IMA-2023

Chania, Crete | September 17-20, 2023

13th International Conference on

Instrumental Methods of Analysis

Modern Trends and Applications

ABSTRACT BOOK

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WELCOME

IMA conferences constitute leading events for analytical chemists and researchers dealing with all applications of instrumental methods of chemical analysis. The series started in 1999 by Laboratory of Inorganic and Analytical Chemistry of the National Technical University of Athens by Professor Maria Ochsenkühn- Petropoulou and it has been biannually organized in Greece, becoming a unique medium for scientists from all over the world to discuss the current developments in the field of Analytical Chemistry, to reflect on new progress and look forward future challenges, as well as to meet, network and forge new scientific interactions.

After the last IMA 2021 which was held as a virtual platform due to the COVID-19 pandemic, IMA conference returns in the traditional fully in-person event. In its 13th part, this cutting-edge international research meeting is hosted on the island of Crete, in Chania, one of the most attractive travel destinations in Greece. IMA 2023 is organized by the Laboratory of Inorganic and Analytical Chemistry, School of Chemical Engineering of the National Technical University of Athens and the Laboratory of Analytical and Environmental Chemistry, School of Mineral Resources Engineering of Technical University of Crete.

The scientific program consists of 11 invited and plenary lectures of leading researchers/ world-renowned experts as well as more than 60 oral presentations and more than 75 poster presentations, covering a wide range of scientific disciplines (environment, food, pharmaceuticals, diagnostics, forensics, archaeometry). In order to encourage scientific exchange and friendship building, we also included a rich social program, including a welcome cocktail, a traditional dinner as well as excursions. The venue of IMA 2023 is one of the well-known five stars hotel, the Minoa Palace Resort Hotel, an excellent host for scientific meetings, conferences, workshops, exhibitions, providing state of the art facilities and the latest audiovisual equipment. Besides the scientific aspects of the scientific program of IMA 2023, you will have a chance to appreciate and explore the exquisite Cretan beaches, to wander around the streets of old town of Chania and its Venetian harbour, to admire well-preserved historical monuments, to cross enchanting gorges, to visit picturesque villages and to taste the so-called Cretan cuisine.

We are very grateful to all members of the organizing committee and International Scientific Advisory Board as well as to “Diazoma Conference and Events” office for all their contributions and hard work for the professional organization of IMA 2023 conference. We are also thankful to our sponsors and exhibitor companies for their support of this meeting.

We strongly believe that you will find IMA 2023 conference a brilliant platform to establish international communications in academic research in Analytical Chemistry as well as to discover and enjoy the treasures of Chania.

Welcome to Chania! Welcome to the IMA 2023 conference!

Assist. Prof. Fotios Tsopelas	**Prof. Maria Ochsenkühn- Petropoulou**	**Prof. Nikolaos Kallithrakas- Kontos**
Laboratory of Inorganic and Analytical Chemistry School of Chemical Engineering National Technical University of Athens	Laboratory of Inorganic and Analytical Chemistry School of Chemical Engineering National Technical University of Athens	Laboratory of Analytical and Environmental Chemistry School of Mineral Resources Engineering Technical University of Crete

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SCIENTIFIC INFORMATION

Topics

Some of the general themes to be covered at IMA-2023 include current trends, developments and applications in:

ANALYTICAL METHODS

- Spectrometric techniques- Mass spectrometry
- Chromatographic and electrophoretic techniques
- Speciation analysis
- Electroanalytical Techniques
- Sensors and Biosensors
- Miniaturized analytical systems (Lab-on-a-Chip)
- Field analysis-Mobile analytical instruments
- Micro- and Nano- fluidics- Paper-based devices
- Thermal analysis
- Sample handling and preparation
- Big analytical data- Chemometrics
- Recent developments on industrial analytical instruments

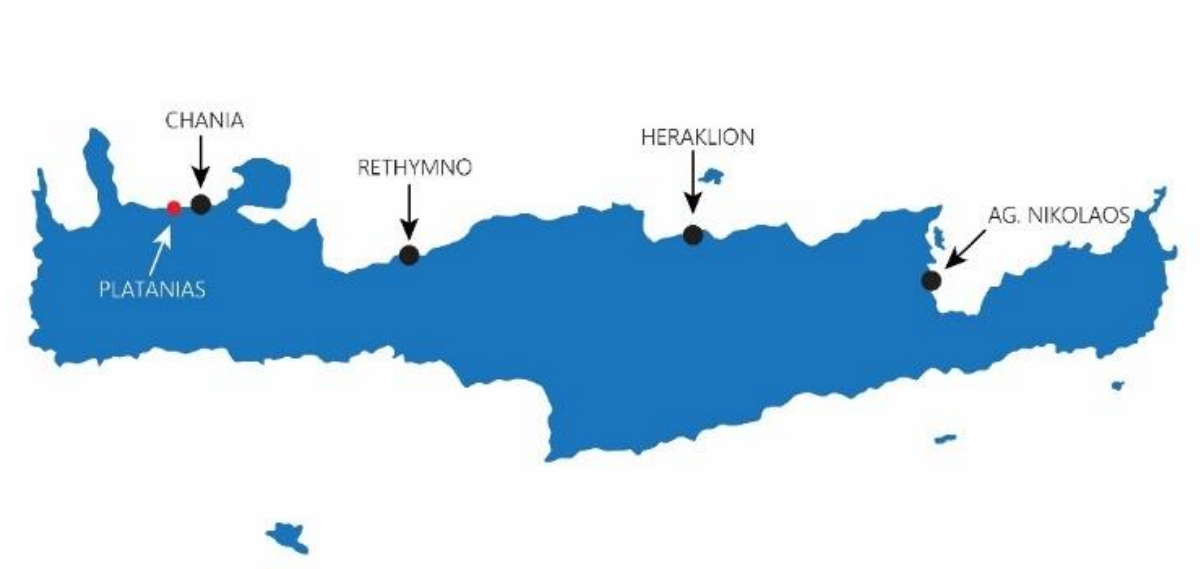
APPLICATIONS

- Environmental Analysis- Ecotoxicology
- Food Analysis
- Pharmaceutical Analysis- Drug Design
- Diagnostics- Point of care systems
- Biomedical and Clinical analysis
- Forensic Science
- Proteomics, Metabolomics, Metallomics
- Archaeometry
- Materials Analysis (e.g. thin layer characterization)
- Quality control-quality assurance in analysis
- Metrology
- Other hot topics (e.g. COVID-19 monitoring)

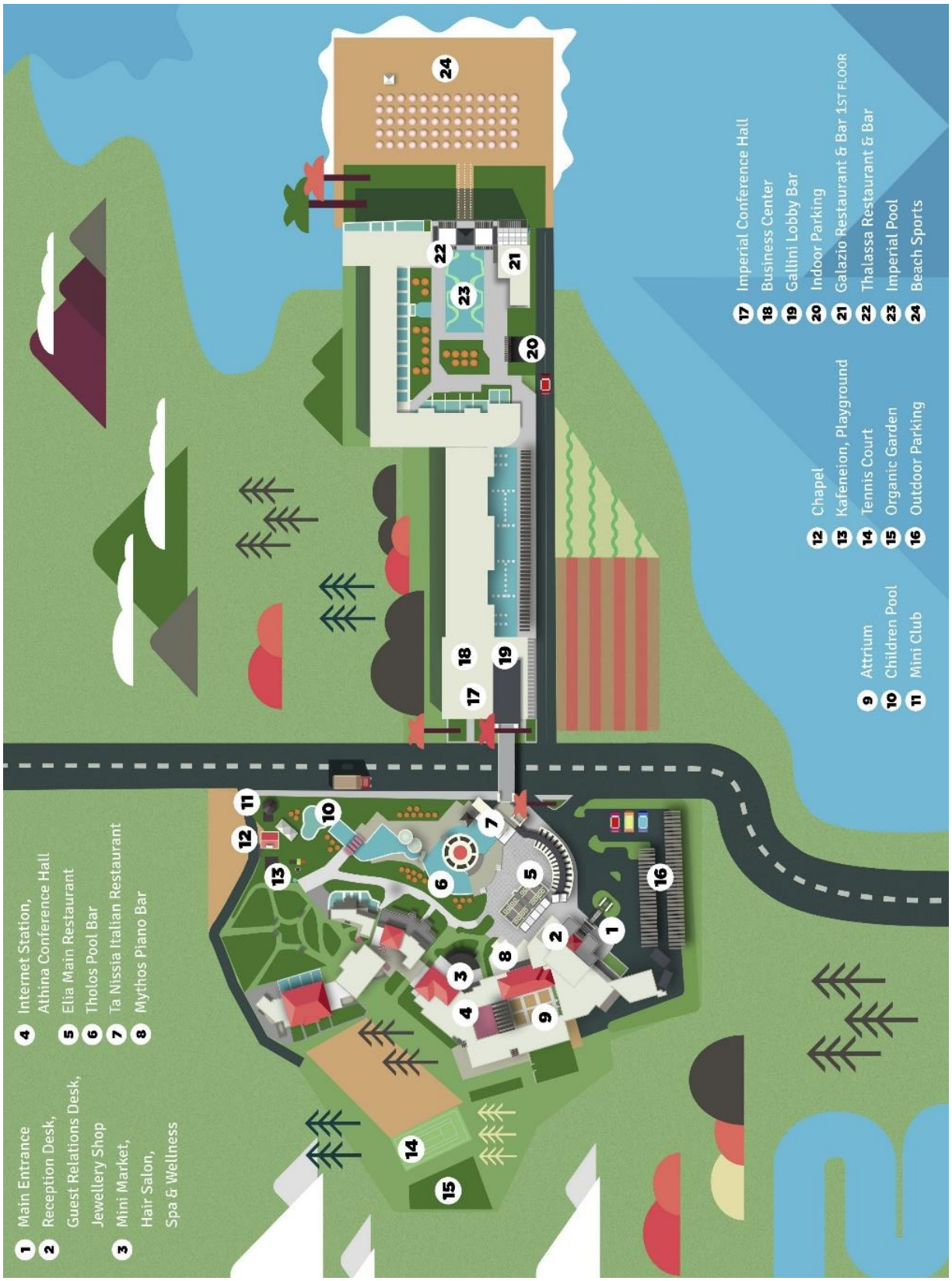
GENERAL INFORMATION

Venue

The conference will be hosted in ***Minoa Palace Resort Hotel***, a luxury 5* beach-side hotel located at the cosmopolitan area of Platanias, 12km west of the picturesque town of Chania and 30min drive from Chania International Airport. Minoa welcomes you to experience the pleasures of indulgence in the most enchanting of settings overlooking the endless azure of the Aegean. The Resort's Congress Hall is a great host for all sorts of corporate events, conferences, workshops & exhibitions, offering flexibility and functionality, as well as state of the art facilities and the latest audiovisual equipment.



Venue map



For more information about the Venue please visit the website: minoapalace.gr

Minoa Palace Resort Hotel
Platanias, Chania, Crete, Greece, 73014 Tel. +30 28210 36500
Email: info@minoapalace.gr

The closest to the conference venue airport is *Chania international airport*. (Please note that Heraklion airport, which is the largest airport in Crete, is more than two hours away from the hotel venue and without any direct and easy or cheap connection with the conference venue.)

How to get to the Venue

Arriving by plane

The **conference venue** is located at **Platanias/Chania, Crete**. During September, Chania is directly connected to several European cities by charter/seasonal flights. Information on destinations can be found in the official website of Chania Airport. Additionally, regular flights from/to Athens International Airport exist daily. You are strongly advised to choose a flight to Chania International Airport. Alternatively, one can land to Heraklion International Airport and reach Chania by bus or car. The driving distance between Heraklion and Chania is 142km.

Arriving by ship

The city of Chania is connected to Piraeus (Athens) daily. The port is in Souda, 7km away from the city center and 21 km away from the Conference Venue (about 20 min driving). You may consult the timetables or book your boat tickets here and here. Information regarding the public bus that connects Souda to Chania city center can be found here.

Bus services

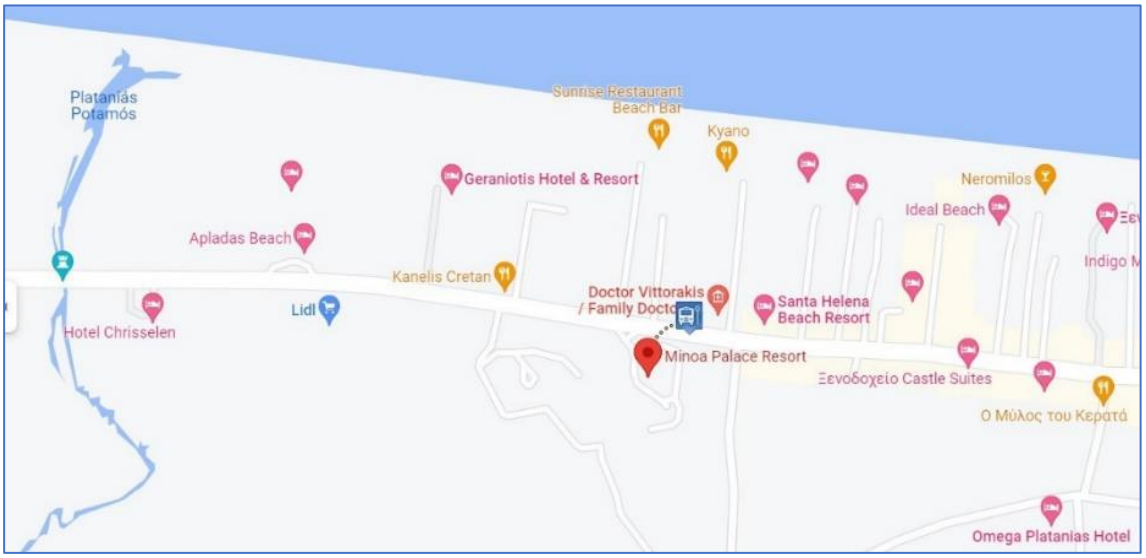
Chania airport → Chania city (Bus station)

Chania airport is located 14km from the city center, and 33.2 km away from the Conference Venue (30-40 min driving). A public bus connects the airport to the city center on a regular basis (line Chania Airport – Chania). The route lasts for 30 minutes approximately, and costs 2.30 €. You may consult the timetables or buy your tickets here

Chania city (Bus station) → Platanias (bus stop MINOA PALACE)

From Chania Bus station there are enough ***routes*** you could get to ***arrive to the Minoa Palace Resort Hotel***. For your convenience we collected here all those routes:

1.**CHANIA-KASTELI**
2.**CHANIA-KOLIMPARI**
3.**CHANIA-PLATANIAS-GERANI**
4.**CHANIA-ZYMVRAGOU**
5.**CHANIA-DELIANA**
6.**CHANIA-RODOPOU**
7.**CHANIA-VOUKOLIES**
8.**CHANIA-PALAIA ROUMATA**
9.**CHANIA-ELAFONISI**
10.**CHANIA-KASTELI-FALASARNA**
11.**CHANIA-PALAIOCHORA**



Taxi services

Moving by taxi is quite common in Crete and prior booking is not required. You may find relevant information and indicative prices in several websites (taxi4crete.gr/taxi-prices-from-chania-airport.html, www.chaniataxi.gr/en/)

The cost of transfer by taxi is approximately the following:

Chania Airport – Chania City Center ~ 25 €

Chania Airport – Conference Venue ~ 48 €

Chania City Center – Conference Venue ~ 20 €

Crete

Crete is the largest island in Greece and the fifth largest in the Mediterranean. It is endowed with an exquisite 1,000-kilometer-long coastline dotted with numerous coves, bays and peninsulas, which afford a multitude of soft, sandy beaches along the infinite blue of the Mediterranean Sea. The island is proud for its longstanding history, spanning from the Minoan civilization (3000 B.C.) until today. Crete welcomes you with its smiling Cretan sun, the sounds of the Cretan lyre, the scents of orange blossom and jasmine, a slice of cool red watermelon and a glass of iced "raki".

Some important archaeological sites of Crete:

The Palace of Knossos

According to tradition, it was the seat of King Minos and the capital of his state. The palace of Knossos is associated with the exciting myths "the Labyrinth and the Minotaur" and "Daedalus and Icarus". References to Knossos, its palace and Minos are made by Homer (the list of ships in Ilias mentions that Crete sent 80 ship under the command of the King of Knossos, Idomeneus, the Odyssey, T 178-9), Thucydides (reference to Minos), Isiodus and Herodotus, Bacchylides and Pindarus, Plutarchus and Diodorus the Sicilian. The city flourished in the Minoan Times (2000 – 1350 B.C.), when it was the most important and populated centre of Crete. It also played an important role and was particularly prosperous in later periods, like the Hellenistic Times. The city of Knossos was constantly populated from the end of the 7th millennium to the Roman Times. In the Neolithic Times there was a stage of technologically developed agricultural life (stone tools and weaving weights). The residents turned from food-collectors into producers (farmers and shepherds) and a there was a trend towards more systematic and permanent settlement. The settlement periods in Knossos succeeded each other and the population of the settlement at the end of the Late Neolithic Period is estimated at 1.000 – 2.000 residents.

The Palace of Phaistos

Phaistos is built on a low hill (altitude of about 100m from sea level), in the south of river Geropotamos (ancient river Lithaios), and dominates the fertile valley of Kato Mesara, which is surrounded by imposing mountains (Psiloritis, Asterousia, Lasithi Mountains). The Libyan Sea extends in the south. Lithaios surrounds the hill of Phaistos in the east and the north and was a source of water supply for the city. The mild and warm climate of the area made the life of its residents comfortable and pleasant. Phaistos was one of the most important centres of the Minoan civilization, and the most wealthy and powerful city of southern Crete. It is mentioned in the texts of ancient writers (Diodorus, Stravon, Pausanius) and Homer. It is one of the three important cities founded in Crete by Minos. According to mythology, the dynasty of Rodamanthus, the son of Zeus and brother of Minos, reigned in it. Homer refers to its participation in the Trojan War and describes it as a "well populated" city. The period of prosperity in Phaistos began with the coming of the Bronze Age in Crete in the middle of the 3rd millennium B.C., when the

foundations of the Minoan civilization were laid. Habitation in Phaistos started in the Neolithic period, as revealed by the foundations of Neolithic houses, tools, statuettes and potsherds discovered under the palace during the excavations. The Neolithic settlement is believed to have covered the top of the hill and its southwestern slope. In the middle of the 3rd millennium B.C. the use of metals began, which favoured the development of the city.

The main cities of Crete

The major cities of Crete (Chania, Rethymno, Heraklion, Agios Nikolaos) were once strategically placed on specific coastal locations of the island to defend against invaders. With a history that starts in prehistoric times and harbours that have always connected the island with other ports of the Mediterranean, the Cretan cities today are modern urban centres that have kept the historical identity of the island alive after countless conquerors have called it their own. In the Middle Ages, the island of Crete passed from the Byzantines to the Arabs, back to the Byzantines and then to Venetians; each one introducing different architectural and cultural elements. Every summer, Crete welcomes thousands of visitors that wish to explore the cities, charming harbours and cultural attractions that seem to be present on every corner.

Chania

In Chania city center one can enjoy the picturesque old harbour, walk around the old town alleys, and enjoy delicious local food in the numerous small restaurants.

Also, there are plenty of option for excursions to Chania region. You could enjoy exotic beaches, like the beach of Balos, which is ranked 35th among the 100 World's best beaches. The Falassarna beach and the Elafonisi peninsula also attract millions of sea-lovers each year.

Less than 1 hour driving from Chania is the famous Samaria gorge, which is the second touristic attraction of Crete (after Knossos Minoan Palace). There are busses every day that can take you from Chania to Samaria gorge.

Discover Crete through the following websites:

incrediblecrete.gr/en/
cretanbeaches.com/en/
youtube.com/watch

SOCIAL EVENTS
(Thursday 21st of September 2023)

Tour to Rethymnon and the Monastery of Arkadi (all day tour)

This tour starts from the Conference Venue Minoa Palace Hotel. At first a visit to the historic Monastery of Arkadi, built in 1587, which is located 23 km east from Rethymno and 80 km east of Chania. Following Arkadi, we will visit the town of Rethymno and enjoy a walk on the picturesque Port, the Venetian Fortress and the narrow winding streets of the old town, which reveal the city's turbulent history. We will be back at the Venue in the evening.

The excursion per person fee of 40.00 euros includes transfers to/from Arkadi Historic Monastery and Rethymno Town with luxury a/c coach, one professional official English-speaking guide per coach and the entrance fee at the monastery and its museum.

Hiking in Imbros Gorge and to Frangokastelo (all day tour)

We depart from the Conference Venue Minoa Palace Hotel. Imbros Gorge is located in the province of Sfakia, south of Chania, and is the third most visited gorge in Crete. It belongs to the E4 European hiking path. The scenery is beautiful, and the low difficulty makes the descent of Imbros ideal for non-experienced hikers. The length of the gorge is 11 km and the course lasts 2-3 hours. After a break to Komitades, the village at the end of the gorge, we will visit Frangokastello, one of the most famous beaches of West Crete, due to the historical Venetian castle on the beautiful beach and the legend of Drosoulites ghosts. It is located 13km east of Hora Sfakion, 80km southeast of Chania, in a small valley south of the White Mountains massif. The main beach of Frangokastelo is truly magnificent, with sand and shallow turquoise waters, ideal for children and families. It is well organized and is quite busy in peak summer months. We will be back at the Venue in the evening.

Light clothing and good walking shoes are important.

The excursion per person fee of 35.00 euros includes transfers to/from Imbros Gorge and Frangokastelo with luxury a/c coach, one professional English-speaking escort per coach and the entrance fee for the gorge.

Visit to the Cave of Agia Sofia and swimming at Elafonissi (all day tour)

We depart from the Conference Venue Minoa Palace Hotel. The Cave is located 47km southwest of Chania, on the western walls of the gorge Topolia, near the main road to Elafonisi. On the left of the cave entrance, there is the small church dedicated to Agia Sophia (Wisdom of God). The entrance of the cave has a width of 25m, while the height reaches 20m in many points, being really huge. The cave has two rooms with different heights, the surface of which is full of stalagmites. The cave was a very important place of worship in the ancient times. In the cave, a clay figurine dating from the 4th century BC has been found. Moreover, Neolithic, Early Minoan, Late Minoan, Classical, Hellenistic and Roman pottery traces have been found. Elafonisi is located 76km west of Chania and 5km south of Chrysoskalitisa Monastery, in the south westernmost tip of Crete. Elafonisi is an oblong peninsula, which often breaks in two parts by water giving the impression of being a separate island. It is a Natura 2000 protected area. The endangered loggerhead sea turtle and several rarer animals and plants find shelter on the island; it is strictly forbidden to remove any plants, animals, shells and sand from the area. The excursion per person fee of 35.00 euros includes transfers with luxury a/c coach and one professional English-speaking escort per coach.

USEFUL CONTACTS

Minoa Palace (VENUE)	0030-2821036500
Chania Bus Station	0030-2821093052
Taxi Chania	0030-2821098700
General Hospital Chania	0030-2821342000
Medical Center- Vittorakis Polyclinic	0030-2821060606
1st Fire Department of Chania	0030-2821079340, 0030-2821063688
Chania Police Station	0030-2821025854

Conference Secretariat
"**Diazoma Conference & Events**"
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13th International Conference on Instrumental Methods of Analysis: Modern Trends and Applications

www.ima2023.gr

Chania, Crete, Greece, 17-20/09/2023

PROGRAM TABLE

Sunday 17th of September 2023

16:00-17:30	*Imperial Hall* *Foyer* **Registration**
17:30-18:30	*Imperial Hall* *Room 1* **Opening Ceremony** (Chairs: F. Tsopelas, M. Ochsenkuehn, N. Kallithrakas)
18:30-19:10	*Imperial Hall Room 1* **Honorary Speaker – Oral Presentation** **G. Hieftje** *Professor, Indiana University* Advanced Spectroscopic Techniques: Origins and Future (Chairs: F. Tsopelas, M. Ochsenkuehn, N. Kallithrakas)
19:10-19:40	*Imperial Hall Room 1* **Invited Oral Presentation 1** **H. Frank** *Prof. Dr., University Bayreuth* Are per- and polyfluoroalkyl substances (PFAS) eternal? (Chairs: F. Tsopelas, M. Ochsenkuehn, N. Kallithrakas)
19:40-20:10	*Imperial Hall Room 1* **Invited Oral Presentation 2** **N. Thomaidis** *Professor, National and Kapodistrian University of Athens* Wastewater surveillance for public health using advanced analytical approaches (Chairs: F. Tsopelas, M. Ochsenkuehn, N. Kallithrakas)
20:30	*Thalassa Restaurant* **Welcome Reception**

Monday 18th of September 2023

09:00-09:30	*Imperial Hall Room 1* **Invited Oral Presentation 3** **S. Pissadakis** *Dr., Foundation for Research and Technology Hellas* Optical fiber chemosensors for trace detection in the gas and liquid phase (Chair: N. Kallithrakas)
09:30-10:45	*Imperial Hall Room 1* **Sensors and Biosensors** *(Various applications except life sciences)* (Chairs: S. Pissadakis, N. Kallithrakas) **OP 1: Dipstick coated with polystyrene-silica core-shell particles for the detection of microbiological fuel contamination** J. Bell, E. Climent, R. Gotor, C. Tobias, P.M. Martin-Sanchez and K. Rurack *Bundesanstalt für Materialforschung und prüfung (BAM)* **OP 2: Fluorescence detection of perfluoroalkyl carboxylic acids with a miniaturised assay** Y. Sun, V. Pérez-Padilla, V. Valderrey, J. Bell, K. Gawlitza and K. Rurack *Bundesanstalt für Materialforschung und prüfung (BAM)* **OP 3: Fabrication of graphene-based Inkjet printed subzero temperature sensor for cold storage monitoring** S. Soni, P. Sathe and D. Gupta *Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology* **OP 4: A home-made 3D printer-based dispensing system for the construction of lateral flow biosensors** P. M. Kalligosfyri[1], S. S. Tragoulias[1], P. Tsikas[1], E. Lamprou[1], T. K. Christopoulos[1,2] and D. P. Kalogianni[1] *[1] Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras* *[2] Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE)* **OP 5: Dipstick-type DNA sensing devices for rapid identification of olive oil cultivar origin** N-M. Christopoulou[1], E. Figgou[2], P. Kalaitzis[2], D. P. Kalogianni[1] and T. K. Christopoulos[1,3] *[1] Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras* *[2] Department of Horticultural Genetics and Biotechnology, Mediterranean Agronomic Institute, Chania* *[3] Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas*
10:45-11:15	**Coffee Break**

11:15-11:45	*Imperial Hall Room 1* **Invited Oral Presentation 4** **A. Escarpa** *Professor, University of Alcala* On-the-fly aptassays for neonatal sepsis diagnosis (Chair: M. Prodromidis)
11:45-12:15	*Imperial Hall Room 1* **Invited Oral Presentation 5** **M. Prodromidis** *Professor, University of Ioannina* Wax screen-printed fabric-based colorimetric microfluidic wearable (bio)sensors for the determination of biomarkers in sweat (Chair: A. Escarpa)
12:15-13:15	*Imperial Hall Room 1* **Sensors and Biosensors: Life Sciences/ Point of care systems** (Chairs: M. Prodromidis, A. Escarpa) **OP 6: Atrazine microfluidic biphasic colorimetric sensor based on barbiturate derivatives microcrystals dislocation** H. L. Nguyen[1], Ch. Rémy[1], S. Le Luyer[1], J. P. Lefévre[1,2], C. Allain[1], I. Leray[1] and C. Mongin[1] *[1] Université Paris-Saclay, ENS Paris-Saclay, CNRS, PPSM* *[2] Conservatoire National des Arts et Métiers* **OP 7: Detection of microRNAs in urine samples by a visual lateral flow assay** E. Lamprou[1], M. Sotiriou[1], P. M. Kalligosfyri[1], D. P. Kalogianni[1] and T. K. Christopoulos[1,2] *[1] Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras* *[2] Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE)* **OP 8: A molecular rapid test for SARS-CoV-2 quantitative detection** P. Maglaras[1], I. Lilis[2,3], F. Paliogianni[3] , V. Bravou[4] and D. P. Kalogianni[1] *[1] Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras* *[2] Department of Physiology, Faculty of Medicine, University of Patras* *[3] Department of Microbiology, Medical School, University of Patras* *[4] Department of Anatomy-Histology-Embryology, Medical School, University of Patras* **OP 9: Multifold improvement of the detectability of lateral flow immunoassays via macromolecular crowding** N-M. Christopoulou, D. P. Kalogianni and T. K. Christopoulos *Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras*
13:30-14:30	**Lunch**
14:30-15:30	*Imperial Hall Room 3* **Poster Session 1** *(See pages 27-32)*

15:30-16:00	*Imperial Hall Room 1* **Invited Oral Presentation 6** **K. Valko** *Professor, Bio-Mimetic Chromatography Ltd* Biomimetic HPLC Measurements of Physicochemical Properties of Compounds to Predict in vivo Distribution and Toxicity (Chair: F. Tsopelas)
16:00-17:30	*Imperial Hall Room 1* **Chromatography: Applications to life sciences and toxicology** (Chairs: K. Valko, F. Tsopelas) **OP 10: UHPLC-FLD/PDA/MS/MS determination of new blood and urinary prognostic biomarkers in hospitalized patients with delta and omicron variant SARS-CoV-2 infection** L. Kujovská Krčmová[1,2], K. Matoušová[1], P. Šmahel[3], M. Skála[4], M. Gančarčíková[1] and B. Melichar[5] *[1] Department of Clinical Biochemistry and Diagnostics, University Hospital Hradec Králové* *[2] Department of Analytical Chemistry, Faculty of Pharmacy in Hradec Kralove* *[3] Department of Infectious Diseases University Hospital Hradec Králové* *[4] Pulmonary Department, University Hospital Hradec Králové* *[5] Department of Oncology, Palacký University, Faculty of Medicine and Dentistry* **OP 11: Quantifying 1000 protein groups per minute of gradient using data-independent acquisition (DIA) on a hybrid quadrupole time-of-flight system** G. Eagle[1] , D. Merkel[3] , N. Morrice[1], I. Batruch[2] and P. Pribil[2] *[1] SCIEX UK* *[2] SCIEX Canada* *[3] SCIEX Germany* **OP 12: CE-ICP-MS/MS in a duty of the changes examination of liposomal cisplatin delivery systems** M. Matczuk, A. Wróblewska and J. Samsonowicz-Górski *Chair of Analytical Chemistry, Faculty of Chemistry, Warsaw University of Technology* **OP 13: Chiral Discrimination in Capillary Electrophoresis: Explore the Potential of Deep Eutectic Solvents and Amino Acid-Based Ionic Liquids** K. A. Ioannou[1], G. D. Ioannou[1], A. Christou[1], I. J. Stavrou[2], M. G. Schmid[3] and C. P. Kapnissi-Christodoulou[1] *[1] Department of Chemistry, University of Cyprus* *[2] Department of Life Sciences, European University Cyprus* *[3] Department of Pharmaceutical Chemistry, Institute of Pharmaceutical Sciences, University of Graz* **OP 14: Determination of cannabinoids in human cerumen by use of UPLC-MS/MS as a potential biomarker for drug use** M. C. Christodoulou[1], M. S. Constantinou[2] , A. P. Louppis[2] , A. Christou[1] , I. J. Stavrou[3] and C. P. Kapnissi-Christodoulou[1] *[1] Department of Chemistry, University of Cyprus* *[2] Analytical Department, MC Analysis Centre LTD* *[3] Department of Life Sciences, European University Cyprus*

	OP 15: Predicting the acute aquatic toxicity of UV-filter compounds used in cosmetic formulations C. Stergiopoulos[1], K. Valko[2] , F. Tsopelas[1] and M. Ochsenkühn-Petropoulou[1] *[1] Laboratory of Inorganic and Analytical Chemistry, School of Chemical Engineering, National Technical University of Athens* *[2] Biomimetic Chromatography Ltd, Stevenage, Hertfordshire* **OP 16: Beyond Conventional Limits: Unlocking Varied Applications with an Innovative LCMS Ionisation Source"** J. Bucek[1], J.-C. Wolf[1], M. Weber[1] and C. Conway[1] *[1] Plasmion GmbH, Germany*
17:45-18:15	**Coffee Break**
18:15-19:00	*Imperial Hall Room 1* **Electroanalytical techniques** (Chairs: T.K. Christopoulos, D. Kalogianni) **OP 17: From a screen-printed electrode to an industrial sensor for on-site measurement of Co and Ni** C. Parat, E. Ricard, S. Le Faucheur and I. Le Hécho *CNRS / Univ Pau & Pays Adour / E2S UPPA, IPREM, UMR5254* **OP 18: What is the most appropriate electrochemical sensor for on-site pesticide analysis?** E. Ricard, D. Bégué, W. Lafargue-Dit-Hauret and C. Parat *CNRS / Univ Pau & Pays Adour / E2S UPPA, Institut des sciences analytiques pour l'environnement et les matériaux, UMR5254* **OP 19: A highly sensitive sensor for glyphosate detection based on the modification of a screen-printed carbon electrode by gold microstructures coated with a nanometric layer of polypyrrole** Q. Palas, E. Ricard, C. Parat, C. Lartigau-Dagron and L. Ronga *CNRS / Univ Pau & Pays Adour / E2S UPPA, IPREM, UMR5254*
19:00-20:00	*Imperial Hall Room 3* **Poster Session 1** *(See pages 27-32)*

Tuesday 19th of September 2023

09:00-09:30	*Imperial Hall Room 1* **Invited Oral Presentation 7** **R. Lobinski** *Professor, IPREM CNRS* Emerging facets of mass spectrometry for elemental speciation (Chair: M. Ochsenkuehn)
09:30-10:00	*Imperial Hall Room 1* **Speciation Analysis (Part I)** (Chairs: R. Lobinski, M. Ochsenkuehn) **OP 20: Mercury speciation in solid matter using thermal release in combination with electrothermal atomic absorption spectrometry** O. Shuvaeva, I. Bekesha and D. Troitskii *Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences* **OP 21: Fish tissue multielement metallobiomolecule profiling method and its application to four commercially important fish species** G. Panagou[1], I. Kalantzi[2], M. Tsapakis[2] and S. A. Pergantis[1] *[1] Department of Chemistry, University of Crete* *[2] Institute of Oceanography, Hellenic Centre for Marine Research*
10:00-10:30	**Coffee Break**
10:30-11:30	*Imperial Hall Room 1* **Speciation Analysis (Part II)** (Chairs: R. Lobinski, M. Ochsenkuehn) **OP 22: Development of a dedicated microsystem coupled to ICP-MS/MS for the selective capture and on-line quantification of uranium-target biomolecules** M. Garcia-Cortes[1], C. Vidaud[2], M. Araya-Farias[3], T. Tran[3] and C. Bresson[1] *[1] Université Paris-Saclay, CEA, Service de Physico-Chimie* *[2] Institut de Biosciences et Biotechnologies d'Aix-Marseille, BIAM, CEA-Marcoule* *[3] Université Paris-Saclay, CNRS, Institut Galien Paris Saclay* **OP 23: Detailed Arsenolipid Determination in BCR Reference Material using HPLC with high-resolution mass spectrometry and ICP-MS** M. Kapsi[1], K. Marmatakis[2], I. Kalantzi[1], M. Tsapakis[1] and S. Pergantis[2] *[1] Institute of Oceanography, Hellenic Centre for Marine Research (HCMR* *[2] Environmental Chemical Processes Laboratory, Department of Chemistry, University of Crete* **OP 24: Novel interference removal strategies using Multi-Quadrupole ICP-MS/MS** H. Ernstberger[1], K. A. Jensen[2], E. Pruszkowski[3] and M. Petrich[4] *[1] PerkinElmer Italy* *[2] Faculty of Environmental Sciences and Natural Resource Management, Norwegian University of Life Sciences* *[3] PerkinElmer United States* *[4] PerkinElmer Germany*

	OP 25: 3 ways to improve your daily lab routine with molecular spectroscopy — from QA/QC to advanced microscopy M. Ries *Thermo Scientific*
11:30-14:45	**Excursion to the city of Chania (Light lunch basket)**
14:45-15:45	*Imperial Hall Room 3* **Poster Session 2** *(See pages 32-36)*
15:45-16:30	*Imperial Hall Room 1* **Associations** (Chairs: Les Ebdon/M. Ochsenkuehn) **OP 26: EXSA: the European X-ray Spectrometry Association** D. Eichert[1,2] on behalf of EXSA Executive Committee[2] *[1] ELETTRA – Sincrotrone Trieste* *[2] Konkoly-Thege M.* **OP 27: The role of the European Association of Professors Emeriti (EAPE)** Sir Les Ebdon *University of Bedfordshire* **OP 28: Why a EuChemS Working Party "Ethics in Chemistry"?** H. Frank *University Bayreuth*
16:30-17:00	*Imperial Hall Room 1* **Invited Oral Presentation 8** **B. Beckhoff** *Dr., Physikalisch-Technische Bundesanstalt* Quantitative Characterisation of Nano- and Microscaled Materials by X-ray Spectrometry (Chair: D. Eichert)
17:00-17:30	**Coffee Break**
17:30-18:45	*Imperial Hall Room 1* **Advanced X-Ray techniques** (Chairs: B. Beckhoff, D. Eichert) **OP 29: XRF under grazing incidence investigations of potential calibration samples for the quantification of heavy elements in particulate matter** L. Borgese[1], P. Cirelli[1], T. Hase[2], and D. Eichert[3] *[1] INSTM - Chemistry for Technologies Laboratory, University of Brescia* *[2] University of Warwick, Department of Physics* *[3] ELETTRA – Sincrotrone Trieste* **OP 30: Laboratory scanning-free GEXRF for the investigation of 2D nanostructures** S. Staeck[1], J. Baumann[1], P. Hönicke[2], K. Andrle[2], Y. Kayser[2], V. Soltwisch[2], N. Wauschkuhn[2], D. Grötzsch[1], J. Weser[2], F. Spikermann[1], G. Goetzke[4], A. Jonas[2], F. Förste[1], I. Mantouvalou[3], H. Stiel[5] and B. Kanngießer[1] *[1] Technical University of Berlin* *[2] Physikalisch-Technische Bundesanstalt*

	[3] *Helmholtz-Zentrum Berlin* [4] *Deutsches Elektronen-Synchrotron DESY* [5] *Max Born Institute* **OP 31: Characterization and calibration of a Bruker S4 T-STAR instrument for virtually standard-less quantitative analysis of aerosol depositions** P.Hönicke[1], B. Beckhoff[1], M. Gottschalk[2], Y. Kayser[1] and S. Seeger[2] [1] *Physikalisch-Technische Bundesanstalt* [2] *Bundesanstalt für Materialforschung und -prüfung* **OP 32: Zinc diffusion in dentine: Investigating elemental gradients and chemical changes at the interface with dental restorations** O. Marushchenko[1,2], F. Lizzi[2], L. J. Bauer[3], H. Elfarraj[2], P. Zaslansky[2] and I. Mantouvalou[1] [1] *Helmholtz-Zentrum Berlin for Materials and Energy* [2] *Dept. of Operative, Preventive and Pediatric Dentistry, Charité – Universitätsmedizin* [3] *Institute for Optics and Atomic Physics, Technical University of Berlin* **OP 33: XRD has changed: Advancing Instrumental Methods of Analysis with Groundbreaking XRD Technology** M. Ziagkos *Analytical Instruments SA*
18:45-19:45	*Imperial Hall Room 3* **Poster Session 2** *(See pages 32-36)*
20:45- 23:00	**Gala dinner**

Wednesday 20th of September 2023

09:00-09:30 — *Imperial Hall Room 1*

Invited Oral Presentation 9

G. Theodoridis *Professor, Aristotle University Thessaloniki*

FoodOmicsGR_RI: Greek National Research Infrastructure for the Comprehensive Characterisation of Foods

(Chair: N. Thomaidis)

09:30-10:45 — **Parallel sessions**

Imperial Hall Room 1

Food Analysis (FoodOmics)

(Chairs: G. Theodoridis, N. Thomaidis, D. Hela)

OP 34: Rapid microbore lipidomic profiling method for the analysis of extra virgin olive oils from different Mediterranean countries by RPLC-TOF/MS. Application of cyclic ion mobility for the isolation of lipid isomers

A. Lioupi[1,2], N. Munjoma[3], T. Liapikos[1,2], L. Gethings[3] and G. Theodoridis[1,2]

[1] Laboratory of Analytical Chemistry, School of Chemistry, Aristotle University of Thessaloniki

[2] FoodOmicsGR Research Infrastructure, AUTh Node, Center for Interdisciplinary Research and Innovation (CIRI-AUTH

[3] Operations, Waters Corporation UK

OP 35: Metabolomics solutions in monitoring nutrition and wellness

O. Begou[1,2,3], G. Theodoridis[1,2] and H. Gika[2,4]

[1] Department of Chemistry, Aristotle University of Thessaloniki

[2] Biomic Auth, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki

[3] ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH

[4] Laboratory of Forensic Medicine and Toxicology, Department of Medicine, Aristotle University of Thessaloniki

OP 36: Elemental metabolomics – Tagging Wheat Sprouts with Rare Earths Elements

L. Papalamprou[1,2], A. Palyvos[1], D.G. Sotirchos[1,2] and C.A. Georgiou[1,2]

[1] Chemistry Laboratory, Department of Food Science and Human Nutrition, Agricultural University of Athens

[2] FoodOmics.GR Research Infrastructure

OP 37: Analysis of pyrrolizidine alcaloids in food

G. Miliadis, C. Kroi and G. Siragakis

TUV Austria Food Allergens Labs

OP 38: Residues of pesticides in the food chain: Are bee products endangered or safe to consumers?

A. Fuente-Ballesteros, J. Bernal and A. M. Ares

Analytical Chemistry Group (TESEA), I. U. CINQUIMA, Faculty of Sciences, University of Valladolid

Imperial Hall Room 2

Materials

(Chairs: I. Gerothanassis, L.A. Tsakanika)

OP 39: Thermal analysis of crystalline diblock copolymers by DSC

S. Bistac, M. Brogly and D. Bindel

Université de Haute Alsace – LPIM

	OP 40: Development of a hybrid portable instrument for assessing the surface state and degradation of monuments: combining LED-Induced Fluorescence, LIBS and Diffuse Reflectance V. Pinon[1], A. Giakoumaki[1], M. Andrianakis[1], K. Hatzigiannakis[1], K. Melessanaki[1], M. Pavlou[2], S. Korosis[2], P. Pouli[1] and D. Anglos[1,3] *[1] Institute of Electronic Structure and Laser, Foundation for Research and Technology* *[2] Ephorate of Antiquities of the City of Athens* *[3] University of Crete, Department of Chemistry* **OP 41: Exploring the Impact of Storage Temperature on PbO and Pb3O4. Aging Characterization with XRD, ATR - FTIR, SAXS and N2 Porosimetry** A. Papadouli[1], N. Pradakis[2], D. A. Gkika[2,3], J. Fantidis[1], M. Maragakis[1], S. Pantazis[4], A. C. Mitropoulos[2,3] and N. Vordos[1] *[1] Department of Physics, International Hellenic University* *[2] Department of Chemistry, International Hellenic University* *[3] Hephaestus Advanced Laboratory, International Hellenic University* *[4] Sunlight Group* **OP 42: Development of Fe3O4-decorated Sn-hydroxide nanocomposites for advanced Cr(VI) capture in drinking water** K. Kalaitzidou, T. Asimakidou and K. Simeonidis *Analytical Chemistry Laboratory, Department of Chemical Engineering, Aristotle University of Thessaloniki*
10:45-11:15	**Coffee Break**
11:15-11:45	*Imperial Hall Room 1* **Invited Oral Presentation 10** **A. Alexopoulou** *Professor, University of West Attica* Hyperspectral Imaging a modern tool for art conservation diagnostics (Chair: Th. Lymperopoulou)
11:45-13:00	**Parallel sessions**
	Imperial Hall Room 1 **Archaeometry** (Chairs: A. Alexopoulou, Th. Lymperopoulou) **OP 43: Spatially resolved analysis of the red pigment Eosin and its photodegradation products by MALDI-MSI in paint samples** K. Janssens[1,2], A. Alvarez-Martín[1,2] and T. Scovacricchi[1] *[1] AXIS Research Group, NANOLab Centre of Excellence, University of Antwerp* *[2] Conservation and Science Department, Rijksmuseum Amsterdam* **OP 44: HPLC studies on shellfish (royal) purple** I. Karapanagiotis *Department of Chemistry, Aristotle University of Thessaloniki* **OP 45: Investigation of spectral markers appropriate for optimized archaeogenetic analysis of ancient dental remains based on Raman scattering and fluorescence spectroscopy techniques** An. Mamali[1,2], A. Philippidis[1], N. Psonis[3], D. Vassou[3], E. Tabakaki[3], A. Nafplioti[3], N. Poulakakis[3,4,5] and D. Anglos[1,2] *[1] Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas (IESL-FORTH)* *[2] Department of Chemistry, University of Crete*

[3] *Foundation for Research and Technology - Hellas (FORTH), Institute of Molecular Biology and Biotechnology (IMBB), Ancient DNA Lab*
[4] *Natural History Museum of Crete (NHMC), School of Sciences and Engineering, University of Crete*
[5] *Biology Department, School of Sciences and Engineering, University of Crete*

OP 46: Towards a multi-analytical methodology based on molecular spectroscopic techniques for the detection and characterization of organic residues in archaeological findings

M. E. Konstantinou[1,2], E. Ralli[2], I. Misyri[2], M. Roumpou[1], A. Philippidis[1], S. Sotiropoulou[1,3], A. Spyros[2], and D. Anglos[1,2]
[1] *Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas (IESL-FORTH)*
[2] *Department of Chemistry, University of Crete*
[3] *School of Applied Arts and Sustainable Design, Hellenic Open University*

OP 47: Advanced spectroscopic and imaging tools with sophisticated robotics and digital repository systems for the analysis, conservation, and documentation of oversized paintings in the framework of an Open Access Conservation Laboratory

K. Hatzigiannakis[1], A. G. Karydas[2], C. Bekiari[3], D. Angelakis[3], A. Terlixi[4], K. Karakasiliotis[5], C. Stentoumis[6], X. Zabulis[3], D. Anglos[1,7], E. Agathonikou[4] and D. Plexousakis[3,8]
[1] *Institute of Electronic Structure and Laser (IESL), FORTH*
[2] *Institute of Nuclear and Particle Physics, N.C.S.R. "Demokritos"*
[3] *Institute of Computer Science (ICS), FORTH*
[4] *National Gallery – Alexandros Soutzos Museum*
[5] *Printec S.A.*
[6] *up2metric P.C.*
[7] *Department of Chemistry, University of Crete*
[8] *Department of Computer Science, University of Crete*

Imperial Hall Room 2

Spectrometry

(Chairs: G. Hieftje, E. Chatzitheodoridis)

OP 48: Towards real-time, on-site monitoring of trace metals in the environment using micro-plasma emission spectroscopy

S. Das[1], K. B. von der Geest[2], A. Mäkinen[2], A. Roost[2], E. Ikonen[1 3] and T. Laurila[2]
[1] *Metrology Research Institute, Aalto University*
[2] *Sensmet Ltd*

OP 49: Utilizing multivariate analysis for the discrimination of athletes' salivary profile using ATR-FTIR spectroscopy

C. Chrimatopoulos[1], E. Pavlou[2], N. Kourkoumelis[2] and V. Sakkas[1]
[1] *Department of Chemistry, School of Sciences, University of Ioannina*
[2] *Department of Medical Physics, Faculty of Medicine, School of Health Sciences, University of Ioannina*

OP 50: PM-IRRAS Surface advanced IR spectrometry: a powerful technique for the characterization of organic and polymer coatings

M. Brogly and S. Bistac
Université de Haute Alsace – LPIM

OP 51: NMR Analytical Perspectives in Natural Products: From Biotransformation Product Dereplication to Protein-Ligand ex-Situ and in-Cell Applications

I. P. Gerothanassis
Section of Organic Chemistry and Biochemistry, Department of Chemistry, University of Ioannina

13:00-14:00	**Lunch**
14:00-15:30	**Parallel sessions**

Imperial Hall Room 1

Environmental

(Chairs: H. Frank, A. Gondikas)

OP 52: Temporal evolution of particulate PAH and Particulate matter concentrations for 6 months in Strasbourg (France)

J. Vaz-Ramos[1,2], A. Becker[1], F. R. Nursanto[1], O. Delhomme[1], M. Millet[1], S. Bégin-Colin[2] and S. Le Calvé[1]

[1] ICPEES – CNRS/University of Strasbourg

[2] IPCMS, UMR-7504 CNRS-Université de Strasbourg

OP 53: Continuous Monitoring of ppb-levels of Formaldehyde: Comparison of Analytical Systems and Development of a Portable Calibration Generator

A. Grandjean[1,2], A. Becker[1], M. Wolf[1], C. Sutter[1], F. Amiet[2], D. Bazin[2] and S. Le Calvé[1]

[1] ICPEES – CNRS/University of Strasbourg

[2] Chromatotec

OP 54: Microfluidic devices for cation detection based on calixarene

I. Leray , A. Depauw, M.H. Ha-Thi, N. Kumar, Q. Pham, C. Remy, J.P. Lefevre and C. Mongin

ENS Paris Saclay PPSM, CNRS

OP 55: Socioeconomic status and public health in Australia: A wastewater-based study

N. Rousis[1,2], Z. Li[3], R. Bade[1], M.S. McLachlan[3], J.F. Mueller[1], J.W. O'Brien[1], B.J. Tscharke[1], N.S. Thomaidis[2] and K.V. Thomas[1]

[1] Queensland Alliance for Environmental Health Sciences (QAEHS), The University of Queensland

[2] Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens

[3] Department of Environmental Science, Stockholm University

OP 56: OxR: A microfluidic instrument to detect reactive oxygen species on terrestrial and planetary environments

C. D. Georgiou[1], E. Chatzitheodoridis[2], E. Kalaitzopoulou[1], P. Papadea[1], M. Skipitari[1], A. Varemmenou[1], H.-A. Stavrakakis[2], I. Markopoulos[4], A. Alexandrou[4] and M. Holynska[5]

[1] Department of Biology, School of Natural Sciences, University of Patras

[2] Department of Geological Sciences, School of Mining and Metallurgical Engineering, National Technical University of Athens

[4] ZEROONE LTD

[5] Materials' Physics & Chemistry Section (TEC-QEE), Technical Reliability and Quality Division (TEC-QE), ESTEC, ESA

OP 57: Shipping pollution in the marine environment: a particulate challenge

A. Gondikas[1,2,3], M. Hassellöv[3], K. Mattsson[3], S. Chen[4] and I.-M. Hassellöv[5]

[1] Creative nano, PC

[2] Department of Geology and Geoenvironment, National and Kapodistrian University of Athens

[3] Department of Marine Sciences, University of Gothenburg

[4] State Environmental Protection Key Laboratory of Environmental Risk Assessment and Control on Chemical Process, School of Resources and Environmental Engineering, East China University of Science and Technology

[5] Department of Mechanics and Maritime Science, Chalmers University of Technology

	Imperial Hall Room 2 **Sample handling** (Chairs: P. Solich, Th. Tsiaka) **OP 58: The use of deep eutectic solvents as sustainable and recyclable solvents for extraction of phenolic compounds from aloe vera rind by-product: Extraction optimization and green metrics** G.I. Ioannou[1], K.A. Ioannou[1], A. Christou[1], I.J. Stavrou[2] and C.P. Kapnissi-Christodoulou[1] *[1] Department of Chemistry, University of Cyprus* *[2] Department of Life Sciences, European University Cyprus* **OP 59: Monitoring of PFAs levels in water using a Solid Phase Extraction coupled with LC/MS-MS analytical method** N. Xanthopoulou, C. Gkementzoglou, D. Alexiadou and G. Seretoudi *EYATH S.A., Thessaloniki Water Supply & Sewerage Company, Thessaloniki Water Treatment Plant Laboratory Department* **OP 60: Sample pretreatment using flow methods** P. Solich, B. Horstkotte, P. Chocholouš, H. Sklenářová and D. Šatínský *Charles University, Faculty of Pharmacy, Dept. of Analytical Chemistry, Hradec Králové* **OP 61: Analyzing ante-mortem and post-mortem biological materials** R. Wietecha-Posłuszny *Laboratory for Forensic Chemistry, Department of Analytical Chemistry, Faculty of Chemistry, Jagiellonian University in Kraków* **OP 62: Qualitative dried blood spots (qDBS) and dried urine spots (DUS): Applications for the accurate determination of biomarkers and illicit drugs** T. Meikopoulos[1,2], O. Begou[1,2,3], Stelios Papazoglou[1,2], H. Gika[2,4] and G. Theodoridis[1,2] *[1] Department of Chemistry, Aristotle University of Thessaloniki* *[2] Biomic AUTH, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki* *[3] ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)* *[4] Laboratory of Forensic Medicine and Toxicology, School of Medicine, Aristotle University of Thessaloniki* **OP 63: Key aspects during the development of analytical sample preparation methods: application to the study of selected pesticides in bee products** Ad. Fuente-Ballesteros, J. Bernal and A. M. Ares *Analytical Chemistry Group (TESEA), I. U. CINQUIMA, Faculty of Sciences, University of Valladolid*
15:30-16:30	*Imperial Hall Room 1* **Closing Ceremony- Awards**

