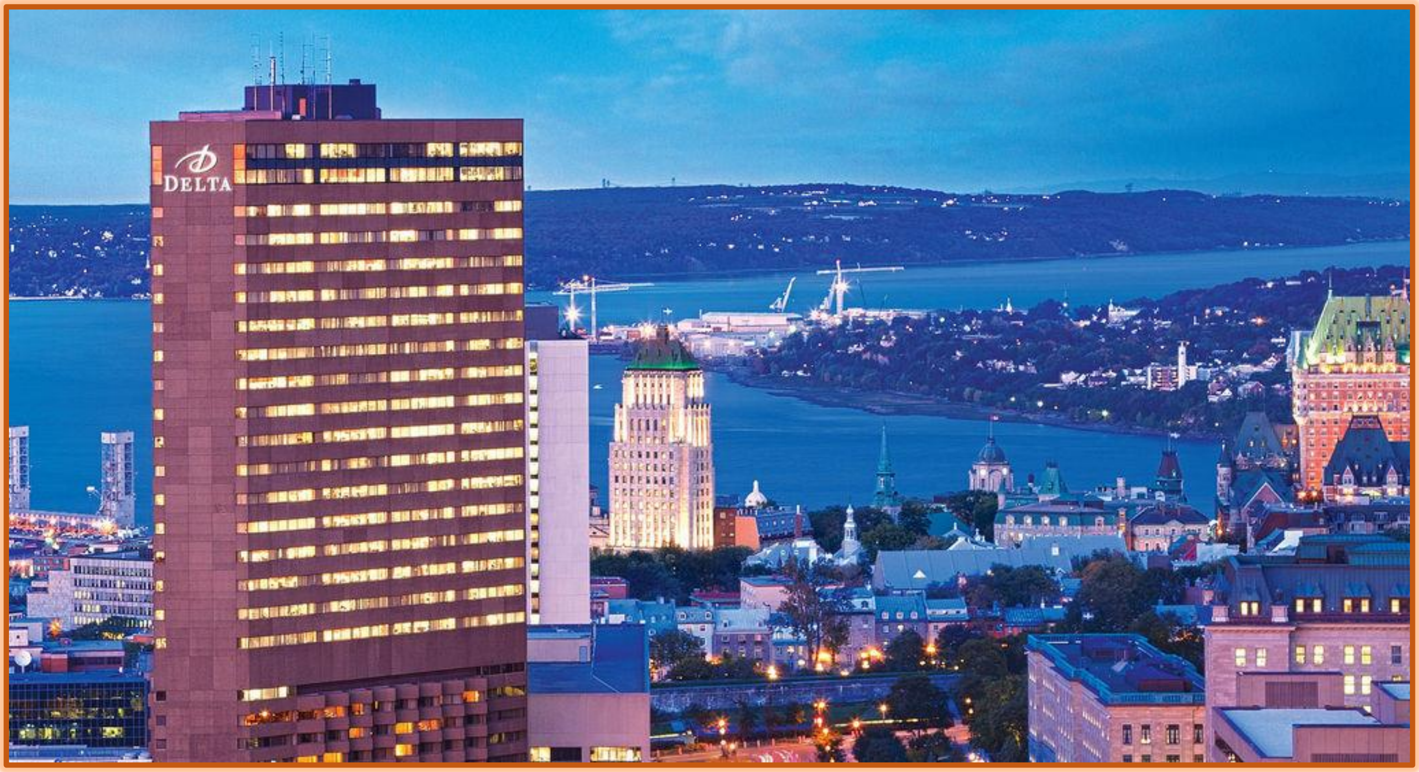
Institut national
de santé publique
Québec
Centre de toxicologie

et / and

CSASS



présentent / present

SpectrAtom
2017

et / and

ICASS 2017

61th International Conference on Analytical Sciences and Spectroscopy

June 19-23 juin, 2017 – Hôtel Delta - Québec, Québec, Canada

PROGRAMME FINAL ET LIVRE DES RÉSUMÉS

FINAL PROGRAM AND BOOK OF ABSTRACTS

Nanoparticle concentration, composition, size and distribution, dissolution and agglomeration tracking – all in under a minute.

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Bienvenue à Spectr'Atom et ICASS 2017

Le comité organisateur est fier de vous accueillir à cette 12ème édition de Spectr'Atom et la 61^{ième} édition d'ICASS à l'hôtel Delta de Québec. Nous espérons que vous allez pouvoir profiter grandement des attraits de notre belle capitale durant votre séjour.

Nous avons bâti pour vous un programme scientifique qui est à la hauteur des éditions passées. Comme vous le savez, cette édition est conjointe avec la 61^{ième} de l'ICASS (conférence internationale sur les sciences analytiques et la spectroscopie) à laquelle vous aurez l'occasion d'assister aux présentations selon vos champs d'intérêts.

Spectr'Atom et ICASS débutent le lundi 19 juin en soirée avec une petite réception amicale près du salon des exposants. Les conférences scientifiques débuteront dès le matin du mardi avec l'accueil officiel suivi de la session « état de l'art et perspectives » présidée par Monsieur Olivier Donard. Spectr'Atom et ICASS seront également agrémentés par des sessions d'affiches et par la présence de nombreux exposants.

Outres les réceptions d'ouverture du lundi et de fermeture du jeudi, quelques activités à l'extérieur de l'hôtel sont prévues dont une soirée le mardi à la microbrasserie l'Inox qui est située à quelques pas de l'hôtel et une croisière sur le fleuve le mercredi afin de contempler les attraits emblématiques de la région (pont de Québec, vue sur le château Frontenac, chutes Montmorency).

Nous espérons que notre programme sera à la hauteur de vos attentes et nous vous souhaitons un séjour agréable parmi nous.

Bon congrès!

Le comité organisateur Spectr'Atom & ICASS

Planification :
Pierre Dumas
Alain LeBlanc
Programmation scientifique :
Patrick Bélanger – Spectr'Atom
Diane Beauchemin – ICASS
Exposants et constructeurs :
David Bisson
Ciprian Cirtiu
Logistique, documentation, articles promotionnels :
Annabelle Dubreuil
Caroline Gourdes
Simon Tardif
Site internet et formulaires en ligne :
Chaoyang Huang et Alizée Rico
Finance :
Jean-François Labranche et Isabelle Royer

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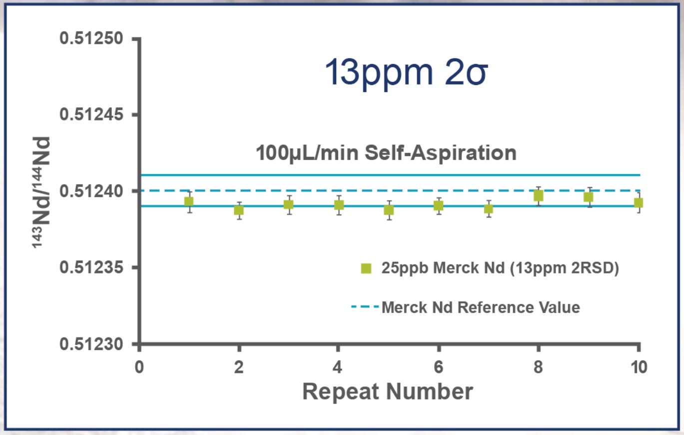
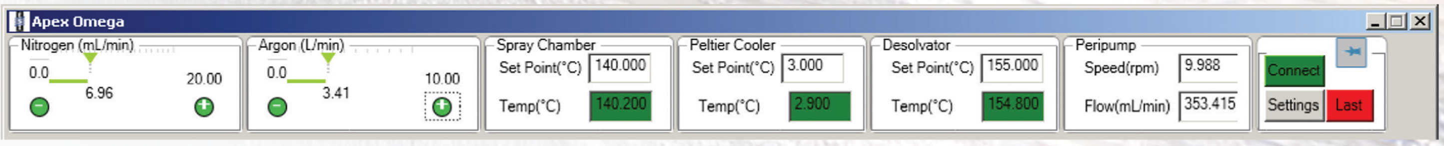


Full Software Control



Nitrogen (mL/min) 0.0 6.96 20.00

Argon (L/min) 0.0 3.41 10.00

Spray Chamber
Set Point(°C) 140.000
Temp(°C) 140.200

Peltier Cooler
Set Point(°C) 3.000
Temp(°C) 2.900

Desolvator
Set Point(°C) 155.000
Temp(°C) 154.800

Peripump
Speed(rpm) 9.988
Flow(mL/min) 353.415

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  - Peltier cooler
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Presented at 2016 Goldschmidt Yokohama
Authors: Nicholas S. Lloyd, Paul Watson, and M. Paul Field

Welcome to the 61st ICASS

The organizing team of the 61st International Conference on Analytical Sciences and Spectroscopy (ICASS) has the pleasure of welcoming you to the Delta Hotel in Québec City. This hotel is a few steps from the gates of Old Québec, the only fortified city in North America, which you may find time to explore. The 61st ICASS is being held in parallel with Spectr'Atom 2017, a conference entirely in French that focuses solely on atomic spectrometry and that ICASS attendees are free to attend.

An impressive program awaits you, which will start with a welcoming reception on Monday June 19, near the exhibition. Two or three parallel sessions will be held from June 20 to June 22 inclusively, with an environmental applications session on the morning of June 23. Two dedicated poster sessions, one for non-students on June 20 and one for student presenters on June 21, will provide a break before two special events. On June 20, attendees are invited to the nearby L'Inox Pub for networking. On June 21, a complimentary boat tour will allow attendees to see several landmarks of Québec city (such as the bridge between Québec and Lévis, the famous Frontenac Castle, and Montmorency Falls).

Our hope is that the program, featuring numerous high-quality presentations and an important exhibition, in combination with the attractive location will make the 61st ICASS an unforgettable event. May you enjoy many fruitful discussions and make several new acquaintances!

61st ICASS Conference Chair
Diane Beauchemin (Queen's University, ON, Canada)

Web Master
Chaoyang Huang (Southern Research Institute, GA, USA)

Organizing committee
Tia Anderlini (Seastar Chemicals, BC, Canada)
Lucas Choma (Queen's University, ON, Canada)
Jack Cornett (University of Ottawa, ON, Canada)
Kingsley Donkor (Thompson Rivers University, BC, Canada)
Doug Evans (Trent University, ON, Canada)
Jesse Greener (Université Laval, QC, Canada)
Alison Holliday (Moravian College, PA, USA)
Lily Huang (Queen's University, ON, Canada)
Ram Lamsal (Queen's University, ON, Canada)
Dominic Larivière (Université Laval, QC, Canada)
Nausheen Sadiq (McGill University, QC, Canada)

Québec City team (from Centre de toxicologie du Québec) :
Planning
Pierre Dumas and Alain LeBlanc

Exhibition
David Bisson and Ciprian Cirtiu

Logistics
Annabelle Dubreuil, Caroline Gourdes and Simon Tardif

Finances
Jean-François Labranche and Isabelle Royer

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Information générale

Bureau d’inscription

Tous les participants (incluant les exposants) doivent se présenter au bureau d’inscription situé à l’entrée du Foyer pour recevoir le matériel du congrès. Votre porte-nom (badge) est votre carte d’entrée pour les sessions, les repas et les activités en soirée. Assurez-vous de toujours le porter.

Présentations orales

Des projecteurs (pour présentations PowerPoint) sont disponibles dans les salles de conférences. Les présentations sont d’une durée de 20 ou 30 minutes, incluant les questions. Une table ronde (scéance plénière) aura lieu à la fin de chaque session.

Affiches

Les panneaux d’affiche seront numérotés tel qu’indiqué dans le programme.

Les affiches doivent être installées avant 9:00 et retirées au plus tard 18:15 le 21 juin (non étudiants) et installées avant 9:00 et retirées au plus tard 17:45 le 22 juin (étudiants). Les auteurs doivent aussi être présents afin d’offrir une présentation de leur affiche le 21 juin de 17:00 à 18:00 (non étudiants) et le 22 juin de 17:00 à 17:30 (étudiants).

General Information

Registration desk

All attendees, speakers and exhibitors are requested to sign in at the registration desk located at the entrance of the Foyer, to pick up the delegate package and the name card (badge) which is mandatory for admission to the sessions, the meals and evening activities.

Oral presentations

Projectors (for PowerPoint presentations) are available in each conference hall. Unless otherwise indicated, presentations are 20 or 40 minutes in lenght, including questions. A Round Table will be held at the end of each session.

Posters

Poster boards will be numbered corresponding to the program.

Posters should be installed by 9:00 and removed by 18:15 on June 20 (non-students) and installed by 9:00 and removed by 17:45 on June 21 (students). The authors must be present to offer a presentation of their posters on June 20 from 17:00 to 18:00 (non-students) and on June 21 from 17:00 to 17:30 (students).

Survol du programme / Program at a glance

Spectr'Atom 2017 🟨

61st ICASS 🟩

Spectr'Atom 2017 & ICASS ⬜

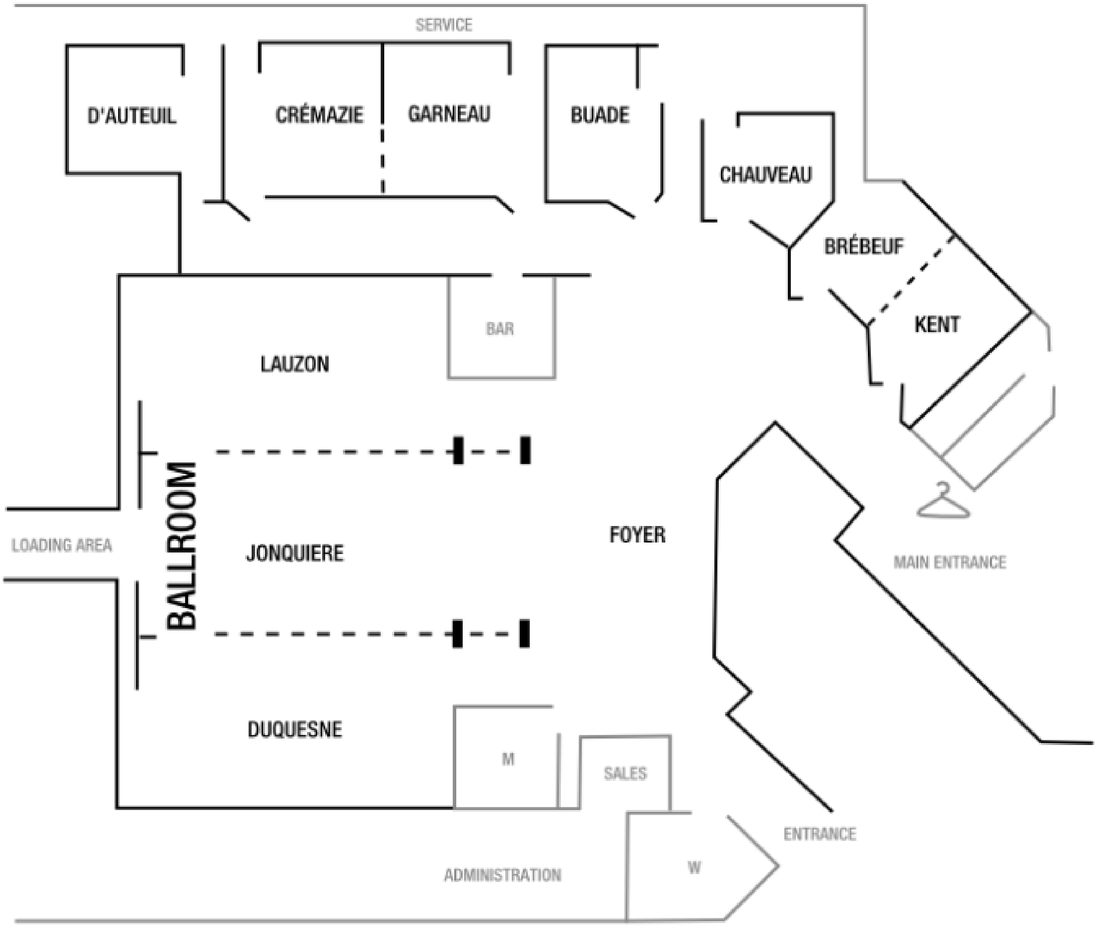
Activité de groupe
Group activity 🟦

Heure - Time	Salle / Room	Lundi / Monday June 19 juin	Mardi / Tuesday June 20 juin	Mercredi/Wednesday June 21 juin	Jeudi/Thursday June 22 juin	Vendredi / Friday June 23 juin
Matinée	Duquesne		Etat de l'art et perspectives	Solutions proposées par les constructeurs	Analyse élémentaire dans le domaine environnemental, minier et alimentaire	Biologie et santé publique
	Crémazie/Garneau		Mass Spectrometry I	Microfluidics I	Image Analysis Workshop	Environmental applications
Morning	Wolfe /Montcalm	Installation des kiosques Booth Set Up **Jonquière/Lauzon** 11:00 - 15:00	Innovations from Manufacturers I	Food safety	Speciation Analysis	
	Brébeuf/Kent			Separations		
12:00 - 13:40	Foyer & Jonquière/Lauzon		Boîte à lunch, exposition et affiches Lunch Box, exhibition	**Nu Instruments** Lunch séminaire Luncheon Seminar	Boîte à lunch Lunch Box Lunch Box CSASS AGM Wolfe/ Montcalm	Clôture de Spectr'atom 2017 End of 61st ICASS
Après-midi	Duquesne		Analyses isotopiques, signature et quantification	Spéciation élémentaire	Nanoparticules	
Afternoon	Crémazie/Garneau		Mass spectrometry II	Microfluidics II	Imaging	
	Wolfe /Montcalm		Innovations from Manufacturers II	Nanomaterials and their analysis	Forensic applications (including complimentary workshop)	
	Brébeuf/Kent		Measurement of radioactive nuclides by Mass Spectrometry			
17:00—18:00			Session d'affiche Poster Session 1*	Session d'affiche Poster Session 2* Temps libre - Free Time	Temps libre Free Time	
18:00 - 19:00			Réseautage Networking (L'Inox) Short course: Inductively Coupled plasma Spectrometry (dinner included) **Brébeuf/Kent**	Croisière sur le fleuve St-Laurent (pas de repas) Départ Hôtel 18:10 Boat ride on the St. Lawrence River (no meal) Hotel departure 6:10 PM		
19:00 - 22:00		Réception d'ouverture de l'exposition Exhibition Opening Reception **Jonquière/Lauzon**			Réception de clôture Closing Reception **Salle de bal** **Ballroom**	

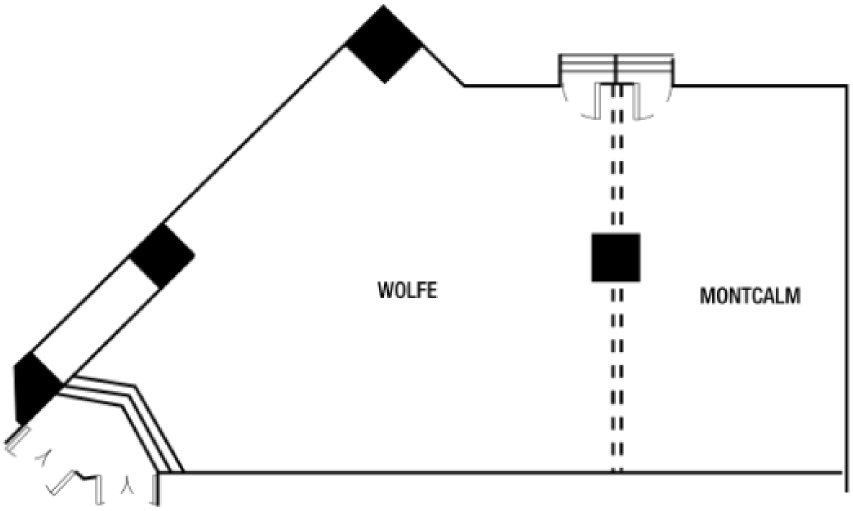
***Les affiches doivent être retirées au plus tard jeudi 13:00 - Posters must be removed by Thursday at 13:00 at the latest**

Delta Québec: Plans des salles / Floor Plans

REZ DE CHAUSSÉE / GROUND FLOOR



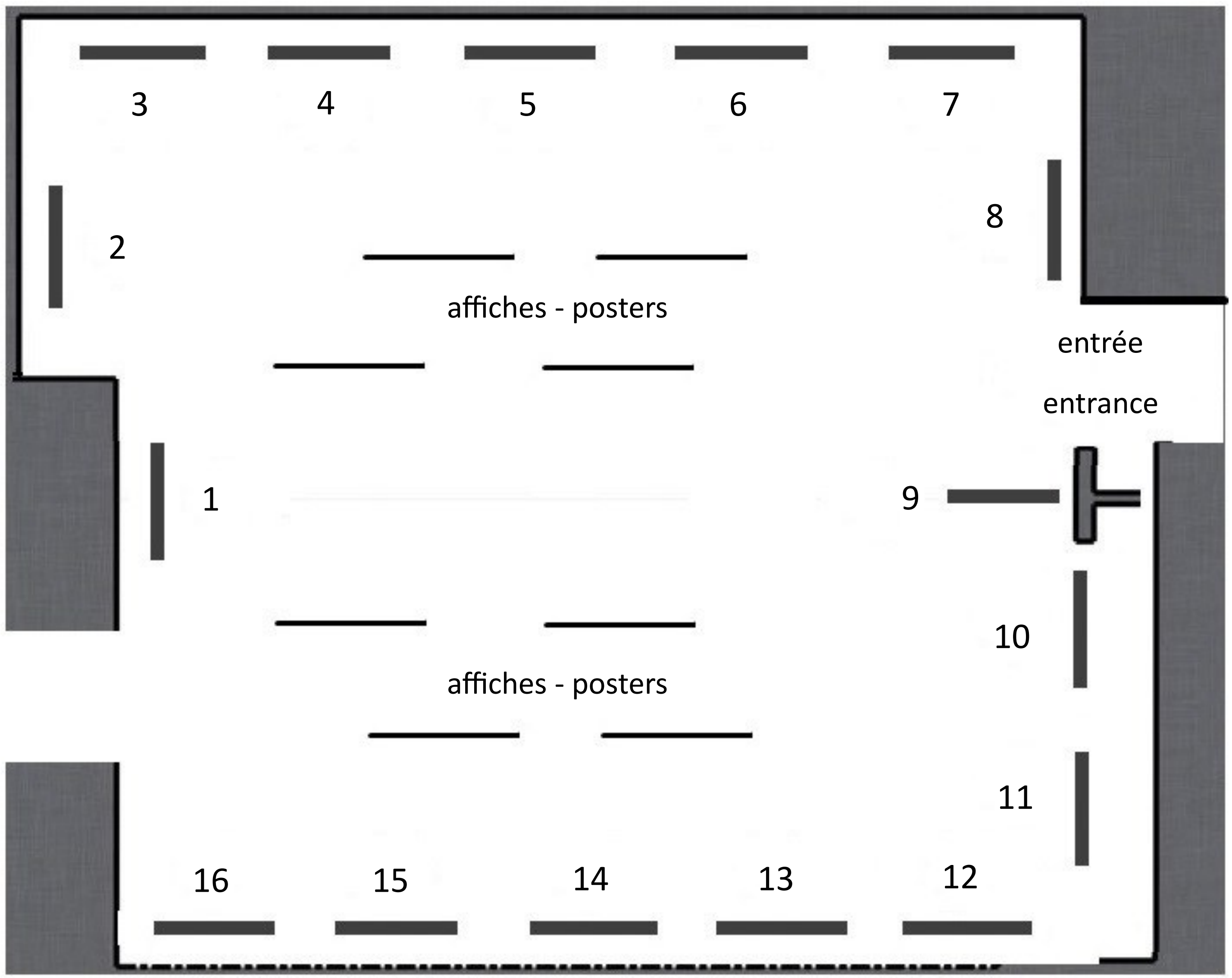
3IÈME ÉTAGE / 3RD FLOOR



SpectrAtom 2017

ICASS 2017

Salle Jonquière/Lauzon Hall



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1	Perkin Elmer
2	Bruker Optics
3	SCP SCIENCE
4	CEM Corporation
5	Agilent
6	ATS Scientific
7	Elemental Scientific
8	Nu Instruments
9	Spectra Analyse
10	ThermoFisher (Canada)
11	Isomass Scientific
12	Glass Expansion
13	Anton Paar
14	Isospark
15	Burgener Research
16	Katanax

Exposants – Exhibitors

(Jonquière/Lauzon)

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Kiosque/Booth 7

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Kiosque/Booth 8

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PCI – Spectra Analyse
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75003 Paris
France
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www.spectraanalyse.com

Kiosque/Booth 10

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Activités de soirée / Evening Activities

Mardi 20 juin - Tuesday June 20 (18:00)

Réseautage- Networking

Bières brassées sur place et menu "Style Pub"
Deux consommations sont offertes à nos participants

Beers brewed on site and Pub Style Menu
Two drinks are offered to all our participants

Brasserie L'Inox (L'Inox Brewpub)
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À cinq minutes à pieds du Delta
A five minute walk from the Delta

Mercredi 21 juin - Wednesday June 21 (17:00-22:00)

Événement Camions Cuisine/Croisière - Food Truck/Boat Ride Event

Stationnement du Delta (arrière de l'hôtel)
Delta parking lot (behind the hotel)

(argent comptant seulement - cash only)

Départ pour le Port à l'avant de l'hôtel à 18:05
Departure for the Harbour in front of the Hotel at 18:05

Jeudi 22 juin - Thursday June 22 (19:00)

Réception de clôture - Closing Reception

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$55 par personne incluant amuses bouches et trois consommations
$55 per person which includes finger foods and three drinks

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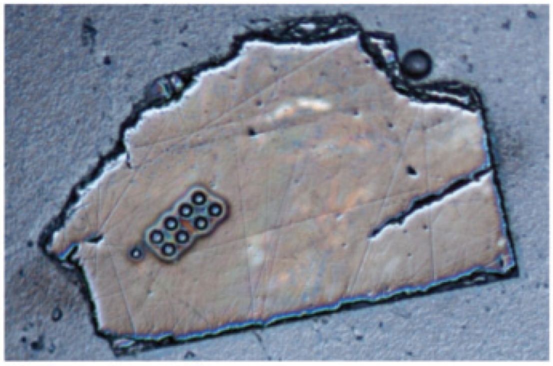


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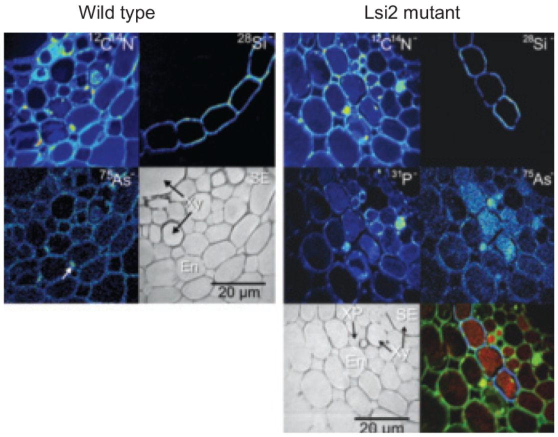
Wild type
Lsi2 mutant
$^{12}C^{14}N$
^{28}Si
^{75}As
SE
Xy
En
20 µm
$^{12}C^{14}N$
^{28}Si
^{31}P
^{75}As
XP
SE
En
Xy
20 µm

Spectr’atom 2017 - Horaire détaillé

Lundi 20 juin 2017		
11:00 à 15:00		**MONTAGE KIOSQUES DES EXPOSANTS** (Salle Jonquière/Lauzon)
19:00		**RÉCEPTION D’OUVERTURE** (Foyer & Salle Jonquière/Lauzon)

Mardi 20 juin 2017		
09:00		**ACCUEIL** par Alain LeBlanc, Diane Beauchemin et Olivier F.X Donard (Salle Duquesne)
ÉTAT DE L'ART ET PERSPECTIVE DE LA SPECTROMÉTRIE ATOMIQUE Président de session : Olivier F.X Donard, Université de Pau, France (Salle Duquesne)		
09:30	O 1-1	**HAUTES PRÉCISIONS, HAUTES SENSIBILITÉS, SPÉCIATION ET ISOTOPIE : DE NOUVELLES OUVERTURES POUR UNE MEILLEURE COMPRÉHENSION DE L’ÉCODYNAMIQUE DES MÉTAUX ET MÉTALLOÏDES DANS L’ENVIRONNEMENT** **Olivier F.X. Donard**, Sylvain Bérail, Emmanuel Tessier, Oriol Baltrons, David Amouroux Center of Mass Spectrometry for Reactivity and Speciation Sciences (MARSS) Institut des Sciences Analytique et de Physicochimie pour l’Environnement et les Matériaux, Université de Pau et des Pays de l’Adour, France
10:00	O 1-2	**STRATÉGIE ANALYTIQUE POUR LA RÉSOLUTION DE PROBLÉMATIQUES RELIÉES À LA PRÉSENCE DE FONDANT DANS UNE SOLUTION PRÉPARÉE PAR FUSION** **Maxime Gagnon**[1], Mathieu Bouchard[2], Mathieu Hamel[2], Dominic Larivière[1]. 1. Département de chimie, Université Laval. 2. Claisse, Québec, Canada
10:20		Pause-café Burgerer
10:40	O 1-3	**UTILISATIONS D’UN MIP-AES AU DÉPARTEMENT DE GÉNIE DES MINES, DE LA MÉTALLURGIE ET DES MATÉRIAUX DE L’UNIVERSITÉ LAVAL : LA DÉCOUVERTE D’UN INSTRUMENT D’ANALYSE ÉLÉMENTAIRE ÉCONOMIQUE ET POLYVALENT** **Keven Turgeon**[1-2], Vicky Dodier[1], Claude Bazin[1], Dominic Larivière[2]. 1 Département de génie des mines, de la métallurgie et des matériaux. 2 Département de chimie, Université Laval.
11:00	O 1-4	**TENEURS EN ELEMENTS TRACES METALLIQUES PRESENTS DANS DES VIANDES ISSUS DE FILIERES BIOLOGIQUE OU CONVENTIONNELLE** **Thiérry Guérin**[1], J. Parinet[1], M. Saint-Hilaire[1], C. Chafey[1], L. Noël[1], B. Minvielle[2], J. Normand[3], A. Travel[4], G. Dervilly-Pinel[5], E. Engel[6] 1 : Université Paris-est, Anses, Laboratoire de Sécurité des Aliments, France; 2 IFIP, La Motte au Vicomte, France, 3 Institut de l’Elevage, Meat Quality Department, Agrapole, France; 4 ITAVI, INRA Centre de Tours, France; 5 LUNAM Université, ONIRIS, LABERCA, NantesFrance; 6 INRA, MASS, France
11:20		Table ronde
12:00		Repas du midi (Foyer & Salle Jonquière/Lauzon)

ANALYSES ISOTOPIQUES, SIGNATURE ET QUANTIFICATION
Président de session : Pierre Dumas, Centre de Toxicologie du Québec, Québec, Canada
(Salle Duquesne)

13:40	O 1-5	**SPÉCIATION DU MERCURE SANGUIN PAR DILUTION ISOTOPIQUE SPME-GC-ICP-MS** **Jean-Francois Bienvenu,** Centre de Toxicologie du Québec, Québec, Canada
14:10	O 1-6	**ANALYSE DU 226-RA ET 210-PB ET ÉLIMINATION DES INTERFÉRENCES RÉSIDUELLES PAR SPECTROMÉTRIE DE MASSE EN TANDEM (ICP-MS/MS).** **Claire Dalencourt**, Kamesh Viswanathan Baskaran, Dominic Larivière Laboratoire de Radioécologie, Université Laval, Québec, Canada
14:30	O 1-7	**SPECIATION, QUANTIFICATION ET ISOTOPIE DES FORMES INORGANIQUES DU SOUFRE EN MILIEU AQUEUX.** **Mathieu Martinez**, Corinne Parat, Isabelle Le Hécho, IPREM, UPPA, Pau, France
14:50		Pause Elemental Scientific
15:10	O 1-8	**L'ÉTALONNAGE INTERNE À L'AIDE D'ISOTOPES ENRICHIS : UNE APPROCHE ALTERNATIVE À LA DILUTION ISOTOPIQUE CONVENTIONNELLE POUR LE DOSAGE D'ÉLÉMENTS MULTI-ISOTOPIQUES PAR ICP-MS** **Pierre Dumas,** Centre de Toxicologie du Québec, Québec, Canada
15:30		Table ronde
17:00 à 18:00		Session d'affiches (non étudiants) (Salle Jonquière/Lauzon)
18:00		Soirée de réseautage à la Microbrasserie L'Inox (coupons pour consommations gratuites offerts sur place) Carte de participant Spectr'Atrom requise

Mercredi 21 juin 2017

LES SOLUTIONS PROPOSÉES PAR LES CONSTRUCTEURS
Président de session : Diane Beauchemin, Queen's University, Dept. of Chemistry, ON, Canada
(Salle Duquesne)

08:30	O 2-1	**OPTIMISATION DU SYSTÈME D'INTRODUCTION D'ÉCHANTILLON EN ICP-IR-MS SUR UN NEPTUNE THERMO** **Laurent Bertal**[1] et Abel Guihou[2], 1 Courtage Analyses Services (Distributeur Glass Expansion), Mont Saint Aignan, France; 2 Cerege, Europôle méditerranée - de l'Arbois, AIX EN PROVENCE, France
09:00	O 2-2	**UN CONDENSÉ DES NOUVELLES TECHNOLOGIES D'ANALYSES INORGANIQUES PAR ICP-OES ET ICP-MS** **Stephan Chady**, Perkin Elmer
09:20	O 2-3	**Solutions par fusion au borate de lithium : pour « convaincre les réfractaires »** **Benoît Bouchard,** Jean-François Nolin, Katanax
09:40		Pause-café Isospark
10:00	O 2-4	**ATTOM, DESCRIPTION, SPÉCIFICITÉS ET APPLICATIONS DE L'ICP-MS HAUTE RÉSOLUTION DE NU INSTRUMENTS** **Ariane Donard**, Benoit Disch, Phil Shaw, Nu Instruments, Wrexham, UK
10:20	O 2-5	**NOVAWAVE – UN CONCEPT INNOVANT DE DIGESTION AUTOMATISEE PAR MICRO-ONDES** **Rachid Choudar**, SCP Science
10:40	O 2-6	**LES NOUVELLES AVANCÉES TECHNIQUES EN LABORATOIRE AVEC LES TECHNOLOGIES AVANCÉES D'ICP COUPLÉ À UN SPECTROMETRE DE MASSE** Daniel Kutscher, Shona McSheehy Ducos, **Michel Alsayegh**, Thermoscientific
11:00		Table ronde
12:00		Repas du midi (Foyer & Salle Jonquière/Lauzon)

SPÉCIATION ÉLÉMENTAIRE
Président de session : Dr Marc Lamoureux
(Salle Duquesne)

13:40	O 2-7	**POTENTIEL DES ANALYSES DE SPÉCIATION POUR LA DISCRIMINATION DE L'ORIGINE GÉOGRAPHIQUE DES VINS ROUGES** **Véronique Vacchina**[1], Bernard Medina[2], Olivier Donard[3], Fabienne Seby[2] 1 UT2A, Pau, France ; 2 Société des Experts Chimistes de France, Paris, France, 3 IPREM, Pau, France
14:10	O 2-8	**SPÉCIATION DU PLATINE EN PRÉSENCE DE MATIÈRE ORGANIQUE NATURELLE** **Geneviève Rioux**, Peter G.C. Campbell, Claude Fortin. 1 INRS-ETE, Québec, Canada
14:30	O 2-9	**SPÉCIATION DES LANTHANIDES EN PRÉSENCE DE LA MATIÉRE ORGANIQUE NATURELLE** **Rahma Rahal**, Peter G. C. Campbell, Claude Fortin 1 INRS-ETE, Québec, Canada
14:50		Pause-café Elemental Scientific
15:10	O 2-10	**SPÉCIATION AQUEUSE DU THORIUM, DU PLOMB ET DE L'URANIUM PAR ÉCHANGE IONIQUE** **Andrei Alexis Largo Sierra**, Peter G. C. Campbell, Claude Fortin INRS-ETE, Québec, Canada
15:30	O2-11	**ANALYSE DE SPÉCIATION DE L'ARSENIC DANS LA FRACTION BIO-ACCESSIBLE POUR L'ÉVALUATION DU RISQUE LIÉ À LA CONSOMMATION DE RIZ DE DIVERS PAYS** Randa Althobiti, Nausheen Sadiq et **Diane Beauchemin**, Queen's University, ON, Canada.
15:50		Table ronde
17:00	**à 17:30**	Session d'affiches (étudiants) (Salle Jonquière/Lauzon)
17:00	**à 18:00**	Événement camions cuisine (Food Trucks) Stationnement de l'Hôtel Delta (derrière l'hôtel)
18:10		Autocar pour se rendre au Port (croisière)
19:00	**à 22:00**	Croisière sur le fleuve St-Laurent (activité gratuite avec Carte de participant Spectr'Atrom)

Jeudi 22 juin 2017

ANALYSE ÉLÉMENTAIRE DANS LE DOMAINE ENVIRONNEMENTAL, MINIER ET ALIMENTAIRE
Président de session : Dominic Larivière, Université Laval, Département de chimie, Québec, Canada
(Salle Duquesne)

08:30	O 3-1	**ANALYSE DU PLUTONIUM À L'ÉTAT D'ULTRA-TRACES DANS DES SÉDIMENTS DE RIVIÈRES DE LA RÉGION DE FUKUSHIMA** **Fabien Pointurier**[1], Hugo Jaegler[1,2], Yuichi Onda[3], Amélie Hubert[1], Anne-Claire Pottin[1], J. Patrick Laceby[2], Olivier Evrard[2] 1 CEA, DAM, DIF, Arpajon, France; 2 Laboratoire des Sciences du Climat et de l'Environnement (LSCE), (CEA/CNRS/UVSQ), Gif-sur-Yvette, France; 3 CRiED, University of Tsukuba, Japon
09:00	O 3-2	**QUELLES METHODES DE MISE EN SOLUTION POUR LES MATRICES SOLIDES ENVIRONNEMENTALES ?** **M. Heller**, A. Habibi, C. Augeray, F. Leprieur IRSN/PRP-ENV/STEME/LTE, Le Vésinet (France)
09:20	O 3-3	**ANALYSE RAPIDE DE RADIUM-226 ET 228 PAR ICP-MS-MS** **Steeve Roberge**[1], Maxime Gagnon[1,2], Charles-Olivier Gilbert [1,2], Nathalie Dassylva[1]. 1 CEAEQ, MDDELCC, Québec, Canada 2 Université Laval, Département de chimie, Québec, Canada
09:40	O 3-4	**SEPARATION AUTOMATISEE ET COUPLAGE AVEC LA MESURE POUR LA QUANTIFICATION RAPIDE DES ACTINIDES ET DE ^{90}SR** **A. Habibi**[1], C. Cossonnet[2], F. Leprieur[1], B. Boulet[2], G. Cote[3], D. Larivière[4] 1 IRSN/PRP-ENV/STEME/LTE, Le Vésinet, France; 2 IRSN/PRP-ENV/STEME/LMRE, Orsay (France), 3 Chimie ParisTech, CNRS, UMR, Laboratoire d'Electrochimie, Chimie aux Interfaces et Modélisation pour l'Energie, Paris, France; 4 Laboratoire de radioécologie, Université Laval, Québec, Canada
10:00		Pause-café Isospark

