# 4TH YOUNG RESEARCHERS' INTERNATIONAL CONFERENCE
## ON CHEMISTRY AND CHEMICAL ENGINEERING

## YRICCCE IV – 2023

## PROGRAMME & BOOK OF ABSTRACTS

JUNE 1 – 3, 2023
DEBRECEN, HUNGARY

# 4TH YOUNG RESEARCHERS' INTERNATIONAL CONFERENCE

## ON CHEMISTRY AND CHEMICAL ENGINEERING

## YRICCCE IV – 2023

June 1 – 3, 2023
Debrecen, Hungary

Organizers:

Published by the Hungarian Chemical Society

ISBN 978-615-6018-16-8

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**Dear Colleagues,**

On behalf of the Organising Committee, I am delighted to cordially invite you to join the 4th Young Researchers' International Conference on Chemistry and Chemical Engineering (YRICCCE IV), which will be held in Debrecen, Hungary during June 1-3, 2023.

This Conference is organised jointly by the Romanian and Hungarian Chemical Societies every two years. The Young Researchers' International Conference on Chemistry and Chemical Engineering conference series was launched in 2016 in Cluj-Napoca, Romania. We were very pleased to be the host of the second conference in Budapest, Hungary in 2018. Since the pandemic brought unexpected changes to our lives, we had to organize the 3rd conference online, but luckily we can return to the face-to-face meeting this year.

The YRICCCE series of conferences offers PhD students, postdocs and young researchers from universities, research institutes and industries the possibility to meet and discuss research topics, to exchange scientific ideas, to inspire new research, and to establish new contacts for closer co-operation.

I hope many young researchers will join us and contribute to the success of the conference.

**Prof. Dr Livia Simon Sarkadi**
Chair of the YRICCCE IV Conference

# Organizing Committee

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University of Debrecen

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**Prof. Dr. Călin Cormoş**

# 4th Young Researchers' International Conference on Chemistry and Chemical Engineering (YRICCCE IV)

### 1-3 June 2023, Debrecen, Hungary

# Programme

## June 1th (Thursday)

12:00 - Registration

14:00 - 14:30 Opening

*Chair: Sándor Kéki*

***Invited Lecture***

14:30 - 15:00 PL1 **Péter Nagy** – *Department of Molecular Immunology and Toxicology and the National Tumor Biology Laboratory, National Institute of Oncology, 1122 Budapest, Hungary*
Control of Cellular Functions Through Protein Cysteine Persulfidation

15:00 - 18:00 Poster session, Flash presentations: P5, P6, P26, P27, P29, P30, P31, P34

18:00 - Welcome

## June 2th (Friday)

*Chair: Livia Simon Sarkadi*

***Invited Lecture***

09:00 - 09:30 PL2 **Adrian-Alexandru Someșan** - *Department of Chemistry, Supramolecular Organic and Organometallic Chemistry Centre (SOOMCC), Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, Romania*
Organometallic compounds of heavy group 14 elements (Sn, Pb) – from ligand design to applications

*Chair: Anca Silvestru*

***Oral Presentations***

09:30 - 09:45 O1 **Cătălin-Eduard Șalgău, Alexandra Pop, Anca Silvestru -** *Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Supramolecular Organic and Organometallic Chemistry Centre, Romania*
Cadmium complexes with organoselenolato ligands. Synthesis and structural characterization

09:45 - 10:00 O2 **Raffaele Fontana, Levente Kiss, Cristian Silvestru** - *Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemistry, Supramolecular Organic and Organometallic Chemistry Centre, Romania*
Synthesis, characterization and evaluation of the catalytic properties of phosphine- and stibine- ligated cyclometalated palladium complexes

10:00 - 10:15 O3 **Anamaria Lavinia Corjuc, Anca Silvestru -** *Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Supramolecular Organic and Organometallic Chemistry Centre, Romania*
Structural aspects in silver complexes with diorganochalcogen ligands of type $(2\text{-}XC_6H_4CH_2)_2E$ (E = S, Se; X = Br, $CH_3$)

10:15 - 10:30 O4 **Maria-Caterina Afloarei, Cristian Silvestru -** *Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Department of Chemistry, Supramolecular Organic and Organometallic Chemistry Centre, Romania*
Synthesis, structural characterization and reactivity of novel organoantimony(III) aryloxides

10:30 - 11:00 Coffee break

*Chair: Adrian-Alexandru Someșan*

***Oral Presentations***

11:00 - 11:15 O5 **Haythem S. Basheer, Mohit Yadav, Janos Kiss, András Sápi, Ákos Kukovecz, Zoltán Kónya** - *Department of Applied and Environmental Chemistry, Interdisciplinary Excellence Centre, Hungary*
Fe-loaded ZnO for sustainable $CO_2$ photocatalysis: A step towards $CO_2$ utilization’’

11:15 - 11:30 O6 **Amin Hassani Moghaddam, Robert Mucsi, Fanni Czirok, András Sápi-** *Department of Applied and Environmental Chemistry, University of Szeged, Hungary*
Effect of $CeO_2$ morphologies On $CO_2$ conversion to CO via revers water gas shift reaction

11:30 - 11:45 O7 **Serra Üneri Haymana; Lajos Nagy; Tibor Nagy; Ákos Kuki; Sándor Kéki -** *University of Debrecen, Faculty of Science and Technology, Department of Applied Chemistry, Hungary*
Development and study of Li-AIR battery using carbon cathode

11:45 - 12:00 O8 **Hanna Judit Szabó, István Lázár, Lajos Daróczi -** *University of Debrecen, Department of Inorganic and Analytical Chemistry, Hungary*
Synthesis of metal nanoparticle-containing aerogels and their potential application as catalysts

12:00 - 12:15 O9 **Balázs Szathmári, Zsolt Kelemen** - *Department of Inorganic and Analytical Chemistry, Faculty of Chemical Technology and Biotechnology, Budapest University of Technology and Economics, Hungary*
Synthesis of carboranyl-siloles – new aiegens

12:15 - 13:30 Lunch

*Chair: Livia Simon Sarkadi*

***Oral Presentations***

13:30 - 13:45 O10 **Zsófi Sajtos, Edina Baranyai, Tamás Varga, Zita Gajdos, A.J. Timothy Jull, Zsuzsa Lisztes-Szabó, Mihály Molnár -** *Atomic Spectroscopy Partner Laboratory, Department of Inorganic and Analytical Chemistry, Faculty of Science and Technology, University of Debrecen, Hungary*
The sweetest time capsules - the MP-AES analysis coupled with AMS age determination of hungarian multifloral honey samples

13:45 - 14:00 O11 **Renáta Németh, Liliána Kata Sznopka, Csenge Orosz, Sándor Tömösközi** - *Budapest University of Technology and Economics, Research Group of Cereal Science and Food Quality, Department of Applied Biotechnology and Food Science, Faculty of Chemical Technology and Biotechnology, Hungary*
Investigation of the techno-functional role of dietary fibers in food matrices based on gluten-free cereals and pseudocereals

14:00 - 14:15 O12 **Kaltrina Berisha, Zsuzsanna Mednyánszky, Hysen Bytyçi, Livia Simon Sarkadi -** *Hungarian University of Agriculture and Life Sciences, Institute of Food Science and Technology, Department of Nutrition, Hungary*
Determination of protein quality of beef sausage

14:15 - 14:30 O13 **Arijit Nath, Geremew Geidare Kailo, Kenbon Beyene Abdisa, Zsuzsanna Mednyánszky, Emőke Szerdahelyi, Attila Csighy, Andras Koris -** *Department of Food Process Engineering, Institute of Food Science and Technology, Hungarian Univer-sity of Agriculture and Life Sciences, Hungary*
Antioxidant and antibacterial activities of peptides by hydrolysis of soybean milk protein by papain

14:30 - 14:45 O14 **Andreea Gostăviceanu, Dana Maria Copolovici -** *"Aurel Vlaicu" University of Arad, Faculty of Food Engineering, Tourism and Environmental Protection and Institute of Technical and Natural Sciences Research-Development-Innovation of "Aurel Vlaicu" University, Romania*
Current applications of antimicrobial peptides

14:45 - 16:00 Poster session

16:00 – 18:00 Sightseeing in Debrecen

19:30 - Dinner

## June 3th (Saturday)

*Chair: Cristian Silvestru*

***Oral Presentations***

09:00 - 09:15 O15 **Lama Ismaiel; Ancuta Nartea; Benedetta Fanesi; Deborah Pacetti; Paolo Lucci; Henry Jaeger** - *Università Politecnica delle Marche, Department of Agricultural, Food and Environmental Sciences, Italy*
Volatile compounds profile of sardines (*sardina pilchardus*) treated with high-pressure processing technology

09:15 - 09:30 O16 **Albert Gashi, György Kenesei, Zsuzsanna Mednyánszky, Livia Simon-Sarkadi -** *Hungarian University of Agriculture and Life Sciences, Department of Nutrition Budapest, Hungary*
Changes in the free amino acid content of sausages due to high hydrostatic pressure treatment

09:30 - 09:45 O17 **Areej Alsobh, Gyula Vatai, Szilvia Bánvölgyi** - *Department of Food Process Engineering, Institute of Food Science and Technology, Hungarian University of Agriculture and Life Sciences, Budapest, Hungary*
Recovery of bioactive anthocyanin pigments from hawthorn fruit by infusion, microwave, and ultrasound-based extraction techniques

09:45 - 10:00 O18 **Yvette Szabó, Márton Szabados, †István Pálinkó, Pál Sipos –** *University of Szeged, Faculty of Science and Informatics, Department of Inorganic, Organic and Analytical Chemistry, Hungary*
Microwave-induced base-catalyzed synthesis of methyl levulinate from levulinic acid

10:00 - 10:15 O19 **Nguyen Thi Phuong Hoang, Ferenc Fodor, Gyula Záray, Anett Endrédi, Christina Streli, Dieter Ingerle, Philipp Ziegler, Martin Radtke, Ana Guilherme Buzanich, Péter Dobosy -** *Institute of Aquatic Ecology, Centre for Ecological Research, Hungary*
Iodine biofortification of cabbage plants cultivating in a hydroponic system

10:15 - 10:30 O20 **Simona Ioniță, Mihaela Deaconu, Roxana-Cristina Popescu, Daniel Lincu, Raul-Augustin Mitran, Cristian Matei, Diana-Iulia Savu, Daniela Berger -** *University "Politehnica" of Bucharest, Faculty of Chemical Engineering and Biotechnology, Romania*
Drug delivery systems based on boronic acid-functionalized silica for cancer therapy

10:30 - 11:00 Coffee break

*Chair: Lucian Pop*

***Oral Presentations***

11:00 - 11:15 O21 **Adelina A. Andelescu, Carmen Cretu, Elisabeta I. Szerb, Anca Silvestru -** *“Coriolan Dragulescu” Institute of Chemistry, Romania*
Water soluble luminescent coordination complexes

11:15 - 11:30 O22 **Simion Bogdan Angyus, Marin Șenilă, Eniko Covaci, Tiberiu Frențiu -** *INCDO-INOE 2000, Research Institute for Analytical Instrumentation, ICIA, Romania*
Diffusive gradients in thin film and electrothermal vaporization capacitively coupled plasma optical emission spectroscopy method for the evaluation of bioavailable Cu, Zn, Cd and Pb fraction in agricultural soils

11:30 - 11:45 O23 **Eniko Covaci; Bogdan Simion Angyus; Marin Senila; Maria Frentiu; Tiberiu Frentiu** – *Babes-Bolyai University, Faculty of Chemistry and Chemical Engineering, Romania*
Greenness and whiteness of small-sized electrothermal vaporization capacitively coupled plasma optical emission spectrometry with *in-situ* diffusive gradients in thin films passive sampling (DGT-SSETV-μCCP-OES)

11:45 - 12:00 Closing remarks

12:00 - Farewell lunch

# Poster section

P1 **Viktória Balla, Viktória Forgács, István Jószai**
*University of Debrecen, Faculty of Medicine, Department of Medical Imaging,*
*Department of Nuclear Medicine and Translational Imaging,*
*4032 Debrecen, Nagyerdei krt. 98.*
Fast chromatographic determination of enantiomeric purity of [$^{11}$C]methionine by pre-column derivatisation method

P2 **Dóra Veronika Barta, Tibor Nagy, Veronika Pardi-Tóth, Gergő Róth, Ákos Kuki, Sándor Kéki**
*University of Debrecen, Faculty of Sciences and Technology, Department of Applied Chemistry, H-4032 Debrecen, Egyetem tér 1, Hungary*
Characterisation of multi-block co-polymers by Mass spectrometria (MS)

P3 **Máté Benedek, Tibor Nagy, Gergő Róth, Ákos Kuki, István Timári, Miklós Zsuga, Sándor Kéki**
*University of Debrecen, Faculty of Science and Technology, Institute of Chemistry*
*H-4032 Debrecen, Egyetem tér 1., Hungary*
Characterization of copolymers using gel permeation chromatography and neural networks

P4 **Diana-Ioana Eftemie[a,B], Teodora Mocanu[c], Sergiu Shova[d], Diana Dragancea[b], Mihai Răducă[a,B], Marius Andruh[a,B]**
[a]*University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, Organic Chemistry, Biochemistry and Catalysis, 030018, Bucharest, Regina Elisabeta Boulevard 4-12, Romania*
[b]*”C. D. Nenitzescu” Institute of Organic and Supramolecular Chemistry of the Romanian Academy, 060023, Bucharest, Splaiul Independenței Street 202B, Romania*
Four novel polynuclear Zn(II) complexes with a Schiff base ligand derived from 2,3-dihydroxybenzaldehyde: synthesis and characterization

P5 **Réka Pálma Erdei[a], László Izsépi [a] , Gyula Batta[a]**
[a]*Department of Organic Chemistry, University of Debrecen,*
*H-4032, Debrecen, Hungary*
Structure and mode of action studies of glycopeptide antibiotics: eremomycin and oritavancin as seen by NMR

P6 **László Bence Farkas[a,b*]; Tamás Milán Nagy[a,b]; Márk Racskó[c]; Attila Borics[d]; István Balázs Tóth[c]; Katalin E. Kövér[a,b]**
*[a]University of Debrecen, Faculty of Science and Technology, Institute of Chemistry, Department of Inorganic and Analytical Chemistry,*
*H-4032, Debrecen, Egyetem tér 1, Hungary*
*[b]ELKH-DE, Molecular Recognition and Interaction Research Group,*
*H-4032, Debrecen, Egyetem tér 1, Hungary*
Targeted binding investigation on living cell samples with saturation transfer triple difference (STTD) NMR method

P7 **Mátyás Fodor[a,b], Zoltán Szűcs[b], Károly Brezovcsik[b]**
*[a]University of Debrecen, Doctoral School of Chemistry*
*4032 Debrecen, Egyetem tér 1., Hungary*
*[b]Institute for Nuclear Research*
*4026 Debrecen, Bem tér 18/c.,*
Terbium isotope production, purification and radiolabelling at the Institute for Nuclear Research

P8 **Antal Galvácsi[a], Csilla Kállay[a], Roland Császár[a], Lajos Nagy[b]**
*[a]Department of Inorganic and Analytical Chemistry, University of Debrecen, H-4032, Hungary*
Interaction of transition metal ions with a prion protein – beta amyloid model peptide

P9 **Isaac Iglesias, Tibor Nagy, Ákos Kuki, Gergő Róth, Zuura Kaldybek Kyzy, Sándor Kéki**
*University of Debrecen, Faculty of Science and Technology, Chemical Department,*
*Egyetem tér 1, 4032, Debrecen, Hungary*
Thermoresponse behavior of nam-nipa block polymer

P10 **Bálint Jávor[1*], Panna Vezse[1], Ádám Golcs[1], Péter Huszthy[1] and Tünde Tóth[1,2]**
*[1]Department of Organic Chemistry and Technology, Budapest University of Technology and Economics, Szent Gellért tér 4, H-1111 Budapest, Hungary*
Enantiodiscriminating Lipophilic Liquid Membrane-Based Assay for High-Throughput Nanomolar Enantioenrichment of Chiral Building Blocks

P11 **Maria-Lorena Jinga[1], Lucian-Gabriel Zamfir[1], Gaudențiu Vărzaru[2], Răzvan Ungurelu[2], Petru Epure[3], Mariana Constantin[1], Iuliana Răut[1], Cristina Firincă[1], Nicoleta Radu[1], Luiza Jecu[1], Mihaela Doni[1], Ana-Maria Gurban[1*]**
*[1]INCDCP-ICECHIM, 202 Spl. Independentei, 060021 Bucharest, Romania*
Comparative study of different nanocomposite materials in the development of biosensors for biogenic amines detection

P12 **Zuura Kaldybek Kyzy, Gergő Róth, Ákos Kuki, Alifya Balqis Zatalini, Miklós Zsuga, Sándor Kéki, Tibor Nagy**
*University of Debrecen, Faculty of Science and Technology, Department of Applied Chemistry, Egyetem tér 1, H-4032, Debrecen, Hungary*
Gel Permeation Chromatography Based Method Development for the Characterization of Thermoresponsive block copolymers

P13 **Zsuzsa Kastal, Bettina D. Balogh, Adrien Balabán, Szilvia Vida, Petra A. Keczán, Tamás P. Szák-Kocsis, Katalin Várnagy**
*University of Debrecen, Egyetem tér 1., H-4032 DEBRECEN, Hungary*
Effect of the Amino Acid Environment of Histidine on the Metal Binding Selectivity of Tau Fragments

