Organized by

University of Ioannina

National Technical University of Athens

20 years

IMA-2019

11th International Conference on Instrumental Methods of Analysis

Modern Trends and Applications

www.ima2019.gr

22-25 September 2019

Grand Serai Hotel

Ioannina, Greece

Abstract Book

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PREFACE

The organizing committee of the IMA-2019 Conference would like to welcome all participants to the 11th International Conference on "Instrumental Methods of Analysis-Modern Trends and Applications", held in Ioannina, Greece, from 22-25 September. The conference is organized by the Department of Chemistry, University of Ioannina and the Lab of Inorganic and Analytical Chemistry, School of Chemical Engineering of the National Technical University of Athens. IMA is a biannual series of conferences that started 20 years ago in 1999 and covers all areas of modern trends and applications of chemical analysis.

During this meeting special emphasis will be given to new developments in analytical instrumentation and novel methods, techniques and applications of chemical analysis. Current analytical trends will be revealed through presentations covering a wide range of techniques in the areas of spectroscopy, atomic and molecular mass spectrometry, electrochemical analysis, chromatographic separations, sensors etc. The trend of using hyphenated techniques along with chemo-metric treatment of complex analytical data has unfolded new perspectives and challenges in chemical analysis, dealing with difficult problems related to modern materials, biological systems, food and environmental micro-pollutants of eco-toxicological interest. Due to the current increasing chemical analysis needs and requirements in the field of Food Science and Technology including quality assurance, safety, authentication and nutritional value, this year's conference will continue to emphasize novel aspects of food analysis research and a **special session is organized by the FoodOmicsGR Research Infrastructure**. Another two special sessions are devoted to state-of the art topics of **Aerosol metrology and X-ray spectroscopy techniques** organized by the **AEROMET EMPIR EURAMET** project and under the auspices of the **EUROPEAN X-RAY SPECTROSCOPY ASSOCIATION (EXSA)**, respectively, where young scientists participating at IMA2019 will receive special awards for their contribution in these fields.

The scientific program includes invited lectures given by outstanding scientists and, oral and posters contributions from researchers from Academia, Research Institutes and the Industry. The program consists of 13 invited and plenary lectures, 15 sessions with oral presentations and close 130 posters in 2 poster sessions. An exhibition of analytical and laboratory equipment will also take place parallel to the conference. At the same time a cultural program with visits to the Castle of Ioannina and Silversmithing Museum, as well as a visit to the traditional village of Metsovo and the lake of Ioannina will render the participants' stay more interesting and enjoyable.
Participants are invited to submit their papers related to their contribution in one of the following scientific journals: *Analytical and Bioanalytical Chemistry, Analyst, Metals, Open Agriculture, Open Chemistry with reference to IMA2019.*

We strongly believe that the discussions and the exchange of ideas among the participants during the 4 days of the conference will make IMA2019 a brilliant platform to initiate new research collaborations, particularly in favor of the young scientists participating in the conference.

We hope you all enjoy the conference and have a memorable stay in Ioannina, looking forward to meet you again at the next IMA2021.

With our best regards

Prof. Triantafyllos A.D. Albanis
Lab. of Analytical & Environmental Chemistry
Department of Chemistry
University of Ioannina

Prof. Maria Ochsenkühn-Petropoulou
Lab of Inorganic and Analytical Chemistry
School of Chemical Engineering
National Technical University of Athens

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The 11th International Conference "IMA 2019-Instrumental Methods of Analysis-Modern Trends and Applications" 22-25 September 2019, Ioannina, Greece is a 4-days scientific meeting covering all areas of modern trends and applications of Chemical Analysis. For the last 20 years IMA has provided an excellent framework for the presentation of new concepts, instruments, methods, systems, and applications in the area of modern chemical analysis. Researchers and scientists from Universities, Research Institutions, State Organizations, and the Industry come together during the meeting to present and discuss the current state of the art in the area of instrumental methods of analysis. At the same time, it provides the grounds for the graduate and post graduate students to present their projects, discuss scientific collaborations with other groups, as well as to explore employment opportunities. An exhibition of analytical instruments and accessories will be also organized in the conference place whereas a number of excursions, tours and social events are included in the program of the IMA 2019.

Topics

Some of the general themes to be covered at IMA-2019 include current trends, developments and applications in:

* Spectrochemical, Electrochemical, Chromatographic, Mass Spectrometric, Microscopic, Imaging and Thermal analysis methods,
* Proteomics, Metabolomics, Metallomics and Elemental Speciation Analysis,
* Chemical- and bio- sensors,
* Field analysis - Mobile analytical instruments,
* Miniaturized analytical systems (Lab-on-a-Chip), micro- and nano- fluidics,
* Immunoassays, Electrophoretic separation techniques,
* Robotics and Automation, Quality control-quality assurance in analysis, Metrology
* Data processing and Chemometrics
* Aerosol Metrology, Environmental, Biomedical (Eco-toxicological, Clinical), Pharmaceutical, Food, and Materials Analysis (Nanomaterials, Smart/ Advanced Materials, Surface Analysis), as well as Archaeometry,
* Analytical chemistry markets and possibilities for commercialization.

Oral presentations

The Scientific Program will include oral presentations and plenary lectures, which will provide an up-to-date presentation of modern trends of Instrumental Methods of Analysis as well as of related subjects of general interest.

Duration of Presentations

- Invited and plenary speakers should plan on a **25 minute long talk** followed by **5 minutes for discussion.**
- For all other oral presentations: presenting authors should plan on a **13 min talk** followed by **2 min for questions and discussion.**

Preparation of Presentations

Presentations should be in Microsoft PowerPoint format (ppt or pptx file) or Adobe Acrobat Reader format (pdf file). Preferably, the widescreen ratio (16:9) should be used. The file should be electronically handed by the speaker to the Slide Reception **at least one session** before his/her presentation.

Poster presentations

Contributed papers describing original research work will be also presented as posters in order to promote efficient discussion on new scientific ideas and results. The presenting authors should **hang their posters in the morning** of their presentation in the **parallel hall "Lord Byron"** and **remove them at the end of the poster session**. The preferable dimensions for posters should be 80 cm x 120 cm (width x height). All posters are required to conform to portrait orientation. Type size should be sufficiently large to allow people to read from 2-3 meters. Posters should be clear and easy to read.

All presentations should be in **English**. Poster and oral presentation will be accepted if **at least one of the authors is registered and present** at the conference for personal communication.

Previous conferences

The past conferences were held in Chalkidiki (1999), Ioannina (2001), Thessaloniki (2003), Iraklion (2005), Patras (2007), Athens (2009), Chania (2011), Thessaloniki (2013), Kalamata (2015) and Heraklion (2017) with 250-300 scientific papers presented by scientists from all over the world at each one.

Best Oral & Poster awards

A competition for the best oral and best poster among the young scientists of the scientific sessions will also take place. These awards will be given to recognize excellence in research and presentation. European X-Ray Spectroscopy Association (EXSA) will also award exceptional contributions to the field of X-ray spectrometry apart from supporting the participation of young scientists in the conference. The winners will be announced during the Closing Ceremony on 25th September at noon.

Journal publication

Participants are invited to submit manuscripts based on their presentations in one of the following journals:

- Analytical and Bioanalytical Chemistry
- Analyst
- Metals
- Open Agriculture
- Open Chemistry

e-Abstract Book

All abstracts of the oral and poster presentations will be included in the e-Abstract Book, which will be available on the conference website: **www.ima2019.gr**.

Venue

IMA-2019 takes place at Grand Serai Hotel, a genuine palace, which combines the traditional style of Ioannina with elements of the Middle East. Ideally positioned in the heart of the city of Ioannina, it is the perfect starting point to discover Ioannina and its many historic monuments and museums, all, within easy reach of the business and commercial district. The Grand Serai Hotel built on a land of 13.000 sq.m, comes to offer a brand new perception of hospitality.

GRAND SERAI HOTEL
Dodonis 33, 45332, Ioannina, Greece
Tel.: +30 2651 0 90550
Website: http://www.grandserai.com

Exhibition

Suppliers of analytical instrumentation and laboratory equipment will exhibit their latest offerings in the Exhibition Area during the Conference. Official opening of the exhibition will take place on 23rd September at 19:00. The exhibition area is outside the lecture area and within the coffee break and lunch areas in the Conference Center of Grand Serai Hotel.

Social Events

Opening Ceremony: 22/9/2019 Grand Serai Hotel, 18.00

Welcome Reception: 22/9/2019 Grand Serai Hotel, 20.30
A get-together Cocktail Reception will take place at Grand Serai Hotel upon completion of the program.

Conference dinner: 24/9/2019 Frontzou Politeia Restaurant, Departure: Grand Serai Hotel, 20:30
The conference dinner celebrating the 20 years of IMA, will be held on September 24th at 21.00 at Frontzou Politeia Restaurant located 2km from the Conference Venue. (Includes transfer from-/to- Grand Serai Hotel)

Half-day tour in Ioannina: 25/9/2019 Departure: Grand Serai Hotel, 14.00 Return: approximately 17:30
(Optional, minimum number of participants required. Info desk available at the Conference Area)
A guided tour around the most important sites of both historical and cultural importance of Ioannina: The Castle of Ioannina, the Byzantine museum and the Silversmithing Museum. (Transfer is included, official English speaking guide and escort)

All day tour to Metsovo: 26/9/2019 Departure: Grand Serai Hotel, 08.30
Return: approximately 17:30

(Optional, minimum number of participants required. Info desk available at the Conference Area)

A post-Conference excursion by bus to the famous traditional village of Metsovo 30 minutes away from Ioannina city. Our guide will walk you to the Averoff Museum and then to Katogi Averof, a local winery where you can have a tour and finally wine degustation in the winery atmospheric cellar. (Transfer is included, official English speaking guide and escort)

Closing Ceremony: 25/9/2019 Grand Serai Hotel, 12.45

Name Badge

All Participants upon confirmation of their registration at the Secretariat will be provided with a **unique Name Badge**. Your personal name badge is your passport to the scientific sessions according to your registration and the exhibition area. All participants are required to wear their badges (visibly) during all sessions. Make sure you will not forget to take always with you this unique name badge.

Certificate of Attendance

All registered participants are entitled to receive a Certificate of Attendance. The **Certificates will be provided electronically** only upon completion of the electronic Evaluation Form. The certificate will be available electronically through the official website of the Conference **(www.ima2019.gr)** using the provided registration barcode.

Liability and Insurance

The Organizers as well as the Organizing-Administrative Bureau of IMA 2019 will assume no liability for injuries or losses of any nature incurred by participants and/or accompanying persons, or for the damage, loss or theft of their personal property during the Conference. Participants are advised to take out their own health, travel and personal insurances.

Organizing-Administrative Bureau/Secretariat

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PROGRAM AT A GLANCE

Sunday, September 22nd 2019

Evergeton Hall	16.30-20.30	Registration
	18.00-20.30	Opening session
	18.00-18.30	Opening Ceremony
	18.30-20.30	Plenary lectures
	20.30	Welcome Reception

Monday, September 23rd 2019

Evergeton Hall	08.15-09.00	Registration
	09.00-09.30	Invited Lecture
	09.30-10.45	X-ray Analysis 1
	10.45-11.30	***Coffee break***
	11.30-12.00	Invited Lecture
	12.00-13.15	**Parallel Sessions**
Evergeton Hall		Food Analysis
Lord Byron Hall		Foodomics
	13.15-14.15	***Lunch***
Lord Byron Hall	14.15-15.15	POSTER SESSION 1 - EXHIBITION
Evergeton Hall	15.15-15.45	Invited Lecture
	15.45-16.45	**Parallel Sessions**
Evergeton Hall		Mass spectrometry
Lord Byron Hall		Metabolomics
Evergeton Hall	***16.45-17.15***	***Coffee break***
	17.15-17.45	Invited Lecture
	17.45-18.30	ICP - MS
Lord Byron Hall	18.30-19.30	POSTER SESSION 1
	19.00	OPENING OF THE EXHIBITION

Tuesday, September 24th 2019

Evergeton Hall	08.15-09.00	Registration
	09.00-09.30	Invited Lecture
	09.30-10.45	**Parallel Sessions**
Evergeton Hall		Chromatography 1
Lord Byron Hall		Sample Handling / Mobile Instruments
	10.45-11.30	***Coffee break***
Evergeton Hall	11.30-12.00	Invited Lecture
	12.00-13.00	**Parallel Sessions**
Evergeton Hall		Materials / Sensors
Lord Byron Hall		Spectrometry 1
	13.00-14.15	***Lunch***
Lord Byron Hall	14.15-15.15	POSTER SESSION 2 – EXHIBITION
Evergeton Hall	15.15-15.45	Invited Lecture
	15.45-16.45	Aerosol Metrology / X-Ray Analysis 2
	16.45-17.15	***Coffee break***
Evergeton Hall	17.15-18.30	Aerosol Metrology / X-Ray Analysis 3
Lord Byron Hall	18.30-19.30	POSTER SESSION 2 - EXHIBITION
	21.00	***CONFERENCE DINNER***

Wednesday, September 25th 2019

Evergeton Hall	08.30-09.00	Registration
	09.00-09.30	Invited Lecture
	09.30-10.30	Chromatography 2 / Spectrometry 2
	10.30-11.00	***Coffee break***
	11.00-11.30	Invited Lecture
	11.30-12.45	Electrochemistry / Archaeometry
	12.45-13.30	Closing Ceremony / Awards
	14.00-17.30	Excursion - Castle-Museums-Ioannina

Thursday, September 26th 2019

	08.30-17.30	Post-Conference Excursion - Metsovo

DETAILED PROGRAM

Sunday, September 22nd 2019

Evergeton Hall

16.30-20.30	Registration
	Opening Session
	T. Albanis, M. Ochsenkühn
18.00-18.30	Opening Ceremony
18.30-20.30	**Plenary Lectures**
	Chair: ***T. Albanis, M. Ochsenkühn***
18.30-19.00	The Evolution of Analytical Atomic Spectrometry ***Sir L. Ebdon***
19.00-19.30	ONE HUNDRED AND FIFTY YEARS OF THE PERIODIC TABLE: Dmitri Mendeleev is recognized as a discoverer and inventor, Chemists become "prophets", and the "entropy" of the chemical knowledge is diminishing ***M. Karayannis***
19.30-20.00	Instrumental Analysis: Dilemmas and Responsibility ***I. Brceski***
20.00-20.30	Ethics in Chemistry and Science: Is it Useful? ***H. Frank***
20.30	***Welcome Reception***

Monday, September 23rd 2019

Evergeton Hall

08.15-09.00		Registration
09.00-09.30		**Invited Lecture** Chair: ***B. Beckhoff, Sir L. Ebdon*** Instrumentation Science: The Third Side of Analytical Chemistry ***G. Hieftje***
09.30-10.45		**Oral Session: X-Ray Analysis 1** Chair: ***B. Beckhoff, Sir L. Ebdon***
09.30-09.45	**OP01**	SYNCHROTRON RADIATION TXRF: STRENGTHS AND CHALLENGES ***D. Eichert***
09.45-10.00	**OP02**	DEVELOPMENTS IN X-RAY DIFFRACTION TECHNOLOGY ***I. Hegedues***
10.00-10.15	**OP03**	IMMOBILIZATION OF HEAVY METALS IN DRINKING WATER: THE ROLE OF METAL (OXY)HYDROXIDES ON SORPTION MECHANISM USING X-RAY ABSORPTIONSPECTROSCOPIES ***F. Pinakidou, M. Katsikini, K. Simeonidis, E. C. Paloura, M. Mitrakas***
10.15-10.30	**OP04**	PORTABLE XRF SPECTROMETRY IN THE FIELD OF CULTURAL HERITAGE ***M. Kaparou, H. Brekoulaki, C. Caliri, S. Fotiou, R. Grethe, V. Kantarelou, E. Kokiasmenou, M. Kontimpa, G. Mastrotheodoros, D. Papadopoulou, F. P. Romano, K. Tsampa, A. G. Karydas***
10.30-10.45	**OP05**	ADVANCES IN X-RAY TECHNOLOGY FOR MATERIALS ANALYSIS ***E. Klothakis***
10.45-11.30		***Coffee break***
11.30-12.00		**Invited Lecture** Chair: ***I. Brceski, V. Sakkas*** Using Instrumental Analysis for Determining Food Authenticity, Adulteration and Food Safety ***I. Malollari***

	12.00-13.15		Parallel Sessions
Evergeton Hall			**Oral Session: Food analysis** Chair: ***I. Brceski, V. Sakkas***
	12.00-12.15	OP06	IDENTIFICATION OF BIO-PHENOLIC PROFILE OF SELECTED NATIVE MONOVARIETAL AND BLENDED FRESHLY PREPARED FRUIT JUICES USING CHROMATOGRAPHIC TECHNIQUES ***J. Llupa, K. Akrida-Demertzi, U. Gašić, D. Topi, P. Demertzis***
	12.15-12.30	OP07	OPTICAL SPECTROSCOPY TECHNIQUES FOR THE CLASSIFICATION AND QUALITY CONTROL OF AGROFOODS ***E. Orfanakis, N. Fragkoulis, R. Kontzedaki, A. Filippidis, A. Zoumi, M. Velegrakis***
	12.30-12.45	OP08	IMMUNOCHEMICAL CONTROL OF RAW MATERIALS' SOURCES IN THE PRODUCTION OF MEAT AND DAIRY FOOD ***E.A. Zvereva, N.I. Smirnova, A.V. Zherdev, B.B. Dzantiev***
	12.45-13.00	OP09	DETERMINATION OF BISPHENOL A IN FOOD SIMULANTS A, B, C AND D1 PERFORMED BY HPLC - FLD AND VALIDATION OF THE METHOD ***K. Nana, C. Proestos, E. Komaitis***
	13.00-13.15	OP10	COMBINED EFFECT OF GASEOUS OZONE AND CITRIC ACID TREATMENT ON QUALITY CHARACTERISTICS AND SHELF LIFE OF PACKAGED FRESH-CUT LETTUCE PRESERVED UNDER REFRIGERATED CONDITIONS ***A. Panou, K. Akrida - Demertzi, P. Demertzis, K. Riganakos***
Lord Byron Hall			**Oral Session: Foodomics** Chair: ***G. Theodoridis, I. Konstantinou***
	12.00-12.20	OP11	FoodOmicsGR NATIONAL RESEARCH INFRASTRUCTURE FOR THE COMPREHENSIVE CHARACTERISATION OF FOODS ***A. Pechlivanis, G. Theodoridis***
	12.20-12.40	OP12	HIGH RESOLUTION MASS SPECTROMETRIC FOODOMICS: FROM BASIC RESEARCH TO INDUSTRIAL APPLICATIONS ***N. Thomaidis***
	12.40-12.55	OP13	FOODOMICS APPROACH TO ASSESS FOOD AUTHENTICITY. TWO PARADIGMS ON GRAPES AND ROYAL JELLY SAMPLES ***C. Virgiliou, D. Kanelis, K. Liva, M. Marinaki, H. Gika, A. Asimopoulou, C. Tananaki, G. Theodoridis***
	12.55-13.10	OP14	HRMS STUDY OF BIOACTIVITY COMPOUNDS DURING EDIBLE OLIVE PROCESSING ***P. Katsianou, G. Koulis, M. Dasenaki, N. Thomaidis***
	13.15-14.15		***Lunch***

Lord Byron

14.15-15.15 **POSTER SESSION 1** *(details in p.17-21)*

P1 01-62 Bioanalytics / Chemometrics / Food Analysis / Foodomics / Mass spectrometry / Metabolomics / X-ray spectroscopy

EXHIBITION

Evergeton

15.15-15.45 **Invited Lecture**

Chair: ***H. Frank, S.A. Pergantis***

Advances in High Resolution Mass Spectrometry for Metal Speciation Analysis

R. Lobinski

15.45-16.45 **Parallel Sessions**

Evergeton Hall

Oral Session: Mass Spectrometry

Chair: ***H. Frank, S.A. Pergantis***

15.45-16.00 **OP15** MASS SPECTROMETRY TECHNIQUES IN FORENSIC TOXICOLOGY
V. Boumba

16.00-16.15 **OP16** DETAILED PHYTOCHEMICAL ANALYSIS OF AN ARTEMISIA ANNUA AND AN ARTEMISIA ABSINTHIUM EXTRACT USING A COMBINATION OF NMR AND HPLC/DAD/MS TECHNIQUES
V.G. Kontogianni, M. Sakka, A. Primikyri, I.P. Gerothanassis

16.15-16.30 **OP17** DETERMINATION OF POLYCHLORINATED BIPHENYLS IN MUSSELS USING QUECHERS IN COMBINATION WITH GC-MS
E. Trantopoulos, V. Boti, T. Albanis

16.30-16.45 **OP18** MAGNETIC SOLID-PHASE EXTRACTION OF PESTICIDES IN NATURAL WATERS USING Fe3O4@SiO2@C18 NANOPARTICLES AS ADSORBENT COUPLED TO GC-MS DETERMINATION
M. Kapsi, V. Sakkas, T. Albanis

Lord Byron Hall

Oral Session: Metabolomics

Chair: ***J. Szpunar, I. Malollari***

15.45-16.15 **OP19** NMR IN NATURAL PRODUCTS: CHEMICAL ANALYSIS OF COMPLEX MIXTURES, BIOANALYTICAL AND METABOLOMICS APPLICATIONS AND DFT NMR STRUCTURES OF ANALYTES
I. Gerothanassis

16.15-16.30 **OP20** NMR-BASED METABOLOMICS OF THE LIPID FRACTION OF ORGANIC AND CONVENTIONAL BOVINE MILK
C. Tsiafoulis, C. Papaemmanouil, D. Alivertis, S. Balayssac, O. Tzamaloukas, M. Malet-Martino, I. Gerothanassis

16.30-16.45 **OP21** UN-TARGETED METABOLOMICS APPROACH FOR THE CHARACTERIZATION, CLASSIFICATION AND MAPPING OF BIOACTIVE COMPOUNDS IN GREEK EXTRA VIRGIN OLIVE OIL
S. Drakopoulou, M. Dasenaki, R. Aalizadeh, A. E. Manola, K. Nikolakis, N. Thomaidis

Evergeton Hall

16.45-17.15 ***Coffee break***

17.15-17.45 **Invited Lecture**

Chair: ***G. Hieftje, N. Thomaidis***

ICP/Electrospray Mass Spectrometry for Studies of the Uptake and Metabolism of Nanoparticles

J. Szpunar

17.45-18.30 **Oral Session: ICP-MS**

Chair: ***G. Hieftje, N. Thomaidis***

17.45-18.00 **OP22** ADVANCEMENTS AND CHALLENGES FOR THE DETERMINATION OF METALS IN INDIVIDUAL CELLS USING SINGLE CELL INDUCTIVELY COUPLED PLASMA – MASS SPECTROMETRY

E. Mavrakis, N. Lydakis-Simantiris, S. A. Pergantis

18.00-18.15 **OP23** SINGLE PARTICLE AND SINGLE CELL ICP-MS ALLOW NEW INSIGHTS TRACKING NANOPARTICLE FATE AND ECOLOGICAL EFFECTS

H. Ernstberger, C. Stephan

18.15-18.30 **OP24** IMPROVEMENTS AND APPLICATIONS OF A NOVEL ORTHOGONAL SONIC-SPRAY IONIZATION SOURCE FOR COUPLING MICROBORE AND CONVENTIONAL HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY TO TANDEM MASS SPECTROMETRY

S. Grafanaki, S. A. Pergantis

Lord Byron

18.30-19.30 **POSTER SESSION 1** *(details in p.17-21)*

P1 01-62 Bioanalytics / Chemometrics / Food Analysis / Foodomics / Mass spectrometry / Metabolomics / X-ray spectroscopy

19.00 **OPENING OF THE EXHIBITION**

POSTER SESSION 1 • P1-01 – P1-62

Bioanalytics / Chemometrics / Food Analysis / Foodomics / Mass spectrometry / Metabolomics / X-ray spectroscopy

P1-01 PREPARATION OF NANOCERIA CONJUGATES FOR BIOANALYTICAL ASSAYS
I. P. Gkini, T. K. Christopoulos

P1-02 CHEMICAL COMPOSITION AND EVIDENCE FOR A SELECTIVE ANTICANCER ACTIVITY OF HELLEBORUS CYCLOPHYLLUS BOISS ON A549 CANCER CELL LINE
P. Yfanti, A. Karkabounas, A. Batistatoy, M. E. Lekka

P1-03 A NOVEL ELECTROCHEMICAL SENSOR BASED ON REDUCED GRAPHENE OXIDE AND MOLECULAR IMPRINTED OVER-OXIDIZED POLYPYRROLE MODIFIED GOLD NANOPARTICLES FOR AMOXICILLINE DETECTION
H. Essousi, H. Barhoumi, S. Karastogianni, S. Girousi

P1-04 DETECTION OF MYCOBACTERIUM AVIUM SUBSPECIES PARATUBERCULOSIS IN INFANT FORMULAS BY CULTURE, PCR AND COMBINED PHAGE-PCR
G. Botsaris, M. Christodoulou, C. Rees

P1-05 INORGANIC ANALYSIS OF TEA SAMPLES USING ENERGY-DISPERSIVE X-RAY FLUORESCENCE SPECTROMETRY AND MULTIVARIATE VARIANCE ANALYSIS
M. Musielak, R. Sitko, B. Walczak

P1-06 FT-IR SPECTROSCOPY IN COMBINATION WITH CHEMOMETRICS FOR THE DETERMINATION OF THE GEOGRAPHICAL ORIGIN OF EXTRA VIRGIN OIL
E. Kakouri, P.K. Revelou, N.S. Sotiropoulou, Ch. Kanakis, C. Pappas, P.A. Tarantilis

P1-07 SPECTROSCOPIC-CHEMOMETRIC METHOD FOR THE INVESTIGATION OF HONEY BOTANICAL ORIGIN
N.S. Sotiropoulou, M. Xagoraris, E. Kakouri, P.K. Revelou, C. Kanakis, C. Pappas, P. A. Tarantilis

P1-08 CHEMISTRY STUDENT'S KNOWLEDGE AND AWARENESS ABOUT BASIC FOOD CONSTITUENTS, THEIR FEATURES AND ROLE
C. Piperidi, K. Akrida-Demertzi, P. Demertzis, G. Tsaparlis

P1-09 EFFECT OF NATURAL PRODUCTS AGAINST FOODBORNE PATHOGENS
C. Michael, G. Botsaris, A. Chrysargyris, V. Goulas, N. Tzortzakis

P1-10 APPLICATION OF MYCOBACTERIOPHAGE FOR RAPID DETECTION AND BIOLOGICAL CONTROL OF MYCOBACTERIA IN DAIRY PRODUCTS: THE CASE OF PARATUBERCULOSIS
N. Markantonis, G. Botsaris

P1-11 IMPROVEMENT OF THE QUALITY OF A GREEK DISTILLATE (TSIPOURO) FROM GRAPES OF THE DEBINA VARIETY WITH THE ADDITION OF SELECTED SUPERFRUITS
K. Gkougkoulis, K. Akrida- Demertzi, P. Demertzis

P1-12 EFFECT OF IRRIGATION ON THE BIOLOGICALLY ACTIVE COMPONENTS OF TOMATOES
R. Tömösközi-Farkas, B. Schmidt-Szantner, M. Nagy-Gasztonyi, P. Milotay

P1-13 A REAL-TIME PCR-BASED METHOD FOR THE IDENTIFICATION OF OLEA EUROPAEA var. SYLVESTRIS (WILD-TYPE OLIVE)
C. Kyriakopoulou, D. Kalogianni

P1-14 ASSESSMENT OF MILK PASTEURIZATION USING A SMARTPHONE OR A CONVENTIONAL DIGITAL CAMERA
A. Sevastou, S. S. Tragoulias, D. P. Kalogianni, T. K. Christopoulos

P1-15 SIMPLE ANALYTICAL METHODOLOGY FOR THE DETERMINATION OF NEONICOTINOID PESTICIDE RESIDUES IN HONEY SAMPLES
S. Pateras, C. Tsoutsi, T. Albanis

P1-16 GREEK HONEY AND MILK SPECTROSCOPIC ANALYSIS: BOTANICAL CLASSIFICATION, ORIGIN DISCRIMINATION AND ADULTERATION STUDIES
N. Fragkoulis, E. Orfanakis, M. Markoulidakis, A. Symianaki, A. Zoumi, M. Velegrakis

P1-17 SPECTROSCOPIC ANALYSIS OF GREEK EXTRA VIRGIN OLIVE OIL: ORIGIN DISCRIMINATION AND ADULTERATION STUDIES
R. Kontzedaki, G. Stavrakakis, G. Sofra-Karanti, E. Orfanakis, N. Fragkoulis, A. Filippidis, S. Mavrakaki, A. Stamataki, M. Velegrakis

P1-18 FATTY ACID PROFILING IN BLOOD OF HEALTHY INDIVIDUALS AND PATIENTS WITH HYPERLIPIDEMIA AND ASSOCIATION
T. Mouskeftara, A. Goulas, A. Asimopoulou, N. Raikos, G. Theodoridis, E. Gika

P1-19 PHYSICOCHEMICAL CHARACTERIZATION OF CASEIN MICELLES FOR NANOFORMULATIONS IN FOOD INDUSTRY
A. Papagiannopoulos, M. D.Charavgi, P.F. Karakousi, I. Tseti, E.D. Chrysina, S. Pispas

P1-20 METABOLOMIC APPROACH FOR GREEK HONEY ORIGIN DISCRIMINATION MAKING USE OF ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY COUPLED TO HIGH RESOLUTION MASS SPECTROMETRY
G. Koulis, P. Katsianou, E. Panagopoulou, C. Proestos, N. Thomaidis

P1-21 SINGLE PARTICLE ICP-MS: NEW PEAK IDENTIFICATION APPROACH FOR ULTRAFAST MEASUREMENT
M. Loula, A. Kana, O. Mestek

P1-22 DETERMINATION OF MACRO- AND MICROELEMENT CONCENTRATIONS IN COAL AND ASH SAMPLE BY ICP-MS
V. Lyubomirova, V. Mihaylova, B. Zlateva, B. Todorov, R. Djingova

P1-23 PHOTOLYTIC AND PHOTOCATALYTIC DEGRADATION OF FUROSEMIDE: KINETICS, IDENTIFICATION OF TRANSFORMATION PRODUCTS AND REACTION PATHWAYS USING LIQUID CHROMATOGRAPHY-ACCURATE MASS SPECTROMETRY (UPLC-MS/MS-LTQ-ORBITRAP)
G. Koutsikou, I. Konstantinou

P1-24 PHARMACEUTICAL RESIDUES IN HOSPITAL WASTEWATERS USING LIQUID CHROMATOGRAPHY COUPLED TO HIGH-RESOLUTION MASS SPECTROMETRY
M. Kapsi, P. Konstas, E. Trantopoulos, Ch. Kosma, A. Karkabounas, V. Boti, I. Konstantinou, T. Albanis

P1-25 COUPLING LIBS TO SSI-MS. INTERFERENCE OF PLASMA FORMATION WITH MASS ANALYSIS
K. Marmatakis, S. A. Pergantis, D. Anglos

P1-26 IN-DEPTH INVESTIGATION OF THE OCCURRENCE OF PER- AND POLYFLUORINATED SUBSTANCES IN TOP PREDATORS AND THEIR PREY EMPLOYING HIGH-RESOLUTION MASS Spectrometry
A. Androulakakis, N. Alygizakis, G. Gkotsis, V. Nikolopoulou, M.-C. Nika, A. Cincinelli, R. Dekker, G. Duke, N. Glowacka, B. Knopf, J. Koschorreck, T. Martellini, P. Movalli, H. Ruedel, R. Shore, G. Treu, J. Slobodnik, N. Thomaidis

P1-27 APPLICATION OF SINGLE PARTICLE INDUCTIVELY COUPLED PLASMA - MASS SPECTROMETRY FOR THE DETECTION AND CHARACTERIZATION OF METAL-CONTAINING NANOPARTICLES IN SEAWATER SAMPLES
M.I. Chronakis, M. Mavrakis, S.A. Pergantis, R.Á. Fernández García, M. Montes - Bayón, J. Bettmer, A. Tsiola, A. Gondikas, M. Tsapakis

P1-28 EVALUATION OF ADVANCED DRINKING WATER TREATMENT PROCESSES BY A COMBINATION OF POWERFUL MASS SPECTROMETRIC TECHNIQUES AND EPR SPECTROSCOPY
M. Antonopoulou, N. Ioannidis, C. Avagianos, T. Kaloudis, T. Triantis, A. Hiskia

P1-29 DETERMINATION OF 12 PHTHALATE ESTERS IN GREEK GRAPE MARC SPIRITS BY LIQUID CHROMATOGRAPHY TANDEM MASS SPECTROMETRY
D. Diamantidou, O. Begou, H. Gika, E. Tsochatzis, S. Kalogiannis, N. Kataiftsi, E. Soufleros, G. Theodoridis, A. Zotou

P1-30 BUILDING A LOCAL LIBRARY OF REFERENCE HPLC CHROMATOGRAMS AND QTOF-MS MASS SPECTRA USING THE MSMLS KIT
D. Diamantidou, P. Katechis, E. Lazaridou, H. Gika, G. Theodoridis

P1-31 ANALYSIS AT TRACE LEVELS OF POLYCHLORINATED BIPHENYLS IN ENVIRONMENTAL WATER SAMPLES BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY
P. Siachoulis, V. Boti, T. Albanis

P1-32 DETERMINATION OF NITROFURAN METABOLITES IN FISH SAMPLES BY MEANS OF LIQUID CHROMATOGRAPHY COUPLED TO HIGH-RESOLUTION-ORBITRAP MASS SPECTROMETRY
E. Trantopoulos, Ch. Kosma, A. Karkabounas, V. Boti, T. Albanis

P1-33 NOVEL MALDI-TOFMS-BASED METHODOLOGY FOR RAPID DETECTION OF PDO FETA CHEESE ADULTERATION
A. Kritikou, D. Damalas, I. Barla, C. Baessmann, N. Thomaidis

P1-34 NON-SPECTRAL INTERFERENCES IN SINGLE-PARTICLE ICP-MS
A. Kaňa, M. Loula, O. Mestek

P1-35 DETERMINATION OF RARE EARTH ELEMENTS OF HIGH CONTENTS IN RARE EARTH ORE USING 5-ACID DIGESTION BY ICP-MS
W. Myung Choi, C. Hun Eum

P1-36 DEVELOPMENT AND VALIDATION OF METHOD FOR DETERMINATION OF TREE NUT ALLERGENS WITH LC-MS/MS
K. Rodi, M. Kostakis, N. Thomaidis, G. Siragakis

P1-37 DEVELOPMENT OF A MULTI-RESIDUE METHODOLOGY FOR THE DETERMINATION OF VETERINARY DRUGS IN ANIMAL FEED BY RP-HPLC-MS/MS
A. Christopoulou, A. Kritikou, M. Dasenaki, N. Thomaidis

P1-38 MARKERS OF OXIDATIVE STRESS AND AMINOACIDS IN INFANT'S SERUM SAMPLES WITH URETEROPELVIC JUNCTION OBSTRUCTION BY STABLE - ISOTOPE DILUTION GC-MS WITH NEGATIVE CHEMICAL IONIZATION
O. Begou, A. Bollenbach, K. Drabert, A. Pavlaki, H. Gika, N. Printza, G. Theodoridis, D. Tsikas

P1-39 CHEMOMETRIC APPROACH TO THE OPTIMIZATION OF HS-SPME/GC-MS PARAMETERS FOR THE DETERMINATION OF MULTICLASS PESTICIDE RESIDUES IN FRUITS AND VEGETABLES
E. Ayeni Kikelomo, L. B. Abdulra'uf

P1-40 A GC-MS METHOD FOR THE DETERMINATION OF FIVE NPS IN WHOLE BLOOD AND THE DETECTION OF SIX NPS IN URINE
A. Alexandridou, T. Mouskeftara, E. Gika, O. Mastrogianni, A. Orfanidis, N. Raikos

P1-41 DETERMINATION OF ROYAL JELLY FREE FATTY ACIDS BY LIQUID CHROMATOGRAPHY-HIGH RESOLUTION MASS SPECTROMETRY
M. G. Kokotou, C. Mantzourani, R. Babaiti, G. Kokotos

P1-42 METABOLOMIC PROFILING OF ZEBRAFISH WITH NMR AND LC-MS/MS AFTER EXPOSURE TO NON-DOPED, N-DOPED AND N,S-DOPED CARBON NANODOTS
K. Pliatsika, T. Chatzimitakos, I. Chousidis, I. Leonardos, C. Stalikas

P1-43 UNTARGETED FECAL METABOLOMICS-BASED ANALYSIS OF CAROB TREATED RATS
O. Begou, O. Deda, H. Gika, I. Taitzoglou, N. Raikos, A. Agapiou, G. Theodoridis

P1-44 METABOLOMICS STUDY OF THE EFFECT OF TOLUENE ON PSEUDOMONAS POTIDA DOT-T1E STRAINS
A. Sayqal

P1-45 METABOLOMICS ANALYSIS FOR THE IN VITRO TOXICITY ASSESSMENT OF COCAINE IN HEPG2
A. Krokos, C. Virgiliou, H. Gkika, N. Raikos, E. Aggelidou, A. Kritis, G. Theodoridis

P1-46 TARGETED AND UNTARGETED METABOLOMICS OF MICE URINE AND FECAL SAMPLES, IN THE DISCOVERY OF ALCOHOL TOXICITY BIOMARKERS
C. Virgiliou, O. Deda, A. Orfanidis, H. Gika

P1-47 XRD CHARACTERIZATION OF CRYSTALLINITY AND PHASE COMPOSITION OF SUBFOSSIL HOLOCENE REINDEER BONES AND ANTLERS FROM THE UST'-POLUY ANCIENT SANCTUARY (WESTERN SIBERIA, RUSSIA)
A. Ryanskaya, D. Kiseleva, P. Kosintsev, O. Bachura, S. Votyakov, N.Fedorova, A. Gusev

P1-48 AN X-RAY SPECTROSCOPY STUDY ON THE MECHANISM OF SB(V) AND CR(VI) ADSORPTION BY TIN AND IRON OXY-HYDROXIDES
G. Papadopoulos, T. Asimakidou, D. Karfaridis, F. Pinakidou, K. Simeonidis

P1-49 EUROPEAN NETWORK FOR CHEMICAL ELEMENTAL ANALYSIS BY TOTAL REFLECTION X-RAY FLUORESCENCE
D. Eichert, L. Borgese

P1-50 NON-INVASIVE COMPOSITIONAL STUDY OF COPPER ALLOY VESSELS FROM THE ARCHAIC CEMETERY OF SINDOS IN THESSALONIKI
C. Katsifas, A. Touloumzidou, G. Zachariadis

P1-51 DEVELOPMENT AND VALIDATION OF A HPLC-PDA METHOD FOR THE DETERMINATION OF OLMESARTAN MEDOXOMIL.
T. Meikopoulos, E. Andriotis, D. Fatouros, N. Mavriki, C. Pourzitaki, G. Theodoridis, H. Gika

P1-52 LIQUID CHROMATOGRAPHY COUPLED TO QUADRUPOLE-ORBITRAP MASS SPECTROMETRY TO INVESTIGATE THE OCCURRENCE OF PHARMACEUTICAL RESIDUES IN NATURAL WATERS
V. Boti, D. Kifokeri, C. Nannou, T. Albanis

P1-53 DETERMINATION OF AMITRAZ, BROMOPROPYLATE, COUMAPHOS AND T-FLUVALINATE RESIDUES IN HONEY BY QUECHERS AND HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY-UV/DAD
E. Gotsi, V. Boti, T. Albanis

P1-54 A GC/MS METHOD FOR THE DETECTION AND QUANTIFICATION OF C12-16 ALKYLDIMETHYLAMINES IN HUMAN BLOOD
E. Brousa, O. Mastrogianni, A. Orfanidis, N. Raikos, H. Zagelidou

P1-55 VALIDATION AND APPLICATION OF METHOD FOR THE DETERMINATION OF PESTICIDE RESIDUES IN NATURAL WATERS AND SEDIMENTS, COUPLED TO GC-MS DETERMINATION
M. Kapsi, V. Sakkas, T. Albanis

P1-56 ANALYTICAL METHODS FOR THE DETECTION OF PHARMACEUTICALS AND THEIR METABOLITES IN SURFACE WATERS
A. Kalogeropoulou, Ch. Kosma, T. Albanis

P1-57 BIORECOVERY OF SCANDIUM AND OTHER RARE EARTH ELEMENTS FROM GREEK RED MUD
K. Kiskira, O. Serifi, G. Lytras, G. Lyberatos, M. Ochsenkuehn-Petropoulou

P1-58 DETERMINATION OF MAJOR ELEMENTS IN BULGARIAN BOTTLED MINERAL WATER
V. Lyubomirova, V. Mihaylova, B. Zlateva-Rangelova, R. Djingova

P1-59 A UHPLC-MS/MS METHOD FOR THE DETECTION AND QUANTIFICATION OF 84 DRUGS OF ABUSE AND PHARMACEUTICALS IN HUMAN BLOOD
A. Orfanidis, H. Gika, G. Theodoridis, O. Mastrogianni, N. Raikos

P1-60 AN EFFICIENT DLLME-GC-MS METHOD DEVELOPED FOR THE DETERMINATION OF MONOHYDROXY AND DIHYDROXY PAHs METABOLITES IN HUMAN URINE
S. Zichová, S. Hrouzková, T. Göen

P1-61 MODIFIED GRAPHENE OXIDE FOR RARE EARTH METALS' PRECONCENTRATION METHOD AFTER DISPERSIVE SOLID PHASE EXTRACTION AND OPTIMIZATION WITH CENTRAL COMPOSITE DESIGN
N. Manousi, E. Deliyanni, G. Zachariadis

P1-62 COMPARISON OF THE DATA OBTAINED BY XRF AND ICP-AES FOR ANALYSIS OF BELT ACCESSORIES DATED TO THE GREAT MIGRATION PERIOD IN BULGARIA
B. Zlateva, D. Lesigyarski, V. Mihaylova, V. Lyubomirova, R. Djingova, I. Kuleff, L. Vagalinski

Tuesday, September 24th 2019

Evergeton Hall

08.15-09.00 Registration

09.00-09.30 **Invited Lecture**

Chair: ***R. Lobinski, D. Hela***

A New Algorithm for Enhancing Chromatographic and Spectroscopic Measurements and Data Processing

E. Rosenberg

09.30-10.45 **Parallel Sessions**

Evergeton Hall

Oral Session: Chromatography 1

Chair: ***R. Lobinski, D. Hela***

09.30-10.00 **OP25** THE UTILITY OF HIGH RESOLUTION MASS SPECTROMETRY & INFORMATICS FOR NATURAL PRODUCT ANALYTICS
I. Riba

10.00-10.15 **OP26** ENHANCED VARIANTS OF MICROEXTRACTION PROCEDURES BASED ON MAGNETIC IONIC LIQUIDS
T. Chatzimitakos, J. Anderson, C. Stalikas

10.15-10.30 **OP27** SYNTHESIS OF AMBERLITE XAD-4 BASED METAL CHELATOR VIA ARYLDIAZONIUM RADICAL ROUTE FOR SOLID PHASE EXTRACTION OF HEAVY METALS FROM GROUNDWATER SAMPLES
A. Alsuhaimi

10.30-10.45 **OP28** FABRIC PHASE SORPTIVE EXTRACTION FOR THE DETERMINATION OF ANTIDEPRESSANT DRUGS IN ENVIRONMENTAL SAMPLES PRIOR TO HPLC-DAD
C. Jimenez Holgado, C. Chrimatopoulos, M. Kalaboka, V. Sakkas

Lord Byron Hall

Oral Session: Sample Handling/Mobile Instruments

Chair: ***J. Barek, M. Prodromidis***

09.30-09.45 **OP29** DNA HYBRIDIZATION ASSAYS AND QUANTITATIVE POLYMERASE CHAIN REACTION USING A SMARTPHONE AS A CHEMILUMINESCENCE IMAGER
P. Kalligosfyri, A. Sevastou, I. Kyriakou, S. Tragoulias, D. Kalogianni, T. Christopoulos

09.45-10.00 **OP30** FLUORESCENCE INSTRUMENTATION FOR RAPID, IN SITU WATER QUALITY ASSESSMENT
N. Adányi, M. Berki, É. Kónya, S. Klátyik, D. Lázár, B. Gémes, D. Csősz, S. Lenk, A. Barócsi, T. L. Csőke, A. Csákányi, L. Domján, G. Szarvas, L. Kocsányi, A. Székács

Lord Byron Hall

10.00-10.15	OP31	PORTABLE DIAGNOSTIC MEDICAL DEVICES UTILIZING FREE-STANDING RESPONSIVE POLYMER FILM-BASED BIOSENSORS AND LOW-COST TRANSDUCERS FOR POINT-OF-CARE APPLICATIONS ***E. Tzianni, J. Hrbac, D. K. Christodoulou, M. I. Prodromidis***
10.15-10.30	OP32	KINETIC STUDY OF PETROLEUM GENERATION USING OPEN-PYROLYSIS ROCK-EVAL ANALYTICAL SYSTEM ***K. Kokkinopoulou, N. Pasadakis***
10.30-10.45	OP33	THE STUDY OF MERCURY ACCUMULATION BY PLANTS DEPENDING ON ITS SPECIATION IN GROWING SUBSTRATE ***O. V. Shuvaeva, M. A. Gustaytis, A. Pohorukova***

Evergeton Hall

10.45-11.30		***Coffee break***
11.30-12.00		**Invited Lecture** Chair: ***I. Gerothanassis, K. Stalikas*** Synthesis Routes for the Preparation of Magnetic Nanoparticles for Health and Environmental Applications ***P. Morales***

12.00-13.00		**Parallel Sessions**

Evergeton Hall

Oral Session: Materials / Sensors

Chair: ***K. Stalikas, K. Simeonidis***

12.00-12.15	OP34	MICROFLUIDIC ANALYTICAL TOOL COUPLING A FLUORESCENT MOLECULAR PROBE AND A MICRO-HYDROCYCLONE FOR THE DETECTION OF WATER CHLORINATION LEVEL ***J. Bell, A. Tillo, J. Bartelmess, V. P. Chauhan, K. Rurack***
12.15-12.30	OP35	LABORATORY EVALUATION OF ULTRAMAFIC ROCKS EXPLOITATION TOWARDS THE PRODUCTION OF ADDED-VALUE PRODUCTS ***E. Tzamos, K. Simeonidis, E. Pagona, X. Ntampou, A. Zouboulis, M. Mitrakas***
12.30-12.45	OP36	LOW-COST "GREEN" SENSORS BASED ON GRAPHITE NANOMATERIALS PREPARED FROM PENCIL LEADS WITH THE AID OF A 3D POSITIONING SPARKING DEVICE FOR THE SENSITIVE DETECTION OF NITROAROMATIC EXPLOSIVES ***M.G. Trachioti, J. Hrbac, D. Hemzal, M.I. Prodromidis***
12.45-13.00	OP37	AUTOMATED INSPECTION OF PMMA COATING ON NON-PATTERNED SILICON WAFERS ***A. Knápek, M. Drozd, M. Matějka, J. Chlumská, S. Král, V. Kolařík***

Lord Byron Hall

Oral Session: Spectrometry 1
Chair: ***K. Valko, I. Gerothanassis***

12.00-12.15 **OP38** DIAGNOSTIC POTENTIAL OF FT-IR-BASED METABOLOMICS FOR THE AUTHENTIFICATION OF LAURUS NOBILIS L. ESSENTIAL OIL IS SUPPORTED BY GC-FID AND GC-MS ANALYSES
M. Papapostolou, S. Ordoudi, S. Kokkini, M. Tsimidou

12.15-12.30 **OP39** COMPARATIVE STUDY OF DATA OBTAINED FOR THE EFSA HEALTH CLAIM 'ON OLIVE OIL POLYPHENOLS' WITH A UHPLC-DAD- FLUORESCENCE PROTOCOL AND A 1H-NMR SPECTROSCOPY PROCEDURE
N. Nenadis, O. Winkelmann, A. Mastralexi, D.L. García-González, T. Gallina-Toschi, M.Z. Tsimidou

12.30-12.45 **OP40** THE LEAN WAY OF CLEANING PHARMACEUTICAL SOILS: A SPECTROSCOPY BASED APPROACH
A. Kumar, J.H. Hyslop, J.J. Leahy, S. Moore

12.45-13.00 **OP41** MONITORING BIOGAS REACTORS USING ANALYTICAL AND MOLECULAR TOOLS
P.G. Kougias, L. Treu, S. Campanaro, X. Zhu, I. Angelidaki

13.00-14.15 ***Lunch***

Lord Byron Hall

14.15-15.15 **POSTER SESSION 2** *(details in p.27-31)*

P2 01-61 Aerosol metrology / Archaeometry / Chemical- and bio-sensors / Chromatography / Environmental analysis / Materials / Mobile analytical instruments / Pharmaceutical analysis / Sample handling / Sensors / Spectrochemical analysis / Thermal analysis

EXHIBITION

Evergeton Hall

15.15-15.45 **Invited Lecture**
Chair: ***D. Eichert, P. Morales***
The EMPIR AEROMET project - dimensional and analytical aerosol metrology based upon different traceability chains
B. Beckhoff

Evergeton Hall

15.45-16.45 **Oral Session: Aerosol Metrology / X-Ray Analysis 2**

Chair: ***D. Eichert, P. Morales***

15.45-16.00 **OP42** QUANTITATIVE ELEMENTAL ANALYSIS OF AMBIENT AEROSOL PARTICLES USING PORTABLE TXRF
S. Seeger, B. Pollakowski-Herrmann, A. Gross, J. Osan, L. Stabile

16.00-16.15 **OP43** AEROMET - THE METROLOGY OF AMBIENT PARTICULATE METALS MEASUREMENTS AND THE EXAMPLE OF THE UK NATIONAL MONITORING NETWORK
S. Goddard, P. Quincey, L. Bregonzio-Rozier, P. Fisicaro, C. Oster, V. Gianotti, M. Laus

16.15-16.30 **OP44** AEROMET PROJECT - PROTOCOL DEVELOPMENT FOR HEAVY METALS ANALYSIS OF COLLECTED AEROSOLS SIZE FRACTIONS
L. Brégonzio-Rozier, C. Oster, P. Fisicaro, F. Gaie-Levrel, S. Goddard, P. Quincey, M. Ochsenkühn-Petropoulou, L.A. Tsakanika, T. Lymperopoulou, F. Tsopelas, K.M. Ochsenkuehn

16.30-16.45 **OP45** DEVELOPMENT AND CHARACTERIZATION OF AEROSOL REFERENCE MATERIALS FOR THE CALIBRATION OF NUCLEAR ANALYTICAL TECHNIQUES
M. Gini, M. Manousakas, V. Kantarelou, V. Vasilatou, M. Chiari, A.G. Karydas, K. Elefteriadis

16.45-17.15 ***Coffee break***

17.15-18.30 **Oral Session: Aerosol Metrology / X-Ray Analysis 3**

Chair: ***P. Morales, P. Quincey***

17.15-17.35 **OP46** LIGHT ABSORBING CARBON MEASUREMENTS ON ATMOSPHERIC AEROSOL PTFE FILTER SAMPLES BY THE MULTI-WAVELENGTH ABSORPTION BLACK CARBON INSTRUMENT (MABI).INTERCOMPARISON WITH OTHER MEASUREMENT TECHNIQUES
K. Eleftheriadis

