

30th International Symposium on Separation Sciences
Univers T Hotel & Cluj-Napoca, Romania



BOOK OF ABSTRACTS



30th International Symposium on Separation Sciences

September 21st – 24th, 2026
Cluj-Napoca, Romania

CASA CĂRȚII DE ȘTIINȚĂ

Editor: Virginia COMAN

Co-Editor: Dan Constantin NIȚĂ, Simion BELDEAN-GALEA

International Symposium on Separation Sciences

Book of Abstracts

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Casa Cărții de Știință
Cluj-Napoca, 2026

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Cluj-Napoca, Romania

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WELCOME to the 30th Edition of ISSS

September 21–24, 2026, Cluj-Napoca



Dear participants of the 30th edition of ISSS,

On behalf of the Scientific and Organizing Committees, we have the honour and great pleasure of extending a warm welcome to the **30th Edition of the International Symposium on Separation Sciences**—an event that, with the exception of the coronavirus pandemic period, has been held annually.

The 30th Edition of the ISSS Symposium is dedicated to all those who promote chemistry among the general public and, in particular, the younger generation, offering them special opportunities to become valuable scientists in the field of separation sciences.

The symposium is highly beneficial for the younger generation, offering them the opportunity to enrich their knowledge regarding recent advances in chromatography, hyphenated separation and detection techniques, and sample preparation methods, as well as to acquire valuable new skills for their careers. Furthermore, participants can establish new connections with colleagues from various universities and countries, while also having the chance to meet internationally renowned scientists.

The 30th Edition of ISSS 2026 focuses on fundamental and practical aspects of separation and detection methods for various compounds from diverse and complex matrices, as well as on hyphenated, multidimensional and miniaturized techniques applied for analytical, preparative and industrial purposes, including new horizons and challenges in separation sciences, accompanied by debates on the theme "Advanced today, conventional tomorrow in separation sciences".

The scientific programme includes two Laureate Plenary Lectures delivered by renowned scientists nominated through a CEGSS selection process for the European Tswett-Nernst Award, 11 Plenary Lectures and 18 Keynote Lectures by invited speakers, as well as 31 Oral Presentations by distinguished senior scientists and researchers in the field of separation sciences. Special attention is paid to the younger generation through 23 Flash Oral Presentations and 17 e-Poster Presentations.

We are pleased to announce that the 30th edition of the ISSS Symposium is attended by approximately 150 registered delegates from 20 countries across Europe and Asia. An exhibition is being held alongside the event, showcasing equipment, columns, and accessories for various separation techniques.

We thank everyone who made the organization of this symposium possible—Babeş-Bolyai University, the Romanian Chemical Society, the National Research Agency, and the Central-European Group for Separation Sciences—as well as the sponsors, exhibitors, media partners, and donors for their financial support. Special thanks go to the members of the Scientific and Organizing Committees for promoting the 30th edition of the ISSS Symposium—a jubilee Edition—and for their varied contributions to the event's success.

We would like to extend our sincere and warm thanks to all the invited speakers who agreed to participate in the symposium and deliver excellent and engaging presentations in the field of separation sciences.

We also extend special thanks to all the participants; they presented excellent abstracts covering all specific areas of separation sciences—ranging from fundamentals to applications in chemistry, biology, pharmacy, medicine, environmental protection, ecology, the food industry, the life sciences, etc.—as well as aspects related to multidimensional separation and hyphenated detection techniques.

The best communications presented by the young generation will be awarded during the symposium after the decision of two international scientific juries, representing both the senior and the young generations.

An exciting social programme is organized, designed to offer participants the opportunity to discover our city, called the *Treasure City*, not only as a place anchored in the past or present, but as a space of coexistence. Exploring Cluj-Napoca can become a fascinating adventure, thanks to the region's distinctive multicultural character.

We look forward to meeting you in Cluj-Napoca at the 30th Edition of the ISSS Symposium—a Jubilee Edition.

Virginia Coman

Simion Beldean-Galea

Symposium Chairs

<https://iss2026.conference.ubbcluj.ro>

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General Information

Symposium Venue

Univers T Hotel, 53-55 Alexandru Vaida Voevod Street

400529 Cluj-Napoca, Romania

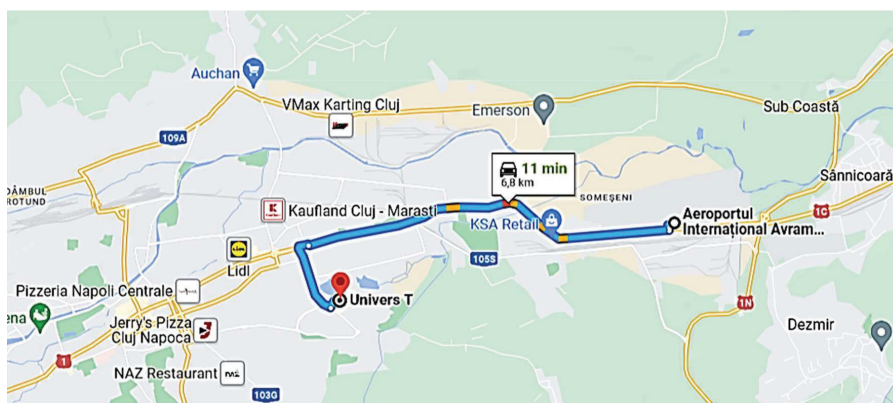
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<https://eng.universt.ro/>

It is very close to the Avram Iancu International Airport (5–10 minute by car).

How to get to “Univers T Hotel” from the Airport



Website: <https://iss2026.conference.ubbcluj.ro>

Registration

At the Venus main Hall of the Univers T Hotel:

Monday, September 21, 2026: 08.00 – 20.00

Tuesday, September 22, 2026: 08.00 – 19.30

Wednesday, September 23, 2026: 08.00 – 19.30

Wednesday, September 24, 2026: 08.00 – 14.00

Badges

Each registered participant and accompanying person must wear their badge to attend scientific sessions, the exhibition, coffee breaks and lunches, as well as to have access to social events.

Symposium language

The symposium language is English. No simultaneous translation is provided.

Key to Lectures & Posters

- LPL – Laureate Plenary Lecture
- PL – Plenary Lecture
- KL – Keynote Lecture
- OP – Oral Presentation
- FOP – Flash Oral Presentation
- eP – e-Poster Oral Presentation

Exhibition

The exhibition, located at the Venus Hall of the Univers T Hotel is open during the whole scientific programme.

Meals

Each participant has breakfast at the hotel where they are staying. Lunches are served at the Hotel Univers T restaurant. Wearing the symposium badge is mandatory for access to Lunch, the Welcome Reception, and the Gala Dinner.

Social Events at Univers T Hotel

Monday, September 21: Welcome Reception, 19.30 – 21.30;

Wednesday, September 23: Gala Dinner, 20.00 – 24.00;

Thursday, September 24: Farewell Reception at 13.00 – 13.30.

Internet connection

Free-of-charge wireless internet access is available in the Symposium area for all registered participants.

Weather

September is a good time to visit Cluj-Napoca. Weather in September is usually nice with temperatures around 22°C.

Welcome to Cluj-Napoca at

30th International Symposium on Separation Sciences



The Organizing Committee is pleased to welcome you at this remarkable international event in Cluj-Napoca, the most important city in Transylvania, named the **TREASURE CITY OF TRANSYLVANIA** due to its two thousand years of history and multicultural meanings.



Until 1974 the city was known Cluj (Claudiopolis in Latin, Klausenburg in German and Kolozsvár in Hungarian); since then, it has been called Cluj-Napoca, to evoke the Roman origins of the settlement, which abounds in archaeological remains. The city is divided in 15 neighborhoods, circularly disposed around the centre, built in a notable Gothic & Baroque architecture.



Having a history with a deep fingerprint over all the aspects of the city life, Cluj-Napoca has a population of approximately 300.000 inhabitants, most of them Romanians, followed by Hungarians, Germans, Jews etc.



Cluj-Napoca is a famous academic and science centre having six state and four private universities. During the academic year, its population is increasing with more than 100.000 students.



Cluj-Napoca is a major touristic attraction thanks to its many charms & opportunities, both ancient & modern, such as historical monuments, churches, museums, libraries, cultural-scientific activities, and more.



“Avram Iancu” International Airport offers scheduled flights connecting the city to major international airport hubs. It is located six km from the city centre.



Cluj-Napoca has a moderate, temperate-continental climate.

Weather in September is usually pleasant, with temperatures around 22°C.

30th International Symposium on Separation Sciences
Univers T Hotel & Cluj-Napoca, Romania



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Victor Constantin MĂRUȚOIU

Victor Constantin Măruțoiu is a member of Writers Union of Romania and serves as a cultural officer for both the "Dumitru Fărcaș" Students' Culture House and the Technical University of Cluj-Napoca. He holds a PhD in Theology, specializing in the New Testament, with a doctoral thesis entitled *New Testament Angelology: A Perspective on Contemporary Biblical Theology* (2014). His academic background includes studies at the Pontifical Gregorian University and the Pontifical University of the Holy Cross in Rome. He has authored 14 poetry volumes, has been featured in 46 anthologies, and has published over 250 articles in literary and cultural journals. His literary contributions have been recognized with 41 awards.

Academic Works: *New Testament Angelology: A Perspective on Contemporary Biblical Theology*, Ecou Transilvan Publishing House, Cluj-Napoca, 2023. *Windows onto the Absolute: An Anthology of Philosophical and Theological Studies*, co-authored with Ionuț Constantin Isac, Romanian Academy (Cluj-Napoca Branch, "George Barițiu" Institute of History, Department of Social and Human Sciences), Casa Cărții de Știință Publishing House, Cluj-Napoca, 2020. *Wooden Churches of Transylvania – Cluj and Sălaj*, edited by Prof. Dr. Constantin Măruțoiu, Prof. Dr. Daniela Popescu, Dr. Ioan Bratu, Prof. Dr. Radu Moraru, and Assoc. Prof. Dr. Luminița Dana Postolache (Contributor), Mega Publishing House, Cluj-Napoca, 2017.

European Cluj-Napoca – History, Tradition, Multiculturalism, and Academic Perspectives

Victor Constantin MĂRUȚOIU

"Dumitru Fărcaș" Students' Culture House, 1-3 Lucian Blaga Square Cluj-Napoca, Romania
Technical University of Cluj-Napoca, 28 Memorandumului Str., Cluj-Napoca, Romania.
victorconstantinmarutoiu@yahoo.com

Keywords: Cluj-Napoca, Education, Architecture, Multiculturalism, Tradition, History

Cluj-Napoca is the heart of Transylvania, pulsating with culture, history, and traditions, while breathing an ethnic, educational, academic, and institutional multiculturalism. The city is a model of harmonious coexistence and continuous evolution. From the early Dacian settlement to the Roman fortress of Napoca, and from the medieval town to today's innovative metropolis, the settlement has functioned as a strategic crossroads for the intersection of nations, ideas, trade, and economic, cultural, and academic relations.

Historical Roots – From Dacian Napoca to the Modern Metropolis:

The area has been settled since the Neolithic period (6000–5500 BC), making it the oldest discovered settlement in Transylvania. It shows remains of the Starčevo-Criș culture discovered in the Mănăștur neighbourhood (a burial site) and on Memorandumului Street, as well as of the Vinča-Turdaș culture from the Lucian Blaga Square site. Archaeological finds also attest to the existence of a settlement (8th century BC) during the Bronze and Iron Ages belonging to the Basarabi culture. The area was inhabited by local tribes, Celts, and Dacians, developing into a Dacian settlement along the course of the Someșul Mic River around 250–100 BC. This was followed by the Roman conquest period (101–106 AD), when it was transformed into a military fort and later granted municipium status by Emperor Hadrian under the name Municipium Aelium Hadrianum Napoca, serving as the capital of the Dacia Porolissensis province. In 168–169 AD, it became a colony, Colonia Aurelia Napoca. In 1173, the County of Cluj (Comitatul Cluj) is mentioned through Thomas, count of Cluj (Thomas comes Clusiensis). In 1241, the Tatar invasion nearly destroyed the locality completely. In 1275, Ladislaus IV the Cuman offered rights to the Saxons who would come and settle in the town of Cluj. In 1316, Charles Robert of Anjou granted benefits and tax exemptions to the town, and in 1405, Emperor Sigismund of Luxembourg, King of Hungary, granted it the status of a free city.

In 1409, public education is first recorded in Cluj with a Catholic school mentioned via *Caspar notarius et rector scholarum*. The year 1443 marks the birth of King Matthias Corvinus in the Matthias House—the future Prince of Transylvania and King of Hungary, and son of the Romanian voivode John Hunyadi (Iancu Corvin de Hunedoara). In 1581, the Transylvanian governor Stefan Báthory established a Jesuit Academy, supporting it with donations. The Treaty of Karlowitz in 1699 marks the moment when Transylvania became a province of the Habsburg Empire, with Cluj becoming an important part of this province. In 1704, General Jean Rabutin destroyed the city walls so that the town would lose its military significance. In 1715, the Citadel (Cetățuia) was erected in the Vauban style, making it the first fortified citadel of this type built in Transylvania. The periods 1790–1848 and 1861–1868 brought Cluj the function of capital of the imperial province of Transylvania, becoming the meeting place of the Transylvanian Diet.

In 1776, Maria Theresa of Austria established a German-language university, which Emperor Joseph II later transformed into a Piarist university with Latin as the language of instruction. During the Austro-Hungarian period, a university with German and Hungarian instruction was established in 1872. Later named the Franz Josef University, it was headquartered where the "Babeș-Bolyai" University stands today.

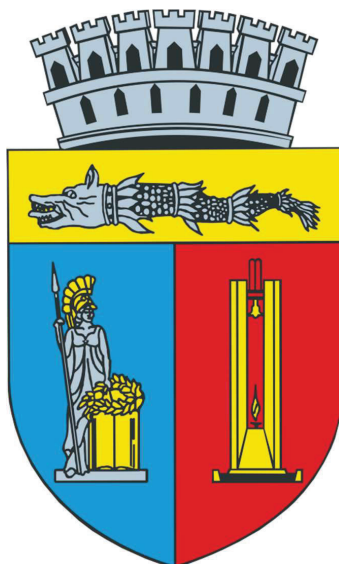
The 20th century brought to the forefront the construction of iconic buildings: the Romanian National Opera and Theatre, the Romanian Orthodox Cathedral in Avram Iancu Square, the Greek-Catholic Cathedral, the Palace of Justice, the Cluj City Hall, the Unitarian High School, and the Palace of Finance. Dating back to the Middle Ages, Saint Michael's Church is a Roman Catholic church built in the Gothic style in the 14th-15th centuries, while the Piarist Church, also known as the Jesuit Church or the University Church dates from the Baroque period, being the first Roman Catholic church built (1718–1724) in Transylvania after the Protestant Reformation. Following the Treaty of Versailles, Cluj became an integral part of Romania in 1918, with a brief period from 1940 to 1944 when it was ceded to Hungary. After World War II, it returned as an integrated part of Romania.

After the 1989 Revolution, the Transfiguration Church (Biserica Schimbarea la Față) was built in Cluj. Its iconostasis was crafted by Silviu Oravitzan from gilded linden wood, and its interior is painted in the mosaic technique by Marko Ivan Rupnik, a Vatican painter.

The Current University Landscape of the city of The Current University Landscape of Cluj-Napoca shows six state universities: Cluj-Napoca shows six state universities: "Babeș-Bolyai" University (UBB)– The largest university in the country, classified as an advanced research and education institution; "Iuliu Hațieganu" University of Medicine and Pharmacy (UMFIH) – A hub of medical excellence that attracts thousands of international students; Technical University of Cluj-Napoca (UTCN) – The main provider of human resources for the IT sector; University of Agricultural Sciences and Veterinary Medicine (USAMV) – A leader in agronomic research and biotechnologies – University of Arts and Design (UAD) & The National Academy of Music "Gheorghe Dima" (ANMGD): The epicentres of creativity, the sciences, music, and visual arts.

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The History of Pharmacy Museum in Cluj-Napoca

Ana-Maria GRUIA

National Museum of Transylvanian History, Pharmacy Museum,
28 Unirii Square, Cluj-Napoca, Romania

ana.gruia@mnit.ro

Key Words: Pharmacy museum, Cultural patrimony, Cluj-Napoca

The Pharmacy Museum in Cluj-Napoca is an integral part of the National Museum of Transylvanian History, showcasing two of its smallest, yet valuable collections: the History of Pharmacy Collection and the Medical Equipment Collection.

The museum occupies spacious areas in the Hintz House, located in the city's Central Plaza (28 Unirii Square), including the rooms of the former Hintz Pharmacy. A pharmacy operated there between the middle of the 18th century and the middle of the 20th century. The Hintz Pharmacy was nationalized in 1949 by the Communist regime, like all private pharmacies and drugstores in Romania, and remained neglected for several years. Then, Professor Valeriu Bologa, a medicine historian, obtained the space for an exhibition of pharmaceutical and medical history. He combined an older history of pharmacy collection, artifacts of folk healing from Romania, as well as objects recovered from nationalized pharmacies from Transylvania.

The location was ideal because the ground-floor interior preserves 18th-century pharmaceutical decorations, mainly a large vault painting with symbols of healing and wellbeing and inscriptions mentioning the owners and different renovation stages. The building retains the structure of traditional pharmacies, with its classic spaces: the *officina*, where products were sold; the *camera materialis*, where raw materials were stored; the laboratory; the cellar; the pharmacist's office; the attic where medicinal plants were dried; and even the pulley in the roof used to lift them into the *herbarium*.

The museum was inaugurated in 1954 and functioned under the successive administration of the University of Medicine and Pharmacy and the History Museum. After the fall of the Communist regime in Romania in 1989, the descendants of the Hintz pharmacists recovered the building and it became private once more. An extensive period of renovations stabilized the entire building between 2018 and 2023. In January 2024, the museum reopened with an expanded and improved exhibition, including new archaeological discoveries (Roman walls, a 19th-century coin hoard, and hundreds of pharmaceutical containers), museum education areas, and multimedia spaces. The museum is state-owned and run, but it rents out part of the ground floor and the basement from Dr. Georg Hintz, the current owner.

The History of Pharmacy Collection includes nearly 7,000 heritage objects of all types: containers made of glass, ceramic, wood, and metal; books; manuscripts; laboratory equipment; pharmaceutical chests and homeopathy kits; works of art; prescriptions; advertisements; and various other objects used in the historic pharmacies of Transylvania. Some 350 artifacts were once part of the Hintz pharmacy, but the origin of several items in the collection is unclear, as the nationalization inventories of 1949 were intentionally imprecise.

Many containers still preserve their *materia medica*, which can be analyzed in detail to discover what treatments Transylvanians used from the 16th to the 20th century. Herbal remedies were often used, but the most interesting ingredients are the old substances of human and animal origin: mummy powder, castor glands, crayfish eyes, cuttlefish bones, and other unusual products.

The complete catalog of the collection, in seven thematic volumes, covering all items entered into the inventory up to December 2022, is fully available online in PDF format in English [1]. The catalog was published as part of a recently implemented exploratory research project. As part of this project, a series of advanced analyses were also carried out, most of them on the contents of the containers inside an 18th-century portable pharmaceutical chest, and the results were published in a separate article [2]. They reveal that a noble Transylvanian family used both simple, local plant medicine, such as mustard, and exotic, complex drugs such as Peruvian Balm and Sennert's bezoar powder, with gold leaf fragments and an extremely high number of ingredients.

The medical equipment collection reflects the medical history of Cluj and includes objects used in its hospitals and medical offices from the late 19th century to the 1980s. The largest group of items was donated in 1997 by Prof. Dr. Pompiliu Manea. The pieces are organized according to different medical specialties, such as dentistry, ophthalmology, radiography, and others. Among the most important objects are an Einthoven electrocardiograph produced in 1915, possibly the oldest in Romania, Röntgen devices and tubes from 1915–1920, and various optical instruments.

The Museum of Pharmacy in Cluj-Napoca offers a variety of services, including a free audio guide in several languages (Romanian, Hungarian, German), video guidance in Romanian sign language, guided tours with specialized museographers, and various museum education workshops. All details regarding visits and the museum's holdings can be found on its website [3].

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History of ISSS Symposia

The origin of the International Symposia on Separation Sciences (ISSS) can be found in the national GC scientific meetings held in Zagreb since 1967, and later on at the Plitvice Lakes until 1988. Over the years, these meetings have expanded to include all chromatographic techniques and other separation techniques. Starting in 1990, these scientific meetings became international, being organized alternately in Bled (Slovenia) and Opatija (Croatia) until 1998. Despite the war affecting parts of Croatia, the participants decided to continue these meetings, benefiting from the support of many scientists from abroad (*i.e.* Slovenia).

During the fourth edition of the ISSS in Opatija in October 1996, the idea of expanding mutual scientific cooperation by inviting similar societies from Bosnia and Herzegovina, Hungary, and Slovakia, with the support of the designated steering committee (Dušan Berek, Bratislava – Slovak Chemical Society; Jože Marsel, Ljubljana – Slovenian Chemical Society; Szabolcs Nyiredy, Budapest – Hungarian Society for Separation Sciences and Nikola Šegudović, Zagreb – Croatian Society of Chemical Engineers).

This idea became a reality in October 1998, at the 5th edition of the ISSS held in Bled, when the Central European Group for Separation Sciences (CEGSS) was founded under the leadership of a steering committee comprising Dušan Berek, Jože Marsel, Branko Nikolin (Sarajevo, Bosnia-Herzegovina), Szabolcs Nyiredy and Nikola Šegudović. During the 3rd Balaton Symposium held in 1999 in Siófok, the CEGSS was extended by the Czech Chemical Society (Pavel Jandera, Pardubice) and in 2000 during the 6th ISSS at Plitvice Lakes (Croatia) it was joined by the Austrian Society for Analytical Chemistry (Wolfgang Buchberger, Linz), Italian Chemical Society (Corrado Sarzanini, Turin), and Polish Chemical Society (Bogusław Buszewski, Toruń).

During the 8th ISSS, Toruń, September 2002, Jože Marsel was replaced by Lucija Zupančič-Kralj from Ljubljana. In October 2006 Szabolcs Nyiredy passed away and in June 2007 he was replaced by Imre Klebovich from Budapest.

In autumn 2007, Modest Gertsyuk from Kiev as a representative of the Ukrainian Chromatographic Society joined CEGSS Steering Committee. In October 2008, Virginia Coman from Cluj-Napoca as a representative of the Romanian Chemical Society adhered to CEGSS Steering Committee, being the tenth member. In September 2019, Živoslav Tešić as a representative of the Serbian Chemical Society joined CEGSS.

In the last part of the year 2025, three societies joined CEGSS as follows: Society of Chemists and Technologists of Macedonia with Jasmina Petreska Stanoeva as a representative, Turkish Chemical Society with Levent Pilet as a representative, and Association of Greek Chemists with Victoria Samanidou as a representative.

CEGSS Steering Committee – 2026

No.	Accession	Corresponding Professional Society	Current National Representative
1	1998	Croatian Society of Chemical Engineers	Tomislav BOLANČA
2	1998	Slovenian Chemical Society	Irena VOVK
3	1998	Slovak Chemical Society	Róbert GÓRA
4	1998	Hungarian Society for Separation Sciences	Krisztián HORVÁTH
5	1999	Czech Chemical Society	Petr ČESLA
6	2000	Austrian Society of Analytical Chemistry	Erwin ROSENBERG
7	2000	Italian Chemical Society	Daniilo CORRADINI
8	2000	Polish Chemical Society	Bogusław BUSZEWSKI*
9	2007	Ukrainian Chromatographic Society	Modest GERTSIUK
10	2008	Romanian Chemical Society	Virginia COMAN**
11	2018	Serbian Chemical Society	Živoslav TEŠIĆ
12	2025	Society of Chemists & Technologists of Macedonia	Jasmina PETRESKA STANOIEVA
13	2025	Turkish Chemical Society	Levent PELIT
14	2025	Association of Greek Chemists	Victoria SAMANIDOU

*President; **Secretary general

Past, Current and Future ISSS Symposia

Symposium	Year	Place	Country	Chairperson
1 st ISSS	1990	Bled	Slovenia	Jože MARSEL
2 nd ISSS	1992	Opatija	Croatia	Srečko TURINA
3 rd ISSS	1994	Bled	Slovenia	Jože MARSEL
4 th ISSS	1996	Opatija	Croatia	Nikola ŠEGUDOVIČ
5 th ISSS	1998	Bled	Slovenia	Jože MARSEL
6 th ISSS	2000	Plitvice	Croatia	Nikola ŠEGUDOVIČ
7 th ISSS (regional)	2002	Pörschach/ Wörthersee	Austria	Wolfgang BUCHBERGER
8 th ISSS	2002	Toruń	Poland	Boguslaw BUSZEWSKI
9 th ISSS	2003	Siófok	Hungary	Szabolcs NYIREDY
10 th ISSS	2004	Opatija	Croatia	Nikola ŠEGUDOVIČ
11 th ISSS	2005	Pardubice	Czechia	Pavel JANDERA
12 th ISSS	2006	Lipica	Slovenia	Lucija ZUPANČIČ-KRALJ
13 th ISSS	2007	Štrbske Pleso	Slovakia	Jozef LEHOTAY
14 th ISSS	2008	Primošten	Croatia	Nikola ŠEGUDOVIČ
15 th ISSS	2009	Siófok	Hungary	Imre KLEBOVICH
16 th ISSS	2010	Roma	Italy	Daniilo CORRADINI
17 th ISSS	2011	Cluj-Napoca	Romania	Virginia COMAN
18 th ISSS	2012	Toruń	Poland	Boguslaw BUSZEWSKI
19 th ISSS	2013	Poreč	Croatia	Tomislav BOLANČA
20 th ISSS	2014	Prague	Czechia	Aleš HORNA, Pavel JANDERA
21 st ISSS	2015	Ljubljana	Slovenia	Irena VOVK
22 nd ISSS	2016	Toruń	Poland	Boguslaw BUSZEWSKI
23 rd ISSS	2017	Vienna	Austria	Erwin ROSENBERG
24 th ISSS	2018	Jasná	Slovakia	Milan HUTTA, Dušan BEREK
25 th ISSS	2019	Łódź	Poland	Joanna KAŁUŻNA-CZAPLINSKA Rafał GŁOWACK
26 th ISSS	2022	Ljubljana	Slovenia	Irena VOVK
27 th ISSS	2023	Cluj-Napoca	Romania	Virginia COMAN Simion BELDEAN-GALEA
28 th ISSS	2024	Messina	Italy	Luigi MONDELLO Daniilo CORRADINI
29 th ISSS	2025	Belgrade	Serbia	Živoslav TEŠIĆ
30 th ISSS	2026	Cluj-Napoca	Romania	Virginia COMAN Simion BELDEAN-GALEA
31 st ISSS	2027	Poznań	Poland	Marcin FRANKOWSKI Anetta ZIOŁA-FRANKOWSKA
32 nd ISSS	2028	Pardubice	Czech Republic	Jana LAVICKA Petr ČESLA

Symposium Aim

The primary aim of the International Symposium on Separation Sciences (ISSS) has always been to provide young researchers with the opportunity to learn more and familiarize themselves with current advances in chromatographic and hyphenated techniques, as well as other methods of separation, detection, and sample preparation.

The symposium connects scientists and users of chromatography, electrophoresis and related or hyphenated separation techniques from academia and industry from around the world giving them the opportunity to present their latest results of the scientific work from different fields of separation sciences and to establish new collaborations.

The symposium brings together scientists and users from academia, research and industry worldwide—specializing in chromatography, electrophoresis, and related or hyphenated separation techniques—offering them the opportunity to present the latest results of their scientific work across various fields of separation science and to establish new collaborations.

ISSS-2026 focuses on fundamental and practical aspects of separation and detection methods for various compounds from diverse and complex matrices, as well as on hyphenated, multidimensional and miniaturized techniques applied for analytical, preparative and industrial purposes, including new horizons and challenges in separation sciences, accompanied by debates on the theme "Advanced today, conventional tomorrow in separation sciences".

Symposium Topics

●Gas chromatography ●Liquid chromatography ●Thin-layer chromatography ●Ion chromatography ●Supercritical fluid chromatography ●Capillary electrophoresis ●Electromigration techniques ●Hyphenated techniques ●Multidimensional separations ●Miniaturised separation techniques ●Sample preparation techniques ●Environmental analysis ●Food analysis ●Pharmaceutical analysis ●Clinical analysis ●Forensic analysis ●Natural product analysis ●Industrial analysis ●Chemometrics ●Others

Scientific Programme

The scientific programme includes:

- Laureate Plenary lectures for the European Tswett-Nernst Prize (2025);
- Plenary & Keynote lectures of invited speakers – recognized scientists;
- Oral, Flash & e-oral Poster presentations – for senior & young scientists, as well as for the young student generation.
- Starting from the paradigms "A solid construction needs a foundation" and "The present and the future can be understood by knowing the past" will take place debates on the theme "Advanced today, conventional tomorrow in separation sciences". At the end of each section, panel discussions will take place on the topics of speeches.
- Symposium language is English (United Kingdom).

LAUREATE PLENARY LECTURES FOR TSWETT-NERNST AWARDS

Gert DESMET, Vrije Universiteit Brussel, Belgium

Imre KLEBOVICH, Semmelweis University, Budapest, Hungary

PLENARY LECTURES

Bogusław BUSZEWSKI, Prof. Jan Czocharlski Kuyavian-Pomeranian Centre, Toruń, PL

Danilo CORRADINI*, National Research Council, Rome, Italy

Erdal DINÇ, Ankara University, Türkiye

Dušan KOVAL, Czech Academy of Sciences, Prague, Czech Republic

Michael LAEMMERHOFER, University of Tuebingen, Germany

Andrei Medvedovici, University of Bucharest, Romania

Erwin ROSENBERG, Vienna University of Technology, Austria

José Juan Santana Rodríguez, University of Las Palmas de Gran Canaria, Spain

Didier THIÉBAUT, French National Centre for Scientific Research, Paris, France

Irena VOVK, National Institute of Chemistry, Ljubljana, Slovenia

KEYNOTE LECTURES

Ramia AL BAKAIN, University of Jordan, Amman, Jordan

Ede BODOKI, University of Medicine and Pharmacy, Cluj-Napoca, Romania

Magdalena BUSZEWSKA-FORAJTA, Nicolaus Copernicus University, Toruń, Poland

Petr ČESLA, University of Pardubice, Czech Republic

Massimo DEL BUBBA, University of Florence, Italy

Hartmut FRANK, University of Bayreuth, Germany

Marcin FRANKOWSKI, Adam Mickiewicz University, Poznań, Poland

Modest GERTSIUK, Academy of Sciences of Ukraine, Kyiv, Ukraine

Róbert GÓRA, Comenius University, Bratislava, Slovakia

Agata KOT-WASIK, Gdańsk University of Technology, Poland

Rajmund MICHALSKI, Polish Academy of Sciences, Zabrze, Poland

Levent PELIT, Ege University, Izmir, Türkiye

Tania SALERNO, University of Messina, Italy

Victoria SAMANIDOU, Aristotle University of Thessaloniki, Greece

Petr TŮMA, Charles University, Prague, Czech Republic

Jérôme VIAL, ESPCI Paris - PSL, Paris, France

Anetta ZIOŁA-FRANKOWSKA, Adam Mickiewicz University, Poznań, Poland

Scientific Information

Scientific programme includes: *Plenary* (30 min.) and *Keynote* (25 min.) lectures given by internationally recognized scientists, *Oral* (20/15/10 min.) of senior and young scientists, and *Flash oral* (5+2 minutes) and *e-Oral poster* (3+2) presentations, including 2 minutes of discussions.

Oral presentation: PowerPoint format (landscape orientation) and saved on an USB Stick (Flash Drive).

Flash oral presentation: 5–10 slides presented in 5 minutes + 2 minutes for discussions; PowerPoint format (landscape orientation) and saved on an USB Stick (Flash Drive).

e-Poster presentation: 3–5 slides (1: title, authors, affiliation, objective; 2-4: experimental, results; 5: conclusions; if necessary, 1–2 more slides) like a regular PowerPoint presentation or using TEMPLATE format; 3-minute presentation and 2-minute discussion.

Flash & e-Poster Competition

The Poster Award Committees (PhD students / seniors) will evaluate the flash & e-Poster oral presentations. Valuable awards will be conferred on Thursday at the Closing Ceremony.

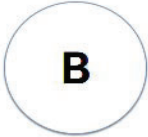
Manuscript Submission

Papers presented at 30-ISSS Symposium will be considered for publication in the official journals of the Symposium, in special issues, *Studia Babeş-Bolyai Universitatis Chemia* (Issue 1/2024) after a peer-review procedure.

Manuscripts will be prepared according to the author instructions of the journal.

The ISSS 2026 Programme contains: 2 Laureate & 11 Plenaries, 18 Keynotes, 31 Orals, 23 Flash-oral and 17 e-oral presentations, presented by senior and young researchers from 20 countries.

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30th International Symposium on Separation Sciences

Univers T Hotel & Cluj-Napoca, Romania



ISSS 2026 – PROGRAMME SCHEDULE

MONDAY – 21 September – REGISTRATION & SECRETARIAT 8:00 – 20:00	
10:00 – 10:30	OPENING CEREMONY
10:30 – 11:30	Laudatio. Two Laureate Plenary Lectures
11:30 – 11:45	Coffee Break, Exhibition
11:45 – 13:30	Session 1 (Plenary, Keynote, Orals)
13:30 – 14:30	Lunch
14:30 – 16:30	Session 2 (Plenary, Keynote, Orals)
16:30 – 17:00	Coffee Break, Exhibition
17:00 – 18:30	Session 3 (Plenary, Keynote, Orals)
18:30 – 19:30	CEGSS Steering Committee Meeting
19:30 – 21:00	WELCOME RECEPTION
TUESDAY – 22 September – REGISTRATION & SECRETARIAT 8:00 – 19:30	
08:30 – 10:30	Session 4 (Plenary, Keynote, Orals)
10:30 – 11:00	Coffee Break, Exhibition
11:00 – 13:00	Session 5 (Plenary, Keynote, Orals)
13:00 – 14:00	Lunch
14:00 – 16:00	Session 6 (Plenary, Keynote, Orals)
16:00 – 16:30	Coffee Break, Exhibition
16:30 – 18:30	Poster Session (Plenary, Keynote, Orals)
WEDNESDAY – 23 September – REGISTRATION & SECRETARIAT 8:00 – 19:30	
08:30 – 10:30	Session 7 (Plenary, Keynote, Orals)
10:30 – 11:00	Coffee Break, Exhibition
11:00 – 13:00	Session 8 (Plenary, Keynote, Orals)
13:00 – 14:00	Lunch
14:00 – 16:00	Session 9 (Plenary, Keynote, Orals)
16:00 – 16:30	Coffee Break, Exhibition
16:30 – 18:30	Session 10 (Plenary, Keynote, Orals)
20:00 – 24:00	GALA DINNER
THURSDAY – 24 September – REGISTRATION & SECRETARIAT 8:00 – 14:00	
08:30 – 10:30	Session 11 (Plenary, Keynote, Orals)
10:30 – 11:00	Coffee Break, Exhibition
11:00 – 12:30	Session 12 (Plenary, Keynote, Orals)
12:30 – 13:30	Closing Ceremony. Farewell Reception

Orals mean: Oral (20, 15, 10 min.), Flash-oral (7 min.) and e-Poster (5 min.) presentations



BOOK OF ABSTRACTS

**Two Laureate Plenary Lectures
for
Tswett-Nernst Awards**



Gert DESMET

Professor Gert Desmet has a Master's degree and PhD in chemical engineering from the Vrije Universiteit Brussel (VUB), Brussels, Belgium, where he currently is a **full professor**. His research mainly focuses on the miniaturization and automation of separation methods, as well as on the investigation and the modeling of flow effects in chromatographic systems. He has been the author or co-author of more than 450 peer-reviewed papers.

He is a past chair of the Chemistry Panel of the Flemish National Science Fund and currently is the Deputy-director of the Solvay Institute for Chemistry. He also is an Associate Editor for the journal "Analytical Chemistry" and was the recipient of an ERC Advanced Grant. He is also a member of the permanent scientific committee of the international HPLC and ISC conference series.

He has won numerous awards, including the Silver Jubilee Medal of the Chromatographic Society of the UK, the JFK Huber Lecture Award from the Austrian Society for Analytical Chemistry, the "American Chemical Society Award for Chromatography", the Istvan Halasz Medal award from the Hungarian Society for Separation Sciences, the A.J.P. Martin medal from the Chromatographic Society of the UK and the Golay Award from Perkin-Elmer.

Assessing the Accuracy of Gaussian Processes in Mapping Chromatographic Responses

Marwan ELKHETTABI¹, Leon NIEZEN¹, Deirdre CABOOTER², Pieter LIBIN¹,
Gert DESMET¹

¹*Vrije Universiteit Brussel Department of Chemical Engineering, Brussels, Belgium;*

²*University of KU Leuven, Department of Pharmaceutical and Pharmacological Sciences, Leuven, Belgium.*

gert.desmet@vub.be

Key Words: Method development, Modeling in chromatography.

Method development (MD) can be defined as the search process to find the best possible chromatographic method, usually the one yielding the desired separation quality in a short (or the shortest) time in a robust part of the design space. When employing algorithmic (and hence automatable) search approaches to find this method, a mathematical goal function (=chromatographic response functions, CRF) describing the quality of the obtained chromatograms is needed to guide the search. For historic reasons, such goal functions are generally referred to as chromatographic response functions (CRFs) in chromatography literature.

The current standard search algorithm to find the method parameters yielding the optimal CRF value is Bayesian optimization (BO), as this automatable search approach does not rely on any a priori knowledge of the CRF landscape. To model (i.e., approximate) the CRF landscape, BO algorithms typically use so-called Gaussian Processes (GPs). A GP is a probabilistic model that defines a distribution of functions rather than, just one single best-fit function.

To give guidance to the future research on computer-aided method development, the present study aimed at quantifying the accuracy with which so-called Gaussian processes (GP) can represent the typical CRF landscapes encountered in chromatographic method development. These are known to be very complex and jagged, with many local depressions and maxima, such that this is a valid research question.

It is found that, for a simple, two-parameter linear gradient, already 50 to 100 experimental scouting runs are needed to have a sufficiently high probability for the GP to find a solution that is reasonably close to the true optimum. But even then, there is always a possibility for a complete failure. This conclusion holds for n=10-component mixtures in an N=10,000 theoretical plate column, and even more for n=20-component mixtures in an N=40,000 column. At the conference, we will also report on potential solutions to this problem.



Imre KLEBOVICH

Professor Imre Klebovich (Pharm.D., Ph.D., D.Sc.) is an **emeritus professor** of Department of Pharmaceutics at Semmelweis University and former Dean of its Faculty of Pharmaceutical Sciences, with a distinguished career spanning academia, industry and scientific leadership.

Dr. Klebovich founded and led the Department of Pharmacokinetics and Drug Metabolism at EGIS Pharmaceuticals for 15 years, after earlier research posts at the Biochemical Institute of the Hungarian Academy of Sciences and Gedeon Richter Ltd. He has held professorial appointments at the Budapest University of Technology and Economics, Pázmány Péter Catholic University.

His research focuses on bioanalytics-radioanalytics, pharmacokinetics, metabolism, biopharmaceutics, bioequivalence, food-drug interactions, *in vitro* dissolution, IVIVC and modified-release drug delivery. He is inventor on 27 patents, author of more than 270 journal papers, 19 books and 25 book chapters, and has delivered over 530 conference lectures. He contributed to the development and registration of three original and 39 generic drugs.

He is the elected chair (2015-2018) of the Permanent Committee on Pharmaceutical Sciences and elected president of the Working Committee on Separation Sciences (2012-2018) of the Hungarian Academy of Sciences and has had long-standing editorial responsibilities with key chromatography and pharmaceutical journals.

His many honours include the Officer's Cross of the Hungarian Order of Merit and a Lifetime Achievement Award from SPDS Mumbai-India, Halász Medal Lifetime Achievement from the Hungarian Society for Separation Science.

Quantifying the Invisible: Radio-bio-analytical Tools in Pharmacokinetic and Drug Metabolite Research

Imre KLEBOVICH

*Semmelweis University, Department of Pharmaceuticals,
7-9 Hógyes Street, H-1092 Budapest, Hungary.
klebovich.imre@semmelweis.hu*

Key Words: Radiochromatography, Bioanalytics, Pharmacokinetics, Drug metabolism, Isotope labelling.

Drug candidates that fail to reveal the full extent of their *in vivo* fate can carry hidden safety and efficacy liabilities, making the "invisible" behavior of a molecule and its metabolites one of the central challenges of preclinical and clinical drug development. Radiolabeled isotopes, principally ^{14}C and ^3H , remain the gold standard for tracing the complete mass balance of a compound because they allow every biotransformation product, regardless of its structure or polarity, to be detected and quantified without the bias introduced by structure-dependent detectors. Over the past decades, the coupling of classical separation platforms, gas chromatography with radioactivity detection (GC-RD), high-performance liquid chromatography with radioactivity detection (HPLC-RD), and on-line and off-line overpressured layer chromatography with radioactivity detection (OPLC-RD/HPTLC-RD), with digital autoradiography (DAR) and the phosphor imaging technique (PIT) has transformed the sensitivity and throughput with which minor and major metabolites can be isolated, purified and quantified from complex biological matrices [1].

The lecture presents an integrated methodological overview of how these radio-bioanalytical tools are combined with hyphenated structural elucidation techniques, LC-MS/MS, LC-NMR and GC-MS, to resolve the identity, concentration-time profile and species-dependent formation of drug metabolites in preclinical and clinical pharmacokinetic studies. Particular emphasis is placed on the role of *in vitro-in vivo* imaging technologies, including MALDI imaging, nanoSPECT/PET and PET/MRI in animal and human models, which extend radiotracer-based quantification from the test tube to the whole organism, and on *in silico* ADME and 3D/4D-QSAR prediction models that guide the selection of Cytochrome P450 isoenzyme-relevant metabolic pathways before radiolabeled studies are undertaken. Representative case studies from bioequivalence, food-drug interaction and modified-release formulation research illustrate how this multi-step workflow, spanning separation, purification, isolation and structure elucidation, generates the quantitative and qualitative evidence required for regulatory submission dossiers [2, 3].

This plenary lecture is delivered on the Nernst-Tswett Award, recognizing a lifetime contribution to the theory, methodology and practical application of separation sciences in pharmacokinetic and drug metabolism research.

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- [2] I. Klebovich. Bioanalytics/radiobioanalytics and imaging techniques in drug metabolism research: Overview of modern aspects and novel techniques, *International Symposium on Scientific and Regulatory Advances in Complex Drugs* (SRACD 2014), Budapest, Hungary, October 27–28, 2014.
- [3] I. Klebovich, The role of radiochromatography in the pharmacokinetic and drug metabolism research (L-12), *13th Balaton Symposium on High-Performance Separation Methods*, Siófok, Hungary, September 2–4, 2023.

Plenary Lectures



Bogusław BUSZEWSKI

Professor Bogusław Buszewski is a graduate of the Maria Curie-Skłodowska University in Lublin (Poland). In 1986 he obtained the PhD degree (STU Bratislava, Czechoslovakia), and in 1992 the DrSc (habilitation). In 1994, he was appointed professor at the Nicolaus Copernicus University in Toruń. He was a scholarship holder of the Alexander von Humboldt Foundation at the University of Tübingen (Germany), a postdoctoral fellow at Kent State University (Ohio, USA) and Kyoto Technical University (Japan) as well as a visiting professor at numerous universities in Europe, Asia, Australia and both America.