P14 **Ghazaleh Khoshroo[a], András Sápi[a]**
[a]*University of Szeged, Interdisciplinary Excellence Center, Department of Applied and Environmental Chemistry, H-6720, Rerrich Béla tér 1, Szeged, Hungary*
Dry Reforming of Methane Based on Transition Metal Catalysts

P15 **Aicha Nour Laouameria[a,b], Mátyás Hunyadi[a], Zoltán Szűcs[a]**
[a]*Institute for Nuclear Research, Atomki, Bem tér 18/c, 4026, Debrecen, Hungary*
[b]*Doctoral School of Chemistry, Faculty of Science and Technology, University of Debrecen, Egyetem tér 1, H-4032 Debrecen, Hungary*
Study of Diffusion Dynamics in PD/RH Alloy

P16 **Valentina Moroșan, Luminița David, Bianca Moldovan**
*„Babeş-Bolyai" University, Faculty of Chemistry and Chemical Engineering,*
*11, Arany Janos Str., 400028 Cluj-Napoca, Romania*
Green sinthesys of bimetallic Ag-Au and Au-Ag nanoparticles and their catalitic activity in the degradation of harmful dyes

P17 **Medárd Kiss-Benkő, Sándor-Balázs Nagy, Márton Szabados, Pál Sipos**
*University of Szeged, Faculty of Science and Informatics, Inorganic, Organic and Analytical Department, H-6720 Szeged, Dom Square 8, Hungary*
Catalytic Activity of Lanthanum Cuprate ($La_2Cuo_4$) in the Synthesis of Triazine Derivatives

P18 **Radu Lucian Silaghi-Dumitrescu, Szilárd-Zoltán Pesek, Maria-Ștefana Lehene, Adrian - Mihai - Vasile Brânzanic**
*Universitatea Babeș-Bolyai din Cluj-Napoca, Facultatea de Chimie și Inginerie Chimică, Strada Arany János 11, Cluj-Napoca 400028*
On the origin of the blue color in the iodine / iodide / starch supramolecular complex

P19 **Raluca – Ioana Rad[a], Adela Meghesan[a], Claudia Cimpoiu[a], Liana Maria Costeab**
[a]*Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University of Cluj-Napoca, Arany Janos Str. 11, RO-400028, Cluj-Napoca, Romania*
Determination of the number and content of pesticides residues found in the vegetables harvested from Transylvanian area

P20 **Ágota Ragyák[1,2], Zita Gajdos[1], A.j. Timothy Jull[3, 5, 6], Mihály Molnár[3], Zsófi Sajtos[1,2], Tamás Varga[3,4], Edina Baranyai[1]**
*[1]Atomic Spectroscopy Partner Laboratory, Department of Inorganic and Analytical Chemistry, Faculty of Science and Technology, University of Debrecen, Egyetem Square 1, H-4032 Debrecen, Hungary*
*[2]University of Debrecen, Doctoral School of Chemistry, Debrecen, Hungary*
Time travel with honeys – the MP-AES analysis coupled with AMS age determination of Hungarian acacia samples

P21 **Aron Rop[a,b], Tibor Nagy[a], Ákos Kuki[a], Sándor Kéki[a]**
*[a]University of Debrecen, Faculty of Science and Technology, Department of Applied Chemistry, H-4032 Debrecen, Egyetem tér, Hungary*
*[b]Macromolecular and Surface Chemistry Research Group, University of Debrecen, Faculty of Science and Technology, Department of Applied Chemistry, H-4032 Debrecen, Egyetem tér , Hungary*
Self-Assembly of Pluronic-Type Amphiphilic Block Copolymers

P22 **Zsófi Sajtos[a], Ágota Zsófia Ragyák[a,B] , Fruzsina Hódi[a], Viktória Szigeti[a], Edina Baranyai[a], Gábor Bellér[c]**
*[a]Atomic Spectroscopy Laboratory, Department of Inorganic and Analytical Chemistry, Faculty of Science and Technology, University of Debrecen, Egyetem Square 1, H-4032 Debrecen, Hungary*
Hydroxymethylfurfural content of old honey samples – does thesticky treat really last forever?

P23 **Balázs Sándor, Ágnes Grenács, Katalin Várnagy**
*University of Debrecen, Egyetem tér 1. H-4032, Debrecen, Hungary*
The effect of serine and threonine on the complex formation and hydrolytic stability of model peptides and the human tub α 1A protein fragment

P24 **Vivien Szabó[a,b], Rebeka Mészáros[c], Pál Sipos[b,D], Márton Szabados[a,B]**
*[a]Department of Organic Chemistry, University of Szeged, H-6720 Szeged, Dóm square 8, Hungary*
*[b]Material and Solution Structure Research Group, Institute of Chemistry, University of Szeged, H-6720 Szeged, Aradi Vértanúk square 1, Hungary*
Synthesis of $Al(OH)_3$ based layered double and triple hydroxides containing manganese, cobalt, nickel, copper and zinc, catalytic use under continuous flow conditions in hydrogenation reaction

P25 **Bence Szakács[a], Tímea Kaszás[a], Tekla Blága[a], Kyle Doherty[b], Éva Juhász-Tóth[a], Trinidad Velasco-Torrijos[b], László Somsák[a], Marietta Tóth[a]**
*[a]University of Debrecen, Department of Organic Chemistry, H-4032 Debrecen, Egyetem tér 1., Hungary*
Transformations of anhydro-aldose oximes into potentially biologically active carbohydrate derivatives

P26 **Melinda Szasz, Dorina Casoni, Claudia Cimpoiu**
*Department of Chemistry, Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Arany Janos No. 11, Cluj-Napoca, Romania*
Similarity of structure and biological activity relationship between antipsychotic drugs and plants with antipsychotic effect

P27 **Melinda TAMAS, Roxana-Alexandra BUTUZA, Anca SILVESTRU**
*Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering,*
*Supramolecular Organic and Organometallic Chemistry Centre,*
*11 Arany János Street, 400028 Cluj-Napoca, Romania*
Diorganotin(IV) complexes with organoselenolato ligands

P28 **Petra Tolvaj, Sándor Kéki, Tibor Nagy**
*University of Debrecen, Faculty of Science and Technology, Department of Applied Chemistry, Hungary, H-4032 Debrecen, Egyetem square 1*
Analysis of cosmetic products by gas chromatography-mass spectrometry and direct-analysis-in-real-time mass spectrometry

P29 **Cătălin Turcu[a,b], Cătălin Maxim[a], Teodora Mocanu[c], Simona Nica[b] and Marius Andruh[a,b]**
[a]*University of Bucharest, Faculty of Chemistry,*
*B-dul Regina Elisabeta, Nr. 4-12, Sector 3, București – 030018 România*
[b]*"C. D. Nenitzescu" Institute of Organic and Supramolecular Chemistry of the Romanian Academy*
*Splaiul Independenței, Nr. 202B, Sector 6, București – 060023 România*
Novel Cu(II) complexes using photoisomerizable ortho-vanilin azo derivatives ligands

P30 **Serra Üneri Haymana, Lajos Nagy, Tibor Nagy, Ákos Kuki, Sándor Kéki**
*University of Debrecen, Faculty of Science and Technology, Department of Applied Chemistry, 4032, Egyetem tér 1, Debrecen/Hungary*
Research and improvement of Li-Air battery applying carbon based cathode

P31 **Rita Végh[a], Mariann Csóka[a]**
[a]*Hungarian University of Agriculture and Life Sciences, Institute of Food Science and Technology, Department of Nutrition, H-1118 Budapest, Somlói street 14-16, Hungary*
Effect of fruit powder fortification on the volatile profile of confectionery products

P32 **Valentin L. Virgil[1,2], Simona Nica[2], Cătălin Maxim[1], Marius Andruh[1,2]**
[1]*University of Bucharest, Faculty of Chemistry, Bulevardul Regina Elisabeta 4-12, Bucharest, Romania*
[2]*"Costin D. Nenițescu" Institute of Organic and Supramolecular Chemistry,*
*Splaiul Independenței nr.202B, 060023, Bucharest, Romania,*
$[Ln_2(hfac)_4(ac)_2(OH_2)_2(OMe)_2]$ – versatile precursor for optical active d-f metal-complexes

P33 **Mohit Yadav[a], Dalibor Tatar[b], Igor Djerdj[b], András Sápi[a], Ákos Kukovecz[a], Zoltán Kónya[a,c]**
*[a]Department of Applied and Environmental Chemistry, Interdisciplinary Excellence Centre, University of Szeged, H-6720, Rerrich Béla Sqr. 1, Szeged, Hungary*
Novel cerium oxide-type high entropy rare earth oxides for photocatalytic $CO_2$ hydrogenation

P34 **Lucian-Gabriel Zamfir[1], Raluca Ianchiș[1], Petru Epure[2], Maria-Lorena Jinga[1], Iuliana Răut[1], Cristina Firincă[1], Nicoleta Radu[1], Mariana Constantin[1], Luiza Jecu[1], Mihaela Doni[1], Ana-Maria Gurban[1,*]**
*[1]National Research & Development Institute for Chemistry &Petrochemistry - ICECHIM; Biotechnology Department, 202 Spl. Independentei, 060021 Bucharest, Romania*
Prospective studies on the development of nanocomposite based electrochemical sensors for the detection of clinically relevant molecules

P35 **Miaomiao Zhang[a], Márta Üveges[a], Judit Tormási[a], Eszter Benes[a], Livia Simon Sarkadi[a*], Réka Vass[b], Sándor G. Vari[c]**
*[a]Institute of Food Science and Technology, Hungarian University of Agriculture and Life Sciences, H-1118 Villányi street 29-43. Budapest, Hungary*
Determination of fatty acid composition in breast milk

# PLENARY LECTURES

# PL1 – PL2

# CONTROL OF CELLULAR FUNCTIONS THROUGH PROTEIN CYSTEINE PERSULFIDATION

**Péter Nagy**

*Department of Molecular Immunology and Toxicology and the National Tumor Biology Laboratory,*
*National Institute of Oncology, 1122 Budapest, Hungary;*
*Department of Anatomy and Histology, Laboratory of Redox Biology,*
*University of Veterinary Medicine, 1078 Budapest, Hungary;*
*Chemistry Institute, University of Debrecen, 4012 Debrecen, Hungary*
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In the field of Redox Biology, cysteine persulfidation (P-Cys-SSH) and polysulfidation (P-Cys-$SS_xH$) is gaining increasing attention as an important posttranslational modification of thiol proteins.

We have shown that persulfidation has a regulatory role on a number of protein functions and recently we also demonstrated their protein protecting properties in cells and *in vivo*. In cellular systems a substantial fraction of important thiol proteins (such as peroxiredoxins, PTP1B, PTEN, KEAP1 or Hsp90) are present in their persulfidated state, which we propose is a preemptive mechanism to prevent them from overoxidation during oxidative stress. We demonstrated that protection is due to formation of perthio-sulfenic, sulfinic and sulfonic acid derivatives (Cys-$SSO_{1\text{-}3}H$), which can be reduced back by the thioredoxin system to the corresponding functional native thiol forms when the stress is over.

We propose that dynamic oxidative persulfidation and enzymatic reduction of functional protein cysteine residues is a general regulatory element in cellular systems. The last part of my presentation will be allocated to show the relevance of this chemistry in cancer biology.

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I acknowledge the support of the National Research, Development and Innovation Fund of the Ministry of Culture and Innovation, under the National Laboratories Program (National Tumor Biology Laboratory (2022–2.1.1-NL-2022-00010)); the Hungarian Thematic Excellence Program (under project TKP2021-EGA-44) and the Eötvös Loránd Research Network – ATE – Laboratory of Redox Biology (grant 15002).

# ORGANOMETALLIC COMPOUNDS OF HEAVY GROUP 14 ELEMENTS (Sn, Pb) – FROM LIGAND DESIGN TO APPLICATIONS

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Organotin(IV) compounds are known for their use as heat stabilizers in PVC industry, catalytic agents (in the formation of urethane foams, silicon rubbers, or esterification) or as biocidal derivatives for more than 60 years.[1]

The organic ligands used for these species have a major impact regarding their catalytic or biologic activity. Thus, an important milestone for organotin(IV) chemistry was the introduction of the 2-($Me_2NCH_2$)$C_6H_4$ moiety which came with various structural particularities[2,3] and potential biological applications for organotin(IV) compounds.[4]

We use this pendant-arm ligand to obtain a rare example of organolead(II) amide and the first organolead(II) boroxide (Figure 1), bringing additional information about the Pb-O bond formation.[5]

On the other hand, our *C*,*O*-chelating ligand was successfully used to isolate novel organotin(IV) derivates, able to act as ligands for other metal centers, giving heterobimetallic complexes (Figure 2).

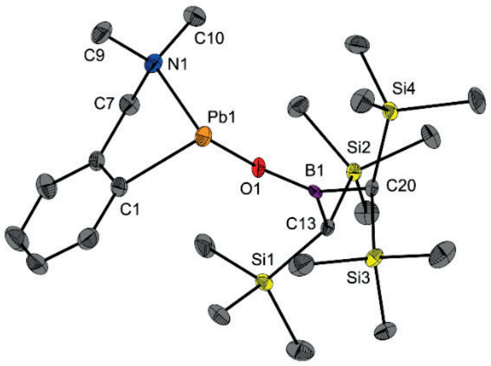

**Figure 1.** Molecular structure of [2-($Me_2NCH_2$)$C_6H_4$]PbOB[CH($SiMe_3$)$_2$]$_2$

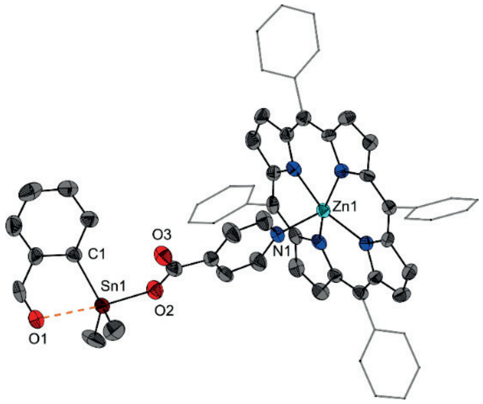

**Figure 2.** Molecular structure of [{2-(O=CH)$C_6H_4$}$Me_2$SnO(O)C$C_5H_4$N-4]ZnTPP

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Financial support from the National University Research Council of Romania UEFISCDI (Research Projects No. PN-IIIP4-ID-PCCF-2016-2-0088/Partner 2, PN-III-P1-1.1-PD-2019-0976.) and from the Babeș-Bolyai University, research project GTC-31835/2020 are highly appreaciated.

# ORAL PRESENTATIONS

## O1 – O23

# CADMIUM COMPLEXES WITH ORGANOSELENOLATO LIGANDS. SYNTHESIS AND STRUCTURAL CHARACTERIZATION

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Recent advances in the development of new precursors for semiconducting materials have attracted a continuously increased interest towards the synthesis of metal complexes with organochalcogen ligands, which might be used to obtain thin films of metal chalcogenides, suitable for optoelectronic devices. Metal complexes for such applications are recommended to have a monomeric structure, thermal stability, and high volatility.[1] Such characteristics can be controlled by using organic groups with donor atoms capable of internal coordination, thus providing an extended coordination sphere around the metal center and either a monomeric structure or only a low degree of association. Metal complexes of type $(RSe)_2M$ (R = 2-$(Me_2NCH_2)C_6H_4$; M = Zn, Cd) were reported to exhibit such particularities due to the nitrogen donor atom in the pendant arm of the organoselenolato ligand.[2]

We report here the synthesis of the new complexes $[Cd(Cl)\{SeC_6H_4(CH_2NMe_2)\text{-}2\}]$, $[Cd(Cl)\{SeC_6H_3(CH_2NMe_2)_2\text{-}2,6\}]$ and $[Cd(SeR)\{N(SiMe_3)_2\}]$ [R = 2-$(Me_2NCH_2)C_6H_4$ or 2-$(CHO)C_6H_4$]. The cadmium complexes were characterized by multinuclear NMR ($^1H$, $^{13}C$, $^{77}Se$) and mass spectrometry. The molecular structures of $[2,6\text{-}(Me_2NCH_2)_2C_6H_3Se]_2[CdCl_4]$ and $[Cd\{SeC_6H_4(CH_2NMe_2)\text{-}2\}\{N(SiMe_3)_2\}]_2$ were determined by single crystal X-Ray diffraction, and strong N→Cd interactions were evidenced.

*Acknowledgements*: The support provided by The National Center for X-Ray Diffraction (Babeş-Bolyai University, Cluj-Napoca, Romania) for XRD determinations and refinement, and the financial support from UEFISCDI (Project PN-III-P4-ID-PCE-2020-1028) are highly acknowledged.

