

CROMATOGRAFÍA Y TÉCNICAS AFINES

SECYTA

SOCIEDAD ESPAÑOLA DE
CROMATOGRAFÍA
Y TÉCNICAS AFINES

46
BOLETÍN DE LA SECYTA
VOLUMEN 46 NÚM. 1 (2025)
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Madrid, 2025, Vol. 46, núm. 1
ISSN 1132-1369

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Diseño de la portada: Pau de Riba

Los autores son responsables del contenido de sus artículos.

EDITORIAL

Queridos socios de la SECyTA,

Escribo estas líneas en los primeros días de septiembre, inmediatamente posteriores a la celebración de nuestra XXIV Reunión Científica, que este año se ha dado en el marco de Euroanalysis 2025. Eso nos ha permitido destacar y reforzar el papel de la cromatografía y otras técnicas separativas en el marco de la química analítica, mostrando los trabajos que realizan nuestros científicos, investigadores y estudiantes a nuestros colegas europeos. Igualmente, hemos podido disfrutar de magníficas comunicaciones de otros ámbitos del análisis químico, que ensanchan nuestra visión de este campo. Deseo agradecer a los organizadores de Euroanalysis 2025, encabezados por la Dra. Anna de Juan, por el esfuerzo realizado para que el congreso haya sido exitoso y de alta calidad científica. Deseo destacar que entre los miembros del Comité Organizador se encontraban algunos socios de SECyTA, como la Dra. Rosa M. Marcé, la Dra. Sílvia Lacorte y el Dr. Cristian Gómez. El número de participantes ha sido elevado (más de 700), de diferentes países, mayoritariamente europeos. El programa ha tenido 6 conferencias plenarias, 21 *keynote lectures* (en 4 sesiones paralelas), 159 comunicaciones orales, además de 88 comunicaciones de jóvenes investigadores, y 430 comunicaciones en forma de póster. Es de destacar que la cromatografía y las técnicas de separación han sido las protagonistas de la primera conferencia plenaria, impartida por el Dr. Frederik Lynen a propuesta de SECyTA, y que algunos de nuestros socios han sido conferenciantes destacados. Como ya es habitual, durante la Reunión se han concedido los premios José Antonio García Domínguez, esponsorizados por Bruker, a las mejores comunicaciones orales y en formato póster. Deseo expresar en estas líneas mi agradecimiento a Bruker en nombre de SECyTA por su soporte constante en la esponsorización de estos premios, que han llegado ya a su XX edición. Este año se ha celebrado también la IV edición del Premio SECyTA a la mejor Tesis Doctoral en Cromatografía y Técnicas Afines, que se otorgó entre las 12 tesis presentadas correspondientes al año 2024. Agradezco el trabajo del jurado que evaluó las Tesis por su esfuerzo y por la labor complicada que supone escoger la mejor entre las tesis, todas ellas de elevada calidad. Enhorabuena a todos los premiados.

Desde estas líneas quiero también informaros de cambios que se han producido en este último periodo. En primer lugar, ha habido algunas substituciones en el Comité Editorial del Boletín: la Dra. Belén Gómara ha sustituido a la Dra. María Luz Sanz y el Dr. Ángel de la Puerta ha sustituido al Dr. Mario Fernández, que se ha jubilado. Junto con ellos, continúan en el Comité la Dra. Ana Cristina Soria y la Dra. Ana Isabel Ruiz. Quiero agradecer a todos ellos el trabajo desinteresado que llevan a cabo para que todos podamos disfrutar de esta revista. Un agradecimiento especial a María Luz y a Mario por todos estos años de dedicación. Con respecto al Boletín, también quiero destacar que, en la Junta de Gobierno del pasado abril, se acordó suspender la impresión en papel a partir de 2026, atendiendo a criterios de uso, sostenibilidad ambiental y eficiencia de recursos. Sin duda, hoy la mayoría de nosotros estamos ya acostumbrados a las revistas en formato digital y esperamos que esta decisión, que fue ratificada en la Asamblea General, sea bien acogida. También estamos en proceso de actualizar la página web para ponerla al día, tanto desde la perspectiva legal (ley de protección de datos, seguridad informática, etc.), como para asegurar su continuidad y facilitar las modificaciones de contenidos. Este proyecto lo está liderando la Dra. Patricia Plaza, vocal de la Junta de Gobierno, a la que agradezco el trabajo que está realizando.

Finalmente, desearía informaros que para el próximo año estamos preparando una reunión de las diferentes sociedades que trabajamos en análisis instrumental en España. La Sociedad Española de Química Analítica (SEQA), la Sociedad Española de Espectrometría de Masas (SEEM), la Sociedad Española de Metabolómica (SESMET), la Sociedad de Espectroscopía Aplicada (SEA) y nuestra Sociedad (SECyTA), realizaremos nuestras reuniones científicas conjuntamente en Salamanca del 21 al 24 de julio, en un único congreso en torno al análisis instrumental. Ya hemos mantenido diferentes reuniones preparatorias y, a partir de ahora, intensificaremos el trabajo, junto con el comité organizador local, encabezado por el Dr. José Luis Pérez Pavón, para que en julio de 2026 podamos disfrutar todos de un interesante congreso, con conferenciantes de alto nivel, en el que podamos dar a conocer nuestras últimas investigaciones. Os iremos proporcionando información a través de los medios habituales (web, correo electrónico, etc.) para que podáis irlos organizando. Espero veros, pues, en Salamanca en el próximo mes de julio.

Un abrazo,

JORDI DÍAZ FERRERO
Presidente de SECyTA

ARTÍCULO

Engineering Functionality: The Role of Smart Materials in Modern Chromatographic Systems

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ABSTRACT

Chromatography remains a cornerstone technique in analytical chemistry, enabling the separation and analysis of complex mixtures. The progress of chromatographic separation technologies is closely linked to the development of stationary phase materials, where particle size, structure, and functionality critically influence column efficiency and selectivity. Recent advances in tailored materials have significantly enhanced the performance of chromatographic systems, improving selectivity and sensitivity. Their integration into packed, monolithic, and open tubular columns has expanded applications in hydrophilic interaction chromatography (HILIC), chiral separations, and catalytic flow systems, among others. This mini-review explores the latest developments (from 2022 to 2025) in the design and application of custom materials for chromatography, focusing on innovations in stationary phases, such as functionalized nanoparticles, hybrid materials, and biomimetic surfaces. The review also highlights key trends, including the integration of nanomaterials, green chemistry principles, among others.

Keywords: Functional Materials; Stationary Phases; Chromatographic Separation; Enantiomers, Isomers, Columns; Porous Frameworks.

1. INTRODUCTION

Chromatographic separation is a fundamental tool in analytical chemistry, widely used for the precise isolation, identification, and quantification of components within complex mixtures. It plays a pivotal role in a wide range of applications, from environmental monitoring to food safety, pharmaceuticals, and biomolecular analysis. The performance of chromatographic systems, particularly high-performance liquid chromatography (HPLC), gas chromatography (GC), and capillary electrochromatography (CEC), is significantly in-

fluenced by the stationary phase materials employed in the columns. These materials determine critical aspects of the separation process, such as column efficiency, selectivity, and resolution. Over the years, substantial advances have been made in improving these materials to enhance the overall efficiency and capacity of chromatographic systems [1, 2].

The efficiency of a chromatographic column is governed by various factors, with the size and structure of the packing material being among the most influential [3]. According to the van Deemter equation, decreasing the particle size of packing materials results in improved separation efficiency by reducing the resistance to mass transfer. This principle has been central to the evolution of chromatographic materials, leading to the development of increasingly smaller packing particles, such as those used in ultra-high performance liquid chromatography (UHPLC). The transition to smaller particle sizes has brought about significant improvements in column performance, enhancing resolution and speed. However, as particle size decreases, the challenge of high back pressure arises, creating significant technical hurdles, especially when pushing materials to the nanoscale [3].

In parallel to these advances in particle size reduction, the exploration of novel functional materials has emerged as a key strategy for improving chromatographic performance. Metal-organic frameworks (MOFs), covalent-organic frameworks (COFs), molecularly imprinted polymers (MIPs), molecular cages, biomolecule-based, and carbon-based materials have gained attention for their tunable properties and versatility [1, 4]. These materials can be engineered to provide high surface areas, selective interactions, and chemical stability, which are crucial for efficient separations. For instance, MOFs are well-known for their large surface area and high porosity, while COFs offer robust structural stability and precise pore size control. MIPs or biorecognition elements are designed for selective molecular interaction, making them ideal for

applications requiring high specificity, such as chiral separation. Recent trends in chromatographic material development involve sophisticated hybridization strategies, where different functional materials are combined to leverage the unique advantages of each [5, 6]. These hybrid materials effectively overcome the limitations of individual components by enhancing stability, flexibility, or selectivity. These innovative hybrid materials are increasingly being incorporated into chromatographic systems, expanding their applications and improving performance across a variety of separation techniques.

Although not classified as a functional material, 3D printing has emerged as a transformative tool in chromatography, enabling the rapid prototyping and customization of column hardware, microfluidic devices, and support structures [7, 8]. This technology facilitates the fabrication of complex geometries and integrated systems that are difficult to achieve through conventional manufacturing methods, offering new possibilities for miniaturization, automation, and cost-effective production in separation science. Recent advances include the printing of monolithic columns and flow distributors with enhanced precision and reproducibility. Moreover, 3D printing allows for the integration of multi-material systems, paving the way for hybrid designs that combine structural components with functional coatings. These developments support the creation of next-generation chromatographic platforms tailored for specific analytical tasks.

This minireview aims to provide an overview of the state-of-the-art and describe the main challenges and gaps during method development using these materials for the recent advances in separation sciences using functional materials. It discusses key materials, such as MOFs, COFs, MIPs, and carbon-based hybrids, with a particular focus on their unique properties and how they can be combined to create more efficient and selective chromatographic systems. Although other chromatographic liquid-coated supports are reported in the literature (including ionic liquids and deep eutectic solvents) [9, 10], this review has focused on the solid materials. Additionally, the review highlights recent case studies in various fields, including environmental monitoring, food safety, biomedical applications, and pharmaceuticals, showcasing the practical applications of these materials. It also addresses the current challenges faced in the integration and commercialization of these advanced materials, including issues related to stability, reproducibility, and scale-up.

This review seeks to offer a broad overview of the potential hybridization and use of functional materials for specific applications within the field of separation science, rather than offering an exhaustive evaluation of the existing literature. To achieve this, a systematic literature search was conducted covering the period from 2022 to 2025. The search was performed using Google Scholar and Scopus, employing the following keywords and their combinations: *functional materials*, *layered double hydroxides*, *molecular cages*, *MOF*, *COF*, *HOF* (hydrogen-bonded organic frameworks), *biosorbents*, *biomolecule*, *MIP*, *aptamer*, *carbonaceous*, *carbon-based*, *nanoparticles*, *silica*, *monoliths*, and *3D-printing*, in conjunction with *chromatographic separation*, *separation*, *chromatography*, *electrochromatography*, *electrophoresis*, *gas chromatography*, and *liquid chromatography*.

2. ORGANIC AND INORGANIC STATIONARY PHASES. TYPES OF FUNCTIONAL MATERIALS

Recent advances in separation science have led to the development of a wide array of functional materials with improved performance over conventional stationary phases. These materials, both organic and inorganic in nature, have been tailored to enhance selectivity, resolution, and robustness across various chromatographic modes, including HPLC, GC, capillary electrochromatography (CEC), and thin-layer chromatography (TLC). **Table 1** summarizes the most recent application in the field [4, 11–64], including MOFs, COFs, MIPs, molecular cages and others explored either as standalone phases or in combination with silica and polymer supports.

Distinguishing the individual role of each component is not always straightforward, as many materials serve multiple functions simultaneously. For instance, contributing to both interaction mechanisms and structural support. Nonetheless, general trends can be highlighted:

- Functional materials (e.g., MOFs, COFs, molecular cages, MIPs) are typically responsible for providing increased interaction sites and selectivity.
- Silica particles and organic monoliths primarily act as mechanical supports, offering column stability, improved fluidics, and packing compatibility with conventional LC formats.

- In most cases, synergetic effects are explicitly or implicitly demonstrated, involving enhancements in chemical stability, mass transfer, multimodal retention, and overall chromatographic performance.

2.1. Porous frameworks and hybrid sorbents for stationary phase design

Metal–Organic Frameworks (MOFs) are a class of crystalline porous materials assembled from metal nodes and organic linkers. Their structural flexibility, tunable pore sizes, and diverse chemistries make them ideal for developing novel stationary phases [65, 66]. In GC, the modulation of particle morphology (e.g., nanoplate vs. nanorod structures) [4, 60] or size [59] has demonstrated improved separation of isomers due to enhanced mass transfer and shape selectivity. In liquid-phase separations such as HPLC or CEC, MOFs can offer additional retention mechanisms through π -stacking, hydrogen bonding, or metal–analyte interactions. However, a common practice is the coupling of MOF with silica particles to pack the resulting hybrid composite in a separation column [55–58]. Furthermore, their capacity for functionalization—such as incorporating chiral ligands or immobilizing biomolecules—allows for customized selectivity in complex separations, including enantioseparation and multi-analyte screening [43, 49, 54, 56, 61, 62].

As an example, Mia *et al.* [62] developed a hybrid monolithic column combining an MOF and a biomolecule to enhance enantioselective chromatographic performance. MOF-5 was grown on a (glycidyl methacrylate)–copolymerized-(ethylene dimethacrylate) (poly(GMA-co-EDMA)) monolith using a layer-by-layer method and functionalized with pepsin through amidation. This pepsin@MOF-5@poly(GMA-co-EDMA) column was used in CEC for the enantioseparation of six basic chiral drugs, showing superior resolution, selectivity, and repeatability compared to pepsin-only columns. The MOF structure also helped stabilize and orient pepsin molecules more effectively, supporting better functional performance and selectivity. This approach is not free from drawbacks involving complex synthesis, potential biomolecule leaching, and limited MOF stability under harsh conditions.

Covalent Organic Frameworks (COFs) are crystalline organic materials with periodic two- or three-dimensional networks formed by strong covalent bonds between light elements (e.g., B, C, N, O) [67]. They

exhibit high surface area, thermal and chemical stability, and low density. Their π -conjugated frameworks make them especially effective for retaining aromatic and planar molecules, and their porous nature facilitates fast analyte diffusion. COFs have shown excellent selectivity and reusability in both GC and LC. Recent studies highlight their role in multimodal separations—combining hydrophobic, hydrogen-bonding, and ionic interactions—making them suitable for analyzing structurally diverse compounds, from vitamins to polyaromatic hydrocarbons. Although they can be used without functionalization [68, 69], several authors have attached this material to silica particles [48, 51–53], and others preferred fluorosubstituents [44, 45] or crown ethers [63]. Liu *et al.* [48] reported a novel SMIP-COF@SiO₂ stationary phase aiming to achieve specific and efficient chromatographic separation of complex analytes, including nucleosides, B vitamins, sulfonamides, alkylbenzenes, phenyl ketones, polycyclic aromatic hydrocarbons (PAHs), and environmental endocrine disruptors. This hybrid material integrates the selective molecular recognition of MIPs with the high surface area and multifunctionality of COFs, enabling multiple retention mechanisms and improved interactions with both hydrophilic and hydrophobic compounds. Analytical results demonstrated superior performance of SMIP-COF@SiO₂ over SMIP@SiO₂ and COF@SiO₂ alone, showing enhanced selectivity, broader applicability, and successful use in real sample matrices such as environmental water and cosmetic products [4].

Molecular cages are discrete, porous, polyhedral structures typically composed of organic or metal–organic building blocks that self-assemble into well-defined cavities. Their intrinsic shape-selectivity, modular structure, and inner functional environments make them attractive as stationary phase materials for chromatography [70, 71]. In GC, molecular cages such as ETTBA-(R,R)-CHDA or metal-organic assemblies like [(Tr₂Pd₃)(CH₃CN)][NO₃]₂ have shown enhanced resolution of halogenated benzenes, esters, and isomeric alkanes by exploiting hydrophobic cavity environments and host–guest interactions [25, 64]. In liquid-phase systems, the coupling of molecular cages with silica particles (e.g., RCC3-GQ@NH₂-SiO₂ or AD-RCC3-R@NH₂-SiO₂) enables their integration into HPLC and reverse-phase (RP)-LC columns, allowing selective retention of nucleosides, amino acids, and chiral compounds through ion exchange, hydrogen bonding, and size-selective effects [26, 41, 42]. The versatility of molecular cages also lies in their synthetic tunability, enabling post-synthetic modifica-

Table 1. Overview of functional materials used in chromatographic separation systems.