His main scientific interests concern separation sciences (HPLC, GC, CZE, FFF, ICP, MALDI, MS), adsorption, columns and stationary phases, sample preparation, environmental and bioanalysis (*-omics*, biomarkers), nanotechnology and chemometrics. He is the author and/or co-author of 16 books (including *Bioanalytics*-Springer), numerous patents and over 770 scientific papers (over 38,000 citations, $h=86$) and a member of the editorial boards of 26 national and international journals. Professor Buszewski is one of the most influential scientists according to the World's Top 1% Scientists List.

Professor Buszewski is the chairman of the Central European Group for Separation Sciences and the honorary chairman of the Analytical Chemistry Committee of the Polish Academy of Sciences. He is an ordinary member of the Polish Academy of Sciences and the European Academy of Sciences and Arts. Awarded by many national and international institutions and organizations (including multiple honoree doctorates, Martin Medal and Awards e.g.: M. Skłodowska Curie, R. Kaliszan, IAAM).

Non-target Analysis of Phospholipids in Egg Yolk Using Quantitative Retention-Chemical Structure Relation and Liquid Chromatography/Triple Quadruple tandem Mass Spectrometry

Bogusław BUSZEWSKI¹⁾, Magdalena BUSZEWSKA-FORAJTA^{1,2)},
Zbigniew DOBRZAŃSKI³⁾, Tadeusz TRZISZKA³⁾

¹⁾prof. J. Czochoński Kuyavian-Pomeranian Science and Technology Center,
Kraśnińskiego str. 4, 87-100 Toruń (Poland);

²⁾Institute of Veterinary Medicine, Nicolaus Copernicus University,
Szosa Bydgoska str. 13, 87-100 Toruń (Poland);

³⁾Wrocław University of Environmental and Life Sciences,
Norwida str. 25, 50-375 Wrocław (Poland).
b.buszewski@centrumczochońskiego.pl

Key Words: Phospholipids, Columns selection, QSRR, LC-MSⁿ.

Natural, active biological compounds constitute a distinct group of molecules that perform essential physiological functions. Their biological activity is closely related to their structural diversity and specific molecular architecture. One important class of such compounds is phospholipids, also known as phosphatides. In addition to glycerol and fatty acids residues, these compounds contain phosphorus components bound to an organic nitrogenous base. As early as 1884, J.L.W. Thudichum stated that "phospholipids are the center, the life, and the chemical soul of the entire bioplasm, both in plants and animals." This concept has inspired the development of analytical strategies aimed at answering the fundamental question: "What determines biological activity?" [1, 2].

Theoretical approaches used to investigate bioactivity include structure-activity relationships (SAR) and quantitative structure-activity relationships (QSAR), as well as quantitative structure-retention relationships (QSRR) [3,4]. These methodologies are based on the assumption that compounds with similar structures exhibit similar biological or physicochemical properties. Therefore, these methods, when complemented by physicochemical descriptors (e.g., lipophilicity, acidity and/or basicity, and related molecular parameters etc.) as well as detailed physicochemical characterization of the surface of new-generation chromatographic stationary phases, are particularly well suited for describing and interpreting the mechanisms involved in chromatographic separation in reversed-phase high-performance liquid chromatography with hydro-organic eluents (RP-HPLC) and hydrophilic interaction liquid chromatography (HILIC) within quantitative structure-retention relationships framework (QSRR).

These aspects are discussed in the context of new-generation chromatographic packings containing variety of functional groups (including amino acids, peptides, and proteins), with particular emphasis placed on identifying correlations between chromatographic selectivity, specificity, and molecular similarity. The characterized and selected stationary phases and chromatographic columns were subsequently applied to the analysis of phospholipids extracted from egg yolk samples derived from both control and experimental groups.

The analyses were carried out using high-performance liquid chromatography coupled with electrospray tandem mass spectrometry (HPLC-ESI-MS/MS). Fatty acyl compositions within 11 classes of egg yolk phospholipids were investigated. Multiple-reaction monitoring mass spectrometry enabled the identification of 123 distinct fatty acyl combinations present in the phospholipid fraction. A substantial proportion of these species contained polyunsaturated fatty acyl chains belonging to the omega-3 and omega-6 families.

Differences were observed between the fatty acyl profiles of hens fed conventional diet and those receiving specialized dietary supplementation. The experimental results were further supported and interpreted using multivariate chemometric analysis.

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Danilo CORRADINI

Danilo Corradini, PhD in chemistry, investigates fundamental and practical aspects of capillary electromigration techniques & HPLC, applied to analytical chemistry, life science, and phytochemistry.

He received education in separation sciences at Yale University (USA), where he served as Postdoctoral fellow in 1983 and 1984, and as Associate researcher in 1986 and Visiting scientist in 1994 & 1996, working with Csaba Horváth, the pioneer of HPLC and eminent separation scientist. He held teaching professorships at the University of Tuscia in Viterbo, Italy (1995–1997; 1999–2006), at Leopold-Franzes Universität of Innsbruck, Austria (1995–1998; 2007), at Johannes Kepler Universität of Linz, Austria (1993–1994), and at University of Siena, Italy (1990–1993). Currently, he serves as Project Investigator of the European Project PATHFOOD (2025–2027) at the Institute of Agricultural Biology and Biotechnology of Consiglio Nazionale delle Ricerche (CNR), in Montelibretti (Rome).

Dr. Corradini is: the chairmen (2025–2027 term) of the Separation Science Group of Società Chimica Italiana (SCI), a Member of the Central European Group for Separation Sciences (CEGSS) since 2011, a Member of the International Strategy & Evaluation Board (ISEB) of the Austrian Drug Screening Institute (ADSI), Innsbruck, Austria, and a Member of the International Scientific Council of the Institute of Analytical Chemistry of the Polish Academy of Science, Toruń, Poland. Previously (from April 2006 to February 2012), he was a Member of the General Scientific Advisory Board of CNR and served in the Scientific Advisory Board of the Institute of Chromatography (1996–2000) and of the Institute for Chemical Methodologies (2002–2008), both belonging to CNR. He was co-chair at the series of the International Symposia on Separation Sciences in 2010 (Rome) and 2024 (Messina).

In recognition of his significant contributions to Analytical Chemistry and Separation Sciences, he has received several awards and honours, including the Csaba Horváth Memorial Award from the Hungarian Society for Separation Science in 2009, the CEGSS Award in 2011, the Arnaldo Liberti Medal from SCI in 2014, the Giovanni Dugo Medal from SCI in 2021, the Prof. Andrzej Waksmundzki Award from the Polish Academy of Sciences in 2023, and the Medal Award for Lifetime Achievements from CEGSS in 2025.

Advances, Strategies and Perspectives of Capillary Electromigration Techniques in Bioanalysis

Danilo CORRADINI

*Italian National Research Council, Institute of Agricultural Biology and Biotechnology (IBBA),
Area Territoriale di Ricerca Roma 1, Strada provinciale 35d, 9 – 00010 Montelibretti (Rome) Italy.
danilo.corradini@cnr.it*

Key Words: Capillary Electrophoresis, Bioanalysis, Electroosmotic Flow, Separation Modes.

Capillary electromigration techniques comprises a pool of microscale separation methods performed in narrow-bore capillary tubes, which are based on the differential migration velocity of the analytes under the action of an electric field. The proper selection of the composition of the background electrolyte (BGE) solution filled within the capillary tube influences both the electroosmotic flow (EOF), which is the electrically driven flow of a liquid within a capillary tube, and the selective separation of the analytes. According to the selected separation mode, either continuous or discontinuous BGE systems are employed, recalling that in continuous systems the composition of BGE is constant along the capillary tube, whereas in discontinuous ones it is varied along the migration path. A given narrow-bore fused-silica capillary (typically 25–100 μm I.D.) can be employed to perform a variety of capillary electromigration techniques, operating under different separation mechanisms, just selecting the proper composition of BGE. On the other hand, other separation modes, such as capillary electrochromatography and capillary sieving electrophoresis, might require the use of dedicated capillaries, either packed or filled with proper material, which act as the stationary phase or the sieving matrix, respectively [1].

This communication provides a retrospective of the techno-scientific progress of capillary electromigration techniques in bioanalysis and discusses fundamental and practical aspects related to the influence of the composition of the BGE on both the separation behavior of biomolecules and the generation of EOF. Most of the investigated BGEs consist of aqueous solutions of buffering agents having the capability of controlling the protonic equilibrium of ionogenic analytes in a wide pH range, while preventing or minimizing their undesirable interactions with the silanol groups on the inner surface of bare fused-silica capillaries [2]. The occurrence of secondary equilibrium in solution between ionogenic analytes and each component of BGE can drastically affect selectivity, which is fundamentally driven by differences in the electrophoretic mobility of the analytes, governed by their effective charge-to-hydrodynamic radius ratios. This implies that selectivity is strongly influenced by the buffering agents, their counterions, and any interacting compounds occurring in the BGE that may alter the net charge or/and the hydrodynamic radius of the analytes. Other factors influencing the electrophoretic behavior of the analytes and, consequently, selectivity, related to the composition of BGE, include buffer concentration and ionic strength, as well as viscosity, temperature and relative permittivity (dielectric constant).

The talk comprises a discussion of practical applications of capillary electromigration techniques to the analysis of biomolecules in complex matrices of vegetable origin. The most recent application is the use of capillary zone electrophoresis (CZE) to investigate the influence of selenium biofortification of different varieties of cabbage (*Brassica oleracea*) on the biosynthesis and accumulation of phytochemicals with various health-promoting effects, such as phenolic compounds and glucosinolates.

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<https://www.pathfood.eu>



Erdal DİNÇ

Prof. Dr. Erdal Dinç is Professor of Analytical Chemistry at the Faculty of Pharmacy, Ankara University, Türkiye. He received his undergraduate degree from Gazi University and his M.Sc. and Ph.D. degrees in Analytical Chemistry from Ankara University.

His research focuses on *drug*, *food*, and *plant analysis*, chromatographic and spectroscopic techniques (HPLC, UPLC, UV-Vis, spectrofluorimetry, and IR spectroscopy), and *chemometrics*.

Throughout his career, he has developed numerous analytical methodologies for the qualitative and quantitative analysis of complex pharmaceutical, biological, food, and environmental samples by integrating spectroscopy, chromatography, multivariate calibration, & mathematical signal processing.

Professor Dinç has introduced several original spectrophotometric methodologies, including:

•*UV double divisor–derivative spectrophotometry*, •*Continuous Wavelet Transform Zero-Crossing (CWT-ZC)*, •*Ratio Spectra-Continuous Wavelet Transform (RS-CWT)*, •*Ratio Spectra-Continuous Wavelet Transform Zero-Crossing (RS-CWT-ZC)*, •*Double Divisor–Continuous Wavelet Transform (DD-CWT)*, •*Double Divisor-Continuous Wavelet Transform Zero-Crossing (DD-CWT-ZC)*, and •*Wavelet-assisted multivariate calibration approaches*.

More recently, his research has advanced toward *wavelet-domain multiway analytical strategies*, introducing a *UV-CWT-PARAFAC double-algorithmic architecture* that transforms conventional spectroscopic measurements into wavelet-domain multiway data for mathematical signal separation and quantitative analysis. His latest work further extends this framework to *wavelet-domain multiway analysis of drug-DNA interactions* based on fractional occupancy (θ).

Professor Dinç has authored 274 *scientific publications*, including 205 *SCI-indexed papers*, 229 *Scopus-indexed papers*, 45 *publications in other international indexing databases*, 5 *conference papers*, and 7 *book chapters*. His publications have received *more than 4.556 citations*. His *h-index* is 36/*Google Scholar*, 3/*Scopus* & 28/*Web of Science*, respectively. He serves as a reviewer for numerous international journals & has given invited & plenary lectures at international scientific meetings.

His current research aims to establish wavelet-domain multiway analytical strategies that complement conventional separation science by introducing mathematical separation as a new analytical paradigm.

Recent Advances in Separation Sciences: From Chromatographic Separation to Chemometric Multiway Spectral Separation in the Wavelet Domain

Erdal DİNÇ

Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06560 Yenimahalle, Ankara, Türkiye.
dinc@ankara.edu.tr

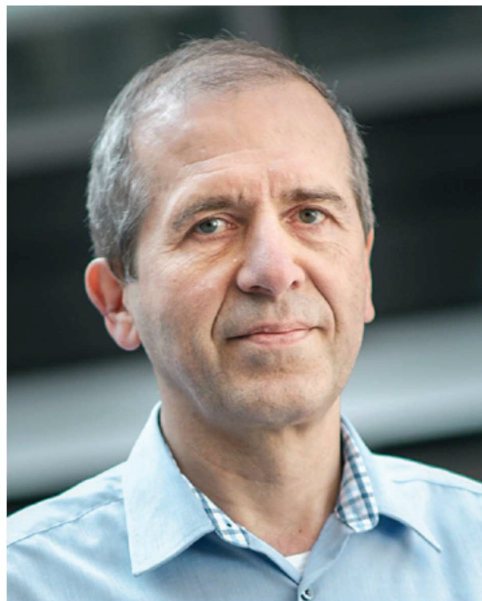
Separation science plays a fundamental role in analytical chemistry and related disciplines by providing reliable methodologies for the separation, identification, and quantitative determination of analytes in different complex matrices. Continuous advances in chromatographic instrumentation, separation technologies, and detection systems have substantially expanded the scope and analytical capabilities of this field, leading to remarkable developments in pharmaceutical, biomedical, food, and environmental analysis [1, 2]. Nevertheless, chromatographic methodologies often require expensive instrumentation, extensive method development, skilled personnel, and time-consuming optimization procedures. In parallel with these developments, chemometrics has become an indispensable component of modern analytical science by providing powerful methodologies for experimental design, optimization, signal preprocessing, multivariate calibration, classification, and mathematical resolution of complex analytical data. Classical multivariate calibration techniques have substantially improved the quantitative prediction of overlapping analytical signals, whereas multiway chemometric methodologies enable the mathematical resolution of complex analytical data through decomposition into chemically meaningful component profiles [3–6].

This lecture highlights the recent evolution of separation sciences from conventional chromatographic separation to chemometric multiway spectral separation in the wavelet domain. Particular emphasis will be placed on a recently developed double-algorithmic framework integrating the Continuous Wavelet Transform (CWT) with Parallel Factor Analysis (PARAFAC). In this framework, conventional two-dimensional analytical measurements are transformed into structured three-way datasets by wavelet-domain dimensional augmentation, enabling subsequent multiway decomposition by PARAFAC. The proposed methodology enables simultaneous chemometric spectral separation, recovery of pure component spectral profiles, estimation of relative concentration distributions, and accurate quantitative analysis without, or with only limited, chromatographic separation [7–10].

Representative applications involving pharmaceutical multicomponent analysis, wavelet-domain multiway spectral resolution of highly overlapping UV spectra, spectrochromatographic analysis, and quantitative drug-DNA interaction studies based on fractional occupancy will be presented to demonstrate the versatility and analytical capability of the proposed methodology. Future perspectives on extending wavelet-domain chemometric multiway spectral separation to chromatographic, spectroscopic, spectrofluorimetric, vibrational spectroscopic, and electroanalytical measurements will also be discussed. The presented framework illustrates how wavelet-domain chemometric multiway spectral separation can complement conventional chromatographic methodologies and contribute to the next generation of separation sciences.

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Václav KAŠIČKA

Václav Kašíčka has received degree RNDr. in physical chemistry at Charles University in Prague in 1979, and PhD. degree in biochemistry at the Institute of Organic Chemistry and Biochemistry, Czechoslovak Academy of Sciences, Prague, in 1985. At this Institute, he is head of the Laboratory of Electromigration Methods (<https://electromigration.group.uochb.cz/en>) since 1995. He is engaged in research and development of electroseparation methods and their application for analysis and characterization of (bio)molecules. He is author/co-author of more than 200 papers in impacted journals, 22 book chapters, and about 180 lectures at the international symposia, with 5101/4031 citations w/w/o self-citations, h-index 40.

He is associated editor of the Journal of Separation Science and the journal Separation Science Plus, member of editorial boards of several of international journals, e.g., Electrophoresis, Current Analytical Chemistry, Current Chromatography, and Separations, and member of permanent Scientific Committees of series of International Symposia ITP YYYY and LACE YYYY. He was secretary of the Steering Committee of the European Society for Separation Science in 2014–2022 and he chairs the Chromatography and Electrophoresis Group of the Czech Chemical Society.

Capillary Electromigration Methods – Powerful Tools for Separation, Analysis and Characterization of Peptides and Proteins

Václav KAŠIČKA¹, Veronika ŠOLÍNOVÁ², Adéla KRÍŽKOVÁ^{1,2}, Petra SÁZELOVÁ¹,
Renáta KONÁŠOVÁ¹, Sille ŠTĚPÁNOVÁ¹, Dušan KOVAL¹

¹*Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences,
Flemingovo náměstí 542/2, 160 00 Prague 6, Czechia;*

²*University of Chemical Technology, Technická 5, 166 28 Prague 6, Czechia.
kasicka@uochb.cas.cz*

Key Words: Capillary Electrophoresis, Isotachopheresis, Affinity electrophoresis, Peptide mapping, Electrokinetic chromatography.

Peptides and proteins belong to the vitally important biopolymers. They act as hormones, hormone and drug receptors, neurotransmitters, enzymes, co-enzymes, enzyme substrate and inhibitors, antigens, antibodies, ionophores, antibiotics and toxins. Based on these activities, many peptide and protein drugs have been developed. During peptide and protein (bio)synthesis or isolation and prior to their biological testing and medical application, their chemical purity has to be checked and their physico-chemical characterization must be performed. In this contribution, high-performance capillary electromigration (CE) methods (zone electrophoresis (CZE), isotachopheresis (CITP), isoelectric focusing (CIEF), affinity electrophoresis (ACE), and micellar electrokinetic chromatography (CMEKC)) will be shown as powerful tools for qualitative and quantitative analysis and physicochemical characterization of peptides and proteins [1-3].

A rational approach has been developed for selection of experimental conditions for CZE analyses of peptides and proteins, e.g. antimicrobial and anorexigenic peptides, peptide and protein hormones, metal binding peptides, monoclonal antibodies, and peptide drugs. It is based on the calculated dependence of the effective charge and specific charge (effective charge divided by relative molecular mass) of peptides and proteins on pH. Ionogenic peptides and proteins were analyzed by CZE as cations in acidic background electrolytes (BGEs) (e.g. 0.5–1.0 M phosphoric acid, 0.5–2 M acetic or formic acid, 50/100 mM Tris-phosphate buffer, pH range 1.0–3.0) or as anions in alkaline BGEs (100/50 mM Tris-acetate, 40/40 mM Tris-tricine or 50/100 mM Tris-borate buffers; pH 7.5–9.5). Nonionogenic peptides, i.e. peptides with blocked or protected ionogenic groups, were analyzed by CMEKC using micellar pseudophases composed of anionic detergent, sodium dodecylsulfate (SDS), or cationic detergent cetyltrimethylammonium bromide (CTAB) in acidic or basic BGEs. The content of counterions of basic or acidic peptides and low-molecular-mass ionic admixtures of peptides, e.g. the rests of acids, bases and salts originating from their synthesis and/or purification procedures, was determined by CITP. Acid-base and electromigration properties of peptides (acidity constants, effective and ionic mobilities, effective charges, isoelectric points and hydrodynamic radii) were investigated by CZE performed in series of BGEs within a wide pH range, 1.5–12.5, and by cationic or anionic mode of CITP.

Peptide mapping of bone proteins by CZE has been applied to distinguish healthy and pathological bone tissues. Strength of interactions of electroneutral cyclic peptides with alkali metal and ammonium cations was studied by ACE and non-covalent bindings of polypeptide hormone, human insulin, with low molecular mass ligands, dopamine, serotonin, arginine, and phenol, were investigated by pressure assisted partial filling ACE.

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Michael LÄMMERHOFER

Michael Lämmerhofer is **Full Professor (W3)** for *Pharmaceutical (Bio-)Analysis* at the *University of Tübingen, Germany* (since 2011). He graduated in *Pharmaceutical Sciences* in 1992 and earned his PhD in *Pharmaceutical Chemistry* in 1996 at the *University of Graz, Austria* (Supervisor: Prof. Wolfgang Lindner). Between 1997 and 2002 he was assistant professor and since 2002 to 2011 associate professor at the *University of Vienna, Institute of Analytical Chemistry*. Between 1999–2000 he spent a year of research as post-doctoral researcher at the *Department of Chemistry of the University of California, Berkeley* (Prof. Frantisek Šveč/ Prof. Jean M. Fréchet). Since 2007, he has been associate editor of *Journal of Separation Science* and since 2024 he is editor-in-chief.

His research interests include bioanalysis (metabolomics and lipidomics), pharmaceutical analysis (impurity profiling, enantioselective analytics), multidimensional separations and biopharmaceuticals analysis (peptides, oligonucleotides, proteins, plasmids), and the development of functionalized separation materials (chiral stationary phases, mixed-mode phases, chemo- & bioaffinity materials, nanoparticles, monoliths).

Lipidomics in Biomedical Research

Michael LAEMMERHOFER, Adrian BRUN, Philipp SEYFRIED, Min SU, Xiaoqing FU, Zijing XU

*University of Tübingen, Institute of Pharmaceutical Sciences,
Auf der Morgenstelle 8, 72076 Tübingen, Germany.
michael.laemmerhofer@uni-tuebingen.de*

Key Words: SWATH, Oxidized phospholipids, Phosphoinositides, Platelet lipidomics.

Lipidomics is a powerful approach in biomedical research that enables the comprehensive profiling of lipid molecules to uncover their roles in cellular signaling, metabolism, and disease pathogenesis. It supports the discovery of diagnostic and prognostic biomarkers, provides mechanistic insights into biological processes, and aids in validating hypotheses from other experimental platforms.

Advances in mass spectrometry, such as data-independent acquisition, ion mobility, and isomer-specific separation techniques, have significantly enhanced the accuracy and depth of lipid identification, particularly for complex and isomeric species, driving progress in areas like inflammation, cancer, and metabolic disorders. Our general untargeted UHPLC-ESI-QTOF-MS/MS lipidomics workflow is based on monophasic lipid extraction with methanol-2-propanol-methyl tert-butylether, reversed-phase LC on CSH C18, data-independent acquisition with SWATH (sequential window acquisition of all theoretical fragment ion mass spectra), and MS/DIAL-based automated data processing followed by manual curation. Typically, 300 to 1000 lipids can be structurally annotated using LipidBlast in silica library matching of experimental deconvoluted mass spectra. Low abundant lipids such as oxylipins and steroids require targeted UHPLC-QqQ-MS/MS analysis to reach the low levels of these signaling molecules. For analyzing challenging lipid classes like phosphoinositide and oxidized phospholipids

New workflows have been established based on studying fragmentation rules, cheminformatics MS spectral library generation and refined data processing software. Applications of our targeted and untargeted lipidomics workflows in collaborative biomedical research projects will be outlined comprising platelet lipidomics [1], muscle dystrophy and lysosomal storage disorders [2], samples from coronary artery disease patients, volunteers of stress studies and female brain imaging study cohorts [3].

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Andrei MEDVEDOVICI

Andrei Medvedovici is currently **Professor** in Separation Sciences at the University of Bucharest, Romania, Faculty of Chemistry, Department of Analytical and Physical Chemistry,

Born in Bucharest, Romania, on November 29th, 1961. *Earned degrees:* B.Sc. in Chemistry (1984) at the Faculty of Chemical Engineering, Chemistry section, Polytechnic Institute of Bucharest; M.Sc. in Analytical Chemistry (1985) at the same institution; Ph.D. in Chemistry (1994) at the Faculty of Chemistry, University of Bucharest. *Study grants:* Pre- and post-doctoral stages at the University of Ghent – Belgium (1991–1992 and 1994–1996). *Professional experience:* Professor at the Faculty of Chemistry, University of Bucharest since 2005; Co-ordinator for Ph.D. theses since 2006; R&D manager (2002–2008) and Scientific Director (2009–2013) at Labormed Pharma, Romania.

Awards: C.D. Nenițescu prize of the Romanian Academy (2009). *Field of interests:* Separation sciences; Sample preparation (LLE, SPE, SPME, SFE); Chromatographic techniques (HPLC, PC-SFC, CGC); Detection in chromatographic techniques (DAD, FLD, RID, ELSD; MS and MS/MS); Automation in chromatography (on-line SPE/HPLC); Multidimensional /comprehensive chromatography (LC/LC; LC/GC; SFC/LC); Hyphenation in separation techniques (LC/MS-MS, SFC/MS-MS, CGC/MS); Development and validation of separation methods; Qualification of the analytical instrumentation.

Application fields: bioanalysis, pharmaceuticals, environmental, food chemistry.

Publications: ISI indexed - 151; cumulated impact factor - 264; non ISI indexed - 14 (10 in international journals); Published courses (University of Bucharest Publishing House) - 5; Chapters in books (international publishers) - 4; Chapters in books (national publishers) - 6; Chapters in international encyclopedias - 10. *Scientometrics:* h-index – 27 (ISI Web of Science), 28 (Scopus), 30 (Research Gate), 32 (Google Scholar).

Member in the Editorial board at Bioanalysis, Journal of Liquid Chromatography & Related Technologies, and The Journal of Environmental Chemistry and Ecotoxicology, Advisory board member for over 15 international journals.

From Classic Liquid-Liquid Extraction to Supramolecular Solvents in Bioanalytical Applications

Andrei MEDVEDOVICI, Mircea-Alexandru COMĂNESCU

University of Bucharest, Faculty of Chemistry, Department of Analytical and Physical Chemistry,
Panduri Ave. # 90–92, Bucharest-050663, Romania.
andrei.medvedovici@chimie.unibuc.ro ; avmedved@yahoo.com

Key Words: Liquid-liquid extraction, Large volume injection in diluents non-miscible with the mobile phase, Supramolecular solvents (SUPRAS), Sample preparation, Bioanalytical methods.

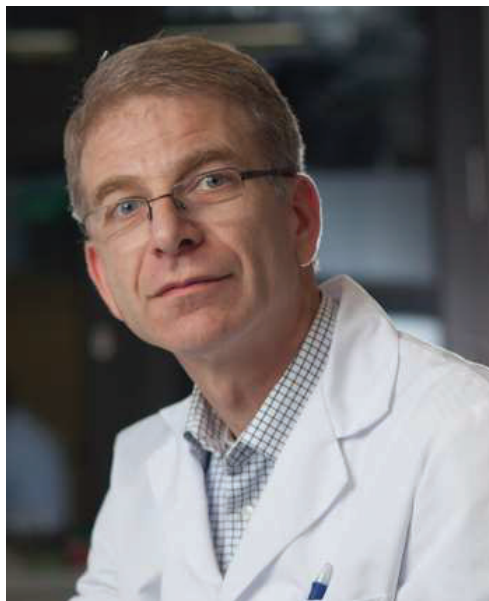
Liquid-liquid extraction (LLE) is certainly the first alternative used for isolating target analytes from complex matrices in bioanalytical applications. The primary advantages are affordability, the ability to tune the polarity characteristics of the extraction solvent(s) with the polarity character of the analyte(s), the potential to optimize the extraction yield through using diverse tools such as the pH of the extracted phase, back-extraction, ion pairing options and salting out effects, and the interesting issue related to sample concentration through solvent evaporation, immediately following the extractant phase isolation. The main drawbacks are the need for relatively high volumes of both sample and extraction phases, the potential harmful health impact relating to the use of toxic organic solvents, extensive sample manipulations which induce an increase in the variability of the resulting quantitative data, affecting the throughput-ness of the whole sample preparation approach, especially when the number of processed samples is considerably high, as it is the case in bioavailability/bioequivalence studies.

The use of specific LLE solvents (including green alternatives) in correlation to the ability of making large volume injection (LVI) in diluents which are not miscible with the mobile phase in liquid chromatography may be the key to the above-mentioned drawbacks. Although such alternative is theoretically forbidden by the chromatographic axiom that *the sample should be dissolved in a solvent fully miscible with the mobile phase and exhibiting less eluotropic force compared to the mobile phase composition at the beginning of the separation process*, it appears that such approaches are feasible in some specific experimental conditions. In fact, LVI of samples prepared in diluents which are not miscible with the mobile phase should be interpreted as an on-line coupling of a LLE stage to the RPLC separation. In such cases, all operations relating to the sample preparation process, including injection, may be realized in a single HPLC vial, with simultaneous extraction & reduction of biological sample volumes.

Relatively recent studies highlighted the possibility of combining the LLE process with size exclusion principles, through the in-situ generation of a new phase resulting from a quacervation process. Ternary systems containing water (usually already in the sample), an organic water-miscible solvent (such as THF, ethyl lactate or *i*-propanol) and a surfactant (i.e. alkanols) first produce reversed micelles which are naturally self-associating as a new phase, separated from the initial aqueous one. Denominated as SUPRAS (supramolecular solvent), such a new phase has the possibility of extracting small polar molecules in the polar cavity of the quacervate, which mainly contains water, and apolar low molecular mass compounds in the apolar sidewalls of the aggregates, which consist of the long alkyl chains. Polar/apolar entities with high molecular masses / volumes do not penetrate in the cavity and/or cavity walls and are thus excluded from the extraction process. This is the case of proteins, glycoproteins and polysaccharides naturally found in biological samples. SUPRAS are highly effective when extracting target analytes from biological matrices. However, a direct LVI of SUPRAS in the RPLC columns should be considered with precaution, as injection volumes are often limited to 20 μ L [1]. Exceeding this threshold may produce serious peak shape alteration. Although exhibiting good size exclusion abilities, SUPRAS are fairly non-selective with respect to the polarity characteristics of low molecular mass extracted compounds. This means that SUPRAS extraction will easily be employed when the chromatographic separation is monitored through highly selective / sensitive detectors (i.e. tandem MS), but has limited use when a simple UV detection is applied. All above-mentioned features will be discussed over the presentation.

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Erwin ROSENBERG

Erwin Rosenberg is **Professor** of Analytical Chemistry and Head of the Research Group for Organic Trace Analysis at the Institute of Chemical Technologies and Analytics of the Vienna University of Technology. Prior to his habilitation in 2000, he has received both his Diploma and PhD degrees from the same university. During the years 2003–2006, he was appointed Guest Professor at the University of Leoben (Austria), and later also had lecturing appointments at the Technical University of Gdańsk, the University of Plovdiv and the University of Thessaloniki.

He is a specialist in the development of chromatographic methods and instrumentation and the pertinent sample preparation procedures for environmental and industrial problems with a particular focus on green and environmentally friendly techniques. More recently, his research interests have focused on the determination of odorous volatile organic compounds, both with relevance to food and consumer products, but also for the purpose of non-invasive medical diagnosis.

He has (co-)authored more than 150 publications in peer reviewed journals that have received more than 3,500 citations (*h*-index of 34), and 14 book chapters related to various aspects of separation sciences, environmental analysis and sample preparation, serves at the Editorial Boards of five analytical and environmental chemistry journals and currently is the Austrian representative in the Central European Group for Separation Sciences (CEGSS).

Analysing the Human Volatilome by Comprehensive Two-Dimensional Gas Chromatography for Early Detection of Lung Cancer

Erwin ROSENBERG¹, Synnöve LEMKE^{1,2}, Esther HEID², Brigitte HOLZER³, Johannes BINTINGER³

¹*TU Wien, Institute of Chemical Technologies and Analytics, 1060 Vienna, Austria;*

²*TU Wien, Institute of Materials Chemistry, 1060 Vienna, Austria;*

³*TU Wien, Institute of Applied Synthetic Chemistry, 1060 Vienna, Austria.*

egon.rosenberg@tuwien.ac.at

Key Words: Breath analysis; Lung cancer; Biomarkers; VOCs; Thermal desorption.

Exhaled breath contains a complex mixture of volatile and semi-volatile organic compounds (VOCs) originating from endogenous metabolism, host–tumor interactions, oxidative stress, and environmental exposures. Lung cancer alters several biochemical pathways that can manifest as distinct VOC fingerprints, offering a noninvasive opportunity for early detection and monitoring [1]. Translating this promise into clinically meaningful performance requires robust sampling, efficient analyte transfer, and sufficient analytical resolving power to disentangle highly complex, low-abundance chemical signatures in humid matrices.

The overall aim of this project is the development of an electronic nose for fast, on-site and non-invasive detection of individual VOCs or VOC patterns for early lung cancer detection. This electronic nose is a hand-held device with a sensor array made selective to certain VOCs or VOC patterns by different tailor-made polymer coatings [2]. To inform the synthesis of more selective polymer materials, but also to identify individual biomarkers for a better understanding of the underlying metabolic pathways, and to provide the chemical data for the training of the electronic nose, comprehensive two-dimensional gas chromatography is proposed with time of-flight mass spectrometric detection (GC×GC-TOF-MS) for the analysis of breath samples.

To this end, human breath samples are collected in 3 L-Tedlar bags, transferred to thermal desorption tubes and thermally desorbed to the GC-MS system. This approach combines simple sample collection with controlled preconcentration, comprehensive two-dimensional separation with high peak capacity and fast, full-spectrum acquisition. Advantages of this strategy, compared to using one-dimensional gas chromatography and/or quadrupole-MS data acquisition are discussed. Identification of low-abundance metabolites clearly benefits from the increased peak capacity of comprehensive separation and the full range data acquisition of TOF-MS. If cryogenic modulation is used instead of flow modulation, also sensitivity can be enhanced over the one-dimensional separation, making this technique fully feasible for biomarker discovery [3].

At this stage, method development is under full swing, and the various considerations of an optimized workflow shall be discussed in detail. No patient samples have been measured yet, and therefore both the training of the electronic nose, as well as the classification of patient samples remain to be carried out in the remaining part of the project. Once this is achieved, the feasibility of the electronic nose for direct detection of lung cancer from patient breath samples will be demonstrated while GC×GC-TOF-MS after thermal desorption analysis of breath samples will continue to serve as a reference and metabolite discovery technique.

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José Juan SANTANA RODRÍGUEZ

Dr. José Juan Santana Rodríguez is **Professor** of Analytical Chemistry at the University of Las Palmas de Gran Canaria (ULPGC) since 1998. He has been an Invited and Visiting Professor at more than twelve universities in Europe, the United States of America, Australia, Japan and South America.

He is author/co-author of over 177 scientific articles in indexed journals, of more than 300 communications to international and national congresses, one book and 12 book chapters.

He has also been, a member of the scientific committee of sixteen international and national conferences, the general chairman of three international symposia and an invited speaker at twenty international conferences.

He has been awarded the “Recognition to Scientific Career Prize” at ULPGC (2019) and he is a permanent member of the Royal Sciences Academy of The Canaries (Spain).

He has been founder and Director of the Institute for Environmental Studies and Natural Resources (i-UNAT) at the University of Las Palmas de Gran Canaria and Dean of Faculty of Marine Sciences of same university.

His research is focused on the Optimization and Development of New Analytical Methodologies for the Determination of Organic Pollutants in Environmental Samples and the Control and Impact of Microcontaminants in Terrestrial and Marine Ecosystems.

Organic Micropollutants in Aquatic Ecosystems: Advanced Chromatographic Analysis and Impact

José Juan SANTANA RODRÍGUEZ

*Universidad de Las Palmas de Gran Canaria, Instituto de Estudios Ambientales y Recursos Naturales
(i-UNAT), 35017 Las Palmas de Gran Canaria, Spain.*

jozejuan.santana@ulpgc.es

Key Words: Organic emerging contaminants, Aquatic ecosystems, Ultra-high-performance liquid chromatography, The Canary Islands.

The quality of the aquatic ecosystems relies heavily on natural and anthropogenic processes. Several problems related to the uptake of pollutants and their subsequent bioaccumulation in organisms have been described worldwide. Therefore, it is essential determine the pollution sources and type of pollutants that are continuously releasing into this natural ecosystem.

One of the new kind of pollutants refers to organic emerging contaminants (OEC) which includes a large number of chemical compounds such pharmaceuticals, personal care products, hormones, flame retardants, etc. The presence of these compounds in aquatic ecosystems may exhibit harmful effects on organisms and there is clear evidence of the repercussions that these substances can have on biological processes in flora and fauna, and even in human beings. Their concentrations in environmental samples are generally very low (ng/L to µg/L), so they do not cause immediate effects on organisms, but prolonged exposure may produce chronic effects on them or more subtle effects such as metabolic or reproductive changes in different species

In this lecture, we present several cases studies about the presence of some families of OEC in different matrices from aquatic systems of an insular region, specifically, the Canary Islands. On the one hand, we focus on the different extraction/preconcentration and determination techniques applied, which include Solid Phase Extraction and Microwave Assisted Extraction and Ultra High-Performance Liquid Chromatography with tandem mass spectrometry, respectively. And, on the other hand, on the monitoring and impact of OEC studied in different locations of this Atlantic archipelago [1, 2, 3].

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Didier THIÉBAUD

Didier Thiébaud is a **Doctor of Pharmacy** and **PhD in Analytical Chemistry**. He was Director of Research at the Centre National de la Recherche Scientifique (CNRS) in the LSABM (Laboratoire Sciences Analytiques, Bioanalytiques et Miniaturisation) in the group of Chemistry Biology Innovation Institute of ESPCI (École supérieure de physique et de chimie industrielles de la Ville de Paris); Paris, PSL University.

During almost forty years, until 2025, his research mainly focused on Supercritical Fluid Chromatography and for more than 25 years on comprehensive two-dimensional chromatography GC×GC. Further to improving the performances of these techniques, he also investigated their hyphenation, their miniaturisation and their application to the analysis of organic compounds in very complex matrices (petroleomics, lipidomics, environment ...) in partnership with academic groups and companies.

He supervised and co-supervised 30 promoted PhD students and authored or co-authored more than 140 publications, 3 books, 8 book chapters and 4 patents. He also served as a president of "Francophone Association of Separation Sciences" (AfSep). Currently Dr. Thiébaud is Honorary Director of Research of the CNRS, Paris, France.

He supervised and co-supervised 30 promoted PhD students and authored or co-authored more than 140 publications, 3 books, 8 book chapters and 4 patents. He also served as a president of the "Francophone Association of Separation Sciences" (AfSep).

Supercritical Fluid Chromatography: the Pros and the Cons after 40 years

Didier THIÉBAUT

*Honorary Director of Research
French National Centre for Scientific Research (CNRS), Paris, France.
didier-r-p-thiebaut@outlook.fr*

Key words: Supercritical fluid chromatography, Pros and Cons.

After doing 40 years of research devoted for a large part to the supercritical fluid chromatography (SFC), it is evidence that SFC has not expanded as one could expect when it started.

This lecture will point out some reasons to try to understand this situation by discussing some features of SFC presented as advantages while the drawbacks were often “forgotten”.

Moreover, despite analytical techniques should be complementary to perform better analysis, competition between separation techniques is a reality: the availability of machines, the price, the investments needed to buy or upgrade systems, the effort to assimilate a different technique, must be considered.

Improvement of separation techniques and their hyphenation to mass spectrometry (MS) must be considered too in order to understand how this competition may have slowed down SFC development.

Capabilities of Ultra-High Performance Liquid Chromatography (UHPLC) for fast and very efficient separations, the implementation of smaller internal diameter columns in routine UHPLC (solvent saving), new column chemistries, optimized interfaces for MS coupling, sample handling etc. have enhanced the power of Liquid Chromatography.

This will be discussed to answer the question, if possible: what is the future of analytical SFC?



Irena VOVK

Res. Prof. Dr. Irena VOVK holds B.Sc., M.Sc. and PhD. in chemistry from the Faculty of Chemistry and Chemical Technology (FCCT), University of Ljubljana. She has been employed at the FCCT (1990–1993), the National Institute of Chemistry (NIC; since 1994, 2008–2020 head of the Department of Food Chemistry; 2017–2021 Quality Council member) and EN-FIST Centre of Excellence (2010–2013, head of the RRP7 group). She is the president of the Food Chemistry Section of the Slovenian Chemical Society (SCS) and its representative in the Central European Group for Separation Sciences (CEGSS) and the Division of Food Chemistry of the European Chemical Society. She has been the representative of the SCS in the European Society for Separation Sciences (EuSSS, 2012–2023).

Research interests: Development of methods based on chromatographic and hyphenated techniques for determination, isolation and identification of bioactive natural compounds. She has been active as the principal investigator of research programme, national, bilateral and European (WP leader) research projects and projects for industry. She participated in 41 scientific and 9 organizing committees of international symposia, 3 times chair (iss2020.si, hptlc2020.si, iss2015.si), once vice-president (CEFood 2022). She is a member of Editorial boards of eight scientific journals. She has been a mentor/co-mentor for academic theses: 7 PhD students, 1 master's and 10 bachelor's.

Bibliography: From 640 bibliographic units, 122 scientific articles, 9 book chapters, more than 50 invited lectures at international symposia and 5 patents.

Awards: "Prometheus of Science for Excellence in Communication" by the Slovenian Science Foundation (2009); "Grand Prize Winner" with Slovenian team at iGEM 2010 competition (MIT, USA, 2010); "Medal and award for achievements in the field of chromatography and related separation techniques" by the CEGSS (2016); Recognition of the Slovenian Chemical Society "for the outstanding contribution as the editor of the journal *Acta Chimica Slovenica*" (2022); "M. Tswett & W. Nernst "Science for Life" Award" by the EuSSS and the CEGSS (2023).

Phytochemicals in Food and Plant Samples – Challenges in Chromatographic and Effect-directed Analyses

Irena VOVK¹, Vesna GLAVNIK¹, Maja BENSA², Breda SIMONOVSKA¹, Živa VIPOTNIK¹,
Etil GUZELMERIC³, Ágnes M. MÓRICZ⁴, Uroš GAŠIČ⁵

¹National Institute of Chemistry, Laboratory for Food Chemistry,
Hajdrihova 19, 1000 Ljubljana, Slovenia;

²University of Ljubljana, Faculty of Health Sciences, Research Institute of Faculty of Health Sciences,
Zdravstvena pot 5, 1000 Ljubljana, Slovenia;

³Yeditepe University, Faculty of Pharmacy, Kayisdagi Cad., Atasehir, 34755, Istanbul, Türkiye;

⁴Plant Protection Institute, HUN-REN Centre for Agricultural Research,
Fehérvári út 132-144, 1116 Budapest, Hungary;

⁵University of Belgrade, Department of Plant Physiology;
National Institute of Republic of Serbia, Institute for Biological Research “Siniša Stanković”,
Bulevar despota Stefana 142, 11060 Belgrade, Serbia.

irena.vovk@ki.si

Key Words: HPTLC, HPLC, Effect-Directed Analysis, Phytochemicals.

The growing demand for novel phytochemical sources, functional foods, and food supplements, together with increasing requirements for food quality and safety assessment, calls for advanced analytical approaches capable of addressing complex plant and food matrices. This lecture will address challenges in the development of methods based on chromatographic and hyphenated techniques. Examples will cover targeted and non-targeted analyses of phytochemicals in plant and food matrices using HPTLC-densitometry, HPTLC-image analysis, HPTLC-MS/MS, (U)HPLC-UV/Vis, and (U)HPLC-MS/MS. Strategies for overcoming challenges related to stability of the analytes, lack of commercial standards and standard reference materials, lack of chromophores, and isomeric structures will be discussed through selected case studies of analyses of phytochemicals from different groups in plant samples (medicinal plants, invasive alien plant species (tree of heaven [1,2,3], Russian vine, Chinese knotweed, Japanese knotweed, Bohemian knotweed and giant knotweed), flower pollen [3,4], etc.) and food samples (e.g., food supplements [7], bee pollen [3,4,6], food waste). Challenges in non-targeted (HP)TLC–EDA analyses of antimicrobial compounds, antioxidants and enzyme inhibitors in crude extracts from different parts of invasive alien plant species, flower pollen and bee pollen will also be presented.

