



**UNIVERSITY
OF LATVIA**

**22nd INTERNATIONAL
SCIENTIFIC CONFERENCE**

“EcoBalt 2021”

Riga, Latvia

October 21–23, 2021



EcoBalt 2021

BOOK OF ABSTRACTS

**22nd INTERNATIONAL
SCIENTIFIC CONFERENCE**

“EcoBalt 2021”

Riga, Latvia

October 21–23, 2021

BOOK OF ABSTRACTS

**ORGANISED BY
UNIVERSITY OF LATVIA
FACULTY OF CHEMISTRY**

International Scientific Conference “EcoBalt 2021”, Riga, Latvia, October 21–23, 2021, Book of Abstracts, University of Latvia Press, 2021. 97 p.

Organisers

The Faculty of Chemistry, University of Latvia

Scientific Committee

Prof. Dr. Chem. Arturs Viksna, University of Latvia (Latvia)

Chair of the conference

Prof. Māris Kļaviņš, University of Latvia (Latvia)

Prof. Vadims Bartkevičs, University of Latvia, BIOR (Latvia)

Prof. Ewa Bulska, University of Warsaw (Poland)

Prof. Viktor Kanicky, Masaryk University (Czech Republic)

Prof. Maja Ramškar, Jožef Stefan Institute (Slovenia)

Prof. Mehmet Yaman, Firat University (Turkey)

Asoc. prof. Ayhan Oral, Çanakkale Onsekiz Mart University (Turkey)

Prof. Aivaras Kareiva, Vilnius University (Lithuania)

Prof. Arūnas Ramanavičius, Vilnius University (Lithuania)

Prof. Ivo Leito, University of Tartu (Estonia)

Dr. Irina Shtangeeva, St. Petersburg University (Russia)

Dr. med. Inese Mārtiņšone, Rīga Stradiņš University (Latvija)

Organizing Committee

Doc. Dr. Chem. Agnese Osīte, University of Latvia

Chair of the Organizing Committee

Asoc. prof., Dr. Chem. Vita Rudoviča, University of Latvia

Dr. Chem. Modris Drille, Latvian Accreditation Bureau

M. Sc. Dace Silarāja, University of Latvia

PhD. Student Māris Bērtiņš, University of Latvia

Dr. Chem. Ingus Pērkons, University of Latvia, BIOR

Working group

M. Sc. Gunita Celma, University of Latvia

PhD. Student Lauma Buša, University of Latvia

PhD. Student Kristaps Saršūns, University of Latvia

PhD. Student Aija Trimdale, University of Latvia

PhD. Student Vitālijs Lazarenko, University of Latvia

B. Sc. Madara Rakšte

Organising committee of conference is not responsible for the information given by authors. Theses are considered for inclusion in the program, the spelling and punctuation are kept without changes.

© University of Latvia, 2021

ISBN 978-9934-18-724-7 (PDF)

<https://doi.org/10.22364/isceb.2021>

CONTENTS

PROGRAMME	10
INVITED SPEAKERS	19
Juris Burlakovs, Ruta Ozola-Davidane, Maris Klavins INNOVATIVE COMPOSITE SORBENTS FOR ORGANIC AND INORGANIC POLLUTANTS REMOVAL FROM AQUEOUS SOLUTIONS IN LANDFILL LEACHATES	20
Markéta Holá, Vojtěch Wertich, Jan Dobeš, Martin Kubeš, Juraj Mozola, Jaromír Leichmann, Viktor Kanický LA-ICP-MS IMAGING WITH FOCUS ON GEOLOGICAL MATERIALS	21
Greta Inkraite, Ramunas Skaudzius, Stasys Tautkus, Aleksej Zarkov, Aivaras Kareiva STUDY OF SUBSTITUTION EFFECTS IN THE YTTRIUM ALUMINIUM GARNET SYNTHESIZED BY ENVIRONMENTALLY BENIGN SOL-GEL SYNTHESIS METHOD	22
Ivo Leito, Asko Laaniste, Koit Herodes ONLINE COURSE AND SOFTWARE FOR LC-MS METHOD VALIDATION	23
Salih Can Süner, Halime Çevikbaş, Seyhan Ulusoy, Gülgün Tinaz, Ayhan Oral PREPARATION OF WOUND HEALING NANOFIBER MATERIAL THAT CONTAINING CINNAMALDEHYDE	24
Arunas Ramanavicius, Eivydąs Andriukonis, Raimonda Celiesiute-Germaniene, Simonas Ramanavicius, Aura Kisielute, Monika Vilkiene, Ieva Mockeviciene, Aurimas Lisauskas, Ieva Kiminaitė, Urte Samukaite-Bubniene DEVELOPMENT OF MICROBIAL FUEL CELLS	25
Maja Remškar, Luka Pirker, Bojana Višić, Anton Gradišek, Agnese Osite AIR POLLUTION BY NANOPARTICLES CAUSED BY USE OF PYROTECHNICS	26
Irina Shtangeeva, Maris Bērtiņš, Arturs Viksna INFLUENCE OF RUBIDIUM ON ACCUMULATION OF MACRO- AND TRACE ELEMENTS IN TWO PLANT SPECIES AND IN THE RHIZOSPHERE SOIL	27
ORAL AND POSTER PRESENTATIONS	28
Lāsma Akūlova, Inese Mārtiņšone, Žanna Martinsone, Laura Komarovska, Anita Seile, Svetlana Lakiša, Ivars Vanadziņš HBM4EU – HUMAN BIOMONITORING INITIATIVE IN LATVIA: STUDY ON PESTICIDE MIXTURES IN ADULT AND CHILDREN POPULATION	29
Līga Avotina, Arturs Zarins, Mihails Halitovs, Larisa Baumane, Aleksandrs Petjukevics, Gunta Kizane THERMAL DECOMPOSITION AND SPECTROMETRIC ANALYSIS OF IRRADIATED KERATINOUS FIBERS	30
Linda Ansone-Bertina, Maris Klavins, Viesturs Ozols, Lauris Arbidans METAL ORGANIC FRAMEWORK COMPOSITES FOR CARBON DIOXIDE CAPTURE	31
Maris Bertins, Agnese Brangule, Vitalijs Lazarenko, Agnese Osite, Arturs Viksna, Gunita Celma POSSIBILITIES FOR INTERFERENCE REDUCTION IN ICP-MS/MS SYSTEM USING HE COLLISION CELL	32

Zane Berzina, Romans Pavlenko, Laura Elina Ikkere, Vadims Bartkevics APPLICATION OF WASTEWATER – BASED EPIDEMIOLOGY FOR TRACKING HUMAN EXPOSURE TO DEOXYNIVALENOL AND ENNIATINS	33
Odeta Brigaitytė, Rasa Šlinkšienė SUITABILITY OF ECOLOGICAL BUCKWHEAT GROATS WASTE FOR FERTILIZER PRODUCTION	34
Zanda Brike, Rita Veilande, Maris Strazds, Kristiana Rancane, Anda Abola, Atis Skudra MERCURY CONCENTRATION IN THE FAECES OF BLACK STORKS	35
Mehmet Veysi Çetiz, Halbay Turumtay, Erdal Kaya, Neriman Özhatay, Emine Akyüz Turumtay INVESTIGATION OF PHYTOCHEMICAL PROPERTIES OF PAEONIA L. GENUS BELONG TO TURKEY'S FLORA	36
Kęstutis Čeplinskas, Andrius Jaskūnas PREPARATION OF MIXED OXIDE CATALYSTS FOR VOLATILE ORGANIC COMPOUND ABATEMENT	37
Merve Danisman, Ayhan Oral SURFACE MODIFICATION OF GRAPHENE OXIDE BY ENZYME CATALYZED REACTION	38
Yusuf Dilgin, Selen Ayaz, Gamze Emir, Serkan Karakaya, Didem Giray Dilgin ELECTROCHEMICAL SENSORS FOR DETERMINATION OF ENVIRONMENTALLY IMPORTANT COMPOUNDS USING DISPOSABLE PENCIL GRAPHITE ELECTRODES	39
Ramunas Diliautas, Aldona Beganskiene, Dovydas Karoblis, Dalis Baltrunas, Kestutis Mazeika, Aleksiej Zarkov, Aivaras Kareiva STRUCTURAL, MORPHOLOGICAL AND MAGNETIC INVESTIGATION OF $Bi_{1-x}Gd_xFe_{0.85}Mn_{0.15}O_3$ SOLID-SOLUTIONS	40
Armands Egleskalns, Ingars Reinholds, Konstantins Bavrins, Gunta Kizane ASSESSMENT OF RADIONUCLIDES IN FORMER SALASPILS NUCLEAR REACTOR COOLING WATER	41
Andrzej Gawor, Andrii Tupys, Anna Ruszczynska, Ewa Bulska APPLICATION OF HR-CS GF MAS FOR FLUORINE DETERMINATION IN BIOLOGICAL SAMPLES	42
Daniela Godina, Kristine Meile, Aivars Zhurins, Arturs Viksna BIO-CHAR CATALYST APPLICATION FOR GLUCOSIDE HYDROLYSIS REACTION	43
Anton Gradišek, Luka Pirker, Anja Pogačnik Krajnc, Urška Gradišar Centa, Jan Malec, Vladimir Radulović, Andreja Jelen, Igor B. Mekjavić, Janez Kovač, Miran Mozetič, Matej Godnič, Metod Čebašek, Tina Bregant, Luka Snoj, Maja Remškar PARTICLE REMOVAL EFFICIENCY OF FACE MASKS DURING THE COVID-19 PANDEMIC	44
Vladlens Grebņevs, Roman Viter, Şahin Altundal, Kārlis Grundšteins, Agnieszka Stołarczyk, Arturs Viksna, Wojciech Simka SOLUTIONS ON THE WAY TO PREPARATION OF CARBONATED TITANIUM IMPLANT COATINGS VIA PLASMA ELECTROLYTIC OXIDATION IN SUSPENSIONS	45
Diana Griesiute, Aivaras Kareiva, Aleksiej Zarkov SYNTHESIS OF $B-Ca_2P_2O_7$ AS AN ADSORBENT FOR THE REMOVAL OF HEAVY METALS FROM WATER	46

Goda Gudinskaitė, Rasa Paleckienė, Rasa Šlinkšienė COMPATIBILITY OF LIQUID FERTILIZERS AND HUMIC SUBSTANCES	47
Laura Elina Ikkere, Iveta Pugajeva, Veronika Šukajeva, Ingus Pērkons WASTEWATER-BASED EPIDEMIOLOGY AS A TOOL FOR PUBLIC HEALTH AND LIFESTYLE ASSESSMENT	48
Greta Inkrataitė, Ramūnas Skaudžius INFLUENCE OF BORON AND MAGNESIUM IONS ON YAG: CE AND LUAG:CE CERAMICS	49
Jakub Karasiński, Andrii Tupys, Ludwik Halicz, Ewa Bulska A NEW METHOD FOR MEASURING GERMANIUM ISOTOPE RATIOS IN MINERALS AND WATER SAMPLES USING MC-ICP-MS AFTER THE FORMATION OF VOLATILE HYDRIDES	50
Dovydas Karoblis, Aleksej Zarkov, Aldona Beganskiene, Aivaras Kareiva PREPARATION OF RUDDLESDEN-POPPER CALCIUM MANGANITES APPLYING MOLTEN SALT SYNTHESIS	51
Vytautas Kavaliauskas, Vilma Olšauskaitė, Audrius Padaruskas HYDROPHOBIC EUTECTIC SOLVENT FOR LIQUID-PHASE MICROEXTRACTION OF PARABENS FROM WATER SAMPLES	52
Aneka Klavina, Ilona Pavlovskā, Agris Auce, Laura Komarovskā, Linda Paegle, Linda Dobkevica, Inese Martisone, Ivars Vanadzins EVALUATION OF SAPROPEL SEDIMENTS FOR MEDICAL PURPOSES	53
Maris Klavins, Marcis Mezulis, Linards Klavins, Viktor Stabnikov, Andrii Marynin, Olena Stabnikova INTERACTION BETWEEN MICROPLASTICS AND CHEMICAL POLLUTANTS	54
Zane Kļaviņa, Arta Bārdule, Ivars Kļaviņš, Zane Lībiete VARIATION IN METHYLMERCURY CONCENTRATIONS IN ENVIRONMENTAL SAMPLES IN FOREST LAND AND WETLANDS WITH ORGANIC SOILS IN LATVIA	55
Zhanymgul Koishybayeva, Abdirash Akilbekov, Abay Ussenov, Anatoli I. Popov, A. Platonenko DFT STUDY OF GALLIUM OXIDE BULK PROPERTIES	56
Agne Kizalaite, Tomas Murauskas, Aleksej Zarkov INSIGHT INTO THE FORMATION OF ZINC WHITLOCKITE: SYNTHESIS, STRUCTURE AND CHARACTERISATION	57
Pille-Riin Laanet, Piret Saar-Reismaa, Merike Vaher ANALYSIS OF SYNTHETIC AND PHYTOCANNABINOIDS USING MICELLAR ELECTROKINETIC CHROMATOGRAPHY	58
K. D. Labsvards, V. Rudovica, J. Rusko, R. Kluga, L. Busa, M. Bertins, J. Naumenko, M. Salajeva, A. Viksna DETERMINATION OF LATVIAN HONEY FLORAL ORIGINS USING IRMS, UHPLC-HRMS, NMR ..	59
Vitālijs Lazarenko, Yelyzaveta Rublova, Raimonds Meija, Jana Andžāne, Vanda Voikiva, Arturs Viksna, Donāts Erts APPLICATION OF INNOVATIVE Bi_2Se_3 THIN FILMS AS ANODES IN AQUEOUS RECHARGEABLE LITHIUM-ION BATTERIES	60

Ilga Lauma Leimane, Jānis Ģibietis DETERMINATION OF NON-FERROUS METALS IN SOIL SAMPLES USING TEST STRIP METHOD	61
Henrieta Markevičiūtē, Nijolē Dukštienē, Valentina Krylova THE STRUCTURAL, MORPHOLOGICAL AND OPTICAL PROPERTIES OF PA6/AG-CD-SE LIGHT-ABSORBING MATERIALS	62
Žanna Martinsone, Lāsma Akūlova, Aneka Kļaviņa, Linda Paegle, Inese Mārtiņšone, Darja Kaļuzņaja, Marija Avota and Ivars Vanadziņš EXPLORING CAUSES, EFFECTS AND POSSIBLE SOLUTIONS FOR CHEMICAL POLLUTION IN THE ENVIRONMENT: CITIZENS' AND EXPERTS' OPINION	63
Inese Martisone, Kristine Sproge, Lasma Akulova, Zanna Martinsone, Linda Matisane HUMAN BIOMONITORING INITIATIVE – FUTURE FOR HUMAN EXPOSURE ASSESSMENT TO CHEMICALS	64
Luīze Terēze Medne, Jānis Ģibietis DETERMINATION OF PHOSPHATES IN SOIL BY RAPID TEST METHOD	65
Austēja Mikolaitienē, Rasa Šlinkšienē EFFECT OF STARCH ADDITIVE ON THE PROPERTIES AND SOLUBILITY OF UREA GRANULES	66
Martina Navrátilová, Andrea Sochová, Daniela Vráblová, Lenka Skálová MONITORING OF ALBENDAZOLE TRANSFER FROM SHEEP DUNG TO FODDER PLANTS AND ADJACENT SOIL BY UHPLC-MS	67
Megija Neimane , Vitālijs Lazarenko , Māris Bērtiņš , Arturs Viksna , Dagnija Lazdiņa, Kristaps Makovskis, Ilze Kārklīņa, Andis Lazdiņš VARIATIONS OF MICRO- AND RARE EARTH ELEMENTS IN THE BOTTOM AND FLY WOOD ASH	68
Estefanija Novicka, Iveta Pugajeva, Ingars Reinholds, Vadims Bartkevics TWO-DIMENSIONAL LIQUID CHROMATOGRAPHY – HIGH RESOLUTION MASS SPECTROMETRY METHOD FOR SIMULTANEOUS MONITORING OF 70 REGULATED AND EMERGING MYCOTOXINS	69
Hans Orru, Triin Veber, Katrin Lang, Inge Ringmets, Tanel Tamm, Marek Maasikmets, Leena Albrecht, Märten Lukk EXPOSURE TO AIR POLLUTION IN THE OIL SHALE REGION IN ESTONIA AND RELATED BIRTH EFFECTS	70
Sergejs Osipovs, Aleksandrs Pučkins DEVELOPMENT OF A METHOD FOR THE TAR ANALYSIS IN CO-PRODUCED GAS	71
Kristaps Oskalns, Maris Bertins, Edgars Selickis, Arturs Viksna APPLICATION OF MULTIFACTOR ANALYSIS FOR DRINKING WATER QUALITY CONTROL IN RIGA CITY	72
Daria Pashneva, Ieva Uogintē, Julija Pauraitē, Agnė Minderytė, Kristina Plauškaitė, Valda Araminienė, Eugenija Farida Dzenajavičienė, Valda Gudynaitė-Franckevičienė, Iveta Varnagirytė-Kabašinskienė, Nerijus Pedišius, Egidijus Lemanas, Tomas Vonžodas, Steigvilė Byčenkienė BLACK CARBON DEPOSITION ON TREE FOLIAGE AN URBAN BACKGROUND IN VILNIUS	73

Matiss Pals, Maris Lauberts, Alexandr Arshanitsa, Arturs Viksna THE OPTIMISATION OF ORGANOSOLV PROCESS OF BARK DELIGNIFICATION PROCESS- WITH FOCUS ON PURIFICATION OF ISOLATED LIGNIN FRACTION	74
Romans Pavļenko, Zane Bērziņa, Mārtiņš Jansons, Vadims Bartkevičs ANALYSIS OF WASTEWATER SAMPLES FOR DETERMINATION OF MYCOTOXINS	75
Ingus Pērkonis, Laura Elina Ikkere, Veronika Šukajeva, Iveta Pugajeva FINGERPRINTING HUMAN PHARMACEUTICALS, ILLICIT DRUGS AND NEW PSYCHOACTIVE SUBSTANCES IN WASTEWATER: A MULTI-METHOD APPROACH	76
Aleksandrs Pučkīns, Sergejs Osipovs ANALYSIS OF POLLUTANTS IN INDUSTRIAL WATER USED FOR COOLING OF CO-PRODUCED GASES	77
Aiga Anna Pudule, Laura Komarovska, Arturs Viksna, Dārta Ūbele, Kārlis Agris Gross NANOSTRUCTURING AMORPHOUS CALCIUM PHOSPHATE: CARBONATE INCLUSION	78
Ingrīda Radveikienė, Gintautas Bagdžiūnas INSIGHTS INTO AN ELECTROCHEMISTRY OF NEUROTRANSMITTERS USING THE CYCLODEXTRINS MODIFIED ELECTRODES	79
Dovilė Ragauskaitė, Rasa Šlinkšienė COFFEE GROUNDS IMPACT ON A RYE GROWTH	80
I. Reinholds, U. Eismonts, K. Saleniece, M. Bertins, A. Viksna, G. Kizane, O. Muter, A. Podjava, A. T. Boginska, S. Gaidukovs, A. Grinbergs EFFECTIVE REMOVAL OF RADIOACTIVE CESIUM FROM CONTAMINATED WATER ENVIRONMENTS BY IN SITU SYNTHESIZED IRON HEXACYANOFERRATE IMOBILIZED ON CELLULOSE ACETATE ESTERS	81
D. Riekstina, A. Egleskalns, G. Kizane, O. Skrypnik, T. Krasta NATURAL RADIOACTIVITY LEVELS IN GRANITE	82
Eleonora Rieksta, Jānis Ģībietis DETERMINATION OF FORMALDEHYDE BY THE "GREEN" RAPID TEST METHOD	83
Artis Robalds RECOVERY OF MICROELEMENTS FROM POTATO JUICE BY BIOSORBENTS	84
Modestas Ružauskas, Elena Bartkienė, Jurga Bernatoniė, Daiva Žadeikė, Arūnas Stankevičius, Vita Lėlė, Vytautė Starkutė, Paulina Zavistanavičiūtė, Juozas Grigas, Eglė Zokaitytė, Arnoldas Pautienius, Gražina Juodeikienė, Valdas Jakštas INFLUENCE OF MULTICOMPONENT NUTRACEUTICAL ON GUT MICROBIOTA IN EXPERIMENTAL ANIMALS	85
Kristaps Saršūns, Kaspars Leduskrasts, Agris Bērziņš, Toms Reķis MODULATION OF LUMINESCENCE SPECTRA VIA SOLID SOLUTION FORMATION OF THIOXANTHONE DERIVATIVES	86
Aina Semjonova, Agris Bērziņš CRYSTALLIZATION AND STABILIZATION OF 2,6-DIMETHOXYPHENYLBORONIC ACID METASTABLE POLYMORPH USING SURFACTANTS	87
Evaldas Simanavičius, Kristina Jančaitienė, Rasa Šlinkšienė DEVELOPMENT OF HYDROPONICS SYSTEMS WITH BIOACTIVE SUBSTANCES	88

Edita Sodaitienė, Audronė Gefenienė, Sigitas Jankauskas, Rimantas Ramanauskas, Romas Ragauskas COMPARATIVE STUDY OF DIFFERENT ADSORBENTS FOR ANODIZED ALUMINUM DYE REMOVAL	89
Viktor Stabnikov, Andrii Marynin, Olena Stabnikova, Maris Klavins THE MICROBIALLY-COATED MICROPLASTICS IN NEUSTONIC WATER-AIR INTERPHASE	90
Aija Trimdale-Deksne, Agris Bērziņš A MULTI-TECHNIQUE APPROACH TO UNDERSTAND THE DIHYDROXYBENZOIC ACID DIFFERENT PROPENSITIES TO FORM SOLID PHASES	91
Valda Valkovska, Liāna Orola ECO-FRIENDLY DYEING OF WOOLLEN YARN USING LATVIAN TRADITIONAL DYE PLANTS	92
Vida Vičkačkaitė, Marija Lukoševičiūtė HEADSPACE-GAS CHROMATOGRAPHIC DETERMINATION OF B-CARYOPHYLLENE IN <i>EPILOBIUM ANGUSTIFOLIUM</i> EXTRACTS	93
Signija Zake, Maris Bertins, Dagnija Lazdina, Karlis Dumins, Arturs Viksna APPLICATION OF NITROGEN AND CARBON STABLE ISOTOPE RATIO MASS SPECTROMETRY FOR NITROGEN CIRCULATION STUDIES DURING CONIFER PLANTING	94
L. Zorza, M. Bertins, K. Saleniece, A. Viksna, A. Grinbergs, O. Muter ACCUMULATION OF CESIUM-133 IN AQUATIC PLANTS AND ITS EFFECT ON THE PHYSIOLOGICAL ACTIVITY OF PLANTS AND AQUATIC MICROORGANISMS	95
A. Zuševica, E. Muižnieks, S. Žigure, S. Celma, T. A. Štāls, K. Dūmiņš, S. Rancāne, D. Lazdiņa HEAVY METAL ACCUMULATION CAPACITY OF VARIOUS LOCAL HERBACEOUS SPECIES COMMUNITIES CULTIVATED IN MUNICIPAL BIOWASTE SUBSTRATE WITH CONSTRUCTION DEBRIS ADMIX	96
Grzegorz Wryk, Agnieszka Borowiec, Iwona Gašiorowska, Katarzyna Stopka, Beata Kondraszuk, Andrzej Gawor, Eliza Kurek, Ewa Bulska AN IMPROVEMENT OF THE ANALYTICAL PROTOCOL OF GLYPHOSATE QUANTIFICATION IN FOOD SAFETY AREA	97

PROGRAMME

21.10.2021

8.45–09.00	Joining the EcoBalt conference ZOOM platform	
First session; Chair: Dr. Agnese Osīte		
09.00–09.20	<p>Prof. Indriķis Muižnieks <i>Rector of University of Latvia</i></p> <p>Prof. Arturs Viksna <i>Faculty of Chemistry</i></p> <p>Uģis Rotbergs <i>Chairman of the Board of the World Wide Fund for Nature;</i> <i>Ambassador of the Institute for Environmental Solutions</i></p>	Opening of the conference
09.20–09.40	<u>Maja Remškar</u> , <i>Luka Pirker, Bojana Višić, Anton Gradišek, Agnese Osīte</i>	AIR POLLUTION BY NANOPARTICLES CAUSED BY USE OF PYROTECHNICS (Invited Speaker)
09.40–10.00	<u>Irina Shtangeeva</u> , <i>Maris Bērtiņš, Arturs Viksna</i>	INFLUENCE OF RUBIDIUM ON ACCUMULATION OF MACRO- AND TRACE ELEMENTS IN TWO PLANT SPECIES AND IN THE RHIZOSPHERE SOIL (Invited Speaker)
10.00–10.15	<u>Mehmet Veysi Çetiz</u> , <i>Halbay Turumtay, Erdal Kaya, Neriman Özhatay, Emine Akyüz Turumtay</i>	INVESTIGATION OF PHYTOCHEMICAL PROPERTIES OF PAEONIA L. GENUS BELONG TO TURKEY'S FLORA
10.15–10.30	<u>Anton Gradišek</u> , <i>Luka Pirker, Anja Pogačnik Krajnc, Urška Gradišar Centa, Jan Malec, Vladimir Radulovič, Andreja Jelen, Igor B. Mekjavić, Janez Kovač, Miran Mozetič, Matej Godnič, Metod Čebašek, Tina Bregant, Luka Snoj, Maja Remškar</i>	PARTICLE REMOVAL EFFICIENCY OF FACE MASKS DURING THE COVID-19 PANDEMIC
10.30–10.45	<u>K. D. Labsvards</u> , <i>V. Rudovica, J. Rusko, R. Kluga, L. Busa, M. Bertins, J. Naumenko, M. Salajeva, A. Viksna</i>	DETERMINATION OF LATVIAN HONEY FLORAL ORIGINS USING IRMS, UHPLC- HRMS, NMR
10.45–11.00	Coffee break, discussions (on-line)	

Second session; Chair: Dr. Ingus Pērkons		
11.00–11.20	<i>Greta Inkrataite, Ramunas Skaudzius, Stasys Tautkus, Aleksej Zarkov, <u>Aivaras Kareiva</u></i>	STUDY OF SUBSTITUTION EFFECTS IN THE YTTRIUM ALUMINIUM GARNET SYNTHESIZED BY ENVIRONMENTALLY BENIGN SOL-GEL SYNTHESIS METHOD (Invited Speaker)
11.20–11.35	<u>Zhanymgul Koishybayeva</u> , <i>Abdirash Akilbekov, Abay Ussenov, Anatoli I. Popov, A. Platonenko</i>	DFT STUDY OF GALLIUM OXIDE BULK PROPERTIES
11.35–11.50	<u>Yusuf Dilgin</u> , <i>Selen Ayaz, Gamze Emir, Serkan Karakaya, Didem Giray Dilgin</i>	ELECTROCHEMICAL SENSORS FOR DETERMINATION OF ENVIRONMENTALLY IMPORTANT COMPOUNDS USING DISPOSABLE PENCIL GRAPHITE ELECTRODES
11.50–12.05	<u>Artis Robalds</u>	RECOVERY OF MICROELEMENTS FROM POTATO JUICE BY BIOSORBENTS
12.05–12.20	<u>I. Reinholds</u> , <i>U. Eismonts, K. Saleniece, M. Bertins, A. Viksna, G. Kizane, O. Muter, A. Podjava, A. T. Boginska, S. Gaidukovs, A. Grinbergs</i>	EFFECTIVE REMOVAL OF RADIOACTIVE CESIUM FROM CONTAMINATED WATER ENVIRONMENTS BY IN SITU SYNTHESIZED IRON HEXACYANOFERRATE IMOBILIZED ON CELLULOSE ACETATE ESTERS
12.20–13.20	Launch break, discussions online	
Third session; Chair: Prof. Vadims Bartkevičs		
13.20–13.40	<u>Juris Burlakovs</u> , <i>Ruta Ozola-Davidane, Maris Klavins</i>	INNOVATIVE COMPOSITE SORBENTS FOR ORGANIC AND INORGANIC POLLUTANTS REMOVAL FROM AQUEOUS SOLUTIONS IN LANDFILL LEACHATES (Invited Speaker)
13.40–13.55	<u>Daniela Godina</u> , <i>Kristine Meile, Aivars Zhurinsh, Arturs Viksna</i>	BIO-CHAR CATALYST APPLICATION FOR GLUCOSIDE HYDROLYSIS REACTION
13.55–14.10	<u>Matiss Pals</u> , <i>Maris Lauberts, Alexandr Arshanitsa, Arturs Viksna</i>	THE OPTIMISATION OF ORGANOSOLV PROCESS OF BARK DELIGNIFICATION PROCESS WITH FOCUS ON PURIFICATION OF ISOLATED LIGNIN FRACTION
14.10–14.25	<u>Hans Orru</u> , <i>Triin Veber, Katrin Lang, Inge Ringmets, Tanel Tamm, Marek Maasikmets, Leena Albrecht, Märten Lukk</i>	EXPOSURE TO AIR POLLUTION IN THE OIL SHALE REGION IN ESTONIA AND RELATED BIRTH EFFECTS

14.25–14.40	<u>Modestas Ružauskas</u> , Elena Bartkienė, Jurga Bernatoniene, Daiva Žadeikė, Arūnas Stankevičius, Vita Lėlė, Vytautė Starkutė, Paulina Zavistanavičiūtė, Juozas Grigas, Eglė Zokaitytė, Arnoldas Pautienius, Gražina Juodeikienė, Valdas Jakštas	INFLUENCE OF MULTICOMPONENT NUTRACEUTICAL ON GUT MICROBIOTA IN EXPERIMENTAL ANIMALS
14.40–14.55	<u>Inese Martisone</u> , Kristine Sproge, Lasma Akulova, Zanna Martinsone, Linda Matisane	HUMAN BIOMONITORING INITIATIVE – FUTURE FOR HUMAN EXPOSURE ASSESSMENT TO CHEMICALS
14.55–15.10	Coffee break, discussions (on-line)	
15.10–17.10	Chair: Lauma Buša POSTER SESSION 1	
15.10–15.15	<u>Linda Ansonė-Bertina</u> , Maris Klavins, Viesturs Ozols, Lauris Arbidans	METAL ORGANIC FRAMEWORK COMPOSITES FOR CARBON DIOXIDE CAPTURE
15.15–15.20	<u>Vytautas Kavaliauskas</u> , Vilma Olšauskaitė, Audrius Padarauskas	HYDROPHOBIC EUTECTIC SOLVENT FOR LIQUID-PHASE MICROEXTRACTION OF PARABENS FROM WATER SAMPLES
15.20–15.25	<u>Luīze Terēze Medne</u> , Jānis Ģībietis	DETERMINATION OF PHOSPHATES IN SOIL BY RAPID TEST METHOD
15.25–15.30	<u>Martina Navrátilová</u> , Andrea Sochová, Daniela Vráblová, Lenka Skálová	MONITORING OF ALBENDAZOLE TRANSFER FROM SHEEP DUNG TO FODDER PLANTS AND ADJACENT SOIL BY UHPLC-MS
15.30–15.35	<u>Ingrīda Radveikienė</u> , Gintautas Bagdžiūnas	INSIGHTS INTO AN ELECTROCHEMISTRY OF NEUROTRANSMITTERS USING THE CYCLODEXTRINS MODIFIED ELECTRODES
15.35–15.40	<u>Eleonora Rieksta</u> , Jānis Ģībietis	DETERMINATION OF FORMALDEHYDE BY THE "GREEN" RAPID TEST METHOD
15.40–15.45	<u>D. Riekstina</u> , A. Egleskalns, G. Kizane, O. Skrypnik, T. Krasta	NATURAL RADIOACTIVITY LEVELS IN GRANITE
15.45–15.50	<u>Ilga Lauma Leimane</u> , Jānis Ģībietis	DETERMINATION OF NON-FERROUS METALS IN SOIL SAMPLES USING TEST STRIP METHOD
15.50–15.55	<u>Valda Valkovska</u> , Liāna Orola	ECO-FRIENDLY DYEING OF WOOLLEN YARN USING LATVIAN TRADITIONAL DYE PLANTS
15.55–16.00	<u>Aija Trimdale-Deksne</u> , Agris Bērziņš	A MULTI-TECHNIQUE APPROACH TO UNDERSTAND THE DIHYDROXYBENZOIC ACID DIFFERENT PROPENSITIES TO FORM SOLID PHASES

16.00–16.05	<u>Aina Semjonova</u> , Agris Bērziņš	CRYSTALLIZATION AND STABILIZATION OF 2,6-DIMETHOXYPHENYLBORONIC ACID METASTABLE POLYMORPH USING SURFACTANTS
16.05–16.10	<u>Henrieta Markevičiūtē</u> , Nijolė Dukštienė, Valentina Krylova	THE STRUCTURAL, MORPHOLOGICAL AND OPTICAL PROPERTIES OF PA6/Ag-Cd-Se LIGHT-ABSORBING MATERIALS
16.10–16.15	<u>Aneka Klavina</u> , Ilona Pavlovska, Agris Auce, Laura Komarovska, Linda Paegle, Linda Dobkevica, Inese Martisone, Ivars Vanadzins	EVALUATION OF SAPROPEL SEDIMENTS FOR MEDICAL PURPOSES
16.15–16.20	<u>Edita Sodaitienė</u> , Audronė Gefenienė, Sigitas Jankauskas, Rimantas Ramanauskas, Romas Ragauskas	COMPARATIVE STUDY OF DIFFERENT ADSORBENTS FOR ANODIZED ALUMINUM DYE REMOVAL
16.20–16.25	Evaldas Simanavičius, <u>Kristina Jančaitienė</u> , Rasa Šlinkšienė	DEVELOPMENT OF HYDROPONICS SYSTEMS WITH BIOACTIVE SUBSTANCES
16.25–16.30	Austėja Mikolaitienė, <u>Rasa Šlinkšienė</u>	EFFECT OF STARCH ADDITIVE ON THE PROPERTIES AND SOLUBILITY OF UREA GRANULES
16.30–16.35	<u>A. Zuševica</u> , E. Muižnieks, S. Žigare, S. Celma, T. A. Štāls, K. Dūmiņš, S. Rancāne, D. Lazdiņa	HEAVY METAL ACCUMULATION CAPACITY OF VARIOUS LOCAL HERBACEOUS SPECIES COMMUNITIES CULTIVATED IN MUNICIPAL BIOWASTE SUBSTRATE WITH CONSTRUCTION DEBRIS ADMIX
16.35–16.40	<u>Zane Kļaviņa</u> , Arta Bārdule, Ivars Kļaviņš, Zane Libiete	VARIATION IN METHYLMERCURY CONCENTRATIONS IN ENVIRONMENTAL SAMPLES IN FOREST LAND AND WETLANDS WITH ORGANIC SOILS IN LATVIA
16.40–16.45	<u>Ramunas Diliautas</u> , Aldona Beganskiene, Dovydas Karoblis, Dalis Baltrunas, Kestutis Mazeika, Aleksej Zarkov, Aivaras Kareiva	STRUCTURAL, MORPHOLOGICAL AND MAGNETIC INVESTIGATION OF Bi _{1-x} Gd _x Fe _{0.85} Mn _{0.15} O ₃ SOLID-SOLUTIONS
16.45–16.50	<u>Vadlens Grebņevs</u> , Roman Viter, Şahin Altundal, Kārlis Grundšteins, Agnieszka Stolarczyk, Arturs Viksna, Wojciech Simka	SOLUTIONS ON THE WAY TO PREPARATION OF CARBONATED TITANIUM IMPLANT COATINGS VIA PLASMA ELECTROLYTIC OXIDATION IN SUSPENSIONS
16.50–16.55	<u>Andrzej Gawor</u> , Andrii Tupys, Anna Ruszczyńska, Ewa Bulska	APPLICATION OF HR-CS GF MAS FOR FLUORINE DETERMINATION IN BIOLOGICAL SAMPLES

16.55–17.00	<u>Līga Avotina</u> , Arturs Zarins, Mihaīls Halitovs, Larisa Baumane, Aleksandrs Petjukevics, Gunta Kizane	THERMAL DECOMPOSITION AND SPECTROMETRIC ANALYSIS OF IRRADIATED KERATINOUS FIBERS
17.00–17.05	<u>Estefanija Novicka</u> , Iveta Pugajeva, Ingars Reinholds, Vadims Bartkevics	TWO-DIMENSIONAL LIQUID CHROMATOGRAPHY – HIGH RESOLUTION MASS SPECTROMETRY METHOD FOR SIMULTANEOUS MONITORING OF 70 REGULATED AND EMERGING MYCOTOXINS
17.05–17.10	<u>Aiga Anna Pudule</u> , Laura Komarovska, Arturs Vīksna, Dārta Ūbele, Kārlis Agris Gross	NANOSTRUCTURING AMORPHOUS CALCIUM PHOSPHATE: CARBONATE INCLUSION
17.10–	Discussions on-line	