Poster Session 1

Monday 18th of September 2023

Imperial Hall Room 3

Sensors and Biosensors – Point of Care Systems – Chromatographic Techniques and Mass Spectrometry – Sample Preparation

1. Sensors and Biosensors

A. Other applications

P. 1: Screening method for discrimination of olive oil from other vegetable oils with a DNA biosensor
N-M Christopoulou[1], V. Mamoulaki[1], A. Mitsiakou[1], E. Samolada[1], D. P. Kalogianni[1], and T. K. Christopoulos[1,2]
[1] *Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras*
[2] *Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE)*

P. 2: Molecular rapid test for detection of tuna fish adulteration
I. P. Gkini[1], P. Christopoulos[1], D. P. Kalogianni[1], T. K. Christopoulos[1,2] and A. Conides[3]
[1] *Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras*
[2] *Institute of Chemical Engineering Sciences / Foundation for Research and Technology Hellas (FORTH/ICE)*
[3] *Hellenic Centre for Marine Research, Institute for Marine Biological Resources*

P. 3: Development of a molecular rapid test for the visual authentication of the fish Sardina pilchardus
M. Kakarelidou[1], P. Christopoulos[1], D. P. Kalogianni[1], T. K. Christopoulos[1 2] and Al. J. Conides[3]
[1] *Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras*
[2] *Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE)*
[3] *Hellenic Centre for Marine Research, Institute for Marine Biological Resources*

B. Life Sciences

P. 4: A sensitive and selective sensor for cancerous exosomes using fluorescent magnetic nanocomposites with graphene oxide-based fluorescence quenching
S. W. Park[1] and Y. K. Jung[1,2]
[1] *Department of Nanoscience and Engineering*
[2] *School of Biomedical Engineering, Inje University*

P. 5: Whole-genome sequencing of SARS-CoV-2: automation in the process of detecting variant evolution of the virus
M. Gancarcikova[1,2], H. Parova[1], M. Berankova[1], L. Rysava[1], L. Krcmova Kujovska[1,3], L. Pavlikova[1], V. Palicka[1] and R. Hyspler[1]
[1] *Department of Clinical Biochemistry and Diagnostics, Charles University, Faculty of Medicine in Hradec Kralove and University Hospital Hradec Kralove*
[2] *University of Pardubice, Faculty of Chemical Technology*
[3] *Charles University, Faculty of Pharmacy in Hradec Kralove*

P. 6: Synthesis and Characterization of Inclusion Complexes of β-Cyclodextrins and Essential Oils of Greek Origin
I. Pitterou[1], E. Kavetsou[1], A. Kalospyros[1], I. Kostopoulou[1], C. Derzekou[1], E. Kontogeorgou[1], T. Armeni[1], D. Daferera[2], P.A. Tarantilis[2], S. Dervisoglou[3], D. Perdikis[3] and A. Detsi[1]
[1] *Laboratory of Organic Chemistry, School of Chemical Engineering, National Technical University of Athens*
[2] *Laboratory of General Chemistry, Department of Food Science & Human Nutrition, School of Food & Nutrition Sciences, Agricultural University of Athens*
[3] *Laboratory of Agricultural Zoology and Entomology, Department of Crop Science, School of Plant Sciences, Agricultural University of Athens*

P. 7: Development of a novel green extraction methodology of nettle using Natural Deep Eutectic Solvents
M. A. Karadendrou[1], E. Nourry[1], A. Tzani[1], T. Lymperopoulou[2], and A. Detsi[1]
[1] Laboratory of Organic Chemistry, School of Chemical Engineering, National Technical University of Athens, Zografou Campus
[2] Processes and Products Quality Control Horizontal Laboratory, Zografou Campus, School of Chemical Engineering, National Technical University of Athens

P. 8: Gas Ion Distillation (GID) and Sequential Ion Processing (SIPRO) as novel techniques in chemical detection: The role of Augmented Reality (AR) in enhancing their applications
F. Tsopelas[1], M. Statheropoulos[1], S. Yli-Kauhaluoma[1], D. Ruiz Lopez[3], G. Eiceman[2] and P. Vaninen[2]
[1] School of Chemical Engineering, National Technical University of Athens
[2] University of Helsinki
[3] ATOS

2. Other clinical (and pharmaceutical) applications

P. 9: The finest smuggler – maximizing the platinum drug loading in liposome nanocarrier
J. Zajda, Z. Wakuła, A. Wróblewska and M. Matczuk
Chair of Analytical Chemistry, Faculty of Chemistry, Warsaw University of Technology

P. 10: Assessment of different methodologies for processing fecal samples in 1H NMR metabolic profiling
K. Tsiantas[1,2], P. Christodoulou[2], M. Matzapetakis[2], M. Zervou[2] and P. Zoumpoulakis[1,2]
[1] Department of Food Science and Technology, University of West Attica
[2] Institute of Chemical Biology, National Hellenic Research Foundation

P. 11: Rapid amplification-free detection of microRNAs based on a tailing reaction and a lateral flow strip test
El. Lamprou , P. M. Kalligosfyri[1] and D. P. Kalogianni
Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras

3. Chromatography (± Mass spectrometry)

P. 12: The potential of Biomimetic Chromatography to predict dermal absorption
A. Georgopoulos, C. Agathokleous, K. Vasileiou, E. Leventaki, B.A. Tsantili- Kakoulidou and F. Tsopelas
Laboratory of Inorganic and Analytical Chemistry, School of Chemical Engineering, National Technical

P. 13: Quantitative determination of aloins A and B in aloe latex and aloe vera-based products - Chemometric classification of aloe vera plants (Aloe Barbadensis Miller) under different conditions
G.I. Ioannou[1], A. Christou[1], I.J. Stavrou[2], C.P. Kapnissi-Christodoulou[1]
[1] Department of Chemistry, University of Cyprus
[2] Department of Life Sciences, European University Cyprus

P. 14: Fecal fatty acid profile of exclusively breast-fed or formula-fed infants
K. Tsiantas[1,2], P. Christodoulou[1], Th. Tsiaka[1], Th. Boutsikou[2], N. Iacovidou[2], V. J. Sinanoglou[1] and P. Zoumpoulakis[1]
[1] Department of Food Science and Technology, University of West Attica
[2] Department of Neonatology, Medical School, National Kapodistrian University of Athens

P. 15: UHPLC-MS analysis of salivary bile acids in non-invasive diagnostics of Barrett's esophagus
V. Dosedělová[1], M. Laštovičková[1], J. Dolina[2], Š. Konečný[2] and P. Kubáň[1]
[1] Institute of Analytical Chemistry of the Czech Academy of Sciences, Brno
[2] University Hospital Brno, Faculty of Medicine, Masaryk University, Brno

P. 16: HPLC-ESI-MS/MS for the determination of Arsenolipids in fish: A new form of arsenic for improved risk assessment
C. M. Drakonaki[1], M. Kapsi[2], I. Kalantzi[2], M. Tsapakis[2] and S. A. Pergantis[1]

[1] *Environmental Chemical Processes Laboratory, Department of Chemistry, University of Crete*
[2] *Institute of Oceanography, Hellenic Centre for Marine Research (HCMR)*

P. 17: Development and validation of targeted UPLC-MS/MS methods to ensure food safety: determination of biogenic amines in tuna fish and coumarin in bakery products

Ar. Lioupi[1,2], Ar. Papaioannou[3], Ch. Virgiliou[2,3], Ach. Iakovakis[4], I. Kaidatzis[4] and G. Theodoridis[1,2]
[1] *Laboratory of Analytical Chemistry, School of Chemistry, Aristotle University of Thessaloniki*
[2] *FoodOmicsGR Research Infrastructure, AUTh Node, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*
[3] *School of Chemical Engineering, Aristotle University of Thessaloniki*
[4] *Veltia Labs for Life, Food Contaminants Laboratory*

P. 18: Development and validation of an LC-ESI-MS/MS method for the trace analysis of Zearalenone in weaned pig bile samples using an IAC-based extraction procedure

I. Bouzouka[1,2], H. Gika[2,3], S. Didos[1,4], P. Tassis[5], D. Floros[5] and A. Argiriou[1,4]
[1] *Institute of Applied Biosciences, Centre for Research and Technology Hellas (CERTH)*
[2] *Laboratory of Forensic Medicine and Toxicology, Medical School, Aristotle University of Thessaloniki*
[3] *Biomic AUTH, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*
[4] *Department of Food Science and Nutrition, School of the Environment, University of the Aegean*
[5] *Clinic of Farm Animals, School of Veterinary Medicine, Aristotle University of Thessaloniki*

P. 19: Development and validation of a UHPLC-MS/MS method for the quantification of the tryptophan pathway-related compounds

M. Kubát[1,2], O. An. Begou[1,3,4], H. Gika[1,5], P. Česla[2] and G. Theodoridis[1,3]
[1] *Biomic AUTH, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki*
[2] *Department of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice*
[3] *Department of Chemistry, Aristotle University of Thessaloniki*
[4] *ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*
[5] *Laboratory of Forensic Medicine and Toxicology, School of Medicine, Aristotle University of Thessaloniki*

P. 20: Metabolic fingerprinting of Muscat of Alexandria of Limnos grape musts during alcoholic fermentation

M. Marinaki[1,2,3], P. Arapitsas[4,5], C. Virgiliou[2,3,6] and G. Theodoridis[1,2,3]
[1] *Laboratory of Analytical Chemistry, School of Chemistry, Aristotle University of Thessaloniki*
[2] *Biomic AUTh, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*
[3] *FoodOmicsGR Research Infrastructure, AUTh Node, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*
[4] *Department of Wine, Vine and Beverage Sciences, School of Food Science, University of West Attica*
[5] *Research and Innovation Centre, Fondazione Edmund Mach*
[6] *School of Chemical Engineering, Aristotle University of Thessaloniki*

P. 21: Identification of transformation products of emerging pollutants formed in photolytic and photocatalytic processes by LC-HR-Orbitrap MS

I. Konstantinou[1,2], V. Boti[1,2], D. Hela[1,2] and T. Albanis[1,2]
[1] *Department of Chemistry, University of Ioannina*
[2] *Institute of Environment and Sustainable Development, University Research and Innovation Center*

P. 22: Determination of perfluorinated compounds in natural waters and wastewaters by solid phase extraction and LC-LTQ/Orbitrap MS

K. Miserli[1], V. Athanasiou[1], V. Boti[1 2], D. Hela[1,2] and I. Konstantinou[1,2]
[1] *Department of Chemistry, University of Ioannina*
[2] *Institute of Environment and Sustainable Development, University Research and Innovation Center of Ioannina*

P. 23: Solid-phase extraction and LC-MS determination of metabolites from biological fluids using magnetic nanoparticles

O. Skyrgiannis[1], C. Virgilliou[1,2], H. Gika[2,3] and K. Simeonidis[1]
[1] *Analytical Chemistry Laboratory, Department of Chemical Engineering, Aristotle University of Thessaloniki*

[2] *Biomic_AUTh, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*
[3] *Department of Medicine, Aristotle University of Thessaloniki*

P. 24: Development and validation of an LC-MS/MS method for the quantitative analysis of 9 steroid hormones in human serum

A. Antoniadou[1,2], T. Meikopoulos[1,2], O. Begou[1,2,3], H. Gika[2,4] and G. Theodoridis[1,2]
[1] *Department of Chemistry, Aristotle University of Thessaloniki*
[2] *Biomic AUTH, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki*
[3] *ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*
[4] *Laboratory of Forensic Medicine and Toxicology, School of Medicine, Aristotle University of Thessaloniki*

P. 25: Improving 4D screening of bile acids in biological samples by Liquid Chromatography – Ion Mobility – High Resolution Mass Spectrometry

C. Virgiliou[1,2], D. Diamantidou[2,3], H. Gika[2,4]and G. Theodoridis[2,3]
[1] *Analytical Chemistry Laboratory, Department of Chemical Engineering, School of Engineering, Aristotle University of Thessaloniki*
[2] *Biomic_AUTh, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*
[3] *Laboratory of Analytical Chemistry, Department of Chemistry, Aristotle University of Thessaloniki*
[4] *School of Medicine, Aristotle University of Thessaloniki*

P. 26: Mass spectrometry metabolite library for 4D Metabolomics. Application to biological samples

A. Lioupi[1], D. Diamantidou[1], T. Zioga[2], A. Koulouri[2], G. Theodoridis[1,3] and C. Virgiliou[2,3]
[1] *Laboratory of Analytical Chemistry, Department of Chemistry, Aristotle University of Thessaloniki*
[2] *Laboratory of Analytical Chemistry, Department of Chemical Engineering, Aristotle University of Thessaloniki*
[3] *Biomic_AUTh, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*

P. 27: Development and validation of a HILIC-MS/MS method for the quantitative analysis of 14 amino acids in dried urine spots (DUS)

T. Meikopoulos[1,2], O. Begou[1,2,3], H. Gika[2,4] and G. Theodoridis[1,2]
[1] *Department of Chemistry, Aristotle University of Thessaloniki*
[2] *Biomic AUTH, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki*
[3] *ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH)*
[4] *Laboratory of Forensic Medicine and Toxicology, School of Medicine, Aristotle University of Thessaloniki*

P. 28: Scandium selective recovery from sulphuric acid leaching solutions by an ion exchange 2-stage procedure using an industrial resin

L.A. Tsakanika, N. Loukas and M. Ochsenkuehn – Petropoulou
Laboratory of Inorganic and Analytical Chemistry, School of Chemical Engineering, NTUA

P. 29: Cyclodextrin- and Cyclofructan-based Chiral Selectors: Evaluation of their Chiral Discrimination Ability in Capillary Electrophoresis for the Enantioseparation of Psychoactive Substances

K. A. Ioannou[1], A. Christou[1], I. J. Stavrou[2], M. G. Schmid[3] and C. P. Kapnissi-Christodoulou[1]
[1] *Department of Chemistry, University of Cyprus*
[2] *Department of Life Sciences, European University Cyprus*
[3] *Department of Pharmaceutical Chemistry, Institute of Pharmaceutical Sciences, University of Graz*

P. 30: Method validation – different approach to pharmaceutical and bioanalytical analysis

L. Matysová[1] and L. Kujovská Krčmová[2]
[1] *Department of Analytical Chemistry, Faculty of Pharmacy in Hradec Králové, Charles University*
[2] *Department of Clinical Biochemistry and Diagnostics, University Hospital Hradec Králové*

P. 31: The possibility of using a dry urine spot to diagnose cerebral creatine deficiency syndromes by tandem mass spectrometry method

H. Jurdáková[1], T. Večereková[1], A. Šalingová[2] and R. Górová[1]

[1] *Comenius University, Faculty of Natural Sciences, Department of Analytical Chemistry*
[2] *National Institute of Children's Diseases, Centre for Inherited Metabolic Disorders*

P.32: HPLC-MS/MS analysis of DINCH plasticizer metabolites in breast milk
R. Górová, A. Oravcová and H. Jurdáková
Department of Analytical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava

P.33: Micellar liquid chromatography in early drug discovery: A Comparative study of the different surfactants
P. Danias[1], A. Pappa[1], A. Tsantili- Kakoulidou[2] and F. Tsopelas[1]
[1] *Laboratory of Inorganic and Analytical Chemistry, School of Chemical Engineering, National Technical University of Athens*
[2] *Department of Pharmaceutical Chemistry, School of Pharmacy, National and Kapodistrian University of Athens*

P. 34: High-Performance PTR-ToF-MS for Detection of ambient Volatile Organic Compounds
O. Zografou[1], C. Kaltsonoudis[2], M. Gini[1], E. Panagiotopoulos[3], A. Lekkas[3], D. Papanastasiou[3], S. Pandis[2,4] and K. Eleftheriadis[1]
[1] *Environmental Radioactivity & Aerosol Tech. for Atmospheric & Climate Impacts, INRaSTES, N.C.S.R. Demokritos*
[2] *Institute of Chemical Engineering Sciences, ICE-HT*
[3] *Fasmatech Science & Technology SA, NCSR Demokritos*
[4] *Department of Chemical Engineering, University of Patras*

4. MS

P. 35: Longitudinal plant health monitoring via HRMS screening workflows
A. Panara, E. Gikas, A. Koupa and N.S. Thomaidis
Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens

P. 36: Pesticide residues tracing control in green leafy vegetables using HRMS technologies
D. Gkountouras[1], V. Botia[2,3] and T. Albanis[1,2,3]
[1] *Department of Chemistry, University of Ioannina*
[2] *Institute of Environment and Sustainable Development, University Research Center of Ioannina (URCI)*
[3] *Unit of Environmental, Organic and Biochemical high-resolution analysis-Orbitrap-LC*

5. Sample Handling

P. 37: Microsampling and modern sample preparation techniques in bioanalysis for clinical research
L. Kujovská Krčmová[1,2], Ch. Suwanvecho[1,2], D. Turoňová[1,2], K. Matoušová[1], M. Matysová[2] and F. Švec[2]
[1] *Department of Clinical Biochemistry and Diagnostics, University Hospital*
[2] *Department of Analytical Chemistry, Faculty of Pharmacy in Hradec Kralove, Charles University*

P. 38: Synthesis, characterization and comparison of four FPSE media for the extraction of antidepressant drugs in aquatic samples
C. Chrimatopoulos, N. Stroutzou, E. Iliadis and V. Sakkas
Department of Chemistry, School of Sciences, University of Ioannina

P. 39: Optimization of ultrasound-assisted extraction (UAE) for the recovery of phenolic compounds from basil and lemon balm byproducts and identification of their phytochemical profile by IR and LC-MS/MS
T. Tsiaka[1], D. Giannis[1], G. Koletsou[1], S. Theofilatos[1], D. Zotos[1], N. Stavropoulou[1], P. Zoumpoulakis[1], I.F. Strati[1], V.J. Sinanoglou[1] and M. Giannakourou[1,2]
[1] *Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica*
[2] *Laboratory of Food Chemistry and Technology, School of Chemical Engineering, National Technical University of Athens*

P. 40: Towards the valorization of distillation byproducts from Mediterranean herbs by implementing ultrasound-assisted extraction (UAE) and experimental design (DOE) models

T. Tsiaka[1], A. Kanioura[1], S. Pilatos[1], I. Roussos[1], G. Vountzouklis[1], N. Stavropoulou[1], E. Gogou[2], P. Zoumpoulakis[1], I.F. Strati[1] , V.J. Sinanoglou[1] and M. Giannakourou[1,2]
[1] Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica
[2] Laboratory of Food Chemistry and Technology, School of Chemical Engineering, National Technical University of Athens

P. 41: Edible oil-based dispersive liquid–liquid microextraction prior to HPLC-UV for the determination of naproxen in milk and dairy products

N. Al Mamari and U. Alshana
Department of Chemistry, College of Science, Sultan Qaboos University

Poster Session 2

Tuesday 19th of September 2023
Imperial Hall Room 3

Environmental Analysis – Food Analysis – Materials Characterization – Archaeometry – Advanced Spectrometric Techniques

1. Environmental Applications

P. 42: Comparison of two Portable and Modular Gas Generators of ppb-levels of Formaldehyde for calibration of analysers and sensors
A. Becker[1], A. Granjean[1,2], C. Sutter[1], M. Wolf[1], F. Amiet[2], D. Bazin[2] and S. Le Calvé[1]
[1] ICPEES – CNRS/University of Strasbourg
[2] Chromatotec

P. 43: Targeted analysis and information data acquisition evaluation for organic contaminants determination
L. Haroune[1], S. Saibi[1] and H. Cabana[2]
[1] Sherbrooke Pharmacology Institute, Sherbrooke University
[2] Sherbrooke University Water Research Group, Department of Civil and Building Engineering

P. 44: Bioleaching of scandium from bauxite residue using different microorganisms
K. Kiskira[1], Th. Lymperopoulou[2], L.A. Tsakanika[1], Ch. Pavlopoulos[3], K. Papadopoulou[3], El. Chatzitheodoridis[4], K.M. Ochsenkühn[1], G. Lyberatos[3] and M. Ochsenkühn-Petropoulou[1]
[1] Laboratory of Inorganic and Analytical Chemistry
[2] Products and Operations Quality Control Laboratory
[3] Laboratory of Organic Chemical Technology, School of Chemical Engineering
[4] Laboratory of Mineralogy, Petrology and Economic Geology, School of Mining and Metallurgical Engineering, National Technical University of Athens

P. 45: Spectroscopic and chemical methods for monitoring humification during composting of vineyard and winery wastes
P. Manoli[1], Il. Rapti[1], Chr. Tzakou[1], G. Patakioutas[2], D. Hela[1, 3]
[1] Department of Chemistry, Laboratory of Industrial Chemistry, University of Ioannina, Greece
[2] Department of Agriculture, University of Ioannina, Greece
[3] Institute of Environment and Sustainable Development, University Research and Innovation Center, 45110, Ioannina, Greece

2. Food Analysis

P. 46: Assessment of enriched oils thermal stability after frying using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy
A.-G. Ioannou, T. Tsiaka, P. Zoumpoulakis and V. J. Sinanoglou
Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica

P. 47: Novel Natural Compounds as Putative Antimicrobials: A Computational Approach
E. Kritsi[1,2], I. Nikolaou[1], M. Markou[1], S. J. Konteles[1], P. Zoumpoulakis[1] and V. J. Sinanoglou[1]
[1] Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica
[2] Institute of Chemical Biology, National Hellenic Research Foundation

P. 48: Assessment of banana quality and shelf-life during ripening by generating prediction models
K. Aouant[1], E. Mouka[1], G. Ladika[1], V. J. Sinanoglou[1] and D. Cavouras[2]
[1] Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology,

University of West Attica
[2] Department of Biomedical Engineering, University of West Attica

P. 49: Comparative evaluation of strawberries fruits and leaves using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy
G. Ladika[1], I. Stephanaki[1], A.-G. Ioannou[1], I. F. Strati[1], V. J. Sinanoglou[1] and D. Cavouras[2]
[1] Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica
[2] Department of Biomedical Engineering, University of West Attica

P. 50: Determination of Heavy Metal in Food using an accredited ICP-MS method
E. Christoforou, D. Stefani, D. Kafouris and E. Christou
State General Laboratory, Ministry of Health

P. 51: Classification of Greek honeys according to their botanical origin using physicochemical properties and macro-elements profile
M.-A. Priakou[1], N. Maragou[2], E. G. Custodio Da Silva[3], M. Kostakis[2], L. Gialouris[1], M. Karvouni[2], A. Kostaki[1], M.-Ch. Serdari[1], E. Nastou[2], E. Kritikou[2], C. Santos Silva[4,5], M. F. Pimentel Avelar[3], N. Thomaidis[2] and M. Dasenaki[1]
[1] Laboratory of Food Chemistry, Chemistry Department, National and Kapodistrian University of Athens
[2] Laboratory of Analytical Chemistry, Chemistry Department, National and Kapodistrian University of Athens
[3] Department of Fundamental Chemistry, Federal University of Pernambuco
[4] Faculty of food sciences and Nutrition and Centre of Biomedical Cybernetics, University of Malta
[5] VTT Technical Research Centre of Finland Ltd

P. 52: Extraction of phenolic compounds from Crocus sativus L. by-products using Box- Behnken experimental design
E. Lykoudi, M. Chatzikonstantinou, T. Tsiaka and I.F. Strati
Department of Food Science and Technology, University of West Attica

P. 53: Study of goat milk adulteration with cow's milk using molecular and physicochemical methods
Th. Georgaraki, D. Houhoula, Ef. Tsakali, M. Chatzikonstantinou, N. Stavropoulou, D. Vougiouklaki and V. J. Sinanoglou
Department of Food Science and Technology, University of West Attica

P. 54: Study of experimental yogurt desserts with mountain tea, and a mixture of saffron, mastic and mountain tea
A. Siozou and I.G. Roussis
Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina

P. 55: Antioxidant and bio- activities of Debina white wine
S. Balaktsi and I.G. Roussis
Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina

P. 56: Quality characteristics of various Greek strained yogurts
S. Chli and I.G. Roussis
Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina

P. 57: Study of enriched white wines with mountain tea and a mixture of saffron and mastic
A. Siozou and I.G. Roussis
Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina

P. 58: Antioxidant and bio- activities of Cabernet Sauvignon and Vlahiko red wines
S. Balaktsi, M. Basalekou and I.G. Roussis
Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina, Greece

P. 59: Comparative analysis of edible fixed (carrier) oils with chromatographic techniques
E. Papakostopoulou, A. Psouni, K. Tsiantas, M. Katsanevaki, A. Venieri, V.J. Sinanoglou and I.F. Strati

Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica

P. 60: Assessment of quality characteristics and oxidative stability of Origanum majorana infused Extra Virgin Olive Oil

M. Katsanevaki, A. Venieri, A. Psouni, E. Papakostopoulou, P.K. Revelou and I.F. Strati
Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica

P. 61: Exploring the quality and safety of extra virgin olive oil using optical spectroscopy

E. Orfanakis[1,2], R. Kontzedaki[1,3], A. Philippidis[1], E. Charitoudi[1,4] and M. Velegrakis[1]
[1] *Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas (IESL-FORTH)*
[2] *Department of Materials Science and Technology, University of Crete*
[3] *Department of Chemistry, University of Crete*
[4] *Department of Physics, University of Crete*

P. 62: The isotopic approach to the authenticity of Cypriot Potatoes for strengthening their identity: Preliminary results

E. Ioannou Papayianni, E. Tzioni, C. Savvidou, C. Louka, C.Damaskinos, M.Tarapoulouzi and R. Kokkinofta
State General Laboratory of Cyprus

3. Archaeometry

P. 63: Characterization and consolidation of limestone using calcium hydroxide/carbonate nanoparticles: a case study in the archaeological site of Pella

K. Marnellou[1], V. Tsiridis[2], M. Stefanidou[2], A. Konstantinidis[2], E. Pavlidou[3], T.D. Karapantsios[1], P.K. Spathis[1] and I. Karapanagiotis[1]
[1] *Department of Chemistry, Aristotle University of Thessaloniki*
[2] *Department of Civil Engineering, Aristotle University of Thessaloniki*
[3] *Department of Physics, Aristotle University of Thessaloniki*

P. 64: A fully automated micro-LIBS system for 2D elemental imaging of marine shells for archaeological research

V. Pinon[1], N. Hausmann[2], D. Theodoraki[2], P. Siozos[1], A. Lemonis[3] and D. Anglos[1,4]
[1] *Institute of Electronic Structure and Laser, Foundation for Research and Technology*
[2] *Leibniz-Zentrum für Archäologie (LEIZA), Leibniz-Forschungsinstitut für Archäologie*
[3] *Biomimetic, Science and Technology Park of Crete*
[4] *University of Crete, Department of Chemistry*

4. Spectrometry

P. 65: Remote LIBS for real time evaluation of the operational condition of polymeric insulators on high voltage power transmission lines

O. Kokkinaki[1], P. Siozos[1], I. Liontos[1], K. Hatzigiannakis[1], M. Andrianakis[1], V. Piñon[1], S. Dellis[2], T. Anagnos[2], N. Mavrikakis[3], K. Siderakis[3], K. Mouratis[4], E. Koudoumas[4], G. Kantemiris[5], S. Couris[5] and D. Anglos[1,6]
[1] *Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas (IESL-FORTH)*
[2] *Raymetrics S.A.*
[3] *Islands Network Operation Department, Hellenic Electricity Distribution Network Operator S.A.*
[4] *Hellenic Mediterranean University, Department of Electrical Engineering*
[5] *Department of Physics, University of Patras*
[6] *Department of Chemistry, University of Crete*

P. 66: Non-destructive spectroscopy combined with chemometrics as a tool for Green Chemical Analysis of lignocellulose

M. Kulp, M. Kuhtinskaja, Ol.-St. Salm, E. Solomina and T. Lukk
Tallinn University of Technology, Dpt. of Chemistry and Biotechnology

P. 67: Optical spectroscopy & chemometrics as an analytical tool in fuel adulteration detection
N. Fragkoulis[1,2], E. Koliou[1,3] and P. Samartzis[1]
[1] *Institute of Electronic Structure and Laser, Foundation for Research and Technology – Hellas (IESL-FORTH)*
[2] *Department of Chemistry, University of Crete*
[3] *Department of Material Science, University of Crete*

P. 68: Analysis of Platinum Group Elements in Water Samples by Energy Dispersive X-Ray Fluorescence
G. Vlamaki and N. Kallithrakas-Kontos
Analytical and Environmental Chemistry Laboratory, School of Mineral Resources Engineering, Technical University of Crete

P. 69: Occurrence of pharmaceuticals residues in surface waters using high resolution mass spectrometry-environmental risk assessment
I. Stavropoulou[1], Ch. Tsoutsi [1,2], and T. Albanis [1,2]
[1]*Department of Chemistry, University of Ioannina*
[2]*University Research Center of Ioannina (URCI), Institute of Environment and Sustainable Development*

P. 70: Risk assessment approach of elemental impurities in in Oral contraceptives pills
Haya S. Al Zeer[1], Monerah A. Altamimy[1], Ahmed I. Al-Ghusn[1], Yahya M. Al Shehry[1], Fahad S. Al Dawsari[1]
[1]*Reference Laboratory for Medicines and Cosmetics (RLMC), Saudi Food and Drug Authority (SFDA), Riyadh 12843-7116, Saudi Arabia*

5. Materials

P. 71: Hydration study of Portland-limestone cements containing aluminum -containing admixtures with a combination of isothermal calorimetry and FTIR spectroscopy
K. Sotiriadis[1], L. Zárybnická[1], P. Mácová[1], A.S. Mazur[2] and P.M. Tolstoy[2]
[1] *Institute of Theoretical and Applied Mechanics of the Czech Academy of Sciences*
[2] *St. Petersburg State University, Center for Magnetic Resonance*

P. 72: Influence of limestone as main constituent in Portland cement on the chloride ingress in pastes exposed to sulfate-chloride solution assessed by Raman and NMR spectroscopy
P. Mácová[1], K. Sotiriadis[1], A.S. Mazur[2] and P.M. Tolstoy[2]
[1] *Institute of Theoretical and Applied Mechanics of the Czech Academy of Sciences*
[2] *St. Petersburg State University, Center for Magnetic Resonance*

P. 73: Optical properties of carbon dots derived from *Posidonia oceanica*
S. Katsantonis[1] and K. V. Kordatos[1]
[1] School of Chemical Engineering, Department of Chemical *Sciences, National Technical University of Athens*

ABSTRACTS ORALS

Honorary Talk

Advanced Spectroscopic Techniques: Origins and Future

Gary M. Hieftje

Department of Chemistry, Indiana University, Bloomington, IN 47405, USA

E-mail: hieftje@indiana.edu

Spectroscopic techniques, like most analytical methods, generally advance by means of an evolutionary process; incremental innovations result in progressive improvements in performance, user-friendliness, and utility. Conveniently, this sort of process lends itself to realistic extrapolation, fostering further innovation and simplifying such practical matters as market prediction and the preparation of "future-oriented" lectures. However, a few advances seem disruptive; they were not earlier anticipated, appear to have come from nowhere, yet have a major impact. Such developments would seem to be impossible to predict. Yet, their origins can be traced, albeit often to unrelated events, external pressures, and unanticipated needs [1]. In this lecture, the origins of several spectroscopic techniques will be examined to identify factors and earlier occurrences that led to their current prominence; in turn, modern needs and pressures (e.g. growing populations, energy shortages, climate change) will be combined with several earlier and recent developments (e.g., artificial intelligence, quantum entanglement, optical modulation) to suggest advanced spectroscopic techniques that are likely to grow in importance and others that might lie on the horizon.

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Invited OP 1

Are Per- and Polyfluoroalkyl Substances (PFAS) Eternal?

H. Frank

Bayreuth Center of Ecology and Environmental Research (BayCEER), University of Bayreuth, D-95440 Bayreuth, Germany

E-Mail: Hartmut.Frank@uni-bayreuth.de

The chemically and thermally highly stable per- and polyfluorinated aliphatic compounds are to be regarded as witness and vestige for future generations of the impact of our industrial civilization, as markers of the anthropocene [1]. A typical example is the extremely stable trifluoroacetate (TFA) which is produced as specialty solvent for fluoropolymer chemistry or as catalyst and reagent in analytical and peptide chemistry, and which arises as atmospheric degradation product of some alternative fluorocarbon refrigerants/propellants [2] or from the mineralization/metabolism of increasingly popular trifluoromethylated pesticides (e.g. trifluralin) or therapeutic agents (e.g. the anti-malaria drug mefloquine) [3]; at the same time, it was surprising when in 1994 TFA was found to occur widely in non-polluted environmental media [4] and to occur naturally in great quantities [5]. Other examples are the per- and polyfluoroalkyl substances which have been in use in the textile and paper industry since more than half a century as „anti-stick“ substances, mainly as water- and grime-repellents for outdoor clothing, for water- and fat-repellent coatings of wrapping papers, and for foamstabilization in fire fighting; they have found numerous other minor applications in the galvanic industry, in the production of fluoropolymers, as additive of specialty lubricants, and they have been used even in cosmetics. Many isomers and homologues (more than 4000) are known, with the two lead compounds perfluorooctanoate (PFOA) and perfluorooctanesulfonate (PFOS) being monitored since the beginning of the century [6,7]; besides originating from industrial spills or fire fighting liquids, they are released in a diffusive way with waste waters and, as persistent organic pollutants, accumulate in the hydrosphere to occur ubiquitously in the aquatic biota [8].

Both chemical classes are under severe scrutiny for being reduced or forbidden in the EU due to their great persistence and potential hazards to human and ecological health; major disputes concerning trace-analytical-method accuracy, the correctness of results, and their interpretation exist; economic and ethical issues associated with regulation are also relevant.

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Invited OP 2

Wastewater surveillance for public health using advanced analytical approaches

Nikolaos S. Thomaidis

Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, 15771, Athens, Greece

E-mail: ntho@chem.uoa.gr

Wastewater-based Epidemiology (WBE) is a non-invasive, continuously developing scientific tool, with the potential for monitoring real-time data on illicit and licit drug consumption, chemical exposure and public health, providing geographical and temporal trends. WBE has been used widely over the last 20 years to reflect the effect of socioeconomic changes and public health crisis on population's mental and physical health. Over the last 3 years, it has gained global attention, for the prevention and control of the COVID-19 pandemic and has been included more systematically in the national surveillance strategies. SARS-CoV-2 genetic traces, parent drugs and their metabolites end up in Wastewater Treatment Plants (WWTPs) and their determination in influents provides data about COVID-19 prevalence and drugs consumption, supporting public health authorities with valuable data. Biomarkers of public health (parent compounds and their metabolites) were identified and quantified from 2010 until today in the WWTP of Attica (Greece), and the detected concentrations were back-calculated into normalized population loads and consumption. LC-MS/MS methodologies and HighResolution Mass Spectrometry (HRMS) accompanied by novel data treatment tools were used to identify known and unknown compounds. In addition, SARS-CoV-2 levels have been monitored daily since 2020 by analyzing influents from the same WWTP, and correlated with chemicals' (e.g. pharmaceuticals, illicit drugs, antimicrobials, surfactants etc.) patterns.

Invited OP 3

Optical fiber chemosensors for trace detection in the gas and liquid phase

Stavros Pissadakis

Foundation for Research and Technology - Hellas (FORTH),
Institute of Electronic Structure and Laser (IESL), N. Plastira 100, Heraklion 70013, GREECE

E-mail: pissas@iesl.forth.gr

Chemosensing is a fundamental functionality of contemporary optical fiber sensors (OFSs), while finding applications in the domains of industrial instrumentation, environmental monitoring, biomedicine, safety/security and defence. For attaining chemosensing functionalities using OFSs, relevant research should be directed into the elaboration of new transduction materials, and into the design and fabrication of sensitive optical platforms for tracing the changes occurring in those transductors. There is a lot of interest grown on optical fiber chemosensors, prompted by the emerging need of portable/wearable sensing devices, which can address a number of cumbersome analytical processes, while offering comparable sensitivity/selectivity and lower operational cost [1]. In this review, advances on the field of optical fiber chemosensors will be presented, examining sensing probes for the detection of organic substances primarily found in the gas phase, while employing a diverse number of transduction materials (oxides, hybrid matrixes, polymers), optical platforms (Bragg and long period gratings, Fabry-Perot resonators), and relevant interaction mechanisms (physisorption, chemisorption or piezotronic effects). Upon combination of transduction materials and optical read-out configuration detectivities of the order of ppm, or lower are achieved, with interaction times varying between few to ten of minutes [2-6]. Additional examples will be given on the use of optical fiber chemosensors in the liquid phase [7-9], where interaction mechanisms and detection protocols differ, since the refractive index and loss figure of the analyte are manifold higher than those of the gas phase, supporting interaction mechanisms of scattering or diffusion.

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Sensors and Biosensors

(Various applications except life sciences)

Oral Presentation 1

Dipstick coated with polystyrene-silica core-shell particles for the detection of microbiological fuel contamination

J. Bell, E. Climent, R. Gotor, C. Tobias, P.M. Martin-Sanchez, and K. Rurack

Bundesanstalt für Materialforschung und prüfung (BAM),
Richard-Willstätter-Str. 11, 12489 Berlin, Germany

E-Mail: jeremy.bell@bam.de

Microbial contamination of fuels by fungi or bacteria poses risks such as corrosion and fuel system fouling, which can lead to critical problems in refineries and distribution systems and has a significant economic impact at every stage of the process. Many factors have been cited as being responsible for microbial growth, like the presence of water in the storage tanks. In fact, only 1 % water in a storage system is sufficient for the growth of microorganisms like bacteria or yeasts, as well as for the development of fungal biomass at the oil/water interface.[1]

This work presents a rapid test for the accurate determination of genomic DNA from aqueous fuel extracts. The detection is based on the use of polystyrene-mesoporous silica core-shell particles onto which modified fluorescent molecular beacons are covalently grafted. These beacons contain in the hairpin loop a target sequence highly conserved in all bacteria, corresponding to a fragment of the 16S ribosomal RNA subunit. The designed single-stranded molecular beacon contained fluorescein as an internal indicator and a quencher in its proximity when not hybridized. Upon hybridization in presence of the target sequence, the indicator and the quencher are spatially separated, resulting in fluorescence enhancement. To perform the assay the developed particles were deposited on different glass fibre strips to obtain a portable and sensitive rapid test. The assays showed that the presence of genomic DNA extracts from bacteria down to 50–70 µg L^{-1} induced a fluorescence response. The optical read-out was adapted for on-site monitoring by fitting a 3D-printed case to a conventional smartphone, taking advantages of the sensitivity of the CMOS detector. Such embedded assembly enabled the detection of genomic DNA in aqueous extracts down to the mg L^{-1} range and represents an interesting step toward on-site monitoring of fuel contamination.[2]

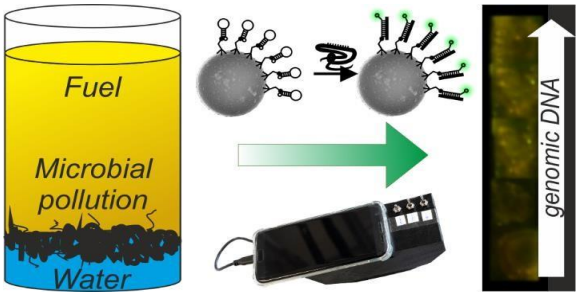

Figure 1. Detection of microbial genomic DNA in aqueous extracts using fluorescent molecular beacons grafted to core/shell particles utilizing a mobile device.

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Oral Presentation 2

Fluorescence detection of perfluoroalkyl carboxylic acids with a miniaturised assay

Yijuan Sun, Víctor Pérez-Padilla, Virginia Valderrey, Jérémy Bell, Kornelia Gawlitza and Knut Rurack

Bundesanstalt für Materialforschung und prüfung (BAM),
Richard-Willstätter-Str. 11, 12489 Berlin, Germany

E-mail: yijuan.sun@bam.de

Per- and polyfluoroalkyl substances (PFAS) are a class of man-made organo-fluorine chemicals that have become environmental contaminants of emerging concern, originating from a variety of materials such as adhesive, stain- and oil-resistant coatings, firefighting foams, etc. The high strength of this C-F bond makes PFAS thermodynamically stable and resistant to (bio)degradation, thus retaining them in the environment over time. Perfluoroalkyl carboxylic acids (PFCAs), one category of the most used PFAS, consist of a fully fluorinated carbon backbone and a charged carboxylic acid headgroup, and have been classified as Substances of Very High Concern (SVHC) and added to the REACH Candidate List due to their persistence in the environment, non-biodegradability and toxicological effects.[1-2] Traditional techniques for the analysis of PFCAs include GC-MS, HRMS and HPLC-based approaches, which are laborious, not portable, costly and require trained personnel. In contrast, fluorescence assays can be designed as easy-to-operate, portable and cost-effective methods with high sensitivity and fast response. Integration of fluorescent probes with an adequately miniaturized assay enables a promising alternative for PFCAs analysis.

Here, a novel guanidine fluorescent probe has been synthesized and fully characterized for the detection of PFCAs in a biphasic extract-&-detect assay. The fluorescent probe was then incorporated into polymeric matrices supported by a red dye-doped SiO_2 nanoparticle to construct a dual-emission sensing platform. Such a system allows precise and selective detection of PFCAs, reducing the interference of competitors, matrix effects and other factors except for the PFCAs. The system was then employed in a droplet-based microfluidic setup which offers a portable and easy to operate detection platform.

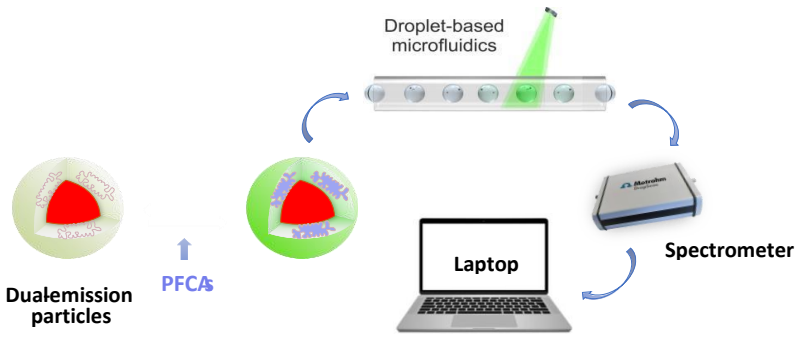

Figure 1. Detection of PFCAs with dual-emission core-shell particles via a droplet-based microfluidic setup

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Oral Presentation 3

Fabrication of graphene-based Inkjet printed subzero temperature sensor for cold storage monitoring

Saurabh Soni[1], Pushkar Sathe[1] and Dipti Gupta[1]

[1]Address- Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology, Bombay, Mumbai, Maharashtra 400076, India

E-mail: diptig@iitb.ac.in

Sub-zero temperature sensor is an ideal candidate for continuous and real-time monitoring of low temperature environments commonly found in the cold storage of food and beverage industries, refrigerators of pharmaceuticals or in polar-regions. Moreover, if such sensors are made flexible in nature, then they can become robust, conformable, wearable and highly stable against mechanical deformation[1-2]. Therefore, in our recent work, we developed highly flexible sub-zero temperature sensors and integrated them with interface electronics to demonstrate their wireless operation. For fabricating the sensors, we used inkjet printing due to its simple processing, volume manufacturing, cost effectiveness and compatibility with large area substrates. The sensor was built by using conductive graphene as temperature sensing material and polydimethylsiloxane (PDMS) elastomer as flexible substrate. The graphene film of thickness ~700 nm was obtained by printing and subsequently photonic curing of commercial graphene ink. The curing improved the conductivity of graphene film up to ~142 Sm^{-1} as shown in figure 1 (a) and resulted in its positive temperature coefficient of resistance within the temperature range between -30^{0}C and 80^{0}C. Photonic curing was also crucial to obtain the printed sensors on flexible substrate. Almost linear relationship was found between the temperature and resistance within the sub-zero range for which the sensitivity of the sensor was estimated to be ~ 0.12 %/°C as shown in figure 1 (b). The sensors demonstrated sufficient flexibility with a bending radius of approximately 25 mm and sustained 200 continuous bending cycles. Finally, we demonstrated the wireless operation of the sensors by wirelessly transmitting and monitoring the real-time temperature data over a smartphone platform. Through the use of inkjet printing and photonic curing, we have achieved a cost-efficient approach to fabricating sub-zero temperature sensors that can withstand high range of temperatures while maintaining their performance.

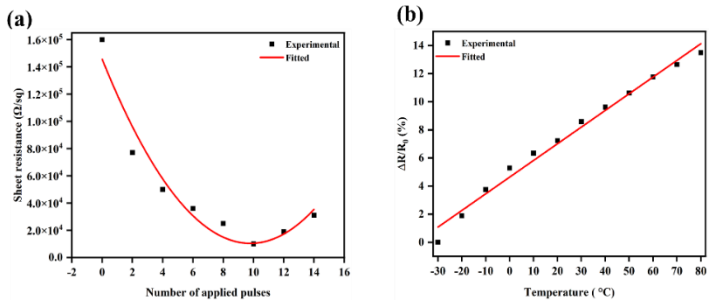

Figure 1. (a) Sheet resistance of printed graphene film at different nos. of applied photonic pulses. (b) Change in resistance (%) of the non-encapsulated sensor with temperature (from -30 to 80 °C),

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Oral Presentation 4

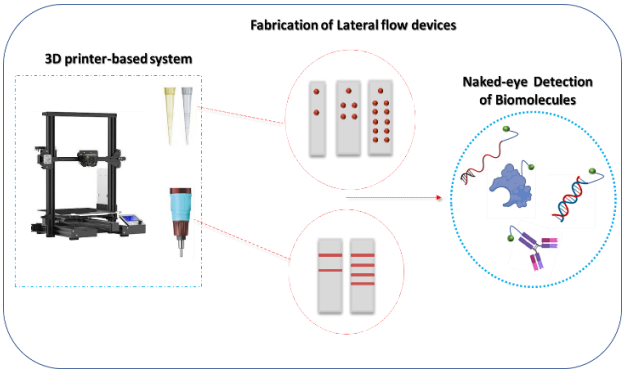
A home-made 3D printer-based dispensing system for the construction of lateral flow biosensors

Panagiota M. Kalligosfyri[1,*], Sotirios S. Tragoulias[1], Panagiotis Tsikas[1], Eleni Lamprou[1], Theodore K. Christopoulos[1,2] and Despina P. Kalogianni[1,*]

[1]Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras, GR26504, Rio, Patras, Greece
[2]Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE), Patras 26504, Greece

E-mail: kalogian@upatras.gr

Lateral flow assays (LFAs), mostly known as rapid tests, are at the forefront of bioanalysis because they combine the simple, fast, low-cost and portable analysis with their great analytical performance. COVID-19 era is one of the recent examples that LFAs proved their usefulness, as the rapid/self-tests became a part of our lives [1-2]. This unprecedented evolution of LFAs, over the last 3 years, requires the exploitation of new technologies and inexpensive materials for easy product manufacturing and fast analysis. Hence, in the present work the 3D printing technology is integrated, for the first time, with cost-effective materials (e.g. rapidographs, pipette tips) for the fabrication of the diagnostic areas of LFAs. We developed a simple and low cost dispensing system of reagents for both testing zones and sensing spots on the LFA. The biosensors were applied for the detection of different biomolecules (proteins, antibodies, single and double stranded DNA sequences). Also LFAs with multiple biosensing zones/spots were constructed for the simultaneous detection of different analytes. Our simple, automated and low-cost proposed system was finally compared with a commercial automated dispenser. The LFAs fabricated by the 3D printer-based system showed similar analytical performance, in terms of detectability and reproducibility, with the LFAs prepared by the commercially available system. In conclusion, we expect that the developed 3D printer-based system could be a very useful alternative that can be adopted by any research laboratory for the construction of biosensing areas of the LFAs for a variety of bioanalytical applications.



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Oral Presentation 5

Dipstick-type DNA sensing devices for rapid identification of olive oil cultivar origin

N-M. Christopoulou[1], E. Figgou[2], P. Kalaitzis[2], D. P. Kalogianni[1], and T. K. Christopoulos[1,3]

[1]Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras, Rio, Patras, Greece 26504
[2]Department of Horticultural Genetics and Biotechnology, Mediterranean Agronomic Institute, Chania (MAICh), Chania, Crete, Greece 73100
[3]Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE), Patras, Greece 26504

E-mail: tchrist@upatras.gr; kalogian@upatras.gr

The identification of the varietal origin of olives and olive oil is of particular importance because their sensorial characteristics and nutritional properties depend on the cultivar. Monovarietal oils have become the centre of interest for producers and consumers. Various DNA markers have been used for olive cultivar identification including genomic microsatellites, RAPD, ISSR, SCAR, AFLP and single-nucleotide polymorphisms (SNP) in combination with electrophoresis, microarrays or fluorescent microspheres and flowcytometry. Contrary to the above, we have developed dipstick-type sensing devices, for rapid identification of olive cultivar. The proposed analytical methodology comprises the following steps: (a) DNA extraction, (b) Quadruplex PCR for simultaneous amplification of two sequences from the cycloartenol synthase gene (179 bp and 170 bp) and two sequences from the lupeol synthase gene (162 bp and 145 bp). (c) Multiplex primer extension reaction using 8 allele-specific primers. A primer is extended only if perfectly complementary to the interrogated sequence. During extension, biotin-modified nucleotides are introduced in the new strands. Characteristic oligonucleotide sequences are attached to the primers for subsequent capture and detection. (d) The extension reaction mixture is applied to the conjugate pad of two dipstick-type DNA sensing devices, each enabling visual detection of 4 alleles of the cycloartenol synthase gene and 4 alleles of the lupeol synthase gene. Each device consists of an absorbing pad, for immersion in the appropriate buffer, a conjugate pad, on which antibiotin antibody-conjugated gold nanoparticles are deposited, and a sensing membrane containing 4 spots of immobilized oligonucleotide sequences. A red spot appears on the sensing membrane only if the primer has been extended, thus denoting the presence of the corresponding allele. The combination of the red spots in the 8 positions of the two sensing devices provides a characteristic DNA code (genotype) of the cultural variety of the olive or olive oil sample. The method was accurate and reproducible when evaluated on the following Greek olive varieties: Koroneiki, Kalamon, Tsounati, Adramytini, Chondrolia, Gaidourelia, Lianolia, Throumbolia and Kothreiki.

Acknowledgement: This research has been co-financed by the European Regional Development Fund of the European Union and Greek national funds through the Operational Program 'Competitiveness, Entrepreneurship and Innovation', under the call 'RESEARCH – CREATE – INNOVATE (project code: T2EDK-02637)'.

Invited OP 4

On-the-fly aptassays for neonatal sepsis diagnosis

A. Escarpa[1], J.M. Gordon[1], L. Arruza[2], M. Moreno[3], M.A. López[1]

[1]Department of Analytical Chemistry, Physical Chemistry, and Chemical Engineering. University of Alcalá, Madrid, Spain.
[2]Division of Neonatology, Instituto del Niño y del Adolescente, Hospital Clínico San Carlos-IdISSC, 28040 Madrid, Spain
[3]Department of Chemistry in Pharmaceutical Sciences, Analytical Chemistry, Faculty of Pharmacy, Universidad Complutense de Madrid. Avda. Complutense, s/n, 28040 Madrid, Spain.

E-mail: alberto.escarpa@uah.es

Diagnosis of neonatal sepsis is very challenging especially in very low birth weight infants, having so small blood volume and given their increased vulnerability to infection due to the immature immune system [1].

Micromotors represent one of the most exciting horizons in micro and nanotechnologies. The utilization of self-propelled micromotors in (bio)-chemical assays has led to a fundamentally new approach where their continuous movement around the sample and the mixing associated effect, greatly enhances the target-receptor contacts and hence the binding efficiency and sensitivity of the assay, even when using a very low sample volume. [2]

While catalytic micromotors covalently functionalized with antibodies have previously been used in the diagnosis of neonatal sepsis in our group [3-5], here we explore the possibilities of aptamers on board on micromotors for this type of diagnosis, due to their high stability, less variability between synthesis batches and very controlled post-production modification all without losing its selectivity and sensitivity.

In this talk, a novel on-the-fly aptassay using catalytic tubular micromotors constituted by graphene oxide-aptamer decorated as a sensing layer, an internal layer of Ni, and a catalytic layer of platinum nanoparticles will be conceptually presented for the determination of interleukin 6 and procalcitonin as relevant sepsis biomarkers [6-7]. The diagnosis capabilities of the MM technology for neonatal sepsis will also be discussed.