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KEYNOTE LECTURES



Ramia AL BAKAIN

Ramia Al Bakain holds a PhD in Analytical Chemistry from Sorbonne Université Pierre et Marie Curie (UPMC), Paris, France. She is a Professor in the Department of Chemistry at the University of Jordan and Visiting Professor at LSABM, ESPCI Paris, France.

Her research focuses on the application of analytical chemistry to develop innovative methods in water, agriculture, and food security. She also works on green techniques for wastewater treatment and sustainable approaches to preserving natural resources. Ramia Al Bakain maintains extensive international research collaborations with institutions in the USA, France, Italy, Austria, Lebanon, Germany and Slovakia. She leads numerous international scientific projects and supervises interdisciplinary teams of graduate students working on water-food-agriculture security challenges in the MENA region. In addition, she is a member in the editorial board of Journal Sustainable Chemistry One World – Elsevier and Science & Technology Nexus Journal.

Ramia has received more than 23 several prestigious international honors and awards, including:

- Elsevier Foundation – ISC3 Green & Sustainable Chemistry Award;
- L'Ordre national du Mérite – *President of the French Republic*;
- L'Oréal-UNESCO Award for Women in Science;
- TWAS Young Arab Scientist (YAS) Prize for Scientific and Technological Achievement in Agricultural and Environmental Sciences;
- Faculty for the Future - The Schlumberger Foundation.

Impact of Sample Handling on the Volatilomic Profile of Medicinal Plants

Ramia AL BAKAIN^{1,2}, Ariane MORTEVEILLE², Mélanie COHEN², Jérôme VIAL²

¹The University of Jordan, School of Science, Department of Chemistry, 1942 Amman, Jordan;

²ESPCI Paris, PSL Research University, UMR CBI, Laboratoire Sciences Analytiques, Bioanalytiques et Miniaturisation, 10 rue Vauquelin, 75231 Paris Cedex 05, France
r.bakain@ju.edu.jo; ramia.bakain@yahoo.com

Keywords: GC–MS, Volatile organic compounds, Medicinal herbs, Extraction techniques.

Medicinal and aromatic plants contain complex mixtures of volatile organic compounds (VOCs). They are widely used in food, cosmetic, pharmaceutical, and aromatherapy applications. However, the characterization of plant volatilomes depends on the extraction methodology employed prior to GC–MS analysis. This work investigates the impact of different extraction approaches on the volatile fingerprints of three representative Jordanian medicinal plants: nutmeg (*Myristica fragrans*), thyme (*Thymus vulgaris*), and rosemary (*Salvia rosmarinus*).

Several extraction techniques coupled to GC–MS were compared, including static headspace (SHS), headspace solid-phase microextraction (HS-SPME), direct immersion SPME (DI-SPME) in water infusion, solvent extraction followed by liquid injection, and direct thermal desorption (TD). Key experimental parameters such as extraction temperature, extraction time, incubation conditions, fiber coating, and salt addition were optimized. Among five tested SPME fibers evaluated, CAR/PDMS and DVB/CAR/PDMS showed the highest extraction efficiencies. Optimal HS-SPME conditions were obtained at 70°C with 5 min incubation and 15 min extraction. The different extraction methods exhibited marked selectivity differences according to analyte volatility and polarity. HS-SPME provided the broadest volatile profiles and the highest number of detected compounds, whereas SHS favored the extraction of the most volatile analytes. Solvent extraction enabled the detection of less volatile compounds not observed in HS-SPME chromatograms.

TD further enhanced extraction efficiency, enabling higher compound coverage compared to liquid injection. The study of plant infusions revealed significant VOCs losses during infusion preparation, particularly for highly volatile terpenes. NaCl addition enhanced HS-SPME extraction through a salting-out effect, especially for semi-volatile compounds of intermediate polarity. Conversely, DI-SPME induced progressive fiber degradation. Quantitatively, (120 vs. 60); (152 vs. 36) and (136 vs. 43) compounds were detected using HS-SPME vs. SHS for nutmeg, thyme and rosemary, respectively. For the extracts, 132, 159 and 132 peaks were detected using TD compared to 106, 120, and 82 for nutmeg, rosemary and thyme, respectively using liquid injection. For dried plant, TD enabled the detection of 245 compounds in thyme using only ~30 mg, compared to 152 using HS-SPME with 500 mg.

These results demonstrate that sample preparation critically influences the GC–MS fingerprint of plant VOCs. The complementarity observed between extraction approaches highlights the importance of selecting extraction strategies according to the targeted chemical space and analytical objectives. This study provides new insights into the optimization of VOC extraction methodologies for plant volatilomic characterization.

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Ede BODOKI

Ede Bodoki, PhD, Pharmacist, is a habilitated Professor of Analytical Chemistry at the Faculty of Pharmacy, Iuliu Hațieganu University of Medicine and Pharmacy, and leader of the Molecular Imprinting and Functional Polymers research group.

With more than 20 years of research experience, he has developed recognized expertise in analytical and bioanalytical chemistry, molecularly imprinted polymers, and drug delivery systems.

His research integrates the development of innovative analytical platforms and functional materials with the elucidation of molecular recognition and interfacial mechanisms using advanced separation techniques, (bio)electroanalysis, molecular spectroscopy, hyphenated analytical methods (HPLC-EC-MS, EC-MS and EC-SERS), and chemometrics for multivariate experimental design and data analysis. All these activities have led to various innovative translational applications in the biomedical, pharmaceutical, and agrochemical fields.

Mechanochemical Molecular Imprinting: Grinding Towards Selectivity

Andreea Elena BODOKI¹, Bogdan-Cezar IACOB², Ede BODOKI²

¹Iuliu Hațieganu University of Medicine and Pharmacy, Faculty of Pharmacy,
Department of Inorganic Chemistry, 400012 Cluj-Napoca, Romania;

²Iuliu Hațieganu University of Medicine and Pharmacy, Faculty of Pharmacy,
Department of Analytical Chemistry, 400349 Cluj-Napoca, Romania.
bodokie@umfcluj.ro

Key Words: Molecular recognition, Molecularly imprinted polymers, Mechanochemistry

Building on our proof-of-concept hybrid photo- and mechanochemically assisted solid-state molecular imprinting strategy [1], we present a systematic study of the mechanochemical parameters governing free-radical, template-assisted polymerization of acrylic monomers under solvent-free or solvent-minimal conditions. Using standardized ball-milling equipment, we elucidate how key variables (grinding media, bulking agent, milling time, mechanical energy input, and trace solvent addition) govern polymerization efficiency, polymer morphology, and molecular recognition performance.

We demonstrate that mechanochemical MIP synthesis operates under fundamentally different principles than solution-phase imprinting, enabling reaction times below 20 min, near-quantitative yields, and enhanced control over polymer architecture. These features translate into readily tunable binding affinity and selectivity of mechanochemically imprinted polymers (MMIPs) [2]. Crucially, we identify an optimal physicochemical window in which minute amounts of a solvent (Liquid Assisted Grinding, LAG) mediate mechanochemical reactivity while preserving high-fidelity recognition motifs. Changes in the LAG environment do not simply alter the overall adsorption capacity of the polymers but modulate a binding landscape whose expression also depends on the molecular characteristics of the rebinding species.

Beyond solvent reduction and environmental benefits, our findings demonstrate that mechanical activation fundamentally reshapes the variables governing molecular imprint formation and recognition. By defining how these variables collectively shape the binding landscape, we establish a basis for moving from empirical optimization towards the rational control of selectivity in mechanochemical molecular imprinting. Coupled with the scalability of milling-based processing, this perspective positions mechanochemical imprinting as a promising route towards sustainable, high-performance molecularly imprinted polymers for analytical, environmental, and biomedical applications.

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Magdalena BUSZEWSKA-FORAJTA

Dr hab. inż. Magdalena Buszevska-Forajta, Professor at Nicolaus Copernicus University in Toruń, is affiliated with the Institute of Veterinary Medicine at Nicolaus Copernicus University and the Kuyavian-Pomeranian Centre for Science and Technology (KPCNT). Her research focuses on analytical chemistry, bioanalysis and metabolomics, combining advanced instrumental techniques with the study of biological and medical processes.

A major area of her scientific interest is the application of metabolomics and biostatistics to investigate mechanisms underlying disease development, particularly chronic non-healing wounds, metabolic disorders and cancer. She also conducts research on the identification of novel biologically active substances and the discovery of potential lead compounds based on ethnopharmacological evidence. Her work includes the isolation and determination of natural bioactive compounds in honey, herbs and fruit.

Her broader research portfolio covers healthy and functional foods, honey-related studies and aquaculture. She applies techniques such as LC-MS/MS, metabolomics, chemometrics and multivariate data analysis to explore the role of metabolites in health, disease and food quality.

Professor Buszevska-Forajta has published in recognised international journals, participated in National Science Centre and European projects, and collaborated with clinical and research teams in Poland and abroad. She is also actively involved in science communication, linking laboratory research, data analysis and practical applications.

Beyond Total Phenolics: Analytical Profiling and Multi-Criteria Design of Mineral–Plant Functional Tonics

Mateusz SUGAJSKI^{1,3}, **Magdalena BUSZEWSKA-FORAJTA**^{2,3}, Bogusław BUSZEWSKI³

¹*Nicolaus Copernicus University in Toruń, Faculty of Chemistry, Department of Environmental Chemistry and Bioanalytics, Gagarina 7, 87-100 Toruń, Poland;*

²*Nicolaus Copernicus University in Toruń, Faculty of Biological and Veterinary Sciences, Institute of Veterinary Medicine, Lwowska 1, 87-100 Toruń, Poland;*

³*Prof. Jan Czocharński Kuyavian-Pomeranian Science and Technology Center, Krasieńskiego 4, 87-100 Toruń, Poland.
m.buszewska@umk.pl*

Key Words: Functional formulation, Mineral water, Polyphenols, Antioxidant capacity, Multi-criteria selection.

The development of functional beverages requires an integrated analytical strategy that links matrix composition, phytochemical profile, stability and biological potential. In this study, Ciechocinek mineral water was used as an active formulation matrix for designing plant-enriched regenerative tonics. The mineral water “Krystynka” was selected as the base matrix after preliminary assessment of formulations containing 30%, 45% and 60% mineral water. Physicochemical parameters, including pH, conductivity, total dissolved solids and mineral character, indicated that the 45% variant provided a balanced compromise between the presence of the mineral matrix and formulation stability.

The plant component system was designed using barberry as a constant component and chokeberry and elderberry as variable components. Barberry, present at 10% in each formulation, served as a model botanical material connecting raw-material screening, extraction optimisation and final tonic design. Chokeberry was introduced as a source of phenolic compounds and reducing capacity, whereas elderberry was used to enhance the phenolic, flavonoid and colour-related profile of the formulations. A panel of 24 mineral–plant formulations was prepared and evaluated using a broad analytical workflow.

The assessment included physicochemical characterisation, total phenolic content, total flavonoid content, antioxidant capacity, marker-compound profiling and formulation stability. Since single analytical parameters were insufficient to identify the most promising variants, a weighted multi-criteria model, WPFF, was applied to integrate chemical, functional and application-related descriptors. The model enabled the selection of leading formulations with the highest functional and technological potential. The selected variants were further subjected to functional validation using an α -amylase inhibition assay, while molecular docking was considered as an additional interpretative tool supporting the relationship between marker compounds and biological activity.

This work demonstrates that functional beverage design should not be based solely on total phenolic or flavonoid content, but rather on an integrated analytical framework combining matrix properties, phytochemical composition, antioxidant potential, stability and target-oriented functional validation. The proposed approach provides a rational basis for developing premium mineral–plant formulations and highlights the role of analytical chemistry in transforming local mineral resources and botanical materials into scientifically supported functional products.



Petr ČESLA

Doc. Ing. Petr Česla is associate professor at the University of Pardubice, Faculty of Chemical Technology, where he received **PhD** in 2007 and finished **habilitation** in 2016.

His research activities include development of liquid phase separation techniques – mainly two-dimensional liquid chromatography, capillary electrophoresis, optimization procedures, and data processing. He has been acting as principal investigator of several projects funded by Czech Science Foundation, focused on two-dimensional LC and CE separations. The latest project was focused on the fraction transfer process in 2D LC and development of active modulation.

He published over 55 original research articles in peer-reviewed journals with more than 1100 citations and H-index 20. He also co-authored two book and three book chapters.

Petr Česla is the representative of the Czech Chemical Society in the Central European Group on Separation Sciences.

Chromatographic Response Functions Revisited: Development of a New Strategy for Gradient Optimization in 2D-LC

Petr ČESLA, Michal KAŠPAR, Sára SVOBODOVÁ,
Pavlaína MUSILOVÁ, Soňa ŘEZKOVÁ

University of Pardubice, Faculty of Chemical Technology, Department of Analytical Chemistry,
Studentská 573, CZ-53210 Pardubice, Czech Republic.
petr.cesla@upce.cz

Key Words: Gradient elution, Optimization, Response functions, Retention modeling,
Two-dimensional LC.

Numerical optimization of gradient elution conditions in high-performance liquid chromatography is traditionally based on retention modeling followed by the evaluation of desired chromatographic criteria, i.e. chromatographic response functions, most commonly those derived from the resolution of critical peak pairs. We have previously demonstrated that retention modeling combined with resolution mapping provides an efficient framework for method development in both reversed-phase liquid chromatography (RP-LC) [1] and hydrophilic interaction liquid chromatography (HILIC) [2]. Despite their widespread use, conventional chromatographic response functions typically describe only selected aspects of separation quality and may not provide a sufficiently comprehensive assessment of complex optimization problems encountered in multidimensional liquid chromatography, and liquid chromatography coupled with tandem mass spectrometry.

To overcome these limitations, we recently introduced the Gradient Score concept, a multi-criteria chromatographic response function integrating chromatographic selectivity, analyte distribution, analysis time, and mass spectrometric acquisition constraints into a single optimization framework [3]. This concept was subsequently extended into a comprehensive workflow for LC-MS/MS method development, encompassing stationary-phase selection, retention modelling, and segmented gradient optimization, while preserving objective and transparent evaluation of multiple performance criteria simultaneously [4]. Furthermore, our recent study combining Linear Solvent Strength (LSS) theory with Quantitative Structure-Retention Relationships (QSRR) demonstrated that retention modelling can provide not only predictive capabilities for method optimization but also valuable mechanistic insight into analyte retention under diverse chromatographic conditions [5].

Building on these developments, the present work revisits the concept of chromatographic response functions in the context of HILIC x RP two-dimensional liquid chromatography. The performance of conventional resolution-based response functions is critically compared with the Gradient Score strategy, and their suitability for gradient optimization in comprehensive two-dimensional separations is evaluated. The goal is to assess whether multi-criteria response functions can provide a more robust and informative basis for gradient optimization than traditional resolution-oriented approaches.

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Massimo DEL BUBBA

Massimo Del Bubba is **Professor** at University of Florence, Department of Chemistry. He is author of 166 papers published in "peer reviewed" international journals indexed on Scopus with more than 5800 citations and H-index of 43.

He has carried out his research mainly in the field of separation science, developing and applying different methods of extraction of organic compounds from the matrix (e.g., liquid/liquid extraction, offline and online solid phase extraction, liquid/solid extraction assisted by ultrasound and microwaves) and using gas chromatography and liquid chromatography coupled with various types of detectors for their instrumental determination. Among these detectors, the use of single quadrupole mass spectrometry with gas chromatography and triple quadrupole mass spectrometry, linear ion trap, Orbitrap ion trap and time-of-flight coupled with liquid chromatography should be highlighted. These techniques have been successfully used for method development and application in multiple areas, including various environmental matrices (e.g. wastewaters, environmental waters, and sludge), foods (e.g., fruits, clams and fish) and biological fluids (i.e. human milk, urine, and blood).

Professor Del Bubba has also a long experience in the application of chemometrics tools for Design of Experiments (DoE), data exploration and interpretation through techniques such as principal component analysis, cluster analysis, partial least square regression, etc. In recent years, his research activity has significantly contributed also to the field of non-targeted analysis (NTA) using liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS). In this domain, he has pioneered two-step prioritization frameworks combining DoE for the online optimization of MS acquisition parameters with multivariate (e.g. PLS-DA-VIP) and univariate statistical tools for offline feature prioritization.

Furthermore, his work encompasses innovative, data-driven methodologies for unbiased candidate compound selection in NTA method development, utilizing molecular fingerprints, precomputed physicochemical properties, predicted environmental mobility, and predicted ionization efficiency to sample extensive chemical spaces (e.g., CompTox).

Understanding the Chemical Space Coverage for Non-Target Analysis: From Unbiased Compound Selection to Advanced Prioritization in LC-HRMS

Massimo DEL BUBBA¹, Lapo RENAI², Giulia BONACCORSO¹, Saer SAMANIPOUR²

¹University of Florence, Department of Chemistry, Via della Lastruccia 3, 50019 Sesto Fiorentino, Florence, Italy;

²University of Amsterdam, van 't Hoff Institute for Molecular Science, 1098 XH Amsterdam, The Netherlands.
massimo.delbubba@unifi.it

Key Words: Non-Target analysis (NTA), Liquid Chromatography–high-resolution mass spectrometry (LC-HRMS), Chemical space coverage, Feature prioritization, Design of experiments (DoE).

Non-target analysis (NTA) based on liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS) has emerged as a crucial tool for exploring the vast and complex chemical space of environmental contaminants and the exposome. However, conventional workflows face two main bottlenecks: (i) selection bias during method development caused by relying on narrow, structurally homogeneous "watch lists" that assume linear structure-retention/ionization relationships, and (ii) sensitivity and data overload challenges when analysing complex matrices, where relevant signals are masked by dissolved organic matter (DOM).

To address the first challenge, an unbiased, data-driven selection strategy was developed to sample representative structures from large chemical libraries, such as the U.S. EPA CompTox database [1]. By incorporating precomputed physicochemical descriptors, elemental mass defects, and machine-learning predictions of environmental mobility and electrospray ionization efficiency, principal component analysis combined with symmetric gridding and structural phase distance filtering yielded Measurable Compound Lists (MCLs). These MCLs significantly expand chemical class diversity, retention index range ($5 < RI < 900$), and mass coverage (100 – 1200 Da) compared to standard monitoring lists, providing a realistic framework for NTA method development and boundary assessment [1].

Building upon this comprehensive space coverage, an advanced two-step prioritization framework was designed for real-world environmental applications, such as evaluating drinking water treatment processes [2]. First, an "online" prioritization was established by applying a Design of Experiments (DoE) optimization to a physicochemical training set of 42 regulatory-relevant contaminants. This optimized critical LC-ESI parameters (mobile phase additives, spray voltage, and source temperature) to maximize feature ionization efficiency and boost sensitivity for large-volume direct injection. Second, an "offline" prioritization combining multivariate (PLS-DA-VIP) and univariate (Wilcoxon post-hoc test) statistics was implemented to isolate statistically significant feature trends. This integrated workflow successfully tracked persistent pollutants (e.g., PFAS and pharmaceuticals), dynamic DOM shifts, and transient transformation byproducts across treatment stages [2].

Together, these complementary strategies bridge the gap between theoretical chemical space mapping and high-performance experimental execution, offering a robust paradigm for expanding measurable coverage and enhancing signal prioritization in exposomic and environmental LC-HRMS workflows.

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Hartmut FRANK

Academic: Doctoral degree 02/73, until 07/74 Research assistant (Tübingen, organic chemistry); 08/74–08/76: Post-doc (visiting assistant professor, Baylor College of Medicine, Houston, TX, USA); 09/76–07/94: Research Scientist, lecturer in Toxicology/Chemistry (Tübingen); 11/86: Habilitation (Tübingen, Chemical Toxicology); 08/94–09/08 Professor in ecotoxicology (Bayreuth), Chair Environmental Chemistry and Ecotoxicology; 09/08–present: **Professor Emeritus**; the long-standing Editor-in-Chief of Toxicological and Environmental Chemistry.

Scientific: Peptide Synthesis, ion chromatography; capillary-GC technology, stationary phases, polysiloxanes, thermostable chiral GC-phases, Chirasil-Val; chromatographic analytical methods in biochemical toxicology, mechanisms, metabolisms, and toxicology of xenobiotics, especially halogenated chemicals; environmental fate of organic chemicals, pathogenic effects of atmospheric pollutants on plants (trees) and of aquatic pollutants on molluscs.

International: Research cooperations: Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 07/81 and 07/83, three months each. School of Chemistry, Australian National University: 12/85, 07/87, 07/89, four months each, Universidade Nova de Lisboa, Portugal, 1984–2008; two – three weeks each year. Oklahoma Medical Research Foundation, Oklahoma City, 11/98–03/99. Teaching appointments: Visiting professor, Vista University Mamelodi, South Africa 1996, 1997; Guest professor, University of Innsbruck, Innsbruck, Austria, 2002–2007; Honorary Professor, South Central University Changsha, China, 2001–2007; Copernicus Guest Professor, University of Ferrara, Italy, Apr.-Sep. 2007; Guest Professor, Chemistry Dep., Free State University, Bloemfontein, South Africa, 2008/2010 four months each; Honorary Professor, Amity University, Noida, India, Nov. 2012.

Trifluoroacetate: Hydrophilic POP of Extreme Persistence

Hartmut FRANK

University of Bayreuth / Bayreuth Center of Ecological & Environmental Research (BayCEER)
30 Universitäts-Str., D-95447 Bayreuth, Germany
hartmut.frank@uni-bayreuth.de

Key Words: Direct/indirect anthropogenic sources/emissions; TFA, PFAS,
Hydrophobicity versus Hydrophilicity

Objective

Numerous plant-protection and bio/insecticides are trifluoromethylated for eco-toxicological performance, potentially forming trifluoroacetate (TFA) contributing indirectly to atmospheric TFA, first detected in the atmosphere in 1995 [1] and the free hydrosphere [2]; certain polyfluorinated substances (PFAS) also result in TFA as end product. Although PFAS have been in use since about 70 years, TFA has been found in the relevant compartments rather late (1995).

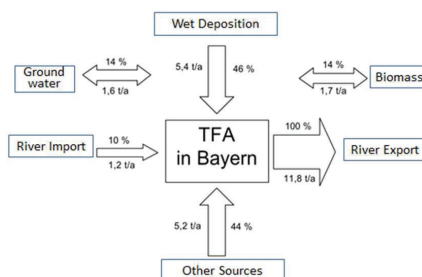
Methods

Briefly, all the materials and the analytical-chemical procedures adopted for trace analysis of PFAS and TFA in the environment – from sampling strategy, sample collection, sample work-up, chromatographic analysis and trace detection – must take unusual physicochemical properties of the analytes into consideration [3]. This means that their ubiquity in all environmental compartments and materials used therein makes trace-analysis difficult; utmost care is needed to avoid mis-analyses.

Results: Also, since some plant-protection agents and biocides may yield trifluoroacetate, its annual environmental budgets (e.g. in the state of Bavaria, Germany) and in oceanic waters have been determined and found to be surprisingly large.

Conclusions

As the ecotoxicological properties of PFAS as well as the lower homologue TFA seem to indicate that their actual ecotoxicological profiles are of low concern; this may change if emissions are continually increased [4, 5].



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Marcin FRANKOWSKI

Professor Marcin Frankowski, PhD, DSc, is a Polish scientist specializing in *analytical and environmental chemistry*. He is affiliated with *Adam Mickiewicz University in Poznań (AMU)*, where he serves as the Head of the *Department of Analytical and Environmental Chemistry* at the Faculty of Chemistry. His scientific work focuses primarily on metal speciation analysis, environmental chemistry, food chemistry, pollution monitoring, and the application of advanced chromatographic and spectrometric techniques as well as hyphenated techniques in analytical chemistry.

Professor Frankowski began his academic career at the Faculty of Chemistry of Adam Mickiewicz University, Poznań, where he obtained his *Master of Science degree in Chemistry in 2005*. In 2009, he earned his PhD in chemical sciences completed under the supervision of Professor Jerzy Siepak. In 2013, he was awarded the degree of *Doctor Habilitatus (DSc)* in chemical.

In recognition of his scientific achievements, he received the title of *Professor of Exact and Natural Sciences in 2023*. International cooperation constitutes an important aspect of his academic career. In 2021, he was appointed *Visiting Professor at Northwest Normal University in Lanzhou, China*, where he participated in doctoral education and contributed to the development of scientific collaboration between Polish and Chinese research institutions.

Professor Frankowski has authored and co-authored around 200 scientific publications in internationally journals. In addition to his research activities, Professor Frankowski has held several important academic and administrative positions. He served as Head of the Water and Soil Analysis Laboratory and, since 2019, has led the Department of Analytical and Environmental Chemistry at AMU.

He is a member of the Polish Chemical Society, Committee on Analytical Chemistry of the Polish Academy, the Chromatography and Related Techniques Group of the Committee of Analytical Chemistry of the Polish Academy of Sciences, and several international scientific and editorial boards.

Advances in Separation and Detection: LC/IC–ICP Hyphenated Techniques

Marcin FRANKOWSKI, Dorota JAKKIELSKA, Anetta ZIOŁA-FRANKOWSKA

Adam Mickiewicz University, Faculty of Chemistry, 8 Uniwersytetu Poznańskiego Str., 61-614 Poznań, Poland.
marcin.frankowski@amu.edu.pl

Key Words: Speciation analysis, Separation methods, ICP-MS, Hyphenated techniques, Toxic elements.

The determination of the chemical speciation of elements such as Al, As, Cr, Hg, Sb, Se, and Sn is essential because their toxicity depends strongly on their chemical form. These elements form numerous inorganic and organic complexes, whose stability and distribution are influenced by factors such as pH, stability constants, ligand concentration, and ligand competition.

Despite significant progress in analytical detection techniques (UV-Vis, FLD, ICP-OES, ICP-MS), the separation stage remains a critical limitation. In particular, there is still a lack of dedicated stationary phases enabling efficient and selective separation of elemental species.

This challenge applies not only to different forms of a single element, but also to complex mixtures containing species of multiple elements. The selection of appropriate chromatographic columns, optimization of mobile phase composition and pH, and adjustment of separation conditions remain highly demanding tasks.

Therefore, the development of novel chromatographic column packings (also as a mix of stationary phases) is essential to achieve more selective and comprehensive separations. This is especially important for advanced hyphenated techniques such as LC/IC-ICP-MS, where improved separation directly enhances the reliability of speciation analysis. The research presents previous and current studies related to the separation and detection of selected elemental species, particularly Al, As, Cr, Sb, and Se, with a primary focus on environmental and food analysis.

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Modest GERTSIUK

Dr. Modest Gertsyuk is **Senior scientist** at the Institute of Environmental Geochemistry National Academy of Sciences (NAS) of Ukraine and Ministry for Emergencies and Affairs of Population Protection from the Consequences of Chernobyl Catastrophe.

Studies: Lviv State University. Franko, Department of Chemistry (1970–1975), Post graduate Institute of Organic Chemistry, Academy of Sciences USSR (1975–1978), Kiev State University. Shevchenko, Faculty of Biology (1982–1989), The Institute of Continuing Education managers and specialist agribusiness, Faculty accounting and audit (1999–2001).

Specialisation: analytical chemistry, chromatography, environmental safety, chemical safety, organic chemistry, bioorganic chemistry, biochemistry, toxicology.

Career: Postgraduate researcher (1975–1978) and Researcher (1978–1987) at the Institute of Organic Chemistry, Academy of Sciences USSR, Researcher at Institute of Bioorganic Chemistry of the Academy of Sciences USSR (1987–1989), Senior researcher at Medved's Institute Ecohygiene and Toxicology. Ministry of Health of Ukraine (1989–1998), Head of Sector of Analytical Chemistry of Polymers and Toxic Wastes at Medved's Institute Ecohygiene and Toxicology. Ministry of Health of Ukraine (1998–2007), Senior researcher at Institute of Environmental Geochemistry, NAS and the MEF of Ukraine (2007–present).

He is also president of the Chromatographic Society of Ukraine, Member of the Steering Committee of the European Society for Separation Science, Member of the Commission of the Hazards Identify Committee on the Hygienic regulation Ministry of Health of Ukraine, Member of the Technical Committee of the State Committee of Ukraine for Technical Regulation and Consumer Policy, and Editor-in-Chief of the Journal of Chromatographic Society.

Chemical-Analytical Investigations of Aqueous Extracts from Products Made of Polymeric Materials

Modest GERTSIUK

*Institute of Environmental Geochemistry of the National Academy of Sciences of Ukraine
34a Academician Palladin Avenue, Kyiv, Ukraine.
chrtgsoc@gmail.com*

Key Words: Polymer materials, Aqueous extracts, Chemical-analytical studies, Sanitary-hygienic assessment.

Relevance and Aim of the Study. The widespread use of plastic products in households, medicine and the food industry has led to stringent requirements for their chemical safety. Polymer matrices often contain residual amounts of unpolymerised monomers, plasticisers, stabilisers and other technological additives that may migrate into contacting media. Water, as a universal solvent, simulates most natural and technological conditions under which plastics are used. The aim of the study is to comprehensively determine the qualitative and quantitative composition of compounds leached into an aqueous medium in order to assess potential toxicological risks and establish whether the products comply with sanitary and hygienic requirements.

Scope of Application and Study Objects. The examination of aqueous extracts is required for a wide range of plastic products. These include containers and packaging for foodstuffs, plastic tableware, containers for storing drinking water and food products, children's products and toys, components of water-supply systems (pipes and fittings), as well as medical devices (syringes, blood transfusion systems, medicine containers and blister packs).

Composition of Aqueous Extracts and Harmful Substances. Depending on the type of polymer and the intended use of the product, water or aqueous simulants are used as extractants, including acetic acid and ethanol solutions. Various toxic components may be identified in aqueous extracts. Products made of polyvinyl chloride (PVC) are characterised by the migration of phthalates (in particular, dibutyl phthalate and diethylhexyl phthalate), which are used as plasticisers, as well as salts of heavy metals such as lead and cadmium. Bisphenol A, a hazardous endocrine disruptor, may leach into water from polycarbonate and epoxy resins. Polystyrene products may release the toxic monomer styrene and aromatic hydrocarbons. Analysis of polyethylene (PE) and polypropylene (PP) extracts may reveal residues of catalysts, antioxidants (e.g. phenolic compounds), and products of thermal degradation of polymer chains, such as formaldehyde and acetaldehyde.

Analytical Methods. A range of modern, highly sensitive methods is used to detect and quantify low concentrations of hazardous substances in aqueous extracts. The principal methods are gas chromatography (GC) and high-performance liquid chromatography (HPLC), which are often coupled with mass spectrometry (GC-MS and HPLC-MS) for the accurate identification of unknown impurities. Heavy-metal concentrations are determined using atomic absorption spectrometry (AAS) or inductively coupled plasma mass spectrometry (ICP-MS). The total content of organic contaminants is assessed using UV spectrophotometry and integral parameters such as permanganate oxidisability and total organic carbon (TOC).

Regulatory Framework. The need for such studies is governed by stringent national and international standards. In Ukraine and the EU Member States, the relevant regulatory framework includes sanitary legislation, the requirements of the Technical Regulations concerning the safety of toys and medical devices, the ISO 10993 series of standards (biological evaluation of medical devices), as well as Commission Regulation (EU) No 10/2011 on plastic materials and articles intended to come into contact with food. The results of aqueous-extract analyses provide the basis for issuing expert opinions on the safety of products for human health.



Róbert GÓRA

Doc. RNDr. PhD. Róbert Góra is **associate professor** at the Comenius University in Bratislava, Faculty of Natural Sciences, Department of Analytical Chemistry. He graduated from the same university and faculty in Bratislava, specializing in analytical chemistry, defended his dissertation in 2004 and completed his habilitation in 2021.

He currently works at the Department of Analytical Chemistry of FNS Comenius University in Bratislava as an associate professor. His scientific activity is primarily focused on the possibilities of combining liquid chromatography methods in the analysis and characterization of natural macromolecules and polymers (humic substances, lignin), on the characterization of natural macromolecules and polymers by liquid chromatography methods, and also on the determination of selected analytes at trace and ultratrace concentration levels by liquid chromatography methods in samples with a complex matrix.

Since 2016, he has been a member of the board of the Slovak Chemical Society (SChemS) for two periods, and in 2021, SChemS nominated him as the representative of Slovak Chemical Society in the Steering Committee of the Central European Group for Separation Sciences (CEGSS).

Characterization of Natural Biomacromolecules by Combination of Linear and Stepwise Gradient Elution in Liquid Chromatography

Róbert GÓRA, Renáta GÓROVÁ

*Department of Analytical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava,
Ilkovičova 6, 84215 Bratislava, Slovak Republic.
robert.gora@uniba.sk*

Key Words: Liquid chromatography, Gradient elution, Natural biomacromolecules, RP-HPLC, SEC

Various natural substances are too complex analytes even for recent highly efficient analytical methods. This primarily includes substances such as humic and fulvic acids and lignin, but also leonardite, alginite and shilagit, which are often part of some nutraceuticals. One research approach is to characterize and analyze such complex systems is based on operational definition. Operationally defined analytes isolated from complex matrices resulted in development of novel combined multidimensional methods based on liquid chromatography separation with potential extension to combinations with electroseparation methods (ESM) and multi-detection (UV-VIS spectrophotometry, spectrofluorimetry, electroanalytical detection) and mass spectrometry (MS). With respect to their supramolecular structure, there is still a lot of controversy about their nature. Reversed-phase high-performance liquid chromatography (RP-HPLC) as prevailing chromatographic method has achieved in the field of analysis and characterization of humic substances and similar molecules only very limited application. Systematic study of orthogonality of novel combined techniques for characterization of operationally defined humic substances (HS) and/or lignin was done. Compatibility of used extreme extractive isolation and separation conditions in HPLC (ion exchange, reversed phase, size-exclusion) with common conditions of various end techniques was tested. Obtained data indicate, that this mode of application of RP-HPLC system could be employed as a separation system for more detailed characterization of such complicated natural macromolecules as analysed samples and obtain so more information about their attributes.

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Agata KOT-WASIK

Professor dr hab. inż. Agata Jolanta Kot-Wasik is professor of Analytical Chemistry at Gdańsk University of Technology, Poland, where she is affiliated with the Department of Analytical Chemistry at the Faculty of Chemistry. Her research focuses on the development and application of advanced analytical strategies for the investigation of environmental contaminants, with particular emphasis on chromatography coupled with tandem and high-resolution mass spectrometry (HRMS). She obtained her PhD at Ghent University, Belgium, and has conducted research at Universities in San Sebastián - Spain, Pau - France, and Cádiz - Spain.

Her scientific work combines analytical chemistry, environmental research, and emerging approaches in metabolomics and lipidomics. She has extensive experience in the analysis of trace organic contaminants in complex environmental matrices, including pharmaceutical residues, emerging pollutants, and their transformation products. A particular focus of her recent research is the application of HRMS-based approaches for comprehensive chemical profiling, identification of previously unrecognized contaminants, and characterization of environmental transformation processes. These approaches provide new opportunities for interpreting complex chemical signatures in wastewater and selecting chemical markers of anthropogenic activity.

Professor Kot-Wasik has authored scientific publications in journals indexed in the Journal Citation Reports, as well as book chapters and academic textbooks. She has led several national research projects, supervised doctoral researchers, and collaborated extensively with scientists from Poland and abroad. She has also held several leadership positions at Gdańsk University of Technology, including Dean of the Faculty of Chemistry.

Decoding Wastewater: High-Resolution Mass Spectrometry for Community Fingerprinting and Selection of Anthropogenic Pollution Markers

Agata KOT-WASIK

*Gdańsk University of Technology, Faculty of Chemistry, Department of Analytical Chemistry,
11/12 Narutowicza Str., 80-233 Gdańsk, Poland.
agawasik@pg.edu.pl*

Key Words: High-resolution mass spectrometry, Identification, Wastewaters, Pollution, Markers

Wastewater represents a unique chemical fingerprint of human activity, reflecting lifestyle, health status, pharmaceutical consumption, and environmental pressures within a community. In recent years, growing attention has been directed towards new and emerging contaminants (NECs), including pharmaceuticals, artificial sweeteners, personal care products, and stimulants, which are continuously released into aquatic environments. Despite their widespread occurrence, the environmental fate, ecotoxicological effects, and removal efficiency of many NECs remain insufficiently understood.

This study explores the potential of environmental metabolomics combined with high-resolution mass spectrometry for comprehensive wastewater characterization and identification of wastewater-specific contamination markers. Long-term monitoring of wastewater and environmental water samples was performed using high-performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry (HPLC-QTOF-MS), supported by targeted HPLC-MS/MS analysis. The applied workflow enabled both non-target profiling of wastewater composition and quantitative determination of selected contaminants.

The results demonstrated the frequent occurrence of pharmaceuticals, artificial sweeteners, and other anthropogenic compounds, confirming their suitability as indicators of wastewater-derived pollution. Elevated levels of selected non-steroidal anti-inflammatory drugs (NSAIDs) and artificial sweeteners were observed during the COVID-19 pandemic period compared with pre-pandemic conditions. Furthermore, SARS-CoV-2 RNA was detected in wastewater samples collected from urban catchments, highlighting the value of wastewater monitoring as a complementary epidemiological surveillance tool.

The presented approach demonstrates how high-resolution mass spectrometry can transform wastewater from a complex environmental matrix into a source of information on community health, lifestyle patterns, and anthropogenic pressures. The study further supports the use of selected emerging contaminants as robust markers for wastewater contamination tracking and environmental assessment.

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Rajmund MICHALSKI

Professor dr hab. Rajmund Michalski works in the Institute of Environmental Engineering of the Polish Academy of Sciences in Zabrze since 1988. His main research concern: ion chromatography and application of hyphenated techniques (IC-ICP-MS, IC-MS) in species analysis (inorganic disinfection by-products, metal/metalloids ions). He is the author of dozens of books, manuscripts and over 190 publications about environmental and food research.

He has undertaken several scholarships abroad (Japan, Tohoku University, 2000–2001) and research placements (Wiesbaden, Germany – 1999, 2002, 2010; Cluj-Napoca, Romania – 2016–2026; Thessaloniki, Greece – 2017; Bilbao, Spain – 2015–2019).

Since 2007, he has been the Polish Academy of Sciences' representative on the ESP EASAC (Environment Steering Panel, European Academies' Science Advisory Council). Since 2016, he has been a member of the PAN Committee on Analytical Chemistry, two Technical Committees within the Polish Committee for Standardisation, and the Polish Chemical Society, as well as Chair of the Scientific Council of the National Chamber of Commerce for the Bottling Industry.

He has received numerous awards, including the prestigious Andrzej Waksmundzki Award of the Analytical Chemistry Section of the Polish Academy of Sciences, and a medal for services to Polish Analytical Chemistry. Since 2020, he has been listed annually in the World's Top 2% Scientists database. Between 2012 and 2016, and again between 2024 and 2026, he served as Deputy Director for Scientific Affairs at the Institute of Physical Chemistry (IPIŚ) of the Polish Academy of Sciences.

New Areas of Applications for Ion Chromatography

Rajmund MICHALSKI

*Institute of Environmental Engineering of Polish Academy of Sciences, Skłodowska-Curie 34, Zabrze, Poland.
rajmund.michalski@ipispan.edu.pl*

Key Words: Ion chromatography, Applications, Environment, Food, Pharmacy.

Ion chromatography, developed over the past 50 years, has significantly revolutionized analytical chemistry, going far beyond the classical determination of simple anions and cations. During this time, the separation technique has undergone a profound evolution in both instrumentations and scope of applications. Its primary field of applications remain water and wastewater monitoring. However, over the past decade, there has been a dynamic expansion of its applications in environmental, food, pharmaceutical, clinical, and different industrial research [1]. Another important area of focus should be the increasingly widespread application of various types of IC in molecular biology and genetics research, including genomics, proteomics, metabolomics, and transcriptomics.

Every year, new models of ion chromatographs with new technological and application solutions enter the market. Innovations focus primarily on automation, miniaturization, ensuring compatibility with at least a dual detection system, and integration with cloud-based solutions [2]. The future of the technology is inextricably linked to the implementation of green chemistry principles through the miniaturization of systems to capillary and "lab-on-a-chip" formats, as well as the implementation of artificial intelligence algorithms for the autonomous optimization of methods and interpretation of results. Technological advances, increasingly stringent regulatory requirements and emerging toxicological data mean that IC will continue to play a key role in environmental, clinical and industrial research in the near future, whilst also opening new areas of applications [3].

The presentation will outline the key advantages and limitations of ion chromatography, and provide an overview of the most significant developments over the last 10 years in terms of new areas of application, technological advances, and the implementation of updated and new international standards based on ion chromatography.

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Acknowledgements

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Levent PELİT

Professor Levent PELİT graduated from Ege University, Faculty of Science, Department of Chemistry in 1998, and completed his master's and then doctoral studies at the Institute of Science, Analytical Chemistry Department of the same university in 2009.

Since 1999, he has been working on the development of electroanalytical, spectroscopic, and chromatographic methods in the Ege University Faculty of Science Department Chemistry and continued his duty as a faculty member after receiving the title of professor in 2022.

He has been involved in the field of analytical separation science, with special emphasis on modern sample preparation approaches, mainly in innovative sorption-based microextraction techniques.

His main basic scientific research areas include the development of analytical methods for the determination of biomarkers for the diagnosis of diseases and the monitoring of environmental pollutants in different matrices. There are many projects, patent applications, and publications involving translational studies on analytical chemistry and separation science.

Determination of Indoor Air Pollutants by Dispersive Liquid Liquid Microextraction

**Levent PELİT^{1,2}, Berfu YİĞRİK^{1,2}, İlayda ÖZKAN^{1,2}, Tuğba YAVUZ¹,
Fusun PELİT, Boguslaw BUSZEWSKI³**

¹*Department of Chemistry, Faculty of Science, Ege University, 35100 Bornova, İzmir, Türkiye*

²*Translational Pulmonary Research Center (Ege TPRC), Ege University, İzmir, Türkiye*

³*Prof. Jan Czocharński Kuyavian-Pomeranian Science and Technology Center,*

4 Krasinskiego str., 87100 Toruń, Poland

levent.pelit@ege.edu.tr

Key Words: Dispersive liquid-liquid microextraction; Air sample analysis; BTEX; Indoor environment

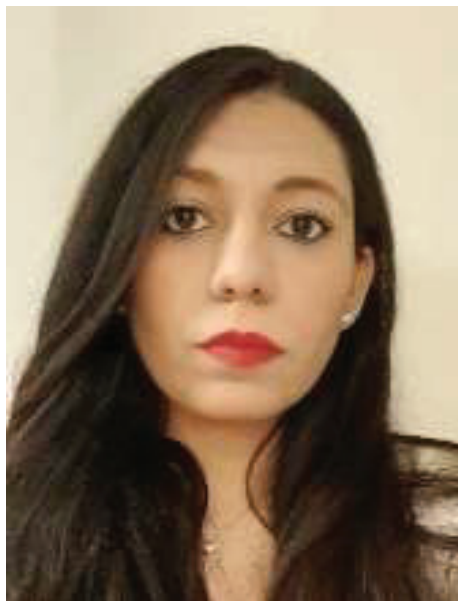
Monitoring volatile organic compounds (VOCs), particularly benzene, toluene, ethylbenzene, p-xylene, and o-xylene (BTEX), is essential due to their detrimental impacts on human health and the environment [1]. BTEX is account for approximately 60–90% of all indoor air pollutants so effective monitoring of them in indoor air is quite important [2]. This study introduces a novel, rapid, and cost-effective method utilizing dispersive liquid–liquid microextraction (DLLME) for analyzing BTEX in indoor air. The procedure involves generating micro-droplets by mechanically dispersing nitrobenzene (NB) as the extraction solvent in water, through which the air sample is passed. After extraction, the phases are separated via centrifugation, and the target analytes are quantified using gas chromatography-flame ionization detection (GC-FID). Under optimized conditions (sampling flow rate: 20 mL/min, sample volume: 200 mL, stirring time: 4 h at 1200 rpm, dispersive liquid volume: 10 mL, temperature: 20–35 °C, and pH: 9), the method demonstrated limits of detection (LOD) ranging from 0.09 to 0.30 ppmv and a linear range of 0.3–300 ppmv. The intraday and interday repeatabilities were between 3.1–8.9% and 8.1–14.4%, respectively. Successfully implemented for indoor air quality monitoring, the method yielded satisfactory recoveries between 94% and 116%. As the first application of DLLME to air sampling, this approach offers notable benefits over conventional methods, including minimal solvent consumption, rapid processing, and a high enrichment factor for trace pollutant analysis.