Material nature	Sorbent specifications	Analytes	Separation system	Remarkable insights	Reference
Metal-organic frameworks (MOFs)					
MOF nanoplates and nanorods	PCN-608	C6 and C8 isomers and chlorotoluene isomers	GC	Modulation of MOF shape and size (scissoring strategy) increases the overall efficiency	[4]
Modified MOF	L-Cys-PCN-224	Amino acids	OT-CEC	Lifetime over 200 injections with good reproducibility (RSD<10%)	[43]
Enzyme@MOF@polymer	Pepsin@MOF-5@poly (GMA-co-EDMA)	Hydroxychloroquine, chloroquine, nefopam, chlorpheniramine, clenbuterol, hydroxyzine	CEC	Enhanced enantiomeric resolution	[62]
Modified MOF	L-His-NH-MIL-53	Racemic drugs (tryptophan, phenylalanine, metoprolol, etc.)	OT-CEC	Enhanced enantiomeric resolution	[61]
Polysaccharide@MOF	4, 5-IMD-Zn@ carboxymethyl β -cyclodextrin	Hydroxychloroquine, ofloxacin, and atenolol	OT-CEC	Enhanced enantiomeric resolution	[49]
MOF	MOF-74 nanoroads	Xylene isomers	GC	Modulating the channel length of the MOFs. Good reproducibility	[60]
MOF	Nano-MIL-103	Benzene isomers, aromatic compounds, and alkanes	GC	Size control of MOF nanoparticles without aggregation	[59]
MOF@silica	ZIF-67/hydrogel@SiO ₂	Positional isomers, Hydrophilic/ionic/hydrophobic analytes	HPLC	Good separation and selectivity due to multiple interaction paths	[58]
IL@MOF@Silica	[BCMIM][Cl-Zr-MOF@SiO ₂	PAHs, phthalates, phenyl ketones, sulfonamides and positional isomers	HPLC	Good stability, repeatability, and reproducibility, no significant matrix effects. Facile preparation	[57]
Carbonaceous/MOF@silica	Fe-CD/MOF-808@SiO ₂	Hydrophilic/hydrophobic/amphiphilic compounds and structural/enantiomeric isomers.	HPLC	Modulation of the retention mechanism with additional interaction sites	[56]
MOF@Silica	MIP-202@NH ₂ -SiO ₂	Positional isomers, sulfonamides, nucleosides/nucleobases and B vitamins	HPLC	Multi-mode separation	[55]
MOF and polymer	Cu ₂ (D-Cam) ₂ Dabco@dopamine polymer	Malic acid	CEC	Improved chiral selectivity	[54]

Material nature	Sorbent specifications	Analytes	Separation system	Remarkable insights	Reference
<i>*Covalent-organic frameworks (COFs)*</i>					
COF@silica	TpPa-1@SiO ₂	PAHs, nucleobases and phenylurea herbicides	RPLC and HILIC	Multi-mode separation	[53]
COF@silica	PA-CA COF@SiO ₂	Chiral pharmaceutical intermediates and chiral drugs	HPLC	Multi-mode separation, greater versatility than commercial columns	[52]
Polymer@COF@silica	MIP@TPB-DVA@SiO ₂	Nucleosides, B vitamins, sulfonamides, alkylbenzenes, phenyl ketones, PAHs and environmental endocrine disruptors	HPLC	Multi-mode separation, tailing phenomenon	[51]
COF@MOF	TpBD/UIO-66-NH ₂	Amino acids, antibiotics, preservatives and sulfonamides	OT-ECE	Multi-mode separation; good reproducibility; preparation was tedious and time-consuming	[47]
COF	(R)-BHTP-COF	Racemic drugs	HPLC	Selectivity and durability	[46]
COF	2D Tph-DHTA	C8 aromatic isomers	GC	Favoured thermodynamics, by slipping stacking, but did not affect the mass transfer	[50]
COF@silica	PFP-COF@NH ₂ -SiO ₂	Phenolic acids, alkaloids and antiviral drugs	HPLC	Modulation of post-synthetic modifications; synthesis tolerable to the order of reagent addition	[44]
Trifluoromethyl-modified COF	TpTFMB-2D-COF	Positional isomers	GC	Easy preparation, high selectivity due to new interaction modes	[45]
Crown ethers and COF	1,1'-binaphyl-20-crown-6-derived dialdehyde and tetraamines with diisopropyl substituent	Letones, epoxides and alkaline substances	OT-CEC	Excellent stability in water, acid and base	[63]
MON@COF@silica	L-cysteine modified chiral MON/COF@SiO ₂	Endocrine disruptors, and pyridoxine	HPLC	Improved permeability, balanced hydrophilicity and hydrophobicity; Multimode	[48]
<i>*Molecular cages*</i>					
Molecular Cage@silica	RCC3-GQ@NH ₂ -SiO ₂	Sulfonamides, nucleosides, acids, and amino acids	HILIC, RPLC Ion Exchange	91 compounds across 15 categories. Can separate nucleosides in just water	[42]
Molecular Cage@silica	AD-RCC3-R@NH ₂ -SiO ₂	Chiral compounds	NPLC	Low concentrations of THF and chloroform effectively improved the separation performance	[26]
Molecular Cage@silica	RCC3-GLD@NH ₂ -SiO ₂	Alkylbenzenes, PAHs, phenols, anilines, sulfonamides, nucleosides, amino acids, sugars, and acids	HILIC, RPLC	Multi-mode separation; Full polarity range; 87 compounds were separated	[41]

Material nature	Sorbent specifications	Analytes	Separation system	Remarkable insights	Reference
Molecular Cage	ETTBA-(R, R)-CHDA	Halogenated benzenes, alkylbenzenes, esters, <i>n</i> -alcohols, <i>n</i> -alkanes, Grob reagent, isomers and racemates	GC	Better performance than commercial homologues with good thermal stability	[25]
Molecular Cage	[(Ti ₂ Pd ₃)(CH ₃ CN)](NO ₃) ₂ + organosulfur ligand	Alkanes and isomeric molecules	GC	Hydrophobic inner cavity with good solubility and stability in aqueous media	[64]
<i>*Organic monolith-based columns*</i>					
Organic monolith	2-naphthylmethacrylate and trimethylolpropane trimethacrylate	Dipeptides and proteins	nano-LC	Good hydrodynamic behaviour	[40]
Modified polymer	MIP(poly-Chitosan)@NH ₂ -AuNPs	Metolachlor	CEC	NH ₂ -AuNPs can provide abundant binding sites and reduce the deformation and collapse of CMIPs' cavities	[20]
Natural polymer	Nylon-6	Urinary extracellular vesicles	HIC	Low-cost and time-efficient (< 20 min) column separation	[27]
Dual-zwitterion hydrophilic monolith	poly(MAMMPS@MPC-co-MBA) or poly(MPC-co-MBA)	Benzoic acid derivatives, nucleobases, nucleosides, phenol derivatives, and amine compounds	HILIC	120,000 plates/m was reached. Retention strength due to the hydrophilicity, while hydrogen bonding and electrostatic interactions played secondary roles	[39]
Polymer@metal	Agarose particles@GMA@Ni NPs	Histidine-tagged proteins	Affinity LC	Fast and efficient separation and purification of target proteins in complex samples with high permeability, low backpressure, and high interfering matrix tolerance	[38]
Derivatized organic monolith	CDs@GMA-based monolith	Neutral, alkaline, and acidic compounds, and Tanaka standard test mixtures	RPLC	Multifactorial retention mechanisms	[37]
Derivatized organic monoliths	Silsesquioxane-based monoliths containing zwitterionic sulfobetaine monomers	Alkylbenzenes, phenolics, aromatic carboxylic acids, nucleobases, nucleosides, and 2-deoxynucleosides	HPLC and HILIC	Multifactorial retention mechanisms; The monomer cannot be changed without affecting the structure of the monolith	[36]
Organic monoliths	MON and MAA-based monolith	PAHs, alkylbenzenes, acidic phenols, basic amines, phenylurea herbicides, parabens, phthalates, and flavonoids	RPLC	Better resolution and selectivity than C18 packed column.	[35]
MIP	EO-co-EDMA attached to mono-dispersed polymer beads	AcT4	HPLC	Key aspect: length of the spacer in a crosslinker. High selectivity	[28]
Organic monolith	L-Cysteine	Dansyl glutamic acid, dansyl aspartic acid, dansyl methionine, and dansyl phenylalanine	HILIC	Low efficiency, due to the lack of surface area and binding site	[18]

Material nature	Sorbent specifications	Analytes	Separation system	Remarkable insights	Reference
<i>*Silica-based columns*</i>					
Derivatized silica monoliths	MIPs@NH ₂ -SiO ₂ monolith	Flavonoids	RPLC	Good separation ability, but it suffered from a poor sensitivity	[21]
Derivatized silica monoliths	Pentafluorophenyl-SiO ₂ monolith	Tocochromanols	RPLC	Reduced back-pressure and better performance than commercial homologues	[19]
Modified silica particles	BEH TM 45 AQ @hydrophilic hybrid organic-inorganic SiO ₂	Double-stranded DNA macromolecule (2-25 kbp)	SC	Rapid separations (under 2 min); They quantify dsRNA impurities	[34]
Polymer@silica	MIP@NH ₂ -SiO ₂	Sulfonamides, ginsenosides, nucleosides, and pesticides	HILIC	Silylation offered better efficiency and resolution	[22]
Modified silica	Triphenyl-SiO ₂	teicoplanin and siRNA patisiran	HPLC, IC and HILIC	Tuning of chromatographic conditions and charge properties are key aspects	[23]
Modified silica	ODS@SiO ₂ @SiO ₂ coreshell microspheres	Small solutes, peptides, and proteins	UPLC	The thickness and pore size of the spheres can be adjusted by varying the reaction time and the particle size of colloidal silica sol	[33]
Modified silica	PTHP-SiO ₂	—	RP-HPLC	Multifunctional material: antibacterial and stationary phase	[24]
Polymer@SiO ₂	NMA and LITFSI	Phthalates	HILIC and RPLC	Stronger hydrophilicity than commercial homologues. Use of lower organic phase content and shorter time	[32]
Protein@silica	Halo-tagged CysLT ₁ R@NH ₂ -SiO ₂	Antraquinones: aloe-emodin, rhein, emodin, chrysophanol, and physcion	Affinity LC	The highest affinity to the receptor indicated the strongest anti-inflammatory effect	[31]
Organic polymer@silica	CS/PAA/ODE hydrogel@SiO ₂	Polar and non-polar analytes. Positional isomers and chiral enantiomers	HILIC/RP-HPLC	Multifunctional; Inhibited swelling due to CS/PAA electrostatic interaction. High stability	[30]
Inorganic-organic silica particles	2D-LDH/CMP@SiO ₂	Positional isomers, Hydrophilic/ionic/hydrophobic analytes	HPLC	Good separation and selectivity due to multiple interaction paths	[29]
<i>*3D-printed columns*</i>					
3D printed Monolith	GMA-based polymer	Biomolecules	Nano-RPLC and HIC	1,000 printed devices with separations in 1 min	[11]
Engineered 3D-printed metal column in a microchip format	Commercial OV-1	Ketones, aromatics, alkanes, and alcohols	microGC	High-hardness die steel enables stable, curved channels and flexible design. Fast, uniform heating suits low-power outdoor analysis	[17]
3D-printed monolith	iminodiacetic acid derived cellulose hydrogel	Polyhistidine-tagged proteins	HPLC	Direct purification from crude lysate with a substantially reduced purification time	[15]

Material nature	Sorbent specifications	Analytes	Separation system	Remarkable insights	Reference
Engineered 3D-printed stain steel column in a microchip format	OV-1	Benzene series compounds, VOCs and gasoline	GC	The assembly can be mass-produced with low cost and the production process is simple and have good repeatability	[16]
Engineered 3D-printed Acrylated column	BMA-based monolith	Proteins	RPLC	Resistance to organic solvents is a key aspect. High pressure resistance	[12]
* Other materials*					
HOF	Chiral HOF-2	Alkanes, n-alcohols, PAHs, and positional isomers	HR-GC	Good column repeatability and reproducibility. Computational studies supported the results	[13]
Extendend pillar[n] arenes	LP6A-C10 and BpP6A-C10	Halogenated benzene, benzaldehyde, phenol and aniline isomers	GC	Better performances over the commercial HP-5 and HP-35 homologues	[14]

Abbreviations: (R)-BHTP-COF; Binaphthyl-based COF; AcT4; AcetylT4; AD-RCC3, homochiral secondary amine molecular cages coated with 3,5-dimethylphenyl carbanate of amylose; BMA, butyl methacrylate; CD, carbon dots; CEC, capillary electrophoresis; CMON, chiral microporous organic network; CS/PAA/ODE, chitosan/polyacrylic acid/octadecene; CysLT₂R, cysteinyl leukotriene receptor type 1; DVA, 2,5-divinylterephthalaldehyde; EO-co-EDMA, ethylene oxide EDMA; ETBBA-(R, R)-CHDA, 4,4'-4''-(ethene-1,1,2,2-tetrayl)-tetra benzaldehyde and (R, R)-diaminocyclohexane; GMA-co-EDMA, (glycidyl methacrylate)-copolymerized-(ethylene dimethacrylate); HIC, hydrophobic interaction chromatography; HILIC, hydrophilic interaction liquid chromatography; HOF, hydrogen-bonded organic framework; HR-GC, high-resolution GC; IC, ion chromatography; IL, ionic liquid; IMAC, immobilized metal ion affinity chromatography; LDH/CMP, layered double hydroxide hybridized with conjugated microporous polymer; LiTFSI, bis(trifluoromethane) sulfonimide lithium; MAMMPs, 3-(4-(methacryloyloxy)methyl)-1-methylpiperidin-1-ium-1-yl)propane-1-sulfonate; MBA, N,N'-methylenebisacrylamide; MOF, metal-organic framework; MON, microporous organic network; MPC, 2-methacryloyloxyethyl phosphorylcholine; NMA, N-methylolacrylamide; NPs, nanoparticles; ODS, octadecyltrichlorosilane; OT-CEC, open tubular capillary electrochromatography; Pa-1, p-phenylenediamine; PA-CA COF, trans-1,2-cyclohexanediamine and (D)-penicillamine COF; PAHs, polycyclic aromatic hydrocarbons; PEG-rhGH, PEGylated recombinant human growth hormone; PFP, pentafluorophenyl; PMACO, poly(maleic acid-alt-1-octadecene; PTHP, poly(tetrahydroxypropan); RC2-CN, cyano-functionalized RC2 molecular cage silica gel; RC23, reduced imine cage; RC23-GLD, epoxy propanol loaded molecular cage; SC, slalom chromatography; SEC, size-exclusion chromatography; Tph-DHTA, 5,10,15,20-tetrakis(4-aminophenyl)-21H,23H-porphyrin and 2,5-dihydroxyterephthalaldehyde; TpTMB 1,3,5-triformylphloroglucinol and 2,2'-bis(trifluoromethyl)benzidine; UPLC, ultra-performance LC.

tions and chiral cavity design, which can be used to optimize interactions with target analytes. However, challenges remain in ensuring uniform coating on supports and minimizing issues such as peak tailing, which may arise from particle heterogeneity or limited phase stability.

Various emerging materials have been explored to enhance chromatographic separation, each offering distinct advantages. MIPs provide high selectivity by mimicking biological recognition, enabling the trace-level detection of drugs and pollutants, especially when combined with porous platforms like COFs or MOFs. However, challenges such as template bleeding and batch variability persist. Nanoparticles, including Ni and Au [20, 38], improve surface interactions and mass transfer, and their functionalization enables targeted affinity separations, though they may suffer from aggregation or pressure instability. Natural sorbents such as cyclodextrins, chitosan, agarose, and nylon-6 bring biocompatibility and low cost to the field, proving usefulness for chiral, protein, or vesicle separations, albeit with limited mechanical stability [20, 27, 37, 38]. HOFs, assembled through non-covalent interactions, offer mild synthesis and good selectivity in high-resolution GC [13], though their sensitivity to humidity can be a drawback. Similarly, pillar[n]arenes, with their rigid, symmetric cavities, excel in separating isomers via host–guest and π –interactions, showing superior performance to commercial columns (HP-5 or HP-35) in GC [14], yet remain underused in liquid-phase systems. Together, these functional materials broaden the toolbox for designing advanced stationary phases, enabling tailored selectivity, multimodal interactions, and application-specific performance across a variety of analytical challenges.

2.2. Organic monolithic-based columns

Organic monoliths are continuous, porous polymer matrices formed *in situ* via thermal or photoinitiated polymerization of monomers and crosslinkers, resulting in a highly permeable network. This structure enables fast flow rates and low backpressure—key advantages over conventional packed columns, particularly in high-throughput and miniaturized systems [72]. The surface chemistry of these monoliths is highly tunable through the choice of monomers, allowing for hydrophobic, hydrophilic, zwitterionic, or aromatic functionalities. Examples such as poly(GMA-co-EDMA), 2-naphthylmethacrylate, and butyl methacrylate-based monoliths have demonstrated ex-

cellent performance in reversed-phase separations of peptides, proteins, and small molecules [28, 39, 40].