17.35-17.45 **OP47** EXSA: European X-ray Spectrometry Association
D. Eichert

17.45-18.00 **OP48** DESIGN AND DEVELOPMENT OF A NEW AEROSOL GENERATION SYSTEM FOR INHALATION EXPOSURE APPLICATIONS
S. Taghvaee, A. Mousavi, M.H. Sowlat, C. Sioutas

Evergeton Hall

18.00-18.15 **OP49** AUTONOMOUS 1.57 MM DIFFERENTIAL ABSORPTION LASER DEVICE FOR REMOTE SENSING OF ATMOSPHERIC CO2
***P. Siozos*, G. Psyllakis, P. Samartzis, M. Velegrakis**

18.15-18.30 **OP50** EDXRF AND XANES AS ANALYTICAL TOOLS FOR NEW MERCURY COMPLEXING MEMBRANES
***N. Kallithrakas-Kontos*, S. Foteinis, E. Vazgiouraki**

Lord Byron Hall

18.30-19.30 **POSTER SESSION 2** *(details in p.27-31)*

P2 01-61 Aerosol metrology / Archaeometry / Chemical-and bio-sensors / Chromatography / Environmental analysis / Materials / Mobile analytical instruments / Pharmaceutical analysis / Sample handling / Sensors / Spectrochemical analysis / Thermal analysis

EXHIBITION

21.00 **CONFERENCE DINNER**

POSTER SESSION 2 • P2-01 – P2-61

Aerosol metrology / Archaeometry / Chemical- and bio- sensors / Chromatography / Environmental analysis / Materials / Mobile analytical instruments / Pharmaceutical analysis / Sample handling / Sensors / Spectrochemical analysis / Thermal analysis

P2-01 CASCADE IMPACTOR SAMPLING HARMONIZED TO NON-DESTRUCTIVE ELEMENTAL ANALYSIS OF AEROSOL PARTICLES
C. Dian, J. Osan, E. Börcsök, L. Stabile, S. Török

P2-02 AEROSOL METROLOGY FOR ATMOSPHERIC SCIENCE AND AIR QUALITY
F. Tsopelas, M. Ochsenkuehn Petropoulou, T. Lymperopoulou, L. A. Tsakanika, K. M. Ochsenkuehn, O. Serifi, C. Stergiopoulos, B. Beckhoff

P2-03 MINERALOGICAL COMPOSITION OF THE BRONZE AGE POTTERY FROM THE KAMENNY AMBAR SETTLEMENT (SOUTHERN URALS, RUSSIA)
A. Ryanskaya, M. Piskareva, D. Kiseleva, S. Panteleeva

P2-04 MINERALOGICAL AND CHEMICAL COMPOSITION OF PREHISTORIC PIGMENTS FROM CAVE PAINTINGS AND PICTOGRAPHS (SOUTHERN URALS, RUSSIA) BY SEM-EDS AND RAMAN SPECTROSCOPY
D. Kiseleva, E. Shagalov, E. Pankrushina, A. Ryanskaya, V. Shirokov

P2-05 ALL-SCREEN-PRINTED INTEGRATED PERMANENT BONDED MAGNETS ELECTROCHEMICAL CELLS
A. Papavasileiou, M. Prodromidis, I. Panagiotopoulos

P2-06 INVESTIGATION OF A MULTIPLEX INJECTOR FOR TIME-RESOLVED GAS CHROMATOGRAPHIC MONITORING
M. Antoniadou, E. Rosenberg, J. Kahr

P2-07 DETERMINATION OF PESTICIDES IN RIVER WATER SAMPLES BY SOLID PHASE EXTRACTION COMBINED WITH HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY/UV DETECTION (HPLC/ UV-DAD)
K. Boushi, V. Boti, T. Albanis

P2-08 ON-LINE EXTRACTION COUPLED TO LIQUID CHROMATOGRAPHIC ANALYSIS OF HYDROPHOBIC ORGANIC COMPOUNDS IN SOILS
A. Votani, T. Choleva, M. Tarara, C. Tziasiou, G. Tsogas, A. Vlessidis, D. Giokas

P2-09 OPTIMIZATION AND VALIDATION OF HPLC METHOD FOR SOME PESTICIDES FROM HUMAN URINE AND COMMERCIAL DOSAGE FORM
W. H. Gebrehiwot, C. Erkmen, B. Uslu

P2-10 BREATH ANALYSIS: A NOVEL NON-INVASIVE TOOL FOR MONITORING RECOVERY AFTER EXERCISE-INDUCED MUSCLE DAMAGE IN HUMANS.
K. Mikedi, E. Moutafis, S. Karma, A. Pappa, A. Krokidas, T. Nomikos

P2-11 QUECHERS-HPLC METHOD FOR AFLATOXIN DETECTION OF FOODS
L. B. Abdulra'uf, A. Sirhan, G. Huat Tan, R. C. S Wong

P2-12 GAS CHROMATOGRAPHY AS A TOOL FOR THE OPTIMIZATION OF DOCOSAHEXAENOIC ACID (DHA) RECOVERY FROM CRYPTHECODINIUM COHNII MICROALGA
M. Stramarkou, A. Chalima, V. Oikonomopoulou, E. Topakas, M. Krokida

P2-13 MICELLAR CHROMATOGRAPHY USING TWEEN-20 AS SURFACTANT: ELUTION MECHANISM AND QUANTITATIVE RETENTION- ACTIVITY RELATIONSHIPS FOR ESTIMATION OF BIOPHARMACEUTICAL PROPERTIES OF STRUCTURALLY-DIVERSE DRUGS
F. Tsopelas, K. Vasileiou, E. Leventaki, A. Tsantili- Kakoulidou

P2-14 THE POTENTIAL OF IMMOBILIZED PLASMA PROTEIN HIGH PERFORMANCE LIQUID CHROMATOGRAPHY TO ESTIMATE ECOTOXICITY OF PESTICIDES
C. Stergiopoulos, F. Tsopelas, M. Petropoulou-Ochsenkuehn

P2-15 INITIATING EFFICIENT SB(V) REMOVAL FOR DRINKING WATER BY A MECHANISM OF REDUCTION/ADSORPTION SEQUENCE
T. Asimakidou, G. Vourlias, K. Kalaitzidou, M. Mitrakas, K. Simeonidis

P2-16 SYNTHESIS AND CHARACTERIZATION OF Ag, ZnO AND AgZnO DECORATED GRAPHENE OXIDE FOR ENVIRONMENTAL APPLICATIONS
N. Adamopoulos, A. Ntziouni, A. Zourou, K. Kordatos

P2-17 GRAPHENE OXIDE/ATTAPULGITE AND GRAPHENE OXIDE/ZEOLITE COMPOSITE HYBRID MATERIALS AS ABSORBENTS IN DYES WASTEWATER TREATMENT
P. Koukakis, N. Adamopoulos, A. Zourou, K. Kordatos

P2-18 SYNTHESIS AND CHARACTERIZATION OF MAGNETIC GRAPHENE OXIDE FOR ENVIRONMENTAL APPLICATIONS
A. Zourou, N. Adamopoulos, A. Ntziouni, K. Kordatos

P2-19 SYNTHESIS AND CHARACTERIZATION OF GRAPHENE OXIDE-CERIA NANOHYBRID MATERIAL
A. Zourou, A. Koniaris, A. Ntziouni, K. Kordatos

P2-20 GRAPHENE OXIDE/β-CYCLODEXTRIN NANOHYBRID AS AN ADSORBENT FOR DYES REMOVAL
A. Zourou, N. Adamopoulos, A. Ntziouni, K. Kordatos

P2-21 MICRO-LIBS MAPPING OF MARINE MOLLUSK SHELLS ENABLES RELIABLE USE OF Mg/Ca AS A TEMPERATURE PROXY
N. Hausmann, I. Malegiannaki, A. Lemonis, P. Siozos, D. Anglos

P2-22 DETERMINATION OF THREE ANTIDEPRESSANT DRUGS BY FABRIC-PHASE SORPTIVE EXTRACTION (FPSE) COUPLED TO HPLC-UV/DAD
C. Chrimatopoulos, C. Jimenez-Holgado, M. Kalampoka, V. Sakkas

P2-23 SILICON LEACHABILITY FROM BAUXITE RESIDUE-THE CASE OF GEL FORMATION
L.A. Tsakanika, T. Lymperopoulou, M. Ochsenkuehn Petropoulou

P2-24 MAGNETIC GRAPHENE OXIDE SOLID-PHASE EXTRACTION OF SELECTED PHARMACEUTICALS FROM ENVIRONMENTAL WATERS
M. Kalampoka, T. Chatzimitakos, C. Stalikas, V. Boti, T. Albanis, V. Sakkas

P2-25 FLUORESCENT CARBON NANODOTS FROM OLIVE OIL PRODUCTION RESIDUES: PREPARATION, CHARACTERIZATION AND ANALYTICAL APPLICATION
N.M. Christopoulou, D. Kalogianni, T. Christopoulos

P2-26 EFFECT OF CARBON ADDITIVE ON SINTERING OF ZIRCONIA CERAMICS
S. Ghyngazov

P2-27 THE EFFECT OF pH ON THE STRUCTURAL AND OPTICAL PROPERTIES OF CARBON QUANTUM DOTS
P. Tsintavi, A. Segos, A. Ntziouni, N. Adamopoulos, L.A. Tsakanika, E. Alexandratou, C. Tsamis, K. Kordatos, A. Zourou

P2-28 UV-FEMTOSECOND DOUBLE-PULSE LIBS FOR THE IN-SITU CHARACTERIZATION OF ITO-BASED THIN FILMS
N. Giannakaris, P. Siozos, S. P. Banerjee, M. Sentis, D. Anglos

P2-29 SYNERGISTIC EFFECTS OF SOLID-PHASE INTERACTIONS IN FERRITE POWDER SYSTEMS UNDER COMPLEX HIGH-ENERGY MECHANICAL AND ELECTRON-BEAM IMPACTS
E. Lysenko, A. Surzhikov, E. Nikolaev

P2-30 FLUORESCENCE INSTRUMENTATION FOR RAPID, IN SITU DETERMINATION OF DISSOLVED ORGANIC MATTER IN WATER
É. Kónya, M. Berki, S. Klátyik, D. Lázár, D. Csősz, S. Lenk, A. Barócsi, T. L. Csőke,A. Csákányi, L. Domján, G. Szarvas, L. Kocsányi, N. Adányi, A. Székács

P2-31 FLUORESCENCE INSTRUMENTATION FOR RAPID, IN SITU DETERMINATION OF ALGAL DENSITY IN WATER
D. Lázár, B. Gémes, S. Klátyik, É. Kónya, M. Berki, D. Csősz, S. Lenk, A. Barócsi, T.L. Csőke, A. Csákányi, L. Domján, G. Szarvas, L. Kocsányi, N. Adányi, A. Székács

P2-32 FLUORESCENCE INSTRUMENTATION FOR RAPID, IN SITU DETERMINATION OF PAHS IN SURFACE WATER
M. Berki, É. Kónya, B. Gémes, S. Klátyik, D. Csősz, S. Lenk, A. Barócsi, T. L. Csőke, A. Csákányi, L. Domján, G. Szarvas, L. Kocsányi, N. Adányi, A. Székács

P2-33 APPLICATION OF ANALYTICAL QUALITY BY DESIGN PRINCIPLES FOR THE DETERMINATION OF ALKYL P-TOLUENESULFONATES IMPURITIES IN APREPITANT BY HPLC. VALIDATION USING TOTAL-ERROR CONCEPT
C. Zacharis, E. Vastardi

P2-34 INSTRUMENTAL ANALYTICAL METHODS AS A TOOL FOR THE EVALUATION OF DEOXYCHOLIC ACID ENCAPSULATION EFFICIENCY IN NATURAL MATRICES USING ELECTROHYDRODYNAMIC PROCESS
M. Panagiotopoulou, S. Papadaki, M. Krokida

P2-35 OCCURRENCE, REMOVAL AND ENVIRONMENTAL RISK ASSESSMENT OF PHARMACEUTICALS IN HOSPITAL AND URBAN WASTEWATERS
P. Martinaiou, E. Trantopoulos, C. Kosma, T. Albanis

P2-36 CHARACTERIZATION OF THE ANTIMICROBIAL ACTIVITY OF HERBAL EXTRACTS FOR REPLACING ANTIBIOTICS IN LIVESTOCK
M.S.G. Kafyra, A. Anastasiadis, M. Krokida

P2-37 DEVELOPMENT AND VALIDATION OF AN RP-HPLC METHOD FOR THE ANALYSIS OF GUAIACOL IN A PHARMACEUTICAL DOSAGE FORM
A. Addoun, C. Chelghoum

P2-38 MAGNETIC MOLECULARLY IMPRINTED POLYMER NANOPARTICLES AS SOLID PHASE EXTRACTION MATRIX IN THERAPEUTIC DRUG MONITORING
M. Nebsen, M. Al-Ghobashy, O. Attallah

P2-39 SYNTHESIS OF MAGNETIC BIMETALLIC Fe-Cu NANOPARTICLES FOR THE DISPERSIVE MICROEXTRACTION OF EMERGING POLLUTANS
A. Vasilas, T. Chatzimitakos, C. Stalikas

P2-40 A NOVEL APPROACH: pH CONTROLLED DISPERSIVE LIQUID-LIQUID MICROEXTRACTION (DLLME) OF PAHS METABOLITES FROM HUMAN URINE
S. Hrouzková, T. Göen, S. Zichová

P2-41 RHODIUM NANOPARTICLES AS PEROXIDASE-MIMETICS FOR THE DETERMINATION OF GLUCOSE
T. Choleva, V. Gatselou, G. Tsogas, A. Vlessidis, D. Giokas

P2-42 DISPERSIVE LIQUID-LIQUID MICROEXTRACTION METHOD FOR HPLC DETERMINATION OF PHENOLIC COMPOUNDS IN CAROB SYRUP
V. Goulas, C. Kalogirou

P2-43 APPLICATION OF DISSOLVABLE LAYERED DOUBLE HYDROXIDES AS AN EXTRACTION MEDIUM OF GOLD NANOPARTICLES PRIOR TO THEIR DETERMINAITON BY ATOMIC ABSORPTION SPECTROMETRY
T. Choleva, D. Giokas

P2-44 DETERMINATION OF HYDRAZINE BY ON-LINE SOLID PHASE EXTRACTION AND DERIVATIZATION USING ZONE FLUIDICS
P. Tzanavaras, C. Zacharis, S. Themistokleous

P2-45 PAPER-BASED DNA BIOSENSOR FOR VISUAL DETECTION OF MILK ADULTERATION
E. Bougadi, D. Kalogianni

P2-46 SYNTHESIS, CHARACTERIZATION AND ANALYTICAL UTILITY OF FREE-STANDING PH RESPONSIVE POLYMER FILMS IN SENSING APPLICATIONS
E. Tzianni, A. Lazanas, M. Trachioti, A. Florou, M. Prodromidis, I. Moutsios, D. Moschovas, M. Karabela, A. Avgeropoulos

P2-47 MICROFLUDIC PLATFORM FOR FUNCTIONALISATION, EXTRACTION AND DETECTION OF PHOSPHORYLATED AMINO ACIDS USING FLUORESCENT SENSORY PARTICLES
S. C. Burnage, J. Bell, W. Wan, K. Rurack

P2-48 ADVANCED SENSORS FOR HEAVY METALS BASED ON MONOELEMENTAL 2D BISMUTHENE AND GRAPHENE NANOCOMPOSITES PRODUCED BY SHEAR-FORCE LIQUID EXFOLIATION
A. Lazanas, A. Paipetis, M. Prodromidis

P2-49 qNMR AS A POWERFUL TOOL FOR PROVIDING PURITY ASSESSMENT AND METROLOGICAL TRACEABILITY
C. Alexopoulos, A. Georgopoulou, P. Giannikopoulou , E. Kakoulides, E. Stathoudaki, V. Schoina, A. Panagiotopoulou

P2-50 NOVEL 1H NMR METHOD FOR THE DETERMINATION OF ANTHOCYANINS IN FRUIT EXTRACTS
V. Goulas, I. Gerothanassis, G. Manganaris

P2-51 RAPID AND SENSITIVE NMR AND MOLECULAR DYNAMICS MAPPING OF SELECTIVE BINDING SITES OF FATTY ACIDS WITH ALBUMIN
I. Gerothanassis, E. Alexandri, A. Primikyri, G. Papamokos

P2-52 FLUORESCENCE SPECTROSCOPY – AN EFFECTIVE TOOL FOR CHARACTERIZATION OF GOLD NANOPARTICLES-PROTEINS CONJUGATES – THE COMPONENTS OF BIOANALYTICAL SYSTEMS
D. Sotnikov, E. Zvereva, A. Zherdev, B. Dzantiev

P2-53 PHOTOCHEMICAL REDUCTION OF SILVER HALIDES FOR THE COLORIMETRIC DETERMINATION OF BIOTHIOLS WITH CONSUMER ELECTRONIC IMAGING DEVICES AS DETECTORS
F. Kappi, M. Tarara, G. Tsogas, A. Vlessidis, D. Giokas

P2-54 HYPER-SPECTRAL RAMAN MAPPING OF MODERN HUMAN ENAMEL AND DENTIN
E. Pankrushina, D. Kiseleva, A. Ryanskaya, A. Lyogkih, N. Ozhgikhina, Y. Mandra

P2-55 ANALYTICAL AND STRUCTURAL STUDIES OF LIPIDS AND RELATED COMPOUNDS WITH THE USE OF NMR AND DFT CALCULATIONS
T. Venianakis, M. Siskos, I. Gerothanassis

P2-56 OPTICAL SCREENING OF BIOTHIOL LEVELS BASED ON ABSORBANCE QUENCHING OF GOLD- COATED SURFACTANT MICELLAR ASSEMBLIES
E. Akrivi, N. Kourkoumelis, A. Vlessidis

P2-57 THERMAL ANALYSIS STUDY OF g-C3N4 PREPARATION USING Al, Al2O3 , Pt/Rh COVERED AND UNCOVERED CRUCIBLES
F. Bairamis, T. Vaimakis, I. Konstantinou, D. Petrakis

P2-58 INVESTIGATIONS OF BIOMATERIALS WITH VIDEO PARTICLE TRACKING MICRORHEOLOGY
A. Papagiannopoulos

P2-59 APPLICATION OF THE QUECHERS TECHNIQUE FOR THE PRE-CONCENTRATION OF MALATHION PESTICIDES IN FRUIT SAMPLES
L. Chimuka, H. Musarurwa, N. Tavengwa

P2-60 MONITORING OF ANTIBIOTICS IN THE PYRENEAN RIVER WATERS USING SOLID-PHASE EXTRACTION UPLC-MS/MS
E. Avramiotis, S. Gozzo, S. Godin, M. Peña Ormad, J. Szpunar

P2-61 ASSESSMENT OF EXPOSURE TO ENDOCRINE DISRUPTING COMPOUNDS USING GAS CHROMATOGRAPHIC-MASS SPECTROMETRIC ANALYSIS OF COMPOSITE FOOD SAMPLES IN A TOTAL DIET STUDY
A. Karakitsou, D. Hela

Wednesday, September 25th 2019

Evergeton Hall

08.30-09.00 Registration

09.00-09.30 **Invited Lecture**

Chair: ***E. Rosenberg, A. Pappa, M. Krokida***

Application of Biomimetic HPLC Properties for the Estimation of Brain to Blood Distribution of Drug Discovery Compounds Including New Modalities

K. Valko

09.30-10.15 **Oral Session: Chromatography 2 / Spectrometry 2**

Chair: ***E. Rosenberg, A. Pappa, M. Krokida***

09.30-09.45 **OP51** BIOMIMETIC CHROMATOGRAPHY: CONDITIONS, ELUTION MECHANISMS AND APPLICATIONS IN EARLY DRUG DISCOVERY

F. Tsopelas, P. Danias, E. Notari, D. Anagnostopoulou, E. Paroutsi, A. Pappa, A.Tsantili - Kakoulidou

09.45-10.00 **OP52** IN-CELL NMR SPECTROSCOPY APPLIED IN THE STUDY OF LIGAND-PROTEIN INTERACTIONS IN LIVING CANCER CELLS

A. Primikyri, N. Sayyad, G. Quilici, E.I. Vrettos, K. Lim, S.W. Chi, G. Musco, I.P. Gerothanassis, A. G. Tzakos

10.00-10.15 **OP53** THE USE OF BIOPARTITIONING MICELLAR CHROMATOGRAPHY TO PREDICT ECOTOXICITY OF PESTICIDES IN AQUATIC ENVIRONMENT

C. Stergiopoulos, F. Tsopelas, M. Ochsenkühn-Petropoulou

10.15-10.30 **OP54** INTERPRETING TOF-SIMS DATA: A HOLISTIC APPROACH

E. Chatzitheodoridis

10.30-11.00 ***Coffee break***

11.00-11.30 **Invited Lecture**

Chair: ***M. Karayannis, K. Ochsenkühn, F. Tsopelas***

Possibilities and Limitations of Electroanalytical Chemistry 60 Years after Nobel Prize for Polarography

J. Barek

Evergeton Hall

11.30-12.45 **Oral Session: Electrochemistry / Archaeometry**

Chair: ***M. Karayannis, K. Ochsenkühn, F. Tsopelas***

11.30-11.45 **OP55** GOLD-SPUTTERED SENSOR FOR THE VOLTAMMETRIC DETERMINATION OF TRACE ARSENIC
A. Economou, J. Gonciarczyk, C. Kokkinos, A. Bobrowski

11.45-12.00 **OP56** 87Sr/86Sr ISOTOPE RATIO DETERMINATION BY MC-ICP-MS USING THE SSB TECHNIQUE FOR ARCHAEOMETRIC PROVENANCE STUDIES
D. Kiseleva, A. Kasyanova, M. Streletskaya, M. Chervyakovskaya

12.00-12.15 **OP57** THE CHALLENGE OF USING PHAGE IN FOOD AND VETERINARY DIAGNOSTICS: DETECTION OF MYCOBACTERIUM AVIUM SUBSPECIES ARATUBERCULOSIS IN INFANT FORMULAS BY CULTURE, PCR AND COMBINED PHAGE-PCR
C. Rees, G. Botsaris

12.15-12.30 **OP58** CHEMICAL COMPOSITION OF BELT ACCESSORIES FROM CENTRAL AND WEST BULGARIA DATED TO THE GREAT MIGRATION PERIOD
D. Lesigyarski, B. Zlateva, L. Traikova, V. Mihailova, V. Bonev

12.30-12.45 **OP59** A COMPUTATIONALLY DESIGNED CARBON PASTE SENSOR FOR SELECTIVE DETERMINATION OF ISOXUPRINE HYDROCHLORIDE IN DIFFERENT MATRICIES
E. S. Elzanfaly, A. S. Saad, M. K. Halimb, K. M. Kelani

12.45-13.30 **Closing Ceremony / Awards**

Chair: ***T. Albanis, M. Ochsenkühn***

14.00-17.30 Excursion - Castle-Museums (Ioannina)

Thursday, September 26th 2019

08.30-17.30 Post-Conference Excursion - Metsovo

SUNDAY, SEPTEMBER 22ND, 2019

EVERGETON HALL

Opening Session

Chair: ***T. Albanis, M. Ochsenkühn-Petropoulou***

PL01 THE EVOLUTION OF ANALYTICAL ATOMIC SPECTROMETRY

L. Ebdon

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In tribute to the 150th anniversary of the Periodic Table, this lecture will show how the various techniques of analytical atomic spectrometry have evolved to enable the determination of most of the elements of the Periodic Table, moving over the years from left to right.

The introduction of flame emission spectrometry in Bunsen's laboratory in the early 1860s, enhanced by Lundegardh's flame photometer, led to simple and direct determination of the alkali and alkaline earth elements. The invention of atomic absorption spectrometry (AAS) is generally attributed to Walsh with acknowledgement being given to Alkemade who also published on the technique in 1955. Together with the subsequent development of atomic fluorescence spectrometry by Winefordner and West, the determination of the elements in groups 1 to 13 and several in groups 14-16 became possible.

Developments in AAS including the use of different flames, vapour generation and graphite furnaces will be reviewed. The use of dc arcs and ac sparks together with direct reading vacuum spectrometers facilitated further extension to more elements in group 16. The development of the inductively coupled plasma by Greenfield and Fassel transformed atomic emission spectrometry, enabling most of the elements measured by AAS to be determined more sensitively and simultaneously.

The breakthrough in the 1980s of inductively coupled plasma- mass spectrometry, based on the research of Gray and Fassel, finally enabled atomic spectrometry to cover virtually all the Periodic Table and the determination of isotopic composition as well.

The importance and utility of all these techniques will be discussed in both a historic and current context.

PL02 ONE HUNDRED AND FIFTY YEARS OF THE PERIODIC TABLE: DMITRI MENDELEEV IS RECOGNIZED AS A DISCOVERER AND INVENTOR, CHEMISTS BECOME "PROPHETS", AND THE "ENTROPY" OF THE CHEMICAL KNOWLEDGE IS DIMINISHING

M.I. Karayannis

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Dmitri Ivanowitsch Mendeleev in 1869, published his proposal for the systematic presentation of the chemical elements. Since then the periodic table, that gave birth, is posted in every chemistry teaching room and is one of the most recognizable symbols of Chemistry. This, in addition to the conditions created for the rapid development of chemistry, has made Mendeleev a discoverer, a **"prophet",** an **inventor** and enabled the chemists to make predictions in their science, a privilege that until then had only the astronomers. It also helped to systematize knowledge, thus enabling the reduction of the **"entropy"** of knowledge in the natural sciences.

The metaphysical alchemy has its roots in ancient Greece with the pre-Socratic philosophers Empedocles, and Heraclitos, who established the concept of the principal elements, **fire, air, water and earth** named ***ρίζες*** (***roots)*** and suggested their opposing properties. Leucippus and Democritus developed their theories of atomism, Aristotle added the fifth element of **ether** and Plato gave **shapes** to all atoms through his platonic solids and used for the first time the word ***"stoiceion"*** (element).

The Arab Jābir ibn Hayyān (Latinized as "Geber"), extended the elemental system in medieval alchemy (8th century), by adding to the five elements, **sulphur**, **mercury and salt** representing metallicity, volatility and solidity respectively.

At the beginning of the 19th c, after consolidating the atomic theory (Dalton), the scientists noticed the relation of the atomic weight (A.W.) of the elements with their properties. The development of chemistry in this direction began to yield when, based on the AVOGADRO's hypothesis, CANNIZZARO succeeded to determine the A.W. of the elements with high accuracy. This enabled **J.W. Döbereiner** (1827), **Alexandre-Émile de Chancourtois, John Newlands** (1862) and **Lohar Meyers** to detect periodicities in characteristic properties of the 56 elements known at that time. Though, Dmitry **Mendeleev** in 1869 is credited for the discovery of the periodic law, the first version of the Periodic Table of elements and the scientist dared to predict the properties of elements yet to be discovered.

The periodic table has been in constant change from its appearance: Expansion, as new elements were discovered, update with new columns, filling of the blank spaces etc. After the discovery of the proton and electron, the quantum-mechanical idea of atomic orbits followed. These findings provided an entirely new kind of logic for the periodic system. Although the basic logic of periodicity did not change, scientists could now see that it was the electron structure that dictated to a large extent the attributes of the table and the similarity of members of the same group.

PL03 INSTRUMENTAL ANALYSIS: DILEMMAS AND RESPONSIBILITY

I. Brčeski

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Instrumental methods of analysis are among the leading ones in analytical chemistry. Essentially, the classical analysis methods have been entirely forgotten and are considered rarity one today. This is somewhat understandable. Instrumental methods can be conducted very quickly, the results are processed by powerful machines using advanced software, so they are quickly available as usable. The areas covered by instrumental techniques are numerous, from typically scientific, to applicative.

Big companies that sell their instruments for expensive sums emphasise all the advantages, with remarks that the machines "basically do everything on their own" and that their usage requires an "operator" who, during an usually 7-day training cycle, begins working on the instrument. For them, the knowledge of the software possibilities is far more important than knowing the characteristics of the substances. In some scientific areas, where the results are analysed by highly educated and narrowly specialised experts, this is not even much of a problem. However, when it comes to the application of the instrumental analytical methods for obtaining results that are particularly important to the public (or court), such as ecochemical examinations, several dilemmas and specific responsibilities may arise there.

Not knowing the origin and nature of the substances being analysed always leads to a certain (bigger or smaller) error. In modern procedures it is even requested that the analyst does not know the sample, but only the code! In order to interpret the results correctly, a good knowledge of the characteristics, the origin, the way of collecting and preparation for analysis of the sample must be had.

Instrumental techniques change very quickly, the time spent on analysing (and thinking about the analysis) shortens, with a tendency of obtaining results for tens of analytical parameters via a single analytical procedure. It also should not be forgotten that they are very expensive. Techniques that were recently considered cutting-edge are rapidly becoming obsolete and replaced with newer ones. A good ICP analyst has barely any or no experience with atomic absorption techniques, those who work on mass spectrometers are not familiar with the mass fragmentation of organic compounds, so, just like with IR spectroscopy (without the knowledge of absorption of functional groups), spectral databases, managed and searched by software, are being used. Of course, results are given in the form of probabilities.

After several years of applying instrumental analysis techniques and tracking the results, the dilemmas multiplied: is so many parameters really necessary in order to characterise something, should it be that expensive, how many techniques should be used to prove a result of particular importance, especially one with a judicial weight, is the analyst aware of the nature of the substances… and does he have time to consider the

problematic itself.

The analytics world of today is unimaginable without instrumental analysis techniques. It is impossible to satisfy the modern demands with the classic procedures, nor should such a possibility be even considered. However it should be known that the flame photometer is the basis of spectroscopical analyses, whereas the analysis of gases should be begun with the Orsat's device… that the knowledge of the substance's characteristics is what makes chemistry divine.

PL04 ETHICS IN CHEMISTRY AND SCIENCE: IS IT USEFUL?

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The practice of chemistry is a key endeavor of men and principal occupation for attainment of material wealth; in fact, even the early proto-chemist has employed chemical methods for adapting to environmental conditions by creating new materials, like metals for weapons for hunting and defense, or pottery for cooking and storage of food. Early men's approach was intuitive and by trial and error; the latter still is, in principle, the way of practicing chemistry in our days.

However, chemists also know that, according to the second law of thermodynamics, every useful, beneficial reaction is inextricably associated with entropic, dis-ordering effects. The enthalpy, the useful fraction of invested energy, can only be maximized (and the entropic fraction in the form of accidents and pollution kept as low as possible) through optimization of each step in the flow of energy and matter. This is true for any ecological or socio-economic systems, even our whole planet: optimization of the positive versus negative effects is in principle the fundamental ability every chemist is trained for, which, in a more general sense, is a matter of ethics. Environmental problem-solving to attain sustainability is a chemical-technological challenge, and, at the same time, an ethical question of balancing group interests under the imperative for social fairness, a main prerequisite for societal-political stability. The respective stakeholders often have different priorities which must be properly considered in order to be socially fruitful. Information exchange - among scientists and between scientists and the public - is the actual means of enabling the transformation of scientific knowledge into technological advances and ultimately into societal wealth. So reliability and truthfulness in communication of research outcomes in journals, as patents, or by other media is of importance for the well-being of a socio-political system. The needed free interplay to find the best balance can only function well under participatory-democratic conditions; ideological constraints make modern scientific-technological systems inefficient.

Thus, scientists must also understand their responsibility for the well-being of the social system they live in. In order to be competent as environmental scientist, besides proper scientific-technical training, education in applied ethics is a core need. Finding a good balance of the diverse positions of stakeholders requires the ability of understanding the view of others, even if opposing and conflictive. For this, besides intellectual capabilities, empathic competence is equally important, requiring a new concept of academic education in environmental science within an ethical, perhaps even spiritual paradigm.

In the lecture, some examples of current practical initiatives towards such improved education and training programs on the European and international level are discussed.

MONDAY, SEPTEMBER 23RD, 2019

EVERGETON HALL

X-ray analysis 1

Chair: ***B. Beckhoff, Sir L. Ebdon***

IL01 INSTRUMENTATION SCIENCE: THE THIRD SIDE OF ANALYTICAL CHEMISTRY

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There are several ways in which scientific investigation can proceed. The traditional "scientific method" is hypothesis-driven; a hypothesis is formulated, a procedure is devised to test the hypothesis, and the results of the test used to determine the validity of the original idea. Unfortunately, this traditional approach generally yields only incremental gains in knowledge. Many of the most important advances arise from true innovation: making connections between areas that had no apparent relationship before.

These innovations are sometimes fostered by new scientific information but sometimes by need. On the one hand, fundamental studies can lead to knowledge that can be profitably applied to areas of current scientific, technical, or societal importance. An example is the emergence of magnetic resonance imaging from its origins in nuclear magnetic resonance spectrometry. From the opposite side, an application can be sufficiently important that it encourages fundamental investigations to help characterize it. The current bioscience revolution is an obvious illustration. Clearly, these activities are both complementary and symbiotic; basic science can lead to the solution of significant applied problems and important present problems can lead to better science. These two approaches — the applied leading the basic and the basic driving the applied — can be considered the two sides of scientific investigation.

Yet, this arrangement does not complete the picture. The translation of basic scientific findings into practical applications and the design of basic experiments to characterize important applications both require a catalyst. That catalyst is often instrumentation. Just as the development of MRI required new devices and tools, so did the decoding of the human genome.It would seem, then, that there are three sides of scientific investigation, in which instrumentation science constitutes an indispensable component. In this presentation, these three sides of scientific investigation will be illustrated with work from our laboratory.

OP01 SYNCHROTRON RADIATION TXRF: STRENGTHS AND CHALLENGES

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Total Reflection X-ray Fluorescence (TXRF) Spectroscopy is one of the most impressive analytical technique providing spectral signatures of materials that can be used to unravel their elemental composition. Within a few seconds and with limited sample preparation, a first characterization of qualitative character can be obtained, whereas thorough and quantitative information will require a full experimental design approach. In addition, differences between the samples or the samples analysis conditions may cause very slight spectral differences that may be difficult to distinguish and/or identify, and that may tremendously affect the reliability and the validity of the results. As such, and despite its apparent versatility and ease-of-use, many issues remain opened in TXRF analysis. These are lying from sample preparation procedures, experimental conditions to related data analysis. Pushing the knowledge limits further in TXRF analysis undoubtedly involves the use of advanced technologies in combination with laboratory equipment and methods. The advent of state-of-the-art analytical research tools, such as synchrotron facilities exploiting the unique qualities of synchrotron radiation (SR), has offered TXRF a new source of unprecedented chemical sensibilities and with high spectral resolution. As SR is being produced over a wide range of energies from the soft (<1 keV) to the hard X-rays (>10 keV), its energy tunability is a strength to excite preferentially selected components of a material, and to assess simultaneously, or by correlation of techniques, the different (bio)chemical and physical properties of the sample. By combining TXRF with X-ray Absorption Spectroscopy (XANES), the speciation and the local structure of the element of interest can be unravelled together with the concentrations of all the elements in presence. In this paper the strengths, drawbacks and challenges of TXRF analysis with a synchrotron source will be highlighted, and illustrated via a few examples from the fields of nanomaterials and biology.

OP02 DEVELOPMENTS IN X-RAY DIFFRACTION TECHNOLOGY

I. Hegedues

Bruker AXS

X-ray Diffraction (XRD) is a powerful analytical technique, which enables detailed analysis of any material from fundamental research to industrial quality control. Application range from phase identification and quantification, to crystal structure determination, to analysis of thin layers as well as stress and texture measurements.

In this talk, we will present an overview of the latest developments in XRD technology, andillustrate the advantages on selected examples:

(i) Kidney stone disease (urolithiasis) affects about 1 in 10 people at some stage in their lives. Different causes can lead to kidney stone formation, and are reflected in the phase-composition of the stones. Using XRD, the crystalline phases are determined and quantified, helping identify the cause of the disease and guide treatment and preventative measures.

(ii) Process and quality control in mining is crucial to reduce costs and environmental impact. For example, XRD is used in iron-ore mining to identify less valuable or problematic minerals and to determine the iron ore composition. The XRD results enable separation of different charges, and crucially, the optimization of reducing agents (coal) and additives required for iron reduction.

(iii) Effective energy storage is a crucial building block in distributed electricity supply from renewable sources and supporting e-mobility. One of the challenges in battery research is the investigation of novel cathode materials during charge- and discharge cycles. In-situ measurements of batteries with XRD benefit from using hard x-ray radiation and large 2D detectors, which allow penetration of battery assemblies and fast data collection respectively.

(iv) High-throughput screening of well-plates is used to accelerate drug development and to improve the quality of pharmaceutical products. In this context, XRD provides a wealth of information for crystallization studies, polymorph screening, structure solution, phase identification and quantification including amorphous content as well as crystallite size determination.

OP03 IMMOBILIZATION OF HEAVY METALS IN DRINKING WATER: THE ROLE OF METAL (OXY)HYDROXIDES ON SORPTION MECHANISM USING X-RAY ABSORPTION SPECTROSCOPIES

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The effective oxidation of As(III) as well as the sorption mechanism of the metal oxyanions onto Fe/Mn (oxy)hydroxides is investigated by means of X-ray Absorption Spectroscopies. Due to the atoms selective character of such techniques, both the adsorbate and absorbent are studied in terms of heavy-metal loading, chemical composition and synthesis pH. In the case of amorphous tetravalent manganese feroxyhyte (TMFx) nanospheres, studied as an efficient As(III)-removal material, the optimum synthesis conditions and chemical composition were determined by the degree of polymerization in the adsorbents' microstructure. Under synthesis into mildly acidic conditions, the change in the polymerization of the metal-oxyhydroxyl chains (metal=Fe, Mn) provides more adsorption sites at edges and corner sites in the bonding environment of Fe and Mn, respectively, thereby enhancing As uptake. After exposure to As-polluted water, similar microstructural changes related to As-bidentate and monodentate geometries are generated: As(V) preferentially occupies the high energy adsorption sites (^{2}C complexes) available in the Mn-oxyhydroxyl groups and the low energy edge sites offered by Fe (^{2}E complexes). Finally, when Fe oxy-hydroxides (FeOOH) are implemented for the removal of As, it is revealed that apart from modifications in the polymerization of the $Fe(O,OH)_6$ chains in the adsorbent, the different As-loading also induces an increase in the ratio of face-/edge-sharing sites. Arsenic (V) species preserve the original oxidation state and form ^{2}C and ^{2}E inner sphere complexes, while As(III) adsorption proceeds only via ^{2}E linkage to the surface.

OP04 PORTABLE XRF SPECTROMETRY IN THE FIELD OF CULTURAL HERITAGE

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The potential of X-ray Fluorescence (XRF) analysis to provide in-situ, non-invasive and simultaneous multi-elemental compositional information is the striking feature of its emerging utilization in the field of Cultural Heritage. Fully exploiting and boosting the technological breakthroughs which offered portability and miniaturization of X-ray detectors and sources (mid- late 90's), the XRF laboratory of the Institute of Nuclear and Particle Physics at NCSR "Demokritos" developed custom-made innovative portable XRF spectrometers motivating the establishment of sustained research collaborative schemes with conservators, curators and archaeologists, but also providing technology transfer and analytical services to cultural heritage end-users. Thus, in the last twenty (20) years, numerous field investigations have been conducted by analyzing and studying unique archaeological/historical collections in Greece and abroad, including Cyprus, Jordan, Syria and Malta.

This contribution is to report recent results of in-situ XRF analysis on different archaeological/historical materials and artifacts stored or exhibited in different sites in Greece, including ancient gold, copper and silver alloys, Mycenaean glass beads and wall-painting pigments, polychromy on marble and wooden panels, colors and pigments in illuminated Byzantine manuscripts, amongst others. Additionally, particular emphasis is to be placed upon methodological developments aimed to support the transition of the XRF technique from its use solely for diagnostic purposes, towards an actual spectrometric technique. In many applications, for example, reliable compositional elemental data can offer a solid ground to study and enlighten the artifacts' manufacture technology and relevant application techniques, allowing a comprehensive comparison with existing databases, whereas through trace element fingerprint analysis the provenance of raw materials can be investigated. Based on case studies, the benefits of quantifying field XRF measurements will be highlighted and discussed in view of major archaeological queries regarding the procurement of raw materials, provenance assignment and technological choices posed when attempting to tackle cultural and societal transformation issues.

OP05 ADVANCES IN X-RAY TECHNOLOGY FOR MATERIALS ANALYSIS

E. Klothakis

During the last years the capabilities of modern analytical x-ray systems have changed dramatically in terms of x-ray sources, optics and detectors, as well as geometries. In this presentation Rigaku will give an overview about hot applications, explain the technique and show typical results that can be expected. The applications include, elemental composition, microscopy, chemical compositions, mapping, coating thickness, stress, texture and more.

IL02 USING INSTRUMENTAL ANALYSIS FOR DETERMINING FOOD AUTHENTICITY, ADULTERATION AND FOOD SAFETY

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Recently has been grown an interesting question of what is authentic food? In other words the customers want to know when is food '*not authentic*'? And what is more important they need a quite realistic answer of these questions. As a matter of fact, the food authenticity issues involved derivative subjects to be clarified, interpreted and settle for best solutions, such as: economically motivated adulteration; false declaration of geographical origin, and false declaration of farming regime / production system.

Analytical techniques in food authentication follow the duty of tracking compounds other than natural, present in food products, keeping in mind the modern definition of the intentional meaning according to which since years the adulteration is… *the fraudulent, intentional substitution or addition of substance in a product for the purpose of increasing the apparent value of the product or reducing the cost of its production'.*

From the National Food Authority has been drawn attention and increased public awareness exposing many bad practical cases, in order to detect the addition of non-permitted substances to meet or enhance specifications, and the addition or substitution of ingredients with lower-valued ones. Doing that, it is needed using and training *for reliable authentication techniques, which at the best of our experience ask for specialized instrumental analysis such as* HPLC, IR spectroscopy, GC MS, IRMS, Hyphenated MS etc.

Searching deeply into the chromatographic techniques, it can be performed the detection of adulteration of *targeted substances such as* - melamine in milk by HPLC; - Sudan dyes in egg yolk by HPLC; -confirmation with a mass spectrometric method. On the other hand, it is of the utmost importance the instrumental detection of partial / total substitution with *cheaper, similar alternatives* by profile of specific classes of compounds or by detection of specific markers, and performing specific analytical protocols of determining practical issues of interest such as: authenticity of fruit juices by LC profiling of polyphenols; authenticity of olive oil and honey, by GC profiling of fatty acids, dealing with example case of study such as: authenticity of fruit juices by HPLC exploiting the fact that different fruits have their own characteristic phenolic compounds.

MONDAY, SEPTEMBER 23RD, 2019

EVERGETON HALL

Food analysis

Chair: ***I. Brceski, V. Sakkas***

OP06 IDENTIFICATION OF BIO-PHENOLIC PROFILE OF SELECTED NATIVE MONOVARIETAL AND BLENDED FRESHLY PREPARED FRUIT JUICES USING CHROMATOGRAPHIC TECHNIQUES

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In recent years, for a significant number of researchers in the world, an important issue is to update the knowledge on the chemical composition and activity of certain ingredients of native monovarietal and blended natural fruit juices in order to allow for the optimum content of prepared fruit juices by cold pressing methods. Solid phase extraction (SPE) combined with high resolution MS chromatographic measurements was used to analyze the phenolic profile in four samples of fruit juices consisting of: (a) Apple; (b) Red fruits (which represent a mixture of apple, pomegranate and beetroot); (c) Plum mixed with blueberry; and (d) Cherry. According to the results of the tests, a total of 35 phenolic compounds were identified, showing a different appearance in our samples, while for each of them the theoretical and experimental exact mass (m / z) and the parameter Δ (ppm) - mean mass accuracy were calculated. The identification of most of the phenolic compounds was performed using standard chemical substances, while the identification of the remaining compounds was done using MS fragmentation. The data from the present study can help to investigate the dependence of nutritional value and other chemical and biological activities of the variety of fruit extracts used in the preparation of different types of juice from their chemical composition, botanical origin as well as their antioxidant and antimicrobial properties.

OP07 OPTICAL SPECTROSCOPY TECHNIQUES FOR THE CLASSIFICATION AND QUALITY CONTROL OF AGROFOODS

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In this contribution we present results obtained in IESL-FORTH by applying optical spectroscopic techniques, (such as Absorption UV-Vis-nIR, Fluorescence spectroscopy and Raman Spectroscopy) combined with machine learning analysis methods for the quick monitoring of the characteristic substances contained in food samples. These techniques have low cost, can provide rapid information and need no special pretreatment of the samples. More specifically, high added value agro-food products such as wine, olive oil and honey, can be analyzed with these spectroscopic techniques, recording a "fingerprint" of the sample in a fast and non-invasive way and providing information about the quality, identification and origin of the products. Currently, wine samples from different wineries were analyzed for the investigation and evaluation of ageing factors of red and white wines from local varieties and for the determination of optimal time and way of maturation in vats and barrels of different type per variety of wine grapes. Furthermore, the detection of the adulteration of extra virgin olive oils (e.v.o.o.) with seed oils and the prediction of organoleptic features of e.v.o.o. were also accomplished. Moreover, honey samples were analyzed and differentiated based on their botanical origin. These studies demonstrate the potential of the optical spectroscopy as a useful tool in the agro-food products' classification and quality control.

OP08 IMMUNOCHEMICAL CONTROL OF RAW MATERIALS' SOURCES IN THE PRODUCTION OF MEAT AND DAIRY FOOD

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Identification of raw materials' sources used in food production is essential to ensure their safety and inform consumers. The use of ad hoc, low grade and allergenic components in food products is a serious problem in modern society. In this regard, the existing tools for controlling sources of food raw materials and confirming their authenticity should be extended to provide rapid screening, including point-of-demand testing without analyzing samples in specialized laboratories.

The report presents the development of immunoanalytical systems for detection of meat and dairy raw materials in food and non-meat additives in meat products. An important issue determining the applicability of immunodetection is the stability of controlled biomarkers after enzymatic and heat treatment. The advantages of troponins, thermostable biomarkers of muscle tissues, were shown. The specificity of various antibodies to troponins was tested. An enzyme-linked immunosorbent assay (ELISA) of troponin I was developed. The ELISA allowed distinguishing mammalian (beef, pork, lamb, horse) and bird (chicken, turkey, duck) meat sources. For dairy raw materials and soy protein, the effect of the sample treatment on immunodetection has been investigated. One-site (competitive) and two-site (sandwich) immunoassays were compared and the best solutions were chosen for the control of (i) native protein molecules or (i) total content of various forms of the processed protein. Kinetic mode of ELISAs of troponin, beta-lactoglobulin, casein, and soybean trypsin inhibitor was evaluated. The assay techniques with a total duration of 30-40 min have been proposed. The applicability of lateral flow immunoassay (LFIA) based on the use of membrane carriers with immobilized immunoreactants were considered. Approaches for highly sensitive quantitative LFIAs were proposed and characterized. Methods for sample preparation of meat and dairy products before immunoassays were comparatively tested.

This study was financially supported by the Russian Science Foundation (grant number 19-16-00108).

OP09 DETERMINATION OF BISPHENOL A IN FOOD SIMULANTS A,B,C AND D1 PERFORMED BY HPLC-FLD AND VALIDATION OF THE METHOD

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Bisphenol A, an endocrine disruptor, is the monomer used to make polycarbonate plastics (PC) so it is widely found in food packaging materials. Complementary to the Regulation (EU) 10/2011, European Commission adopted the Regulation (EU) 2018/213 prohibiting migration of BPA found in varnishes and coatings intended to come into contact with infant food. The aim of this work was to develop and validate a fit for purpose method for the determination of BPA following overall migration in aqueous food simulants (A, B, C and D1) from plastic materials and articles intended to come into contact with food. Determination of total migration was carried out by article filling with the corresponding simulator and contact temperature and time conditions at 2 hours at 70 °C. Qualitative and quantitative determination of BPA was performed by a High Performance Liquid Chromatographer (HPLC) coupled to a Fluorometric Detector (FLD). The analysis resulted in fast elution time of BPA (around 4 minutes) by using a C18 column applied. The method was validated; LODs and LOQs varied from 0.42 to 2.12 μg L^{-1} and 1.31 to 6.43 μg L^{-1} respectively. Recovery, precision, trueness, linearity, uncertainties, repeatability, reproducibility fulfilled all the requirements set by ISO 17025. Trueness of the method developed, regarding A and B simulators, was proved by the successful interlaboratory test (Proficiency test) that we participated in (z-scores in simulants A and B were 0.60 and 0.33 respectively). This research resulted in a rapid, cost effective and environmental friendly green method for BPA specific determination.

OP10 COMBINED EFFECT OF GASEOUS OZONE AND CITRIC ACID TREATMENT ON QUALITY CHARACTERISTICS AND SHELF LIFE OF PACKAGED FRESH-CUT LETTUCE PRESERVED UNDER REFRIGERATED CONDITIONS

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Ozone (O_3) is formed in the stratosphere from the effect of solar ultraviolet radiation to atmospheric oxygen and the electrical discharges created during the thunderstorms. Ozone has a strong oxidative capacity that makes it a powerful disinfectant for food processing, as it can destroy bacteria, fungi, spores and viruses. Its oxidative capacity depends on factors such as concentration and exposure time, temperature, relative humidity, chemical composition of food and microbial load. In the present study, the combined effect of gaseous ozone and citric acid treatment on quality characteristics and shelf life of fresh-cut lettuce packaged under passive modified atmosphere conditions and stored under refrigeration was investigated. Lettuce samples were treated with 1% w/v citric acid, ozone at concentrations of 0.5, 1.0 and 1.5 ppm and ozone plus citric acid at the same concentrations, for 45 minutes. All samples were packaged in PET//LLDPE bags and stored. Headspace analysis, color parameters (L*, a* and b*), pH, microbiological tests (total viable, yeasts and molds and *Enterobacteriaceae* counts), volatile constituents and overall visual quality were monitored during storage. Oxygen consumption rate was significantly reduced ($p<0.05$) by 1.0 ppm ozone and by citric acid treatment compared to control sample. Carbon dioxide production rate and total viable counts were affected significantly by 0.5 and 1.0 ppm ozone treatment. Treatment with 1.5 ppm ozone and with citric acid caused significant reduction in *Enterobacteriaceae* counts. No one treatment affected significantly color parameters and pH. Concentration of trans-2-hexenal (produced by the oxidative degradation of fatty acids) was decreased in all treatments during cold storage. Samples treated with citric acid, 0.5 ppm ozone and 0.5 ppm ozone plus citric acid presented better overall visual quality until the last day of storage.

MONDAY, SEPTEMBER 23RD, 2019

LORDON BYRON HALL

Foodomics

Chair: ***G. Theodoridis, I. Konstantinou***

OP11 FoodOmicsGR NATIONAL RESEARCH INFRASTRUCTURE FOR THE COMPREHENSIVE CHARACTERISATION OF FOODS

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National infrastructure **FoodOmicsGR_RI** aims to coordinate the actions of research teams from eight Greek Universities and Research Centers in a network that will support the method development and implementation of dietary studies and comprehensive characterization of foodstuff. **FoodOmicsGR_RI** combines food/nutrition science with the most advanced analytical techniques, bioinformatics and field/application sciences. The main objective is the comprehensive mapping of the food content, the assessment of their distinct value and the study of the effect of nutritional intervention on the metabolic-proteomic profile of biological samples of consumers and animal models.