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Acknowledgements

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Tania SALERNO

Dr. Tania M. G. Salerno is a **Researcher** in Analytical Chemistry at the University of Messina. She obtained her Bachelor's and master's degrees in Chemistry at the University of Catania, followed by a PhD in Chemical Sciences at the University of Messina in 2018. Her academic and research background is multidisciplinary, including Materials Chemistry, Physical and Organic Chemistry. From 2019 to 2021, she worked as Technical Director and specialist in separation techniques at BeSep s.r.l., gaining expertise in liquid and gas chromatography coupled with infrared spectroscopy.

Since December 2021, she has been a Researcher in Analytical Chemistry at the Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina. She also teaches Analytical Chemistry in the Bachelor's degree course in Nutraceutical Sciences and Functional Foods (SNAF) and Advanced Mass Spectrometry to PhD students in chemical sciences.

Her research focuses on the analysis and characterization of complex matrices of forensic, cosmetic, food, and environmental interest. Her expertise includes chromatography, spectroscopy, mass spectrometry, analytical method development and validation, and the use of innovative hyphenated techniques, particularly GC-FTIR, HPLC-FTIR.

Up to date she is author of 35 paper in peer-reviewed journal, and about 30 conference contribution between oral and poster communications.

From Separation to Identification: Exploring the Potential of Chromatography Coupled to IR Spectroscopy

Tania M. G. SALERNO¹, Luigi MONDELLO^{1, 2}

¹*University of Messina, Messina Institute of Technology c/o Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, Viale G. Palatucci 13, 98168 – Messina, Italy;*

²*Chromaleont s.r.l., c/o Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Viale G. Palatucci 13, 98168 – Messina, Italy.
tsalerno@unime.it*

Key Words: Gas chromatography, Liquid chromatography, Infrared spectroscopy, Solid deposition interface.

Chromatography combined with infrared spectroscopy represent a powerful approach for the separation and identification of chemical compounds.

In particular, the hyphenated techniques gas chromatography–infrared spectroscopy (GC–IR) and liquid chromatography–infrared spectroscopy (LC–IR) bring together the separation capabilities of chromatographic methods with the information (molecular and structural) obtained from infrared spectra. It is indeed well known that IR spectroscopy can provide valuable evidence for the identification of functional groups and, in many cases, help distinguish compounds with very similar structures or closely related isomers.

While GC–FTIR has long been applied to the characterization of volatile and semi-volatile compounds. More recent developments in LC–FTIR instrumentation and interfacing strategies have extended the technique toward compounds that are non-volatile, thermally sensitive, or unsuitable for gas-phase analysis.

This keynote will explore the fundamental concepts and practical application of chromatography coupled to IR approaches, together with instrument developments, (i.e. the use of a solid deposition interface) . The presentation will highlight how the combined use of chromatographic separation coupled to infrared spectroscopy can provide complementary structural information and strengthen the identification of challenging analytes in modern analytical chemistry.

To this extent, examples from forensic science, pharmaceutical analysis, food chemistry and biotechnology will demonstrate how the effective combination of these techniques can contribute to the characterization of complex samples.



Victoria SAMANIDOU

Dr. Victoria Samanidou is **Full Professor**, Director of the Laboratory of Analytical Chemistry and Vice-President of the School of Chemistry of Aristotle University of Thessaloniki, Greece.

Her research interests focus on the development of green sample preparation methods using microextraction techniques based on sorptive extraction prior to chromatographic analysis.

She has co-authored more than 350 articles and reviews, 100 opinions/commentaries/forum articles and 65 chapters in scientific books or tutorials. She is in the editorial board member of more than 35 scientific journals and guest editor in around 50 special issues.

Since 2020 she is included in the 2% top world scientists in the field of Analytical Chemistry (career and single year) published in PLOS Biology based on citations from SCOPUS (h-index 54). She has also been included in several Power Lists of the Analytical Scientist magazine.

She has been the Leader of Working Group 1 Science and Fundamentals of EuChemS-DAC Sample Preparation Study Group and Network (2021–2025).

Till end of July 2026, she was the president of the Research Ethics Committee of Aristotle University of Thessaloniki.

From 2016 to 2024 she has been the President of the Steering Committee of the Association of Greek Chemists-Regional Division of Central & Western Macedonia.

Since January 2026 she is the representative of the Association of Greek Chemists in CEGSS.

<https://www.chem.auth.gr/en/staff/vsamanidou/>

Antibiotics Determination in Complex Matrices: from Extraction to Green(Er) Microextraction

Victoria SAMANIDOU

*Aristotle University of Thessaloniki, Laboratory of Analytical Chemistry, School of Chemistry,
54124 Thessaloniki, Greece.
samanidu@chem.auth.gr*

Key Words: Antibiotics; Green sample preparation; Microextraction.

Antibiotics are extensively used in both human and veterinary medicine. Their use has led to their occurrence as residues in food products, in environmental samples, as well as in biological matrices. Till now various traditional extraction techniques have been proposed in literature. These mainly include liquid–liquid extraction (LLE) and solid-phase extraction (SPE) in column or dispersive format.

However, these approaches are often tedious, time-consuming, and most importantly they consume high solvent volumes. Therefore, in recent years microextraction techniques have been developed.

These miniaturized and green(er) sample preparation approaches have been applied in novel analytical methods to align with the demands of Green Analytical Chemistry and Green Sample Preparation guidelines.

Among them, Fabric Phase Sorbent Extraction and Capsule Phase Microextraction have proved to be an efficient transition to microextraction approaches and have been introduced in the analysis of various complex matrices: biosamples, food samples, environmental waters etc.

Overall, the transition from conventional extraction methods to microextraction approaches reflects current trends toward green analytical chemistry, enabling rapid, cost-effective, and environmentally sustainable determination of antibiotics. Moreover, the advances in novel sorbent materials are expected to further improve sensitivity, selectivity, and applicability across diverse food and biological matrices.



Petr TŮMA

Petr Tůma, RNDr. Ing., PhD, is a **Full Professor** of Analytical Chemistry at the Department of Hygiene of the Third Faculty of Medicine of Charles University, Prague, Czech Republic.

He received his PhD in Analytical Chemistry from the Faculty of Science, Charles University, in 2003. His research expertise encompasses capillary and microfluidic chip electrophoresis, capacitively coupled contactless conductivity detection, and the development of portable electrophoretic instrumentation for clinical and biological applications.

His current research focuses on the automated online coupling of capillary electrophoresis with microdialysis sampling for *in vivo* and bioanalytical monitoring.

Professor Tůma has authored and co-authored 114 publications in peer-reviewed impact-indexed journals (74 as first or corresponding author), accumulating a cumulative impact factor of 420. He is also the author of 6 chapters in international monographs (Elsevier, Springer) and holds 2 patents. His work has received over 2,550 citations, achieving an h-index of 30 (Web of Science).

3D Printing for the Fabrication of PDMS Microfluidics and the Design of Online Interface Between Capillary Electrophoresis and Microdialysis

Petr TŮMA

*Charles University, Third Faculty of Medicine, Department of Hygiene,
Ruská 87, Prague 10, 100 00 Prague, Czech Republic.
petr.tuma@lf3.cuni.cz*

Key Words: Capillary electrophoresis, Clinical samples, Microdialysis, Microfluidics, On-line coupling

3D printing using stereolithography (SLA) is newly used for the laboratory fabrication of PDMS microfluidics. SLA is employed to produce open molds with a system of stretched fibers, which are filled with a polymerization mixture and left to cure thermally. The mold is then removed, the fibers are pulled out, and finally, the inner surface of the microfluidics channels is hydrophilized by ozonation. The proposed procedure can be used to produce two-, three-, four-, and multi-way connectors, mixers, or flow gating interfaces (FGI), which are applied in capillary electrophoresis (CE) and in the laboratory processing of microliter sample volumes [1].

The manufactured PDMS microfluidics ensure easy connection of fused silica capillaries and tubes in a wide range of outer diameters, which can be continuously varied from 2 millimeters to a minimum size of 100 μm . The connection between the microfluidics and the capillaries is watertight and tested for pressures up to 100 kPa. Furthermore, integrated PDMS microfluidics are used as FGI for the construction of an online connection between a flow-through sampling technique and a CE instrument.

The developed online connection is tested for sequential analysis of a mixture of Gly and Ala with an RSD of 0.8% for migration time and 2.5% for peak area. In the next phase, an online connection between CE and microdialysis is established, which is applied to determine the amino acid profile in human serum and breast milk from several mammals, and to monitor metabolites over time in cell cultures [2–3].

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Acknowledgements

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Jérôme VIAL

Dr. Jérôme Vial is associate professor at ESPCI Paris PSL since 1999 and **full professor since 2023**. He has coauthored more than 130 papers in the field of separation sciences and chemometrics (h-index =35, Google Scholar). He supervised and co-supervised 23 PhD students.

After around ten years of research on the elaboration of novel stationary phases for GC on chip, professor Vial is currently working in multidimensional separations and more especially in GC×GC.

His research, often conducted in close partnership with the industry, deals with the main concerns of our society. Therefore, for example, he has developed analytical workflow to elucidate the detailed composition of renewable gases and to monitor the solvent degradation in post combustion CO₂ capture processes.

For medical diagnosis purposes, professor Vial is working on analytical methodologies, from sampling to data processing, to identify volatile biomarkers of pathologies. He also developed strategies to characterize pyrolysis oils within the frame of tire valorization. Recently, he built partnerships with Brazil and Jordan to elucidate the volatile profile of endemic plants with an objective of healthcare and medical applications.

Always, professor Vial tried to use analytical chemistry to answer societal and industrial needs in a transdisciplinary approach.

GCxGC-ToF-MS to Characterize Emissions of Materials likely to be used for Human volatolome Sampling

**Jérôme VIAL¹, Elsa BOUDARD^{1,2}, Nabil MOUMANE²,
José DUGAY¹, Didier THIÉBAUT¹**

¹PSL Research University, ESPCI Paris, UMR CBI, Laboratoire Sciences Analytiques, Bioanalytiques et Miniaturisation, 10 rue Vauquelin, 75231 Paris Cedex 05, France ;

²SenseBioTek Health-Care, 21 Grande rue, 78240 Aigremont, France.

jerome.vial@espci.psl.eu

The present study provided an exhaustive examination of VOC emissions originating from 13 different raw materials susceptible to being used in the sampling of the human volatolome and encompassing both polymeric and non-polymeric compositions.

To achieve this aim, direct thermodesorption coupled with comprehensive two-dimensional gas chromatography/time-of-flight mass spectrometry (TD-GC×GC/ToFMS) was considered. For each material, we reported the total number of detected peaks, an estimation of the total volatile organic compound (TVOC) concentration, the distribution of VOC emissions across different chemical families, the minimum and maximum individual concentrations, as well as hypotheses regarding the origins of some specific VOCs depending on the material considered.

The findings from this investigation allowed a classification of the materials in three main groups and revealed that materials, such as silicone and polyurethane, could emit an extensive array of VOCs, with up to 2000 chromatographic peaks detected, and emissions of total volatile organic compounds (TVOCs) reaching levels of 5.4 µg/g and 9.8 µg/g, respectively.

In the case of polyamide, some VOCs could be related to potential reagents involved in its synthesis. While highlighting materials that should be used with caution depending on the topic and target analytes, this study identified materials that exhibited minimal VOC emissions, such as polytetrafluoroethylene, aluminum, and stainless steel, after an adequate conditioning step including cleaning with ethanol.

The selected analytical technique, TD-GC×GC/ToFMS, proved its relevance to identify and characterize semi-quantitatively VOC emissions from those materials. Such information was essential within the frame of the development of a body odor sampling system, but could also be useful for other purposes.

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Anetta ZIOŁA-FRANKOWSKA

Anetta Ziola-Frankowska is **Professor, PhD, DSc**, at the Adam Mickiewicz University (AMU), Faculty of Chemistry, in Poznań. She is a Polish scientist specializing in *analytical, environmental, and biomedical chemistry*. She is recognized as an accomplished analytical chemist whose work combines methodological innovation with practical applications in environmental protection, food safety, and biomedical research. Her scientific contributions have strengthened the development of modern analytical chemistry and expanded understanding of the occurrence and impact of trace elements in environmental and biological systems.

She graduated in 2002 at the same University and Faculty in Poznań, obtaining a Master of Science degree in *Environmental Chemistry*. In 2004, she completed postgraduate studies in *Environmental and Food Pollution Analysis* at the Gdańsk University of Technology. She earned her PhD in 2008 with the dissertation "*Determination of Aluminum in Environmental Samples in the Aspect of Fractionation and Speciation Analysis*". In 2017, she obtained habilitation with the thesis "*Application of Chemical Analytics in Biological and Environmental Research*." Throughout her career, Professor Ziola-Frankowska has contributed significantly to interdisciplinary research linking chemistry, environmental sciences, medicine, and toxicology.

She has authored and co-authored numerous scientific papers published in recognized journals in analytical chemistry, environmental monitoring, toxicology, and biomedical sciences. Her highly cited studies concern environmental contamination, trace element determination, aluminum and arsenic speciation, water quality assessment, and elemental composition of human tissues and skeletal materials. She conducts scientific research within numerous inter-university collaborations in Poland and abroad (USA, China). She coordinated and participated in several national and international projects (*Horizon 2020 Marie Skłodowska-Curie Programme*) and educational projects for young people. She also organized scientific events (European Researchers' Night, Poznań Festival of Science and Arts) and other numerous promotional activities within the AMU Faculty of Chemistry.

Preliminary HPLC-ICP-MS Speciation of Water- and Fat-Soluble Arsenic Species Using Synthesized Standard

Anetta ZIOLA-FRANKOWSKA, Dorota JAKKIELSKA, Marcin FRANKOWSKI

Adam Mickiewicz University, Faculty of Chemistry, 8 Uniwersytetu Poznańskiego Str., 61-614 Poznań, Poland.
anettazf@amu.edu.pl

Key Words: Foods, Arsenic forms, Chromatography, HPLC-ICP-MS

Chromatography continues to play a central role in separation science, particularly in the determination of toxic elements and their chemical forms in complex matrices. In the context of food safety and environmental monitoring, arsenic remains a critical contaminant due to its high toxicity and widespread occurrence. Importantly, its toxicity strongly depends on its chemical speciation, making advanced chromatographic approaches essential for accurate risk assessment.

In this study, we synthesized two arsenolipids, AsFA 362 and AsHC 360, which we then used in an attempt to develop a method for simultaneous analysis of both water-soluble species [As(III), As(V), AsB and DMA] and fat-soluble species (arsenolipids: AsFA 362 and AsHC 360). This approach aimed to enable a more accurate assessment of environmental contamination and health risks linked to the consumption of arsenic-containing foods by introducing a method that allows the determination of a higher number of toxic species in just one run. We performed the analyses qualitatively, using mostly standards, but real food samples, including algae, salmon and tuna, were also used.

To our knowledge, this is the first study that aimed to develop a method for simultaneous determination of water- and fat-soluble arsenic species by reversed-phase high-performance liquid chromatography (RP-HPLC) with inductively coupled plasma mass spectrometry (ICP-MS). The use of ion-exchange columns in combination with a C18 column allowed us to fully separate the arsenolipids and to partially separate the water-soluble arsenic species. It demonstrates the potential of the developed method for the simultaneous analysis of water-soluble arsenic species, specifically the highly toxic As(III) and As(V), alongside fat-soluble arsenic species – arsenolipids. We believe that, despite certain limitations, the methodological insights presented contribute to the advancement of chromatographic techniques and provide a valuable foundation for future developments in arsenic speciation analysis in food and environmental matrices.

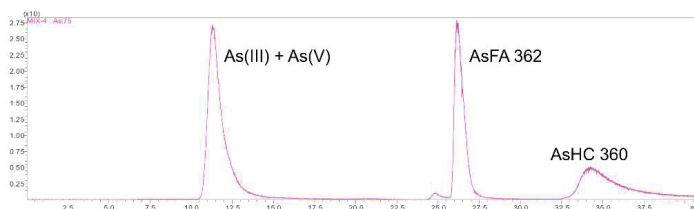


Figure 1. Chromatogram of the mix of 4 arsenic species — As(III), As(V), AsFA 362 and AsHC 360, 1 mg L⁻¹, prepared in methanol; t_{R1} = 11.279, t_{R2} = 26.139, t_{R3} = 34.250. Gradient (0.4 mL min⁻¹) with after column dilution (0.7 mL min⁻¹, 1% nitric acid): 0–4 min, 0% B; 4–6 min, 0→100% B; 6–39 min, 100% B; 39–40 min, 100→0% B; 40–41 min, 0% B. Mobile phase A: 20 mmol L⁻¹ ammonium acetate in water (pH=9.2). Columns: Thermo Scientific Dionex IonPac CG5A, Thermo Scientific Dionex IonPac AS22 and Shimadzu Shim-pack Scepter C18-120 (4.6×150 mm, 3 µm). Injection volume: 10 µL.

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 DOI: [10.3390/foods15132304](https://doi.org/10.3390/foods15132304)

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Oral Presentations

OP-01 – OP-29

OP-01 – OP-03 (20 minute)

OP-04 – OP-16 (15 minute)

OP-17 – OP-29 (10 minute)

Eco-Friendly Extraction of Phenolic Compounds from Cypriot Carob Leaves of *Ceratonia siliqua* L. and Tubers of *Asphodelus ramosus* L. Using Natural Deep Eutectic Solvents: Process Optimization and Phytochemical Characterization

Katerina A. IOANNOU¹, Amalia-Maria POLITI², Panagiotis PAPAGEORGIS^{2,3},
Constantina STAVRIDOU⁴, Efremia HADJISOLOMOU⁴, Christina PITTA⁴,
Dimitrios SARRIS⁵, Androulla N. MILIOTOU^{6,7}, Panoraia I. SIAFAKA^{2,3},
Constantina P. KAPNISSI-CHRISTODOULOU¹, Ioannis J. STAVROU^{2,3}

¹University of Cyprus, Department of Chemistry, Nicosia, Cyprus;

²EUC Research Centre, Diogenous 6, Egkomi, 2404, Nicosia, Cyprus;

³European University Cyprus, Diogenous 6, Egkomi, 2404, Nicosia, Cyprus;

⁴Agricultural Research Institute, P.O. Box 22016, 1516 Nicosia Cyprus;

⁵KES Research Centre, Grevenon 2, 1055, Nicosia, Cyprus;

⁶University of Nicosia Research Foundation, 46 Makedonitissas Avenue, 2417, Nicosia, Cyprus;

⁷University of Nicosia, 46 Makedonitissas Avenue, 2417, Nicosia, Cyprus.

ioannou.katerina@ucy.ac.cy

Key Words: NaDES, Ultrasound-assisted extraction, Polyphenols, Antioxidants, Response surface methodology.

This study explores the optimization of a sustainable extraction approach for bioactive compounds from the leaves of *Ceratonia siliqua* L. and the tubers of *Asphodelus ramosus* L., two plant species widely distributed in Cyprus. Ultrasound-assisted extraction (UAE) was combined with natural deep eutectic solvents (NaDESs) for the effective and eco-friendly isolation of polyphenols.

Response surface methodology (RSM) was applied to investigate the effects of solvent-to-solid ratio, extraction time, temperature and NaDES water content on polyphenol extractability and the antioxidant activity of the extracts. A comprehensive characterization of the phenolic composition of the optimum extracts was achieved using spectrophotometric, titrimetric and chromatographic methods. Spectrophotometric assays enabled a rapid screening and determination of total phenolic, flavonoid, triterpenoid and polysaccharide content, while the *in vitro* antioxidant activity was evaluated in terms of DPPH and ABTS free radical inhibition and ferric-reducing antioxidant power (FRAP). Total tannin content was determined using a titrimetric method.

Chromatographic analysis further enabled the identification and quantification of the main polyphenolic compounds in the NaDES extraction medium. The results demonstrate that the proposed eco-friendly extraction approach effectively recovers bioactive compounds from Cypriot *Ceratonia siliqua* L. leaves and *Asphodelus ramosus* L. tubers and highlights their potential for the development of pharmaceutical formulations with skin-healing applications.

Acknowledgments

The project EXCELLENCE/0524/0466 is implemented within the framework of the Cohesion Policy Programme 'THALIA 2021–2027', co-funded by the European Union through the Research and Innovation Foundation.

Beyond Signal-to-Noise: Practical and Statistical Challenges in LC-MS/MS Method Evaluation and Data Reporting

Paweł KUBICA, Dominika OSIECKA, Tomasz MAJCHRZAK

*Gdańsk University of Technology, Faculty of Chemistry, Department of Analytical Chemistry, Gdańsk, Poland.
pawel.kubica@pg.edu.pl*

Key Words: Mass spectrometry, Signal-to-Noise, Calibration curve, LOD, LOQ.

Liquid chromatography coupled with tandem mass spectrometry is widely regarded as a selective and sensitive analytical platform, especially when operated in multiple reaction monitoring mode. Nevertheless, several commonly applied validation and data-processing practices in LC-MS/MS methods may lead to oversimplified or even misleading conclusions. This presentation focuses on three practical issues that arise at the interface between chromatographic separation, mass spectrometric detection and statistical treatment of quantitative data.

The first issue concerns the use of signal-to-noise ratio for estimating limits of detection and quantification. Although S/N criteria are still frequently reported, their interpretation in MRM-based methods is often problematic [1]. The apparent noise level may depend on peak integration, smoothing, baseline selection, acquisition parameters, ion selection and vendor-specific algorithms. In highly selective MS/MS traces, the baseline may not represent classical chromatographic noise, and therefore S/N-based LOD and LOQ values can be difficult to reproduce and poorly related to true quantitative performance. More robust alternatives include approaches based on replicate low-level matrix-fortified samples, calibration statistics, prediction intervals, precision profiles and predefined acceptance criteria for accuracy and precision at the lower end of the working range.

The second issue is the evaluation of matrix influence. Matrix effects are often assessed by comparing calibration slopes obtained in solvent and in matrix; however, slope comparison alone does not always provide sufficient evidence of matrix-related bias. A statistically sound assessment should consider the entire calibration model, including slope, intercept, residual variability, lack of fit and uncertainty of estimated parameters [2]. Regression-based comparison, curve parallelism, confidence intervals and analysis of covariance can help distinguish between a practically relevant matrix effect and random variation in calibration data. This is particularly important when matrix influence changes across the concentration range or when internal standards only partially compensate for ion suppression or enhancement.

The third issue concerns the use of weighted calibration. LC-MS/MS calibration data are frequently heteroscedastic, with variance increasing with concentration and relative error becoming most critical near the LOQ. In such cases, unweighted regression may provide visually acceptable linearity while producing biased back-calculated concentrations at low levels. The choice of weighting factor should therefore be justified by residual analysis, accuracy profiles and performance of calibrators and quality control samples across the whole range, rather than by routine preference.

Finally, these statistical choices directly affect how results should be reported. Limits, concentrations, recoveries and validation parameters should be presented with appropriate significant figures, reflecting method precision rather than artificial numerical certainty. Overall, reliable LC-MS/MS quantification requires not only optimized instrumentation, but also transparent, statistically defensible data evaluation.

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Digital Scent Signature

Štěpán URBAN

*University of Chemistry and Technology Prague, Faculty of Chemical Engineering,
Department of analytical chemistry, Technická 5, 166 28 Prague 6 – Dejvice, Czech Republic.
Stepan.Urban@vscht.cz*

Key Words: Digital scent signature, Human body scent, GC×GC.

Detailed chemical analyses of human scent evidence using GC×GC indicates more than hundreds of thousands of varied chemical scent compounds present in any scent sample. These scent compounds can be formally divided into three groups: primary, secondary and tertiary compounds, where the primary compounds are genetically designated. The concentration ratios of these primary compounds make the unambiguous identification of persons possible. Moreover, the chemical analyses provide a great deal of additional information about the providers of these scent samples, such as ethnic origin, gender, blood group, degenerative illnesses, etc.

In this study, the immense identification potential of the human scent samples was utilized to create a special digital code, a so-called digital scent signature that involves all the essential information about the scent provider. These digital scent signatures enable the creation of a database and of course they can be compared to one another by a special computer program.

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Can Separation Sciences Address Consumers' Food Safety Concerns?

Maja BENSA¹, Mojca JEVŠNIK PODLESNIK², Irena VOVK³

¹University of Ljubljana, Faculty of Health Sciences, Research Institute of Faculty of Health Sciences, Zdravstvena pot 5, 1000 Ljubljana, Slovenia;

²University of Ljubljana, Faculty of Health Sciences, Department of Sanitary Engineering, Zdravstvena pot 5, 1000 Ljubljana, Slovenia;

³National Institute of Chemistry, Laboratory for Food Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia.
maja.bensa@zf.uni-lj.si

Key Words: Food safety, Consumer's concerns, Food analysis, Chemical hazards.

Food safety is a global public health priority due to emerging food safety risks and recurrent foodborne outbreaks. Many food safety challenges are connected with climate change and affect multiple levels of our food system, including consumers' food safety concerns. This presentation will include findings on Slovenian consumers' food safety concerns, an overview of food safety hazards in the European Union, and examples of food safety irregularities discovered with chromatographic analysis of compounds related to chemical hazards. Consumer food safety concerns in Slovenia were investigated using a mixed-methods approach combining a validated online questionnaire (n = 1621) [1] and focus group discussions (n = 40, interviews in small groups), conducted both in person and online. The study covered a variety of aspects from novel foods to persistent food hazards. Questionnaire participants were most concerned about food fraud, heavy metal contamination, and pesticide residues, whereas focus group participants were most concerned about food production practices, various chemical and biological hazards. The top-ranking food safety hazards in the EU were evaluated using the Rapid Alert System for Food and Feed (RASFF) for the period 2017-2025 [2]. Consumer concerns were compared with the patterns of food safety hazards and non-compliances reported through RASFF. Additionally, in connection to chromatographic analysis of compounds/groups of compounds related to chemical hazards in foods selected recent examples of non-compliances found in foods on the Slovenian and EU markets will be presented. These findings highlight the importance of both chemical analysis for ensuring food safety and transparent communication with consumers in order to build trust in food safety.

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Preparation of Celery Extracts by Means of Supercritical CO₂ Extraction

Andrea BOGYOR¹, Zair IBRAIMOV², Bagashar ZHAKSYBAY², Rustam TOKPAYEV²,
Graziella TURDEAN¹, Alexandra CSAVDĂRI^{1,3}

¹*Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemical Engineering,
11 Arany János Str., 400028 Cluj-Napoca, Romania;*

²*Al-Farabi Kazakh National University, Center of Physical and Chemical Methods of Research and Analysis,
96A Tole bi Street, 050012 Almaty, Kazakhstan;*

³*Al-Farabi Kazakh National University, Faculty of Chemistry and Chemical Technology,
Department of Analytical, Colloidal Chemistry and Technology of Rare Elements,
71 Al-Farabi Avenue, 050040 Almaty, Kazakhstan.
andrea.bogyor@ubbcluj.ro*

Key Words: *Apium graveolens*, Supercritical CO₂ extraction, Extract characterization.

Celery (*Apium graveolens*) is a plant of high commercial significance. Its leaves, stalks and roots may be used as dish flavouring additives, or may represent the base of various phytopharmaceutical products. Its biological proprieties are well documented [1]: prevention of coronary and vascular diseases, or antioxidant, anti-inflammatory, anticancer, antimicrobial, and antifungal effects, respectively. However, the biologically active phytochemical composition of any celery-derived product is strictly related to its method of preparation.

The purpose of this work was to investigate the effect of 3 supercritical carbon dioxide extraction parameters on the characteristics of the extracts [2]. Hence, 15 extracts were prepared by using solid dry mixtures of celery leaves and stalks, while varying the CO₂ pressure, its flow rate and percentage of the alcoholic co-solvent, respectively. A wide range of descriptors was used to assess the quality of extracts as well as the performance of extraction [3]. Among these are: extract density, dry residue content, total phenolic content, antioxidant activity, and extraction kinetics. Gas chromatography coupled with mass spectrometry was used to determine the chemical composition of obtained extracts. The obtained data were analysed by means of statistical tools in order to draw the appropriate conclusions.

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Determination of Endocrine Disruptors in Reclaimed Wastewater and Surface Waters by SPME Optimized through Chemometric Approaches and GC/MS Analysis

**Simona DI BONITO¹, Luca RIVOIRA¹, Massimo DEL BUBBA²,
Mihail Simion BELDEAN-GALEA³, Maria Concetta BRUZZONITI¹**

¹*University of Turin, Department of Chemistry, Via Pietro Giuria 7, 10125, Turin, Italy;*

²*University of Florence, Department of Chemistry "Ugo Schiff",*

Via della Lastruccia 3, 50019, Sesto Fiorentino (FI), Italy;

³*Babeş-Bolyai University, Faculty of Environmental Science and Engineering, Cluj-Napoca, Romania.*

simona.dibonito@unito.it

Key Words: SPME-GC/MS, Endocrine-disrupting compounds, Water reuse, Experimental design.

The reuse of treated wastewater for irrigation is encouraged by recent EU Regulation 741/2020, as it represents a key strategy for sustainable water resource management. The safe reuse of treated wastewater is mandatory and requires the preparation and authorization of a risk management plan in which chemical and biological risks are properly addressed according to the intended use scenario. Among the chemical compounds that may compromise water quality, bisphenol A (BPA) and 4-nonylphenol (4-NP) are of increasing concern due to their persistence and potential effects on human and environmental health.

Due to the lack of a unique protocol for the simultaneous determination of these compounds, and with the aim of improving the detection capabilities of existing methods reported in the literature, this work aimed to develop a solid-phase microextraction (SPME, polyacrylate fiber) method coupled with gas chromatography–mass spectrometry (GC–MS). To optimize the extraction efficiency, a two-step chemometric approach was employed using a Full Factorial Design (2³), followed by a Central Composite Design, investigating the effects of temperature (40–90°C), extraction time (10–40 min), and salinity (NaCl, 0–15% w/v). The optimized method was validated in terms of linearity, limits of detection (LOD), limits of quantification (LOQ), and precision. LOD and LOQ values were 7.8 ng/L and 24 ng/L for 4-NP, and 0.3 µg/L and 0.9 µg/L for BPA, respectively. Good repeatability and reproducibility were achieved, with intra-day RSD values ranging from 7.7% to 9.0% and inter-day RSD values of 8.1% and 9.6% for 4-NP and BPA, respectively.

The method was successfully applied to the screening of wastewater treatment plant effluents and surface waters intended for irrigation. As a reliable analytical tool, it supports the monitoring of BPA and 4-NP in water, thereby contributing to safer agricultural practices and the preservation of vital ecosystem services.

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Profiling the Glucosinolate Response to Selenium Biofortification in Two Diverse *Brassicaceae* Crops by an UHPLC-MS/MS Study

Enrica DONATI¹, Zeineb ATURKI¹, Giovanni D'ORAZIO¹, Lázaro-Armando PÉREZ-ACOSTA², Mercè LLUGANY³, María-Jesús SÁNCHEZ-MARTÍN², Danilo CORRADINI¹

¹*Italian National Research Council, Institute of Agricultural Biology and Biotechnology (IBBA), Area Territoriale di Ricerca Roma 1, Strada Provinciale 35d, 9 – 00010 Montelibretti (Rome), Italy;*

²*Universitat Autònoma de Barcelona, Faculty of Science, Department of Chemistry, GTS Research Group, 08193 Bellaterra, Spain;*

³*Universitat Autònoma de Barcelona, Faculty of Bioscience, Plant Physiology, BABVE, 08193 Bellaterra, Spain. enrica.donati@cnr.it*

Keywords: Selenium biofortification, Glucosinolates, *Brassicaceae*, UHPLC-MS/MS, Metabolomics.

Dietary selenium (Se) intake is largely dependent on the Se content in soil where vegetable and feed crops are cultivated. Agronomic biofortification offers an effective strategy to increase Se intake through the diet, as plants efficiently convert inorganic Se into bioavailable organic forms, such as selenoamino-acids. Beyond increasing Se content, recent research highlights that Se-biofortification modulates the biosynthesis of specialized key metabolites, particularly sulphur-rich compounds like glucosinolates (GSLs), which are characteristic secondary metabolites of the *Brassicaceae* family, known for their health-promoting properties [1].

In this regard, the present work aims to assess the influence of selenium biofortification on the biosynthesis and accumulation of glucosinolates in two diverse *Brassicaceae* crops, specifically Savoy and Tuscan cabbage. GSLs were extracted from mature leaves of treated and control plants, employing a 70% (v/v) methanol-water solution at 70 °C. The extracts were analysed by UHPLC-MS/MS using a XSelect Premier HSS T3-C18 column with a binary gradient of water and acetonitrile, both containing 0.1% (v/v) formic acid. GSLs quantification was performed in Multiple Reaction Monitoring (MRM) mode, using specific transitions for the quantification and confirmation of target analytes.

The obtained results demonstrate that selenium biofortification significantly alters the glucosinolate profile in both Tuscan and Savoy cabbage, exerting a cultivar-specific modulation on their composition. These findings provide essential insights for developing optimised agronomic protocols to enhance the beneficial properties of these Brassica crops.

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Integrated ^1H -NMR, LC–UV and Nano-LC–MS Profiling of Primary and Secondary Metabolites in Globe Artichoke Plant Parts

Giovanni D'ORAZIO, Enrico SERNI, Giuseppe SCIOLI, Anatoly P. SOBOLEV

*Italian National Research Council, Institute of Agricultural Biology and Biotechnology (IBBA),
Area Territoriale di Ricerca Roma 1, Strada provinciale 35d, 9 – 00010 Montelibretti (Rome), Italy.
giovanni.dorazio@cnr.it*

Key Words: Polyphenols, Artichoke, nano-LC, NMR, Metabolic profile.

Globe artichoke (*Cynara cardunculus* L. subsp. *scolymus*) is a well-recognized source of bioactive compounds, yet most studies focus on a single edible part and rely on one analytical technique. Here we present a three-level analytical workflow that integrates ultrasound-assisted extraction, ^1H NMR spectroscopy, nano-LC–UV–MS, and analytical-scale LC–UV for the comprehensive characterization of hydroalcoholic extracts from four anatomical parts: stems, large basal leaves, outer bracts, and the edible globe.

^1H NMR was used to quantify primary metabolites and selected phenolic acids, revealing marked differences among plant parts in total soluble content and in the relative abundance of sugars, amino acids, organic acids, and polyols. LC–UV profiling at 280, 325, and 349 nm provided a rapid comparison of phenolic families across fractions. Nano-LC–MS, interfaced via nanoflow electrospray ionization, afforded high-sensitivity detection of individual caffeoyl- and dicaffeoylquinic acids together with luteolin- and apigenin-based glycosides, including low-abundance species undetectable/recognizable by LC–UV.

The use of miniaturized chromatography, low-flow nanospray, and reduced solvent volumes in sample preparation is fully consistent with a Green Analytical Chemistry framework, without compromising separation efficiency or detection sensitivity. Taken together, this multi-platform strategy delivers a comprehensive metabolite profile across edible and non-edible artichoke fractions and offers a practical, sustainable template for the valorisation of complex plant matrices.

Carbon-Based Sensitive Matrix for Heavy Metals Electrochemical Determination

Carmen Ioana FORT, Graziella Liana TURDEAN

*Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemical Engineering,
Centre of Electrochemistry and Non-conventional Materials, 11, Arany Janos St., 400028 -Cluj-Napoca, Romania
ioana.fort@ubbcluj.ro*

Key Words: Modified electrodes, Heavy metals detection, Environmental analysis

A wide range of materials, including carbon-based frameworks [1], clays [2], and various metal oxides [3], are routinely employed in electrochemical research, particularly in electrode design. These components are often introduced as surface modifiers because they can markedly improve electrochemical performance by enlarging the active area, enhancing electrical conductivity, and strengthening catalytic activity. Although carbon-based nanocomposites have been extensively explored for developing modified electrodes, the incorporation of the Bi-carbon nanocomposite offers a set of unique benefits, providing an additional pathway for advancing the overall efficiency and responsiveness of electrochemical electrodes.

Glassy carbon electrodes (GCEs) modified with Bi-carbon nanocomposite demonstrate strong potential for the electrochemical determination of heavy metals (Pb^{2+} and Cd^{2+}). The Bi-carbon-based electrodes were fabricated through a straightforward drop-casting procedure. Their electrochemical characteristics, together with their analytical performance parameters – such as detection limit, sensitivity, and selectivity toward heavy metals - were thoroughly evaluated using cyclic voltammetry, electrochemical impedance spectroscopy, and square-wave anodic stripping voltammetry.

The electroanalytical assessment of the Bi-carbon-modified GCE demonstrated a remarkably low detection limit, high sensitivity, strong operational stability, and excellent reproducibility for heavy metal ions determination. When tested on real water samples, the electrode showed accurate and consistent measurements, confirming its robust analytical performance and underscoring its suitability for practical, real-world sensing applications.

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Sampling and GC×GC Characterization of Trace Volatile Organic Compounds in H₂ and CO₂ Matrices for Renewable Gas Integration

David GARCÍA GALLEGO¹, Claudia PAIJENS², Sandy BSAIBES²,
José DUGAY¹, Jérôme VIAL¹

¹UMR CBI, Laboratoire des Sciences Analytiques, Bioanalytiques et Miniaturisation (LSABM),
ESPCI Paris – PSL, 10 rue Vauquelin, 75231 Paris Cedex 05, France;

²NaTran R&I, 1 Rue du Commandant d'Estienne d'Orves, 92390, Villeneuve-la-Garenne, France.
david.garcia-gallego@espci.fr

Key Words: Comprehensive 2D gas chromatography, Renewable gas, Sampling, Thermodesorption, Volatile organic compounds.

Different families of volatile organic compounds (VOCs) can be present in H₂ and CO₂ streams and may differ according to the production pathway. Even at trace levels, these compounds may interfere with odorants, reduce combustion efficiency, or contribute to infrastructure corrosion [1]. However, little information exists on the nature of VOCs present in H₂ and CO₂, especially depending on gas production pathways. A deeper characterization is therefore required to better manage these gases and ensure the gas quality levels required for high-purity applications.

In the context of the energy transition, H₂ and CO₂ are central to achieving net-zero by 2050, as targeted by the European Union and France's National Low-Carbon Strategy [2]. H₂ produced by electrolysis serves as a low-carbon feedstock or energy carrier, while captured CO₂ can be used for the production of synthetic methane, fuels, or chemicals.

This study develops an analytical workflow for detecting and semi-quantifying trace VOCs in H₂ and CO₂ matrices. Sampling is performed using stainless steel adsorption tubes packed with an adsorbent phase (e.g., Tenax TA), which retain VOCs while the major gases pass through. High chromatographic resolution is achieved with thermal desorption coupled to comprehensive two-dimensional gas chromatography and time-of-flight mass spectrometry (TD-GC×GC-ToFMS). A non-polar Rxi-5ms column combined with a semi-polar DB-1701 column provides sufficient orthogonality to obtain a detailed chemical fingerprint of the trace VOCs [3].

Data processing is performed using ChromaTOF for BT software (LECO), enabling chromatographic deconvolution. In parallel, ChromaTOF SYNC was evaluated as an alternative workflow, allowing batch processing and chromatogram alignment based on retention indices within a unified dataset. Both software were applied to the same dataset in order to assess whether comparable results are obtained, as well as to evaluate data consistency and processing efficiency.

The method enables trace level distribution of different VOCs families such as alkanes, aromatics and halogenated compounds. Semi quantification through external calibration with one representative compound per family provides the distribution of VOC levels. These results will support the development of dedicated VOC databases and the identification of marker compounds for data driven assessment of VOC occurrence in H₂ and CO₂ streams.

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Monitoring of Pharmacologically Active Dyes in Wastewater Using Passive Sampling: Opportunities and Challenges

Kamila MITROWSKA, Katarzyna SIELSKA, Monika GRZESIAK

*National Veterinary Research Institute (PIWet), Department of Chemical Research of Food and Feed,
al. Partyzantów 57, 24-100 Puławy, Poland.
kamila.mitrowska@piwet.pulawy.pl*

Key Words: Malachite green, Contamination, WWTP, Aquatic environment.

Pharmacologically active dyes (PADs), such as malachite green, crystal violet, and methylene blue, are of increasing concern in aquatic environments due to their persistence and potential toxicological effects on ecosystems and human health. These compounds have historically been used as antiseptics and veterinary therapeutics in aquaculture; however, their use in food-producing animals is prohibited in the European Union due to suspected carcinogenicity. In addition, their widespread application as industrial dyes contributes to their continuous release into wastewater systems and wastewater treatment plants (WWTPs), where conventional treatment processes often fail to ensure complete removal [1–3].

Based on our previous studies, passive sampling has proven effective for monitoring PADs in surface waters, particularly when using Chemcatcher® devices with weak cation exchange (WCX) sorbents. However, its application to wastewater remains largely unexplored, representing a significant opportunity for advancing monitoring strategies in more complex matrices. Passive samplers enable the determination of time-weighted average (TWA) concentrations, providing a more representative assessment of fluctuating, low-level contamination compared to conventional grab sampling.

The implementation of passive sampling in wastewater presents both opportunities and challenges. Compared with surface waters, wastewater systems have higher contaminant loads, matrices with greater chemical complexity (high organic load, surfactants, suspended solids, colloids), and variable hydraulic conditions (high turbulence near inlets, stagnant zones in tanks). These factors can increase fouling, alter sorption behaviour, and introduce uncertainty in sampling rates (Rs). In addition, heterogeneous flow conditions in WWTPs lead to site-specific boundary-layer effects, complicating Rs estimation and reducing the reliability of laboratory-based calibrations. As a result, in situ calibration is often necessary, although it may still limit quantification to semi-quantitative levels.

Further methodological challenges include optimising deployment time, which is typically shorter in wastewater due to biofouling and high particulate loads. While temperature effects appear limited, the influence of microbial activity remains poorly understood. The impact of pH is compound-specific and closely linked to analyte ionisation and sorbent properties, which is particularly relevant for cationic PADs retained on ion-exchange phases.

Finally, while passive sampling provides robust TWA concentrations, estimating mass loads requires integrating flow data, which are often unavailable in sewer networks. Overall, this work highlights the potential of passive sampling as a monitoring tool for PADs in wastewater, while critically addressing the methodological limitations that must be considered for reliable application in complex environmental systems.