10:20	O 3-5	**COMPARAISON DES SPECTROMÉTRIES XRF ET ICP-AES POUR L’ANALYSE ÉLÉMENTAIRE DANS LES VÉGÉTAUX À TRAVERS LA MÉTHODE DU PROFIL D’EXACTITUDE** **Pierre Masson**, Dominique Orignac, Patrice Soule, Thierry Dalix, Guillaume Daugey. INRA-USRAVE, Centre de Recherches de Bordeaux-Aquitaine, Cedex, France
10:40	O 3-6	**GÉOCHIMIE DU RADIUM DANS LES EAUX SOUTERRAINES NATURELLES DU SUD-EST DU NOUVEAU-BRUNSWICK** François Lagacé, Delphine Foucher, Céline Surette, **Olivier Clarisse,** Université de Moncton, NB, Canada
11:00		Table ronde
12:00		Repas du midi (Foyer) ou Lunch conférence Nu Instruments (Duquesne) – repas léger offert
12:00	**à 14:00**	Démontage kiosques des exposants (Salle Jonquière/Lauzon)
NANOPARTICULES Président de session : Ciprian Mihai-Cirtiu, Centre de Toxicologie du Québec, Québec, Canada (Salle Duquesne)		
13 :40	O 3-7	**"TENDANCES DANS L'ANALYSE "SINGLE PARTICLE ET SINGLE CELL ICP-MS" : DE LA DÉTECTION DANS LES MATRICES COMPLEXES À LA QUANTIFICATION EN NOMBRE DE PARTICULES ET DU CONTENU EN MÉTAL DANS LES ORGANISMES UNICELLULAIRES INDIVIDUELS"** **Stephan Chady**, Perkin Elmer
14:10	O 3-8	**AMÉLIORATION DES LIMITES DE DÉTECTIONS POUR LA MESURE PAR SP-ICP-MS AVEC L’HR-ICP-MS ATTOM PAR L’UTILISATION D’UN DESOLVATEUR ET DU MODE « PSEUDO RÉSOLUTION »** **Ariane Donard**, Benoit Disch, Phil Shaw, Nu Instruments, Wrexham, UK
14:30	O 3-9	**DÉVELOPPEMENT ET VALIDATION D’UNE MÉTHODE ANALYTIQUE ICP-MS EN MODE « SINGLE PARTICLE » (SP-ICP-MS) POUR L’ANALYSE DE NANOPARTICULES (NP) DE DIOXYDE DE TITANE (TIO2) DANS LES MILIEUX BIOLOGIQUES »** **Samantha Salou**, Ciprian Mihai-Cirtiu, Centre de Toxicologie du Québec, Québec, Canada
14:50		Pause-café Glass Expansion
15:10	O 3-10	**ANALYSE DES IMPURETES ELEMENTAIRES ET DES NANOPARTICULES DE TIO2 DANS DES PRODUITS COSMETIQUES PAR UNE COMBINAISON DE TECHNIQUES** **Fabienne Séby**[1], Inmaculada De La Calle[1,2], Marlène Klein[1], Mathieu Menta[1] 1 UT2A/ADERA, Pau, France; 2 Universidad de Vigo, Spain.
15:30	O 3-11	**ÉVALUATION DE LA STABILITÉ DE NANOPARTICULES D’OXYDE DE ZINC PAR SINGLE-PARTICLE ICP-MS** **Laurie Fréchette-Viens**, Madjid Hadioui, Kevin J. Wilkinson. Université de Montréal, Canada
15:50		Table ronde
19:00		Réception de clôture (disponible sur achat d’un coupon de 55,00$)

Vendredi 23 juin 2017

BIOLOGIE ET SANTÉ PUBLIQUE Président de session : Patrick Bélanger, Centre de Toxicologie du Québec, Québec, Canada (Salle Duquesne)		
08:30	O 4-1	**INFLUENCE DE LA COMPOSITION DE LA MATIÈRE ORGANIQUE DISSOUTE SUR LA MOBILITÉ ET LA BIODISPONIBILITÉ DU MERCURE** Céline **Guéguen**[1], Vaughn Mangal[1], Ben Stenzler[2], Alexandre Poulain[2] 1 Trent University, Peterborough, ON, Canada; 2 University of Ottawa, Ottawa ON, Canada,
09:00	O 4-2	**DETERMINATION DU MERCURE DANS LES URINES. RESULTATS DE LA COMPARAISON INTER-LABORATOIRES OELM** **Josianne Arnaud**[1], C. Weykamp[2], M.Gonzales-Estecha[3], M Patriarca[3], S Koetsier[4] 1 CHUGA, France; 2 Queen Beatrix Hospital, The Netherlands, 3 Istituto Superiore di Sanità, Italie; 4 RCPAQAP Chemical Pathology, Australia,

09:20	O 4-3	**MÉTHODE D'ANALYSE DU CHROME HEXAVALENT DANS LES GLOBULES ROUGES PAR ICP MS/MS** **Sébastien Gagné,** Centre de Toxicologie du Québec, Québec, Canada
09:40	O 4-4	**LES ANALYSES INORGANIQUES ET L'AIDE AU DIAGNOSTIC VÉTÉRINAIRE OU QUAND ON N'APPELLE PAS UN CHAT UN CHAT** **Nathalie Ouellet**, DLEAA, Québec, Canada
10:00		Pause-café Agilent
10:20	O 4-5	**IMAGERIE QUANTITATIVE DU PLATINE DANS DES TISSUS BIOLOGIQUES PAR LA-ICP MS** Carine Arnaudguilhem[1], Marion Larroque[3], Olivia Sgarbura[4], François Quenet[4], Brice Bouyssière[1], Christian Larroque[2], **Sandra Mounicou**[1] 1 CNRS/ UNIV PAU & PAYS ADOUR, Institut des Sciences Analytiques et de Physico-Chimie pour l'Environnement et les Matériaux, PAU, France ; 2 IRCM/INSERM, ICM Val d'Aurelle, France 3 ICM/ Unité de Recherche Translationnelle, Campus Val d'Aurelle, France 4 ICM/ Service Chirurgie A2, Campus Val d'Aurelle, France
10:40		Table ronde
11:30		Fermeture des conférences


Agilent ICP-MS
Agilent ICP-QQQ
Agilent AA
Agilent MP-AES
Agilent ICP-OES

61ST ICASS FINAL PROGRAM

MONDAY, JUNE 19, AFTERNOON

11:00-15:00 Set-up of exhibition - *Jonquière/Lauzon*

19:00-22:00 Exhibition opening reception – *Foyer & Jonquière/Lauzon*

TUESDAY, JUNE 20, MORNING

Innovations from manufacturers I – *Wolfe/Montcalm*

Organizers and co-Chairs: Lucas Choma and Diane Beauchemin

9:00 (**(I009)** MIR AND FIR ANALYSIS OF INORGANIC SPECIES IN A SINGLE DATA ACQUISITION. **Sergey Shilov**, Mathias Keßler, Xia Stammer, Bruker Optics

9:20 **(I027)** INTRODUCING AGILENT'S SECOND GENERATION ICP-MS/MS, THE 8900 QQQ FOR UNPRECEDENTED SPECTRAL INTERFERENCE CONTROL, EXTREME HIGH SENSITIVITY, PERFECT ISOTOPIC SIGNATURES, AND MUCH MORE. **Pamela Wee**, Agilent Technologies Canada Inc.

9:40 **(I005)** HANDLING INTERFERENCES IN THE MODERN LABORATORY WITH ADVANCED TRIPLE QUADRUPOLE ICP-MS TECHNOLOGY. Daniel Kutscher, Shona McSheehy Ducos, Maura Rury. Thermo Fisher Scientific. Presented by: **Michael Plantz**

10:00 Burgerer Coffee Break - *Foyer*

10:40 **(I031)** ELEMENTAL ANALYSIS BY MASS SPECTROMETRY: SOLUTION FROM NU INSTRUMENTS, HR-ICP-MS ATTOM AND GDMS ASTRUM. **Benoit Disch**, Ariane Donard, Phil Shaw, Nu Instruments

11:00 **(I052)** HIGH SENSITIVITY TIN SPECIATION USING A NEW GC INTERFACE WITH SECTOR FIELD HIGH RESOLUTION ICP-MS. **Peter Stow**, Isomass Scientific Inc.

11:20 **(I053)** NEXION 2000 ICP-MS – ANY MATRIX, ANY INTERFERENCE, ANY PARTICLE SIZE. **Andrew Rams**, PerkinElmer Inc.

11:40 **(I022)** CHOOSING THE PROPER SAMPLE INTRODUCTION SYSTEM TO ALLEVIATE INTERFERENCES IN ICP. **Jerry Dulude** and Ryan Brennan, Glass Expansion

12:00 Lunch – *Foyer* & Exhibition Hall and Poster session - *Jonquière/Lauzon*

Mass Spectrometry – *Crémazie/Garneau*

Organizer: Kingsley Donkor

Co-Chairs: Paul Mayer and Alexander Donald

9:00 **(I008)** THE QUANTITATIVE MASS SPECTROMETRIC ANALYSIS OF MICROBIAL METABOLISM OF DIETARY GLYCOCONJUGATES. **Zandberg, Wesley F[1];** Noestheden, Matthew[1]; Vicaretti, Sara D[1]; Gibson, Deanna[2]; Wylie, Aaron D[1]. University of British Columbia, Okanagan Campus; Department of [1]Chemistry and [2]Biology.

9:40 **(I019)** CARACTERISATION OF BIOACTIVE CRANBERRY FRACTIONS BY MASS SPECTROMETRY APPROACHES. Marie-Claude Denis[1], Yves Desjardins[2], André Marette[2], Pascal Dubé[2], Stéphanie Dudonné[2], Edgard Delvin[1], Emile Levy[1], **Alexandra Furtos**[1], [1]Université de Montréal, Montréal, QC H3T 1C5, [2]Institute of Nutraceuticals and Functional foods (INAF), Université Laval, QC G1V 0A6

10:00 Burgerer Coffee Break - *Foyer*

10:40 **(I081)** LC/ESI-MS METHOD FOR DETERMINATION OF POTENTIALLY-RELEVANT FATTY ACIDS IN BEEF. **Kingsley K. Donkor**[1], Laiel C. Soliman[1], Elizabeth M. Andrucson[1], Bruno Cinel[1], John S. Church[2], Thompson Rivers University, Department of Chemistry[1] and Department of Natural Resource Sciences[2] , Kamloops, BC

11:00 **(I045)** MECHANISM AND CONTROL OF THE SELECTIVE FRAGMENTATION OF PROTEIN IONS. Huixin X. Wang,[1] Michael G. Leeming,[2] **W. Alexander Donald**[1], [1] School of Chemistry, UNSW Sydney, Australia; [2] School of Chemistry, University of Melbourne, Australia

11:40 **(I017)** DEVELOPMENT OF LC-QQQ-MS METHODS FOR CHARACTERIZATION OF REGENERABLE AMINE SOLVENTS USED IN CO2 CAPTURE. **S. Gallant**, A. Furtos, K. C. Waldron. Department of Chemistry, Université de Montréal.

12:00 Lunch – *Foyer* & Exhibition Hall and Poster session - *Jonquière/Lauzon*

TUESDAY, JUNE 20, AFTERNOON

Innovations from manufacturers II – *Wolfe/Montcalm*

Organizers and co-Chairs: Lucas Choma and Diane Beauchemin

13:40 **(I020)** FTIR SPECTROELECTROCHEMISTRY: NEW ASSESSORIES AND APPLICATIONS. **Sergey Shilov**, Matthias Kessler, Bruker Optics

14:00 **(I016)** THE AGILENT 5110 ICP-OES: ROBUST – POWERFUL – FAST. **Wayne Blonski**, Agilent Technologies Canada Inc.

14:20 **(I065)** ADVANCES IN ICP-OES HARDWARE AND OPTICAL DESIGN. **Dion Tsourides**. Spectro Ametek.

14:40 **(I067)** SELECTING THE OPTIMUM SAMPLE INTRODUCTION SYSTEM FOR ICP-OES ANALYSIS OF DIFFICULT SAMPLES. **Sergei Leikin**. Texas Scientific Products

15:00 Elemental Scientific Coffee Break - *Foyer*

15:40 **(I059)** NEW TECHNIQUES FOR PREPARING PLASTICS AND POLYMERS BY MICROWAVE SAMPLE PREPARATION. Tina Restivo, Austin Thornton, Bob Lockerman, and Michael Howe, CEM Corporation. Presented by: **Bill MacLuckie**

16:00 **(I064)** ADVANCES IN MICROWAVE SAMPLE PREPARATION: TRADITIONAL AND MODERN DAY DESIGNS FOR TRACE METALS ANALYSIS. **Parag Bhargava** and Gilles Groulx, ATS Scientific Inc. 4030 Mainway, Burlington, ON Canada

16:20 **(I069)** *Easy***PREP** SAMPLE HANDLER, AUTOMATION OF TEDIOUS LIQUID TRANSFER TASKS. **John Dykeman**, SCP SCIENCE

16:40 End of session

17:00-18:00 Non-student poster session (authors present) - *Jonquière/Lauzon*

18:00-22:00 Short course on Inductively Coupled Plasma Spectrometry (dinner included in course registration fee) – *Brébeuf/Kent*

or

18:00 Relaxed Networking at L'Inox Brewpub

Mass Spectrometry – *Crémazie/Garneau*

Organizer: Kingsley Donkor

Co-Chairs: Wesley Zandberg and Kingsley Donkor

13:40 **(I058)** INVESTIGATION OF THE UNIMOLECULAR REACTIONS OF IONIZED POLYCYCLIC AROMATIC HYDROCARBONS**.** Brandi West, Alicia Sit, Sabria Mohamad, Eduardo Solano, Jake Burner, Yardley Paige Cuthbert, Iden Djavani-Tabrizi and **Paul M. Mayer**. Department of Chemistry and Biomolecular Sciences, University of Ottawa; Sarah Rodriguez, Christine Joblin. Université de Toulouse III, Toulouse, France; Andras Bodi, Patrick Hemberger: Paul Sherrer Institut, Villigen, Switzerland

14:00 **(I018)** THE DEVELOPMENT OF AN AIR TREATMENT UNIT FOR IMPROVED REAL TIME MSMS MONITORING OF VOLATILE ORGANIC COMPOUNDS.

Alexandre Ouellet, Marco Li Fraine, Christophe Romiguière, Annie Michaud, Dominic Lortie, Jean-François Boily and Patrick Avon, Centre d'expertise en analyse

environnementale du Québec, MDDELCC; 850, boulevard Vanier, porte Sud, Laval, QC

14:40 **(I033)** MONITORING UPTAKE OF A DNAZYME MOTOR BY LIVING CELLS USING ICP-MS. Hanyong Peng, Xing-Fang Li, X. Chris Le, **Hongquan Zhang**. Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and Pathology, University of Alberta, Edmonton, Alberta, T6G 2G3, Canada

15:00 Elemental Scientific Coffee Break - *Foyer*

15:40 **(I011)** ANALYSIS OF NEONICOTINOIDS AND PARTICLE BOUND PESTICIDES IN ATMOSPHERIC SAMPLES BY LIQUID CHROMATOGRAPHY-TANDEM MASS SPECTROMETRY. **Renata Raina-Fulton**, Asal Behdarvandan. University of Regina, Department of Chemistry and Biochemistry.

16:00 **(I062)** DEVELOPMENT OF ANALYTICAL TECHNIQUES TO STUDY THE HUMAN MICROBIOME, Daniel Figeys, University of Ottawa. Presented by: **Zhibin Ning**

16:40 End of session

17:00-18:00 Non-student poster session (authors present) - *Jonquière/Lauzon*

18:00-22:00 Short course on Inductively Coupled Plasma Spectrometry (dinner included in course registration fee) – *Brébeuf/Kent*

or

18:00 Relaxed Networking at L'Inox Brewpub

<u>Measurement of radioactive nuclides by mass spectrometry</u> – *Brébeuf/Kent*

Organizers: Dominic Larivière, Jack Cornett and Doug Evans

co-Chairs: Jack Cornett and Doug Evans

13:20 **(I078)** RADIOCHEMICAL SEPARATIONS FOR UNUSUAL SAMPLE MATRICES. **Ralf Sudowe**, Department of Environmental & Radiological Health Sciences, Colorado State University

14:00 **(I077)** MEASURING ULTRA-TRACE PLUTONIUM CONCENTRATIONS IN ARCTIC SEAWATER. Andy Z. Zhou, Xiaolei. Zhao, Daniel Sauve, Chris Charles and **R. Jack Cornett**, A.E. Lalonde Laboratory for Accelerator Mass Spectrometry, University of Ottawa, Ottawa, Canada.

14:20 **(I084)** NEW METHODOLOGY TO RELEASE ^{129}I FROM CHARCOAL SAMPLES. **Barbara Francisco** and Robert Jack Cornett, AEL-AMS Laboratory, Advanced Research Complex, University of Ottawa. 25 Templeton Street, Ottawa, ON, K1N 6N5.

14:40 **(I048)** DETERMINATION OF ^{210}Pb IN WATER SAMPLES BY ICP-MS/MS AFTER CLOUD POINT EXTRACTION USING CROWN ETHERS. **Guillaume Blanchet-Chouinard** and Dominic Larivière, Radioecology laboratory, Chemistry Department, Laval University.

15:00 Elemental Scientific Coffee Break - *Foyer*

15:40 **(I073)** ONLINE SEPARATION AND DETERMINATION OF ^{226}RA AND TRACE METALS FROM MINING WASTEWATER AND FRACKING WATER. **Wei Wang** and Douglas Evans, School of Environment, Trent University, Peterborough, ON Canada

16:00 **(I079)** A NEW RAPID TECHNIQUE TO MEASURE ^{226}RA CONCENTRATIONS IN WATER. Andy Z. Zhou, Xiaolei. Zhao and **R. Jack Cornett**, A.E. Lalonde Laboratory for Accelerator Mass Spectrometry, University of Ottawa, Ottawa, Canada.

16:20 **(I047)** A CPE METHOD TO PRE-CONCENTRATE AND EXTRACT RADIONUCLIDES FROM ENVIRONMENTAL MATRICES. **Anthony Tremblay** and Dominic Larivière, Radioecology laboratory, Chemistry Department, Laval University.

16:40 **(I074)** THE ACCURATE DETERMINATION OF RADIONUCLIDES WITHOUT PRIOR CHEMICAL SEPARATION OF INTERFERENCES USING AN AGILENT ICP-MS/MS. **Pamela Wee**, Agilent Technologies Canada Inc.

17:00 End of session

17:00-18:00 Non-student poster session (authors present) - *Jonquière/Lauzon*

(I001) SAMPLE PREPARATION METHODS FOR DETERMINATION OF PHTHALATE ESTERS IN FOOD SAMPLES BY GAS CHROMATOGRAPHY. **Wanna Kanchanamayoon** and Sutthirak Uansiri, Creative Chemistry and Innovation Research Unit, Department of Chemistry, Faculty of Science, Mahasarakham University, MahaSarakham 44150, Thailand.

(I015) NANOPARTICLE SIZE AND ZETA POTENTIAL USING TUNEABLE NANOPORE RESISTIVE PULSE SENSING (TRPS) TECHNOLOGY. **Mary-Luyza Avramescu**[1], Pat .E. Rasmussen[1,2], [1]Environmental Health Science and Research Bureau, Environmental and Radiation Health Sciences Directorate, HECSB, Health Canada, Ottawa, ON, [2]Earth and Environmental Sciences Department, University of Ottawa, Ottawa, ON

(I061) SPECIATION ANALYSIS OF ARSENIC IN MILK: METHOD DEVELOPMENT AND APPLICATION TO THE FRENCH SURVEILLANCE PLAN CONCERNING MILK CONTAMINATION BY ARSENIC SPECIES. A. Leufroy, R. Chekri, J. Zinck, N. Marchond, **T. Guérin** and P. Jitaru

(I066) DEVELOPMENT AND APPLICATION OF A NOVEL ANALYTICAL APPROACH BASED ON ASYMMETRIC FLOW FIELD FLOW FRACTIONATION COUPLED TO ICP-MS FOR TIO_2 NANOPARTICLES DETERMINATION IN FOOD. Lucas Givelet[a], D. Boutry[a], S. Motellier[a], P. Jitaru[b], **T. Guérin**[b] and J-F. Damlencourt[a], [a] CEA Grenoble, Laboratoire de Recherche en Nanosécurité, Grenoble, France ; [b] Université de Paris-Est, Anses, Laboratoire de Sécurité des Aliments, Maisons-Alfort, France

(I089) DEVELOPMENT OF METHODS FOR THE CHARACTERIZATION OF A 12 M KOH ZINCATE FUEL FOR GREEN ENERGY BACKUP SYSTEMS USING FLOW INJECTION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY**. Tia Anderlini** and Diane Beauchemin**,** Department of Chemistry. Queen's University, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada

18:00-22:00 Short course on Inductively Coupled Plasma Spectrometry (dinner included in course registration fee) – *Brébeuf/Kent*

or

18:00 Relaxed Networking at L'Inox Brewpub

WEDNESDAY, JUNE 21, MORNING

Food safety – *Wolfe/Montcalm*

Organizers and co-Chairs: Nausheen Sadiq and Diane Beauchemin

8:40 **(I054)** CHROMIUM SPECIATION ANALYSIS IN DAIRY AND CEREAL PRODUCTS BY HPLC-ICPMS. **T. Guérin**[1], F. Hernandez[1], N. Bemrah[1], F; Cormant[1], F. Séby[2], L. Noël[1], P. Jitaru[1], [1]Université Paris-est, Anses, Laboratoire de Sécurité des Aliments, Maisons-Alfort, France ; [2]UT2A, Pau, France.

9:20 **(I050)** INORGANIC ARSENIC SPECIATION IN RICE AND RICE-BASED PRODUCTS USING HYDRIDE GENERATION ATOMIC ABSORPTION SPECTROMETRY (HG AAS). **Dirce Pozebon**, Greice Magalhães dos Santos, Camila Cerveira and Diogo P. de Moraes. Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves 9500, 91501-970, Porto Alegre, RS, Brazil

9:40 **(I087)** INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY WITH ON-LINE LEACHING: A METHOD TO ASSESS THE MAXIMUM BIO-ACCESSBLILITY OF TOXIC AND ESSENTIAL ELEMENTS IN WHEAT FROM SAUDI ARABIA. **Randa Althobiti** and Diane Beauchemin, Department of Chemistry. Queen's University, 90 Bader Lane. Kingston, Ontario K7L 3N6, Canada.

10:00 Isospark Coffee Break - *Foyer*

10:40 **(I051)** MULTIELEMENT DETERMINATION IN VEGETABLES USING LA-ICP-MS. **Valderi Luiz Dressler**, Matheus A. G. Nunes. Department of Chemistry, Federal University of Santa Maria, Av. Roraima 1000, 97105-900, Santa Maria, RS, Brazil.

11:00 **(I049)** DEVELOPMENT OF LC-MS/MS BASED PROTOCOLS FOR THE NON-TARGETED ANALYSIS OF FOOD CONTAMINANTS**. Stéphane Bayen**, L. Tian, A. von Eyken, Department of Food Science and Agricultural Chemistry, McGill University, 21111 Lakeshore, Ste Anne de Bellevue, QC

11:20 **(I046)** NON-TARGETED IDENTIFICATION OF ORGANIC MIGRANTS FROM REUSABLE PLASTIC BOTTLES USING LC-MS: INFLUENCE OF THE DATA POST-PROCESSING. **L.Tian***, S.* Bayen, Department of Food Science and Agricultural Chemistry, McGill University, 21111 Lakeshore, Ste Anne de Bellevue, QC

11:40 **(I090)** MULTI-ELEMENTAL RISK ASSESSMENT OF TOXIC AND ESSENTIAL ELEMENTS IN OAT CEREAL USING ION EXCHANGE CHROMATOGRAPHY COUPLED TO INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Nausheen Sadiq** and Diane Beauchemin, Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada

12.00 Lunch – *Foyer* & Exhibition Hall and Poster session - *Jonquière/Lauzon,*
Nu Instruments Luncheon Seminar - *Duquesne*

Separations

Organizer and Chair: Alison Holliday

9:00 **(I032)** CAPILLARY AND MICROCHIP ELECTROPHORESIS FOR FLUORESCENCE-BASED ASSAYS OF ENZYME ACTIVITY IN *DICTYOSTELIUM*. Kathy Rodogiannis, Jessica T. Duong, Kunwei Yang, and **Michelle L. Kovarik**. Department of Chemistry, Trinity College, 300 Summit St. Hartford, CT 06106.

9:40 **(I039)** INVESTIGATION BY LIQUID CHROMATOGRAPHY OF A MIXED-MODE STATIONARY PHASE BASED ON BILE ACID OLIGOMERS AS INVERTIBLE AMPHIPHILIC POCKETS. **V. Dionne-Dumont**, M. Zhang, N. Lévaray, X.X. Zhu and K.C. Waldron, Départment de chimie, Université de Montréal

10:00 Isospark Coffee Break - *Foyer*

10:40 **(I036)** AUTOMATED ENZYME MICROREACTOR FABRICATION FOR PROTEOMICS APPLICATIONS: EVALUATION BY CZE, HPLC AND MS. G. Ghafourifar, A. Fleitz, B. Fleury and **K.C. Waldron**. Department of Chemistry, Université de Montréal, Montréal, QC.

11:20 **(I040)** CAPILLARY ELECTROPHORESIS FOR DETECTION OF PEPTIDE FOLDING INTERMEDIATES. John D. Barr,[1] Amanda M. Miller,[1] Liuqing Shi,[2] David E. Clemmer,[2] and **Alison E. Holliday**[1], [1]Department of Chemistry, Moravian College, Bethlehem, PA

12:00 Lunch – *Foyer* & Exhibition Hall and Poster session - *Jonquière/Lauzon,*
Nu Instruments Luncheon Seminar - *Duquesne*

COMPLIMENTARY WORKSHOP

Image Analysis – *Crémazie/Garneau*

Instructor: Jesse Greener

9:00 **(W1)** Image analysis workshop using powerful open-access image analysis software, ImageJ. Participants will gain hands on experience to analyse sample data sets, which include 2D, 3D images and videos. Various concepts will be covered related to: (i) setting up your workspace environment, (ii) image display enhancements and (iii) image manipulation and analysis, and (iv) special topics.

12:00 Lunch – *Foyer* & Exhibition Hall and Poster session - *Jonquière/Lauzon,*
Nu Instruments Luncheon Seminar - *Duquesne*

WEDNESDAY, JUNE 21, AFTERNOON

Nanomaterials and their analysis – *Wolfe/Montcalm*

Organizers and co-Chairs: Ram Lamsal and Diane Beauchemin

13:40 **(I026)** ANALYSIS OF SMALL NANOPARTICLES BY SP-ICP-MS- LOWER SIZE DETECTION LIMITS THROUGH INSTRUMENTAL IMPROVEMENTS AND DATA TREATMENT. Madjid Hadioui and **Kevin J. Wilkinson**. Biophysical Environmental Chemistry Group, Department of Chemistry, University of Montreal, QC

14:00 **(I097)** SYNTHESIS OF BIMETALLIC HOLLOW AgM NANOPARTICLES, STRUCTURE AND COMPOSITION ANALYSIS. **Josée R. Daniel**,[1] Sadegh Yazdi,[2] Lauren McCarthy,[2] Emilie Ringe[2] and Denis Boudreau[1], [1]Département de chimie et Centre d'optique, photonique et laser (COPL), Université Laval, Québec (QC), G1V 0A6, Canada; [2]Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, 77005, USA.

14:20 **(I055)** ADVANCEMENTS IN SINGLE PARTICLE ICP-MS – SIGNIFICANT INSTRUMENT SETTINGS AND THEIR IMPLICATIONS ON DATA QUALITY. Chady Stephan, Samad Bazargan, Hamid Badiei, Aaron Hineman**, Andrew Rams**. PerkinElmer Inc., Woodbridge, ON

14:40 **(I043)** SIZE AND NUMBER QUANTIFICATION OF Ag NANOPARTICLES IN NATURAL WATERS USING SINGLE PARTICLE ICP-MS. **Karla Newman**, Water Quality Center, Trent University, 1600 West Bank Drive, Peterborough, ON

15:00 Elemental Scientific Coffee Break - *Foyer*

15:40 **(I056)** SP-ICP-MS TECHNIQUE FOR THE ANALYSIS AND THE STABILITY STUDY OF METAL NANOPARTICLES IN BIOLOGICAL FLUIDS. **Ciprian M Cirtiu**, Institut National de Santé Publique du Québec, Centre de Toxicologie du Québec.

16:00 **(I021)** SINGLE CELL ICP-MS ANALYSIS: QUANTIFYING THE UPTAKE OF METALS BY UNICELLULAR ORGANISMS ON A CELLULAR LEVEL. Ruth Merrifield[1], Lauren Amable[2], Jamie Lead[1], **Andrew Rams**[3], Chady Stephan[3], [1]Center for Environmental NanoScience and Risk (CENR), Department of Environmental health sciences, Arnold School of Public Health, University of South Carolina, Columbia SC, [2]Division of Intramural Research, National Institute on Minority Health and Health Disparities, National Institutes of Health, 9000 Rockville Pike, Bethesda, Maryland, 20892, [3]PerkinElmer Inc. Shelton, CT

16:20 **(I068)** GRAPHENE QUANTUM DOTS: DEPOSITION ON POLYDOPAMINE-MODIFIED TiO_2 NANOPARTICLES. **Edward P.C. Lai** and Kaiyu Wang, Department of Chemistry, Carleton University, Ottawa, ON

16:40 **(I083)** SINGLE PARTICLE INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY METHOD FOR THE CHARACTERIZATION OF PLATINUM NANOPARTICLES FOR FUEL CELL APPLICATIONS. **Ram P. Lamsal**[a], Sadaf Tahamasebi[a], Gregory Jerkiewicz[a], Stève Baranton[b], Christophe Coutanceau[b], Aaron Hineman[c], Chady Stephan[c] and Diane Beauchemin[a], [a]Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada; [b]Université de Poitiers IC2MP, 4 Rue Michel Brunet, B27, TSA 51106, 86073 Poitiers cedex 9, France; [c]Perkin Elmer Canada, 501 Rowntree Dairy Rd, Unit 6, Woodbridge, ON, L4L 8H, Canada

17:00 End of session

17:00-17:30 Student poster session (authors present) - *Jonquière/Lauzon*

17:00-18:00 Food Truck Event in Hotel Parking Lot (behind the Hotel)

18:05 Bus boarding in front of the hotel (destination Québec Harbour)

19:00-22:00 Complimentary boat tour (no meal included)

Imaging – *Crémazie/Garneau*

Organizer and Chair: Jesse Greener

13:40 **(I041)** SUPER-RESOLUTION FLUORESCENCE MICROSCOPY AS A TOOL FOR THE CHARACTERIZATION OF CELLULOSE NANOSTRUCTURE. Mouhanad Babi and **Jose Moran-Mirabal**, Department of Chemistry and Chemical Biology, McMaster University

14:20 **(I012)** REAL-TIME IMAGING OF pH VARIATIONS IN MICROCHANNELS USING FLUORESCENT NANOPARTICLES. **Jérémie Asselin**, Mazeyar P. Gashti, Denis Boudreau, Jesse Greener. Université Laval.

14:40 **(I006)** EVALUATION OF NANOPARTICLE DISPERSION USING DIFFERENT MICROSCOPIC TECHNIQUES, **R. Lussier**, Université Laval

15:00 Elemental Scientific Coffee Break - *Foyer*

15:40 **(I024)** FORM SINUSOIDAL WAVES LAMINAR CO-FLOW IN MICRO DEVICES BY USING MICRO-MANAGER TO CONTROL FLOW RATE. **Nan Jia**, Jesse Greener, Department of Chemistry and Centre de recherche sur les matériaux avancés (CERMA), Université Laval, Québec, QC

16:00 **(I029)** CONFOCAL LASER SCANNING MICROSCOPY AND ELECTROCHEMICAL STUDY ON MICROFLUIDIC MICROBIAL FUEL CELL. **Mehran Abbaszadeh Amirdehi**, Jesse Greener, Université Laval, Québec, QC

16:20 **(I035)** THE USE OF MICRO-IMAGING TECHNIQUES TO ANALYZE BIOFILM DEVELOPMENT DATA IN MICROCHANNEL. **Farnaz Asayesh**, Jesse Greener, Department of Chemistry, Laval University, Quebec, QC

16:40 **(I037)** A COMBINED OPTICAL MICROSCOPY AND INFRARED SPECTRAL MICROSCOPY APPROACH FOR *IN-SITU* STUDYING OF BIOFILMS. **Mohammad Pousti**, Jesse Greener, Department of Chemistry, Laval University, Quebec, QC

17:00 End of session

17:00-17:30 Student poster session (authors present) - *Jonquière/Lauzon*

17:00-18:00 Food Truck Event in Hotel Parking Lot (behind the Hotel)

18:05 Bus boarding in front of the hotel (destination Québec Harbour)

19:00-22:00 Complimentary boat tour (no meal included)

17:00-17:30 Student poster session (authors present) - *Jonquière/Lauzon*

(I007) IMPROVING THE ANALYTICAL PERFORMANCE OF ETV-ICPOES VIA A MIXED-GAS PLASMA. **Guilherme L. Scheffler**,[a] Dirce Pozebon,[a] and Diane Beauchemin[b]. [a.] Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves, 9500, 91501-970 Porto Alegre, RS, Brazil. [b.] Department of Chemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada.

(I044) CLOUD POINT EXTRACTION OF PLUTONIUM IN FISH TISSUES COUPLED TO ALPHA SPECTROMETRY. **Alexa Leblanc** and Dominic Larivière, Radioecology laboratory, Chemistry Department, Laval University.

(I082) SINGLE PARTICLE ANALYSIS USING MIXED-GAS INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY, **Lucas Choma** and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada.

(I088) INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY WITH ON-LINE LEACHING TO ASSESS THE MAXIMUM BIO-ACCESSBLILITY OF TOXIC AND ESSENTIAL ELEMENTS IN NATURAL TOOTHBRUSH FROM SAUDI ARABIA. **Randa Althobiti** and Diane Beauchemin, Department of Chemistry. Queen's University, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada

(I094) ASSESSMENT OF NI-BASED ELECTRODE STABILITY IN ALKALINE FUEL CELLS THROUGH THE DEVELOPMENT OF ICP-MS METHODS FOR BASIC ELECTROLYTE SOLUTIONS. **Alexa Mainguy**, Nausheen Sadiq and, Diane Beauchemin* Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K6L 3N6

(I092) PRE-CONCENTRATION OF NICKEL IN ALKALINE FUEL CELL ELECTROLYTE FOR ANALYSIS BY INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY. **Suhaylah Sequeira** and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6

(I075) NOVEL DESIGN OF INFRARED-HEATED INTEGRATED SAMPLE INTRODUCTION SYSTEM FOR IMPROVING ANALYTICAL PERFORMANCE OF INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY. **Ahmed Al Hejami** and Diane Beauchemin, Chemistry Department, Queen's University, Kingston, Ontario, Canada

(I095) SLURRY NEBULIZATION AND INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY WITH A MIXED-GAS PLASMA FOR THE ANALYSIS OF VEGETATION SAMPLES. **R. Teuma-Castelletti** and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6

17:00-18:00 Food Truck Event in Hotel Parking Lot (behind the Hotel)

18:05 Bus boarding in front of the hotel (destination Québec Harbour)

19:00-22:00 Complimentary boat tour (no meal included)

THURSDAY, JUNE 22, MORNING

Speciation analysis – *Wolfe/Montcalm*

Organizers and co-Chairs: Nausheen Sadiq and Diane Beauchemin

9:00 **(I070)** TOWARDS UNDERSTANDING OF METHYLMERCURY TOXICITY**, Z. Gajdosechova**[a,b], M. M. Lawan[a], D. S. Urgast[a], A. Raab[a], K. G. Scheckel[c], E. Lombi[d], P. M. Kopittke[e], K. Loeschner[f], E. H. Larsen[f], G. Woods[g], A. Brownlow[h], F. L. Read[i], J. Feldmann[a], E. M. Krupp[a], [a]TESLA, University of Aberdeen, UK. [b]NRC, Ottawa, Canada [c]US EPA, National Risk Management Research Laboratory, Cincinnati, USA. [d]Future Industries Institute, University of South Australia, South Australia. [e]School Agriculture and Food Sciences, The University of Queensland, Australia. [f]National Food Institute, Technical University of Denmark, Denmark. [g]Agilent Technologies UK. [h]SAC Wildlife Unit, UK. [i]Oceanlab, University of Aberdeen, UK

9:40 **(I071)** TRACE METAL SPECIATION IN A MULTIVITAMIN CANDIDATE REFERENCE MATERIAL. **Kelly LeBlanc**, Lucia D'Ulivo, Kenny Nadeau, Indumathi Pihillagawa Gedara, Lu Yang, Zoltan Mester. National Research Council of Canada.

10:00 Isospark Coffee Break - *Foyer*

10:40 **(I014)** METAL SPECIATION IN NATURAL WATERS USING HIGH RESOLUTION MASS SPECTROMETRY. **C. Guéguen**, T. Nguyen Quoc, V. Mangal. Trent University, Peterborough, ON.