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Invited OP 5

Wax screen-printed fabric-based colorimetric microfluidic wearable (bio)sensors for the determination of biomarkers in sweat

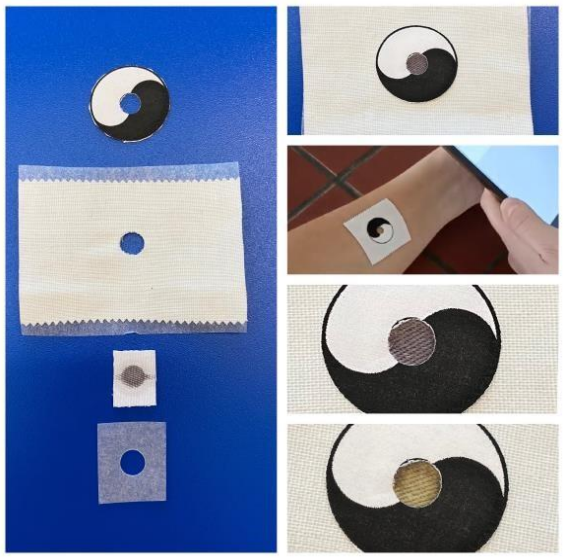
Mamas I. Prodromidis

Laboratory of Analytical Chemistry, University of Ioannina, 45 110 Ioannina, Greece E-mail: mprodrom@uoi.gr

Wearable sensors for healthcare monitoring offer a non-invasive, real-time analysis of biological samples. Fabric (cloth) is a very promising material for the development of wearable (bio)sensors due to its low cost, ability to transport fluid via capillary forces, flexibility, high tensile strength and durability, and biocompatibility. Hence, cloth is an ideal material for the development of economical and user-friendly diagnostic devices. The fabrication of cloth-based microfluidics has been implemented with various methods, such as weaving, wax-transfer printing, manual rubbering with solid wax through a screen, paper-aided wax printing, photolithography and stitching.

Here, we present the formulation of a screen-printing compatible wax-based thixotropic ink and the fabrication of low-cost microfluidic-based ink on cloth with an automatic, high throughput screen printing technique.

We have developed colorimetric wearable fabric-based (bio)sensors for the determination of different biomarkers in sweat. Sweat chloride, urea and pH are essential biomarkers, since they constitute indicators for cystic fibrosis, kidneys' malfunction, and dehydration. Research on the wax-based ink composition was accomplished by preparing inks in different solvents, thixotropic polymer solutions, and wax types and quantities.



Sweat analytes were determined by analyzing the color parameters of RGB and L*a*b* color spaces of the assay zones. The proposed colorimetric procedure for the determination of chloride ions depends on the chemical reaction between the chloride ions and silver chromate that causes the discoloration of silver chromate. The detection range was 10-100 mmol/L chloride which covers the normal range of chloride ions in sweat. For the determination of urea and pH, a shared approach was followed, based on the color change of a pH indicators blend. In the case of urea, enzymatically produced ammonia, due to the hydrolysis of urea in presence of urease, causes pH changes that relate linearly with the concentration of urea in sweat. Analytical data were calculated by the color analysis of images obtained by a scanner or a mobile phone using the open access software ImageJ.

Our future goal is to expand the application of our fabric-based wearable biosensors at other important biomarkers, thus enabling health experts and untrained users to monitor and manage health issues in a facile way outside the laboratory.

Sensors and Biosensors

(Life sciences/ Point of care systems)

Oral Presentation 6

Atrazine microfluidic biphasic colorimetric sensor based on barbiturate derivatives microcrystals dislocation

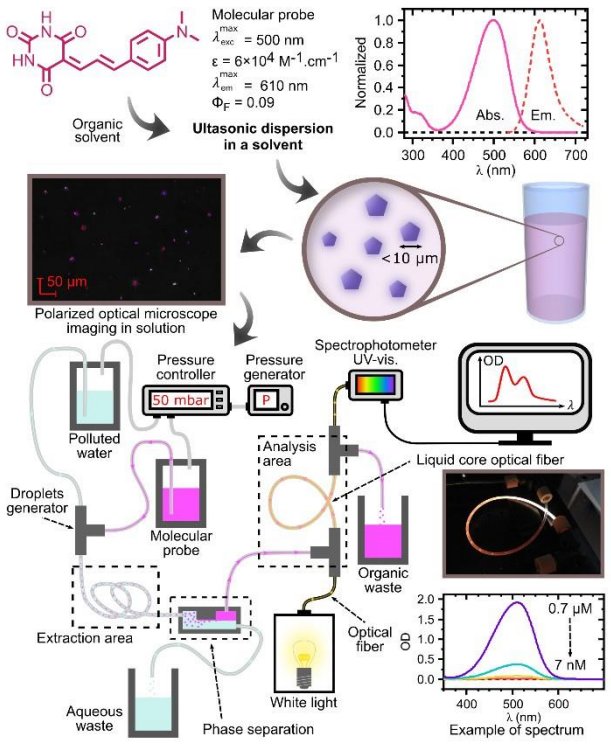
Hanh Linh Nguyen[1], Charlotte Rémy[1], Simon Le Luyer[1], Jean Pierre Lefévre[1,2], Clémence Allain[1], Isabelle Leray[1], Cédric Mongin[1]

[1] Université Paris-Saclay, ENS Paris-Saclay, CNRS, PPSM, 91190, Gif-sur-Yvette, France
[2]Conservatoire National des Arts et Métiers, 75003 Paris, France

E-mail: cedric.mongin@ens-paris-saclay.fr

The detection of polluting species in the environment (water, soil, air, food, manufactured products) is a major public health and environmental issue. Nowadays, many substances are classified as probable carcinogens, reprotoxic or mutagenic, while their utilization remains highly developed. This is particularly the case for certain herbicides/pesticides used in the agrifood industry such as glyphosate, atrazine or dicamba. The presence of residues in finished products, soils or water is strictly regulated by environmental standards, which tend to be more and more restrictive. However, if control standards are required, the available analytical techniques must match. This involves the development of analytical techniques that both address the issues of sensitivity, reliability and cost.

Among all the compounds available, Atrazine has been extensively employed in the intensive agri-food industry as herbicides over the past five decades. Despite its banning in the European Union since 2003 it is still in use in numerous countries around the world and it is widely present in the environment due to its remarkable retention in soil and poor solubility in water. This compound as well as its degradation products are highly toxic, potentially endocrine disruptor and carcinogenic.[1]



Therefore, to achieve efficient Atrazine quantification, numerous methods have been reported.[2-7] Here we present another approach using a microfluidic sensor based on phase-extraction combined with colorimetric recognition by micro- crystalline barbiturate derivatives.[8]

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Oral Presentation 7

Detection of microRNAs in urine samples by a visual lateral flow assay

Eleni Lamprou[1], Markos Sotiriou[1], Panagiota M. Kalligosfyri[1], Despina P. Kalogianni[1,*], Theodore K. Christopoulos[1,2]

[1]Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras, GR26504, Rio, Patras, Greece

[2]Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE), Patras, 26504, Greece

E-mail: kalogian@upatras.gr

MicroRNAs, along with circulating tumor DNA, circulating cancer cells and exosomes, are novel biomarkers in liquid biopsy applications. These biomarkers can be found in various body fluids such as saliva, urine, blood and cerebrospinal fluid. MiRNAs are particularly challenging analytes due to their very small size (18-25 nt) and their instability. Several methods have been already reported for miRNAs analysis. However, most of the methods are expensive and time consuming. On the other hand, biosensors have come to front in order to reduce the cost, the analysis time, the extensive sample preparation and the expensive instrumentation. Nanomaterials have also been exploited in biosensors for signal enhancement. In this context, we have developed a lateral flow assay for the visual detection of miRNAs in urine samples. MiR-21 and miR-let-7a were used as models for assay development The method includes i) isolation of miRNAs form urine samples, ii) amplification of miRNAs by reverse transcription – polymerase chain reaction (RT-PCR) and iii) detection of the amplified products by the lateral flow assay. Gold nanoparticles were used as reporters for visual detection. As low as 10^2-10^3 copies of miR-21 and 10^2-10^4 copies of miR-let7a spiked in urine samples were detectable by the this lateral flow assay. The proposed strip-based assay is simple and rapid, and provides visual detection by naked eye with good detectability and repeatability with %CVs < 4.5%. The proposed strip is also universal, meaning that it can be applied for the detection of any other miRNA sequence by simply changing the nucleic acids sequences used for amplification and detection.

Acknowledgements: This research has been co-financed by the European Regional Development. Fund of the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call RESEARCH – CREATE – INNOVATE (project code:T2EDK-02196)».

Oral Presentation 8

A molecular rapid test for SARS-CoV-2 quantitative detection

Panagiotis Maglaras[1], Ioannis Lilis[2,3], Fotini Paliogianni[3], Vasiliki Bravou[4] and Despina P. Kalogianni[1,*]

[1]Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras, GR26504, Rio, Patras, Greece

[2]Department of Physiology, Faculty of Medicine, University of Patras, 26504 Rio, Patras, Greece

[3]Department of Microbiology, Medical School, University of Patras, Rio, Patras, Greece

[4]Department of Anatomy-Histology-Embryology, Medical School, University of Patras, 26504 Rio, Patras, Greece

E-mail: kalogian@upatras.gr

The pandemic of COVID-19 have brought self-/rapid tests in the very forefront and proved their grate usefulness. Developing novel COVID-19 detection methods is very important as rapid and accurate diagnosis is crucial to control the current pandemic and also the acquired knowledge can be exploited for future outbreaks [1-2]. We have here developed a novel rapid strip test for visual and quantitative detection of SARS-CoV-2. The novelty lies on the use of a DNA internal standard/competitor of SARS-CoV-2 sequence for quantification. The method includes i) RT-PCR of specific nucleic acid sequence, ii) hybridization of the PCR products to complementary DNA probes and iii) detection with the rapid test using gold nanoparticles conjugated to anti-biotin antibody as reporters for visual detection. The proposed test provided rapid visual detection and simultaneous quantification of SARS-Cov-2 virus in nasopharyngeal swab samples with high specificity, detectability and repeatability. Less than 10 copies of the virus was detectable by the rapid quantitative test. This novel molecular rapid test is simple and cost-effective, and it comprises a promising diagnostic tool.

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Oral Presentation 9

Multifold improvement of the detectability of lateral flow immunoassays via macromolecular crowding

N-M. Christopoulou[1], D. P. Kalogianni[1], and T. K. Christopoulos[1]

[1]Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras, Rio, Patras, Greece 26504

E-mail: tchrist@upatras.gr

Lateral flow immunoassays (LFIA) provide low-cost, simple, portable, and rapid point-of-need testing and therefore they have found numerous applications in health, environmental and food sectors. Usually, the user only needs to apply the sample on the device and wait for a short time for the results. During the COVID-19 pandemic, hundreds of millions of self-tests/rapid tests were (and still are) performed, every day, exclusively by LFIA, a fact that undoubtedly proves the unique advantages of LFIA. The weakness, however, of the immunosensors of this type is their low detection capabilities. A pressing challenge in LFIA is to improve detectability without compromising assay simplicity and practicality. Contrary to current strategies, that focus on improving detection capability through the synthesis and introduction of novel labels and/or multistep protocols, we have exploited, for the first time, the macromolecular crowding effect to modify and regulate the microenvironment of LFIA, thus promoting the interactions that are responsible for analyte recognition and signal generation while the solution migrates through the confining pores of the strip-pads by capillary forces. Because both infectious diseases and food allergies are, globally, major issues of public concern, as target analytes to investigate the effect of macromolecular crowding on the detectability of LFIA we chose the nucleoprotein of SARS-CoV-2 (the virus responsible for COVID-19), the *Streptococcus pyogenes* (Strep-A) antigen and the peanut allergen. The effect of >15 water soluble macromolecular crowding agents of various molecular masses and concentrations was studied. At the optimum conditions a 5-10-fold improvement of the signal was achieved reproducibly for all analytes without affecting the background, i.e., the nonspecific binding of the labeled particles to the test zone of the strips. The proposed approach is complementary to other methods of improving the sensitivity by using novel labels. Because biomacromolecular interactions have a fundamental role in all types of biosensors, we foresee that the proposed strategy will also find applications in other biosensors and analytical devices.

Invited OP 6

Biomimetic HPLC Measurements of Physicochemical Properties of Compounds to Predict in vivo Distribution and Toxicity

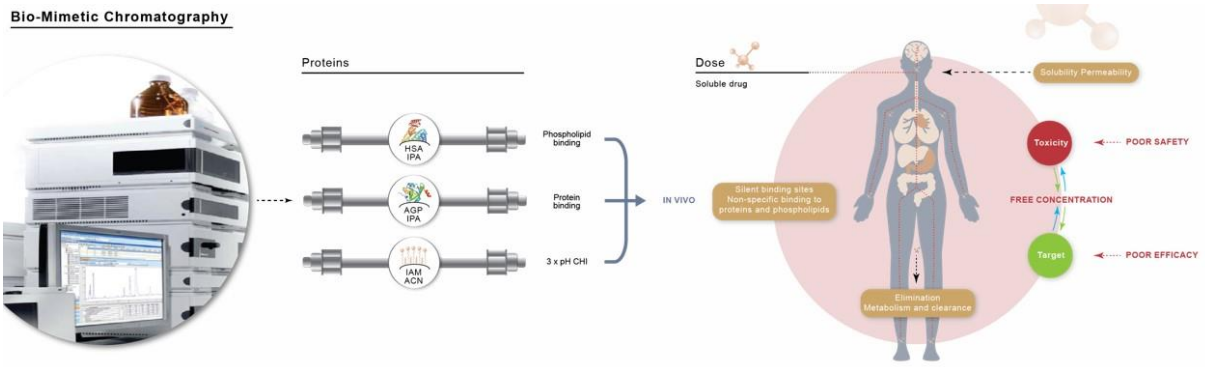
K. Valko[1] and B. Calvin[2]

[1]Bio-Mimetic Chromatography Ltd, BTC Stevenage, Herts SG1 2DX, United Kingdom
[2]Aseda Sciences, Kurz Purdue Technology Center 1281 Win Hentschel Blvd, Suite 1570
West Lafayette, IN 47906-4337, USA

E-mail: Klara_Valko@bio-mimetic-chromatography.com

The chromatographic separation principle is suitable for measuring the physicochemical properties of compounds using generic HPLC methods with standardized retention times. When phospholipids (IAM, immobilized artificial membrane) and proteins (albumin and glycoprotein) are used as stationary phases, the measured data can be used for predicting the toxicity and in vivo distribution of compounds. Thus, compounds' volume of distribution, brain tissue binding, lung retention, skin penetration, phospholipidotic and cardiotoxicity potential can be predicted.

These measurements will be part of an AI/machine learning (ML) platform developed by AsedaSciences®, which will integrate other high-content cellular and zebrafish embryo toxicity screens. The chromatographic, cellular and zebrafish screening results and associated MLbased predictions and visualization will be available on an AWS cloud-based platform called 3RnD®. Scientists from any academic Institution or drug discovery company will be able to compare the results for their own compounds to a library of thousands of compounds, helping to predict toxicity risk earlier. This approach helps scientists select safer scaffolds, understand SAR's impact, and prioritize safer compounds, improving R&D productivity by preventing later-stage attrition.



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Chromatography: Applications to life sciences and toxicology

Oral Presentation 10

UHPLC-FLD/PDA/MS/MS determination of new blood and urinary prognostic biomarkers in hospitalized patients with delta and omicron variant SARS-CoV-2 infection

L. Kujovská Krčmová[1,2], K. Matoušová[1], P. Šmahel[3], M. Skála[4], M. Gančarčíková[1], B. Melichar[5]

[1]Department of Clinical Biochemistry and Diagnostics, University Hospital Hradec Králové, Sokolská 581, Hradec Králové, 500 05, Czech Republic
[2]Department of Analytical Chemistry, Faculty of Pharmacy in Hradec Kralove, Charles University, Akademika Heyrovského 1203/8, 500 05, Hradec Králové, Czech Republic
[3]Deparment of Infectious Diseases University Hospital Hradec Králové, Sokolská 581, Hradec Králové, 500 05, Czech Republic
[4]Pulmonary Department, University Hospital Hradec Králové, Sokolská 581, Hradec Králové, 500 05, Czech Republic
[5]Department of Oncology, Palacký University, Faculty of Medicine and Dentistry, Olomouc, I.P. Pavlova 6, 77900, Olomouc, Czech Republic

E-mail: Lenka.Kujovska@fnhk.cz.

Inflammatory biomarkers neopterin, kynurenine, and tryptophan and their ratio were investigated, and evaluated their prognostic significance in hospitalized patients with COVID19. In 2021-22, we studied 108 hospitalized patients with COVID-19 at University Hospital Hradec Kralove, Czech Republic. Both variants, delta, and omicron were studied. Blood and urine sampling for the determination of selected markers were set at the beginning of the hospitalization. UHPLC-FLD/PDA/MSMS sensitive and specific methods were used for the determination.
Urinary and serum neopterin levels correlated ($r=0.775$, $p<0.0001$). We observed statistically significant ($p<0.05$) higher levels at admission of serum kynurenine/tryptophan ratio, neopterin, and kynurenine in the patients who needed oxygen therapy in the future during the hospitalization. Urinary markers measured at the beginning of the hospitalization were in group with a bad prognosis significantly higher. Blood markers confirmed the same trend as urinary. From our investigation, elevated neopterin, kynurenine, and kynurenine/tryptophan ratio at admission correlate with disease severity and bad prognosis, and it is possible to use urine as a noninvasively sampled bioliquid. Detailed data will be presented.

Acknowledgements: This work was supported by the Ministry of Health of the Czech Republic, grant nr. NU22- A- 108.

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Oral Presentation 11

Quantifying 1000 protein groups per minute of gradient using data-independent acquisition (DIA) on a hybrid quadrupole time-of-flight system

Gina Eagle[1], Dietrich Merkel[3], Nick Morrice[1], Ihor Batruch[2], Patrick Pribil[2]

[1]SCIEX, UK
[2]SCIEX, Canada
[3]SCIEX, Germany
Email: dietrich.merkel@sciex.com

High-throughput proteomic analysis has long been the goal of many researchers, and this workflow has been shown to work well using the Evosep One HPLC system when coupled to a variety of mass spectrometry systems. Data-independent acquisition (DIA) has become the standard method of analysis with many researchers. Using DIA on a hybrid quadrupole time-of-flight (QTOF) system gives incredible speed and sensitivity with very high quantitative precision, especially when the quantitation is performed on the MS2 transitions. It has been previously shown using a combination of the Evosep One and a QTOF system that impressive numbers of proteins can be identified and quantified from standard cell lysate digests using DIA. Here, we present this workflow using a conventional UPLC system at 5mL/min. The gradients used were designed to approximate the active gradient used on the Evosep One system, and cell lysate digests were separated on a 150 mm x 0.3 mm microflow column in trap/elute mode. A trap/elute method was designed using a 5-minute active gradient and 11 minutes total run time to mimic the Evosep 100 SPD method. Using human cell lysates of K562 and HeLa and a 200 ng on-column load, approximately 5,000 protein groups could be quantified using DIA, which is approximately 1,000 protein groups per minute of active gradient. These analyses were very robust with about 90%95% of proteins being quantified with a CV <20%. These analyses were not restricted to human cell lines, as impressive data were also obtained with a yeast proteome sample where over 3,100 protein groups could be quantified in 5 minutes. To visualize the data obtained from DIA-NN software, we used a cloud-based software suite to import the .tsv output file, followed by statistical analyses to show differential protein expression.

Oral Presentation 12

CE-ICP-MS/MS in a duty of the changes examination of liposomal cisplatin delivery systems

M. Matczuk, A. Wróblewska, J. Samsonowicz-Górski

Chair of Analytical Chemistry, Faculty of Chemistry, Warsaw University of Technology, Stanisława Noakowskiego 3, 00-664 Warsaw

E-mail: magdalena.matczuk@pw.edu.pl

Although cisplatin is an anticancer drug often used in the chemotherapy of various malignancies for many years, its non-selective transportation into cells results in severe therapy side effects. Non-toxic nanomaterials such as liposomes can be used to provide targeted delivery of this drug. In addition, biocompatibility (similarity to cell membranes), biodegradability, ease of synthesis and surface modification, and the ability to adjust the degree of drug encapsulation distinguish them from other nanomaterials considered as drug nanocarriers.

Moreover, ten liposomes–anticancer drug systems have already been approved for marketing, but none contain cisplatin in their composition. This situation may have resulted from using ineffective analytical tools for their characterization. Therefore, the goal of the study was, on the one hand, to develop a straightforward procedure for the formation of liposomes and effective encapsulation of the drug inside them and, on the other hand, to optimize the analytical method for their monitoring employing capillary electrophoresis (CE) combined with inductively coupled plasma tandem mass spectrometry (ICP-MS/MS).

However, the CE-ICP-MS technique has already been utilized to study liposome–cisplatin systems, the ICP tandem mass spectrometer has not been employed till now. Due to the applied apparatus configuration, the developed method can be used not only for the qualitative and quantitative monitoring of changes in the systems mentioned above but also for portraying their interactions with proteins, which opens up new analytical possibilities in the study of the trafficking mechanisms of these chemical entities.

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Oral Presentation 13

Chiral Discrimination in Capillary Electrophoresis: Explore the Potential of Deep Eutectic Solvents and Amino Acid-Based Ionic Liquids

K. A. Ioannou[1], G. D. Ioannou[1], A. Christou[1], I. J. Stavrou[2], M. G. Schmid[3], C. P. Kapnissi-Christodoulou[1*]

[1]Department of Chemistry, University of Cyprus, 1678 Nicosia, Cyprus

[2]Department of Life Sciences, European University Cyprus, 2404 Nicosia, Cyprus

[3]Department of Pharmaceutical Chemistry, Institute of Pharmaceutical Sciences, University of Graz, 8010 Graz, Austria

E-mail: ckapni1@ucy.ac.cy

"New psychoactive substances" (NPS) have recently gained great attention, as many of them are not listed in several national drug legislation as illegal substances. This has, in turn, led to an exponential increase in their derivatives. Slight modifications of the molecular structures of previously banned recreational drugs provide a wide variety of alternative, non-prohibited, synthetic derivatives with similar psychoactive properties [1]. Due to the existence of a stereogenic center in the structure of many NPS, there are two enantiomers for each drug, which one enantiomer may be active, while the other may be less active, inactive, or has adverse effects [1,2]. During this study, the effect of the combined use of amino acid-based ionic liquids (AAILs) and deep eutectic solvents (DESs) with either cyclodextrin- (CD) or cyclofructan- (CF) based chiral selectors (CSs) for the chiral separation of amphetamine derivatives was investigated. A non-significant improvement in enantiomeric separation of target analytes was observed when AAILs were combined with either CF or CD. On the other side, outstanding results were obtained using the dual CM-β-CD/DES system, highlighting the existence of a synergistic effect. Specifically, the dual CM-β-CD/DES system improved the enantiomeric resolution of amphetamine derivatives. The addition of 0.5% v/v of ChCl-EG to the BGE increased the resolution values of amphetamine (AMP), methamphetamine (MA) and 3-fluorethamphetamine (3-FEA) from 1.4, 1.1, 1.0 to 1.8, 1.8, and 1.5, respectively, leading to baseline separations for all amphetamine derivatives under study. This was not the case for the CF/DES dual system, which exhibited a worse separation of amphetamines, indicating an antagonistic effect. In addition, the proposed method can be successfully applied for the enantiomeric separation of more challenging species and then examine the pharmacological and toxicological activity of the individual enantiomers.

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Oral Presentation 14

Determination of cannabinoids in human cerumen by use of UPLCMS/MS as a potential biomarker for drug use

M. C. Christodoulou[1], M. S. Constantinou[2], A. P. Louppis[2], A. Christou[1], I. J. Stavrou[3], C. P. Kapnissi-Christodoulou[1*]

[1]Department of Chemistry, University of Cyprus, 1678 Nicosia, Cyprus

[2]Analytical Department, MC Analysis Centre LTD, 2563 Nicosia, Cyprus

[3]Department of Life Sciences, European University Cyprus, 2404 Nicosia, Cyprus

[*]Corresponding author. Tel.: (357) 22 892774; E-mail address: ckapni1@ucy.ac.cy

Over the years, conventional biological specimens such as urine, whole blood, and saliva have been commonly used for drug testing in the fields of toxicological and forensic analysis. In recent years though, there has been an increase in the use of alternative matrices such as nails, hair, breath, and cerumen, as they can provide additional information about the timeline of a drug use, but also, information of individual's health status, dietary habits, exposure to pollutants, as well as ethnicity and gender. In this study, a UPLC-MS/MS method was developed and validated for the determination of the concentrations of several cannabinoids in cerumen, including cannabidiol (CBD), cannabinol (CBN), Δ^9-tetrahydrocannabinol (Δ^9-THC), cannabichromene (CBC), cannabigerol (CBG), and 11-Nor- 9-carboxy- tetrahydrocannabinol (THC-COOH). The method was applied to samples collected from 14 cannabis users. Based on this study, in twelve out of fourteen cases, Δ^9-THC was found to be positive, while in six cases, three major cannabinoids, CBN, CBG and Δ^9-THC, were quantified at concentrations of 0.02–0.21 μg g^{-1}, 0.01–0.24 μg g^{-1} and
0.01–4.86 μg g^{-1}, respectively. In addition, a detection window for the substances Δ^9THC, CBN and CBG, in cerumen, was defined, with Δ^9-THC reaching a maximum detection frame of up to fifteen days after smoking 0.5 g of marijuana cigarette. The collected data were further evaluated by the use of ANOVA-one-way analysis. A significant difference in earwax production was observed between cannabis users and non-users ($p<0.05$). However, factors such as age, frequency, and the last time of use did not affect earwax production. They had though a significant impact on cannabinoid concentrations.

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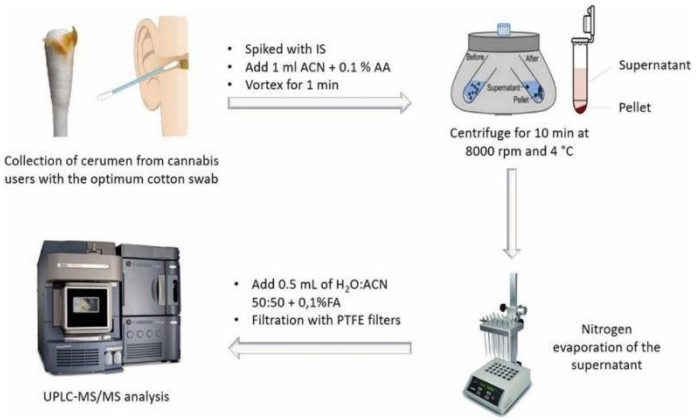

Figure 1: The whole experimental procedure until the analysis by UPLC-MS/MS.

Oral Presentation 15

Predicting the acute aquatic toxicity of UV-filter compounds used in cosmetic formulations

C. Stergiopoulos[1], K. Valko[2], F. Tsopelas[1], and M. Ochsenkühn-Petropoulou[1]

[1]Laboratory of Inorganic and Analytical Chemistry, School of Chemical Engineering, National Technical University of Athens, Greece
[2]Biomimetic Chromatography Ltd, Stevenage, Hertfordshire, UK

E-mail: chrisxp3@hotmail.com

Sun exposure is one of the most important factors in extrinsic skin ageing. The effects of sunlight on the skin are profound. They are estimated to account for up to 90% of visible skin ageing, particularly in people without the natural protection associated with higher levels of melanocytes in the skin. In 2005 more than 300 products were on sale claiming sun protection [1], containing more than 25 UV filter chemicals. Most sun protection products work by absorbing, reflecting, or scattering sunlight. Chemical UV filters have to be approved by FDA in the USA and are used in various sunscreen and cosmetic products. Sunscreen products can enter the marine environment directly (swimming & bathing) and indirectly (wastewater discharges). Because wastewater treatment plants cannot efficiently remove high concentrations of the organic UV-filters, and the natural degradation of these compounds is slow, they occur in the environment. Various studies describe adverse effects of UV filters on the marine environment and marine organism, including mortality, growth inhibition and reproduction failure due to endocrine disruption, coral bleaching and accumulation in food chains [2]. In our previous publications, the aquatic toxicity of pharmaceuticals has been modeled using the various measured and calculated properties of compounds [3]. It was found that using biomimetic HPLC measurements, compounds binding to phospholipids and proteins can be used to predict their aquatic toxicity. Biomimetic HPLC measurements using an immobilized artificial membrane (IAM), alpha-1-acid glycoprotein (AGP) and humans serum albumin (HSA) stationary phases provide a fast and reliable measurement of compounds' properties that can be related to their toxicity [4]. In this work, the phospholipid and protein binding of 13 compounds that are used in various sunscreen products were measured and their aquatic toxicity was predicted using published model equations [5]. It is highlighted that the UV-filter effect is and should not be related to the lipophilicity of the compounds that can consequently lead to their aquatic toxicity. The aforementioned conclusion could help in selecting those UV-filter compounds that have the smallest potential risk to the environment and the aquatic life in natural waters.

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Oral Presentation 16

Beyond Conventional Limits: Unlocking Varied Applications with an Innovative LCMS Ionisation Source"

J. Bucek[1], J.-C. Wolf[1], M. Weber[1] and C. Conway[1]

[1]Plasmion GmbH, Am Mittleren Moos 48, Augsburg, DE-86157, Germany

E-mail: jan.bucek@plasmion.de

The Cold Plasma Ionisation Source, commercially available as SICRIT® (Soft Ionisation by Chemical Reaction in Transfer), is a plug-and-play add-on compatible with any atmospheric pressure mass spectrometer (AP-MS) on the market. Its soft ionisation is founded on a combination of APPI, APCI, and ESI, which unlocks a brand-new potential for ionising a wide range of analytes using just one simple and user-friendly device. When looking at the applications, various possibilities emerge. In example a direct, fast, and fully quantitative screening, with target compounds ranging from illicit drugs [1] to PFAs [2] or food products [3], [4] may be a choice to develop a robust high-throughput MS-based approach.

Furthermore, SICRIT® makes typical LCMS coupling easier by delivering clean spectra with minimalistic fragmentation. This has already proven beneficial in the analysis of various types of lipids [5].

Lastly, a completely unique and innovative approach involves coupling GC to atmospheric mass spectrometry – a method typically used for LCMS. Not only does this break the status quo of the previously strictly separated GCMS and LCMS applications, but it primarily opens a way to use a soft and sensitive ion source where only EI and CI could have been applied before.

On top of all these advancements, the impact of replacing helium with hydrogen as a GC carrier gas, resulting in up to 50% faster analysis, will be presented [6].

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Electroanalytical techniques

Oral Presentation 17

From a screen-printed electrode to an industrial sensor for on-site measurement of Co and Ni

C. Parat, E. Ricard, S. Le Faucheur and I. Le Hécho

CNRS / Univ Pau & Pays Adour / E2S UPPA, IPREM, UMR5254, 2 avenue Pierre Angot, 64000 Pau, France

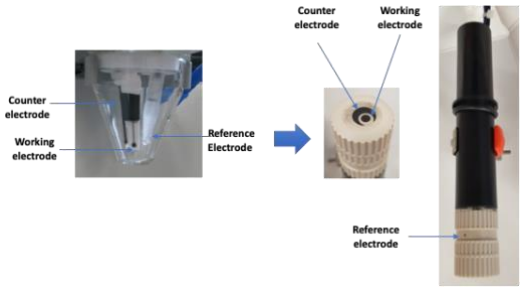
E-mail: corinne.parat@univ-pau.fr

In recent years, an increasing number of portable systems or kits for the *in situ* analysis of contaminants such as metals or pesticides have appeared on the market, but none of them allow for long-term monitoring in the field. There are many reasons for the lack of such a system, one of the main ones being the complexity of designing a robust and sensitive sensor for the targets of interest, that can be handled by unskilled personnel. Our team has overcome this challenge by transforming a conventional 3-electrode system (a working screen-printed carbon electrode (SPCE), a reference electrode and a counter electrode) into an all-in-one sensor for use in a flow measurement system for on-site trace metal monitoring.

The first part of this work focused on the modification of the 3-electrode system (Figure 1) to provide a robust and easy-to-handled sensor that allows the application of sensitive methods such as voltammetric methods. The main challenge in the design of the sensor concerned the working electrode, since, according to our specifications, this electrode must be easily replaceable for maintenance and usable for different metal monitoring application. The second part of the work focused on the simultaneous detection of Co and Ni by modifying the working surface SPCE with a bismuth film (Bi-SPCE). The detection of Co and Ni was carried out in 3 steps: (i) the Ni and Co ions were first complexed with dimethylglyoxime, (ii) the complexes were then accumulated on the surface of the Bi-SPCE and (iii) the stripping step was performed using linear scan voltammetry (LSV) [1]. Finally, the probe was tested on the pilot rivers of Lacq (Total Energies), a facility consisting of 16 artificial channels filled by the Gave de Pau river (France). During one month, the new sensor was deployed in the channels spiked with Co and Ni at 3 different concentrations (3, 6 and 30 µg/L).

This campaign has shown the robustness of the sensor in a real environment, its stability over 24 hours and its sensitivity to concentration variations, but also a strong effect of temperature on the Co signal. In summary, this device, which integrates sampling, filtration and measurement in a single step, has emerged as a promising tool for monitoring metal concentration in aquatic ecosystems.

A



B

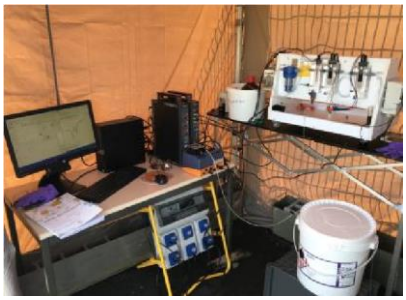


Figure 1. A - From SPCE to industrial sensor [2]; **B** – On-site measurement device

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Oral Presentation 18

What is the most appropriate electrochemical sensor for on-site pesticide analysis?

E. Ricard[1], D. Bégué[1], W. Lafargue-Dit-Hauret[1] and and C. Parat[1]

[1]CNRS / Univ Pau & Pays Adour / E2S UPPA,
Institut des sciences analytiques pour l'environnement et les matériaux, UMR5254, 2 avenue Pierre Angot, 64000 Pau, France

Email: estelle.ricard@univ-pau.fr

The analysis of pesticides in freshwater is a complex field of activity involving several steps, from sample collection to laboratory analysis, and requiring qualified personnel. To overcome these drawbacks, the development of sensors has been carried out, leading to increasingly complex electrochemical platforms to improve sensitivity and/or selectivity. The most efficient sensors are biosensors, based on antibodies or aptamers [1]. However, this type of sensor requires precise working conditions (temperature and composition of the analysis solution) which are not compatible with an on-site measurement. The analytical challenge is to develop a robust sensor that is easy to use for a field application and with a good sensitivity.

The purpose of these works was therefore to detect different pesticide molecules by means of a simple electrochemical platform with little or no modification. Two substrates, ie a carbonbased screen printed electrode (SPCE) and a gold modified SPCE, and 4 targeted molecules (glyphosate, diuron, isoproturon, thiabendazole) were selected. Each combination was tested under different analytical conditions in order to obtain the best sensitivity. Based on the work of Ren et al. [2] who showed the impact of Au nanostructure morphology on As(III) detection, different Au structures were also compared in terms of sensitivity and stability for the glyphosate detection. In parallel, a theoretical study aiming to model the interaction between each molecule with different electrode substrates has been performed.

Coupled experimental and theoretical investigations showed that (i) the sensitivity of the sensor could be improved by careful selection of the electrode substrate and the analytical conditions based on the chemical characteristics of the target and that (ii) a simple plateform resulted in a robust and easy-to-use sensor.

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Oral Presentation 19

A highly sensitive sensor for glyphosate detection based on the modification of a screen-printed carbon electrode by gold microstructures coated with a nanometric layer of polypyrrole

Q. Palas, E. Ricard, C. Parat, C. Lartigau-Dagron and L. Ronga

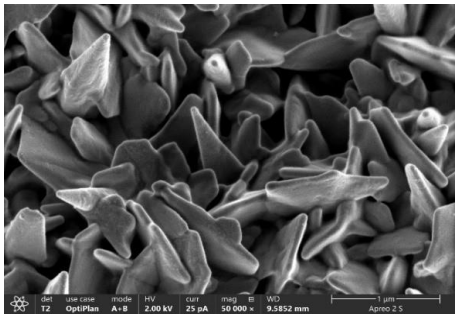
CNRS / Univ Pau & Pays Adour / E2S UPPA, IPREM, UMR5254, 2 avenue Pierre Angot, 64000 Pau, France
E-mail: quentin.palas@univ-pau.fr

Glyphosate, an extensively used herbicide, is frequently detected in surface waters and drinking water sources, leading to concerns about its potential impacts on human health and the environment. The International Agency for Research on Cancer (IARC) has classified glyphosate as "probably carcinogenic to humans," further intensifying these concerns. Consequently, there is an urgent need to develop techniques to continuously monitor the amount of glyphosate in drinking water.

Based on the previously reported evidence that glyphosate can be detected onto gold surface [1], a gold modified screen-printed electrode (Au-SPCE) was developed to directly detect glyphosate. By working on the structuration of the gold layer, this sensor showed a limit of detection (LOD) of 5µmol/L and a linear dynamic range from 10 µmol/L to 100 µmol/L. However, this detection range didn't respect the French limit for glyphosate in drinking water of 5 nmol/L.

In order to reach this limit (or to improve the LOD), this Au-SPCE was modified by the electrodeposition of a very thin polypyrrole layer (PPy), this polymer being previously used as a molecular-imprinted polymer for glyphosate [2-3]. Therefore, the electropolymerization of pyrrole on Au-SPCE in the presence of glyphosate was investigated and the ability of the derived electrode to directly detect glyphosate was assessed. Relevant structural properties of the electrode were highlighted by scanning electron microscopy (SEM) (Figure 1A) and the chemical composition of the layer was studied by X-ray photoelectron spectroscopy (XPS). This new reusable electrode allowed femtomolar detection of glyphosate in acetate buffer solution at pH 4.5 (Figure 1B), which appears promising for detection in drinking water.

a)



b)

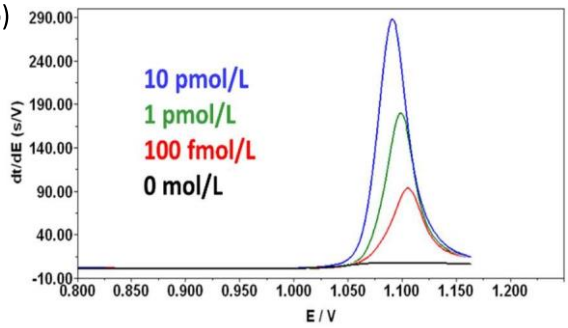


Figure 1. PPy-Au-SPCE: a) Scanning electron microscopy (50 000X), b) Potential stripping amperometryin the presence of different concentrations of glyphosate (100 fM-10 pM in 0.1 mol/L of acetate buffer at pH=4.5).

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Invited OP 7

Emerging facets of mass spectrometry for elemental speciation

Ryszard Lobinski[1]

[1] Institute of Analytical and Physical Chemistry for the Environment and Materials (IPREM), National Research Centre of France (CNRS), Hélioparc, 2, av. Pr. Angot, 64053 Pau, France
E-mail: Ryszard.Lobinski@cnrs.fr

The introduction of hyphenated techniques based on the coupling of a chromatographic separation technique with an element-selective atomic spectrometric was a game-changer in the field of chemical speciation analysis owing to the dramatic decrease of detection limits and increase in molecular specificity based on the retention time matching [1].

Inductively coupled plasma mass spectrometry (ICP MS) in particular, has gained a prominent place as detection technique. In combination with HPLC it allowed a number of exploratory studies for metal species and remains a fundamental technique in the field of metallomics [2].

Recently, the developments in high-resolution Fourier transform mass spectrometry have opened new horizons in studies of metal-binding species. The principal challenge of characterizing metal chelators in real world complex systems is the complexity of the organic mixture and the trace concentrations of specific metal chelates. High-resolution mass spectrometry approaches are able to overcome these issues by resolving molecular features across a large mass range and providing accurate mass information that can be used to identify isotope patterns for elements of interest.

The possibility to produce a cascade of product ion mass spectra to at least the MS4 level with the preservation of the isotopic pattern and the sub-ppm mass accuracy largely facilitates the elucidation of structure in de novo identification. There is, however, need for a careful optimization of analytical protocols in order to eliminate (or at least to account for) the formation of artefact metal complexes during chromatography and electrospray ionization.

Finally, an additional dimension to speciation analysis has been recently offered by ionmobility mass spectrometry which is particularly attractive for monoisotopic elements [3].

The lecture discusses the very recent contributions of different state-of the art mass spectrometric techniques (ICP MS/MS, FT MS and ion-mobility mass spectrometry) for speciation analysis in environmental chemistry, nutrition and life-sciences.

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Speciation Analysis

Part I

Oral Presentation 20

Mercury speciation in solid matter using thermal release in combination with elecrothermal atomic absorption spectrometry

O. Shuvaeva, I. Bekesha, D. Troitskii

Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences,
3, Lavrentiev prospect, Novosibirsk 630090, Russia

E-mail:olga@niic.nsc.ru

Mercury is an element involved in global processes occurring in Biosphere, the distribution of which in natural environments strongly depends on its chemical form. For this reason, the development of methodology for mercury speciation in various media is of particular value. In these terms the solid samples are the most problematic as traditionally used conventional analytical procedures include the species isolation from the matrix followed by their subsequent separation and element-selective detection. At that the extraction of the analytes is most critical stage, which may be accompanied by their loss or transformation. Moreover, it does not allow the isolation of water-insoluble species, for example, mercury sulfide. Therefore, the direct analysis with application of the thermal release as separation stage in combination with electrothermal atomic absorption detection (TR-ETA-AAS) seems very promising. At present moment, a number of issues remain that hinder its practical application as a reliable analytical technique.

In present work the thermal behavior of the most common mercury species as pure substances were studied as a starting point using a commercial instrument RA-915$^+$ (Lumex, Russia) modified by adding a module providing continuous increase in temperature with a subsequent stop until the thermal peak is formed. It was shown on the example of the mixture of methylmercury and mercury chlorides, mercury sulfide and mercury sulfate that the transformation of the studied compounds occurs under thermal exposure, which leads to a change in their physicochemical characteristics, but does not prevent their baseline separation [1]. The programmable heating and diluting by Al_2O_3 to eliminate matrix effects has been applied for analysis of real natural samples and standard reference materials (Fig.1). As a result the detection limits at the level of 2-5 ng (as mercury) were achieved.

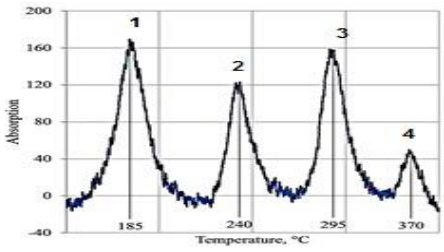

Fig.1. Thermospecrum of the mixture of $HgCl_2$,(1) CH_3HgC (2)l, HgS(3) and $HgSO_4$ (4) diluted by Al_2O_3 (1:4). Heating rate 15°C·min^{-1};Ar flow 0.2 L·min^{-1}

This work was supported by Russian Science Foundation (grant ID: 22-27-00684)

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Oral Presentation 21

Fish tissue multielement metallobiomolecule profiling method and its application to four commercially important fish species

G. Panagou[1], I. Kalantzi[2], M. Tsapakis[2] and S. A. Pergantis[1]

[1]Department of Chemistry, University of Crete, Heraklion, Greece

[2]Institute of Oceanography, Hellenic Centre for Marine Research, Heraklion, Greece

E-mail: georginapanagou@gmail.com

As seafood consumption is increasing rapidly showing an annual increment of approximately 3.1% from 1961,[1] it is crucial to evaluate health risks associated with high metal concentrations. However, knowledge of total metal concentrations in fish does not reveal much about metal species, metal distribution amongst biomolecules (metallobiomolecules), and thus the detailed metal behaviour in terms of toxicity and bioavailability.[2]

In this study, we report on the development of a novel extraction method for removing intact metallobiomolecules and inorganic metal species from freeze-dried fish tissue. This enables the extraction of sarcoplasmic proteins, such as heme proteins, and metallobiomolecules, soluble in low ionic strength aqueous buffers.[3] Extracts were analyzed by using online size exclusion chromatography with inductively coupled plasma mass spectrometry (SEC-ICP-MS). Using this approach metallobiomolecules are separated based on their molecular weight and selectively detected by their metal content and in some cases their heteroatom (S, P) content.

Metallobiomolecule chromatographic size profiles from the application of this methodology have been obtained for As, Se, Ni, Zn, Cu, Fe, Co, Mn, Cr, Cd, and Tl species in tissue extracts of four commercially important fish species: common pandora (*Pagellus Erythrinus*), red mullet (*Mullus barbatus*), European hake (*Merluccius merluccius*) and anchovy (*Engraulis encrasicolus*) collected between North Evia and Central Greece region. A quantitative approach is also being developed. These fish species have been previously analyzed for their total metal concentrations in tissues and intestines,[4][5] however, no information about their corresponding metallobiomolecule content has been provided.

Our results indicate a correlation between the metallobiomolecule profile of fish species and their habitat (benthic or pelagic). In addition, the correlation of each metallobiomolecule profile with fish gender was investigated. This approach is expected to contribute to further studies related to fish consumption risk assessment, studies of metal homeostasis in fish, environmental metal contamination studies, and even discovering optimum conditions required for the well-being of farmed fish.

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Acknowledgements

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Speciation Analysis

Part II

Oral Presentation 22

Development of a dedicated microsystem coupled to ICP-MS/MS for the selective capture and on-line quantification of uranium-target biomolecules

Marta Garcia-Cortes[1,$], Claude Vidaud[2], Monica Araya-Farias[3,#], Thuy Tran[3], Carole Bresson[1]

[1]Université Paris-Saclay, CEA, Service de Physico-Chimie, 91191, Gif-sur-Yvette, France
[2]Institut de Biosciences et Biotechnologies d'Aix-Marseille, BIAM, CEA-Marcoule, 30207 Bagnols Sur Cèze, France
[3] Université Paris-Saclay, CNRS, Institut Galien Paris Saclay, 91400, Orsay, France.
[$] Current address: Dpt. Analytical Chemistry, Faculty of Chemistry, Universidad Complutense de Madrid, 28040, Madrid,Spain
[#] Current address: Univ Paris Saclay, Dept Medicaments & Technol Sante MTS, CEA, INRAE,SPI, F-91191 Gif Sur Yvette, France

E-mail: carole.bresson@cea.fr

Uranium (U) is a ubiquitous element in the environment due to natural origin or anthropogenic activities. In case of contamination, the biokinetics of uranium is well described but the molecular mechanisms responsible for its toxicity are still poorly understood. The identification of proteins binding specifically uranium in its uranyl form (UO_2^{2+}) and the characterization of UO_2^{2+} interactions with these targets are essential to describe the mechanisms leading to its deleterious effects, and to develop selective decorporating agents.

Thanks to the implementation of Immobilized Metal Affinity Chromatography (IMAC) on micro-beads [1], several target proteins of UO_2^{2+} have been successfully isolated from extracts of human kidney-2 (HK-2) and dopaminergic (SH-SY5Y) cells [2] and recently from root and shoot extracts of Arabidopsis thaliana [3]. Nevertheless, this strategy still requires quite significant volumes of sample to perform replicates of analysis and induces consumption of toxic materials and waste production.

In order to address these issues, we have downscaled the IMAC method through the development of a separation microsystem [4] and its coupling to inductively coupled plasmatandem mass spectrometry (ICP-MS/MS). In particular, a functionalized monolithic support was synthetized *in situ* and locally anchored in the microchannels of a glass chip, to ensure the UO_2^{2+} immobilization needed for the IMAC separation mode. Based on a phosphorylated monolith dedicated to the preconcentration of phosphopeptides [5], we have adapted the composition of the reaction mixture of the support synthesis to reach appropriate properties such as permeability, porosity or specific area, consistent with our microsystem. Then, we have developed an *ad-hoc* on-line quantification method through the coupling of microsystem to ICP-MS/MS, to determine the UO_2^{2+} immobilization ratio within the microchannels and the performance of the on chip-IMAC method to capture reference proteins selective for UO_2^{2+}. For this, we took advantage of the ICP-MS/MS technology that enables the on-line simultaneous monitoring of the signals of U and the heteroatoms such as sulfur and phosphorous, naturally contained in the proteins selectively captured and eluted from the functionalized micro-channels. Hence, the proof of concept of the IMAC miniaturized method and the gain provided by the downscaling have been demonstrated.

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Oral Presentation 23

Detailed Arsenolipid Determination in BCR Reference Material using HPLC with high-resolution mass spectrometry and ICP-MS

M. Kapsi[1], K. Marmatakis[2], I. Kalantzi[1], M. Tsapakis[1] and S. Pergantis [2]

[1]Institute of Oceanography, Hellenic Centre for Marine Research (HCMR), Gournes - Pediados, Heraklion 70014, Crete,
[2]Environmental Chemical Processes Laboratory, Department of Chemistry, University of Crete, Heraklion 71003, Crete

E-mail: m.kapsi@hcmr.gr

Arsenic containing-lipids (arsenolipids) are novel natural products recently shown to be widespread in fish and marine food [1]. They are likely naturally biosynthesized by algae by a process of oxidative methylation. Fish is a major food; therefore, the concentration of compounds such as arsenolipids needs to be determined. This particularly challenging due to difficulty in isolating them from the lipid matrix and the lack of suitable standards and analytical techniques for their determination [2]. In this study, the certified reference material (CRM) BCR-627 Tuna Fish Tissue (4.8 ± 0.3 mg As per kg) was investigated for its AsLp content, both those that have already been identified as well as unknown forms. The objective is to provide detailed characterization of AsLp species present in a readily available reference material and thus enable its broader use for AsLp determinations in fish and other AsLp-related research conducted by the scientific community. Sample preparation involved extraction of AsLp with pyridine and purification with SPE using a silica gel column and methanol as elution solvent [3]. Gradient elution reversed-phase HPLC on-line with ICP-MS and ESI-Orbitrap-MS was used to gain information on the speciation of non-polar AsLp in BCR-627. The highresolving power of the Orbitrap was essential to identify and distinguish the all the arsenic species present in BCR-627, as indicated by the overlay of the ICP-MS elemental chromatograms and the accurate mass molecular ion signals from the ESI-orbitrap MS. Using this approach more than twenty AsLp were identified in extracts of BCR-627 including arseniccontaining fatty acids (AsFAs) and hydrocarbons (AsHCs). Both ESI-MS and ESI-MS/MS accurate mass spectra confirmed the proposed molecular compositions. All analyte elemental compositions were identified with a mass error less than 1.5 ppm. Among the AsLp detected, nine compounds have not been previously identified in BCR-627 in previous studies. Optimized parameters for AsLp speciation analysis, structure characterization and AsLp concentrations (μg As/g) of the different arsenic species will be presented. An approach for overlaying gradient elution reversed phase HPLC-ESI-MS accurate mass chromatograms, with those obtained using the same chromatography with ICP-MS detection will be presented. Up to 95% methanol in the mobile phase could be introduced into the ICP-MS without any need to add an O_2 gas.

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The research project was supported by *the Hellenic Foundation for Research and Innovation (H.F.R.I.)* under the "2nd Call for H.F.R.I. Research Projects to support Post-Doctoral Researchers" (Project Number: 692).

Oral Presentation 24

Novel interference removal strategies using Multi-Quadrupole ICP-MS/MS

H. Ernstberger[1], K. A. Jensen[2], E. Pruszkowski[3], and M. Petrich[4]

[1]PerkinElmer, Viale dell'Innovazione 3, 20126 Milano, Italy
[2]Faculty of Environmental Sciences and Natural Resource Management, Norwegian University of Life Sciences, 1432 Ås, Norway
[3]PerkinElmer, 940 Winter St., Waltham, MA 02451, United States
[4]PerkinElmer, Ferdinand-Porsche-Ring 17, 63110 Rodgau, Germany

E-mail: helmut.ernstberger@perkinelmer.com

The need for effective interference removal in ICP-MS has prompted over time a number of instrumental innovations permitting the use of collision or reaction gases. Recently, the specificity provided by a Multi-Quadrupole ICP-MS/MS system has resulted in new possibilities for interference removal and ionized cell gas removal. Following on outline of the key features of a Multi-Quadrupole ICP-MS/MS system, recently collected data on reactivity for a variety of reaction gases will be presented and the possibilities for novel interference removal strategies discussed.

Oral Presentation 25

3 ways to improve your daily lab routine with molecular spectroscopy — from QA/QC to advanced microscopy

M. Ries[1] and M. Klimovic[1]

[1]Thermo Fisher Scientific GmbH, Im Steingrund 4-6, 63303 Dreieich, Germany
E-mail: Maximilian.ries@thermofisher.com

Vibrational spectroscopy techniques hold significant interest in diverse applications, spanning QA/QC labs, forensic institutes, university research, and R&D departments across various industries. The molecular information extracted from vibrational spectra recorded through infrared and Raman spectroscopic techniques serves as a unique fingerprint of molecular properties and content distribution in mixtures. It also acts as a quality indicator for product monitoring and enables the identification of unknown materials based on their molecular signatures.

Nonetheless, the portfolio of instruments, techniques, and applications in this field is continuously expanding, rendering it challenging to comprehend without specialized expertise. The purpose of this presentation is to introduce Thermo Fisher Scientific's portfolio of infrared and Raman instruments, encompassing a wide range of applications. Additionally, the presentation will provide insights into software features and highlight microscopy solutions tailored to address advanced spectroscopic challenges.