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# SYNTHESIS, CHARACTERIZATION AND EVALUATION OF THE CATALYTIC PROPERTIES OF PHOSPHINE- AND STIBINE-LIGATED CYCLOMETALATED PALLADIUM COMPLEXES

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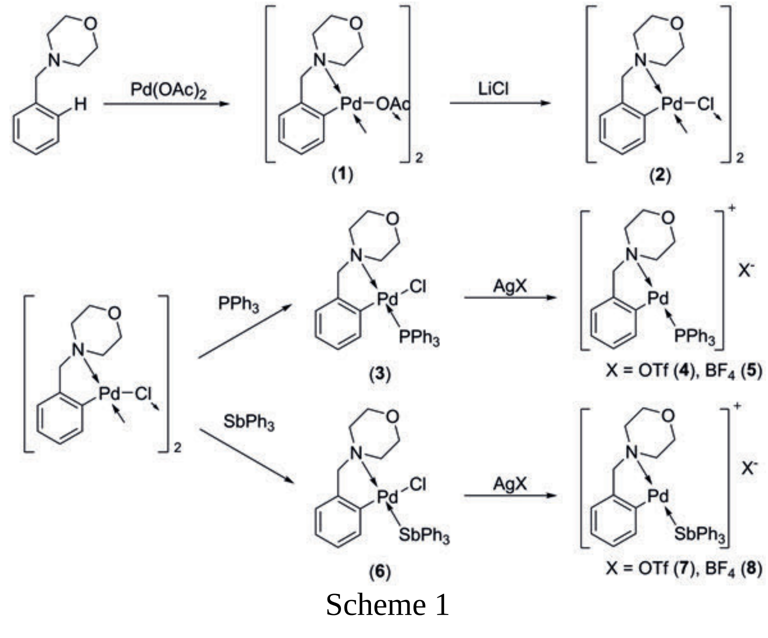
Cyclometalated palladium(II) compounds have attracted increasing attention in organometallic chemistry, finding applications in organic synthesis and in catalysis. Several groups have focused their research in this area, enhancing and tuning the palladacycles catalytic capabilities, by modifying their electronic and steric properties.[1] On this basis many efforts were made to develop highly effective catalysts for reactions such as Suzuki cross-coupling and homocoupling of phenylboronic acids to obtain nonsymmetric and symmetric compounds, respectively.[2]

The main objectives of this research work concern (*i*) the design and synthesis of a new series of neutral and ionic compounds containing the five-membered palladacycle fragment $[2\text{-}\{O(CH_2CH_2)NCH_2\}C_6H_4]Pd(II)$ in which the palladium is coordinated to different donor atoms (P and Sb) in the ancillary ligand (Scheme1), (*ii*) their structural characterization by multinuclear NMR in solution and single-crystal X-ray diffraction, and (*iii*) evaluation of their catalytic properties towards homocoupling and Suzuki cross-coupling reactions.



Scheme 1

*Acknowledgements:* This work was supported by a grant of Ministry of Research and Innovation, CNCS - UEFISCDI, project number PN-III-P4-ID-PCE-2020-2651.

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# STRUCTURAL ASPECTS IN SILVER COMPLEXES WITH DIORGANOCHALCOGEN LIGANDS OF TYPE $(2\text{-}XC_6H_4CH_2)_2E$ (E = S, Se; X = Br, $CH_3$)

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Silver complexes attracted a continuously increased interest for their applicability in various fields, *e.g.* as antimicrobial and antibacterial agents,[1] catalysis or co-catalysis for organic transformations, or as precursors for silver chalcogenides. The biological uses of silver compounds are based not only on the specific activity, but also on their low toxicicy.[2]

We focused our research work on the coordination behaviour of diorganochalcogen ligands of type $(2\text{-}BrC_6H_4CH_2)_2E$ [E = S (**L1**), Se (**L2**)] $(2\text{-}CH_3C_6H_4CH_2)_2E$ [E = S (**L3**), Se (**L4**)] towards silver. The four ligands were prepared by reacting 2-bromobenzil bromide or 2-methylbenzil bromide with the corresponding sodium chalcogenide, based on adapted literature procedures.[3] All four compounds were employed in reactions with silver salts, namely $AgNO_3$, AgOTf and $AgClO_4$ in a 1:1 or a 1:2 molar ratio, thus resulting in complexes of type [Ag(X)(L}] and $[Ag(X)(L)_2]$, respectively, where X = $ONO_2$, $OSO_2CF_3$, or $OClO_3$ and L = **L1** – **L4**. The purity, the solution behaviour and the solid-state structure of the ligands and the silver complexes were investigated by analytical methods: mass spectrometry, multinuclear NMR, molar conductivity and IR spectroscopy. For selected compounds, the molecular structures were determinate by single-crystal-X-ray diffraction. The molar conductivity for $10^{-3}$ mol/L MeOH solutions showed a behaviour as 1:1 electrolytes for the silver complexes, while the single-crystal X-ray diffraction studies revealed the attachment of the inorganic ligands $X^-$ to silver by O─Ag interactions.

*Acknowledgements*: The support provided by The National Center for X-Ray Diffraction (Babeș-Bolyai University, Cluj-Napoca, Romania) for XRD determinations and refinement, and the financial support from UEFISCDI (Project PN-III-P4-ID-PCE-2020-1028) are highly acknowledged.

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# SYNTHESIS, STRUCTURAL CHARACTERIZATION AND REACTIVITY OF NOVEL ORGANOANTIMONY(III) ARYLOXIDES

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The organometallic chemistry of antimony(III) has produced significant achievements in both fundamental and applied chemistry in the last few decades. Notable achievements have been obtained in a wide range of topics, including but not limited to efficient fixation of $CO_2$ by organoantimony(III) oxo-species, C−H bond activation, as well as applications in catalysis. The area of organoantimony(III) alkoxides and aryloxides, however, is poorly developed, with relatively few examples published so far.[1-4]

A series of new organoantimony(III) aryloxides, $[2\text{-}(Me_2NCH_2C_6H_4)]_2Sb(OAr)$ (**3**), $[2\text{-}(Me_2NCH_2C_6H_4)]Sb(OAr)Cl$ (**5**), $[2\text{-}(Me_2NCH_2C_6H_4)]Sb(OAr)_2$ (**6**) and $[\{2\text{-}(Me_2NCH_2C_6H_4)\}Sb(OAr)]_2O$ (**7**) (Ar = 2,4,6-$Cl_3C_6H_2$), were synthesised using two different synthetic pathways and were structurally characterised. The stability in solution and sensitivity to moisture of these compounds as well as the reactivity of compounds **3**, **6** and **7** towards $CO_2$ was investigated.

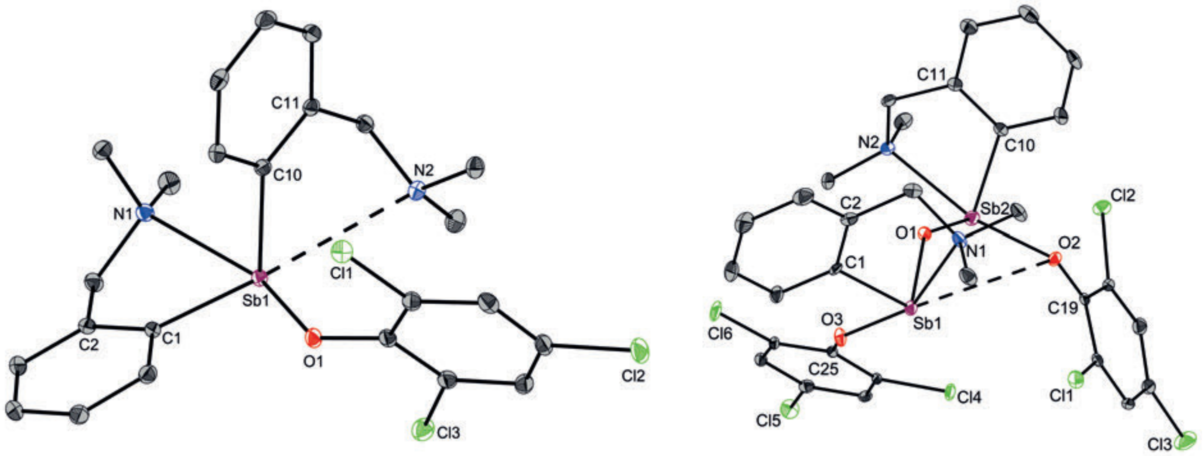

Figure 1. Molecular structures of compounds (**3**) (*left*) and (**7**) (*right*).

*Acknowledgements:* This work was supported by a grant of Ministry of Research and Innovation, CNCS - UEFISCDI, project number PN-III-P4-ID-PCE-2020-2651.

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# FE-LOADED ZNO FOR SUSTAINABLE $CO_2$ PHOTOCATALYSIS: A STEP TOWARDS $CO_2$ UTILIZATION''

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## Abstract

This study investigates the synthesis and characterization of iron loaded zinc oxide (ZnO) as a photocatalyst for $CO_2$ photoreduction. Two different synthesis methods, hydrothermal and wet impregnation, are compared and the photocatalytic activity of the resulting samples is evaluated under both UV and visible light irradiation. Various characterization techniques, such as XRD, TEM and UV-Vis diffuse reflectance spectroscopy are used. The study finds that Fe wet impregnation method significantly improves the photocatalytic activity of the iron-loaded ZnO under both UV and visible light irradiation, compared to the ZnO with iron loaded through the hydrothermal method. However, the iron-loaded ZnO synthesized through the hydrothermal method also shows some photocatalytic activity. The study focuses on the application of photocatalysis for $CO_2$ photoreduction using RWGS as a model reaction. Overall, the study provides valuable insights into the synthesis and characterization of iron-loaded ZnO as a photocatalyst for $CO_2$ photoreduction and highlights the importance of synthesis method on photocatalytic activity.

**Keywords:** Photocatalysis, $CO_2$ reduction, RWGS, UV/Visible light irradiation.

# EFFECT OF CEO$_2$ MORPHOLOGIES ON CO$_2$ CONVERSION TO CO VIA REVERS WATER GAS SHIFT REACTION

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Carbon dioxide is an abundant carbon feedstock, and there exists a sustainable interest in methods for its utilization. CeO$_2$ with different shapes including Hollow sphere, Nanorods, two types of Mesoporous were prepared with different methodologies (hydrothermal, solgel, and impregnation) and applied to support Cu particles. The obtained samples were tested for the reverse water-gas shift (RWGS) reaction under the reaction conditions, V(H$_2$): V (CO$_2$) = 4:1. In order to reveal the core factors affecting the catalytic performance, the physicochemical properties of the catalysts were analyzed by XRD, BET, SEM, TEM, and H$_2$-TPR techniques. The Cu/CeO$_2$-hollow sphere sample exhibited the best catalytic performance among the as-prepared catalyst with approximately 99% CO selectivity. It is owing to CeO$_2$-hollow sphere catalyst has the largest surface area, pore size, and pore volume which are vitally crucial for CO$_2$ catalytic reaction.

**Keywords:** CeO$_2$, Different morphologies, Copper, Reverse water-gas shift reaction, CO$_2$ hydrogenation

# DEVELOPMENT AND STUDY OF Li-AIR BATTERY USING CARBON CATHODE

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## Abstract

A new, recheargeable lithium-air battery was constructed and tested using 3D printer for printing the Swagelok-type polypropylene (PP) cell body. Two different types of carbon based cathodes which were charcoal and vulcan carbon cloth were applied; and metal lithium was used as anode. The anode and cathode compartments were separated by polypropylene membrane and 1.0 M Li-trifilate dissolved in propylene carbonate was applied as electrolyte. To prevent any damage of PP membrane and to ensure the appropriate amont of electrolyte cotton membranes immersed in electrolyte were placed on both sides of the PP membrane in case of charcoal cathode. However, for vulcan carbon cathode, only one cotton membrane was applied in the lithium anode compartment.

To test and compare the two cells with different cathodes the cyclic voltammetry, impedance spectroscopy and cycling test measurements were performed using 0.05 mAcm$^{-2}$-0.1 mAcm$^{-2}$ current densities. It was found that the charcoal cathode could provide higher capacity and lifetime than the vulcan carbon; the Coulomb efficiency was approximately 100% over 200 (Fig. 1) and 60 cycles for the charcoal and vulcan carbon cathods, respectively.

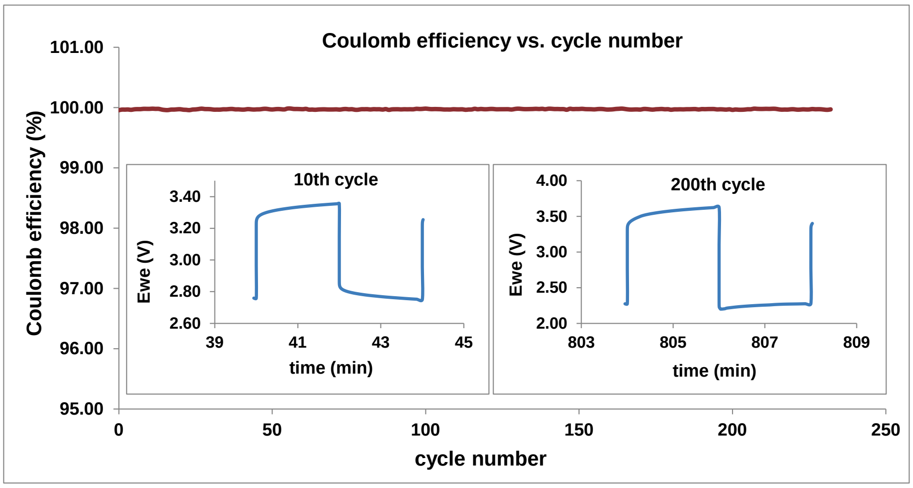

Figure 1: Coulomb efficiency and cycles using charcoal as cathode

*Acknowledgements:* Project no. RRF-2.3.1-21-2022-00009, titled National Laboratory for Renewable Energy has been implemented with the support provided by the Recovery and Resilience Facility of the Europian Union within the framework of Programme Széchenyi Plan Plus. Thanks for the financial support provided by the Mol Group, Hungary.

# SYNTHESIS OF METAL NANOPARTICLE-CONTAINING AEROGELS AND THEIR POTENTIAL APPLICATION AS CATALYSTS

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In recent years, various fields have focused on metal nanomaterials because of their unique properties. To date, metal nanoparticles (NPs) have been synthesized using three methods: physical (mechanical methods and vapor methods) chemical and biological approaches. Among these methods, the chemical approach is the most common. In a typical chemical synthesis process, metal NPs are synthesized via the reduction of a metal in the salt form to its metallic form in an aqueous phase.[1] In this work, Au NPs, Ag NPs and Ag-Cu NPs were prepared and characterized by using UV–Vis spectroscopy and transmission electron microscopy (TEM) techniques

Aerogels are suitable for forming nanocomposites with metal nanoparticles due to their structure. Immobilization of nanoparticles in a chemically resistant aerogel matrix would offer the possibility of combining the advantages of an immobilized catalyst and a highly porous and easily penetrable solid support.[2] The production of aerogels consists of three main steps: sol-gel synthesis, aging and supercitical drying. Unfortunately, the synthetic conditions of the sol-gel process led to rapid aggregation of the citrate-stabilized nanoparticles and the loss of catalytic activity. It has been found that certain organic solvents and atmospheric $CO_2$ have significant effect on aggregation but cannot be entirely excluded under standard synthetic conditions. Testing several types of polymeric materials resulted in the solution, in which polyvinylpirrolidone (PVP) served as a protecting polymer which prevented the formation of larger aggregates.[3]

The catalytic activity of the as-prepared nanocomposite aerogels and the synthesized Au NPs, Ag NPs, and Ag-Cu NPs as catalysts were evaluated via the reduction of p-nitro phenol by sodium hydroborate monitored by UV-Vis. Nitrophenols are difficult to be biodegraded, which causes toxic threat to aquatic lives and amphibians, including human beings.

*Acknowledgements:* This publication was supported by the GINOP-2.3.2-15-2016-00041 project. The work was co-financed by the European Union and the European Regional Development Fund.

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# SYNTHESIS OF CARBORANYL-SILOLES – NEW AIEGENS

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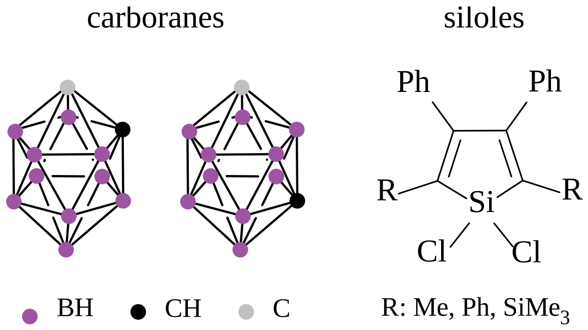
Aggregation-induced emission (AIE) is an abnormal phenomenon observed with certain molecules. It is receiving intense research interest due to its bright prospects in material science and biological technology[1]. This unique behavior was first described in the case of siloles.[2] Most of these compounds do not show significant fluorescence in diluted solution because nonradiative relaxation occurs due to the rotation of the different substituents of the silole ring. These rotational motions are hindered in the aggregate state; the fluorescence could be recovered in the aggregate or solid state.[3] Later, the same behavior was described in the case of the 3-dimensional o-carborane compounds. Still, unlike siloles, the AIE behavior could be attributed to C-C bond vibration within the cluster framework.[4]



Questions arise about how the system derived from combining the two types of AIE active compounds behave. In this work, we have successfully synthesized nine new carboranyl-silole molecules and investigated their photophysical behavior. Based on our results, these compounds show AIE properties and are potentially suited for optoelectric appliances.