“We acknowledge support of this work by the project «FoodOmicsGR Comprehensive Characterisation of Foods» (MIS 5029057) which is implemented under the Action Reinforcement of the Research and Innovation Infrastructure <http://www.antagonistikotita.gr/epanek_en/proskliseis.asp?id=28&cs=>, 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)”

OP12 HIGH RESOLUTION MASS SPECTROMETRIC FOODOMICS: FROM BASIC RESEARCH TO INDUSTRIAL APPLICATIONS

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During the last decade, food industry is facing a major breakthrough due to the development and application of high-throughput omics technologies in food analysis (foodomics). Through holistic food analysis approaches, authenticity, health claims, quality and safety are connected to food components. In particular, high resolution mass spectrometry (HRMS) has proved to demonstrate excellent analytical performance, allowing the determination of a wide range of target micro-constituents and assisting the identification for both non-targeted and targeted ("suspect") compounds. The exploration of food adulteration and the assurance of geographical and botanological origin of food products are only a few research areas that HRMS-based foodomics can apply to, holding promise for the discovery of potential (bio)markers in relation to food authenticity and food safety. In our laboratory, integrated target, suspect and non-target screening workflows based on LC/GC-QToF-MS, LC-TIMS-QToFMS and MALDI-ToFMS have been developed and applied to a wide variety of food matrices. Extensive databases were developed including targeted endogenous food metabolites (619 compounds), as well as a wide "suspect" MS-ready database, including thousands of natural products. QSRR models were developed for the retention time prediction of "unknown" compounds under RPLC and HILIC elution modes and a Retention Time Index (RTI) system was developed for interlaboratoy harmonization of LC-HRMS screening. Data analysis and evaluation in non-target HRMS screening workflow was significantly assisted using advanced data processing tools combined with advanced chemometric techniques, like Affinity Propagation for clustering, Ant Colony Optimization (ACO) for feature selection and Random Forest for prediction (ACO-RF/RF). The developed workflows have been implemented in different food authenticity studies, like the varietal discrimination or the discrimination of organic and conventional Extra Virgin Olive Oils, the characterization of honey based on its botanological and geographical origin, the detection of milk and feta adulteration and the detection of juice-to-juice adulteration. Furthermore, different applications of MS-based metabolomics have been used to answer challenging issues of the food industry, like questions on the packaging material migration, composite food analysis and new (bio)markers for fish freshness (in refrigerated products) and many more other examples.

"We acknowledge support of this work by the project «FoodOmicsGR Comprehensive Characterisation of Foods» (MIS 5029057) which is implemented under the Action Reinforcement of the Research and Innovation Infrastructure <http://www.antagonistikotita.gr/epanek_en/proskliseis.asp?id=28&cs=>, 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)"

OP13 FOODOMICS APPROACH TO ASSESS FOOD AUTHENTICITY. TWO PARADIGMS ON GRAPES AND ROYAL JELLY SAMPLES

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Food authenticity is a global issue, with extensive economic, social, health and environmental impacts. The intention of fraud high quality food products is to mislead consumers by adding sub-standard and cheaper grades for financial gain. Such activity can involve harmful, or unfit for human consumption food products mislabelled or misdescribed in some form. Metabolomics (both targeted and untargeted) and specifically Foodomics represents a field that offers the ability to assess food safety and quality at every stage of production to ensure food safety for human consumption. It is the discipline that studies food and nutrition through the application and integration of advanced omics technologies to improve consumer's well-being, health, and knowledge. Likewise, foodomics can play a major role in the investigation of different topics closely related to food traceability, such as authenticity, thanks to the discrimination of expected and unexpected metabolites in a specific food product.

An untargeted LC-HRMS profiling method was applied to map metabolic profile of grapes collected from three vineyards from Lemnos Island at different days and of must during every day of alcoholic fermentation and monitor their differentiation among vineyards, grape ripening periods and throughout alcoholic fermentation period. Current developments on mass triple quadrupole instrumentation along with advanced software capabilities resulted in development of tailored-made targeted metabolomics methods able to (semi)- quantify tens of analytes of specific interest in a single injection and provide solid, quantitative and unambiguous data. Such a method was developed in our lab and applied to Royal Jelly samples in order to assess differences in the metabolic content of samples from artificial bee feeding with protein and sugar supplements compare to non-feeding.

"We acknowledge support of this work by the project «FoodOmicsGR Comprehensive Characterisation of Foods» (MIS 5029057) which is implemented under the Action Reinforcement of the Research and Innovation Infrastructure <http://www.antagonistikotita.gr/epanek_en/proskliseis.asp?id=28&cs=>, 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)"

OP14 HRMS STUDY OF BIOACTIVITY COMPOUNDS DURING EDIBLE OLIVE PROCESSING

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Olives are the fruits of the olive tree (Olea Europaea) and they are largely consumed mostly in the Mediterranean countries. Table olives belong in high value foodstuff due to their great content of bioactive compounds, related to many biological properties such as antioxidant activity. Raw olives cannot be consumed due to the presence of the bitter glycoside, oleuropein and many processing methods have been developed worldwide in order to produce a safe and comestible product [1]. Thus, the determination of the bioactive profile of olives during processing is of great importance as it is strictly connected to the nutritional and commercial value of the product. For this purpose, an in-house UPLC-ESI-QTOFMS methodology was developed in order to determine the bioactive profile of table olives.

Two types of experiments were conducted in order to study the variation of bioactive compounds during edible olive processing. The first one consists of two stages of debittering with diffusion of olives in water, while the second one includes one stage of debittering with the use of dry salt. For these experiments three different varieties of olives were utilized. A database consisting of 49 phenolic compounds, encountered in olives, was used in order to identify and quantify these compounds in all samples. The target screening approach was performed using Bruker TASQ 1.4 software. The identification criteria were mass accuracy, retention time, isotopic fitting as well as MS/MS fragments. The quantification of phenolic compounds was performed using standard calibration curves. After the debittering steps, a reduction of bitter secoiridoids such as oleuropein was reported, along with simultaneous increase in the content of their hydrolysis products (hydroxytyrosol, tyrosol). The daily intake of edible olives corresponding to a health claim according the Regulation 432/2012 of the European Commission was calculated, exploiting their health promoting role.

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This research has been financed by the Region of the North Aegean through the program “Novel wide-scope research for the promotion of N. Aegean olive oil and olive products through the designation of their unique characteristics and bioactive content”.

IL03 ADVANCES IN HIGH RESOLUTION MASS SPECTROMETRY FOR METAL SPECIATION ANALYSIS

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The introduction of coupled methods combining a chromatographic separation step with element-specific detection, most often by inductively coupled plasma mass spectrometry (ICP MS), has been a decisive factor in the rapid progress of metal speciation analysis. The success of these methods depends critically on the chromatographic separation power and the purity of peaks used for quantification. Therefore, the approach shows considerable limitation in the analysis of complex matrices as well as in the cases when standards of the analytes are unavailable.

The ultimate proof of the species identity can be obtained by its molecular signature confirmed by the fine isotopic structure. It can be achieved if the separation is good enough to distinguish species with masses differing by one electron. Hence, the analytical challenge is shifted from the chromatographic peak capacity to the peak capacity in a mass spectrum. The detected feature is not the elemental but the molecular isotopic pattern of the analyte compound.

Resolution powers down to a single electron mass and below can be obtained by Fourier transform mass spectrometry, either using ion cyclotron resonance (FT-ICR) or orbital trap (FT-Orbitrap), which has opened new horizons in speciation studies of metal or metalloid- containing compounds at trace concentration levels. The lecture discusses the opportunities offered by FT-MS approaches for speciation analysis. The effect of data acquisition and treatment parameters (transient duration, magnitude vs. absorption mode, search for metal isotope patterns in data sets) will be discussed. Sensitivity, resolution, risk for false positives/negatives, and quantification strategies will be compared with canonical procedures using the ICP MS detection. In particular, comprehensive approaches aiming the identification of a large number of metal or metalloid containing species in a single run (metallomics) will be discussed.

MONDAY, SEPTEMBER 23RD, 2019

EVERGETON HALL

Mass spectrometry

Chair: ***H. Frank, S. A. Pergantis***

OP15 MASS SPECTROMETRY TECHNIQUES IN FORENSIC TOXICOLOGY

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A forensic toxicology laboratory is called to analyze a variety of biological specimens, such as hair, urine, blood, and oral fluid. The biological matrices of these specimens pose varying screening challenges, which demand a continuing research on the development of more innovative methodologies to reduce analyses time, enhance sensitivity, and enable the detection of more substances, while increasing the capacity of laboratories to offer a range of services. Health clinics, psychiatric hospitals, prisons, and physician practices working in addiction medicine are examples of institutions benefiting from such services.

The most important analytical technique used in toxicological forensic analysis is mass spectrometry. Mass spectrometry coupled with chromatography techniques is preferred for the identification of new drugs or metabolites, through screening analysis, providing excellent precision, accuracy, and sensitivity. Toxicological drug screening, also known as general unknown analysis—a broad screening method that screens for a broad range of substances, is traditionally conducted with GC-MS techniques. However in recent years it has been steadily replaced by liquid chromatography coupled to mass spectrometry (LC-MS) methods. The main reason LC-MS is increasingly favored over GC-MS is the reduction in sample preparation time. However, sample complexity complicates the identification among compounds with similar fragmentation patterns, along with the problems caused by ionization chemical suppression. On the other hand, new psychoactive substances are breaking into the market at a rapid rate, which means some drugs may be missing from the current mass spectra libraries. Therefore, recent and future developments in mass spectrometers should be followed by the creation of new softwares in order to improve simplicity and robustness in the identification of drugs, and simultaneously, new methods must be constantly developed, so laboratories can keep pace with the new psychoactive substances market.

OP16 DETAILED PHYTOCHEMICAL ANALYSIS OF AN *ARTEMISIA ANNUA* AND AN *ARTEMISIA ABSINTHIUM* EXTRACT USING A COMBINATION OF NMR AND HPLC/DAD/MS TECHNIQUES

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Artemisia annua (Asteraceae), which has been used for many centuries in Chinese folk medicine for the treatment of fever and malaria, is the only natural source of artemisinin. Artemisinin-based combination therapies have been recommended worldwide as first-line treatment of falciparum malaria [1]. The ability to detect artemisinin and its known analogues in plant extracts is an especially difficult task since the compounds are present in very low concentrations, are thermolabile, and lack UV or fluorescent chromophores [2].

As a follow-up of our studies on the use of NMR spectroscopy in mixture analysis of plant extracts [3,4], NMR methods were implemented for the simultaneous determination and quantification of artemisinin and its analogues and flavonoids in an *Artemisia annua* extract. The analytical results were confirmed with HPLC/DAD/MS measurements. Also an *Artemisia absinthium* extract, selected from wild populations growing in Epirus (Greece), was analyzed and the transformation of its major component in a solution with chloroform-d was observed using NMR spectroscopy.

In this work the combination of 2D $^{1}H–^{13}C$ HSQC with the $^{1}H–^{13}C$ HMBC techniques allows the rapid, systematic, and complete assignments of artemisinin and five of its analogues along with flavonoids, camphor and an aromatic ketone (in total 13 compounds) in a complex diethyl ether *A. annua* plant extract. The identification of 11 compounds was confirmed using LC/DAD/ESI-MS^{n} (camphor and aromatic ketone were not identified). Qualitative and quantitative results obtained using an NMR method are described. The results were found in good agreement with those obtained with the use of the time consuming HPLC-DAD and LC-MS/MS, for the compounds that standards were available.

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OP17 DETERMINATION OF POLYCHLORINATED BIPHENYLS IN MUSSELS USING QUECHERS IN COMBINATION WITH GC-MS

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Polychlorinated biphenyls (PCBs) are organic chlorine compounds with the formula $C_{12}H_{10-x}Cl_x$ and have been widely used as dielectric and coolant fluids in electrical apparatus. Because of their longevity, PCBs are still widely in use, even though their manufacture has declined drastically since the 1960's when they have been demonstrated to cause a variety of adverse health effects. They have been shown to cause cancer in animals as well as a number of serious non-cancer health effects in animals such as effects on nervous system and reproductive system. Studies in humans support evidence for potential carcinogenic and non-carcinogenic effects of PCBs. Therefore, PCB production was banned by United States federal law in 1978 and by the Stockholm Convention on Persistent Organic Pollutants in 2001. Persistent organic pollutants such as PCBs are repeatedly detected in marine waters and biota. Mussels are filter feeders leading to their use as biological indicators for the monitoring and evaluation of pollution in the studied ecosystems. Therefore, the aim of the present study was the development of an analytical method for the simultaneous determination of fourteen (14) widely used PCBs in mussel samples from North Western Greece. More specifically, a QuEChERS extraction method followed by GC-MS methodology was applied. Good linearity was obtained in all cases exhibiting excellent coefficients of determination (R^2). The method precision achieved in terms of repeatability and within-lab reproducibility was low enough, expressed as relative standard deviation (R.S.D.). Recoveries obtained were satisfactory for all metabolites (above 70%) while limits of detection found at the low ppb level (1 ppb - 10 ppb). The proposed methodology was successfully applied to determine the pollutant load of mussels from seawater ecosystems near aquaculture facilities in North Western Greece.

OP18 MAGNETIC SOLID-PHASE EXTRACTION OF PESTICIDES IN NATURAL WATERS USING Fe3O4@SiO2@C18 NANOPARTICLES AS ADSORBENT COUPLED TO GC-MS DETERMINATION

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The occurrence of pesticides and their conversion products in aquatic system is one of the major environmental problems worldwide. These residues may cause long-term adverse effects to the aquatic environment, and even harm human life. Sample pre-treatment procedures are crucial for the whole analysis process, which aim at enriching targeted analytes and eliminating matrix effect. Magnetic solid-phase extraction (MSPE), has drawn extensive attention in sample preparation in recent years [1- 2]. Is a new mode of SPE based on the adoption of magnetic nanoparticles (MNPs) as sorbents, at micro- or nano-scale and shows great advantages in separation science. A rapid magnetic solid-phase extraction (MSPE) method coupled to Gas Chromatography-Mass Spectrometry (GC-MS) was developed for the simultaneous extraction of ten pesticides belonging to various categories (insecticides, herbicides and fungicides) in environmental water samples. The magnetic Fe_3O_4@SiO_2@C18 nanoparticles were synthesized by coprecipitation of Fe^{2+} and Fe^{3+}ions, at alkaline conditions, under hydrothermal treatment and used as adsorbents of MSPE. The proposed method is optimized by means of experimental design and response surface methodology. Under optimal conditions, the MSPE-GC-MS method presented fast simple separation and analysis, and excellent linearity in the range of 6.4-5000.0 ng/L, with coefficients of determination (R^2) higher than 0.9901 for all compounds. Moreover, the performance of the MSPE method was compared to a conventional SPE and the MSPE method was comparable. Finally, the optimized method was applied in a case-control study carried out in Rivers Aliakmonas, Loudias and Axios (Macedonia Region-North Greece). The magnetic Fe_3O_4@SiO_2@C18 composites based MSPE method proved promising for convenient and efficient determination of pesticides in environmental water samples.

MONDAY, SEPTEMBER 23RD, 2019

LORDON BYRON

Metabolomics

Chair: ***J. Szpunar, I. Malollari***

OP19 NMR IN NATURAL PRODUCTS: CHEMICAL ANALYSIS OF COMPLEX MIXTURES, BIOANALYTICAL AND METABOLOMICS APPLICATIONS AND DFT NMR STRUCTURES OF ANALYTES

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A critical overview of recent analytical developments of NMR spectroscopy in natural products will be provided with emphasis in the following applications:

(i) chemical analysis of extracts without isolation or derivatization steps [1], including 'in situ' direct monitoring of dynamic changes of metabolites [2], enzymatic reaction products [3], real time biotransformation monitoring [4] and metabolomics analysis [5].

(ii) "in-cell" NMR in decoding the apoptotic activity of flavonoids [6] and artemisinin with the Bcl-2 family of proteins and

(iii) quantum chemical calculations of high resolution structures of analytes in solution based on NMR chemical shifts [7].

Acknowledgments

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OP20 NMR-BASED METABOLOMICS OF THE LIPID FRACTION OF ORGANIC AND CONVENTIONAL BOVINE MILK

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Origin and quality identification in dairy products is an important and challenging issue. The objective of the present work (1) was to compare the metabolite profile of the lipid fraction of organic and conventional bovine milk using NMR metabolomics analysis. ^{1}H NMR and 1D TOCSY NMR methods were performed on extracted lipid fraction of lyophilized milk: 14 organic and 16 conventional retail milk samples (collected monthly) and 64 (58 conventional and 6 organics) from the farm milk samples collected over a 14-month longitudinal study in Cyprus. Data were treated with multivariate methods (PCA, PLS-DA) and a normalization of the data series was proposed, thus each analyte was expressed as % content in the lipid fraction of each sample resulting group discrimination (Figure). Moreover, minor components were identified and quantified and modification of the currently used equations was proposed. Results showed discrimination between organic and conventional milk produced in Cyprus with differences mainly being assigned to specific fatty acids. Increased % content of conjugated (9-*cis*,11-*trans*)18:2 linoleic acid (CLA), α-linolenic acid, linoleic acid, allylic protons and total unsaturated fatty acids (UFA) and decreased % content for caproleic acid were observed in the organic samples compared to the conventional ones. The present work confirms that lipid profile is affected by contrasting management system (organic vs. conventional) and supports the potential of NMR-based metabolomics for the rapid analysis and authentication of the milk.

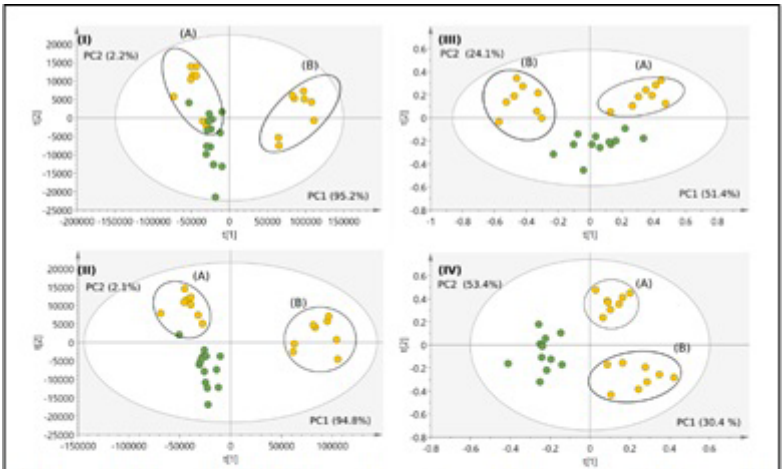

Figure. PCA and PLS-DA analyses Score plots on the UNor and NorCont data of the lipid fraction of organic and conventional processed (P) milk samples. (I) PCA score plot and (II) PLS-DA score plot of UNor procedure, (III) PCA score plot and (IV) PLS-DA score plot of the NorCont procedure. Yellow circles for conventional and green circles for organic samples; conventional milk samples consisted of: (A), 1.5% fat content and (B), 3.0 % fat content.

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OP21 UN-TARGETED METABOLOMICS APPROACH FOR THE CHARACTERIZATION, CLASSIFICATION AND MAPPING OF BIOACTIVE COMPOUNDS IN GREEK EXTRA VIRGIN OLIVE OIL

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Extra virgin olive oil (EVOO) has been declared as a main component of the Mediterranean diet, both for its distinctive taste, but foremost for its high nutritional value. Due to its beneficial nutritional properties, olive oil is often subjected to economically motivated adulteration (EMA). Health claim established for the polyphenols of olive oil (Commission Regulation (EU) 432/2012), indicating that olive oil polyphenols contribute to the protection of blood lipids from oxidative stress, has raise awareness for the quality assurance of the olive oil authenticity and has also contributed to the further in-depth study of bioactive compounds. The present study focuses on the characterization and the classification of Greek EVOOs, identifying their bioactive compound profile following an un-targeted metabolomics approach. More specifically, a number of 452 Greek EVOO samples were collected from North Aegean islands, varying in terms of variety, cultivar, agronomic techniques and processing technologies. Their bioactive metabolic fingerprint was determined using ultra-performance liquid chromatography-quadrupole time of flight mass spectrometry (UPLC-QToF-MS). New compounds were detected and identified through suspect screening with an in-house MS-ready database of 1600 compounds that have been previously reported to exist in olive oil. The data set was treated using advanced chemometric techniques, achieving adequate classification and mapping of the samples as well as the identification of unique biomarkers that could indicate olive oil origin, cultivar and techniques applied during the olive oil production.

Acknowledgement:

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MONDAY, SEPTEMBER 23RD, 2019

EVERGETON HALL

ICP-MS

Chair: ***G. Hieftje, N. Thomaidis***

IL04 ICP/ELECTROSPRAY MASS SPECTROMETRY FOR STUDIES OF THE UPTAKE AND METABOLISM OF NANOPARTICLES

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The extensive use of metal-containing nanoparticles in an increasing number of applications is leading to their release into the environment. Their interaction with plants may affect plants physiological processes and eventually lead to the bioaccumulation of nanoparticles, and products of their metabolism, in the animal and human food chain. In this context, the investigation of the behaviour of the nanoparticles throughout the whole process of interaction with plants - uptake, bioaccumulation, translocation and possible metabolism - is needed. However, such a challenge requires the use of a number of techniques providing complementary information.

The lecture presents the results obtained for studies of the interaction of a number of metal (Pt and Pd) and metal oxide (ZnO and CeO_2) NPs with plants. Owing to a multi-technique analytical approach based on elemental (ICP) and molecular (ESI) mass spectrometry, the behaviour of the NPs could be investigated throughout the whole process: (i) the stability of NPs in growth media was studied by single particle inductively coupled plasma mass spectrometry (SP-ICP-MS); (ii) the bioaccumulation of NPs was determined by conventional ICP-MS after acid digestion; (iii) the physicochemical form of the nanoparticles taken up by plants was characterized by SP-ICP-MS after enzymatic digestion of different plant organs; (iv) the species created within the plant as a result of the NPs metabolism were identified by (two-dimensional) liquid chromatography coupled to ICP-MS and electrospray ionization Orbitrap MS^n (ESI Orbitrap MS^n) and, finally, (v) the localization on of the metal within the plant tissue was investigated by laser ablation (LA)- ICP-MS.

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OP22 ADVANCEMENTS AND CHALLENGES FOR THE DETERMINATION OF METALS IN INDIVIDUAL CELLS USING SINGLE CELL INDUCTIVELY COUPLED PLASMA - MASS SPECTROMETRY

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Inductively coupled plasma-mass spectrometry (ICP-MS) is a major analytical technique in the field of metallomics, mainly because of its high sensitivity, low interferences and thus low detection limits. While there is a multitude of studies reporting on the use of ICP-MS in conventional mode, that is by analyzing a sample following acid-digestion, in order to determine the total metal concentration in tissues or cell cultures, questions on whether this metal concentration is distributed in a uniform pattern (homogenously) amongst the cells still remain. Single Cell ICP-MS (SC ICP-MS) attempts to fill this gap by quantitating metals in individual cells, and thus offers insight regarding metal uptake on a per cell basis.

The operation of SC ICP-MS involves the introduction of dilute cell suspensions (10^5cells mL^{-1}) into a high-temperature argon plasma mainly through, but not limited to, a pneumatic nebulizer. Upon arriving to the plasma, each single cell is atomized to its constituent elements, the elements and their isotopes are ionized and the resulting ions are detected as a single pulse above a constant background. The latter requires fast data acquisition and the application of extremely low dwell times (ms to μs range) in order to capture the cell detection events which range from 0.2-0.6 ms.

In this work, unicellular cultures of *Chlamydomonas reinhardtii*cells are exposed to different concentrations of pentavalent arsenic [As(V)] as arsenate, tetravalent selenium [Se(IV)] as selenite and hexavalent [Se(VI)] as selenate, and each cell culture will be analyzed for their As and Se content with ICP-MS in Single Cell and Conventional mode. In addition to the analysis of a relatively robust in terms of osmotic stress cell line like *Chlamydomonas reinhardtii*, attempts will be carried out to expand the technique's measurement capability to determine the iron (Fe) content of mouse macrophages, a mammalian-type cell line, by enhancing the technique's tolerance towards conventional buffers and common cultivation media. Finally, attempts will be made in providing improved SC ICP-MS validation by improving the existing calibration procedures.

OP23 SINGLE PARTICLE AND SINGLE CELL ICP-MS ALLOW NEW INSIGHTS TRACKING NANOPARTICLE FATE AND ECOLOGICAL EFFECTS

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Monitoring the presence of engineered, natural or incidental nanomaterials, particularly metallic or metal-containing nanoparticles (NPs) in environmental systems is essential to understand their potential ecotoxicological implications. To date, it has been challenging to detect and quantitatively analyze the concentration of metallic or metal-containing NPs in environmental samples.

Here we developed a fast and simple protocol to monitor the concentrations of NPs in environmental waters. Fast scanning techniques allow for the quantitative analysis of a full suit of elements leading to multi-element analysis via SP-ICP-MS in a single sample acquisition. The particle size, concentration and distribution, along with the dissolved concentration, is quantified for each element. With the aid of all matrix sample dilution (AMS), an online sample dilution with argon, this multi-element analysis is possible in all environmental samples from tap water to sea waters without prior dilution making it an ideal tool for the environmental monitoring of NPs.

For ecological studies, Single Cell ICP-MS enabled us to assess the interaction of metal-containing nanoparticles at the individual cell. It allows the monitoring of both intrinsic (nutrient) metals within the cell as well as the uptake or adsorption of contaminant metals or NPs within environmental systems.

The talk will explain how to operate single particle ICP-MS and single cell ICP-MS for nanoparticle analysis. Application examples of single particle and single cell ICP-MS will be discussed.

OP24 IMPROVEMENTS AND APPLICATIONS OF A NOVEL ORTHOGONAL SONIC-SPRAY IONIZATION SOURCE FOR COUPLING MICROBORE AND CONVENTIONAL HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY TO TANDEM MASS SPECTROMETRY

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The aim of this study was the development of an interface for the efficient coupling of microbore and conventional high performance liquid chromatography to Sonic- spray ionization Mass spectrometry (SSI- MS). For this purpose we examined the use of a voltage- free cylindrical rod in order to bend the spray coming from the SSI nebulizer around the rod and into the ion inlet orifice of the mass spectrometer. A significant difference of this newly developed SSI interface compared to the recently introduced electrospray based Unispray™ [1] source is that no electrical potential is applied to the cylindrical rod. The data obtained in the study were acquired using a triple quadrupole mass spectrometer TSQ Quantum (Thermo Scientific), fitted with a homebuilt SSI source to which a cylindrical rod has been added off- axis to the spray. The nebulizer used with the Sonic- spray ionization source was placed at a 90^{o} angle to the mass spectrometer inlet. This source allows for enhanced sensitivity and the ability to operate under high flow rates ranging from 50-800 μL min^{-1}. It therefore enables for the convenient coupling of conventional and microbore HPLC columns to a mass spectrometer. Several examples using HPLC with this new SSI interface for the analysis of various types of samples, including amino acids separations, arsenic speciation analysis, as well as metabolomics analysis, will be presented. Analytical figures including limits of detection, robustness, accuracy and stability will be presented, as well.

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P1-01 PREPARATION OF NANOCERIA CONJUGATES FOR BIOANALYTICAL ASSAYS

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Enzymes, such as phosphatase, peroxidase and galactosidase, are used extensively as reporters in bioanalytical assays, especially immunoassays and nucleic acid hybridization assays, due to the signal amplification introduced through substrate turnover. The aim of the present work is to exploit the oxidase-like catalytic properties of cerium oxide nanoparticles for the preparation of reporters for protein and DNA assays. Because the biotin-avidin interaction is of fundamental importance for the development of antibody- and nucleic acid-based assays we prepared nanoceria-streptavidin conjugates that maintain both the oxidase-like activity of nanoceria and the high affinity of streptavidin for biotinylated molecules. We investigated various approaches of synthesis and surface modification of cerium nanoparticles with -COOH groups starting from aqueous solutions of $Ce(NO_3)_3$. One synthetic approach involved controlled alkaline precipitation in a 25% NH_3 solution in the presence of ethylene glycol (at 60 ^oC) followed by sodium citrate treatment. The optimum oxidase activity of nanoceria was at a Ce^{3+}: citrate molar ratio of 6:5. The average diameter of nanoceria was found, by transmission electron microscopy (TEM), to be 2.4 nm. In another synthetic approach we mixed Ce^{3+} with polyacrylic acid (PAA, Mr=1800) followed by controlled alkaline precipitation. The optimum Ce^{3+}:PAA ratio was 10:1 and the average size of nanoceria was 1.5 nm. The oxidase activity of nanoceria was assessed by using 0.5 mM 3,3,5,5'-tetramethylbenzidine (TMB) as a chromogenic substrate at an optimum pH of 4.5. The synthesized nanoceria was conjugated to 12 mg/mL streptavidin using 0.24 g/mL N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride. The conjugate was purified from the free streptavidin and free nanoceria by size exclusion chromatography on a Sephacryl S200 column. The functionality of the conjugate was evaluated by using microtiter wells coated with biotinylated albumin. The absorbance was measured at 450 nm by a microplate photometer.

Acknowledgement

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search 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).

P1-02 CHEMICAL COMPOSITION AND EVIDENCE FOR A SELECTIVE ANTICANCER ACTIVITY OF HELLEBORUS CYCLOPHYLLUS BOISS ON A549 CANCER CELL LINE

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Plant extracts are becoming popular sources for bioactive compounds. In the present study we determined the chemical profile and investigated the ability of *Helleborus cyclophyllus* Boiss methanol extract to induce cell death on a human lung adenocarcinoma cell-line (A549). The type of cell death and the selectivity of this activity towards cancer cells were investigated using a primary human lung fibroblasts' (PHLF) cell line, as a model of normal-healthy cells.

The chemical composition of the methanol extract was assessed by preparative high performance liquid chromatography (HPLC) followed by liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis, using the Orbitrap hybrid mass analyzer. To monitor the effect of *H. cyclophyllus* extract on the morphology of A549 cells and PHLF, a dose- and time-dependent experiment was conducted. After treatment, cells stained by haematoxylin-eosin and observed by an optical microscope.

The phytochemical analysis revealed the presence, among others, of hellebrin, hellebrigenin, deglucohellebrin, 20-hydroxyecdysone, polypodine b and 2-deoxy-D-ribono-1,4-lactone. A549 cells exposed for 3 and 6 h to the extract showed a wavy cell membrane and the formation of vesicles (Ectosomes). However, after 24 h of exposure, A549 cells were detached. The formation of a big vesicle into the cell cytoplasm (thanatosome), the margination and compression of the nucleus at the periphery of the cell, the presence of binucleated cells and the formation of apoptotic bodies were observed. Untreated A549 cells and PHLF were not affected. According to our best of knowledge, this sequence of events leading selectively cancer cells to apoptosis, has not been reported before.

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P1-03 A NOVEL ELECTROCHEMICAL SENSOR BASED ON REDUCED GRAPHENE OXIDE AND MOLECULAR IMPRINTED OVER-OXIDIZED POLYPYRROLE MODIFIED GOLD NANOPARTICLES FOR AMOXICILLINE DETECTION

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An electrochemical sensor for amoxicillin (AMX) detection based on reduced graphene oxide (RGO), molecular imprinted overoxidized polypyrrole (MIOPPy) modified with gold nanoparticles (AuNPs) is described in this work. The electrochemical behavior of the imprinted and non-imprinted polymer (NIP) was carried out by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The structure and morphology of the prepared MIP sensor were characterized by scanning electron microscopy (SEM), UV-Visible (UV-Vis), Fourier transform infrared spectroscopy (FTIR) and its experimental parameters such as monomer and template concentration, pH buffer solution, incubation time of AMX and AuNPs, scan rate as well as electropolymerization scan cycles were investigated and optimized to improve the sensor's performance. The peak current obtained at the MIP electrode was proportional to the AMX concentration in the range from 10^{-8} to 10^{-3} mol L^{-1} with a detection limit (LOD) and sensitivity of 9.55×10^{-9} mol L^{-1} and 2.28×10^{-6} µA mol^{-1} L, respectively. It was also found that this sensor exhibited reproducibility and excellent selectivity against molecules with similar chemical structures. Besides, the analytical application of the AMX sensor confirms the feasibility of AMX detection in milk and human serum.

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P1-04 DETECTION OF MYCOBACTERIUM AVIUM SUBSPECIES PARATUBERCULOSIS IN INFANT FORMULAS BY CULTURE, PCR AND COMBINED PHAGE-PCR

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Mycobacterium avium subspecies *paratuberculosis* (MAP), the causative agent of Johnes disease in cattle and other ruminants, may have a role in the development of Crohn's disease in humans. The presence of MAP in infant powder milk has been demonstrated in the past by both culture and PCR based methods and can be due to process contamination or the survival of the organism in the powder matrix during the manufacturing process. MAP can form clumps, making it more heat resistant and given also the coating with milk proteins and fat, viable cells could escape besides oven's efficacy. The objective of this study was to investigate different infant milk-based formulas for the presence of MAP by culture and PCR and also the combined phage-PCR method which is rapid, sensitive and can giving a fast indication for the presence of viable mycobacteria in the samples. A total of 35 samples from a total of ten different producers were analyzed. Following reconstitution and decontamination all samples were cultured for MAP onto Herrold's Egg Yolk Agar with Amphotericin, Nalidixic Acid, Vancomycin, with Mycobactin J and incubated for a period of 6 months. Samples were also processed through an IS900 PCR assay to identify the presence or verify the absence of MAP DNA. Finally, reconstituted samples were processed through the phage amplification assay and the plaques were extracted for PCR identification. Phage-PCR assay detected viable MAP in 13% (4/32) of PIF samples. Culture detected viable MAP in 9% (3/32) PIF samples, all of which were also phage-PCR positive. Direct IS900 PCR detected MAP DNA in 22% (7/32) of PIF samples. The presence of MAP in infant formulas highlights the need to decrease the risk of exposure for infants and young children by assuring that skim milk intended for the manufacture of formulas is be from MAP free herds.

P1-05 INORGANIC ANALYSIS OF TEA SAMPLES USING ENERGY-DISPERSIVE X-RAY FLUORESCENCE SPECTROMETRY AND MULTIVARIATE VARIANCE ANALYSIS

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In this work, samples of green and black *Camellia sinensis* tea were analyzed using the energy-dispersive X-ray fluorescence spectrometry. Each sample was measured in the form of leaves, loose powder and pellets (52 samples of each type), to see the influence of sample preparation on reliability of the results. Twenty elements were determined in most of 156 samples. The accuracy of the results was evaluated by measuring certified reference materials in two forms, the loose powder and pellets. Since the pellets gave the most accurate and precise results, further studies were conducted based on them only. Evaluation of statistical significance of the fermentation process on the element composition of tea samples was performed, based on the ANOVA Simultaneous Component Analysis (ASCA) [1]. Distribution of the null hypothesis (obtained based on permutation test) clearly showed that the fermentation process is statistically significant (at the significance level 0.05) and it affects the content of elements in the studied black and green tea samples. The bootstrapping method used to calculate the confidence intervals of the principal components loadings allows identification of elements relevant to differentiation of the analyzed tea types. The performed study gives evidence that inorganic analysis based on the X-Ray fluorescence followed by multivariate analysis of variance allows differentiation of the green and fermented tea samples.

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P1-06 FT-IR SPECTROSCOPY IN COMBINATION WITH CHEMOMETRICS FOR THE DETERMINATION OF THE GEOGRAPHICAL ORIGIN OF EXTRA VIRGIN OIL

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Olive oil is a typical Mediterranean food product. Due to its high nutritional value its consumption is being increasing. Greek regions produce one of the best extra virgin olive oil (EVOO) qualities worldwide. Since EVOO from certain regions have an added value, they may reach a higher market price. Thus, cases of frauds and misleading information concerning their origin are frequent. In this regard, nowadays quality and authenticity topics are of major concern not only for manufactures and customers but also for administrative authorities. Although various quality control methods do exist, methods that determine the origin of an olive oil remain a challenging problem. In this regard the development of new and/or improved, quick and low-cost analytical methods to ensure authenticity and origin of olive oil is imperative. FT-IR technique in combination with chemometric analysis is among the most promising analytical methods for determining the geographical origin of food products. FT-IR spectroscopy allows fast and non-destructive analysis of samples. The resulting spectrum is characteristic of each sample and provides its chemical ''fingerprint''. The aim of the present study is to classify EVOO produced from different Greek regions using FT-IR spectroscopy and chemometrics. Samples from Lakonia (n=10), Messinia (n=16) and Heraklion areas (n=12), provided from local producers, were analysed. FT-IR spectra were recorded using attenuated total reflectance (ATR) device on a Nicolet 6700 FT-IR spectrometer. Discriminant analysis was performed using SPSS software v. 23.0 and TQ Analyst software ver. 8.0.0.245. The 1779-1704 cm^{-1}, 1216-1043 cm^{-1} and 781-659 cm^{-1} spectral regions were used for both analysis. Results showed that FT-IR analytical technique along with chemometrics analysis may be successfully used to determine the geographical origin of an olive oil.

P1-07 SPECTROSCOPIC-CHEMOMETRIC METHOD FOR THE INVESTIGATION OF HONEY BOTANICAL ORIGIN

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Fourier-transformed infrared spectroscopy (FT-IR) is a well-established technique for the analysis of the physical-chemical parameters of honey. The authentication of botanical origin of honey is of high importance since it affects its commercial value. In this study FT-IR spectra of 36 honey samples from three honey types (eight thyme, 13 pine, 15 fir) were obtained in triplicates without any sample pretreatment, using a Nicolet 6700 FT-IR in the attenuated total reflectance (ATR) mode with DTGS detector. Collection and processing of spectral data was carried out using OMNIC ver. 7.3. Botanical origin discrimination was achieved performing discriminant analysis (DA) using two software packages, the TQ Analyst software ver. 8.0.0.245 and the SPSS ver. 23.0 software. Samples were divided in three groups (thyme, pine, fir) and the spectral region 1760-650 cm^{-1} was used for the discrimination. A chemometric model was developed by the TQ Analyst using 31 honey samples for calibration and 5 samples for validation. 14 principal components were used which described 100 % of variability. Correct classification was accomplished for the 87.1 % of samples and 80.0 % of the validation set samples were correctly classified. Using the SPSS, two different independent discriminant functions were computed by canonical discriminant analysis. The Wilks λ values for the two discriminant functions were 0.162 and 0.563, indicating a good discriminant power of the model. Eigenvalues suggest that the first discriminant function was more discriminating with high canonical correlation (0.844) which explained 76.1 % of the total variance. The percentages of correct classification and validation were 83.3 % and 58.3 %. The obtained DA results are very promising and indicate the potential use of FT-IR spectroscopy and chemometrics as a rapid, low-cost method for the discrimination of different honey types.

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P1-08 CHEMISTRY STUDENT'S KNOWLEDGE AND AWARENESS ABOUT BASIC FOOD CONSTITUENTS, THEIR FEATURES AND ROLE

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We present part of a doctoral thesis about third-year chemistry students' knowledge and awareness of the main food constituents. The study was conducted for two consecutive academic years (2014-15 and 2015-16), in the Department of Chemistry of the University of Ioannina, within the context of a laboratory course on "Food Analysis and Technology". Students were informed in advance about the research character of the study, while the voluntary nature of their participation and the fact that their anonymous participation would have no consequence on their overall assessment and marking of the course were made clear to them. A sample of 110 students answered a questionnaire on carbohydrates, while another sample of 113 students answered a questionnaire on proteins and fats. Concerning carbohydrates, the questions dealt with their characteristics, the reasons why we eat them, and the consequences for the human health of eating foods rich in carbohydrate. The role of fiber in nutrition has also been analyzed. As for proteins, the questions concerned their characteristics and the reasons why we eat them, including questions about soybeans. Finally, with regard to fat, we considered lipids, saturated, mono- unsaturated and poly-unsaturated fatty acids, the quality of the various animal and vegetable fats and vegetable oils, and the reasons for the presence and avoidance of trans-fatty acids in foods. The results showed that the students generally had satisfactory to excellent knowledge and awareness of the topics under consideration.

P1-09 EFFECT OF NATURAL PRODUCTS AGAINST FOODBORNE PATHOGENS

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Worldwide, many people are suffering from foodborne illnesses caused by microbial pathogens whereas other consumers are demanding food products without chemicals which they believe are harmful for their health. Furthermore, another broad problem nowadays is the antimicrobial resistance towards several antimicrobials which can lead to 'super bugs'. Thus, the use of new methods and substances in food processing and packaging for a safer food whilst prolonging its shelf-life is pivotal. These food related issues can be overcome by using natural substances as antimicrobials and preservatives additives in foods. Essential oils (EO's) derived from plants are natural substances that have antimicrobial properties and could be a great alternative dealing with these issues. Therefore, aim of this study was to investigate the antimicrobial effect of three essential oils, deriving from plants, against 12 foodborne pathogens. Carvacrol, Eugenol and *Pistacia lentiscus* essential oils were examined for their antimicrobial effect. *Pistacia lentiscus* leafs were left to dry before extracting the essential oil using hydrodistillation and then characterized for its components with Gas Chromatography/Mass Spectrometry (GC/MS). Disk diffusion assay was performed by adding pure EO's to paper disks located in BHI agar plates previously inoculated with the tested microbes. Broth microdilution method performed in 96 well plates with BHI agar while stock solutions of the EO's were diluted in 20% DMSO. Preliminary results showed that all EO's had antimicrobial effect against the tested foodborne pathogens and the results for Minimum Bactericidal concentration (MBC) and Minimum Inhibitory concentration (MIC) values showed significant antimicrobial activity of the EO's against *Listeria spp.* with inhibition up to 300 μg/ml in some cases and total inhibition at 600 μg/ml.

P1-10 APPLICATION OF MYCOBACTERIOPHAGE FOR RAPID DETECTION AND BIOLOGICAL CONTROL OF MYCOBACTERIA IN DAIRY PRODUCTS: THE CASE OF PARATUBERCULOSIS

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Paratuberculosis is a chronic debilitating enteritis of domestic ruminants and other animals caused by *Mycobacterium avium* subspecies *paratuberculosis* (MAP). The bacterium can be excreted in faeces and milk of infected animals. It has long been suspected that exposure to MAP is an important contributing agent, to the development of Crohn's disease in humans. Bacteriophage are viruses infecting only bacteria; thus, do not harm animals and humans. This study applies strictly lytic mycobacteriophage for detection and potential control of paratuberculosis as an example of how other mycobacterial diseases can also be challenged. A potential strategy is to block the source of pathogens in the animal and human populations. To achieve this, firstly, a rapid and sensitive method needs to be developed for the detection of viable MAP. The classical methods for detection are culture based, time consuming and not very sensitive. PCR-based methods are rapid and more sensitive, but they are not able to distinguish between live and dead cells. A rapid and sensitive phage-PCR method was developed, which detects viable mycobacteria in milk and dairy products. The samples are infected with mycobacteriophage which infect only living mycobacteria. An agent which destroys the non-adsorbed phages is then applied to the samples. Following culture on a lawn of sensor cells the formation of plaques is a positive indication for the presence of mycobacteria in the sample examined. DNA extraction from the plaques followed by specific PCR can identify the *Mycobacterium* spp. cells as MAP. Additionally, a lytic mycobacteriophage was examined for the depuration of artificially contaminated milk with *Mycobacterium smegmatis* (MS). Preliminary data from the application of mycobacteriophage suggest at least 2 log reduction after just 8 hours of treatment.

P1-11 IMPROVEMENT OF THE QUALITY OF A GREEK DISTILLATE (TSIPOURO) FROM GRAPES OF THE DEBINA VARIETY WITH THE ADDITION OF SELECTED SUPERFRUITS

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Superfruits are characterized as foods with supposed health benefits, as they contain unique components such as high amounts of antioxidants, polysaccharides, and species-specific phytonutrients. It is reported that they act as antioxidant, detoxifying means and as boosters of the immune system. In the present study, the effect of the addition of selected superfruits [dry golden berries, dry fruits of crataegus (hawthorn) and hippophae] on the quality characteristics of a distillate (tsipouro) from grapes of the debina variety was investigated. Addition was done at concentrations of 1, 3 and 5% and the samples were kept at 20 and 30°C for up to seven months. The antioxidant capacity of the samples was measured using DPPH (2,2-diphenyl-2-picrylhydrazyl) method and the determination of the total phenols was carried out using Folin-Ciocalteu method. The identification and quantification of the volatile constituents were performed by means of solid-phase microextraction (SPME) coupled to gas chromatography/mass spectrometry (GC/MS). In all samples an increase in antioxidant capacity was observed, as a function of time, concentration of added superfruits and temperature, compared to the original distillate. Of the samples studied, the largest increase in antioxidant capacity and total phenols content was found in the distillates to which dry fruits of crataegus and hippophae were added. Also, a number of additional volatile compounds were detected in the spirits studied, compared to the original ones. Most of these substances are thought to have a positive effect on the aromatic profile of the product. The sensory examination showed that the samples to which superfruits were added, exhibit better organoleptic properties. In conclusion, the addition of superfruits to the distillates can have a beneficial effect on human health and can also lead to better acceptance of these products by consumers.

P1-12 EFFECT OF IRRIGATION ON THE BIOLOGICALLY ACTIVE COMPONENTS OF TOMATOES

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Tomato, an annual horticultural plant with worldwide distribution and high economic value, offers beneficial effects to human health through its high content in natural antioxidants including phenolic compounds, vitamins and other nutrients. It has been reported that the levels of the health promoting bioactive compounds and the antioxidant activity of tomato extracts are strongly influenced by agronomic aspects, particularly the genotype, ripening stage, etc. Moreover, it is widely recognized that the protective role of tomato consumption is due to the synergistic effect among the different classes of antioxidants.

The aim of our work was to evaluate the influence of technological (irrigation) and seasonal factors on the content of different secondary metabolites. In our 3-year series of experiments we investigated the effect of irrigation on a Hungarian tomato variety, originated form field experiment. Tomatoes, harvested in the same maturity state were tested for lycopene, beta carotene, tocopherol derivatives, antioxidant capacity and total polyphenol content. Reversed phase HPLC-DAD method were used for quantification of carotenoid components and Vitamin C, normal phase HPLC-FLD method was applied for tocopherol compounds. We investigated the antioxidant capacity (DPPH) and total polyphenol content with classical photometric methods. According to the discriminant analysis, the various years could be distinguished by analysis of secondary metabolites. We found a correlation between the irrigation and the amount of vitamin C and tocopherols. The same effect was found between the concentration of tocopherols and lycopene and Vitamin C content.

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P1-13 A REAL-TIME PCR-BASED METHOD FOR THE IDENTIFICATION OF OLEA EUROPAEA var. SYLVESTRIS (WILD-TYPE OLIVE)

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The wild-type of olive tree, *Olea europaea var Sylvestris* or oleaster, is the ancestor of cultivated olive trees, while it is one of the oldest agricultural tree crops worldwide. It is considered to have more beneficial nutrients for human heath than the common cultivated type of olive (*Olea europaea L.*), leading to a higher nutritional and financial value. For this reason, wild-olive type is very vulnerable to fraud for economic profit. As common- and wild-type olive have similar phenotypes, there is a need to establish criteria to distinguish the wild-type from the cultivated olive. Genetic variations between the two species have been studied using randomly amplified polymorphic DNA (RAPD), amplified fragment length polymorphism (AFLP) and cytoplasmic (chloroplast and mitochondrial) DNA markers, inter-simple and simple sequence repeats (ISSRs and SSRs). In this work, a new method has been developed for the discrimination of *Olea europaea var Sylvestris* from *Olea europaea L*. The method is based on the detection of different nucleotide polymporphisms (SNPs) present in the wild-olive's chloroplastic genome by real-time PCR (Polymerase Chain Reaction). The method includes DNA isolation form olive leaves or oil that is then subjected two amplification using a species-specific primer that contains at its 3' end the SNP of interest and a common primer. The amplicons are detected in real time using the fluorescence DNA intercalating dye, SYBR-Green I. Finally, with this method, we were able to detect as low as 1% content of wild-type olive in binary DNA mixtures of the two olive species.

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P1-14 ASSESSMENT OF MILK PASTEURIZATION USING A SMARTPHONE OR A CONVENTIONAL DIGITAL CAMERA

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The measurement of alkaline phosphatase (ALP) activity is used as a verifying method for pasteurization of dairy products. Alkaline phosphatase exhibits greater thermal resistance than pathogenic bacteria present in milk, therefore its inactivation indicates the destruction of all pathogenic bacteria in milk products. The U.S. and European public health limit for alkaline phosphatase is 350 mU/L. Several methods have been developed for ALP determination with most common the colorimetric, fluorometric and chemiluminometric ones. In the present study we have developed chemiluminometric methods using a smartphone or a digital camera as detectors. As samples, we used pasteurized cow and sheep milk spiked with ALP as well as mixtures of pasteurized and raw (non-pasteurized) milk. Chemiluminescence images acquired by the smartphone and the digital camera were analyzed by the ImageJ software. The signal-to-background ratios at the level of 200 mU/L, for images captured by smartphone, were 3.7 and 2.8 for cow and sheep milk, respectively, while with the digital camera the respective ratios were 7.3 and 5.4. The coefficients of variation (CV) at 200 mU/L, with smartphone as detector, were 8.3% and 4.9% for cow and sheep milk, respectively. For images by digital camera the CVs were 7.9 % and 3.6% for cow and sheep milk respectively. The linearity extends up to 900 mU/L. The lowest detectable percentage of raw milk in pasteurized milk is 0.01% with signal-to-background ratios 2.3 for cow milk and 6.6 for sheep milk in smartphone images and 3.9 for cow milk and 13.2 for sheep milk in images by digital camera. Quantification studies showed that the method can achieve the detection of lower concentrations than the permissible limit of 350 mU/L in a short and low cost protocol.

P1-15 SIMPLE ANALYTICAL METHODOLOGY FOR THE DETERMINATION OF NEONICOTINOID PESTICIDE RESIDUES IN HONEY SAMPLES

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Bees are critically important in the environment, sustaining biodiversity by providing essential pollination for a wide range of crops and wild plants. The majority of crops grown in the European Union depend on insect pollination. They contribute to human health and wellbeing directly through the production of honey and other food and feed supplies such as pollen, wax, propolis and royal jelly. Honey is a natural product produced by Apis mellifera bees and its composition is mainly depended by the floral origin of the nectar. During its production and harvesting, honey may be contaminated by pesticides applied in agriculture and distributed in the environment. These contaminants may be carried on bee bodies or with the forages to the hive, from where they eventually find their way into honey. Honey is a food product with world-wide consumption especially among children and in terms of food safety concern it must be free of chemical contaminants. Among the proposed culprits are pesticides called neonicotinoids, which are supposed to be less harmful to beneficial insects and mammals than the previous generation of chemicals. In view of the important ecological and economic value of bees, there is a need to monitor and maintain healthy bee stocks, not just nationally, but globally. Owing to the complex nature of the honey matrix, there is a consensus on that efficient sample preparation; detection and identification are important aspects of analytical methods to determine pesticides in honey.

This work is focused on the applicability of QuEChERS sample preparation methodology combined with HPLC-DAD for the analysis of 7 neonicotinoid pesticides in honey samples. Good linearity (R^2>0.98) was observed in the 0.01-5 mg/Kg concentration range with RSD values 0.16-6.5%. The method allowed detection of the tested compounds at concentrations below the maximum residue limits required by European and international regulations.

