

CONGRESO INTERNACIONAL

XXX ENCONTRO GALEGO - PORTUGUÉS DE QUÍMICA

PONTEVEDRA

GALICIA - ESPAÑA

18, 19 y 20 de Noviembre 2026

LIBRO DE RESÚMENES



SPQ

ASOCIACIÓN DE QUÍMICOS DE GALICIA

Colexio Oficial de Químicos de Galicia

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Noviembre 2026

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PRÓLOGO

Foi no ano 1985, cando se estableceu un vínculo entre os químicos do norte de Portugal e de Galicia organizando aquel I ENCONTRO GALEGO PORTUGUÉS DE QUÍMICA. Xa pasaron 37 anos daquel primeiro ENCONTRO que os profesores José Luis Costa Lima, José Luis Figueiredo, Gonzalo Vázquez Uña, Juan Vieites Bautista de Sousa, Pelayo Rubido Muñiz e José Varela Cardama puxeron en marcha.

Neste ano 2026, os ENCONTROS xa celebran a súa 30 ª edición e faino na cidade de Pontevedra. Cidade que na que se levaron a cabo numerosos congresos de bo e grato recordo. Pontevedra é unha cidade monumental chea de arte e historia e, tras Santiago de Compostela, posúe o mellor Centro Histórico de Galicia.

Este ano celebramos o Congreso na Fundación ABANCA. No centro mesmo da cidade de Pontevedra, edificio cheo de historia, que foi centro económico da cidade de Pontevedra e hoxe convertido en centro cultural da cidade..

Sempre, sen perder de vista que a química é unha ciencia que abarca todas as facetas da vida e, tamén, sirve de base para outras disciplinas e, entre todas, poder facer unha sociedade mais xusta e próspera, este XXX ENCONTRO GALEGO PORTUGUÉS DE QUÍMICA volve a unir a todas as persoas que fixeron e fan da química a súa profesión. A Comisión Directiva do Congreso desexa, como sempre, que este punto de encontro as persoas asistentes teñades un lugar e un tempo onde compartir os vosos traballos e experiencias para seguir traballando, xuntos, e abrindo novos camiños para a vosa vida laboral e, tamén, novos camiños para a química.

A química, nestes momentos, afronta retos importantes: contaminación do planeta, a intelixencia artificial, desenvolvemento dunha industria química sostible. Retos que están abrindo novos e interesantes campos de traballo. A química, como ciencia central que é, necesita de todas as persoas que traballades e investigades en calquera dos moitos campos e especialidades desta fermosa disciplina e os ENCONTROS son o tipo de congresos onde podemos ver a evolución e os avances de química. Tanto a Sociedade Portuguesa de Química e a súa Delegación Norte, como o Colexio Oficial de Químicos de Galicia e a Asociación de Químicos de Galicia manteñen vivos estes ENCONTROS coa esperanza de aportar o noso grao de arena para que teñades ese espazo de comunicación e intercambio de experiencias para que sigades facendo da química unha profesión fermosa e frutífera para a sociedade.

Espero que os desexos cos que vides a este XXX ENCONTRO GALEGO PORTUGUÉS DE QUÍMICA se vexan cumpridos.

Dr. Manuel Rodríguez Méndez
Decano Colexio Oficial de Químicos de Galicia.

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El Colegio Oficial de Químicos de Galicia y la Comisión Organizadora del XXX Encontro Internacional Galego-Portugués de Química, desean manifestar su agradecimiento a la Fundación ENCE por su colaboración:



LOCALIZACIÓN DEL XXX ENCONTRO INTERNACIONAL GALEGO PORTUGUÉS DE QUÍMICA

Pontevedra: Situada en la provincia de Pontevedra (Galicia, España), es la capital de la provincia homónima y una de las principales ciudades del noroeste peninsular. Con una población de 83 114 habitantes (INE 2023), es el segundo municipio más poblado de la provincia, tras Vigo, y uno de los principales centros administrativos, culturales y de servicios de Galicia. La ciudad constituye el núcleo de un área urbana que integra varios municipios de su entorno y desempeña un importante papel como eje territorial de las Rías Bajas. Geográficamente se localiza en la margen oriental de la ría de Pontevedra, en el suroeste de Galicia, a unos 60 km al sur de Santiago de Compostela y aproximadamente a 28 km al noreste de Vigo. El término municipal abarca una superficie de 118,3 km², con una densidad de población aproximada de 702 habitantes por km². Además, Pontevedra es reconocida internacionalmente por su modelo urbano, caracterizado por la amplia peatonalización de su centro histórico y por sus políticas de movilidad sostenible, que la han convertido en un referente del urbanismo a nivel europeo.

INFORMACIONES VARIAS

El Encontro se celebrará en la sede Afundación Pontevedra, Rúa Augusto González Besada, 2 - 36001 Pontevedra, Galicia, España



SEDE AFUNDACIÓN PONTEVEDRA

La Sede Afundación Pontevedra, ubicada en la plaza de San José, fue rehabilitada e inaugurada en 2006 bajo la dirección del arquitecto pontevedrés César Portela, quien concibió un proyecto basado en la integración de la tradición arquitectónica del inmueble con la estética del siglo XXI. El edificio, construido en distintas fases entre 1944 y 1974, conserva sus históricas fachadas de piedra, que se combinan con una gran cristalera posterior, aportando una imagen contemporánea. En su interior destaca un amplio vestíbulo iluminado por un gran óculo central que conecta las diferentes estancias y actúa como una prolongación del espacio público de la plaza. Con una superficie aproximada de 12 000 metros cuadrados, el edificio alberga un auditorio con capacidad para 737 personas, una sala de conferencias, salas de reuniones y de exposiciones, además de otros espacios multifuncionales destinados a actividades culturales, sociales y empresariales.

PARA COMER LOS DÍAS DEL CONGRESO:

La oferta gastronómica de Pontevedra combina la tradición culinaria gallega con propuestas modernas y asequibles. El casco histórico concentra numerosos restaurantes, tabernas, cafeterías y bares de tapas donde es posible degustar productos típicos como el pulpo, las empanadas, los mariscos y pescados de la ría, las carnes de calidad o los quesos y embutidos de la región, todo ello acompañado por los vinos de la Denominación de Origen Rías Baixas, especialmente el albariño.

A menos de diez minutos a pie de la Sede Afundación se encuentra una amplia oferta de establecimientos para todos los presupuestos. Muchos de ellos ofrecen menú del día (aprox. 14-15 €) entre semana, además de raciones, platos combinados y bocadillos a precios asequibles, lo que convierte a la ciudad en un destino ideal para disfrutar de la cocina local sin realizar un gran desembolso. Entre las opciones recomendadas figuran Los Castellanos, Bodegón Arca, Taberna de Félix, Alcrique y Savoy Restobar, todos ellos situados en el centro histórico o en sus inmediaciones. La amplia oferta de terrazas y locales de ambiente universitario convierte además la ciudad en un lugar ideal para compartir comidas y cenas durante el congreso.



Los Castellanos	3 min	Clásico del centro. Muy buena opción para comidas informales, raciones y platos combinados.
Bodegón Arca	5 min	Muy popular entre locales. Comida casera abundante y excelente relación calidad-precio.
Taberna de Félix	5 min	Ideal para tapas, bocadillos y raciones. Ambiente desenfadado.
Alcrique	6 min	Cocina casera con buena relación calidad-precio y menú entre semana.
Savoy Restobar	7 min	Dispone de menú del día y suele ser una buena opción si se busca algo un poco más elaborado sin disparar el presupuesto.

CÓMO LLEGAR A PONTEVEDRA

Pontevedra cuenta con excelentes conexiones por carretera y ferrocarril con las principales ciudades de Galicia y del resto de España. Además, dispone de tres aeropuertos internacionales a menos de una hora y media de distancia, lo que facilita el acceso tanto para asistentes nacionales como internacionales.

✈️ EN AVIÓN

Pontevedra no dispone de aeropuerto propio, pero se encuentra próxima a tres aeropuertos:

Aeropuerto de Vigo (VGO): situado a unos 30 km de Pontevedra (aprox. 30 minutos en coche). Es la opción más cercana y ofrece vuelos nacionales y algunas conexiones internacionales.

Aeropuerto de Santiago-Rosalía de Castro (SCQ): a unos 75 km (aprox. 1 hora). Es el aeropuerto gallego con mayor número de conexiones nacionales e internacionales.

Aeropuerto de Oporto (OPO, Portugal): a unos 170 km (aprox. 2 horas). Constituye una excelente alternativa para vuelos internacionales y de bajo coste.

🚆 EN TREN

La estación de Pontevedra cuenta con servicios de Media Distancia y Alta Velocidad (AVE/Avlo/Alvia) que la conectan con Madrid, Santiago de Compostela, A Coruña, Vigo y otras ciudades gallegas.

La estación se encuentra a unos 15-20 minutos a pie de la Sede Afundación

🚌 EN AUTOBÚS

La estación de autobuses está situada junto a la estación de tren, lo que facilita los transbordos. Existen conexiones frecuentes con las principales ciudades gallegas y con numerosas ciudades españolas.

Además, la Praza de Galicia, situada en pleno centro urbano, es uno de los principales puntos de parada de autobuses urbanos e interurbanos y se encuentra a escasos minutos de la Sede Afundación.

🚗 EN COCHE

Pontevedra está comunicada por la AP-9, eje principal del corredor atlántico gallego, que enlaza la ciudad con Vigo, Santiago de Compostela, A Coruña y Ferrol. También dispone de acceso mediante la A-52 hacia Ourense y Madrid.

En las inmediaciones de la Sede Afundación existen varios aparcamientos públicos de pago.

📍 Cómo llegar desde la estación a la sede

🚶 Estación de tren/autobuses → Sede Afundación: 15-20 min a pie

Transporte Público Urbano e Interurbano de Pontevedra

https://pontevedra.gal/transporte-publico/

La parada más próxima a la Sede Afundación es Praza de Galicia, situada a apenas 2-3 minutos a pie. La línea 2 conecta este punto con la estación de tren y autobuses, entre otros destinos.

INFORMACIÓN SOBRE EL CONGRESO

RECEPCIÓN

La oficina de información y la recepción para retirar la documentación del Encontro, estará localizada en el vestíbulo de la Facultad de Química, en la planta baja. Permanecerá abierta durante todos los días de su celebración.

EQUIPAMIENTO DE PROYECCIONES

Las salas de conferencias están equipadas con ordenador y cañón de proyección. Cada orador deberá transferir el fichero de su presentación al ordenador de la sala que le corresponda, con la antelación suficiente. Siendo aconsejable se realice en la sesión anterior.

PRESENTACIONES ORALES

Las conferencias plenarias tendrán una duración de 45-50 minutos más 10 minutos para preguntas.

La duración de las comunicaciones orales será de 10 minutos más 5 minutos para resolución de dudas. Se solicita a todos los oradores que cumplan el tiempo estipulado, a fin de evitar retrasos en el programa.
Se recomienda que las presentaciones se hagan en formato pdf o PowerPoint.

POSTERS

Deberán colocarse el primer día, primera sesión y retirarse el último, tras el acto de clausura, por los propios autores de la comunicación. Se solicita a los autores de los trabajos presentados, estén presentes junto a los mismos durante la sesión de discusión.

SALAS DEL CONGRESO

El congreso tendrá lugar en 3 salas de la Sede de AFundación en Pontevedra, Auditorio, Sala de Conferencias y Aula

Planta Baja: Auditorio
4ª planta: Sala de Confeencias
5ª planta: Aula y Catering

CENA DEL ENCONTRO

La cena del ENCONTRO tendrá como protagonista el cocido gallego, uno de los platos tradicionales de la gastronomía gallega, especialmente típico de los meses de otoño e invierno, la cena se celebrará el día 19 de noviembre a las 21:30 horas en el Comedor del Hotel Galicia Palace, (https://www.galiciapalace.com/), Avda. de Vigo, 3 - 36003 Pontevedra. Con un coste de 40 € por persona.

Sede Afundación → Hotel Galicia Palace: 8-10 min a pie

MENÚ
Primer plato:
Caldo gallego o sopa de cocido.
Plato principal:
Cocido con lacón, oreja, ternera, costilla salada,
cacheira, chorizo cebollero, chorizo de carne y pollo, acompañado de grelos,
repollo, garbanzos y patata.
Postre:
Filloa caramelizada rellena de crema.
Bebidas:
Café, aguas, cervezas o vino Rectoral de Amandi.

PROGRAMA DEL XXX ENCONTRO INTERNACIONAL GALEGO PORTUGUÉS DE QUÍMICA

SALAS		Planta
A	Auditorio	baja
B	Sala de Conferencias	4ª
C	Aula	5ª

CATERING	5ª
POSTERS	baja

DÍA	HORA	SALAS			
		PLENARIAS SALA A	A	B	C
18	10:00 - 11:45	INSCRIPIÓN Y RECEPCIÓN			
		COLOCACÓN DE PÓSTERS			
	11:45- 12:15	A	SESIÓN DE APERTURA.		
	12:15-13:15		CONFERENCIA PLENARIA		
	13:15 - 13:45	TIEMPO con Prof. Thomas R. Cech			
	13:45		AMB01	QA01	QS01
	14:00		AMB02	QA02	QS02
	14:15-16:00	COMIDA			
	16:00		AMB03	QA03	QS03
	16:15		AMB04	QA04	QS04
	16:30		AMB07	QA05	QS05
	16:45		AMB08	QA06	QS06
	PAUSA: 10 minutos				
	17:00 - 17:45	CP1			
	17:45 - 18:15	COFFEE BREAK + POSTERS			
	18:15		AMB05	QA07	QS07
	18:30		AMB06	QA08	QS08
	18:45		AMB09	QA09	QS09
	19:00		AMB10	QA03	QS10
	19:15		AMB11	QA10	NN06

DÍA	HORA	SALAS			
		PLENARIAS SALA A	A	B	C
19	9:45		AMB12	QA11	NN02
	10:00		AMB13	QA12	NN03
	10:15		ALM04	QA13	NN04
	10:30		AMB15	QA14	NN05
	10:45		AMB16	QA15	NN01
		PAUSA: 10 minutos			
	11:10		AMB17	QA16	NN07
	11:25		AMB18	QA17	QT01
	11:40		AMB19	QA18	QT02
	11:55		AMB20	QA19	QT03
	11:55 - 12:40	CP2			
	12:40 - 13:15	COFFEE BREAK + POSTERS			
	13:15		AMB21	CAT01	QI08
	13:30		AMB22	CAT02	QI01
	13:45		AMB23	CAT03	QI02
	14:00		AMB24	CAT04	QI03
	14:00 - 16:00	COMIDA			
	16:00		AMB25	CAT05	QI04
	16:15		AMB26	CAT06	QI05
	16:30		AMB27	CAT07	QI06
	16:45		AMB28	CAT08	QI07
	17:00 - 17:45	CP3			
	17:45 -18:15	COFFEE BREAK + POSTERS			
	18:15		AMB29	CAT09	BB09
	18:30		AMB30	CAT10	BB01
	18:45		AMB31	CAT11	BB02
	19:00		AMB32	CAT12	BB03
	21:00	CENA DEL ENCONTRO			

DÍA	HORA	SALAS			
		PLENARIAS SALA A	A	B	C
20	9:45		AMB33	EDU02	BB04
	10:00		POL01	EDU01	BB05
	10:15		ALM01	EDU03	BB06
	10:30		ALM02	QO01	BB07
	10:45		ALM03	QO02	BB08
	10:45 - 10:55	PAUSA: 10 minutos			
	10:55		ALM04	QO03	
	11:10		ALM05	QO04	CAT13
	11:25		ALM06	QO05	BB10
	11:40		ALM07	QO06	BB11
	11:40 - 12:30	CP4			
	12:30 - 13:00	COFFEE BREAK + POSTERS			
	13:00		AMB14	QO07	BB12
	13:15		ALM09	QO08	IND01
	13:30		ALM10	QO09	IND02
	13:45		ALM11	QO10	IND03
	14:15 - 16:00	COMIDA			
	16:00 - 16:15	RETIRADA DE POSTERS			
	16:00		ALM12	QO11	IND04
	16:15		ALM13	QO12	IND05
	16:30		ALM14	QO13	IND06
	16:45		ALM15	QO14	IND07
	17:00		ALM16	QO15	IND08
	17:15		ALM17	QO16	QF01
	17:30	PAUSA: 10 minutos			
	17:40	A	CLAUSURA DEL CONGRESO		

RELACIÓN DE CONFERENCIAS PLENARIAS

CONFERENCIA APERTURA:

Prof. Thomas R. Cech

Premio Nobel de Química, 1989

RNA Is More than a Messenger: The Chemistry and Biochemistry of Noncoding RNAs

CP 1 **Prof. Pedro Góis**

Facultade de Farmacia. Universidade de Lisboa.

Boronic Acids: A Useful Functional Platform for Chemical Biology

CP 2 **Prof. Cláudia Silva**

Facultade de Engenharia. Universidade do Porto

Engineering Carbon Nitride Nanomaterials for Photocatalytic Applications

CP 3 **Prof. Diego Peña Gil**

CiQUS - Departamento de Química Orgánica. Universidade de Santiago de Compostela

When organic chemistry meets surface science: from single-molecule characterizationto exotic carbon-based nanostructures

CP 4 **Prof. Isabel Pastoriza**

CINBIO - Facultade de Química. Universidade de Vigo

From Nanochemistry to Molecular Detection

RELACIÓN DE COMUNICACIONES

CONFERENCIAS PLENARIAS

CONFERENCIA DE APERTURA

Prof. Thomas R. Cech

RNA Is More than a Messenger: The Chemistry and Biochemistry of Noncoding RNAs

CP 1 **Prof. Pedro Góis**

Boronic Acids: A Useful Functional Platform for Chemical Biology

CP 2 **Prof. Cláudia Silva**

Engineering Carbon Nitride Nanomaterials for Photocatalytic Applications

CP 3 **Prof. Diego Peña Gil**

When organic chemistry meets surface science: from single-molecule characterizationto exotic carbon-based nanostructures

CP 4 **Prof. Isabel Pastoriza**

From Nanochemistry to Molecular Detection

COMUNICACIONES

Química Alimentaria

Oral

ALM01	Composición nutricional y compuestos bioactivos en el almez (Celtis australis L.), un fruto tradicional de la Dieta Mediterránea.	Patricia García-Herrera, José Ignacio Alonso Esteban, Samuel Fernández-Tomé, María Cortes Sánchez-Mata, Montaña Cámara, Patricia Morales, Virginia Fernández, Rosa María Cámara, Lorena González-Zamorano, Laura Aceituno, Manuel Pardo de Sanatayana
ALM02	Effect of acylation on the interaction of anthocyanins with pea, soy and yeast proteins under mildly alkaline conditions	Ziqi Guo, Catarina Ferreira, Susana Soares, Victor Freitas, Joana Oliveira
ALM03	Yeast Protein-Chitosan Coacervation: effect of pH, biopolymer ratio, and ionic strength	Ana Rita Pereira, Ana Fernandes, Nuno Mateus, Victor de Freitas
ALM04	Bee4Cheese Project: From Green Extraction of Propolis for Preservation of Traditional Cheese	Artem Drogalin, David Almeida, Aritson Tolentino, Paula Rodrigues, M. Natália D.S. Cordeiro, Miguel Vilas-Boas, João Reis, Soraia I. Falcão, Andreia F. Peixoto
ALM05	Valorização do bagaço de Vaccinium ashei: Efeito da secagem por liofilização e por ar quente na sua composição nutricional e química	Syed Waqas Ali Bacha, Matilde Rodrigues, Alexandre Gonçalves, A. Tadeu Alves, Joana S. Amaral, Cristina Caleja, Lillian Barros
ALM06	Wheat Fermented Beverages: Phenolic Composition, Antioxidant Activity and Evolution of Immunogenic Gluten Peptides During Digestion	Pardellas-Soto, Jorge; Casanova-Salvador, Paula; Martínez-Carballo, Elena; Pérez-Gregorio, Rosa
ALM07	Determinação do perfil de triacilglicerol em ovos a partir de um método otimizado de ASAP-MS/MS	Mariana S. Leoncio, Victor H. M. Cruz, Jessica S. Pizzo, Patrícia D.S. Santos, Geovane A. R. Silva, Oscar O. Santos e Jesuí V. Visentainer
ALM08	Development and optimization of propolis-carob particle-stabilized Pickering emulsions	Liandra Gracher-Teixeira, Bruna Dias, Luiza A. Oumura, Arantzazu Santamaria-Echart, Isabel Reinas, Maria-Filomena Barreiro

ALM09	Development of Pickering Emulsions Stabilized by Astaxanthin-Based Solid Dispersion Particles for Food Analogs	Luiza A. Oumura, Liandra Gracher-Teixeira, Bruna Dias, Arantzazu Santamaria-Echart, Isabel Reinas, Bogdan Demczuk Jr., Maria-Filomena Barreiro
ALM10	Impact of Maturation on the Nutritional Profile, Phytochemical Composition and Bioactive Potential of Persimmon (Diospyros kaki L.)	S. Rocha, L. Barros, M. de Almeida, B. Paulos, F. Mandim, B. Albuquerque, A. Gonçalves, A.P. Pereira, E. Pereira
ALM11	From by-product to food: valorisation of lentil tofu residue into granola, farofa and a cereal bar	Maria Eduarda Cordeiro, Tayse F.F. da Silveira, Rossana V.C. Cardoso, Rafael Sprea, Manuel Ângelo Rodrigues, Lillian Barros
ALM12	Chemical Structure of Procyanidins and Polysaccharides Governs Their Interactions at Oral Interfaces	Mónica Jesus, Elisabete Coelho, Elsa Brandão, Nuno Mateus, Victor de Freitas, Susana Soares
ALM13	Caraterização morfológica e fitoquímica de microvegetais de espinafre biofortificados com selénio inorgânico	Alexis Pereira, Maria Inês Dias, M. Beatriz P. P. Oliveira, José Pinela
ALM14	Fermented red grape juices: influence of in vitro model design on gut microbiota modulation	Ana R. Monteiro, Ana Faria, José Capelo, Edgard Relaño de la Guia, Mikel Roldan, Carolina Cueva, M. Victoria Moreno-Arribas, Iva Fernandes
ALM15	Techno-functional, rheological, and pasting properties of gluten-free rice flour enriched with Scolymus hispanicus L. root powder	Beatriz H. Paschoalinotto, Miguel A. Prieto, Spyridon A. Petropoulos, Joanna Harasym, Maria Inês Dias
ALM16	Estratégias de cultivo e otimização da biofortificação de cogumelos do género Pleurotus com ferro: O projeto Nutr&ssencial	Maria G. Leichtweis, Roberto A. Costa, Bruno Melgar, Maria Inês Dias, Pablo A. García, José Pinela, Carla Pereira
ALM17	Caracterização integrada do cultivo e da qualidade dos morangos para o desenvolvimento de sistemas de produção controlados por inteligência artificial: o projeto SUSTAiN	Maria G. Leichtweis, Ruth Rodríguez-Ramos, Carolina Campos, Jorge Paiva, Sara Rodrigues, Susana Araújo, Higor Rosse, Khadija Sabiri, Infância Maria Lima Barreira Rocha, José Alberto Martins Gonçalves, Carla Pereira, Maria Inês Dias

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ALM18	Judías carillas: composición nutricional de un alimento tradicional consumido en el área mediterránea	Patricia García-Herrera, José Ignacio Alonso Esteban, Samuel Fernández-Tomé, María Cortes Sánchez-Mata, Montaña Cámara, Patricia Morales, Virginia Fernández, Rosa María Cámara, Lorena González-Zamorano, Laura Aceituno, Manuel Pardo de Sanatayana
ALM19	BEVEGAL — Ultrasound-Assisted Formulation of Plant-Based Beverages from Galician Chestnut and Faba de Lourenzá	J. A. Custodio-Mendoza, M. R. Pérez-Gregorio, P. Reboredo-Fernandez, E. Martinez-Carballo
ALM20	Assessment of Environmental Contaminants in Innovative Canned Seafood Products	Sara Sousa, Juliana Pais-Costa, Helena Oliveira, Amparo Gonçalves, Beatriz Fernandes, Carmo Serrano, António Marques, Maria Leonor Nunes, Valentina F. Domingues, Cristina Delerue-Matos
ALM21	Subcritical Water Extraction of Bioactive Compounds from Portuguese Cabbage (Brassica oleracea) By-products for Sustainable Aquafeed Ingredients	B. J. Azeredo, E. F. Vieira, V. F. Domingues, M. J. Ramalhosa, C. Delerue-Matos
ALM22	Da capacidade antioxidante à proteção lipídica: avaliação de extratos de macroalgas em condições de oxidação acelerada	F. Santos, Valentina F. Domingues, C. Soares, M. J. Ramalhosa, H. Augusto, C. Delerue-Matos

ALM23	Cerrando el ciclo agroalimentario: recuperación asistida por ultrasonidos de antioxidantes a partir de hojas y tallos de pimiento	Matilde Rodrigues, María Carpena, M. Beatriz P.P. Oliveira, Celestino Santos-Buelga, Miguel A. Prieto, José Pinela
ALM24	Validación analítica de un método enzimático para la cuantificación de azúcares totales en vinos y bebidas espirituosas	Soledad Muniategui Lorenzo, Isabel Turnes Carou, Alba Núñez López, Iago Neira García, Jaime. Fernández-Paz
ALM25	Towards a low-cost flow-based method for selenium quantification in common bean	Jacinta Santos, Tânia C. F. Ribas, Marta W. Vasconcelos, António O. S. S. Rangel, Carla S. Santos, Raquel B. R. Mesquita
ALM26	Formation and Characterization of Insoluble Anthocyanin–λ-Carrageenan Complexes: Interactions, Thermal Stability, and Release Behaviour	Ana Fernandes, Tomás Garrido, Ana Rita Pereira, Hiléia K.S. Souza, Nuno Mateus, Victor de Freitas
ALM27	Efeito da secagem na composição nutricional de farinhas produzidas com mirtilos de refugo	Syed Waqas Ali Bacha, S. Coelho-Fernandes, A. Padrão, Matilde Rodrigues, L. Rocha, A.P. Pereira, A. Gama, A. Tadeu Alves, L. Barros, J. S. Amaral, A. Gonçalves, C. Caleja
ALM28	Zearalenone in Commercially Available Beers: Quantitative Assessment and Consumer	Anaëlle Boissonnet, Eloïse Brunesseaux, Maria N. Vaz, Sofia C. Duarte, Ana Paiva, Maria J. Campos, André M. P. T. Pereira, Liliana J. G. Silva, Angelina Pena
ALM29	Comparative Analysis of Fatty Acid Profiles in Eggs from Different Production Systems and Cooking Treatments	Mariana S. Leoncio1, Victor H. M. M. da Cruz, Geovani Yoti Braz Nakamura, Oscar O. S. Junior1, Camila Rodrigues, Jesui V. Visentainer
ALM30	A sequential injection analysis method for the determination of nitrites and nitrates in processed meats	Catarina C. Sousa*, Tânia C. F. Ribas, Maria J. M. Nunes, Paula Teixeira, António O. S. S. Rangel
ALM31	Effect of anthocyanin incorporation route on the functional performance of gelatin-based intelligent films	Bruna Dias, Liandra Gracher-Teixeira, Ana C. Lima, Arantzazu Santamaria-Echart, Maria-Filomena Barreiro
ALM32	One-factor-at-a-time screening of the alcoholic fermentation of astringent persimmon must for vinegar production	F. Mota, A.P. Pereira, T. Montes, B. Paulos, L. Barros, E. Pereira*, A. Gonçalves
ALM33	Lentil (Lens culinaris Medik.) tofu: a high-protein, low-fat alternative to soy tofu	Maria Eduarda Cordeiro, Tayse F.F. da Silveira, Manuel Ângelo Rodrigues, Lillian Barros, Rossana V.C. Cardoso
ALM34	Caracterização comparativa dos perfis de compostos fenólicos de microvegetais de acelga e espinafre	Alexis Pereira, Maria Inês Dias, M. Beatriz P. P. Oliveira, José Pinela
ALM35	From glucosinolates to isothiocyanates: the chemical characterisation of salad rocket	Ruth Rodríguez-Ramos, Beatriz H. Paschoalinotto, Antonio V. Herrera-Herrera, Bárbara Socas-Rodríguez, Célia Cabral, Maria Inês Dias
ALM36	Effect of NPK fertilisation on the chemical profile and the in vitro antioxidant properties of Portulaca oleracea L. leaves and stems	Beatriz H. Paschoalinotto, Ruth Rodríguez-Ramos, Mikel Añibarro-Ortega, Nikolaos Tzortzakis, Lillian Barros, Maria Inês Dias
ALM37	Cultivation of glucosinolate-enriched Brassicas for the development of functional pasta products	Beatriz H. Paschoalinotto, Ruth Rodríguez-Ramos, Cláudia Novais, C. Cabral, M. I. Dias
ALM38	Perfil de aminoácidos em produtos derivados do leite: efeito da maturação	Susana Machado, Sara Maia, Liliana Espirito Santo, Wemerson de C. Oliveira, Matheus A. P. Pedroso, Neila S. P. dos S. Richards, M. Beatriz P. P Oliveira, Rita C. Alves

ALM39	Valorizing Portuguese propolis extracts as functional ingredients in cereal snack bars	Sandra Barbosa, Ana R. Circuncisão, Francimara Marques, Maria F. Sousa, Cristina Almeida-Aguiar, Susana M. Cardoso.

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AMB02	Green-synthesis of ZVI particles from plant extracts for phosphate removal	Iñaki Beceiro-Cillero, Sarah Fiol, Juan Antelo, Xosé Lois Otero
AMB03	Waste into Water Treatment: Red Onion Peel as a Natural Coagulant	Ana R. Oliveira, Inês S. Moreira, Cidália M. S. Botelho, Ricardo M. Ferreira
AMB04	Circular Valorisation of Iron-Functionalised Pine Bark Biosorbents after Textile Wastewater Treatment	Beatriz Pacheco, Cidália Botelho, Salomé Soares, Ricardo M. Ferreira*
AMB05	Caracterización de compuestos orgánicos volátiles en la atmósfera de un área industrial: Puertollano (España)	Elena Molina, Cristian Chacón, Pilar Martín, Sagrario Salgado, Laura Solé, Laura Vallecillos
AMB06	Implicaciones atmosféricas del uso del 2-butoxietanol como aditivo en la formulación de biocombustibles	Cristian Chacón, Elena Molina, Sagrario Salgado, Pilar Martín
AMB07	Dynamic Adsorption and Regeneration Behavior of Strong-Base Anion-Exchange Resins in Pd(II)/Zn(II) Chloride Systems	Filipa S. Brito, Eduardo L. Oliveira, Hugo A. M. Bacelo, Vanessa R. A. Ferreira, Helena M. V. M. Soares
AMB08	Hemotoxic effects of emerging bisphenol analogues in human erythrocytes	Inês Santos, Lara Vieira, Carina Proença, Eduarda Fernandes, Marisa Freitas
AMB09	From Structure to Performance: Pt(IV) and Pd(II) Adsorption on Next-Generation Anion-Exchange Resins	Vanessa R. A. Ferreira*, Hugo A. M. Bacelo, Mariana B. Rodrigues, Filipa S. Brito, Helena M.V.M. Soares
AMB10	Bioconcreto autorreparable: comportamiento frente a la formación y sellado de fisuras	Guevara Garcia, Paulina; Flores, Francisco; Guanín Carrión, Nahomi; Tenelema Quinatoa, Melany; Ugsha Chugchilan, Pacha
AMB11	Biomass-Derived Furans as a Platform for Sustainable Synthesis and Green Chemistry Education	Mariana Peixoto, Daniel-Almeida Santos, Teresa M. V. D. Pinho e Melo, Marta Pineiro
AMB12	Avocado Seed Valorisation for Water Treatment	Inês S. Moreira, Mariana Letra, Sofia Mota, Cidália Botelho, Ricardo M. Ferreira
AMB13	Design and Development of Potent HIV Protease Inhibitors Based on a Biorenewable Scaffold	Xavier Cruz Correia, Dominique Schols, Ivo E. Sampaio-Dias
AMB14	From renewable biopolymers to functional fibers: advanced electrospinning of Chitosan-PCL nanocomposites for textile dye adsorption	Óscar Martínez-Rico, Ángeles Domínguez, Begoña González
AMB15	Rapid capture and recovery of Nd, Tb and Dy from water using pristine Kraft lignin: a response surface approach	Helder F. Martins, Rodrigo C. Almeida, Diogo L. Mateus, Thiago Silva, André M. da Costa Lopes, Eduarda Pereira, Bruno Henriques
AMB16	Assessment of Chromium Contamination in Aquatic Environments near Tannery Industries: A Portuguese Case Study	Liliana J. G. Silva, Angelina Pena, Maria J. Campos, André M. P. T. Pereira
AMB17	Photosensitizers and Hybrid Materials for the Photodynamic Disinfection of Water	Carlos J. P. Monteiro, Ana S. M. Joaquinito, Cristina J. Dias, Nuno M. M. Moura, M. Amparo F. Faustino
AMB18	Unlocking Microalgal Polysaccharides Through Sustainable Extraction Strategies for Aquafeed Applications	Ana Luísa Rebelo, Luís F. Baião, Marta Monteiro, Sofia A. Costa Lima

AMB19	Rare earth removal from simulated magnet and lamp waste using a microporous niobium–iron silicate	Thiago Silva, Joana Sousa, David Oliveira, Bruno Henriques, João Rocha, Daniela Tavares, Eduarda Pereira
AMB20	Valorization of white grape pomace through targeted recovery of phenolic acids using conventional and hydrotropic solvents	Iván Montenegro, Elena Gómez, Ángeles Domínguez, Begoña González
AMB21	Evaluación energética y ambiental de materiales de aislamiento sostenibles para edificios mediante simulación térmica dinámica y análisis del ciclo de vida	Khalid Azizi
AMB22	Lipid profile and antimicrobial activity of by-products of the winemaking process: the case of grape pomace and stems	Marlene Machado, Sara Maia, Juliana Peixoto, Helena Ferreira, Fernanda Cosme, Fernando Nunes, M. Beatriz P. P. Oliveira, Rita C. Alves
AMB23	Tuning Supercritical CO_2 Extraction of Ruscus aculeatus L. Fruits: Influence of Polar Modifiers on Extract Fractionation and Chemical Profiles	Y. Dulyanska, L.A.E. Batista de Carvalho, M. J. Barroca, F. J. Gonçalves, R. P. F. Guiné, C.I.A.V. Santos
AMB24	Liquefaction Process Optimization and Bio-Polyols Characterization of Ruscus aculeatus L. Branches	Y. Dulyanska, L.A.E. Batista de Carvalho, M. J. Barroca, F. J. Gonçalves, R. P. F. Guiné, C.I.A.V. Santos
AMB25	Valorization of Moroccan geomaterials into low-cost ceramic membranes: optimization using response surface methodology (Box-Behnken design)	Khaoula Benzaboul, Rajae Kharbouch, Mounia Baidou, Soukaina El Abbadi, Hajar El Moustansiri, Joaquim Esteves Da Silva, Abdelmjid Bouazizi, Mohamed Douma
AMB26	Materiales Avanzados para la Construcción Sustentable: Aportes de la Ingeniería de los Materiales a la Innovación	Dra. Elisabeth Viviana Lucero Baldevenites
AMB27	An integrated extraction-to-formulation approach for propolis-based lip care using hydrophobic NaDES	Nicolas Justus, Maria F. Sousa, Sandra Barbosa, Ana R. Circuncisão, Cristina Almeida-Aguiar, Maria João Sousa, Paulo C. Kirnev, Susana M. Cardoso
AMB28	Ultrasound-Assisted Extraction of Phenolic Compounds with Antioxidant Properties from Grape Stalks: Process Optimization by Response Surface Methodology	Sara Maia, Thiago F. Soares, M. Beatriz P. P. Oliveira, Rita C. Alves
AMB29	Compound Wind–Solar Generation Deficits and Joint Electricity Price–Carbon Stress in Peninsular Spain	Danial Esfandiary Abdolmaleki, Pastora María Bello Bugallo
AMB30	Evaluación de Soluciones basadas en la Naturaleza (SbN) para la adaptación climática y resiliencia en Galicia	Alicia García Delgado, Pastora María Bello Bugallo
AMB31	Transformando emisiones en materias primas: el papel del CCUS en la producción sostenible de metanol	Marianny D, Álvarez Rodríguez, Ignacio Bañeres Estribano, Pastora M. Bello Bugallo
AMB32	Riesgos operacionales y ambientales inherentes a la aquatermólisis en la recuperación térmica del crudo en la Faja Petrolífera del Orinoco	Arturo J. Calvo Tiapa, Pastora M. Bello Bugallo
AMB33	Más allá del pozo: desafíos conjuntos para una gestión integrada en la explotación de la Faja Petrolífera del Orinoco bajo un esquema de recuperación térmica	Arturo J. Calvo Tiapa, Pastora M. Bello Bugallo

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AMB35	Removal of Nutrients and Veterinary Pharmaceuticals from Agricultural Effluents by Adsorption on Advanced Substrates: The LIFE4FARMS Project	Elisabete C. D'Oliveira, Sílvia A. B. S. de Quadros
AMB36	Synthesis and Characterization of rGO/TiO_2 on flexible substrates for use as electrode in DSSCs	B. Asenjo1, M.P. Alcacera, and J.F. Trigo
AMB37	Synthesis and Characterization of Pb free perovskite based films obtained by sol-gel method.	B. Asenjo
AMB38	Grafitización catalítica asistida por microondas de biocarbones derivados de residuos: hacia la producción de biografitos circulares	Ana M. Ares-Fuentes, José Antonio Marcotegui, Alfonso Echave, Érik Aguirre, Eduardo Olariaga, Iera Gorostiaga, Javier Echevarría
AMB39	Valorización de subproductos agroalimentarios mediante pirólisis continua asistida por microondas para la producción de gas rico en H_2 y CO	Ana M. Ares-Fuentes, José Antonio Marcotegui, Alfonso Echave, Erik Aguirre, Aritz Estévez, Iera Gorostiaga, Javier Echeverría, Adur Ruiz
AMB40	Almond and walnut shells as alternative lignocellulosic raw materials for particleboard production	Simão Silva, Paulo Magalhães, Luísa H. Carvalho, Valentina F. Domingues
AMB41	Monitoring PFAS Occurrence in Potentially Contaminated Soils from Galicia (NW Spain) by UPLC-MS/MS	Santiago Feijoo-Montenegro, Ivan Carabante, Andrea L. Tasca, Juan Antelo, Carmela Monterroso, Sarah Fiol
AMB42	Seasonal co-occurrence of microplastics and phthalates in atmospheric particulate matter (PM10) at an urban traffic site	João Pinto da Costa, Sónia da Rocha, Ana Paço, Khawla Chouchene, Carolina Dias, Joana Barata, Anabela Pereira, Alexandra Nunes, Vânia Martins, Susana Marta Almeida, Teresa Rocha-Santos, Mário Cerqueira
AMB43	Purification of Ethyl Biodiesel Based on Circular Economy Principles through Adsorption Using Residual Biomass-Based Materials	Gabrielly C. Belarmino, Paulo Brito, Ana Queiroz, António E. Ribeiro, Maria Carolina Sérgi Gomes
AMB44	Geochemical characterization and organic matter distribution in sediments from the Ría de Ferrol	Tomás Cumbraos-Díaz, Juan Antelo, María Santiso, Guillermo Díaz-Agras, Ramiro Tato, Marcos P. Señarís, María Candás, Andrés de Solaún, Carmela Monterroso, Sarah Fiol, Xosé L. Otero
AMB45	Estudio del efecto de aditivos sobre las propiedades fisicoquímicas y las emisiones atmosféricas de purines porcinos	María Fernández, Cristian Chacón, Elena Molina, Sagrario Salgado, Pilar Martín
AMB46	Una aproximación al muestreo de grandes volúmenes de agua para monitorizar microplásticos	J.M. Andrade-Garda, E. Llavero-López, A. López-Rosales, J. Terán-Baamonde, J. Lejo-Santiago, S. Muniategui-Lorenzo, Jose L. Cereijo-Arango, Jorge J. Delgado-Martín
AMB47	Chemometric challenges to identify microplastics in environmental samples	J.M. Andrade-Garda, C. Román-Zas, A. López-Rosales, E. Llavero-López, B. Fuente-Ferreiro, S. Muniategui-Lorenzo
AMB48	Behavior and mechanism of terbuthylazine adsorption on polyethylene microplastics in the marine environment	María José González-Castro, David Fernández-Álvarez, Soledad Muniategui- Lorenzo, María Elisa Beceiro-González
AMB49	Cell-dependent cytotoxicity of bisphenol A and its substitutes: evidence from human hepatic, immune and erythrocyte models	Carina Proença, Inês Santos, Lara Vieira, Marisa Freitas, Eduarda Fernandes

AMB50	Desempeño de compuestos fúngicos para aplicaciones constructivas no estructurales: caracterización de Pleurotus ostreatus y Ganoderma lucidum	Guevara Garcia, Paulina; Duchicela, Jessica; Alpusig, Cinthya; López, Jessica; Cóndor, Kevin; Toapanta, Sebastián
AMB51	Immunotoxic effects of bisphenol A analogues on human neutrophils	Lara Vieira, Carina Proença, Inês Santos, Eduarda Fernandes, Marisa Freitas
AMB52	Reuse of organic waste as sustainable adsorbents for the removal of sertraline in aqueous systems	Maria Fernanda Lauterio Coelho, Camila Zoe Correa, Paulo Brito, Ana Queiroz, António E. Ribeiro
AMB53	Different technologies for the extraction of polysaccharides from Ulva spp. using green solvents	L. Veitía-de-Armas, V. Ruiz Valencia, M. Dolati, M.D. Torres, H. Domínguez
AMB54	Monitoring the WWTP at Porto airport - design of a µPAD for determination of nitrogen-based ions	Mafalda G. Pereira, Mariana S. Cruz, Sofia Rocha, António O. S. S. Rangel, Raquel B. R. Mesquita
AMB55	Optimized ultrasonication-redox depolymerization for controlled production of low molecular weight ulvan and carrageenan	V. de Santos, K.L. Baltrusch, M.D. Torres, H. Domínguez
AMB56	Aqueous matrix contaminated with antidepressants: Adsorption via activated charcoal from walnut shell	Karla C. A. Varela, Elisângela Düsman, Paulo Brito, Ana Queiroz, António E. Ribeiro
AMB57	A sustainable alternative for the selective synthesis of 2-aminoquinolines using porous ZnO/carbon composites	M. Al Bahri, S. Morales-Torres, L.M. Pastrana-Martínez, F. J. Maldonado-Hódar, E. Pérez-Mayoral
AMB58	Functional biomass-derived hydrothermal carbons highly efficient and selective for the green dihydroquinazolinone synthesis	M. Al Bahri, A. J. López Peinado, M. Adame-Pereira, Carlos J. Durán-Valle, E. Pérez-Mayoral
AMB59	Porphyrin-Functionalised Silica Materials for Water Decontamination: Metal Ion Adsorption	Nuno M. M. Moura, Chahrazad El Abiad, Y. Draoui, Smaail Radi, M. Amparo F. Faustino, M. Graça P. M. S. Neves
AMB60	HVO (Hidrobiodiesel) Frente a Diesel	M.C. Fernández-Feal, B. Sánchez-Fernández, L.R. Sánchez-Fernández
AMB61	Hydrothermal Zeolitization of Fly Ash-Based Geopolymers and Their Composites with Biomass-Derived Activated Carbon for Carbamazepine Removal	Lívia Firmani, Ana Paula Ferreira, José A. Peres, Jose L. Diaz de Tuesta, Helder T. Gomes
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AMB64	Effect of solvent on the microwave-assisted extraction of bioactive compounds from Melipona flavolineata geopropolis	Fernanda W. F. Bezerra, Luiza H. da S. Martins, Maria D. Torres, Herminia Domínguez, Renan C. Chisté
AMB65	Effect of Nitrogen Addition to the Headspace on the Extraction of Bioactive Compounds from Mentrasto (Ageratum conyzoides) by Autohydrolysis	Carolina Fernandes, Maria D. Torres, Herminia D. González, Ana Carolina de Aguiar
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AMB69	Valorization of viticulture surplus from the Douro Demarcated Region: fatty acid and vitamin E profiles	Marlene Machado, Fernanda Cosme, Fernando Nunes, M. Beatriz P. P. Oliveira, Rita C. Alves
AMB70	Ultrasound-assisted extraction as a tool for grape pomace valorization: Optimization of phenolic recovery and antioxidant activity	Sara Maia, Thiago F. Soares, Juliana A. Barreto Peixoto, M. Beatriz P. P. Oliveira, Rita C. Alves
AMB71	Functional biomass-derived hydrothermal carbons highly efficient and selective for the green dihydroquinazolinone synthesis	M. Al Bahri1, A. J. López Peinado, M. Adame-Pereira, Carlos J. Durán-Valle, E. Pérez-Mayoral
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AMB73	Antimicrobial Activity of Neat Natural Deep Eutectic Solvents and Propolis Extracts	Nicolas Justus, Maria F. Sousa, Sandra Barbosa, Ana R. Circuncisão, Cristina Almeida-Aguiar, Izamara de Oliveira, Maria João Sousa, Paulo C. Kirnev, Susana M. Cardoso
AMB74	Preparação de MOF-5 a partir de resíduos de PET para valorização catalítica do CO2	Susana Guimarães, Salete S. Balula, Ana M.G. Silva, Carlos R. Gomes, Luís Cunha-Silva
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AMB76	Vulnerabilidad de recursos críticos en baterías para vehículos eléctricos: una aportación a la identificación de retos futuros	Yago Pérez Rey, Ângelo Adão Monteiro, Laura Blanco García, Pastora M. Bello Bugallo, Jose Manuel Vila Abad
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AMB78	Is the European Union capable of ensuring a sustainable supply of raw materials for the energy transition?	Adrián Costas Coello, Laura Blanco García, Pastora M. Bello Bugallo, Jose Manuel Vila Abad
AMB79	Low-carbon enhanced oil recovery in the Orinoco Oil Belt: Integrating CCUS, CO_2-EOR and renewable steam generation for extra-heavy oil production	Adrián Costas Coello, Arturo J. Calvo Tiapa, Marianny D. Álvarez Rodríguez, Pastora M. Bello Bugallo
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AMB83	Análisis multicriterio de teledetección para la implementación de una microrred fotovoltaica en Lonhe, Cuanza Sul, Angola	Ângelo Adão Monteiro, Adilson Domingos Caetano, Pastora Maria Bello Bugallo

Bioquímica y Biotecnología

Oral

BB01	Spray Incorporating Peptide- and Peptidomimetic-Based Ionic Liquid Conjugates for Topical Applications	Inês Costa, Ana Gomes*, Mariana Ferreira, Paula Gameiro & Paula Gomes
BB02	Lipophilic and phenolic profiling of Galactites tomentosus: insights into an underexplored thistle	A.C.S. Veríssimo, P. B. Andrade, D.C.G.A. Pinto
BB03	Subcritical Water Extraction for the Sustainable Valorization of Mediterranean Brown Seaweeds and the Recovery of High-Value Compounds	Sheyma Inoubli*, Wided Megdiche-Ksouri, Leila Ktari, Riadh Ksouri, Fethi Mensi, María Dolores Torres, Céline Laroche, Herminia Domínguez
BB04	Effect of Subcritical Water Extraction Temperature on the Chemical Composition and Structural Characteristics of Fractions from the Green Seaweed Chaetomorpha linum	Nour Aslouj, Sheyma Inoubli, Wided Megdiche-Ksouri, Leila Ktari, Fethi Mensi, María Dolores Torres, Céline Laroche, Riadh Ksouri, Herminia Domínguez
BB05	Chemical Interactions at the Oral Interface: Nanoscale Mapping of Astringency in Cell-Based Models	I. M. Ferreira, F. A. Carvalho, A. S. Fernandes, N. C. Santos, S. Soares
BB06	Chemical diversity of astringents shapes mechanosensitive Ca^{2+} signalling in a human Merkel cell-based model	Sara A. Martins, Joana P. Guedes, Susana Soares
BB07	From Galloylation to Oral Retention: Chemical Drivers of Interindividual Variability in Black Tea Astringency	Joana P. Guedes, Sara A. Martins, Ricardo Franco-Duarte, Elsa Brandão, Susana Soares
BB08	Purification of antileukemic biopharmaceuticals using carbon xerogels	Francisco M. Moreira; Rita A.M. Barros; Rui S. Ribeiro; Ana P.M. Tavares; Raquel O. Cristóvão; Cláudia G. Silva; Joaquim L. Faria
BB09	Valorization of coffee silverskin as a functional food ingredient: in vitro assessment of its anti-metabolic syndrome potential	Juliana A. Barreto-Peixoto, Cláudia Silva, Nelson Andrade, M. Beatriz P. P. Oliveira, Fátima Martel, Rita C. Alves
BB10	Functional biomembranes based on polysaccharides and polyphenols to improve oral mucositis	Ana Carolina Alves, Joana Guedes, Luís Cruz, Susana Soares
BB11	Optimization of propolis extraction from Montesinho Natural Park towards sustainable cosmetic ingredients	Maria F. Sousa, Nicolas Justus, Sandra Barbosa, Ana R. Circuncisão, Cristina Almeida-Aguiar, Izamara de Oliveira, Maria C. Ribeiro, Maria J. Sousa, Olívia Pereira, Susana M. Cardoso.
BB12	Molecular Dynamics Simulations of the Temperature Dependence of Early Amyloid-β42 Oligomerization	Gabriel Martins, Cristiano Rocha, Nuno Galamba

Poster

BB13	Estudio de la adsorción superficial de sulfametoxazol en nanopartículas de óxido de circonio mediante espectrometría vibracional	E. Felipe de la Torre, P. Rodríguez Rodríguez, A.J. Aller, R. López González, F.J. Pereira García
BB14	Solid–Liquid Extraction of Gramicidin from Aneurinibacillus aneurinilyticus Fermentations Using PBS and Membrane Technology: Effect of Agitation Rate	N. Russo-Martínez, X. Vecino, A.B. Moldes, J.M. Cruz
BB15	Real-Time Kinetic Absorbance Microplate Assay for Monitoring Acinetobacter baumannii-Phage Infection	Joana L. A. Miranda, Aurora Silva, Fátima Barroso, Júlia M. C. S. Magalhães
BB16	Organ-specific phytochemical profiles of Galactites tomentosus	A.C.S. Veríssimo, P. B. Andrade, D.C.G.A. Pinto
BB17	Exploring the Effect of Cinnamomum burmannii on Blood Coagulation	Mohammed Benhamou, Vanessa Paula1, Josiana Vaz , Olivia Pereira, Mª João Sousa

BB18	Effects of Choline Salt–Urea DES Formulations on Bovine Carbonic Anhydrase II: Experimental and Molecular Dynamics Analysis	Daniel J. M. Agostinho, Matheus M. Pereira, Mariana Emilia Ghica
BB19	MALDI-TOF-MS profiling of Gramicidin S analogue extracts: effects of culture medium and storage temperature on the stability of mass spectral profiles	N. González-Fernández, A. López-Prieto, J.M. Cruz and A.B. Moldes
BB20	Consensus QSAR modeling for virtual screening of acetylcholinesterase inhibitors	Cláudia Novais, Carlos S. H. Shiraishi, Carla Pereira, Celestino Santos Buelga, Rui Abreu
BB21	Evaluation and Optimization of Seed Disinfection and Germination Protocols in Eruca sativa and Brassica oleracea var. acephala	Cláudia Novais, Ailine Fortes Alves, Maria João Sousa, Carla Pereira, Maria Inês Dias
BB22	Effects of De Novo Peptides on Aβ42 Oligomerization: Molecular Dynamics Insights	Cristiano Rocha, Gabriel Martins, Nuno Galamba

Catálisis y Fotocatálisis

Oral

CAT01	Integrated advanced oxidation processes for salicylic acid degradation using Graphene Oxide/ZnO/$BaSnO_3$	Flávio H. C. Boldrin, César A. F. M. P. Lico, Ikaro Tessaro, Bruno H. B. Silva, Laila G. Andrade, Camilla G. Mascarenhas, Diogo G. Abreu, Pedro H. L. N. A. Santos, Nuno P.F. Gonçalves, Tito Trindade, Liana A. Rodrigues
CAT02	Tailored Cu-Doped ZnO Nanoparticles for Enhanced Photocatalytic Degradation: Optimization of Cu Doping and Immobilization on 3D Printed Scaffolds	Chiara Grassi, Tito Trindade, Corrado Barani, Gigliola Lusvardi, Alfonso Zambon, Nuno P. F. Gonçalves
CAT03	Bauxite residue-derived Fe_2O_3/g-C_3N_4 composites for photocatalytic degradation of emerging water pollutants	Caroline M. B. Araujo, Pedro F. T. Neves, Rui M. Novais, Tito Trindade, Nuno P. F. Gonçalves
CAT04	Sustainable Magnetic Biochar Catalysts for Glycerol Valorization to Solketal	Ó. Pellaumail, C.N. Dias, S.M. Bruno, L. Dias, B. Gholamahmadi, S.S. Balula and F. Mirante
CAT05	Blue Light, Blue Dye: Photocatalytic Guanylation of Sulfonylthioureas	Manuel J. Verganista, Augusto C. Tomé, Carlos M. Monteiro, Nuno R. Candeias
CAT06	Microwave-assisted green synthesis of nanomaterials for photocatalysis	Amanda Martinello Neres de Souza, Daniel Luiz Stamm Baldisserotto, Heloise Dendena, Daniel Eduardo Weibel
CAT07	Effect of Support Nature on the Catalytic Performance of Cobalt Based Fischer–Tropsch Catalysts	Thais Berberich, Claudia Magalhães, Bruno Machado, Dânia Constantino, Helder T. Gomes, Joaquim Faria
CAT08	Electrochemical synthesis of ligand-free transition-metal clusters for sustainable redox catalysis	José M. Blanco Trillo, Selene Giráldez Ferreira, Xabier Lesta Yáñez, Violeta barca neukötter, M. Arturo López Quintela, Carlos Vázquez Vázquez.
CAT09	Estabilidade e reutilização aprimoradas de fotocatalisadores à base de Ag3PO4 por meio de um compósito magnético Fe3O4/HDL/Ag3PO4/AgBr	Fabiano Scolfaro Cheri, Geovânia Cordeiro de Assis, Antonio Carlos Silva Costa Teixeira
CAT10	A Multimodal Machine Learning Framework for Photocatalyst Design in Hydrogen Production	Ana Luísa Machado, Cláudia Silva, Maria José Sampaio, Idelfonso B. R. Nogueira
CAT11	3D-Printed Photocatalytic Immobilised Systems for Green Hydrogen Production	Isabel S.O. Barbosa, Maria A.O. Silva, Yaidelin A. Manrique, Joana C. Lopes, Maria J. Sampaio, Joaquim L. Faria, Ricardo J. Santos, Cláudia G. Silva
CAT12	Enhancing Photocatalytic Hydrogen Evolution through RuO2 modified Graphitic Carbon Nitride	Joana P. Ramos, Joana C. Lopes, Geovânia C. Assis, Joaquim L. Faria, Maria J. Sampaio, Cláudia G. Silva

CAT13	Visible-light-driven photocatalytic ammonia-to-hydrogen process using g-C3N4-based materials	Rafael C. Carneiro, Joana C. Lopes, Goran Dražić, Maria J. Sampaio, Joaquim L. Faria, Cláudia G. Silva

Poster

CAT14	Catalytic ozonation of salicylic acid using atmospheric air and a Carbon Xerogel/ZnO/$BaSnO_3$ catalyst	Flávio H. C. Boldrin, Ikaro Tessaro, Bruno H. B. Silva, Laila G. Andrade, Camilla G. Mascarenhas, Diogo G. Abreu, Pedro H. L. N. A. Santos, Tito Trindade, Liana A. Rodrigues
CAT15	Activity–Selectivity Trade-Off in Cobalt Fischer–Tropsch Catalysts Supported on Si-Modified Alumina	Thais Berberich, Claudia Magalhães, Bruno Machado, Dânia Constantino, Helder T. Gomes, Joaquim Faria
CAT16	Removal of sulfamethoxazole and paracetamol by Fe-containing polymeric membranes: CWPO versus persulfate activation	Kurtebayeva A.A., Silva A.S., Álvarez-Torrellas S., Gomes H.T., Kalmakhanova M.S.
CAT17	Role of TiO_2 Crystalline Phases in Light-Driven H2 Evolution over RuO_2/g-C_3N_4-based Photocatalysts	Joana P. Ramos, Matilde M. Vilela, Geovânia C. Assis, Joana C. Lopes, Joaquim L. Faria, Cláudia G. Silva, Maria J. Sampaio
CAT18	Development of Ag3PO4/g-C3N4 Photocatalysts for the Removal of Organic Pollutants	Fabiano S. Cheri, Geovânia C. de Assis, Cláudia G. Silva, Joaquim L. Faria, Antonio Carlos Teixeira, Maria J. Sampaio

Enseñanza de la Química

Oral

EDU01	La necesidad de matematizar conceptos de química	Ana María Gayol Gonzalez, Sandro Javier González Lafarga, Sandra Marcela Vera
EDU02	From Spectra to Exoplanets: Introducing Astrochemistry in Primary Education	Juan Carlos Ferreira Nolasco
EDU03	Análisis curricular y enfoque CTSA en las pruebas de la Olimpiada Gallega de Química: potencial para el Flipped Learning y la IA	Juan José Sanmartín Rodríguez, José Manuel Andrade Garda

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EDU04	É urgente preparar a geração futura para uma posição ativa relativamente aos oceanos	Teresa Maria De Oliveira Garcia; Luz Parallé, Sérgio Rodrigues
EDU05	Energy for a Sustainable Future: Exploring New Educational Approaches	Laura Blanco Garcia, Pastora Bello Bugallo

Química Industrial e Ingeniería Química

Oral

IND01	Engineering trade-offs in biosurfactant recovery from a corn-derived stream: A comparative pilot-scale study of diffusion dialysis vs electrodialysis	X. Vecino, M. Reig, J.M. Cruz, J.L. Cortina, A.B. Moldes
IND02	Methane/Hydrogen Separation Using a Hierarchically Structured 3D-Printed Porous Carbon Monolith	Laura Bueno, Jose A. C. Silva, Adriano Henrique
IND03	Phenolic-rich purified extracts from Paulownia tomentosa fruits: formulation of starch films for potential health applications	Francisco Díaz-Seoane, Lenka Molčanová, M. Dolores Torres, Eloi Funtané, José María Funtané, Karel Šmejkal, Herminia Domínguez
IND04	Barrier Performance of Natural Rubber Aqueous Dispersion Coatings for Paperboard	Maylee Saavedra, Ricardo Lourido, José Quibén, Ramón Moreira
IND05	BIOCO_2PRO: engineering feedstocks for flexible biogenic CO_2 and syngas production	Isabel B. Calhau, Patrícia Braga, Luís A. C. Tarelho, Athanasios Papadopoulos, Valter Silva
IND06	Experimental Determination and Machine Learning Modeling of Amino Acid Solubility in Aqueous Electrolyte Solutions	S. P. Pinho, P. H. Hamasaki, C. A. Piske, O. Ferreira, M. A. R. Martins, D. O. Abranches and J. A. P. Coutinho

IND07	Acidogenic Fermentation of Lipid Industry Wastes as a Sustainable Valorization Strategy	André Oliveira, Júlia Chegão, Sílvia Petronilho, Mário Coelho, Ricardo Magalhães, Luísa S. Serafim
IND08	Beyond Conventional Re-Refining: Supercritical CO_2 for the Recovery of Challenging Waste Lubricating Oil Streams	C.I.A.V. Santos, L.M. Gando-Ferreira

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IND09	Producción continua de biochar a escala industrial mediante pirólisis a vacío en reactor Auger: criterios de selección de biomasa y aplicación en tintas conductoras para electrodos serigrafiados (SPE)	Manuel Santiago Melón Guntín, David Sucunza Sáenz, Antonio Berná Galiano, Sergio David Gonzalez Egido
IND10	Compostos bioativos sustentáveis derivados de microalgas e cianobactérias para aplicações cosmecêuticas e nutracêuticas (SMACC+)	Legido José Luis, Mourelle Lourdes, Ocampo, Víctor, Domínguez, Herminia, Granja, Luana, Torres, Mª Dolores, Principe, Tonia, Betancor, Abenchara, Barreiro, Filomena, García Vaquero, Marco, Alsamhi, Saeed, O´Brolchain, Niall, Monteiro, Laura, Brito, Gonçalo, Picot, Laurent, Bardor, Muriel
IND11	Efecto de la proporción HPMC:MC sobre las propiedades físicas y oxidativas de oleogeles de aceite de colza	Mario Lama, Amaya Franco-Uría, Ramón Moreira
IND12	Reología de las masas y características de magdalenas de harina de yuca elaboradas con mantequilla o aceite con y sin gelación	Mario Lama, Santiago Arufe, Amaya Franco-Uría, Ramón Moreira
IND13	Influence of Fishery By-Product Type and Hydrolysis Conditions on the Obtention of Protein Hydrolysates and Antioxidant Bioactive Peptides	Sofia Viciana-Mosquera, Noelia López Cotelo, Amaya Franco-Uría, Maria López Pedrouso, José Antonio Vázquez, Jorge Sineiro, Luis T. Antelo, Daniel Franco
IND14	Influence of Rosin and Zinc Oxide on the Structure and Rheology of Natural Rubber Aqueous Dispersions	Maylee Saavedra, Ricardo Lourido, José Quibén, Ramón Moreira
IND15	Valorización de residuos agroforestales para la fabricación de bandejas de celulosa moldeada	De Castro Alves, Lisandra, Espinosa Victor, Eduardo, Francisco Fuentes, J.L., Quintero Sánchez, Manuel
IND16	Linking physicochemical properties and heavy-metal adsorption in biomass-derived carbons through multivariate analysis	Joseph I. Ramírez-Hernández, Diego Gómez-Díaz, M. Sonia Freire, Julia González-Álvarez
IND17	Fig and Almond Pruning Biomass as Low-Cost Adsorbents for Nitrate Removal from Aqueous Solution	Yesica VIcente, Ángela Muñoz, Patricia Gómez, Diego Gómez-Díaz, M. Sonia Freire, Julia González-Álvarez
IND18	3D Printing of Biodegradable Hydrogels for Lutein Incorporation	Madalena Marques, Sofia Saraiva, Rafael C. Rebelo, Carlos Paula, Mariana Emilia Ghica
IND19	Procesos de modelización/simulación en la síntesis y purificación de un ester de amilo	José Canosa, Julio Rufo, Beatriz Lorenzo, Juan Ortega

Nanoquímica y Nanotecnología

Oral

NN01	Quantum Heterojunctions Enabling Textile All-in-One Photo-Supercapacitors	João M. O. Silva, André M. Pereira, Clara R. Pereira, Joana S. Teixeira
NN02	Role of the Electrogenerated Hydrophilic Carbon in the Formation, Stability and Activity of Pd nanoparticles	Andreia Veloso*, Cristina Oliveira
NN03	Surfactant-free colloidal syntheses of metal nanoparticles: challenges and opportunities for catalysis and beyond	Javier Eiroa Soto and Jonathan Quinson

NN04	Multifunctional Smart Security Labels for Anti-Counterfeiting Textiles	Marta S. Nunes, Ana R. Sousa, Felippe Gonçalves, M. Helena Silva, Tomás Gonçalves, Clara R. Pereira, André Pereira
NN05	Smart Photoswitchable Organic-Inorganic Hybrid Nanomaterials for Light-Responsive Textile Applications	Gabriela Werdan, Joana S. Teixeira, Clara R. Pereira
NN06	Development of Nanoformulations for Oral Administration and Treatment of Crohn's Disease	Rita F. R. Cardoso; Clarisse Lopes; Ana Rita Saraiva; Cláudia Machado; Joana Moreira; Francisco Otero-Espinar; Miguel Pinto; Carlos Fernandes
NN07	Biomimetic Non-Lamellar Lipid Nanoparticles for Bioactive Compound Delivery	Ana Amorim, Sofia Oliveira, Ana Isabel Barbosa, Ibraheem Yousef, Cláudia Nunes, Andreia Granja, Salette Reis

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NN08	Purpurin 18-Assisted Formation of Gold Nanoparticles on WS_2 Nanoflakes for Cancer Therapy	Noelia González-Ballesteros, Melissa Santi, Evie L. Papadopoulou, Francesco Bonaccorso, Franca Bigi, Giancarlo Salviati and M Carmen Rodríguez-Argüelles
NN09	Carbon Nanomaterials as Photo-Active Materials in Textile All-in-one Photo-Supercapacitors	João M. O. Silva, Gonçalo M. Araujo, André M. Pereira, Clara R. Pereira, Joana S. Teixeira
NN10	Cysteamine-Functionalized ZnPPIX for Integration with PVP-Stabilized Silver Nanoparticles: Optical and Photochemical Characterization	Santos D.M.L, Ribeiro M.J.G, Marmo. V.L.M, Raniero L. J, Soreto S
NN11	Exploring Liposomal NanoSystems for Delivery of Triphenylphosphonium Derivatives	Rita F. R. Cardoso, Clarisse Lopes, Joana Moreira, Barbara Nunes, Cláudia Sampaio Machado, Miguel Pinto, Fernando Cagide and Carlos Fernandes
NN12	Electrochemical synthesis of ligand-free iron clusters: ascorbic acid oxidation and antibacterial evaluation	José M. Blanco Trillo, Blanca Domínguez Loidi, Selene Giráldez Ferreira, Xabier Lesta Yáñez, M. Arturo López Quintela, Carlos Vázquez Vázquez.
NN13	From milk cream to functional nanocarriers: a sustainable approach for curcumin delivery	Ana D. Torres, João Albuquerque, Filipa Soares, Cláudia Nunes, Salette Reis
NN14	From Sea to Skin: Dunaliella salina Nanoparticle-Loaded Hydrogels for Skin Hydration and Regeneration	Tito Teixeira, Maria Antónia Salgado, Sofia A. Costa Lima
NN15	Ingeniería de Nanomateriales para el Almacenamiento Sostenible de Energía: Retos y Perspectivas Emergentes	Dra. Elisabeth Viviana Lucero Baldevenites
NN16	Development of Sustainable Lignin-Based Nanoplatforms with Magnetothermal and Optical Properties	Manuel Antonio González Gómez, Yolanda Piñeiro y José Rivas

Química de Polímeros

Oral

POL01	Desenvolvimento e caracterização de matrizes biopoliméricas para revestimentos alimentares	Tayna C. B. Souza, B. Nogueira, Catarina P. Gomes,1 Custódio Lobo Roriz, Isabel P. Fernandes,Rolando C. S. Dias, Miguel A. Prieto, Filipa A. Fernandes, Sandrina A. Heleno,

Poster

POL02	Design and synthesis of perchlorotriphenylmethyl radical-based covalent triazine framework for lithium-ion storage	Tianshu Zhang, Arindam Mal, Manuel Souto
POL03	PVC Insulation, Elongation and Product Robustness	Sandra Matos, Ana Luís

POL04	Potencial de diferentes quitosanos para o desenvolvimento de revestimentos alimentares	Tayna C. B. Souza, Catarina P. Gomes, Custódio Lobo Roriz, Izamara de Oliveira, Isabel P. Fernandes, Rolando C. S. Dias, Miguel A. Prieto, Filipa A. Fernandes, Sandrina A. Heleno
POL05	Shrinking Process Optimization	Sandra Matos, Guilherme Ferreira
POL06	From Wheat Straw to Functional Food Packaging: Cellulose- and Lignin-Stabilized Pickering Emulsions for Sustainable Coatings	Eduardo Espinosa, Esther Rincón, De Castro Alves, Lisandra, Francisco Fuentes, J.L, Quintero Sánchez, Manuel

Química Analítica

Oral

QA01	From conventional water sampling to a miniaturized solid phase extraction sampling strategy for metal ions monitoring	Tânia C. F. Ribas*, Inês O. M. S. Dias, Raquel B. R. Mesquita, António O. S. S. Rangel
QA02	Reliable lithium quantification in waters with ionic strength: ICP-OES method validation and uncertainty assessment	Raquel T. Fernandes, Daniela S. Tavares, Eugénio Soares, João Rocha, Eduarda Pereira
QA03	Orfinas Emergentes em Amostras de Drug Checking: Identificação e Elucidação Estrutural	Bárbara F. C. Barra; Joana R. P Pereira; Ana S. D. Ferreira; Gonçalo C. Justino; Rui M. Almeida; Hans Oeri; Alexandre Quintas; Nuno R. Neng
QA04	Dispositivo analítico basado en papel asistido por smartphone para la detección colorimétrica de azúcares reductores en miel	Vanesa Romero, Alicia Carro, Carlos Bendicho, Isela Lavilla, Francisco Pena-Pereira
QA05	Desarrollo de una sonda fluorescente basada en puntos de carbono sintetizados mediante UV/H_2O_2 para la detección de bisfenol A en alimentos	Alberto Abalde-Pujales, Vanesa Romero, Francisco Pena-Pereira, Carlos Bendicho, Isela Lavilla
QA06	Determinación colorimétrica cinético-catalítica de vanadio mediante un dispositivo microfluídico tridimensional basado en papel	N. Villarino, E. Treviño, I. Lavilla, C. Bendicho, F. Pena-Pereira
QA07	Towards Integrated Wine Analysis: Automated Determination of Carbon Dioxide and Sulphur Dioxide	Bartłomiej Trojanowski , Tania C.F. Ribas, Raquel. B.R. Mesquita, Antonio O.S.S.
QA08	Development of a 3D-microfluidic paper-based analytical device for phosphate determination with smartphone-based colorimetric detection	Inmaculada De la Calle-González*, José Manuel Graña-Dosantos, Francisco Pena-Pereira
QA09	Electrochemical DNA-based biosensors to discriminate against the rs1065852 SNPs genotypes associated with drug-resistant epilepsy	Renata Santos, Stephanie L. Morais, João Pacheco, Henri Nouws, Hygor Fernandes, Giovanny Pinto, M. León-Vázquez, D. San Juan-Orta, Karen L. Benítez-Rodríguez, I. Ruíz-Santillán, Iris Feria-Romero, M. Fátima Barroso
QA10	Sustainability-by-Design Sample Preparation for Thermal-Processing Contaminants in Infant Foods	J. A. Custodio-Mendoza, M. R. Pérez-Gregorio, M. Llompart, A. M. Carro, E. Martinez-Carballo
QA11	Integrated One Health Monitoring Tool for On-Site Nitrate and Nitrite Analysis	Francisca T. S. M. Ferreira, António O. S. S. Rangel, Raquel B. R. Mesquita
QA12	Aplicación de LA-ICP-MS á análise de mostras líquidas: determinación de elementos traza en leite	Domínguez-Robles I., Herbello-Hermelo P., Domínguez-González R., Bermejo-Barrera P., Moreda-Piñeiro A.
QA13	Flow-based method for glyphosate monitoring in well water samples for human consumption	Juliana I. S. Aguiar, António O. S. S. Rangel, Raquel B. R. Mesquita
QA14	A sequential injection chromatographic approach for molecular weight screening of protein hydrolysates	Raquel Teixeira, Tânia C. F. Ribas, André Almeida, Manuela Pintado, António O. S. S. Rangel

QA15	Desenvolvemento dun método para a determinación de nanopartículas de cerio e ferro en material particulado atmosférico	González-Barcia Sheila, Pumares-Guntín Elena, Barciela-Alonso María Carmen, Moreda-Piñeiro Antonio, Peña-Vázquez Elena, Vázquez-García María José
QA16	Addressing gadolinium contamination from hospital effluents: A sustainable approach for protecting aquatic water quality	Eduarda Pereira, Daniela S. Tavares, Rosa Freitas, Tito Trindade, Raquel Fernandes, Thiago Silva, João Rocha
QA17	Electrochemical Procedures Coupled To CYP450 Metabolism For Control And Environment Risk Analysis Of Transdermal Patches	José Pedro Silva, Célia G. Amorim, Alberto da Nova Araújo
QA18	Plataformas sensoras baseadas em pontos quânticos e polímeros molecularmente impressos imobilizados em suportes sólidos: desenvolvimento, reconhecimento molecular e aplicações	Eduarda Rodrigues, Rafael C. Castro, Ana Margarida L. Piloto, João L. M. Santos e David S. M. Ribeiro
QA19	Caracterización de gasolinas mediante el perfil de hidrocarburos (HCs) ligeros saturados (C1-C7) de la fase de vapor	Luis Alejandro Díaz Flores, Pablo Hugo Zárraga Luqueño, Telma Gloria Castro Romero, Ma. Amparo Martínez Arroyo, Lara Bárbara Cuesta Castillo

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QA20	SENTINEL Project: Analytical Characterization of Emerging Nitazene Opioids	Bárbara F. C. Barra, Joana R. P. Pereira, Mariana P. Madeira, Sara F. Amaral, Daniela R. Ferreira, Marisa H. Maria, Joana Couceiro, Patrícia Serra, Helena Gaspar, Alexandre Quintas, Nuno R. Neng
QA21	Targeting Emerging Nitazenes: Development and Validation of a GC–MS/MS Method for Drug Checking Samples	Joana R. P Pereira; Bárbara F. C. Barra; Suzana Fonseca; Alexandre Quintas; Nuno R. Neng
QA22	Identifying the Botanical Origin of Honeys: Single-walled carbon nanotube-based genosensors for the detection of Erica arborea in honey samples	Stephanie L. Morais, Marlene Santos, Ana L. Teixeira, Valentina F. Domingues, Cristina Delerue-Matos, M. Fátima Barroso
QA23	New chemosensor and nano-liquid chromatography for the determination of phenols in environmental waters	M.C. Prieto-Blanco, B. Monforte-Gómez, P. Campíns-Falcó
QA24	Validación de un método automatizado basado en volumetría potenciométrica para la determinación de la acidez total en vinos	María José González-Castro, Julia María Medín-Crespo, Iago Neira, Jaime Fernández-Paz
QA25	Chiral Resolution and Biological Activity of Novel Terpene-Based Cannabinoids	Gabriel V. L. Marques, Rita M.G. Santos, Irene Pereira, Cristina P.R Xavier, Carla Fernandes, Maria Emília Sousa, Renata B. de Oliveira
QA26	Optimización de separaciones por HPLC mediante diseños experimentales Box–Behnken y Doehlert	E. Felipe de la Torre, N. Porto González, P. Ablanedo Ablanedo, A.J. Aller, R. López González, F.J. Pereira García
QA27	Diseño y optimización de un método de preconcentración de etinilestradiol y estriol mediante microextracción líquido-líquido dispersiva asistida por ultrasonidos (ua-dllme) para su análisis por fluorimetría	I. Martínez-Garrido, E. Felipe-de la Torre, S. Martínez-Mendoza, R. López, A.J. Aller, F.J. Pereira, L.C. Robles.
QA28	Determinação simultânea de amoxicilina e ácido clavulânico em formulações farmacêuticas usando pontos quânticos de $AgInS_2$ e quimiometria	Rafael C. Castro, Ricardo N. M. J. Páscoa, Eduarda Rodrigues, João L. M. Santos, David S. M. Ribeiro

QA29	Sondas fluorescentes combinadas de pontos quânticos e análise quimiométrica para a determinação cinética de cloranfenicol em formulações farmacêuticas	David S. M. Ribeiro, Ricardo N. M. J. Páscoa, Eduarda Rodrigues, João L. M. Santos, Rafael C. Castro
QA30	Sensor Raciométrico Baseado em Membranas Molecularmente Impressas para a Deteção no Local do CA 19-9	Eduarda Rodrigues, Ana Xu, Paula Sampaio, Rafael C. Castro, David S. M. Ribeiro, Ana Margarida L. Piloto e João L. M. Santos
QA31	Towards Online CO_2 Monitoring in Power Transformers: Evaluation of NDIR Sensors Detection in Spiked Oil Samples	Inês N. Vilhena, Vítor R. Costa, Roberto Laranjeira1, Denis R. Santos, João Piteira, Hugo M. Oliveira
QA32	Gas sensors characterization for dissolved gas analysis of power transformer oil	Vítor R. Costa, Inês N. Vilhena, Roberto Laranjeira, Denis R. Santos, João Piteira, Hugo M. Oliveira
QA33	Análisis de componentes principales (PCA) del perfil de hidrocarburos y su aplicación en la caracterización de diésel	Luis Alejandro Díaz Flores, Adolfo Jesús Chávez Cortez, Telma Gloria Castro Romero, Ma. Amparo Martínez Arroyo, Lara Bárbara Cuesta Castillo

Química Física

Oral

QF01	Exploring the Solid-State Landscape of Leflunomide: Polymorphism and Multicomponent Systems	Nuno A. S. Santos, João A. Baptista, João Canotilho, M. Ermelinda S. Eusébio, Ricardo A. E. Castro, Teresa M. R. Maria

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QF02	Estudo microcalorimétrico do crescimento de Pediococcus acidilactici em meio de cultura enriquecido	Gómez, Carmen , Franco, Javier, Lago, Natividad, Legido, José Luis, Pardellas-Soto, Jorge, Veiga-Sans, Sonia, Pérez-Gregorio, Rosa
QF03	From Pyrazines to Bipyridines: Structural and Spectral Parallels Across Leflunomide Multicomponent Assemblies	Nuno A. S. Santos, João A. Baptista, João Canotilho, M. Ermelinda S. Eusébio, Ricardo A. E. Castro, Teresa M. R. Maria

Química Inorgánica

Oral

QI01	A mononuclear Dy-N3O5 complex with single-molecule magnet behavior	P. Oreiro-Martínez, E. García-Gorraiz, J. Corredoira-Vázquez, A.M. García-Deibe, M. Fondo
QI02	Assessing Charge Transfer in Halogen Bonds: A Comparative Study Using OP/TOP, QTAIM, and LVM Descriptors	Rachel A. Maia, Carlos V. Santos-Jr, Julio Corredoira-Vazquez, Ricardo L. Longo, Albano N. Carneiro Neto, Renaldo T. Moura-Jr
QI03	Synthesis, structure, and in vitro cytotoxicity of a dinuclear Cu(II) complex based on a bis(thiosemicarbazone) ligand	I. Velo-Heleno, A. Luzardo, S. Fernández-Fariña, R. Pedrido, A. M. González-Noya
QI04	Synthesis of Platinum Complexes based on Gemcitabine and Cytidine	Giulia Orsini, Ines Leitão, Ana Petronilho
QI05	Rutenio(II) e Tiosemicarbazonas: novas prespectivas na loita contra o cancro de mama triple negativo.	Mónica Martínez Estévez, Ezequiel Vázquez López, Soledad García Fontán, Isolda Romero Canelón
QI06	Coordination behavior and reactivity of $\{M(CO)_3\}^+$ (M = Tc, Re) complexes bearing thiosemicarbazone-carborane ligands	Irene Vázquez Carballo, Maximilian Roca Jungfer, Antonio Sousa Pedrares
QI07	Substituent Effects on C–C and C–H Bonding: A Multi Descriptor Investigation via Electron Density Overlap	Robson F. Silva, Rachel A. Maia, Carlos V. Santos-Jr, Albano N. Carneiro Neto, Renaldo T. Moura-Jr
QI08	Valorização de resíduos PET e CO2 através da preparação do MOF Co-BDC para a produção de carbonatos cíclicos	Susana Guimarães, Salete S. Balula, Ana M.G. Silva, Carlos R. Gomes4, Luís Cunha-Silva

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QI09	JoyAI: A machine learning approach for predictions of ligand excitation energies in lanthanide-based complexes	Rachel A. Maia, Emanuel E. M. Feitosa, Maria M. S. Silva, Carlos V. Santos-Jr, Julio Corredoira-Vazquez, Ricardo L. Longo, Albano N. Carneiro Neto, Renaldo T. Moura-Jr
QI10	A route to zinc(II) helical complexes from bishydrazones	I. Velo-Heleno, M. Rodríguez-Padrón, M. Martínez-Calvo, C. Núñez, L. Rodríguez-Silva, M. Maneiro
QI11	Gold(I)-NHC Complexes Derived from Uracil and Cytosine: Synthesis, Characterization and Potential Applications	Giulia Romeo, Ana Petronilho
QI12	Study and comparison of the stability of two iminophosphorane ligands: carborane versus organic	Irene Vázquez Carballo, Antonio Sousa Pedrares
QI13	Modulating Defect States in Real-Sized Lanthanide-Doped Nanoparticles	Robson F. Silva, Rachel A. Maia, Carlos V. Santos-Jr, Albano N. Carneiro Neto, Renaldo T. Moura-Jr
QI14	Machine learning applied to the magneto-optical properties of lanthanide metal complexesMachine learning applied to the magneto-optical properties of lanthanide metal complexes.	Breogán Lago-López; Julio Corredoira-Vázquez; Albano N. Carneiro Neto
QI15	Machine Learning-Driven Prediction of Judd-Ofelt Parameters and Hypersensitive Ratios in Europium(III) Complexes	Daniel Nieto-Pastoriza, Julio Corredoira-Vazquez, Renaldo T. Moura, Matilde Fondo, Albano N. Carneiro Neto

Química Orgánica

Oral

QO01	Continuous-Flow Synthesis and Process Optimization of MANIO:A Scalable Route to a Promising p53-Targeting Anticancer Agent	Margherita Gajo, Maria I. L. Soares1, Lucília Saraiva2, Teresa M. V. D. Pinho e Melo1
QO02	From organic chemistry lab to the sea: exploring 3,4-dihydroxyxanthone as a sustainable antifouling agent	Bruno S. M. Loureiro, Catarina Costa, Ana R. Sampaio, Raquel Ruivo, Ana Sara Gomes, Joana Almeida, Marta Correia da Silva
QO03	Valorização de grafite reciclada através da incorporação de óxido de grafeno em betão	Luís M. G. Ferreira, Rita Silva, Ricardo Pereira, Maria Regufe, Dulce Geraldo, Susana P. G. Costa
QO04	Validation of Quantum Chemistry Predictions. Quinoidal-Base Tautomers in Anthocyanins and Related Compounds	Pereira, Rui; Mahmoodi, Hanieh; Basílio, Nuno; Lima, João C. ; Outis, Mani.; De Freitas, Victor; Cruz, Luis; Pina, Fernando
QO05	N,N-dimethylformimidamide Purines as new fluorescent platforms: Synthesis, photophysical properties and quantum chemical calculations	Jorge M. Gonçalves, Elisabete M. S. Castanheira, Paulo J. G. Coutinho, Alice M. Dias
QO06	Challenges and breakthroughs in developing potent antifungal and halochromic dyes: tackling the problem of selective synthesis	Mariana P. Silva, Bárbara Silva, Inês Costa, Paulo J. G. Coutinho, Eugénia Pinto, Alice M. Dias
QO07	Spectroscopic Characterization of Dynamic Complexes between Anthocyanins and a Boronic Acid-Chalcone Receptor	Mariana Cunha, Victor de Freitas, Luís Cruz
QO08	Discovery of First-in-Class Melanostatin-Based Ago-Allosteric Modulators of Dopamine D2 Receptors	Hugo F. Costa Almeida; Xavier C. Correia; Sara C. Silva-Reis; Beatriz L. Pires-Lima; Vera M. Costa; Eddy Sotelo, José E. Rodríguez-Borges; Ivo E. Sampaio-Dias
QO09	Molecular Engineering of Porphyrin–PAHs for Functional π-Conjugated Materials In-Solution and On-Surface	Ana R. Monteiro, Marina Vázquez-Carballo, Diego Peña

QO10	Fluorescent probes for Efficient Assays for Measuring Inhibition of Penicillin Binding Protein 3 (PBP3) Transpeptidases	Ignacio E Tobal; Helen G Smith; Stephen A. Marshal; Alistair J. M. Farley; Christopher J. Schofield
QO11	Silyl-Prins cyclization with ketones: stereoselective construction of C2-quaternary stereocenters in polysubstituted tetrahydropyrans	L. G. Parte, L. F. Peña, C. Díez-Poza, A. Barbero
QO12	Ferrocene-Core Hybrid Molecules: A Synthetic Strategy Toward Novel Oxacycles for Targeted Cancer Therapeutics	L. Pedraza, L. Arribas, A del Campo-Balguerías, C. Alonso-Moreno, E. López, A. Barbero
QO13	Synthesis of diketopyrrolopyrrole-derived maleimides — new turn-on fluorescent probes for detecting biothiols	Gonçalo F. Oliveira, Augusto C. Tomé1
QO14	Porphyrin–AZT Conjugates: Synthesis and Photophysical Evaluation	Telma B. Olival, Oscar D. Rodrigues, Carlos J. P. Monteiro, M. Amparo F. Faustino
QO15	Impact of regioisomerism in bianthracene-bis-porphyrin chiral conjugates	Marina Vázquez Carballo, Ana R. Monteiro, and Diego Peña
QO16	(–)-Quinic acid as a natural chiron for the photocatalyzed synthesis of spirolactones	Carina J. N. Caires, Carlos A. M. Afonso, Nuno R. Candeias

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QO17	Synthesis, characterization and in vitro dissolution testing of a dihydropyrimidinone obtained via the biginelli multicomponent reaction	Marcos Vinicios da Silva, Sérgio Scherrer Thomasi, Luciana de Matos Alves Pinto
QO18	Synthesis of novel 4-(bis(4-(dialkylamino)phenyl)amino) phthalonitrile derivatives	Gonçalo F. Oliveira; Leandro M. O. Lourenço
QO19	Mechanochemical Hetero-Diels-Alder Reactions of In Situ Generated Azoalkenes with 2,5-Dimethylfuran: A Sustainable Synthetic Approach	Ângela Marques, Teresa M. V. D. Pinho e Melo, Marta Pineiro
QO20	Bis(trimethylsilyl) Peroxide-Mediated α-Chlorination of Acetophenones	Flávio Figueira*, Francisco Domingues, Nuno R. Candeias
QO21	A Streamlined and Sustainable One-Pot Route to cis-4-Hydroxy-L-Prolyl Amides	Ivo E. Sampaio-Dias, Xavier C. Correia, Hugo F. Costa-Almeida, Beatriz L. Pires-Lima, Sara C. Silva-Reis, Xerardo García-Mera

Química y Salud

Oral

QS01	From Photochemistry to Phototoxicity: Linking the Photochemical Behavior of Food-Derived Chromophores to Cellular Response in Melanoma Cells	Patrícia Correia, Sofia Aleixo, Nuno Mateus, Victor Freitas and Iva Fernandes
QS02	From β-Keto Reduction to Neurotoxicity: Cytotoxic and Oxidative Effects of Dihydropentedrone and Dihydromethylone in SH-SY5Y Cells	Carolina Mourão; Ana Sofia Almeida; Bárbara Silva; Fernando Remião; Carla Fernandes
QS03	Translating the mind: a point-of-care electrochemical platform for miR-151a-3p in neurodevelopmental disorders	Eduarda Pereira, Renata Santos, Farzaneh Jahantigh, Stephanie L. Morais, Catarina Prior, Marlene Santos, João G. Pacheco, Ana Luísa Teixeira, M. Fátima Barroso
QS04	Point-of-care quantification of salivary alpha-amylase using a vertical flow µPAD for stress monitoring in humans and pigs	Maria M. P. Melo, María Botía, José Joaquín Cerón, António O. S. S. Rangel, Raquel B. R. Mesquita
QS05	Light-Activated Zinc(II) Phthalocyanines for Enhanced Antimicrobial Photodynamic Inactivation of Gram-Positive Bacteria	Daiane N. Maronde, José E. R. Borges, Adelaide Almeida, Leandro M. O. Lourenço

QS06	Design and Synthesis of Fluorinated Analogues of a Non-Nitrocatechol COMT Inhibitor for Neuroprotection in Dopaminergic Degeneration	Inês Silva, Daniel Chavarria, Fernanda Borges, Sofia Benfeito
QS07	The First Sila-Derivatives of Vitamin D: Synthesis and Biological Application in Triple-Negative Breast Cancer Therapy	Maria B. Igreja-Cardoso, Sara C. Silva-Reis, José E. Rodríguez-Borges, Ivo E. Sampaio-Dias
QS08	First-in-Class Melanostatin Hybrids as Potent Modulators of the Dopamine D2 Receptors with Neuroprotective Activity	Beatriz L. Pires-Lima, Sara C. Silva-Reis, Xavier C. Correia, Hugo F. Costa-Almeida, Xerardo García-Mera, Nuno Vale, José E. Rodríguez-Borges, Ivo E. Sampaio-Dias
QS09	Chemical Modification of the Anti-EGFR Monoclonal Antibody with 11-Mercaptoundecanoic Acid: UV–Vis and FTIR Characterization	Santos D.M.L, Ribeiro M.J.G, Marmo. V.L.M, Raniero L. J, Soreto S
QS10	Preliminary Mechanistic Studies of New Pyrimidine-Based Compounds for Osteosarcoma Therapy	Pereira, A. B., Teixeira, S., Santos, I., Ferreira de Oliveira, J. M. P., Fernandes E., Carvalho, M. A.

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QS11	Innovación molecular en la Química Cosmética	Ana María Gayol González, Juan José Sanmartín Rodríguez.
QS12	Hypericin- Synthesized Metal Nanoparticles as Anticancer Green-Light-Activated Agents in 3D Tumor Models	Noelia González-Ballesteros, Melissa Santi, Raquel Rey-Méndez, Andrea Marranci, Franca Bigi, Giancarlo Salviati , Filippo Fabbri and M Carmen Rodríguez-Argüelles
QS13	Del residuo al valor: extracción asistida por microondas de compuestos bioactivos a partir de hojas y tallos de berenjena	Matilde Rodrigues, María Carpena, M. Beatriz P.P. Oliveira, Celestino Santos-Buelga, Miguel A. Prieto, José Pinela
QS14	Electrochemical microRNA-based biosensor for predicting therapeutic response in castration-resistant prostate cancer	Eduarda Pereira, Marlene Santos, Ana Luísa Teixeira, M. Fátima Barroso
QS15	Melanostatin-Amantadine Conjugates as Potent Positive Allosteric Modulators of Dopamine D2 Receptors	Daiane N. Maronde, Maria B. Igreja-Cardoso, Sara C. Silva-Reis, Xavier C. Correia, Hugo F. Costa-Almeida, Beatriz L. Pires-Lima, José E. Rodríguez-Borges, Ivo E. Sampaio-Dias
QS16	Synthesis of Neuroprotective Agents Targeting Dopaminergic Degeneration and Ferroptosis	Inês Silva, Daniel Chavarria, Fernanda Borges, Sofia Benfeito
QS17	Decoupling Neuroprotection from MAO-B Inhibition through Bioisosteric Replacement of Rasagiline	Maria B. Igreja-Cardoso, Sara C. Silva-Reis, Xavier C. Correia, Hugo F. Costa-Almeida, Gabriel M. Azevedo, Vera M. Costa, Damijan Knez, Stanislav Gobec, José E. Rodríguez-Borges, Ivo E. Sampaio-Dias
QS18	Fine-Tuning Glypromate Neuroprotection: Synthesis and Biological Evaluation of Novel Peptide-Drug Conjugates	Hugo F. Costa Almeida; Sara C. Silva-Reis; Xavier C. Correia; Vera M. Costa; José E. Rodríguez-Borges; Ivo E. Sampaio-Dias
QS19	Synthesis and Neurotoxicity Profile of Pyridine-Based Melanostatin Derivatives Targeting Parkinson's Disease	Beatriz L. Pires-Lima, Nuno Vale, Xerardo García-Mera, José E. Rodríguez-Borges, Ivo E. Sampaio-Dias
QS20	Biodegradability of Glucocorticoids: Chemical Stability and Environmental Fate	Ângela do Ó, E. Manuela Garrido, Alexandra Gaspar, Jorge Garrido
QS21	Zein-Coated SPION-Based Paclitaxel Release Systems for Pancreatic Cancer Applications	Jacinta Santos, Sofia Saraiva, Nuno R. Ferreira, Andreia Romeiro, Mariana Emilia Ghica

QS22	Development of Melanostatin Azapeptides with Improved Biochemical Stability	Xavier Cruz Correia, Hugo F. Costa-Almeida, Sara C. Silva-Reis, Beatriz L. Pires-Lima, Vera M. Costa, Xerardo García-Mera, José E. Rodríguez-Borges, Ivo E. Sampaio-Dias
QS23	Building Blocks for Novel 3-Hydroxypyridin-4-One Chelators: Towards Biomedical Metal Coordination and Critical Raw Materials Recovery	Ângela do Ó, Jorge Garrido, E. Manuela Garrido, Alexandra Gaspar
QS24	Development of Conformationally Constrained Peptides as Potent Positive Allosteric Modulators of the Dopamine D2 Receptor	Ivo E. Sampaio-Dias, Hugo F. Costa-Almeida, Xavier C. Correia, Beatriz L. Pires-Lima, Marialessandra Contino, Maria Grazia Perrone, Giovanni Graziano, José Brea, María I. Loza, Eddy Sotelo, Ana Reis-Mendes, Vera M. Costa, Xerardo García-Mera, José E. Rodríguez-Borges
QS25	Revisiting Fluoroquinolones: New Chemistry, New Antibacterial Possibilities	Ângela do Ó; Alexandra Gaspar, Jorge Garrido, Manuela Garrido , Manuela Machado, Eduardo Soares

Química Teórica

Oral

QT01	WFS4PLAS: simulating microplastic adsorption	Raul E. Dias, Susana L. H. Rebelo, Alexandre L. Magalhães
QT02	Ion Structure and Dynamics in Ionic Liquids Confined within MXene Electrodes: Molecular Insights into Supercapacitor Charging	I.V. Voroshylova, V. Koverga, M.N.D.S. Cordeiro, V.B. Ivanistsev
QT03	Green-Solvent Extraction of Propolis: Experimental Assessment and Machine Learning Prediction of Total Phenolic Content	David L. Almeida, Artem Drogalin, Amit Kumar Halder, M. Natália D.S. Cordeiro, Andreia F. Peixoto

Póster

QT04	Structure–Activity Relationship Analysis of Novel Synthetic Opioids Using Molecular Docking	Sara F. Amaral, Bárbara F. C. Barra, Alexandre Quintas, Nuno R. Neng, Patrícia Serra
QT05	Molecular dynamics study of PVA/H3PO4 polymer electrolyte: the role of the proton in structure and transport	Andreia P. Fonseca, M. Natália D. S. Cordeiro, Clara R. Pereira, Iuliia V. Voroshylova

Seguridad Química

Póster

SQ01	Compuestos BTEX en residuos de tanques de almacenamiento de gas natural	M.C. Fernández-Feal, B. Sánchez-Fernández, L.R. Sánchez-Fernández

CONFERENCIAS PLENARIAS

RNA Is More than a Messenger: The Chemistry and Biochemistry of Noncoding RNAs

Thomas R. Cech, PhD
Distinguished Professor of Biochemistry, U. of Colorado Boulder, Colorado, USA
Nobel Prize in Chemistry, 1989

Prof. Cech will present two examples where RNA is not functioning in its traditional role as a messenger. The first concerns catalytic RNAs, called “ribozymes.” This research led to the Nobel Prize in Chemistry in 1989. The second example concerns recent unpublished research in which RNA controls the activity of a gene-silencing protein in the human cell nucleus. This work relies on cryogenic electron microscopy and A.I. Throughout his talk, Prof. Cech will emphasize the importance of thinking like a chemist – e.g., molecular structure, hydrogen bonding, metal ions, transition states, kinetics and thermodynamics – for understanding the mechanisms of biochemical processes essential for life.

Boronic Acids: A Useful Functional Platform for Chemical Biology

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Boronic acids (BAs) possess a rich and dynamic coordination chemistry, often characterized by the interconversion of the central boron atom between an uncharged trigonal planar structure and an anionic sp^3-hybridized borate species. This versatility allows for the judicious selection of ligands to construct a wide array of boron complexes (Bcomplexes) with unique molecular architectures and diverse properties.

The stability of boron-based reversible covalent bonds is highly influenced by factors such as pH and the concentration of endogenous molecules like carbohydrates and glutathione. Additionally, aromatic boronic acids are well-known to undergo rapid oxidation to phenols in the presence of reactive oxygen species. This distinctive reactivity profile provides an additional layer of utility for BAs, enabling the design of materials that incorporate mechanisms to respond to specific chemical stimuli.

Such responsiveness is particularly valuable in the discovery and development of new drugs for complex diseases, including cancer, neurodegeneration, and inflammation, which are often characterized by these chemical triggers as key molecular hallmarks. This presentation will focus on the use of boronic acids in the synthesis of Bcomplexes, highlighting their potential as well-defined, stimuli-responsive molecular platform.[1-4].

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Engineering Carbon Nitride Nanomaterials for Photocatalytic Applications

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The transition to sustainable chemical processes requires efficient catalytic systems that operate under mild conditions with minimal environmental impact. Graphitic carbon nitride (g-C_3N_4) has emerged as a promising metal-free semiconductor for photocatalytic and photo-biocatalytic applications due to its visible-light activity, chemical stability, abundance, and simple synthesis. This work presents a comprehensive strategy for engineering carbon nitride nanomaterials through rational design, structural modification, and integration into advanced catalytic systems for environmental, energy, and biomedical applications. Engineered carbon nitride materials were successfully applied in diverse photocatalytic processes. In water treatment, they promote visible-light-driven degradation of micropollutants, including photo-Fenton reactions with in situ H_2O_2 generation [1]. For solar fuel production, g-C_3N_4-based systems efficiently reform biomass-derived substrates to produce hydrogen, including in seawater, demonstrating their robustness and sustainability [2]. Additional applications include photocatalytic organic synthesis and nitrogen-cycle processes such as ammonia production. Hybrid systems combining g-C_3N_4 with enzymes such as glucose oxidase exhibit enhanced catalytic efficiency, stability, and reusability while enabling synergistic light-driven biotransformations. These materials further show cytocompatibility and potential for biomedical-inspired applications [3]. To facilitate practical implementation, catalysts were immobilized on structured supports and integrated into innovative photoreactors. Mesostructured reactor designs combined with computational fluid dynamics (CFD) modeling improve light distribution, mass transfer, and scalability, supporting real-world deployment [4]. Overall, this presentation highlights the versatility of engineered carbon nitride nanomaterials as a platform for sustainable photocatalysis. Integrating advanced materials design with reactor engineering demonstrates a pathway toward efficient, scalable, and environmentally friendly catalytic technologies (Fig. 1).

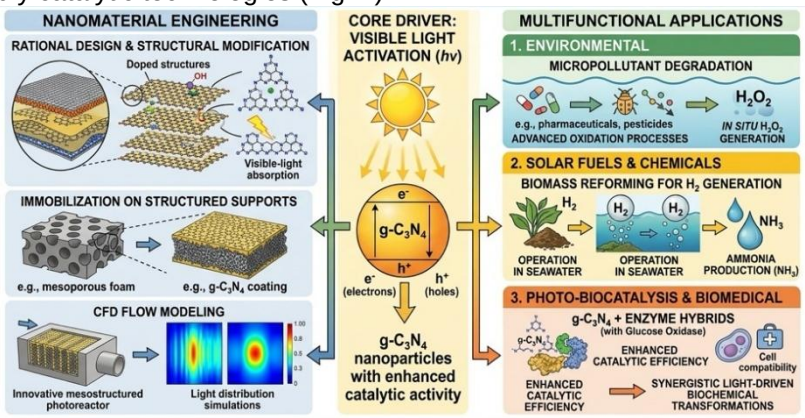


Fig.1. Carbon nitride photocatalysis.

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When Organic Chemistry Meets Surface Science: From Single-Molecule Characterization To Exotic Carbon-Based Nanostructures

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Keywords: *nanographenes, molecular materials, on-surface synthesis, single-molecule reactions, scanning probe microscopy*

The interplay between organic chemistry and surface science allows atomically precise characterization, synthesis, and manipulation of carbon-based nanostructures. Advances in scanning probe microscopy and on-surface synthesis have unlocked new routes to obtain fascinating nanographenes,[1] exotic and highly reactive molecules, and controlled single-molecule reactions.[2] Importantly, these developments open access to transformations inaccessible to solution-phase chemistry such as the indenyl coupling (Figure 1a)[3] or the preparation of well-defined porphyrin oligomers (Figure 1b).[4] This talk focuses on recent advances of our group at the interface between organic chemistry and surface science that have contributed to the resolution of long-standing chemical challenges.

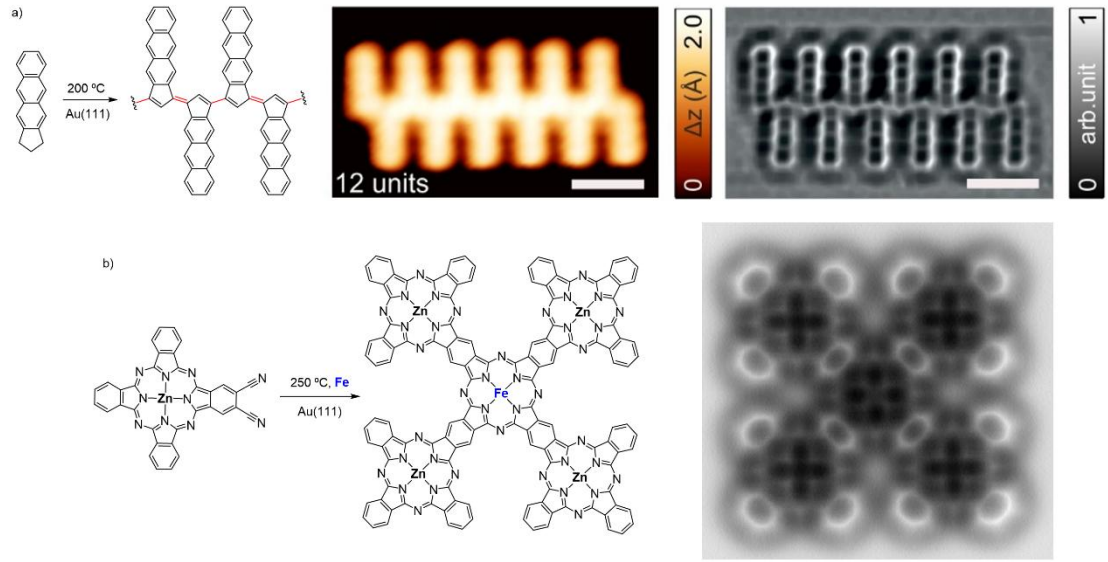


Figure 1. a) On-surface indenyl coupling.[3] b) Phthalonitrile cyclotetramerization.[4]

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From Nanochemistry to Molecular Detection

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The ability to manipulate matter at the nanoscale has opened unprecedented opportunities to control how light interacts with materials. Among the most remarkable examples are plasmonic nanoparticles, metallic nanostructures capable of concentrating light at nanoscale and generating intense electromagnetic fields. These unique optical properties have transformed plasmonics into a powerful platform for ultrasensitive molecular detection through Surface-Enhanced Raman Scattering (SERS).
Over the last two decades, advances in colloidal nanochemistry have enabled the precise control of nanoparticle size, shape, composition, and surface chemistry. Such synthetic control is not merely a chemical challenge; it directly determines the optical response of the nanomaterials and their performance in sensing applications.
In this lecture, I will discuss how fundamental concepts in colloidal synthesis and nanoplasmonics have converged to enable the rational design of SERS-active nanomaterials. I will highlight the intimate relationship between nanoparticle structure and optical properties, illustrating how nanoscale engineering translates into improved analytical performance. Finally, I will present recent advances in the application of plasmonic nanostructures to chemical sensing, bioanalysis, and molecular diagnostics, showing how the precise control of matter at the nanometer scale is contributing to the development of new tools for addressing challenges in different fields.