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# THE SWEETEST TIME CAPSULES – THE MP-AES ANALYSIS COUPLED WITH AMS AGE DETERMINATION OF HUNGARIAN MULTIFLORAL HONEY SAMPLES

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Our former study highlights that acacia honey can be successfully applied for long-term environmental assessment as old samples keep inorganic compounds preserved as well as they serve as a proper material for radiocarbon dating. Good agreement was observed between the radiocarbon activity of the acaica honeys and the atmospheric bomb-peak that was used for calibration. In present study the time-dependent elemental composition and AMS dating results of 36 rape, sunflower and multifloral honey samples are presented, collected between 1985 and 2018 in geographically close locations. Elemental concentration data were gained by MP-AES method. Based on the elemental analysis we concluded that bee products regardless the type provide useful environmental information of the previous decades, such as the decreasing trend of airborne Pb emission can be traced. However, radiocarbon results agree less with the atmospheric bomb peak. Random offsets were observed in the specific radiocarbon activity of the honey samples. FTIR-ATR analysis was used to gain a deeper knowledge regarding the organic material composition of the honey samples. Results indicate that neither the inorganic composition nor the organic constituents show corresponding pattern to the AMS deviation. Even the 5-(Hydroxymethyl)furfural content following the expected age trend in acacia honeys has no such pattern in present sample series. This work indicates that rape and sunflower honey samples are not as reliable materials for radiocarbon dating as acacia honeys. Thus, the complex application of honey samples for environmental reconstruction requires the species-separated investigation of bee products to reveal their adaptability for assessment approaches.

*Acknowledgements*: The research was supported by the European Union and the State of Hungary, co-financed by the European Regional Development Fund in the project of GINOP-2.3.2-15-2016-00009 'ICER'. E. Baranyai and Z. Sajtos are grateful for the financial support of the János Bolyai Research Scholarship of the Hungarian Academy of Sciences and for the support of the ÚNKP-20-5 (Bolyai+) and ÚNKP 22-4-1 New National Excellence Program of the Ministry of Innovation and Technology from the source of the National Research, Development and Innovation Fund of Hungary.

# INVESTIGATION OF THE TECHNO-FUNCTIONAL ROLE OF DIETARY FIBERS IN FOOD MATRICES BASED ON GLUTEN-FREE CEREALS AND PSEUDOCEREALS

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Both from a nutritional and technological point of view, the properties of various fiber components can be significantly different, which can also be greatly influenced by food processing technology. Cereals and pseudocereals have been the basis of human nutrition for thousands of years, which are also excellent sources of dietary fibers. Their most significant fiber components are pentosans (arabinoxylans, AX) and β-glucans. The techno-functional properties of AXs have already been investigated in many studies in wheat and rye-based matrices, based on which interactions with gluten proteins are assumed[1,2]. However, there are still severeal open ended questions regarding the role of AX in food matrices. Much less information is available about β-glucan functionality compared to AXs, drawing attention to the need of performing comprehensive studies in this area.

The basic assumption of the current research is that different fibers play a complex role in affecting the properties of food matrices (e.g.: dough) based on cereals and pseudocereals. However, it is questionable to what extent and how particular fiber components influence the technological properties in matrices of different composition, in the absence of gluten proteins.

The aim of this work was to investigate the techno-functional properties of arabinoxylan and β-glucan cereal fibers in different gluten-free cereal and pseudocereal based model dough systems, as well as to study the possible intermolecular interactions with other matrix constituents, like proteins and starch). Different approaches were used to investigate the role of individual dietary fiber components. On the one hand, the studied fiber component was added to native flours. In this case, the flour components can be tested in their original state, but they might interfere the identification of the impact of the dosed fiber components. Based on another approach, flour was fractionated into its main components (proteins, starch) and then composed repeatedly (reconstituted) by mixing the fractions in correct proportion to create a cleaner, simpler model system. By a reduction-reoxidation process of dough, which has already been successfully applied to wheat[3], possible disulfide and other covalent bonds formed during dough mixing can be broken with reducing agents, then reassembled by oxidation. Thereby the incorporation of the component in question into the protein-starch matrix can be investigated.

The results of the research work can contribute to a more comprehensive understanding of the structural role of dietary fibers in food matrices based on gluten-free cereals and pseudocereals, as well as to the development of healthier gluten-free bakery and pasta products with increased dietary fiber content.

This research work supported by the ÚNKP-22-4-II-BME-129 New National Excellence Program of the Ministry for Culture and Innovation from the source of the National Research, Development and Innovation Fund and is the part of the BME-EGA-02 - TKP2021 project supported by the Ministry for Innovation and Technology of Hungary from the National Research, Development and Innovation Fund.

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# DETERMINATION OF PROTEIN QUALITY OF BEEF SAUSAGE

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Beef meat is one of the most nutritious foods that contains a variety of nutrients, including high-quality protein. Traditional Kosovan sausage is a dried, precooked, non-fermented sausage. The aim of this study was to determine the nutritional quality of traditional beef sausages based on proteinogenic amino acid and free amino acid composition. The Automatic Amino Acid Analyzer (AAA400 Ingos Ltd., Prague, Czech Republic) equipped with an Ionex Ostion LCP5020 cation-exchange column (22×0.37 cm) was used to determine amino acids after hydrolyzation (6 M HCl, 24 h), and free amino acids after extraction with 10% trichloroacetic acid. Ala (15.56%), Leu (13.28%), Gly (8.64%), Pro (8.41%), Ser (8.26%), and Val (7.65%) were the main protein building amino acids. Essential amino acids made up 44.30% of total amino acids. Beside the protein building amino acids, the content of free amino acids was relatively high accounted around 10% of total amino acid content. Ala (22.81%), Glu (11.61%), Leu (9.19%), and Lys (7.67%) were the most abundant free amino acids. The results show that taditional Kosovan beef sausage has a high nutritional value and is a good source of amino acids essential for human health.

*Acknowledgements*: The authors acknowledge the Hungarian University of Agriculture and Life Sciences's Doctoral School of Food Science and Stipendium Hungaricum Scholarship for the support in this study!

# ANTIOXIDANT AND ANTIBACTERIAL ACTIVITIES OF PEPTIDES BY HYDROLYSIS OF SOYBEAN MILK PROTEIN BY PAPAIN

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Soybean (*Glycine max*) milk protein (SMP) has been recognized as a high-quality source of protein because it contains all of the essential amino acids necessary for human diet and nutrition. Contradictorily, soybean proteins are listed among the “big 8” allergens due to the presence of linear and conformational epitopes in protein structure. Therefore, to produce peptises from SMP is a considerable attractive. The objective of the investigation was to prepare peptides with antioxidant and antibacerial activities by papain hydrolysis of SMP by continuous-mode membrane bioreactor.

The process was started with 720 mL of soybean milk (initial volume), pH 7, and 80 mL of sterile enzyme solution. Therefore, it may be said that the membrane bioreactor was started with 0.9 $g{\cdot}L^{-1}$ of papain and 25 $g{\cdot}L^{-1}$ of soybean milk protein. In the bioreactor, temperature 50 °C was maintained in the experiment. In the membrane separation unit, constant operational TMP 3 bar and retentate flow rate ($Q_r$) 100 $L{\cdot}h^{-1}$ were maintained. Membrane permeates with constant volume were collected in fraction basis and the volume level of soybean milk in the bioreactor was maintained constant through level-controller and constant supply of enzyme-free soybean milk. Membrane bioreactor was operated for 12 h. Antioxidant capacity and antibacterial activity were measured in membrane permeate, collected at every time fraction. To understand the molecular weight of soybean proteins and soybean-based peptides, sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) was performed by a vertical electrophoresis system. Antioxidant capacity was measured by ferric reducing ability of plasma (FRAP) and 2,2-Diphenyl-1-picrylhydrazyl (DPPH) assays. The antibacterial activity (zone of inhibition) against *Bacillus cereus* was noted in membrane permeate by agar-diffusion method. Peptides with antioxidant capacity and antibacterial activity were produced by papain hydrolysis of SMP in membrane bioreactor.

It was found that initially, permeate flux was high, subsequently reduced and eventually became asymptotic with filtration time due to the formation of concentration polarization on membrane surface. When the static turbulence promoter was not used inside of the membrane tube, initial permeate flux ($J_o$) and specific energy consumption ($E_s$) were 2.8 $L{\cdot}m^{-2}{\cdot}h^{-1}$ and 31 $kW{\cdot}h{\cdot}m^{-3}$, respectively. Those values were changed to 8.7 $L{\cdot}m^{-2}{\cdot}h^{-1}$ and 38 $kW{\cdot}h{\cdot}m^{-3}$ when the static turbulence promoter was applied inside of the membrane tube. The static turbulence promoter created turbulence in working fluid, offered tangential and centrifugal forces, increased velocity and vorticity of fluid across the membrane surface, which reduced deposition of solutes on membrane surface (concentration polarization) and increased permeate flux. Specific energy consumption during the static turbulence promoter-implemented filtration process was lower compared to the filtration without that device. It was found that the antioxidant capacity and zone of inhibition by permeate from membrane, collected at different fractions during the whole period, increased over time. As the membrane bioreactor was operated with a continuous supply of soybean milk into the bioreactor and sufficient amount of papain, more soybean milk proteins were hydrolyzed over time and permeated through porous channel of membrane in a continuous way.

# CURRENT APPLICATIONS OF ANTIMICROBIAL PEPTIDES

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The discipline of biomedicine has undergone significant development in recent years. New treatments have been discovered that may be able to combat incurable diseases. Cancer is a major public health concern and one of the leading causes of death around the globe. Due to the toxicity of current treatments and the frequently acquired resistance of tumor cells, novel treatment methods have been sought, with an emphasis on more specific targeted cell therapies. Due to their capacity to bind to multiple types of cancer cells and their blood vessels, peptide technology are considered efficient for cancer treatment[1,2]. Bacterial infections represent a further global health concern. The threat posed by bacterial drug resistance is growing, necessitating the contemplation of alternative treatments. Thus, antimicrobial peptides (AMPs), which are omnipresent, are oligopeptides that can pass through the inner and outer membranes of microorganisms. Antifungal, antiviral, and anticancer properties are also attributed to these AMPs[3]. The applications of different peptides and the involvement of peptide-based therapeutics in clinical trials will be discussed.

*Acknowledgments:* This work was supported by a grant from the Ministry of Research, Innovation and Digitization,
CNCS - UEFISCDI, project number PN-III-P4-PCE-2021-0639, within PNCDI III.

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# VOLATILE COMPOUNDS PROFILE OF SARDINES (*SARDINA PILCHARDUS*) TREATED WITH HIGH-PRESSURE PROCESSING TECHNOLOGY

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High-pressure processing (HPP) is an innovative non-thermal technology in the food processing sector exhibiting an excellent capacity for microbial inactivation, improving the shelf life of food products and preserving their quality[1]. Sardines are the most relevant pelagic fish of the Mediterranean Sea and their chemical composition is considered to be a source of multiple bioactive compounds such as ω3 polyunsaturated fatty acids, especially eicosapentaenoic (EPA) and docosahexaenoic (DHA) acids, and antioxidants[1]. However, sardines are prone to microbial spoilage and lipid oxidation during food processing and storage. Furthermore, sardines and the chemical changes such as lipid oxidation that might be induced during HPP treatments are not well covered in the literature.

The aim of this work is to evaluate the extent of lipid oxidation in sardine fillets after different HPP treatments, i.e., samples pressurized at 400 and 600 MPa for 1, 2.5, 5, and 10 minutes, and subsequently stored at (+4°C) for 0, 7, and 14 days. Treated samples and control ones were subjected to lipid extraction at the storage days. All the extracted lipids were analyzed for volatile compounds using headspace solid phase micro-extraction (HS-SPME), together with gas chromatography-mass spectrometry[2,3].

The preliminary results showed alterations in the studied lipid dependent on the intensity of pressure and its duration. Volatile secondary oxidation products such as ketones and aldehydes (including alkanals, alkenal, alkadienals, and aromatic aldehydes) were present at the end of the storage period.

HPP conditions seemed to have an impact on the presence of oxidized products while improving the shelf-life of fresh sardines. However, there was no notice of lipid rancidity in the pressurized samples stored for up to 14 days at (+4°C). Eventually, high-pressure processing is a solution to preserve sardines and maintain their antioxidant content.

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# CHANGES IN THE FREE AMINO ACID CONTENT OF SAUSAGES DUE TO HIGH HYDROSTATIC PRESSURE TREATMENT

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The free amino acid (FAA)composition of meat products contributes to the flavor, taste and quality of the product during storage. This study aimed to evaluate the effect of high hydrostatic pressure (HHP) treatment on the formation of free amino acids in different types of sausages (chicken, pork and mangalica sausages) during storage. The samples were treated with 600 MPa pressure for 5 minutes and stored at 12 -16°C for five weeks. Free amino acids were determined using an automated amino acid analyzer, after extraction with 10% trichloroacetic acid. A total of 26 amino acids were identified, with glutamic acid, alanine, leucine, lysine, and 1-methyl-histidine as the major FAA in all sausage samples. Results showed that the content of branch chain amino acids (BCAA-Leu, Ile, Val), sulfur-containing amino acids (SAA-Met, Cys), and aromatic amino acids (AAA- Phe, Tyr) was highest in mangalica sausages (BCAA:17.72-25.01%; SAA: 2.92-4.10%; AAA: 4.14-5.10%), followed by chicken (BCAA:17.90-19.69%; SAA: 2.77-3.04%; AAA: 3.59-4.15%) and pork sausages (Bcaa:14.01-15.95%; SAA: 2.20-2.62%; AAA: 3.14-4.08%) in both control and HHP-treated samples. Depending on the type of sausage and the storage time, the HHP treatment had a variable effect on the amino acid content. HHP treatment increased the levels of BCAA, SAA, and AAA in pork sausages. HHP treatment, on the other hand, reduced the amino acid content of chicken sausage from the first to the fifth week of storage. HHP treatment had no characteristic effect on mangalica sausage. The findings of this study provide useful insights into the effects of HHP treatment on the nutritional composition of sausages and emphasize the importance of taking the type of sausage and storage time into account when assessing the impact of HHP on food quality.

*Acknowledgements*: The authors acknowledge the Hungarian University of Agriculture and Life Sciences's Doctoral School of Food Science and Stipendium Hungaricum Scholarship for the support in this study!

# RECOVERY OF BIOACTIVE ANTHOCYANIN PIGMENTS FROM HAWTHORN FRUIT BY INFUSION, MICROWAVE, AND ULTRASOUND-BASED EXTRACTION TECHNIQUES.

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The present study aimed to evaluate the efficient extraction techniques for recovering superior-quality anthocyanins from hawthorn fruit. Infusion, ultrasound-assisted, and microwave extraction techniques were carried out using different solvents (methanol, ethanol, and isopropanol). The results of the anthocyanin concentration, co-pigmenting compounds, color values, and antioxidant activities of hawthorn fruit extracts suggested that the ultrasound technique is superior to other techniques, which gave a total anthocyanin content (TAC) of (0.152, 0.143, and 0.097 mg/100 g) using methanol, ethanol, and isopropanol respectively. It was also shown that methanol extract is better than the other solvents extract. In addition, the color pattern (L*a*b*) of the extracts was measured. Generally, the trends of the lightness (L*) values, and the values of yellowness or blueness (b*) were lower than the control sample, while the values of redness or greens (a*) were higher than the control sample which has values of (L*=54.65, b*=18.22, a* =-10.54). In brief, the obtained results show the potential of hawthorn fruit as a source of anthocyanin pigments, with potential uses in various industrial fields, such as food, pharmaceutical, and cosmetics.

**Keywords:** Hawthorn fruit, Anthocyanins, Infusion, ultrasound-assisted, Microwave

*Acknowledgement:* The authors acknowledged the European Union and the European Social Fund (grant agreement no. EFOP-3.6.3- VEKOP-16-2017-00005), the Tempus Public Foundation under the Stipendium Hungaricum Scholarship Program for their financial support to our project.

# MICROWAVE-INDUCED BASE-CATALYZED SYNTHESIS OF METHYL LEVULINATE FROM LEVULINIC ACID

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In todays' infrastructure the integration of biodiesel and bioethanol proved to be one of the increasingly popular application of the biomass for fuel production as renewable carbon source. Despite the advantages, too high amount of food ingredients are consumed for the synthesis of the first generation biofuels. This realization led the researchers to turn to the improvement of second generation biofuels. For the synthesis of these, lignocellulose is used as raw material, which is widely available and can be transformed into numerous products[1]. Levulinic acid[2] is a product formed during cellulose degradation and is a platform molecule. The alkyl-levulinates formed from the levulinic acid alkylation are promising applicants as biodiesel additives[3].

The aim of our research was to synthesize methyl levulinate from levulinic acid using dimethyl carbonate as methylating agent. Despite the fact that levulinic acid is used widely, only few articles can be found in the literature about this method. Even though, dimethyl carbonate is considered green, it is a weak methylating agent, for this reason it needs long reaction time (4 hours) and high temperatures (160-200°C). Considering this characteristic microwave irradiation was applied to examine its potential for milder reaction conditions.

In our work with the assist of microwave irradiation we managed to decrease the initial temperature and reaction time. According to our results at 120°C 1 hour, at 90°C (around boiling point) 4 hours is enough to reach 90% methyl levulinate yield. Furthermore, we decreased the necessary catalyst amount (to 1/8) and the dimethyl carbonate solvent/reactant amount (to ½). Another remarkable aspect of our results, that we observed a stable intermediate which is not yet described in the literature. This intermediate was examined using different techniques such as: XRD, FT-IR, $^{1}$H-NMR, $^{13}$C-NMR, and GC-MS.

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# IODINE BIOFORTIFICATION OF CABBAGE PLANTS CULTIVATING IN A HYDROPONIC SYSTEM

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Iodine is an essential trace element in the human diet being involved in the synthesis of thyroid hormones. The recommended daily intake for iodine ranges between 90 and 270 µg; 90 µg – young children (1–8 years), 120 µg – older children (9–13 years), 150 µg – adults, and 220–270 µg pregnant and lactating woman[1,2]. Iodine deficiency affects ca. 2.2 billion people worldwide, therefore it is an important challenge to find a plant-based source of iodine, which would provide the recommended dietary allowance[3].