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Furan-Based Thin-Film Microextraction System for Urinary Lung Cancer Metabolomics

Füsun PELİT^{1,2}, İlknur ERBAS^{1,2}, Tuğberk Nail DİZDAS^{1,2}, Nazlı Mert ÖZÜPEK³, Esra SAKRAK⁴, Durmuş ÖZDEMİR⁵, Özlem GOKSEL^{6,2}, Yasemin BASBINAR³, Tuncay GOKSEL^{6,2}, Levent PELİT^{1,2}

¹Ege University, Faculty of Science, Department of Chemistry, 35100 Bornova, İzmir-Türkiye;

²Ege University Translational Pulmonary Research Center (EgeSAM), İzmir-Türkiye;

³Dokuz Eylül University, Institute of Oncology, Department of Translational Oncology, İzmir-Türkiye;

⁴Ege University, Drug Development & Pharmacokinetic Research & Application Center İzmir-Türkiye;

⁵İzmir Institute of Technology, Department of Chemistry, İzmir-Türkiye;

⁶Ege University, Faculty of Medicine, Department of Pulmonary Medicine, Division of Immunology and Allergy, İzmir-Türkiye.

fusun.okcu@ege.edu.tr

Key Words: Thin-film microextraction, Electrochemical polymerization, Furan coating, Urinary metabolomics, Lung cancer; LC–MS/MS.

Early diagnosis of lung cancer remains a major clinical challenge due to the lack of reliable, non-invasive biomarkers. Urinary metabolomics has emerged as a promising approach for biomarker discovery; however, efficient and reproducible sample preparation remains a critical limitation. In this study, an electrochemically prepared furan-coated thin-film microextraction (TFME) platform was developed and coupled with LC–MS/MS for targeted urinary metabolomic analysis in lung cancer [1].

Furan was electropolymerized onto stainless-steel blades to obtain a stable extraction coating. The coating morphology and chemical structure were characterized using SEM and FTIR analyses. A high-throughput 96-well TFME workflow was established, and extraction conditions were optimized by evaluating sample pH, desorption solvent, and adsorption time. Eighteen clinically relevant metabolites were simultaneously determined by LC–MS/MS [2].

The developed TFME method demonstrated excellent analytical performance, providing satisfactory recoveries (100±16%), low limits of detection and quantification, and good repeatability for all target metabolites. The optimized extraction conditions consisted of sample pH 12, aqueous formic acid-based desorption solvent, and 150 min adsorption time. These conditions enabled efficient extraction of metabolites with diverse physicochemical properties while minimizing matrix effects.

The proposed workflow was successfully applied to urine samples collected from 53 lung cancer patients and 100 healthy volunteers. Multivariate statistical analysis revealed distinct metabolic differences between the two groups. Principal component analysis demonstrated clear clustering trends, while PLS-DA achieved robust discrimination between healthy controls and lung cancer patients. Several metabolites, including nicotinamide, alanine, and amino acid-related compounds, showed significant alterations associated with lung cancer metabolism.

Overall, the electrochemically prepared furan-coated TFME platform provides a robust, reproducible, and high-throughput sample preparation strategy for urinary metabolomics. The developed analytical workflow offers considerable potential for non-invasive biomarker discovery and future clinical applications in lung cancer diagnosis.

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Exploring the Skin Volatolome by TD-GC×GC-TOFMS to Identify Signatures of Skin Cancer

Kleidisa RRUSHKA^{1,2}, Eva DÉMONGEOT², Nabil MOUMANE²,
Nathalie GAGEY-EILSTEIN², Yves ROZENHOLC³, José DUGAY¹, Jérôme VIAL¹

¹ESPCI Paris, PSL Research University, UMR CBI, Laboratoire des Sciences Analytiques, Bioanalytiques et Miniaturisation, 10 rue Vauquelin, 75231 Paris Cedex 05, France;

²SenseBioTek, 21 grande rue, 78240 Aigremont, France;

³Biostatistique, Traitement et Modélisation des données biologiques, BioSTM - UMS CNRS 3612 - U INSERM 25, Université Paris Cité, Paris, France.

kleidisa.rrushka@espci.fr

Key Words: Skin volatolome, Volatile organic compounds, TD-GC×GC-TOFMS, Biomarkers.

The skin volatolome, defined as the set of volatile organic compounds (VOCs) emitted by the skin, reflects the physiological state of the body and may contain disease-specific signatures[1]. While dogs' extremely sensitive sense of smell is capable of detecting variations of volatile profile during the occurrence of certain diseases, it only provides a binary response and doesn't allow identification of the compounds involved, thus justifying the use of advanced analytical methodologies. In this context, this study aims to explore the skin volatolome of patients with skin cancer in order to identify discriminating volatile signatures using thermodesorption followed by comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (TD-GC×GC-TOFMS).

In a first step, Skin VOCs are collected using the SkinVOCs® device, based on an adsorbent polymer support applied to the skin via a specific patch delimiting the area of interest. After passive adsorption, the compounds are thermally desorbed and then separated and identified by GC×GC-TOFMS[2]. This allows the simultaneous separation and detection of several hundred compounds per sample. The clinical protocol, in progress, includes the sampling and analysis of three main types of skin cancer and a group of healthy controls, allowing comparisons between patients and healthy subjects. It also enables evaluation of differences across cancer types, as well as between lesional and clinically healthy area within the same individual.

Given the high density of information in GC×GC chromatograms, data processing represents a critical step. In first attempt, ChromaTOF Tile[3] was used to identify statistically significant compounds based on Fisher ratio. However, due to the large size of the cohort and the extended analytical period, retention time shifts were observed, leading to limitations in Tile processing. In particular, peak misalignment caused some compounds to be partially or completely excluded from predefined tile regions, resulting in false negatives and potentially misleading lists of significant features. In addition, the output frequently contained redundant features corresponding to the same compound with varying peak areas, complicating feature selection and increasing ambiguity in downstream analysis. An alternative workflow, ChromaTOF Sync, enables batch processing and chromatogram alignment based on retention indices within a unified dataset. Nevertheless, it requires substantial manual intervention, which limits its applicability to large cohorts.

To overcome these limitations, an automated data processing workflow was developed in R Studio, specifically designed to account for retention time variability and large-scale datasets. The implemented methodology automatically identifies discriminant features between groups. Preliminary results, evaluated using supervised chemometric methods such as Random Forest, demonstrate a clear discrimination between sampled areas from diseased patients. This automated pipeline replaces time-consuming manual curation with a reproducible and scalable strategy, better suited for large clinical studies conducted over extended periods, while ensuring full control over processing parameters.

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Does a Vegetarian Smell Different Than an Omnivore?

Veronika ŠKEŘÍKOVÁ, Ulrika MALÁ, Lenka JÁNOŠÍKOVÁ, Štěpán URBAN

*University of Chemistry and Technology Prague, Faculty of Chemical Engineering,
Department of analytical chemistry, Technická 5, 166 28 Prague 6 – Dejvice, Czech Republic.
Veronika.Skerikova@vscht.cz*

Key Words: Human body scent, GC×GC, Diet.

Diet is one of the most significant factors that accompany a person daily throughout life. Its composition is reflected in the metabolism of individual tissues, in the health of the digestive tract and ultimately in the biochemical state of the organism. Less obvious consequences of long-term dietary habits include their reflection in human body odor. The odor profile of an individual is simultaneously shaped by several variables, including genetics, hormonal status, environment and diet, which is the subject of this work. Diet can change the composition of metabolites entering the sweat glands and change the spectrum of volatile organic compounds that are excreted from the skin surface.

The investigation of this relationship extends to several scientific disciplines. From a medical perspective, it opens space for non-invasive diagnostics and monitoring of metabolic status through skin odorants, and from a forensic olfactronics perspective, it represents an information source for profiling the originator of the odor signature, because long-term dietary habits are among the stable characteristics of an individual. A deeper understanding of this relationship could contribute to the refinement of identification procedures and at the same time provide insight into how everyday lifestyle is reflected in a biological manifestation hidden from ordinary perception.

This study aimed to verify whether skin scent profiles can distinguish long-term meat consumers from individuals on a meat-free diet. The experimental part involved 18 volunteers, from whom scent samples were collected from the palms and subsequently analysed using GC×GC-MS. The data were reduced to a ratio matrix of peak areas and divided into a training set and a test set. The Mann-Whitney U test, applied exclusively to the training set, identified statistically significant ratios that were used in principal component analysis, cluster analysis, and *k*-NN classification. The analysis revealed two main clusters reflecting the two volunteer groups, Omnivores and Vegetarians. The groups were separated along the first principal component, and the projection of the test samples into this defined space confirmed that the identified ratio system correctly assigns samples even outside the training set. Cluster analysis independently confirmed this division with clusters corresponding to the dietary groups, and the *k*-NN classifier achieved an accuracy of 71.25%. The findings support the hypothesis that skin scent profiles reflect long-term dietary habits.

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Molecular Docking Analysis of Gallic Acid, Pyrogallol and Resorcinol with Sleep- and CR-Regulating Protein Targets in a *Drosophila* Model of Fragile X Syndrome

Sara MILOJEVIC¹, Nikola MITOVIC², Maja STOJKOVIC¹, **Tomislav TOSTI**³,
Dragana PROTIC¹

¹University of Belgrade, Faculty of Medicine, Department of Pharmacology, Clinical Pharmacology and Toxicology, Dr. Subotica-starijeg 1, Belgrade, Serbia;

²University of Belgrade, Faculty of Medicine, Department of Pathophysiology, Belgrade, Serbia;

³University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Njegoseva 12, Belgrade, Serbia.
tomislav.tosti@ihtm.bg.ac.rs

Key Words: Gallic Acid, Molecular docking, *Drosophila melanogaster*, *Rac1*, Fragile X syndrome.

As a naturally occurring polyphenol characterized by low toxicity and the capacity to modulate neuronal signaling, gallic acid (GA) offers significant pharmacological potential for the management of sleep and circadian rhythm (CR) disturbances, which are hallmark features of fragile X syndrome (FXS).

Previous behavioral results from our laboratory demonstrated that GA modulates sleep and CR in the *Drosophila melanogaster* model of FXS, and as the potential targets - *Rac1*, *bsk*, *Jra*, *Cyfp*, and *Dscam* regulatory genes were detected via integrative bioinformatic analysis. The present study utilizes molecular docking to characterize the binding interactions of the GA and its metabolites pyrogallol and resorcinol with protein products of these sleep- and CR-related genes in the *Drosophila melanogaster* model of FXS. Three-dimensional protein structures were sourced from the Protein Data Bank, followed by preparation in UCSF ChimeraX including water removal, addition of hydrogen atoms, and energy minimization. Ligand structures for GA, resorcinol and pyrogallol, were retrieved from PubChem. Simulations were executed using AutoDock Vina within the SAMSON Connect platform, and results were evaluated based on binding affinity (kcal/mol) and interaction profiles visualized in PyMOL.

Docking results for GA identified the highest binding affinity for the Ras-related protein (encoded by *Rac1*, -5.73 kcal/mol), followed by JNK protein kinase (encoded by *bsk*, -5.58 kcal/mol) and the cell adhesion molecule *Dscam1* (-5.50 kcal/mol). Proteins *Cyfp* and *Jra* exhibited lower affinities of -4.55 kcal/mol and -3.73 kcal/mol, respectively. For the metabolite resorcinol, Ras-related protein again showed the strongest interaction (-5.25 kcal/mol), followed by *Cyfp* (-4.82 kcal/mol) and *Dscam1* (-4.47 kcal/mol). Similarly, pyrogallol demonstrated the highest affinity for Ras-related protein (-5.37 kcal/mol), with *Cyfp* at -4.76 kcal/mol and *Dscam1* at -4.46 kcal/mol. Comparative analysis revealed that, while products of the *Rac1* and *Cyfp* maintained consistent affinities across the parent compound and its metabolites, *Dscam1* showed a marked reduction in binding affinity for metabolites compared to GA.

These findings suggest that GA may influence sleep and CR through a structured interface of signaling genes and their protein products. This pilot study identifies Ras-related protein encoded by *Rac1* as the target with the highest interaction potential; however, further comprehensive molecular evaluations remain essential to validate our findings and confirm the underlying mechanisms.

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The Application of Hansen Solubility Parameters: Solvent Selection in Dispersive Liquid-Liquid Microextraction of Phthalates and its Combination with GC Analysis of Medicines

Igor ZAKHARKIV, Maryna ZUI

*Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Street, City of Kyiv, Ukraine, 01601.
maryzuy@knu.ua*

Key Words: Hansen solubility parameters, Microextraction, Gas chromatography, Phthalates, Analysis of medicines

Phthalate esters or phthalates are widely used as plasticizers in polymer production to enhance flexibility, stability, pliability and durability. Because phthalates are not chemically bound to the polymer matrix, they can easily leach from plastics into the environment and living organisms. It is well established that phthalates act as priority environmental toxicants, endocrine disruptors, and allergens, with some exhibiting carcinogenic effects. Consequently, monitoring their concentration in various products is essential. For instance, the maximum contaminant level (MCL) for DBP and DEHP in drinking water is set at 6–8 µg/L in the USA and EU countries.

Liquid extraction and microextraction represent classical sample preparation methods. This work applies the Hansen solubility theory to select the most effective organic solvents for dispersive liquid-liquid microextraction (DLLME). Based on literature data for the Hansen solubility parameters of dimethyl, diethyl, dibutyl, and dioctyl phthalates (DMP, DEP, DBP, and DOP), the solubility parameters for diisobutyl and diethylhexyl phthalates (DiBP and DEHP) were calculated using the group-contribution approach proposed by Panayiotou and Stefanis [1]. Using these solubility parameters, the "solubility distance" R_A between the organic solvent and the analyte was determined to evaluate analyte solubility in the chosen solvents

According to Hansen solubility theory, a smaller "solubility distance" R_A between the analyte and the solvent (or solvent mixture) indicates more efficient extraction into the organic phase. For example, replacing pure chloroform with a chloroform–acetonitrile mixture reduces the R_A value for DBP from 5.7 to 2.7. This enhancement leads to near-quantitative extraction of DBP and other phthalates, achieving extraction recoveries of 91–97%.

This study demonstrates that adding two organic solvents of different polarities to an aqueous analyte solution during DLLME results in an extraction phase containing both solvents: a polar one (e.g., acetonitrile) and a non-polar one (e.g., chloroform). Specifically, when chloroform serves as the extraction solvent, the polar solvent content in the resulting extraction phase ranges from 14% for isopropanol to 30% for acetone.

Liquid extraction is known to proceed via the formation of analyte–solvent solvates. IR spectroscopy revealed a shift of 10–20 cm^{-1} in the bands corresponding to the C=O and C–O stretching vibrations of the DMP ester group C-(C=O)-O in various organic solvents compared to the DMP. This shift indicates the formation of hydrogen and dipole–dipole bonds within the solvates. Polar solvents, such as acetonitrile and acetone, exerted the most significant effect on the IR band maxima, confirming their primary role in solvate formation.

Consequently, a binary chloroform–acetonitrile mixture was optimized for the quantitative extraction of DiBP, DBP, and DEHP from liquid pharmaceuticals (nasal drops packaged in plastic bottles). The phthalate concentrations determined by GC-FID were confirmed by GC-MS. The developed method demonstrates high accuracy and reproducibility, with a relative standard deviation (RSD) not exceeding 7.0%.

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Development and Validation of a Quantitative HPTLC Method for Monitoring Sequential Carbohydrate Hydrolysis

Julia BAUMLI^{1,2}, Cipriana TCACI¹, Claudia CIMPOIU^{1,2}

¹Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, Cluj-Napoca, Romania;

²Babeş-Bolyai University, Research Center for Advanced Chemical Analysis, Instrumentation & Chemometrics - ANALYTICA, Cluj-Napoca, Romania.

julia.baumli@ubbcluj.ro

Key Words: Quantitative HPTLC, Sequential hydrolysis, α -Amylase, α -Glucosidase, Starch digestion.

High-performance thin-layer chromatography (HPTLC) combines parallel sample analysis with chromatographic separation, direct visualization, and quantitative evaluation of individual analytes [1]. These characteristics are particularly useful for monitoring enzymatic carbohydrate hydrolysis, where several mono- and oligosaccharides may be formed simultaneously and cannot be individually evaluated by conventional reducing-sugar or glucose assays [2]. The aim of this study was to develop and validate a quantitative HPTLC method for product-resolved monitoring of sequential enzymatic hydrolysis, using starch digestion as a model application. To the best of our knowledge, this is the first quantitative HPTLC workflow integrating α -amylase (EC 3.2.1.1) and α -glucosidase (EC 3.2.1.20) hydrolysis within the same sequential digestion model.

The analytical workflow involved pancreatic α -amylase hydrolysis followed by α -glucosidase-mediated conversion of the resulting oligosaccharides into glucose. Chromatographic and enzymatic conditions were optimized to obtain reproducible hydrolysis profiles suitable for quantitative analysis. The developed system enabled the separation of glucose, maltose, maltotriose, and maltotetraose. Maltose was selected as a representative quantitative marker for the α -amylase stage, whereas glucose was used to evaluate the complete sequential hydrolysis process.

Chromatographic separation was performed on HPTLC silica gel 60 F₂₅₄ plates using acetonitrile–iso-propanol–water (6:1.5:2.5, v/v/v) as the optimized mobile phase. Detection was carried out after derivatization with aniline – diphenylamine – orthophosphoric acid reagent [3]. The method was validated for maltose and glucose and showed suitable selectivity, calibration performance, sensitivity, precision, accuracy, and robustness. The obtained results confirmed that both markers could be reliably quantified within the selected working range and used to monitor variations in product formation during the two enzymatic stages.

Potato, maize, rice, and tapioca starches were analyzed to demonstrate the applicability of the method to substrates with different hydrolysis behaviours. Acarbose was used as a reference inhibitor to evaluate changes in product formation during both enzymatic stages. The method enabled quantitative comparison of substrate-dependent hydrolysis and inhibition profiles, while chromatographic separation allowed residual oligosaccharides to be directly observed after the α -glucosidase step.

Application of the method revealed clear substrate-dependent differences in hydrolysis and acarbose-mediated inhibition. During the α -amylase stage, tapioca and maize starches showed the highest apparent susceptibility to inhibition, with IC₅₀ values of 24.5 ± 0.5 and 28.2 ± 0.5 μ M, respectively, whereas potato starch showed the lowest susceptibility (IC₅₀ = 48.0 ± 0.7 μ M). Following the α -glucosidase step, maize and tapioca starches again exhibited the lowest glucose-based IC₅₀ values, while rice starch required a higher acarbose concentration to reach 50% inhibition. The chromatographic profiles also revealed residual maltotetraose after the second enzymatic stage, illustrating the additional information provided by product-resolved analysis.

The developed HPTLC method provides a rapid, micro-scale, and analytically informative platform for product-resolved monitoring of sequential carbohydrate hydrolysis. Although demonstrated using starch digestion, the proposed workflow may be further adapted to other substrates and samples generating the investigated mono- and oligosaccharides.

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Pyrolysis-GC-MS for the Identification and Quantification of Microplastics in Complex Matrices via Hydrogen Peroxide Digestion

Giulia BONACCORSO¹, Ilaria COLZI², Donatella FIBBI³, Massimo DEL BUBBA¹

¹University of Florence, Department of Chemistry, Via della Lastruccia, 3, 50019, Sesto Fiorentino, Italy;

²University of Florence, Department of Biology, Via Micheli 1, 50121 Florence, Italy

³G.I.D.A. S.p.A., Via Baciacavallo 36, 59100 Prato, Italy

giulia.bonaccorso@unifi.it

Key Words: Microwave digestion, Wastewater, Blue crab, Design of experiment, Pollen.

This study evaluates the analytical performance of pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS) for the simultaneous identification and quantification of eight target microplastics (MPs) in highly challenging matrices: wastewater, blue crab, and pollen. To mitigate severe organic matter interferences, dedicated digestion protocols utilizing 30% hydrogen peroxide (H₂O₂) were developed. Under optimized conditions, this reagent efficiently oxidizes the organic without compromising the integrity of the MP [1], breaking down exclusively into non-toxic by-products (water and oxygen).

A microwave-assisted digestion (MAD) procedure was implemented for wastewater analysis, significantly accelerating sample filtration rates. This method yielded an average apparent recovery of 67 ± 19%, with significant matrix effects (|ME| > 30%) limited to a few cases. Environmental screening revealed widespread contamination from polyethylene, polyvinyl chloride, polypropylene, polyamide, polycarbonate, and polystyrene.

The H₂O₂-based MAD protocol has also been successfully adapted for blue crab pulp (body and claws), achieving recovery and matrix effect values ranging from 25% to 84% and from -29% to 64%, respectively. This has enabled the quantification of polyethylene and polyamide in the order of tens of ng/mg fresh weight.

Finally, to overcome the limited availability of pollen samples, a miniaturised ultrasound-assisted digestion method (0.75 mL of H₂O₂ per mg of sample) was developed, using 1–2 mg of matrix. Optimised using Design of Experiments (DoE) by varying temperatures and contact times, the efficiency of matrix degradation was validated by analysing the chemical oxygen demand (COD). Under optimal conditions (maximum temperature and duration), a remarkably low residual COD (10–20 mg/L) was achieved, confirming extensive removal of organic matter.

Overall, this comprehensive study demonstrates the high versatility of H₂O₂-based pre-treatments combined with Py-GC-MS as a reliable platform for monitoring microplastics in complex matrices.

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Effect of Viscosity Parameter on Mineral and Vitamin Composition of *Olea europaea* L. Leaf Extracts

Eda BÜKER^{1,2}, Dorina CASONI³

¹*Gazi University, Faculty of Pharmacy, Department of Basic Pharmaceutical Sciences, Ankara, Türkiye, Emniyet, Taç Sokağı Street, No:3, 06330 Yenimahalle/Ankara, Türkiye;*

²*Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, Enzymology and Applied Biocatalysis Research Center, 11 Arany János Str., 400028 Cluj-Napoca, Romania;*

³*Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemistry, 11 Arany János Str., 400028 Cluj-Napoca, Romania.
edabiyik@gazi.edu.tr, eda.biyik@ubbcluj.ro*

Key Words: Minerals, *Olea europaea* L., Phytomedicine, Viscosity, Vitamins.

This study demonstrated that viscosity can serve as a basis for standardized selection of extracts targeting a specific mineral and vitamin profile. To determine the effect of viscosity on the plant extracts from the mixture of leaves of *Olea europaea* L. Ayvalik and Gemlik cultivars grown on the Western Side of Türkiye, in Koprubasi, Manisa, three extracts were obtained using the cold maceration and cold evaporation methods under low-vacuum conditions at three different viscosities.

The extracts were a valuable source of minerals, as shown by ICP-OES results, and vitamins, as shown by HPLC results. High-viscosity extraction yielded higher quantity of Ca, Mg, Na, P minerals and B1, B2, B3, B6, C, and K1 vitamins, allowing their use as an additional dietary source of important elements. The low level of potentially toxic elements in leaves and their insignificant transfer in extracts confirms the environmental safety of plant material, supporting the conclusion that *O. europaea* leaves grown in the natural and climatic conditions of Koprubasi are not only effective but also safe phytotherapeutic raw materials. The ANOVA results revealed that inter-viscosity differentiation affected the accumulation of high levels of minerals and vitamins in the plant extracts using the cold maceration method. High viscosity positively affected mineral extraction efficiency because it can increase solvent diffusivity and penetration into plant cell walls. In the vitamin composition of the extracts, low viscosity was inversely correlated with the concentrations of analyzed vitamins.

To assess the phytotherapeutic uses of the studied extracts, the obtained extracts were consumed by volunteers with diabetes mellitus. When the extract was consumed 30 minutes before meals each day, the blood glucose levels of the patients were more balanced.

It should be noted that this study did not include a sensory evaluation on the extracts. Future studies should further conduct sensory evaluations of extracts with different viscosities and to test the potential link between viscosity and health benefits, thereby confirming their quality and health-related properties.

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Functionalized Biomimetic Materials for Capillary Electrophoresis: Modulating Electroosmotic Flow and Protein Interactions for Nanobody Specific Separation and Quantification

Tristan CORBALAN¹, Yoann LADNER¹, Margaux CLAVIE¹, Mehdi AHMAD²,
Gilles SUBRA¹, Philippe RONDARD³, Pierre André LAFON³, Catherine PERRIN¹

¹IBMM, University of Montpellier, CNRS, ENSCM, 34293 Montpellier, France;

²ICGM, University of Montpellier, CNRS, ENSCM, 34293 Montpellier, France;

³IGF, University of Montpellier, CNRS, Inserm, 34090 Montpellier, France.

tristan.corbalan@umontpellier.fr

Key Words: Capillary electrochromatography, Biomimetic material, Analytical method development, Surface imprinting.

The quantification of biomolecules in complex biological media remains a significant analytical challenge due to matrix effects, low analyte concentrations, and limited sample volumes. These constraints are particularly critical for nanobodies, which are present in trace amounts yet hold considerable therapeutic potential. Capillary electrophoresis, owing to its high efficiency, automation and low sample consumption, represents a powerful approach for addressing these challenges.

In this context, we developed a biomimetic strategy based on molecularly imprinted polymers incorporating silylated amino acid derivatives, designed to reproduce the selective interactions found in biological recognition processes by forming cavities complementary in shape and composition to the template analyte [1,2]. Leucine, arginine, serine and tyrosine were selected as functional monomers, as they are primarily represented at antibody paratopes and play key roles in molecular recognition.

The biomimetic material was synthesized directly inside a fused silica capillary within 60 minutes, enabling their direct integration into a CE workflow. Analyses were performed with injection volumes as low as 5 nL, highlighting the suitability of the method for scarce biological samples.

Initial studies conducted on model proteins in phosphate buffer at pH 7 demonstrated excellent selectivity and retention behavior, confirming the effectiveness of the imprinting strategy. Further optimization of key parameters, including migration velocity, capillary internal diameter and polymerization conditions, enabled the system to achieve an imprinting factor of 5. These further optimizations were carried out on a therapeutic relevant molecule, the nanobody Nb-DN1, highlighting the potential of the approach for clinically significant targets. These results can be put into perspective with those reported in literature, that show imprinting factor of 1.9 for the capture of lysozyme [3].

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A Case Study for Celery Drying Kinetics

Alexandra CSAVDĂRI^{1,2}, Andrea BOGYOR¹, Graziella TURDEAN¹

¹Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemical Engineering, 11 Arany János Street, 400028 Cluj-Napoca, Romania;

²Al-Farabi Kazakh National University, Faculty of Chemistry and Chemical Technology, Department of Analytical, Colloidal Chemistry and Technology of Rare Elements, 71 Al-Farabi Avenue, 050040 Almaty, Kazakhstan.
alexandra.csavdari@ubbcluj.ro

Key Words: *Apium graveolens*, Convective drying, Kinetic modeling.

Despite the widespread use of forced convective drying for fruits and vegetables, studies at moderate temperatures and comparative analyses of different plant parts under identical conditions remain limited. This study addresses the respective gaps by comparing the thin-layer drying behaviour of celery leaves and stalks at 40, 50, and 60°C [1].

Drying kinetic rate laws were determined from gravimetric measurements. Although leaves dried faster than stems, higher temperatures significantly reduced drying time in both cases. Among six evaluated kinetic models [2], the parabolic model was selected as the most suitable due to its strong predictive performance and simplicity.

ANOVA statistical testing results confirmed that both drying temperature and plant part significantly affected the process, while their interaction was not significant. Model parameters reflected these findings, with two coefficients showing temperature dependence. Effective moisture diffusivity increased with temperature and was approximately three orders of magnitude higher in stalks than in leaves. As a result, stalks exhibited a 34% lower activation energy and lower specific energy consumption, demonstrating that stalk drying is more energy-efficient than leaf drying.

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Untargeted Metabolite Profiling of Exhaled Breath Condensate for the Identification of Potential Lung Cancer Biomarkers

Ebru ÇALKAN YILDIRIM¹, Füsun PELİT^{1,2}, Korcan KORBA³, Nazlı MERT⁴,
Tuncay GÖKSEL^{1,5}, Yasemin BAŞPINAR⁴, Levent PELİT^{1,2}

¹Ege University, Translational Pulmonary Research Center (Ege-SAM), 35100, İzmir, Türkiye;

²Ege University, Faculty of Science, Department of Chemistry, 35040 İzmir, Türkiye;

³Ege University, Faculty of Chemical Engineering, Engineering Department, 35040, İzmir, Türkiye;

⁴Dokuz Eylül University, Institute of Oncology, Department of Translational Oncology,
35340, Balçova, İzmir, Türkiye;

⁵Ege University, Faculty of Medicine, Department of Pulmonary Medicine, 35100, Bornova, İzmir, Türkiye.

ebrucalkanyildirim09@gmail.com

Keywords: Exhaled breath condensate, Lung cancer, Untargeted metabolomics, Biomarker discovery, Liquid chromatography-quadrupole time-of-flight mass spectrometry.

A non-invasive biological matrix, exhaled breath condensate (EBC), contains metabolites derived from the respiratory tract and has emerged as a promising source of biomarkers for investigating diseases such as lung cancer [1, 2]. Some of the studies reveal that, mass spectrometry-based metabolomic profiling of EBC has demonstrated potential for identifying metabolic alterations associated with lung cancer [2, 3]. In this study, an untargeted metabolomics approach was applied to identify differences between the EBC metabolomic profiles of lung cancer patients and healthy individuals.

The study included 18 patients with lung cancer and 21 healthy individuals. EBC samples were collected under controlled conditions using a custom-designed borosilicate glass condenser operated at -20 °C. Metabolomic analysis was performed by liquid chromatography coupled with quadrupole time-of-flight mass spectrometry (LC-QTOF/MS) in electrospray ionization data-independent acquisition (ESI-DIA) mode. The acquired data were processed using Signpost MS software for peak detection, feature extraction, retention time alignment, and normalization. Principal component analysis (PCA), hierarchical clustering, Random Forest classification, and metabolic pathway analyses were performed to evaluate differences in metabolomic profiles.

PCA demonstrated partial separation between lung cancer and healthy control samples, particularly along the first principal component. Hierarchical clustering revealed that specific metabolomic features exhibited different abundance patterns between the groups. Random Forest analysis demonstrated discrimination between the groups, with an overall classification accuracy of 92.6%. Functional pathway analysis using Mummichog and Gene Set Enrichment Analysis revealed significant alterations in the tricarboxylic acid (TCA) cycle, glycolysis/gluconeogenesis, and pyruvate metabolism. These findings suggest that central energy metabolism is particularly affected in the EBC metabolomic profile associated with lung cancer.

In conclusion, high-resolution mass spectrometry-based untargeted metabolomic analysis of EBC enabled the identification of reproducible metabolic differences between lung cancer patients and healthy individuals. The findings support the potential of EBC as a non-invasive biological matrix for lung cancer metabolomics research and the identification of candidate metabolomic features.

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A Novel Rapid UPLC–PDA Method for the Simultaneous Determination of Estradiol Valerate and Dienogest in Tablets

Erdal DİNÇ¹, Adem MERT^{1,2}

¹Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06560 Yenimahalle, Ankara, Turkey;

²Gaziantep University, Naci Topçuoğlu Vocational School, 27310 Şehitkamil, Gaziantep, Turkey.
ademmert@gantep.edu.tr

Key Words: Estradiol valerate, Dienogest; UPLC–PDA, Simultaneous determination, Pharmaceutical quality control.

Estradiol valerate (EV) and dienogest (DG) are widely used in combined oral formulations for contraception and the treatment of heavy menstrual bleeding [1, 2]. Their low dosage levels require rapid, selective, and reliable analytical methods for routine pharmaceutical quality control. In this study, a novel ultra-performance liquid chromatography coupled with photodiode array detection (UPLC–PDA) method was developed and validated for the simultaneous determination of EV and DG in commercial tablet formulations.

Chromatographic separation was performed on a Waters ACQUITY UPLC BEH C18 column (2.1×100 mm, 1.7 µm) maintained at 40°C. Isocratic elution was achieved using water–acetonitrile–0.08 M ammonium carbonate buffer (8:74:18, v/v/v) at a flow rate of 0.36 mL/min. The injection volume was 1.0 µL, and the total analysis time was 3.50 min. Detection was carried out at 222.2 nm for EV and 304.8 nm for DG. Under the optimized chromatographic conditions, DG and EV were eluted at retention times of 0.73 and 2.41 min, respectively, with excellent peak resolution.

The analytical procedure was validated according to the ICH Q2(R2) guideline [3]. Recovery values ranged from 99.3 to 99.5% for EV and from 100.6 to 102.8% for DG. Intraday and interday precision studies demonstrated satisfactory repeatability, with relative standard deviation values below 2.5%. Analysis of ten independently prepared tablet sample solutions produced mean concentrations of 10.01 ± 0.12 µg/mL for EV and 10.00 ± 0.14 µg/mL for DG, corresponding to 100.1% and 100.0% of the nominal working concentrations, respectively.

The proposed UPLC–PDA method combines rapid chromatographic separation, excellent analytical performance, and low solvent consumption, making it a practical and reliable alternative for the routine quality control of combined pharmaceutical formulations containing estradiol valerate and dienogest.

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Development of a Multi-Interaction Adsorbent for μ -SPE of Polycyclic Aromatic Hydrocarbons in Urine Samples

İlknur ERBAŞ^{1,2}, Füsün PELİT^{*1,2}, Tuğberk Nail DİZDAŞ^{1,2}, Tülin Deniz ÇİFTÇİ¹

¹Ege University, Faculty of Science, Department of Chemistry, 35040 Bornova, İzmir, Türkiye;

²Ege University, Translational Pulmonary Research Center (EgeSAM), 35040, Bornova, İzmir, Türkiye.
ilknurbgtr@gmail.com

Key Words: Polycyclic aromatic hydrocarbons, Micro-solid phase extraction (μ -SPE), Multi-interaction adsorbent; Urine analysis, Gas chromatography-mass spectrometry.

Polycyclic aromatic hydrocarbons (PAHs) are widespread environmental contaminants mainly originating from incomplete combustion and anthropogenic activities. Human exposure occurs through inhalation, dietary intake, and dermal contact, raising concern due to the carcinogenic, mutagenic, and genotoxic properties of several PAHs. However, their determination in biological samples remains analytically challenging due to low concentrations, hydrophobicity, and complex matrix effects [1].

In this study, a Fe–Mn nanocomposite-coated resin was developed as a multi-interaction adsorbent for micro-solid phase extraction (μ -SPE) of PAHs from urine samples followed by gas chromatography–mass spectrometry (GC–MS) analysis [2]. The adsorbent was prepared by Fe(II) activation of the resin surface, followed by oxidative deposition using KMnO_4 and subsequent NaBH_4 treatment. SEM characterization revealed a heterogeneous and porous surface with a compact metal oxide layer, providing favorable adsorption sites for multiple interactions with PAHs, including π – π interactions, hydrogen bonding, and van der Waals forces.

The μ -SPE procedure was systematically optimized using a multivariate experimental design. Eleven experimental variables were initially screened using a Plackett–Burman design, followed by optimization of the most influential factors using a Box–Behnken response surface design. The final conditions consisted of 0.05 g adsorbent, 10 mL urine at pH 4, 20 min ultrasonic-assisted extraction, 7.5 min centrifugation, and desorption with 200 μL toluene for 20 min. The optimized μ -SPE–GC–MS method was successfully applied to the determination of 18 priority PAHs in urine samples. Adsorption equilibrium studies were predominantly described by the Freundlich isotherm model, supporting heterogeneous and multilayer adsorption on the Fe–Mn-modified surface.

The developed method was further applied to investigate differences in urinary PAH profiles and their potential relevance to biological exposure and disease-associated discrimination. Among the evaluated PAHs, anthracene exhibited the strongest discriminatory performance, with an AUC of 0.829 (95% CI: 0.756–0.901, $p < 0.001$), 73.3% sensitivity, and 83.8% specificity. Overall, the developed Fe–Mn nanocomposite-based μ -SPE–GC–MS approach provides an efficient and miniaturized strategy for PAH determination in complex urine matrices, demonstrating potential for biomonitoring, exposure assessment, and investigation of disease-associated PAH profiles.

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Untargeted LC-HRMS Profiling and Data-Processing Workflow for the Resolution and Discrimination of Complex Wheat Metabolomes

Sara MOROZZI¹, Lapo RENAI², Leonardo VERDI³,
Simone ORLANDINI³, Massimo DEL BUBBA¹

¹University of Florence, Department of Chemistry, Sesto Fiorentino, Italy;

²University of Amsterdam, Van't Hoff Institute for Molecular Science, Amsterdam, The Netherlands;

³University of Florence, Department of Agriculture, Food, Environment, and Forestry, Florence, Italy.
sara.morozzi@unifi.it

Key Words: Non-targeted analysis, LC-HRMS, Metabolites.

The comprehensive characterization of complex food matrices, such as the wheat metabolome, represents a significant analytical challenge due to the wide dynamic range and chemical diversity of the constituents. In this context, non-targeted analysis (NTA) approaches relying on Liquid Chromatography coupled with High-Resolution Mass Spectrometry (LC-HRMS) are essential to maximize peak capacity and ensure the detection of a broad spectrum of metabolites [1].

This study presents an optimized LC-HRMS untargeted platform combined with a data-processing workflow to resolve and identify molecular features capable of discriminating wheat samples based on variety and geographical origin. Twenty-two grain samples, encompassing two cultivars grown across four distinct Italian regions from 2022 to 2024, were subjected to metabolite extraction (focusing on the polyphenolic fraction) and subsequent LC-HRMS analysis.

To handle the high dimensionality and complexity of the resulting raw chromatographic data, a rigorous pre-processing pipeline was implemented, including blank subtraction, retention time alignment, replicate averaging, zero imputation, log-transformation, and median scaling. To filter the most statistically significant features from the unresolved background and co-eluting peaks, a parametric post hoc Games-Howell test was applied for multiple comparisons across two distinct lines: (i) cultivar differentiation and (ii) geographical provenance.

The filtered features were characterized based on their isotopic patterns and exact MS/MS fragments, allowing formula assignment and structural elucidation of potential biomarkers (e.g., specific polyphenols). The integration of high-efficiency liquid chromatography with advanced data-filtering strategies proved to be a powerful tool for unraveling complex matrices, demonstrating how tailored separation and processing workflows can successfully drive food traceability and authenticity compliance.

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Microplastic Determination in European Waters: The WATERPATH Project Experience

Luca RIVOIRA¹, Simona DI BONITO¹, Michela COIA¹, Massimo DEL BUBBA²,
Mihail Simion BELDEAN-GALEA³, Maria Concetta BRUZZONITI¹

¹University of Turin, Department of Chemistry, Via Pietro Giuria 7, 10125, Turin, Italy;

²University of Florence, Department of Chemistry "Ugo Schiff", Sesto Fiorentino, Italy;

³Babeş-Bolyai University, Faculty of Environmental Science and Engineering, Cluj-Napoca, Romania.

luca.rivoira@unito.it

Key Words: Microplastics, Sample preparation, Microplastic separation, Waters, WATERPATH project

The reliable determination of microplastics in water matrices requires selective sample-preparation and particle-separation steps before final identification or polymer-specific confirmation can be achieved. In surface waters, drinking-water resources and wastewater-treatment streams, microplastic particles must be isolated from complex suspended matter while minimising contamination, losses and matrix-dependent bias. From the perspective of separation sciences, the analytical challenge therefore includes the development of robust particle-isolation and classification workflows able to generate comparable data across matrices of varying complexity.

Within the WATERPATH EU-project, a monitoring campaign was started in selected European water matrices, including Italian surface waters from the Arno and Po river basins, and Romanian drinking-water and wastewater-treatment systems located along the Mureş River basin.

Samples collected between autumn and winter were processed using matrix-adapted protocols for microplastic isolation and morphological classification, distinguishing fibres from non-fibrous particles and evaluating particle-size distributions.

Microplastic abundance in the Arno River ranged from 4.8 to 14.8 MPs/L in October and from 3.7 to 7.1 MPs/L in January, showing generally lower winter values while maintaining a downstream increase towards the lower river course. In the Po River, concentrations ranged from 1.2 to 4.5 MPs/L in October and from 1.5 to 11.5 MPs/L in January, with the highest value observed at the Turin site during winter. In Romania, concentrations decreased from 5.0 MPs/L at the Mureş River intake to 0.8 MPs/L after drinking-water treatment. In comparison, the wastewater-treatment plant reduced microplastic abundance from 18.7 to 5.0 MPs/L, corresponding to estimated removal efficiencies of 83.3% and 73.2%, respectively.

Fibres were the dominant morphological class in all the matrices, accounting for approximately 90–95% of isolated microplastics in the Arno samples, 89–93% in the Po/Turin samples and 85.6% in the Romanian samples. Particle-size distributions were mainly sub-millimetric to millimetric, with occasional larger items reaching several millimeters.

These results underline the importance of harmonized separation-based sample preparation and particle classification for reliable comparison of microplastic contamination through European waters.

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LC-MS/MS analysis of various pharmaceuticals and metabolites in the Drinking Water Production and Wastewater Treatment Systems of Târgu Mureş City, Romania

**Robert TÖTÖS¹, Mihaela-Cătălina POPOVICI², Vlad-Alexandru PĂNESCU²,
Ioana BLESNEAG³, Maria-Virginia COMAN²**

¹*Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, 11 Árány Janos Str.,
RO-400028 Cluj-Napoca, Romania;*

²*"Raluca Ripan" Institute for Research in Chemistry, Babeş-Bolyai University, 30 Fântânele Str.,
RO-400294 Cluj-Napoca, Romania;*

³*Faculty of Medicine, "George Emil Palade" University of Medicine, Pharmacy, Science and Technology,
38 Gh. Marinescu Str., RO-5401438, Târgu Mureş, Romania.
robert.totos@ubbcluj.ro*

Key Words: LC-MS/MS, Wastewater analysis, Pharmaceutical residues, Emerging pollutants.

Ensuring clean drinking water and maintaining efficient wastewater treatment are among the most pressing challenges in modern environmental analytics and separation science. The daily use of pharmaceuticals, preservatives and antifungal agents in food, household chemicals in modern consumer society introduces anthropogenic micropollutants into the aquatic ecosystem.

There is a major socio-economic paradoxon which should be highlighted. Over the recent decades, Europe, and specifically the Central and Eastern European region, has experienced an escalating process of deindustrialization. A significant portion of traditional, high-emission industrial manufacturing has gradually declined or relocated from the continent. The chromatographic analysis of environmental samples from the Târgu Mureş collection system and also from other regions, reveals surprisingly that the concentration of the investigated pollutants shows no decline despite the de-creasing industrial and heavy factory emissions - results in accordance with the European trend [1–3].

Due to the extremely low concentration range (ng/L) and the presence of interfering matrix components, a liquid chromatography-tandem mass spectrometric method (ESI source MRM mode) was used in this study. Samples were pre-concentrated using solid-phase extraction (SPE). The chromatographic separation was performed using an Agilent 1200 series HPLC system on a reversed-phase (Phenomenex Synergi 4u Polar-RP) column using gradient elution (water/actonitrile), while detection was carried out with an Agilent 6410B tandem mass spectrometer.

The LC-MS/MS method provided excellent selectivity along with low limits of quantification (LOQ ~4 ng/ml), enabling precise tracking of the target compounds. Small amounts of the diuretic Hydrochlorothiazide can be found in wastewater samples before and also after treatment. From macrolide antibiotics Azithromycin and Clarithromycin are present in significant amounts, also detectable in drinking water in very small amounts (below limit of quantitation but well above limit of detection). Worrying are however the amounts of the antidepressant Venlafaxine and its metabolite O-desmethyl-venlafaxine and the antihypertensive Candesartan and its metabolite O-desethyl-candesartan. The results clearly demonstrate that continuous monitoring remains indispensable for future risk assessment and the development of more efficient purification technologies if required.