Despite these strengths, organic monoliths traditionally suffer from lower surface areas and susceptibility to swelling or shrinkage in certain solvents, which can affect reproducibility. However, recent advances—many reflected in **Table 1**—showcase how these limitations can be addressed through post-polymerization modifications and the integration of functional fillers. For instance, the incorporation of carbon dots [37], MIPs [20], or MOFs [54, 62] has significantly enhanced their interaction capacity, selectivity, and mechanical robustness. Additionally, zwitterionic monoliths, such as those based on poly(2-methacryloyloxyethyl phosphorylcholine copolymerized with N,N'-methylenebisacrylamide, poly(MPC-co-MBA) [39], offer strong hydrophilic interaction capabilities, reaching plate counts as high as 120,000 plates/m. Functionalized monoliths with cyclodextrins or silsesquioxanes expand retention modes through host–guest or electrostatic mechanisms as well [36, 37]. For instance, a polymer brush-assisted immobilized metal affinity chromatography (IMAC) composite was developed using superporous agarose particles as the support, flexible copolymer brushes to enhance ligand density, and Ni²⁺-chelated iminodiacetic acid (IDA) as recognition elements [38]. The superporous structure provides high permeability and low backpressure, while the polymer brushes allow for dense and stable ligand presentation, significantly improving binding efficiency through multiple coordination interactions. The composite effectively separates His-tagged proteins from complex biological samples, even in the presence of high concentrations of interfering substances. Additionally, its thermo-responsive properties enable modulation of protein binding by temperature changes, introducing an extra level of control. This material offers key advantages in separation science, including high selectivity, fast mass transfer, and adaptability to complex matrices. However, limitations include the relatively complex synthesis process and potential ligand leaching during prolonged use.

2.3. Silica-based columns

Silica is widely regarded as the gold standard in LC, valued for its high mechanical strength, controlled porosity, narrow particle size distribution, and excellent surface chemistry [73, 74]. Its surface silanol groups can engage in hydrogen bonding, ion-exchange, and

polar interactions, making bare silica particularly effective for normal-phase and HILIC. Functionalization with chemically bonded groups—such as C18, phenyl, amino, or cyano moieties—further extends its utility to reversed-phase and selective separations [19, 23, 24]. Despite its broad applicability, native silica suffers from chemical instability at extreme pH values (typically < 2 and > 8), which can result in surface degradation, dissolution, or structural collapse.

To overcome these limitations, recent developments have focused on creating hybrid organic–inorganic silica materials and composite phases, many of which are summarized in **Table 1**. These include the incorporation of advanced functional materials such as MOFs, COFs, molecular cages, and MIPs, which enhance silica chemical robustness and extend its selectivity and retention mechanisms [21, 22, 26, 29–31, 41, 42, 48, 51–53, 55–58]. The most promising preparation methods for these hybrid materials include:

- Surface grafting or *in situ* growth of functional materials (MOFs, COFs, MIPs) onto silica particles: This method ensures good adherence and coverage, enhancing stability and reproducibility (e.g., MOF-808@SiO₂, COF@SiO₂, RCC3-GQ@NH₂-SiO₂).
- Sol-gel and co-precipitation methods: Used for materials like MIP-202@SiO₂ or ZIF-67@hydrogel@SiO₂, these allow uniform distribution of the sorbent onto silica, enabling multi-mode separation via hydrogen bonding, π -interactions, or ion exchange.
- Layer-by-layer assembly: This approach is often applied when biofunctionalization is required (e.g., pepsin@MOF-5@poly(GMA-co-EDMA)) for precise control over the surface architecture and selectivity.
- Click chemistry and post-synthetic modification: These strategies facilitate the attachment of specific ligands, fluorinated groups, or crown ethers to silica-bound frameworks, enhancing selectivity and performance.
- Core-shell strategies (e.g., SiO₂@SiO₂ microspheres): With precise control of shell thickness and porosity, they enable high-efficiency separations with low backpressure, offering tunability and reproducibility.

For example, PFP-SiO₂ monoliths [19] offer enhanced π - π interactions and reduced backpressure for

hydrophobic analytes, while amino-functionalized silica supports electrostatic interactions with nucleic acids and charged pharmaceuticals. Likewise, biomolecule-silica hybrids, such as those functionalized with pepsin or cyclodextrins, demonstrate high selectivity in enantioseparation or host-guest interactions (see **Table 1**). Several examples listed in **Table 1**—such as RCC3-GQ@NH₂-SiO₂, MIP@NH₂-SiO₂, or COF@SiO₂—illustrate the breadth of strategies used to transform silica into a multifunctional stationary phase platform, capable of accommodating multimodal separation mechanisms and performing well in complex matrices.

To overcome the common issues of incomplete shell coating and poor reproducibility in silica particles, Tang *et al.* [33] performed a mechanistic study to optimize shell formation of SiO₂@SiO₂ core-shell silica microspheres (CSSMs). It was found that ureido modification of the silica core surface significantly lowers its Zeta potential (to -20.1 to -4.8 mV), promoting the uniform deposition of urea-formaldehyde/silica nanoparticle coacervates and leading to more consistent and dense shell growth. Control over parameters such as pH, temperature, reaction time, and water content further improved uniformity and scalability, enabling semi-preparative yields up to 50 g. The shell thickness and pore size could be tuned by adjusting reaction time and the colloidal silica sol particle size. After surface modification with octadecyltrichlorosilane, the resulting CSSMs demonstrated high separation efficiency and low column backpressure as stationary phases in RPLC and UHPLC, effectively separating small molecules, peptides, and proteins. Advantages of this approach include tunability, improved batch reproducibility, and scalability, offering a viable alternative to traditional layer-by-layer methods. Limitations lie in the requirement for careful surface modification and the sensitivity of shell formation to surface potential.

Another example is published by Zhong *et al.* [21] where kaempferol molecularly imprinted monolithic columns (MIMCs) were successfully prepared by surface imprinting on silica monoliths (**Figure 1**), offering a homogeneous pore structure, high surface area (> 100 m²/g), porosity ($\sim 74\%$), and good permeability. Using a straightforward three-step process—monolith synthesis, surface functionalization, and imprinting polymerization—these columns enabled selective chromatographic separation of flavonoids from Ginkgo leaf hydrolysate. Among the different functionalized supports evaluated, ami-

no-modified silica monoliths ($\text{SiO}_2\text{-NH}_2$) exhibited superior chromatographic performance, achieving near-baseline separation of structurally similar flavonoids such as kaempferol, genistein, isorhamnetin, and quercetin. However, when applied in solid-phase extraction (SPE), the thiol- and vinyl-functionalized monoliths outperformed the amino-functionalized ones, providing cleaner extracts with fewer retained impurities. Despite excellent selectivity, the $\text{SiO}_2\text{-NH}_2$ -based MIMC showed limited sensitivity, with a relatively poor limit of detection, suggesting room for improvement in analytical applications. Nevertheless, this study underscores the value of surface imprinting strategies on monolithic supports as a promising route for developing highly selective stationary phases for the separation and analysis of target compounds in complex matrices.

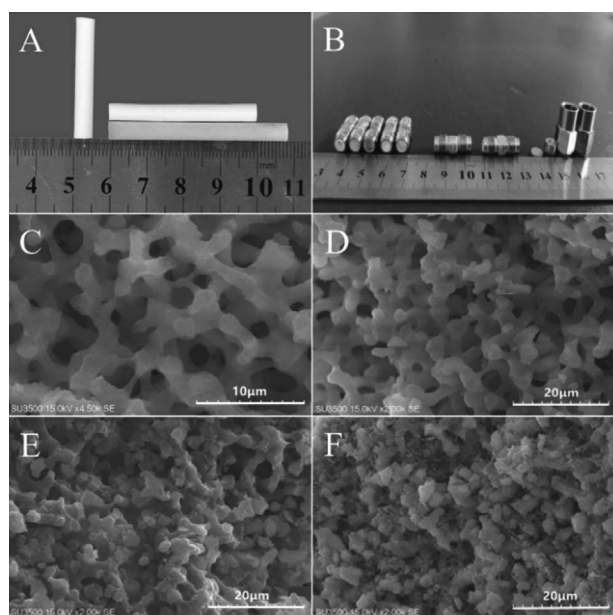


Figure 1. Optical images and micrographs of silica-based columns. (A, B) Appearance morphology. (C) SEM images of SiO_2 , (D) $\text{SiO}_2\text{-NH}_2\text{-MIP}$, (E) $\text{SiO}_2\text{-SH-MIP}$, (F) $\text{SiO}_2\text{-CC-MIP}$. Reproduced from [21] with permission from John Wiley & Sons Copyright® 2025.

These advances confirm that silica, while a mature material, continues to evolve as a central scaffold for next-generation chromatographic stationary phases when combined with nanostructured or biomimetic components. Its adaptability ensures continued relevance across diverse analytical challenges, from environmental analysis to pharmaceutical profiling.

2.4. 3D Printing in Chromatographic Separation

While not a functional material itself, 3D printing has recently emerged as a transformative tool in the development of chromatographic systems, and for that, it is worth mentioning some examples [7, 8]. This technique enables the precise fabrication of custom-designed stationary phase supports, column housings, and microfluidic architectures, which can significantly influence separation performance. As shown in **Table 1**, several examples demonstrate how 3D-printing has been applied to create monolithic columns, metal-based microchips, and customized polymer formats for the efficient separation of proteins, small molecules, and volatile organic compounds, among others [11, 12, 15–17].

The main advantages of 3D printing lie in its geometry control, rapid prototyping, and ability to integrate multiple functions (e.g., flow channels, sorbent beds, connectors) into a single device. Materials used range from GMA-based polymers and acrylates to commercial particles, depending on the separation mode and chemical resistance required. Although 3D printing does not introduce new chemical interactions like MOFs or COFs, it enhances the versatility and applicability of existing functional materials by enabling their incorporation into optimized structures. These formats are particularly attractive for miniaturized systems, on-site analysis, and high-throughput platforms, where conventional fabrication methods fall short.

Wen *et al.* [11] reported a scalable manufacturing strategy for HPLC media that integrates stereolithography 3D printing with porogenic chemistry (**Figure 2**). This enables parallel production of media with consistent macroporous structures and high reproducibility (2.04 % retention time variation across 1,000 columns). The media supports fast separations of proteins and antibodies in reversed-phase and hydrophobic interaction chromatography. Scaling up from analytical to preparative purification was achieved with minimal extra cost or method changes, exemplified by isolating 12 mg of hemeproteins in 8 minutes and processing liter-scale fermentations in 7 hours on a single 20 mm column. Automated production and precise microstructure replication allow excellent method transfer and scalable manufacturing without specialized expertise, offering significant potential for rapid, customizable separation and purification in biosynthesis and pharmaceutical fields. However, despite its advantages, this approach may face limita-

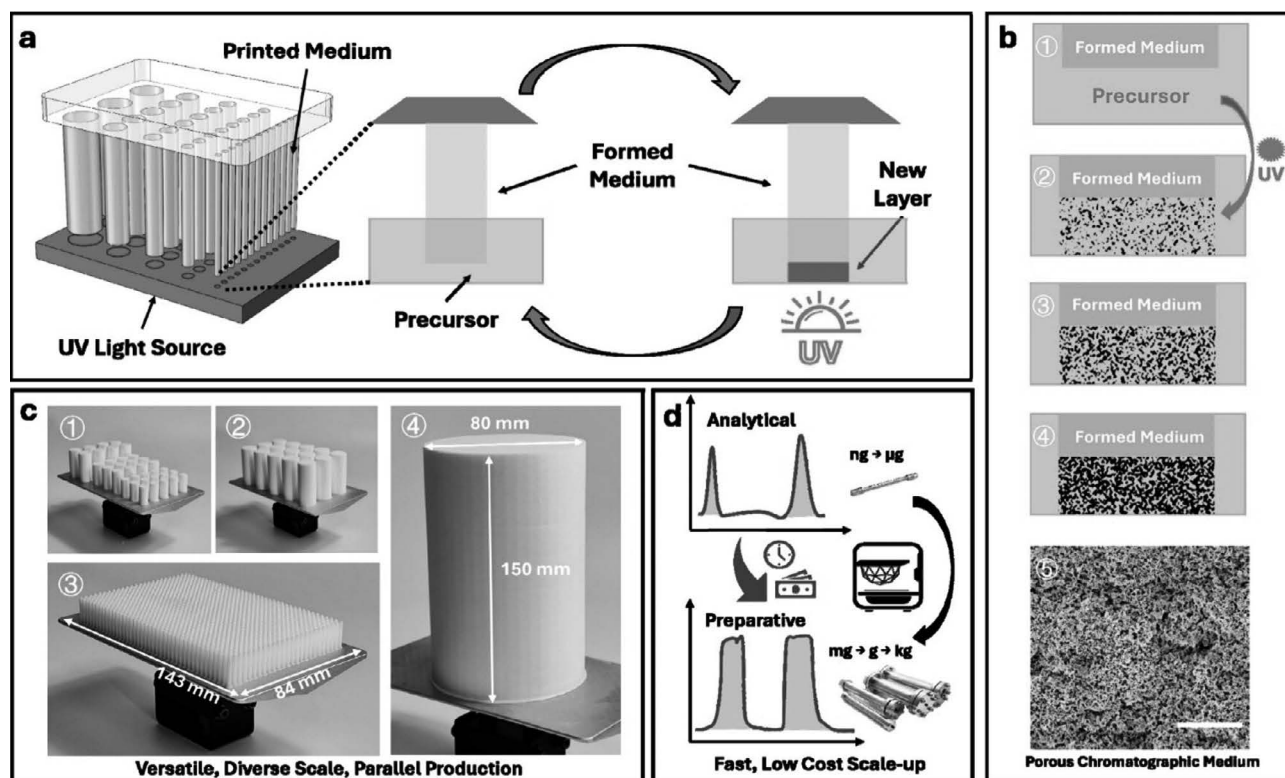


Figure 2. Stereolithographic 3D printing of HPLC stationary phase. (a) Liquid crystal display and digital light processing 3D-printing process for HPLC media. (b) Pore formation mechanism: 1—homogeneous precursor, 2—UV-initiated polymer nuclei, 3—microglobule growth, 4—porous structure formation, 5—SEM image (scale bar: 20 μm). (c) Versatile column formats: 1—analytical (8.5–15 mm i.d.), 2—preparative (20.8 mm i.d.), 3—SPE (1.5 mm i.d., 1000/batch), 4—wide-bore (80 mm i.d.); all printed on 143 $\times$ 84 mm² plates. (d) Scalable, low-cost production and method development using printed media. Reproduced from [11] with permission from the American Chemical Society Copyright® 2025.

tions such as the initial cost and accessibility of high-resolution stereolithography printers, potential constraints in the range of printable chemistries compatible with porogenic formulations (organic solvents), and challenges in scaling beyond certain column dimensions or complex geometries.

3. CURRENT CHALLENGES AND FUTURE OUTLOOK

Despite significant progress, several challenges hinder the widespread use of advanced functional materials in chromatography. Stability remains a concern, especially for MOFs and COFs that degrade under moisture or extreme pH. Reproducibility and scale-up are also problematic, as many synthesis methods are complex and not easily standardized, limiting commercial translation.

Integration into existing platforms is another hurdle—lab-scale successes often fail to transfer to conventional column formats or automated systems. Additionally, the field must address green chemistry concerns, promoting sustainable synthesis routes and biodegradable materials.

Looking forward, bioinspired hybrids (e.g., enzyme–MOF) and 3D-printed materials offer customized solutions with improved performance. The use of AI-based tools to design and predict effective material combinations could accelerate discovery, reduce development time, and enhance application-specific selectivity.

4. CONCLUSIONS

The integration of functional materials into chromatographic stationary phases has opened new avenues

for improving separation efficiency, selectivity, and versatility. Materials such as MOFs, COFs, molecular cages, MIPs, nanoparticles, and natural sorbents offer diverse and tunable interactions with target analytes, enabling the resolution of complex mixtures, including isomeric, chiral, and trace-level compounds. Their ability to introduce multimodal retention mechanisms—ranging from π -interactions and hydrogen bonding to molecular recognition and ion exchange—has significantly enhanced the analytical power of both GC and LC.

Recent strategies involving hybridization with silica or incorporation into organic monoliths have further expanded the applicability of these materials, as reflected in **Table 1**. Moreover, enabling technologies such as 3D-printing are pushing the boundaries of column design and format flexibility, allowing the practical implementation of advanced materials in compact, efficient, and customizable platforms. While most advanced materials reviewed are still at the experimental stage, some are approaching commercial viability (especially silica-based hybrid supports), with potential for near-future translation into market-ready stationary phases.

Acknowledgments

This study was funded by grant PID2021-125459OB-I00 funded by MCIN/AEI/10.13039/501100011033 and by “ERDF A way of making Europe”.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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NOTICIAS DE LA SECyTA

EUROANALYSIS 2025 Y XXIV REUNIÓN CIENTÍFICA DE LA SECyTA (53.ª REUNIÓN CIENTÍFICA DEL GCTA)

Euroanalysis 2025, which will take place in the **Barcelona International Convention Centre** in Barcelona from August 31st to September 4th, aims to be a forum to share knowledge and experience, a think tank and a place to promote Analytical Chemistry networking. It is the conference of the Division of Analytical Chemistry (DAC) of European Chemical Society (EuChemS) and this Edition is organized by the **Catalan Chemical Society** and the **Spanish Society of Chromatography and Related Techniques (SECyTA)** will incorporate the XXIV Edition of its annual Meeting within Euroanalysis 2025. The motto of the conference will be **Analytics 5.0: answering societal challenges**.