P1-16 GREEK HONEY AND MILK SPECTROSCOPIC ANALYSIS: BOTANICAL CLASSIFICATION, ORIGIN DISCRIMINATION AND ADULTERATION STUDIES

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Quality control in food products is of great importance nowadays. It is often associated with modern analytical methods and procedures which are expensive, time consuming, usually destructive for the sample. Different approaches have been employed with techniques that are of low cost, non-destructive, can provide rapid information and need no special pretreatment of the samples. At IESL-FORTH, we apply optical spectroscopic techniques [Fluorescence, Absorption (UV-Vis-NIR), FT-IR and Raman Spectroscopy] coupled with analysis through machine learning-based modeling for the quick monitoring of the characteristic substances contained in food samples. In this contribution, there are studies concerning commercially available milk samples, differing in animal species and fat content. Optical Spectroscopy has been applied so as to correlate the samples with the different animal origin and the fat percentage. Furthermore, sheep milk samples from different breeding sites in Crete have been studied in order to be discriminated according to the feeding practices. Another product we investigated is honey. We accomplished the distinction of the botanical origin and the correlation with pollen analysis data. These studies demonstrate the potential of the optical spectroscopy as a useful tool in the agro-food products' quality control and as a competent alternative to the classical analytical methods.

P1-17 SPECTROSCOPIC ANALYSIS OF GREEK EXTRA VIRGIN OLIVE OIL: ORIGIN DISCRIMINATION AND ADULTERATION STUDIES

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Lately there has been an increasing demand and strong export activity related to agricultural products, which have a high added value, mainly olive oil. The ultimate goal is the production and distribution of high quality olive oil. Many procedures have been developed in order to assess the quality of olive oil. At the Institute of Electronic Structure and Laser of FORTH optical spectroscopic techniques [Absorption (UV-Vis-NIR), Fluorescence and Raman spectroscopy] coupled with machine learning techniques are applied in order to study the olive oil. In this work we present results obtained by applying optical spectroscopic techniques in extra virgin olive oil (E.V.O.O.) samples from various regions in Greece. Optical spectra were recorded for the investigation of olive oil's origin. Moreover, since the adulteration of extra virgin olive oil with low-quality and inexpensive seed oil is a serious problem in the market, mixtures of E.V.O.O.with different types of seed oils were studied. Their analysis showed low detection limits. Finally, a correlation of tasting results, with spectroscopic data was carried out. These techniques are of low cost, need no special pretreatment of the samples and are capable of providing rapid information and are able to stand as an innovative alternative to the conventional analytical techniques.

P1-18 FATTY ACID PROFILING IN BLOOD OF HEALTHY INDIVIDUALS AND PATIENTS WITH HYPERLIPIDEMIA AND ASSOCIATION

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PNPLA3, CAT, CETP and ABCB1 are enzymes and transfer proteins involved in the metabolism of lipids, and common polymorphisms in their respective genes (rs738409, rs1001179, rs708272 and rs2032582 respectively) have been shown to affect blood lipid homeostasis. The purpose of this study was to develop and validate a rapid and reliable method for the quantitative determination of fatty acids in blood, with gas chromatography and flame ionization detector and then examine their association with the afore mentioned polymorphisms. Twenty FA (C14:0, C15:0, C15:1, C16:0, C16:1, C17:0, C17:1, C18:0, C18:1cis, C18:2cis, C20:0, C20:1, C20:2 C20:3, C20:4, C20:5, C23:0, C24:0, C24:1, C22:6) were determined in blood after their extraction by Folch method and esterification with CH_3OH/HCl. The analysis was performed by GC-FID. The parameters of accuracy, precision, linearity, limit of detection, limit of quantification and stability of the analytes were evaluated and were found within the acceptable limits.

The developed method was successfully applied to the analysis of blood clinical samples in a population of healthy and patients with hyperlipidemia carriers of the major genotypes of rs2032582, rs738409, rs1001179, rs708272 (n=109). The differentiation in fatty acid profile was studied between the two groups following stratification according to all genotypes and within the same group between the different genotypes for each separate polymorphism. PLS-DA models were constructed for the discrimination of the groups (p value of CV Analysis was <0.05) and identification of potential biomarkers (VIP values). ROCs were constructed for the evaluation of the models (AUC values while box plots and heatmaps summarizing the potential correlations were obtained. Based on these it was found that differences in the concentrations of C14: 0, C16: 0, C16: 1, C18: 1, C18: 2 between healthy and patients were in almost all cases significant

P1-19 PHYSICOCHEMICAL CHARACTERIZATION OF CASEIN MICELLES FOR NANOFORMULATIONS IN FOOD INDUSTRY

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Caseins form colloidal particles in the form of micelles and represent about 80% of the bovine milk proteins. They fall in the category of intrinsically disordered milk proteins and the elucidation of their structure-function relationships in aqueous solutions is of great research interest, in view of their biological relevance, as well as their broad commercial and pharmaceutical applications. Casein micelles can be regarded as natural nano-capsules, which effectively deliver nutrients. Therefore, there is a number of studies reported in the literature describing their potential to be utilized as nano-carriers of biologically active agents such as drugs and nutrients. In this work, we use biophysical and biochemical methods to investigate new functionalized caseins with encapsulated pharmaceutical ingredients. Light scattering methods are combined with X-ray diffraction and spectroscopy to relate the structure at the molecular level to the morphological characteristics at the micellar level as a function of solution conditions (e.g. pH and temperature) using commercially available caseins as reference. Caseins characterization in solution and in bulk aim at developing preparation protocols for the establishment and optimization of the formulation of these market-oriented pharmaceutical nano-carriers. The importance of the combination of a series of experimental techniques in order to control and fine-tune the stability and function of these protein-based pharmaceutical formulations is demonstrated in this work.

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P1-20 METABOLOMIC APPROACH FOR GREEK HONEY ORIGIN DISCRIMINATION MAKING USE OF ULTRA- HIGH PERFORMANCE LIQUID CHROMATOGRAPHY COUPLED TO HIGH RESOLUTION MASS SPECTROMETRY

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Honey is a foodstuff which is subjected to various deceitful practices, such as addition of syrups or mislabelling due to its high price in the market. It is widely known that honey obtained from specific plants is strictly associated with unique organoleptic and/or health beneficial properties [1]. Another important factor influencing the quality of the product is the provenance in which is produced. Hence, the evaluation and verification of honey authenticity is a task of paramount importance for the producers, consumers and regulatory bodies. Untargeted metabolomics using UPLC-ESI-QTOF MS is a powerful approach for the simultaneous analysis of many compounds as well as identify new biomarkers which can discriminate the samples according to their origin. A generic extraction protocol was utilized in order to obtain the whole metabolic profile of the samples. The developed method was applied to 135 Greek honey samples from 5 different botanical origins. Most of the samples are unifloral while some other are polyfloral. The non-target screening approach was performed using Bruker Metaboscape 3.0 software which incorporates sophisticated tools for profiling, statistical analysis and compound identification. At First, the peak list with the masses of interest was obtained and multivariate statistical analysis was ensued to spot some new markers which can differentiate the samples according to their origin. For the selected peaks the most plausible molecular formula(s) were determined using SmartFormula in which thresholds of mass accuracy and isotopic pattern are taken into account. To determine the most likely molecular structure for the selected peaks we used Compounds Crawler which searches public databases as well as in silico fragmentation software (Metfrag) which are incorporated in the software.

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P1-21 SINGLE PARTICLE ICP-MS: NEW PEAK IDENTIFICATION APPROACH FOR ULTRAFAST MEASUREMENT

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Single particle inductively coupled plasma mass spectrometry (sp-ICP-MS) is a method for sizing and quantification of inorganic nanoparticles (NPs). The method is based on analyzing a highly diluted NP dispersion and recording the signal with high frequency. The NPs enter the spectrometer individually and each of them is recorded as a peak in the transient signal of the observed m/z. Number of such peaks is proportional to NP number concentration and their area is proportional to the third power of NP diameter. Modern spectrometers are capable of measuring with high sampling frequencies, i.e. short dwell times. Commonly, dwell time 100 µs can be used, however, some spectrometers can measure with dwell time as short as 10 µs. The shorter is the dwell time, the more points are recorded per peak. This can improve analytical parameters of the method, but it can cause some difficulties, too. When short dwell time is applied, more points are recorded per peak, but signal intensity in each of the points is lower. When analyzing small NPs with low signals, short dwell times can cause that a zero-value point appears inside the peak. In extreme cases, the peak can fall apart entirely and multiple low-intensity peaks are observed instead of a single peak, which leads to significant distortion of results in terms of both NP diameter and number concentration.

In this work, we tested new data evaluation approaches to overcome these problems and enable meaningful analyzes with short dwell times. Approach based on separation of peaks by 50 or preferably 100 µs of continuous zero-values showed very good results and was able to eliminate the distortion of results.

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P1-22 DETERMINATION OF MACRO- AND MICROELEMENT CONCENTRATIONS IN COAL AND ASH SAMPLE BY ICP-MS

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The use of coal as energy source may cause serious environmental impact resulting in contamination of soil, water and air due to pollutant emissions A large amount of ashes produced from burning of coal is generated in Bulgaria each year as industrial waste. Most of these ashes can lead to dispersion of potentially toxic elements, REE etc. in the surrounding groundwater and soil. In this study using inductively coupled plasma mass spectrometry (ICP-MS) the concentrations of 53 elements have been determined in coal and coal ashes, collected from a thermal power plant and mines in south-western Bulgaria. Samples were digested using mixture of different acids. The concentrations of macroelements Al, Ba, Ca, Fe, K, Mg, Mn, Na, P, Si and Ti were determined using a correction factor (RPa) to reduce the analytical signal. Two certified reference materials NBS 1632 and NBS 1635 were used to examine the accuracy of the method. Sodium (up to 0.22 wt.%), magnesium (up to 0.58 wt.%), aluminum (up to 4 wt.%), calcium (up to 13%), potassium (up to 0.7 wt.%) and iron (up to 4%) concentrations were found in coal and ashes samples. Total REE concentrations ranging from 8 to 82 ppm in the coal and ash samples were lower than the average worldwide values for various coal ashes deposits globally. In addition, the concentration of the most hazardous trace elements As, Bi, Cd, Co, Ni, Pb, Sb, Th and U in analyzed samples was significantly low.

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P1-23 PHOTOLYTIC AND PHOTOCATALYTIC DEGRADATION OF FUROSEMIDE: KINETICS, IDENTIFICATION OF TRANSFORMATION PRODUCTS AND REACTION PATHWAYS USING LIQUID CHROMATOGRAPHY-ACCURATE MASS SPECTROMETRY (UPLC-MS/MS-LTQ-ORBITRAP)

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In the present study the photolytic and photocatalytic degradation of furosemide, a widely used diuretic drug, have been investigated. Furosemide has been detected both in sewage treatment plants and rivers at concertation levels more than 100 ng/L, therefore its environmental fate has to been examined. Liquid chromatography-accurate mass spectrometry (UPLC-MS/MS-LTQ-Orbitrap) was implemented for the identification of the transformation products (TPs). The photolytic and photocatalytic experiments were conducted under simulated solar light (suntest simulator, 300 W, C_{FUR}= 10 mg/L). Photolysis of furosemide followed apparent first-order model with rate constant of k_{app}= 0.025 min^{-1}, revealing the formation of six TPs (two of which were identified for the first time) mainly via the cleavage of the furanylmethyl group (TP1), dehalogenation (TP3), dehalogenation-hydroxylation (TP2), followed by oxidation and/or decarboxylation pathways (TP4, TP5, TP6). Photocatalysis of furosemide by graphitic carbon nitride as photocatalyst (50 mg/L) and TiO_2 for comparison purposes followed also apparent first-order model with rate constant of k_{app}= 0.192 min^{-1} and $k_{appTIO2}$=0.137 min^{-1}, respectively. Four TPs (TP1, TP2, TP5, TP7) have been identified using both catalysts. All TPs were degraded after 240 min of irradiation. TP1, TP2, TP6 and TP7 were characterized as early stage products, followed typical bell-shaped curves attaining peak concentrations at 5-45 min while TP3, TP4 and TP5 were characterized as secondary TPs, showing maximum concentrations in more prolonged irradiation times (90-240 min). Based on the above results, the photocatalytic degradation using both photocatalysts is an effective process for water decontamination from high priority pharmaceuticals such as furosemide.

P1-24 PHARMACEUTICAL RESIDUES IN HOSPITAL WASTEWATERS USING LIQUID CHROMATOGRAPHY COUPLED TO HIGH-RESOLUTION MASS SPECTROMETRY

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Environmental occurrence, distribution and transportation of Pharmaceutical Active Compounds (PhACs) in the aquatic environment, has been reported in numerous research articles and reviews, worldwide. Wastewater treatment plants (WWTPs) have been considered as one of the main inputs of PhACs into the environment, since after the treatment considerable amounts can be transferred to surface waters either due to insufficient removal efficiencies or, if high removals are attained, concentrations up to ng/L and μg/L can still be found, depending on the compounds' mass loadings. In order to assess the environmental loadings of PhACs in the aquatic environment of Epirus region, a monitoring program took place in the WWTP of the University Hospital of Ioannina city. For this purpose an analytical method was developed and validated, for the simultaneous determination of 35 pharmaceuticals in the influent and the effluent of the WWTP. Analytical methodology was based on ultra-high performance liquid chromatography-Orbitrap high-resolution mass spectrometry, after solid-phase extraction through Oasis HLB cartridges. Six sampling campaigns took place from October 2018 to March 2019. The results showed that concentrations of the target pharmaceuticals in the influents ranged between <LOQ and 46666.9 ng/L, while in the effluents between <LOQ and 2844.9 ng/L. Furthermore, removal efficiencies of the target compounds in the WWTP were estimated and the results showed that eliminations ranged between negative values (e.g. carbamazepine) up to 100% (e.g. caffeine). Finally, an assessment of the environmental risk of the target compounds took place, providing important information on the distribution and fate of these contaminants in the aquatic environment.

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P1-25 COUPLING LIBS TO SSI-MS. INTERFERENCE OF PLASMA FORMATION WITH MASS ANALYSIS

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The combination of laser induced breakdown spectroscopy with sonic-spray ionization (SSI) mass spectrometry (MS) is a promising tool for fast and straightforward analysis providing both the elemental composition and the molar mass of metal-organic compounds and metal containing biomolecules. [1] The analysis relies on the use of pneumatic nebulizer to generate aerosol spray form the analyte solution in water/acetonitrile. The aerosol is fed into the inlet of the mass spectrometer at a constant flow, 15-20 μL/min, and mass spectra are collected. In parallel, it is interrogated, at a repetition rate of 5-10 Hz, by pulses from a nanosecond laser (Nd:YAG, λ = 1064nm) that give rise to the formation of strongly emitting plasma, off of which time-resolved LIBS spectra are recorded. In the present study we have examined how and what extent formation of plasma, taking place at the region between the nebulizer edge and the mass spectrometer inlet, might influence the recorded mass spectrum. For example, diatomic molecules, such as OH, generated in the plasma plume can lead to gas phase cluster formation. The effect is related to sample matrix and is evident in presence of free metal ions, while it is minimized in the case of covalently bonded molecules or co-ordination compounds. We explored possible reaction pathways of the OH radicals with analytes having aromatic rings. It is shown that the ablation process has some, but clearly not significant interference, with the molecular MS measurements, and can further be reduced with proper synchronization settings that enable collection of mass spectra out of phase with respect to the plasma events.

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P1-26 IN-DEPTH INVESTIGATION OF THE OCCURRENCE OF PER- AND POLYFLUORINATED SUBSTANCES IN TOP PREDATORS AND THEIR PREY EMPLOYING HIGH-RESOLUTION MASS SPECTROMETRY

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Environmental Specimen Banks (ESBs), scientific collections (SC) and Natural History Museums (NHMs) have conducted systematic and opportunistic sampling campaigns for decades, collecting various tissues from apex predators (e.g. raptors, otters, seals) and their prey (e.g. fish). Sample collections are guided by standardised protocols and operate under well-controlled conditions to allow for retrospective chemicals investigations. Analysis of top predators and their prey samples by high-throughput analytical methods such as high-resolution mass spectrometry (HRMS) and non-target screening (NTS) is a new and developing field. The EU funded LIFE APEX project (LIFE17 ENV/SK/000355, 2018-2022, www.lifeapex.eu) was initiated to bring together sample collections and analytical laboratories with the objective to apply generic sample preparation and instrumental methods and generate contaminant data for top apex predators and their prey in support of chemicals management. In context of this study, 67 recent specimens from northern Europe (United Kingdom, Germany, Netherlands and Sweden) were retrieved from ESBs, SCs and NHMs and were analyzed for the presence of per- and polyfluorinated substances, employing wide-scope target and suspect screening methods. All samples were lyophilized before analysis in order to enhance extraction efficiency, improve the precision and achieve lower detection limits. The analytes were extracted from the dry matrices through generic methods of extraction, using an accelerated solvent extraction, followed by clean-up through solid phase extraction. The extracts were analyzed by both liquid and gas chromatography coupled to HRMS, using electrospray and atmospheric pressure ionization techniques (LC-ESI-QToF and GC-APCI-QToF). Samples were screened for 30 per- and polyfluorinated substances using target screening and 3425 using suspect screening. Results indicate wide-spread occurrence and high potential of bioaccumulation of per- and polyfluorinated sub-

stances in top predators and their prey.

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P1-27 APPLICATION OF SINGLE PARTICLE INDUCTIVELY COUPLED PLASMA - MASS SPECTROMETRY FOR THE DETECTION AND CHARACTERIZATION OF METAL-CONTAINING NANOPARTICLES IN SEAWATER SAMPLES

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With the increasing production and use of nanomaterials, along with rising public awareness, comes the need for their determination in environmental systems. Seawater is likely to receive anthropogenic nanomaterial input through various sources and, as a result, it is critical to efficiently and quantitatively detect nanomaterials in such systems using high-throughput analytical techniques. One of the most sensitive analytical techniques available for the determination of metals in liquids is Inductively Coupled Plasma - Mass Spectrometry (ICP - MS). More specifically for the determination of metal-containing nanomaterials, single particle - ICP - MS (spICPMS) has been used extensively not only for their detection but also for the quantification of an array of their parameters. However, the direct analysis of untreated seawater samples necessitates frequent maintenance of the ICP-MS instrument due to buildup of salt residues on the sample introduction cones, which is time consuming and hampers the methods applicability for high-throughput analysis. Our previous work has demonstrated the development of an on-line dilution system that tackles most of such problems for the determination of Ag nanoparticles in seawater (Toncelli et al). In this analytical approach the seawater sample is transferred to the tip of the ICP-MS pneumatic nebulizer through a fused silica capillary, where it is diluted by a makeup flow of deionized water. With this system no sample pre-treatment is required, saving time and ensuring detection stability and nanoparticle physicochemical characteristics' integrity. In the present work, the method is applied to monitor nanomaterials and track behaviour in seawater samples taken for a mesocosm experiment studying the effect of Ag nanoparticles and ionic Ag on microbial planktonic community dynamics. In addition, the approach is used to provide a preliminary investigation into the presence of natural, anthropogenic and incidental metal-containing nanomaterials (multi-elemetal analysis) in the seawater environment of Santorini Island.

P1-28 EVALUATION OF ADVANCED DRINKING WATER TREATMENT PROCESSES BY A COMBINATION OF POWERFUL MASS SPECTROMETRIC TECHNIQUES AND EPR SPECTROSCOPY

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The production of drinking water with good aesthetic characteristics (taste and odor (T&O)) is one of the main contemporary challenges for the water industry. In the last decades, advanced oxidation processes (AOPs) were established as promising methods for T&O control in drinking water. In the present study, emerging UV-based advanced oxidation processes were evaluated for the efficient removal of recalcitrant T&O compounds that can cause problems in the aesthetic characteristics of the water. Special attention was paid to homogeneous processes such as UV-A/Cl2, which have higher potential for real large-scale applications than other AOPs. Specifically, the activation of several oxidants, widely used in drinking water treatment plants, by ultraviolet (UV) or solar irradiation can be an alternative and efficient technology. The performance of the studied processes was evaluated by using a combination of powerful mass spectrometric techniques such as HR-LC-MS, GC-MS and electron paramagnetic resonance (EPR) spectroscopy. Numerous different structures of transformation products (TPs) were identified by HR-LC-MS and GC-MS. Accurate mass measurements were employed to discriminate the structures among isomers formed during the degradation process. EPR spectroscopy in combination with the spin trapping technique was used to identify the photoinduced reactive species, which were produced during the applied processes. The significant role of HO. radicals in the degradation process was proved. Overall results of this study show that effective degradation of T&O compounds in ultrapure and real drinking water samples can be achieved using the employed UV-based AOPs.

Acknowledgement

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P1-29 DETERMINATION OF 12 PHTHALATE ESTERS IN GREEK GRAPE MARC SPIRITS BY LIQUID CHROMATOGRAPHY TANDEM MASS SPECTROMETRY

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An Ultra High Performance Liquid Chromatography-Tandem Mass Spectrometry (UHPLC-MS/MS) method has been developed for the determination of twelve phthalate esters (PAEs) in grape marc spirits' samples. The separation was performed on a U-VD-Spher PUR 100 C18-E (100 mm x 2.0 mm, 1.8 μm) column by gradient elution and followed by positive electrospray ionization as well as multi-reaction monitoring provided by a triple-quadrupole tandem mass spectrometer. The proposed method was validated in terms of the detection (LOD) and quantification limits (LOQ), the linearity ranges, and the intra- and inter- day precision and accuracy of the analysis. The detection limits ranged from 0.3 to 33.3 μg L^{-1}. The accuracy of the method was assessed by recovery experiments resulting in values from 81.6-109.6%. The standard addition method was used for quantification and the Student's t-test was carried out to evaluate the matrix effect.

Finally, the method was successfully applied to the analysis of phthalate esters in grape marc spirits samples, selected from various regions in Greece and Cyprus. The total 45 samples were analyzed directly without any pretreatment procedure. All PAEs proved to be present at least once in the analyzed grape marc spirits samples, except only in cases of diphenyl (DPhP) and diisodecyl phthalate (DiDP). Only bis-(2-ethylhexyl) phthalate (DEHP) appeared in 3 specimens, in concentration above Specific Migration Limits (SML) established by the European Union, Framework Regulation (EU) No 1935/2004 [1] and Commission Regulation (EU) No 10/2011 [2]. Despite the detection of DEHP, at concentrations higher than its SML, in a limited number of samples, the largest number of Greek spirits is classified as safe for human consumption, which is confirmed by the reports of the State General Laboratory.

P1-30 BUILDING A LOCAL LIBRARY OF REFERENCE HPLC CHROMATOGRAMS AND QTOF-MS MASS SPECTRA USING THE MSMLS KIT

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MSMLS (Mass Spectrometry Metabolite Library) is a collection of high purity (>95%) small biochemical molecules, that span a broad range of primary metabolism, in an economical, ready-to-use format. The library can provide retention times and spectra for key metabolic compounds, help in the optimization of the analytical mass spectrometry protocols, qualify and quantify sensitivity and limits of detection.

In this work, a local Metabolite Library has been developed for liquid chromatography-mass spectrometry metabolomics applications. For this purpose, 7 polypropylene plates in 96 well format were analyzed with injections of simple mixtures in an ultra-performance liquid chromatography system combined with a quadrupole time-of-flight mass spectrometer (UHPLC-QTOF). The chromatographic separation was performed on a Supelco Ascentis® Express AQ-C18 (100 2.1mm, 2.7 μm) HPLC column by gradient elution, and followed by both positive and negative electrospray ionization. MS data were acquired from 70 to 1000 Da using two MS^E functions simultaneously. In function 1, low collision energy (LE) of 10 eV was used for the acquisition of precursor ions $[M+H]^+$ and $[M+H]^-$, in MS^E 2 function a high energy ramp from 20 to 30 eV (HE) was applied in order to fragment all ions transmitted for optimal fragmentation data. Data was corrected during acquisition using an external reference (Lock-SprayTM) of leucine-enkephalin via a lockspray interface, generating a reference ion at 556.2850 Da ($[M+H]^+$) for positive ion mode and at m/z 554.2850 Da ($[M-H]^-$) in negative ion mode to ensure accurate mass measurements over a wide dynamic range. Chromatographic and MS attributes of the analyte peaks (i.e. retention time, parent and daughter ions) provided useful analytical information for every given compound. The MLSDiscovery software tool was used to build the local standard library, supporting the extraction, manipulation, and storage of the data generated when using MLS plates.

P1-31 ANALYSIS AT TRACE LEVELS OF POLYCHLORINATED BIPHENYLS IN ENVIRONMENTAL WATER SAMPLES BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY

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During the last two decades, the presence of persistent organic pollutants (POPs), including polychlorinated biphenyls (PCBs), in natural aquatic environments has been considered as an emerging issue due to their high degree of persistence, bioaccumulation and toxicity. Despite regulatory action in the 1970s, trace residues of these chemicals are still present at appreciable concentrations in aquatic ecosystems. A variety of adverse effects have been described on wildlife and human for these contaminants as endocrine disruption, developmental impairment, reproductive dysfunction and carcinogenesis. PCBs have been classified as carcinogenic to humans by the International Agency for Research on Cancer (IARC) (group 1) and United States Environmental Protection Agency (US EPA) (group B2) [1]. The aim of this study was to evaluate the potential occurrence of PCBs residues (PCB 28, 31, 52, 101, 118, 138, 153 and 180) in the aquatic environment of Arachthos River (Epirus region, N.W. Greece). For this purpose, several sampling points were selected from Arachthos springs to its estuaries at Amvrakikos Gulf with a view to determine PCBs concentration levels and further to assess the risk associated with their residues posed to the studied ecosystem. In the present study, solid phase extraction (SPE) technique followed by gas chromatography tandem mass spectrometric analysis (GC-MS) was applied. SPE methodology was shown to be linear over a wide range of concentration, exhibited satisfactory repeatability, and reached limits of detection usually in the low ppt range. Recoveries obtained were above 82.5% for all analytes. The proposed method proved to be applicable to the routine analysis of water samples of different origins (river and sea water) taken in the course of a year.

[1] M. Petrovic, M. Sremacki, J. Radonic, I. Mihajlovic, B. Obrovski, M. Vojinovic Miloradov, Science of the Total Environment, 644, 2018, 1201-1206.

P1-32 DETERMINATION OF NITROFURAN METABOLITES IN FISH SAMPLES BY MEANS OF LIQUID CHROMATOGRAPHY COUPLED TO HIGH-RESOLUTION-ORBITRAP MASS SPECTROMETRY

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Nitrofurans (NFs) are synthetic antibiotic drugs exhibiting broad spectrum activities and have been widely used as veterinary medicines or as feed additives in industrial farming of food-producing animals. Aquaculturists also use NFs to treat diseases found in aquatic animals, such as fish, shrimp, and crabs. The four most widely used NFs in veterinary medicine are nitrofurantoin (NFT), furazolidone (FZD), nitrofurazone (NFZ) and furaltadone (FTD) which all contain a characteristic 5-nitrofuran ring. After intake, NFs are extensively metabolized into their corresponding metabolites (NFMs), identified as 1-amino-hydantoin (AHD), 3-amino-2-oxazolidone (AOZ), semicarbazide (SEM) and 3-amino-5-methyl-morpholino-2-oxazolidinone (AMOZ), for nitrofurantoin, furazolidone, nitrofurazone and furaltadone, respectively. NFs and their metabolites are suspected to possess carcinogenic and mutagenic potency, therefore their application in food and animal production was banned in the EU in 1995 and in the USA in 2002. A minimum required performance level (MRPL) of 1 μg kg^{-1}, for each nitrofuran metabolite in meat product has been established by the EU. Nevertheless, NFs are still being used to treat animal diseases in some countries because of their efficiency, availability and relatively low cost. Since parent NFs are extensively metabolized to tissue-bond metabolites, recent analytical methods have been focused on the determination of the NFMs instead of the parent compounds. An analytical methodology combining derivatization for pretreatment, neutralisation and LLE for extraction, was developed and evaluated exhibiting excellent performance for the all the target metabolites. The detection and quantification of the target compounds in fish samples were carried out using the innovative Hybrid LTQ Orbitrap mass spectrometry technology. The ultimate purpose was the successful application in the field of fish sample analysis from aquacultures in North Western Greece.

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P1-33 NOVEL MALDI-TOFMS-BASED METHODOLOGY FOR RAPID DETECTION OF PDO FETA CHEESE ADULTERATION

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"Feta" is a Protected Designation of Origin (PDO) Greek cheese, ripened in brine, produced exclusively from pasteurized sheep's milk or sheep's and goat's milk (up to 30%). The worldwide recognition of Feta is attributed to its special sensory characteristics, rendering as one of the Greece's most important exports. However, in the dairy industry, cow's milk is frequently admixed with sheep's milk during the manufacture of ovine cheeses due to the lower yield of ewes combined with the lower price of cow's milk. Due to its high economic impact, fraud control is therefore vital, especially for PDO high-grade cheeses made entirely from sheep's/goat's milk. To assess the authenticity of dairy products and defend consumers' health, a European Reference Methodology (ERM) was established to detect cow proteins in dairy products, based on gel isoelectric focusing (IEF) technique. Nevertheless, this method is time-consuming and suffers from interpretation difficulties due to overlapping of species-specific bands. In the present work, a fast and sensitive matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOFMS)-based methodology has been developed for the detection of "feta" cheese adulteration. Dedicated procedures were set up for the analysis of corresponding protein and/or peptide components (dilution of skimmed samples, protein tryptic digestion, ultrafiltration etc.). Pure cows', goats' and sheep's milk and cheese samples as well as binary mixtures were analyzed. Evaluation of potential species-specific markers was carried out utilizing the protein/peptide profiles. To the best of our knowledge, this is the first study reported in the literature to detect "feta" cheese adulteration using MALDI-TOFMS. The method was developed in agreement with the requirements of Reg. 273/2008 and provides substantially low LODs and short-time analysis. Consequently, it could be proposed as a second generation ERM for pure milk/cheese authentication.

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P1-34 NON-SPECTRAL INTERFERENCES IN SINGLE-PARTICLE ICP-MS

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Single-particle inductively coupled plasma mass spectrometry is powerful technique recently used for the analysis of nanoparticles (NPs) of metals, non-metals, or their compounds. This work demonstrates the effect of sodium chloride and carbon-related non-spectral interferences on the analysis of arsenic and silver NPs by this method.

Non-spectral interferences caused by sodium lead to under-estimation of As and Ag NPs diameter by about 7 % and 15 % at NaCl concentration of 450 mg L^{-1} and about 28 % and 41 % at NaCl concentration of 4500 mg L^{-1}, respectively, in comparison to aqueous NPs dispersions. Sodium non-spectral interferences also lead to about a 9 % lower number of detected NPs for dispersions of both As and Ag NPs in 4500 mg L^{-1} NaCl as a consequence of lower transport efficiency owing to high NaCl content. On the contrary, measurement of NPs in matrices containing methanol gives results where Ag and As NPs diameter is over-estimated by about 3 % and 15 % at a methanol content of 1 % (v/v) and about 6 % and 20 % at a methanol content of 2 % (v/v), respectively, in comparison to aqueous NPs dispersions. In addition, the organic carbon species behave as surfactants and increase the transport efficiency; this leads to an over-estimation in the determined number concentration of NPs by about 17 % for Ag NPs and about 10 % for As NPs at a methanol content of 5 % (v/v) in comparison to aqueous NPs dispersions.

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P1-35 DETERMINATION OF RARE EARTH ELEMENTS OF HIGH CONTENTS IN RARE EARTH ORE USING 5-ACID DIGESTION BY ICP-MS

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At present, rare earth elements (REEs) are one of the valuable resources with increasing use worldwide. Therefore, the technology to analyze REEs among rare earth ore which contain large amounts of rare earths is an important technology for the utilization of REEs. In this study, determination of REEs in rare earth ore using 5-acid digestion by ICP-MS was studied by comparing 4-acid digestion method without using alkali fusion method in rare earth ore containing more than 6 wt.% T-REEs. To ensure the quantification of REEs, rare earth ore reference materials were compared ICP-MS results with each other using the 4-acid digestion method using hydrochloric acid, nitric acid, hydrofluoric acid, perchloric acid, and 5-acid digestion method with added sulfuric acid. The experiment found that the digestion method, which was digested by adding sulfuric acid compared to the 4-acid digestion method, had a more satisfactory recovery for REEs. Analysis of REEs by 5-acid digestion method and ICP-MS shows that the matrix effect, such as 157Gd, 158Gd, 159Tb, 166Er, 172Yb, 174Yb, 175Lu present in relatively trace quantities by media containing 139La, 140Ce, 141Pr, and 142Nd coexist in rare earth ore. To overcome this, Inter-elements correction (IEC) method was used. As a result, the recovery of REEs results was 96 to 103 % compared to the certified value of the reference material, and the relative standard deviation of the analysis results was less than 3%. Additional study shall be made to apply this method to samples of other metals and materials containing high-concentration rare earths elements.

P1-36 DEVELOPMENT AND VALIDATION OF METHOD FOR DETERMINATION OF TREE NUT ALLERGENS WITH LC-MS/MS

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Allergy is an intense response of the immune system due to a type of antigen, the allergen. Allergens may be found in different foods and refer to proteins or peptides responsible for the allergenic activity. Most of these allergens are generally resistant to food processing. For example, peanut allergens are the most common cause of fatal anaphylaxis caused by food because, heat treatment of the food can increase their allergenicity and the reactions can be activated by some micrograms of the proteins. This research aims at the determination of allergenic proteins from nuts present in foods, such as chocolates, with ultra-High Performance Liquid Chromatography - tandem mass spectrometry (uHPLC-MS/MS). Until now, ELISA was been applied to allergen determination. LC-MS/MS technique is regarded as a new approach to detect multiple allergens. In this study an uHPLC-MS/MS method was developed and applied for the simultaneous identification and determination of the traces of tree nut allergens (peanut, pecan, pistachio, hazelnuts). Method's protocol includes extraction of protein, trypsin digestion, purification with SPE and LC-MS/MS injection. Method's parameters, such as time of digestion, were optimized. Moreover, LC-MS/MS detection was achieved based on subsequent peptides generated by enzymatic digestion. Specifically, for every peptide (two for every allergenic protein), the molecular mass and their two products were determined. Despite, time-consuming sample preparation, the developed method has many advantages. The method is characterized by high sensitivity, low limits of detection and it can provide simultaneous analysis of multiple tree nut allergens in a single preparation and a single injection step.

P1-37 DEVELOPMENT OF A MULTI-RESIDUE METHODOLOGY FOR THE DETERMINATION OF VETERINARY DRUGS IN ANIMAL FEED BY RP-HPLC-MS/MS

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Veterinary drugs are widely used in animal production to treat diseases, prevent infection and promote growth of animals. Veterinary drug residues might find their way into animal-based food products and subsequently the consumer through the food chain, causing adverse health effects for both animals and humans (e.g allergic reactions, development of bacterial resistance, carcinogenesis, etc). Illegal or improper use of medicated feeding stuffs or unintentional cross-contamination are the most frequent pathways for residue occurrence. Although different EU legal frameworks have established Maximum Residue Limits (MRLs) for antibiotic and anthelmintic residues in food of animal origin, no official legislation has been set for feed control limits so far. Therefore, detecting and monitoring of these compounds in animal feed is of high importance for controlling contamination within the food-processing chain. The most challenging analytical part in multi-residue veterinary drug determination is their isolation from the feed matrix as they present different physicochemical properties. The aim of this study was the development of a multi-class and multi-residue methodology for the determination of a wide variety of veterinary drugs, including tetracyclines, sulfonamides, quinolones, b-lactams, macrolides, benzimidazoles, amphenicols, anthelmintics and avermectins, among others, using Reversed Phase High Pressure Liquid Chromatography-tandem Mass Spectrometry (RP-HPLC-MS/MS). A thorough optimization of the sample preparation protocol was performed, and different extraction and cleanup procedures were tested. The method was validated in agreement with the guidelines of Commission Decision 2002/657/EC achieving substantially low LODs and short-time analysis.

P1-38 MARKERS OF OXIDATIVE STRESS AND AMINOACIDS IN INFANT'S SERUM SAMPLES WITH URETEROPELVIC JUNCTION OBSTRUCTION BY STABLE -ISOTOPE DILUTION GC-MS WITH NEGATIVE CHEMICAL IONIZATION

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The most common cause of chronic kidney disease (CKD) in infants is congenital anomalies of the urinary tract and particularly obstructive nephropathy. Despite the fact that ureteropelvic junction obstruction (UPJO) is the most common obstructive nephropathy fundamental questions regarding its mechanism, assessment and treatment remain still unanswered. The aim of the present study was to separate neonates and infants with UPJO from healthy ones based on their serum metabolic profile and also to distinguish surgical from non-surgical cases. The ultimate goal was to extract specific serum biomarkers that will allow early diagnosis of renal dysfunction in the specific population through targeted and quantitative metabolomics-based analysis. Serum samples were collected from 21 patients preoperatively, 22 patients with mild stenosis treated conservatively, and 15 healthy controls. The median age of the participants in all 3 groups was 2 months and all had normal creatinine values. Samples were subjected to two targeted metabolomics analyses by electron- capture negative-ion chemical ionization Gas Chromatography - Mass Spectrometry (ECNICI - GC-MS) method for the quantification of malondialdehyde (MDA), Nitrite and Nitrate as pentafluorobenzyl derivatives and of amino acids and their derivatives as *N*-pentafluoropropionic amides of methyl esters. Analyses of the serum samples revealed a clear separation with a statistically significant difference between the three groups. Univariate statistical analysis highlighted homoarginine (hArg) (pValue 0.03), asymmetric dimethylarginine (ADMA) (pValue 0.04) and malondialdehyde (MDA) (pValue 0.02) as potential biomarkers for UPJO, enabling the discrimination of patients who required surgery from those followed by systematical monitoring as well as from healthy controls.

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P1-39 CHEMOMETRIC APPROACH TO THE OPTIMIZATION OF HS-SPME/GC-MS PARAMETERS FOR THE DETERMINATION OF MULTICLASS PESTICIDE RESIDUES IN FRUITS AND VEGETABLES

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An HS-SPME method was developed using multivariate experimental designs, which was conducted in two stages. The significance of each factor was estimated using the Plackett-Burman (P-B) design, for the identification of significant factors, followed by the optimization of the significant factors using central composite design (CCD). The multivariate experiment involved the use of Minitab® statistical software for the generation of a 2^{7-4} P-B design and CCD matrix. The method performance evaluated with internal standard calibration method produced good analytical figures of merit with linearity ranging from 1 - 500 µg/kg with correlation coefficient greater than 0.99, LOD and LOQ were found between 0.35 and 8.33 µg/kg and 1.15 and 27.76 µg/kg respectively. The average recovery was between 73 % and 118 % with relative standard deviation (RSD = 1.5 - 14 %) for all the investigated pesticides. The multivariate method helps to reduce optimization time and improve analytical throughput.

P1-40 A GC-MS METHOD FOR THE DETERMINATION OF FIVE NPS IN WHOLE BLOOD AND THE DETECTION OF SIX NPS IN URINE

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New psychoactive substances are gaining space in illicit drug markets worldwide. NPS are classified into different chemical classes. They are often designed to have similar structures with their ''traditional'' and banned analogues, as to display similar pharmacological actions and to be 'legal'. The aim of this project was to develop and validate a method for the detection and quantification of five NPS such as synthetic cathinones, opioids and cannabinoids. Mephedrone, 3,4-MDPV, AH-7921, JWH-018 and AM-2201 were quantified in whole blood samples and the same compounds plus methylone were detected in urine samples by GC-MS. Thestudy for the optimum sample preparation method showed that derivatization was not necessary before analysis. The method showed good linearity for all analytes within a concentration range from 0.005 to 2 μg/mL, with LODs ranging from 0.002 to 0.08μg/mL in blood and from 0.002 to 0.08μg/mL in urine and LOQs from 0.005 to 0.25μg/mL in blood. Accuracy was within acceptable limits with %bias ranging from -11.16% to +18.87%for inter-assay studyand from -17.97% to +20.06% for intra-assay study. Precision was found to be between 2.59% and 17% (CV%) for intra-assay study and from 6.04% to 13.72% (CV%) for inter-assay study. Also, an interlaboratory assessment took place for three samples containing all compounds at three concentration levels. The results of the two laboratories being involved, agreed with a correlation coefficient of 0.9954. No matrix effect or carryover was observed in both matrices, whereas the analytes were found to be stable in samples during two freeze-thaw cycles at -18 ^{o}C and in the sample extracts at 4 ^{o}C for two days. The developed method can be used for the reliable and fast quantification of five NPS in blood and the detection of six NPS in urine; thus, it could be a supporting tool in a clinical or forensic toxicology lab.

P1-41 DETERMINATION OF ROYAL JELLY FREE FATTY ACIDS BY LIQUID CHROMATOGRAPHY-HIGH RESOLUTION MASS SPECTROMETRY

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Royal jelly (RJ) has been used since ancient times in traditional medicine, and it is currently used as a functional food and in pharmaceuticals and cosmetics. It is a white-yellowish, acidic colloid, which contains 3-8% lipids. RJ fatty acids are medium-chained (8-10 carbon atoms) free fatty acids, terminally and/or internally hydroxylated, with terminal mono- or dicarboxylic acid functionalities, either saturated or monounsaturated at the 2-position. *trans*-10-Hydroxy-2-decenoic acid is the predominant fatty acid in RJ and its amount varies depending on the origin of the jelly and characteristics of the bee. Usually the RJ fatty acids are determined by gas chromatography-mass spectrometry (GC-MS). However, such a method requires the conversion of free fatty acids into the corresponding trimethylsilyl derivatives. We present here a method for the determination of RJ free fatty acids by liquid chromatography-high resolution mass spectrometry (LC-HRMS) avoiding any derivatization step. LC-MS/MS measurements were performed with an ABSciex Triple TOF 4600 combined with a micro-LC Eksigent and an autosampler. Electrospray ionization in negative mode was used for the MS experiments. Halo C18 2.7 μm, 90 Å, 0.5 × 50 mm^2 (Eksigent) was used as a column and the mobile phase consisted of a gradient (A: acetonitrile/0.01% formic acid/isopropanol 80/20 v/v; B: H_2O/0.01% formic acid). Two simple extraction protocols, one employing methanol and the other a mixture of diethyl ether-isopropanol (50:1 v/v), were studied. The later was employed for the real samples. The method was validated and applied in five samples of Greek RJ. Our method allows the rapid determination of the major free fatty acids in royal jelly samples, namely *trans*-10-hydroxy-2-decenoic acid, 10-hydroxy-decanoic acid, 3-hydroxy-decanoic acid, decanedioic acid and 2-dodecenedioic acid.

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P1-42 METABOLOMIC PROFILING OF ZEBRAFISH WITH NMR AND LC-MS/MS AFTER EXPOSURE TO NON-DOPED, N-DOPED AND N,S-DOPED CARBON NANODOTS

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Recently, nanomaterials have become a rapidly developing field of research due to their numerous advantages and tremendous potential in biomedical, environmental and energy applications. Carbon nanodots (CNDs) are a new class of carbon nanomaterials with a size <10 nm that recently emerged and have drawn significant attention. Since their discovery, CNDs have found many applications in the fields of chemical (bio) sensing, bioimaging, nanomedicine and photocatalysis. However, a concern arises over their transport, transformation and fate after their release in the environment. Also, their toxicity on (marine) organisms and humans was recently addressed as an important issue.

In this study, the toxic effects and metabolic alterations of Zebrafish (*Danio rerio*) were assessed after exposure to CNDs. Owing to their unique, favorable characteristics (i.e. high fecundity, small size, rapid generation time, optical transparency during early embryogenesis) zebrafish is a distinguished vertebrate model for biomedical research and (eco)toxicology. In order to obtain a holistic view of the effect of heteroatoms on the toxicity of CNDs, we employed CNDs from citric acid, either pristine or doped with nitrogen and nitrogen/sulfur. Toxicity studies yielded the following results: LD_{50} values: 555 μg mL^{-1}, 400 μg mL^{-1} and 150 μg mL^{-1} for non-doped, N-doped and N,S-doped CNDs, respectively, highlighting that heteroatoms can dramatically increase the toxicity of the CNDs. To obtain insight into the metabolic alterations that occur in zebrafish upon exposure to CNDs, a metabolomic workflow was employed that combines ^{1}H-NMR spectroscopy, LC-MS/MS and online, free-access databases. Numerous differences in the metabolic pathways were recorded in all cases. A typical example is the activation of alanine, aspartate and glutamate metabolism, aminoacyl-tRNA biosynthesis, butanoate metabolism, D-glutamine and D-glutamate metabolism, glutathione metabolism, selenoamino acid metabolism, valine, leucine and isoleucine degradation pathways and deactivation of starch and sucrose metabolism, glycine, serine and threonine metabolism, among others, after exposure to 150 μg mL^{-1} N,S-doped CNDs. Our findings underline the importance to study further the impact of CNDs upon the environmental organisms.

P1-43 UNTARGETED FECAL METABOLOMICS-BASED ANALYSIS OF CAROB TREATED RATS

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Ceratonia siliqua L. Fabaceae, known as the carob, is native to the eastern Mediterranean countries and its products are widely used in the diet of people living in Mediterranean Europe, Middle East and North Africa. Carob is considered to be of great economic significance and of high nutritional value as it is fat-free, rich in fibers, flavonoids, sugars, D-pinitol, proteins, vitamins, antioxidants and several important minerals. A plethora of studies have demonstrated the beneficial effect of carob against different diseases, such as diabetes, cancer, diarrhea, metabolic syndrome, hyperlipidemia, etc. However, only few applied metabolomics-based methods have investigated the beneficial effects of carobs in everyday diet. In the present study 8 male Wistar rats were treated with carob powder via water consumption (10 g powder / L) for a 15 days period and their fecal metabolic profile were compared to those of 8 non-treated (controls) by UHPLC-HR MS. The aim was to investigate changes in the metabolic signatures on the basis of carobs diet. Chromatographic separation was performed on an Acquity HSS T3 column by A: acetonitrile, 0.1% formic acid and B: H_2O, 0.1% formic acid. An LTQ Orbitrap MS acquired profiling data in both positive and negative ionization mode and data were extracted by XCMS. Preliminary results from multivariate and univariate statistical analyses, revealed a clear separation in the fecal metabolic content of treated rats vs controls in the first and last day of treatment, indicating metabolic alterations deriving by nutritional intervention with carobs. The dietary intervention was proven to be a strong differentiating factor affected metabolic pathways associated with cellular energy production.

Acknowledgments

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P1-44 METABOLOMICS STUDY OF THE EFFECT OF TOLUENE ON PSEUDOMONAS POTIDA DOT-T1E STRAINS

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Efflux pumps are critically important membrane components that play a crucial role in strain tolerance in Pseudomonas putida to antibiotics and aromatic hydrocarbons that result in these toxicants being expelled from the bacteria. Here, the effect of propranolol on P. putida was examined by sudden addition of 0.2, 0.4 and 0.6 mg mL-1 of this β-blocker to several strains of P. putida, including the wild type DOT-T1E and the efflux pump knockout mutants DOT-T1EPS28 and DOT-T1E-18. Bacterial viability measurements reveal that the efflux pump TtgABC plays a more important role than the TtgGHI pump in strain tolerance to propranolol. Mid-infrared spectroscopy was then used as a rapid, high-throughput screening tool to investigate any phenotypic changes resulting from exposure to varying levels of propranolol. Multivariate statistical analysis of these MIR data revealed gradient trends in resultant ordination scores plots, which were related to the concentration of propranolol. MIR illustrated phenotypic changes associated with the presence of this drug within the cell that could be assigned to significant changes that occurred within the bacterial protein components. To complement this phenotypic fingerprinting approach metabolic profiling was performed using gas chromatography mass spectrometry to identify metabolites of interest during the growth of bacteria following toxic perturbation with the same concentration levels of propranolol. Metabolic profiling revealed that ornithine, which was only produced by P. putida cells in the presence of propranolol, presents itself as a major metabolic feature that has important functions in propranolol stress tolerance mechanisms within this highly significant and environmentally relevant species of bacteria.

Biography

Ali Sayqal has completed his PhD at the age of 31 years from University of Manchester and postdoctoral studies from University of Manchester School of Chemistry. He is the Head of Applied Science Research Centre. He has published 7 papers in reputed journals and he is a consultant at the two Holy Mosques Institute for Hajj and Umrah Research.

P1-45 METABOLOMICS ANALYSIS FOR THE IN VITRO TOXICITY ASSESSMENT OF COCAINE IN HEPG2

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The toxicity of cocaine and its metabolites has been a subject of study for many years since cocaine is one of the most common drugs of abuse. The majority of studies focus on the determination of cocaine and its metabolites in biological matrixes in order to determine cocaine abuse. In the current project, the toxicity of cocaine on human liver cancer cell line (HepG2) is assessed. Cocaine toxicity (LC_{50}) on HepG2 cells was experimentally calculated using an XTT assay at different concentrations from 0.1 mM to 10 mM. Afterwards metabolic profiling was performed in HepG2 cells to study the cytotoxic activity of cocaine at the estimated LC_{50} at three different time points (3h, 24h and 48h after). Cell medium was collected and frozen at -24°C, then the wells were washed three times with PBS and the metabolism was stopped with the addition of 2 mL of ACN: MeOH: H_2O, 50:30:20 (v/v). The mixture was collected using a cell scraper and after freezing for 20 min at -24°C. The collected samples of the extracellular and intracellular material were further analyzed with a validated HILIC LC-MS-MS method for targeted metabolomics analysis. The chromatographic analysis was performed in ACQUITY Amide column with A: ACN:H_2O 95:5 v/v 10 mM ammonium formate, and B: H_2O: ACN 70:30 v/v 10 mM ammonium formate. The triple quadrupole performed MRM acquisition for the detection of more than 100 hydrophilic metabolites of different metabolic pathways. The obtained data were further processed and PLS-DA and OPLS-DA models were constructed for the discrimination of the groups and the identification of potential biomarkers in the extracellular and intracellular samples; clear separation was found between cocaine affected and the control samples. Following studies will include also untargeted metabolomics analysis using GC-MS and reversed phase LC-Q-TOF analysis in positive and negative mode.

P1-46 TARGETED AND UNTARGETED METABOLOMICS OF MICE URINE AND FECAL SAMPLES, IN THE DISCOVERY OF ALCOHOL TOXICITY BIOMARKERS

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Metabolomics-based analysis has proven to be a reliable tool in biomarker discovery and in the elucidation of biochemical mechanisms. Alcohol health-related problems can occur at different levels of severity, from mild to life-threatening, such as cirrhosis of the liver, increased cardiovascular disease, malignant neoplasm, hepatic steatosis. The aim of the project is to study the metabolic profile of mice urine and fecal samples in order to gain new insight in the biochemical mechanism of alcohol toxicity in animal models.