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Rapid UPLC Method for the Simultaneous Determination of Aspirin and Clopidogrel in Combined Tablet Formulation

Asiye ÜÇER^{1,2}, Erdal DİNÇ¹

¹Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry,
06560 Yenimahalle, Ankara, Türkiye;

²Ankara Yıldırım Beyazıt University, Faculty of Pharmacy, Department of Analytical Chemistry,
06010 Etlik, Keçiören, Ankara, Türkiye.
aucer@aybu.edu.tr

Key Words: Aspirin, Clopidogrel, UPLC–PDA, Simultaneous determination, Pharmaceutical analysis, Method validation.

Aspirin is an important active pharmaceutical compound widely used because of its analgesic, antipyretic, anti-inflammatory, and antithrombotic properties [1]. Clopidogrel is an antiplatelet medication used to prevent serious blood clots [2]. Aspirin and clopidogrel are commonly administered in combination for the prevention and treatment of cardiovascular diseases [3, 4]. Therefore, rapid, reliable, and economical analytical methods are required for the routine quality control of combined pharmaceutical formulations.

In this study, a rapid ultra-performance liquid chromatography coupled with photodiode array detection (UPLC–PDA) method was developed and validated for the simultaneous determination of aspirin and clopidogrel in combined tablet formulations. Chromatographic separation was achieved on an ACQUITY UPLC BEH C18 column (2.1×50 mm, 1.7 µm) using a mobile phase consisting of acetonitrile–methanol–0.08 M HCl (26:13:61, v/v/v). The flow rate was 0.32 mL/min, the column temperature was maintained at 55°C, and detection was performed at 223 nm. Complete chromatographic separation of aspirin and clopidogrel was achieved within 1.8 min.

The proposed method was validated according to ICH guidelines with respect to linearity, sensitivity, precision, accuracy, selectivity, and robustness. Excellent linearity was obtained over the concentration range of 4–20 µg/mL for both analytes. The limits of detection and quantification were 0.36 and 1.21 µg/mL for aspirin and 0.36 and 1.19 µg/mL for clopidogrel, respectively. Recovery studies performed using synthetic mixtures yielded mean recoveries of 101.9 ± 2.27% for aspirin and 101.7 ± 1.76% for clopidogrel, demonstrating satisfactory accuracy and precision. The method was successfully applied to the assay of commercial tablet formulations without interference from tablet excipients.

The short analysis time, efficient chromatographic separation, low solvent consumption, and satisfactory analytical performance demonstrate that the proposed UPLC–PDA method is a practical and cost-effective alternative for the high-throughput routine quality control of combined aspirin and clopidogrel tablet formulations.

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Integrated Chemical and Phenotypic Assessment of Wastewater-Impacted Coastal Waters in Gran Canaria: Linking Multiresidue UHPLC-QToF Screening and Antibiotic Susceptibility Profiles

Tanausú VEGA-MORALES, Zoraida SOSA-FERRERA,
José Juan SANTANA-RODRÍGUEZ

Universidad de Las Palmas de Gran Canaria (ULPGC), Instituto Universitario de Estudios Ambientales y Recursos Naturales (i-UNAT), 35017 Las Palmas de Gran Canaria, Spain
tanausu.vega@ulpgc.es

Key Words: Wastewater, Coastal waters, Emerging contaminants, UHPLC-QToF-MS, Antimicrobial resistance.

In water-scarce insular regions like Gran Canaria (Canary Islands, Spain), the intensive reuse of treated wastewater and its disposal via submarine outfalls represent critical pathways for environmental contamination [1]. These matrices act as vectors for contaminants of emerging concern (CECs), including antibiotics, which drive the proliferation and dissemination of antibiotic-resistant bacteria (ARB) and antibiotic resistance genes (ARGs) [2,3]. Consequently, this continuous discharge poses a severe threat to vulnerable coastal ecosystems and public health.

This study evaluates the occurrence of organic contaminants and phenotypic antimicrobial resistance in WWTP effluents and receiving coastal waters in Gran Canaria Island, Spain. Two complete sampling campaigns were planned in March and June 2026, covering selected WWTP effluents and adjacent coastal areas influenced by wastewater discharges. Chemical characterization was performed by solid-phase extraction followed by UHPLC-QToF-MS. Data were acquired in MSE mode over the m/z 80–1200 range and processed using a targeted workflow including more than 50 contaminants of emerging concern, such as pharmaceuticals, antibiotics, UV filters, plastic additives and other anthropogenic markers. In parallel, microbiological analyses focused on the isolation and quantification of fecal indicator bacteria, including *Enterococcus* spp. and Enterobacteriaceae, as well as environmentally relevant bacteria such as *Pseudomonas* spp, were carried out. Representative isolates were subjected to antimicrobial susceptibility testing by disk diffusion.

Results from the first sampling campaign, carried out in March 2026, showed the occurrence of multiple anthropogenic contaminants in WWTP effluents and impacted coastal waters, supporting the role of wastewater discharges as relevant sources of chemical pressure. Phenotypic resistance was also observed in several bacterial isolates. *Pseudomonas* spp. showed resistance to clinically relevant antibiotics, including cefepime, ciprofloxacin and gentamicin in selected samples, while coliform isolates showed resistance mainly to ampicillin. *Enterococcus* spp. displayed resistance to erythromycin, tetracycline and sulfamethoxazole/trimethoprim in wastewater-impacted samples. The June 2026 campaign will allow the evaluation of temporal variability in both chemical contamination patterns and phenotypic resistance profiles.

Overall, this combined chemical and microbiological data set provides a comprehensive assessment of wastewater's impact in vulnerable insular environments. Also, this integrated strategy may help identify priority monitoring indicators and support improved surveillance frameworks for coastal areas affected by wastewater discharges.

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Flash Oral Presentations

01–23

Three-Way Modeling of Kinetic Absorbance Measurements of Drug–AgNP Interactions for the Quantification of Acetylcysteine in Tablets

Erdal DİNÇ¹, Burcu Zeynep BULGUROĞLU^{1,2,3}

¹Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry,
06560 Yenimahalle, Ankara, Türkiye;

²Ankara University, Graduate School of Health Sciences, Department of Analytical Chemistry,
06110 Dışkapı, Ankara, Türkiye;

³Zonguldak Bülent Ecevit University, Faculty of Pharmacy, Department of Analytical Chemistry,
67600 Kozlu, Zonguldak, Türkiye.
b.bulguroglu@beun.edu.tr

Keywords: Acetylcysteine, Silver nanoparticles, Kinetic spectrophotometry, Three-way analysis, PARAFAC.

In this study, a three-way chemometric strategy was developed for the selective quantification of acetylcysteine (AC) in commercial tablets. Since AC lacks a suitable chromophore for direct UV-Vis spectroscopic determination, an AgNP-based complex-sensing approach was developed to generate a measurable optical response through the interaction of AC with silver nanoparticles (AgNPs) synthesized specifically for this study [1].

Following AC-AgNP interaction, UV-Vis absorption spectra were recorded over 225–1000 nm at 0, 5, 10, 15, 20, and 25 min. While the conventional spectroscopic method used the AC-AgNP response measured at a single reaction time of 5 min, the proposed multiway strategy simultaneously utilized all six kinetic spectra. The resulting wavelength $\times$ time $\times$ sample data were arranged as a third-order tensor and decomposed by parallel factor analysis (PARAFAC) [2].

PARAFAC mathematically resolved the overlapping contributions of AgNPs and the AgNP-AC complex and provided chemically interpretable spectral, kinetic, and relative concentration profiles. The spectral and kinetic profiles characterized the resolved components and their time-dependent behavior, respectively, whereas the relative concentration profile was used for quantitative determination of AC in tablets. Thus, incorporation of the kinetic dimension enabled multiway mathematical resolution of the overlapping spectral system [2, 3].

The PARAFAC calibration was linear over 16.32–65.28 $\mu\text{g/mL}$, with a correlation coefficient of 0.9993. Analysis of commercial tablet sample solutions gave $595.70 \pm 6.65 \mu\text{g/mL}$ (RSD 1.12%) by the PARAFAC approach, compared with $591.28 \pm 9.22 \mu\text{g/mL}$ (RSD 1.56%) obtained by the conventional 5-min spectroscopic method. The proposed AgNP-based complex sensing-kinetic UV-PARAFAC strategy demonstrates the analytical advantage of incorporating the kinetic dimension for mathematical resolution of overlapping spectral contributions and selective quantification of AC in pharmaceutical preparations.

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Optimization of a Green QuEChERS Approach for Extraction and Quantification of Thirty-Four Priority Organic Micropollutants in Tomatoes through Experimental Design and Multiple Response Optimization

Maria Concetta BRUZZONITI¹, Giasmin CECCONI¹, Massimo DEL BUBBA², Luca RIVOIRA¹

¹*University of Turin, Department of Chemistry, Via Pietro Giuria 7, 10125, Turin, Italy;*

²*University of Florence, Department of Chemistry "Ugo Schiff",*

Via della Lastruccia 3, 50019, Sesto Fiorentino (FI), Italy.

mariaconcetta.bruzzoniti@unito.it

Key Words: Tomatoes, Micropollutants, QuEChERS, Experimental design, AGREE.

The analysis of chemical contamination in highly consumed fruits and vegetables, such as tomatoes, poses a complex analytical challenge. The contamination of polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), and nitro-PAHs raises serious health concerns due to their airborne deposition and uptake from polluted soils and water sources. The current analytical methods used to investigate organic contamination in tomatoes are time-consuming, non-simultaneous, and often not environmentally friendly. Furthermore, the study of nitro-PAHs in tomatoes has not been extensively explored, yet.

Considering these circumstances, this research introduces a QuEChERS-based approach, combined with gas chromatography/mass spectrometry, to simultaneously detect 16 PAHs, 14 PCBs, and 4 nitro-PAHs in three different tomato cultivars of wide consumption (*Rio Grande*, *Beefsteak*, *Vine*). To determine the optimal extraction conditions, this study examines the effects of extraction solvents, namely dichloromethane, cyclohexane, and acetone, as well as four d-SPE phases for extract purification, utilizing advanced experimental design coupled with multiple response and optimization.

The optimized protocol uses cyclohexane extraction, followed by a double purification step using primary secondary amine (PSA) and octadecyl silica, and sulfuric acid oxidation. The protocol allows to achieve recoveries of 60–120% (RSD% < 15%), with good repeatability (inter-day precision <15%) and minimal matrix effects (<16%).

The greenness of the protocol over existing literature methodologies was assessed by a recently developed open-source tool (AGREE, Analytical GREENness Metric Approach and Software). Finally, the protocol developed is successfully applied to the analysis of authentic tomato samples obtained from a local Italian market.

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Polyaniline-Based Microextraction Blades for Metabolomics Studies

Melda Nur BELELI^{1,2}, Ilknur Erbas^{1,2}, Esra Şakrak³, Tuğberk Nail Dizdas^{1,2}, Füsün Pelit^{1,2}

¹Ege University, Faculty of Science, Department of Chemistry, İzmir, Türkiye;

²Ege University, Translational Pulmonary Research Center (EgeSAM), İzmir, Türkiye;

³Ege University, Drug Development and Pharmacokinetic Research and Application Center, İzmir, Türkiye.
fusun.okcu@ege.edu.tr

Key Words: Thin-film microextraction, Electrochemical polymerization, Polyaniline coating, LC–MS/MS

Metabolites are the end products of metabolic processes occurring in biological systems and exhibit dynamic changes in biological samples in response to diseases, environmental factors, and physiological conditions. Accurate and reliable metabolomic analyses are of great importance for biomarker discovery and the elucidation of disease mechanisms [1]. Conventional sample preparation methods are generally time-consuming, require large volumes of organic solvents, and present limitations in terms of environmental sustainability. Therefore, there is a growing need for novel metabolomic sample preparation strategies that are rapid, environmentally friendly, and selective [2].

In this study a thin-film microextraction (TFME) blades produced by electropolymerization was performed for use in metabolomic analyses. Homogeneous, durable, and high-surface-area polyaniline film coatings were fabricated on conductive stainless-steel substrates. Surface morphologies of TFME blades have been characterized by scanning electron microscopy (SEM), and Fourier Transform Infrared Spectroscopy (FTIR).

Both the electropolymerization parameters and extraction conditions were optimized using chemometric approaches. Initially, influential factors were screened using the Plackett–Burman design (PBD), followed by further optimization employing the Box–Behnken design (BBD). The target metabolites selected for this study are proline, hypoxanthine, phenylalanine, valine, alanine, and nicotinamide, which have previously been reported as promising metabolic biomarkers for lung cancer. The calibration curves showed good linearity, with correlation coefficients (R^2) exceeding 0.98, while the RSD values ranged from 5% to 17%. The accuracy of the proposed method was evaluated using spiked urine samples.

Overall, the electrochemically prepared furan-coated TFME platform provides a robust, reproducible, and high-throughput sample preparation strategy for urinary metabolomics. The developed analytical workflow offers considerable potential for non-invasive biomarker discovery and future clinical applications in lung cancer diagnosis.

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UV-Vis Spectrophotometric Method for Acrylamide Quantification in Food Samples via Selective Reaction with L-Cysteine

Dorina CASONI, Debora CÂMPAN

*Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemistry,
11 Arany János Str., 400028 Cluj-Napoca, Romania.
dorina.casoni@ubbcluj.ro*

Key Words: Acrylamide, UV-Vis spectrometry, L-Cysteine, Ninhydrin, Analytical method development

Acrylamide is a heat-induced food contaminant formed predominantly through the Maillard reaction in carbohydrate-rich foods processed at high temperatures. Because of its potential neurotoxic and carcinogenic effects, the development of rapid, reliable, and cost-effective analytical methods for its determination is an important objective for food safety monitoring [1-3].

In this study, a new method based on UV-Vis spectrometry was developed and validated for the determination of acrylamide in food samples. The proposed method is based on the selective reaction between acrylamide and L-cysteine, followed by spectrophotometric quantification of the excess unreacted L-cysteine through its reaction with ninhydrin by producing a pink chromophore measured at 560 nm.

The experimental parameters including reagent concentrations, reaction time and reaction temperature, were optimized to obtain maximum sensitivity and reproducibility. The method exhibited a broad linear working range of 35.54-355.40 $\mu\text{g mL}^{-1}$ for acrylamide determination. Validation studies demonstrated good analytical performance, with a limit of detection (LOD) of $11.68 \pm 0.14 \mu\text{g mL}^{-1}$ and a limit of quantification (LOQ) of $38.94 \pm 0.16 \mu\text{g mL}^{-1}$. The recovery between 100.11% and 101.21%, obtained using fortified samples at four concentration levels indicated an excellent method accuracy.

The applicability of the method was further demonstrated using fortified biscuit extracts, confirming the potential of proposed spectrophotometric method for food analysis. Compared with conventional chromatographic techniques, the proposed procedure requires simpler instrumentation, lower operating costs, and shorter analysis times while maintaining satisfactory analytical performance.

Consequently, the developed UV-Vis spectrophotometric method represents a promising alternative for routine screening of acrylamide in food analysis laboratories where advanced chromatographic instrumentation is not readily available.

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Classification of Pollen Types Based on VOC Profiles Using High-Resolution GC-Orbitrap

Ebru ÇALKAN YILDIRIM^{1,2}, Berfu YİĞRIK^{1,2}, Senol ALAN³, İshak Özel TEKİN⁴,
Özlem GÖKSEL^{1,5}, Tuncay GÖKSEL^{1,5}, Levent PELİT^{1,2}

¹Ege University, Translational Pulmonary Research Center (Ege-SAM), 35100, Bornova, İzmir, Türkiye;

²Ege University, Department of Chemistry, Faculty of Science, 35040 Bornova, İzmir, Türkiye;

³Zonguldak Bulent Ecevit University, Faculty of Science, Department of Biology, 67630 Zonguldak, Türkiye;

⁴Zonguldak Bulent Ecevit University, Faculty of Medicine, Department of Immunology,
67630 Zonguldak, Türkiye;

⁵Ege University, Faculty of Medicine, Department of Pulmonary Medicine, 35100, Bornova, İzmir, Türkiye.

ebrucalkanyildirim09@gmail.com

Keywords: Pollen type identification, Volatile fingerprint, GC-orbitrap, Solid phase microextraction, Chemometrics.

Pollen grains contain a complex mixture of volatile organic compounds (VOCs) that may provide characteristic chemical fingerprints for distinguishing different pollen types. Previous studies have demonstrated that pollen samples of different botanical origins exhibit distinct volatile profiles and that selected VOCs may serve as potential markers for pollen identification and discrimination [1–3]. The present study aimed to evaluate the potential of high-resolution GC-Orbitrap mass spectrometry combined with chemometric analysis for the characterization and classification of different pollen samples.

A total of 25 different pollen samples were investigated. For this purpose, an appropriate amount of pollen was placed into a headspace (HS) vial and incubated at 50°C for 15 min. Subsequently, a CAR/PDMS/DVB solid-phase microextraction (SPME) fiber was exposed to the headspace. After sampling at the same temperature for 15 min, the extracted volatile organic compounds (VOCs) were thermally desorbed in the inlet block of the gas chromatograph at 220°C for 5 min. The desorbed VOCs were then detected using the full-scan acquisition mode (m/z range of 40–450) of the Orbitrap mass spectrometer. Each sample was analyzed in triplicate.

The resulting chromatographic and mass spectral data were evaluated using principal component analysis (PCA), hierarchical cluster analysis (HCA), and differential analysis. A total of 365 chromatographic and mass spectral features were detected across the pollen samples. PCA revealed differences in volatile profiles among the pollen types, with PC1 and PC2 explaining 21.5% and 11.4% of the total variance, respectively. Furthermore, hierarchical cluster analysis (HCA) proved highly effective in classifying a wide variety of pollen types, showing distinct and consistent clustering based on their taxonomic similarities.

Overall, high-resolution GC-Orbitrap-based VOC profiling combined with multivariate statistical analysis revealed characteristic chemical differences among the pollen samples. The results indicate that VOC fingerprinting may provide a powerful complementary analytical approach for pollen classification and chemical characterization.

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Hydrophobic Deep Eutectic Solvent-Based Liquid–Liquid Microextraction for Trace Analysis of Bisphenol A in Environmental Waters

İlknur ERBAŞ^{1,2}, Neval BAYCAN³, Füsün PELİT^{1,2}

¹Ege University, Faculty of Science, Department of Chemistry, 35040 Bornova, İzmir, Türkiye;

²Ege University, Translational Pulmonary Research Center (Ege-SAM), 35100, Bornova, İzmir, Türkiye;

³Dokuz Eylül University, Faculty of Engineering, Department of Environmental Engineering, 35160, Buca, İzmir, Türkiye.

ilknurbgtr@gmail.com

Key Words: Hydrophobic deep eutectic solvents (HDES), Bisphenol A (BPA), LC–MS/MS, Green chemistry, Water pollution.

Bisphenol A (BPA) is an endocrine-disrupting compound that poses direct and indirect risks to human health and the environment. Its determination in surface and wastewater samples is analytically challenging because BPA is generally present at low concentrations, requiring an effective preconcentration step prior to instrumental analysis [1]. With the increasing emphasis on green chemistry, considerable attention has been directed toward the development and application of environmentally friendly solvents.

Deep eutectic solvents (DESs) have emerged as a promising class of green solvents for the extraction and separation of target compounds from various sample matrices [2]. DESs are typically formed by combining two or more components through hydrogen-bonding interactions, resulting in a eutectic system with a melting point lower than those of the individual components. Their favorable physicochemical properties and reduced dependence on conventional volatile organic solvents make them attractive alternatives for sample preparation.

In this study, a hydrophobic deep eutectic solvent-based liquid–liquid microextraction (HDES-LLME) method was developed for the extraction and preconcentration of BPA from environmental water samples. The aim was to establish a simple, rapid, cost-effective, and low-solvent-consumption approach as an alternative to conventional sample preparation techniques. A hydrophobic DES was prepared in the laboratory and employed as the extraction phase in the LLME procedure.

Considering the number of experimental variables potentially affecting extraction performance, a Plackett–Burman design was initially applied to screen the investigated parameters. Based on the magnitude of the standardized effects, HDES volume, HBA/HBD molar ratio, and centrifugation time were identified as the most influential variables and subsequently optimized using a Box–Behnken design. The optimum conditions were determined as an HDES volume of 100 μ L, an HBA/HBD molar ratio of 1:1, and a centrifugation time of 15 min.

Under the optimized conditions, the developed method exhibited good analytical performance, with a coefficient of determination (R^2) of 0.9955 and a limit of detection (LOD) of 0.39 ng mL⁻¹. Precision, expressed as relative standard deviation, ranged from 2.8% to 6.9%. The accuracy of the method was evaluated using spiked river water samples, resulting in satisfactory recoveries ranging from 94% to 97%. These results demonstrate that the proposed HDES-LLME method provides an efficient and environmentally favorable approach for the extraction and trace-level determination of BPA in environmental water samples.

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Nutritional and Bioactive Profiling of Medlar (*Mespilus germanica* L.) Fruits and Leaves for Functional Food Development

Doru Ion NISTOR¹, Miuta Rafila FILIP², Mihaela Cecilia VLASSA²,
Crina Carmen MUREȘAN¹, Romina Alina MARC¹

¹University of Agricultural Sciences and Veterinary Medicine, Faculty of Food Science and Technology,
Food Engineering Department, Cluj-Napoca 400372, Romania;

²Babeș-Bolyai University, "Raluca Ripan" Institute for Research in Chemistry, Analytical Chemistry Laboratory,
30 Fântânele Street, Cluj-Napoca, 400294, Romania.
miuta.filip@ubbcluj.ro

Key Words: Medlar fruits and leaves, Organic acids, Polyphenolic compounds, Carbohydrates, Antioxidant capacity.

Mespilus germanica L., commonly known as medlar, is an underutilized fruit species belonging to the Rosaceae family with a long history of use in traditional gastronomy and folk medicine [1].

In recent years, growing consumer interest in natural foods rich in health-promoting compounds has renewed attention toward medlar as a valuable source of nutrients and bioactive constituents. Owing to its unique phytochemical composition, medlar has considerable potential for incorporation into functional foods, nutraceutical formulations, and natural antioxidant ingredients [2, 3].

The present study investigated the nutritional and bioactive composition of *Mespilus germanica* L. fruits and leaves harvested at three developmental stages. Carbohydrates, organic acids, total polyphenolic compounds (TPC), total flavonoid content (TFC), and antioxidant activity (DPPH and ABTS assays) were evaluated using chromatographic and spectrophotometric methods.

The results revealed marked differences between fruits and leaves.

In fruits, fructose was the predominant carbohydrate (4.24–9.80 mg/100 g fresh weight), while TPC and organic acids ranged from 3.38–24.95 mg/100 g and 97.23–287.14 mg/100 g fresh weight, respectively. Leaves showed a considerably richer phytochemical profile, with glucose levels of 6.38–13.02 mg/100 g, organic acids of 829.48–1687.38 mg/100 g, TPC of 129.03–174.89 mg/100 g, and TFC of 1248.96–1618.93 mg/100 g fresh weight. The high phenolic content was associated with strong antioxidant activity, with DPPH values of 9406.87–9790.98 $\mu\text{mol TE}/100\text{ g}$ and ABTS values of 7349–9572 $\mu\text{mol TE}/100\text{ g}$ fresh weight.

The high levels of phenolic compounds, flavonoids, and organic acids, together with the strong antioxidant activity observed, highlight the potential of medlar-derived materials as functional ingredients. Medlar fruits may be utilized in the development of functional beverages, fruit-based products, and nutraceutical formulations, while the leaves could serve as a sustainable source of natural antioxidants and phytochemicals for food fortification. These findings support the valorization of *Mespilus germanica* L. as a promising resource for the development of innovative functional foods with added health benefits.

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Excompan Software System for Large Substances Datasets Automated Expert Evaluation

Mykola GERTSIUK¹, Modest GERTSIUK²

¹State University of Information and Communication Technologies, Kyiv, Ukraine;

²Institute of Environmental Geochemistry of National Academy of Sciences of Ukraine, Kyiv, Ukraine.

m.gertsyuk@duikt.edu.ua

Key words: ExComPan, Toxicity assessment, Data automation, PubChem, PubMed.

The developed ExComPan software addresses the labor-intensive challenge of interpreting chemical substances large datasets within mixtures context by automating toxicological risk assessments. By integrating data from PubChem and PubMed, the system enables users to perform high-precision substance selection based on structural descriptors and evaluate their aggregate impact relative to established appropriate standards.

In contemporary analytical chemistry, there is an escalating demand for the expert interpretation of substances lists, particularly in the context of complex mixture characterization. This process often requires handling large data sets, which presents significant challenges. Most commonly, data processing is performed in Excel, resulting in increased workload and longer research times, research time and possible inaccuracies possibility, related to lack of information. These factors highlight the necessity for more efficient approaches to evaluate mentioned data.

Such issues can be addressed through automated solutions, such as ChemSteer, ECOSAR, EPI Suite, GaBi Sphera Solutions, SimaPro, USETox, ToxTool, etc. [1]. However, despite the advantages of automation, the software mentioned also has certain drawbacks:

- All mentioned software demonstrates insufficient efficiency when used for toxic emissions evaluation in their impact on environment.

- A limitation, which appears in frames of exploitation lifecycle [1].

To eliminate the disadvantages mentioned, an ExComPan (Expert Compounds Panel) e-system that allows conducting research evaluation has been developed.

The core functionality of the developed software is based on a conceptual framework for the automated toxicity assessment of individual chemical substances and mixtures. Currently, the system utilizes the Independent Action (IA) model, which operates under the assumption that mixture components exert their effects through distinct, non-interactive biological pathways. The assessment protocol identifies hazardous constituents by comparing concentration levels against established regulatory standards or by cross-referencing known toxicological profiles within the integrated database.

While this approach provides a robust baseline, its predictive power is limited by the inherent constraints of the IA model. The integration of advanced sorting and filtering(selection) capabilities allows for the systematic grouping of substances based on structural or functional similarities.

From user's perspective user interface appears as table that contains substances list with such chemical characteristics (*substance name, formula and BruttoFormula, substance saturation, compound class*), input data (*substance concentration – in case if concentration data is presented*), toxicity characteristics (*such value data as LD50*), and hygienic (danger) characteristics (*such values as MAC, or TLV*).

The software is implemented as a web-based platform, integrating a curated internal database with global repositories such as PubChem and PubMed. Currently, the internal database serves as the primary source for substance-specific parameters used in toxicity estimations. Due to the inherent heterogeneity and ambiguity of raw data in PubChem, we have adopted a manual synchronization protocol with internal database to ensure the high fidelity of chemical descriptors and toxicological benchmarks within our system. Integration with PubMed facilitates targeted bibliometric analysis, enabling researchers to retrieve peer-reviewed literature selected by specific chemical compounds or functional groups. Described mentions may be shown as a conceptual diagram on Figure 1.

Future developments aim to transition from a localized data storage model to a fully synchronized, real-time API integration with PubChem and PubMed, retrieving necessary chemical data. A software user interface is shown at Figure 2.

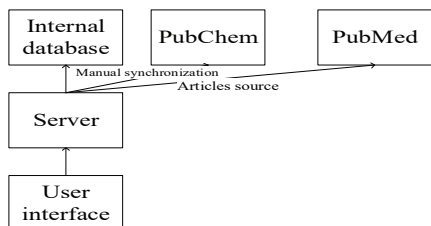


Figure 1. ExComPan conceptual diagram.

Name	Formula	Brutto Formula	Saturation	Compound Class	Toxicity level	Danger level
Pentadecane		C ₁₅ H ₃₂	Alkane	Alkane	⚠️ Toxic	⚠️ Toxic
Ethanol		C ₂ H ₆ O	Alkane	Ketone	⚠️ Toxic	⚠️ Toxic
Cyclohexane		C ₆ H ₁₂	Alkane	Cycle	⚠️ Toxic	⚠️ Toxic
Benzyl acetate		C ₁₅ H ₁₈ O ₂	Alkane	Heterocycle	⚠️ Toxic	⚠️ Toxic
Octanone		C ₈ H ₁₆	Alkane	Alkane	⚠️ Toxic	⚠️ Toxic
Butene		C ₄ H ₈	Alkane	Ether	⚠️ Toxic	⚠️ Toxic

Figure 2. ExComPan resulting table interface.

Mentioned user interface is structured into three functional modules designed for high-level data interpretation:

- Toxicological Profiling Dashboard:** A comprehensive data grid containing physicochemical properties, toxicity/hygienic indices for each mixture component. This module features automated hazard and toxicity level indicators, with integrated multi-parameter sorting capabilities to facilitate comparative analysis.
- Structural and Chemical Selection Engine:** To refine the search space, the system provides advanced selection based on:
 - Elemental:** Isolation of substances based on specific atoms within the molecular formula (Brutto formula).
 - Categorisation** by specific compound classes (e.g., phenols, aliphatic hydrocarbons, etc.).
 - Saturation:** Selection based on the double/triple bonds or aromaticity, allowing for reactivity-based clustering.
- Mixture Toxicity Assessment Panel:** A dedicated synthesis module that displays the aggregate toxicity markers for the multi-component system, providing a holistic view of the mixture's hazardous potential.

The ExComPan software framework offers a robust solution for the high-throughput processing of complex chemical datasets, effectively overcoming the throughput bottlenecks inherent in manual data interpretation. By operationalizing toxicological assessment models and establishing a curated integration with PubChem and PubMed, the system facilitates high-fidelity hazard characterization for both discrete analyses and multicomponent matrices.

This platform significantly reduces analytical lead times and extends the functional lifecycle of traditional computational tools. By providing specialized modules for selection based on structural descriptors and chemical ontology, ExComPan empowers researchers to isolate critical parameters and elucidate the toxicological profiles of complex chemical systems with enhanced precision and efficiency.

Upcoming iterations will prioritize the implementation of Concentration Addition (CA) predictive models. Unlike the current IA approach, the CA model accounts for dose-additive effects among components with similar Modes of Action (MoA), providing a more ecologically and physiologically relevant assessment of chemical mixtures.

Parallel to this, we aim to evolve our data acquisition strategy from manual synchronization to a full-scale API integration with PubChem. This will enable real-time retrieval of dynamic data. By automating the ingestion of these parameters, the system will offer a high-throughput, adaptive environment for the predictive toxicology of emerging contaminants.

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HPTLC, HPTLC-DPPH and HPTLC-MS/MS Analyses of *Fallopia* species Extracts

Vesna GLAVNIK¹, Irena VOVK¹, Živa VIPOTNIK¹, Simona STRGULC KRAJŠEK²

¹National Institute of Chemistry, Laboratory for Food Chemistry, 19 Hajdrihova, SI-1000 Ljubljana, Slovenia;

²University of Ljubljana, Biotechnical Faculty, Depart. of Biology, 101 Jamnikarjeva, SI-1000 Ljubljana, Slovenia.
vesna.glavnik@ki.si

Key Words: Invasive alien plant species, Phenolic compounds, HPTLC, HPTLC-MS/MS.

Japanese knotweed (*Fallopia japonica* Houtt.), giant knotweed (*Fallopia sachalinensis* Ronse Decr.) and their interspecific hybrid Bohemian knotweed (*Fallopia bohemica* J. Chrtek & A. Chrteková) J.P. Bailey as well as Russian-vine (*Fallopia baldschuanica* (Regel) Holub) and Chinese knotweed (*Fallopia multiflora* (Thunb.) Haraldson), invasive alien plant species, represent huge environmental and economic problems.

Despite their large biomass these plant species are unexplored source of bioactive compounds. The aim of this study was to examine differences between the extracts of Japanese knotweed, giant knotweed, Bohemian knotweed, Russian-vine and Chinese knotweed prepared from different plant parts of the same plant species, different year of collection at the same location and at different locations. Chemical profiles of investigated extracts were obtained from HPTLC silica gel plates after post-chromatographic derivatization with 4-dimethylaminocinnamaldehyde (DMACA) [1] detection reagent.

Profiles of DPPH radical scavenging activities of the extracts were obtained by effect-directed analysis, performed on the developed HPTLC silica gel plates by post-chromatographic application of 2,2-diphenyl-1-picrylhydrazyl (DPPH•) reagent. HPTLC-MS/MS analyses of inflorescence extracts were performed on HPTLC silica gel plates that were pre-developed twice [2] (to eliminate impurities causing ion suppression of the compounds of interest) before the application of extracts and development with toluene-acetone-formic acid (3:6:1, v/v) [2] as for HPTLC-DMACA and HPTLC-DPPH analyses. HPTLC-DPPH•-image analysis and HPTLC-DPPH•-densitometry in fluorescence mode (FLD), HPTLC-DMACA-image analysis and HPTLC-DMACA-densitometry in absorption mode (Vis), confirmed differences among crude extracts of plant materials from the different plant parts of the same plant species, different plant species as well as different years on the same location and different locations. HPTLC-MS/MS results also showed differences between inflorescence extracts of different species and complemented the results of our previous HPTLC-MS/MS analyses of Japanese knotweed [2-5], giant knotweed [4] and Bohemian knotweed [4] rhizomes [2-5] and leaves [4,6].

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Trace Analysis of Bisphenols and Parabens in Human Plasma by RP-HPLC-MS/MS

Miroslav KUBÁT, Lucie NOVOTNÁ, Petr ČESLA

*University of Pardubice, Faculty of Chemical Technology, Department of Analytical Chemistry,
Pardubice, Czech Republic.
miroslav.kubat@upce.cz*

Key Words: Trace analysis, Bisphenols, Parabens, RP-HPLC-MS/MS, Human plasma, Biomonitoring

Endocrine-disrupting chemicals (EDCs) are exogenous substances that interfere with hormonal signalling and thereby affect physiological regulation, development, and reproduction. Bisphenols (e.g. BPA and structural analogues) and parabens (alkyl esters of p-hydroxybenzoic acid) are widely used synthetic EDCs of concern because they are ubiquitous in consumer products and the environment, leading to human exposure via diet, dermal contact, and inhalation. Human plasma is a relevant matrix for biomonitoring because it reflects internal exposure and can be linked to potential systemic effects.

Trace-level quantification of bisphenols and parabens in plasma is analytically challenging due to matrix complexity, low analyte concentrations, matrix effects, and the risk of pre-analytical contamination, which is particularly critical for ubiquitous compounds such as BPA. Robust workflows therefore require selective sample preparation, stringent blank control, and sensitive, selective detection.

Here, we present a targeted RP-HPLC–MS/MS method for selected bisphenols and parabens in human plasma. Chromatographic separation is performed under reversed-phase gradient conditions using aqueous ammonium acetate and acetonitrile, with a 20-minute total cycle time including column re-equilibration. Detection is carried out in multiple reaction monitoring (MRM) mode.

Sample preparation is intentionally simple and high-throughput, comprising protein precipitation with acetonitrile, centrifugation, and spin-filtration, without an additional pre-concentration step. Recovery and matrix effects were evaluated for the final procedure and benchmarked against alternative liquid–liquid extraction (LLE) and solid-phase extraction (SPE) approaches. A procedural blank was processed with every batch, and background signals were subtracted when present to avoid misinterpretation due to laboratory contamination. Validation showed linearity from 0.1 to 500 µg/L and limits of detection of 0.1–2.5 µg/L. Analyte stability was assessed, and intra- and inter-day accuracy and precision met acceptance criteria across three concentration levels (≤15%).

Acknowledgements

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A Flexible Multi-Criteria Approach to Targeted LC-MS/MS Method Optimization

Michal KAŠPAR, Pavlína MUSILOVÁ, Petr ČESLA

University of Pardubice, Faculty of Chemical Technology, Department of Analytical Chemistry,
Studentská 95, 532 10 Pardubice, Czech Republic.
michal.kaspar@upce.cz

Key Words: Gradient score, LC-MS/MS, Multi-criteria optimization, Method development, Phenolic compounds.

Targeted LC-MS/MS methods developed for large analyte panels require a balance between chromatographic performance and tandem mass spectrometric acquisition constraints. Because separation quality, analysis time, peak shape, and acquisition feasibility are commonly evaluated using independent criteria, the selection of optimal conditions can remain subjective. This work presents a flexible multi-criteria framework based on the Gradient Score (GS), which combines selected chromatographic and MS/MS descriptors into a single normalized response.

The approach was evaluated using 65 phenolic compounds analyzed by reversed-phase liquid chromatography coupled with triple-quadrupole tandem mass spectrometry in scheduled multiple reaction monitoring mode. Ten stationary phases and a set of linear and segmented gradient programs were compared. Depending on the optimization task, GS was assembled from configurable subcriteria describing gradient time, overlap of scheduled detection windows, separation of predefined critical analyte pairs, peak broadening, and the distribution of analyte retention times across the usable chromatographic window. Each subcriterion was transformed by min-max normalization and combined using user-defined weights, enabling objective ranking of experimental conditions under different analytical priorities.

For stationary-phase screening, the framework identified phases providing a favorable compromise between critical-pair resolution, peak width, and analyte distribution under two independent linear gradients. The selected phase was subsequently used for retention modeling based on three linear gradients and for the design of segmented gradient profiles. Retention predictions were verified using independent validation gradients, and the resulting profiles were ranked by GS while considering both chromatographic quality and scheduled MRM acquisition demands. The final method achieved broad analyte coverage within a short analysis time without excessive overlap of detection windows.

Compared with the original fixed GS formulation introduced for phenolic profiling during coffee roasting [1], the present framework allows both the included descriptors and their relative weights to be adapted to the analytical objective. The proposed approach therefore provides a transparent, transferable, and automation-ready strategy for rational optimization of targeted LC-MS/MS methods.

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Determination of Aromatic Hydrocarbons in Air by Ti₃AlC₂ Based SPME Fiber

**Duygu Oğuz KILIÇ^{1,2,3}, İlayda ÖZKAN^{2,3}, Berfu YİĞRİK^{2,3}, Gül KAYA⁴,
Kasim OCAKOĞLU⁴, Levent PELİT^{2,3}**

¹Izmir Institute of Technology (IZTECH), Center for Materials Research, Bornova, İzmir, Türkiye;

²Ege University, Faculty of Science, Department of Chemistry, 35040 İzmir, Türkiye;

³Ege University, Translational Pulmonary Research Center (Ege-SAM), 35040, İzmir, Türkiye;

⁴Tarsus University, Faculty of Engineering, Department of Engineering Fundamental Sciences, Tarsus, Türkiye.
duyguoguz@iyte.edu.tr

Key Words: Ti₃AlC₂ solid phase microextraction fiber, Volatile organic compounds, Air analysis, Gas chromatography.

Despite their significant toxicological risks, some volatile organic compounds (VOCs) are extensively utilized across various industries including plastics, polymers, fuels, pharmaceuticals, and agricultural chemicals due to their high chemical reactivity and excellent solvent properties. Given their environmental persistence and adverse health effects, these compounds are classified as priority pollutants, mandating rigorous monitoring at sub-ppm levels [1]. Although highly sensitive chromatographic and spectroscopic techniques (e.g., GC-FID/MS, HPLC, and UV-Vis/FT-IR) are widely employed for their determination, the ultra-trace concentrations in environmental samples typically require a robust sample preconcentration step. Solid-phase microextraction (SPME) has emerged as a highly preferred, green chemistry-compliant alternative for this purpose, as it significantly minimizes or entirely eliminates the use of organic solvents [2]. While commercially available SPME fibers are generally employed for such applications, their use is often hindered by significant drawbacks, including mechanical fragility, limited thermal stability, and a short lifespan. To overcome these inherent limitations, nanomaterial-based SPME fibers have been intensively investigated as highly promising alternatives.

The accurate profiling of volatile aromatic compounds, particularly BTEX (benzene, toluene, ethylbenzene, and xylenes), in air samples is of critical importance. Originating primarily from vehicular exhaust and industrial emissions, these ubiquitous contaminants pose severe public health risks, highlighted by the established carcinogenicity of benzene. By seamlessly integrating with gas chromatography (GC) and streamlining sample preparation, SPME fiber provides a rapid, cost-effective, and highly reliable solvent-free method to directly extract and concentrate these trace-level atmospheric pollutants.

In this study, novel SPME fibers coated with various nanomaterials specifically black phosphorus, Cr₂CTx/Cr MXene, and Ti₃AlC₂ MAX phase were developed, and their extraction affinities for VOCs of varying polarities were evaluated. The Ti₃AlC₂ MAX-based SPME fiber demonstrated superior extraction efficiency for aromatic VOCs. Following the systematic optimization of critical sampling parameters, including extraction time, temperature, and sample volume, the proposed method successfully achieved the detection of atmospheric BTEX compounds at sub-ppm levels. The optimized method was successfully utilized for the quantitative analysis of BTEX in real air samples.

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Comparative Studies on the Determination of Trifluoroacetic Acid by Ion Chromatography

Rajmund MICHALSKI¹, Joanna KOŃCZYK², Katarzyna STAHL¹,
Paulina PECYNA-UTYLSKA¹, Edward MUNTEAN³

¹*Institute of Environmental Engineering of Polish Academy of Sciences,
34 Skłodowska-Curie Street, Zabrze, Poland;*

²*Jan Długosz University in Częstochowa, Institute of Chemistry, Faculty of Science & Technology,
13/15 Armii Krajowej Street, Częstochowa, Poland;*

³*University of Agricultural Sciences & Veterinary Medicine, Faculty of Food Sciences & Technology,
Food Sciences Department, 3-5 Calea Mănăştur, Cluj-Napoca, Romania.*

rajmund.michalski@ipispan.edu.pl

Key Words: Trifluoroacetic acid, Ion chromatography, Methodology, Water.

The number of new substances subject to legal regulation is steadily increasing in line with new toxicological knowledge and advances in analytical chemistry. Currently, the focus is on, amongst others, microplastics and compounds from the group of poly- and perfluoroalkyl acids (PFAS), including trifluoroacetic acid (TFA). The latter is a breakdown product of PFAS found in refrigerants, agrochemicals, medicines and fluoropolymer precursors. It is therefore ubiquitous in the air, water, food and consumer products [1].

TFA dissolves readily in water and organic solvents and is highly persistent and mobile in the environment. In the food industry, TFA-based materials are widely used in food packaging. The first reports of PFAS toxicity date back to the early 1950s. It was only with the rapid development of analytical chemistry and toxicology that it became possible to detect the presence of PFAS and TFA in various materials and to realise the scale of the problems associated with them. Scientific research has shown that the accumulation of certain PFAS in the human body can lead to health problems [2].

In 2020, the EFSA published a document on the occurrence of PFAS in food. However, it did not issue an opinion on human consumption of TFA. It did, however, set the dietary intake threshold for TFA at 4.4 ng/kg body weight [3]. The aim of the study was to develop a simple method for determining TFA in water, using ion chromatography with conductometric detection, which is accessible in routine laboratories.

For this purpose, ion chromatographs from the following manufacturers were used: Metrohm, Dionex, Shimadzu, and Shine. As part of the optimisation of the methodologies, analytical columns, eluents, eluent flow rates and injection volumes appropriate for the manufacturer were used. Detection was conducted in each case by suppressed conductivity detector. The results obtained were sufficiently satisfactory to be considered suitable for the determination of toxic TFA ions in water in the presence of other inorganic anions.

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LC-MS/MS Determination of Five Alkylphenols in E-Cigarette Refill Liquids: Method Development and Validation

Dominika OSIECKA, Maria LUBIŃSKA, Paweł KUBICA

*Gdańsk University of Technology, Chemical Faculty, Department of Analytical Chemistry,
G. Narutowicza Street 11/12, 80-233, Gdańsk, Poland.
dominika.osiecka@pg.edu.pl*

Key Words: E-cigarette refill liquids, LC-MS/MS, Alkylphenols, Endocrine-disrupting chemicals.