COMUNICACIONES ORALES

QUÍMICA ALIMENTARIA

Composición nutricional y compuestos bioactivos en el almez (*Celtis australis* L.), un fruto tradicional de la Dieta Mediterránea

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La Dieta Mediterránea, Patrimonio Cultural Inmaterial desde el año 2010, es reconocida por sus beneficios para la salud, así como por su valor sociocultural y su contribución a la sostenibilidad ambiental. Este modelo alimentario se caracteriza por el predominio de alimentos de origen vegetal y el consumo de productos locales, lo que favorece prácticas agrícolas tradicionales y una menor huella ambiental. Entre los frutos silvestres consumidos tradicionalmente en el Mediterráneo se encuentra la almecina, el fruto del almez, un árbol caducifolio que presenta un fruto de 8-12 mm, en drupa redondeada y con largo pedúnculo, color negro azulado en la madurez. Se distribuye por el sur de Europa, oeste de Asia, noroeste de África y región macaronésica. Se encuentra en riberas y otros ambientes mediterráneos de la península ibérica, más frecuente en el este y sur y en Baleares [1].

A pesar de ser un alimento consumido de forma tradicional en el área mediterránea, existen escasos estudios acerca de su composición nutricional y compuestos bioactivos, por lo que el objetivo principal del presente trabajo es determinar su composición nutricional, capacidad antioxidante, compuestos fenólicos totales y familias fenólicas presentes en este fruto.

Para ello se realizó el análisis de la composición centesimal, utilizando para ello métodos oficiales para el análisis de alimentos [2]: humedad (desecación a 100 ªC), cenizas (incineración por vía seca, a 500 ºC), proteínas (método Kjehldahl), grasa total (extracto etéreo mediante método Soxhlet), fibra (método enzimático-gravimétrico), hidratos de carbono disponibles totales y azúcares solubles totales (método colorimétrico de la antrona, con o sin hidrólisis previa).
La capacidad antioxidante (Folin-Ciocalteu) y compuestos fenólicos totales (Fast-Blue BB) y familias fenólicas [3] se estudiaron aplicando el método QUENCHER, con el fin de incluir la contribución de sustancias de bajo peso molecular (como los compuestos fenólicos), así como antioxidantes poco solubles.

Algunos de los resultados muestran que la almecina destaca por su contenido en fibra dietética insoluble (13,7 g/100 g), y por presentar un claro sabor dulce debido al contenido en azúcares solubles (39,5 g/100 g). En relación con los compuestos bioactivos, destaca el contenido en antocianinas totales (11,9 mg cianidina-3-glucósido/100 g), siendo superior al presente en el fruto del cerezo silvestre (4,7 mg cianidina-3-glucósido/100 g) aunque por debajo de otros dos frutos (25,6 y 210,1 mg cianidina-3-glucósido/100 g, para fresa y arándano, respectivamente) [3].

Agradecimientos

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Effect of acylation on the interaction of anthocyanins with pea, soy and yeast proteins under mildly alkaline conditions

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Anthocyanin colour depends on molecular structure and pH. The position of acylated sugars influences the persistence of blue species [1], while pH-dependent equilibria and degradation pathways shape anthocyanin spectral behaviour [2]. We recently showed that pH-modulated complexation of malvidin-3-*O*-glucoside with bovine serum albumin enhanced blue colour formation and stability under alkaline conditions [3]. However, it is unknown whether plant- and yeast-derived proteins, which are more suitable for food applications, can stabilise blue anthocyanin species, and what role acylation plays in this process. Here, we compared the interactions of pea protein isolate (PPI), yeast protein extract (YPE) and soy protein isolate (SPI) with an acylated peonidin, peonidin-3-(6″-caffeoyl-6‴-feruloylsophoroside)-5-glucoside (PN-Ac), and a non-acylated analogue, peonidin-3-glucoside (PN), at mildly alkaline conditions (pH 8 and 9).

UV-Vis spectra of each anthocyanin alone and in the presence of increasing concentrations of PPI (0.055-2.75 mg/mL), YPE (0.0422-2.11 mg/mL) or SPI (0.0606-3.03 mg/mL) were recorded at pH 8 and 9 in 30-fold-diluted Theorell-Stenhagen universal buffer at 25 °C. Fluorescence spectra were also recorded to probe binding.

At pH 8, all three proteins altered the absorption of PN-Ac in a concentration-dependent manner, accompanied by bathochromic shifts, whereas PN mainly exhibited changes in absorbance intensity. At pH 9, PN-Ac absorbance at 607 nm increased with protein concentration, with YPE producing the largest increase at the highest tested concentrations; PN exhibited a smaller absolute increase at the same wavelength (Fig. 1A-L). After 24 h, PN-Ac mixtures with higher protein concentrations retained greater visible absorbance than PN-Ac alone, whereas PN mixtures showed lower absolute absorbance near 607 nm than the corresponding PN-Ac mixtures.

These results show that acylation may influence the protein-induced stabilisation of blue species under mildly alkaline conditions, supporting the design of acylated anthocyanin-protein systems for colour modulation in foods.

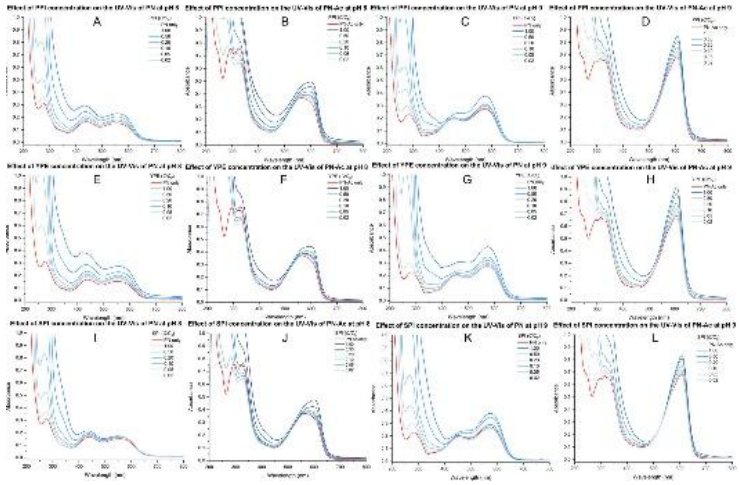


Fig.1. UV-Vis spectra of PN and PN-Ac in the presence of increasing concentrations of PPI (A-D), YPE (E-H) and SPI (I-L) at pH 8 and 9.

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Yeast Protein-Chitosan Coacervation: effect of pH, biopolymer ratio, and ionic strength

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Proteins and polysaccharides are key components of food matrices, and their interactions can modulate the matrices' physicochemical and functional properties. Complex coacervation, a liquid–liquid phase separation process primarily driven by electrostatic interactions between oppositely charged macromolecules, offers a versatile strategy for food applications, including encapsulation of bioactive compounds, controlled release, stabilization of food systems, texture and rheological modulation, and active packaging development [1–3].

This work proposes the formation of coacervates between yeast (*Saccharomyces cerevisiae*) protein extract (YPE) and chitosan (CH), focusing on optimizing coacervation conditions and elucidating molecular-level interactions. YPE represents a valuable protein source with a favourable amino acid profile and is recognized as safe by regulatory authorities [4]. YPE exhibited a protein content above 60%, and an isoelectric point at pH 3.7 was revealed by ζ-potential analysis. Turbidity measurements performed at different pH values (4.0, 5.0, and 6.0) and ionic strengths (10, 100, and 250 mM) demonstrated a pH- and CH:YPE ratio-dependent coacervation behaviour. At pH 4.0 and 5.0, only minor changes in turbidity were observed upon CH addition, whereas at pH 6.0, turbidity varied significantly with the CH:YPE ratio (Fig.1). Optimal coacervation ratios decreased with increasing ionic strength, suggesting electrostatic interactions as the driving force for coacervate formation. FTIR analysis revealed changes in the amide I (1640 cm^{-1}), amide II and III bands, as well as in the hydroxyl/amino region (3000–3300 cm^{-1}), suggesting the involvement of protein functional groups in electrostatic interactions, hydrogen bonding, and hydrophobic interactions during YPE–CH coacervate formation. Secondary structure analysis further revealed pH-dependent conformational rearrangements with distinct structural profiles at pH 6.0 compared with pH 4.0 and 5.0. The microstructure of CH:YPE coacervates (1% w/w, optimal ratio 0.04:1), as well as of the individual biopolymers, was investigated by scanning electron microscopy and revealed a more porous and homogeneous microstructure at pH 6.0, with smaller pores, whereas at pH 4.0, a continuous, lamellar morphology resembling CH suggested weaker biopolymer interactions. Overall, this study highlights the potential of complex coacervation to bridge chemistry and food science in the development of sustainable and rationally designed protein-based materials.

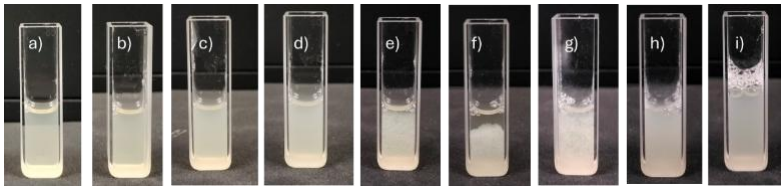


Fig.1. Visual appearance of CH-YPE (1% w/w) mixtures at pH 6 with increasing CH ratios from (a) 0.001:1 to (i) 0.1:1. Turbidity and phase separation indicate coacervate formation.

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Bee4Cheese Project: From Green Extraction of Propolis to the Preservation of Traditional Cheese

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Propolis, a resinous by-product of beekeeping, is globally recognised for its biological activity and growing commercial value.[1] In parallel, Portugal has a long-standing tradition of artisanal cheese production, valued nationally and internationally for its cultural significance and distinctive sensory qualities. Building on these two regional assets, the BEE4CHEESE project applies Green Chemistry principles to valorise propolis as a natural preservative for traditional cheeses, replacing conventional, solvent-intensive extraction with greener alternatives.

Ultrasound-assisted extraction (UAE) was adopted as the core green technology, reducing extraction time and energy consumption while improving mass transfer. Several solvent systems were screened, including conventional solvents (ethanol and glycerol) and natural deep eutectic solvents (NADES) composed of biodegradable, food-grade components. Among these, lactic acid/1,2-propanediol and menthol/1,2-propanediol NADES performed best, yielding up to ~167 mg GAE/g of total phenolics and ~65 mg QE/g of flavonoids — comparable to, or exceeding, the ethanolic benchmark. The UAE protocol was further scaled up to 500 g of raw propolis with extraction yields above 80%, confirming its robustness beyond lab scale.[2]

These results show that food-grade, bio-based solvents can replace ethanol without compromising extraction efficiency, while enabling industrial-scale processing. The resulting extracts are now being evaluated as natural antimicrobial coatings for traditional cheese wheels — directly linking green extraction technology to the preservation of an artisanal food product and reinforcing the potential of green chemistry in sustainable agri-food value chains.

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Valorização do bagaço de *Vaccinium ashei*: Efeito da secagem por liofilização e por ar quente na sua composição nutricional e química

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O bagaço de mirtilo (*Vaccinium ashei*), principal subproduto gerado durante a produção de sumos[1], permanece uma fonte valiosa de nutrientes e compostos bioativos, apesar de ser obtido a partir de frutos fora de calibre[2]. A sua adequada estabilização é essencial para preservar a sua qualidade e promover a sua valorização como ingrediente alimentar funcional. Assim, este estudo pretendeu avaliar o efeito da liofilização e da secagem por ar quente na composição nutricional e química do bagaço de mirtilo proveniente de frutos fora de calibre.

As amostras, fornecidas pela GreenFactor (Braga, Portugal) foram posteriormente estabilizadas por liofilização (BPL) ou secagem por ar quente a 45 ºC (BPD). A cor instrumental (CIELAB: *L**, *a** e *b**) foi avaliada, seguida da determinação da composição centesimal (proteína, gordura, cinzas e hidratos de carbono) de acordo com os métodos oficiais da AOAC. Os açúcares livres e os ácidos orgânicos foram analisados por HPLC acoplada a detetores de índice de refração (HPLC-RI) e de arranjo de díodos (HPLC-DAD), respetivamente. O perfil de ácidos gordos foi determinado por cromatografia gasosa com deteção por ionização de chama (GC-FID), após derivatização em ésteres metílicos de ácidos gordos (FAME).

O BPL apresentou uma tonalidade ligeiramente mais avermelhada (*a** = 14 ± 1) do que o BPD (*a** = 11,9 ± 0,4), enquanto a luminosidade (*L** = 20,0 ± 0,5) e a tonalidade amarela (*b** = 4,7 ± 0,1 e 4,0 ± 0,1, respetivamente) foram semelhantes entre os tratamentos. Em base de peso seco, os teores de proteína foram de 3,4 ± 0,1% e 3,6 ± 0,1% no BPL e BPD, respetivamente, enquanto os teores de gordura e cinza foram aproximadamente de 2,0 e 0,039 g/100g, respetivamente, em ambas as amostras. A frutose e a glucose foram os açúcares livres predominantes, apresentando a glucose teores de 9,00 g/100 g em ambas as amostras, enquanto a frutose apresentou valores de 8,5 ± 0,1 g/100 g e 8,0 ± 0,1 g/100 g no BPL e BPD, respetivamente. O ácido málico foi o ácido orgânico predominante, com teores totais de ácidos orgânicos de 3,9 ± 0,6 g/100g no BPL e 4,7 ± 0,2 g/100 g no BPD. Os ácidos linoleico (C18:2n-6) e oleico (C18:1n-9) foram os ácidos gordos predominantes. Os ácidos gordos polinsaturados representaram 49,2 ± 0,4% e 49,2 ± 0,3% do total de ácidos gordos no BPL e BPD, respetivamente.

De um modo geral, a liofilização e a secagem por ar quente resultaram em composições nutricionais e químicas globalmente semelhantes, tendo sido observadas apenas pequenas diferenças na cor. Estes resultados indicam que ambos os métodos de secagem são adequados para a estabilização do bagaço de mirtilo antes da sua valorização como ingrediente alimentar funcional de valor acrescentado, contribuindo para a utilização sustentável de mirtilos fora de calibre no contexto de uma abordagem de bioeconomia circular.

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Wheat Fermented Beverages: Phenolic Composition, Antioxidant Activity and Evolution of Immunogenic Gluten Peptides During Digestion

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Human dietary preferences are increasingly shifting towards healthy, safe, resilient, and sustainable diets. In this context, harnessing autochthonous microbiota represents a promising research avenue for developing innovative, future-oriented foods that combine nutritional quality with enhanced functional properties. Fermentation by lactic acid bacteria (LAB) has been proposed as an effective strategy to promote the release and transformation of phenolic compounds, thereby enhancing the functional properties of cereal-derived foods and beverages [1]. Furthermore, LAB-mediated proteolysis can modify wheat gluten proteins, potentially reducing their immunoreactivity while generating peptides with biological activity [2]. Against this background, the present study investigated autochthonous wheat strains to produce probiotic-rich wheat-based beverages (PWBBs). An integrated approach was used to characterise phenolic composition, antioxidant activity, gluten immunoreactivity, and immunogenic peptide fate during in vitro gastrointestinal digestion.

PWBBs were prepared using two enzymatic pretreatments and fermented with selected LAB strains, individually or in consortia. Phenolic content, antioxidant activity, and phenolic composition were assessed using spectrophotometric and mass spectrometry-based methods. Gluten content and protein profiles were evaluated by competitive ELISA and Western blotting, respectively. Following in vitro gastrointestinal digestion, bioaccessible fractions were analysed by LC–MS/MS, and immunogenic peptides were characterised using SearchGUI and PeptideShaker.

Fermentation yielded beverages with diverse phenolic profiles and enhanced antioxidant capacity. Competitive ELISA and Western blotting revealed extensive gluten hydrolysis, with a trend towards greater protein degradation in beverages subjected to extended enzymatic pretreatment. Significant differences were observed in the release of immunogenic peptides *in vitro* after mimicking the human digestion depending on the treatments. Extended enzymatic pretreatment promoted substantial gluten hydrolysis before fermentation, limiting the additional reduction in immunoreactive peptides achieved during subsequent fermentation and directly affect the immunogenic peptides bioaccesibility. In contrast, beverages subjected to shorter enzymatic pretreatment exhibited a more pronounced reduction in immunoreactive peptides following fermentation, particularly when fermented with *L. casei.* These findings highlight the importance of optimising the interplay between enzymatic pretreatment and microbial fermentation to modulate gluten-derived peptide profiles.
Overall, this study demonstrates the potential of autochthonous LAB strains as biotechnological tools for developing fermented wheat-based beverages with enhanced antioxidant properties and modified gluten immunoreactivity. This approach could contribute to sustainable cereal valorisation strategies while advancing the development of innovative fermented foods with improved functional properties.

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Determinação do perfil de triacilglicerol em ovos a partir de um método otimizado de ASAP-MS/MS

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Atualmente, sistemas de criação mais conscientes com o bem-estar animal têm conquistado espaço no mercado [1]. No entanto, é importante considerar como os diferentes sistemas de criação podem impactar a qualidade e perfil nutricional de seus produtos derivados [2]. Considerando esse panorama, a técnica de espectrometria de massas em tandem com sonda de análise de sólidos atmosféricos (ASAP-MS/MS) oferece grandes vantagens por sua simplicidade, velocidade, custo-benefício e eliminação de etapas morosas de preparo de amostras [3]. Assim, o presente trabalho teve como objetivo avaliar o potencial da técnica na obtenção do perfil de triacilglicerol (TAG) de ovos provenientes de diferentes sistemas de criação.

Foram obtidos três lotes de ovos grandes oriundos de galinhas poedeiras criadas em sistemas orgânicos (OE), convencionais (SE), livres de gaiola (CE), criação solta (FE), e enriquecidos com ômega-3 (WE). Três gemas de cada sistema e lote foram separadas e homogeneizadas em um *pool* de amostra. Para determinação dos lipídeos totais (LT), as amostras foram extraídas através do método Bligh and Dyer [4], seguida por esterificação e determinação dos ácidos graxos (AG) por GC-FID. A determinação direta do perfil de triacilgliceróis (TAGs) em condições otimizadas da técnica de ASAP-MS/MS.

Os principais TAGs continham na estrutura de glicerol os ácidos palmítico (P), palmitoleico (Po), esteárico (S), oleico (O) e linoleico (L). Os quatro TAGs mais abundantes em todas as amostras foram PLL, PoOO/PoSL/POL, POO and SSO, concordando com a composição em AGs das amostras. Os TAGs majoritários foram 54:1 (TAG SSO) em WE (10,62%) e 52:4 (TAG PLL/PoOL) em CE (9,67%). A análise de correlações não demonstrou diferença ($p < 0,05$).

Dessa forma, a metodologia proposta se mostrou eficiente para a determinação rápida e confiável do perfil de TAGs em gema. Entretanto, estudos futuros com maior número de amostras são necessários, para identificação de possíveis marcadores lipídicos ou a construção de uma digital lipídica mais abrangente.

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Development and optimization of propolis-carob particle-stabilized Pickering emulsions

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Pickering emulsions, stabilized by solid particles at the oil-water interface, have attracted increasing interest in food applications, particularly through the use of particles derived from natural materials [1,2]. This study aimed to develop and optimize oil-in-water Pickering emulsions using propolis-carob particles (ProAlf) produced via the solid dispersion technique, with a focus on maximizing the emulsified layer.

Propolis-carob particles (ProAlf) were prepared using the solid dispersion technique and explored as particulate stabilizers for oil-in-water Pickering emulsions. The particles were characterized using zeta potential measurements, Fourier-transform infrared (FTIR) spectroscopy, wettability, particle size distribution, and colorimetric analyses. Emulsions were formulated according to a central composite rotatable design comprising 11 experiments, varying particle concentration (3.38-7.62 %, w/v) and oil volume fraction (0.36-0.64). The emulsion layer percentage (EL) was used as the response variable, and emulsion morphology was evaluated by optical and confocal microscopy. A quadratic model was fitted to assess the influence of the formulation variables.

Experimental EL values ranged from 77.1% to 100%, and the fitted quadratic model showed an R^2 of 0.9872. Validation experiments showed good agreement between predicted and experimental EL values: 100% and 97% (V1), 93.57% and 94% (V2), and 100% and 100% (V3), respectively. Among the formulations evaluated, the emulsion containing 5.5% (w/v) ProAlf particles and an oil volume fraction of 0.64 achieved 100% EL and was selected for further characterization, including color analysis, optical and confocal microscopy, droplet size measurements, and rheological evaluation.

Overall, the results highlight the potential of ProAlf particles to develop fully emulsified oil-in-water emulsions. The optimization approach provides a basis for further characterization and the development of innovative food formulations using propolis-carob particles, e.g., a chocolate mousse.

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Development of Pickering Emulsions Stabilized by Astaxanthin-Based Solid Dispersion Particles for Food Analogs

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The global food industry is currently driven by heightened consumer demand for nutritional health, sustainable sourcing, and "clean label" formulations [1]. In this context, Pickering emulsions have emerged as a technically superior alternative to traditional surfactant-based systems [2]. Astaxanthin, a xanthophyll carotenoid, stands out as a high-potential candidate for these systems due to its potent antioxidant properties and red color [3].

In the present research, astaxanthin-based particles were produced using the solid dispersion technique to serve as stabilizers for Pickering emulsion systems. The experimental work includes the characterization of the solid particles by determining particle size distribution, zeta potential, water contact angle, colorimetry, and Fourier-Transform Infrared Spectroscopy (FTIR). Subsequently, the resulting emulsions were analyzed to determine their morphological characteristics, droplet size, creaming index, chromatic properties, and rheological behavior.

The astaxanthin solid dispersion particles' emulsifying potential was successfully demonstrated through both particle characterization and the stability of the resulting emulsion. The FTIR spectra suggested the incorporation of astaxanthin into the carrier matrix and possible interactions between the formulation components. The particles showed a volume-weighted mean diameter (D[4,3]) of 1.51 ± 0.01 µm, a zeta potential below -30 mV, and a water contact angle of 109 ± 5.4°. Together, these properties supported their potential as Pickering emulsion stabilizers, which was subsequently confirmed by the stability of the resulting emulsions.

Oil-in-water Pickering emulsion formation was confirmed via confocal microscopy. During 30 days of storage, the emulsion remained physically stable, with no visible phase separation and only minor variations in the volume-weighted mean droplet diameter (D[4,3]) and microstructure. The low total color difference ($\Delta E^* = 0.71$) indicated negligible color changes during storage.

The present work introduces a novel approach to emulsion stabilization using astaxanthin-based particles that serve as both a Pickering stabilizer and a food colorant, contributing to the development of food products that mimic conventional ones while offering a natural, simplified ingredient profile suitable for various diets and aligned with current market trends.

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Impact of Maturation on the Nutritional Profile, Phytochemical Composition and Bioactive Potential of Persimmon (*Diospyros kaki* L.)

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Persimmon (*Diospyros kaki* L.) is a seasonal fruit of considerable nutritional interest, whose chemical composition and bioactive properties vary throughout maturation. This process involves physiological and biochemical changes that influence the nutritional profile, and in chemical contents, as well as the antioxidant capacity of the fruit. These changes may also depend on the cultivar and astringency type, thereby affecting the physicochemical characteristics and overall fruit quality [1,2]. Understanding these variations is essential for assessing persimmon quality and identifying the maturation stages most suitable for its food-related valorisation. In this context, this study aimed to characterize and compare the nutritional and chemical composition of firm and soft persimmons at different maturation stages, while assessing their antioxidant potential and the toxicity of their extracts. The study sought to investigate variations associated with persimmon type and maturation stage, providing insights into fruit quality and supporting the evaluation of extract safety for potential food-related applications. The nutritional composition of the fruits was determined according to official AOAC methods, including moisture, protein, ash and total fat contents, as well as carbohydrate content and energy value. Individual organic acids were analysed by ultra-high-performance liquid chromatography coupled with diode-array detection (UPLC-DAD), while individual sugars were quantified by high-performance liquid chromatography with refractive index detection (HPLC-RI). Fatty acid composition was determined by gas chromatography coupled with flame ionization detection (GC-FID). The antioxidant activity of the extracts was assessed using the ORAC (oxygen radical absorbance capacity) and TBARS (thiobarbituric acid reactive substances) assays. Additionally, extract toxicity was evaluated to further characterize their biological safety.
The results revealed variations in the nutritional composition of persimmon according to ripening stage. Analysis of the sugar profile identified fructose and glucose in the samples, while sucrose was also detected in some cases. Variations in sugar profiles were observed between the two persimmon types, firm and soft, and across different ripening stages. The ORAC and TBARS assays indicated antioxidant activity in the extracts analysed. Overall, the nutritional and chemical composition of persimmon varies according to fruit type and ripening stage, highlighting the importance of these factors in determining fruit characteristics and quality.

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From by-product to food: valorisation of lentil tofu residue into granola, farofa and a cereal bar

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Lentil tofu production generates a solid residue that retains about half of the initial seed mass. Within the 3Rs project, this work aimed to reuse this residue in ready-to-eat foods, following a zero-waste approach.

The freeze-dried residue was characterised and incorporated into a sweet granola (oats, natural sweeteners), a savoury farofa (toasted crumb seasoned with garlic, herbs and vegetable oils) and a cereal bar. Proximate composition [1], total dietary fibre and fatty acid profile (GC-FID) [2] were determined, as well as the water activity (a^w) of the cereal bar (mean ± SD, n = 3). The samples were subjected to in vitro gastrointestinal digestion (INFOGEST [3]), and the growth of four probiotic strains (*Bifidobacterium animalis* subsp. *lactis* Bb-12, *Lacticaseibacillus casei, Lactobacillus acidophilus* LA-5 and *Lactiplantibacillus plantarum*) on the digested samples was monitored by optical density (620 nm, 48 h), using glucose, fructo-oligosaccharides (FOS) and inulin as references.

The residue was rich in dietary fibre (45 ± 3 g/100 g), with 13.8 ± 0.3 g protein and 1.6 ± 0.1 g fat/100 g. All three products met the “high fibre” claim of Regulation (EC) No 1924/2006 [4]: farofa (50.0 ± 0.8 g/100 g), granola (13.8 g/100 g) and cereal bar (10.3 g/100 g). Protein ranged from 14.0 g/100 g (granola) to 21.7 g/100 g (farofa); farofa and cereal bar also qualified as “high protein” (>20% of energy) and granola as “source of protein” (~15%). Energy ranged from 301 (cereal bar) to 364 kcal/100 g (granola). The residue lipids were 56% polyunsaturated, with an n-6/n-3 ratio of 3.9; in the products, the fatty acid profile reflected the added ingredients (cereal bar: 61% oleic acid). The cereal bar had an a^w of 0.89, typical of intermediate-moisture foods. All samples supported the growth of the four strains: the residue reached maximum OD values (2.1–2.2), higher than FOS (1.5–1.8) and close to inulin (2.3–2.5), and the granola was similar to inulin (2.3–2.6), suggesting a prebiotic potential. Reusing the residue turned a by-product into nutritious, fibre-rich foods, closing the lentil processing cycle.

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Chemical Structure of Procyanidins and Polysaccharides Governs Their Interactions at Oral Interfaces

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Grape-seed procyanidins are oligomeric and polymeric flavan-3-ols whose degree of polymerisation, interflavan linkages and distribution of phenolic hydroxyl groups shape their non-covalent interactions with oral constituents. Hydrogen bonding and hydrophobic association with salivary proteins and mucosal components can contribute to astringency [1]. Polysaccharides may alter these interactions through direct association with procyanidins, thereby competing with oral binding sites, or through association with preformed polyphenol–protein complexes that limits their precipitation [2]. Their monosaccharide composition, glycosidic architecture, branching, charge and molecular size are therefore plausible determinants of binding modulation, although the contributions of individual structural features remain to be established.

We investigated how five chemically distinct polysaccharide families - arabinogalactan, xanthan gum, arabinoxylan, xyloglucan and mannoprotein - modulate grape-seed procyanidin binding across oral models of increasing complexity: isolated salivary proteins, human tongue epithelial cells (HSC-3), and HSC-3 with mucosal pellicle and salivary proteins. Procyanidins were pre-incubated with each polysaccharide to simulate a food matrix modulation before contact with oral surfaces. Procyanidins bound to oral models were quantified by colorimetric assay and HPLC, with and without polysaccharides.

Xanthan gum and arabinoxylan significantly decreased procyanidin binding to oral models. The magnitude of this effect differed between polysaccharide types and between fractions of the same polysaccharide, indicating a dependence on polysaccharide identity/structure and the composition of the oral interface. For xanthan gum fractions, chain length was a key determinant in the epithelial model (HSC3), while side-chain were more relevant in salivary protein-containing models.
These results highlight polysaccharide molecular architecture as a candidate driver of procyanidin partitioning between solution and oral surfaces; targeted structural characterisation and binding studies will be required to identify the responsible chemical features. Xanthan gum and arabinoxylan emerge as promising ingredients for modulating procyanidin–oral component interactions in polyphenol-rich formulations.

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Caraterização morfológica e fitoquímica de microvegetais de espinafre biofortificados com selénio inorgânico

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Os microvegetais têm despertado crescente interesse devido ao seu valor nutricional e à presença de diversos compostos bioativos [1]. O selénio (Se) é um micronutriente essencial para a saúde humana, cuja ingestão inadequada constitui uma preocupação nutricional em diversas regiões do mundo. Neste contexto, a biofortificação de microvegetais com Se surge como uma estratégia promissora para aumentar o aporte alimentar deste elemento, podendo também influenciar o crescimento e a composição fitoquímica das plantas [2,3]. Assim, o presente estudo teve como objetivo avaliar os efeitos de diferentes formas e concentrações de Se nas características morfológicas, no perfil químico e na atividade antioxidante *in vitro* de microvegetais de espinafre (*Spinacia oleracea* L. cv. Lorelay).

As sementes foram semeadas em tabuleiros contendo vermiculite e cultivadas numa câmara de crescimento sob iluminação fluorescente, com um fotoperíodo de 16 h de luz/8 h de escuro, temperatura de 20–25 °C e humidade relativa de aproximadamente 60%. Os microvegetais foram irrigados com uma solução nutritiva NPK (3:1:6), sem adição de Se (controlo) ou suplementada com selenito ou selenato de sódio em diferentes concentrações (10, 20 e 40 µM Se), incluindo ainda um tratamento com uma mistura de ambas as formas inorgânicas (20 µM Se). Aos 14 dias após a sementeira, os microvegetais foram colhidos e avaliados quanto às suas características morfológicas e colorimétricas. A composição fitoquímica foi caracterizada através da determinação dos perfis de açúcares solúveis, ácidos orgânicos, tocoferóis, ácidos gordos, compostos fenólicos e saponinas, recorrendo a diferentes técnicas cromatográficas. O teor de Se nas plantas foi determinado por espetroscopia de absorção atómica. A atividade antioxidante foi avaliada através de ensaios *in vitro*.

Os tratamentos de biofortificação influenciaram as características morfológicas e colorimétricas, bem como a composição fitoquímica dos microvegetais, com respostas dependentes da forma química e da concentração aplicada. O selenato de sódio, particularmente a 40 µM Se, favoreceu o crescimento em altura e promoveu uma maior acumulação de Se. Por sua vez, os tratamentos com selenito de sódio proporcionaram uma coloração verde mais intensa e, de um modo geral, aumentaram os teores de açúcares solúveis e ácidos gordos. A suplementação com selenito, nas concentrações de 20 e 40 µM Se, proporcionou os maiores teores de α-tocoferol e de compostos fenólicos, incluindo flavonoides, respetivamente. A atividade antioxidante variou em função do ensaio *in vitro* utilizado e da forma de Se aplicada. Em geral, os resultados demonstram que a forma química e a concentração de Se influenciam o crescimento, a sua acumulação e a composição fitoquímica dos microvegetais de espinafre, constituindo fatores relevantes para a otimização das estratégias de biofortificação.

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Fermented red grape juices: influence of *in vitro* model design on gut microbiota modulation

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Growing interest in healthier dietary choices has encouraged the development of foods and beverages with reduced sugar content, as part of strategies to address obesity and type 2 diabetes [1]. In this context, yeast-driven alcoholic fermentation offers a food-processing strategy that extends beyond sugar reduction, reshaping the chemical composition of fruit matrices by transforming existing compounds and producing additional metabolites [2]. These changes may influence the interactions between (poly)phenol-rich beverages and the gut microbiota, whose metabolic activity contributes to the conversion of dietary (poly)phenols into metabolites that may impact obesity-related risk factors [3]. Thus, understanding how fermentation modifies these interactions requires consideration of both the resulting matrix composition and the subsequent transformations that occur during gastrointestinal digestion.

In this work, non-fermented and yeast-fermented red grape juices were compared to characterize differences in matrix composition and investigate their implications for downstream *in vitro* gut microbiota studies. Targeted analyses revealed marked differences in phenolic and organic acid profiles, along with a significant reduction in sugar content in fermented juices compared with the non-fermented matrix. To assess matrix–microbiota interactions under different experimental conditions, two complementary in vitro approaches were used: (i) a static colonic fermentation model involving direct matrix-microbiota exposure, and (ii) a dynamic gastrointestinal system (simgi®) incorporating simulated gastrointestinal digestion before colonic fermentation.

Microbiota modulation by the juices differed between the static and dynamic models, with distinct changes in microbial composition, short-chain fatty acid production, and phenolic metabolite profiles. Overall, these findings highlight that the effects of fermented fruit-based beverages extend beyond sugar reduction and that their interactions with the gut microbiota depend on both matrix composition and experimental conditions. Integrating gastrointestinal digestion into *in vitro* studies may therefore provide a more comprehensive understanding of these interactions and support the evaluation of beverages developed for potential metabolic health applications.

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Techno-functional, rheological, and pasting properties of gluten-free rice flour enriched with *Scolymus hispanicus* L. root powder

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The demand for gluten-free products requires innovative formulations that overcome the nutritional and techno-functional limitations of rice flour, such as its low fibre content and the challenges associated with its rapid retrogradation [1,2]. Wild Edible Plants (WEPs) offer a sustainable and effective strategy for addressing these issues within the agrifood sector [3]. *Scolymus hispanicus* L. (golden thistle) is a WEP, known for its climate resilience and roots rich in fibre and bioactive compounds, which make this plant an optimal source of promising functional ingredients [4].

This study investigated the incorporation of *S. hispanicus* root powder (SHP) into rice flour (RF) at substitution levels of 10%, 20%, and 30%. The functional impact of SHP was assessed through techno-functional properties, including the water absorption index (WAI), swelling power (SP), water-holding capacity (WHC), water absorption capacity (WAC), water solubility index (WSI), oil absorption capacity (OAC), hydrophilic/lipophilic index (HLI), emulsifying activity (EA), emulsion stability (ES), foaming capacity (FC), foaming stability (FS), and least gelation concentration (LGC). Pasting profiles were evaluated using a Rapid Visco Analyzer (RVA), rheological behaviour was assessed through frequency sweeps, and texture profile analysis (TPA) was performed.

Results indicated that SHP incorporation significantly enhanced hydration capacities while reducing peak and final viscosities, primarily due to starch dilution and fibre-water competitive interactions. Rheological analysis confirmed that, despite a decrease in viscoelastic moduli (*G'* and *G"*), the blended matrices sustained stable, solid-like networks. Furthermore, TPA revealed that 20–30% SHP formulations yielded softer, more cohesive, and highly elastic structures, effectively attenuating starch retrogradation. Ultimately, *S. hispanicus* emerges as a viable functional ingredient capable of optimizing the rheological and textural performance of gluten-free matrices, thereby driving the diversification and qualitative enhancement of gluten-free flours.

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Estratégias de cultivo e otimização da biofortificação de cogumelos do género *Pleurotus* com ferro: O projeto Nutr&ssencial

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A biofortificação de cogumelos com minerais constitui uma estratégia para o desenvolvimento de ingredientes alimentares com composição nutricional diferenciada. Os cogumelos do género *Pleurotus* apresentam interesse neste contexto devido à sua utilização alimentar e à capacidade de acumulação de minerais durante o crescimento [1,2]. No âmbito do projeto Nutr&ssencial, pretende-se desenvolver e otimizar estratégias de cultivo para a produção de cogumelos biofortificados com ferro, avaliando simultaneamente o desempenho produtivo e a capacidade de bioacumulação deste elemento. Numa primeira fase, foi realizado um ensaio exploratório envolvendo três espécies, nomeadamente *Pleurotus ostreatus*, *P. citrinopileatus* e *P. djamor*, submetidas a diferentes condições de suplementação com ferro, prolina e dextrose. Foram avaliadas duas fontes de ferro, sulfato de ferro(II) ($FeSO_4 \cdot 7H_2O$) e uma formulação comercial de ferro quelatado, procurando investigar a influência da forma química do mineral e da disponibilidade de nutrientes no desenvolvimento fúngico e na biofortificação. A prolina foi incluída pelo seu potencial papel na resposta ao stress oxidativo e pela hipótese de contribuir para os mecanismos de captação e acumulação de ferro pelo micélio, enquanto a dextrose foi considerada como fonte adicional de carbono. A avaliação preliminar do desempenho produtivo evidenciou diferenças entre as espécies, destacando-se *P. citrinopileatus* pela frutificação mais rápida e robusta, enquanto *P. djamor* apresentou corpos frutíferos menos densos. Estas observações fundamentaram a seleção de *P. citrinopileatus* para a continuidade dos estudos. Num segundo ensaio, exclusivamente com *P. citrinopileatus*, foram estabelecidas diferentes combinações de fontes de ferro e suplementação com prolina e dextrose, visando aprofundar a avaliação da influência destes fatores no desempenho produtivo e na bioacumulação mineral. Os cogumelos foram produzidos em sacos de cultivo sob condições ambientais controladas, com registo da massa fresca dos corpos frutíferos por saco e por colheita, para determinação da eficiência biológica (EB, %). Após a colheita, as amostras foram congeladas, liofilizadas e trituradas, para posterior quantificação do teor de ferro por espectrometria de absorção atómica (AAS).

A integração dos resultados de eficiência biológica e concentração de ferro nos corpos frutíferos permitirá avaliar a influência das condições experimentais na produtividade e na capacidade de bioacumulação mineral. A aplicação da metodologia de superfície de resposta (RSM) permitirá identificar combinações de fatores que favoreçam a produção de cogumelos biofortificados com ferro, procurando conciliar o enriquecimento mineral com um desempenho produtivo adequado. As condições selecionadas servirão de base à posterior caracterização nutricional, química e bioativa dos cogumelos, bem como à avaliação do seu potencial de utilização como ingredientes no desenvolvimento de alternativas alimentares de base não animal.

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Caracterização integrada do cultivo e da qualidade dos morangos para o desenvolvimento de sistemas de produção controlados por inteligência artificial: o projeto SUSTAiN

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O morangueiro (*Fragaria* spp.) é uma cultura de elevada importância económica, cuja produtividade e qualidade dos frutos são influenciadas por fatores ambientais [1]. O projeto SUSTAiN visa desenvolver um sistema inteligente de cultivo hidropónico em ambiente controlado, integrando sensores IoT que permitam a monitorização e controlo em tempo real dos parâmetros críticos como humidade, temperatura, luminosidade, pH, e condutividade elétrica em tempo, fortalecendo a agricultura de precisão em ambientes controlados, iluminação inteligente com ajuste automático de espectros e intensidade de luz, suportado por IA, para otimizar o crescimento em diferentes estágios de desenvolvimento e algoritmos IA para ajustar dinamicamente os parâmetros de cultivo. A monitorização dos parâmetros ambientais e nutricionais permitirá ajustar as condições de cultivo às necessidades das plantas, promovendo a otimização da produção e do uso de recursos. Os dados ambientais, produtivos e de qualidade dos frutos serão integrados para desenvolver modelos de IA que apoiem a gestão e o controlo adaptativo do sistema. No âmbito da avaliação experimental, serão estudadas quatro cultivares de morangueiro, considerando o cultivo em sistema semi-hidropónico e condições de produção convencional em campo. Serão acompanhados parâmetros morfológicos, fisiológicos e produtivos ao longo dos ciclos vegetativo e reprodutivo (desenvolvimento das plantas, floração, frutificação, número e dimensão dos frutos e o rendimento por planta). A qualidade dos morangos será avaliada através de parâmetros físicos (massa, calibre, textura e cor (CIELAB), avaliação da composição centesimal (AOAC) e mineral (AAS), determinação de açúcares livres (HPLC-RI), ácidos orgânicos (UFLC-PDA), perfis de ácidos gordos (GC-FID), tocoferóis (HPLC-FL), e compostos fenólicos (HPLC-DAD-MS). A atividade antioxidante (TBARS e OxHLIA) permitirá complementar a caracterização do potencial bioativo dos frutos. A integração dos resultados permitirá relacionar as condições de cultivo com o desenvolvimento das plantas, a produtividade e a qualidade dos frutos, identificando diferenças entre cultivares e sistemas de produção, promovendo uma produção mais eficiente e sustentável ao longo do ano.

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QUÍMICA AMBIENTAL Y SOSTENIBLE

Salinity-driven adsorption kinetics and process optimization of Reactive Brilliant Blue removal using untreated eggshell waste

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Textile effluents are especially difficult to treat efficiently due to the presence of high concentrations of dissolved salts and reactive dyes. In this context, the valorization of agro-industrial by-products as biosorbents has emerged as a sustainable strategy, which allows for the recovery of waste and the remediation of wastewaters [1,2]. Despite the significant adsorption capacity of eggshells for anionic dyes, the impact of salinity on the adsorption kinetics and process optimization is still not well understood [3].

In this work, the adsorption of Reactive Brilliant Blue (RBB) onto untreated ground eggshells was investigated using a Box–Behnken experimental design combined with Response Surface Methodology (RSM). Seventeen experimental conditions were established to investigate the effects of initial dye concentration (10-30-50 mg L^{-1}), sorbent dosage (0.25-0.75-1.25 g), salinity (0-25-50) and contact time (1-192 h). Process performance was interpreted through reduced polynomial models and kinetic modelling.

Salinity was an important factor affecting dye removal during the early stage of adsorption (ANOVA, $p < 0.001$), favoring faster adsorption rates and allowing removal efficiencies close to 100% within 24–48 h. However, this effect gradually weakened after ca. 72 h, while sorbent dosage remained the only consistently significant variable throughout the process. Reduced mathematical models adequately predicted dye removal up to 72 h (R^2 = 0.69–0.86). Furthermore, comparison of the kinetic models obtained for the seventeen experimental conditions revealed that kinetic behaviour varied according to the operational conditions, highlighting the combined influence of salinity, sorbent dosage and dye concentration on adsorption performance.

Numerical optimization predicted maximum removal efficiencies approaching 100%, with desirability values close to unity under practical operating conditions. The results obtained demonstrate untreated eggshell waste as an efficient and sustainable biosorbent for textile wastewater treatment with salinity as a key operational parameter controlling the adsorption kinetics and process optimization. The combined application of Response Surface Methodology and kinetic modelling provides a practical framework for optimizing biosorption processes under conditions representative of real textile wastewaters.

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Green-synthesis of ZVI particles from plant extracts for phosphate removal

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Eutrophication is one of the main environmental problems nowadays. With the rapid population growth during the last century, the use of synthetic fertilizers has become essential. Consequently, this has caused the release of significant amounts of N and P into the aquatic environment through leaching, to the point of exceeding safe planetary boundaries [1]. This has led to widespread eutrophication, posing a risk to human health and the integrity of aquatic ecosystem [2]. Therefore, various mitigation strategies have been tested, ranging from the reduction in the use of fertilizers to the direct removal of nutrients. However, these solutions show significant limitations, including their complex implementation and high environmental or economic cost [3].

In this work, we evaluated various forms of zero-valent iron (ZVI) synthesized using plant extracts as eco-friendly adsorbents for phosphate sequestration from eutrophicated waters. Three plant species commonly found in Galicia were chosen: *Rubus ulmifolius*, *Urtica dioica* and *Eucalyptus globulus*. Leaf extracts were prepared and subsequently mixed at a 2:1 proportion with a 0.1 M $FeSO_4$ solution to promote the reduction of Fe(II) to ZVI. The resulting particles were characterized and their ability to retain phosphate in aqueous medium was evaluated. Thus, adsorption isotherms were obtained at 1-500 µM of PO_4 and pH 4 and 7, as well as pH edge experiments conducted over a pH range of 4-9 and PO_4 concentrations of 25, 50 and 100 µM. The adsorption isotherms were simulated using the Freundlich, Langmuir and Langmuir-Freundlich models, and the adsorption capacity of the ZVI particles were compared with other forms of Fe phases, more extensively studied, such as ferrihydrite.

Results revealed a higher Fe content in the ZVI particles produced from *U. dioica* (10.4%), followed by those from *R. ulmifolius* (6.6%) and *E. globulus* (3.5%). The adsorption isotherms, fitted using the Langmuir model, showed that ZVI particles obtained with *U. dioica* had a maximum adsorption capacity ranging from 270 to 417 mg_{PO4}/g_{ZVI}. These values were up to 30 times higher than those observed for the ZVI particles from *R. ulmifolius* and *E. globulus*. Similar trends were observed in pH edges, with ZVI particles from *U. dioica* showing the highest adsorption rates, especially at higher phosphate concentrations. Overall, higher adsorption rates were observed under acidic conditions (pH 4 to 6), followed by an adsorption decrease as pH increased. This reduction was more pronounced above pH 7, especially for the ZVI particles produced from *U. dioica*.

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Waste into Water Treatment: Red Onion Peel as a Natural Coagulant

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Fruit and vegetable processing generates both lignocellulosic residues and high-strength wastewaters containing suspended particles, colour and organic matter. Red onion peel is particularly rich in phenolic compounds and represents a promising feedstock for the production of tannin-based coagulants [1-3]. This work investigated aqueous extraction of tannins from red onion peel and the subsequent application of chemically modified extracts to the primary treatment of real wastewater from the same industrial sector.

Extraction was evaluated through a three-factor Box-Behnken design, varying temperature (30-90 °C), time (10-60 min) and solid-to-liquid ratio (1:50-1:16.5). Temperature significantly increased the recovery of total phenolics and condensed tannins, whereas the solid-to-liquid ratio significantly affected only total phenolics. A model-guided condition of 90 °C, 60 min and 0.060 g/mL was experimentally validated, yielding 903 mg catechin equivalents per gram of extract. The resulting extract was modified through a Mannich reaction, and formulations prepared with different volumes of Mannich solution were evaluated by jar tests using centrifuged industrial wastewater. Their performance was compared with Tanfloc, $FeCl_3$ and $Al_2(SO_4)_3$.

The best overall formulation, prepared with twice the reference volume of Mannich solution, achieved 82% turbidity removal at 45 mg/L and pH 5.92. This value was close to that obtained with a commercially available biocoagulant (Tanfloc) (87.5% at 100 mg/L) and higher than those obtained with FeCl3 (71.7% at 30 mg/L) and $Al_2(SO_4)_3$ (75.3% at 25 mg/L). In addition to turbidity removal, the treatment reduced true colour by at least 56%, UV254 by 55.5%, filtered total organic carbon by 42% and chemical oxygen demand by 64%. A formulation prepared with three times the reference Mannich-solution volume also achieved 78.8% turbidity removal at only 10 mg/L, revealing a relevant balance between removal efficiency and reagent dose. These findings demonstrate the potential of red onion peel as a source of functional tannins for primary treatment of agro-food wastewater, while simultaneously promoting residue valorisation and reducing the organic load entering the subsequent biological treatment stage.

Table 1. Performance of tannin-based and conventional coagulants in food-processing wastewater treatment.

Coagulant	Optimum pH	Optimum dose (mg/L)	Removal at 30 min (%)	Removal at 60 min (%)
Optimum 1.5×	6.93	5	56 ± 3	60 ± 2
Optimum 2×	5.92	45	80.0 ± 0.5	82 ± 2
Optimum 3×	6.84	10	78 ± 2	79 ± 3
Tanfloc	4.92	100	80 ± 3	87.5 ± 0.7
Ferric chloride	5.84	30	69 ± 4	72 ± 3
Aluminium sulphate	5.84	25	74 ± 2	75 ± 2

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Circular Valorisation of Iron-Functionalised Pine Bark Biosorbents after Textile Wastewater Treatment

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Textile wastewater treatment by adsorption can generate spent materials whose subsequent management influences the overall sustainability of the process. This work investigated an integrated approach in which pine bark was converted into an iron-functionalised biosorbent for textile wastewater treatment and subsequently valorised in cementitious materials. Pine bark was prepared as powder (<0.5 mm) and granules (1.0–2.0 mm), functionalised with 10% (w/w) Fe and thermally treated at 400 °C under N_2/H_2. Adsorption performance was initially evaluated using a synthetic textile effluent containing three dyes and subsequently validated with a real industrial effluent.

High colour-removal efficiencies were obtained for both biosorbent formats. For the synthetic effluent, increasing the biosorbent dosage from 5 to 10 g/L increased colour removal from 88.7 to 99.2%. More importantly, high efficiency was maintained with the real textile effluent, reaching 90.9 ± 0.7% and 89.1 ± 4% colour removal for granular and powdered biosorbents, respectively, after 48 h. SEM–EDS revealed morphological and compositional changes associated with Fe functionalisation, thermal treatment and adsorption, supporting the interaction between the engineered pine-bark surface and wastewater constituents [1,2].

After treatment, the spent biosorbents were incorporated into cementitious roof-tile specimens as partial sand replacements at 2, 5 and 10%. Incorporation did not compromise the maximum load under the tested conditions, with the 5% powdered-biosorbent formulation reaching 0.426 kN compared with 0.301 kN for the control. Moreover, preliminary 30-day immersion tests in distilled water indicated negligible Fe release. These results demonstrate the potential of a circular treatment strategy in which a forestry residue is first used for wastewater remediation and subsequently redirected towards a secondary application in construction materials.

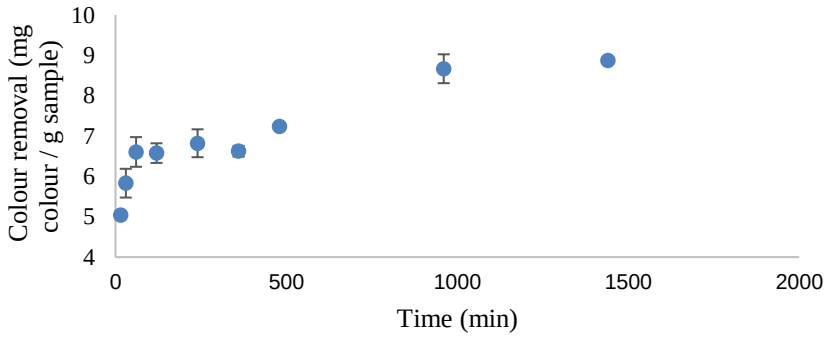


Fig.1. Apparent colour reduction of textile effluent using granular Fe-functionalised pine bark at 5 g/L.

Acknowledgments
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Caracterización de compuestos orgánicos volátiles en la atmósfera de un área industrial: Puertollano (España)

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Los compuestos orgánicos volátiles (COVs) son compuestos de especial relevancia en los estudios de calidad del aire por sus efectos ambientales y sobre la salud. Son liberados a la atmósfera desde diferentes fuentes, tanto naturales como antropogénicas, entre las que destacan las actividades industriales, el tráfico rodado y el uso de disolventes. Además, los COVs participan, junto con los óxidos de nitrógeno y en presencia de radiación solar, en procesos fotoquímicos que contribuyen a la formación de ozono troposférico [1,2]. En este trabajo se caracterizó la distribución espacial y temporal de COVs en Puertollano (Ciudad Real), municipio que alberga un importante complejo industrial y energético de Repsol dedicado al refino de petróleo, la producción química y la generación de energía.

Se determinaron 60 COVs mediante muestreo pasivo con tubos axiales rellenos de Carbopack X y posterior análisis por desorción térmica acoplada a cromatografía de gases y espectrometría de masas (TD-GC-MS) [3,4]. El muestreo se realizó en cuatro emplazamientos urbanos de Puertollano: Barriada 630 (P1), Rampas Mecánicas (P2), Almacén Municipal (P3) y Campo de Fútbol (P4), seleccionados para representar diferentes grados de influencia urbana, de tráfico e industrial, durante ocho periodos consecutivos de 14 días entre octubre de 2025 y enero de 2026.

Los perfiles mostraron un claro predominio de alcanos ligeros y compuestos aromáticos, aunque con diferencias entre emplazamientos. El isopentano alcanzó en algún periodo un valor máximo cercano a 50 µg m^{-3} en P2 y el estireno presentó concentraciones destacables, especialmente en P1 y P3, donde superó los 20 µg m^{-3}. En P4 se registró la concentración máxima de benceno, 9,49 µg m^{-3}, mientras que P3 destacó por la mayor diversidad de compuestos, incluyendo compuestos oxigenados y organoclorados.

La evolución temporal mostró variaciones entre los periodos de muestreo. El muestreo 3 (07/11-21/11) presentó la mayor contribución relativa de pentanos, aproximadamente un 37 % de la concentración total de COVs, indicando un mayor peso de los hidrocarburos ligeros en este periodo, mientras que el muestreo 5 (05/12-19/12) registró las mayores concentraciones globales de COVs. Este último periodo coincidió con la fase final de una parada programada del área de destilación del complejo petroquímico, durante la cual las operaciones de puesta en marcha podrían haber contribuido a incrementos puntuales de emisiones. El análisis de las relaciones xilenos/etilbenceno (X/E) y tolueno/benceno (T/B) indicó un predominio de aportes asociados a fuentes vehiculares, así como un carácter relativamente reciente de las masas de aire y un escaso envejecimiento fotoquímico [5]. Por otro lado, el análisis de T/B frente a la concentración de benceno apuntó además a aportes asociados a la combustión de biomasa o carbón [6], posiblemente relacionadas con la influencia de la planta de biomasa del entorno.

En cuanto a los efectos sobre la salud, los hidrocarburos aromáticos constituyeron la principal contribución al riesgo no cancerígeno. El riesgo cancerígeno estimado fue mayoritariamente bajo o moderado, siendo el benceno y el cloroformo los principales contribuyentes.

En conjunto, se observaron diferencias en la distribución de los COVs entre emplazamientos y periodos de muestreo, asociadas a distintas fuentes de emisión.

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Implicaciones atmosféricas del uso del 2-butoxietanol como aditivo en la formulación de biocombustibles

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El desarrollo de biocombustibles ha impulsado la investigación de aditivos oxigenados capaces de mejorar sus propiedades y favorecer la combustión. Entre ellos, los hidroxiéteres presentan interés por combinar un grupo alcohol y un grupo éter en su estructura [1]. En particular, el 2-butoxietanol se ha estudiado como aditivo del biodiésel para mejorar sus propiedades y su comportamiento durante la combustión [2]. No obstante, la detección de este tipo de compuestos en los gases de escape de motores alimentados con mezclas de diésel y biodiésel pone de manifiesto su posible emisión por combustión incompleta [3]. Por ello, para evaluar las implicaciones ambientales de su uso es necesario conocer su persistencia atmosférica y las consecuencias de su transformación química.

En la atmósfera, los hidroxiéteres reaccionan con el radical hidroxilo (·OH), el radical nitrato ($\cdot NO_3$) durante la noche y los átomos de cloro (Cl) presentes en zonas costeras e industriales. Estas reacciones generan productos oxigenados y pueden contribuir, a través de los procesos fotoquímicos posteriores, a la formación de ozono troposférico. Una rápida eliminación atmosférica no implica necesariamente un impacto ambiental despreciable, ya que los productos presentan su propia reactividad y persistencia. Por tanto, es necesario combinar el estudio cinético con la identificación de los productos de degradación [4]. En el caso del 2-butoxietanol, la información disponible se concentra principalmente en las reacciones con el ·OH; los escasos datos cinéticos sobre su reacción con $\cdot NO_3$ y la ausencia tanto de estudios cinéticos como de estudios de productos de la reacción con átomos de Cl motivaron esta investigación, con el objetivo de ampliar el conocimiento sobre el comportamiento de este tipo de compuestos en la atmósfera.

Las constantes de velocidad de las reacciones del 2-butoxietanol con el $\cdot NO_3$ y los átomos de Cl se determinaron mediante el método relativo utilizando espectroscopía infrarroja por transformada de Fourier (FTIR), a 298 ± 5 K y 720 ± 10 torr. Los valores obtenidos fueron $(8{,}16 \pm 1{,}59) \times 10^{-15}$ y $(4{,}33 \pm 0{,}28) \times 10^{-10}$ cm^3 $molécula^{-1}$ s^{-1}, respectivamente. Durante el estudio de productos de la reacción con Cl, realizado en aire sintético y en ausencia de NO_X, se identificaron formaldehído, propanal, formiato de 2-hidroxietilo y formiato de butilo, interpretándose las posibles rutas de formación con apoyo del generador de mecanismos MechGen [5]. Los resultados se contextualizaron comparándolos con otros hidroxiéteres y evaluando la capacidad predictiva de los métodos de relación estructura-actividad [6]. Asimismo, se estimaron los tiempos de vida atmosféricos y el potencial de creación de ozono fotoquímico [7], tanto de estos compuestos como de los productos de degradación conocidos de las reacciones del 2-butoxietanol con los oxidantes atmosféricos.

Las predicciones cinéticas mostraron una concordancia global razonable con los datos experimentales. Los hidroxiéteres considerados presentaron tiempos de vida estimados del orden de horas y una capacidad intermedia de formación de ozono. Algunos productos de degradación mostraron un mayor potencial de formación de ozono o una mayor persistencia. Estos resultados contribuyen a evaluar las implicaciones atmosféricas de los aditivos en biocombustibles, considerando tanto su eliminación como los contaminantes secundarios perjudiciales generados.

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Dynamic Adsorption and Regeneration Behavior of Strong-Base Anion-Exchange Resins in Pd(II)/Zn(II) Chloride Systems

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The recovery of palladium from spent automotive catalysts is essential for strengthening circular material flows and reducing the environmental burdens associated with primary PGM production [1]. This work investigates the continuous-mode adsorption and elution behavior of four strong-base anion-exchange resins: Purolite SPA260127E, DuPont Amberlyst A26, Purolite Purogold A194, and DOW XZ 91419 (SPA, A26, A194, XZ, respectively) using a Pd/Zn chloride solution formulated to reflect the competitive conditions of gasoline-catalyst leachates, where Zn is the major co-leached species that influences the selectivity of resin for Pd. Breakthrough experiments indicated significant differences in dynamic retention, with SPA resin exhibiting the highest Pd breakthrough volume (110 BV), followed by A26, A194, and XZ resins. Zn retention was also strongly resin-dependent, highlighting the importance of resin morphology and the charge and specific interactions of the $PdCl_4^{2-}$ and $ZnCl_3^-$ species in governing adsorption. Elution studies demonstrated that adsorption strength does not predict regenerability: although SPA resin showed the highest Pd uptake, only 57 *wt.*% was recovered with 1 mol/L NaOH, whereas XZ resin enabled nearly quantitative Pd elution (>99 *wt.*%) despite its low dynamic retention. Water proved effective for selective Zn stripping, while NaOH promoted Pd desorption through hydroxide-induced ligand exchange. All resins produced eluates with Pd purity above 99 *wt.*%, confirming the high selectivity of the elution strategy.

The choice of resin depends on the intended application. SPA resin offers the highest Pd(II) adsorption capacity but shows poor regeneration, making it less suitable for cyclic operation. XZ resin regenerates efficiently and allows nearly complete Pd elution, but its low adsorption capacity limits its use when high metal uptake is required. A26 resin provides a balanced compromise between Pd adsorption performance and regenerability, making it a suitable option for continuous hydrometallurgical Pd recovery from multi-element leachates.

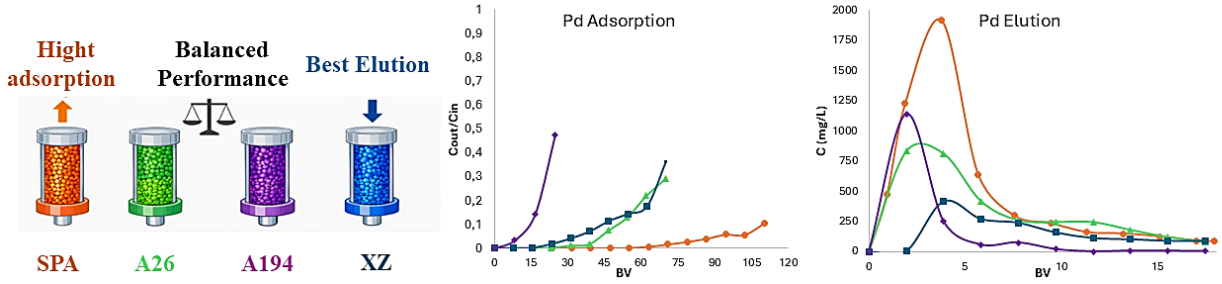


Fig. 1. Graphical overview of the comparative adsorption–elution performance of strong-base anion-exchange resins (SPA, A26, A194, and XZ) for Pd(II) recovery.

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Hemotoxic effects of emerging bisphenol analogues in human erythrocytes

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Bisphenols are synthetic chemicals widely used in the manufacture of consumer products, and are structurally characterized by the presence of two hydroxyphenyl groups. Among them, bisphenol A has been the most extensively produced and studied, particularly due to its widespread application in polycarbonate plastics and epoxy resins. Increasing regulatory restrictions and concerns over the potential adverse effects of bisphenol A have driven the development and use of structurally related analogues [1], although little is known about their potential adverse effects in humans. Erythrocytes represent a particularly relevant cellular target for investigating the hematotoxic effects of environmental chemicals. As the most abundant cells in the bloodstream, they are continuously exposed to circulating xenobiotics and are particularly dependent on membrane integrity, redox homeostasis, and tightly regulated intracellular calcium levels to maintain their functionality and survival [2,3]. Disruption of these processes may promote premature erythrocyte damage and removal from circulation.

This study aimed to compare the hemotoxic effects of ten structurally related bisphenols, namely, bisphenols A, A-DMA, AF, AP, B, BP, E, F, M, and S, on human erythrocytes and to characterize the cellular events underlying the observed erythrocyte injury. To this end, hemolysis, phosphatidylserine (PS) externalization, intracellular calcium accumulation, reactive species (RS) generation, and total glutathione (GSH) levels were assessed.

Our findings revealed distinct patterns of erythrocyte injury among bisphenol analogues, suggesting that structurally related compounds can affect erythrocytes through different pathways. Bisphenols AF and M promote eryptosis through oxidative stress-related mechanisms, whereas AP and BP induced erythrocyte alterations without a significant increase in RS and decrease of total GSH levels, suggesting the involvement of alternative mechanisms. Among the compounds tested, bisphenol M exhibited the broadest hemotoxic profile, inducing multiple erythrocyte alterations, including hemolysis, PS translocation, intracellular calcium accumulation, RS generation, and GSH depletion.

Overall, these findings demonstrate substantial differences in the hemotoxic potential of structurally related bisphenol A analogues and highlight the need to consider the toxicological profiles of individual bisphenols when evaluating their use as bisphenol A alternatives.

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From Structure to Performance: Pt(IV) and Pd(II) Adsorption on Next-Generation Anion-Exchange Resins

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Recovering platinum group metals (PGMs) from secondary resources is increasingly important for reducing the environmental burdens of primary mining and promoting sustainable material cycles, yet achieving selective removal of Pt and Pd from dilute chloride leachates remains a central challenge in hydrometallurgical processing [1].

This work investigates the adsorption of Pt(IV) and Pd(II) chlorocomplexes onto two strongly basic anion-exchange resins—a newly engineered quaternary ammonium resin (Purolite SPA260127E, SPA) and a commercial benchmark (Amberlyst A26, A26) [2]. Structural characterization revealed distinct pore architectures, with SPA resin exhibiting a uniform mesoporous network and higher functional group density, while A26 resin displayed a heterogeneous macroporous structure (Fig. 1). Kinetic experiments showed faster Pd(II) uptake for both materials, with SPA resin presenting more homogeneous diffusion behavior. Equilibrium data fitted Redlich–Peterson and Sips models, indicating mixed monolayer adsorption and surface heterogeneity. SPA evidenced the highest adsorption capacities (1.8 mmol·g^{-1} for Pt(IV) and 2.6 mmol·g^{-1} for Pd(II)) in multi-element chloride systems. Post-adsorption SEM/EDS and XPS analyses further confirmed this enhanced performance, revealing higher metal loadings in SPA resin and clear evidence of ion-exchange between $R_4N^+Cl^-$ groups and anionic chlorometalate species, such as $[PdCl_4]^{2-}$ and $[PtCl_6]^{2-}$, consistent with its more accessible mesoporous structure and favorable surface chemistry.

Taken together, these results reveal clear structure–performance relationships and establish SPA resin as a highly efficient and potential resin for the selective recovery of PGMs from complex hydrometallurgical streams.

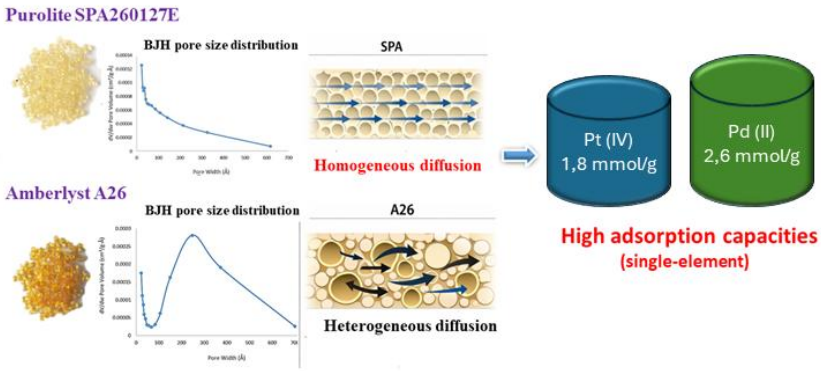


Fig. 1. Graphic overview of the structural features of the anion-exchange resins and the corresponding Pt(IV) and Pd(II) adsorption performance of the SPA resin.

Acknowledgment

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Bioconcreto autorreparable: comportamiento frente a la formación y sellado de fisuras

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Las fisuras en el hormigón facilitan el ingreso de agua, dióxido de carbono, cloruros y otros agentes agresivos, acelerando procesos como la corrosión del acero de refuerzo, la pérdida de resistencia y la disminución de la vida útil de las estructuras [1] (Wong et al., 2024). En este contexto, el bioconcreto constituye una alternativa sostenible para favorecer la autorreparación de fisuras mediante la Precipitación de Carbonato de Calcio Inducida por Microorganismos (MICP). Esta investigación evaluó el comportamiento de un bioconcreto elaborado con *Bacillus subtilis* y lactato de calcio, considerando la evolución de las fisuras controladas, la formación de carbonato de calcio y la viabilidad bacteriana dentro del hormigón.

Se fabricaron especímenes cilíndricos de hormigón convencional y bioconcreto, de 150 mm de diámetro y 300 mm de altura, conforme a los procedimientos establecidos para la elaboración y curado de probetas de hormigón normas ecuatorianas NTE INEN 1573, 2010 y ASTM C192/C192M. En la mezcla de hormigón se incorporó *Bacillus subtilis* y lactato de calcio como fuente de nutrientes, manteniendo condiciones homogéneas de dosificación, mezclado, compactación y almacenamiento. Las probetas fueron sometidas a curado por inmersión durante 28 días. Posteriormente, se generaron fisuras controladas y otras mediante cargas parciales de compresión, como resultado del comportamiento natural del material. El proceso de autocuración fue monitoreado bajo condiciones controladas de humedad y temperatura.

Los resultados evidenciaron la aparición progresiva de depósitos blanquecinos en el interior y los bordes de las fisuras. La observación microscópica permitió identificar estructuras cristalinas compatibles con carbonato de calcio, mientras que el análisis mediante microscopía electrónica de barrido y espectroscopía de energía dispersiva de rayos X (SEM-EDS) confirmó la presencia predominante de calcio, carbono y oxígeno en los precipitados, además al realizar la verificación con tinción de Gram y tinción de endosporas, confirmó la permanencia de *Bacillus subtilis* dentro del bioconcreto después del fraguado y endurecimiento, evidenciando la resistencia de la bacteria a las condiciones alcalinas, la baja disponibilidad de nutrientes y las presiones osmóticas características de la matriz cementicia [2], [3]

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Biomass-Derived Furans as a Platform for Sustainable Synthesis and Green Chemistry Education

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Biomass-derived furans have emerged as attractive renewable building blocks for the development of sustainable synthetic methodologies due to their availability, reactivity and structural diversity [1]. In particular, hetero-Diels-Alder (HDA) reactions involving nitrosoalkenes constitute an efficient strategy for the synthesis of oxygen- and nitrogen-containing heterocycles [2,3].

In this work, the reactivity of several biomass-derived furans and bis-furans towards nitrosoalkenes generated *in situ* from α-bromo oximes was investigated under mechanochemical conditions. Solvent-free ball milling promoted the formation of HDA cycloadducts in good to excellent yields while reducing reaction times and eliminating the need for organic solvents. The influence of structural features of the dienophile, namely electronic properties and linker architecture in bis-furan systems, was evaluated.

The results showed that reactivity is strongly dependent on both electronic and steric effects. Electron-rich substrates displayed enhanced reactivity, with 2,5-dimethylfuran affording the corresponding furo-oxazine in 93% yield. The synthetic utility of the obtained cycloadducts was further demonstrated through DBU-mediated rearrangements leading to 6*H*-1,2-oxazines and functionalized pyridines, providing access to structurally diverse heterocyclic scaffolds from renewable starting materials through short synthetic sequences.

The model reaction was also translated into an undergraduate Green Chemistry laboratory experiment, where students evaluated the sustainability of mechanochemical and solution-based methodologies using green metrics and computational toxicology tools. This research-led educational activity highlights the potential of mechanochemistry as a platform for integrating synthetic chemistry, environmental impact assessment and safety evaluation within chemistry curricula.

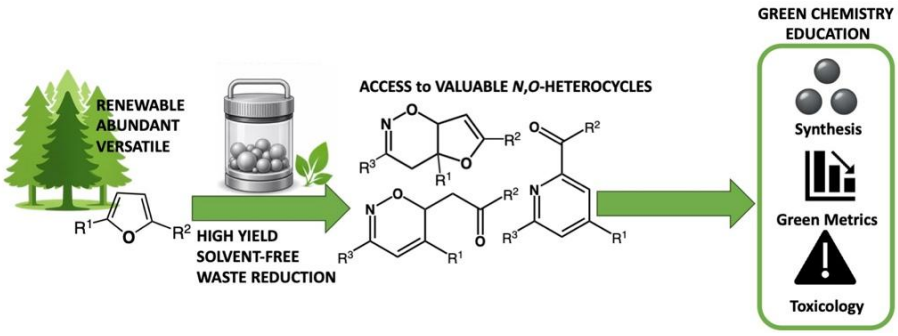


Fig.1. From Research in Sustainable Synthesis to Green Chemistry Education.

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Avocado Seed Valorisation for Water Treatment

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The increasing demand for processed vegetables presents an environmental challenge associated with the treatment of the organic-rich wastewater. Potato and carrot processing generates effluents containing high concentrations of starch, suspended solids, and colloidal organic matter, resulting in elevated turbidity and chemical oxygen demand (COD) [1]. Although coagulation–flocculation is widely employed for wastewater clarification [2], conventional chemical coagulants can generate substantial amounts of sludge, highlighting the need for more sustainable alternatives. In this context, avocado seeds, an abundant agro-industrial by-product rich in proteins, carbohydrates, and phenolic compounds [3], represent a promising source of natural biocoagulants. This study investigated the production of avocado-seed biocoagulants via dilute hydrochloric acid extraction, optimising time (10–60 min), temperature (30–90 ºC), and concentration (0.02–0.06 g/L). Jar Tests assessed clarification of real food-processing wastewater, comparing extracts with aluminium sulphate and organic commercial (Tanfloc) coagulants, and demonstrated coagulation activity. A 76% turbidity removal was obtained at 150 mg/L extract concentration and 90 min of sedimentation, while a 400 mg/L extract concentration reached 61% removal after 60 min. Comparatively, *Tanfloc* achieved 63% removal at 20 mg/L, whereas aluminium sulphate was ineffective under the tested conditions. These findings demonstrate the potential of avocado seed extracts as an alternative biocoagulant for food-processing wastewater treatment, achieving clarification comparable to that achieved by *Tanfloc* under the studied conditions.

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Design and Development of Potent HIV Protease Inhibitors Based on a Biorenewable Scaffold

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Highly active antiretroviral therapy (HAART) remains the most effective therapeutic strategy for managing human immunodeficiency virus (HIV) infection, significantly reducing viral replication, morbidity, and mortality.[1] Among the antiretroviral agents used in HAART, protease inhibitors such as Darunavir target the HIV protease enzyme, thereby preventing the maturation of newly formed viral particles.[1] Despite their therapeutic effectiveness, the synthesis of complex protease inhibitors often involves multiple synthetic steps, considerable solvent and reagent consumption, and significant waste generation, emphasizing the need for more sustainable synthetic strategies.[2]

In this work, we present a comparative sustainable chemistry assessment of the synthesis of the bis-tetrahydrofuran alcohol (bis-THF) scaffold found in Darunavir and a newly developed biorenewable scaffold proposed as an alternative structural platform for HIV protease inhibitors. Established synthetic approaches to the bis-THF moiety reported in the literature were evaluated alongside our newly developed methodology using a range of green chemistry metrics.

The new scaffold is derived from a biorenewable starting material through a concise two-step synthetic sequence, affording a 71% overall yield and 100% enantiomeric purity. In addition to its synthetic and sustainability benefits, the scaffold displays biological relevance, as demonstrated by a novel Darunavir analogue incorporating this structural motif, which exhibits HIV protease inhibition in the low nanomolar range.

Overall, this study combines synthetic efficiency, renewable feedstocks, green chemistry metrics, and biological activity to assess the potential of the new scaffold as a more sustainable alternative to the conventional Darunavir-derived framework. The results highlight how the use of biorenewable molecular platforms can simultaneously streamline synthetic routes and provide structurally suitable scaffolds for the development of potent HIV protease inhibitors.

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From renewable biopolymers to functional fibers: electrospinning of Chitosan-PCL nanocomposites for textile dye adsorption

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Water contamination from synthetic dyes used in textile finishing processes poses a major environmental challenge. To address this issue, this work presents high-performance, reusable electrospun nanocomposites designed for textile effluent remediation.

To resolve the intrinsic mechanical fragility of pure chitosan without burying its reactive surface sites within a bulk matrix, an asymmetric layered architecture combining chitosan (formulated with polyethylene oxide and cellulose nanocrystals) and poly(ε-caprolactone) (PCL) was fabricated. The resulting composite integrates the structural ductility and wet stability of the PCL backing layer with the high surface accessibility and hydrophilicity of the chitosan layer.

In batch adsorption experiments with the reactive dye Remazol Brilliant Blue R, the layered membranes achieved rapid decolorization with removal efficiencies exceeding 98% across concentrations up to 200 mg/L. The adsorption behavior conformed to pseudo-second-order kinetics and the Langmuir isotherm model, reaching a maximum monolayer capacity of 69.5 mg/g at 25°C governed by electrostatic attraction and hydrogen bonding. Furthermore, the membranes demonstrated reusability over at least three consecutive cycles with partial dye recovery in alkaline medium. These results demonstrate the potential of tailored biopolymer-based electrospun architectures as sustainable, mechanically robust solutions for wastewater treatment in circular textile ecosystems.

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Rapid capture and recovery of Nd, Tb and Dy from water using pristine Kraft lignin: a response surface approach

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Rare earth elements (REEs) such as neodymium (Nd), terbium (Tb) and dysprosium (Dy) are critical raw materials for Nd–Fe–B permanent magnets and other low-carbon technologies, and their recovery from secondary resources has become a strategic priority in Europe [1]. Because conventional hydrometallurgical routes are reagent-intensive, low-cost biosorbents able to pre-concentrate REEs from dilute aqueous streams are a promising complementary approach [2]. In this work, Kraft lignin (KL) isolated by CO_2 precipitation from industrial *Eucalyptus urograndis* black liquor [3] was evaluated, without any chemical modification, for the simultaneous removal of Nd, Tb and Dy from multielement aqueous solutions.

A three-factor, three-level Box-Behnken design combined with response surface methodology [4] was used to assess the effects of initial REE concentration (0.5–10 µmol/L per element), KL dose (50–500 mg/L) and salinity (0–30, NaCl) at pH 5.7–6.3 and 295 K. Sorption was fast, with most of the uptake occurring within the first 3 h. Removal decreased with increasing REE concentration and salinity and increased with KL dose. All quadratic models were statistically significant (R^2 = 0.899–0.983), and the predicted optimum (0.5 µmol/L REE, zero salinity, 500 mg/L KL) yielded removals above 86% after only 15 min. An independent validation under these conditions confirmed complete removal (≈100%) of the three elements after 1 h (Table 1). Maximum observed uptakes were 3.13, 5.51 and 5.19 mg/g for Nd, Tb and Dy, respectively, suggesting preferential retention of the heavier REEs. FT-IR spectra of pristine and REE-loaded KL showed that the lignin backbone was preserved and pointed to carboxylate and phenolic oxygen groups as the main binding sites, consistent with a surface complexation mechanism.

Desorption with 0.5 M HNO_3 for 3 h recovered approximately 78% of Nd and 73% of Tb and Dy. Overall, these results highlight unmodified KL, an abundant by-product of the pulp and paper industry, as a promising bio-based sorbent for rapid REE capture and recovery, and support its future assessment in real REE-bearing effluents and leachates.

Table 1. Removal of Nd, Tb and Dy by KL under the optimum conditions (0.5 µmol/L REE, salinity 0, 500 mg/L KL), maximum observed uptake and recovery with 0.5 M HNO_3 (3 h).

Element	Predicted removal, 1 h (%)	Observed removal, 1 h (%)[a]	$q_{max,obs}$ (mg/g)[b]	Recovery (%)
Nd	86.4	≈100	3.13	≈78
Tb	91.2	≈100	5.51	≈73
Dy	91.5	≈100	5.19	≈73

[a] Independent validation experiment (n = 2). [b] Maximum uptake observed across the experimental domain.

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Assessment of Chromium Contamination in Aquatic Environments near Tannery Industries: A Portuguese Case Study

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Environmental contamination arising from industrial activities remains a major global concern, with tannery operations recognized as one of the principal sources of chromium (Cr) release into aquatic environments [1]. Chromium occurs in several oxidation states, exhibiting markedly different levels of mobility, bioavailability, and toxicity, thereby posing significant risks to both aquatic ecosystems and human health. In Portugal [2], the Alcanena region represents a notable hotspot of tannery activity, hosting approximately 60 leather-processing industries. This study investigated total Cr concentrations in the Alviela River and the Carvalho Stream, with particular emphasis on the influence of a local wastewater treatment plant (WWTP) receiving tannery effluents.

Water samples were collected upstream and downstream of the WWTP discharge point and analysed using graphite furnace atomic absorption spectrometry and inductively coupled plasma optical emission spectrometry. The analytical method achieved a detection limit of 0.33 μg L^{-1}.

The highest Cr concentration (560 μg L^{-1}) was measured in the Carvalho Stream downstream of the WWTP discharge, clearly demonstrating the contribution of treated tannery effluents to local chromium contamination. In the Alviela River, downstream concentrations ranged from 8 to 50 μg L^{-1}, with several values exceeding both the predicted no-effect concentration (PNEC) for aquatic organisms and the drinking-water safety threshold of 25 μg L^{-1}. Notably, elevated chromium concentrations were still detected approximately 5 km downstream of the discharge point, indicating the persistence and downstream transport of chromium contamination within the river system.

To the best of our knowledge, this is the first study to document the current extent of chromium contamination associated with tannery effluents in the Alcanena region. The results provide compelling evidence of the continuing environmental pressure exerted by this industrial sector, demonstrating that chromium contamination persists for at least 5 km downstream of the WWTP discharge. These findings highlight the urgent need for enhanced monitoring programmes and more effective pollution mitigation strategies to protect aquatic ecosystems and water resources.

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Photosensitizers and Hybrid Materials for the Photodynamic Disinfection of Water

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Wastewater, particularly from hospitals, is a major route for the release of pathogenic and antibiotic-resistant bacteria into the environment, and conventional disinfection methods have known limitations, including the formation of toxic by-products. Photodynamic inactivation (PDI) combines a photosensitizer (PS), visible light and dioxygen to generate reactive oxygen species (ROS) that damage multiple microbial targets, making the development of resistance unlikely.

This communication will show how cationic porphyrins can be designed for water disinfection. The number and distribution of positive charges and the nature of the *meso* substituents determine the efficiency against Gram-negative bacteria [1]. Selected cationic porphyrins inactivated faecal bacteria in urban wastewater [2] and clinical multidrug-resistant bacteria in hospital wastewater [3], and repeated treatments did not induce resistance [4].

To allow recovery and reuse of the PS, cationic porphyrins were coupled to silica-coated magnetic nanoparticles, affording hybrids that are removed with a magnet and remain active over several cycles [5,6]. Because unrecovered material may reach crops irrigated with treated wastewater, the effect of a porphyrin–Fe_3O_4 hybrid on wheat was also evaluated, with no apparent phytotoxicity at low doses and short-term exposure [7]. The remaining challenges for application will be briefly discussed.

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Unlocking Microalgal Polysaccharides Through Sustainable Extraction Strategies for Aquafeed Applications

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Prioritisation of sustainability has led to the development of new extraction techniques that lower energy use, enable the use of less hazardous solvents, and can help minimise waste, while ensuring efficient conversion of biomass into the desired bioactive compounds. Polysaccharides extracted from algae exhibit promising bioactivity, including immunomodulatory and antioxidant effects, making them attractive functional feed ingredients to improve fish health and disease resistance in aquaculture. The objective of this study was to produce polysaccharide-enriched extracts from microalgae *Chlorella vulgaris* and *Dunaliella salina*, applying three different aqueous methods, whilst comparing the extraction performance and characterising the extracts. Afterwards, their biocompatibility was assessed in toxicity assays conducted on zebrafish larvae 3 days post-fertilization.

Three extraction methods: conventional hot-water extraction (HWE), ohmic heating extraction (OHE), and ultrasonic-assisted extraction (UAE), were applied to freeze-dried microalgal biomass suspensions at 50 g L^{-1}. Carbohydrate content was quantified by the sulphuric acid/UV spectrophotometry methodology, antioxidant activities by ABTS and FRAP assays, and functional groups by ATR-FTIR spectroscopy. OHE resulted in greater extraction yields for both algae species, but the content of carbohydrates was less, indicating co-extraction of a broader range of compounds. For the ABTS assay, HWE and UAE extracts showed IC_{50} values below 3 mg mL^{-1} for *D. salina*, and below 1 mg mL^{-1} for *C. vulgaris.* For the FRAP assay, HWE and UAE extracts showed relevant antioxidant activity. ATR-FTIR spectra displayed characteristic glycosidic linkage bands and confirmed β-glucans (894 cm^{-1}) in UAE extracts for both algae.

All zebrafish larvae survived exposure to OHE extracts at 0.1, 0.5 and 1.0 mg mL^{-1} for both species, whereas extracts from HWE and UAE caused high mortality at concentrations ≥ 0.5 mg mL^{-1}. Overall, UAE emerged as the most promising method for both species, combining high yield with strong radical-scavenging and reducing capacities. However, the concentration-dependent mortality observed at higher doses suggests potential toxicity, warranting further assays to verify biological activity at lower, non-lethal concentrations. The environmental sustainability of these methods will be evaluated using established greenness metrics grounded in core sustainable chemistry principles.

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Rare earth removal from simulated magnet and lamp waste using a microporous niobium–iron silicate

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End-of-life magnets and fluorescent lamps are secondary sources of rare earth elements (REEs), whose uptake by microporous Nb–Fe silicates has previously been demonstrated in spiked waters [1]. Extending this evaluation to mixtures representing these wastes, this study investigated REE removal by $Na_{2.9}(Nb_{1.55}Fe_{0.45})Si_2O_{10}\cdot xH_2O$, combining process optimisation with sorption kinetics [2].

Response surface methodology with a Box–Behnken design was applied to mineral water containing nine REEs, assessing pH (4–8), initial concentration (1–5 µmol/L per element) and sorbent dose (20–180 mg/L). At the predicted optimum (pH 4.2, 1.8 µmol/L per element and 179 mg/L sorbent), measured removals after 6 h were 88.2 % for Nd and 66.1 % for Y, against predictions of 100 % for both, revealing a larger prediction discrepancy for Y.

In synthetic mixtures simulating permanent magnet and lamp phosphor waste, at pH 4 and 180 mg/L sorbent, Nd and Y removals reached 97.7 and 96.7 %, respectively, after 1 h at initial concentrations of 5 µmol/L of the respective target element. Increasing these concentrations to 50 µmol/L reduced removal to 85.5 % for Nd and 74.3 % for Y after 48 h. Uptake was best described by the Elovich model for Nd and the pseudo-second-order model for Y, although these fits do not establish a specific sorption mechanism. The results support simultaneous REE uptake from the tested mixtures; evaluation in real leachates, together with desorption and reuse studies, remains necessary to assess recovery-process applicability.

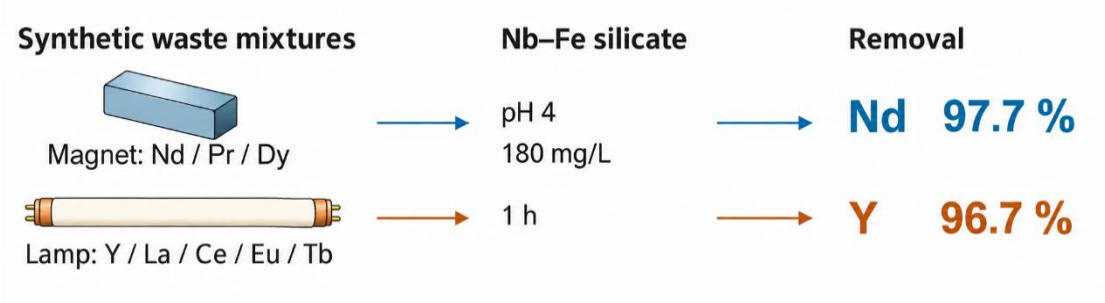


Fig. 1. REE removal from simulated waste mixtures; initial Nd or Y: 5 µmol/L [2].

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Valorization of White Grape Pomace Through Targeted Recovery of Phenolic Acids Using Conventional and Hydrotropic Solvents

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Grape pomace, the main by-product of the winemaking process, represents an abundant and underutilized source of polyphenols [1,2]. These bioactive compounds are widely recognized for its antioxidant, anti-inflammatory, and antimicrobial properties, among others, offering high-value applications across the food, pharmaceutical, and cosmetic industries [3]. In this regard, conventional solvent extraction methods are routinely used to obtain polyphenol-rich extracts; however, the selective recovery of specific compounds remains a significant challenge due to their structural similarity [4]. Within this framework, this work presents the selective extraction of targeted polyphenols from white grape pomace (Albariño) using both conventional solvents and an aqueous hydrotropic system of food grade citric acid.

Winemaking waste was kindly supplied by Albamar winery (Cambados, Pontevedra). After drying and grinding the raw grape pomace, solid-liquid extractions were performed with methanol, ethanol, pure water and an aqueous hydrotropic mixture of 5 wt% citric acid. Subsequently, the extracts were characterized in terms of total phenolic content (TPC) and antioxidant capacity (AC), and submitted to HPLC-MS/MS analysis to explore their polyphenolic composition.

Results showed that the 5 wt% citric acid hydrotropic solution provided the extract with the highest TPC and AC values. For its part, methanolic extracts yielded a higher TPC but slightly lower AC than the water extract, whereas ethanolic extracts achieved the lowest values. HPLC profiles evidenced the broad-spectrum extraction capacity of methanol and ethanol towards polyphenolic compounds, whereas pure water preferentially recovered phenolic acids, accounting for 90.8 % of the total polyphenolic fraction. In terms of total quantified polyphenolic, methanol achieved the highest yield of 35.6 mg/100 g pomace, while water attained 3.7 mg/100 g pomace. Notably, extraction with 5 wt% citric acid doubled the polyphenol recovery to 7.3 mg/100 g pomace, maintaining the selectivity towards phenolic acids (85.6 %).

Overall, while methanol and ethanol acted as broad-spectrum extractants for diverse polyphenols and pure water preferentially recovered phenolic acids, the 5 wt% citric acid hydrotropic system successfully enhanced extraction efficiency while maintaining high selectivity. These results underscore the hydrotropic potential of citric acid to selectively separate targeted polyphenolic fractions from white grape pomace.

Acknowledgements

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Evaluación energética y ambiental de materiales de aislamiento sostenibles para edificios mediante simulación térmica dinámica y análisis del ciclo de vida

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El elevado consumo energético del sector de la edificación es una de las principales fuentes de emisiones de gases de efecto invernadero, especialmente en zonas climáticas con importantes necesidades de calefacción y refrigeración [1] . Por lo tanto, mejorar el rendimiento térmico de los edificios mediante el uso de materiales aislantes eficientes es una estrategia clave para reducir la demanda energética y mejorar el confort térmico [2]. Sin embargo, la evaluación de estos materiales suele limitarse a su rendimiento energético durante su uso, sin considerar suficientemente su impacto ambiental a lo largo de su ciclo de vida. El objetivo de este trabajo es evaluar de forma integrada el rendimiento energético y ambiental de diferentes materiales aislantes aplicados a edificios, con el fin de identificar las soluciones que ofrecen el mejor compromiso entre eficiencia energética e impacto ambiental. La metodología adoptada se basa en un enfoque combinado. En primer lugar, se realizan simulaciones térmicas dinámicas con el software TRNSYS en un edificio residencial de referencia, considerando diferentes escenarios de aislamiento, incluyendo materiales convencionales y de origen biológico. Estas simulaciones permiten evaluar la demanda energética anual del edificio. En segundo lugar, se realiza un análisis del ciclo de vida (ACV) de los materiales de aislamiento mediante el software openLCA, evaluando su impacto ambiental a través del potencial de calentamiento global (PCG). Los resultados muestran que todos los materiales aislantes reducen significativamente el consumo energético respecto al edificio sin aislamiento. El poliuretano presenta el menor consumo energético anual, pero también el mayor PCG, mientras que el cáñamo presenta el menor impacto ambiental. El corcho expandido ofrece un equilibrio favorable entre ambos criterios, combinando un bajo consumo energético con un reducido impacto ambiental. Estos resultados subrayan la importancia de integrar criterios energéticos y ambientales para orientar la selección de materiales de aislamiento hacia soluciones más sostenibles.

Palabras clave: Aislamiento térmico, rendimiento energético de la edificación, evaluación del ciclo de vida (ACV), simulación térmica dinámica, materiales sostenibles.

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Lipid profile and antimicrobial activity of by-products of the winemaking process: the case of grape pomace and stems

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The winemaking process generates large amounts of by-products that may contain valuable compounds, such as phenolics, tannins, fatty acids, and vitamin E, which may be potentially used in the cosmetic industry due to their antioxidant, moisturizing, anti-inflammatory, and antimicrobial properties [1]. The present study aimed to characterize the fatty acid composition and vitamin E profile of grape pomace and stems and to evaluate the antimicrobial activity of extracts obtained from these by-products.

Nine stem and four pomace samples from different grape varieties and terroirs were freeze-dried and ground before chemical analysis. The lipid content was determined using the Soxhlet method (AOAC 991.36). For vitamin E and fatty acid analysis, lipids were extracted using a cold extraction method, according to Alves et al. [2] and analysed by RP-HPLC-FLD-DAD and GC-FID, respectively [3]. Freeze-dried extracts of grape stems and pomace were obtained by microwave-assisted extraction under optimized conditions (stems: 9.54 min, 74.55% ethanol, and 47.17 °C; pomace: 39.80 min, 40.61% ethanol, and 70 °C). The preliminary antimicrobial activity was assessed against *Candida albicans* and *Staphylococcus aureus* by agar diffusion assay. The minimum inhibitory concentration (MIC) was subsequently determined against *S. aureus* using the broth microdilution method.

The results showed differences in lipid content between the two grape by-products (pomace: 5.24 -14.56 % dw; stems: 0.63 - 1.72 % dw). Six vitamin E vitamers (α-, γ-, and δ-tocopherol, α-, β-, γ-tocotrienol) were identified in stems and pomace, with α-tocopherol being the most abundant (4.50 - 22.64 mg/kg dw), except in one variety of pomace (Vinhão - Vinhos Verdes), where γ-tocotrienol was the most abundant (17.04 mg/kg dw). Linoleic (C18:2n6c) and palmitic (C16:0) acids were the most abundant fatty acids in the stems, whereas linoleic (C18:2n6c) and oleic (C18:1n9c) acids predominated in the pomace. The extracts exhibited inhibitory activity against *Staphylococcus aureus*, with minimum inhibitory concentration (MIC) values ranging from 1.56 to 6.25 mg/mL. In the agar diffusion assay, no inhibition zones were observed against *C. albicans* These results support the valorization of grape pomace and stems as sources of valuable compounds, contributing to circular economy approaches in the cosmetic industry.

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Tuning Supercritical CO_2 Extraction of *Ruscus aculeatus* L. Fruits: Influence of Polar Modifiers on Extract Fractionation and Chemical Profiles

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The selective recovery of natural compounds from plant matrices is an important strategy for developing sustainable extraction processes. *Ruscus aculeatus* L. contains chemically diverse phytoconstituents, including steroidal saponins, flavonoids and phenolic compounds[1]. Supercritical CO_2 extraction, particularly when combined with modifiers, offers a promising approach for recovering bioactive compounds[2].

This study investigates the influence of water and ethanol as extraction modifiers on on the chemical profiles of extracts obtained from *R. aculeatus* fruit pulp and seeds. Extractions were performed using $scCO_2$ and modified solvent systems, followed by chemical screening using complementary thin-layer chromatography (TLC) systems. Pure CO_2 predominantly yielded profiles associated with low-polarity compounds, whereas water- and ethanol-assisted extraction produced distinct patterns, suggesting the recovery of a wider range of phytochemicals (Figure 1). Seed extraction yielded two distinct phases, including an oil-rich fraction. TLC analysis of samples containing these fractions revealed chromatographic profiles potentially consistent with fatty acids and other lipophilic compounds, highlighting the oil-rich fraction as a promising source of functional lipids for food formulations. The TLC profiles further suggested the possible presence of phenolic acids, flavonoid-related compounds, and terpenoids, warranting further investigation of their biological properties and food applications.

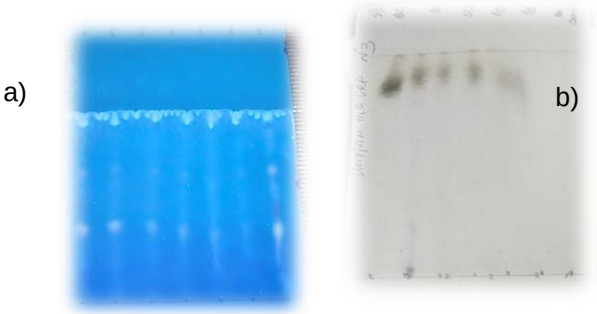


Fig.1. TLC of extracts obtained by using $scCO_2$+H_2O binary co-solvent system: (a) in S2-based and (b) chloroform-based system.

The combination of $scCO_2$ extraction and complementary TLC systems provides a rapid, cost-effective approach to assessing the influence of plant matrix and co-solvent on extract composition, supporting the potential valorization of R. aculeatus pulp and seeds for food-related applications.

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Liquefaction Process Optimization and Bio-Polyols Characterization of *Ruscus aculeatus* L. Branches

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The development of bio-based polymers has attracted significant scientific interest, driven by the growing demand for sustainable materials. Polyalcohol liquefaction is a thermochemical process, which has gained increasing attention as an efficient route for converting biomass residues into valuable intermediates, among them resins, adhesives, polyurethane foams, and other polymeric materials [1]. In this context, *Ruscus aculeatus L.* (Butcher's Broom), a native Portuguese plant traditionally used in medicine, represents a potentially valuable lignocellulosic resource for biomass valorization [2]. The main contribution of this work is to reinforce the eco-valorization of *Ruscus aculeatus* L. by thoroughly investigating and optimizing the liquefaction of its branches to produce bio-based polyols and by evaluating their suitability as precursors for polyurethane foams. Moreover, the novelty of this work lies in the exploration of *Ruscus aculeatus* as an unconventional and underutilized lignocellulosic resource, whereas biomass liquefaction for polyol production is already widely studied. Liquefaction experiments were conducted using a jacketed batch reactor Parr 5100, with a total volume of 600 mL supplied by Parr Instruments Co. (Moline, IL, USA). For each run, 10 g of oven-dried material, previously milled to a particle size range of 0.250–0.420 mm, was loaded into the reactor. To assess the influence of particle size on liquefaction efficiency, additional experiments were carried out using biomass fractions classified as >40, 40–60, 60–80, and <80 mesh. Biomass solubilization and the conversion of cellulose, hemicellulose, and lignin are strongly dependent on the elevated temperatures used because these temperatures promote the cleavage of polysaccharide glycosidic linkages and the scission of ether bonds in lignin structures. This interpretation is supported by the results, which demonstrate a noticeable increase in the liquefaction yield as temperature rises: from 39% at 140 °C to 67% at 160 °C, and to 92% at 180 °C. The data confirm that increasing the temperature significantly increases the liquefaction yield. This effect is slightly more pronounced between 140 °C and 160 °C, when the liquefaction yield increases by 28 percentage points, compared with an increase of 25 percentage points between 160 °C and 180 °C. The variation in hydroxyl number with the temperature of liquefaction was studied for polyols liquefied at temperatures of 140 °C, 160 °C, and 180 °C, for a constant period of 60 min. The results show that the hydroxyl number of the polyol liquefied at 140 °C is the highest, at 1038 mg KOH·g−1. As the temperature increases from 140 °C to 160 °C, a decrease to 932 mg KOH·g^{-1} is observed, and there is a further decrease to 916 mg KOH·g^{-1} for 180 °C. This trend is particularly significant because it contrasts with the increase in liquefaction yield. While higher temperatures promote more extensive depolymerization and solubilization, they simultaneously reduce the hydroxyl number per unit mass of product. Furthermore, the FTIR-ATR spectra of the polyols produced from Ruscus branches at different liquefaction temperatures show the typical absorption bands of lignocellulosic-derived polyols, with noticeable variations in intensity as a function of temperature. These variations, mainly focused on the broader band centered at ca. 3360 cm^{-1}, assigned to the O–H stretching vibrations, reflecting the formation of hydroxyl-containing compounds during depolymerization, as well as on the absorption bands around 2930 and 2870 cm^{-1} corresponding, respectively, to antisymmetric and symmetric stretching vibrations of the aliphatic $–CH_2$ and $–CH_3$ groups typical of the presence of aliphatic chains originating from degraded polysaccharides and lignin side chains. These spectral changes indicate progressive chemical transformations during liquefaction [3]. A weak but discernible band around 1730 cm^{-1} is assigned to C=O stretching vibrations of ester and/or carbonyl groups, while the signal observed near 1600 cm−1, associated with aromatic C=C stretching vibrations mainly derived from lignin structures, almost disappears during liquefaction. These changes indicate the progression of the liquefaction process. However, FTIR analysis mainly provides qualitative information, and therefore these observations should be interpreted as indicative trends rather than definitive structural evidence. Overall, the results highlight the critical role of liquefaction conditions in tailoring polyol properties for specific applications. The findings confirm the strong potential of *Ruscus aculeatus* L. as a sustainable raw material for bio-based polyols, while also emphasizing the importance of process optimization to balance reactivity, stability, and processability in industrial applications [4].

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Valorization of Moroccan geomaterials into low-cost ceramic membranes: optimization using response surface methodology (Box-Behnken design)

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Ceramic membranes are chemically and thermally stable, but their high costs limit their use in water treatment [1]. Local natural resources offer a sustainable and inexpensive route to producing them [1]. Morocco has abundant and inexpensive geomaterials that can reduce this cost. In this work, porous ceramic membrane supports were prepared from Moroccan geomaterials pozzolan, bentonite and diatomite, together with a natural $CaCO_3$ additive, using uniaxial dry pressing and a low sintering temperature (850-1050 °C). A three-factor Box-Behnken design was used to optimize sintering temperature, bentonite content (5-15%), and pore-forming additive content (0-20%) for porosity, water permeability, and mechanical strength. The materials were characterized by XRF, XRD, and FTIR analysis.

Statistical analysis (ANOVA) gave significant models for the three responses. Multi-response optimization with the desirability function gave optimal conditions of 1050 °C, 15% bentonite, 20% pore-forming agents, offering the best balance between porosity 37.49%, water permeability 1300.95 $L.h^{-1}.m^{-2}.bar^{-1}$, and mechanical strength 25.28 MPa, confirmed experimentally. XRD of the optimal membrane showed newly formed phases such as anorthite, indicating the decomposition of $CaCO_3$ and the reaction between resulting CaO and the aluminosilicates [2]. SEM revealed interconnected pores and well-developed sintering necks, without cracks, consistent with the measured porosity and strength.

These results show that suitable membrane supports can be made from local raw materials at low firing temperature, offering a sustainable and low-cost route for water treatment.

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Materiales Avanzados para la Construcción Sustentable: Aportes de la Ingeniería de los Materiales a la Innovación

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La construcción sustentable constituye una de las principales estrategias para reducir el impacto ambiental asociado al crecimiento urbano y al desarrollo de infraestructuras. En este contexto, la ingeniería de los materiales desempeña un papel fundamental mediante el diseño y la optimización de materiales avanzados capaces de mejorar la eficiencia estructural, energética y ambiental de las edificaciones. Los avances recientes han impulsado el desarrollo de hormigones de baja huella de carbono, materiales compuestos reforzados, cementos alternativos, materiales reciclados y soluciones bioinspiradas que contribuyen a disminuir el consumo de recursos naturales y las emisiones de gases de efecto invernadero. [1].

Asimismo, la incorporación de materiales reciclados y el aprovechamiento de residuos industriales favorecen la implementación de modelos de economía circular en el sector de la construcción, promoviendo la reutilización de recursos y la reducción de residuos.[2]

Por otra parte, los cementos de bajo carbono y las nuevas formulaciones basadas en arcillas calcinadas y materiales suplementarios permiten mantener un adecuado desempeño mecánico al tiempo que reducen significativamente las emisiones asociadas a su producción{3]

En conjunto, estas innovaciones evidencian que la ingeniería de los materiales constituye un eje estratégico para la transición hacia una construcción más sostenible, resiliente y alineada con los objetivos globales de desarrollo sostenible (Fig. 1).



Fig.1. Impacto ambiental en la construcción

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An integrated extraction-to-formulation approach for propolis-based lip care using hydrophobic NaDES

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More sustainable cosmetic ingredients require extraction strategies that reduce conventional solvent use and simplify downstream processing. Although propolis is widely used in natural cosmetics, ethanolic extracts are poorly suited for anhydrous lip-care products. Hydrophobic natural deep eutectic solvents (NaDES) represent a promising alternative, combining efficient bioactive extraction with direct compatibility with lipid-based formulations [1,2]. This study aimed to evaluate the potential of a NaDES-based propolis extract as a functional ingredient in lip balms, focusing on physical and oxidative stability.