For this purpose, a long-term animal experiment was conducted with 38 C57BL/6 mice (8-10 weeks old) of both genders separated into control and ethanol (5% v/v) *ad libitum* feeding groups, with *Lieber-DeCarli* diet for 8 weeks. Urine and fecal samples were collected in two time points (at 10^{th} and 20^{th} day after the beginning of the alcohol administration), while tissues were collected at post mortem. The animal experiment was conducted in agreement with the current national and European legislation (N. 2015/1992, ΠΔ 56/2013, European guideline 2010/63). Both targeted and untargeted methods were applied for a comprehensive metabolic profiling of fecal samples while only targeted analysis was applied for urine samples due to low sample volume availability. An *in house* HILIC UHPLC-MS/MS method was applied for the detection of 101 polar metabolites, including sugars, amino acids, organic acids, amines, etc, in a single run of 40 min. Additionally UHPLC- QTOF-MS analysis was performed to study differences in lipids and non-polar metabolites in fecal samples. Data were processed using TargetLynx (Waters) and XCMS. Both multivariate and univariate statistical analysis were accomplished using SIMCA-P 13.0, MS Excel for Windows and R programming language. Despite some limitations such as heterogeneity of fecal samples and low volume of urine samples, we could reveal a multitude of disturbances in the polar, non-polar and semi-polar metabolic content of the samples due to the alcohol intervention by both targeted and untargeted approaches. The biochemical pathways of major precursors that are essential for the energy production were significantly affected by the ethanol consumption. Mainly perturbations in amino acids metabolism were revealed based on studies results.

Acknowledgments

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P1-47 XRD CHARACTERIZATION OF CRYSTALLINITY AND PHASE COMPOSITION OF SUBFOSSIL HOLOCENE REINDEER BONES AND ANTLERS FROM THE UST'-POLUY ANCIENT SANCTUARY (WESTERN SIBERIA, RUSSIA)

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The Ust'-Poluy settlement sanctuary (Salekhard) is one of the most important archaeological sites of the Bronze-Iron Age in the Yamal region of Russia, which combined the entire epochs of ancient people's life. In the present work, the structural features of the bones and antlers of subfossil reindeer (Rangifer tarandus L., 1758) from the Subarctic of Western Siberia (Ust'-Poluy archaeological monument) and modern individuals (Polar Urals) were studied using X-ray diffraction (XRD). The reindeer bone and antler fragments were powdered manually in a jasper mortar and analyzed by XRD using a Shimadzu XRD-7000 powder X-ray diffractometer with Cu Kα radiation (λ=1.5406 Å) operating at 40 kV and 30.0 mA. XRD patterns were collected across the angular range of 20-70°. The preliminary qualitative phase analysis of the bones was conducted using the ICDD PDF-2 database. To perform the quantitative full profile analysis and unit cell lattice parameters determination of the bones and antlers, the digitized XRD patterns were analyzed according to the Rietveld method using the Sietronics SiroQuant software.

Crystallinity index (CI) was determined as the full width at half maximum (FWHM) of the apatite 002 reflection in degrees 2θ. The average size of coherently diffracting domains (otherwise referred to as crystallites) was determined: the length using the 002 reflection, and the width using the 300 reflection. FWHMs of 002 and 300 principal reflections corresponding to apatite crystallites were measured after background subtraction and correction for the instrument function. Considering that strain broadening is negligible, true crystallite sizes were determined from the Scherrer equation. Refined apatite unit cell parameters correspond to carbonated apatite. Obtained crystallite dimensions and crystallinity indices are in a good agreement with the values for subfossil bones.

The work was carried out at the Geoanalyst Center for Collective Use and supported by RFBR grant No. 18-35-00462.

P1-48 AN X-RAY SPECTROSCOPY STUDY ON THE MECHANISM OF Sb(V) AND Cr(VI) ADSORPTION BY TIN AND IRON OXY-HYDROXIDES

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This work attempts to elucidate the occurring mechanisms that explain the efficiency of inorganic adsorbents oriented to the removal of antimony and hexavalent chromium from drinking water, by means of XPS and XAFS measurements. In particular, Sn(II)-based oxy-hydroxides were optimized to capture Cr(VI) by initiating its reduction to the insoluble Cr(III) form. The XPS analysis of the adsorbent, after its use in water treatment, on the Cr 2p peak range revealed the exclusive presence Cr(III) obtained in two binding variations attributed to oxide and hydroxylated configuration on the solid's surface. The first contribution is related to inner-sphere bidentate mononuclear (edge sharing) of oxide complexes whereas hydroxylated complexes contribute to binuclear (corner sharing) ones as XAFS measurements indicated. Uptake of the very mobile Sb(V) oxy-ions was realized by Fe(III)/Sn(II) oxy-hydroxide nanocomposites which succeed to reduce the pentavalent form into Sb(III) and enable its adsorption by the iron-based phase. The occurrence of the reduction/adsorption sequence is validated by measurements in the Sb 4d peak which shows Sb(III) as the only contributing form. In both cases, surface tin appears in the Sn(II) and Sn(IV) oxidation states after its partial oxidation through participation in the reduction of Cr(VI) and Sb(V).

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P1-49 EUROPEAN NETWORK FOR CHEMICAL ELEMENTAL ANALYSIS BY TOTAL REFLECTION X_-RAY FLUORESCENCE

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The COST Action CA 18130, "European Network for Chemical Elemental Analysis by Total Reflection X-Ray Fluorescence" [1], acronym ENFORCE-TXRF, aims to coordinate research and building capacity in the field of elemental analysis by total reflection X-ray fluorescence spectroscopy (TXRF) in order to develop and assess new tools, protocols, methodologies, and instrumentation for the screening and accurate determination of elemental and co-elemental presences, occurrences and concentrations. The elements targeted are ranging from potentially toxic elements and heavy metals, to nutrients, beneficial elements and to trace elements, with their delicate threshold between deleterious exposure and beneficial effect. Such analysis may have tremendous repercussions in quality control practices and even in establishing new regulatory policy. This Action will create an infrastructure for scientific communication, exchange and collaboration to enhance technical standards, and advance measurement science. This will foster new research activities and will allow to combine the various partners' related expertise in chemistry, physics, life science and engineering. This network will provide the information and tools to maximize European competitiveness in forming and attracting talented scientists, supporting new sources and capabilities that improve research productivity, quality, dissemination, efficiency, and career development.

The activities will enable breakthrough scientific developments leading to new concepts and products, increasing Europe's research and innovation capacities, and supporting European Commission regulation organizations in crucial fields as environmental protection, food safety, life science, and nanotechnologies. ENFORCE TXRF will create well-organized and sustainable partnerships. ENFORCE-TXRF has formally started on March 13th 2019 with its first Managing Committee meeting and will remain in force for the next 4 years. This Action is opened to all researchers interested in contributing in the TXRF field of research, worldwide.

[1] https://www.cost.eu/actions/CA18130/#tabs|Name:overview

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P1-50 NON-INVASIVE COMPOSITIONAL STUDY OF COPPER ALLOY VESSELS FROM THE ARCHAIC CEMETERY OF SINDOS IN THESSALONIKI

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The present study focuses at the non-invasive determination of the chemical composition of copper alloy vessels from an archaeological site of Central Macedonia, the archaic cemetery (6th - early 5th BC) of Sindos in Thessaloniki through the implementation of the Energy Dispersive micro-X-Ray Fluorescence (EDμXRF) spectrometry. It concerns twenty-three (23) copper alloy vessels of everyday or symposium use which belong to a variety of shapes. They were unearthed in well dated contexts during controlled excavations of the Archaeological Service. Since the option of sampling in ancient artefacts is limited, the use of non-invasive analytical techniques like EDμXRF is compulsory. Furthermore, the possibility of taking dozens or even hundreds of measurements from different parts of the artefacts, the multi-element rapid analysis, the absence of sample preparation procedures (e.g. dissolution), the optical inspection through cameras and the differentiation of the diameter of the incident beam establish EDμXRF as one of the most widespread analytical techniques in the field of archaeometallurgical studies.

The aims of the present study are: a) to determine the composition of the alloy used for the construction of the vessels as well as the differentiation according to each part of the object, b) to examine the effect of the alloying elements and impurities to the castability and formability of vessels, c) to ascertain the access of the ancient Macedonian technicians of the Archaic era to raw materials and d) to investigate the manufacturing technology of that certain period in ancient Macedonia. The present study is a part of a wider archaeometric project regarding the evolution of the metalworking at the area of the ancient Macedonia, from the Archaic to the Hellenistic era, in order to create a database of analytical data for their composition.

P1-51 DEVELOPMENT AND VALIDATION OF A HPLC-PDA METHOD FOR THE DETERMINATION OF OLMESARTAN MEDOXOMIL

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Olmesartan medoxomil (OLM) is an angiotensin II type 1 (AT(1)) receptor antagonist (angiotensin receptor blocker [ARB]) that inhibits the actions of angiotensin II on the renin-angiotensin-aldosterone system, which plays a key role in the pathogenesis of hypertension. A novel High-Pressure Liquid Chromatography- Photodiode Array (HPLC-PDA) method has been developed for the determination of the prodrug Olmesartan Medoxomil, in tablets and in dissolution test samples. The chromatographic separation was performed on a XTerra MS C18 (2.1mm × 50mm, 3.5µm) column with a mobile phase consisting of solvent (A) water: methanol, 95:5% v/v (0.1% formic acid, 10 mM ammonium formate) and solvent (B) acetonitrile. The applied gradient elution consists of two isocratic steps: 0-2 min 85% solvent A, 2-5 min 70% solvent A, 5-6 min 85% solvent A where returned to the initial condition, followed by column re-equilibration. The proposed method was validated in terms of the limit of detection (LOD) and the limit of quantification (LOQ), of intra- and inter- day precision, and accuracy. The stability of the drug in solutions was also studied. The accuracy was estimated by recovery experiments, resulting in the range of 98-106,6%., and the intra- and inter- day precision was between 0,3%-0,82% and 0,59%-2,31% RSD, respectively. LOD and LOQ determined to be 0.25 mg/L and 0.83 mg/L, respectively. Standard solutions of OLM were found to be stable in ACN: H_2O, 60:40 (v/v) at -18 ^{o}C for a period of 1 month. The method was developed with the aim to be applied for drug content determination in various sample types. The method is fast, simple, accurate and easy to perform for routine analysis of the prodrug Olmesartan Medoxomil.

P1-52 LIQUID CHROMATOGRAPHY COUPLED TO QUADRUPOLE-ORBITRAP MASS SPECTROMETRY TO INVESTIGATE THE OCCURRENCE OF PHARMACEUTICAL RESIDUES IN NATURAL WATERS

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The focus for water pollution research has recently been shifted from the conventional organic priority pollutants to the so-called emerging contaminants while many of them are not regulated yet. This category of pollutants includes a variety of substances with both industrial and domestic applications but quite different potential harmful effects. Among others, pharmaceuticals, personal care products and disinfectants are included. Pharmaceuticals comprise a group of chemical compounds, including complex molecules with different functional groups, physicochemical and biological properties. The presence of residual pharmaceuticals in the aquatic environment is an important environmental issue. Since the drugs are designed to cause biological responses, they could pose a risk to organisms in their natural environment. In this study, the presence of selected pharmaceutical compounds (paracetamol, phenazone, ketoprofen, budenosonide and atenolol) in surface waters was investigated. Six sampling points along the aquatic system of the River Louros, close to the city of Ioannina (Epirus, NW Greece), were selected for the assessment of their pollutant load. Analytical method was based on solid-phase extraction (SPE) of water samples, using Oasis HLB cartridges, followed by high performance liquid chromatography coupled to Orbitrap high resolution mass spectrometry (HPLC-LTQ/Orbitrap-MS). The methodology exhibited good analytical characteristics with recoveries over 65% for all analytes (R^2 >0.9990, LOQs between 1.5 and 11.0 ng/L). Results revealed the presence of only paracetamol (although in levels below LOQ) in two out of six sampling stations. The proposed analytical methodology proved to be fast, easy, effective and reliable for the systematic monitoring of pharmaceuticals residues in natural waters.

Acknowledgments

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P1-53 DETERMINATION OF AMITRAZ, BROMOPROPYLATE, COUMAPHOS AND T-FLUVALINATE RESIDUES IN HONEY BY QUECHERS AND HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY-UV/DAD

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Acaricides are applied in agriculture as phytosanitary products against pests and in apiculture to control the bee parasite Varroa destructor [1]. Bee products can be contaminated from different sources. The contamination can arise from beekeeping practices or from the environment. The acaricide use is a common worldwide practice in honey cultivation to protect the production. Nevertheless, their presence decreases honey safety band quality and affects the human health. Therefore, it is important to set up an easy, reliable, and rapid analytical method for determining such compounds in honey. In the present study a method based on QuEChERS extraction [2] and analysis by high performance liquid chromatography on a C18 reversed-phase column with UV/diode array detection (HPLC-UV/DAD) was applied. Isocratic elution system was used with acetonitrile-water (80:20 v/v) containing 0.01M acetic acid as mobile phase while the selected compounds (amitraz, bromopropylate, coumaphos and τ-fluvalinate) were detected at 249, 233, 313 and 254 nm, respectively. This method, combined with accurate and sensitive detection, allowed quantification and confirmation at the low level of 10 μg kg^{-1}, with recoveries ranging between 78 and 103%. The analytical method was optimized in terms of the type and the amount of the sorbent materials and afterwards validated with a view to be applied to commercial honey products. Consumer's representative honey products (32 samples in total) were purchased from local markets of Epirus region, N.W. Greece. Organic honey samples were also included.

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P1-54 A GC/MS METHOD FOR THE DETECTION AND QUANTIFICATION OF C12-16 ALKYLDIMETHYLAMINES IN HUMAN BLOOD

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N,N-dimethyldodecylamine is produced from lauryl alcohol and dimethylamine. C12-16 alkyldimethylamines is used as an intermediate for manufacture of amineoxides and quarternary amino compounds. The subsequent products are used as disinfectants; detergents; dyeing auxiliaries, wetting agents, antistatic agents and bleaching agents in textile industry; pharmacy; corrosion inhibitors; fuel oil antiicing. The aim of this study was the development and validation of a GC-MS method for the determination of C12-16 alkyldimethylamines in blood and finally its application in postmortem blood samples.

Analysis of the amines was performed on a gas chromatograph Agilent Technologies 7890A with a MS 5975C inrXL, EI/CI MSD with Triple-Axis detector, after liquid-liquid extraction. Five different organic solvents (Butyl Acetate, ethyl acetate, dichloromethane, n-hexane and n-heptane) were used for the optimization of the extraction procedure. A QuEChERS step was applied (20mg MgSO4, 5mg NaCl), pH was adjusted at 12 (5mg K2CO3).Samples were then vortexed, centrifuged and directly injected into the GC/MS system. The quantification of the amines was done by sSCAN mode, using 58 as the quantifier ion for the three compounds. Hexane was the solvent of choice for the extraction procedure. The validation of the method was performed on spiked blood samples for the evaluation of selectivity, carry-over, limit of detection (LOD), limit of quantification (LOQ), recovery, accuracy and precision (RSD%) and the evaluation of the validation results was found satisfactory. A rapid, sensitive and reliable method was developed for the determination of C12-C16 alkyldimethylamines in blood after optimization experiments and finally successfully applied to a real blood sample from a suicide attempt.

P1-55 VALIDATION AND APPLICATION OF METHOD FOR THE DETERMINATION OF PESTICIDE RESIDUES IN NATURAL WATERS AND SEDIMENTS, COUPLED TO GC-MS DETERMINATION

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A number of pesticides are used in aquaculture to treat sea lice or control weeds and algae. The determination of the residues of pesticides is one of the major challenges for the preservation and sustainability of the environment [1]. It is very important due to the risks that these compounds offer to human health, besides their persistence in the environment and their tendency to bio-accumulation. It is therefore, needed to be monitored for a better knowledge of its fate. Pesticides that are more hydrophobic tend to be detected more frequently in sediment. Thus, measuring pesticides in sediment is important for tracking their fate in the environment and evaluating for potential toxicity [2]. The main objectives of this study were to develop rapid and accurate screening multi-residue pesticide methods on the basis of Solid Phase Extraction (SPE) technique for the determination of 10 pesticides in water samples and on the basis of QuEChERS technique for the sediments. The target compounds were determined by Gas Chromatography coupled with Mass Spectrometry (GC-MS). The method was validated in terms of accuracy, precision, linearity, detection and quantification limits. The recovery percentages obtained for the pesticides in water at three different concentration levels, ranged between 73.2 to 101.2%, with relative standard deviations below 9.3%. The corresponding results from the sediment ranged between 69.5 to 122.7% with relative standard deviations below 11.2%. The limits of detection for the pesticides in water and sediment were below 12 ng L^{-1} and 9 mg kg^{-1}, respectively. The optimized methods were applied in Epirus region (North-Western Greece) to determine the concentration level of the target compounds in sea water and sediment samples. The analytical methodologies exhibited excellent analytical characteristics and proved to be reliable for the estimation of the pollutant load in sea water and sediment samples from marine aquaculture.

P1-56 ANALYTICAL METHODS FOR THE DETECTION OF PHARMACEUTICALS AND THEIR METABOLITES IN SURFACE WATERS

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Pharmaceuticals, among the emerging contaminants, are the most relevant group of substances for the possible impact on aquatic ecosystems due to their universal use and chemico-physical properties. Pharmaceuticals consumed by humans are continuously discharged in aquatic environments through urban effluents. Several classes of pharmaceuticals such as antibiotics, non-steroidal, anti-inflammatory drugs, β-blockers, antipsychotics, cholesterol lowering drugs, anticonvulsants, and hormones have indeed been widely detected in surface waters near major cities around the world. The present study describes the development of a highly selective and sensitive analytical method using solid phase extraction (SPE) followed by UHPLC-LTQ-Orbitrap-MS methodology for the determination of some frequently prescribed pharmaceuticals and their metabolites in surface waters. The analytes were separated on a Fortis Diphenyl column (2.6 μm, 50x2.1 mm) using gradient elution in positive (+ESI) and negative (-ESI) ionization mode. A number of 26 pharmaceuticals and 6 metabolites were selected. Pharmaceuticals positively ionized: sulfamethoxazole, sulfamethoxypyridazine, sulfadiazine, sulfapyridine, sulfamethazine, sulfamethizole, sulfaquinoxaline, sulfathiazole, erythromycin, trimethoprim, oxolinic acid, oxytetracycline, amoxicillin, caffeine, paracetamol, fluoxetine, carbamazepine, sertraline, venlafaxine, phenazone, citalopram and their metabolites: N-acetylsulfamethoxazole, norfluoxetine, carbamazepine-10,11-epoxide, N-desmethylsertraline, O-desmethylvenlafaxine. Pharmaceuticals negatively ionized: diclofenac, ibyprofen, triclosan, florfenicol, tolfenamic acid and one metabolite: 2-hydroxy-ibyprofen. In order to optimize the extraction method, five different cartridges were tested: Oasis HLB, Oasis MCX, C8-CNW, C18-CNW and Telos and the results showed that most of the compounds exhibited higher recoveries using Oasis HLB.

Acknowledgements

«This research is co-financed by Greece and the European Union (European Social Fund- ESF) through the Operational Programme «Human Resources Development, Education and Lifelong Learning» in the context of the project “Strengthening Human Resources Research Potential via Doctorate Research” (MIS-5000432), implemented by the State Scholarships Foundation (IKY)». The authors would like to thank the Unit of Environmental, Organic and Biochemical high resolution analysis-ORBITRAP-LC-MS of the University of Ioannina for providing access to the facilities.

P1-57 BIORECOVERY OF SCANDIUM AND OTHER RARE EARTH ELEMENTS FROM GREEK RED MUD

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The crucial dependency on critical raw material (CRM) and its supply risk is a growing concern for EU in the recent years. Among the CRMs, rare-earth elements (REEs) are considered to be by far the riskiest supply. Red mud (RM), a hazard by-product of the alumina production, is a waste material produced in huge quantities by the mining industry [1]. It contains a considerable amount of REEs, in particular Scandium (Sc), which represents more than 95% of the economic value of REEs in RM [2]. The annual production of RM in Greece is up to 750,000 metric tons with around 1 kg REEs/ton RM [3]. Biotechnology can play an important role based on the understanding of living organisms and their interaction with different REEs [4]. This study centered on the development of a novel bioleaching process for the recovery of Sc and other REEs from RM supplied from Aluminium of Greece, as an alternative approach to selective acid leaching. Heterotrophic organisms produce organic acids and thus dissolve the solid matrix of RM making the REEs available for simple physical extraction. The study is focused on the characterization of microbial diversity of RM, collection of isolates and screening, the optimization of the bioleaching process and the Life Cycle Assessment (LCA) and Life Cycle Cost Analysis (LCC) of the process.

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P1-58 DETERMINATION OF MAJOR ELEMENTS IN BULGARIAN BOTTLED MINERAL WATER

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Water analysis plays a decisive role in the regulations that determine the water quality levels. Because of the significance of clean water for human health, water analysis is critical for determining both elements present at high and trace concentrations. Besides being able to simultaneously analyze many elements, quadrupole ICP-MS also offers high sensitivity over a wide linear range and low detection limits. However, the direct determination of macro components (alkaline and alkaline earth elements, as well as Al, Fe, Mn, P, Si) in natural waters using ICP-MS is hampered by their low ionization potential and high concentration ranges in which they are present in water samples.

In the presents study the possibilities of two approaches: cold plasma conditions at reduced plasma frequency and introduction of a rejection parameter (RPa) to suppress the signal intensity were studied and their ability to extend the linear ranges of macro components were evaluated. The optimization study demonstrated that the introduction of Rpa is preferable, the most serious advantages being the wider linear range, the ability to suppress signal intensity selectively on a per-isotope basis and the possibility for application the method in simultaneous macro- and microelements analysis. This method has been applied for ICP-MS determination of Na, K, Ca, Mg, Al, Fe, Mn, P and Si in several brands of bottled mineral waters purchased from the commercial network of Bulgaria. The accuracy of the determination was evaluated by ICP-OES measurement.

Acknowledgements

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P1-59 A UHPLC-MS/MS METHOD FOR THE DETECTION AND QUANTIFICATION OF 84 DRUGS OF ABUSE AND PHARMACEUTICALS IN HUMAN BLOOD

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The present study reports the development of a method for the detection and quantification of drugs and medicines in human blood. Forensic and Clinical toxicology labs face a big number of cases most of which require fast delivery of trustworthy, accurate results. These needs in combination with the fact that blood is the basic and most important biological specimen for such analysis, lead to the necessity for a fast, reliable screening method for a large number of target molecules in human blood (postmortem or clinical). Chromatography was performed by an ACQUITY UPLC H-Class System (Waters Corporation) on an Acquity BEH C18 column (150 × 2.1 mm i.d., 1.7 µm; Waters) and a gradient of MeOH over H_2O with a total analysis time of 17 minutes for 84 drugs and pharmaceuticals. MS/MS detection of analytes and IS was carried out on a Xevo TQD system (Waters, UK) and MRM mode was applied for the detection and quantification of all analytes. The target compounds comprise opiates, cocaine, cannabinoids, amphetamines, benzodiazepines, antipsychotics, antidepressants, barbiturates, hypnotics, antiepileptic and NPS. Sample pretreatment process was also studied. The validation of the method was performed on spiked blood samples for the evaluation of selectivity, carry-over, limit of detection (LOD), limit of quantification (LOQ), recovery, matrix effect, accuracy and precision (RSD%). The proposed method was applied in our labs for the analysis of numerous forensic cases of chronic drug abusers collected post mortem. In conclusion, this new method is a useful and powerful tool in toxicologist's hands because it is fast, simple, trustworthy and covers a range of drugs very important for the daily practice of the toxicology lab. Application of the method can provide an answer whether a blood sample is positive in any of the 84 tested drugs, and provide solid quantitative results.

P1-60 AN EFFICIENT DLLME-GC-MS METHOD DEVELOPED FOR THE DETERMINATION OF MONOHYDROXY AND DIHYDROXY PAHs METABOLITES IN HUMAN URINE

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Polycyclic aromatic hydrocarbons (PAHs) are a class of environmentally persistent organic compounds which are mainly formed through incomplete combustion of organic molecules. PAHs are highly lipophilic and soluble in organic solvents. Several national and international organizations have evaluated their toxicity, and 16 PAHs have been defined to be of the most significant concern to potential exposure and adverse health effects (EPA 1977). The most common biomarkers of PAHs exposure are their urinary monohydroxylated metabolites (OHPAHs). Urine is an easily available sample which is accessible in large volumes by direct collection by the donors as well as it is a useful matrix for analysis of quickly metabolized and excreted chemicals. The demand for selective and sensitive analytical methods for the determination of PAHs metabolites in human biological samples has been recently increasing. Independently of the suitable analytical technique, sample preparation such as extraction, clean-up, and preconcentration steps are required for the isolation OHPAHs from urine to reach the concentration levels which are necessary for its determination in such a complex biological matrix. We propose a dispersive liquid-liquid microextraction (DLLME) followed by gas chromatography and mass spectrometric detection with quadrupole analyzer (GC-MS), for the determination of 15 hydroxylated PAHs metabolites of naphthalene, fluorene, phenanthrene, anthracene and pyrene in human urine. In comparison with other techniques, this method has the advantage of fast, selective and environmentally friendly microextraction. The determination of mono and dihydroxy metabolites of PAHs at the trace concentration levels is the most important advantage of this method.

Acknowledgement

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P1-61 MODIFIED GRAPHENE OXIDE FOR RARE EARTH METALS' PRECONCENTRATION METHOD AFTER DISPERSIVE SOLID PHASE EXTRACTION AND OPTIMIZATION WITH CENTRAL COMPOSITE DESIGN

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Since its discovery in 2004, graphene has received worldwide attention and until today it has several applications. Graphene has been used for the separation of organic substances by π-π interaction due to the extensive presence of benzene rings. Moreover, because of its oxygen containing active sites, graphene oxide is suitable for binding with metal ions, such as rare earth metals (REEs). Rare earth metals have been extensively used in agriculture as fertilizer, growth promoters and feed additives. Today, because of their characteristics they gain more and more attention in various industrial fields, such as electronics, superconductors, catalysts, and ceramics. Therefore, the concentration of those elements has increased in environmental and biological samples and finally impaired human health by food chain accumulation. Herein, a novel graphene oxide derived material was prepared for the preconcentration of REEs. Modification took place to increase the capacity of the material. After characterization it was applied for the dispersive solid phase extraction (d-SPE) of rare earth metals followed by inductively coupled plasma atomic emission mass spectrometry detection (ICP-MS). Central Composite design and Derringer's type desirability function were employed for the optimization of the adsorption and desorption steps. The proposed method was validated in terms of linearity, LOD, LOQ, accuracy, within-day precision and between-day repeatability. Adsorption capacity, effect of co-existing ions and reusability of the material were also studied. The d-SPE method is simple, rapid, sensitive and it can be used for the analysis of La, Pr, Yb, Ce, Er, Eu, Sm, Dy, Nd, Tb, Gd, Ho and Tm in complex matrices.

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P1-62 COMPARISON OF THE DATA OBTAINED BY XRF AND ICP-AES FOR ANALYSIS OF BELT ACCESSORIES DATED TO THE GREAT MIGRATION PERIOD IN BULGARIA

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Chemical analyses using modern instrumental techniques are widespread in the field of archaeometry, and instruments often used for this purpose present both destructive and non-destructive techniques. In the last 10-15 years special attention is paid on portable XRF spectrometers, usually used for *in situ* analyses at the archaeological sites or in museum expositions. Furthermore, the increasing availability of portable XRF devices, as well as their moderate cost when compared to laboratory-based techniques, more frequently allows the incorporation of chemical examinations in material culture studies. Such analyses, however, have limitations and cannot answer all questions that have arisen. On the other hand, combining several instrumental techniques with different characteristics can produce quite satisfactory results.

In this work are presented the results obtained from analysis of a number of belt accessories dated to the Great Migration Period in Bulgaria (3rd-7th c. AD). The analysis was carried out by ICP-AES (Perkin Elmer Optima 6000 DV) and p-XRF (Bruker, S1 Titan), and the data were compared by the methods of multivariate statistics for consistency in terms of source determination (metal alloys) and individual element concentrations. Both instruments identified the same type metal alloys, but individual element comparisons showed significant differences. However, these differences are irrelevant to alloy type identification and can be resolved through instrument cross calibration. Even with a lower sensitivity, the p-XRF was found suitable for determining the main compounds and some of the microelements, especially for samples that are valuable from historical and archaeological point of view and therefore the non-destructive technique is more appropriate for their investigation.

Acknowledgments

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Invited Lecture

IL05 A NEW ALGORITHM FOR ENHANCING CHROMATOGRAPHIC AND SPECTROSCOPIC MEASUREMENTS AND DATA PROCESSING

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To most analytical chemists, the Fourier transform is known for its ability to improve the signal-to-noise ratio of analytical measurements by multiplexing the original analytical signal which is much used in signal and image processing. Far less known among chemists is that the Fourier transform is just one of several related linear transformations. While the Fourier transform reconstructs the original signal from sines and cosines; the other transforms are based on other periodic functions.

The Hadamard transform is the most common of these alternative transforms. Based on square waves rather than on sines and cosines, this transform finds applications in three different areas in analytical chemistry. First, it is used to multiplex or encode analytical signals, so that many signals can be measured simultaneously - mainly with the aim of the improving the S/N ratio. Second, the transform is used in multiplexed imaging where spatially resolved information is obtained without focusing a high-intensity source on a sample. Finally, the Hadamard transform is used in data transformation. Information is relocated so that signal compression can be performed without loss of essential features of the data set.

In this presentation, we will discuss the use of the Hadamard transform for processing data from a gas chromatograph with a fast modulating multiplexing sample inlet. Multiplexing is not used here as a means of improving the S/N ratio of faint signal features, but to record chromatograms of transient signals with higher time resolution than that of sequential measurements. This is done by injecting the sample according to a pseudo-random binary sequence, and decomposition of the resulting signal into a matrix of individual chromatograms. A new algorithm of decomposing the data matrix will be presented and compared to earlier published approaches.

Acknowledgments

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TUESDAY, SEPTEMBER 24TH, 2019

EVERGETON HALL

Chromatography 1

Chair: ***R. Lobinski, D. Hela***

OP25 THE UTILITY OF HIGH RESOLUTION MASS SPECTROMETRY & INFORMATICS FOR NATURAL PRODUCT ANALYTICS

I. Riba

Senior Applications Chemist, WATERS Ltd

Advances in the performance and functionality of mass spectrometry systems have allowed a more accurate and in-depth analysis of natural products. Whilst enhancements to the mass spectrometer are extremely valuable, the combination with ion mobility separation adds a new dimension to any analysis, improving confidence in results.

Waters' mass spectrometry systems, particularly with seamless incorporation of ion mobility separation, are routinely used in compound profiling and adulteration studies. The production of scientific libraries, in association with collaborators, including mass, product ion, retention time and collision cross-section information play an important role in the accuracy and precision of the Waters' natural products solution.

Here, we will describe the use of the Waters' natural products solution in profiling and screening.

OP26 ENHANCED VARIANTS OF MICROEXTRACTION PROCEDURES BASED ON MAGNETIC IONIC LIQUIDS

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An ongoing trend in microextraction in chemical analysis is the use of ionic liquids (ILs). A more advanced concept of IL-based microextraction is the magnetic separation of the ILs from the analyzed matrix. In this context, the employment of magnetic ILs (MILs) in microextraction has been rendered easier and new microextraction modes have become available.

In this study, we developed two variants of common microextraction procedures, using the $[P66614^{+}][Dy(III)(hfacac)^{4-}]$ MIL. The first approach is a dispersive liquid-liquid microextraction procedure which combines a water insoluble solid support and the MIL in a one-pot, pH-modulated procedure for the microextraction of triazines and sulfonamides. The newly developed analytical method enjoys the benefits of sensitivity (limits of quantification: 0.034-0.091 μg L^{-1}) and precision (relative standard deviation: 5.2-8.1%), while good recoveries (i.e., 89-101%) were achieved from a lake water and an effluent from a municipal wastewater treatment plant.

The second approach is a matrix solid-phase extraction procedure, which employs MIL for the first time. Because of its magnetic properties, the MIL can be harvested directly after the extraction step, using a magnet, while its hydrophobic nature makes it possible the extraction of pesticides from raw vegetables of high water content. The limits of quantification achieved with the developed procedure were between 0.002 and 0.009 mg kg^{-1}, lower than the general maximum residue limits established for pesticides by the EU 62/2018 European Commission legislation. Good precision ((relative standard deviation: 5.2-7.1%), good recoveries (i.e., 94-101%) and low matrix effect (between -13% and 14%) and simplicity, complement the advantages of the developed procedure. Overall, the two developed procedures pave the way for more challenging applications.

Acknowledgements

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OP27 SYNTHESIS OF AMBERLITE XAD-4 BASED METAL CHELATOR VIA ARYLDIAZONIUM RADICAL ROUTE FOR SOLID PHASE EXTRACTION OF HEAVY METALS FROM GROUNDWATER SAMPLES

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A simple chemical functionalization for styrene polymeric substrate and a like via aryldiazonium salts radical has been used to anchor 8-hydroquinidine (8-HQ) moieties onto Amberlite XAD-4beads. the coupling approach involves the generation (in situ) of nitroaniline aryldiazonium salt in presence of hypophosphorous acid which is co-valently grafted onto Amberlite XAD-4. Subsequently, the 8-HQ chelator is added via standard diazo coupling. The successfulness of the synthesized resin was confirmed by (ATR-IR), (TGA) and (XPS). The risen was packed into cartridges and used with standard solid phase extraction (SPE) apparatus for the extraction of trace metals; Co (II), Ni (II) and Cu (II) from groundwater samples prior to their measurement by (ICP-MS). The resin exhibited more than 90% enhancement in capacity exchange relative to the plain Amberlite XAD-4. Under the optimum conditions the sorption capacity of the sorbent was 0.366, 0.265 and 0.328 (mM/g) for Co (II), Ni (II) and Cu (II) respectively. The sorbent showed efficient performance when applied for SPE of trace metals from groundwater real samples from AlMadinah AlMumnawarah, Saudi Arabia.

OP28 FABRIC PHASE SORPTIVE EXTRACTION FOR THE DETERMINATION OF ANTIDEPRESSANT DRUGS IN ENVIRONMENTAL SAMPLES PRIOR TO HPLC-DAD

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Every year, hundreds of tons of organic pollutants reach the environment through several types of waters (drinking water, groundwater, surface water treated) and many of these compounds have harmful effects on the aquatic ecosystem. Thus, there is an urgent need to rapidly detect water pollution in the field. Different miniaturized methodologies based on solid phases as extracting sorbent have been applied in order to reduce cost and simplify the extraction procedure. In this work, a rapid, simple and green method for the extraction and pre-concentration of three psychoactive drugs that are commonly used in the treatment of mental diseases (citalopram, clozapine and sertraline) was developed using a novel extraction process, Fabric Phase Sorptive Extraction (FPSE) coupled to high performance liquid chromatography-photodiode array detection (HPLC-DAD). FPSE is a novel, highly sensitive, efficient and solvent minimized sample preparation technique that integrates the advantages of sol-gel coating technology and the rich surface chemistry of different fabrics such as cellulose, polyester and fiberglass. Parameters like pH, sample volume, extraction time, elution time and elution solvent which affect the efficiency of the FPSE, were evaluated in depth with the employment of experimental design and Response Surface Methodology (RSM). The chromatographic separation was carried out using a mobile phase consisted of methanol and water acidified with phosphate buffer of pH 3.0 at a flow rate 0.3 mL/min on a Fortis-SpeedCore C18 50x2.1 mm, 2.6 μm column.

Characterization of the materials and surfaces was carried out by FT-IR, contact angle and roll-off angle measurements, differential scanning calorimetry and optical microscopy.

The method shows good linearity, with RSD of less than 6%. Absolute recoveries higher than 60% were obtained for the studied compounds.

TUESDAY, SEPTEMBER 24TH, 2019

LORDON BYRON

Sample handling / Mobile Instruments

Chair: ***J. Barek, M. Prodromidis***

OP29 DNA HYBRIDIZATION ASSAYS AND QUANTITATIVE POLYMERASE CHAIN REACTION USING A SMARTPHONE AS A CHEMILUMINESCENCE IMAGER

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Polymerase chain reaction (PCR) is a fundamental technique in nucleic acid analytical chemistry. PCR entails *in vitro*exponential amplification of DNA/RNA sequences enabling ultra-low detection levels in complicated sample matrices. Quantitative competitive PCR has found widespread applications in the health, food and environmental sectors. The determination of the amplification products has been based on electrophoresis, fluorometry, chemiluminometry, mass spectrometry and flow-cytometry. All the above methods require costly equipment and highly qualified personnel. In this work, we introduce the smartphone as a low-cost chemiluminescence imager for the development of *(a)* DNA hybridization assays and *(b)* quantitative competitive PCR assays (QCPCR). For the hybridization assay, a specific oligonucleotide probe was immobilized in microtiter wells and allowed to hybridized with biotinylated denatured dsDNA target. The hybrids were determined by adding an avidin-peroxidase conjugate in combination with a chemiluminogenic substrate. The emitted light was detected by a smartphone and the results were compared with a conventional digital camera and a microtiter-plate luminometer (with a photomultiplier). The limits of detection of the DNA target based on the smartphone, digital camera and luminometer were 1.6, 2.4 and 1 pmol/L, respectively. For QCPCR, a suitable dsDNA internal standard (competitor), with the same size and same primer binding sites as the target sequence, was synthesized and 5000 molecules were added to each amplification reaction. The amplification products from the target and competitor were determined by the hybridization assay and the ratio of the smartphone-obtained signals were related to the number of target DNA copies in the sample prior to PCR. Smartphone-based QCPCR showed an analytical range from 137 to $9x10^5$ copies of target DNA. The CVs for the QPCR ranged from 7-17%.

Acknowledgement

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OP30 FLUORESCENCE INSTRUMENTATION FOR RAPID, IN SITU WATER QUALITY ASSESSMENT

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Due to emerging water sovereignty problems, water quality assessment plays an important role in our century both at local and global scales. As water quality refers to chemical, physical and biological characteristics of water, the development of a portable, rapid device for the determination and visualisation of the main parameters of waters is even more needed for such complex analyses. For this purpose, we developed a family of fluorimeters for *in situ* determination of water quality. The modular structure of the instrument offers the possibility to determine various water quality parameters by using direct and immunofluorescence techniques. A short insight into an instrumentation development aiming the use of fluorescence techniques to measure different chemical and biological parameters will be discussed.

For the first application a standard cuvette is used. The sample is excited with a Xenon flash lamp combined with an optical bandpass filter. Fluorescence is measured with a high-sensitivity, TE cooled CCD fiber-optic spectrometer or a photomultiplier tube combined with a set of optical interference filters for the measurement of biological and chemical oxygen demand (BOD/COD), total organic carbon (TOC) and the presence of polycyclic aromatic hydrocarbons (PAHs).

The second application fits to 96-well microplate format. The samples are illuminated with high power LEDs of different wavelengths and the emitted fluorescence is measured with silicon photodiodes having large active area to determine the density of phytoplankton and phytobenthic algae based on chlorophyll-*a* (Chl-*a*) content.

Acknowledgment

This research was supported by the National Research, Development and Innovation Fund of Hungary within the National Competitiveness and Excellence Program NVKP_16-1-2016-0049.

OP31 PORTABLE DIAGNOSTIC MEDICAL DEVICES UTILIZING FREE-STANDING RESPONSIVE POLYMER FILM-BASED BIOSENSORS AND LOW-COST TRANSDUCERS FOR POINT-OF-CARE APPLICATIONS

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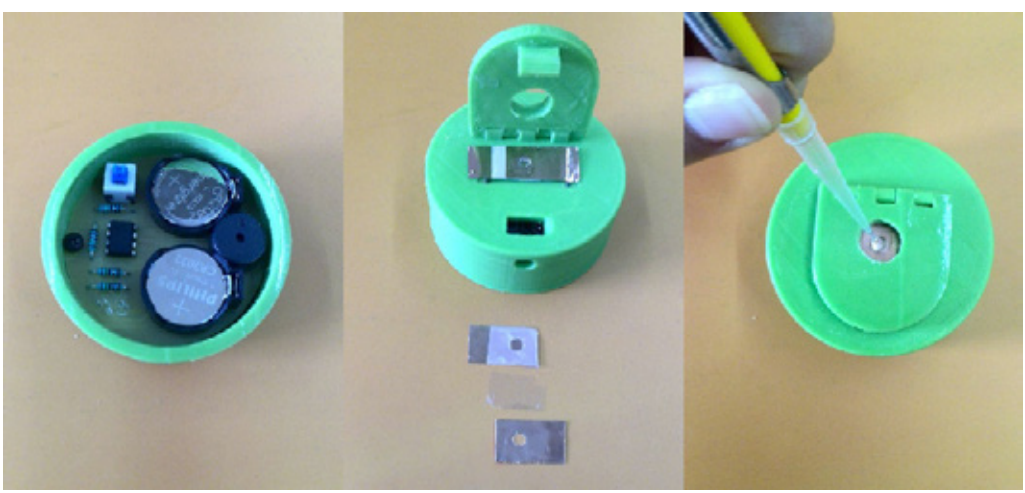
Herein, we describe a novel type of medical diagnostic devices able to provide reliable clinical measurements at resource-limited or poor settings, where centralized laboratory facilities are in short supply, and for use at home. The diagnostic devices employing novel free-standing responsive polymer-based biosensors and newly devised transduction and measuring principles. Diagnostic devices include a single microfluidic vertical channel and their operation is based on the measurement of the time required the infinite electric resistance between two, uncontacted, conductive layers to reach a finite value as a result of the selective degradation of the responsive polymer membrane by the target analyte (biochemical index).



The concept is demonstrated by utilizing a pH-responsive membrane, a copolymer of methylmethacrylate and methacrylic acid (Eudragit S100), modified with the enzyme urease. The device was successfully tested for the determination of urea directly in untreated, undiluted urine samples. In this case, membrane degradation is caused by the enzymatically produced ammonia according to the chemical equation: Urea + H_2O -(urease)® CO_2 + $2NH_3$. In addition, a near-patient detection of Helicobacter pylori in bioptic samples is also demonstrated.

The proposed diagnostic devices can be used as a generic platform for the point-of-care analysis of a large variety of biochemical indices, in accordance with the “ASSURED” criteria set by the world health organization (WHO). Wide scope applicability can be achieved by the proper combination of responsive polymer membranes and enzymes that will be immobilized onto the surface of the membranes. Medical diagnostic devices have been designed to have small size, light weight, and low power consumption.

Acknowledgements

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: T1EDK-03341).

OP32 KINETIC STUDY OF PETROLEUM GENERATION USING OPEN-PYROLYSIS ROCK-EVAL ANALYTICAL SYSTEM

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Basin and petroleum system modeling, which leads to the assessment of hydrocarbons' resources, requires kerogen thermal transformation kinetics as input for the reconstruction of generation history. In most industrial studies, reaction rates and frequency factors are selected from literature data, describing kerogens of similar origin and environment of deposition. It has been shown that this approach leads to significant inaccuracies. Alternatively, thermal decomposition reactions may be studied with thermal gravimetry (TG) experiments at various heating rates to approximate hydrocarbon generation processes allowing the thermal energy required for hydrocarbon generation under differing geological conditions to be inferred. Rock-Eval (RE) analytical pyrolysis method has been widely accepted as industry standard method in petroleum exploration studies to identify kerogen type and maturation level, while RE pyrolysis curve (S2) may be used to generate reaction kinetics. The method provides pyrolysis data in a rapid and sensitive way to obtain and as it has been shown, it estimates accurately the kinetic parameters. The kinetics of the thermal decomposition of kerogen are typically described as a series of independent and parallel 1st order quasi-irreversible reactions and expressed by a distribution of activation energy with a single fixed frequency factor. This assumption seems to be oversimplified; nevertheless, it is supported by observations of the source rock maturation in nature. In this work, a sample set of six source rocks from Greek Ionian zone were used to demonstrate the ability of the RE method to provide accurate kinetic data, comparable to the ones obtained from time-consuming and costly laboratory pyrolysis experiments. Kinetic data for the examined kerogens is reported. Furthermore, the influence of the matrix (inorganic content, presence of bitumens) was studied, using samples pretreated respectively, by HCl treatment and organic solvent extraction. The results indicate that organofacies' variations affect the accuracy of hydrocarbons' generation model.

OP33 THE STUDY OF MERCURY ACCUMULATION BY PLANTS DEPENDING ON ITS SPECIATION IN GROWING SUBSTRATE

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Despite the fact that phytotechnologies are used rather intensively in world practice both for cleaning contaminated areas and for extracting valuable components, the main attention is usually focused on their practical application, and to a lesser extent touches upon scientific problems focused on the study and understanding of the essence of the bioaccumulation phenomenon. Unfortunately the relationship between the chemical form of the element in substrate and the efficiency of its extraction by plants is not discussed in the literature. To clarify the question the present work was concentrated in the study of the dependence mercury accumulation efficiency by plants in natural and man-made environments on its chemical form. The speciation of mercury as well as of the products of its transformation in growing substrate was performed using the hyphenation of thermal release technique with electrothermal atomic absorption detection (TR-ETA-AAS) which were previously developed by the authors [1]. The maim advantage of this approach consists in direct analysis of the solid environmental samples (soils, plants etc.) without prior dissolving. As a result it was shown that a series of mercury extractability depending on the initially introduced species can be represented as the following: $CH_3Hg^+ > Hg^{2+} > HgS$. Moreover, it was also found that the chemical forms of mercury in substrate undergo to the transformation in time.

Reference

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IL06 SYNTHESIS ROUTES FOR THE PREPARATION OF MAGNETIC NANOPARTICLES FOR HEALTH AND ENVIRONMENTAL APPLICATIONS

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Ferrimagnetic iron oxide nanoparticles (magnetite or maghemite) have been the subject of an intense research, not only for fundamental studies but also for their potentiality in a wide spread number of practical applications such as the biomedicine and environmental areas. Most of these studies were focused on nanoparticles with spherical morphology but recently there is an emerging interest on anisometric nanoparticles. This talk is focused on the synthesis routes for the production of uniform anisometric magnetite/maghemite nanoparticles with different morphologies like cubes, rods, disks, flowers and many others [1]. We analyzed those procedures, detected the key parameters governing the production of these nanoparticles with particular emphasis in the role of the ligands in the final nanoparticle morphology. Finally, the impact of each morphology on the different applications are analysed in detail.

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TUESDAY, SEPTEMBER 24TH, 2019

EVERGETON HALL

Materials / Sensors

Chair: ***K. Stalikas, K. Simeonidis***

OP34 MICROFLUIDIC ANALYTICAL TOOL COUPLING A FLUORESCENT MOLECULAR PROBE AND A MICRO-HYDROCYCLONE FOR THE DETECTION OF WATER CHLORINATION LEVEL

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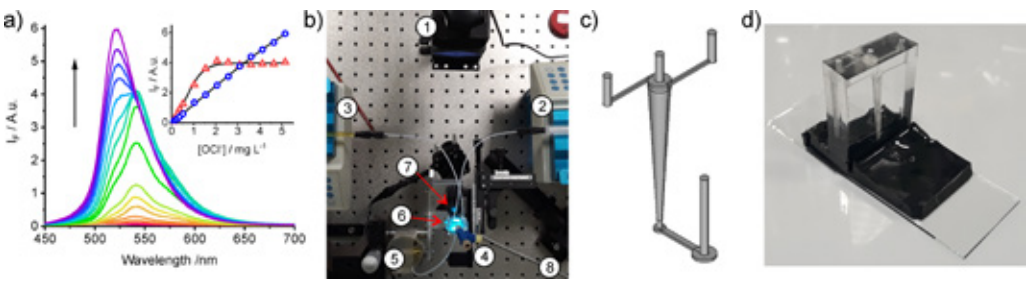
Chlorination of pool water and wastewater, in food and pharmaceutical production, as well as in pesticide and paper manufacturing is a routinely used technique. However, the amount of chlorine in water must be strictly adjusted, to ensure enough concentration to kill pathogenic bacteria and viruses, while preventing too high concentrations inducing negative effects on human health. As an indicator, a molecular fluorescent probe based on a BODIPY structure was designed. This indicator exhibits a sensitive and selective fluorescence response upon increasing concentrations of hypochlorite in aqueous solvent mixtures. Real-time analyses became possible after the integration of this fluorescent indicator into newly designed 2D & 3D microfluidic chips incorporating a passive sinusoidal mixer and a micro-hydrocyclone, respectively. A comparison of the two microfluidic systems, including their ability to prevent accumulation or circulation of microbubbles, has shown excellent fluidic behaviour for the micro-hydrocyclone device. This system was distinctly more robust against gas bubbles, showed a higher signal gain and allowed to halve the limit of detection to 0.02 mg L^{-1}. The use of the 3D system to quantify the chlorine content of pool water samples for sensitive and quantitative chlorine monitoring has been demonstrated.



OP35 LABORATORY EVALUATION OF ULTRAMAFIC ROCKS EXPLOITATION TOWARDS THE PRODUCTION OF ADDED-VALUE PRODUCTS

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In magnesite-producing mines, the initial extraction of the ore is followed by a series of processes for the separation of magnesite from the host ultramafic rock, with the latter considered the by-product of the separation processes. Due to the serpentinization of the ultramafic rocks and the consequent alteration of the primary minerals olivine and/or pyroxene mainly to secondary minerals of the serpentine group, the physicochemical properties of these by-products are degraded and their economic and commercial exploitation is currently limited. The purpose of this study, is the qualitative and quantitative characterization of rocks hosting magnesite ore deposits and their evaluation regarding the possibility of upgrading their properties using various treatment methods (e.g. thermal) under the frame of circular economy. For this purpose, samples of various grades were collected from "Rachoni" magnesite mine of "Grecian Magnesite SA" company in Gerakini, Chalkidiki, Greece. Initial investigation and evaluation of the samples was carried out in order to develop appropriate laboratory and industrial technology for the conversion of these wastes into a commercial product (dunite) with added value. On this purpose, X-ray diffractometry analysis was extensively applied as a tool to initially identify the geological origin and the mineralogical content of the collected samples and then, understand the structural changes observed during thermal treatment. Further information on the mechanism for preferable formation of dunite were received by Thermogravimetric and Differential Thermal Analysis (TG-DTA).

Overall, samples consisting mainly of serpentine ($Mg_2Si_2O_5(OH)$) and forsterite (Mg_2SiO_4) were the most promising to undergo a suitable thermal treatment (>680 °C) and upgrade their physicochemical characteristics. Particularly, the transformation proceeds by the decomposition of serpentine towards the formation of a "second generation" forsterite. Such reaction becomes more favorable in the excess of magnesium as determined in magnesite-rich samples.