Alkylphenols (APs) are a group of chemicals widely used in industry as antioxidants, heat stabilizers and additives in the manufacture of polymers, lubricants, rubber, plastics and phenolic resins. Due to their estrogenic activity, APs are classified as endocrine-disrupting chemicals (EDCs) [1]. Consequently, nonylphenol (NP) is not included in the Union List of substances authorised for use in plastic food-contact materials and is prohibited in cosmetic products under Regulation (EC) No. 1223/2009 [2]. In contrast, despite inhalation representing one of the most direct routes of human exposure and e-cigarette aerosol being in direct contact with the respiratory mucosa, no regulations currently address the presence of alkylphenols in e-cigarette refill liquids.

Building upon our previous finding of bisphenol A in e-cigarette refill liquids, another endocrine-disrupting phenolic compound [3], the present study aimed to develop extraction procedure followed by LC-MS/MS analysis for the determination of five alkylphenols – 4-nonylphenol, 4-tert-octylphenol, 4-octylphenol, 4-pentylphenol and 4-hexylphenol – in e-cigarette refill liquids. Method development focused on covering two major analytical challenges: matrix effects caused by the propylene glycol (PG) and vegetable glycerol (VG), the primary constituents of e-liquids, and chromatographic separation of structurally similar APs. Chromatographic conditions were optimized to achieve baseline separation of analytes, including the positional isomers octylphenol and 4-tert-octylphenol.

To overcome the challenging PG/VG matrix, a simple sample preparation procedure based on salting-out-assisted liquid-liquid extraction inspired by QuEChERS principles was developed. Unlike conventional QuEChERS applications developed for water-based matrices, e-cigarette refill liquids consist primarily PG and VG, which are readily co-extracted into acetonitrile and cause pronounced matrix effects during LC–MS/MS analysis. The MgSO_4 and NaCl addition effectively limited the transfer of PG and VG, while matrix-matched calibration ensured reliable trace-level determination of APs

The method showed good linearity over the concentration range of 0.05 to 1.5 ng per g of e-liquid. The method was validated and recoveries ranged from 83 to 107%, while coefficients of variation (CVs) did not exceed 10%. The validated method was successfully applied to the analysis of commercially available e-cigarette refill liquids.

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Development of a GC-MS Method for the Determination of Emerging Pesticides in Water Samples

**Vlad-Alexandru PĂNESCU¹, Mihaela-Cătălina POPOVICI¹, Maria-Virginia COMAN¹,
Mihail Simion BELDEAN-GALEA²**

¹ Babeş-Bolyai University, "Raluca Ripan" Institute for Research in Chemistry,
30 Fântânele Str., RO-400294 Cluj-Napoca, Romania;

²Babeş-Bolyai University, Faculty of Environmental Science and Engineering,
30 Fântânele Str., RO-400294 Cluj-Napoca, Romania.
vlad.panescu@ubbcluj.ro

Key Words: Emerging pesticides, Water samples, Gas chromatography-mass spectrometry, Solid-phase extraction.

The aim of this work is to develop a method for the determination of ten pesticides mentioned in the EU watch lists as emerging contaminants, namely aclonifen, difenoconazole, epoxiconazole, imazalil, ipconazole, irgarol, miconazole, quinoxifen, tamoxifen and triclosan by solid phase extraction and GC-MS analysis.

In order to cover a wide polarity spectrum, two extraction cartridges (Oasis MCX and Oasis WAX) connected in series were used for solid phase extraction. The elution of the compounds was done separately for each cartridge with different solvent mixtures to obtain a satisfactory recovery. The identification of the compounds was done in selected ion monitoring (SIM) mode. The developed method shows a good linearity with R^2 ranging between 0.9981 and 0.999, a good precision with an RSD ranging between 1.32 and 5.67%, and detection limit ranging between 1.23 and 5.63 ng/L. For extraction, one liter of water, acidified at pH 3.9 and filtered through a 0.45 µm Millipore membrane was passed through the two cartridges and eluted with 5 mL of the solvent mixture for each cartridge. After elution, the extracts were unified, evaporated to dryness under a nitrogen stream and reconstituted in 2 mL of methanol for analysis.

The developed protocol was applied for the determination of these pesticides in four types of water, namely river water, drinking water, wastewater and treated wastewater samples collected from Drinking Water Production and Wastewater Treatment Systems of Târgu-Mureş City, Romania. Three sets of samples were collected in October 2025, February and July 2026 in order to study the incidence and variability of these compounds over time. The results obtained showed the presence of triclosan in nine samples with concentrations ranging between 0.47 and 135.1 ng/L, irgarol in one sample with a concentration of 48.1 ng/L, ipconazole in one sample with a concentration of 6.56 ng/L, and imazalil in three samples with concentrations ranging between 87.97 and 308.73 ng/g.

The study highlights the need to monitor these types of pesticides in order to obtain sufficient data to assess exposure and health risk associated with consumption through drinking water.

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LC-MS/MS Monitoring of Various PFAS in the Drinking Water Production and Wastewater Treatment Systems of Târgu Mureș City, Romania

**Mihaela-Cătălina POPOVICI¹, Vlad-Alexandru PĂNESCU¹,
Simina Ioana BELDEAN-GALEA², Maria-Virginia COMAN¹**

¹Babeș-Bolyai University, "Raluca Ripan" Institute for Research in Chemistry,
30 Fântânele Str., RO-400294 Cluj-Napoca, Romania;

²Iuliu Hațieganu University of Medicine and Pharmacy, Faculty of Dental Medicine,
8 Victor Babeș Str., RO-400347 Cluj-Napoca, Romania.
mihaela.herghellegiu@ubbcluj.ro

Key Words: Forever Contaminants, PFAS, Water Samples, LC-MS/MS, Direct Injection.

Poly- and perfluoroalkylated compounds (PFAS) constitute a large category of organofluorinated compounds, characterized by pronounced chemical stability, refractoriness to degradation and amphiphilic properties (hydrophobic and lipophobic). The long persistence in ecosystems, correlated with their high potential for bioaccumulation, has determined the international authorities to classify PFAS in the category of "persistent pollutants" or "forever contaminants" [1]. Human exposure, mainly achieved through the ingestion of drinking water, is associated with a variety of health effects, including developmental issues, disruptions in lipid metabolism and the endocrine system, and serious conditions such as cancer, immune system toxicity, liver damage, and reproductive toxicity [2].

In this context, the optimization of analytical methods with high sensitivity and selectivity becomes an imperative priority. This work describes an LC-MS/MS analysis method for the simultaneous determination of 20 PFAS compounds in river and drinking water samples, using a simplified sample preparation procedure. The determinations were performed using an LC-MS/MS system with a PFAS delay column and coupled to a Triple Quadrupole mass spectrometer equipped with an electrospray ionization source (negative ESI), and gradient mobile phase elution.

For the analysis, water samples were filtered through a 0.45 µm nylon membrane, then diluted with methanol in a ration water sample:methanol of 60:40 (v/v), internal standard addition, vortexing for 15 min and injected directly into the LC system. The performance parameters of the method show good linearity with correlation coefficients R^2 above 0.99 in the concentration range 1.5–50 ng/L, a limit of quantification between 1.25 and 1.5 ng/L, respectively a good degree of recovery between 80% and 120%. A solution containing 16 stable isotopic-labelled compounds (free acid) was used as an internal standard, and the identification of the compounds was done by the MRM (multiple reaction monitoring) method.

The analysis method was applied for the analysis of drinking water, river water and wastewater treatment plant effluent samples collected in three time periods October 2025, February and July 2026 from the Drinking Water Production and Wastewater Treatment Systems of Târgu Mureș City, Romania, demonstrating the viability of this method for the analysis of real samples, in accordance with the selectivity and sensitivity requirements imposed by European legislation.

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Development and Validation of a Liquid Chromatographic Tandem Mass Spectrometric Method (LC–MS/MS) for the Determination of Bisphenols and Parabens in Menstrual Products after Solid-Phase Extraction

Pavlos VOUTSAS, Natasa KALOGIOURI, **Victoria SAMANIDOU**

*Aristotle University of Thessaloniki, School of Chemistry, Laboratory of Analytical Chemistry,
Thessaloniki, GR-54124, Greece.
samanidu@chem.auth.gr*

Key Words: Bisphenols, Parabens, Menstrual products, SPE, LC-MS/MS

Abstract

Menstrual products present a potential source of exposure to endocrine-disrupting chemicals (EDCs), while limited information is provided on product labels regarding their composition[1,2]. In this research, a novel method was developed and validated for the determination of parabens (PBs) and bisphenols (BPs) in menstrual products, including pads, panty liners, and tampons, to assess potential chemical exposure and product safety.

Methods

Sample preparation was optimized by evaluating extraction solvent, solvent volume, extraction time, SPE sorbent, and elution conditions. Extraction was achieved using only 2 mL of methanol and 15 min ultrasonication, followed by Oasis HLB solid-phase extraction and LC–MS/MS ESI analysis. Compounds were analyzed using a Shimadzu LCMS-8060RX system equipped with an ESI source and an XBridge® BEH C18 XP column (2.5 μ m, 3.0 $\times$ 100 mm) operated at 40°C and 0.3 mL/min. Gradient elution was performed using water and methanol as mobile phases, with detection carried out by LC-MS/MS in negative ESI mode using multiple reaction monitoring (MRM). DES was used as an internal standard to correct for instrumental variability, injection repeatability, and ESI signal fluctuations. Linearity was assessed over 1–100 ng/mL using ordinary least-squares regression. Sensitivity was evaluated by S/N ratios, with LOD and LOQ calculated as 3 $\times$ (S/N) and 10 $\times$ (S/N), respectively. Accuracy, precision, and matrix effects were evaluated at selected concentration levels using RR%, RSD%, and ME%, respectively.

Results

All analytes showed good linearity ($R^2 > 0.99$) over the concentration range of 1–100 ng/mL. The LOQ was found to be 1 ng/mL and the LOD at 0.2 ng/mL for validation and real sample analyses. Relative recoveries ranged from 83.9–112.2%, meeting the 80–120% acceptance criteria and demonstrating good accuracy. Precision was also satisfactory, with RSD% values below 20% at the LOQ and below 15% at higher validation levels. The average RSD% across all validation levels remained below 10%, confirming good method reproducibility. The proposed method demonstrated good greenness, analytical performance, and practical applicability, achieving MoGAPI, RAPI, and BAGI scores of 78, 77.5, and 67.5, respectively. The validated method was applied to commercially available menstrual products. BPA was detected in every sample analyzed, although generally at low concentrations (up to 68 ng/g) whereas the remaining BPs were absent or present only at trace levels. In contrast, PBs were more frequently detected, particularly in scented products, with methylparaben and propylparaben reaching concentrations of 3635 and 2052 ng/g.

Conclusions

Although most samples showed low BP and PB concentrations, frequent exposure may still pose potential risks, highlighting the importance of product safety certification and transparency.

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The Fate of Lycopene and other Carotenoids from Feed to Egg in two Laying Hen Set-ups

Andrew CASSAR¹, Mauro BUTTIGIEG¹, Adrian BUGEJA DOUGLAS¹,
Slavica BLAGOJEVIĆ², **Tomislav TOSTI**³, Everaldo ATTARD¹

¹University of Malta, Institute of Earth Systems, Division of Rural Sciences and Food Systems,
Msida MSD2080, Malta;

² University of Belgrade, Faculty of Pharmacy, Department of Physical Chemistry and Instrumental Methods,
Belgrade, Serbia;

³University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Njegoseva 12, Belgrade, Serbia.
tomislav.tosti@ihfm.bg.ac.rs

Key Words: Egg, Lycopene, Carotenoids, Tomato powder, Egg yolk.

Eggs are a nutritious food, providing a balanced source of essential amino acids, fatty acids, minerals and vitamins. The nutritional and physicochemical characteristics of eggs can be influenced by the composition of laying hens' diets and by dietary supplementation with bioactive compounds. The aim of this study was to determine the effect of tomato powder on egg weight, egg length and width, yolk colour, carotenoid content, polyphenol content and antioxidant content when given to laying hens as a feed additive.

The study analysed 576 eggs from two experimental trials involving laying hens fed diets supplemented with 0, 2, 4 or 6 g tomato powder per 100 g feed. Tomato supplementation did not significantly affect egg weight or shape. Yolk colour intensity increased from 5 in the control group to 14 in the 6 g/100 g feed group by the end of the experiment, with comparable trends observed under farm conditions.

Physicochemical analysis showed a significant increase in yolk carotenoid content during the feeding trial. Using UV–Vis spectrophotometry after extraction with a hexane–acetone–ethanol (2:1:1) solvent system, the study detected substantial concentrations of lycopene, β -carotene and lutein. The highest values were observed under isolated conditions (43.84, 35.49 and 41.05 mg/kg, respectively), while slightly lower concentrations were recorded under farm conditions (35.49, 34.21 and 36.43 mg/kg, respectively). These results indicate that carotenoids from dietary tomato powder were effectively transferred to the egg yolk.

The study found that chlorophyll A and B accumulated in the yolk at much lower concentrations than the major carotenoids.

Total polyphenol content, determined by the Folin–Ciocalteu assay, did not differ significantly among the dietary treatment groups, ranging from 108 mg/g (group fed 6 g/100 g) to 316 mg/g (control group) across both experimental systems.

Antioxidant scavenging activity was assessed using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) method. The highest value, 26.16 mg/100 g, was found in week 8 in the control group of the farm experiment, while the lowest value, 18.62 mg/100 g, was found in week 4 in the 6 g group of the farm experiment.

This study indicates that lycopene and other carotenoids, which may be present in industrial food wastes, can be easily incorporated as a feed additive. At these dietary concentrations, lycopene enhances the other carotenoids present in the egg yolk.

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HPLC-MS Method Development for the Analysis of Polar Low Molecular Weight Metabolites

Barbora TOŠOVSKÁ, Petr ČESLA

University of Pardubice, Faculty of Chemical Technology, Department of Analytical Chemistry,
Studentská 573, 532 10 Pardubice, Czech Republic.
barbora.tosovska@student.upce.cz

Key Words: HILIC, HPLC-MS, Bioinert columns, Polar metabolites.

Low molecular weight polar metabolites play a fundamental role in cellular metabolism and provide valuable insights into physiological and pathological processes. The analysis of these compounds remains one of the major challenges in liquid chromatography due to their high polarity, limited retention in reversed-phase liquid chromatography, and undesirable interactions between analytes and metal surfaces, particularly in the case of phosphorylated metabolites. Hydrophilic interaction liquid chromatography (HILIC) coupled with mass spectrometry (MS) represents a suitable approach for the analysis of these metabolites. However, the efficiency, robustness, and reproducibility of the method strongly depend on careful optimization of chromatographic conditions, particularly the selection of the stationary phase and column hardware [1, 2].

The aim of this study was to develop and optimize an HPLC-MS method based on HILIC separation for the analysis of polar low molecular weight metabolites involved in mitochondrial metabolism, including tricarboxylic acid cycle intermediates and adenine nucleotides. As part of the method development, HILIC separation conditions were optimized, especially the mobile phase composition, buffer concentration, and gradient elution to improve chromatographic selectivity and compatibility with MS. In addition, three HILIC columns were compared: the conventional InfinityLab Poroshell 120 HILIC-Z column and two bioinert columns with different stationary phases, InfinityLab Poroshell 120 HILIC-Z PEEK-Lined and XBridge Premier BEH Amide.

The comparison showed that the use of bioinert column hardware reduced undesirable interactions between analytes and metal surfaces, resulting in improved peak shape, higher MS signal intensity, and increased method sensitivity and reproducibility compared with conventional column hardware. Furthermore, the different stationary phases exhibited different retention and selectivity characteristics, highlighting the importance of stationary phase selection in HILIC method development. The results show that the combination of optimized HILIC conditions and bioinert column hardware contributes to reliable and sensitive HPLC-MS analysis of challenging polar metabolites.

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UHPLC-MS/MS Analyses and Spectrophotometric Assays of Japanese Knotweed Extracts Obtained from Accelerated Solvent Extraction

Živa VIPOTNIK¹, Vesna GLAVNIK¹, Uroš M. GAŠIĆ², Maja BENSA³, Irena VOVK¹

¹National Institute of Chemistry, Laboratory for Food Chemistry,
Hajdrihova 19, SI-1000 Ljubljana, Slovenia;

²National Institute of Republic of Serbia, Institute for Biological Research "Siniša Stanković",
Department of Plant Physiology, University of Belgrade,
Bulevar despota Stefana 142, RS-11108 Belgrade, Serbia;

³University of Ljubljana, Faculty of Health Sciences, Research Institute of Faculty of Health Sciences,
Zdravstvena pot 5, SI-1000 Ljubljana, Slovenia.
ziva.vipotnik@ki.si

Key Words: Phenolic compounds, Accelerated solvent extraction, UHPLC-MS/MS, Antioxidant activities.

Japanese knotweed (*Fallopia japonica* Houtt.), ranked among the world's 100 most invasive alien plant species in Europe and North America, exerts a severe negative impact on ecosystems, but at the same time represents a massive and valuable biomass with an unexplored source of bioactive secondary metabolites.

This study investigated the optimization of Accelerated Solvent Extraction (ASE) to simultaneously maximize Total Phenolic Content (TPC) and DPPH radical scavenging activity (RSA) from Japanese knotweed leaf matrices. Response Surface Methodology (RSM) based on a Custom D-Optimal Design was applied to evaluate the individual and interactive effects of extraction temperature (60 – 140°C) and solvent composition (acetone, methanol, ethanol, water, and their aqueous mixtures). Based on the experimental matrix, 35 runs were performed. Analysis of Variance (ANOVA) demonstrated that the quadratic models for both TPC and DPPH inhibition were highly significant ($p < 0.05$) with strong coefficients of determination ($R^2 > 0.95$), confirming robust predictive capacity.

The optimal extraction temperature was highly dependent on the chosen solvent system. At 80°C, the highest yields were achieved using 100% methanol (46.9 ± 0.9 mg GAE/g TPC, 53% RSA), 80% methanol (62.3 ± 0.7 mg GAE/g TPC, 24% RSA), and 70% acetone (18.7 ± 0.6 mg GAE/g TPC, 44% RSA). Conversely, a lower temperature of 60°C was optimal for 100% ethanol (75.7 ± 0.2 mg GAE/g TPC, 24% RSA) and 70% methanol, which yielded the highest overall phenolic concentration (98.2 ± 0.7 mg GAE/g TPC, 52% RSA). Elevated temperatures were required for 70% ethanol at 120°C (62.5 ± 0.6 mg GAE/g TPC, 61% RSA), while pure water reached its optimum at 140°C (36.1 ± 0.9 mg GAE/g TPC, 36% RSA). Complementary UHPLC-MS/MS profiling successfully identified 85 distinct bioactive compounds, including phenolic acids, flavonoids (flavan-3-ols, flavones, flavanones), stilbenes, and anthraquinones.

These findings demonstrate that optimized ASE is a highly efficient strategy to valorize invasive Japanese knotweed biomass into targeted, high-value functional bioactive compounds.

Acknowledgements

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Eco-friendly synthesis of Ag/Ag₂O Nanoparticles using *Eryngium planum* L. Extract and their Antioxidant & Antimicrobial Activity

Adriana-Maria ANDREICA¹, Mihaela Cecilia VLASSA¹, Ioana PERHAIȚA¹,
Rahela CARPA², Maria COROȘ³, Ioan PETEAN⁴

¹Babeș-Bolyai University, Raluca-Ripan Institute for Research in Chemistry, 400294 Cluj-Napoca, Romania;

²Babeș-Bolyai University, Faculty of Biology and Geology, Molecular Biology and Biotechnology Department, 400084 Cluj-Napoca, Romania;

³National Institute for Research and Development of Isotopic and Molecular Technologies, 400293 Cluj-Napoca, Romania;

⁴Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, 400084 Cluj-Napoca, Romania.

mihaela.vlassa@ubbcluj.ro

Key Words: Green synthesis, Silver/silver oxide nanoparticles, *Eryngium planum*, Antioxidant activity, Antimicrobial activity.

This study reports the eco-friendly green-synthesis of silver/silver oxide nanoparticles (Ag/Ag₂O NPs) using an aqueous extract from the aerial parts of *Eryngium planum* L. as both a reducing and stabilizing agent [1].

Reaction parameters including pH, temperature, extract-to-precursor ratio, and reaction time, were systematically optimized and monitored through UV-Vis spectroscopy [2]. FTIR analysis identified the organic functional groups responsible for the reduction of silver ions and subsequent capping of the nanoparticles. Morphological and structural characterization by AFM revealed spherical Ag/Ag₂O NPs with an average diameter of 27 nm, while TGA/DTA confirmed the thermal decomposition of the plant-derived biomolecules adsorbed onto the nanoparticle surface. Quantitative assays demonstrated that the synthesized Ag/Ag₂O NPs possessed significantly higher total phenolic (TPC) and total flavonoid (TFC) contents compared to the crude aqueous extract [3]. Also, the nanoparticles exhibited superior antioxidant capacity in both DPPH and ABTS radical scavenging assays [4]. Furthermore, antimicrobial screening revealed enhanced inhibitory activity against five pathogenic strains, encompassing four distinct bacterial strains (*Staphylococcus aureus*, *Escherichia coli*, *Enterococcus faecalis*, *Pseudomonas aeruginosa*) and one fungal strain (*Candida albicans*).

The antimicrobial activity of Ag/Ag₂O NPs against *candida* has higher antifungal efficacy than the antibiotic in the mixture. These results underscore the potential of *E. planum*-mediated Ag/Ag₂O NPs as potent antioxidant and antimicrobial agents for biomedical applications.

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A Simple and Cost-Effective Method for the Determination of Organic Tomatoes

Nergis İlayda ÖZKAN^{1,2}, Uluç Yarkın SİPAHİ^{1,2}, Duygu Selin TURAN³, Berfu YİĞRİK^{1,2},
Lara HIŞMAN⁴, Asel Zehra MULCAR⁴, Can ARAT⁴, Gölgen Bahar ÖZTEKİN⁴,
Burak ORDİN³, Levent PELİT^{1,2}

¹Ege University, Faculty of Science, Department of Chemistry, 35040 Bornova, İzmir, Türkiye;

²Ege University, Translational Pulmonary Research Center (EgeSAM), 35040, Bornova, İzmir, Türkiye;

³TAKEV High School, Altievler Mah. Vakıf Sk. No:3 35320 Sahilevleri, İzmir, Türkiye;

⁴Ege University, Faculty of Agriculture, Department of Horticulture, 35040 Bornova, İzmir, Türkiye.

levent.pelit@ege.edu.tr

Key Words: Gas chromatography, Volatile organic compounds, Volatile inorganic compounds, Atmospheric dielectric barrier discharges optical emission detector.

The increasing consumer demand for organic agricultural products has driven the need for reliable analytical methods to verify their authenticity and prevent food fraud. Currently, the authentication of organic products typically relies on sophisticated techniques such as isotope ratio mass spectrometry (IRMS) or targeted multi-residue pesticide analyses. However, these conventional methods present significant drawbacks, including high operational costs, complex and time-consuming sample preparation steps, and the requirement for highly specialized instrumentation.

To overcome these inherent limitations, there is a growing interest in developing simple, rapid, and cost-effective alternatives. Volatile organic compounds (VOCs) play a crucial role in the sensory quality and metabolic response of agricultural crops. In tomatoes, the VOC profile is highly sensitive to cultivation practices; variations in soil management, fertilization, and environmental stress between organic and conventional farming systems significantly alter the emission of specific secondary metabolites. Consequently, the comprehensive profiling of these emissions often referred to as "odor fingerprinting" has emerged as a powerful discriminatory tool. By evaluating the holistic VOC signatures rather than targeting individual markers, it is possible to successfully classify tomatoes based on their agricultural origin. This odor fingerprinting approach not only bypasses the disadvantages of traditional methods, but also offers a robust/reliable strategy for the chemical characterization/authentication of tomatoes.

In this study, the VOC fingerprinting of the conventional and organic tomatoes was obtained after head space solid phase microextraction gas chromatography flame ionization detector (HS-SPME-GC-FID) method. Following the homogenization step, the tomato homogenate was centrifuged at 5000 rpm for 5 min, and a 2 mL aliquot of the supernatant was transferred into a 20 mL headspace (HS) vial containing 0.4 g of NaCl. After incubation at 55°C for 10 min, VOC extraction step was carried out by using a CAR/PDMS/DVB SPME fiber for 15 min. Subsequently, the fiber was introduced into the GC injection port, and the adsorbed VOCs were desorbed at 225°C for 5 min.

The analysis of detected VOCs was performed using the Python-programming language. The scikit-learn library was used for implementing the Support Vector Machine, Random Forest, Principal Component Analysis, and LOOCV procedures; SciPy was used for one-way ANOVA F-tests; and stats models were employed for false discovery rate (FDR) correction. The best-performing model (all 214 VOCs) achieved 90.0% accuracy, an AUC of 0.991, and strong statistical significance confirmed by a 200-iteration permutation test ($p = 0.005$).

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Determination of Volatile Compounds by Laboratory-Made Plasma Detector

Nergis İlayda ÖZKAN^{1,2}, Bilge Nur KARA^{1,2}, **Berfu YİĞRİK**^{1,2}, Samed GÜMÜŞ³,
Yavuz ÖZTÜRK³, Erkan Zeki ENGİN³, Sefer Haşım BURGAZ⁴, Alper ÇETİNEL⁴,
Denizcan KÖSEOĞLU⁵, Metin BİLGE³, Aytaç KARADAĞ⁶, Levent PELİT^{1,2}

¹Ege University, Faculty of Science, Department of Chemistry, 35040 İzmir, Türkiye;

²Ege University, Translational Pulmonary Research Center (Ege-SAM), 35040, İzmir, Türkiye;

³Ege University, Faculty of Engineering, Department of Electrical and Electronics Engineering,
35040, Bornova, İzmir, Türkiye;

⁴Ege University, Faculty of Science, Department of Physics, 35040, İzmir, Türkiye;

⁵AltraFlora Natural Extracts Inc., Zafer Mahallesi, 1033. Sokak, No: 16A, 20020 Merkezefendi, Denizli, Türkiye;

⁶IstWest AVM, IstWest Çarşı, Yenibosna Merkez Mahallesi, Değirmenbahçe Caddesi, No:17A1,
34130 Bahçelievler, İstanbul, Türkiye.

berfuyigrik@gmail.com

Key Words: Gas chromatography, Volatile organic compounds, Volatile inorganic compounds, Atmospheric dielectric barrier discharge optical emission detector.

Determination of inorganic and organic volatile compounds in environmental (indoor atmosphere) or biological matrices (exhaled breath) quite important [1]. In this step, key parameters is the detector used in gas chromatographic system for the determination of analytes. Unlike conventional gas chromatography (GC) detectors, which often require a compromise between universality and sensitivity, plasma-based detectors offer unique analytical capabilities [2, 3]. While the widely used flame ionization detector (FID) is blind to permanent gases, water, and most inorganic compounds, and the thermal conductivity detector (TCD) suffers from limited sensitivity, plasma detectors provide near-universal detection at trace (sub-ppm/ppb) levels. Furthermore, in contrast to the electron capture detector (ECD) and FID, plasma-based systems eliminate the need for radioactive sources and hazardous combustible gases like hydrogen, typically utilizing only an inert discharge gas such as helium or argon. This enables the simultaneous, highly sensitive, and safe profiling of both organic and inorganic species in complex matrices a task that traditionally requires the coupling of multiple conventional detectors. Therefore, conducting research on plasma detectors, which are among the next-generation detector systems, is of great importance.

In this study, a atmospheric dielectric barrier discharge (DBD) plasma-based optical emission detector was designed and integrated into a gas chromatography (GC) system for the chromatographic determination of some volatile organic and inorganic compounds such as methane, ammonia, hydrogen, in air samples. The best performance was obtained for methane. Under the optimized experimental conditions, the developed method achieved a limit of detection (LOD) of 53 ppm for CH₄. The repeatability of the method was evaluated with a relative standard deviation (RSD) of 13.1%, demonstrating acceptable analytical performance. The results indicate that the proposed GC–DBD optical emission detection system provides a reliable and cost-effective approach for methane analysis. Furthermore, the developed system shows considerable potential for future applications involving the simultaneous determination of chemically diverse gaseous compounds by further optimization of the detection system.

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e-POSTER PRESENTATIONS

01–17

ITS2 eDNA Metabarcoding Reveals Distinct Fungal Communities Across Soil Trajectories in a Remediated Former Cooking-Plant

Maria-Anastasia ABRUDAN¹, Emanuela D. TIODAR², Cristina L. VĂCAR²,
Zoltan R. BALÁZS^{1,2,3}, Dorina PODAR^{1,2}

¹*Babeş-Bolyai University, Faculty of Biology and Geology, Department of Molecular Biology and Biotechnology, Cluj-Napoca, Romania;*

²*Babeş-Bolyai University, Centre for Systems Biology, Biodiversity and Bioresources (3B), Cluj-Napoca; Romania;*

³*Babeş-Bolyai University, Doctoral School of Integrative Biology, Cluj-Napoca, Romania.
dorina.podar@ubbcluj.ro*

Key Words: eDNA, Metabarcoding, Fungi, Soil remediation, Polycyclic aromatic hydrocarbons (PAHs).

Intensive industrial activity has left numerous sites worldwide with soils contaminated by persistent pollutants. Such contamination can pose long-term ecological risks and may require remediation to support ecosystem recovery. The present study focused on a historically contaminated site located within a former coking-plant area in Homécourt, north-eastern France, affected by polycyclic aromatic hydrocarbons (PAHs) and metals [1]. The objective was to assess the extent of ecological recovery by comparing four soil trajectories and evaluating associations between fungal community composition and present-day soil physicochemical properties. Approximately two decades after the remediation interventions in the treatment area, soil fungal communities were characterised using ITS2 eDNA (Internal Transcribed Spacer 2 environmental DNA – a genetic marker) metabarcoding.

Four areas were considered distinct soil trajectories, each reflecting a different history of contamination, remediation, and vegetation development. Control was a contaminated area under natural attenuation, without active remediation. The Treatment area underwent thermal desorption in 2003 and pedological engineering in 2007 and is currently grass-covered. Reference Forest and Reference Grassland represented, respectively, a forest and a natural grassland with no history of contamination.

Twenty independently collected composite soil samples were analysed, with five biological replicates per trajectory. Fungal alpha and beta diversity were estimated, and the association between community composition and the measured physicochemical context was examined.

Observed fungal richness was lower in Treatment than in both reference trajectories, whereas Shannon and Inverse Simpson diversity did not differ significantly. Fungal community composition differed significantly among all four trajectories. Treatment was distinct from Control and both reference trajectories. A significant association was also detected between fungal composition and a subset of the measured present-day soil physicochemical properties. Because these properties contained overlapping information, their contributions were interpreted collectively rather than independently.

Treatment was characterised by a fungal assemblage distinct from Control and both reference trajectories. Because environmental history, vegetation and soil conditions varied simultaneously among the investigated areas, the observed differences represent multifactorial trajectory-level associations rather than causal effects of a single factor. ITS2 eDNA metabarcoding therefore complements physicochemical assessment by revealing biological differences among soils with distinct environmental histories.

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GC–MS-Based VOC Profiling of Poultry Cecal Content as an Analytical Tool for Assessing Low-Dose Antibiotic Exposure in Broiler Chickens

**Magdalena BUSZEWSKA-FORAJTA^{1,2}, İknur ERBAŞ³, Ebru ÇALKAN YILDIRIM³,
Berfu YİĞRIK³, Małgorzata OLEJNIK¹, Levent PELIT³**

¹*Nicolaus Copernicus University in Toruń, Faculty of Biological and Veterinary Sciences,
Institute of Veterinary Medicine, Lwowska 1, 87-100 Toruń, Poland*

²*Prof. Jan Czocharński Kuyavian-Pomeranian Science and Technology Center,
Kraśińskiego 4, 87-100 Toruń, Poland*

³*Ege University, Faculty of Science, Department of Chemistry, Division of Analytical Chemistry,
Bornova, 35100 İzmir, Türkiye
m.buszevska@umk.pl*

Key Words: GC–MS, Volatile organic compounds, Cecal content, Low-dose antibiotics, One health.

The aim of this study was to compare faecal volatile organic compound (VOC) profiles of healthy chickens and chickens exposed to antibiotic treatment. Faecal samples were collected on day 7 after antibiotic administration, homogenised, stored at –80°C and analysed using HS-SPME–GC–Orbitrap MS. A 500 mg portion of each sample was used for VOC profiling, and the acquired data were processed using Compound Discoverer.

A total of 233 GC–EI features were detected. Principal component analysis showed a group-related distribution of samples, with PC1 and PC2 accounting for 29.5% and 8.3% of the total variance, respectively. Differential analysis identified 35 features meeting $p < 0.05$ and $|\log_2 \text{fold change}| \geq 1$; 25 showed higher and 10 lower signals in the antibiotic-treated group. Twenty-eight features remained significant after multiple-testing correction.

Tentative annotations included methionol and several mono- and sesquiterpenes. The observed pattern may reflect antibiotic-associated changes in microbial sulphur-amino-acid metabolism and in the biotransformation of plant-derived dietary compounds.

The results show that antibiotic treatment was associated with a distinct faecal VOC profile seven days after administration. HS-SPME–GC–Orbitrap MS may therefore provide a useful complementary approach for detecting antibiotic-associated changes in gut-related metabolic activity.

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Sorption of Venlafaxine: Comparison of MIP and NIP

Kristina TOLIĆ ČOP, **Leona ČAKIĆ**, Luka OBULJEN, Dragana MUTAVDŽIĆ PAVLOVIĆ

*University of Zagreb, Faculty of Chemical Engineering and Technology,
19 Trg Marka Marulića, 10 000 Zagreb, Croatia.
lcakic@fkit.unizg.hr*

Key Words: Venlafaxine, Sorption, Molecularly Imprinted Polymers, Imprinting Factor.

Pharmaceuticals as emerging contaminants have been in the spotlight of scientific research for some time due to the lack of efficient removal technologies, their continuous unmonitored release into the environment, persistence in aquatic systems, and limited regulatory measures. New technologies and approaches are being developed to achieve selective and efficient removal of emerging contaminants, with molecularly imprinted polymers representing one of the most promising alternatives. Molecularly imprinted polymers are materials with tailor-made binding sites that are structurally compatible with the template molecule.

This study investigates differences in venlafaxine sorption performance on MIP and NIP. The molecularly imprinted polymer was synthesized by bulk polymerization using venlafaxine, DMSO, MAA, EGDMA, and AIBN as the template, solvent, functional monomer, cross-linker, and initiator, respectively. The polymerization solution was purged with N₂ and cured for 24 h at 60°C. The non-imprinted polymer was synthesized under the same conditions, without adding the template molecule. The MIP was washed using Soxhlet extraction with a MeOH:HAc (9:1, v/v) mixture until the venlafaxine peak was no longer detected by HPLC.

The examined sorption parameters included pH, temperature, ionic strength, and sorbent mass. The effect of pH was investigated at pH values of 4, 7, and 9. Higher pH values favored the sorption process due to electrostatic interactions between the negatively charged MIP surface and positively charged venlafaxine molecules. The effect of temperature was investigated at 25, 30 and 35°C. Sorption onto the MIP was enhanced at higher temperatures, whereas sorption onto the NIP was favored at lower temperatures. Ionic strength experiments were carried out using 0.001, 0.01, and 0.1 M NaCl. Both sorbents showed reduced sorption at higher NaCl concentrations. The effect of sorbent mass was investigated with 2.5, 5, 7.5, and 10 mg of sorbent. Increasing the sorbent mass resulted in improved sorption performance. The imprinting factor was calculated for all experiments.

Acknowledgements

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How HT-GC/MS and HT-GC×GC/MS Can Help for the Detailed Characterization of Heavy Distillation Volatile Fractions from Pyrolysis Oils

Xiangdong CHEN^{1,2}, Carlos RINCON², José DUGAY¹, Benoît GADENNE², Michel SABLIER¹, Arianne MORTEVEILLE¹, Jérôme VIAL¹

¹ESPCI Paris, PSL Research University, UMR CBI, Laboratoire des Sciences Analytiques, Bioanalytiques et Miniaturisation, 10 rue Vauquelin, 75231 Paris Cedex 05, France;

²MFP Michelin, Place des Carmes Deschaux, 63040 Clermont-Ferrand CEDEX 09.
xiangdong.chen@espci.fr / jerome.vial@espci.psl.eu

Key Words: Pyrolysis oil, HT-GC/MS, GC×GC.

The continuous growth of the human population, coupled with the rising demand for transportation, has resulted in higher tire consumption and, consequently, greater tire waste generation. In response, various tire waste management strategies have been explored in recent decades, particularly focusing on two main forms of valorization: material and energy recovery. Among these, tire pyrolysis has emerged as a well-established treatment method, enabling the production of value-added raw materials such as pyrolysis oils. According to literature, pyrolysis oils are a complex matrix containing high amounts of aliphatic, aromatic and heterocyclic compounds (usually more than thousands of compounds and some of them have similar boiling points). For this reason, distillation of pyrolysis oils is commonly performed to simplify the matrix and to obtain different fractions for targeted valorization processes including reuse as materials or fuels. However, previous studies have shown that the presence of heteroatomic compounds in these oils can hinder their effective utilization. For example, sulfur and nitrogen compounds are sources of toxic and corrosive gases such as SO_x and NO_x [1]. Therefore, detailed characterization of heteroatomic compounds within the distillation fractions of pyrolysis oils is essential for optimizing their downstream applications.

The characterization of the volatile fraction of pyrolysis oils has been previously conducted by two-dimensional gas chromatography combined with time-of-flight mass spectrometry (GC×GC/TOFMS, Leco). In this approach, distillation fractions with boiling points up to 369 °C were successfully eluted using our developed analytical protocol. However, due to the limited upper temperature tolerance of the polar column, heavier fractions could not be eluted. Moreover, the use of a nitrogen cryogenic modulator restricts the analysis of high-molecular weight compounds in these fractions.

To characterize the heavy fraction (369°C–509°C) of pyrolysis oils, the first step of this study involved developing a high-temperature gas chromatography–mass spectrometry (HT-GC/MS) protocol. Specific experimental conditions were optimized, including the selection of the column, as well as the temperatures of the oven, transfer line, and MS source. This protocol was then adapted to establish a high-temperature two-dimensional gas chromatography–mass spectrometry (HT-GC×GC/MS) method using a fluidic modulator (INSIGHT flow modulator, SepSolve) to prevent the trapping of high-molecular-weight compounds. This approach enabled the acquisition of two-dimensional chromatograms of the heavy fractions, which complement the previous GC×GC/TOFMS results.

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qPCR-based Quantification of *merA* Gene for Screening Microbial Resistance to Mercury within the Rhizosphere of Plants Native to Polluted Sites

Mihai C. GRIMM^{1,3}, Emanuela D. TIODAR^{2,3}, Horia L. BANCIU^{2,3}, Dorina PODAR^{2,3}

¹*Babeş-Bolyai University, Doctoral School of Integrative Biology, Cluj-Napoca, Romania;*

²*Babeş-Bolyai University, Department of Molecular Biology and Biotechnology, Cluj-Napoca, Romania;*

³*Babeş-Bolyai University, Centre for Systems Biology, Biodiversity and Bioresources(3B,) Cluj-Napoca, Romania.*

mihai.grimm@ubbcluj.ro / dorina.podar@ubbcluj.ro

Key Words: Bioremediation, *Diplotaxis muralis*, *Lotus tenuis*, Phytoremediation.

Mercury (Hg) contamination affects almost 10% of European soils [1], posing risks to ecosystem and human health and requiring urgent remediation. For large contaminated areas, conventional interventions such as thermal desorption are costly and impractical, driving interest in microorganisms-assisted phytoremediation. Such techniques involve the use of plant species native to contaminated sites, alongside their associated rhizosphere microbial communities as cost-effective and scalable alternatives. Central to this approach is the microbial resistance to Hg, largely mediated by the mercuric reductase, encoded by *merA* gene. This detoxification mechanisms involves the transformation of Hg²⁺ to a less toxic form of mercury, Hg⁰. However, no standardised method for screening plant species and their associated rhizosphere microorganisms suitable for phytoremediation approaches exists.

This study aimed to develop a qPCR-based method for quantifying *merA* gene abundance in the rhizosphere soil, for comparing Hg-resistance potential between different plant species. The two most dominant herbaceous plant species from a historically contaminated site were selected for analysis, *Lotus tenuis* and *Diplotaxis muralis*.

Gene copy number of *merA* was quantified by qPCR using specific primers with amplification efficiency and specificity verified by melt curve. Gene copy numbers were normalised per unit soil mass (dry weight). *merA* was detected in 83% of *D. muralis* samples and in 100% of *L. tenuis* samples. For *L. tenuis*, control samples from a non-contaminated site were analyzed and *merA* was absent in all with one exception.

This qPCR-based quantification of rhizosphere *merA* abundance provides a preliminary study for screening plant species for their potential to be used in phytoremediation strategies, based on their associated rhizosphere potential to withstand mercury toxicity. Broadly, this approach offers a practical selection criterion for phytoremediation approaches, ahead of costlier laboratory work.

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A Gas Chromatographic Approach for the Monitoring of PFAS in Water Samples

Anastasia KORPETI, Natalia MANOUSHI, Erwin ROSENBERG

*Vienna University of Technology, Institute of Chemical Technologies and Analytics,
Getreidemarkt 9/164, 1060, Vienna, Austria.
anastasia.korpeti@tuwien.ac.at*

Key Words: Gas Chromatography, PFAS, Water samples, Derivatization.

Per- and polyfluoroalkyl substances (PFAS) are synthetic fluorinated compounds that are used in industrial applications because of their high stability and resistance to degradation. Because of their environmental persistence and bioaccumulation, PFAS are commonly detected in wastewater, biosolids, and composts. Wastewater treatment plants (WWTPs) are important monitoring points for PFAS since they collect water from landfill leachates, stormwater, domestic, agricultural and industrial effluents [1].

They may also introduce PFAS into the environment through effluent discharge to surface water, land application of biosolids and disposal of residuals as well as air emissions [2]. Due to the associated environmental and health concerns, the analysis of wastewater samples from WWTPs is important. The aim of this study was to develop an analytical method based on extraction and derivatization to determine PFAS, specifically perfluoroalkyl carboxylic acids (PFCAs) in wastewater samples using gas chromatograph with tandem mass spectrometry (GC-MS/MS). Fluorinated acids are ionic, stable and therefore nonvolatile, which makes them unsuitable for direct analysis by gas chromatography.

Therefore, derivatization prior to GC analysis is required to convert the polar acid into a neutral and more volatile derivative. Different reagents were tested including N,O-bis(trimethylsilyl) trifluoroacetamide, trimethyl sulfonium hydroxide, isobutyl chloroformate, trimethyl silyl diazomethane, tetraalkylammonium salts, trimethyl orthoformate, triethyl orthoformate with the benzyl bromide showing superior performance.

The reaction conditions were comprehensively optimized for the selective and sensitive determination of perfluoroalkyl acids in wastewater samples.

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Quality Control of Natural Vinegar Based on Lactic and Acetic Acid Content

Olena KONOPLITSKA, Valentyna LEVCHYK

*Taras Shevchenko National University of Kyiv, Faculty of Chemistry, Department of Analytical Chemistry,
Hetmana Pavla Skoropadskoho Street, 12, City of Kyiv, Ukraine.
valentynalevchyk@gmail.com*

Keywords: Vinegar, HPLC, Acetic acid, Lactic acid, Food authenticity.