22.10.2021

8.45–09.00	Joining the EcoBalt conference ZOOM platform	
Fourth session; Chair: Prof. Arturs Vīksna		
09.00–09.20	<u>Markéta Holá</u> , Vojtěch Wertich, Jan Dobeš, Martin Kubeš, Juraj Mozola, Jaromír Leichmann, Viktor Kanický	LA-ICP-MS IMAGING WITH FOCUS ON GEOLOGICAL MATERIALS (Invited Speaker)
09.20–09.40	Salih CAN SÜNER, Halime ÇEVİKBAŞ, Seyhan ULUSOY, Gülğün TINAZ, <u>Ayhan ORAL</u>	PREPARATION OF WOUND HEALING NANOFIBER MATERIAL THAT CONTAINING CINNAMALDEHYDE (Invited Speaker)
09.40–09.55	<u>Merve Danisman</u> , Ayhan Oral	SURFACE MODIFICATION OF GRAPHENE OXIDE BY ENZYME CATALYZED REACTION
09.55–10.15	<u>Ingus Pērkons</u> , Laura Elīna Ikkere, Veronika Šukajeva, Iveta Pugajeva	FINGERPRINTING HUMAN PHARMACEUTICALS, ILLICIT DRUGS AND NEW PSYCHOACTIVE SUBSTANCES IN WASTEWATER: A MULTI-METHOD APPROACH
10.15–10.25	Coffee break, discussions (on-line)	
Fifth session; Chair: Assoc. prof. Agris Bērziņš		
10.25–10.40	Jakub Karasiński, <u>Andrii Tupys</u> , Ludwik Halicz, Ewa Bulska	A NEW METHOD FOR MEASURING GERMANIUM ISOTOPE RATIOS IN MINERALS AND WATER SAMPLES USING MC-ICP-MS AFTER THE FORMATION OF VOLATILE HYDRIDES

10.40–11.00	<u>Arunas Ramanavicius</u> , <i>Eivydas Andriukonis, Raimonda Celiesiute-Germaniene, Simonas Ramanavicius, Aura Kisieliute, Monika Vilkiene, Urte Samukaite-Bubniene</i>	DEVELOPMENT OF MICROBIAL FUEL CELLS (Invited Speaker)
11.00–11.15	<u>Žanna Martinsons</u> , <i>Lāsma Akūlova, Aneka Kļaviņa, Linda Paegle, Inese Mārtiņšone, Darja Kaļūznaja, Marija Avota, Ivars Vanadziņš</i>	EXPLORING CAUSES, EFFECTS AND POSSIBLE SOLUTIONS FOR CHEMICAL POLLUTION IN THE ENVIRONMENT: CITIZENS' AND EXPERTS' OPINION
11.15–11.30	<u>Lāsma Akūlova</u> , <i>Inese Mārtiņšone, Žanna Martinsons, Laura Komarovska, Anita Seile, Svetlana Lakiša, Ivars Vanadziņš</i>	HBM4EU – HUMAN BIOMONITORING INITIATIVE IN LATVIA: STUDY ON PESTICIDE MIXTURES IN ADULT AND CHILDREN POPULATION
11.30–11.45	<u>Zanda Brike</u> , <i>Rita Veilande, Maris Strazds, Kristiana Rancane, Anda Abola, Atis</i>	MERCURY CONCENTRATION IN THE FAECES OF BLACK STORKS
11.45–12.00	<u>Vitālijs Lazarenko</u> , <i>Yelyzaveta Rublova, Raimonds Meija, Jana Andžāne, Vanda Voikiva, Arturs Viksna, Donāts Erts</i>	APPLICATION OF INNOVATIVE Bi ₂ Se ₃ THIN FILMS AS ANODES IN AQUEOUS RECHARGEABLE LITHIUM-ION BATTERIES
12.00–12.40	Launch break, discussions (on-line)	
Sixth session; Chair. Prof. Māris Kļaviņš		
12.40 – 13.00	<u>Ivo Leito</u> , <i>Asko Laaniste, Koit Herodes</i>	ONLINE COURSE AND SOFTWARE FOR LC-MS METHOD VALIDATION (Invited Speaker)
13.00-13.15	<u>Laura Elina Ikkere</u> , <i>Iveta Pugajeva, Veronika Šukajeva, Ingus Pērcons</i>	WASTEWATER-BASED EPIDEMIOLOGY AS A TOOL FOR PUBLIC HEALTH AND LIFESTYLE ASSESSMENT
13.15–13.30	<u>Zane Berzina</u> , <i>Romans Pavlenko, Laura Elina Ikkere, Vadims Bartkevics</i>	APPLICATION OF WASTEWATER – BASED EPIDEMIOLOGY FOR TRACKING HUMAN EXPOSURE TO DEOXYNIVALENOL AND ENNIATINS
13:30–13.45	<u>Maris Bertins</u> , <i>Agnese Brangule, Vitalijs Lazarenko, Agnese Osite, Arturs Viksna</i>	POSSIBILITIES FOR INTERFERENCE REDUCTION IN ICP-MS/MS SYSTEM USING He COLLISION CELL
13.45–14.00	<u>Signija Zake</u> , <i>Maris Bertins, Dagnija Lazdina, Karlis Dumins, Arturs Viksna</i>	APPLICATION OF NITROGEN AND CARBON STABLE ISOTOPE RATIO MASS SPECTROMETRY FOR NITROGEN CIRCULATION STUDIES DURING CONIFER PLANTING

14.00–14.15	<u>Kristaps Oskalns</u> , Maris Bertins, Edgars Selickis, Arturs Viksna	APPLICATION OF MULTIFACTOR ANALYSIS FOR DRINKING WATER QUALITY CONTROL IN RIGA CITY
14.15–14.30	<u>Kristaps Saršūns</u> , Kaspars Leduskrasts, Agris Bērziņš, Toms Rekis	MODULATION OF LUMINESCENCE SPECTRA VIA SOLID SOLUTION FORMATION OF THIOXANTHONE DERIVATIVES
14.30–14.45	Coffee break, discussions (on-line)	
14.45–16.25	Chair: Kristaps Saršūns POSTER SESSION 2	
14.45–14.50	<u>Maris Klavins</u> , Marcis Mezulis, Linards Klavins, Viktor Stabnikov, Andrii Marynin, Olena Stabnikova	INTERACTION BETWEEN MICROPLASTICS AND CHEMICAL POLLUTANTS
14.50–14.55	<u>Vida Vičkačkaitė</u> , Marija Lukoševičiūtė	HEADSPACE-GAS CHROMATOGRAPHIC DETERMINATION OF β -CARYOPHYLLENE IN EPILOBIUM ANGUSTIFOLIUM EXTRACTS
14.55–15.00	<u>Grzegorz Wryk</u> , Agnieszka Borowiec, Iwona Gąsiorowska, Katarzyna Stopka, Beata Kondraszuk, Andrzej Gawor, Eliza Kurek, Ewa Bulska	AN IMPROVEMENT OF THE ANALYTICAL PROTOCOL OF GLYPHOSATE QUANTIFICATION IN FOOD SAFETY AREA
15.00–15.05	<u>Pille-Riin Laanet</u> , Piret Saar-Reismaa, Merike Vaher	ANALYSIS OF SYNTHETIC AND PHYTOCANNABINOIDS USING MICELLAR ELECTROKINETIC CHROMATOGRAPHY
15.05–15.10	<u>Dovilė Ragauskaitė</u> , Rasa Šlinkšienė	COFFEE GROUNDS IMPACT ON A RYE GROWTH
15.10–15.15	<u>Agne Kizalaite</u> , Tomas Murauskas, Aleksej Zarkov	INSIGHT INTO THE FORMATION OF ZINC WHITLOCKITE: SYNTHESIS, STRUCTURE AND CHARACTERISATION
15.15–15.20	<u>Dovydas Karoblis</u> , Aleksej Zarkov, Aldona Beganskiene, Aivaras Kareiva	PREPARATION OF RUDDLESDEN-POPPER CALCIUM MANGANITES APPLYING MOLTEN SALT SYNTHESIS
15.20–15.25	<u>Greta Inkrataitė</u> , Ramūnas Skaudžius	INFLUENCE OF BORON AND MAGNESIUM IONS ON YAG:Ce AND LuAG:Ce CERAMICS
15.25–15.30	Goda Gudinskaitė, <u>Rasa Paleckienė</u> , Rasa Šlinkšienė	COMPATIBILITY OF LIQUID FERTILIZERS AND HUMIC SUBSTANCES
15.30–15.35	<u>Diana Griesiute</u> , Aivaras Kareiva, Aleksej Zarkov	SYNTHESIS OF β -Ca ₂ P ₂ O ₇ AS AN ADSORBENT FOR THE REMOVAL OF HEAVY METALS FROM WATER

15.35–15.40	<u>Odeta Brigaitytė</u> , Rasa Šlinkšienė	SUITABILITY OF ECOLOGICAL BUCKWHEAT GROATS WASTE FOR FERTILIZER PRODUCTION
15.40–15.45	<u>Daria Pashneva</u> , Ieva Uogintė, Julija Pauraitė, Agnė Minderytė, Kristina Plauškaitė, Valda Araminienė, Eugenija Farida Dzenajavičienė, Valda Gudynaitė-Franckevičienė, Iveta Varnagirytė-Kabašinskienė, Nerijus Pedišius, Egidijus Lemanas, Tomas Vonžodas, Steigvilė Byčenkienė	BLACK CARBON DEPOSITION ON TREE FOLIAGE AN URBAN BACKGROUND IN VILNIUS
15.45–15.50	Kęstutis Čeplinskas, <u>Andrius Jaskūnas</u>	PREPARATION OF MIXED OXIDE CATALYSTS FOR VOLATILE ORGANIC COMPOUND ABATEMENT
15.50–15.55	<u>Megija Neimane</u> , Vitālijs Lazarenko, Māris Bērtiņš, Arturs Viksna, Dagnija Lazdiņa, Kristaps Makovskis, Ilze Kārklīņa, Andis Lazdiņš	VARIATIONS OF MICRO- AND RARE EARTH ELEMENTS IN THE BOTTOM AND FLY WOOD ASH
15.55–16.00	<u>Armands Egleskalns</u> , Ingars Reinholds, Konstantins Bavrins, Gunta Kizane	ASSESSMENT OF RADIONUCLIDES IN FORMER SALASPILS NUCLEAR REACTOR COOLING WATER
16.00-16.05	<u>Romans Pavlenko</u> , Zane Bērziņa, Mārtiņš Jansons, Vadims Bartkevičs	ANALYSIS OF WASTEWATER SAMPLES FOR DETERMINATION OF MYCOTOXINS
16.05–16.10	<u>Sergejs Osipovs</u> , Aleksandrs Pučkīns	DEVELOPMENT OF A METHOD FOR THE TAR ANALYSIS IN CO-PRODUCED GAS
16.10–16.15	<u>Aleksandrs Pučkīns</u> , Sergejs Osipovs	ANALYSIS OF POLLUTANTS IN INDUSTRIAL WATER USED FOR COOLING OF CO-PRODUCED GASES
16.15–16.20	<u>L. Zorza</u> , M. Bertins, K. Saleniece, A. Viksna, A. Grinbergs, O. Muter	ACCUMULATION OF CESIUM-133 IN AQUATIC PLANTS AND ITS EFFECT ON THE PHYSIOLOGICAL ACTIVITY OF PLANTS AND AQUATIC MICROORGANISMS
16.20– 16.25	<u>Viktor Stabnikov</u> , Andrii Marynin, Olena Stabnikova, Maris Klavins	THE MICROBIALLY-COATED MICROPLASTICS IN NEUSTONIC WATER-AIR INTERPHASE
16.25	Discussions on-line, conference closing	

23.10.2021

For on-line videos please visit the conference web page	<u>EcoBalt2021</u>
---	---

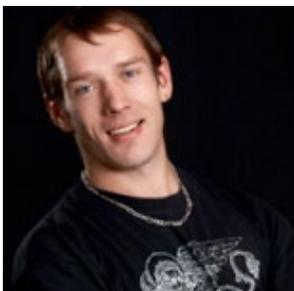
EcoBalt 2021 SPONSORS



INVITED SPEAKERS

Dr. Juris Burlakovs

University of Latvia (Latvia)



Dr. Markéta Holá

Masaryk University, Brno (Czech Republic)



Prof. Habil. Dr. Aivaras Kareiva

Vilnius University (Lithuania)



Prof. Dr. Ivo Leito

Tartu University (Estonia)



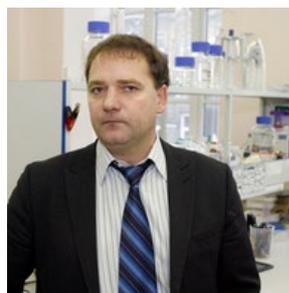
Prof. Dr. Ayhan Oral

Çanakkale Onsekiz Mart University (Turkey)



Prof. Habil. Dr. Arūnas Ramanavičius

Vilnius University (Lithuania)



Prof. Dr. phys. Maja Remškar

Jožef Stefan Institute (Slovenia)



Dr. Irina Shtangeeva

St. Petersburg State University (Russia)



INNOVATIVE COMPOSITE SORBENTS FOR ORGANIC AND INORGANIC POLLUTANTS REMOVAL FROM AQUEOUS SOLUTIONS IN LANDFILL LEACHATES

Juris Burlakovs¹, Ruta Ozola-Davidane¹, Maris Klavins¹

¹ Department of Environmental Science, University of Latvia, Riga, Latvia

The study reveals the development of appropriate innovative sorbents based on clay material for arsenic and *p*-nitrophenol sorption using iron oxy-hydroxide and surfactant modification. Natural and manufactured clay were chosen for comparison of modification efficiency to obtain the best sorption results for As (V) and *p*-nitrophenol. Obtained results indicate that modification of clay with iron compounds and various surfactants significantly improve the sorption capacity of newly developed materials used for sorption of inorganic and organic compounds from aqueous solutions in landfill leachates.

Natural clay minerals have received a lot of attention as potential sorbents, because of their abundance, cost-effectiveness, high sorption and ion-exchange properties [1]. Clay minerals can be modified using different approaches to obtain innovative materials for application as sorbents in the removal of inorganic and organic pollutants from leachates, wastewater, groundwater and soil [2, 3]. Modification with surfactants improves hydrophobization needed if interaction with low polarity organic molecules is necessary, but chemical modification with inorganic species, e.g., hydrated iron supports the physical improvement of sorption and ion exchange process in order to benefit the treatment of media from inorganic pollutants [4]. Materials achieved better properties for specific remedial applications regarding heavy metals and metalloids, prepared organoclays from hydrophilic montmorillonite by intercalating cationic or nonionic surfactants can interact with organic molecules of differing polarity and serve as immobilizers for organic molecules and toxicants, e.g., phenols and NOCs. Further studies will reveal improved properties to benefit landfill leachate treatment, wastewater engineering and environmental remediation industries.

Acknowledgement. The research was supported by project No.1.1.1.2/VIAA/3/19/531 "Innovative technologies for stabilization of landfills-diminishing of environmental impact and resources potential in frames of circular economy".

References

1. Zhang, L.; Zhang, B.; Wu, T.; Sun, D.; Li, Y. *Colloids and Surfaces A: Physicochem. Eng. Aspects*. **2015**, 484, 118-129.
2. Lee, S. M.; Tiwari, D. *Applied Clay Science*. **2012**, 59-60, 84-102.
3. Burlakovs, J.; Karklina, A.; Karpovics, A.; Klavins, M. *Material Science and Applied Chemistry*. **2013**, 29, 137-141.
4. Lee, S. M.; Laldawngliana, C.; Tiwari, D. *Chemical Engineering Journal*. **2012**, 195-196, 103-111.

Contact person: Juris Burlakovs, Faculty of Geography and Earth Sciences, University of Latvia, Raina Blvd. 19, LV 1586, Riga, Latvia, phone: +371 28469044, e-mail: juris.burlakovs@lu.lv

LA-ICP-MS IMAGING WITH FOCUS ON GEOLOGICAL MATERIALS

Markéta Holá¹, Vojtěch Wertich², Jan Dobeš¹, Martin Kubeš², Juraj Mozola², Jaromír Leichmann², Viktor Kanický¹

¹ Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

² Department of Geological Sciences, Faculty of Science, Masaryk University, Brno, Czech Republic

Inorganic analysis of geological samples of various origins, compositions and states is the basis for study in the field of geochemistry. The most common is bulk analysis of rocks, minerals or water using a wide range of analytical techniques. Gradually, surface techniques such as backscattered electron imagery (BSE), X-ray micro-analysis or LA-ICP-MS became an integral part of solution bulk analyses. A more detailed method for elemental distribution has become imaging (mapping) of selected areas on the sample, which replaces or complements local spot analysis. Nowadays, the creation of elemental maps of minerals becomes an integral part of the study of their heterogeneity, element mobility, major or trace elemental distribution or dating [1]. Thanks to microscopic scale imaging techniques, it is possible to decipher geological processes and environment evolution of an area represented by analysed samples.

An example of geoinaging is a study focused on uranium ore sample with its utilization in exploration, mining and processing of uranium ore, "fingerprinting" of uranium ore concentrates and also in technologies used in nuclear waste repositories due to similarities in chemical composition between uraninite and spent nuclear fuel [2]. A method of LA-ICP-MS was applied to create images revealing distribution and possible migration of elements and isotopes in samples of uranium ore. Elemental/isotopic imaging can display presence and distribution of selected isotopes causing structural defects and thus can help to better understand the evolution of geological processes, and to identify the structures responsible for uranium migration. The images can also provide essential information for the provenance study of analysed uranium ore samples.

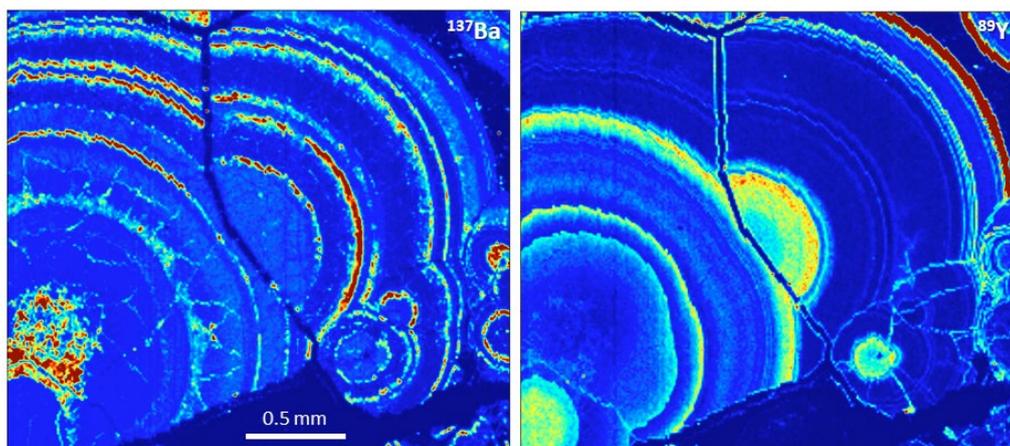


Figure 1. Distribution of Ba and Y in uraninite obtained by LA-ICP-MS. Normalised intensities in cps, blue colour as minimum, red as maximum.

References

1. Chew, D.; Drost, K.; Marsh, J. H.; Petrus, J. A. *Chem. Geol.* **2021**, 559, 119917.
2. Spano, T. L.; Simonetti, A.; Balboni, E.; Dorais, C.; Burns, P. C. *Applied Geochemistry.* **2017**, 84, 277-285.

Contact person: Markéta Holá, Kamenice 5, 625 00 Brno, Czech Republic, phone: +420 54949 4285, e-mail: mhola@sci.muni.cz

STUDY OF SUBSTITUTION EFFECTS IN THE YTTRIUM ALUMINIUM GARNET SYNTHESIZED BY ENVIRONMENTALLY BENIGN SOL-GEL SYNTHESIS METHOD

Greta Inkrataite¹, Ramunas Skaudzius¹, Stasys Tautkus¹, Aleksej Zarkov¹, Aivaras Kareiva¹

¹ Institute of Chemistry, Vilnius University, Vilnius, Lithuania

Over the last few decades, environmentally benign sol-gel synthesis techniques have been used to prepare variety of different mixed-metal oxides. The sol-gel process is used to obviate the experimental difficulties and chemical inhomogeneity associated with conventional ceramic processing. In the ideal situation, the homogeneity in an amorphous gel which, on subsequent pyrolysis, yields the complex oxide directly, providing that segregation and partial crystallization can be prevented.

The compound $3Y_2O_3 \cdot 5Al_2O_3$ is referred to as yttrium aluminium garnet ($Y_3Al_5O_{12}$, YAG) and adopts the cubic garnet structure. When doped with a transition metal or lanthanide ions, YAG represents an important solid-state laser material widely used in luminescence systems, window materials for a variety of lamps and for fibre-optic telecommunication systems [1-4].

In this work the synthesis of polycrystalline Ce^{3+} -doped yttrium aluminium garnet (YAG: Ce^{3+}) substituted with different amounts of Ti^{4+} and Ca^{2+} ions by the sol-gel process is described. YAG powders were characterized by XRD analysis, FTIR spectroscopy and scanning electron microscopy. The luminescent properties of synthesized compounds were investigated as well. White powders were obtained by heating the precursor gels at 180 °C, and then calcinating at 1000 °C for 10 h. The XRD and FTIR results showed that during simultaneous Ti^{4+} and Ca^{2+} co-doping the monophasic $Y_{3-x}Ca_xAl_{5-y}Ti_yO_{12}$ garnet was obtained at certain substitutional level of calcium for yttrium and titanium for aluminium. It was demonstrated that the substitution by aforementioned ions had no or little effect on the morphology of synthesized specimens, as in all cases the crystallites 5-30 μm in size were formed. According to measured emission and excitation spectra we can conclude that the luminescence was seriously quenched in YAG: Ce^{3+},Ca^{2+} and YAG: Ce^{3+},Ca^{2+},Ti^{4+} , but the YAG: Ce^{3+},Ti^{4+} samples showed the characteristic emission of cerium with highest intensity for the $Y_{2.985}Ce_{0.015}Al_{5-y}Ti_yO_{12}$ sample with $y = 0.15$.

Acknowledgement. Authors would like to thank Andrius Pakalniskis for helpful discussions and Romuald Nanevic for technical assistance. This work was supported by a Research grant NEGEMAT (No. S-MIP-19-59) from the Research Council of Lithuania.

References

1. Skaudzius, R.; Zalga, A.; Kareiva, V. *Materials Science (Medžiagotyra)*. **2008**, *14*, 193-197.
2. Pavasaryte, L.; Katelnikovas, A.; Momot, A.; Reekmans, G.; Hardy, A.; Van Bael, M.; Adriaensens, P.; Yang, T. C. K.; Kareiva, A. *J. Lumin.* **2019**, *212*, 14-22.
3. Laurikenas, A.; Sakalauskas, D.; Marsalka, A.; Raudonis, R.; Antuzevics, A.; Balevicius, V.; Zarkov, A.; Kareiva, A. *J. Sol-Gel. Sci. Technol.* **2021**, *97*, 479-487.
4. Pakalniskis, A.; Marsalka, A.; Raudonis, R.; Balevicius, V.; Zarkov, A.; Skaudzius, R.; Kareiva, A. *Optic. Mater.* **2021**, *111*, 110586.

Contact person: Aivaras Kareiva, Institute of Chemistry, Vilnius University, Naugarduko 24, LT-03225 Vilnius, Lithuania, phone: +370 61567428, e-mail: aivaras.kareiva@chgf.vu.lt

ONLINE COURSE AND SOFTWARE FOR LC-MS METHOD VALIDATION

Ivo Leito¹, Asko Laaniste¹, Koit Herodes¹

¹ University of Tartu, Institute of Chemistry, Ravila 14a, 50411 Tartu, Estonia

This presentation is about an education-related activity in process here at UT: web-based course “*LC-MS Method Validation*” (https://sisu.ut.ee/lcms_method_validation/) and a software tool – *ValChrom* – linked with it.

LC-MS Method Validation is a practice-oriented on-line course on validation of analytical methods, specifically using LC-MS as technique. The course introduces the main concepts and mathematical apparatus of validation, covers the most important method performance parameters and ways of estimating them. The course is largely based on two-part tutorial review on validation of liquid chromatography–mass spectrometry methods [1, 2]. The course contains lectures, practical exercises and numerous tests for self-testing. In spite of being introductory, this course intends to offer sufficient knowledge and skills for carrying out validation for the most common LC-MS analyses in routine laboratory environment. The real-life analysis situations for which there are either examples or self-tests, are for example pesticide analyses in fruits and vegetables, perfluoroalkyl acids in water, antibiotics in blood serum, glyphosate and AMPA in surface water.

ValChrom is a software tool, which on one hand teaches how validation (first of all for chromatographic methods) should be done and on the other hand helps professionals with experiment planning and calculations of performance parameters in order to reduce the time and effort involved. *ValChrom* enables validation according to specific Guideline documents, e.g., Eurachem, EMA, ICH, . . . and combination of requirements from different guidelines. It „walks the user through validation“ of his/her specific method and automatically creates the experiment plan on the basis of information about method parameters and requirements entered by the user. The user will have a good overview of all the performance parameters and possibility to generate detailed reports. It is accessible from anywhere and is free of charge. At this stage, *ValChrom* is still a work in progress, but sufficient amount of functionality is already available, so that it can already be used as a tool for teaching and also offers great help for actual validation experiments.

References

1. Kipper, K.; Oldekop, M. L.; Evard, H.; Herodes, K.; Ravio, P.; Leito, I. Tutorial review on validation of liquid chromatography–mass spectrometry methods: Part I. *A. Anal. Chim. Acta.* **2015**, *870*, 29-44.
2. Kipper, K.; Oldekop, M. L.; Evard, H.; Herodes, K.; Ravio, P.; Leito, I. Tutorial review on validation of liquid chromatography–mass spectrometry methods: Part II. *A. Anal. Chim. Acta.* **2015**, *870*, 8-28.

Contact person: Ivo Leito; e-mail: ivo.leito@ut.ee

PREPARATION OF WOUND HEALING NANOFIBER MATERIAL THAT CONTAINING CINNAMALDEHYDE

Salih Can Süner¹, Halime Çevikbaş², Seyhan Ulusoy², Gülgün Tinaz³, Ayhan Oral⁴

¹ Department of Chemistry and Chemical Processing, Lapseki Vocational School, Canakkale Onsekiz Mart University, 17800, Canakkale, Turkey

² Department of Biology, Suleyman Demirel University, 32260 Isparta, Turkey

³ Department of Basic Pharmacy Sciences, Faculty of Pharmacy, Marmara University, Istanbul, Turkey

⁴ Department of Chemistry, Faculty of Art and Science, Canakkale Onsekiz Mart University, 17020 Çanakkale, Turkey

Cinnamaldehyde is derived from cinnamon bark. Cinnamaldehyde (CA) is widely used in food, pharmaceutical, biomedical, and cosmetics industries thanks to its excellent antibacterial effects, and strong antioxidant properties. Poly (Lactic acid)-gelatin hybrid nanofiber was used as a carrier for CA because polymer nanofiber is biocompatible, has a high specific surface area, and high porosity, which can enhance the affect of CA onto the surface. The insertion of gelatin into the Poly (lactic acid) matrix has changed the solubility of the matrix. The optimization of nanofiber preparation was performed and the nanofiber matrix was prepared by using electrospinning. The nanofiber matrices were characterized by using Scanning Electron Microscopy. The nanofibers were evaluated for their antibacterial and anti-biofilm activity against *P. aeruginosa* using crystal violet assay. The results demonstrated that nanofibers can effectively inhibit 72.2% of *P. aeruginosa* biofilm formation. The nanofibers exhibited remarkable antibacterial properties against *Staphylococcus aureus* and *Pseudomonas aeruginosa*.

Thus, our study showed that CA-loaded nanofibers may have applications as wound dressing materials and for use in other biomedical applications.

Contact person: Salih Can Süner, e-mail: salihcansuner@comu.edu.tr

DEVELOPMENT OF MICROBIAL FUEL CELLS

Arunas Ramanavicius^{1,2}, Eivydas Andriukonis^{1,2}, Raimonda Celiesiute-Germaniene², Simonas Ramanavicius^{1,2}, Aura Kisieliute², Monika Vilkiene³, Ieva Mockeviciene³, Aurimas Lisauskas⁴, Ieva Kiminaitė⁴, Urte Samukaite-Bubniene^{1,2}

¹ Department of Physical Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko st. 24, LT-03225, Vilnius, Lithuania

² Laboratory of Nanotechnology, State Research Institute Center for Physical Sciences and Technology, Sauletekio ave 3, LT-10257 Vilnius, Lithuania

³ Lithuanian Research Centre for Agriculture and Forestry, Instituto al. 1, Kėdainių r. sav. Lithuania

⁴ Lithuanian energy institute, Laboratory of combustion processes, Breslaujos st. 3, LT-44403 Kaunas, Lithuania

This presentation focuses on the development of microbial biofuel cells and shows the way how very similar principles, which are applied for the design of biosensors and some other bioelectronics-based devices can be applied for the design of biofuel cells [1]. Some attention will be paid to charge transfer aspects in biofuel cells [1]. The most of microorganism-based amperometric biosensors shows poor specificity, but this drawback can be well exploited in the design of microbial biofuel cells because this enables to consume wider range of chemical fuels [2]. The efficiency of the charge transfer is among the most challenging and critical issues during the development of any kind of biofuel cells [3]. In the most cases particular redox mediators and nanomaterials are applied for the facilitation of charge transfer from applied biomaterials towards biofuel cell electrodes [4]. Some improvements in charge transfer efficiency can be achieved by the application of conducting polymers (CPs), which can be used for the immobilization of enzymes and in some particular cases even for the facilitation of charge transfer [2,4,5]. In this presentation charge transfer pathways and mechanisms, which are suitable for the design of biosensors and in biofuel cells are discussed. The ways for the modification of cell-wall/membrane by conducting polymers in order to enhance charge transfer efficiency of microorganisms, which can be potentially applied in the design of microbial biofuel cells, are outlined [3-5]. The biocompatibility-related aspects of conducting polymers with microorganisms are overviewed.

References

1. Andriukonis, E.; Celiesiute-Germaniene, R.; Ramanavicius, S.; Viter, R.; Ramanavicius, A. From Microorganism-based Amperometric Biosensors towards Microbial Fuel Cells. *Sensors*. **2021**, *21*, 2442.
2. Rozene, J.; Morkvenaite-Vilkonciene, I.; Bruzaite, I.; Dzedzickis, A.; Ramanavicius, A. Yeast-based microbial biofuel cell mediated by 9,10-phenanthrenequinone. *Electrochimica Acta*. **2021**, *373*, 137918.
3. Ramanavicius, S.; Ramanavicius, A. Conducting Polymers in the Design of Biosensors and Biofuel Cells. *Polymers*. **2021**, *13*, 49.
4. Ramanavicius, S.; Ramanavicius, A. Charge transfer and biocompatibility aspects in conducting polymers based enzymatic biosensors and biofuel cells. *Nanomaterials*. **2021**, *11*, 371.
5. Bruzaite, I.; Rozene, J.; Morkvenaite-Vilkonciene, I.; Ramanavicius, A. Towards Microorganism-based Biofuel Cells: The Viability of *Saccharomyces cerevisiae* Modified by Multiwalled Carbon Nanotubes. *Nanomaterials*. **2020**, *10*, 954.

AIR POLLUTION BY NANOPARTICLES CAUSED BY USE OF PYROTECHNICS

Maja Remškar^{1,2}, Luka Pirker^{1,2}, Bojana Višić^{1,3}, Anton Gradišek¹, Agnese Osīte⁴

¹ Solid State Physics Department, Jožef Stefan Institute, Ljubljana, Slovenia

² Faculty of Mathematics and Physics, University in Ljubljana, Slovenia

³ Center for Solid State Physics and New Materials, Institute of Physics Belgrade, Belgrade, Serbia

⁴ Department of Analytical Chemistry, University of Latvia, Riga, Latvia

Fireworks and other pyrotechnic devices with light effects and spectacular explosions are often used to celebrate different events due to their aesthetic and entertainment value. Effects connected to the smoke and noise are undesired side effects usually neglected by pyrotechnics enthusiasts. While dog owners attempt to protect their pets from such celebrations, and bird watchers to get prohibition of fireworks, members of the general population bring their children to enjoy the light spectacle. Unfortunately, they do not consider the local atmosphere pollution arising from the toxic combustion by-products. In addition, explosions portrayed in cartoons, together with the fireworks and sparklers as advertised in the media, influence the celebration habits, from birthday parties, wedding ceremonies to other festivities. As an example, sport events frequently start or finish with fireworks, while pyrotechnic articles are still occasionally used by fans during games although their use is formally forbidden.

We will present results from measurements of air pollution by aerosols during New Year fireworks in Ljubljana, during a football match at the local stadium between two national rivals and of indoor air pollution by particles during combustion of sparklers. The measurements have been performed using a scanning mobility particle sizer and a low-pressure cascade impactor. The collected particles were chemically analysed by X-ray energy dispersive analysis, scanning electron microscopy, and mass spectrometry. It was found that all three types of pyrotechnics caused a strong increase in the number concentration of aerosols but with a different outreach, from several km in the case of New Year firework to several metres during the combustion of sparklers. The concentrations of nanoparticles between 80 nm and 150 nm in size measured at 2.8 km from the firework platform during New Year in Ljubljana clearly increased shortly after the firework. Public data have shown an increase in concentrations of heavy metals typical for pyrotechnics (Cu, Sr, Ba) in PM₁₀ even several days after the firework event. Beside carbon, the chemical analysis of the collected aerosols revealed the presence of typical elements used in pyrotechnic devices, like Mg, Al, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Rb, Sr, Sn, Ba, and Pb. The indoor combustion of a single sparkler has increased the total concentration of the aerosols for at least 150 times with respect to the background level. More than 10 % of the metals (Ba, Fe, Al) from the sparklers have been released into the local atmosphere in form of aerosols with the diameter of 100 nm or smaller [1]. Use of pyrotechnic articles and torches at a football match caused an increase in the number concentration of aerosols up to 12-fold. The estimated cumulative dose of the inhaled particles by the players during the match was about 300% higher than the dose one would get in a low-pollution environment [2].

References:

1. Remškar, M.; Tavčar, G.; Škapin, S. D. *Air Qual Atmos Health*. **2015**, *8*, 205-211.
2. Pirker, L.; Gradišek, A.; Višić, B.; Remškar, M. *Atmos. Environ.* **2020**, *233*, 117567-10.

Contact person: Maja Remškar, Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia, phone: +386 1 4773961, e-mail: maja.remškar@ijs.si

INFLUENCE OF RUBIDIUM ON ACCUMULATION OF MACRO- AND TRACE ELEMENTS IN TWO PLANT SPECIES AND IN THE RHIZOSPHERE SOIL

Irina Shtangeeva¹, Maris Bērtiņš², Arturs Viksna²

¹ Institute of Earth Sciences, St. Petersburg University, St. Petersburg, Russia

² Department of Analytical Chemistry, University of Latvia, Riga, Latvia

Introduction. Environmental pollution is a serious problem all around the world. Over the past decades, several well-known heavy metals have received much attention of researchers, and new information has been collected on their toxicity. However, knowledge of the biogeochemistry of many other potentially toxic trace elements is scarce, though an increase of concentration of any element in soil can lead to negative consequences for plants. Among other poorly-studied trace elements is rubidium (Rb). Information about environmental chemistry of Rb, a chemical analogue of K, an essential plant nutrient, is still scarce. The aim of the research was to assess the impact of root exudates of two widely distributed plant species that belong to different botanical taxa: couch grass (monocot) and dandelion (dicot) on the concentrations of macro- and trace elements in the plants and in rhizosphere soil of the plants when the plants grow separately and close to each other in non-contaminated soil and in the soil spiked with RbCl.

Methods. A field trial was performed in a park in St. Petersburg, Russia. For the experiment we used two plots located close to each other. One of the plots served as a control (soil at the plot was spiked with ordinary water), soil at another plot was spiked with RbCl. The plants and rhizosphere soil were collected three times during a day. The concentrations of C and N in the soil samples were determined by Vario Micro Cube (Elementar). For determination of concentrations of Al, As, Ba, Ca, Cd, Ce, Co, Cr, Cu, Fe, Ga, K, La, Mg, Mn, Na, Ni, P, Pb, Rb, Sc, Se, Sr, V and Zn was used Agilent 8900 ICP-QQQ Inductively Coupled Plasma Mass Spectrometer with Micromist nebuliser.

Results and Discussion. During daytime, total amount of C and N in the rhizosphere soil of couch grass and dandelion was found to be constantly decreasing. Similar variations were also found for Mg, Al, V, Ga, and As. The concentrations of some other elements (Na, Se, La, and Ce) showed a maximum value in the middle of day. These variations might be due to changes in the soil temperature. Contamination of soil by RbCl negatively affected the concentrations of several elements in the rhizosphere soil of couch grass and dandelion. The impact was more marked when the plants grow far from each other. Both plants were capable of accumulating large amounts of Rb. The bioaccumulation of Rb resulted in statistically significant variations in the concentrations of several elements in roots and leaves of the plants. The element concentrations in both plants also varied in the course of the day. The variations were different for couch grass and dandelion and were not the same for the plants growing separately and close to each other. Although couch grass and dandelion were grown in the same site and collected simultaneously, the concentrations of many elements in the plants differed significantly. More differences were found between concentrations of elements in leaves of the two plant species.