Organizing Committee

- Anna de Juan, from *Universitat de Barcelona*, and member of the board of the *Catalan Chemical Society*.
- Rosa Maria Marcé, from *Universitat Rovira i Virgili*, and vice president of the *Catalan Chemical Society*.
- Elisabet Fuguet, from *Universitat de Barcelona*.
- Manel Alcalà, from *Universitat Autònoma de Barcelona*.
- Anna Rigol, from *Universitat de Barcelona*.
- Sònia Sentellas, from *Universitat de Barcelona*.
- Manuela Hidalgo, from *Universitat de Girona*.
- Silvia Lacorte, from *Institute of Environmental Assessment and Water Research, CSIC*.
- Cristian Gómez-Canela, from *Universitat Ramon Llull*.

Plenary speakers

- **Federic Lynen. Ghent University, Belgium.** *Temperature responsive and per-aqueous liquid chromatography: new solutions for more sustainable multidimensional high performance liquid chromatography.*
- **Laura Lechuga. CSIC, Spain.** *Revolutionizing point-of-care diagnostics with nanophotonic biosensors.*
- **Marek Tbiszewski. Gdańsk University of Technology, Poland.** *Greenness metrics and assessments.*

- **Elia Psillakis. Technical University of Crete, Greece.** Winner of Robert Kellner Award Lecture.
- **Günter Gauglitz. University of Tübingen, Germany.** Winner of the DAC Award.

History Lecture

- **Miquel Esteban. Universitat de Barcelona, Spain.**

Keynote speakers

- **Soledad Cárdenas. University of Cordoba, Spain.** *Sustainable sample preparation: from planar extraction devices to affordable ambient mass spectrometry interfaces.*
- **Alegría Carrasco-Pancorbo. University of Granada, Spain.** *Advancing food metabolomics: analytical strategies, main areas of interest and examples of innovative applications.*
- **Costanza Cucci. Italian National Research Council (IFAC-CNR) of Florence, Italy.** *Reflection hyperspectral imaging for artworks and archaeological assets: state of the art and perspectives.*
- **Elena Domínguez Vega. Leiden University Medical Center, The Netherlands.** *Digging into the multifaceted variability of (auto)antibody molecules using novel MS-based approaches.*
- **Peter Eichhorn. Merck Healthcare KGaA.** *Bi-analytical strategies for antibody-based therapeutics in drug discovery and development.*
- **Kim Esbensen.** *WHY do we need a Theory of Sampling (TOS) for analysis?*
- **Javier Hernández-Borges. University of La Laguna, Spain.** *From influent to effluent: understanding microplastic distribution in wastewater treatment.*
- **Hans-gerd Janssen. Unilever/Wageningen University, The Netherlands.** *Advances in chromatography, mass spectrometry and data processing: Their influence on food analysis.*
- **Koen Janssens. University of Antwerp, Belgium.** *Looking at works of art with X-ray eyes: non-destructive spectroscopic imaging and analysis.*

- **Dimitria Lambropoulou. Aristotle University of Thessaloniki, Greece.** *Suspect and Non-Target Analysis for determination of emerging contaminants in water and food samples.*
- **Ivo Leito. University of Tartu, Estonia.** Excellence in analytical chemistry: A joint master's programme.
- **Martina Marchetti-Deschmann. TU Wien, Institut für Chemische Technologien und Analytik, Austria.** *Mass spec imaging: a comprehensive view of molecular insights.*
- **Agata Michalska. University of Warsaw, Poland.** *Adding colour to ion sensing.*
- **Encarnación Moyano. University of Barcelona, Spain.** *Mass spectrometry: a game changer in analytical chemistry.*
- **Claudia Paoletti.** *The new frontiers in food and feed risk assessment.*
- **Rodolfo J. Romañach. University of Puerto Rico, Puerto Rico.** *Innovation and collaboration for process analytical technology and advanced pharmaceutical manufacturing.*
- **Agnieszka Smolinska. University of Maastricht, The Netherlands.** *Where scent meets diagnosis: data-driven volatolomics and chemometrics.*
- **Joanna Szpunar. CNRS, France.** *Mass spectrometry approaches to the analysis of nano- and microplastics.*
- **Frantisek Svec. Charles University in Hradec Kralove, Czech Republic.** *Organic polymer-based nanofibers as an advanced format of sorbents for sample preparation in HPLC.*
- **Romà Tauler. IDAEA-CSIC, Spain.** *Non-target chemometric analysis of MS data.*
- **Oscar Yanes. University of Rovira i Virgili, Spain.** *From mass spectrum to structure: accelerating metabolite identification with AI and cloud computing.*

Preconference courses

Several courses will be taught the first day of the Conference, that will take place at the historical Building of the Universitat de Barcelona. The courses will be taught by experts in each field. The courses are the following:

- **Hyperspectral Imaging: modalities and hardware.** José Manuel Amigo and Martina Marchetti Deschmann.

- **Hyperspectral imaging: software and data analysis.** José Manuel Amigo and Rodrigo Rocha.
- **Basic Chemometrics.** Federico Marini and Agnieszka Smolinska.
- **Advanced chemometrics.** Federico Marini and Agnieszka Smolinska.
- **Why analysis needs the Theory of Sampling (TOS): The importance of the "before analysis" domain.** Kim H. Esbensen.
- **Introduction to liquid chromatography-ion mobility-mass spectrometry.** Encarna Moyano.
- **New trends in bioanalysis.** Raluca-Ioana van Staden.

Awards

- Awards **José Antonio García-Domínguez of the SECyTA** and sponsored by Bruker to the 2 best young oral and poster presentations related to separation techniques.
- Award of **Grupo de Ciencia y Tecnologías (Bio)Analíticas** of the **Spanish Royal Society of Chemistry.**
- Award of the **EuChemS-DAC Sample Prep Study Group and Network** to the best poster presentation in sample treatment.
- Awards of the **American Chemical Society** to young presentations.

Special Volume of Analytical and Bioanalytical Chemistry

A special issue of Analytical and Bioanalytical Chemistry will be dedicated to publishing papers presenting the results shown in Euroanalysis2025.

Grants

Several scientific societies offer grant for attending the conference: SECyTA, Sociedad de Espectroscopia Aplicada (SEA), Sociedad Española de Espectrometría de Masas (SEEM), Sociedad Española de Química Analítica (SEQA), the Divisions of Analytical Chemistry of the German Chemical Society (GDCh), the Royal Society of Chemistry, and the Società Chimica Italiana.

NUEVOS SOCIOS

2096

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4.ª EDICIÓN DEL PREMIO SECyTA A LA MEJOR TESIS DOCTORAL EN CROMATOGRAFÍA Y TÉCNICAS AFINES (Aprobado por la Junta de Gobierno de la SECyTA el 1 de abril de 2025)

La Sociedad Española de Cromatografía y Técnicas Afines (SECyTA) convoca, en su 4.ª edición en 2025, el premio SECyTA a la mejor Tesis Doctoral. Este premio tiene por objeto reconocer el mérito científico de las tesis doctorales realizadas por los socios de la SECyTA sobre Cromatografía y sus Técnicas Afines.

El premio se regirá por las siguientes bases:

1. Habrá un único premio indivisible en el que se entregará al ganador un diploma acreditativo y un cheque nominativo de 1.000 €. El premio podrá ser declarado desierto. El jurado podrá otorgar excepcionalmente un accésit, que consistirá en un diploma acreditativo y 500 €, en el caso que lo considere necesario.
2. Podrá optar al premio cualquier socio de la SECyTA que haya defendido su tesis doctoral entre el 1 de enero y el 31 de diciembre de 2024.
3. Los candidatos deben ser socios de SECyTA en la fecha de la defensa de la Tesis Doctoral, con una antigüedad mínima de un año en relación a la fecha de cierre de esta convocatoria y deberán estar al corriente del pago de la cuota de la Sociedad en la fecha de convocatoria del presente premio.
4. Las candidaturas deberán remitirse a la secretaria de la SECyTA por correo electrónico (secretaria@secyta.es) antes del **30 de abril de 2025**, incluyendo la siguiente documentación en un fichero comprimido o a través de una plataforma de envío de grandes ficheros (WeTransfer, Google Drive, Dropbox, etc.):
 - Carta de solicitud de participación en el premio.
 - Certificado acreditativo de la fecha de defensa de la tesis doctoral.
 - Ejemplar de la tesis doctoral en formato pdf.
 - *Curriculum Vitae* del candidato (en formato normalizado de la FECYT)
 - Resumen de la tesis doctoral, destacando aquellos aspectos más relevantes de su aportación científica en el área de las técnicas

separativas/cromatográficas y afines (máximo 2 páginas^[1]).

- Foto del candidato con la finalidad de su publicación en el Boletín de SECyTA, caso de ser premiado.
 - Anexo con una relación de las publicaciones y comunicaciones a congresos relacionadas directamente con la Tesis doctoral, incluyendo los indicios de calidad (área JCR, índice de impacto, posición en el área, número de citas) de las aportaciones que se presenten como artículos científicos.
5. El jurado del premio estará formado por entre 3-5 investigadores expertos, nombrados por la Junta de Gobierno de la Sociedad, que no tengan publicaciones comunes con los candidatos presentados.
 6. Las decisiones del jurado se tomarán por votación secreta y serán inapelables.
 7. Los criterios de concesión se basarán en la calidad y el carácter innovador de la investigación científica llevada a cabo por cada participante.
 8. El fallo del jurado se comunicará con suficiente antelación antes de la reunión científica de SECyTA y en esta edición el premio se entregará durante la celebración de la XXIV Reunión Anual de la SECyTA que se celebrará en Barcelona del 31 de agosto al 4 de septiembre de 2025.
 9. En el Acto de entrega del premio, se invitará al/la ganador/a a realizar una breve presentación de su Tesis doctoral (máximo 5 min.) que resuma las principales aportaciones y conclusiones. Además, en el periodo de 12 meses siguientes a la aceptación del premio se deberá presentar un artículo para ser publicado en el boletín de la Sociedad.
 10. La concurrencia a este premio supone la aceptación de las bases del mismo.

NÚRIA FONTANALS TORROJA
Secretaria de la SECyTA

^[1] En el caso de una tesis escrita en otra lengua diferente a castellano o inglés se aportará un resumen extendido (máximo 4 páginas) escrito en cualquiera de estos dos idiomas.

PREMIO SECyTA A LA MEJOR TESIS DOCTORAL EN CROMATOGRFÍA Y TÉCNICAS AFINES

4.ª Edición del Premio SECyTA a la mejor Tesis Doctoral en Cromatografía y Técnicas Afines

El pasado 1 de abril de 2025, la Junta de la SECyTA aprobó la convocatoria de la 4.ª edición de los Premios SECyTA a la mejor Tesis Doctoral en Cromatografía y Técnicas Afines, información que fue puesta en conocimiento de todos los socios mediante correo electrónico, web y redes sociales el día 7 de abril.

Una vez llevado a cabo todo el proceso descrito en las bases, el jurado creado para tal efecto emitió su veredicto el día 9 de julio de este año, en el que se destaca “el elevado carácter innovador y calidad científica de todas las tesis doctorales presentadas a esta edición de los Premios”. El veredicto final fue el siguiente:

Premio SECyTA a la mejor Tesis Doctoral defendida en 2024 concedido a la tesis titulada ***Enantiomeric analysis of drugs and/or amino acids by nano-se-***

parative techniques. Improving the selectivity in chiral capillary electrophoresis using ionic liquids and deep eutectic solvents in combination with cyclodextrins, defendida por la **Dra. Sandra Salido Fortuna**, dirigida por las Dras. María Castro Puyana y María Luisa Marina Alegre, y presentada en la Universidad de Alcalá en 2024.

Asimismo, teniendo en cuenta la elevada calidad científica y carácter innovador en Cromatografía y Técnicas Afines del resto de tesis doctorales presentadas, se acuerda conceder el accésit que prevé la convocatoria de esta 4.ª edición en su punto 1 a la Tesis Doctoral titulada ***Determination of organic contaminants using new materials and solvents from a green analytical chemistry perspective***, defendida por la **Dra. Cecilia Ortega Zamora**, dirigida por los Dres. Javier Hernández Borges y Javier González Sálamo, y presentada en la Universidad de La Laguna en 2024.

Resumen tesis Premio Mejor Tesis SECyTA 4.ª Edición del Premio, convocatoria de 2024



Enantiomeric analysis of drugs and/or amino acids by nano-separative techniques. Improving the selectivity in chiral capillary electrophoresis using ionic liquids and deep eutectic solvents in combination with cyclodextrins

Autora: **Sandra Salido Fortuna**

Directores: Dras. María Castro Puyana y María Luisa Marina Alegre

Grupo de investigación: Técnicas de (Micro)Separación, Universidad de Alcalá

Fecha de la defensa: 12 de julio de 2024

El análisis enantioselectivo representa uno de los desafíos más relevantes en la Química Analítica, debido a la necesidad de diferenciar y cuantificar los enantiómeros de compuestos quirales en distintos sectores (farmacéutico, biomédico, alimentario y medioambiental), ya que la actividad biológica, farmacológica o toxicológica de cada uno de esos enantiómeros puede diferir de forma significativa en entornos quirales. En este contexto, el objetivo principal de la Tesis Doctoral fue el desarrollo de metodologías de separación quiral utilizando técnicas nano-separativas, como electroforesis capilar (CE) y nano-cromatografía líquida (nano-LC) para dar solución a problemas analíticos reales mediante procedimientos sostenibles, eficientes y de bajo coste.

Una parte importante de la Tesis se centró en el desarrollo de nuevos métodos enantioselectivos por CE para una amplia variedad de compuestos de interés, incluyendo fármacos (licarbazepina, indacaterol, o ketorolaco) y aminoácidos. La optimización de parámetros experimentales se realizó mediante el empleo de diseños experimentales de superficies de respuesta para maximizar la resolución enantiomérica y minimizar los tiempos de análisis.

Tras la validación, los métodos desarrollados se emplearon en el análisis de formulaciones farmacéuticas, suplementos dietéticos y muestras biológicas. Un aspecto novedoso fue la investigación del mecanismo de reconocimiento quiral en CE mediante la

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combinación de técnicas experimentales (RMN y modelización molecular) que permitió una comprensión más profunda de las interacciones específicas enantiómero-selector, aportando datos clave para el entendimiento de sistemas enantioselectivos.

Otro de los retos científicos abordados, fue la búsqueda de nuevos selectores quirales o aditivos para desarrollar sistemas enantioselectivos novedosos. El empleo de líquidos iónicos quirales basados en aminoácidos (AAILs) y disolventes eutécticos profundos (DESS) en CE se estudió por ser considerados una opción respetuosa con el medio ambiente. Estos compuestos, en general, permitieron mejorar la selectividad, modulando el flujo electroosmótico y favoreciendo las interacciones selector quiral-analito. Su empleo junto a CDs mejoró significativamente la selectividad, resolución y eficacia del sistema de separación, abriendo nuevas posibilidades para la química verde aplicada a las separaciones enantioméricas. Se validaron y aplicaron distintas metodologías, empleando dichos compuestos, a la determinación de fármacos (lacosamida, sulconazol y econazol) en formulaciones farmacéuticas.

Empleando nano-LC, se abordó la evaluación del potencial de una fase estacionaria quiral (amilosa tris(3-cloro-5-metilfenilcarbamato)) para separaciones quirales de fármacos considerados contaminantes emergentes. La optimización de la fase móvil permitió realizar separaciones rápidas, con alta resolución y buena selectividad y, además, se realizó una estrategia de microextracción líquido-líquido basada en el uso de acetato de isoamilo, un compuesto natural, permitiendo la preconcentración de los analitos en muestras de agua de río.

En conjunto, los resultados obtenidos en esta Tesis presentan una contribución integral e innovadora al campo de las separaciones quirales, abordando tanto el desarrollo de nuevos sistemas de separación como su aplicación directa a muestras reales, en contextos farmacéuticos, biomédicos, medioambientales y alimentario. Además, se refuerza el valor de las técnicas nano-separativas como herramientas clave en la Química Analítica moderna, y se abren nuevas vías para el diseño de metodologías limpias y selectivas en el ámbito de la separación y cuantificación de enantiómeros en una amplia variedad de matrices.