Acknowledgments

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OP36 LOW-COST "GREEN" SENSORS BASED ON GRAPHITE NANOMATERIALS PREPARED FROM PENCIL LEADS WITH THE AID OF A 3D POSITIONING SPARKING DEVICE FOR THE SENSITIVE DETECTION OF NITROAROMATIC EXPLOSIVES

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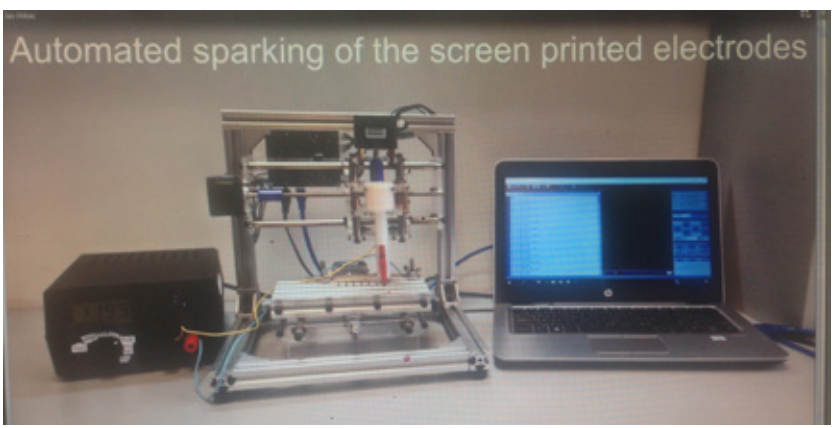
We report on the straightforward preparation of graphite nanomaterials (GNMs) through a direct graphite-to-substrate electric discharge at ambient conditions at 1.2 kV between pencil leads and low-cost graphite screen-printed electrodes (SPEs). The so-modified sparked GNM-SPE was characterized by Raman spectroscopy, scanning electron microscopy, cyclic voltammetry, and electrochemical impedance spectroscopy. GNM-SPE sparked electrodes endowed sensitivity to plain SPEs to the cathodic voltammetric detection of various nitroaromatic explosives. Different commercially available pencil leads including "graphite pencil" (Faber−Castell, Castell 9000) of different degrees of hardness (4H, 2H, HB, 2B and 4B), "high-purity graphite leads" (Pilot, ENO−G, HB), "needle-crystal leads" (Uni-ball, Uni, HB) and "nanodiamonds leads" (Uni-ball, Nano−Dia, HB) were examined. Taking as criterion the highest response to the electro reduction of 2,4,6-trinitrotoluene (TNT), Castell 9000 (2B) pencil was selected as optimum. SPEs that have been modified with 200 sparking cycles showed an excellent repeatability (RSD_{50ppb} = 1.8%, n=5), reproducibility (RSD_{10ppb} = 3.0% και RSD_{50ppb} = 2.8%, n=5) and linear response over the concentration range 1−100 ppb TNT. Data fit the equation I (μA) = (0.0137 ± 0.0002) [TNT(ppb)] − (0.0043 ± 0.0020), R^2 = 0.9989, while the limit of detection based on the 3σ/m criterion was calculated 0.44 ppb. The interference effect of other nitroaromatic explosives and masking compounds, which are used to hinder the detection of TNT, was extensively investigated.



Moreover, GNM-SPE sparked electrodes were successfully applied to the determination of TNT in drinking water samples fortified with 2, 5 and 10 ppb TNT. Recovery was from 101±8 to 109±7%. Results demonstrated a new type of GNM-SPE low cost electrodes lend themselves to extremely simple preparation while offering enhanced detection capabilities and a wide-scope of applicability. Remarkably, GNM-SPE sparked electrodes can be prepared on-demand, within 3-4 min, through a totally green and solution-free method that requires only a pencil lead and a power supply.

OP37 AUTOMATED INSPECTION OF PMMA COATING ON NON-PATTERNED SILICON WAFERS

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Quality control of the resist coating on the silicon wafer is one of the major task prior the exposition of patterns into the resist layer. Thus, the ability to inspect and identify the physical defect in the resist layer plays an important role. The absence of any unwanted defect in resist is an ultimate requirement for preparation of precise and functional micro- or nano-patterned surfaces. Currently used wafer inspection systems is mostly used in semiconductor or microelectronic industry to inspect non-patterned or patterned wafers in order to achieve production with high yield. Typically, they are based on acoustic micro imaging, optical imaging or electron microscopy. This paper presents design of a custom optical based inspection device for small batch lithography production that allows scanning a wafer surface with an optical camera and by analyzing the captured images to determine the coordinates (X, Y), size and type of the defects in the resist layer. In addition, a software that is responsible for driving the scanning device and for advanced image processing is presented.

TUESDAY, SEPTEMBER 24TH, 2019

LORDON BYRON HALL

Spectrometry 1

Chair: ***K. Valko, I. Gerothanassis***

OP38 DIAGNOSTIC POTENTIAL OF FT-IR-BASED METABOLOMICS FOR THE AUTHENTICATION OF LAURUS NOBILIS L. ESSENTIAL OIL IS SUPPORTED BY GC-FID AND GC-MS ANALYSES

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The essential oil (EO) of the leaves of the evergreen *L. nobilis* L. tree (bay leaves) is traditionally used in food and pharmaceutical industry due to its antioxidant and antimicrobial properties. Its composition is dominated by 1,8-cineole although its levels may vary largely. Authentication is thus necessary to avoid adulteration problems. Powerful separation techniques such as gas chromatography (GC) that are routinely applied for EO composition analysis and detection of adulteration have been also used for bay leaf EO. Spectroscopic investigation in the mid-infrared (MIR) region that provides a rapid, reproducible and non-destructive option for quality control and authentication of natural products has found scarce applications for bay leaf EO so far. In our study, FT-MIR spectra of EOs produced in the laboratory (0.08-1.4 mL) from botanically identified bay leaves were acquired using a liquid transmission cell, pre-processed and used as fingerprint for "authentic bay leaf EO" (n = 97). The spectral dataset was enriched with data for commercial bay leaf EOs and commercial EOs of different botanical origin. Exploratory analysis through chemometrics (e.g. interval-Principal Component Analysis) provided diagnostic evidence in certain sub-regions e.g. 1100-1160 and 1700-1760 cm^{-1}, indicative of O-CH_3 but also ketone C=O stretching vibrations. Identification of major metabolites in the studied EOs via GC-FID and GC-MS analyses supported the aforementioned results. Overall, the proposed approach for FT-IR-based metabolomic analysis seems promising for the authentication of *L. nobilis* L. EO.

Acknowledgment: 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:T1EDK-04174)» and by the project "Upgrading the Plant Capital (PlantUp)" (MIS 5002803) 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).

OP39 COMPARATIVE STUDY OF DATA OBTAINED FOR THE EFSA HEALTH CLAIM 'ON OLIVE OIL POLYPHENOLS' WITH A UHPLC-DAD- FLUORESCENCE PROTOCOL AND A 1H-NMR SPECTROSCOPY PROCEDURE

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The interest in olive oil phenolic compounds, namely the derivatives of oleuropein and ligstroside, led to numerous publications on their analysis which is dominated by liquid chromatographic approaches. Approval of the health claim on 'olive oil polyphenols' regarding 'protection of blood lipids from oxidative stress' raised analytical concerns for the determination of the 5 mg of hydroxytyrosol and its derivatives (e.g. oleuropein complex and tyrosol)/20 g oil using existing procedures. Such concern was due to the complexity of the derived chromatograms and poor peak resolution. These issues are mainly due to the fact that: (i) oleocanthal and oleacein react with methanol and water, common solvents used for the phenol extraction and constituents of the mobile phase during their chromatographic separation, resulting to artefact formation, (ii) the instability of oleuropein and ligstroside aglycones when coming in contact with common chromatographic stationery phases [1]. Consequently, the analysis is challenging. To address these issues, some researchers propose the simplification of the phenolic profile applying acidic hydrolysis to the isolated polar fraction, that give rise only to simple hydroxytyrosol and tyrosol. Others, propose the use of specialized techniques of high capital cost, namely ^{1}H-NMR after extraction of target compounds with deuterated acetonitrile [1,2]. In the present study the same virgin olive oils were analysed using a fit for the purpose UHPLC -diode array procedure [2] and a ^{1}H-NMR procedure. Data comparison in absolute values and statistical treatment highlight pros and cons of the two analytical procedures.

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Acknowledgments

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OP40 THE LEAN WAY OF CLEANING PHARMACEUTICAL SOILS: A SPECTROSCOPY BASED APPROACH

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Quality control and product safety are of the utmost importance in the manufacturing of pharmaceutical products. As a result, cleaning verification is one of the essential components in Good Manufacturing Practice (GMP) standard.[1,2] However the rigorous nature of the process poses a huge scientific and economic problem for the pharma industry as a bulk amount of potential manufacturing time is lost to the process of cleaning, verification and validation. Also cleaning processes have not yet achieved the same level of advancement as their manufacturing or packaging counterparts and are still adopted randomly or chosen simply based on what has been used in the past thus adding up to the inefficiency.

Here in this work, we report a materials science-based approach for the study of interaction between the pharmaceutical soils and the detergents coupled with a lean way of collecting and analyzing data for the development of an efficient cleaning process. An in-depth characterization of the soil was carried out using various spectroscopic methods such as UV-Vis spectroscopy, Raman spectroscopy, and FT-IR spectroscopy, conductivity and pH measurements, powder X-ray diffraction (PXRD) analysis and particle size studies. Once the soil was characterized, interaction between the soil and active ingredients of the detergent was studied using UV-Vis spectroscopy, Raman spectroscopy, and FT-IR spectroscopy to find the optimum detergent for different kind of soils. Lean way of collecting and analyzing the data helped in identifying optimal cleaning parameters for both the products and equipment to be cleaned. Processes optimized through the selection of the best cleaning agents/parameters reduced residues to the lowest risk level and provided a high assurance of safety to patients. The cleaning time was also reduced significantly, thus improving the production efficiency.

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OP41 MONITORING BIOGAS REACTORS USING ANALYTICAL AND MOLECULAR TOOLS

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One of the main inhibitions in biogas digesters is attributed to the accumulation of Long Chain Fatty Acids (LCFA). Therefore, an accurate and on-time monitoring of the process is necessary to avoid any imbalances that can lead to severe economic and environmental problems. In this study we combined modern analytical and molecular tools to map the performance of manure-based biogas reactors during an adaptation process to LCFA rich feedstock. Replicate biogas reactors processing cattle manure were subjected to a radical change of influent composition by adding into it unsaturated fatty acid (Na-Oleate). As expected, the methane production was enhanced and after a period with accumulated volatile fatty acids (VFA) the process recovered to the initial VFA and pH levels. Metagenomic analysis showed that the addition of LCFA shifted the microbial community into a more specialised consortium specialised in performing fatty acids degradation. Syntrophic bacteria belonging to *Syntrophomonas* genus proliferated, outcompeting other members of *Syntrophomonadaceae* family. In respect to the archaeal community, it was demonstrated that the predominant methanogenic pathway was hydrogenotrophic as supported by the high abundance of *Candidatus* Methanoculleus thermohydrogenotrophicum.

Acknowledgements

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TUESDAY, SEPTEMBER 24TH, 2019

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Aerosol Metrology / X-ray analysis 2

Chair: ***D. Eichert, P. Morales***

IL07 THE EMPIR AEROMET PROJECT - DIMENSIONAL AND ANALYTICAL AEROSOL METROLOGY BASED UPON DIFFERENT TRACEABILITY CHAINS

B. Beckhoff

Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany on behalf of the AEROMET consortium

Measurements of aerosol particles are vital for enforcing EU air quality regulations to protect human health, and for research on climate change effects. Although metrics such as PM10 and PM2.5 are currently in use, the level of uncertainty of aerosol metrics in general is too high and the traceability is insufficient. The EURAMET EMPIR AEROMET project having 21 European partners (see www.aerometproject.com) aims to improve the uncertainty of particle mass, size and number concentration measurements and the characterization of regulated components in airborne particles as needed by EU air quality monitoring networks. Regulatory bodies, air quality networks and instrument manufacturers all require the improvement of air quality monitoring, however there is currently a lack of traceable calibration standards and harmonised calibration procedures for measuring airborne PM. In addition, methods measuring PM10 and PM2.5 within the EU Air Quality Directive need improving to ensure the comparability of local data measured by instruments relying on different working principles (e.g. gravimetry vs. optical spectroscopy). Therefore, reference methods and calibration procedures for instruments are to be developed. The elemental composition analysis of aerosols is required in existing regulations to understand origins, behaviour, environmental fate and impacts (e.g. effects on health and climate). Current methods for the quantification of regulated aerosol components (e.g. EC/OC/TC, metals, anions, and cations) are notoriously inflexible in terms of time and spatial resolution and do not meet requirements concerning detection sensitivity and flexibility for monitoring the temporal and spatial variability of air pollution. Therefore, the project works on validated methods for the determination of major components of PM as well as on an infrastructure for the calibration of Mobility Particle Size Spectrometers and Condensation Particle Counters based on international standards. Modern SI-traceable x-ray spectroscopy offers opportunities to improve the chemical analysis of aerosols directly at their emission sources. It needs to be combined with adequate sampling methods aiming at establishing a rugged in-situ method.

The project is supported by the EMPIR initiative of the European Union's Horizon 2020 program, through grant agreement 16ENV07 AEROMET.

OP42 QUANTITATIVE ELEMENTAL ANALYSIS OF AMBIENT AEROSOL PARTICLES USING PORTABLE TXRF

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A reliable analysis of aerosol particles is crucial for enforcing EU air quality regulations to protect human health, and for research on climate change effects [1]. Although metrics such as PM_{10} and $PM_{2.5}$ are currently in use, the level of uncertainty of aerosol metrics is too high and the traceability is insufficient. Within the AEROMET project [2] procedures are developed aiming at reducing the uncertainties of particle mass, size, and number concentration measurements including the characterization of regulated components in airborne particles. Here, we present an approach how to improve the uncertainty of in particle mass concentration measurements by mobile total reflection x-ray fluorescence (TXRF) analysis. The combination of TXRF and aerosol sampling techniques - traced back to reference-free synchrotron radiation-based XRF - enables a quantitative quasi real-time analysis of element mass concentrations in ambient air. During in-field campaigns, the monitoring of size dependent mass concentrations of specific elements in ambient aerosols was tested for the first time under dynamic conditions. This approach allows a direct time and size-resolved analysis without laborious digestion steps and a reduced risk of contamination.

Aerosol particles were sampled in a 13-stage DLPI impactor on acrylic discs. TXRF analysis was performed on-site with the transportable spectrometer S2 PICOFOX (Bruker Nano GmbH). The TXRF quantification was based on internal standardization. At moderate air pollution levels (PM_{10} 20 µg/m³) sampling times of less than 2 hours were enough to detect elements in different particle size bins below 10 µm. The on-site approach and the high sensitivity of TXRF enables the observation of rather quick changes in the quantity and distribution of elements in an ambient aerosol on the day of sampling. For example, the analysis of morning and afternoon sampling shifts reveals the occurrence of Fe, Ca and Si in different size bins and their temporal change in respective mass concentrations over the day while the distributions of several other elements remain unchanged.

[1] Directive 2008/50/EC published on the European Commission Ambient Air Quality website: *http://ec.europa.eu/environment/air/quality/existing_leg.htm.*

[2] *http://www.aerometproject.com/*

OP43 AEROMET - THE METROLOGY OF AMBIENT PARTICULATE METALS MEASUREMENTS AND THE EXAMPLE OF THE UK NATIONAL MONITORING NETWORK

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Air quality monitoring of ambient air is essential to minimise the exposure of the general population to toxic substances such as heavy metals, and thus the health risks associated with them. In the UK, ambient air is monitored under the UK Heavy Metals Monitoring Network for a number of heavy metals in PM_{10}, including nickel (Ni), arsenic (As), cadmium (Cd) and lead (Pb) to ensure compliance with the limit and target values specified in the EU Air Quality and Fourth Daughter Directives. In terms of analytical metrology, the directives require results to be produced according to a reference method that involves the acid digestion of samples followed by metals determination using ICP-MS (Inductively-Coupled Plasma - Mass Spectrometry) or AAS (Atomic Absorption Spectrometry), but most modern air quality laboratories use ICP-MS. These spectrometric instrumental techniques are specified because they meet the sensitivity requirements of the directives.

This presentation will outline the overall operation of the national UK metals network, which comprises 25 monitoring sites around the UK. At each site a Partisol sampler collects PM_{10} onto cellulose filters, which are then returned to the laboratory at NPL, then prepared and analyzed according to the reference method using ICP-MS. The operating principles of ICP-MS will be explained. Metals concentrations in ambient air are reported for 12 metals, including the 4 directive metals. Our analysis procedure is governed by numerous quality assurance and control measures to provide confidence in the final concentrations generated. This essential role of good metrological practise is currently being developed further with our colleagues in the AEROMET project.

OP44 AEROMET PROJECT - PROTOCOL DEVELOPMENT FOR HEAVY METALS ANALYSIS OF COLLECTED AEROSOLS SIZE FRACTIONS

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Due to their contribution to adverse health effects, even at the low concentrations found in ambient air, heavy metals in ambient particulate matter (aPM) need to be measured regularly by conducting PM sampling on filters (2004/107/EC directive). These filters have to be analysed by a reference method to measure heavy metal concentrations in aPM (EN 14902:2005). Among the reference methods, Inductively-Coupled Plasma - Mass Spectrometry (ICP-MS) is the most used technique by air quality laboratories for lead (Pb), cadmium (Cd), arsenic (As) and nickel (Ni) measurement in the PM10 fraction of aPM.

The smaller the size of aPM the deeper the penetration into the respiratory tract, it is therefore important to properly evaluate heavy metals levels on different collected size fractions. In the frame of the AEROMET project (http://www.aerometproject.com), an aerosol generation and collection protocol development was proposed for ICP-MS analysis of aerosols collected with different size fractions (PM2.5 and PM10 fractions) using a LNE well characterised material. This generation has to be stable and reproducible in order to ensure the production of reference aerosol loaded filters for specific sampling time and size fraction. Preliminary results will be presented.

The loaded filters will then be distributed among the project partners and analysed in order to develop protocols for heavy metals analysis of collected aerosol size fractions on filters and carry out comparative evaluation of reference ICP-MS and XRF methods.

OP45 DEVELOPMENT AND CHARACTERIZATION OF AEROSOL REFERENCE MATERIALS FOR THE CALIBRATION OF NUCLEAR ANALYTICAL TECHNIQUES

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Elemental analysis of Particulate Matter (PM) samples collected on filter media, is an analytical task that remains challenging. Many factors contribute to this fact, such as the very low concentrations of the analytes, the non-uniform deposition of the sample on the substrate, the matrix effects due to the PM particle size and the reactive species that may lead to artifact formation. Analysis of this type of samples is very important not only in environmental monitoring but also in aerosol chemistry.

The standards that are usually used for the calibration of nuclear techniques such as XRF and PIXE, are vacuum-deposited single metals or single compound salts onto films. However, these standards do not resemble neither the substrates that are typically used for aerosol sampling and PM matrix, nor the very low elemental concentrations of ambient PM samples and the spectral interreferences that usually appear in the analysis of real PM samples.

In the framework of the IAEA TC Project RER/1/008 “Supporting Air Quality Management”, reference samples on filter media were prepared from Dust Certified Reference Materials deposited in Polytetrafluoroethylene filters (PTFE). Two Certified Reference Materials were used: the 2854 and the 2853 NIST CRMs. According to the producer of the CRMs, the minimum sample mass for the certified values to be valid should be 100 mg. Taking into account that this loading would produce samples with concentrations outside the range of ambient samples, lower mass was used for the preparation of the reference materials. The produced standards were subsequently checked for the homogeneity andthe reproducibility of the deposited mass onto the membrane filters by means of small beam XRF spectrometry and PIXE at an internationally recognized expert laboratory (LABEC Lab, INFN, Florence). The results of the analytical characterization and validation of these aerosol reference materials will be reported.

TUESDAY, SEPTEMBER 24TH, 2019

EVERGETON HALL

Aerosol Metrology / X-ray analysis 3

Chair: ***P. Morales, P. Quincey***

OP46 LIGHT ABSORBING CARBON MEASUREMENTS ON ATMOSPHERIC AEROSOL PTFE FILTER SAMPLES BY THE MULTI-WAVELENGTH ABSORPTION BLACK CARBON INSTRUMENT (MABI). INTERCOMPARISON WITH OTHER MEASUREMENT TECHNIQUES

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Source apportionment studies are based in the various chemical fingerprints of aerosol species originating from different sources. The detailed analysis and chemical characterization of aerosol samples collected on filters is the common practice for the identification of several major and trace metals, ions and organic tracers with their concentrations ranging over several orders of magnitude. In many instances, where real time data for black carbon are not available, there are limitations obtaining information for the carbonaceous fraction usually concerning the filter material. The Multi-wavelength Absorption Black Carbon Instrument (MABI) introduced by ANSTO (Cohen et al., 2000) is a non-destructive optical transmission method for deriving equivalent Black Carbon mass (eBC) on Teflon filters. It is based on a basic principles calibration taking into account a well-defined mass absorption coefficient and has been used extensively in source apportionment studies. In the absence of a primary standard for aerosol absorption, the problems associated with the optical response of aerosol particles embedded in filter material and the high variability and uncertainty of mass absorption coefficients (Petzold et al., 2013) an intercomparison study was performed in Athens to assess the MABI response with respect to concurrent measurements by well-known field instruments for aerosol absorption, eBC. In general a very good correlation among the different techniques is observed for a variety of aerosol loads in the Demokritos suburban station in Athens. The observed variability is discussed in view of current state of the art knowledge regarding source aerosol types and filter loading.

Acknowledgement:

This work is partly conducted for the 16ENV02 Black Carbon project of the European Union funded through the European Metrology Programme for Innovation and Research (EMPIR). EMPIR is jointly funded by the EMPIR participating countries within EURAMET and the European Union. The IAEA Regional Project RER7011 is also acknowledged

OP47 EXSA: EUROPEAN X-RAY SPECTROMETRY ASSOCIATION

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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 devices 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 co-organizes summer schools as well as dedicated workshops on novel and emerging X-ray spectrometry topics.

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. The next application period for EXSA's Young Scientist Award will start in **November 2019** and end on **February 2020**. For further information see **www.exsa.hu**.

EXSA gathers more than 100 members from academia and industry and is sponsored and supported by more than 10 companies.

EXSA is supporting the Fundamental Parameters Initiative and its workshops (https://www.exsa.hu/fpi.php), an essential requirement for accurate quantitative X-ray Analysis.

Since its foundation, EXSA has supported more than 50 workshops and conferences, among which the IMA Conference 2019.

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

OP48 DESIGN AND DEVELOPMENT OF A NEW AEROSOL GENERATION SYSTEM FOR INHALATION EXPOSURE APPLICATIONS

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The aim of this study was to develop an innovative setup for generating aerosols that perfectly resemble ambient particulate matters (PM) in terms of physical and chemical characteristics. To this end, a high volume sampler was used to collect ambient PM on filters; followed by the extraction of collected filters in Milli-Q water. As an alternative approach, we also captured the ambient particles directly into the Milli-Q water, using the versatile aerosol concentration enrichment system (VACES)/aerosol-into-liquid collector tandem technology. Afterward, we employed HOPE nebulizers to re-aerosolize the aqueous PM slurries derived from both approaches. The size distribution of generated aerosols were then investigated by the means of a scanning mobility particle sizer (SMPS) in conjunction with a condensation particle counter (CPC) to assure the similarity of nebulized particles to those of ambient ones in terms of physical properties. In addition, the ambient and re-aerosolized samples were chemically analyzed for elemental and organic carbon (EC/OC), water soluble organic carbon (WSOC), polycyclic aromatic hydrocarbons (PAHs), metals and trace elements, and inorganic ions. Results from this study indicated that we can effectively recover the water soluble components of ambient PM (e.g., water-soluble inorganic ions, and water-soluble organic matter) by re-aerosolizing the aqueous extracted PM slurry. However, the water insoluble portions of ambient PM (e.g., EC, PAHs, and some of the redox-active metal elements) were not well reconstructed using this approach. On the other hand, we were able to perfectly reconstruct all constituents of ambient PM by using the VACES/aerosol-into-liquid collector tandem technology for collecting ambient PM directly into the Milli-Q water. These results corroborate the superiority of using the VACES/aerosol-into liquid collector tandem technology for preparing PM slurries, which can further be used in our aerosol generation configuration to generate physically and chemically stable aerosols that perfectly resemble ambient PM.

OP49 AUTONOMOUS 1.57 MM DIFFERENTIAL ABSORPTION LASER DEVICE FOR REMOTE SENSING OF ATMOSPHERIC CO_2

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Measurement of atmospheric CO_2 concentrations is critical in order to observe the sources and sinks of CO_2 emission on continental and regional scales. The CO_2 concentration measurement is quite complicated and requires sophisticated instrumentation and laboratory equipment. Several research groups have developed experimental lidar systems but the complexity of the instruments has prevented of using them widely. Moreover, research efforts on atmospheric CO_2 measurements have been reported of cw lasers which reflected however, from a hard target at known distance in a differential absorption arrangement.

OP50 EDXRF AND XANES AS ANALYTICAL TOOLS FOR NEW MERCURY COMPLEXING MEMBRANES

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X-ray absorption near-edge structure (XANES) spectroscopy and Energy Dispersive X-Ray Fluorescence (EDXRF) were was employed as complementary analytical techniques for the evaluation of new produced mercury complexing membranes. EDXRF was used for a relatively quick scanning of membrane mercury collection yield as well as their specificity to mercury and avoidance of interfering from other ion competition. XANES was used to determine the chemical binding between divalent inorganic mercury Hg(II) ions and the polymer-based membranes, functionalized with various organic ligands. Membranes were prepared by mixing the membrane matrix with suitable solvent, complexing ligand, ionophore and plasticizer. The produced liquid was used to make a thin film on a Mylar® substrate; this film was used for mercury collection from water solutions and for EDXRF analysis. For XANES analysis a similar film was produced on the surface of a quartz reflector that it was used for mercury complexation before XANES analysis in TXRF mode. The XANES experiments took place in the Elettra Sincrotrone of Trieste (Italy). The complexing abilities of the selected ligands were proved and the effect of various ligands on the mercury atoms were recorded.

Acknowledgements: Thanks are expressed to the International Atomic Energy Agency (IAEA) for providing funding through the coordinated research project G42005. We greatly appreciate the beamtime awarded by IAEA and the Elettra Sincrotrone Trieste.

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Aerosol metrology / Archaeometry / Chemical- and bio- sensors / Chromatography / Environmental analysis / Materials / Mobile analytical instruments / Pharmaceutical analysis / Sample handling / Sensors / Spectrochemical analysis / Thermal analysis

P2-01 CASCADE IMPACTOR SAMPLING HARMONIZED TO NON-DESTRUCTIVE ELEMENTAL ANALYSIS OF AEROSOL PARTICLES

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Adequate characterization of atmospheric particulate matter covers both size and chemical composition information. Size distribution of elemental concentrations is important for climate and health effect of aerosols. In the framework of the European project AEROMET (Aerosol metrology for atmospheric science and quality) the task of our research group is to harmonize size-fractionated sampling technique with total-reflection X-ray fluorescence (TXRF) elemental analysis. A special cascade impactor sampling method was developed allowing collection of particles directly onto Si wafers ideally suited for TXRF due to their excellent surface roughness. Such backing can be used for complementary techniques, scanning electron microscopy (SEM) and Raman spectrometry. The applied 9-stage May type cascade impactor covers a wide size range of 70 nm to 16 µm, partly covering ultrafine particles. The collection efficiency at different impactor stages was tested using aerosols generated from solutions with size distribution measured with a scanning mobility particle sizer (SMPS). Ambient samples were collected from 20 min to 4 hours in suburban Budapest (Hungary) and in urban Cassino (Italy). Parallel monitoring of black carbon by an aethalometer and the size distribution using an SMPS was performed. Collective elemental analyses of the sampled particles were carried out using TXRF in laboratory and using synchrotron radiation (SR) at Elettra (Trieste, Italy). For calibration of TXRF, standards imitating deposited microparticles were used, prepared using photolitography or a nanoliter injector. For transition metals, detection limits of 100 pg/m^3 were reached for laboratory TXRF. Based on SEM observations the soot particles were most abundant on the 70-180 nm range. As obtained by TXRF, the maximum concentrations of elements related to high-temperature processes (e.g. K - biomass combustion, Zn - traffic) were found in the 180-300 nm fraction. By combination of cascade impactor sampling and complementary analytical techniques, the time variation of aerosol composition can be followed.

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Measurements of airborne particulate matter constitute an important tool for environmental investigations especially in terms of the impact of atmospheric pollution to human health and the design of the appropriate measures and legislation. Usually, investigations focus on PM_{10} και $PM_{2.5}$ particles (particulates with aerodynamic diameter less than 10 μm and 2.5 μm, respectively). Such studies usually suffer from high uncertainty of measurements as well as insufficient traceability. The project "AEROMET" aims to properly address and propose solutions for such issues. Participants in "AEROMET" project involve 21 entities from 15 E.U. countries, mainly National Metrological Institutes (NMIs) with PTB (Physikalische-Technische Bundesanstalt, Germany) acting as coordinator. Laboratory of Inorganic and Analytical Chemistry of NTUA participates as external funded partner. Specific aims of AEROMET project are as follows in individual work packages (WP, Work Packages):

1. Design and development of a novel aerosol mixing chamber producing stable reference aerosol for reasons of calibration of automated instruments for PM_{10} and $PM_{2.5}$ particulates and the validation of methods for quantification of their composition (WP1).

2. Application of traceable validated methods for quantification of different forms of carbon (i.e. elemental (EC), organic (OC) and total carbon (TC)) as well as cations and toxic elements, such as As, Cd, Pb, Ni and Hg (WP2).

3. Development of calibration procedures for Mobility Particle Size Spectrometers (MPSS) and Condensation Particle Counters (CPCs) (WP3).

4. Use of mobile X-ray spectrometers for the real time and on-site quantification of the composition of particulates. Results will be compared with reference methods (e.g. ICP-MS). Sampling and in-situ measurements using TXRF have been performed in an urban area (Cassino, Italy) and in a suburban background area (Budapest, Hungary) (WP4).

5. Design and construction of substrates using nanomaterials for the measurement of fine and ultrafine particulates (UFP) (WP5).

Acknowledgment

This work is supported by the EMPIR (European Metrology Program for Innovation and Research) program, co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation program. The work is done in the frame of the 16ENV07 AEROMET project.

P2-03 MINERALOGICAL COMPOSITION OF THE BRONZE AGE POTTERY FROM THE KAMENNY AMBAR SETTLEMENT (SOUTHERN URALS, RUSSIA)

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Ceramic vessels and their fragments are the most common archaeological finds. The study of the pottery mineralogical composition is important for determining maximum firing temperatures and its redox atmosphere. These parameters can provide useful information about the achieved technological level of pottery skill of ancient society. The aim of the work is to assess the composition and firing temperatures of Sintashta type ceramics from the Kamenny Ambar Bronze Age fortified settlement (21-17 centuries BC, Southern Urals, Russia) using X-ray diffraction. XRD diffraction patterns were obtained using the SHIMADZU XRD-7000 X-ray diffractometer. The operational conditions were as follows: copper radiation in the range of Bragg angles 2Θ 3-70, recording speed 1°/min. Preliminary qualitative X-ray diffraction analysis was carried out according to the basic reflexes using the ICDD Powder Diffraction File-2 database. Quantitative full-profile X-ray diffraction analysis was carried out using SiroQuant Software (Sietronics, Australia).

X-ray diffraction analysis of ceramics from the Kamenny Ambar Bronze Age fortified settlement (Southern Urals) showed that ceramics include quartz, mica (muscovite), chlorite, potassium feldspar (microcline), plagioclase (albite), tremolite, pyrite and rutile. Dolomite and calcite may be present as raw material for moulding or as a part of lean additives (shell and grog mixed with shell). Talc is the main component of additives and is found in large quantities in all studied samples. By the presence of chlorite, calcite and the absence of newly formed high-temperature phases, it can be concluded that firing temperature is quite low (for a number of samples doesn't exceed 650°C, and for some others in the range of 650-800°C). The obtained data generally don't contradict the results of technological analysis of ceramics, and in some cases allow for its clarifying and supplementing.

The work was carried out at the "Geoanalitik" Center for Collective Use and supported by RSF grant No. 16-18-10332.

P2-04 MINERALOGICAL AND CHEMICAL COMPOSITION OF PREHISTORIC PIGMENTS FROM CAVE PAINTINGS AND PICTOGRAPHS (SOUTHERN URALS, RUSSIA) BY SEM-EDS AND RAMAN SPECTROSCOPY

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This paper presents the results of studying the elemental and mineral composition of pigments from a number of cave paintings and pictographs (Southern Urals, Russia) using SEM-EDS, Raman microspectroscopy and XRD. SEM images and elemental mapping of carbon sputtered samples were performed using JEOL JSM-6390LV with INCA Energy 450 EDS with accelerating voltage of 20 kV. Raman spectra were obtained using Horiba Jobin Yvon LabRam-HR Evolution using 488 nm Ar laser excitation and 600 grooves/mm grating in the range 0-2000 cm^{-1}. Space resolution was up to 1 μm. Mineral phase identification was carried out using KnowItAll (Bio RAD) and RRUFF.INFO databases. XRD diffraction patterns of rocks and minerals were obtained using SHIMADZU XRD-7000 X-ray diffractometer. The operational conditions were as follows: copper radiation in the range of Bragg angles 2Θ 20-70, recording speed 1°/min, 40 kV and 30 mA. Preliminary qualitative X-ray diffraction analysis was carried out according to the basic reflexes using the ICDD Powder Diffraction File-2 database. Quantitative full-profile X-ray diffraction analysis was carried out using SiroQuant Software (Sietronics).

It has been shown that the main inorganic components of the pigments are goethite and hematite-containing ochres and carbon, most likely derived from burnt bone; organic binder is likely of animal origin. The technology of dye manufacture could include the stage of thorough grinding of inorganic raw materials with a binder, and the application of paint could occur in layers. For the images of open-air pictographs, the presence of calcium oxalates, formed as a result of the interaction of organic components with rock matter, is characteristic, which can perform a stabilizing function and protect pigments from weathering and reliably fix the dye to the substrate.

The work was carried out at the UB RAS "Geoanalytic" Center for Collective Use within IGG UB RAS state assignment 18-118053090045-8.

P2-05 ALL-SCREEN-PRINTED INTEGRATED PERMANENT BONDED MAGNETS ELECTROCHEMICAL CELLS

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Electrochemical (voltammetric or impedimetric) magneto assays have rapidly increased in recent years thanks to the efficient and simple separation capability afforded by a magnetic field. Their operation is based on the use of magnetic beads or magnetic nanoparticles, thereafter magnetic particles (MPs), sized from some nm to a few μm, as support to perform the assay. MPs consist of a paramagnetic or superparamagnetic core, mainly based on different iron oxide forms such as magnetite (Fe_3O_4) and maghemite (γ-Fe_2O_3, ferrimagnetic), which are covered with suitable protective layers to prevent their aggregation. The use of MPs in analytical chemistry offers significant advantages as the target analyte is preconcentrated on the surface of MPs, while the magnetic assisted manipulation by using external magnets allows easy separation of the magnetic particles-analyte complex from the matrix of the sample to the electrode surface, resulting in the reduction of matrix effects and the increase of the selectivity of the assay. To this end, a number of specially designed experimental setups, such as magnetic electrode shafts, single or multi positions magnetic supports, electrochemical cells integrated with electromagnets positioned underneath the active surface of the working electrode etc. have been developed aiming to offer the necessary magnetic field. These setups however are relatively costly and of course are not indicated for use in on-site applications. Here in, we introduced for the first time the development of low-cost, disposable screen-printed electrochemical cells integrated with screen-printed permanent bonded magnets that serve as alternatives to conventional magnets, magnetic supports or external electromagnets. All screen-printed integrated permanent bonded magnets-graphite sensors hold promise for the development of low-cost advanced sensors for chemical analysis in the field. Details on the fabrication, characterization and analytical utility of these novel magnet-electrode combined sensors will be presented

P2-06 INVESTIGATION OF A MULTIPLEX INJECTOR FOR TIME-RESOLVED GAS CHROMATOGRAPHIC MONITORING

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Multiplexing is a technique that allows the introduction of one or more samples at specified time intervals. Its concept includes a specified random sample introduction and a mathematical data processing (Hadamard transform) to obtain the single/averaged chromatogram. It has been used for S/N ratio and sample throughput improvements in many analytical methods using capillary electrophoresis, fluorescence imaging, gas and liquid chromatography and others. Apart from this use, it can also provide information on the time resolved chromatograms and, thus, be used for monitoring of reactions that can take place in a specific situation. Most important aspects for optimization in a multiplexing method are the sample introduction and the data processing. Ideally, multiplex injection is performed with a fast sample introduction system to have the best results after final data processing. Previous reports combined multiplexing and gas chromatographic systems (GC) with flame ionization (FID) or mass spectrometric detectors (MS). This work uses a multiplexing-GC system with the He-plasma-based barrier discharge ionization detector (BID). Previous investigations have shown its superior sensitivity in comparison with other well-established GC detectors such as the thermal conductivity (TCD) or flame ionization (FID) detector. The detector is particularly efficient when analysing low molecular compounds, halogenated or oxygenated compounds. This set up can be suitable for the monitoring of lithium-ion batteries (LIBs) electrolyte degradation products which can alter the characteristics of the electrochemical cell or form volatile and hazardous emissions. This work investigates the efficiency of a lab made injector after optimisation of critical parameters like flow and injection time. The practical and data processing method limitations as well as possible ways to overcome these are discussed for the monitoring of LIB degradation products under abuse conditions (overcharging).

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P2-07 DETERMINATION OF PESTICIDES IN RIVER WATER SAMPLES BY SOLID PHASE EXTRACTION COMBINED WITH HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY/ UV DETECTION (HPLC/ UV-DAD)

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In the present study a solid phase extraction (SPE) method has been applied for the simultaneous determination of six pesticides of interest in river water using high-performance liquid chromatography coupled to ultraviolet detector, serial photodiodes (HPLC / UV-DAD). The six pesticides included Chlorothalonil (235 nm), Cyprodinil (270 nm), Kresoxym-methyl (220 nm), Mepanipyrim (270 nm), Propargite (225 nm) and Pyriproxyfen (220 nm) and were selected in terms of their frequent use in agricultural activities around the study area. Several sampling points were selected along the Drin River in Albania. The Drin is a river in Southern and Southeastern Europe with two distributaries one discharging into the Adriatic Sea and the other one into the Buna River. The river and its tributaries form the Gulf of Drin, an ocean basin that encompasses the northern Albanian Adriatic Sea Coast. Agilent's C18 cartridges were applied for the preconcentration of the samples. The elution of the target compounds was carried out with a mixture of 5 ml ethyl acetate: methanol (1:1 v/v) followed by 5 ml of ethyl acetate. The method was validated in terms of the analytical characteristics showing good linearity and exhibiting quantification limits at the low ppt levels. Recoveries obtained were in the range of 62% to 96% and 61% to 91% for all analytes in distilled and river water respectively. The analytical methodology was further applied to determine the seasonal variation (autumn, winter, spring, summer) of the target analytes' levels in five (5) sampling stations along the Drin River, in Albania.

P2-08 ON-LINE EXTRACTION COUPLED TO LIQUID CHROMATOGRAPHIC ANALYSIS OF HYDROPHOBIC ORGANIC COMPOUNDS IN SOILS

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This work aims to evaluate the application of on-line extraction coupled to liquid chromatographic analysis (OLE-LC) for the extraction of non-polar organic compounds from complex solid matrices. OLE-LC is a new sample preparation approach that is based on the direct coupling of dynamic extraction to on-line liquid chromatographic analysis using a simple re-configuration of HPLC instrumentation without the need for additional apparatus or devices. Specifically, the sample loop of a conventional HPLC injection valve is replaced with an extraction vessel containing the solid sample. Upon injection, the mobile phase flows through the extraction vessel and accomplishes the dynamic extraction of the analytes, assisted by the high pressure developed in the HPLC system. The eluted analytes are directly transferred to the HPLC column for separation and analysis. In this manner, sample pretreatment is significantly simplified since steps such as cleaning, solvent exchange, filtration and drying of the extracts are no longer required. Despite these advantages, however, OLE-LC has only been used as a qualitative analysis tool for obtaining a fingerprint of sample composition. What is more, the experimental parameters pertaining to its operation and performance have not been investigated. In this work we provide a detailed study of the experimental parameters related to the efficiency of both the extraction and chromatographic separation and elucidate its use also as a quantitative analysis approach of complex samples.

P2-09 OPTIMIZATION AND VALIDATION OF HPLC METHOD FOR SOME PESTICIDES FROM HUMAN URINE AND COMMERCIAL DOSAGE FORM

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Pesticides help improve the quality and quantity of crops produced. However, pesticides can cause environmental problems. For example, humans are exposed to pesticide residues in food and other environmental media. High performance liquid chromatography (HPLC), in particular reversed-phase liquid chromatography (RP-LC), has long established itself as a pertinent technique in the pharmaceutical industry. In this study RP- HPLC method was developed and optimized for the determination of clorothalonil (CLO), dinobuton (DIN) and buprofezin (BUP) in different water samples, tomato and soil samples. RP- HPLC analysis was performed with Kinetex C18 (150 × 4.6 mm ID × 5 µm) (Phenomenex, USA) analytical column with 1 mL min^{-1} flow rate of mobile phase which consisted of acetonitrile: 10 mM (pH: 6.54) ammonium acetate buffer solution in the ratio of 75:25 (v/v) at 25 ^{0}C. Injection volume of the samples was 10 µL and the wavelength of the detector was set at 254 nm for monitoring all analytes. Calibration graphs showed a good linearity with a coefficient of determination (R^2) of at least 0.999 for three pesticides. Intraday and interday precision (expressed as RSD%) were lower than 1.16%. The developed methods were demonstrated to be simple and rapid for the simultaneous determination of CLO, DIN and BUP in human urine and commercial dosage form containing only CLO. Recovery values are in the range between 99.4 and 106.80% for CLO, 95.9 and 104.4 for DIN and 98.5 and 104.8 for BUP in human urine. Recovery value is in the range between 94.1 and 97.1% for CLO in commercial dosage form.

P2-10 BREATH ANALYSIS: A NOVEL NON-INVASIVE TOOL FOR MONITORING RECOVERY AFTER EXERCISE-INDUCED MUSCLE DAMAGE IN HUMANS

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Breath Analysis has been used as a novel technique for studying a number of health-related issues in humans over the last decades. Expired air contains hundreds of Volatile Organic Compounds (VOCs) that could provide us with valuable information on one's health status. In the current work, the potential of using Breath Analysis for monitoring recovery after physical exercise by measuring indices of oxidative stress, is examined. Exercise-induced oxidative stress and related muscle damage is an undesirable situation for athletes and fast recovery is crucial. So far, monitoring the degree of recovery is done using ergo-physiological methods and blood analysis. Breath analysis is examined in this work as an alternative method, mainly due to its non-invasive character and the absence of sampling frequency limitations. For that purpose, a controlled experiment was carried out involving triggering of exercise-induced oxidative stress to a group of healthy volunteers of mild physical activity and monitoring of oxidative stress related indices in their expired air and serum before and after exercise. The volunteers followed a preparation protocol regarding diet and hygienic and an eccentric exercise protocol able to induce oxidative stress. Expired air samples were collected from volunteers in Tedlar bags, before exercise and 1h and 24h after exercise. Samples were analyzed by thermal desorption gas chromatography-mass spectrometry. VOCs related to oxidative stress, including alkanes (nonane, decane, dodecane, tetradecane), aldehydes (nonanal, decanal) and isoprene, were targeted in expired air analysis and their concentration pattern over time was studied. Findings were compared to the results of the analysis of biochemical markers of exercise-induced muscle damage, inflammation and oxidative stress (creatine kinase, IL-6, protein carbonyls, malonil dialdehyde), in serum. Future application of breath analysis in intervention studies aiming to investigate the effectiveness of various food supplements in the recovery after exercise, will be critically evaluated from the results.

P2-11 QUECHERS-HPLC METHOD FOR AFLATOXIN DETECTION OF FOODS

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A Quick, Easy, Cheap, Effective, Rugged and Safe (QuEChERS) method for the analysis of aflatoxins in food samples was developed. The preliminary work focused on optimizing sample pretreatment conditions, such as the extraction solvents, the type and amount of drying agents, the extraction time, and the solvent-sample ratio. A mixture of methanol/acetonitrile (60:40, v/v%) provided better recoveries in the range of 71.8 - 107.7 % at spike levels of 1.5 -50 microgram/kilogram, with relative standard deviation (RSDs) lower that 15%. The developed QuEChERS-HPLC method was found to be more precise when compared with fluorometric method. A total of 669 domestic and imported food samples in Jordan were analyzed for their aflatoxins contents and peanut and peanut butter samples were found to have highest incidence of contamination (10 contaminations) followed by pistachio nut samples (6 contaminations) and sesame seed samples (2 contaminations).

P2-12 GAS CHROMATOGRAPHY AS A TOOL FOR THE OPTIMIZATION OF DOCOSAHEXAENOIC ACID (DHA) RECOVERY FROM CRYPTHECODINIUM COHNII MICROALGA

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Docosahexaenoic acid (DHA) represents an omega-3 polyunsaturated fatty acid (PUFA) with important health benefits. *Crypthecodinium cohnii (C. cohnii)* microalga is one of the major DHA sources thanks to its unique fatty acid composition and fast growth rates. For the recovery of PUFAs from microalgae, solvent extraction techniques are widely employed. Specifically, ultrasound-assisted extraction (UAE) represents an environmentally benign technique with high efficiency. In the present work, UAE of DHA from *C. cohnii* was performed using different solvents (hexane, hexane: isopropanol (2:3) and 2-butanol) and under different conditions (extraction time: 5, 10 and 15 min solvent/biomass ratio: 10, 20 and 30 and ultrasound power: 150, 450 and 750 W). Gas Chromatography (GC) protocols were developed for qualitative and quantitative evaluation of *C. cohnii* PUFA content, focusing on DHA, as a decision making tool for the selection of the optimum extraction solvent and conditions. The results of GC analysis showed that hexane: isopropanol (2:3) was the optimum solvent. In addition, the results of the extraction parameters scanning demonstrated that the extraction power did not significantly affect the yield, ranging from 82.2 to 86.7%, while the extraction time and the solvent/biomass ratio were found to be more crucial parameters. In conclusion, UAE using hexane: isopropanol with the suitable conditions significantly improved the yields and preserved the high quality of DHA.

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P2-13 MICELLAR CHROMATOGRAPHY USING TWEEN-20 AS SURFACTANT: ELUTION MECHANISM AND QUANTITATIVE RETENTION- ACTIVITY RELATIONSHIPS FOR ESTIMATION OF BIOPHARMACEUTICAL PROPERTIES OF STRUCTURALLY-DIVERSE DRUGS

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The use of liquid chromatography to model pharmacokinetic properties in early drug discovery is based on the similarities governing chromatographic and biological processes. Indeed, several pharmacokinetic properties are the outcome of a dynamic distribution of drugs between aqueous phases and membranes or tissues. Progress in HPLC column technology succeeded in immobilizing phospholipids and different types of proteins (e.g. Human Serum Albumin (HSA) or alpha1- acid glycoprotein (AGP)) on a silica gel skeleton to produce immobilized artificial membrane (IAM) chromatography and protein-based stationary phases, respectively. Another type of biochromatography is Biopartitioning Micellar Chromatography (BMC), employed by the use of a traditional hydrophobic stationary phase (e.g. C-18) and aqueous mobile phases in presence of a surfactant above its critical micellar concentration. The neutral polyoxyethylene (23) lauryl ether (Brij-35) is the first and most widely implemented surfactant. Other popular surfactants for use in MLC include sodium dodecyl sulfate, sodium deoxycholate, cetyltrimethylammonium bromide and polyethylene glycol sorbitan monolaurate (Tween).

In the present investigation, retention factors of about 60 structurally- diverse drugs on micellar chromatography were measured using Tween 20 as surfactant in aqueous mobile phase at pH 7.4 and 5.5. The retention factors were compared with octanol- water partition (logP) and distribution coefficient as well as retention factors measured on Immobilized Artificial Membrane (IAM) chromatography and biopartitioning micellar chromatography using Brij-35 as surfactant, measured in our previous investigations. Finally, retention factors of the present investigation were employed to construct relationships with Caco-2 cell lines permeability, Human Oral Absorption (%HOA) and Plasma Protein Binding (%PPB) data taken from literature. As additional molecular descriptors, Molecular Weight (MW), Topological Polar Surface Area (TPSA) as well as Abraham's hydrogen-bond acidity (A) and basicity (B), positively (F^+) and negatively (F^-) molecular fraction were tried.

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P2-14 THE POTENTIAL OF IMMOBILIZED PLASMA PROTEIN HIGH PERFORMANCE LIQUID CHROMATOGRAPHY TO ESTIMATE ECOTOXICITY OF PESTICIDES

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The use of biomimetic and physicochemical measurements, such as lipophilicity, to help rationalise the behaviour of experimental molecules in biological environments is an important facet of environmental science. Lipophilicity measurements are demonstrably unreliable for poorly soluble compounds. However, reversed phase high pressure liquid chromatographic (HPLC) methodologies using C-18 columns provide an effective and reliable replacement, irrespective of solubility. As several ecotoxicological properties involve a dynamic distribution of xenobiotics between aqueous environment and tissues of aquatic organisms, HPLC can be used in order to predict environmental risk indices. Biomimetic chromatography has the advantage of combining simulation of the biological environment with fast measurements, while it is economic and user friendly and requires only a small amount of analyte. Immobilized protein chromatography uses biomimetic stationary phases consisting of immobilized plasma proteins, such as human serum albumin (HSA) and alpha-1 acid glycoprotein (AGP). Therefore, it attracts great interest in the pharmaceutical industry since proteins can bind a remarkable variety of drugs impacting their delivery and efficacy. It is also proven not only that there is a trend between protein binding and compound lipophilicity, but also that strong binding of drugs can cause drug safety issues or several adverse effects. In the present work, the potential of immobilized human serum albumin (HSA) HPLC to predict ecotoxicity of pesticides is studied for the first time. More specifically, the elution of a set of 39 structurally diverse pesticides is tested by HSA-HPLC and their retention is obtained. Retention factors determined with 10% organic modifier (2-propanol), as well as extrapolated to pure aqueous phase are used to establish relationships with ecotoxicity data for various organisms obtained from the literature (US EPA). Additional physicochemical parameters are also tested regarding their impact on modeling. The obtained models are then compared with those derived with octanol-water partitioning.

P2-15 INITIATING EFFICIENT SB(V) REMOVAL FOR DRINKING WATER BY A MECHANISM OF REDUCTION/ADSORPTION SEQUENCE

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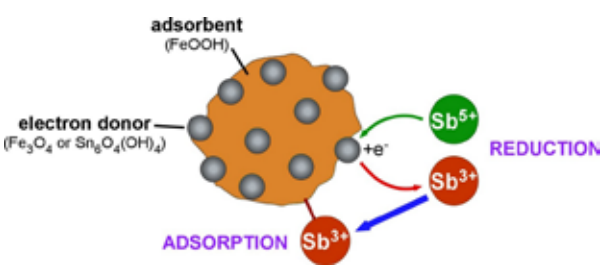
In an attempt to overcome the difficulties related to the efficient capture of Sb(V), this work introduces an alternative approach based on the intermediate reduction to the Sb (III) followed by its non-reversible adsorption on typical iron oxy-hydroxides (Figure 1). To this direction, an iron oxy-hydroxide (FeOOH) optimized for high Sb (III) uptake was combined either with iron oxide (Fe_3O_4) or tin oxy-hydroxide ($Sn_6O_4(OH)_4$) nanoparticles that serve as a reducing agents and a carrier of the FeOOH. The synergy of the two phases in the nanocomposite enables a much better performance for Sb(V) removal in compliance with the drinking water regulations and the requirements for long-term chemical stability and low-cost preparation. The reducing potential of the nanocomposites increases almost proportionally to the percentage of Fe_3O_4 and $Sn_6O_4(OH)_4$. The ability of such phases to operate as electron donors enables the reduction of Sb(V) to Sb(III) oxy-ions which are then captured by the iron oxy-hydroxide that shows higher affinity to antimonite species. It is important to note that the efficiency of these adsorbents is extended to the low residual concentrations range including the drinking water regulation limit for antimony. Suggestively, the uptake capacity of the Fe_3O_4/FeOOH (50 %wt.) corresponding to a Sb(V) residual concentration of 5 μg/L is found to be 0.4 mg/g However, further increase in the Fe_3O_4 content does not improve efficiency. The magnetic response of Fe_3O_4 is another important advantage of this system related to the possibility for alternative application schemes in water treatment based on magnetic separation. Optimum composition in the $Sn_6O_4(OH)_4$/FeOOH nanocomposite is observed at much lower tin oxy-hydroxides percentages <30 % wt. This is attributed to the combination of higher reducing potential but much lower affinity of $Sn_6O_4(OH)_4$ to the secondary formed Sb(III) species. XPS studies verify the occurring of the assumed "reduction-adsorption" mechanism introduced by the studied nanocomposites. In particular, the majority of adsorbed antimony is found in the trivalent state and mostly located in the neighborhood of Fe^{3+} ions indicating their attachment to the FeOOH surface. Such preliminary results set the application of reducing-FeOOH nanocomposites among the first adsorption processes with practical interest in Sb(V) removal.