Contact person: Irina Shtangeeva, St. Petersburg University, Universitetskaya nab. 7/9, St. Petersburg, Russia phone: +78126876122, e-mail: shtangeeva@gmail.com

ORAL AND POSTER PRESENTATIONS

HBM4EU – HUMAN BIOMONITORING INITIATIVE IN LATVIA: STUDY ON PESTICIDE MIXTURES IN ADULT AND CHILDREN POPULATION

Lāsma Akūlova¹, Inese Mārtiņšone¹, Žanna Martinsone¹, Laura Komarovska¹, Anita Seile¹,
Svetlana Lakiša¹, Ivars Vanadziņš²

¹ Laboratory of Hygiene and Occupational Diseases, Rīga Stradiņš University, Dzirciema 16, Rīga, LV-1007

² Institute of Occupational Safety and Environmental Health, Rīga Stradiņš university, Dzirciema 16, Rīga, Latvia, LV-1007

Introduction. Pesticides and their mixtures are identified as one of the priority substances in the HBM4EU (Human Biomonitoring for EU) initiative and human biomonitoring data is needed to further evaluate safe exposure levels [1]. The aim of the study is to determine the presence of various pesticide mixtures in human body and their potential effects on human health.

Methods. The study methods consist of survey and suspect screening for pesticides and their metabolites. Total sample size is 400 urine samples – 200 from non-spraying season (spring 2020) and 200 from spraying season (summer 2020). Study participants were 50 adult-child pairs living in vicinity of agricultural lands (less than 250m) and 50 adult-child pairs living at least 500m away from agricultural lands. Sample analysis was carried out in INRAE Toxalim, France, using chromatography-high resolution mass spectrometry profiling. Urine sample analysis for both seasons is carried out, but, due to high amount of metabolites, additional time is needed to interpret the possible sources of pesticide mixtures.

Results and discussion. Since the possible ways of pesticide contamination are several – via inhalation, ingestion and skin, dietary and living conditions as well as social parameters were evaluated during survey. Questions of socioeconomic factors, health and consumer habits (where subjects buy their products or whether they grow some in their garden), whether they use pesticides/insecticides in their garden, if they have been in contact with pets or other animals and whether they have treated animals or themselves with anti-parasitic/insecticide products were asked, as well as a food diary for the past 24h prior urine sample collection was gathered. In a large study carried out in the Netherlands [2], pesticide concentrations decreased slightly with distance, but not all results were in line with this statement, therefore other contamination ways (especially dietary habits and contacts with pets/animals) should be further explored.

Conclusions. Although living near agricultural lands that are treated with pesticides could have potential health effects, this study could prevent speculations on this topic. Other exposure ways should be investigated such as personal or pet anti-parasitic and insecticide treatment and dietary habits. The survey data will give additional information on study participants health, consumer and other habits, which will be used to better interpret and identify the possible contamination ways of pesticides in the study group.

References

1. Greet Schoeters RL. Scoping documents for 2021 for the first and second second round HBM4EU priority substances. **2020**.
2. Vermeulen RCH, Wenneker M, van de Zande J, Figueiredo D. Research on exposure of residents to pesticides in the Netherlands OBO flower bulbs. Available: https://www.researchgate.net/publication/332353646_Research_on_exposure_of_residents_to_pesticides_in_the_Netherlands_case_study_flower_bulbs#fullTextFileContent (accessed September 24, 2021).

Contact person: Lāsma Akūlova, Dzirciema street 16, Riga, Latvia, LV-1007, phone: +371 29437702, e-mail: lasma.akulova@rsu.lv

THERMAL DECOMPOSITION AND SPECTROMETRIC ANALYSIS OF IRRADIATED KERATINOUS FIBERS

Liga Avotina¹, Arturs Zarins^{1,2}, Mihails Halitovs^{1,3}, Larisa Baumane^{1,4}, Aleksandrs Petjukevics⁵,
Gunta Kizane¹

¹ Institute of Chemical Physics, University of Latvia, Riga, Latvia

² Faculty of Natural Sciences and Mathematics, Daugavpils University, Daugavpils, Latvia

³ Department of Human Physiology and Biochemistry, Riga Stradiņš University, Riga, Latvia

⁴ Latvian Institute of Organic Synthesis, Riga, Latvia

⁵ Institute of Life Sciences and Technology, Daugavpils University

Activated carbon fibers can be used for various filtering systems. In order to improve the filtering process, radiation modification of the materials can be applied. The main feature and advantage of radiation initiation is capability to generate active intermediate products in the solid phase [1].

Fibers from commercially available carded sheep wool were irradiated with gamma rays, Cobalt-60 source, absorbed doses 9.7-10.2 kGy, 52.5-54.5 kGy and 102.7-103.7 kGy, in order to modify their structure. Free radicals in non-irradiated and irradiated fibers were analysed by means of electron spin resonance spectrometry (ESR). For analysis of chemical bonds Fourier transform infrared spectrometry (FTIR) was used. Mass changes together with analysis of chemical bonds of released gases were analysed with thermogravimetry/differential thermal analysis device combined with Fourier transform infrared spectrometer (TG/DTA-FTIR). For analysis of thermal decomposition products quadrupole mass spectrometry (QMS) was used.

A superposition of three radicals eumelanine, pheomelanine and sulphur-centred radical [2-4] gives a narrow, asymmetric signal with a g-value 2.00768 and line width 9 G. At lower magnetic field characteristic Fe³⁺ signal with a g-factor 2.1 is detected. Irradiation of fibers causes increase of the signal with g-factor 2.007 and formation of new signal with g-factor 2.2 as well as signals of sulphur-centred radicals [2]. In TG/DTA-FTIR analysis mass decrease of non-irradiated fibers reaches 100%, while irradiated: 80-90%. Thermal decomposition can be divided in 3 main steps corresponding to desorption of water, release of sulphur containing compounds and oxidation/decomposition of organic compounds within the fibers. QMS spectra give information about decomposition process under vacuum conditions.

Obtained results show that irradiation causes changes in the content of free radicals, while thermal decomposition characteristics of irradiated fibers remain similar to non-irradiated.

Acknowledgement. Research is performed within the frames of ERDF project No: 1.1.1.1./20/A/155 "Development of novel and innovative composite materials with enhanced sorption properties from renewable biological natural resources available in the Republic of Latvia for commercial air purification filtration systems".

NATIONAL
DEVELOPMENT
PLAN 2020



EUROPEAN UNION
European Regional
Development Fund

INVESTING IN YOUR FUTURE

References

1. Porubská, M., et al. *Polymer Degradation and Stability*. **2015**, *111*, 151-158.
2. Chikvaidze, E.N., et al. *Magn. Reson.Chem.* **2014**, *52*, 377-382.
3. Strzelczak, G. et al. *Nukleonika*. **2013**, *58(4)*, 505-509.
4. Paulin, J. V. et al. *J.Phys.Chem. B*. **2019**, *123*, 1248-1255.

Contact person: Liga Avotina, Jelgavas str.1, +371 29617232, liga.avotina@lu.lv

METAL ORGANIC FRAMEWORK COMPOSITES FOR CARBON DIOXIDE CAPTURE

Linda Ansone-Bertina¹, Maris Klavins¹, Viesturs Ozols¹, Lauris Arbidans¹

¹ Department of Environmental Science, University of Latvia, Riga, Latvia

Based on the scientific literature, the CO₂ concentration in the atmosphere has significantly increased in the last 40 years (Ghanbari et al. 2020). The high levels of CO₂ emissions lead to global warming, therefore the development and application of effective CO₂ capture and sequestration techniques are of immense importance, to minimize CO₂ emissions thus protect the environment, decrease the rise of climate temperature (Ghanbari et al. 2020). Different porous materials like zeolites, activated carbon, metal-oxide molecular sieves, aluminophosphates, activated alumina silica gel, pillared clays, carbon nanotubes, inorganic and polymeric resins, porous organic materials, porous metal-organic frameworks are used as adsorbents for CO₂ capture. Metal organic frameworks (MOFs) are a class of compounds based on metal ions that via coordination bonding bind to organic ligands to form 1-, 2- or 3-dimensional structures and are characterized by porosity. Robust 3D structure, high surface area, controllable pore structure makes MOFs promising materials for CO₂ capture and sequestration. To improve CO₂ sorption different MOF modification approaches including pre-synthesis and post-synthesis as well as the synthesis of MOF composites are used. MOF composites may provide stronger interaction between CO₂ and composite material, higher volume of porosity, higher thermal and water stability, etc.

According to the scientific literature, 3 MOFs were synthesized: CuBTC (Israr et al. 2016), UTSA-16 (Abdoli et al. 2019), and UiO-66(Zr)-(COOH)₂ (Yang et al. 2013). CuBTC synthesis was performed by ultra-sonication, while UTSA-16 and UiO-66(Zr)-(COOH)₂ synthesis were performed using conventional – hydrothermal reaction conditions. The MOF composites were synthesized using the appropriate MOF synthesis methods with the addition of the potential composite material – montmorillonite, aerosil, and biochar. MOF composites have been characterized and their ability to sorb CO₂ has been determined using TGA. The obtained results indicate that all CuBTC composites have higher sorption capacity than CuBTC alone, while composites of UTSA-16 and UiO-66(Zr)-(COOH)₂ have lower sorption capacity than the appropriate MOF alone. Sorbed amount of CO₂ increased from 2.4 mmol/g of CuBTC to 2.6 mmol/g of CuBTC@montmorillonite, 3.7 mmol/g of CuBTC@aerosil, and 5.6 mmol/g of CuBTC@biochar. Although composite addition has not improved CO₂ sorption abilities of UTSA-16 and UiO-66(Zr)-(COOH)₂, montmorillonite is the most potential composite material for UTSA-16 and the obtained results of UiO-66(Zr)-(COOH)₂ are close to all studied materials only slightly higher for the biochar composite.

Acknowledgement. Research is supported by the ERDF project "Innovation of the waste-to-energy concept for the low-carbon economy: Development of novel carbon capture technology for thermochemical processing of municipal solid waste (Carbon Capture and Storage from Waste - CCSW)".

References

1. Ghanbari, T.; Abnisa, F.; Ashri Wan Daud, W. M. *Sci. Total. Environ.* **2020**, *707*, 135090.
2. Abdoli, Y.; Razavian, M.; Fatemi, S. *Appl. Organometal. Chem.* **2019**, *33(8)*, 35004.
3. Israr, F.; Kim, D. K.; Kim, Y.; Oh, S. J.; Chun, W. *Ultrasonics Sonochemistry.* **2016**, *29*, 186-193.
4. Yang, Q.; Vaesen, S.; Ragon, F.; Wiersum, A. D.; Wu, D.; Lago, A.; Devic, T.; Martineau, C.; Taulelle, F.; Llewellyn, P. L.; Jobic, H.; Zhong, C.; Serre, C.; De Wiereld, G.; Maurin, G. *Angew.Chem. Int.Ed.* **2013**, *52*, 1-6.

Contact person: Linda Ansone-Bertina, Department of Environmental Science, University of Latvia, Jelgavas st.1, Riga, Latvia, LV-1004, phone: +37129856693, e-mail: linda.ansone-bertina@lu.lv

POSSIBILITIES FOR INTERFERENCE REDUCTION IN ICP-MS/MS SYSTEM USING HE COLLISION CELL

Maris Bertins¹, Agnese Brangule², Vitalijs Lazarenko¹, Agnese Osite¹, Arturs Viksna¹, Gunita Celma¹

¹ University of Latvia, Faculty of Chemistry, Jelgavas iela 1, LV-1004, Riga, Latvia

² Riga Stradiņš University, Department of Pharmaceutical Chemistry, Dzirciema iela 16, LV-1007, Riga, Latvia

Nowadays one of the most powerful multi-element analysis techniques is an inductively coupled plasma mass spectrometry (ICP-MS) method, but it suffers from some very well-documented spectral interferences which can be very problematic when some samples of different complex matrices and origins are analysed. Polyatomic (or molecular) ions at the same m/z ratio as the analyte of interest are the reason for different interferences to a wide range of elements to be determined.

At this moment ICP-MS is a standard analytical technique for the measurement of many elements in different kinds of environmental samples (water, soil, plants, etc.) as well as pharmaceuticals and other materials and it is not imaginable without collision/reaction cell but some spectral interferences still create problems for the determination of several elements. Use of some other isotope with lower natural occurrence or dilution can decrease these interferences, but some industries like semiconductor production or pharmacology require low detection limits and complex chemicals with high purity.

Some devices like Agilent 8900 ICP-TripleQuad features a tandem MS/MS configuration, which consists of two scanning quadrupole mass analysers on either side of a collision/reaction cell. This configuration enables to use of ICP-MS in MS/MS mode in which it is possible to resolve difficult spectral interferences in a wide range of sample types using reactive cell gases like O_2 , H_2 , NH_3 , etc. MS/MS mode also can be used for the more difficult elements and problematic interferences that can be encountered in routine analysis, for example, food, sludge, soil, wastewater, and pharmaceuticals.

This study aimed to evaluate the possibilities to decrease the impact from polyatomic interferences when using ICP-MS/MS system equipped with a He collision cell.

In this study, several SRM's were analyzed (Lichen (IAEA 336), Algae (IAEA 392), Algae (IAEA 413), White Cabbage (BCR 679), Sewage sludge (LGC 6181), and Air filters (LGC A2-1365). Measurements were done with Agilent 8900 ICP-MS QQQ) equipped with a micro-mist nebulizer and He collision cell (He gas flow 5.0 mL min^{-1}). Measurements were done in both using single MS and tandem MS/MS.

Results of this study showed that it is possible to significantly decrease quantification limits for ^{28}Si measurements using ICP-MS/MS together with He collision cell while it is impossible to measure using a single MS system due to high interference from atmospheric nitrogen (N_2 , $m/z = 28$). Better results are also obtained for measurements for ^{39}K , where some imprecision of measurements can be due to $^{38}\text{Ar}^1\text{H}$ ($m/z = 39$). Better results are also obtained when measuring Na, W, Mo, Cl, and S.

Acknowledgement. Research is supported by the Project "Strengthening the doctoral capacity of the University of Latvia within the framework of the new doctoral model" with project identification No.8.2.2.0 / 20 / I / 006, LU registration No. ESS2021 / 434, co-financed by the European Social Fund.

Contact person: Māris Bērtiņš, e-mail: Maris.Bertins@lu.lv

APPLICATION OF WASTEWATER – BASED EPIDEMIOLOGY FOR TRACKING HUMAN EXPOSURE TO DEOXYNIVALENOL AND ENNIATINS

Zane Berzina^{1,2}, Romans Pavlenko^{1,2}, Laura Elina Ikkere², Vadims Bartkevics^{1,2}

¹ Department of Analytical Chemistry, University of Latvia, Riga, Latvia

² Institute of Food Safety, Animal Health and Environment “BIOR”, Riga, Latvia

Wastewater-based epidemiology (WBE) is a promising biomonitoring approach with the potential to provide direct information on human intake and exposure to food and environmental chemicals. WBE based on the normalisation method using a population biomarker 5-hydroxyindoleacetic acid (5-HIAA) is the aim of this study. This type of normalization technique has been previously used to detect various other compounds and adjusting different population biomarkers¹, but to the best of our knowledge this is the first study tracking human exposure to mycotoxins.

For six weeks (from late June to early August) every working day a wastewater (WW) sample was collected from influent in a sewage treatment plant. Free deoxynivalenol was determined in all WW samples. Average deoxynivalenol concentration in WW samples was 52 ± 9 ng/L and median – 53 ± 9 ng/L. Based on average 5-HIAA excretion – 6.9 mg/day per person and determined 5-HIAA content in the samples (in average 14.6 ± 2.8 μ g/L) an intake of deoxynivalenol by the population in Riga was estimated at 0.036 mg/day per person.

Based on Joint FAO/WHO Expert Committee on Food Additives² provisional maximum tolerable daily intake 0.070 mg/day/person (considering a mean weight of 70 kg for adult >18 years) is not exceeded, although European Food Safety Authority (EFSA) for chronic dietary exposure has set a limit of 0.015 – 0.071 mg/day/person³ that might raise a concern for human health.

With a 100% frequency of detection Enniatin B and B1 was detected in WW samples and 90% of samples contained Enniatin A, but 86% - Enniatin A1. Concentrations were in the range of 0.02 – 27.7 ng/L. Beauvericin was detected at LOQ levels in 14% of samples.

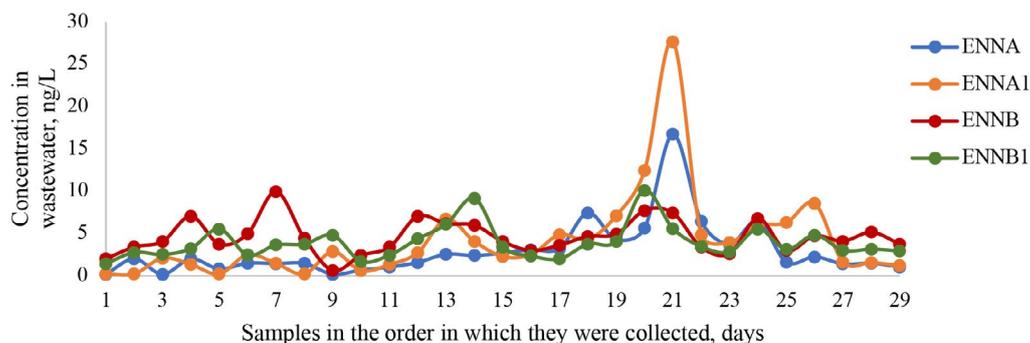


Figure 1. Changes in Enniatin concentrations over time in WW

References

1. Hou, C.; Chu, T.; Chen, M.; Hua, Z.; Xu, P.; Xu, H.; Wang, Y.; Liao, J.; Di, B. Application of multi-parameter population model based on endogenous population biomarkers and flow volume in wastewater epidemiology. *Sci. Total Environ.* **2021**, 759, 143480.
2. Joint FAO/WHO Expert Committee on Food Additives. Meeting (72nd : 2010 : Rome, Italy), World Health Organization & Food and Agriculture Organization of the United Nations. (2011). Safety evaluation of certain contaminants in food: prepared by the Seventy-second meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). World Health Organization.
3. Annual Report of the EFSA Journal 2013.

This work was supported by the Latvian Council of Science under project No. lzp-2020/2-0128.

Contact person: Zane Berzina, phone: +371 29136039, e-mail: zane.berzina@bior.lv

SUITABILITY OF ECOLOGICAL BUCKWHEAT GROATS WASTE FOR FERTILIZER PRODUCTION

Odeta Brigaitytė¹, Rasa Šlinkšienė¹

¹ Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania

One of the parts of the European Commission's Green Course strategy is field-to-table strategy. Nevertheless, it is important that food production is not limited by this. Therefore, in Lithuania, as in the whole of Europe, more and more attention is paid to the creation of a closed circuit and the sustainability of all ecosystems. The changing lifestyle and priorities of people determine the need for organic, nutritious agricultural products. In Lithuania, buckwheat, a very nutritious, undemanding plant with a very wide range of applications in the food industry, meets all these criteria. Innovative companies, such as UAB Ekofrisa, not only produce high-value food products, but also meet energy needs by burning biomass waste at biofuel filling stations. This results in a large amount of organic buckwheat husk ash, which contains some of the nutrients needed by plants (potassium, phosphorus, calcium, etc.). Due to the high dust content, its direct use for plant fertilization is problematic. On the other hand, fertilization with plant waste not only increases economic efficiency, but also slows down soil degradation, increases the amount of organic matter in the soil. All this enables scientists to develop innovative products and make technological decisions [1, 2].

After evaluating the research of ash (sunflower husks, rapeseed stalks) carried out by the Department of Physical and Inorganic Chemistry [3], various types of waste from buckwheat groats production (leftover biomass, untreated buckwheat husks, cleaned buckwheat husks) were investigated in this work. Standard and adapted methodologies for the study of chemical elements and physical properties were used for the analysis of raw materials.

Depending on the nature of waste, it was found to contain different concentrations of potassium, phosphorus, calcium, magnesium, carbon, trace elements (Fe, Mn, Zn, Cu, Co) and heavy metals (Cr, Ni, Pb, Cd). The granulometric composition (Figure 1) and other properties (bulk density, pH, etc.) of these raw materials also differ.

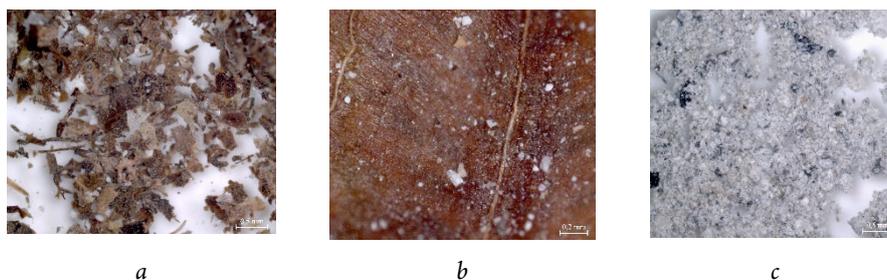


Figure 1. Optical view of: a – buckwheat groats waste biomass; b – buckwheat husk; c – buckwheat husk ash.

The obtained results suggest that all types of waste from the production of buckwheat groats can be used as raw materials for the production of granular compound fertilizers.

References

1. Tilvikienė V. *Production of alternative biomass sources (including alternative protein production sources and technologies) in primary agriculture: technological solutions, their use for bioeconomy development purposes - energy, feed, food*. Akademija, Lithuania: LAMMC, 2020.
2. Chojnacka, K.; Moustakas, K.; Witek-Krowiak A. *Bioresource Technology*. 2020, 295.
3. Paleckienė, R.; Sviklas, A. M.; Šlinkšienė, R.; Štreimikis, V. *Polish Journal of Environmental Studies*. 2010, 19(5), 973-979.

Contact person: Odeta, Brigaitytė, Radvilėnų str. 19, Kaunas, phone: +370 67559881, e-mail: odeta.brigaityte@ktu.lt

MERCURY CONCENTRATION IN THE FAECES OF BLACK STORKS

Zanda Brike¹, Rita Veilande¹, Maris Strazds², Kristiana Rancane¹, Anda Abola¹, Atis Skudra¹

¹ Institute of Atomic Physics and Spectroscopy, University of Latvia, Riga, Latvia

² Institute of Biology, University of Latvia, Riga, Latvia

Birds are widely used as bio monitors to assess the state of the environment, for example, environmental pollution levels. Monitoring may be done by using various indicators, such as blood, feathers, faeces, eggs and eggshells [1]. Non-invasive methods are especially important when working with endangered species.

Mercury (Hg) is a well-known environmental pollutant that may accumulate in aquatic ecosystems, reaching harmful concentrations. Common contaminants include organic mercury compounds, especially methylmercury, which are known to bio-accumulate and bio-magnify in the food chain [2]. As a piscivorous bird, the Black stork (*Ciconia nigra*) is at risk for higher mercury intake than non-piscivorous birds.

In this study, for the first time, we report mercury concentration measurements of black stork faeces from various nesting sites in Latvia. Adult storks do not look after their youth all the time, when hatchlings have reached a certain age (on average about 2–3 weeks). This allows to differentiate between droppings from the parents (in spring, before hatching) and chicks (in summer, when parents do not defecate near the nest). We have analysed 19 faecal samples from 18 nesting sites using an atomic absorption spectrometer with Zeeman correction Lumex RA-915M and its attachment for pyrolytic combustion. Samples have been collected in 2020 and 2021, twice a year – in the spring and in the summer.

We found that mercury concentrations varied from 16 to 522 ng/g in spring samples and from 10 to 170 ng/g in summer samples. In 7 nests the Hg concentration in the spring samples was higher than in the summer samples, in 7 nests the highest value was for the summer samples, and for 5 nests the concentration levels were similar in both the spring and the summer.

Preliminary results show that excrements of black storks contain some amount of mercury and that concentrations differ between nesting sites.

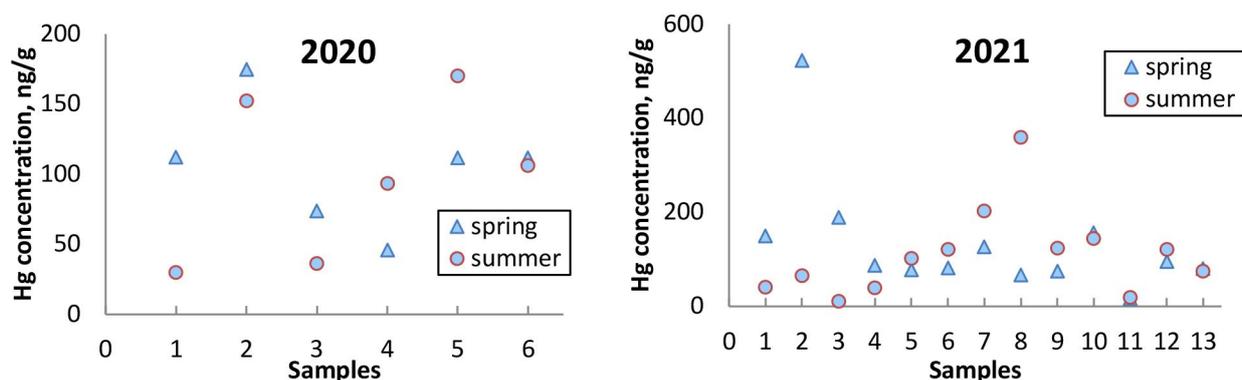


Figure 1. Comparison of Hg mean concentration in black storks feces in summer and spring for years 2020 and 2021.

Acknowledgment. This work was supported by the Latvian Council of Science No. lzp-2020/1-0005.

References

1. Abola, A., et al. *Proceedings of the 13th International Scientific and Practical Conference*. **2021**, 1, 12-16.
2. Harding, G.; Dalziel, J.; Vass, P. *PLOS ONE*, **2018**, 13(7).

Contact person: Zanda Brike, phone: +371 29821918, e-mail:zanda.brike@gmail.com

INVESTIGATION OF PHYTOCHEMICAL PROPERTIES OF PAEONIA L. GENUS BELONG TO TURKEY'S FLORA

Mehmet Veysi Çetiz¹, Halbay Turumtay², Erdal Kaya³, Neriman Özhatay⁴, Emine Akyüz Turumtay⁵

¹ Department of Molecular Biology and Genetic, Usak University, Usak, TURKEY

² Department of Energy systems Engineering, Karadeniz Technical University, Trabzon, TURKEY

³ Atatürk Horticultural Central Research Institute, Yalova, TURKEY

⁴ Faculty of Pharmacy, Eastern Mediterranean University, Turkish Republic of Northern Cyprus

⁵ Department of Chemistry, Recep Tayyip Erdogan University, Rize, TURKEY

The genus *Paeonia* includes 52 recognized members (36 species, 15 subspecies and 1 variety) worldwide, 9 species and 4 subspecies are registered Turkey, and is mainly distributed in temperate regions of Asia, southern Europe and western North America [1]. The *Paeonia* species are known for their rich chemical composition and their compounds have various medicinal properties which extensive phytochemical studies and pharmacological activity analyzes have been carried out over the past few decades as growing popularity of *Paeonia* plants for their medicinal and nutritional values. Among the various parts of *Paeonia*, the root is of particular interest to phytochemists for its medicinal uses. Root's includes valuable monoterpene, flavonoids, tannins, stilbenes, triterpenoids and steroids, and phenols have also been reported [2]. Modern pharmacological studies have shown that compounds and extracts obtained from plants of this genus have a wide range of biological activities, adding antioxidant, antitumor, anti-viral and etc. effects. For instance, against in vitro Moloney Mouse Leukemia Virus Reverse Transcriptase a study has shown that the total extracts (SPME-EO and HD-EO) were evaluated for their inhibition against Moloney Mouse Leukemia Virus Reverse Transcriptase (M-MLV-RT) using a primer extension assay (measurement of dATP single nucleotide addition). M-MLV-RT could not add a single nucleotide to the 14-mer primer in the presence of total extracts (both EO extracts, and the SPME and HD total EO extracts) were found to have a strong inhibitory effect on M-MLV-RT. [2]. In summary, we hypothesize that Peony may be a therapeutic drug candidate for the prevention of viral diseases such as against HIV and Hepatitis B viruses. For this reason, further research in this direction is needed to fully support this potential.

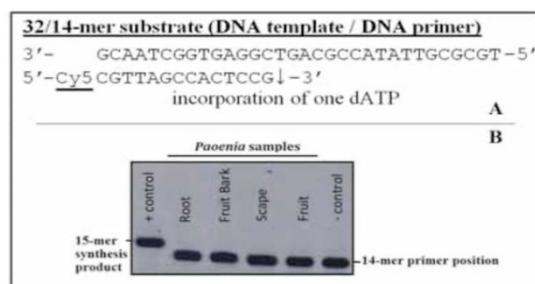


Figure 1. Inhibition Effects of parts of *Paeonia daurica* total extracts by Primary Extension Assay. A; Synthetic DNA substrate, B; gel image of M-MLV RT DNA polymerase activity assay.

Acknowledgement. The authors acknowledge the financial support from The Scientific and Technical Research Council of Turkey (TUBITAK-120Z502).

References

- Orhan, I.; Demirci, B.; Omar, I.; Siddiqui, H.; Kaya, E.; Choudhary, M. I.; Genc-Ecevit, G.; Oñazhatay, N.; Şener, B., Başer, K. H. C. *Pharmaceutical Biology*. **2010**, *48*(1), 10-16.
- Demir, A.; Turumtay, H.; Sandalli, A.; Baykal, H.; Atamovs, V.; Sandalli, C.; Turumtay, E. *Fresenius Environmental Bulletin*. **2021**, *30*(6), 5616-5624.

Contact person: Mehmet Veysi ÇETİZ, e-mail: mehmetveysi.cetiz@usak.edu.tr

PREPARATION OF MIXED OXIDE CATALYSTS FOR VOLATILE ORGANIC COMPOUND ABATEMENT

Kęstutis Čeplinskas¹, Andrius Jaskūnas¹

¹ Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania

Catalytic oxidation of volatile organic compounds (VOCs) is the most cost-effective abatement method of low concentration pollutants in the air. Catalysts are usually prepared by wet impregnation method, when catalytically active sites are formed through the two-step process: adsorption of active component salts on the selected support and their thermal destruction by calcination [1]. Precious metals, especially platinum, are the most active in catalytic oxidation of VOCs, but its price and low abundance forces to look for alternatives among transition metal oxides and their mixtures. Mixed metal oxides showed great potential in the field of VOC oxidation, because competitive adsorption of several components on the support leads to the larger, less energetically uniform and more catalytically active surface of calcined catalyst [2]. Highest catalytic activity is often achieved when the content of active component reaches around 10 %, so it is necessary to evaluate competitive adsorption of selected components and evaluate their adsorptive capacities as well as distribution of active components after calcination.

During these studies, catalysts were prepared on γ -Al₂O₃ support using solutions of Cu, Co and Cr nitrates. Recent experiments showed, that CuO is one of the most active and selective components among transition metal oxides for VOC oxidation. Therefore, mixed oxide catalysts were prepared specifically on its basis: impregnation solutions maintained constant (50 g/L) Cu concentration in all mixtures, while Cr and Co concentrations varied from 10 to 50 g/l. After impregnation, saturated support pellets were dried, then calcined and XRD analysis indicated that CuO, Co₃O₄ and Cr₂O₃ were formed as active components on the surface of γ -Al₂O₃. AAS analysis of solutions and calcined samples showed that adsorption of primary element – Cu is not limited by presence of co-adsorbing ions and even slight increase of adsorptive capacity was observed - from 45.91 mg/g for single Cu adsorption to 68.24-67.98 mg/g and 60.87-49.07 mg/g for Cu-Co and Cu-Cr adsorption respectively. High chromium concentrations decrease pH of solutions drastically, which affects adsorption of Cu unfavorably. Adsorption of additives – Co and Cr proceeds similarly in single component and co-adsorption conditions: adsorption capacities for Co and Cr are in the range of 7.04-41.03 mg/g and 11.20-30.07 mg/g respectively, when impregnation concentrations increase from 10 to 50 g/L.

Aforementioned capacities leads to the total content of the active components being in the range of 9.5-14.1 % for Cu-Co and 9.26-10.53 % for Cu-Cr pair, which is completely satisfactory for preparation of supported catalysts. Influence of co-adsorption was evaluated with Langmuir, Freundlich, Dubinin-Radushkevich (D-R), Temkin and Elovich models that are derived on various premises, so each fit of the model by linear regression analysis can confirm or disprove those assumptions. Adsorption modeling resulted in Freundlich isotherm being the best fit for both Co and Cr, which indicates the formation of several layers of adsorbate and adsorption proceeding in several steps covering the entire surface of pellet, which was also confirmed by optical microscopy. Furthermore, D-R model indicated, that co-adsorption of Cu and Co decreases activation energy of Co adsorption from 10.9 kJ/mol to 7.8 kJ/mol.

References

1. Munnik, P.; de Jongh, P.E.; de Jong K.P. *Chem. Rev.* **2015**, *115*(14), 6687-6718.
2. Gawande, M. B.; Pandey, R. K.; Jayram, R.V. *Catal. Sci. Technol.* **2012**, *2*(6), 1113-1125.

Contact person: Andrius Jaskūnas, Radvilėnų 19, Kaunas, Lithuania, +37037457070, e-mail: andrius.jaskunas@ktu.lt

SURFACE MODIFICATION OF GRAPHENE OXIDE BY ENZYME CATALYZED REACTION

Merve Danisman¹, Ayhan Oral²

¹ Department of Chemistry and Chemical Processing Technologies, Bayramic Vocational School, Canakkale Onsekiz Mart University, 17700, Canakkale, Turkey

² Department of Chemistry, Faculty of Sciences and Arts, Canakkale Onsekiz Mart University, 17020, Canakkale, Turkey

Graphene has attracted extensive attention because of its unique electronic, thermal, mechanical, optical properties [1]. GO, an oxidized form of graphene is an important material for the development of polymer nanocomposites due to presence of oxygenated functionalities such as hydroxyl, epoxide, carbonyl and carboxyl groups [2]. Surface modification of GO allows it to disperse more easily in water, organic solvents and different matrices which is advantageous for combining GO with ceramic or polymer matrices to improve the material properties [1]. In generally, chemical methods are used for surface modification, however, there is a possibility that these methods may contain chemical contamination [3]. As is well-known, enzymes are highly efficient and specific catalysts. Enzymatic methods, which are more modern and environmentalist and advantageous compared to chemical techniques, have become increasingly important in recent years [4]. For these reasons, in this study, enzymatic surface modification process by lipase enzyme catalysis with methacrylic acid was studied on the surface of graphene oxide. Modified particles have been characterized by Fourier Transform Infrared Spectrophotometer (FTIR), Scanning Electron Microscope (SEM) and Thermogravimetric Analysis (TGA).

Acknowledgement. The authors gratefully acknowledge financial support from Çanakkale Onsekiz Mart University, Scientific Research Projects Coordination Unit (FDK-2020-3297).

References

1. Peng, S.; Liu, C.; Fan, X. Surface Modification of Graphene Oxide by Carboxyl- Group: Preparation, Characterization, and Application for Proteins Immobilization. *Integrated Ferroelectrics*. **2015**, 163, 42-53.
2. Sharma, R.; Mahto, V.; Vuthaluru, H. Synthesis of PMMA / modified graphene oxide nanocomposite pour point depressant and its effect on the flow properties of Indian waxy crude oil. **2019**, 235, 1245-1259.
3. Wang, J.; Liang, G.; Zhao, W.; Zhang, Z. Enzymatic surface modification of PBO fibres. *Surface and Coatings Technology*. **2017**, 201(8), 4800-4804.
4. Karaki, N.; Aljawish, A.; Humeau, C.; Muniglia, L.; Jasniewski, J. Enzymatic modification of polysaccharides: Mechanisms, Properties, And potential applications: A review. *Enzyme and Microbial Technology*, **2016**, 90, 1-18.

Contact Person: Merve Danisman, phone: +902867732512, e-mail: mervedanisman@comu.edu.tr

ELECTROCHEMICAL SENSORS FOR DETERMINATION OF ENVIRONMENTALLY IMPORTANT COMPOUNDS USING DISPOSABLE PENCIL GRAPHITE ELECTRODES

Yusuf Dilgin¹, Selen Ayaz¹, Gamze Emir¹, Serkan Karakaya¹, Didem Giray Dilgin²

¹ Çanakkale Onsekiz Mart University, Science and Arts Faculty, Department of Chemistry, 17100 Çanakkale-Turkey

² Çanakkale Onsekiz Mart University, Faculty of Education, Department of Mathematics and Science, Chemistry Education Programme, 17020 Çanakkale-Turkey

Pencil leads are consisted of graphite, clay and wax and their percentage can be changed Pencil leads are made of graphite, clay and wax and their percentages can vary depending on the hardness of the leads. For example, there are 74% graphite, 20% clay and 5% wax in the tip of the 2B type pen, which we frequently use in our work. Recently, pencil graphite electrodes (PGE) have found a great attention in the electroanalytical studies, because they offer several advantages such as high electrochemical reactivity, ease of surface modification, high stability, low cost, disposable electrode material, and avoidance of time-consuming polishing procedures [1-3]. Although bare or pretreated PGEs have been widely used in electrochemical sensor/biosensor studies, these electrodes generally offer the poor sensitive and selective results for the detection of many analytes due to their low electrocatalytic activities In order to obtain more sensitive and selective results, PGE surface has been modified with a suitable electrocatalyst or electron mediator in the fabrication of electrochemical sensors/biosensors. In this context, modified PGEs have been widely used in the electrochemical determination of many environmental or pharmaceutical compounds.