Associations

Oral Presentation 26

EXSA: the European X-ray Spectrometry Association

D. Eichert[1,2] on behalf of EXSA Executive Committee[2]

[1]ELETTRA – Sincrotrone Trieste, S.S. 14 Km 163.5 in Area Science Park, 34149 Basovizza, Trieste, Italy
[2]Konkoly-Thege M. út 29-33. 26.ép.fsz.11., H-1121 Budapest, Hungary

E-mail: diane.eichert@elettra.eu, excom@exsa.hu

X-ray spectrometry field of research is composed by many X-ray based techniques, which allows to shed some light into the properties of matter, in a complementary way. From micro-analytical to spatially nanoresolved technique, and time-resolved to energy-resolved technique, a plethora of investigations can be undertaken for various types of materials, and in many fields of research. For instance, X-ray fluorescence techniques are used qualitatively as well as quantitatively for sensitive and simultaneous elemental analysis. XRS is especially well-fitted for contributing in addressing some global challenges such as in Energy, Nanoelectronics, Health, and Environment as well as for Cultural Heritage.

EXSA is a non-profit organization founded in 2004 for promoting cooperation and scientific exchanges between X-ray spectroscopists and analysts within Europe. It brings together users of X-ray spectrometry in various fields of research as well as manufacturers of X-ray instrumentation and developers of X-ray methodologies. EXSA aims to stimulate interaction and communication between young and experienced scientists, between academia and industry, thus fostering scientific progress and innovation.
EXSA supports the participation of talented young scientists in scientific events and coorganizes summer schools as well as dedicated workshops on novel and emerging X-ray spectrometry topics. In 2021, EXSA has put together its 1st Virtual Conference on X-ray Spectrometry, with four hot topics: XRS in environmental applications, XRS for novel materials including batteries, nanostructures, etc.; Instrumental development for XRS and its applications, and Fundamental parameters (https://www.exsa.hu/conf2021/). In October this year, EXSA is organising together with the LNHB (Laboratoire National Henry Becquerel, CEA Saclay, France), a school and workshop week event, on quantitative methods in X-ray Spectrometry. Details and programs of the past editions may be found at www.exsa.hu/quant2017 and www.exsa.hu/quant2019.
EXSA awards scientists for their exceptional contributions to the field of X-ray spectrometry. Two awards for young X-ray spectrometrists and one award for outstanding scientific achievements are bestowed usually during the EXRS conferences.
EXSA is supporting the Fundamental Parameters Initiative and its workshops (https://www.exsa.hu/fpi.php), aiming for better knowledge of FPs as an essential requirement for accurate quantitative X-ray Analysis.
EXSA gathers more than 125 members from academia and industry and is sponsored by more than 12 companies. Since its foundation, EXSA has supported more than 60 workshops and conferences, among them the IMA Conference 2019 and 2021.

For more information, please visit www.exsa.hu.

Oral Presentation 27

The role of the European Association of Professors Emeriti (EAPE)

Professor Sir Les Ebdon

President EAPE and Emeritus Professor, University of Bedfordshire, University Square, Luton, Bedfordshire, LU1 3JU, UK

Email: Les.ebdon@beds.ac.uk

Technological developments of the last 40 years, such as the world-wide web and artificial intelligence, have meant that information and disinformation have become commonplace. This places a premium on wisdom and the ability to discern fact from fantasy. Those academics who have been recognised as of professorial calibre but have now retired from paid employment, Professors Emeriti, have a great capital of knowledge and understanding that has often been under-utilised. Accordingly a group of distinguished Professors Emeriti, under the leadership of the famous Greek cardiologist Professor Dennis Cokkinos, established the European Association of Professors Emeriti (EAPE) some six years ago. The Association seeks to create or preserve ties amongst academics and retired professors all over Europe and world-wide. EAPE looks to encourage collaboration, research and academic meetings both virtual and in person. EAPE publishes, quarterly a prestigious Bulletin and holds a major Congress biennially. This talk will expand on the aims and achievements of EAPE and discuss its plans for the future. The COVID-19 pandemic has taught us that the role of the expert is not obsolete despite the democratisation of information and this theme will be further explored.

Oral Presentation 28

Why a EuChemS Working Party "Ethics in Chemistry"?

H. Frank

University Bayreuth

Email: Hartmut.Frank@uni-bayreuth.de

Science and technology strongly shape modern societies and their conditions, nationally and globally. Chemistry is a key science and technology in this process, contributing directly and indirectly to advancement of the wealth of nations. But the quantitative growth of material turnover also entails new risks. It is in the interest of chemists (as well as the societies at large including other scientists/professionals) to participate in finding the proper balance, together with policy makers, regulators, and agitators for sustainable and sound (chemical) progress, also for the sake of our reputation and acceptance by society. Therefore, awareness of the ethical, social and cultural dimensions of practicing chemistry is in the interest of us chemists and of society as a whole:

By

- Contributing to the professional discussion of chemistry-related ethical issues (Science Ethics)

- Elaborating codes of conduct, approaches of “good scientific practice”, and “chemical ethos” (Professional Ethics)

- Sharpening the awareness of chemists for ethical, social and legal implications of their professional practice, integrating these topics into education of chemists.

Invited OP 8

Quantitative Characterisation of Nano- and Microscaled Materials by X-ray Spectrometry

Burkhard Beckhoff

Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany
email: Burkhard.Beckhoff@PTB.de

Traceable characterization methods allow for the accurate correlation of the functionality or toxicity of nanomaterials with the underlaying chemical, structural or physical material properties. These correlations are required for the directed development of advanced materials at both the nano- and microscales to reach target functionalities such as conversion efficiencies or selective sensitivities. The reliable characterization of these materials requires techniques that often need to be adapted to the nano- or microscaled dimensions of the samples with respect to both the spatial dimensions of the probe and the instrumental or experimental discrimination capability. The traceability of analytical methods revealing information on chemical material properties relies on reference materials or qualified calibration samples, the spatial elemental distributions of which must be very similar to the nanomaterial of interest. At the nano- and microscales, however, there exist only few well-known reference materials. An alternate route to establish the required traceability lays in the physical calibration of the analytical instrument's response behavior and efficiency in conjunction with a good knowledge of the various interaction probabilities. This SI-traceable approach for x-ray spectrometry has been established by Germany's metrology institute PTB. For the elemental analysis, speciation, and coordination of nanomaterials, such a physical traceability can be achieved for x-ray spectrometry. This requires the radiometric calibration of energy- and wavelength-dispersive x-ray spectrometers as well as the reliable determination of atomic x-ray fundamental parameters using such instrumentation. In different operational configurations the information depths, discrimination capability and sensitivity of x-ray spectrometry can be considerably modified while preserving its traceability allowing for the characterization of surface contamination as well as interfacial thin layer and nano- or microparticle chemical compositions. Furthermore, time-resolved and hybrid approaches provide access to analytical information on batteries under operando conditions or allow to reveal dimensional information such as in elemental or species depth profiles of nanomaterials. Application examples for the characterization of advanced materials at the nanoscale and for the qualification of calibration samples that can employed in laboratory x-ray instruments will be provided.

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Advanced X-Ray techniques

Oral Presentation 29

XRF under grazing incidence investigations of potential calibration samples for the quantification of heavy elements in particulate matter

Laura Borgese[1], Paola Cirelli[1], Thomas Hase[2], and Diane Eichert[3]

[1]INSTM - Chemistry for Technologies Laboratory, University of Brescia, via Branze 38, 25123 Brescia, Italy [2]University of Warwick, Department of Physics, Coventry CV4 7AL, United Kingdom [3]ELETTRA – Sincrotrone Trieste, S.S. 14 Km 163.5 in Area Science Park, 34149 Basovizza, Trieste, Italy

E-mail: diane.eichert@elettra.eu

Particulate matter (PM) is among the six primary environmental pollutants, and its associated health risks well established. The situation is critical, with less than 30% of the global population exposed to $PM_{2.5}$ levels below the threshold recommended by the World Health Organization (WHO), with additional PM monitoring, characterization and controls needed.

PMs are traditionally collected onto filtering membranes (filters), and their mass amounts and composition determined. X-Ray Fluorescence (XRF) techniques (including variants such as Total Reflection XRF, TXRF) present interesting and more sustainable alternative to reference techniques as AAS or ICPs, giving comparable results and probing the filters directly without the need to digest them. PM filters can also be prepared with the Smart Store® method [1], which encloses the collected filters between two polymeric layers. This process avoids material losses, contaminations, and allows the sample to be preserved. Used with a TXRF spectrometer, the method has been shown to be suitable for elemental quantification of PMs [2]. To determine the PMs' elements of interests, such as Class 1 human toxicants (Pb, Hg, As, Cd), environmental scientists need reliable and accurate elemental analysis techniques underpinned by calibration procedures employing fit-for-purpose reference materials (RM). Unfortunately, RM representative of PM filters are crucially lacking (NIST CRM 2783 excepted), with no adequate concentration ranges for PMs covering the targeted applications.

Here, we present data from a set of calibration samples realized by nebulizing a solution of a reference material with a particle generator and collecting the obtained aerosols onto a filter. By varying the nebulization time and changing the concentration of the solution, filters loaded with a wide range of elemental masses may be obtained. Filters were then prepared according to the Smart Store® method and characterized with XRF under grazing incidence conditions. We compared these results with solutions, with the same composition, deposited as droplets onto a carrier and characterized using TXRF. Formally, the nebulized residues on the filters prepared with the Smart Store® do not satisfy the conditions underpinning quantitative TXRF, but we demonstrate that the retrieved net intensities may be used to build an external calibration curve, and allow for quantification procedures for PMs captured on air filters at environmentally relevant levels.

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Oral Presentation 30

Laboratory scanning-free GEXRF for the investigation of 2D nanostructures

S. Staeck[1], J. Baumann[1], P. Hönicke[2], K. Andrle[2], Y. Kayser[2], V. Soltwisch[2], N. Wauschkuhn[2], D. Grötzsch[1], J. Weser[2], F. Spikermann[1], G. Goetzke[4], A. Jonas[2], F. Förste[1], I. Mantouvalou[3], H. Stiel[5] and B. Kanngießer[1]

[1]Technical University of Berlin, BLiX, Hardenbergstr. 36, 10623, Berlin, Germany
[2] Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany
[3]Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany
[4]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany
[5]Max Born Institute, Max-Born-Str. 2A, 12489 Berlin, Germany

E-mail: steffen.staeck@tu-berlin.de

The ability to characterize nanostructures such as multilayers or more complex 2D structures is becoming increasingly important with the ever-growing device complexity in the semiconductor industry and the miniaturization of feature sizes. Grazing-emission X-ray fluorescence spectroscopy (GEXRF) [1] provides a tool to characterize these structures nondestructively with spatial and elemental sensitivity [2]. Current development strives for laboratory spectrometers, which may be utilized for process-engineering without the need for access to large-scale facilities.

GEXRF is based on conventional X-ray fluorescence spectroscopy; with GEXRF the detection angle is varied around the glancing angle to modulate the information depth of the fluorescence signal. Self-interference of the fluorescence photons furthermore modulates the resulting signal and is instrumental for the sensitivity of the method. This provides information about the elemental depth distribution of the sample down to the sub-nm scale. The angle dependent XRF signal can then be fitted with a sample model to obtain the sample parameters of interest [3]. When using a pixelated 2D detector, the method can be utilized scanning-free (SF-GEXRF).

In this work, SF-GEXRF demonstration experiments on multilayers and nanogratings will be presented, which have been performed at the Berlin Laboratory for innovative X-ray Technologies (BLiX). The applied laboratory setup and measurement results in the soft [4] and tender X-ray range will be discussed with respect to current challenges and analytical opportunities.

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Oral Presentation 31

Characterization and calibration of a Bruker S4 T-STAR instrument for virtually standard-less quantitative analysis of aerosol depositions

P. Hönicke[1], B. Beckhoff[1], M. Gottschalk[2], Y. Kayser[1], S. Seeger[2]

[1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany
[2]Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin, Germany

Grazing-Incidence X-ray fluorescence (GIXRF) analysis is a very powerful technique for the indepth analysis of many types of technologically relevant samples, e.g., nanoparticle depositions, shallow dopant profiles or thin layered samples. The method is suitable also for a quantitative analysis of the elemental composition in an airborne particulate matter sample with some benefits over total reflection XRF, which is more common in aerosol science [1]. With the availability of commercial bench-top instruments, capable of performing TXRF and GIXRF, quantitative elemental analysis of aerosol samples from cascade impactors can easily be employed.
However, the quantification of the sample, whose structure and mass loading may vary from accumulations of particles up to layers depending on the stage of a cascade impactor used, particle composition, collection time and pollution level, requires structure-dependent information and a profound knowledge of the geometrical parameters of the instrument's setup. For a most accurate quantification without using reference or calibration specimen representative of the experimental samples, the incident beam geometry as well as the detector aperture need to be known. Together they determine the incident angle dependent so-called effective solid angle of detection which is a key parameter for quantitative and meaningful data analysis.
In this work, we demonstrate how these instrumental parameters can be determined for a Bruker S4 T-STAR instrument [2] using a well-known calibration sample, and how this knowledge can be used to perform virtually standard-less quantitative GIXRF on various types of samples including aerosol samples collected with cascade impactors.

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Oral Presentation 32

Zinc diffusion in dentine: Investigating elemental gradients and chemical changes at the interface with dental restorations

Oleksandra Marushchenko[1,2], F. Lizzi[2], L. J. Bauer[3], H. Elfarraj[2], P. Zaslansky[2], and I. Mantouvalou[1]

[1]Helmholtz-Zentrum Berlin for Materials and Energy, Berlin, Germany;
[2]Dept. of Operative, Preventive and Pediatric Dentistry, Charité – Universitätsmedizin Berlin, Germany;
[3]Institute for Optics and Atomic Physics, Technical University of Berlin, Germany.

E-mail: oleksandra.marushchenko@charite.de

Dentine, a vital component of teeth composed of carbonated hydroxyapatite (cHAP) and collagen fibers, contains micron-sized dentinal tubules [1]. Dental materials used for tooth restoration often come into close contact with dentine, leading to the diffusion of elements through the tubules and potential changes in chemical and structural properties. Zinc is a naturally occurring trace element in teeth as well as a common component of dental fillings. Therefore, understanding the mechanisms of Zn diffusion and the role of elemental gradients in the interzone between restorations and normal dentine is of particular interest.

X-ray methods are successfully used to characterize both tooth tissues and dental restorative materials. Micro-X-ray fluorescence spectroscopy (μ-XRF) known as a non-destructive method for 2D elemental imaging with a spatial resolution in the micrometer range, was used to detect diffusion of elements from the dental restoration material to the tooth interior [2].

XANES (X-ray Absorption Near Edge Structure) is a spectroscopic technique that provides detailed information about the local atomic environment and electronic structure of materials. By analyzing X-ray absorption spectra at specific distances in relation to the interface between filling and dentine, the chemical environment of elements, such as zinc is rendered feasible. In this study, a model system was established using bovine teeth with artificially placed filling material (Life™, Kerr; Gutta Percha) containing high levels of zinc. Significant diffusion of Zn, hundreds of microns into the bulk of the tooth, was detected and localized after a year of aging with μXRF (*Fig.1*).

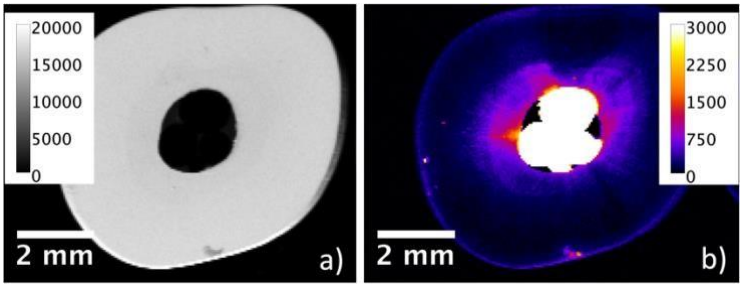

Figure 1: Ca(a) and Zn(b) distribution in a bovine tooth slice, 11 months after placing of the Gutta percha filling. μXRF images, intensities given in net peak counts.

The results of the several μ-XRF/XANES measurements will be presented, shedding light on the diffusion behavior of Zn. The multimethod approach employed in this study offers several advantages in understanding the microchemistry of dentine and its interface with dental restorations.

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Oral Presentation 33

XRD has changed: Advancing Instrumental Methods of Analysis with Groundbreaking XRD Technology

Minos Ziagkos[1]

[1]Analytical Instruments SA, Tzavella 9, Chalandri 15231

E-mail: mziagkos@analytical.gr

For more than 60 years, Bruker has created innovative analytical instruments, to support the scientific community, as well as the users in Industry. Our analytical solutions stand for cutting edge technology and highest performance. While we are providing top technology for scientists worldwide, over the past decades, we have more and more focused, on making the latest analytical methods, also accessible to a broader group of users. At the forefront of this endeavor for accessibility are our benchtop instruments. Although they come with a smaller footprint than our landmark full sized systems, they share with them the same analytical instrument DNA, including the focus on data quality, robust hardware design and reliable results. Today we are happy to introduce a new member of our benchtop solution family, the D6 PHASER. The D6 PHASER is the base of a new world of X-Ray Diffraction solutions with compact size and unparalleled flexibility.

Invited OP 9

FoodOmicsGR_RI: Greek National Research Infrastructure for the Comprehensive Characterisation of Foods

Georgios Theodoridis[1, 2]

[1]Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, 54124, Greece [2]Biomic_AUTH, CIRI, Balkan Center, 10 Km Thermi-Thessaloniki, Greece

E-mail: gtheodor@chem.auth.gr

Foodomics combines food and nutrition sciences with advanced analytical techniques and bioinformatics, in a hypothesis-free approach toward characterization of the food composition or food consumers' biofluids. Foodomics, addresses scientific challenges such as food authentication, traceability, improvement of food produce, food quality and nutritional value. This holistic approach employs cutting-edge technologies and big data. New knowledge is generated, highlighting previously unknown associations of biomolecules with the studied phenotype.

FoodOmicsGR_RI is a national research infrastructure that aims to perform and aid omics research in agri-food sector in the Greek research environment. This field is of high importance for the country and its agriculture and primary sector. Because of the unique landscape Greece exhibits a diverse and rich portfolio of local/national products and foods. Therefore, the central scope of FoodOmicsGR_RI is to support the Greek agri-food sector by generating robust data on the composition and nutritional value of the local produce, thereby increasing product's position, market demand and provide a higher revenue for the producers. The infrastructure comprises eight (8) Greek Universities and Research Centers. Analytical groups and food specialist groups comprise a team of 80 staff and newly recruited researchers from 20 scientific disciplines. Our work included the establishment of FoodOmicsGR food database, a public searchable database with more than 18000 entries, with concentration values for ca 900 metabolites found in 26 Greek foods. We will also present our results on the development of LC-MS methods for the characterization, mapping and classification of Greek foods. Finally, we will briefly discuss application of the technology in the study of diet and nutrition and their impact in health and wellness [1].

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Food Analysis (FoodOmics)

Oral Presentation 34

Rapid microbore lipidomic profiling method for the analysis of extra virgin olive oils from different Mediterranean countries by RPLC-TOF/MS.

Application of cyclic ion mobility for the isolation of lipid isomers.

Artemis Lioupi[1,2], Nyasha Munjoma[3], Theodoros Liapikos[1,2], Lee Gethings[3] and Georgios Theodoridis[1,2]

[1]Laboratory of Analytical Chemistry, School of Chemistry, Aristotle University of Thessaloniki, 54124, Thessaloniki, Greece
[2]FoodOmicsGR Research Infrastructure, AUTh Node, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, 57001, Greece
[3]Operations, Waters Corporation, Stamford Avenue, Wilmslow, SK9 4AX, United Kingdom

E-mail: gtheodor@chem.auth.gr

Lipidomic approaches are widely applied in food science research with an emphasis on ensuring the quality and nutritional value of products. This work, describes the development of an UPLCHRMS method with a microbore UPLC C8 column (1.0 × 50 mm, with 1.7 μm diameter particles) for the lipidomic analysis of extra virgin olive oil samples with analysis times of 5 min/sample. Compared to a 20-min conventional method, the newly proposed method achieves a 75 % saving in mobile phase consumption and injection volumes of 0.2 μL. The method was applied for the analysis of extra virgin olive oil samples from different regions of Greece, Israel, Palestine, Spain and Cyprus and significant differences in triglycerides/markers of geographical origin were detected. Additionally, statistically significant differentiations were observed in lipids between samples from different regions of Greece (Halkidiki, Kavala, Peloponnese, Crete). The quality control samples from each country were analysed also with a cyclic ion mobility mass spectrometer and important examples of the isolation of lipid isomers are presented.

Oral Presentation 35

Metabolomics solutions in monitoring nutrition and wellness

O. Begou[1,2,3], G. Theodoridis[1,2] H. Gika [2,4]

[1]Department of Chemistry, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[2]Biomic Auth, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki, Innovation Area of Thessaloniki, Thermi 57001, Greece
[3]ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, 57001, Greece
[4] Laboratory of Forensic Medicine and Toxicology, Department of Medicine, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

E-mail: olgabegou@thetabiomarkers.com

Metabolomics has emerged as valuable tool for monitoring nutrition and wellness. By analyzing the small molecules (metabolites) present in biological samples, such as blood or urine, metabolomics enables a comprehensive assessment of an individual's metabolic profile. In that frame, the term "nutrimetabolomics" has emerged that describes the applications of metabolomics in nutritional studies. This approach can provide insights into dietary intake, nutrient metabolism, identify food-derived biomarkers, inter-individual variability in metabolizing foods in health and disease states and overall provide important insights on the wellness status of individuals. Hence metabolomics-based nutritional monitoring can identify specific metabolites associated with dietary patterns or nutrient deficiencies, offering personalized feedback and guidance for optimizing dietary choices and helping to track disease progression, and facilitate preventive healthcare strategies. With advancements in analytical techniques and data analysis methods, metabolomics solutions hold great potential in improving nutrition assessment, wellness monitoring, and personalized healthcare. Our group has implemented a plethora of research studies regarding nutrition and wellness monitoring using both targeted and untargeted omics protocols. We have developed advanced analytical methods on LC-MS/MS, GC-MS and/or LC-TIMS-QTOFMS platforms. These projects include 1) the investigation of the effect of carob consumption by monitoring the urine and fecal metabolic profile of Wistar rats, 2) the analysis of specific exercise biomarkers in athlete's urine with the aim to improve their athletic performance through diet modification 3) the development of methods using non-invasively collected biological samples such as dry urine spots. The latter can facilitate human-centric at home sampling of biofluids allowing tailored nutritional interventions. This work aims to provide an update on the applications of metabolomics to personalize nutrition and to deliver tailored and clinically relevant applications aiding in the advancement of nutritional science.

Acknowledgment:
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Oral Presentation 36

Elemental metabolomics – Tagging Wheat Sprouts with Rare Earths Elements

L. Papalamprou[1,2], A. Palyvos[1], D.G. Sotirchos[1,2], C.A. Georgiou[1,2]

[1]Chemistry Laboratory, Department of Food Science and Human Nutrition, Agricultural University of Athens, 75 Iera Odos, 118 55 Athens, Greece
[2]FoodOmics.GR Research Infrastructure, Greece

E-mail: cag@aua.gr

Rare earths (REEs) tagging could identify production site and reassure consumers on food authenticity. Tagging with minimal amounts of REEs is feasible by the ultra-low detection limits of –Omic analytical techniques. Minimal loads and the luck of any biochemical activity render tagging with REEs safe and well accepted by the consumers. Rare earth elements and specifically Gadolinium (Gd) was assimilated in wheat sprouts and studied through ICP-MS. The dose response, time evolution, length and dry weight of sprouts were measured. Results show a linear increase in the assimilation of Gd in wheat as we increase the dose of Gd in the watering solution. There is also a big increase in the Gd concentration on the sixth day of watering, nearly 2 times higher than the fifth day. The lowest concentration of Gd resulted in the greatest growth of sprouts, 25% more than the highest concentration, whereas the lowest concentration resulted in approximately the same weight, 5% difference, with the control. Our goal is to make a 14 bite number of the 14 REEs that can code up to 16.000 combinations. Further aim is the production of dairy products tagged with REEs from the milk of sheep fed with the wheat sprouts that are loaded with REEs. Next experiments are with Dysprosium and then with the 12 other REEs [1].

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Oral Presentation 37

Analysis of pyrrolizidine Alcaloids in food

G. Miliadis, C. Kroi, G. Siragakis

TUV Austria Food Allergens Labs

E-mail: christina.kroi@tuvaustria.com

Pyrrolizidine alkaloids (PAs) are a group of naturally occurring alkaloids based on the structure of pyrrolizidine. They are produced by plants as a defense mechanism against herbivorous insects. More than 660 PAs have been identified in plants and about half of them show hepatotoxicity. It is estimated that 3% of flowering plants contain PAs. They are detected in pollen, tea, oregano, herbal infusions, herbal food supplements, honey, but also in products of animal origin as milk, dairy products, eggs, meat and meat products. EFSA CONTAM committee has issued scientific opinion that of possible danger for human health associated with exposure to pyrrolizidine alkaloids, especially for those who consume often and in large quantities, teas, and herbal infused beverages, and in particular for the younger groups of population. Furthermore, the committee concluded that there is potential concern for the health of children and infants who consume large amounts of honey. It set a recommended value of 237 mg/kg body weight per day to evaluate the carcinogenicity risks from PAs. The EU maximum levels for total PAs in various herbs, infusions, etc. are defined in Regulation 2040/2020 (EU) and range from 0.001 mg/kg in tea for infants to 1mg/kg in oregano, and from 0.4 to 0.5 mg/kg in other herbal infusions (dried product). In the present study, a method was developed for the extraction of PAs from various foods using acidified methanolic solution and the determination of PAs using internal standard method with LC-MS/MS. The method was validated and accredited for 31 compounds of the PAs class in herbs and cereals. Accuracy was estimated by recovery and values found were 61-120% in cereals and 60-125% in herbs. Accuracy was also verified by successful participation in 3 proficiency tests. Reproducibility was estimated by %RSD and its values were found ≤19.8% in cereals and ≤16.8% in herbs. The expanded uncertainty was found 40% with its main component being the intra-laboratory reproducibility. The limit of detection was found 0.005 mg/kg and the limit of quantification 0.016 mg/kg. In our laboratories 367 samples were recently analysed for PAs, in 185 of which concentrations of PAs were detected; 210 samples were oregano, 147 of which contained detectable concentrations and 74 of them were above the legal limits. These figures are 35% higher than corresponding exceedances of other toxicologically significant substances. Concentrations of PAs in oregano reached up to 94.7 mg/kg. In other products, in cumin 41% of the samples were above the legal limits. These significant numbers of samples with PAs exceeding the legal limits proves that the analysis of food for PAs is necessary for the protection of the consumer.

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Oral Presentation 38

Residues of pesticides in the food chain: Are bee products endangered or safe to consumers?

Adrián Fuente-Ballesteros, José Bernal, Ana M. Ares

Analytical Chemistry Group (TESEA), I. U. CINQUIMA, Faculty of Sciences, University of Valladolid, 47011, Valladolid, Spain

E-mail: adrian.fuente.ballesteros@uva.es

There is significant concern surrounding the health status of beehives, with bee losses being attributed to various factors, including inadequate framing practices or climate change. Pesticides can be found in beehives, either due to beekeepers utilizing them to control the damaging effects of the Varroa mite or their potential accumulation in wax, which is directly in contact with other bee products. Recent food alerts have raised concerns about the safety of these products, as the presence of pesticides, especially acaricides, in honey poses a risk to consumers. Potential effects may include skin and eye irritation, respiratory problems, allergic reactions, or even more severe health issues in cases of acute poisoning or chronic exposure. Consequently, there is a need for efficient, selective, and sensitive methods to determine pesticide residues in bee products.

Different analytical methods involving solvent extraction, QuEChERS (*Quick, Easy, Cheap, Effective, Rugged and Safe*) and *clean-up* steps followed by a further gas chromatography-mass spectrometry determination were proposed and validated to determine seven of the most frequently detected pesticides (atrazine, chlorpyrifos, chlorfenvinphos, α-endosulfan, bromopropylate, coumaphos, and τ-fluvalinate) in Spanish bee products such as bee pollen [1], beeswax [2], and honey [3]. Pesticide residues were analyzed in bee pollen samples from local supermarkets and experimental apiaries finding six positive samples in chlorfenvinphos (0.030-
0.035 mg/kg), α-endosulfan (0.077 mg/kg), coumaphos (0.042 mg/kg), and τ-fluvalinate (0.010-0.097 mg/kg). In most cases, concentrations were higher than those authorized by current legislation. These results are consistent with studies on beeswax and honey. Beeswaxes were analyzed and τ-fluvalinate (up to 569 mg/kg) was found in most of the samples, followed by coumaphos (up to 2350 mg/kg), chlorfenvinphos (up to 165 mg/kg) and chlorpyrifos (up to 274 mg/kg). Similarly, residues of τ-fluvalinate were found in honeys from rosemary, multifloral and oak. Nevertheless, these concentrations were in all cases below the established maximum residue level in honey and other apiculture products according to European Commission. Due to the detection of several acaricide residues in bee matrices, it is necessary to develop analytical methods to monitor them to ensure their safety and the protection of human welfare.

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Materials

Oral Presentation 39

Thermal analysis of crystalline diblock copolymers by DSC

S. Bistac[1], M. Brogly[1] and D. Bindel[1]

[1]Université de Haute Alsace – LPIM, 68093 Mulhouse Cedex, France

E-mail: sophie.bistac-brogly@uha.fr

Polyethylene-block-polyethylene glycol copolymers (PE-b-PEG) are amphiphilic copolymers, with a hydrophilic PEG block and a hydrophobic PE block. Morever, both blocks are able to crystallize into two distinctive crystalline phases. The objective of this work is to study the organization of PE-b-PEG copolymers containing different ration of PE and PEG blocks, and to analyse the effect of the copolymers composition on their crystalline properties .

The effects of the molecular weight and the weight ratio of the two polymer blocks on the PEb-PEG crystallinity will be evidenced by the characterization of various PE-b-PEG copolymers of different compositions. Crystallinity degree of each block will be determined by Differential Scanning Calorimetry (DSC). The morphology and the growth rate of the both crystalline phases of each block are also investigated by optical microscopy (polarized light) equipped with a hot-stage device. In order to evidence the influence of the blocks ratio, the results obtained for PE-b-PEG copolymers are compared with the crystalline organization of the PE and PEG homopolymers. The PE/PEG blocks ratio of the copolymers varies from 17/83 to 77/23 (weight/weight). The experimental results evidenced that the crystallization of the PE block is closer to PE homopolymer when the copolymer contains more than 50.wt % of PE sequences. Inversely, for PE-b-PEG copolymers containing more than 50.wt % of PEG, the PEG block crystalline organization is similar to the PEG homopolymer. An important hindrance of each block on the crystallization growth rate of the other block has been evidenced. When the ratio of one block is increased, the crystallization of this block is favoured, the crystallization of the other block is hindered, and could even be totally prevented. These results, relative to crystalline organization of PE-b-PEG diblock copolymers could allow to better understanding of the organization and crystallization of each block when the copolymers will be adsorbed on a solid substrate, or at liquid interface, for surfactant applications.

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Oral Presentation 40

Development of a hybrid portable instrument for assessing the surface state and degradation of monuments: combining LED-Induced Fluorescence, LIBS and Diffuse Reflectance

V. Pinon[1], A. Giakoumaki[1], M. Andrianakis[1], K. Hatzigiannakis[1], K. Melessanaki[1], Maria Pavlou[2], Serafeim Korosis[2], P. Pouli[1] and D. Anglos[1,3]

[1]Institute of Electronic Structure and Laser, Foundation for Research and Technology, Nikolaou Plastira 100, 70013, Vassilika Vouton, Heraklion, Crete, Greece
[2]Ephorate of Antiquities of the City of Athens, Makriyianni 2-4, 11742 Athens, Greece
[3]University of Crete, Department of Chemistry, Voutes University Campus, P.O. Box 2208, 70013, Heraklion, Crete, Greece

E-mail: vpinon@iesl.forth.gr

Monuments are subject to various environmental and human-induced factors, leading to the gradual formation and deposition of crusts on their surface such as biodeterioration, atmospheric pollution crusts, corrosion products, patinas, etc. Additionally, monuments can exhibit chromatic layers, either intrinsic to their architectural characteristics (e.g., wall paintings) or as a result of external influences. Given that these deposits can have aesthetic but also structural implications, a comprehensive characterization of the state of the monument becomes crucial before deciding on the future conservation approach. However, the compositional diversity of these layers (biological, organic, inorganic) often necessitates the application of multiple complementary analytical techniques, preferably non-destructive and applicable in situ.
To address these requirements, we have developed a hybrid portable instrument integrating three different spectroscopic techniques: LED-Induced Fluorescence for biodeterioration detection and discrimination, Laser-Induced Breakdown Spectroscopy (LIBS) for elemental analysis of pigments, metals/metal corrosion, and inorganic crusts, and Diffuse Reflectance Spectroscopy for molecular analysis of pigments and coloured layers.
In this study, we will present the design, components and performance of the newly-developed hybrid system. In a first stage, various archaeological objects and fragments from monuments and sites of Athens (stones, ceramics, metals, wall paintings) were analysed in the laboratory to evaluate the system's performance prior to field application. The results of these analyses helped the fine-tuning of experimental parameters for each technique but also the definition of an analysis methodology. Preliminary results indicate that this hybrid instrument is a valuable tool for conservators, heritage scientists, archaeologists, and others, as it enables rapid, portable, and effective characterization of a wide range of materials present on monument surfaces.

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Oral Presentation 41

Exploring the Impact of Storage Temperature on PbO and Pb_3O_4. Aging Characterization with XRD, ATR - FTIR, SAXS and N_2 Porosimetry.

A. Papadouli[1], N. Pradakis[2], D. A. Gkika[2,3], J. Fantidis[1], M. Maragakis[1], S. Pantazis[4], A. C. Mitropoulos[2,3] and N Vordos[1,*]

[1]Department of Physics, International Hellenic University, St. Lucas, 65404, Kavala, Greece
[2]Department of Chemistry, International Hellenic University, St. Lucas, 65404, Kavala, Greece
[3]Hephaestus Advanced Laboratory, International Hellenic University, St. Lucas, 65404, Kavala, Greece
[4]Sunlight Group, Neo Olvio 672 00 Xanthi, Greece

E-mail: nvordos@physics.ihu.gr

Lead-based batteries can include varying concentrations of PbO (α-PbO and β-PbO), and Pb_3O_4. To assess the influence of storage temperature on their structural composition, samples of PbO and Pb_3O_4 were analyzed. Four different characterization techniques were involved for the analysis, Attenuated Total Reflection-Fourier Transform Infrared (ATR-FTIR), X-ray Diffraction (XRD), N_2 Porosimetry (BET method), and Small Angle X-ray Scattering (SAXS) [1]–[4].The overarching objective of this study is to draw correlations between these structural modifications and battery performance. Experimentally thermal impact on physiochemical properties of PbO and minimum was assessed at 20, 30, 40, 50 and 55^{0}C. Briefly samples were left to dry in borosilicate glass discs on constant temperatures $\pm 1^0C$ for two days continuously. In XRD analysis (5°-90° range with a step of 0.01° degrees/sec), the presence of many peaks indicated the poly-crystalline structure of minimum differentiating slightly at 50°C drying condition (Fig. 1.). Prominently, peaks at 840 [cm^{-1}] and 1010 [cm^{-1}] in ATR-FTIR analysis (32 scans/sample, 4000-700 [cm^{-1}] range) suggest the existence of lead oxides. With temperature rising, certain absorption bands intensity change. This can be attributed to alternation in vibrational molecular states indicating changes in the chemical or physical properties of material. For the N_2 porosimetry analysis, measurements were taken at 10 points within the BET region after overnight sample degassing (25°C). The effect of temperature led to an approximate 10 - 20% variation in the specific surface area (m^2/gr) of the analyzed samples. SAXS analysis was performed in a rig system (CuKa, λ=0.15056nm) at 1.5m detector-to-sample distance for 7200 sec exposure time. In the Porod region, a peak emerges at 1.2nm accompanied by slight variations in the slopes suggesting changes in surface roughness, interfacial area, and fractal dimensions of the scattering entities within the sample.

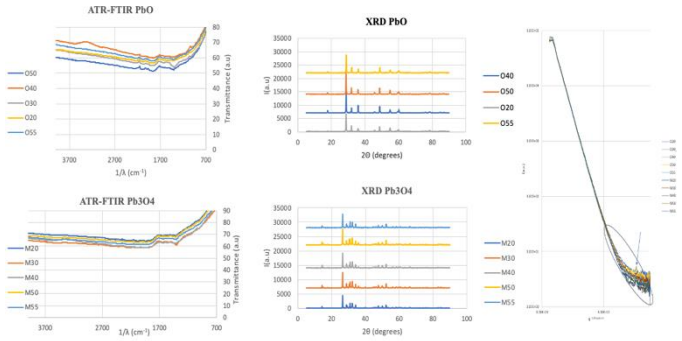

Fig. 1. ATR-FTIR, XRD and SAXS spectra of Lead Oxide (PbO) and Minium (Pb_3O_4) for different drying temperatures. O20: PbO dried at 20°C, O30: at 30 °C, O40: at 40 °C, O50: at 50 °C and O55:at 55°C. M20: Minimum dried at 20°C, M30: at 30 °C, M40: at 40 °C, M50: at 50 °C and M55:at 55°C.

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Oral Presentation 42

Development of Fe_3O_4-decorated Sn-hydroxide nanocomposites for advanced Cr(VI) capture in drinking water

K. Kalaitzidou, T. Asimakidou, K. Simeonidis

Analytical Chemistry Laboratory, Department of Chemical Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

E-mail: ksime@physics.auth.gr

A nanomaterial consisting of bivalent tin chloroxy-hydroxide (abhurite) known for its high reducing potential, was combined with magnetically responding iron oxide (Fe_3O_4) nanoparticles to deliver a novel class of water treatment adsorbents able to capture high-valent forms of pollutants through a reducing/precipitation mechanism. Synthesis of such nanocomposites involved the continuous flow precipitation of the tin phase using $SnCl_2$ as precursor and the oxidative precipitation of $FeSO_4$ to collect Fe_3O_4 nanoparticles. Optimized preparation approaches for each constituent were combined with different ways to produce a proper material which preserves the efficiency and the magnetic properties of abhurite and magnetite, respectively. The separate preparation of each component and then, after partial dehydration, high-energy sludge homogenization was found to be the best alternative to overcome the intense chemical and surface interactions during materials' growth. According to this sequence, the abhurite phase was precipitated into large aggregates of hierarchically deposited nanocrystals in the form of skein-like spherical structures with dimensions in the range 5-30 μm, whereas 30-40 nm spherical Fe_3O_4 nanoparticles were homogeneously deposited in the interlayer area of abhurite. The developed Fe_3O_4-decorated abhurite spheres were further evaluated for their capacity to promote hexavalent chromium uptake at concentrations complying with drinking water demands (regulation limit 25 μg/L) as well as with sufficient magnetization enabling the separation of the solid at the end of the purification procedure. Particularly, the efficiency of the nanocomposite decorated with 5 % Fe_3O_4 nanoparticles was estimated to be above 8 mg/g which is a very good value considering the efficiency of pure abhurite and the fact that the nanocomposite is featured with magnetic properties. As the Fe_3O_4 content increased, the efficiency drops proportionally reaching around 4 mg/g for the 40 % nanocomposite. Advanced materials characterization by X-ray absorption and photoelectron spectroscopy indicated that the high performance of Fe_3O_4-decorated abhurite to capture aqueous Cr(VI) forms is based on transformation into insoluble Cr(III) species incorporated onto the adsorbent's surface layer.

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Invited OP 10

Hyperspectral Imaging combined with spectrometric techniques as a useful tool for art conservation diagnostics

Athina Georgia Alexopoulou[1]

[1]ARTICON Lab Conservation Promotion of Visual Art, Book and Archival Material, Faculty of Applied Arts and Culture, University of West Attica, Ag. Spyridonos , Egaleo Park Campus, Egaleo 12243, Attiki, Greece

E-mail: athfrt@uniwa.gr

Today, technology in the field of art diagnostics, and in particular hyperspectral imaging techniques with an emphasis in the non-visible region of the spectrum, are the spearhead of non-destructive examination, constituting a valuable tool at the service of art historians, archaeologists, conservators, engineers and researchers. Non-destructive methods, as noninvasive, non-contact techniques, are attractive green tech solutions since they are environmentally friendly, do not require sampling, have quick in situ application, do not involve consumables or waste materials, have very low energy consumption as well as the ability of post-processing imaging data. So, they offer the advantage of examining a wide range of objects (easel and panel paintings, wall paintings, archival material, ceramics, stone, etc.), thus supporting a multidisciplinary approach, documentation, analysis and protection of works of art, giving significant additive value.

Hyperspectral imaging is in increasing demand in the field of art conservation, art history and archaeology judging by the number of recent reviews on the subject from the conservation and archaeology community. Even though these techniques are important by themselves, they exhibit a special dynamic potential when combined with modern advanced techniques from the field of analytical chemistry and computer science which help them answer complex issues.

Hyperspectral imaging collects images of an object in a series of spectral windows being distinct between them only regarding the spectral channels they operate, giving both spatial and spectral information. With the increased number of bands and speed of acquisition, they are applied qualitatively for band to band comparison in order to identify areas of different material composition, natural degradation of material, previous conservation interventions and in particular revealing underdrawings and preparatory sketches [1,2]. They can operate in UV, visible, NIR reflectance and fluorescence mode from 380 to 1000nm. Furthermore, modern InGaAs detectors which have a spectral sensitivity that ranges in the near infrared from 10001700nm can be used to extend and exploit the spectral range [3].

Through selective case studies in the field of ceramics, archaeological monuments and historical pigments the author intends to demonstrate that spectral imaging techniques combined with spectrometric methods, in particular XRF and SEM-EDAX, can be considered as a useful tool for art conservation diagnostics. It and can offer many more possibilities compared to what the common user imagines, provided that the application of the methods take into account the specific characteristics of the material and exploit its properties.

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Archaeometry

Oral Presentation 43

Spatially resolved analysis of the red pigment Eosin and its degradation products by MALDI-MSI

K. Janssens[1,2], A. Alvarez-Martín[1,2] and T. Scovacricchi [2]

[1]AXIS Research Group, NANOLab Centre of Excellence, University of Antwerp, Belgium [2]Conservation and Science Department, Rijksmuseum Amsterdam, The Netherlands

E-mail: koen.janssens@uantwerpen.be

In the last two decades, the field of Conservation Science has gained considerable attention in museums and cultural institutions with the aim to better preserve our cultural heritage for future generations. Until recently, the perception of the discoloration of works of art has been based on the empirical observation and experience of artists and conservators. However, over the last 10 years, major advances in non-invasive spectroscopic methods and imaging techniques have made it possible to investigate in great detail the chemical mechanisms involved in (mainly inorganic) pigment deterioration [1].
To identify organic pigments and study their degradation behaviour, in many cases, traditional mass spectrometry (MS) techniques coupled to liquid or gas chromatography are used. However, the sample preparation required for chromatographic separation implies the dissolution of the paint sample and with that the obliteration of its layered structure. This makes it difficult to properly track down original organic pigments and their degradation products within stratified paint layer samples.

One organic pigment frequently employed by late 19th – early 20th century painters such as Vincent Van Gogh and James Ensor is geranium lake. The organic chromophore molecule in this pigment is eosin, an analogue of fluorescein with 4 Br-substituents, that exhibits a fairly rapid loss of color when exposed to ambient light [2,3].

Recently, within the AXIS research group, a new research line was started, centered on spatially resolved 2D distribution analysis of organic compounds by Matrix Assisted Laser Desorption Ionization - Mass Spectrometry Imaging (MALDI-MSI). Here, we show for the first time the potential of MALDI-MSI to investigate the correlation between spatially resolved molecular information with the discoloration process of oil paintings. This allows for the analysis of paint cross-sections with a lateral resolution of around 10 µm, without loss of ionization efficiency due to topography effects. The method is used to study oil paint samples containing a mixture of organic and inorganic pigments, such as eosin and lead white; the multistep degradation process of the eosin molecules can be closely studied via MALDI-MSI.

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Oral Presentation 44

HPLC studies on shellfish (royal) purple

I. Karapanagiotis

Department of Chemistry, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

E-mail: karapana@chem.auth.gr

Shellfish purple, also known as Tyrian purple and royal purple, has been used since the early Late Bronze Age, according to scientific studies which reported the identifications of purple pigments in mural paintings of the Aegean [1]. These Aegean settlements are older than Tyre. Since then, shellfish purple has been used in the Mediterranean until the cease of the Byzantine empire and the conquest of Constantinople by the Ottomans [2].

In the Mediterranean basin there are three molluscan species which are sources of the purple pigment and therefore could have been used in heritage objects of the area: *Hexaplex trunculus* L. (*Murex trunculus*), *Bolinus brandaris* L. (*Murex brandaris*) and *Stramonita haemastoma* (*Thais haemastoma*). The chemical compositions of the pigments which can be produced from the three molluscan species is discussed in this paper. High Pressure Liquid Chromatography (HPLC) coupled to a Photo Diode Array detector (PDA) revealed that all three molluscan species contain the same colouring compounds, that are indigotin (IND), indirubin (INR), 6′bromoindirubin (6′MBIR), 6-bromoindirubin (6MBIR), 6-bromoindigotin (MBI), 6,6′dibromoindigotin (DBI) and 6,6′-dibromoindirubin (DBIR). The relative (%) integrated HPLC peak areas were measured and showed that *M. brandaris* and *T. haemastoma* gave HPLC results which are similar to each other and comparable to HPLC profiles which were collected for *M. trunculus* extracts.

The aforementioned results, are compared with corresponding HPLC data which were collected for small samples extracted from several cultural heritage objects dating from the Minoan to the Byzantine period, in an attempt to identify the specific molluscan species used in the objects of antiquity. Moreover, the effects of ageing, induced primarily by the UV radiation, are discussed in light of recently published results [3]. Finally, the HPLC results are used to discuss issues related to the production technology of the purple pigment which flourished in the past in the Mediterranean.

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Oral Presentation 45

Investigation of spectral markers appropriate for optimized archaeogenetic analysis of ancient dental remains based on Raman scattering and fluorescence spectroscopy techniques

Angeliki Mamali[1,2], Aggelos Philippidis[1] and Demetrios Anglos[1,2]

[1]Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas (IESL-FORTH), 700 13 Heraklion, Crete, Greece

[2]Department of Chemistry, University of Crete, 700 13 Heraklion, Crete, Greece

E-mail: filagg@iesl.forth.gr

Ancient DNA (aDNA) and protein analysis of human remains (bones, teeth) is a very promising research field exploring a plethora of different topics related to human evolution and past societies [1]. Ancient DNA analysis generates exclusive data that cannot be retrieved otherwise, nonetheless, it normally requires -at least partial- destruction of valuable and unique archaeological samples. The destructive nature of aDNA analysis constitutes a major drawback when extracting DNA from valuable and rare samples, especially in cases where DNA preservation is poor resulting in low -if any- DNA yield. For this reason, alternative methods to select samples, which are the most promising for archaeogenomics analysis are obviously of great importance. In this context, molecular spectroscopies can complement archaeogenomics analysis in a time and cost-efficient manner [2].

In this study, Raman and fluorescence spectroscopy techniques were employed for investigating ancient dental samples. We establish spectral indicators that can be correlated to the organic content (e.g.collagen) and further can be used to predict aDNA preservation levels in ancient human dental samples. The first step of the research is the application of spectroscopic methods as sensitivity probes associated with the DNA preservation level that will be determined via aDNA analyses prior to spectroscopic applications. This work will help to the determination of relevant spectral indicators and statistically supported thresholds, which can accurately discriminate between DNA-rich and DNA-poor dental samples. Afterward, and in the second step of our research, we will apply the methodology developed to detect the most suitable specimens for aDNA analysis. Raman and fluorescence techniques will act as screening tools for archaeogenomics analysis. We expect that this pre-selection will ensure that ancient DNA analysis is performed only on those samples, which are most likely to yield high amounts of endogenous DNA. This study enhances the capability of spectroscopic methods as reliable, fast, low cost and non-destructive screening tools for endogenous DNA preservation in archaeological teeth. The preliminary results show that we can select the best candidates for meaningful archaeogenomics analysis.

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Oral Presentation 46

Towards a multi-analytical methodology based on molecular spectroscopic techniques for the detection and characterization of organic residues in archaeological findings

Maria Eleni Konstantinou[1,2], Evangelia Ralli[2], Ioanna Misyri[2], Maria Roumpou[1], Aggelos Philippidis[1], Sophia Sotiropoulou[1,3], Apostolos Spyros[2], and Demetrios Anglos[1,2]

[1]Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas (IESL-FORTH), 700 13 Heraklion, Crete, Greece

[2]Department of Chemistry, University of Crete, 700 13 Heraklion, Crete, Greece [3]School of Applied Arts and Sustainable Design, Hellenic Open University
E-mail: mek@iesl.forth.gr

Systematic sampling and analysis of organic residues, found typically, yet not exclusively, as material remains adsorbed in the walls of archaeological ceramic containers, have enabled archaeologists, over the past three decades, to obtain significant information concerning the use and processing of natural products in antiquity, and have also stirred up conversations about implications of the data generated. Chromatographic techniques utilizing different detection schemes (GC, GC-MS, HPLC, LC-MS), often combined with isotopic analysis (GC-c-IRMS, IRMS) have been widely applied in the context of archaeological residue analysis, given their high sensitivity and selectivity, allowing reliable analysis of complex and even highly degraded archaeological samples. Nonetheless, these techniques are destructive and moreover require copious and time-consuming sample preparation steps, eventually limiting the number of samples amenable to analysis. Molecular spectroscopic techniques, on the other hand, could offer alternative, faster approaches to chemical analysis that would enable efficient screening and characterization of organic remains found either as amorphous deposits or trapped in inorganic matrices. The implementation of spectroscopic techniques could ensure in many ways availability of samples for future analysis, as well as allow assessment of their state of preservation, guiding further analytical steps.
The work presented in this paper outlines a case study focusing on the detection and characterization of organic residues preserved within the matrix of archaeological pottery of different shapes from Bronze Age Crete and also soil samples sampled from a ritual-related context in Akrotiri (Thera) dated to the Late Bronze Age. Our primary aim is to work out a multi-analytical methodology utilizing FTIR, micro-Raman, Fluorescence and NMR spectroscopies for the characterization of molecular species that are reported as biomarkers of specific natural products. It has been demonstrated that these biomarkers can survive in the archaeological record and in different burial environments, exhibiting specific spectral features that can be assessed through molecular spectroscopic techniques. Moreover, a refined residue analysis protocol has been developed and spectral libraries for specific compounds and plant/animal species have been generated through the examination of samples from modern materials, such as pine resins, beeswax and plant oil all typical of the Mediterranean region. Model samples have also been submitted to artificial ageing to develop suitable reference spectra and provide insights into the degradation pathways and their effect on the spectra produced. Spectroscopic results of archaeological ceramic and soil samples preserving residues, according to GC-MS analysis, are used for validation purposes. The selected spectroscopic techniques complement each other and we hope that our study will highlight the potential of routine utilization of spectrochemical analytical tools in archaeometry laboratories, also facilitating analysis of residues that cannot be sampled off of archaeological objects or excavation sites.

Oral Presentation 47

Advanced spectroscopic and imaging tools with sophisticated robotics and digital repository systems for the analysis, conservation and documentation of oversized paintings in the framework of an Open Access Laboratory

K. Hatzigiannakis[1], A. G. Karydas[2], C. Bekiari[3], D. Angelakis[3], A. Terlixi[4], K. Karakasiliotis[5], C. Stentoumis[6], X. Zabulis[3], D. Anglos [1,7], E. Agathonikou[4], D. Plexousakis [3,8]

[1] Institute of Electronic Structure and Laser (IESL), FORTH, P.O. Box 1385, 71110 Heraklion, Crete, Greece.

[2] Institute of Nuclear and Particle Physics, N.C.S.R. "Demokritos", Patr. Gregoriou E & 27 Neapoleos Str, 15341 Agia Paraskevi, Athens, Greece.

[3] Institute of Computer Science (ICS), FORTH, P.O. Box 1385, 71110 Heraklion, Crete, Greece.

[4] National Gallery – Alexandros Soutzos Museum,50 Vasileos Konstantinou str., 116 34, Athens.

[5] Printec S.A., 7-7A Poseidonos Ave. & Lokridos Str., 18344, Moschato

[6] up2metric P.C., Michail Mela 21, GR-11521, Athens, Greece

[7] Department of Chemistry, University of Crete, P.O. Box 2208, GR 710 03, Heraklion, Crete, Greece.

[8.] Department of Computer Science, University of Crete, P.O. Box 2208, GR 710 03, Heraklion, Crete, Greece.

E-mail: kostas@iesl.forth.gr..

The analysis of precious and delicate objects, such as paintings, requires advanced spectroscopic and imaging tools, operating remotely and non-invasively. The output of these tools has to be processed in a synergetic way to allow thorough study of the materials and the techniques applied for the construction of the artwork. In the case of oversized paintings, the use of these analytical tools requires the complementary implementation of robotic equipment driven by sophisticated software to enable access to the whole area of the painting as well as accurate positioning.