To achieve this, propolis from Montesinho Natural Park (Portugal) was extracted at 10% (w/w) by ultrasound-assisted extraction using a hydrophobic NaDES composed of menthol and lauric acid (ML, 4:1). A central composite design was employed to investigate the effects of extraction time, water content, and ultrasound amplitude. The selected conditions (15 min, 40% water, 60% amplitude) yielded an extract with substantial antioxidant activity (DPPH 273.35 ± 7.93; ABTS 200.20 ± 2.40 mg AA/g propolis), and a total flavonoid content (TFC) of 102.96 ± 0.69 mg QE/g propolis. UHPLC-DAD-ESI/MS analysis revealed a phenolic profile particularly rich in chrysin, pinobanksin, galangin, pinocembrin, and CAPE. A scale-up NaDES batch maintained or slightly improved responses (TFC 112.82 ± 1.80 mg QE/g).

Three anhydrous lip balms containing beeswax, coconut and almond oil were formulated: F1 incorporated the ML-propolis extract at 1%, as the bioactive ingredient, F2 contained ML at the same proportion as a solvent control, and F3 consisted of the emollient base without either propolis or NaDES. Physical stability was assessed by vibration and centrifugation tests, freeze-thaw cycling, thermal stress at 5 and 45 °C and light exposure, using texture profile and CIELAB color analyses in all. Oxidative stability was measured by Rancimat method at 90 °C. All formulations were homogeneous and free of phase separation at baseline. The oxidation induction time of F1 (66.38 ± 4.24 h) was about 2.5-fold higher than F2 (26.41 ± 0.59 h) and F3 (25.82 ± 3.32 h), showing that the protection came from propolis constituents and not from the solvent. F1 also remained physically stable in the density, vibration and centrifugation tests, with moderate texture changes under thermal stress but generally smaller than those of the base. Color changes were slight at 5 and 45 °C, but prolonged light exposure caused visible discoloration in all formulations (ΔE > 5), highliting the need for light-protective packaging. Consumer testing indicated good acceptance, while estimated raw-material and packaging costs were low relative to participants' stated willingness to pay. Overall, these results support NADES-based propolis extracts as promising green, directly incorporable antioxidant ingredients for natural, sustainable lip care products.

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Ultrasound-Assisted Extraction of Phenolic Compounds with Antioxidant Properties from Grape Stalks: Process Optimization by Response Surface Methodology

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The winemaking industry generates substantial quantities of solid by-products, with grape stalks being one of the major residues generated during the destemming process. However, they remain largely undervalued.

Aligned with circular bioeconomy principles, this study aimed to optimize an ultrasound-assisted extraction (UAE) process to recover antioxidant phenolic compounds from grape stalks. A Central Composite Design combined with Response Surface Methodology was employed to investigate the effects of three independent variables: solid-to-liquid ratio (400–1200 mg/100 mL), extraction time (5–15 min), and ethanol concentration in the extraction solvent (20–80%). Extraction efficiency was assessed based on total phenolic (TPC), total flavonoid (TFC), and total anthocyanin contents (TAC), as well as antioxidant activity (using DPPH• scavenging and FRAP assays).

Across all response variables, extraction time and ethanol concentration were identified as the most influential factors. Optimal conditions were established at 459.37 mg/100 mL, 11.57 min, and 39.39% ethanol in water (v/v), yielding 14.48 mg GAE/g for TPC, 8.14 mg CE/g for TFC, 0.2595 mg C3GE/g for TAC, and antioxidant capacities of 28.21 mg TE/g and 163.85 µmol FSE/g for DPPH• scavenging and FRAP assays, respectively. Experimental validation confirmed high model reliability.
Overall, these results highlight the importance of tailoring UAE conditions to the grape stalk matrix to optimize phenolic recovery. The optimized process provided extracts with good antioxidant properties, confirming the potential of this winemaking by-product as a sustainable source of functional ingredients.

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Compound Wind–Solar Generation Deficits and Joint Electricity Price–Carbon Stress in Peninsular Spain

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Abstract
Wind and solar power have become central to Spain's electricity mix, but periods of weak generation from both sources can overlap. Such conditions may place additional pressure on electricity markets while increasing reliance on carbon-intensive generation. Recent studies have examined renewable-energy droughts [1,2] and the influence of renewable electricity on wholesale prices [3,4]. However, the relationship between concurrent generation deficits and the simultaneous occurrence of high electricity prices and carbon intensity deserves closer examination.

This study investigates this relationship in Peninsular Spain using historical electricity-system and market data. Periods of unusually low wind and solar generation are examined alongside changes in wholesale electricity prices and the carbon intensity of electricity production. The analysis compares overlapping generation deficits with other operating conditions, while considering the influence of electricity demand, fuel prices and seasonal variation. Particular attention is given to whether economic and environmental pressures tend to occur together during these periods, rather than treating price and emissions as unrelated outcomes.

The study aims to establish whether concurrent wind–solar deficits are associated with a distinct pattern of market and carbon stress. Examining these two dimensions together may offer a clearer picture of the challenges facing Spain's increasingly renewable electricity system and their implications for energy-security planning.

Keywords: Renewable energy deficits; Wind–solar generation; Electricity prices; Carbon intensity; Energy security; Spain.

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Evaluación de Soluciones basadas en la Naturaleza (SbN) para la adaptación climática y resiliencia en Galicia

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Frente a la creciente frecuencia de eventos climáticos extremos y sus impactos en cascada sobre los ecosistemas gallegos, la adopción de medidas de adaptación efectivas constituye una prioridad estratégica. Las investigaciones recientes señalan que las infraestructuras convencionales, como los diques de mampostería o barreras físicas artificiales, presentan limitaciones frente a la variabilidad climática, posicionando a las Soluciones Basadas en la Naturaleza (SbN) como alternativas eficientes y sostenibles a largo plazo.

Esta investigación evalúa la efectividad técnica y socio-ambiental de un catálogo de SbN, tecnologías de naturalización e infraestructura verde adaptadas a las especificidades biogeográficas de Galicia. El trabajo analiza intervenciones clave como la aplicación de acolchados orgánicos y la siembra de coberturas herbáceas de germinación rápida tras incendios, las cuales han demostrado que reducen la erosión laminar y el arrastre de cenizas entre un 70 y un 90% al fijar el suelo y absorber el exceso de nitratos solubles y amortiguan el impacto de las primeras lluvias torrenciales. Asimismo, se evalúa la protección y restauración de bosques de ribera, que actúan como trampas naturales de sedimentos y biofiltros hídricos, evitando la llegada masiva de cenizas y contaminantes a los cauces fluviales y rías.

A través de métricas de sostenibilidad e indicadores de efectividad basados en el análisis de ciclo de vida (ACV), la investigación demuestra cómo la integración de SbN incrementa la capacidad de retención de agua y protege los servicios ecosistémicos esenciales. El trabajo proporciona un catálogo tipificado de SbN diseñadas para el territorio gallego, ofreciendo soporte técnico directamente aplicable a la Estratexia Galega de Cambio Climático e Enerxía 2030 y la directiva europea de infraestructuras verdes, contribuyendo a la protección del sector primario y a la resiliencia socioeconómica regional.

PALABRAS CLAVE:
Cambio climático | Adaptación | Soluciones Basadas en la Naturaleza (SbN) | Infraestructura verde | Resiliencia territorial

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Transformando emisiones en materias primas: el papel del CCUS en la producción sostenible de metanol

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Dentro del abanico de tecnologías de captura, utilización y almacenamiento de carbono (CCUS), la utilización química del CO_2 destaca por integrar la mitigación climática con los principios de la economía circular mediante la transformación de emisiones en materias primas de valor añadido [3] [4]. En este contexto, la conversión catalítica de CO_2 capturado en metanol constituye una alternativa prometedora para la descarbonización de sectores intensivos en emisiones, como la industria cementera, siderúrgica y química [1] [4] [5]. El metanol es considerado además una materia prima estratégica e intermediario clave para la producción de e-combustibles y numerosos productos químicos, favoreciendo la reincorporación de corrientes gaseosas residuales al ciclo productivo industrial y reduciendo la dependencia de recursos fósiles [3] [4] [7].

Sin embargo, el despliegue técnico y la viabilidad ambiental de la síntesis de metanol a partir de CO_2 presentan importantes desafíos asociados al elevado consumo energético del proceso y a la significativa demanda de hidrógeno renovable [2] [3] [4]. Para garantizar una contribución real a la sostenibilidad, resulta esencial cuantificar con precisión las emisiones netas evitadas mediante metodologías rigurosas de Análisis de Ciclo de Vida (ACV) [1] [4]. Esta evaluación debe considerar tanto la energía empleada en la captura del CO_2 como las emisiones asociadas a la producción de hidrógeno verde [2] [4], asegurando que el sistema proporcione beneficios ambientales netos frente a las rutas convencionales y evite el traslado de impactos a otras etapas de la cadena de valor.

Esta estrategia de valorización del carbono se encuentra alineada con la iniciativa europea Towards an Ambitious Industrial Carbon Management for the EU [6] y con el marco regulatorio establecido por el Net-Zero Industry Act [7], que reconocen la utilización del CO_2 como un elemento estratégico para fortalecer la competitividad industrial y avanzar hacia la neutralidad climática. La integración de estos procesos en los instrumentos regulatorios de emisiones industriales y en el esquema de Mejores Técnicas Disponibles (BAT/MTD) favorece la transformación de residuos en recursos útiles [5] [7]. En conjunto, la producción sostenible de metanol ejemplifica la evolución del CCUS desde una herramienta de mitigación de emisiones hacia un eje estratégico para el desarrollo de la química sostenible [4] [6] [7].

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Riesgos operacionales y ambientales inherentes a la aquatermólisis en la recuperación térmica del crudo en la Faja Petrolífera del Orinoco

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La Faja Petrolífera del Orinoco (FPO) alberga uno de los mayores volúmenes de crudo pesado y extrapesado del mundo. Su explotación mediante técnicas de Recuperación Mejorada de Hidrocarburos (Enhanced Oil Recovery, EOR) de base térmica, como el Drenaje Gravitacional Asistido por Vapor (Steam Assisted Gravity Drainage, SAGD), se fundamenta en el incremento de la temperatura del yacimiento para reducir la viscosidad del crudo. Bajo estas condiciones tienen lugar procesos de aquatermólisis asociados a la interacción entre el vapor inyectado y las fracciones pesadas del petróleo [1]. Estas reacciones modifican la estructura química de resinas y asfaltenos, favoreciendo la transformación de compuestos organoazufrados y la reducción de la viscosidad del crudo [2].

A diferencia de estudios centrados en los impactos generales de las tecnologías EOR térmicas, el presente trabajo analiza específicamente los riesgos operacionales y ambientales derivados de la aquatermólisis como mecanismo químico subyacente. El primer frente de riesgo corresponde a la generación de sulfuro de hidrógeno (H_2S) durante la transformación térmica de compuestos azufrados presentes en las fracciones pesadas del petróleo [3]. La producción de este gas está estrechamente relacionada con las condiciones de temperatura y presión del proceso [3]. Asimismo, el incremento de la severidad térmica favorece una mayor generación de H_2S bajo condiciones de vapor sobrecalentado [4]. Debido a su elevada toxicidad y a su carácter corrosivo, este compuesto constituye uno de los principales riesgos asociados a las operaciones de recuperación térmica [3]. El segundo frente de riesgo está asociado a los efectos de los gases ácidos sobre la integridad de los sistemas de producción. La presencia de H_2S puede acelerar mecanismos de corrosión en tuberías, pozos e instalaciones superficiales [3]. Adicionalmente, la evolución química inducida por la aquatermólisis puede generar condiciones operacionales menos favorables para la gestión de los procesos térmicos [2]. Estas circunstancias obligan a incorporar estrategias específicas de monitoreo y control durante la operación de proyectos EOR.

La expansión de las tecnologías térmicas plantea desafíos crecientes para la gestión ambiental y operacional de los campos petroleros [5]. En el contexto de la Faja Petrolífera del Orinoco, la planificación coordinada de las operaciones constituye un elemento relevante para mitigar riesgos y optimizar el aprovechamiento de los recursos disponibles [6]. Entre las medidas preventivas recomendadas destacan el monitoreo continuo de H_2S mediante sistemas automáticos de detección, la selección de materiales resistentes a ambientes corrosivos, la optimización del ratio vapor-petróleo (Steam Oil Ratio, SOR) para limitar la severidad térmica y la incorporación de sistemas de captura y tratamiento de gases ácidos. Estas acciones son fundamentales para avanzar hacia una explotación más segura y ambientalmente responsable de los recursos de la FPO.

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Más allá del pozo: desafíos conjuntos para una gestión integrada en la explotación de la Faja Petrolífera del Orinoco bajo un esquema de recuperación térmica

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La Faja Petrolífera del Orinoco (FPO) concentra uno de los mayores volúmenes de crudo pesado y extrapesado del mundo. Su explotación mediante técnicas de Recuperación Mejorada de Hidrocarburos (Enhanced Oil Recovery, EOR) de base térmica, como el Drenaje Gravitacional Asistido por Vapor (Steam Assisted Gravity Drainage, SAGD), depende de la generación masiva de vapor para reducir la viscosidad del crudo mediante procesos de aquatermólisis [2]. Este proceso puede generar simultáneamente emisiones atmosféricas y corrientes líquidas residuales que comparten un mismo origen operacional y que, sin embargo, suelen evaluarse de forma independiente. La producción de vapor requerida por las tecnologías EOR térmicas constituye una fuente relevante de emisiones de gases de efecto invernadero asociadas al consumo energético del proceso [4]. Además, la aquatermólisis favorece la generación de sulfuro de hidrógeno (H_2S) durante la transformación térmica de compuestos organoazufrados presentes en el crudo [1]. La presencia de este gas representa un desafío adicional para la gestión ambiental y la seguridad operacional debido a su toxicidad y carácter corrosivo [1].

La recuperación térmica también demanda volúmenes de agua significativamente superiores a los requeridos en esquemas de producción convencionales [4]. Como consecuencia, se generan corrientes de agua producida que pueden contener gases disueltos, sales y restos de hidrocarburos derivados del proceso de extracción. La gestión inadecuada de estas corrientes puede incrementar el riesgo de afectación de recursos hídricos a través de problemas de integridad en los pozos o deficiencias en los sistemas de disposición y control ambiental [3]. En el caso de la FPO, la gestión fragmentada de los bloques de explotación plantea retos adicionales para el seguimiento integrado de los impactos ambientales asociados a la recuperación térmica [6]. Asimismo, los compromisos globales de mitigación climática ponen de manifiesto la necesidad de mejorar el control de emisiones derivadas de actividades energéticas intensivas en carbono [5].

Este trabajo propone una revisión integrada de los riesgos asociados al agua y al aire en la FPO, identificando puntos de control comunes relacionados con la gestión del vapor, la integridad de pozos y el tratamiento de aguas de producción. Como resultado esperado, se plantea el desarrollo de indicadores socioambientales integrados y de un marco de monitoreo regional que contribuya a una gestión más coordinada de los impactos asociados a la explotación térmica de crudos pesados.

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BIOQUÍMICA Y BIOTECNOLOGÍA

Spray Incorporating Peptide- and Peptidomimetic-Based Ionic Liquid Conjugates for Topical Applications

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The topical treatment of infected and complicated wounds remains a major clinical challenge, with current approaches often failing to provide both patient comfort during application and effective antimicrobial activity without contributing to the growing problem of bacterial resistance. In this context, there is a pressing need for innovative topical therapies that combine efficacy, safety, and ease of application. [1]

Peptides and peptidomimetics have emerged as promising platforms for the development of such therapies, owing to their structural versatility and broad spectrum of biological activities. Our research focuses on the design, synthesis, and biological evaluation of peptide-based compounds and their peptidomimetic derivatives, with particular emphasis on their potential for the treatment of skin infections and impaired wound healing. [2,3]

The aim of this work is to develop an innovative topical spray formulation for wound management that combines antimicrobial and wound-healing properties. By integrating these complementary activities into a single therapeutic approach, the formulation is intended to provide an effective, safe, and patient-friendly alternative for the treatment of chronic wounds, while potentially reducing the pressure for antimicrobial resistance.

The peptide/peptidomimetic-based compounds displayed promising antimicrobial activity, and the resulting spray formulations retained antimicrobial efficacy. In particular, the developed formulation showed activity against *Staphylococcus aureus*, demonstrating that the polymer-based spray system can effectively deliver peptide-based antimicrobial agents. These findings support the potential of this approach as a versatile topical delivery platform and provide a promising basis for the development of innovative treatments for chronic wounds.

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Lipophilic and phenolic profiling of *Galactites tomentosus*: insights into an underexplored thistle

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Thistle refers to a type of wild, herbaceous, thorny plant, primarily belonging to the Apiaceae, Dipsacaceae, and Asteraceae families. It is commonly found on agricultural land, pastures, fallow land, and waste land, for example in the Beira Baixa area of Portugal. Since these plants have no use in agriculture or for feeding animals, they are regarded as unwanted weeds by local farmers and have to be removed, which brings about extra costs. *Galactites tomenosus* is one of such plants. It is therefore important to look into alternative methods of giving these plants value and to help with the region's development.

For hundreds of years different species of thistle have been employed in traditional medicine for the treatment of a variety of diseases since they have anti-inflammatory, antibacterial, antipyretic, cytotoxic, and antidiabetic properties. The properties in question are most commonly used when the thistle is prepared by means of infusion, decoction, or boiling [1]. Research has investigated the bioactive properties of various thistle species and has given promising results [2].

The phytochemical profile and any associated bioactivities of *Galactites tomentosus* have never been investigated. The present study is concerned with promoting underexplored thistles, with a special focus on *Galactites tomentosus*, by means of a phytochemical analysis and the identification of bioactive compounds. To achieve this, the plants were harvested and their various parts (flower, leaf, stem, and root) were separated, dried and then macerated. Extracts were prepared from each of the parts using both hexane and ethanol and these were analysed by GC-MS and HPLC-DAD-MS, respectively. The lipophilic composition showed the presence of compounds such as lupeol and its derivatives in the flower, stem and leaf, one of which was a lupeol derivative that was predominant in the flower and occurred at a quantity of 128 µg/mg extract. The results regarding the polyphenolic composition show that compounds such as apigenin, luteolin and kaempferol derivatives are present.

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Subcritical Water Extraction for the Sustainable Valorization of Mediterranean Brown Seaweeds and the Recovery of High-Value Compounds

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Brown algae represent a valuable renewable resource with considerable potential for the development of high-value, nutrient-rich food products. Their incorporation into food formulations offers opportunities to modify existing products by removing, reducing, increasing, adding, or replacing specific ingredients and additives, potentially enhancing their nutritional value and health-promoting properties (Cofrades et al., 2017). Furthermore, algae are a promising source of natural antioxidant and antibacterial compounds that may serve as nutraceutical ingredients, contributing to improved food quality and safety (Polat et al., 2021).

The present study aims to investigate the potential of the Mediterranean brown seaweeds *Sargassum vulgare* and *Padina pavonica* as sources of bioactive compounds and value-added bioproducts. Subcritical water extraction was employed as a sustainable extraction technology to recover antioxidant-rich extracts, proteins, carbohydrate fractions, and alginates.

The brown seaweeds *S. vulgare* and *P. pavonica*, harvested from the Tunisian coast, were subjected to subcritical water extraction under non-isothermal conditions over a temperature range of 120–220 °C, using a liquid-to-solid ratio (LSR) of 30:1. Calcium alginates were subsequently precipitated from the resulting liquid extracts by adding $CaCl_2$ (1%). The recovered calcium alginates were characterized in terms of molecular weight distribution and rheological properties to assess their structural and functional characteristics. The remaining alginate-depleted extracts were further analyzed to determine their total phenolic, sulfate, and protein contents, as well as their antioxidant capacity, in order to evaluate the potential of the seaweeds as sources of bioactive compounds and value-added products.

The results highlight the potential of *S. vulgare* and *P. pavonica* as promising sources of bioactive compounds. Subcritical water extraction offers a sustainable approach to recovering antioxidant-rich extracts and valuable polysaccharide fractions, including alginates with potential functional applications. Overall, this study supports the valorization of Mediterranean brown seaweeds as renewable marine resources for the development of high-value products and the advancement of sustainable biorefinery strategies.

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Effect of Subcritical Water Extraction Temperature on the Chemical Composition and Structural Characteristics of Fractions from the Green Seaweed *Chaetomorpha linum*

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Marine macroalgae have attracted increasing scientific interest as sources of bioactive compounds [1]. Among green seaweeds, *Chaetomorpha linum* is a promising source of polysaccharides with potential biological activities [2]. Subcritical water extraction (SWE) offers an environmentally friendly approach to recovering these compounds by exploiting the properties of water under subcritical conditions. In particular, extraction temperature is a critical parameter influencing extraction efficiency and the chemical characteristics of the recovered fractions [3, 4].

This study investigated the influence of SWE temperature on the extraction yield and chemical composition of solid and liquid fractions obtained from *C. linum*. Prior to extraction, the raw biomass was characterized in terms of its mineral, lipid, sulfate, and carbohydrate contents. SWE was subsequently performed at temperatures ranging from 120 to 220 °C.

The resulting fractions were characterized to determine extraction yields and monosaccharide composition. Following acid hydrolysis, the monosaccharide profiles were analyzed by high-performance liquid chromatography (HPLC) and compared with those of the raw biomass to evaluate changes in carbohydrate composition induced by the extraction process. The liquid fractions were further analyzed for total phenolic content, antioxidant capacity, protein content, and sulfate content. In addition, the molecular size distribution of polysaccharides in the solid fractions was investigated using high-performance size-exclusion chromatography (HPSEC).

Overall, this work provides insights into the influence of extraction temperature on the recovery and structural characteristics of compounds from *C. linum.* The chemical characterization of the resulting fractions supports further investigation of this green seaweed as a potential source of bioactive ingredients.

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Chemical Interactions at the Oral Interface: Nanoscale Mapping of Astringency in Cell-Based Models

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Astringency is a complex oral tactile sensation, commonly described as tightening, puckering, or roughness, that influences the sensory acceptance of plant-based foods [1]. Although traditionally associated with the precipitation of salivary proteins by astringent molecules, its molecular basis also involves interactions at the saliva-mucin-epithelium interface and changes in interfacial lubrication [2]. Differences in chemical composition and molecular interactions at the oral cavity may therefore contribute to distinct perceptual subqualities, ranging from puckering to velvety sensations [3,4].

This study investigated how chemically distinct astringents interact with model oral surfaces and modify their nanoscale properties. Previous research has demonstrated that these compounds can induce significant biophysical alterations in epithelial membranes, specifically affecting hydration, lipid packing, and membrane tension [5]. The selected stimuli comprised black tea extract (BTE, a flavanol (catechin)-rich polyphenolic mixture associated with puckering), alum (an aluminium salt associated with aggressive dryness), and quercetin galactoside (QGal, a glycosylated flavonol associated with velvety smoothness). Their contrasting chemical characteristics provide a basis for comparing compound-surface adsorption and the resulting interfacial effects. Two human oral cell lines, HSC-3 (tongue squamous cell carcinoma) and TR146 (buccal mucosa), were studied in cell-only systems and in models incorporating mucosal pellicle and human saliva to assess the influence of the oral biochemical environment.

Adsorption assays were combined with atomic force microscopy (AFM) to relate compound retention at the oral interface to changes in surface topography, friction, and nanoscale mechanical behaviour. Adsorption was compound-dependent and modulated by the saliva, indicating that interfacial affinity cannot be considered independently of the surrounding molecular environment. AFM measurements showed that QGal and alum significantly modified the measured surface properties of epithelial cells, whereas BTE-induced changes were most evident in the mucosal pellicle- and saliva-containing model. These contrasting responses suggest that the chemical nature of the astringent and the composition of the oral interface jointly govern the observed nanoscale effects.

Salivary proteins and molecular signatures associated with these interfacial changes were identified by liquid chromatography-tandem mass spectrometry (LC–MS/MS) analyses. By integrating adsorption measurements, AFM-derived surface properties, and chemically defined oral-interface models, this approach advances the investigation of compound-interface relationships underlying astringency and may inform the rational design of plant-based food formulations toward desirable astringent subqualities.

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Chemical diversity of astringents shapes mechanosensitive Ca^{2+} signalling in a human Merkel cell-based model

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Astringency is a dry, puckering oral tactile sensation elicited by chemically diverse substances, notably polyphenolic tannins and aluminium salts such as alum [1]. Their molecular properties and interactions with oral constituents are central to understanding astringency. Although salivary protein-polyphenol complexation and precipitation are established mechanisms [2], they do not fully explain how astringent chemicals generate a tactile response. Psychophysical evidence implicates trigeminal rather than gustatory innervation [3], suggesting that astringent-induced physicochemical changes at the oral epithelial interface activate mechanotransduction pathways. However, candidate polymodal channels, including TRPV2 and TRPC5, are inhibited rather than activated by tannic acid [4].

Merkel cells are oral touch-sensing cells that employ Piezo-dependent mechanotransduction [5]. To investigate whether chemically distinct astringents elicit different cellular responses, we established a human Merkel cell-derived *in vitro* assay and quantified intracellular Ca^{2+} dynamics using the fluorescent probe Fluo-4 and a high-throughput fluorescence-image plate reader (FLIPR) platform. We compared tannic acid, an astringent polyphenol mixture with multiple potential interaction compounds, with alum, an astringent aluminium salt, and included caffeine as a bitter, non-astringent control.

The cells displayed mechanosensitive Ca^{2+} signalling: fluid shear stress induced Ca^{2+} transients attenuated by extracellular Ca^{2+} chelation with EGTA and by the mechanosensitive-channel inhibitor GsMTx4 [6]. The Piezo1 agonist Yoda1 also produced an EGTA-sensitive Ca^{2+} influx [7]. Chemical exposure revealed distinct dose–response profiles: tannic acid and alum elicited concentration-dependent Ca^{2+} responses, with apparent EC_{50} values of 2.7 and 631 µM, respectively, whereas caffeine was inactive under the tested conditions.

The two astringents exhibited different pharmacological response patterns, consistent with different modes of physicochemical perturbation at the cell interface. At lower concentrations, tannic acid-induced signalling depended on extracellular Ca^{2+} and was sensitive to GsMTx4; at higher concentrations, the response was no longer significantly reduced by EGTA, suggesting a recruitment of intracellular Ca^{2+} stores. In contrast, alum produced a steep, threshold-like concentration–response relationship, with marked GsMTx4 sensitivity but limited inhibition by EGTA alone. Combined EGTA and GsMTx4 treatment produced the greatest reduction for both compounds. For the first time, we gather observations that support a mechanism in astringency in which chemically dependent interactions at the membrane interface couple to mechanosensitive Ca^{2+} signalling and intracellular Ca^{2+} mobilisation.

Overall, the results reveal compound-dependent relationships between astringent chemistry, concentration–response behaviour and cellular Ca^{2+} signalling. By distinguishing polyphenol- and aluminium salt-induced activation profiles, this assay provides a chemical–biological framework for investigating the mechanisms of astringency and for future structure–activity studies in more complex three-dimensional oral mucosa models.

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From Galloylation to Oral Retention: Chemical Drivers of Interindividual Variability in Black Tea Astringency

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How the molecular structures of black tea (BT) phenolic compound (PC) govern their partitioning between saliva and oral surfaces remains a key chemical question in astringency research. Although astringency has traditionally been attributed to PC-induced precipitation of salivary proteins (SPs), this mechanism alone cannot explain pronounced interindividual differences in perceived intensity [1].

BT provides a chemically diverse system for examining structure-dependent interactions. During tea oxidation, flavan-3-ols such as (–)-epigallocatechin gallate (EGCG) and (–)-epicatechin gallate (ECG) undergo oxidative transformations that generate, among other products, theaflavins such as theaflavin-3,3′-digallate (TFdG) and theasinensins such as theasinensin A (TSA). Differences in galloylation, molecular size and phenolic hydroxyl-group distribution influence the potential for hydrogen bonding and hydrophobic association with proline-rich proteins (PRPs), mucins and glycoproteins at the oral mucosal interface [2,3]. This provides a molecular basis for investigating selective PC retention beyond bulk protein precipitation.

To relate BT PC chemistry to oral retention and perception, adsorption of individual PC onto the tongue epithelium was quantified *in vivo* by HPLC in 16 volunteers and examined alongside sensory responses, SP precipitation, salivary physiology, and mucin transcript and protein measurements. These results were compared with established *in vitro* oral models based on tongue HSC-3 and buccal TR146 cells, with or without a mucosal pellicle [4,5]. Across the models, EGCG, ECG, TFdG and TSA predominated in the adsorbed PC fraction, whereas non-galloylated epicatechin and epigallocatechin contributed less. The mucosal pellicle increased total PC retention 4- to 13-fold (e.g., HSC-3: 11 to 45 µg/mL). TFdG was the only individual compound to reach its reported sensory detection threshold [6], suggesting that the perceptual astringency response cannot be assigned solely to one adsorbed PC. PRPs were the predominant proteins in the precipitated proteins.

Among the studied variables, the variables associated with perceived intensity changed with BT concentration: at lowest concentration, mucin proteins were the key driver; at intermediate concentrations, salivary flow and SP precipitation were the most important variables; and, at highest concentration the key variable was epithelial PC adsorption. This concentration dependence is consistent with a changing balance between protein–PC association in saliva and retention at the mucosal interface; pellicle saturation remains a mechanistic hypothesis to be tested.

These findings identify selective adsorption and concentration-dependent oral partitioning of structurally distinct tea PC as complementary chemical determinants of astringency. Linking PC composition with salivary and mucosal interfacial chemistry may support targeted modulation of BT mouthfeel and the formulation of plant-based products.

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Purification of antileukemic biopharmaceuticals using carbon xerogels

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L-asparaginase (ASNase) is an enzyme of vital importance for the treatment of acute lymphoblastic leukaemia and for food processing [1,2]. However, the complex and expensive nature of the ASNase purification process is the limiting factor in making life-saving treatments affordable and accessible to anyone [3]. To address this bottleneck, researchers need to develop newer ASNase purification processes that are cheaper, simpler, and capable of meeting purity requirements [4]. This work aimed to develop and evaluate a new ASNase purification method based on carbon xerogels (CXs). Accordingly, CXs with mesopore diameters of 6.7, 11.7 and 24.0 nm were synthesised and used in batch purification to evaluate purification performance and the effect of textural properties. The purification factor (PF) was determined as the ratio of the specific activity of ASNase after and before purification. CX regeneration strategies based on pH, ionic strength, surfactants, and temperature were evaluated. Afterwards, the best-performing CX was evaluated for implementation in a semi-continuous ASNase process using a packed-bed adsorption column with a bed height of 5 cm. All results were confirmed by sodium dodecyl sulphate polyacrylamide gel electrophoresis. Purification performance of CXs increases with both mesopore size and pore volume, with the CX with the largest average mesopore diameter (24.0 nm) achieving the highest purification performance (PF=3.0). This correlation may be explained by the combined effect of two factors. First, greater accessible surface area results in increased protein adsorption capacity. Second, differences in size between the impurities and ASNase influence their diffusion through the porous network, with smaller impurities diffusing more rapidly than the larger ASNase. As a result, impurities are adsorbed faster and to a greater extent than ASNase. Among all regeneration methods, only thermal treatment at 350 °C under N_2 yielded a regenerated adsorbent capable of purifying ASNase in a consecutive purification cycle (PF = 2.2). In semi-continuous operation, ASNase was purified by the packed column for at least 3 h, reaching a maximum PF of 17.5 during the initial minutes and approximately 2.0 for the remainder of the operation. After the regeneration of the packed CXs, the column purified ASNase for 3 h, reaching a maximum PF of 8.2 and a mean PF of 1.8. Overall, our findings demonstrate the potential of CXs in purifying ASNase laying the foundations for the development of a simple and cost-effective ASNase purification process.

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Valorization of coffee silverskin as a functional food ingredient: *in vitro* assessment of its anti-metabolic syndrome potential

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Coffee consumption has been associated with protective effects against metabolic syndrome (MetS), a cluster of metabolic disorders that includes hyperglycemia, dyslipidemia, obesity, and chronic low-grade inflammation [1]. These effects seem to be related to its richness in chlorogenic acids (CGA) and caffeine, which are known for their antidiabetic, anti-inflammatory, and anti-lipogenic effects [1,2]. Similarly, coffee silverskin (CS), the major by-product of coffee roasting industries, is a source of these bioactive compounds, so it has great potential to be valorized as a functional food ingredient, even though it is still underexploited and mainly discarded, representing an environmental concern [2]. Therefore, this study aimed to investigate the anti-MetS potential of a CS extract *in vitro*, having in view its valorization. The CS sample consisted of a blend of Arabica and Robusta CS, representative of the main by-product generated by Portuguese coffee roasting industries. A CS extract (CSE) was prepared by aqueous ultrasound-assisted extraction and freeze-dried. The extract was chemically characterized by RP-HPLC-DAD regarding caffeine and CGA content, and its effects were tested in three cell lines: intestinal epithelial cells (Caco-2), hepatocytes (HepG2) and adipocytes (3T3-L1). The uptake of radiolabelled glucose (^{3}H-D-glucose, ^{3}H-DG) and fructose (^{14}C-fructose, ^{14}C-FRU) was assessed by liquid scintillation counting [2]. The expression levels of key genes involved in sugar and lipid metabolism (*GLUT2*, *GLUT5*, *SGLT1*, *ACC*, *FAS*, *SREBP-1c*, and *ChREBP*) were evaluated by RT-qPCR. Anti-inflammatory effects were assessed by quantifying NO and NAG levels with spectrophotometric assays [4]. CSE presented 39 mg/g of caffeine and ~12 mg/g of CGA, mainly 5-CQA (~8 mg/g). In Caco-2 cells, CSE significantly reduced ^{3}H-DG and ^{14}C-FRU uptake, as well as the gene expression of GLUT2, GLUT5, and SGLT1. In HepG2 cells, CSE significantly decreased the expression of *FAS* and *ChREBP*. CSE also significantly decreased NO levels in HepG2 cells but not NAG levels. In Caco-2 cells, however, it significantly increased both NO and NAG levels. No effects on ^{3}H-DG uptake or on NO and NAG levels were observed in 3T3-L1 cells. The reduction of intestinal sugar uptake and the downregulation of intestinal sugar transporters suggest an antidiabetic potential. The downregulation of FAS, a key enzyme in *de novo* lipogenesis, and of ChREBP, a transcription factor that regulates both lipid and sugar metabolism, suggests an anti-lipogenic potential and a possible additional contribution to an antidiabetic potential at the hepatic level. However, the inflammatory effects of CSE depended on the cell line, being anti-inflammatory in HepG2 cells and pro-inflammatory in Caco-2 cells. Overall, CSE showed promising anti-MetS potential *in vitro*. Thus, these results support the valorization of coffee silverskin as a sustainable functional food ingredient, although further *in vivo* studies and clinical trials should be performed.

Acknowledgments

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Functional biomembranes based on polysaccharides and polyphenols to improve oral mucositis

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Oral mucositis is a frequent and debilitating complication of chemotherapy and radiotherapy, particularly in patients receiving treatment for head and neck cancers. This condition can cause severe pain, difficulty eating or drinking, increased susceptibility to infections, and a marked reduction in patients' quality of life [1]. This study aimed to develop and evaluate functional biomembranes based on polysaccharides and plant-derived polyphenols for a potential application in oral mucositis treatment.

Biomembranes based on pectin, carboxymethylcellulose, and pullulan were developed, with tannic acid and Pea Butterfly flower Extract (PBE) selected for incorporation. Cytocompatibility and wound closure were evaluated using the HSC-3 and TR146 oral cell lines. The resulting biomembranes were characterized regarding their thickness, appearance, colour properties, mechanical properties, and disintegration time behaviour in human saliva.

The selected polysaccharides successfully formed biomembranes, with the results varying according to the polymer matrix. Pullulan, carboxymethylcellulose, and pectin showed favourable cytocompatibility both alone and following the incorporation of tannic acid at 1% (w/w, relative to polymer mass) or PBE at concentrations ranging from 10-50% (w/w). In the wound healing assay, pullulan demonstrated the best results, reducing the wound closure time in HSC-3 cells compared with the control. However, the incorporation of tannic acid markedly increased the wound closure time in both cell lines; 10% PBE did not significantly affect the wound closure, and 50% PBE also increased the wound closure to some extent, depending on the polymeric matrix and cell line.

The resulting biomembranes exhibited thicknesses varying from 9-17 µm and different mechanical behaviours in terms of tensile strength, resistance to extension and elongation at break. Their disintegration behaviour also varied depending on the polymer matrix and the protein concentration of the saliva used.

In summary, polysaccharide-based biomembranes incorporating two classes of polyphenols were successfully developed and evaluated *in vitro*. Further characterization of the biomembranes, including studies of compound release, anti-inflammatory and antioxidant activities, mucoadhesion and interactions with the oral mucosal environment, will be important to further establish the potential of these biomaterials for oral mucositis management.

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Optimization of propolis extraction from Montesinho Natural Park towards sustainable cosmetic ingredients

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Propolis is a bee-produced resinous substance, known for its antioxidant, healing, anti-inflammatory, and antimicrobial properties, making it a promising natural source of functional ingredients [1]. However, extraction conditions strongly influence the recovery and concentration of its bioactive constituents. This study aimed to optimize maceration conditions for the recovery of bioactive compounds from propolis sourced from Montesinho Natural Park (Portugal) and to evaluate the potential of the most promising extracts as a natural dermo-cosmetic ingredients in liquid soap formulations. To achieve this, ground propolis was characterized according to ISO 24381:2023 and macerated in ethanol 70% (v/v) (ME70) or monopropylene glycol (MMPG) at three propolis concentrations (10, 20, and 30% w/w). Extraction kinetics were monitored over 30 days by determining total phenolic content using the Folin-Ciocalteu assay, total flavonoid content using the $AlCl_3$ assay, and antioxidant activity using the $DPPH^{\bullet}$ and $ABTS^{+\bullet}$ radical scavenging assays. Raw propolis showed low ash (0.8%) and wax (7.3%) contents, indicating high quality. For both solvents, increasing propolis concentration resulted in higher phenolic and flavonoid contents and greater antioxidant activity per mL of extract. Based on kinetic profiles, 30% (w/w) propolis and 5 days of maceration were selected. Under these conditions, MMPG outperformed ME70 in total phenolic content (57.5 vs. 49.6 mg GAE/mL), total flavonoid content (23.5 vs. 18.4 mg QE/mL), and antioxidant activity (DPPH: 88.4 vs. 78.1 mg AAE/mL and ABTS: 86.1 vs. 75.4 mg AAE/mL), respectively. Both extracts revealed high inhibitory (MIC), bactericidal (MBC) and fungicidal (MFC) activities. ME70 showed slightly higher inhibitory potential against *Staphylococcus aureus, Salmonella enterica, and Candida albicans*, while MMPG exhibited stronger bactericidal activity against *Pseudomonas aeruginosa*, *S. aureus*, and *Cutibacterium acnes*, and better selectivity in non-inhibiting the skin-protective *Staphylococcus epidermidis*. Besides this, UHPLC-DAD-ESI/MS analysis revealed similar qualitative profiles for both extracts, with 44 tentatively identified compounds, predominantly flavonoids (chrysin, pinocembrin, galangin, pinobanksin) and phenolic acids (caffeic acid, *p*-coumaric acid, ferulic acid) and their methyl-esters. Following incorporation at 5% into a liquid soap formulation, the extracts contributed to maintain suitable pH (~ 6.0) and viscosity during storage, especially at 5 ºC, while also showing promising bactericidal potential against *C. albicans*, *Escherichia coli*, *S. aureus*, and *C. acnes*. Overall, optimized maceration yielded concentrated, bioactive Montesinho propolis extracts with potential as natural antiseptic ingredients for sustainable dermo-cosmetic applications.

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Molecular Dynamics Simulations of the Temperature Dependence of Early Amyloid-β42 Oligomerization

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We used molecular dynamics simulations to investigate how temperature modulates hydrophobic interactions and β-sheet formation in CHARMM36m model of a monomer, dimer and a tetramer of Aβ42 [1]. For the isolated monomer, increasing temperature leads to an increase in intramolecular contacts, promoting hydrogen-bonding and secondary-structure reorganization toward β-sheet and turn motifs. Analysis of the dimer and tetramer of Aβ42 reveals increased conformational heterogeneity at high temperatures, suggesting a smaller-than-expected configurational entropy penalty upon association. Thus, whereas monomers undergo temperature-induced compaction, enhancing intramolecular interactions, including the formation of β-sheets, in the dimer and tetramer, hydrophobic stabilization is redirected toward aggregation, promoting cross β-sheet formation, peptide elongation, and the emergence of spherical conformations. Notably, the residues that stabilize intramolecular β-sheets in the monomer (approximately sequences 16-22 and 29-36) overlap with those that form cross β-sheet motifs in the aggregates, suggesting that intramolecular β-sheet formation is intrinsically linked to aggregation propensity. These results, in close agreement with earlier NMR measurements of the monomer and protofibrils, reveal a competition between intra- and intermolecular hydrophobic interactions, with intermolecular interactions ultimately becoming more favorable than the intramolecular interactions that stabilize monomer solvation.

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CATÁLISIS Y FOTOCATÁLISIS

Integrated advanced oxidation processes for salicylic acid degradation using Graphene Oxide/ZnO/$BaSnO_3$

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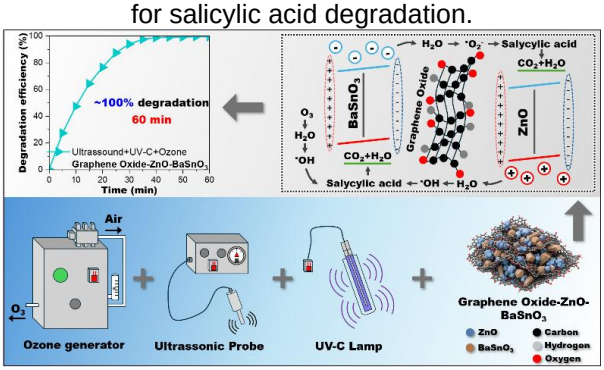
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The increasing occurrence of emerging contaminants has driven the development of more efficient and versatile treatment strategies, with advanced oxidation processes (AOPs) receiving particular attention [1]. However, the application of individual AOPs may be limited under challenging conditions, encouraging the integration of complementary processes. In this study, a multifunctional graphene oxide/ZnO/$BaSnO_3$ catalyst was developed for the combined application of heterogeneous photocatalysis, piezocatalysis, and catalytic ozonation using salicylic acid (SA) as a model emerging contaminant. The graphene oxide (GO) was synthesized by a modified Hummers method, and the composite was subsequently prepared via precipitation method. The resulting composite was characterized by powder X-ray diffraction (XRD), transmission electron microscopy (TEM), and diffuse reflectance spectroscopy (DRS), confirming the formation of the desired crystalline phases and a band gap of 3.22 eV [2, 3]. Based on its structural and optical characteristics, a GO-stabilized Z-scheme heterojunction was proposed. The individual and combined processes were subsequently evaluated to assess their synergistic effects on SA degradation. The simultaneous application of photocatalysis, piezocatalysis, and catalytic ozonation provided the highest performance, achieving complete degradation of 10 mg L^{-1} SA within 60 min. The integration of these processes therefore has the potential to increase both the degradation efficiency and operational versatility of AOP-based systems, highlighting the catalyst as a promising platform for the treatment of emerging contaminants under different operating conditions [4].

Fig.1. Schematic representation of the integration of piezocatalysis, heterogeneous photocatalysis (UV-C), and catalytic ozonation using the GO/ZnO/$BaSnO_3$ catalyst, including the proposed Z-scheme heterojunction for salicylic acid degradation.



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Tailored Cu-Doped ZnO Nanoparticles for Enhanced Photocatalytic Degradation: Optimization of Cu Doping and Immobilization on 3D Printed Scaffolds

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Clean water scarcity and wastewater contamination present urgent global health and environmental issues, directly aligning with Goal 6 of the UN 2030 Agenda for Sustainable Development. In this context, combining advanced nanotechnology with sustainable materials offers a highly promising pathway toward efficient and scalable water remediation. This work reports the systematic synthesis, structural optimization, and photocatalytic evaluation of Cu-doped ZnO nanoparticles designed for the effective degradation of organic pollutants in aqueous environments. The nanoparticles were synthesized via a controlled chemical precipitation method utilizing citric acid as a chelating and capping agent to tailor particle size and morphology. To investigate the role of copper content, various doping concentrations were incorporated into the zinc oxide matrix. [1] The insertion of copper atoms introduced intermediate energy levels within the electronic band structure of ZnO, which effectively suppressed electron-hole recombination and significantly enhanced photocatalytic efficiency under UV light irradiation. Experimental results demonstrated that the formulation with 0.1 wt.% Cu doping achieved superior catalytic performance, attaining maximum degradation of acetaminophen within 2 hours, far outperforming pristine ZnO. To overcome the practical limitations associated with nanoparticle recovery in slurry systems, 3D printed porous ceramic-like scaffolds were fabricated via direct ink writing. [2] Bio-derived amorphous silica was incorporated into the 3D printable aluminosilicate matrix to serve as an effective anchoring network for the nanoparticles. [3] The optimized Cu-doped ZnO nanoparticles were successfully immobilized onto the 3D printed scaffolds via dip-coating, creating high-surface-area catalytic structures. This study demonstrates a sustainable strategy integrating agricultural waste upcycling, additive manufacturing, and tailored nanomaterials for advanced water treatment applications.

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Bauxite residue-derived Fe_2O_3/g-C_3N_4 composites for photocatalytic degradation of emerging water pollutants

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Bauxite residue (BR) is an industrial by-product generated during alumina production, rich in metal oxides, including iron oxides, whose complex composition and alkalinity pose challenges for its recycling, proper disposal and sustainable management. Thus, the incorporation of BR into photocatalytic materials offers an opportunity to simultaneously valorize an industrial residue and develop more efficient functional materials for water remediation [1,2]. In this work, Fe_2O_3/g-C_3N_4 composites were prepared by thermal polymerization of melamine incorporating BR at mass fractions of 0.1, 0.2, and 0.3 wt.%. The photocatalytic performance of the composites was evaluated using ciprofloxacin (CIP) and acetaminophen (ACT) as emerging pollutants under both UV (365 nm) and visible (405 nm) light irradiation.

X-ray diffraction confirmed the presence of Fe_2O_3 crystalline phases in the BR-containing materials, while SEM, FTIR, UV–Visible spectroscopies, and zeta potential measurements were used to investigate their morphological, structural, optical, and surface properties. The incorporation of BR significantly enhanced the degradation of CIP and ACT compared with pristine g-C_3N_4, under both irradiation conditions evaluated. For example, for ACT incorporating only 0.1 wt.% BR (g-C_3N_4/0.1%BR) significantly increased the degradation efficiency from 55.2% (pristine g-C_3N_4) to over 96% after 2 h of UV irradiation. Under visible light, the BR-containing composite achieved a 2-fold increase in degradation efficiency relative to the pristine (Fig.1). For CIP, 99.4% of degradation was achieved in 2 h under visible light, and complete CIP removal was achieved after only 1 h under UV irradiation.

The enhanced performance demonstrates the potential of the BR-derived Fe_2O_3/g-C_3N_4 ultra-low loading composites as photocatalysts for the degradation of emerging water pollutants. Future studies will investigate their performance in real water matrices and their immobilization onto additively manufactured scaffolds for continuous-flow photocatalytic applications [3].

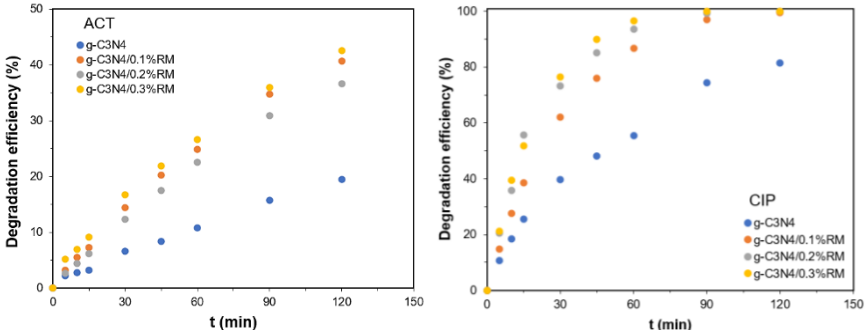


Fig. 1. Degradation efficiencies for ACT and CIP using different catalysts under visible light irradiation.

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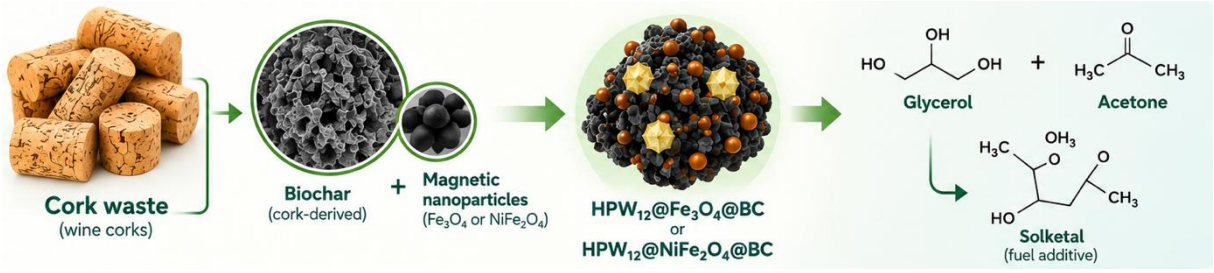
Sustainable Magnetic Biochar Catalysts for Glycerol Valorization to Solketal

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The development of sustainable and low-cost catalysts from renewable and waste-derived resources is an important challenge for advancing greener catalytic processes. In this work, heterogeneous magnetic catalysts were developed by combining pyrolyzed industrial residues (cork stoppers) as porous biochar supports with the highly active heteropoly acid (phosphotungstic acid, HPW_{12}). Magnetic functionality was introduced through the incorporation of Fe_3O_4 or $NiFe_2O_4$ nanoparticles, enabling the recovery of the catalysts after reaction. The resulting composites were characterized by FTIR-ATR, SEM-EDS, ICP-OES, BET, XRD, potentiometric titration, and magnetometry. Their catalytic performance was evaluated in the acetalization of glycerol with acetone for the production of solketal, a valuable fuel additive and an important product for the valorization of glycerol generated as a by-product of biodiesel production. The catalytic results showed that the nanoparticles strongly influenced the reaction performance. In particular, HPW_{12}@Fe_3O_4@BC composite exhibited a higher pore size than HPW_{12}@$NiFe_2O_4$@BC composite, favoring the accessibility of the active sites and leading to the best catalytic performance, with up to 87% of glycerol conversion and 97% of solketal selectivity after only 5 min at 60 °C, under a solvent-free system. The catalyst exhibited promising reusability, highlighting the potential of waste-derived magnetic biochars as low-cost and recyclable catalytic materials for glycerol valorization. This approach combines waste valorization, catalyst recovery, and the production of value-added fuel additives, contributing to the development of more sustainable processes for the biodiesel industry.

Fig.1. Schematic illustration of the conversion of waste cork into biochar-supported magnetic HPW_{12} catalysts (HPW_{12}@Fe_3O_4@BC and HPW_{12}@$NiFe_2O_4$@BC) and their application in glycerol acetalization with acetone for solketal production.



Acknowledgments

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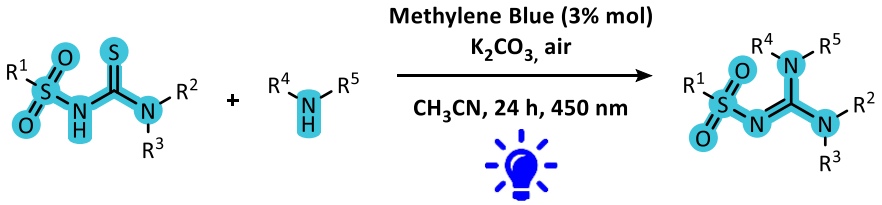
Blue Light, Blue Dye: Photocatalytic Guanylation of Sulfonylthioureas

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Developing sustainable and mild methodologies for constructing nitrogen-rich functionalities remains a central goal in modern organic synthesis. Guanidine motifs are prevalent in pharmaceuticals, agrochemicals, catalysts, superbases, superpotent sweeteners, and bioactive natural products.[1] However, their installation by traditional methods often relies on conditions with a high E-factor, generating stoichiometric amounts of byproducts (e.g., from EDC[2] or the Mukaiyama reagent[3]), or on toxic reagents such as $HgCl_2$.[4]

Herein, we report a blue-light-mediated guanylation of sulfonylthioureas enabled by methylene blue (MB), an inexpensive, commercially available organic photocatalyst. Under blue LED irradiation, the reaction proceeds under mild, metal-free conditions, providing access to sulfonylguanidines from sulfonylthioureas and readily available amines.

Using a model sulfonylthiourea and morpholine, we optimized key reaction parameters, including the photocatalyst, base, and solvent, affording the desired product in 78% yield after 24 h at room temperature. Under the optimized conditions, yields across the substrate scope, including primary and secondary amines, anilines, and different sulfonylthioureas, ranged from 9% to 91%, highlighting the method's robustness and potential as a greener alternative to classical guanylation protocols. Efforts to elucidate the reaction mechanism will also be presented.



Scheme 1. Photocatalytic synthesis of sulfonylguanidines aided by Methylene Blue.

Acknowledgements
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Microwave-assisted green synthesis of nanomaterials for photocatalysis

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Carbon quantum dots (CQDs) have been widely studied in photocatalysis, biomedicine, etc. due to their tunable optical properties, non-toxicity, low-cost synthesis, biocompatibility and strong photoluminescence [1]. Among the various synthesis routes, microwave (MW) irradiation stands out for its eco-friendly nature. Microwave synthesis can be done in less time than hydrothermal synthesis, uses non-toxic reagents, and promotes a more uniform heating of the solution [2].

In this work, we report the green synthesis of highly fluorescent CQDs from chitosan with acetic acid (AA-CQD) and glycerol with iron chloride (GFe-CQD) under MW irradiation using a conventional household oven [3]. The CQDs are characterized by UV–Vis absorption, photoluminescence spectroscopy (PL) and transmission electron microscopy (TEM), revealing blue emission and nanoscale particle sizes suitable for photocatalytic applications. Building on these results, TiO_2 nanoparticles are prepared via MW-assisted routes [4] and characterized by X-ray diffraction (XRD) and diffuse reflectance spectroscopy (DRS) to correlate crystal structure and electronic properties with photocatalytic behavior.

PL analysis of AA-CQDs and GFe-CQDs showed typical fluorescence centered at 460–465 nm (λ_{ex} = 390 nm), differing only in intensity. UV–Vis analysis showed an absorbance peak at approximately 240 nm for GFe-CQDs and 285 nm for AA-CQDs. TEM analysis revealed CQD sizes of 11.3 nm for AA-CQDs and 11.1 nm for GFe-CQDs. XRD showed that the MW-derived TiO_2, prepared from the water-stable precursor TiBALDH in an open beaker, is amorphous as synthesized and becomes phase-pure anatase after calcination (550 °C, 3 h) [5]; DRS gave an optical band gap of ~3.18 eV.

GFe-CQDs are then combined with TiO_2 by impregnation [3], and the composite is evaluated in photocatalytic hydrogen evolution (Hg–Xe lamp, 164 W, 3.5 h, methanol 11.8 % v/v as hole scavenger). The MW-derived TiO_2 produced 2.30 µmol g^{-1} h^{-1} of H_2, 1.56 times more than commercial P25 (1.47 µmol g^{-1} h^{-1}), and the TiO_2@CQD composite reached 4.05 µmol g^{-1} h^{-1}, 2.75 times the P25 value. A single household microwave oven thus yields both components of an active photocatalyst, with the chitosan-derived CQDs raising the H_2 evolution of bare TiO_2 by about 75 %.

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Effect of Support Nature on the Catalytic Performance of Cobalt-Based Fischer–Tropsch Catalysts

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The transition toward a more sustainable and low-carbon energy system has renewed interest in technologies for the production of synthetic fuels and chemicals from alternative carbon resources. Fischer–Tropsch synthesis (FTS), which converts synthesis gas into hydrocarbons, represents a versatile route for the production of high-quality fuels and valuable chemicals. Its integration with syngas obtained from renewable resources further strengthens its potential within future sustainable fuel production schemes [1,2]. Cobalt-based catalysts are particularly attractive for FTS due to their high activity, high selectivity toward long-chain hydrocarbons, and relatively low water–gas shift activity [2,3]. However, their catalytic performance is strongly dependent on catalyst formulation, particularly on the properties of the support. Beyond providing surface area for the dispersion of cobalt nanoparticles, the support can influence reducibility, metal–support interactions, mass transport, and catalyst stability, ultimately affecting FTS performance and product selectivity [2-4]. Therefore, understanding the relationship between support properties and catalytic performance is essential for the rational design of efficient cobalt-based FTS catalysts.

In this work, cobalt catalysts supported on materials with markedly different properties, including modifeid carbon nanotubes (CNTs), Si-modified alumina-based supports, and zeolite, were investigated under Fischer–Tropsch synthesis conditions. Their catalytic performance was evaluated in terms of cobalt-normalized CO conversion (CTY) and selectivity toward CH_4, C_2–C_4, and C_{5+} hydrocarbons. The chain-growth probability (α) was also determined to evaluate the influence of the support on hydrocarbon chain propagation. The results reveal a pronounced effect of the support on both catalytic activity and product distribution. Oxide-supported catalysts generally exhibited higher cobalt-normalized activity, reaching a CTY of 6.4 10^{-5}·mol_{Co}^{-1}·s^{-1}, while CNT-supported catalysts showed a strong dependence on surface treatment. Selected CNT catalysts favored heavier hydrocarbons, reaching 96.7% C_{5+} selectivity and α values up to 0.82, while suppressing methane formation. These results highlight the key role of support selection and modification in tuning the balance between cobalt-specific activity and hydrocarbon chain growth in FTS.

Acknowledgements

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Electrochemical synthesis of ligand-free transition-metal clusters for sustainable redox catalysis

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Atomically precise metal clusters exhibit size-dependent electronic structures and reactivity that make them promising catalysts for challenging chemical transformations[1]. Building on previous experience in the electrochemical synthesis of Ag and Cu clusters[2][3], this work explores the extension of this approach towards ligand-free transition-metal systems based on earth-abundant elements.

Electrochemically generated Fe and Ni species have been investigated as catalytic systems for complementary redox transformations. The Fe system promotes the oxidation of ascorbic acid, whereas Ni species catalyse the reduction of 4-nitrophenol in the presence of a reducing agent. Spectroscopic and elemental characterization was used to investigate the species generated under different electrochemical conditions and to establish relationships between their physicochemical properties and catalytic behaviour.

The results demonstrate that electrochemical synthesis provides a simple aqueous route to generate catalytically active transition-metal clusters without the use of conventional molecular ligands or stabilizing agents. The complementary redox activity observed for Fe and Ni highlights the potential of this strategy for developing low-cost catalysts based on earth-abundant metals.

This work establishes a new research direction focused on the electrochemical generation of ligand-free transition-metal clusters and their application in sustainable catalysis, with future perspectives towards environmental relevant remediation and catalytic hydrogen production.

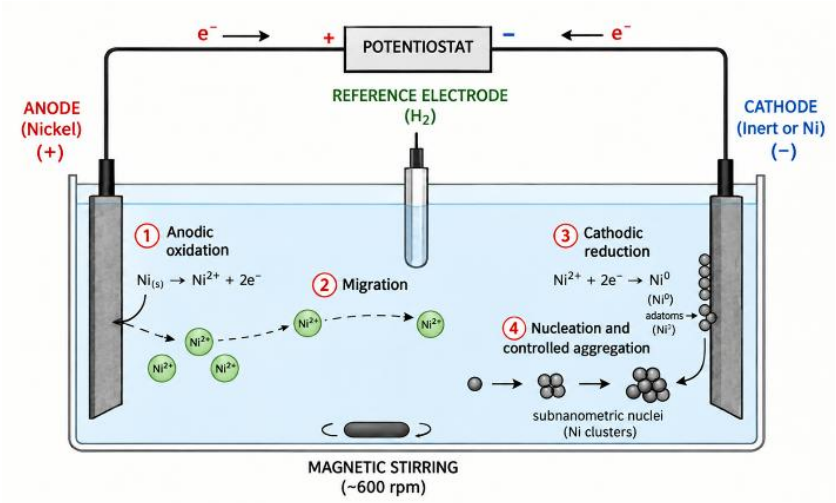


Fig.1. Schematic illustration of the electrochemical synthesis of nickel nanoclusters in aqueous solution in the absence of stabilizing agents

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Estabilidade e reutilização aprimoradas de fotocatalisadores à base de Ag_3PO_4 por meio de um compósito magnético Fe_3O_4/HDL/Ag_3PO_4/AgBr

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A presença de fármacos em ambientes aquáticos representa um desafio para o tratamento de águas residuárias, impulsionando o desenvolvimento de tecnologias avançadas de remediação [1]. Nesse contexto, a fotocatálise heterogênea apresenta potencial para a degradação de contaminantes orgânicos, embora a aplicação do Ag_3PO_4 seja limitada pela fotocorrosão e pela perda de atividade durante a reutilização [1]. Assim, este trabalho teve como objetivo desenvolver um compósito fotocatalítico magnético constituído por Fe_3O_4, hidróxido duplo lamelar (HDL), Ag_3PO_4 e AgBr, visando melhorar sua estabilidade operacional e facilitar sua recuperação [2].

As análises de difração de raios X (DRX) confirmaram a presença das fases constituintes do compósito, enquanto a caracterização textural revelou área superficial específica de 175,75 m^2g^{-1}, sugerindo maior capacidade de adsorção e disponibilidade de sítios ativos. As imagens de microscopia eletrônica de varredura (MEV) evidenciaram morfologia granular e aglomerada. As medidas fotoeletroquímicas indicaram densidade de fotocorrente de aproximadamente 6–7 μA cm^{-2}, sugerindo favorecimento da separação e do transporte de cargas. Adicionalmente, o menor diâmetro de semicírculo no diagrama de Nyquist indicou menor resistência à transferência de cargas em comparação com os precursores. O band gap de 1,75 eV, o menor entre os materiais caracterizados, sugere menor energia necessária para a excitação eletrônica. A fotoluminescência indicou baixa recombinação radiativa dos portadores de carga, enquanto os resultados de espectroscopia de fotoelétrons excitados por raios X (XPS) foram compatíveis com os estados químicos esperados. A ressonância paramagnética eletrônica (EPR) indicou a formação de radicais hidroxila (•OH) e superóxido (O_2•$^-$) sob irradiação, espécies potencialmente envolvidas na degradação do contaminante.

A atividade fotocatalítica foi avaliada utilizando-se 50 mg de catalisador em 50 mL de solução aquosa de acetaminofeno (ACT) a 5 mg L^{-1}, sob irradiação UV–Vis, com monitoramento por cromatografia líquida de alta eficiência (HPLC). O Ag_3PO_4 puro apresentou 63% de remoção de ACT, com constante cinética aparente de 0,017 min^{-1}, enquanto o compósito Fe_3O_4/HDL/ Ag_3PO_4/AgBr alcançou remoção semelhante (63%), com constante de 0,012 min^{-1}. O sistema Ag_3PO_4/AgBr apresentou aproximadamente 51% de remoção. Embora o compósito quaternário tenha apresentado menor velocidade cinética que o Ag_3PO_4 puro, sua maior estabilidade ao longo de quatro ciclos consecutivos de reutilização evidencia uma vantagem operacional relevante. Além disso, sua recuperação magnética com o auxílio de um ímã simplifica a separação do catalisador da solução tratada. Dessa forma, a integração das quatro fases constitui uma estratégia promissora para desenvolver fotocatalisadores que conciliem eficiência de remoção, estabilidade operacional e facilidade de recuperação no tratamento de águas contaminadas por fármacos.

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A Multimodal Machine Learning Framework for Photocatalyst Design in Hydrogen Production

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Driven by the global energy transition, hydrogen (H_2) is a promising energy carrier due to its high energy density and zero-carbon combustion [1]. Photocatalytic water splitting is an attractive production route, enabling solar-to-H_2 conversion [2]. However, photocatalyst design for H_2 evolution is hindered by complex structure-property relationships, sparse datasets and a lack of models jointly handling multimodal inputs and physically coupled targets [3,4]. To bridge this gap, this work presents a multimodal foundation model for photocatalyst screening integrating four pretrained encoders, i.e. MatSciBERT, mat2vec, CHGNet and Magpie with matminer, via cross-attention and FiLM fusion.

Training follows a two-stage strategy. In the first stage, a joint multi-head phase trains simultaneously on band gap (E_g), band edges: E_C (Conduction Band Minimum) and E_V (Valence Band Maximum), Fermi energy (E_F), gap-type classification and application-level targets across 30 982 Materials Project entries and 606 curated H_2 evolution rate labels (R_{H_2}). In the second stage, a deployment specialisation fine-tunes this backbone towards R_{H_2} prediction while retaining bulk-electronic auxiliary heads. Secondary application targets, dielectric constant (ε_∞) and CO_2 photoreduction rate (R_{CO_2}), are included to assess embedding generalisability. Domain informed prediction heads embed known semiconductor physics through learned softmax gates, a band-structure consistency regularisation term enforces physical validity and temperature scaled Monte Carlo-dropout provides calibrated uncertainty estimates [5].

Joint training achieves R_{H_2} R^2 = 0.817, rising to R^2 = 0.860 after deployment specialisation. Band-structure predictions are strong across E_C (R^2 = 0.907), E_V (R^2 = 0.924) and E_F (R^2 = 0.823). Also, they remain self-consistent with 0.098 eV. Gap-type classification achieves an accuracy of 0.767 (direct-gap F1 = 0.538), improvable to F1 = 0.562 via class weighted retraining. Temperature scaling corrects the systematically underestimated intervals, achieving approximately 98 % empirical coverage on the H_2 test set. This is slightly above the 95 % target, reflecting a conservative bias that is expected given the small test size. Secondary targets confirm representation transferability, with ε_∞ R^2 = 0.911 and R_{CO_2} R^2 = 0.974 upon specialisation. The final model is a unified screening tool with physically self-consistent, multi-target and uncertainty-quantifies predictions to accelerate photocatalytic H_2 materials discovery.

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3D-Printed Photocatalytic Immobilised Systems for Green Hydrogen Production

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This work presents a novel approach to photocatalytic hydrogen (H_2) production by combining photocatalyst immobilisation with Additive Manufacturing (AM), addressing key limitations associated with conventional suspended photocatalytic systems [1].

Two photocatalysts, TiO_2 and thermally exfoliated g-C_3N_4 (GCN-T), both coupled with a Pt co-catalyst, were synthesised and immobilised onto complex 3D-printed structures designed to maximise the irradiated surface area [1,2].

A hybrid immobilisation strategy, combining 3D printing with subsequent dip coating, provided the best photocatalytic performance. Among the tested structural configurations (FLEX, STAR, MONO), the FLEX structure achieved the highest H_2 production due to its enhanced light exposure.

Comparative studies using methanol, glycerol, and glucose as sacrificial reagents showed similar H_2 generation for Pt/TiO_2 across all three. At the same time, Pt/GCN-T exhibited a clear trend: methanol > glycerol > glucose, attributed to the complexity of the sacrificial molecules.

Overall, the results demonstrate the potential of AM for the rational design and fabrication of high-performance immobilised photocatalytic systems, providing a promising and scalable strategy for sustainable H_2 production.

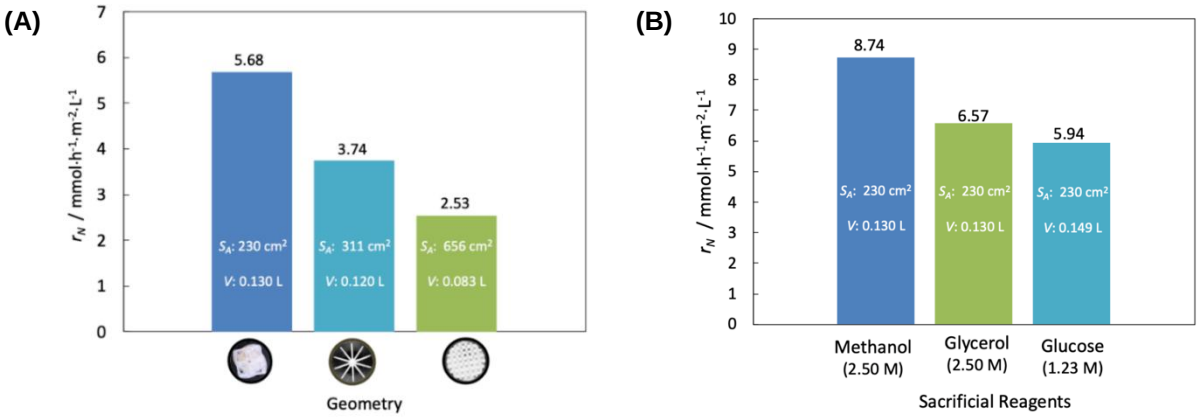


Fig.1. (A) Normalised hydrogen production rate (*rN*) using: FLEX- i–Pt/TiO2–1.0, STAR-i-Pt/TiO2 –1.0 and MONO-i-Pt/TiO2–1.0; The experiments were conducted using a methanol aqueous solution (2.50 M), under irradiation of the UV- LED system. (B) Normalised hydrogen production rates (*rN*) using the FLEX-i–Pt/GCN-T–1.0 structure and different sacrificial reagents. Inside each bar there is the reaction volume (*V*) and the structure's surface area (SA). The experiments were conducted under irradiation of the Vis-LED system.

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Enhancing Photocatalytic Hydrogen Evolution through RuO_2-modified Graphitic Carbon Nitride

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The sustainability of hydrogen (H_2) depends entirely on how it is produced. Green H_2 remains costly and technologically challenging, motivating the search for more efficient, low-cost production pathways, such as photocatalytic H_2 evolution. Graphitic carbon nitride (g-C_3N_4) is a metal-free photocatalyst with high stability and low cost. Still, its activity is often limited by high charge-carrier recombination rates and a low specific surface area [1]. To improve its activity, heat treatments and the use of cocatalysts are often employed to enhance the surface area and the charge-carrier dynamics, respectively [2]. Thus, in this work, both approaches were studied by synthesising two series of binary photocatalysts combining ruthenium oxide (RuO_2) with bulk g-C_3N_4 (gCN) or thermally exfoliated g-C_3N_4 (gCNT).

g-C_3N_4 was synthesised by thermal polymerisation of dicyandiamide in a muffle furnace. The resulting bulk material was subsequently thermally exfoliated. Binary RuO_2/gCN and RuO_2/gCNT photocatalysts with different RuO_2 loadings (0.2–5.0 wt. %) were prepared by wet impregnation. For this purpose, gCN or gCNT was added to an aqueous dispersion of $RuCl_3$ at 70 °C until partial solvent evaporation. After washing and drying, the materials were calcined at 400 °C. All synthesised materials were extensively characterised using several techniques. Photocatalytic experiments were performed using an LED system with a fixed excitation wavelength of 370 nm for 2 h under an N_2 atmosphere, with a catalyst load of 0.5 g L^{-1} and triethanolamine (0.2 M) as the electron donor. H_2 production was monitored by online gas chromatography.

Regarding the optical properties of the materials, the incorporation of RuO_2 led to a slight increase in the catalysts' light absorption, which is highly desirable in photocatalysis, and a substantial decrease in photoluminescence, suggesting suppressed charge-carrier recombination. The surface area of the gCNT catalysts was, as expected, significantly higher than that of the gCN materials, confirming the separation of g-C_3N_4 layers upon thermal treatment. Overall, the gCNT catalysts outperformed the bulk ones in H_2 production, likely due to the increase in the number of available active sites and improved mass-transfer mobility at the catalyst surface. The 0.5 wt.% RuO_2/gCNT photocatalyst showed the best performance among the synthesised materials, achieving an H_2 production rate of 5063 μmol g_{cat}^{-1} h^{-1}, while no H_2 was detected using neat RuO_2, pristine bulk and exfoliated g-C_3N_4. These results confirm the cocatalytic role of RuO_2, which enhances charge separation and provides active sites for proton reduction, thereby boosting H_2 production under mild conditions and contributing to the design of more efficient photocatalytic systems.

Acknowledgements

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Visible-light-driven photocatalytic ammonia-to-hydrogen process using g-C_3N_4-based materials

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Ammonia (NH_3) is considered a potential hydrogen (H_2) carrier, given its advantageous properties, including high H_2 content (17.8%), thermodynamically favourable decomposition and established infrastructure [1]. Developing a visible-light-driven photocatalytic pathway could enable the cracking of NH_3 under mild conditions, in contrast to conventional methods that rely on high-temperature thermocatalysis. Graphitic carbon nitride (g-C_3N_4) is a well-researched, visible-light-active photocatalyst with tunable properties, suitable for driving the reaction. This research investigates the potential of exfoliated g-C_3N_4 (GCN-T) loaded with metal particles (M/GCN-T, M = Au, Pd, Ru) for the photocatalytic cracking of NH_3 to H_2. All photocatalysts were prepared by the incipient wetness impregnation method, in which a solution containing a metal precursor was added dropwise to GCN-T under sonication. The photocatalytic activity was evaluated using a glass batch reactor and a four-LED system with a peak emission of 420 nm. An ammonium hydroxide solution (NH_4OH, 0.5 M NH_3) served as the source of NH_3. Pd/GCN-T showed the highest H_2 generation of 0.8 mmol/g_{cat} after 6 h of irradiation, at a catalyst loading of 1 g/L. The same material also exhibited the highest NH_3 conversion of 36%, followed by Ru/GCN-T and Au/GCN-T. The superior activity of Pd/GCN-T seems to be related to the predominant presence of metal single atoms, which maximise metal atom utilisation and enhance electronic properties [2]. Electrochemical analysis showed that Pd/GCN-T had the lowest electrochemical impedance among the tested materials, indicating lower charge-transfer resistance. It exhibited the highest current at both the reduction and oxidation potentials. Time-resolved photoluminescence decay analysis showed that Pd/GCN-T exhibited the strongest lifetime shortening, suggesting improved charge separation and efficient charge transfer from GCN-T to Pd atoms [3]. The decomposition mechanism of NH_3 is hypothesised to initiate with the formation of $\cdot NH_2$ radicals through the oxidation of NH_3 by photogenerated holes in the valence band. The detection of hydrazine (N_2H_4) supports this hypothesis, as N_2H_4 may result from the self-coupling of $\cdot NH_2$ radicals. Further oxidation of N_2H_4 by photogenerated holes may lead to the formation of N_2. Finally, H^+ species are reduced to H_2 by photogenerated electrons in the conduction band [4].

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ENSEÑANZA DE LA QUÍMICA

La necesidad de matematizar conceptos de química

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Este trabajo aborda la dificultad de enseñar contenidos químicos cuando los estudiantes carecen de una base matemática consolidada [1]. Para solucionarlo, instrumentamos la matematización del pH mediante un taller interdisciplinar basado en el aprendizaje situado [2, 3] y la teoría socioepistemológica *Aprender Matemática*. Esta metodología transita por tres etapas para construir el conocimiento: intuitiva (contextual), operacional e institucionalización del contenido.

La propuesta, iniciada en instituciones educativas de Argentina, se adaptó a la Formación Profesional en la Xunta de Galicia (España) con alumnos de entre 17 y 19 años, atendiendo a su currículo [6], conocimientos previos y emociones [4]. La experiencia combinó dos encuentros de laboratorio en el IES Xunqueira 1, tareas asincrónicas y una defensa virtual, utilizando Padlet [5] y Canva para deconstruir el error y trabajar colaborativamente.

Habitualmente, el estudio del pH (equilibrio, teorías ácido-base, constantes) se limita a la química, generando un aprendizaje memorístico o meramente técnico respecto a los cálculos. Frente a esto, nuestra propuesta articuló:

1. Etapa intuitiva: Clasificación cuali-cuantitativa del pH de elementos cotidianos (agua de mar local, limón, café,gaseosa, producto de limpieza) con tiras reactivas.
2. Matematización: Aplicación de aritmética, álgebra (intervalos reales, ecuaciones, logaritmos, notación científica) y estadística (variables y valor mediano).

La interacción digital y el enfoque situado desperto un gran interés. El alumnado logró una comprensión significativa y diseñó infografías de alta calidad sobre el pH en Galicia con un sólido sustento químico-matemático. El éxito de la experiencia demuestra el valor del trabajo colaborativo, el aprendizaje situado [2] y las metodologías STEM [7], por lo que proponemos replicar esta estrategia de trabajo interárea en otras unidades curriculares.

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From Spectra to Exoplanets: Introducing Astrochemistry in Primary Education

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Astrochemistry is currently undergoing a particularly exciting period, driven by major advances in spectroscopy and by facilities such as the James Webb Space Telescope (JWST), which are revealing the chemical composition of interstellar environments, planetary systems and exoplanet atmospheres. Future missions such as ESA's Ariel will further expand this field by systematically characterising the atmospheres of a large and diverse population of exoplanets. These developments provide an opportunity to bring contemporary chemistry and astronomy into the classroom from an early age.

This communication presents the development and implementation of an educational programme introducing astrochemistry in primary education. The programme was initially piloted and refined during the 2025/26 school year with several primary school classes visiting the Planetário do Porto – Centro Ciência Viva, and is now being further implemented at the Agrupamento de Escolas de Vilela, Portugal.

The programme uses light and spectroscopy as the central link between chemistry and astronomy, progressing from familiar observations of colour and light to the interpretation of spectra and the identification of chemical elements and molecules in astronomical objects.

Through practical and inquiry-based activities, pupils explore why stars have different colours, how light can be decomposed into a spectrum, how different chemical elements produce characteristic spectral signatures, and how scientists use these signatures to investigate the Sun, stars and, ultimately, the atmospheres of exoplanets. Contemporary missions such as JWST and Ariel are used to connect simple classroom experiments with current frontiers in scientific research.

The communication will describe the educational design, the activities developed, the experience gained during the initial pilot phase, and the ongoing implementation during the 2026/27 school year. It will discuss the potential of astrochemistry as an interdisciplinary context for introducing concepts from chemistry, physics and astronomy, while promoting curiosity, scientific inquiry and STEM engagement among young learners.

Keywords: Astrochemistry; Spectroscopy; Primary Education; STEM Education; Exoplanets; Science Education

Análisis curricular y enfoque CTSA en las pruebas de la Olimpiada Gallega de Química: potencial para el Flipped Learning y la IA

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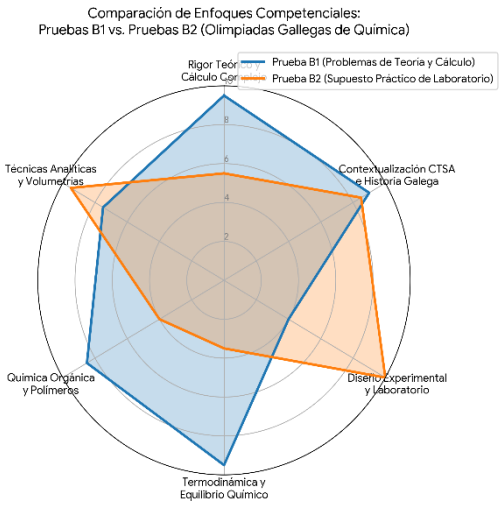
Introducción y objetivos. La preparación de las Olimpiadas de Química se basa, sobre todo, en la resolución repetitiva de problemas. Hay poca investigación sobre metodologías activas en contextos de alta exigencia. Este trabajo, primera fase de una investigación más amplia, reúne evidencias para diseñar un programa de preparación basado en *Flipped Learning* e inteligencia artificial (IA). Se analiza el rendimiento histórico del alumnado y el contenido de las pruebas, y se contrasta con la literatura.

Metodología. Se realizó un análisis documental de las pruebas de las Olimpiadas Gallegas de Química (2013-2026), categorizando cada enunciado según el currículo de 2.º de Bachillerato en Galicia[1], los ejes temáticos de la Química, el enfoque CTSA (Ciencia, Tecnología, Sociedad y Ambiente) y las competencias evaluadas. Los resultados se contrastaron con la revisión de la literatura.

Resultados. La **prueba A** (2013-2026) cubre los contenidos esenciales de la Química de Bachillerato, alineados con los currículos oficiales: estequiometría, estructura atómica y periodicidad, enlace y fuerzas intermoleculares, y reactividad y equilibrio. Evalúan la destreza de cálculo, la comprensión conceptual y el razonamiento crítico.

La **prueba B1** combina rigor técnico con ajuste al currículo gallego. Mediante contextos interdisciplinares (historia, industria, patrimonio, dilemas medioambientales), integran estructura atómica, termodinámica, equilibrios, electroquímica y química orgánica, y exigen transferir conocimientos a situaciones nuevas.

La **prueba B2**, centrada en supuestos prácticos de laboratorio, es coherente con las anteriores, evalúan el diseño de montajes, la preparación de disoluciones, la seguridad y el tratamiento de datos.



Las pruebas B1 y B2 integran además de forma transversal el enfoque CTSA (economía circular, vertidos industriales, acidificación oceánica, calidad del agua, bulos toxicológicos), fomentando la concienciación ambiental[2] y una ciudadanía crítica.

Conclusión. Las pruebas de las Olimpiadas Gallegas de Química van más allá del cálculo algorítmico: combinan cobertura curricular, razonamiento conceptual, competencia experimental y enfoque CTSA. Esta riqueza contrasta con una preparación basada en la repetición de problemas y justifica el diseño de un programa con *Flipped Learning* e IA que desarrolle esas competencias, a validar en las siguientes fases de la investigación.

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QUÍMICA INDUSTRIAL E INGENIERÍA QUÍMICA

Engineering trade-offs in biosurfactant recovery from a corn-derived stream: A comparative pilot-scale study of diffusion dialysis vs electrodialysis

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Transitioning toward a circular bioeconomy requires sustainable downstream technologies capable of efficiently recovering high-value compounds from complex agro-industrial side streams. Corn steep water (CSW), an abundant by-product of corn wet milling, contains significant concentrations of naturally synthesized biosurfactants (BS) and organic metabolites. Within the framework of the EMCOBIOS project, this study presents a pilot-scale (TRL 5) comparative assessment of two distinct membrane separation technologies operated in closed-loop mode for BS valorisation from CSW: diffusion dialysis (DD) and electrodialysis (ED).

Although both technologies rely on selective membrane transport, they exhibit fundamental differences in mass transfer driving forces, resulting in distinct purification efficiencies, operational kinetics, and final product characteristics. DD [1], employing regenerated cellulose membranes (6-8 kDa cut-off) under a concentration gradient, achieved a BS recovery yield of 60 g/kg CSW after 72-hour period. The passive separation mechanism proved selective retaining high-molecular-weight ionic fractions (m/z 950 and 1156) to produce an extract with excellent physicochemical properties, including a critical micelle concentration (CMC) of 0.14 g/L and a contact angle of 10.7° on glass, indicating superior surface activity and wetting performance. In contrast, ED employed an electric-field-driven transport across ion-exchange membranes to intensify mass transfer, reducing the purification time by nearly 90% down to 8 hours. Although the ED-recovered BS exhibited slightly lower surface activity (CMC 0.18 g/L and contact angle 14.2°), ED system enabled multi-product biorefinery integration by simultaneously co-recovering high-value secondary products, specifically lactic acid and potassium hydroxide [2]. Furthermore, synthetic ion-exchange membranes in ED displayed superior resistance to microbial fouling compared to the biodegradable cellulose membranes employed in DD.

Overall, these findings establish clear criteria for technology selection based on industrial goals: DD maximises surfactant quality and purity for high-end applications, whereas ED optimises throughput, robustness, and multi-product valorisation. This work offers a validated framework for decision-making in sustainable biorefineries upgrading renewable, corn-derived streams.

Acknowledgments

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Methane/Hydrogen Separation Using a Hierarchically Structured 3D-Printed Porous Carbon Monolith

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Efficient CH_4/H_2 separation is key to producing high-purity H_2 from steam methane reforming (SMR), which accounts for most of the global hydrogen production [1], and to recovering H_2 from natural gas grids blended with hydrogen [2]. Pressure swing adsorption (PSA) is a leading route, but it demands adsorbents that combine high CH_4 uptake with negligible H_2 adsorption [3]. Structured adsorbents such as 3D-printed carbon monoliths offer open channels that lower pressure drop and enhance mass transfer relative to pellets.

Here, a hierarchically structured 3D-printed carbon monolith, synthesized by stereolithographic [4], is assessed for CH_4/H_2 separation through fixed-bed breakthrough experiments under conditions relevant to PSA (303–343 K and up to 3000 kP). H_2 behaved as an essentially non-adsorbing species, whereas CH_4 was strongly adsorbed, reaching 7.4 mol·kg^{-1} at 3000 kPa and 303 K. Binary CH_4/H_2 breakthrough experiments (25:75, 50:50 and 90:10 vol.%) were carried out at 303 K and 100 and 3000 kPa (Fig.1 shows the 50:50 case), together with ten consecutive adsorption/desorption cycles. The corresponding working capacities were 3.0, 4.1 and 5.4 mol·kg^{-1}. The CH_4 equilibrium data was satisfactorily modelled by the Dual-Site Langmuir model, with the fitted parameters implemented in Aspen Adsorption to simulate the breakthough curves. A pressure-dependent linear driving force (LDF) model was used, giving rise to a k_{LDF,CH_4} value of 0.24 s^{-1} at 100 kPa. These results show that structured 3D-printed carbon monoliths are effective adsorbents for CH_4/H_2 separation, combining selective CH_4 capture with negligible H_2 uptake.

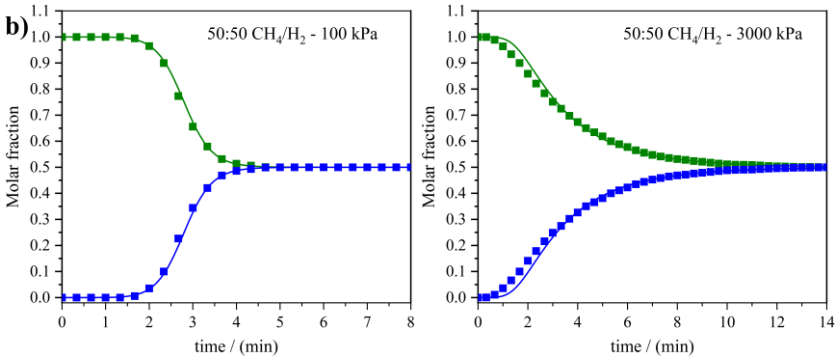


Fig.1. CH_4/H_2 binary breakthrough curves on the 3D-printed carbon monolith at 303 K for a 50:50 vol.%. Left: 100 kPa; right: 3000 kPa. Symbols represent experimental data and continuous lines represent numerical simulations.

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Phenolic-rich purified extracts from *Paulownia tomentosa* fruits: formulation of starch films for potential health applications

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Paulownia is a tree genus native to southeastern Asia, where it has been cultivated for decorative, cultural, and medicinal purposes for over 2000 years. This species possesses a variety of bioactive compounds in various plant structures, including phenolic acids, lignans, terpenoids and flavonoids in various plant structures. Verbascoside is a phenilpropanoid compound present in this species significantly studied for its beneficial properties. Plants with high concentrations of this molecule have been used in medicine for anti-inflammation and anti-microbial therapy [1].

This study focuses on *Paulownia tomentosa* fruits purified extracts obtained via mechanical pressing and autohydrolysis after a microwave hydrodiffusion and gravity and ultrasonic bath extraction treatment using non ionic polymeric resins. These extracts as well as commercial phenolic additives known to be present on these fruits (verbascoside, diplacol [2]) were used to formulate starch films. No sequential biorefinery approach has been reported for *P. tomentosa* fruits, an underexplored plant part, and no studies comparing complex fractions with isolated phenolics from were found in film literature.

Pressed juice and autohydrolysis phenolic purified fractions used for film formulation presented Total Phenolic Compound values of 42.41 g GAE/g dry extract and 37.8 g GAE/g dry extract, and Trolox Equivalent Antioxidant Capacity of 75.58 g TEAC/g dry extract and 92.13 g TEAC/g dry extract, respectively. Mainly verbascoside and phenyl propanoid glycosides were identified in the pressed juice fraction, and chlorogenic acid in the autohydrolysis fraction. The addition of the autohydrolysis fraction to starch films increases storage module and stabilizes both moduli, likely because of the presence of phenolic acids [3] supporting its potential use in protective coatings requiring improved structural integrity. Verbascoside reduces the storage module value; whereas pressed juice desorption fraction produces a stronger plasticizing effect, likely because of the combined action of this molecule and sugars and oligosaccharides, being more suitable for coatings or release matrices than verbascoside alone. Higher concentrations of pressed juice contributed to matrix structuring, leading to a decrease in the glycerol addition. Hydroalcoholic films (10% EtOH) were formulated in order to effectively disperse diplacol. Both moduli were decreased by approximately a hundred fold due to ethanol addition. Overall, *P. tomentosa* fractions demonstrated dual functionality: enhancing mechanical strength or promoting flexibility, depending on the fraction and formulation, therefore suitable for various health related applications.

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Barrier Performance of Natural Rubber Aqueous Dispersion Coatings for Paperboard

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Natural rubber aqueous dispersions offer a renewable route for producing functional paperboard coatings and reducing dependence on petroleum derived barriers. This work evaluated how rosin resin and zinc oxide (ZnO) influenced resistance to water, grease and water vapour in paperboard coated with natural rubber aqueous dispersions.

Four dispersions containing 0 or 30 parts per hundred rubber (phr) rosin and 0 or 7.25 phr ZnO were prepared and identified as R0_Zn0, R0_Zn7.25, R30_Zn0 and R30_Zn7.25. The dispersions were applied to paperboard at a dry coat weight of approximately 6.5 $g \cdot m^{-2}$. Liquid water absorptiveness was determined using the $Cobb_{1800}$ method, grease resistance was evaluated with coloured extra virgin olive oil evaluating the penetration to the other side of the paper and water vapour transmission rate (WVTR) was measured using a gravimetric cup method.

The uncoated paperboard showed a $Cobb_{1800}$ value of approximately 90 $g \cdot m^{-2}$. The ZnO free coatings produced only a limited reduction, with values close to 80 $g \cdot m^{-2}$. By contrast, ZnO reduced $Cobb_{1800}$ to 38 $g \cdot m^{-2}$ without rosin and 27 $g \cdot m^{-2}$ with rosin. R30_Zn7.25 therefore reduced liquid water absorption by approximately 70% regarding to the uncoated substrate. These results identify ZnO as the main component responsible for improving liquid water resistance, with the greatest reduction obtained when ZnO and rosin were combined. Similar improvements after ZnO incorporation have been reported for coated kraft paper [1].

Grease penetration occurred after approximately 1 h in the uncoated paperboard. No penetration was observed during the first 8 h for R0_Zn0, R0_Zn7.25 or R30_Zn0, while R30_Zn7.25 showed no visible penetration throughout the 24 h evaluation period. Thus, every natural rubber coating improved grease resistance, but the combined incorporation of rosin and ZnO provided the highest performance. Previous studies have likewise shown that complementary components can improve the grease resistance of natural rubber coatings [2].

All coated samples also reduced water vapour transmission. WVTR decreased from approximately 77 $g \cdot m^{-2} \cdot day^{-1}$ for the uncoated paperboard to 38–45 $g \cdot m^{-2} \cdot day^{-1}$ after coating, corresponding to reductions of approximately 42–51%. No significant differences were observed among the four formulations according to Tukey's test ($p > 0.05$). Therefore, the formation of the natural rubber coating layer was more relevant than rosin or ZnO content for reducing water vapour transmission, in agreement with previous natural rubber coatings reported for paper substrates [3].

Overall, natural rubber aqueous dispersions formed coatings that improved the three barrier properties evaluated. ZnO was essential for increasing resistance to water, whereas the combination of ZnO and rosin provided the highest grease resistance. R30_Zn7.25 showed the most favourable overall balance, combining the lowest $Cobb_{1800}$ value, no grease penetration during 24 h and a WVTR comparable to the other coated formulations.

Acknowledgements
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BIOCO$_2$PRO: engineering feedstocks for flexible biogenic CO_2 and syngas production

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Residual biomass is increasingly recognized as a promising renewable energy resource, encompassing wastes from forestry, agriculture, industry, and municipal activities. Among thermochemical conversion technologies, gasification offers a versatile pathway for the energy valorization of biomass and the sustainable utilization of biogenic carbon [1]. However, its efficient operation depends strongly on the physicochemical and thermochemical characteristics of the feedstock.

In Portugal, extensive forest resources and mandatory forest management and fire-prevention activities generate significant quantities of forest residues, which often lack viable valorization pathways [2]. In addition, refuse-derived fuel (RDF) and sewage sludge represent potentially relevant secondary feedstocks, although their application in gasification is constrained by factors such as high ash content, moisture, inorganic matter, and heterogeneous composition. Co-gasification with residual forest biomass therefore represents a promising approach to enhance their valorization while addressing waste-management challenges. Accordingly, selected forestry and municipal residues were investigated as potential feedstocks for gasification.

The feedstocks were characterized to determine their physicochemical and thermochemical properties and to assess their suitability for gasification. Among the materials evaluated, residual pine biomass (*Pinus pinaster*) exhibited the most favorable characteristics for use as the primary feedstock. Based on ash and moisture contents, an initial sludge incorporation of 5 wt.% is recommended, combined with 95 wt.% residual forest biomass. For RDF, its more favorable energy-related properties support an initial incorporation of approximately 10 wt.%, providing a suitable basis for evaluating its valorization potential under representative gasification conditions.

Overall, the results demonstrate the potential of co-gasification to valorize heterogeneous residual streams while supporting the sustainable management of forest and municipal wastes. These findings provide an important basis for the first phase of BIOCO$_2$PRO (Figure 1), which aims to reduce emissions and waste through the integrated valorization of biogenic CO_2 and recovered lithium from Li_2CO_3 production, while simultaneously enabling green H_2 production.

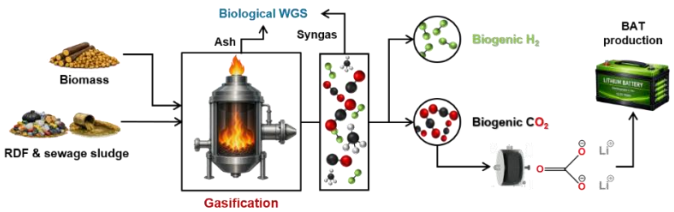


Figure 1: Flowchart of BIOCO$_2$PRO project

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Experimental Determination and Machine Learning Modeling of Amino Acid Solubility in Aqueous Electrolyte Solutions

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The solubility of compounds such as amino acids in aqueous solutions is of great value and interest to fields including chemical engineering, biochemistry, separation processes, and the pharmaceutical industry. The presence of electrolytes promotes significant changes in the solubility behavior of these compounds, generating phenomena described as salting-in and salting-out effects [1]. These variations depend intrinsically on the nature and characteristics of the amino acid, the type of ion present (monovalent or divalent), the salt concentration, the type of solvent, and the specific solute-ions-solvent interactions.

This work reports experimental solubility measurements of glycine and L-isoleucine in aqueous solutions containing the electrolytes KCl, NaCl, KBr, NaBr, $C_7H_5NaO_3$, and Na_2CO_3 at 298.15 K, covering a wide range of concentrations. The experimental data were also used to develop computational models based on Gaussian Processes (GP), integrated with the COSMO software as a continuum solvent model, aiming to analyze, predict, and validate the thermodynamic behavior of these systems.

The profiles obtained demonstrated a distinct response of the salting-in and salting-out mechanisms for each amino acid. This behavioral divergence highlighted the direct impact of polarity, functional group specificity, and electrolyte-induced pH changes in the medium.

GP modelling was used both to predict solubility and to critically assess experimental data through comparison with literature values, helping to identify potential discrepancies [2]. The values predicted by the computational model and the measurements obtained in the laboratory showed excellent agreement, confirming the robustness and accuracy of both approaches. Combining solid–liquid equilibrium measurements with machine learning provide a useful framework for predicting amino acid solubility and investigating ion-specific effects in aqueous solutions.

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Acidogenic Fermentation of Lipid Industry Wastes as a Sustainable Valorization Strategy

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Lipid industry waste has increased significantly, with spent frying oil (SFO) and the wastewater generated during the cleaning of SFO transport tanks (TTWW) standing out due to their difficult treatment, requiring effective valorization strategies [1]. This study aims to explore the possibility of using SFO and TTWW as substrates for acidogenic fermentation (AF) to produce short-chain organic acids (SCOAs). SFO was composed of 97.9% triacylglycerides, mainly esterified oleic (49.1%), linoleic (26.6%) and linolenic (14.5%) acids, with a chemical oxygen demand (COD) of 1032.14 g COD/L. TTWW exhibited a carbohydrate content of 67%, with glucose as the main constituent, and a COD of 90.04 g COD/L. Four wastewater treatment plant (WWTP) sludges were tested as inocula, two aerobic (AES and AESER) and two anaerobic (ANS and ANSER), with varying food-to-microorganism (F/M) ratios of 1:1, 1:2, 2:1 and 3:1 g COD/g Volatile Suspended Solids (VSS) and assays with pH control at 5.5 and 10.5 used ANS as inoculum, at a F/M ratio of 1:2. Assays using TTWW as substrate leading the highest acidification degrees and SCOAs mixtures of acetic, propionic, butyric and valeric acids, while SFO-based assays mainly produced acetic and propionic acids, while pH-controlled experiments broadened the SCOAs spectrum without significantly increasing yields. A continuous stirred tank reactor (CSTR) operating with TTWW revealed a production of mainly propionic and acetic acids, highlighting shifts in metabolic patterns under continuous larger volumes operation. The progressive increase of feeding ratio led to biomass growth and SCOAs production increase, with butyric acid also being obtained for a F/M ratio of 4:1. This work demonstrates the feasibility of converting SFO and TTWW into valuable SCOA-rich streams, highlighting their potential integration into sustainable bioprocesses.

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Beyond Conventional Re-Refining: Supercritical CO_2 for the Recovery of Challenging Waste Lubricating Oil Streams

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The increasing thermal, oxidative and tribological demands of modern engines have driven the development of more sophisticated lubricant formulations, incorporating synthetic base stocks and advanced additive packages. Among these, ester-containing components introduce functional groups that may undergo saponification under alkaline treatment conditions [1], compromising conventional re-refining operations. This change in chemical composition gives place to segregarion of specific waste lubricant oil streams that are difficult to process using its established regeneration technology.

This work explores supercritical carbon dioxide ($scCO_2$) as a chemically mild and tunable solvent for the selective recovery of valuable oil fractions from complex multisource waste lubricating oils (WLOs), including streams presenting limitations for conventional regeneration. Unlike chemically reactive treatment routes, $scCO_2$ extraction relies on pressure-dependent solvent properties to promote physical separation while minimizing undesirable chemical transformations.

Experimental investigations were conducted using a high-pressure extraction system to evaluate the influence of operating conditions and feedstock characteristics on extraction performance and oil recovery. Particular attention was given to the relationship between feedstock heterogeneity, solvent selectivity and the recovery of valuable oil fractions, with a view to extending regeneration opportunities to chemically challenging waste streams. Regeneration yields achieved 60 to 80%, depending on feedstock characteristics and operating conditions [2]. The recovered fractions were characterized through physicochemical and compositional analyses, demonstrating quality parameters and compositional profiles approaching those of commercial base oils.

By addressing an emerging industrial challenge associated with the evolving chemical composition of lubricants, this study investigates the potential of $scCO_2$ extraction to expand the range of WLOs suitable for circular recovery. The proposed approach contributes to the development of selective and resource-efficient separation strategies, supporting the transition towards more adaptable and sustainable lubricant regeneration processes.

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NANOQUÍMICA Y NANOTECNOLOGÍA

Quantum Heterojunctions Enabling Textile All-in-One Photo-Supercapacitors

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Wearable electronics and smart textiles still rely on rigid, compact energy storage devices that must be recharged by an external power source. Integrating energy conversion and storage directly into textiles would increase the autonomy of electronic devices in applications ranging from outdoor equipment, such as backpacks and tents, (Figure 1) to defense and workwear.[1]

This work focuses on the development of an all-in-one textile photo-supercapacitor (PSC) that harvests solar energy, converts it into electrochemical energy and stores it in a single device, rather than pairing a separate harvester with a storage unit. The integrated design reduces size, improves flexibility and simplifies the overall architecture.[2]
A heterojunction of carbon dots (CDs) and semiconductive nanoparticles (S-NP), and the corresponding *ex-situ* materials were synthesized by precipitation/hydrothermal scalable methods. CDs were chosen due to their high biocompability, strong photoluminescence, tunable electronic levels and abundant surface functional groups, while S-NPs provide a semiconducting interface that assists charge separation under illumination. These particles were mostly amorphous (observed by XRD), with hydrodynamic diameters of 4 ± 1 nm for the CQDs and 3 ± 1 nm for the S-NPs (determined by DLS). Additional characterization included scanning transmission electron microscopy, zeta potential measurements, UV–Vis spectroscopy and fluorescence spectroscopy.

Symmetric planar textile PSCs (7.5 cm^2 active area) were assembled using an ink of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) mixed with oxidized-carbon nanotubes coated onto textile substrates. CD, S-NPs or C@S-NP heterojunction were used as photoactive layer. Polyvinyl alcohol/H_3PO_4 as selected as the solid-gel electrolyte. A reference device without photoactive materials was also fabricated. The resulted devices were evaluated by electrochemical impedance spectroscopy, cyclic voltammetry, galvanostatic charge–discharge methods.
C@Si-based PSC showed a specific capacitance of 887.3 $mFcm^{-2}$ (at 1mV s^{-1}, vs. 735.0 mF cm^{-2} for reference device), presenting an energy density of 7.48 µW h cm^{-2} at 15.62 µW cm^{-2}. Interestingly, this photo-active textile device photogenerated 23.9 mV, equivalent to 178% improvement over non-photoactive device.

These results show that the C@Si heterojunction enhances photovoltage generation and charge storage in an all-in-one flexible device, paving the way for the next generation of self-powered wearables.



Fig.1. Schematic representation of the device assembled and possible application.

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Role of the Electrogenerated Hydrophilic Carbon in the Formation, Stability and Activity of Pd nanoparticles

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The development of stable electrocatalysts with ultralow noble-metal loading remains a major challenge for sustainable electrochemical technologies.
In a previous study, we demonstrated that electrogenerated hydrophilic carbon nanomaterial (EHC) generated in tartaric medium (EHC-tartaric) [1] could reduce Pd^{2+} ions to palladium nanoparticles (PdNPs), while simultaneously acting as a support for the resulting nanoparticles [2]. However, the electrochemical activity of the PdNPs was found to be unstable along the time. Even though, it was significantly improved in the presence of a carbon nanomaterial electrogenerated in phosphate medium, EHC-phosphate.