In this study, we described the use of disposable PGEs in the determination of some environmentally important compounds such as pesticides (Chlorpyrifos, trifluralin), heavy metal ions (Cd^{2+}), and some toxic compounds (hydrazine, formaldehyde, sulfide ions). Moreover, in our studies modified PGEs were used in flow injection analysis (FIA) system for the first time. It was concluded that, the integration of PGEs with FIA offers the development of cheap, sensitive, selective, disposable and faster electrochemical sensors, various analytes.

References

1. Torrinha, Á.; Amorim, C. G.; Montenegro, M. C. B. S. M.; Araújo, A. N. *Talanta*. **2018**, *190*, 235-247.
2. Akanda, M. R.; Sohail, M.; Aziz, M. A.; Kawde, A. N. *Electroanalysis*. **2016**, *28*(3), 408-424.
3. Kawde, A. N.; Baig, N.; Sajid, M. *RSC Advances*. **2016**, *6*(94), 91325-91340.

Contact person: Yusuf Dilgin, Canakkale Onsekiz Mart Univ. Science and Art Faculty, Department of Chemistry, 17100, Çanakkale, phone: +905336563973, e-mail: ydilgin@comu.edu.tr

STRUCTURAL, MORPHOLOGICAL AND MAGNETIC INVESTIGATION OF $\text{Bi}_{1-x}\text{Gd}_x\text{Fe}_{0.85}\text{Mn}_{0.15}\text{O}_3$ SOLID-SOLUTIONS

Ramunas Diliautas¹, Aldona Beganskiene¹, Dovydas Karoblis¹, Dalis Baltrunas², Kestutis Mazeika², Aleksej Zarkov¹, Aivaras Kareiva¹

¹ Institute of Chemistry, Vilnius University, Vilnius, Lithuania

² Center of Physical Sciences and Technology, Vilnius, Lithuania

Out of a large family of known multiferroic materials, the bismuth ferrite (BiFeO_3) remains the most important one. This material is antiferromagnetic and ferroelectric way below room temperature with high Neel ($T_N=370$ °C) and Curie ($T_C=810$ °C) [1] temperatures. While being the perfect candidate for incorporation to practical devices, this material still has some disadvantages, like leakage problems, which lead to low resistivity, due to nonstoichiometry or defect-related issues [2]. Furthermore, phase-pure bismuth ferrite is difficult to prepare, because of the formation of Bi-rich or Fe-rich impurity phases [3]. In order to avoid those issues, the substitution of either Bi^{3+} or Fe^{3+} as well as co-doping of both elements can be performed. In our case, we replaced 15 % of Fe^{3+} ions with Mn^{3+} ions, because in our previous study [4] at this concentration structural changes occurred. And Bi^{3+} ions were substituted by Gd^{3+} ions due to the fact that gadolinium ions are magnetically active, which could lead to new magnetic interactions.

In the present study, $\text{Bi}_{1-x}\text{Gd}_x\text{Fe}_{0.85}\text{Mn}_{0.15}\text{O}_3$ (with x varying from 0 to 1) solid solutions were prepared by an environmentally friendly, cheap and non-toxic sol-gel technique using ethylene glycol as a complexing agent. Three different annealing temperatures (500 °C, 650 °C and 800 °C) were chosen for the formation of final products. For phase purity evaluation X-ray diffraction and Mössbauer spectroscopy analysis were performed. For morphology estimation and particle size determination scanning electron microscopy (SEM) was carried out. Additionally, FT-IR and Raman spectroscopy, as well as thermogravimetric analysis (TGA) studies, were implemented.

Acknowledgment. This work was supported by a Research grant BUNACOMP (No. S MIP-19-9) from the Research Council of Lithuania.

References

1. Teague, J. R.; Gerson, R.; James, W. J. *Solid State Commun.* **1970**, *8*(13), 1073-1074
2. Park, T. J.; Papaefthymiou, G. C.; Viescas, A. J.; Moodenbaugh, A. R.; Wong, S. S. *Nano Lett.* **2007**, *7*(3), 766-772.
3. Catalan, G.; Scott, J. F. *Adv. Mater.* **2009**, *21*(24), 2463-2485.
4. Karoblis, D.; Diliautas, R.; Mazeika, K.; Baltrunas, D.; Niaura, G.; Talaikis, M.; Beganskiene, A.; Zarkov, A.; Kareiva, A. *Mater.* **2021**, *14*(17), 4844.

Contact person: Ramunas, Diliautas, Naugarduko st. 24, Vilnius, phone: +37069831217, e-mail: ramunas.diliautas@stud.chgf.vu.lt

ASSESSMENT OF RADIONUCLIDES IN FORMER SALASPILS NUCLEAR REACTOR COOLING WATER

Armands Egleskalns^{1,2}, Ingars Reinholds^{1,2,3}, Konstantins Bavrins³, Gunta Kizane^{1,2}

¹ Institute of Chemical physics, University of Latvia, Riga, Latvia

² Faculty of Chemistry, University of Latvia, Riga, Latvia

³ Institute of Food Safety, Animal health and Environment "BIOR", Riga, Latvia

The radioactive waste waters from cooling systems of nuclear reactors may accumulate different long-living radionuclides such as Cs-137, tritium (H-3). The beta emitting H-3 nuclide with half-life 12.3 years commonly is produced as a result of the neutron nuclear reaction with deuterium [1], while it is considered as "less" toxic to that of gamma emitting nuclides Co-60 and Cs-137. Japan recently announced plans to discharge over 1.2 million tons of radioactive water from the Fukushima Daiichi Nuclear Power Plant (FDNPP) into the Pacific Ocean, whereas long term effect may have dramatical impact on environment [2]. There is need for more reliable strategies for safe removal and isolation of nuclear wastes containing H-3 and more toxic nuclides. This problem is attributed also to the Latvian situation, where in the old Salaspils nuclear reactor territory H-3 rich cooling water wastes are located.

The aim of this study was to evaluate the strategy recently reported by the Koyoto University (Koyanaka et al. 2019) based on lithium manganese oxide (LiMn_2O_4) spinel structure sorbents, which were used for the decontamination of tritiated water wastes [3]. This study and other recent reports have indicated to benefits of such spinel-based structures for Li-H exchanges resulting in partly hydrogenated spinel structures, which may activate protium-deuterium and protium – tritium ion exchanges. In our study cellulose acetate (CA) has been tested as the fiber matrix for the attachment of such sorbents modified for the adsorption of H-3 from nuclear waters. Within preliminary experiments based on hydrogenated commercial LiMn_2O_4 it was confirmed by liquid scintillation technique that H-3 contents were notably reduced tritiated water. The further study was dedicated to the development of magnetic composites based on CA and LiMn_2O_4 - iron oxide (Fe_3O_4) at different concentrations up to 25 wt% to improve the separation efficiency. The research demonstrates higher tritium adsorption qualities of acid-hydrolysed lithium-manganese oxide paired with cellulose acetate in comparison to pure LiMn_2O_4 .

By promoting magnetic properties of hybrid sorbent with different ferrous oxides, it allows to collect tritiated sorbent without further contaminating sample water.

The results of conducted study suggest that inorganic sorbents modified with acid use Li-H exchange mechanism which subsequently is followed by H-T exchange in spinel structure of sorbent.

Acknowledgement. The study was financially supported by the Latvian Council of Science, project No. lzp-2020/2-0213 "Application of modified cellulose fiber sorbents for the concentration of radioactive hydrogen (tritium) and other radionuclides from contaminated environments and evaluation of toxicity: approbation of the approach in Latvia for the decontamination of stored nuclear reactor water wastes".

References

1. Taylor, P. A. Physical, chemical, and biological treatment of groundwater at contaminated nuclear and NORM sites. *Woodhead Pub.* **2015**, 237.
2. Zhao, C., et al. Transport and dispersion of tritium from the radioactive water of the Fukushima Daiichi nuclear plant. *Marine Pollution Bulletin.* **2021**, 169, 112515.
3. Koyanaka, H.; Fukutani, S.; Miyatake, H. Tritium separation from heavy water using a membrane containing deuterated manganese dioxide. *Journal of Radioanalytical and Nuclear Chemistry.* **2019**, 322(3), 1889-1895.

Contact person: Armands Egleskalns, 1 Jelgavas iela, Riga, Latvia, LV-1004, phone: +37128242479, e-mail: armands.egleskalns@lu.lv

APPLICATION OF HR-CS GF MAS FOR FLUORINE DETERMINATION IN BIOLOGICAL SAMPLES

Andrzej Gawor¹, Andrii Tupys¹, Anna Rusczyńska¹, Ewa Bulska¹

¹ Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland

Nowadays growing attention is paid to the control of fluorine content in samples of biological origin as it is present in the form of various biologically active organic compounds. Due to the chemically-rich matrix of biological tissues, the determination of fluorine becomes a challenging task. Furthermore, a required complex sample preparation procedure makes the determination of the low contents of F by ion chromatography UV-Vis or ion-selective electrodes not possible [1]. High-resolution continuum source graphite furnace molecular absorption spectrometry (HR-CS GF MAS) seems to be the best option for this purpose due to its high robustness to matrix interferences, especially in the presence of carefully selected modifiers. In this work the possibility of quantitative determination of F in water and animal tissues was examined by measuring the molecular absorption of gallium monofluoride (GaF) at 211.248 nm with the use of a commercially available HR-CS GF MAS system [2]. Experimental conditions for the sensitive and precise determination of fluorine were optimized, including the time/temperature program as well as the composition of modifier mixture combined mode of modification. Under the conditions of fluoride present in the sample was stabilized up to 600 °C, and the optimum vaporization temperature for GaF was 1540 °C. Palladium and zirconium deposited onto the graphite surface served as solid modifiers; sodium acetate and ruthenium modifiers were added directly to the sample. The limit of detection and the characteristic mass of the method were 0.43 µg/L and 8.7 pg, respectively. The proposed procedure was validated by the use of certified reference materials of lake water and animal tissue. The acceptable recovery was obtained proving the possibility of application for samples with similar matrix.

References

1. Gawor, A.; Tupys, A.; Rusczyńska, A.; Bulska, E. An Improved Methodology for Determination of Fluorine in Biological Samples Using High-Resolution Molecular Absorption Spectrometry via Gallium Fluorine Formation in a Graphite Furnace. *Appl. Sci.* **2021**, *11*, 5493;
2. Gawor, A.; Konopka, A.; Rusczyńska, A.; Pączek, L.; Gajewski, Z.; Bulska, E. Molecular absorption and mass spectrometry for complementary analytical study of fluorinated drugs in animal organisms. *J. Anal. At. Spectrom.* **2020**, *35*, 1840–1847.

Contact person: Andrzej Gawor, Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland; phone: +48 22 55 26 705; e-mail: agawor@chem.uw.edu.pl

BIO-CHAR CATALYST APPLICATION FOR GLUCOSIDE HYDROLYSIS REACTION

Daniela Godina^{1,2}, Kristine Meile¹, Aivars Zhurinsh¹, Arturs Viksna²

¹ Latvian State Institute of Wood Chemistry, Dzerbenes 27, LV-1006 Riga, Latvia

² University of Latvia, Jelgavas 1, LV-1004 Riga, Latvia

Biomass is a type of renewable resources that can be used for obtaining of energy, carbon-containing chemicals and materials. Biochar based solid acid catalysts is a promising alternative to mineral acid in biomass hydrolysis and dehydration due to its high reaction activity, recyclability and also low cost [1]. In this work several glucosides were used as model compounds to characterize hydrolysis process of glucosidic compounds found in biomass derived products such as bio-oil.

For the glucoside hydrolysis experiments we used 3 structurally different glucoside standards – ascorbylglucoside, salicin and methyl- β -D-glucopyranoside. Based on the previously obtained results with cellobiose hydrolysis to glucose using bio-char catalysts [2] we used catalyst with the best catalytic activity – sulfonated bio-char that was obtained via fast pyrolysis process (BC-Py-H₂SO₄). Reaction was done under pressurised conditions at 3 different temperatures – 103, 110 and 120 °C. The reaction time was 1, 2, 3, 5, 8 and 24 h. The mass ratio of glucoside and catalyst were 1:5. Qualitative and quantitative measurements of glucosides, glucose and their degradation products were done using UHPLC system.

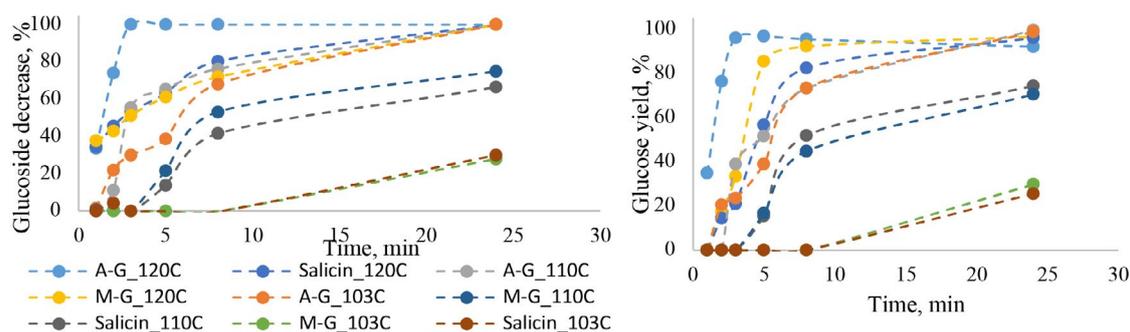


Figure 1. Glucoside decrease and glucose yield after hydrolysis at different temperatures in time intervals.

The data in Figure 1 show that the fastest hydrolysis of glycosides takes place at 120 °C. Ascorbyl glycoside at 103 and 110 °C undergoes complete hydrolysis of glycoside to glucose after 24 h, but at 120 °C glycoside undergoes complete hydrolysis after 3 h. Methyl- β -D-glucopyranoside undergoes partial hydrolysis at 103 °C only after 24 h to form 26% glucose, and at 110 °C after 5 h partial hydrolysis undergoes 16% glucose and after 24 h produces 74% glucose. If the hydrolysis is performed at a temperature of 120 °C, then glycoside degradation is observed, as the reduction of the glycoside content is 38%, but no glucose is formed as a degradation product. A similar pattern is observed for salicin as for methyl- β -D-glucopyranoside. Hydrolysis of salicin at 120 °C after 1 h shows degradation of the glycoside, with a 34% reduction in the amount of glycoside, but glucose is not formed as a degradation product for this glycoside either.

References

1. Fraga, A.; Do C.C.; Quitete, P. B.; Ximenes, V. L.; Sousa-Aguiar, E. F.; Fonseca I. M.; Rego, A. M. B.; *Mol. J. Catal. A Chem.* **2016**, *422*, 248-257.
2. Godina, D.; Meile, K.; Zhurinsh, A. *RSC Adv.* **2021**, *11*, 18259-18269.

Contact person: Daniela Godina, Latvian State Institute of Wood Chemistry, Dzerbenes 27, LV-1006 Riga, Latvia, phone: +371 26811949, e-mail: daniela.godina@kki.lv

PARTICLE REMOVAL EFFICIENCY OF FACE MASKS DURING THE COVID-19 PANDEMIC

**Anton Gradišek¹, Luka Pirker¹, Anja Pogačnik Krajnc¹, Urška Gradišar Centa¹, Jan Malec¹,
Vladimir Radulović¹, Andreja Jelen¹, Igor B. Mekjavič¹, Janez Kovač¹, Miran Mozetič¹,
Matej Godnič², Metod Čebašek³, Tina Bregant⁴, Luka Snoj¹, Maja Remškar¹**

¹ Jozef Stefan Institute, Ljubljana, Slovenia

² Novo Mesto General Hospital, Novo Mesto, Slovenia

³ Hyla d.o.o., Ljubljana, Slovenia

⁴ CIRIUS, Kamnik, Slovenia

At the onset of the Covid-19 pandemic, the world faced a dire lack of PPE, and in particular face masks. As studies quickly demonstrated, the SARS-CoV-2 virus primarily spreads through droplets (aerosols) that are released when breathing, talking, and coughing. Therefore, masks are the first line of protection to slow the spread of the virus. They act as a barrier against the dispersion of droplets and at the same time protect the wearer against the aerosols already present in the surrounding air.

In spring 2020, we started investigating different properties of face masks and improvised protection equipment with a special focus on the particle removal efficiency. We used a scanning mobility particle sizer to measure the number concentration of a standard aerosol powder passing through a mask mounted on a manikin head in a special chamber. The results show high filtration efficiency of FFP2, FFP3, and certified surgical masks for all sizes of tested particles, while protection efficiency of washable masks depends on their constituent fabrics [1].

Furthermore, we have demonstrated that ionizing radiation (both gamma and electron beam) can be used for emergency sterilization of FFP2 and FFP3 masks, provided that the respirators are recharged afterwards [2].

References

1. Pogačnik Krajnc, A.; Pirker, L.; Gradišar Centa, U.; Gradišek, A.; Mekjavič, I. B.; Godnič, M.; Remškar, M. Size-and Time-Dependent Particle Removal Efficiency of Face Masks and Improvised Respiratory Protection Equipment Used during the COVID-19 Pandemic. *Sensors*. **2021**, *21*(5), 1567.
2. Pirker, L.; Krajnc, A. P.; Malec, J.; Radulović, V.; Gradišek, A.; Jelen, A.; Snoj, L. Sterilization of polypropylene membranes of facepiece respirators by ionizing radiation. *Journal of membrane science*. **2021**, *619*, 118756.

Contact person: Anton Gradišek, e-mail: anton.gradisek@ijs.si

SOLUTIONS ON THE WAY TO PREPARATION OF CARBONATED TITANIUM IMPLANT COATINGS VIA PLASMA ELECTROLYTIC OXIDATION IN SUSPENSIONS

Vladlens Grebņevs^{1,2}, Roman Viter³, Şahin Altundal³, Kārlis Grundšteins³, Agnieszka Stolarczyk², Arturs Vīksna¹, Wojciech Simka²

¹ Department of Analytical Chemistry, University of Latvia, Riga, Latvia

² Faculty of Chemistry, Silesian University of Technology, Gliwice, Poland

³ Institute of Atomic Physics and Spectroscopy, University of Latvia, Riga, Latvia

Plasma electrolytic oxidation (PEO) is a relatively novel electrochemical method for preparation of porous chemically modified oxide coatings on metallic substrates, gaining popularity in the last decade particularly. Due to use of voltages higher than 100 V, simplicity and financial availability of technology, utilization of PEO opens wide horizons in improvement of metallic product surface properties, finding applications in materials science, construction, metallurgy, aviation, shipbuilding etc.

Regarding perspectives in human biomaterial field in 2020s, PEO seems to be powerful tool to make a quantum leap in chemical identity of implants to natural bone tissue since it allows to incorporate carbonates. As practice shows, attempts to prepare carbonated calcium phosphate coatings on titanium substrates using such widespread techniques as magnetron sputtering, plasma spraying and sol-gel, have failed or appeared to be ineffectual. Among the main reasons the following can be mentioned: high costs, unrequired properties of resulting product as well as chemical properties of carbonates themselves - low solubility in water and alkaline medium, degradation to carbon dioxide in acids, thermal instability and others.

The important feature of PEO that enables carbonate transfer to the surface of coating without side reactions is possibility to conduct the process in a suspension bath in opposition to conventional phenomena occurring in liquid homogeneous systems. More precisely, negatively charged suspended particles are able to migrate to the positive anode and undergo inert or partly reactive incorporation to porous oxide layer. However, the practical applicability runs into the lack of investigations on optimal conditions for successful incorporation of carbonate particles. Also referring to PEO in suspensions on the whole, no systematic information has been provided before on regularities how incorporation of different solid particles influence coating properties.

The aim of current research was to perform preliminary PEO investigations in suspensions assessing possibilities of carbonate particle incorporation, detecting factors influencing properties of obtained materials and finding appropriate solutions to overcome emerging difficulties. For proper comparison of results various physicochemical methods were involved in characterization of sample surface and cross-sectional parameters – Raman and EDX spectroscopy, roughness and contact angle measurements, SEM and SBF tests. Results showed that such factors as suspension pH, concentration of base electrolyte, carbonate-containing particle size, crystallinity, synthesis method and chemical composition play a vital role in formation of coatings with required characteristics for implantology purposes and right variation of those can have synergic effect.

References

1. Krzakała, A., Kazek-Kęsik, A., Simka, W. (2013). *RSC Advances*, 3 (43), 19725-19743.
2. Lu, X., Mohedano, M., Blawert, C., Matykina, E. *et.al.* (2016). *Surface and Coatings Technology*, 307, 1165-1182.

Contact person: Vladlens Grebņevs, Jelgavas street 1-617 (Riga, Latvia), +371 20241113, vladlens.grebnevs@lu.lv

SYNTHESIS OF β - $\text{Ca}_2\text{P}_2\text{O}_7$ AS AN ADSORBENT FOR THE REMOVAL OF HEAVY METALS FROM WATER

Diana Griesiute¹, Aivaras Kareiva¹, Aleksej Zarkov¹

¹ Institute of Chemistry, Vilnius University, Vilnius, Lithuania

Nowadays, water purification is of essential importance due to increased contamination, which brings a serious risk to public health and other forms of life on the earth. In order to reduce the contamination, there are various techniques and sorbents [1-4]. Nevertheless, the search for and development of new materials for the fast and efficient removal of pollutants from water remains the task of the highest priority.

Calcium phosphates (CPs) are the class of materials that have a huge potential in environmental applications such as water treatments. These materials can be used for the removal of both organic pollutants such as dyes and antibiotics and heavy metal ions [5]. The most frequently utilized CP for the application for removal of heavy metals from water is calcium hydroxyapatite (HAp) [6]. This compound is known very well for its ability to incorporate easily different isovalent and aliovalent ions [7]. However, there are no reports on the adsorption properties of calcium polyphosphates like calcium pyrophosphate ($\text{Ca}_2\text{P}_2\text{O}_7$). The aim of this work is to develop a synthesis method for the preparation of β - $\text{Ca}_2\text{P}_2\text{O}_7$ and to estimate its adsorption properties toward different metal ions (Al^{3+} , Cd^{2+} , Co^{2+} , Cu^{2+} , Fe^{2+} , Mn^{2+} , Ni^{2+} , Pb^{2+} , Sn^{2+} , Sr^{2+} and Zn^{2+}).

In the present work, single-phase β - $\text{Ca}_2\text{P}_2\text{O}_7$ was synthesized by a wet precipitation process followed by thermal treatment. Initial powders were synthesized using $\text{Ca}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ and $(\text{NH}_4)_2\text{HPO}_4$ as starting materials. The precursors were dissolved separately in deionized water and solutions were mixed together. The obtained precipitates were filtered and dried, resulting powders were annealed at 800 °C. Physicochemical properties of the sorbent were characterized by means of X-ray diffraction (XRD) analysis, Fourier transform infrared spectroscopy (FTIR), thermal analysis (TGA/DSC), scanning electron microscopy (SEM) and low temperature adsorption–desorption of nitrogen (BET method).

The results showed that obtained material consisted of porous plate-like particles with micrometer dimensions. The sorption properties of the obtained material were studied for different metal ions in model aqueous solutions. It was determined that β - $\text{Ca}_2\text{P}_2\text{O}_7$ demonstrates the highest adsorption capacity for Pb^{2+} and Sn^{2+} , while the lowest capacities were observed towards Sr^{2+} , Ni^{2+} and Co^{2+} ions. The optimal pH value for the removal of Pb^{2+} ions was determined to be 2, which is related to the low solubility of β - $\text{Ca}_2\text{P}_2\text{O}_7$ at this pH. The adsorption capacity towards Pb^{2+} ions were calculated as high as 120 mg g⁻¹.

References

1. Ivanets, A. I.; Kitikova, N. V.; Shashkova, I. L.; Oleksiienko, O. V.; Levchuk, I.; Sillanpää, M. J. *Environ. Chem. Eng.* **2014**, *2*, 981–987.
2. Kondo, Y.; Goto, T.; Sekino, T. *RSC Adv.* **2020**, *10*, 41032-41040.
3. Ahmad, S. Z. N.; Wan Salleh, W. N.; Ismail, A. F.; Yusof, N.; Mohd Yusop, M. Z.; Aziz, F. *Chemosphere.* **2020**, *248*, 126008.
4. Melnyk, I. V.; Pogorilyi, R. P.; Zub, Y. L.; Vaclavikova, M.; Gdula, K.; Dabrowski, A.; Seisenbaeva, G. A.; Kessler, V. G. *Sci. Rep.* **2018**, *8*, 13.
5. Goto, T.; Cho, S. H.; Ohtsuki, C.; Sekino, T. *J. Environ. Chem. Eng.* **2021**, *9*, 105738.
6. Hernández-Cocoletzi, H.; Salinas, R. A.; Águila-Almanza, E.; Rubio-Rosas, E.; Chai, W. S.; Chew, K. W.; Mariscal-Hernández, C.; Show, P. L. *Environ. Technol. Innov.* **2020**, *20*, 101109.
7. Šupová, M. *Ceram. Int.* **2015**, *41*, 9203-9231.

Contact person: Diana Griesiute, Institute of Chemistry, Vilnius University, Naugarduko 24, LT-03225 Vilnius, Lithuania, e-mail: diana.griesiute@chgf.vu.lt

COMPATIBILITY OF LIQUID FERTILIZERS AND HUMIC SUBSTANCES

Goda Gudinskaitė¹, Rasa Paleckienė¹, Rasa Šlinkšienė¹

¹ Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania

The ever-increasing intensity of agriculture is causing irreversible qualitative changes in the soil. Soil conservation and improvement is a priority of EU agro-environmental policy. However, this is also one of the most difficult challenges for agriculture. Various ways for sustainable agriculture are proposed. One way to provide arable soil with humic substances is through the use of humic extracts. Humic substances (HS) can be defined as "a general category of naturally occurring, biogenic, heterogeneous organic substances that can generally be characterized as being yellow to black in color, of high molecular weight (MW), and refractory" [1]. Various raw materials can be used to extract humic substances. Those include sedimentary minerals (coal, lignite, shale), peat, compost or sapropel. Humic substances from different sources have different compositions and biological effects depending on their chemical structure and physico-chemical properties [2]. Extracts of humic substances already having industrial application in the world are extracted from leonardites and used alone or in combination with mineral fertilizers.

In this work dry humic materials were used: Huminrich Huplus Potassium Humate Fulvic glossy powder and Huminrich Huplus soluble humic acid glossy flakes. Solutions of different concentrations were prepared from these materials. The obtained solutions were analyzed, the properties of the obtained solutions (pH, crystallization temperature, density, viscosity, electrical conductivity) were determined. The prepared solutions were found to contain insoluble matter, so sedimentation analyzes were performed (Figure 1).



Figure 1. Sedimentation analyzes of HS solutions (5, 10, 15, 16, 17, 18, 19, 20% – left to right).

The sediment layer depends on the concentration and ranges from 0.5 to 2 ml. The resulting solutions are not stable and tend to delaminate. The obtained concentrates of humic substances were used to enrich liquid micronutrient fertilizers made of copper, zinc, manganese and molybdenum salts. The same delamination effect is observed when the addition of HS solutions to micronutrient fertilizers is added. Mixing again gives an even distribution of the components throughout the volume.

References

1. Sparks, D. L. *Chemistry of Soil Organic Matter, Environmental Soil Chemistry* (Second Edition), Academic Press, **2003**, 75-113.
2. Fuentes, M.; Baigorri, R.; González-Gaitano, G. *et al. J Soils Sediments*. **2018**, *18*, 1389-1399.

Contact person: Rasa Paleckienė, Radvilėnų str. 19, Kaunas LT-50254, Lithuania, phone: +370 37 457070,
e-mail: rasa.paleckiene@ktu.lt

WASTEWATER-BASED EPIDEMIOLOGY AS A TOOL FOR PUBLIC HEALTH AND LIFESTYLE ASSESSMENT

Laura Elina Ikkere^{1,2}, Iveta Pugajeva¹, Veronika Šukajeva¹, Ingus Pērkonis¹

¹ Institute of Food Safety, Animal Health and Environment “BIOR”, Lejupes iela 3, Riga, Latvia

² University of Latvia, Faculty of Chemistry, Jelgavas iela 1, Riga, Latvia

During the last decade growing interest has been shown towards new approach in wastewater analysis – wastewater-based epidemiology. It is based on the analysis of specific human metabolic excretion products (biomarkers) in wastewater as indicators of consumption or population exposure to different substances by normalisation of analyte influent concentration to per capita mass loads using the daily flow and the size of the population within wastewater treatment plant (WWTP) catchment boundaries. However, estimation of population size is a major source of uncertainty in the wastewater-based epidemiology. Introducing a population biomarker in the sample analysis may significantly reduce errors in the backcalculation associated with population estimation and wastewater volume measurement [1].

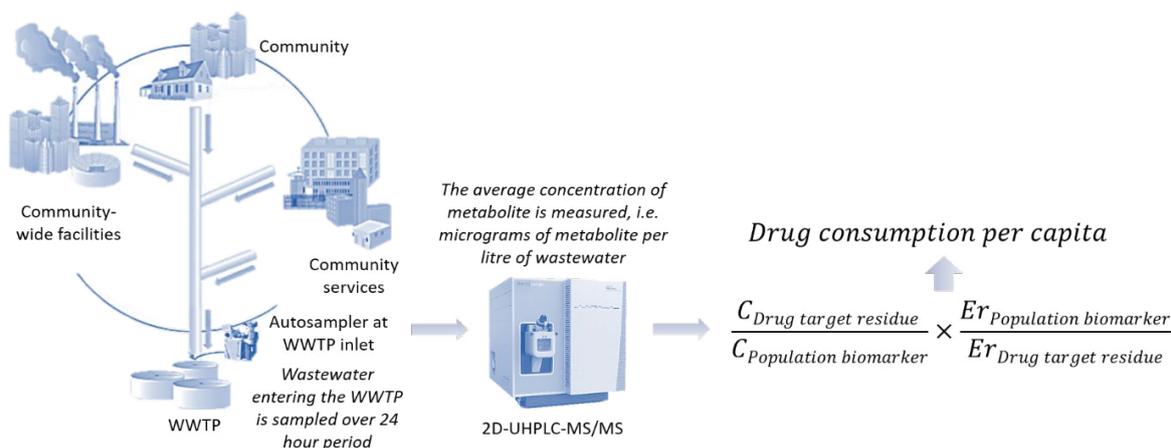


Figure 1. Scheme of wastewater-based epidemiology.

In the present study a total of 62 compounds, including pharmaceuticals and their metabolites, as well as lifestyle and population biomarkers were determined in wastewater influent samples. Sample preparation was carried out by SPE and dilute-and-shoot approaches. Quantitation was performed by 2D-UHPLC-MS/MS. Both short-term and year-long trends were assessed by measuring grab samples each workday over 6-week period and 24-hour composite samples every week starting from December 2020, respectively. 43 compounds were present in the wastewater samples, representing antibiotics, nonsteroidal anti-inflammatory drugs, antihypertensives and others.

Acknowledgement. The research was part of project “Elaboration of new methodology using ultra high-resolution mass spectrometry for assessing public health via wastewater-based epidemiology” (Nr. lzp-2020/2-0150) funded by Latvian Council of Science.

References

1. Choi, P. M.; Tschärke, B. J.; Donner, E.; O’Brien, J. W.; Grant, S. C.; Kaserzon, S. L.; Kaserzon, S.L.; Mackie R.; O’Malley E.; Crosbie N. D.; Thomas K.V.; Mueller, J. F. Wastewater-based epidemiology biomarkers: Past, present and future. *Trends Analyt. Chem.* **2018**, *105*, 453-469.

Contact person: Laura Elina Ikkere, Lejupes 3, Riga, phone: +371 26477009, e-mail: ikkere.laura@gmail.com

INFLUENCE OF BORON AND MAGNESIUM IONS ON YAG: CE AND LUAG:CE CERAMICS

Greta Inkrataitė¹, Ramūnas Skaudžius¹

¹ Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania

In order to convert high-energy radiation, such as gamma or X-rays, into a visible light, a certain type of material is needed. Such compounds are usually referred to as scintillators. Over the years many different candidates to fit the requirements were examined. However, compounds with garnet structure have attracted a particularly large amount of attention [1]. Cerium doped yttrium and lutetium aluminum garnets (YAG:Ce, LuAG:Ce), have high density, high thermal stability, a rather intensive emission/excitation and high quantum efficiency which are needed for a good scintillator. However, further optimization and improvement is still needed especially on the shortening of the decay time. One way to approach this problem is to alloy the aforementioned compounds with different elements, such as boron and magnesium [2, 3].

In this work we describe the synthesized YAG and LuAG garnets that are doped with 0.5% cerium that are additionally doped with 5% of boron and / or 0.03% of magnesium. The initial powders of garnets were synthesized Sol-Gel method. Ceramics were obtained using hydrostatic pressure. Boron and additional doping by magnesium are expected to improve required luminescent properties. Selected sol-gel method determines the homogeneity of compounds and low temperatures of synthesis. Phosphor coatings were analyzed by X-ray diffraction analysis and scanning electron microscopies. Emission, excitation spectra and decay times have been investigated as well.

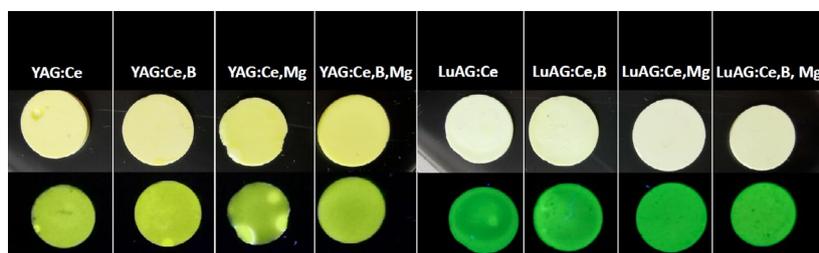


Figure 1. Ceramics of different garnets in day light and under 365 nm excitation.

References

1. Machado, I. P.; Teixeira V. C., *et al. J. Alloys Compd.* **2019**, 777, 638-645.
2. Foster, C.; Koschan M., *et al. J. Cryst. Growth.* **2018**, 486, 126-129.
3. Lucchini M. T.; Baganov O., *et al. J. Lumin.*, **2018**, 194, 1-7.

Contact person: Greta Inkrataitė, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko st. 24, LT-03225 Vilnius, Lithuania, phone: +370 52193105, e-mail: greta.inkrataite@chgf.vu.lt

A NEW METHOD FOR MEASURING GERMANIUM ISOTOPE RATIOS IN MINERALS AND WATER SAMPLES USING MC-ICP-MS AFTER THE FORMATION OF VOLATILE HYDRIDES

Jakub Karasiński¹, Andrii Tupys¹, Ludwik Halicz^{1,2} and Ewa Bulska¹

¹ Biological and Chemical Research Centre, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland

² Geological Survey of Israel, 32 Y. Leybowitz st., 9692100 Jerusalem, Israel

Germanium is a trace element with the average content in rocks and minerals of the earth's crust of around 1 mg kg⁻¹. Germanium has five isotopes that occur naturally with atomic masses 70, 72, 73, 74, 76 and relative abundances of 21.23, 27.66, 7.72, 35.94 and 7.45%, respectively [1]. Only few works have been published about changes in Ge isotope composition so far mainly due to its low content and a number of limitations in measuring performance [2].

In order to perform Ge isotope analysis by multicollector inductively coupled plasma mass spectrometry (MC-ICP-MS), we found out that it is necessary to isolate the analyte before measurements. Method for the accurate measurement of Ge isotope ratio in water and natural geological solid phase samples using MC-ICP-MS right after the Ge hydride generation was developed. The procedure is based on the liquid-liquid extraction of germanium in order to separate those species which can cause the decomposition of germanium hydride or limit its formation. It was shown that neither extraction nor evaporation causes analyte losses and thus isotopic fractionation. Standard-Sample Bracketing method was applied to correct instrumental bias and mass discrimination effect. The application of time resolved mode of measurements enabled to choose analytical signals with best parameters and improved the precision of results. Adjusting the pH value of solutions by using acetic buffer increased the sensitivity nearly 5 times in comparison to the conditions for germanium hydrides generation proposed by other authors. It is worth mentioning that the developed method is much quicker and simpler, does not require laborious separation of germanium using ion-exchange resins and thanks to its high sensitivity it enables determination of Ge isotopic ratio in samples with its relatively low content. The isotopic ratio values for ⁷⁴Ge/⁷⁰Ge were measured in selected standard reference materials for which expected values were found in GeoREM database. It was demonstrated that precision and trueness of the proposed method are equally good or even better than methods earlier proposed in literature. This procedure was also successfully applied to the isotopic analysis of natural water samples with relatively high contents of germanium.

References

1. De Laeter, J. R.; Böhlke, J. K.; De Bièvre, P.; Hidaka, H.; Peiser, H. S.; Rosman, K. J. R.; Taylor, P. D. P. Atomic weights of the elements. Review 2000 (IUPAC Technical Report). *Pure Appl. Chem.* **2003**, 75, 683-800.
2. Rouxel, O. J.; Luais, B. Germanium Isotope Geochemistry. *Rev. Mineral. Geochem.* **2017**, 82, 601-656.