In the framework of the NSFR project "PROTEAS" (MIS 5069984), a toolbox, comprised of Macro XRF (MA-XRF), Hyperspectral, Fluorescence and Infrared Imaging, has been employed for the comprehensive investigation of oversized paintings. This toolbox is augmented with the utilization of a robotic system constructed with conventional hardware but driven with innovative machine vision software which enables accurate and repeatable access to oversized paintings. Additionally, the robotic system is capable of facilitating conservation processes. The toolbox is complemented with a digital platform for the detailed documentation of the analytical and conservation actions, the handling and the presentation of these data.

The activities of the PROTEAS project will be held in an Open Access Laboratory, settled in the premises of National Gallery of Athens - Alexandros Soutzos Museum, which will establish a channel for the communication between experts on heritage analysis and conservation and allow the public to attend the diagnostic and restoration procedures and understand the importance and complexity of protecting Cultural Heritage objects.

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Keywords: Robotic system, database, Macro XRF (MA-XRF), Hyperspectral Imaging, Fluorescence Imaging, Infrared Imaging, Open-Access Laboratory, Paintings, Artworks, Cultural Heritage, Heritage Science.

Spectometry

Oral Presentation 48

Towards real-time, on-site monitoring of trace metals in the environment using micro-plasma emission spectroscopy

Sudatta Das[1], Kalle Blomberg von der Geest[2], Ari Mäkinen[2], Aappo Roost[2], Erkki Ikonen[1,3], and Toni Laurila[2]

[1]Metrology Research Institute, Aalto University, Maarintie 8, 02150 Espoo, Finland
[2]Sensmet Ltd, Moreentie 15L 6, 90620 Oulu, Finland.
[3]VTT MIKES, VTT Technical Research Centre of Finland Ltd, Tekniikantie 1, 02150 Espoo, Finland

E-mail: Sudatta.das@aalto.fi

Contamination of toxic metals in the environment calls for continuous monitoring to identify and limit their abundance in trace and ultra-trace levels. The standard analytical techniques from Atomic Absorption Spectroscopy to Inductively Coupled Plasma optical emission spectrometry or Inductively coupled plasma-mass spectrometry techniques are extensively practiced for metal detection in laboratories. Those sophisticated techniques offer high sensitivity and sequential analysis of multiple metals at the cost of complex and expensive instrumentation, high power, and supply of inert gas. Such requirements make the systems bulky, expensive, and incompatible for on-site applications.

This inadequacy leads us to report on a novel and compact online trace metal analyzer that can simultaneously detect up to 30 metals at the sub-μg/L range in aqueous solutions. The analyzer is based on Micro-plasma Optical Emission Spectroscopy [1], where the microdischarge is created directly inside the water sample thus eliminating the use of carrier gas or nebulizer. The simple and compact design makes the analyzer robust and portable for field measurement. The performance of the analyzer is evaluated with lithium, nickel, and copper dissolved in deionized water leading to the detection limits of 0.1 μg/L, 0.2 μg/L, and 0.1 μg/L, respectively. The measurement uncertainty expressed in terms of relative standard deviation is less than 5% for each metal. The developed technique demonstrates high capacity for real-time metal analysis in process water applications, quantitative measurements of aerosol composition, water quality analysis at power plants and in semiconductor industries.

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Oral Presentation 49

Utilizing multivariate analysis for the discrimination of athletes' salivary profile using ATR-FTIR spectroscopy

C. Chrimatopoulos[1], E. Pavlou[2], N. Kourkoumelis[2] and V. Sakkas[1]

[1]Department of Chemistry, School of Sciences, University of Ioannina, Ioannina, 45110, Greece
[2]Department of Medical Physics, Faculty of Medicine, School of Health Sciences, University of Ioannina, Ioannina, 45110, Greece

E-mail: v.sakkas@uoi.gr

Sport science is rising in interest quickly by assisting athletes to improve their performance with minimum health effect [1]. Blood and urine are the most common biofluids in physical exercise metabolic analyses, but the interest of the scientific community in non-invasive biological fluids sampling is increasing [2]. Saliva composition is strongly correlated with physical exercise, providing useful information about the athlete's physical condition [3]. In this study, 57 male athletes were participated with different physical condition level, while salivary profile of them was studied via infrared spectroscopy (ATR-FTIR), and analysed using multivariate analyses (PCA and PLS-DA). Chemometric discrimination of spectral salivary profile was successfully accomplished with unsupervised PCA, before and after physical exercise, as well as between athletes being in different physical condition level (low vs. high). Moreover, PLS-DA (supervised chemometric tool) was utilised to create a stricter classification/prediction model. This technique presented extremely promising results for the discrimination of athletes' fitness level (Fig. 1), having an accuracy of 93%. To our knowledge, ATR-FTIR spectroscopy combined with multivariate analysis was used for the first time to estimate physical condition level of athletes.

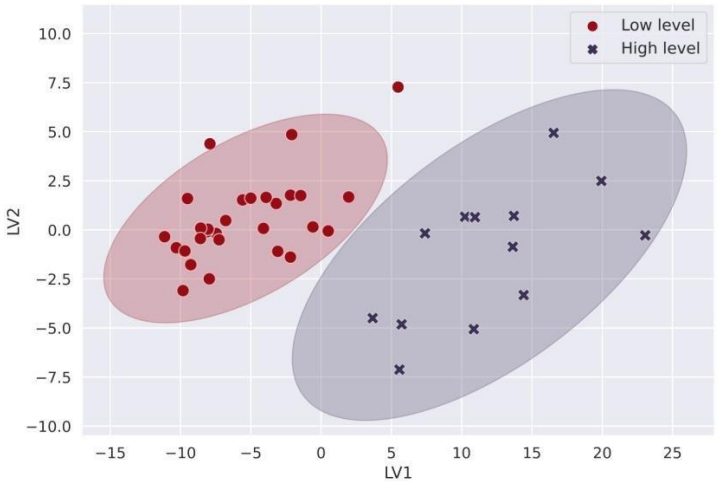

Figure 1. Partial Least Squares - Discriminant Analysis (PLS-DA) for the two groups of athletes (low level vs. high level).

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Oral Presentation 50

PM-IRRAS Surface advanced IR spectrometry: a powerful technique for the characterization of organic and polymer coatings

M. Brogly[1] and S. Bistac[1]

[1]Université de Haute Alsace – LPIM, 68093 Mulhouse Cedex, France

E-mail: maurice.brogly@uha.fr

Polymer coating deposition on a wide variety of engineering substrates has gained significant attention. Coatings are tailored to provide and improve specific characteristics, such as corrosion, chemical, wear and weathering resistance. Characterization of polymer coatings requires the use of specific characterization techniques. Polarization-Modulation InfraRed Reflection Absorption Spectroscopy (PM-IRRAS) is an innovative and original vibrational spectroscopy that is used for "in situ" reflectivity experiments to characterize organic[1] or polymer[2] coatings deposited as thin films on reflective metallic substrates and access the mechanism of thin film formation and further structuration of polymer chains at interfaces. Due to the polarization modulation of the incident IR wave, its reflection at the interface according to surface selection rules increases the sensitivity of the spectral response, allowing determination of molecular orientation, organization, structuration or crystallization effects after polymer chains adsorption. Atomic force microscopy (AFM) analyses were also performed on the same polymer coatings in order to access the surface topology and to evidence amorphous and crystalline phases if any. Three case studies will be more precisely highlighted. First, the study of the kinetic of a film-forming process of an adhesive emulsion will be described on the basis of IR surface reflectivity measurements. The diffusion process of the different species (water, polymer, additives) during the film-drying is evidenced and the specific interactions responsible for the thermodynamic miscibility and for the film-forming are quantified. Second, the adsorption and grafting from solution of adhesion promoters, that are dedicated organic molecules used in hybrid materials to improve stress transfer between organic polymer matrix and the reinforcing element, is described. PM-IRRAS contribute to understanding the mechanisms that govern adsorption, growth of these ultra-thin layers on inorganic substrates. Results show that alkyl chains conformational anisotropy for adsorbed states is detected and calculation of the tilt angle of the grafted molecule depends on the nature of the substrate, but mainly on the nature of the anchoring group functionalities. Third, the directed adsorption, structuration and crystallization of thin polymer films will be described. Various polymers were adsorbed by spin-coating on metallic substrates. The surface chemistry (hydrophilic/hydrophobic) of the substrates was controlled by chemical grafting and its influence on the organization/structuration of adsorbed polymer chains was then studied. Results show first that the competition between polymer/polymer and polymer/substrate interactions has a direct effect on the chains orientations and conformations and thus surface morphologies, and second that substrate surface chemistry alters the balance between these interactions significantly.

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Oral Presentation 51

NMR Analytical Perspectives in Natural Products: From Biotransformation Product Dereplication to Protein-Ligand ex-Situ and in-Cell Applications

Ioannis P. Gerothanassis

Section of Organic Chemistry and Biochemistry, Department of Chemistry, University of Ioannina, Ioannina, GR, 45110, Greece

E-mail: igeroth@uoi.gr

In this lecture recent developments of natural abundance ligand-observed NMR methods in the field of natural products will be summarized [1]. Representative examples will be provided on: (a) real-time in-tube enzymatic biotransformations of natural products, with the use or not of immobilized enzymes [2]. (b) Ligand-macromolecular interactions, with the use of saturation transfer difference (STD) NMR, inter-molecular transfer NOEs for PHArmacophore Mapping (INPHARMA) NMR, in combination with computational methods [3]. Emphasis will be given in investigating conformational flexibility of mono- and polyunsaturated free fatty acids bound to human serum albumin [3] and the anti-apoptotic protein Bcl-2. (c) Ligand interactions with the anti-apoptotic family of Bcl-2 proteins in living cells without the need of isotope labelling techniques [4].

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Environmental

Oral Presentation 52

Temporal evolution of particulate PAH and Particulate matter concentrations for 6 months in Strasbourg (France)

J. Vaz-Ramos[1,2], A. Becker[1], F. R. Nursanto[1], O. Delhomme[1], M. Millet[1], S. Bégin-Colin [2] and S. Le Calvé[1]

[1]ICPEES – CNRS/University of Strasbourg, 25 rue Becquerel, Strasbourg, France
[2]IPCMS, UMR-7504 CNRS-Université de Strasbourg, 23 rue du Lœss, CEDEX 2, 67034 Strasbourg, France
E-mail: s.lecalve@unistra.fr

Air quality is a topic that has gained more and more interest in the last decades, as pollutants present in the air are responsible for causing deleterious effects on human health, as well as impacting the environment [1]. Among these pollutants, polycyclic aromatic hydrocarbons (PAH) are constituted by two or more aromatic rings and are widespread environmental contaminants formed during incomplete combustion or pyrolysis of organic material. The presence of polycyclic aromatic hydrocarbons (PAHs) and particulate matter (PM) in the air is known to provoke deleterious effects on human health [2,3]. This work focused on the monitoring of PM and PAHs in the air over 6 months in a peri-urban site in Strasbourg (France), using a three-stage cascade impactor and a particle analyser allowing PM1, PM2.5 and PM10 discrimination. Meteorological conditions were monitored to study their influence on the pollutant levels.
During the first month, the average PM10 concentration of the cascade impactor and particle analyser varied from 11.8 to 80.2 $\mu g/m^3$ and 10.6 to 220.2 $\mu g/m^3$, respectively [4]. The PAH total concentration ranged from 1.1 to 7.6 ng/m^3 and a predominance of 5- and 6-ring PAHs was observed. PAHs were also more abundant in finer particles (PM1). Specifically, identified PAHs are traffic tracers suggesting that vehicular emission was one of its main sources during this period. Two pollution episodes, associated with either a Saharan dust wind episode or traffic pollution, were observed, and led to PM10 and PM2.5 surpassing the daily limit values established by the European Union despite the traffic limitations according to the COVID restrictions. The total PAH concentrations were the highest during these periods suggesting PAHs might be bound to and transported via dust particles [4].
In the following five months, PAH concentrations were significantly lower. A sharp drop in PAH concentrations was observed in the middle of May, which could be explained by the shutdown of the collective domestic heating systems in the neighboring residential areas. This would suggest that, outside of specific pollution episodes, PAHs are mainly emitted from collective domestic heating systems and that car emissions are relatively limited.

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Oral Presentation 53

Continuous Monitoring of ppb-levels of Formaldehyde: Comparison of Analytical Systems and Development of a Portable Calibration Generator

A. Grandjean[1,2], A. Becker[1], M. Wolf[1], C. Sutter[1], F. Amiet[2], D. Bazin[2] and S. Le Calvé[1]

[1]ICPEES – CNRS/University of Strasbourg, 25 rue Becquerel, Strasbourg, France
[2]Chromatotec, 15 Rue d'Artiguelongue, Saint-Antoine, France

E-mail: s.lecalve@unistra.fr

Since humans spend most of their routine time indoors, accurate and continuous monitoring of indoor air pollutants is crucial to understand and prevent airborne diseases. In indoor air, aldehydes mainly originate from construction materials such as plywood, insulating materials, paints, etc. [1]. Formaldehyde, the most abundant one, is classified as carcinogenic category 1B under European Regulation (EC) No 1272/2008. An exposure limit of 30 µg/m^3 for chronic exposure has been established. Considering its hydrophilic properties and its high reactivity, formaldehyde is a challenging molecule to measure as well as to generate precisely/steadily [2]. The accuracy of an analysis is highly dependent on the quality of the calibration step. In this work, three ways of gaseous formaldehyde generation and three formaldehyde analysers were evaluated. The three sources used were: a permeation system using an aqueous formaldehyde solution, a paraformaldehyde permeation tube heated at 50 or 60°C and supplied by a constant flow of nitrogen, and a gaseous formaldehyde cylinder.

First, the formaldehyde solution and the permeation tubes were used for a laboratory-controlled intercomparison of two analysers: a portable microanalyser based on the derivatization of formaldehyde for continuous fluorometric detection, and an Automatic Gas 2D-chromatograph equipped with a thermodesorption unit and flame ionization detector (auto-TD-GC-FID) [3]. Their performance was studied, with a focus on humidity interference. The auto-TD-GC-FID response was influenced by the presence of humidity in the air while the microanalyser was not.

In a second intercomparison study, the microanalyser was successfully challenged at low concentrations, from 2.5 to 21 µg m^{-3}. Gaseous formaldehyde originated from a certified permeation tube or a certified cylinder. When using this certified permeation tube, the HPLC used as the reference method measured concentrations 30% lower than the expected theoretical values, showing that its formaldehyde emission rate must be accurately (re)determined.

To improve the in-situ calibration procedure of (trans)portable formaldehyde analysers, a portable calibration generator and a transportable high-performance liquid chromatography (HPLC) for gaseous formaldehyde monitoring were developed. The transportable HPLC system using 2,4-dinitrophenylhydrazine (DNPH) sampling tubes based on the reference method ISO 16000-3 allowed laboratory or on-site calibration of the generator. The portable generator consists of a permeation tube inserted in a 200 cm^3 oven heated at 50 or 60°C and supplied by a constant flow of nitrogen in the range of 30 – 100 mL min^{-1}. It was designed to achieve low formaldehyde generation, good portability, and fast stabilisation for on-field calibration. It generated very stable concentrations from 33 to 290 µg m^{-3} over several months.

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Oral Presentation 54

Microfluidic devices for cation detection based on calixarene

I. Leray[1], A. Depauw[1], M.H. Ha-Thi,[1,] N. Kumar[1], Q. Pham[1], C. Remy[1], J.P. Lefevre[1,] C. Mongin

[1] ENS Paris Saclay PPSM(CNRS, , 4 avenue des Sciences, 91190 Gif Sur Yvette

The selective and sensitive detection of alkali cations and amines is of great interest in various fields including medecine and environment. Potassium involves in the transmission of nerve impulses. Monitoring the potassium concentration in brain tissues should be very interesting in order to understand several neurological diseases such epilepsy. The detection of Cs^+ ions is of great importance due to its intrinsic toxicity and its ability to displace potassium from muscles and red blood cells. [1] The major source of cesium involves nuclear waste materials. Also the detection of amines is of great interest because of their involvement in various diseases.

Different types of techniques have been employed for the detection of metal ions, however, the approach based on chemically derived fluorescent sensors has their own advantages, including non-destructive nature, high sensitivity and applicability to the bio-systems [2, 3]. As for concern of alkali metal ions detection, the cationic complex forming characteristic of crown ethers offer horizon to design optical chemosensors for these ions. Calix[4]arene appended with crown loops have been shown to exhibit high selectivity for alkali metal ions [4]. Therefore, we employed calix[4]arene scaffold to develop fluorescence chemosensors for the detection of alkali matal ions such as K^+ and Cs^+ ions. [5,6, 7]. Regarding the amine detection calix[6]arene funnels offer a selective receptor for primary amines[8]. In this context, several systems including development of microfluidic chips are presented.

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Oral Presentation 55

Socioeconomic status and public health in Australia: A wastewater-based study

Rousis N.[1,2], Li Z.[3], Bade R.[1], McLachlan M.S.[3], Mueller J.F.[1], O'Brien J.W.[1], Tscharke B.J.[1], Thomaidis N.S.[2], Thomas K.V.[1]

[1]Queensland Alliance for Environmental Health Sciences (QAEHS), The University of Queensland, 20 Cornwall Street, Woolloongabba, QLD 4102, Australia
[2]Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, 15771 Athens, Greece
[3]Department of Environmental Science, Stockholm University, SE-106 91 Stockholm, Sweden

E-mail: nrousis@chem.uoa.gr

Analysis of untreated municipal wastewater is recognized as an innovative approach to assess population exposure to or consumption of various substances. Currently, there are no published wastewater-based studies investigating the relationships between catchment social, demographic, and economic characteristics with chemicals using advanced non-targeted techniques. In this study, fifteen wastewater samples covering 27% of the Australian population were collected during a population Census. The samples were analyzed with a workflow employing liquid chromatography high-resolution mass spectrometry and chemometric tools for non-target analysis. Socioeconomic characteristics of catchment areas were generated using Geospatial Information Systems software. Potential correlations were explored between pseudo-mass loads of the identified compounds and socioeconomic and demographic descriptors of the wastewater catchments derived from Census data. Markers of public health (e.g., cardiac arrhythmia, cardiovascular disease, anxiety disorder and type 2 diabetes) were identified in the wastewater samples by the proposed workflow. They were positively correlated with descriptors of disadvantage in education, occupation, marital status and income, and negatively correlated with descriptors of advantage in education and occupation. In addition, markers of polypropylene glycol (PPG) and polyethylene glycol (PEG) related compounds were positively correlated with housing and occupation disadvantage. High positive correlations were found between separated and divorced people and specific drugs used to treat cardiac arrhythmia, cardiovascular disease, and depression. Our robust non-targeted methodology in combination with Census data can identify relationships between biomarkers of public health, human behaviour and lifestyle and socio-demographics of whole populations. Furthermore, it can identify specific areas and socioeconomic groups that may need more assistance than others for public health issues. This approach complements important public health information and enables large-scale national coverage with a relatively small number of samples.

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Oral Presentation 56

OxR: A microfluidic instrument to detect reactive oxygen species on terrestrial and planetary environments

Georgiou Christos[1], Chatzitheodoridis Elias[2], Kalaitzopoulou Electra[1], Papadea Polyxeni[1], Skipitari Marianna[1], Varemmenou Athina[1], Stavrakakis Hector-Andreas[2], Markopoulos Ioannis[4], Alexandrou Aggelos[4], Holynska Malgorzata[5]

[1]Department of Biology, School of Natural Sciences, University of Patras; [2] Department of Geological Sciences, School of Mining and Metallurgical Engineering, National Technical University of Athens; [4] ZEROONE LTD, Athens,
Greece; [5] Materials' Physics & Chemistry Section (TEC-QEE), Technical Reliability and Quality Division (TEC-QE), ESTEC, ESA

E-mails: c.georgiou@upatras.gr; eliasch@metal.ntua.gr

Reactive Oxygen Species (ROS), such as metal superoxides ($O_2^{\bullet-}$; e.g., KO_2), metal peroxides (O_2^{2-}; e.g., K_2O_2), and potential generators of hydroxyl radicals ($^{\bullet}OH$) are formed by intense UV and cosmic radiation as well as by micrometeorite impact on the Moon's surface, on planet Mars, and on other planetary bodies. Under these conditions, chemical bonds in minerals break, making their surfaces highly reactive. The produced ROS species are highly reactive also in contact with organic compounds, and the latter cannot retain their structure and integrity. The developed instrument, OxR (Oxygen Release), is a small microfluidic device that can detect and identify different types of ROS in terrestrial and planetary soils and regoliths, allowing the exploration for ROS-free soils, which could have preserved putative life and biosignatures on other planets, or simply existing organics, or to identify contaminated soils on Earth with chemicals that produce ROS, i.e., to be used for agricultural purposes or resolving other environmental issues caused by fine mechanical breaking of mineral surfaces. An important planetary application is the identification of ROS-free soils on Mars that can be sampled for future sample return missions.

OxR measures ROS through the release of oxygen upon their reaction with water. Catalysis on MnO_2, i.e., on pyrolusite, releases additional oxygen due to the dissociation of hydrogen peroxide (H_2O_2) that has been formed already in the reaction of ROS with water. Highly toxic free hydroxyl radicals ($^{\bullet}OH$) can be also detected spectroscopically. To test the instrument, we have produced Lunar and Mars soil and dust simulants, or dusts produced from actual Lunar meteorites. Experiments on those materials using lab-applicable specific chemical assays demonstrated that oxygen release exceeds by at least 3 times the value acquired by Viking during the Gas Exchange Experiment of the 1976 Viking mission to Mars. Also, the release of $^{\bullet}OH$ is observed to be at the same order with past studies on Mars-like Atacama and Mojave soils. The increased release of oxygen is a significant outcome, because it supports ISRU of oxygen on planetary surfaces for respiration of astronauts or as a propulsion gas. For that, we have invented the concept of "oxygen farming" which we intent to apply on the Lunar surface. Additionally, the methods we propose can be used to remediate ROS-rich soils.

Disclaimers

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Oral Presentation 57

Shipping pollution in the marine environment: a particulate challenge

A. Gondikas[1,2,3], M. Hassellöv[3], K. Mattsson[3], S. Chen[4], and I.-M. Hassellöv[5]

[1]Creative nano, PC, Metamorfosi, 14451 Athens, Greece

[2]Department of Geology and Geoenvironment, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, 15771 Athens, Greece

[3]Department of Marine Sciences, University of Gothenburg, BOX 461, SE-405 30 Gothenburg, Sweden

[4]State Environmental Protection Key Laboratory of Environmental Risk Assessment and Control on Chemical Process, School of Resources and Environmental Engineering, East China University of Science and Technology, Shanghai 200237, PR China

[5]Department of Mechanics and Maritime Science, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden

E-mail: a.gondikas@creativenano.gr

Shipping has been traditionally considered an environmentally friendly means of transportation, a perspective that is challenged in recent years. Scientific evidence on air quality impacts has led the International Maritime Organization to put in place regulations for limiting atmospheric pollution from shipping [1]. Scrubbers are highly efficient in capturing sulphur species from ship exhaust gas and are currently the most popular sulphur abatement technology in large ships. In short, seawater is fed in the scrubber and brought in contact with the exhaust gas, allowing mass transfer of components from the gaseous into the water phase; the resulting effluent is returned to the sea with or without pre-treatment. In addition to sulphur, scrubbers are highly efficient in removing particulate matter from the exhaust gas, which is likely to contain hazardous elements, such as metallic and organic pollutants [2-3]. Furthermore, antifouling paints on the underwater body of the ship are designed with toxic properties, in order to prevent biological growth and build-up of drag, which reduces speed and increases fuel consumption when the ship is in motion. Ship paint microplastics containing biocides, such as the metals copper and zinc, and particles containing tin (residues from old or current use of tributyl-tin ship hull paints) raise concerns on the environmental impacts from ships and smaller boats [4-5]. What is common in the cases of scrubber effluent and antifouling paints is the direct release of particles loaded with pollutants. It is therefore imperative to determine the fate and transport of particles from ships into the marine environment. The determination of physical and chemical properties of these particles is a crucial step, prior to testing toxicological effects on marine organisms and applying models to predict their transport in the ocean. In this work, we present advantages and disadvantages of analytical methods for monitoring particle emissions from ships in the marine environment, with a focus on scrubber effluent and antifouling paints. A comprehensive methodological approach is presented, which is based on automated scanning electron microscopy with energy dispersive spectroscopy for particles retained on 10 μm pore-size membranes and single-particle inductively coupled plasma mass spectroscopy for filter-passing particles. The superiority of correlative microscopy is discussed for the former particle populations.

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Sample Handling

Oral Presentation 58

The use of deep eutectic solvents as sustainable and recyclable solvents for extraction of phenolic compounds from aloe vera rind by-product: Extraction optimization and green metrics

G.I. Ioannou[1], K.A. Ioannou[1], A. Christou[1], I.J. Stavrou[2], C.P. Kapnissi-Christodoulou[1]

[1]Department of Chemistry, University of Cyprus, 1678 Nicosia, Cyprus
[2]Department of Life Sciences, European University Cyprus, 2404 Nicosia, Cyprus

Email: ckapni1@ucy.ac.cy

In this study, an optimized environmentally friendly procedure was performed to enhance the sustainable utilization of phenolic antioxidants derived from aloe vera rind by-product. The procedure entailed the utilization of ultrasound-assisted extraction (UAE) in combination with deep eutectic solvents (DESs). A total of eleven different DESs and three conventional solvents were employed as extraction media for polyphenolic compounds. Choline chloride-citric acid (ChCl-CA) was selected as the optimal extractant due to its extraction efficiency in relation to the total phenolic content. The operating conditions of UAE were optimized and modelled by use of response surface methodology, with the aim of maximizing the yield of total phenolics and antioxidant capacity. The optimal operational parameters for the UAE procedure were determined to be 16.5 min, 74% DES and solvent to solid ratio equal to 192. HPLC analysis was performed on the optimum extract, revealing significant levels of phenolics present in the aloe rind. Efficient recovery of the extracted antioxidants was successfully accomplished through the utilization of solid-phase extraction (SPE) with polyamide cartridges. The ChClCA DES exhibited excellent recycling capability with a yield of over 90% through SPE. Finally, the greenness of the method was evaluated using the AGREE and AGREEprep metrics. The results obtained from the green approaches highlighted the sustainability and the greenness of the proposed extraction procedure for the aloe by-product.

Oral Presentation 59

Monitoring of PFAs levels in water using a Solid Phase Extraction coupled with LC/MS-MS analytical method

Nikoletta Xanthopoulou[1], Chrysa Gkementzoglou[1], Despoina Alexiadou[1], Georgia Seretoudi[1]

[1]EYATH S.A., Thessaloniki Water Supply & Sewerage Company, Thessaloniki Water Treatment Plant Laboratory Department

E-mail: nxanthopoulou@eyath.gr

Per- and polyfluoroalkyl compounds (PFAs) are a huge class of nearly 10,000 anthropogenic contaminants that are persistent, bioaccumulative and toxic. Due to their attractive physicochemical properties, thermal and chemical stability, they are used in numerous industrial and consumer products in everyday life.[1,2,3] Their ubiquitous presence and resistance to degradation have led to their detection in the aquatic environment, rainwater, drinking water and consequently animals and humans[4].

Their abundance led to their inclusion in the new European Drinking Water Directive (DWD) with a parametric value of 100 ng/L per compound and a maximum method detection limit of 30 ng/L. Thus, an analytical method for the determination of the 20 PFAs included in the DWD, bearing four- to thirteen-carbon chains with either carboxylic or sulfonic acid, was developed based on ISO 21675:2019, for drinking and surface water samples. This method was validated according to ISO 17025:2017. Method Detection Limits vary between 0.49-10.37ng/L. Reproducibility varies between 4-22%, recovery between 75-134% and uncertainty between 10-52% for both matrices.

Monthly monitoring of PFAs levels was carried out since September 2021, for drinking water samples from the city of Thessaloniki and its water resources (Aravissos springs and Aliakmonas river). In all drinking water samples, PFAs levels were below 10ng/L while in untreated water samples PFAs were detected in levels below 20ng/L. These results strongly indicate that there is no substantial PFAs pollution for the city drinking water.

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Oral Presentation 60

Sample pretreatment using flow methods

P. Solich[1], B. Horstkotte[1], P. Chocholouš[1], H. Sklenářová[1] and D. Šatínský[1]

[1]Charles University, Faculty of Pharmacy, Dept. of Analytical Chemistry, Hradec Králové, Czech Republic
E-mail: solich@faf.cuni.cz

Recently, green sample preparation has become of great interest to an increasing number of scientists and many attempts have been undertaken to automate such preparation procedures. The automation of the sample pretreatment step, in particular analyte extraction, enhances procedural repeatability, decreases the risk for human errors, and minimizes the need for manipulation with organic solvents and other reagents. To automate different extraction procedures, flow techniques as highly versatile tools, above all Sequential Injection Analysis (SIA) [1], and applying the principles of flow methods on other platforms, have been one of the main approaches used for this task. In this field, various extraction methodologies have been developed based on liquid-liquid extraction in its basic, miniaturized form, and also in dispersive format. Modified SIA systems have been used for their applications in the field of environmental and biological samples analysis. Sample pretreatment using solid phase extraction is based on universal or selective sorbents including restrictive access materials, molecularly imprinted polymers, and nanomaterials. Extraction procedures have been automated in SIA systems with sorbents used in the form of prepacked micro-columns or taking advantage of the Bead-Injection approach, i.e. using a sorbent suspension as a renewable packing material in the miniaturized SIA-related Lab-On-Valve format [2]. Head-space extraction was also developed in the single-drop format for the analysis of volatile analytes using a second SIA-related approach Lab-in-syringe [3]. All these sample pretreatment methods can be used in combination with on-line determination using the same flow system or hyphenated with chromatographic systems. Outstanding examples will be discussed to demonstrate how flow techniques can improve the sample pretreatment and preparation steps.

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Oral Presentation 61

Analyzing ante-mortem and post-mortem biological materials

Renata Wietecha-Posłuszny[1]

[1]Laboratory for Forensic Chemistry, Department of Analytical Chemistry, Faculty of Chemistry, Jagiellonian University in Kraków, Gronostajowa St. 2, 30-387 Kraków, Poland

Email: renata.wietecha-posluszny@uj.edu.pl

Keywords: green metrics, forensic chemistry, psychoactive substances, biological samples, green assessment

The subject of this presentation is an overview of selected methods of sample preparation and analysis, in particular effective extraction techniques used for the isolation of psychoactive substances from biological materials used in toxicological-forensic analyzes. The process of preparing a sample for analysis is one of the first and critical stages of its analysis, which regardless of further phases of proceeding with the sample, determines the quality and reliability of the results of chemical analysis. This step is often time-consuming and requires the consumption of large quantities of reagents. The innovative such as: solid phase microextraction and miniaturization allow not only to reduce their quantity, but also to perform the analysis using small amounts of the sample, which is often available in limited quantities in forensic analysis [1,2]. Moreover one of the most important stages in the development of a new analytical method is its validation and assessment of greenness using the appropriate metric. In the present study, the White Analytical Chemistry (WAC) concept [3] and the ChlorTox Scale [4] were used to assess the methods of forensic and toxicological analysis from various angles.

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Oral Presentation 62

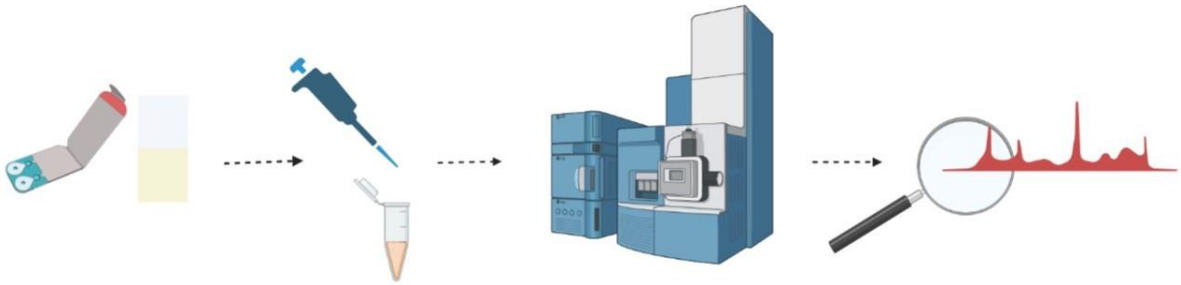
Qualitative dried blood spots (qDBS) and dried urine spots (DUS): Applications for the accurate determination of biomarkers and illicit drugs

T. Meikopoulos[1,2], O. Begou[1,2,3], Stelios Papazoglou[1,2], H. Gika[2,4], G. Theodoridis[1,2]

[1]Department of Chemistry, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[2]Biomic AUTH, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki, Innovation Area of Thessaloniki, Thermi 57001, Greece
[3]ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, 57001, Greece
[4]Laboratory of Forensic Medicine and Toxicology, School of Medicine, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

E-mail: meikthom@chem.auth.gr

Dried matrix spot (DMS) is a sampling technique in which a small volume of biological fluid is collected using a particular filter paper. DMS analysis is widely employed over the last decade, in fields such as biomarker research and toxicology. An alternative to analysing native liquid urine is employing dried urine spots (DUS), with the advantages of simplicity, stability, and cost-efficiency. Amino acids determination from DUS is of high potential for biomarker research since it enables simple sample collection, long-term preservation, convenient transit, and compatibility with a variety of analytical procedures. For the DUS application, an efficient method for the quantification of 14 amino acids was developed. Moreover, the advantages of blood microsampling is very appealing for a variety of bioanalysis applications. This technique is less invasive than the normal venipuncture, making it particularly suitable for sample collection, among neonates, the elderly, and patients requiring frequent and repetitive testing. For the qualitative dried blood spots (qDBS) applications, Capitainer qDBS device was used. Two validated methods were developed. The first one, aimed to the accurate and reproducible determination of 4 different ceramides, while the other one intends to quantitatively determine 12 acyl-carnitines. Boths methods provide accurate results for such metabolites which are implicated in regulation of diverse cellular processes i.e., cardiovascular diseases, type 2 diabetes, and others. Finally, a qDBS application was employed, defining 23 illicit drugs in a short term analysis with a quick and easy sample pretreatment protocol.



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Oral Presentation 63

Key aspects during the development of analytical sample preparation methods: application to the study of selected pesticides in bee products

Adrián Fuente-Ballesteros, José Bernal, Ana M. Ares

Analytical Chemistry Group (TESEA), I. U. CINQUIMA, Faculty of Sciences, University of Valladolid, 47011, Valladolid, Spain

E-mail: adrian.fuente.ballesteros@uva.es

No official methods for evaluating pesticide residues in bee products are available. There is a myriad of methods in the scientific literature that can be used, and they are usually selected based on the materials and equipment available in the laboratory. Nevertheless, the complex composition of bee products requires the development of matrix-specific sample preparation methods which must be selective and provide acceptable recovery values and matrix effect. Different sample preparation methods such as QuEChERS (*Quick, Easy, Cheap, Effective, Rugged & Safe*), SPE (*Solid-Phase Extraction*), SE (*Solvent Extraction*), DLLME (*Dispersive Liquid-Liquid Microextraction*), and SPME (*Solid-Phase Microextraction*) have been proposed and applied to analyze contaminant residues in bee products.

When designing sample preparation methods for studying pesticides in bee products, it is crucial to consider specific fundamental aspects: i) optimization of sample amount to be able to determine analytes at low concentration levels, ii) accurate selection of the extraction solvent (polarity, ratio, and volume), iii) optimization of the order of the steps and their characteristics (volume, time, and temperature) and iv) benefits of using salts to favor the transfer of acaricides or cleaning sorbents to reduce the matrix effect. Considering these indications, two useful approaches to evaluate acaricide residues are QuEChERS and SE methods. These sample treatments have been optimized, and the corresponding methods that comprised gas chromatography-mass spectrometry (GC-MS) were validated in different bee products [1,2]. Pesticides, mainly acaricides, from beeswax were determined by using a modified QuEChERS method involving an extraction with an acetic acid in acetonitrile mixture followed by dispersive solid-phase extraction (enhanced matrix removal lipid, and a polishing step). Similarly, bee pollen was also analyzed by a modified QuEChERS method but employing an ethyl acetate and cyclohexane as extractant and a mixture of salts for the *clean-up* step. Two sample treatments were needed for honeys concerned with their different composition influenced by the botanical origin. An efficient and simple sample treatment with low solvent consumption was selected consisting of single solvent extraction with an ethyl acetate and cyclohexane mixture for light honeys, and a double extraction for dark honeys. It can be concluded that the combination of the above-mentioned sample treatments with GC-MS was confirmed to be an optimal methodology for the analysis of acaricide residues in different bee products.

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ABSTRACTS POSTERS

Poster Session 1

Sensors & Biosensors
A. Other Applications

P.1 Screening method for discrimination of olive oil from other vegetable oils with a DNA biosensor

N-M Christopoulou[1], V. Mamoulaki[1], A. Mitsiakou[1], E. Samolada[1], D. P. Kalogianni[1], and T. K. Christopoulos[1,2]

[1]Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras, Rio, Patras, Greece 26504
[2]Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE), Patras, Greece 26504

E-mail: tchrist@upatras.gr ; kalogian@upatras.gr

Because of its unique sensorial characteristics, nutritional advantages and health benefits, olive oil, the key component of the Mediterranean diet, commands a much higher price than other edible oils with significant benefits for the economy of producing countries. As a result, it becomes a prime target for fraudulent activities. The most frequent adulteration of olive oil involves mixing with less expensive vegetable/seed oils. Therefore, there is a high research activity on the development of analytical methods for detection of vegetable oils present in olive oil. Compared to small metabolites whose profile is affected by environmental conditions, DNA offers the advantages of high stability and specificity. In this work, we have developed a molecular rapid test for the discrimination of olive oil from sunflower, soya, corn, sesame, hazelnut, and almond oils. Following DNA extraction, we performed a PCR using a single pair of primers to amplify a sequence (~179 bp) of the *rbcl* gene from the seven oils. The amplified DNA was then subjected to a multiplex extension reaction by DNA polymerase using specific oligonucleotide primers that enable discrimination of oil species. Detection of the products was achieved by a single DNA biosensor that captures all the products of the extension reaction through hybridization with immobilized oligonucleotide probes. Only the extended products, however, carry biotin moieties to enable detection with antibody-functionalized gold nanoparticles. The results appear as red spots on the membrane of the sensor. Each spot represents a specific plant oil, thus allowing spatial discrimination and simultaneous detection of seven different plant species/oils. As low as 5% of adulteration of olive oil in binary mixtures with hazelnut, sesame, soya and corn were detected by the multiplex strip, while 10% of adulteration was detected for almond and sunflower, all with very good reproducibility. [The authors VM, AM and ES contributed equally to this project].

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P.2 Molecular rapid test for detection of tuna fish adulteration

I. P. Gkini[1], P. Christopoulos[1], D. P. Kalogianni[1], T. K. Christopoulos[1,2], and A. Conides[3]

[1]Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras, Rio, Patras, Greece 26504

[2]Institute of Chemical Engineering Sciences / Foundation for Research and Technology Hellas (FORTH/ICE), Patras, Greece 26504

[3]Hellenic Centre for Marine Research, Institute for Marine Biological Resources, 46.7 km Athens-Sounion, Mavro Lithari, 19013 Anavyssos, Attika, Greece

E-mail: tchrist@upatras.gr; kalogian@upatras.gr

Tuna is a beneficial food, very light in calories and highly recommended for a balanced diet. Due to the continuous increase in the demand for tuna, especially for culinary preparations of the bluefin tuna species in fresh or processed forms, and its comparatively high market price, there is a pressing need to develop analytical methods for the detection of adulteration of tuna with other lower priced fish. In the present work we have developed a simple, fast, and lowcost molecular method for visual detection of bluefin tuna species (BFT) adulteration. The three species studied were Thunnus thynnus (BFT), Thunnus albacares and Katsuwonus pelamis. The method is based on the construction of a DNA biosensor comprising an immersion pad, a conjugate pad, a sensing membrane, and an absorbent pad. The membrane consists of a control zone, containing biotinylated albumin, and a test zone with immobilized capture oligonucleotide (oligo-dT). DNA was isolated from fresh and cooked fish samples followed by PCR to amplify sequences of the D-loop region for Thunnus albacares, the Cytb gene for Katsuwonus pelamis and the NADH5 for BFT. The PCR products were hybridized (15 min) with specific, dA-tailed probes. We prepared gold nanoparticle-antibiotin antibody conjugates for hybrid detection. The hybridized solution and the conjugates were applied to the conjugate pad. The signal was observed in 15 min. The effect of the amount (fmol) of PCR products on the intensity of the test zone was studied for the three species in the range of 0-100 fmol, in triplicate. The results were reproducible. The biosensor can detect 1.6, 6.3 and 12.5 fmol PCR product from albacares, pelamis and BFT, respectively. Cross-reactivity studies confirmed that the probe of one species does not hybridize with DNA from the other two species. The method was evaluated using mixtures of fresh tissue PCR products and mixtures of DNA isolates from heat-treated tissues at adulteration percentages of 1-100 %. The three most ordinary case adulterated mixtures were tested, i.e., albacares with pelamis, BFT with pelamis and BFT with albacares. The findings show that the method can detect 1% of adulteration by naked eye.

Acknowledgements: The research presented herein was conducted in the frame of the research project "DNASEEKER- Innovative prototype genetic method for the identification of fish species for the Greek fishery products processing industry" (MIS 5072570), co-funded by the Greek Government Operational Program for Fisheries and Sea 2014–2020 and the EU EMFF.

P.3 Development of a molecular rapid test for the visual authentication of the fish *Sardina pilchardus*

Myrto Kakarelidou[1], Panagiotis Christopoulos[1], Despina P. Kalogianni[1,*], Theodore K. Christopoulos[1,2,*] and Alexis J. Conides[3]

[1]Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras, Rio, Patras 26504, Greece
[2]Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE), Patras 26504, Greece
[3]Hellenic Centre for Marine Research, Institute for Marine Biological Resources 46.7 km Athens-Sounion, Mavro Lithari, 19013 Anavyssos, Attika, Greece

E-mail: kalogian@upatras.gr

Fish adulteration is a major global concern. Adulteration refers to the substitution of a particular fish sample with another fish of lower price and nutritional value, especially in processed fish-based products, for economical profit. Sardines are one of the most consumed and vulnerable to adulteration product worldwide. Thus, the development of analytical methods for fish adulteration are of great interest. Molecular methods are the preferred ones due to DNA stability in fresh, processed and canned products. In this project, we have developed a molecular rapid test for fish authentication. In detail, the adulteration of *Sardina pilchardus* with *Sardinella aurita*, the most common species used for sardines adulteration, was detected. The detection was visual, by naked eye, using colored nanoparticles as reporters, while the analysis with the rapid test was completed within 10 min. As low as 3 fmol of PCR product of *Sardinella aurita* and 1% of adulteration in binary PCR mixtures were detected by the proposed test. The test was finally applied for the detection of adulteration in processed binary fish mixtures (boiled, salted and canned) being able to detect down to 5% of adulteration. The proposed test is rapid and simple, providing very good detectability and reproducibility. This test is also universal, meaning that it can be applied for the detection and identification of other fish species.

Acknowledgements: The research presented herein was conducted in the frame of the research project "DNASEEKER- Innovative prototype genetic method for the identification of fish species for the Greek fishery products processing industry" (MIS 5072570), co-funded by the Greek Government Operational Program for Fisheries and Sea 2014–2020 and the EU EMFF.

B. Life Sciences

P.4 A sensitive and selective sensor for cancerous exosomes using fluorescent magnetic nanocomposites with graphene oxide-based fluorescence quenching

Seok Won Park[1], Yun Kyung Jung[1,2*]

[1]Department of Nanoscience and Engineering & [2]School of Biomedical Engineering, Inje University, Gimhae 50834, Republic of Korea

E-mail: ykjung9@inje.ac.kr

Exosomes have various tumor-specific proteins and are considered important biomarkers for early diagnosis of cancer [1]. However, previous exosome detection technologies have limitations such as the requirement of expensive equipment and complicated procedures [2]. In this study, fluorescence-emitting carbon quantum dots (CQDs) and magnetic nanoparticles were fabricated and incorporated into a single fluorescent magnetic nanocomposite (FMN) by the help of polymer. And, an anti-epithelial cell adhesion molecule (EpCAM) aptamer was conjugated to the FMN to detect the EpCAM overexpressed on the surface of cancerous exosomes. Fluorescence of FMNs was quenched by fluorescence resonance energy transfer (FRET) between anti-EpCAM aptamer-conjugated FMN and graphene oxide (GO). Upon reaction with cancerous exosomes, anti-EpCAM aptamer-conjugated FMNs moved away from the GO and their fluorescence was reignited. At concentrations of $0 – 128 \times 10^3$ particles/μL of cancerous exosomes, the fluorescence recovery increased linearly, successfully demonstrating the detection and isolation of cancerous exosomes from real samples. The FMN developed in this study can be used as a valuable platform that can detect and separate cancer-related biomolecules as well as various disease-related molecules.

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P.5 Whole-genome sequencing of SARS-CoV-2: automation in theprocess of detecting variant evolution of the virus

M. Gancarcikova[1,2], H. Parova[1], M. Berankova[1], L. Rysava [1], L. Krcmova Kujovska[1,3], L. Pavlikova[1], V. Palicka[1], R. Hyspler[1]

[1]Department of Clinical Biochemistry and Diagnostics, Charles University, Faculty of Medicine inHradec Kralove and University Hospital Hradec Kralove, Czech Republic
[2]University of Pardubice, Faculty of Chemical Technology, Czech Republic
[3]Charles University, Faculty of Pharmacy in Hradec Kralove, Czech Republic E-mail:

marketa.gancarcikova@fnhk.cz

Next-generation sequencing (NGS) technology has been successfully used to trace the origin and understand the evolution of infectious agents, investigate transmission, but also to find effective treatment. The high demands on diagnostic laboratories during pandemics have resulted in the implementation of automation of the complex steps involved in the preparation of NGS libraries. By whole-genome sequencing of SARS-CoV-2, the etiologic agent of Covid-19 disease, 6,765 SARS-CoV-2 genomes isolated from nasopharyngeal swabs or bronchoalveolar lavages of Covid-positive patients were sequenced at the University Hospital Hradec Kralove between 2021/05 and 2022/11 as part of a national surveillance strategy. Commercial kits CleanPlex® SARS-CoV-2 Panel for Illumina (Paragon Genomics) and Swift Normalase™ Amplicon SARS-CoV-2 Panels (Swift Biosciences) were used to prepare the amplicon library with process automation using Biomek Automated Workstation (Beckman Coulter) or NGS Bravo (Agilent Technologies). Sequencing was performed on the MiSeq platform (Illumina), secondary analysis was performed using the Bioxsys COVID application (aligned to GenBank NC_045512.2), and the Nextstrain (https://clades.nextstrain.org/)and Pangolin (https://pangolin.cog-uk.io/) application databases were used for phylogenetic assignment. A total of 6,133 genomic sequences (identity > 90%, N content < 5%, coverage ≥ 20x) were uploaded to the global GISAID database (https://gisaid.org/). Detailed data will be presented. The automation of NGS library preparation [1] represents a high-throughput and robust system with standardized results and concurrently a unique tool in an efficient strategy to monitor SARS-CoV-2 variants in real-time, track the evolution of virus dynamics, and identify variants of potential clinical significance.

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P.6 Synthesis and Characterization of Inclusion Complexes of β-Cyclodextrins and Essential Oils of Greek Origin

I. Pitterou[1], E. Kavetsou[1], A. Kalospyros[1], I. Kostopoulou[1], C. Derzekou[1], E. Kontogeorgou[1], T. Armeni[1], D. Daferera[2], P.A. Tarantilis[2], S. Dervisoglou[3], D. Perdikis[3], A. Detsi[1]

[1]Laboratory of Organic Chemistry, School of Chemical Engineering, National Technical University of Athens, Zografou Campus, 15780 Athens,Greece

[2]Laboratory of General Chemistry, Department of Food Science & Human Nutrition, School of Food & Nutrition Sciences, Agricultural University of Athens, 11855, Athens, Greece

[3]Laboratory of Agricultural Zoology and Entomology, Department of Crop Science, School of Plant Sciences, Agricultural University of Athens, 11855, Athens, Greece

E-mail: adetsi@chemeng.ntua.gr

Essential oils (EOs) are component mixtures, consisting mainly of non-polar low molecular weight metabolites, such as terpenoids, phenolic-derived compounds, and aliphatic components. These oils are typically derived from aromatic plants and exhibit a wide range of biological activities, including antibacterial, antioxidant, antifungal, insecticidal, and antiviral properties. However, EOs contain delicate and volatile molecules that are susceptible to degradation during manufacturing or treatment processes, primarily due to unfavorable factors like heat, humidity, light, and oxygen. Nanoencapsulation creates a protective barrier between the desired molecules and the surrounding environment, ensuring their preservation and enhancing their stability. The aim of the present study was to encapsulate EOs from Greek aromatic plants, (*Mentha pulegium*, *Ocimum basilicum,* and *Origanum majorana*) in βcyclodextrin (β-CD) and chemically modified β-CD matrices (hydroxypropyl-β-cyclodextrin (HP-β-CD) and methyl-β-cyclodextrin (Me-β-CD)) through the formation of inclusion complexes (ICs) using the co-precipitation and kneading methods. The resulting ICs exhibited nanoscale sizes ranging from 90.5 ± 7.8 nm to 465.0 ± 0.3 nm, polydispersity index ranging from 0.348 ± 0.019 to 0.473 ± 0.032, and satisfactory stability in suspension (-32.4 ± 1.7 mV to -11.7 ± 0.6 mV). The process yield was satisfactory, ranging between 71.1% and 87.4%, while the inclusion efficiency ranged from 18% to 98.48%. The in vitro release studies of selected ICs were conducted using GC-MS and a sustained release profile was observed with an initial burst effect in the first hour. The release kinetics were better described by the Higuchi equation whereas the release mechanisms were predicted to be erosion and diffusion.

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P.7 Development of a novel green extraction methodology of nettle using Natural Deep Eutectic Solvents

M.-A. Karadendrou[1], E. Nourry[1], A. Tzani[1], T. Lymperopoulou[2], and A. Detsi[1]

[1]Laboratory of Organic Chemistry, School of Chemical Engineering, National Technical University of Athens, Zografou Campus, 15780 Athens, Greece

[2] Processes and Products Quality Control Horizontal Laboratory, Zografou Campus, School of Chemical Engineering, National Technical University of Athens, 15780 Athens, Greece

E-mail: adetsi@chemeng.ntua.gr

Nettle (*Urtica dioica* L.) is a wild herbaceous plant that has been greatly used over the years as a traditional medicine to treat various diseases and consists a rich source of bioactive compounds with numerous medicinal, nutritional and cosmetic properties[1]. The aim of the present study is the development and optimization of a greener methodology for the extraction of phytochemicals from nettle.

For the development of the process, natural deep eutectic solvents (NaDES) were used as extraction media. NaDES are a new class of green solvents that comprise of two or more naturally-occurring compounds. They have recently emerged as promising extraction solvents due to the numerous advantages that they offer, such as high extraction yields, stabilization of the obtained extracts and protection of the extracted compounds[1-4].

In the present work, different NaDES were synthesized, structurally characterized and examined for their ability to extract bioactive compounds from nettle. The NaDES extracts were evaluated regarding their total flavonoid (TFC) and phenolic (TPC) content, as well as their antioxidant activity. The solvent screening indicated that the most potent extraction solvent was the NaDES derived from betaine and glycerol.

The optimization of the extraction methodology was investigated by performing Experimental Design applying a symmetrical three-level Box-Behnken design with selected independent variables the extraction temperature, the NADES-to-water and the solid-to-solvent ratio. The TPC and TFC of the extracts, as well as their DPPH radical scavenging ability were selected as response variables. The phytochemical profile of the optimum NADES-extract was further studied by performing HPLC analysis. The results were compared with an extract derived by extraction using a conventional hydroethanolic solution, revealing a higher amount of the identified bioactive compounds in the NaDES extract.