EHC-phosphate may act as a **support for PdNPs,** given the ability of its constituent units to form continuous films upon solvent evaporation [3]. In addition, its surface functional groups, particularly **carbonyl and hydroxyl groups,** may interact directly with the Pd surface contributing to nanoparticle stabilization. Thus, EHC-phosphate may act not only as a support but also, potentially, as a **ligand.**

To investigate the role of EHC-phosphate in the formation, stability and electrochemical activity of PdNPs, the nanoparticles were synthesized using sodium borohydride ($NaBH_4$) as a non-carbon-based reducing agent. This approach eliminates the contribution of EHC-tartaric as a reducing agent, allowing the specific influence of EHC-phosphate to be assessed. Its effect was investigated by adding the carbon nanomaterial either during PdNP formation or after nanoparticle synthesis (Pd-EHC), with the results compared to those obtained in the absence of EHC (Pd).

The resulting Pd–EHC nanocomposites were evaluated towards the **oxygen reduction reaction (ORR)** and the reduction / oxidation of hydrogen peroxide (H_2O_2). Remarkably, the nanocomposites exhibited an **"oxygen-memory" effect**, maintaining a significant reduction current under deoxygenated conditions.

Overall, these findings highlight the potential role of EHC-phosphate in controlling the formation, stabilization and electrochemical properties of Pd nanoparticles, while suggesting that its dual function as a **support and ligand** may contribute to their enhanced electrochemical performance. This approach opens new perspectives for the development of **low-cost and sustainable nanocatalysts** for advanced electrochemical applications.

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Surfactant-free colloidal syntheses of metal nanoparticles: challenges and opportunities for catalysis and beyond

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Nanomaterials present unique properties that make them extremely attractive for applications in chemical synthesis, energy conversion, water/air treatment, optics, sensing, electronics, medicine and many more. However, there is still room for improvement to address various challenges related to the **controlled synthesis** of nanoparticles (NPs) [1,2]. In this talk, we will give an overview of some research from the *Nanomaterials Engineering for Sustainable Technologies* (NEST) research group that recently moved to the University of A Coruña, Galicia, Spain.

We will first discuss and challenge the actual need for various chemicals such as additives, ligands, capping agents, surfactants, stabilizers, polymers etc., selected rather empirically to date in colloidal syntheses of metal NPs by wet chemical approaches [1]. We will show with the example of our developed ethanol-mediated [3,4] and revisited $NaBH_4$-mediated synthesis [5-7] that very simple surfactant-free syntheses can be developed at room temperature in water-based solvents for gold (Au) and silver (Ag) NPs [8]. Despite the apparent simplicity of the methods without added stabilizers, the colloids are extremely stable over time and size control is easily achieved by various strategies [3-13]. The syntheses also scale up well to 1 L of solutions at relatively concentrated solutions of metal (e.g. 0.5 mM of Au) [3,5].

We will then illustrate how those surfactant-free colloidal syntheses can serve as ideal building blocks towards more complex materials with the example of core@shell Au@Ag nanoparticles [8]. We will also show that the knowledge gained on studying alcohol-mediated synthesis in aqueous solvent can be extended to non-aqueous systems [13,14]. Finally, we will show how the synthesis methods pushed up to revisit some concepts in the stabilization of the colloids for instance regarding the effects of cations [15]. We will give a glimpse or our recent results using those syntheses for self-driving laboratories and data-driven discovery of materials [16]. All these recent results open new avenues for material design.

The surfactant-free nanoparticles are also ideal for applications where a clean surface would be needed such as in catalysis or medicine. In particular, we will illustrate how the materials obtained are relevant for energy conversion with the example of the electrocatalytic alcohol-oxidation [5,12], as well as water treatment with model reactions for water purification such as the 4-nitrophenol degradation [5,17] but also dyes degradation with the case studies of Methylene Blue or Congo Red [7].

Overall, the talk will give background on the promising features of surfactant-free colloidal syntheses of NPs and their possible use for fundamental and applied research.

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Multifunctional Smart Labels for Anti-Counterfeiting Textiles

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Counterfeiting is a growing global threat that affects multiple sectors of the economy and compromises product authenticity, competitiveness, and consumer trust [1]. Although digital passports and smart security labels (e.g. QR codes, RFID tags, holograms) are widely used to validate goods and services throughout the value chain [2], increasingly sophisticated counterfeiting networks demand more advanced technological security solutions.

This work presents a novel multifunctional coding system for textile applications, which integrates optical and electrochemical features into QR-based smart labels to enhance anti-counterfeiting protection. Functional nanomaterials with tailored optical (carbon dots) and electrochemical (carbon-based materials) features were synthesized *via* liquid-phase approaches and characterized through ultraviolet–visible, infrared, fluorescence and Raman spectroscopies, X-ray diffraction, magnetometry, scanning/transmission electron microscopies and electrochemical measurements. The materials were incorporated in functional inks and coated onto textile substrates using well-implemented industrial printing techniques. Smart sensing elements and QR-based security labels were fabricated (Figure 1) and their (multi)functional performance and security features assessed.

The security labels performance and capability were evaluated considering material type, pattern configuration and textile substrate. The generated QR codes combined conventional QR-readable information with additional security features embedded in the functional inks, and demonstrated reliable readability through standard smartphone applications. The approach resulted in the creation of a new textile security label that combined for the first time optical and electrochemical functionalities. The integration of complementary physical responses significantly enhanced coding versatility and security potential, demonstrating strong applicability for advanced anti-counterfeiting solutions.



Fig.1. QR code printed on cotton fabric using a developed functional ink.

Funding

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Smart Photoswitchable Organic-Inorganic Hybrid Nanomaterials for Light-Responsive Textile Applications

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Tungsten trioxide (WO_3) has attracted interest as a promising light-responsive nanomaterial due to the easy modulation of its size and morphology, high thermal stability and low cost. When incorporated in textiles, WO_3 has been used in wearable UV/sunlight devices, camouflaging and fashion [1]. However, its slow coloration/bleaching rates and low color variation hinder the scope of applications [2]. Looking to surpass these limitations, in this work WO_3 was hybridized with different organic and inorganic photoresponsive compounds to produce new smart nanomaterials with fast response to UV/sunlight radiation, high color reversibility, palette diversity, and phosphorescence. The hybrid WO_3-based organic-inorganic light-responsive nanomaterials were prepared by sustainable synthesis methods, including *in situ* solvothermal hybridization and mechanochemical synthesis (ball-milling), with the use of organic nitrospiro-based molecules and inorganic pigments. The resulting materials were incorporated in pastes based on two different binders, polyurethane and polyacrylate, and coated onto cotton fabrics to produce photoswitchable textiles with modulated photochromic performance. The nanomaterials were characterized in terms of morphology, structure, chemical composition and light-induced color switching properties by scanning electron microscopy, energy dispersive X-ray spectroscopy, X-ray diffraction, Fourier transform infrared spectroscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, and colorimetry.

Under UV light (λ = 365 nm) irradiation, the fabrics coated with hybrid WO_3-based nanomaterials exhibited a wider color variety, lower coloration and bleaching times in comparison to the parent nanomaterial, as well as phosphorescence. The most promising fabric (Fig. 1) reached a maximum total color difference ΔE^* = 31.9 in only 15 min, presenting green phosphorescence and an orange to blue transition when exposed to UV and sunlight. Upon exposure to water, the fabric underwent accelerated bleaching within 30 seconds. The photochromic response of these nanomaterials shedded light into the potential of organic-inorganic hybrids for wearable devices, UV light sensors and anticounterfeiting applications.

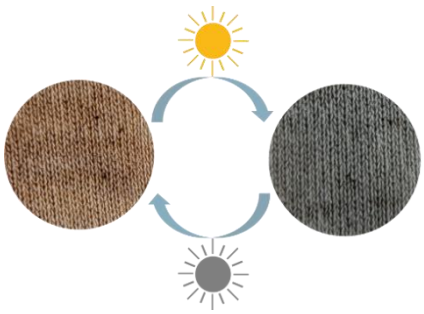


Fig.1. Cotton fabric coated with an optimized tungsten oxide hybrid dispersed in polyurethane, before and after exposure to UV light (λ = 365 nm).

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Development of Nanoformulations for Oral Administration and Treatment of Crohn's Disease

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Crohn's disease (CD) is a chronic inflammatory bowel disease for which there is currently no cure, although several pharmacological treatments are available to control inflammation and manage symptoms. Methotrexate (MTX) is an antifolate and immunomodulatory drug used in CD to suppress excessive immune responses, reduce intestinal inflammation, and induce and maintain disease remission. However, its therapeutic application is limited by poor aqueous solubility, low intestinal permeability, variable oral bioavailability, and potential systemic toxicity, including hepatotoxicity and myelosuppression. These limitations highlight the need for improved drug delivery strategies, such as lipid-based nanoformulations, to enhance oral drug delivery, improve therapeutic efficacy, and minimise adverse effects.[1] In recent years, the encapsulation of drugs in nanoformulations has emerged as a promising strategy to overcome biological barriers and improve drug delivery.[2] This work aimed to develop and characterize lipid-based nanoformulations for oral administration of MTX, with particular emphasis on solid lipid nanoparticles (SLN) and nanostructured lipid carriers (NLC), to overcome MTX-related oral delivery drawbacks and potentially improve its therapeutic efficacy. The NLC- and SLN-based nanoformulations were prepared by emulsion-solvent evaporation and double emulsion methods, respectively.[3-5] The nanoformulations were characterized in terms of key physicochemical properties, association efficiency, drug loading capacity, and their stability under storage conditions (4°C and room temperature), as well as under gastrointestinal conditions. Their interaction with mucins and MTX release profile were also investigated. In addition, preliminary *in vitro* cell viability evaluation, as well as *in vivo* survival assays using *Caenorhabditis elegans*, were performed.

The nanoformulation SLN@MTX exhibited mean particle size of approximately 157.40 nm with an association efficiency of 77.19 ± 4.61% (drug loading capacity of 1.38 ± 0.08%), while NLC showed particle size of XXX and association efficiency of 41.26 ± 8.47%. Overall, SLNs exhibited a more favorable physicochemical profile than NLC, showing higher colloidal stability under storage conditions and maintaining a comparatively homogeneous particle population under gastrointestinal conditions and in the presence of mucins. Also, SLN@MTX showed a limited drug release profile, with only approximately 10–20% of the encapsulated MTX released over 96 hours. Preliminary *in vitro* celular studies showed no significant reduction in cell viability after 4hours of exposure to SLN@MTX in Caco-2 cells, while survival rates above 88.89% were observed in *Caenorhabditis elegans*. Thus, these findings identified SLN as the most promising lipid system investigated in this work for the incorporation and oral administration of MTX. However, further optimization of drug release and additional biological studies are needed to establish its potential for the treatment of Crohn's disease.

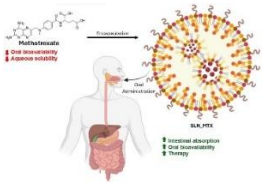


Fig.1. Schematic representation of the main goal of the work. Created with BioRender.com.

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Biomimetic Non-Lamellar Lipid Nanoparticles for Bioactive Compound Delivery

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Non-lamellar nanoparticles are lipid-based platforms that are emerging in the nanomedicine field due to their outstanding properties and versatility. Their non-lamellar nature offers them complex internal structures, resulting in high surface areas, effective drug protection, and stability. Their composition can be tailored, allowing the incorporation of components that enhance application-specificity. Additionally, biocompatible and biodegradable lipids can be used, aligning with green chemistry principles and planetary health.

The aim of this work was to produce biomimetic non-lamellar lipid nanosystems and explore their potential for the delivery of bioactive compounds across different applications, particularly cancer therapy and cosmetics.

Nanoparticles with application-specific biomimetic features were produced and optimized. The developed nanosystems were characterized in terms of physicochemical properties, including size, polydispersity, zeta potential, and encapsulation efficiency. Further structural and morphological characterization was performed by SAXS and Cryo-TEM. Stability, biocompatibility, anticancer activity, antioxidant activity, and cellular uptake were assessed, as well as permeation across appropriate biological barriers. Biological interactions were evaluated by synchrotron-based FTIR.

The biomimetic nanoplatforms exhibited suitable sizes, low polydispersity, and high compound loading. Stability was maintained for at least 6 weeks upon storage. The nanoparticles were cytocompatible in L929, HaCaT, bEnd.3, and U251 cells, while encapsulation enhanced cytotoxicity by up to 4-fold compared to the free drug in U251 cells. Additionally, high uptake by U251 cells and good permeation across an *in vitro* BBB model were observed. Their versatility was further evidenced by the preservation of the encapsulated bioactive compound's antioxidant activity, alongside good permeation across porcine skin, and induction of changes in the lipid organization of the *stratum corneum* and epidermis.

Overall, these findings suggest that the developed biomimetic non-lamellar lipid nanoparticles are promising delivery systems, emphasizing the versatility of this type of nanosystem for different biomedical applications.

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QUÍMICA DE POLÍMEROS

Desenvolvimento e caracterização de matrizes biopoliméricas para revestimentos alimentares

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Os revestimentos alimentares à base de biopolímeros naturais constituem uma alternativa de interesse para a conservação de alimentos e para a redução de embalagens plásticas [1]. Neste contexto, este trabalho teve como objetivo o estudo do desenvolvimento de formulações binárias de quitosano/alginato de sódio (QA) e quitosano/carragenina (QC) para aplicação como revestimentos alimentares.

Prepararam-se quatro formulações de QA e QC a 1%, com e sem glicerol (0,5%), utilizando a proporção 50:50 (*v*/*v*). As soluções filmogénicas foram avaliadas quanto ao comportamento reológico e à atividade antimicrobiana e utilizadas para obter filmes por evaporação do solvente, que, posteriormente, foram caracterizados por FTIR, microscopia ótica e ensaios de tração, avaliando-se ainda a permeabilidade ao vapor de água, a solubilidade em água e o grau de inchamento.

As soluções filmogénicas sem glicerol de QA apresentaram maior pseudoplasticidade que QC, com índices de escoamento (*Power Law*) de 0,42 ± 0,01 e 0,49 ± 0,02, respetivamente. Os perfis antibacterianos foram iguais, exceto frente a *Yersinia enterocolitica*, para a qual QC apresentou CMI e CMB de 1,25 mg/mL, em comparação com 2,5 mg/mL para QA. O FTIR demonstrou formação de complexos em ambas as amostras, e a microscopia revelou textura rugosa e ligeiramente fibrosa em QA e densa, com agregados, em QC. Nas propriedades mecânicas, o glicerol reduziu o alongamento na rutura de 5 ± 3% para 16 ± 3 % em QA e de 8 ± 3% para 28 ± 10% em QC, tornando os filmes mais flexíveis. Quanto à solubilidade em água, os filmes sem glicerol apresentaram valores inferiores, sendo QA (11,1 ± 0,2%) o mais baixo em relação a QC (17 ± 1%), e a adição de glicerol aumentou a solubilidade das duas misturas para 24 ± 2% em QA e 42 ± 6% em QC. Relativamente ao grau de inchamento QA sem glicerol apresentou maior absorção (1337 ± 57%) em relação a QC (141 ± 23%). Com glicerol, o inchamento diminuiu para 947 ± 56% em QA, enquanto QC manteve um valor próximo do observado sem plastificante (133 ± 43%). A permeabilidade ao vapor de água foi menor em QA ($4 \pm 1 \times 10^{-11}$ g/(m·s·Pa)) que em QC ($5{,}4 \pm 0{,}3 \times 10^{-11}$ g/(m·s·Pa)), sem glicerol. A incorporação do plastificante não aumentou este parâmetro em QA, mas elevou-o para $7 \pm 2 \times 10^{-11}$ g/(m·s·Pa) em QC.

O estudo evidenciou variabilidade em alguns parâmetros dos filmes, em função da composição e da adição de glicerol. Assim, as formulações apresentam potencial para aplicações diferenciadas, devendo ser selecionadas conforme as necessidades de cada alimento e validadas nas condições de conservação pretendidas.

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QUÍMICA ANALÍTICA

From conventional water sampling to a miniaturized solid phase extraction sampling strategy for metal ions monitoring

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Traditional monitoring of metal ions in water commonly relies on the collection and transport of large-volume samples to the laboratory, followed by preservation, storage, and extensive sample preparation prior to instrumental analysis. These workflows are often labor-intensive, require significant reagent consumption, and may compromise sample integrity due to physicochemical and biological changes occurring during storage and transport. Furthermore, conventional pre-treatment procedures, such as liquid-liquid extraction and off-line solid-phase extraction, increase analysis time, generate additional waste, and introduce potential sources of contamination and analyte loss. From a logistical perspective, the handling, transport, and storage of large numbers of bulky water samples can also be challenging, requiring considerable space, increasing operational costs, and limiting the feasibility of large-scale or remote monitoring campaigns.

To address the limitations associated with conventional sampling procedures, we developed miniaturized sampling strategies based on solid-phase extraction (SPE) for the in-situ collection of metal ions was explored. In this context a sampling device for cadmium monitoring was developed and the same approach was extended to enable the simultaneous sampling of copper, iron and zinc ions. By immobilizing the target analyte/s directly onto a solid sorbent at the sampling site, the proposed approach combines analyte sampling, matrix clean-up, and analyte enrichment into a single step. In addition, the reduced generation of chemical waste, lower transportation requirements, and the possibility of reusing the extraction materials support the principles of green analytical chemistry and sustainable environmental monitoring. Overall, these portable and resource-efficient strategies represent a promising alternative to conventional water sampling procedures for the monitoring of metal ions in aquatic systems.

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Reliable lithium quantification in waters with ionic strength: ICP-OES method validation and uncertainty assessment

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Lithium is a strategic raw material for rechargeable batteries, and its reliable determination in water is important for assessing potential resources and supporting recovery processes. However, ionic matrices may compromise analytical performance [1,2]. This work aimed to validate an inductively coupled plasma optical emission spectrometry (ICP-OES) method for lithium determination at approximately 670 nm in saline water matrices. Calibration standards were prepared with 5 g L^{-1} NaCl, and seawater samples were diluted to the same salinity to provide comparable analytical conditions [3].

Five independent six-level calibrations (5–500 µg/L) confirmed linearity by the Mandel test ($\alpha = 0.05$), with correlation coefficients ≥ 0.999944. Weighted linear regression was adopted to account for heterogeneous response variances. Blank-based detection and quantification limits were 0.677 and 2.050 µg/L, respectively, and the operational quantification limit was established at 5 µg/L. Repeatability ranged from 0.58 to 1.40 % RSD, while intermediate precision ranged from 1.84 to 3.61 % RSD. Eleven spike-recovery tests across the calibration range yielded recoveries of 91.51–103.08 %, meeting the 90–110 % acceptance criterion. Relative mean biases for two commercial reference solutions were −2.46 and −1.29%, supporting method trueness.

The relative expanded measurement uncertainty, estimated from intermediate precision, bias and reference-value uncertainty using an ISO 11352-based approach [4], was 7.79 % ($k = 2$). Together, these results demonstrate that the method provides reliable lithium quantification within the investigated concentration range and matrix conditions, with documented precision, trueness and measurement uncertainty.

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Orfinas Emergentes em Amostras de Drug Checking: Identificação e Elucidação Estrutural

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O surgimento de novos opioides sintéticos (NSOs) é uma preocupação para a saúde pública que vem crescendo, devido à rápida diversificação estrutural destes compostos [1]. Na sequência das medidas legislativas implementadas pela China na estrutura central dos nitazenos, em julho de 2025, tem levado ao surgimento de NSOs. Uma dessas classes é a das benzimidazol-2-onas, também designadas por orfinas. O seu aparecimento representa um desafio para a vigilância toxicológica e para os serviços de drug checking, particularmente devido à necessidade de uma identificação rápida e inequívoca de compostos estruturalmente novos [2]. A SR-17018 (5,6-dicloro desmetilclorfina) é uma orfina com elevada afinidade pelos recetores opioides, cujo aparecimento recente no mercado ilícito reforça a necessidade de monitorização desta classe [3]. Neste contexto, o presente trabalho teve como objetivo identificar e caracterizar dois novos análogos de SR-17018 detetados em amostras de rua recolhidas por um serviço de drug checking. A elucidação estrutural foi realizada através da combinação de cromatografia gasosa acoplada à espectrometria de massa em tandem (GC-MS/MS), espectrometria de massa de alta resolução (HRMS) e espectroscopia de ressonância magnética nuclear (NMR). A abordagem analítica permitiu a identificação e elucidação estrutural de dois novos análogos de SR-17018, 6-cloro desmetilclorfina e 5,7-dicloro desmetilclorfina). Estes resultados permitiram a identificação e avaliação de NSOs, reforçando a importância do papel dos serviços de drug checking na deteção de substâncias emergentes.

Agradecimentos

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Dispositivo analítico basado en papel asistido por smartphone para la detección colorimétrica de azúcares reductores en miel

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La autenticidad y calidad de la miel están asociadas a su contenido de azúcares reductores, principalmente glucosa y fructosa, que representan aproximadamente el 90–95% del total de azúcares [1]. Dado que la miel es uno de los productos alimentarios más adulterados a nivel mundial, el desarrollo de herramientas analíticas rápidas, accesibles y sostenibles es esencial para el control de calidad y la prevención del fraude.

En este trabajo se desarrolla un dispositivo analítico basado en papel (PAD) tipo *spot-test*. El PAD se combina con detección asistida por smartphone para determinar colorimétricamente los azúcares reductores totales en miel, expresados como la suma de glucosa y fructosa [2]. El método propuesto emplea una plataforma de papel hidrofílico biodegradable y un consumo mínimo de reactivos, apoyando principios analíticos verdes y sostenibles. La metodología se basa en la reacción de Benedict. La reacción colorimétrica consiste en una reacción redox entre el Cu(II) del reactivo de Benedict y los grupos reductores de los monosacáridos. Como resultado se forma óxido cuproso (Cu_2O) y aparece un color verde cuya intensidad depende de la concentración de azúcares reductores presentes en la muestra. Las imágenes de la reacción colorimétrica realizada en el PAD se adquirien bajo iluminación controlada empleando la cámara de un smartphone y se procesan digitalmente con la aplicación web gratuita Trigit. La cuantificación se logró monitorizando los cambios en el canal azul del espacio de color RGB, proporcionando una respuesta lineal en el intervalo de concentración de 50–400 mg/L (Fig. 1), con límites de detección y cuantificación de 11 mg/L y 37 mg/L, respectivamente, y una desviación estándar relativa inferior al 8% (n = 3). El método se aplicó al análisis de doce muestras comerciales de miel, mostrando buena concordancia con los valores declarados en las etiquetas. Además, el método se validó utilizando un material de referencia certificado y se comparó con el método oficial AOAC Lane–Eynon [3].

El método propuesto ofrece un enfoque rápido, simple, económico, accesible y respetuoso con el medio ambiente para cuantificar el contenido total de azúcares reductores en miel, requiriendo únicamente equipamiento básico de laboratorio. Su compatibilidad con la detección mediante smartphone facilita la adquisición y el análisis de datos, convirtiendo el método en una herramienta práctica de cribado para la evaluación de la calidad de la miel en laboratorios pequeños o no especializados antes de realizar análisis centralizados.

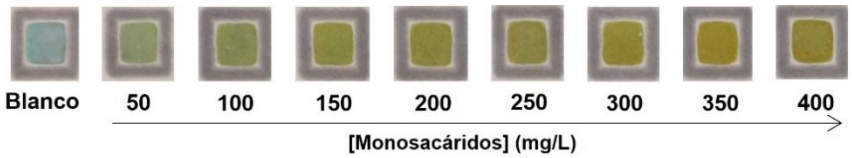


Fig.1. Imágenes del PAD tipo *spot-test* para cada estándar de calibración.

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Desarrollo de una sonda fluorescente basada en puntos de carbono sintetizados mediante UV/H2O2 para la detección de bisfenol A en alimentos

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El control de contaminantes en los alimentos es de gran importancia para garantizar su calidad, así como para prevenir problemas de salud y toxicidad. En particular, la presencia de bisfenol A (BPA) en alimentos genera gran preocupación debido a su comportamiento como disruptor endocrino. El BPA es un compuesto sintético, utilizado principalmente como monómero para producir plástico de policarbonato y resinas epoxi, que tienen numerosas aplicaciones en los recipientes de almacenamiento. La exposición al BPA a través de la cadena alimentaria puede producirse cuando el monómero residual migra hacia los alimentos envasados, por ejemplo, desde el recubrimiento interior de las latas. La Unión Europea (UE) y la Autoridad Europea de Seguridad Alimentaria (EFSA) establecen, respectivamente, un límite específico de migración de 0,05 mg kg^{-1} de alimento y una ingesta diaria tolerable de 2 ng kg^{-1} de peso corporal al día. Teniendo en cuenta los bajos niveles recomendados, el desarrollo de métodos analíticos rápidos y sensibles, capaces de detectar el BPA en matrices alimentarias, reviste un gran interés para la evaluación de la seguridad alimentaria [1]. En este trabajo se ha desarrollado una sonda fluorescente de tipo *turn-off*, basada en puntos de carbono (CDs) para la determinación de BPA en alimentos enlatados [2].

La estrategia propuesta se basa en la integración de la síntesis de CDs y detección de BPA en una única etapa (2 min), simplificando el procedimiento y reduciendo el tiempo necesario para llevar a cabo el análisis. La generación *in situ* de CDs fluorescentes se realiza bajo irradiación UV en presencia de H_2O_2. La descomposición fotoasistida del H_2O_2 favorece la formación de radicales hidroxilo, que contribuyen al desarrollo de la respuesta fluorescente del nanomaterial basado en carbono [3]. Por el contrario, la síntesis en presencia de BPA da lugar a una disminución de la fluorescencia (*turn-off*). El BPA actúa como "*scanvenger*" de los radicales hidroxilo inhibiendo su efecto catalítico. Así, la disminución de la intensidad de fluorescencia de los CDs es dependiente de la concentración BPA, y esta respuesta permite el reconocimiento y la cuantificación del BPA.

En condiciones optimizadas, el método proporcionó un límite de detección de 8,8 µg kg^{-1} y un límite de cuantificación de 29,4 µg kg^{-1}. El método se aplicó con éxito al análisis de muestras de alimentos en conserva (maíz dulce, guisantes, champiñones, berberechos y atún). Asimismo, se realizaron estudios de recuperación, obteniéndose valores comprendidos entre el 97% y el 105%, con una desviación estándar relativa del 4%. La estrategia fotoasistida propuesta combina, de forma simultánea, la síntesis de nanomateriales y el reconocimiento químico, ofreciendo una herramienta potencial de cribado para la determinación de BPA y sus análogos en muestras de alimentos, con aplicaciones en seguridad alimentaria y control de calidad. El procedimiento propuesto requiere un bajo consumo de muestra y reactivos, permitiendo una elevada frecuencia de análisis de muestras.

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Determinación colorimétrica cinético-catalítica de vanadio mediante un dispositivo microfluídico tridimensional basado en papel

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La detección de iones metálicos en muestras medioambientales mediante sistemas analíticos portátiles sigue suponiendo un reto. En este sentido, los dispositivos analíticos basados en papel constituyen una alternativa atractiva, si bien su limitada sensibilidad restringe su aplicabilidad directa a la determinación de metales a niveles de concentración elevados. En consecuencia, a menudo se requieren procedimientos de preconcentración previos para poder determinar metales a niveles traza. Aunque dichos procedimientos pueden mejorar el rendimiento analítico, también suponen un aumento de la complejidad del análisis y reducen la simplicidad y la portabilidad de estas alternativas, limitando así su aplicabilidad [1]. Una estrategia potencial para solventar esta limitación consistiría en la implementación de reacciones colorimétricas catalizadas de modo selectivo por el ión metálico a determinar, caracterizadas por su elevada sensibilidad, en dispositivos analíticos basados en papel.

En este trabajo se ha desarrollado un método colorimétrico cinético-catalítico que utiliza un dispositivo analítico microfluídico tridimensional origami basado en papel (3D-µPAD) para la determinación de vanadio. El método analítico propuesto se basa en la actividad catalítica del vanadio en la oxidación del ácido gálico causada por el bromato en condiciones ácidas. Esta reacción produce un compuesto coloreado que puede detectarse directamente en las zonas de reacción del 3D-µPAD.

Las medidas cuantitativas se realizaron mediante análisis de imágenes digitales obtenidas con un *smartphone*, utilizando tanto calibración a tiempo fijo como calibración mediante velocidades iniciales. Ambas estrategias mostraron características analíticas satisfactorias, incluyendo límites de detección en el intervalo de 3,1 a 3,6 µg/L y límites de cuantificación entre 10,3 y 12,0 µg/L. Además, los métodos mostraron respuestas lineales en intervalos de concentración que se extendían hasta los 500 µg/L. La repetibilidad y la precisión intermedia, expresadas como desviación estándar relativa, fueron inferiores al 7,2 % y al 7,5 %, respectivamente. El método propuesto también ofreció una elevada capacidad de procesamiento de muestras, con un rendimiento estimado que oscilaba entre 48 y 96 muestras por hora. La validación del método se llevó a cabo utilizando seis materiales de referencia certificados con matrices de distinta complejidad (agua de mar, sedimentos, suelo y lodos industriales). Los resultados obtenidos con ambos métodos de calibración coincidieron satisfactoriamente con los valores de referencia certificados con un nivel de confianza del 95 % [2].

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Towards Integrated Wine Analysis: Automated Determination of Carbon Dioxide and Sulphur Dioxide

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Carbon dioxide and sulphur dioxide are important parameters in wine production and quality control. Carbon dioxide affects the sensory characteristics and effervescence of wines, whereas sulphur dioxide is widely used during winemaking due to its antioxidant and antimicrobial properties. Despite their importance, both compounds are commonly determined using separate analytical procedures, which may increase analysis time, reagent consumption and sample handling.

Gas-diffusion membrane separation combined with flow-based analysis has previously been demonstrated as an effective approach for isolating volatile analytes from complex wine matrices. Atanassov et al. applied membrane gas-diffusion units in flow injection analysis (FIA) for the spectrophotometric determination of CO_2 and SO_2 in wines [1]. Subsequently, Segundo and Rangel incorporated a gas-diffusion membrane unit into a sequential injection analysis (SIA) system for the determination of SO_2 in wines [2]. These studies demonstrated the potential of membrane-based separation in automated wine analysis and provided the basis for further development of flow systems integrating the determination of both analytes.

In the present work, a membrane gas-diffusion separator was integrated into a sequential injection análisis(SIA) system for the determination of CO_2 and SO_2 within a single automated analytical platform. Carbon dioxide transferred through the membrane into an acceptor solution containing bromothymol blue (BTB), where the resulting pH change was monitored spectrophotometrically. Sulphur dioxide was transferred into a malachite green solution and determined based on the corresponding decrease in absorbance. The entire analytical sequence, including sample and reagent handling, gas-diffusion separation and signal acquisition, was controlled using GlobalLab software.

The analytical conditions were optimized experimentally, and the developed system was evaluated with respect to the influence of the major potential interferents present in wine. The method was subsequently applied to the analysis of 12 different Portuguese wines. The concentrations obtained using the developed SIA system showed good agreement with those determined using the corresponding reference methods: the Ripper method for SO_2 and potentiometric titration following sample alkalization for CO_2. Representative results for three selected wine samples are presented in Table 1, illustrating the agreement between the proposed system and the reference procedures.

The obtained results demonstrate that membrane gas-diffusion separation combined with SIA enables the automated determination of CO_2 and SO_2 in real wine samples using a single analytical platform. The system provides effective separation of volatile analytes from the wine matrix, reduces manual sample handling and reagent consumption, and produces results consistent with conventional reference procedures. The proposed approach therefore represents a promising tool for rapid and automated wine analysis.

Table 1. Comparison of CO_2 and SO_2 concentrations determined in three representative Portuguese wines using the proposed SIA system and the corresponding reference methods.

CO_2								
Wine sample	Wine type	Reference mean [g/L]	Reference SD [g/L]	Proposed mean [g/L]	Proposed SD [g/L]	Absolute bias [g/L]	Relative bias [%]	Recovery [%]
Senhor da Vinha	Red	0.455	0.025	0.430	0.025	-0.025	-5.437	94.563
Linhas Tortas 2024	Red	0.447	0.034	0.474	0.050	0.026	5.892	105.892
Chardonnay	White	1.483	0.094	1.447	0.089	-0.035	-2.393	97.607
SO_2								
Wine sample	Wine type	Reference mean [mg/L]	Reference SD [mg/L]	Proposed mean [mg/L]	Proposed SD [mg/L]	Absolute bias [mg/L]	Relative bias [%]	Recovery [%]
Senhor da Vinha	Red	205.026	3.922	210.900	3.382	5.874	2.865	102.865
Linhas Tortas 2024	Red	48.302	2.369	52.339	1.297	4.037	8.359	108.359
Chardonnay	White	94.928	4.298	88.672	6.425	-6.256	-6.590	93.410

Agradecimientos
Este apartado se colocará después de la figura o tabla [Arial 9 pt]

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Development of a 3D-microfluidic paper-based analytical device for phosphate determination with smartphone-based colorimetric detection

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Phosphate is essential for plant growth in agriculture. However, an excess of this anion in different water bodies may produce eutrophication due to algae proliferation [1]. The limit of discharge in urban wastewater is 0.5 mg phosphorus/L in cities with fewer than 150,000 inhabitants, and 0.7 mg phosphorus/L in cities with a population of ≥ 150,000 inhabitants (Directive 2024/3019) [2]. Thus, the determination of phosphate in environmental samples is crucial. In our work [3], we designed a colorimetric 3D-µPAD based on the UV-vis spectrophotometric standardized method 4500-P E [4]. The assay relied on the formation of a blue-colored product (molybdenum blue) in the detection area of the 3D-µPAD in the presence of phosphate. The designed 3D-µPAD enabled the simultaneous processing of a blank and a standard or a sample, in duplicate, thus minimizing potential inconsistencies associated with the luminosity changes and digitization step. Experimental parameters, including geometric aspects of the 3D-µPAD, digitization and image processing conditions, the amount of chemicals preloaded in the 3D-µPAD, and the reaction time, were fully optimized. An exhaustive interference study was performed. The shelf life of the device was evaluated under different storage conditions, and the effect of incorporating reagents such as ethylene glycol and p-toluenesulfonic acid into preloaded 3D-µPADs was assessed. Under optimal conditions, the assay exhibited a working range of 4-25 mg P/L. The limits of detection (LOD) and quantification (LOQ) were 0.015 mg P/L and 0.05 mg P/L, respectively. The repeatability and intermediate precision of a 5 mg P/L standard were 4.8 % and 7.1 %, respectively. The proposed colorimetric assay has been successfully applied to phosphorous determination in waters, soils and sediments, obtaining recoveries ranging from 94 to 107 %. The ready-to-use 3D-µPAD showed a greener profile than the standard method for phosphate determination, being affordable, easy-to-use, and suitable for citizen science applications.

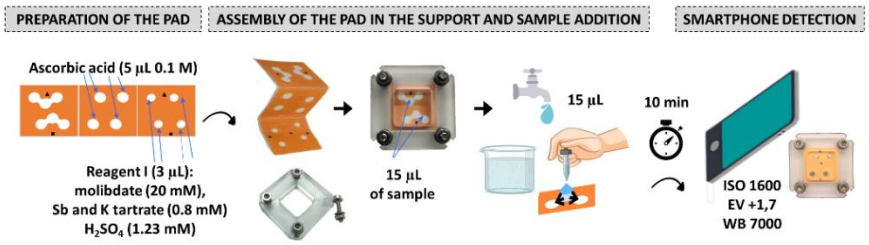


Fig.1. Scheme of the designed 3D-µPAD for phosphate analysis.

Acknowledgements
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Electrochemical DNA-based biosensors to discriminate against the rs1065852 SNPs genotypes associated with drug-resistant epilepsy

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Epilepsy is a chronic, heterogeneous neurological disorder characterized by the occurrence of at least two seizures, that affects over 50 million people worldwide [1]. Anti-seizure medication is administrated to reduce morbidity and mortality, however nearly one-third of patients can develop drug-resistance, leading to more seizures. Recent pharmacogenomic studies reported an association between the single-nucleotide polymorphism (SNP) rs1065852 (*CYP2D6**10) and the poor treatment response [2]. So, the early identifying of this SNP could help with the treatment outcome. In this study, a disposable electrochemical biosensor was developed to discriminate the three genotypes linked to the rs1065852 SNP: wild-type homozygous (C/C), heterozygous (C/T), and mutant homozygous (T/T). The sensor's methodology results from the enzymatic hybridization reaction between purified DNA containing the *CYP2D6**10 SNPs, obtained from healthy and epileptic volunteers, and a synthetic complementary probe immobilized on screen-printed gold electrodes. Chronoamperometric measurements were used to optimize each step. This sensor successfully distinguished the current intensities between the purified DNA fragments corresponding to the C/C, C/T, and T/T genotypes. The electrochemical results were then confirmed by DNA sequencing. These findings demonstrate that the disposable electrochemical DNA-based biosensor offers a sensitive and cost-effective approach for detecting the rs1065852 genotypes and may support the early identification of patients with drug-resistant epilepsy.

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Sustainability-by-Design Sample Preparation for Thermal-Processing Contaminants in Infant Foods

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The analysis of thermal-processing contaminants in infant foods requires efficient sample preparation strategies capable of addressing complex lipid- and protein-rich matrices while minimizing environmental impact [1-3]. This work presents a set of sustainability-by-design analytical workflows based on miniaturization and microextraction for the determination of relevant processing contaminants in infant foods [1-3].

Five complementary approaches were developed according to analyte class and separation technique. Maillard-related contaminants, including acetamide, acrylamide and glycidamide, were determined by µ-QuEChERS-DLLME-GC-MS within situ derivatization. Carbonyl compounds associated with lipid oxidation were analyzed by gas-diffusion microextraction coupled to HPLC-UV, complemented by HS-SPME-GC-MS for broader coverage of volatile carbonyls and α-dicarbonyls. A direct µ-QuEChERS-UHPLC-MS/MS strategy using sustainable materials was applied to 3-MCPDE, 2-MCPDE and glycidyl esters, avoiding conventional hydrolysis or transesterification steps. PAHs were determined by µ-dSPE-DLLME-GC-MS using reduced extraction volumes and tailored clean-up for fat-rich matrices [1-3].

Across the workflows, miniaturization and microextraction reduced sample and solvent use, consumables, waste, and processing steps while maintaining analytical robustness in complex infant-food matrices. Low-volume extraction, reduced-scale clean-up, and sustainable sorbents further supported greener sample preparation without compromising performance..

Overall, these methodologies illustrate the potential of sustainability-by-design sample preparation for greener contaminant monitoring in infant foods. Miniaturized and microextraction-based workflows provide versatile alternatives for improving the environmental performance of food safety analysis while preserving fit-for-purpose analytical capabilities.

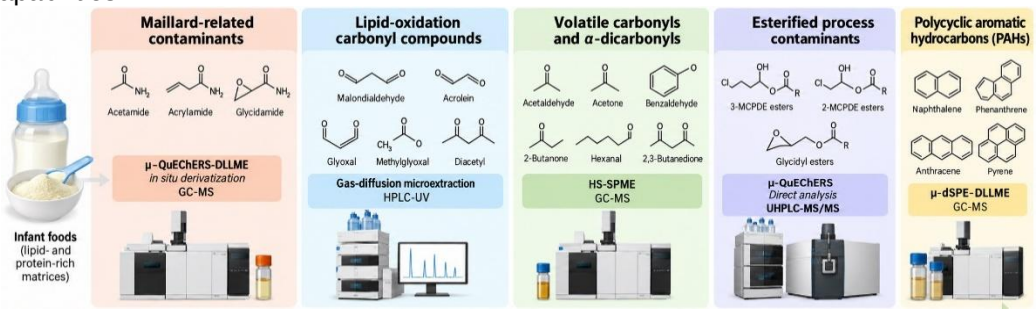


***Fig 1**. Sustainability-by-design workflows for infant food analysis.*

Agradecimientos

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Integrated One Health Monitoring Tool for On-Site Nitrate and Nitrite Analysis

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Nitrate and nitrite are two nitrogen ions that can be present in natural waters and can impact human health, creating a link between environmental contamination and public health. In rural areas, nitrogen fertilisers may leach into groundwater, consequently increasing nitrate levels in well water. The concentration of nitrate also relates to microbiological growth, so European directives state that the concentration in waters should not be above 50 mg/L (800 µM), established as the maximum admissible limit [1]. In urine, nitrite not only reflects individual exposure but can also give insightful information on the diagnosis of diseases such as urinary tract infection. Monitoring both matrices together is a practical illustration of the One Health concept, yet it is rarely feasible outside the laboratory.

The PHsense project aims to develop innovative microfluidic sensor devices for rapid, on-site monitoring of public health biomarkers in natural water and in non-invasively collected biological fluids.
Within this project, we developed a multilayer microfluidic paper-based analytical device (µPAD) for the quantification of nitrate and nitrite in both well water and urine samples. Nitrite is detected directly via the Griess reaction, which produces a pink-coloured product proportional to the nitrite concentration. For nitrate detection, zinc powder embedded in one of the paper layers reduces nitrate to nitrite as the sample flows vertically through the device layers, so the same colourimetric reaction is used for nitrate determination. The design addresses the ASSURED criteria for point-of-need testing: low cost, no instrumentation, simple operation, and rapid results.

In well water, nitrate was quantified from 98.7 to 2000 µM, with a limit of detection (LOD) of 29.6 µM, and nitrite was quantified from 2.8 to 44.0 µM, with a LOD of 0.83 µM. In urine, the linear ranges were 120 to 2000 µM for nitrate (LOD 35.9 µM) and 6.2 to 40.0 µM for nitrite (LOD 1.8 µM). The accuracy of the devices was validated by comparison with a reference method and through recovery studies. Additionally, the developed µPAD enabled evaluation of the efficiency and accuracy of a commercial filtration pitcher by testing multiple well water samples with different nitrate and nitrite levels, before and after the pitcher filtration.

The designed paper-based sensor offers a simple, portable approach to on-site screening of nitrate and nitrite in environmental and biological samples, supporting faster public health decisions.

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Aplicación de LA-ICP-MS á análise de mostras líquidas: determinación de elementos traza en leite

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A ablación láser acoplada á espectrometría de masas con plasma acoplado inductivamente (LA-ICP-MS) constitúe unha ferramenta de gran interese para a caracterización elemental de materiais sólidos. Permite levar a cabo unha análise multielemental de gran resolución espacial, empregando unha mínima cantidade e preparación de mostra.

A aplicación desta técnica centrouse tradicionalmente en matrices xeolóxicas, metálicas, vítreas e cerámicas. Mais as súas abundantes vantaxes, están impulsando a procura de estratexias que permitan estender o seu uso a matrices ambientais, biolóxicas e alimentarias.

O obxectivo deste traballo é a optimización e aplicación dun método de solidificación de mostras líquidas que permita levar a cabo a análise do contido de elementos traza en diferentes mostras de leite.

A primeira parte consistiu en levar a cabo a optimización da metodoloxía, baseada na preparación de pequenas gotas de leite inmobilizadas nunha matriz de xelatina porcina mediante un proceso de solidificación controlada. Esta estratexia permitiu obter un soporte sólido e reproducible, axeitado para a súa análise directa mediante ablación láser. Durante a etapa de optimización avaliouse a influencia de diferentes parámetros experimentais, incluíndo o contido de xelatina (10 %), a enerxía do láser (0.4 J cm^{-2}), a velocidade de varrido (20 µm s^{-1}) e o tamaño do punto de ablación (50 µm).

A continuación, avaliáronse as principais características analíticas do método, incluíndo os límites de detección (LOD) e cuantificación (LOQ), a exactitude e a precisión, esta última estudada tanto a nivel intragota como intergota. Para a avaliación da exactitude e da trazabilidade da resposta analítica, empregouse o material de referencia certificado ERM®-BD151.

Finalmente, levouse a cabo a aplicación do método a mostras reais. Empregáronse mostras de leite materno maduro e intermedio, fórmulas infantís de distinta composición, leites de vaca comerciais con variedade de materia graxa, leites sen lactosa e bebidas de orixe vexetal.

Os resultados obtidos demostran a adecuación da metodoloxía desenvolvida para a determinación de elementos traza en leite mediante LA-ICP-MS. Impulsando así o emprego desta técnica para análises en matrices líquidas e permitindo explorar novas aplicacións nutricionais e clínicas.

Flow-based method for glyphosate monitoring in well water samples for human consumption

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Glyphosate is widely used as an agricultural herbicide, raising significant concerns regarding groundwater leaching and consequent drinking water quality. Private well water sources in rural areas are particularly vulnerable as they routinely bypass municipal monitoring and treatments, exposing domestic consumers to potential health risks.

Standard chromatographic techniques, such as HPLC or LC-MS/MS, are the usual reference methods for glyphosate determination. However, these methods are expensive, rely on toxic solvents, and require complex instrumentation and skilled operators. To address these shortcomings, a flow injection system coupled with spectrophotometric detection was developed. This approach is based on an indirect catalytic reaction: free Cu^{2+} catalyses the oxidation of TMB by H_2O_2 into a blue product and in the presence of glyphosate, the latter complexes with Cu^{2+}, inhibiting the oxidation of TMB, causing a decrease in absorbance proportional to glyphosate concentration. The developed FIA method was optimized to maximise analytical performance, namely by studying physical and chemical parameters. Physical parameters included the flow rate of each channel, reaction coil length, and manifold configuration by the placement of reaction reactors and the confluence points. The chemical parameters evaluated were the concentration of all reagents involved, Cu^{2+}/buffer, TMB/ethanol, and H_2O_2, as well as the sample volume injected. Afterwards, a final parameter was tested: the reaction temperature with the inclusion of a hot bath. Currently ongoing is the validation process of the optimised FIA method, which already enables a rapid, and environmentally friendly alternative with strong potential as a high-throughput screening platform for routine glyphosate monitoring in domestic well waters.

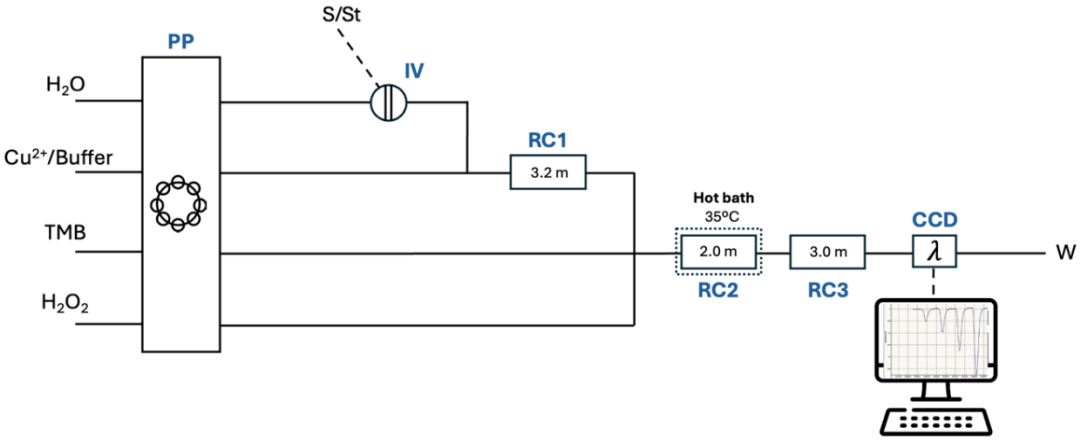


Fig.1. Schematic diagram of FIA manifold for glyphosate determination. PP: peristaltic pump; S/St: sample or standard injection; IV: injection valve; RC1: reaction coil 1 (3.2 m); RC2: reaction coil 2 (2.0 m heated at 35ºC); RC3: reaction coil 3 (3.0 m at room temperature); CCD: spectrophotometric detector (λ = 653 nm); W: waste.

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A sequential injection chromatographic approach for molecular weight screening of protein hydrolysates

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European Union regulations on feed additives increase the need for rapid and reliable analytical tools for the characterization of protein hydrolysates [1]. Conventional approaches based on high-performance liquid chromatography (HPLC) are robust but may involve high operational costs, complex instrumentation, and long analysis times.

In this work, a low-pressure size-exclusion chromatographic method based on sequential injection analysis (SIA) was developed and optimized for molecular weight screening of protein hydrolysates, with a particular focus on the 10 kDa threshold. The main experimental parameters affecting chromatographic performance were evaluated, including flow rate, chromatographic column dimensions, standard solution concentration, and sample volume. The selected conditions included a flow rate of 0.325 mL min^{-1}, a 10 cm column with a 3.17 mm internal diameter, a standard solution concentration of 0.10 mg mL^{-1}, and a sample volume of 150 µL.

The optimized method was applied to protein hydrolysates from different sources, namely swine, black soldier fly (BSF), and fish. Distinct chromatographic profiles were obtained relative to a 10 kDa molecular weight marker, demonstrating the system's ability to differentiate the hydrolysates according to their molecular weight distribution. The proposed approach provides a miniaturized, automated, and cost-effective alternative for rapid molecular weight screening of protein hydrolysates.

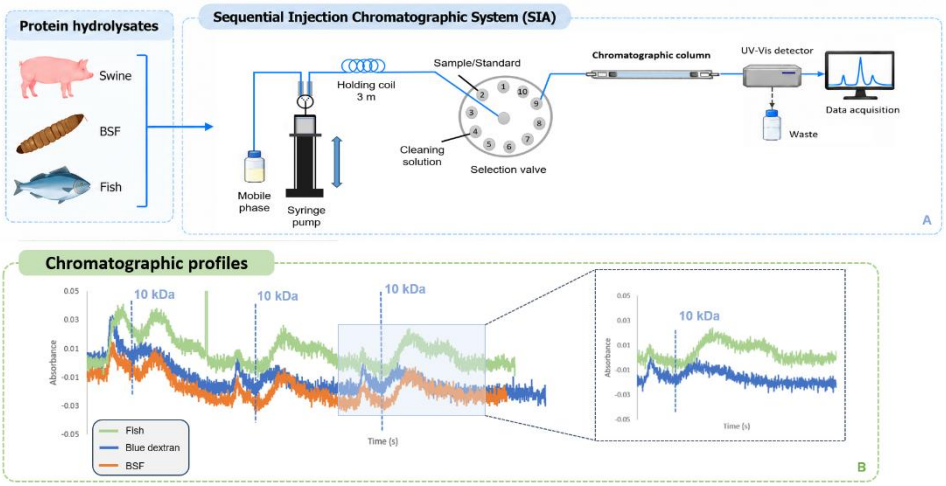


Fig.1. Sequential injection chromatographic system for hydrolysates molecular weight screening (A), and representative chromatographic profiles of protein hydrolysates in triplicate (B).

Acknowledgments
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Desenvolvemento dun método para a determinación de nanopartículas de cerio e ferro en material particulado atmosférico

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O material particulado atmosférico (PM) constitúe unha das principais preocupacións ambientais e de saúde pública asociadas á contaminación atmosférica urbana. O reducido tamaño das partículas finas ($PM_{2,5}$) favorece a súa penetración nas vías respiratorias e pode contribuír á aparición de efectos adversos sobre a saúde. Dentro do material particulado, a presenza de nanopartículas metálicas suscita un interese crecente, particularmente aquelas asociadas ás emisións derivadas do tráfico. Entre estas nanopartículas, as de cerio (CeNPs) e as de ferro (FeNPs) poden chegar á atmosfera como consecuencia do emprego de aditivos nos combustibles diésel, dos procesos de combustión ou do desgaste de compoñentes asociados ás actividades dos vehículos.

O obxectivo deste traballo foi desenvolver e optimizar unha metodoloxía para a extracción e caracterización de CeNPs e FeNPs presentes en mostras de PM_{10} e $PM_{2,5}$ recollidas en filtros de fibra de cuarzo.

En primeiro lugar, realizouse unha análise do contido total de Ce e Fe mediante espectrometría de masas con plasma de acoplamento indutivo (ICP-MS) tras unha dixestión ácida asistida por microondas (HNO_3/H_2O_2). As medidas realizáronse en modo KED (*Kinetic Energy Discrimination*) empregando He como gas de colisión, e a calibración levouse a cabo mediante o método de adición estándar (0,5- 50 µg L^{-1}) e empregando o Rh como patrón interno.

Para a determinación das nanopartículas presentes no PM, empregouse a extracción asistida por ultrasóns utilizando hidróxido de tetrametilamonio (TMAH) como axente extractante. Optimizáronse diferentes parámetros que afectan ao proceso de extracción, como a concentración e o volume de TMAH e o tempo de sonicación. As condicións óptimas foron 5 mL de TMAH ao 2,0 % e 2 h de sonicación para as CeNPs, mentres que para as FeNPs empregáronse 5 mL de TMAH ao 3,0 % durante 1 h. Posteriormente, os extractos filtráronse empregando filtros de celulosa de 5,0 µm e as nanopartículas caracterizáronse mediante espectrometría de masas con plasma de acoplamento indutivo no modo *single particle* (spICP-MS).

As metodoloxías optimizadas foron finalmente aplicadas a mostras reais de PM_{10} e $PM_{2,5}$, permitindo a determinación e caracterización de nanopartículas de cerio e ferro presentes no material particulado atmosférico.

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Addressing gadolinium contamination from hospital effluents: A sustainable approach for protecting aquatic water quality

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Gadolinium (Gd) has emerged as a contaminant of increasing environmental relevance due to the widespread use of Gd-based contrast agents (GBCAs) in magnetic resonance imaging. Following administration, these highly stable complexes are largely excreted and enter wastewater streams, including hospital effluents. Conventional wastewater treatment is not specifically designed to retain these compounds, favouring their transfer to receiving waters and the development of anthropogenic Gd anomalies in aquatic systems. This study assessed a magnetic sorption-based treatment as a potential strategy to reduce Gd loads before their discharge into the environment.

The influence of operational and water-chemistry parameters relevant to treatment performance was investigated, including initial Gd concentration, sorbent dose, salinity and contact time. Gd removal increased with the amount of sorbent available and was influenced by the initial contaminant concentration, while the effect of salinity became less pronounced when sufficient sorption capacity was provided. Under favourable treatment conditions, Gd removal exceeded 90 % within 1 h in both freshwater and saline media (Figure 1). In kinetic assays performed under intermediate experimental conditions, removal reached 89 % after 3 h and increased to 94% after 48 h [1]. In a more chemically complex mineral-water matrix containing nine rare-earth elements, 78 % of Gd was removed after 3 h, increasing to 83,5 % after 6 h and 87,5 % after 48 h, despite competition from co-occurring ions [2].

These findings demonstrate that magnetic sorption can provide an efficient and operationally simple option for limiting the transfer of anthropogenic Gd to aquatic environments. Rather than focusing only on downstream remediation, the results support the development of targeted treatment steps for Gd-containing wastewaters close to major emission sources. In healthcare settings where GBCAs are routinely used, reducing Gd loads before discharge could help limit their environmental dispersion and decrease the pressure of hospital-derived effluents on the chemical quality of receiving waters. Further validation using real hospital wastewater will be important to assess implementation under environmentally realistic conditions.

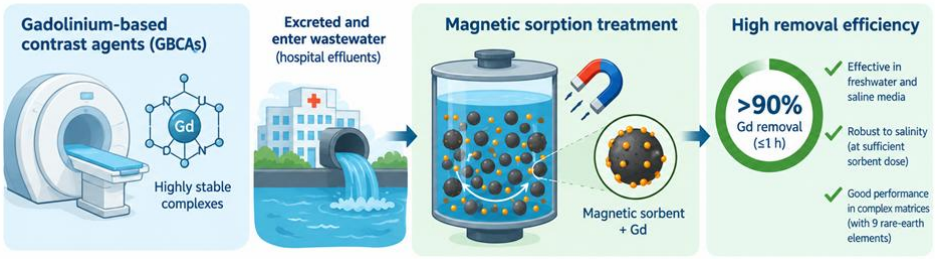


Fig.1. Gd removal by magnetic sorption under different water conditions.

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Electrochemical Procedures Coupled To Cyp450 Metabolism For Control And Environment Risk Analysis Of Transdermal Patches

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Transdermal patches are widely used for the sustained delivery of pharmaceutical compounds through the skin, offering advantages such as bypassing first-pass metabolism, good adherence to treatment, and adaptability to different drugs [1]. However, their use also contributes to the growing presence of pharmaceutical compounds and metabolites in aquatic environments, partly due to improper disposal after use. This contamination poses environmental concerns, as several drugs have negatively impacted local biota [2].

This work describes the development of an electrochemical analytical method for the in vitro control of progesterone formulations and assessment of after-use contamination levels in aquatic biomes. This is achieved through a microfluidics platform containing an electrode with a progesterone permselective membrane and gel encapsulated Cytochrome P450, for metabolic assessment. The optimized membrane exhibited electrochemical response towards progesterone, producing a linear signal inversely proportional to its concentration, in the 10^{-7} to 10^{-2} µM range. Furthermore, a signal increase was observed when the progesterone flows through the gel network containing the enzyme. The proposed method enables rapid detection of progesterone and evaluation of its metabolic degradation rate, providing a portable and low waste alternative for drug presence screening in water bodies, before and after metabolic degradation [3].

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Plataformas sensoras baseadas em pontos quânticos e polímeros molecularmente impressos imobilizados em suportes sólidos: desenvolvimento, reconhecimento molecular e aplicações

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As tecnologias de diagnóstico e de monitorização descentralizadas são essenciais para expandir o acesso aos cuidados de saúde e à monitorização ambiental [1]. Neste contexto, os sensores fluorescentes destacam-se pela elevada sensibilidade, rapidez e potencial de portabilidade [2]. Estas plataformas precisam de um elemento sensor, em que os pontos quânticos (QDs), devido às suas propriedades únicas, constituem transdutores óticos promissores para estas aplicações. No entanto, os QDs não apresentam seletividade molecular intrínseca, o que limita a sua fiabilidade em matrizes complexas e torna necessária a integração de elementos de reconhecimento [3, 4].

Para alcançar este objetivo, os QDs são frequentemente combinados com elementos de reconhecimento molecular, como anticorpos [3] e polímeros molecularmente impressos (MIPs) [4]. Os MIPs são recetores artificiais que, por meio de cavidades específicas, mimetizam o reconhecimento de anticorpos, oferecendo elevada seletividade, maior estabilidade química, menor custo e maior robustez no armazenamento. A investigação recente tem-se centrado cada vez mais na imobilização de sistemas QD–MIP em suportes sólidos [5], com o objetivo de desenvolver plataformas de deteção portáteis e de utilização simples para aplicação no local de prestação de cuidados de saúde.

Embora as nanoestruturas QD–MIP imobilizadas em substratos sólidos demonstrem um desempenho analítico promissor, ainda persistem desafios relacionados com a eficiência de imobilização, a preservação da fluorescência, a acessibilidade dos sítios de reconhecimento e a reprodutibilidade analítica, cuja resolução é essencial para a aplicação destes sistemas em condições reais.

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Caracterización de gasolinas mediante el perfil de hidrocarburos (HCs) ligeros saturados (C_1-C_7) de la fase de vapor

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El objetivo de este trabajo fue caracterizar muestras de gasolina mediante el perfil hidrocarburos ligeros saturados (C_1-C_7) de la fase de vapor del combustible. La metodología consistió en una implementación y rápida del método ASTM D2163-23ε1, el cual está diseñado para la determinación de hidrocarburos ligeros C_1-C_5 en muestras de gas licuado de petróleo (GLP). El muestreo de gasolina consistió en 63 muestras (31 de tipo regular y 32 de tipo premium), obtenidas en 32 estaciones de servicio de cuatro marcas mexicanas (OXXO, Petro 7, PEMEX y Mobil). Cada muestra se diluyó al 5 % en metanol y se analizó la fase de vapor producida en una relación líquido-gas 2:1 V/V. El análisis cuantitativo de los hidrocarburos se realizó por normalización de área (% A), considerando los compuestos con un porcentaje de área cromatográfica mayor al 10 %. La concentración de los hidrocarburos se analizó por promedio y gráficos de cajas (boxplot). Los resultados mostraron que cada tipo de gasolina presentó un perfil de hidrocarburos característico, identificando cuatro hidrocarburos mayoritarios (isobutano, n-butano, isopentano y n-pentano) en todas las muestras analizadas. El análisis de los datos evidenció que las muestras de gasolina regular presentaron menor dispersión en la concentración de n-butano e isopentano en comparación con las muestras de gasolina premium. En cuanto a las marcas comerciales, los perfiles de tres marcas de gasolina regular presentaron similitudes, mientras que la cuarta mostró diferencias respecto a las demás. La metodología analítica demostró viabilidad para caracterizar el tipo de gasolina e identificar las similitudes entre marcas de combustible, exclusivamente analizando la fase vapor. Esta contribución metodológica representa una herramienta complementaria al control de calidad del combustible; para medir o monitorear las emisiones de HCs ligeros debido a la evaporación de gasolina; o como una estrategia analítica para evaluar la pureza relativa de la gasolina o del fraccionamiento del petróleo a nivel industrial.

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QUÍMICA-FÍSICA

Exploring the Solid-State Landscape of Leflunomide: Polymorphism and Multicomponent Systems

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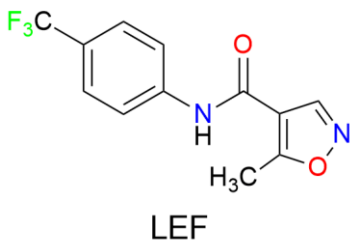
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Oral solid dosage forms are widely used in pharmaceutical therapy. However, the poor aqueous solubility of many active pharmaceutical ingredients can limit their oral bioavailability and, consequently, their therapeutic efficacy [1]. In this context, the study of the solid-state, namely polymorphism and multicomponent systems, is a fundamental strategy for optimizing relevant physicochemical properties without modifying the chemical identity of the drugs [2,3].

Leflunomide (LEF), Figure 1 (a), a disease-modifying antirheumatic drug used in the treatment of rheumatoid arthritis, exhibits poor aqueous solubility and is administered exclusively in the form of oral tablets. Given that its solid-state behaviour remains relatively underexplored, particularly regarding polymorphism and multicomponent systems, LEF is an ideal target for this type of investigation [4,5].

In this work, three polymorphic forms of LEF were characterised by powder X-ray diffraction (PXRD) and attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR), leading to the identification of a new crystalline form (Form III) and an amorphous phase. A complementary study using differential scanning calorimetry and polarized light thermomicroscopy provided insight into the thermodynamic relationships among the polymorphs, Figure 1 (b). In addition, through extensive mechanochemical screening, sixteen multicomponent systems (fifteen crystalline and one coamorphous) were identified and characterized by PXRD and ATR-FTIR. The determination of the crystal structures of six of these systems by single-crystal X-ray diffraction allowed for a detailed analysis of their intermolecular interactions and supramolecular arrangements.

(a)



(b)

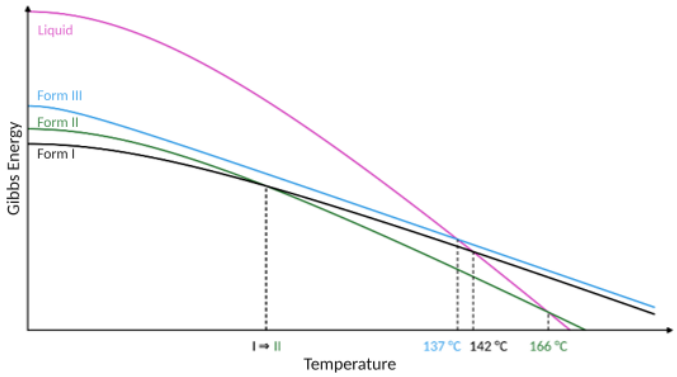


Fig. 1. (a) Molecular structure of leflunomide (b) Representation of Gibbs energy as a function of temperature for the three polymorphic forms of LEF.

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QUÍMICA INORGÁNICA

A mononuclear Dy-N_3O_5 complex with single-molecule magnet behavior

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Molecular magnetism has emerged as an attractive research field due to the potential of single-molecule magnets (SMMs) for applications in high-density information storage and quantum technologies [1].

Lanthanoid-based SMMs are particularly promising owing to their strong magnetic anisotropy. In this context, the electrostatic model proposed by Rinehart and Long established a relationship between the coordination geometry and the magnetic anisotropy of lanthanoid ions [2]. For oblate ions such as Dy^{3+}, highly axial coordination environments are expected to maximize magnetic anisotropy.

Among the geometries investigated for Dy^{3+} based SMMs, pentagonal and hexagonal bipyramidal environments are particularly attractive due to their strong axial character [3]. However, achieving these coordination geometries in stable coordination compounds remains challenging. Therefore, the rational design of suitable ligands is essential for controlling the coordination environment around the lanthanoid ion and optimizing its magnetic properties.

Herein, we report the synthesis, structural, and magnetic characterization of a mononuclear Dy^{3+} complex featuring a slightly distorted hexagonal bipyramidal N_3O_5 coordination environment. Alternating-current (ac) magnetic susceptibility measurements reveal slow relaxation of the magnetization under zero applied dc magnetic field, confirming its SMM behavior.

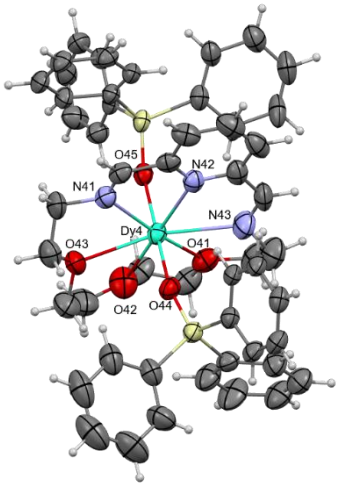


Fig.1. Ellipsoids diagram of $[Dy(L^{N3O3})(Ph_3SiO)_2]^+$ cation in $\{[Dy(L^{N3O3})(Ph_3SiO)_2](BPh_4)\}\cdot 0.81CH_2Cl_2$.

Acknowledgements

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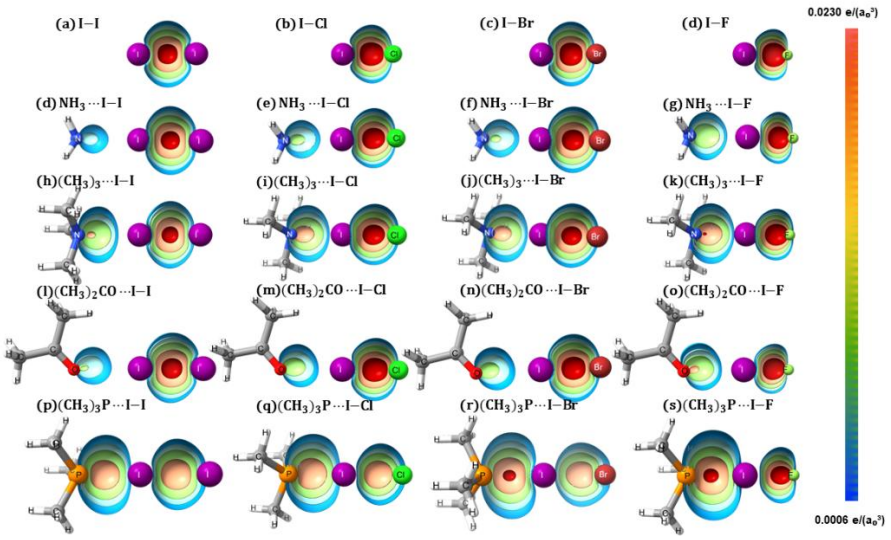
Assessing Charge Transfer in Halogen Bonds: A Comparative Study Using OP/TOP, QTAIM, and LVM Descriptors

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Halogen bonds (XBs) are fundamentally driven by electrostatic interactions (the σ-hole) [1,2] and Mulliken's charge-transfer (CT) model [3]. While orbital overlap explains the characteristic linear directionality of XBs [4], its direct quantification remains scarce. To address this, we quantified orbital overlap in 28 X−I···B complexes (X = I, Cl, Br, F; B = diverse Lewis bases) using the Overlap Model (OP/TOP) [5-7], alongside QTAIM, LVM, and NBO analyses. Calculations at the ωB97X-D3/def2-TZVP level revealed strong convergence across all models. We demonstrate that XB strength is highly dependent on the polarizability and electronegativity of X, and the basicity of B. Stronger bases (e.g., PMe_3, NMe_3) yield stronger XBs with higher electron density, whereas weaker bases form less pronounced interactions. XB strengthening is intrinsically linked to increase the nB→σ*(I−X) charge transfer, greater electron sharing (evidenced by overlap descriptors), and higher local force constants. The overlap density maps $\rho_{OP}(r)$ visually illustrate this progression (see Fig. 1). These strong correlations validate applied methodologies and underscore the significant covalent contribution to halogen bonding.

Fig.1. Overlap density maps $\rho_{OP}(r)$ for systems with halogen bonds.



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Synthesis, structure, and in vitro cytotoxicity of a dinuclear Cu(II) complex based on a *bis*(thiosemicarbazone) ligand

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Colorectal cancer presents a major global health challenge that must be considered a growing epidemic in the 21st century. The limited therapeutic options with proven efficacy highlight the urgent need for new treatment strategies, driving the search for effective metallodrugs that target altered copper homeostasis in tumor cells. [1] In this context copper(II) complexes emerge as a feasible alternative to expand the therapeutic arsenal against colorectal cancer.

Here, we report the electrochemical synthesis and structural characterization of a novel dinuclear copper(II) complex, [Cu_2(L)(OH)], featuring an exogenous bridging hydroxo group derived from atmospheric oxygen. Electrochemical analysis revealed a quasi-reversible Cu(II)/Cu(I) redox process ($E_{1/2}$=-0.726 V vs. Ag/AgCl), suggesting potential selectivity under hypoxic conditions. In vitro cytotoxic assays against human colorectal adenocarcinoma cells (HCT-8) yielded an IC_{50} of 8.9 µM (Neutral Red assay) and 14.5 µM (WST-1 assay). This antiproliferative activity is comparable to clinical agents like cisplatin, oxaliplatin, 5-fluorouracil, and irinotecan, positioning copper(II) *bis*(thiosemicarbazone) complexes as promising anticancer candidates.

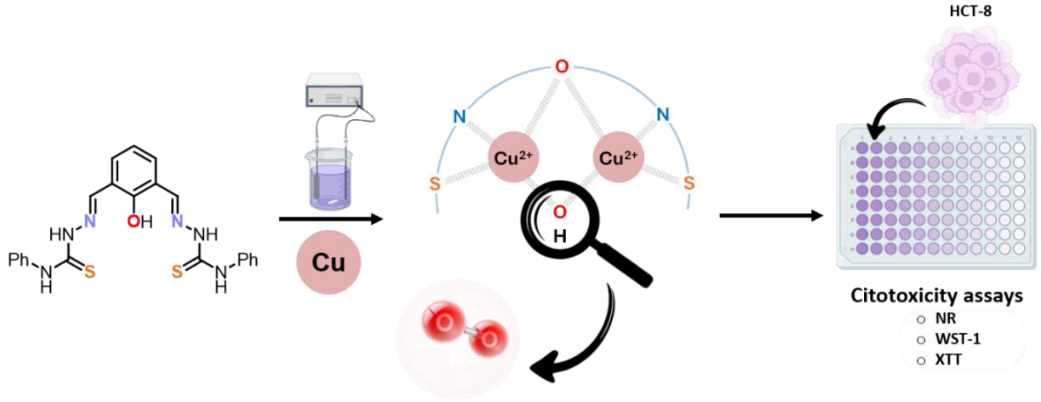


Fig.1. Synthesis of the copper(II) complex with the exogenous hydroxyl group and its cytotoxicity studies.

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Synthesis of Platinum Complexes based on Gemcitabine and Cytidine

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Nucleosides play a fundamental role in cellular physiology, serving as essential components in processes such as DNA and RNA synthesis, metabolic regulation, and cell signaling. Nucleoside derivatives represent an important class of anticancer agents and can be used in combination therapy to enhance therapeutic efficacy through complementary mechanisms of action. However, combination therapies are often problematic due to the different pharmacokinetics of individual drugs.[1] One promising strategy to circumvent these issues is the combination of cytotoxic functionalities in one single molecule through organometallic derivatization of nucleosides. In this context, platinum-based drugs represent the most widely used class of anticancer agents and have been fundamental in advancing cancer therapy.[2]

Studies have demonstrated that gemcitabine and cisplatin exert synergistic effects on non-small cell lung cancer, breast cancer, and ovarian cancer.[3] Moreover, the combination of these agents represents an established therapeutic option for patients with locally advanced or metastatic pancreatic cancer.[4] Our group has previously reported the synthesis and biological evaluation of platinum (II) complexes derived from uridine and deoxyuridine.[5] Inspired by these findings, and based on our previous work, we examined the synthesis of platinum complexes containing gemcitabine derivatives aiming for their use as anticancer drugs. Due to their structural similarities, the synthesis of platinum-based cytosine and deoxy-cytosine complexes was also explored. The results of this work will be presented in this communication.

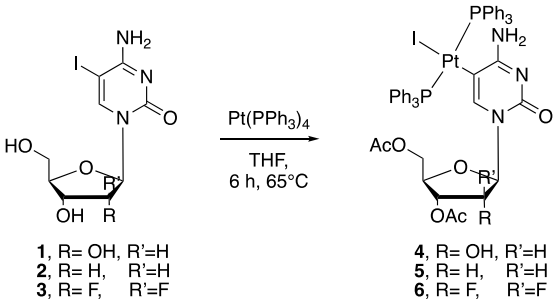


Fig.1. Synthesis of Platinum (II) pyrimidine nucleosides by oxidative addition

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Rutenio(II) e Tiosemicarbazonas: novas prespectivas na loita contra o cancro de mama triple negativo.

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O uso de fármacos anticanceríxenos baseados en platino, como o cisplatino, está limitado polos seus efectos secundarios y a emerxente aparición de resistencias, o que está conducindo a búsqueda de alternativas con terapias baseadas en metais. Os complexos de Rutenio emerxeron como prometedores candidatos debido ás súas favorables propiedades farmacolóxicas, incluíndo baixa toxicidade, unha rica química redox, e a capacidade para atacar tanto aos tumores primarios como aos metastásicos. [1]

En particular, os complexos organometálicos de areno-Ru(II) do tipo [Ru(η⁶-areno)L_x] chamaron a atención debido á súa versatilidade estrutural e á súa actividade biolóxica axustable. A incorporación de ligandos bioactivos como as tiosemicarbazonas (TSCs), as cales coordínanse a través de átomos dadores N,S, ofrecen vantaxes adicionais, xa que estes ligandos posúen propiedades anticanceríxenas intrínsecas e poden modular a estabilidade, reactividade e captación celular dos complexos resultantes. [2]
O cancro de mama triplo negativo representa un subtipo agresivo de cancro de mama con limitadas opción terapéuticas. A liña celular MDA-MB-231 é un modelo amplamente usado para esta enfermidade, caracterizada por unha alta invasividade e resistencia aos tratamentos convencionais, o que a fai especialmente adecuada para avaliar novos axentes anticanceríxenos.

Neste traballo, informamos da síntese e caracterización dunha serie de complexos de Ru(II) de formula xeral **[Ru(η⁶-p-cimeno)(κ²-N,S-TSC)]** xunto coa investigación da súa estabilidade baixo condicións fisiolóxicas e a súa actividade citotóxica *in vitro* contra as células MDA-MB-231.

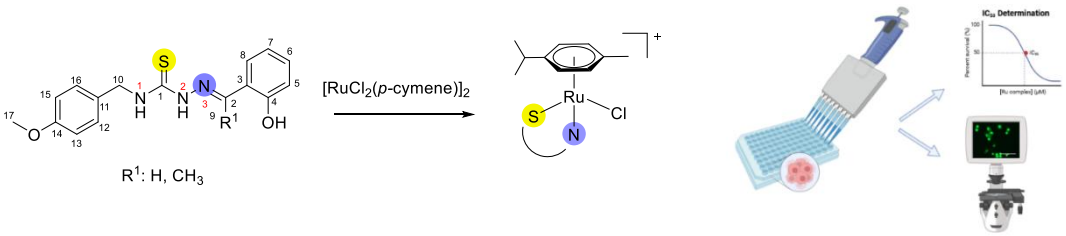


Fig.1. Esquema de e estudio biolóxico.

Agradecementos
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Coordination behavior and reactivity of $\{M(CO)_3\}^+$ (M = Tc, Re) complexes bearing thiosemicarbazone-carborane ligands

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Thiosemicarbazones represent a versatile class of ligands in coordination chemistry, attracting interest due to their diverse biological activities and pharmacological potential.[1,2] Despite the extensive variety of TSC derivatives investigated to date, no examples incorporating a carborane moiety have been reported, despite their significant potential to modulate biological properties for medicinal applications.[3]

It is well established that metal complexation often alters and enhances the biological profile of thiosemicarbazones, frequently resulting in superior anticancer potency compared to the uncoordinated ligands. Consequently, metal complexes of carboranyl-functionalized TSCs provide an interesting framework for designing targeted, biologically active compounds. In particular, complexes featuring the rhenium tricarbonyl core, $\{Re(CO)_3\}^+$, exhibit tunable biological activity and utility in bioimaging applications through their radioactive $\{Tc(CO)_3\}^+$ analogs.[4-6] Thus, in this contribution the coordination behaviour of a carboranyl-thiosemicarbazone ligand towards the organometallic *fac*-$\{M(CO)_3\}^+$ (M=Tc, Re) core is described.

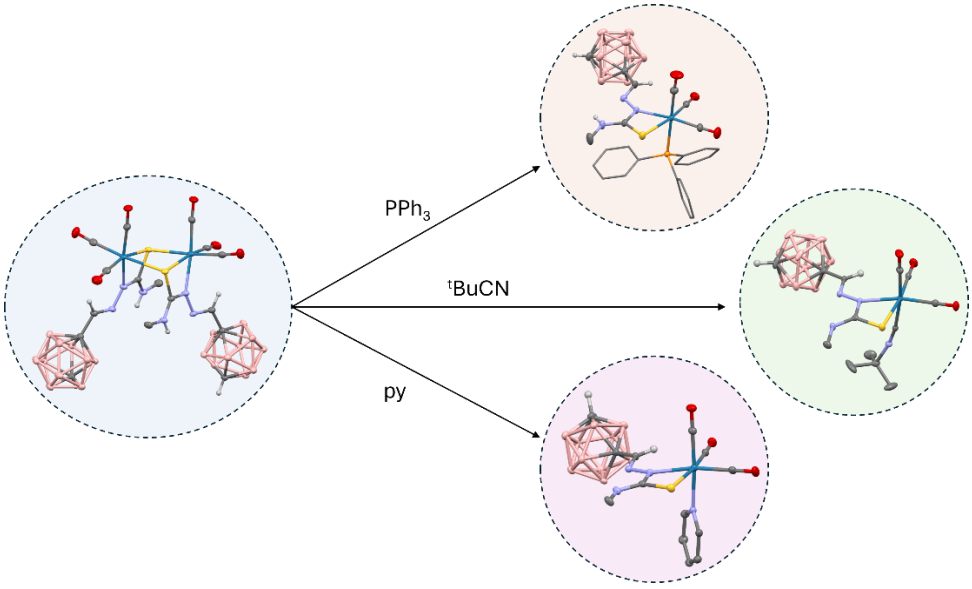


Fig.1. Coordination behavior of some examples of *fac*-$\{M(CO)_3\}^+$ complexes.

Acknowledgements

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Substituent Effects on C–C and C–H Bonding: A Multi-Descriptor Investigation via Electron Density Overlap

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Understanding how structural modifications affect chemical bonds is important for relating molecular structure to chemical properties. Simple organic molecules provide suitable models for investigating these effects in a controlled manner [1].The addition of substituents can modify the electronic distribution of chemical bonds, affecting their polarity, electron density, and covalency through inductive and resonance effects [2–4]. In this study, HmC–CXHn systems (X = $N(CH_3)_2$, NH_2, CN, or NO_2) were investigated using Local Vibrational Mode (LVM), Quantum Theory of Atoms in Molecules (QTAIM), Electron Localization Function (ELF), and Natural Bond Orbital (NBO) approaches [5,6] to evaluate changes in bonding properties. The results show that C–C and C–H bonds are affected by the substituent electronic effects. Electron-donating groups generally increase bond lengths and overlap density, while electron-withdrawing groups promote bond shortening and lower overlap density. Increasing C–C unsaturation is accompanied by higher ΔE^2 values and increased occupation of π-type antibonding orbitals, as reflected by the OCC (orbital occupation) values of π_1^* and π_2^*. The $N(CH_3)_2$ and NH_2 substituted systems exhibit higher second-order perturbation energies, ΔE^2, indicating stronger donor–acceptor stabilization, whereas the CN substituted systems generally show lower ΔE^2 values. NO_2 is the only substituent that increases the local (LVM) force constants regardless of C–C bond order. The overlap density maps, $\rho_{OP}(r)$, further illustrate these changes in electron sharing and bonding character (see Fig. 1)

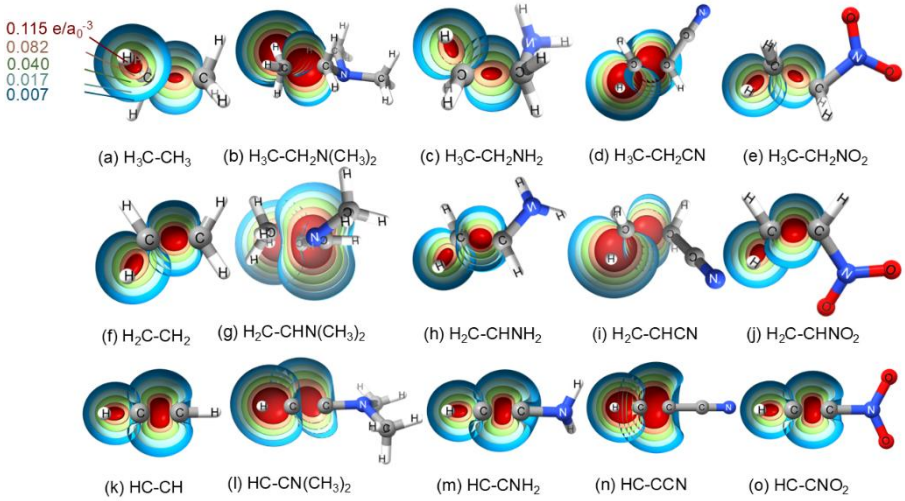


Fig.1. Maps of the overlap density, $\rho_{OP}(r)$, for various HmC–CXHn systemsç

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Valorização de resíduos PET e CO_2 através da preparação do MOF Co-BDC para a produção de carbonatos cíclicos

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A acumulação de resíduos plásticos nos ecossistemas constitui um problema ambiental significativo, agravado pela persistência de polímeros como o poli(tereftalato de etileno) (PET), cuja fragmentação pode originar microplásticos .[1]. Paralelamente, o aumento da concentração atmosférica de dióxido de carbono (CO_2) contribui para o aquecimento global, reforçando a necessidade de estratégias que permitam a sua captura e valorização química.

Neste contexto, as estruturas metal-orgânicas (MOFs) destacam-se pelas suas elevadas áreas superficiais, porosidade ajustável e potencial aplicação na adsorção de CO_2 e na catálise heterogénea. A utilização de ácido tereftálico recuperado a partir de resíduos de PET como ligando orgânico na síntese destes materiais constitui uma abordagem de economia circular, promovendo simultaneamente a valorização de resíduos plásticos e do CO_2.[2], [3]

Este trabalho teve como objetivo valorizar resíduos de PET e CO_2 através da recuperação de ácido tereftálico (H_2BDC) por hidrólise assistida por aquecimento óhmico e da sua utilização na síntese do MOF Co-BDC. A caracterização e a pureza do ligando recuperado foram investigadas por ressonância magnética nuclear (RMN) e espectroscopia de infravermelho por transformada de Fourier (FT-IR). A utilização de H_2BDC recuperado permitiu obter o material do tipo MOF cristalino, denominado Co-BDC, demonstrando a viabilidade da preparação de MOFs catalíticos de baixo custo.

O material preparado foi caracterizado por difração de raios X de pós, FT-IR, microscopia eletrónica de varrimento acoplada à espectroscopia de raios X por dispersão de energia (SEM-EDS), análise termogravimétrica e isotérmicas de adsorção-dessorção de N_2. Por fim, a atividade catalítica do Co-BDC foi avaliada na reação de cicloadição de CO_2 com epicloridrina, visando a produção de carbonatos cíclicos com potencial aplicação como aditivos de combustíveis[4] .

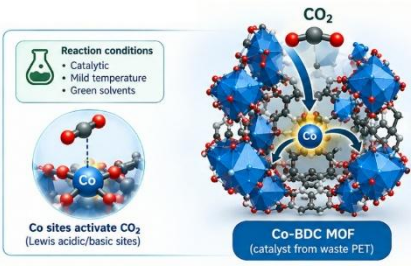


Figura 1. Esquema de ação da estrutura de Co-BDC para a captura de CO_2 com fim catalítico.

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QUÍMICA ORGÁNICA

Continuous-Flow Synthesis and Process Optimization of MANIO: A Scalable Route to a Promising p53-Targeting Anticancer Agent

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Colorectal cancer (CRC) is a major global health challenge, driving the development of novel therapeutic strategies such as the reactivation of the p53 tumor suppressor protein. In this context, MANIO, (3*S*)-6,7-bis(hydroxymethyl)-5-methyl-3-phenyl-1*H*,3*H*-pyrrolo[1,2-*c*]thiazole, is a "best-in-class" p53 activator capable of restoring the function of both wild-type and mutant p53 proteins, thereby exhibiting significant anticancer potential [1]. To overcome the synthetic bottlenecks that limit the preclinical translation, this work integrates synthetic route optimization and continuous-flow technology to enable an efficient, sustainable, and scalable production of MANIO.

The previously reported four-step batch synthesis of MANIO was limited by the final ester reduction step by hazardous reaction conditions and a modest yield of up to 56% [2]. Thus far, an optimized reducing protocol has been developed, providing a safer, more robust, and more reproducible process with an improved yield of 83%. In parallel, a continuous-flow approach was also developed to address batch scalability issues and enhance process efficiency [3,4]. Once reagent solubility limitations were resolved, the key 1,3-dipolar cycloaddition step was successfully translated to flow conditions, reducing the reaction time drastically from 4 h in batch to only 45 min in flow while yielding the pure MANIO precursor in 85% yield (Fig. 1). In this communication, we present our ongoing efforts to adapt the fully optimized synthetic sequence to continuous-flow conditions, to achieve gram-scale production of MANIO. This will enable detailed studies of p53-MANIO interaction studies by NMR and support the development of nanostructured lipid carrier (NLC)-based formulation. Collectively, these efforts are intended to advance MANIO toward clinical translation as a novel p53-targeting therapeutic candidate for colorectal cancer.

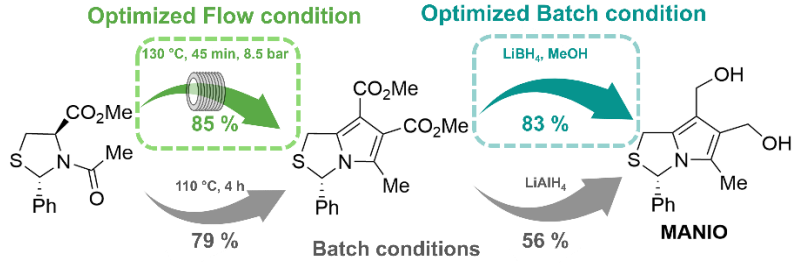


Fig.1. Optimized final steps: continuous-flow 1,3-dipolar cycloaddition and ester reduction.

Acknowledgments

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From organic chemistry lab to the sea: exploring 3,4-dihydroxyxanthone as a sustainable antifouling agent

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Marine biofouling remains a major challenge for submerged structures, increasing maintenance costs and causing several environmental impacts. The development of effective and safe antifouling compounds, combined with cost-effective production, is therefore highly desirable [1]. 3,4-Dihydroxyxanthone (3,4-DOHX) has shown promising antifouling properties and an eco-friendly profile [2]. This study aimed: i) to explore alternative synthetic methodologies to increase the sustainability of the 3,4-DOHX synthesis, ii) to study compatibility with commercial coatings, and iii) to perform in situ antifouling efficacy tests in the Atlantic Ocean.

Despite the same atom economy (67%), the optimized route demonstrated better performance in terms of Green and Sustainable Chemistry, with the use of recyclable ionic liquids, instead of the corrosive and expensive reagent $AlCl_3$, with shorter reaction times and energy consumption with the use of microwave heating, and with the replacement of a reaction step with a toxic organic solvent with a low-cost and solvent-free step [3] . 3,4-DOHX was incorporated into a commercial rosin-based marine coating (Raffaello Eco from Boero). Good compatibility between 2% of 3,4DOHX and the polymeric matrix was observed. The prepared coating exhibited a uniform morphology and greater surface hydrophilicity after incorporating the compound and was applied to standardized acrylic substrates. After being submerged for several months at a depth of 1.5 meters, a delay in macrofouling was observed in prototypes coated with 3,4-DOHX-containing coatings, compared with those without 3,4-DOHX. This work, combining the optimization of the antifouling additive through Green Chemistry principles, with marine performance assessment, contributes to both SDG12 (responsible production) and SDG14 (protect life below water).

Keywords: antifouling, green organic chemistry, xanthone

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Valorização de grafite reciclada através da incorporação de óxido de grafeno em betão

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A incorporação de óxido de grafeno (GO) no betão tem suscitado interesse devido ao potencial para melhorar as propriedades mecânicas e físico-químicas deste material. A adição deste nanomaterial tem sido associada a uma maior resistência mecânica e durabilidade, bem como a uma menor permeabilidade a espécies potencialmente corrosivas [1,2]. Adicionalmente, o aumento da resistência à compressão, promovido pela presença de GO na matriz cimentícia, tem sido apontado como uma possível estratégia para reduzir a quantidade de cimento utilizada na produção de betão, contribuindo, consequentemente, para a diminuição das emissões de poluentes associadas à sua produção [1].

O GO pode ser sintetizado a partir de grafite, por métodos químicos que envolvem processos de oxidação e esfoliação. Atualmente, a empresa b.again (dstgroup) recupera grafite da massa negra obtida durante a reciclagem de baterias de ião-lítio em fim de vida. A valorização deste material em novas aplicações representa uma oportunidade para fomentar a economia circular e contribuir para o desenvolvimento de materiais mais sustentáveis.

Neste trabalho, sintetizou-se GO a partir de grafite reciclada através do método de *Hummers improved* e comparou-se as suas propriedades com as de GO de origem comercial [3]. As amostras foram caracterizadas pelas espectroscopias de infravermelho com transformada de Fourier e reflexão total atenuada (ATR-FTIR), Raman, ultravioleta-visível (UV-Vis) e fluorescência de raios X (XRF). Adicionalmente, avaliou-se o efeito da incorporação do GO sintetizado a partir de grafite reciclada no desempenho do betão, através da determinação da resistência à compressão e da massa volúmica, bem como da caracterização microestrutural por microscopia eletrónica de varrimento (SEM) e espectroscopia de raios X por dispersão em energia (EDS). Aos 28 dias, o betão com GO proveniente de grafite reciclada apresentou um aumento da resistência à compressão de 18% relativamente ao betão sem GO e de 2% relativamente ao betão contendo GO comercial de referência. A incorporação de GO resultou ainda num aumento da massa volúmica de, aproximadamente, 2% relativamente ao betão sem GO. A possibilidade de reduzir o teor de cimento através da incorporação de GO foi também avaliada, mediante uma redução simultânea de 10% das quantidades de cimento e de água (de modo a manter o rácio água/ligante). Aos 28 dias, não foram observadas diferenças estatisticamente significativas entre a resistência à compressão do betão contendo GO e menos 10% de cimento e água e a do betão de referência, sem GO e sem redução do teor de cimento.

Este estudo demonstra o potencial de valorização da grafite recuperada de baterias de ião-lítio em fim de vida através da sua conversão em GO e posterior incorporação no betão, promovendo simultaneamente o desenvolvimento de materiais de construção com desempenho melhorado e uma utilização mais circular e sustentável dos recursos.

Agradecimientos
Este trabalho contou com o apoio da Fundação Portuguesa para a Ciência e Tecnologia (FCT), no âmbito do financiamento estratégico ao Centro de Química da Universidade do Minho (CQ-UM/UM, UID/00686/2025, https://doi.org/10.54499/UID/00686/2025), e das empresas dst s.a., b.again e tbetão, mediante o acesso às suas instalações de investigação, equipamento e amostras necessários para a realização deste trabalho.

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Validation of Quantum Chemistry Predictions. Quinoidal-Base Tautomers in Anthocyanins and Related Compounds

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Anthocyanins are natural flavonoids with unique multistate color profile. [1] These properties have been explored for multiple applications, including functional materials, biosensors and medicinal products. [1] The theoretical investigation of the color properties of quinoidal anthocyanidin monomers is a powerful tool for predicting absorption features and their environment-dependent shifts. [2] However, experimental validation is crucial for the legitimacy of the theoretical models applied.

This study presents quantum-chemical calculations for the quinoidal-base tautomers of anthocyanins and related compounds, and the respective experimental validation. [4] The tautomers of the quinoidal-base form in anthocyanins and 3-deoxyanthocyanidins and their contributions to the color of the neutral quinoidal base were analyzed for the anthocyanins malvidin 3,5-O-diglucoside (bearing two hydroxyl substituents) and malvidin 3-O-glucoside, as well as for the synthetic 3-deoxyanthocyanin apigeninidin (bearing three hydroxyl substituents). The microstates associated with these tautomers were defined, model compounds of apigeninidin were synthesized, and the corresponding acid–base equilibria were studied by stopped-flow and conventional spectrophotometry. It was concluded that, for species with two hydroxyl substituents, only the tautomer deprotonated at position 7 is present; for species with three hydroxyl substituents, tautomer 7 remains the major form, but the tautomer deprotonated at position 5 is significant (approximately 18%). In all cases, the tautomer deprotonated at position 4′ can be neglected.

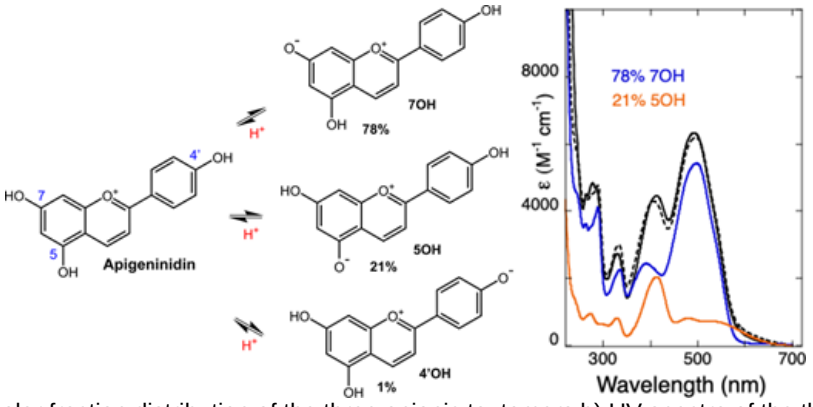


Figure 1: a) Molar fraction distribution of the three anionic tautomers b) UV spectra of the three individual monohydroxylated flavylium cation compared to the UV spectra of apigeninidin.

Acknowledgments

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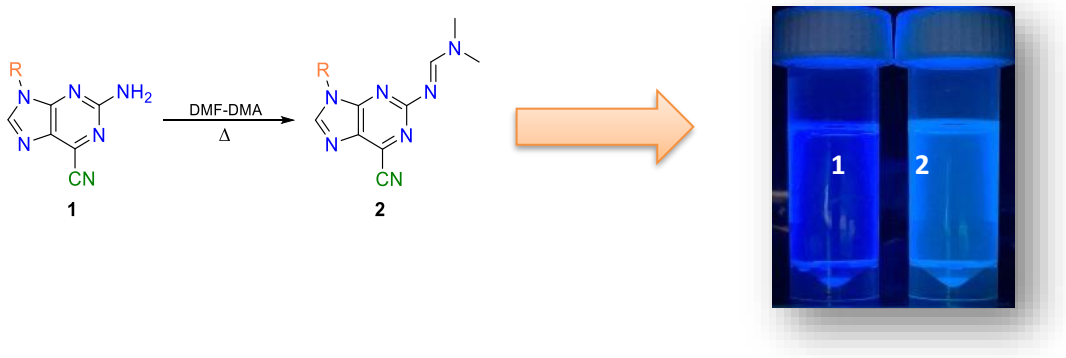
N,N-dimethylformimidamide Purines as new fluorescent platforms: Synthesis, photophysical properties and quantum chemical calculations

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Fluorescence has been widely used as a tool to shed light on cellular processes and responses to stimuli/insults [1]. Fluorescent nucleoside analogues (FNAs) are included in this group of molecules, featuring important characteristics, such as small size and potential to interact with the cellular machinery, or even to be incorporated in nucleic acids [2]. Despite their potential, FNAs have yet to find a place in bioimaging, largely owing to their generally inadequate spectral properties (e.g. absorption and emission in the UV region).

In previous work of our research group, highly fluorescent 2-amino-6-cyanopurines were obtained by a simple and efficient method [3]. However, the absorption and emission wavelengths remain in the blue region close to UV, which can induce photodamage and technical hindrances. To overcome this limitation, a new set of 6-cyanopurines with a *N,N*-dimethylformimidamide group at C-2 were synthesized from the 2-amino-6-cyanopurines through a one-step method, leading to improved photophysical properties. To gain some insight into the structural and electronic molecular properties of both ground state (S_0) and first excited singlet state (S_1), TDDFT calculations [4] of electronic and vibrational structure were also performed.

In this communication, the synthesis and characterization of the newly prepared purines will be presented. The photophysical properties determined in different media will be discussed and compared with theoretical results obtained by TDDFT calculations.



Acknowledgements
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Challenges and breakthroughs in developing potent antifungal and halochromic dyes: tackling the problem of selective synthesis

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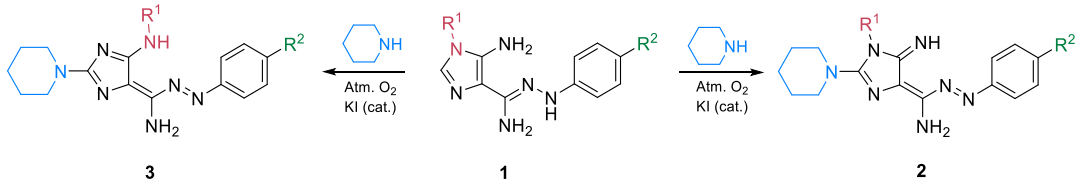
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Fungal infections present significant morbidity and mortality in immunocompromised individuals. To mitigate this problem, the World Health Organization defined a priority list of fungal pathogens, to guide research development and public health action. This list includes *Cryptococcus neoformans* in the critical priority group and *Pichia kudriavzevii* (*Candida krusei*) in the medium priority group [1]. The threat of antimicrobial resistance, particularly antifungal, is an arising challenge when battling fungal infections, creating a demand for new antifungal agents. This led our group to develop novel 2-aminoimidazole azo dyes **2** and **3** (**Scheme 1**) with potent antimicrobial activity against pathogenic yeasts (MICs as good as 2 mg/mL against *C. neoformans* and 4 mg/mL against *C. krusei*) [2,3].

In addition to the great potential as antifungal agents, these azo dyes exhibit unusual green and purple colours, showing a significant redshift in their UV-Vis absorption spectrum when compared to traditional azo dyes, which makes them valuable tools for biomedical applications [4]. They also present interesting halochromism within the biological window. Moreover, the structures of these two classes of azo dyes are extremely tuneable, as changes in R^1 and especially R^2 substituents can lead to significant change in colorimetric and antimicrobial properties.

This communication will dive into the unique properties of these molecules and the challenges of their syntheses, as the two classes possess common intermediate compounds, leading to problems in selectivity. The contribution of *ab initio* molecular quantum mechanics calculations will also be explored, as it was essential to understanding the stability and reactivity of the intermediate compounds and target products, thus guiding the selective synthesis of each class of azo dyes.



Scheme 1. Synthesis of azo dyes **2** and **3** from amidrazones **1.**

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Spectroscopic Characterization of Dynamic Complexes between Anthocyanins and a Boronic Acid-Chalcone Receptor

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Boronate–diol interactions have emerged as powerful tools in molecular recognition, controlled drug delivery, and sensing applications. Plant-based polyphenols are relevant bioactive molecules that could benefit from this chemistry for the development of smart systems [1]. However, studies investigating their interactions, particularly those involving pH-responsive anthocyanin dyes and boronic acid derivatives, remain limited in the literature [2].

In this work, we conducted systematic spectroscopic studies (UV–Vis, fluorescence, NMR) to evaluate the binding behavior between a synthesized boronic acid–chalcone receptor and structurally diverse anthocyanins. The preliminary results enabled the estimation of association binding constants and demonstrated a dynamic, pH-dependent, and structure-driven interaction mode between the receptor and the anthocyanins.

These findings provide valuable insights for the development of smart biomaterials, such as films and membranes, designed to host and release polyphenol-like bioactive molecules in a self-regulated manner triggered by pH variations. Such systems could have promising applications in innovative food packaging solutions.

Acknowledgments

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Funding

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Discovery of First-in-Class Melanostatin-Based Ago-Allosteric Modulators of Dopamine D_2 Receptors

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Melanostatin (MIF-1) is an endogenous positive allosteric modulator (PAM) of the dopamine D_2 receptors (D_2R),[1] representing a promising pharmacological lead for the treatment of Parkinson's disease and other dopamine-related central nervous system disorders. However, its peptide nature limits its clinical application, motivating the development of structurally optimized analogs.[2]

In this work, a novel series of MIF-1 derivatives incorporating alicyclic β-amino acids cispentacin and its unsaturated synthetic precursor 2-aminocyclopent-3-ene-1-carboxylic acid was designed, synthesized, and pharmacologically evaluated to study the impact of ring flexibility and stereochemistry on D2R modulation.[3] Functional assays in transfected human D_2R in CHO cells showed that only cispentacin-based analogs **8b** and **9b** retained activity, significantly enhancing dopamine (DA) potency by 4.2- and 4.3-fold at 0.01 nM, while MIF-1 was inactive at this concentration. At 1 nM, while compound **9b** showed a comparable reduction of EC_{50} to that of MIF-1 (3.8- versus 3.7-fold), compound **8b** reduced the EC_{50} of DA by 9.2-fold, significantly surpassing MIF-1. Furthermore, in the absence of DA, compound **8b** displayed intrinsic agonist activity, establishing the first MIF-1-based compound with ago-allosteric activity.

Cytotoxicity assessment in dopaminergic differentiated human SH-SY5Y cells demonstrated that the most active compounds showed no meaningful cytotoxicity at 100 μM, supporting a favorable preliminary safety profile. Overall, this study broadens the structural diversity of MIF-1-derived modulators, identifying alicyclic scaffolds as key structural motifs for enhancing D_2R allosteric modulation. These findings provide a foundation for the development of next-generation therapeutics targeting dopaminergic dysfunction.