In this work iodine biofortification of cabbage was investigated cultivating plants in hydroponic system containing iodine in concentration of 0.01-1.0 mg/L as potassium iodide or potassium iodate. During the experiment plant physiological properties (chlorophyl content, photosynthetic efficiency), biomass production, concentration changes of iodine- as well selected essential elements were investigated.

Results showed that iodine addition had no effect on the photosynthetic efficiency and chlorophyll content. Biomass production was stimulated by the iodide treatment in all dosages, while applying iodate this phenomenon was observed only in low concentrations, above 0.5 mg /L the yield was reduced. Increasing iodine concentrations in the nutrient solutions resulted in higher iodine content in all plant parts, the presence of iodide caused 2-7 times higher accumulation compared with the iodate treatment and it was established that and highest concentration was observed in the roots, lowest in the edible plant tissues. Type of the iodine treatment had different impact on the essential element transport, applying iodide in the nutrient solution the concentration of all elements was decreased, while adding 1.0 mg/L iodate the transport was stimulated compared with the control plants.

Acknowledgements: This research was supported by the National Research Development and Innovation Office (PD 132242).

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# DRUG DELIVERY SYSTEMS BASED ON BORONIC ACID-FUNCTIONALIZED SILICA FOR CANCER THERAPY

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Novel approaches regarding cancer therapy are based on targeting cancerous cells, avoiding side effects of classical chemotherapeutic agents, as well as enhancing their effects on the targeted cells[1,2]. Mesoporous silica nanoparticles (MSN) are versatile, biocompatible platforms that can accommodate guest molecules and various functional groups, for developing systems for cancer therapy applications[3]. MSN have high specific surface area, large pore volume and tailored pore array. Boronic acid derivatives have the capacity to target sialic acid receptors overexpressed by breast cancer cells, due to its capacity to reversibly form boronic esters with diols and triols[4].

In this work, several boronic acid-functionalized MSN were obtained and characterized as delivery systems for doxorubicin. The boronic acid moieties were grafted on the surface of MSN. Two types of silica carriers were employed in order to study their influence on the functional group binding, as well as on chemotherapeutic agent release.

The physicochemical properties of both carriers and drug-loaded materials were evaluated through various characterization techniques. Biological effects of developed drug delivery systems on BJ dermal cells and BT474 breast cancer cell line were also assessed.

*Acknowledgements:* The financial support of the UEFISCDI funding agency (Romania) through project no. PED 576/2022 is greatly appreciated.

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# WATER SOLUBLE LUMINESCENT COORDINATION COMPLEXES

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## Abstract:

Water-soluble coordination complexes based on *d*-block metal centers are attracting a continuously growing interest for catalytic and biological applications due to their unique properties such as environment-responsive ligand exchange kinetics, diverse photochemical and photophysical properties, and the ability to form specific interactions with biomolecules.[**1,2**]

Oligopyridines as ligands, are of interest in medicine because: i) they are able to form stable complexes with various d-block metal ions by dπ→pπ* bonding, ii) their planar structure makes them suitable to intercalate DNA, iii) the chelation of a metal may result in luminescent compounds suitable as bioimaging agents or as photosensitizers for photodynamic therapy, etc. [**3,4**]

On this background, herein we report the synthesis and characterization of some new water soluble heteroleptic *d*-block metal complexes. The compounds were characterized by elemental analysis and molar conductivity, IR, $^1$H-NMR and UV-Vis spectroscopy.

Some of the complexes also presented lyotropic liquid crystalline properties and their mesomorphic behaviour in water were investigated by polarized optical microscopy (POM) using the Lawrence penetration method and showed the ability to self-assemble into chromonic phases in water at room temperature.

*Acknowledgements*: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-PD-2021-0427, within PNCDI III.

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# DIFFUSIVE GRADIENTS IN THIN FILM AND ELECTROTHERMAL VAPORIZATION CAPACITIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROSCOPY METHOD FOR THE EVALUATION OF BIOAVAILABLE CU, ZN, CD AND PB FRACTION IN AGRICULTURAL SOILS

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The diffusive gradient in thin films (DGT) technique is used in environmental chemistry as a passive sampling tool for assessment of trace metal contaminants in water, soil and sediment[1,2]. DGT was proposed by Davison and Zhang[3] for *in situ* separation of bioavailable fraction of inorganic contaminants. Determination of bioavailable fraction gives a more accurate risk assessment of exposure posed by toxic metals in the environment than their total metal content[3]. In this work, the DGT technique was used for the extraction of bioavailable Cu, Zn, Cd and Pb from soil samples, and determination by fully miniaturized and cost-effective electrothermal vaporisation - capacitively coupled microplasma optical emission spectrometer (ETV-µCCP-OES) built in our laboratory. The method was validated by analysing soil reference materials (CRMs). The soil CRMs were digested using microwave-assissted *aqua regia* extraction for the determination of the pseudo-total metals concentrations. The digested solutions were appropriately diluted and brought to a neutral pH. DGT devices with Chelex resin gels (DGT Research, Lancaster, UK) were imersed in these solution for a known period. At retrieval, the metals acumulated by resin gels were eluted in nitric acid 1M, and then analysed by ETV-µCCP-OES. CRM analysis showed good recoveries and thus the method was considered accurate for 95% confidence level. Good liniarities were obtained for the accumulation of metals over the 48 hours of deployment period. For bioavailable fraction determination in the soil sample, the assembled DGT device was deployed in the moist soil sample (80-90% of the maximum water holding capacity) for 48 h at 20 ± 2 °C, followed by elution as mentioned above. The unique features of the ETV-µCCP-OES instrumentation coupled with DGT passive sampling offer several advantages compared to traditional laboratory scaled instruments (low cost, low power and Ar consumption). Also the evaluation of figures of merit revealed that the method is sensitive and suitable for the determination of total and bioavailable of several trace metals concerning the risk exposure for the environment and agricultural crops.

*Acknowledgements:* This work was supported by a grant of the Romanian Ministry of Research and Innovation, CNCS/CCCDI-UEFISCDI, contract nr. 733PED/2022, project number PN-III-P2-2.1-PED2021-0151, within PNCDI III.

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# GREENNESS AND WHITENESS OF SMALL-SIZED ELECTROTHERMAL VAPORIZATION CAPACITIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY WITH *IN-SITU* DIFFUSIVE GRADIENTS IN THIN FILMS PASSIVE SAMPLING (DGT*SSETV-µCCP-OES)

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The aim of this work was the greenness and whiteness degree assessment of a fully miniaturized instrumentation based on small-sized electrothermal vaporization capacitively coupled plasma microtorch optical emission spectrometry (SSETV-µCCP-OES) for the simultaneous determination of Cu, Zn, Cd, Pb and Hg in surface water after *in-situ* passive sampling on diffusive gradients in thin films (DGT) device. The DGT-SSETV-µCCP-OES method was evaluated in comparison with classical methods of analysis based on graphite furnace atomic absorption spectrometry (GF-AAS), used for Cu, Zn, Cd and Pb determination, and thermal decomposition atomic absorption spectrometry (TD-AAS) for Hg determination, with or without DGT passive sampling. The methods greenness was evaluated using the AGREEprep metric, developed by Wojnowski *et al.*[1], while the whiteness based on the Red-Green-Blue (RGB-12) algorithm, developed by Nowak et al.[2], that assesses not only the greenness of a method, that takes into account the toxicity and quantity of reagents, but also the figures of merit of the analytical method (limit of detection, limit of determination, precision and accuracy), time- and cost-efficiency and instrumentation functionality. The DGT-SSETV-µCCP-OES method was based on metals accumulation from surface water on the DGT devices with Chelex-100 resin for a period of 7 days, followed by elution in 1 mL of 1 mol $L^{-1}$ $HNO_3$ solution and determination. The method provided red/green/blue/white scores of 100/80/98/93%. The high red score was obtained because of the substantial improvement of the limits of detection by the use of DGT (0.01 µg $L^{-1}$ for Cd, Zn and Hg, 0.02 µg $L^{-1}$ for Cu and 0.07 µg $L^{-1}$ for Pb) and very good precision and accuracy of the method. The 80% green score was attributed due to the sampling method type (*in-situ*), very low energy consumption for sample preparation and analysis (1 W/sample), and low amounts of toxic reagents used and waste generated. The 98% blue score was due to the fully miniaturized instrumentation equipped with a low-resolution microspectrometer, simultaneous determination of the five elements with a relative high speed of analysis (2-3 minutes per sample). Overall, the DGT-SSETV-µCCP-OES method resulted in a whiteness degree of 93%, better than those obtained for GF-AAS and TD-AAS without DGT passive sampling.

*Acknowledgements:* This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2021-0151, within PNCDI III. Contract number 733PED/2022.

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# POSTER PRESENTATIONS

## P1 – P35

# FAST CHROMATOGRAPHIC DETERMINATION OF ENANTIOMERIC PURITY OF [$^{11}$C]METHIONINE BY PRE-COLUMN DERIVATISATION METHOD

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[$^{11}$C]methionine is used for PET diagnosis of brain tumors in University Hospital of Debrecen. Determination of enantiomeric purity is a critical quality parameter for release of this radiopharmaceutical for human use. For this purpose, the European Pharmacopoea recommends a thin layer chromatographic method based on separation of D- and L-isomers on chiral stationary phase.[1] However, the analysis could be performed cost effectively using reversed-phase HPLC and pre-column derivatization method in case of [$^{18}$F]fluoroethyl-tyrosine.[2] In this work a derivatization procedure with *N*-isobutyryl-L-cysteine (IBLC) and *o*-phthalaldehyde (OPA) was applied for liquid chromatographic determination of enantiomeric purity of [$^{11}$C]methionine. Our goal was to develop an ultra-performance liquid chromatography (UPLC) method with short measurement time and to achieve at least 1.5 peak resolution of D- and L-[$^{11}$C]methionine.

Examinations were performed on Waters *I*-Class UPLC system which consisted of the following units: pump, autosampler, degasser, column manager, UV-Vis, and radioactivity detector. Acquisition and data processing were performed with Empower software. Analytical grade chemicals of Merck and VWR were used for method development and validation processes. Aqueous and acetonitrile solutions of phosphoric acid, formic acid and trifluoroacetic acid were used for mobile phase. The composition of binary solvent mixtures and gradient times were optimized. For stationary phase the following analytical columns were applied: Waters BEH C18 100 x 2.1 mm, 1.7 μm, Waters BEH C18 50 x 2.1 mm, 1.7 μm, Waters CSH C18 150 x 2.1 mm, 1.7 μm, Kinetex XB-C18 50 x 4.6 mm, 2.6 μm.

According to the optimized analytical procedure Waters BEH C18 50 x 2.1 mm, 1.7 μm column is recommended to apply. Aqueous solution of formic acid (0.1% m/m) and 0.1% m/m formic acid in acetonitrile were used for mobile phases. At the start of the measurement, the ratio of acetonitrile of the eluent was increased from 0 to 95% in 5 min. The flow rate was adjusted to 0.6 ml/min. The temperature of the column was maintained at 30°C. The injection volume was 2 μL. The measurement time was 4 minutes. During sample preparation the radiopharmaceutical, 10 mg/mL of IBLC in 250 mM borate buffer (pH 10.2) and 3.5 mg/mL OPA in dioxane was mixed in ratio of 1:6:3. The obtained L-L- and L-D-diastereomers were separated with resolution of higher than 2. The validation of the developed method was performed in accordance with the ICH and GMP guidelines. We examined linearity, recovery, and limit of detection (LOD) to implement validation which resulted in values that complied with recognized standards. Validation parameters were as follows: $R^2>0.99$, $RSD_{\%}<5\%$, LOD=20 MBq/mL. In conclusion the developed method is suitable for specifying the enantiomeric purity of the [$^{11}$C]methionine radiopharmaceutical using pre-column derivatization procedure.

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# CHARACTERISATION OF MULTI-BLOCK CO-POLYMERS BY MASS SPECTROMETRIA (MS)

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The properties of copolymers are more alterable with a higher number of monomer units and their applicability is also extensible. What makes them more useful is the ability to combinate the properties of the monomers. To fine-tune the structure of copolymers controlled polymerization procedures, to understand the structure-property relation special analytical procedures are required. Soft ionization methods such as the matrix-assisted laser desorption/ionization (MALDI) (1), (2) and the electrospray ionization (ESI) (3), have opened the way for the mass spectrometric (MS) characterization of intact polymers and copolymers(4),(5). Mass spectrometry (MS) is capable of providing information on individual polymer chains. However, the analysis of copolymers is challenging due to the expected enormous numbers of peaks in the spectrum. Furthermore, overlaps raise difficulties in identifying.

In the field of multi-block copolymers the mentioned problems are cumulative, the reason that the number of blocks is more than two. With the help of mass spectrometry we are capable of separating the components of copolymers, based on the m/z values. Therefore we can get detailed information on the length and distribution of the blocks.

The aim of that work is to establish a method to analyze the sequence and the individual blocks of multi-block copolymers. To reach this, the forthcoming block copolymer has been examined: 4-Acryloylmorpholine, N-Diaectoneacrylamide, N-Isopropylacrylamide and N,N-Dimethylacrylamide tetra block copolymer. The degree of polymerization was designed to be 8 5 5 5 and 10 10 10 10. These were produced with RAFT (Reversible addition−fragmentation chain-transfer) polymerization which allowed the synthesis of the well-defined block length. And it's established that the size of the blocks and their distribution is definable and it is well-matched with the planned evaluations.

*Acknowledgements:*The work was supported by the GINOP-2.3.3-15-2016-00021 projects and by Thematic Excellence Program (TKP2020-NKA-04) of the Ministry for Innovation and Technology in Hungary. The projects were co-financed by the European Union and the European Regional Development Fund. Furthermore, this paper was also supported by Grant No. FK-132385 from National Research, Development and Innovation Office (NKFI). Thanks for the financial support provided by the Mol Group, Hungary.

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# CHARACTERIZATION OF COPOLYMERS USING GEL PERMEATION CHROMATOGRAPHY AND NEURAL NETWORKS

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Gel permeation chromatography (GPC) is a commonly used technique for the analysis of polymers and copolymers, but it cannot provide important information such as the composition of copolymers[2]. We have developed a method based on gel permeation chromatography and neural networks (ANN) for the detailed characterisation of copolymers. This was based on GPC measurements with different polarity eluents to determine the measured mass averages and their variations in different solvents. Detailed characterization of the copolymers was performed by MALDI-TOF[1] and NMR measurements. Artificial intelligence (neural network) was used to process the data obtained from the GPC measurements and the polymer properties obtained from the detailed characterisation. The target values for the neural networks were the data measured by MALDI-TOF mass spectrometry and NMR spectroscopy, while the input data set was the results obtained by GPC. Our GPC-ANN method was demonstrated by the analysis of different polyoxamers, namely polyethylene oxide (PEO)-polypropylene oxide (PPO) block copolymers. We also generated two neural networks. *ANN_1* operates in a wider mass range (1000-12500 Da) and has two output parameters ($M_\mathrm{n}$ and EO%), while the more accurate *ANN_2* operates in a narrower mass range (max. 5000 Da) and has seven output parameters (two average molecular weights, the mass % ethylene oxide content and the average number of repeating units - four parameters). The main advantage of our work is that the data obtained from GPC, MALDI-TOF MS and $^1$H-NMR can be used to create a database that can be extended with additional experimental results, and the mass range and accuracy of the neural nets can be further improved.

*Acknowledgements:* The work was supported by the GINOP-2.3.3-15-2016-00021 projects and by Thematic Excellence Program (TKP2020-NKA-04) of the Ministry for Innovation and Technology in Hungary. The projects were co-financed by the European Union and the European Regional Development Fund. Furthermore, this paper was also supported by Grant No. FK-132385 from National Research, Development and Innovation Office (NKFI). Thanks for the financial support provided by the Mol Group, Hungary.

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# FOUR NOVEL POLYNUCLEAR ZN(II) COMPLEXES WITH A SCHIFF BASE LIGAND DERIVED FROM 2,3-DIHYDROXYBENZALDEHYDE: SYNTHESIS AND CHARACTERIZATION

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The Schiff base ligands are known for their ability to form with Zn(II), different complexes with various nuclearities[1], which make them suitable candidates for applications in catalysis[2], fluorescence-based OLED devices[3] or biology[4]. Numerous Schiff bases used as ligands in this type of complexes are derived from *o*-vanilline[1], but another interesting, structurally related, aldehyde, which can generate multinuclear metal complexes, is 2,3-dihydroxybenzaldehyde. In literature there are several Zn(II) polynuclear complexes with bicompartmental Schiff base derived from 2,3-dihydroxybenzaldehyde[5], but as far as we know, there is only one tetranuclear Zn(II) complex resulted by 1:1 condensation reaction between this aldehyde and a diamine[6].

Hence, four new Zn(II) complexes were synthesized using as a ligand a Schiff base formed by the condensation of 2,3-dihydroxybenzaldehyde with monoamines, such as 3-amino-1-propanol ($H_3\mathbf{L^1}$) or 2-(2-aminoethyl)pyridine ($H_2\mathbf{L^2}$) and Zn(II) salts: $[Zn_{12}\mathbf{L^1}_{10}Cl_2(MeOH)]$ (**1**), $[Zn_4\mathbf{L^2}_2(H\mathbf{L^2})_2](ClO_4)_2$ (**2**), $[Zn_4\mathbf{L^2}_2X_4]$ (X = acetate (**3**) or pivalate (**4**)). All compounds have been characterized by single crystal and powder X-ray diffraction, UV-VIS and IR spectroscopies. Also, photoluminescence analysis of this complexes reveal that compounds **3** and **4** present fluorescent properties.