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P.8 Gas Ion Distillation (GID) and Sequential Ion Processing (SIPRO) as novel techniques in chemical detection: The role of Augmented Reality (AR) in enhancing their applications

F. Tsopelas[1], M. Statheropoulos[1], Sari Yli-Kauhaluoma[2], Dario Ruiz Lopez[3], G. Eiceman[2] and P. Vaninen[2]

[1] School of Chemical Engineering, National Technical University of Athens
[2] University of Helsinki, Finland
[3] ATOS

e-mail: stathero@chemeng.ntua.gr

Gas Ion Distillation (GID) and Sequential Ion Processing (SIPRO) are two novel analytical techniques developed in the framework of the challenging FETOPEN project GIDPROVIS [1]. GID is based on the pre-fractionation of chemicals as ions at ambient pressure. The technique can separate mixtures through differences in reaction chemistry of gas phase ions [2] and targets in replacing gas chromatography in separations performed in milliseconds to few seconds. SIPRO is based on processing ions of individual chemicals. The ions are fragmented in air at ambient pressure using strong electric fields, providing structurally significant molecular information. After the fragmentation step the separation of ions is performed by classical drift time ion mobility spectrometry (IMS) providing spectra that identify chemical compounds. The combination of GID/SIPRO when miniaturized is expected to bring GC/MS or GC/IMD to the field for robust, reliable, ultra-fast detection, identification and monitoring providing sensors network-like applications for ambient environment monitoring in security, safety but also in recreation. Installing such networks of chemical detectors in different areas will allow monitoring chemically the ambient environment through various devices and gadgets. Mobile phones are included. To address the challenge of sharing the data and information in a meaningful and efficient way to both operational people and civilians, Augmented Reality (AR) has been used. The message directed from the system are different to operational and to the public. Four levels of messages have been defined; data, information, knowledge and "wisdom". Practically, information and knowledge are directed to civilians using special platforms and depending on the situation (security, safety, recreation, education). For security purposes the "Toolbox" platform is used. However, AR has been used for recognition of the objects through the AI software and the camera of the gadget used. This option allows for finding out the possible source of chemical emissions and the direction and the size of the plume. In the framework of the project the human perception of the chemical risk was examined [3] and particularly how symbols, pictograms and others means transfer the chemical risk to operational people and the public. The results of extensive interviews have shown, among others, difficulties in recognizing the type and extend of chemical risks through established pictograms and symbols.

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2. Other Clinical (or pharmaceutical) applications

P.9 The finest smuggler – maximizing the platinum drug loading in liposome nanocarrier

J. Zajda, Z. Wakuła, A. Wróblewska and M. Matczuk

Chair of Analytical Chemistry, Faculty of Chemistry, Warsaw University of Technology, Stanisława Noakowskiego 3, 00-664 Warsaw

E-mail: Joanna.Zajda@pw.edu.pl

Over 40 years ago, the most known metal-based drug, cisplatin, was introduced to clinical practice, and it is still the leading active substance. Despite numerous advantages, chemotherapy, with its use, is associated with severe side effects caused by indiscriminate uptake into normal and cancerous cells [1]. Hence, intensified efforts have been undertaken to provide safe and effective therapies by employing nanocarrier-based drug's targeted delivery systems (DTDSs). Such systems offer the preferential accumulation of cisplatin in cancer cells and reduce adverse side effects. Considering superior biocompatibility and biodegradability, adjustability, flexibility, and ease of functionalization, liposomes composed of lipid bilayer spherical membranes are gaining more interest as nanocarriers [2].

The efficient and reproducible synthesis of liposomes on a large scale yielding stable vesicles of defined properties and high drug loading is of paramount importance. A simple and fast solvent-injection method enables the synthesis of liposomes in a size range appropriate for passive targeting [3,4]. However, the encapsulation efficiency of hydrophilic drugs such as cisplatin, which takes place during the synthesis, is relatively low. Therefore, various approaches aiming for increased Pt-drug loading have been explored within this study. In particular, liposome synthesis conditions have been optimized (e.g., incubation buffer composition, lipid composition, organic solvent), and the feasibility of subsequent freeze-thaw or lyophilization-rehydration procedures have been verified. The encapsulation efficiency of cisplatin and stability of DTDS was determined by capillary electrophoresis hyphened with inductively coupled plasma tandem mass spectrometry (CE-ICP-MS/MS) that guaranteed low limits of detection for metallodrug and nanocarrier and offered high resolution and separation in the mild conditions preventing vesicle's disruption.

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P.10 Assessment of different methodologies for processing fecal samples in 1H NMR metabolic profiling

Konstantinos Tsiantas[1,2], Paris Christodoulou[2], Manolis Matzapetakis[2], Maria Zervou[2] and Panagiotis Zoumpoulakis[1,2]

[1]Department of Food Science and Technology, University of West Attica, Ag. Spyridonos, 12243 Egaleo, Greece

[2]Institute of Chemical Biology, National Hellenic Research Foundation, 48, Vas. Constantinou Ave., 11635 Athens, Greece

NMR-based metabolomics is recognized as a potent analytical platform for comprehending the intricate connections between the gut microbiota and the health status of the host. However, fecal samples have recently gained more attention in comparison to urine or blood matrices, highlighting the importance of generating reliable and consistent data. Fecal samples contain a complex mixture of metabolites, including those derived from the gut microbiota and the host. The choice of extraction protocol can significantly impact the quality and quantity of metabolites obtained for analysis. Therefore, systematic investigation and optimization of fecal metabolite extraction protocols are essential to ensure accurate and reproducible results in NMR metabolomics studies focused on fecal samples.

On these grounds, this study evaluates the effect of different sample processing methodologies (i.e., crude extraction, ultrafiltration, freeze-drying) as well as different pulse sequences (1D NOESY presat and CPMG), on the diversity and abundance of metabolites extracted. The evaluation of various protocols was conducted using human fecal samples obtained from the OSTEOME clinical study, which investigates the effects of a nutraceutical supplement, rich in prebiotics, on osteopenia.

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P.11 Rapid amplification-free detection of microRNAs based on a tailing reaction and a lateral flow strip test

Eleni Lamprou[1], Panagiota M. Kalligosfyri[1] and Despina P. Kalogianni[1,*]

[1]Analytical/Bioanalytical Chemistry & Nanotechnology Group, Department of Chemistry, University of Patras, GR26504, Rio, Patras, Greece

E-mail: kalogian@upatras.gr

MicroRNAs (miRNAs) have emerged as new biomarkers for liquid biopsy applications. MiRNAs are present in a variety of bodily fluids and have been linked to various physiological and pathological processes. Several methods and biosensors, especially the ones that exploit nanomaterials, have been developed for miRNA analysis and are based on target amplification, target recycling or signal amplification. We have herein developed a new lateral flow test in combination with a tailing reaction, which enables the visual detection of microRNAs sequences, bypassing the need of an initial target amplification step. In detail, miRNAs molecules are subjected firstly to a tailing reaction incorporating a poly(A) tail at the 3′ of the microRNA sequences by a poly(A) RNA polymerase. The tailed products were then hybridized to a biotinylated complementary DNA probe and detected by a lateral flow test. The hybrids were captured by immobilized poly(dT) sequences onto the test zone of the strip through the poly(A) tail of the microRNAs, while gold nanoparticles conjugated to anti-biotin antibody were accumulated at this zone, through anti-biotin Ab-biotin interaction, forming a visual red spot. A second red spot is also formed at the control zone of the strip by immobilized biotin moieties to confirm the proper function of the test. MiR-let-7a was used here as a model. As low as 500 fmol of miR-let-7a was detected by the proposed rapid strip test. In conclusion, the detection of microRNAs is visual by naked eye, there is no need for microRNA amplification, while the proposed lateral flow strip test is universal and can be applied for the detection of any microRNA sequence.

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3. Chromatography (+ Mass spectrometry)

P.12 The potential of Biomimetic Chromatography to predict dermal absorption of drugs

A. Georgopoulos, C. Agathokleous, K. Vasileiou, E. Leventaki, B. A. Tsantili- Kakoulidou and F. Tsopelas

[1]Laboratory of Inorganic and Analytical Chemistry, School of Chemical Engineering, National Technical University of Athens, Iroon Polytechniou 9, 15780 Athens, Greece.

E-mail: ftsop@central.ntua.gr

The term "biomimetic chromatography" or simply "biochromatography" refers to liquid chromatography employed for the simulation of biological processes. In liquid chromatography, dissolved in the mobile phase chemicals participate in a dynamic equilibrium between mobile and stationary phase and their elution expresses their distribution coefficients between the two phases. In living organisms, tissues and membranes constitute the stationary phase and liquids (e.g. general circulation) the mobile phase. The successful simulation of a biological process requires the selection of appropriate chromatographic conditions (mainly mobile and stationary phase) and retention factors can be used in the so called quantitative retention- activity relationships (QRAR), a useful tool in early drug design [1]. Retention indices of three types of biomimetic chromatography have been included in QRARs; Immobilized Artificial Membrane (IAM) chromatography, Immobilized Plasma Protein Chromatography and Micellar Liquid Chromatography (MLC). In the latter case, MLC uses reversed-phase stationary phases in combination with micellar mobile phases prepared by the addition of surfactants above their critical micelle concentration [2].

The present work refers to a comparative performance of IAM and micellar chromatography using different surfactants, as well as traditional n-octanol/ water partitioning (logP), to predict dermal absorption of drugs. For this purpose, retention factors measured on IAM.PD.DD2 stationary phase as well as on a reversed-phase stationary phase using neutral polyoxyethylene (23) lauryl ether (Brij-35), Tween-20, Tween-80 and Triton X-100, the anionic sodium dodecyl sulfate (SDS) and the cationic cetyltrimethylammonium bromide (CTAB) as well as logP were evaluated as a measure for dermal absorption. Physicochemical/ molecular descriptors, such as Molecular Weight, Topological Polar Surface Area, Number of Rotatable Bonds, Abraham's Hydrogen Bond Acidity and Basicity was also tested.

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P.13 Quantitative determination of aloins A and B in aloe latex and aloe verabased products - Chemometric classification of aloe vera plants (*Aloe Barbadensis Miller*) under different conditions

G.I. Ioannou[1], A. Christou[1], I.J. Stavrou[2], C.P. Kapnissi-Christodoulou[1]

[1] Department of Chemistry, University of Cyprus, 1678 Nicosia, Cyprus
[2] Department of Life Sciences, European University Cyprus, 2404 Nicosia, Cyprus

E-mail: ckapni1@ucy.ac.cy

The medicinal properties of aloe vera are attributed to its bioactive compounds found in the latex. In particular, aloe emodin, and aloins A and B, present in the aloe latex, are known for their laxative action. This study aims to develop a simple HPLC method for their determination. In addition, the correlation between these compounds with regards to the plant's environmental conditions and the leaf's location within the plant was examined.Aloe vera plants under different conditions and thirteen aloe-based products were analyzed by use of HPLC-DAD in combination with chemometrics. Each leaf from the plants was studied separately for its content in compounds with a laxative effect. The developed method was performed with a C18 column and the total analysis time was 22 minutes. It was observed that, in contrast with fieldcultivation plants, the concentrations of aloins in potted plants follow a specific pattern based on the position of the leaves. It was also observed that climatic and environmental conditions have a significant impact on the concentrations of aloins. Principal Component Analysis was performed to evaluate correlations among measurements. The model was able to separate the aloe plants based on their seasonal variation and growing conditions. Finally, it was observed that aloins were detected in just two out of thirteen products, and their total concentration surpassed the maximum levels set by EU legislation. The findings of this research work offer valuable insights into the variability of aloins in different in leaves at different position and plants exposed to various conditions.

P.14 Fecal fatty acid profile of exclusively breast-fed or formula-fed infants

Konstantinos Tsiantas[1,2], Paris Christodoulou[1], Thalia Tsiaka[1], Theodora Boutsikou[2], Nicoletta Iacovidou[2], Vassilia J. Sinanoglou[1] and Panagiotis Zoumpoulakis[1]

[1] Department of Food Science and Technology, University of West Attica, Ag. Spyridonos, 12243 Egaleo, Greece

[2] Department of Neonatology, Medical School, National Kapodistrian University of Athens, 157 72 Athens, Greece

E-mail: ktsiantas@uniwa.gr

Indisputably, breast milk is considered by WHO the most complete type of nutrition for all infants since it contains several compounds (i.e., complex proteins including antibodies, essential lipids, vitamins and carbohydrates such as human milk oligosaccharides – HMOs) with unique properties such as the normal growth of the infant, the enhancement of immune and nerval response as well as the establishment of a healthy gut microbiota. Meanwhile, the development of next generation infant formulas has placed particular emphasis on incorporating some of the beneficial functional properties of breast milk. Thus, this study evaluates the fecal fatty acid profile of infants that followed different dietary approaches, aiming to further provide insights on the effects of infant nutrition on gut microbiota. Briefly, fecal samples (N= 116) were collected in four different time points (Day 3, Day 15, Day 60 and Day 90) and in turn extracted and analyzed using gas chromatography coupled with a flame ionization detector (GC-FID). More than fifteen fatty acids were identified and quantified. Data matrix was then subjected to multivariate statistical analysis using MetaboAnalyst 5.0. More specifically, Unsupervised Principal Component Analysis (PCA) was applied in order to acquire a comprehensive insight and visualize any relation (trends-outliers) among samples. A step further, the data set was subjected to OPLS-DA analysis in order to improve model visualization and interpretation. Overall, results indicate a similar fecal fatty acid profile irrespective of the two dietary approaches.

P.15 UHPLC-MS analysis of salivary bile acids in non-invasive diagnostics of Barrett's esophagus

V. Dosedělová[1], M. Laštovičková[1], J. Dolina[2], Š. Konečný[2], P. Kubáň[1]

[1]Institute of Analytical Chemistry of the Czech Academy of Sciences, Brno, Czech Republic
[2]University Hospital Brno, Faculty of Medicine, Masaryk University, Brno, Czech Republic

E-mail: Vera.Dosedelova@gmail.com

Barrett's esophagus is a serious condition characterized by a replacement of damaged epithelium cells by intestinal-type cells, which is caused by frequent reflux episodes, that is, backflow of the acidic gastric and duodenal contents into the esophagus [1]. The exact mechanism of disease progression has not been resolved, but bile acids, a group of compounds necessary for lipid digestion, were suggested to contribute to the pathology [2-3]. Routine diagnosis of Barrett's esophagus is performed by invasive endoscopy with sample collection and subsequent histological examination [1]. In this work, levels of bile acids in saliva were investigated because bile acids are not currently analyzed by clinicians, even though they might serve as a non-invasive tool in the diagnostics of Barrett's esophagus.

We present development and optimization of methodology for saliva collection, sample preparation and bile acid analysis by reversed-phase ultra-high-performance liquid chromatography - mass spectrometry (UHPLC-MS). Saliva samples were collected by spitting into a plastic container. Sample preparation involved protein precipitation using methanol and solid-phase extraction to purify and enrich bile acids in samples. A sensitive UHPLC-MS method was developed for the quantification of unconjugated and glycine-conjugated bile acids. In a pilot study, levels of bile acids were significantly higher in saliva from patients with Barrett's esophagus (n = 10) compared to healthy volunteers (n = 10). Moreover, highresolution MS and ion mobility were utilized for the investigation of fragmentation patterns and the identification of new bile acids in saliva. Based on ion mobility, accurate mass, and product ion spectra, taurine-conjugated bile acids and a sulfate conjugate were identified in saliva from healthy volunteers. A larger clinical study including taurine-conjugated bile acids will be performed in future research to validate the applicability of salivary bile acids in non-invasive diagnostics of Barrett's esophagus.

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P.16 HPLC-ESI-MS/MS for the determination of Arsenolipids in fish: A new form of arsenic for improved risk assessment

C. M. Drakonaki[1], M. Kapsi[2], I. Kalantzi[2], M. Tsapakis[2] and S. A. Pergantis[1]

[1]Environmental Chemical Processes Laboratory, Department of Chemistry, University of Crete, Voutes Campus, Heraklion, 70013, Greece
[2]Institute of Oceanography, Hellenic Centre for Marine Research (HCMR), Gournes - Pediados, Heraklion, 71003, Greece

E-mail: spergantis@uoc.gr

Fish constitute a major portion of the diet for Greek people. Although they are an excellent source of nutrients, they also uptake toxic metals and metalloids from their environment and their food. More specifically, arsenic (As) and its species are biotransformed and bioaccumulated within marine organisms, leading to possible toxic effects following their consumption by humans. The extent of such effects depends on the As species and concentrations present, therefore necessitating arsenic speciation analysis for risk assessment purposes.[1][2]
Four fish species (Mullus Barbatus, Merluccius Merluccius, Pagellus Erythrinus, Engraulis Encrasicolus) from North Evia, Greece were selected as samples, due to the possibly higher concentration of As from industrial processes taking place around this area. Regarding organic arsenic species, they can be divided into two main groups: water-soluble and lipid-soluble, also known as arsenolipids (AsLp). Some groups of arsenolopids are arsenic-containing hydrocarbons (AsHCs), arsenic-containing fatty acids (AsFAs) and arsenic-containing phospholipids (AsPLs).[3] Considering their toxicity, recent in vitro studies have reported toxic effects for AsLp, specifically AsHCs.[4]
This study focuses on the determination of AsLp using HPLC-ESI-Orbitrap-MS/MS, HPLCESI-QQQ-MS/MS and HPLC-ICP-MS, and their comparison. Comparisons are also conducted between the fish AsLp profiles and concentrations. In addition, As mass balance data obtained using microwave digestion and ICP-MS will be discussed.[5]

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P.17 Development and validation of targeted UPLC-MS/MS methods to ensure food safety: determination of biogenic amines in tuna fish and coumarin in bakery products

Artemis Lioupi[1,2], Aristea Papaioannou[3], Christina Virgiliou[2,3], Achilleas Iakovakis[4], Ioannis Kaidatzis[4] and Georgios Theodoridis[1,2]

[1]Laboratory of Analytical Chemistry, School of Chemistry, Aristotle University of Thessaloniki, 54124, Thessaloniki, Greece
[2]FoodOmicsGR Research Infrastructure, AUTh Node, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, 57001, Greece
[3]School of Chemical Engineering, Aristotle University of Thessaloniki, 54636, Thessaloniki, Greece
[4]Veltia Labs for Life, Food Contaminants Laboratory, Thessaloniki, 57022, Greece

E-mail: gtheodor@chem.auth.gr

This work describes the development of targeted UPLC-MS/MS methods for the detection of biomarkers related to food safety. For the above purpose, two separated methods were developed for the detection of coumarin in bakery products and biogenic amines such as histamine, tyramine, putrescine and cadaverine in fish products. With regards to biogenic amines, a HILIC column was utilised to enhance retention of polar molecules. A simple sample preparation procedure was followed using the solvent mixture MeOH/H_2O (50/50, v/v), 0.1% acetic acid for protein precipitation and analyte extraction. Intra- and inter-day accuracy ranged from 88.0% (Cad) to 102.7% (Tyr) and from 85.0% (Cad) to 99.8 % (Tyr), respectively. Intra- and inter-day precision ranged from 0.4% (Tyr, Put) to 3.3% (His) and from 0.7% (Tyr) to 5.0% (Cad), respectively. Limits of detection (LOD) and limits of quantification (LOQ) varied from 0.0009 to 0.0940 mg/kg and from 0.0030 mg/kg to 0.3100 mg/kg, respectively, depending on the analyte. The method applied to tuna fish samples with the aim to evaluate any toxic effect linked to biogenic amines in foods. Herein, is also described the development of a fast and efficient RPLC-MS/MS method for the analysis of coumarin in bakery products (cereal, biscuits, flour, crème, and brioche). Different extraction solvent systems were tested with the aim of achieving selective and reliable determination of coumarin in all matrices. The solvent mixture MeOH: H_2O (80:20, v/v) showed improved extraction efficiency and repeatability for coumarin with recoveries reaching 101.3%. Intra- and inter-day accuracy ranged from 95.1% to 111.0% and from 93.5% to 112.3%, respectively. The method showed satisfactory sensitivity with a quantitation limit (LOQ) of 0.0053 ng/mL. The developed approach underwent proficiency testing, and its uncertainty was assessed. Both methods were applied successfully for the quantitation of the analytes in products sold in Greek markets to evaluate their levels according to the current EU legislation in force. According to the results, markers were quantified above the regulated concentration limits in several products indicating the need for application of such sensitive, robust, fast and cost-effective methods in routine analysis of food quality and safety laboratories.

P.18 Development and validation of an LC-ESI-MS/MS method for the trace analysis of Zearalenone in weaned pig bile samples using an IAC-based extraction procedure.

I. Bouzouka[1,2], H. Gika[2,3], S. Didos[1,4], P. Tassis[5], D. Floros[5], A. Argiriou[1,4]

[1] Institute of Applied Biosciences, Centre for Research and Technology Hellas (CERTH), 57001, Thermi, Thessaloniki, Greece

[2] Laboratory of Forensic Medicine and Toxicology, Medical School, Aristotle University of Thessaloniki, 54124, Thessaloniki Greece, Greece

[3] Biomic AUTH, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center B1.4, Thessaloniki GR 57001, Greece

[4] Department of Food Science and Nutrition, School of the Environment, University of the Aegean, 81400, Myrina, Lemnos, Greece

[5] Clinic of Farm Animals, School of Veterinary Medicine, Aristotle University of Thessaloniki, 54627 Thessaloniki, Greece

E-mail: ibouzouka@certh.gr

Zearalenone (ZEN) is a nonsteroidal mycotoxin produced by Fusarium fungi and pigs among others are the most vulnerable to its estrogenic effects. Contaminated products can cause significant economic losses and pose a risk to animals and humans. Particularly in pigs, symptoms of hyperestrogenism have been reported even at concentrations below 1 mg/kg.(1) To prevent these effects, methods for reliable determination of ZEN at low concentrations in food and feed are needed thus methods' sensitivities down to the sub ppb levels are required to enable accurate risk assessment and studies on ZEN metabolism.

In this study, bile samples from weaned pigs were studied to investigate the presence of ZEN due to contamination. Based on enterohepatic circulation, ZEN may be present in bile for a longer period of time than in blood.(2) Additionally, when blood concentrations are low or nondetectable, bile may be the preferred matrix since the concentration of ZEN and its metabolites in bile is substantially greater, as reported in several investigations, due to the accumulation of ZEN and its metabolites in bile.(3) The aim of the present study was to develop an analytical method for the determination of ZEN at low concentrations in bile or other biological fluids. An UHPLC coupled to a Q Exactive Focus™ Orbitrap Mass Spectrometer was employed. The chromatographic separation was achieved under a water-methanol gradient elution and single ion monitoring (SIM) acquisition was performed using the negative ionization mode. For method development, different sample preparation conditions and different MS parameters were evaluated. The optimum protocol comprises an SPE by the use of immunoaffinity columns (IAC). The recoveries were in the range of 83-113 % and an LOQ of 0.03 ppb was achieved. Precision and accuracy were within acceptable values in the working concentration range. The method has been successfully used for the quantitative determination of ZEN in weaned pig bile samples from a feeding trial with two groups (positive and negative control). The method can be used to trace ZEN exposure of pigs and possibly other farm animals, if the corresponding feed is no longer available for analysis.

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P.19 Development and validation of a UHPLC-MS/MS method for the quantification of the tryptophan pathway-related compounds

Miroslav Kubát[1,2], Olga Angeliki Begou[1,3,4], Helen Gika[1,5], Petr Česla[2] and Georgios Theodoridis[1,3]

[1]Biomic AUTH, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki, Innovation Area of Thessaloniki, Thermi 57001, Greece
[2]Department of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentska 573, CZ-53210 Pardubice, Czech Republic
[3]Department of Chemistry, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[4]ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, 57001, Greece
[5]Laboratory of Forensic Medicine and Toxicology, School of Medicine, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

E-mail: gtheodor@chem.auth.gr

Tryptophan is an essential amino acid that is involved in various physiological and pathological processes. Its metabolites are generated through different pathways, such as the kynurenine, serotonin, and indole pathways. These metabolites can modulate neuronal, immune, and gut functions. Alterations in tryptophan metabolism are associated with depression, Alzheimer's disease, neuroinflammatory diseases, inflammatory bowel diseases, metabolic disorders, and cancer. Liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) is a powerful technique that can provide a comprehensive and sensitive analysis of tryptophan metabolism. Many LC-MS/MS methods have been developed for measuring tryptophan and its metabolites in biological samples, such as serum, urine, cerebrospinal fluid, and stool. Although most of the tryptophan pathway-related compounds were detected in human faeces, many of them remain unquantified. Stool analysis provides a non-invasive method to study the gut microbiome and its metabolic functions, potentially leading to the development of personalized therapeutic strategies and interventions targeting gut-related disorders. Here, we present a UHPLC-MS/MS method for the separation and quantification of homovanillic acid, hippuric acid, tryptophan, kynurenic acid, tyrosine, serotonin, citrulline, arginine, norepinephrine, phenylalanine, dopamine, xanthine, glutamic acid, glutamine, acetylcholine, anthranilic acid, hypoxanthine, nicotinic acid, nicotinamide, γ-aminobutyric acid, and trimethylamine-N-oxide in human faeces. Chromatographic separation was performed in hydrophilic interactions (HILIC) mode on an Acquity UPLC BEH Amide Column (130Å, 1.7 µm, 2.1 mm × 150 mm), with a mobile phase consisting of a binary solvent system, where solvent A was ACN:H_2O, 95:5 v/v, 10 mM $HCOONH_4$, 0.1 % HCOOH, pH = 4 and B was ACN:H_2O, 30:70 v/v, 10 mM $HCOONH_4$, 0.05 % HCOOH, pH = 6.5. MS/MS detection was carried out on a Xevo TQD system (Waters, UK) operating in positive electrospray ionization mode. Stool samples were collected in commercially available tubes, where different extraction solvents and solvent ratios were tested for the optimum extraction of all analytes. The extraction recovery, LOD, LOQ, linearity, precision, accuracy, and stability for each analyte were evaluated. The method was used for the quantification of the tryptophan pathway-related metabolites in human faeces.

P.20 Metabolic fingerprinting of Muscat of Alexandria of Limnos grape musts during alcoholic fermentation

M. Marinaki[1,2,3], P. Arapitsas[4,5], C. Virgiliou[2,3,6] and G. Theodoridis[1,2,3]

[1] Laboratory of Analytical Chemistry, School of Chemistry, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[2] Biomic AUTh, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center B1.4, 10thkm Thessaloniki-Thermi Rd, P.O. Box 8318, GR 57001, Thessaloniki, Greece
[3] FoodOmicsGR Research Infrastructure, AUTh Node, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center B1.4, 10th km Thessaloniki-Thermi Rd, P.O. Box 8318, GR 57001, Thessaloniki, Greece
[4] Department of Wine, Vine and Beverage Sciences, School of Food Science, University of West Attica, Ag. Spyridonos str, Egaleo, 12243, Athens, Greece
[5] Research and Innovation Centre, Fondazione Edmund Mach, via E. Mach 1, 38010 San Michele all'Adige, Italy
[6] School of Chemical Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
E-mail: cvirgiliou@cheng.auth.gr

Muscat of Alexandria is one of the most floral and aromatic white grape cultivars, and the variety most cultivated on Limnos Island, producing popular appellation of origin sweet and dry wines. The vineyard region and the vinification process are of the most important factors contributing in wine's quality. The aim of this study is to fingerprint for the first time the metabolome of Muscat of Alexandria grape musts during alcoholic fermentation using a LCMS based untargeted single-batch method.

The metabolomic fingerprint of 71 grape musts, sampled by 3 wineries of Limnos Island, 8 tanks and 2 vintages (2019, 2020) in 9 time points during alcoholic fermentation, was analysed with a LC-MS based metabolomics protocol by an UHPLC-timsTOF-MS instrument, both in ESI+ and ESI- mode [1–3]. Blanks and QC samples were analyzed every 7 samples during batch analysis and a simple sample preparation, including centrifugation, filtration and dilution, was performed. Multivariate statistical analysis was performed to monitor the behaviour of grape musts during fermentation and biomarker analysis revealed the trend of the identified metabolites. Correlations were used for the annotation of unknown features, and the data provided indications for the behaviour of N-containing compound during alcoholic fermentation for the first time, while the trends of acids, flavonoids, phenolics, hydroxycinnamates and several important for wines' quality analytes were studied during fermentation.

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P.21 Identification of transformation products of emerging pollutants formed in photolytic and photocatalytic processes by LC-HR-Orbitrap MS

I. Konstantinou[1,2], V. Boti[1,2], D. Hela[1,2] and T. Albanis[1,2]

[1]Department of Chemistry, University of Ioannina, 45110, Ioannina, Greece
[2]Institute of Environment and Sustainable Development, University Research and Innovation Center, 45110, Ioannina, Greece

E-mail: iokonst@uoi.gr

The pollution of aquatic environment by organic micro-pollutants constitutes nowadays one of the most significant environmental problems. Hence, it is necessary to study their transformation and removal from aquatic matrices. Considering the relevance and importance of photochemical processes in the environmental fate and protection technologies for organic micropollutants, the pesent study deals with the identification of transformation products and mechanistic aspects of photolytic-photocatalytic degradation processes for selected organic micropollutants frequently detected in aqueous media. In this direction, the photolytic degradation of clothianidin (CLTH) insecticide in suspensions and aqueous extracts of hydrochar particles as well as the photocatalytic degradation by g-C_3N_4 catalysts was studied. CLTH is widely used and due to its physicochemical properties has been detected in surface and groundwater while it has been included in priority pollutant lists for aquatic systems.

The photolytic-photocatalytic degradation experiments of CLTH were performed with simulated sunlight irradiation (Suntest apparatus). First-order kinetics was followed in all cases. Regarding photodegradation of CLTH in the presence of HC suspensions and aqueous extracts, the degradation kinetics is reduced compared to that in distilled water except the case of 200 mg L^{-1} HC aqueous suspension. The photodegradation rate in aqueous extracts with 50 and 100 mg L^{-1} HC particles concentration was higher compared to the rate in corresponding suspensions while the inverse trend was observed for the degradation rate using 200 and 400 mg L^{-1} HC concentration. Fast degradation was observed using g-C_3N_4 catalysts with $t_{1/2}$<60 min. Transformation products (TPs) of CLTH have been determined using liquid chromatography-high resolution accurate mass spectrometry of (LC-MS-Orbitrap). Six TPs have been identified in all matrices and processes, i.e. photolysis in distilled water, HC aqueous extracts and HC aqueous suspensions and photocatalysis in distilled water. Major TPs in distilled water was TZMU while in HC water extracts were TMG, and MAI. The relative TPs profiles depend on the substrate denoting direct and indirect photolysis routes taking place in different degrees in the presence or absence of HC particles. Finally, the toxicity assessment of CLTH TPs was assessed by Microtox bioassay and in silico (ECOSAR) methods. Corresponding investigations contribute to a better understanding of photochemical processes in the environmental fate and removal processes of emerging contaminants.

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P.22 Determination of perfluorinated compounds in natural waters and wastewaters by solid phase extraction and LC-LTQ/Orbitrap MS

K. Miserli[1], V. Athanasiou[1], V. Boti[1,2], D. Hela[1,2] and I. Konstantinou[1,2]

[1]Department of Chemistry, University of Ioannina, 45110, Greece
[2] Institute of Environment and Sustainable Development, University Research and Innovation Center of Ioannina, 45110, Greece

E-mail: iokonst@uoi.gr

Perfluorinated compounds (PFCs) are a group of environmental contaminants that are used since 1950s in various applications and can be divided into four main categories including perfluoroalkyl carboxylate acids (PFCAs), perfluoroalkyl sulfonates (PFASs), perfluoroalkyl sulfonamides (PFSAs) and fluorotelomer alcohols (FTOHs) [1]. Wastewater treatment plants (WWTPs) are considered the major source of PFCs in the environment while industrial discharges, landfills, atmospheric deposition, agricultural runoff, firefighting training sites are secondary sources by direct or indirect routes entering the aquatic environment [2]. The monitoring of PFCs was assessed by applying solid phase extraction (SPE) protocols followed by ultra-highperformance liquid chromatography–high-resolution linear ion trap Orbitrap mass spectrometry (UHPLC-LTQ/Orbitrap MS), operated in negative ionization mode, in order to investigate 18 multiclass PFCs in distilled (DW), lake water, seawater and wastewater samples. All the analytical methods were validated in terms of linearity, recovery, intra and inter-day precisions, uncertainty (%U)/Horrat ratio at two spiking levels, matrix-effects (ME), process efficiency (PE) and limits of detection and quantification (Table 1). Finally, the developed methods were applied successfully in water samples from different aquatic systems of Greece and wastewater samples from municipal and hospital WWTP in Ioannina city, revealing maximum concentrations for FOSA 14 ng L^{-1}, PFDoA 16 ng L^{-1} in secondary influent wastewater with 100% removal in secondary effluent, for PFBA 11 ng L^{-1} in secondary effluent and for PFOA 160 ng L^{-1} in hospital secondary wastewater effluent. Traces of PFCs compounds were detected in lake samples in the range from 0.3 ng L^{-1} to 1.6 ng L^{-1}.

Table 1: Method performance parameters for two spiking concentration levels.

18 PFCs		%Recovery (n=5)	LOD (ng L^{-1})	%RSD (n=5)	%U	%ME	%PE
Wastewater	10 ng L^{-1}	66 - 95	0.02 - 0.76	< 20	< 32	< ± 30	51 - 95
	100 ng L^{-1}	73 - 98		< 20	< 22.63		66 - 102
Lake/ DW	10 ng L^{-1}	45 – 99/ 75 - 98	0.04 – 0.75	< 20	< 32	< ± 49	54 – 99/ 52 - 114
	50 ng L^{-1}	49 – 108/ 78 - 110	0.01 – 0.13	< 20	< 25		77 – 106/ 64 - 112

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P.23 Solid-phase extraction and LC-MS determination of metabolites from biological fluids using magnetic nanoparticles

O. Skyrgiannis[1], C. Virgilliou[1,2], H. Gika[2,3], K. Simeonidis[1]

[1]Analytical Chemistry Laboratory, Department of Chemical Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[2]Biomic_AUTh, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center, 57001, 10th km Thessaloniki-Thermi, Thessaloniki, Greece
[3]Department of Medicine, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

E-mail: ksime@physics.auth.gr, cvirgiliou@cheng.auth.gr

Amino acids are essential building blocks of human life, playing important roles in a multitude of different biological processes. Therefore, monitoring of their levels in biological samples provides a way to determine occurring biochemical reactions and indirectly understand the presence of uncommon mechanisms or developing diseases. Owing to their chemical affinity with metabolites such as amino acids, magnetite (Fe_3O_4) nanoparticles, whether as bare or functionalized, have been proposed as a challenging substrate to promote the solid-phase extraction of targeted metabolites and the enrichment of analytes met at very low concentrations. Their magnetic response provides an extra advantage toward facile recovery after dispersion in the sample fulfilling also the demand for green chemistry practices in analytical chemistry. This study evaluates the potential of Fe_3O_4 nanoparticles to extract and analyze major amino acids from patients urine samples by developing a simple and rapid treatment protocol. Bare Fe_3O_4 nanoparticles sized around 40 nm were synthesized through the oxidative precipitation of $FeSO_4$ in a microwave-heated continuous flow method maintaining pH level 11.5. A quantity of nanoparticles was introduced into the sample and contacted under stirring for few minutes before their separation by a permanent magnet. Captured amino acids were leached from nanoparticles using a mixture of citric buffer solution and acetonitrile. The detection of amino acids in the recovered solution was determined using liquid chromatography coupled to mass spectrometry (LC-MS/MS). Optimization of the protocol included the definition of the particles dispersion and leaching time, the pH of the sample, the particles dose and the leaching buffer solution.

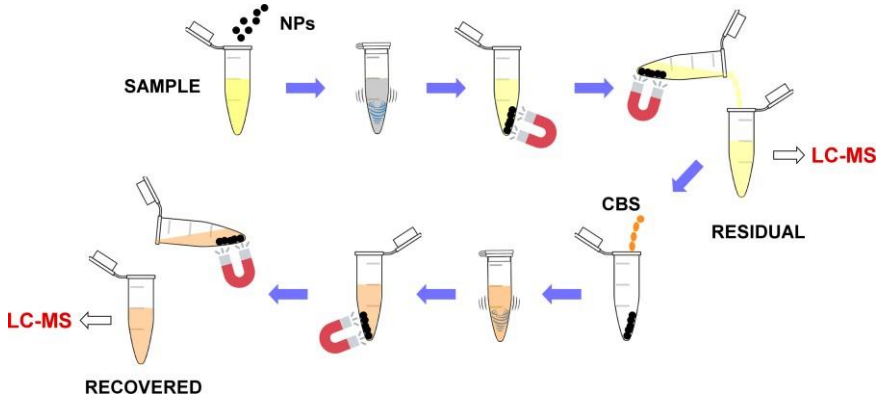

Figure 1. Steps involved in the solid-phase extraction of amino acids by Fe_3O_4 nanoparticles.

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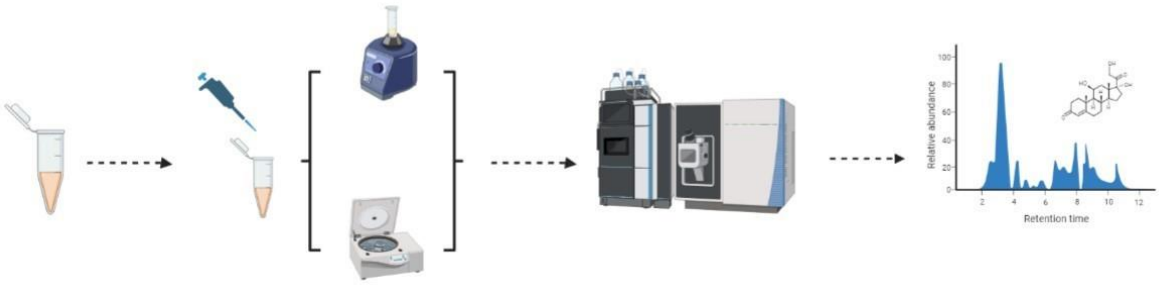
P.24 Development and validation of an LC-MS/MS method for the quantitative analysis of 9 steroid hormones in human serum

A. Antoniadou[1,2], T. Meikopoulos [1,2], O. Begou [1,2,3], H. Gika [2,4], G. Theodoridis [1,2]

[1]Department of Chemistry, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[2]Biomic AUTH, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki, Innovation Area of Thessaloniki, Thermi 57001, Greece
[3]ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, 57001, Greece
[4]Laboratory of Forensic Medicine and Toxicology, School of Medicine, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece

E-mail: olgabegou@thetabiomarkers.com

Steroid hormones are endogenous compounds that are formed from cholesterol by enzymatic processes in the placenta, gonads, and adrenal glands. Three cyclohexane rings and a cyclopentane ring compose the fundamental structure of all steroids, which function as neuroendocrine regulators of physiological development or even immune response and metabolic stress. Accurate determination of steroids remains an important topic for a variety of studies and end-points. The aim of this study was to develop a simple, rapid, and reliable method for the detection and quantitation of 9 steroid hormones in human serum. Analysis was performed on a Bruker Elute™ UHPLC coupled to an EVOQ™ LC-TQ Elite MS/MS system. The mass spectrometer operated in positive electrospray ionization mode (+ESI) for all analytes. Separation was carried out using an Acquity UPLC C18 BEH column (1.7 µm,100 mm x 2.1 mm), and mobile phases solvents were 0.1% formic acid (FA) in water and 0.1% FA in methanol. Sample preparation was performed via liquid liquid extraction (LLE), while different extraction solvents and solvent ratios were investigated for the pre-treatment of serum. One millilitre of MTBE was found to be the most suitable extraction solvent, with extraction recovery ranging from 85.8% to 111.8%. Similar results were obtained for matrix effect assessment, found within the acceptable criteria. Limit of quantification (LOQ), limit of detection (LOD), intra- and inter- day accuracy and precision were evaluated in terms of method validation. The obtained results were very satisfactory; the developed method can be a useful tool for the serum steroid profiling and the investigation of the mechanisms of steroid-related diseases.



P.25 Improving 4D screening of bile acids in biological samples by Liquid Chromatography – Ion Mobility – High Resolution Mass Spectrometry

C. Virgiliou[1,2], D. Diamantidou[2,3], H. Gika[2,4], G. Theodoridis[2,3]

[1]Analytical Chemistry Laboratory, Department of Chemical Engineering, School of Engineering, Aristotle University of Thessaloniki, 54 124, Thessaloniki, Greece
[2]Biomic_AUTh, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center, B1.4, Thessaloniki, 10th km Thessaloniki-Thermi Rd, P.O. Box 8318, GR 57001
[3]Laboratory of Analytical Chemistry, Department of Chemistry, Aristotle University of Thessaloniki, 541 24, Thessaloniki, Greece
[4]School of Medicine, Aristotle University of Thessaloniki, Thessaloniki, 54124, Greece

E-mail: gtheodor@chem.auth.gr

Bile acids (BA) are among the most important classes of biological molecules in the digestive system and have been linked to several diseases, including diabetes, metabolic disruption, and colorectal cancer. Their similarities in structure and polarity result in similar chromatographic retention times and MS patterns, and thus their annotation in biological matrices is particularly challenging. Ion Mobility offers an additional dimension of separation and when combined with liquid chromatography becomes an attractive tool in isomeric separation. Herein, we developed a LC-IM-MS method to determine 32 BAs in fecal and serum samples.

All standards were distributed in a 96-well plate (BACSMLS Sigma Library) and were prepared by diluting each well with methanol:H_2O 50:50 v/v, at the final concentration of 10 mg L^{-1}. The chromatographic separation was achieved on an ACQUITY BEH C8 column (1.7 μm, 100 mm × 2.1 mm) using a modified 15 min gradient programme developed by Sarafian et al. [4]. The mobile phase was consisted of solvent A: acetonitrile:H_2O 10:90 v/v with 1mM ammonium formate and formic acid (pH = 4.2), and solvent B: acetonitrile:2-propanol 50:50 v/v. Highresolution mass spectrometry was carried out on a timsTOF mass spectrometer (Bruker, Germany) operating in negative ionization mode (ESI).

The BAs were found to ionize readily and [M-H^-] was the main ion form. RSD values were calculated after triplicate measures of CCS values and were below 0.3% in all cases. Chromatographic separation was achieved for the majority of the compounds, and TIMS allowed to separate co-eluted isomers. The developed method was successfully applied in human aqueous and lyophilized fecal samples, and human serum. In total, 15 BAs were annotated using MetaboScape® software (Bruker, Germany). ^{TIMS}CCS values reported here were comparable between different laboratories, demonstrating the capability for confident interlaboratory annotations.

Acknowledgements: The work was part of the project "FoodomicsGR_RI Comprehensive Characterization of Foods" (MIS 5029057) which is implemented under the Action "Reinforcement of the Research and Innovation Infrastructure", funded by the Operational Programme Competitiveness. Entrepreneurship and Innovation (NSRF 2014-2020) and co-financed by Greece and the European Union (European Regional Development Fund).

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P.26 Mass spectrometry metabolite library for 4D Metabolomics. Application to biological samples.

A. Lioupi[1], D. Diamantidou[1], T. Zioga[2] A. Koulouri[2], G. Theodoridis[1,3] and C. Virgiliou[2,3]

[1]Laboratory of Analytical Chemistry, Department of Chemistry, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[2]Laboratory of Analytical Chemistry, Department of Chemical Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[3]Biomic_AUTh, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center, B1.4, Thessaloniki, 10th km Thessaloniki-Thermi Rd, P.O. Box 8318, GR 57001

E-mail: cvirgiliou@cheng.auth.gr

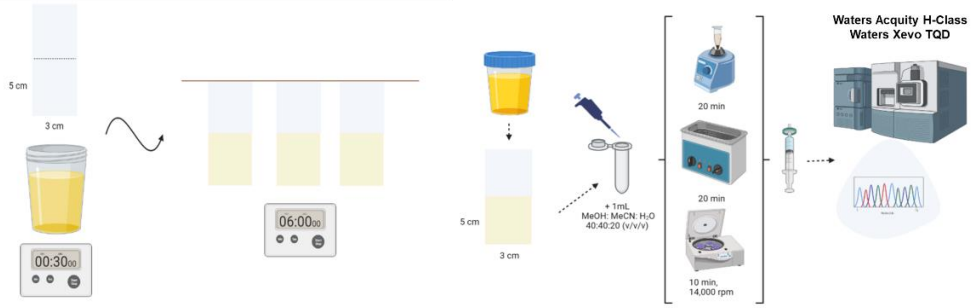
Untargeted metabolomics investigations necessitate gathering a comprehensive range of metabolic information from every sample under analysis. As a result, these approaches typically employ highly specific and efficient analytical techniques including both reversed-phase (RP) and hydrophilic interaction liquid chromatography (HILIC) combined with mass spectrometry. This work describes the development of an ion mobility-enhanced spectral library for small molecule analysis. Accurate measurements of collision cross section (CCS), retention time (RT), and mass-to-charge ratio (*m/z*) values for individual small molecules significantly accelerate the process of curating and constructing a reference 4D library for efficient sample annotation in high throughput analysis. An untargeted metabolomics TIMS TOF/MS method was developed for the comprehensive profile of biological samples with emphasis on molecules with low molecular mass. Examples of metabolite identification and isomer isolation with ion mobility are presented. The developed library enabled also the identification of important metabolites/markers of different diseases found in human urine by RPLC-Tims-TOF-MS analysis. The method was also applied in the study of food adulteration of honey samples.

P.27 Development and validation of a HILIC-MS/MS method for the quantitative analysis of 14 amino acids in dried urine spots (DUS)

T. Meikopoulos[1,2], O. Begou[1,2,3], H. Gika[2,4], G. Theodoridis[1,2]

[1]Department of Chemistry, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
[2]Biomic AUTH, Bioanalysis and Omics Lab, Centre for Interdisciplinary Research of Aristotle University of Thessaloniki, Innovation Area of Thessaloniki, Thermi 57001, Greece
[3]ThetaBiomarkers, Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Thessaloniki, 57001, Greece
[4]Laboratory of Forensic Medicine and Toxicology, School of Medicine, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
E-mail: olgabegou@thetabiomarkers.com

The analysis of amino acids in urine holds significant importance in various areas of healthcare and research, as it provides valuable insights for a number of questions such as diagnosing metabolic disorders, assessing nutritional status, evaluating kidney function, and monitoring treatment response. Identifying specific amino acids as biomarkers may contribute to the development of diagnostic tests or therapeutic interventions. The storage and transportation of liquid urine specimens constitutes a major concern, especially in cases of sampling from remote areas. Dried urine spots (DUS), an alternative to analysis native liquid urine, offers advantages of convenience, stability, and cost-effectiveness. DUS allows easy sample collection, long-term storage, easy transportation and compatibility with various analytical techniques, making it a promising method for amino acid analysis and biomarker investigations. The aim of the present study was to develop an efficient method for the quantitative analysis of 14 amino acids in dried urine spots (DUS) and to evaluate its clinical applicability in human cohort(s). Different extraction solvents and solvent ratios were investigated for the pre-treatment of the urine spot that was collected using different filter papers. Accuracy, precision, extraction recovery, matrix effect, and short- and long-term stability were also evaluated. DUS extraction efficiency was compared with the typical urine amino acids analysis. The monitoring of all analytes and their corresponding isotopically labelled internal standards was based on the detection of the charged ions [M+H]+ in positive electrospray ionization mode using an Acquity H-Class linked to a Xevo TQD instrument (Waters). Separation was carried out using an Acquity UPLC BEH HILIC column (1.7 μm, 150 mm x 2.1 mm), where mobile phases constituted of ACN:H_2O, 95:5 v/v, 10 mM $HCOONH_4$, (pH= 3) and ACN:H_2O, 30:70 v/v, 10 mM $HCOONH_4$, (pH = 3). One millilitre of ACN:MeOH:H_2O, 40:40:20 v/v/v, was found to be the optimum extraction solvent, with recovery ranging from 89.2% to 111%. The obtained results showed that DUS offers an enticing substitute for bioanalysis and amino acid quantification.



Acknowledgments: This work was financially supported by the project "Innovative biofunctional foods and products based on Greek endemic herbs and kiwi: development – analysis – classification".

P.28 Scandium selective recovery from sulphuric acid leaching solutions by an ion exchange 2-stage procedure using an industrial resin

L.A. Tsakanika,N. Loukas and M. Ochsenkuehn - Petropoulou

Laboratory of Inorganic and Analytical Chemistry, School of Chemical Engineering, NTUA

E-mail: btsakanika@gmail.com

Red mud or bauxite residue is the industrial by-product of Bayer method of bauxite processing. It is rich in major elements, especially iron, but also in numerous trace elements, some of which are of high techno-economic interest, such as rare earths (scandium, yttrium and lanthanides). Some of the rare earths including scandium have been identified as Critical Raw Materials (CRMs) due to their high demand for high-tech materials and the scarcity of their economically exploitable resources. The utilization of red mud as a low-cost secondary raw material for the recovery of scandium with appropriate separation techniques could be a challenge for the further utilization of this industrial by-product with economic benefits for the aluminium industry.

The present study focused on the investigation and optimization of scandium selective recovery from the major elements, such as iron, which coexists in pregnant leaching solutions, by ion exchange procedure using an industrial cationic resin. The pregnant leaching solution (S/L 2-10%: Sc ~1-4 $mg \cdot L^{-1}$ and Fe ~300-1200 $mg \cdot L^{-1}$) was obtained after red mud leaching with sulphuric acid [1]. The efficiency of the resin was studied and the optimum separation conditions were found by studying several variables in batch and column experiments.

Batch experiments showed that in leachates of 1M H_2SO_4 and solid/liquid (S/L) 2% a 2:1 ratio (feed solution to resin) is suitable for scandium and iron quantitative adsorption about 93% and 87% respectively in 10 min. For more concentrated leachates (solid/liquid 10%), lower ratios 0.6-1:1 are required and the equilibrium is reached faster (2-10 min) regardless of the feed solution-resin ratio due to higher concentrations of analytes. The resin capacity for scandium was found in the range of 1.7-2.2 $\mu g \cdot g^{-1}$. In column experiments, after resin loading with feed solution of S/L 10%, scandium selective recovery is achieved in two sequential stages based on previous works with nitric acid solutions [2,3]: a) elution with HCl solutions for iron removal, b) elution with H_2SO_4 solutions for scandium quantitative recovery. The ratio of 1:1 (feed solution/resin) was chosen as the most suitable. Breakthrough curves of scandium and iron were constructed and the operating and total capacity were calculated. For scandium, they were found 4.24 and 20.5 $\mu g \cdot mL^{-1}$ respectively. The elution curves were also conducted for both stages. 1.5M HCl and a ratio of 3:1 were selected for almost total removal of iron (about 100%) with low scandium losses (4%). In the next stage, 2M H_2SO_4 and a ratio of 2:1 were chosen achieving higher rates (91%) for scandium selective recovery compared to 1M H_2SO_4 (80%). As it was proved, the use of sulphuric acid as both leaching agent and eluent does not cause any problem in scandium adsorption and selective recovery and good results can be obtained.

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P.29 Cyclodextrin- and Cyclofructan-based Chiral Selectors: Evaluation of their Chiral Discrimination Ability in Capillary Electrophoresis for the Enantioseparation of Psychoactive Substances

K. A. Ioannou[1], A. Christou[1], I. J. Stavrou[2], M. G. Schmid[3], C. P. Kapnissi - Christodoulou[1*]

[1]Department of Chemistry, University of Cyprus, 1678 Nicosia, Cyprus
[2]Department of Life Sciences, European University Cyprus, 2404 Nicosia, Cyprus
[3]Department of Pharmaceutical Chemistry, Institute of Pharmaceutical Sciences, University of Graz, 8010 Graz, Austria

E-mail: ckapni1@ucy.ac.cy

Synthetic cathinone and amphetamine derivatives have attracted considerable scientific attention as many of them are not listed in several national drug legislation as illegal substances. Like numerous pharmaceutical compounds, illicit drugs, including NPS, exhibit chirality which results in the presence of two enantiomers for each drug. These enantiomers can demonstrate different pharmacological activity and metabolic and pharmacokinetic characteristics. Therefore, analytical methods, capable of differentiating enantiomers, are of great importance. During this study, a simple, reliable, and easy-to-prepare electrophoretic method was developed for the enantioseparation of ten NPS (amphetamine and cathinone derivatives). Several electrophoretic parameters were examined for the optimization of separation conditions, including the type and concentration of the CS (cyclodextrin- and cyclofructan-based CSs were utilized) and the concentration and pH of the BGE. The use of cyclofructan-based CSs for the enantiomeric separation of NPS was established and demonstrated excellent results. Sulfated cyclofructan-6 (SCF-6) and sulfated cyclofructan-7 (SCF-7) exhibited remarkable enantioselective ability for amphetamine and cathinone derivatives, respectively. Under the determined optimal electrophoretic conditions, ten psychoactive substances were enantiomerically separated using 1 mM SCF-6 for the amphetamine derivatives and 1 mM SCF-7 for the cathinone derivatives dissolved in an aqueous solution of 20-mM monobasic sodium phosphate at pH 2.5, a temperature of 25 °C, and an applied voltage of 25 kV. In addition, the method was validated by estimating the intra- and interday precision [1].

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P.30 Method validation – different approach to pharmaceutical and bioanalytical analysis

L. Matysová[1], L. Kujovská Krčmová[2]

[1]Department of Analytical Chemistry, Faculty of Pharmacy in Hradec Králové, Charles University, Czech Republic
[2]Department of Clinical Biochemistry and Diagnostics, University Hospital Hradec Králové, Czech Republic

E-mail: Ludmila.matysova@faf.cuni.cz

The validation procedure of methods for pharmaceutical analysis is different from validation of methods for bioanalysis.
This different approach is based on the fact, that while for pharmaceuticals the values of analytes are expected and more or less known, the opposite is true for biological material (normal and pathological levels of biological markers may differ significantly, etc.).
For example - for bioanalytical method validation are different limits for parameters.
In linearity – at least 75% of the calibration standards should be ± 15% of the nominal value.
For accuracy and precision is limit ± 15% of the nominal value, but under the LLOQ is limit ± 20% of nominal value. The requirement for selectivity is - the absence of interfering components is accepted where the response is less than 20 % LLOQ for an analyst. The details will be presented on my poster.