P2-16 SYNTHESIS AND CHARACTERIZATION OF Ag, ZnO AND AgZnO DECORATED GRAPHENE OXIDE FOR ENVIRONMENTAL APPLICATIONS

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Graphene Oxide (GO) is a versatile nanomaterial derived from the oxidization and exfoliation of graphite, providing high specific area and making it ideal for environmental applications like organic compound and heavy metal removal. The “defects” of GO, meaning the functional oxygen groups added in the oxidization process, such as hydroxyls, carboxyl groups etc., can be utilized for the modification of GO, depending the needs of an application. Ag and ZnO are known for their photocatalytic and anti-microbial aspects which can increase the overall performance and effectiveness when combined with GO, while small particles of the metals/ metal oxides are spread on the large surface and in-between the GO sheets. In this work, three different nano-hybrid materials (GO-Ag, GO-ZnO, GO-AgZnO) have been synthesized, characterized and analyzed. The experimental procedure started with the synthesis of the GO via a modified Hummer’s method. Following with a self-assembly solvothermal process for the decoration of GO with each individual metal and their combination. After the synthesis, the nano-hybrid materials where characterized by X-ray diffraction analysis (XRD), Fourier-transform infrared spectroscopy (FTIR), Thermogravimetric analysis (TGA), Raman spectroscopy and Scanning electron microscopy (SEM). The results were analyzed and compared to pinpoint the differences between the GO-Ag, GO-ZnO and the GO-AgZnO hybrid. The main goal of this study was to synthesize and analyze the GO-AgZnO, something that has been successfully done.

P2-17 GRAPHENE OXIDE/ATTAPULGITE AND GRAPHENE OXIDE/ZEOLITE COMPOSITE HYBRID MATERIALS AS ABSORBENTS IN DYES WASTEWATER TREATMENT

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In recent years, dye's pollution has attracted the attention of the scientific community due to their toxicity to humans as well as the environment in general. Industrial wastewater containing dyes have various toxic effects on humans such as allergies or even cancer. Therefore, it is of outmost importance that those wastewaters must be treated for the removal of these toxic organic dyes. Over the years, many treatments have been applied, such as precipitation, ion exchange, membrane filtration, absorption and others. Among all these methods, absorption is the most popular, mainly because of its flexibility, low cost and simplicity. In this study, attapulgite (ATP) from the Ventzia Basin, Western Macedonia, Greece, clinoptilolite (CLI) and Graphene Oxide (GO), were used to synthesize and utilize two different hybrid materials that can be applied in water treatment as absorbents. Also, "Congo Red" (CR) organic dye was used to determine the absorption capability of the GO/ATP and GO/CLI composites. Both composite hybrid materials were synthesized by a simple hydrothermal method. This method is relatively eco-friendly as no harmful or high toxicity reagents were used during the synthesis process. The properties of the composite materials were examined, by means of X-ray powder diffraction (XRD) and Fourier Transform infrared spectroscopy (FT-IR). Also, their absorption capabilities were determined, via UV-Vis spectroscopy, measuring the concentration in water solutions before and after the materials were applied.

P2-18 SYNTHESIS AND CHARACTERIZATION OF MAGNETIC GRAPHENE OXIDE FOR ENVIRONMENTAL APPLICATIONS

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Nowadays, the widespread industrial activity is responsible for the generation of serious environmental issues, such as water pollution. Organic dyes have been widely used in many industrial fields, such as textiles, paper, coatings and leather. It is known that most of them are highly toxic and can cause carcinogenic effects on human beings even at low concentrations. Consequently, their removal has become a global concern over the last century. So far, numerous efforts have been developed for organic dyes removal, such as adsorption, photo-chemical degradation, coagulation flocculation, oxidation, as well as, catalytic ozonation. Among these techniques, adsorption is the most popular due to its simplicity and low cost. Therefore, it is very important to develop adsorbents with high adsorption capacity and fast separation rates for treating large volumes of wastewater. In recent years, carbon based nanomaterials, such as graphene oxide (GO), have drawn considerable attention because of their high surface area and chemical stability. However, the separation or recovery of GO adsorbent in heterogeneous systems still remains a steep challenge. Considering this point, the combination of GO with magnetic nanoparticles is an ideal option for an easy separation process, as it could be easily retrieved by applying an external magnetic field. This work is focused on the synthesis of magnetic GO-$CuFe_2O_4$ nanohybrid by a facile solvothermal route and its characterization through XRD, FT-IR, TGA, SEM, as well as, TEM. Furthermore, this study evaluated the performance of GO-$CuFe_2O_4$ nanohybrid in the removal of Congo Red (CR) dye from aqueous solution, using UV-Vis spectroscopy.

P2-19 SYNTHESIS AND CHARACTERIZATION OF GRAPHENE OXIDE-CERIA NANOHYBRID MATERIAL

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Nowadays, graphene has attracted the interest of the scientific community because of its excellent physical and chemical properties. It is a flat one atom thick layer, consisting of sp^2 hybridized carbon atoms arranged in a hexagonal lattice. Graphene oxide (GO), which possesses the characteristics of graphene, shows a great promise for the fabrication of nanoscale structures. Due to the fact that GO contains a range of reactive oxygen functional groups (e.g., carboxylic acids, hydroxyl, and carbonyl groups), it can be easily modified with a number of organic or inorganic compounds in order to achieve desired final properties. In the present work, GO was successfully modified with cerium dioxide (CeO_2) (otherwise ceria) nanoparticles. CeO_2 is an attractive rare earth metal oxide which has been intensively studied in several areas, such as catalysis, fuel cells, supercapacitors, gas sensors, etc. The combination of GO with CeO_2 nanoparticles not only does it prevent GO from agglomeration due to π-π interactions, but also helps the formation of metal oxide nanostructures with uniformly dispersed controlled morphologies, suppressing the agglomeration of CeO_2. More specifically, in this work the incorporation of CeO_2 nanoparticles onto GO nanosheets was accomplished by the electrostatic self-assembly method. The final GO-CeO_2 nanohybrid was characterized via X-Ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT-IR), Thermogravimetric Analysis (TGA), micro Raman Spectroscopy, as well as, Field Emission Scanning Electron Microscopy (FESEM).

P2-20 GRAPHENE OXIDE/β-CYCLODEXTRIN NANOHYBRID AS AN ADSORBENT FOR DYES REMOVAL

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Nowadays, more than 100.000 commercial dyes are used in various industrial fields, such as textiles, paper, printing, rubber, plastics, cosmetics, leather tanning and food processing. It is known that about 10%-15% of all dyes used in the industry are lost in the wastewater during processing. Owing to their high thermal and chemical stability, most of them are resistant to degradation by light, heat, and oxidants in nature. Therefore, dyes removal from wastewater has become a significant issue worldwide. Among the numerous efforts which have been developed for dyes removal, adsorption is the most favorable due to its simplicity and low cost. In recent years, carbon based nanomaterials, such as graphene oxide (GO), have been used as adsorbents because of their high surface area and chemical stability. In order to enhance the adsorption capacity of these nanomaterials, their combination with β-cyclodextrin (β-CD) has been considered an ideal option. β-CD is a cyclic oligosaccharide consisting of seven a-D-glucose units connected through α-(1,4) linkages and it has a hydrophilic exterior and a hydrophobic interior. Due to its structure, β-CD is capable of forming stable host-guest inclusion complexes with various aromatic molecules by virtue of series of weak intermolecular forces. The objective of this study is the synthesis of a GO/β-CD nanohybrid through a facile hydrothermal method. The final nanohybrid was characterized through XRD, FT-IR, TGA, as well as, Nitrogen Porosimetry. Moreover, this study evaluated the performance of GO/β-CD nanohybrid in the removal of Congo Red (CR) dye from aqueous solution, using UV-Vis spectroscopy.

P2-21 MICRO-LIBS MAPPING OF MARINE MOLLUSK SHELLS ENABLES RELIABLE USE OF Mg/Ca AS A TEMPERATURE PROXY

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Mollusc shells constitute valuable biogeochemical archives based on seasonal variability records imprinted in their growth increments as elemental composition or isotope variations. Their availability along modern and ancient shorelines as well as their good preservation facilitate climatic analyses at a high temporal and spatial resolution. They are commonly analysed using oxygen isotope ratios (δ18O) or elemental ratios (e.g. Mg/Ca, Sr/Ca, Ba/Ca) which are correlated to the variations of environmental temperature. However, the lack of fast methods limits analysis to low numbers of shells, and thus reduces significantly the statistical value of results. The use of micro-LIBS mapping facilitates acquisition of spatially extensive elemental maps and opens up prospects for handling large numbers of samples. In these studies, we have employed a custom-made LIBS microscope and concentrated on recording Mg/Ca ratio maps across sections of aragonitic or calcitic shells. Maps provide information regarding the season of death, as well as season dependent annual minima and maxima, but furthermore enable one to understand whether the recorded variations are specific to research location or individual specimens and thus avoid misinterpretations. Still obtaining absolute estimates of temperature based on Mg/Ca ratios is not straightforward. However, combining these high resolution data from samples that show meaningful seasonality patterns with one or two measurements of oxygen isotope analysis (performed on the same sample) gives rise to true temperature variation mapping and provides the means to access previously uninterpretable climate proxies on a large scale.

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P2-22 DETERMINATION OF THREE ANTIDEPRESSANT DRUGS BY FABRIC-PHASE SORPTIVE EXTRACTION (FPSE) COUPLED TO HPLC-UV/DAD

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Depression is one of the most common chronic or recurrent mental illnesses in modern society. It is often characterized by inattention, reduced self-confidence, pessimism, guilt, sleep disturbance, self-harm, and ultimately suicide. The determination of antidepressant drugs in environmental samples is particularly useful since these chemicals are not commonly monitored in the environment but have the potential to be released in high quantities and cause adverse ecological and/or human health effects. Current trend in sample preparation involves the use of novel sample preparation procedures. Among them Fabric-Phase Sorptive Extraction (FPSE), a current and up-to-date technique of solid sorbent-based microextraction, is regarded to be a simple, sensitive, and fast analytical technique. This work reports a novel fabric-phase sorptive extraction protocol, coupled to High-Performance Liquid-Chromatography-Diode Array Detection (FPSE-HPLC-DAD) for the simultaneous extraction, preconcentration and analysis of three antidepressants, namely, bupropion, mirtazapine and sertraline, in natural water samples. The selected antidepressants were well resolved by using a Fortis C18 column (50 mm x 2.1 mm) at 25 °C and methanol and phosphate 0.03% buffer in gradient elution mode within 15 min. Two FPSE media, Whatman filter and Fiber glass Whatman filter, coated with different sol-gel sorbent chemistries having different polarities and selectivities were studied, polyethylene glycol (PEG) and polyethylene glycol - polypropylene glycol - polyethylene glycol triblock copolymer (PEG-PPG-PEG). Fiber glass Whatman filter coated with PEG-PPG-PEG media was found to be the most efficient extraction media for the analytes of interest in the intended study. Relative recovery values ranged between 60-80% for all target analytes while the developed method provides satisfactory limit of detection of less than 3.22 μg/μL.

P2-23 SILICON LEACHABILITY FROM BAUXITE RESIDUE - THE CASE OF GEL FORMATION

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Bauxite residue is the alkaline fine sized byproduct of bauxite digestion for alumina production from Bayer process. The byproduct is rich in numerous major, minor and trace elements. The extraction of valuable elements of techno-economical interest can be a profitable route for the utilization of byproduct. Hydrometallurgical treatment with mineral acids is the most common method for trace elements recovery such as scandium and other rare earths. However, the method is not selective because of major elements co-extraction usually in large amounts. Among others main elements, silicon high concentration in pregnant solution at low pH causes handling problems due to gel formation hindering the following purification and isolation processes. In the present work silicon leachability from greek bauxite residue is investigated applying the optimum leaching conditions for scandium extraction with sulfuric acid. The optimum values were presented in details elsewhere [1]. The determination of silicon is performed by an ICP-OES. Gel formation is also studied as a function of time for different leaching parameters (molarity, solid/liquid ratio, addition of agent e.t.c.). Gel formation is caused due to the presence of silica in the solution as silicic acid (H_4SiO_4) at pH<7. The monomers connect to form polysilicic acid and colloids result to gel formation, as they entrap liquid inside their structure [2]. Aiming at gel re-dissolving different ways (dilution, attack with concentrated sulfuric acid, sodium hydroxide or hydrogen peroxide) are further investigated.

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P2-24 MAGNETIC GRAPHENE OXIDE SOLID-PHASE EXTRACTION OF SELECTED PHARMACEUTICALS FROM ENVIRONMENTAL WATERS

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Pharmaceuticals constitute one of the most important emerging classes of environmental pollutants. They are a prominent group of emerging contaminants frequently found in wastewater effluents and wastewater-impacted aquatic environments. Therefore, it is necessary to develop simple and reliable methods for their determination. Several analytical processes and many methods have been used for the pretreatment of pharmaceutical residues in different matrices. Magnetic solid-phase extraction (MSPE) received much attention in the last decade. It is based on the adsorption of target analytes by dispersing magnetic adsorbent into liquid sample, followed by magnetic separation with the help of external permanent magnet. In recent years, graphene-based magnetic composites have attracted tremendous research interest owing to promising properties together with the ease of processability and functionalization render graphene-based magnetic composites to be ideal adsorbents in magnetic solid-phase extraction. In our study, a magnetic adsorbent Fe_3O_4/reduced graphene oxide was prepared for the determination of selected pharmaceuticals (antibiotics, antidepressants and antipsychotics) in environmental waters. To fulfil the need of ultra-sensitivity the MSPE was combined with ultra-high performance liquid chromatography (UHPLC) coupled to hybrid Q-Orbitrap high-resolution full-scan mass spectrometry (HRMS). Under the optimized conditions the method showed a good linear response in the concentration range of three orders of magnitude ($r^2 \geq 0.9878$). Limits of quantification were at ppt levels for the majority of the analytes and recoveries of 54.1%-109.1% were achieved at different spiked levels.

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P2-25 FLUORESCENT CARBON NANODOTS FROM OLIVE OIL PRODUCTION RESIDUES: PREPARATION, CHARACTERIZATION AND ANALYTICAL APPLICATION

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We used olive oil production residues, such as olive leaves, olive cake, crushed olive stones and fine combustion particles (fine char) for the synthesis of fluorescent carbon dots (CDs) through hydrothermal processing. CDs were prepared in water, in aqueous solution of ethylenediamine and in aqueous solution of cysteamine. The hydrothermal temperature and time were investigated in the range of 150-180 ^{o}C from 3 to 48 h. The morphology of CDs was studied by transmission electron microscopy. The CDs were nearly spherical with sizes from 3-7 nm. The functional groups of the CD preparations were studied by FTIR. The presence of hydroxyl and carboxyl groups and epoxy groups on the surface offers great water solubility. The CD preparations exhibited fluorescence excitation-dependent emission. The excitation maximum was 320-340 nm. The emission spectra exhibit large Stokes shifts of 70-80 nm. The fluorescence quantum yields of CDs prepared in water, ethylenediamine and cysteamine were 2%, 6.7% and 12%, respectively. The fluorescence remained constant at various ionic strengths corresponding to 0-1 M NaCl. The effect of pH on the fluorescence of CD preparations was studied in the range of 2.5 to 12. The effect of the presence of 32 inorganic ions on the fluorescence spectra of CDs was also studied. Furthermore, studies have been carried out demonstrating that carbon nanodots can be used for the quantitative determination of Fe^{3+} and CrO_4^{2-} in the range of 5-100 μM based on the quenching properties of these ions. In conclusion, the present study creates new prospects for the transformation of widely available and environmentally harmful materials to high added-value analytical tools.

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P2-26 EFFECT OF CARBON ADDITIVE ON SINTERING OF ZIRCONIA CERAMICS

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Using the technique of dilatometry, sintering of zirconium ceramics from nano powder doped with carbon nanotubes has been investigated. A composite of zirconia powder and carbon nanotubes in a ratio of 85 to 15% was made by mechanical stirring in a planetary mill. Compacts with a diameter of 9 mm and a thickness of 3 mm were made by uniaxial static pressing. The effects of the additive were determined by the method of comparing the characteristics of the ceramics without the additive and with the additive. It was found that the addition of carbon nanotubes greatly facilitates the process of pressing. Press samples at the same time more resistant to mechanical destruction. It is shown that the shrinkage process of carbon-doped samples is identical to that of sintering pure zirconia ceramics. However, by changing the carbon concentration and pressing pressure, you can effectively manage the porosity of the finished ceramics, which allows it to be used as a material for biomedicine. So, at a pressure of more than 700 MPa, the porosity of the ceramic doped with carbon is 30% greater than the porosity at a pressure of 80 MPa. It was also found that if the porous ceramics is processed with an intense pulsed electron beam, its subsurface layer becomes nonporous and has a higher microhardness.

P2-27 THE EFFECT OF pH ON THE STRUCTURAL AND OPTICAL PROPERTIES OF CARBON QUANTUM DOTS

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The discovery of carbon quantum dots (CQD's) was a random occurrence, isolated as a fluorescent byproduct during the synthesis of carbon nanotubes. CQD's are nanocrystals with generally spherical shape, they have attracted considerable and growing scientific and technological interest. This interest is also reflected by the almost exponential growth of scientific articles published about this subject. But it is mainly due to the unique physical properties of CQD's and especially their photoluminescence, which seems to be directly related to the energy levels of the CQD's. In biology, they have been used for the construction of bio-sensors. In medicine, they have been used to diagnose and treat cancer. Finally, in optoelectronics there are applications of CQD's in transistors, lasers, LEDs, etc. In this work the effect of pH on the structural and optical properties of nitrogen and sulfur doped CQD's is investigated. For the preparation of CQD's were used thiourea and citric acid, while the synthesis of CQD's was carried out in a microwave reactor. The reaction conditions were: temperature 200 ° C, pressure 40 bar and power 800 W for one hour. The existence of organic groups on the surface of the CQD's before pH change was confirmed by FTIR technique. Then, the initial samples of quantum dots were treated in different pH (pH range: 3.0 -10.0) using buffer solutions, in order to determine the modification in the functional groups of the CQD's. The characterization of their structural and chemical properties was performed by the FTIR technique. The study of the optical properties of the resulting CQD's solutions was carried out using PL and UV-Vis.

P2-28 UV-FEMTOSECOND DOUBLE-PULSE LIBS FOR THE IN-SITU CHARACTERIZATION OF ITO-BASED THIN FILMS

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Performing compositional analysis and depth-resolved profiling of nanometer-scale samples (thin films) is a demanding task and requires the use of sophisticated techniques. Furthermore, if this type of analysis is to be done in the context of a production line in an industrial environment, additional requirements are imposed having to do with speed of analysis and ability to run such diagnostics in situ. Laser-Induced Breakdown Spectroscopy (LIBS) has been investigated as a potential technology for rapid analysis of materials at different depths of thin film structures. A main challenge in this application is the need to achieve efficient analysis of each layered film with just a single sequence of pulses. This translates to the requirement of recording reliably good emission signals which arise from a single laser-plasma event that samples material volumes as low as 5 - 80 μm^3 corresponding to elemental mass quantities down to 10 picograms. In an effort to maximally exploit the optical energy of each laser pulse for generating an intense plasma, hence enhancing the analytical capacity of the proposed method, we have examined the possibility of performing Double-pulse (DP) LIBS which involves ablation of the sample with a pair of pulses temporally separated by a few tens of picoseconds. The current work concentrates on the use of UV-Femtosecond-DP-LIBS (λ = 248 nm, tpulse = 450 fs) for the characterization of multi-layered thin films, of relevance to industrial applications, exploring critical measurement parameters and attempting to establish optimum conditions for performing minimally invasive depth-profile analysis. The results on indium-tin oxide (ITO) films indicate increase of the emission by as high as a factor of 3-5, depending on pulse energy and spectral transition properties, when DP-LIBS is used in comparison to (single-pulse) SP-LIBS, demonstrating that the proposed double-pulse approach is a promising one for the characterisation of nanofilms.

P2-29 SYNERGISTIC EFFECTS OF SOLID-PHASE INTERACTIONS IN FERRITE POWDER SYSTEMS UNDER COMPLEX HIGH-ENERGY MECHANICAL AND ELECTRON-BEAM IMPACTS

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The solid-phase synthesis is the main method of commercial production of ferrites, which requires high temperatures and long times to manufacture multicomponent ferrites with homogeneous compositions. In particular, the efficiency of solid-phase synthesis can be increased by application of specific methods that allow the reagents to be activated directly in the process of synthesis. As previously shown, a heating of precursors by an intensive electron beam is an efficient method for solid-state reactions intensification. It is also known that a mechanical activation in high energy ball mills is a popular technique to prepare the powders with disordered structure and fine fraction. The aim of this work is to investigate the synergistic effects of solid-phase interactions in ferrite powder systems under complex high-energy mechanical and electron beam impacts that include the grinding and activation of powder reagents in an AGO-2S planetary mill and subsequent heating by an electron beam with energy above 1 MeV using ILU-6 accelerator. The microstructure of ferrites was studied using the Brüner, Emmett, Teller and laser diffraction methods as well as X-ray diffraction and scanning electron microscopy analyses. The homogeneity of the phase composition of the obtained samples was investigated using a new method of analysis based on thermomagnetic measurements [1]. It was established that a high energy electron beam heating of mechanically activated ferrite reagents allows to accelerate the solid-state reactions at synthesis and thus to obtain ferrite powders with final composition at significantly lower temperatures and times of synthesis. It was found that this approach makes it possible to combine the both technological stages of synthesis and sintering in one stage of treatment, consisting in a heating of press-samples by a high-energy electron beam to a sintering temperature.

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P2-30 FLUORESCENCE INSTRUMENTATION FOR RAPID, IN SITU DETERMINATION OF DISSOLVED ORGANIC MATTER IN WATER

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Water management is of increasing importance due to decreasing availability of drinking water and increasing water quality problems, and quality assessment is an essential task in the control of water resources. Reference standard methods for determination of quality parameters (conductivity, pH, temperature, turbidity) as well as chemical oxygen demand (COD), biological oxygen demand (BOD) and total organic content (TOC) are available as laboratory methods. In the recent decades fluorescence spectroscopy has been intensively applied in the analysis of dissolved organic matter (DOM), in hope to extend analytical capacities with *in situ* methods. Such determinations are possible, because some DOM fractions are fluorescent, and these fractions can be further classified into tryptophan-like and tyrosine-like substances. A portable, modular structured instrument was developed for rapid determination of the most important water quality parameters by using direct fluorescence techniques. In our system the sample in a standard quartz cuvette is excited with a Xenon flash lamp combined with an optical bandpass filter. The fluorescence is measured with a high-sensitivity, thermoelectric cooled CCD fibre-optic spectrometer or a photomultiplier tube combined with a set of optical interference filter. The fluorescence of the solutions tryptophan and tyrosine were excited at 256 and 276 nm, when emitted at 311 nm, 335 nm and 377 nm. A “fingerprint map” is established from the chemometric processing of signals obtained from the results of corresponding characteristic emission wavelengths. Both the newly developed module and the analytical procedure are validated on the basis of appropriate reference measurements.

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P2-31 FLUORESCENCE INSTRUMENTATION FOR RAPID, IN SITU DETERMINATION OF ALGAL DENSITY IN WATER

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Algal bloom is a key water quality problem, associated with eutrophication of surface water and leading to toxicity problems due to phytotoxins. To extend current methods to assess algal density and composition, our novel excitation fluorescence method was assessed to determine the density of phytoplankton and phytobenthic algae by chlorophyll-a-content. The utility of novel devices for laser induced fluorescence of chlorophyll-a detection (FluoroMeter Module (FMM) in two- (CFM) and four-channel (CFM4ch) versions) was tested on green/blue/diatom algae. To select optimal excitation wavelengths, fluorescent emission spectra of the algal species tested were taken. The intensity of excitation chlorophyll-a-fluorescence (the maximal level of fluorescence emitted by algal cells upon darkness adaptation) was determined at 690 and 735 nm. Limits of detection and quantitation (LODs, LOQs) were compared among both the algal species studies and the instrument types used, the utility of various analytical 96-well microplates (transparent/white/black), the effects of test volumes and dark incubation durations were evaluated. Density measurements of green algae allowed good to excellent LOD and LOQ values ($LOD_{FMM}=4.01*10^6$, $LOD_{CFM}=1.15*10^5$, $LOD_{CFM4Ch}=2.22*10^3$; $LOQ_{FMM}=8.12*10^6$, $LOQ_{CFM}=2.65*10^5$, $LOQ_{CFM4Ch}=5.67*10^4$ cell/ml). Detection sensitivity occurred to be favourable also for the blue alga species studied ($LOD_{FMM}=8.26*10^7$, $LOD_{CFM4Ch}=4.46*10^6$ cell/ml). In contrast, substantial improvements in the detectability of the density of diatoms were not observed for LODs or LOQs. Correlations among algal densities detected by fluorimetry and by reference techniques (e.g., Bürker chamber, optical density devices, extractive chlorophyll-a content determination) have been evaluated. Excellent correlations (R>0.98) between chlorophyll-a-fluorescence in all fluorimeters and all reference methods were observed for green/blue algae. For diatoms, however, FMM signals showed no proportional increase with chlorophyll-a-content in the sample, and high correlation with the reference methods was achieved only by CFM4Ch.

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P2-32 FLUORESCENCE INSTRUMENTATION FOR RAPID, IN SITU DETERMINATION OF PAHS IN SURFACE WATER

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Polycyclic aromatic hydrocarbons (PAHs) consisting of two or more condensed aromatic rings are ubiquitous environmental pollutants. Many PAH substances have been proven to have toxic, carcinogenic and mutagenic properties. They are deposited from the atmosphere into surface waters by sedimentation and precipitation, and they also emerge as soil pollutants via groundwaters. Directive 2008/105 / EC of the European Parliament and of the European Council sets strict environmental quality standards (EQS) to regulate the annual average value (AA) and the maximum allowable value (MAC) of PAHs in surface waters. AA-EQS values are 0.05 µg/l for benzo[a]pyrene, 0.03 µg/l for Σ benzo[b]fluoranthene + benzo[k] fluoranthene and 0.002 µg/l for Σ benzo[g,h,i] perylene + indeno[1,2,3-cd]pyrene. A portable, modular structured instrument was developed for rapid determination of the most important PAHs by using direct fluorescence techniques. The sample is excited with a Xenon flash lamp combined with an optical bandpass filter at a specific UV wavelength range (250-330 nm). Fluorescence is measured with a high-sensitivity, TE cooled CCD fiber-optic spectrometer or a photomultiplier tube combined with a set of optical interference filters in the range of 330 nm; 370 nm; 390 nm; 430 nm; 460 nm. A “fingerprint map” is established from the chemometric processing of signals obtained from the results of corresponding characteristic emission wavelengths. Both the newly developed module and the analytical procedure are validated on the basis of appropriate reference measurements.

This research was supported by the National Research, Development and Innovation Fund of Hungary within the National Competitiveness and Excellence Program NVKP_16-1-2016-0049.

P2-33 APPLICATION OF ANALYTICAL QUALITY BY DESIGN PRINCIPLES FOR THE DETERMINATION OF ALKYL P-TOLUENESULFONATES IMPURITIES IN APREPITANT BY HPLC. VALIDATION USING TOTAL-ERROR CONCEPT

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In this research we report the development of a simple and robust liquid chromatographic method for the quantification of two genotoxic alkyl sulphonate impurities (namely methyl p-toluenesulfonate and isopropyl p-toluenesulfonate) in Aprepitant API substances using the Analytical Quality by Design (AQbD) approach. Following the steps of AQbD protocol, the selected critical method attributes (CMAs) were the separation criterions between the critical peak pairs, the analysis time and the peak efficiencies of the analytes. The critical method parameters (CMPs) included the flow rate, the gradient slope and the acetonitrile content at the first step of the gradient elution program. Multivariate experimental designs namely Plackett-Burman and Box-Behnken designs were conducted sequentially for factor screening and optimization of the method parameters. The optimal separation conditions were estimated using the desirability function. The method was fully validated in the range of 10-200% of the target concentration limit of the analytes using the "total error" approach. Accuracy profiles – a graphical decision-making tool – were constructed using the results of the validation procedures. The beta-expectation tolerance intervals did not exceed the acceptance criteria of ± 10%, meaning that 95% of future results will be included in the defined bias limits. The relative bias ranged between − 1.3-3.8% for both analytes, while the RSD values for repeatability and intermediate precision were less than 1.9% in all cases. The achieved limit of detection (LOD) and the limit of quantification (LOQ) were adequate for the specific purpose and found to be 0.02% (corresponding to 48 μg g^{-1}in sample) for both methyl and isopropyl p-toluenesulfonate. As proof-of-concept, the validated method was successfully applied in the analysis of several Aprepitant batches indicating that this methodology could be used for routine quality control analyses.

P2-34 INSTRUMENTAL ANALYTICAL METHODS AS A TOOL FOR THE EVALUATION OF DEOXYCHOLIC ACID ENCAPSULATION EFFICIENCY IN NATURAL MATRICES USING ELECTROHYDRODYNAMIC PROCESS

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Deoxycholic acid (DCA) is a naturally occurring, bile acid, and has been studied extensively for its lipolytic action [1, 2]. However, until today, its applications are limited to injectable formulations making it inaccessible to the general public. The encapsulation of DCA in natural matrices via the electrohydrodynamic process is an innovative solution, as the micro- and nano- fiber or particle structures produced, exhibit good mechanical properties, protection of the bioactive compound from exogenous factors and the possibility of its gradual release into the body. The electrohydrodynamic process avoids the use of toxic solvents while ensuring the quality and stability of the thermo-sensitive components thanks to its operation at ambient temperature [3, 4]. In the present work DCA was encapsulated in Polylactic acid (PLA) (0.4 % w/v in acetone), a natural, biodegradable and biocompatible polymer [5], using the coaxial electrospinning process. The morphology (shape, size) of the encapsulation product was studied using Scanning Electron Microscopy (SEM) while the complex formations and generally the type of interactions between the polymer matrix and the encapsulated substance (physical or chemical encapsulation) were examined with Attenuated Total Reflectance Infrared spectroscopy (ATR-FTIR). In addition, the thermal behavior of the complexes was evaluated by Differential Scanning Calorimetry (DSC) to assess the stability of the generated structures. At the same time, the encapsulation efficiency was determined using Ultraviolet/Visible spectroscopy (UV/Vis) with the aid of a standard curve made for DCA with this method, while the size distribution of the electrospun structures was measured through a Laser diffraction particle size analyzer to assess the uniformity and the possible need for optimization of the encapsulation process.

P2-35 OCCURRENCE, REMOVAL AND ENVIRONMENTAL RISK ASSESSMENT OF PHARMACEUTICALS IN HOSPITAL AND URBAN WASTEWATERS

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Pharmaceuticals are a broad group of chemical compounds, including complex molecules with a variety of different functional groups, physicochemical and biological properties. They can enter the environment through many streams, including the outflows of sewage treatment plants and the drainage of waste from sources such as livestock breeding units. An additional source of pharmaceuticals in urban wastewater is the inappropriate disposal of unused or expired drugs. In the present study, the occurrence, removal and environmental risk assessment of ten pharmaceutical compounds, were studied in wastewater treatment plants (WWTPs) in north and northwestern Greece. These pharmaceuticals belong to different treatment categories and include bupropion, venlafaxine, mirtazapine, sertraline, citalopram, caffeine, triclosan, carbamazepine, diazepam and clozapine. They have been selected due to their high usage rate but also because of their proven presence both in wastewater treatment plants and the aquatic environment. The samples were collected from the University hospital of Ioannina and three urban wastewater treatment plants in north and northwestern Greece (Ioannina city, Grevena city and town of Chalastra). Analytical methodology was based on gas chromatography coupled to mass spectrometry (GC-MS) detection after the application of a solid phase extraction (SPE) step. The results showed that the most often detectable compounds were caffeine, triclosan and venlafaxine. High concentration levels of caffeine, up to 22142.1 ng/L were found, so caffeine was a dominant compound. Bupropion, mirtazapine, citalopram, diazepam and clozapine were the less frequently detected compounds and their concentrations ranged from levels between below quantification limit and 87.2 ng/l. In addition, removal rates were up to 99 %. Furthermore, environmental risk assessment was estimated by calculating the risk quotient (RQ) for aquatic organisms such as algae, fish and daphnia. Finally, high levels of acute and chronic toxicity were observed for triclosan (RQ>1).

P2-36 CHARACTERIZATION OF THE ANTIMICROBIAL ACTIVITY OF HERBAL EXTRACTS FOR REPLACING ANTIBIOTICS IN LIVESTOCK

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In the framework of this study microwave and ultrasound assisted extraction of herbs was examined to evaluate through instrumental methods of analysis such as High Performance Liquid Chromatography (HPLC) and UV-Vis spectrophotometry the efficiency of the proposed techniques in providing extracts with high antimicrobial activity for replacing the conventional antibiotics in animal feed. More specific, the raw materials that were used, were Magnolia officinalis, pills of citrus fruits such as lemon and orange and green tea seeds. Based on the literature, the applied extraction protocols were the most effective for extracting the antimicrobial compounds, while solvents such as methanol, ethyl acetate, petroleum ether were used. The Ph was adjusted to 2 using acetic acid. According to the HPLC and UV-Vis measurements that conducted, Magnolia officinalis can be very effective in the treatment against the resistant bacteria of the livestock such as Vancomycin- Resistant- Enterococci (VRE) and Methicillin-Resistant- Staphylococcus Aureus (MRSA) due to the high content of Magnolol and Honokiol [1,2]. On the other hand HPLC proved the high content of alkaloids and citrus flavonoids in orange and lemon pill, proving a potential antibacterial and antifungal activity especially for Listeria Monocytogenes, Salmonella sp. and Campylobacter jejuni [3,4] . Finally green tea seeds, it was proved to have same properties as citrus fruit pill, containing polyphenols (such as catechins, flavonoids) and alkaloids. The obtained extracts will be used as pre-mixes for animal feed replacing the conventional chemical antibiotics. Thus the EU legislation for incorporating the extracts into the feed was also examined, providing information regarding the final product requirements and the chemical that should be used during every step of the extraction procedure.

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P2-37 DEVELOPMENT AND VALIDATION OF AN RP-HPLC METHOD FOR THE ANALYSIS OF GUAIACOL IN A PHARMACEUTICAL DOSAGE FORM

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Development of simple and reliable analytical methods is of paramount importance for quality control laboratories. The main criterions that are usually requested are time and cost. Guaiacol, a natural antiseptic and expectorant compound, is used as an active substance in liquid formulation medicines in association with other active substances such as Codeine or Pholcodine. The analysis of guaiacol is carried out mainly by GC/FID method. However, it possesses some drawbacks that make it not suitable for routine analysis. First, an extraction step is required. Second, lower recovery extraction may occur after the extraction procedure. Third, important quantity of hazardous solvent like chloroform is used during the extraction. And fourth, the analysis time is relatively high (t_r ~ 25 min). Hence, it could be argued that the GC/FID method is a time and solvent-consuming technique that is not appropriate for the routine laboratory analysis. The purpose of this work was to develop, a fast and effective rp-HPLC method as an alternative approach for the analysis of guaiacol in liquid formulation. After many trials and errors, the optimum chromatographic conditions were determined. The mobile phase composition consisted in a mixture of phosphate buffer pH 3/acetonitrile/methanol (425/425/150 v/v/v). The maximum wavelength was set at 276 nm. The analyte was eluted on a C18 column (250 mm length, 4.6 mm I.D, 5 µm). The developed method was then validated according to the ICH guidelines. Specificity test showed no interferences with the excipients. The LOD and LOQ were 0.06 and 0.15 µg mL^{-1} respectively. The response factor versus analyte concentration was found linear (R^2 > 0.999) in the range of 9.6-14.4 µg mL^{-1}. The analysis time (t_r = 3.49 min) and the validation parameters of precision, robustness, recovery and formulation assay indicated that the developed method is suitable for the laboratory routine analysis.

P2-38 MAGNETIC MOLECULARLY IMPRINTED POLYMER NANOPARTICLES AS SOLID PHASE EXTRACTION MATRIX IN THERAPEUTIC DRUG MONITORING

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In this study, a novel, economic cost, computer- aided design technique was proposed for the synthesis of two molecularly imprinted polymers (MIP) on magnetic Fe_3O_4 nanoparticles (NPs). The synthesized magnetic molecularly imprinted polymer nanoparticles (Fe_3O_4@MIPs NPs) were evaluated for the extraction of their template drugs - the antiepileptic drug levteracetam (LEV) and the antileukemic agent 6-mercaptopurin (6-MP) - from plasma samples as a mean of sample purification and enrichment prior to chromatographic analysis of these drugs in therapeutic drug monitoring. Adsorption experiments were carried out to determine the optimum conditions of extraction including the type of solvent, extraction time, pH and amount of adsorbent. Adsorption isotherms were best fitted to Langmuir model in the studied cases and adsorption kinetics were modeled with pseudo second order kinetics. The synthesized Fe_3O_4@MIPs NPs just needed 30 min to reach the adsorption equilibrium with maximum adsorption capacities of 26.04 mg/g for LEV and 1mg/g for 6-MP. For therapeutic drug monitoring of LEV, a validated HPLC method was developed and utilized in combination with the proposed sample preparation technique to provide a fast and reliable approach for analysis of LEV in plasma samples. On the other hand, a validated LC-MS/MS method was utilized for the simultaneous determination of 6-MP and its active metabolite thioguanine (TG) after their simultaneous extraction using the proposed Fe_3O_4@MIPs NPs. The satisfactory results obtained proved that the Fe_3O_4@MIPs NPs can be a vital alternative to more traditional extraction techniques for biological samples pre-concentration.

P2-39 SYNTHESIS OF MAGNETIC BIMETALLIC Fe-Cu NANOPARTICLES FOR THE DISPERSIVE MICROEXTRACTION OF EMERGING POLLUTANS

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In the past decade, the use of nanoparticles as a sorbent in sample preparation procedures has been a rising and promising trend. Among the various nanomaterials, the use of magnetic nanomaterials made feasible the development of new, advanced sample preparation techniques and more efficient analytical methods. Benzophenones are the most common ingredients as UV filters in cosmetic formulations (i.e. sunscreens) and are potentially toxic as well as they may pose significant estrogenic and/or anti-androgenic activity. Phenols exist mainly in typical effluents of agro-industrial wastes and even at low concentrations the exhibit harmful effects on organisms. Pesticides are well known environmental contaminants owing to their toxicity and bioaccumulation. Pharmaceuticals are not only toxic for many organisms but also, they can even promote bacterial resistance to antibiotics. In present study, we synthesized iron-copper bi-metallic, magnetic nanoparticles and examined their applicability as a new sorbent for the dispersive microextraction of certain classes of pesticides, phenols, benzophenones and pharmaceutical compounds from environmental aqueous matrixes. Copper was selected because of its high affinity with aromatic compounds and iron in order to render the nanoparticles magnetic. The results reveal that only a small quantity of iron-copper nanoparticles (i.e. 5 mg) can almost quantitatively extract mixture of (4-nitrophenol, 3-methyl-4-nitrophenol, benzophenone-6, fenbufen, benzophenone-8, parathion methyl, trifluralin, at a concentration of 30 mg L^{-1} in less than 10 min. This showcases the great potential of iron-copper magnetic nanoparticles to serve as an efficient sorbing material in microextraction procedures.

P2-40 A NOVEL APPROACH: pH CONTROLLED DISPERSIVE LIQUID-LIQUID MICROEXTRACTION (DLLME) OF PAHS METABOLITES FROM HUMAN URINE

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Gas chromatography-mass spectrometry (GC-MS) using quadrupole analyser with electron ionization is currently the method of choice in organic analysis covering a wide range of applications in a broad spectrum of samples. However, one of the significant limitations which restrict the achievement of its optimal sensitivity is the signal suppression due to matrix interferences introduced by the presence of co-extracted compounds during the sample preparation procedure. Co-extracted matrix components may cause several problems, including inaccurate quantitation, decreased method ruggedness, low analyte detectability, and even reporting false positive or negative results. Careful optimization of GC-MS parameters may result in a reduction but rarely complete elimination of the matrix effect. For ionisable compounds, the DLLME efficiency could be modulated by aqueous phase/urine pH adjustment. In this study, 15 PAHs metabolites with different pKa values were selectively extracted by a small amount of chloroform serving as an extraction solvent at the pH 5.0 of the urine sample. All samples were enzymatically hydrolysed due to the transformation of glucuronidated metabolites into free compounds. Chromatographic separation and detection were improved by using derivatization with N-methyl-N-(trimethylsilyl) trifluoroacetamide (MSTFA). We evaluated various ways of pH adjustment with a focus on suitable puffer. In general, the most suitable pH of urine sample was in the range of 3.55 - 4.75, which correspond with the proper pH for the urine hydrolysis (pH 4.0 - 4.5) as well as the silylation reaction, which is driven by a good leaving group, which means a leaving group with low basicity. The pH was adjusted by 0.5 mL of 0.4 M acetate buffer before enzymatic hydrolysis of urine and by the same volume of the same buffer before extraction. This method provides effective compensation of matrix co-extractants in the extract, thus a high selectivity, sensitivity and accuracy were achieved.

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P2-41 RHODIUM NANOPARTICLES AS PEROXIDASE-MIMETICS FOR THE DETERMINATION OF GLUCOSE

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This work reports the use of rhodium nanoparticles (RhNPs) as catalytic labels for sensitive colorimetric assays by exploiting their intrinsic peroxidase-mimetic activity. RhNPs catalyze the oxidation of the peroxidase substrate 3,3,5,5-tetramethylbenzidine (TMB) in the presence of H_2O_2 producing a blue reaction product with a maximum absorbance at 652 nm. The calculated kinetic parameters indicate high affinity of RhNPs for both the substrate TMB and H_2O_2. Based on these findings, a sensitive and selective colorimetric method was designed for the determination of glucose with a linear response between 5 to 125 μM and detection limits as low as 0.75 μM. Due to the lack of reactivity of RhNPs towards saccharides, thiols, amino acids and ascorbic acid the method excels exceptional selectivity in complex samples and was used for the determination of glucose in human blood plasma and soft drinks with very satisfactory results in terms of sensitivity and reproducibility.

P2-42 DISPERSIVE LIQUID-LIQUID MICROEXTRACTION METHOD FOR HPLC DETERMINATION OF PHENOLIC COMPOUNDS IN CAROB SYRUP

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The carob syrup is a traditional Mediterranean product that is produced from carob fruits. In general, it comprises a high proportion of sugars namely sucrose, fructose and glucose (> 65%) and amounts of bioactive compounds as polyols, fibers and phenolic compounds. This alternative sweetener has attracted the interest of food industry due to its energy density and glycaemic index as well as the presence of bioactive phenolics. The analysis of phenolics in carob syrup involves the elimination of matrix components as it is a highly supersaturated solution sugars and the preconcentration of analytes. The goal of this work was to develop a fast and inexpensive dispersive liquid-liquid microextraction (DLLME) method suitable to the determination of phenolic compounds in carob syrup. For the implementation of DLLME optimization, an artificial syrup reflecting the main components of carob syrup was prepared. This solution was spiked with four phenolic acids and three flavonoids at 1 μg g^{-1}. Initially, chloroform, dichloromethane and bromebenzene was evaluated as extractant solvent; whereas the efficacy of methanol, acetone and acetonitrile as disperser solvent was also determined. Furthermore, the volumes of extractant (300, 450 and 600 μL) and disperser solvents (400, 600 and 800 μL) were optimized to increase further the recoveries of phenolics. Results showed a great impact of nature and volume of extraction and dispersive solvents on the recovery of phenolics from carob syrup. Results showed the exhaustive extraction for investigated analytes was achieved using 450 μL chloroform as extractant solvent and 800 μL methanol as disperser solvent. The recovery of gallic acid, the major phenolic compound, and flavonoids was higher than 98%, while the recoveries of hydroxycinnamic acids were between 85% and 99%. Overall, the proposed DLLME method in combination with HPLC is a useful analytical tool for the determination phenolic compounds in carob syrup.

P2-43 APPLICATION OF DISSOLVABLE LAYERED DOUBLE HYDROXIDES AS AN EXTRACTION MEDIUM OF GOLD NANOPARTICLES PRIOR TO THEIR DETERMINAITON BY ATOMIC ABSORPTION SPECTROMETRY

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This work reports the use of magnesium-aluminum layered double hydroxides (LDH) for the liquid phase extraction of gold nanoparticles (AuNPs) form water samples. LDH were formed in-situ in the aqueous sample solution under strongly alkaline conditions entrapping and co-precipitating AuNPs which are then re-dissolved under acidic conditions. To enable the application of atomic spectroscopy the extracts were ultra-centrifuged to separate AuNPs from the bulk aqueous phase containing the dissolved aluminum and magnesium species. The AuNPs were finally re-dissolved in HNO_3/HCl or HNO_3 and determined by flame atomic absorption spectrometry (FAAS) or electrothermal atomic absorption spectrometry (ETASS), respectively. Interestingly, the dissolution and centrifugation steps enabled the separation of gold ions form AuNPs thus enabling the speciation of gold species in the sample without the need of masking agents or other sample pretreatment procedures. The method enables the determination of AuNPs at concentration levels as low as 0.6 nM and 0.4 pM with FAAS and ETAAS respectively, with satisfactory reproducibility (RSD=7%, n=3) and recoveries higher than 80%.

P2-44 DETERMINATION OF HYDRAZINE BY ON-LINE SOLID PHASE EXTRACTION AND DERIVATIZATION USING ZONE FLUIDICS

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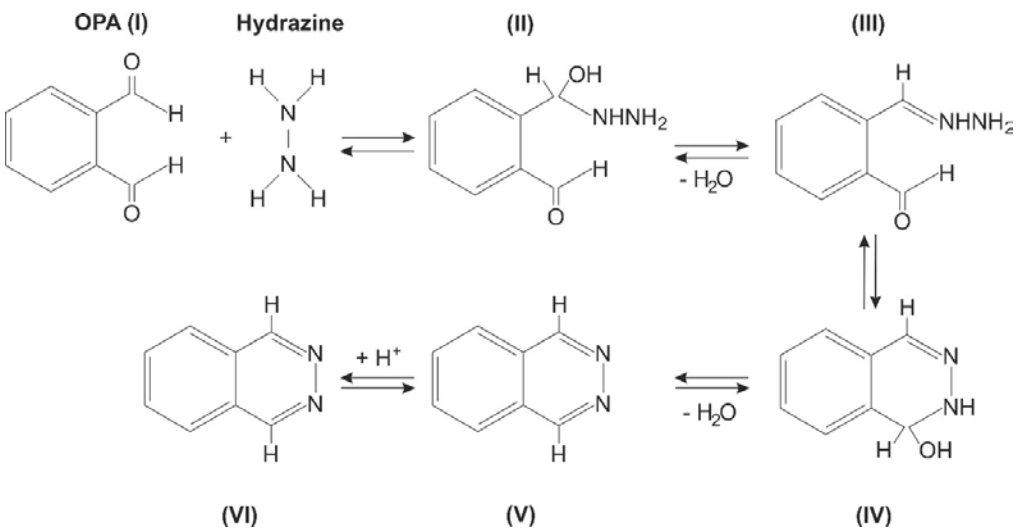
In the present study we report a fully automated method for the determination of the genotoxic impurity hydrazine in allopurinol active pharmaceutical ingredient (API) based on the concept of zone-fluidics. Hydrazine reacts on-line with o-phthalaldehyde in a unique way, that is in acidic medium (pH < 1.5) and in the absence of nucleophylic reagents, to form a highly fluorescent hydrazone (318/376 nm). The combination of a 120 s long stopped-flow step at elevated temperature (70 °C) offered adequate sensitivity (LOD = 1 μg L^{-1}) to meet the low pharmacopoeia limits for the selected application. The analyte was separated efficiently from the excess of the API by on line solid phase extraction using a Hydrophilic-Lipophilic technology sorbent that provided direct retention of the more hydrophobic API without the need of wetting/conditioning steps. Percent recoveries ranged between 94.3 and 105.9 %.



P2-45 PAPER-BASED DNA BIOSENSOR FOR VISUAL DETECTION OF MILK ADULTERATION

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Dairy products are vulnerable to adulteration with milk derived from different animal-species of lower cost and thus of lower nutritional value. Some adulterants, such as bovine milk, may contain serious allergens or other hazard ingredients. For these reasons, controls are of great demand to protect consumers from economical fraud, as well as from health risks. This project reports the development of an easy, rapid, specific and sensitive DNA-based biosensor for milk authenticity tests of dairy products. DNA was isolated form dairy products, such as milk and yogurt, purchased from local stores. The isolated DNA was subjected to Polymerase Chain Reaction (PCR) to amplify animal-specific DNA sequences. The PCR products were then detected by the DNA biosensor. The detection was accomplished by the accumulation of gold nanoparticles at the test zone of the biosensor forming a visual red spot in the presence of target DNA. A second red spot was formed at the control zone to confirm the proper function of the sensor. The biosensor was applied for the detection of bovine species in binary mixtures of cow milk in sheep's and goat's yogurt, respectively. The proposed method offered very good detectability, as we were able detect as low as 3.1 fmol of PCR product specific to the three-animal species and 0.01% content of bovine milk in binary yogurt mixtures.

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P2-46 SYNTHESIS, CHARACTERIZATION AND ANALYTICAL UTILITY OF FREE-STANDING PH RESPONSIVE POLYMER FILMS IN SENSING APPLICATIONS

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Herein, we report on the synthesis of copolymers of methacrylic acid (ME) and methylmethacrylate (MMA) with an increased amount of ester and at different molecular weights in order to investigate the critical pH at which the resulting copolymers are degraded. For this purpose, different polymerization methods were examined while the resulting copolymers were extensively studied by various morphological and physico-chemical techniques (SEM, NMR, GPC, CV, EIS and contact angle measurements). Results were compared with those of Eudragit® S100 polymer, a commercially available pH responsive copolymer of randomly distributed ME-MMA, in which the ratio of the free carboxyl groups to the ester groups is approx. 1:2. Eudragit® S100 is degraded at pH>7. Polymer solutions of different concentrations (4-15% v/w) were prepared in THF or in a blend of isopropanol/DDW (97/3 v/v), while the casting of free-standing membranes was conducted with the aid of a wet film applicator (1 to 8 mil, URAI). By using a newly devised analytical device and a new measuring principle, a comprehensive study of the kinetics of membrane degradation at various concentrations of NH_3, which was used as a model compound, was conducted. The analytical device (we call it BioPoC) includes a single microfluidic vertical channel and its operation is based on the measurement of the time required the infinite electric resistance between two, uncontacted, conductive layers to reach a finite value as a result of the selective degradation of the pH-responsive polymer membrane by the target analyte. Results indicate that the time required for membrane degradation is concentration dependent while the detection range can be tuned by the thickness of the membrane. BioPoC represents a new generation of diagnostic devices based on stimuli-responsive polymers. Appropriate combinations of enzyme(s) and responsive polymer films could extend the use of the proposed technology for the determination of a wide range of biochemical indices in biological samples.