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Molecular Engineering of Porphyrin–PAHs for Functional π-Conjugated Materials In-Solution and On-Surface

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Porphyrins (PORs) are versatile molecular building blocks for organic electronics owing to their structural rigidity, chemical stability, distinctive photophysical properties, and metal-coordination capabilities.[1] Their incorporation into extended π-extended conjugated architectures offers opportunities to modulate electronic delocalization and charge transport.[2] In this context, polycyclic aromatic hydrocarbons (PAHs) provide structurally defined building blocks for the bottom-up synthesis of advanced carbon-based nanostructures, including nanographenes (NGs) and graphene nanoribbons (GNRs).[3] Combining PORs and PAHs therefore provides a versatile strategy for developing functional π-conjugated materials with tailored electronic properties and molecular recognition capabilities.[4]

Here, we present our recent advances in the bottom-up synthesis of atomically precise POR-PAHs, exploring complementary approaches both in-solution (ISS) and on-surface synthesis (OSS). In solution, we investigate the construction of π-extended molecular hybrids by coupling metalated PORs with structurally defined PAH scaffolds, including bianthracene (BA)- and dicyclopentaanthracene (DCPA)-based systems (**Fig. 1**). In parallel, selected molecular precursors are investigated on Au(111) surfaces to assess their potential for OSS, exploiting surface-assisted cyclodehydrogenation and subsequent coupling reactions to access extended π-conjugated structures. By tailoring precursor symmetry, functionalization patterns, and reactive termini, this work explores different synthetic routes towards structurally precise hybrid architectures that combine the electronic properties of carbon-based nanostructures with the distinctive photophysical and coordination properties of PORs, with potential applications in chemical sensing and molecular electronics.

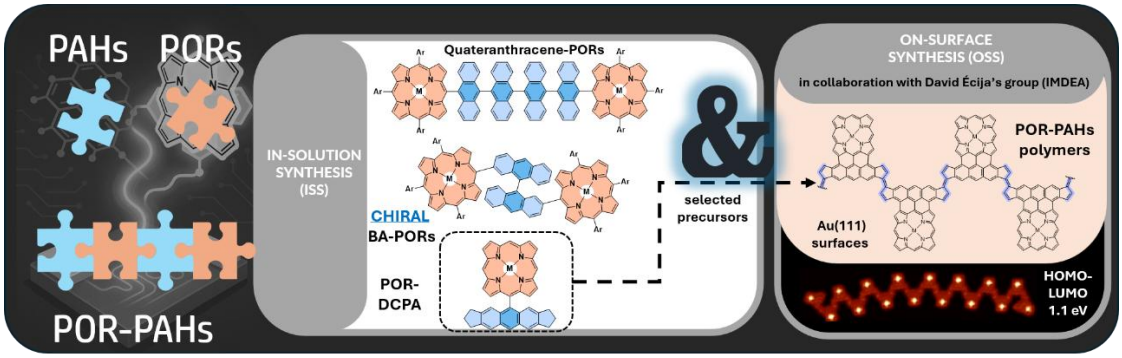


Fig.1. Bottom-up synthesis of POR-PAHs (in-solution and on-surface).

Agradecimientos
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Fluorescent probes for Efficient Assays for Measuring Inhibition of Penicillin Binding Protein 3 (PBP3) Transpeptidases

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β-Lactam antibiotics remain among the most important antibacterial agents and exert their activity through covalent inhibition of penicillin-binding proteins (PBPs), key enzymes involved in bacterial peptidoglycan biosynthesis. However, relatively few efficient methods are available for quantitatively assessing PBP inhibition, limiting the characterisation and development of new antibacterial agents.[1-3]

Here, we report a fluorescence-based assay for the rapid determination of second-order inhibition rate constants (kinact/KI) for PBP3 transpeptidases. The method employs **FC5** (Fig 1), a cephalosporin-derived probe that releases fluorescent umbelliferone following covalent reaction with the PBP active-site serine. The assay was applied to PBP3 enzymes from clinically relevant Gram-negative bacteria, including *Acinetobacter baumannii*, *Escherichia coli*, *Klebsiella pneumoniae* and *Pseudomonas aeruginosa*, enabling efficient comparison of representative penicillins, cephalosporins, monobactams and carbapenems.

The fluorescence results were supported by protein-observed mass spectrometry competition experiments. In addition, X-ray crystallographic structures of *P. aeruginosa* PBP3 in complex with ertapenem, doripenem and biapenem provided structural insight into how differences in carbapenem substitution influence PBP3 recognition and reactivity.

This methodology provides a convenient platform for profiling PBP inhibition and may facilitate the development of new β-lactam and non-β-lactam transpeptidase inhibitors with improved antibacterial properties.

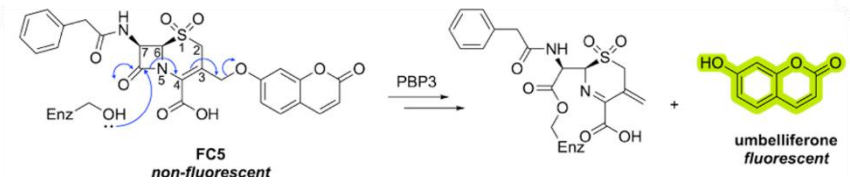


Fig.1. A fluorescence-based assay for penicillin-binding protein (PBP) transpeptidase activity employing FC5, a non-fluorescent cephalosporin-derived probe that, upon reaction with PBP3, releases umbelliferone from the C3 position, generating a fluorescent signal.

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Silyl-Prins cyclization with ketones: stereoselective construction of C2-quaternary stereocenters in polysubstituted tetrahydropyrans

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Heterocyclic compounds are part of the structure of numerous biologic and pharmacologically active natural products [1]. Therefore, the study and development of new methodologies that could be applied for the selective synthesis of polysubstituted heterocycles is of great importance [2]. In recent years, our research group has focused on the use of silylated compounds in Prins cyclization as a method for synthesizing different oxacycles [3].

Recently, our research group has published the use of cyclopropylsilyl alcohols as nucleophiles in silyl-Prins cyclization for the synthesis of tetrasubstituted tetrahydropyrans [4]. Herein we report an unprecedented Prins cyclization protocol capable of engaging non-activated ketones, delivering quaternary stereocenters with high stereoselectivity, and accommodating diverse Lewis acid counterions (Figure 1) [5].

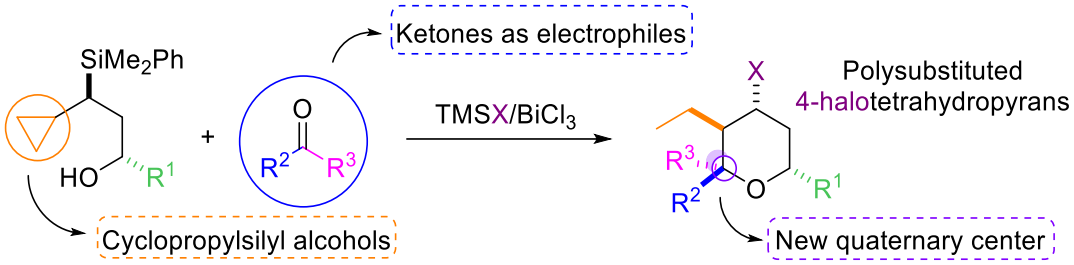


Fig.1. Study of silyl-Prins cyclization between cyclopropylsilyl alcohols and ketones

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Ferrocene-Core Hybrid Molecules: A Synthetic Strategy Toward Novel Oxacycles for Targeted Cancer Therapeutics

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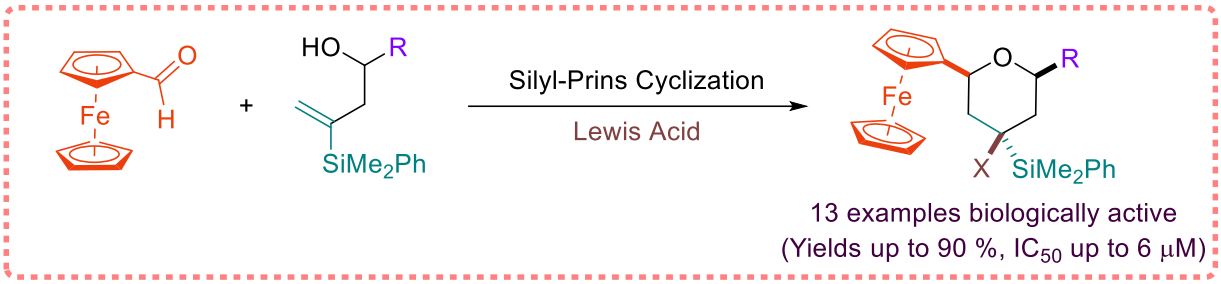
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Ferrocene is an organometallic compound that has demonstrated remarkable versatility in a wide range of applications, including asymmetric catalysis and medicinal chemistry. In recent years, the incorporation of the ferrocene moiety into bioactive molecules has emerged as a powerful strategy to enhance their pharmacological properties, particularly their anticancer activity [1]. In this context, ferrocene–oxacycle structures have shown promising cytotoxic profiles, highlighting their potential as therapeutic candidates [2].

Herein, we report the synthesis of novel tetrahydropyran-ferrocene derivatives through a Silyl-Prins cyclization reaction, a robust and efficient methodology for the construction of oxygenated six-membered rings [3]. The synthetic approach involves the reaction of a ferrocene-based aldehyde precursor with a variety of vinylsilanes, including halogenated substrates, under mild Lewis acid catalysis. This strategy enables rapid access to structurally diverse ferrocenyl tetrahydropyrans in good yields and with high functional group tolerance.

The obtained compounds are currently being evaluated for their antiproliferative activity against triple-negative breast cancer (TNBC) cell lines. This study aims to expand the chemical space of ferrocene-containing bioactive molecules and to identify new candidates with promising anticancer properties.

Fig.1. Synthesis of tetrahydropyran–ferrocene derivatives via Silyl–Prins cyclization, affording halogenated oxacyclic hybrids.



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Synthesis of diketopyrrolopyrrole-derived maleimides — new turn-on fluorescent probes for detecting biothiols

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Diketopyrrolopyrroles (DPP) are a class of synthetic organic dyes and pigments first synthesized in 1974. These compounds exhibit excellent photophysical properties, such as high Stokes shifts and high fluorescence quantum yield, as well as high thermal and photostability. Furthermore, the optical properties of these compounds can be easily tuned by alkylation of the lactam units or by functionalization of the aromatic rings [1,2].

Biothiols play important roles in human health that, when the concentration of these compounds is disrupted, it is usually due to a disease, namely neurodegenerative diseases or tumours. Thus, the monitoring of the concentration of these compounds can be a valuable approach for the early diagnosis of these diseases [3,4].

In this work [5], Pigment Red 254 was functionalized to yield two maleimide-substituted DPP derivatives, which act as turn-on probes for cysteine, homocysteine or glutathione. These compounds achieved limits of detection in the nanomolar range (18 nM) within 5 minutes.

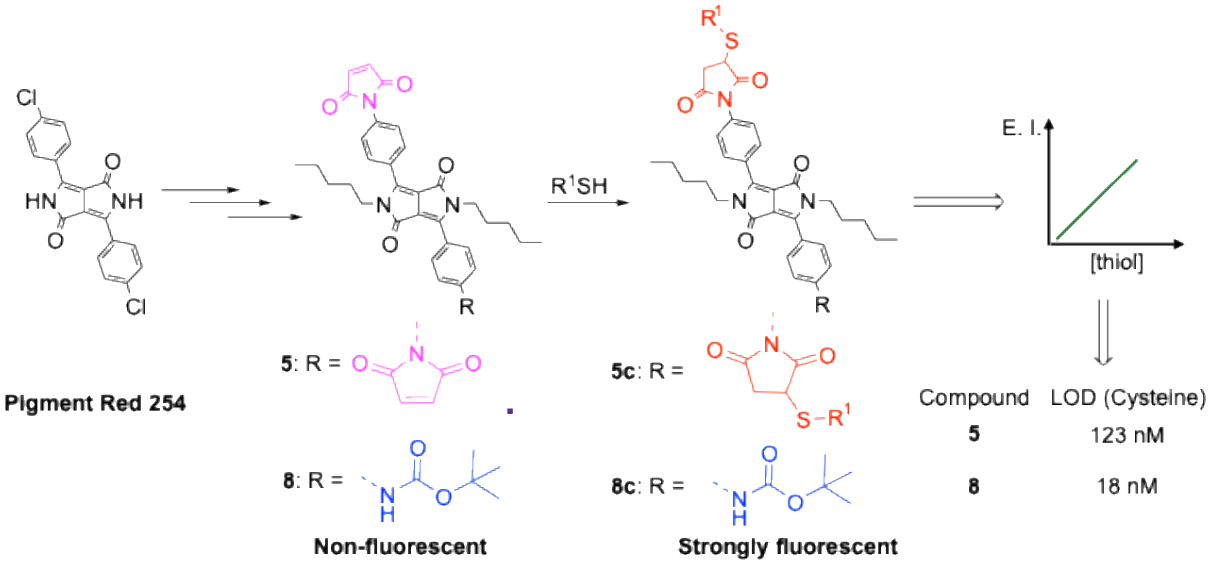


Fig.1. Synthesis of maleimide-substituted DPP **5** and **8** and their limits of detection for cysteine.

Acknowledgments
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Porphyrin–AZT Conjugates: Synthesis and Photophysical Evaluation

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Photodynamic therapy (PDT) is an emerging therapy that combines a photosensitizer (PS), light of a specific wavelength in the visible region, and dioxygen (O_2). The interaction of these three components leads to the generation of reactive oxygen species (ROS), namely singlet oxygen ($^1O_2$) [1]. Porphyrins have been extensively explored as PS due to their ability to be functionalized with various types of structures and molecules with proven biological activity [2], [3]. The conjugation of antiviral agents with PS is a promising strategy aimed at enhancing antiviral response and controlling viral infections [4-6].

In this work, porphyrin derivatives containing AZT units, an antiviral drug used to treat HIV, were synthesized. In this oral communication, the synthesis, structural characterization and photophysical evaluation of these derivatives will be discussed.

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Impact of regioisomerism in bianthracene-bis-porphyrin chiral conjugates

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The development of chiral π-conjugated nanomaterials has attracted growing attention due to their potential to generate chirality-dependent optical and electronic phenomena. Within this context, porphyrins (PORs) play a particularly important role due to their strong absorption, versatile photophysical properties and stability. Recently, increasing interest has focused on integrating achiral PORs with chiral aromatic systems, such as nanographenes and polyaromatic hydrocarbons (PAHs), enabling the development of π-extended moieties with promising chirality-dependent photophysical and electronic properties. Such systems hold considerable potential for wide range of research fields, such as optoelectronics, spintronics and biological imaging. [1-3]

In this work, we report the synthesis of two novel axially chiral bianthracene-bis-POR conjugates, in which a chiral bianthracene scaffold connects two POR chromophores through two different porphyrin possitions, *meso* and *β*, giving rise to two regioisomers (**Figure 1**). The resulting racemic mixtures were fully characterized by mass spectrometry, NMR and UV-Vis spectroscopies. The corresponding enantiomers were subsequently separated by chiral HPLC, and their chiroptical properties were studied in detail by circular dichroism (CD) spectroscopy. The CD results suggest that regioisomerism plays a key role in the optoelectronic properties of these conjugates, highlighting the importance of molecular connectivity in their chiroptical response. These findings establish new avenues for the rational design of bis-POR chiral platforms and enable the fine-tuning of their chiroptical properties. Such his might be highly appealing for a wide variety of research fields, such as optoelectronics, spintronics, and biological imaging.

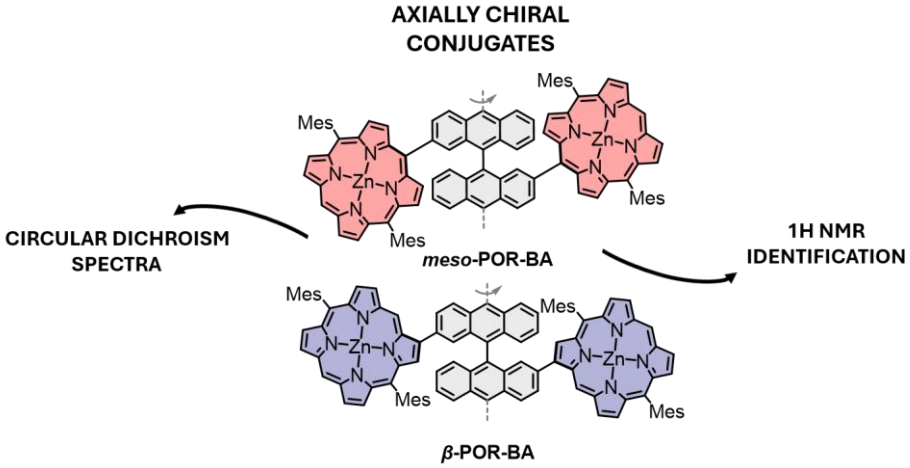


Fig.1. *meso* and *β* chiral bianthracene-bis-POR conjugates and their respective CD and ^{1}H NMR spectra.

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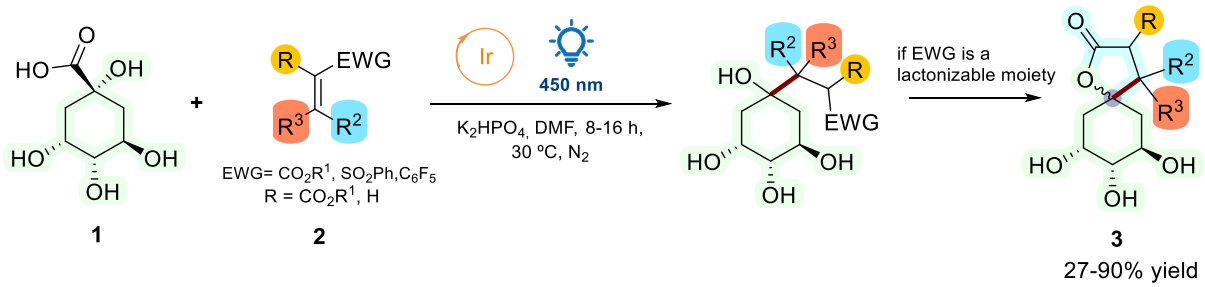
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(–)-Quinic acid as a natural chiron for the photocatalyzed synthesis of spirolactones

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Photocatalyzed Giese reactions are photoredox-mediated radical conjugate additions that enable sustainable synthetic routes by adding alkyl radicals to electron-deficient olefins, particularly when using visible light.[1] Among the radical precursors employed, carboxylic acids and their derivatives are particularly attractive due to their availability and ability to generate alkyl radicals through photochemical decarboxylation under mild conditions.[2] In this context, quinic acid (QA), naturally available in its enantiomerically pure form, represents an attractive chiron for the synthesis of new compounds. However, its structural modification often requires harsh reaction conditions and hazardous reagents, highlighting the need for milder and more sustainable approaches.[3] Such strategies are particularly relevant for the synthesis of γ-lactones and their spiro derivatives, which exhibit a range of biological activities, including anti-inflammatory, antiviral, antibiotic, and anticancer effects, making them valuable scaffolds in drug design. Developing greener, more efficient and stereocontrolled methods is crucial for exploring new derivatives and providing environmentally friendly solutions in drug development.[4], [5]

Combining all these aspects, we started a study of a promising and versatile transformation where QA (**1**), is used as a radical precursor for a photocatalyzed decarboxylative Giese-type conjugate addition with an alkylidene malonate (**2**), followed by lactonization to afford spirolactones (**3**) (**Scheme 1**). Optimization of this reaction was done through an extensive screening of photocatalysts, solvents and bases. Preliminary results reveal the impact of vicinal hydroxyl group protection of QA moiety on diastereoselectivity, thereby pointing to a promising platform for the development of stereocontrolled radical transformations and the synthesis of biologically relevant spirocyclic scaffolds.



Scheme 1. Standard conditions for QA tandem photocatalyzed decarboxylative Giese-addition followed by lactonization with QA.

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QUÍMICA Y SALUD

From Photochemistry to Phototoxicity: Linking the Photochemical Behavior of Food-Derived Chromophores to Cellular Response in Melanoma Cells

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Despite being traditionally valued for their antioxidant properties, several naturally occurring chromophores can absorb radiation and generate reactive oxygen species (ROS) upon light exposure [1-3]. In this study, curcumin, sodium copper chlorophyllin, riboflavin and quercetin were comparatively evaluated under standardized blue-light irradiation (405 nm) to investigate how their photochemical properties translate into cellular photodynamic responses and to establish their relative photodynamic efficiency.

The compounds were first characterized by UV–visible spectroscopy, and their photostability was evaluated by UHPLC after irradiation. Intracellular singlet oxygen production was assessed by confocal microscopy using SO Green™ 520AM Singlet Oxygen Sensor. Photodynamic activity was evaluated in A375 and B16-F10 melanoma cells under two treatment configurations: compounds were either removed after 1 h of pre-incubation to eliminate the extracellular/unbound fraction before irradiation or retained in the medium during irradiation. Long-term proliferative capacity was further investigated by clonogenic analysis.

Overall, curcumin showed the most effective and persistent photodynamic response, combining strong acute phototoxicity (70% loss of cellular viability at 3 µM) with pronounced inhibition of long-term colony formation (a 76% reduction in colony number following irradiation in the presence of 1.5 µM curcumin). Cellular retention, subcellular localization and/or interaction with photodamage-sensitive targets may contribute substantially to the observed activity. Its lipophilic character and ability to generate ROS other than singlet oxygen may further contribute to the photoinduced response. Riboflavin, despite being the least photostable of the four compounds, with substantial depletion of the parent peak accompanied by the formation of new species (lumichrome and lumiflavin), exhibited the strongest intracellular singlet oxygen-related response but substantially lower phototoxicity when the extracellular compound fraction was removed, demonstrating that ROS generation alone does not determine cellular photodynamic efficacy.

By applying a common characterization framework under identical blue-light irradiation conditions, this study enables a more meaningful comparison of structurally distinct food-derived chromophores and provides insight into the multifactorial nature of their photodynamic responses. These findings provide a basis for evaluating food-derived chromophores in blue-light-mediated photodynamic strategies, with potential downstream applications in skin-related and antimicrobial approaches.

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From β-Keto Reduction to Neurotoxicity: Cytotoxic and Oxidative Effects of Dihydropentedrone and Dihydromethylone in SH-SY5Y Cells

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Synthetic cathinones are new psychoactive substances whose toxicological evaluation has traditionally focused on parent compounds; however, increasing evidence suggests that metabolites may substantially contribute to overall biological effects and toxicity [1]. Their metabolic pathways include *N*-demethylation, *O*-demethylation, and β-keto reduction [2,3], yet the toxicological impact of these metabolites remains underexplored. Notably, carbonyl-reduced metabolites may exhibit higher cytotoxicity than their parent cathinones [4]. This work aimed to evaluate the cytotoxicity of the β-hydroxy metabolites dihydromethylone (DHM) and dihydropentedrone (DHP) and to assess the potential involvement of oxidative stress in DHP-induced cytotoxicity.

DHP and DHM were synthesized by $NaBH_4$-mediated reduction of the β-keto group of the corresponding parent cathinones [5]. Cytotoxicity was assessed in dopaminergic-differentiated SH-SY5Y cells after 24 h exposure using the Neutral Red uptake assay, and EC_{50} values were determined by nonlinear regression. Based on its cytotoxicity profile, DHP was further evaluated for intracellular reactive oxygen and nitrogen species (ROS/RNS) production using the DCFH-DA probe.

Both metabolites induced a concentration-dependent decrease in cell viability. DHP displayed greater cytotoxic potency, with an EC_{50} of 1423 µM, whereas DHM presented an EC_{50} of 3259 µM. Compared with previously reported values for the parent cathinones (~3000 µM) [6], DHP was more cytotoxic than pentedrone, while DHM showed a cytotoxicity profile similar to methylone. DHP exposure at 250 and 750 µM did not significantly alter ROS/RNS levels, whereas 1500 µM, close to its EC_{50}, induced a significant 13.7% increase in DCF fluorescence ($p < 0.0001$).

These findings indicate that β-keto reduction does not necessarily result in detoxification. The increased cytotoxic potency of DHP and the significant ROS/RNS production observed near its EC_{50} suggest that oxidative stress may contribute to its cytotoxicity, reinforcing the importance of including phase I metabolites in the toxicological assessment of synthetic cathinones.

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Translating the mind: a *point-of-care* electrochemical platform for miR-151a-3p in neurodevelopmental disorders

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Neurodevelopmental disorders, including Attention-Deficit/Hyperactivity Disorder (ADHD) and Autism Spectrum Disorder (ASD), affect millions of individuals worldwide; however, their diagnosis still relies heavily on subjective behavioral assessments defined in the DSM-5 [1]. This clinical challenge may lead to misdiagnosis, underscoring the urgent need for objective biomarkers. Circulating microRNAs (miRNAs) have emerged as promising candidates due to their critical roles in neural plasticity and their stability in biofluids [2]. Recent evidence highlights miR-151a-3p as a potential non-invasive biomarker, showing direct association with both disease diagnosis and therapeutic response [3].

This work presents the development of a disposable, label-free electrochemical biosensor designed for *point-of-care* miR-151a-3p screening. Specific DNA capture probes were immobilized onto the biosensor surface, with the entire assembly and hybridization events characterized by Cyclic-, Square-Wave Voltammetry, and Electrochemical Impedance Spectroscopy. Key experimental parameters, including probe density, self-assembled monolayer and hybridization conditions were optimized to maximize the charge-transfer resistance (R_{ct}) response and surface coverage.

Results demonstrate that the biosensor platform achieves high specificity, successfully discriminating the target miR-151a-3p from non-complementary sequences. Current efforts focus on validating its performance directly in complex biological matrices. Overall, this platform provides a cost-effective and rapid-response analytical approach, laying the groundwork for decentralized and objective screening tools in clinical neurodevelopmental care.

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Point-of-care quantification of salivary alpha-amylase using a vertical flow µPAD for stress monitoring in humans and pigs

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Salivary alpha-amylase (AMY) is a biomarker of nervous system activity, increasingly used to monitor physical and psychological stress in humans and animals. Additionally, it has also been associated with other health conditions, such as attention-deficit/hyperactivity disorder (ADHD) in children. However, conventional methods for AMY quantification, namely spectrophotometry assay, rely on expensive equipment, long processing times, and laboratory infrastructure, which limits their use in point-of-care settings. Since saliva is a biological fluid of non-invasively collection, as it can be collected without specialized operators and through a painless procedure, it makes frequent monitoring possible when combined with a simple analytical method.

In this work, a simple, fast, and low-cost microfluidic paper-based analytical device (µPAD) was developed for the colorimetric quantification of AMY in saliva. The method relies on the enzymatic hydrolysis of starch by AMY, followed by the iodine-starch reaction, in which the intensity of the blue colour decreases as AMY activity increases. The device was assembled without complex fabrication procedures, by stacking two layers of filter paper discs inside a laminating plastic pouch, while using a vertical flow approach for sample loading. Samples react with starch for 5 minutes, after which an iodine solution is added for a 15-minute colorimetric reaction, resulting in a total analysis time of 20 minutes and a sample volume of only 50 µL.

The µPAD showed a linear range of 10.0-50.0 U/mL (after sample dilution), with a limit of detection of 2.53 U/mL and a limit of quantification of 8.42 U/mL. After assembly, the devices remained stable for 60 days at room temperature, and the consumables cost was as low as 0.17 € per device (with 24 reading units). Validation with real human and porcine saliva samples confirmed the applicability of the proposed µPAD as an environmentally friendly and affordable point-of-care tool for salivary AMY monitoring, with potential use in stress assessment in humans and in welfare monitoring in veterinary contexts, namely in pigs.

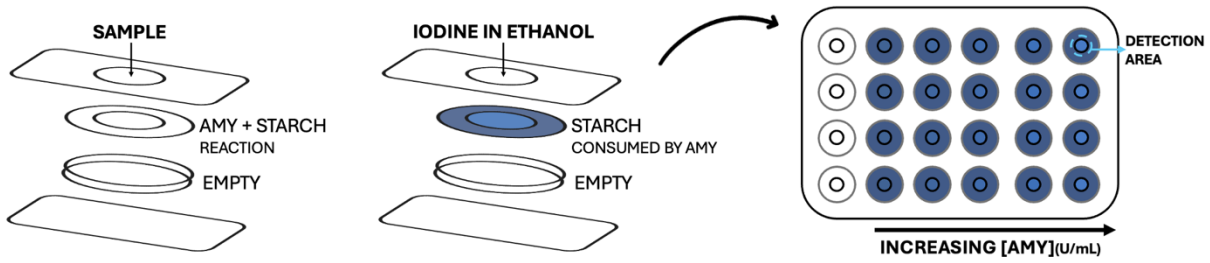


Fig.1. Schematic representation of the µPAD and the reaction principle for AMY determination in saliva, and the resulting coloured complexes and detection areas

Acknowledgments

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Light-Activated Zinc(II) Phthalocyanines for Enhanced Antimicrobial Photodynamic Inactivation of Gram-Positive Bacteria

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Antimicrobial resistance drives the search for alternatives, including antimicrobial photodynamic inactivation (aPDI), which combines a photosensitizer (PS), light, and molecular oxygen to inactivate bacteria [1,2]. In this context, zinc(II) phthalocyanines (ZnPc) dyes are attractive PS due to their photophysical properties, while the incorporation of boronic acid functionalities offers the opportunity to tune their molecular structure and biological performance [3].

This study investigated the aPDI of three boronic acid-functionalized ZnPcs against *Staphylococcus aureus*. The compounds included a tetrasubstituted (ZnPc **1**) and two octasubstituted derivatives (ZnPcs **2** and **3**). Antimicrobial performance was evaluated at concentrations of 5.0 and 10.0 μM under white light irradiation (100 mW cm^{-2}) for up to 60 min, both in the absence and presence of potassium iodide (KI) as a coadjuvant [3].

Antimicrobial efficacy depended on molecular structure and KI presence. ZnPc **1** achieved bacterial reductions of up to 7 Log units, while ZnPc **2** showed the highest activity, reaching the detection limit within 15 min with KI addition. In contrast, fluorinated ZnPc **3** exhibited moderate activity. These findings highlight the potential of boronic acid-functionalized ZnPcs, particularly ZnPc **2**, combined with KI coadjuvant, to enhance light-driven inactivation of Gram-positive bacteria.

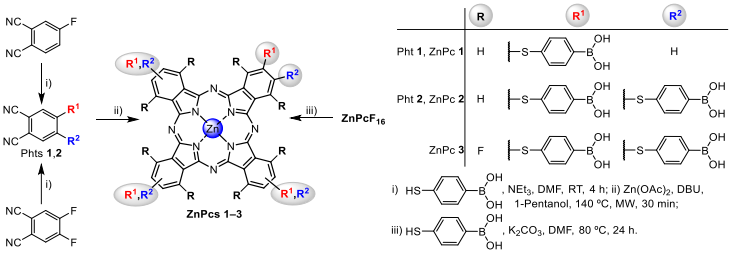


Fig. 1. Synthesis of boronic acid-based zinc(II) phthalocyanines (ZnPcs **1**–**3**).

Funding
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Design and Synthesis of Fluorinated Analogues of a Non-Nitrocatechol COMT Inhibitor for Neuroprotection in Dopaminergic Degeneration

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Dopaminergic degeneration and increased dopamine metabolism contributes to dopamine deficiency in neurodegenerative diseases such as Parkinson's disease [1]. The current therapeutic strategies aim to restore dopaminergic neurotransmission through the co-administration of the dopamine precursor L-DOPA and catechol-O-methyltransferase (COMT) inhibitors [2]. Although these approaches offer symptomatic relief, they do not halt the progression of neurodegeneration and raise concerns regarding long-term efficacy and toxicity [3]. This work aims to expand the library of COMT inhibitors through the synthesis and biological evaluation of analogues of Compound 9, a novel, selective COMT inhibitor with neuroprotective properties previously developed by our research team [4].

The synthetic approach involves a Michael addition of a protected 3-hydroxy-4H-pyran-4-one to appropriately substituted primary arylamines under mild acidic conditions, followed by a deprotection step to obtain the final compounds. The structures of the final products were confirmed by nuclear magnetic resonance (NMR) spectroscopy. The obtained compounds were subsequently evaluated for their inhibitory activity against rat liver membrane-bound COMT (MB-COMT) and assessed for their drug-like properties. The results obtained so far will be presented in this communication.

This work aims to expand the library of COMT inhibitors and explore the potential of the synthesized analogues for further development.

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The First Sila-Derivatives of Vitamin D: Synthesis and Biological Application in Triple-Negative Breast Cancer Therapy

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Breast cancer remains one of the most frequently diagnosed types of cancer worldwide and continues to be a major cause of cancer-related mortality.[1] Despite significant therapeutic advances, the development of more effective and safer treatment strategies remains an important challenge. Vitamin D receptor (VDR) signalling regulates several processes relevant to tumour development and progression, including cell proliferation, differentiation, and apoptosis, supporting the investigation of VDR modulation as a therapeutic approach.[2,3] Calcitriol (1,25-dihydroxyvitamin D_3) is the active form of vitamin D and exhibits antiproliferative activity in several cancer models.[2,3] However, its therapeutic application is limited by hypercalcaemia at therapeutically relevant doses.[2,3] Vitamin D analogues capable of maintaining VDR activity while reducing hypercalcaemic effects therefore represent a relevant strategy to overcome this limitation.

In this context, carbon-to-silicon substitution was explored for the first time in vitamin D analogues as a bioisosteric strategy to improve their biological profile.[4] Six novel sila-vitamin D analogues were therefore designed by replacing the C25 carbon atom of the calcitriol side chain with silicon and synthesised via a Wittig-Horner approach. Their interaction with VDR was evaluated through ligand-binding and transcriptional activity assays, while X-ray crystallographic studies were performed to characterise the complexes formed by the sila-analogues and the VDR ligand-binding domain. Competitive binding assays demonstrated that the sila-analogues retained high affinity for VDR, with IC_{50} values comparable to those of calcitriol, and structural analysis further revealed additional interactions between the modified side chains and the VDR ligand-binding domain, contributing to the stabilisation of the active VDR conformation. Despite retaining transcriptional activity, the analogues showed significantly reduced hypercalcaemic activity in mice after 21 days of treatment compared with calcitriol. The analogues also significantly reduced the proliferation of triple-negative breast cancer cells (MDA-MB-231), and Sila-**3–6** further enhanced the antiproliferative effect of paclitaxel in both 2D and 3D culture models.

These findings establish silicon incorporation as a valuable strategy to preserve VDR activity while addressing a major limitation associated with calcitriol, supporting further preclinical development of sila-vitamin D analogues for anticancer applications.

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First-in-Class Melanostatin Hybrids as Potent Modulators of the Dopamine D_2 Receptors with Neuroprotective Activity

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Current therapy for Parkinson's disease (PD) is constrained by the long-term complications of levodopa, creating a clear need for new strategies to modulate dopaminergic signaling.[1] Melanostatin (MIF-1) has attracted attention as a privileged scaffold for dopamine D_2 receptor (D_2R) modulation due to its intrinsic positive allosteric modulatory activity.[1] However, its potency and drug-like properties must be improved before clinical translation.

In this work, nicotinic acid (Nic), a vitamer of vitamin B_3, was used as a proline (Pro) bioisostere, synthesizing twelve novel vitamin B_3-MIF-1 hybrids.[1] Nicotinoyl-L-leucylglycinamide (**6c**) emerged as the lead compound, increasing dopamine potency 5.11-fold at 0.01 nM and protecting dopaminergic-differentiated SH-SY5Y cells against neurotoxicity induced by 50–100 μM of 6-OHDA.[1]

Additionally, Pro-to-Nic substitution showed no cytotoxicity in HepG2, reduced P-glycoprotein-mediated efflux, and preserved β-turn conformational propensity, supporting improved oral drug-like properties.[1] Taken together, these results position **6c** as the first dual-acting MIF-1 derivative and establish Nic as a privileged Pro surrogate for next-generation MIF-1-based PD therapeutics.[1]

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Chemical Modification of the Anti-EGFR Monoclonal Antibody with 11-Mercaptoundecanoic Acid: UV–Vis and FTIR Characterization

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The chemical functionalization of monoclonal antibodies is a relevant strategy for the development of hybrid systems for future biomedical applications. In this study, the chimeric anti-EGFR monoclonal antibody (cetuximab), obtained from the commercial drug Erbitux®, was used considering its availability and acquisition cost. The objective was to chemically modify the antibody with 11-mercaptoundecanoic acid (MUA).

For antibody purification and extraction, Amicon Ultra-0.5 centrifugal filters with a 3 kDa molecular weight cutoff were used at 14,000 × g for 30 min at 21 °C, followed by successive washes with ultrapure water. Chemical modification was performed through a coupling reaction using EDC and sulfo-NHS, with the aim of forming amide bonds between the carboxyl groups of MUA and the available amine groups on the antibody [1,2]. The samples were characterized by ultraviolet-visible (UV–Vis) spectroscopy and Fourier-transform infrared (FTIR) spectroscopy.

After purification, the UV–Vis spectra showed absorption bands at approximately 220 and 270 nm. Following MUA modification, these bands shifted to 225 and 271 nm, respectively, with an increase in absorbance. The A260/A280 ratio was approximately 1.10. FTIR analysis showed a shift in the amide II band from 1541 to 1523 cm^{-1}, while the amide I band remained at 1637 cm^{-1} and the amide III band shifted slightly from 1238 to 1236 cm^{-1}. C–H stretching bands were observed between 2876 and 2961 cm^{-1}. A subtle spectral change was also observed in the 2500–2600 cm^{-1} region, which is associated with S–H stretching [3–5]

The UV–Vis and FTIR results indicate spectral changes associated with MUA treatment. The shift in the amide II band, together with the changes in the C–H and S–H regions, supports the proposed chemical modification, although further analyses are needed to confirm covalent attachment [3–5]. These findings provide a starting point for subsequent studies on the conjugation of the modified antibody with metallic nanoparticles for the development of hybrid systems with potential biomedical applications [4].

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Preliminary Mechanistic Studies of New Pyrimidine-Based Compounds for Osteosarcoma Therapy

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Osteosarcoma is the most common and aggressive primary bone malignancy of mesenchymal origin. It affects predominantly children, adolescents and young adults, with a second smaller incidence peak in older people. This type of cancer is characterized by heterogeneity, chemoresistance and a high rate of metastasis, mostly to the lungs and occasionally to bone or lymph nodes. According to the Sarcoma Foundation of America, there are 4110 new cases and 2210 deaths estimated for 2026 in the United States. [1-5]

The standard care of osteosarcoma has remained unchanged and relies on surgical resection combined with neoadjuvant and adjuvant chemotherapy, typically including doxorubicin, cisplatin and high doses of methotrexate [1,2,3,5]. Although this approach has proven effective in non-metastatic osteosarcomas, with a 5-year survival rate of approximately 69%, therapeutic options for metastatic/recurrent osteosarcoma remain limited, as this rate falls considerably to 33%. [4]

Considering the limited improvement in survival outcomes for patients with osteosarcoma over the past four decades, there is an urgent need to develop innovative and more effective therapeutic strategies [1-3]. In this study, the aim of our research group was to explore pyrimidine-based compounds as a novel class of therapeutics for osteosarcoma.

A series of new alkylated pyrimidine-based compounds was synthesized and tested *in vitro* for their activity against the 143B osteosarcoma cell line. Following 48-hour treatment, cell viability and growth were evaluated using resazurin and sulforhodamine B assays, respectively. The derivative bearing a 4-($HOCH_2CH_2CH_2$)O substituent exhibited the most pronounced anti-osteosarcoma activity compared with the other derivatives tested. The first mechanistic studies performed using Annexin V/PI and cell-cycle analyses showed that this derivative induces apoptosis and causes cell-cycle arrest.

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QUÍMICA TEÓRICA

WFS4PLAS: SIMULATING MICROPLASTIC ADSORPTION

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The rapid spread of microplastics in aquatic ecosystems has triggered significant concern regarding their adverse effects on environmental and global health, particularly as viable solutions have yet to emerge. Once dispersed, microplastics can exist for hundreds of years [1], being ingested by organisms and accumulating in the food chain [2]. Membrane solutions are among the most promising methodologies for wastewater treatment, but current processes remain expensive and mostly rely on fossil-fuel-derived polymers and non-green solvents [3].

The WFs4Plas project aims to develop sustainable membrane systems based on functionalized wood fibers (WFs) and other carbon-based materials for the efficient removal of microplastics from water, coupled with their catalytic depolymerization. This objective is pursued through an integrated approach that combines experimental techniques with computational modelling. Molecular models of cellulose Iβ, graphene sheets, and lignin surfaces have been constructed in the presence of representative polyethylene terephthalate (PET), polystyrene (PS), and nylon 6 to evaluate adsorption behavior. These insights support the rational design of advanced membrane materials, reducing dependence on fossil-derived resources while enhancing microplastic remediation efficiency. Furthermore, weathered polymers are also being modelled to simulate real microplastics affected by the environment. These findings will guide the experimental simultaneous task being performed by other researchers in WFs4Plas.

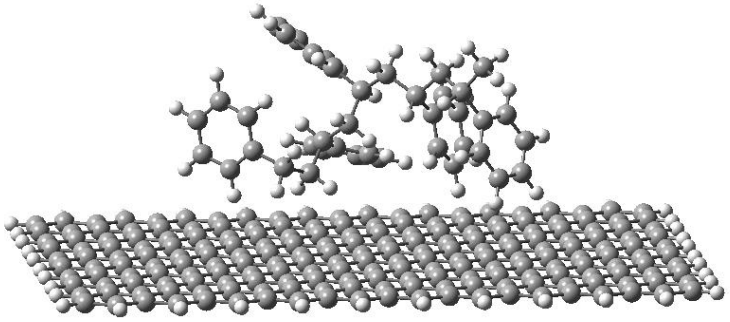


Fig.1. Polystyrene interacting with a graphene surface.

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Ion Structure and Dynamics in Ionic Liquids Confined within MXene Electrodes: Molecular Insights into Supercapacitor Charging

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Electric double layer capacitors (EDLCs) are promising energy storage devices for applications requiring rapid charge and discharge. Their performance is governed by the molecular organization of ions at electrified interfaces, which is strongly influenced by pore confinement, electrode properties, and electrolyte structure. [1,2] Here, we employ atomistic molecular dynamics simulations under constant potential conditions [3] to investigate ion arrangement, dynamics, and charging mechanisms in MXene-based supercapacitors.

Model systems consisting of slit-pore MXene electrodes filled with the ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate were studied for different pore widths, applied potentials, and surface terminations. [4] MXene electrodes functionalized with F, Cl, Br, O, S, and OH groups were considered to elucidate the role of surface chemistry in controlling ion organization within confined ionic liquids. The effects of confinement and electrode termination were analyzed through ion density distributions, interfacial layering, charge distribution, and ion mobility.

The simulations reveal that both pore dimensions and MXene surface chemistry strongly influence ionic packing and charging behavior. Surface terminations modify ion-electrode interactions, interfacial ordering, and the balance between charge accumulation and ion transport. These results provide molecular level insights into the charging mechanisms of MXene-based EDLCs and highlight the importance of considering electrode chemistry together with confinement effects when understanding energy storage at electrified interfaces.

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Green-Solvent Extraction of Propolis: Experimental Assessment and Machine Learning Prediction of Total Phenolic Content

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Ultrasound-assisted extraction (UAE) provides an efficient approach for recovering bioactive compounds from propolis, but selecting suitable solvents and extraction conditions remains challenging due to the chemical diversity of solvent systems [1]. This study investigated ultrasound-assisted extraction of Bragança propolis using conventional hydroethanolic and alternative green solvents, combined with machine learning (ML) to predict total phenolic content (TPC) and identify the factors governing extraction efficiency.

Several ethanol-free alternatives were evaluated, such as glycerol, 1,2-propanediol, lactic acid-based mixtures and ethyl lactate, among others. Among the alternative solvents, ethyl lactate achieved the highest TPC (181 mg GAE g^{-1}) and TFC (72 mg QE g^{-1}) under the evaluated conditions.

To investigate the relationships between solvent chemistry and TPC, a dataset comprising 86 observations done on our lab, including 25 distinct solvent mixtures was assembled using COSMO-RS-derived molecular descriptors and experimental extraction parameters. Six descriptors derived from sigma profiles characterized molecular regions associated with hydrogen-bond donor, non-polar and hydrogen-bond acceptor interactions [2]. Nine non-linear regression algorithms were evaluated using five-fold cross-validation, grid-search hyperparameter optimization and a mixture-out training/test split to assess generalization to previously unseen solvent mixtures. The Gradient Boosting Regressor achieved a cross-validated $Q^2$of 0.689 and a test-set $R^2$of approximately 0.90, with a mean absolute error of approximately 11.7 mg GAE g^{-1}. SHapley Additive exPlanations (SHAP) identified the molecular descriptors as the most influential predictors [3]. The most influential was the non-polar descriptor S3, with higher values generally associated with increased predicted TPC, this relation was inverse on H-bond acceptors such as S6.

Overall, integrating experimental extraction with interpretable ML provides a framework for identifying promising green solvent systems, understanding the influence of solvent chemistry and extraction conditions to further identify promising candidates that can lead to the development of efficient propolis extraction processes for potential food and cosmetic applications.

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QUÍMICA ALIMENTARIA

Judías carillas: composición nutricional de un alimento tradicional consumido en el área mediterránea.

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La judía carilla (*Vigna unguiculata* L. Walp. subsp. *unguiculata*) es una leguminosa de origen africano y consumida en la zona mediterránea desde la antigüedad. Actualmente se encuentra ampliamente distribuida, existiendo referencias bibliográficas de su consumo en Asia o América [1, 2]. Se trata de una planta herbácea trepadora de hojas trifoliadas y color verde brillante. Los tallos son volubles y soportan las inflorescencias de flores de color blanco-crema. El fruto es una legumbre alargada y estrecha, con semillas arriñonadas blancas con una mancha negra alrededor del hilo [3]. Su composición ha sido previamente estudiada en otras zonas del mundo, pero no existen datos bibliográficos acerca de la composición de las semillas procedentes de la península ibérica. Por ello, el presente trabajo tiene como objetivo el análisis de la composición centesimal de judía carilla: humedad, sales minerales (cenizas), proteínas, grasa total, fibra alimentaria [4], e hidratos de carbono disponibles totales [5] en muestras de semillas procedentes de dos localidades distintas (Aldeanueva de la Vera, Cáceres y Velayos, Ávila). Los resultados obtenidos (Figura 1) fueron comparados con los correspondientes a la judía blanca (*Phaseolus vulgaris* L.), cuyos datos se obtuvieron de tablas de composición de los alimentos (BEDCA). Destaca el contenido en fibra e hidratos de carbono, superior al presente en la judía blanca.

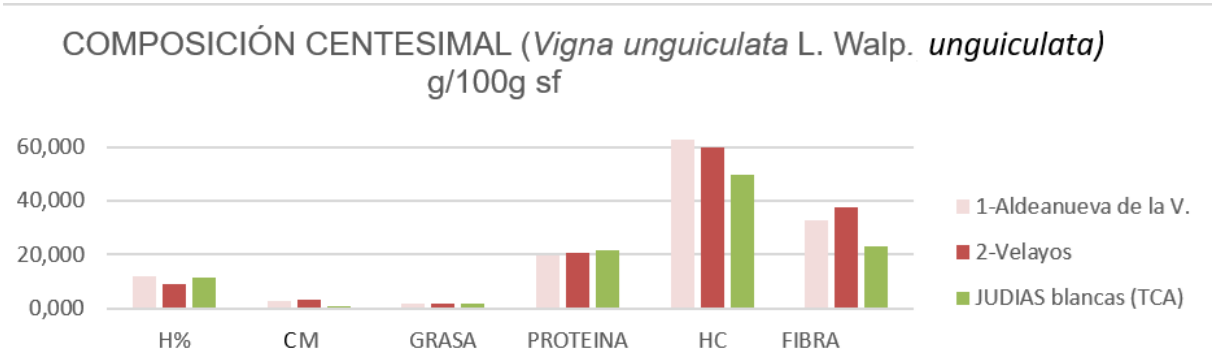


Fig.1. Composición nutricional de las judías carillas frente a la judía blanca. H%: porcentaje de humedad; CM: contenido mineral; HC: hidratos de carbono totales

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BEVEGAL — Ultrasound-Assisted Formulation of Plant-Based Beverages from Galician Chestnut and Faba de Lourenzá

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The growing demand for plant-based foods has increased interest in alternative raw materials with high nutritional value and regional identity [1]. In this work, non-fermented plant-based beverages were developed from two Galician protected raw materials [2-3], chestnut and Faba de Lourenzá, using ultrasound-assisted processing as a sustainable technological strategy.

A stepwise optimization approach was followed. Conventional soaking was first compared with ultrasound-assisted soaking, followed by evaluation of a post-soaking ultrasound treatment and the influence of particle-size reduction order. Processing conditions were subsequently optimized through a 12-run asymmetric experimental design considering soaking ratio and time, ultrasound time and temperature, and cooking time. Antioxidant capacity (DPPH), total phenolic content (Folin-Ciocalteu), soluble protein content (BCA), and 24 h colloidal stability were used as response variables. The optimized beverages were further characterized in terms of rheological behavior, proximate and elemental composition, proteins, sugars, vitamins, organic acids, phenolic compounds by HPLC-QTOF-MS/MS, and volatile compounds by HS-SPME-GC-MS. Protein digestibility and phenolic bioaccessibility were also evaluated using the INFOGEST in vitro digestion model.

Ultrasound-assisted soaking reduced processing time from 24 h to 1 h while improving bioactive and protein-related responses. Further ultrasound treatment enhanced antioxidant capacity and stability, with pre-ultrasound grinding improving extractability and reproducibility. Chestnut beverages showed higher antioxidant activity, phenolic retention and stability, whereas Faba de Lourenzá beverages had higher protein content and more structured pseudoplastic behavior. After in vitro digestion, chestnut fractions were enriched in tannin-related compounds, while Faba de Lourenzá showed enrichment in phenolic acids and glycosylated flavonoid/isoflavone-related compounds. SDS-PAGE indicated partial proteolysis after digestion.



***Fig 1**. The BeVeGal project logo.*

Overall, ultrasound-assisted processing combined with experimental design provides an effective strategy for obtaining differentiated plant-based beverages from locally relevant Galician raw materials. The approach simultaneously reduces processing time and promotes the recovery of compounds of nutritional and functional interest, supporting the valorization of chestnut and Faba de Lourenzá in the development of sustainable plant-based foods.

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Assessment of Environmental Contaminants in Innovative Canned Seafood Products

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Portugal is among the largest consumers of fishery and aquaculture products in the European Union, with an apparent consumption of approximately 54 kg per capita per year [1]. Canning, therefore, represents an important method of seafood preservation and distribution, offering extended shelf life, room-temperature stability, and convenience to consumers. As part of the BlueBioeconomyPact project (vertical WP4 FOOD) six innovative canned products with reduced sodium content were developed by lowering the amount of salt used, partially replacing sodium chloride with potassium chloride or microencapsulated flavouring ingredients, along with two ready-to-eat canned meals based on Atlantic chub mackerel, legumes and vegetables. As fish and other marine-derived ingredients can contain significant levels of environmental contaminants that pose potential risks to human health and represent a broader public health concern [2], the objective of this study was to evaluate the chemical safety of these products.

A total of 40 environmental contaminants, including organochlorine pesticides, polychlorinated biphenyls, brominated flame retardants, organophosphorus pesticides, organophosphate esters, and dioxins, were assessed using a single QuEChERS extraction and dispersive solid-phase extraction clean-up. Quantification was performed by gas chromatography flame photometric detection and electron capture detection. The method was validated for linearity, method detection and quantification limits, precision, recovery, matrix effect, and relative combined measurement uncertainty following the European Commission's SANTE guidelines [3,4].

Trace levels of contaminants were detected in only two of the six canned products. Tris(2-ethylhexyl) phosphate (TEHP) was detected in canned tuna with microencapsulates of lemon and pepper, while hexachlorobenzene (HCB), tributyl phosphate (TnBP), and TEHP were detected in the canned mackerel ready-to-eat meal. All detected concentrations were below the applicable European Commission regulatory limits [5]. Overall, these results indicate that the developed canned products complied with safety requirements and indicate no apparent chemical safety concern for the target contaminants.

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Subcritical Water Extraction of Bioactive Compounds from Portuguese Cabbage *(Brassica oleracea)* by-products for Sustainable Aquafeed Ingredients

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The global aquaculture industry is undergoing a “Blue Transformation”, driving the search for sustainable and functional feed ingredients to reduce reliance on finite marine resources and mitigate environmental impacts [1]. Brassica oleracea by-products represent an underutilised resource within a circular economy framework [2, 3]. They contain bioactive compounds, particularly glucosinolates (GLS), which upon enzymatic hydrolysis generate isothiocyanates (ITCs) with antioxidant and immunomodulatory properties [4]. However, careful process control is required to minimise the formation of undesirable goitrogenic compounds and nitriles [5].

This study aimed to optimise subcritical water extraction (SWE) of bioactive compounds from cabbage (Brassica oleracea var. costata) for potential use as a functional aquafeed additive. A Box-Behnken design (17 runs) investigated temperature (100–200 °C), time (20–60 min), and pressure (40–100 bar). Total phenolics (TPC), total flavonoids (TFC), total carotenoid content (TCC), and isothiocyanates (ITCs) were quantified, along with antioxidant activity evaluated by ABTS, DPPH, and FRAP assays.

All responses were adequately described by significant quadratic models ($p < 0.001$; adjusted $R^2 = 0.932–0.981$). Temperature was the dominant factor affecting most responses. Within the investigated domain, multi-response optimisation identified 200 °C, 58.9 min, and 40.0 bar as the optimal conditions (desirability = 0.948), with predicted TPC of 79.55 mg GAE/g extract, TCC of 0.795 mg/g extract, and ITCs of 23.26 mg AITC eq./g extract. Within the SWE design, TPC was strongly correlated with ABTS, DPPH, and FRAP responses ($r = 0.984–0.991$; Benjamini–Hochberg-adjusted $p < 0.001$), supporting a close association between phenolic recovery and antioxidant activity.

High-temperature SWE promoted the recovery of several bioactive compounds and generated extracts with high antioxidant potential. The optimised process therefore represents a promising strategy for valorising cabbage by-products as functional ingredients for aquafeed applications. Future studies should focus on in vivo feeding trials and life cycle assessment to further evaluate the biological efficacy and environmental sustainability of the proposed approach [6–8].

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Da capacidade antioxidante à proteção lipídica: avaliação de extratos de macroalgas em condições de oxidação acelerada

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As macroalgas constituem uma fonte promissora de compostos com propriedades antioxidantes [1]. Contudo, a capacidade antioxidante determinada por ensaios químicos não se traduz necessariamente em proteção eficaz de matrizes lipídicas [2]. Num estudo anterior, dez macroalgas comerciais foram submetidas a extração com água subcrítica (SWE; 140 e 190 °C) e a extração assistida por ultrassons (UAE; 10 e 20 min), tendo a SWE a 190 °C originado, em geral, os teores mais elevados de compostos fenólicos totais e capacidade antioxidante [1]. O presente trabalho avaliou a capacidade funcional desses extratos de inibir a oxidação lipídica em óleos alimentares sob condições de armazenamento acelerado [3].

Os extratos de dez espécies de macroalgas (quatro castanhas, duas verdes e quatro vermelhas) foram incorporados em óleo de girassol, frequentemente utilizado na indústria conserveira, e armazenados a 45 °C por 16 dias. A oxidação foi monitorizada aos 4, 8, 12 e 16 dias através da determinação do índice de peróxidos (PV), do valor de p-anisidina (ipA), das substâncias reativas ao ácido tiobarbitúrico (TBARS) e do índice de oxidação total (TOTOX). O óleo sem antioxidante e o butil-hidroxitolueno (BHT) foram utilizados como controlos. O efeito da espécie, das condições de extração e do tempo de armazenamento foi avaliado estatisticamente e complementado pela determinação de índices de proteção relativamente ao óleo e ao BHT.

A resposta oxidativa dependeu fortemente da espécie, da condição de extração e do tempo de armazenamento. O PV apresentou interação significativa entre extração × tempo em todas as espécies, enquanto o TBARS também foi marcadamente dependente do tempo. Em contraste, o ipA e o TOTOX apresentaram padrões de extração mais estáveis em várias espécies. A análise integrada das 40 combinações espécie × extração revelou perfis distintos de proteção primária e secundária. O extrato de *Palmaria palmata* obtido por UAE durante 10 min conferiu a maior proteção global contra a oxidação primária, enquanto o extrato de *Porphyra dioica* obtido nas mesmas condições apresentou o melhor desempenho global relativamente à oxidação secundária. Estes resultados contrastam com a superioridade da SWE a 190 °C observada anteriormente em ensaios de TPC, FRAP e ABTS, demonstrando que uma elevada capacidade antioxidante química não implica necessariamente maior eficácia numa matriz lipídica [2].

Os resultados evidenciam a importância de avaliar antioxidantes naturais em sistemas alimentares reais através de marcadores complementares das diferentes fases da oxidação. A seleção de *P. palmata* e *P. dioica* para estudos subsequentes foi sustentada pelos seus perfis de proteção específicos e complementares.

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Cerrando el ciclo agroalimentario: recuperación asistida por ultrasonidos de antioxidantes a partir de hojas y tallos de pimiento

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La creciente generación de residuos agrícolas ha impulsado la búsqueda de estrategias de valorización sostenible en el marco de la bioeconomía circular. En este contexto, el cultivo de pimiento (*Capsicum annuum* L.) genera cantidades considerables de biomasa vegetal al final del ciclo productivo, que permanece en gran medida infrautilizada a pesar de su riqueza en fitoquímicos con propiedades antioxidantes y potencial inhibidor frente a enzimas asociadas a la diabetes [1]. El aprovechamiento de esta biomasa como fuente de compuestos bioactivos de alto valor añadido requiere tecnologías de extracción eficientes y sostenibles. Entre ellas, la extracción asistida por ultrasonidos (UAE) constituye una alternativa prometedora, ya que favorece la disrupción de las estructuras celulares mediante cavitación acústica, facilita la liberación de compuestos intracelulares y permite reducir el tiempo de extracción y el consumo de disolventes [2,3]. Por ello, el presente estudio tuvo como objetivo optimizar las condiciones de UAE para la recuperación de compuestos bioactivos a partir de biomasa aérea de pimiento (hojas y tallos) al final del ciclo productivo. Para ello, se aplicó un diseño compuesto central combinado con metodología de superficie de respuesta (RSM), utilizando como variables independientes la amplitud de ultrasonidos (20–100%) y la proporción de etanol en el disolvente (0–100%, *v/v*). Como variables de respuesta se evaluaron el rendimiento de extracción, el contenido fenólico total y la actividad antioxidante *in vitro* mediante los ensayos DPPH, ABTS y de inhibición del blanqueamiento de la crocina. Aunque el trabajo experimental se encuentra todavía en curso, se espera ajustar modelos polinómicos capaces de describir adecuadamente el proceso de UAE e identificar las condiciones óptimas de extracción. Estas condiciones serán posteriormente verificadas experimentalmente mediante extracciones realizadas en las condiciones predichas y la comparación entre las respuestas experimentales y las predichas. El extracto obtenido en las condiciones optimizadas será posteriormente caracterizado para identificar y cuantificar sus compuestos fenólicos individuales. En conjunto, este trabajo pretende establecer un proceso de UAE verde y optimizado para la obtención de extractos ricos en compuestos fenólicos y con actividad antioxidante a partir de biomasa aérea de pimiento al final del ciclo productivo, contribuyendo a su valorización sostenible y a su potencial aprovechamiento como fuente de ingredientes de alto valor añadido para futuras aplicaciones en el sector agroalimentario.

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Validación analítica de un método enzimático para la cuantificación de azúcares totales en vinos y bebidas espirituosas

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La determinación del contenido en azúcares constituye un parámetro de gran relevancia en el control de calidad de vinos y bebidas espirituosas, debido a su influencia en las características organolépticas, la clasificación comercial y el cumplimiento de la legislación vigente [1].

En este trabajo se aborda la validación de un método enzimático automatizado mediante el analizador Y15 de Biosystems [2], para la determinación de azúcares totales en vinos y bebidas espirituosas, conforme a los requisitos establecidos en la norma UNE-EN ISO/IEC 17025:2017 [3], evaluándose los principales parámetros de desempeño analítico: linealidad, límites de detección y cuantificación, precisión, exactitud e incertidumbre de medida.

Los resultados obtenidos mostraron una linealidad adecuada en el intervalo estudiado (0,8-400,0 g/L). Los límites de detección y cuantificación permiten una correcta determinación de azucares en las matrices de estudio. La precisión, evaluada en términos de repetibilidad y precisión intermedia demuestra que el método es capaz de proporcionar resultados fiables y reproducibles. La exactitud se evaluó mediante estudios de recuperación analítica, participación en ejercicios intercomparativos, y comparación con un método de referencia, mostrando en todos los casos valores satisfactorios. También se evaluó la incertidumbre estimada resultando adecuada para el uso previsto, confirmando la fiabilidad del método para la determinación de azúcares totales en las matrices analizadas. Por último, también se estableció un plan de control de calidad interno que permita verificar el correcto funcionamiento del método y detectar posibles desviaciones durante su aplicación rutinaria.

La metodología propuesta presenta ventajas operativas asociadas a su automatización, permitiendo realizar los análisis de forma eficiente y fiable, con un reducido consumo de muestra y reactivos. Estas características contribuyen a incrementar la capacidad analítica y optimizar los tiempos de procesamiento. Se demuestran la idoneidad del método enzimático para su incorporación a la rutina analítica de un laboratorio de análisis de rutina.

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Towards a low-cost flow-based method for selenium quantification in common bean

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Selenium (Se) is an essential micronutrient for humans and animals, but the gap between deficiency and toxicity is narrow [1]. Legumes are protein-rich and, as most Se occurs in protein-bound forms, they are a strategic target for Se biofortification. Selenium can benefit plants by modulating antioxidant enzymes (glutathione peroxidase and glutathione S-transferase), regulating reactive oxygen species, and maintaining cellular thiol homeostasis [2]. This improves photosynthesis, nutrient homeostasis, and reduce toxic metal uptake [2, 3]. However, excess Se causes oxidative stress and impaired development [1, 2, 3]. Understanding this sensitive Se equilibrium in legumes depends on accurate, routine quantification, which is limited by the cost and operating requirements of conventional methods, namely ICP-MS, hydride generation AAS and HPLC-ICP-MS.

Spectrophotometric methods usually offer better cost-effectiveness because they do not require expensive equipment or high operating costs. In this work, we chose a colorimetric reaction based on the oxidation of iodide by Se in an acidic medium, with starch as the chromogenic reagent, because it uses inexpensive reagents and simple spectrophotometric detection [4]. Combining the colour reaction with a flow analysis approach can improve the method further, as flow techniques provide controlled reaction conditions, reduced reagent consumption, and high sample throughput. In this context, this work aimed to develop and optimise a sequential injection spectrophotometric method based on the KI-starch reaction for Se determination in common bean (*Phaseolus vulgaris* L.). Method optimisation covered physical (flow rates, reaction coil lengths) and chemical (reagent concentration, masking agents) parameters to achieve the best analytical performance for future Se quantification in common bean.

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Formation and Characterization of Insoluble Anthocyanin–λ-Carrageenan Complexes: Interactions, Thermal Stability, and Release Behaviour

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Anthocyanins are natural pigments with antioxidant properties, but their application in food systems is constrained by their sensitivity to environmental conditions. Complexation with charged biopolymers offers a strategy to improve their stability and modulate their release. However, the formation and functional properties of insoluble anthocyanin-based complexes remain insufficiently explored.

This study investigated the formation of insoluble complexes between blackberry anthocyanin extract (BAE) and λ-carrageenan (λ-CRG), focusing on the interactions involved, structural morphology, thermal stability, and anthocyanin release behaviour. The anthocyanin profile of BAE was characterized, with cyanidin-3-*O*-glucoside identified as the predominant compound.

Optimal complex formation was achieved at pH 3 and a λ-CRG/BAE weight ratio of 0.05. FTIR-ATR analysis supported the occurrence of electrostatic interactions and structural rearrangements upon complexation, consistent with the association between positively charged anthocyanins and negatively charged sulfate groups of λ-CRG. Scanning electron microscopy revealed a porous, network-like morphology, while thermal analysis indicated enhanced thermal resistance compared with the free extract. Release studies showed limited anthocyanin diffusion over 8 h and were consistent with a Fickian diffusion model. The diffusional exponent (*n*) varied with pH and ionic strength, indicating that the release behaviour was influenced by the surrounding medium.

These findings establish a relationship between complex formation, material structure, thermal stability, and anthocyanin release, highlighting the potential of insoluble anthocyanin–λ-carrageenan complexes as a strategy for improving anthocyanin stability and modulating their release in food-related applications.

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Efeito da secagem na composição nutricional de farinhas produzidas com mirtilos de refugo

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A cultura do mirtilo em Portugal tem registado um crescimento significativo nos últimos anos, no entanto, uma parte relevante da colheita não cumpre os requisitos necessários para comercialização em fresco, sobretudo ao nível do estado de maturação e calibre. Estes mirtilos de refugo, dependendo das suas características, são encaminhados para a alimentação animal (categoria A), para a indústria de congelação (categoria B) ou para a destilação (categoria C). Contudo, estes frutos contêm quantidades elevadas de compostos bioativos que podem ser valorizados pela criação de novos produtos de valor acrescentado e, assim aumentar a sustentabilidade da cadeia produtiva dos mirtilos. Assim, neste estudo, as três categorias de mirtilos foram desidratadas, e caracterizadas quanto à sua composição nutricional de modo a selecionar as categorias mais promissoras para o desenvolvimento de uma farinha de mirtilo.

As diferentes categorias de mirtilos, fornecidas pela GreenFactor (Braga, Portugal) foram estabilizadas por liofilização e por secagem por ar quente a diferentes temperaturas (40º C; 45º C; 50º C; 55º C e 60º C). Após o processo de desidratação, as amostras foram trituradas para obtenção da farinha e esta foi analisada quanto à sua cor (CIELAB: *L**, *a** e *b**) e composição centesimal (cinzas, proteína e gordura) de acordo com os métodos oficiais de análise da AOAC.

O teor de humidade de todas as farinhas analisadas variou entre 14 – 18% (p=0,54), sendo ligeiramente superior nas amostras desidratadas a 40 e 45ºC. A farinha obtida com os mirtilos da categoria A apresentou cerca de 1,6 vezes mais quantidade de proteína do que as restantes categorias (4,00 *vs* 2,39 e 2,66 g/100g em base húmida respetivamente, $p < 0,0001$) bem como o maior teor de cinzas (1,26 *vs* 1,04 e 1,03 %, respetivamente). O teor de gordura das farinhas não foi influenciado nem pelo processo nem pelas temperaturas de secagem. O efeito mais evidente da temperatura de secagem foi no parâmetro cor (*a** aumenta de 6,0 a 40 °C para 11,8 a 60 °C; $R^2 = 0,87$; $p < 0,0001$), apresentado uma tonalidade mais avermelhada nas farinhas obtidas com mirtilos desidratados a temperaturas mais altas. As farinhas obtidas com os mirtilos liofilizados foram as que apresentaram cor mais clara, pois apresentam valor de *L** mais alto. A liofilização reduziu o teor de cinzas (0,94 vs 1,17 %; $p = 0,011$) e não alterou o de proteína ou gordura. A interação categoria × temperatura foi significativa na maioria das variáveis.

De um modo geral, a liofilização e a secagem por ar quente, bem como as temperaturas de secagem testadas, influenciaram significativamente alguns parâmetros nutricionais das diferentes amostras de farinhas. No entanto, de modo a confirmar o efeito global da secagem na composição nutricional das farinhas, é necessário complementar estes dados com análises adicionais, nomeadamente a quantificação total de fibras e hidratos de carbono.

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Zearalenone in Commercially Available Beers: Quantitative Assessment and Consumer

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Zearalenone (ZEN) is a mycotoxin commonly found at low concentrations in foods consumed on a daily basis, including beer, one of the most widely consumed alcoholic beverages. This mycotoxin is produced by fungi of the genus *Fusarium*. Several studies have shown that ZEN can cause hyperoestrogenism, resulting in reproductive disorders in several animal species, including humans [1].

This study aimed to quantitatively assess the mycotoxin content in 134 commercially available beer samples in order to evaluate Portuguese consumers' exposure risk. Sample analysis was performed using a commercial immunoassay (RIDASCREEN Zearalenon), and risk assessment was conducted using a deterministic approach. In this study, beers were classified into different categories, allowing the relationship between ZEN content and the type of beer produced to be assessed.

The Estimated Daily Intake (EDI) was calculated according to three scenarios (best-case, worst-case and average). Across all beer samples, the EDI estimates for the best- and worst-case scenarios showed substantial variability (0.7122 ng/kg body weight/day and 7.3758 ng/kg body weight/day, respectively), with markedly different values between scenarios. In the best-case scenario, the values for each beer category were homogeneous (0.7 ng/kg body weight/day), indicating a limited influence of beer type on ZEN intake when contamination levels are low. In the worst-case scenario, the values were also relatively homogeneous (7.3758 ng/kg body weight/day), with the exception of non-alcoholic beers (3.1548 ng/kg body weight/day) and craft and ALE beers (6.2497 ng/kg body weight/day). Non-alcoholic beers therefore stood out as having notably lower ZEN levels compared with the other categories. Overall, all estimated values were substantially below the Tolerable Daily Intake (TDI) of 250 ng/kg body weight/day.

Thus, considering daily beer consumption alone, exposure to ZEN does not appear to represent a health hazard to consumers. Although ZEN intake through beer consumption was low, the contribution of other dietary sources that may contain this mycotoxin should also be considered in order to obtain a more comprehensive estimate of overall exposure. Future research could therefore benefit from a broader assessment of ZEN exposure through biomonitoring approaches.

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Comparative Analysis of Fatty Acid Profiles in Eggs from Different Production Systems and Cooking Treatments

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Omega-3 intake is consistently low in Western diets, which are typically rich in omega-6 fatty acids (FAs) [1,2]. The food industry has explored food enrichment to increase omega-3 intake and improve the dietary balance between omega-6 and omega-3 fatty acids, as this imbalance is linked to higher rates of inflammatory, autoimmune, and allergic diseases [3,4,5]. This study aims to quantify the FA profile of egg yolks from indoor-reared (IR), organic (OR), and omega-3-enriched (OE) production systems, and determine the effect of household cooking methods on omega-3 FAs profile.

One hundred large eggs from each system were purchased from local retailers across Paraná (Brazil) and divided into five treatment groups: raw, boiled, fried, scrambled, and omelet. Cooking treatments were performed to represent typical household practices. Lipid were extracted using the Bligh and Dyer [6] method, followed by esterification and FA analysis using gas chromatography with flame ionization detection (GC-FID).

The FA profiles were mainly composed of oleic, palmitic, linoleic, and stearic acids, with differences observed among production systems and cooking methods. IR eggs had the highest total saturated FA content (55.24 ± 0.71 mg g^{-1}), followed by OR (38.77 ± 17.78 mg g^{-1}) and OE (27.45 ± 1.23 mg g^{-1}). A similar trend was observed for total monounsaturated FAs, with the highest level in IR (86.77 ± 1.51 mg g^{-1}), followed by OR (60.44 ± 26.05 mg g^{-1}) and OE (37.53 ± 1.22 mg g^{-1}). In contrast, polyunsaturated FA content was highest in OR (23.81 ± 11.59 mg g^{-1}), followed by IE (19.64 ± 0.87 mg g^{-1}) and OE (13.51 ± 0.67 mg g^{-1}). In raw egg yolks, the contents of α-linolenic acid (ALA), eicosapentaenoic acid (EPA), and docosapentaenoic acid (DPA) did not differ significantly among the three production systems ($p > 0.05$). However, docosahexaenoic acid (DHA) content was significantly higher in OE (0.96 ± 0.16 mg g^{-1}) than in IR (0.29 ± 0.01 mg g^{-1}) and OR (0.37 ± 0.20 mg g^{-1}). Cooking significantly affected omega-3 content in eggs. Across cooking methods, OE showed higher or similar omega-3 levels comparable to IR, although values for OE and OR were often similar after cooking.

Overall, OE and OR eggs showed similar omega-3 fatty acid contents after cooking, suggesting that household cooking may compromise the nutritional advantage of enriched eggs. These findings highlight the need to optimize enrichment strategies, potentially through the inclusion of antioxidants such as vitamin E and selenium, to improve oxidative stability and preserve omega-3 FAs during typical cooking practices.

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A sequential injection analysis method for the determination of nitrites and nitrates in processed meats

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Nitrates and nitrites are widely used in processed meat products for microbiological safety, color development, and product stability [1]. However, concerns about potential health risks and increasingly strict European regulations highlight the need for reliable, efficient, and sustainable analytical methods to monitor their concentrations [1,2]. In this context, a sequential injection analysis (SIA) methodology, previously developed for water analysis [3], was adapted, optimized, and validated for the determination of nitrite and nitrate in processed meat products, including ham, spicy chourizo, and bacon. The proposed system combines automatic sample and reagent handling with spectrophotometric detection based on the Griess reaction at 540nm. Nitrite was determined directly, whereas nitrate was previously reduced to nitrite using a copperized cadmium column integrated into the analytical manifold [3].

The SIA methodology demonstrated satisfactory analytical performance, with limits of detection of 0.45 and 6.32 µmol/L and limits of quantification of 1.50 and 21.1 µmol/L for nitrite and nitrate, respectively. It should also be highlighted that the analytical method was applied to the determination of the aforementioned analytes in processed meat extracts after a complex extraction procedure. Therefore, interference studies were carried out to assess the impact of the sample extraction matrix on analyte quantification. The results demonstrated that matrix effects remained below 10% for both analytes, indicating that the matrix did not statistically interfere with the determination.

Overall, the developed SIA methodology represents a simpler, miniaturized, automatic, and cost-effective alternative for monitoring nitrite and nitrate in processed meat products. By combining analytical efficiency with reduced resource consumption and waste generation, this approach supports routine food quality control and contributes to more sustainable analytical practices in food industry [4].

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Effect of anthocyanin incorporation route on the functional performance of gelatin-based intelligent films

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The development of intelligent packaging systems based on natural pH-sensitive compounds offers a promising approach for the visual monitoring of food freshness [1]. In this context, anthocyanins are particularly attractive due to their pH-dependent color behavior. However, their stability can influence the color response and functional performance of the resulting materials, making it an important consideration for their application in intelligent packaging [2].

In this work, the effect of the anthocyanin incorporation strategy on the properties of gelatin-based intelligent films was evaluated. Black carrot anthocyanins were incorporated into gelatin films either as a free extract (GAE) or within a water-in-oil-in-water (W/O/W) double emulsion system (GDE). A gelatin (G) film without anthocyanins was used as control. The resulting films were characterized in terms of color, thickness, transparency, water vapor permeability, water contact angle, mechanical properties, Fourier-transform infrared spectroscopy (FTIR) and antioxidant activity.

Both anthocyanin-containing films exhibited a clear pH-dependent color response, with transitions from reddish to purple, bluish and brownish tones as pH increased. The incorporation strategy influenced the film properties: GDE films showed greater thickness (232.4 µm) and lower transparency (4.16 %) than GAE films (166.4 µm and 9.80 %, respectively). Moreover, GDE films showed higher antioxidant activity (48.10 % DPPH inhibition) compared to GAE films (22.22 %). Regarding mechanical properties, GDE films showed a lower Young's modulus (0.72 GPa) than GAE films (0.98 GPa), while no significant differences in water vapor permeability were observed derived from the incorporation route. The GDE films also showed improved pigment retention in aqueous media while maintaining their pH-responsive behavior. The functional performance of the films was further evaluated through food application tests. In yogurt, the color difference was approximately $\Delta E = 7.0$ for GAE and $\Delta E = 4.0$ for GDE, indicating a more pronounced color shift and higher pigment migration in the film containing free extract. During chicken breast storage, the pH increased from 5.82 to 6.8, accompanied by color changes in both films, with ΔE values of approximately 35.59 and 24.90 obtained for GAE and GDE, respectively. Overall, the results demonstrate that the anthocyanin incorporation route plays an important role in determining the physicochemical and functional properties of gelatin-based intelligent films. The double emulsion approach reduced pigment migration and improved color stability while maintaining the pH-responsive behavior required for freshness-monitoring applications.

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One-factor-at-a-time screening of the alcoholic fermentation of astringent persimmon must for vinegar production

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Astringent persimmon (*Diospyros kaki* L.) from Douro region (Portugal) has little commercial value but is rich in fermentable sugars and bioactive compounds, making it a candidate raw material for fruit vinegar. A one-factor-at-a-time (OFAT) approach identified the variables most relevant in its alcoholic fermentation, as a first step towards process optimisation.

Eight factors were varied one at a time relative to a control assay, related to fruit processing (pressing; crushing), viscosity control (pectinase; 1:3 dilution with glucose solution), microbial control (25 mg/L SO_2 at pH 3.5; 1.6-fold inoculum; thermal sterilisation), fruit ripeness (unripe; overripe), yeast strain (Fermol Charmat; Complet killer Fru), nutrient supplementation (Enovit, 0.3 g/L), initial pH control (3.5) and temperature (25 °C). Fermentations were followed by daily mass loss and characterised at the end by °Brix, pH, total and volatile acidity (OIV), reducing sugars (DNS) and ethanol (ebulliometry).

Thermal sterilisation led to heat-induced gelation of the must. The control and twelve variations completed fermentation in 4–12 days, with °Brix falling from 15.6-18.5 to 4.3-6.0 and residual reducing sugars of 1.2-8.8 g/L. Volatile acidity (VA) discriminated the conditions best: 0.24 g/L in the control versus 4.02, 3.18 and 3.66 g/L with crushing, no pectinase and Fermol Charmat, respectively, with concurrent increases in total acidity (8.40, 6.68 and 7.73 vs. 3.68 g/L), suggesting acetic acid accumulation during the alcoholic phase. Ethanol was 11.1 % v/v in the control and 6.3-8.7 % v/v in the variations, except the glucose-compensated dilution (11.9 %), with the lowest values (6.3–7.5 %) in the three assays with VA >3 g/L. Unripe and stemmed fruit did not confer good organoleptic properties.

No single-factor change improved on the control in terms of VA. Overripe fruit, 25 °C and 25 mg/L SO_2 at pH 3.5 performed comparably (4-5 days; VA ≤0.66 g/L), whereas crushing, omitting pectinase and the alternative strain markedly increased VA and lowered ethanol. Ebulliometric ethanol is biased by volatile acidity and interactions were not assessed, so the results are descriptive and identify no optimum. A two-level factorial design is proposed for the categorical factors with the largest effects (processing, pectinase, yeast strain) and a response surface design for the continuous factors (SO_2 dose, initial pH, temperature, inoculum size, initial sugar), with VA, HPLC-quantified ethanol, duration and sensory quality as responses.

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Lentil (*Lens culinaris* Medik.) tofu: a high-protein, low-fat alternative to soy tofu

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Lentil is an underused legume in Portugal, and its use in plant-based foods could reduce dependence on imported soy. Within the 3Rs project, this work aimed to develop a tofu-type product from lentils and to characterise its nutritional quality.

The tofu was produced by thermal coagulation of an aqueous lentil extract and was compared with a commercial soy tofu (control). Proximate composition was determined by AOAC methods [1], the fatty acid profile by GC-FID [2] and water activity (a^w) by direct measurement. Results are expressed on a fresh-weight basis (mean ± SD, n = 3).

The lentil tofu contained 87 ± 1 g moisture, 4.41 ± 0.02 g protein, 0.107 ± 0.009 g fat, 0.38 ± 0.02 g ash and 8 ± 1 g carbohydrates per 100 g, with an energy value of 52 ± 4 kcal/100 g. Protein supplied about 34% of the energy, so the product meets the "high protein" and "low fat" claims of Regulation (EC) No 1924/2006 [3]. Compared with the commercial soy tofu, lentil tofu had a slightly higher protein content (4.41 vs. 3.9 g/100 g), about 97% less fat (0.107 vs. 3.25 g/100 g) and 19% less energy (52 vs. 64 kcal/100 g). Polyunsaturated fatty acids made up 55% of the lipid fraction, mainly linoleic (39.5%) and α-linolenic (12.1%) acids, giving a favourable total n-6/n-3 ratio of 2.5. Its high a^w (0.96) requires refrigerated storage. Lentil tofu is therefore a nutritionally competitive, locally produced alternative to soy tofu.

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Caracterização comparativa dos perfis de compostos fenólicos de microvegetais de acelga e espinafre

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Os microvegetais têm despertado crescente interesse científico e comercial devido ao seu valor nutricional, ao teor de compostos bioativos e às características sensoriais [1,2]. Entre estes compostos, destacam-se os polifenóis, aos quais têm sido atribuídas diversas atividades biológicas, incluindo propriedades antioxidantes, antimicrobianas e anti-inflamatórias, com potenciais benefícios para a saúde humana [2,3]. A acelga (*Beta vulgaris* L. var. *cicla*) e o espinafre (*Spinacia oleracea* L.) são espécies de interesse alimentar da família Amaranthaceae, cuja composição fitoquímica tem sido amplamente estudada em plantas adultas. Contudo, a informação sobre os seus perfis fenólicos na fase de microvegetal, particularmente numa perspetiva comparativa, permanece limitada. Neste contexto, o presente estudo teve como objetivo produzir microvegetais de acelga e espinafre em condições de cultivo interior e caracterizar e comparar os respetivos perfis de compostos fenólicos.

As sementes foram semeadas em tabuleiros de germinação contendo vermiculite e cultivadas numa câmara de crescimento *walk-in* com iluminação fluorescente, sob um fotoperíodo de 16 h de luz/8 h de escuro, a uma temperatura de 20–25 °C e humidade relativa de aproximadamente 60%. Os microvegetais de espinafre e acelga foram irrigados com uma solução nutritiva NPK (3:1:6) e colhidos aos 14 e 17 dias após a sementeira, respetivamente. Após a preparação de extratos hidroetanólicos, os perfis de compostos fenólicos foram caracterizados por cromatografia líquida de alta eficiência com deteção por arranjo de díodos e espetrometria de massa com ionização por *electrospray* (HPLC-DAD-ESI/MS).

Os flavonoides constituíram a principal classe de compostos fenólicos identificada em ambas as espécies, embora tenham sido observadas diferenças nos respetivos perfis. Nos microvegetais de acelga, verificou-se a predominância de derivados de vitexina, enquanto nos de espinafre se destacaram os derivados de spinacetina e patuletina. Estes resultados evidenciam diferenças na composição fenólica das duas espécies e reforçam o potencial destes microvegetais como fontes alimentares de flavonoides com propriedades antioxidantes e anti-inflamatórias [2,3]. Estudos futuros deverão avaliar a composição nutricional destes microvegetais, nomeadamente os teores de vitaminas e minerais essenciais, bem como as suas propriedades bioativas.

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From glucosinolates to isothiocyanates: the chemical characterisation of salad rocket

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Glucosinolates (GSLs) are sulphur-containing secondary metabolites naturally present in plants of the Brassicaceae family; they are precursors of biologically active substances, particularly isothiocyanates (ITCs), which are widely recognised for their anti-inflammatory, antioxidant, and metabolic-regulating capacity [1]. These compounds have gained much attention due to their beneficial health effects, making necessary the chemical characterisation of *Brassica* vegetables [2]. In this sense, the analysis of these compounds poses a challenge, as extraction conditions can affect the stability of GSLs.

The aim of this study is to develop analytical methods for the determination of GSLs and ITCs in salad rocket (*Brassica eruca* L.). Based on a comprehensive literature review, various extraction protocols will be investigated – either those that preserve the intact structure of the GSLs or, conversely, those that promote their hydrolysis into ITCs. The extraction performance will be evaluated in terms of efficiency and yield to choose the most appropriate conditions for the analysis of both families of compounds. The validation will be carried out for calibration, sensitivity, precision, and accuracy. The separation, identification, and quantification of the target analytes will be conducted through HPLC-DAD-IT-MS.

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Effect of NPK fertilisation on the chemical profile and the *in vitro* antioxidant properties of *Portulaca oleracea* L. leaves and stems

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Interest in wild species such as purslane (*Portulaca oleracea* L.) is growing in response to the demand for functional foods and sustainable agricultural practices [1]. NFT (Nutrient Film Technique) hydroponic cultivation offers the advantage of precisely controlling the availability of essential macronutrients, such as nitrogen (N), phosphorus (P), and potassium (K) [2]. Manipulating NPK ratios directly affects the content of primary and secondary compounds across different parts of the plant matrix (such as stems and leaves) [3]. Therefore, this study investigated the combined effects of nitrogen (100 and 200 ppm), phosphorus (47, 70, and 105 ppm), and potassium (250, 350, and 525 ppm) on the chemical profile by gravimetric and chromatographic methods of purslane leaves and stems, alongside the *in vitro* antioxidant properties by measuring lipid peroxidation (TBARS) and oxidative haemolysis (OxHLIA) of their hydroethanolic extracts.

The leaves contained higher levels of proteins, while the stems showed higher amounts of fibre and carbohydrates. Furthermore, combining high levels of P and K (105 and 525 ppm, respectively) does not appear to affect the ash, crude protein, or fat profile of purslane leaves, irrespective of the N concentration. Palmitic acid (C16:0) was the most abundant SFA in the plant tissues. However, high P: K ratios favoured a higher relative proportion of omega-6 (C18:2n6, linoleic acid) and omega-3 (C18:3n3, α-linolenic acid). The content of free sugars was more abundant in the stems, whereas the content of tocopherols (α- and γ-tocopherols) was higher in the leaves. Oxalic acid was found to be the most prevalent organic acid, with higher concentrations observed in the stems compared to the leaves. Notably, its content in leaves was reduced to levels considered safe for consumption, depending on the nutrient solution applied. Oleraceins A and C were the alkaloids quantified in both parts of the purslane. Leaf extracts demonstrated greater antioxidant capacity, particularly in the OxHLIA assay, as they exhibited lower IC_{50} values than the positive control.

Overall, these findings demonstrate that targeted hydroponic nutrient modulation significantly enhances the nutritional and functional profile of *P. oleracea*, solidifying its role as a sustainable and versatile food source.

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Cultivation of Glucosinolate-Enriched *Brassicas* Using Plant Tissue Culture and Hydroponic Systems for the Development of Functional Pasta Products

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Intensive agricultural practices place increasing pressure on natural resources, highlighting the need for sustainable food production strategies [1]. In this context, controlled cultivation of *Brassica* species through plant tissue culture and hydroponic systems offers an innovative approach to producing biomass enriched in glucosinolates (GSLs), valuable plant secondary metabolites [2]. Glucosinolates are sulphur-containing compounds that can be hydrolysed by myrosinase following tissue disruption, generating biologically active products, including isothiocyanates (ITCs). Among these, sulforaphane and indole-3-carbinol have attracted considerable attention for their potential antioxidant and chemopreventive properties. However, GSL accumulation and conversion depend on plant species, cultivation conditions, and processing, making production optimisation essential [3]. This project aims to integrate *in vitro* and hydroponic cultivation strategies to enhance GSL production in *Brassica* biomass and explore its application in functional pasta development. Post-harvest handling and sustainable extraction technologies will be investigated to maximise compound recovery while preserving their bioactivity. GSL profiles and, where feasible, their hydrolysis products will be characterised using HPLC-DAD/ESI-MS. The enriched plant material will subsequently be incorporated into pasta formulations, whose technological, physicochemical and sensory properties will be evaluated. Particular attention will be given to compound stability and potential bioaccessibility following processing. By integrating controlled plant production, sustainable extraction, and food innovation, this project seeks to valorise Brassica biomass and develop pasta products with enhanced phytochemical value.

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Perfil de aminoácidos em produtos derivados do leite: efeito da maturação

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A maturação é uma etapa determinante para a qualidade dos queijos, durante a qual ocorrem transformações bioquímicas que influenciam as suas características nutricionais e sensoriais. O perfil de aminoácidos constitui um parâmetro relevante para caracterizar a composição proteica destes produtos e avaliar possíveis efeitos do processo de fabrico e do tempo de maturação. Neste contexto, este estudo teve como objetivo avaliar a evolução do perfil e da concentração de aminoácidos em queijos de leite de vaca dos tipos Colonial (QC) e Iogurtado (QI).

Os queijos, produzidos com culturas *starter* (QC) ou iogurte natural (QI), foram maturados a 5 °C e analisados aos 10, 20, 30 e 40 dias. Após hidrólise e derivatização automática (com OPA/3-MPA e FMOC), os aminoácidos foram determinados por HPLC com deteção por fluorescência. Os resultados foram analisados por ANOVA de dois fatores ($p < 0,05$).

Identificaram-se 17 aminoácidos nas amostras, observando-se perfis de aminoácidos totais semelhantes nos dois tipos de queijo. O teor proteico foi de 21,4% no QC e 20,4% no QI. Ao fim de 40 dias, a concentração total de aminoácidos aumentou 39,22% no QC e 23,52% no QI. O ácido glutâmico apresentou as concentrações mais elevadas (33,5-47,8 mg/g no QC e 36,1-45,3 mg/g no QI), seguido da leucina e da prolina. Em conjunto, estes três aminoácidos representaram cerca de 42% dos aminoácidos totais em ambos os tipos de queijo, considerando todos os tempos de maturação. O triptofano apresentou as menores concentrações (1,9-2,1 mg/g no QC e 1,7–1,9 mg/g no QI). De uma maneira geral, o tempo de maturação influenciou significativamente 14 dos 17 aminoácidos, enquanto a interação entre o tempo e o tipo de queijo foi significativa para a histidina e o triptofano.

Conclui-se que o tempo de maturação é o principal fator associado às alterações do perfil de aminoácidos, embora alguns apresentem respostas distintas consoante o tipo de queijo.

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Valorizing Portuguese propolis extracts as functional ingredients in cereal snack bars

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The growing demand for convenient foods with enhanced nutritional and functional properties has encouraged the incorporation of natural bioactive ingredients into cereal-based products [1]. Bee products offer promising opportunities for food innovation, with honey and propolis contributing mainly to nutritional composition, while propolis provides mainly phenolic compounds with antioxidant potential. However, propolis incorporation into food formulations remains challenging due to its poor solubility and intense organoleptic characteristics, which may compromise consumer acceptance [2]. In this context, this study aimed to investigate the impact of propolis extract incorporation on the physicochemical, functional, and sensory properties of cereal snack bars.

Portuguese propolis was extracted by maceration in 70% ethanol at a concentration of 30% (w/w), followed by solvent evaporation. The resulting extract was incorporated into cereal snack bars containing honey, pollen, chestnut cream, nuts and seeds. Three formulations were evaluated: a control without propolis extract (SP), and two formulations containing 0.5% (P1X) and 1.0% (P2X) propolis extract. Moisture and protein contents, surface color (CIELab system), total phenolics content (Folin-Ciocalteu assay), total flavonoids content ($AlCl_3$ assay), and antioxidant activity ($DPPH^{\bullet}$, $ABTS^{\bullet+}$, $NO^{\bullet}$, and FRAP) were assessed. Phenolic compounds were further investigated by UHPLC-DAD-ESI/MS, while sensory acceptance was evaluated by 20 untrained panelists.

The results showed that propolis enrichment did not significantly affect moisture (6.0-6.2%) and protein (10.9-12.2%) contents but induced small changes in surface color ($\Delta E > 2$). Total phenolics increased significantly from 0.075 g GAE/100 g in SP to 0.12 and 0.14 g GAE/100 g in P1X and P2X, respectively, corresponding to increases of 60% and 87%. The propolis-enriched formulations also exhibited higher flavonoid levels and antioxidant capacities. DPPH antioxidant capacity increased from 0.23 g AAE/100 g in SP to 0.28 and 0.30 g AAE/100 g in P1X and P2X, respectively. Similar trends were observed for ABTS and FRAP, although differences between P1X and P2X were not statistically different. UHPLC-DAD-ESI/MS analysis identified characteristic propolis bioactive compounds in the enriched bars, including ferulic acid, pinobanksin, pinocembrin, chrysin, galangin, and caffeic acid phenylethyl ester (CAPE). Sensory evaluation suggested a slight reduction in aroma and flavor with increasing propolis concentration, although all formulations maintained good overall acceptance.

Overall, these findings highlight the potential of Portuguese propolis for developing naturally enriched cereal bars, with 0.5% incorporation providing a favorable balance between phytochemical enrichment, antioxidant activity, and sensory quality.

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QUÍMICA AMBIENTAL Y SOSTENIBLE

Potential of Limpet Shell Sand (*Patella aspera*) for Phosphorus Recovery from Livestock Effluents in the Azores: A Physicochemical Review and Theoretical Proposition

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Phosphorus recovery ($P\text{-}PO_4^{-3}$) from livestock effluents constitutes a priority to mitigate eutrophication and promote nutrient recycling. In the Azores Archipelago (a key dairy cattle farming hub in Portugal), the management of phosphorus-rich agricultural effluents intersects with the challenge of managing naturally acidic volcanic soils, in which applied phosphorus is irreversibly retained by iron and aluminum oxides. Concurrently, the consumption of limpets (*Patella aspera*) generates tons of unutilized residual shell waste annually [1]. This work presents a literature review and a proposed theoretical circular economy model to evaluate the physicochemical feasibility of converting these shells into reactive sand to treat effluents and produce a phosphate fertilizer/soil conditioner for volcanic soils.

Shell sand can act as a reactive bed for heterogeneous nucleation. The interfacial dissolution of $CaCO_3$ [$CaCO_3(s) + H^+ \rightleftharpoons Ca^{2+} + HCO_3^-$] releases Ca^{2+} into the grain boundary layer [2]. In alkaline livestock effluents (pH 8–9), orthophosphate (predominantly HPO_4^{2-}) undergoes chemisorption at calcium sites [$>CO_3\text{–}Ca^+ + HPO_4^{2-} \rightleftharpoons >CO_3\text{–}Ca\text{–}HPO_4^-$] [3], inducing the crystallization of phosphate phases (Amorphous Calcium Phosphate and Hydroxyapatite) anchored onto the sand grain itself [4]. The continuous dissolution of the biomineral consumes precipitation acidity, maintaining a self-regulating buffer pH (8,5–9,8). As process limitations, the literature points to competition from bicarbonate (which induces non-specific calcite co-precipitation), the inhibitory effect of Mg^{2+} on crystallization, and organic matter [5].
Mineralogically, the shell of Patella aspera contains aragonite (a metastable polymorph more soluble than pure calcite) [6]. In acidic volcanic soils, the accelerated dissolution of aragonite by H^+ ions can induce the release of Ca^{2+} and HCO_3^-, raising the rhizospheric pH and preventing the irreversible fixation of phosphorus [7]. Ecotoxicologically, literature data demonstrate that heavy and trace metals (Fe, Zn, Cu, Cd, Ni, Co accumulate in the soft tissues of the mollusk rather than in the mineral matrix of the shell. However, shells from polluted estuarine zones present a risk of enrichment in manganese (Mn, up to 130,5 µg/g) and iron [8].

In conclusion, although the theoretical model highlights the potential of *Patella aspera* shell sand to integrate a circular economy cycle in the Azores, its practical viability depends on overcoming major physicochemical and operational challenges. The presence of organic matter, competition for bicarbonate, and the inhibitory effect of ions such as Mg^{2+} can affect the kinetics of phosphorus precipitation and the stability of the formed mineral phases. Future research is recommended to focus on: i) experimental validation of the model at bench and pilot scales using real livestock effluents; ii) studying the kinetics of phosphorus release and acidity neutralization in local volcanic soils; and iii) detailed ecotoxicological and mineralogical characterization of the biomineral, ensuring the technology's efficiency and environmental safety prior to full-scale application.

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Removal of Nutrients and Veterinary Pharmaceuticals from Agricultural Effluents by Adsorption on Advanced Substrates: The LIFE4FARMS Project

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The contamination of water resources by intensive livestock effluents constitutes a growing threat due to the chemical persistence of emerging organic micropollutants, such as antibiotics and hormones, associated with high nutrient levels (nitrogen and phosphorus). The European project LIFE4FARMS proposes to mitigate this impact through the Wet4Agro system, an enhanced Nature-Based Solution (eNBS). This work presents the chemical foundations and surface interaction mechanisms envisioned for this system, which aims at the simultaneous removal of pollutants under different edaphoclimatic conditions, with prototypes installed in the Czech Republic and the Azores.

The application of filter beds composed of advanced inorganic substrates with high porosity and surface accessibility — such as pumice and ceramic shards — directly addresses the evidence that conventional materials have low retention capacity and saturate rapidly, making the use of special high-sorption substrates indispensable to ensure the effective and sustained removal of nutrients in constructed wetlands.[1]. From the perspective of surface chemistry, the removal process will be governed by physical and chemical adsorption phenomena (physisorption and chemisorption), regulated by pH-dependent electrostatic interactions, Van der Waals forces, and ion exchange at the solid-liquid interface. Preliminary laboratory-scale kinetic studies indicate that the adsorption of amphoteric compounds such as tetracycline onto pumice is highly efficient across a wide pH range, following pseudo-second-order models and Freundlich isotherms, suggesting multilayer adsorption on heterogeneous surfaces.[2].

The project's chemical monitoring will focus on evaluating degradation and retention efficiency, with estimated targets exceeding 70% for total nitrogen (via coupled biological nitrification/denitrification processes within the biofilm) and 80% for pharmaceutical residues[3]. The quantification and speciation of analytes in complex wastewater matrices will be conducted using advanced Analytical Chemistry techniques, employing solid-phase extraction (SPE) followed by high-performance liquid chromatography coupled to tandem mass spectrometry (HPLC-MS/MS) for micropollutants, and automated spectrophotometric methods for nutrient monitoring.

In conclusion, the LIFE4FARMS project will validate the feasibility of geo-available materials as green and eco-efficient adsorbents. The Wet4Agro system is expected to provide a sustainable and low-cost technological solution for agricultural decontamination and water resource protection in the Czech Republic and the Azores.

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Synthesis and characterization of rGO/TiO_2 on flexible substrates for use as electrode in DSSCs

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Dye-sensitized solar cells (DSSCs), also known as Grätzel cells[1], stand out about other devices for being easy to handle, ecological, fast to manufacture, use of simple materials, good use of solar radiation and less sensitive to temperature rise, so these technologies are promising when compared to conventional silicon cells [2].
Currently, PCE values in DSSCs are reaching up to 15.2% [3], so their performance needs to be increased to make them more competitive.
DSSCs consist of three main components: a photoanode (wide band gap semiconductors such as TiO_2), an electrolyte (a redox pair such as iodide/triiodide (I^-/I_3^-)), and a counter electrode (CE), which is usually fluorine-doped tin oxide (FTO) glass with platinum. Incorporating reduced graphene oxide (rGO) into TiO_2 is an alternative to improve electron transport and lifetime.
Some authors [4] have found that doping TiO_2 with other elements results in an increase in the efficiency of the solar cell. In this work, TiO_2 doped with commercial reduced graphene oxide (rGO) was synthesized and deposited on flexible substrates (polyethylene terephthalate, PET) by Spin coating to study its chemical and physical properties, homogeneity, adhesion to the substrate, etc.

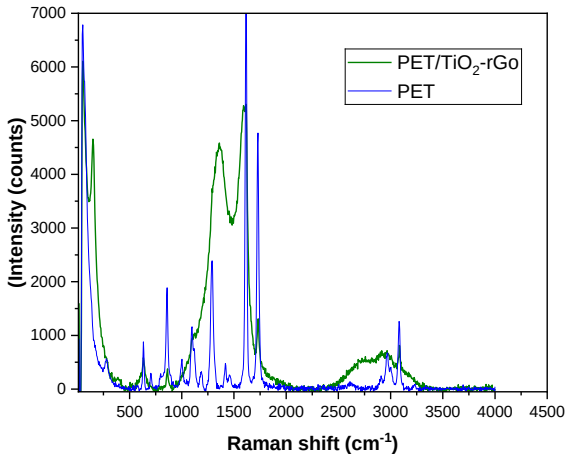


Fig.1. Raman spectrum of the flexible substrate (PET) and TiO_2 doped rGO/PET.

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Synthesis and Characterization of Pb free perovskite based films obtained by sol-gel method.

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TiO_2 and ZnO are oxides whose wide band gap energies, large surface area, high conduction band edge, chemical stability, and charge carrier mobilities make them suitable for use in photovoltaic devices, optoelectronics, catalysis, etc.

Dye-sensitized solar cells (DSSCs) consist of a photoanode, a counter electrode, and an electrolyte located between them. The photoanode, composed of dye-sensitized semiconductor nanoparticles deposited on a conductive glass (FTO) substrate, is where the conversion of light into electricity begins. Its main function is to absorb the electrons generated when the dye captures light and transport them to the external circuit. The most commonly used photoanodes are titanium oxide (TiO_2) [1] and zinc oxide (ZnO).
In the solar cell, the ZnO film [2] is prone to photocorrosion and dye desorption; however, when combined with TiO_2, its stability as a photoelectrode increases.
Therefore, zinc titanates, being composed of the binary system TiO_2–ZnO, they can be used as an electron transport layer, interfacial material, or photoanode component, especially in these new generation solar cells [3].

In this study, thin films of Zn and Ti were synthesized and deposited onto glass using the centrifugal coating technique for use in this type of solar cell. The resulting films were characterized using scanning electron microscopy (SEM), X-ray diffraction, infrared spectroscopy and Raman spectroscopy.

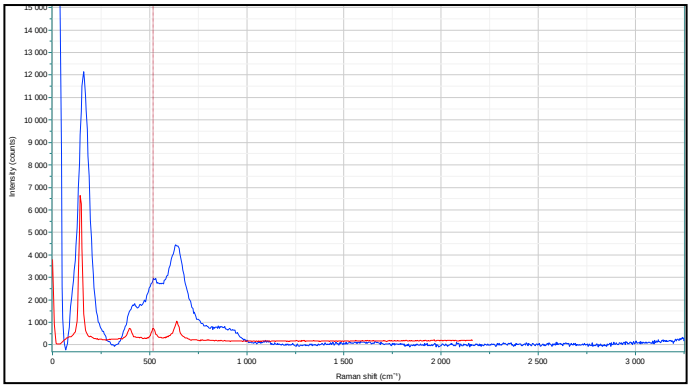


Fig.1. Raman spectrum of the TiO_2 (red) and TiO_2–ZnO with heat treatment (blue).

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Grafitización catalítica asistida por microondas de biocarbones derivados de residuos: hacia la producción de biografitos circulares

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La transformación de residuos de biomasa en materiales carbonosos de alto valor añadido constituye una estrategia relevante para avanzar hacia una economía circular del carbono y reducir la dependencia de materias primas fósiles críticas en aplicaciones energéticas y electroquímicas. Sin embargo, la grafitización convencional suele requerir tratamientos térmicos severos (≥ 2500 °C), limitando su viabilidad económica y dificultando su integración en procesos de valorización de residuos. En este contexto, el proyecto BIOGRAFITOMW investiga una ruta alternativa de grafitización catalítica a baja temperatura asistida por microondas (MW) orientada a la obtención de biografitos circulares a partir de diferentes residuos de biomasa [1].

Para el escalado del proceso a nivel semiindustrial, se desarrolló una configuración basada en un sistema de reactores MW multimagnetrón, en el que el biocarbón obtenido por pirólisis es posteriormente sometido a tratamiento termo-catalítico en presencia de 15–20 % en peso de Fe_2O_3 comercial [2]. La configuración permite suministrar hasta 7.2 kW al reactor de grafitización y trabajar en una atmósfera reductora generada durante el propio proceso de conversión, minimizando la necesidad de agentes reductores externos. Se estudiaron biocarbones procedentes de diferentes residuos, incluyendo hueso de aceituna, posos de café, cascarilla de avena y residuos celulósicos. La influencia de la temperatura, potencia MW, tiempo de tratamiento, atmósfera y naturaleza del precursor se evaluó mediante espectroscopía Raman, empleando la relación de intensidades (I_D/I_G) como indicador del grado de desorden/reorganización de la estructura carbonosa.