Contact person: Andrii Tupys, Biological and Chemical Research Centre, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland; phone: +48 22 55 26 705; e-mail: atupys(at)cnbc.uw.edu.pl

PREPARATION OF RUDDLESDEN-POPPER CALCIUM MANGANITES APPLYING MOLTEN SALT SYNTHESIS

Dovydas Karoblis¹, Aleksej Zarkov¹, Aldona Beganskiene¹, Aivaras Kareiva¹

¹ Institute of Chemistry, Vilnius University, Vilnius, Lithuania

Materials with perovskite (general formula ABO_3) structure have been extensively investigated for a long time due to their high variety of different physical properties and wide areas of application. This class of compounds has a vast diversity of structural variations, including the Ruddlesden-Popper phase. This layered perovskite oxide has the general formula $A_{n+1}B_nO_{3n+1}$ and consists of alternating AO and ABO_3 layers. The calcium manganite-based $CaO(CaMnO_3)_m$ ($m = 1, 2, 3, \infty$) compounds are an example of a material with a Ruddlesden-Popper structure.

This compound is considered one of the most eminent thermoelectric materials [1]. Different synthetic approaches have been applying for the preparation of calcium manganite-based materials, including solid-state with high oxygen pressure annealing [2] or Pechini sol-gel method [3]. To the best of our knowledge, there is no research regarding the preparation of calcium manganite-based $CaO(CaMnO_3)_m$ ($m = 1, 2, 3, \infty$) compounds by molten salt synthesis.

In the present work, $CaMnO_3$ -based materials were prepared by applying the molten salt synthetic technique for the first time. Different annealing conditions (time, temperature), as well as various ratios between salt and Ca/Mn precursors, were chosen for the selective preparation of final products. Few characterization techniques, including X-ray diffraction, FT-IR spectroscopy, and scanning electron microscopy (SEM), were implemented in order to examine possible morphological and structural changes.

Acknowledgments. This work was supported by a Research grant BUNACOMP (No. S MIP-19-9) from the Research Council of Lithuania.

References

1. He, J.; Liu, Y.; Funahashi, R. *J. Mater. Res.* **2011**, *26*(15), 1762-1772.
2. MacChesney, J. B.; Williams, H. J.; Potter, J. F.; Sherwood, R. C. *Phys. Rev.* **1967**, *164*(2), 779.
3. Fawcett, I. D.; Sunstrom IV, J. E.; Greenblatt, M.; Croft, M.; Ramanujachary, K. V. *Chem. Mater.* **1998**, *10*(11), 3643-3651.

Contact person: Dovydas, Karoblis, Naugarduko st. 24, Vilnius, phone: +370 62126186,
e-mail: dovydas.karoblis@chgf.vu.lt

HYDROPHOBIC EUTECTIC SOLVENT FOR LIQUID-PHASE MICROEXTRACTION OF PARABENS FROM WATER SAMPLES

Vytautas Kavaliauskas¹, Vilma Olšauskaitė¹, Audrius Padarauskas¹

¹ Department of Analytical and Environmental Chemistry, Vilnius University, Vilnius, Lithuania

Parabens (esters of *p*-hydroxybenzoic acid) are widely used as preservatives in food, cosmetic and pharmaceutical products [1]. Recently, it has been proven that parabens are genotoxic, disrupt the endocrine system, and probably cause breast cancer [2]. Due to an increased use of preservatives, more and more parabens end up in surface and ground waters, since they are not completely metabolised in the human body nor completely removed during wastewater treatment.

In the present work, hydrophobic eutectic solvent composed of tetrahexylammonium chloride and trifluoroacetic acid (molar ratio 1:2) was employed for liquid-phase microextraction of four parabens (methylparaben, ethylparaben, propylparaben and butylparaben) from water samples. The extracts were analyzed by HPLC using an Agilent 1290 Infinity II LC system (Agilent, Waldbronn, Germany) equipped with a ternary pump, thermostatted column compartment, photodiode array detector and autosampler. InfinityLab Poroshell 120 EC-C18 (3.0 × 150 mm, 2.7 μm, Agilent) column was used in the experiments. Separations were performed at a flow rate of 0.5 mL/min under linear gradient elution with acetonitrile (ACN)/water mobile phase. The initial composition of the mobile phase for parabens was 50% ACN, and it was changed to 100% ACN in 6 min. Naphthalene was used as an internal standard. The injection volume was 10 μL and the detection wavelength was set at 230 nm.

The effects of main parameters, such as sample volume, eutectic solvent volume, extraction time and salt concentration, on the extraction efficiency of parabens were investigated. For the final microextraction experiments, 10 mL of water sample was placed into a 15 mL glass centrifuge tube and spiked with naphthalene at 20 μg/L. Then 100 μL of eutectic solvent was added and the mixture was shaken manually for 30 s, resulting in the formation of emulsion. The phases were separated by centrifugation at 3000 rpm for 5 min, the upper aqueous phase was removed using a syringe, the residue was dissolved in 50 μL acetonitrile and analyzed using HPLC technique.

Under optimized extraction conditions, the enrichment factors ranged from 89 to 95. Calibration curves were linear ($R^2 \geq 0.997$) for a concentration level between 0.50 and 500 μg/L. The detection limits were in the range 0.10 - 0.16 μg/L. Finally, the method was applied for the determination of parabens in environmental water samples. Average recoveries of spiked samples were in the range from 93% to 105% with satisfactory precision (RSDs lower than 7.4%). The obtained results indicate that the developed method is a promising alternative for the rapid enrichment and determination of parabens in aqueous samples.

References

1. Bledzka, D.; Gromadzinska, J.; Wasowicz, W. *Environ. Int.* **2014**, *67*, 27-42.
2. Harvey, P.W.; Darbre, P. *J. Appl. Toxicol.* **2004**, *3*(24), 167-176.

Contact person: Vytautas Kavaliauskas, Naugarduko 24, LT-03225, Vilnius, Lithuania, phone: +370 5 2193119, e-mail: vytautas.kavaliauskas@chf.vu.lt

EVALUATION OF SAPROPEL SEDIMENTS FOR MEDICAL PURPOSES

**Aneka Klavina¹, Ilona Pavlovskā¹, Agris Auce¹, Laura Komarovskā¹, Linda Paegle¹,
 Linda Dobkevica², Inese Martisone¹, Ivars Vanadzins¹**

¹ Institute of Occupation Safety and Environmental Health, Riga Stradiņš University, Riga, Latvia

² Institute of Biology, University of Latvia, Riga, Latvia

The growing trends in the use of biological materials call for greater use of local resources, and the availability of natural and sustainable materials is one of the priorities worldwide. Freshwater sapropel is a common natural material in lake basins in Latvia, but is still not sufficiently studied. The main goal of the project was to conduct a detailed and systematic studies on the therapeutic properties of sapropel obtained in Latvia lakes, to elevate its scientifically based use in medicine and to develop new therapeutic procedures and services, as well as to advocate the development of new exportable products.

The results include the survey, sampling depths and processing, evaluation of external signs, physical, chemical and biochemical parameters and evaluation of microbiological indicators, detection of pollution factors (pesticide residues, heavy metal concentration). Biologically active components from the sapropel samples was extracted using the alkaline method. Sapropel extracts were characterized by organic carbon content (TOC), humic (HA) and fulvic acid (FA) concentrations, trace metal concentrations and antioxidant activity (TAS).

Lake ↓	pH	Total concentration (mg/ml)				Metal concentration, mg.kg							Microbiology, Uncertainty ±15,40	
						Heavy				Trace				
		TOC	HA	FA	TAS	Pb	Cd	Ni	Co	Mn	Fe	Zn	CFU/g	Isolated species
Zeilu	7.8	126.4	160.2	74.3	0.75	2.60	0.1	11.8	5.0	0.18	19.7	0.04	2,65 x 10 ⁶	<i>Serratia fonticola</i> / <i>Pseudomonas veronii</i> / <i>Pseudomonas chlororaphis</i>
Mazais Kivdalošs	7.3	129.1	167.8	72.9	0.87	2.66	0.2	18.4	8.2	0.09	10.3	0.10	2,0 x 10 ⁵	<i>Pseudomonas veronii</i>
Ivsku	8.0	106.5	113.1	76.5	0.32	3.10	0.2	3.1	1.7	0.13	4.8	0.08	1,1 x 10 ⁵	<i>Paenibacillus amylolyticus</i> / <i>Aeromonas bestiarum</i>
Dunakla	8.0	104.3	138.4	44.5	0.47	5.23	0.2	15.3	5.7	0.16	4.4	0.04	2,3 x 10 ⁷	<i>Aeromonas sobria</i> / <i>Pseudomonas marginalis</i> / <i>Brevundimonas diminuta</i>
Audzeli	7.1	125.4	161.8	70.0	1.03	5.84	0.2	25.2	6.3	0.67	32.3	0.08	2,1 x 10 ⁵	<i>Acinetobacter johnsonii</i>

Organoleptically sapropel samples found predominantly dark brown, because of plankton, plants and connected with peat existence and high organic matter. The heavy metals –Pb, Cd, Co, Ni - were present in all samples, but none of the metals exceed maximum acceptable level. Despite the fact that no active pathogens have been identified in the untreated sapropel samples, the CFU exceeds the limit allowed by EU cosmetic standards in all sapropel samples. It is necessary to reduce CFU/g in raw sapropel by sterilization or by adding preservatives before using it in cosmetic or medical applications. The concentration of HA and FA and the antioxidant levels varies strongly between the lakes. It was found that TAS level is considerably higher in organic sapropel extracts.

Within the framework of this study, guidelines for the extraction of sapropel "Methodology for the Development of Industrial Mining" have been developed. As a result, these guidelines set out the steps to be taken to ensure that the sapropel samples obtained retain their original properties.

Contact person: Aneka Klavina, Dzirciema street 16, Riga, LV 1007, phone +371 28467321, e-mail: aneka.klavina@rsu.lv

INTERACTION BETWEEN MICROPLASTICS AND CHEMICAL POLLUTANTS

**Maris Klavins¹, Marcis Mezulis², Linards Klavins¹, Viktor Stabnikov³, Andrii Marynin⁴,
Olena Stabnikova^{3,4}**

¹ Department of Environmental Science, University of Latvia, Riga, Latvia

² Department of Analytical Chemistry, University of Latvia, Riga, Latvia

³ Department of Biotechnology and Microbiology, National University of Food Technologies, Kyiv, Ukraine

⁴ Advanced Research Laboratory, National University of Food Technologies, Kyiv, Ukraine

Microplastics are ubiquitous environmental pollutant of growing concern. As they are stable, can be found even in remote sites where anthropogenic activities are low and their presence is steadily increasing. Of especial importance are accumulation of microplastic particles in the aquatic environments as thus their presence reflect pollution levels in river catchments, but as a result with complex interactions, microplastics can accumulate in river and lake sediments. When released, microplastics interact with many other chemicals present in the environment, including organic and inorganic substances. Microplastics support development of microorganisms on their surface and thus major change of their behavior in environment take place. During such interactions of key importance are the surface properties and functionalities of microplastics as well as environmental processes, such as aging of plastic material. The aim of our study is to compare the sorption mechanisms of environmental pollutants on microplastics in conditions close to real aquatic environment, considering major role of dissolved organic matter (DOM) of natural as well as anthropogenic environment. The sorption mechanisms including, hydrophobic interactions, electrostatic interactions, pore filling are discussed as well as the impact of the DOM properties are discussed.

Acknowledgement. Research supported by Latvian-Ukrainian Joint Programme of Scientific and Technological Cooperation project “The microbially-coated microplastics in neustonic water-air interphase and their environmental impacts on aquatic biotopes”.

Contact person: Maris Klavins, Department of Environmental Science, University of Latvia, Raina blvd 19, Riga, LV 1586, Latvia.
Tel.: +371 29307090; e-mail: maris.klavins@lu.lv

VARIATION IN METHYLMERCURY CONCENTRATIONS IN ENVIRONMENTAL SAMPLES IN FOREST LAND AND WETLANDS WITH ORGANIC SOILS IN LATVIA

Zane Kļaviņa^{1,2}, Arta Bārdule¹, Ivars Kļaviņš^{1,2}, Zane Libiete¹

¹ Latvian State Forest Research Institute “Silava”, Salaspils, Latvia

² Department of Environmental Science, University of Latvia, Riga, Latvia

The reliance of Latvian national economy on the forest sector, combined with the new EU legislation that will likely result in stricter forest protection measures, at the same time necessitating transition to bio-based economy (EU Forest Strategy 2021, EU Biodiversity Strategy to 2030), will likely result in intensified forest management in some areas, and knowledge about the impact of different management measures on environmental quality is needed. Mercury (Hg) and its methylation are among the chief concerns related to the impact of land management practices on water quality, and both forestry and wetland restoration measures may have a certain input (e.g., [1-3]). While the problem is topical also in Latvia, data on Hg concentrations in various environments is scarce. Our study strives to fill some of the information gaps, by analysing methylmercury (MeHg) concentrations in water and sediments of small peatland forest streams, as well as in topsoil in wetlands with different management regimes.

In the 2018-2019, water and sediment samples were taken in eight small watercourses in experimental forests of the Kalsnava Forest district, and organic soil samples were taken at 0-10 cm soil layer in 22 research sites in wetlands in different regions of Latvia. The sampling sites were subject to disturbances of various type and severity. MeHg concentrations were determined at the Institute of Food Safety, Animal Health and Environment “BIOR” (Latvia) using GC-ICP-MS method.

Seasonally, the highest mean MeHg concentrations in water were found in spring and summer, but the highest mean MeHg concentrations in sediments were found in summer and autumn (Figure 1). No statistically significant differences in MeHg concentration in water between disturbed (beaver dam removal, ditch cleaning) and undisturbed sites were detected, but MeHg concentration in sediment samples was statistically higher in undisturbed sites. If the MeHg concentrations in organic soil samples from wetlands with different management regimes (forests, peat extraction sites, commercial berry plantations, raised bogs, transitional mires; Figure 1) were compared, the highest mean MeHg concentrations were found in raised bogs and drained Norway spruce forests.

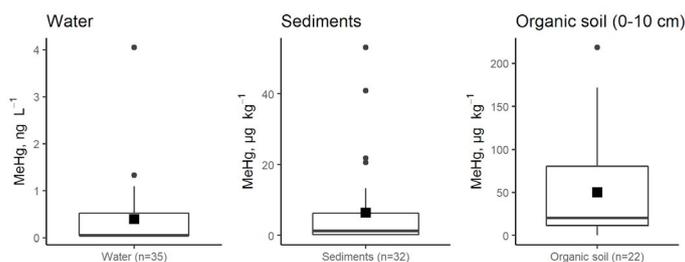


Figure 1. Variation in MeHg concentrations in water and sediment samples from small watercourses in forest land and in organic soil samples from wetlands with different management regimes in Latvia. In the boxplots, the median is shown by the bold line, the mean is shown by the black square, dots outside the box and whiskers represent outliers of the datasets.

Acknowledgment. This work was supported by the Latvian Council of Science project No. lzp-2018/1-0434 “Interaction of microbial diversity with methane turnover and mercury methylation in organic soils”.

References

1. Porvari, P.; Verta, M.; Munthe, J.; Haapanen, M. *Environ. Sci. Technol.* **2003**, *37*, 2389-2393.
2. Bishop, K.; Allan, C. J.; Bringmark, L.; Garcia, E.; Hellsten, S., et al. *Journal of the Royal Swedish Academy of Forestry and Agriculture.* **2009**, *148*, 9-23.
3. Eklöf, K.; Lidskog, R.; Bishop, K. *Ambio*, **2016**, *45*, 163-174.

Contact person: Zane Kļaviņa, Rigas str. 111, Salaspils, Latvia, LV-2169, phone: +371 67942555, e-mail: zane.kalvite@silava.lv

DFT STUDY OF GALLIUM OXIDE BULK PROPERTIES

Zhanymgul Koishybayeva¹, Abdirash Akilbekov¹, Abay Usenov¹, Anatoli I. Popov^{1,2},
A. Platonenko²

¹ L. N. Gumilyov Eurasian National University, Nur-Sultan, Kazakhstan

² Institute of Solid State Physics, University of Latvia, Riga, Latvia

The recent focus on climate change and global warming has generated tremendous worldwide interest in reducing carbon dioxide (CO₂) emissions into the environment. The main source of CO₂ emissions from human activities is energy conversion, especially the combustion of fossil fuels to generate electricity, heat and transport [1,2].

Emissions from fossil fuel combustion can be significantly reduced in both the energy and transportation industries if the combustion conditions are effectively monitored using semiconductor gas sensors. As we know, gallium oxide (β -Ga₂O₃) is promise material for sensor applications. Thus, the first-principle study of electronic structure pure and defective β -Ga₂O₃ is very important point on the way of detail understanding of sensor characteristics.

In this work, we are investigated the crystal structure, lattice parameters and intrinsic defects of β -Ga₂O₃, and their formation energy at atomic level by first principles calculations.

The crystal structure of β -Ga₂O₃ was investigated, where $a \perp c$, $b \perp c$, and the angle between the a and c axes is 104°. Lattice parameters are $a = 12.2$ Å, $b = 3.04$ Å, $c = 5.80$ Å. Having a monoclinic (C2/m) structure, a crystal has two unique Ga and three unique O sites as shown on Figure 1.

The formation energy of oxygen (V_{O}) and gallium (V_{Ga}) vacancies in β -Ga₂O₃ as well as their charge transition levels have been calculated. As result, V_{Ga1} has lower formation energy than V_{Ga2} : 10 eV vs 12 eV at oxygen-rich condition. At the same time, the transition levels lie rather high than 0.7 eV above the valence band, which makes gallium vacancies deep acceptors. In the case of oxygen vacancies, calculations give the ionization energies above 1 eV for all three types of V_{O} . Therefore, oxygen vacancies are so-called deep donors.

Calculations of the charge transition levels revealed that all three types of oxygen vacancies are deep donors and cannot be responsible for the n-type conductivity in Ga₂O₃. However, they can compensate acceptors by giving them their electrons. Similar results were obtained for all types of gallium vacancies, which are deep acceptors with high formation energies.

References

1. Gurney, K. R., *et al.* High Resolution Fossil Fuel Combustion CO₂ Emission Fluxes for the United States. *Environmental Science & Technology*. **2009**, 43, 5535-5541.
2. Rao, A. B.; Rubin, E. S. A Technical, Economic, and Environmental Assessment of Amine-Based CO₂ Capture Technology for Power Plant Greenhouse Gas Control. *Environmental Science & Technology*. **2002**, 36, 4467-4475.

Contact person: Zhanymgul Koishybayeva, L.N. Gumilyov ENU, 2 Satpaeva str. Nur-Sultan, email: zhanymgul.k@gmail.com

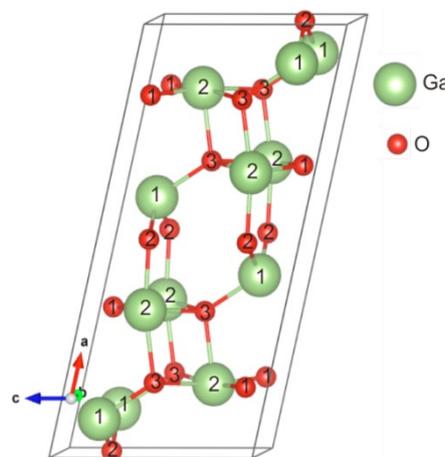


Figure 1. Schematic representation of crystal structure of monoclinic β -Ga₂O₃.

INSIGHT INTO THE FORMATION OF ZINC WHITLOCKITE: SYNTHESIS, STRUCTURE AND CHARACTERISATION

Agne Kizalaite¹, Tomas Murauskas¹, Aleksej Zarkov¹

¹ Institute of Chemistry, Vilnius University, Vilnius, Lithuania

Magnesium whitlockite ($\text{Ca}_{18}\text{Mg}_2\text{H}_2(\text{PO}_4)_{14}$) is the second most abundant mineral in natural bone tissue, accounting for 20–35 wt% of it [1]. In recent years this compound attracted more and more attention in fields of bone regeneration and tissue engineering due to its excellent biocompatibility and osteogenic capability [2]. Incorporation of biologically active ions into the whitlockite structure could result in superior biological performance and expanded clinical application of the material. Promising potential substituent in whitlockite is Zn, which can enhance the rate of metabolic processes, encourage cellular proliferation and osteogenic differentiation [3] and give antibacterial properties to calcium phosphates [4]. These properties can accelerate bone regeneration processes and decrease the infection rate.

In the present work, pure-phase whitlockite powders containing Zn ions ($\text{Ca}_{18}\text{Zn}_2\text{H}_2(\text{PO}_4)_{14}$) were successfully obtained and investigated. Calcium hydrogen phosphate dihydrate and zinc acetate dihydrate were used as starting materials to synthesize zinc whitlockite powders using hydrothermal synthesis method. Synthesis was performed at 200 °C temperature for 3 h. It was shown that particle size and shape can be controlled by synthesis conditions. Synthesised compounds characterization was performed using X-ray diffraction (XRD), Fourier-transform infrared spectrometry (FTIR), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). Scanning electron microscopy (SEM) was used to characterize the morphology of the particles. Rietveld analysis was employed for calculations of lattice parameters.

Acknowledgement. This was supported by a Research grant BUNACOMP (No. S-MIP-19-9) from the Research Council of Lithuania.

References

1. Cheng, H.; Chabok, R., *et al. Acta Biomater.* **2018**, *69*(1), 342-351.
2. Jang, H. L.; Bin Zheng, G., *et al. Adv. Healthc. Mater.* **2015**, *5*(1), 128-136.
3. Sevari, S.; Kim J. K., *et al. ACS Appl. Mater. Inter.* **2021**, *13*(30), 35342-35355.
4. Fadeeva, I. V.; Gafurov, M. R., *et al. BioNanoSci.* **2017**, *7*(2), 434-438.

Contact person: Agne Kizalaite, Naugarduko g. 24, Vilnius, Lithuania, e-mail: agne.kizalaite@chgf.vu.lt

ANALYSIS OF SYNTHETIC AND PHYTOCANNABINOIDS USING MICELLAR ELECTROKINETIC CHROMATOGRAPHY

Pille-Riin Laanet¹, Piret Saar-Reismaa¹, Merike Vaher¹

¹ Department of Chemistry and Biotechnology, Tallinn University of Technology, Tallinn, Estonia

Synthetic cannabinoids are the largest group of compounds currently monitored in Europe by the European Monitoring Centre for Drugs and Drug Addiction. Synthetic cannabinoids are substances that mimic the effects of THC, which is primarily responsible for the psychoactive effects of cannabis. Since the beginning of 2000s, herbal smoking mixtures including considerably varied amounts of different synthetic cannabinoids have been sold, typically under the name *Spice*. The compounds are usually mixed with or sprayed onto the plant material. The use of synthetic cannabinoids has caused many serious health problems and mass poisonings. [1] Therefore, the monitoring institutions need reliable methods for the analysis of products containing these compounds likely to cause great harm to users.

The objective for this research was to develop a new method for the detection of four synthetic cannabinoids and two phytocannabinoids from plant materials using micellar electrokinetic chromatography with UV-absorbance detection (MEKC-UV). Compounds analysed in this research were JWH-018, JWH-073, JWH-200, JWH-250, CBD and THC. Optimisation of the method included both the background electrolyte and CE parameters, and was achieved through the execution of two consecutive Box-Behnken experimental plans. Primary validation was conducted to determine the performance characteristics. Selectivity study of several plants was executed and different solvents for extraction compared to decide on a fitting sample pre-treatment process. Limits of detection and quantification were 3.0 mg/L and 5.0 mg/L for all synthetic cannabinoids and 3.7 mg/L and 6.2 mg/L for both phytocannabinoids.

As a result of this research a novel MEK-CUV method was developed, which enables the differentiation of plant materials containing synthetic or phytocannabinoids employing a water-based background electrolyte system. Quantification of four synthetic cannabinoids and qualification of two phytocannabinoids was achieved.

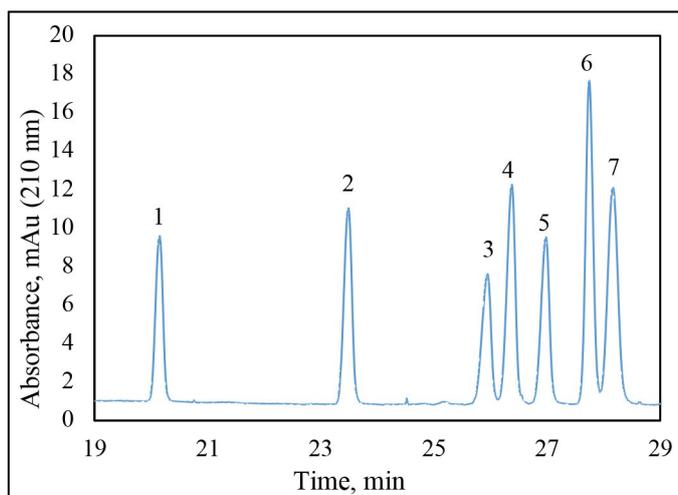


Figure 1. Electropherogram achieved using the novel MEKCUV method. Identification: 1 – IS, 2 – JWH-200, 3 – JWH-250, 4 – JWH-073, 5 – JWH-018, 6 – THC, 7 – CBD.

Acknowledgement. This work was supported by Estonian Centre of Analytical Chemistry (AKKI).

References

1. European Monitoring Centre for Drugs and Drug Addiction, “Synthetic cannabinoids in Europe,” 2017.

Contact person: Pille-Riin Laanet, e-mail: pilleriin.laanet@ttu.ee, phone: +3726204325, Akadeemia tee 15, 12618, Tallinn, Estonia.

DETERMINATION OF LATVIAN HONEY FLORAL ORIGINS USING IRMS, UHPLC-HRMS, NMR

K. D. Labsvards^{1,2}, V. Rudovica¹, J. Rusko^{1,2}, R. Kluga¹, L. Busa¹, M. Bertins¹, J. Naumenko¹, M. Salajeva¹, A. Viksna¹

¹ University of Latvia, Faculty of Chemistry, Jelgavas street 1, LV-1004 Riga, Latvia

² Institute of Food Safety, Animal Health and Environment “BIOR”, Lejupes street 3, LV1076, Riga, Latvia

EU does not have enough locally produced honey, so a large proportion has to be imported from outside the EU, which offers relatively cheaper honey. The floral origin of honey is also an important indicator of product quality, which determines the price. Bees are able to collect monofloral honey from rapeseed (*Brassica napus*), linden (*Tilia cordata*), heather (*Ericaceae vulgaris*), buckwheat (*Fagopyrum esculentum*), clover (*Trifolium repens*) and willow (*Salix cinerea*) for the honey of geographical origin of Latvia.

In order to determine the suitability of different instrumental methods for the recognition of such monofloral honey types, only IRMS, UHPLC-HRMS, NMR analyzes were performed and the results were processed using chemometric methods [1-2]. Melissopalynology analyzes and various instrumental methods were performed on 62 honey samples of Latvian origin. IRMS was performed to determine the carbon isotope ratio. The $\delta^{13}\text{C}$ values are expressed relative to VPDB. UHPLC-HRMS was performed to quantify 33 different polyphenols, flavonoids and plant hormones. NMR working frequency of 300 MHz was performed to acquire ¹H-NMR spectra. A combined analysis of the principal components was performed, from the results obtained in the IRMS experimental course and the organic compounds quantified by the UHPLC-HRMS method.

Preliminary results after reduction of the variables indicated that organic compounds such as p-hydroxybenzoic acid, p-coumaric acid and rutin, which have already been found in the honey of Latvian origin, could be used to identify monofloral buckwheat honey [3]. Other IRMS results suggest that the $\delta^{15}\text{N}$ isotope can be used to identify heather honey among Latvian honey samples, but NMR has the potential to recognize a mixture of several flower honey compositions.

Acknowledgement. This research was funded by grant “Recognition of monofloral honey of Latvian origin using nuclear magnetic resonance, chromatographic, isotope ratio mass spectrometry and chemometric methods” grant Nr. LZP-2020/2-0200.

References

1. Drivelos, S. A.; Danezis, G. P.; Halagarda, M.; Popek, S.; Georgiou, C. A. Geographical origin and botanical type honey authentication through elemental metabolomics via chemometrics. *Food Chem.* **2021**, 338, 127936.
2. Ghanavati, S. N.; Javaheran, M. Y.; Marini, F.; Nescatelli, R.; Biancolillo, A. Classification of honey applying high performance liquid chromatography, near-infrared spectroscopy and chemometrics. *Chemom. Intell. Lab. Syst.* **2020**, 202, 104037.
3. Rusko, J.; Vainovska, P.; Vilne, B.; Bartkevics, V. Phenolic profiles of raw mono- and polyfloral honeys from Latvia, *J. Food Compos. Anal.* **2021**, 98, 103813.

Contact person: Krišs Dāvids Labsvārds, phone: +371-26395784, e-mail: kriss_davids.labsvards@lu.lv

APPLICATION OF INNOVATIVE Bi_2Se_3 THIN FILMS AS ANODES IN AQUEOUS RECHARGEABLE LITHIUM-ION BATTERIES

**Vitālijs Lazarenko¹, Yelyzaveta Rublova¹, Raimonds Meija¹, Jana Andžāne¹, Vanda Voikiva¹,
Arturs Viksna², Donāts Erts¹**

¹ Institute of Chemical Physics, University of Latvia, Raina blvd. 19, LV-1586, Riga, Latvia

² University of Latvia, Faculty of Chemistry, Raina blvd. 19, LV-1586, Riga, Latvia

For recent decades lithium-ion batteries (LIBs) have dominated the world marketplace as the most promising energy storage device due to their great advantages – high energy density, long cycle life and high energy efficiency. On the other hand, the use of non-aqueous electrolytes (e.g. LiBF_4 , LiPF_6) in the LIBs poses a hazard to the environment as in the contact with the ambient environment they are flammable and explosive. Alternatively, to reduce the cost of production and increase the safety standards for batteries aqueous electrolytes (e.g. LiNO_3 , Li_2SO_4) could be used. In 1994 Dahn and his research group demonstrated for the first time the concept and possible perspectives of rechargeable lithium-ion batteries (ARLIBs) where lithium aqueous electrolytes were used. Bi_2Se_3 is a unique material with a layered structure that has already shown great performances as an anode in LIBs by using non-aqueous lithium electrolytes. Perhaps, Bi_2Se_3 can also be a promising candidate as anode for ARLIBs.

The aim of this research was to investigate the electrochemical properties of Bi_2Se_3 thin film by using lithium aqueous electrolytes. For this research LiNO_3 electrolyte which is more electrochemically stable than commonly used Li_2SO_4 and LiCl and can be prepared in high concentrations (>8 M) was selected. Bi_2Se_3 thin films were synthesized using the physical vapour deposition method. For the electrochemical measurements, such as, cycling voltammetry, electrochemical impedance spectroscopy and galvanostatic charge/discharge were performed. To analyse the surface morphology and chemical composition of Bi_2Se_3 thin films, a scanning electron microscope equipped with energy-dispersive X-ray spectroscopy was used.

Results of this study demonstrated that the formation of solid electrolyte interphase (SEI) layer on the Bi_2Se_3 thin film surface improves anode stability and provides higher Li^+ intercalation/deintercalation reversibility and diffusion. Intensive galvanostatic charge/discharge measurements demonstrated a high specific capacity of Bi_2Se_3 thin film.

Contact person: Vitālijs Lazarenko, phone: +371 26649122, e-mail: vitalijs.lazarenko@lu.lv

DETERMINATION OF NON-FERROUS METALS IN SOIL SAMPLES USING TEST STRIP METHOD

Ilga Lauma Leimane¹, Jānis Ģibietis²

¹ Department of Analytical Chemistry, University of Latvia, Riga, Latvia

² Enola Chemical Co., Ltd., Riga, Latvia

Non-ferrous metals in soil are important microelements for different kinds of plants, however insufficient or excessive concentrations of these metals can disturb the growth of plants. Conventional households use various soil substrates, supplements, fungicides and other horticultural products on a daily basis, which can significantly affect the concentration of various elements in the soil. Quantitative or semi-quantitative determination by the test strip method would be a useful way to analyse such soils. Tests strips have a lower accuracy than traditional quantification methods, but very accurate results are not so essential for conventional household use.

In this work the possibility of using of water quality test strips for the determination of monovalent and divalent copper, and divalent manganese in soil was performed. Soil extracts were obtained by three different extractants: nitric acid, potassium chloride and sulfamic acid solutions. Aside from conventional soil samples, special soil samples were also prepared by preliminary treating soil with horticulturally used products such as Bordeaux solution and potassium permanganate. Flame atomic absorption spectrometry (FAAS) was used as reference method. The results of measurements performed by the test strip method were recorded with a colour reflection densitometer. Based on calibration results, the copper and manganese concentrations of the test samples were determined from the colour index M that was measured by the densitometer.

Nitric acid extract displayed the most accurate results in comparison to the reference method for the determination of copper, while the results of KCl and sulfamic acid were lower. In the case of manganese, both nitric acid and sulfamic acid extracts gave relatively successful results, while those of KCl extract were significantly lower. The copper concentration in the sample treated with Bordeaux solution increased significantly, the strip test method results differ from the FAAS in value of about several hundred milligrams, since the accuracy of the test strips decreases at higher ion concentrations. In the case of KMnO_4 , the concentration of manganese in the sample increased by a few tens of milligrams, as the concentration of permanganate solution that is commonly used in agriculture is very low.

In conclusion, the test strip method gives sufficiently accurate results for the determination of copper and manganese at lower ion concentrations and gives approximate results at higher concentration. Extraction procedure was elaborated for application of conventional water quality test strips for analysis of soil samples and the prototype of reagent kit was designed.

Contact person: Jānis Ģibietis, phone: +371 29236869, e-mail: janis@enola.lv

THE STRUCTURAL, MORPHOLOGICAL AND OPTICAL PROPERTIES OF PA6/AG-CD-SE LIGHT-ABSORBING MATERIALS

Henrieta Markevičiūtė¹, Nijolė Dukštienė¹, Valentina Krylova¹

¹ Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania

Ordered films of nanoscale sized inorganic semiconductors within the polymers are of major interest in optoelectronics as light emitting devices [1] or photovoltaics [2], since semiconducting nanoparticles, incorporated into a processable polymer film, are easy to handle, process and manipulate [3]. The present work aims to synthesize and characterize PA6/Ag-Cd-Se composites. These composites were obtained applying different chemical synthesis methods: the PA6/Se via chemical bath deposition (CBD), the PA6/Cd-Se by successive ionic layer adsorption and reaction (SILAR) and the PA6/Ag-Cd-Se by cation exchange (CE) method. In order to have a deep understanding of the relationship between the composition and the end-use properties of polyamide-6-based selenium nanocomposites, we mainly focused on the description of the microstructure, morphology and optical properties of obtained composites. The XRD analysis of samples was performed on the Bruker Advance D8 diffractometer. SEM/EDS measurements were performed by using a Hitachi S-3400N microscope equipped with the Bruker Quad 5040 EDS system. AFM experiments were carried out at room temperature using a NanoWizard[®]3 NanoScience microscope. The UV-Vis spectrum (200 to 1100 nm) was recorded using a Spectronic Genesys 8 UV/Visible spectrophotometer with compensation for PA6 absorption.

In PA6/Se composite selenium formed at the end of the reaction was amorphous. The diffraction peaks positions in PA6/Cd-Se composite were mainly indexed as a hexagonal CdSe (JCPDS#77-2307) and a monoclinic Se₈ (JCPDS#71-528), respectively. PA6/Ag-Cd-Se composite XRD patterns showed a complex film crystalline composition with the hexagonal CdSe, the orthorhombic Ag₂Se (JCPDS#24-1410) and the metallic Ag (JCPDS#03-1472) peaks, respectively.

The diffractograms of PA6/Ag-Cd-Se also displayed monoclinic selenium. Obtained composites exhibit heterogeneous surface morphology: isolated particles of amorphous selenium, pyramidal-like single crystals and submicron-sized particles of no specific-shape observed on PA6/Se, PA6/Cd-Se, and PA6/Ag-Cd-Se surfaces, respectively. The investigated composites are direct band semiconductors (Table 1). Relatively high Urbach energy values indicate the formation of disordered structures, which correlates with heterogeneous surface morphology and composition.

Finally, we have succeeded in fabricating PA6/Se, PA6/Cd-Se, and PA6/Ag-Cd-Se composites with a direct optical band gaps in the visible spectral range, which appear to be promising candidates for optoelectronic components.

Table 1. The fundamental absorption edge (λ_g), optical band gap ($E_{\text{op.g}}$), Urbach energy (E_U) and steepness parameter (σ) of studied composite materials.

Composite	λ_g , nm	$E_{\text{op.g}}$, eV	E_U , eV	σ
PA6	278	4.46	1.32	0.0195
PA6/Se	555	2.23	0.094	0.237
PA6/Cd-Se	606	2.05	0.397	0.0646
PA6/Ag-Cd-Se	757	1.64	0.695	0.0369

References

1. Park, Y.; Advincula, R.C. *Chem. Mater.* **2011**, *23*(19), 4273-4294.
2. Liu, R. *Materials.* **2014**, *7*(4), 2747-2771.
3. Luccio, T. D.; Piscopiello, E.; Laera, A. M.; Antisari, M. V. *Mater. Sci. Eng. C.* **2007**, *27*(5-8), 1372-1376.