Objective

Vinegar is a 4–12% aqueous solution of acetic acid with a wide range of applications, including use as a condiment and as a household cleaning agent. Depending on its production method, vinegar can be classified as natural or synthetic. Synthetic vinegar is produced by diluting acetic acid derived from non-food raw materials and may contain harmful impurities, including aldehydes and traces of heavy metals. Natural vinegar is produced by a two-stage fermentation process and, in addition to acetic acid, contains other organic acids such as lactic, tartaric, malic, and citric acids, as well as vitamins B, C, and E. Among the non-volatile organic acids present in natural vinegar, lactic acid is the most abundant, being formed mainly during alcoholic fermentation. Counterfeit natural vinegar is typically produced by adding fruit juices, flavourings, or colourants to synthetic vinegar. Therefore, verifying the authenticity of vinegar by determining its organic acid composition, particularly lactic and acetic acids, is important. High-performance liquid chromatography (HPLC) is the most widely used method for determining organic acids in food products because of its high sensitivity, reproducibility, resolution, and short analysis time.

Methods

Identification and quantification of the studied organic acids was carried out by the HPLC method with a diode-array detector (DAD) on a C18 column.

Results

Using acetonitrile and 0.025 M sodium dihydrogen phosphate buffer (pH 3.0) in a 1:99 v/v ratio as the mobile phase provided optimal separation of lactic and acetic acids. The effects of mobile phase flow rate, column temperature, and detection wavelength were investigated. The analytical performance of the developed method was evaluated under the optimized chromatographic conditions. The detection limits for lactic and acetic acids were 0.09 and 0.6 mg/mL, respectively. The limits of quantification were 0.27 mg/mL for lactic acid and 1.8 mg/mL for acetic acid.

Conclusions

The developed HPLC method was successfully applied to the analysis of lactic and acetic acids in natural and table vinegar samples. The proposed HPLC method was validated and found to be suitable for distinguishing natural vinegar from synthetic vinegar based on organic acid composition.

Incorporation of Fabric Phase Sorptive Extraction Membranes onto a 3D-Printed Modified Drone Sampler for the Collection of Volatile Organic Compounds from Air Samples prior to GC-MS Analysis

Natalia MANOUSHI¹, Tobias SCHÜFTNER², Sebastian STEINER¹, Marco ANNERL^{1,3}, Abuzar KABIR⁴, Erwin ROSENBERG¹

¹*Vienna University of Technology, Institute of Chemical Technology and Analytics, Getreidemarkt 9/164, 1060 Vienna, Austria;*

²*Vienna University of Technology, Institute of Applied Physics, Vienna, Austria;*

³*Competence Center CHASE GmbH, Ghegastrasse 3, 1030 Vienna, Austria;*

⁴*Florida International University, Global Forensic and Justice Center (GFJC), Department of Chemistry and Biochemistry, Miami, FL, USA.*

natalia.manousi@tuwien.ac.at

Key Words: FPSE, VOCs, Air, Wildfires, Unmanned aerial vehicles.

Biomass burning can typically occur in wildfires or controlled burns of wildland and agricultural fuels and it can result in a large source of volatile organic compounds (VOCs). The main source of these VOC emissions can be attributed to the pyrolysis of wood polymers that form biomass including cellulose, hemicellulose, and lignin. These VOCs can exhibit certain toxicity and thus sampling during a wildfire can pose a threat to human health and their safety.

To overcome this limitation unmanned aerial vehicles or drones can be employed and combined with different sampling techniques for the collection of VOCs. In this work, fabric phase sorptive extraction (FPSE) was used for the first time for the sampling of VOCs released from wood pyrolysis. This technique utilizes permeable and flexible fabric substrates coated with a sol-gel organic-inorganic sorbent and it can be used for the sampling and sample preparation of different matrices.

For this purpose, a 3D-printed unit was developed and incorporated onto a drone to accommodate the sampling membranes. Afterwards, the main parameters affecting the performance of the FPSE sampling protocol were optimized. Accordingly, different desorption and sample introduction techniques were investigated, with solid-phase microextraction (SPME) being selected prior to analysis by gas chromatography mass-spectrometry (GC-MS).

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Simplified Determination of Traces of Explosives and their Degradation Products in Environmental Samples using Picric Acid as a Model

Anastasiia MOSENDZ, Veronika SKALOZUB, Maryna ZUI

*Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Street, 01601, Kyiv, Ukraine.
anastasiiamosendz@knu.ua*

Key Words: HPLC, SPE, Toxicants, Green chemistry, Extraction.

The determination of explosives is the priority of safety in most countries. Despite that, contamination of the territories and water by explosions often remains secondary problem. The removal of the immediate blast and other hazard will inevitably take priority over environmental considerations [1]. The analysis of the contaminated areas after the elimination of the hazard is important for the safety of life, ensuring the possibility of drinking water or growing crops. The simplification of the procedure and development of cheaper sensitive methods can lead to more thorough environmental control and more data being gathered about pollution.

The popular method of GC-MS, HPLC-MS require expensive equipment as well as the resources for each of analysis and high cost of maintaining the equipment. While HPLC-UV is not suitable for on-site analysis, it can provide more detailed, reliable information, while being more available and cost-effective compared to mass-spectroscopy. The effective sample preparation can ensure desired sensitivity and be designed for simple clean-up of various types of samples.

Due to safety and legal reasons, in this study the picric acid, also known as trinitrophenol – nitroaromatic semi-polar molecule – was used as model substance.

The method using SPE was developed, with the cartridge type being chosen between the common C18 sorbents by few different brands, and more suited for polar compounds C8 and HLB sorbents. The Oasis HLB cartridges shown the best results. This is consistent with the literature data about determination of explosives, focused on clean-up of motor oil-based samples [2]. As the samples were water based, the optimal pH level was chosen, and the addition of buffer solution was necessary. The optimal pH indicated if the ionised or molecular form is better absorbed, and the difference shows that acidity of sample may decrease the extraction.

The experiment showed that picric acid was not eluting with water or methanol, so these solvents are suited for washing cartridge before elution with acetonitrile. Volumes of samples and eluate were optimized to increase concentration efficient. The larger sample volumes can be used, in order to increase the preconcentration coefficient and decrease the fluctuation of results related to inhomogeneous sample. Meanwhile the elution is better with limited volume (2 mL of acetonitrile) as it is enough to elute most of the analyte and avoid unnecessary dilution.

Using Waters e2695/2998, HPLC was done in isocratic mode with 30% acetonitrile and 70% water at Kromasil C18 and Spherisorb Phenil columns, both giving the sufficient peak symmetry and the retention time around 2 min. The picric acid detection was done by PDA at 360 nm, and the 210-400 nm range was monitored for other possible compounds. The recovery was above 85%, allowing to reach the limit of quantification at 0.1 µg/L.

The standard addition method was used to validate the method of environmental samples' analysis. In addition, the use of in-lab-synthesized materials was considered with development of method based on SBSE (Stir Bar Sorptive Extraction), in search for the sample preparation requiring less complex equipment.

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LC–PDA–MS/MS Characterization of Phytochemical Changes in *Clitoria ternatea* L. Extract during Simulated Gastrointestinal Digestion

Ribi Ramadanti MULTISONA¹, Petr ČESLA², Barbora TOŠOVSKÁ²,
Michal KAŠPAR², Anna GRAMZA-MICHAŁOWSKA¹

¹Poznań University of Life Sciences, Faculty of Food Science and Nutrition, Department of Gastronomy Science and Functional Foods, Wojska Polskiego 31, 60-624 Poznań, Poland;

²University of Pardubice, Faculty of Chemical Technology, Department of Analytical Chemistry, Studentská 573, CZ-532 10 Pardubice, Czech Republic.
ribi.multisona@up.poznan.pl

Key Words: *Clitoria ternatea* L., LC–PDA–MS/MS, Phytochemical profiling, Simulated gastrointestinal digestion.

Clitoria ternatea L. flowers contain a diverse range of bioactive compounds, particularly ternatin anthocyanins and flavonoid glycosides [1], whose structural diversity presents analytical challenges for comprehensive characterization. While the phytochemical composition of *C. ternatea* has been extensively reported, limited information is available on changes in individual compounds during gastrointestinal digestion. This study aimed to characterize digestion-induced changes in the phytochemical profile of *C. ternatea* extract using liquid chromatography coupled with photodiode array detection and tandem mass spectrometry (LC–PDA–MS/MS).

An aqueous *C. ternatea* extract was subjected to sequential simulated gastrointestinal digestion comprising oral, gastric, and intestinal phases in a temperature-controlled glass bioreactor [2]. Samples collected before digestion and after each digestive stage were analysed using a reversed-phase LC–PDA–MS/MS method employing a diphenyl stationary phase and gradient elution [3] to separate structurally related anthocyanins and flavonoid glycosides. Tentative compound identification was achieved by integrating chromatographic retention behaviour, UV–Vis absorption spectra, molecular ions, and diagnostic MS/MS fragmentation patterns.

The analytical workflow enabled comprehensive phytochemical profiling throughout the digestion process. Ternatin-type anthocyanins and kaempferol derivatives were consistently detected in the undigested extract as well as after gastric and intestinal digestion. In contrast, quercetin derivatives were not detected in the undigested extract but became detectable following gastric digestion, where quercetin 3-(2G-rhamnosylrutinoside), quercetin 3-neohesperidoside, quercetin 3-rutinoside, and quercetin 3-glucoside were tentatively identified. Following intestinal digestion, only quercetin 3-(2G-rhamnosylrutinoside) remained detectable, demonstrating stage-dependent changes in the detectable flavonoid profile.

The developed LC–PDA–MS/MS workflow proved effective for resolving and characterizing structurally related phytochemicals in a complex plant matrix and enabled detailed monitoring of digestion-dependent compositional changes. These findings demonstrate the applicability of chromatographic profiling for investigating phytochemical stability and transformation during simulated gastrointestinal digestion and provide a foundation for future studies on the behaviour of plant-derived bioactive compounds.

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Polymer-Derived Micropollutants in Municipal Wastewater Treatment Plants

**Alina POHL, Malwina TYTŁA, Czesława ROSIK-DULEWSKA, Michał BODZEK,
Rajmund MICHALSKI**

*The Institute of Environmental Engineering of the Polish Academy of Sciences,
34 Skłodowskiej-Curie Street, 41-819 Zabrze, Poland.
alina.pohl@ipispan.edu.pl*

Key Words: Phthalates, Wastewater treatment plants, Mass balance.

Wastewater treatment plants (WWTPs) are an important component of the environmental cycle of micropollutants. Among substances present in wastewater and sewage sludge, increasing attention is being paid to compounds originating from plastics. These materials contain various additives, such as plasticizers, stabilizers, and flame retardants, which provide them with desired functional properties. However, some of these substances exhibit endocrine-disrupting properties, raising growing environmental concerns. The variable efficiency of micropollutant removal leads to their emission into surface waters with treated effluents or their accumulation in sewage sludge [1]. Therefore, understanding their fate and assessing their removal efficiency are essential for evaluating their environmental impact.

The aim of this study was to evaluate the mass balance of commonly used plasticizers—phthalates (PAEs)—in a municipal wastewater treatment plant. The concentrations of dimethyl phthalate (DMP), diethyl phthalate (DEP), diisobutyl phthalate (DiBP), dibutyl phthalate (DBP), benzyl butyl phthalate (BBP), bis(2-ethylhexyl) phthalate (DEHP), and di-n-octyl phthalate (DOP) were determined using gas chromatography coupled with mass spectrometry (GC-MS). Samples were collected during the summer season from a municipal wastewater treatment plant operating in a mechanical–biological–chemical system located in southern Poland.

The conducted mass balance showed that the average daily load of total phthalates entering the WWTPs was 634.1 g/d. Approximately 32.4% of the incoming load was discharged with treated wastewater, while 17.9% accumulated in sewage sludge. The largest contribution to this fraction was associated with more hydrophobic compounds, such as DEHP and BBP, which show a high affinity for the solid phase. The remaining portion, accounting for nearly 49.7% of the total load, may have undergone biodegradation and/or transformation during treatment processes. The highest contribution of these processes was observed for DMP and DEP, which according to literature data are more biodegradable due to their lower molecular weight and simpler chemical structure [2].

The results confirm that wastewater treatment plants constitute an important barrier by reducing the emission of phthalates into the aquatic environment, however, they do not ensure their complete removal.

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Analysis and Characterization of Acid-base Properties of Newly Synthesized Steroid Derivatives by Capillary Electrophoresis

Veronika ŠOLÍNOVÁ, Barbora SLAVÍKOVÁ, Eva KUDOVÁ, Václav KAŠIČKA

*Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences,
Flemingovo náměstí 542/2, 160 00 Praha 6, Czech Republic.
solinova@uochb.cas.cz*

Key Words: Acidity constant, Capillary electrophoresis, Neurosteroids, Electrophoretic mobility.

Neurosteroids (NSs) are naturally occurring steroid molecules synthesized in the brain from cholesterol. They rapidly modulate neuronal activity by interacting with receptor systems. Understanding their mechanisms of action is essential for the development of new therapies for neurological and psychiatric disorders, including Alzheimer's disease, epilepsy, and depression [1,2]. However, the molecular and physicochemical bases of their effects remain insufficiently understood. Recently, five new synthetic analogues of naturally occurring NSs have been prepared. Four of them contained an oxadiazole ring, in which protonation of a nitrogen atom leads to the formation of a stabilized cationic species through charge delocalization within the heterocyclic system. The fifth compound contained a carboxylic acid group that, upon deprotonation, forms a resonance-stabilized carboxylate anion. The aim of this study was to investigate the acid–base properties of these compounds using capillary electrophoresis (CE).

CE experiments were performed in an Agilent CE 7100 System analyzer (Agilent, Waldbronn, Germany). Analyses were carried out in a fused-silica capillary with an outer polyimide coating (ID/OD 50/375 μm ; total/effective length 420/335 mm) obtained from Polymicro Technologies. The analyzed compounds were dissolved in methanol, injected hydrodynamically at 30 mbar for 10 s, and detected using a UV–Vis spectrophotometric detector set at 200 nm.

Firstly, all compounds were analyzed by CE and their purity was verified. Secondly, the dependences of the effective electrophoretic mobilities of the analyzed compounds on pH were determined using a series of background electrolytes (BGEs) in the pH range 2.25–7.25, at a constant ionic strength of 25 mM and a constant temperature of 25°C. To accelerate the measurements, an external pressure of 30–50 mbar was applied. From these dependences, the mixed acidity constants, $pK_{a,\text{mix}}$, corresponding to the activity of hydroxonium cations (pH) and to the ionic strength of 25 mM, together with the actual ionic mobilities of the monovalent cationic and anionic forms of the analyzed compounds, were determined by nonlinear regression analysis of the experimental data. In a subsequent step, the mixed acidity constants, $pK_{a,\text{mix}}$, were recalculated to the thermodynamic acidity constants, $pK_{a,\text{th}}$, using the Debye–Hückel theory as described in [3]. The absolute values of the actual ionic mobilities were in the range $(22.7\text{--}30.7) \times 10^{-9} \text{ m}^2/\text{V/s}$ for all analyzed compounds. The obtained thermodynamic pK_a values for the basic oxadiazole group in four compounds ranged from 4.46 to 4.79, whereas the pK_a value for the acidic carboxyl group of the fifth compound was equal to 4.17. From these values, it follows that at physiological pH 7.0–7.5, the compounds containing the oxadiazole ring are predominantly uncharged, whereas the compound containing the carboxylic group is negatively charged.

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Negative Thermal Gradient Gas Chromatography using the Wavemaker Concept

Sebastian STEINER, Felix FRANK, Bernhard KLAMPFL, Erwin ROSENBERG

¹Institute of Chemical Technologies and Analytics, TU Wien, Vienna, Austria.
s.steiner@tuwien.ac.at

Key Words: Gas chromatography, Fast gas chromatography, Negative thermal gradient

Gas chromatography (GC) is a well-established separation technique whose fundamental operating principle has remained largely unchanged for decades. Conventional GC relies on oven-based heating of long columns at constant temperatures or using a temperature program to reduce the retention for less volatile analytes, reducing the total run time. However, even with a temperature program, run times can still lie upwards of 30 minutes. Another possible way of making the separation faster is the use of shorter columns, albeit, at the cost of reduced separation efficiency [1].

Going beyond conventional GC, a negative thermal gradient can be applied spatially, meaning analytes are injected at the hottest point of the column while moving into subsequently cooler regions during their separation. This introduces an additional peak sharpening effect, which makes it possible to combine the speed of fast GC approaches with the separation efficiency of conventional GC. In this work, we propose an innovative approach for chromatography by which a moving thermal gradient can be introduced by heating individual segments of the column. This enables the transport of the analytes on a thermal wave while separating the analytes based on their retention, improving separation speed by up to two orders of magnitude [2, 3].

All of this makes the application of a negative thermal gradient a promising new way of combining speed and resolution in gas chromatography. Based on this, the Wavemaker provides a practical implementation of this concept through dynamic, segment-wise heating, enabling controlled studies of NTGC (negative thermal gradient gas chromatography) that challenge classical scaling relationships in gas chromatography.

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Capillary Electrophoretic Determination of Acid-Base Properties of Photoresponsive Inhibitors of Poly(ADP-ribose) Polymerase 1

Sille ŠTĚPÁNOVÁ, Miroslav KAŠPAR, Kristýna JELÍNKOVÁ, Zlatko JANEBA, Václav KAŠIČKA

*Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences,
Flemingovo nám. 542/2, 160 00 Prague 6, Czechia.*

sille.stepanova@uochb.cas.cz

Key Words: Acidity constant, Capillary electrophoresis, Photoactive compounds.

Photopharmacology is a field that combines photochemistry and pharmacology, and uses light to control the biological activity of molecules. By activating a drug at a specific location or time, one can minimize off-target effects and increase the maximum deliverable dose. The aim of this study was to apply capillary electrophoresis (CE) for determination of the acidity constant (pK_a) of ionogenic pyrrolidine group of three potential photoresponsive inhibitors of poly(ADP-ribose) polymerase 1 (PARP1), a cancer-relevant target, to characterize their protonation states during switching experiments [1].

CE experiments were performed in ProteomeLab PA800 (Beckman-Coulter) using the internally uncoated fused silica capillary with the total/effective length of 40.5/30.1 cm, and the ID/OD of 50/375 μm . The analyzed compounds were partially soluble in methanol at concentrations of 0.16–0.25 mg/100 μL . They were introduced into the capillary hydrodynamically (13.8–20.7 mbar $\times$ 10–20 s, 5.1–15.4 nL injected), and detected by UV-absorption at 200 nm.

For the determination of acidity constants of studied compounds, their effective mobilities were measured in a series of aqueous background electrolytes within a pH range 1.71–5.74 at constant temperature (25°C) and constant ionic strength (25 mM). From the pH dependences of their effective mobilities, their mixed acidity constants (related to the activity of hydroxonium cations (pH) and 25 mM ionic strength) were determined by the non-linear regression analysis. Then, the mixed acidity constants were recalculated to the thermodynamic acidity constants employing the Debye-Hückel theory as described in [2].

CE data was used for the pK_a determinations with the assistance of two programs, commercial program Origin and freeware AnglerFish [3]. With the latter program, also the limiting ionic mobilities were determined, from which the hydrodynamic radii of analyzed compounds were calculated.

CE was demonstrated to be a suitable method for the investigation of acid-base properties even if very small amounts of analytes were available. Similar thermodynamic pK_a values for studied compounds were obtained by both programs, they were in the range of 3.78–4.31. The limiting mobilities of investigated compounds were in the range of $(18.5\text{--}21.8) \times 10^{-9} \text{ m}^2/\text{V/s}$ while the hydrodynamic radii between 0.44–0.52 nm.

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Passive Sampling for Ni Determination in Water Using PVC-based Polymer Inclusion Membrane

Marin ȘENILĂ, Simion Bogdan ANGYUS, Enikő Kovács,
Otto TODOR-BOIER, Lăcrimioara ȘENILĂ

INCDO-INOE Research Institute for Analytical Instrumentation, 67 Donath, 400293, Cluj-Napoca, Romania.
marin.senila@icia.ro

Key Words: Polymer inclusion membrane; Metal separation; Sample pretreatment; Passive sampling

Polymer inclusion membranes (PIMs) have emerged as an advanced membrane separation technology, particularly for metal ion separation [1]. Their high selectivity, cost-effectiveness, operational simplicity, and ability to combine extraction and stripping in a single step make them an attractive and sustainable alternative to conventional separation methods. Owing to their recyclability and versatility, PIMs have found broad applications in analytical chemistry, wastewater treatment, and metal recovery [2, 3].

Nickel is recognized as a potentially toxic element, even at low concentrations, highlighting the need for efficient removal technologies. In this study, a novel PIM incorporating 1-alkyltriazole as the carrier was developed for the selective extraction of Ni(II) ions from wastewater. The stability constants and partition coefficients of Ni(II)-alkyltriazole complexes were determined to evaluate the carrier–metal interactions. Membrane transport studies were performed to determine the initial fluxes, selectivity coefficients, and recovery factors for Ni(II), Pd(II), and Zn(II). Transport experiments employed a donor solution containing 5 mg/L Ni(II), with feed and receiving phase flow rates ranging from 1.5 to 3.5 cm³/min. The membrane performance was evaluated at 20 and 30°C.

The developed membrane exhibited excellent transport properties, achieving approximately 84% extraction of Ni(II) from the feed solution under the investigated conditions. These findings demonstrate that PIMs incorporating 1-alkyltriazole are effective and promising materials for the selective removal and recovery of Ni(II) ions from aqueous solutions.

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Long-Term Effects of Two Remediation Strategies on Soil Bacterial Communities: Contaminant Removal versus Ecological Approach

**Emanuela D. TIODAR¹, Cristina L. VĂCAR¹, Zoltan R. BALÁZS^{1,2},
Carmen A. ROBA³, Dorina PODAR^{1,2}**

*¹Babeş-Bolyai University, Centre for Systems Biology, Biodiversity and Bioresources (3B),
Cluj-Napoca, Romania;*

²Babeş-Bolyai University, Department of Molecular Biology and Biotechnology, Cluj-Napoca, Romania;

*³Babeş Bolyai University, Faculty of Environmental Sciences and Engineering, Cluj-Napoca, Romania.
dana.tiodar@ubbcluj.ro.*

Key Words: eDNA, Metals, Pollution, Remediation, Soil microbiota.

Soil contamination by heavy metals and polycyclic aromatic hydrocarbons (PAHs) poses persistent risks to ecosystem and human health, yet the long-term effectiveness of different remediation strategies in reducing contaminant pressure remains poorly characterized. This study compares two contrasting remediation approaches at contaminated sites, two decades after implementation, using soil microbial community profiling as a sensitive bio-indicator of residual contaminant impact and remediation success.

At the Homécourt site (France), a former coking plant had introduced PAHs alongside Cd and Hg into the soil. Remediation combined thermal desorption for contaminant elimination with pedological reconstruction and grassland establishment. At the Moldova Nouă site (Romania), decades of copper mining resulted in elevated soil Cu, Zn, Pb, and As. Here, removal of contaminants was not performed; remediation consisted of revegetation through perennial grassland and afforestation.

Soil bacterial diversity and community composition were characterized by environmental DNA (eDNA) metabarcoding, applied as an indirect diagnostic tool to assess residual contaminant impact on ecosystem recovery. Treated plots were compared to untreated contaminated - controls and unimpacted - reference soils, by evaluating both alpha and beta diversity

Results show divergent outcomes reflecting differences in contaminant removal versus containment. At Homécourt, thermal desorption yielded soils with significantly elevated bacterial richness relative to references, but community composition was clearly distinct, structured by nutrient and physical soil properties rather than by residual PAH signatures, indicating effective contaminant elimination but incomplete ecological equivalence. At Moldova Nouă, where metals were not removed, richness did not differ significantly across groups, treated communities resembled more closely the reference soil communities than at Homécourt, yet community structure continued to reflect a persistent metal contamination gradient, confirming incomplete remediation despite vegetation establishment.

These findings illustrate a key trade-off between remediation approaches: engineered, contaminant-removal strategies (e.g., thermal desorption) can effectively eliminate target pollutants but are costly, spatially limited, and may leave chemically "cleaned" soils supporting novel, non-analog biological communities. Nature-based, containment-oriented strategies leave residual contamination detectable through its ecological signature, but may better preserve natural recovery trajectories. Environmental DNA-based diversity metrics are proposed as a complementary, sensitive tool for evaluating long-term remediation performance along standard chemical monitoring.

Acknowledgements

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Optimization of Reagent Volumes for ICP-MS Trace Metal Analysis in Environmental Reference Materials

Cristina-Lorena VĂCAR¹, Dan-Constantin NIȚĂ², Dorina PODAR^{1,3}

¹Babeș-Bolyai University, Centre for Systems Biology, Biodiversity and Bioresources (3B),
3-5 Clinicilor St., 400015 Cluj-Napoca, Romania;

²Babeș-Bolyai University, Institute for Research, Development and Innovation in Applied Natural Sciences,
Cluj-Napoca, Romania;

³Babeș-Bolyai University, Department of Molecular Biology and Biotechnology,
1 Kogălniceanu Str., 400084 Cluj-Napoca, Romania.

cristina.vacar@ubbcluj.ro / dorina.podar@ubbcluj.ro

Key Words: Acid digestion, ICP-MS, Reference material, Trace metal extraction, Recovery efficiency.

Environmental sample analysis is critical for monitoring ecosystem health and assessing toxic or essential metal pollution pathways. This monitoring requires precise quantification, which depends on effective sample digestion prior to instrumental analysis. Sample mass is often limited and different matrices react uniquely. The aim was to evaluate the effect that different volume of reagents used for microwave digestion of various small mass matrices have on the elemental extraction efficiency.

Four certified reference materials, soil (ERM-CC141), root (IPE 143), leaves (NIST 1547), and mussel tissue (ERMCE278K), were digested using an Anton Paar Multiwave 5000 system. All samples were prepared and analyzed in duplicate. For the soil matrix, 0.1 g sample was treated with variable volumes of HCl (0.5, 1.0, or 1.5 mL, EMSURE grade, 37%) and brought to a final volume of 6 mL with HNO₃ (EMSURE grade, 65%), followed by a microwave program consisting of a 10-minute ramp to 180°C and a 30-minute hold. Conversely, biological matrices (0.2 g) were digested using 6 mL HNO₃ combined with variable volumes of H₂O₂ (1.0, 1.5, or 2.0 mL, Suprapur grade, 30%), utilizing a 20-minute microwave ramp to 180°C and a 15-minute hold. Target elements (Cr, Mn, Fe, Co, Ni, Cu, Zn, Cd, Pb) were subsequently quantified via ICP-MS QQQ (triple quadrupole inductively coupled plasma mass spectrometry, Agilent 8900).

Reagent volumes did not statistically alter elemental extraction efficiencies within any of the tested matrix. Pooled recoveries for Mn (106.9 ± 4.6%), Fe (106.7 ± 5.9%), Co (95.7 ± 5.4%), Cu (104.3 ± 5.2%), and Zn (106.4 ± 4.1%) demonstrated high accuracy and method reproducibility (mean ± SD, n = 12). In the soil matrix Cr recovery was suppressed (51.0 ± 0.9%, mean ± SD, n = 3), likely due to its trapping within acid-resistant silicate minerals. Conversely, Cr recovered efficiently in biological matrices (107.5 ± 9.2%, mean ± SD, n = 6). For the leaf matrix quantitative recoveries were achieved for Mn, Fe, Cu, and Zn (100.6%–110.2%), whereas Cd exhibited significant under-recovery down to 68.8%. An isolated Pb over-recovery spike of 139.0% was attributed to an accidental contamination event.

This optimization study demonstrates that using well homogenized low mass samples and minimum volumes of reagent successfully achieves optimum elemental recoveries across diverse matrices, confirming that minimal inputs of HCl and H₂O₂ are sufficient, though extraction efficiencies remain constrained by soil silicate mineral boundaries and biological tissue matrix effects.

Acknowledgements

The research is funded by the Horizon Europe project ARAGORN (Achieving Remediation and Governing Restoration of contaminated soils Now) under grant agreement 101112723.

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Beátrix-Aletta DEMJÉN – Deputy Managing Editor, MDPI Romania

Studied at the Faculty of Chemistry and Chemical Engineering at Babeş-Bolyai University in Cluj-Napoca, where she earned a Bachelor's degree in Chemical Engineering and completed a Master's degree in Advanced Chemistry.

Joined MDPI in December 2020 as an Assistant Editor. Throughout her career at the company, she has taken on progressively broader responsibilities, moving into the role of Section Managing Editor and developing extensive experience in editorial management, scientific publishing, and journal operations.

Since 2024, she has served as Deputy Managing Editor, supporting the development and management of several MDPI journals, including *Molecules*, *Colloids and Interfaces*, *Oxygen*, *Nitrogen*, *Purification*, and *JNT*.

Alexandra-Georgiana BAJDAN – Deputy Managing Editor at MDPI Romania

She completed her bachelor's degree in chemical engineering at the Faculty of Engineering in Foreign Languages, University Politehnica of Bucharest. She has a Master's Degree in Biomaterials for Tissue Engineering from the Faculty of Engineering in Foreign Languages, University Politehnica of Bucharest.

She has joined MDPI in 2020 as an Assistant Editor. In 2022, started working as a Deputy Managing Editor, focusing on building strong, trusting relationships with journal collaborators, handling external and ethical requests, and representing MDPI at events.

MDPI Academic Publishing Workshop – Artificial Intelligence in Publishing

Beátrix-Aletta DEMJÉN and Alexandra Georgiana BĂJDAN

*MDPI Open Access Romania, 77 Bulevardul 21 Decembrie 1989, 400604 Cluj-Napoca
demjen@mdpi.com ; bajdan@mdpi.com*

Key Words: Artificial intelligence, Open access publishing, AI in academic publishing, Academic publishing.

Throughout the years, artificial intelligence (AI) has gained terrain in all aspects related to our lives, including the publishing industry. People rapidly adapted to its usage as it is offering new possibilities for content creation, editing, translating or results presentation. As AI tools are introduced to various platforms and websites, even software that assists authors or editors it is important to raise a discussion on how and where it could be used and to establish some guidelines that ensure that the scientific accuracy is well maintained while technology is progressing. As the accessibility and usage of AI grew, this raises important questions on its ethical usage and impact on the publishing process.

The current work aims to provide an overview on different types of AI systems and how they are used in publishing, how various people implied in the publication process could use it effectively and problems that could arise from the involvement of generative AI.

We will also take a closer look to the ethical and scientific risks associated with the use of AI in publishing; The importance to check how AI companies use the data that is provided, content ownership aspects and data sharing possibilities and limitations. To be able to use AI responsibly we will discuss some of the journal's requirements and useful tips on how to disclose AI usage. Last, we will showcase how publishers are responding to the new challenges this technology is bringing in the current academic publishing landscape.

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Cezara POPA

Site Head STADA Romania

As a major pillar of Romania's pharmaceutical industry, STADA's site in Turda represents one of the largest foreign greenfield investments made in the country over the last 30 years. Representing a total investment of €70 million, including €21 million in state aid, the state-of-the-art facility currently employs over 400 people from Cluj, Alba, and Mureș counties.

The site houses 3 specialized labs for microbiology, physical-chemical testing, and quality control, with operations running across 12 advanced production lines supported by an automated warehouse. With an annual capacity of around 150 million medicine packages, STADA Turda ensures access to high-quality medicines for patients and partners in over 20 European countries.

Expanding Access to Healthcare: STADA Romania's Contribution through Generics, Specialty and Consumer Healthcare

Cezara POPA

STADA M&D SRL, 10 Trascăului Street, 401135 Turda, Cluj County, Romania
cezara.popa@stada.ro

Healthcare sustainability depends on broad patient access to safe, effective and affordable treatments. Guided by STADA's purpose, Caring for People's Health as a Trusted Partner, the presentation explores how STADA Romania improves access to healthcare through its Generics, Specialty and Consumer Healthcare portfolios.

It will also showcase the company's manufacturing footprint, highlighting the production site in Turda as well as the laboratories in Turda and Timișoara, which support quality and patient-focused healthcare solutions.



Improving Recovery and Reproducibility with Inert LC Column Hardware

Mihaela MUTZ

Laboratorium SRL, Strada Baia nr. 16, Sector 1, București, Romania
mihaela.mutz@laboratorium.ro

Key Words: Inert Column Hardware, Non-Specific Adsorption, MaxPeak Premier, Metal-Sensitive Analytes, Liquid Chromatography.

Non-specific adsorption of metal-sensitive analytes onto stainless-steel column hardware is a persistent source of poor recovery, reduced sensitivity and inconsistent reproducibility in liquid chromatography. This work evaluates an inert hardware platform (MaxPeak Premier, Waters Corporation) that introduces a hybrid organic/inorganic surface layer between the metal and the mobile phase, minimizing the electrostatic and chelation interactions responsible for these losses [1]. The same validated column chemistries used on conventional hardware (e.g., XBridge BEH C18) are retained, so no change in method development is required while the source of adsorption is addressed at the hardware level.

Two case studies illustrate the practical impact. Recovery of deferoxamine, a strongly iron-chelating drug, was substantially improved on inert hardware compared to standard stainless-steel columns [2].

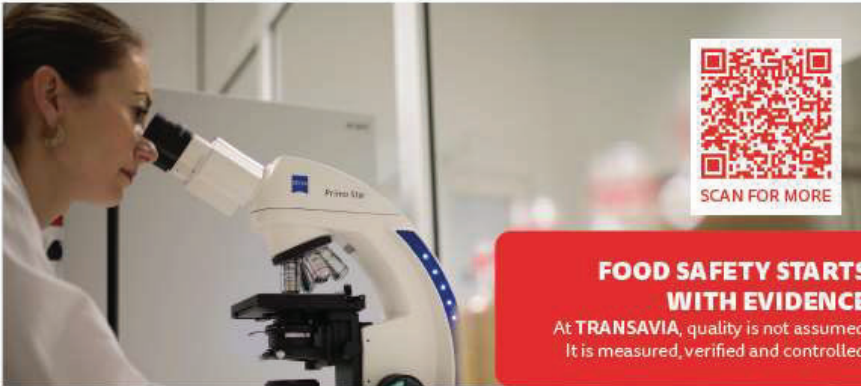
In a USP assay for acetaminophen in cough syrup, retention-time reproducibility improved from 1.59% RSD on stainless steel to 0.09% RSD on the inert platform. Comparable recovery gains were observed for AMPcP and adenosine phosphates under isocratic reversed-phase conditions.

The inert hardware is now available across a broad selectivity space, spanning hybrid and silica-based chemistries from HPLC to UHPLC particle sizes [3], indicating that hardware-level inertness offers a direct, broadly applicable solution for metal-sensitive analyses relevant to pharmaceutical, environmental, food and clinical laboratories.

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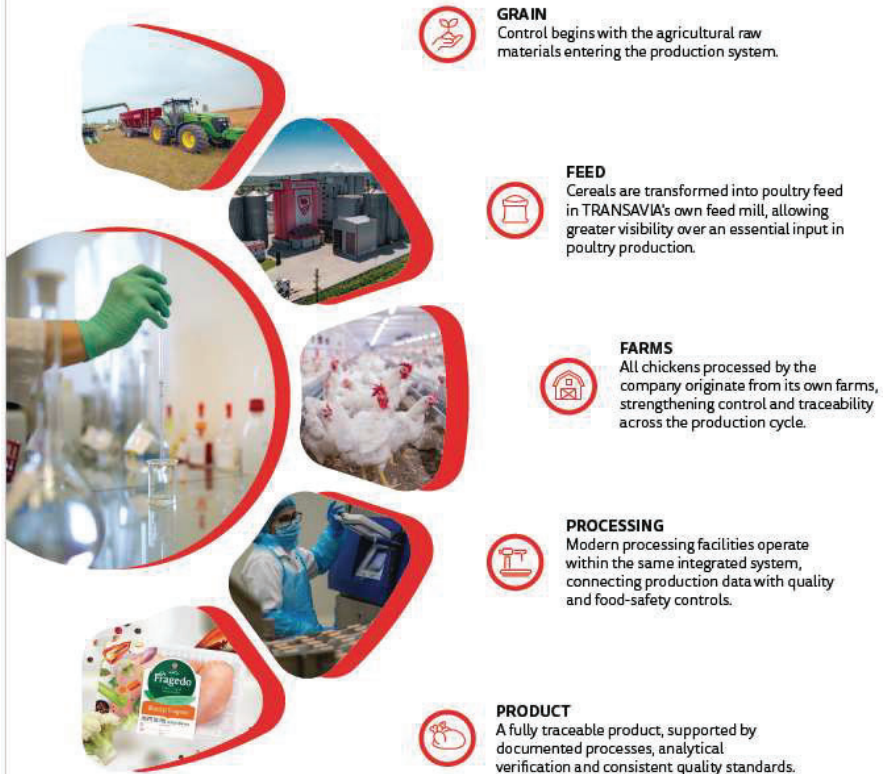
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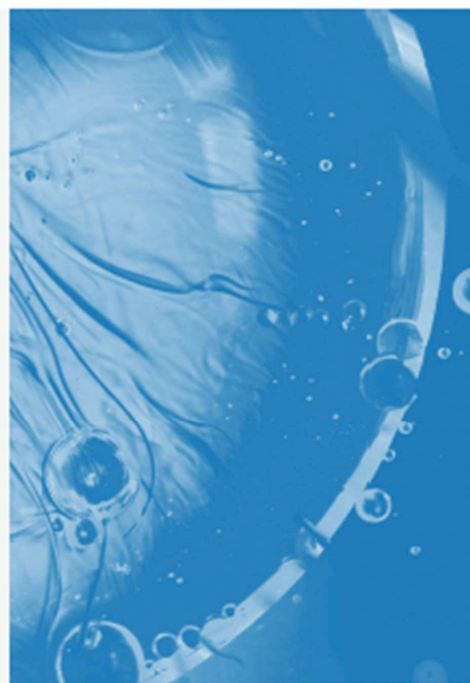


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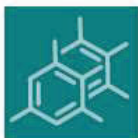
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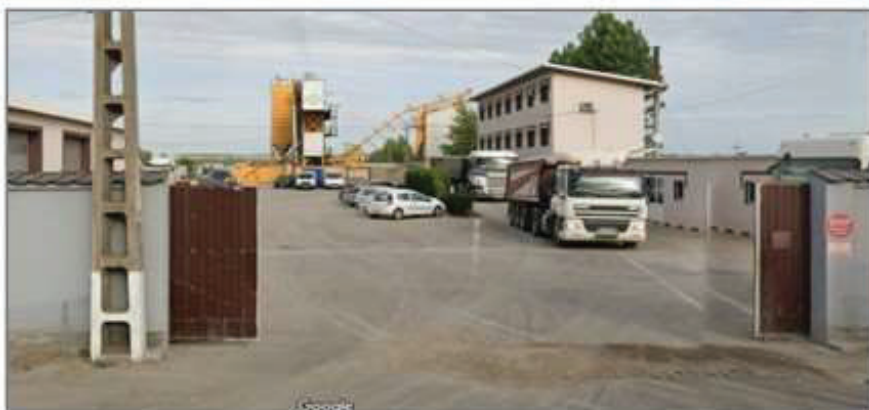
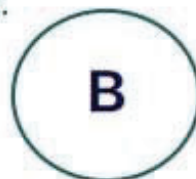
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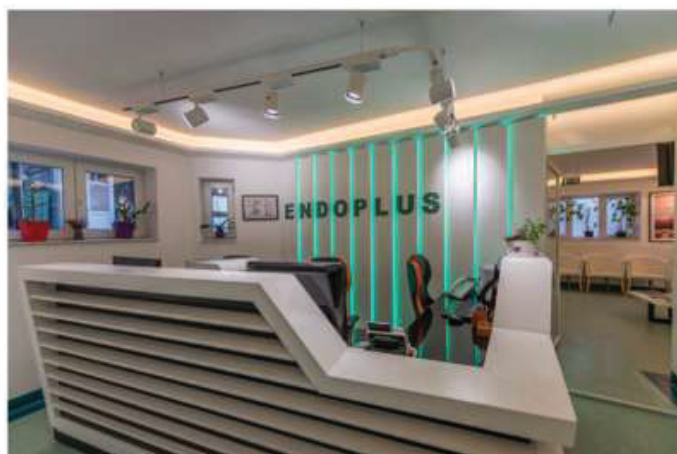
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brings together specialists from various fields related to urology — trained to the highest standards — to provide patients with comprehensive, personalized, & specialized services within a pleasant atmosphere defined by safety and responsibility.



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MOTTO:
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priority
—
Your
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TOPOLOVENI

The magiun factory in Topoloveni has a considerable history: it was established in 1914 and was the first factory of its kind in the country, known as the "Cooperative of Topoloveni" where magiun was produced from plums & other fruits.

After being taken over by the Sonimpex Serv Com trading company in 2001, the magiun factory was put back into operation under technological conditions adapted to international standards, which led to progress in product quality and national and international recognition of this quality.

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<https://www.magiun-sonimpex.ro>



TOPOLOVENI



- What does Topoloveni Plum Jam contain?
100% fruit, no added sugar, 0% chemicals.

It can also be consumed by people with diabetes, subject to the approval of their attending physician, according to the study conducted at the National Institute of Diabetes, Nutrition and Metabolic Diseases "Prof. Dr. N.C. Paulescu".



- How do I identify genuine Topoloveni products?

Each Topoloveni jar bears a mark that represents a guarantee of quality: the logo of Supplier of the Royal House of Romania. It is one of the surest ways to distinguish our products from other products in supermarkets that have "Topoloveni" in the name.



Topoloveni Rose Petal Jam, with no added sugar, is a natural delight, like a secret garden full of roses ...



Customer relations:

Mobile: (+4)0731.144.109

<https://www.magiun-sonimpex.ro>

E-mail: comenzi@magiun-sonimpex.ro

Pharmacy Museum – integral part
National Museum of Transylvania
History muzeul
farmaciei



The Pharmacy Museum, a true treasure of the history of medicine and pharmacy, was reopened in 2025 following a period of renovation & expansion (2018-2023). It shows the story of the evolution of pharmacy and medicine in Transylvania. The museum building, one of the city's jewels, is a historical and architectural monument built in the 16th century. It housed Cluj's oldest pharmacy open to the public, named *At Saint George's*, documented as early as 1573.



Hintz House



Established in 1954, the Pharmacy Museum was subsequently designated as the History Collection of Pharmacy. It originated from a donation of Transylvanian pharmaceutical artifacts by Professor Gyula Orient (1869-1940) and was later enriched by other valuable donations illustrating pharmaceutical activity in Transylvania of the 16th–19th centuries.

Hintz House, named after its last owner, shows inside pharmaceutical furnishings dating back to the 18th century – unique pieces in Romania. The ground floor houses the premises of the old pharmacy (1750 to 1949). The building preserves the traditional pharmacy layout: *officina* (sales area), *materialis camera* (storing raw materials), *laboratory*, *cellar*, *pharmacist's office*, *attic* (drying medicinal plants), *roof-mounted pulley* (hoisting plants up to the attic).

<https://muzeulfarmaciei.mnit.ro>

— MISSION of PHARMACY MUSEUM —

- ◆ to present & research attitudes towards health, illness and the body in Transylvania over time, focusing on hygiene importance & disease prevention
- ◆ to preserve & valorize a specialized & rare heritage collection of over 7000 items of the history of pharmacy & over 200 pieces of old medical equipment.





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<https://chem.ubbcluj.ro/~studiachemia/>

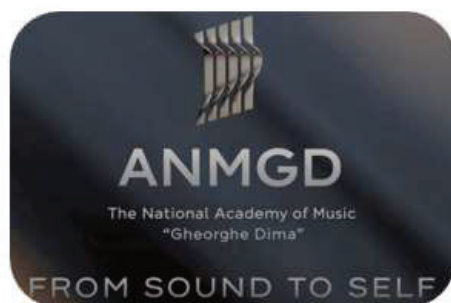
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<https://anmgd.ro/en>

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