Resumen tesis Accésit Mejor Tesis SECyTA 4ª Edición del Premio, convocatoria de 2024



Determination of organic contaminants using new materials and solvents from a green analytical chemistry perspective

Autora: **Cecilia Ortega Zamora**

Directores: Dres. Javier Hernández Borges y Javier González Sálamo

Grupo de investigación: Applied Analytical Chemistry (AChem), Universidad de La Laguna

Fecha de defensa: 26 de junio de 2024

Una de las principales tendencias en Química Analítica es el desarrollo de metodologías de extracción eficientes y sostenibles basadas en los principios de la Química Analítica Verde (GAC). En este sentido, en esta Tesis Doctoral se diseñaron y evaluaron nuevos disolventes de punto eutéctico ultra-bajo naturales (NADESS) y polímeros sensibles a estímulos como fases de extracción para la determinación de diferentes contaminantes emergentes y persistentes (plastificantes, fármacos, hidrocarburos aromáticos policíclicos, bifenilos policlorados y plaguicidas, entre otros) en muestras ambientales, alimentarias y biológicas. Estos nuevos materiales mostraron una capacidad de extracción comparable a la de los convencionales, reduciendo significativamente su impacto ambiental al ser parcial o totalmente biodegradables.

En lo que respecta a los NADESS, se prepararon y caracterizaron disolventes cuasi-hidrofóbicos a partir de mentol o fenchol combinados con ácido acético, y se aplicaron en procedimientos de microextracción líquido-líquido dispersiva de muestras acuosas sin emplear disolventes de dispersión. Además, se desarrolló una versión mejorada basada en la solidificación de la gota orgánica, lo que amplió su aplicabilidad a matrices más complejas y facilitó la manipulación de la gota tras la extracción. Se prepararon también varias mezclas eutécticas a diferentes relaciones molares a partir de los mismos compuestos para mejorar la robustez del método.

Por otro lado, se introdujo por primera vez el uso de polímeros autodegradables en preparación de

muestra, diseñados para despolimerizarse bajo estímulos específicos tras su uso. Se sintetizaron y caracterizaron dos tipos de sorbentes poliméricos: los polímeros de cadena escindible y los polímeros dinámicos covalentes, que demostraron una alta eficiencia en técnicas miniaturizadas de extracción en fase sólida dispersiva. Además, estos materiales presentan la ventaja de degradarse en fragmentos de baja o nula toxicidad o, incluso, en sus compuestos originales al aplicar estímulos adecuados. En el caso del polímero de cadena escindible, se comprobó también que el producto obtenido tras su degradación podía ser repolimerizado permitiendo obtener el polímero original.

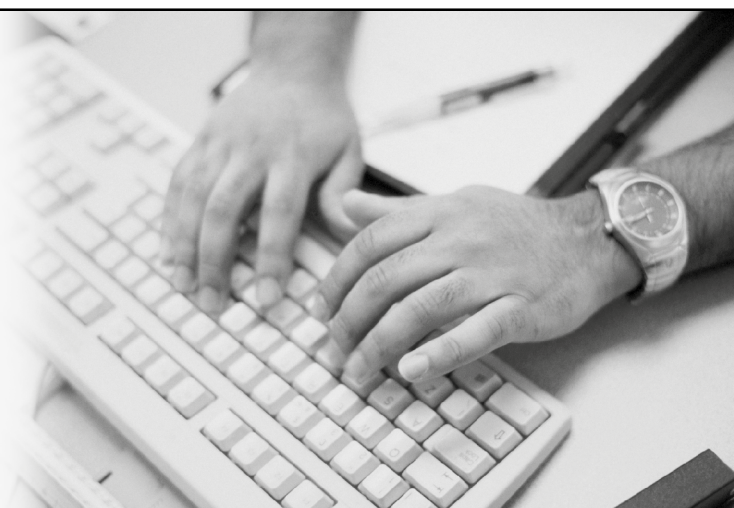
Los procedimientos desarrollados fueron optimizados, validados y aplicados al análisis de muestras acuosas, incluyendo diferentes tipos de aguas, bebi-

das y orina. La separación y detección de los contaminantes objeto de estudio se llevó a cabo utilizando cromatografía de líquidos de alta y ultra-alta eficacia o cromatografía de gases acopladas a diferentes detectores tanto convencionales como de espectrometría de masas. Además, la sostenibilidad de los métodos fue evaluada mediante diferentes métricas basadas en la GAC, en la Preparación de Muestra Verde y en la Química Analítica Blanca, obteniendo puntuaciones favorables cuando se consideraba exclusivamente la etapa de preparación de muestra.

En conjunto, esta Tesis Doctoral proporciona diversas soluciones innovadoras y sostenibles para la preparación de muestras, contribuyendo al avance de la GAC y al diseño de procedimientos analíticos más respetuosos con el medio ambiente.

NOTA DE REDACCIÓN

*Desde el Comité Editorial
os animamos a que nos enviéis
toda aquella información que
consideréis de interés
(premios, jubilaciones, etc.)
para su difusión entre
los lectores del boletín.*



DOS SOCIAS DE LA SECyTA DISTINGUIDAS POR LA REVISTA *THE ANALYTICAL SCIENTIST*

Un año más, la revista *The Analytical Scientist* ha publicado su "Power List" de 2025. En el número de julio, se ha hecho pública la lista correspondiente a este año, denominada en esta ocasión "Leading Voices Edition". Cada año, la revista pregunta a las personas de la "Power List" cuáles son los mayores desafíos a los que se enfrenta la ciencia analítica: la visibilidad, el talento y la sobrecarga de datos suelen ser temas recurrentes. En 2025, se ha sumado a la lista la agitación económica y política —especialmente en torno a la financiación de la investigación—, que presenta dificultades serias propias y, además, amplifica los desafíos ya existentes. A fin de obtener nuevas ideas y soluciones frente a estos desafíos, en 2025, la revista ha dado un giro a su "Power List". En lugar del proceso habitual de nominaciones, la revista ha invitado a los participantes a responder una de tres preguntas cruciales para el campo. Un panel de expertos ha seleccionado posteriormente y a ciegas los 30 pensamientos más originales y argumentos más convincentes frente a estas preguntas, cuyos autores han conformado la "Power List" de 2025.



Coral Barbas es la Directora del Centro de Metabólica y Bioanálisis (CEMBIO), Universidad CEU San Pablo, Madrid.



Lourdes Ramos es Investigadora Científica del Departamento de Análisis Instrumental y Química Ambiental, Instituto de Química Orgánica General (IQOG-CSIC), Madrid.

Este año es un enorme placer el poder contar entre estas voces que lideran la respuesta a los desafíos de la ciencia analítica con dos socias de la SECyTA. En concreto, la Dra. Coral Barbas (CEMBIO, Universidad CEU San Pablo) y la Dra. Lourdes Ramos (IQOG-CSIC), miembros destacados de la SECyTA. Ambas investigadoras han sido seleccionadas para la "Power List" de 2025 por su visión sobre qué debería hacerse para ayudar a que la ciencia analítica alcance protagonismo como la piedra angular de toda buena ciencia y sobre cómo ayudamos a los científicos analíticos de hoy a convertirse en los líderes científicos del mañana, respectivamente. En el enlace de la noticia (<https://theanalyticalscientist.com/power-list/2025/>) se tiene acceso a la visión de estas investigadoras sobre cómo dar respuesta a estos desafíos concretos.

Desde aquí queremos dar a ambas socias de la SECyTA nuestra más sincera enhorabuena por esta merecida distinción.



CONGRESOS CELEBRADOS

24th European Meeting On Environmental Chemistry (EMEC 24)

The European Meeting on Environmental Chemistry (EMEC) takes place annually on behalf of the Association of Chemistry and the Environment (ACE). In 2024, EMEC was hosted by the University of Alicante in Spain from 26th to 29th November. The scientific programme of EMEC 24 was extensive, featuring 2 plenary lectures, 7 keynote lectures, 4 sponsor lectures, 25 oral communications, 25 oral presentations by young researchers, and 140 poster communications. A total of 197 delegates from 32 countries registered for the meeting. The conference benefitted from the support of SECyTA, which participated as a collaborating association.

On the evening of Tuesday 26th November, delegates gathered at the Museum of the University of Alicante for a welcome cocktail and a string-quartet concert. The following morning, the opening ceremony took place in the Auditorium of the University of Alicante. Teresa Lana, Secretary of the University of Alicante, introduced the meeting co-chairs, Lorena Vidal and Antonio Canals, and the ACE representatives. The first scientific talk of the day was a plenary lecture by Pedro Jiménez-Guerrero. His presentation, 'Climate Change and Air Pollution: Two Silent Killers,' explained how climate change and air pollution are linked and why both pose serious risks to human health. He reminded the audience that nearly everyone breathes polluted air and that more than eight million premature deaths each year are linked to air pollution. He argued that we must address both climate change and pollution together to protect public health.

In the first oral session, Silvia Lacorte described how samples of blood and eggs from gulls, flamingos and owls can be used to monitor environmental contaminants such as per- and polyfluoroalkyl substances (PFAS), polychlorinated biphenyls (PCBs), and polycyclic aromatic hydrocarbons (PAHs). Next, Gerhard Lammel spoke about the environmental behaviour of the sixteen PAHs listed by the United States Environmental Protection Agency (US EPA). Later, José Solà-Gullón presented his work on turning carbon dioxide into formate and formic acid using electrochemical methods.

After a coffee break, the second session on environmental monitoring began. The session included six oral communications, although one was cancelled. It opened with Albert T. Lebedev, who presented his work on semi-volatile organic pollutants in the Polar Arctic atmosphere. Using long-term passive sampling combined with gas chromatography coupled with high-resolution mass spectrometry, his team identified benzoic acid as the compound present at the highest concentrations. The remaining talks covered a variety of environmental pollutants: Karolina Czarny-Krymiński discussed the degradation of bisphenols by green algae and cyanobacteria; Evgeny Bulatov presented the application of passive samplers for monitoring contaminants in water, including pharmaceuticals and pesticides; and Marta Turull focused on the detection of metal pollutants.

A shared lunch at the University restaurant gave delegates an opportunity to continue their discussions in an informal setting. In the afternoon, the session chaired by Albert T. Lebedev and Polonca Trebše opened with presentations from conference sponsors. Emanuele Ceccon of Restek Corporation discussed the latest methods for analysing PFAS and the regulatory landscape, while Julio Lluch of LECO Corporation talked about enhancing non-targeted analysis using comprehensive two-dimensional gas chromatography coupled with high-resolution mass spectrometry in environmental samples. A poster session rounded off the formal programme of the day, providing an opportunity for further discussion and exchange among participants. Later, delegates registered for a guided tour of the historic centre of Alicante departed, while the rest took part in a workshop for early-career researchers about tips and resources in finding the right postdoctoral position.

On Thursday, the day began with three keynote lectures. Lourdes Ramos opened the session with a presentation on persistent organic pollutants, followed by Ana Rita Lado, who explored contaminants of emerging concern, ranging from pharmaceuticals to personal care products, emphasising the role of enantioselectivity in the environment. The final keynote in this session, delivered by José Juan Santana, examined organic UV filters, a type of personal care

product, as markers of anthropogenic micropollution. The morning continued with several oral communications covering agro-environmentally friendly processes, advances in food chemistry, environmental modelling and monitoring, as well as developments in green chemistry and sustainable approaches. After lunch, the young researchers' oral presentations began, divided into two parallel sessions: one in the main auditorium and the other in an upstairs classroom. Presentations in the auditorium highlighted green chemistry strategies, alongside contributions on environmental monitoring and environmental technologies. After the second poster session, the conference gala dinner took place at the Meliá Alicante Hotel, bringing a close to a full day of scientific debate and networking.

On Friday, the eleventh oral session began with two keynote lectures. Francisco Javier Vilaplana presented biochemical strategies for the valorisation of agrifood side streams within a circular primary-production framework, explaining how residues from agricultural processing can be converted into valuable bioproducts. Manuel Miró then discussed the role of microplastics as vectors for plastic-additive chemicals, showing how small polymer particles can transport harmful substances through the environment. Two further talks that morning, given by representatives of Agilent Technologies and Bruker Daltonics, focused on microplastic analysis and PFAS detection, reinforcing earlier discussions in the conference.

The final scientific session focused on environmental technologies. At midday, the ACE held its General Assembly, to which all EMEC 24 participants were invited. As part of their conference registration,

delegates already held full ACE membership for 2025. During the Assembly, a new Executive Board was elected for the 2025–2029 period, and plans for upcoming meetings were announced: EMEC 25 will be hosted in Crete, Greece, and EMEC 26 in Klaipėda, Lithuania.

After a farewell brunch, the second and final plenary lecture was delivered by Eleftheria Psillakis, chairwoman of EMEC 25. She spoke on cigarette water leachates as an overlooked environmental issue. The closing ceremony began with the announcement of the young scientist awards. I was honoured to receive the Best Poster Communication Prize for Young Researchers, sponsored by Restek Corporation, and I would like to express my gratitude to the Scientific Committee and to Restek for this recognition.

Overall, EMEC 24 brought together researchers to share advances in environmental chemistry, from pollutant monitoring to sustainable technologies. Beyond the scientific sessions, the meeting encouraged collaboration and the exchange of ideas, reinforcing its role as a key forum for addressing environmental challenges. Finally, I extend my gratitude to SECyTA for providing the grant that enabled me to attend this meeting.

ANDRÉS DUQUE VILLAVERDE

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Participation in the 21st Annual International Conference of the Metabolomics Society (Metabolomics 2025, Prague, Czech Republic)

I had the privilege of attending the 21st Annual International Conference of the Metabolomics Society, held from 22nd-26th June 2025, in the historic and picturesque city of Prague (Czech Republic). The conference took place at the Prague Congress Centre, a large neo-functionalist building located in the Nusle district, originally known as the Palace of Culture of Prague. The venue, set on the edge of the Nusle Valley and near the iconic Nusle Bridge, offered impressive facilities and panoramic views of the city, contributing to a memorable scientific environment. This event is one of the most important annual gatherings in the metabolomics field, bringing together leading researchers, technology developers, and young scientists from around the world to share the latest advances, challenges, and opportunities across all domains of metabolomics.

The conference offered an intense and highly enriching scientific program. The event opened on Sunday 22nd June with a series of pre-conference workshops that provided participants with valuable training on advanced and emerging methodologies. Among the several workshops I attended, I would like to highlight the session titled 'W6: Demystifying Stable Isotope Labelling Metabolomics', presented by Dr. James MacRae (The Francis Crick Institute, UK) and Dr. Bart Ghesquière (KU Leuven, Belgium). The session focused on the application of stable isotope labelling to investigate metabolic pathways in both *in vitro* and *in vivo* systems, and how this approach can provide insights into metabolic fluxes that are not accessible through conventional untargeted metabolomics. The workshop covered essential aspects of experimental design, including selection of isotopic tracers (e.g., [U-¹³C₆]glucose, ¹³C-glutamine, ¹³C-acetate), labeling duration, routes of administration, and technical considerations for both bolus and continuous infusion strategies. On Monday 23rd June I also had the opportunity to attend the Career Night Roundtable Discussion, a dynamic session designed to provide early-career researchers with insights into various professional pathways in metabolomics. The panel featured international experts from academia, industry, and governmental research institutions who shared their experiences and advice on topics such as postdoctoral opportunities, transitioning between sectors, leadership in science, and grant writing. It was an inspiring session that offered practical guid-

ance and a global perspective of scientific career development.

The following days were structured around plenary lectures, thematic oral sessions, poster sessions, sponsor exhibitions, and panel discussions. The plenary sessions addressed current challenges in clinical metabolomics, large-scale data integration, standardization of analytical workflows, and sustainability in omics sciences. Throughout the conference, parallel oral sessions were held on topics such as computational metabolomics, plant and food metabolomics, environmental applications, lipidomics, and novel analytical technologies. These sessions showcased cutting-edge work, including advances in ion mobility spectrometry, high-resolution mass spectrometry, data annotation pipelines, and integration with proteomics and transcriptomics. I found the oral communications on lipidomics especially stimulating, as they offered updated perspectives on quantitative workflows, new extraction protocols, and data interpretation strategies.

During the poster sessions, I had the opportunity to present my research work titled 'Decoding the Lipidome of Human Seminal Plasma in the Context of Male Infertility'. The study, developed within the framework of my PhD at the Centre of Metabolomics and Bioanalysis (CEMBIO) of the Faculty of Pharmacy (CEU-San Pablo University) and led by Prof. Coral Barbas, explores lipid-based biomarkers in human seminal plasma using untargeted lipidomics strategies (LC-QTOF-MS), aiming to gain mechanistic insight into male subfertility. Our methodological comparison of four extraction protocols revealed that the Matyash method provides the best performance for both polar and non-polar lipid species. We successfully annotated over 230 lipids across 20 subclasses. The presentation generated valuable feedback and led to engaging discussions with researchers working in clinical bioanalytics and lipidomics. Several attendees expressed interest in our curation pipeline.

Besides the scientific program, the conference included social events, such as welcome receptions and the gala dinner held in a historical venue in Prague. These activities provided an excellent opportunity to meet young and senior scientists, share ideas, and explore potential collaborations. I also had the chance

INFORMACIONES

to speak informally with experts from academic and industrial settings, which was both motivating and insightful for the development of my career in analytical and biomedical research.