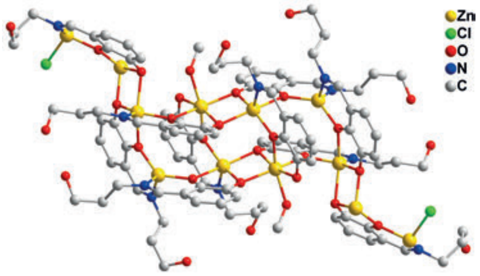

**Figure 1**. Molecular structure of compound **1**

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# STRUCTURE AND MODE OF ACTION STUDIES OF GLYCOPEPTIDE ANTIBIOTICS: EREMOMYCIN AND ORITAVANCIN AS SEEN BY NMR

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Antibiotic resistance emerges as a worldwide public health problem. Therefore, development of new glycopeptide antibiotics[1] is necessary. Oritavancin is a semisynthetic chloro-eremomycin derivative, that has been approved by the FDA against Gram-positive bacteria, including *methicillin*-resistant *Staphylococcus aureus* (**MRSA**). Structure and mode of action studies of glycopeptide antibiotics are often supported by $^{1}H$ and $^{13}C$ NMR techniques. Here, we show that $^{15}N$ labelling of eremomycin opens a new avenue for NMR studies.

We show, that $^{15}N$ relaxation ($T_1$,$T_2$, NOE) provides more insight into the internal dynamics[2] of NH amides. Global correlation times derived from the same data set prove, that adding cell-wall analogue peptide *N-Ac-D-Ala-D-Ala*[3] to eremomycin, induces eremomycin tetramers and octamers from the dimers abundant in the absence of ligand. Diffusion NMR method (DOSY) led to the same conclusion. Oritavancin also forms asymmetric strong dimers in aqueous solution, however adding dipeptide ligand causes precipitation, suggesting possible higher oligomerisation states.

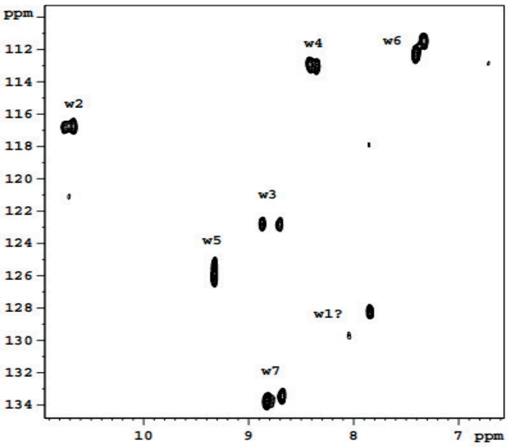

**Figure 1: $^{15}N/^{1}H$ spectra of $^{15}N$-eremomycin.**

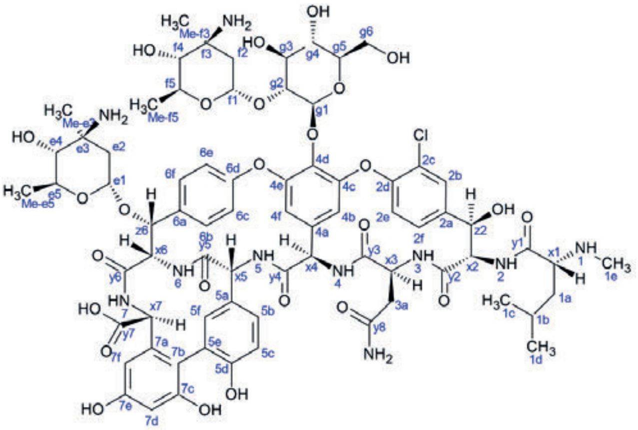

**Figure 2: The structure of eremomycin.**

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# TARGETED BINDING INVESTIGATION ON LIVING CELL SAMPLES WITH SATURATION TRANSFER TRIPLE DIFFERENCE (STTD) NMR METHOD

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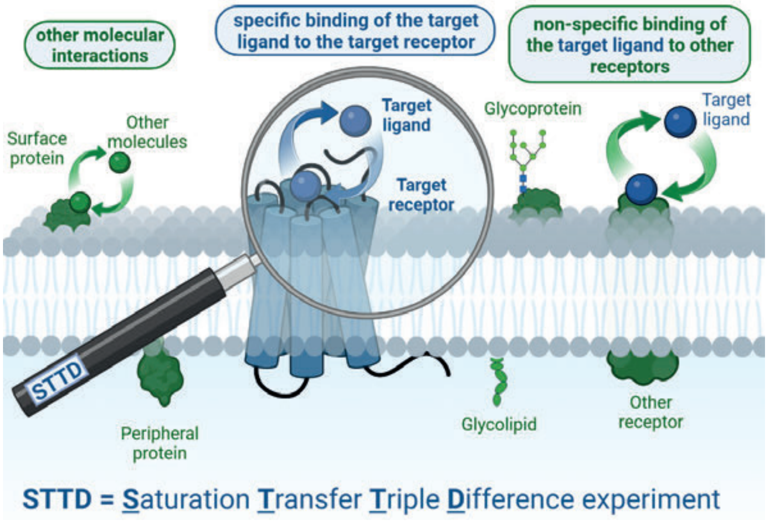
The saturation-transfer difference (STD) NMR experiment is a widely used technique for characterizing interactions between small molecules and target proteins (receptors, enzymes) in solution due to its robustness and easy implementation[1].

The cellular environment, however, is way more complex and contains many compounds such as metabolites, osmolytes, other proteins, nucleic acids and lipids, depending on the specifics of the cellular(sub)-system.

In order to probe the interaction of a target ligand with the target membrane-bound protein in their natural environment[2], we have developed a novel STD NMR strategy. The saturation transfer triple difference (STTD) method is purging the resulting $^1$H STD spectrum from the non-specific binding contribution of the target ligand as well as from the interactions of other molecules.

With this method, we studied the interaction between endomorphin-2 and μ-opioid receptor mutants in a cellular environment.



*1.Figure:* Targeted-observation with the saturation transfer triple difference (STTD) method

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# TERBIUM ISOTOPE PRODUCTION, PURIFICATION AND RADIOLABELLING AT THE INSTITUTE FOR NUCLEAR RESEARCH

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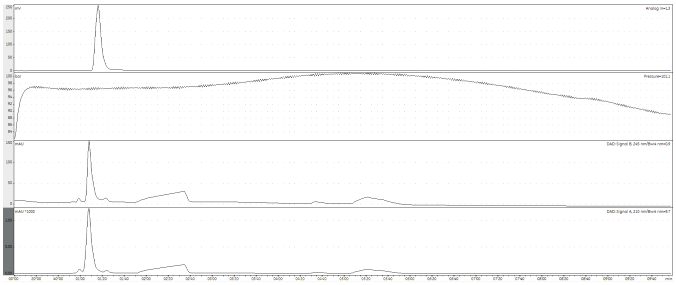
Terbium is an interesting element, because it has numerous radioisotopes, with possibility for applications in α (Tb-149), β- (Tb-161), Auger-electron therapy (Tb-161) as well as SPECT (Tb-155, Tb-161) and PET (Tb-152) diagnostics.[1]

Coupled with the fact that terbium also has a stable isotope (Tb-159) and that it has fluorescent properties allows for some interesting applications, such as optical imaging after UV-excitation. This phenomenon is well known an has even been utilized to create light sources.[2]

Radioisotopes of terbium can be produced from the corresponding gadolinium isotopes via cyclotron, with proton irradiation, by (p,n) reactions. Natural gadolinium contains Gd-154 - Gd-158 isotopes, in 2-25% amounts. Enriched gadolinium-oxide pellets can be irradiated to obtain purer samples, and alternatively neutron-irradiation can also be exploited, using reactors.

Hereby the authors will present the research carried out in the Institute for Nuclear Research (ATOMKI) regarding this topic. Our goal was to develop a method for separation of terbium radioisotopes from bulk gadolinium metal ions, following the dissolution of solid $Gd_2O_3$ target after irradiation, as well as radiolabelling of chelator molecules, and affibodies with terbium isotopes, and studying the characteristics of the produced moieties.

The same labelling was attempted at different conditions, and followed by HPLC UV/vis and scintillation detector. A chromatogramof a failed labeling attempt is included as an example.



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# INTERACTION OF TRANSITION METAL IONS WITH A PRION PROTEIN - BETA AMYLOID MODEL PEPTIDE

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Transition metal ions such as Cu(II) and Zn(II) play an important role in many key biological processes, thus their dysregulation and accumulations are a common pathological hallmark of many neurodegenerative disorders for instance Alzheimer’s disease and prion disease. The above-mentioned metal ions by coordinating with proteins, including amyloid-β and the human prion, are able to induce their aggregation leading to the formation of senile plaques.[1]

Protein oxidation represents a major pathway of protein degradation. Oxidation reactions are significantly affected by protein sequence and structure. Additional complexities are introduced when oxidation reactions are catalyzed by transition metals. Such reactions may predominantly affect amino acid residues directly involved in metal binding or located in the close vicinity of the metal-binding site. Metal catalyzed oxidation (MCO) can lead to damaged bio-molecules and this is implicated in oxidative stress, biological aging and neurodegenerative diseases. MCO of proteins is mainly a site-specific process in which only one or a few amino acids at the metal-binding sites of the protein are preferentially oxidized.[2]

The complex formation processes and the oxidation of PrP has been widely studied in our research group.[3]In the continuation of this work, beta-amyloid peptide is in the focus of my research. The studied fragment ($NH_2$-GTHSAKHA-$NH_2$) represents a transition between these two classes, because this prion protein mutant also contains the N-terminal amino group. This model peptide contains the prion protein’s two metal binding sites (namely $His^{96}$ and $His^{111}$) relatively close to each other and a free amino group.

The interaction of the peptide with copper(II), nickel(II) and zinc(II) ions were studied at 1:1 and 2:1 metal to ligand ratios. The deprotonation constants of the peptide and the stability constants of the formed complexes were determined by pH-potentiometry. UV-Visible and CD spectroscopy were used for identifying the coordinating donor atoms and for determining the structures of the formed complexes. Mono and dimer species are formed in every system, furthermore mixed metal complexes are also present in the Cu(II)-Ni(II)-$NH_2$-GTHSAKHA-$NH_2$ solution.

The oxidation of the above-mentioned model peptide in the Cu(II):peptide system was studied in the physiological pH range by the addition of $H_2O_2$ in the presence and absence of ascorbic acid by HPLC-ESI-MS. Singly and doubly oxidized products formed, in which the oxidation of one or two histidine residues occurred. The place of oxidation was determined by MS/MS method.

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# THERMORESPONSE BEHAVIOR OF NAM-NIPA BLOCK POLYMER

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Smart materials are a novelty technology nowadays due to the great number of applications in biosensing, biotechnology, chemical separation, drug delivery, etc, due to the capacity of responding to external stimulus by exposure to pH, light, electric and magnetic fields, and temperature. The change of the phase of an acrylamide block by temperature can be used for tunning another polymer block to improve the properties[1]. In this case, the aim of our research is to study the thermoresponse behavior of a diblock poly N-Acryloylmorphine (NAM) and N-isopropylacrylamide (NIPA) at different degree of polymerization (DP) and differnet composition. The polymers were synthetized via reversible addition–fragmentation chain transfer (RAFT) polymerization method, which allows to control the molecular weight and get a low polydispersity at different degree of polymerization. To characterize the block polymers, the matrix-assisted laser desorption/ionization (MALD-TOF MS) mass spectrometric measurements were carried out to determine the number- and weight average molecular weights and polidispersity[2]. Concerning the study of the thermoresponse, the samples were subjected to dynamic light scattering (DLS) analyis, in which the samples were diluted in water keeping a constant concentration of 10 mg/ml in order to analyze the change of the structure by the exposure to the temperature. The DLS results, showed a general tendency for the different ratio of DP of pNAM/pNIPA content, as the amount of NIPA was added, the temperature for the thermoresponse decreases and the formation of agregates arises, confirming that increasing the temperature the block pNIPA loses the solubility in water. Most of the samples exhibited agregation point values of 32 degree Celsius, which is related to the thermoresponse NIPA characeristic[3]. However increasing the length of the pNAM block, the cloud point were incresed. Higher effect was found at high pNAM:pNIPA ratio. The self-assambly property of this block polymer can be used specillay for the release of encapsulated drugs and biomedical applications.

*Acknowledgements:* The work was supported by the GINOP-2.3.3-15-2016-00021 projects and by Thematic Excellence Program (TKP2020-NKA-04) of the Ministry for Innovation and Technology in Hungary. The projects were co-financed by the European Union and the European Regional Development Fund. Furthermore, this paper was also supported by Grant No. FK-132385 from National Research, Development and Innovation Office (NKFI). Thanks for the financial support provided by the Mol Group, Hungary.

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# ENANTIODISCRIMINATING LIPOPHILIC LIQUID MEMBRANE-BASED ASSAY FOR HIGH-THROUGHPUT NANOMOLAR ENANTIOENRICHMENT OF CHIRAL BUILDING BLOCKS

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## Abstract

The reported optical resolution method was designed to support high-throughput enantioseparation of molecular building blocks obtained by automated small-scale synthetic methods. Lipophilic esters of common resolving agents were prepared and used as liquid membranes on the indifferent polymer surface of a microtiter assay. Chiral model compounds were enriched in one of the enantiomers starting from the aqueous solutions of their racemic mixture. Enantiodiscrimination was provided by forming diastereomeric coordination complexes of lipophilic enantiopure esters with the enantiomers of the chiral building blocks inside the liquid membranes. This enantiomeric recognition resulted in a greater distribution ratio of the preferred isomer in the membrane phase, thus the process enables a simultaneous enantioenrichment of the solutions outside the membrane. This poster reports a novel microplate-integrated stereoselective membrane enrichment technique satisfying the need for automatable enantioseparation on a subpreparative scale.

*Acknowledgments:* Special thanks to Greg Prikler for the discussions that inspired this work. The authors express their thanks to Dániel Ster and Rita Molnárné Bernáth for their helpful technical support. Thanks to Szabolcs László for his help in characterizing the new compounds and to Melinda Mihalec for her contribution in evaluating the spectroscopic data

# COMPARATIVE STUDY OF DIFFERENT NANOCOMPOSITE MATERIALS IN THE DEVELOPMENT OF BIOSENSORS FOR BIOGENIC AMINES DETECTION

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Biogenic amines (BAs) represent a group of low molecular weight organic compounds, occuring in a chemical, biochemical or microbial degradation process of the amino acids that are present in all eukaryotic cells[1,2]. The accumulation of significant amounts of BAs in food usually occurs due to the fermenting microorganisms that possess amino acid decarboxylase activity[2]. In plants, BAs play an important role in the plant grows and development, their concentrations increasing under environmental stressor factors. In addition, polyamines have a big positive impact, such as increasing the nitrogen resource and longevity in cellular functions. For example, putrescine results through arginine and ornithine's decarboxylation, participating in plants development and contributing to tolerance for abiotic stress, like high and low temperatures, drought and salinity[3,4].

Different carbon-based nanocomposite materials have been used for the development of electrochemical biosensors for sensitive and rapid detection of putrescine. The electrochemical sensitive platforms have been developed by modification of the carbon screen-printed electrodes (SPEs) with nanocomposite materials based on singled or multi walled carbon nanotubes, nanoribbons, Prussian blue and enzyme, diamine oxidase (DAO) using physical deposition or entrapment in different matrices, such as ionic liquids, sol-gel or polymeric films. Cyclic voltammetry (CV), amperometry and electrochemical impedance spectroscopy (EIS) were used to characterize the electrochemical properties of the modified sensors, while surface morphology of the functionalized active surfaces was studied using SEM and FTIR spectroscopy.

The modification of SPEs with nanocomposite materials provides an electroconductive network and a large active surface of the sensors, thus accelerating the transfer of electrons, allowing a sensitive detection of putrescine.

*Acknowledgements:* This work was funded by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2021-1942, contract no 662/2022– AMI-FOOD. The authors acknowledge the support received within the project POC-A1-A1.2.3-G-2015-P_40_352-SECVENT, Sequential processes to close bioeconomy side stream and innovative bioproducts resulted from these, contract 81/2016, SMIS 105684, subsidiary project 2638/2022 and through the Projects to finance excellence in RDI, Contract no. 15PFE /2021.

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# GEL PERMEATION CHROMATOGRAPHY BASED METHOD DEVELOPMENT FOR THE CHARACTERIZATION OF THERMORESPONSIVE BLOCK COPOLYMERS

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The relevance of thermoresponsive block copolymers has steadily grown over many decades and most part of the work has been dedicated to developing temperature-sensitive macromolecules that can be crafted into new smart materials. Thermoresponsive copolymers have garnered significant interest due to their ability to undergo reversible changes in solubility, swelling, and other physical properties in response to changes in temperature[1,2]. These properties make thermoresponsive copolymers promising candidates for use in drug delivery, tissue engineering, and other biomedical applications.