Los tratamientos realizados entre 521 y 810 °C durante aproximadamente 1–3 h produjeron una modificación significativa de la estructura de los biocarbones, con valores finales de (I_D/I_G) comprendidos entre 0.94 y 2.37. Los menores valores se obtuvieron bajo condiciones fuertemente reductoras y, en determinados precursores, a temperaturas superiores a 700 °C. El valor mínimo, (I_D/I_G = 0,94), se obtuvo para un biocarbón procedente de residuo celulósico tratado en presencia de CO_2, mientras que los materiales derivados de la mezcla hueso de aceituna/posos de café alcanzaron valores próximos a la unidad. En un ensayo específico, la incorporación de un 20 % de Fe_2O_3 redujo el (I_D/I_G) del precursor desde 5.97 hasta aproximadamente 1.50, junto con una mayor definición de la banda G y una menor contribución relativa de las estructuras desordenadas.

Estos resultados demuestran la viabilidad de utilizar el calentamiento MW combinado con catálisis mediante Fe_2O_3 para favorecer el reordenamiento de biocarbones derivados de residuos a temperaturas inferiores a las habitualmente asociadas a procesos convencionales de grafitización. La estrategia integra la valorización de residuos, el aprovechamiento de una materia prima renovable y la producción de materiales carbonosos de mayor valor añadido, constituyendo una alternativa prometedora para una ruta más sostenible hacia biografitos circulares. La posterior caracterización estructural, textural y electroquímica permitirá determinar el grado de grafitización alcanzado y evaluar su idoneidad para aplicaciones de almacenamiento y conversión de energía.

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Valorización de subproductos agroalimentarios mediante pirólisis continua asistida por microondas para la producción de gas rico en H_2 y CO

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La valorización de subproductos agroalimentarios mediante procesos termoquímicos constituye una estrategia de interés para avanzar hacia modelos de economía circular y producción descentralizada de vectores energéticos renovables. La elevada heterogeneidad de estos residuos, junto con su contenido variable de humedad, material mineral y compuestos orgánicos, dificulta su conversión eficiente mediante tecnologías convencionales. En este contexto, la pirólisis y gasificación asistidas por microondas (MW) ofrecen una alternativa basada en calentamiento volumétrica y selectivo, con potencial para intensificar la conversión de biomasa y favorecer la generación de gases combustibles [1]. El objetivo de este trabajo es evaluar experimentalmente un sistema continuo de pirólisis/gasificación asistida por MW desarrollado a escala piloto para la valorización de subproductos agroalimentarios y determinar las condiciones de operación que permitan obtener una corriente gaseosa rica en H_2 y CO susceptible de posterior acondicionamiento y valorización energética o química.

Como etapa previa al diseño del proceso, se caracterizaron tres subproductos agroalimentarios de diferente naturaleza: cascarilla de avena, alperujo y tierras decolorantes agotadas. La cascarilla de avena presentó las características más favorables para la generación de gas combustible, con aproximadamente 8% de humedad, 70-72% de materia volátil y 2-4% de cenizas, además de un contenido de carbono de 40-43%. El alperujo presentó una elevada humedad (69-76%), mientras que las tierras decolorantes mostraron una elevada fracción mineral (57-70% de cenizas), evidenciando la necesidad de adaptar la estrategia termoquímica a la composición específica de cada subproducto [2].

A partir de estos resultados se diseñó y construyó el reactor RPMW1, integrando simulación electromagnética, calentamiento multimagnetrón, alimentación continua, y monitorización de gases *on-line*, operando a presión atmosférica. Los ensayos experimentales con cascarilla de avena en régimen continuo revelaron un perfil de conversión altamente estable a lo largo de seis horas de operación. El sistema alcanzó un régimen estacionario térmico entre 660 °C y 835 °C. Bajo estas condiciones estables, se constató una producción sostenida de gas con fracciones volumétricas medias de CO (10–19%) e H_2 (12–20%). Este comportamiento es consistente con la contribución de reacciones secundarias de gasificación del *char* y de Boudouard, favorecidas por el calentamiento volumétrico y selectivo mediante microondas. Los resultados demuestran la viabilidad de la conversión continua de subproductos agroalimentarios mediante MW y proporcionan parámetros experimentales para el desarrollo de una segunda etapa de tratamiento y acondicionamiento del gas, orientada a su valorización energética y química. Esta estrategia contribuye a integrar la valorización de residuos con la producción de vectores energéticos renovables dentro de un enfoque de economía circular.

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Almond and walnut shells as alternative lignocellulosic raw materials for particleboard production

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The growing demand for particleboards places increasing pressure on wood resources and highlights the need for alternative lignocellulosic raw materials. In 2024, global particleboard production reached approximately 1.23 × 10^8 m^3 [1], corresponding to about 7.69 × 10^3 km^2 of panels, assuming a thickness of 16 mm. This area is equivalent to around 77 times the area of Lisbon and 13 times the area of Madrid, highlighting the high demand for lignocellulosic raw materials. At the same time, almond and walnut production in the Iberian Peninsula reached approximately 4.60 × 10^5 t and 3.12 × 10^4 t, respectively [2], generating substantial quantities of shell residues. The valorisation of these agro-industrial by-products as alternative raw materials for particleboard production could contribute simultaneously to reducing wood consumption and promoting waste valorisation within a circular bioeconomy framework.

This study aimed to evaluate almond shells (AS) and walnut shells (WS) as partial substitutes for wood in particleboard production. The residues were dried, milled and sieved to obtain particle sizes suitable for incorporation into the core layer of the panels. Their particle size distribution, moisture content, pH, buffering capacity, chemical composition and thermal behaviour were characterized. Almond and walnut shells showed similar chemical profiles, with Klason lignin contents of 52.10 ± 2.16% and 50.07 ± 0.10%, cellulose contents of 43.41 ± 1.10% and 41.79 ± 0.47%, and hemicellulose contents of 44.58 ± 1.10% and 41.48 ± 0.47%, respectively.

Preliminary three layers particleboards (thickness of 16 mm) were produced by replacing 10% and 30% of the wood in the core layer with AS or WS. Control panels without residue incorporation were also produced. Two pressing times, 90 s and 120 s, were evaluated to assess the influence of processing conditions on panel performance. The panels were tested for density (EN 323), moisture content (EN 322), thickness swelling (EN 317), internal bond strength (EN 319), bending strength (EN 310) and modulus of elasticity (EN 310). The main results obtained for panels pressed for 120 s are summarized in Table 1.

Table 1. Main properties of particleboards produced with almond shell (AS) and walnut shell (WS).

Panel type	Time (s)	Density (kg/m³)	MOR (MPa)	MOE (MPa)	IB (MPa)	TS (%)
Control	120	682 ± 6	13.0 ± 0.5	2033 ± 196	0.59 ± 0.25	25.9 ± 1.1
AS 10%	120	685 ± 13	12.8 ± 0.1	2006 ± 217	0.66 ± 0.06	22.9 ± 0.8
AS 30%	120	713 ± 17	11.2 ± 0.8	1703 ± 159	0.64 ± 0.03	23.5 ± 1.0
WS 10%	120	683 ± 10	13.4 ± 0.4	1983 ± 156	0.68 ± 0.03	22.9 ± 1.1
WS 30%	120	713 ± 17	11.0 ± 0.5	1733 ± 110	0.58 ± 0.04	23.9 ± 0.7

Increasing shell incorporation to 30% reduced mechanical performance, while thickness swelling remained below the control. Overall, 10% incorporation provided the best balance between wood replacement and panel performance. Based on the technical requirements evaluated so far, almond and walnut shells show promising potential for partial wood replacement in particleboard production.

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Monitoring PFAS Occurrence in Potentially Contaminated Soils from Galicia (NW Spain) by UPLC-MS/MS

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Per- and polyfluoroalkyl substances (PFAS) are a large group of synthetic fluorinated compounds characterized by high chemical and thermal stability, due to the strength of their carbon-fluorine bond [1]. The extensive use of PFAS in industrial and commercial applications, including aqueous film-forming foams (AFFF), combined with their resistance to degradation processes, has resulted in their widespread occurrence and persistence in the environment [2]. In this context, the development of reliable analytical methods for their determination in soils allows the assessment of their presence, distribution and potential sources.

This work is part of the *PFASTOP* project, which focuses on the occurrence and environmental behaviour of PFAS in soil-water-plant systems. The proposed method for PFAS quantification in soils is based on methanol extraction followed by a solid-phase extraction (SPE) for the purification of the samples. A total of twenty PFAS compounds were quantified in soil extracts by ultra-performance liquid chromatography coupled with tandem mass spectrometry (UPLC-MS/MS), using internal standards to monitor the analytical performance.

The extraction procedure was applied to soil samples collected from different sites in Galicia (Spain) with potential PFAS contamination. These included areas surrounding airports, where the use of AFFF represents a potential source of PFAS contamination in soils and groundwater [2]. Additionally, samples were collected from a landfill that had previously been affected by a wildfire. Landfills are considered important sources of PFAS release into the environment, as these compounds can leach from a wide range of PFAS-containing products, including plastics and textiles, disposed of over time [3]. Samples were also collected from soils amended with technosols and sewage sludge, which may represent additional sources of PFAS contamination. This work represents a first step towards the characterization of PFAS occurrence in Galician soils and will contribute to the development and application of analytical procedures for their environmental assessment.

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Seasonal co-occurrence of microplastics and phthalates in atmospheric particulate matter (PM_{10}) at an urban traffic site

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Urban road traffic is increasingly recognized as an important source of non-exhaust particulate emissions arising from tire and brake wear, road-surface abrasion, and the resuspension of deposited material [1]. These processes release a complex mixture of airborne contaminants, including plastic-derived material and associated additives, such as phthalates [2,3]. Traffic-dominated urban environments may therefore represent relevant hotspots for the simultaneous occurrence of these emerging contaminants. However, knowledge of their co-occurrence and temporal variability in urban air remains limited, with previous studies reporting inconsistent seasonal patterns [4,5].

Herein, we assessed the co-occurrence of suspected airborne microplastics and phthalates at an urban traffic site in Lisbon, Portugal, across different seasons. Particulate matter (PM_{10}) was collected on quartz-fibre filters using a high-volume sampler. Suspected microplastics were extracted following oxidative digestion and density separation, stained with Nile Red, and quantified by fluorescence stereomicroscopy. Phthalates were solvent-extracted and quantified by GC-MS targeting seven priority analytes.

Results showed that suspected airborne microplastics were most prevalent during autumn and occurred at their lowest concentrations during spring. Conversely, phthalates were detected in greater numbers and at higher concentrations during spring. These contrasting seasonal patterns may reflect differences in atmospheric partitioning and transport, as well as seasonal variations in source strength, given that suspected microplastics and phthalates may originate, at least partly, from different sources.

Overall, this study shows that urban traffic environments may constitute hotspots for simultaneous exposure to suspected airborne microplastics and plastic additives. It also highlights the complexity of establishing seasonal patterns for these contaminants and the need for further research using integrated urban air monitoring approaches that combine particle-based and chemical indicators. Such approaches may improve our understanding of the sources and dynamics of these emerging contaminants and support the development of more effective mitigation strategies and regulatory initiatives

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Purification of Ethyl Biodiesel Based on Circular Economy Principles through Adsorption Using Residual Biomass-Based Materials

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Biodiesel is a renewable and biodegradable alternative to fossil diesel and can be produced from low-cost residual feedstocks such as waste cooking oil (WCO). However, crude biodiesel contains impurities, including free glycerol, residual alcohol, catalyst, soaps, and water, which must be removed to meet quality standards such as EN 14214 and ASTM D6751 [1]. Wet washing, the conventional purification route, is effective but may consume 3-10 L of water per litre of biodiesel and generates effluents with high biochemical oxygen demand (BOD) and chemical oxygen demand (COD) [1]. Dry purification by adsorption avoids water use, can be applied in continuous systems, and, when the adsorbents are derived from agro-industrial waste, aligns with the principles of the circular economy [1,2].

This work aims to evaluate the purification of ethyl biodiesel, produced from WCO, by adsorption in a fixed-bed column, with emphasis on glycerol removal. Three bioadsorbents previously prepared by the research group are evaluated: activated carbon from almond shell chemically activated with H_3PO_4, with and without a washing step, and carbon from olive pit obtained by physical activation. The adsorbents are characterised by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), Brunauer–Emmett–Teller (BET) surface area and pore-size analysis, point of zero charge (PZC), isoelectric point (IEP), and scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM-EDS). The biodiesel will be analysed before and after purification for free glycerol (colorimetric method by ultraviolet-visible spectrophotometry) and fatty acid ethyl esters (gas chromatography with flame ionisation detection, GC-FID) [3,4].

Column experiments will be performed at different feed flow rates to obtain breakthrough curves, from which breakthrough time, saturation time, and adsorption capacity will be determined. The experimental data will be described using the Thomas, Yoon-Nelson, and Adams-Bohart models [5]. This study is expected to contribute to an alternative, water-free biodiesel purification route based on residual biomass, supporting sustainability and waste valorisation.

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Geochemical characterization and organic matter distribution in sediments from the Ría de Ferrol

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Shellfishing is one of the main economic activities on the coastal areas of Galicia. The high productivity of this region is related to its geomorphology, particularly the presence of rias, which create certain hydrodynamic and sedimentary conditions that promote the transport and accumulation of nutrients, making possible the growth of bivalve populations. However, during the last decades the productivity of most of the shellfish fisheries have shown a noticeable decline, probably due to the rise of temperatures and the acidification of water, as well as pollutant deposition and eutrophication processes.

In this context, the project BIVAFERROL addresses the integral study of the environmental quality of the sediments in the Ría de Ferrol. Specifically, this work focuses on the geochemical characterization of the sediments, particularly on the distribution and accumulation of the organic matter across different parts of the ria. One of the proposed hypothesis relates the accumulation of organic matter with changes in the ria hydrodynamics following the construction of the outer harbour, as alterations in sediment circulation and transportation patterns may have favoured the deposition and accumulation of organic matter in the sediments. The microbial degradation of this organic matter may lead to high oxygen consumption, causing the development of anoxic conditions that can negatively affect the development and survival of bivalves. (1,2)

To verify this hypothesis, a geochemical characterization was carried out on sediments collected at different depths from more than 80 sampling points distributed along the ria. The analyses included general physiochemical parameters, such as pH or redox potential, as well as organic and inorganic carbon, total nitrogen and total sulphur contents. The results were represented using cartographic tools to identify geochemical distribution patterns, compare them with historical data and evaluate possible relationships between the changes on the sedimentary dynamic and the accumulation of organic matter.

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Estudio del efecto de aditivos sobre las propiedades fisicoquímicas y las emisiones atmosféricas de purines porcinos

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La gestión de los purines porcinos constituye un importante reto ambiental debido a la generación de emisiones gaseosas y compuestos odoríferos durante su almacenamiento [1]. Entre ellos se encuentran principalmente el amoníaco (NH_3), metano (CH_4) y diferentes compuestos orgánicos volátiles (COV) y sulfurados, algunos de los cuales presentan bajos umbrales olfativos y contribuyen de forma importante a los problemas de olor asociados a las explotaciones ganaderas [2].

En este trabajo se estudió experimentalmente la aplicación de aditivos como estrategia para modificar las propiedades fisicoquímicas del purín y evaluar su posible efecto sobre las emisiones. Se estudiaron carbonato cálcico, un aditivo comercial de composición mayoritariamente carbonatada, zeolita y sepiolita. Los materiales fueron caracterizados mediante diferentes técnicas, como la difracción de rayos X y el método BET. Además, el perfil de COV se analizó cualitativamente mediante microextracción en fase sólida acoplada a cromatografía de gases-espectrometría de masas (SPME-GC-EI-TOFMS). Se realizaron dos experimentos con purines porcinos. En el primero se utilizaron muestras de purín de fosa y de balsa, en las que se evaluó la evolución del pH y la conductividad eléctrica (CE) y se compararon sus perfiles de COV. En el segundo experimento se utilizaron únicamente muestras de purín de fosa y se estudió la evolución del pH, la CE y la demanda química de oxígeno (DQO), así como la evolución temporal de los COV.

Los resultados mostraron diferencias en el comportamiento de los distintos aditivos. En el primer experimento, el purín de balsa presentó una menor respuesta a los tratamientos que el purín de fosa. En el segundo experimento, la zeolita y, especialmente, la sepiolita permitieron mantener valores de pH inferiores respecto al blanco. Este comportamiento resulta de interés, ya que el pH influye en el equilibrio entre amonio (NH_4^+) y NH_3 y, por tanto, en el potencial de volatilización del amoníaco[1]. La conductividad eléctrica presentó variaciones entre los tratamientos, aunque sin una tendencia clara. En cuanto a la DQO, la zeolita y la sepiolita mostraron una tendencia hacia valores más bajos, lo que podría asociarse a un menor potencial de formación de CH_4. Por último, el análisis mediante SPME-GC-EI-TOFMS mostró una reducción de las señales de COV, más importante en el caso de la zeolita y la sepiolita, que indica una disminución de los compuestos asociados al olor.

El comportamiento observado parece estar relacionado con las propiedades superficiales de los materiales. La sepiolita, con la mayor área superficial (189,6 m^2/g), presentó los resultados más prometedores, mientras que la zeolita (36,18 m^2/g) también mostró una tendencia favorable frente a los materiales carbonatados, con áreas superficiales considerablemente menores (1,86 y 3,26 m^2/g). La sepiolita presenta además especial interés por su elevada disponibilidad en España, único país productor de la Unión Europea [3]. Aun así, es necesario mejorar el diseño experimental para confirmar las tendencias observadas.

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Una aproximación al muestreo de grandes volúmenes de agua para monitorizar microplásticos

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La contaminación por microplásticos (MPs) en sistemas acuáticos está estrechamente relacionada con su transporte desde fuentes terrestres. Entre ellas cabe citar al tráfico rodado (fuente relevante de partículas procedentes del desgaste de neumáticos) y los residuos plásticos liberados indebidamente al medio ambiente. Tanto los fragmentos grandes como los MPs se movilizan por la escorrentía y redes de drenaje, para llegar a los y sistemas fluviales, alcanzando finalmente los ambientes costeros. Dado que el número de MPs en los cauces fluviales de Galicia es reducido su estudio requiere sistemas de muestreo capaces de recoger volúmenes representativos de agua (además de ser portátiles para permitir trabajo de campo).

En este trabajo se presenta el diseño y aplicación de un sistema de muestreo portátil basado en bombeo y filtración en cascada 1 mm, 300 µm, 100 µm, .20 µm), adecuado al estudio de MPs. El sistema cumple los requisitos básicos de las guías internacionales ASTM D8332-20 e ISO 5667-27:2025, pudiendo adaptarse con cambios sencillos para la metodología europea (Commission Delegated Decision (EU) 2024/1441). La zona de estudio para testar el sistema se sitúa en el tramo final de la cuenca del río Mero (embalse de Cecebre, A Coruña), con tramos eminentemente rurales y tramos con influencia urbana, incluyendo la desembocadura en la Ría do Burgo (A Coruña). En cada punto de muestreo se tomaron 100 L de agua. Las torres de tamices se trasladan al laboratorio, de donde se retiran los filtrados. Posteriormente se determinan los MPs mediante espectroscopía infrarroja basada en láser de cascada cuántica (QCL-IR).

Los resultados preliminares indican niveles bajos de MPs en los cauces: 8 MPs/L (3 km antes de la desembocadura, adyacente a la entrada de una planta de depuración de agua); 7 Mps/L (0.5 km antes de la desembocadura del río Mero, A Barcala, O Burgo). Los polímeros predominantes son: PP, PET, PE, PU, ABS, PVC.

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Chemometric Challenges To Identify Microplastics In Environmental Samples

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Microplastic (MP) pollution has become a major environmental concern due to the widespread occurrence and persistence of polymer residues in a broad range of environmental compartments. Despite significant progress in their analytical characterization, identifying MPs reliably remains challenging. Infrared and Raman spectroscopy are widely used for this purpose, typically by comparing the spectrum of an unknown particle with those included in spectral libraries. However, environmental MPs may undergo physical degradation, photochemical oxidation and biofouling, while additives, sample treatment and measurement conditions may further modify their spectra, hindering reliable identification.

While conventional spectral library searching provides a simple, straightforward approach for MP identification, its performance depends strongly on the representativeness of the spectral collection, matching criteria, identification thresholds and spectral preprocessing. Chemometric methods provide alternative strategies for exploiting spectral information and improving polymer discrimination. Current applications range from conventional multivariate classification methods (cluster analysis, LDA, etc.) to machine learning and deep learning approaches, including KNN, PLS-DA, random forests, SVM and neural networks.

Notwithstanding their potential, several challenges still limit their application to environmental samples. Several factors may compromise the transferability of models, including spectral variability, insufficient representation of weathered polymers, limited datasets and differences in measurement conditions. Robust external validation (along with representative spectral datasets) using real environmental samples are therefore essential for developing reliable and harmonized chemometric strategies for MP identification.

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Behavior and mechanism of terbuthylazine adsorption on polyethylene microplastics in the marine environment

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In recent times, the increase in the presence of microplastics in the oceans has become a significant environmental concern, as these polimers have a negative impact on ecosystems and act as vectors for other contaminants that can be adsorbed onto their surface. For this reason, numerous studies have been conducted on the adsorption of organic substances by microplastics, but for triazine herbicides, these studies are scarce [1]. Triazines are a group of contaminants that are present in the ten most-used herbicide formulations in Europe. Although they are highly water soluble, it has been observed that coastal systems have little capacity to degrade these compounds. This study is focused on the behaviour and adsorption mechanisms of terbuthylazine on pristine and aged polyethylene (PE) microplastics simulating both wet marine conditions and conditions on the dry part of beaches. Polyethylene, a polyolefin derived from the polymerisation of ethylene, is by far the most widely used plastic in the packaging industry [2]. Terbuthylazine is an herbicide formally classified as a priority substance for presenting a significant risk to waters due to its regular use and persistence [3].

The kinetics and adsorption isotherms of terbuthylazine on pristine and aged MPs were studied using a batch procedure. The method was based on putting 25 mg of the polymer in contact with 25 mL of the of terbuthylazine standard solution prepared in synthetic seawater. The tube was placed in an incubator at 25 ± 2 °C and kept shaking at 150 revolutions per minute (rpm) for a certain period of time. All sorption experiments were carried out in triplicate and three controls (MPs free) were also performed to control any loss caused by terbuthylazine degradation, volatilization or sorption to surfaces. The tubes were centrifuged at 2500 rpm for 15 min to separate the MPs from the aqueous fraction and terbuthylazine remaining in solution was analysed by liquid chromatography. The kinetic studies were carried out using a 5 mg/L terbuthylazine standard solution, taking supernatant samples at different time intervals (3, 6, 24, 48, 72, and 144 h). For the adsorption isotherms study, five different concentrations were used (0.5, 1, 2, 4, and 5 mg/L), which were left stirring for 72 h to reach adsorption equilibrium.

The results show that the roughness and specific surface area of aged microplastics increase their adsorption capacity compared to pristine microplastics. Furthermore, adsorption capacity increases significantly with wet aging compared to dry aging, probably because the aging process under marine conditions is more energetic.Once the experiment was completed, the percentage adsorbed from the initial concentration was 52.4% for wet-aged PE, 27.7% for dry-aged PE, and 12.6% for pristine PE.For the three MPs, the sorption kinetic data fit well with the second-order kinetic model ($R^2 \geq$ 0,995) although the kinetic profiles revealed that sorption rates are also controlled by intraparticle diffusion model.

Regarding the study of terbuthylazine adsorption mechanisms, it has been observed that all three microplastics conform to the Henry model ($R^2 \geq$ 0,993), a mechanism dominated by hydrophobic interactions. In the case of aged microplastics, it is noteworthy that, due to the high R^2 values ($R^2 \geq$ 0,994) and the parameter *n* values were less than 1, they also conform to the Freundlich model, indicating that the surface of these microplastics presents a heterogeneous surface concerning terbuthylazine adsorption points.

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Cell-dependent cytotoxicity of bisphenol A and its substitutes: evidence from human hepatic, immune and erythrocyte models

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Bisphenol A (BPA) is a recognised metabolism-disrupting chemical (MDC), associated with obesity, type 2 diabetes and metabolic dysfunction-associated steatotic liver disease (MASLD), and acting on the liver, adipose tissue and pancreas to alter glucose and lipid homeostasis. Regulatory restrictions have driven its replacement by structural analogues whose toxicological profiles remain far less characterised. Available evidence indicates that several are not safer alternatives, showing comparable or greater cytotoxicity and metabolism-disrupting activity. Given the central role of the liver in metabolic homeostasis and the relevance of circulating immune and blood cells as direct targets of systemic exposure, assessing the effects of BPA analogues in human hepatic, immune and erythroid cellular models is important for defining their cytotoxic and metabolic safety profiles. This study aimed to compare the cytotoxicity of BPA and its analogues BPAF, BPM and BPAP in HepG2 cells, human neutrophils and erythrocytes.

HepG2 were exposed to BPA, BPAF, BPM and BPAP (0 - 25 µM) for 24h, and viability was assessed by the sulforhodamine B (SRB) assay. Human neutrophils were isolated from whole blood of healthy donors by the gradient density centrifugation method [1]. Human neutrophils were incubated with BPA (0 - 100 µM), BPAF, BPAP (0 - 50 µM) and BPM (0 - 25 µM) for 1 h. Cytotoxicity was assessed by flow cytometry using annexin V-FITC/propidium iodide (PI) double staining, allowing discrimination between viable, apoptotic and necrotic cells. Erythrocytes were isolated from the blood of healthy donors by differential centrifugation [2] and exposed to the bisphenols under study (0 - 100 µM, except BPM which was 0 -25 µM) for 5 h. After centrifugation, the supernatant was transferred to a 96-well plate, and the absorbance was measured at 540 nm in a microplate reader.

While BPA showed no cytotoxicity in any of the three cell models at the concentrations tested, its substitutes exhibited distinct concentration- and cell-dependent effects. BPM, BPAP and BPAF reduced HepG2 cell viability at 25 µM, whereas neutrophils displayed differential sensitivity, with cytotoxicity occurring at 12.5, 25 and 50 µM, respectively. In erythrocytes, BPM induced haemolysis at 12.5 and 25 µM and BPAP at 100 µM, while BPAF remained non-haemolytic.

Overall, BPA substitutes were more cytotoxic than BPA, with distinct cell-dependent profiles. Notably, BPM was the most cytotoxic, affecting hepatic, immune and erythroid cells. These findings challenge the assumption that BPA analogues are safer alternatives and highlight the importance of assessing their cytotoxicity across different human cell types to establish appropriate non-cytotoxic concentration ranges.

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Desempeño de compuestos fúngicos para aplicaciones constructivas no estructurales: caracterización de *Pleurotus ostreatus y Ganoderma lucidum*

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Los compuestos basados en micelio fúngico ofrecen una vía para valorizar sustratos lignocelulósicos en productos livianos, pero su desempeño depende de la especie, el sustrato y las condiciones de fabricación; la humedad y la variabilidad mecánica siguen siendo desafíos para su aplicación en construcción [1],[2]. Este estudio caracterizó y comparó bloques, ladrillos y planchas obtenidos con *Pleurotus ostreatus (PO)* y *Ganoderma lucidum (GL)* frente a materiales convencionales mediante ensayos físicos, mecánicos, térmicos, de inflamabilidad y acústicos, con procedimientos basados en normas INEN, ISO y ASTM. Algunas pruebas de fuego y acústica se adaptaron por disponibilidad de equipamiento. La literatura confirma que variar la composición y el procesamiento modifica de forma importante la absorción y resistencia [1],[3].

Los ladrillos de micelio presentaron absorción de agua de 57,42% (PO) y 62,95% (GL). La resistencia a compresión fue: 0,12 y 0,53 MPa en ladrillos. En las planchas de G. lucidum, el ensayo exploratorio de llama pequeña reportó propagación inferior a 150 mm y ausencia de gotas o partículas inflamadas; el trabajo asignó clasificación D, d0. Su potencial radica en la sostenibilidad y propiedades de aislamiento.

Los resultados delimitan el uso actual de estos materiales a posibles aplicaciones no estructurales, requiriendo protección frente a humedad y durabilidad. Los materiales de micelio son una alternativa prometedora, económica y ecológica para aplicaciones no estructurales en construcción.



Fig.1. Ladrillo convencional y ladrillos y planchas de micelio

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Immunotoxic effects of bisphenol A analogues on human neutrophils

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Bisphenols are widely used synthetic chemicals, with bisphenol A being extensively incorporated into consumer products and associated with multiple adverse health effects, including cytotoxicity and endocrine disruption. Restrictions on bisphenol A have promoted the use of alternative bisphenol analogues [1], although their toxicological effects, particularly on immune cells, remain poorly understood. Neutrophils are the most abundant circulating leukocytes and a key component of the innate immune response. Their defense mechanisms, including neutrophil extracellular trap (NET) release and reactive species (RS) production, are tightly regulated by intracellular signaling pathways [2]. Therefore, bisphenol-induced alterations in these responses may compromise neutrophil function highlighting the need to investigate the effects of emerging bisphenol analogues in this cellular model.

This study aimed to characterize the effects of selected structurally related bisphenol A analogues, namely bisphenols A-DMA, AF, AP, B, BP, E, F, M, and S, on cell viability, apoptosis, necrosis, NET release, and oxidative burst in freshly isolated human neutrophils.

Among the ten bisphenols evaluated, bisphenols AF, AP, B, BP, and M significantly affected neutrophil cell death. In addition, bisphenols AF, AP, BP, and M significantly enhanced NET release, with BP and M eliciting the most pronounced responses. Under basal conditions, bisphenols AF, AP, M, and S significantly increased intracellular RS production, with M already inducing a significant effect at the lowest concentration evaluated. Under PMA-stimulated conditions, used to mimic an inflammatory state, bisphenols AF and S further enhanced RS production beyond that induced by PMA alone.

Bisphenol A analogues differentially disrupted key neutrophil functions, including cell survival, NET release, and oxidative responses. These findings challenge the assumption that bisphenol A substitutes are inherently safer and raise concerns about their potential to interfere with innate immune responses, reinforcing the need for a comprehensive assessment of the immunotoxicity of emerging bisphenols.

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Reuse of organic waste as sustainable adsorbents for the removal of sertraline in aqueous systems

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Pharmaceutical residues have been increasingly detected in wastewater and receiving waters, where persistence after conventional treatment may contribute to chronic aquatic exposure. Recent studies have documented the occurrence of antidepressants in wastewater and receiving waters, assessed their removal and environmental risks, and related wastewater mass loads to prescription volumes [1–3]. Sertraline is a relevant target because its ionisable amine and aromatic structure influence its environmental behaviour and interactions with adsorbent surfaces. Hence, in this study, sertraline hydrochloride was selected as the target pollutant for removal by adsorption using biomass-derived activated carbons, combining purification with sustainable agro-industrial waste valorisation [4].

Although biomass-derived adsorbents show potential, differences in the precursors, activation route, selected analytical method, and experimental conditions complicate comparisons of results. Olive stone, walnut shell, and almond shell were selected as lignocellulosic residues with the potential to produce porous carbonaceous materials. $ZnCl_2$-activated adsorbents from these precursors were previously prepared within the research group [5–7]. Bourafa et al. demonstrated that olive-stone waste can be converted into CO_2-activated biochar and hydrochar for pharmaceutical removal, supporting the inclusion of this precursor in the preliminary assessment [8]. This project will compare the materials' performance in controlled synthetic aqueous solutions and identify the most promising adsorbent.

Initially, the materials will be evaluated in batch experiments under common conditions, with sertraline hydrochloride quantified by HPLC-DAD. The selected adsorbent will then undergo kinetic, equilibrium, and thermodynamic analyses, as well as Box-Behnken response-surface optimisation. The expected outcome is an evidence-based analysis that links sertraline's environmental relevance to the sustainable reuse of agro-industrial waste and identifies the main removal conditions. The experimental pathway is shown in Fig. 1.

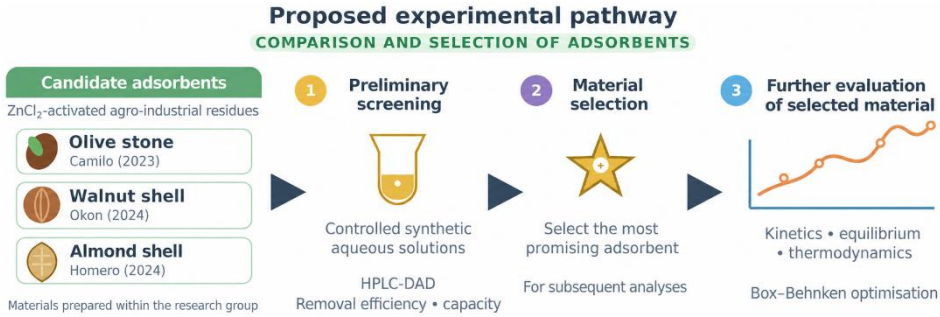


Fig. 1. Proposed experimental pathway for assessing $ZnCl_2$-activated biomass-derived adsorbents for sertraline hydrochloride removal.

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Different technologies for the extraction of polysaccharides from Ulva *spp*. using green solvents

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Green macroalgae are an important source of bioactive compounds with potential applications in food, pharmaceutical, and biotechnological fields. Among them, the genus *Ulva* is particularly relevant due to its widespread availability and valuable composition, including polysaccharides, proteins, pigments, and phenolic compounds [1,2]. Ulvan, a sulfated polysaccharide located in the cell walls of *Ulva* species, is one of their major bioactive components [3]. For this reason, selecting an appropriate extraction method is important for recovering Ulvan while maintaining an efficient process [3-5]. In this study, different extraction technologies were employed to obtain ulvan, including an Ultrasound Bath, Ultrasound, and Autohydrolysis at various extraction temperatures, using thermal water as the extraction agent and deionized water as a control. A solvent/biomass ratio of 1:30 (w:w) was used, along with specific extraction conditions for each technology: Ultrasound Bath (T: 35–45°C, t: 1 h, f: 80 kHz, A: 100%), Ultrasound (T: 55–65°C, t: 5 min, A: 100%, cycle: 0.5), and Autohydrolysis (T: 150–170°C). The highest extraction yields were 16.63%, 19.15%, and 26.49% for the aforementioned technologies, respectively. These yields were higher than the results obtained with the deionized water control, which were 14.63%, 13.02%, and 25.82%. Overall, the results indicate that the extraction conditions affected the recovery from Ulva biomass, with autohydrolysis giving the highest yield among the tested methods.

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Monitoring the WWTP at Porto airport - design of a µPAD for determination of nitrogen-based ions

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The city of Porto has been awarded Europe's Leading City Destination in 2025 by the World Travel Awards [1], as a consequence of the increasing number of tourists. Consequently, there has been a significant increase in air traffic at Porto Airport, Francisco Sá Carneiro Airport. In 2025, the airport handled 16.9 million passengers [2] and kept growing in 2026, with approximately 3.48 million passengers during the first quarter of the year, representing an 8.3% increase compared with the same period in 2025 [3]. Maintaining high operational efficiency while complying with environmental requirements is particularly relevant and the airport sustainability is crucial. In this context, we aimed to design new monitoring tools to enable an in-situ, fast accurate analysis of airport interest areas, namely wastewater treatment plant.

The airport already operates a wastewater treatment plant (WWTP), following environmental guidelines, and its current monitoring relies on off-site laboratory analysis using expensive instrumentation and trained personnel, which limits measurements frequency. In this context, we developed a microfluidic paper-based analytical device (µPAD) to enable a simple, low-cost, in-situ monitoring of water samples at previously established sampling points across the airport. These sampling points were established in collaboration with Porto Airport Sustainability and Environment department, to cover WWTP and its sources: terminal wastewater, aircraft bluewaters (wastewater from aircrafts) and both in and out of the WWTP. The target analytes, nitrogen-based ions namely ammonia and nitrate are the primary targets, as WWTP performance indicators. Monitoring the different samples refered can provide valuable anticipation of impact in the WWTP operation, which is fundamental to have an informed decision in potential improved to a WWTP with tertiary treatment.

The µPADs methods provide a simpler, user friendly and highly portable alternative for in-situ analysis. Additionally, they provide rapid, low-cost and decentralised monitoring capacity, contributing to improved environmental monitoring and sustainability at Porto Airport.

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Optimized ultrasonication-redox depolymerization for controlled production of low molecular weight ulvan and carrageenan

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Abstract

Sulfated polysaccharides from marine sources, such as ulvan and carrageenan, exhibit promising biological and functional properties. However their high molar mass and limited solubility restrict broader biomedical, agricultural, and industrial applications. This study develops a sequential ultrasonication (US) and hydrogen peroxide–ascorbic acid (H_2O_2/AH_2) redox treatment as a scalable and controllable strategy for depolymerizing ulvan and carrageenan. Depolymerization kinetics and key operational variables were evaluated.

For ulvan, US followed a one-phase exponential decay model, rapidly reducing apparent weight-average molar mass (Mw) and achieving a 50% reduction within 12.9 min at 60% amplitude and 0.64 W/mL. The redox step was accurately described by a quadratic regression model, identifying temperature, reaction time, and redox system-to-ulvan ratio as the main factors. The combined US–redox process reduced Mw from 1058 to 31.7 kDa within 60 min, whereas acid hydrolysis control (0.1 M HCl) reduced Mw only from 1022 to 429 kDa under equivalent treatment time. Optimal depolymerization conditions predicted an H_2O_2/AH_2 ratio of 3.5, redox system/ulvan ratio of 4, 60 °C, and 85.5 min, yielded a 15 kDa product within the model's 95% prediction interval. After TFF concentration and spray drying, HPSEC confirmed no significant change in molar mass distribution or Mw. FTIR and ^{13}C-^{1}H NMR analyses revealed that depolymerized and spray-dried ulvan retained functional groups and structure, with hydrolysis occurring only at anomeric centers without significant side reactions.

For carrageenan, a two-step process combining ultrasonic pretreatment with a H_2O_2–AH_2 redox system efficiently produced low-molecular-weight carrageenan (LMWC). Ultrasonication rapidly reduced molecular weight, homogenized polymer size, and preserved functional groups, as confirmed by HPSEC, rheology, FTIR, and ^{1}H NMR. Depolymerization kinetics followed a two-phase model, with the most energy-efficient ultrasonication at 60% amplitude for 8.67 min (54.2% Mw reduction, 218.8 J/mL). Redox-assisted depolymerization was optimized via a quadratic model, showing strong effects of temperature and time, while intermediate reagent ratios maximized efficiency. Scaling from 150 mL to 2.2 L retained performance, producing ~9.35 kDa LMWC with lower polydispersity, reduced reagent consumption, and faster processing than mild-acid hydrolysis controls. The purified fraction exhibited enhanced antioxidant activity (IC_{50} 0.96 g/L, 270 mg Trolox equivalents/g).

Overall, the sequential US–H_2O_2/AH_2 approach offers a scalable, well-controlled route to tailor low-molar-mass sulfated polysaccharides for specific applications, outperforming conventional acid treatments and providing a robust alternative to enzymatic depolymerization.

Acknowledgements
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Aqueous matrix contaminated with antidepressants: Adsorption via activated charcoal from walnut shell

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Emerging contaminants are substances that have only recently been documented in the scientific literature or that lack established environmental standards, thus bypassing conventional regulatory control [1]. Among them, pharmaceuticals and personal care products assume a prominent position [2]. They enter the environment through industrial, domestic, and hospital effluents, agrochemicals, sewage sludge, landfill leachates, and septic tanks [3], and their presence at trace concentrations hinders toxicological assessment and risk management. Wastewater treatment plants, the central link between emission sources and receiving water bodies, were designed to remove organic matter, nutrients, and suspended solids rather than complex organic micropollutants; residues of these compounds or of their metabolites may therefore reach surface waters and, potentially, drinking water [4].

Antidepressant consumption more than doubled between 2013 and 2023 in several OECD countries [5]. These drugs have been detected in raw wastewater worldwide at total concentrations between 72.62 and 5011.8 ng L^{-1}. Their discharge has been associated with bioaccumulation and with physiological and behavioural alterations in non-target organisms [6].

In this context, the present work addresses five neuronal monoamine reuptake inhibitors: duloxetine, fluoxetine, paroxetine, sertraline, and venlafaxine. All are predominantly protonated at environmental pH, yet their sorption behaviour differs: sertraline showed the highest sorption coefficient in primary sludge (3.5×10^4 L kg^{-1}) [7], whereas venlafaxine, the most hydrophilic, showed the lowest sorption coefficient [8]. On the other hand, walnut shell-derived activated carbons, obtained from an agricultural by-product in line with circular economy principles, have reached surface areas above 1200 m^2 g^{-1} and performance competitive with commercial activated carbons [9,10]. However, most studies evaluate isolated compounds, and those comparing single and multicomponent systems show that competition for active sites depends on the adsorbent–drug pair [11]. No study on the adsorption of antidepressant mixtures onto walnut shell carbon was identified. Furthermore, only seven articles applied HPLC-DAD to the simultaneous determination of antidepressants, mostly in biological matrices, and none quantified them in real water samples. Hence, this study aims to investigate the application of an activated charcoal (synthesized from walnut shells activated with zinc chloride) for the removal, by adsorption in an aqueous matrix, of a mixture of frequently used neuropsychiatric drugs. A methodology is proposed that encompasses quantification by HPLC-DAD, as well as kinetic and equilibrium studies.

Acknowledgements
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A sustainable alternative for the selective synthesis of 2-aminoquinolines using porous ZnO/carbon composites

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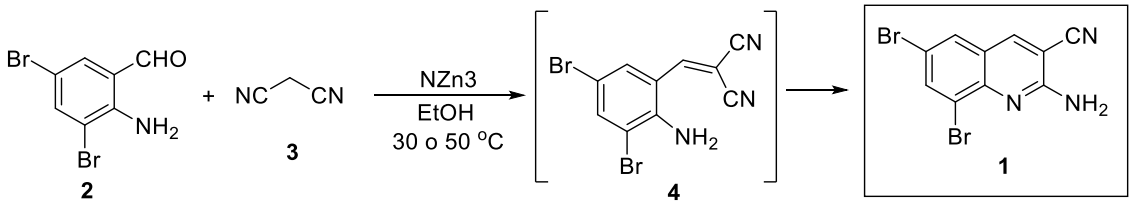
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Aminoquinolines are pharmaceutical scaffolds being the subject of extensive research because of their variety of biological activities; antimalarial, antitumor, and antibacterial activity, among them.
In other sense, Zinc oxide (ZnO) is an attractive material for catalytic applications characterized by its low cost, low toxicity, and high chemical stability. The use of porous supports such as activated carbons (ACs) often improves both dispersion of ZnO particles and surface area favoring the reactant access to active sites [1].

This communication presents a series of ZnO/carbon composites applied to the sustainable synthesis of 2-aminoquinolines (**1**) by reacting 2-amino-3,5-dibromobenzaldehyde (**2**) and malononitrile (**3**) in EtOH, as a recognized green solvent (Scheme 1).



Scheme 1. Synthesis of 2-aminoquinoline (**1**) from 2-amino-3,5-dibromobenzaldehyde (**2**) and malononitrile (**3**), in EtOH, catalyzed by ZnO/carbon composites.

In all cases, the formation of intermediate (**4**) was observed which is transformed into the reaction product (**1**) over time. Both the amount of catalyst used, and the reaction temperature directly impacted into conversion and selectivity to quinoline (**1**). Higher conversion values were observed when increasing the catalyst amount whereas the reaction temperature is a key factor driving the selectivity to quinoline (**1**).

It is important to note that catalyst porosity plays a significant role in the process. Intermediate (**4**) was preferentially formed when using microporous ZnO/carbon composite, at short reaction times, whereas the mesoporous sample favors the formation of quinoline (**1**), suggesting enhanced diffusion of both reactants and products.

In summary, this communication presents for the first time a series of easily prepared carbonaceous materials containing supported ZnO nanoparticles active in the synthesis of 2-aminoquinoline (**1**). The obtained results strongly suggest that the catalyst porosity and temperature have a direct impact on reaction selectivity.

Acknowledgements
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Functional biomass-derived hydrothermal carbons highly efficient and selective for the green dihydroquinazolinone synthesis

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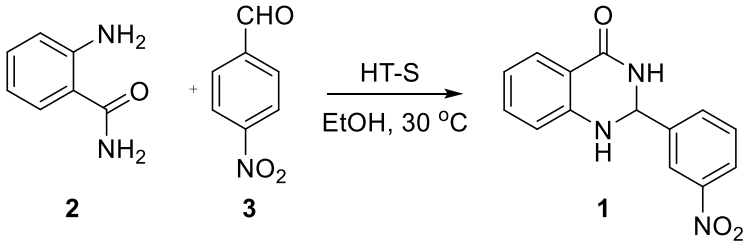
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Nitrogen-containing heterocycles are found in a wide variety of biologically active natural products, as well as in synthetic drugs and pharmaceutical products [1]. Specifically, 2,3-dihydroquinazolinones are *N*-heterocycles that exhibit a great variety of biological activities; antiviral, anticancer, antimicrobial, antihypertensive, anti-inflammatory, and antihistamine activities, among others.

This communication presents a family of acidic catalysts based on biomass-derived carbon materials easy to prepare and highly efficient in the sustainable and selective synthesis of 2,3-dihydroquinazolinones (**1**) from 2-aminobenzamide (**2**) and 4-nitrobenzaldehyde (**3**).



Scheme 1. Synthesis of 2,3-dihydroquinazolinone (**1**) from 2-aminobenzamide (**2**) and 4-nitrobenzaldehyde (**3**), catalyzed by HT-S at 30 °C in EtOH.

The materials under investigation were prepared via the hydrothermal method using sucrose in the presence or in the absence of a commercial activated carbon with subsequent H_2SO_4 treatment. All the prepared carbonaceous materials proved active in the synthesis of 2,3-dihydroquinazolinone (**1**), the reaction proceeding with high conversion values. Both the amount of catalyst used and the reaction temperature had a direct impact on the selectivity to (**1**).

Catalyst acidity plays a crucial role in the course of the reaction in such a manner that the most acidic catalyst (pH = 1.9 and 24% oxygen content) afforded the dihydroquinazolinone (**1**) with a quantitative yield after a reaction time of only 60 min while in the presence of a sample showing a lower acidity (pH = 4.4 and 5.6% oxygen content), both conversion and selectivity decreased considerably. These results strongly suggest that sulfonic or sulfate groups, as detected by IR spectroscopy, are behind the observed reactivity.

All these results are also supported by a computational study carried out by DFT calculations.

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Porphyrin-functionalized silica materials for water decontamination: metal ion adsorption

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Tetrapyrrolic macrocycles, particularly porphyrins and related derivatives, are highly versatile compounds due to their tunable structures, extended π-conjugation, and remarkable coordination and photophysical properties. These features have supported their use in catalysis, sensing, solar energy conversion, and biomedicine. More recently, porphyrins have also attracted interest in environmental remediation, namely for the removal of toxic metal ions from contaminated waters.

The affinity and selectivity of porphyrinic systems towards metal ions can be modulated through appropriate structural modifications. When immobilised onto silica, these macrocycles give rise to hybrid adsorbent materials that combine the metal-binding ability of porphyrins with the advantages of a solid support, including high surface area, chemical stability, easy separation from aqueous media, and potential reuse [1–4].

This communication presents selected studies developed by our group on porphyrin-functionalized silica materials for the adsorption of metal ions from aqueous solutions. The influence of porphyrin structure, silica functionalization, and metal-ion coordination ability on adsorption performance will be discussed, highlighting the potential of these hybrid materials as reusable platforms for sustainable water decontamination.

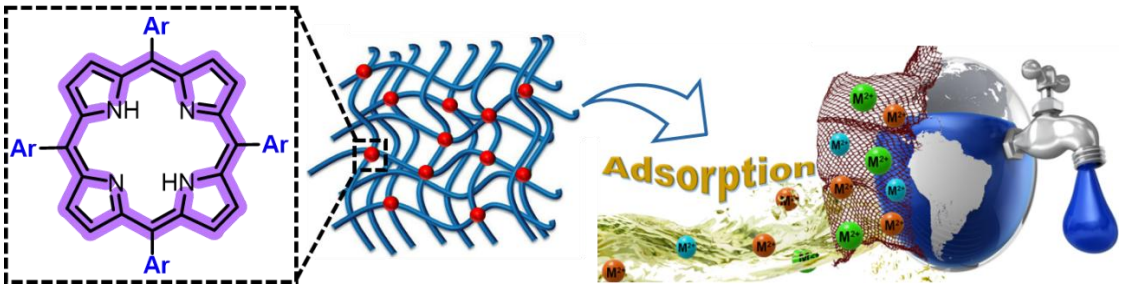


Fig. 2. Porphyrin-functionalized silica materials for metal-ion adsorption from aqueous media.

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HVO (Hidrobiodiesel) Frente A Diesel

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Es un error común confundir el HVO (Aceite Vegetal Hidrotratado) con el biodiésel (FAME) y el diésel convencional; el HVO un producto parafínico sintético [1].

La comercialización del HVO en España está en plena evolución regulatoria. A diferencia de otros países europeos donde el HVO100 está plenamente integrado en el mercado de combustibles, en España su regulación se ha ido desarrollando progresivamente al amparo de la legislación europea sobre energías renovables.

El Plan Nacional Integrado de Energía y Clima (PNIEC) 2023-2030 [2] fija objetivos ambiciosos de incorporación de energías renovables en el transporte, lo que impulsa directamente la adopción del HVO y otros biocombustibles avanzados. La normativa europea de referencia, la Directiva de Energías Renovables (RED III) [3], establece que los biocombustibles avanzados como el HVO deben suponer una proporción creciente del consumo de energía en el transporte.

En este trabajo se analizan, a lo largo de un año, muestras de gasóleo y HVO destinado al funcionamiento de grupos electrógenos; a la vez que se toman muestras de HVO comercializado, bajo distintos nombres comerciales, por distintas petroleras en estaciones de servicio para consumo en transporte.

De forma sencilla, se puede afirmar que el HVO funciona igual de bien o incluso mejor en ciertos aspectos que el gasóleo convencional y es significativamente más sostenible, es un sustituto directo de alto rendimiento con una huella de carbono mucho menor; las claves fundamentales:

- Rendimiento equivalente (o superior): alto número de cetano (superior al del diésel fósil), una combustión más limpia y eficiente, mejor rendimiento en frío.
- Mayor sostenibilidad: El HVO reduce las emisiones de gases de efecto invernadero/CO2 en todo su ciclo de vida hasta en un 90% en comparación con el diésel fósil.
- Menos emisiones locales: Produce menos partículas, óxidos de nitrógeno (NOx) y azufre, lo que mejora la calidad del aire.
- Origen renovable: Se produce a partir de residuos, grasas animales y aceites vegetales usados, lo que lo convierte en una alternativa a la economía circular.

El gasóleo convencional y el HVO son totalmente miscibles y compatibles entre sí. Esto significa que pueden mezclarse en cualquier proporción sin problemas técnicos y utilizarse en motores diésel sin modificaciones, ya que el HVO es un combustible parafínico de alta calidad que funciona como sustituto directo aunque “no es adecuado para todos los vehículos”

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Hydrothermal Zeolitization of Fly Ash-Based Geopolymers and Their Composites with Biomass-Derived Activated Carbon for Carbamazepine Removal

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In this study, fly ash-based geopolymers (GP_M) were synthesized and hydrothermally treated with 2.0 M NaOH (70°C, 24h) to promote in situ zeolitization (GP_HT2.0). A geopolymer–carbon composite (GP_AC) was also prepared by incorporating activated carbon obtained from winery grape pomace (AC_WGP) and subjected to the same hydrothermal treatment (GP_AC_HT2.0). XRD confirmed the formation of Na-faujasite in the GP_HT2.0, and BET analysis revealed a substantial increase in specific surface area from 30 $m^2\ g^{-1}$ for the untreated geopolymer to 181 $m^2\ g^{-1}$ after hydrothermal treatment. In the composite, the treatment increased the surface area from 48 to 139 $m^2\ g^{-1}$, although no zeolitic phase was detected. Finally, the adsorption performance was evaluated using carbamazepine as a model pharmaceutical. Adsorption kinetics were best described by the pseudo-second-order model, with **equilibrium adsorption capacity** (q_e) of 4.2, 29.4, 39.7 and 30.6 mg g^{-1} for GP_M, GP_HT2.0, GP_AC and GP_AC_HT2.0, respectively. Adsorption isotherm data were better fitted by the Langmuir model (q_{max} = 7.8, 10.3, 10.4 and 23.4 mg g^{-1}, respectively), indicating predominant monolayer adsorption. The zeolitized geopolymer (GP_HT2.0) showed an approximately sevenfold higher carbamazepine uptake than the untreated one (GP_M), while combining activated carbon with hydrothermal treatment (GP_AC_HT2.0) gave the highest Langmuir capacity. These results show that waste-derived zeolitic geopolymers and geopolymer–carbon composites are promising adsorbents for pharmaceutical removal from wastewater.

Tabla 1. Textural properties analysis for the materials

Sample	S_{BET} ($m^2\ g^{-1}$)	$S_{Langmuir}$ ($m^2\ g^{-1}$)	S_{mic} ($m^2\ g^{-1}$)	S_{ext} ($m^2\ g^{-1}$)	V_{total} ($cm^3\ g^{-1}$)
FA	13	248	-	1	0.010
GP_M	30	232	-	7	0.074
GP_HT2.0	181	527	68	113	0.195
AC_WGP	427	632	254	173	0.225
GP_AC	48	188	12	36	0.110
GP_AC_HT2.0	139	138	77	62	0.138

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Influence of heating at high temperatures on the behavior of concrete with incorporation of Diatomaceous Earths

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Summary

The growing demand for sustainable construction materials has encouraged the valorisation of industrial waste and the reduction of conventional raw material consumption. In this context, residual diatomaceous earth (RDT) from the wine industry represents a promising alternative for partial cement or sand replacement in concrete. This study investigates the influence of high-temperature exposure, relative humidity, and cooling time on the residual compressive strength of concrete incorporating RDT. Three compositions were analysed: reference concrete (REF), concrete with 10% cement replacement by RDT (RC), and concrete with 5% sand replacement by RDT (RA). Specimens were exposed to temperatures of 20, 200, 400, and 600 °C under relative humidity conditions of 65%, 77.5%, and 90%, and their compressive strength was evaluated after 0, 24, and 48 h of cooling. Overall, temperature was identified as the main factor influencing residual compressive strength, with strength decreasing as exposure temperature increased. Nevertheless, the RDT-containing compositions generally showed promising performance compared with the reference concrete, particularly RA, which exhibited higher initial compressive strength. As illustrated in Figure 1, under the specific condition of 600 °C and 90% relative humidity, RA retained approximately 35% of its initial compressive strength, reaching a residual strength of around 15 MPa after 48 h of cooling. This result highlights the potential of partial sand replacement with RDT to preserve residual mechanical performance following severe thermal exposure. Overall, the findings support the valorisation of this wine-industry residue as a supplementary raw material for more sustainable concrete, while highlighting the importance of considering environmental and post-heating conditions when assessing its performance.

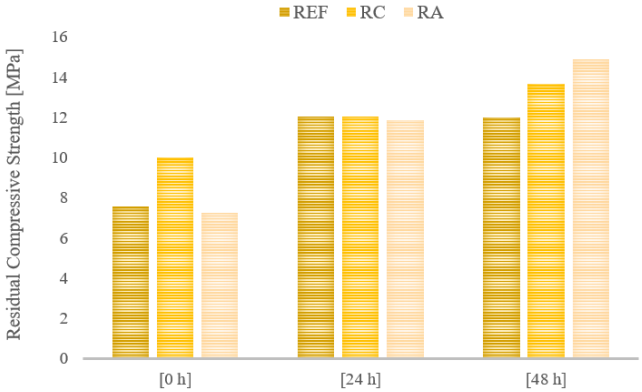


Figure 1: *Resistance* residual compression, at 0, 24 and 48 hours, 600°C and humidity of 90%.

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Unlocking the Value of Shrimp By-Products through Sustainable Extraction Strategies

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Shrimp processing generates significant amounts of by-products which represent valuable sources of biopolymers and bioactive compounds.[1] Their valorisation through sustainable extraction strategies offers opportunities to reduce waste while promoting the recovery of high-value compounds within a circular bioeconomy framework.

This work explores alternative extraction strategies for the recovery of chitosan and astaxanthin from shrimp by-products, focusing on the use of extraction media with potential environmental advantages. For chitosan production, different processing approaches were investigated, involving citric acid and a deep eutectic solvent, followed by alkaline deacetylation. The obtained materials were evaluated in terms of their physicochemical properties, including solubility and structural characteristics. Both processing approaches demonstrated potential for the successful recovery of chitosan from shrimp by-products.

In parallel, the recovery of astaxanthin and other carotenoids was explored using alternative extraction media, including oils and deep eutectic solvents. These approaches were investigated as potential alternatives to conventional organic solvent-based extraction methods, with particular emphasis on the recovery of carotenoid-rich extracts and their stability over time. Preliminary results showed that different extraction media enabled the recovery of carotenoid-containing extracts, with storage conditions playing an important role in their stability.

Overall, this study highlights the potential of exploring complementary extraction strategies for the recovery of distinct high-value compounds from shrimp processing residues. By targeting both biopolymers and carotenoids, these approaches contribute to a more comprehensive valorisation of marine by-products, supporting resource efficiency and the development of sustainable processing strategies.

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Effect of solvent on the microwave-assisted extraction of bioactive compounds from *Melipona flavolineata* geopropolis

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Geopropolis produced by stingless bees constitutes a complex organic-mineral matrix with potential as a source of bioactive compounds [1]. The efficiency of recovering these compounds depends on the technique employed and the characteristics of the solvent [2]. Microwave-assisted extraction (MAE) enables enhanced mass transfer and reduced processing time, offering the potential to obtain bioactive extracts through more sustainable routes [3].

The objective of this study was to evaluate the effect of solvent nature on the recovery of bioactive compounds from *Melipona flavolineata* geopropolis using microwave-assisted extraction (MAE). Systems using water (MW-H_2O; 100–220 °C) and ethanol (MW-EtOH; 100–180 °C) were evaluated. The extracts were characterized in terms of total phenolic content (TPC), total flavonoid content (TFC), and antioxidant capacity using ABTS, FRAP, and DPPH methods.

The extraction response depended on the solvent nature and temperature. In MW-H_2O extraction, the highest TPC and TFC values were obtained at 200 °C, reaching 2348.17 ± 86.19 mg GAE/100 g and 463.30 ± 5.02 mg QE/100 g, respectively. Under this condition, the antioxidant capacity was 23.50 ± 2.03 mM TE/100 g (ABTS) and 14.90 ± 0.22 g AA/100 g (FRAP), while DPPH inhibition was 90.60 ± 1.42%. For MW-EtOH, the highest TPC values occurred at 180 °C (2385.22 ± 73.38 mg GAE/100 g), along with 162.52 ± 3.67 mg QE/100 g (TFC), 54.09 ± 1.88 mM TE/100 g (ABTS), 31.46 ± 0.67 g AA/100 g (FRAP), and 94.12 ± 0.71% DPPH inhibition. Although water favored the recovery of phenolic compounds and flavonoids under more severe hydrothermal conditions, 70% ethanol yielded a higher antioxidant response in the ABTS and FRAP assays at the condition of highest TPC.

The results demonstrate that solvent polarity, combined with dielectric heating, modulates the recovery and functional profile of the extracted compounds, showing that the composition of geopropolis extracts can be tailored through the selection of MAE conditions. Thus, solvent selection can serve as a strategy to direct the chemical and functional profile of geopropolis extracts, contributing to the sustainable utilization of this Amazonian matrix.

Table 1. Comparison of the main results obtained by microwave-assisted extraction.

Condition	TPC (mg GAE/100 g)	FTC (mg QE/100 g)	ABTS (mM TE/100 g)	FRAP (g AA/100 g)	DPPH (% inhibition)
MW-H_2O - 200 °C	2348.17 ± 86.19	463.30 ± 5.02	23.50 ± 2.03	14.90 ± 0.22	90.60 ± 1.42
MW-EtOH - 180 °C	2385.22 ± 73.38	162.52 ± 3.67	54.09 ± 1.88	31.46 ± 0.67	94.12 ± 0.71

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Effect of Nitrogen Addition to the Headspace on the Extraction of Bioactive Compounds from Mentrasto (*Ageratum conyzoides*) by Autohydrolysis

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Mentrasto (*Ageratum conyzoides*) is a common medicinal herb in Brazil. Although the health benefits of mentrasto have been previously documented in the literature, its potential as a source of bioactive compounds and its technological applications remain underexplored. Consequently, the development of green extraction processes based on different technologies, such as autohydrolysis using water as a solvent, represents a promising approach. This study aimed to assess the influence of nitrogen addition to the headspace during autohydrolysis on the recovery of bioactive compounds from dried and milled mentrasto (DMM), as assessed by global extraction yield (X_0), total reducing capacity (TRC), and antioxidant capacity (FRAP).

Autohydrolysis was performed at 200 and 220 °C using water as the solvent at a solvent-to-feed ratio of 1:30. Prior to each run, the extraction vessel headspace was purged with nitrogen gas from a pressurized cylinder for 30 s by opening a control valve to displace the air. The valve was then closed, retaining the nitrogen in the headspace throughout the process. A non-isothermal heating–cooling profile was employed, with heating discontinued immediately upon reaching the target temperature. All extracts were characterized regarding X_0, TRC, and FRAP. X_0 was determined gravimetrically after oven drying the extracts until constant mass. TRC was evaluated using the Folin–Ciocalteu method and expressed as mg gallic acid equivalents (GAE)/g DMM [1], whereas FRAP was determined by the ferric reducing antioxidant power assay and expressed as mg Trolox equivalents (TE)/g DMM [2].

As shown in Table 1, the global yield (X_0) and Total Reducing Capacity (TRC) differed significantly between the temperatures evaluated (200 and 220 °C). At 200 °C, nitrogen had no significant effect on either response, whereas at 220 °C, the highest X_0 and TRC values were obtained in the absence of nitrogen, indicating that the inert atmosphere did not enhance overall extraction performance. In contrast, FRAP values increased significantly in the presence of nitrogen at 220 °C. This result may be associated with the reduced availability of oxygen under the inert atmosphere, which can limit oxidative reactions and contribute to the preservation of compounds with antioxidant capacity. This hypothesis is consistent with previous findings showing greater phenolic stability under nitrogen atmospheres [3].

Therefore, although a nitrogen-filled headspace during autohydrolysis did not influence the increase in Xo and TRC, its use may represent a strategy to minimize oxidative degradation during high-temperature processing, thereby opening new possibilities for preserving bioactive compounds exposed to these conditions.

Table 1. Characterization of the extracts obtained under different extraction conditions.

Conditions	X_0 (%)	TRC (mg GAE/g DMM)	FRAP (mg TE/g DMM)
200 °C	34.60 ± 1.10^{c}	$25.41\pm0,53^{c}$	48.28 ± 1.38^{c}
200 °C + N	34.19 ± 1.56^{c}	25.12 ± 1.21^{c}	52.70 ± 1.79^{c}
220 °C	46.06 ± 1.69^{a}	40.67 ± 1.78^{a}	64.91 ± 2.06^{b}
220 °C+ N	39.00 ± 1.03^{b}	33.45 ± 1.27^{b}	74.58 ± 3.12^{a}

Different letters in the same column indicate statistically significant differences between values ($p < 0.05$).

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From Plants to Plant Protection: Green Solvent Extraction of Olive Pomace Biocompounds for Sustainable Phytopathogen Control

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Olive pomace, a major by-product of the olive oil industry, represents a promising source of bioactive compounds with potential applications in sustainable plant protection [1,2]. Beyond waste valorization, the recovery of naturally occurring phytochemicals offers an opportunity to develop plant-derived alternatives for controlling bacterial diseases. Among these, *Xylella fastidiosa* and *Erwinia amylovora*, two Gram-negative phytopathogens responsible for economically significant crop losses, represent relevant targets for exploring the antimicrobial potential of olive-derived compounds.

This study investigates the selective recovery of functional biocompounds from olive pomace using supercritical carbon dioxide ($scCO_2$), with and without polar co-solvents, aiming to establish relationships between extraction conditions, chemical composition, and potential biological activity. Olive pomace samples with different moisture contents were subjected to $scCO_2$ extraction using neat CO_2 and modified solvent systems incorporating water or ethanol. The resulting extracts were examined using thin-layer chromatography under complementary elution and visualization conditions to investigate differences in chemical profiles. Preliminary chromatographic observations revealed multiple detectable constituents and responses consistent with the presence of phenolic compounds, highlighting the compositional complexity of the recovered fractions. Complementary molecular modelling studies investigate the interactions of three representative olive-derived compounds, hydroxytyrosol, oleic acid, and coniferyl alcohol, with a model Gram-negative bacterial membrane. Selected to represent distinct chemical families and physicochemical properties, these compounds provide a molecular-level basis for exploring their membrane affinity, partitioning behaviour, and potential effects on membrane organization.

By integrating green solvent fractionation with molecular-level investigations, this work establishes a framework for identifying olive pomace-derived fractions with potential applications against X. *fastidiosa* and E. *amylovora*. The proposed approach connects agro-industrial waste valorization with sustainable crop protection, advancing a circular strategy in which plant-derived compounds are recovered and investigated for their potential to protect plants.

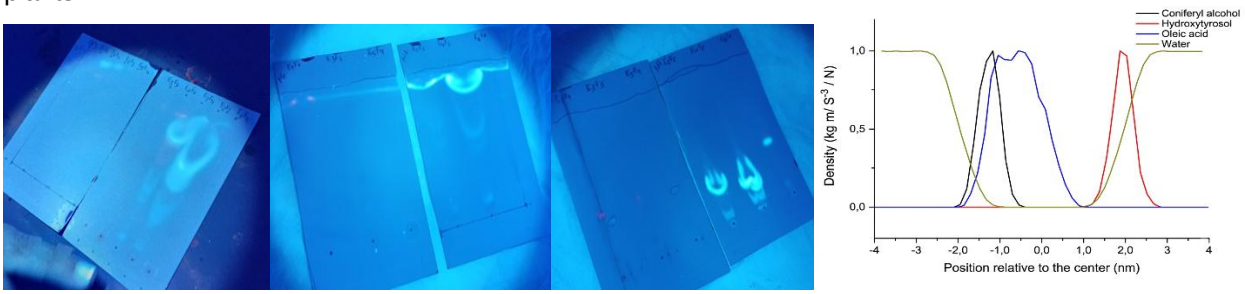


Figure 1 – Complementary experimental and computational characterization of olive pomace extracts. TLC fingerprinting under UV highlights compositional differences among extracts obtained under different supercritical extraction conditions, while molecular dynamics simulations (right) reveal distinct membrane partitioning of representative biocompounds.

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Experimental Assessment of PV Soiling Losses and Cleaning Profitability: The NOOR IV Solar Plant Case Study

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Dust accumulation on photovoltaic (PV) modules represents a major operational challenge, particularly in arid and semi-arid environments, where soiling can significantly reduce PV performance and energy yield [1] [2]. This study experimentally assesses the impact of dust accumulation on PV performance and evaluates the techno-economic profitability of cleaning operations at the NOOR IV photovoltaic power plant in Ouarzazate, Morocco. The experimental study was conducted over a complete 18-day cleaning cycle using two identical 325 Wp polycrystalline PV modules. One module was used as a reference and cleaned daily, while the second followed the cleaning cycle applied at the solar plant. Solar irradiance, short-circuit current, and open-circuit voltage were monitored to quantify the progressive effect of dust accumulation on PV electrical performance. The results showed that power losses increased progressively with dust accumulation, reaching approximately 13.5% at the end of the cleaning cycle. Over the complete experimental period, the average potential power gain associated with cleaning was estimated at 7.4%. The corresponding gross energy gain was estimated at 4240 Wh/m²/month. Considering the cleaning costs and the economic assumptions adopted in the study, the net economic benefit was approximately 2.95 MAD/m²/month. When extrapolated to the entire NOOR IV photovoltaic field, this represents an estimated net economic gain of approximately 1,252,570 MAD per month. These findings highlight the importance of considering site-specific soiling losses when defining operation and maintenance strategies for large-scale PV installations. Optimizing cleaning frequency can contribute to recovering energy losses while maintaining economically viable PV plant operation under dusty environmental conditions.

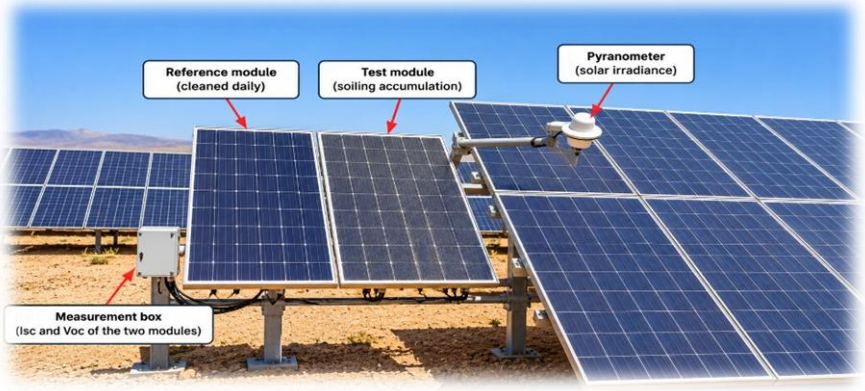


Fig.3. Experimental setup for evaluating PV soiling losses at the NOOR IV solar plant.

Keywords: Photovoltaic systems; Soiling losses; Dust accumulation; PV cleaning; Energy performance; Techno-economic analysis.

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Sustainable Valorisation of Chestnut Shells in Innovative Cosmetic Applications

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The generation of agro-industrial waste is an increasing environmental challenge, particularly in the chestnut industry, where *brulage* treatments applied during industrial freezing produce significant quantities of shell residues. In Trás-os-Montes, Portugal, a major European chestnut-producing region, this underexploited biomass offers opportunities for sustainable valorisation within a circular economy framework [1].

Within the scope of the CyChest project, this work explores the sustainable valorisation of *brulage*-treated chestnut shells through the recovery of bioactive compounds and their subsequent incorporation into value-added cosmetic products [2,3].

The biomass was initially characterised by FTIR, TGA, and NMR analyses, confirming the presence of cellulose, lignin, and phenolic compounds associated with antioxidant activity. Different extraction techniques, including maceration, Soxhlet extraction, ultrasound-assisted extraction (UAE), and supercritical CO_2 extraction, were evaluated and compared in terms of extraction yield, total phenolic and flavonoid contents, antioxidant capacity, and chemical profile. Among the methods investigated, UAE provided the best compromise between extraction efficiency and energy consumption. Chemical characterisation of the extracts revealed oleic acid as the predominant compound, followed by L-ascorbic acid, linoleic acid, γ-sitosterol, and long-chain alkanes. The most promising extract was subsequently microencapsulated by complex coacervation to enhance its stability and facilitate its incorporation into cosmetic formulations. The resulting spherical microcapsules exhibited both mononucleate and polynucleate morphologies while preserving the antioxidant activity of the encapsulated extract. Incorporation of the microcapsules into a commercial serum further improved its antioxidant performance.

These findings demonstrate the potential of chestnut shell residues as a sustainable source of high-value bioactive compounds for cosmetic applications, contributing to resource efficiency, circular bioeconomy strategies, and the economic valorisation of chestnut-producing regions.

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Valorization of viticulture surplus from the Douro Demarcated Region: fatty acid and vitamin E profiles

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Portugal's wine sector is suffering from an overproduction crisis, worsened by a decline in world consumption and the build-up of stocks in wineries. With purchase prices falling below operating costs, the grape harvest has become financially unviable for many winegrowers, who are forced to leave tonnes of grapes in the vineyards [1]. Therefore, it is important to redirect the surplus to alternative industries by utilising grapes for biotechnological and ecological purposes. Converting this raw material into natural juices, food concentrates, cosmetic extracts, and bioenergy emerges as a viable circular economy strategy to mitigate agricultural waste and provide supplementary income. Thus, the aim of this study was to characterise two red grape varieties (Touriga Nacional and Tinta Roriz) from the Douro Demarcated Region in terms of their vitamin E and fatty acid profiles.

Five grape samples were collected from Douro Superior and Cima Corgo. Grapes were separated from bunches, freeze-dried, and ground. Lipid content was determined using the Soxhlet method (AOAC 991.36). For vitamin E and fatty acid analyses, lipids were extracted by a cold extraction method according to Alves et al. [2]. Vitamin E profile was analysed by RP-HPLC-FLD-DAD, and fatty acids were converted into fatty acid methyl esters (FAME) via alkaline and acid transmethylation, using KOH (0.5 M in methanol) and BF_3 (14% in methanol), and analysed by GC-FID [3].

Results confirmed a low lipid content in the grapes, from 0.09 to 2.41% (dw, dry weight), with Touriga Nacional having the highest values. This range is in accordance with grape composition, mainly constituted by reducing sugars (glucose and fructose), whereas lipids are a minor constituent and mainly in the seeds [4]. Six vitamers of vitamin E, α-, γ- and δ-tocopherol and α-, β- and γ-tocotrienol, were identified with α-tocopherol as the most abundant (2.14-13.20 mg/kg dw). Touriga Nacional showed higher total vitamin E concentrations (17.65-20.47 mg/kg dw) compared to Tinta Roriz (6.39-7.83 mg/kg dw). The major fatty acids of grapes were linoleic (C18:2n6c) and oleic (C18:1n9c) acids.

In conclusion, the significant content of bioactive lipophilic compounds in the grape samples confirms their high potential for application in the cosmetic and nutraceutical industries, transforming viticultural waste into a sustainable economic opportunity.

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Ultrasound-assisted extraction as a tool for grape pomace valorization: Optimization of phenolic recovery and antioxidant activity

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The wine industry is one of the oldest and most economically relevant agri-food sectors, with around 7 million hectares of vineyards worldwide and a global wine production of approximately 227 million hectoliters in 2025. However, this sector generates large amounts of grape pomace, composed of skins, residual pulp, seeds, and stalks, which corresponds to 20–30% of the original grape mass and reaches an estimated 10.5–13.1 million tons per year, representing both an environmental concern and an underexploited resource. In recent years, grape pomace has been recognized as a promising raw material for sustainable value chains, as it is rich in bioactive compounds, particularly polyphenols (e.g., phenolic acids, flavonols, flavan-3-ols, anthocyanins, and stilbenes), with recognized bioactive properties, namely antioxidant activity [1]. Therefore, recovering these compounds can be considered an opportunity to reduce waste and add value to the wine production chain, in line with circular economy principles. To achieve this sustainably, the extraction process must be efficient, fast, and environmentally friendly. Ultrasound-assisted extraction (UAE) is a green technology that uses acoustic cavitation to disrupt plant cell walls, increasing extraction yields while reducing time, solvent consumption, and thermal degradation [2]. This study aimed to develop and optimize a UAE method to recover phenolic compounds from grape pomace, using a Central Composite Design combined with Response Surface Methodology. Three factors were evaluated: solid-to-liquid ratio (400–1200 mg/100 mL), extraction time (5–15 min), and ethanol proportion in the hydroethanolic solvent (20–80%, v/v). The extracts were characterized for total phenolic, total flavonoid, and total anthocyanin contents (TPC, TFC, and TAC, respectively), and their antioxidant potential was determined by DPPH$^{\bullet}$ radical scavenging and ferric reducing antioxidant power (FRAP) assays. Extraction time and ethanol concentration were the most influential variables for all responses. The optimal conditions were established at 475.19 mg/100 mL, 12.88 min, and 58.18% (v/v) ethanol. Under these conditions, the extracts reached 32.62 mg GAE/g (TPC), 17.65 mg CE/g (TFC), 0.98 mg C3GE/g (TAC), 47.44 mg TE/g (DPPH$^{\bullet}$), and 388.51 μmol FSE/g (FRAP). Experimental validation confirmed the predictive accuracy of the models. Overall, these results support the use of UAE as an effective strategy to convert grape pomace from waste into a bioeconomy resource, providing antioxidant-rich extracts with several potential applications, such as in the food, nutraceutical, and cosmetic sectors.

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Functional biomass-derived hydrothermal carbons highly efficient and selective for the green dihydroquinazolinone synthesis

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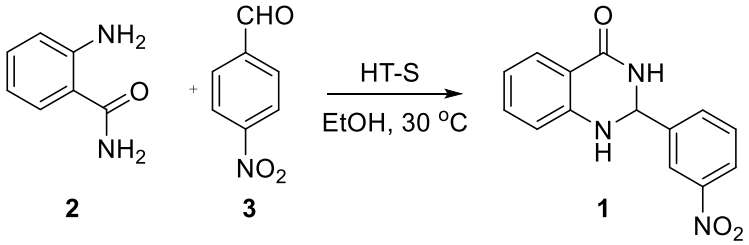
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Nitrogen-containing heterocycles are found in a wide variety of biologically active natural products, as well as in synthetic drugs and pharmaceutical products [1]. Specifically, 2,3-dihydroquinazolinones are *N*-heterocycles that exhibit a great variety of biological activities; antiviral, anticancer, antimicrobial, antihypertensive, anti-inflammatory, and antihistamine activities, among others.

This communication presents a family of acidic catalysts based on biomass-derived carbon materials easy to prepare and highly efficient in the sustainable and selective synthesis of 2,3-dihydroquinazolinones (**1**) from 2-aminobenzamide (**2**) and 4-nitrobenzaldehyde (**3**).



2 **3** **1**

Scheme 1. Synthesis of 2,3-dihydroquinazolinone (**1**) from 2-aminobenzamide (**2**) and 4-nitrobenzaldehyde (**3**), catalyzed by HT-S at 30 °C in EtOH.

The materials under investigation were prepared via the hydrothermal method using sucrose in the presence or in the absence of a commercial activated carbon with subsequent H_2SO_4 treatment. All the prepared carbonaceous materials proved active in the synthesis of 2,3-dihydroquinazolinone (**1**), the reaction proceeding with high conversion values. Both the amount of catalyst used and the reaction temperature had a direct impact on the selectivity to (**1**).

Catalyst acidity plays a crucial role in the course of the reaction in such a manner that the most acidic catalyst (pH = 1.9 and 24% oxygen content) afforded the dihydroquinazolinone (**1**) with a quantitative yield after a reaction time of only 60 min while in the presence of a sample showing a lower acidity (pH = 4.4 and 5.6% oxygen content), both conversion and selectivity decreased considerably. These results strongly suggest that sulfonic or sulfate groups, as detected by IR spectroscopy, are behind the observed reactivity.

All these results are also supported by a computational study carried out by DFT calculations.

Acknowledgements

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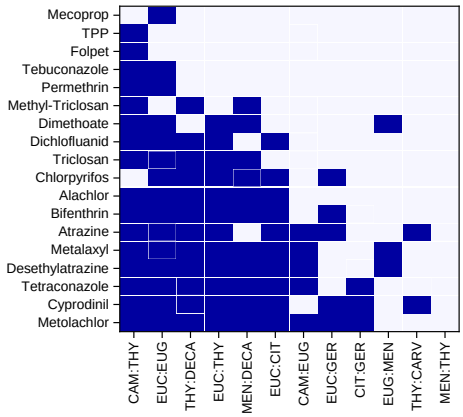
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Physical Stability and Chromatographic Viability of Hydrophobic Deep Eutectic Solvents for Environmental Analysis

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Hydrophobic deep eutectic solvents (HDES) offer a key advance over conventional organic solvents in green analytical chemistry [1]. In this study, was evaluated the preparation and physical stability [2] of HDES mixtures for liquid-liquid microextraction [3] of 18 contaminants. Precursors such as organic acids, ammonium salts, and terpenes were combined in specific molar ratios; camphor and eucalyptol act strictly as hydrogen bond acceptors (HBA). The preparation was carried out under heating (60 °C) and agitation, followed by a 12-hour resting period at room temperature to classify the physical state (homogeneous liquid, cloudy liquid, phase separation, precipitate, or solidified material).
Screening demonstrated that mixtures based on quaternary ammonium salts (e.g., TBAB:HEXA) are prone to aqueous leaching, resulting in volumetric loss, while combinations such as CAM:CINN solidified at room temperature. However, systems such as CAM:THY and EUC:EUG formed stable homogeneous liquids, becoming excellent options for liquid-liquid microextraction assays. 200 µL of each HDES was dispersed in 4 mL of aqueous sample (2.5 $mg \cdot L^{-1}$ of the target analytes). After homogenization and centrifugation for phase separation, the mixtures operated as the supernatant extracting phase, with the exception of the EUC:EUG system, which exhibited a density higher than that of water.
Extracts (1.5 µL) were analyzed by GC-MS (Agilent 6890/5973B) in SCAN mode using pulsed splitless injection and a DB-5MS column. The current findings confirm that the hydrophobicity of HDES is a critical variable that discards supramolecular networks susceptible to disruption by hydration. The performance and selectivity of the solvents that passed the physical screening in the simultaneous detection of the analytes are illustrated in Figure 1.

Figure 1. Heatmap showing the extraction performance of the different HDESs for 18 environmental contaminants. Precursor abbreviations: CAM (camphor), THY (thymol), EUC (eucalyptol), EUG (eugenol), DECA (decanoic acid), CINN (cinnamic acid), MEN (menthol), CIT (citronellol), GER (geraniol), and CARV (carvacrol).



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Antimicrobial Activity of Neat Natural Deep Eutectic Solvents and Propolis Extracts

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Propolis is a natural, complex natural source of bioactive compounds with antimicrobial potential, but the activity of natural deep eutectic solvent (NaDES)-based extracts may reflect both the contributions from solvent and the compounds recovered from propolis [1,2]. This study evaluated the antimicrobial activity of five neat NaDES and their respective NaDES-based propolis extracts to investigate differences in their inhibitory and microbicidal properties. The NaDES systems comprised proline:citric acid (PCA_1, 1:1;), proline:citric acid (PCA_2,2:1), monopropylene glycol:citric acid (4:1; PGCA), menthol:lauric acid (4:1; ML), and betaine:citric acid (1:2; BCA). Minimum inhibitory (MIC) and minimum bactericidal (MBC) concentrations were determined by broth microdilution against Gram-negative bacteria (*Escherichia coli*, *Pseudomonas aeruginosa*, and *Salmonella enterica*), Gram-positive bacteria (*Staphylococcus aureus* and *Cutibacterium acnes*) and the yeast *Candida albicans*.

Among the neat NADEs, all systems except PGCA inhibited the tested bacteria at 0.78% (v/v), with MBCs generally matching the corresponding MICs. Higher MBCs were required against *C. acnes* for the PCA_1, ML, and PCA_2 systems. Against *C. albicans*, PCA_1, BCA, and PCA_2 exhibited MIC/(MBC/MFC) values of 0.78%, whereas ML and PGCA required 6.25%. The NaDES-based propolis extracts exhibited distinct antimicrobial profiles, with PGCA and ML systems showing the most notable inhibitory activity. PGCA system showed MICs of 0.63 mg/mL against *S. enterica* and 1.25 mg/mL against *S. aureus* and, particularly against *C. albicans 1.25 mg/mL)*, despite the absence of detectable antibacterial and low antifungal activity in the corresponding NaDES, which suggests suggesting a contribution from propolis-derived compounds. Similarly, ML exhibited MICs of 0.63 mg/mL against *S. aureus* and 1.25 mg/mL against *S. enterica* and *C. albicans*. Although inhibitory activity was observed, higher concentrations were generally required to achieve bactericidal and fungicidal effects, while *E. coli* and *C. acnes* exhibited the lowest susceptibility to the propolis extracts. Overall, these findings highlight differences in antimicrobial activity between neat NaDES and their respective NaDES-based propolis extracts, particularly noticed for PGCA system. It is suggested that propolis-derived constituents, such as phenolic compounds may contribute to the inhibitory activity of the extracts. These findings emphasize the importance of considering both the extraction medium and the recovered compounds when evaluating NaDES-based propolis extracts and justify a further evaluation of this extracts as potential multifunctional topical ingredients, including preservative-efficacy and safety testing.

Acknowledgments
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Preparação de MOF-5 a partir de resíduos de PET para valorização catalítica do CO_2

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A rápida acumulação de resíduos plásticos constitui um problema ambiental crítico, originando resíduos persistentes nos ecossistemas. Os resíduos de garrafas de poli(tereftalato de etileno) (PET) representam uma preocupação ecológica significativa, devido às limitações da sua reciclagem após dispersão no ambiente. A hidrólise química de resíduos de PET constitui uma estratégia viável para a recuperação de materiais, permitindo a obtenção de ácido tereftálico (H_2BDC) [1], que pode posteriormente ser utilizado como ligando na síntese de estruturas metal-orgânicas porosas (MOFs) [2], [3].Por outro lado, o dióxido de carbono (CO_2) é um dos principais gases com efeito de estufa, cuja emissão excessiva, decorrente da atividade humana, contribui significativamente para as alterações climáticas. O principal objetivo deste trabalho consiste em estudar a hidrolise de resíduos de PET em condições ambientalmente sustentáveis, privilegiando a utilização de solventes verdes e metodologias energeticamente eficientes. O H_2BDC recuperado será posteriormente combinado com centros metálicos, neste trabalho, o zinco, para a preparação do MOF-5. Este último foi posteriormente investigado como catalisador heterogéneo para a conversão e valorização de CO_2.
O material MOF-5 preparado foi caracterizado por difração de raios X de pós, FT-IR, microscopia eletrónica de varrimento acoplada à espectroscopia de raios X por dispersão de energia (SEM-EDS), análise termogravimétrica e isotérmicas de adsorção-dessorção de N_2. Por fim, a atividade catalítica do MOF-5 foi avaliada na reação de cicloadição de CO_2 com epicloridrina, visando à produção de carbonatos cíclicos com potencial aplicação como aditivos de combustíveis.[4].

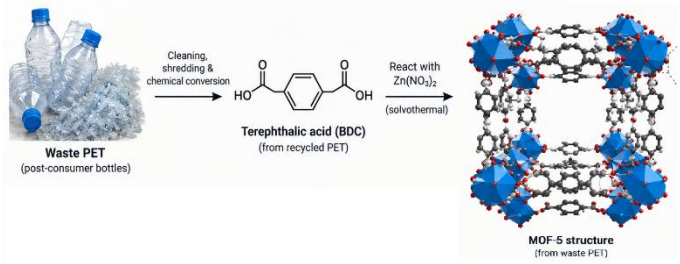


Figure 1. Esquema da abordagem para a valorização de resíduos de PET na forma de estruturas porosas do tipo MOF-5

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Integrated assessment of interconnected climate risks and cascading effects at the regional level in Galicia

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Climate change in Galicia poses complex challenges that do not occur in isolation, but are interconnected. Most studies address environmental threats from a sectoral perspective, however, it is important to analyse how these events are triggered and amplified through cascade effects and feedback loops.
This research evaluates a methodological framework for multi-risk assessment adapted to the Galician biogeographical context, focusing on the chain of impacts linking the terrestrial, aquatic and coastal environments. A clear example of this chain reaction is the sequence:
Episodes of drought and heatwaves > increased severity of forest fires > drastic loss of vegetation cover and soil degradation > soil sealing and loss of infiltration capacity > torrential run-off and the transport of ash and sediments into river basins > biogeochemical alteration and eutrophication of the estuaries > direct impact on marine biodiversity, socio-economic activities and public health.
Recent research shows how the increase in the duration of droughts and the vapour pressure deficit intensifies the severity of large forest fires, causing the volatilisation of organic matter and the formation of hydrophobic layers on the soil surface. As the soil's infiltration capacity is drastically reduced, torrential rainfall triggers immediate runoff, carrying large quantities of ash, nitrogen, phosphorus and sediment into river basins. This flow reaches the estuaries, disrupting their biogeochemical balance, causing water turbidity and leading to eutrophication and localised anoxia, which directly affect marine biodiversity, phytoplankton photosynthesis and the survival of shellfish beds and aquaculture.
By integrating climate, hydrological and land-use databases, the study identifies the most vulnerable areas and delineates critical risk hotspots where steep slopes, fine-grained soils and high socio-economic dependence on shellfish gathering converge. The resulting regional map provides useful tools for preventive spatial planning and risk management at a regional level, fully in line with the Galician Strategy on Climate Change and Energy 2030 and the National Climate Change Adaptation Plan (PNACC), helping to safeguard public health and the socio-economic resilience of the primary sector in Galicia.

KEYWORDS:
Climate change | Cascading effects | Feedback loops | Adaptation

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Vulnerabilidad de recursos críticos en baterías para vehículos eléctricos: una aportación a la identificación de retos futuros

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La compra de vehículos eléctricos, impulsada por las recientes políticas de descarbonización del transporte, ha experimentado un gran aumento en los últimos años [1,2]. Sin embargo, pese a prometer menores emisiones y una menor dependencia de los combustibles fósiles, estos vehículos presentan problemas relacionados con las baterías que utilizan o, más concretamente, con los materiales que las componen. Actualmente, estos sistemas de almacenamiento de energía se basan, en su mayoría, en el litio, además de otros materiales críticos como el níquel, el cobalto o el manganeso, considerados así por la Unión Europea en el Reglamento 2024/1252 [3]. La alta demanda de estos materiales, junto a sus dificultades de extracción y suministro, generan un conflicto en la transición a los nuevos vehículos eléctricos. Una de las estrategias más extendidas para suplir este problema consiste en una mejora de la infraestructura de reciclaje de estas baterías, favoreciendo así una economía circular [2]

El presente trabajo se centra en analizar la evolución prevista para las baterías en los vehículos eléctricos, en términos tanto de su composición química como de sus ventajas y desventajas, estudiando desde las ya comunes en este ámbito NMC, NCA y LFP, hasta las tecnologías más novedosas de estado sólido. Para ello, se realizará una revisión bibliográfica de publicaciones científicas, informes técnicos y normativa europea, que permitirán evaluar los futuros desafíos asociados a estas tecnologías. Además, se analiza el problema generado por la escasez de los materiales críticos necesarios en su fabricación, cómo estos pueden suponer una barrera para la transición hacia medios de transporte más sostenibles y qué estrategias se están siguiendo para suplir sus carencias.

La revisión realizada muestra que la evolución tecnológica de las baterías puede reducir, de forma notable, la presión sobre los materiales críticos. En el caso de China, la introducción de baterías de litio-azufre y de estado sólido podría reducir la demanda de estos materiales hasta un 60% en 2040, en el escenario más favorable. El litio, sin embargo, sigue siendo un problema, ya que su demanda continúa en aumento y el reciclaje no permite cubrirla. En cambio, otros materiales como el níquel, el cobalto, el manganeso o el grafito sí podrían cubrir toda su demanda mediante reciclaje [4]. Asimismo, los resultados de un estudio realizado en Estados Unidos indican que, para limitar el calentamiento global a menos de 2ºC, el suministro mundial de litio debería crecer un 35% anual hasta 2035 en un escenario sin reciclaje de materiales críticos [5]. En conjunto, estos resultados ponen de manifiesto la importancia de mejorar la gestión de estas tecnologías durante todo su ciclo de vida, lo que podría contribuir a reducir la dependencia de las materias primas vírgenes.

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Textile waste valorisation for a circular economy: a systematic review of material recovery and waste conversion pathways

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Textile waste amounts to about 92 million tons globally, spread over the various stages of a product's lifecycle. An increase in the generation of textile waste driven by swift consumption patterns and expansion of the textile manufacturing industry has resulted in significant environmental challenges and the need for sustainable recovery strategies [1]. Conventional disposal practices such as landfilling and incineration often result in low-value resources and contribute to environmental pollution [2].

In this context, valorisation of textile waste provides promising opportunities to recover fibres, polymers, chemicals, and energy-rich products by supporting the transition towards a circular economy.

This work presents the biodegradable polymers which is used for the manufacture of fishing gears. It elaborates the primary raw materials, methods used for the manufacturing, and the new initiatives in the market for replacing non biodegradable fishing gears.

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Is the European Union capable of ensuring a sustainable supply of raw materials for the energy transition?

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The global transition towards renewable energy sources and electrification is essential to mitigating climate change. However, this transition requires large quantities of specific raw materials. Key technologies, including high-capacity batteries and electric vehicle motors, rely heavily on materials such as lithium, nickel, cobalt, manganese, graphite, aluminium, copper and rare earth elements [1]. The supply chains of these materials are vulnerable due to the geographical concentration of extraction and refining activities in a limited number of countries [2], raising concerns about supply security and the long-term deployment of these technologies.

This study examines strategies to be implemented to secure and diversify the supply of critical raw materials in the European Union, as well as potential alternative materials and technologies. To this end, a literature review was conducted based on reports published over the last decade from international organizations such as the IEA, the JRC or the EU itself, focusing on current recycling strategies, new extraction and refining projects, supply diversification and research aimed at improving existing technologies and developing new ones.

The results indicate that the European Union's future supply security will depend mostly on the implementation of the Critical Raw Materials Act [3], which establishes benchmarks for 2030. These include meeting at least 10% of the EU's annual consumption of strategic raw materials through domestic extraction, 40% through processing within the EU, and 25% through recycling. The Act also aims to ensure that no more than 65% of the EU's annual consumption of each strategic raw material at any relevant stage of processing comes from a single third country [4]. The review suggests that meeting these benchmarks will require progress across all stages of the value chain, with processing showing the largest gap. These measures are complemented by research and innovation initiatives supported by programs such as Horizon Europe. Current research focuses on improving existing technologies and developing alternatives that could reduce dependence on these critical raw materials, including solid-state batteries and next-generation permanent magnets [5]

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Low-carbon enhanced oil recovery in the Orinoco Oil Belt: Integrating CCUS, CO_2-EOR and renewable steam generation for extra-heavy oil production

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The global energy transition is driving the need to reduce emissions associated with hydrocarbon production, particularly in heavy and extra-heavy oil reservoirs where Enhanced Oil Recovery (EOR) processes exhibit high carbon intensities. Conventional thermal recovery methods, such as Cyclic Steam Stimulation (CSS) and Steam-Assisted Gravity Drainage (SAGD), require large quantities of steam generated through natural gas combustion, representing one of the major sources of greenhouse gas emissions in these operations [4]. At the same time, Carbon Capture, Utilization and Storage (CCUS) technologies have emerged as a promising pathway for reducing emissions associated with petroleum production [2]. Likewise, carbon dioxide enhanced oil recovery (CO_2-EOR) can increase hydrocarbon recovery while simultaneously promoting long-term geological storage of CO_2 under suitable reservoir conditions [5].

Although these approaches have been extensively studied independently, relatively few studies have explored their integration within a unified low-carbon petroleum production strategy [2]. This work proposes the conceptual framework Hybrid Low-Carbon Enhanced Oil Recovery Systems (HLCEOR), designed to combine carbon capture, CO_2-EOR, and renewable steam generation through Concentrated Solar Power (CSP) and geothermal energy sources. Using the Orinoco Oil Belt as a conceptual case study, a methodology based on technical, environmental, and governance indicators is developed to assess the potential emission reductions associated with hybrid advanced recovery systems [6].

The conceptual analysis suggests that integrating CCUS technologies with renewable steam generation could substantially reduce the carbon intensity of extra-heavy oil production [1]. In addition, opportunities exist to increase geological CO_2 storage within suitable reservoirs [5]. A reduction in fossil fuel consumption during thermal recovery operations may also be achieved through the incorporation of renewable energy sources for steam production [4]. However, the magnitude of these benefits will depend on several factors, including reservoir suitability for long-term CO_2 storage [5], the availability of carbon capture and transportation infrastructure [2], and the existence of regulatory frameworks specifically designed for CCUS-EOR deployment [4]. The HLCEOR framework represents an initial contribution to the development of petroleum production strategies aligned with decarbonization objectives [3] and provides a conceptual roadmap for the future implementation of low-carbon EOR systems in heavy oil provinces.

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Panorama de la dependencia de materias primas críticas en la Unión Europea: el papel de las tecnologías limpias, el ecodiseño y el reciclaje

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En 2024 la Unión Europea estableció un marco para garantizar el suministro de materias primas fundamentales [1], e impulsó la implantación industrial de tecnologías de cero emisiones netas [2]. En este marco se pretende reducir la dependencia de otros países que monopolizan el suministro de materias primas. Incrementar la circularidad de éstas mediante tecnologías limpias, ecodiseño y reciclaje, se plantea como una contribución clave para alcanzar dicho objetivo. Una vía todavía poco explorada para alcanzar una mayor circularidad en el ámbito energético es el reciclaje de algunos materiales críticos de difícil obtención [3]. Según datos de la Comisión Europea la tasa actual de circularidad, una medida de que porcentaje de materiales son reciclados en lugar de desechados, se encuentra alrededor del 12%. Este valor se quiere duplicar al 24% para el año 2030 [4]

El propósito de este trabajo es hacer un análisis de las distintas técnicas de reciclaje y estrategias de ecodiseño existentes que puedan contribuir a una transición energética limpia. El estudio se centra, principalmente, en los equipos y componentes asociados a las tecnologías limpias, debido al margen de mejora que presentan en términos de circularidad. Para ello, se examinan soluciones orientadas a mejorar la recuperación de los principales materiales críticos (litio, cobalto, níquel y tierras raras). Además, también se estudia reducir la demanda de materias primas y prolongar la vida útil de los productos con el fin de identificar alternativas que favorezcan un uso más eficiente de los recursos.

Los resultados del análisis muestran que los avances en el reciclaje de estos materiales se concentran en torno a las baterías de iones de litio [4], mientras que otras tecnologías, como los imanes permanentes, los sistemas de hidrógeno y las células fotovoltaicas, reciben comparativamente menor atención por parte de la comunidad científica. Para abordar esta situación, se proponen distintas estrategias, como diversificar las tecnologías limpias para reducir los posibles cuellos de botella energéticos y de residuos, orientar la investigación hacia la reducción de la demanda de materiales y desarrollar sistemas que permitan prolongar su vida útil. Asimismo, el ecodiseño constituye una estrategia clave de la economía circular, al incorporar criterios ambientales y de sostenibilidad a lo largo de todo el ciclo de vida de los productos [1, 2]. No obstante, los estudios recientes indican que muchos proyectos innovadores en ecodiseño y reciclaje se encuentran todavía en fases de desarrollo tecnológico intermedias (TRL 3–8) [5]. Por ello, el apoyo mediante subvenciones públicas podría favorecer su desarrollo e implementación, contribuyendo a una economía más circular y a una transición energética sostenible.

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The Orinoco Oil Belt as a Strategic Source of Critical Minerals: Towards an Integrated Hydrocarbon, Vanadium and Nickel Co-Production Model

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The global energy transition is driving a growing demand for critical minerals required for energy storage technologies, electrification, and industrial decarbonization. Among these, vanadium and nickel occupy a strategic position due to their application in redox flow batteries, lithium-ion batteries, and advanced alloys. At the same time, the Orinoco Oil Belt (OOB), one of the world's largest accumulations of extra-heavy crude oil, contains significant concentrations of both elements associated with metalloporphyrins, asphaltenes, and heavy petroleum fractions [5]. Previous studies have demonstrated that these metals become progressively concentrated during heavy oil upgrading and refining processes [1]. Their enrichment in petroleum coke-derived ashes and other processing residues has also been documented [2]. The recovery of vanadium from petroleum coke ash has been extensively investigated through different extraction routes [3]. Likewise, the simultaneous recovery of vanadium and nickel from enriched ash streams has been demonstrated using hydrometallurgical processes [4]. These findings indicate that selected petroleum residues may represent valuable secondary sources of critical raw materials.

While existing research has primarily focused on metallurgical recovery technologies from petroleum coke, fly ash, and other heavy oil-derived residues [2], the strategic, regulatory, and governance implications of such recovery pathways have received comparatively limited attention. This work proposes a reinterpretation of the Orinoco Oil Belt not only as a petroleum-producing province but also as a hybrid energy-mineral system. To support this perspective, the concept of Critical Minerals Associated with Hydrocarbons (CMAH) is introduced, referring to strategically important minerals present within petroleum systems and recoverable through production, upgrading, or residue treatment activities. Building upon this concept, the framework of Strategic Energy-Material Systems (SEMS) is proposed, whereby petroleum systems can simultaneously generate hydrocarbons [1], critical minerals [2], additional economic value [3], and circular economy benefits [4].

The results of the conceptual analysis suggest that recovering vanadium and nickel from metal-enriched petroleum residues could contribute simultaneously to energy security [1], diversification of critical mineral supply chains [2], and industrial waste valorization [4]. The study also identifies regulatory challenges arising from the absence of governance mechanisms specifically designed for resources located at the intersection of the petroleum and mining sectors. Consequently, a conceptual roadmap is proposed for the development of governance frameworks adapted to hybrid energy-material systems. This approach could transform the Orinoco Oil Belt into an international reference case for integrated energy production, critical mineral recovery, and circular economy strategies within the broader context of the energy transition. The CMAH and SEMS concepts constitute a preliminary contribution to the emerging discussion on governance of strategic resources in complex industrial systems and provide a new perspective on the potential role of metal-rich petroleum provinces in future global critical mineral supply chains.

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Baterías de nueva generación para la transición energética: Avances tecnológicos, retos y perspectivas de sostenibilidad

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La creciente integración de energías renovables en los sistemas eléctricos ha incrementado la necesidad de tecnologías de almacenamiento energético eficientes, seguras y sostenibles. Entre estas tecnologías, las baterías electroquímicas desempeñan un papel fundamental al facilitar la gestión de la intermitencia de fuentes renovables como la energía solar y eólica, contribuyendo además a la electrificación del transporte y a la descarbonización de la economía [2]
Este trabajo analiza las principales tecnologías de almacenamiento mediante baterías, incluyendo las de ion-litio y alternativas emergentes como las de estado sólido, sodio-ion, litio-azufre y flujo redox, destacando su potencial para mejorar la seguridad, el rendimiento y la sostenibilidad del sector [4]. Asimismo, evalúa los desafíos asociados a los materiales críticos, como litio, níquel, cobalto y grafito, y el papel de la economía circular, basada en la reutilización y el reciclaje, como estrategia para reducir los impactos ambientales y reforzar la seguridad de suministro [3,4]
Los resultados obtenidos de la revisión bibliográfica muestran que la innovación tecnológica y el desarrollo de modelos de economía circular serán factores determinantes para garantizar la sostenibilidad futura del almacenamiento energético a gran escala. En particular, la mejora de los procesos de reciclaje, la recuperación de materiales críticos y la implementación de sistemas de segunda vida para baterías permitirán aumentar la eficiencia en el uso de recursos y fortalecer la resiliencia de las cadenas de suministro [1,2]
Finalmente, se concluye que las baterías de nueva generación representan una tecnología clave para alcanzar los objetivos de neutralidad climática establecidos por la Unión Europea, aunque aún persisten desafíos significativos relacionados con la eficiencia, la durabilidad, la seguridad, la disponibilidad de materiales críticos y la sostenibilidad de la cadena de suministro. El futuro del sector dependerá tanto de los avances tecnológicos en nuevas químicas de baterías como de la consolidación de estrategias de economía circular que permitan un aprovechamiento más eficiente de los recursos disponibles [1,3]

Palabras clave: almacenamiento energético, baterías de ion-litio, baterías de estado sólido, materiales críticos, economía circular, energías renovables, movilidad eléctrica, transición energética.