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P.31 The possibility of using a dry urine spot to diagnose cerebral creatine deficiency syndromes by tandem mass spectrometry method

H. Jurdáková[1], T. Večereková[1], A. Šalingová[2] and R. Górová[1]

[1]Comenius University, Faculty of Natural Sciences, Department of Analytical Chemistry, Ilkovičova 6, 842 15 Bratislava, Slovak Republic
[2]National Institute of Children's Diseases, Centre for Inherited Metabolic Disorders, Limbová 1, 833 40 Bratislava, Slovak Republic

E-mail: helena.jurdakova@uniba.sk

Creatine deficiency syndromes (CDS) are a group of inborn errors of metabolism and include disorders of creatine synthesis and transport. A common feature of these syndromes is a lack of creatine in the brain, which causes neurological diseases. The CDS group includes two autosomal recessive disorders of creatine synthesis - arginine glycine amidinotransferase (AGAT) and guanidinoacetate methyltransferase (GAMT) enzyme deficiency, as well as an Xlinked creatine transporter (CRTR) deficiency disorder. The determination of creatine and guanidinoacetic acid (GAA) as specific biomarkers of CDS is significant from the point of view of establishing the correct diagnosis and treatment [1,2].
When determining the content of creatine in urine, the disadvantage is its instability and increasing concentration over time due to bacterial contamination. If the creatine determination in urine sample is not carried out immediately after collection, it is necessary to freeze the sample immediately and reduce the number of thaws to a minimum [3,4].
This work is aimed at investigating the possibility of using a dry urine spot to determine the concentration of creatine, GAA and creatinine in urine sample using tandem mass spectrometry and testing the stability of these analytes in a liquid matrix and in a dry urine spot at different storage temperatures.
The results show that GAA and creatinine are stable analytes in the liquid matrix as well as in dry urine spot. Creatine is stable at room temperature for only about 3 hours in liquid matrix, then its concentration increases and after 24 hours it is more than 3 times higher. In dry urine spot creatine is stable within 24 at room temperature, and more than 3-fold increase in concentration was noted after a week, when stored at 4°C it was a 1.5-fold increase after a week. All analytes show a good stability when stored at -20°C.
Using a certified reference material of lyophilized urine at three different concentration levels were evaluated intraday precision (up to 2,9% for creatine, 3,8% for GAA and 2,1% for creatinine), interday precision (up to 3,4% for creatine, 4,4% for GAA and 3,0% for creatinine), and accuracy (up to 10.3%, 13,5 % and 6,1% for creatine, GAA and creatinine respectively) for a dry urine spot method. Detection limits for creatine, GAA and creatinine were at 0.005 mmol/L, 0.005 mmol/L and 0.12 mmol/L, and quantification limits at 0.018 mmol/L, 0.016 mmol/L and 0.40 mmol/L, respectively.
Dry spot urine samples of two patients with GAMT deficiency were also analysed.

Acknowledgment
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P.32 HPLC-MS/MS analysis of DINCH plasticizer metabolites in breast milk

R. Górová, A. Oravcová and H. Jurdáková

Department of Analytical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 842 15 Bratislava, Slovak Republic

E-mail: renata.gorova@uniba.sk

Human biomonitoring is the best tool for identifying, controlling and preventing exposure of the population to environmental chemical pollutants [1]. Di(isononyl) cyclohexane-1,2dicarboxylate (DINCH) gradually replaces phthalates used as plasticizers in many consumer products, especially in food packaging, children's toys and medical devices due to its more favorable toxicological profile [2]. Adverse effects such as thyroid hyperplasia and renal toxicity have been observed in animal models only at relatively high doses [2]. However, as the DINCH production and usage have been rapidly increased, the rate of exposure is increased accordingly, so biomonitoring of exposure is important mainly in sensitive population cohorts such as children in early life. By breastfeeding, the mother can transfer potentially toxic chemicals to which the mother has previously been exposed. It is important to identify trends in contamination and take public health measures [3]. As biomarkers of exposure to DINCH are used mainly two oxidized metabolites, hydroxy- (OH-MINCH) and carboxy- (cx-MINCH) cyclohexane-1,2-dicarboxylic acid monoesters. The aim of this work was to study breast milk sample pretreatment prior to HPLC-MS/MS determination of these two metabolites. RP-HPLC measurements were performed using C-18 stationary phase and mobile phases A (water with 0.05% acetic acid) and B (ACN with 0.05% acetic acid), with gradient elution from 90% A to 100% B at a flow rate of 0.23 ml/min. A short treatment column was placed in front of the analytical column for online SPE. Triple quadrupole mass spectrometer with HESI ion source operated in negative mode was utilized for measurements, monitoring selective mass transitions for each analyte and corresponding isotopicaly labeled standards.

Pretreatment procedures were assessed for overall pretreatment efficiency based on the recovery of cx-MINCH and OH-MINCH from the matrix and on the matrix effects in the ionization source of mass spectrometer. We examined aqueous fraction of milk obtained after centrifugation, and extracts to ethylacetate and mixture of ethylacetate and hexane. Pretreatment efficiency obtained for aqueous milk phase and ethylacetate extracts were very similar at the level of 50 %, after adding hexane into the extraction solution the recovery decreased by half. Our results indicated that extraction to examined organic solvents did not bring any improvement of pretreatment method efficiency, the procedure was more laborious and time consuming. On the basis of HPLC-MS/MS analysis of aqueous phase of milk samples we estimated limits of quantification (as signal-to-noise ratio 10) for cx-MINCH 0.03 µg/l and for OH-MINCH 0.12 µg/l.

Acknowledgements

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P.33 Micellar liquid chromatography in early drug discovery: A comparative study of the different surfactants

P. Danias[1], A. Pappa[1], A. Tsantili- Kakoulidou[2] and F. Tsopelas[1]

[1]Laboratory of Inorganic and Analytical Chemistry, School of Chemical Engineering, National Technical University of Athens, Iroon Polytechniou 9, 15780 Athens, Greece.
[2]Department of Pharmaceutical Chemistry, School of Pharmacy, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, 1571 Athens, Greece.

E-mail: ftsop@central.ntua.gr

The use of liquid chromatography to model Absorption- Distribution- Metabolism- Elimination and Toxicology of chemicals is based on the similarity between chromatographic and biological processes. Both are governed by a dynamic distribution of chemicals between mobile and stationary phases and both retention on a chromatographic column as well as ADMET properties are the outcome of the distribution between the two phases. In the case of organisms, the general circulation/ blood can be considered as the mobile phase, while tissues and membranes are the stationary phase. Hence, liquid chromatography under appropriate conditions (i.e. pH, temperature, presence of electrolytes) can mimic biological processes and it is known as "biomimetic chromatography" or "biochromatography". Retention factors have been served as appropriate indices to be included in several quantitative retention- activity relationships for the estimation of ADMET properties in early drug design [1]. Three types of biomimetic chromatography have been developed; Immobilized Artificial Membrane (IAM) chromatography, Plasma Protein Chromatography and Micellar Liquid Chromatography (MLC). MLC uses reversed-phase stationary phases in combination with micellar mobile phases prepared by the addition of surfactants above their critical micelle concentration. The neutral polyoxyethylene (23) lauryl ether (Brij-35) is the first and most widely implemented surfactant, while the neutral Tween-20, Tween-80 and Triton X-100, the anionic sodium dodecyl sulfate (SDS) and the cationic cetyltrimethylammonium bromide (CTAB) have also been used. However, there is a lack of comparatives studies concerning the most appropriate surfactant to estimate individual ADMET properties.

The present work refers to a comparative investigation of 6 different surfactants, namely the neutral Brij-35, Tween-20, Tween-80 and Trion X-100, the anionic SDS as well as the cationic CTAB in respect to their ability to model ADMET properties. In all cases, extrapolated to pure aqueous phase retention factors, $\log k_w$, were determined. The underlying retention mechanism was scrutinized by considering the relationship of $\log k_w$ with octanol- water partitioning with other physicochemical descriptors expressing electrostatic interactions and hydrogen bonding. Similarities/ dissimilarities between IAM and MLC retention and logP were investigated by Principal Component Analysis (PCA) and Liner Solvation Energy Relationships (LSER). Finally, a comparative study was carried out for models constructed for cell permeability, human oral absorption and plasma protein binding based on logP as well as retention factors on IAM chromatography and MLC using the 6 different surfactants.

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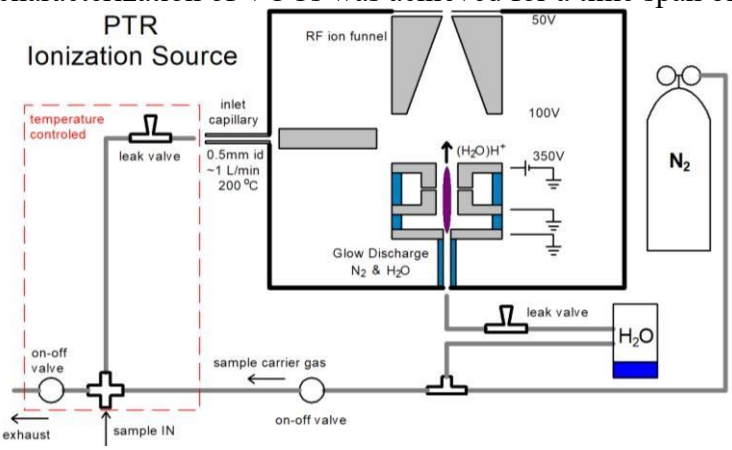
P.34 High-Performance PTR-ToF-MS for Detection of ambient Volatile Organic Compounds

Olga Zografou[1], C. Kaltsonoudis[2], M. Gini[1], E. Panagiotopoulos[3], A. Lekkas[3], D. Papanastasiou[3], S. Pandis[2,4], and K. Eleftheriadis[1]

[1]IEnvironmental Radioactivity & Aerosol Tech. for Atmospheric & Climate Impacts, INRaSTES, N.C.S.R. "Demokritos", 15341 Athens, Greece
[2]Institute of Chemical Engineering Sciences, ICE-HT, Patras, 26500, Greece
[3]Fasmatech Science & Technology SA, NCSR Demokritos, 15310, Athens, Greece
[4]Department of Chemical Engineering, University of Patras, Patras, 26504, Greece

E-mail: o.zografou@ipta.demokritos.gr

A newly developed ionization source was coupled to a Time of Flight Proton Transfer Reaction Mass Spectrometer for detection of volatile organic compounds. An enlarged inlet capillary enables the maximization of sampling, improving the instrument's sensitivity. Analyte ions introduced into vacuum are in direct contact with the plasma and interactions between analyte species, and low energy electrons (~10eV) is the main mechanism responsible for ionization, and with minimal fragmentation. The dominant form of ionization was proton transfer or electron removal with a sample m/z plus one or sample m/z resulting, respectively. The optimized transfer line consists of a set of ion guides (octapole, quadrupole, and hexapole), a high-vacuum lens and a beam forming slit focus that transfer the ion beam to the ToF section. The mass resolving power (M/dM) of the oToF mass analyzer at 500 Th is 20,000 (fwhm).
The instrument was deployed for measurements of atmospheric gases at the DEM suburban station in Athens (member of GAW and part of ACTRIS and PANACEA). Concurrent measurements included particle size distribution, real-time chemical composition of PM_1, greenhouse gases and EC/OC and XRF analysis of $PM_{2.5}$ collected on filters through highvolume samplers. Real-time characterization of VOCs was achieved for a time span of one month.



The instrument's high resolution and sensitivity is evident from the results, which also suggest high robustness. A broad range of analytes can be measured with very low limits of detection, even in the order of 5 ppt in some cases.

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4. MS

P.35 Longitudinal plant health monitoring via HRMS screening workflows

A. Panara[1], E. Gikas[1], A. Koupa[1] and N.S. Thomaidis[1]

[1] Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, 15771 Athens, Zografou GR-15771, Greece

e-mail: ntho@chem.uoa.gr

In the modern era, significant efforts have been made towards implementing more environmentally friendly procedures, like composting, to mitigate the negative effects of intensive agricultural practices. Two fertilizers (onion-based and mushroom based) via hydrolysis of the compost from the corresponding raw materials were produced. These fertilizers, which have been previously comprehensively chemically characterized [1], were applied to tomato leaves at 5 time points (t=0, t=15, t=30, t=45, and t=60 days) based on the life cycle of the tomato plant in order to monitor plant health and growth. The experimental design employed dividing the number of individual plant units into two groups, which have been irrigated with the onion-based and the mushroom-based fertilizer, respectively. Control samples were also used at each time point to eliminate confounding parameters that are produced due to the plant's normal growth. After the harvesting, the plant leaves were frozen using liquid nitrogen and consequently extracted using aq. MeOH (70:30,v/v).

The analysis was performed via UPLC-qTOFMS (Bruker Daltonics) using an Acclaim RSLC 120 C18 column (2.2 μm, 2.1 × 100 mm) in both ionization modes (± ESI). Data dependent (DDA/AutoMS) and data independent (DIA/bbCID) acquisition modes have been utilized in conjunction with open-source software (MS-DIAL and MZmine) to ascertain the mining of the maximum number of features. Statistical analysis, including ANOVA Simultaneous Component Analysis (ASCA) and Multivariate Empirical Bayes (MEBA) for longitudinal monitoring, has been employed to highlight the features being differentiated among the different irrigation conditions and time points. Metabolites related to plant growth belonging to several chemical classes were identified, proving the efficacy of the fertilizer products. Furthermore, the efficiency of the analytical and statistical workflows utilized has also been demonstrated.

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P.36 Pesticide residues tracing control in green leafy vegetables using HRMS technologies

Dimitrios Gkountouras[1], Vasiliki Boti[1,2,3] and Triantafyllos Albanis[1,2,3]*

[1]Department of Chemistry, University of Ioannina, Ioannina, 45110, Greece
[2]Institute of Environment and Sustainable Development, University Research Center of Ioannina (URCI), Ioannina, 45110, Greece
[3]Unit of Environmental, Organic and Biochemical high-resolution analysis-Orbitrap-LC-MS, Ioannina, 45110, Greece

*E-mail: talbanis@uoi.gr

Healthy dietary habits encourage the consumption of a vast number of vegetables and especially leafy greens. For this reason, monitoring of pesticides in chlorophyll-rich matrices is an issue of high importance, concerning that the presence of pesticide residues in green commodities is a very common phenomenon. In this study, a complete workflow of analysis was performed, including a primal step of non-targeted suspect analysis of approximately 400 pesticide compounds and transformation products, following a sequent target analysis level of confirmation of over 30 widely used pesticides. As preparation procedure, QuEChERS method of extraction was employed after validation for the analysis of 25 samples of packaged leafy green vegetables, commercially distributed in all over Greece. The QuEChERS method proved to be massively efficient in extracting the chosen pesticides, with recoveries above 70%, excellent linearity ($R^2 > 0.99$), and extraordinary precision (RSDs < 20%). Limits of quantification for the most analytes reached concentrations lower than 10 μg/Kg, meeting the established maximum residue limits by the European Commission. Ultra-high performance liquid chromatography combined with a hybrid LTQ/Orbitrap HRMS was applied for analysis. Ultimately, this approach is expected to provide added value in the perspective of tracing emerging contaminants such us pesticides in popular food matrices, without prior data, in order to be enlisted as an initial safeguard for the preservation of food commodities of high quality and appropriate for consumption.

Keywords: HRMS, green leafy vegetables, QuEChERS, pesticides.

5. Sample Handling

P.37 Microsampling and modern sample preparation techniques in bioanalysis for clinical research

L. Kujovská Krčmová[1,2], Ch. Suwanvecho[1,2], D. Turoňová[1,2], K. Matoušová[1], M. Matysová[2], F. Švec[2]

[1]Department of Clinical Biochemistry and Diagnostics, University Hospital, Sokolská 581, Hradec Kralové, 500 05, Czech Republic

[2]Department of Analytical Chemistry, Faculty of Pharmacy in Hradec Kralove, Charles University, Akademika Heyrovskeho 1203/8, 500 05, Hradec Kralove, Czech Republic

E-mail: Lenka.Kujovska@fnhk.cz.

The main goal of clinical research is to improve knowledge about diseases, to develop diagnostic methods for new treatments and medical devices to provide better patient care. Liquid chromatography is one of the modern techniques that allow to identify and quantify a variety of biological molecules that can be used as biomarkers to investigate complex interaction between the disease and therapy[1].
The preanalytical phase is one of the key parts in the analysis of biological samples. This phase includes sampling, transport, sample preparation, and storage before analysis for non-urgent samples. This entire process is the most time consuming and a source of errors.
Not all modern procedures are suitable for clinical research and practice. The same applies to current trends in liquid chromatography.
The aim of our study was to find optimal solution for patients in clinical studies with the main effort to small sample volume, simplicity, green friendly, medical staff safety, and price. We tested various new, modern commercially available microsampling devices for dry blood spots and dry plasma spots. In sample preparation, µ-SPE pipette tips and DPX based on various chemistries and principles were tested, and their potential usage in clinical research was evaluated. As the best WAX-S XTR pipette tip containing an ion exchanger and salt were selected. All these new preanalytical techniques in combination with modern UHPLC-MS/MS methods could serve as modern tools in clinical research and practice [2].

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P.38 Synthesis, characterization and comparison of four FPSE media for the extraction of antidepressant drugs in aquatic samples

C. Chrimatopoulos, N. Stroutzou, E. Iliadis and V. Sakkas

Department of Chemistry, School of Sciences, University of Ioannina, Ioannina, 45110, Greece

E-mail: v.sakkas@uoi.gr

Depression is one of the most common mental disorders that people suffer. Antidepressant drugs, as the major treatment, end up in surface waters having disastrous outcomes in human health and/or environment [1]. Fabric-Phase Sorptive Extraction (FPSE) is a modern and ecofriendly two-step sample preparation technique. FPSE uses as an extraction medium a natural or synthetic substrate that is chemically coated with an ultra-thin layer of a hybrid organicinorganic sol-gel solution [2].

The aim of the study was the synthesis and comparison of four different FPSE media for the extraction of antidepressants drugs in aquatic samples. Cellulose fiber filter (C) and fiberglass filter (FG) were used as substrates. Two different polymers were tested for the synthesis of sol-gel solutions, polyethylene glycol (PEG 300) and poly(ethylene glycol)-blockpoly(propylene glycol)-block-poly(ethylene glycol) (PEG-PPG-PEG 5.800), namely. Adsorption and desorption/recovery efficiencies were studied for the four FPSE media (Fig. 1). FG-PEG 300 was found to have the best performance for the extraction of antidepressants. Finally, characterization of the optimum medium (FG-PEG 300) was followed the synthesis with FTIR spectroscopy, SEM and EDS analysis.

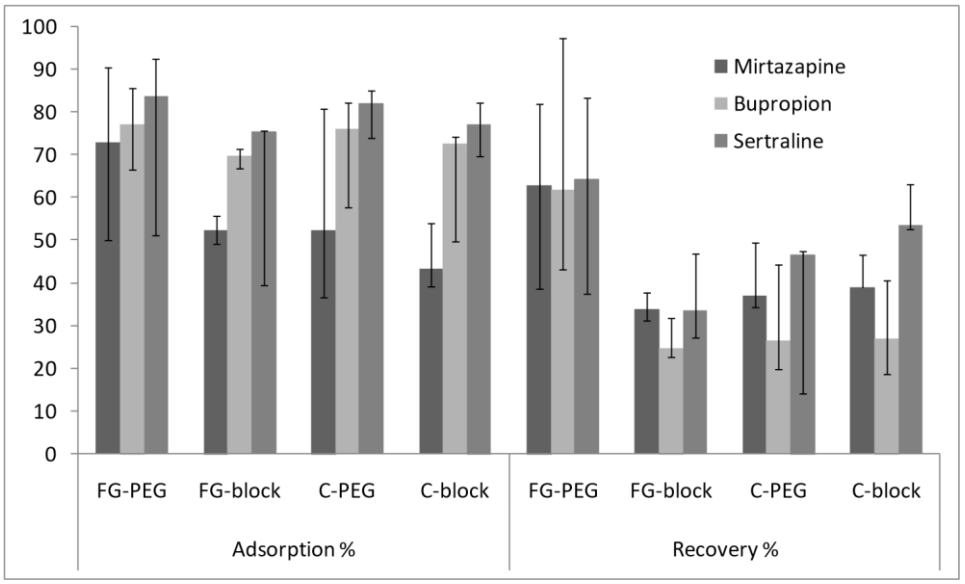

Figure 1. Test series of the Fabric Phase Sorptive Extraction of three antidepressants using four different FPSE media.

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P.39 Optimization of ultrasound-assisted extraction (UAE) for the recovery of phenolic compounds from basil and lemon balm byproducts and identification of their phytochemical profile by IR and LC-MS/MS

T. Tsiaka[1], D. Giannis[1], G. Koletsou[1], S. Theofilatos[1], D. Zotos[1], N. Stavropoulou[1], P. Zoumpoulakis[1], I.F. Strati[1], V.J. Sinanoglou[1], M. Giannakourou[1,2]

[1]Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica, Ag. Spyridonos, 12243 Egaleo, Greece
[2]Laboratory of Food Chemistry and Technology, School of Chemical Engineering, National Technical University of Athens, Iroon Polytechniou 5, 15780 Athens, Greece

E-mail: tsiakath@uniwa.gr

Following the precepts of the current market, the cultivation of Mediterranean aromatic plants is skyrocketing mainly due to the increasing demands for essential oil production, resulting also in the co-generation of large amounts of solid by products, rich in bioactive compounds, such as polyphenols, carotenoids, etc. [1]. Therefore, the purpose of the present study is (a) the optimization of ultrasound-assisted extraction (UAE) for the recovery of phenolic compounds, a non-conventional eco-friendly extraction technique, from basil (*Ocimum basilicum*) and lemon balm (*Melissa officinalis*) distillation byproducts and (b) the assessment of their phytochemical profile using infrared spectrometry (IR) and liquid chromatography-tandem mass spectrometry (LC-MS/MS) [2]. According to the results of Box-Behnken design [3], the total phenolic content (TPC) of lemon balm was maximized at lower values of % ethanol content and solvent/material ratio and at higher extraction time and ultrasound (US) power, while % ethanol content as well as the interaction of extraction time and US power were the most significant factors for the optimization of phenolic content in basil extracts. The antiradical and antioxidant activity of the optimized extracts of the two aromatic plants and their byproducts was also determined using 2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS•+) and ferric reducing antioxidant power (FRAP) assays, respectively, showing good correlation with the TPC results. In particular, the plant extracts contained higher TPC, antioxidant and antiradical activities compared to the corresponding byproducts, generated after hydrodistillation, while basil biomass was richer in phenolics compared to lemon balm solid residues. Furthermore, different varieties/types and harvesting time seems to affect the TPC values of plant byproducts. In the case of basil byproducts, large leaf basil byproducts showed higher TPC, ABTS and FRAP values than fine leaf basil byproducts, while the byproducts produced by the basil harvested in late autumn exhibited increased phenolic content compared to those cropped in early autumn. Moreover, IR and LC-MS/MS spectra revealed the presence of phenolic acids, flavonoids, caffeic acids, triterpenes, salvianolic acids, phenol and flavonoid derivatives.

Acknowledgments: Part of this research has been co-financed by the European Union and Greek national funds through the Operational Program «Competitiveness, Entrepreneurship and Innovation», under the call «RESEARCH-CREATE-INNOVATE» (project code: T2EDK-02569).

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P.40 Towards the valorization of distillation byproducts from Mediterranean herbs by implementing ultrasound-assisted extraction (UAE) and experimental design (DOE) models

T. Tsiaka[1], A. Kanioura[1], S. Pilatos[1], I. Roussos[1], G. Vountzouklis[1], N. Stavropoulou[1], E. Gogou[2], P. Zoumpoulakis[1], I.F. Strati[1], V.J. Sinanoglou[1], M. Giannakourou[1,2]

[1]Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica, Ag. Spyridonos, 12243 Egaleo, Greece

[2]Laboratory of Food Chemistry and Technology, School of Chemical Engineering, National Technical University of Athens, Iroon Polytechniou 5, 15780 Athens, Greece

E-mail: tsiakath@uniwa.gr

Lately, the valorization of plant byproducts and their conversion to high-added value cooproducts forms a major pillar of sustainability and circular economy. In order to align with the principals of these concepts, current research focuses on the recovery of bioactive constituents (i.e. phenolic compounds, terpenes, flavonoids, etc.) with potential antimicrobial and antioxidant properties, from the byproducts generated after the distillation of medicinal and aromatic herbs [1]. Thus, the primary aim of the present work was the optimization of ultrasound-assisted extraction (UAE) using experimental design (DOE) models [2] for the recovery of phenolic compounds from the solid distillation biomasses of yarrow (*Achillea millefolium*), rosemary (*Salvia rosmarinus*) and elder (*Sambucus nigra*). In particular, a 27-run Box-Behnken design was applied to evaluate the effects of ethanol content (% v/v), extraction time (min), solvent-to-material ratio (mL/g) and ultrasound power (%) on the total phenolic content (TPC) of plant extracts and their byproducts, as determined by Folin-Ciocalteu method. In addition, the antiradical and antioxidant activities of herbs solid residues were determined by 2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS•+) and ferric reducing antioxidant power (FRAP) methods, respectively, and the results of these two assays were correlated with the phenolic content of byproducts extracts. The outcomes of the spectrophotometric assays were further supported by the interpretation of the Attenuated Total Reflection-Infrared Spectroscopy (ATR-IR) spectra [3], which confirmed that herb byproducts constitute a valuable underexploited source of bioactive ingredients, that can be used as novel natural food additives.

Acknowledgment: Part of this research has been co-financed by the European Union and Greek national funds through the Operational Program «Competitiveness, Entrepreneurship and Innovation», under the call «RESEARCH-CREATE-INNOVATE» (project code: T2EDK-02569).

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P.41 Edible oil-based dispersive liquid–liquid microextraction prior to HPLCUV for the determination of naproxen in milk and dairy products

Najoud Al Mamari and Usama Alshana

Department of Chemistry, College of Science, Sultan Qaboos University, 123 Al Khod, Muscat, Oman

E-mail: u.alshana@squ.edu.om

Edible oils (EO) have a high potential as green extraction solvents for liquid–liquid microextraction due to the numerous benefits they have, which include renewability, biodegradability, non-toxicity, low volatility, low price, tunable viscosity and compatibility with many analytical techniques. The use of EO, in their intact form, as extraction solvents has been illustrated in the literature for the extraction of several elemental [1] and molecular [2] analytes. Nevertheless, neither their use in liquid–liquid microextraction nor with HPLC has been reported. In this study, edible oil-based dispersive liquid–liquid microextraction is proposed prior to HPLC-UV for the extraction and determination of naproxen. Optimum chromatographic conditions were achieved with a reversed-phase column (i.e., C18, 3 μm, 120 Å, 2.1 × 150 mm). The analyte was separated from the matrix constituents at ambient temperature using acetonitrile (A) and 0.10% (v/v) phosphoric acid (B), 40:60 (A:B, v/v) as the mobile phase, at a flow rate of 0.50 mL min^{-1} and an injection volume of 20.0 μL. Naproxen was monitored at 230.0 nm. Optimum extraction conditions were realized using 300 μL of almond oil as the extraction solvent and 1000 μL of acetonitrile as the disperser solvent at 3.0 min extraction time. Back-extraction of naproxen into 200 μL of 10.0% (v/v) acetonitrile in phosphate buffer (pH 7.00) within 2.0 min enabled direct injection of the back-extraction solution into the instrument. The limit of detection was found as 0.020 μg g^{-1}. A good linearity was achieved with coefficients of determination above 0.9976. The proposed method was used for the determination of naproxen in milk and dairy products (i.e., cow milk, fresh laban, labneh, white cheese and yogurt) with percentage relative recoveries higher than 92.0% and percentage relative standard deviations below 8.3%.

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Poster Session 2
Environmental Applications

P.42 Comparison of two Portable and Modular Gas Generators of ppb-levels of Formaldehyde for calibration of analysers and sensors

A. Becker[1], A. Granjean[1,2], C. Sutter[1], M. Wolf[1], F. Amiet[2], D. Bazin[2] and S. Le Calvé[1]

[1]ICPEES – CNRS/University of Strasbourg, 25 rue Becquerel, Strasbourg, France
[2]Chromatotec, 15 Rue d'Artiguelongue, Saint-Antoine, France

E-mail: s.lecalve@unistra.fr

According to a 2020 German study, air pollution is the leading cause of mortality in the world before AIDS, smoking and parasitic and infectious diseases [1]. Air pollution is now the biggest environmental health risk in the world. indoor air quality has become a societal issue and major environmental impact, insofar as a citizen spends 80% of his time in closed environments. Volatile Organic Compounds (VOCs) are pollutants frequently found in indoor environments. Among these VOCs, formaldehyde, which is a recognized carcinogen by the WHO, is a major indoor air pollutant due to its multiple sources (materials, combustion, etc.) [2]. Our recent work has led to portable air formaldehyde analysers [3-5]. However, all quality analysis is based on prior, precise, and reliable calibration.

This work aims at developing and validating under laboratory-controlled conditions two gas mixture generation devices designed for easy on-site or laboratory calibration of analytical instruments dedicated to air monitoring, such as analysers or sensors [6].

The first portable device, which has been validated for formaldehyde, is based on the diffusion of liquid formaldehyde through a short microporous interface with an air stream to reach nonHenry equilibrium gas–liquid dynamics. The geometry of the temperature-controlled assembly has been optimised to allow easy change of the aqueous solution, keeping the microporous tube straight. The formaldehyde generator has been coupled to an on-line formaldehyde analyser to monitor the gas concentration generated as a function of the liquid formaldehyde concentration, the temperature, the air gas flow rate, and the microporous tube length. Our experimental results show that the generated gaseous formaldehyde concentration increase linearly between 10 and 1740 µg m^{-3} with that of the aqueous solution ranging between 0 and 200 mg L^{-1} for all the gas flow rates studied, namely 25, 50 and 100 mL min^{-1}.

The second portable device is based on the diffusion of formaldehyde by a paraformaldehyde permeation tube. This formaldehyde generator has been coupled with an on-line formaldehyde analyser to monitor the generated gas concentration based on temperature, air gas flow and humidity. Our experimental results show that the gaseous formaldehyde concentration generated increases between 34 and 291 µg m^{-3} for temperatures of 50 and 60°C for all the gas flow rates studied, namely 30, 50, 70 and 100 mL min^{-1}.

These techniques developed here are the only ones allowing to operate with a low flow such as 25 to 100 mL min^{-1} while generating a wide range of concentrations (10–1000 µg m^{-3}) with very good precision.

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P.43 Targeted analysis and information data acquisition evaluation for organic contaminants determination

Lounès Haroune[1]*, Sabrina Saibi[1], Hubert Cabana[2]

1. Sherbrooke Pharmacology Institute, Sherbrooke University, Sherbrooke, QC, Canada
2. Sherbrooke University Water Research Group, Department of Civil and Building Engineering,

E-mail: lounes.haroune@usherbrooke.ca

Trace organic contaminants (TrOCs) present in wastewater pose a significant environmental concern due to their potential adverse effects on aquatic ecosystems. This study aimed to comprehensively evaluate the occurrence, removal efficiency, and ecotoxicological implications of TrOCs in a conventional wastewater treatment plant (WWTP). Daily samples of influent, effluent, and biosolids were collected and analyzed over a 20-day period.

Quantitative analysis of 70 selected TrOCs was conducted using liquid chromatography coupled to a hybrid triple quadrupole/linear ion trap mass spectrometer. Additionally, a qualitative meta-analysis using information data acquisition (IDA) was performed to evaluate over 6000 TrOC spectra comprehensively. Finally, the ecotoxicological risks were evaluated using a toxic unit (TU) approach.

Results revealed the presence of diverse TrOCs in the WWTP, with acetaminophen and caffeine being the most prominent compounds in the influent, reaching concentrations of approximately 2000 ng L-1. However, both compounds were effectively removed during the treatment process. Interestingly, carbamazepine and carbendazim exhibited a contrasting behaviour, showing higher concentrations in the effluent (52.5 and 614 ng L-1, respectively) compared to the influent (8.52 and 146 ng L-1, respectively). The IDA meta-analysis confirmed these observations and identified pharmaceutical compounds as the predominant contaminants across all matrices, highlighting significant contamination of biosolids with over 90 detected compounds. Ecotoxicological risk assessment based on TUs indicated weak to moderate risks associated with the detected TrOCs. These findings underscore the potential ecological impacts and emphasize the need for effective monitoring strategies to minimize their release into the environment.

This study provides valuable insight into the occurrence, removal efficiency, and ecotoxicological implications of TrOCs in a conventional WWTP. The results contribute to our understanding of TrOC dynamics and emphasize the importance of robust analytical characterization. Further research is warranted to identify emerging TrOCs and their derivatives better, thereby addressing potential environmental risks and enhancing wastewater treatment strategies.

P.44 Bioleaching of scandium from bauxite residue using different microorganisms

K. Kiskira[1], Th. Lymperopoulou[2], L.A. Tsakanika[1], Ch. Pavlopoulos[3], K. Papadopoulou[3], Elias Chatzitheodoridis[4], K.M. Ochsenkühn[1], G. Lyberatos[3] and M. Ochsenkühn-Petropoulou[1]

[1]Laboratory of Inorganic and Analytical Chemistry;
[2]Products and Operations Quality Control Laboratory;
[3]Laboratory of Organic Chemical Technology, School of Chemical Engineering
[4]Laboratory of Mineralogy, Petrology and Economic Geology,School of Mining and Metallurgical Engineering,
National Technical University of Athens, Iroon Polytechniou 9, Zografou campus, 15773 Athens, Greece

E-mail: kirki.kis@gmail.com

In recent years, the European Union has become increasingly concerned about its reliance on critical raw materials (CRMs) and the risk of their supply. Rare-earth elements (REEs) are widely regarded as having the most uncertain supply of any CRMs. Bauxite Residue (BR) an alkaline by-product, from the Bayer process for alumina production, is considered aσ hazardous material due to its volume and alkalinity and its disposal is a major global environmental issue [1]. REEs and other important metals can be extracted from BR as a secondary source. Sc extraction from BR has been investigated mostly by hydrometallurgical methods using different mineral acids such as nitric, hydrochloric and sulfuric acids [2]. Biotechnologies, such as bioleaching, can play an essential role in metal recovery because of their operational flexibility and low energy requirements [3,4]. The aim of this study was the investigation and comparison of a bioleaching procedure using pure cultures of the fungus *Aspergillus niger* and the bacterium *Acetobacter tropicalis,* both producing various organic acids [3,4]. The optimization of the process was performed by testing different parameters such as BR solid to liquid (S/L) ratio, biomass production, final pH, percentage recovery of Sc and the organic acids produced by the microorganisms. ICP-OES was used for the determination of Sc in all leachate solutions, while HPLC was used for the identification of organic acids. BR was analysed, before and after bioleaching, using XRD. The materials' micro-morphology was also evaluated using optical microscopy and SEM. In a one-step bioleaching procedure at 1% S/L for 20 days, the maximum Sc extraction was 42% with the use of *Acetobacter tropicalis,* while at the same conditions, 46% recovery was achieved with the use of *Aspergillus niger.* Even though, the use of fungus resulted in slightly higher Sc recovery, biosorption phenomena were observed, making it difficult to distinguish between the different bioprocesses. Easier to control and faster microbial growth was reported with the use of bacterium and no biosorption was observed. Acetic, oxalic, and citric acids were the most abundant organic acids generated by both microorganisms. The results show a synergetic effect of the diverse organic acids generated by the microorganisms. Optimization of the bioleaching process is in progress, aiming to minimize the incubation time and to maximize Sc recovery for up-scaling the bioleaching process for Sc extraction from BR.

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P.45 Spectroscopic and chemical methods for monitoring humification during composting of vineyard and winery wastes

Panagiota Manoli[1], Ilaeira Rapti[1], Christina Tzakou[1], Georgios Patakioutas[2], Dimitra Hela[1,3]

[1] Department of Chemistry, Laboratory of Industrial Chemistry, University of Ioannina, 45110, Ioannina, Greece

[2] Department of Agriculture, University of Ioannina, 47100, Kostakioi, Arta, Greece Address

[3] Institute of Environment and Sustainable Development, University Research and Innovation Center, 45110, Ioannina, Greece

E-mail: dchela@uoi.gr

Composting is an environmentally friendly practice that helps reducing the environmental footprint of winemaking by minimizing winery waste release in the environment as well as carbon emission from vineyard pruning burning, while producing a valuable amendment for soil enrichment in vineyards or other agricultural settings. The physicochemical and spectroscopic characteristics of the compost are important tools for assessing its maturity and stability in order to be used for various purposes. The combination of classical analytical methods and advanced instrumental methods can provide more conclusive information about the humification progrees during composting [1]. In the present work, compost samples after the co-composting of wine lees and organic vine pruning were analyzed on a monthly basis during a composting process. Also, the effect of adding wine lees with lower total phenolic content (TPC) after modification, on the quality of the final product was investigated. The average values of TPC measured by the Folin-Ciocalteu method were low, denoting stability of compost organic matter. In all compost samples N, C and H were determined while C/N ratio exhibited values less than 20, that were similar between the two types of samples and that decreased during the composting process leading to a stable final product. The humification process is often indicated by the changes in the components of the dissolved organic matter (DOM) during composting. The spectroscopic UV-visible ratio (E4/E6) decreased in line with the humification progress. Low E4/E6 ratios showed the presence of larger humic acid molecules or higher condensation degree. ATR-FT-IR spectroscopy was also applied in order to determine the changes in functional groups of organic substances in compost samples.The ratios of absorbance at 1650/2845, 1525/2925 and 2920/1640 were also calculated showing the changes at organic matter content and confirmed the aromaticity increase by the biosynthesis of humic-like and fulvic-like substances**.** Also, fluorescence excitation-emission matrix spectroscopy with parallel factor analysis (PARAFAC) was used in order to contribute to the maturity evaluation of compost. and a three-factor model was applied. Three fluorercent components were identified C 1 protein like components (280 /340) C2 humic like components (350)/450) and fulvic-like substances C3 (325/400). These results evidenced the dissolved organic matter humification.[2] The studied composts presented a stable and humified organic matter suitable for agronomic use in the aspect of circular economy.

Keywords: compost, wine lees, spectroscopic methods, maturity

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Food Analysis

P.46 Assessment of enriched oils thermal stability after frying using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy

A.-G. Ioannou, T. Tsiaka, P. Zoumpoulakis and V. J. Sinanoglou*

Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica, Agiou Spyridonos, 12243 Egaleo, Greece

E-mail: vsina@uniwa.gr

During the past decades, edible oils' enrichment has been considered as the major focus of numerous research studies in order to achieve their thermal stability and protection against oxidation. The majority of these research projects focused on the enrichment of edible oils with natural or synthetic antioxidants to increase their oxidation resistance. Therefore, the current study aims to examine the effect of frying process on the thermal stability of oils enriched with bioactive compounds compared to non-enriched ones (controls), using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR). Gallic acid, ascorbic acid and oenological tannins were selected as bioactive constituents for the oils' enrichment and then, were added at optimized concentrations in olive pomace and sesame oils. Next, the enriched and control oil samples were subjected to frying and oil aliquots were collected at predetermined time intervals (5,11,15,25 and 35 minutes of heating) for ATR-FTIR analysis. Subsequently, the obtained FTIR spectra of the examined oils were subjected to normalization, ATR correction, and smoothing using Quad-Cupic Savitsky Golay method and then, were interpreted in terms of their characteristic bands. The FTIR spectra were further processed using statistical tools, in order to relate the frying duration with the characteristic IR bands' intensities. More specifically, the relative changes of the spectra band intensities, at the predetermined time intervals, as well as the ratio of the bands recorded at 722 and 966 cm^{-1} (out-of-plane vibration of *cis* and *trans* –HC=CH− group of disubstituted olefins, respectively) were determined. Afterwards, the obtained results were correlated and classified from 0% (for non-oxidized samples) to 100% (for the most degraded oil sample). The received results, pinpointed the degradation levels of the studied oils as well as the effect of the individual bioactive compounds on the thermal stability of the enriched oils. Interestingly, the used bioactive compounds were sorted, in terms of their effectiveness in the oils' protection accordingly: gallic acid, ascorbic acid and oenological tannins. Moreover, the above results indicate the efficiency of ATR-FTIR technique to evaluate the effect of oil enrichment with bioactive compounds in (a) oil oxidation and (b) *cis* to *trans* fatty acids conversion, which are common indicators of oil degradation.

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P.47 Novel Natural Compounds as Putative Antimicrobials: A Computational Approach

E. Kritsi[1,2], I. Nikolaou[1], M. Markou[1], S. J. Konteles[1], P. Zoumpoulakis[1] and V. J. Sinanoglou[1]

[1] Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica, Agiou Spyridonos, 12243 Egaleo, Greece

[2] Institute of Chemical Biology, National Hellenic Research Foundation, 48, Vas. Constantinou Ave., 11635 Athens, Greece

E-mail: vsina@uniwa.gr

In packaged foods, the growth and survival of pathogenic microorganisms can cause serious foodborne diseases, compromising the safety and the quality of the food product. Particularly, bacteria such as, *Salmonella spp.* and *Escherichia coli* can affect one in six people annually, leading to approximately 128,000 hospitalizations and 3,000 deaths, with about $90 billion in the USA [1]. Until today, pasteurization and the use of antibiotics are at the forefront of pathogenic microorganisms confrontation. However, the degradation of organoleptic characteristics of food products and the resistance to antibiotics highlight the urgent need to discover novel agents that overcome these issues [2]. Towards this direction, compounds of natural origin possess a prominent position due to their structural diversity and complexity which appoint them as favourable starting materials in the discovery of small molecules.

Therefore, the present study attempts to identify natural compounds, potential inhibitors of the Topoisomerase IV (TopoIV) enzyme of the pathogenic bacterium *Escherichia coli (*E. coli). To fulfill this scope, the natural compounds included to the "Specs" library (https://www.specs.net/) were filtered and subjected to molecular docking studies, aiming to calculate their bind affinity into the *E. coli* TopoIV enzyme (Figure 1). The results assessment revealed six natural compounds in a prominent position as potential inhibitors. In a further step, the selected compounds will be purchased and their *in vitro* inhibitory activity will be evaluated with the ultimate goal of their application in packaged foods.

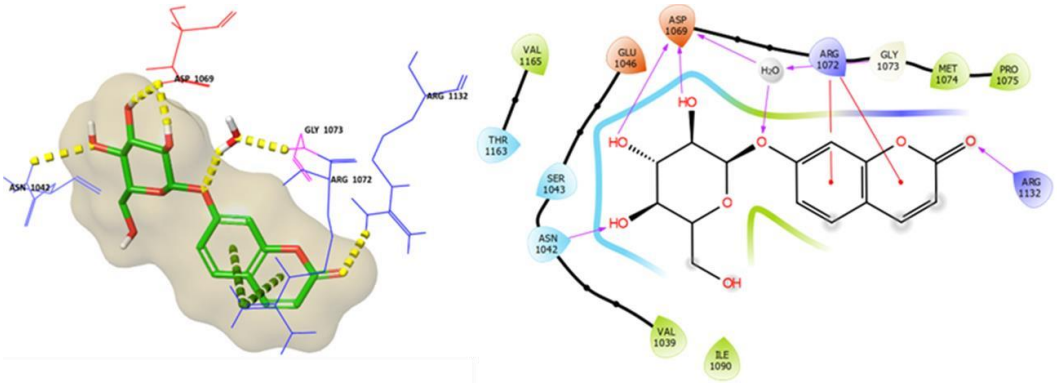

Figure 1: Representative binding pose of Skimmin at the active site of *E. coli* TopoIV enzyme.

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P.48 Assessment of banana quality and shelf-life during ripening by generating prediction models

K. Aouant[1], E. Mouka[1], G. Ladika[1], V. J. Sinanoglou[1] and D. Cavouras[2*]

[1] Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica, Agiou Spyridonos, 12243 Egaleo, Greece.
[2] Department of Biomedical Engineering, University of West Attica, Agiou Spyridonos, 12243 Egaleo, Greece

E-mail: cavouras@uniwa.gr

The fruits and vegetables' quality in relation to the ripening degree is one of the most important issues to be investigated in order to ensure consistent quality for consumers and to minimize post-harvest spoilage. Therefore, the aim of the present study was the predictive models' development in order to assess the ability of textural features, from image analysis on banana peel, to predict shelf life and fruit quality parameters during ripening. More specifically, textural features calculated from images of banana peel [a* (redness/greenness), b* (yellowness/blueness), mean value, standard deviation (std), skewness, contrast (con), dissimilarity (dis), energy, homogeneity, Angular Second Moment (ASM), Short Run Emphasis (SRE), Long Run Emphasis (LRE), and Run Length Non-Uniformity (RLN)] [1] were correlated with physicochemical quality parameters of banana flesh [Brix, firmness, total phenolic content (TPC), titratable acidity (TA), moisture and water activity (a_w)], to estimate banana shelf life and ripening process, during storage throughout a period of 21 days. The results showed that the a* and b* values of banana peel are good indicators of Brix and firmness values of banana flesh (R^2 >0.7). Moreover, the gradient boosting regressor model was employed to predict the banana ripening degree in relation to storage day, from textural and physicochemical features multiple regression, with R^2 0.999. Furthermore, using the same regressor model the quality of banana flesh was predicted, through Brix, firmness, TPC, and TA values during ripening, from the values of textural features of the banana peel by multiple regression, with R^2 >0.98. The predictive model application, using ~~the~~ image analysis resulting features, may be used as a tool for estimating the quality and shelf life of fruits.

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P.49 Comparative evaluation of strawberries fruits and leaves using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy

G. Ladika[1], I. Stephanaki[1], A.-G. Ioannou[1], I. F. Strati[1], V. J. Sinanoglou[1] and D. Cavouras[2*]

[1] Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica, Agiou Spyridonos, 12243 Egaleo, Greece.
[2] Department of Biomedical Engineering, University of West Attica, Agiou Spyridonos, 12243 Egaleo, Greece

E-mail: cavouras@uniwa.gr

The strawberry is one of the most economically important fruits worldwide and is characterized by unique organoleptic properties and important nutritional value. The cultivated strawberry (Fragaria x ananassa), one of the newest domesticated plants, cultivated since the early 18th century in Europe [1]. The present study was conducted to evaluate comparatively the phytochemicals profile from strawberry (Fragaria × ananassa) fruits and leaves using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR). ATRFTIR is a widely used, rapid, direct and non-destructive analytical technique to identify the functional groups present in plant materials and to elucidate the structure of their phytochemical constituents. The interpretation of ATR-FTIR spectra bands, ranged among 4000-499 cm^{-1}, revealed the presence of characteristic compounds in fruits and leaves of strawberry, such as physical pigments, aromatic compounds, esters, polyphenols, and carbohydrates. The most important findings are summarized below. The intensities at 2922, 2854, 1472 and 1462 cm^{-1} related to C(sp^3)-H stretching and bending vibrations, which are associated with the presence of chlorophyll [2] and aliphatic compounds, exhibited significant higher values in strawberry leaves than in fruits. The bands at 3630 and 1687 cm^{-1}, which are corresponded to the OH stretch in phenols and to C=O stretch of ketone group in chlorophyll, respectively, as well as the bands at 1420 and 966 cm^{-1} which are related to the bending vibrations of *cis*-C(sp^2)-H in chlorophyll and of *trans*–HC=CH– in carotenoids, respectively, were detected only in strawberry leaves. Moreover, the bending vibration of hydroxyl group, present in water at 1635 cm^{-1} [3], showed significant higher intensities in strawberry fruits than in leaves. Finally, the bands at 1238, 1105 and 1030 cm^{-1} which are related to the stretching vibrations of C–O in esters, organic acids and carbohydrates [4], displayed significant higher intensities in strawberry fruits than in leaves. Therefore, ATR-FTIR technique can successfully and non-destructively evaluate the phytochemical profile of fruits and vegetables, finding significant applications in their quality control.

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P.50 Determination of Heavy Metal in Food using an accredited ICP-MS method

E. Christoforou[1], D. Stefani[1], D. Kafouris[1] and E. Christou[1]

[1]State General Laboratory, Ministry of Health, 44 Kimonos St, 1451 Nicosia, CYPRUS

E-mail: echristoforou@sgl.moh.gov.cy

An accredited method using inductively coupled plasma mass spectrometry (ICP-MS) was applied for the determination of lead, cadmium and mercury in several food categories such as fish and mammals' meat, molluscs, milk, honey, fruits and vegetables, grains and grain products and foods for infants and children. Method performance characteristics were determined after spiking blank samples. The mean recoveries of lead, cadmium and mercury in different spiked samples, as well as the relative standard deviations for repeatability and reproducibility and limits of detection and quantification were in agreement with the requirements of the EU legislation for the control of contaminants and similar to those published by other researchers. Heavy metals concentrations ranged from 0.0002 to 0.379 mg kg^{-1}. It was observed that for some food categories up to 96% of the samples were contaminated with at least one of the three metals (Figure 1), but only a very low percentage of samples (1%) exceeded the maximum limits of the EU legislation. As regards to the presence of mercury and cadmium in the tested foodstuffs, the most contaminated food categories were found to be fish meat and molluscs respectively. The analysis of lead in food showed lower concentrations compared to cadmium and mercury, and it was more uniformly distributed to all food categories with a range between 35 and 67% of positive samples (Figure 1).

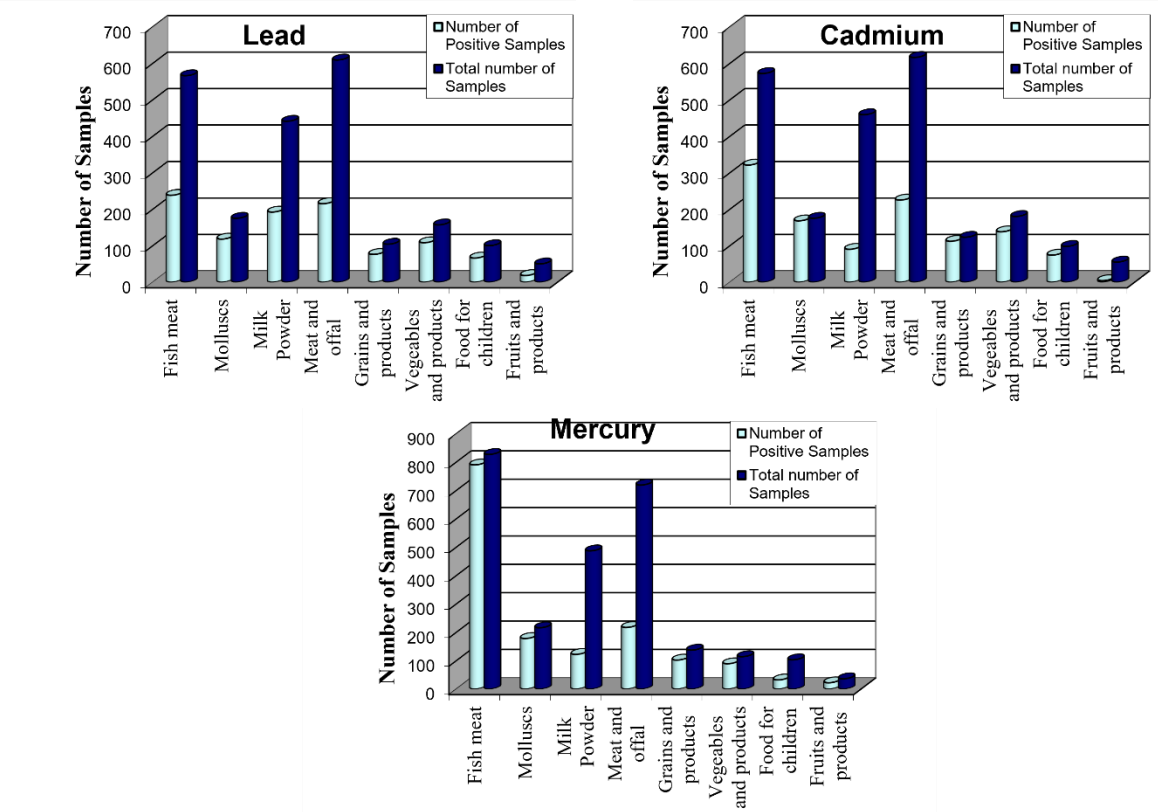

Figure 1. Heavy metals occurrence in selected food categories in Cyprus.