In this work, NAM - NIPA-based water-soluble block copolymers with varying degrees of polymerization synthesized (Mn: , pNAM%: ) using reversible addition/fragmentation chain transfer (RAFT) polymerization and characterized MALDI – TOF – MS (mass spectrometry)[3]. The characterization of copolymers is challenging with the gel permeation chromatography (GPC) technique since the hydrodynamic radius of copolymers depends on the Mn and composition. For copolymers there are no standard materials thus there is a strong need to develop methods for detailed characterization. We have developed a GPC-based method, where copolymers were measured with two different eluents, which is capable of identifying the molecular weight and composition. Such a method helps in the development of block copolymer-based functional materials.

*Acknowledgements:* The work was supported by the GINOP-2.3.3-15-2016-00021 projects and by Thematic Excellence Program (TKP2020-NKA-04) of the Ministry for Innovation and Technology in Hungary. The projects were co-financed by the European Union and the European Regional Development Fund. Furthermore, this paper was also supported by Grant No. FK-132385 from National Research, Development and Innovation Office (NKFI). Thanks for the financial support provided by the Mol Group, Hungary.

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# EFFECT OF THE AMINO ACID ENVIRONMENT OF HISTIDINE ON THE METAL BINDING SELECTIVITY OF TAU FRAGMENTS

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Alzheimer's disease (AD) is a progressive neurodegenerative disorder, it leads to the decline of motor and cognitive functions. Pathophysiological changes involving abnormal protein aggregation in the central nervous system characterise AD. While aggregation of amyloid-β (Aβ) leads to the formation of extracellular amyloid plaques, aggregates of hyperphosphorylated Tau protein form intracellular neurofibrillary tangles.[1] Previous studies also justified that metal ions such as Cu(II), Zn(II), Fe(II) are accumulated in the brain of AD patients and contribute to the hyperphosphorylation of Tau protein, leading to cell impairment.[2] Tau protein contains 12 histidine amino acids in the sequence which provide high metal binding affinity to Tau and its various peptide fragments. These residues with metal binding ability are well-separated and several other coordinating side chains are also available close to the histidyl sites.[3] However, the characterisation of the metal binding sites of Tau protein have not adequately been clarified yet. Additionally as a result of metal ion and peptide interaction, metal ion, e.g. Cu(II) can also catalyze the oxidation of peptides. Metal ion-catalyzed oxidation plays a role in the formation of reactive oxygen species (ROS), contributing towards oxidative stress.[2]

The systematic investigation of Tau fragments containing the possible metal binding sites began a few years ago in our research group.[4-6] As a first step we investigated the metal complexes of histidyl containing fragments from the N-termini (Tau(9-16), Tau(26-33)) and R3 region (Tau(326-333)). In the continuation of this work, different fragments and mutant peptides were studied that contain seryl, threonyl and prolyl residue close to the histidyl sites: Ac-ATMHQD-$NH_2$ (Tau(29-34) mutant), Ac-AQPHTEI-$NH_2$ (Tau(91-97)), Ac-KTDHGA-$NH_2$ (Tau(385-390)), Ac-SPRHLS-$NH_2$ (Tau(404-409)), as these groups can the change complex formation processes of the peptides.

Furthermore the Cu(II)-catalysed oxidation of the mentiond peptides was investigated and electrochemical studies of Cu(II) complexes were performed in order to examine the possibility of ROS formation.

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# DRY REFORMING OF METHANE BASED ON TRANSITION METAL CATALYSTS

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Significant releases of greenhouse gases, which can induce global climate changes as well as environmentally harmful pollutant emissions, have mainly originated from some carbon-containing fossil fuel combustions such as coal, natural gas, and petroleum. In recent years, the development of renewable energy sources and the reduction of greenhouse gas emissions have become increasingly urgent global issues. The conversion of $CH_4$ and $CO_2$, the two main major greenhouse gases into synthesis gas is the focus of academic and industrial research. One of the possibilities to achieve this goal is to react the $CH_4$ and $CO_2$ with each other. The $CH_4$ can react with $CO_2$ as a reductant - by techniques including Dry reforming (DR), to produce the industrially important syngas ($CO + H_2$ mixture).

In this research, Dry reforming of methane with carbon dioxide has been investigated in atmospheric pressure, at 650°C, using transition metal catalysts (Ni, Co, Fe). The results indicate that trimetallic catalysts improved the catalytic performances.

**Keywords:** Dry reforming of methane, Syngas, Ni-Co-Fe, Transition metal catalyst, Trimetallic catalysts.

# STUDY OF DIFFUSION DYNAMICS IN PD/RH ALLOY

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Auger-emitting radionuclides have potential for the therapy of cancer due to their high level of cytotoxicity and short-range biological effectiveness, which makes them suitable for treating micrometastases while sparing normal tissues. Several radioisotopes of the platinum group metals (PGM) emit Auger electrons, such as $^{192}$Ir, $^{193m,195m}$Pt, and $^{103}$Pd which emit Auger electrons during its decay [1]. These isotopes can be produced via cyclotron by irradiation of the platinum group metals, such as, Os, Ir, Rh. The separation process of these radioisotopes usually is carrying out by the "wet chemistry", which is an unusual difficult and time/human power consuming due to the extreme chemical inertness of these elements. The aim objective of this study is the design and construction of radionuclide separation equipment employing dry distillation method for platinum group metals, first optimized on $^{103}$Pd.

$^{103}$Pd is produced by the irradiation of $^{103}$Rh with protons at the MGC-20 cyclotron of ATOMKI. During the proposed dry distillation process the $^{103}$Pd atoms randomly distributed in the Rh matrix must be extracted and deposited on a substrate suitable for the subsequent chemical processing. The main parameter governing the process at a given temperature is the diffusion constant of Pd in Rh matrix, which is not available in the literature. In order to appropriately adjust the operational parameters of the distiller, we have to measure the diffusion constant. Therefore, we've prepared samples of Rh foils with 100 nm thick Pd layer deposited on their surface using magnetron sputtering vapor deposition technique. One sample was kept for the control and one was annealed at 900 °C for 1 hour in a vacuum furnace. The Pd-Rh interface of both samples was analyzed with depth profiling measurements using SIMS/SNMS (Secondary Ion/Neutral Mass Spectrometry). The preliminary results showed a developed intermixing of the two elements, which is a useful data for designing the subsequent systematic measurements.

A separation test was also done with the distiller to probe the temperature settings for an effective separation of the two metals. We used a mixture of Rh and Pd powders with equal mass amount. An approximate amount of the mixture was filled in a BN (Boron nitride) crucible and heated to a temperature range of 1500-1700 $^{o}$C. The deposition surface was a 50 µm-thick Nb foil, which was then analyzed with the scanning electron microscope. The EDX data showed the presence of Pd on the surface of the Nb foil, while that of the Rh was found below the sensitivity threshold of the analyzer.

We propose the novel concept of diffusion driven extraction of radionuclides produced by irradiation of PGM targets at the cyclotron. Diffusion and evaporation rates, chemical and radionuclide impurities will be optimized by engineering structural and physical parameters.

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# GREEN SINTHESYS OF BIMETALLIC Ag-Au AND Au-Ag NANOPARTICLES AND THEIR CATALITIC ACTIVITY IN THE DEGRADATION OF HARMFUL DYES

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Green methods of synthesizing bimetallic nanoparticles of Ag with Au core and Au with Ag core using the aquous *Lycium barbarum* fruit extract as source of bioactive compounds were developed and the catalytic activity of the nanoparticles was evaluated (Figure 1). *Lycium barbarum* fruits (goji berry or wolfberrry) are rich sources of polyphenolic compounds that can both reduce silver and gold ions and stabilize the formed nanoparticles.[1,2,3] The biosynthesis of the bimetallic nanoparticles was accomplished in a two steps process : first the sinthesys of the monometallic nanoparticles was carried out and then the sinthesys of the bimetallic nanoparticles. The synthesized nanoparticles were evaluated using UV-Vis spectral analysis, which show specific absorption peaks at 530-540 nm for gold and 415-430 nm for silver. Further the catalytic ability of the nanoparticles in the degradation of Brilliant blue FCF by $NaBH_4$ was evaluated.[3] The results shown an increase of the degradation rate for both Ag-Au and Au-Ag nanoparticles for Brilliant Blue FCF dye.

The methods presented are enviromental friendly methods of obtaining nanoparticles and the catalytic activity of the obtained nanoparticles can represent an usefull tool for pollution control.

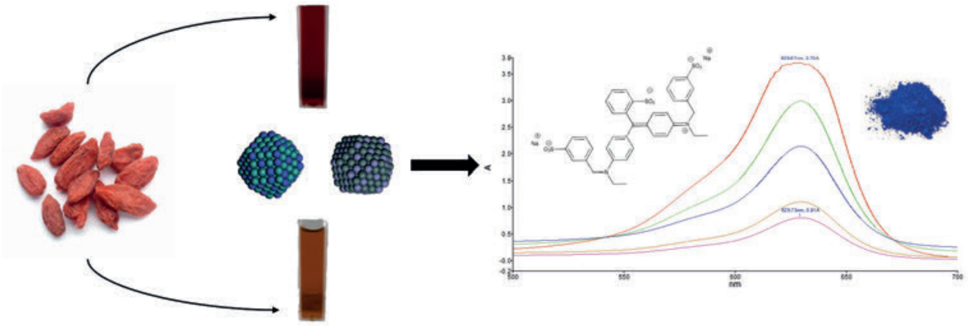

**Figure 1**. Sinthesys of nanoparticles and degradatios spectra of Brilliant Blue FCF dye

*Acknowledgments: Financial support from CNCS-UEFISCDI, Romania, project number PN-III_P1.1.1-TE-2021-0511*

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# CATALYTIC ACTIVITY OF LANTHANUM CUPRATE ($La_2CuO_4$) IN THE SYNTHESIS OF TRIAZINE DERIVATIVES

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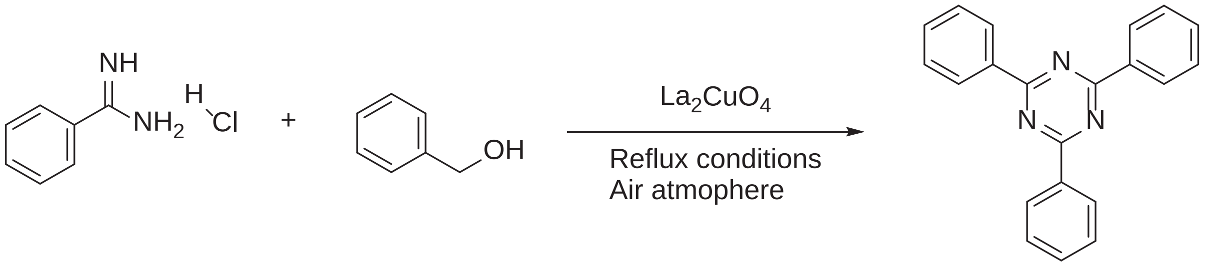
Rare earth oxides play an irreplaceable role in many important catalytic reactions, especially as solid catalysts or adsorbents, mainly as supports and additives[1]. Currently, rare earth catalytic materials proved to be useful in areas like petroleum chemical industry, the catalytic combustion of fossil fuels, automotive emissions control, the purification of industrial waste air, and solid solution fuel cells[2]. However, in liquid phase organic reactions there haven't been much progress seen.

In this work the catalytical activity of $La_2CuO_4$ perovskite was investigated in the synthesis of 1,3,5-triazine derivatives between amidine hydrochlorides and alcohols in air. The catalyst was synthesized by sol-gel method known in the literature, and characterized *via* X-ray diffraction analysis (XRD), infrared spectroscopy (IR), scanning and transmission electron microscopy (SEM and TEM). During our investigation both the catalyst and base loading were optimized. Excellent selectivity was achieved towards the triazine derivatives with as low catalyst loading as 2.5 mol%.



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# ON THE ORIGIN OF THE BLUE COLOR IN THE IODINE / IODIDE / STARCH SUPRAMOLECULAR COMPLEX

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## Abstract

Iodide plays an important role in the formation of the starch–iodine complex. The iodine-derived species in the macromolecular helix from a polyiodide chain is responsible for the blue color. Several experiments have been made in order to establish the length of the polyiodide chain. Such experiments used saturated starch, iodine aqueous solution 1mM, iodine-iodide aqueous solution, iodide aqueous solution, glucose, starch 0.5%, alcohol 0.1N, methanol 10mM.

By the computational study of the polyiodide chain, it has been encountered an equilibrium between the polyiodide chains, as complexes with amylose, and the iodine and iodide in the preparative solution. In consequence, changing the concentrations causes changes of their relative populations.

Molecular orbital calculations, geometry optimizations and single point calculations were realized using the B3LYP DFT functional and the TD-SCF method coupled with def2svp, all calculations being performed using the GAUSSVIEW 5.0.9 package, and the molecular orbitals were visualized using the GAUSSVIEW 5.0.9 package.

The experiments with iodine and the TD-DFT calculations gave additional information regarding iodine-iodide solution, the color of iodine solution, addition of anions, of amylase, the color of iodine chains, the reaction of starch.

# DETERMINATION OF THE NUMBER AND CONTENT OF PESTICIDES RESIDUES FOUND IN THE VEGETABLES HARVESTED FROM TRANSYLVANIAN AREA

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In this paper, we aimed to determine the content of pesticide residues in several vegetable matrices from the Transylvania area, taking as a starting point the National Summary Report on Pesticide residues in Romania, issued by European Food Safety Authority (ESFA) from 2019, 2020 and 2021. In the selection of the studied vegetable matrices, the concentration and number of pesticides reported by EFSA were taken into account, respectively: lettuce, spinach, parsley, cucumbers.

Two other aspects that were taken into account in the selection of vegetables for the study were the type of vegetables most consumed for the purpose of detoxification and whether they are declared organic or not.

Due to the acceptable performance parameters combined with properties of easy and quick handling was chose mini-Luke modified extraction method as the most favorable in the pesticide residues analysis from all studied vegetables.

The analysis of the extracts was carried out by LC – TQ – MS with Jet Stream high sensitivity ion source, in positive and negative mode, using a method by which 240 pesticides can be identified and quantified.

The LC method was validated for cucumber in terms of linearity, accuracy, limit of detection (LOD) and limit of quantification (LOQ) and a good linearity with correlation coefficients higher than 0.98 was obtained. Among pesticide residues with highest quantities above the Maximum Residue Level (MRL) found in the selected vegetables, were carbendazim, piraclostrobin and thiophanate-methyl.

The results suggest that buying produce from certificate markets and farmers or even cultivate the produce in their personal garden can be a sustainable solution for the environment and living things and also providing and contributing to a “green” future.

# TIME TRAVEL WITH HONEYS – THE MP-AES ANALYSIS COUPLED WITH AMS AGE DETERMINATION OF HUNGARIAN ACACIA SAMPLES

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Honeys are excellent indicators of the environment, several studies show that the elemental content of honey entirely depends on the botanical and geographical origin, but the information is incomplete regarding time-dependent composition changes. Twenty-six acacia and four honey samples with unknown botanical origin were collected between 1958-2018 and analysed for elemental composition by microwave plasma optical emission spectrometry (MP-AES). The elemental analysis was coupled with independent dating method by accelerator mass spectrometry (AMS) to determine the real age of the honey samples and test the possibility of radiocarbon based dating of bee products, which has not been applied before.

According to the analytical measurements and statistical analysis, we can conclude that the elemental composition shows change with time in the acacia honey during the last five decades. We have proven that honey preserves information of previous times and thus can be applied as an environmental indicator in reconstruction studies by analysing the non-degradable mineral content. Our results further show that acacia honey is a suitable material for radiocarbon dating, proved by the results compared to the atmospheric radiocarbon bomb-peak. The presented new approach for investigations of honey by radiocarbon-based age determination coupled with elemental analysis can be used in biological, dietary, archaeological or other multidisciplinary studies as well. Some samples show slightly depleted radiocarbon content, based on these results, honey could be used for atmospheric monitoring.

*Acknowledgements:* The research was supported by the European Union and the State of Hungary, co-financed by the European Regional Development Fund in the project of GINOP-2.3.2-15-2016-00009 'ICER'. Zsófi Sajtos was Supported by the ÚNPK 20-3-II. new national excellence program of the ministry for innovation and technology from the source of the national research, developement and innovation fund. E. Baranyai is grateful for the financial support of the János Bolyai Research Scholarship of the Hungarian Academy of Sciences and for the support of the ÚNKP-20-5 (Bolyai+) New National Excellence Program of the Ministry of Innovation and Technology from the source of the national research, developement and innovation fundof Hungary.

# SELF-ASSEMBLY OF PLURONIC-TYPE AMPHIPHILIC BLOCK COPOLYMERS

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Self-Assembly is a process in which a system of pre-existing components forms an organized structure or pattern because of specific, local interactions among the components themselves without external direction. The self-assembly of Pluronic-type amphiphilic block copolymers are driven by interactions of hydrophobic PPO chain and hydrophilic PEO chain in selective solvent proper for one block and poor for the other e.g., water.[1] The self-assembled structures in solution can be probed using a wide range of analytical techniques e.g., Surface tension, rheology and Light scattering techniques.[2]

A series of five triblock copolymers of Mn >5000g/mol was dispersed in water at varying copolymer concentrations and the micellization monitored at a fixed temperature of 37°C using Dynamic Light Scattering. We found that above a certain unique concentration (critical micelle concentration) for each copolymer, spherical micelles were formed having hydrodynamic diameter less than 100nm. The size of micelles remained constant with the increase in concentration above the critical micellization concentration indicating their stability. The detection of these micelles is indicated by apparent rise in scattering intensity of laser light.