Contact person: Henrieta Markevičiūtė, Radvilėnų str. 19, Kaunas, Lithuania, phone: +370 62917619, e-mail: henrieta.markeviciute@ktu.lt

EXPLORING CAUSES, EFFECTS AND POSSIBLE SOLUTIONS FOR CHEMICAL POLLUTION IN THE ENVIRONMENT: CITIZENS' AND EXPERTS' OPINION

Žanna Martinsone¹, Lāsma Akūlova¹, Aneka Kļaviņa¹, Linda Paegle¹, Inese Mārtiņšone¹,
Darja Kaļūznaja², Marija Avota² and Ivars Vanadzīns¹

¹ Laboratory of Hygiene and Occupational Diseases, Institute of Occupational Safety and Environmental Health, Rīga Stradiņš University, Dzirciema 16, Rīga, Latvia, LV-1007

² Department of Occupational and Environmental Health, Rīga Stradiņš University, Dzirciema 16, Rīga, Latvia, LV-1007

Nowadays chemical pollution is strongly linked to human population. People consume vast amounts of food, water, energy – creating environmental pollution caused by unsafe use and management of chemicals (building materials, cleaning agents, perfumes, deodorants, insecticides control and personal care products etc.) at households level and in general. The aim of this study is to determine citizens' and experts' opinion regarding potential causes, exposure levels and prevention of chemical pollution in Latvia.

This pilot study was supported by Rīga Stradiņš University grant "Exploring Causes, Effects and Possible Solutions for Chemical Pollution in the Environment: Citizens' and Experts' Views". The pilot study data was received via focus groups interviews (<90 min) from individuals (N=36 (12 men, 24 women; age: 19–52) living in Riga/Rigas' peri-urban area. In total 5 citizen focus group (October – November 2019, February 2020) and 3 expert interviews (from governmental, educational and non-governmental organizations) were held. Interviews included topics on chemical pollution, waste management, environmental information availability and health effects of environmental pollution.

The main problems identified by respondents were lack of information and environmental education, infrastructure provision and access to the services, responsibility and environmental management (e.g. hazardous waste, large garbage management, the meaning of chemical product labelling. The importance of cost, infrastructure provision, availability of the service, functionality and effectiveness, simplicity, example, ecological safety and origin were highlighted as essential issues for chemical pollution managing in future as well. [1] Product and brand marketing, reviews and recommendations, also personal factors: environmental friendliness and increased environmental awareness influence the choices and actions regarding chemical products. [2]

The improvement of public environmental knowledge and access to information via schools, informative materials, and relevant applications for smartphones, advertisement and social campaigns, as well as supporting of eco-innovation is needed. Detailed monitoring and research on sewage, surface and groundwater quality monitoring, ambient and indoor air quality even at households, and human biomonitoring should be done.

References

1. Akūlova, L.; Bukina, A.; Martinsone, Ž. Environmental Management Challenges and Possible Solutions Regarding Chemical Pollution Caused by Households in Latvia: A Qualitative Pilot Study. *Environmental and Climate Technologies*. **2020**, *24*(3), 534-544.
2. Akūlova, L.; Bukina, A.; Martinsone, Ž. Factors influencing eco-friendly choices and environmentally sustainable action taking regarding chemical product usage in households, Latvia: A Pilot study. *Daugavpils Universitātes 62. Starptautiskās zinātniskās konferences rakstu krājums*. Available: https://dukonference.lv/files/978-9984-14-925-7_62_konf_kraj_A_Dabaszin.pdf

Contact person: Žanna Martinsone, Dzirciema street 16, Riga, Latvia, LV-1007, phone: +371 26157562, e-mail: zanna.martinsone@rsu.lv.

HUMAN BIOMONITORING INITIATIVE – FUTURE FOR HUMAN EXPOSURE ASSESSMENT TO CHEMICALS

Inese Martisone¹, Kristine Sproge¹, Lasma Akulova¹, Zanna Martinsone¹, Linda Matisane¹

¹ Institute of Occupation Safety and Environmental Health, Riga Stradiņš University, Riga, Latvia

People are exposed to a complex mixture of chemicals in their daily lives through the environment, consumer products, food and drinking water and at work. The human biomonitoring is one of the tools how to assess the associated health impacts of chemical mixtures to human health and improve risk assessment of chemical. In the case of established biomonitoring system in the country there is possibility to analyze data at the level of the individual and human biomonitoring data can inform medical treatment or guidance on the need to reduce exposure.

In the 2017 in the Europe started HORIZON 2020 project “Human Biomonitoring initiative for Europe Union” (HBM4EU). The main objective for Human Biomonitoring initiative is to generate evidence on the causal links between human exposure to chemicals and health outcomes and in work with chemical risk assessors adapt chemical risk assessment methodologies to use human biomonitoring data and to account for the contribution of multiple external exposure pathways to the total chemical body burden. Create limit values for human health and environment protection.

The purpose is not only to create new guidance limit values for the chemical under concern and communicate new knowledge to policy makers for effective implementation in a legal act, but as well as to evaluate the effectiveness of existing policies.

Riga Stradins university researchers are participating in the two HBM4EU subprojects: “Joint survey of pesticides (SPECIMEn study)” under WP-15 and “E-waste study” under WP-8. More information available: [HBM4EU – science and policy for a healthy future](#)

Contact person: Inese Martinsone, Dzirciema street 16, Riga, LV 1007, phone +371 29404158, e-mail: inese.martinsone@rsu.lv

DETERMINATION OF PHOSPHATES IN SOIL BY RAPID TEST METHOD

Luīze Terēze Medne¹, Jānis Ģībietis²

¹ Department of Analytical Chemistry, University of Latvia, Riga, Latvia

² Enola Chemical Co., Ltd., Riga, Latvia

Options for applying water quality rapid tests for detecting phosphates in soil samples were studied, looking at the best available soil phosphorus detection method. The official method used by the Ministry of Agriculture laboratories [1] has been used as the reference method [1].

Two phosphate detection test systems were used in the experiments – **Phosphate Test Strips** (*Industrial Test Systems*) and **Phosphate Low Range Checker Colorimeter** (*Hanna Instruments*). Soil sample extraction was performed with deionised water, 0,5 M potassium chloride solution, 0,5 M, 0,1 M and 0,01 M hydrochloric acid and 0,1 M, 0,01 M sulfamic acid solution.

The found P_2O_5 content in all soil samples was proportional to the reference method results, but its value was influenced by the used extraction media. Both rapid tests show similar results for all extractions, but the colorimeter can produce more accurate results than the visual test, as its accuracy is limited by visual reading of the colour.

The most immediate results of the reference method were obtained by extraction of soil samples for 5 minutes with a solution of 0,01 M sulfamic acid. The P_2O_5 content thus determined by the Phosphate Low Range Checker system is 1,2 to 1,4 times higher than that determined by the reference method while the Phosphate Test Strips method overlaps the results of the reference method following errors in visual reading (Figure 1).

Using the results of this study, a prototype of the phosphate rapid test supplement (extraction) kit was designed, which would be useful for the determination of phosphates in soil for small farms and hobby purposes as an alternative to laboratory tests.

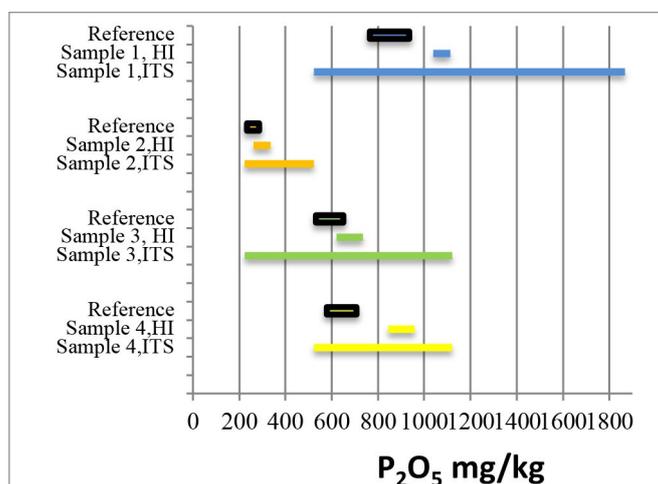


Figure 1. Comparison of the results of both rapid tests and reference analysis for soil samples 1-4 (5 min extraction with 0,01 M sulfamic acid solution) HI – Phosphate Low Range Checker Colorimeter (*Hanna Instruments*)
ITS – Phosphate Test Strips (*Industrial Test Systems*).

References

1. Zemkopības ministrija. Augsnes agroķīmisko analīžu metodes. Available: https://zm.gov.lv/public/ck/files/ZM/kartibas/ZMk_21_2014p6.pdf

Contact person: Jānis Ģībietis, phone: +371 29236869, e-mail: janis@enola.lv

EFFECT OF STARCH ADDITIVE ON THE PROPERTIES AND SOLUBILITY OF UREA GRANULES

Austėja Mikolaitienė¹, Rasa Šlinkšienė¹

¹ Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Lithuania

The Green Economy course of EU provides a macro-economic approach to sustainable economic growth, and encouraged sustainable Consumption and Production. Very important is investment into such economic activities, infrastructure and assets that allow reduced carbon emissions, and prevention of the loss of biodiversity and ecosystem services. Therefore more importance is placed on re-use of nutrients and biofertilisers and on the increase of efficiency of plant nutrients [1]. Approximately 30–40% of fertilisers used are lost, plants do not have enough time to absorb them due to rapid fertiliser solution. Fertilisers washed from the soil cause environmental problems. The intention is to create fertiliser, the solubility of nutrients whereof would conform to the plants' needs. An innovative field in fertiliser research is to obtain controlled-release fertilisers with a biodegradable substance from renewable raw materials [2, 3].

The aim of this study is to investigate the possibilities of microalgae using to produce efficient fertilizers. Raw materials mixtures were granulated by wet granulation method (the liquid phase-binder was sprayed onto the dry materials powder) and using a laboratory drum granulator-dryer. The biggest problems are caused by nitrogen leaching from concentrated fertilizers, so in the work urea was granulated with various binders: starch, starch + polyvinyl acetate and starch + polyvinyl acetate + glycerol. The strength, moisture, homogeneity (Figure 1) and dissolution rate of the obtained fertilizer granules were studied.

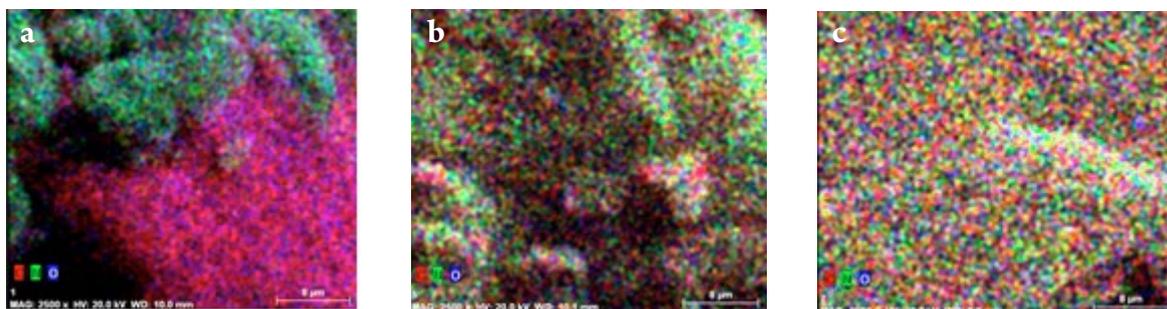


Figure 3. SEM maps of elements (C, N, O): *a* – starch; *b* – starch+polyvinyl acetate; acetate; *c* – starch+polyvinyl acetate+glycerol.

It was found that the use of the additive does not significantly increase the strength of the granules, the moisture content of the granules is up to 2%. Analyzing the results is important to mention that the dissolution rate of the granules with the additive is lower than that of pure urea. Consequently, such nitrogen fertilizers should reduce the negative impact on water pollution.

References

1. Sutton, M. A.; Bleeker, A.; Howard, C. M. *et al.* Our Nutrient World: The challenge to produce more food and energy with less pollution. **2013**.
2. Lawrencja, D., Wong, S. K., Low, D. Y. S, *et al.* Controlled Release Fertilizers: A Review on Coating Materials and Mechanism of Release. *Plants*. **2021**, *10*(2). 238.
3. Chojnacka, K.; Moustakas, K.; Witek-Krowiak, A. Bio-based fertilizers: A practical approach towards circular economy. *Bioresource Technology*. **2020**, 295.

Contact person: Rasa Šlinkšienė, Radvilėnų str. 19, Kaunas, Lithuania, +37037457070, e-mail: rasa.slinkisien@ktu.lt

MONITORING OF ALBENDAZOLE TRANSFER FROM SHEEP DUNG TO FODDER PLANTS AND ADJACENT SOIL BY UHPLC-MS

Martina Navrátilová¹, Andrea Sochová¹, Daniela Vráblová¹, Lenka Skálová¹

¹ Department of Biochemical Sciences, Faculty of Pharmacy in Hradec Králové, Charles University, Czech Republic

Introduction. Albendazole (ABZ), a broad-spectrum benzimidazole anthelmintic drug, is used in livestock and humans to treat gastrointestinal worms. Antihelmintics are administered to the animals as a preventative measure and across the board. Drugs used in livestock farming mainly enter the environment directly via excrements on the pastures or via manure from treated animals used for the fertilization of fields. Laboratory experiments showed that plants could uptake and even biotransform ABZ from dung under laboratory-controlled conditions, but it was not known if these were present under real field conditions. This study monitors the transfer of ABZ and its main transformation products (TPs) albendazole sulfoxide (ABZ-SO) and albendazole sulfone (ABZ-SO₂) from the dung of treated sheep to common fodder plants *Medicago sativa* and *Trifolium pratense* and adjacent soils. This was observed from different distances (plants, soil) and depths (soil) to which compounds could spread from dung piles.

Methods. A UHPLC-MS method for analysis of ABZ, ABZ-SO and ABZ-SO₂ has been developed and validated. To ensure that the method is suitable for its intended use, the method validation was performed according to SANTE/11813/2017. The parent drug and TPs were extracted from field samples by using two extraction methods: modified QuEChERS (EN 15662) for soil and LLE based on ethyl acetate for plants.

Results. Our study successfully detected the presence of ABZ TP (ABZ-SO and ABZ-SO₂) in the soil-plant system. Even two months after the first contact of fodder with faeces, ABZ-SO was still present in plants and connected soil.

Conclusions. In general, drugs might be a significant source of micropollutants in the environment. These chemicals could be found in soil and groundwater where it is possible for plants to uptake them. This entails the risk of spreading veterinary drugs on agricultural land with potential risk to ecosystems.

Acknowledgment. The study was supported by Charles University in Prague, project GAUK no. 1136120.

Contact person: Martina, Navrátilová, Akademika Heyrovského 1503, Hradec Králové, 500 05, Czech Republic, phone: + 420 495 067 449, e-mail: navratimart@faf.cuni.cz.

VARIATIONS OF MICRO- AND RARE EARTH ELEMENTS IN THE BOTTOM AND FLY WOOD ASH

**Megija Neimane¹, Vitālijs Lazarenko¹, Māris Bērtiņš¹, Arturs Viksna¹, Dagnija Lazdiņa²,
Kristaps Makovskis², Ilze Kārklīņa², Andis Lazdiņš²**

¹ University of Latvia, Faculty of Chemistry, Jelgava street 1, Riga, Latvia

² Latvian State Forest Research Institute "Silava", Riga street 111, Salaspils, Latvia

Wood ash is biomass obtained by the combustion of wood products (wood chips, logs, etc.). The main production of wood ash in large quantities is through the combustion of wood for the production of heat (e.g., factories) and energy (e.g., boiler houses). By combustion process, wood products produce ~6-10% ash from the total weight of wood and contain a high amount of macro- and microelements. Furthermore, several studies have shown that wood ash might also contain rare earth elements.

Nowadays, wood ash is used for various purposes. In several European Union countries, wood ash is used in road construction and asphaltting works. However, the most common application of wood ash is as a fertilizer for agricultural and forest soil. The high content of macro- and micro- elements in the wood ash ensures plants with the necessary nutrients and reduces soil acidity. Rare earth elements promote plant growth and increase crop yields. The use of wood ash can create biocycle, increase the amount of renewable energy, reduce the number of landfill sites and CO₂ emissions.

Wood ash is divided into two main types – bottom ash and fly ash. Bottom ash is the coarsest and granulated ash fraction with particle size from 0.4 mm to 4.7 mm that contains impurities (stones, sands, etc.). Fly ash is the finest fraction with particle size from 12 μm to 250 which contains inorganic compounds and a small amount of unburned carbon.

The aim of this research was to evaluate micro- and rare earth element content in the bottom and fly wood ash. Both types of wood ash samples were collected from boiler houses from the different parts of Latvia in 2014. Wood ash samples were extracted in concentrated HNO₃ by using a mechanical shaker, then the resulting solution was diluted with deionized water and filtered. The micro- and rare earth element content were determined by ICP-MS (Agilent 8900 ICP-QQQ) analysis method. The pH and electrical conductivity were also determined in the extract in the deionized water.

Obtained results show that wood ash is a highly basic material (pH > 12). The electrical conductivity of bottom ash is higher than fly ash. The content of Al, Mn, Zn, Cr, Cd and Pb in the fly ash is ~2-6 times higher than in the bottom ash. However, the content of Cu, Ni, V and As are ~2 times higher in the bottom ash. Rare earth elements content in the bottom ash is ~2-3 times higher than in the fly ash.

Acknowledgement. This study has been supported by LSFT financed research topic "Research program on improvement of forest growth conditions" (Agreement No 3.5.5-5.1-000z-101-16-31).

Contact person: Megija Neimane, phone: +371 26097159, e-mail: megijaneimane@gmail.com

TWO-DIMENSIONAL LIQUID CHROMATOGRAPHY – HIGH RESOLUTION MASS SPECTROMETRY METHOD FOR SIMULTANEOUS MONITORING OF 70 REGULATED AND EMERGING MYCOTOXINS

Estefanija Novicka^{1,2}, Iveta Pugajeva², Ingars Reinholds², Vadims Bartkevics^{1,2}

¹ Department of Analytical Chemistry, University of Latvia, Riga, Latvia

² Institute of Food Safety, Animal Health and Environment "BIOR", Riga, Latvia

Tea is one of the most popular and widely consumed beverages in the world (being the leading drink after water in terms of consumption). Unlike other types of tea, Pu-erh belongs to the best known post-fermented teas, which need a long time of maturation to be considered ripened. It is unique due to the microbial postfermentation process, which may last from several months to many years, resulting in potential fungal contamination, but there have been very few studies on multi-mycotoxin occurrence in Pu-erh teas, generally because of problems with analytical method development for this complex matrix [1, 2].

In recent years, two-dimensional liquid chromatography (2D-LC) has raised a significant interest in the field of separation science. It is based on combining two solid phases to achieve higher separation power and peak capacity. 2D-LC is mostly applied in the case of sophisticated interactions and pronounced matrix effects [3]. Generally, there are two most commonly used modes of *online* 2D-LC separation including comprehensive and heart-cutting analysis. The main advantage of heart-cutting technique is that first and second dimension run times are decoupled and can be operated closer to optimal conditions without any time constraints on the second-dimension separation, providing higher peak resolution [4].

The aim achieved during this work was to expand the scope of mycotoxins detectable within one analytical method and improve selectivity of the method using chromatographic separation by 2D-LC technique. Finally, this fully automated, sensitive and reliable *online*-heart-cutting two-dimensional liquid chromatography method coupled with time-of-flight high resolution mass spectrometry (2D-LC-TOF-HRMS) for the determination of 70 emerging and regulated mycotoxins in Pu-erh tea was fully validated according to the performance criteria set in the European Union (EU) guidelines and applied for the analysis of 20 Latvian Pu-erh teas.

The most frequent occurrence (100%) among 19 detected mycotoxins was determined for deoxynivalenol (DON) and its metabolites (D3G, 3-AcDON and 15-AcDON) with the highest content for DON reaching the maximum of 8946 µg/kg in the raw Pu-erh tea material.

References:

1. Sedova, I.; Kiseleva, M.; Tutelyan, V. *Toxins*. **2018**, *10*(11), 444.
2. Yashin, A.; Nemzer, B.; Combet, E.; Yashin, Y. *J. Food Res.* **2015**, *4*(3), 56-88.
3. Wang, Y. Q.; Tang, X.; Li, J. F.; Wu, Y. L.; Sun, Y. Y.; Fang, M. J.; Wu, Z.; Wang, X. M.; Qui, Y. K. *J. Chromatogr. A.* **2017**, *1519*, 145-151.
4. Yang, Y.; Zhang, Y.; Wei, C.; Li, J.; Sun, W. *Talanta*. **2018**, *187*, 252-258.

Contact person: Estefanija Novicka, phone: +371 26628269, e-mail: estefanija.novicka@gmail.com

EXPOSURE TO AIR POLLUTION IN THE OIL SHALE REGION IN ESTONIA AND RELATED BIRTH EFFECTS

**Hans Orru¹, Triin Veber¹, Katrin Lang¹, Inge Ringmets¹, Tanel Tamm¹, Marek Maasikmets²,
Leena Albrecht³, Märten Lukk³**

¹ Institute of Family Medicine, University of Tartu, Tartu, Estonia

² Estonian Environmental Research Centre, Tallinn, Estonia

³ Estonian Health Board, Tallinn, Estonia

Despite improved air quality in the oil shale region in Ida-Viru County, Estonia across the years, a quarter of the population still see air pollution within their place of residence being rated as posing a high or very high risk to their children's health. Also, scientific research indicates health effect of fine particles (PM_{2.5}) at concentrations far below limit values set by the European Union. Among the pollutants, the impact which can be caused by the oil shale industry is characterized best in Ida-Viru County by exposure to PM_{2.5}. Current study aimed to see how the air pollution has been affecting risk of birth effects: babies born prematurely (<37 weeks) and/or having low birth weight (≤2500 g).

During the analysis birth data was retrieved from Estonian birth registry for 2004–2018. The air pollution exposure was assessed with combination of measured (indicating temporal variation) and modelled (indicating spatial variation) concentrations of pollutants. The association were studied with logistic regression analysis.

The proportion of babies, which are born preterm, is highest in Ida-Viru County (5.9%) among all the Estonian counties. Health inequality levels also reflected in the form of lower birth weights, being 125 g lower in Ida-Viru County in comparison to the average figures for the other Estonian regions. The analysis showed that exposure PM_{2.5} during the first trimester increased the risk of a preterm birth, while exposure in the third trimester increased the risk of a low birth weight. In terms of the latter indicator, though, the impact on birth weight was only evident in Ida-Viru County. Other pollutants, which were also studied, had no significant effect (such as PM₁₀ or NO₂), or had a less significant effect (such as B(a)P), or provided controversial results (such as for benzene). The risk of a preterm birth – as well as of a low birth weight – were also increased by living within a ten-kilometre radius of the oil shale industry. Moreover, the study showed indicate that the closer the mother's residence to the oil shale industry (equal to or less than 3 km, 5 km, or 10 km), the poorer are the birth indicators.

As significant drivers for such birth effects include air pollution, as well as various socio-demographic factors, it is equally important to limit pollutant emissions and to improve the living environment in Ida-Viru County as a whole. In order to reduce pollutant emissions, the oil shale companies should use the best available technology (BAT) to achieve their goals, as the risk of preterm births and low birth weights has been shown to be higher within the vicinity of an operational oil shale industry site. Furthermore, levels of awareness in local people as well as policy makers and physicians need to be raised within the region which is suffering most from such levels of impact by air pollution on birth indicators. We believe that improving the health of the people of Ida-Viru County should be an essential part of fair transition with-in the European Green Deal, as health inequality levels here are significant in the area and begin already before birth.

Contact person: Hans, Orru, Ravila 19, Tartu 50409, Estonia, phone: +372 7374203, e-mail: hans.orrut@ut.ee

DEVELOPMENT OF A METHOD FOR THE TAR ANALYSIS IN CO-PRODUCED GAS

Sergejs Osipovs¹, Aleksandrs Pučkīns¹

¹ Department of Applied Chemistry, Daugavpils University, Daugavpils, Latvia

Introduction. The biggest problem with discarding old tires is that they contain chemicals and heavy metals that leach into the environment as the tires break down. Some of these chemicals are carcinogenic and mutagenic. One of the methods for solving the problem is pyrolysis of old tyres. Pyrolysis dissolves waste and also produces useful by-products. In this case, gas, liquid and solid phases are formed. Gas mixture containing tar, among other components. Traditional methods for tar sampling are based on cold solvent-trapping coupled with solvent absorption in impingers.

Methods. The present work focuses on a solid-phase adsorption (SPA) method for determining the concentration of tar compounds. A modified sampling device consisting of 500 mg of amino-phase sorbent and 100 mg of activated coconut charcoal was chosen as optimal for sampling tar (including its volatile organic compounds) in gas produced in tyre pyrolysis. For research in a real life context, the double-layered fixed-bed reactor situated in eastern Latvia (Daudavpils region) was used. Varying volumes of pyrolytic gas were drawn through the adsorbents, and the total amount of tar was then compared to the number of its individual component compounds.

Tar was sampled at the pyrolytic gas temperature of 250 °C. It was drawn through the adsorbent cartridges at the flow rate of 100 mL min⁻¹ for various periods of time, namely 1, 2, and 3 min, resulting in 100, 200, and 300 mL of the pyrolytic gas being drawn through the adsorbents respectively.

Results. Both sorbents were analyzed separately. All heavy compounds of the tar are completely adsorbed on amino-phase adsorbent, and light compounds of the tar, such as benzene and toluene, are partially adsorbed on this amino-phase adsorbent, and partially on activated coconut charcoal. The total amounts of each compound were calculated, as well as the tar on both sorbents. The results were converted to normal cubic meters of pyrolytic gas. The dependence of the concentration of the total tar and some of its compounds on both sorbents on the volume of the pyrolytic gas passed through them has been investigated. It was concluded that the volume of pyrolytic gas had little or no effect on the total amount of tar found on both adsorbents. For example, when 100 mL of pyrolytic gas was passed through the adsorbents, the total tar concentration was 7348 ± 228 mg m⁻³; when 200 mL was collected, the concentration was 7412 ± 302 mg m⁻³; and at 300 ml the concentration was 7395 ± 269 mg m⁻³.

Conclusions. Testing the device consisting of 500 mg of the amino-phase adsorbent and 100 mg of activated coconut charcoal in real life conditions, along with varying volumes of the pyrolytic gas drawn through the adsorbents, gave results that were comparable in the total amounts of both tar and its individual component compounds. However, with an increase of the volume of pyrolytic gas drawn through the adsorbents, greater amounts of benzene, toluene, and other light compounds pass through the amino-phase adsorbent and are collected on the activated coconut charcoal. An increased volume of pyrolytic gas leads to a growing number of compounds detected and identified on the amino-phase adsorbent. It appears reasonable to take into account the concentration of tar in the pyrolytic gas while selecting the volume of gas for sampling, as well as whether it is necessary to detect those individual tar compounds whose concentration is very small.

Contact person: Sergejs Osipovs, Parades 1A, Daugavpils, Latvia, phone: +371 26163221, e-mail: sergejs.osipovs@du.lv

APPLICATION OF MULTIFACTOR ANALYSIS FOR DRINKING WATER QUALITY CONTROL IN RIGA CITY

Kristaps Oskalns^{1,2}, Maris Bertins¹, Edgars Selickis², Arturs Viksna¹

¹ University of Latvia, Faculty of Chemistry, Jelgavas iela 1, LV-1004, Riga, Latvia

² Joint Water Quality Control laboratory, Riga Water Ltd., Bauskas iela 209, LV-1076, Riga, Latvia

In the centralized drinking water supply network of Riga, water is supplied from five water treatment stations, four of which are underground water pumping stations: “Baltezers”, “Baltezers II”, “Rembergi”, “Zakumuīža” and one is the surface water treatment station “Daugava”. The chemical composition of the water produced in these stations is different. The quantity and quality of water supplied are monitored daily, but the Riga water supply network is very long (~ 1482 km) and in some places, variable water quality is possible, which is influenced by several factors, such as rapid pressure change, slow water flow, etc.

Water quality in the supply network may change due to various factors and not always significant changes in drinking water quality can be assessed by only one indicator, for example, the pH value in the center of Riga may change depending on the water origin, but the quality may meet the requirements. Therefore, when planning the control of drinking water quality, it is very important to identify as many measurable parameters as possible by including them in multifactor analysis methods. If significant changes are found in several parameters of the analysed sample, it is necessary to perform a more in-depth study of the causes of these changes. One of the reasons for the changes in the quality indicators for the drinking water of the city of Riga is the change of the place of origin of the supplied water – the water supply is provided from another water treatment station. In this case, it would be important to know the origin of the drinking water sample.

In this study drinking water of Riga city was classified and evaluated the possibilities of authentication using principal component analysis. Eight different samples were taken at four different times in period of time from 2020 and 2021. Each sample was analysed for pH, conductivity and sulphate, chloride, calcium content. Using analysed data Larson and Langelier indexes were calculated for determining water corrosivity.

Obtained results showed that using the analysis of the main components, it is possible to classify Riga drinking water into six groups – Baltezers, Zakumuīža, Daugava, Daugava and Baltezers, Baltezers and Zakumuīža and mixed water of all stations. When classifying drinking water in the city of Riga, four groups are formed: water with moderately corrosive properties and the ability to dissolve the protective layer of calcium carbonate, water with no corrosive properties and which tends to slightly precipitate calcium carbonate forming a protective layer, water with a tendency to form a protective layer of calcium carbonate, but characterized by strong corrosivity according to the Larson index and mixed type drinking water (groundwater and surface treated drinking water) with highly corrosive properties and a tendency to slightly dissolve the protective layer of calcium carbonate. Using the analysis of the main components, it is possible to determine the place of origin of drinking water samples taken from the Riga centralized water supply and also to estimate the intensity of mixing of water prepared by different stations.

Contact person: Kristaps Oskalns, e-mail: oshkalns@gmail.com

BLACK CARBON DEPOSITION ON TREE FOLIAGE AN URBAN BACKGROUND IN VILNIUS

Daria Pashneva¹, Ieva Uogintė¹, Julija Pauraitė¹, Agnė Minderytė¹, Kristina Plauškaitė¹, Valda Araminienė², Eugenija Farida Dzenajavičienė³, Valda Gudynaitė-Franckevičienė², Iveta Varnagirytė-Kabašinskienė², Nerijus Pedišius³, Egidijus Lemanas³, Tomas Vonžodas³, Steigvilė Byčenkienė¹

¹ SRI Center for Physical Sciences and Technology (FTMC), Saulėtekio ave. 3, Vilnius, Lithuania

² Lithuanian Research Centre for Agriculture and Forestry, Instituto av. 1, Kėdainiai distr., Lithuania

³ Lithuanian Energy Institute, Breslaujos str. 3, Kaunas, Lithuania

Black carbon (BC) is a primary particulate aerosol component derived from incomplete combustion processes and have impact on regional and global climate change, air quality, public health and ecosystems [1] including increased temperatures, accelerated ice and snow melt, and disruptions to precipitation patterns. Mounting scientific evidence suggests that reducing current emissions of BC can provide nearterm climate benefits, particularly for sensitive regions such as the Arctic. Because of the strong warming potential and short atmospheric lifetime of BC, BC mitigation offers an opportunity to address key climate effects and slow the rate of climate change. However, BC reductions cannot substitute for reductions in long-lived greenhouse gases (GHGs). The main sources of BC in urban areas are traffic and heating [2] climate and human health. In this study, equivalent black carbon (eBC). Green infrastructure (especially urban trees) plays an important role in improving air quality [3]. This study investigates potential influence of urban trees on BC removal by *Norway spruce* and silver birch along with the BC formation, mass concentration and source apportionment. Measurements were performed during July-October 2020 at an urban background station in Vilnius. The aethalometer (A Magee Scientific Company Aethalometer model AE31) provided continuous real-time measurements of BC mass concentration. Transmission electron microscopy (Tecnai G2 F20 X-TWIN, resolution 0.25-0.102 nm) in combination with energy scattering X-ray spectroscopy (EDX) was used to characterize and obtain detailed information on the morphology, size, and elemental composition of individual aerosol particles deposited on leaf of silver birch (*Betula pendula* Roth) and needle of Scots pine (*Pinus sylvestris* L.). This study has shown that traffic (54 %) and firewood and agro-biomass burning are both significant contributors to BC emissions during the warm season in urban background area in the period of June-October 2020. BC aerosol particles were found in all samples of leaves and needles as a result of the condensation mechanism during combustion. The diameter of primary particles ranged from 24 nm to 30 nm on leaves of silver birch, and from 32 nm to 44 nm on spruce needles. Larger agglomerates were found on the needles of conifers than on broadleaf trees, as they form a thicker epicuticular wax layer and are more efficient in accumulating BC. The present work confirmed the role of BC traffic mitigation in urban areas and improving emissions reduction efficiency for solid biomass burning. This work was carried out in the framework of the project "Investigation of aerosol black carbon emissions from biomass incineration units and deposition on tree foliage" (RTO Lithuania).

References

1. U.S. EPA, "Report to Congress on Black Carbon," *Dep. Inter. Environ. Relat. Agencies Appropriations Act, 2010*. Available: <https://www3.epa.gov/airquality/blackcarbon/2012report/fullreport.pdf>.
2. Helin, A., *et al.*, Characteristics and source apportionment of black carbon in the Helsinki metropolitan area, Finland, *Atmos. Environ.* **2018**, *190*, 87-98.
3. Barwise, Y. Designing vegetation barriers for urban air pollution abatement : a practical review for appropriate plant species selection, *npj Clim. Atmos. Sci.* **2014**, 1-19.

Contact person: Daria Pashneva, phone: +370 60455746, e-mail: daria.pashneva@ftmc.lt

THE OPTIMISATION OF ORGANOSOLV PROCESS OF BARK DELIGNIFICATION PROCESS-WITH FOCUS ON PURIFICATION OF ISOLATED LIGNIN FRACTION

Matiss Pals^{1,2}, Maris Lauberts², Alexandr Arshanitsa², Arturs Viksna¹

¹ University of Latvia, Faculty of Chemistry, Jelgavas iela 1, Riga, Latvia

² Latvian State Institute of Wood chemistry, Dzerbenes iela 27, Riga, Latvia

Residual bark, after non lignin phenolic extraction, is a valuable resource suitable for further fractionation in terms of effective lignin and carbohydrates obtaining. A promising environmentally friendly approach for residual bark processing is *Organosolv* delignification using alcohols-water mixtures as a solvent. This approach allows obtaining of lignin with low degree of condensation and high solubility in organic solvents and high amounts of reactive functional groups, that is suitable for further use in various polymeric material obtaining. Lipophilic compounds are the dominant group of admixtures present in separated aspen bark lignin fraction. To obtain pure lignin from aspen bark total processing scheme has to be optimized to include pre-treatment and post-treatment methods of admixture separation. Complete processing scheme is shown in figure 1.

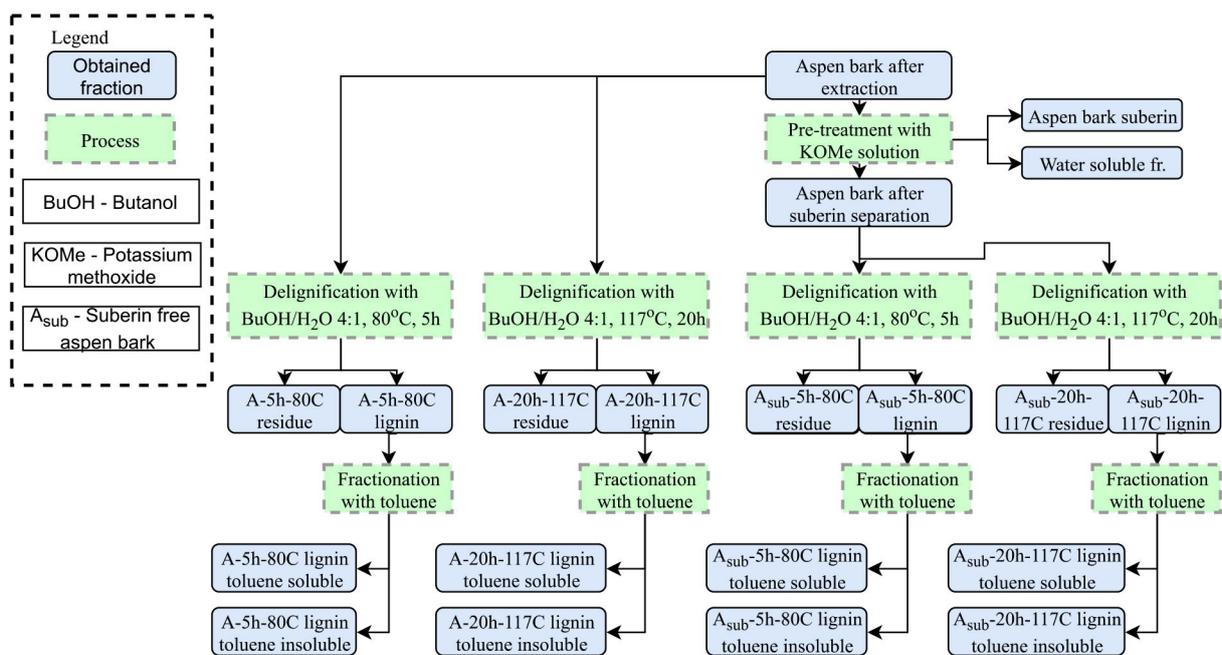


Figure 1. Proposed pathways *Organosolv* delignification of extracted bark.

All obtained fractions were characterized by using analytical pyrolysis, FTIR and GC-FID methods in terms of lignin content, carbohydrate content as well as lipophilic admixture content. Obtained results show that by combining pre-treatment and post-treatment of lignin fractions, it is possible to decrease significantly the content of non-lignin impurities in isolated fractions of aspen bark lignin.