11:20 **(I072)** OVERCOMING CHALLENGES OF Hg SPECIES QUANTIFICATION IN PETROLEUM HYDROCARBONS. **Z. Gajdosechova**[a,b], M. S. Boskamp[a], F. Lopez-Linares[c], J. Feldmann[a], E. M. Krupp[a]. [a]TESLA, University of Aberdeen, UK , [b]NRC, Ottawa, Canada, [c]Chevron Energy Technology Company, USA

11:40 **(I091)** SPECIATION ANALYSIS OF NICKEL IN ALKALINE FUEL CELL ELECTROLYTE BY ION CHROMATOGRAPHY COUPLED TO INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Nausheen Sadiq**, Sadaf Tahmasebi, Gregory Jerkiewicz and Diane Beauchemin, Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada

12:00 Lunch – *Foyer* & CSASS Annual General Meeting – *Wolfe/Montcalm*

12:00-14:00 Dismantling of exhibition

Microfluidics I – *Crémazie/Garneau*

Organizer and Chair: Jesse Greener

9:00 **(I060)** HIGHLY-MINIATURIZED AND LOW POWER POTENTIOSTAT FOR ON-CHIP ELECTROCHEMICAL SENSING. [1]Jessy Mathault, [1,2] Samuel Morneau-Gamache, [1]Elnaz Ghodsevali, [1]Hamza Landari, [3]Mounir Boukadoum, [2]Élodie Boisselier, [1]**Amine Miled**, [1]LABioTRON Bioeng. Research Laboratory, ECE Dept. Université Laval, Québec, QC.

9:40 **(I010)** LOCALIZED QUANTIFICATION OF pH USING FLUORESCENT NANOSENSORS IN SINGLE-PARTICLE TRACKING ANALYSES. **Jérémie Asselin**, Denis Boudreau, Université Laval.

10:00 Isospark Coffee Break - *Foyer*

10:40 **(I025)** HYDRODYNAMIC EFFECTS ON BIOFILM AT THE BIOINTERFACE USING A MICROFLUIDIC ELECTROCHEMICAL CELL: CASE STUDY OF PSEUDOMONAS SP. **Mirpouyan Zarabadi**[1], François Paquet-Mercier[1], Steve Charette[2], Jesse Greener[1], Département de chimie[1] and Département de biochimie, de microbiologie et de bio-informatique[2], Faculté des sciences et de génie, Université Laval, Québec, QC

11:00 **(I063)** SPINNING FLUIDS FOR POINT-OF-CARE DIAGNOSTICS. **Maurice Boissinot**, CHU de Québec-Université Laval

11:40 **(I023)** PHOTOTHERMAL MICROFLUIDIC CANTILEVER DEFLECION SPECTROSCOPY REFLECTING CLUSTERING MECHANISM OF ETHANOL WATER MIXTURES. **M. S. Ghoraishi**, J. E. Hawk, T. Thundat, Chemical and Material Engineering Department, University of Alberta, Canada

12:00 Lunch - *Foyer* & CSASS Annual General Meeting – *Wolfe/Montcalm*

12:00-14:00 Dismantling of exhibition

THURSDAY, JUNE 22, AFTERNOON

Forensic Applications – *Wolfe/Montcalm*

Organizers and co-Chairs: Lily Huang and Diane Beauchemin

13:40 **(I076)** TRACE ELEMENT AND ISOTOPE ANALYSES OF MICRO-SOLDERING LEAD-BASED METAL ASSOCIATED TO IMPROVISED EXPLOSIVE DEVICE (IED) BY ICP-MS, AND FORENSIC ASSOCIATION WITH ORIGIN. **Claude Dalpé** and Nigel G.R. Hearns. Royal Canadian Mounted Police, National Forensic Laboratory Services, Ottawa, Canada.

14:20 **(I002)** PAINT IDENTIFICATION USING VIBRATIONAL SPECTROSCOPY FROM MIR TO THz SPECTRAL RANGE. **Sergey Shilov**, Tom Tague, Pang Wang, Bruker Optics, 19 Fortune Dr., Billerica, MA, USA.

14:40 **(I042)** FORENSIC ANALYSIS OF AUTOMOTIVE PAINT CHIPS FOR VEHICLE MANUFACTURER, COLOUR AND YEAR OF PRODUCTION USING ELECTROTHERMAL VAPORIZATION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY. **L. Huang** and D. Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K6L 3N6

15:00 Glass Expansion Coffee Break - *Foyer*

15:40 **(I093)** FORENSIC ANALYSIS OF HUMAN NAIL FOR GENDER AND ETHNICITY USING ELECTROTHERMAL VAPORIZATION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY. A. Schug and **D. Beauchemin**, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K6L 3N6

16:00 **(W2) COMPLIMENTARY WORKSHOP:** FORENSIC SCIENCE AND REVERSE ENGINEERING UNING VIBRATIONAL SPECTROSCOPY. **Sergey Shilov**, Bruker Optics, USA

17:00 End of session

19:00-22:00 Closing Reception (ticket required) - *Duquesne*

Microfluidics II – *Crémazie/Garneau*

Organizer and Chair: Jesse Greener

13:40 **(I028)** RELEASE OF MESOPOROUS SILICA PARTICLES BY FREE STANDING PH SENSITIVE MEMBRANES. **Nan Jia**,[a] Erica Rosella,[a] Estelle Juèrea,[b] Freddy Kleitza,[b] Jesse Greener[a], [a]Department of Chemistry and Centre de recherche sur les matériaux avancés (CERMA), Université Laval, Québec, Québec G1V 0A6, Canada, [b]Institute of Inorganic Chemistry – Functional Materials, University of Vienna, Währinger Straße 42, 1090 Vienna, Austria.

14:00 **(I003)** A MULTILAYER FLOW MODEL FOR NON-INTRUSIVE BIOFILM VISCOSITY MEASUREMENTS. J. Greener,[1] M. Parvinzadeh Gashti,[1] A. Eslami,[2] M. P. Zarabadi,[1] and **S. M. Taghavi**[2] Departments of Chemistry[1] and Chemical Engineering[2], Université Laval, 1045 Ave. de la Médecine, Quebec, Quebec G1V 0A6

14:40 **(I038)** SPECTROSCOPIC IMAGING IN MICROCHANNELS FOR STUDIES OF BIOFILMS. **Mohammad Pousti**, Jesse Greener, Department of Chemistry, Laval University, Quebec, QC

15:00 Glass Expansion Coffee Break - *Foyer*

15:40 **(I030)** ELECTROCHEMICAL IMAGING FOR MICROFLUIDICS: A FULL-SYSTEM APPROACH. **Mehran Abbaszadeh Amirdehi**, Jesse Greener, Université Laval, Québec, QC

16:00 **(I034)** MICROFLUIDIC CO-FLOWS FOR A SELF-STANDING COLLAGEN MEMBRANE SYNTHESIS. **Erica Rosella**[a], Nan Jia[a], Diego Mantovani[b], Jesse Greener[a], [a]Dept. of Chemistry, Laval University, Quebec city, QC, G1V 0A6, [b]Lab. of Biomaterials and Bioengineering, CRC-I, Dept. of Min-Met--Materials Eng. & CHU Research Center, Laval University, Quebec

16:20 **(I096)** GONE BUT NOT FORGOTTEN: PATTERNING AND ENHANCED BIOFILM GROWTH BY TEMPORARILY WALL ADHERED BUBBLES IN MICROFLUIDIC FLOW CELLS. **Jesse Greener**, Department of Chemistry, Laval University.

17:00 End of session

19:00-22:00 Closing Reception (ticket required) - *Duquesne*

FRIDAY, JUNE 23, MORNING

Environmental applications – *Crémazie/Garneau*

Organizers and co-Chairs: Tia Anderlini and Diane Beauchemin

9:00 **(I086)** NOVEL EXPERIMENTAL APPROACH FOR ATRAZINE-SOIL CHEMISTRY MODELS. **Marc Lamoureux**, Donald S. Gamble, and Hanan Malibari, Department of Chemistry, Saint Mary's University, Halifax, NS, B3H 3C3

9:40 **(I013)** IN SITU VIBRATIONAL SPECTROSCOPY FOR ENVIRONMENTAL APPLICATIONS RELATED TO ARSENIC REMOVAL TECHNOLOGIES. **Hind A. Al-Abadleh**. Department of Chemistry and Biochemistry, Wilfrid Laurier University, Waterloo, ON N2L 3C5

10:00 Agilent Coffee Break - *Foyer*

10:40 **(I080)** FORMATION, UPTAKE AND METABOLISM OF SELENIUM SPECIES BY FRESHWATER ALGAE. **Dirk Wallschläger**, Kelly LeBlanc, Sarah D'Amario and Denina Simmons. Trent University, Peterborough, ON.

11:20 **(I004)** DIRECT ANALYSIS OF AIR FILTERS FOR TOXIC ELEMENTS SCREENING USING A MIXED-GAS PLASMA AND ETV-ICPOES. **Guilherme L. Scheffler**,[a] Nausheen Sadiq,[b] Dirce Pozebon,[a] and Diane Beauchemin[b]. [a.]Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves, 9500, 91501-970 Porto Alegre, RS, Brazil. [b.]Department of Chemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada.

11:40 **(I085)** INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY COUPLED TO A MULTI-MODE SAMPLE INTRODUCTION SYSTEM WITH AN INFRARED HEATED PRE-EVAPORATION TUBE FOR THE ANALYSIS OF WASTE WATERS. **Tia Anderlini** and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada

12:00 End of the 61st ICASS


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Résumés de Spectr'Atom 2017
en ordre de présentation

(O = Oral, A = Affiche)

O 1-1

HAUTES PRÉCISIONS, HAUTES SENSIBILITÉS, SPÉCIATION ET ISOTOPIE : DE NOUVELLES OUVERTURES POUR UNE MEILLEURE COMPRÉHENSION DE L'ÉCODYNAMIQUE DES MÉTAUX ET MÉTALLOÏDES DANS L'ENVIRONNEMENT

Olivier F.X. Donard, Sylvain Bérail, Emmanuel Tessier, Oriol Baltrons, David Amouroux
Center of Mass Spectrometry for Reactivity and Speciation Sciences (MARSS)
Institut des Sciences Analytique et de Physicochimie pour l'Environnement et les Matériaux, Université de Pau et des Pays de l'Adour, France

La spectrométrie atomique nécessite l'atomisation de l'élément pour pouvoir l'étudier. Mais il est maintenant reconnu et accepté que les éléments dans les échantillons étudiés existent sous différentes formes physicochimiques. Les formes chimique des éléments leurs confèrent leurs propriétés en ce qui concerne leurs aspects essentiels ou caractère toxique. De la même façon, leurs formes chimiques vont étroitement conditionner leurs transferts et devenir dans les différents compartiments de l'environnement. Il faut donc extraire le maximum d'information de l'analyse « inorganique ». Le développement récent des méthodes couplées (chromatographies liquides ou gazeuses) avec l'ICP/MS (Inductively Coupled Plasma/Mass Spectrometry) a permis de faire des avancées considérables dans ce sens et ouvert de nouvelles voies en ce qui concerne la compréhension et l'impact des formes chimiques des métaux dans l'environnement et tous les secteurs de l'agroalimentaire et de l'industrie. Dans la même dynamique, le développement de l'ICP/MS à Multicollection permet aussi maintenant d'avoir une mesure fiable et précise de la signature isotopique des éléments non traditionnels. L'isotopie fait partie du concept de spéciation définie au sens de l'IUPAC. Nous avons développé de nouvelles approches en combinant aussi les méthodes de séparation (chromatographie en phase gazeuse) couplées à l'ICP/MS à Multicollection. Cela nous permet maintenant d'associer une signature isotopique à une forme chimique dans un élément et même échantillon ce qui permet de poser ainsi de nouvelles questions fondamentales.

Le développement de méthodes couplées permets maintenant de faire la détermination totale du Hg en ultra Traces au niveau de quelques ng/L comme le couplage avec une chromatographie avec injection avec de gros volume permets aussi de faire la spéciation du Hg (Hg°, Hg inorganique et formes méthylées) au niveau de quelques ng/L également. Enfin, les stratégies de pré-concentration en ligne avec désorption directe en ICP/MS à Multicollection, en développement, permettront d'entrevoir de faire la détection du Pb, Cd, Cu, et autres éléments d'intérêt pour la directive européenne cadre sur l'eau directement au niveau du ng/L. Tous ces résultats ont été réalisées également grâce à une gestion avancée des signaux transitoires afin d'obtenir les meilleures précisions possibles dans des conditions d'intégrations difficiles. L'ensemble de ces avancées permettront d'ouvrir de nouveaux champs d'investigation dans le domaine de l'environnement et des milieux aquatiques qui sont fragiles On sera bientôt en mesure d'associer isotopies, origine, et formes chimiques ce qui amènera un éclairage nouveau pour déconvoluer les mécanismes de réactivité et transferts des métaux et métalloïdes dans les différents compartiments de l'environnement.

O 1-2

STRATÉGIE ANALYTIQUE POUR LA RÉSOLUTION DE PROBLÉMATIQUES RELIÉES À LA PRÉSENCE DE FONDANT DANS UNE SOLUTION PRÉPARÉE PAR FUSION

Maxime Gagnon[1], Mathieu Bouchard[2], Mathieu Hamel[2], Dominic Larivière[1].
1. Département de chimie, Université Laval. 2. Claisse, Québec, Canada

Les analyses par plasma à induction (ICP) ou par micro-ondes (MIP) sont parmi les méthodes d'analyses les plus fiables et les plus communes pour la détermination de métaux, incluant ceux pertinents pour le domaine minier. Ces appareils sont polyvalents et permettent des analyses multiélémentaires avec d'excellentes sensibilités. Cependant, l'introduction d'échantillons solide par ces approches atomiques nécessite une mise en solution (complète ou partielle) préalable de ces derniers. De nombreuses études comparatives ont été publiées concernant ces modes de mises en solution pour divers analytes. Pour des matrices et des éléments réfractaires, la fusion permet généralement une mise en solution plus complète et de façon plus rapide que les autres approches énumérées précédemment. Néanmoins, la digestion par fusion possède certaines limitations reliées à la mesure des métaux. Celles-ci incluent la pureté du fondant ainsi que la charge élevée en sel qui peuvent influencer la qualité des résultats analytiques et la durée de vie de certaines pièces d'équipement.

Par conséquent, il est donc essentiel de réduire la charge en sel des échantillons dissout par fusion avant leur introduction dans le système d'analyse. Ceci peut être effectué à l'aide d'approches analytiques basées sur des principes de séparation chromatographiques. Pour ce projet, le défi sera de valider la compatibilité entre la fusion au peroxyde de sodium automatisée et la séparation chromatographique pour certains métaux pour des analyses par MP-AES.

O 1-3

UTILISATIONS D'UN MIP-AES AU DÉPARTEMENT DE GÉNIE DES MINES, DE LA MÉTALLURGIE ET DES MATÉRIAUX DE L'UNIVERSITÉ LAVAL : LA DÉCOUVERTE D'UN INSTRUMENT D'ANALYSE ÉLÉMENTAIRE ÉCONOMIQUE ET POLYVALENT

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Depuis deux ans, le département de génie des mines, de la métallurgie et des matériaux de l'Université Laval possède un spectromètre à émission atomique à plasma induit par micro-onde (MP-AES 4200) de Agilent Technologies. Depuis son acquisition, cet instrument a permis de produire des analyses élémentaires pour différentes applications de recherche académique dans le domaine minier, de la métallurgie et environnemental. La présentation fait le survol de l'utilisation du MP-AES et des résultats pour différentes applications. Dans le domaine de la production des éléments de terres rares (ETR), l'instrument permet de générer des analyses élémentaires pour le minerai initial, les étapes de traitement du minerai et la séparation des ETR par extraction par solvant. Le MP-AES permet d'analyser avec justesse la majorité des ETR et des impuretés (Fe, Mg, Ca,…). Dans le domaine de la production du fer, le MP-AES est adéquat pour l'analyse du concentré haute teneur en fer, mais aussi de l'alimentation et des rejets du procédé. Dans le domaine de la production de l'or, l'instrument permet l'analyse de faible teneur en or dans les solutions de cyanuration. En raison de ses faibles coûts d'utilisation et sa polyvalence dans les nombreux domaines des mines et de la métallurgie, le MP-AES est devenu un instrument indispensable à l'avancement des projets de recherches du département.

O 1-4

TENEURS EN ELEMENTS TRACES METALLIQUES PRESENTS DANS DES VIANDES ISSUS DE FILIERES BIOLOGIQUE OU CONVENTIONNELLE

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Dans une note publiée en 2011, le conseil scientifique pour l'agriculture biologique souligne que 95% des consommateurs français citent la santé comme premier motif d'achat des produits « Bio ». Aucune étude scientifique ne démontre cependant clairement le bien-fondé de ces allégations. La question se pose par exemple pour les produits d'origine animale, qui sont susceptibles d'être contaminés par des micropolluants environnementaux, des mycotoxines ou des antibiotiques. Le projet SOMEAT a pour ambition de fournir des données scientifiques objectives pour évaluer les bénéfices et risques éventuels des systèmes de production de viande biologique au regard notamment de leurs teneurs en contaminants.

L'objectif de cette présentation est de vous révéler les teneurs en éléments traces métalliques (Cd, Pb, Hg, As Cu et Zn) obtenues dans 325 échantillons de muscles ou de foies de bovins, porcs et volaille issus de filières biologique ou conventionnelle d'élevages français.

Même si aucun dépassement des teneurs réglementaires (Rég. (EC) No 1881/2006) en Pb et en Cd n'a été observé, que les teneurs en contaminants (Pb, Cd, As et Hg) sont souvent très faibles et proches des limites de quantification, pour certains de ces éléments, une différence statistique significative a été observée entre les muscles ou foies issus de ces 2 filières. Des analyses en composantes principales ont été réalisées afin de tenter d'expliquer ces différences.

O 1-5

SPÉCIATION DU MERCURE SANGUIN PAR DILUTION ISOTOPIQUE SPME-GC-ICP-MS

Jean-Francois Bienvenu, Centre de Toxicologie du Québec, Québec, Canada

L'utilisation du mercure ne date pas d'hier et il est présent sous plusieurs formes dans notre environnement (métallique, organique et inorganique). Chacune de ces formes n'a pas le même degré de toxicité, et pour cette raison il est important de connaitre la quantité de chacune des formes présentes dans un échantillon. La spéciation des formes de mercure est obtenue par chromatographie en phase gazeuse suite à un échantillonnage par micro-extraction en phase solide automatisé. Être avant-gardistes apporte son lot de problématiques lors du développement de méthode d'analyse sur un nouvel instrument. Lors de cette présentation nous verrons quelques-uns des défis rencontrés par l'équipe du CTQ lors du développement et de la validation d'une méthode de spéciation des formes du mercure sanguin par SPME-GC-ICP-MS qui est présentement utilisée pour l'enquête canadienne sur les mesures de santé (ECMS) en collaboration avec le gouvernement du Canada.

O 1-6

ANALYSE DU 226-RA ET 210-PB ET ÉLIMINATION DES INTERFÉRENCES RÉSIDUELLES PAR SPECTROMÉTRIE DE MASSE EN TANDEM (ICP-MS/MS).

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Laboratoire de Radioécologie, Université Laval, Québec, Canada

La mesure de certains radionucléides est nécessaire pour déterminer le risque radiochimique que représentent certains échantillons environnementaux ou androgènes. Bien que l'analyse spectroscopique du radium 226 et du plomb 210 soit largement utilisée et présente des limites de détection et de quantification relativement faibles, la possibilité d'un instrument unique pour l'analyse de tous les paramètres environnementaux est séduisante.

Cependant pour atteindre des limites de quantification du même ordre que la spectrométrie alpha, il est souvent nécessaire de faire intervenir des modules tels que l'APEX pour permettre d'augmenter la sensibilité instrumentale. Ces modules, bien que largement répandus et utilisés pour augmenter les performances sont rarement compatibles avec des instruments de routine.

C'est pourquoi, nous avons mis en place deux nouvelles méthodes instrumentales sur un ICP-MS/MS 8800 d'Agilent Technologies ; une pour le radium 226 et une pour le plomb 210. L'utilisation de la spectrométrie de masse en tandem couplée à une cellule de réaction et/ou de collision nous a permis de discriminer les interférences potentielles afin d'obtenir une mesure sélective de l'analyte. Lorsque ces méthodes sont couplées à des méthodes d'extraction, les limites de quantifications et de détection mesurée répondent aux exigences gouvernementales.

O 1-7

SPECIATION, QUANTIFICATION ET ISOTOPIE DES FORMES INORGANIQUES DU SOUFRE EN MILIEU AQUEUX.

Mathieu Martinez, Corinne Parat, Isabelle Le Hécho, IPREM, UPPA, Pau, France

La spéciation et la composition isotopique du soufre (δ34S) sont d'un grand intérêt pour l'étude du mécanisme de sulfato-réduction bactérien qui a lieu dans les eaux souterraines et qui fait intervenir différentes molécules soufrées telles que : SO42-, SO32-, S2O32- et HS-. L'ICP-MS à multi-collecteurs (MC-ICP-MS) a été mis en oeuvre dans un certain nombre d'études pour la détermination des isotopes stables du soufre. Un avantage majeur de cette technique est la possibilité de réaliser des couplages entre le MC-ICP-MS et différents systèmes de séparation ou d'introduction de l'échantillon (ablation laser, chromatographie liquide et gazeuse). Le challenge analytique est de mettre au point un couplage entre la chromatographie liquide et le MC-ICP-MS permettant d'obtenir la signature isotopique du soufre en tenant compte de sa spéciation au sein d'un même échantillon. Les difficultés liées à ce couplage sont multiples : il faut éviter un fractionnement isotopique lors de l'analyse, le biais de masse instrumental doit être corrigé et le δ34S doit être calculé à partir d'un signal transitoire. Dans ce but, une méthode de séparation chromatographique (échange d'ions) a été développée. A ce jour, cette méthode permet de séparer SO42-, SO32- et S2O32- (voir figure 1) ; une optimisation est en cours afin d'inclure HS- à la méthode. Cette technique couplée à un HR-ICP-MS ou un TQ-ICP-MS permet une quantification précise de chaque espèce. Le couplage avec un MC-ICP-MS permettra de calculer leur δ34S. Les étapes du développement de la méthode de séparation chromatographique, les premiers résultats de quantification dans des échantillons d'eaux souterraines naturelles et les travaux préliminaires obtenus par couplage LC-MC-ICP-MS seront présentés.

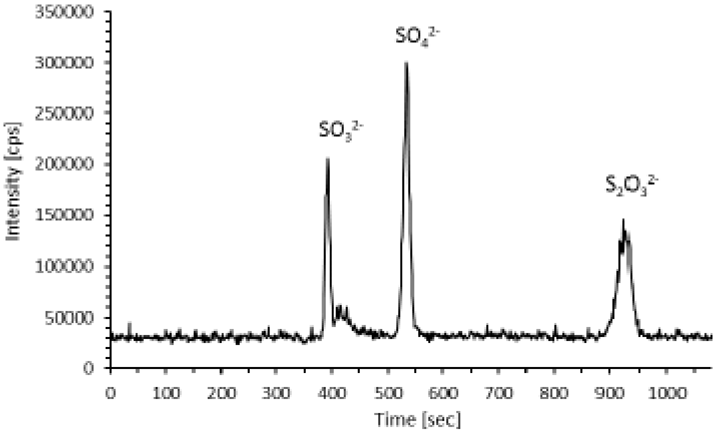

Figure 1: Analyse LC-ICP-HRMS d'une solution contenant 100 ppb-S de SO_3^{2-}, SO_4^{2-} et $S_2O_3^{2-}$.

O 1-8

L’ÉTALONNAGE INTERNE À L’AIDE D’ISOTOPES ENRICHIS : UNE APPROCHE ALTERNATIVE À LA DILUTION ISOTOPIQUE CONVENTIONNELLE POUR LE DOSAGE D’ÉLÉMENTS MULTI-ISOTOPIQUES PAR ICP-MS

Pierre Dumas, Centre de Toxicologie du Québec, Québec, Canada

La dilution isotopique est reconnue en métrologie comme une technique d’étalonnage primaire qui permet d’atteindre un haut niveau de précision et d’exactitude. Cette approche quantitative rigoureuse est généralement réservée à des dosages nécessitant la meilleure fiabilité analytique possible, telle que la certification de matériaux de référence. Elle s’avère cependant peu populaire pour l’analyse de routine, étant souvent jugée trop exigeante à réaliser.

L’auteur propose ici une stratégie d’étalonnage alternative à la dilution isotopique conventionnelle basée n’ont pas sur la quantité ajoutée d’un élément isotopiquement enrichi, mais sur l’utilisation de l’isotope enrichi à titre d’étalon interne pour les autres isotopes de l’élément. En combinant cet étalon interne à une courbe d’étalonnage conventionnelle, on obtient une courbe d’étalonnage par dilution isotopique (CEDI) aux propriétés inédites. La courbe réponse ainsi obtenue par ICP-MS/MS, de type polynomial degré 4, s’est avérée indépendante aux effets de matrices biologiques (sang, urine, plasma, tissus) pour le sélénium et le mercure, mais surtout stable sur une période de plusieurs mois voir même années, tout en fournissant une précision analytique de l’ordre de ± 2 % d’erreur.

L’efficacité de cette stratégie à a été mise à profit par le laboratoire afin de valider par CEDI-ICP-MS/MS la fiabilité des valeurs désignées par consensus en sélénium et en mercure dans les matériaux d’essais d’aptitude de leur programme d’assurance de la qualité externe QMEQAS

Cette nouvelle approche a pour mérite de faire bénéficier l’analyste, des mêmes avantages de la dilution isotopique conventionnelle, tout en simplifiant la procédure d’étalonnage, favorisant ainsi l’intégration de l’étalonnage par dilution isotopique aux analyses de routine.

O 2-1

OPTIMISATION DU SYSTÈME D'INTRODUCTION D'ÉCHANTILLON EN ICP-IR-MS SUR UN NEPTUNE THERMO

Laurent Bertal[1] et Abel Guihou[2],
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La première phase montre l'intérêt du débitmètre TruFlo de Glass Expansion pour mesurer l'influence des variations de température sur le débit d'échantillon entrant dans l'ICP. Les conséquences sur les mesures étant mises en évidence, la seconde phase décrit l'utilisation de la chambre thermostatée ISOMIST à la place du système d'origine et ses avantages en termes de stabilité, mais aussi de rendement analytique.

Dans une note publiée en 2011, le conseil scientifique pour l'agriculture biologique souligne que 95% des consommateurs français citent la santé comme premier motif d'achat des produits « Bio ». Aucune étude scientifique ne démontre cependant clairement le bien-fondé de ces allégations. La question se pose par exemple pour les produits d'origine animale, qui sont susceptibles d'être contaminés par des micropolluants environnementaux, des mycotoxines ou des antibiotiques. Le projet SOMEAT a pour ambition de fournir des données scientifiques objectives pour évaluer les bénéfices et risques éventuels des systèmes de production de viande biologique au regard notamment de leurs teneurs en contaminants.
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O 2-2

UN CONDENSÉ DES NOUVELLES TECHNOLOGIES D'ANALYSES INORGANIQUES PAR ICP-OES ET ICP-MS

Stephan Chady, Perkin Elmer

Single Particle ICP-MS (SP-ICP-MS) est devenue une méthode reconnue pour l'analyse de nanoparticules dans divers types d'échantillons tels que biologiques, environnementaux et industriels. Plusieurs paramètres et conditions instrumentales affectent la justesse, la précision et la reproductibilité de l'analyse dont l'effet matrice, le niveau du bruit de fond, l'efficacité de transport, le temps de lecture ainsi que le type de système d'introduction utilisé. L'intégration du signal joue un rôle primordial dans la qualité des données générées – intégration « intensité de signal vs aire de pic ». En se basant sur la technique SP-ICP-MS, Single Cell ICP-MS (SC-ICP-MS) vient de se développer comme étant une technique qui permet de mesurer le contenu en particules ou en fraction ionique dans des organismes unicellulaires. SC-ICP-MS nécessite un système d'introduction dédié qui permet de livrer des organismes unicellulaires de quelques microns de taille au plasma de l'ICP-MS.

O 2-3

Solutions par fusion au borate de lithium : pour « convaincre les réfractaires »

Benoît Bouchard, Jean-François Nolin, Katanax

La fusion au borate de lithium est reconnue dans le domaine de la spectroscopie par fluorescence aux rayons X (XRF) pour la qualité des résultats obtenus lors de l'analyse des disques de verre. Les vertus de cette technique de digestion sont par contre encore assez mal connues aux fins des analyses ICP. Il est en fait possible de tirer profit de tous les avantages de la digestion dans la matrice de bore-lithium dans le but d'obtenir des solutions pour les analyses liquides (ICP, AA) au lieu de disques de verre.

Pour ne mentionner que certains d'entre eux, nous dénotons entre autre la simplicité de cette technique (minimisant la quantité de manipulations), la sécurité (système entièrement automatisé sans utilisation d'acide fluorhydrique), la rapidité (obtention de solutions en moins de 20 minutes), ainsi que la facilité de digestion des matrices géologiques à caractère réfractaire telles que les aluminosilicates, la céramique, la porcelaine, la brique, la zircone, l'argile, la magnésie, etc.

Cette présentation traitera des avantages marqués que nous offre la préparation des échantillons par fusion, comparée à d'autres techniques de mise en solution telles que la digestion par acides ou par micro-onde.

O 2-4

ATTOM, DESCRIPTION, SPÉCIFICITÉS ET APPLICATIONS DE L'ICP-MS HAUTE RÉSOLUTION DE NU INSTRUMENTS

Ariane Donard, Benoit Disch, Phil Shaw, Nu Instruments, Wrexham, UK

L'AttoM de Nu Instruments est un ICP-MS haute résolution entièrement conçu et construit pour fournir les meilleures performances et la meilleure fiabilité grâce à sa flexibilité et à sa facilité d'utilisation pour la mesure de rapports élémentaires et de rapports isotopiques. L'instrument permet notamment d'obtenir des précisions les plus fines sur des rapports isotopiques du fait de sa capacité à balayer rapidement entre les isotopes d'intérêt sur une plage de masse relative de 40% sans qu'il soit nécessaire de changer le champ magnétique. La tension d'accélération, la tension ESA et les optiques ioniques utilisées pour la focalisation du faisceau sont maintenues constants pendant l'acquisition. Seuls les optiques ioniques FastScan situées à l'entrée et à la sortie de l'aimant varient, ils sont utilisés pour dévier rapidement les isotopes sélectionnés séquentiellement pour l'acquisition de données. Le mode LinkedScan permet de combiner le balayage de l'aimant et l'utilisation des optiques ioniques Fastscan pour pouvoir effectuer une mesure de l'ensemble de la gamme de masse (Li-U and U-Li) en 220 ms. Ce mode est notamment très apprécié pour la mesure de signaux transitoires où le nombre de cycle par mesure est un paramètre essentiel. Plusieurs spécificités techniques de l'instrument et différentes exemples d'applications seront discutées.

O 2-5

NOVAWAVE – UN CONCEPT INNOVANT DE DIGESTION AUTOMATISEE PAR MICRO-ONDES

Rachid Choudar, SCP Science

NovaWAVE est un système de digestion et d'extraction complètement automatisé, disposant de douze mini cavités micro-ondes permettant le traitement simultané de un à douze échantillons dans des tubes en Quartz calibre ou en Fluoropolymère. La température de chaque échantillon est suivie en continu par un détecteur infrarouge pour chacune des positions qui transmet l'information au système de contrôle qui lui-même pilote la source de puissance de chaque mini cavité ce qui permet d'appliquer plus ou moins d'énergie selon la réaction dans le tube. Le NovaWAVE dispose d'un logiciel flexible et facile à utiliser permettant l'assignation d'un mode opératoire spécifique à chacun des échantillons digérés en simultané. Le logiciel opérant le NovaWAVE permet de préserver l'intégrité et la traçabilité des méthodes et données générées lors des séquences de digestion. Le haut volume d'échantillons que peut traiter le NovaWAVE résulte de sa conception unique et de sa totale automatisation.

O 2-6

LES NOUVELLES AVANCÉES TECHNIQUES EN LABORATOIRE AVEC LES TECHNOLOGIES AVANCÉES D'ICP COUPLÉ À UN SPECTROMETRE DE MASSE

Daniel Kutscher, Shona McSheehy Ducos, **Michel Alsayegh**, Thermoscientific

Les laboratoires utilisant la spectrométrie de masse au plasma couplé inductivement (ICP-MS) ont plus que doublé au cours des dernières années. Cette popularité grandissante est surtout dû à sa convivialité. Plusieurs raison techniques, commerciales et de productivité expliquent aussi cette popularité. Les appareils d'ICP-MS de nos jours possèdent une sensibilité accrue, une grande gamme dynamique linéaire et une capacité à traiter des types d'échantillons de différentes matrices. Plusieurs outils connexes peuvent aujourd'hui permettre de faire de la spéciation, de l'ablation laser ou de la dilution à partir du même logiciel puissant. Le logiciel peut aussi gérer les interférences et faire le contrôle de la qualité tant en production qu'en milieu règlementaire.

O 2-7

POTENTIEL DES ANALYSES DE SPÉCIATION POUR LA DISCRIMINATION DE L'ORIGINE GÉOGRAPHIQUE DES VINS ROUGES

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3 IPREM, Pau, France

La traçabilité du vin est devenue un enjeu majeur à la fois pour les consommateurs et les producteurs. En effet, à cause de son prix de vente élevé, c'est un produit fortement sujet aux fraudes. Les analyses de traçabilité sont, entre autres, réalisées par le dosage des éléments trace. Ces-dernières peuvent effectivement varier en fonction des sols sur lesquels la vigne a poussé mais également en fonction des pratiques agricoles. Ces différentes origines peuvent donc potentiellement influer sur la spéciation des éléments trace. L'objectif de notre travail était donc vérifier si les analyses de spéciation pouvaient être plus discriminantes que les analyses des teneurs totales.

Dans un premier temps, le développement et la validation des méthodes de spéciation de différents métaux (As, Se,…) dans le vin rouge seront décrits. Puis l'application de ces méthodes à l'analyse de vins rouges de différentes origines géographiques sera présentée. Finalement, le traitement statistique de ces données permettra de conclure quant à la pertinence d'utiliser les analyses de spéciation pour discriminer l'origine géographique du vin rouge.

O 2-8

SPÉCIATION DU PLATINE EN PRÉSENCE DE MATIÈRE ORGANIQUE NATURELLE

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Les concentrations d'éléments du groupe platine mesurées dans l'environnement ont augmenté durant les dernières décennies. Cette augmentation est principalement causée par l'utilisation de ces métaux dans les convertisseurs catalytiques des automobiles. Afin d'évaluer le risque environnemental de ces métaux en milieu naturel, la présence de ligands tels que la matière organique naturelle doit être considérée. En effet, la matière organique naturelle lie fortement les éléments du groupe platine, et elle peut donc modifier la biodisponibilité de ces éléments en les complexant. L'objectif de ce projet de maîtrise est d'étudier la spéciation du platine et du palladium en présence de matière organique naturelle (Suwannee River humic acid) et de vérifier l'influence de la matière organique naturelle sur l'absorption et la toxicité de ces métaux chez l'algue verte unicellulaire Chlamydomonas reinhardtii. La première étape du projet consiste donc à quantifier la complexation du platine et du palladium par la matière organique naturelle. Pour ce faire, deux méthodes ont été envisagées: la dialyse à l'équilibre et l'ultrafiltration partielle. La dialyse s'étant avérée difficilement reproductible, ce sont donc les résultats de spéciation obtenus par ultrafiltration partielle qui seront présentés ici. Ces résultats sont comparés à ceux obtenus à l'aide du modèle thermodynamique WHAM afin de vérifier sa capacité à estimer la complexation du Pt et du Pd par la matière organique naturelle. Dans ce projet, les concentrations expérimentales sont sélectionnées afin de représenter les conditions observées en milieu naturel. Ainsi, les concentrations de matière organique naturelle choisies sont inférieures à 5 mg C/L tandis que les concentrations de Pt et de Pd sont inférieures à 300 nM. Les expériences de spéciation sont réalisées à pH 5 dans un milieu de culture simplifié contenant des ions majeurs. La deuxième étape du projet consistera à exposer Chlamydomonas reinhardtii aux milieux caractérisés par ultrafiltration partielle et quantifier la bioaccumulation et les effets.

O 2-9

SPÉCIATION DES LANTHANIDES EN PRÉSENCE DE LA MATIÉRE ORGANIQUE NATURELLE

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Une augmentation des concentrations environnementales des lanthanides est anticipée, due à une utilisation et une exploitation de plus en plus importantes de ces métaux. Pour évaluer les risques environnementaux que posera cette augmentation de concentrations, il faudra tenir compte de la composition du milieu récepteur. L'un des paramètres importants qui peuvent moduler la toxicité de ces métaux vis-à-vis des organismes aquatiques est la matière organique naturelle (MON). Ce ligand peut complexer les lanthanides, ce qui devrait réduire leur biodisponibilité et avoir un effet sur leur internalisation et par conséquent leur toxicité.

Dans une étude réalisée dans notre laboratoire, la toxicité des lanthanides pour l'algue unicellulaire Chlorella fusca a été déterminée dans des milieux synthétiques. Cependant, ces milieux synthétiques ne contenaient pas de MON. Donc la première étape de ce projet consiste à caractériser la complexation des lanthanides par la MON (SRHA : Suwannee River Humic Acid) en utilisant la technique de dialyse à l'équilibre. Le modèle WHAM sera aussi utilisé afin d'estimer la spéciation de ces métaux en présence de la SRHA. Les résultats expérimentales obtenus seront comparés à ceux obtenus par WHAM et la technique d'échange ionique l'IET.

Les concentrations des lanthanides utilisées seront comprises entre 10 et 1000nM, et celles de la matière organique naturelle seront comprises entre 1 et 5 mg C/L. Les concentrations de lanthanides ont été mesurées par ICP-OES, et seront présentées dans une présentation orale.

Pour évaluer la toxicité des lanthanides en présence de la matière organique, les algues seront exposées à différentes concentrations des métaux, tout en considérant leur spéciation dans le milieu. La quantité des lanthanides internalisée, le taux de croissance algale ainsi que le rendement cellulaire final seront suivis.