These social activities provided an excellent environment to reconnect with fellow researchers. In particular, I had the pleasure of meeting again many early-career scientists I had first encountered during the *European School for Metabolomics (EUSM2024)*, held in June 2024 at the University of Granada. It was extremely rewarding to share how our respective research projects had progressed since that date. Additionally, I was glad to meet and interact with several fellow members of the Young Researchers Group of the Spanish Society for Metabolomics (Jóvenes de la SESMet), to which I also belong. The group includes PhD and Master's students, as well as junior postdoctoral researchers from diverse metabolomics backgrounds.

Attending Metabolomics 2025 has been a remarkable milestone in my PhD journey. It has not only enabled me to present and discuss my work at an international level, but also to learn from leading scientists, explore emerging tools and trends, and broaden my scientific network. I am particularly grateful to the Spanish Society of Chromatography and Related Techniques (SECyTA) for granting me financial support through a travel grant, which made my participation possible. The knowledge and experience gained during this conference will undoubtedly contribute to the improvement of my ongoing research and future scientific output.

LUZ ALONSO-DASQUES

PhD Student

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University Madrid (Spain)*

NOTA DEL COMITÉ EDITORIAL

Desde el Comité Editorial del Boletín de la SECyTA queremos comunicaros los cambios en cuanto a su composición que, a partir de este número, tendrán lugar. Despedimos con cariño a Mario Fernández del Instituto de Química Orgánica General (CSIC) quien, con gran compromiso y dedicación, ha desempeñado un papel destacado, no sólo dentro del Boletín, sino como webmaster y gestor de redes sociales de la SECyTA. Por otra parte, agradecemos la incorporación de Belén Gómara, del mismo Instituto, quien debido a su experiencia en la Junta de la SECyTA y en otras actividades organizadas por nuestra Sociedad, sin duda será una aportación de gran utilidad a nuestro Boletín. ¡Bienvenida, Belén!

CALENDARIO DE ACTIVIDADES

1. **ISSS 2025: 29th International Symposium on Separation Sciences**
25-27 de septiembre de 2025. Belgrado (Serbia)
Chair: **Ž. Tešić**
<https://isss2025belgrade.rs/>
2. **PREP 2025: 37th International Symposium on Preparative and Process Chromatography**
29 de septiembre-2 de octubre de 2025. Filadelfia (EE. UU.)
Chairs: **O. Dapremont, S. Menegatti y N. Vecchiarello**
<https://www.prep2025.org/>
3. **21st International Workshop on Emerging HRMS and LC-MS Applications in Environmental Analysis and Food Safety**
7-8 de octubre de 2025. Ottawa (Canadá)
Chair: **D. Aga**
<https://lcmsms2025.ca/>
4. **Dioxin 2025: 45th International Symposium on Halogenated Persistent Organic Pollutants (POPs)**
1-6 de noviembre de 2025. Antalya (Turquía)
Chair: **P. Kurt-Karakus**
<https://www.dioxin2025.org/default>
5. **μTAS 2025: 29th International Conference on Miniaturized Systems for Chemistry and Life Sciences - Micro-Total Analysis Systems**
2-6 de noviembre de 2025. Adelaida (Australia)
Chairs: **M. Breadmore, R. Guijt y C. Priest**
<https://microtas2025.org>
6. **SETAC Europe 36th Annual Meeting**
17-21 de mayo de 2026. Maastricht (Países Bajos)
Chair: **N. van den Brink**
<https://www.setac.org/discover-events/global-meetings/setac-europe-36th-annual-meeting.html>
7. **ISCC 2026: 44th International Symposium on Capillary Chromatography y 21st GCxGC Symposium**
17-22 de mayo de 2026. Riva del Garda (Italia)
Chairs: **L. Mondello y P. Sandra**
<https://iscc44.chromaleont.it/>
8. **HTC-19: 19th International Symposium on Hyphenated Techniques in Chromatography and Separation Technology**
26-29 de mayo de 2026. Leuven (Bélgica)
Chairs: **S. Eeltink, F. Lynen, D. Cabooter**
<https://htc-19.com/>
9. **HPLC 2026: 55th International Symposium on High Performance Liquid Phase Separations and Related Techniques (HPLC 2026)**
6-11 de junio de 2026. Indianápolis (EE. UU.)
Chairs: **J. Anderson y T. Maloney**
<https://hplc2026-symposium.org/>
10. **ECC10: 10th EuChemS Chemistry Congress**
12-16 de julio de 2026. Amberes (Bélgica)
Chairs: **C. De Bie y T. Vranken**
<https://euchems2026.eu/>
11. **IMSC 2026: 26th International Mass Spectrometry Conference**
22-28 de agosto de 2026. Lyon (Francia)
Chairs: **I. Fournier e I. Compagnon**
<https://imsc26.com/>
12. **ISC 2026: 35th International Symposium on Chromatography**
6-10 de septiembre de 2026. Praga (República Checa)
Chairs: **M. Holčápek y L. Nováková**
<https://www.isc2026.org/>

ARTÍCULOS DE INTERÉS

Herramientas para la evaluación de métodos analíticos

Las métricas para la evaluación de métodos analíticos han atraído un enorme interés por parte de la comunidad analítica, y es cada vez más común su utilización en artículos científicos de este ámbito.

En un momento donde el desarrollo de métodos cada vez más sostenibles ha pasado a ser una prioridad, el empleo de estas herramientas ha tenido un impacto muy positivo e inmediato en las publicaciones de Química Analítica. Gracias a su implementación, se ha cuestionado el empleo, sin justificación objetiva, de adjetivos como *environmentally friendly*, *sustainable* o *green* a la hora de designar nuevas metodologías. Además, dichas métricas han permitido guiar a los grupos de investigación sobre cómo se pueden mejorar sus trabajos para conseguir que sean más seguros para el/la investigador/a y para el medio ambiente.

No obstante, y pese a su cada vez mayor popularidad, su empleo ha generado también controversia. Así, si bien la simplicidad es una de sus virtudes, ésta puede también favorecer su manejo sin un conocimiento previo suficiente, lo que incrementa aún más la subjetividad de los resultados obtenidos. Por otro lado, la creación de cada vez más herramientas con pequeñas modificaciones sobre las existentes puede acabar por confundir y desmotivar a nuevos/as potenciales usuarios/as.

El objetivo de esta reseña es pues, comparar tres de las herramientas más utilizadas para la evaluación de métodos analíticos, comparando su facilidad de uso y los aspectos considerados en dicha evaluación, con el fin de guiar al personal usuario que todavía no esté familiarizado con este tipo de métricas, o que quiera profundizar sobre su aplicación.

AGREE—Analytical GREENness Metric Approach and Software

Francisco Pena-Pereira, Wojciech Wojnowski, Marek Tobiszewski (2020). *Analytical Chemistry*, 92, 10076-10082

La aplicación AGREE se puede decir que es una de las responsables de la elevada popularidad de este tipo

de métricas. Gracias a su interfaz *user friendly* y a un diseño simple, es de las herramientas más empleadas junto con su versión centrada en la preparación de muestra (AGREEprep).

En la Figura 1, podemos ver que la aplicación AGREE cuenta con 12 apartados correspondientes a cada uno de los principios de la Química Analítica Verde. Todos los apartados cuentan con el mismo peso para la evaluación, aunque se pueden modificar manualmente, justificándolo en función de la pretendida aplicación. En el centro de la gráfica se muestra un número entre el 0 y el 1, donde el 0 correspondería a un método poco “verde” y el 1 a uno muy “verde”. Sin embargo, es necesario señalar que el valor obtenido por estas herramientas no se debe interpretar como un valor absoluto, requiriéndose su comparación con metodologías previas a la hora de objetivar las potenciales mejoras de las metodologías propuestas.

Otra de las ventajas de esta métrica es el algoritmo que utiliza para calcular el valor final, ya que, como veremos más adelante, muchas otras métricas emplean modelos de selección de unas 3-4 opciones, lo que limita la diferenciación de los resultados.

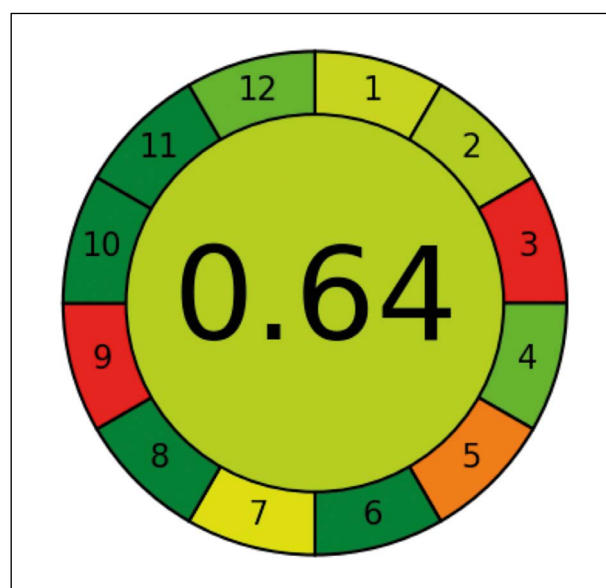


Figura 1. Evaluación de un método analítico realizado con la herramienta AGREE.

Modified GAPI (MoGAPI) Tool and Software for the Assessment of Method Greenness: Case Studies and Applications

Fotouh R. Mansour, Justyna Plotka-Wasyłka, Marcello Locatelli (2024). *Analytica*, 5, 451-457

El GAPI original es una de las aplicaciones pioneras y otra de las responsables de la popularización de este tipo de herramientas. El GAPI, como observamos en

la Figura 2, nos presenta 5 pentágonos correspondientes a distintos parámetros a evaluar dentro del proceso analítico: muestreo (a), preparación de muestra (b y c), reactivos y disolventes (d), instrumentación (e). Cada triángulo es un ítem para evaluar, en el que se despliegan 3-4 opciones para elegir y, en función de la selección, aparecerá el triángulo en rojo (poco sostenible), amarillo (intermedio) y verde (sostenible).

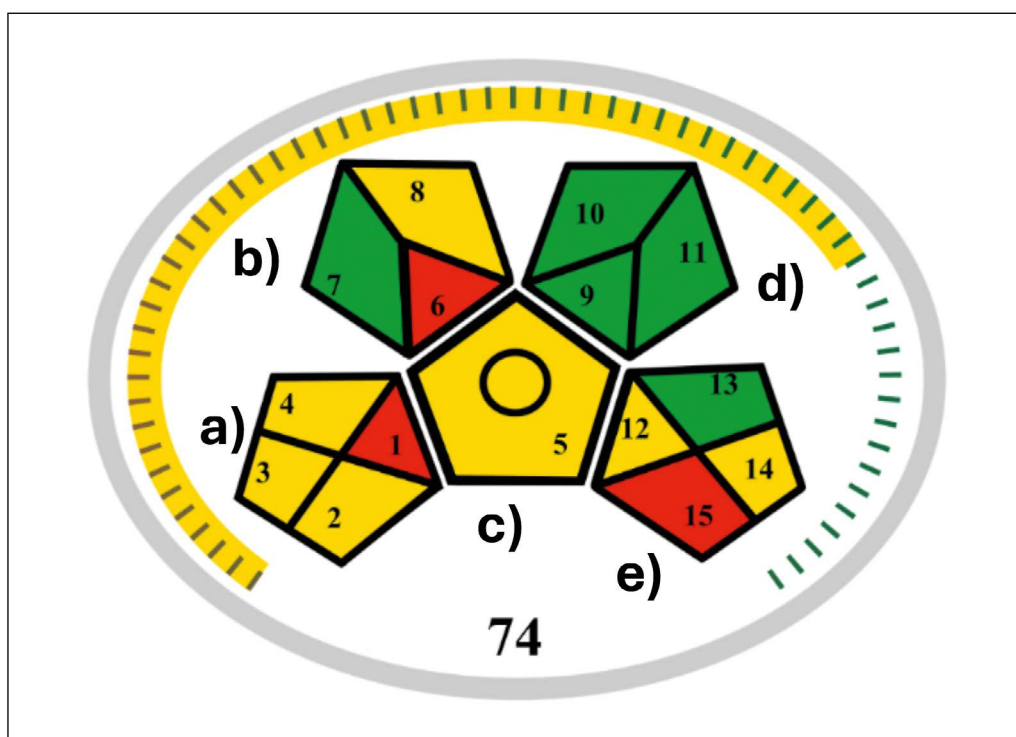


Figura 2. Evaluación de un método analítico realizado con la herramienta MoGAPI.

Años más tarde, aparecería el COMPLEXGapi, añadiendo un hexágono en la parte inferior, donde se evalúan otras etapas previas, como la síntesis del material.

Pese a cubrir la totalidad del procedimiento analítico y su sencillez de manejo, todavía contaba con una serie de desventajas. Una de las más relevantes, era la ausencia de un dato cuantitativo. Aunque hemos hablado en apartados anteriores que el valor numérico no debe interpretarse como un valor absoluto, éste facilita su comparación con métodos previos descritos en la bibliografía. Además, basar el sistema en un código de colores lo hace poco inclusivo para personas con visibilidad reducida u otro tipo de discapacidades visuales.

Finalmente, aparecieron el MoGAPI (Fig. 2) y ComplexMoGAPI, los cuales sí incluían un sistema de evaluación numérica sin necesidad de pasos adicionales para el/la usuario/a.

Sin embargo, todavía persisten algunos problemas, como el hecho de que los resultados deriven de la selección de 3-4 opciones, lo que provoca que, por ejemplo, un método que use 10,1 mL de disolvente no sea considerado como verde, mientras que uno que emplee 9,9 mL, sí lo sea. A pesar de ello, es de destacar el esfuerzo para ir mejorando la herramienta a lo largo de los años, en lugar de ir creando nuevas y diferentes métricas en su lugar.

Blue applicability grade index (BAGI) and software: a new tool for the evaluation of method practicality

Natalia Manousi, Wojciech Wojnowski, Justyna Płotka-Wasyłka, Victoria Samanidou (2019). *Green Chemistry*, 25, 7598

La última aplicación, no trata de evaluar el carácter “verde” del método y se centra más en la Química Analítica “Azul”, más enfocada en la practicidad, el factor económico y la eficiencia de los métodos analíticos. Este parámetro solía pasar más desapercibido, pero, gracias a esta herramienta, ha ganado mucha más presencia en los artículos de Química Analítica.

La aplicación BAGI se ha convertido en una de las más utilizadas, ya que es la única que se centra en la practicidad de forma exclusiva y, al igual que pasaba para las dos aplicaciones previas, su interfaz es simple y fácil de manejar.

En la Figura 3 se muestra un ejemplo de una evaluación con BAGI. En el centro del diagrama aparece un valor entre 25 y 100, correspondiendo 25 a un método poco práctico y 100 a uno muy práctico. Tal y como describe el trabajo, un método con una puntuación por encima de 60 ya puede ser considerado como práctico, pero, como se ha hecho mucho hincapié en esta reseña, no se deben considerar como absolutos los resultados obtenidos y siempre deben ser contextualizados y comparados con los de métodos previos.

En este caso, existe un código de intensidad de color, donde un azul más intenso indica que el ítem evaluado es más práctico. Por otro lado, al igual que ocurría en el GAPI, cada ítem nos da una selección de 3-5 posibilidades, aunque en este caso suelen ser

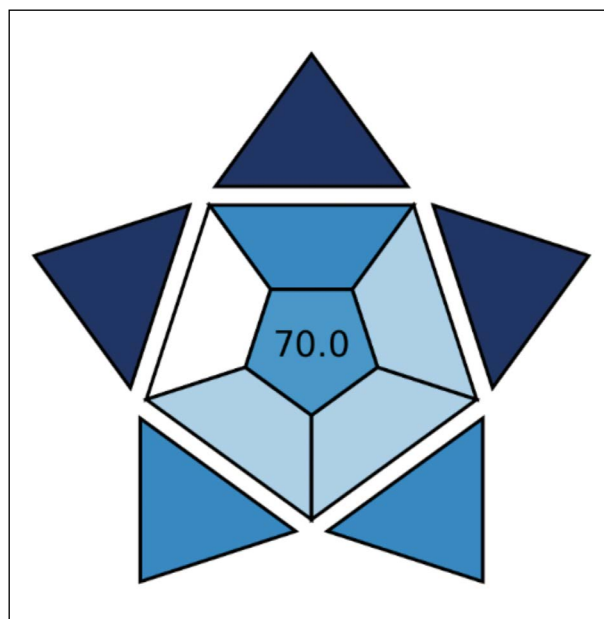


Figura 3. Evaluación de un método realizado con la herramienta BAGI.

variables más cualitativas, por lo que está más justificado.

En cuanto a sus virtudes, además de la sencillez, cabe mencionar el hecho de que esta herramienta hace distinciones en cuanto al volumen de muestra en función de su procedencia, diferenciando si son biológicas o no, lo que puede ser también de interés para determinadas aplicaciones.

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INSTRUMENT: PEGASUS® BTX

EXPAND YOUR PFAS ANALYSIS— SCREEN FOR TARGETS AND IDENTIFY UNKNOWN SIMULTANEOUSLY

Key Words: PFAS, GC-MS, HR-MS, TOFMS, Environmental Analysis, Pollutants, Emerging Substances, Non-target, NTS, Screening.