Contact person: Matiss Pals, Latvian State Institute of Wood Chemistry, Dzerbenes 27, LV-1006 Riga, Latvia, phone: +371 28330283, e-mail: matiss.pals@kki.lv

ANALYSIS OF WASTEWATER SAMPLES FOR DETERMINATION OF MYCOTOXINS

Romans Pavļenko^{1,2}, Zane Bērziņa^{1,2}, Mārtiņš Jansons², Vadims Bartkevičs^{1,2}

¹ Faculty of Chemistry, University of Latvia, Riga, Latvia

² Institute of Food Safety, Animal Health and Environment "BIOR", Riga, Latvia

Mycotoxins are a large group of various structural compounds and biological exposures, and they are made by various groups of fungi. Mycotoxins are considered a global health, agriculture, and economical threat. Most mycotoxins are chemically stable, they survive storage and processing, and could even remain in cooked food, so humans are mainly exposed through direct ingestion of contaminated foods. Mycotoxins are metabolised by the liver and/or kidney, depending on their type and their metabolized products are excreted in the urine. Wastewater based epidemiology is a novel biomonitoring approach for tracking human exposure to mycotoxins. Therefore, sensitive and selective wastewater sample preparation and instrumental method was developed by several authors [1].

Within the current study the main parameters of the analysis were optimised for the determination of mycotoxins which were detected in wastewater samples – deoxynivalenol, beauvericin, enniatin A, enniatin A1, enniatin B and enniatin B1. Quadrupole tandem mass spectrometry was selected for the quantification of these compounds.

13 analytical columns were compared by the sorption coefficient and the number of theoretical plates. The best result of separation for deoxynivalenol was achieved using Hypercarb column, and for others – Kinetex PFP column.

Five solid phase extraction (SPE) columns (Strata X, Strata-C18, Oasis HLB, Strata Basic Screen, and Strata ABW) were compared. Three sample volume 333 mL, 666 mL, and 1000 mL were compared. Matrix effects were compared, and it was found that ion suppression effects were observed for almost all compounds. The method precision ranged from 1.3 to 7% for different mycotoxins. At stability test was not found any significant analyte degradation after storage for 2 weeks at -18 and +4 °C.

The developed method has lower limit of detections than other studies performed so far, for example, in this study LOD of deoxynivalenol is 1.9 ng/L, for beauvericin is 0.039 ng/L and for ENNs' are 0.044 – 0.14 ng/L, and for the first time the detection of mycotoxin from the enniatin group was achieved [2].

References

1. Gracia-Lor, E.; Zuccato, E.; Hernández, F.; Castiglioni, S. Wastewater-Based Epidemiology for Tracking Human Exposure to Mycotoxins. *J. Hazard. Mater.* **2020**, 382, 1-7.
2. Schenzel, J.; Schwarzenbach, R. P.; Bucheli, T. D. Multi-Residue Screening Method To Quantify Mycotoxins in Aqueous Environmental Samples. *J. Agric. Food Chem.* **2010**, 58(21), 11207-11217.

This work was supported by the Latvian Council of Science under project No. lzp-2020/2-0128.

Contact person: Romans Pavļenko, Lejupes Street 3, Riga, Latvia, phone: +371 22351223, e-mail: romans.pavlenko@bior.lv

FINGERPRINTING HUMAN PHARMACEUTICALS, ILLICIT DRUGS AND NEW PSYCHOACTIVE SUBSTANCES IN WASTEWATER: A MULTI-METHOD APPROACH

Ingus Pērkonis¹, Laura Elīna Ikkere^{1,2}, Veronika Šukajeva^{1,2}, Iveta Pugajeva¹

¹ Institute of Food Safety, Animal Health and Environment "BIOR", Lejupes iela 3, Riga, LV-1076, Latvia

² University of Latvia, Faculty of Chemistry, Jelgavas iela 1, Riga LV-1004, Latvia

The main concept of sewage biomarker analysis is that a representative sample of wastewater acts as surrogate pooled urine sample from the combined population [1]. Hence, wastewater is a treasure trove of biological and chemical information, and continuous monitoring of biomarkers may unravel time-trends of multiple factors affecting community-wide health and behaviour.

In our study we focused on human pharmaceuticals, illicit drugs, new psychoactive substances (NPS) and major metabolites of these bioactive compounds. Considering that the physicochemical properties of these substances are extremely diverse, a multi-method approach was explored. We developed three high-resolution mass spectrometry (HRMS) based methods on Orbitrap-MS and FT-ICR-MS platforms, that utilize different sample introduction techniques: direct infusion, reversed-phase liquid chromatography (RP-LC) and hydrophilic interaction liquid chromatography (see Figure 1.).

In case of targeted analysis, a reference standard is crucial for the confirmation purposes. Yet, such standards for illicit drugs and NPS are difficult to obtain and store due to legislative measures and limited commercial availability. Thus, the method was developed and applied without the use of reference standards. Optimization steps of the suspect screening workflow relied on a selection of "off-target" analytes (e.g., pesticides, biogenic amines, mycotoxins, etc.), which acted as proxies, mimicking the chemical diversity of the actual suspect substances. To lower the rate of false-positive hits, tentative identification of suspect compounds was performed using several criteria: accurate mass (<5 ppm) and isotopic pattern (from 20 to 50 %) are in accordance to the theoretical values and at least two fragment ions can be matched against experimental MS/MS spectra from the database (i.e., METLIN and Mass Bank of North America).

The developed multi-method approach was used for the selected biomarker in real samples collected regularly within a period of eight months from the main wastewater treatment plant in Riga, Latvia. The results of study revealed population's behaviour at various stages of COVID-19 pandemic.

References

1. Reid, M. J.; Baz-Lomba, J. A.; Ryu, Y.; Thomas, K. V. Using biomarkers in wastewater to monitor community drug use: A conceptual approach for dealing with new psychoactive substances. *Science of The Total Environment*. **2014**, 487, 651-658.

Contact person: Ingus Perkonis, Lejupes iela 3, Riga, LV-1076, Latvia, phone: +371 67620513, e-mail: ingus.perkonis@bior.lv

Human pharmaceuticals, illicit drugs, new psychoactive substances and major metabolites of these compounds

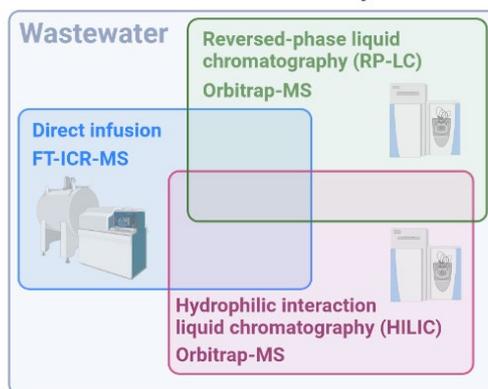


Figure 1. A schematic representation of the developed multi-method approach.

ANALYSIS OF POLLUTANTS IN INDUSTRIAL WATER USED FOR COOLING OF CO-PRODUCED GASES

Aleksandrs Pučkīns¹, Sergejs Osipovs¹

¹ Department of Applied Chemistry, Daugavpils University, Daugavpils, Latvia

Introduction. Pyrolysis dissolves waste and also produces useful by-products. In this case, gas, liquid and solid phases are formed. Gas mixture containing tar, among other components. Water scrubbing technology is used for pyrolytic gas purification. The disadvantage of this technology is that tar components gradually accumulate in the water. Most exposed to this process the readily soluble light heterocyclic aromatic compounds of tar, as well as heavy polyaromatic compounds of tar. Some light aromatic tar compounds, the content of which is usually very high in the pyrolytic gas, are present in small amounts in the cooling and cleaning water. In the pyrolytic gas purification process, not only does the total amount of tar in the cooling and cleaning water increase, but also the ratio of the individual tar compounds to each other changes, especially the heaviest polyaromatic tar compounds accumulate, which leads to problems. Further purification and use of the cooling and rinsing water itself.

Methods. Cooling water from the scrubber for analysis was sampled at the pyrolytic gas temperature of 250°C three times – after 5, 10, and 15 pyrolysis cycles. The analysed tar components were extracted from water using dichloromethane. To 100 mL of water was added 4 mL of dichloromethane and was shaken for 30 minutes. The procedure was repeated three times from the same sample to increase yield. The extracts were then combined and concentrated using a rotary evaporator, filtered through syringe filters and injected into GC-MS.

Results. The concentrations of individual tar compounds in cooling and cleaning water increase in different ways with increasing pyrolysis cycles. For example, for light aromatic tar compounds, poorly soluble in water, such as benzene and naphthalene, when pyrolysis cycles are tripled, their concentration in cooling and cleaning water increases only 1.69 and 1.57 times, respectively. But for light heterocyclic aromatics tar compounds readily soluble in water, such as phenol, m-cresol, p-cresol, and 2,3-xyleneol, with an increase in pyrolysis cycles by three times, their concentration in cooling and cleaning water increases by 2.54, 2.63, 2.48, and 2.74 times, respectively. Likewise, for heavy polyaromatic tar compounds poorly soluble in water, the increase in concentrations in cooling and cleaning water with an increase in pyrolysis cycles occurs significantly more than for light tar compounds. For example, for tar compounds such as pyrene, chrysene, and coronene, when pyrolysis cycles triple, their concentration in cooling and cleaning water increases 2.69, 1.91, and 2.52 times, respectively.

Conclusions. Cooling and cleaning water, in the process of contact with pyrolytic gas, gradually accumulates readily soluble light heterocyclic aromatics tar compounds, as well as heavy polyaromatic tar compounds. Some light aromatics tar compounds, the content of which is usually very high in pyrolytic gas, are present in small quantities in cooling and cleaning water. In the process of purification of pyrolytic gas, not only does the total amount of tar in the cooling and cleaning water increase, but also the ratio of individual tar compounds to each other changes, especially accumulating the heaviest polyaromatic tar compounds, which leads to problems of further purification and utilization of the cooling and cleaning water itself.

Contact person: Aleksandrs Pučkīns, Parades 1A, Daugavpils, Latvia, phone: +371 25949235, e-mail: aleksandrs.puckins@du.lv

NANOSTRUCTURING AMORPHOUS CALCIUM PHOSPHATE: CARBONATE INCLUSION

Aiga Anna Pudule¹, Laura Komarovska², Arturs Viksna², Dārta Ūbele¹, Kārlis Agris Gross¹

¹ Institute of Materials and Surface Engineering, Riga Technical University, Riga, Latvia

² Dept. of Analytical Chemistry, University of Latvia, Riga, Latvia

Amorphous calcium phosphate (ACP) is an alluring compound with many possibilities for different compounds to be designed as it welcomes ion substitution. In biomaterials, carbonate ion substitution not only makes ACP more similar to bone, but it also enhances the bioactivity and solubility, making it more suitable for biomedical processing routes. In this study, we have compared three nanostructuring pathways - heating in a furnace, and hydrothermal processing in water or steam – to determine:

- a) the capacity for ACP to form monophasic apatite of seven different Ca/P molar ratio (1.67, 1.8, 2.0, 2.2, 2.4, 2.6, 2.8) powders;
- b) CO₃²⁻ inclusion in ACP structure and arrangement in the ACP structure; and
- c) the total CO₃²⁻ content in ACP powders with various Ca/P molar ratio.

The intention is to provide an insight into the various nanostructuring possibilities and outcomes, that contribute to the design of patient specific biomaterials in the future.

ACP powders were synthesized by precipitation and freeze-drying. The obtained powder and nanostructured samples were characterized by X-ray diffraction (XRD) and Fourier transform infra-red spectroscopy (FTIR) to determine the stability of amorphous phase and chemical bonding. Nanostructuring was done by heating samples in a furnace in air at 700 for 2h and hydrothermally heating at 150 for 2h. Nanostructured samples were investigated in more detail by FTIR deconvolution of the 800-900 cm⁻¹ CO₃²⁻ peak to determine ion inclusion in the ACP structure with various Ca/P molar ratios. In addition, carbon mass fraction analysis showed the CO₃²⁻ ion content with various Ca/P molar ratio ACP powders.

Results show that the amorphous phase can be retained up to a Ca/P ratio of 2.6. Nanostructuring approaches showed that all approaches (heating in the furnace, and hydrothermal processing in water) resulted in monophasic apatite up to Ca/P of 2.0, however hydrothermal processing in steam maintained stability even up to Ca/P of 2.2. FTIR deconvolution showed all 3 types of CO₃²⁻ substitution with the non-apatitic form as the most often occurring for non-structured samples, however, nanostructuring of ACP decreases non-apatitic CO₃²⁻ inclusion. Total carbonate ion content in ACP powders increased linearly with the Ca/P molar ratio.

References

1. Yasar, O. F., Liao, W.C., Stevansson, B., Edén, M., *J.Phys.Chem.C.*, **2021**, 125(8), 4675–4693.

Contact person: Aiga Anna Pudule, Paula Valdena 3/7, Riga, Latvia, phone: +371 27107475, e-mail: aiga-anna.pudule@rtu.lv

INSIGHTS INTO AN ELECTROCHEMISTRY OF NEUROTRANSMITTERS USING THE CYCLODEXTRINS MODIFIED ELECTRODES

Ingrida Radveikienė¹, Gintautas Bagdžiūnas¹

¹ Group of Supramolecular Analysis, Institute of Biochemistry, Life Sciences Centre, Vilnius University, Saulėtekio av. 7, LT-10257, Vilnius, Lithuania

Neurotransmitters (NTs) play a key role in the regulation of physiological and behavioral functions such as sleep, mood, memory, etc. [1]. Hence, various analytical tools have been reported for the determination of NTs in biological matrices. However, the selective detection of NMs in human body is a difficult task because they have very similar chemical and physical properties [2]. In turn, electrochemical sensors based on cyclodextrins (CDs) as the molecules with cavities have been applied to analyze biomedical and pharmaceutical analytes [3].

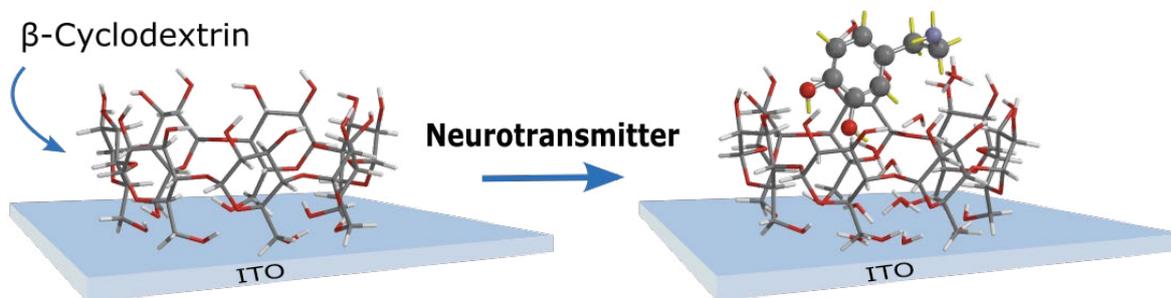


Figure 1. The ITO electrode coated by β -CD and schematic analysis of NTs.

In this work, indium tin oxide (ITO) electrodes were coated with a monolayer of β -CD and γ -CD monolayers (β - or γ -CD/ITO) and characterized (Figure 1). The NTs such as adrenalin, serotonin, dopamine and melatonin were analyzed in this work. Electrochemical analysis of the NTs using the β - or γ -CD/ITO as the working electrodes was carried out by cyclic voltammetry (CV) at different pH of 4.1, 7.0, 9.0 and 12.0. Additionally, to estimate the association energies, the host–guest systems of the NTs in CDs as the supramolecular assemblies were computed using density-functional theory (DFT).

Acknowledgement. This work was supported by the Research Council of Lithuania (grant number: S-MIP-20-45).

References

1. Banerjee, S.; McCracken, S.; Hossain, M. F.; Slaughter, G. *Biosensors*. **2020**, *10*(101), 1-18.
2. Yin, B.; Zhai, H. L.; Zhao, B. Q.; Bi, K. X.; Mi, J. Y. *Bioelectrochemistry*, **2021**, *139*, 1-7.
3. Lenik, J. *Current Medicinal Chemistry*. **2017**, *24*, 2359-2391.

Contact person: Ingrida Radveikienė, Vilnius, Lithuania, phone: +370 63929685, e-mail: ingrida.jurkeviciute@gmc.vu.lt

COFFEE GROUNDS IMPACT ON A RYE GROWTH

Dovilė Ragauskaitė¹, Rasa Šlinkšienė¹

¹ Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Lithuania

Urbanization is closely linked to the food industry. According to the Food and Agriculture Organization of the United Nations (FAO), global food waste reached 1.3 billion tones (one third of total production for human consumption) [1]. Food waste includes all waste generated in the food chain: during the stages of cultivation, harvesting, processing, storage, transportation and consumption. The disposal of biodegradable organic waste and its accumulation in landfills poses a variety of environmental, economic and social problems [2]. The scientific literature suggests that coffee grounds are not only high in calories but are rich in a variety of chemical elements and compounds that could be used and applied to other industries [3], e.g., coffee grounds can be used in agriculture – as an alternative organic fertilizer that improves chemical and physical properties of the soil and promotes plant growth. Portuguese researchers studied the influence of fresh and composted coffee grounds on the growth of lettuce (*Lactuca sativa*). The results showed that both fresh and composted coffee grounds improved lettuce growth compared to the control sample, but this was greatly influenced by the coffee grounds to soil ratio. The best results were obtained when fresh coffee grounds accounted for 2.5–5% of the total weight of the mixture and 10% for composted one. The use of more than 10% of fresh coffee grounds resulted in a slowing of plant growth [4].

This research analyses the spent coffee grounds additive impact on rye (*Secale cereale* L.) growth.

During the research coffee grounds were mixed with soil. Five different composition mixtures were prepared: 0 %, 2 %, 4 %, 6 % and 8 % of coffee grounds were added to the soil, respectively. Mixture with no coffee grounds was considered as a control.

The grown rye was cut, then weighed. The length of each stem was measured and the number of leaves was determined. Results showed that the addition of coffee grounds has a negative effect on rye growth.

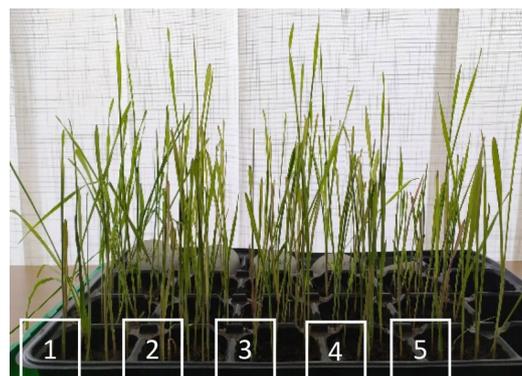


Figure 4. *Secale cereale* L. grown in mixtures with: 1–0; 2–2; 3–4; 4–6; 5–8 % of coffee grounds additive.

References

1. The Food and Agriculture Organization of the United Nations (FAO).
2. Sharholy, M.; Ahmad K.; Gauhar, M.; Trivedi, R. Municipal solid waste management in Indian cities – A review. *Waste management*. **2008**, *28*, 459-467.
3. Campos-Vega, R.; Loarca-Pina, G.; Vergara-Castaneda, H. A.; Oomah, B. D. Spent coffee grounds: A review on current research and future prospects. *Trends in Food Science & Technology*. **2015**, *45*(1), 24-36.
4. Gomes T.; Pereira, J. A.; Ramalhosa, E.; Casal S.; Baptista, P. *Effect of fresh and composted spent coffee grounds on lettuce growth, photosynthetic pigments and mineral composition*. In VII Congreso Ibérico de Agroingeniería y Ciencias Hortícolas, Madrid. **2013**.

Contact person: Dovilė Ragauskaitė, Radvilėnų pl. 19, Kaunas, Lithuania, phone: +37037457070, e-mail: dovile.ragauskaite@ktu.lt

EFFECTIVE REMOVAL OF RADIOACTIVE CESIUM FROM CONTAMINATED WATER ENVIRONMENTS BY IN SITU SYNTHESIZED IRON HEXACYANOFERRATE IMOBILIZED ON CELLULOSE ACETATE ESTERS

I. Reinholds^{1,2}, U. Eismonts^{1,2}, K. Saleniece^{1,2}, M. Bertins³, A. Viksna³, G. Kizane¹, O. Muter^{1,4}, A. Podjava³, A. T. Boginska³, S. Gaidukovs⁵, A. Grinbergs^{1,4}

¹ Institute of Chemical Physics, University of Latvia, Riga, Latvia

² Faculty of Medicine, University of Latvia, Riga, Latvia

³ Faculty of Chemistry, University of Latvia, Riga, Latvia

⁴ Institute of Microbiology & Biotechnology, Riga, Latvia

⁵ Faculty of Material Science and Applied Chemistry, Institute of Polymer Materials, Riga, Latvia

The aim of this research was to develop polymer sorbents for the removal of radioactive cesium (Cs-137) from water samples.

Cs-137 is one of the most long-living gamma radiation emitting radionuclides (half-life >30.2 years) that may spread in the environment after nuclear incidents and may accumulate in the water residues of nuclear reactors. Structural exchange potential of Cs to potassium (K) raise concerns of human health risks and need sufficient individual protection and antidotes.

The Prussian blue (PB) is common name of hexacyanoferrate class compounds, which depending on the conditions of preparation can be classified into soluble PB and insoluble PB. The zeolitic-like insoluble form, e.g., iron hexacyanoferrate presents some defects in its cubic lattice resulting the vacancies that make PB capable of trapping radioactive and nonradioactive Cs, thallium, and other toxic metals [1].

Within experimental part, different reaction routes for the synthesis of micro to nanoscale PB solid forms were tested. The optimized conditions based on ultrasound treatment allowed to obtain in-situ immobilized PB sorbent on cellulose acetate (CA) materials (CA-PB).

CA as one of the most common litters in the form of cigarette butts has raised attention due to the recycling and reusability studies. Commercial cigarette butts were tested as potential membrane filters compared with other types of CA including nano-CA fibers. The method for the removal of plasticizing agents with remaining fiber structure was developed.

The obtained CA-PB sorbent materials were characterized using spectroscopy and microscopy methods (FTIR, SEM, etc.) as well as the stability under different temperature and pH conditions were evaluated to determine capability of sorbents for the removal of cs from water samples. The optimization of the adsorption capacity was tested by using non-radioactive Cs salts. The efficiency of sorbent material was confirmed using IC-PMS method.

Developed materials were successfully applied for removal of Cs from real contaminated samples with determined Cs-137 contents.

Acknowledgement. The research was funded from the Latvian Council of Science: Project No. lzp-2020/2-0213 "Application of modified cellulose fiber sorbents for concentration of radioactive hydrogen (tritium) and other radionuclides from contaminated environments and evaluation of toxic properties: approbation of the method for purification of water residues from nuclear reactors stored in Latvia.

References

1. Estelrich, J.; Busquets, M. A. Prussian blue: A safe pigment with zeolitic-like activity. *International Journal of Molecular Sciences*. **2021**, *22*(2), 780.

Contact person: Ingars Reinholds, Jelgavas 1, Riga, Latvia, phone: +371 26802448, e-mail: ingars.reinholds@lu.lv

NATURAL RADIOACTIVITY LEVELS IN GRANITE

D. Riekstina^{1,2}, A. Egleskalns^{2,3}, G. Kizane², O. Skrypnik², T. Krasta¹

¹ Institute of Solid State Physics, University of Latvia, Riga, Latvia

² Institute of Chemical Physics, University of Latvia, Riga, Latvia

³ Department of Chemistry, University of Latvia, Riga, Latvia

Natural radionuclides K-40, and Th-232, U-238 decay chain products contained in building materials are the main source of radiation dose received by population and the only source of indoor radiation exposure. Present work contains results of the study of natural radionuclide level, activity index I (Bq/kg) and dose rate in different granite. Knowledge of natural radioactivity level in this material is important to reduce harmful effects of ionizing radiation. As yet, Latvia is one of a few EU countries in which no one has performed comprehensive measurements of natural radionuclide contents in these materials [1, 2].

The aim of this study was to obtain data on the content of natural radionuclides in various granite materials used in Latvia in order to determine their compliance with the relevant Latvia and EU regulations.

The dose rate was measured using a calibrated radiometer Inspector Radiation Alert and ranged from 0.16 to 0.80 microSv/h for different granite materials.

Concentration of K-40 and Th-232, U-238 gamma radioactivity in granite and marble samples were determined using the high resolution HPGe gamma-spectrometer Ortec. Uncertainty of measurements was within the range of 3–10 %, the minimal detectable activity – 0.3 Bq/kg. Credibility of obtained results is ensured by the quality assurance and control according to the main requirements of ISO/IEC 17025 standard.

Results of measurements have shown that the concentration of natural radionuclides in granite materials exceeds the limits allowed by Latvian national regulations.

Acknowledgement. The study was financially supported by the University of Latvia project “Implementation of international obligations in cooperation with the IAEA”, ZD2013 / AZ64.

References

1. Nuccetelli, C.; Risica, S., *et al. J. Radiol. Prot.* **2012**, 32, 349-358.
2. Trevisi, R.; Risica, S., *et al. J. Environ. Radioact.* **2012**, 105, 11-20.

Contact person: Gunta Kizane, 1 Jelgavas street, Riga, Latvia, LV-1004, phone: +3712927 4714, e-mail: gunta.kizane@lu.lv

DETERMINATION OF FORMALDEHYDE BY THE "GREEN" RAPID TEST METHOD

Eleonora Rieksta¹, Jānis Ģībietis²

¹ Department of Analytical Chemistry, University of Latvia, Riga, Latvia

² Enola Chemical Co., Ltd., Riga, Latvia

Rapid test methods were studied for the detection of formaldehyde in the aquatic environment, including pharmaceutical and cosmetic preparations.

A long-known specific photometric method for the determination of formaldehyde by chromotropic acid by heating in concentrated sulphuric acid [1]. It has been selected as a reference method. However, this method is not suitable for conducting rapid tests outside the laboratory because of the danger and the use of substances harmful to the environment.

The green method is based on the reaction of formaldehyde with chromotropic acid in the presence of magnesium sulphate to form a stable Mg^{2+} /cyclotetrachromotropylen complex[2]. Calibration graphs were obtained by spectrophotometric determination of formaldehyde with chromotropic acid in sulfuric acid (as reference) and the green method.

Based on several principles of green chemistry, it was chosen to create a rapid test kit, where one reagent was replaced by another – more environmentally friendly – substance in the reaction, as well as the reaction was accelerated with microwave energy.

The result is a rapid test for the determination of formaldehyde in aqueous solutions, based on a modified green method, which is assisted by microwave energy. With the help of this rapid test it is possible to determine the mass concentration of formaldehyde in various aqueous solutions starting from 3 mg / L in 10-15 minutes. The "green" method is environmentally friendly, selective and much safer than the standard method with sulfuric acid.

References

1. Eegriwe, E. Reaktionen und reagenzien zum nachweis organischer verbindungen iv). *Zeitschrift für Anal. Chemie.* **1937**, 110, 22-25.
2. Gasparini, F.; Weinert, P. L.; Lima, L. S.; Pezza, L.; Pezza, H. R. *J. Braz. Chem. Soc.* **2008**, 19(8), 1531-1537.

Contact person: Jānis Ģībietis, phone: +371 29236869, e-mail: janis@enola.lv

RECOVERY OF MICROELEMENTS FROM POTATO JUICE BY BIOSORBENTS

Artis Robalds

Institute of Food Safety, Animal Health and Environment "BIOR", Riga, Latvia

Biosorbents are biomass-based adsorbents, which have been applied to remove wide range of substances (e.g., heavy metals, dyes and pharmaceuticals) from polluted waters [1-3]. Sometimes, the aim of the treatment process is not only the removal of the particular substance from the solution, but also the recovery of it, so that it could be re-used later. Probably, the most typical example is the recovery of gold ions, and different biosorbents have been applied, such as seaweed bladder wrack [4]. Recovery of rare earth elements has also gained significant interest in recent years [5].

In this study, it was evaluated, whether it is possible to recover microelements (with a focus on copper) from potato juice (a by-product of a starch production) by several biosorbents, namely, wheat bran, pea skins, buckwheat husks and others. There is an assumption that saturated biosorbents (i.e., biosorbents after adsorption) later could be used as an animal feed supplement or soil fertilizer. Similar approach has been proposed by a research group from Poland, and they have used synthetic solutions containing metal ions for the saturation of biosorbents [6].

To evaluate adsorption potential of selected biosorbents batch scale adsorption studies were conducted. 0.5 grams of the selected biosorbent were mixed in 50 mL conical flasks (24h, 120 RPM, room temperature) with 45 ml of mL potato juice from. The maximum adsorption capacity towards copper ions was determined by isotherm studies (concentration of copper ions in the solution ranging from 0.1 to 500 mg/L). Wet digestion procedure was applied for the determination of micro and macroelements in potato juice (both prior and after adsorption), using ICP-MS. More details can be found in the work by Reinholds and co-workers [7].

Results indicate that biosorbents can remove up to 54.4 % of copper ions from potato juice relatively fast. Meanwhile, the removal of zinc ions reached only 13.5 % and in some cases was even washed out from biosorbent. The concentration of Na, Mg, K and Ca increased in the potato juice after the adsorption, when adsorption performance of different adsorbents was tested, i.e., washout of these elements took place, indicated a potentially strong roll of cation exchange in the overall biosorption process.

Acknowledgment. This work was supported by the European Regional Development Fund (project agreement No. 1.1.1.2/16/I/001, research proposal No. 1.1.1.2/VIAA/2/18/248).

References

1. Giri, D. D.; Alhazmi, A.; Mohammad, A.; Haque, S.; Srivastava, N.; Thakur, V. K.; Gupta, P. D. B. *Chemosphere*, **2022**, 287(1), 132016.
2. Saravanan, P.; Josephraj, J.; Thillainayagam, B. P. *Environ. Nanotechnol. Monit. Manag.* **2021**, 16, 100560.
3. Oba, S. N.; Ighalo, J. O.; Aniagor, C. O.; Igwegbe, C. A. *Sci. Total Environ.* **2021**, 780, 146608.
4. Mata, Y. N.; Torres, E.; Blázquez, M. L.; Ballester, A.; González, F.; Muñoz J. A. *J. Hazard. Mater.* **2009**, 166(2-3), 612-618.
5. Barcelos da Costa, T.; Carlos da Silva, M. G.; Vieira, M. G. A. *J. Hazard. Mater.*, **2022**, 421, 126742.
6. Kowalczyk, P.; Ligas, B.; Skrzypczak, D.; Mikula, K.; Izydorczyk, G.; Witek-Krowiak, A.; Moustakas, K.; Chojnacka, K. *Environ. Pollut.* **2021**, 268, 115937.
7. Reinholds, I.; Rusko, J.; Pugajeva, I.; Berzina, Z.; Jansons, M.; Kirilina-Gutmane, O.; Tihomirova, K.; Bartkevics, V. *Foods*. **2020**, 9, 93.

Contact person: Artis Robalds, Lejupes iela 3, LV-1076, Riga, Latvija, phone: +37126769597 e-mail: artis.robalds@bior.lv

INFLUENCE OF MULTICOMPONENT NUTRACEUTICAL ON GUT MICROBIOTA IN EXPERIMENTAL ANIMALS

Modestas Ružauskas¹, Elena Bartkienė², Jurga Bernatoniene³, Daiva Žadeikė⁴, Arūnas Stankevičius⁵, Vita Lėlė², Vytautė Starkutė², Paulina Zavistanavičiūtė², Juozas Grigas⁵, Eglė Zokaitytė², Arnoldas Pautienius⁵, Gražina Juodeikienė³, Valdas Jakštas⁶

¹ Microbiology and Virology Institute, Lithuanian University of Health Sciences, Kaunas, Lithuania

² Department of Food Safety and Quality, Lithuanian University of Health Sciences, Kaunas, Lithuania

³ Institute of Pharmaceutical Technologies, Lithuanian University of Health Sciences, Kaunas, Lithuania

⁴ Department of Food Science and Technology, Kaunas University of Technology, Kaunas, Lithuania

⁵ Department of Anatomy and Physiology, Lithuanian University of Health Sciences, Kaunas, Lithuania

⁶ Institute of Pharmaceutical Technologies, Lithuanian University of Health Sciences, Kaunas, Lithuania

Introduction. Nutraceuticals are dietary supplements containing concentrated bioactive compounds found in a variety of foods and presented in a pharmaceutical form. Nutraceuticals are used for health benefits however, their positive influence should be proved by scientific evidence [1]. Microbiome is very important functional component [2], therefore the aim of the study was to investigate the influence of newly developed nutraceutical on microbial changes in the gut of experimental animals.

Methods. Nutraceutical included essential oils (*Origanum vulgare*, *Mintha piperita*, *Thymus vulgaris*), bovine colostrum, *Lactobacillus uvarum* and *L. casei* bacterial strains and apple pomace. 16 weaned-off piglets as experimental animals were used: half of them were fed by conventional feed (control group) and another half by conventional feed plus 30g of nutraceutical daily, for four weeks. Metagenomics were performed with the aim to explore microbial community changes. General blood indices and weight gain data were also compared.

Results and Discussion. Before the experiment the microbial composition in the feces of both animal groups were similar. The most prevalent genera included *Prevotella*, *Clostridium* and *Barnesiella*. At the end of the experiment significant changes in microbial composition between the groups were recorded: the amount of probiotic bacteria was much higher in the experimental group of animals. The amount of *Bifidobacterium* increased 1.9 times, *Streptococcus* – 2.6 times, *Enterococcus* – 1.5 times, *Bacillus* – 3 times and *Faecalibacterium* – 1.6 times. The amount of two probiotic genera *Escherichia* and *Lactobacillus* however, has decreased (by 2.3 and 1.9 times respectively) although the general percental amount of these two genera overall was low in both groups. The decreased amount of some bacteria may be explained by increased numbers of other bacterial species. During the study significant increase of immunoglobulin G in the blood sera of experimental animals was also recorded. Weight gain and cholesterol level in blood has no significant differences among the groups.

Conclusion. Nutraceuticals containing essential oils, lactic acid bacteria, bovine colostrum and fruit production by-products is promising tool for altering of microbial composition by increasing the number of probiotic bacteria in the digestive tract.

References

1. Schmitt, J. Nutraceuticals: is there good science behind the hype? *Br. J. Clin. Pharmacol.* **2013**, 75, S85-S87.
2. Valdes, A. M.; Walter, J.; Segal, E.; Spector, T. D. Role of the gut microbiota in nutrition and health. *BMJ.* **2018**, 361-2179.

Contact person: Modestas Ružauskas, Tilžės g. 18, Kaunas, 47181, Lithuania, phone: +370 61515240, e-mail: modestas.ruzauskas@lsmuni.lt

MODULATION OF LUMINESCENCE SPECTRA VIA SOLID SOLUTION FORMATION OF THIOXANTHONE DERIVATIVES

Kristaps Saršūns¹, Kaspars Leduskrasts², Agris Bērziņš¹, Toms Reķis¹

¹ Faculty of Chemistry, University of Latvia, Jelgavas street 1, Riga, Latvia

² Latvian Institute of Organic Synthesis, Aizkraukles iela 21, Riga, Latvia

Solid solutions (SS) are single multicomponent solid phases for which the constituent component ratio can vary in continuum. Along with the composition, also properties of solid solutions are modulated. The changes in composition are often accompanied by a continuous change in some physical and/or chemical properties (e.g., density, solubility, melting point), and more complex properties such as non-linear optical properties, solid-state luminescence, and phosphorescence properties, that are composition-dependent [1, 2].

Several thioxanthone (TXANT) derivatives (Figure 1) were selected as model compounds because of their physico-chemical properties and chemically similar structures, in which the different atom (R) may not significantly affect the dominant intermolecular interactions [2].

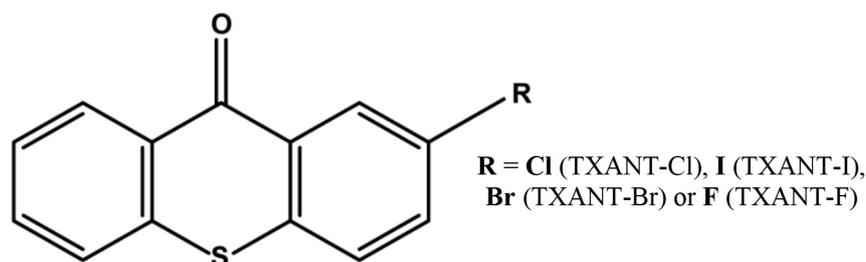


Figure 1. Molecular structure of thioxanthone derivatives.

In this study we explore solid solution formation in thioxanthone derivative systems, namely, 2-iodo-thioxanthone : 2-chlorothioxanthone / 2-bromthioxanthone and 2-fluorothioxanthone : 2-chlorothioxanthone / 2-bromthioxanthone. Solid solutions have been identified and characterized using powder X-ray diffraction and thermal methods of analysis. Their composition limits are summarized in respective two component phase diagrams. The compounds have been selected based on reported room-temperature solid-state luminescence phenomena. Photoluminescence spectra of all crystalline phases in powder form were recorded to see how they change with respect to those of the pure substances known from the literature. This confirmed that technologically relevant properties can be modulated via solid solution formation and therefore can be modulated in a continuous fashion [3].