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P2-47 MICROFLUDIC PLATFORM FOR FUNCTIONALISATION, EXTRACTION AND DETECTION OF PHOSPHORYLATED AMINO ACIDS USING FLUORESCENT SENSORY PARTICLES

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The reliable identification and quantification of phosphorylated amino acids, peptides and proteins is one of the key challenges in contemporary bioanalytical research, noteworthy, to diagnose and treat diseases at an early developmental stage [1]. Miniaturised sensing devices like microfluidic chips combined with “smart” detection chemistry, simple data assessment, processing and presentation are very attractive for benchtop use in clinical environments [2]. We developed novel synthetic probes targeting phosphorylated amino acids, based on core-shell microparticles consisting of a silica core coated with a molecularly imprinted polymer (MIP) shell, Figure 1 [3]. These “plastic antibodies” are extremely robust, resist denaturing solvents and elevated temperatures, can be reproducibly produced at low cost, and potentially overcome many of the practical problems in current bioanalytical detection strategies. The MIP layer contains a fluorescent probe monomer (Figure 2), binds selectively to phosphorylated tyrosine (pTyr) with a significant imprinting factor higher than 3.5 and responds with a “lighting-up” of its fluorescence accompanied by the development of a strongly red-shifted emission band toward the analyte. In analogy to our previous work [4], the bead-based ratiometric detection scheme has also been successfully transferred to a microfluidic chip format to demonstrate its applicability to rapid assays. Such a miniaturized device could yield an automated pTyr measurement system in the future. The setup was built by coupling a modular microfluidic system [5] for amino acid functionalisation (Fmoc protection) and, as shown in Figure 3, a multi-layer PDMS/Teflon/glass microfluidic chip [6] for buffering, extraction (micropillars co-flow extraction) and selective adsorption on the MIP core-shell particles. A miniaturized optical assembly for low-light fluorescence measurements was also developed. Based on small opto-electronic parts and optical fibres, the emission from the MIP particles upon addition of pTyr concentrations from 0.5 - 200 µM could be monitored in real-time (Figure 4).

P2-48 ADVANCED SENSORS FOR HEAVY METALS BASED ON MONOELEMENTAL 2D BISMUTHENE AND GRAPHENE NANOCOMPOSITES PRODUCED BY SHEAR-FORCE LIQUID EXFOLIATION

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Inorganic layered materials, also known as “graphene-like” inorganic analogues, have emerged as a new and versatile source of nanomaterials. Due to their thickness-dependent physical properties they have drawn an enormous scientific interest as regards their exfoliation and the potential use of the exfoliated two-dimensional crystals to attractive new applications in various industrial and technological sectors. This work reports for the first time, the use of low dimensional Bismuthene/Graphene hybrid films as electrode’s modifiers for the ultra-sensitive determination of Pb(II) and Cd(II) ions in the sub microgram-per-liter level by using anodic stripping voltammetry. Bulk Bismuth was exfoliated by a shear-force liquid phase exfoliation method, at 5 °C, in the presence of 5 mg/mL of sodium cholate that plays a dual role as both a solution medium for the exfoliation process and a stabilizer to prevent the restacking of the exfoliated layers. The effect of the rotation speed on the morphology and electrocatalytic properties of each particular material was investigated with Raman spectroscopy, scanning electron microscopy and various electrochemical techniques. Compared with bulk Bi/Graphene hybrid film-modified glassy carbon electrodes (GCEs), exfoliated Bismuthene/Graphene hybrid film-modified GCEs exhibited remarkably enhanced detection capabilities and limits of detection at the sub microgram-per-liter level. This work provides for the first time data on the facile preparation of 2D monoelemental bismuthene, which can be easily cast into films offering highly sensitive sensors. In addition, it triggers the development of advanced sensors based on other pnictogens.

P2-49 qNMR AS A POWERFUL TOOL FOR PROVIDING PURITY ASSESSMENT AND METROLOGICAL TRACEABILITY

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Since most analytical quantitative techniques are compound-dependent, the reliable quantification of organic substances constitutes a very challenging task. For example, purity determination by liquid chromatography combined with UV, DAD or fluorescence detectors always requires a traceable reference of the compound. However, for many organic compounds, certified reference materials are not yet available. Therefore, the mass fraction of an organic compound is usually determined by measuring all potential impurities (such as structure related organic compounds, water, residual volatile compounds and inorganic impurities) and calculating the purity by subtracting the sum of the impurity values from a total of 100%. This technique, called the mass-balance approach, implies that all potential impurities could be resolved and measured by a chromatographic method, assuming that the impurities produce the same detector response as the target analyte, which is often not the case. An alternative to this time-consuming process is using a primary method, such as NMR. By taking advantage of NMR's capability to provide structural information and of its direct proportional relationship between resonance intensity and number of nuclei, the qNMR technique was used to provide results that are traceable to the International System of Units (SI) via appropriately certified internal standards. In our contribution, a series of application of ^{1}H qNMR on a variety of organic molecules, is described. The parameters of the NMR experiment are described, the purity assessments for ethanol, pyributicarb, zearalenone and benzo[a]pyrene by ^{1}H qNMR are provided and the elaboration of the respective uncertainty budgets are presented. Our data indicate that the qNMR method can be used to perform accurate, simple, and rapid analysis of target analyte content that is traceable to the SI.

P2-50 NOVEL 1H NMR METHOD FOR THE DETERMINATION OF ANTHOCYANINS IN FRUIT EXTRACTS

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Anthocyanins are one of the most important group of pigments in the plant kingdom and are responsible for diverse pigmentation in flowers, fruits and vegetables. Furthermore, anthocyanins play important role for human health as they are correlated with antioxidant and anti-cancer effects. They are hydroxylated and methoxylated derivatives of phenyl-2-benzopyrylium or flavylium salts. Their basic structure of the aglycone form is a C6-C3-C6 carbon skeleton, whereas they mostly found glycosylated derivatives in nature. The determination of anthocyanins is usually performed with the coupling of separation technique as liquid chromatography with UV-Vis spectroscopy or mass spectrometry. In the present study, we describe a novel and rapid determination of anthocyanins in crude plant fruit extracts without any previous separation step. ^{1}H-NMR spectra showed that the resonance of H-4 can be used to discriminate anthocyanins in fruit extracts as it appears at 8.2-8.6 ppm, a non-overcrowded region of spectra. Results also indicated that the resonance of H-4 is depended on the substitution of anthocyanin skeleton and the discrimination of anthocyanins in a complex mixture is feasible. In a next step, the effect of pH on the chemical shift of H-4 was investigated as the anthocyanins are involved in a series of pH-dependent equilibria giving rise to different chemical species due to their ionic nature. Results demonstrated that pH values influences the chemical shift as well as the resolution of highlighting the need to pH adjustment of the sample at pH=3.0. Cyanidin-3-*O*-rutinoside, cyanidin-3-*O*-glucoside, peonidin-3-*O*-rutinoside, and pelargonidin-3-*O*-rutinoside were found in samples. A drift in chemical shifts of H-4 resonance was observed due to the copigmentation of anthocyanins with other organic compounds or metallic ions. This difficulty was overtaken with spiking. Overall, the present method exploits the diagnostic peak of H-4 for the determination of anthocyanins in fruit samples without any previous separation step.

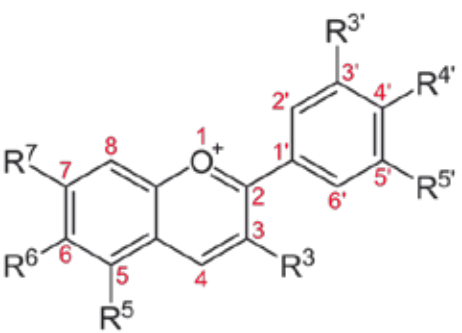

Figure 1. Basic structure of anthocyanins.

P2-51 RAPID AND SENSITIVE NMR AND MOLECULAR DYNAMICS MAPPING OF SELECTIVE BINDING SITES OF FATTY ACIDS WITH ALBUMIN

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An NMR approach based on saturation transfer difference (STD) and Tr-NOESY techniques is reported, for the first time, for mapping interactions and specific binding sites of fatty acids with non-labelled bovine serum albumin (BSA) through competition experiments with drugs of known binding sites. The analytical method was applied to caproleic acid, oleic acid (Fig. 1A), linolenic acid, linoleic acid, linoleic acid methyl ester, cis-9, trans-11 CLA. From the analysis of the experimental data it appears that only free fatty acids but not the methyl esters interact with the BSA protein. The experimental NMR data were used as constraints in molecular dynamic simulations (Fig. 1B). This combined methodology may find promising applications in the field of lipid research.

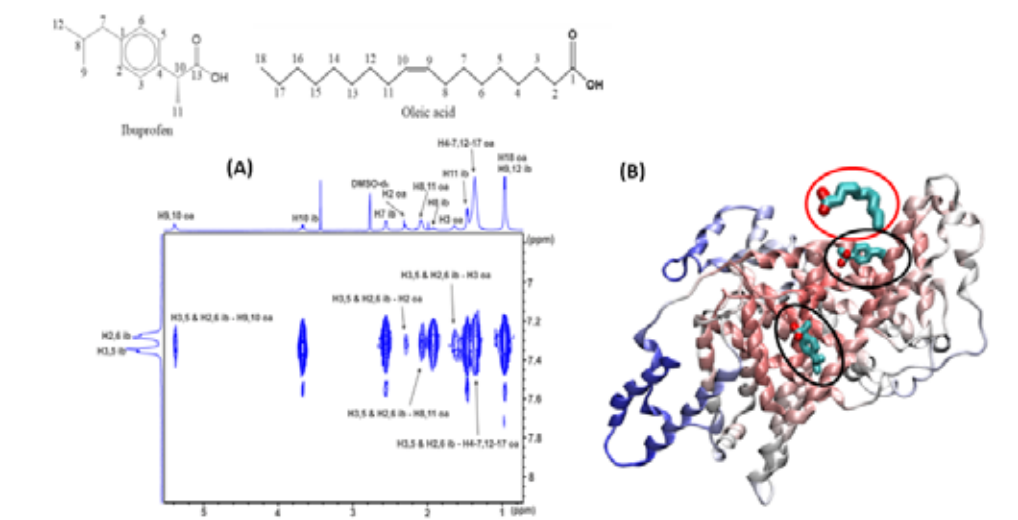

Figure 1. (A) Tr-NOESY NMR spectrum of oleic acid and ibuprofen (molar ratio 1:1.1) with BSA protein in PBS buffer in D_2O with 10% DMSO-d_6 (T = 310K, number of scans = 56, experimental time = 4h 20min). **(B)** Human Serum Albumin (cartoon representation) in complex with Ibuprofen. (PDB code: 2BXG). Deprotonated caproleic acid (up in red ellipse-representation licorice) replaced the ibuprofen molecules (two molecules in black ellipse -representation licorice) adopting constraints dictated by NMR experiments. The resulting structure was the initial input for fully atomistic MD simulations.

Acknowledgments

E. Alexandri acknowledges financial support from the Greek State Scholarships Foundation (MIS5000432).

P2-52 FLUORESCENCE SPECTROSCOPY - AN EFFECTIVE TOOL FOR CHARACTERIZATION OF GOLD NANOPARTICLES-PROTEINS CONJUGATES - THE COMPONENTS OF BIOANALYTICAL SYSTEMS

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Gold nanoparticles (GNPs) modified with biomolecules are extensively used in various modern bioanalytical systems as detection agents. Their practical demand is due both to the optical properties of the carrier particle, modulated by localized surface plasmon resonance processes, and to the possibility of the carrier being functionalized by antibodies or other receptor molecules to effectively detect the target analyte. In this regard, the issues of assessing the composition and functional activity of nanoparticles - biomolecule composites are extremely important. We have studied the composition of the conjugates of GNPs and of two proteins (immunoglobulins G and serum albumin), which are most often used for bioanalytical purposes. GNPs were synthesized by the Turkevich - French method. The diameters of GNPs obtained under different conditions ranged from 20 to 50 nm (according to transmission electron microscopy). The aggregation of proteins was controlled by the flow field fraction method. To estimate the protein/GNP ratio, we used the method based on fluorescence spectroscopy. The composition of the obtained conjugates was compared depending on the concentration of the protein during the synthesis and the pH of the immobilization medium. Immunoglobulin G is efficiently sorbed on the GNPs over the pH range from 4 to 10, whereas the effective binding of serum albumin of low protein concentrations is observed only in acidic (pH <7) medium. The conditions, leading to the production of either monolayer or multilayer products, are established. Based on the data obtained, a new model of protein shell formation around GNPs has been proposed and conditions for obtaining conjugates with maximal binding capacity in immunochromatography were determined.

This study was financially supported by the Ministry of Science and Higher Education of the Russian Federation (grant agreement No. 14.613.21.0080 on 22.11.2017, unique identifier RFMEFI61317X0080).

P2-53 PHOTOCHEMICAL REDUCTION OF SILVER HALIDES FOR THE COLORIMETRIC DETERMINATION OF BIOTHIOLS WITH CONSUMER ELECTRONIC IMAGING DEVICES AS DETECTORS

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This work describes a novel approach for the determination of free biothiols in biological fluids based on silver-halide formation and analytical detection with broadly-available imaging devices (i.e. flatbed scanners). The method is based on the ability of biothiols to bind to silver ions and dissociate the silver halide crystals thus changing the photosensitivity of silver halide crystal suspensions. Quantification of biothiols is accomplished using a flatbed scanner operating in transmittance mode by measuring the light intensity transmitted through the silver halide suspension while physiologically relevant biothiol levels can be inspected by the unattended eye by monitoring the colorimetric transitions of the silver halide suspension. The applicability of this low-cost method is demonstrated in the determination of biothiols in biological samples, such as urine and blood plasma, with satisfactory analytical features in terms of sensitivity, selectivity and reproducibility. The developed assay was successfully applied to the determination of free biothiols in urine and blood plasma samples with detection limits less than 10 μM, satisfactory recoveries (92-97%), good reproducibility (6.7-8.8%) and exceptional selectivity against other major components of biological fluids.

P2-54 HYPER-SPECTRAL RAMAN MAPPING OF MODERN HUMAN ENAMEL AND DENTIN

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Raman spectroscopic techniques are widely used to study the local molecular structure and its defects of modern human and animal bones and teeth, as well as fossil and archaeological hard tissues. Phosphate biominerals of human tooth enamel and dentin consist mainly of $Ca_{10}(PO4)_6(OH)_{10}$ hydroxyapatite and are characterized by complex variable microstructure, morphology and chemical composition. Here, Raman spectroscopy registers the molecular and ionic vibrations of mineral compounds, such as phosphate, carbonate, and hydro-phosphate ions, as well as numerous vibrations from the proteinaceous matrix. The morphology, chemical composition and structure of enamel and dentine are the main factors determining tooth resistance to carious and non-carious lesions. The aim of the work is to perform the hyper-spectral Raman mapping of human dental hard tissues revealing the local structural differences between sound teeth and the teeth affected with dental diseases (Stainton-Capdepont syndrome, hypoplasia, erosion). Raman mapping is performed using Horiba Jobin Yvon LabRam-HR Evolution based on a confocal Raman microscope, using 632.8 nm He-Ne excitation, an Olympus 100× objective (NA = 0.9, focus size ≈1 μm diameter) with power on sample of about 2 mW. Spectra are obtained using a 600 grooves/mm grating providing the lateral resolution better than 2 μm. The spectrometer calibration was guided along the Rayleigh line and the emission lines of a neon lamp. The results obtained substantiate the structural variations in intact and affected teeth as the degree of bioapatite disorder. The changes observed in the degree of mineralization and their manifestation through the full width at half maximum and peak position of P-O stretching vibration at ~960 cm^{-1} and C-H stretching vibration at ~2940 cm^{-1} are the sensitive probes of the local structural environment.

The work was carried out at the Geoanalyst Center for Collective Use and funded by RFBR grant No. 18-35-00462.

P2-55 ANALYTICAL AND STRUCTURAL STUDIES OF LIPIDS AND RELATED COMPOUNDS WITH THE USE OF NMR AND DFT CALCULATIONS

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High resolution NMR spectroscopic techniques including ^{1}H, ^{13}C and ^{31}P NMR have been successfully employed as a structural and analytical tool for unsaturated fatty acids [1]. In the present work a selective 1D TOCSY [2,3] has been established as a reliable method for the positional isomerism in monounsaturated fatty acids (18:1) which is based on the quantification of 1D TOCSY integrals of diagnostic resonances, upon selective excitation of the composite olefinic protons. The relative TOCSY integrals of α-CH_2/CH_3, β-CH_2/CH_3, CH_2=CH-C$\underline{H}_2$/α-CH_3 and CH_2=CH-C$\underline{H}_2$/CH_3 protons were found to be: (i) practically insensitive to the exact setting of the pulse repetition time for values of 2.7 to 5.6 x T_1 of the longest relaxation times which are due to CH_3 terminal groups; (ii) practically insensitive to the *cis/trans* geometric isomerization and (iii) strongly dependent on the position of the double bond. Selective 1D TOCSY, therefore, can serve as a rapid and reliable analytical and structural approach for the profiling of unsaturated C=C positional isomerism. In this work, also, structural determination of model compounds of free fatty acids in $CHCl_3$ was performed with DFT calculations based on ^{1}H chemical shifts and compared to X-ray crystallographic data. The values of the chemical shifts of the structures based on X-ray crystallographic data diverge from experimental chemical shifts significantly. It can be concluded that the DFT method that was used can provide accurate structural determination of the above compounds in solution which is more precise than that obtained by the use of single crystal X-ray crystallography.

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P2-56 OPTICAL SCREENING OF BIOTHIOL LEVELS BASED ON ABSORBANCE QUENCHING OF GOLD- COATED SURFACTANT MICELLAR ASSEMBLIES

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This work describes a method for the optical screening of total free biothiol levels in biological fluids. The method is based on the strong affinity of biothiols for gold ions which are coated on cationic surfactant micelles through electrostatic interactions. The electrostatic attraction of gold ions on the hydrophilic surface of cationic micelles produces an intense absorbance peak at 380 nm which is quenched in the presence of biothiols such as cysteine, glutathione and homocysteine because biothiols complex gold ions and release them from the surface of the micelles. This phenomenon causes a linear decrease in the absorbance of the solutions at 380 nm in the concentration range from 10-100 μg L^{-1} enabling the determination of biothiols at concentrations lower than 10 μg L^{-1} with good reproducibility (RSD=5%, n=5). The method was initially benchmarked to the determination of biothiols in artificial urine and blood plasma samples with satisfactory recoveries (i.e. >90% in urine and >85% in plasma).

P2-57 THERMAL ANALYSIS STUDY OF g-C3N4 PREPARATION USING Al, Al2O3 , Pt/Rh COVERED AND UNCOVERED CRUCIBLES

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The most attractive method for preparation of g-C_3N_4 has been the thermal condensation of nitrogen-rich precursors, such as urea, melamine, cyanamide, thiourea, trithiocyanucic acid, etc., because of the simplicity and use of cheap and readily available precursors. The polymeric material g-C_3N_4 was prepared by thermal condensation process using urea as precursor compound. X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier-transformed infrared spectroscopy (FT-IR) techniques were used for the physicochemical characterization of g-C_3N_4 powder. The results confirmed the successful synthesis of g-C_3N_4 at the temperature range examined bearing mesoporous and packed layered structure. Thermogravimetry (TGA) and differential scanning calorimetry (DSC) analyses were performed to examine the effect of the crucible used for g-C_3N_4 synthesis. TGA was performed with a heating rate of 10°C/min from 25 to 800°C. The covered and uncovered crucibles used were: Al, Al_2O_3 and Pt/Rh. Thermal analysis revealed the transformation of the precursor material to g-C_3N_4 through several steps. From the thermal analysis results it can be concluded that Al crucibles are the most effective for both polymerization step and the produced quantity of g-C_3N_4.

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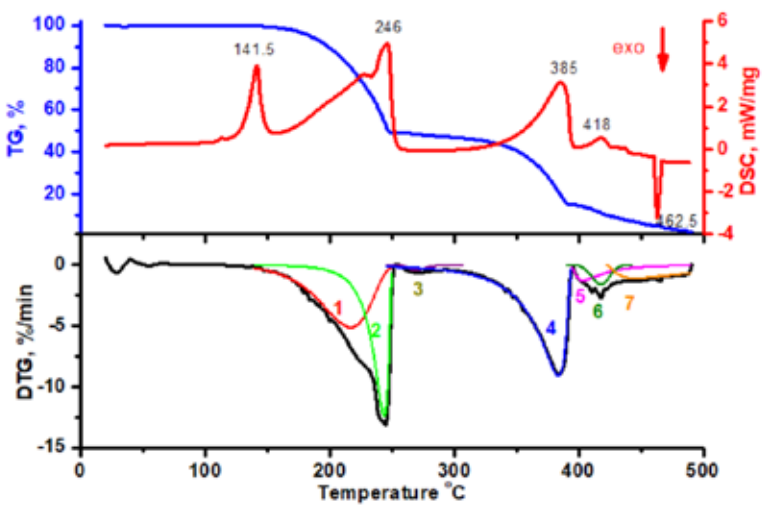

Diagram 1: Thermal Analysis curves of urea thermal treatment in Al open crucible.

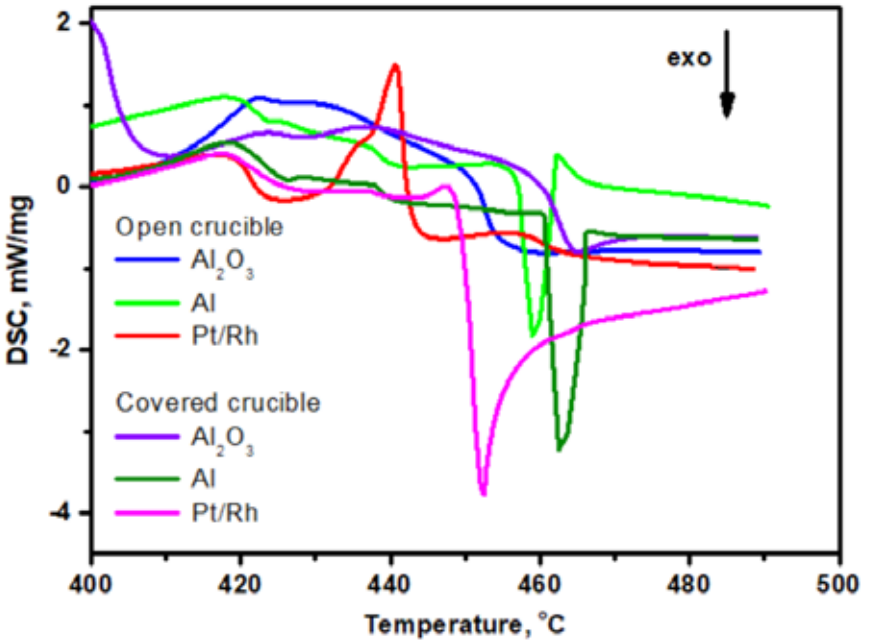

Diagram 2: DSC curves, at selected temperature ranges, in covered and uncovered Al_2O_3, Al and Pt/Rh crucibles.

P2-58 INVESTIGATIONS OF BIOMATERIALS WITH VIDEO PARTICLE TRACKING MICRORHEOLOGY

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Microrheological techniques have been developed to investigate rheological properties of soft materials with spatial sensitivity at the micro and nano scales [1]. Special examples include, the mapping of the mechanical properties inside live cells [2], the trapping ability of human respiratory mucus [3] and the correlation of cells and extracellular matrix mechanics with the grade and stage of tumors[4]. Microrheology methods investigate the motion of probe particles inside biomaterials and with the advantages of very small sample amounts, local measurements and extended time (or frequency) range. We report on the analysis of Xanthan Gum solutions [5] that are important in modern food science as viscosity modifiers and bioactive substance carriers. We probe the self-similar nature of Xanthan viscoelasticity and fully characterize its behaviour at different salts either in the native or in the renatured state. Based on this treatment we apply our methodology on complexes of Xanthan with the cationic surfactant dodecyltrimethylammonium bromide (DTMAB) [6] and DNA solutions. We apply Cox-Merz rule to relate the linear viscoelasticity to the shear-thinning behaviour [7]. In this work we demonstrate how video particle tracking microrheology probes the local rheology and is a technique that complements bulk rheology and expands our understanding in multi-length scale biomaterials.

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P2-59 APPLICATION OF THE QUECHERS TECHNIQUE FOR THE PRE-CONCENTRATION OF MALATHION PESTICIDES IN FRUIT SAMPLES

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Malathion is an organophosphate pesticide that is an irreversible inhibitor of the enzyme cholinesterase and is widely used in agriculture to control pests in fruits. In areas close to farms applying it, it ends up in water bodies that can be used as drinking water sources. In this work, the concentrations of malathion in fruits were determined using UV-Vis spectrophotometry prior to pre-concentration using QuEChERS. The Z-sep$^+$/PSA sorbent combination was used for the d-SPE clean-up, and extraction was done using acetonitrile during QuEChERS. The extracted malathion was then hydrolysed under basic conditions followed by the reaction with potassium bromate. This reaction caused the development of an orange-yellow colour, thereby making the mixture UV-active. The absorbance of the mixture was then measured using a UV-Vis spectrophotometer at a wavelength of 415 nm. The QuEChERS parameters, which included type and volume of extraction solvent, type and mass of sorbents, and centrifugation rate, were optimised prior to application of the developed method to real fruit samples. The linear range was from 0.1 to 0.9 mg kg^{-1} while the coefficient of determination (R^2) was 0.9999. The limit of detection (LOD) for malathion was found to be 0.017 mg kg^{-1} and the limit of quantification was 0.05 mg kg^{-1}. The orange samples were found with no malathion residues when the developed method was applied to them while the concentrations of malathion in apple and pear samples were 0.07 mg kg^{-1} and 0.09 mg kg^{-1} respectively.

P2-60 MONITORING OF ANTIBIOTICS IN THE PYRENEAN RIVER WATERS USING SOLID-PHASE EXTRACTION UPLC-MS/MS

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The discovery of antibiotics is considered one of the greatest scientific and medical achievements of the 20th century. However, these special drugs have been increasingly threatened by the emergence, dissemination, and persistence of antibiotic resistance, which is worsened by excessive and inappropriate use of antibiotics on humans and animals and their subsequent occurrence into the environment. The identification, characterization and monitoring of these compounds in the environment are crucial to assess their dynamics and potential toxicological effects on ecosystems [1]. The study area, the POCTEFA territory covering the Spanish Communities of Aragon, Catalonia, Basque Country and Navarre, and the French regions of New Aquitaine and Occitania is characterized by intense animal farming; livestock farms are its main rural economic engine. For example, out of 41.5M of pigs registered in Spain and France, 38% are in the POCTEFA territory. They are the largest emitters of veterinary antibiotics to the environment and the main responsible for the indirect exposures, due to their presence in meat and their direct emission to freshwaters. The analytical method developed to control these emerging pollutants consists of solid-phase extraction preconcentration of antibiotics followed by their separation by Ultra Performance Liquid Chromatography (UPLC) and tandem MS detection using a QExactive hybrid quadrupole-Orbitrap mass spectrometer. The species of interest can be followed within 25 mins of a chromatographic run. The detection limits achieved for most of the species are in the range of 5-100 ng/l. The presentation reports results obtained for compounds representing different categories of antibiotics observed in the POCTEFA area. The most abundant species found were fluoroquinolones present in 70% of sampling points studied.

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Acknowledgements

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P2-61 ASSESSMENT OF EXPOSURE TO ENDOCRINE DISRUPTING COMPOUNDS USING GAS CHROMATOGRAPHIC-MASS SPECTROMETRIC ANALYSIS OF COMPOSITE FOOD SAMPLES IN A TOTAL DIET STUDY

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A significant number of pesticides that are widely used in agriculture function as endocrine disrupting chemicals (EDCs). Humans can be exposed to ECDS via the food consumption with adverse health effects. There is a growing concern that maternal, fetal and childhood exposure to EDCs could play a larger role in the causation of many endocrine diseases and disorders than previously believed. There is a need for quick and reliable analytical methodologies for the large scale determination of pesticides in complex food matrices that could work as an effective tool for food controls as well as for performing dietary risk assessments. The present study combines the dispersive solid phase extraction methodology and GC-MS for the determination of 104 pesticides and metabolites with endocrine disrupting activity, in composite samples based on model Mediterranean diet. The prepared composite sample contained 51% fruits and vegetable, 15% dairy products 7% meat and fish, 23% dry commodities and 4% olive oil and olives. For the extraction and cleanup, liquid partitioning with acetronitrile combined with matrix dispersion using sorbents (PSA, C18, carbon black) was applied. The recoveries ranged from 70 to 119% for the 89% of the analytes at three concentration levels (between 30 and 1000 μgkg^{-1}). RSD and Intra-Day RSD were below 20% for more than 98% of the analytes. The GC-MS method provided good linearity ($R^2 > 0.996$) for the 90% of the compounds. Linearity was studied using triplicate matrix-matched standards at five concentrations (10-500 $\mu g\ L^{-1}$). More than 80% of the studied pesticides presented soft matrix effects (Δ±20%). The LODs were < $2\mu gkg^{-1}$(S/N=3) for more than 92% of the analytes. LOQs (S/N=10) were below 10 μgKg^{-1}. The method was applied to one year food monitoring program in Western Greece. Over 1200 samples of raw food were collected composing a sum 39 composite total diet samples. The results of the monitoring program were used for the assessment of consumers' risk due to the exposure to pesticide residues via the Mediterranean diet. The dietary risk was estimated at chronic level using the determined pesticide residue levels and the mean consumption data of the Mediterranean Diet in Greece (1721g day-1). The National Theoretical Maximum Dietary Intake (NTMDI) and the National Estimated Dietary Intake (NEDI) were calculated for each detected analyte and were compared with the corresponding acceptable daily intake (ADI) levels. The NEDI was found below the ADI in all cases .The Cumulative risk was determined for the samples with two or more detected ECDs applying the Hazard Index (HI) and Cumulative Risk Index (CRI) models. HI was less than one and CRI was more than one for all cases indicating acceptable risk.

WEDNESDAY, SEPTEMBER 25TH, 2019

EVERGETON HALL

Chromatography 2 / Spectrometry 2

Chair: ***E. Rosenberg, A. Pappa, M. Krokida***

IL08 APPLICATION OF BIOMIMETIC HPLC PROPERTIES FOR THE ESTIMATION OF BRAIN TO BLOOD DISTRIBUTION OF DRUG DISCOVERY COMPOUNDS INCLUDING NEW MODALITIES

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The biomimetic binding characteristics of drug discovery compounds can be measured using chemically bonded protein and phospholipid stationary phases in HPLC. The methodology has been reviewed [1] and applied in drug discovery [2]. The derived albumin, glycoprotein and phospholipid binding data can be used in mathematical models to estimate *in vivo*distribution of compounds. It has been demonstrated that the methodology can be applied not only for small synthetic drug discovery compounds but also for compounds with molecular weight larger than 500, such as peptides and macrocycles [3].

A good model has been found for estimating the brain tissue binding of over 100 drug discovery compounds for which the brain tissue binding was measured using equilibrium dialysis method. Similarly, good model has been found for the estimation of the total plasma protein binding of compounds using the biomimetic HPLC binding data. Based on these two models the brain to plasma distribution ratio can be calculated that has been shown to provide a good differentiation between brain penetrant and non-penetrant compounds.

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OP51 BIOMIMETIC CHROMATOGRAPHY: CONDITIONS, ELUTION MECHANISMS AND APPLICATIONS IN EARLY DRUG DISCOVERY

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High Performance Liquid Chromatography (HPLC) is a powerful analytical technique based on the differentiation in the elution of different compounds through a chromatographic column by the flow of a mobile phase. Thus, 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. As several pharmacokinetic properties involve a dynamic distribution of drugs between general circulation and tissues, HPLC can be used to predict pharmacokinetic properties, provided that stationary phases contain a biologically relevant agent. Progress in HPLC column technology succeeded in immobilizing phospholipids and different types of proteins (e.g. Human Serum Albumin (HSA) or alpha1- acid glycoprotein (AGP)) on a silica gel skeleton to produce immobilized artificial membrane (IAM) chromatography and protein-based stationary phases, respectively. Another type of biochromatography is Biopartitioning Micellar Chromatography (BMC), employed by the use of a traditional hydrophobic stationary phase (e.g. C-18) and aqueous mobile phases in presence of a surfactant above its critical micellar concentration.

This presentation is devoted to the use of biomimetic chromatography under appropriate conditions, the underlying retention mechanisms and applications to the early drug discovery. For this purpose, a large data set of over than 90 structurally- diverse drugs was investigated using IAM, HSA, AGP and BMC. Retention factors were compared with octanol- water partition and distribution coefficients, while the role of electrostatic interactions was explored. Interrelation of retention factors obtained on the different stationary phases was also performed. Finally, representative applications of the obtained biomimetic chromatographic indices to estimate representative pharmacokinetic properties are presented. Among others, models for the prediction of Human Oral Absorption (%HOA), Plasma Protein Binding (% PPB) and Blood- Brain Barrier penetration were constructed. Additional molecular descriptors were tested in the models in order to improve their predictive performance.

OP52 IN-CELL NMR SPECTROSCOPY APPLIED IN THE STUDY OF LIGAND-PROTEIN INTERACTIONS IN LIVING CANCER CELLS

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In-cell NMR spectroscopy is a noninvasive analytical technique, which reveals structural and conformational information for the study of protein-protein and ligand-protein interactions directly in the intracellular environment of living cells, at the atomic level, under physiological conditions [1,2]. This methodology has been successfully applied in the analysis of ^{15}N isotope-labeled proteins, overexpressed in *E. coli*, where ^{1}H-^{15}N HSQC in-cell NMR is performed directly in intact cells. However, current methodologies are inadequate at charting intracellular interactions of nonlabeled proteins [3].

Herein, we describe for the first time the application of in-cell NMR analytical methodology in the monitoring of the interaction of a bioconjugate of quercetin with the antiapoptotic protein Bcl-2 inside living human cancer cells without requiring prior isotopic labeling of the target protein. STD and Tr-NOESY NMR were employed to evaluate the direct binding of the ligand to the nonlabeled Bcl-2 protein intracellularly, which was further validated *in vitro* [4]. All the aromatic protons of the ligand were found to interact with receptors intracellularly, whereas competition experiments with a selective inhibitor of Bcl-2 clearly indicated the direct binding of the bioconjugate to the BH3 domain of the protein. Tr-NOESY in-cell NMR was recorded to investigate the preferred conformation of bound quercetin-alanine. Two new Tr-NOE crosspeaks of the ligand inside the intact cells were detected, suggesting the adaption of a new conformation of the bioconjugate upon binding. This approach has proved a very promising strategy for the real-time screening of the interaction profiling of drugs with their therapeutic targets in their native cellular environment in living eukaryotic cells, paving the way to the new field of intracellular rational drug design [4].

Acknowledgments

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OP53 THE USE OF BIOPARTITIONING MICELLAR CHROMATOGRAPHY TO PREDICT ECOTOXICITY OF PESTICIDES IN AQUATIC ENVIRONMENT

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Agricultural development has led a parallel growth in the use of chemical agents for plague controls, which are known as pesticides. These compounds are released into the environment dispersing in various environmental media and provoking serious health problems. Therefore, there is a need of evaluating the potential hazard of pesticides for risk assessment. Aquatic toxicity tests are current methods applied by the European community for ecotoxicity estimation. The experimental determinations are difficult, time-consuming, and expensive. Chromatography poses a powerful technique for the measurement of physicochemical parameters of organic compounds. Chromatographic retention has proven to be a good surrogate to logP measurements due to the higher accuracy and easier experimental performance. Opposite to conventional RPLC systems, micelles have proven to be more adequate chemical models for biomembranes, due to their amphiphilic properties. Biopartitioning micellar chromatography (BMC) is a liquid chromatographic system that uses surfactant solutions above the critical micelle concentration as micellar mobile phases and C18 reversed stationary phases. BMC retention has been used to describe several biological activities and ecotoxic parameters. In the present work, the potential of BMC to predict ecotoxicity of pesticides in aquatic organisms is studied. For this reason, the retention of 39 pesticides is determined by BMC. Polyoxyethylene(23) lauryl ether (Brij35), sodium dodecyl sulfate (SDS) and cetrimonium bromide (CTAB) are used as different surfactants on a Discovery RP-18 column. In all cases, extrapolated to pure aqueous phase retention factors ($\log k_w$) are determined. The results are then combined by statistical software with ecotoxicity data for aquatic organisms obtained from the literature (US EPA) in order to establish relationships. Furthermore, additional physicochemical parameters affecting modeling are tested. The predictive performance of BMC with the use of every surfactant is then compared with each other, as well as with the one of octanol-water partitioning.

OP54 INTERPRETING TOF-SIMS DATA: A HOLISTIC APPROACH

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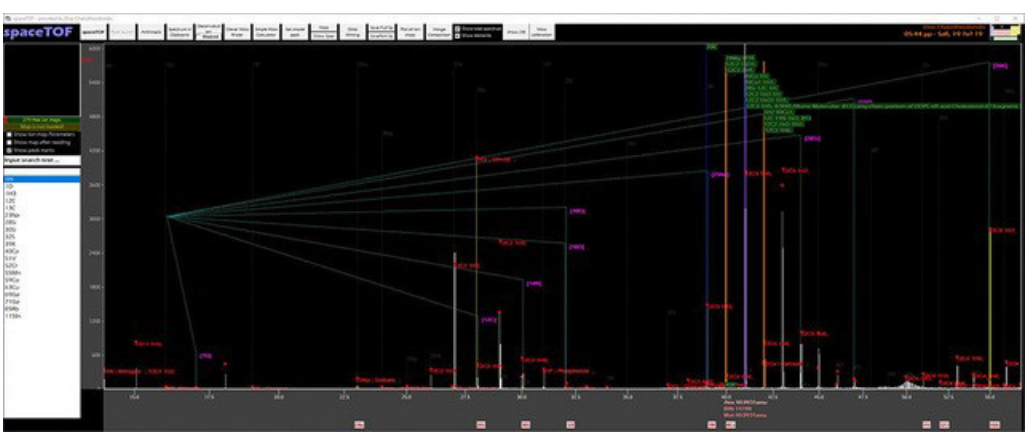
TOF-SIMS spectra are especially complicated because they generally have a very large number of peaks, with many mass interferences. Although high mass resolving power assists in deconvolving overlapping peaks, it also increases their number significantly. Even when a good mass calibration is applied, still many peaks remain unidentified. Here, we will demonstrate a holistic approach to interpret TOF-SIMS mass spectra. Our spectra have been acquired with tow high mass resolving power TOF-SIMS instruments of the University of Manchester. We acquired arrays of spectra in beam scanning mode from a number of reference samples, and natural terrestrial and extraterrestrial samples (i.e., meteorites). The focus of this work is, firstly, on demonstrating that a single mass calibration is not enough to easily identify all peaks with ease, but rather, two mass calibrations are required, one for the atomic and one for the molecular ionic species. Secondly, we will demonstrate that interpretation is more straightforward when molecular ions are grouped according to their molecular species (i.e., hydrocarbons), extracted and plotted by peak intensity or area; then, systematic patterns are revealed that could be used as chemical signatures to identify different molecular species with their ionic fragments. Processing of all spectra is done with “spaceTOF”, a software developed in-house (see image for a screenshot). We use this technique in the search for biosignatures of fossilised life in terrestrial and extraterrestrial samples. This is an actual topic in the search for extraterrestrial life and the discipline of astrobiology.



WEDNESDAY, SEPTEMBER 25TH, 2019

EVERGETON HALL

Electrochemistry / Archaeometry

Chair: ***M. Karayannis, K. Ochsenkühn, F. Tsopelas***

IL09 POSSIBILITIES AND LIMITATIONS OF ELECTROANALYTICAL CHEMISTRY 60 YEARS AFTER NOBEL PRIZE FOR POLAROGRAPHY

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The aim of this contribution is to show practical applications of modern voltammetric and amperometric techniques for monitoring of submicromolar concentrations of electrochemically active organic compounds (environmental pollutants, food components and pollutants, biomarkers of exposure, treatment or illness, etc.). It will be demonstrated that by using novel electrode materials either bare (solid amalgams, bismuth, antimony, various forms of carbon films or pastes, carbon nanoparticles, boron doped diamond etc.) or chemically (e.g. molecularly imprinted polymers), enzymatically, or DNA modified, modern voltammetric/amperometric methods can offer faster, cheaper and sufficiently selective and sensitive alternative to fascinating possibilities of modern spectrometric and separation methods. And in a way to renew old glory of polarographic methods presenting great progress in the time of Jaroslav Heyrovsky. Attention will be paid to combination of electrochemical methods with preliminary separation using solid phase extraction or thin layer chromatography, hollow fibre microextraction, membrane separation etc., with measurements in flowing systems (flow injection analysis or HPLC with electrochemical detection) and to new arrangements increasing attractiveness of modern electroanalytical methods to practical laboratories, point of care analysis, on site (field) analysis, large scale monitoring of biologically active organic compounds, etc. It will be demonstrated that even now, 60 years after Nobel Prize for polarographic method of analysis, the basic underlying ideas and the approach to solving analytical problems is worth of following. This will be demonstrated on recently developed voltammetric/amperometric methods in our UNESCO Laboratory of environmental electrochemistry. The activities of Task Force Electroanalytical Chemistry established by Division of Analytical Chemistry of European Chemical Society will be mentioned as well.

Acknowledgement

This research was supported by the Czech Science Foundation (GACR project No. 17-03868S).

OP55 GOLD-SPUTTERED SENSOR FOR THE VOLTAMMETRIC DETERMINATION OF TRACE ARSENIC

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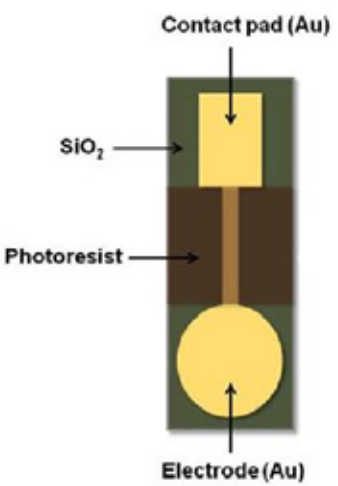
It is generally acknowledged that Au is one of the best electrode materials for the detection of As(III) after preconcentration and stripping voltammetry. Solid Au or electroplated thin-film Au electrodes have been traditionally used for this purpose [1-3]. This work describes a novel microfabricated Au electrochemical sensor that addresses the limitations of existing conventional Au electrodes, is semi-disposable and offers scope for mass-production. The fabrication approach combines sputtering of a 100 nm-thick Au film on an oxidized silicon wafer with photolithography for the definition of sensor geometry (Figure 1).

The sensor was optimized for the detection of As(III) at trace levels. The preconcentration time, the preconcentration potential, the composition of supporting electrolyte and the stripping waveform were studied. Total arsenic was determined by reduction of As(V) to As(III) using $NaBH_4$. The interference study revealed that Cu(II) produces a stripping peak that overlaps with the arsenic peak and various approaches were assessed to alleviate this interference.

The sensor exhibited linear calibration plots in the studied concentration range (2-150 μg L^{-1} of As(III)) with good linearity (R^2> 0.99) while a sub-μg L^{-1} limit of detection for As(III) was obtained for 240 s of preconcentration. The response was stable for more than 100 preconcentation/stripping cycles allowing operation in the semi-disposable mode.



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OP56 87Sr/86Sr ISOTOPE RATIO DETERMINATION BY MC-ICP-MS USING THE SSB TECHNIQUE FOR ARCHAEOMETRIC PROVENANCE STUDIES

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Measuring the natural abundance of isotopes and variations in their ratios in the archaeological hard tissues (such as bones and teeth) can provide important information about the evolution and migration of humans and animals and their origin. Strontium isotopes are among the most effective for characterizing the prehistoric mobility of humans and animals.

$^{87}Sr/^{86}Sr$ isotopic ratio incorporates into the surrounding biosphere from underlying bedrocks and is practically not fractionated by biological organisms. Since Sr can replace Ca in the hydroxyapatite crystal lattice of bones and teeth, $^{87}Sr/^{86}Sr$ ratio can be directly attributed to the isotopic ratio of the geochemical province where humans and animals reside.

The work presents the method of $^{87}Sr/^{86}Sr$ isotope ratio analysis in biogenic apatite by multicollector (MC) ICP-MS using the standard-sample bracketing (SSB) technique with preliminary chromatographic separation of Sr.

All works were performed in cleanrooms (ISO 6, 7) of the Zavaritsky Institute of Geology and Geochemistry, UB RAS. A highly selective strontium-specific Triskem SR resin was used for Sr chromatographic separation. Sr isotopic composition measurements were performed by the SSB technique using a NIST SRM 987 by MC ICP-MS Neptune Plus (Thermo Fischer, Germany). The analysis of Bone Meal SRM 1486 and Bone Ash SRM 1400 standard reference materials was carried out, and the expanded uncertainty was calculated. For NIST Bone Ash 1400, $^{87}Sr/^{86}Sr = 0.7133 \pm 0.0004$, and for NIST Bone Meal 1486 $^{87}Sr/^{86}Sr = 0.7094 \pm 0.0002$, which is in an excellent agreement with the GeoReM Database data (0.7131-0.7134) and (0.709269-0.70964), respectively.

The developed method was applied to the strontium isotope analysis of animal and human teeth and bones as well as ancient textiles from a number of archaeological sites in Russia.

The work was carried out at the "Geoanalitik" Center for Collective Use and supported by RSF grant No. 16-17-10283.

OP57 THE CHALLENGE OF USING PHAGE IN FOOD AND VETERINARY DIAGNOSTICS: DETECTION OF MYCOBACTERIUM AVIUM SUBSPECIES PARATUBERCULOSIS IN INFANT FORMULAS BY CULTURE, PCR AND COMBINED PHAGE-PCR

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Mycobacterium avium subspecies *paratuberculosis* (MAP), the causative agent of Johnes disease in cattle and other ruminants, may have a role in the development of Crohn's disease in humans. The presence of MAP in infant powder milk has been demonstrated in the past by both culture and PCR based methods and can be due to process contamination or the survival of the organism in the powder matrix during the manufacturing process. MAP can form clumps, making it more heat resistant and given also the coating with milk proteins and fat, viable cells could escape besides oven's efficacy. The objective of this study was to investigate different infant milk-based formulas for the presence of MAP by culture and PCR and also the combined phage-PCR method which is rapid, sensitive and can giving a fast indication for the presence of viable mycobacteria in the samples. A total of 35 samples from a total of ten different producers were analyzed. Following reconstitution and decontamination all samples were cultured for MAP onto Herrold's Egg Yolk Agar with Amphotericin, Nalidixic Acid, Vancomycin, with Mycobactin J and incubated for a period of 6 months. Samples were also processed through an IS900 PCR assay to identify the presence or verify the absence of MAP DNA. Finally, reconstituted samples were processed through the phage amplification assay and the plaques were extracted for PCR identification. Phage-PCR assay detected viable MAP in 13% (4/32) of PIF samples. Culture detected viable MAP in 9% (3/32) PIF samples, all of which were also phage-PCR positive. Direct IS900 PCR detected MAP DNA in 22% (7/32) of PIF samples. The presence of MAP in infant formulas highlights the need to decrease the risk of exposure for infants and young children by assuring that skim milk intended for the manufacture of formulas is be from MAP free herds.

OP58 CHEMICAL COMPOSITION OF BELT ACCESSORIES FROM CENTRAL AND WEST BULGARIA DATED TO THE GREAT MIGRATION PERIOD

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The belt accessories style have accommodated to fashion of their era and are thus very important chronological indicators. They carry potential information about social status, gender and ethnicity of the owner as well as about commercial contacts and production centers. Studies of the development of belt accessories from the period of Late Antiquity (or the Great Migration Period) in Bulgaria lag significantly with respect to the large amount of finds of this kind.

In the present study a set of copper alloy buckles collected from several archaeological museums in Central and West Bulgaria were analyzed using both X-ray Fluorescence and Inductively Coupled Plasma - Atomic Emission Spectrometry. The finds were dated to the 3rd-7th centuries CE. Concentrations of 14 elements were determined (As, Bi, Co, Cd, Cu, Fe, Mn, Ni, P, Pb, Sb, Se, Sn, Zn) applying an external calibration strategy using well characterized matrix-matched standards and standard reference materials with similar chemical and physical properties as the artifacts analyzed. The investigated belt accessories were made predominantly of brass with various concentrations of Zn (from 4 to more than 15 %), however additions of tin and lead in moderate concentrations are common, which suggests that part of the items were made by adoption of older bronze or brass artifacts. By analyzing different structural parts of the buckles we show that they were made using alloys with a strictly defined composition. For example rivets were prepared from a nearly pure copper or copper alloy containing brass and tin in significantly lower concentrations than the main body of the buckle. Statistical treatment of the data obtained show separation of the analyzed buckles in several groups according to the elemental composition that match to a great extent the typological and geographical characterization of the artifacts.

Financed by the National Science Fund of Bulgaria under the Contract No. DN 10-15/2016

OP59 A COMPUTATIONALLY DESIGNED CARBON PASTE SENSOR FOR SELECTIVE DETERMINATION OF ISOXUPRINE HYDROCHLORIDE IN DIFFERENT MATRICIES

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The presence of validated sensitive and selective analytical methods is mandatory during the different stages of drug registration process to fulfill the requirements of regulatory authorities. Such methods shall be used to determine drugs in their raw material, dosage form, dissolution media and plasma (for invivo studies). In this work a sensitive and selective potentiometric method using a carbon paste sensor was developed to determine isoxsuprine hydrochloride (ISX); a drug used for cerebral and peripheral vascular diseases; in different matrices in presence of four of its photothermal degradation products reported to impair liver and kidney functions. Initial screening experiment was carried out to select paste components affecting the sensor performance. Secondly, the R-studio was used to establish a two level four factor fractional factorial experimental design for optimization of the sensor composition. The studied factors included categorical factors such as the ion-exchanger, plasticizer and ionophore type and amount. Eight experiments were carried out and the outputs measured included the Nernstian slope, limit of detection and correlation coefficient. The optimized carbon paste sensor formed of tetrakis- [3,5-bis (trifluoro- methyl) phenyl] borate (2.5 wt%), calix [8] arene (1 wt%) in 47 wt% graphite plasticized with 47 wt% dioctyl phthalate produced a Nernstian slope of 59.71 mV/decade, LOD of 9.20×10^{-7} M and a correlation coefficient approaching unity in the concentration range of 4.76×10^{-6} to 1×10^{-2} M. Sensor performance was measured as per IUPAC guidelines and the method was validated according to the ICH validation parameters. The proposed sensor was efficiently used for the determination of ISX in raw material, VASCULAR® market formulation and biological fluids (human plasma and urine). Moreover, the low cost, direct, real time analysis characteristics of the developed method enabled its application as a superior eco-friendly alternative inline dissolution analyzer for ISX tablets compared to the USP official method.

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Index of Authors

A

B

C

D

E

F

G

H

I

J

K

L

M

N

O

P

Q

R

S

T

U

V

W

X

Y

Z

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