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O 2-10

SPÉCIATION AQUEUSE DU THORIUM, DU PLOMB ET DE L'URANIUM PAR ÉCHANGE IONIQUE

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En vertu du rôle important que joue l'ion métallique libre dans l'accumulation et la toxicité des métaux chez les organismes aquatiques, de nouvelles techniques analytiques de dosage sont recherchées. Une de ces techniques fait appel à une résine échangeuse d'ions. Cette technique a été utilisée avec succès avec plusieurs ions divalents tels que Cd, Co, Cu, Ni et Zn en présence de différents ligands (synthétiques et naturels) mais aussi avec Ag et récemment avec plusieurs lanthanides tels que La, et Eu. Dans ce projet, nous examinons la capacité de la Technique d'Échange Ionique (TÉI) pour déterminer les concentrations d'ions libres du Pb, du Th et de l'UO2 en solution. Les premiers résultats ont été obtenus à une force ionique relativement faible (I = 0.1 M NaNO3) et à pH 4.0, 5.0 et 6.0 dans lesquels la spéciation des métaux est relativement simple. Dans le cas du plomb des analyses ont été fait à pH 7.0 et 8.0 dans le but d'observer l'influence de la présence d'hydroxo-complexes sur la sélectivité de la technique à l'ion libre. Les résultats préliminaires indiquent que dans un milieu acide des coefficients de distribution de Pb2+ sont presque identiques alors que ceux de l'UO22+ augmentent avec le pH, suggérant une interférence de la part d'un complexe. Des essais préliminaires ont montré que le thorium possède une forte affinité pour la résine donc cet effet n'a cependant pas permis d'obtenir de résultats à des pH > 4. Pour cet élément, l'augmentation de la force ionique à 0.3 M (NaNO3) est donc nécessaire afin de pouvoir atteindre un équilibre. Les modifications à apporter à l'approche expérimentale ainsi que des résultats sur la sélectivité de la résine en présence des ligands, telles que le citrate, NTA et la matière organique dissous (acide fulvique) seront présentés.

O 2-11

ANALYSE DE SPÉCIATION DE L'ARSENIC DANS LA FRACTION BIO-ACCESSIBLE POUR L'ÉVALUATION DU RISQUE LIÉ À LA CONSOMMATION DE RIZ DE DIVERS PAYS

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Comme la toxicité de l'arsenic dépend de sa forme chimique et que seule la portion bio-disponible (i.e. entrant dans le système sanguin) peut avoir des effets toxiques, une évaluation réaliste du risque lié à la consommation d'aliments ne peut simplement être basée sur la concentration totale en arsenic ou même sur une analyse de spéciation. La portion bio-accessible (i.e. dissoute dans le système gastro-intestinal) doit être considérée car elle correspond à la portion bio-disponible dans le pire cas. Dans cette étude, une méthode de lixiviation fut utilisée pour obtenir la portion bio-accessible d'échantillons de riz du Moyen-Orient, des États-Unis et de l'Inde, qui fut ensuite analysée par chromatographie ionique couplée à la spectrométrie à plasma à couplage inductif pour mesure la concentration de chaque espèce d'arsenic. Les résultats obtenus par une méthode de lixiviation en ligne ainsi que par une méthode conventionnelle montrent que la concentration totale, la bio-accessibilité et la spéciation de l'arsenic varient d'un échantillon de riz à l'autre. La cuisson peut aussi changer la distribution des espèces d'arsenic. Toutefois, dans tous les cas, laver le riz avant de le cuire réduit de manière significative la quantité d'arsenic bio-accessible. Cela constitue donc une façon simple de diminuer le risque.

O 3-1

ANALYSE DU PLUTONIUM À L'ÉTAT D'ULTRA-TRACES DANS DES SÉDIMENTS DE RIVIÈRES DE LA RÉGION DE FUKUSHIMA

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L'accident de Fukushima a produit une pollution radioactive qui s'est déposée sur les sols et sédiments de la Préfecture de Fukushima au nord-est du Japon. Plusieurs équipes ont détecté des ultra-traces de plutonium dans des échantillons de sols, sédiments et végétaux à proximité de la centrale (jusqu'à quelques km).

L'objectif de cette étude est de suivre les variations spatio-temporelles de la concentration en plutonium dans des sédiments de rivière et des sols prélevés à des distances de plusieurs dizaines de km de la centrale afin d'évaluer les dynamiques des particules de sédiments marqués par les retombées de la centrale dans les bassins versants côtiers du Japon. Cette étude est menée en collaboration avec le Laboratoire des Sciences du Climat et de l'Environnement (LSCE – Unité Mixte CEA/CNRS/Université, France) et le Center for Research in Isotopes and Environmental Dynamics de l'Université de Tsukuba, Japon.

Les analyses consistent en un traitement chimique complet suivi d'une mesure isotopique par ICPMS à secteur magnétique simple collection (Thermo « Element XR ») ou par ICPMS multi-collection (Thermo « Neptune Plus »). Etape clé de l'analyse, le traitement chimique consiste en une dissolution de l'échantillon suivi d'extractions, purifications et concentrations du plutonium et de l'uranium contenus dans environ 5 grammes de sol ou sédiment. Les séparations sont effectuées par chromatographie anioniques et par chromatographie d'extraction. Les ICPMS utilisés sont optimisés en sensibilité (> 108 cps par µg·L-1 de 238U) afin d'obtenir des limites de détection inférieures au fg (1 femtogramme = 10-15g) pour les différents isotopes du plutonium. Les quantifications sont réalisées par dilution isotopique avec un traceur de 244Pu. Les rapports isotopiques 240Pu/239Pu, 241Pu/239Pu et 242Pu/239Pu sont mesurés avec une précision suffisante pour discriminer le plutonium issue de la centrale de Fukushima de celui des retombées globales des essais nucléaires atmosphériques. Ces derniers ont engendré à la surface du globe un marquage en plutonium généralisé qui se caractérise par des rapports isotopiques relativement constants et bien connus.

Cette présentation décrit largement les méthodes d'analyse utilisées, aussi bien le traitement chimique que la mesure isotopique. Quelques résultats de mesure sont également donnés.

O 3-2

QUELLES METHODES DE MISE EN SOLUTION POUR LES MATRICES SOLIDES ENVIRONNEMENTALES ?

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La quantification des radionucléides par ICP-MS dans les matrices solides environnementales (sols, végétaux terrestres et aquatiques, poissons,…) nécessite une étape préalable de mise en solution des échantillons. L'objectif de cette première étape est d'obtenir une solution homogène. Les méthodes dites « classiques » de mise en solution par bains d'acides chauffés sont couramment utilisées dans les laboratoires de radiochimie. Ces méthodes, bien que faciles à mettre en œuvre, ne permettent pas systématiquement une digestion totale des échantillons, notamment en présence d'oxydes réfractaires ou bien de particules chaudes émises lors d'accidents nucléaires. D'autre part, l'utilisation de grands volumes d'acides concentrés et chauffés constituent une importante source d'exposition au risque chimique pour le personnel des laboratoires.

Des alternatives à ces méthodes « classiques » existent. Le choix de la technique dépend de la matrice à analyser, des propriétés du ou des radionucléides recherchés et des performances à atteindre en termes de limites de quantification. Ainsi, dans le cadre de l'analyse des radionucléides dont la période est longue (uranium, thorium) ou dans un contexte accidentel ayant entraîné une contamination significative de l'environnement, de petites prises d'essais suffisent pour la quantification par ICP-MS. Dans ce cas, le four à micro-ondes classique ou la fusion alcaline peuvent être mis en œuvre. En revanche, ces techniques ne sont pas adaptées pour les analyses réalisées dans le cadre des programmes de surveillance radiologique de l'environnement ou des études radioécologiques qui nécessitent des prises d'essais plus élevées afin d'atteindre des limites de quantification plus basses compatibles avec les niveaux d'activités recherchés. Pour ces prises d'essais plus importantes, jusqu'à 10 grammes, l'utilisation de systèmes de mise en solution semi-ouverts ou de four à micro-ondes grande capacité constituent des alternatives pertinentes.

L'objectif de cette communication est de présenter les différents systèmes de mise en solution testés par l'Institut de radioprotection et de sûreté nucléaire puis d'analyser leurs avantages et leurs inconvénients pour la quantification de différents radionucléides par ICP-MS.

O 3-3

ANALYSE RAPIDE DE RADIUM-226 ET 228 PAR ICP-MS-MS

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Le Centre d’expertise en analyse environnementale du Québec (CEAEQ) est le laboratoire du ministère du Développement durable de l’Environnement et de la Lutte contre les changements climatiques (MDDELCC). La mission du CEAEQ est de garantir la disponibilité, la qualité et la continuité de l’expertise en analyse environnementale au Québec. Au Québec il n’existe aucune norme règlementaire pour le radium-228 alors que le radium-226 est normé dans le Règlement sur la qualité de l’eau potable et dans la Directive 019 sur l’industrie minière qui encadre les rejets de cette l’industrie. Il n’existe aucun laboratoire spécialisé en radioactivité au Québec et jusqu’à tout récemment il n’y avait aucun laboratoire accrédité pour l’analyse du radium-226. Les méthodes d’analyse radiométriques d’analyse par spectrométrie gamma et alpha et bêta permettent la quantification des radionucléides selon leurs propriétés de rayonnement et demande une expertise spécifique à ce domaine. Cependant, l’augmentation de la sensibilité instrumentale des ICP-MS et ICP-MS/MS permet maintenant de réaliser des analyses de métaux en traces et ultra-traces et d’être appliqué à des radio-isotopes de période radioactive supérieure à 1000 ans tout en atteignant des performances analytiques équivalentes à celles des méthodes radiométriques. Le CEAEQ a ainsi développé une méthode rapide d’analyse de radium-226 et 228 dans différentes matrices d’eau. Cette méthode est accréditée selon la norme ISO 17025 et a permis de réaliser avec succès différents essais inter-laboratoires. Elle a aussi permis au MDDELCC d’effectuer des vérifications de radium-226 dans des d’échantillons d’eau potable, des contrôles de rejets miniers et d’établir des niveaux de fond des eaux souterraines de différentes régions du Québec.

O 3-4

SEPARATION AUTOMATISEE ET COUPLAGE AVEC LA MESURE POUR LA QUANTIFICATION RAPIDE DES ACTINIDES ET DE ^{90}SR

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En cas de crise nucléaire, en phase d’urgence comme en phase post-accidentelle, les radionucléides potentiellement rejetés dans l’environnement devront être rapidement quantifiés afin de répondre aux attentes des pouvoirs publics locaux et nationaux. Une grande réactivité des laboratoires d’analyse est donc indispensable afin de fournir aux gestionnaires de crise, dans les meilleurs délais, les données nécessaires à l’évaluation des conséquences radiologiques d’un accident sur les personnes (mesures de protection des populations à mettre en place) et sur l’environnement (niveau de contamination des territoires). Parmi ces radionucléides, la contribution des émetteurs alpha et bêta à la dose interne peut être très importante et induire de sévères dommages en cas d’ingestion ou d’inhalation.

Les protocoles actuellement utilisés pour la quantification des actinides et de 90Sr dans le cadre de la surveillance radiologique de l'environnement en France sont très performants et permettent d'atteindre des limites de détection très basses. La mise en œuvre de ces protocoles est cependant laborieuse et les délais de traitement chimique et d'analyse associés peuvent nécessiter plusieurs semaines pour certains radionucléides.

Au cours de ces dernières années, les publications présentant de nouvelles stratégies pour mettre en place des méthodes visant à augmenter le nombre d'échantillons traités se sont multipliées. Néanmoins, aucune étude visant à quantifier les actinides et 90Sr avec un protocole de séparation unique et automatisé couplé en ligne à la mesure n'a été publiée.

Pour être prêt à répondre efficacement à ses missions dans le cadre d'une crise radiologique et, in fine, limiter ainsi l'exposition des populations aux rayonnements alpha et bêta, l'IRSN a développé une nouvelle méthode permettant une réduction importante des délais d'analyse actuels.

Cette méthode permet la quantification rapide des isotopes des actinides (234, 235, 236, 238U, 230, 232Th,
239, 240Pu, 237Np, 241Am and 244Cm) et de 90Sr dans les échantillons de l'environnement (eaux et solides).
Pour les échantillons solides (prise d'essai jusqu'à 0,7 g), la première étape consiste en une mise en solution rapide, automatisée et complète par fusion alcaline.
L'étape de séparation chromatographique est précédée par une étape de purification par co-précipitation. La séparation est réalisée avec un module de chromatographie liquide spécialement adapté aux besoins du protocole développé. Ce module est composé de 9 vannes et de 3 colonnes par échantillon. Les colonnes sont remplies avec les résines TEVA®, TRU et Sr, afin de permettre la séparation de tous les interférents. Les vannes permettent d'installer jusqu'à 30 colonnes et donc de traiter jusqu'à 10 échantillons sans réutilisation des résines afin d'éviter toute contamination croisée.

Les performances de la séparation automatisée ont été optimisées avec un plan d'expérience factoriel et les résultats ont été traités avec le logiciel Minitab®. Cette nouvelle méthode de séparation est couplée en ligne à un ICP-MS pour la quantification. Après optimisation, la séparation chromatographique automatisée couplée en ligne à l'ICP-MS permet de quantifier les éléments d'intérêt dans 10 échantillons en 24 heures dont ~ 12 heures d'automatisation totale (sans intervention des opérateurs). En complément, le système de séparation automatisée mis en place permet également de récolter la fraction contenant le strontium pour une éventuelle quantification de 89Sr et de 90Sr avec une méthode de mesure nucléaire.

En conclusion, ce couplage permet d'abaisser drastiquement les limites de détection des isotopes artificiels des éléments étudiés. Par ailleurs, d'excellentes performances en termes de rendements chimiques, de fidélité et de justesse ont été obtenues. La rapidité de cette nouvelle méthode, en comparaison avec les méthodes classiques actuelles, la rend incontournable pour des besoins de mesures en situation d'incident ou d'accident nucléaire associés où les délais de rendu de résultats sont très contraints.

O 3-5

COMPARAISON DES SPECTROMÉTRIES XRF ET ICP-AES POUR L'ANALYSE ÉLÉMENTAIRE DANS LES VÉGÉTAUX À TRAVERS LA MÉTHODE DU PROFIL D'EXACTITUDE

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En l'absence de toute méthode normalisée, la norme ISO 17025 demande à un laboratoire de valider ses méthodes analytiques en interne. Cette validation est habituellement réalisée à travers un lot d'échantillons de concentrations différentes pour lesquelles des critères analytiques prédéfinis doivent être vérifiés. Parmi ces critères, l'exactitude – qui regroupe justesse et précision – est d'une importance capitale pour l'analyse quantitative.

Dans ce but, la méthode du profil d'exactitude représente une approche de la validation qui a l'avantage d'utiliser à la fois une méthode statistique globale combinant justesse et précision à travers le calcul d'un intervalle de tolérance des mesures, et une interprétation graphique simple qui permet la prise de décision. La comparaison de cet intervalle avec des limites acceptables fixées par l'utilisateur détermine la validité du domaine de mesure pour la méthode et l'incertitude des futurs résultats d'analyse.

Cette étude décrit le calcul des intervalles de tolérance, à partir de la précision intermédiaire, pour la mesure d'éléments minéraux dans les végétaux par la spectrométrie de fluorescence des rayons X, directement sur l'échantillon à l'état solide. Les profils ont été obtenus à partir d'un lot de 6 échantillons certifiés, analysés chaque semaine pendant 5 semaines. Les résultats ont été comparés à ceux obtenus par spectrométrie d'émission atomique par plasma à couplage inductif (ICP-AES) après mise en solution des échantillons, qui est la méthode de référence du laboratoire.

La spectrométrie de fluorescence des rayons X est une bonne façon d'obtenir des résultats assez justes et précis très rapidement. Elle reste cependant moins juste que la spectrométrie ICP-AES, moins sensible aux effets de matrice mais aussi plus lente.

O 3-6

GÉOCHIMIE DU RADIUM DANS LES EAUX SOUTERRAINES NATURELLES DU SUD-EST DU NOUVEAU-BRUNSWICK

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Le radium, un radionucléide associé à la chaîne de désintégration de l'uranium, est un élément naturellement présent dans le sous-sol terrestre notamment dans le schiste. Si le développement technologique récent permet l'exploitation du gaz de schiste jusqu'alors inaccessible, il augmente aussi l'accessibilité et la mobilité de nouveaux contaminants. Parmi ces nouveaux contaminants, le radium est un indicateur prometteur pour caractériser l'impact environnemental de l'industrie gazière. L'enrichissement de ce contaminant dans les écosystèmes perturbés serait alors révélateur d'un impact anthropique. Idéalement, l'indicateur choisi doit être spécifique à l'impact que l'on désire mesurer, être sensible aux très fines perturbations anthropiques, avoir une variabilité saisonnière et géographique limitée, ainsi qu'un comportement chimique bien caractérisé. Finalement, les concentrations de référence de cet indicateur (préalable à la perturbation du milieu naturel) doivent être déterminées. C'est dans ce contexte que nous avons établi les concentrations de référence en radium dans les aquifères souterrains du sud-est du Nouveau-Brunswick : 68 puits privés des comtés de Kent, King et Albert ont été échantillonnés et

analysés. Pour 9 d’entre eux, la variabilité temporelle du radium a été déterminée sur une échelle pluriannuelle. Nos résultats démontrent des variabilités géographiques et saisonnières du radium des plus limitées et des niveaux de concentrations moyens très faibles (env. 0,1 pg/L). Finalement, la concentration en radium mesurée est fortement influencée par les propriétés géochimiques intrinsèques des aquifères (pH, conductivité, Fe, Mn, Ba, Sr, Mg, Ca). Les résultats de cette étude serviront à établir la pertinence de cet élément radioactif comme indicateur d’impact environnemental en prévision d’un futur développement de l’industrie des gaz de schiste dans la province.

O 3-7

"TENDANCES DANS L'ANALYSE "SINGLE PARTICLE ET SINGLE CELL ICP-MS" : DE LA DÉTECTION DANS LES MATRICES COMPLEXES À LA QUANTIFICATION EN NOMBRE DE PARTICULES ET DU CONTENU EN MÉTAL DANS LES ORGANISMES UNICELLULAIRES INDIVIDUELS"

Stephan Chady, Perkin Elmer

Single Particle ICP-MS (SP-ICP-MS) est devenue une méthode reconnue pour l’analyse de nanoparticules dans divers types d’échantillons tels que biologiques, environnementaux et industriels. Plusieurs paramètres et conditions instrumentales affectent la justesse, la précision et la reproductibilité de l’analyse dont l’effet matrice, le niveau du bruit de fond, l’efficacité de transport, le temps de lecture ainsi que le type de système d’introduction utilisé. L’intégration du signal joue un rôle primordial dans la qualité des données générées – intégration « intensité de signal vs aire de pic ». En se basant sur la technique SP-ICP-MS, Single Cell ICP-MS (SC-ICP-MS) vient de se développer comme étant une technique qui permet de mesurer le contenu en particules ou en fraction ionique dans des organismes unicellulaires. SC-ICP-MS nécessite un système d’introduction dédié qui permet de livrer des organismes unicellulaires de quelques microns de taille au plasma de l’ICP-MS.

O 3-8

AMÉLIORATION DES LIMITES DE DÉTECTIONS POUR LA MESURE PAR SP-ICP-MS AVEC L’HR-ICP-MS ATTOM PAR L’UTILISATION D’UN DESOLVATEUR ET DU MODE « PSEUDO RÉSOLUTION »

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Du fait de leur propriété novatrices, les nanoparticules sont de plus en plus utilisées dans l’industrie. Leur introduction dans l’environnement et les questions posées concernant l’effet néfaste potentiel pour la santé humaine entraine la nécessité de développer des méthodes capables de caractériser ces matériaux. La méthode « Single Particle » -ICP-MS (SP-ICP-MS) a été prouvé ces dernières années comme étant un outil de mesure efficace pour le comptage et la mesure de la taille de nanoparticules. L’ICP-MS haute résolution de Nu Instruments l’AttoM offre la possibilité de mesurer un signal avec un dwell time aussi rapide que 10 µs (sans interruption). La combinaison entre l’acquisition de signal rapide, sa haute sensibilité et la possibilité de supprimer l’effet d’interférences en augmentant la résolution font de l’AttoM un instrument idéal pour cette méthode. Grace à sa haute efficacité de transmission l’AttoM permet déjà d’obtenir des limites de détections en mode d’introduction classique par nébulisation (6 nm pour Au, Ag, CeO). Dans ce travail, l’utilisation d’un desolvateur pour améliorer les limites de détections est discuté

(4 nm pour Au, Ag, CeO). La distinction entre l'efficacité de transport d'échantillon et l'efficacité de transmission ionique est étudiée pour expliquer l'augmentation de la sensibilité. La capacité d'augmenter la résolution sur l'AttoM est discuté pour la mesure de nanoparticules de Fe_2O_3 pour s'affranchir d'interférences. La possibilité de choisir la fente source et collecteur de manière indépendante permet d'obtenir une « pseudo résolution » La limite de détection atteignable pour ce type de nanoparticule est discutée.

O 3-9

DÉVELOPPEMENT ET VALIDATION D'UNE MÉTHODE ANALYTIQUE ICP-MS EN MODE « SINGLE PARTICLE » (SP-ICP-MS) POUR L'ANALYSE DE NANOPARTICULES (NP) DE DIOXYDE DE TITANE (TIO2) DANS LES MILIEUX BIOLOGIQUES »

Samantha Salou, Ciprian Mihai-Cirtiu, Centre de Toxicologie du Québec, Québec, Canada

L'utilisation de NPTiO2 est de plus en plus répandue. Leur fabrication considérable et l'usage croissant, suscitent actuellement des préoccupations majeures quant aux risques sanitaires potentiels. En effet, les sources d'exposition sont diverses, ainsi les NP sont susceptibles de traverser les barrières biologiques, d'être distribuées dans le corps humain via le sang et ainsi de s'accumuler dans divers organes ou encore d'être transformées/excrétées. Il est donc indispensable de les mesurer et de déterminer leurs propriétés dans les fluides biologiques. La métrologie actuelle permettant une telle caractérisation est limitée de part son manque de sensibilisé et spécificité. La SP-ICP-MS apparaît comme une technique novatrice et prometteuse pour l'analyse des NP dans des matrices complexes. Elle fournit des informations quant à la présence d'ions dissous/NP, la taille/distribution en taille, les concentrations en nombre/masse, nous permettant ainsi d'évaluer l'exposition humaine. Le développement méthodologique repose sur l'utilisation de matériaux de référence NIST de NPTiO2. Des paramètres instrumentaux tels que le temps d'intégration du signal, le type de nébuliseur, le débit du gaz de nébulisation, la distance entre la torche et le cône échantillonneur seront optimisés afin obtenir le maximum de signal pour l'élément d'intérêt. Ensuite la méthode sera validée selon une approche quantitative impliquant la détermination des paramètres suivants : limite de détection et quantification, plage de travail en taille et concentration, précision, exactitude et robustesse. Étant donné qu'il n'existe pas de matériaux de référence pour les milieux biologiques disponibles commercialement, la méthode des échantillons enrichis (matrice biologique enrichie avec des matériaux de référence NIST) sera utilisée pour la détermination des paramètres de validation. La méthode, sensible et robuste, rapide et fiable, répondra ainsi au grand besoin qui existe actuellement en matière d'évaluation de l'exposition aux NP. Ce projet devrait aboutir au développement et à la validation d'une méthode d'analyse innovante qui servira de base de référence pour la métrologie des NP dans les milieux biologiques.

O 3-10

ANALYSE DES IMPURETES ELEMENTAIRES ET DES NANOPARTICULES DE TIO2 DANS DES PRODUITS COSMETIQUES PAR UNE COMBINAISON DE TECHNIQUES

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Les produits cosmétiques font maintenant partie de notre vie quotidienne et sont de ce fait soumis à la réglementation européenne N° 1223/2009. En ce qui concerne les substances inorganiques concernées par cette directive, un certain nombre d'éléments est pris en compte ainsi que la présence de nanoparticules (NPs). Seules les NPs de TiO_2 sont autorisées en tant que filtre solaire et leur ajout aux produits cosmétiques doit être indiqué par la mention (nano) sur l'étiquette. Malgré la mise en place de cette réglementation, la caractérisation des NPs dans les cosmétiques reste difficile, notamment en raison de matrices complexes.

Une étude a donc été conduite afin de pouvoir proposer une méthode de caractérisation de NPs utilisable en routine. Dans cet objectif, 16 produits cosmétiques et/ou d'hygiène corporelle couramment utilisés ont été sélectionnés (shampoings (3), crèmes solaires (2), différentes crèmes hydratantes avec ou sans filtres solaires (6), sérums hydratant (2), dentifrices (2) et baume à lèvres (1)). Dans un premier temps, le contenu en impuretés élémentaires a été dosé après minéralisation acide par ICP-AES ou ICP-MS, selon les niveaux de concentrations. Aucune substance dont l'utilisation est prohibée n'a été détectée mais des teneurs importantes de titane ont parfois été mises en évidence, notamment dans les crèmes solaires, certaines crèmes hydratantes, un dentifrice et le baume à lèvres. La méthode de Diffusion Dynamique de la Lumière (DLS) ayant montré la présence de NPs, la taille de nanoparticules métalliques a été définie plus précisément par SP-ICP-MS en comparant deux méthodes de préparation, l'utilisation d'un tensioactif (SDS) et une méthode de dégraissage avec de l'hexane. Il a été montré que les particules de TiO_2 sont présentes dans tous les produits dans lesquels Ti a été mesuré avec des tailles comprises entre 50 et 120 nm. L'utilisation d'hexane est préférable pour la mise en suspension des NPs, l'extraction avec le SDS ayant tendance à légèrement surestimer la taille en raison probablement de son adsorption à la surface des NPs.

O 3-11

ÉVALUATION DE LA STABILITÉ DE NANOPARTICULES D'OXYDE DE ZINC PAR SINGLE-PARTICLE ICP-MS

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Les nanoparticules d'oxyde de zinc (ZnO NP) sont parmi les plus utilisées en industrie. Leur production croissante dans divers secteurs comme les produits de consommation et l'agriculture mène inévitablement à leur présence accrue dans l'environnement alors que leur risque écologique y est méconnu. Ce problème est en partie causé par les faibles concentrations auxquelles elles s'y trouvent, qui sont inférieures aux limites de détection des techniques analytiques classiques. Une technique récemment développée, nommée « single-particle ICP-MS » (SP-ICPMS), est cependant prometteuse pour détecter et caractériser les nanoparticules métalliques à des concentrations réalistes pour l'environnement (<ppb). Dans le cas des ZnO NP toutefois, la grande présence de zinc ionique en solution est problématique puisqu'elle masque le signal des plus petites particules. Une solution à ce problème est l'utilisation d'un couplage en série de l'ICP-MS avec une résine échangeuse d'ions. Ce montage permet de retirer notamment le zinc dissous avant l'acquisition, et ainsi d'éviter la perte du signal des particules. L'utilisation d'un ICP-MS à secteur magnétique à grande sensibilité et d'une fenêtre d'acquisition de signal (dwell time) de 50 µs ont mené à la détection de très petites particules, avec des tailles allant jusqu'à 19 nm. Ces conditions ont permis l'étude de la stabilité des ZnO NP sur 48 h en fonction de leur type d'enrobage, de leur concentration initiale ainsi que du milieu auquel elles sont exposées. Nous montrons entre autres que, en présence de matière organique, la dissolution des ZnO NP est rapide et importante.

O 4-1

INFLUENCE DE LA COMPOSITION DE LA MATIÈRE ORGANIQUE DISSOUTE SUR LA MOBILITÉ ET LA BIODISPONIBILITÉ DU MERCURE

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La matière organique dissoute (MOD) joue un rôle clé dans la spéciation et la biodisponibilité du mercure dans les systèmes aquatiques naturels. Les études précédentes ont surtout porté sur la capacité des substances humiques à complexer le mercure mais le récent développement de la spectrométrie de masse à haute résolution (HRMS) (e.g. Orbitrap, FT ICR MS) permet de mieux comprendre la composition de la MOD et en particulier de ses principaux agents chelatants. Dans ce papier, la biodisponibilité du mercure basée sur un bioreporteur luminescent est étudiée en fonction de la composition des ligands organiques produits par les algues (Chlorella vulgaris, Chlamydomonas reinhardtii and Scenedesmus obliquus) déterminés par HRMS. La MOD d'origine planctonique est riche en azote, soufre et en structures aliphatiques. Les agents chelateurs du mercure produits par Chlamydomonas sont dominés par des composés peu polaires et de plus grand poids moléculaire comparativement à ceux produits par les algues d'eau douce (Chlorella et Scenedesmus). Les expériences de biodisponibilité basées sur un bioreporteur luminescent (gram negative E. coli) montrent que les composés de faible poids moléculaire sont déterminants dans la biodisponibilité du Hg en milieu oxique. Nos résultats démontrent l'importance de la composition structurelle de la MOD planctonique sur la biodisponibilité du mercure.

O 4-2

DETERMINATION DU MERCURE DANS LES URINES. RESULTATS DE LA COMPARAISON INTER-LABORATOIRES OELM

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La détermination du mercure urinaire est particulièrement délicate du fait de la volatilité de cet élément et de la matrice urinaire. Le mercure urinaire a été inclus dans la comparaison interlaboratoires OELM (Occupational and Environmental Laboratory Medicine) en Avril 2012 avec une tolérance ±30% pour des concentrations > 10 µg/l et ±3 µg/l pour des concentrations inférieures. Les résultats restent assez médiocres comparés à d'autres circuits tels que PCI et QMEQAS. Dans ce travail nous avons analysé les résultats obtenus entre Avril 2012 et mars 2017. Trois actions ont été réalisées. Les échantillons ont été acidifiés à partir d'Avril 2015. En Mars 2016, il a été demandé aux participants de doser le mercure urinaire dans les 4 heures suivant la décongélation des échantillons. Un des échantillons du cycle 2016-2017 a été traité avec ou sans ajout d'acide sulfamique et triton. L'addition d'acide dégrade la récupération des ajouts (74.2 vs 68.4%, $p<0.0001$), ne modifie pas les coefficients de variation et le pourcentage de laboratoire ayant des performances satisfaisantes. L'addition d'acide sulfamique et de triton n'empêche pas la perte du mercure ajouté à l'échantillon natif (39.4±13.0 vs 43.1±14.7µg/l, $n=28$ participants, $p=0.26$ pour un ajout de 62.4µg/l). Cette perte intervient très rapidement, principalement durant le transport à température ambiante, les échantillons identiques dosés à plusieurs mois d'intervalle ne montrant pas de différence significative de concentration ($n=58$ échantillons en double, $p=0.12$).

O 4-3

MÉTHODE D'ANALYSE DU CHROME HEXAVALENT DANS LES GLOBULES ROUGES PAR ICP MS/MS

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Le chrome hexavalent [Cr (VI)] représente un problème de santé publique bien connu. Plusieurs publications font état de sa mesure dans les eaux de consommation ou les eaux souterraines. Toutefois peu de méthodes font la mesure du Cr (VI) directement dans le sang, car suivant l'absorption par les globules rouge, ce dernier est réduit en chrome trivalent [Cr (III)], non toxique. Une fois réduit en Cr (III), il n'est plus possible de faire une distinction entre le Cr (III) provenant d'une réduction du Cr (VI) et le Cr (III) provenant d'autres sources.

La méthode que nous avons développée au CTQ permet de faire la détermination du chrome total à provenant des globules rouges à l'aide d'une procédure standardisée de séparation et de lavage des globules rouges lors de la collection des échantillons. Comme seuls les formes anioniques essentiellement chromates et dichromates basées sur le Cr (VI), ont la faculté de traverser la barrière cellulaire des globules rouges, la concentration totale de chrome à l'intérieur des globules rouges est représentatives, au moment du prélèvement, du niveau d'exposition cumulatif moyen des dernières semaines d'un individu à une source de Cr (VI).

Cette présentation fait un survol de la méthode en présentant les fondements de la méthode, les contraintes techniques du processus de lavage, l'évaluation des interférences instrumentales sur la masse atomique du chrome. La validation de la méthode ainsi que l'importance des sources de contamination potentielles seront également abordés.

O 4-4

LES ANALYSES INORGANIQUES ET L'AIDE AU DIAGNOSTIC VÉTÉRINAIRE OU QUAND ON N'APPELLE PAS UN CHAT UN CHAT

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Le rôle du Laboratoire d'expertises et d'analyses alimentaires (LEAA) en matière de protection de la santé publique s'exerce par le biais des services analytiques et de l'expertise scientifique qu'il offre aux différents intervenants du secteur bioalimentaire. Bien qu'on associe les analyses réalisées au LEAA aux activités de surveillance et de contrôle de la qualité des aliments, il existe un volet analytique tout aussi important visant à soutenir les médecins vétérinaires chargés de l'amélioration de la santé et du bien-être animal. Le travail du LEAA consiste alors à fournir un support au diagnostic. Or, sur le plan méthodologique, les objectifs et contraintes liés à cette catégorie d'analyses diffèrent souvent de ceux dont on tient compte pour doser les contaminants dans les aliments. Dans le cas du dosage des éléments inorganiques, le nombre de paramètres d'intérêt, l'étendue des plages de concentration et l'exotisme de certaines matrices requièrent des ajustements méthodologiques.

En effet, le nombre d'éléments toxiques qu'il est d'usage de surveiller de façon systématique dans les aliments est faible. Le dosage de ces contaminants est réalisé sur des plages de concentrations restreintes puisqu'ils ne sont présents qu'à l'état de traces dans les matrices alimentaires. Les couples contaminant-matrice sont bien établis, les interférences causées par les matrices, connues et contrôlées, et les paramètres de performance des méthodes, adaptés aux exigences règlementaires. En contrepartie, le profil élémentaire recherché dans les matrices biologiques provenant des vétérinaires est beaucoup plus large, car en plus d'identifier les éléments traces, on souhaite évaluer la qualité de l'alimentation animale. L'étalonnage pour chaque élément doit être suffisamment étendu pour contenir les concentrations symptomatiques de carences et les teneurs résultant d'expositions aigües. Par ailleurs, les profils d'interférences peuvent être très variables d'une espèce à l'autre, même pour une même matrice biologique. Les approches utilisées pour répondre aux exigences de l'aide au diagnostic varient selon la technique instrumentale employée. Elles font appel, sans s'y limiter, à l'observation du signal en temps réel et à la réalisation de profils semi-quantitatifs pour l'identification des interférences, de même qu'à l'usage de la cellule à collision/réaction pour leur contrôle. D'autre part, la régression pondérée, disponible sur la plupart des plateformes instrumentales, permet une quantification adéquate sur une très large gamme de concentrations.

O 4-5

IMAGERIE QUANTITATIVE DU PLATINE DANS DES TISSUS BIOLOGIQUES PAR LA-ICP MS

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L'étude de la distribution des métaux sur une coupe mince de tissus permet de progresser dans la compréhension des processus biologiques complexes impliquant les métaux. Les techniques de bioimagerie, combinant une résolution spatiale (µm) et la sensibilité de la spectrométrie de masse à plasma, telle que l'ablation laser couplée à l'ICP MS (LA-ICP MS), offrent un grand potentiel pour cette problématique. La préparation d'échantillon est relativement directe puisque les échantillons de tissus sectionnés en couche mince (5-200 µm) sont soit incorporés dans la paraffine, soit coupés congelés et déposés sur une lame. Cependant, une des plus grandes difficultés en bio-imagerie par LA-ICP MS est le développement d'une stratégie de quantification fiable. En effet l'échantillon est analysé en couche mince sans aucune étape préalable d'homogénéisation. Ainsi la variation de la composition des échantillons biologiques, même entre plusieurs couches minces successives, entraine des problèmes au niveau de l'analyse en LA-ICP MS (ablation du matériel, transport du matériel ablaté vers l'ICP MS, stabilité de l'ICP MS et dérive du signal élémentaire dû à l'effet matrice et dépôts dans la source ICP).
Cette communication présente l'avancée des développements réalisés pour l'imagerie quantitative par LA-ICP MS du platine (Pt) issu des médicaments anticancéreux et des éléments endogènes (Cu, Zn, Fe) dans des coupes fines de tissus mous. La méthodologie développée repose sur l'utilisation de films polymériques dopés avec des solutions métalliques permettant la quantification des éléments présents dans les tissus. Ces films sont réalisés par spin-coating sur des lames de verre. Parallèlement, seuls des films contenant l'étalon interne métallique sont recouverts du tissu biologique puis l'ensemble est échantillonné par ablation laser. Les limites de détection de l'ordre du µg g-1 obtenues pour le Pt (ainsi que pour Cu et Zn) permettent de quantifier le Pt dans les tissus à une résolution spatiale de l'ordre de 75µm2. Cette méthodologie appliquée à l'analyse de tissus tumoraux permet notamment d'étudier (i) la pénétration du médicament dans les tumeurs et donc l'efficacité du traitement à base de Pt et (ii) le microenvironnement métallique des tumeurs.

A 1

L'ORIGINE DU MÉTHANE ET DU CARBONE INORGANIQUE DISSOUS DANS L'EAU PAR L'ANALYSE ISOTOPIQUE DU CARBONE.

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Une méthode d'analyse des ratios isotopiques du carbone (δ13C) a été développée dans le but d'analyser le méthane (CH4) et le carbone inorganique dissous (CID) dans l'eau. Cette méthode de pointe, nous permet de quantitativement extraire et analyser à l'état gazeux et en simultané les concentrations et les signatures isotopiques du CH4 et CID, afin d'obtenir l'origine du CH4 (thermogénique ou biogénique) lorsque mise en relation avec les proportions de méthane, éthane et propane. Puisque l'exactitude des mesures isotopiques des composés dissous dans l'eau est essentielle pour l'interprétation des résultats obtenus, une calibration isotopique fût mise en place afin de confirmer la justesse des résultats à des concentrations aussi basses que 2 µg/L de CH4 et 80 µg/L de CID dissous dans l'eau. Puisque la production de standards de méthane dissous est laborieuse, la validation méthodologique en rapport avec la concentration et les signatures isotopiques du CH4 a été effectuée à l'aide d'une comparaison inter-laboratoire (n = 4) sur des échantillons d'eau provenant du réseau du suivi des eaux souterraines du Québec. La documentation des niveaux de bases et l'origine du méthane dissous de ce même réseau a débuté en 2013-2014. L'ensemble de la méthodologie utilisé, et la mise en perspective des signatures du CID, du CH4 et des ratios des concentrations du CH4 sur les concentrations d'éthane et de propane dans la détermination de la source du gaz seront présentées.

A 2

NOUVELLE APPROCHE D'OPTIMISATION DES CONDITIONS EN ICP-MS POUR UNE MÉTHODE DE SPÉCIATION DU MERCURE DANS LE SANG PAR ID-GC-ICP-MS

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Les systèmes d'introduction du ICP-MS en mode gazeux et liquide présentent de nombreuses différences. En plus d'une configuration distincte, les conditions maximales d'analyse sont grandement influencées par la matrice utilisée. Lorsque le ICP-MS est utilisé en alternance (configuration LC et GC), il est nécessaire d'effectuer l'optimisation des paramètres instrumentaux fréquemment. En mode GC, il est également nécessaire d'être exactement dans les mêmes conditions instrumentales que lors de l'analyse.