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Análisis multicriterio de teledetección para la implementación de una microrred fotovoltaica en Lonhe, Cuanza Sul, Angola

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La transición energética en Angola requiere soluciones descentralizadas que permitan mejorar el acceso a la electricidad en las zonas rurales, donde las limitaciones de la red eléctrica convencional dificultan el suministro energético. En este contexto, las microrredes fotovoltaicas constituyen una alternativa prometedora, cuya implementación requiere identificar emplazamientos adecuados desde el punto de vista ambiental, topográfico y de infraestructura [1,2]. El objetivo de este estudio es identificar áreas aptas para la implantación de microrredes fotovoltaicas en Lonhe, provincia de Cuanza Sul, Angola, mediante la integración de técnicas de teledetección y análisis multicriterio en un sistema de información geográfica (SIG).

La metodología se basa en el procesamiento de imágenes Sentinel-2 L2A, utilizando las bandas espectrales B2, B3, B4 y B8 para generar composiciones en falso color y calcular el índice de vegetación de diferencia normalizada (NDVI). Asimismo, se consideran las características de la cobertura del suelo y la presencia de cuerpos de agua y zonas ambientalmente sensibles como elementos relevantes para la selección de emplazamientos. Las variables se normalizan y combinan mediante una combinación lineal ponderada (*Weighted Linear Combination*, WLC), lo que permite generar un mapa de aptitud espacial para la implantación de sistemas fotovoltaicos [3]

Los resultados cartográficos permiten diferenciar zonas con distintos niveles de aptitud, destacando las áreas con menor cobertura vegetal y menor presencia de restricciones ambientales como emplazamientos potencialmente favorables, frente a los cuerpos de agua y las zonas ambientalmente sensibles, que se consideran áreas restringidas. En conjunto, el estudio muestra el potencial de la integración de la teledetección y el análisis multicriterio como herramienta de apoyo a la planificación energética rural y a la identificación preliminar de emplazamientos para microrredes fotovoltaicas. Como líneas futuras de investigación, se plantea incorporar modelos digitales de elevación, datos de radiación solar y validaciones de campo para reforzar la evaluación de la idoneidad de las áreas identificadas.

Palabras clave: teledetección; análisis multicriterio; sistemas de información geográfica; microrredes fotovoltaicas; transición energética.

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BIOQUÍMICA Y BIOTECNOLOGÍA

Estudio de la adsorción superficial de sulfametoxazol en nanopartículas de óxido de circonio mediante espectrometría vibracional

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El sulfametoxazol (SMX) es un antibiótico sulfonamídico de amplio uso clínico, cuya adsorción sobre materiales sólidos depende de diversos factores fisicoquímicos, entre ellos el pH y las características superficiales del adsorbente [1]. En este trabajo se estudia la adsorción de SMX sobre nanopartículas de óxido de circonio (ZrO_2-NP) a distintos valores de pH, con el objetivo de identificar las condiciones que favorecen la carga del antibiótico en la superficie y comprender las interacciones fármaco–nanopartícula implicadas.

La caracterización del sistema se llevó a cabo mediante espectroscopías de absorción infrarroja por transformada de Fourier (FTIR) y UV-Vis (UV-Vis) y espectrometría Raman, empleando estas técnicas de forma complementaria para caracterizar la interacción del SMX con la superficie de las ZrO_2-NP y evaluar la adsorción en función del pH.

Los resultados muestran que el pH desempeña un papel determinante en el proceso de adsorción, observándose una mayor interacción del SMX con las nanopartículas a pH ácido, mientras que en condiciones básicas se produce una disminución significativa de la adsorción, en concordancia con la dependencia del proceso respecto a la especiación del SMX y a las interacciones superficiales [2]. Este comportamiento puede relacionarse con el estado de protonación del SMX y con la modificación de las propiedades superficiales del ZrO_2-NP en función del pH.

El estudio proporciona información sobre la naturaleza de la interacción SMX–ZrO_2-NP, constituyendo una base para la evaluación de estas nanopartículas como potencial plataforma para sistemas de administración de antibióticos.

Solid–Liquid Extraction of Gramicidin from *Aneurinibacillus aneurinilyticus* Fermentations Using PBS and Membrane Technology: Effect of Agitation Rate

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Gramicidin is an antimicrobial peptide with potential applications against multidrug-resistant microorganisms. Its scalable production requires the identification of suitable fermentation conditions and the implementation of mild, efficient solid–liquid extraction strategies for product recovery. This study evaluated the effect of agitation rate on gramicidin production by *Aneurinibacillus aneurinilyticus* and on its recovery through a PBS-based solid–liquid extraction protocol, followed by membrane dialysis and lyophilization.

A. aneurinilyticus was cultivated in tryptic soy broth (TSB) at 37 °C and an initial pH of 6.0, using a 1 L working volume in both experiments. Two agitation rates, 180 and 300 rpm, were compared. After fermentation, solid residues were recovered by centrifugation, washed with Milli-Q water, and subjected to solid–liquid extraction with phosphate-buffered saline (PBS) under agitation at room temperature for 2 h, following a protocol previously applied to the mild desorption of cell-bound biosurfactants. The PBS extract was separated by centrifugation, dialyzed using a 6-8 kDa molecular-weight-cut-off membrane, and freeze-dried. Gramicidin presence was assessed by chromatographic analysis.

At 180 rpm, PBS extraction yielded 0.249 ± 0.067 mg/mL of dialyzed lyophilized extract, corresponding to an estimated recovery of 249 ± 67 mg/L. At 300 rpm, a 12.5 ± 0.5 mL aliquot yielded 1.95 ± 0.05 mg of dried extract, equivalent to 0.156 mg/mL and 156 mg/L. Although the culture medium, temperature, initial pH, working volume, and extraction protocol were comparable, the higher extract recovery obtained at 180 rpm suggests that agitation rate may influence gramicidin production, oxygen transfer, cell physiology, or extraction efficiency. Chromatographic analysis confirmed the presence of gramicidin in the recovered fractions.

These preliminary results indicate that 180 rpm may be a more suitable agitation condition for gramicidin recovery under the evaluated conditions. The PBS-based solid–liquid extraction, dialysis, and lyophilization workflow provides a mild, solvent-reduced alternative for recovering biomass-associated antimicrobial peptides and can support further optimization of gramicidin production.

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Real-Time Kinetic Absorbance Microplate Assay for Monitoring *Acinetobacter baumannii*-Phage Infection

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Acinetobacter baumannii is the most common pathogen causing ventilator-associated pneumonia (VAP) and is difficult to treat in critical care [1]. Early diagnosis is complicated by nonspecific symptoms and limited diagnostic options, often resulting in empirical antibiotic use and contributing to the development of drug-resistant strains [2]. Therefore, there is an urgent need for rapid, sensitive, and cost-effective diagnostic tools. Biosensors, particularly those employing bacteriophages as recognition elements, offer promising solutions due to their selectivity, stability, and ease of production, making them ideal for point-of-care diagnostics [3,4].

Studying phage-bacteria interactions is crucial for designing this intended diagnostic probe. Here, we present a rapid, efficient, high-throughput microplate-based kinetic absorbance assay for quantitatively assessing bacteria–phage interactions. The method enables real-time monitoring of phage-mediated bacterial lysis across multiple samples, providing precise measurements of lysis time and capacity. Kinetic absorbance profiles support robust comparisons among phage strains and bacterial hosts and allow determination of the phage concentration required to lyse a bacterial suspension of known density. It can also be used to study the multiplicity of infection (MOI), defined as the ratio of phage particles to host bacterial cells at the start of infection. By streamlining these measurements, the assay enables rapid comparison of bacteriophage strains and, when needed, evaluation of phage-cocktail efficacy against different bacterial pathogens.

In this work, we investigated the interactions between *Acinetobacter baumannii* DSMZ 25645 (G7 strain) and four susceptible phages: DSMZ 108246, *Acinetobacter* phage vB_AbaM-Bhz15 (Myovirus); DSMZ 108247, *Acinetobacter* phage vB_AbaP-Bhz16 (Podovirus); DSMZ 108588, *Acinetobacter* phage vB_AbaP-Bhz21 (Podovirus); and DSMZ 108589, *Acinetobacter* phage vB_AbaM-Bhz22 (Myovirus). Bhz15 and Bhz16 phages have previously been reported to act effectively in combination against *A. baumannii* [5]. Based on this finding, we used the developed microplate-based kinetic absorbance assay to evaluate Bhz15 and Bhz16 individually and in combination with the other phages acquired for the G7 strain, Bhz21 and Bhz22.

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Organ-specific phytochemical profiles of *Galactites tomentosus*

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Thistles are herbaceous, spiny plants commonly regarded as weeds and mainly belonging to the Apiaceae, Dipsacaceae and Asteraceae families. In agricultural areas of Beira Baixa, Portugal, some of these plants have little use as crops or animal feed, and they must be removed, resulting in additional costs for local farmers. However, studies on related species have documented traditional medicinal uses, diverse phytochemical constituents and biological activities [1–3], suggesting opportunities for their valorization. Among these plants, *Galactites tomentosus* was investigated to compare the phenolic composition of its flowers, leaves, stems and roots.

The four organs were separated, dried and subjected to maceration with hexane and ethanol. Ethanolic extracts were analysed by HPLC–DAD–MS^n, and phenolic constituents were identified from their chromatographic, UV and mass spectral characteristics. GC–MS data from the corresponding hexane extracts provided information on the lipophilic composition of the different organs.

The phytochemical profiles differed among organs. Apigenin and luteolin were detected in both flowers and leaves. Flowers also contained compounds identified as apigenin-*O*-deoxyhexosyl-hexoside, apigenin-*O*-glucuronide and luteolin-*O*-glucuronide, and methoxylated luteolin derivatives, whereas leaves contained caffeoylquinic and dicaffeoylquinic acids, along with quercetin-*O*-rutinoside and quercetin-*O*-glucoside. Quercetin-*O*-rutinoside was also found in stems, while caffeoyl hexosides were detected across all three aerial organs. Root extracts contained compounds tentatively assigned as mono-, di- and tricaffeoylquinic acids. Pentacyclic triterpenes, including lupeol and amyrin derivatives, were detected in flowers, leaves and stems but were not detected in roots. Sterols occurred in all four organs, with campesterol detected in stems and roots and stigmastanol only in roots.

These findings highlight differences in the chemical composition of the four organs and provide a basis for selecting extracts for further compound characterization and biological evaluation, supporting the valorization of *Galactites tomentosus*.

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Exploring the Effect of *Cinnamomum burmannii* on Blood Coagulation

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Abstract

Cinnamomum burmannii is a medicinal plant extensively recognized for its broad spectrum of pharmacological activities. Given the growing need for safer natural alternatives to synthetic anticoagulants, commonly associated with bleeding complications, drug interactions, and resistance, this study aimed to evaluate the in vitro anticoagulant activity of hydroalcoholic extracts derived from different aerial parts (leaves, stems, and cork) using both animal and human plasma models.

Preliminary phytochemical screening revealed the presence of phenols, tannins, terpenoids, and proteins. Quantitative analysis showed a high total phenolic content (467.5 ± 6.4 mg GAE/g) and flavonoid content (8.32 ± 0.18 mg QE/g), particularly in the cork sample. Essential oil yields reached 4.67% in cork and 0.5% in leaves and stems.

Our findings demonstrate that the hydroalcoholic extract of C. burmannii exhibits a significant anticoagulant effect, characterized by a dose-dependent prolongation of coagulation time. In vitro assays revealed a marked extension of clotting parameters across both intrinsic and extrinsic pathways, including clotting time (CT), prothrombin time (PT), and activated partial thromboplastin time (aPTT/TCK). These effects may be attributed to the plant's richness in secondary metabolites, which could influence coagulation factors by enhancing antithrombin activity, inhibiting fibrinogenesis, and/or reducing fibrinogen levels.

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Keywords

Cinnamomum burmannii, blood coagulation, natural anticoagulants, medicinal plants, alternative therapies.

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Effects of Choline Salt–Urea DES Formulations on Bovine Carbonic Anhydrase II: Experimental and Molecular Dynamics Analysis

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Bovine carbonic anhydrase II (CA II) is a zinc-dependent metalloenzyme whose function is sensitive to the surrounding chemical environment [1]. Although deep eutectic solvents (DES) have been investigated as reaction media for carbonic anhydrase [2], their effects on enzyme activity and structure remain formulation-dependent. This study combines experimental assays and molecular dynamics (MD) simulations to evaluate CA II in aqueous media containing urea, choline chloride (ChCl), choline acetate (ChOAc), choline dihydrogen citrate (ChDHC), and the corresponding 1:2 choline salt:urea DES formulations.

Apparent esterase activity was determined by p-nitrophenyl acetate hydrolysis following exposure to 1 M individual compound or DES formulation solutions, with approximately tenfold dilution during the assay. The activity of CA II in each media was compared with that obtained in phosphate buffer (control). Time- and temperature-dependent functional stability was assessed for the control, urea and ChCl conditions. Complementary 250 ns MD simulations of the 1 M aqueous systems characterized conformational deviation, compactness, hydrogen bonding, residue-level mobility, and the local Zn^{2+}-coordination and protein–solvent environments.

Urea and ChCl individually maintained initial activity broadly comparable to the control (46.3 ± 6.5 mU/mL). By contrast, ChCl:Urea (19.3 ± 1.7 mU/mL) and ChOAc:Urea (12.8 ± 0.7 mU/mL) retained only approximately 42% and 28% of control activity, respectively, despite not being strongly acidic. ChDHC-containing systems showed negligible apparent activity under acidic conditions (pH ≈ 4). At room temperature, all evaluated conditions led to loss of activity over 14 days, although ChCl exhibited the most favourable descriptive retention profile. At 45 °C, urea showed pronounced activity loss (26% retention after three days), whereas ChCl retained 95% at day three but showed no sustained advantage over the control at day seven. MD simulations indicated preservation of the overall fold, compactness and intraprotein hydrogen-bond network, alongside formulation-dependent changes in local flexibility, including near the catalytic Zn^{2+} environment.

Together, these results show that reduced CA II activity in the investigated DES formulations can coexist with an apparently preserved global protein structure. Changes in the local solvent environment may contribute to this structure–function divergence. Together, these findings highlight that preservation of the global protein structure does not necessarily ensure retention of enzymatic activity, providing a foundation for future studies aimed at elucidating the molecular factors governing CA II performance in choline–urea-based media.

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MALDI-TOF-MS profiling of Gramicidin S analogue extracts: effects of culture medium and storage temperature on the stability of mass spectral profiles

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Gramicidin S (GS) is a cyclic antibiotic peptide with broad-spectrum antimicrobial activity. However, its hemolytic toxicity limits its systemic use, motivating the investigation of GS analogues for potential antimicrobial applications. Exploring alternative fermentation media may also contribute to the development of more sustainable biotechnological processes. In this context, *Aneurinibacillus aneurinilyticus* CECT 9939, isolated from Corn Steep Liquor (CSL), an agro-industrial by-product from the corn-milling industry, is a promising producer of GS-related compounds [1]. Previous work identified GS analogues in extracts obtained from this microorganism, supporting further investigation of these microbial preparations [2]. This study investigated the influence of culture medium and storage temperature on the mass spectral profiles of GS analogue extracts using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS). *A. aneurinilyticus* was cultivated for 7 days in Tryptone Soy Broth (TSB) and TSB supplemented with 400 g/L FeedStimulants CSL (TSB+CSL). Following fermentation, the extracts were obtained according to a previously standardized extraction protocol [3]. Mass spectral profiles of GS analogue extracts were compared by MALDI-TOF-MS between culture medium at time 0 (T0), and after 15 days of storage at 4 ºC, room temperature (RT), and 60 ºC. In both cases a commercial GS reference standard was included.

The results indicated that at T0, the culture medium was associated with differences in the relative GS analogue profiles while MALDI-TOF-MS profiles showed relative stability during storage under the conditions tested. The relative distribution of five mass signals (1112, 1126, 1140, 1154, and 1168 Da) was largely preserved. HPLC-PDA analysis, which was used as a potential validation method, showed no detectable decrease in total peptide concentration, even after storage at 60 ºC. Comparison of relative analogue abundances obtained by HPLC-PDA and MALDI-TOF-MS revealed a strong linear correlation (R=0.93), while Bland–Altman analysis yielded a bias close to zero. Overall, the results support MALDI-TOF-MS as a rapid complementary approach for monitoring changes in the mass spectral profiles of GS analogue extracts during storage, alongside chromatographic quantification.
This study provides insights into the influence of culture medium on the mass spectral profiles of GS analogue extracts and the effect of storage temperature on their stability over time. The findings may help guide further molecular characterization of the detected compounds and subsequent investigations into the antimicrobial activity and cytotoxicity of the extracts.

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Consensus QSAR modeling for virtual screening of acetylcholinesterase inhibitors

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Acetylcholinesterase (AChE) plays a significant role in neurodegenerative diseases, particularly Alzheimer's disease (AD). This enzyme hydrolyzes acetylcholine, terminating cholinergic neurotransmission. In AD, cholinergic dysfunction is associated with cholinergic neuron degeneration and reduced acetylcholine levels, making AChE inhibition a relevant approach to combat neurodegenerative diseases [1]. In this study, we developed a virtual screening approach based on quantitative structure-activity relationship (QSAR) models to identify and prioritize potential AChE inhibitors from a library of commercially available compounds.

To develop the models, we collected and curated biological activity data from the ChEMBL database and selected an initial dataset of 6,040 compounds. Of these, we classified 1,336 as active and the rest as inactive. We calculated Morgan molecular fingerprints for each compound and used them to develop and evaluate different machine learning algorithms. Based on five-fold cross-validation performance, we built a consensus QSAR model combining Logistic Regression, Random Forest, and Support Vector Machine [2-4], achieving an AUC value of 0.908.

The model was then applied to the commercial MolPort in-stock library, consisting of approximately 6.27 million compounds. After applying the computational selection criteria, we identified 7,781 AChE inhibitor candidates. Of these, 531 had a consensus score of 0.60 or higher, including seven confirmed natural products, 86 natural product analogs, and 438 synthetic compounds.

The results demonstrate the potential of consensus QSAR models for the virtual screening of large chemical libraries and for prioritizing compounds with potential AChE inhibitory activity. Identifying these candidates provides a basis for selecting compounds for subsequent experimental studies, which are necessary to confirm the computationally predicted biological activity.

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Evaluation and Optimization of Seed Disinfection and Germination Protocols in *Eruca sativa* and *Brassica oleracea var. acephala*

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The establishment of *in vitro* plant cultures depends on obtaining aseptic and viable plant material. Seed disinfection is a key step in reducing microbial contamination while preserving seed viability and germination capacity [1]. This study aimed to evaluate seed disinfection and germination conditions for *Eruca sativa* and *Brassica oleracea* var. *acephala*, as an initial step towards their *in vitro* establishment, propagation and future biomass production. Disinfection and germination protocols were adapted from previously described methodologies for *E. sativa* [2] and *B. oleracea* var. *acephala* [3]. Different disinfection conditions were tested by varying exposure time to commercial bleach containing approximately 5% sodium hypochlorite (NaClO), the number of drops of Tween, and the inclusion of a 70% ethanol treatment. Both seed species were rinsed with autoclaved water between disinfection solutions. Germination was assessed on 0.9% (w/v) agar prepared with distilled water, with or without the addition of sucrose, and on half-strength Murashige and Skoog (½ MS) medium.

For *E. sativa*, germination rates of 33% and 34% were recorded on 0.9% agar and on 0.9% agar supplemented with 2% sucrose, respectively. No germination was observed on ½ MS medium (0%), where brown spots developed around the seeds during the assessment period. The most effective disinfection treatment consisted of a 15 minute exposure to 60 mL of commercial bleach, with five drops of Tween and no ethanol treatment. No contamination was observed under these conditions, and germination reached 41% on agar with water. For *B. oleracea* var. *acephala*, germination reached approximately 85% on 0.9% agar, compared with 55% on agar supplemented with 3% sucrose. The best disinfection results were obtained following a 12 minute exposure to 60 mL of commercial bleach, with six drops of Tween, followed by a 1 minute treatment with 70% ethanol. No contamination was observed following this treatment, whereas disinfection periods shorter than seven minutes were insufficient to prevent contamination in some seeds.

These results highlight species-specific responses to the disinfection and germination conditions tested. The protocols identified provide a basis for the *in vitro* establishment of both species, supporting their subsequent propagation and future biomass production

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Effects of De Novo Peptides on Aβ42 Oligomerization: Molecular Dynamics Insights

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Proteins perform essential biological roles through balanced molecular interactions, yet disruption of these interactions can promote harmful aggregation. In Alzheimer's disease, amyloid-β42 (Aβ42) aggregation forms toxic oligomeric, and fibrillar assemblies implicated in neurotoxicity [1]. Short peptides based on the KLVFF region of Aβ42 (residues 16-20) have been explored as recognition elements and aggregation modulators [2-4]. Despite this work, the interactions driving early Aβ42 assembly remain difficult to target. Deep-learning algorithms for *de novo* protein design has opened the way for novel *in silico* strategies to develop peptide binders against hotspots [5].

Here, four *de novo* peptides of sizes ranging between 7 and 15 residues, using different constrained sequences of the Aβ42 peptide and a common hotspot region (residues 16-22) were generated using RFdiffusion, combined with ProteinMPNN and AlphaFold. The Aβ($_{16}$KLVFFAE$_{22}$) sequence and Aβ($_{16}$KLVFF$_{20}$-KKKKKK) were also studied as reference peptides. Molecular dynamics simulations showed that the shorter designs formed cross-β structures with the hotspot, whereas the longer designs adopted α-helical conformations. Peptide effects were assessed on CHARMM36m (C36m) Aβ42 tetramers at a 1:1 peptide-to-monomer ratio at 310 and 370 K.

Although none of the peptides prevented the formation of all possible oligomeric species (i.e., dimer, trimer, and tetramer), several, selectively inhibited or delayed tetramer formation within the simulation timescale, resulting in less compact assemblies. The underlying mechanisms differed among peptides, with some altering intermolecular β-sheet organization through persistent interactions with the C-terminal region and others influencing tetramer formation with limited participation in βsheet interactions. The behavior of the peptides 16-22 and the 16-20-KKKKKK closely reproduced experimental observations [3,4]. At high temperatures none of the peptides precluded tetramerization, suggesting that enhanced hydrophobic interactions outweigh peptide-mediated inhibition. Notably, charged peptides showed the strongest effects on tetramer formation, indicating an important role for electrostatic interactions in inhibiting Aβ42 aggregation. Overall, these results show that *de novo* peptides can modulate early Aβ42 assembly in a sequence and condition dependent manner.

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CATÁLISIS Y FOTOCATÁLISIS

Catalytic ozonation of salicylic acid using atmospheric air and a Carbon Xerogel/ZnO/$BaSnO_3$ catalyst

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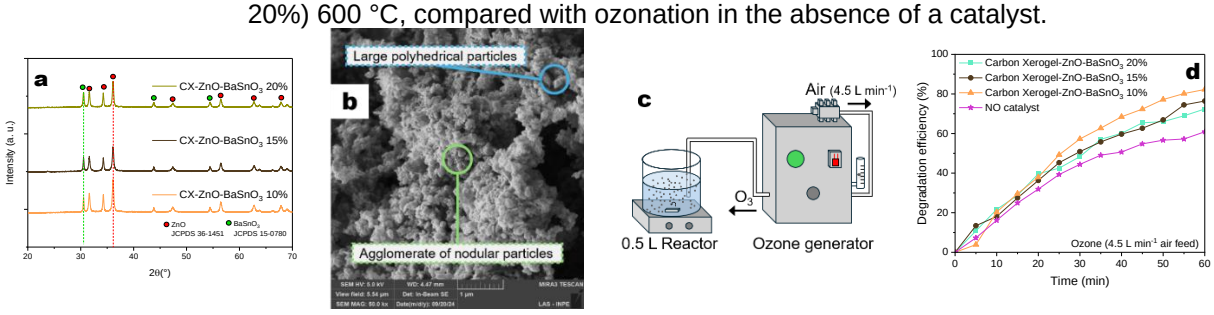
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Emerging contaminants have become a major scientific concern in recent decades, driving the development of effective treatment processes and catalytic materials for their removal. Catalytic ozonation is a widely investigated approach; however, ozone generation commonly relies on oxygen-enriched feeds, which may increase process costs and resource requirements [1, 2]. In this context, this study investigated the catalytic ozonation of salicylic acid (SA) using atmospheric air as the ozone feed (4.5 L min^{-1}) and a carbon xerogel/ZnO/$BaSnO_3$ (CX/ZnO/$BaSnO_3$) catalytic system. The composite combines materials previously reported as promising for heterogeneous photocatalysis, with the present study extending their application to catalytic ozonation [3, 4]. Composites containing 10–20 wt.% $BaSnO_3$ were synthesized by a precipitation route, using previously synthesized $BaSnO_3$, to evaluate the influence of perovskite content on catalytic performance. X-ray diffraction confirmed the formation of the expected crystalline phases for all compositions, while scanning electron microscopy of the 10% composite revealed agglomerated nodular particles associated with larger polyhedral structures. Among the investigated materials, CX/ZnO/$BaSnO_3$ 10% showed the highest catalytic performance, achieving over 80% degradation of SA (10 mg L^{-1}) within 60 min. The other composites also achieved degradation above 70% under the same conditions, consistently outperforming ozonation in the absence of a catalyst. These results demonstrate the effectiveness of the CX/ZnO/$BaSnO_3$ 10% composite for catalytic ozonation using atmospheric air as the ozone feed, while highlighting its potential as a multifunctional catalyst for integration with other advanced oxidation processes.

Fig.1. (a) X-ray diffraction patterns of CX-ZnO-$BaSnO_3$ (10–20%) 600 °C; (b) scanning electron microscopy (SEM) micrograph of CX-ZnO-$BaSnO_3$ 10% (50 kx); (c) experimental setup used for the degradation experiments; and (d) salicylic acid (10 mg L^{-1}) degradation by catalytic ozonation using CX-ZnO-$BaSnO_3$ (10–20%) 600 °C, compared with ozonation in the absence of a catalyst.



Acknowledgments

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Activity–Selectivity Trade-Off in Cobalt Fischer–Tropsch Catalysts Supported on Si-Modified Alumina

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Fischer–Tropsch synthesis (FTS) is a versatile route to produce synthetic fuels and valuable chemicals through the conversion of syngas. The possibility of producing syngas from renewable resources has renewed interest in FTS as part of sustainable fuel production strategies [1]. The performance of the FTS catalysts is strongly influenced by the properties of its support, which affect cobalt dispersion, reducibility, metal–support interactions, and stability [2,3]. Alumina is widely employed as a support for cobalt FTS catalysts due to its high surface area, suitable pore structure, and mechanical stability. Nevertheless, metal-support interactions may lead to the formation of hardly reducible cobalt species, decreasing the availability of metallic cobalt active sites [3,4]. Modification of alumina with silica has therefore been investigated as a strategy to tune these interactions and the physicochemical properties of the support, potentially affecting both activity and hydrocarbon selectivity [4,5].

In this work, cobalt catalysts supported on Si-doped alumina with different Si contents and textural properties were evaluated under FTS conditions and benchmarked against a commercial alumina-supported cobalt catalyst. Their catalytic performance was assessed in terms of cobalt-normalized CO conversion (CTY), selectivity toward CH_4, C_2–C_4 and C_{5+} hydrocarbons and chain-growth probability (α). The commercial catalyst exhibited the highest cobalt-normalized activity (CTY = 10.38 10^{-5}·mol_{Co}^{-1}·s^{-1}) and a chain-growth probability of α = 0.76. The Si-doped alumina catalysts presented lower CTY values but consistently higher C_{5+} selectivity (92.4–93.3%) than the commercial catalyst (91.0%). The formation of light C_2–C_4 hydrocarbons were also reduced from 3.2% for the commercial catalyst to 1.0–1.9% for the Si-modified systems. Furthermore, variations in the C_5-C_{11} and C_{12}-C_{20} fractions among the modified supports demonstrate the influence of support composition and textural properties on the hydrocarbon distribution. Overall, the results reveal a clear activity–selectivity trade-off and demonstrate the potential of Si-modified alumina for tailoring product selectivity in cobalt-based FTS catalysts.

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Removal of sulfamethoxazole and paracetamol by Fe-containing polymeric membranes: CWPO versus persulfate activation

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Sulfamethoxazole (SMX) and paracetamol (PCM) were removed from water using polymeric membranes prepared by phase inversion with magnetic activated carbon (MAC2.5) or a composite filler of MAC2.5 and $MnFe_2O_4$-modified clay. Membranes were cast in distilled water (DW) or in a water–isopropanol (IPA) coagulation bath and tested in continuous mode (C_0 = 10 mg/L, flow rate 0.5 mL/min, 60 °C, pH 3.5, 120 min), considering three removal processes: adsorption, catalytic wet peroxide oxidation (CWPO) and sodium persulfate (SPS) activation [1]. The results obtained are presented in Table 1.

Blank membranes removed only 7–10% of SMX and 8–13% of PCM in adsorption tests. Adding MAC2.5 markedly increased adsorption, reaching 42–43% (SMX) and 48–49% (PCM) for MAC2.5-IPA after 120 min, without reaching a plateau. In CWPO, iron-containing membranes removed 20–31% of SMX and 25–45% of PCM, never exceeding adsorption removal. Clay-containing membranes consumed H_2O_2 most intensively without a proportional gain in SMX removal [2].

SPS was far more effective: iron-containing membranes removed 75–83% of SMX within 15 min and 86–95% of PCM after 120 min, with residual persulfate falling to 0.1–0.2 of its initial value. Blank membranes removed only 10–14% and did not consume persulfate, confirming activation at the Fe-containing components. Fe leaching was low (0.11–0.23 mg/L for SMX; 0.02–0.05 mg/L for PCM). Radical identities were not determined.

Under the conditions studied, the ranking of removals was SPS oxidation > adsorption ≈ CWPO. The IPA bath improved adsorption and CWPO. SEM images (Fig. 1) show the pore structure [3].

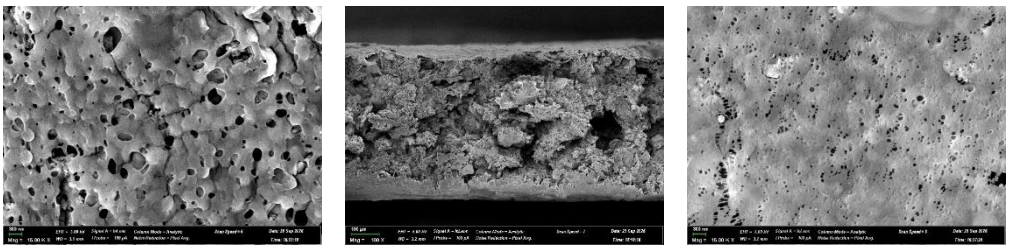


Fig. 1. SEM micrographs of the membranes: (a) surface and (b) cross-section of MAC2.5-IPA; (c) surface of MAC2.5+Clay-IPA.

Table 1. Final removal (%) of SMX and PCM after 120 min.

Membrane	Ads. SMX	Ads. PCM	CWPO SMX	CWPO PCM	SPS SMX	SPS PCM
MAC2.5-DW	~28	~41	~22	~25	~80	94–95
MAC2.5-IPA	42–43	48–49	~31	~45	82–83	~86
MAC2.5+Clay-DW	~20	~43	~20	38–39	80–81	94–95
MAC2.5+Clay-IPA	~40	52–53	20–24	~44	80–81	94–95

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Role of TiO_2 Crystalline Phases in Light-Driven H_2 Evolution over RuO_2/g-C_3N_4-based Photocatalysts

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Heterogeneous photocatalysis offers a promising route for H_2 evolution under mild operating conditions, yet the development of more efficient photocatalysts remains essential for viable implementation. Graphitic carbon nitride (g-C_3N_4) is a widely studied semiconductor due to its high stability, low cost and simple preparation. However, its efficiency is still limited by low surface area and fast charge-carrier recombination. Furthermore, combining g-C_3N_4 with other semiconductors, such as TiO_2 and RuO_2, has been reported to form heterojunctions with improved charge-carrier mobility [1]. In this work, ternary photocatalysts of RuO_2/g-C_3N_4/TiO_2 (referred to as RCNTi-T, where T = 400 – 900 °C) were synthesised using TiO_2 calcined at different temperatures to explore the influence of the TiO_2 crystalline phases on H_2 evolution.

g-C_3N_4 was produced through thermal polymerisation of dicyandiamide [2], while TiO_2 was synthesised by a sol-gel method [3]. The resulting TiO_2 samples were calcined under air flow for 3 h at different temperatures (400, 500, 600, 700, 800 and 900 °C). Ternary photocatalysts were then prepared by wet impregnation using TiO_2 calcined at each temperature, while maintaining a fixed g-C_3N_4/TiO_2 mass ratio (1:1). For this purpose, the g-C_3N_4/TiO_2 mixtures were added to an aqueous RuCl3 dispersion at 70 °C until partial solvent evaporation. After washing and drying, the materials were calcined at 400 °C to obtain ternary photocatalysts containing 1 wt.% RuO_2. All photocatalysts were characterised using several techniques and tested with a four-LED system at a fixed excitation wavelength of 370 nm. The photocatalytic experiments were performed for 2 h under an N_2 atmosphere, using a catalyst load of 0.5 g L^{-1} and triethanolamine (0.2 M) as the sacrificial electron donor. H_2 production was monitored by online gas chromatography.

Although the catalysts showed significant differences in photoluminescence emission, no clear trend with the TiO_2 calcination temperature was identified. The RCNTi-500 catalyst showed the highest H_2 production rate of 9701 μmol g_{cat}^{-1} h^{-1}, followed by RCNTi-400, while a progressive decrease in H_2 production was detected for photocatalysts prepared with TiO_2 calcined above 500 ºC. This trend is consistent with changes in TiO_2 crystalline phases reported in the literature [3]: increasing calcination temperatures favour the formation of rutile over anatase. These results highlight the important role of TiO_2 crystallinity in the photocatalytic performance, reinforcing the need to tailor TiO_2 phase composition.

Acknowledgements

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Development of Ag_3PO_4/g-C_3N_4 Photocatalysts for the Removal of Organic Pollutants

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Heterogeneous photocatalysis has attracted considerable interest for the treatment of contaminated water due to its ability to degrade organic pollutants through the generation of reactive species [1]. In this context, the development of photocatalysts with high efficiency and stability remains one of the main challenges [1]. Silver phosphate (Ag_3PO_4) exhibits high photocatalytic activity under visible-light irradiation, showing great potential for the degradation of organic pollutants [2,3]. However, its application is limited by low stability due to photocorrosion during the photocatalytic process [3]. One strategy to overcome this limitation is to form heterojunctions with other semiconductors, such as graphitic carbon nitride (g-C_3N_4), a material characterised by chemical stability, visible-light absorption, and ease of preparation [4]. The combination of Ag_3PO_4 with g-C_3N_4 may promote the separation and transfer of photogenerated charge carriers, reducing their recombination and potentially improving photocatalytic efficiency while minimising photocorrosion. Therefore, this study aimed to synthesise Ag_3PO_4/g-C_3N_4 composites with different g-C_3N_4 contents and evaluate their performance using Rhodamine B (RhB) as a model compound.

The g-C_3N_4 was synthesised from dicyandiamide by microwave-assisted thermal treatment [4]. The Ag_3PO_4/g-C_3N_4 composites were prepared by sonicating g-C_3N_4 in water, followed by the addition of $AgNO_3$, stirring for 1 h, and the dropwise addition of Na_2HPO_4. Materials with different g-C_3N_4 contents (0.5, 10, 35, 60, and 90%) were prepared, along with pure Ag_3PO_4 for comparison. The resulting precipitates were centrifuged and dried at 70 ºC for 12 h. The photocatalytic performance of the materials was evaluated by degrading RhB (5 mg L^{-1}) using a photocatalyst concentration of 1 g L^{-1}.

Preliminary results showed that the composites with lower g-C_3N_4 contents (0.5% and 10%) exhibited better photocatalytic performance, achieving nearly complete degradation of RhB in less than 3 min under visible-light irradiation (λ_{exc} = 420 nm). This work will present the results of reproducibility and reusability tests to investigate the influence of g-C_3N_4 incorporation on Ag_3PO_4 stability and the mitigation of its photocorrosion. Characterisation techniques will also be employed to evaluate the physicochemical properties of the materials and elucidate their relationship with photocatalytic performance.

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ENSEÑANZA DE LA QUÍMICA

É urgente preparar a geração futura para uma posição ativa relativamente aos oceanos

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Têm sido publicados vários alertas para a crise dos oceanos [1], com base no registo de várias situações de crise ambiental e as consequências da inação ou do atraso para a humanidade e o planeta. Cuidar dos oceanos e travar a sua destruição tornou-se um dever que é urgente implementar.

De facto, perante a urgência de travar a destruição dos oceanos é preciso deixar a atitude passiva de apenas identificar os problemas, e agir.

Assim a literacia oceânica, com aprendizagem prática e contacto direto, utilização de novas tecnologías de investigação, incentivo ao empreendedorismo a resolução de problemas e desenvolvimento de competencia e liderança ambientais, é fundamental.

O estudo dos oceanos faz-se, de acordo com os programas de todos os países estudados: (Portugal, Espanha, França e Itália), desde a infância, com uma abordagem lúdica que evolui, na faixa etária dos 12 aos 15 anos, para uma abordagem sustentável relativamente à água doce! Os oceanos passam a ser tema de estudo, na disciplina de ciências naturais como habitat e parte do ecosistema de uma miríade de seres vivos e materia inorgánica.

Sendo a pré-adolescencia a fase em que os alunos estão preparados para iniciar o desenvolvimento do espírito crítico, de acordo com vários pedagogos nomeadamente Piaget, Paulo Freire, Lev Vigotsky o seu interesse pelo meio ambiente especialmente pelos oceanos pode ser incrementado na escola.
O ensino do tema “oceanos” pode entrar em todos os curricula das disciplinas de ciências exatas: matemática, ciencias naturais e físico-química.



Fig.1. Vista do Oceano Atlântico a partir do aquário Augusto Nobre. Antes, centro de investigação em biología marinha. Vê-se o tanque exterior onde se encontravam animais marinhos de grande porte, em exposição. O aquário foi a casa do mar destruída pelo mar.

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Energy for a Sustainable Future: Exploring New Educational Approaches

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Energy plays a fundamental role in modern society, supporting everyday activities, industrial processes and technological development. However, the energy required to produce goods and provide services often goes unnoticed by individual consumers, making it difficult to assess its environmental impact and understand the importance of sustainable energy use [1]. In this regard, hands-on experiments and inquiry-based learning are key to helping students better understand energy use and its environmental impact. Educational studies have also highlighted the value of exploring topics such as product life cycles and renewable energy technologies to connect scientific concepts with real-world sustainability challenges [2-4].

This work proposes the development of two low-cost, hands-on educational and training activities aimed at exploring energy and sustainability through practical science education. Designed for different educational levels, the activities will combine experimentation, observation and guided reflection to introduce key concepts related to energy use, efficiency and environmental impact. One activity will focus on engaging younger students through accessible, age-appropriate scientific exploration, while the other will encourage older students to critically examine energy consumption and the role of individual choices in promoting more sustainable practices. Both activities will prioritize simple materials, accessibility and implementation in classroom settings.

By translating abstract scientific concepts into tangible learning experiences, these activities aim to foster scientific curiosity, strengthen energy literacy and promote environmental awareness among students. Adapting experimental approaches to different age groups can help make the challenges associated with energy consumption more accessible and encourage critical thinking about sustainable solutions. Ultimately, this initiative seeks to highlight the value of practical science education in empowering future generations to understand energy-related challenges and contribute to a more sustainable society.

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QUÍMICA INDUSTRIAL E INGENIERÍA QUÍMICA

Producción continua de biochar a escala industrial mediante pirólisis a vacío en reactor Auger: criterios de selección de biomasa y aplicación en tintas conductoras para electrodos serigrafiados (SPE)

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El auge de la inteligencia artificial y el desarrollo tecnológico ha intensificado el uso de materias primas no renovables (minerales como el grafito y metales como aditivos) para la fabricación de componentes electrónicos y almacenamiento energético. La búsqueda de materias primas alternativas y renovables, especialmente materiales carbonosos, sostenibles requiere superar la brecha existente entre el laboratorio y la producción industrial continua.[1]

El objetivo de este trabajo es demostrar la viabilidad técnica y operativa de la producción continua de biochar a escala industrial, empleando un reactor de pirólisis tipo Auger a vacío. El proceso fue validado y optimizado utilizando siete biomasas residuales con diversa composición de celulosa, hemicelulosa y lignina, lo que permitió establecer los parámetros químicos clave de selección de materia prima para maximizar la calidad del material de carbono [2-3]. Los biochars producidos se caracterizan fisicoquímicamente mediante análisis termogravimétrico (TGA), microscopía electrónica de barrido (SEM) y superficie (BET), para determinar su morfología y electroquímicamente mediante ciclo-voltamperometría (CV), formulando tintas conductoras con el biochar producido y depositándolo sobre electrodos serigrafiados (*screen-printed electrodes*, SPE) [4] para determinar su rendimiento en baterías y supercondensadores.

Fig.1. Planta de pirólisis tipo Auger



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Compostos bioativos sustentáveis derivados de microalgas e cianobactérias para aplicações cosmecêuticas e nutracêuticas (SMACC+)

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O O projeto Compostos Bioativos Sustentáveis Derivados de Microalgas e Cianobactérias para Aplicações Cosmecêuticas e Nutracêuticas (SMACC+) (https://smacc+.eu) é um projeto de cooperação europeia focado no desenvolvimento de compostos bioativos sustentáveis e de elevado valor acrescentado, derivados de microalgas e cianobactérias, para aplicações cosmecêuticas e nutracêuticas. O projeto promove processos biotecnológicos ecoeficientes, abordagens de economia circular e a substituição de aditivos sintéticos por alternativas naturais, seguras e eficazes. Cofinanciado pelo Fundo Europeu de Desenvolvimento Regional (FEDER) no âmbito do Programa Interreg Atlântico e coordenado pela Universidade de Vigo, o projeto tem um orçamento total de 2,8 milhões de euros, dos quais 2,1 milhões de euros são provenientes do FEDER. O projeto reúne nove parceiros da Área Atlântica, incluindo universidades, organizações de investigação e empresas inovadoras, combinando a excelência científica com a experiência industrial. Os parceiros do projeto são: CINBIO – Univ. Vigo, La Rochelle Université, University College Dublin, Instituto Tecnológico de Canarias, Instituto Politécnico de Bragança, University of Galway, Alga Biologics, Finnova Foundation e A4F – Algae for Future. Os objetivos do projeto são: a) Promover a adoção de soluções sustentáveis baseadas na biotecnologia com recurso a microalgas. b) Transferir o conhecimento científico para a indústria e para a sociedade. c) Fomentar a colaboração entre investigadores, empresas, estudantes e decisores políticos. d) Aumentar a consciencialização pública sobre os benefícios da biotecnologia azul.

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Efecto de la proporción HPMC:MC sobre las propiedades físicas y oxidativas de oleogeles de aceite de colza

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Uno de los principales desafíos de la industria alimentaria es mejorar la calidad nutricional de los alimentos mediante la reducción del contenido de grasas saturadas y trans. En este contexto, los oleogeles, estructuras formadas por un organogelador en donde se atrapa aceite, constituyen una alternativa prometedora [1]. La hidroxipropilmetilcelulosa (HPMC) es uno de los estructurantes más utilizados debido a las buenas propiedades que confiere a estos sistemas [2]. En cambio, la metilcelulosa (MC) ha sido poco estudiada con este fin, mientras que su combinación con HPMC no ha sido investigada. Por ello, este trabajo evaluó las propiedades estructurales y oxidativas de oleogeles elaborados con mezclas de HPMC (80–120 cP) y MC (4000 cP), utilizando aceite de colza.

Los oleogeles se elaboraron mediante el método indirecto "*emulsion-template*". Para ello, se prepararon emulsiones O/W al 50% p/p, que posteriormente se deshidrataron mediante secado convectivo a 80 ºC. El sólido obtenido se homogeneizó para formar el oleogel. Se estudiaron cinco sistemas con distintas relaciones en peso de HPMC:MC (2,00:0; 1,50:0,50; 1,00:1,00; 0,46:1,54 y 0:2,00), manteniendo constante la concentración total de estructurante en 2% p/p en la emulsión. La caracterización estructural incluyó barridos reológicos de deformación (0,01–1%; 1 Hz), frecuencia (0,1–10 Hz; 0,1% de deformación) y temperatura (25–80 ºC; 0,1% de deformación; 1 Hz). Adicionalmente, se realizó un análisis de perfil de textura (TPA) para determinar dureza, adhesividad, cohesividad y elasticidad, aplicando una deformación del 50% sobre muestras de 19 mm de diámetro con una sonda cilíndrica de 25 mm y una celda de carga de 5 kg. También se evaluó la retención de aceite (OBC) mediante centrifugación. Finalmente, la oxidación primaria y secundaria se evaluaron 12 h después de la obtención del oleogel mediante el índice de peróxidos (IP) y el valor de *p*-anisidina (AV), respectivamente.

La región viscoelástica lineal superó en todos los casos el 0.1% de deformación. Todos presentaron un comportamiento tipo gel ($G' > G''$) y una baja dependencia de la frecuencia, lo que indica una estructura organizada y estable. Los módulos más elevados correspondieron al oleogel de HPMC y disminuyeron progresivamente con su reemplazo por MC, alcanzando los valores más bajos para el oleogel de únicamente MC. Las rampas de temperatura evidenciaron pocos cambios estructurales en todo el rango de estudio, además de curvas de calentamiento y enfriamiento prácticamente superpuestas. De forma consistente con la reología, la dureza disminuyó de 11,57 a 6,02 kPa al reemplazar HPMC por MC. Esta sustitución también produjo geles más cohesivos, pero menos adhesivos y elásticos. Asimismo, el OBC disminuyó del 89 al 71%, mostrando una relación directa entre la respuesta reológica, la dureza y la capacidad de retención de aceite.

En general, los oleogeles presentaron una baja oxidación, con valores de IP entre 7,3 y 9,4 meq O_2/kg y de AV entre 2,1 y 5,4. Los valores más bajos correspondieron al sistema de HPMC y aumentaron con su reemplazo por MC, aunque todos los sistemas mantuvieron una buena calidad oxidativa. En conclusión, el uso combinado de estructurantes celulósicos permitió obtener oleogeles con diferentes propiedades estructurales y niveles de oxidación similares, facilitando el diseño de oleogeles adaptados a distintas aplicaciones alimentarias.

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Reología de las masas y características de magdalenas de harina de yuca elaboradas con mantequilla o aceite con y sin gelación

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La demanda de alimentos saludables y sin gluten ha impulsado el uso de harinas alternativas, como la harina de yuca, en productos de panadería [1]. No obstante, la ausencia de gluten plantea desafíos tecnológicos que pueden abordarse con el uso de hidrocoloides como la hidroxipropilmetilcelulosa (HPMC) [2]. Asimismo, los oleogeles representan una alternativa a las grasas sólidas para mejorar el perfil nutricional [3]. En este trabajo se elaboraron magdalenas de harina de yuca con aceite, oleogel de HPMC o mantequilla, con el objetivo de evaluar el efecto de la fase oleosa sobre las propiedades reológicas de las masas y las características del producto final, además de la relación entre ambas.

Los oleogeles se prepararon mediante el método indirecto "*emulsion-template"* a partir de emulsiones aceite/agua (o/w, 50% p/p) de aceite de colza y HPMC (80–120 cP, 2% p/p en emulsión). Se elaboraron 4 formulaciones de masas según la fase oleosa: aceite de colza (C1), aceite de colza con HPMC en polvo (C2), oleogel (C3) y mantequilla (C4). Las masas se caracterizaron a 25 ºC mediante barridos de deformación (0,001–10%; 1 Hz) y frecuencia (0,01–10 Hz; 0,05% de deformación), curvas de flujo (0,01–100 s^{-1}) y ensayos de fluencia-recuperación (0,3 Pa durante 5 y 15 min de recuperación). En las magdalenas se determinaron el volumen específico por desplazamiento de semillas de colza y el perfil de textura (TPA) mediante compresión al 50%, analizando dureza, cohesividad, elasticidad y masticabilidad.

Todas las masas presentaron un comportamiento predominantemente elástico (G´ > G´´), con una corta región viscoelástica lineal (<0,08% de deformación) y un aumento progresivo de los módulos reológicos en el orden C1 < C2 < C3 < C4, evidenciando una mayor estructuración por la incorporación de HPMC, especialmente como oleogel, mientras que la mantequilla generó la red más consistente. Las formulaciones mostraron comportamiento pseudoplástico y una viscosidad acorde con la tendencia observada para los módulos, atribuida al fortalecimiento de las interacciones entre hidrocoloide, proteínas y agua, siendo más pronunciado en el oleogel, mientras que en la mantequilla se relacionó con la mayor complejidad estructural del sistema. Las curvas de flujo se ajustaron al modelo de Sisko y los ensayos de fluencia-recuperación fueron consistentes con los obtenidos mediante SAOS.

En la magdalena, C1 presentó el mayor volumen específico, mientras que la incorporación de HPMC en polvo o como oleogel, disminuyó este parámetro, probablemente porque la mayor estructuración y viscosidad de la masa limitaron la expansión de las burbujas durante el horneado. C4 mostró el menor volumen específico, asociado a su elevada viscosidad. Asimismo, el HPMC aumentó la dureza y la masticabilidad, características generalmente poco deseables en ese tipo de productos, y redujo ligeramente la cohesividad y la elasticidad. La mantequilla produjo valores intermedios de dureza y masticabilidad. En conclusión, la incorporación de HPMC en la concentración estudiada incrementó la estructuración de las masas, pero afectó negativamente algunas propiedades de las magdalenas, reduciendo su volumen específico y aumentando su dureza. Por ello, futuros estudios deberían evaluar menores concentraciones de HPMC para minimizar estos efectos.

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Influence of Fishery By-Product Type and Hydrolysis Conditions on the Obtention of Protein Hydrolysates and Antioxidant Bioactive Peptides

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Fish discards are a portion of the total catch that is returned to the sea due to their lack of commercial value [1]. The European Commission has established a series of goals to reduce the number of discards to ensure the obtention of the economic benefit of fishing [2].

Fish protein hydrolysates (FPH) are considered a promising source of bioactive peptides with potential health-promoting properties. Their antioxidant and antihypertensive activities make them especially attractive ingredients for the development of functional foods. In addition, their production from fishery by-products and fishing discards contributes to the valorization of underutilized marine resources and promotes a more sustainable use of these raw materials [3].

In this study, the dissolved protein concentration (Lowry assay) and antioxidant activity (ABTS, DPPH & FRAP assays) of different fish protein hydrolysates from Atlantic chub mackerel (*Scomber colias*) were evaluated to assess the influence of the hydrolysate source (skin and bones vs. heads) and the presence or absence of pH control and hydrolysis time control. For the Lowry assay, 1 g of FPH was resuspended in 10 mL of distilled water and maintained at 4 °C for 2 h. The suspension was then centrifuged at 13,500 rpm (≈12,200 × g) for 30 min and filtered through a 0.45 µm syringe filter. For the ABTS and DPPH assays, protein concentrations of 10 g/L and 20 g/L, respectively, were used.

The results showed that hydrolysis time and pH control influenced both protein solubility and antioxidant activity, although an increase in soluble protein content did not necessarily correspond to enhanced antioxidant activity. The response varied depending on the type of by-product and hydrolysis conditions, with longer hydrolysis times not always resulting in improved antioxidant properties. These findings highlight the importance of optimizing hydrolysis conditions according to the specific raw material and target bioactivity.

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Influence of Rosin and Zinc Oxide on the Structure and Rheology of Natural Rubber Aqueous Dispersions

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Natural rubber is an attractive renewable raw material for paperboard coatings and can be employed as substitute of plastic coatings. The conversion of natural rubber compounds into aqueous dispersions to be applied as coating requires effective control of particle size and flow behaviour. Both properties depend on interactions among the polymer matrix, resin, mineral particles, and crosslinking components. This work investigated the influence of rosin resin and zinc oxide (ZnO) on particle size distribution and rheological behaviour in natural rubber aqueous dispersions prepared using ACTEGA Artística technology [1].

Natural rubber compounds containing 0 or 30 parts per hundred rubber (phr) rosin were mixed with kaolin and antioxidant at 150 °C. The solid compounds were converted into aqueous dispersions at 65 °C and conditioned to 40 wt.% solids using crosslinking solutions without or with ZnO. Four formulations were obtained: R0_Zn0, R0_Zn7.25, R30_Zn0, and R30_Zn7.25. Three independent batches per formulation were analysed by laser diffraction and rheological tests at 25 °C.

Before conditioning, all batches showed a homogeneous appearance without visible agglomerates. In the absence of rosin, the main particle population remained centred at approximately 5–7 µm and was only slightly affected by ZnO. The dispersions containing 30 phr rosin showed a more complex distribution. The presence of rosin split the population in two, around 2 and 18 µm, shifting from predominantly smaller to larger with the presence of ZnO. Strain sweeps showed predominantly elastic behaviour within the linear viscoelastic region. Rosin produced a Rosin produced like a plasticizer effect, reducing both the elastic (G´) and viscous (G´´) moduli whereas ZnO increased the initial elastic response. Without rosin, G′ at the yield point increased from 10 to 26 Pa after ZnO addition, although the linear region became shorter. Frequency sweeps also confirmed a mainly elastic response. Rosin decreased G′ and G″, while ZnO resulted in higher G′ values. R30_Zn0 showed a crossover at 4 rad·s^{-1}, whereas R30_Zn7.25 maintained G′ > G″ throughout the measured range.

All formulations exhibited shear thinning behaviour, in agreement with previous studies on natural rubber latex [2]. The dispersions without rosin showed negligible hysteresis, indicating an almost reversible response during the applied shear cycle. Rosin introduced a clear dependence on shear history. In the rosin containing system, ZnO reduced the hysteresis area by approximately 50%, indicating a lower dependence on previous shear conditions. Similar behaviour has been associated with disruption and partial recovery of colloidal structures during consecutive shear ramps [3].

Overall, rosin produced softer dispersions with greater dependence on shear history, whereas ZnO promoted a more persistent elastic response and reduced hysteresis in the presence of rosin. The combination of both components also caused the greatest changes in particle organization. These findings show that the liquid properties of natural rubber aqueous dispersions can be controlled through formulation composition.

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Valorización de residuos agroforestales para la fabricación de bandejas de celulosa moldeada

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Este trabajo se desarrolló en el marco del proyecto PRIMA BIOMEDPACK («Sistemas de envasado para prolongar la vida útil de los alimentos mediterráneos mediante soluciones innovadoras y circulares basadas en una biorrefinería en cascada multiproducto de residuos agroalimentarios»), cuyo objetivo es desarrollar soluciones de envasado sostenibles a partir de recursos renovables.

Se utilizaron pastas celulósicas obtenidas a partir de paja de trigo, poda de olivo y sarmiento de vid. Estas pastas se caracterizaron morfológicamente y se compararon con una pasta kraft comercial de eucalipto. Posteriormente, se prepararon mezclas formadas por un 70 % de pasta comercial y un 30 % de cada una de las pastas procedentes de los residuos. Tras el refino, las mezclas se emplearon para fabricar bandejas mediante un proceso de termoformado que incluyó la formación por vacío, el prensado en frío y el prensado final en caliente.

Las bandejas obtenidas se evaluaron considerando su procesabilidad, comportamiento mecánico y capacidad de absorción de agua y aceite. Los resultados mostraron que las características morfológicas de las fibras influyeron significativamente tanto en el proceso de fabricación como en las propiedades finales de las bandejas. Entre las formulaciones estudiadas, la mezcla que contenía pasta de paja de trigo presentó el mejor equilibrio global entre procesabilidad y prestaciones.

Los resultados demuestran el potencial de la paja de trigo, la poda de olivo y el sarmiento de vid como fuentes alternativas de fibra para la fabricación de envases de celulosa moldeada. Su aprovechamiento permite valorizar residuos agroforestales y avanzar hacia soluciones de envasado más sostenibles y alineadas con los principios de la economía circular.



Fig.1. Bandejas producidas con las formulaciones evaluadas.

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Linking physicochemical properties and heavy-metal adsorption in biomass-derived carbons through multivariate analysis

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Biomass-derived activated carbons represent a sustainable and low-cost alternative for the removal of metal ions from aqueous streams. However, their adsorption behavior depends simultaneously on multiple textural and surface-chemical properties, making it difficult to identify the main factors governing material performance when each descriptor is analyzed independently. In this work, multivariate analysis techniques were applied to the physicochemical characterization data of 14 carbon materials produced from olive stones (OS) and almond shells (AS). The dataset included non-activated carbons and materials chemically activated with KOH, H_3PO_4 and $ZnCl_2$ at different carbon/activating-agent ratios evaluated for the adsorption of Cu^{2+} and Pb^{2+} under varying initial metal concentrations and adsorbent doses [1].

Pearson correlation analysis first revealed a high degree of interdependence among several physicochemical properties, particularly among descriptors related to pore structure. Principal component analysis (PCA) was subsequently performed on standardized physicochemical variables, considering one independent observation per carbon material. The first principal component was mainly associated with the development of the porous structure, with important contributions from BET surface area, total pore volume and average pore diameter. The second component was primary related to differences in surface composition of Zn, Cl and P. Finally, the third component reflected variations in surface mineral composition and acid-base properties with notable contributions from surface Ca content and pH. Unsupervised K-means analysis further confirmed the strong differentiation induced by the activation process. The cluster comprising the KOH-activated carbons was characterized by higher surface areas, pore volumes, and average pore diameters and, under comparable experimental conditions, showed the highest Cu^{2+} and Pb^{2+} adsorption capacities. These results demonstrate that unsupervised multivariate techniques can identify chemically meaningful structures within complex adsorbent-characterization datasets and provide a complementary approach for relating activation strategy, material physicochemical properties, and adsorption performance.

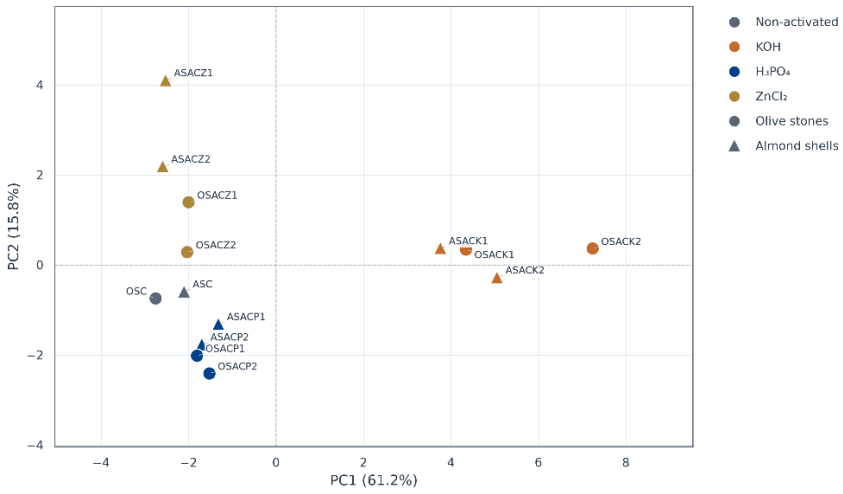


Fig.1. PCA score plot of biomass-derived carbons based on their physicochemical properties.

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Fig and Almond Pruning Biomass as Low-Cost Adsorbents for Nitrate Removal from Aqueous Solutions

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Nitrate pollution is one of the major challenges affecting the quality of surface and groundwater resources, primarily due to the intensive use of nitrogen-based fertilizers and discharges from agricultural and livestock activities. High nitrate concentrations can lead to eutrophication and pose risks to human health, making their removal a matter of considerable environmental concern. Among the available treatment technologies, adsorption has attracted significant attention because of its simplicity, effectiveness, and ease of implementation. In this context, the direct use of biomass residues, without prior carbonization or activation treatments, has emerged as a sustainable and cost-effective alternative. Materials such as rice husks, lignocellulosic wastes, pruning residues, and other agro-industrial by-products contain surface functional groups capable of interacting with nitrate anions, enabling their removal from aqueous solutions [1,2]. Furthermore, the valorization of these residues helps reduce waste management costs and promotes circular economy strategies aimed at developing more sustainable water treatment technologies [2].

In this study, the potential of two biomass residues, namely fig and almond pruning sawdust, has been evaluated due to the large quantities generated annually. For this purpose, adsorption equilibrium and kinetics experiments were performed under various conditions (initial nitrate concentration, adsorbent dosage and pH) for evaluating the separation process. Almond biomass showed higher nitrate removal percentage than fig biomass at concentrations below 400 mg L^{-1} (Fig. 1). Indeed, the adsorption efficiency of almond pruning remained close to 100% for initial concentrations up to 250 mg L^{-1} at pH=14. However, nitrate removal decreased with increasing, especially for almond pruning, which may be attributed to the saturation of available adsorption sites. In addition, increasing pH enhanced nitrate removal for both materials. The higher nitrate removal showed by almond sawdust may be related to differences in elemental composition and surface functional groups identified by FTIR compared with fig sawdust. The porous structure characteristics do not seem to play a relevant role, given that the specific surface area is higher for fig tree pruning biomass (31.4 m^2/g) than for almond tree pruning biomass (12.7 m^2/g).

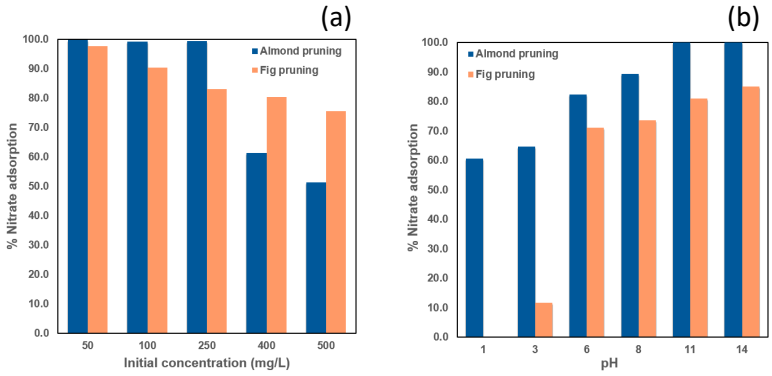


Fig.1. Effect of initial concentration at pH of 14 (a) and of pH at initial concentration of 250 mg/L (b) on nitrate adsorption by almond and fig pruning sawdust (adsorbent dose, 10 g/L; 50ºC and time,150 min)

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3D Printing of Biodegradable Hydrogels for Lutein Incorporation

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Hydrogels derived from natural sources, particularly those based on chitosan, have gained substantial attention in the biomedical field due to their superior swelling capacity, bicompatibility, biodegradability, antimicrobial and antifungal properties, that make them ideal candidates for tissue engineering, wound dressing and drug delivery [1].

Nevertheless, pure chitosan suffers from poor mechanical integrity and limited printability [2]. To adress these drawbacks blending chitosan with pectin, an anionic, biodegradable polysaccharide with high gelling capacity [3], enable the formation of polyelectrolyte complexes (PECs) driven by electrostatic interaction that improve the overall performance of the hydrogel. Furthermore, post-printing ionic crosslinking with sodium tripolyphosphate (TPP) ensures mechanical stability and structural fidelity during post-processing and handling.

In the present work, 3D-printed chitosan-pectin hidrogels were synthesized shaped by 3D printing, and crosslinked with TPP to encapsulate lutein. As a dietary carotenoid with proven efficacy in mitigating retinal nerve degeneration, cataracts, and age-related macular degeneration [4], lutein exhibits low bioavailability after digestion due to its susceptibility to degradation by light, heat, and oxidation.

To optimize printability, several inks were formulated using different chitosan-to-pectin ratios while maintaining a fixed total polymer concentration of 5.5% (w/v), followed by comprehensive rheological characterization. After 3D printing, the resulting hydrogels were evaluated through FTIR spectroscopy, swelling assays, and SEM to investigate matrix porosity. Lastly, following carotenoid incorporation, the delivery performance was evaluated via *in vitro* release studies.

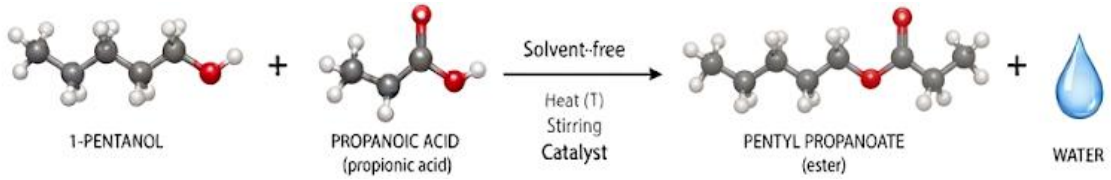
Agradecimientos
This work was developed within the framework of project 3DBIOGEL4HEALTH – “Exploring the 3D Bioprinting for Design of Novel Biodegradable Hydrogels as Lutein Carriers” (Ref. 2023.12614.PEX), financed by national funds through the Fundação para a Ciência e a Tecnologia (FCT). Additional funding was provided through projects with the following references: LA/P/0112/2020, UID/00285/2025, UID/00102/2025, UID/PRR/00102/2025, and UID/PRR2/00102/2025.

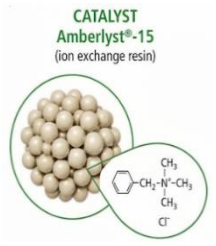
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Procesos de modelización/simulación en la síntesis y purificación de un ester de amilo

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El **propanoato de pentilo (**PP**)** es un biosolvente utilizado en diversos sectores industriales[1] que presenta una eficiencia comparable a la de otros disolventes convencionales. La ruta de síntesis habitual para su producción se realiza mediante el clásico proceso de esterificación cuyo esquema es:





Es conocido que estos procesos se realizan en medio acido actuando como catalizador. Pero, la eliminación del ácido inorgánico empleado suele generar diversos problemas, como corrosión en los equipos, toxicidad, y otros residuos no deseados. Por ello, con el fin de lograr un proceso sostenible, se empleó la Amberlite-15 como catalizador, que es una resina de intercambio iónico suministrada por Merck. De esta forma, con este trabajo se comparó la eficacia de este catalizador con los resultados obtenidos al emplear una enzima utilizada en síntesis orgánica (Lypozime-435) y especialmente en procesos de esterificación.[2,3]

La reacción se llevó a cabo en ausencia de disolvente en un reactor discontinuo, con agitación y calentamiento desde el exterior, ver Figura 1. La toma de micromuestras y la temperatura del medio se realizó de forma automática, utilizando un programa de control propio realizado al efecto. Se trabajó a presión atmosférica (~ 98 kPa) y a dos temperaturas de 50 y 70 ºC, considerando únicamente una relación molar inicial de reactivos: x_0, alcohol / x_0, ácido = 1, esto es, equivalente a la estequiométrica. Se utilizó una carga de catalizador del 10 % con respecto a la masa inicial de ácido. Los resultados mostraron que la reacción transcurre más rápidamente, alcanzando una conversión cercana al 65 %, cuando se utiliza la temperatura más elevada de 70 ºC.

Los datos cinéticos se correlacionaron utilizando una ley de velocidad reversible de segundo orden y el modelo establecido finalmente se utilizó para simular el proceso de producción del PP mediante el simulador en abierto DWSM© (Fig. 2), con el fin de evaluar la viabilidad técnica de la ruta de producción más práctica. Los resultados de la simulación mostraron que la purificación del PP, siguiendo la ruta propuesta, es viable lográndose una pureza del éster puro cercana al 99 %. Por todo lo realizado, en base a la ruta de trabajo basada en la terna experimentación-modelización-simulación, se concluye que el trabajo proporciona una contribución valiosa para el avance en el escalado de este proceso específico, e incluso extrapolable a otros casos de producción de ésteres.

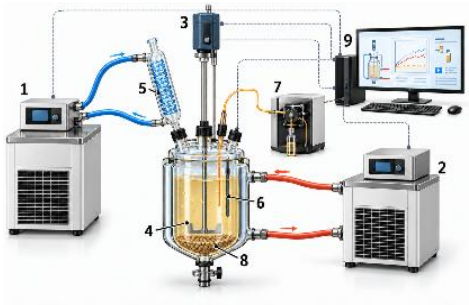


Fig. 1. Instalación experimental

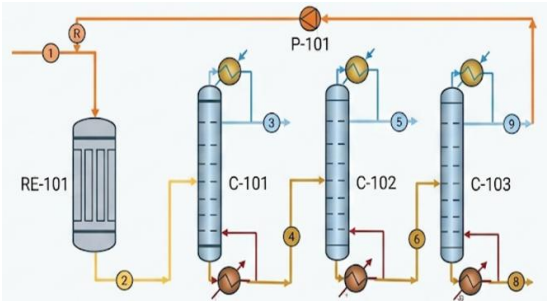


Fig. 2. Proceso de simulación

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NANOQUÍMICA Y NANOTECNOLOGÍA

Purpurin 18-Assisted Formation of Gold Nanoparticles on WS_2 Nanoflakes for Cancer Therapy

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The integration of two-dimensional transition metal dichalcogenides (TMDCs), metal nanoparticles, and natural photosensitizers represents a promising strategy for the development of multifunctional nanosystems for combined cancer therapies. In this context, tungsten disulfide (WS_2) nanoflakes provide a high surface-area platform with strong X-ray attenuation and photothermal properties, while gold nanoparticles (AuNPs) can further enhance radiation-matter interactions and provide plasmonic functionality [1]. The incorporation of natural photosensitizers such as Purpurin 18 (Pur18) may additionally promote reactive oxygen species (ROS) generation, providing opportunities for synergistic therapeutic effects [2]. Herein, we report a rapid one-pot synthesis of AuNPs decorated WS_2 nanoflakes functionalized with Pur18 (WS_2AuPur18). The synthesis was performed at room temperature within 1 h by combining WS_2 nanoflakes, $HAuCl_4$, and Pur18 in a one-pot reaction. A control system containing WS_2 and $HAuCl_4$, but without Pur18, was prepared under identical conditions to investigate the influence of the natural photosensitizer on AuNP formation and deposition. The resulting materials were characterized by UV-Vis spectroscopy, fluorescence spectroscopy, transmission electron microscopy (TEM), and high-resolution TEM (HRTEM). ROS generation was evaluated using ABDA and DPBF assays. TEM analyses revealed the presence of AuNPs on the WS_2 surface in both systems. However, the WS_2AuPur18 exhibited a higher AuNP coverage across the nanoflake surface, together with smaller and more homogeneous nanoparticles compared with the control WS_2Au system. Quantitative analysis of a significant number of nanoparticles (>200) confirmed this difference, with an average AuNPs diameter of 11.2±3.0 nm for WS_2Au and 9.4±2.0 nm for WS_2AuPur18. These results suggest that Pur18 plays a role in the nucleation and growth of AuNPs during the one-pot synthesis, promoting the formation of smaller and more homogeneously distributed nanoparticles.
The combination of WS_2, AuNPs, and Pur18 within a single nanostructure provides a multifunctional platform with potential for photothermal, photodynamic, and radiotherapy applications. Their biological activity and cytotoxicity are currently being evaluated in different cancer cell lines to assess their potential for cancer therapy.



Fig.1. Schematic representation of the one-pot synthesis of WS_2AuPur18.

Acknowledgments
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Carbon Nanomaterials as Photo-Active Materials in Textile All-in-one Photo-Supercapacitors

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With the growing demand for energy-storage solutions that combine longer lifetimes, higher efficiency and more compact designs, together with the increasing focus on renewable energy, interest in green energy technologies has intensified. Photo-supercapacitors (PSCs) are one such technology, as they harvest sunlight, convert it into electrochemical energy and store it in a single device.[1]

In this work, carbon-based nanomaterials were synthesised from urea and citric acid at different mass ratios (25:75, 50:50 and 75:25 wt%) and two temperatures (180 °C and 200 °C) by a scalable microwave method (Fig. 1). All carbon-based samples were characterised by X-ray diffraction (XRD), which showed a pattern characteristic of an amorphous structure, and by dynamic light scattering, which gave an average hydrodynamic size of about 300 nm. Fourier-transform infrared spectroscopy with attenuated total reflectance (FTIR-ATR), UV–Vis spectroscopy, fluorescence spectroscopy and zeta potential measurements were used to assess chemical composition, optical properties and colloidal stability.

The 50:50 urea/citric acid sample prepared at 200 °C was selected and used to dope a poly(vinyl alcohol)/H_3PO_4 solid-gel electrolyte in 0, 0.25, 0.50, 1.0, 2.0 and 4.0 %(v/v). The resulting films were characterised by FTIR-ATR and XRD and then incorporated as electrolyte into planar devices fabricated using cotton-based textiles coated with poly(3,4-ethylenedioxythiophene) polystyrene sulfonate and oxidised carbon nanotubes as electrodes. The assembled devices were evaluated by cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy. The best-performing device, prepared with 2% doping, delivered an energy density of 0.63 μWh cm^{-2} and a power density of 137.86 μW cm^{-2}. Under visible-light irradiation, the doped device generated 69.0 mV, compared with 1.80 mV for the undoped electrolyte, corresponding to a 38-fold increase.

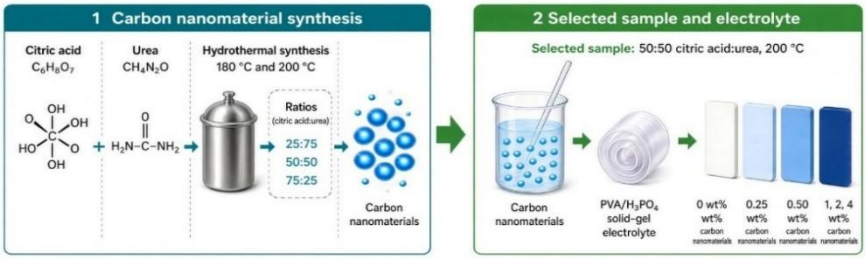


Fig.1. Visual summary of the work done.

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Cysteamine-Functionalized ZnPPIX for Integration with PVP-Stabilized Silver Nanoparticles: Optical and Photochemical Characterization

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Photodynamic therapy (PDT) is a promising approach for biomedical applications, based on the activation of photosensitizers (PS) by light to promote the generation of reactive oxygen species (ROS), including singlet oxygen ($^1O_2$) [1]. The association of PS with metallic nanoparticles has sparked interest in the development of hybrid systems with complementary optical and physicochemical properties [2]. In this context, this study investigated the functionalization of zinc protoporphyrin IX (ZnPPIX) through an EDC/sulfo-NHS mediated coupling reaction and its association with silver nanoparticles (AgNPs), subsequently stabilized with poly(N-vinylpyrrolidone) (PVP).

ZnPPIX was prepared in a DMSO/NaOH (50% v/v) medium, subjected to sonication and centrifugation, and functionalized with cysteamine to introduce thiol groups to promote its association with AgNPs. These were synthesized by the chemical reduction of silver nitrate with sodium borohydride, using citric acid as a modulating agent. After the incorporation of functionalized ZnPPIX, the suspension was kept under agitation for 24 hours at 25 °C, followed by the addition of PVP (40 kDa). The system was characterized by UV–Vis, fluorescence, and FTIR spectroscopies, dynamic light scattering (DLS), electrophoretic light scattering (ELS), and transmission electron microscopy (TEM). The generation of $^1O_2$ was indirectly evaluated by the photobleaching of ABDA under 420 nm irradiation, with a power of 43 mW [3].

The UV–Vis spectra showed the plasmonic band of the AgNPs at approximately 396 nm and an absorption contribution near 418 nm after the incorporation of ZnPPIX, consistent with the presence of FS. Fluorescence was observed between 570 and 680 nm, with changes after association with the nanoparticles. The FTIR spectra revealed modifications in the bands at 1367, 1427, and 1470 cm^{-1}, associated with vibrations of the porphyrin macrocycle, as well as changes in the region of 2882–2987 cm^{-1}, related to aliphatic C–H stretching. These changes are consistent with the proposed functionalization.

The polydispersity index (PDI) increased from 0.247 in the initial AgNPs to 0.574 after the incorporation of functionalized ZnPPIX and 0.845 after the addition of PVP. The zeta potential varied from −23.3 to −36.9 mV and, subsequently, to −22.7 mV. Despite the greater heterogeneity indicated by DLS, the TEM images revealed approximately spherical nanoparticles, with a size close to 20 nm and without evident agglomerates in the observed regions. The ABDA assay showed photobleaching under irradiation, consistent with the photosensitized generation of $^1O_2$. Together, the results demonstrate spectroscopic and colloidal changes after the incorporation of the FS and indicate photodynamic activity, justifying further studies of the hybrid ZnPPIX–AgNPs system for potential PDT applications.

Acknowledgments
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Exploring Liposomal NanoSystems for Delivery of Triphenylphosphonium Derivatives

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Quaternary phosphonium compounds, namely triphenylphosphonium derivatives (TPPs), have demonstrated antimicrobial and antifungal activity against resistant strains.[1] However, their cytotoxicity in human cells constitutes a limitation to clinical application, highlighting the need to develop delivery strategies that allow improving their safety profile.[1] In this context, nanoscale delivery systems, particularly liposomes, emerge as a promising approach, allowing modulation of the release of encapsulated compounds and potentially minimizing off-target cytotoxic effects.[2]

In this work, liposomes composed of dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) were developed, incorporating TPP derivatives with different alkyl chain lengths (Cx-TPPs; x = 8, 10, 12, 14 and 16 carbon atoms), through thin lipid film hydration method.[3] The nanoformulations were characterized in terms of particle size and zeta potential using dynamic light scattering and electrophoretic light scattering, respectively, while association efficiency was determined by ultra-high performance liquid chromatography. Additionally, stability in storage conditions was evaluated, as well as the behavior of the nanoformulations under different pH conditions and in the presence of mucins. The cytotoxicity of the free and encapsulated compounds was investigated in normal human dermal fibroblasts (NHDF) and in human hepatocellular carcinoma cells (HepG2), using resazurin and sulforodamine B assays.

The results demonstrated the successful incorporation of the different Cx-TPP derivatives into DPPC liposomes, with association efficiencies (AE%) ranging from 48% to 92%, resulting in nanoformulations with sizes smaller than 300 nm and zeta-potential influenced by the alkyl chain length. The nanoformulations showed stability during a storage period of up to eight weeks, also showing the ability to interact with mucins and greater stability under slightly acidic to neutral pH conditions. Additionally, the most promising nanoformulations demonstrated reduced cytotoxicity compared to their respective free compounds in both cell lines evaluated.

Overall, the results obtained demonstrate that DPPC liposomes constitute a promising strategy for the encapsulation of Cx-TPP derivatives, combining adequate physicochemical properties with reduced cytotoxicity. These results support the potential of these systems as delivery platforms for compounds with antimicrobial activity, contributing to the development of nanoformulations with an improved safety profile.

Acknowledgments

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Electrochemical synthesis of ligand-free iron clusters: ascorbic acid oxidation and antibacterial evaluation

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Iron nanoclusters are emerging as promising platforms for catalysis and biomedical applications due to their low cost, biocompatibility and unique electronic and surface properties. In this context, the absence of stabilizing ligands is particularly attractive, as it leaves surface sites accessible for substrate interaction and avoids ligand-induced inhibition of activity. Building on our recent advances in ligand-free electrochemical methodologies[1], [2], this work focuses on the synthesis, characterization and dual-functional evaluation of iron clusters generated in aqueous media without conventional stabilizing agents.

The obtained iron species were characterized by complementary spectroscopic and analytical techniques, including UV-Vis and fluorescence spectroscopy and ICP analysis. Their functional performance was then assessed in two complementary contexts. First, their catalytic behaviour was probed through ascorbic acid oxidation, a reaction linked to ROS generation and oxidative stress. The clusters showed high catalytic efficiency, establishing relationships between the electrochemical generation conditions and their redox catalytic behaviour. Second, their antibacterial activity was tested against *E. coli*, showing up to 65% reduction in the bacterial population at the assayed concentrations. Notably, while some samples displayed correlation between ascorbate oxidation and antibacterial activity, others did not, indicating that ROS-mediated mechanisms are not solely responsible for the observed bacterial inhibition.

These results position earth-abundant iron nanoclusters as promising multifunctional materials, combining low-cost sustainable catalysis with antibacterial activity that warrants further structural optimization.

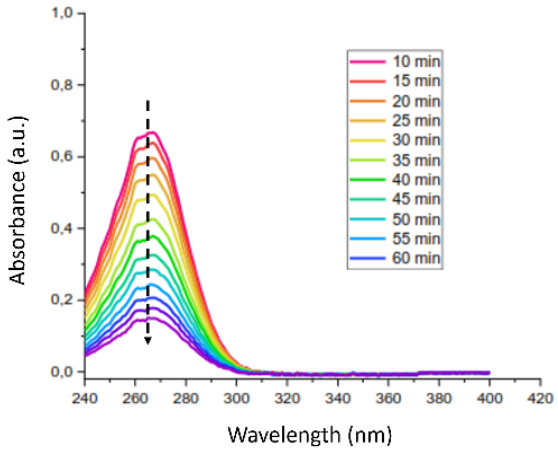


Fig.1. UV-Vis monitoring of ascorbic acid at 265 nm in the presence of Fe clusters

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From milk cream to functional nanocarriers: a sustainable approach for curcumin delivery

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The development of sustainable food technologies requires innovative strategies to valorize underutilized resources and to improve the stability, delivery, and functionality of bioactive compounds. Milk, a widely consumed food and a complex biological system, offers promising opportunities in this context. In particular, milk fat globules and their associated membrane components represent a valuable yet underexplored resource for developing biocompatible nanocarriers.

This work explores the conversion of milk cream into milk fat globule-based nanocarriers (MiGloN) to encapsulate and deliver bioactive compounds in functional foods [1]. The approach valorizes a dairy-derived resource through a simple, organic-solvent-free production process that combines milk fat with food-compatible surfactants and uses sonication to produce nanoscale dispersions. Unlike approaches based on purified milk fat, this strategy retains the protein components associated with milk fat globules, thereby contributing to nanocarrier stability and biological interactions.

MiGloN remain stable for up to ten months at room temperature and show resistance to simulated gastrointestinal conditions, supporting their potential for oral delivery applications. Furthermore, the absence of cytotoxic effects at concentrations up to 2.5 mg/mL and their non-hemolytic behavior provide encouraging initial evidence of biocompatibility. The resulting nanocarriers exhibit promising physicochemical properties and inherent antioxidant activity. These characteristics are particularly relevant for functional food applications, in which carrier stability, compatibility with food ingredients, and the protection of sensitive bioactive compounds are important considerations.

The lipid-rich composition of MiGloN provides a promising environment for incorporating hydrophobic compounds such as curcumin. Its encapsulation within these nanocarriers improves its dispersion in aqueous media and helps protect it against degradation, thereby supporting its incorporation into food matrices and oral formulations. Curcumin is of particular interest because, despite its recognized antioxidant activity and potential health benefits, its poor water solubility and limited stability pose significant challenges to its effective incorporation into aqueous food products. The combination of curcumin with nanocarriers that also exhibit antioxidant activity further provides an interesting opportunity to develop multifunctional food formulations.

By combining the valorization of dairy resources with solvent-free processing and the development of functional nanocarriers, this work contributes to more sustainable approaches to food formulation. MiGloN offer a promising platform for incorporating sensitive bioactive compounds into functional foods and nutritional supplements, potentially enhancing their stability and delivery while creating added value from milk-derived materials. In particular, the use of MiGloN to deliver curcumin offers a promising approach to addressing the formulation challenges of poorly water-soluble bioactive compounds while creating added value from milk-derived materials.

Funding
This work received financial support from the PT national funds (FCT/MECI, Fundação para a Ciência e Tecnologia and Ministério da Educação, Ciência e Inovação) through the project UID/50006/2025 DOI 10.54499/UID/50006/2025 - Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos.

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From Sea to Skin: *Dunaliella salina* Nanoparticle-Loaded Hydrogels for Skin Hydration and Regeneration

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Dunaliella salina is a microalga recognized for its rich content of bioactive compounds, such as polar lipids and carotenoids, which exhibit health-promoting properties, including antioxidant activity of particular interest for skin care. The sustainable exploitation of these bioactives within blue biotechnology requires the development of suitable delivery systems capable of improving their stability and enhancing their functionality. This work aimed to develop D. salina extract-loaded lipid nanoparticles and to incorporate them into a polymeric hydrogel for skin hydration and regeneration.

The lipids and pigments were extracted using a conventional organic solvent method based on the Bligh and Dyer procedure, with a lipid yield of 5.7 ± 0.7 % (dry weight). The antioxidant activity of the extract with and without pigments was evaluated using DPPH, ABTS and FRAP assays, revealing significant antioxidant capacity. Gas chromatography analysis showed a lipid extract dominated by saturated C16–C18 fatty acids and, with a relevant proportion of palmitic acid (16:0) and unsaturated fatty acids represented largely by α-linolenic acid (18:3n-3), indicating the presence of nutritionally and functionally valuable marine lipids.

To improve delivery, stability and applicability, the extracts were incorporated into lipid nanoparticles composed of Precirol® ATO 5 as the solid lipid matrix and Tween®80 as surfactant, produced by hot emulsification followed by sonication. The nanoparticles presented a particle size of 204.3 ± 19.4 nm, a polydispersity index of 0.253 ± 0.037 and a zeta potential of −13.7 ± 2.3 mV, demonstrating the formation of stable and homogeneous nanosystems. *D. salina* extract-loaded nanoparticles were further evaluated for their stability during storage and under processing conditions.

A formulation suitable for topical application was obtained by incorporation of the nanoparticles into a hydrogel composed of polyvinylpyrrolidone (PVP), sodium alginate (10 %, w/v) and glycerol. Alginate, a marine-derived polysaccharide, provides a biocompatible, water-retaining gel network known to support wound healing, while PVP acts as a film-forming and humectant agent that improves spreadability and skin adhesion. Glycerol acts as a humectant and plasticizer, enhancing moisture retention and gel flexibility. Combined with the antioxidant activity of the encapsulated bioactives, this hybrid system is designed to promote skin hydration, reinforce the barrier function and support tissue regeneration. The rheological behaviour of the nanoparticle-loaded hydrogel was evaluated by rotational (flow curves) and oscillatory (amplitude and frequency sweeps) measurements, determining viscosity, storage (G′) and loss (G″) moduli and the linear viscoelastic region, in order to assess the effect of nanoparticle incorporation on gel structure, shear-thinning behaviour and suitability for cutaneous application. Skin permeation and retention of the bioactives were studied in Franz diffusion cells using porcine ear skin, quantifying the amounts retained in the skin layers as well as the ones permeated into the receptor compartment, to confirm local delivery with limited systemic passage. Overall, this work highlights the potential of *D. salina*-based nanosystems in hydrogels as sustainable, marine-derived ingredients for skin care.

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Ingeniería de Nanomateriales para el Almacenamiento Sostenible de Energía: Retos y Perspectivas Emergentes

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La transición energética global exige el desarrollo de tecnologías capaces de almacenar energía de forma eficiente, segura y sostenible. En este contexto, los nanomateriales funcionales han emergido como una alternativa estratégica para mejorar el rendimiento de dispositivos de almacenamiento energético, especialmente en baterías recargables, supercondensadores y sistemas híbridos.

La reducción de dimensiones a escala nanométrica permite incrementar la superficie específica activa, optimizar el transporte de carga y mejorar la cinética electroquímica de los materiales. Entre los sistemas más estudiados destacan los óxidos metálicos nanoestructurados, los materiales basados en carbono, el grafeno y los compuestos híbridos multifuncionales. Estas estructuras presentan propiedades únicas derivadas de fenómenos de confinamiento electrónico y de la elevada interacción superficial con los medios circundantes.

Los avances recientes en síntesis mediante procesos sol-gel, métodos hidrotermales y estrategias de autoensamblaje han permitido obtener materiales con morfologías controladas, elevada estabilidad estructural y mejores capacidades de almacenamiento energético. Asimismo, la incorporación de enfoques de química verde está favoreciendo la producción de nanomateriales con menor impacto ambiental, reduciendo el uso de reactivos tóxicos y el consumo energético asociado a los procesos de fabricación.

Sin embargo, persisten desafíos relacionados con la escalabilidad industrial, la estabilidad a largo plazo y la evaluación integral del ciclo de vida de estos materiales. El desarrollo futuro dependerá de la integración de criterios de sostenibilidad, economía circular y diseño inteligente de materiales avanzados.



Fig.1. La nanotecnología da una nueva dimensión a la transformación renovable

Agradecimientos

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Development of Sustainable Lignin-Based Nanoplatforms with Magnetothermal and Optical Properties

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The development of sustainable and multifunctional nanomaterials has attracted increasing attention as an environmentally responsible approach to advanced nanotechnology. Lignin, an abundant natural biopolymer derived from lignocellulosic biomass, represents a promising renewable resource for the design of functional hybrid nanostructures [1].

In parallel, superparamagnetic iron oxide nanoparticles (SPIONs) have attracted considerable interest due to their unique magnetic properties, relatively low toxicity, and potential biocompatibility, making them promising candidates for a wide range of technological and biomedical applications [2].

Their ability to generate heat under alternating magnetic fields makes them suitable for magnetic hyperthermia [3]. However, their colloidal stability and biological interactions are strongly influenced by their surface chemistry and coating composition. In this regard, lignin offers a sustainable and versatile alternative for the surface functionalization of SPIONs, potentially providing additional functionalities while promoting the development of environmentally friendly magnetic nanoplatforms.

In this work, sustainable lignin-based magnetic nanoplatforms incorporating SPIONs were developed and characterized, combining the intrinsic optical properties of lignin with the magnetic response of iron oxide nanoparticles. Their physicochemical characteristics and multifunctional properties were systematically investigated.

The resulting nanoplatforms exhibited magnetothermal activity under an alternating magnetic field, together with intrinsic autofluorescence without the need for external fluorescent dyes. Furthermore, in vitro cytotoxicity assays revealed a favorable cellular response under the experimental conditions evaluated. These findings highlight the potential of lignin-based magnetic nanoplatforms as sustainable and multifunctional materials combining magnetothermal and optical properties with promising preliminary cytocompatibility.

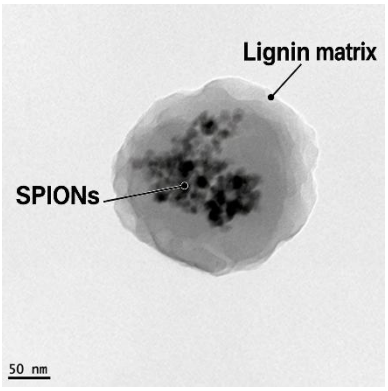


Fig. 1. TEM image of lignin-based magnetic nanoplatforms showing SPIONs embedded within the lignin matrix

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QUÍMICA DE POLÍMEROS

Design and synthesis of perchlorotriphenylmethyl radical-based covalent triazine framework for lithium-ion storage

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Perchlorotriphenylmethyl (PTM) radicals[1] have been extensively studied due to their high stability, luminescent properties, and electroactive behavior. Although a limited number of PTM-based covalent organic frameworks (COFs) have been reported,[2] their application as organic electrodes for lithium-ion battery (LIB) systems remains largely unexplored. In this study, a PTM radical-based triazine COF (PTMR-CTF) was synthesized and fully characterized using various spectroscopic techniques. The presence of PTM radicals within the framework was confirmed by electron paramagnetic resonance (EPR) spectroscopy. Additionally, the electroactive nature of PTMR-CTF was demonstrated by reversible redox peaks observed in solid-state cyclic voltammetry (CV). Ongoing investigations are focused on evaluating this material as anode for lithium-ion storage.

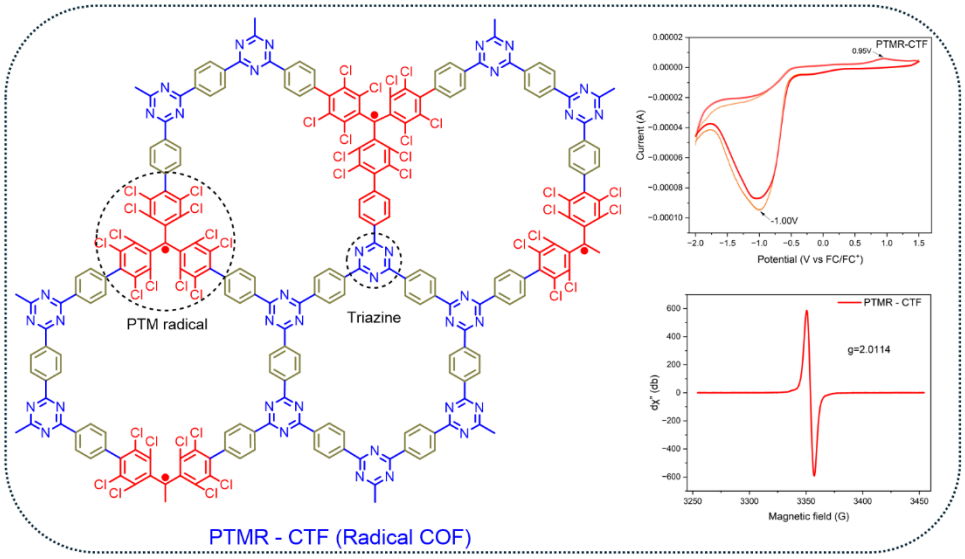


Figure1: Structure and selected characterization of PTMR-CTF

Agradecimientos
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PVC Insulation, Elongation and Product Robustness

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Abstract:

PVC insulation elongation within specification may act as a hidden contributor to quality and reliability issues in automotive antenna cable assemblies. Traditional qualification methods evaluate material properties and manufacturing parameters independently, against their respective specifications. However, interactions between compliant material characteristics and process tolerances may create hidden sources of variation that impact product quality and reliability.
The aim of this study proposes a robustness-based approach to assess how variations in material mechanical properties, within approved specifications, interact with manufacturing parameters to influence product performance.
The objective is to establish a framework for identifying hidden contributors to quality variation and support the transition from compliance-based qualification toward robustness-based reliability assessment and investigate whether specification-compliant material and process variations interact to reduce robustness and increase product performance variability.



Fig.1. Antenna cable

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Potencial de diferentes quitosanos para o desenvolvimento de revestimentos alimentares

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O quitosano destaca-se pela biodegradabilidade, capacidade filmogénica e atividade antimicrobiana [1]. Contudo, as diferenças no grau de desacetilação e na viscosidade podem influenciar o seu desempenho em revestimentos alimentares híbridos. Assim, avaliou-se a influência do grau de desacetilação (85% e 90%) e da classe de viscosidade (100 e 600 mPa·s) na atividade antimicrobiana do quitosano e nas propriedades físico-químicas dos filmes.

Foram preparadas soluções de quitosano a 1% (*m*/*v*) em ácido acético a 0,5% (*v*/*v*), obtendo-se os filmes por evaporação do solvente. Para as soluções filmogénicas, avaliou-se a viscosidade e a atividade antimicrobiana por microdiluição, com determinação da concentração mínima inibitória (CMI), bactericida (CMB) e fungicida (CMF), frente a contaminantes alimentares. A caracterização dos filmes incluiu espectroscopia de infravermelho com transformada de Fourier (FTIR) e determinação da espessura, do grau de inchamento, da permeabilidade ao vapor de água, da humidade e da cor.

As soluções apresentaram viscosidades de 50 ± 1 – 62,3 ± 0,3 mPa·s e de 311 ± 53 – 349 ± 3 mPa·s nas classes de 100 e 600, respetivamente. Na avaliação antimicrobiana, o quitosano 90/100 apresentou CMI de 0,47 mg/mL frente *Listeria monocytogenes* e *Staphylococcus aureus*, e o 85/100 de 0,94 mg/mL frente *Pseudomonas aeruginosa* e *Salmonella enterica*. A inibição dos fungos ocorreu apenas a 7,5 mg/mL, sem atividade fungicida no intervalo testado. Nos filmes, o FTIR indicou a presença de grupos acetilados e aminas sem demonstrar diferenças qualitativas. Quanto ao comportamento perante a água, o inchamento variou entre 345 ± 61% no 90/600 e 765 ± 133% no 90/100, enquanto a permeabilidade ao vapor de água apresentou valores próximos entre amostras, ligeiramente inferiores nos quitosanos com 90% de desacetilação. A espessura dos filmes variou entre 17 ± 0,3 e 19 ± 0,4 µm, observando-se valores ligeiramente inferiores nos filmes com maior grau de desacetilação. Quanto à cor, os filmes da classe 600 apresentaram valores de a^* ligeiramente superiores e de b^* mais negativos, sem uma tendência clara associada ao grau de desacetilação.

Estes resultados preliminares indicam que o quitosano 90/100 é o mais promissor para desenvolver revestimentos alimentares binários, devido à sua baixa viscosidade e elevada atividade antibacteriana. Contudo, o grau de inchamento mais elevado sugere avaliar se a combinação com outros polímeros permite reduzir o inchamento dos filmes sem comprometer a atividade antimicrobiana.

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Shrinking Process Optimization

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Abstract:

One of the biggest issues on automotive industry related with manufacturing process is the watertightness of welded splices. Watertightness is mainly related to splice configuration (number of wires welded), insulation material of wires, it compatibility with polyolefin tubes and the parameters defined during shrinking process. Shrinking is a mechanical process where the adhesive materials fill the voids or pores of the surfaces and hold surfaces together by interlocking. Adhesion occurs by the adhesive flowing and filling micro-cavities on the substrate. When the adhesive then hardens, the substrates are held together mechanically. The adhesive must not only wet the substrate, but also have the right rheological properties to penetrate pores and openings in a reasonable time. The surface of a substrate is never truly smooth but consists of a maze of peaks and valleys. According to the mechanical theory of adhesion, in order to function properly, the adhesive must penetrate the cavities on the surface, displace the trapped air at the interface, and lock-on mechanically to the substrate.
The surface roughness aids in adhesion by increasing the total contact area between the adhesive or sealant and the adherent. Increasing the actual area of contact will increase the total energy of surface interaction by a proportional amount. Thus, the mechanical theory generally suggests that roughening of surfaces is beneficial because there is mechanical interlocking and it increases the total effective area over which the forces of adhesion can develop. However, roughening is only effective if the adhesive wets the surface well.
Since good adhesion can occur between smooth adherent surfaces as well, it is clear that while interlocking helps promote adhesion, it is not really a generally applicable adhesion mechanism. Pretreatment methods applied on surfaces enhance adhesion. These pretreatments (especially plastic surface treatments) result in micro roughness on the adherend surface, which can improve bond strength and durability by providing mechanical interlocking. Beyond mechanical interlocking, the enhancement of the adhesive joint strength due to the roughing of the adherend surface may also result from other factors such as formation of a larger surface, improved kinetics of wetting and increased plastic deformation of the adhesive.
The proposal of our study is a realization of a model of the sealing function according to the configuration and the process variations that will be demonstrated by: y=f(x). With this definition we expect to have improved process optimum setting to make it more robust, capability prediction and identification of most risky configurations and improved quality control conditions.

Keywords: shrinking process, process control, process variation

From Wheat Straw to Functional Food Packaging: Cellulose- and Lignin-Stabilized Pickering Emulsions for Sustainable Coatings

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The transition towards sustainable food packaging requires renewable materials with improved barrier and functional properties. This study explores an integrated wheat straw biorefinery approach to produce fiber-based packaging coated with beeswax Pickering emulsions stabilized by two lignocellulosic nanomaterials: cellulose nanofibers (CNF) and lignin nanoparticles (LNPs).

Cellulosic pulp was obtained from wheat straw and converted into paper sheets, while cellulose fractions and lignin recovered from black liquor were separately processed into CNF and LNPs. Beeswax-in-water emulsions were formulated using either stabilizer, and applied as coatings onto the resulting paper substrates. Additionally, curcumin was incorporated into CNF-stabilized emulsions to provide antioxidant functionality. Emulsion stability, droplet size, mechanical performance, water interactions, vapor transmission, and antioxidant activity were investigated.

CNF-stabilized formulations containing 0.25% CNF and 20% beeswax enabled curcumin encapsulation with an efficiency of 82.67%. Their application reduced water vapor transmission from approximately 37 to 18 g m^{-2} h^{-1} without curcumin, or 27 g m^{-2} h^{-1} with curcumin, while increasing antioxidant activity. LNP-stabilized coatings enhanced surface hydrophobicity, reduced water and oil absorption, and improved tear and burst resistance. However, these coatings increased water vapor transmission, highlighting formulation dependent trade-offs. Both systems exhibited limitations in certain mechanical properties, emphasizing the need for further optimization.

The comparative assessment provides insight into how stabilizer chemistry influences coating performance and specific end-use suitability. Overall, this work demonstrates the complementary potential of cellulose and lignin nanomaterials derived from a common agricultural residue to create functional fiber-based food packaging, while identifying critical performance parameters for future development and potential industrial implementation.

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QUÍMICA ANALÍTICA

SENTINEL Project: Analytical Characterisation of Emerging Nitazene Opioids

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The re-emergence of nitazenes, a highly potent class of novel synthetic opioids (NSOs), represents a significant analytical challenge due to their structural diversity, high potency, and increasing presence in illicit drug markets. Originally synthesised in the mid-20th century but never approved for clinical use, nitazenes have reappeared since 2019, with an increasing number of structurally diverse analogues being identified worldwide. Their high potency, in some cases exceeding that of fentanyl, together with their occurrence at low concentrations in complex samples, highlights the need for sensitive and selective analytical strategies [1,2]. The SENTINEL project, “Predictive Analysis and Monitoring of Emerging Opioids Derivatives – Nitazenes Analogues”, focuses on the analytical characterisation and monitoring of emerging nitazene opioids. The project combines chromatographic separation, mass spectrometric analysis, structural characterisation, and complementary computational approaches to investigate the chemical properties and analytical behaviour of these compounds. Emphasis is placed on the characterization of mass spectrometric fragmentation patterns and the development and optimization of sensitive and selective methodologies for the detection of nitazenes and newly emerging analogues. This work investigates the characteristic fragmentation patterns of nitazenes using gas chromatography–tandem mass spectrometry (GC–MS/MS), with particular emphasis on the identification of diagnostic product ions and fragmentation pathways associated with different structural features. The resulting fragmentation profiles provide valuable information for compound characterisation and differentiation of structurally related nitazene analogues. By establishing robust analytical strategies for the characterisation and detection of emerging nitazenes, SENTINEL contributes to improving analytical preparedness for the continuous emergence of new synthetic opioids and highlights the role of modern analytical chemistry in the investigation of rapidly evolving chemical threats.

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Targeting Emerging Nitazenes: Development and Validation of a GC-MS/MS Method for Drug Checking Samples

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The global unregulated drug market is increasingly affected by nitazenes, a class of novel synthetic opioids structurally distinct from fentanyl and associated with extreme potency and a high risk of fatal overdoses. Several analogues are reported to be hundreds to thousands of times more potent than morphine or even fentanyl. Nitazenes frequently appear as adulterants or in counterfeit pharmaceuticals, increasing the likelihood of unintentional exposure. Their detection remains analytically challenging, as conventional screening techniques often fails to identify these compounds and their typically low concentrations require highly sensitive instrumentation [1-3]. This work aimed to develop and validate a method for monitoring 22 nitazene analogues in drug checking samples (powders and tablets). The sample preparation consisted of methanol extraction, followed by sonication and filtration before analysis by gas chromatography coupled to tandem mass spectrometry (GC-MS/MS). The analysis was performed in multiple reaction monitoring (MRM) mode, with three transitions per analyte, to ensure adequate selectivity and sensitivity. Additionally, the full scan mode was used to enable the identification of potential adulterants or new unidentified nitazenes. The method achieved efficient chromatographic resolution within 30 minutes, with low detection and quantification limits (< 5 µg/mL), good linearity (r^2 > 0.99) and suitable precision and accuracy (RSD % < 15 % and Bias < 20 %, respectively). Overall, this validated method provides a robust and valuable analytical tool for nitazene detection, strengthening forensic and drug-checking capabilities.