P.51 Classification of Greek honeys according to their botanical origin using physicochemical properties and macro-elements profile

Maria-Anthi Priakou[1], Niki Maragou[2], Erklaylle Gabriely Custodio Da Silva[3], Marios Kostakis[2], Loukas Gialouris[1], Maria Karvouni[2], Areti Kostaki[1], Maria-Christina Serdari[1], Elena Nastou[2], Evangelia Kritikou[2], Carolina Santos Silva[4,5], Maria Fernanda Pimentel Avelar[3], Nikolaos Thomaidis[2] and Marilena Dasenaki[1]*

[1]Laboratory of Food Chemistry, Chemistry Department, National and Kapodistrian University of Athens, Panepistimiopolis Zographou, 15771 Athens, Greece
[2]Laboratory of Analytical Chemistry, Chemistry Department, National and Kapodistrian University of Athens, Panepistimiopolis Zographou, 15771 Athens, Greece
[3]Department of Fundamental Chemistry, Federal University of Pernambuco, Recife, PE, Brazil
[4]Faculty of food sciences and Nutrition and Centre of Biomedical Cybernetics, University of Malta, Msida, Malta
[5]VTT Technical Research Centre of Finland Ltd, Tekniikantie 1, 02150 Espoo

E-mail: mdasenaki@chem.uoa.gr

Honey is an ancient food which is largely consumed worldwide due to its unique nutritional and medicinal properties. As well-established in the literature, honey composition is greatly influenced by the botanical and geographical origin and environmental climatic conditions[1]**.** One of honey's main quality parameters is its botanical origin, and its price is often related to that, making its authentication an issue of high concern for consumers and a very important challenge for food scientists. In this context, the present work aims to study the classification of Greek honeys according to their botanical origin, based on the macro-elements profile and their physicochemical parameters. Class Modeling methods were applied, such as SIMCA and DD-SIMCA. 265 Greek honey samples, belonging to different varieties, were analyzed and the pH, moisture, electrical conductivity and acidity values were determined, as well as the concentrations of Na, K, Ca and Mg. The analysis of the macro-elements was performed using Microwave Plasma Atomic Emission Spectrometry (MP-AES), a technique that has gained interest due to its multi-element capability, extensive linear dynamic range and very rapid analysis.[1] Among the macro-elements, K presented the highest concentrations for all tested honey varieties, with values ranging between 49,6 – 7584 mg/kg. One-class-classification models were built for fir, oak, pine, arbutus, chestnut, heather, orange and thyme honeys, determining training and prediction sets for each variety. Overall, very promising results were found for oak, fir, orange, pine and thyme honeys for which classification models with more than 75% true negatives and 83% true positives were obtained.

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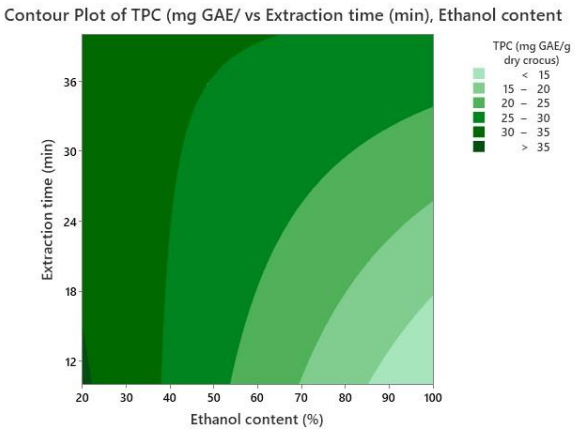
P.52 Extraction of phenolic compounds from *Crocus sativus L.* by-products using Box- Behnken experimental design

E. Lykoudi[1], M. Chatzikonstantinou[1], T. Tsiaka[1] and I.F. Strati[1]

[1]Department of Food Science and Technology, University of West Attica, Egaleo, 12243, Greece

E-mail: fst18684049@uniwa.gr

Crocus sativus L. is a monocotyledonous herbaceous triploid plant. The dried stigmas of the plant produce the most expensive spice in the world, commercially known as saffron, which has been reported in folk medicine for the protection of cardiovascular, nervous, respiratory, renal, digestive and endocrine functions. Its main constituents, crocin, picrocrocin, and safranal are responsible for color, taste, and aroma, respectively [1]. Response surface methodology (RSM) was used for the process optimization as it allows the evaluation of the effect of multiple variables and their interactions on the output variables with reduced number of trials. Ultrasound assisted extraction (UAE) of the main polyphenols was optimized for the following factors (process variables): a) ethanol content (%) in water/ethanol solvent mixture, b) extraction time (min), c) US power (%), and d) solvent/ material ratio (mL/g), with the aid of Box-Behnken experimental design. The experimental design involved three factors (process variables) each at three equidistant levels (-1, 0, +1) and the response variable was the total phenolic content (TPC), as determined by a micromethod of Folin–Ciocalteu's colorimetric assay [2]. The optimized conditions, according to the experimental design, were found to be: 20% ethanol content in water/ethanol solvent mixture, 10 min, 80% US power, and 40 mL/g solvent/material ratio. Moreover, Ferric Reducing Antioxidant Power (FRAP) assay and scavenging activity on 2,2'-Azino-bis-(3-ethylbenzothiazoline-6-sulfonic acid) radical ($ABTS^{\bullet+}$) were determined in selected extracts of plant by-products in order to assess the antioxidant capacity (expressed as mg $FeSO_4*7H_2O$/100 mL) as well as the antiradical activity [expressed as Trolox equivalents (TE)/100 mL].



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P.53 Study of goat milk adulteration with cow's milk using molecular and physicochemical methods

[1]Theoni Georgaraki[1], Dimitra Houhoula[1], Efstathia Tsakali[1], M. Chatzikonstantinou[1], Natalia Stavropoulou[1], Despina Vougiouklaki[1] and Vassilia J. Sinanoglou[1*]

Department of Food Science and Technology, University of West Attica, Agiou Spyridonos, 12243 Egaleo, Greece

E-mail: fst18684049@uniwa.gr

Goat milk is considered as a high-nutritional food, mainly rich in fat, proteins, vitamins and minerals with significant nutritional and health benefits for consumers [1]. The value of goat's milk is high and its fraudulent adulteration with other available sources of milk of lower value, such as cow's milk is very common nowadays, mainly aimed at increasing profit [2]. The aim of this study was to detect the goat milk adulteration with cow milk using physicochemical and molecular techniques and statistical analysis. Specifically, Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR), color measurement, specific gravity, and cryoscopy, as well as DNA molecular analysis using the Polymerase chain reaction (PCR) technique in combination with electrophoresis, were used. Blends of goat milk with different percentages of cow milk were prepared by mixing goat milk with cow milk in different concentrations (5, 15, 25 and 35% v/v). The goat and cow milk samples and their mixtures were analysed at ambient temperature. The most interesting findings are summarized below. ATRFTIR results revealed higher intensities at the regions 1638 cm^{-1} (amide-I), 1545 cm^{-1} (amideII), and 1030-1070 cm^{-1} (nucleic acids, phospholipids, phosphorylated proteins and lactose) for goat milk. Moreover, the ratios of the bands 1638:1545, 1157:1030, 1157:1070 and 1070:1030, cm^{-1} showed significant changes as the proportion of cow in the goat milk increased, proving the importance of these indicators for cow adulteration detection. In addition, the other techniques used gave satisfactory results for the detection of goat milk adulteration with cow's milk. Moreover, DNA analysis can detect the adulteration of goat milk with cow milk with high sensitivity both qualitatively and quantitatively. In conclusion, results demonstrate that the combination of the above quick, easy, and non-destructive techniques is a promising methodology which could be applied for the adulteration detection in milk and dairy products.

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P.54 Study of experimental yogurt desserts with mountain tea, and a mixture of saffron, mastic and mountain tea

A. Siozou and I.G. Roussis

Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina, Greece
Email: iroussis@uoi.gr

Yogurt has gained a positive perception by the consumers as a functional dairy product with a simple flavour. The enrichment of yogurt with herbs/aromatic plants is of both research and commercial interest. Herbs/aromatic plants contribute to human health and to the flavour of the products [1, 2, 3].
In the present work, experimental cow yogurt desserts prepared by the addition of mountain tea from Epirus (EMT), and a mixture of saffron, mastic and mountain tea from Epirus (SMEMT) were studied. Yogurt desserts (YD) with EMT exhibited higher pH values and lower syneresis compared with control yogurt (CY). Antioxidant activity was determined by the Folin, FRAP and DPPH assays. Methanolic extracts of YD with EMT exhibited higher antioxidant activity than CY. Similar results obtained for scavenging of hydroxyl radicals by methanolic extracts. Aqueous extracts of YD with EMT exhibited higher anti-inflammatory activity (LOX assay) than CY. All the above activities observed in a dose dependent manner indicating the positive effect of EMT. YD with SMEMT exhibited higher antioxidant activity (Folin, FRAP, DPPH assays), higher scavenging of hydroxyl radicals, and higher anti-inflammatory activity than YD with GMT indicating the positive effect of saffron and mastic. All the above activities were followed during storage of yogurt and yogurt desserts for up to 50 days. Volatile profiles were determined by SPME GC-MS method. YD with GMT exhibited higher levels of many terpenoids such as alpha-pinene, camphene, beta-pinene, o-cymene than CY. YD with SMGMT exhibited higher levels of many volatile compounds such as alpha-thujene, alpha-pinene, camphene, beta-myrcene, beta-pinene, benzene 1-methoxy-2-methyl-, o-cymene, d-limonene, d-linalool, cis-verbenol, isopinocarveol, myrtenol, d-verbenone than YD with GMT. All experimental yogurt and yogurt desserts evaluated as products of very good organoleptic quality.

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P.55 Antioxidant and bio- activities of Debina white wine

S. Balaktsi and I.G. Roussis

Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina, Greece
Email: iroussis@uoi.gr

White wines exhibit significant antioxidant and bio-activities, even though lower than red [1,2,3]. Debina variety is cultivated at Zitsa (Epirus, Greece) and Debina dry white wine is PDO Zitsa. The aim of the present work was to estimate antioxidant and bio-activities of Debina wine, and also of Malagousia and Robola white wines for comparison purposes.

Phenolic and thiol antioxidants, antioxidant activity, scavenging of hydroxyl radicals and antiinflammatory activity of white wines were evaluated. Debina wines after fermentation, after bottling and six months after bottling were examined. Moreover, two Debina wines from different wineries, one Malagousia and one Robola wine, all after bottling, were also examined. Total free sulphydryls of Debina wine decreased during storage for 6 months (period after bottling), while decrease was not observed for o-diphenols, and flavanols. Antioxidant activity was stable or increased during the above period, as estimated by the Folin and FRAP assay respectively. Scavenging of hydroxyl radicals as well as anti-inflammatory activity (LOX assay) increased during storage of Debina wine for six months. During the period after fermentation to bottling all the above parameters were stable or increased. Debina, Malagousia and Robola wines after bottling exhibited differences in their levels of total free sulphydryls and phenolics (phenolic index, o-diphenols, flavanols) as well as in their antioxidant activities (Folin and FRAP assays). However, these differences were distributed among these wines. Both Debina wines exhibited higher scavenging capacity of hydroxyl radicals than Malagousia and Robola wines. Anti-inflammatory activity of the four wines studied followed the order Debina II > Robola > Debina I = Malagousia. Present results indicate that Debina wine exhibits significant antioxidant, scavenging and anti-inflammatory activities, stable for several months and similar or higher to those of other white wines,

Table 1. Scavenging of hydroxyl radicals (SHR) and anti-inflammatoty activity (AIA) of 15fold diluted white wines.

	Debina I	Debina II	Malagouzia	Robola
SHR, mg/L as caffeic acid	$333^{C} \pm 5$	$385^{D} \pm 22$	$83^{A} \pm 4$	$149^{B} \pm 4$
AIA, %	$22.5^{A} \pm 2.5$	$49.5^{C} \pm 2.3$	$19.0^{A} \pm 1.0$	$39.0^{B} \pm 2.0$

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P.56 Quality characteristics of various Greek strained yogurts

S. Chli and I.G. Roussis

Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina, Greece
Email: iroussis@uoi.gr

Yogurt has gained a positive perception by the consumers as a functional dairy product with a simple flavour [1, 2, 3]. In the present work, the effect of storage time on quality characteristics of cow strained yogurt was studied. Moreover, quality characteristics of Greek cow strained yogurts with various fat content from different areas (Epirus, Macedonia, Thessaly) were evaluated.

Yogurts with typical or lower fat content were storage at 4 ^{o}C for 3, 20, 40, 60 days. Syneresis decreased during the period 3-20 days, while remained constant during next periods. Antioxidant activity (Folin assay) as well as peptide content (Lowry and Bradford assays) of yogurt water extracts increased during storage. Volatiles were determined by SPME GC-MS methodology. Among them carbonyl compounds exhibited changes in their levels during storage, and terpenes decreased. Levels of acids C4-C10 were stable during storage, while acetic acid was produced during first period of storage.

Yogurts produced in different areas exhibited differences in syneresis and peptide content (Lowry and Bradford assay), as well as in antioxidant activities of both water and methanolic extracts (Folin FRAP, and DPPH assay, respectively). These differences can be attributed to differences in yogurt making technologies. Yogurts exhibited differences in the levels of several volatiles such as diacetyl, hexanal, acids and some terpenes. Differences in some terpenes such as limonene may be correlated with the areas where yogurts were produced.

Table 1. The antioxidant activity of strained yogurts with 2 % and 6 % fat during storage.

	Days	2 % Fat	6 % Fat
FRAP assay (mg gallic acid / Kg strained yogurt)	3d	3,21 ^{aA} ± 0,09	3,18 ^{aA} ± 0,30
	20d	3,2 ^{aA} ± 0,5	3,14 ^{aA} ± 0,19
	40d	3,18 ^{aA} ± 0,02	3,12 ^{aA} ± 0,12
	60d	2,92 ^{aA} ± 0,22	3,08 ^{aA} ± 0,02

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P.57 Study of enriched white wines with mountain tea and a mixture of saffron and mastic

A. Siozou and I.G. Roussis

Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina, Greece
Email: iroussis@uoi.gr

White wines exhibit significant antioxidant and bio-activities, even though lower than red. Debina variety is cultivated at Zitsa (Epirus, Greece). The enrichment of foods with herbs/aromatic plants is of both research and commercial interest. Herbs/aromatic plants contribute to human health and to the flavour of the products [1, 2, 3, 4]. In the present work, Debina wines prepared by the addition of mountain tea from Epirus (EMT), and a mixture of saffron and mastic (SM) were studied.

Two different wines each with higher and lower sulphur dioxide levels were used. Free SO_2 levels varied from 10.2 to 93.9 mg/L. Control wines and enriched wines were analysed after storage for 0, 2 and 7 weeks.

All enriched wines exhibited higher levels of o-diphenols and similar levels of flavanols in comparison with their control wines. The absorbance at 420 nm of enriched wines were higher than their controls. EMT and SM addition inhibited the decrease of flavanols and o-diphenols during wine storage indicating that they retard the oxidative browning. All enriched wines exhibited higher antioxidant activity (Folin, FRAP, DPPH assays) than their controls at any sampling time, indicating the potential replacement of part of SO_2 by the addition of EMT and SM. Enriched wines exhibited higher scavenging of hydroxyl radicals and anti-inflammatory activity in comparison with their controls at any sampling time indicating the potential positive effect of EMT and SM addition on health related properties of the products. Volatile profiles of wines were determined by SPME GC-MS methodology. Enriched wines exhibited higher levels of volatiles such as some terpenes than control wine. Control and enriched wines evaluated as products of very good organoleptic quality.

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P.58 Antioxidant and bio- activities of Cabernet Sauvignon and Vlahiko red wines

S. Balaktsi, M. Basalekou and I.G. Roussis

Laboratory of Food Chemistry, Department of Chemistry, University of Ioannina, Greece Email: iroussis@uoi.gr

Red wines exhibit significant antioxidant and bio-activities [1,2,3]. Cabernet Sauvignon is a well-known variety which in Greece first cultivated in the regions of Metsovo and Atalanti. Vlahiko a promising indigenous variety cultivated mainly at Zitsa, Epirus. The aim of the present work was to estimate antioxidant and bio-activities of Cabernet Sauvignon and Vlahiko red wines over two vintages. For this reason, color intensity, phenolic and thiol antioxidants, antioxidant activity, scavenging of hydroxyl radicals and anti-inflammatory activity were evaluated.

Cabernet Sauvignon wines exhibited statistically significantly higher values of color intensity, total phenolic index and concentrations of o-diphenols, hydroxycinnamic acids, flavanols and tannins than Vlahiko ones, while all wines exhibited similar levels of anthocyanins.

Cabernet Sauvignon and Vlahiko wines exhibited statistically significant differences on their antioxidant and bio-activities. For Vlahiko the antioxidant activity was $1908^{a} \pm 140$ mg/L and $467^{a} \pm 6$ mg/L in gallic acid as estimated by the Folin and FRAP assays respectively, while for Cabernet Sauvignon it was $3809^{b} \pm 170$ mg/L and $885^{b} \pm 26$ mg/L in gallic acid. Hydroxyl radicals' scavenging for Vlahiko was $1930^{a} \pm 400$ mg/L in caffeic acid, while for Cabernet Sauvignon it was $4190^{b} \pm 230$ mg/L in caffeic acid. The % inflammatory activity, for Vlahiko was $36^{b} \pm 5$ % inhibition while for Cabernet Sauvignon it was $21.5^{a} \pm 2.5$ % inhibition.

Antioxidant and bio-activities of Cabernet Sauvignon wines from Metsovo and Atalanti did not differ significantly, as well as of Vlahiko wines from two wineries from Zitsa. In conclusion, wines from both varieties present hydroxyl radical's scavenging and
inflammatory activity. Moreover, a statistically significant difference between the two varieties was observed, with Cabernet Sauvignon wines presenting higher antioxidant activity and hydroxyl radical's scavenging. On the other hand, Vlahiko wines showed higher inflammatory activity. The geographical origin of the grapes and/or the winemaking technology was not found to statistically influence neither the antioxidant activity nor the hydroxyl radical's scavenging or inflammatory activity of the wines.

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P.59 Comparative analysis of edible fixed (carrier) oils with chromatographic techniques

E. Papakostopoulou[1], A. Psouni[1], K. Tsiantas[1], M. Katsanevaki[1], A. Venieri[1], V.J. Sinanoglou[1] and I.F. Strati[1]

[1]Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica, 122 43 Egaleo, Greece

E-mail: fiqs21031@uniwa.gr

Fixed or carrier oils are typically used in the cosmetics and pharmaceutical industries; however,with increasing consumer demand for healthier and alternative plant-based oils, edible fixed (carrier) oils are becoming increasingly popular in the food industry [1]. This comparative studyaims to identify differences in the fatty acid profile of fixed (carrier) oils, obtained either fromseeds or kernels. The Fatty acid methyl esters (FAME) of total lipids of 26 edible fixed oils were analyzed using an Agilent 6890 Series Gas Chromatograph paired with a flame ionisationdetector (FID). The chromatograph was equipped with a DB-23 capillary column (60m x 0.25mm i.d., 0.15 μm film) (50%- Cyanopropyl-methylpolysiloxane) from Agilent Technologies [2].

Table 1 Representative fatty acids (% composition) of examined fixed oils

Fixed Oils	Fatty Acids composition (%)				
	16:0	**18:0**	**18:1**	**18:2**	**18:3**
Almond oil	6.1	3.8	**68.8**	14,7	ND
Apricot kernel oil	5.6	1.5	64.5	23.6	0.1
Avocado kernel oil	**18.5**	0.8	57.5	8.2	0.6
Black seed oil	11.1	3.3	22.4	50.6	0.2
Canola oil	4.4	1.8	52.5	21.5	**10.0**
Carrot oil	10.3	6.4	38.3	40.2	0.3
Chia seed oil	8.8	3.7	7.7	20.6	**54.3**
Coconut oil	7.8	3.1	4.3	0.9	ND
Coffee bean oil	8.9	4.8	22.4	55.2	0.1
Evening primrose oil	5.8	2	6.6	**75.4**	0.4
Grapeseed oil	**52.2**	36.1	3.4	5.9	ND
Hazelnut oil	6.9	2.2	**71.6**	13.8	0.1
Linseed oil	6	4.3	19.9	15.6	**48.5**
Macadamia oil	7.6	2.7	49.9	2.1	0.2
Milk Thistle oil	8	5.4	20.7	53.5	0.2
Mustard seed oil	**15.6**	2.6	64.0	9.6	0.6
Peanut oil	8.4	2.6	56.7	26.4	0.1
Pine cone oil	4.8	2.6	22.6	**63.4**	0.2
Plum kernel oil	5.3	1.8	**66.5**	20.1	0.1
Pomegranate oil	9.9	2.8	**65.8**	9.8	0.7
Poppy seed oil	10.6	2.2	39.9	35.4	0.7
Pumpkin oil	10.8	5.6	26.8	45.2	2
Sea buckthorn oil	**33.4**	1.3	28.5	2.7	1.3
Sesame oil	8.1	5.8	36.8	44.1	0.4
Soybean oil	10.9	5.5	25.9	48.6	5.8
Walnut oil	6.5	2.7	15.4	**58.7**	**10.2**

Hazelnut oil presented the highest percentage of oleic acid, followed by almond. plum and pomegranate oil, (Table 1). The highest percentage of linoleic acid was noticed in evening primrose oil, followed by pine cone oil and walnut oil. Chia seed oil, followed by linseed, walnut and canola oil, contained considerable amounts of linolenic acid. C16:0 and C18:0 were the predominant saturated fatty acids (SFA) found in grapeseed oil, sea buckthorn, avocado kernel andmustard seed oil. Coconut oil contained significant amount of SFA , especially C12:0 (55.5%), C14:0 (19.3%) and C10:0 (8.2%). Conclusively, it is observed that fixed oils derived from seeds tend to have higher percentage of mono- or poly- saturated fatty acids, necessary for maintaining proper body function, compared to the respective oils derived from kernels.

Edible fixed oils could be further investigated for additional quality parameters as well as for their oxidative stability in order to evaluate their suitability for food industry and for potential health benefits to consumer.

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P.60 Assessment of quality characteristics and oxidative stability of *Origanum majorana* infused Extra Virgin Olive Oil

M. Katsanevaki[1], A. Venieri[1], A. Psouni[1], E. Papakostopoulou[1], P.K. Revelou and I.F. Strati[1]

[1]Laboratory of Chemistry, Analysis & Design of Food Processes, Department of Food Science and Technology, University of West Attica, 122 43 Egaleo, Greece

E-mail: fiqs21031@uniwa.gr

Recently, flavor infused olive oils are gaining relevance in the food industry, especially in the section of gourmet products [1], although, according to the International Olive Oil Council standards, they are considered seasonings [2]. The purpose of the present study was to assess the effect of aromatic herbs in quality characteristics and thermal stability of Extra Virgin Olive Oil (EVOO). For this reason, EVOO samples infused with *Origanum majorana*, at two different concentration levels (20 g/L and 40 g/L), were analyzed for acidity value, color parameters, chlorophyll and β-carotene content, as well as for oxidative stability through the Rancimat method, at two different time periods (0 and 14 days of storage). The acidity of all EVOO samples was not significantly affected by the aromatization. Color measurement in all samples ranged from 1.0-1.3 Red, 35.0-38.0 Yellow, 0 Blue and 0.3-0.8 Neutral Lovibond units in the Lovibond RBYN scale; whereas chlorophyll and β-carotene content increased both with *Origanum majorana* concentration and storage time. The enrichment of EVOO with *Origanum majorana* at the concentration level of 40 g/L resulted in an increase of induction time by 14%, compared to the control, after 14 days of storage. The results of the present study point out that the enrichment of EVOO with aromatic herbs could have a positive effect on oil's sensory and quality characteristics, as well as on its oxidative stability.

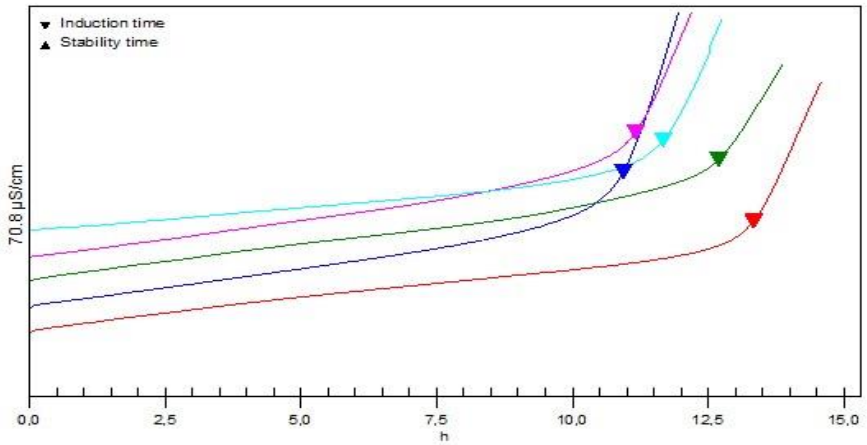

Figure 1: *Conductance (µS/cm) to heating time (h) evolution measurements for EVOO samples [light blue line:*

Control; purple line: EVOO+EVOO+20.0 g/L O.M. (14 days); red line: EVOO+40.0 g/L 20.0 g/L O.M. (0 day); green line: EVOO+40.0 g/L O.M. (0 day); blue line: O.M. (14 days)].

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P.61 Exploring the quality and safety of extra virgin olive oil using optical spectroscopy

Emmanouil Orfanakis[1,2], Renate Kontzedaki[1,3], Aggelos Philippidis[1], Eleni Charitoudi[1,4] and Michalis Velegrakis[1]

[1]Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas (IESL-FORTH), 70013 Heraklion, Greece
[2]Department of Materials Science and Technology, University of Crete, 70013 Heraklion, Greece
[3]Department of Chemistry, University of Crete, 700 13 Heraklion, Crete, Greece
[4]Department of Physics, University of Crete, 70013 Heraklion, Greece

E-mail: filagg@iesl.forth.gr

Extra virgin olive oil (EVOO) has been declared a main component of the Mediterranean diet; it is correlated with health benefits due to its high nutritional value. The health benefits of extra virgin olive oil (EVOO) are attributed to its unique composition, which is primarily a result of its high content of monounsaturated fatty acids and minor substances such as phenolic compounds, which present antioxidant and anti-inflammatory properties [1]. These benefits can often be invalidated through contamination with pollutants and adulterants. In order to secure the safety and quality of EVOO, the implementation of a rapid, low cost and easily adaptable on-site method is essential. Optical spectroscopy techniques provide an alternative analytical approach to food analysis. In this approach, we will present the application of optical spectroscopy in combination with statistical analysis as a tool for EVOO analysis in terms of quality and safety. Specifically, Raman spectroscopy provides a clear classification of organic and conventional olive oils and further into high and low quality. The samples were prior evaluated by a certified tasting panel. Moreover, the detection of benzo[a]pyrene, a polycyclic aromatic hydrocarbon, at different concentrations in EVOO was achieved by the application of fluorescence spectroscopy. Furthermore, samples of EVOO spiked with lubricant oils and the detection limit of fluorescence spectroscopy were also investigated. The results demonstrate the power of Raman and fluorescence spectroscopy as analytical tools for monitoring the quality and safety of EVOO samples.

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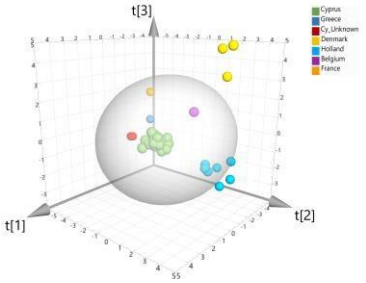
P.62 The isotopic approach to the authenticity of Cypriot Potatoes for strengthening their identity: Preliminary results

E. Ioannou Papayianni, E. Tzioni, C. Savvidou, C. Louka, C.Damaskinos, M.Tarapoulouzi and R. Kokkinofta

State General Laboratory, P.O.Box 28648, Nicosia, Cyprus
E-mail: eioannou@sgl.moh.gov.cy, sglsnif@cytanet.com.cy

Local products are an integral part of an area's local heritage as they contribute to the adoption of a region's "identity", creating bonds between its products, their unique characteristics and the special geoclimatic conditions existing in the region. Recently, the consumers have diverted their interest towards local and traditional products, which possess unique quality characteristcs. The increased demand of these products is an economic opportunity for areas that are able to diversify and properly promote their local products.

The authenticity study of the potatoe are of a great importance, due to the fact that its geographical origin has not been widely investigated. Given the economic importance of potato production, establishing the origin of unknown commercial samples declared as Cypriot is particularly important for Cypriot producers. In the study presented here, stable isotope ratios were studied in order to develop a potato provenance methodology. The potato starch has been broken down with the aid of α-amylase to soluble drextrines and oligosaccharide. Ethanol fermedation of hydrolized potato starch was carried out with Saccharomyces cerevisiae. The combined information from isotopic ratios of $^{13}C/^{12}C$ and $^{18}O/^{16}O$ by IRMS and D/H by SNIF-NMR spectroscopy in potatoes ethanol, has been observed to create a unique isotopic fingerprinting of the samples studied. The conclusions obtained from the chemometric analysis of the above results are very promising, for the protection of local production. It is believed that the differentiation of local potatoes is related to the unique geological and climatic conditions existing in the island.



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3.Archaeometry

P.63 Characterization and consolidation of limestone using calcium hydroxide/carbonate nanoparticles: a case study in the archaeological site of Pella

K. Marnellou[1], V. Tsiridis[2], M. Stefanidou[2], A. Konstantinidis[2], E. Pavlidou[3], T.D. Karapantsios[1], P.K. Spathis[1] and I. Karapanagiotis[1*]

[1]Department of Chemistry, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece
[2]Department of Civil Engineering, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece
[3]Department of Physics, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

*E-mail: karapana@chem.auth.gr

Limestone is the main construction material in the archaeological site of Pella, the capital of ancient Macedonia and the birthplace of Alexander the Great. The goal of this research is to test the protective efficacy that calcium hydroxide or modified carbonate nanoparticles can offer to limestone. The former (hydroxide) nanoparticles were purchased from the market whereas the latter (modified carbonate) nanoparticles were produced in the laboratory.
Prior to conservation studies a physicochemical characterisation of Pella's stone was carried out using samples which were collected from the archaeological site. Porosity, specific gravity, water absorption coefficient and compressive strength of the stone samples were measured. Moreover, scanning electron microscopy (SEM) equipped with energy-dispersive X-rays (EDX) was employed to carry out elemental analysis.
Two products were tested for the conservation of limestone. First, CaLoSiL® IP a stone consolidator, which contains calcium hydroxide nanoparticles (from 50 to 250 nm) stably dispersed in *iso*-propanol, was applied onto limestone specimens. Four different concentrations (from 5 to 25 g/L) of CaLoSiL were prepared and applied for comparative purposes. The wet and dry uptakes were measured, followed by colourimetric and porosity measurements. The durability of the treatment was tested using the tape peeling test, whereas the effect of the consolidator on the mechanical properties of limestone were evaluated using a Vicker's microindentation instrument.
In a second conservation approach, calcium carbonate particles in the form of waste marble powder were functionalised with stearic acid. The modified powder obtained superhydrophobicity which is an important property for conservation products of heritage monuments, as these are threatened by rainwater-induced degradation mechanisms. The protective efficacy of the modified particles is currently tested in comparison to CaLoSiL.

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P.64 A fully automated micro-LIBS system for 2D elemental imaging of marine shells for archaeological research

V. Pinon[1], N. Hausmann[2], D. Theodoraki[2], P. Siozos[1], A. Lemonis[3] and D. Anglos[1,4]

[1]Institute of Electronic Structure and Laser, Foundation for Research and Technology, Nikolaou Plastira 100, 70013, Vassilika Vouton, Heraklion, Crete, Greece
[2]Leibniz-Zentrum für Archäologie (LEIZA), Leibniz-Forschungsinstitut für Archäologie, Mainz, Germany
[3]Biomimetic, Science and Technology Park of Crete, Heraklion, Crete, 70013, Greece
[4]University of Crete, Department of Chemistry, Voutes University Campus, P.O. Box 2208, 70013, Heraklion, Crete, Greece

E-mail: vpinon@iesl.forth.gr

Chemical analysis of mollusc shells provides valuable information for paleoclimatic studies, offering insights into past environmental conditions, including sea surface temperature. Furthermore, the elemental analysis of shell remains collected from archaeological sites allows for the extraction of information regarding the season during which the shells were collected as a food source by the population residing in those sites. Understanding the season of shell collection contributes to our knowledge of settlement life, gathering practices, collection environments, and the seasonality of occupation. While stable isotope analysis is commonly used to determine sea surface temperature and season of collection, it is a time-consuming, destructive, and expensive process. An alternative method involves estimating sea surface temperature from the ratio of magnesium (Mg) to calcium (Ca) concentration [1-2]. Mollusc shells are primarily composed of calcium carbonate, but magnesium is incorporated in a process affected by the sea surface temperature, thus replacing some calcium ions. However, the ratio of these two elements is also affected by the internal mechanisms of the shells. Therefore, ensuring an accurate interpretation of results and enhancing the statistical value of the obtained information requires analysis of a substantial number of samples.

In this study, we present a practical example of a new Laser-Induced Breakdown Spectroscopy (LIBS) system for elemental imaging of carbonate shells. Compared to previous systems with similar objectives, our acquisition process has been considerably accelerated, achieving a rate of approximately 76 spectra per second at a resolution of 30 μm, 10-15 times faster. We have also improved the software capabilities by incorporating a point-and-click interface and ensuring the laser beam remains safely confined within the housing, thereby creating a safer working environment.

One of the primary advantages of LIBS is analysis speed, ease, and repeatability, allowing researchers to reassess sampling parameters, such as resolution or the number of spectra taken per location. This capability enhances the analytical detail of paleoclimatic data, a benefit not available with many other methods that are more destructive or time-consuming.

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4.Spectometry

P.65 Remote LIBS for real time evaluation of the operational condition of polymeric insulators on high voltage power transmission lines

O. Kokkinaki[1], P. Siozos[1], I. Liontos[1], K. Hatzigiannakis[1], M. Andrianakis[1], V. Piñon, S. Dellis[2], T. Anagnos[2], N. Mavrikakis[3], K. Siderakis[3], K. Mouratis[4], E. Koudoumas[4], G. Kantemiris[5], S. Couris[5] and D. Anglos[1,6]

[1]Institute of Electronic Structure and Laser, Foundation for Research and Technoloy-Hellas (IESL-FORTH), P.O. Box 1385, GR 71110 Heraklion, Crete, Greece

[2]Raymetrics S.A., 32 Spartis, Metamorfosis, GR 14452, Athens, Greece

[3]Islands Network Operation Department, Hellenic Electricity Distribution Network Operator S.A., GR71307, Heraklion, Crete, Greece

[4]Hellenic Mediterranean University, Department of Electrical Engineering, P. O. Box 1939, GR 71004, Heraklion, Crete, Greece

[5]Department of Physics, University of Patras, GR 26504, Patras, Greece

[6]Department of Chemistry, University of Crete, P.O. Box 2208, GR 71003, Heraklion, Crete, Greece

E-mail: olga@iesl.forth.gr

Polymer-based composite insulators constitute basic components of overhead high voltage power transmission lines, due to their superior operational performance, especially under pollution conditions, in comparison with the traditional ceramic or glass insulators. However, the long-term exposure of polymeric insulators to environmental, electrical and mechanical stress may lead to gradual degradation of their insulation properties due to ageing. In order to safeguard the reliability of the power transmission lines, we have demonstrated the feasibility of remote Laser Induced Breakdown Spectroscopy (LIBS) technique as a diagnostic tool for the evaluation of the type and the physical condition of field-aged composite insulators [1]. In the framework of the project PoweR-LIBS (IMS 5131360) we are presenting a fielddeployable, transportable, integrated Remote LIBS (R-LIBS) system, which has been developed for the real-time evaluation of the insulators in service, without removing them from the network. The R-LIBS system is designed on the basis of a typical stand-off configuration scheme, it is placed on the ground, and analysis is performed in the range of 2040 meters. Targeting and focusing a Q-switched Nd: YAG laser beam (at 1064 nm) on the insulators' surface results in plasma emission, which is collected by a Newtonian-type telescope and analyzed by a high- resolution portable spectrometer in the 250-450 nm spectral range.

Remote LIBS spectra have been recorded upon irradiation of 25 field-aged polymeric insulators and 12 artificially-aged insulators, under the same experimental conditions. The insulators differ in the chemical composition of the polymeric material, their operation time, and the degree of degradation (due to pollution and/or electrical stress). R-LIBS spectra and data of the characterization of the physicochemical and electrical properties of the insulators have been processed using machine learning algorithms. Results demonstrate the robustness of our presented R-LIBS method as an efficient tool for the fast and reliable prediction of the performance of the insulators.

The project is co-financed by the European Regional Development Fund of the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call RESEARCH – CREATE - INNOVATE (project code: T2EDK-02717).

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P.66 Non-destructive spectroscopy combined with chemometrics as a tool for Green Chemical Analysis of lignocellulose

Maria Kulp, Maria Kuhtinskaja, Olivia-Stella Salm, Evelin Solomina, Tiit Lukk

Tallinn University of Technology, Dpt. of Chemistry and Biotechnology, Akadeemia tee 15, Tallinn, Estonia

E-mail: maria.kulp@chemnet.ee

The trend in the modern world is to replace fossil fuels with green energy sources in order to reduce their environmental impact. The biorefinery industry, within this premise, needs to establish quantitative and qualitative analytical methods to better understand lignocellulosic biomass composition and structure. The classical "wet" chemistry methods are currently still preferred to yield accurate and precise results. However, traditional analysis methods are tedious, time consuming, require large sample sizes, involve a considerable consumption of energy and produce a significant amount of hazardous substances.

The advantage of using vibrational spectroscopic techniques, such as attenuated total reflectance Fourier transform mid infrared spectroscopy (ATR-FTIR) [1], is the possibility of evaluating the composition of lignocellulosics by analysing small amounts of samples and developing non-destructive, simple, fast and direct determination methods. The use of this technique meets trends in wood analysis to develop green methods that generate fast responses with no consumption of reagents or solvents, and consequently less environmental impact. Moreover, non-destructive spectroscopy potentially enables the simultaneous analysis of several analytes in a single run, with a consequent saving of reagents and time.

Exploratory and quantitation methods employing vibration spectroscopic techniques require the joint use of chemometric tools. Multivariate statistical analysis including principal component analysis (PCA), hierarchical cluster analysis (HCA), linear discrimination analysis (LDA) or partial least squares regression (PLSR) are often applied [2,3].

In present study 90 samples of three different wood species (pine, spruce and birch) grown in Estonia were characterized by wet chemistry analysis (acid-soluble and acid-insoluble lignin, metal and organic element contents, extractives) and ATR-FTIR spectroscopy. Obtained chemical and spectroscopic data was subjected for chemometric analysis. For estimation of the place of grow or the source of origin of unknown wood samples the discrimination of wood samples was achieved by using principal component analysis (PCA) and linear discrimination analysis (LDA). Moreover, PLS multivariate calibration models allied to variable selection methods were developed and cross-validated to quantify the total and acid soluble lignin and the content of extractives. Although a wide range of input parameters (i.e., various wood species) was used, highly satisfactory results were obtained with the root-mean-square errors of 2-5 % for all parameters.

This study shows the potential of non-destructive IR spectroscopy combined with multivariate analysis methods for a quick identification, classification and evaluation of the chemical composition of lignocellulose, providing green alternative to classical "wet" chemical analysis.

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P.67 Optical spectroscopy & chemometrics as an analytical tool in fuel adulteration detection

N. Fragkoulis[1,2], E. Koliou[1,3], P. Samartzis[1]

[1] Institute of Electronic Structure and Laser, Foundation for Research and Technology – Hellas (IESL-FORTH), N. Plastira 100, Heraklion, Crete 70013, Greece

[2] Department of Chemistry, University of Crete, Heraklion, Crete 70013, Greece [3] Department of Material Science, University of Crete, Heraklion, Crete 70013, Greece

E-mail: nfragkoulis@iesl.forth.gr

Fuel adulteration is a problem with repercussions to the environment and the economy. Classical analytical techniques, such as NMR, liquid and gas chromatography, have been used to detect adulteration [1, 2]. These techniques, although very precise, tend to be expensive and time consuming. In this contribution we present an alternative approach, coupling optical spectroscopy and chemometrics. We compare the performance of five spectroscopic techniques (UV & NIR absorption, FT-IR, Raman and Fluorescence) in detecting adulteration of premium gasoline samples with regular gasoline. The spectroscopic data were analyzed using Partial Least Squares (PLS) regression. UV, NIR, and Fluorescence exhibit R^2 values over 95% with error values below 10%, while FTIR and Raman have similar R^2 with higher error. This study demonstrates the potential of optical spectroscopy as a fast, simple and low-cost way of studying fuel adulteration, complementary to the currently used methods.

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P.68 Analysis of Platinum Group Elements in Water Samples by Energy Dispersive X-Ray Fluorescence

G. Vlamaki and N. Kallithrakas-Kontos

Analytical and Environmental Chemistry Laboratory, School of Mineral Resources Engineering, Technical University of Crete, University Campus, GR-73100 Chania, Greece

E-mail: kalli@mred.tuc.gr

The term “platinum group metals” (PGM) includes six transition noble metals of the 5th and 6th periods of the periodic table (Ruthenium (Ru), Rhodium (Rh), Palladium (Pd), Osmium (Os), Iridium (Ir) and Platinum (Pt)) that are often found together in various minerals. For the last years, PGM have been included in the list of the ten most expensive metals with Rh being the most expensive of them. Their important applications in high-tech products as well as their excellent catalytic properties have attracted a particular interest in these metals, including in the recycling sector, while their potential environmental impact is increasingly being investigated [1]. Energy Dispersive X-Ray Fluorescence (EDXRF) could be a very interesting method for PGM analysis, especially from their L x-ray lines (for Pt, Ir, Os). Considering liquid samples, the expected concentrations are very low, so an improvement of the minimum detection limit is needed.
In recent years, the application of novel complexation membranes has achieved an excellent improvement of these detection limits in the case of aqueous solutions (including seawater) [2]. In the present work we present the first results from the application of this preconcentration method to the analysis of PGE; among them, emphasis was given on the analysis of platinum [3] which was used as a "paradigm" for all the others. At the same time, the experimental selections given, and the difficulties encountered in such analyses are highlighted. In the case of Pt a minimum detection limit less than 100 ppt (parts per trillion) in 250 ml of drinking water was achieved in 20 min analysis and the effort to improve is ongoing for all PGM. Figure 1 shows the spectrum from the analysis of tap ~~a~~ water sample, doped with platinum of 20 ppb concentration under the conditions indicated in the figure caption.

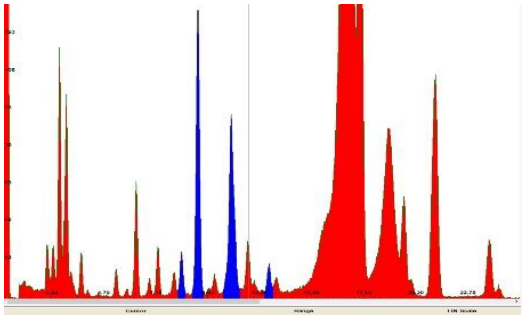

Figure 1. Analysis of 250 mL tap water spiked with 20 ppb Pt for 5 min.

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P.69 Occurrence of pharmaceuticals residues in surface waters Using high resolution mass spectrometry-environmental risk Assessment

I. Stavropoulou[1], Ch. Tsoutsi[1,2], and T. Albanis[1,2]

[1]Department of Chemistry, University of Ioannina, 45110 Ioannina, Greece
[2]University Research Center of Ioannina (URCI), Institute of Environment and Sustainable Development, Ioannina 45110, Greece

E-mail: htsoutsi@uoi.gr

Contamination of water resources by pharmaceutical residues is one of the major challenges for the preservation and sustainability of the environment. In the last decade, traces of pharmaceuticals, typically at levels in the nanograms to low micrograms per liter range, have been reported in the water cycle, including wastewater and surface waters. Pharmaceuticals residue analysis in environmental samples has received increasing attention, resulting in many environmental monitoring programs for a broad range of these substances. The main objective of this study was the occurrence of 35 pharmaceutical residues in surface waters from different sampling points along the aquatic systems of Lake Pamvotis and the River Kalamas, (Epirus, Greece), while the monitoring program was carried out from April 2022 until March 2023. In addition, it was necessary to study the occurrence of these compounds in the effluent of wastewater treatment plants (WWTPs) in Ioannina city, as it outflows into the studied water system. For this purpose, two different solid-phase extraction (SPE) extraction methods were applied, one for the wastewater and the other for the lake, river, and sea water. The detection of pharmaceutical compounds was carried out using liquid chromatography coupled with high-resolution mass spectrometry, using a hybrid orbitrap mass analyzer (LC-LTQ/Orbitrap MS). The detected compounds included amisulpride, caffeine, carbamazepine, citalopram, fenofibrate, mirtazapine, o-desmethyl venlafaxine, paracetamol, and venlafaxine. Caffeine was the dominant compound, with the highest concentrations of 432.6 ng/L. Finally, the assessment of the environmental risk (acute and chronic) for the detected compounds was estimated calculating risk quotients (RQs) for different aquatic organisms (fish, invertebrates, and algae). In most cases, the results indicated low and moderate risk (RQ<0.1 and RQ<1, respectively), except for fenofibrate with RQ=2.9 for algae and paracetamol with RQ=6.9 for invertebrates, indicating high risk.

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P.70 Risk assessment approach of elemental impurities in Oral contraceptives pills

Haya S. Al Zeer[1], Monerah A. Altamimy[1], Ahmed I. Al-Ghusn[1], Yahya M. Al Shehry[1], Fahad S. Al Dawsari[1].

[1]Reference Laboratory for Medicines and Cosmetics (RLMC), Saudi Food and Drug Authority (SFDA), Riyadh 12843-7116, Saudi Arabia

E-mail: Haya.s.z555@gmail.com

Background: Drug products may threaten human health if they contain elemental impurities. These impurities can result from various sources, such as residual catalysts intentionally introduced during synthesis or interactions with processing machinery or container/closure systems. One of the sources of exposure to chemical toxicity is pharmaceutical contraceptives, which can cause chemical accumulation in the body, copper toxicity, and oxidative stress. Additionally, these contraceptives may severely affect the gut and vaginal microbiomes, hepatic function, and nutrient status. Combination oral contraceptives (COCs), the most commonly prescribed birth control pills for women, contain two synthetic steroid hormones, estrogen and progesterone. However, COCs have been associated with various toxic effects. As elemental impurities can lead to various toxic effects, their levels in drug products should be monitored and controlled. Exposure to toxic metals can cause various health issues, including psychiatric symptoms that may mimic various psychiatric disorders, resulting in the prescription of psychoactive drugs or other unnecessary therapies. This study aims to determine unacceptable levels of elemental impurities in certain types of COCs based on the International Council for Harmonization (ICH) guidelines. The presence of certain elemental impurities would require a risk assessment.

Method: The study selected eleven drug products from hormonal contraceptive classes, known to have psychiatric side effects, for analysis using Inductively Coupled Plasma Mass Spectrometry (ICP-MS). The analytical method followed the United States Pharmacopeia official method outlined in general chapter

〈233〉 Elemental Impurities—Procedures. Sample preparation and instrument setup were conducted based on the same chapter. The data was analyzed using Power BI © 2023 Microsoft 365 and Microsoft Excel®.

Conclusion: Based on the results of the drugs tested, none of them exceeded the permissible daily exposure or unacceptable levels of elemental impurities mentioned in ICH and USP. However, elemental impurities are still noteworthy and could be considered for further analytical investigations. Despite some products containing the same active substances and excipients, the presence of elemental impurities with varying concentrations among the target samples raises questions. Some drugs contain class 1 or 2A elements in small amounts, and some manufacturers intentionally add elements from class 2B or 3 during the synthesis of Active Pharmaceutical Ingredients (API). Therefore, conducting a risk assessment is essential and includes other industrial and pharmacoeconomic aspects, such as whether the element was intentionally added, which is a crucial point in pharmaceutical risk management. It is vital to note that risk assessment and risk management in pharmaceuticals do not solely depend on toxicological data; several other factors, such as drug accessibility, drug shortage, pharmacoeconomics, and industrial aspects, must also be considered. Therefore, we strongly recommend establishing targeted risk-based postmarket programs to investigate elemental impurities in pharmaceuticals.

5. Materials

P.71 Hydration study of Portland-limestone cements containing aluminum containing admixtures with a combination of isothermal calorimetry and FTIR spectroscopy

K. Sotiriadis[1], L.Zárybnická[1], P. Mácová[1], A.S. Mazur[2], P.M. Tolstoy[2]

[1]Institute of Theoretical and Applied Mechanics of the Czech Academy of Sciences, Prosecká 809/76, CZ-19000 Prague, Czech Republic

[2] St. Petersburg State University, Center for Magnetic Resonance, Universitetsky pr. 26, RU-198504 Petergof, St. Petersburg, Russia

E-mail: zarybnicka@itam.cas.cz

The building industry is an increasingly developing sector. The significant environmental footprint of the production processes of cementitious materials calls for urgent solutions to optimise concrete composition and extend its service life [1–4]. Portland-limestone cements serve this goal as their clinker content is reduced; however, they are known for their susceptibility to cold and humid sulfate-containing environments. The use of calcined clays as mineral admixtures in the binder improves the durability of Portland-limestone cement concrete against chemical attack. This is because of the silicon- and alumina-rich composition of these reactive materials that modifies the structure of cement hydrates [5–7].

This paper aims to highlight the effect of such composition on the hydration of Portland-limestone cement by comparing two cement pastes prepared from type CEM II/A-LL (LA) and CEM II/B-LL (LB) cements that were admixed with either metakaolin (MK) or aluminum hydroxide (AH). The hydration study was performed with isothermal calorimetry and FTIR spectroscopy. The water-to-binder ratio of the paste was set to 0.45; a 10% substitution level of cement with the admixtures (by binder mass) was selected. The pozzolanic reaction between MK and the portlandite produced during cement hydration leads to the formation of Si-rich C(A-)S-H, which is more resistant to sulfate attack [5,7]. Due to the aluminum-rich composition of MK, additional calcium aluminate hydrates form during hydration, while aluminum is incorporated in the silicate chains of cement hydrates. AH was used for comparison with MK, i.e., to "exclude" the effect of silicon. Silicon-rich nature will differentiate the FTIR signal of Si-O-Si/Si-O-Al bonds in the C-(A-)S-H. The hydration is affected because of the use of MK/AH. The understanding of the hydration process of the used binders is a key to assess the final durability properties.

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P.72 Influence of limestone as main constituent in Portland cement on the chloride ingress in pastes exposed to sulfate-chloride solution assessed by *P.68* Raman and NMR spectroscopy

P.Mácová[1], K.Sotiriadis[1], A.S.Mazur[2] and P.M. Tolstoy[2]

[1] Institute of Theoretical and Applied Mechanics of the Czech Academy of Sciences, Prosecká 809/76, CZ-19000 Prague, Czech Republic

[2] St. Petersburg State University, Center for Magnetic Resonance, Universitetsky pr. 26, RU-198504 Petergof, St. Petersburg, Russia

E-mail: macova@itam.cas.cz

The durability of cementitious materials in aggressive environments is of significant concern in civil engineering practice [1–3]. This study aims to investigate the microstructural changes occurring in two different cement pastes made from type CEM I ordinary Portland cement (PC) and type CEM II/B-LL Portland limestone cement (PLC), during exposure to sulfate-chloride solution and, therefore, assess the chloride ingress in relation to the presence of limestone in the cement. The cylindrical specimens were exposed to a sulfate-chloride solution and a solution containing only chlorides for 5 months at low temperature (5℃). Subsequently, the changes in microstructure at different depths were analysed using micro-Raman spectroscopy, ^{29}Si solid-state nuclear magnetic resonance (ss NMR) spectroscopy, and X-ray powder diffraction (XRPD).
The results revealed notable variations among the different combinations of cements and corrosive environments. The distribution of phases within the hydrated pastes shows significant influence of the presence of limestone in cement and sulfates in the corrosive solution closer the specimen's surface, indicating degradation of main binding phase (C−S−H) and the formation of crystalline products (gypsum, ettringite, thaumasite, Friedel's salt).
The findings highlight the influence of Ca/Si ratio of the cement used, and the presence of sulfates in the solution on the resistance against chloride ingress.

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P.73 Optical properties of carbon dots derived from *Posidonia oceanica*

S. Katsantonis[1] and K. V. Kordatos[1]

[1]School of Chemical Engineering, Department of Chemical Sciences, National Technical University of Athens, 9 Iroon Polytechniou Str., 15780 Athens, Greece

E-mail: spyroskatsantonis@mail.ntua.gr

Posidonia oceanica is a seagrass species that is encountered in the Mediterranean Sea and is characterized by long strip-like leaves. The leaves of *Posidonia oceanica* are a great source of carbon, since they mainly consist of structural carbohydrates (cellulose, hemicellulose) and lignin. The aim of this work is the synthesis of carbon dots (CDs) from *Posidonia oceanica* leaves and the investigation of their optical properties. CDs are a class of carbon nanomaterials with size less than 10 nm and possess many functional groups on their surface. Different types of CDs were successfully synthesized via a hydrothermal method using various quantities of lignocellulose, which was isolated from *Posidonia oceanica* leaves. The synthesized materials were characterized using a variety of instrumental methods of analysis, including Ultraviolet-Visible spectrometry (UV-Vis), Photoluminescence (PL) and FourierTransform Infrared spectroscopy (FT-IR).