La nouvelle approche permet l'ajustement des paramètres du ICP-MS par infusion et ce, directement avec l'élément d'intérêt sous forme volatile. Il en résulte un signal continu et relativement stable qui permet de vérifier l'alignement, les débits de gaz et les paramètres électroniques rapidement. Étant très similaire aux conditions expérimentales, l'optimisation est spécifique à l'analyse effectuée pour obtenir une meilleure performance instrumentale. La procédure proposée est rapide, simple et efficace.

A 3

PROBLÉMATIQUE DE L'ANALYSE DE L'ÉTAIN DANS LES CHEVEUX PAR ICP-MS

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Le dosage de l'étain dans les cheveux peut servir comme indicateur d'exposition et l'analyse par ICP-MS est une technique de choix de par sa sensibilité et sa spécificité. Pour doser l'étain dans les cheveux, l'échantillon doit être minéralisé au préalable. Les essais menés au CTQ démontrent qu'une digestion basique offre de bien meilleurs résultats qu'une digestion acide.

A 4

ANALYSES DE METAUX A L’ETAT DE TRACES DANS LES CIRCUITS DES CENTRALES NUCLEAIRES PAR ICP-MS

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La limitation de la corrosion rencontrée dans les centrales à réacteurs à eau sous pression (REP) a pour but de maintenir les centrales dans un état sûr et performant, tout en limitant les coûts de maintenance.
Une surveillance des produits de corrosion ainsi que des polluants des circuits des centrales est ainsi assurée par les exploitants selon des spécifications définissant les fréquences et les valeurs limites à respecter.
Dans ce contexte, le département laboratoire du CEIDRE d’EDF a développé une méthode de dosage des métaux dans les différents circuits des centrales REP par ICP-MS. L’ICP-MS est une technique multi-élémentaire rapide et précise qui permet de descendre à des limites de quantification inférieures au µg/L. La procédure de dosage développée permet l’analyse de différents métaux : Na, Mg, Al, Ca, Fe, Cr, Co, Cu, Ni, Zn, Pb sur des gammes allant de 0,1 µg/L à 20 µg/L.
L’optimisation des conditions analytiques pour limiter les interférences (choix et réglages des gaz de collision en fonction des circuits, étalons internes) ainsi que l’évaluation des performances de la méthode validée seront présentés.

A 5

COMPARAISON DES SPECTROMÉTRIES XRF ET ICP-AES POUR L'ANALYSE ÉLÉMENTAIRE DANS LES VÉGÉTAUX À TRAVERS LA MÉTHODE DU PROFIL D'EXACTITUDE

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En l'absence de toute méthode normalisée, la norme ISO 17025 demande à un laboratoire de valider ses méthodes analytiques en interne. Cette validation est habituellement réalisée à travers un lot d'échantillons de concentrations différentes pour lesquelles des critères analytiques prédéfinis doivent être vérifiés. Parmi ces critères, l'exactitude – qui regroupe justesse et précision – est d'une importance capitale pour l'analyse quantitative.

Dans ce but, la méthode du profil d'exactitude représente une approche de la validation qui a l'avantage d'utiliser à la fois une méthode statistique globale combinant justesse et précision à travers le calcul d'un intervalle de tolérance des mesures, et une interprétation graphique simple qui permet la prise de décision. La comparaison de cet intervalle avec des limites acceptables fixées par l'utilisateur détermine la validité du domaine de mesure pour la méthode et l'incertitude des futurs résultats d'analyse.

Cette étude décrit le calcul des intervalles de tolérance, à partir de la précision intermédiaire, pour la mesure d'éléments minéraux dans les végétaux par la spectrométrie de fluorescence des rayons X, directement sur l'échantillon à l'état solide. Les profils ont été obtenus à partir d'un lot de 6 échantillons certifiés, analysés chaque semaine pendant 5 semaines. Les résultats ont été comparés à ceux obtenus par spectrométrie d'émission atomique par plasma à couplage inductif (ICP-AES) après mise en solution des échantillons, qui est la méthode de référence du laboratoire.

La spectrométrie de fluorescence des rayons X est une bonne façon d'obtenir des résultats assez justes et précis très rapidement. Elle reste cependant moins juste que la spectrométrie ICP-AES, moins sensible aux effets de matrice mais aussi plus lente.

A 6

AMELIORATION DES LIMITES DE DETECTIONS POUR LA MESURE PAR SP-ICP-MS AVEC L'HR-ICP-MS ATTOM PAR L'UTILISATION D'UN DESOLVATEUR ET DU MODE « PSEUDO RESOLUTION »

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Du fait de leur propriété novatrices, les nanoparticules sont de plus en plus utilisées dans l'industrie. Leur introduction dans l'environnement et les questions posées concernant l'effet néfaste potentiel pour la santé humaine entraine la nécessité de développer des méthodes capables de caractériser ces matériaux. La méthode « Single Particle » -ICP-MS (SP-ICP-MS) a été prouvé ces dernières années comme étant un outil de mesure efficace pour le comptage et la mesure de la taille de nanoparticules. L'ICP-MS haute résolution de Nu Instruments l'AttoM offre la possibilité de mesurer un signal avec un dwell time aussi rapide que 10 µs (sans interruption). La combinaison entre l'acquisition de signal rapide, sa haute sensibilité et la possibilité de supprimer l'effet d'interférences en augmentant la résolution font de l'AttoM un instrument idéal pour cette méthode. Grace à sa haute efficacité de transmission l'AttoM permet déjà d'obtenir des limites de détections en mode d'introduction classique par nébulisation (6 nm pour Au, Ag, CeO). Dans ce travail, l'utilisation d'un desolvateur pour améliorer les limites de détections est discuté (4 nm pour Au, Ag, CeO). La distinction entre l'efficacité de transport d'échantillon et l'efficacité de transmission ionique est étudiée pour expliquer l'augmentation de la sensibilité. La capacité d'augmenter la résolution sur l'AttoM est discuté pour la mesure de nanoparticules de Fe2O3 pour s'affranchir d'interférences. La possibilité de choisir la fente source et collecteur de manière indépendante permet d'obtenir une « pseudo résolution » La limite de détection atteignable pour ce type de nanoparticule est discutée.

A 7

ANALYSE DE SPÉCIATION SIMULTANÉE DE CHROME, ARSENIC ET SELENIUM DANS LA FRACTION BIO-ACCESSIBLE D'ÉCHANTILLONS DE RIZ POUR L'ÉVALUATION DU RISQUE

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Il existe plus de 40 000 types différents de riz [1], dont plusieurs sont connus pour contenir des quantités importantes d'arsenic inorganique, c'est-à-dire la forme la plus toxique. Étant donné qu'un régime composé principalement de riz est partagé par plus de 3 milliards de personnes [1], l'évaluation du risque posé par l'arsenic, le chrome, le sélénium et d'autres éléments toxiques dans le riz est importante. Une méthode in vitro simple développée précédemment [2] a été utilisée pour évaluer la bio-accessibilité maximale des différents éléments toxiques (Cd, Pb) et potentiellement toxiques (As, Se et Cr). La méthode implique une lixiviation en continu séquentielle en ligne d'une petite quantité d'échantillon (0,2 g) avec de la salive, du suc gastrique et du suc intestinal artificiels, tout en détectant continuellement les éléments libérés par spectrométrie de masse à plasma à couplage inductif (ICPMS). L'analyse simultanée de spéciation de Cr, As et Se dans les lixiviats fut ensuite faite par chromatographie ionique couplée à ICPMS. Dans cette affiche, la méthode sera décrite en détail et les résultats obtenus pour l'analyse des trois variétés de riz seront rapportés, y compris la vérification du bilan massique par comparaison de la somme des concentrations d'espèces avec les quantités totales bio-accessibles mesurées par lixiviation en ligne avec ICPMS.

[1] Rice Association: Varieties, (2004).
[2] N. Horner and D. Beauchemin, Anal. Chim. Acta, 758, 28 (2013).

A 8

OPTIMISATION D'UNE MÉTHODE D'EXTRACTION ACIDE DES ÉLÉMENTS DE TERRE RARE DANS LES RÉSIDUS DE BAUXITE

Julie Rochette, Dominic Larivière, Laboratoire de Radioécologie, Département de chimie, Université Laval, Québec, Canada

L'objectif de cette recherche vise le développement d'une méthode d'extraction acide qui permet d'extraire sélectivement les éléments de terre rare tout en minimisant les éléments majeurs de la matrice de boues rouges. Initialement, une digestion complète a été effectuée afin de connaître les concentrations des éléments présents dans la matrice des boues rouges. Par la suite, des digestions avec des acides dilués (chlorhydrique, nitrique et sulfurique) ont été effectuées à différents pH, températures et temps de chauffages. Les éléments de terre rare ont été analysés par ICP-MS/MS tandis que les éléments majeurs par ICP-OES. Dans le but de simplifier les extractions, une technique de statistique a été utilisée, c'est-à-dire le plan factoriel. Cette technique permet de varier plusieurs paramètres en même temps, en plus de vérifier l'interconnectivité des paramètres étudiés.

Lors de ces extractions, un pourcentage acceptable des éléments de terre rare est extrait préférentiellement aux autres constituants de la matrice. Suivant l'étape de dissolution, une extraction liquide- liquide avec le ligand de type diglycolamide est effectuée afin de séparer les éléments entre eux. Afin d'optimiser la séparation, le plan factoriel est encore utilisé.


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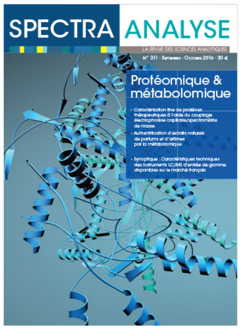
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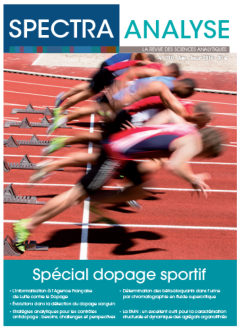
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Abstracts of invited and contributed presentations

(P = Poster, W = Workshop, S = Short Course)

Complimentary workshops

W1

IMAGE ANALYSIS. **Jesse Greener**, Université Laval, Département de chimie, Québec, QC (jesse.greener@chm.ulaval.ca)

Increasingly, analytical sciences are focused on generating information-dense data sets to maximise the impact of research endeavours. High-resolution, quantitative, spatially resolved data is readily acquired by modern instrumentation, which ranges from standard microscopy to spectral imaging systems. Proper management, analysis and representation of these data sets are critical to their efficient use. In this workshop, Professor Jesse Greener will lead an image analysis workshop using powerful open-access image analysis software, ImageJ. Participants will gain hands on experience to analyse sample data sets, which include 2D, 3D images and videos. Various concepts will be covered related to: (i) setting up your workspace environment, (ii) image display enhancements and (iii) image manipulation and analysis, and (iv) special topics. Specifically, participants will learn:

(i) File management, manipulation of bit-depth, global image calibrations
(ii) Look up tables, image overlays, stacking images (for time series, z-stacks, λ-stacks)
(iii) Image calculations, intensity profiles, background correction for uneven lighting situations, and recording simple macros, and batch editing.

Participants are encouraged to bring their laptops preloaded with imageJ software which can be freely downloaded here. Example files will be made available to participants during the session. This session will be held in the spirit of a laboratory class, where participants are expected to take notes and work on exercises provided. The time of the session will be announced shortly, and total length will be a half day.

W2

FORENSIC SCIENCE AND REVERSE ENGINEERING UNING VIBRATIONAL SPECTROSCOPY. **Sergey Shilov**, Bruker Optics, USA (Sergey.Shilov@bruker.com)

Molecular spectroscopy (infrared and Raman) is among the most powerful tools in the forensic science and reverse-engineering process. Each molecule has a unique infrared and Raman signature, providing great specificity in the identification. The distribution of components can also be determined by collecting infrared and Raman images of the product in question. Vibrational spectroscopy will be presented as an important tool in determining the chemical composition of unknown materials and compounds with the goal of reducing or even eliminating the product development cycle. The following topics will be explored:

-Sample preparation techniques
-Product disassembly and analysis
-The role of FTIR and Raman microanalysis
-Chemical imaging and depth profiling

Examples will be shown demonstrating the chemical identification process using infrared and Raman spectroscopy, including a live demonstration. Attendees are encouraged to bring samples of interest for analysis. Please, e-mail to Jaclyn.Scanlon@bruker.com to register.

Short course

S1

INDUCTIVELY COUPLED PLASMA SPECTROMETRY. **Diane Beauchemin,** Queen's University, Kingston, ON (diane.beauchemin@chem.queensu.ca)

The inductively coupled plasma (ICP) is widely used as an emission source in optical emission spectrometry (OES) and as an ion source in mass spectrometry (MS). In its standard configuration, with a nebulization system, it enables multi-elemental analysis of solutions with a wide linear dynamic range. During this short course, the fundamental principles of the ICP will be briefly reviewed along with how to optimize the ICP operating conditions for robustness, i.e. freedom from matrix effects. The source of the remaining limitations will also be discussed along with simple strategies to alleviate them. Topics will include:

- Nebulization process
- Processes occurring in the ICP
- Selection of operating conditions and robustness indicator
- Calibration strategies
- Low-cost alternative sample introduction strategies
    - Flow injection
    - Vapour generation

The features of each approach will be highlighted using selected examples of applications.

I001 P

SAMPLE PREPARATION METHODS FOR DETERMINATION OF PHTHALATE ESTERS IN FOOD SAMPLES BY GAS CHROMATOGRAPHY. **Wanna Kanchanamayoon** and Sutthirak Uansiri, Creative Chemistry and Innovation Research Unit, Department of Chemistry, Faculty of Science, Mahasarakham University, MahaSarakham 44150, Thailand. (wanna.s@msu.ac.th)

A simple and environmental friendly method for determination of four phthalate esters were developed by headspace solid-phase microextraction (HS-SPME) and ultrasound-assisted low density solvent based dispersive liquid-liquid microextraction (USADLLME). Four phthalate esters are dimethyl phthalate (DMP), diethyl phthalate (DEP), di-n-butyl phthalate (DnBP) and di(2-ethylhexyl phthalate (DEHP). HS-SPME with polydimethylsiloxane/divinylbenzene (PDMS/DVB) fiber was used for extraction of phthalate esters in edible oil and soft drink samples. The enrichment factor (EF) showed in the range of 11-17 in vegetable oil and 37-848 in soft drink samples. USADDLME was developed for determination of phthtlate esters in drinking water samples. A low density solvent, toluene was selected as extraction solvent, a mixture of 15 µL toluene and 100µL methanol (disperser solvent) was rapidly injected into water samples. A cloudy solution was formed after ultra-sonication for 5 min, and then centrifuged at 5000 rpm for 5 min. Under the optimum conditions, the enrichment factors were found in the range of 29-67. The two proposed methods were successfully applied for trace analysis of four phthalate esters in real samples.

I002

PAINT IDENTIFICATION USING VIBRATIONAL SPECTROSCOPY FROM MIR TO THz SPECTRAL RANGE. **Sergey Shilov**, Tom Tague, Pang Wang, Bruker Optics, 19 Fortune Dr., Billerica, MA, USA (Sergey.Shilov@bruker.com)

Identification of different paints is in high demand in the forensic community. A commonly used technique for paint identification involves the comparison of infrared spectra of an unknown paint against a spectral library. Inorganic pigments have characteristics bands in the Far IR (FIR) range below 400 cm^{-1} (~12THz) while polymer binders have distinctive spectral features in the Mid-IR spectral range (4000-400 cm^{-1}). Measuring both ranges allows accurate paint identification.

Spectra of different paint samples were acquired using spectrometer that allows measurements from 6000 to 50 cm^{-1} (1.5 THz) in one step without exchanging optical components. Simultaneous identification of a paint binder and pigment was performed using multicomponent spectral searching. Library of most common pigments in MIR-THz range will be presented and the methods of data pretreatment will be discussed in details. Examples will include analysis of the art objects and investigations of samples collected at the crime scene.

I003

A MULTILAYER FLOW MODEL FOR NON-INTRUSIVE BIOFILM VISCOSITY MEASUREMENTS.

J. Greener,[1] M. Parvinzadeh Gashti,[1] A. Eslami,[2] M. P. Zarabadi,[1] and **S. M. Taghavi**[2] Departments of Chemistry[1] and Chemical Engineering[2], Université Laval, 1045 Ave. de la Médecine, Quebec, Quebec G1V 0A6, Canada (Seyed-Mohammad.Taghavi@gch.ulaval.ca)

We develop a mathematical fluid mechanics model to quantify biofilm layer average viscosities in a nonintrusive way. To do so, we employ straight, low-aspect ratio micro flow cells to support biofilm attachment and preferential accumulation at the short sidewall. The model is semi-analytical and takes advantages of a multilayer concept. The model inputs are experimental measurements of biofilm dimensions and average speed and the typical model outputs are biofilm viscosity and velocity profiles, with a reasonable time resolution. Through strongly limiting biases related to non-Newtonian biofilm properties (e.g., shear dependent viscosity), our method makes the study of biofilm mechanical properties possible. Using our method, we interestingly show that in 50 h from inoculation to early maturation stages, biofilm viscosity may grow by over 2 orders of magnitude.

I004

DIRECT ANALYSIS OF AIR FILTERS FOR TOXIC ELEMENTS SCREENING USING A MIXED-GAS PLASMA AND ETV-ICPOES.

Guilherme L. Scheffler,[a] Nausheen Sadiq,[b] Dirce Pozebon,[a] and Diane Beauchemin[b]. [a.]Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves, 9500, 91501-970 Porto Alegre, RS, Brazil. [b.]Department of Chemistry, Queen's University, Kingston, ON K7L 3N6 (guilherme.scheffler@ufrgs.br)

A fast analytical method for screening toxic elements in particulate matter on air filters was developed using electrothermal vaporization coupled to inductively coupled plasma optical emission spectrometry (ETV-ICPOES) and using small air filter pieces directly deposited into graphite boats. First, univariate optimization of CHF_3 reaction gas flow rate (0-10 mL/min), pyrolysis temperature (200-900ºC) and vaporization temperature (1200-2400ºC) was carried out to ensure proper ashing of the filter matrix and quantitative release of the analytes. To maximize sensitivity, a mixed-gas ICP was created by adding 0.45 L/min of N_2 to the outer plasma Ar gas. A multivariate optimization of the main parameters influencing sensitivity was then carried out using a factorial design and yielded 7 mL/min CHF_3, 0.1 L/min carrier gas and 0.2 L/min by-pass gas. Quantification was performed by external calibration using increasing amounts of solid certified reference material (NIST1648a, urban particle matter). To verify the accuracy, 10 cm^2 (~ 0.30 g) filter squares were digested in 2 mL of concentrated HNO_3 for 48 h, diluted to 20 mL with high-purity water and the resulting solution was analysed by liquid nebulization ICPOES or ICP mass spectrometry (ICPMS). The average concentrations found for the analytes investigated (Al, Ti, V, Cr, Ni, Cu, As, Se, Sr, Mo, Cd, Sb and Pb) were in the range of 1.50-14,000 µg/g. The results obtained using ETV-ICPOES (direct solid sampling) and ICPOES or ICPMS (after digestion) were in agreement in most cases. Additional studies included leaching investigations to check the bio-accessibility of toxic elements using simulated saliva and gastric juice as well as lung fluid.

I005

HANDLING INTERFERENCES IN THE MODERN LABORATORY WITH ADVANCED TRIPLE QUADRUPOLE ICP-MS TECHNOLOGY. Daniel Kutscher[1], Shona McSheehy Ducos[1], Maura Rury[2]. [1]Thermo Fisher Scientific, Hanna-Kunath-Straße 11, Bremen, Germany 28199. [2]Thermo Fisher Scientific, 168 Third Avenue, Waltham, MA 02451. (Daniel.Kutscher@thermofisher.com) Presented by: **Michael Plantz**

Inductively Coupled Plasma Mass Spectrometry (ICP-MS) has grown in popularity over the past few decades to become the technique of choice for both cutting edge research and routine analysis of trace elements. Its high sensitivity, wide linear dynamic range, and its ability to process almost every element in the periodic table make it applicable to a wide variety of sample types. A significant drawback to this technique is the production of false positive data due to overlapping isobaric and polyatomic interferences. These interferences have the most direct effect on data quality and can have significant implications, particularly in regulatory applications. Data from a new triple quadrupole ICP-MS will be presented which features enhanced interference removal and better limits of detection in challenging matrices compared to an equivalent single quadrupole instrument. The new instrument achieves the lowest limits of detection in a variety of challenging matrices, for a variety of challenging analytes, with a minimum of effort.

I006

EVALUATION OF NANOPARTICLE DISPERSION USING DIFFERENT MICROSCOPIC TECHNIQUES, **R. Lussier**, Université Laval (renaud.lussier.1@ulaval.ca)

The incorporation of inorganic nanoparticles in polymeric matrix is known to modify the properties of the material. Such nanocomposites can be produced for enhancing mechanical properties of a polymer, its conductivity or to confer properties of the particle to the material such as surface plasmon or magnetic susceptibility. In order to understand the mechanical effect of a filler into a polymer, one must understand the interactions involved between the components of the system. Electron microscopy, because of its high resolution, is the preferred way to observe nanoparticles, but polymer/nanoparticle blends are must harder to image using electron microscopy. The aim of this study is to image iron oxide nanoparticles/elastomeric polydimethylsiloxane blends used in the fabrication of deformable membranes. This enable to correlate the dispersion of the particles with the mechanical properties measured. While optical microscopy yields lower resolutions, the acquisition is simpler and quicker than using electron microscopy. Bright field and dark field optical microscopy are used to image our blends and the particle analysis are compared. Scanning electron microscopy is used to get further insight of the interparticle separation. A critical comparison of the different techniques is made in regards of our needs for understanding the material’s behavior.

I007 P

IMPROVING THE ANALYTICAL PERFORMANCE OF ETV-ICPOES VIA A MIXED-GAS PLASMA.

Guilherme L. Scheffler,[a] Dirce Pozebon,[a] and Diane Beauchemin[b]. [a.]Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves, 9500, 91501-970 Porto Alegre, RS, Brazil. [b.]Department of Chemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada. (guilherme.scheffler@ufrgs.br)

To improve the analytical performance of electrothermal vaporization (ETV) coupled to inductively coupled plasma optical emission spectrometry (ICPOES), a robust mixed-gas Ar-N_2 plasma was created by introducing 0.4 L/min N_2 in the plasma outer gas and 20 mL/min N_2 as a sheathing gas around the aerosol carrier flow. Under re-optimized CHF_3 reaction gas flow rate (8 mL/min), Ar carrier flow rate (0.15 L/min) and Ar by-pass flow rate (0.50 L/min), peak area from the ETV transient signal improved 2.5 fold on average compared to when using an Ar ICP, the improvement being greater for ionic than atomic emission lines. To compensate for sample loading effects on the plasma, point-by-point internal standardization with Ar 763.511 nm was done. Overall, detection limits (3σ) improved 10 fold on average while sensitivity improved by a factor of 4 in comparison to an Ar ICP. External calibration using increasing amounts of SS-2 soil certified reference material (CRM) allowed the accurate analysis of soil CRMs (Montana soil NIST2710, Montana soil 2711 and SS-1) according to a Student's t test at the 95% confidence level. The lower suppression of the argon emission line in the mixed-gas plasma confirms the higher robustness of this plasma compared to an Ar ICP.

I008

THE QUANTITATIVE MASS SPECTROMETRIC ANALYSIS OF MICROBIAL METABOLISM OF DIETARY GLYCOCONJUGATES.

Zandberg, Wesley F[1]; Noestheden, Matthew[1]; Vicaretti, Sara D[1]; Gibson, Deanna[2]; Wylie, Aaron D[1]. University of British Columbia, Okanagan Campus; Department of [1]Chemistry and [2]Biology. (wesley.zandberg@ubc.ca).

The past decade has seen significant advances made in the use of mass spectrometry (MS) to qualify the relative changes in the glycans present in biological samples. However, these approaches are limited due to the vastly different MS response factors for structurally related glycans. This is especially problematic in instances where glycan substrate-product relationships are desired. Our research on two case studies will be presented to highlight our efforts to surmount this limitation: (1) the impact of yeast metabolism on glycosidically-bound flavour compounds in grapes during fermentation and (2) the metabolism of free milk glycans by gastrointestinal (GI) bacteria in neonates. Both pleasing and unpleasant wine flavour precursors are bound as non-detectible (by taste/smell) glycosides in grapes; these are released by microbial enzymes whose activities are closely linked to the exact chemical nature of the glycan portion of these glycoconjugates. Thus, a clearer understanding of the glycosides present in grapes, and how these are processed during fermentation, is essential for controlling the sensory profile of wines. Likewise, milk glycans perform a plethora of health-promoting effects in infants that are very closely linked to their structually-dependent metabolism by GI bacteria. Our research has led to the identification of a previously unidentified glycosylated grape metabolite thought to be linked to "smoke-taint'' in wines made from forest fire-exposed grapes. As well, nine unreported human milk glycans have also been putatively identified. Recent progress will be discussed.

I009

MIR AND FIR ANALYSIS OF INORGANIC SPECIES IN A SINGLE DATA ACQUISITION.

Sergey Shilov, Mathias Keßler, Xia Stammer, Bruker Optics, 19 Fortune Drive, Billerica, MA 01821 (Sergey.Shilov@bruker.com)

The extension of the mid IR towards the far IR spectral range below 400 cm^{-1} is of great interest for molecular vibrational analysis for inorganic and organometallic chemistry, for geological, pharmaceutical, and physical applications, polymorph screening and crystallinity analysis as well as for matrix isolation spectroscopy. In these cases, the additional far infrared region offers insight to low energy vibrations which are observable only there. This includes inorganic species, lattice vibrations or intermolecular vibrations in the ordered solid state.

The spectral range of a FTIR spectrometer is defined by the major optical components such as the source, beamsplitter, and detector. The globar source covers a broad spectral range from 8000 to 20 cm^{-1}. However a bottle neck exists with respect to the beamsplitter and detector. To extend the spectral range further into the far IR and THz spectral ranges, one or more additional far IR beam splitters and detectors have been previously required. Two new optic components have been incorporated in a spectrometer to achieve coverage of both the mid and far infrared in a single scan: a wide range MIR-FIR beam splitter and the wide range DLaTGS detector that utilizes a diamond window. The use of a standard SiC IR source with these components yields a spectral range of 6000 cm^{-1} down to 50 cm^{-1} in one step for all types of transmittance, reflectance and ATR measurements. Utilizing the external water cooled mercury arc high power lamp the spectral range can be ultimately extended down to 10 cm^{-1}. Examples of application will include emission in MIR-THz range, identification of pains, additives in polymers and polymorphism studies.

I010

LOCALIZED QUANTIFICATION OF pH USING FLUORESCENT NANOSENSORS IN SINGLE-PARTICLE TRACKING ANALYSES. **Jérémie Asselin**, Denis Boudreau, Université Laval. (jeremie.asselin.1@ulaval.ca)

The development of nanotechnologies for sensing applications has helped improve significantly analytical parameters like limits of quantification, sensitivities and dynamic ranges of detection for different ions and biomolecules. Notably, architectures such as core-shell particles with plasmon-enhanced fluorescence present a distinctive scattering signature and an increased luminescence brightness, theoretically, these probes could be tracked with limited photobleaching, and better temporal and spatial resolutions. In this work, we characterized a fast-response pH nanosensor in microscopy using a nanoparticle tracking analysis (NTA) technique. Different compositions of silver-core and silica-shell particles were compared to achieve maximal signal and sensitivity. Measurements of the scattering from the metallic core allowed tracking of the probes in buffered solutions while the fluorescence intensity allowed quantification of local pH values. Calibration curves were compared with spectrofluorimetric experiments made in bulk suspensions and normalized by concentration values acquired with NTA. The application of these bright nanosensors could be advantageous in biomedical research, where specific organelles can be targeted with a complementary surface functionalization and their activity followed in function of changes in the local intracellular pH.

I011

ANALYSIS OF NEONICOTINOIDS AND PARTICLE BOUND PESTICIDES IN ATMOSPHERIC SAMPLES BY LIQUID CHROMATOGRAPHY-TANDEM MASS SPECTROMETRY.

Renata Raina-Fulton, Asal Behdarvandan. University of Regina, Department of Chemistry and Biochemistry. (Renata.raina@uregina.ca)

A liquid chromatography-positive ion electrospray ionization-tandem mass spectrometry (LC-ESI^+-MS/MS) method for the analysis of neonicoitinoids or selected metabolites have been developed for a wide range of sample matrices including atmospheric samples. Neonicotinoids partition between the gas and particle phase in the atmosphere. A high-volume semi-volatile air sampler is used for collection of the particle phase fraction of pesticides (on filters) and gas phase fraction on atmospheric sorbent materials such as polyurethane foam and XAD-2. A new LC-MS/MS method has been developed for the simultaneous analysis of a wide range of neonicotinoid insecticides (acetamiprid, clothianidin, dinotefuran, imidacloprid, nitenpyram, sulfoxaflor, thiacloprid and thiamethoxam), selected degradation products or metabolites (clothianidin, 6-chloronicotinic acid, N-desmethyl acetamiprid, N-desmethyl thiamethoxam, imidacloprid-olefin and imidacloprid-urea) as well as other fungicides that have been detected in the particle phase including strobilurin fungicides and azole fungicides. A chemical class-specific approach is used to obtain better recoveries for neonicotinoids than with multiresidue pesticide methods. Sample preparation includes accelerated solvent extraction of solid sorbent materials used in atmospheric sampling, pre-concentration, and solid-phase extraction. Detection limits for neonicotinoid insecticides and strobilurin fungicides ranges 0.5-2.0 ng/mL (0.5-2.0 pg/m^3) with these methods adaptable to other sample matrices.

I012

REAL-TIME IMAGING OF pH VARIATIONS IN MICROCHANNELS USING FLUORESCENT NANOPARTICLES.

Jérémie Asselin, Mazeyar P. Gashti, Denis Boudreau, Jesse Greener. Université Laval. (jeremie.asselin.1@ulaval.ca)

Measurements of pH values in confined environments are a challenge for biomedical researches. Recently, developments in microfluidics have allowed impressive control of *in-vitro* conditions for the growth and analytical probing of cell cultures. In this work, a microfluidic platform with a fluorescent nanoparticle-based sensor is demonstrated for real-time, ratiometric pH imaging of biofilms. Sensing is accomplished by a thin patterned layer of covalently bonded $Ag@SiO_2$+FiTC nanoparticles on an embedded planar glass substrate. After validation experiments, the device was used to monitor pH changes at the attachment surface of a biofilm of the oral bacteria, *Streptococcus salivarius*. By controlling flow and chemical concentration conditions in the microchannel, biochemical and mass transport contributions to the Stephan curve could be probed individually. This opens the way for the analysis of separate contributions to dental cavities due to localized acidification directly at the biofilm tooth interface. Moreover, a method for creating pH maps in microchannels containing liquid/liquid and liquid/gas phases comprised of water and CO_2 is demonstrated. It is based on a glass slide coated with nanoparticles exhibiting metal-enhanced fluorescence. The time resolution is better than 500 ms, limited by the fluidic control. This quantitative technique opens the way for new in situ measurements of physical dissolution and chemical reactions in dynamic CO_2 gas-liquid systems.

I013

IN SITU VIBRATIONAL SPECTROSCOPY FOR ENVIRONMENTAL APPLICATIONS RELATED TO ARSENIC REMOVAL TECHNOLOGIES. **Hind A. Al-Abadleh**. Department of Chemistry and Biochemistry, Wilfrid Laurier University, Waterloo, ON N2L 3C5. (halabadleh@wlu.ca).

As advances in nanotechnology are taking place in an effort to build a sustainable and green future economy, it is becoming increasingly important to conduct fundamental research into the surface chemistry of nanomaterials to fully realize their potential in pollutants removal from water resources. In general, molecular-level understanding of processes at the liquid/solid interface demands using simple model systems and in situ techniques such attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR). This presentation will focus on the surface chemistry of hematite nanomaterials with inorganic and organic species of arsenic under environmentally-relevant conditions. Iron is one of the ubiquitous elements found in natural and engineered materials in the oxide and hydroxide forms. The structure of surface arsenic complexes was elucidated from spectral data collected as a function of time, concentration, pH(D) coupled with DFT calculations. Adsorption rates of arsenicals were measured and correlated with the structure of surface complexes. The infrared spectral data were complemented by flow calorimetric measurements to gain insight into surface charge and heats of adsorption. The thermodynamics of surface processes were modeled using the triple layer surface complexation model. We will show how the high affinity of iron oxide nanoparticles towards arsenic compounds in aqueous environments has implications on the mobility of these pollutants in geochemical environments, and design of arsenic removal technologies from industrial wastewater.

I014

METAL SPECIATION IN NATURAL WATERS USING HIGH RESOLUTION MASS SPECTROMETRY. **C. Guéguen**, T. Nguyen Quoc, V. Mangal. Trent University, Peterborough, ON, CANADA. (celinegueguen@trentu.ca)

The chemical speciation and bioavailability of Hg and Fe are markedly influenced by their complexation with dissolved organic matter (DOM) in aquatic environments. The recent development and application of ultrahigh resolution Orbitrap and Fourier transform ion cyclotron resonance mass spectrometry (FT ICR MS) coupled with electrospray ionization allow the identification of individual metal-DOM complexes. In this study, we detected and characterized natural dissolved organic ligands that bind Fe and Hg in the Arctic Ocean and algal cultures. The major complexes were identified based on both exact molecular mass and patterns of metal stable isotope distributions detected by FT ICR MS. Heteroatomic compounds (CHON and CHONS) were found to be one of the most important ligands for Fe and Hg binding, respectively. Although these organic ligands represent a small fraction of the total DOM, their unambiguous presence would help us understand specific roles of DOM in controlling Fe and Hg chemical speciation and biological uptake in natural aquatic environments.

I015 P

NANOPARTICLE SIZE AND ZETA POTENTIAL USING TUNEABLE NANOPORE RESISTIVE PULSE SENSING (TRPS) TECHNOLOGY. **Mary-Luyza Avramescu**[1], Pat .E. Rasmussen[1,2], [1]Environmental Health Science and Research Bureau, Environmental and Radiation Health Sciences Directorate, HECSB, Health Canada, Ottawa, ON, [2]Earth and Environmental Sciences Department, University of Ottawa, Ottawa, ON (mary-luyza.avramescu@canada.ca)

Methods for physicochemical characterization of engineered nanomaterials dispersed in biological fluids are in high demand to improve understanding of toxicology test results. Tuneable Nanopore Resistive Pulse Sensing (TRPS) was evaluated for its ability to determine size, surface charge (zeta potential), and number concentration for individual nanoparticles and also mixtures of different size populations of nanoparticles suspended in Phosphate Buffered Saline (PBS) solution. In the TRPS method, individual nanoparticles (suspended in a fluid) pass through size-controlled pores that are tuned using a combination of pressure and voltage. Each nanoparticle creates a "blockade" signal of ionic current which is measured and converted to particle diameter, surface charge, and concentration. The TRPS technology compared well with traditional Dynamic Light Scattering (DLS) technology using two different types of polystyrene particles in four different sizes (60nm, 100nm, 200nm and 400nm). Experiments showed that size and zeta potential results for negatively-charged carboxylated polystyrene (CPC) and near-neutral polystyrene (CPN) obtained with TRPS confirmed results obtained using DLS. For example, TRPS showed a monomodal particle distribution with size and zeta potential results similar to DLS for CPC with nominal size 100 nm (124nm and -17mV by TRPS vs 129nm and -17mV by DLS) and CPN with nominal size 100 nm (99nm and -12mV by TRPS vs 108nm and -11mV by DLS). A unique advantage of TRPS is that it permits characterization of individual size populations in polymodal dispersions (which DLS cannot do). TRPS revealed a bimodal particle size distribution in NIST 1898 nano-TiO_2 certified reference material with a more abundant 123 nm fraction (88%) and a less abundant 238 nm fraction (12%). In contrast, DLS was capable of identifying only one peak (129nm). Despite its advantages, TRPS is a very labour-intensive technique compared to DLS, and its application appears to be limited to neutral physiological electrolytes. Therefore, TRPS is a very useful complementary method for verifying and/or “fine-tuning” other physical-chemical characterization methods.

I016

THE AGILENT 5110 ICP-OES: ROBUST – POWERFUL – FAST. **Wayne Blonski**, Agilent Technologies Canada Inc. (wayne.blonski@agilent.com)

The Agilent 5110 ICP OES Synchronous Vertical Dual View instrument is uniquely placed within the market as a leader in speed, innovation and robust performance. The many features of this instrument will be discussed and demonstrated with examples from generated data related to gold analysis. Topics will include: hardware overview, software overview, applet software tool, and the IntelliQuant full spectral scan feature.

I017

DEVELOPMENT OF LC-QQQ-MS METHODS FOR CHARACTERIZATION OF REGENERABLE AMINE SOLVENTS USED IN CO2 CAPTURE.

S. Gallant, A. Furtos, K. C. Waldron. Department of Chemistry, Université de Montréal. (karen.waldron@umontreal.ca)

The post-combustion capture of CO2 in the energy industry can be achieved using aqueous amine-based solvents. During the process, which is followed by release of the gases as a pure stream and solvent regeneration, many species are formed including degradation products. These species, amines primarily and nitrosamines, need to be characterized on an on-going basis for both monitoring and improvement in the process, resulting in both economic and environmental benefits. Our objective is to develop liquid chromatography-mass spectrometry (LCMS) approaches to characterize the main degradation products in various solvent samples used for CO2 capture. Many of these products are unknown and thus we need efficient LC methods and high-resolution MS and MS/MS detection for confident peak identification. Classical reversed-phase columns were tested but the highly hydrophilic nature of the samples led to many unretained products. New column technologies for hydrophilic analytes, like HILIC, are showing promise to achieve our first goal of maximizing the separation before identifying all peaks. This presentation will discuss the method development used and the preliminary results for separating standard samples that contain a selection of degradation species known in the aqueous amine solvents, as well as real samples that contain unknown species.

I018

THE DEVELOPMENT OF AN AIR TREATMENT UNIT FOR IMPROVED REAL TIME MSMS MONITORING OF VOLATILE ORGANIC COMPOUNDS.