Background and Description

Research into the prevalence of per- and polyfluoroalkyl substances (PFAS) —also known as ‘forever chemicals’ due to their high stability in our environment and food chain— continues to grow. At the same time, regulatory control of these species in our water and food supplies continues to gain momentum. However, analysis of PFAS in complex environmental samples can be challenging due to the enormous number and variety of PFAS chemicals. New analytical methods must be developed to monitor PFAS in the environment.

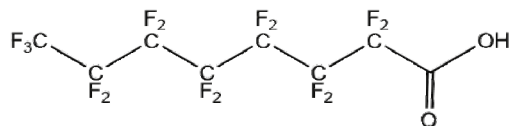


Figure 1. PFAS Sources.

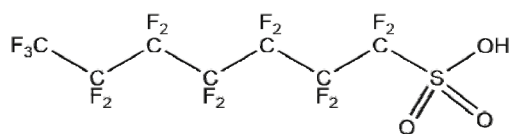
This application note focuses on the rapidly expanding area of PFAS analysis and highlights how screening for known PFAS targets, as well as discovering and identifying unknown PFAS chemicals, can be performed using high-performance Gas Chromatography with Time-of-Flight Mass Spectrometry (GC-TOFMS). New libraries are being developed to facilitate the screening of these pollutants in samples.

Sources and Types of PFAS

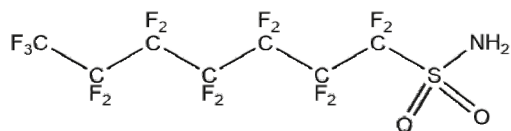
A huge array of products, that we use and are exposed to daily, contain PFAS (Figure 1). There are thousands of different PFAS molecules used in the industries producing these materials. PFAS have been categorized into different groups depending on their functionality. For example, PFAS that are currently screened by LC-MS and GC-MS methods include perfluoroalkylcarboxylic acids (PFCA), perfluoroalkanesulfonates (PFSA), perfluoroalkanesulfonamides (FASA), and fluorotelomer alcohols (X:2FTOH). The perfluorinated sections (alkyl backbone), vary in length and may be branched. Several representative, commercially available PFAS are provided (Figure 2): 1) Perfluoro-



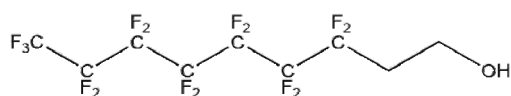
Perfluorooctanoic acid (PFOA)



Perfluorooctanesulfonic acid (PFOS)



Perfluorooctanesulfonamide acid (PFOSA)



Octylfluorotelomer ethanol (8:2 FTOH)

Figure 2. Examples of some common PFAS types (some available as analytical standards).

rooctanoic acid (PFOA), 2) Perfluorooctanesulfonic acid (PFOS), 3) Perfluorooctanesulfonamide (PFOSA), and 4) 2-perfluorooctyl ethanol (8:2FTOH).

PFAS Screening Using GC-TOFMS

With huge numbers of PFAS varieties in existence, the use of powerful screening technologies is vital. For volatile and semi-volatile PFAS analysis, GC-TOFMS is ideal, due to the ability to collect sensitive, full mass range data at high acquisition rates. This allows a variety of

real-world sample matrices to be analyzed, such as a set of commercially available 'Anti-Fog and Demisting,' products. These products contain a variety of PFAS as indicated by Stapleton and coworkers.¹ Simultaneous target and non-target screening (NTS) of these products was performed using a **LECO Pegasus® BTX GC-TOFMS** system. For example, analysis of an anti-fog spray product (Figure 3), revealed some known target PFAS compounds, but also an array of unknowns as well. Electron ionization-Mass spectrometry (EI-MS) spectral fragmentation indicated that they could be assigned as PFAS candidates.

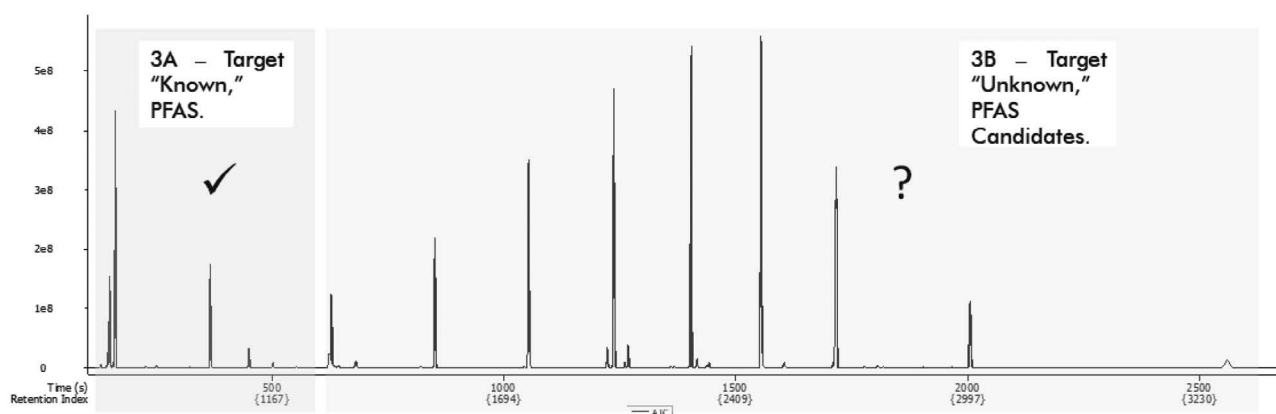


Figure 3. Simultaneous target and non-target screening of a commercially available 'anti-fog' spray. Sections of 'known' PFAS targets (3A highlighted in green) and 'unknown' PFAS candidates (3B highlighted in grey) are displayed.

The presence of five PFAS target compounds (Figure 3A) was confirmed using analytical standards and similarity matching to NIST 2023 mass spectral

and retention index (RI) library entries. These five species are highlighted in the zoomed-in section of the chromatogram and table below (Figure 4).

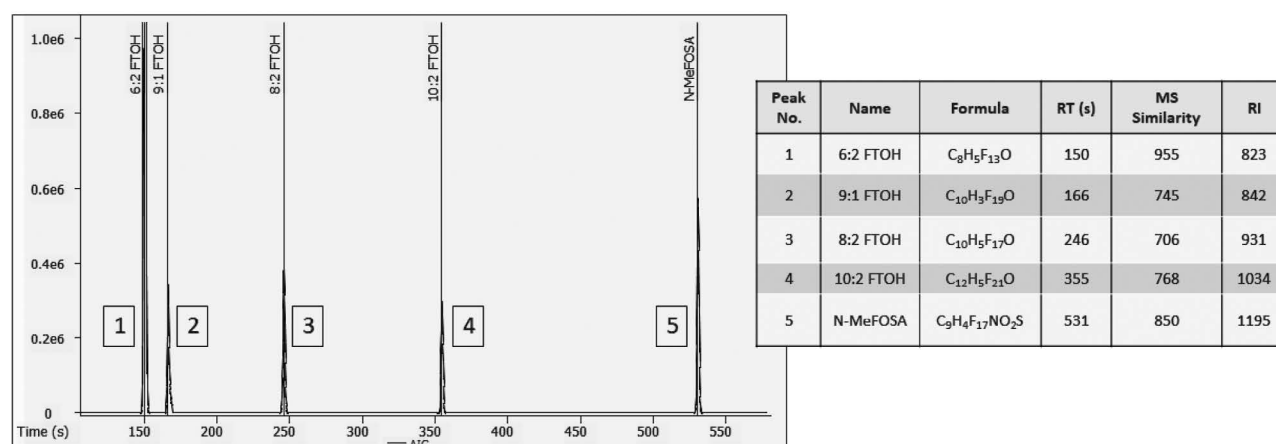


Figure 4. A zoomed-in section of the chromatogram is highlighted in Figure 3A, showing five target PFAS species that were identified using standards and library data. Nomenclature used corresponds to the alkyl chain of the perfluorinated and functional group sections of the compounds. For example, 6:2 FTOH represents a perfluorinated 6-carbon backbone tail with an ethanol head.

In addition to the target PFAS molecules found, the non-target data collected also revealed several other components (Figure 3B), which were judged to be possible PFAS candidates. The nine most prominent peaks showed similar mass spectral fragmentation, indicating the presence of fluoroalkyl and ethoxy groups. However, elution times were spread out rather evenly as the GC temperature gradient increased,

suggesting a homologous series of PFAS. To investigate the identification of these species, further analysis was performed using a **LECO Pegasus HRT+** high resolution, accurate mass GC-TOFMS system, equipped with a **Multi-Mode Ion Source® (MMS®)**. This ion source allows electron ionization (EI), as well as positive and negative chemical ionization (PCI and NCI), to be performed.

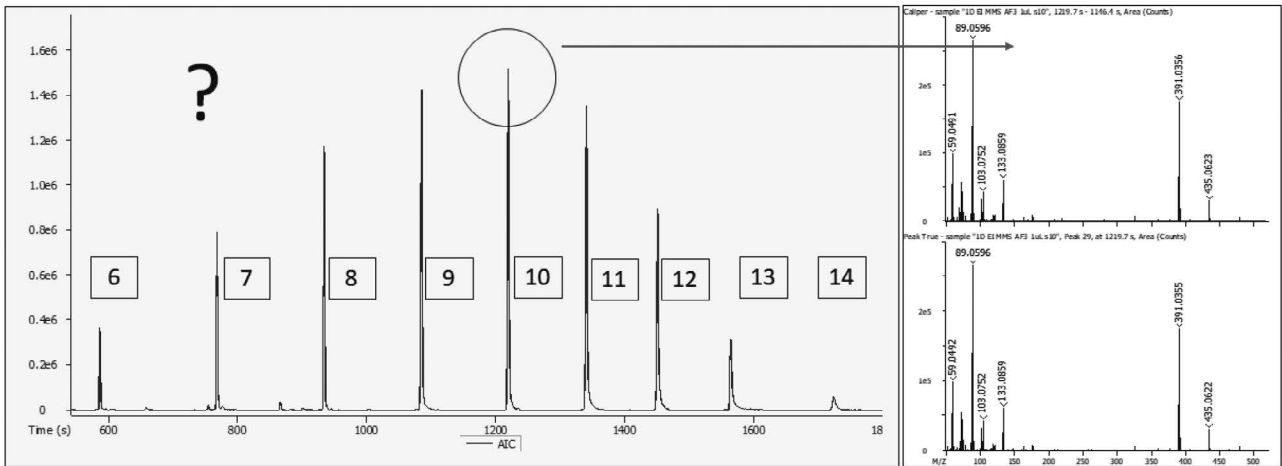


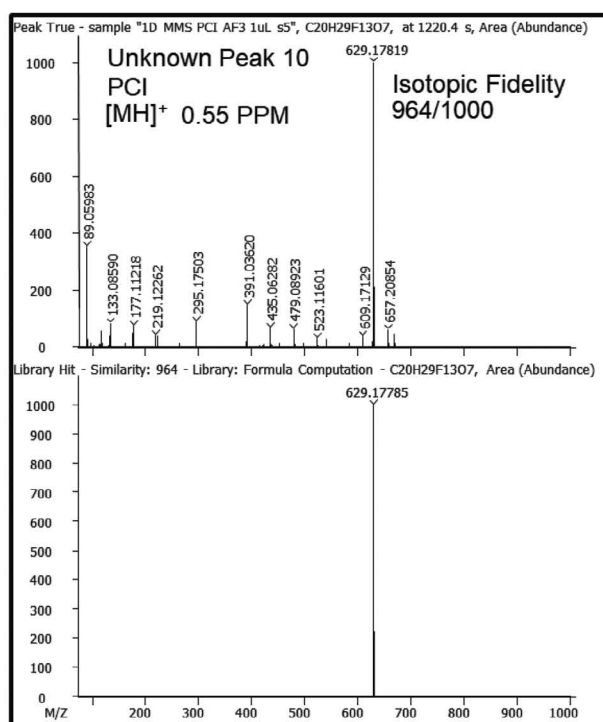
Figure 5. 5A) The chromatogram section featuring unknown PFAS candidates, peaks 6-14. 5B) The EI mass spectra for peak 10.

The most prominent unknown peaks (6-14, Figure 5A) all showed very similar EI mass spectral accurate mass fragments (Figure 5B, representative MS spectrum for unknown 10), which was useful in confirming the possibility that they were PFAS candidates. To obtain further structural information and to identify the species with higher confidence, positive chemical ionization data was collected, facilitating the generation of intense protonated molecular adducts.

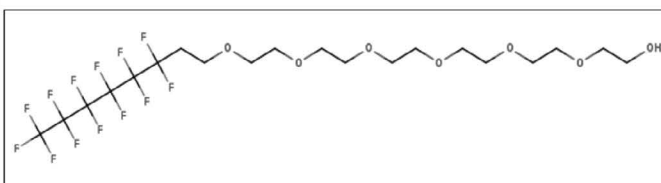
The generation of accurate mass molecular ion data provided formulas for $[MH]^+$, $[M+CH]^+$, and $[M+CH]^+$ adducts with mass accuracies of less than ± 1 ppm, and allowed strong tentative identification of the unknown compounds to be a group of fluorotelomer ethoxylates (FTEOs), as shown for peak 10 (Figure 6), via a search of the EPA CompTox Chemicals Database.² The list of similarly strong tentative identification formulas for this PFAS class —reached using the same process for peaks 6-14— is provided below (Table 1).

Table 1. Unknown peaks 6-14, tentatively identified as a class of fluorotelomer ethoxylates (FTEOs), PFAS compounds.

Peak	Name	Formula	Molecular Mass
6	2-(2-(2-(Perfluorohexyl)ethoxy)ethanol	C ₁₂ H ₁₃ F ₁₃ O ₃	452.0657101
7	2-[2-(2-(2-(Perfluorohexyl)ethoxy)ethoxy)ethoxy]ethoxy]ethanol	C ₁₄ H ₁₇ F ₁₃ O ₄	496.0919251
8	2-[2-(2-[2-(2-(Perfluorohexyl)ethoxy)ethoxy]ethoxy)ethoxy]ethoxy]ethanol	C ₁₆ H ₂₁ F ₁₃ O ₅	540.1181399
9	2-[2-(2-(2-[2-(2-(Perfluorohexyl)ethoxy)ethoxy]ethoxy)ethoxy)ethoxy]ethoxy]ethanol	C ₁₈ H ₂₅ F ₁₃ O ₆	584.1443546
10	2-[2-(2-(2-[2-(2-(Perfluorohexyl)ethoxy)ethoxy]ethoxy)ethoxy)ethoxy]ethoxy]ethoxy]ethanol	C ₂₀ H ₂₉ F ₁₃ O ₇	628.1705694
11	23-(Perfluorohexyl)-3,6,9,12,15,18,21-heptaaoxatricosan-1-ol)	C ₂₂ H ₃₃ F ₁₃ O ₈	672.1967841
12	26-(Perfluorohexyl)-3,6,9,12,15,18,21,24-octaoxahexacosan-1-ol)	C ₂₄ H ₃₇ F ₁₃ O ₉	716.2229989
13	29-(Perfluorohexyl)-3,6,9,12,15,18,21,24,27-nanoxanonacosan-1-ol)	C ₂₆ H ₄₁ F ₁₃ O ₁₀	760.2492136
14	32-(Perfluorohexyl)-3,6,9,12,15,18,21,24,27,30-decaoxadotriacontan-1-ol)	C ₂₈ H ₄₅ F ₁₃ O ₁₁	804.2754284



Ion	Formula	m/z obs	m/z calc	PPM
[MH] ⁺	C ₂₀ H ₃₀ F ₁₃ O ₇	629.17785	629.17819	0.55
[M+C ₂ H ₅] ⁺	C ₂₂ H ₃₄ F ₁₃ O ₇	657.20915	657.20854	-0.92
[M+C ₃ H ₅] ⁺	C ₂₃ H ₃₄ F ₁₃ O ₇	669.20915	669.20952	0.56



Name:

2-{2-(2-(2-(2-(Perfluorohexyl)ethoxy)ethoxy)ethoxy]ethanol

EPA CompTox ID: DTXSID901339320

Molecular Formula: C₂₀H₂₉F₁₃O₇

Molecular Mass: 628.170569 g/mol

Figure 6. PCI Data and structural determination of unknown peak 10, using ChromaTOF® software with high-resolution accurate mass data for molecular adducts and subsequent search of the molecular formula with the EPA CompTox Chemicals Database.

Conclusion

Meeting the growing environmental research and regulatory needs for PFAS analysis requires the use of powerful technologies to screen for known targets and to detect and identify unknown PFAS candidates. Here, sub-nominal mass GC-TOFMS, allowed simultaneous, full mass range, highly sensitive target, and NTS screening for PFAS in Anti-Fog/Demisting products, detecting a variety of both known PFAS and unknown PFAS candidates. The use of accurate mass GC-HR-TOFMS technology with EI and CI capabilities facilitated strong tentative identifications of the unknowns to be a class of fluorotelomer ethoxylates (FTEOs). This approach, together with the results ob-

tained, suggests that these technologies are an ideal choice for screening and identification of volatile and semi-volatile PFAS, in an array of sample types in complex matrices.