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Identifying the Botanical Origin of Honeys: Single-walled carbon nanotube-based genosensors for the detection of *Erica arborea* in honey samples

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High-value food products are extremely susceptible to fraudulent practices. As the number of reports on food fraud increases, major concerns regarding the quality, safety and authenticity of food ingredients have emerged. Honey, for instance, is a product frequently subjected to adulteration due to its rich nutritional profile, numerous health benefits and its potentially high market price [1]. One of the most common forms of honey fraud involves the mislabeling of its botanical and/or geographical origin, which is especially relevant in terms of honey quality because many of the honey's desirable characteristics are associated with its floral source [2]. Therefore, there is a pressing need for the development of a reliable and efficient analytical tool to verify the botanical origin of honey.

In this study, an electrochemical biosensing platform based on screen-printed carbon electrodes modified with single-walled carbon nanotubes (SWCNT) was developed to detection the genomic DNA of *Erica arborea* – the white heather plant – in commercial honey samples. By examining public genetic databases, a DNA-target probe specific to *E. arborea*, together with its complementary sequence, were selected and designed. The sensing strategy behind this sensor results from the sandwich DNA hybridization reaction between the purified genomic DNA extracted from the commercial honey and its complementary probe. To enable enzymatic amplification and enhance the electrochemical response, the complementary probe was cut in two smaller fragments and functionalized with an amine (NH_2) group and fluorescein isothiocyanate (FITC).

The amplified electrochemical response, measured by chronoamperometry, demonstrated a linear range from 0.01 nM to 1.00 nM. Furthermore, the developed biosensor was successfully employed to identify the residual genomic heather DNA in the commercial honey. These results were then validated by real-time quantitative PCR. Hence, SWCNT-based genosensors are a promising and sensitive analytical strategy for the botanical origin authentication of honey.

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New chemosensor and nano-liquid chromatography for the determination of phenols in environmental waters

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Phenol and its derivatives can be found in the environmental waters due to their use in industrial and agricultural activities and, subsequently, to their incomplete removal of the wastewaters. The toxicity of some phenolic compounds poses a risk to aquatic medium and alert about their potential introduction in food chain. Different analytical strategies for their determination were proposed in which chromatographic methods and colorimetric sensors based on new materials were between the most relevant [1-2]. Here, both techniques were proposed and qualified their potential use in water analysis. A new assay for in place analysis and nano liquid chromatography for lab were presented. Both procedures are developed considering sustainable and green chemistry.

In this work, ten phenols which include bisphenol A, phenol and chloro-, amino-, methyl- phenols were derivatized using 4-aminoantipyrine (4-AAP), a known derivatizing agent. The reaction in basic medium was performed using a 1 mL sample solution yielding a color change to yellow at dark orange. As a novelty, we proposed a chemosensor using this classic reaction inside a porous three-dimensional matrix composed of polydimethylsiloxane (PDMS), tetraethyl orthosilicate (TEOS) and zeolite, like a sponge which retain inside the 4-AAP (Z@TEOS@PDMS@AAP) [3]. For the simultaneous determination of phenolic compounds in multiple samples, the sponge is placed in a multi-walled microplate, 4-AAP reacted in contact with analytes and the change of color was quantified through the SPECTROFREE software application for smartphones. The analytical characteristics of chemosensor were compared to those obtained for the solution derivatization with similar results for the linearity and the limits of detection for two model compounds (phenol and bisphenol A). In order to improve LODs, a previous stage to derivatization using solid phase extraction (SPE) was optimized. When a 100 mL sample volume were processed, an elution volume of 200 µL ethanol was optimized for standards and seawater samples of Valencian coast. Thereby, LODs of phenol and bisphenol A were 10 ng/mL and 20 ng/mL, respectively.

In addition, a chromatographic method using in-tube solid-phase microextraction coupled to nano-liquid chromatography (IT-SPME-nano LC-DAD) was presented. The IT-SPME system for on-line concentration was composed of two valves (a manual injection valve of six ports and an automatic valve of 10 ports with a TEOS-MTEOS capillary). A C18 column and elution gradient (acetonitrile/water) achieved to separate a multicomponent standard with seven phenols (3-aminophenol, resorcinol, phenol, *o,m*-cresol, 2-chlorophenol, 4-chlorophenol) for screening of environmental samples. For a more efficient purification and preconcentration, the samples were treated by a micro-SPE system composed of sorbent immobilized into syringe. Seawater samples collected in “Ría de Arousa” (Galiza, Spain) were analyzed. 2-chlorophenol may be present in nine of eleven samples and 4-chlorophenol in six of them.

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Validación de un método automatizado basado en volumetría potenciométrica para la determinación de la acidez total en vinos

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La determinación de la acidez total constituye un parámetro analítico de relevancia crítica en la evaluación de la calidad de los productos vitivinícolas, dado su impacto sobre las propiedades organolépticas del vino, su estabilidad microbiológica y cumplimiento normativo. En este sentido, el Reglamento 1308/2013 (2013) [1] de la Comisión, establece que el análisis físico químico de los vinos debe incluir, entre otras características, la determinación de la acidez total, así como tener en cuenta los métodos de análisis recomendados y publicados por la Organización Internacional de la Viña y el Vino (OIV).

La OIV define la acidez total del vino como el conjunto de sus ácidos titulables hasta alcanzar un pH de 7 frente a una solución alcalina estándar, omitiendo el CO_2 [2]. Los ácidos orgánicos aportan frescura, estabilidad y, por supuesto, acidez. La forma reglamentaria y más extendida de expresar la acidez total en vinos es en gramos de ácido tartárico por litro de muestra. Según el Reglamento (UE) 1308/2013 (2013) [1], la acidez total en vinos tiene que superar la concentración de 3,5 g/L.

El proceso de validación se diseñó siguiendo las directrices de la norma UNE-EN ISO/IEC 17025 [3] y las recomendaciones de la guía de la OIV-OENO 418-2013 [4]. El método evaluado puso de manifiesto un rendimiento analítico óptimo en todos sus parámetros de desempeño.

- En primer lugar, los ensayos de precisión mostraron una reducida variabilidad tanto en condiciones de repetibilidad como de precisión intermedia, siendo la diferencia máxima entre medidas inferior a los límites estipulados por las directrices de la OIV.
- La exactitud del procedimiento quedó confirmada mediante el análisis de material de control interno y los resultados alcanzados en los ejercicios de intercomparación de BIPEA, en los que se registraron valores de $|Z| \leq 2{,}0$ en la totalidad de las determinaciones, así como mediante el estudio de la recuperación, obteniendo valores de entre un 94% y un 100%.
- En lo referente a la robustez, se confirmó que la metodología mantiene un comportamiento estable y una notable consistencia analítica frente a pequeñas variaciones.
- La comparación directa con la volumetría clásica evidenció una sólida correlación entre ambas técnicas, tanto para muestras de vino comerciales (R^2 = 0,9733), como para muestras de sidras (R^2 = 0,9881). Los resultados obtenidos han demostrado que ambos métodos son estadísticamente comparables ($\alpha \leq 0{,}05$).

El método potenciométrico automatizado aporta la ventaja de eliminar la subjetividad del operador en la apreciación del punto final, aspecto de especial relevancia en matrices con intensa coloración como los vinos tintos. Adicionalmente, el elevado grado de automatización del sistema contribuye a optimizar la capacidad operativa del laboratorio y a reducir el consumo de reactivos. En conclusión, el método potenciométrico constituye una alternativa fiable, eficiente y precisa para su integración inmediata en la rutina analítica de LAFIGA. La totalidad de los datos obtenidos no sólo constatan la competencia técnica del procedimiento, sino que proporcionan la documentación necesaria para su futura acreditación por la Entidad Nacional de Acreditación (ENAC) bajo la norma UNE-EN ISO/IEC 17025.

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Chiral Resolution and Biological Activity of Novel Terpene-Based Cannabinoids

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Cannabinoids, such as nabilone, cannabidiol (CBD), and Δ⁹-tetrahydrocannabinol (Δ^9-THC), have demonstrated significant therapeutic potential for clinically challenging conditions in multiple pathology models [1]. Due to the pharmacological potential of CBD, novel terpene-based CBD analogs were synthesized [2]. The synthetic methods used to prepare these analogs are not enantioselective, resulting in mixtures of enantiomers. As chirality can influence the biological and toxicological properties of bioactive compounds, the individual evaluation of enantiomers is important for understanding their pharmacological profiles [3].

In this work, the chiral resolution of two enantiomeric pairs of synthesized terpene-based CBD (RAC3 and RAC6Ab) was performed by analytical liquid chromatography using an amylose tris(3,5-dimethylphenylcarbamate) column under normal-phase elution with *n*-hexane/ethanol as mobile phase. The chromatographic conditions were successfully scaled up and applied to achieve preparative separation and collect highly pure enantiomeric fractions, achieving enantiomeric ratios higher than 99%.

Four enantiomerically pure terpene-based CBD were evaluated for their antitumor effects on the human breast cancer cell line MDA-MB-231, a highly aggressive and invasive triple-negative breast cancer (TNBC) cell line, through a resazurin assay. MDA-MB-231 cells were treated with compounds for 48 hours, and their half-maximal inhibitory concentration (IC_{50}) was then determined. Results demonstrated enantioselectivity between the two RAC3 enantiomers in inhibiting the metabolic activity of MDA-MB-231 cells (IC_{50} = 46.57 μM for RAC3 1(+) and IC_{50} = 27.28 μM for RAC3 2(-). On the other hand, both RAC6Ab enantiomers showed only modest differences in their ability to inhibit MDA-MB-231 metabolic activity, with IC_{50} = 48.86 μM for RAC6Ab 1(+) and IC_{50} = 45.90 μM for RAC6Ab 2(-). These results indicate that RAC3 2(-) exhibited the strongest antitumor potential against MDA-MB-231 cells.

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Optimización de separaciones por HPLC mediante diseños experimentales Box–Behnken y Doehlert

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La optimización de procesos de separación mediante cromatografía líquida de alta resolución (HPLC) constituye un problema complejo debido a la influencia simultánea de múltiples variables experimentales. En este contexto, el diseño de experimentos (DOE) permite estudiar el efecto de los factores de control sobre las respuestas de interés, reduciendo el número de experimentos necesarios frente a los procedimientos convencionales de optimización [1].

En este trabajo se estudia la aplicación y comparación de dos diseños experimentales de superficie de respuesta, Box–Behnken y Doehlert [2], para la optimización de la separación mediante HPLC de cinco β-bloqueantes: acebutolol, atenolol, labetalol, nadolol y propranolol, en forma de principio activo. La separación se llevó a cabo mediante HPLC, al que se encontraba acoplado un detector de diodos en serie (PDA). Para ambos diseños se estudiaron como variables de control el pH, el caudal de la fase móvil y el contenido de modificador orgánico (acetonitrilo) de la fase móvil. Como respuestas cromatográficas se consideraron el mayor tiempo de retención de los cinco analitos y la menor resolución entre picos del cromatograma.

A partir de los resultados experimentales obtenidos para cada diseño, se desarrollaron modelos matemáticos que permitieron establecer la relación entre las variables de control y las respuestas cromatográficas. El análisis estadístico y la optimización de los modelos se efectuaron mediante el programa *Stat-Ease,* estableciendo como objetivo la maximización de la resolución cromatográfica y la minimización del tiempo de retención. Las condiciones óptimas de separación obtenidas fueron pH 4.6, 33 % de acetonitrilo (ACN) y un caudal de 0.922 mL/min para el diseño Box–Behnken, mientras que para el diseño Doehlert se obtuvieron un pH de 6.385, un 40.4 % de ACN y un caudal de 0.906 mL/min.

La comparación de las predicciones obtenidas mostró que el diseño Box–Behnken alcanzó una mayor resolución mínima, mientras que el diseño Doehlert presentó un menor tiempo de retención máximo. Estos resultados ponen de manifiesto las diferencias entre ambos diseños en la optimización de las respuestas cromatográficas.

Agradecimientos

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Diseño Y Optimización De Un Método De Preconcentración De Etinilestradiol Y Estriol Mediante Microextracción Líquido-Líquido Dispersiva Asistida Por Ultrasonidos (UA-DLLME) Para Su Análisis Por Fluorimetría

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Los estrógenos etinilestradiol y estriol juegan un papel relevante tanto en la salud humana, ya que son muy importantes en fisiología humana, como en el medioambiente, puesto que son considerados contaminantes y no se pueden eliminar en plantas de tratamiento de aguas [1].

En este trabajo se ha desarrollado un método de cuantificación de estas hormonas aplicando la variante de la microextracción líquido-líquido dispersiva asistida por ultrasonidos (UA-DLLME) para preconcentrar y/o separar los analitos. La metodología diseñada supone una ventaja frente a la DLLME convencional, puesto que elimina el uso del disolvente dispersante, característico de este tipo de microextracción, haciéndolo más respetuoso con el medio ambiente [2]. Se trata de una metodología interesante para estos analitos, dado que no se han encontrado referencias previas que apliquen de forma simultánea la UA-DLLME y la fluorescencia para el análisis de estrógenos.

Para la detección de las hormonas en los extractos se empleó la fluorimetría, que permite obtener información cuantitativa con una sensibilidad muy elevada. Con el objetivo de caracterizar fluorimétricamente las hormonas, se efectuó una serie de estudios preliminares, incluyendo, entre ellos, la emisión de ambas hormonas en los diferentes disolventes orgánicos que se utilizarían para la extracción posteriormente. Para aumentar la eficacia del método, se optimizaron las variables que lo afectan, como el pH, la concentración de sales, el tiempo y frecuencia de sonicación y el tiempo de centrifugación, para cada hormona, probando con dos disolventes: el acetato de n-butilo y el octanol.

Se aplicó el método optimizado a formulaciones farmacéuticas de ambas hormonas encontrando resultados positivos para uno de ellos. Finalmente, se compararon los LOD y LOQ obtenidos para ambas hormonas y los mejores disolventes, obteniéndose métodos altamente sensibles.

Agradecimientos

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Determinação simultânea de amoxicilina e ácido clavulânico em formulações farmacêuticas usando pontos quânticos de $AgInS_2$ e quimiometria

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A deteção multiplexada, na qual se avaliam simultaneamente múltiplos analitos no mesmo ensaio, ou a deteção múltipla de um único analito numa matriz de amostras complexa repleta de espécies interferentes, tem despertado, nos últimos anos, interesse na comunidade analítica [1]. Para além disso, as respostas de fotoluminescência (PL) podem ser processadas por modelos quimiométricos adequados, permitindo extrair informações analíticas que possibilitam a deteção precisa e seletiva de múltiplos alvos numa única análise de amostra [2].

Devido ao uso clínico generalizado da sua formulação combinada, a determinação simultânea e exata de amoxicilina (AMX) e ácido clavulânico (CLA) em formulações farmacêuticas é essencial, o que exige o desenvolvimento de metodologias analíticas simples, rápidas, económicas e fiáveis. Neste trabalho, desenvolveu-se um método espetrofluorométrico inovador para a determinação simultânea de AMX e CLA em formulações farmacêuticas, baseado numa deteção multiplexada, utilizando pontos quânticos de $AgInS_2$ passivados com ácido mercaptopropiónico (MPA-$AgInS_2$ QDs) como sondas de PL, combinados com análise quimiométrica.

Sintetizaram-se e avaliaram-se vários QDs para alcançar a máxima sensibilidade para ambos os analitos, tendo sido observados diferentes mecanismos de interação para cada um deles. Aplicou-se um planeamento experimental fatorial completo para garantir resultados robustos e avaliar os efeitos principais e as interações entre os dois analitos. Os dados cinéticos de fluorescência adquiridos foram modelados pelo método *unfolded partial least squares* (U-PLS). A otimização dos modelos U-PLS envolveu o estudo de diferentes regiões espetrais, revelando que a utilização da região espetral completa permitiu obter os melhores resultados, com exatidões de 2% para a AMX e de 11% para o CLA, em termos de erro relativo de previsão (REP).

Este método foi comparado com o método cromatográfico oficial da USP, não se tendo observado diferenças estatisticamente significativas, o que valida a exatidão e a fiabilidade do método desenvolvido. Esta metodologia analítica, simples, rápida e económica, pode servir como alternativa valiosa ao método cromatográfico oficial, eliminando a necessidade de solventes tóxicos.

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Sondas fluorescentes combinadas de pontos quânticos e análise quimiométrica para a determinação cinética de cloranfenicol em formulações farmacêuticas

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A combinação de nanomateriais fluorescentes com diferentes características de emissão permite desenvolver sondas de emissão dupla para a determinação de princípios ativos em formulações farmacêuticas. A análise da informação cinética de fotoluminescência (PL) com métodos quimiométricos poderá melhorar a capacidade analítica destas plataformas, permitindo explorar padrões de resposta que não são acessíveis através de medições convencionais num único instante [1,2].

Neste trabalho, desenvolveu-se uma plataforma de deteção por PL de emissão dupla, combinando pontos quânticos de carbono (CDs) e pontos quânticos ternários de $AgInS_2$ (AIS QDs) funcionalizados com ácido mercaptopropiónico (MPA), para a determinação quantitativa de cloranfenicol, recorrendo a métodos quimiométricos na análise de dados. Inicialmente, sintetizaram-se e avaliaram-se individualmente pontos quânticos de diferentes naturezas, tais como CDs, CdTe QDs e AIS QDs. Foram avaliadas a sua fotoestabilidade, a resposta de PL na presença do analito, bem como a evolução temporal da interação com o antibiótico (cinética). Posteriormente, foram desenvolvidas e comparadas duas sondas de emissão dupla, CDs/MPA-CdTe e CDs/MPA-$AgInS_2$, selecionadas com base nas características de emissão dos respetivos componentes. Os dados cinéticos de PL foram tratados pelo método *unfolded partial least squares* (U-PLS), explorando a informação multidimensional dos espectros adquiridos ao longo do tempo. A sonda CDs/MPA-$AgInS_2$ apresentou o melhor desempenho global, considerando o compromisso entre sensibilidade, fotoestabilidade e biocompatibilidade, uma vez que não contém cádmio. A otimização dos modelos U-PLS envolveu a avaliação do tempo de aquisição cinética e de diferentes regiões espetrais. Os resultados demonstraram que a quantificação pode ser realizada nos primeiros 5 minutos de interação, utilizando o espectro de emissão completo da sonda. Adicionalmente, observaram-se diferentes mecanismos de interação para cada nanomaterial na sonda combinada: estático para a interação CDs/cloranfenicol e dinâmico para a interação MPA-$AgInS_2$/cloranfenicol. Esta complementaridade de resposta contribui para a discriminação da informação analítica através da abordagem quimiométrica.

A metodologia proposta foi aplicada com sucesso à determinação de cloranfenicol em formulações farmacêuticas comerciais, apresentando resultados exatos e figuras de mérito analítico favoráveis. Esta abordagem constitui uma alternativa promissora para a quantificação rápida de cloranfenicol, combinando sondas fluorescentes de emissão dupla, informação cinética e análise quimiométrica, com potencial para o desenvolvimento de metodologias analíticas mais sustentáveis.

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Sensor Raciométrico Baseado em Membranas Molecularmente Impressas para a Deteção no Local do CA 19-9

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Este trabalho visa desenvolver um biossensor para a deteção do antigénio carboidrato 19-9 (CA 19-9), um biomarcador utilizado no acompanhamento clínico de doentes com cancro do pâncreas, cujos níveis séricos podem estar elevados (>37 U/mL) [1]. Apesar das suas propriedades óticas favoráveis, incluindo elevada fluorescência, estabilidade química e sensibilidade, os pontos quânticos (QDs) utilizados como sondas fluorescentes podem apresentar limitações associadas à monitorização de uma única emissão, tornando as medições suscetíveis a interferências e variações nas condições de leitura [1, 2].

Para minimizar estas limitações, foi desenvolvido um sensor de emissão dupla baseado na imobilização, numa membrana de poliamina, de pontos quânticos de CdTe com emissão amarela (y-QDs), funcionalizados com polímeros de impressão molecular, e de pontos de carbono com emissão azul (b-CDs). Os y-QDs atuam como sondas sensíveis ao CA 19-9 [2], enquanto os b-CDs atuam como referência interna [3]. A ligação do biomarcador às cavidades de reconhecimento molecular dos polímeros de impressão induz a inibição seletiva da fluorescência dos y-QDs, enquanto a emissão dos b-CDs permanece essencialmente inalterada. A alteração relativa entre as duas emissões origina uma mudança de cor visível de amarelo/verde para azul, permitindo a deteção ratiométrica do biomarcador.

O sensor permitiu quantificar o CA 19-9 num intervalo linear de 4–400 U mL^{-1}, com um limite de deteção de 0,056 U mL^{-1} em amostras de soro diluídas 100 vezes. O sistema apresentou ainda boa seletividade e estabilidade fotoquímica a curto prazo, demonstrando potencial para o desenvolvimento de plataformas fluorescentes de deteção ratiométrica de biomarcadores.

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Towards Online CO_2 Monitoring in Power Transformers: Evaluation of NDIR Sensors Detection in Spiked Oil Samples

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Dissolved gas analysis (DGA) is a method used to diagnose the condition of power transformers by analyzing the type and concentration of gases dissolved in the transformer oil and correlating this information with potential defects. This is currently used to detect early faults and avoid costly operations and prolonged maintenance work. DGA in transformer oil is usually analyzed using detection techniques such as gas chromatography (GC), in accordance with the ASTM 3612 standard [1]. This provides analysis with very high accuracy and repeatability. However, these methods require manual *in-situ* sampling and have the disadvantage of having to be performed in a laboratory environment, given the complexity of the equipment [2].

In this work, two NDIR sensors were used: a Non-Dispersive Infrared (NDIR) pyroelectric detector (PyrIQ Evaluation KIT, InfraTec) with a 3D-printed gas sample chamber and a printed circuit board (PCB) with a commercial NDIR (INIR2-CD5) sensor. A GC-BID (gas chromatography coupled with dielectric barrier discharge detector) was used to monitor the performance of the sensors. The experimental procedure was developed and conducted with the aim of preparing transformer oil samples with a concentration range of 0 – 20000 ppm of dissolved CO_2 using different bubbling times (0, 1, 2, 4, 8 min). For this purpose, 100% CO_2 was dissolved into the transformer oil using a CO_2-filled balloon with a syringe attached and with its tip placed into the oil.

The samples of transformer oil were analysed by GC-BID: a blank oil sample and a spiked sample with the oil bubbling, using the setup shown in **Fig. 1a**. The analysed samples were the headspace of the transformer oil that, when heated, released the dissolved CO_2. This analysis proved that the method was functional and controllable (concentrations in the range 0 – 20000 ppm of CO_2 were measured), as only the spiked sample had a CO_2 peak in the chromatogram (**Fig. 1b**). The same method was used with the NDIR sensor integrated in the PCB (**Fig. 1c**) and compared with the NDIR pyroelectric sensor, obtaining a coefficient of variation (CV) of 7.7%. In future experiments, this method can be expanded to CO, CH_4, and H_2 and validated with the GC-BID.

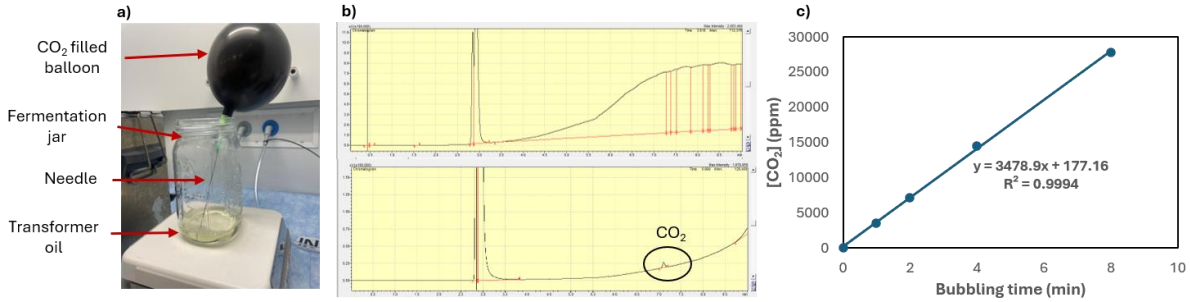


Fig.1. a) Setup for the transformer oil bubbling of 100% CO_2 with a balloon and a syringe; **b)** GC-BID chromatogram, blank oil sample (top), spiked oil sample (bottom); **c)** CO_2 DGA analysis calibration curve with INIR2-CD5 sensor.

Acknowledgements

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Gas sensors characterization for dissolved gas analysis of power transformer oil

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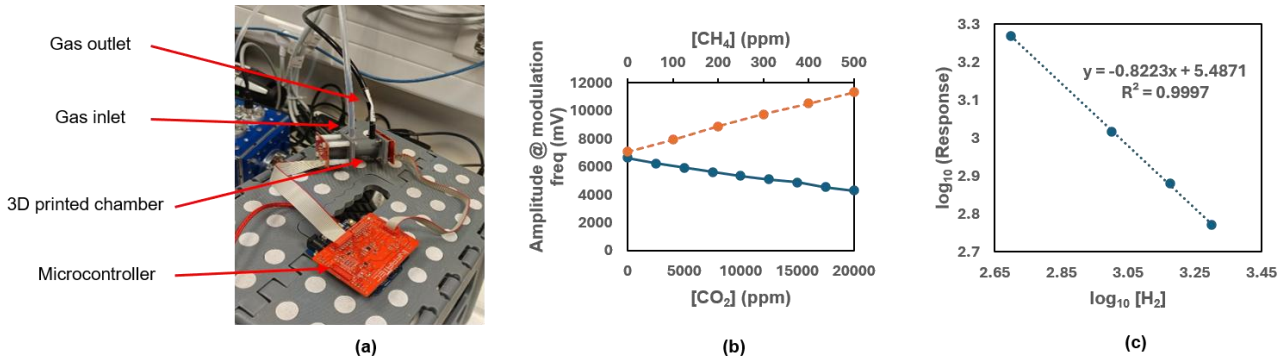
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Dissolved gas analysis (DGA) diagnoses power transformer faults by correlating dissolved gases concentration, like CO_2, CH_4, H_2 and other hydrocarbons, with overheating, arcing, and partial discharge malfunctions. Conventional techniques, such as gas chromatography (GC), are accurate and repeatable but require manual sampling and complex laboratory equipment, limiting on-site monitoring [1].

Non-dispersive infrared (NDIR) sensors detect gases through characteristic IR absorption and are widely used for CO_2, CO, and CH_4, but cannot directly detect H_2 due to its lack of IR absorption [2]. This work presents an NDIR system comprising an IR source, a 3D-printed gas chamber, and a lithium tantalate ($LiTaO_3$) pyroelectric detector with a multi bandpass filters. Gas concentrations are determined through IR attenuation (experimental setup shown in Fig. 1). The sensor was characterized up to 50,000 ppm of CO_2 and 500 ppm CH_4, achieving R^2 values of 0.9954 for CO_2 within the ATE project's target range (up to 20,000 ppm) and 0.9985 for CH_4, respectively.

A second set of CO_2 (also NDIR-based), CO, and H_2 sensors (Metal Oxide-based in both cases) was characterized in a 15.24 × 15.24 × 15.24 cm^3 chamber with controlled gas delivery via a mass flow controller (MFC) (Fig. 1). The MQ-7 (CO), INIR2-CD5 (CO_2), and SB-19-00 (H_2) sensors were integrated into a PCB for further flask-lid installation. The CO_2 reached 50,000 ppm with R^2 = 0.997 (within the target range of 20,000 ppm), while the CO and H_2 reached 2,000 ppm with R^2 values of 0.9703 and 0.9997, respectively.

Fig.1. ***(a)*** Components of the IR sensor setup. ***(b)*** CO_2 (solid line) and CH_4 (dotted line) NDIR sensor calibration curves. ***(c)*** H_2 Metal Oxide sensor calibration curve.



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Análisis de componentes principales (PCA) del perfil de hidrocarburos y su aplicación en la caracterización de diésel

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El objetivo de este trabajo fue caracterizar muestras de diésel a partir del perfil de hidrocarburos saturados de la fase líquida del combustible y el análisis de componentes principales (PCA). Para ello, las condiciones cromatográficas se configuraron para realizar una determinación rápida de hidrocarburos (25 min) por cromatografía de gases acoplada a espectrometría de masas (GC-MS). La separación de los analitos se realizó en una columna DB-5ms (30 m, 0.25 mm de diámetro interno y 0.25 µm de fase), identificando los hidrocarburos saturados de la serie homóloga, del decano al eicosano (C_{10}-C_{20}); las áreas cromatográficas de cada hidrocarburo identificado se utilizaron como variables de entrada para el PCA. El muestreo consistió en 19 muestras de diésel, obtenidas en estaciones de servicio de cuatro marcas en México: OXXO, Petro 7, PEMEX y Mobil. Cada muestra se diluyó al 5 % en metanol y se analizó por GC-MS. Los resultados mostraron que las cuatro marcas de diésel presentaron un perfil de hidrocarburos similar, sin embargo, el análisis por PCA evidenció que tres marcas de diésel presentaron similitudes en cuanto a las cargas (loadings) de hidrocarburos, mientras que la cuarta mostró diferencias respecto a las demás. La marca de diésel diferente mostró una puntuación diferenciada (score), y una mayor respuesta cromatográfica de hidrocarburos pesados a partir de hexadecano (nC_{16}), lo cual se corroboró en los cromatogramas. Esta propuesta analítica demostró viabilidad para caracterizar el tipo de diésel e identificar las similitudes entre marcas de combustible, exclusivamente analizando la respuesta analítica de los hidrocarburos mayoritarios en la fase líquida. Esta contribución metodológica representa una herramienta cualitativa complementaria al control de calidad del combustible, que puede utilizarse para mapear la composición química del diésel o del fraccionamiento del petróleo.

Agradecimientos

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QUÍMICA FÍSICA

Estudo microcalorimétrico do crescimento de *Pediococcus acidilactici* em meio de cultura enriquecido

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O *Pediococcus acidilactici* é uma bactéria láctica Gram-positiva utilizada na fermentação de alimentos. As culturas bacterianas produzem energia como resultado do metabolismo bacteriano. A taxa de produção de calor é uma medida adequada da atividade metabólica dos organismos e dos seus componentes. Embora o calor produzido pelas bactérias seja muito pequeno, a sua reprodução exponencial num meio de cultura permite a deteção de calor através de microcalorimetria. Neste estudo, analisámos o comportamento microcalorimétrico de *Pediococcus acidilactici* utilizando um microcalorímetro Calvet [1], técnica descrita em trabalhos anteriores [2,3]. As estirpes bacterianas utilizadas foram isoladas a partir de trigo Tocayo spp. cultivado em condições ecológicas em Cuenca (Espanha) e posteriormente caracterizado em termos de atividade probiótica, resistência a antibióticos, atividade enzimática, produção de EPS, capacidade antioxidante e agregação a IEB. Como meio de cultura, utilizamos caldo de soja e caseína digerido com CO_2, que é o meio de cultura mais utilizado na prática clínica hospitalar. O calorímetro contém duas células de aço inoxidável (experimental e de referência). O microcalorímetro de Calvet está ligado a um sistema de aquisição de dados através de uma interface remota [4]. As medições são realizadas com um microvoltímetro ligado a um microcontrolador ESP32, que transmite os dados para um servidor remoto utilizando o protocolo MQTT. As experiências foram conduzidas com concentrações finais de 10^7 UFC/mL e uma temperatura constante de 298,15 e 310,15 K foi mantida dentro do microcalorímetro. Registando a diferença de potencial térmico ao longo do tempo, foram obtidas curvas de crescimento de *Pediococcus acidilactici.*

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From Pyrazines to Bipyridines: Structural and Spectral Parallels Across Leflunomide Multicomponent Assemblies

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Among the various drug delivery routes, the oral pathway remains the most widely utilised. However, many active pharmaceutical ingredients exhibit poor aqueous solubility, which severely limits their oral bioavailability and therapeutic efficacy [1]. Crystal engineering offers a promising strategy to address these limitations. Multicomponent systems, structures composed of two or more molecular species that interact through noncovalent bonds in a defined stoichiometric ratio, have attracted significant interest, as they may possess distinct physicochemical properties relative to the starting materials, while preserving the therapeutic effect of the drug [2].

Leflunomide (LEF), Figure 1, is a poorly water-soluble disease-modifying antirheumatic drug used in the treatment of rheumatoid arthritis [3]. Following previous observations of molecular interactions between LEF and pyrazine derivatives, this study investigated the formation of multicomponent systems between LEF and four bipyridine-based compounds, specifically 2,2-bipyridyl (22B), 4,4-bipyridyl (44B), 1,2-bis(4-pyridyl)ethane (BPA) and E-1,2-di(4-pyridyl)ethylene (BPE), Figure 1 (b).

Three multicomponent systems with nominal LEF molar ratios of 2:1 were obtained by mechanochemical grinding using 44B, BPA and BPE. Subsequent solution crystallisation of the ground mixtures led to the formation of an additional system with 22B and a further crystalline phase involving LEF and 44B. All solid phases were characterised by X-ray powder diffraction and Fourier-transform infrared spectroscopy. The similarities between the infrared spectra of these systems and those of previously reported LEF-pyrazine systems are consistent with similar hydrogen-bonding environments and potentially comparable supramolecular arrangements.

The crystal structure of LEF-44B (2:1) system obtained by solution crystallisation was determined by single-crystal X-ray diffraction. Interestingly, this crystalline phase was only obtained when crystallisation was performed using a 1:2 molar ratio mixture of LEF:44B, whereas using a mixture with a 2:1 molar ratio yielded only a physical mixture.

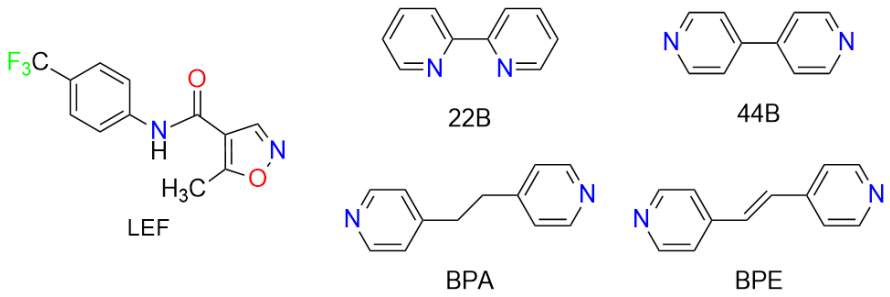


Fig. 1. Molecular structure of leflunomide (LEF), 2,2-bipyridyl (22B), 4,4-bipyridyl (44B), 1,2-bis(4-pyridyl)ethane (BPA) and E-1,2-di(4-pyridyl)ethylene (BPE).

Acknowledgments

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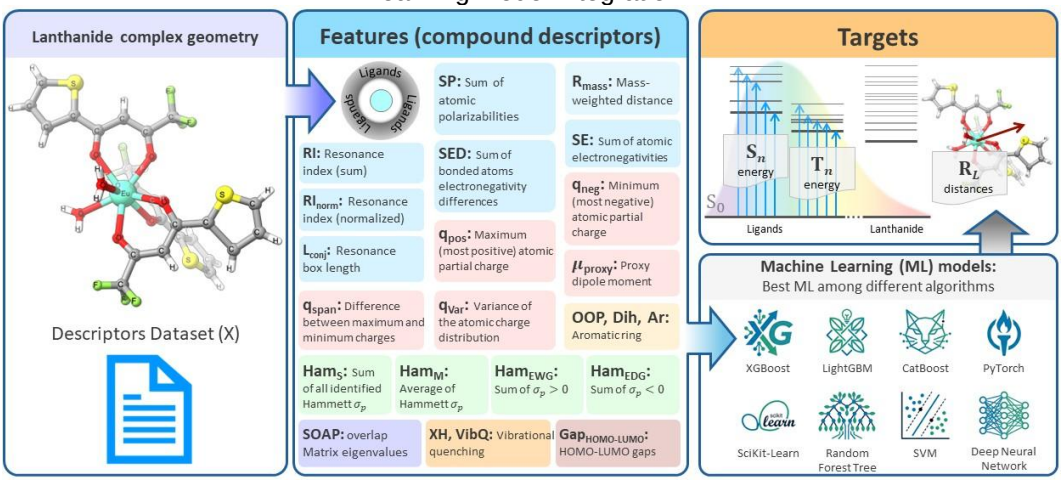
JoyAI: A machine learning approach for predictions of ligand excitation energies in lanthanide-based complexes

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Modeling lanthanide luminescence requires the determination of non-radiative energy transfer rates between organic ligands and the central lanthanide ion [1]. Within the JOYSpectra web platform (http://www.joyspectra.com.br or http://www.joyspectra.eu) [2], this theoretical framework relies on accurate singlet (S_1) and triplet (T_1) excitation energies. Although Density Functional Theory (DFT) can provide reliable excitation energies, its high computational cost limits its applicability to large-scale screening. To overcome this limitation, JoyAI, a graph-based artificial intelligence tool (Fig. 1), was developed and integrated into the test version of JOYSpectra to rapidly predict these energies. In the present study, we systematically benchmark the performance of the JoyAI module when coupled with geometries obtained from fast computational methods. The evaluation protocol involved re-optimizing the geometries of the coordination compounds in the JoyAI training dataset using the GFN2-xTB method. The resulting geometries were subsequently used as inputs to JoyAI to predict S_1 and T_1 excitation energies, which were evaluated against reference values obtained at the M06/def2-TZVP DFT level. The deviations between the JoyAI predictions based on semiempirical geometries and the DFT reference values were generally within 5–10%. This level of accuracy is compatible with the energy ranges required for modeling energy-transfer processes in lanthanide complexes.

Fig.1. Schematic representation of the JoyAI architecture, highlighting descriptor extraction and machine learning model integration.



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A route to zinc(II) helical complexes from *bis*hydrazones

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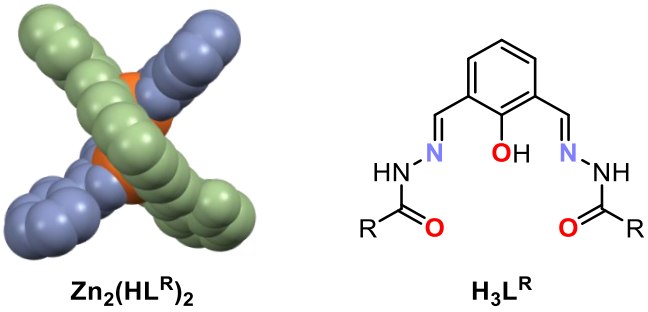
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Designing artificial helical complexes from biologically involved-metal ions is a major goal of Metallosupramolecular Chemistry.[1] In this context, dinuclear zinc(II) helicates, derived from ligands such as thiosemicarbazones and hydrazones, are of significant interest for their potential biological applications.[2],[3] These include the induction of cytotoxic activity against cancer cells and the design of new metallodrugs acting by DNA intercalation mechanisms. In addition, these artificial metallostructures demonstrated to possess technological potential, including luminescent emission, chiral detection, and the design of stimulus-responsive materials through reversible structural interconversions.[4]

Herein, we report the electrochemical synthesis and structural characterization of two new dinuclear zinc(II) helical complexes, $[Zn_2(HL^R)]_2$, derived from two *bis*hydrazone ligands.



$Zn_2(HL^R)_2$ H_3L^R

Fig.1. Zinc(II) helical complexes (left) derived from *bis*hydrazone ligands (right).

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Gold(I)-NHC Complexes Derived from Uracil and Cytosine

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Gold-based compounds have attracted considerable interest in medicinal chemistry due to their promising anticancer properties. In particular gold(I) N-heterocyclic carbene complexes have been investigated for their ability to interfere with cellular redox homeostasis, including through inhibition of thioredoxin reductase (TrxR), leading to oxidative stress and cell death [1]. More recently, gold complexes have also emerged as promising candidates for the induction of immunogenic cell death (ICD). Notably, a rationally designed redox-active Au(I) N-heterocyclic carbene (NHC) complex was shown to induce characteristic ICD biomarkers, including calreticulin exposure, ATP secretion and HMGB1 release [2], providing a potential link between direct cytotoxicity and stimulation of antitumor immune responses [3, 4].

Nucleobases represent attractive scaffolds for the development of bioactive compounds, as demonstrated by the widespread use of nucleobase and nucleoside analogues in anticancer and antiviral therapy [5]. Their structural versatility and biological relevance also make them valuable scaffolds for the design of metal-based compounds with potential therapeutic applications. In this context, we have developed a series of gold(I)–N-heterocyclic carbene (NHC) complexes based on uracil and cytosine, aiming for their biological application.

We functionalized uracil and cytosine with imidazole derivatives to prepare NHC precursors with different substituents, thereby tuning the steric and electronic properties of the resulting complexes. In this communication we will discuss the synthesis and the characterization of the corresponding gold complexes.

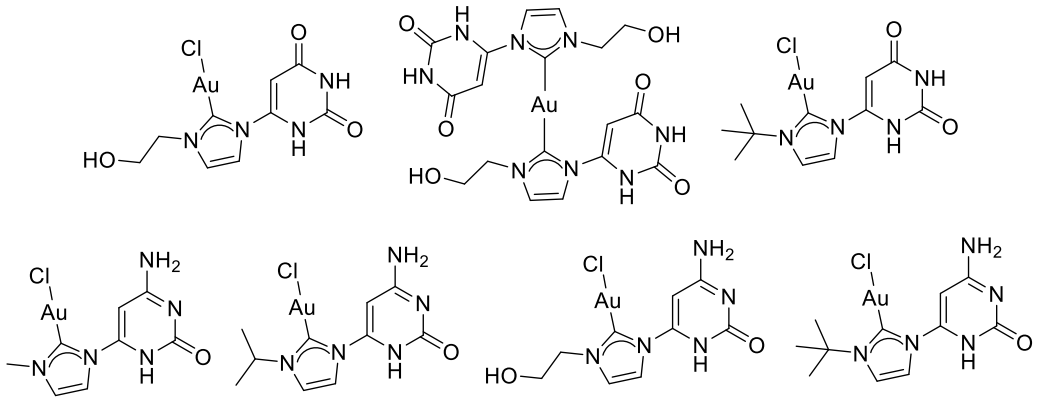


Fig.1. Synthesized gold(I)-complexes based on uracil and cytosine.

Agradecimientos
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Study and comparison of the stability of two iminophosphorane ligands: carborane versus organic

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The compounds known as thiosemicarbazones (TSCs) constitute a highly versatile and promising class of ligands in coordination chemistry. They are of great pharmacological interest due to their diverse biological properties, including antiparasitic, antifungal, antiviral, antibacterial, and antitumor activities, among others [1,2]. Consequently, they currently form part of numerous biologically active compounds [3].

Despite the wide variety of studied TSC derivatives, no examples of thiosemicarbazone derivatives containing either a carborane or an iminophosphorane group in any position have been reported in the literature, notwithstanding the compelling potential pharmacological applications these could offer.

Taking this into account, this communication presents the first example of a potential thiosemicarbazone ligand functionalized with both before mentioned groups, carborane and iminophosphorane (Figure 1), along with the study of its stability compared to its purely organic analog.

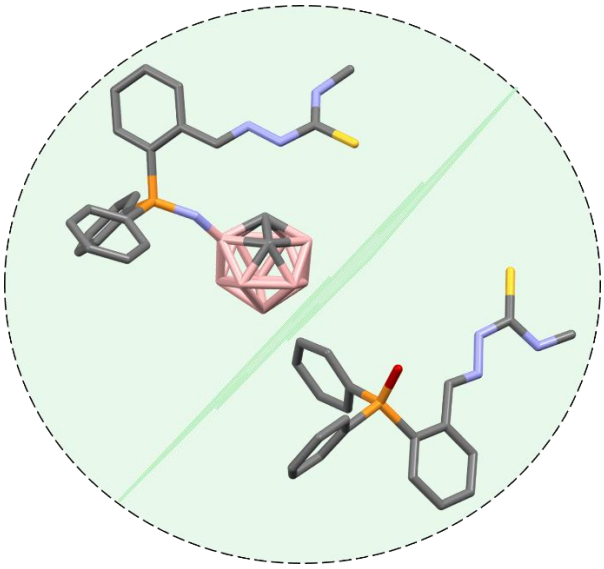


Fig.1. The two fragments compared in this contribution.

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Modulating Defect States in Real-Sized Lanthanide-Doped Nanoparticles

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Surface defect states act as energy reservoirs that significantly influence upconversion luminescence in rare-earth-doped nanoparticles [1]. Since lanthanide incorporation inherently favors vacancy formation [2], characterizing these states is crucial to understanding energy-transfer and multiphonon relaxation processes. In this ongoing project, we investigate real-sized β-$NaYF_4$ core-shell nanoparticles doped with the Yb^{3+}/Er^{3+} pair and their underlying energy transfer mechanics (Figure 1). We are developing a theoretical methodology to map specific multi-charge vacancy states intrinsic to the fluoride matrix (e.g., V_F, V_Y). Calculations are performed using Density Functional Theory (GGA-PBE+U) to accurately describe the highly correlated 4f electrons. By integrating these defect formation energies with computational models of real-sized core-shell geometries, we aim to extract Ln^{3+}-Ln^{3+} distance distributions and modified energy transfer rates. This developing framework seeks to predict how native vacancy charge states trap migrating energy (Figure 1), providing robust predictions to optimize lanthanide-doped nanomaterials for photonics and bioimaging.

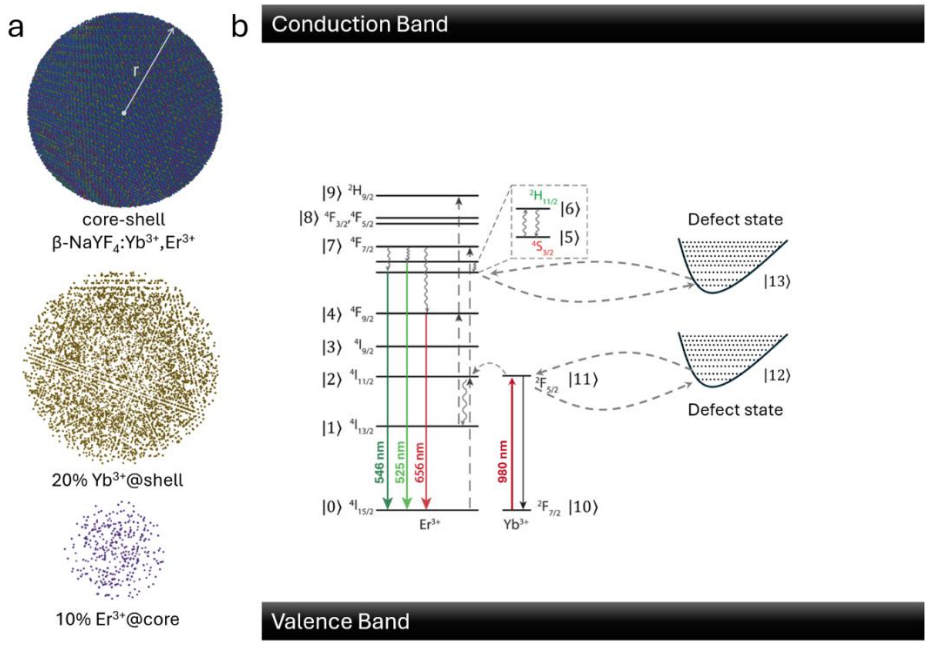


Figure 1. (a) Computational structural model of a β-$NaYF_4$ core-shell nanoparticle, detailing the complete geometry alongside the isolated 20% Yb^{3+} doped shell and the 10% Er^{3+} doped core. (b) Energy level diagram illustrating the 980 nm upconversion mechanism for the Yb^{3+}/Er^{3+} pair, highlighting the proposed two-way energy transfer dynamics between the lanthanide 4f states and localized intrinsic defect states (|12⟩, |13⟩) acting as energy reservoirs within the host bandgap.

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Machine learning applied to the magneto-optical properties of lanthanide metal complexes

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Lanthanide coordination compounds are promising candidates for molecular information storage, spintronics, and multifunctional devices [1]. However, establishing reliable magneto-structural correlations remains challenging due to their complex electronic structures, strong magnetic anisotropy, and extreme sensitivity to local coordination environments [2].

Here, we will apply machine learning approaches (ML, e.g., XGBoost, Artificial Neural Networks) to predict the magnetic properties of Dy^{3+}-based single-molecule magnets (SMMs). A comprehensive database of published crystal structures and experimental magnetic data will be constructed to train and validate these predictive models [3]. By extracting selected structural and coordination-environment descriptors, we expect to identify key magneto-structural correlations, targeting the effective energy barrier for magnetization reversal (U_{eff}) and the blocking temperature (T_B) as the primary predictive variables (Figure 1).

These models will be integrated into the JOYSpectra platform (http://www.joyspectra.eu). Users can directly upload crystal structures to automatically extract relevant molecular descriptors and generate rapid magnetic property predictions (Figure 1). This automated approach facilitates magneto-structural analysis and accelerates the rational design of new lanthanide-based materials, with future expansions targeting the prediction of optical properties for multifunctional molecular systems.

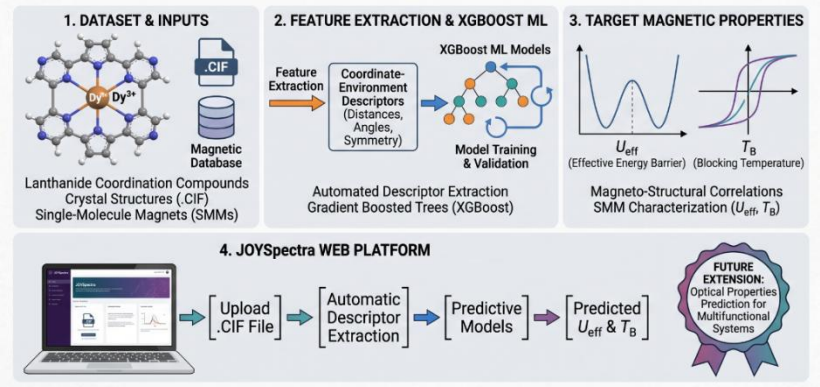


Figure 1. Workflow of the ML architecture for predicting magneto-optical properties in lanthanide complexes. Crystallographic data (CIFs) are processed to extract coordination-environment descriptors, which feed XGBoost models to predict key Single-Molecule Magnet (SMM) parameters (U_{eff}, T_B). The predictive ML model will be integrated into the JOYSpectra platform for automated magneto-structural analysis and rational material design.

Acknowledgements
A.N.C.N. acknowledges support from the Ramón y Cajal programme RYC2024-048927-I, funded by MICIU/AEI/10.13039/501100011033 and the European Union ESF+. This work was also supported by project INCT-LumiNanoTec (CNPq, Brazil) under Grant No. 408501/2024-3. J.C.V thanks Xunta de Galicia for his postdoctoral fellowship (ED481D-2025/006).

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Machine Learning-Driven Prediction of Judd-Ofelt Parameters and Hypersensitive Ratios in Europium(III) Complexes

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The luminescent performance of Europium(III) coordination compounds is heavily governed by the structural symmetry and electronic nature of the local coordination environment. The hypersensitivity ratio (*R2*) (historically termed the asymmetry ratio) and Judd-Ofelt intensity parameters serve as critical metrics for mapping 4f-4f transitions and rationalizing these photophysical properties [1].

In this work, we developed a comprehensive dataset by extracting Judd-Ofelt parameters and experimental *R2* ratios from a diverse library of emission spectra. Because the dynamic coupling mechanism governing hypersensitive transitions is highly dependent on the polarizability of the surrounding ligands [1], Density Functional Theory (DFT) calculations will be performed to compute localized ligand polarizabilities (α). These DFT-derived polarizabilities were subsequently fitted to the experimental *R2* values and integrated into the dataset alongside precise crystallographic structural features for each complex.

Building upon this structural and electronic dataset, the next step is the application of advanced machine learning architectures, including XGBoost, artificial neural networks, and graph-based models, to model the photophysical behavior of the target complexes. These predictive algorithms are capable to map the complex, non-linear relationships between the structural and polarizability inputs and the resulting *R2* and Judd-Ofelt parameters. The result of this computational pipeline aims to provide a robust, data-driven framework for anticipating the emission intensities of lanthanide complexes directly from structural features, which will be further incorporated in the JOYSpectra web platform (http://www.joyspectra.eu), accelerating the rational design of novel luminescent materials.

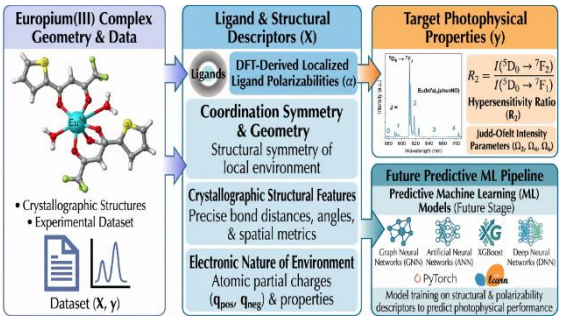


Figure 1. Schematic workflow for predicting Europium(III) photophysical properties. Crystallographic data (left) are parameterized into structural and electronic descriptors, including DFT-derived ligand polarizabilities and coordination symmetry (center). These descriptors will feed future machine learning algorithms (bottom right) to directly predict target luminescent properties (top right), specifically the R2 and Ω_λ.

Acknowledgements

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QUÍMICA ORGÁNICA

Synthesis, Characterization And In Vitro Dissolution Testing Of A Dihydropyrimidinone Obtained Via The Biginelli Multicomponent Reaction

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The low aqueous dissolution of the dihydropyrimidinone DHPM-S limits its performance in aqueous media. This study aimed to investigate the interaction between DHPM-S and β-cyclodextrin (β-CD) using ^{1}H NMR to evaluate the effect of complexation at molar ratios of 1:1 and 1:2 on the in vitro dissolution profile. The inclusion complexes were prepared by lyophilization and characterized by ^{1}H NMR spectroscopy using a 400 MHz spectrometer in DMSO-d_6. Dissolution tests were performed using samples equivalent to 6.0 mg of DHPM-S in 10 mL of ultrapure water, under stirring in a water bath at 37 ± 0.2 °C for 480 min. Aliquots were collected at 5-min intervals, filtered, and analyzed by UV–Vis spectrophotometry at 308 nm.

The ^{1}H NMR spectrum (Fig. 1) of the DHPM-S, was obtained and compared with literature data, confirming its synthesis.

In the dissolution assay (Fig. 2), free DHPM-S exhibited 1.72% dissolution at 30 min and 13.10% at 480 min, with T_{50} > 480 min. The 1:1 complex exhibited 8.00% dissolution at 30 min, reached T_{50} at approximately 170 min, and achieved 62.32% dissolution at 480 min. The 1:2 complex showed the highest initial dissolution, at 15.95% after 30 min, but reached only 17.85% at 480 min, without attaining 50% dissolution during the assay (T_{50} > 480 min). The ^{1}H NMR results are consistent with the formation of interacting systems between DHPM-S and β-CD, as indicated by minor changes in chemical shifts and spatial proximity correlations between the components. Among the systems evaluated, the 1:1 complex exhibited the best overall dissolution profile, increasing final dissolution from 13.10% to 62.32% and reducing T_{50} to approximately 170 min. Increasing the β-CD proportion in the 1:2 complex did not result in sustained improvement in dissolution throughout the assay. As a future prospect, this work aims to evaluate the biological potential of the drug-both in its free form and when complexed with cyclodextrin-regarding its antileishmanial activity. This research will be conducted in collaboration with the Faculty of Pharmacy at the University of Lisbon, in Portugal. It is expected that the results will be positive and that the coumpond will demonstrate efficacy in reducing the effects of leishmaniasis, thereby contributing to the development of more effective therapeutic solutions for neglected tropical diseases.

Fig.1. ^{1}H NMR spectrum of DHPM-S.

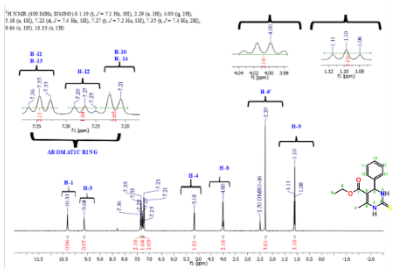
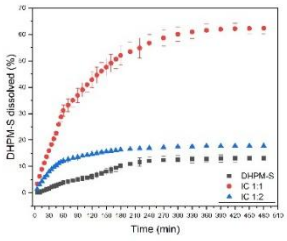


Fig.2. *In vitro* dissolution assay.



Acknowledgments

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Synthesis of novel 4-(bis(4-(dialkylamino)phenyl)amino) phthalonitrile derivatives

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Renewable energy is starting to provide a significant amount of energy to the electrical grids around the word, particularly solar photovoltaics [1]. However, despite saving in emissions while generating energy, the process of obtaining the crystalline silicon used in classical solar cells is quite energy demanding [2]. In the search for alternatives, perovskite solar cells become quite relevant, as they are significantly cheaper to produce, however, their stability remains an issue. Phthalocyanines can be a solution for this issue due to their hydrophobicity protecting the perovskite from humidity and allowing increasing photovoltaic efficiencies [3].

Introducing electron donating groups in the peripheral α,β-positions of phthalocyanines has proved beneficial in achieving high photovoltaic efficiencies [4].Thus, in this work, a series of 4-(bis(4-aminophenyl)amino)phthalonitrile derivatives were synthesized and characterized by spectroscopical techniques, which may be useful for the synthesis of phthalocyanines with strong electron donating groups in the β-positions.

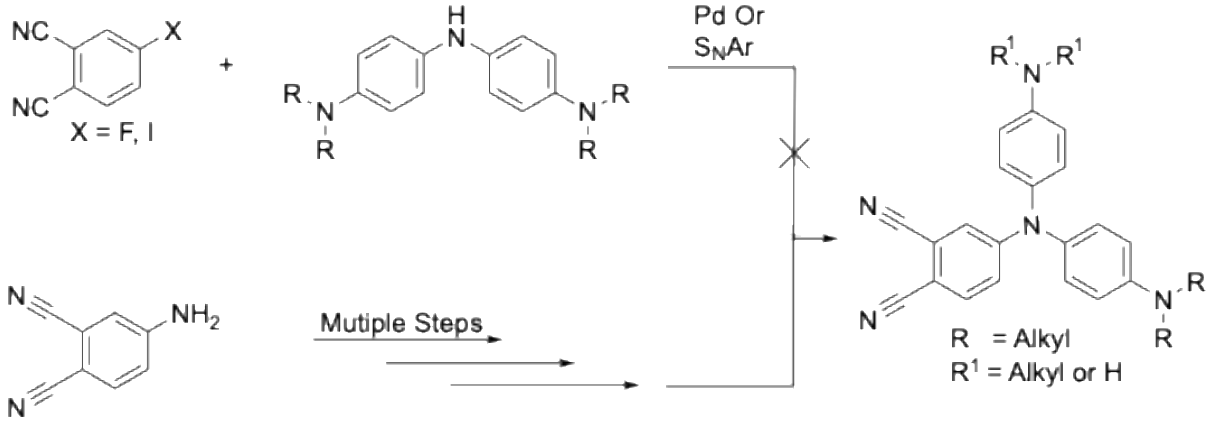


Fig.1. Synthesis of alkylated 4-(bis(4-aminophenyl)amino)phthalonitrile

Funding
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Acknowledgments
Thanks to the University of Aveiro and FCT/MCTES (Fundação para a Ciência e a Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior) for the financial support LAQV–REQUIMTE (UID/50006/2025, DOI: 10.54499/UID/50006/2025), and COMPETE2030-FEDER-00799000, funded by FCT/MCTES through national funds. G. F. Oliveira thanks FCT for their research fellow (Ref: BI/UI104/12677/2025).

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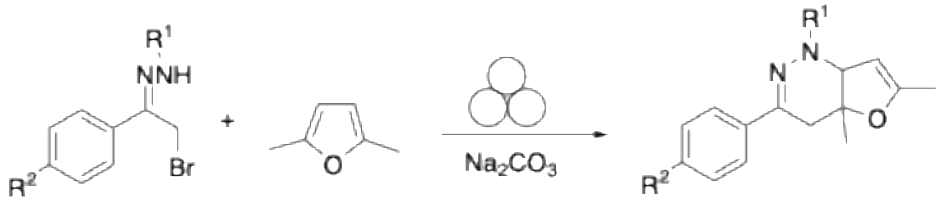
Mechanochemical Hetero-Diels-Alder Reactions of In Situ Generated Azoalkenes with 2,5-Dimethylfuran: A Sustainable Synthetic Approach

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The pursuit of sustainable synthetic methodologies has led to growing interest in mechanochemistry, which has emerged as a powerful synthetic tool with considerable potential to improve the environmental sustainability of chemical processes [1]. In parallel, hetero-Diels-Alder (HDA) reactions involving azoalkenes constitute an efficient strategy for the synthesis of nitrogen-containing heterocycles [2,3]. The combination of mechanochemistry with biomass-derived furans and the unique reactivity of azoalkenes offers a promising route to the environmentally benign synthesis of valuable N-heterocyclic scaffolds.

To evaluate the efficiency of mechanochemical conditions for the HDA reaction between in situ generated azoalkenes and 2,5-dimethylfuran, a series of α-halohydrazones was employed as azoalkene precursors under ball-milling conditions. Mechanochemical synthesis afforded the desired furan-tetrahydropyridazines in excellent yields (84-94%) after only 1-2 h of milling. The highest yields were obtained for the fluoro- and nitro-phenyl substituted derivatives (94% and 92%, respectively). In contrast, the corresponding conventional procedures required significantly longer reaction times (23-28 h) and, in some cases, resulted in lower yields, particularly for the nitro derivative (59%). Green metrics analysis demonstrated a clear environmental advantage for mechanochemistry, with E-factor values ranging from 1.3 to 3.2. EcoScale assessments further confirmed the superior sustainability of the mechanochemical approach.

Overall, these results demonstrate that mechanochemical activation provides an efficient and sustainable platform for promoting HDA reactions of azoalkenes with biomass-derived furans. Beyond enhancing reaction efficiency, this solvent-free methodology aligns with the principles of green chemistry by minimizing waste generation while maintaining excellent yields. The combination of operational simplicity, broad applicability, and favourable sustainability metrics highlights the potential of mechanochemistry as a valuable strategy for the development of sustainable syntheses of nitrogen-containing heterocyclic compounds.



R^1 = 2,4-dinitrophneyl or CO_2tBu
R^2 = H, F, Br or NO2

Fig.1. Synthesis of tetrahydropyridazines

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Bis(trimethylsilyl) Peroxide-Mediated α-Chlorination of Acetophenones

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The α-functionalisation of aromatic ketones provides access to versatile intermediates for the synthesis of structurally diverse organic compounds. In particular, α-chloroketones are useful building blocks for heterocyclic frameworks of potential pharmaceutical interest [1]. Previous studies have demonstrated condition-dependent reactivity of bis(trimethylsilyl) peroxide (BTMSP) [2] towards carbon nucleophiles [3], as well as the influence of reagent stoichiometry and aromatic substitution on acetophenone halogenation using other reagent systems [4]. Herein, we investigated the α-chlorination of acetophenone and substituted acetophenones using a reagent system comprising BTMSP, trimethylsilyl chloride and a base (Fig. 1). Reaction optimisation focused on varying base identity, solvent and reagent stoichiometry to identify conditions that improve product yields for the substrates examined. Product formation was quantified by NMR spectroscopy using an internal standard, enabling comparison across reaction conditions and assessment of substrate-dependent reactivity.
The findings are discussed in relation to possible pathways involving substrate silylation and the generation of chlorinating species in the reaction mixture. The involvement of peroxysilyl intermediates and the distinction between ionic and radical pathways in the present system remain under investigation. The resulting α-chloroketones offer opportunities for subsequent diversification towards heterocyclic structures relevant to bioactive compound discovery [1]. Overall, this study explores silyl peroxide-mediated aromatic ketone functionalisation and identifies experimental parameters to guide further methodological and mechanistic development.



Fig.1. Silyl peroxide-mediated α-chlorination of acetophenones.

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This work was developed within the scope of the Project UID/50006/2025-Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos (DOI: 10.54499/UID/50006/2025) and FCT is gratefully acknowledged for the funded project BiSiPe4Tame (COMPETE2030-FEDER-00753500), supported by FEDER and the Foundation for Science and Technology.

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A Streamlined One-Pot Route to *cis*-4-Hydroxy-L-Prolyl Amides

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cis-4-Hydroxy-L-proline (*cis*-Hyp) is a rare yet highly valuable stereoisomer of 4-hydroxy-L-proline found in natural products such as phallotoxins from Amanita mushrooms.[1] Owing to its unique stereochemistry, *cis*-Hyp has emerged as an attractive scaffold for pharmaceutical and cosmeceutical applications.[1] However, its high cost and the limitations of current synthetic approaches have restricted its broader use in drug development.

In this work, we disclose a streamlined, sustainable, and highly efficient one-pot methodology for the preparation of *cis*-Hyp amides from readily available *trans*-4-hydroxy-L-proline (*trans*-Hyp), without the need for peptide coupling reagents or capping steps (Figure 1).[1] The sequence involves stereoinversion of *trans*-Hyp through an intramolecular Mitsunobu reaction, followed by lactone aminolysis as an efficient strategy for amide bond formation. A broad range of nucleophiles can be employed, including primary, secondary, and aromatic amines, amino alcohols, amino acid derivatives, and dipeptides, affording 25 examples in 76-97% overall yield, without isolation of intermediates and with complete diastereoselectivity.[1,2] The methodology is readily scalable, providing yields of up to 91%, and can be extended to a three-step telescoped process incorporating an additional *O*-silylation step, affording an 83% overall yield.[1,2] Compared with traditional stepwise approaches, this strategy offers greater operational simplicity, improved atom economy, and reduced waste generation.[1,2] The synthetic utility of the method was further demonstrated through the formal synthesis of a bioactive compound with antiamnesic properties.[1,2]

Overall, this streamlined and sustainable protocol provides efficient access to *cis*-Hyp-containing peptides and supports their broader exploration in peptide research.

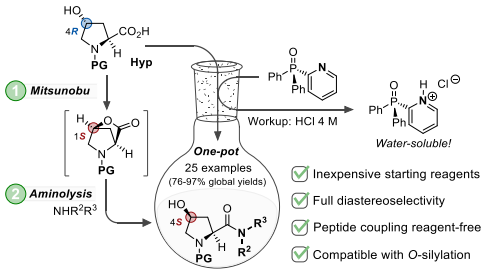


Fig.1. A streamlined one-pot assembly of *cis*-Hyp from readily available *trans*-Hyp.

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QUÍMICA Y SALUD

Innovación molecular en la Química Cosmética

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La química cosmética contemporánea ha evolucionado significativamente mediante el diseño de sistemas avanzados de liberación de principios activos. El objetivo de esta revisión fue analizar los mecanismos de penetración cutánea y la estabilidad oxidativa de ingredientes lábiles incorporados en matrices coloidales modernas. A través de una revisión sistemática de la literatura científica reciente, se evaluó el comportamiento termodinámico de diversas formulaciones tópicas en el estrato córneo.

Los resultados demuestran que la encapsulación de antioxidantes en nanopartículas lipídicas y liposomas incrementa su biodisponibilidad epidérmica hasta en un 40%, protegiéndolos de la degradación ambiental [1]. Asimismo, la integración de la química verde ha permitido sustituir polímeros acrílicos sintéticos por biopolímeros vegetales, optimizando la reología del producto [2]. Los ensayos ecotoxicológicos confirman que estas nuevas matrices reducen drásticamente los efectos adversos y la sensibilización celular [3].

En conclusión, la sinergia entre la ingeniería coloidal y la dermatología molecular es fundamental para el desarrollo de cosméticos de alta predictibilidad terapéutica. El futuro del sector radica en la personalización molecular de los vehículos de entrega, garantizando la convergencia entre eficacia clínica, seguridad del consumidor y sostenibilidad ambiental.

Palabras clave: Biodisponibilidad, Liposomas, Penetración cutánea, Química cosmética, Sostenibilidad

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Hypericin- Synthesized Metal Nanoparticles as Anticancer Green-Light-Activated Agents in 3D Tumor Models

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Photodynamic therapy (PDT) has emerged as a promising strategy for cancer treatment, although its efficacy strongly depends on the properties of the photosensitizer and its ability to generate reactive oxygen species (ROS) upon light activation [1]. Nanoparticle-based systems offer an opportunity to modulate these properties and improve the therapeutic performance of photosensitizers [2]. In this study, hypericin (Hyp), a natural photosensitizer with both reducing and oxidating properties [3], was exploited for the direct synthesis of gold and silver nanoparticles, Au@Hyp and Ag@Hyp, respectively. The nanomaterials were comprehensively characterized, and their photochemical behavior was investigated using complementary assays for singlet oxygen and total ROS generation. Despite their similar synthetic origin, the two systems displayed markedly different photophysical properties. Ag@Hyp showed enhanced ROS generation compared with free Hyp, whereas Au@Hyp exhibited a reduction in ROS production, demonstrating the influence of the metallic component on the photodynamic behavior of the photosensitizer. The biological activity of the systems was subsequently evaluated in HT-29 colorectal adenocarcinoma, MIA PaCa-2 pancreatic adenocarcinoma, and GL-261 glioblastoma cells. Following green-light irradiation, Ag@Hyp produced a stronger cytotoxic response than free Hyp, with the magnitude of the effect depending on the cell type. In particular, MIA PaCa-2 cells showed a pronounced and sustained response, while GL-261 cells exhibited an earlier decrease in viability. The photodynamic effect of Ag@Hyp was associated with increased intracellular ROS generation, DNA damage, and activation of apoptotic pathways. Importantly, Ag@Hyp was also investigated in 3D tumor spheroids, where light activation significantly delayed tumor growth, providing evidence of its activity in a model that better reproduces key features of the tumor microenvironment. Overall, these findings demonstrate that the direct synthesis of silver nanoparticles with Hyp can enhance its photodynamic performance and highlight Ag@Hyp as a promising candidate for light-triggered cancer therapy.

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Del residuo al valor: extracción asistida por microondas de compuestos bioactivos a partir de hojas y tallos de berenjena

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La creciente generación de subproductos agrícolas ha impulsado la búsqueda de estrategias de valorización sostenible en el marco de la bioeconomía circular. En este contexto, el cultivo de berenjena (*Solanum melongena* L.) genera cantidades considerables de biomasa aérea al final del ciclo de cultivo, que permanece en gran medida infrautilizada a pesar de su riqueza en compuestos fenólicos y otros fitoquímicos antioxidantes y con potencial inhibidor frente a enzimas asociadas a la diabetes [1]. El aprovechamiento de esta biomasa como fuente de compuestos bioactivos de alto valor añadido requiere tecnologías de extracción eficientes y respetuosas con el medio ambiente [2]. Entre ellas, la extracción asistida por microondas (MAE) constituye una alternativa prometedora, ya que favorece un calentamiento rápido del sistema disolvente-matriz, mejora la disrupción celular y reduce el tiempo de procesado [3]. Por ello, el presente estudio tuvo como objetivo optimizar las condiciones de MAE para la recuperación de compuestos bioactivos a partir de hojas y tallos de berenjena. Como etapa previa a su valorización, la biomasa vegetal fue sometida a un análisis de residuos de plaguicidas mediante extracción QuEChERS, limpieza por dSPE y análisis por LC-MS/MS, con el fin de evaluar su seguridad química y su idoneidad para la posterior valorización. La optimización se realizó mediante un diseño compuesto central combinado con metodología de superficie de respuesta, utilizando como variables independientes la temperatura de extracción (60–180°C) y la proporción de etanol en el disolvente (0–100%, *v/v*). Como variables de respuesta se evaluaron el rendimiento de extracción, el contenido fenólico total y la actividad antioxidante *in vitro*, evaluada mediante los ensayos DPPH, ABTS y de inhibición del blanqueamiento de la crocina. Aunque el trabajo experimental se encuentra todavía en curso, se espera ajustar modelos polinómicos capaces de describir adecuadamente el proceso de MAE e identificar las condiciones óptimas de extracción. Las condiciones óptimas predichas por los modelos serán posteriormente verificadas experimentalmente mediante extracciones realizadas en dichas condiciones y la comparación entre las respuestas experimentales y las predichas. El extracto obtenido en las condiciones óptimas será posteriormente caracterizado para identificar y cuantificar sus compuestos fenólicos individuales. En conjunto, este trabajo pretende establecer un proceso de MAE verde, seguro y optimizado para la obtención de extractos ricos en compuestos fenólicos a partir de biomasa aérea de berenjena, contribuyendo a su valorización sostenible y a su potencial aprovechamiento en aplicaciones alimentarias, farmacéuticas y cosméticas.

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Electrochemical microRNA-based biosensor for predicting therapeutic response in castration-resistant prostate cancer

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Therapeutic resistance is a major challenge in prostate cancer (PC) treatment, since molecular changes associated with resistance may occur before clinical progression is detected by conventional methods [1]. Minimally invasive biomarkers are an essential support for PC patients monitoring, due to their potential to detect emerging resistance at early stages and to enable monitoring throughout treatment. Therefore, circulating microRNAs (miRNAs) emerge as promising candidates, combining high stability in biofluids with key regulatory roles in disease progression and therapeutic resistance [2].

In this work, we aim to develop of an electrochemical biosensor for the detection of a characterized panel of circulating miRNAs associated with treatment response and resistance in castration-resistant prostate cancer (CRPC). The sensing strategy is based on the functionalization of the electrode surface with specific probes, allowing miRNA recognition to be translated into an electrochemical signal. The electrode interface and experimental conditions will be optimized to achieve high sensitivity and selectivity, while advancing the development of a *point-of-care* platform suitable for analysis in clinical settings.

The combination of a characterized and well-defined miRNA panel with electrochemical detection may represent a promising strategy for monitoring molecular changes associated with PC treatment resistance. In the longer term, this approach could support the development of rapid and minimally invasive tools for longitudinal monitoring of treatment response in CRPC, allowing earlier detection of resistance and more timely therapeutic decisions, ultimately supporting personalized patient management.

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Melanostatin-Amantadine Conjugates as Potent Positive Allosteric Modulators of Dopamine D_2 Receptors

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Current therapies for Parkinson's disease rely on direct dopamine receptor activation, which is often accompanied by motor complications and loss of efficacy over time. Allosteric modulation of dopamine D_2 receptors (D_2R) offers a more refined alternative, as shown by melanostatin, an endogenous neuropeptide that acts as a positive allosteric modulator (PAM) of the D_2R.[1] However, its peptide nature limits its development as a drug, mainly due to poor gastrointestinal absorption and susceptibility to enzymatic degradation.[1,2]

This study explored a bioconjugation strategy based on the lipophilic bullet approach to optimize the pharmacological activity and physicochemical properties of melanostatin. Two bioconjugates of melanostatin with amantadine (adamantan-1-amine) were synthesized via peptide bond formation, obtaining conjugate **1** and the corresponding carbamate derivative **2**, and were evaluated using functional assays at human D_2R. At 0.01 nM, the conjugates enhanced dopamine potency by 3.3- and 4.9-fold, with EC_{50} values of 26.39 ± 3.37 nM and 17.82 ± 4.24 nM, respectively.[3] Cytotoxicity was assessed in differentiated SH-SY5Y cells using the MTT reduction assay.[3] Conjugate **1** showed no significant cytotoxicity up to 200 µM, whereas conjugate **2** induced a slight but statistically significant reduction in cell viability at the highest concentration tested.[3]

Overall, these findings support amantadine-based conjugation as a promising strategy for developing potent melanostatin-derived D_2R PAMs and warrant further investigation of their pharmacological and therapeutic potential.

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Synthesis of Neuroprotective Agents Targeting Dopaminergic Degeneration and Ferroptosis

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Parkinson's disease (PD) is associated with the degeneration of dopaminergic neurons and alterations in dopamine metabolism [1]. Catechol-O-methyltransferase (COMT) inhibitors are used to improve dopaminergic neurotransmission, but the long-term safety of new compounds remains an important consideration [2,3]. Following the development of Compound 9, a novel selective COMT inhibitor with neuroprotective properties by our research team [4], this work focuses on the synthesis of its predicted phase I metabolites to support the characterization of its metabolic profile and safety.

The synthetic approach involves a Michael addition between a protected 3-hydroxy-4H-pyran-4-one and appropriately substituted primary arylamines, followed by a deprotection step. Reaction conditions are being optimized to improve yields and minimize byproduct formation. The results obtained to date will be presented in this communication.

This study complements the development of new COMT inhibitor analogues by investigating the potential metabolites of Compound 9, contributing to a broader understanding of its metabolic profile and supporting its further pharmacological development.

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Decoupling Neuroprotection from MAO-B Inhibition through Bioisosteric Replacement of Rasagiline

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Parkinson's disease (PD) is a progressive neurodegenerative disorder characterised by the selective loss of dopaminergic neurons, driven in part by oxidative stress arising from mitochondrial dysfunction and dopamine metabolism.[1] Rasagiline combines potent, irreversible inhibition of monoamine oxidase B (MAO-B), a mechanism central to its use in PD, with a broader pharmacological profile that extends beyond dopaminergic modulation.[2,3] In particular, neuroprotective activity has consistently been reported across several experimental models.[2,3] Although both properties are associated with the same scaffold, whether they are intrinsically linked remains unclear.

Clarifying whether these properties can be uncoupled is particularly relevant for understanding which structural features of the rasagiline scaffold are responsible for neuroprotection independently of MAO-B inhibition. To address this question from a structural perspective, an indane-to-azaindane bioisosteric replacement was explored within the rasagiline scaffold.[4] Two novel azaindane isosteres, *rac*-**2a** and *rac*-**2b**, were synthesised and evaluated for MAO inhibition and neuroprotective activity in dopaminergic differentiated SH-SY5Y cells exposed to paraquat. Despite a marked attenuation in MAO-B inhibitory activity (IC_{50} shifting from submicromolar to the tens of micromolar range) and the absence of the time-dependent inhibition characteristic of rasagiline, both azaindane derivatives retained neuroprotective activity, with *rac*-**2b** showing greater neuroprotection than rasagiline under the evaluated conditions.

The distinct pharmacological profiles resulting from this bioisosteric modification demonstrate that neuroprotective activity can be preserved despite a pronounced reduction in MAO-B inhibition. By uncoupling these two activities through a defined structural change, these findings provide new insights into the molecular determinants underlying rasagiline-associated neuroprotection and support azaindane bioisosterism as a valuable approach for exploring MAO-independent neuroprotection.

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Fine-Tuning Glypromate Neuroprotection: Synthesis and Biological Evaluation of Novel Peptide-Drug Conjugates

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Glypromate (GPE, glycyl-L-prolyl-L-glutamic acid) is an endogenous neuropeptide with reported neuroprotective properties, but its peptide nature limits its therapeutic potential.[1] In this work, a series of Glypromate-based peptidomimetics was investigated to determine how structural modifications influence cytotoxicity and neuroprotective activity.[2] The compounds explore different structural features, including replacement of L-proline with L-pipecolic acid, functionalization of the glutamate residue at either the α- or γ-carboxyl group, and conjugation with bioactive amines relevant to neurodegenerative disease therapy.

The compounds were first evaluated for cytotoxicity in differentiated SH-SY5Y cells, after which those displaying suitable viability profiles were assessed for neuroprotection against 6-hydroxydopamine (6-OHDA)-induced toxicity. Several proline-based conjugates significantly counteracted 6-OHDA-induced loss of cell viability, with compounds **2a**, **2c**, **3a**, **3b** and **6b** showing significant neuroprotective effects. Among them, compound **3b**, containing memantine conjugated at the α-carboxyl position of glutamate, displayed the strongest response, showing a 2.3-fold improvement in neuroprotective activity compared with the parent GPE peptide.

Structure-activity relationship analysis indicated that neuroprotection was influenced by both the nature of the conjugated bioactive amine and the site of functionalization. Furthermore, replacement of L-proline with L-pipecolic acid was generally detrimental to both cytotoxicity and neuroprotective activity, highlighting the importance of conformational restriction within the peptide scaffold.
Overall, these findings identify key structural features governing GPE-derived neuroprotection and support the development of optimized peptidomimetics as potential neuroprotective agents.

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Synthesis and Neurotoxicity Profile of Pyridine-Based Melanostatin Derivatives Targeting Parkinson's Disease

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Parkinson's disease (PD) is characterized by the progressive loss of dopaminergic neurons in the substantia nigra, causing dopamine deficiency and the cardinal motor symptoms of tremor, rigidity, and bradykinesia.[1,2] Levodopa remains the first-line therapy, but its chronic use often leads to dyskinesias and motor fluctuations, highlighting the need for complementary approaches.[1,2] Melanostatin (MIF-1, L-Pro-L-Leu-Gly-NH_2), an endogenous neuropeptide, acts as a positive allosteric modulator of dopamine D_2 receptors, which may enhance dopaminergic signaling in early PD and potentiate levodopa response, possibly allowing lower doses.[3,4] However, its peptidic nature limits its pharmacokinetic profile, motivating the development of non-peptidic analogs with improved metabolic stability and oral bioavailability.[3,4]

In this context, pyridine derivatives have been explored as prolyl mimetics owing to their structural versatility and ability to reach the central nervous system as well as their neuroprotective potential.[4] Building on this, in this work we synthesized twelve novel pyridine-based MIF-1 analogs. Cytotoxicity screening in differentiated SH-SY5Y cells showed that methyl ester analogs were markedly cytotoxic, whereas the corresponding amides displayed a favorable safety profile for neuronal applications. This structure–cytotoxicity relationship offers a useful guide for optimizing the toxicological profile of pyridine-based MIF-1 derivatives and sets the stage for evaluating their PAM activity, contributing to the development of safer and more effective therapies for PD.

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Biodegradability of Glucocorticoids: Chemical Stability and Environmental Fate

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Glucocorticoids (Fig. 1) are widely used pharmaceutical compounds due to their anti-inflammatory and immunosuppressive properties. Their occurrence in the environment has raised concerns regarding pharmaceutical persistence and the potential consequences of continuous environmental exposure [2]. Understanding the biodegradability of these compounds is therefore important for assessing their environmental fate and supporting the development of more sustainable approaches to pharmaceutical use and management [3].

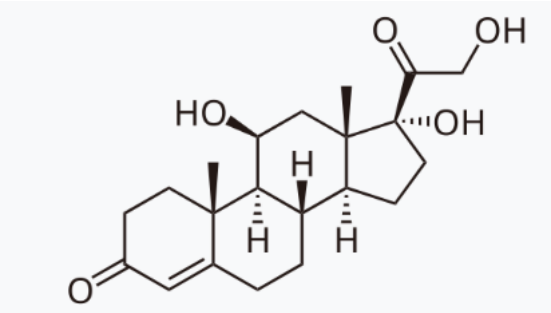


Fig.1. Chemical structure of cortisol, an endogenous glucocorticoid

This study investigated the biodegradability of selected glucocorticoids using a soil sample as the biological inoculum. Biodegradability assays were conducted to assess the susceptibility of the compounds to biological degradation under the experimental conditions employed. The results showed that no biodegradation was observed for the glucocorticoids investigated, suggesting that these compounds may persist in the tested soil-based system.
To further explore the influence of biological conditions on their degradation, additional experiments using alternative inoculum sources are currently underway. These investigations aim to determine whether different microbial communities may promote glucocorticoid biodegradation and to provide a broader understanding of the factors governing their environmental fate.
This work contributes to the chemical assessment of pharmaceutical biodegradability and highlights the importance of investigating glucocorticoid persistence under different biological conditions. The findings may support future research into the environmental behavior of pharmaceutical compounds and their implications for environmental and human health.

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Zein-Coated SPION-Based Paclitaxel Release Systems for Pancreatic Cancer Applications

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Pancreatic ductal adenocarcinoma (PDAC) is associated with one of the lowest survival rates in oncology, partly due to its acidic, dense, and desmoplastic tumor microenvironment, which acts as a physical barrier to conventional chemotherapy [1, 2]. The use of superparamagnetic iron oxide nanoparticles (SPIONs) in nanomedicine represents a promising theranostic approach for targeted drug delivery [3]. However, the conventional synthesis of these nanoparticles often involves toxic reagents and harsh conditions [4].

The main objective of this study was to develop and characterize SPIONs through green synthesis using aqueous and hydroethanolic extracts of *Salvia officinalis* and *Urtica dioica*, and to compare their features with those prepared by conventional chemical synthesis. The optimized systems were subsequently functionalized with the biopolymer zein for the encapsulation of the chemotherapeutic drug paclitaxel (PTX).

The analysis of the extracts by high-performance liquid chromatography (HPLC) and UV–Vis spectroscopy showed that hydroethanolic extraction is more effective in providing bioactive compounds with reducing and stabilizing properties. Structurally, X-ray diffraction (XRD) confirmed the presence of magnetite crystalline cores smaller than 10 nm, characteristic of superparamagnetic behavior. Scanning electron microscopy (SEM) revealed the formation of spherical structures following the incorporation of magnetite into the polymeric matrix, while zeta potential analysis showed a shift in surface charge from positive to negative values, indicating an effective interaction between the SPIONs and zein.

In vitro assays evaluating the PTX release profile demonstrated a continuous and controlled release of approximately 90% of the drug under acidic conditions simulating the tumor microenvironment. Combining the principles of green chemistry with the use of biopolymers represents a promising approach for the development of nanocarriers, offering new therapeutic perspectives for overcoming the physiological barriers associated with PDAC.

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Development of Melanostatin Azapeptides with Improved Biochemical Stability

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The gold standard for Parkinson's disease therapy is based on enhancing dopamine levels in the central nervous system through the administration of levodopa.[1] However, long-term treatment with this drug is associated with serious side effects that may exacerbate the motor symptoms of the disease.[1] Melanostatin, an endogenous neuropeptide, acts as a positive allosteric modulator (PAM) of dopamine D_2 receptors, making it clinically relevant for the treatment of Parkinson's disease and other dopamine-related disorders.[2] Nevertheless, due to its biochemical nature, this neuropeptide presents inadequate pharmacokinetic properties, limiting its potential clinical application.[2]

This project aims to overcome the pharmacokinetic limitations of melanostatin through the development of azapeptides based on the rational replacement of the proline residue with an aza-proline scaffold. This subtle but effective strategy was used to generate a library of 24 melanostatin derivatives. Functional pharmacological assays at dopamine D_2 receptors showed that the melanostatin azapeptides exhibit potent PAM activity, reducing the EC_{50} of dopamine by up to 8.8-fold and outperforming the parent neuropeptide at 1 nM. Furthermore, melanostatin azapeptides showed no cytotoxicity in differentiated SH-SY5Y cells at 100 µM, suggesting a favourable therapeutic window. In addition, these azapeptides did not interact with *h*ERG channels. Preliminary pharmacokinetic studies also demonstrated a 4.7-fold improvement in microsomal stability. Overall, these findings support the potential of melanostatin azapeptides as a new generation of therapeutic agents for Parkinson's disease.

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Building Blocks for Novel 3-Hydroxypyridin-4-One Chelators: Towards Biomedical Metal Coordination and Critical Raw Materials Recovery

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The development of versatile metal chelators is of growing interest in both biomedical research and the sustainable management of critical raw materials. From the coordination of biologically relevant metal ions to the selective separation and recovery of valuable metals, tailored chelating agents offer opportunities to address challenges in health and resource sustainability.
The 3-hydroxypyridin-4-one scaffold offers a versatile framework for developing metal chelators with therapeutic and biomedical applications. Its clinical utility is exemplified by deferiprone, an orally active drug used to treat iron overload [1]. Other derivatives have been investigated as potential neuroprotective, antimicrobial and anticancer agents, while tris(3-hydroxypyridin-4-one) ligands have been developed to coordinate gallium-68 in targeted positron emission tomography (PET) radiotracers [2,3].
In this work, 3-hydroxypyridin-4-one derivatives were successfully synthesised using more sustainable synthetic approaches. These methodologies provide access to versatile molecular building blocks while seeking to reduce the environmental impact of the synthetic process. The iron-chelating ability of the resulting compounds was assessed and compared with that of ethylenediaminetetraacetic acid (EDTA) and catechol-based compounds, providing an initial evaluation of their metal-binding properties and potential as chelating agents.
The combination of sustainable synthesis and preliminary functional assessment establishes a basis for further structural optimisation and investigation of these compounds. Beyond their potential relevance to biomedical applications involving iron coordination, these derivatives may also serve as starting points for the development of tailored ligands for the selective separation and recovery of critical raw materials.
Overall, this work highlights the potential of sustainable synthetic strategies to expand the chemical diversity of 3-hydroxypyridin-4-one-based compounds and support the development of new chelating systems for biomedical research and resource recovery.

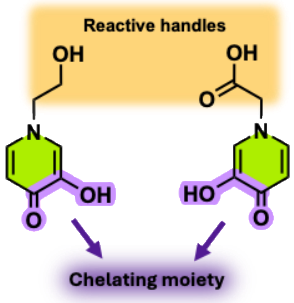


Fig.1. 3-Hydroxypyridin-4-one derivatives

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Development of Conformationally Constrained Peptides as Potent Positive Allosteric Modulators of the Dopamine D_2 Receptor

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Melanostatin (MIF-1) is a short endogenous neuropeptide that acts as a positive allosteric modulator (PAM) with high selectivity for the dopamine D_2 receptor (D_2R), highlighting its therapeutic potential for dopamine-related disorders of the central nervous system, including depression, drug abuse, obesity, tardive dyskinesia, restless legs syndrome, and Parkinson's disease (PD).[1,2] Previous studies have shown that replacement of the L-proline residue of MIF-1 with L-pipecolic acid affords bioactive derivatives with preserved PAM activity.[1]

In this work, we further investigated the role of the L-proline residue in the PAM activity of MIF-1 by merging structural features of L-proline and L-pipecolic acid into a conformationally constrained bridged scaffold, namely (1*R*,3*S*,4*S*)-2-azanorbornane-3-carboxylic acid. A series of 16 bridged MIF-1 derivatives was synthesized and pharmacologically evaluated using functional D_2R assays.[2] Four compounds markedly enhanced dopamine potency, producing up to a 6.6-fold shift and reaching dopamine EC_{50} values as low as 0.01 nM, consistent with potent PAM activity.[2] Furthermore, studies in human dopaminergic SH-SY5Y neuronal cells revealed no neurotoxicity at concentrations up to 200 µM, while the new derivatives displayed improved pharmacokinetic properties compared with the parent neuropeptide.[2]

Overall, these findings establish conformational restriction through a bridged proline mimetic as a promising strategy for the development of highly potent D_2R PAMs and support their further exploration for the treatment of dopamine-related disorders.

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Revisiting Fluoroquinolones: New Chemistry, New Antibacterial Possibilities

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Antimicrobial resistance (AMR) is a major global health challenge that is increasingly undermining the effectiveness of available antibacterial therapies. Although fluoroquinolones remain an important class of broad-spectrum antibiotics, the emergence and spread of bacterial resistance underscore the need for new derivatives with improved antibacterial properties.[1,2] Modifying established antibacterial scaffolds offers a valuable way to explore chemical diversity and identify promising compounds for further development.[3] This work describes the design, synthesis, and preliminary antibacterial screening of a small library of fluoroquinolone derivatives based on ciprofloxacin.

We investigated two strategic chemical modifications at C-3 and C-7 of the ciprofloxacin backbone, attaching heteroaromatic substituents via amide coupling or palladium-catalysed Suzuki–Miyaura cross-coupling. We isolated and characterised seven final compounds by NMR.

We assessed antibacterial activity against Gram-positive and Gram-negative bacteria, using ciprofloxacin as the reference antibacterial agent. An initial single-point screening assay identified compounds for subsequent determination of minimum inhibitory concentrations (MICs) and minimum bactericidal concentrations (MBCs).

Overall, the C-7 series displayed the most promising antibacterial profiles, whereas the C-3 series showed more variable and generally less favourable activity. Differences between derivatives highlighted the influence of both the modification site and the heterocyclic substituent on antibacterial performance.

These findings support further investigation of C-7 substituted fluoroquinolones as starting points for antibacterial optimisation. Future studies will prioritise evaluation against resistant bacteria and cytotoxicity assessment.

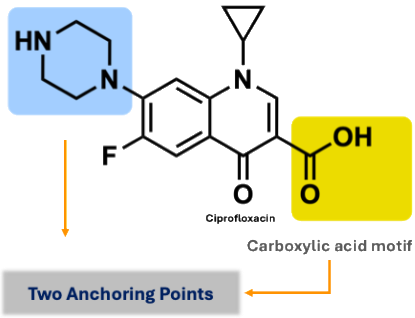


Figure 4. Ciprofloxacin strategic chemical modifications at C-3 and C-7

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QUÍMICA TEÓRICA

Structure–Activity Relationship Analysis of Novel Synthetic Opioids Using Molecular Docking

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The continuous emergence of novel psychoactive substances (NPS), specifically highly potent novel synthetic opioids (NSOs) like fentanyl, nitazene, and orphine analogs, presents a critical challenge for forensic toxicology and public health. Due to their extreme potency, often hundreds of times greater than morphine, there is an urgent need for predictive tools to characterize their interaction with biological targets before these compounds become highly prevalent in the illicit market [1]. Developed under the framework of the SENTINEL Project, this study presents an in silico computational toxicology platform focused on the human μ-opioid receptor (MOR). Target receptor preparations and a comprehensive ligand library encompassing emerging synthetic opioid families are constructed. Molecular docking simulations are executed to identify receptor-ligand binding modes, predicting binding affinities, and evaluate specific molecular interactions within the MOR binding pocket [2,3]. Structural analysis and projection of key physicochemical properties are carried out to map structural requirements for receptor activation. By systematically modelling these interactions, we investigate Structure-Activity Relationship (SAR) trends across the diverse compound families. This molecular-level insight enables the identification of key structural modifications that modulate receptor engagement, helping to anticipate the pharmacological profiles of newly emerging analogs This computational docking approach provides forensic and toxicological sciences with a robust predictive modelling platform. By delivering early predictive data on receptor affinity and SAR of emerging opioids, this work supports early-warning surveillance systems within the SENTINEL Project, enabling proactive public health and regulatory responses.

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Molecular dynamics study of PVA/H_3PO_4 polymer electrolyte: the role of the proton in structure and transport

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Gel polyelectrolytes based on poly(vinyl alcohol) (PVA) doped with acidic, neutral or alkaline species are widely used in flexible and wearable supercapacitors and in self-chargeable devices that combine energy harvesting and storage [1,2]. Among these, phosphoric acid-doped PVA stands out for its high ionic conductivity, chemical stability and ease of handling, which make it attractive for wearable applications [2]. Optimising such devices requires understanding nanoscale mechanisms that remain largely unknown, such as ion transport within the electrolyte and the dynamics of water adsorption and desorption.

Although extensive molecular dynamics (MD) investigations have been conducted on phosphoric acid-doped polymer electrolytes such as those based on polybenzimidazole [3] and Nafion [4], the molecular-level behaviour of the PVA/H_3PO_4 system remains largely unexplored. A key question is whether the structural and transport properties of this electrolyte are governed solely by the presence of ionic charge or whether they also depend on the ability of the proton to form hydrogen bonds with the polymer matrix. MD simulations provide access to structural and dynamical information that is challenging to obtain experimentally, including hydrogen-bonding networks and the individual diffusion behaviour of each species.

In this work, MD simulations were performed using the GROMACS package to reproduce the experimentally studied PVA:H_3PO_4 aqueous formulation. Three systems were investigated, differing in the representation of the acid: (i) undissociated molecular H_3PO_4; (ii) the reaction products of the first dissociation, H_3O^+ and $H_2PO_4^-$, which dominate at the pH of this formulation, considering further deprotonation to HPO_4^{2-} and PO_4^{3-} statistically insignificant for the given system size; and (iii) sodium dihydrogen phosphate, in which H^+ was replaced by Na^+. This design isolates the effect of the cation and of the protonation state on the hydrogen-bond network established between the polymer and the phosphate species.

The results indicate that the molecular and dissociated acid systems exhibit essentially identical polymer-chain conformations, despite the presence of ions only in the latter. In contrast, replacing the proton by Na^+ significantly modifies both the polymer conformation and the mobility of the dihydrogen phosphate anion. These findings indicate that it is the hydrogen-bond donating ability of the cation, rather than the presence of ionic charge alone, that governs structure and transport in this electrolyte. By identifying the molecular origin of this behaviour, this work opens new perspectives for the rational design of next-generation polymer electrolytes for self-chargeable wearable devices.

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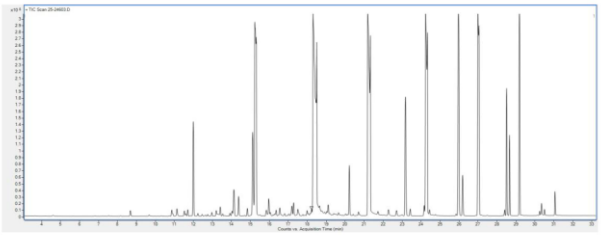


SEGURIDAD QUÍMICA

Compuestos Btex En Residuos De Tanques De Almacenamiento De Gas Natural

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Los hidrocarburos volátiles presentes en los residuos de los tanques de gas natural representan una mezcla compleja de compuestos orgánicos ligeros que permanecen en forma líquida, condensada o gaseosa atrapada tras el almacenamiento o vaciado del tanque. Aunque el gas natural comercial es principalmente metano, los residuos (lodos, condensados y fondos de tanque) concentran fracciones de hidrocarburos más pesados y Compuestos Orgánicos Volátiles (COV) [1] que plantean serios riesgos para la seguridad, la salud y el medio ambiente.



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Los residuos acumulados en los tanques de almacenamiento o terminales de gas natural suelen contener:

- Gases licuados y fracciones ligeras.
- Hidrocarburos No Metánicos (NMHC) [2].
- Compuestos BTEX: Benceno, Tolueno, Etilbenceno y Xilenos; hidrocarburos aromáticos altamente volátiles, tóxicos y, en el caso del benceno, carcinógenos reconocidos.
- Condensados del gas natural (GNL/GNC).: Mezclas de hidrocarburos líquidos de baja densidad que se separan del gas por cambios de presión y temperatura.

La presencia de estos COV entraña ciertos riesgos asociados [3]:

- Riesgo de explosión e inflamabilidad: Debido a su alta presión de vapor, estos hidrocarburos pasan fácilmente a la fase gaseosa a temperatura ambiente. Cualquier chispa o fallo en la inertización del tanque durante tareas de mantenimiento o purga puede causar explosiones violentas.
- Toxicidad para la salud laboral: La inhalación de vapores acumulados de benceno o tolueno provoca efectos crónicos en el sistema nervioso y la médula ósea.
- Emisiones fugitivas e impacto ambiental: La liberación o venteo de estos gases contribuye de forma directa a la formación de ozono troposférico y a la contaminación atmosférica.

El trabajo, tras determinar el contenido en COV de varios residuos de tanques de almacenamiento de gas natural en buques gaseros, demuestra la importancia de analizar el contenido en BTEX de los mismos como paso previo a su limpieza por parte de personal especializado; al objeto de gestionar adecuadamente los riesgos derivados a su exposición.

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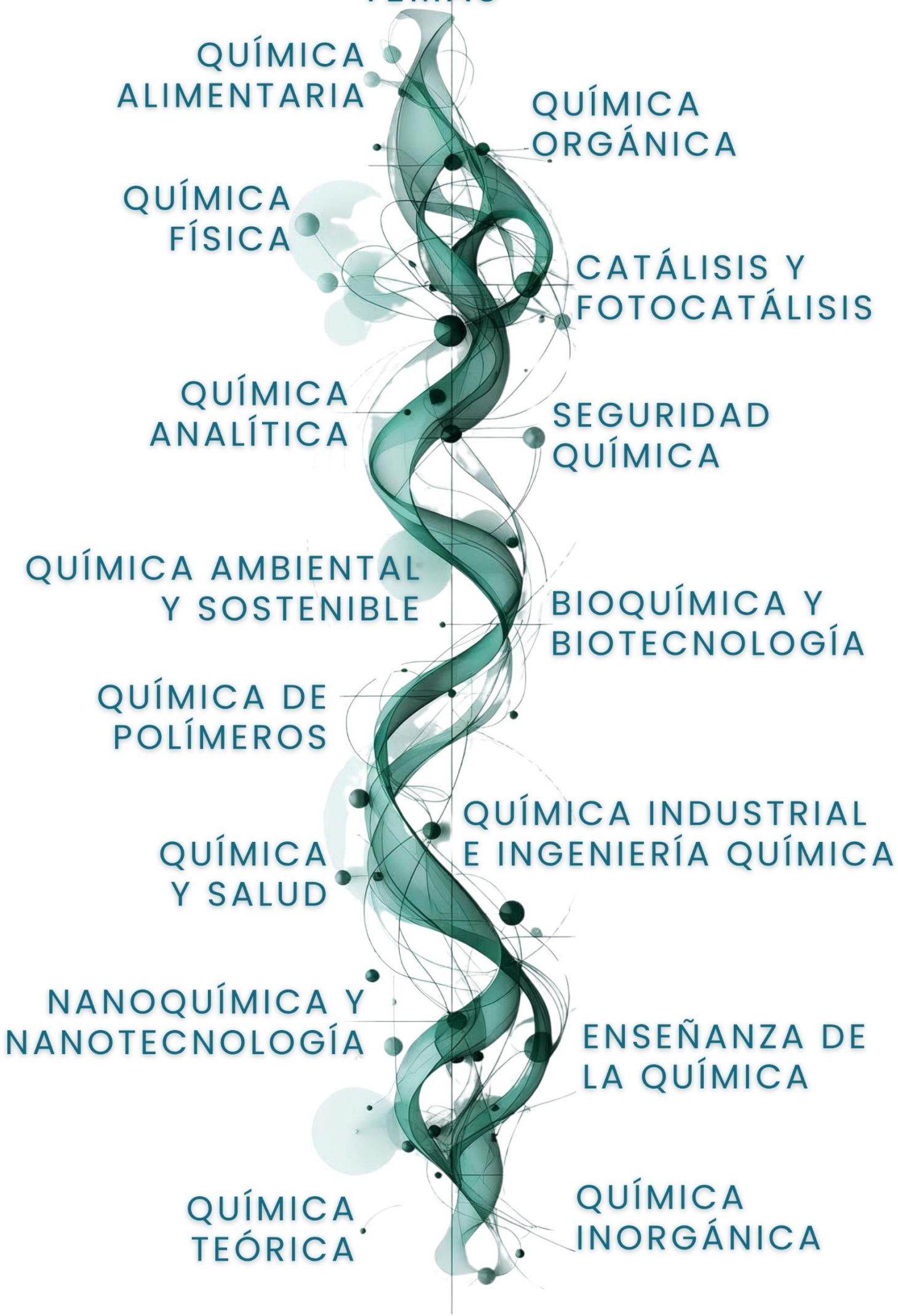
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