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The monitoring of volatile organic compounds (VOCs) in air is usually performed using specialized sampling and gas chromatography techniques. True real time analysis and quantification of VOCs in ambient air is increasingly important in cases of industrial emissions assessment and environmental emergencies. Our Division operates a TAGA Mobile Laboratory whose main analytical instrument is a customized APCI-MSMS. The MS response for various VOCs was analyzed over time and found to be unstable due to fluctuating atmospheric conditions. Since water, naturally present in ambient air, is used as the reactive gas for the ionization of VOCs, a custom built air treatment MS peripheral was designed and assembled to control the temperature (T) and the absolute humidity (AH) of the sampled air prior to the ionization source of the MS. An assessment of the air treatment peripheral use for the analysis of various VOCs shows an attenuation of the influence of atmospheric conditions on the MS response when compared to the analysis of the same standards done without T and AH control. More importantly, controlling the T and AH of the sampled air enables the creation of more reproducible calibration curves for various VOCs allowing for more reliable and ultimately faster quantification in continuous real time APCI-MSMS VOCs monitoring conditions.

I019

CARACTERISATION OF BIOACTIVE CRANBERRY FRACTIONS BY MASS SPECTROMETRY APPROACHES. Marie-Claude Denis[1], Yves Desjardins[2], André Marette[2], Pascal Dubé[2], Stéphanie Dudonné[2], Edgard Delvin[1], Emile Levy[1], **Alexandra Furtos**[1], [1]Universite de Montreal, Montreal, QC H3T 1C5, [2]Institute of Nutraceuticals and Functional foods (INAF), Universite Laval, QC G1V 0A6 (Alexandra.furtos@umontreal.ca)

Increasing evidence indicates that fruits contain functional nutrients with several preventive and therapeutic health benefits. Among them, cranberries have recently received attention as a result of their association with protection against urinary tract infections, glycemic response improvement and cardiovascular risk prevention, but with limited focus on gastrointestinal health. In this study, cranberry extracts have been separated in three fractions of low, medium and high molecular weight. The potential effects of these fractions on intestinal Caco-2/15 epithelial cells was evaluated and an obvious reduction in oxidative stress and inflammation was observed. A combination of LC-MS/MS (on a Synapt G2-S from Waters) and MALDI-TOF (on an ultrafleXtreme from Bruker Daltonics) methods were used to characterize the polyphenolic species responsible for the observed biological activity. Reversed phase and hydrophilic interaction liquid chromatography (HILIC) coupled to high-resolution mass spectrometry were first used to generate empirical formulae for the species identified in the 3 fractions. Additionally, MALDI-TOF/TOF was performed on the medium and high fractions in order to obtain complementary information on larger size oligomers. The LC-MS analysis revealed that the low molecular weight fraction was essentially constituted of small absorbable phenolic acids and some anthocyanins. The medium fraction was mostly composed of anthocyanin and flavonols and also procyanidins monomers, dimers and small oligomers. A particular attention was paid to characterizing the high molecular weight fraction in view of its dominant antioxidant and anti-inflammatory actions noted on intestinal epithelial cells exposed to various stressors. It contained for the most part flavonols and procyanidins, the latter essentially composed of oligomers and polymers. Procyanidin oligomers/polymers up to DP16 were identified by both HILIC-LC-MS and MALDI-TOF approaches.

I020

FTIR SPECTROELECTROCHEMISTRY: NEW ASSESSORIES AND APPLICATIONS. **Sergey Shilov**, Matthias Kessler, Bruker Optics, 19 Fortune Dr., Billerica, MA, USA (Sergey.Shilov@bruker.com)

The combination of FT-IR spectroscopy with electrochemistry offers insight in the molecular change during electrochemical reactions in an addition to the electrochemical response of the studied media. This method can be applied for investigations of electrolytes or reactions at electrode surfaces. New accessories for the spectroelectrochemical studies will be presented. Accessories can be configured for the reflection-absorption or for the attenuated total reflectance (ATR) measurements. IR reflection-absorbance spectroscopy (IRRAS) set-up is used for the studies of the electrolyte and the electrode surface while ATR configuration is used to analyze the electrode surface without strong influence of the electrolyte. Optimization of spectroelectrochemical setup and details of communication between the potentiostat and the FTIR spectrometer will be discussed. Example of applications will include electro oxidation of metal-organic complexes, alcohols, and glycerol.

I021

SINGLE CELL ICP-MS ANALYSIS: QUANTIFYING THE UPTAKE OF METALS BY UNICELLULAR ORGANISMS ON A CELLULAR LEVEL.

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The manufacture and use of products containing metals or metallic nanoparticles (NPs) has been increasing over the years. Some of these products are designed to biologically interact, in the case of medical or anti-bacterial products, while others are not, such as paints, fuel additives, and sunscreens. In either case, the interaction of metals on a cellular level is inevitable whether targeted or accidental (environmental) exposure. Accurately measuring exposure levels and cellular uptake of metallic products can be challenging due instrumental limitations or biological diversity. Metal concentrations are often measured as the ensemble of the entire cell population through acid digestion with no information on the distribution of metal in the cell population.

Single cell ICP-MS (SC-ICP-MS) is a new ICP-MS technique based on single particle ICP-MS (SP-ICP-MS), which allows for the measurement of the metal content of individual unicellular organisms in attograms (10^{-18} g) per cell. SC-ICP-MS allows for the quantification of both exposure concentration and dose to unicellular organisms in both environmental and human health studies with minimal sample preparation and at relevant metal exposure concentrations. Furthermore, SC-ICP-MS allows for the quantification of both metal concentration within the cell as well as the number of cells containing that metal, permitting the measurement of intrinsic metal as well as the uptake of both dissolved and nanoparticulate (NP) metals. Here we will discuss the challenges faced with experimental design and methods for SC-ICP-MS, along with two examples highlighting the use of SC-ICP-MS in both the medical and environmental communities. Firstly, we will describe the use of SC-ICP-MS to measure the uptake of the metal-containing chemotherapy drug, cisplatin. Secondly, we will describe the uptake of dissolved and NP gold into various strains of flagellated freshwater algae.

I022

CHOOSING THE PROPER SAMPLE INTRODUCTION SYSTEM TO ALLEVIATE INTERFERENCES IN ICP.

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The proper selection of sample introduction components is critical to mitigate matrix effects in the analysis of trace and ultratrace metals in ICP spectrometry. In this paper, we will discuss how the appropriate nebulizer, spray chamber, torch and other ancillary accessories can be used to reduce interferences and improve accuracy.

I023

PHOTOTHERMAL MICROFLUIDIC CANTILEVER DEFLECION SPECTROSCOPY REFLECTING CLUSTERING MECHANISM OF ETHANOL WATER MIXTURES. **M. S. Ghoraishi**, J. E. Hawk, T. Thundat, Chemical and Material Engineering Department, University of Alberta, Canada (ghoraish@ualberta.ca)

Understanding liquid properties in small scale has become important in recent decades. Aqueous mixtures of alcohol have been under investigation among biologists, physicists, chemists and engineers since such a mixture is a typical prototype for biomolecules, micelle formation, and structural stability of proteins (to name a few). Protein stability for example can be affected by solute-solute, solvent-solvent and solvent-solute interactions. As a result, Short chain alcohols such as EtOH have been used as a simple model for understanding of more complex aqueous biomolecules. The structure of ethanol conformers effects absorption bands of C-C-O stretch in IR spectrum. Presence of anti conformer lead to strong absorption band around 1045 cm-1 related to C-C-O stretch while gauche conformers absorption related to the same stretch is approximately 40 cm^{-1} further. In this letter we study vibrational energy peaks of EtOH water binary mixtures using micromechanical calorimetric spectroscopy using bimaterial microfluidic cantilevers (BMC). The IR spectra of EtOH-water are experimentally collected employing a BMC as concentration of EtOH changes from 20–100 wt%. Voigt function is used to deconvolute spectrums and average peak maxima of each peak are plotted for both anti and gauche conformers as a function of concentration. As concentration of EtOH varies in the mixture, considerable shifts in the wavenumber at IR absorption peak maxima are reported. The experimentally measured shifts in the wavenumber at IR absorption peak maxima are related to changes in dipole moment (μ) of EtOH at different concentration. IR absorption wavenumber shows proportionality to ($1/\mu$). The relationship between IR absorption wavenumber for both anti and gauche conformers of EtOH, and inverse dipole moment, $1/\mu$, of EtOH at different concentrations follows a power law dependence agreeing with a least squares agreement of 92% for anti and 97% for gauche conformers. Our technique offers a platform to investigate dipole effect on molecular vibrations of mixtures in confined picoliter volumes, previously unexplored with other analytical techniques due to limitations of volume under study.

I024

FORM SINUSOIDAL WAVES LAMINAR CO-FLOW IN MICRO DEVICES BY USING MICRO-MANAGER TO CONTROL FLOW RATE. **Nan Jia**, Jesse Greener, Department of Chemistry and Centre de recherche sur les matériaux avancés (CERMA), Université Laval, Québec, QC G1V 0A6, Canada (jesse.greener@chm.ulaval.ca)

Micro-Manager is a powerful tool to combine microscope with other hardware such as pump, stage or shutter. It provides more possibilities for researchers to get image data more efficient and accurate. Here we demonstrate a way to crate sinusoidal standing waves at the interface of two solution in X shape micro channel by using Micro-Manager to control solution flow rate. Different period of sinusoidal waves image data can be obtained automatically by applying different frequency or flow rate. And the sinusoidal waves can be standing waves in specific condition. This study will help to fabricate villi like chitosan membrane by in situ generation of pH gradients, which can mimic the human intestinal environment and has great potential in numerous field such as drug development and in vitro human intestinal model study.

I025

HYDRODYNAMIC EFFECTS ON BIOFILM AT THE BIOINTERFACE USING A MICROFLUIDIC ELECTROCHEMICAL CELL: CASE STUDY OF PSEUDOMONAS SP.

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Electrochemical impedance spectroscopy (EIS) has been previously applied to verify the trend of bacterial cells attachment and biofilm formation. Various bioelectrical modeling for electroactive and non-electroactive biofilm were used to identify the electrode/electrolyte and the electrode / bacteria / electrolyte interfaces. The anchoring biofilm layer is expected to exhibit a different response to environmental stresses than for portions in the bulk, due to the protection from other strata and the proximity to the attachment surface. In this project, in situ EIS measurements of biocapacitance and bioresistance of Pseudomonas sp. biofilms were conducted during the growth phase and under different shear flow conditions. Distinct, but reversible changes to the amount of biofilm and its structure at the attachment surface were observed during the application of elevated shear stress. Following the application of extreme shear stresses, complete removal of significant portions of biofilm outer layers occurred, but this did not change the measured quantity of biofilm at the electrode attachment surface.

I026

ANALYSIS OF SMALL NANOPARTICLES BY SP-ICP-MS- LOWER SIZE DETECTION LIMITS THROUGH INSTRUMENTAL IMPROVEMENTS AND DATA TREATMENT.

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Single particle ICP-MS is a promising technique used to determine nanoparticle (NP) concentrations and size distributions in environmental and biological media. It is generally acknowledged that the smallest nanoparticles are the most reactive and thus are likely to pose the greatest environmental and biological risk. The lower limit of particle sizes that can be detected by SP-ICP-MS will depend on the signal to noise, which is often limiting for the lighter elements or highly soluble nanoparticles. For example, using a quadrupole ICP-MS, size distributions are only possible for TiO2 nanoparticles above □60 nm. Three strategies have been employed in our lab in order to increase S:N: (i) the use of a sector field instrument; (ii) the generation of dry aerosols and (iii) the removal of dissolved metal. For example, by coupling a desolvatation membrane to a quadrupole ICP-MS, it was possible to increase measurement sensitivity in order to enable the determination of TiO2 NP as small as 26.3 nm. The use of a sector field ICP-MS increased sensitivity further (49Ti: 35 cps/ppt in wet mode; 890 cps/ppt in dry mode), allowing us to attain sizes as small as 15.6 nm. Since the detection of very small NP is also influenced by the background (instrumental and dissolved metal), results will also be presented on the data treatment and reduction of dissolved metal.

I027

INTRODUCING AGILENT'S SECOND GENERATION ICP-MS/MS, THE 8900 QQQ FOR UNPRECEDENTED SPECTRAL INTERFERENCE CONTROL, EXTREME HIGH SENSITIVITY, PERFECT ISOTOPIC SIGNATURES, AND MUCH MORE.

Pamela Wee, Agilent Technologies Canada Inc. (pamela.wee@agilent.com)

Since its launch in 2012 as the world's first ICP-MS/MS, the Agilent 8800 QQQ rapidly established itself in diverse industries from routine production labs to advanced research to manufacturing. Based on an uncompromised design, the two full-size hyperbolic quadrupole mass filters (QMF) in the Agilent ICP-QQQ guarantees an abundance sensitivity on the order of E-10, unmatched by any ICP-MS. Simply by using the MS/MS mode, wing overlaps are eliminated. Chemical pre-separation cannot remove wing overlaps from a massive spectral peak of the same elemental ion. Both full QMFs deliver better than unit mass resolution. These are critical for the successful resolution of spectral interferences using gas phase ion chemistry in a reaction cell which resides between the QMFs. Cell gases are chosen for the resolution of spectral interferences, for the provision of adequate sensitivity for reliable calibration, and for fast sample throughput. "Real world samples" contain co-existing elements that can react with the cell gases, creating unwanted product ions that cause new interferences. Simply by setting the first QMF to one desired mass, say at M amu, all ions with masses $\leq$ (M – 1) and $\geq$ (M + 1) are prevented from entering the cell. When using reactive gases (such as O_2 and NH_3) either to shift the interference or to shift the analyte, getting the correct isotopic signatures ensures that all spectral interferences are resolved. With the new Agilent 8900 QQQ, sensitivities are doubled without compromising the already low CeO^+/Ce^+ and Ce^{++}/Ce^+ ratios, background decimated, matrix tolerance enhanced to 25% NaCl, 100-fold increase in detector dynamic range, faster detector dwell times, and faster cell gas switching. In addition to interference resolution, instrument conditions conducive to long term stability will also be discussed. Many examples will be shown.

I028

RELEASE OF MESOPOROUS SILICA PARTICLES BY FREE STANDING PH SENSITIVE MEMBRANES.

Nan Jia,[a] Erica Rosella,[a] Estelle Juèrea,[b] Freddy Kleitza,[b] Jesse Greener[a], [a]Department of Chemistry and Centre de recherche sur les matériaux avancés (CERMA), Université Laval, Québec, Québec G1V 0A6, Canada, [b]Institute of Inorganic Chemistry – Functional Materials, University of Vienna, Währinger Straße 42, 1090 Vienna, Austria. (jesse.greener@chm.ulaval.ca)

Here we demonstrate a proof of concept idea that uses microfluidics to form well defined chitosan membranes loaded with mesoporous silica nanoparticles (MCM-48-type), which can be released on demand. The membranes are stable under very high flow rates of PBS buffer, but can be steadily eroded by applying an acid to either side of the membrane. Release rate can be tuned based on membrane synthesis conditions and pH of the trigger solution. The approach has the potential to add smart drug delivery functionality to membranes for special applications in organs on a chip and other areas of regenerative medicine.

I029

CONFOCAL LASER SCANNING MICROSCOPY AND ELECTROCHEMICAL STUDY ON MICROFLUIDIC MICROBIAL FUEL CELL.

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A microbial fuel cell (MFC) is a bio-electrochemical device which bacteria catalyze redox reactions, convert the energy stored in substrates to usable electricity. The MFC is a promising power source, but it remains a great challenge to increase its low power density to make it a viable source of energy in practical applications.[1] The image monitoring of biofilms on the surface of electrode using CLSM microscopy is a standard technique in biofilm research. coupling between produced current and microscopy results provide this opportunity to monitor biofilm parameters such as surface coverage, biomass, and biofilm roughness. [5] We will use a microfluidic system in this case to take advantages of CLSM for on-chip monitoring of biofilm. The advantages of microfluidic MFC in compare to conventional MFC (dual chamber) is that we can use do on chip CLSM measurement with a very thin coverslip. So, it is not necessary to bring the electrode out of channel or use a glovebox system for anaerobic bacteria. We can do measurement without destroying the sample. The cell voltage is related on the quantity of bacteria at the time on the surface of electrode. Hence the confocal laser scanning microscopy (CLSM) were obtained after the experiments. The electrode-adhered *G. Sulfurreducens* biofilm samples were stained with a LIVE/DEAD BacLight staining kit and imaged by CLSM. Preliminary results illustrate the biofilm analysis in different layers.

1. Logan, Bruce E. Microbial fuel cells. John Wiley & Sons, 2008.
2. McLean, Jeffrey S., et al. Environmental science & technology 44.7 (2010): 2721-2727.

I030

ELECTROCHEMICAL IMAGING FOR MICROFLUIDICS: A FULL-SYSTEM APPROACH.

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Electrochemical imaging is developed as a new chemical imaging modality for microfluidics. The technique is based on multipoint voltammetry using an embedded 20x10 microelectrode array implemented on a customized printed circuit board (PCB). Electrode durability was enhanced by chemical modification of the electrode surfaces, which enabled continuous, stable use for over 2 months. A system-level approach enables automatic measurement calibration, data acquisition and data processing through a graphical user interface. Following data processing, redox currents and peak positions are extracted from location-specific voltammagrams and converted into pixels of an “electrochemical image”. The system is demonstrated by imaging steady-state and dynamic laminar flow patterns of flow-confined solutions of the redox pairs $Fe(CN)_6^{3-/4-}$ or multi-redox environments that include coflowing $Ru(NH_3)_6^{2+/3+}$ solutions. Images obtained are compared with flow simulations and optical images for validation. A strategy to achieve measurements with spatial resolution smaller than individual electrodes is also demonstrated as an avenue to enhance image spatial resolution in some cases. It is expected that this new approach to chemical imaging will expand the applicability of microfluidics in certain areas of chemistry and biology without requiring electochemistry specialists.

I031

ELEMENTAL ANALYSIS BY MASS SPECTROMETRY: SOLUTION FROM NU INSTRUMENTS, HR-ICP-MS ATTOM AND GDMS ASTRUM. **Benoit Disch**, Ariane Donard, Phil Shaw. Nu Instruments, Unit 74 Clywedog Road South, Wrexham Industrial Estate, Wrexham, LL13 9XS, UK. (ariane.donard@nu-ins.com)

Mass spectrometry is a well-established technique for the characterisation of major and trace elements in the environment and in industry. In this presentation, solutions from Nu Instrument will be presented including two systems, the AttoM HR-ICP-MS and the Astrum GDMS.The AttoM HR-ICP-MS is a double-focusing single-collector instrument of forward Nier-Johnson geometry which features the unique FastScan Ion Optics. The instrument is entirely purpose designed and built to provide the best performance and reliability coupled with flexibility and ease-of-use for precise and accurate elemental and isotope ratio analysis. The instrument can also be used to rapidly scan/jump between isotopes of interest over a 40% relative mass range without the necessity to change the magnetic field or acceleration voltage. For this mode the magnet is parked in the middle of the mass range of selected isotopes (known as 'park mass'). Acceleration voltage, ESA voltage and ion optics used for beam focusing are kept constant during the acquisition. Only the FastScan Ion Optics located at the entrance and exit of the magnet are varied, being used to rapidly deflect the selected isotopes sequentially onto the magnet park mass for data acquisition. Several applications such as laser ablation, quantitative analysis and nanoparticles will be presented. The Nu Astrum is the latest generation of HR-GDMS instruments developed to be the benchmark in GDMS. The instrument was designed in conjunction with the users of the most widely-used and field-proven instrument, the VG9000. The best design concepts of this system were combined with advances in sample cell design, control electronics and pumping technology to produce a high performance new instrument designed specifically for ultra-trace analysis of impurities. Characteristics and applications will be presented.

I032

CAPILLARY AND MICROCHIP ELECTROPHORESIS FOR FLUORESCENCE-BASED ASSAYS OF ENZYME ACTIVITY IN *DICTYOSTELIUM*. Kathy Rodogiannis, Jessica T. Duong, Kunwei Yang, and **Michelle L. Kovarik**. Department of Chemistry, Trinity College, 300 Summit St. Hartford, CT 06106. (michelle.kovarik@trincoll.edu.)

Many enzyme assays are based on fluorescence signals from fluorogenic, FRET-based, or fluorescently-tagged reporter substrates. While well-established fluorogenic substrates are available, a limitation of these reporters is that only the product species, and not the reactant species, is detectable, making it difficult to determine the effect of variation in reporter loading. Measurements based on spectral changes in signal with enzyme activity, such as FRET assays, address this issue since both the reactant and product species are fluorescent; however, these measurements require highly specialized substrates. In contrast, substrates with a simple fluorescent tag are more readily designed and modified, but require physical separation to distinguish reactants from products. I will describe our efforts to use capillary and microchip electrophoresis separations to enhance the utility of fluorogenic and fluorescently-labeled substrate reporters. In particular, we are applying these tools to measure oxidative stress and protein kinase activity in the social amoeba *Dictyostelium discoideum* with the goal of single-cell analysis of enzyme activity in these cells.

I033

MONITORING UPTAKE OF A DNAZYME MOTOR BY LIVING CELLS USING ICP-MS.

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Synthetic DNA motors have great potential to mimic natural protein motors in cells; but the operation of synthetic DNA motors in living cells remains challenging. Herein, we report a DNAzyme motor that operates in living cells in response to a specific intracellular target. The motor system is constructed on a 20-nm gold nanoparticle (AuNP) decorated with hundreds of substrate strands serving as DNA tracks and dozens of DNAzyme molecules each silenced by a switch strand. Interaction of a target molecule with the switch strand turns on the DNAzyme motor, initiating the autonomous walking of the motor along the AuNP. To operate in living cells, the DNA motor system must be readily taken up by living cells. We used ICP-MS to evaluate the cellular update of the DNAzyme motor system, because ICP-MS enables highly sensitive detection of AuNPs. Our results showed when 0.2 nM AuNP and 2 h incubation were used, each cell took up about 3.2×10^4 AuNPs, which is approximately equivalent to 13 nM AuNP in the cell.

I034

MICROFLUIDIC CO-FLOWS FOR A SELF-STANDING COLLAGEN MEMBRANE SYNTHESIS.

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Microfluidics laminar flow patterning has recently been exploited for *in situ* microfabrication of polymer membranes[1]. Collagen is well known for biomedical applications due to its biocompatibility[2]. In this work we feature a flow-templated growth of collagen membrane in microfluidics device. A side-by-side co-flowing stream of buffer solution at pH 10 and collagen solution at pH 3.5 generated pH gradients at the interface of the two solutions. As the localized pH at the interface match with pKa of the molecule, collagen started to jellified (ca. 7.4). A solid self-standing collagen membrane spanned in the X-shape microfluidic device was completely formed within ten minutes. Bright field microscopy was used to observe the modification of bulk properties of the membrane (size, swelling coefficient, density) by the modulation of the synthesis parameters (pH and flow rates). X-Ray diffraction pattern was collected to confirm the crystallinity of the collagen membrane under the flow. The degradation process of the membrane was investigated by the presence of flow. Finally, 3T3 cells were seeded into the synthesized membranes suggest the capability of the membrane to support cell growth and proliferation. We expect this fabricated construct to be applied in cellular signaling studies and in the development of organs-on-a chip device.

1) Luo, X.; et al. *Lab on a Chip.* 2010, *10*, 59–65.
2) Boccafoschi, F. et al. *Macromol*. *Biosci*. 2007, *7*, 719726.

I035

THE USE OF MICRO-IMAGING TECHNIQUES TO ANALYZE BIOFILM DEVELOPMENT DATA IN MICROCHANNEL. **Farnaz Asayesh**, Jesse Greener, Department of Chemistry, Laval University, Quebec, QC, G1V 0A6 (Farnaz.Asayesh.1@ulaval.ca)

Bacterial biofilms are formed from surface-adhered bacteria surrounded by an extracellular polymeric substrate (EPS). Despite laminar-flow templating approach that can confine biofilm growth in the lateral directions within a microchannel, biofilms tend to also grow upstream toward the nutrient source. This eventually causes the contamination of upstream tubing, which undermines accurate specification of experimental conditions. Here, we present a microfluidic device with 63 mm for length and 2 mm width for head and body, 250 um for neck which modulates the upstream flow velocity as a mechanism to stop backward growth and inlet contamination for long-duration experiments. For this purpose, we have to observe changes in biofilm development during the whole experiment inside the microchannel. However, limited field of view made it impossible to observe the entire channel. Therefore, an automatic stage has been used to monitor biofilm changes in time throughout the whole channel, the acquisition time is 1h and the experiment last for 72hrs. After gathering all the images, ImageJ has been used for stitching images, each image has individual spatio temporal measurement of optical density which automatically applies background correction. At the end, we have clear observation of biofilm behavior in the entire microchannel during complete experiment.

I036

AUTOMATED ENZYME MICROREACTOR FABRICATION FOR PROTEOMICS APPLICATIONS: EVALUATION BY CZE, HPLC AND MS. G. Ghafourifar, A. Fleitz, B. Fleury and **K.C. Waldron**. Department of Chemistry, Université de Montréal, Montréal, QC. (karen.waldron@umontreal.ca)

Enzymatic digestion of proteins is an important sample preparation step in bottom-up protein sequencing. By using immobilized proteolytic enzymes over soluble formats, higher enzyme:substrate ratios can be used to accelerate digestion while avoiding unwanted autolysis products that can lead to ionization suppression in peptide mass mapping. Many linking chemistries and solid supports work well to immobilize enzymes. However, a simple method to achieve this in microfluidic channels is less obvious. This presentation will show our progress in making glutaraldehyde-crosslinked enzyme in batch form and “in-situ” to fabricate an immobilized enzyme microreactor (IMER). Our long-term goal is to develop simple IMER methods for microfluidic platforms that eliminate the need to pack solid-phase particles. In the short term, single capillary IMERs of dimensions 0.25 mm ID x 43 cm have been prepared using an Agilent CE system to deliver the regents needed for IMER fabrication, followed by the substrate. Digests collected at the outlet were analysed by CZE-UV, CZE-MS or HPLC-MS and the peptide maps were used to assess efficiency of the fabrication/ digestion using peptide and protein standards. Small IMERSs (0.25 mm ID x 3 cm) were fabricated manually and imaged by confocal laser scanning fluorescence microscopy. This showed that immobilized chymotrypsin was mostly near the inner walls but also extended a few tens of nanometers into the centre of the microreactor suggesting that a significant amount of immobilized enzyme was present.

I037

A COMBINED OPTICAL MICROSCOPY AND INFRARED SPECTRAL MICROSCOPY APPROACH FOR *IN-SITU* STUDYING OF BIOFILMS. **Mohammad Pousti**, Jesse Greener, Department of Chemistry, Laval University, Quebec, QC, G1V 0A6, Canada (mohammad.pousti.1@ulaval.ca)

Optical microscopy has been the primary in situ characterization tools due to its compatibility with transparent microfluidic devices and its ability to provide spatially-resolved information. In recent years, different types of microscopy including optical, fluorescence and laser scanning methods offered new ways of improving our knowledge in biofilm related subjects. But all of these techniques lacks giving chemical informations of biofilm components. Hence, improving new methods for acquiring chemical information is vital. For monitoring biofilm in real-time, analytical methodologies need to be further developed. Here we introduce a fast, low-cost, label-free and reliable Infrared (IR) imaging technique for in situ analysis of biofilms inside microfluidic channels. This technique incorporates advantages of previous methods for IR imaging, and it includes an automatic stage driven by a stepper motor for positioning the microfluidic device in different positions relative to the probe beam. Furthermore a home-made optical microscope is fixed on top of microchannel to visually guide us and complement IR data. We programed the stage movement to be synchronized with IR and optical microscope acquisition so that at each position we have both IR and optical spatio temporal information.

I038

SPECTROSCOPIC IMAGING IN MICROCHANNELS FOR STUDIES OF BIOFILMS. **Mohammad Pousti**, Jesse Greener, Department of Chemistry, Laval University, Quebec, QC, G1V 0A6, Canada (mohammad.pousti.1@ulaval.ca)

Biofilms are surface-attached communities of bacteria, encased in an extracellular matrix of secreted proteins, carbohydrates and DNA. The vast majority of all bacteria on Earth exist in a biofilm format. They are also becoming an important biomaterial for applications ranging from bioreactors to energy production. Microfluidics is accelerating biofilm research as a general platform for manipulation and study of biofilms. However, for further development, new in situ analytical methodologies are needed. Specifically, for chemical analysis biofilms and chemical by-products at different positions are required. Here we introduce a fast, low-cost and reliable method for acquiring 1D maps with microfluidic devices by attenuated total reflection infrared (ATR-IR) spectroscopy. The system includes a home-built automatic ATR-IR stage for moving the microfluidic/ATR assembly to different positions relative to the probe beam. Furthermore, a customized micro-imaging system is coupled to the platform add complementary data. We demonstrate this approach in two acquisition modes: parallel measurements of multiple microchannels containing biofilms at different ionic strength environments and 1D maps of biofilms down the length of a single channel. Future directions will be discussed.

I039

INVESTIGATION BY LIQUID CHROMATOGRAPHY OF A MIXED-MODE STATIONARY PHASE BASED ON BILE ACID OLIGOMERS AS INVERTIBLE AMPHIPHILIC POCKETS.

V. Dionne-Dumont, M. Zhang, N. Lévaray, X.X. Zhu and K.C. Waldron, Département de chimie, Université de Montréal (karen.waldron@umontreal.ca)

Novel bile acid-based oligomers that can form invertible amphiphilic host-guest pockets in solution were synthesized then grafted onto silica particles of 6 micron diameter. The molecular pocket formed by the oligomers is capable of inverting itself to form either a hydrophobic or hydrophilic cavity depending on the polarity of the eluent as a result of their amphiphilic nature and conformational flexibility of the linker between monomers. Changes in the mobile phase polarity thus allow us to switch the chromatographic separation mode between normal and reversed phase. Alteration of the experimental conditions can be used to adjust retention and selectivity. Moreover, the molecular pockets can potentially act as a chiral selector in certain separations based on previous reports for a monomeric bile acid-based stationary phase. This presentation will describe our efforts to characterize the novel materials in different modes, such as HILIC and reversed phase. The chromatographic performance of the new mixed-mode stationary phases was evaluated by studying the effect of eluent composition, pH, buffer concentration of the mobile phase and column temperature. The reproducibility of our capillary column packing technique will also be discussed.

I040

CAPILLARY ELECTROPHORESIS FOR DETECTION OF PEPTIDE FOLDING INTERMEDIATES.

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In non-polar environments, polyproline takes on an all-*cis* helical structure (PPI); upon introduction to an aqueous environment, it folds into an all-*trans* helical structure (PPII). Due to the high energetic barriers of the *cis-trans* isomerization, this folding takes place over a much longer timescale than most peptide folding. Recently, intermediates along the folding transition pathway were observed for the 13-mer polyproline peptide using ion mobility spectrometry-mass spectrometry (IMS-MS). However, as IMS is a gas-phase separation technique, questions remained about reporting of solution-phase phenomena. Mechanistically, capillary electrophoresis (CE) is the solution-phase analogue of IMS, and it allows for direct separation and observation of charged species in solution. Using CE with UV/Vis detection, we have observed intermediates in the transition between PPI and PPII for polyproline-13. Although we resolve fewer intermediates than observed in IMS, summation of IMS features allows us to demonstrate that the same profile of species as a function of time is being observed with both techniques. We have since followed the PPI→PPII transition of a variety of different length polyprolines; intermediates are only observed when the polyproline peptide is of sufficient length.

I041

SUPER-RESOLUTION FLUORESCENCE MICROSCOPY AS A TOOL FOR THE CHARACTERIZATION OF CELLULOSE NANOSTRUCTURE. Mouhanad Babi and **Jose Moran-Mirabal**, Department of Chemistry and Chemical Biology, McMaster University, 1280 Main Street West, Hamilton, ON L8S 4M1 (mirabj@mcmaster.ca)

Cellulose, a major structural component of plant cell walls, is Earth's most abundant biopolymer and an attractive material for the production of biodegradable and renewable products, such as biofuels and bioplastics. Manufacturing these products often entails the chemical or biochemical breakdown of cellulose, a process that is limited by its crystalline structure. To better understand these manufacturing processes and improve their efficiency, we require insight into the nanoscale structure of cellulose and the mechanism of its depolymerization. In this work, direct stochastic optical reconstruction microscopy (dSTORM) was used to study the structure of fluorescently-labelled bacterial microcrystalline cellulose (BMCC) at the nanoscale. Super-resolution imaging unveiled repeating patterns of high and low fluorophore density on BMCC microfibrils that are hypothesized to represent dislocations (disordered) and crystalline regions of cellulose. Grafting cellulose using different dyes or labelling reactions produced similar patterns, suggesting that the fluorescent patterns are labelling chemistry-independent, and are instead encoded within the native cellulose structure. The length of the dark regions was measured and their distribution was found to correlate with the length of cellulose nanocrystals produced by short hydrolysis treatments. The length of the microfibril dark regions were also determined to be independent on the concentration of dye during the grafting procedure, strongly suggesting that the observed labelling patterns are due to naturally encoded crystalline and disordered regions in cellulose microfibrils. A fluorescently-labeled cellulase – CBHI-Cy5 – bound to labelled BMCC was imaged in the same way and the results show that the enzyme does not exhibit any preferential binding to either the crystalline or disordered cellulose regions. Understanding the nanostructure of cellulose will allow us to improve cellulose manufacturing processes and give insight into how plant cells assemble, restructure and degrade their cell wall.

I042

FORENSIC ANALYSIS OF AUTOMOTIVE PAINT CHIPS FOR VEHICLE MANUFACTURER, COLOUR AND YEAR OF PRODUCTION USING ELECTROTHERMAL VAPORIZATION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY. **L. Huang** and D. Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K6L 3N6 (diane.beauchemin@chem.queensu.ca)

Forensic analysis demands fast and simple methods of identification, as samples could be time-sensitive and prone to contamination. A direct solid sampling method, electrothermal vaporization (ETV), coupled with a trace elemental analytical technique, inductively coupled plasma-optical emission spectrometry (ICPOES), is proving useful for forensic analysis. Its direct solid sampling capabilities decreases sample processing time and contamination, as very little sample preparation is required. The inorganic information obtained can then be used to identify and match samples using linear discriminant analysis (LDA), a probability statistical method derived from Bayes' theorem. Using this method, small pieces of paint flakes were correctly matched to their respective manufacturer, colour, and year of production to help solve hit-and-run cases.

I043

SIZE AND NUMBER QUANTIFICATION OF SILVER NANOPARTICLES IN NATURAL WATERS USING SINGLE PARTICLE ICP-MS. **Karla Newman**, Water Quality Centre, Trent University, 1600 West Bank Drive, Peterborough, ON (karlanewman@trentu.ca)

Silver nanoparticles (Ag NPs) are being incorporated into many consumer products. Since Ag NPs can be released from these products and then enter domestic wastewater, there is a growing concern regarding the potential impacts of Ag NPs on aquatic ecosystems. However, the concentrations in surface waters are likely to be low (<0.5 ng L^{-1}) and the detection of Ag NPs at these low concentrations remains a challenge that can only be addressed by developments in analytical instrumental and sample preparation methods. Here, the parameters and conditions that limit the accurate measurement of particle sizes and number concentrations for Ag NPs were evaluated using a high sensitivity magnetic sector ICP-MS in single particle mode and dwell times of 10 to 100 μs. Accurate particle sizing *and* number quantification was achieved using dwell times ≤ 50 μs and a maximum particle frequency of 200 events s^{-1}. The composition and the shape of the sample vials used for the preparation and storage of NP standards and samples were shown to influence both particle sizes and numbers. Silver NPs stored in clear glass vials had increased rates of particle dissolution due to photo-assisted oxidation on the glass surface. Digestive ripening of Ag NPs, whereby smaller particles grow at the expense of larger ones, was also observed for both amber and clear glass vials. Polypropylene (PP) and perfluoroalkoxy (PFA) vials, and polymeric membranes (Nylon, cellulose acetate) used for sample filtering, were found to present a relatively inert surface, with no changes in the measured particle size distribution. However, these materials were prone to surface adsorption of NPs. Protocols were developed to address these challenges and characterise Ag NPs in a range of surface waters.

I044 P

CLOUD POINT EXTRACTION OF PLUTONIUM IN FISH TISSUES COUPLED TO ALPHA SPECTROMETRY. **Alexa Leblanc** and Dominic Larivière, Radioecology laboratory, Chemistry Department, Laval University. (alexa.leblanc.1@ulaval.ca)

This presentation will highlight the methodological development of a simplified approach to extract and quantify plutonium from fish tissues by alpha spectrometry and ICP-MS. To do this, a cloud point extraction method (CPE) approach is used. This method allows the actinides to be separated from the matrix and preconcentrated in a small volume of surfactant. The use of a selective ligand makes it possible to form a complex with plutonium and which is extracted into the micelles. The ligand P, P-di (2-ethylhexyl) of methanediphosphonic acid (H_2DEH[MDP]) is used because it has a high extraction affinity for actinides and especially for plutonium. Since plutonium is a long-half-life alpha emitter, analyses can be performed by alpha spectroscopy or by ICP-MS, depending whether or not the isotopic composition is required. However, prior to cloud point extraction and analysis, fish samples are treated to eliminate water and organic matter that can interfere with micelle formation. The various stages required for the mineralisation, the CPE preconcentration and finally the detection by alpha spectrometry or ICP-MS will be presented for the analysis of large quantities (> 500 g) of fresh fish tissues.

I045

MECHANISM AND CONTROL OF THE SELECTIVE FRAGMENTATION OF PROTEIN IONS.

Huixin X. Wang,[1] Michael G. Leeming,[2] **W. Alexander Donald**[1], [1] School of Chemistry, UNSW Sydney, Australia; [2] School of Chemistry, University of Melbourne, Australia. (w.donald@unsw.edu.au)

Whole protein mass spectrometry (MS) is an emerging approach in which intact protein ions can be isolated and fragmented without proteolytic digestion. The primary advantage of intact protein MS is that degradation products, sequence variants, and different combinations of post-translational modifications can be distinguished. However, a key challenge is that ion fragmentation methods generally result in non-specific dissociation, which can significantly limit protein identification because ion signal is diluted between hundreds of fragment ions.

We have discovered that protein ions in very high charge states (CSs) dissociate selectively in higher-energy collision-induced dissociation (HCD). As CS increases, the extent of fragmentation and sequence coverage decreases significantly. This is attributable to predominantly non-specific cleavages at lower CSs while selective fragmentation is observed at higher CSs. By comparing measured cleavage sites to calculated protonation sites, these data indicate that “mobile” protons drive fragmentation. At lower CSs, where basic sites are protonated, additional collision energy is required to mobilize protons onto backbone sites for fragmentation. At sufficiently high CSs, protons are localized on backbone residues prior to HCD. Thus, highly selective fragmentation occurs near the predicted sites of backbone protonation.