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2. United States Environmental Protection Agency, Computational Toxicology Chemicals Dashboard: <https://comptox.epa.gov/>

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APPLICATION NEWS

Nexis GC-2030 combined with Polyarc reactor

DETERMINATION OF LITHIUM-ION BATTERY ELECTROLYTE COMPOSITION WITH POLYARC MICROREACTOR

Waldemar Weber¹, Omar Mayorga¹, Rebecca Kelting¹, Nerea Lorenzo Parodi¹

¹ Shimadzu Europa GmbH.

User Benefits

- High accuracy quantitative determination of electrolyte composition.
- Result directly from one measurement without external and internal calibration.

Introduction

The production of the electrolytes for lithium-ion batteries takes place at different places globally. For quality assurance it is essential to determine the precise composition of organic carbonates. Variations in their composition can significantly affect battery performance and safety. Accurate analysis ensures that manufacturers can maintain consistent quality and meet the stringent requirements of the industry, leading to more reliable and efficient energy storage solutions.

The producers typically provide the weight percentages (%w) as the given composition. To determine this composition different analytical technologies can be used, typically GC-FID, GC-MS, LC or NMR. All of these technologies (except for NMR) have one thing in common: they all provide molecule-dependent responses. In other words, to determine the weight percentages (%w), an external calibration with all expected compound standards would need to be performed.

This is a common practice and typically does not pose a problem in routine operations. Nevertheless, for semi-routine and non-routine laboratories this leads to a significant time investment. In this article,

we present a new, highly accurate GC-based method without the need for external or internal calibrations.

The Polyarc system has a catalytic microreactor that enhances gas chromatographs with flame ionization detectors (FIDs) by converting all organic compounds to methane molecules prior to their detection by the FID, therefore converting the FID into a quantitative carbon detector (QCD). An additional advantage of this approach is that by eliminating complex calibrations, the accuracy of quantification is significantly enhanced.

Sample Preparation and Measurement

25 μ L LIB electrolyte with 1M LiPF₆ has been diluted with 1 mL dichloromethane and centrifuged for 5 min at 8500 rpm. The centrifuged solution was transferred into a 2 mL GC glass vial and measured by GC-2030 with Polyarc reactor.

The Package

For this application, a Shimadzu GC-2030 with liquid sampler AOC-30i (Figure 1, left) and Polyarc reactor (Figure 1, right part) was used.

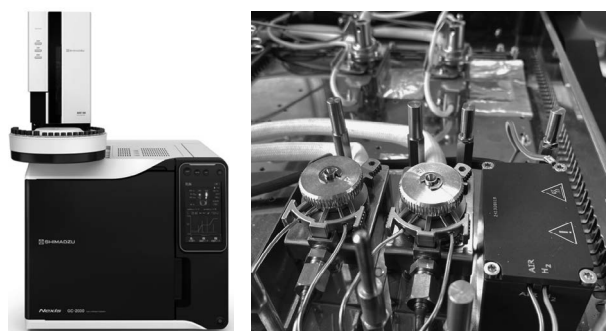


Figure 1. Shimadzu GC-2030 with AOC-30i (left) and Polyarc reactor (right).

The recommended analytical hardware and software configuration is listed below.

- **Main Unit.** Nexis GC-2030 gas chromatograph with FID-2030 detector and Polyarc catalytic microreactor.
- **Accessory.** AOC-30i liquid sampler.
- **Main Consumables.** SH-5 column (30 m $\times$ 0.25 mm $\times$ 0.25 μ m; P/N 221-75701-30).
- **Software.** LabSolutions LCGC.

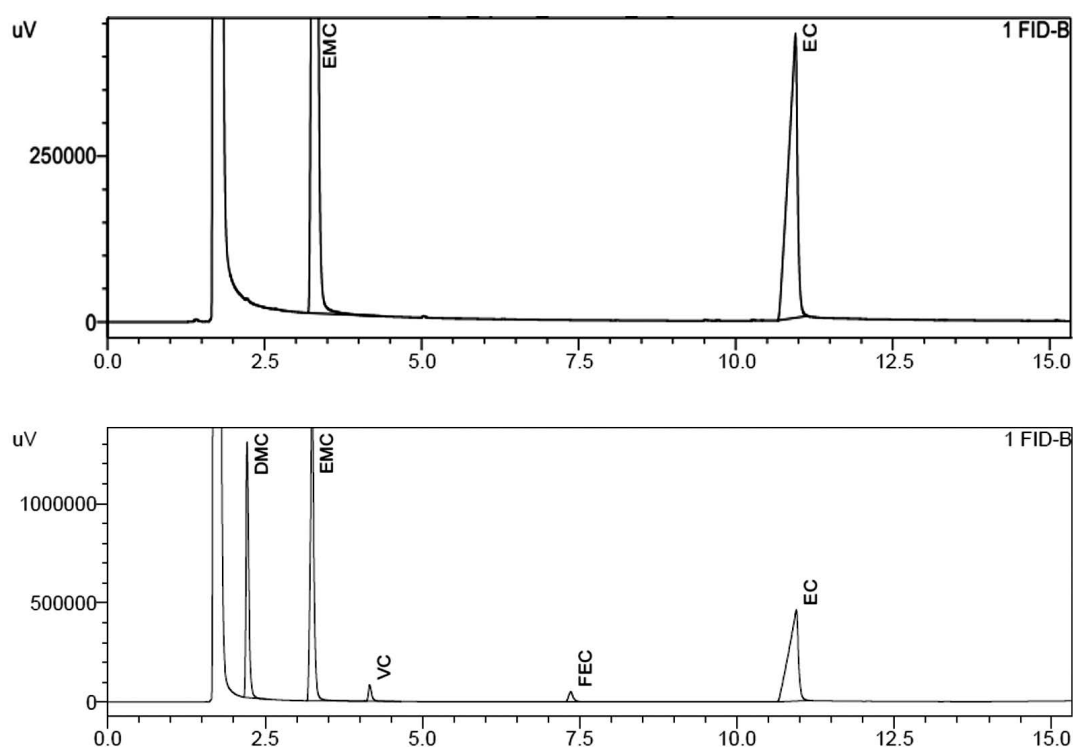


Figure 2. Obtained chromatograms of two measured LIB electrolytes.

Results and Discussion

The obtained results of two different measured electrolytes are shown in Figure 2.

The two measured electrolytes are slightly different in composition of main carbonates and additives. Both represent quite typical products often used for LIBs manufacturing. For both a manufacturer's specification of the weight percentage (%w) is available. The original specifications may slightly differ from the really quantified values. The reason for that is the native decomposition and rearrangement of carbonates already during the storage. As long as the decomposition occurs only on a small scale, it does not have any impact on the quality of the electrolytes.

Since the Polyarc reactor converts all substances to methane before the FID, providing a molecule-independent response, the calculation of weight percentages (%w) using this approach is very straightforward. Basically, the software integrates the related compounds (main compounds and additives) peak areas and calculates the % of areas out of these values. The obtained % of areas are at the same time the needed %w of all integrated compounds.

This technology even does not require an accurate and precise sample preparation, the sample amount should just not overload the reactor and FID. Not presented within this application note, but a possible feature is the calculation of decomposition/purity grade. In that case the sum of peak areas of the target components are compared to the sum of peak areas of the unknown components in a percentage relationship. These two % areas are then the %w between the targeted compounds and destruction decomposition products (or impurities) in the electrolyte.

The calculated %w of the investigated electrolytes in comparison to the manufacturer specifications are shown in Table 1. The electrolytes were measured three times to calculate the %RSD.

The results shown in Table 1 demonstrate a very high accuracy in the RSD of weight percentage calculations, with all components being <1%. The correlation between the calculated weight percentages and those provided by the manufacturers also shows a very good agreement. Minor differences arise, as mentioned earlier, due to prior storage, transportation, and sample preparation. Overall, Table 1 clearly indicates that a reliable correlation between the meas-

Table 1. Obtained results for %w calculations.

Compound		DMC	EMC	DEC	VC	FEC	EC
Sample 1	Peak area average	n.d	11969890	n.d	n.d	n.d	4430757
	%RSD	—	0.2	—	—	—	0.5
	Calculated %w	—	73%	—	—	—	27%
	Specified %w	0	70%	0	0	0	30%
Sample 2	Peak area average	3894856	6076716	n.d	294409	263520	4918256
	%RSD	0.8	0.6	—	0.8	0.5	0.7
	Calculated %w	25.2%	39.3%	—	1.8%	1.7%	32%
	Specified %w	27-29%	35-37%	0	1.7-2.5%	1.7-2.5%	34-38%

ured values and the specifications is possible, thus ensuring a dependable quality assurance analysis.

Conclusion

This application demonstrated the suitability of the Shimadzu GC-2030 with Polyarc reactor to fulfil a

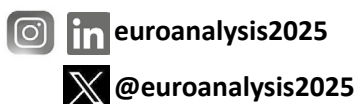
common request for the quality assurance of LIB electrolytes. Within only one measurement and without any additional time it is possible to obtain high accuracy results. Polyarc reactor is an important add-in to a classical GCMS analysis in this field, where the MS is used for confirmation and identification and the Polyarc-FID as a detector for the reliable quantification of sample composition.

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NOVEDADES TÉCNICAS



DISOLVENTES DE ALTA PUREZA PARA ANÁLISIS DE PFAS

Los compuestos perfluoroalquilados y polifluoroalquilados (PFAS, por sus siglas en inglés) han emergido como contaminantes globales de gran preocupación debido a su persistencia, bioacumulación y potenciales efectos adversos para la salud humana y el medio ambiente.

Estos compuestos químicos sintéticos, con enlaces carbono-flúor, extremadamente estables, han sido utilizados durante décadas en la fabricación de envases, recubrimientos antiadherentes, ropa, etc., pero se les atribuyen ciertos riesgos para la salud humana.

Ante este creciente enfoque regulatorio y legislativo, ha aumentado la necesidad de realizar análisis precisos y libres de contaminantes de fondo. Debido a la amplia presencia de estos compuestos en la vida cotidiana, esto se ha convertido en un desafío para los laboratorios de análisis.

El análisis de PFAS requiere técnicas sensibles y específicas. Entre los métodos más empleados se destaca la cromatografía de líquidos de alta resolución acoplada a espectrometría de masas (LC-MS/MS), que permite identificar y cuantificar diversos PFAS en muestras ambientales y biológicas. La preparación de muestras frecuentemente involucra procesos de extracción en fase sólida (SPE) para concentrar y limpiar los analitos de interés. La selección adecuada de materiales y solventes es fundamental para evitar contaminaciones cruzadas y resultados falsos positivos,

dado que los PFAS pueden estar presentes incluso en materiales de laboratorio.

Scharlab presenta su nueva gama desarrollada específicamente para el análisis de PFAS. Estos disolventes han sido fabricados, purificados y envasados para garantizar la ausencia de compuestos perfluoroalquilados y polifluoroalquilados. El análisis de estos compuestos se realiza con técnicas de LC-MS/MS, por lo que son aptos también para estas técnicas. A su vez, garantizan unos niveles de estos compuestos por debajo de los límites establecidos por la EPA 533 y EPA 537.1. <https://www.scharlab.com/es/es/productos-quimicos/disolventes-para-analisis-de-pfas>

Para más información sobre estos compuestos y cómo tratarlos, apúntate a nuestro webinar técnico de **PFAS en muestras medioambientales y alimentarias: ¿Cuáles son los retos?**

Apuntate aquí:



NORMAS DE PUBLICACIÓN

La revista *Cromatografía y Técnicas Afines (CTA)* (ISSN 1132-1369) es el boletín de la Sociedad Española de Cromatografía y Técnicas Afines (SECyTA) cuya función es la de ser un medio de comunicación entre sus miembros, los profesionales que trabajan en cromatografía y técnicas relacionadas y las empresas del sector.

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4. Informaciones (congresos, reuniones, cursos, nuevas tesis doctorales y otros acontecimientos de interés).
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6. Novedades y notas técnicas (sección de información de los nuevos productos y/o aplicaciones de las empresas colaboradoras con la SECyTA).
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CTA publica artículos relacionados con técnicas analíticas (de separación, de identificación, etc.), bien sobre investigaciones en las propias técnicas o sobre aplicaciones de las mismas. Los autores de los artículos recibirán una compensación económica (**300 euros**) por cada artículo publicado en CTA.

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Para publicar artículos en CTA **no** es necesario ser socio de la SECyTA.

El idioma de la revista y, por tanto de escritura de los artículos, es el castellano, aunque se admiten también artículos en inglés.

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Los trabajos deberán estar escritos a doble espacio, con un tamaño de fuente de 10 ó 12 pt y cada página deberá ir numerada. El tamaño de los trabajos

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ana.ruiz@csic.es, acsoria@iqog.csic.es,
angeldelapuerta@iqog.csic.es, bgomara@iqog.csic.es

Los trabajos de investigación no deberán haberse publicado previamente. Antes de su publicación todos los trabajos serán revisados por especialistas en el tema, quienes juzgarán la conveniencia de su publicación o propondrán a los autores las modificaciones oportunas.

Título: Deberá ser conciso y reflejar el contenido del trabajo. A continuación se citará el nombre de los autores con la dirección completa de cada uno de ellos, incluyéndose también el correo electrónico y teléfono del autor al que deberá remitirse la correspondencia.

Resumen: De 100 a 150 palabras reflejando de forma clara y concisa el propósito y los resultados más relevantes del artículo.

Texto principal: los trabajos originales de investigación seguirán el formato tradicional, incluyendo **Introducción, Materiales y Métodos, Resultados y Discusión, Conclusiones y Bibliografía.**

Bibliografía: Las referencias bibliográficas aparecerán en el texto entre paréntesis con el apellido de los autores y el año (e.g. Bianco y Edwards, 2008). Si son más de dos autores, se citará el apellido del primero seguido por "y col.," y el año de publicación (e.g. García-Pérez y col., 2007). Si se citan varias referencias juntas se separarán por punto y coma (e.g. Smith y col., 1980; Brit y col., 1985). Al final del artículo las referencias serán ordenadas por orden alfabético con el siguiente formato:

- 1) Hirota, T., Ohki, K., Kawagishi, R., Kajimoto, Y., Mizuno, S. *Hypertens. Res.* 2007 (30), 489-496.
- 2) Venter, J. C. "The Emission of Sulfur to the Remote Atmosphere" en *The Biogeochemical Cycling of Sulfur and Nitrogen* (Eds. J. N. Galloway y col.). D. Reidel Publishing Co., Dordrech, Holland (1985), p. 346.

Tablas: Se enviarán con un breve encabezamiento y numeradas según el orden de aparición en el texto.

Figuras: Se enviarán en un archivo diferente, separadas y numeradas por orden de aparición en el texto. Las leyendas deberán incluirse al final del artículo a continuación de la bibliografía.

NUEVAS TESIS DOCTORALES

En esta sección se incluyen resúmenes en español de las Tesis Doctorales que se han defendido en los últimos 12 meses. La extensión no debe ser superior a 300 palabras incluyendo título de la tesis, lugar y fecha de defensa y directores de la misma. Sería conveniente incluir una foto del doctor.

El número de resúmenes estará condicionado al espacio disponible para esta sección dentro del Boletín.

INFORMACIÓN BIBLIOGRÁFICA - ARTÍCULOS DE INTERÉS

En esta sección se incluye una revisión de tres artículos recientes y de diferentes autores sobre un tema de interés dentro del ámbito de la cromatografía y técnicas afines. Estas contribuciones serán remuneradas con **75 euros**.

NOTAS TÉCNICAS

Las empresas colaboradoras de la SECyTA pueden contribuir en esta sección con información técnica (nuevos desarrollos, aplicaciones, etc.) en el campo de la cromatografía y técnicas afines. Deberán remitirse a la redacción de CTA con anterioridad a los días **1 de mayo** (para el primer número) y **1 de noviembre** (para el segundo).

NOVEDADES TÉCNICAS

Las empresas colaboradoras de la SECyTA disponen en cada número de una página gratuita para informar sobre las novedades de sus productos. La extensión máxima de los originales será 3 DIN A4 mecanografiados a doble espacio, pudiéndose incluir algunos gráficos y fotografías en blanco y negro (no más de tres). Los plazos de envío serán los indicados en las Notas técnicas.

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La adjudicación de los espacios disponibles destinados a publicidad se realizará por riguroso orden de petición.

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CTA agradecerá toda la información que reciba de sus lectores sobre asuntos de interés general dentro del campo de la cromatografía y técnicas afines (cursos, conferencias, congresos, ofertas de trabajo, informes sobre el trabajo de grupos españoles y extranjeros, reseñas de libros o cualquier tipo de colaboración).

A su vez, CTA publicará, en la medida de lo posible, respuestas de especialistas a todas aquellas cuestiones concretas que formulen los lectores en relación con sus problemas en el laboratorio o con asuntos relacionados en general con la cromatografía y técnicas afines.

Para cualquier cuestión relacionada con CTA pueden ponerse en contacto con:

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