Acknowledgement. This work has been supported by the Latvian Council of Science, project "Crystal engineering of pharmaceutical multicomponent phases for more efficient crystalline phase design", project No. lzp-2018/1-0312 and University of Latvia foundation through "Mikrotikls" doctoral scholarship in the field of natural and medical sciences.

References

1. Lusi, M. *Crystal Growth & Design*. **2018**, 18(6), 3704-3712.
2. Saršūns, K.; Bērziņš, A.; Reķis, T. *Crystal Growth & Design*. **2020**, 20(12), 7997-8004.
3. Wen, Y.; Liu, H.; Zhang, S.; Gao, Y.; Yan, Y.; Yang, B. *J. Mater. Chem. C*. **2019**, 7, 12502-12508.

Contact person: Kristaps Saršūns, Jelgavas street 1 (Riga, Latvia), phone: +371-22354160, e-mail: kristaps.sarsuns@lu.lv

CRYSTALLIZATION AND STABILIZATION OF 2,6-DIMETHOXYPHENYLBORONIC ACID METASTABLE POLYMORPH USING SURFACTANTS

Aina Semjonova¹, Agris Bērziņš¹

¹ Department of Physical Chemistry, University of Latvia, Riga, Latvia

Physical properties such as solubility [1] and bioavailability [2, 3] of active pharmaceutical ingredients (API) can significantly depend on the polymorphic form. Many APIs have low solubility in water and use of a metastable polymorphic form can enhance the solubility and bioavailability [4]. However, metastable forms have lower stability and often they can very rapidly transform to a stable form. The use of crystallization additives is one of the empirical methods. It can stabilize metastable forms [5, 6] and also promote their nucleation in a crystallization [7].

In this study, 2,6-dimethoxyphenylboronic acid (2,6-MeOPheBA) was used as a model substance to investigate the ability of surfactants as an additive to allow the crystallization of the metastable form. 2,6-MeOPheBA exists as two polymorphs⁸ (see Figure 1.).

In this study both 2,6-MeOPheBA polymorphs were characterized using thermal analysis to determine the relative stability of polymorphs. 2,6-MeOPheBA was crystallized under different conditions by performing evaporation and cooling crystallization from different solvents. Solid forms obtained in the crystallization were characterized with powder X-ray diffraction. After evaluation of the polymorphic outcome in crystallization from pure solvents, toluene was selected for additive (surfactant) screening. Surfactants with divergent intermolecular interaction possibilities were used as additives. Surfactants improving the likelihood for crystallization of the metastable form were studied further under different crystallization conditions.

Form I, the stable polymorph, contains boronic acid homodimers, but form II, the metastable polymorph, – hydrogen-bonded catamer synthon. Surfactants Span 20 and OGP promoted crystallization of metastable form and its stabilization in evaporation crystallization. New unstable polymorph III was obtained in presence of Span 20 and OGP. Form III rapidly transforms to form II.

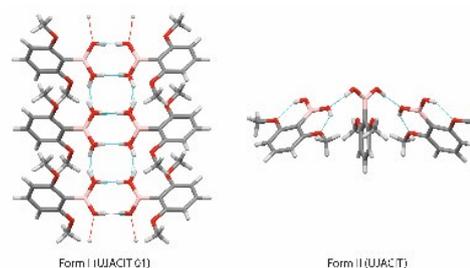


Figure 1. Hydrogen bonding in crystal structures of 2,6-MeOPheBA polymorphs.

References

1. Okabe, N.; Kyoyama, H. *Acta Crystallogr. Sect. E Struct.* **2001**.
2. Haisa, M., *et al. Acta Crystallogr. Sect. B.* **1982**.
3. Braun, D. E., *et al. Cryst. Growth Des.*
4. Gdaniec, M., *et al. Acta Crystallogr. Sect. C Cryst. Struct. Commun.* **1994**.
5. MacGillivray, L. R.; Zaworotko, M. J. *J. Chem. Crystallogr.* **1994**.
6. Mazurek, J., *et al. Acta Crystallogr. Sect. E Struct.* **2007**.
7. Sarma, B., *et al. Cryst. Growth Des.* **2010**.
8. Varughese, S.; Desiraju, G. R. *Cryst. Growth Des.* **2010**.

Contact person: Aina Semjonova, Jelgavas iela 1, Riga, Latvia, e-mail: ainasemjonova@gmail.com

DEVELOPMENT OF HYDROPONICS SYSTEMS WITH BIOACTIVE SUBSTANCES

Evaldas Simanavičius¹, Kristina Jančaitienė¹, Rasa Šlinkšienė¹

¹ Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania

Considering that human world population will reach about 9 billion by the year 2050 [1], it appears clear that food security is one of the pivotal themes of the new millennium and, reasonably, the most urgent challenge for the agricultural sector. However, it should be considered that the progressive drop of fertile soil surface, due to environmental pollution and urbanization phenomena [2], greatly complicates the context. Therefore, about 3.5% of the worldwide area cultivated under tunnels and greenhouses for vegetables production adopts the soilless agriculture techniques based on hydroponic solution (such as floating systems, nutrient film technique (named also NFT) – or aeroponics) [3].

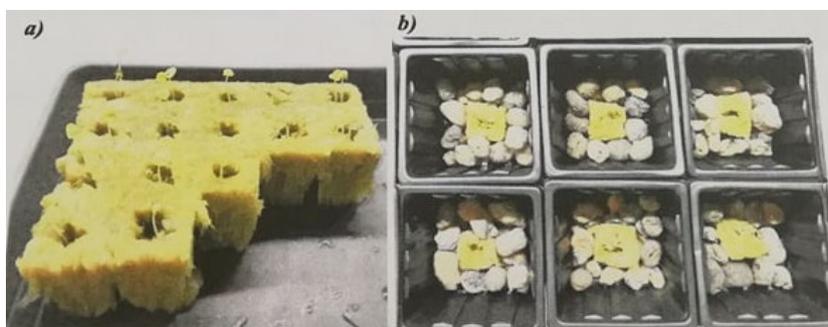


Figure 1. Lemon balm seeds after 2 weeks of germination in stone wool cubes (a) and plant pots with stone wool air expanded clay granules (b).

In the course of this work, liquid concentrated fertilizers of grades 1-8-22, 11-0-0 with calcium and magnesium and microelements were prepared, the diluted solutions of which with the addition of bioactive substances were used as nutrients solutions for growing lemon balm (Figure 1). Hydroponic cultivation technology has also been developed, which has been used to grow lemon balm to reduce the concentration of liquid concentrated fertilizers in nutrient solutions by 10 %, 20 %, 30 % and 40 % at the expense of the "Humicop". During the work, immersion solution of hydroponic cultivation technology was developed and presented. In this technology is recommended to keep a constant volume in the plant-growing vessel during vegetation period by constantly adding water. The fertilizers can be circulated in a closed circle until the electrical conductivity reaches a critical value, and nutrients concentration will be lower be established normal.

References

1. Tilman, D.; Cassman, K. G.; Matson, P. A.; Naylor, R.; Polasky, S. Agriculture sustainability and intensive production practices. *Nature*. **2002**, *418*, 671-677.
2. Chen, J. Rapid urbanization in China: a real challenge to soil protection and food security. *Catena*. **2007**, *69*, 1-15.
3. Hickman, G. International greenhouse vegetable production – Statistics. Mariposa, CA, USA: Cuesta Roble Greenhouse Vegetable Consulting. **2016**.

Contact person: Kristina Jančaitienė; Radvilėnų rd. 19, LT-50254; phone: +370 68848757; e-mail: kristina.jancaitiene@ktu.lt

COMPARATIVE STUDY OF DIFFERENT ADSORBENTS FOR ANODIZED ALUMINUM DYE REMOVAL

Edita Sodaitienė¹, Audronė Gefenienė¹, Sigitas Jankauskas¹, Rimantas Ramanauskas¹, Romas Ragauskas¹

¹ Center for Physical Sciences and Technology, LT-10257 Vilnius, Lithuania

Surfaces of anodized aluminum usually are colored both for technical and decorative purposes [1]. Metal complex organic dyes, widely applied for aluminum coloring, contain not only aromatic ligands but also heavy metals [2]. Therefore, the dye-contaminated wastewater should be treated to prevent the environmental pollution [3]. Adsorption has become one of the most frequently used technologies for the treatment of colored water [4]. Waste materials are employed as cheap substitutes to remove organic dyes [5]. In our study, groundwater treatment waste (GWTW) obtained from the drinking water supply station in Vilnius has been successfully utilized for the decoloration of the metal complex dye solutions. Commercial adsorbents of various types, including activated carbon NORIT PK 1–3, macroporous resins (weak base Macronet MN 150, non-ionic Macronet MN 200, strong acid Macronet MN 500), and mixed bed resin PMB 101 were also used to assess their adsorption capability. The chromium complex anionic dye removal rate and efficiency using different adsorbents was determined in batch experiments considering not only degree of solution decoloration but also chromium adsorption capacity (Figure 1). More than 96 % of the dye color can be removed in the first 3 min using a natural nano-adsorbent GWTW. The adsorptive properties of GWTW are comparable with those of the powdered activated carbon. The adsorption of the dye by the tested granular polymeric materials increases over time, but even after 60 min, it does not equal the removal efficiency achieved with GWTW. On the basis of obtained results, GWTW could be considered as sustainable material for the fast pre-treatment of dye-contaminated water.

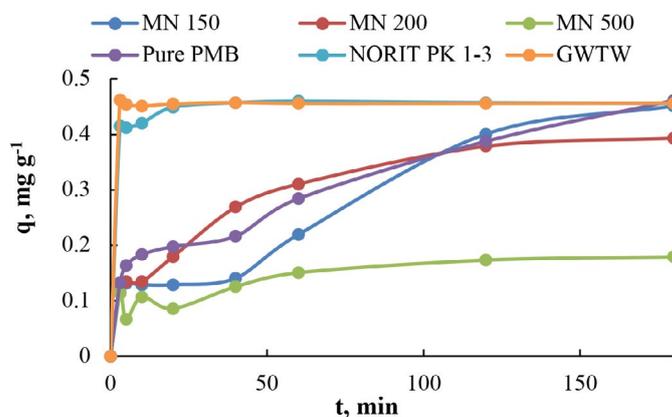


Figure 1. Effect of contact time on chromium adsorption using different adsorbents.

References

1. Chang, C. C.; Chiang, F. C.; Chen, S. M., Thangavelu, K., Yang, H. J. *Int. J. Electrochem. Sci.* **2016**, *11*, 2142-2150.
2. Hou, P.; Shi, C.; Wu, L.; Hou, X. *Microchem. J.* **2016**, *128*, 218-225.
3. Collivignarelli, M. C.; Abb, A.; Miino, M. C.; Damiani, S. *J. Environ. Manage.* **2019**, *236*, 727-745.
4. El-sayed, M. E. A. *Sci. Total Environ.* **2020**, *739*, 139903.
5. Haddad, B.; Mittal, A.; Mittal, J.; Paolone, A.; Villemin, D.; Debdab, M.; Mimanne, G.; Habibi, A.; Hamidi, Z.; Boumediene, M.; Belarbi, E. H. *Chem. Data Collect.*, **2021**, *33*, 100717.

Contact person: Edita Sodaitienė, Saulėtekio av. 3, Vilnius, phone: +370 5 264 8843, e-mail: edita.zubryte@ftmc.lt

THE MICROBIALLY-COATED MICROPLASTICS IN NEUSTONIC WATER-AIR INTERPHASE

Viktor Stabnikov¹, Andrii Marynin², Olena Stabnikova^{1,2}, Maris Klavins³

¹ Department of Biotechnology and Microbiology, National University of Food Technologies, Kyiv, Ukraine

² Advanced Research Laboratory, National University of Food Technologies, Kyiv, Ukraine

³ Department of Environmental Science, University of Latvia, House of Nature, Riga, Latvia

Plastic pollution has become one of the most widespread recalcitrant environmental contaminants. In 2016 annual plastic production was 322 million tons, and it is expected that its production will increase up to 33 billion tons by 2050 [1]. It is estimated that 76% of total plastics produced are landfilled or spread in the natural environment. Plastics with the size less than 5 mm in length are considered as microplastics (MPs). MPs are constantly present in fresh and marine water systems. It becomes a main source of anthropogenic pollution of the oceans and its concentration in highly contaminated rivers could be up to 100 mg/L.

Bacterial cells are usually concentrated in the surface microlayer at the air-water interface in the natural water bodies forming bacterioneuston. Bacteria concentration can be increased by the addition of a source of nutrients with hydrophobic properties in water. An example of microbial optical density change (measured by microphotometer MKF) due to increasing of hexadecane concentration in water sample is shown on Figure.

Bacterioneuston community may also include antibiotic, resistant or pathogenic variants whose concentrations in the bacterioneuston may be some thousand times higher than in the underlying layers of water. It is possible to obtain high concentration of bacteria in bacterioneuston by their adhesion on the carrier with high hydrophobic properties [2].

Major water-polluting microplastics are polyethylene and polypropylene with lower than water density. Therefore, they are concentrated in the neustonic layer near the water-air interface altogether with hydrophobic cells and spores of bacteria. This can cause environmental and public health problems because the floating micro- and nanoparticles of plastics could be coated with biofilm of hydrophobic and often putative pathogenic bacteria [3]. So, impacts of even small quantities of microplastics in aquatic environments must be accounted for considering their accumulation in microlayer at the water-air interface. Sampler for collection of water from a few micrometers layer of water-air interface was proposed to be used for microplastic study.

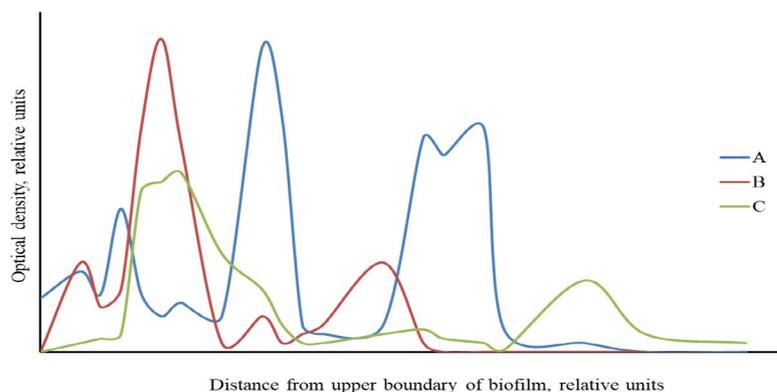


Figure 1. Microbial optical density at different concentration of hexadecane, % (v/v) in water: 0.008 (A), 0.08 (B) and 0.8 (C).

References

1. Bellasi, A., Binda, G., Pozzi, A., Galafassi, S., Volta, P., Bettinetti, R. (2020). *Environments*, 7 (4), 30.
2. Stabnikova, O.V. *Micbobiol. zh.*, 60 (2), 85-90.
3. Bowley, J., Baker-Austin, C., Porter, A., Hartnell, R., Lewis C. (2021). *Trends Microbiol.*, 29 (2), 107-116.

Acknowledgements: Research supported by Latvian-Ukrainian Joint Programme of Scientific and Technological Cooperation project “The microbially-coated microplastics in neustonic water-air interphase and their environmental impacts on aquatic biotopes”

Contact person: Viktor Stabnikov, Department of Biotechnology and Microbiology, National University of Food Technologies, Volodymyrskaya Str., 68, Kyiv, 01601, Ukraine. Tel.:+380 509336327; E-mail: vstabnikov1@gmail.com.

A MULTI-TECHNIQUE APPROACH TO UNDERSTAND THE DIHYDROXYBENZOIC ACID DIFFERENT PROPENSITIES TO FORM SOLID PHASES

Aija Trimdale-Deksne¹, Agris Bērziņš¹

¹ University of Latvia Faculty of Chemistry, Jelgavas iela 1, Riga, Latvia

Dihydroxybenzoic acids[1-8] (diOHBA) are small organic molecules. The arrangement of the hydroxyl groups in the benzene ring has a significant effect on the propensity of diOHBAs to form different solid phases when crystallized from the solution. A combined study using crystal structure and molecule electrostatic potential surface analysis, as well as an exploration of molecular association in solution using spectroscopic methods and molecular dynamics simulations were used to determine the possible mechanism of how the location of the phenolic hydroxyl groups affect the diversity of solid phases formed by the diOHBAs.

The crystal structure analysis showed more commonalities than differences between the diOHBAs, and showed that the classical carboxylic acid homodimers and ring-like hydrogen bond motifs consisting of six diOHBA molecules are prominently present in almost all analyzed crystal structures. However, hydrogen bonds formed by phenolic hydroxyl groups expressed the most pronounced impact on the propensity of diOHBAs to form different solid forms. Additionally, the non-ortho-substituted diOHBAs have an even distribution of ESP extrema, resulting in the formation of intermolecular interactions, allowing for the incorporation of guest molecules.

The differences of molecule behaviour in the solution was observed as different propensity to form associated species, namely, associates linked by interaction between carboxyl group and phenolic hydroxyl group or two phenolic hydroxyl groups as well as stacked molecule pairs. Both experimental spectroscopic investigations and molecular dynamics simulations indicated that the higher abundance of phenolic hydroxyl group associates can be linked to a higher solvate formation propensity as these features are exhibited by diOHBAs having no hydroxyl group in ortho position. However, none of the employed analysis indicated towards prominent presence of carboxylic acid homodimers in the solution. For more information please see Pharmaceutics article (Doi: 10.3390/pharmaceutics13050734).

Acknowledgment. This research has been supported by the Latvian Council of Science, project "Crystal engineering of pharmaceutical multicomponent phases for more efficient crystalline phase design" (project No. lzp-2018/1-0312.4).

References:

1. Okabe, N.; Kyoyama, H. *Acta Crystallogr. Sect. E Struct.* **2001**.
2. Haisa, M., et al. *Acta Crystallogr. Sect. B.* **1982**.
3. Braun, D. E., et al. *Cryst. Growth Des.* **2011**.
4. Gdaniec, M., et al. *Acta Crystallogr. Sect. C Cryst. Struct. Commun.* **1994**.
5. MacGillivray, L. R.; Zaworotko, M. J. *J. Chem. Crystallogr.* **1994**.
6. Mazurek, J., et al. *Acta Crystallogr. Sect. E Struct.* **2007**.
7. Sarma, B., et al. *Cryst. Growth Des.* **2010**.
8. Varughese, S.; Desiraju, G. R. *Cryst. Growth Des.* **2010**.

Contact person: Aija Trimdale-Deksne, Jelgava street 1, e-mail – aija.trimdale@lu.lv

ECO-FRIENDLY DYEING OF WOOLLEN YARN USING LATVIAN TRADITIONAL DYE PLANTS

Valda Valkovska¹, Liāna Orola¹

¹ Department of Physical Chemistry, University of Latvia, Riga, Latvia

Nowadays, the public interest in natural dyeing is related to cultural heritage, green lifestyle and eco-economy. Natural dyestuffs are biodegradable, non-toxic, non-carcinogenic and less allergenic in comparison with synthetic dyes [1]. The popular dye plants of Latvia summarized in the listing of plant dyes are: black alder (*Alnus glutinosa*), perforate St John's-wort (*Hypericum perforatum*), silver birch (*Betula pendula*), golden marguerite (*Anthemis tinctoria*), beet (*Beta vulgaris*), onion (*Allium cepa*), madder (*Rubia tinctorum*), scented Mayweed (*Chamomilla recutita*), pedunculate oak (*Quercus robur*) [2]. Plant-based dyestuffs are a sustainable renewable resource, that can provide a wide range of colours.

Natural dyes have a better affinity for adsorption in protein-based materials than cellulosic materials [3]. Mordants improve the dye uptake and fastness properties of the dye. Metallic mordants (potassium aluminium sulfate, ferrous sulfate, copper sulfate) are the most commonly used in natural dyeing processes due to the formation of coordination complexes and their ability to create a variety of shades than natural mordants (tannins). The textile dyeing industry produces a large amount of wastewater. In addition, it is contaminated with synthetic dyes, metallic mordants and other components [4].

The objective of this study was to dye woollen yarn using native plants and characterize extracts of dyestuffs by ultra high-performance liquid chromatography coupled with a diode array detector and mass spectrometry (UHPLC-DAD-MS). Dried dye plants (onion peels; perforate St John's-wort, meadowsweet and marjoram flowers) were soaked in deionised water, slowly heated to 90 °C and continued heating for two hours. After dyestuffs extraction, a mixture was filtered and used for the dyeing. Unmordanted yarn was dyed at 80–90 °C for two hours, rinsed with water and dried.

The study will present results of the chemical analysis of dyestuffs extracts. The phytochemical screening of the dyeing solutions of the plants showed presence of flavan-3-ols, flavanols, phenolic acids and other compounds.

References

1. Mirjalili, M.; Nazarpour, K.; Karimi, L. *Journal of Cleaner Production*. **2011**, *19*, 1045-1051.
2. Karlson, A. *The Yearbook of Balkan and Baltic Studies*. **2019**, *2(1)*, 87-100.
3. Shahid, M.; Shahid-UI, I.; Mohammad, F. J. *J Clean Prod*. **2013**, *53*, 310-331.
4. Lohtander, T.; Arola, S.; Laaksonen, P. *Color. Technol*. **2019**, *136(1)*, 3-14.

Contact person: Valda Valkovska, University of Latvia, Faculty of Chemistry, Jelgavas str 1, Riga, LV-1004, Latvia, phone: +37126733922, e-mail: valda.valkovska@lu.lv

HEADSPACE-GAS CHROMATOGRAPHIC DETERMINATION OF β -CARYOPHYLLENE IN *EPILOBIUM ANGUSTIFOLIUM* EXTRACTS

Vida Vičkačkaitė¹, Marija Lukoševičiūtė¹

¹ Department of Analytical and Environmental Chemistry, Vilnius University, Vilnius, Lithuania

Epilobium angustifolium is a plant widely used in non-traditional medicine as it demonstrates analgesic and antiinflammatory activity, anticancer properties, treats gastrointestinal disorders, mucous membrane lesions, improves the speed of wounds healing, swelling [1]. *Epilobium angustifolium* is rich in biologically active compounds including phenols, flavonoids, terpenes, aliphatic acids, sterols [2], however, until now, little attention has been paid to its volatile components. To our knowledge, there is only one study on the presence of β -caryophyllene in *Epilobium angustifolium* [3].

It is possible that β -caryophyllene is responsible for the unique therapeutic properties of *Epilobium angustifolium* as its pharmacological properties (analgesic, antioxidant, anti-inflammatory, antidepressant, cancer cell growth inhibitory effect) [4] largely coincide with those of *Epilobium angustifolium*.

β -Caryophyllene is soluble in oils thus the extract of *Epilobium angustifolium* in edible oils is not only of a pleasant specific aroma, but probably also should demonstrate the healing effect. Thus quick and reliable method of β -caryophyllene determination in edible oils is required.

We suggest determine β -caryophyllene by applying headspace gas chromatography (HS-GC).

Standard β -caryophyllene solutions were prepared in coconut oil. An influence of headspace vial heating temperature, heating time, sample quantity on β -caryophyllene peak area was examined and optimal HS-GC conditions were determined. The calibration curve obtained under optimal conditions was linear up to 10 mg/g, the correlation coefficient was 0.999, the detection limit was 60 μ g/kg, RSD (at 0.1 mg/g, n = 5) was 3.8%.

The technique was applied for β -caryophyllene determination in extract of *Epilobium angustifolium* in sunflower oil. The extract was prepared by mixing of 1 g of dried *Epilobium angustifolium* with 10 g of sunflower oil and keeping the mixture in the dark for 14 days. Sunflower oil extract was found to contain 1.3 mg/kg of β -caryophyllene.

The obtained results demonstrate that the suggested technique allows fast, simple and reliable determination of β -caryophyllene in *Epilobium angustifolium* extracts in edible oils.

References

1. Ostrovska, H.; Oleshchuk, O.; Vannini, S.; Cataldi, S.; Albi, E.; Codini, M.; Moulas, A.; Marchyshyn, S.; Beccari, T.; Ceccarini, M. R. *The EuroBiotech Journal*. **2017**, *1*(2), 126-131.
2. Kukina, T. P.; Frolova, T. S.; Salnikova, O. I. *Chemistry of Natural Compounds*. **2014**, *50*(2), 233-236.
3. Kaškonienė, V.; Maruška, A.; Akuneca, I.; Stankevičius, M.; Ragažinskienė, O.; Bartkuvienė, V.; Kornyšova, O.; Briedis, V.; Ugenskienė, R. *Natural Product Research*. **2016**, *30*(12), 1373-1381.
4. Francomano, F.; Caruso, A.; Barbarossa, A.; Fazio, A.; La Torre, C.; Ceramella, J.; Mallamaci, R.; Saturnino, C.; Iacopetta, D.; Sinicropi, M. S. *Appl. Sci*. **2019**, *9*, 5420.

Contact person: Vida Vičkačkaitė, Department of Analytical and Environmental Chemistry, Vilnius University, Naugarduko St. 24, Vilnius, Lithuania, phone: +37052193124, e-mail: vida.vickaackaite@chf.vu.lt

APPLICATION OF NITROGEN AND CARBON STABLE ISOTOPE RATIO MASS SPECTROMETRY FOR NITROGEN CIRCULATION STUDIES DURING CONIFER PLANTING

Signija Zake¹, Maris Bertins¹, Dagnija Lazdina², Karlis Dumins², Arturs Viksna¹

¹ University of Latvia, Faculty of Chemistry, Jelgavas iela 1, LV-1004, Riga, Latvia

² Latvian State Forest Research Institute 'Silava', 111 Rigas Street, LV-2169, Salaspils, Latvia

For us, the living organisms, nature provides all the necessary conditions and environment to survive. Like animals, the full growth of plants is ensured by many elements, such as nitrogen, carbon, oxygen, etc. Also, nitrogen is one of the most common elements in the atmosphere of the earth, which is found not only in the air but also in soil and water, and plants.

Plants uptake nitrogen from the soil in the form of nitrates or ammonia, so when fertilization is applied, a soil improver with ammonia or nitrate-containing compounds is often used. However, this is not the only way to bring nitrogen into the soil, one of the other ways is to use amino acids. In this study one of the amino acids - arginine was used as additional fertiliser.

Application of light stable isotope ratio mass spectrometry (IRMS, EA Eurovector elementanalyser, and Nu Horizon massspectrometer) for determination of nitrogen isotope ratios in different types of plants and their respective parts makes it possible to draw conclusions about the nitrogen uptake by the plant. This method can be used to determine which soil improver is more suitable for the plant (which bears higher yields than others).

The aim of this study was to evaluate the effect of the addition of arginine phosphate in specific plots and the nitrogen cycle, as well as on changes in $d^{15}N$ values in both pine and spruce needles. Soil and conifer samples were taken from 4 different forest type plots (grass-type, peat-type, dam-type and, peat-type).

Before this study it has been hypothesized that conifers will absorb nitrogen from the arginine phosphate-containing fertiliser as their sole source of nitrogen, thus changing the nitrogen isotope ratio values of these plants and becoming closer to the applied improver. However, evaluating the obtained results, such a tendency was observed in only two of the four plots, that is, for dam-type forest and forage-type forest. On the other hand, in the other two areas (for grass-type forest and narrow-leaved peat-type forest) there is an increase in nitrogen isotope ratios, which is not related to the applied fertiliser, as their values also increase in control samples. The obtained results indicate that only spruce seedlings have taken up active nitrogen and that the applied remedy could be the only source of their nitrogen, which is indicated by an increase in the amount of nitrogen and a decrease in $d^{15}N$ values. In the case of pine plants, however, this is not the only source of nitrogen, as their nitrogen growth is less pronounced and $d^{15}N$ values increase, similar to the control samples.

Contact person: Signija Zake, e-mail: signija.zake@lu.lv

ACCUMULATION OF CESIUM-133 IN AQUATIC PLANTS AND ITS EFFECT ON THE PHYSIOLOGICAL ACTIVITY OF PLANTS AND AQUATIC MICROORGANISMS

L. Zorza^{1,2}, M. Bertins⁴, K. Saleniece^{2,3}, A. Viksna⁴, A. Grinbergs^{1,2}, O. Muter^{1,2}

¹ Institute of Microbiology & Biotechnology, University of Latvia, Riga, Latvia

² Institute of Chemical Physics, University of Latvia, Riga, Latvia

³ Faculty of Medicine, University of Latvia, Riga, Latvia

⁴ Faculty of Chemistry, University of Latvia, Riga, Latvia

Natural cesium is present in the environment in only one stable form, as the isotope ¹³³Cs. Radioactive forms of cesium (¹³⁴Cs and ¹³⁷Cs) are produced by the fission of uranium in fuel rods during the normal operation of nuclear power plants, or when nuclear weapons are exploded. Radioisotopes of cesium with a relatively long half-life emit harmful beta and gamma radiation thus creating environmental risks [1].

Cesium can bioaccumulate in both aquatic and terrestrial food chains [2]. Cs in aquatic ecosystems is able to accumulate both from nutrient sources and from cesium, which is dissolved in water and suspended in solid particles and sediments. Cs acts in a similar way to essential elements in organisms, such as potassium, which greatly facilitates the entry of cesium inside the cell [3;4]. The mechanisms of radioactive cesium isotope accumulation in the cells of organisms are known to be identical to non-radioactive forms, therefore accumulation tests can be performed using ¹³³Cs [1].

The aim of this study was to determine the accumulation rate of ¹³³Cs by aquatic plants, as well as to determine the enzymatic activity of aquatic plants and microorganisms after being exposed with ¹³³Cs in various concentrations.

In our research, four aquatic macrophytes (*Bakopa* sp., *Elodea* sp., *Ceratophyllum* sp., *Limnobium* sp.) in a self-sustaining aquarium water were exposed to 1 μM, 10 μM and 1000 μM ¹³³Cs as cesium chloride (CsCl) for 10 days, at 23° C, under natural light conditions. The concentration of ¹³³Cs and other metals in the liquid phase and their accumulation in aquatic plants were determined by gas chromatography. Accumulation of ¹³³Cs and other metals in plant biomass was shown to be species- and metal-specific. Plant response to the metal accumulation was evaluated by a range of enzyme groups, which are involved in antioxidant activities and metabolism. In particular, peroxidase, dehydrogenase and guaiacol peroxidase activity were measured in the crude plant extracts, which were prepared from non-treated plants and after 10 day incubation with CsCl. The kinetics of enzyme reactions were highly dependent on the initial concentration of ¹³³Cs in aquatic environments, as well as on plant species. The data on ¹³³Cs accumulation in aquatic plants and their response to the metal stress provided new knowledge on the mechanisms of metal-plant interrelations, which will be implemented in water treatment technologies, particularly, for removal of radioisotopes.

Acknowledgement The research was funded from the Latvian Council of Science: Project No. lzp-2020/2-0213 "Application of modified cellulose fiber sorbents for concentration of radioactive hydrogen (tritium) and other radionuclides from contaminated environments and evaluation of toxic properties: approbation of the method for purification of water residues from nuclear reactors stored in Latvia.

References

1. Burger, A.; Lichtscheidl, I. Stable and radioactive cesium: A review about distribution in the environment, uptake and translocation in plants, plant reactions and plants' potential for bioremediation. *The Science of the total environment*. **2018**, *618*, 1459-1485.
2. Rowan, D. J. Cesium bioaccumulation by aquatic organisms. *The Science of the total environment*. **1998**.
3. Allaye-Chan, A. C., et al. Seasonal concentrations of cesium-137 in rumen content, skeletal muscles and feces of caribou from the Porcupine herd: lichen ingestion rates and implications for human consumption. *Rangifer*. **1990**, 17-24.
4. Remy, E., et al. The major facilitator superfamily transporter ZIFL2 modulates cesium and potassium homeostasis in Arabidopsis. *Plant & cell physiology*, **2015**, *56*(1), 148-162.

Contact person: Laura Žorža, Jelgavas 1, Riga, Latvia, phone: +371 26608947, e-mail: laura.zorza@lu.lv

HEAVY METAL ACCUMULATION CAPACITY OF VARIOUS LOCAL HERBACEOUS SPECIES COMMUNITIES CULTIVATED IN MUNICIPAL BIOWASTE SUBSTRATE WITH CONSTRUCTION DEBRIS ADMIX

A. Zuševica¹, E. Muižnieks¹, S. Žigure¹, S. Celma¹, T. A. Štāls¹, K. Dūmiņš¹, S. Rancāne¹, D. Lazdiņa¹

¹ Latvian State Forest Research Institute “Silava”

Biodegradable waste that comes from general waste often contains a lot of heavy metals. Fast-growing tree plantations with herbaceous plants as phytoaccumulators can be planted to perform soil remediation of heavy metal. Phytoaccumulation studies generally focus on the ability of one species to accumulate pollution, but in the context of ecosystems and biodiversity, it would be better to choose local species that grow in communities.

The aim of this study was to determine the phytoaccumulation of different cultivated and local grassland plant species in a potentially contaminated substrate and how it is affected by the presence of construction debris in the soil. Species communities with nitrophilic grass species – *Lolium perenne*, *Festuca pratensis*, *Phleum pratense* – as well as combination of nitrophilic grass and *Brassicaceae* genus species – *Dactylis glomerata*, *Raphanus sativus* subsp. *oleiferus*, *Sinapis alba* – showed the largest decrease of heavy metal (Zn, Cd, Pb, Cu) content in the soil and one of the largest accumulations in aboveground parts of the plant after vegetation season. Those species could be cultivated together with willows and poplars which are already well known as fitoremediants. Heavy metal accumulation was lower in species communities with crops – buckwheat, field beans – and legume communities. The plants capacity to absorb the heavy metals from contaminated soil depended on species composition and the presence of construction debris.

Acknowledgements. This study has been supported by Ltd Getlini ECO financed research “Development of recommendations for the establishment of composting fields for biodegradable waste compost obtained from municipal waste – by creating tree plantations with herbaceous plants“.

Contact person: Austra Zuševica, e-mail: austra.zusevica@silava.lv

AN IMPROVEMENT OF THE ANALYTICAL PROTOCOL OF GLYPHOSATE QUANTIFICATION IN FOOD SAFETY AREA

**Grzegorz Wryk¹, Agnieszka Borowiec¹, Iwona Gąsiorowska¹, Katarzyna Stopka¹,
Beata Kondraszuk¹, Andrzej Gawor¹, Eliza Kurek¹, Ewa Bulska¹**

¹ Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw,
Żwirki i Wigury 101, 02-089 Warsaw, Poland

Glyphosate (CAS No 1071-83-6; N-(phosphonomethyl)glycine) is one of the most widely used herbicides with applications in agriculture, forestry, industrial weed control, lawn, garden, and aquatic environments [1]. In plants, glyphosate disrupts the shikimic acid pathway through inhibition of the enzyme 5-enolpyruvylshikimate-3-phosphate (EPSP) synthase. The resulting deficiency in EPSP production leads to reductions in aromatic amino acids that are vital for protein synthesis and plant growth [2]. Glyphosate is absorbed across the leaves and stems of plants and is translocated throughout the plant. It concentrates in the meristem tissue [1].

Glyphosate has been thoroughly assessed by Member States, the European Chemicals Agency (ECHA) and the European Food Safety Authority (EFSA) in recent years. In the European Union (EU), maximum residue levels (MRLs) have been established for glyphosate, which are set for most plant and animal commodities at the limit of quantification (LOQ) of 0.1 mg/kg and 0.05 mg/kg, respectively. European Union approval for glyphosate as an active substance in plant protection products expires in 2022 [3]. Due to constantly changing legislating and market requirements for food safety, there is a need to develop new analytical protocol for glyphosate quantification with low detection limits.

The quantification of glyphosate residues is very challenging because of the highly polar and amphoteric nature of the molecule, the low molecular weight, the high water solubility and the lack of chromophores. For these reasons, glyphosate is one of the few pesticides which are not amenable to the multiresidue methods typically employed in pesticide residue analysis. In this work, we present an improved methodology for glyphosate quantification using high-performance liquid chromatography coupled with tandem mass spectrometry. The method was validated based on SANTE/12682/2019 [4] requirements on four different matrices: apple, buckwheat, blueberries and rapeseed. The method's validation was evaluated through a series of assessments to determine the accuracy, precision, linearity, matrix effect, limit of detection (LOD), and limit of quantification (LOQ). The mean recoveries for all matrices were within 70%–120% at three fortification levels, including the LOQ. The LOQ was 0.01 mg/kg and the expanded measurement uncertainty was estimated to be <50%. The proposed method was successfully applied in accredited laboratory of University of Warsaw (number of accreditation: AB 1525) in routine analysis in food safety area.

References

1. Tomlin, C. D. S. *The Pesticide Manual: A World Compendium, 14th ed. British Crop Protection Council: Hampshire. 2006*, 545-548.
2. Vencill, W. K. E. *Herbicide Handbook, 8th ed. Weed Science Society of America: Lawrence. 2002*, 231-234.
3. Commission Implementing Regulation (EU) 2017/2324 of 12 December 2017 renewing the approval of the active substance glyphosate in accordance with Regulation (EC) No 1107/2009 of the European Parliament and of the Council concerning the placing of plant protection products on the market.
4. Analytical Quality Control and Method Validation Procedures for Pesticide Residues Analysis in Food and Feed; EU Reference Laboratories for Residues of Pesticides; SANTE/12682/2019.

Contact person: Grzegorz Wryk, address: Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland; phone: +48 516 182 313, e-mail: gwryk@cnbc.uw.edu.pl