Our results indicate that low CSs are desirable for obtaining extensive sequence information for deep sequence characterization. Alternatively, HCD of high CSs can result in the formation of selective sequence ions, which can be used as “sequence tags” for protein identification. Now, the “optimal” CSs of protein ions can be predicted to enable selective and controlled dissociation for generating sequence tags with maximum sensitivity.

I046

NON-TARGETED IDENTIFICATION OF ORGANIC MIGRANTS FROM REUSABLE PLASTIC BOTTLES USING LC-MS: INFLUENCE OF THE DATA POST-PROCESSING.

L.Tian, *S.* Bayen, Department of Food Science and Agricultural Chemistry, McGill University, 21111 Lakeshore, Ste Anne de Bellevue, QC H9X 3V9 (stephane.bayen@mcgill.ca)

The use of food simulants is a common approach to assess the leaching of potentially harmful chemicals into food or drink from food packaging and other food contact materials. Food simulants (e.g. water/ethanol or acetic acid solutions) are used in place of actual food, providing a simpler and more systematic tool to study chemical migration. In this study, water/ethanol was used as a food simulant to extract organic migrants from >20 plastic bottles. Extracts were analyzed using high performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry (HPLC-QTOF-MS). Both MS and MS/MS data were recorded and explored to (i) identify chemical migrants and (ii) compare different types of bottles (e.g. "BPA-free" or not, transparent vs colored). In this presentation, we will discuss the influence of data processing on the identification of features (organic migrants) specific to each type of bottles.

I047

A CPE METHOD TO PRE-CONCENTRATE AND EXTRACT RADIONUCLIDES FROM ENVIRONMENTAL MATRICES. **Anthony Tremblay** and Dominic Larivière, Radioecology laboratory, Chemistry Department, Laval University. (anthony.tremblay.3@ulaval.ca)

It can be challenging to measure the concentration of radionuclides using mass spectrometry when these concentrations are in the "parts per trillion" range. Yet, radionuclides can cause health problems even at these low concentrations, especially alpha-emitting radionuclides with a short half-life. This is why we are developing methods to rapidly extract and pre-concentrate radionuclides at the ultra-trace level in an environmental matrix to be able to measure their concentration. The method consists of a cloud point extraction of target radionuclides coupled with an ICP-MS. The cloud point extraction system developed is composed of a mix of non-ionic (Triton X-114, Triton X-100) and ionic (cetyltrimethylammonium bromide) surfactants. The target radionuclides are extracted by forming stable complexes with chelating agents chosen for their selective behavior towards one or a couple of radionuclides targeted by the method. The complexes formed are electronically neutral and tend to go inside the micelles, in the organic phase. By separating the small volume of surfactant rich phase from the aqueous phase of the solution, we achieve the pre-concentration and the extraction of the target radionuclides. The final goal of the project is to simplify the cloud point extraction method and make it robust enough that it can be performed as a routine analysis. Therefore, work is being done to automatize the method, to make it more efficient. Works is also being done to achieve a back-extraction of the radionuclides, so that the organic phase isn't injected in the instrument. A sequential system that could extract two or more target elements from the same sample using two different cloud point extraction systems is also in progress.

I048

DETERMINATION OF ^{210}Pb IN WATER SAMPLES BY ICP-MS/MS AFTER CLOUD POINT EXTRACTION USING CROWN ETHERS. **Guillaume Blanchet-Chouinard** and Dominic Larivière, Radioecology laboratory, Chemistry Department, Laval University. (guillaume.blanchet-chouinard.1@ulaval.ca)

Isotopes such as ^{90}Sr, ^{137}Cs ^{210}Pb and ^{210}Po, if measured in our environment, can be significant contributors to radiation exposure. The potential radiotoxicity of lead-210 originates from its relatively long half-life ($t_{1/2}$ = 22,3y), the high energy associated with its progeny, such as Po-210, and chemical similarity to alkaline earth elements. This last feature of lead-210 makes him difficult to separate from complex environmental matrices. The maximum acceptable concentration for Lead-210 in drinking water is 0,1 Bq/L, the lowest amongst the naturally occurring radionuclides, which pose a challenge for its rapid and precise determination by radiometric and mass spectrometric approaches.

Therefore, the biggest challenge for ^{210}Pb determination is to find an effective way to selectively extract and preconcentrate this radionuclide. Several selective preconcentration techniques such as co-precipitation exist for such tasks. Recently, cloud point extraction (CPE) has been used for the isolation and enrichment of radionuclides in a variety of matrices. The concept of CPE consists in the aggregation of surfactants containing the analyte of interest based on changes in experimental conditions (e.g. temperature). Crown ethers, that have already demonstrated their great affinity for lead with other kinds of extraction have been investigated to provide selectivity to the system. This presentation will highlights to analytical developments of a CPE methodology for the detection of traces of ^{210}Pb in environmental matrices.

I049

DEVELOPMENT OF LC-MS/MS BASED PROTOCOLS FOR THE NON-TARGETED ANALYSIS OF FOOD CONTAMINANTS. **S. Bayen**, L. Tian, A. von Eyken, Department of Food Science and Agricultural Chemistry, McGill University, 21111 Lakeshore, Ste Anne de Bellevue, QC H9X 3V9, Canada (stephane.bayen@mcgill.ca)

Food contaminant analysis has benefitted from rapid developments in the fields of chromatography and mass spectrometry, in terms of quantification and sample throughput. In the last decade, the innovation brought by the usage of accurate mass measurements led to a more robust identification of unknown molecules in complex matrices. Accurate mass analysis is used to identify 'known unknowns' through search in chemical databases, but is also used as a tool for mining for non-previously reported chemical structures. The identification of small molecules in tissues using non-targeted analysis has been applied mainly in the plant/animal sciences and the biomedical area, and non-targeted studies on food toxicants remain scarce. The development of unbiased, standardized protocols is therefore necessary to study contaminants in the complex food matrices. In this talk, examples will be provided to demonstrate how accurate-mass quadrupole time-of-flight LC/MS can be used to analyze specific target contaminants, while simultaneously recording high resolution MS and MS/MS data for other small molecules, providing additional key food safety and quality information.

I050

INORGANIC ARSENIC SPECIATION IN RICE AND RICE-BASED PRODUCTS USING HYDRIDE GENERATION ATOMIC ABSORPTION SPECTROMETRY (HG AAS). **Dirce Pozebon**, Greice Magalhães dos Santos, Camila Cerveira and Diogo P. de Moraes. Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves 9500, 91501-970, Porto Alegre, RS, Brazil. (dircepoz@iq.ufrgs.br)

Rice is an important food for billions of people worldwide, whereas rice-based foods are usually consumed by individuals intolerant to gluten (celiac people), lactose, and other allergies. The celiac disease may affect up to 1% of the western population, mainly children and individuals over 65 years old. Arsenic is 10 times higher in rice grain than in other cereals. This toxic element is mainly present as As(III), As(V), and dimethylarsenate (DMA) in rice, comprising 90% of the total As content; the remainder As is in the form of monomethylarsonate (MMA). High performance liquid chromatography (HPLC) hyphenated with inductively coupled plasma mass spectrometry (ICP-MS) has usually been employed for As speciation in rice and rice products. However, the DMA and MMA species are considered of low toxicity and therefore only the inorganic arsenic (iAs) concentration monitoring in rice and rice products is necessary. In this sense, for the sake of simplicity, non chromatographic methods of iAs speciation are nowadays recommended. The hydride generation atomic absorption spectrometry (HG AAS) technique is proposed in the present study. Selective generation of As(III) is achieved with 0.1% (m/v) $NaBH_4$ and 10 mol L^{-1} HCl. Total inorganic arsenic (As(III) + As(V)) is determined by As(V) pre-reduction (with KI + ascorbic acid in 1.2 mol L^{-1} HCl) followed by determination at the same conditions used for As(III). The As species are extracted with 0.28 mol L^{-1} at 90 ^{o}C (heating on hot plate or microwave oven) for 90 minutes. The limits of quantification meet the current legislation. The feasibility of the methodology is demonstrated for iAs speciation in rice and rice products (solid and liquids). Acknowledgements to CNPq and CAPES.

I051

MULTILEMENT DETERMINATION IN VEGETABLES USING LA-ICP-MS. **Valderi Luiz Dressler**, Matheus A. G. Nunes. Department of Chemistry, Federal University of Santa Maria, Av. Roraima 1000, 97105-900, Santa Maria, RS, Brazil. (vdressler@gmail.com)

Element contents in vegetables may come not only from the soil itself, but also from sources like fertilizers, solid and liquid waste, and industrial emissions. Excessive accumulation of elements, mainly in edible parts, can lead consequences for food quality and safety. Therefore, it is essential to monitor food quality, given that vegetables is one of the main sources of nutrients for humans and other animals. Besides, vegetables can also be a source of toxic elements. Different techniques can be used for elemental determination in plant but, in general, the sample must be in solution. Sample decomposition is a time consuming step and prone to analyte loses and contamination. Laser ablation-inductively coupled plasma mass spectrometry (LA-ICP-MS) allows the direct analysis of solid samples, with minimum sample handling. Multielemental determination capability, low limit of detection (LOD) and high spatial resolution are other characteristics of LA-ICP-MS. In the present work we proposed the use of the LA-ICP-MS technique for total (bulk) element determination and spatial distribution (bioimaging) of elements in vegetables. Tea leaves and Brazil nuts samples were analyzed. Calibration strategies using certified reference materials and paper discs spiked with the analytes as matrix matched standards, with and without use of ^{13}C as internal standard, were evaluated. The quality assurance of results was established by applying the proposed method to the analysis of botanical CRMs and samples. After instrumental parameters optimization, elements like As, Cd, Co, Cr, Cu, Mn, Ni, Pb, Se, Sr, V and Zn were determined. The method precision (RSD) was better than 20% and LOD values ranged from 0.05 to 0.81 μg g^{-1}. Overall, by using LA-ICP-MS method it was possible to obtain bioimages of element distribution and determine the bulk element concentration in the samples. Acknowledgements to CNPq and CAPES.

I052

HIGH SENSITIVITY TIN SPECIATION USING A NEW GC INTERFACE WITH SECTOR FIELD HIGH RESOLUTION ICP-MS. **Peter Stow**, Isomass Scientific Inc., 140, 5700 - 1 Street S. W., Calgary, Alberta T2H 3A9 (pstow@isomass.com)

Purpose: To evaluate the performance of a new interface between Sector Field Inductively Coupled Plasma Mass Spectrometry (SF ICP-MS) and Gas Chromatography (GC) for tin speciation.

Methods: The Thermo Scientific ELEMENT XR HR-ICPMS and the Thermo Scientific TRACE 1310 GC were seamlessly connected by the Thermo Scientific GCI 200 Interface.

Results: The GCI 200 Interface can be quickly and easily installed. By means of the flexible and light design of the heated transfer line, the ICP-MS torch position can be easily tuned without being affected by the weight of the interface. We show how a stable temperature profile and the absence of cold spots avoids condensation and peak broadening. 14 Tin species are well separated. Because of the high acceleration voltage of Sector Field ICP-MS this technique is extremely sensitive. In combination with its low backgrounds, this leads to the low detection limits required for sensitive tin speciation analysis.

I053

NEXION 2000 ICP-MS – ANY MATRIX, ANY INTERFERENCE, ANY PARTICLE SIZE.

Andrew Rams, PerkinElmer Inc., Woodbridge, ON (Andrew.Rams@perkinelmer.com)

Laboratories around the world continue to push forward with needs for greater sensitivity, robustness, versatility, and throughput out of their instrumentation. PerkinElmer continues to strive to meet these needs through new advancements that enable researchers and laboratory professionals to meet their goals. The introduction of the new NexION 2000 ICP-MS which features an array of innovative technologies that combine to deliver a versatile and high-performance instrument provides the platform needed to expand analytical expectations. New aspects of the NexION 2000 will be discussed with supporting data provided. Various applications making use of these features will be presented as well.

I054

CHROMIUM SPECIATION ANALYSIS IN DAIRY AND CEREAL PRODUCTS BY HPLC-ICPMS.

T. Guérin[1], F. Hernandez[1], N. Bemrah[1], F; Cormant[1], F. Séby[2], L. Noël[1], P. Jitaru[1], [1]Université Paris-est, Anses, Laboratoire de Sécurité des Aliments, Maisons-Alfort, France ; [2]UT2A, Pau, France. (thierry.guerin@anses.fr)

Chromium (Cr) is a metal widely distributed throughout the Earth's crust and the most commonly forms found are Cr(III) and Cr(VI). Cr(III) has long been considered as an essential nutrient for human health whereas Cr(VI) is carcinogenic to humans. The most important contribution to the overall exposure of total chromium in the general population is through food. To improve risk assessment on the presence of chromium, there is a need to accurately determine the content of Cr(III) and Cr(VI) in food.

The aim of this work is to develop specific and very sensitive methods to determine Cr(VI) and Cr(III) in dairy and cereal products, which are the main contributors to total chromium dietary exposure. Experimental designs were used to better optimize the separation and extraction of Cr species while estimating the influence of the most important parameters and their interactions.

In the absence of certified reference material for Cr(VI) or Cr(III) determination in food, the method was validated using spiked samples. Analytical performances were assessed in terms of linearity, specificity, sensitivity, accuracy, repeatability and intermediate precision.
The two methods were then applied to the determination of Cr(VI) or Cr(III) in dairy and cereal products of different brands and origins. Additionally, these results were used to evaluate the exposure of the French population to Cr(VI) or Cr(III).

I055

ADVANCEMENTS IN SINGLE PARTICLE ICP-MS – SIGNIFICANT INSTRUMENT SETTINGS AND THEIR IMPLICATIONS ON DATA QUALITY. Chady Stephan, Samad Bazargan, Hamid Badiei, Aaron Hineman**, Andrew Rams**. PerkinElmer Inc., Woodbridge, ON (Andrew.Rams@perkinelmer.com)

The characterization, sizing, and quantification of metal-based nanoparticles (NP) in a variety of matrices using single particle-inductively coupled plasma-mass spectrometry (SP-ICP-MS) is becoming increasingly popular due to the sensitive nature of the technique. Novel reaction cell optimizations, instrument settings, and data processing techniques are used to explore the benefits of continuous data acquisition rates as fast as 105 Hz (or 10 µs dwell times).

This talk presents data on the various significant instrument settings and their implications on nanoparticle characterization. Information on instrument setup, sample prep and transport efficiency on data quality is given. The effect of varying the dwell time and its influence on particle integration, particle counting, particle sizing, and background signal is discussed. Data describing the use of Dynamic Reaction Cell (DRC) design in handling short-lived transient events while managing spectral interferences is also introduced.

I056

SP-ICP-MS TECHNIQUE FOR THE ANALYSIS AND THE STABILITY STUDY OF METAL NANOPARTICLES IN BIOLOGICAL FLUIDS. **Ciprian M Cirtiu**, Institut National de Santé Publique du Québec, Centre de Toxicologie du Québec. (ciprian-mihai.cirtiu@inspq.qc.ca)

Metal nanoparticles (MNP) are widely used in various fields, including biomedical, especially for diagnostics, surgery and medicine. Regardless their application, it is crucial to understand the stability, fate and biodistribution in biological media once the human body is exposed. Many techniques (microscopy, spectroscopy, chromatography, etc) are available for the detection and characterization of NP in their raw state but they are not all suitable for biological media. ICP-MS, a high specific and sensitive technique has been widely used in last decades for the analysis of metals, and more recently for the analysis of NP upon digestion of samples containing NP. However, important information is lost when proceeding through digestion of NP, such as size, size distribution and shape. Single Particle-ICP-MS (SP-ICP-MS) has emerged as a technique for NP characterization and quantification. Here, the capability of the SP-ICP-MS technique to analyze Au and TiO2 NP in blood and urine, two complex biological matrices is presented. A NexION 300S ICP-MS from PerkinElmer with a Nano Application module integrated in the Syngistix software is used for data collection and processing. Furthermore, SP-ICP-MS was used to investigate the stability of Au NP by tracking their change in size and measuring the free ion concentrations that could potentially be released through dissolution.

I057

MS COMPATIBLE SAMPLE PREPARATION TECHNIQUES FOR DEEP COVERAGE PROTEOME ANALYSIS.

Fei Fang, Qun Zhao, Huiming Yuan, **Lihua Zhang**, Yukui Zhang. Dalian Institute of Chemical Physics, Chinese Academy of Sciences. (lihuazhang@dicp.ac.cn) **WITHDRAWN**

To achieve the deep-coverage proteome analysis, we proposed an ionic liquid based FASP protocol (i-FASP), by which with 1-dodecyl-3-methylimidazolium chloride (C12Im-Cl), both soluable and insoluable proteins could be efficiently extracted from cells, and denatured simultaneously at 95°C with DTT added, followed by on-filter alkylation, digestion and desalting. Different from the typical FASP protocol, most C12Im-Cl could be easily removed by ammonium bicarbonate. Contributed by the stronger extraction and solubilization efficiency of C12Im-Cl than SDS, and the higher biocompatiblity with tryptic digestion, the identified protein and membrane protein number in HeLa cells was obviously improved within reduced time. Furthermore, such a protocol was successfully applied in the label-free based quantitation of human liver tissues, and showed superiority to traditional FASP method.

Besides, to improve the throughput for proteome sample preparation, we developed a hollow fiber membrane-aided fully automated sample treatment (FAST) method, by which samples could be denatured, reduced, desalted and digested in 20 min via “one-stop” service. Through the on-line combination of FAST with nano-LC-ESI-MS/MS, we further established a fully integrated platform for high-throughput proteome quantification, and demonstrated its capacity to analyze sub-nanogram starting materials.

I058

INVESTIGATION OF THE UNIMOLECULAR REACTIONS OF IONIZED POLYCYCLIC AROMATIC HYDROCARBONS.

Brandi West, Alicia Sit, Sabria Mohamad, Eduardo Solano, Jake Burner, Yardley Paige Cuthbert, Iden Djavani-Tabrizi and **Paul M. Mayer**. Department of Chemistry and Biomolecular Sciences, University of Ottawa; Sarah Rodriguez, Christine Joblin. Université de Toulouse III, Toulouse, France; Andras Bodi, Patrick Hemberger: Paul Sherrer Institut, Villigen, Switzerland (pmmayer@uottawa.ca)

Carbon-based macromolecules are an important constituent of interstellar material, comprising 10-20% of the carbon in the galaxy. They play an important role in the physical and chemical evolution of the photodissociation regions of the galaxy due to ultraviolet emissions from stars. These macromolecules can take the form of polyaromatic hydrocarbons (PAHs) or other, aromatic-based molecular systems but their complete characterization remains allusive. Over the past 25 years of the so-called PAH hypothesis these molecules have been argued to be involved in shielding organic reactions in the interstellar medium (ISM) and playing an active role catalyzing these reactions, especially H_2 formation. We have been exploring the dissociation dynamics of ionized PAHs by a combination of tandem mass spectrometry (collision induced dissociation) and imaging photoelectron photoion coincidence spectroscopy (iPEPICO). The presentation will review the advantages of the two approaches to ion reaction dynamics and highlight the challenges faced when studying this class of molecules.

I059

NEW TECHNIQUES FOR PREPARING PLASTICS AND POLYMERS BY MICROWAVE SAMPLE PREPARATION. Tina Restivo, Austin Thornton, Bob Lockerman, and Michael Howe, CEM Corporation. Presented by: **Bill MacLuckie**

Traditional acid digestion of many polymers have typically involved the use of a sulfuric acid char step in order to dehydrate the polymer and break the cross linkages. This is followed by a second step of oxidation with nitric acid. This is a tedious process and the sulfuric acid step raises the viscosity of the liquid, which is not friendly to ICP-MS analysis. Other techniques such as dry ashing samples prior to taking up in dilute acids and very costly high pressure apparatus have also been attempted but each has their own difficulties.

We will prepare a variety of polymeric samples by traditional cost effective microwave digestion without the use of sulfuric acid or dry ashing steps. Analysis will be reported using ICP-OES and ICP-MS analysis. Spike recovery data as well as data derived from standard reference materials will be presented and discussed.

I060

HIGHLY-MINIATURIZED AND LOW POWER POTENTIOSTAT FOR ON-CHIP ELECTROCHEMICAL SENSING. [1]Jessy Mathault, [1,2] Samuel Morneau-Gamache, [1]Elnaz Ghodsevali, [1]Hamza Landari, [3]Mounir Boukadoum, [2]Élodie Boisselier, [1]**Amine Miled**, [1]LABioTRON Bioeng. Research Laboratory, ECE Dept. Université Laval, Québec, QC, Research Centre for Advanced Materials (CERMA), Université Laval, QC, [2]Ophthalmology department, Faculty of Medicine, Université Laval, Québec, QC, [3]CoFaMic, Université du Québec à Montréal, QC, Canada

Potentiostat miniaturization was taking a lot of interests for years/decades ago. Different approaches and architectures have been proposed to achieve different potentiostat functionalities. In some cases, the sensitivity was very critical, in others the dimensions of the system or power consumption for embedded systems are more critical. In this presentation we present our research lab work related to a potentiostat architecture to detect a wide range of reduction-oxidation currents, while exhibiting low-power consumption and low-noise operation. Different architectures have been designed. In one architecture we used a discrete electronic design configuration based on counter/reference-based potentiostat using gold plated electrode array with advanced signal processing approach to extract peak position and amplitude. In another approach we used a CMOS-based design to achieve a 5 μA sensitivity and 0.99 linearity. The total power consumption was under 55 μW. The complete system was assembled on a 20 mm x 20 mm platform that includes the potentiostat chip, the electrode terminals and an instrumentation amplifier for redox current buffering, once converted to a voltage by a series resistor. In addition, embedded electrodes and a microfluidic chamber (8 mm x 8 mm) was designed on the system. The system was successfully tested with ferricyanide, a stable electroactive compound, and validated with dopamine, a popular neurotransmitter. The system was tested with dopamine (1 μM and 0.1 mM). The detected current varied between 60 μA and 100 μA. On the other hand, when the concentration was between 0.1 mM and 10 mM, the detected current was in the range of 100 μA to 840 μA. Thus, we observed two linear behaviors: one with 0.074 μA/mM at high concentration and 404.04 μA/mM at low concentration with carbon screen printed electrodes.

I061 P

SPECIATION ANALYSIS OF ARSENIC IN MILK: METHOD DEVELOPMENT AND APPLICATION TO THE FRENCH SURVEILLANCE PLAN CONCERNING MILK CONTAMINATION BY ARSENIC SPECIES. A. Leufroy, R. Chekri, J. Zinck, N. Marchond, **T. Guérin** and P. Jitaru (petru.jitaru@anses.fr)

The presence of arsenic species in foodstuff is a matter of concern at national and European level. Apart from the trace metals (Pb, Cd and Hg) currently regulated by EU, arsenic species and particularly inorganic arsenic (As(III) + As(V)) have become of interest in the last years due to their high toxicity. At present, among all arsenic species present in food, maximum level is imposed by EU only for inorganic arsenic in rice and some rice derivatives. Nevertheless, the milk is currently one of the foodstuffs of concern in terms of contamination with arsenic species due to its large consumption by the general population, particularly by children. This is confirmed by the implementation in 2016 of a national surveillance plan in France for inorganic arsenic in milk. Therefore, obtaining occurrence data in terms of arsenic speciation in milk at national and European level is necessary in order to assess more accurately the toxicological impact of this element via milk consumption. This is a challenging task from analytical point of view given that arsenic species are present in milk at extremely low levels (generally < 1 µg/kg) and also because of the complexity of the milk matrix, which may seriously hamper the method analytical performances.

This study presents primarily the development and the validation of a method for arsenic speciation analysis in various types of milk by anion exchange chromatography coupled to an iCAP Q (Thermo) inductively coupled plasma mass spectrometer (AE-HPLC-ICP-MS). The extraction of arsenic species from the milk matrix was carried out using a mixture of HNO_3 1% (v/v) + H_2O_2 1% (m/m) in a closed microwave system. H_2O_2 is used here to oxidize As(III) to As(V), which allows the measurement of the entire fraction of inorganic arsenic as As(V). The various arsenic species were separated by using an IonPac AS7 ion exchange column (250 × 4 mm; 10 µm particles). Method validation was carried out by means of the accuracy profile using spiked milk matrices. The method was further applied to the analysis of the samples of the national French surveillance plan (2016) concerning arsenic speciation in milk.

I062

DEVELOPMENT OF ANALYTICAL TECHNIQUES TO STUDY THE HUMAN MICROBIOME, **Daniel Figeys**, University of Ottawa (dfigeys@uottawa.ca)

Host–microbiome interactions have been linked to a growing list of diseases such as inflammatory bowel diseases (IBD), obesity, diabetes, etc.. Inflammatory bowel disease (IBD) is a chronic inflammatory disorder, consisting of two predominant subtypes, ulcerative colitis (UC) and Crohn's disease (CD). The exact mechanism by which this disease arises is unknown, however it is believed to emanate through a combination of an exaggerated immune response in a genetically susceptible host, triggered by environmental factors. We are interested in studying the molecular changes that occurs in host and microbiota during gut dysbiosis using different omics approaches with a particular. Here, we will present some of our new analytical techniques for the study of the microbiome by metaproteomics.

I063

SPINNING FLUIDS FOR POINT-OF-CARE DIAGNOSTICS. **Maurice Boissinot**, CHU de Québec-Université Laval. Maurice.Boissinot@crchul.ulaval.ca

Our team developed the first real-time PCR molecular diagnostic tests to be cleared by the US FDA. These tests are now fabricated in Quebec City within a manufacturing facility employing over 300 skilled workers and distributed worldwide by BD diagnostics for the diagnosis of infectious diseases. However, this first generation of commercial real-time PCR tests needs to be performed in a central laboratory.

In the hope of performing molecular testing closer to patients, we decided to automated and simplify liquid handling using microfluidics. This presentation will explain the basics of centripetal microfluidic approaches we developed in order to integrate all steps required for sample processing, nucleic acid amplification, multiplex optical detection, and result output usable by clinicians. The audience will have an overview of the revolutionary fluidic technology currently commercialized by Quebec City start-up GenePOC inc. for the rapid detection and identification of microbes at point-of-care.

I064

ADVANCES IN MICROWAVE SAMPLE PREPARATION: TRADITIONAL AND MODERN DAY DESIGNS FOR TRACE METALS ANALYSIS. **Parag Bhargava** and Gilles Groulx, ATS Scientific Inc. 4030 Mainway, Burlington, ON Canada L7M 4B9

Closed-vessel microwave digestion has long been recognized as one of the most effective sample prep technique for the digestion of samples for metals analysis by ICP-OES or ICP-MS. Historically these systems have been mostly of traditional microwave designs, usually with rotors with individual samples contained in many separate vessels. This approach is often successful; however in some cases, incomplete digestions at lower temperatures (180°C-220°C) can result in substantial amount of total organic carbon in the digested solution. This organic carbon build up inside ICP-OES or ICP-MS causes issues which requires extensive cleaning, replacement of tubes etc.

Milestone’s patented Single Reaction Chamber (SRC) microwave technology, incorporated in the UltraWAVE, integrates all of the benefits of closed-vessel microwave digestion while making sample preparation fast, easy, effective, and of the highest quality. In this system, all samples are digested simultaneously in one large Teflon lined stainless steel chamber in individual vials (disposable glass, quartz or TFM) with loose fitting caps. The presence of stainless steel chamber allows the UltraWAVE to achieve very high temperature and pressure (300°C and 199bar) during the digestions. Thus, complete digestion of a wide variety of sample matrices can be achieved with the largest sample size (up to 15 grams dry weight) and minimum acid usage (3-5 mL per sample). Many types of samples with different acid chemistries and sample weights can be digested in a single run.

The presentation will give an overview of the traditional closed vessel system and SRC technology along with successful application examples for both types of systems.

I065

ADVANCES IN ICP-OES HARDWARE AND OPTICAL DESIGN. **Dion Tsourides**. Spectro, Ametek. (Dion.tsourides@ametek.com)

A revolutionary improvement in Optical ICP spectroscopy will be described. The use of a ORCA based high-resolution ICP-OES spectrometer coupled to the first and only excitation source featuring a fast and convenient selection of axial plasma or radial plasma observation in a single instrument — without any optical compromise.

Designed for use in the most demanding and diverse elemental applications, this novel design easily surpasses the performance limitations of conventional ICP-OES instruments — dramatically improving sensitivity, stability, and precision, while lowering operating costs with the introduction of innovative components, unique capabilities, and optimum flexibility (VUV down to 130nm).

I066 P

DEVELOPMENT AND APPLICATION OF A NOVEL ANALYTICAL APPROACH BASED ON ASYMMETRIC FLOW FIELD FLOW FRACTIONATION COUPLED TO ICP-MS FOR TIO_2 NANOPARTICLES DETERMINATION IN FOOD. Lucas Givelet[a], D. Boutry[a], S. Motellier[a], P. Jitaru[b], **T. Guérin**[b] and J-F. Damlencourt[a], [a] CEA Grenoble, Laboratoire de Recherche en Nanosécurité, Grenoble, France ; [b] Université de Paris-Est, Anses, Laboratoire de Sécurité des Aliments, Maisons-Alfort, France (lucas.givelet@cea.fr)

Titanium dioxide (TiO_2) is a synthetic dye for food known as E171 being used to enhance the white colour or brightness. Recent studies showed that this food additive is partially present at a nanoscale size (<100 nm) but it is difficult to have representative size distribution of a whole batch using microscopy technique. In this study, Asymmetric Flow-Field-Flow-Fractionation (AF4) coupled to Inductively Coupled Plasma – Mass Spectrometry (ICP-MS) was investigated to determine the size distribution of E171 in liquid state. AF4 allows the particles separation based on their size and their zeta potential (electrostatic interaction). The aim of this work is the development of a method for the TiO_2 characterization in food with AF4-ICP-MS. First investigations were focused on electrostatic studies. For that, several parameters were tested like the pH, the ionic strength and the addition of surfactant in the eluent. This work allows to find conditions for which NPs are not agglomerated/aggregated and NPs are not adsorbed to the AF4 membrane. A Zetasizer Nano ZSP instrument was used to measure the zeta potential and the hydrodynamic diameter of TiO_2 NPs in suspension in different media. The zeta potential of AF4 common membrane (Regenerated Cellulose, 10 kDa) was measured by using an electrokinetic analyser SurPASS.

Our results confirm that the zeta potential of particles and membranes are significantly impacted by the pH, the ionic strength and the nature of the surfactant. Indeed, eluent combinations seems promote electrostatic repulsion (same zeta potential electrostatic sign) like Sodium Dodecyl Sulfate (SDS) with $NaNO_3$ at 1 mM or Triton X-100 (Tx-100) at pH > 5 and $NaNO_3$ at 1mM. Moreover, the hydrodynamic diameter measurements of particles revealed that the FL-70 is the surfactant for which particles are the least aggregated. This preliminary study allowed us to select a liquid carrier for the future AF4-ICP-MS experiments. Real tests with the AF4 tool are under progress to confirm if there is a raise of recovery and an optimal separation of TiO_2 nanoparticles with the selected parameters.

I067

SELECTING THE OPTIMUM SAMPLE INTRODUCTION SYSTEM FOR ICP-OES ANALYSIS OF DIFFICULT SAMPLES. **Sergei Leikin**. Texas Scientific Products. (sergei@txscientific.com)

Modern ICP-OES analytical instrumentation offers good performance parameters: sensitivity, robustness and reliability. At the same time analysis of many matrices by ICP-OES is often challenged by the High Salt and particulate content in the real world samples. Quite often these analyses also require reaching low detection limits. That is why choosing the optimum sample introduction system to utilize the high analytical potential of today's ICP spectrometers still remains very critical task.

The most common concentric type nebulizers suffer from frequent clogging in presence of even tiny particles and require daily maintenance when running high salt matrices. These problems were effectively addressed by applying sample introduction system with nonconcentric Nebulizer types: OptiSolids XL ™, OptiMist ® and E2 (Enhanced Efficiency) Modified Lichte. Performance data for a number of challenging applications including High Salt industrial waters, Agricultural Soil and Fertilizer Extracts, environmental with low detection limits requirements as well as specialty organic chemicals, used Oils and Greases will be presented.

I068

GRAPHENE QUANTUM DOTS: DEPOSITION ON POLYDOPAMINE-MODIFIED TiO_2 NANOPARTICLES. **Edward P.C. Lai** and Kaiyu Wang, Department of Chemistry, Carleton University, Ottawa, ON K1S 5B6

Graphene quantum dots (GQDs) possess many excellent properties of graphene and quantum dots. They have the good strength and conductivity of graphene. Their quantum confinement effect is particularly evident to exhibit good photoluminescence properties. GQDs can be synthesized by pyrolysis of citric acid. The synthesis method were optimized with regards to the pyrolysis time, pyrolysis temperature, and solution pH. The GQDs was characterized using Fourier transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM) and fluorescence spectroscopy. The synthetic GQDs were used to detect metal oxide nanoparticles in water. Titanium dioxide nanoparticles were first modified by adding dopamine. FTIR analysis confirmed a coating of polydopamine (PDA) on each nanoparticle surface. GQDs could then be immobilized on the PDA-modified TiO_2 nanoparticles by 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide in MES buffer. The resultant TiO_2-PDA-GQDs nanoparticles emitted weaker photo-luminescence together with a red shift of the maximum emission wavelength. Standard calibration produced a curve that was best fitted with a 2nd-order polynomial equation. TEM with energy dispersive X-ray analysis revealed the small GQDs (~3.3 nm) deposited on the surface of TiO_2 nanoparticles (>20 nm). Next, graphene oxide (GO) was demonstrated to drive the synthesis of GQDs. Dialysis of the GO-driven GQDs through a 8K-10K MWCO cellulose membrane yielded unexpected changes to the emission intensity as well as the Rayleigh scattering intensity.

I069

*Easy***PREP** SAMPLE HANDLER, AUTOMATION OF TEDIOUS LIQUID TRANSFER TASKS.

John Dykeman, SCP SCIENCE (jdykeman@scpscience.com).

The *Easy***PREP** Sample Handler from **SCP SCIENCE**, is a robotic liquid delivery system that permits laboratory tasks to be automated. Many repetitive procedures such as acid dispensing, normalization, sample transfer are time consuming and tedious for laboratory staff. As well, automation provides highly reproducible results and precision for liquid handling.

*Easy***PREP** is designed to work with laboratory protocols so has much flexibility in terms of vessel type and size, from standard autosampler tubes, and digestion tubes to microwave digestions vessels.

The presentation will provide details of the many functions and capabilities of the *Easy***PREP** Sample Handler from **SCP SCIENCE.**

I070

TOWARDS UNDERSTANDING OF METHYLMERCURY TOXICITY

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Toxic effects of Hg species and their modes of action are under considerable scrutiny, predominantly due to the capability of MeHg to cross the blood-brain barrier and selectively damage the central nervous system. There is ample evidence of similarities in the metabolic pathways of Hg and Se through their significant correlations in internal organs of animals, which gave grounds for more in depth investigations and led to identification of HgSe as the final product of Hg detoxification.

A comprehensive study of Hg's impact on Se species was conducted on the livers and brains collected from the pod of 21 stranded pilot whales. CV-AFS and HR-ICP-MS were used for analysis of total Hg and Se, respectively. Mercury speciation was performed using GC-ICP-MS whilst HPLC-ICP-MS/ESI-MS was used for Se speciation. Spatial co-localization was visualized by LA-ICP-MS, HgSe was identified by synchrotron XAS while sp-ICP-MS provided information on the size distribution of formed HgSe aggregates.

The results show that as a consequence of MeHg detoxification, Se-methionine, the selenium pool in the system is depleted in the efforts to maintain essential levels of Se-cysteine. The detoxification mechanism is fully developed from the early age of the animals, with particulate Hg found already in juvenile tissues. This study provides evidence of so far unreported depletion of the bioavailable Se pool, a plausible driving mechanism of demonstrated neurotoxic effects of MeHg in the organism affected by its high dietary intake.

I071

TRACE METAL SPECIATION IN A MULTIVITAMIN CANDIDATE REFERENCE MATERIAL.

Kelly LeBlanc, Lucia D'Ulivo, Kenny Nadeau, Indumathi Pihillagawa Gedara, Lu Yang, Zoltan Mester. National Research Council of Canada. (Kelly.LeBlanc@nrc-cnrc.gc.ca)

For the certification of new multivitamin reference materials at the National Research Council Canada (NRC), the speciation of trace metals in the multivitamin tablets was examined. Extraction and analysis methods for cyanocobalamin (vitamin B_{12}) and selenomethionine (from selenized yeast) were optimized on a "per tablet" basis, using standard addition for quantification to account for matrix effects. High-performance liquid chromatography (HPLC) was found to be sensitive to sample matrix, thus sample cleanup and/or significant dilution was required before analysis. HPLC was followed by element-specific detection using inductively-coupled plasma triple quadrupole mass spectrometry (ICP-QQQ-MS) to enhance sensitivity by eliminating matrix and plasma interferences, particularly on ^{80}Se. NIST's SRM 3280 (multivitamin/multielement tablets) and NRC's CRM SELM-1 (selenium enriched yeast) were used as reference during these analyses.

I072

OVERCOMING CHALLENGES OF Hg SPECIES QUANTIFICATION IN PETROLEUM HYDROCARBONS.

Z. Gajdosechova[a,b], M. S. Boskamp[a], F. Lopez-Linares[c], J. Feldmann[a], E. M. Krupp[a]. [a]TESLA, University of Aberdeen, UK , [b]NRC, Ottawa, Canada, [c]Chevron Energy Technology Company, USA. (Zuzana.Gajdosechova@nrc.ca)

The corrosive properties of Hg require its constant monitoring within the petrochemical industry, however owing to the matrix complexity and the dynamic behavior of the analyte, Hg speciation and species quantification remain challenging.

Four crude oil samples were analysed using GC-ICP-MS and thee quantification methods were evaluated; external calibration, standard addition and species-specific isotope dilution mass spectrometry (SS-IDMS).

The external calibration method showed strong solvent dependence, while quantification using standard addition method was hindered by formation of an emulsion during the derivatisation step. SS-IDMS allowed for quantification InHg in all four samples however, it also revealed positive bias in quantification of InHg caused by HgS particles. It was postulated that HgS nanoparticles present in the crude oil might undergo alkylation during the derivatisation step resulting in the overestimation of InHg concentration. This study highlights the advantages of SS-IDMS, which proves to be a robust approach for the analysis of Hg in crude oils.

I073

ONLINE SEPARATION AND DETERMINATION OF ^{226}RA AND TRACE METALS FROM MINING WASTEWATER AND FRACKING WATER. **Wei Wang** and Douglas Evans, School of Environment, Trent University, Peterborough, ON Canada (weiwang@trentu)

Comparing to the traditional methods for low level ^{226}Ra determinations which require long sample holding time or long detection time, an online solid-phase extraction method combined with ICP-MS to separate and purify low level ^{226}Ra from samples with complex matrixes, such as fracking water (up to 20% of total dissolved solid TDS) and mining wastewater with high level of transition metals, is developed in this study. In addition, using this system certain trace elements from the sample can be determined during the separation of Ra from the sample matrix. AG 50w x8 cation exchange resin, Sr Spec resin and Nobias Chelate resin were used in a flow injection system which was programed to control the purification and pre-concentration of Ra and inline dilution of other elements. Different sample loops and various volumes of resins were used, based on the level of TDS in the samples. Method optimization achieved high Ra recovery with samples contains different matrices, and acceptable method detection limits of ^{226}Ra were achieved from different sample volumes. In addition, this method also achieved up to1000 times online dilution for other trace metals. There is large potential to apply this system to online determination of other radionuclides.

I074

THE ACCURATE DETERMINATION OF RADIONUCLIDES WITHOUT PRIOR CHEMICAL SEPARATION OF INTERFERENCES USING AN AGILENT ICP-MS/MS. **Pamela Wee**, Agilent Technologies Canada Inc.

This paper summarizes the accomplishments-to-date of the Agilent ICP-MS/MS in the direct determination of the radionuclides, $^{90}\mathrm{Sr}^+$, $^{129}\mathrm{I}^+$, $^{137}\mathrm{Cs}^+$, $^{238}\mathrm{Pu}^+$, $^{239}\mathrm{Pu}^+$, and $^{236}\mathrm{U}^+/^{238}\mathrm{U}^+$ ratios by tandem mass spectrometry with chemical resolution using gas-phase ion chemistry.

The ICP-MS/MS configuration consists of a collision reaction cell (CRC) between two quadrupole mass filters, Q1 and Q2. The abundance sensitivity afforded by tandem MS is better than 10^{-10}, eliminating wing overlaps of $^{127}\mathrm{IH}^+$ on $^{129}\mathrm{I}^+$ and $^{238}\mathrm{U}^+$ on $^{237}\mathrm{Np}^+$ and $^{239}\mathrm{Pu}^+$.

The CRC is filled with a gas that reacts with the analyte and its interferences at different rates. When the reaction kinetics favour the analyte, the analyte is converted to a molecular ion which is then measured in “mass-shift” mode. The interference from $^{235}\mathrm{UH}^+$ on $^{236}\mathrm{U}^+$ was circumvented by oxidizing U with O_2. The $^{236}\mathrm{U}^+/^{238}\mathrm{U}^+$ ratio was determined as a $^{236}\mathrm{U}^{16}\mathrm{O}^+/^{238}\mathrm{U}^{16}\mathrm{O}^+$ ratio.

When the reaction kinetics favour the interferent, the interferent is converted to another form and the analyte is measured at its elemental mass (the “on-mass” mode). Differences in the oxidizing efficiencies of N_2O, O_2, CO_2 were used to discriminate interferences Ba^+ from Cs^+, $^{90}\mathrm{Zr}^+$ from $^{90}\mathrm{Sr}^+$, and $^{239}\mathrm{U}^+$ from $^{239}\mathrm{Pu}^+$, respectively. The $^{238}\mathrm{U}^+$ interference on $^{238}\mathrm{Pu}^+$ was removed by reacting U^+ to amine cluster ions by a blend of 10% NH_3/90% He. The $^{129}\mathrm{Xe}^+$ interference on $^{129}\mathrm{I}^+$ was removed by charge transfer reaction with O_2.

Q1 is unique to the Agilent ICP-MS/MS: it is a unit mass resolution mass spectrometer, operated under vacuum, and precedes the reaction cell. This configuration is vital for the successful and simple implementation of chemical resolution in ICP-MS. Results from the efforts of many scientists will be presented.

I075 P

NOVEL DESIGN OF INFRARED-HEATED INTEGRATED SAMPLE INTRODUCTION SYSTEM FOR IMPROVING ANALYTICAL PERFORMANCE OF INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY. **Ahmed Al Hejami** and Diane Beauchemin, Chemistry Department, Queen's University, Kingston, Ontario, Canada
(*diane.beauchemin@chem.queensu.ca*)

A pneumatic sample introduction system (consisting of a nebulizer and spray chamber) is still considered the Achilles' heel of inductively coupled plasma (ICP) spectrometry, as only around 5% of the sample can be introduced into plasma. A simple approach to enhance sample transport efficiency is pre-evaporation of the sample aerosol, which leads to improved sensitivity, detection limit and plasma robustness. In this presentation, a new design of infrared (IR)-heated sample introduction system will be described: a baffled cyclonic spray chamber was modified so as to allow an IR heating lamp to be inserted in the centre of the spray chamber for more effective heating. The new system is simple and compact so as to fit easily in the torch box. This presentation will compare this new IR-heated integrated sample introduction system to the regular one in terms of sensitivity, detection limit, plasma robustness and precision.

I076

TRACE ELEMENT AND ISOTOPE ANALYSES OF MICRO-SOLDERING LEAD-BASED METAL ASSOCIATED TO IMPROVISED EXPLOSIVE DEVICE (IED) BY ICP-MS, AND FORENSIC ASSOCIATION WITH ORIGIN. **Claude Dalpé** and Nigel G.R. Hearns. Royal Canadian Mounted Police, National Forensic Laboratory Services, Ottawa, Canada. (claude.dalpe@rcmp-grc.gc.ca).

The measurement of lead (Pb) isotopes by ICP-MS has been recently applied to a homicide case where a tentative association was found between a fabrication tool used by the suspect and debris at the crime scene originating from an IED. The short time period afforded to the RCMP to develop the analytical protocol placed the forensic application on the edge of acceptability as evidence at court, and the trial Judge ruled the scope of data was insufficient to suitably evaluate the uniqueness of the association. Trace Evidence Services of the RCMP consequently decided to drive this expertise further by analyzing a broad variety of commercially available Pb solders, using both trace element analysis of impurities and Pb-isotope analysis, to fully characterize these materials and provide sufficient chemical markers for discrimination. The goal is to build a reliable database of household solders based on peer-reviewed spectrochemical methods to use in future criminal investigations. Thus far, preliminary results indicate that four Pb isotopes 204, 206, 207, 208Pb, the 204/206Pb and 208/206Pb, are the most discriminant ratios with a two relative standard deviations (2RSD's) better than 0.33 and 0.13 %, respectively. The use of 207/206Pb (0.12% RSD) can be valuable when plotted against 204/206Pb to discriminate solder samples as well.

I077

MEASURING ULTRA-TRACE PLUTONIUM CONCENTRATIONS IN ARCTIC SEAWATER.

Andy Z. Zhou, Xiaolei. Zhao, Daniel Sauve, Chris Charles and **R. Jack Cornett**, A.E. Lalonde Laboratory for Accelerator Mass Spectrometry, University of Ottawa, Ottawa, Canada. (Jack.cornett@uottawa.ca)

^{239,240}Pu is found in the marine environment from the worldwide nuclear weapon detonations and reprocessing plant releases in the past 50 years. To monitor the Pu concentration in the Arctic Ocean, a sensitive AMS method was developed for measuring ^{239,240}Pu. In this method, a known concentration of ^{242}Pu was added to 20 L seawater as the yield tracer. The Pu was then precipitated into 400 mg $Fe(OH)_3$ and was re-dissolved in 10 mL HNO3 to reduce its sample volume. After Pu was separated from U by chromatographic extraction, the solid sputter targets for AMS measurements were made from NdF_3 coprecipitation and mixing with a large excess of PbF_2. PuF_3^- ions were extracted from the SO-110 ion source and Pu3$^+$ ions were counted in a gaseous ionization detector. The detection limit was <2 fg for ^{239}Pu and ^{240}Pu with a sensitivity of >50 CPS per pg. The AMS ^{239,240}Pu atom ratios were similar to the global fallout ratio of 0.18. The highest ^{239,240}Pu concentrations were measured in the Arctic Ocean were from water layers between 600 and 800 m. The lowest ^{239,240}Pu concentrations were measured in the surface waters.

I078

RADIOCHEMICAL SEPARATIONS FOR UNUSUAL SAMPLE MATRICES.

Ralf Sudowe, Department of Environmental & Radiological Health Sciences, Colorado State University (ralf.sudowe@colostate.edu)

Most current radioanalytical protocols have been developed for the analysis of air, water, soil and bioassay samples. While these protocols build the foundation of operational environmental monitoring, recent years have shown a renewed need for procedures that can be applied to more unusual samples. Techniques are, for example, lacking for samples that could potentially be encountered in the aftermath of a nuclear incident. Due to the likelihood of such an event occurring in an urban or metropolitan area, it is crucial to have procedures that can be used to rapidly and accurately separate and determine radioactive materials from matrices such as concrete, steel, and glass. Another need for improved sample analysis methods became apparent in the aftermath of the reactor accident at the Fukushima Nuclear Power Plant. The elevated salinity of sea and ocean water results in a complex matrix that hinders the isolation, characterization, and determination of the radioisotopes of interest. As a result there is a severe lack in methods that would allow the rapid determination of alpha and pure beta-emitting radionuclides in ocean water. This presentation will discuss recent research aimed at developing analytical protocols involving extraction chromatography that can be applied to such types of samples.

I079

A NEW RAPID TECHNIQUE TO MEASURE ^{226}RA CONCENTRATIONS IN WATER. Andy Z. Zhou, Xiaolei. Zhao and **R. Jack Cornett**, A.E. Lalonde Laboratory for Accelerator Mass Spectrometry, University of Ottawa, Ottawa, Canada. (Jack.cornett@uottawa.ca)

Radium-226 is a naturally occurring ubiquitous radionuclide produced in the radioactive decay series of U-238. We developed a new rapid and extremely sensitive method of measuring Ra-226 in drinking water utilizing Accelerator Mass Spectrometry (AMS). Ra-226 was co-precipitated with BaBeF4 since this precipitate is very stability and has extremely low solubility. Mixed with PbF_2 and compresses into a copper target, the mixed solid showed a great electrical and thermal conductivity in the AMS Cs+ sputter ion source. Dilutions series measurements agreed with expected values with an external error of 5%. The detection limit of this AMS method was very low -3 fg (1.1×10-4 Bq) with a sensitivity of >20 counts per second (CPS) per pg. We performed a survey of Ra-226 concentration in water and bottled water. The Ra-226 concentration in all samples was considerably less than the Canadian water quality guidelines.

I080

FORMATION, UPTAKE AND METABOLISM OF SELENIUM SPECIES BY FRESHWATER ALGAE. **Dirk Wallschläger**, Kelly LeBlanc, Sarah D'Amario and Denina Simmons. Trent University, Peterborough, ON. (dwallsch@trentu.ca)

The interaction of algae with inorganic selenium (Se) species in impacted fresh waters has been studied extensively in the past, due to the propensity of Se to accumulate in aquatic food chains and cause reproductive effects in top predators, which is believed to involve organic Se species like selenomethionine (SeMet). However, many past studies have been conducted at unrealistic concentration levels, due to the use of outdated analytical methods. We have developed LC-ICP-MS and LC-ES-MS-MS methods with low ng/L detection limits, allowing us to study these processes at more realistic concentration levels. Our studies show that green freshwater algae take up selenate, a common inorganic Se species in impacted waters, transform it into a number of known inorganic (e.g. selenocyanate) and organic Se species (like SeMet), and release those back into the surrounding waters. We also identified a number of unknown organic Se compounds formed and released by the algae, such as various SeMet oxidation products, in laboratory and field experiments. Further studies on the fate of the released metabolites show that selenite may not be available for (re-)uptake and metabolism by the tested algal species, questioning its relevance for Se bioaccumulation. Finally, we present some data on the effect of hydrochemical conditions on the (re-)uptake of SeMet, indicating that nitrate inhibits SeMet uptake at concentrations typical of impacted ecosystems.

I081

LC/ESI-MS METHOD FOR DETERMINATION OF POTENTIALLY-RELEVANT FATTY ACIDS IN BEEF. **Kingsley K. Donkor**[1], Laiel C. Soliman[1], Elizabeth M. Andrucson[1], Bruno Cinel[1], John S. Church[2], Thompson Rivers University, Department of Chemistry[1] and Department of Natural Resource Sciences[2] , Kamloops, BC. (kdonkor@tru.ca)

A method was developed to separate, identify, and quantify twenty-eight fatty acids of potential health relevance using liquid chromatography/electrospray ionization-mass spectrometry (LC/ESI-MS). Several experimental factors were investigated including the mobile phase composition and the elution gradient of the liquid chromatographic step. The major advantage of the proposed method is that the optimized conditions enabled baseline separation of three pairs of fatty acid isomers that are otherwise challenging to separate. The limits of detection ranged from 0.01 to 0.26 mg L^{-1} for the analytes and average recovery (mean, $n = 4$) was found to be 102 ± 12%. In addition, the proposed method was validated using a quality control standard mix of fatty acids which yielded acceptable precision and accuracy. Fatty acid concentrations in conventional grain-fed and organic grass-fed beef were determined, and the results indicate that grass-fed beef have a lower omega-6 to omega-3 ratio (1.6 – 2.8) compared to grain-fed beef (9.3 – 13.5). Principal component analysis (PCA) was applied on the resulting data to find correlation between significant fatty acids and the diet of beef samples.

I082 P

SINGLE PARTICLE ANALYSIS USING MIXED-GAS INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY, **Lucas Choma** and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada.

While inductively coupled plasma mass spectrometry (ICP-MS) is a more widely used method for single particle analysis for the detection and quantification of nanoparticles (1-100 nm), ICP optical emission spectrometry (OES) can be applied to single particle analysis and microparticles (>100 nm). Due to the increased use of nano/microparticles in applications such as fuel cells, cosmetics, and pharmaceuticals, single particle analysis is becoming an area of increased interest. While aspirating a dilute solution of particles, each droplet should only carry one particle, so that measurements are performed on a "particle by particle" basis.

During this poster presentation, the use of a mixed-gas plasma in combination with SP analysis will be explored using an $Ar\text{-}N_2\text{-}N_2$ or $Ar\text{-}N_2\text{-}H_2$ plasma in order to increase sensitivity through greater power density and transfer of energy from the bulk plasma to the central channel. These results will be compared to those obtained using conventional robust Ar conditions. Since larger particles may sink to the bottom of the sample, the use of a surfactant will also be explored to mitigate this effect and to achieve a monodispersed suspension of particles.

I083

SINGLE PARTICLE INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY METHOD FOR THE CHARACTERIZATION OF PLATINUM NANOPARTICLES FOR FUEL CELL APPLICATIONS. **Ram P. Lamsal**[a], Sadaf Tahamasebi[a], Gregory Jerkiewicz[a], Stève Baranton[b], Christophe Coutanceau[b], Aaron Hineman[c], Chady Stephan[c] and Diane Beauchemin[a], [a]Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada; [b]Université de Poitiers IC2MP, Equipe "Catalyse et Milieux" Non-Conventionnels, 4 Rue Michel Brunet, B27, TSA 51106, 86073 Poitiers cedex 9, France; [c]Perkin Elmer Canada, 501 Rowntree Dairy Rd, Unit 6, Woodbridge, ON, L4L 8H, Canada

Because nanoparticles (NPs) have larger specific surface area than their bulk solid counterparts they are increasingly usee in a wide range of industrial applications, in particular in fuel cell technology. Research aim at improving the design of fuel cells by increasing the electrochemically active surface area through the loading of NPs of different sizes on a substrate. Thus, there is a need to not only determine the NP mass concentration, but also estimate their size and size distribution. In recent years, single particle inductively coupled plasma mass spectrometry (spICPMS) has emerged as a reliable tool for quantification of metallic NPs suspended in aqueous medium, and for size measurement and determination of the size distribution pattern if their density, shape and composition are known. In this study, we examined the performance of spICPMS for in-house (laboratory) synthesized platinum (Pt) NPs having a nominal diameter of 10 nm, as verified by transmission electron microscopy (TEM). A NexION 350D ICPMS, operating in single particle mode by using the Syngistix^{TM} Nano Application module was used for data collection and processing. From the size histogram, the mean was calculated to be 12 ± 2 nm, in good agreement with TEM measurements, with a corresponding size detection limit of 6 nm.

I084

NEW METHODOLOGY TO RELEASE ^{129}I FROM CHARCOAL SAMPLES. **Barbara Francisco** and Robert Jack Cornett, AEL-AMS Laboratory, Advanced Research Complex, University of Ottawa. 25 Templeton Street, Ottawa, ON, K1N 6N5. (bbaf@hotmail.com)

A new methodology is developed to release ^{129}I from charcoal presented in air filters. Carbon in air filters is used to removes odors by trapping them in the pores of the activated carbon. Then, the goal of this project is quantify the amount of ^{129}I that is absorbed in the charcoal. A new experimental system is set up. Crushed charcoal sample with HNO_3 concentrated, labeled with ^{125}I, is heated and the vapor formed is trapped into $AgNO_3$ solution. Thus, an iodine precipitate was formed, treated and analysed under AgI crystals, by AMS and ^{129}I was measured by ^{129}I/^{127}I atomic ratio. Before a precipitation treatment, ^{125}I in solutions is analysed by Wizard Gamma Counting (Perkin Elmer) for recovery calculations. ^{125}I recoveries found in charcoals samples ranged from 69 to 100%. The amount of ^{129}I ranged from 3.82E+07 to 1.64E+09. These results show that the proposed methodology and the new experiment set up, could be used for this purpose.

I085

INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY COUPLED TO A MULTI-MODE SAMPLE INTRODUCTION SYSTEM WITH AN INFRARED HEATED PRE-EVAPORATION TUBE FOR THE ANALYSIS OF WASTE WATERS. **Tia Anderlini** and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada

An improved method for greater sample introduction efficiency and enhanced analytical performance is explored by coupling an infrared (IR) heated multimode sample introduction system (MSIS) to inductively coupled plasma optical emission spectrometry (ICPOES). A pre-evaporation tube surrounded by an IR-heated ceramic rope was inserted between the MSIS and torch to improve on previous related methods of pre-evaporation. This research was conducted in all three MSIS modes (nebulisation mode, hydride generation mode, and dual mode) and on two different ICPOES instruments. Comparisons were made between conventional set-ups in terms of sensitivity, detection limit, precision, and robustness. By tracking both hydride-forming and non-hydride forming elements, the effects of heating in combination with hydride generation were probed. Finally, optimal methods were validated by analysis of certified reference materials of waste water. Of particular interest are the improvements found for Be when MSIS(IR) is compared to conventional MSIS, indicating that beryllium hydride could be produced with the addition of heat. Overall improvements in analytical capabilities throughout this work are correlated to HG enhancing sensitivity in hydride-forming elements (i.e. when compared to PN), the hydrogen by-product of MSIS HG improving plasma excitation efficiency, and the pre-evaporation of the aerosol resulting in preserved water vapour for further improved plasma excitation characteristics and reduced sample droplet size.

I086

NOVEL EXPERIMENTAL APPROACH FOR ATRAZINE-SOIL CHEMISTRY MODELS. **Marc Lamoureux**, Donald S. Gamble, and Hanan Malibari, Department of Chemistry, Saint Mary's University, Halifax, NS, B3H 3C3 (marc.lamoureux@smu.ca)

This paper will present a new approach to study the distribution of Atrazine between the dissolved, labile sorbed, and non-labile sorbed phases when Atrazine is in contact with soil particles in an aqueous soil slurry. In particular, the sorption-desorption kinetics is studied using a novel combination of off-line filtration and on-line micro-extraction filtration cell with an HPLC equipped with UV-VIS detection system. This combination of filtration system allows the study of the time-dependent concentration of Atrazine in three different compartment (dissolved, labile sorbed, and non-labile sorbed phases). This approach allows us to meet two related objectives that support future kinetics and mechanism modelling. One was to establish a data base of analysed soil components. The other was to produce time dependent pesticide soil data related to the analysed soil components. Sorption kinetics results will be presented and discussed in the context of developing sorption-desorption models with better predictability.

I087

INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY WITH ON-LINE LEACHING TO ASSESS THE MAXIMUM BIO-ACCESSIBILITY OF TOXIC AND ESSENTIAL ELEMENTS IN WHEAT FROM SAUDI ARABIA. **Randa Althobiti** and Diane Beauchemin, Department of Chemistry. Queen's University, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada (diane.beauchemin@chem.queensu.ca)

Wheat is one of the main ingredients for all bread and bakery industries and thus one of the most consumed cereals in Saudi Arabia, which must be investigated both from nutritional and toxicological points of view. For the first time, a continuous leaching method performed on-line with inductively coupled plasma mass spectrometry (ICPMS) was applied to wheat samples to assess the maximum bio-accessibility of several trace elements. This method involves sequential leaching of the samples with artificial saliva, gastric juice and intestinal juice while continuously monitoring the released elements by ICPMS. The results, which were compared to those obtained by a conventional batch method, show that the bio-accessibility of the investigated elements varies from element to element among the samples. For example, the highest bio-accessible concentration of Pb by the batch method was 780 ± 80 ng/g and 1340 ± 300 ng/g for Nakleeh and Noqrah wheat samples, respectively, corresponding to 88% and 95% bio-accessibility. Another example is the bio-accessible concentration of Cd, which was 410 ± 30 ng/g and 1360 ± 200 ng/g for Qassim and Safeer wheat samples, corresponding to a 60% and 90% bio-accessibility. Using bio-accessible concentrations, realistic recommendations can be made to help ensure the safety of wheat for people’s diet.

I088 P

INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY WITH ON-LINE LEACHING TO ASSESS THE MAXIMUM BIO-ACCESSBLILITY OF TOXIC AND ESSENTIAL ELEMENTS IN NATURAL TOOTHBRUSH FROM SAUDI ARABIA. **Randa Althobiti** and Diane Beauchemin, Department of Chemistry. Queen's University, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada (diane.beauchemin@chem.queensu.ca)

Meswak (or Siwak) is a wood stick that is used by millions of people in various parts of the world, particularly in the Kingdom of Saudi Arabia, as an oral hygiene tool. These natural toothbrushes, which are inexpensive and simple to use, are not only excellent tools for cleaning teeth but are then swallowed to benefit from their broad range of properties. However, they are sold with no packaging in a heavily polluted area of Saudi Arabia. Because the use of contaminated meswak is a potential health concern, a continuous leaching method, coupled on-line with inductively coupled plasma mass spectrometry (ICPMS), was used on natural toothbrush samples to assess the maximum bio-accessibility of several trace elements. This method involves sequential leaching of the samples with artificial saliva, gastric juice and intestinal juice while continuously monitoring the released elements by ICPMS. Results obtained from the polluted and unpolluted meswak showed that the majority of Cr, Ni, Cu, Zn and As was leached by saliva but, in contrast, the majority of Cd and Pb was leached by gastric juice. Furthermore, they indicate that the bio-accessibility of toxic elements ranged from 70% to 100% in unpolluted meswak, and was 50% to 100% in polluted meswak. Samples collected from polluted areas typically have the highest concentrations. The ongoing work will chiefly focus on improving the understanding of meswak safety in Saudi Arabia.

I089 P

DEVELOPMENT OF METHODS FOR THE CHARACTERIZATION OF A 12 M KOH ZINCATE FUEL FOR GREEN ENERGY BACKUP SYSTEMS USING FLOW INJECTION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY.

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The overall analysis of a 12 M KOH zincate fuel, which is used in green energy backup systems is explored using inductively coupled plasma optical emission spectrometry (ICPOES). By employing various techniques, including flow injection analysis, various dilutions with external calibration, and standard additions, a final procedure was formulated for the verification of K concentration, as well as the measurement of additives (Al, Fe, Mg, In, Si), corrosion products (such C from CO_3^{2-}), and Zn particles both in and filtered from solution. Furthermore, the effects of exposing the potassium zincate electrolyte fuel to air were assessed, demonstrating how potassium carbonate precipitate formation could affect the elemental concentrations in the fuel over time. In doing so, a final novel method for the fast and sequential elemental analysis of all components of a highly corrosive base and its exposure by-product was established.

I090

MULTI-ELEMENTAL RISK ASSESSMENT OF TOXIC AND ESSENTIAL ELEMENTS IN OAT CEREAL USING ION EXCHANGE CHROMATOGRAPHY COUPLED TO INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY.

Nausheen Sadiq and Diane Beauchemin, Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada (diane.beauchemin@chem.queensu.ca)

Numerous studies have been conducted on the arsenic content of rice and rice-related products. Studies on baby food have considered several organic compounds, such as aflatoxins and fumonisins, but not the potentially toxic content of baby foods at the elemental level. Similarly, oat cereal has only been studied in the past for organic compounds [1]. This study looks at a popular brand of oat cereal in order to determine: 1) If there is a comparable amount of As and other potentially toxic elements in oat cereal and in rice cereal; 2) If these levels are higher than levels obtained in rice cereals; and finally 3) If the levels of inorganic As are higher than the limits set by the US Food and Drug Administration in baby rice cereal. Although concentrations were typically lower than what was obtained for baby rice cereal, the bio-accessibility for the batch method was close to 90%, which is a cause for concern.

[1] Rubert, J., Soler, C. & Mañes, J. (2012). Food Chemistry, 133, 176-183.

I091

SPECIATION ANALYSIS OF NICKEL IN ALKALINE FUEL CELL ELECTROLYTE BY ION CHROMATOGRAPHY COUPLED TO INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY.

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Significant research is nowadays focused on the development of alkaline fuel cell technology, as cheaper metals than platinum, which are stable in NaOH and KOH matrices, may then be used as catalysts. Nickel, of which Canada is a major producer, is an example of such a metal. In order to develop a suitable fuel cell, information is needed about the electrochemical reactions taking place, which may be inferred through a determination of the chemical form of any dissolved Ni in the electrolyte. However, such analysis has never been performed. During this presentation, a new speciation analysis method involving ion chromatography coupled to inductively coupled plasma mass spectrometry (ICPMS) will be presented. The high sensitivity of ICPMS allows the detection of minute amounts of Ni. Using CG10 and CS10 guard and analytical cation exchange columns, respectively, Ni^{2+} is eluted isocratically using a 0.55 M HCl mobile phase, within 10 min following injection of a 0.1 M NaOH solution containing 50 ng/mL of Ni. Application of this speciation analysis method to sample solutions obtained following an increasing number of cyclic voltammetry cycles (to simulate fuel cell operation) revealed that the only detected species was Ni^{2+} with an estimated concentration of less than 20 ng/mL.

I092 P

DIRECT SPECIATION ANALYSIS OF ARSENIC IN SOLIDS BY ELECTROTHERMAL VAPORISATION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY.

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The usual method for the speciation analysis of solid samples involves an extraction followed by injection of the extract onto a chromatographic system with detection by inductively coupled plasma (ICP) spectrometry. The extraction step can be time-consuming and may result in the conversion of an element from one species to another, rendering results inaccurate. It would be beneficial to perform speciation analysis directly from a solid sample to minimize opportunities for species inter-conversion. Preliminary results indicate that this can be achieved by coupling electrothermal vaporization (ETV) to ICP optical emission spectrometry (OES). Samples of the fern *Pteris vittata* grown in arsenic contaminated soil were analyzed. Using a ramping temperature program, multiple peaks were observed in the temporal profile. These peaks occurred in two distinct groups, a low temperature group from 200ºC to 600ºC and a high temperature group from 1300ºC to 2000ºC. These peak groups can be further separated with variations in the temperature program such as precise selection of vaporization temperatures and increased ramping time. Analysis of certified reference materials with similar matrices and previous speciation results for *Pteris vittata* suggest that the low temperature peak group contains dimethylarsinic acid (DMA) and As(V) while the high temperature peak group contains As(III).

I093

FORENSIC ANALYSIS OF HUMAN NAIL FOR GENDER AND ETHNICITY USING ELECTROTHERMAL VAPORIZATION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY.

A. Schug and **D. Beauchemin**, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K6L 3N6

The forensic analysis of nail clippings by electrothermal vaporization (ETV) coupled to inductively coupled plasma optical emission spectrometry (ICPOES) was performed in an attempt to identify gender and ethnicity. Nail clippings were cleaned with acetone and then high-purity water before being left to air-dry. They were simply placed in graphite boats for insertion into the ETV graphite furnace. Qualitative measurements were conducted in combination with multivariate analysis to infer gender and ethnicity. Peak areas of the resulting ETV-ICPOES transient signals were computed, following internal standardization with an argon emission line (763.511 nm) to compensate for sample loading effects on the plasma. The resulting peak area was finally corrected for sample mass before being used for multivariate analysis. Principal component analysis (PCA), which could not accurately identify gender or ethnicity of all the samples, was first performed to reduce the dimensionality of the multidimensional data set and select the elements with the highest loading scores. Linear discriminant analysis (LDA) ascribed gender with a 90% success rate using Zn, Fe and K, and correctly identified ethnicity of all the samples using Li, Mo, S, Cr, As, Sb, Cd and Cu.

I094 P

ASSESSMENT OF NI-BASED ELECTRODE STABILITY IN ALKALINE FUEL CELLS THROUGH THE DEVELOPMENT OF ICP-MS METHODS FOR BASIC ELECTROLYTE SOLUTIONS.

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The goal of this work was to develop methods for the analysis of KOH and NaOH electrolyte used in alkaline fuel cells in order to assess the stability of new Ni-based electrodes being developed. Given that the sample introduction system of an inductively coupled plasma mass spectrometry (ICP-MS) instrument is made of glass and that the ICP torch is made of quartz, which can both be attacked by hydroxides, alkaline solutions were neutralized off-line by adding acid, or on-line through merging of an acidic solution. These neutralization processes, paired with the use of flow injection into a stream of high purity water, allows for the use of the regular glass sample introduction system and quartz injector. The sensitivity and detection limit for Ni and other elements that would be present in the electrolyte solutions were determined for each approach, to establish which is best suited for the analysis of basic solutions by ICP-MS. These analyses revealed that offline neutralization yields the lowest limits of detection (LOD). In an acidic water matrix, values in the ng/L range are obtained for these elements. When comparing matrices of 0.5 M NaOH and KOH for this method, the lowest LOD values are obtained when using KOH, with all LODs being equal to or less than 10 µg/L for the elements of interest. In addition, potential matrix effects arising from the significant concentration of neutralization salt by-products in a range of 0 M to 2 M were assessed, as suppression effects may result from increasing alkaline concentrations. Additional considerations were given to the operating conditions of the ICP-MS instrument and to consumable costs associated with using solutions with a high salt concentration. Indeed, both the sampler and skimmer cones undergo considerable degradation, significantly increasing operation and analyses costs.

I095 P

SLURRY NEBULIZATION AND INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY WITH A MIXED-GAS PLASMA FOR THE ANALYSIS OF VEGETATION SAMPLES.

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Total digestions of solid samples for analysis by inductively coupled plasma (ICP) spectrometry requires harsh acids and high temperatures. Even with these potentially dangerous conditions, incomplete digestions are common. Solid sampling methods such as electrothermal vaporization and laser ablation avoid digestion steps but are costly and do not have cheap and readily available calibration standards. By grinding material into very fine particles, solid samples may be dispersed in aqueous solutions by surfactants. This forms quasi-stable slurries that can be directly nebulized for analysis by inductively coupled plasma mass spectrometry.[1] This work optimized mixed gas plasma conditions for the reduction of matrix effects as described by Makonnen and Beauchemin[2]. This allowed the slurries to be calibrated against commercial aqueous standards diluted with surfactant. When the method was applied to Hard Red Spring Wheat Flour (NIST CRM #8437) good agreement was found with concentrations of the certified elements tested. The method is thus promising for the total analysis of solid samples without conducting an acid digestion.

(1) Ebdon, L.; Foulkes, M.; Sutton, K. Slurry Nebulization in Plasmas. *J. Anal. At. Spectrom.* **1997**, *12* (2), 213–229.
(2) Makonnen, Y.; Beauchemin, D. An argon–nitrogen–hydrogen mixed-gas plasma as a robust ionization source for inductively coupled plasma mass spectrometry. *Spectrochim. Acta Part B At. Spectrosc.* **2014**, *99*, 87–93.

I096

GONE BUT NOT FORGOTTEN: PATTERNING AND ENHANCED BIOFILM GROWTH BY TEMPORARILY WALL ADHERED BUBBLES IN MICROFLUIDIC FLOW CELLS.

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Low aspect ratio, hydrophobic microfluidic flow cells were used to temporarily trap microbubbles during inoculation of *Pseudomonas sp.* bacterial biofilms. Contrary to intuition, surfaces which were temporarily blocked by bubbles could drastically enhance biofilm growth, despite bubble elimination as much as a day earlier. The resulting biofilm patterns were dependant on the inoculation state of the surface, with ring patterns observed for bubbles formed on clean surfaces and continuous patterns for bubbles formed on inoculated surfaces. In both cases, bubble-patterned biofilms were more homogeneous than for biofilms formed in the absence of bubbles. High resolution confocal laser scanning microscopy (CLSM) was used to examine the nature of bacteria-bubble interactions. It is concluded that the underlying mechanism for the observed growth enhancement was related to bacterial trapping by the bubble.

I097

SYNTHESIS OF BIMETALLIC HOLLOW AGM NANOPARTICLES, STRUCTURE AND COMPOSITION ANALYSIS. **Josée R. Daniel**,[1] Sadegh Yazdi,[2] Lauren McCarthy,[2] Emilie Ringe[2] and Denis Boudreau[1], [1]Département de chimie et Centre d'optique, photonique et laser (COPL), Université Laval, Québec (QC), G1V 0A6, Canada; [2]Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, 77005, USA.

Plasmonic nanomaterials have found applications in multiple fields such as catalysis, molecular sensing, imaging and single molecule spectroscopy, among others. The performance of a given nanomaterial in terms of absorption, scattering or local electric field enhancement can be optimized for a specific application by controlling physical properties such as size, shape and composition. In this context, hollow bimetallic nanostructures provide additional variables, including shell thickness and metallic component ratio, which can be manipulated to finely tune the plasmonic and optical properties of the structures. Galvanic replacement is an efficient and versatile synthesis strategy for the preparation of hollow and semi-hollow nanostructures with enviable plasmonic properties. This presentation will discuss our recent progress on the synthesis of hollow bimetallic nanostructures using silver nanoparticles as sacrificial templates and partial galvanic replacement by more noble metals (Au, Pd, Pt) and their characterization. These structures could find applications in various fields such as reprogrammable sensors, responsive materials, optical memory units, molecular sensing, cellular imaging and *in situ* microscopy of chemical reactions.


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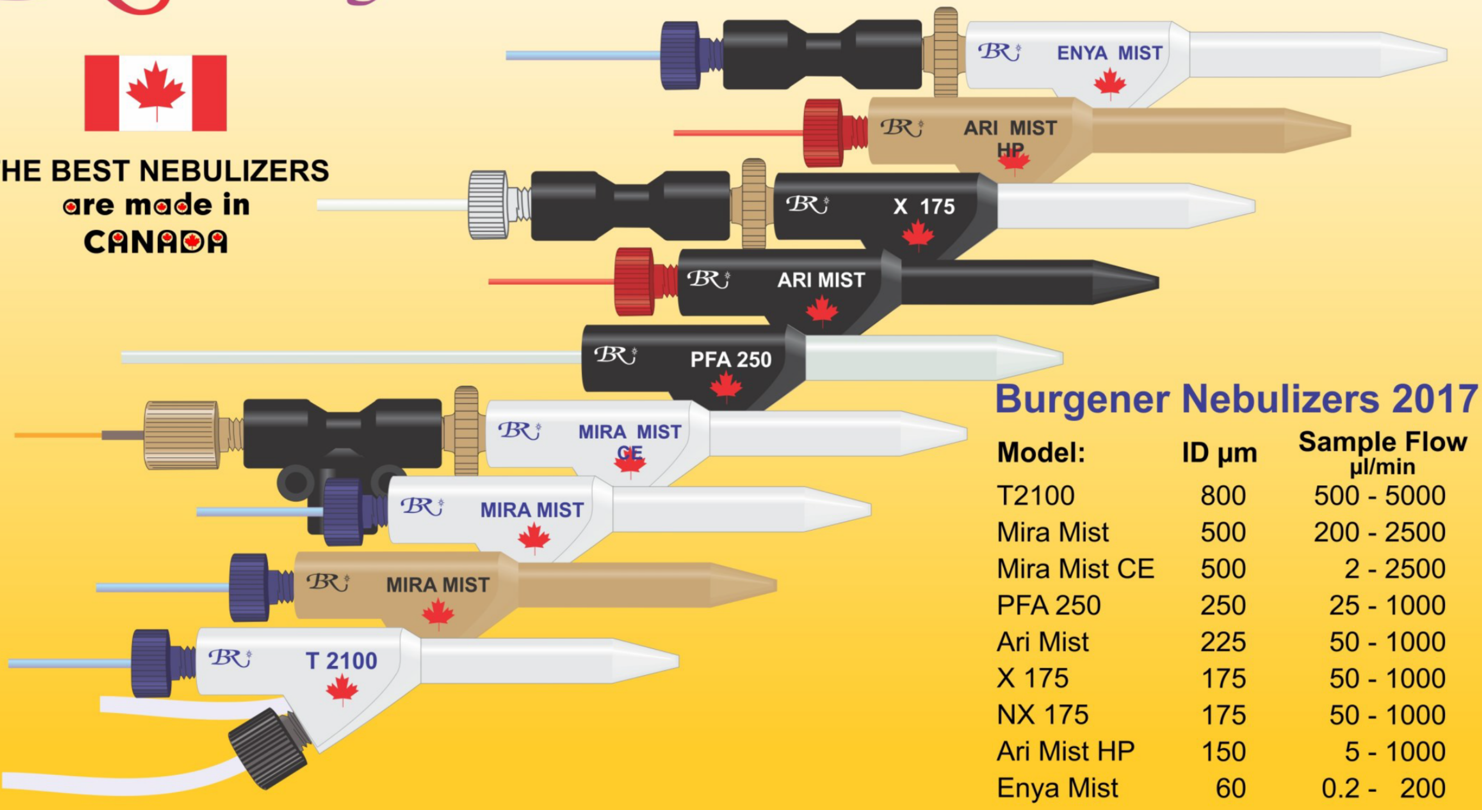
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