The knowledge of behavior of triblock copolymers in solutions at physiological body temperature may inform the application of self-assembled structures like micelles to be used as drug carriers for targeted drug delivery considering that the size of micelles is in nanomeric scale (<100nm) and thus can easily penetrate narrow body blood vessels. Moreover, the stability of these micelles above critical micellization concentration is important in the application point of view.

*Acknowledgements:* The work was supported by the GINOP-2.3.3-15-2016-00021 projects and by Thematic Excellence Program (TKP2020-NKA-04) of the Ministry for Innovation and Technology in Hungary. The projects were co-financed by the European Union and the European Regional Development Fund. Furthermore, this paper was also supported by Grant No. FK-132385 from National Research, Development and Innovation Office (NKFI). Thanks for the financial support provided by the Mol Group, Hungary.

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# HYDROXYMETHYLFURFURAL CONTENT OF OLD HONEY SAMPLES – DOES THESTICKY TREAT REALLY LAST FOREVER?

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Honey is widely thought to be a food source with indefinite shelf life - this statement is challenged in present work by analysing the 5-hydroxymethylfurfural (HMF) content of a unique sample series of old aparian products. Acacia, rape and sunflower honeys origiated from 1959 to 2020 were analysed for HMF content collected and stored appropriately by hungarian beekeepers and honey museums. Since the small amount of the unique sample series we scaled down and optimized the original spectrophotometric method by White from 1979.[1] The HMF concentration of the acacia honeys vary in a wide range (9-1320 mg/kg honey), but tendentially increase with storage time (age of the sample). Since the handling and storage parameters, the species and the region of origin in this series are the same for the samples it is safe to assume that the measured aparian products differed only in the storage period. The HMF content of acacia honeys of different ages from Western Hungary (Gór and Mesterháza) were excellently approximated by a quadratic equation. However, the rape and sunflower honeys show a remarkably high offset compared to the expected trendline. There is no observable pattern in their HMF level plotted against the year of collection

*Acknowledgements*: The research was supported by the European Union and the State of Hungary. E. Baranyai and Z. Sajtos are grateful for the financial support of the János Bolyai Research Scholarship of the Hungarian Academy of Sciences and for the support of the ÚNKP-20-5 (Bolyai+) and ÚNKP 22-4-1 New National Excellence Program of the Ministry of Innovation and Technology from the source of the National Research, Development and Innovation Fund of Hungary.

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# THE EFFECT OF SERINE AND THREONINE ON THE COMPLEX FORMATION AND HYDROLYTIC STABILITY OF MODEL PEPTIDES AND THE HUMAN TUB α 1A PROTEIN FRAGMENT

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Interaction of metal ions and proteins, peptides, amino acids are essential in the human body and it is important to understand the processes taking place, which can be reversible like the coordination, or even irreversible ones could also occur like the oxidative reactions or the hydrolytic processes.

Investigations of amino acids and basic model peptides and their complex formation processes with transition metal ions, like Cu(II), Ni(II), Zn(II), Co(II), Cd(II), Pd(II), Pt(II), Hg(II), etc. were thoroughly described before. In case of peptides, anchor groups are responsible for the capture of the metal ion and further amide nitrogens are also bond as pH increases. During solution equilibrium and spectroscopic measurements, reversible complex formation processes are assumed in the presence of nickel(II) ions. However, in the below defined motif enables other reactions between the metal ions and the peptide, furthermore it is assumed; a non-coordinating side chain of serine or threonine residue is responsible for the exceptional behaviour.

Structure altering effect of these sequences were observed in case of -(S/T)XH- motifs through the circular dichroism spectra of their 4N nickel complexes[1,2] and in the presence of the nickel(II) ion, selective hydrolysis of the peptide also occurs.[3] It is important to observe that the described reaction was detected at higher temperature and mostly after several hours, if the pH was slightly basic.

Numerous natural proteins contain the -(S/T)XH- motif, highlighted one of the most interesting one, the HUMAN TUB α 1A. It is well known that the polymerization of the α and ß TUB-monomers results in the formation of the microtubules in the human brain. However, in case of neurodegenerative diseases, the opposite process, the disintegration of the microtubules was observed. The previously mentioned sequence can be found as the environment of His8 and His192 in the HUMAN TUB α 1A protein. Description of processes, which could take place between the metal ions and the TUB natural protein fragments are important, because it may contribute to understanding the role of metal ions in the development of Alzheimer's Disease (AD) or Parkinson's Disease.

In our work, we studied the structural change of the formed complexes and the possibility of hydrolysis under the conditions of solution equilibrium and spectroscopic measurements in case of -SXH- model peptides and the natural TUB fragment. The role of serine/threonine can be the facilitation of hydrolytic processes by the formation of a defined complex geometry; however, this preliminary step is not enough in each case for the final cleavage of the peptide.

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# SYNTHESIS OF AL(OH)$_3$ BASED LAYERED DOUBLE AND TRIPLE HYDROXIDES CONTAINING MANGANESE, COBALT, NICKEL, COPPER AND ZINC, CATALYTIC USE UNDER CONTINUOUS FLOW CONDITIONS IN HYDROGENATION REACTION

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Layered double hydroxides (abbreviated as LDHs) and layered triple hydroxides (abbreviated as LTHs) are a group of the anionic clays. Their layered structure consists of divalent and trivalent metal hydroxides. The replacement of divalent metals with trivalent ones results in positively charged layers which are naturalized by negatively charged counter ions intercalating in the interlayer region besides water molecules. Owing to the basicity of their surface these materials are important for many modern applications such as polymer additives or (photo)catalysts. [1]

Gibbsite, $\gamma$-Al(OH)$_3$ is one of the mineral forms of aluminum hydroxide. Its structure is like the above-mentioned conventional LDHs, forming stacked sheets of linked octahedra. Each aluminum ion bonds to six hydroxide groups, two aluminum octahedra share one hydroxide group. The binding strength between the sheets comes from weak residual bonds. In the octahedra, wisely selected positively charged cations can be incorporated thus creating a whole new and yet not so investigated group of the LDHs. The incorporation has several limiting factors due to the size of the octahedral holes. In addition to the ionic radii of the metal ions wished to be incorporated, their solvation enthalpies are also decisive. [2, 3]

In our work, we aimed to synthesize various members of this aluminum hydroxide based non-conventional LDH group with the incorporation of Mn(II), Co(II), Ni(II), Cu(II), Zn(II) ions into the octahedra. Furthermore, we wished to investigate the catalytic properties of these materials by using them under continuous flow conditions in the hydrogenation of cinnamaldehyde in liquid phase. To understand the catalytic contribution of these high Al(III) and low transition metal containing LDHs and LTHs, conventional LDHs were also synthesized for comparative reasons.

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# TRANSFORMATIONS OF ANHYDRO-ALDOSE OXIMES INTO POTENTIALLY BIOLOGICALLY ACTIVE CARBOHYDRATE DERIVATIVES

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*Candida albicans* is a dimorphoric yeast which can exist in a commensal state in the mucosae and gastrointestinal tract.[1] *C. albicans* becomes pathogenic in immunocompromised patients under various conditions, such as superficial and systemic infections.[2] The high pathogenicity of *Candida* species may be related to their adherence to the host organism. The cell surface glycans are important receptors for *C. albicans* and warrant the development of anti-adherence ligands that can mimic them, thus disrupting *C. albicans* - epithelial cell interactions.[3] Very recently, a series of divalent sugar derivatives were tested to show that galactosyl derivatives with triazole linker units connected to an aromatic core are efficient inhibitors of *Candida albicans* adherence.[4]

In our research group a two-step synthetic procedure was elaborated for the preparation of anhydro-aldose oximes from anhydro-aldononitriles: reduction of glycosyl cyanides then *in situ* trapping of the intermediate imine by semicarbazide and a transimination reaction in the presence of hydroxylamine-hydrochloride.[5] Oximes can be applied to generate *in situ* nitrile oxide either by a halogenation/base induced elimination sequence or oxidation by NaOCl. This reactive intermediate can react as a 1,3-dipole with C-C double and triple bonds and C-N triple bonds in dipolar cycloadditions to form heterocyclic compounds.

Based on these preliminaries, we plan to systematically study the reactions of nitrile oxides derived from anhydro-aldose oximes to form glycopyranosylidene-spiro- and *C*-glycosyl-heterocyclic compounds, which can be novel potential anti-adherence agents against *C. albicans* as well as glycogen phosphorylase and galectin inhibitors.

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The research was supported by the National Research, Development and Innovation Office under the project PD 142641, by the ÚNKP-22-3-I-DE-390 New National Excellence Program of the Ministry for Innovation and Technology from the source of the National Research, Development and Innovation Fund, and by the European Cooperation in Science and Technology under the project CA18132.

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# SIMILARITY OF STRUCTURE AND BIOLOGICAL ACTIVITY RELATIONSHIP BETWEEN ANTIPSYCHOTIC DRUGS AND PLANTS WITH ANTIPSYCHOTIC EFFECT

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Antipsychotics drugs are the prescribed treatment to ameliorate schizophrenia symptoms, but they have severed limitation for treatment of negative and cognitive symptoms and induce drug-related adverse effects[1]. For selected antipsychotic drugs authorized in Romania (Haloperidol, Risperidone, Aripiprazole, Olanzapine and Quetiapine) the experimental determination of lipophilicity was carried out by thin-layer chromatography using the mobile phase acetonitrile-water with increasing percentage of acetonitrile and 0.2% formic acid in each case. Lipophilicity parameters ($R_{M0}$) were determined from retention data ($R_f$ values) on four types of reversed phase using RP-18, CN, DIOL and NH2 chromatographic plates[2,3,4]. The determined lipophilicity parameters were discussed in terms of the structure-lipophilicity relationships with topological polar surface area (TPSA) and bioactivity estimated by computational methods[5]. A literature search was conducted for active principle from plants with antipsychotic effect, bioactivity estimated by computational methods and discussed in term of correlation with structure and bioactivity of antipsychotic drugs[5,6,7,8,9].

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# DIORGANOTIN(IV) COMPLEXES WITH ORGANOSELENOLATO LIGANDS

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Organotin(IV) compounds attracted a considerable increased interest over last years due to their potential biological properties (antibacterial or antitumor agents) and their applications as precursors for nanomaterials for optoelectronics.[1] On the other hand, various organoselenium compounds were intensively studied for their antioxidant and antiproliferative properties, or they were used as immunomodulators and antiinflamatory or antidepressant drugs.[2]

Our recent research interest was focused on the synthesis and structural characterization of organotin compounds with organoselenolato ligands with potential for biological applications. In order to increase the stability of the organotin compounds we used aromatic organic groups bearing pendant arms with nitrogen donor atoms capable of N→E intramolecular interactions, *e.g.* $2\text{-}(Me_2NCH_2)C_6H_4$.

We report here on the synthesis and structural characterization of several homo- and heteroleptic diorganotin(IV) complexes with organoselenolato ligands of type $pzCH_2CH_2Se^-$ (pz = pyrazole). Compounds of type $RR'Sn(SeCH_2CH_2pz)_2$ ($R = 2\text{-}(Me_2NCH_2)C_6H_4$, R' = Me, $^n$Bu, Ph, $2\text{-}(Me_2NCH_2)C_6H_4$) were prepared by reacting $RR'SnCl_2$ with $Na[SeCH_2CH_2pz]$ in a 1:2 molar ratio and they were characterized by multinuclear NMR and mass spectrometry.

*Acknowledgements*: The financial support of UEFISCDI, Project PN-III-P4-ID-PCE-2020-1028 is highly acknowledged.

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# ANALYSIS OF COSMETIC PRODUCTS BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY AND DIRECT-ANALYSIS-IN-REAL-TIME MASS SPECTROMETRY

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In our work different types of decorative cosmetics with different prices have been investigated by GC-MS and DART-MS analysis. These samples are complex mixtures showing high variation in their chemical composition. We focused on the volatile compounds to compare the cosmetics as the most common allergens[1] (fragnances and preservatives) are falling in this category.

All the samples were extracted by methanol and acetone applying an ultrasonic bath. Fifteen different samples were studied and numerous compounds were identified. We found paraben derivatives in many samples, which are usually applied as a preservative in cosmetics, however, they show potential endocrine disruptor effects[2].

In the European Union, the parabens that are allowed in products have a quantitative limit (0.4 m/m% for single ester and 0.8 m/m% for mixture of esters[3]. To measure the amount of parabens in our samples, we used DART-MS, as this method is capable of providing data within second, however it is semi-quantitative. We used paraben standards purchased from Sigma-Aldrich.

During the research we did not identify any prohibited components and all samples adhered to the quantitative regulations but some chemicals are currently under assessment by the European Chemicals Agency.

*Acknowledgements:* The work was supported by the GINOP-2.3.3-15-2016-00021 projects and by Thematic Excellence Program (TKP2020-NKA-04) of the Ministry for Innovation and Technology in Hungary. The projects were co-financed by the European Union and the European Regional Development Fund. Furthermore, this paper was also supported by Grant No. FK-132385 from National Research, Development and Innovation Office (NKFI). Thanks for the financial support provided by the Mol Group, Hungary.

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# NOVEL Cu(II) COMPLEXES USING PHOTOISOMERIZABLE *ortho*-VANILIN AZO DERIVATIVES LIGANDS

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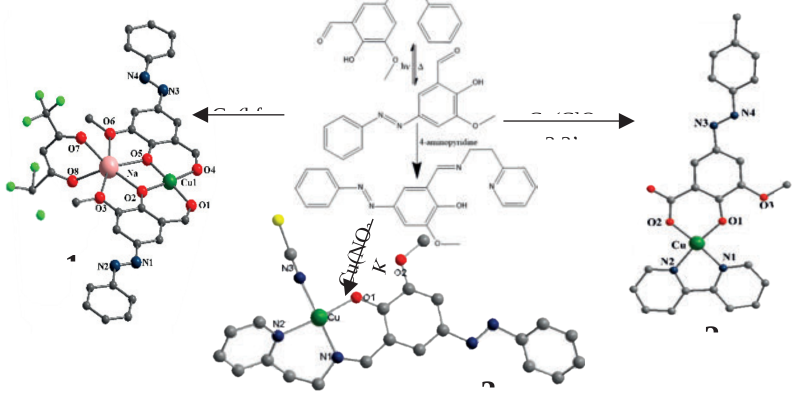
*Ortho*-vanilin (IUPAC: 2-hydroxy-3-methoxybenzaldehyde) posseses a rich coordination chemistry due to the possibility of easily forming Schiff base compounds.[1] The popularity of the Schiff base derivatives arises from the asymmetric bicompartimental pockets which can assemble homo- and heterometallic complexes.[2]

As a continuation of our work, we functionalize *o*-vanilin with azobenzene derivatives in order to develop photoswitchable organic and coordination compounds. For this purpose, we synthesized (E)-2-hydroxy-3-methoxy-5-(phenyldiazenyl)benzaldehyde ($HL_1$), (E)-2-hydroxy-3-methoxy-5-(*p*-tolyldiazenyl)benzaldehyde ($HL_2$) and 2-methoxy-4-((E)-phenyldiazenyl)-6-((E)-((2-(pyridin-2-yl)ethyl)imino)methyl)phenol ($HL_3$). By reaction with different copper salts, two types of mononuclear complexes are formed. For example, reaction of $HL_1$ with $[Cu(hfac)_2]\cdot H_2O$ yields $[Cu(L_1)_2Na(hfac)]$,(**1**). If the reaction is performed with $Cu(ClO_4)_2\cdot 6H_2O$, $HL_2$ and 2,2'-bipyridine as co-ligand, copper(II) manifests its oxidative properties and *in situ* oxidation of the aldehyde group occurred with the formation of the coresponding carboxylic acid,(**2**). If a Schiff base is used as organic ligand, in reaction with $Cu(NO_3)_2\cdot 3H_2O$, a mononuclear Cu(II) complex, (**3**), is formed in the presence of KSCN as co-ligand.



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# RESEARCH AND IMPROVEMENT OF Li-AIR BATTERY APPLYING CARBON BASED CATHODE

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*Abstract:* A new, recheargeable lithium-air battery which has Swagelok-type polypropylene (PP) cell body was printed using 3D printer and tested. Charcoal and vulcan carbon cloth were applied as cathode compartments; and metal lithium was used as anode. The anode and cathode parts were separated by polypropylene membrane immersed in electrolyte which was propylene carbonate containing 1.0 M Li-trifilate salt. Two pieces of cottons were also immersed in electrolyte and put on both sides of the PP membrane for charcoal cathode to prevent any damage of PP membrane and to provide the enough amount of electrolyte. However, when vulcan carbon was applied as cathode, only one cotton was applied in the lithium anode. The cyclic voltammetry, impedance spectroscopy and cycling test measurements were carried out using 0.05 $mAcm^{-2}$-0.1$mAcm^{-2}$ current densities to test and compare the two cells by using both cathodes. It was obtained that the charcoal cathode provided higher capacity and lifetime than the vulcan carbon cathode; the Coulomb efficiency was approximately 100% over 200 cycles for the charcoal cathode and 60 cycles in the case of vulcan carbon cathod.

*Acknowledgements:* Project no. RRF-2.3.1-21-2022-00009, titled National Laboratory for Renewable Energy has been implemented with the support provided by the Recovery and Resilience Facility of the Europian Union within the framework of Programme Széchenyi Plan Plus. Thanks for the financial support provided by the Mol Group, Hungary.

# EFFECT OF FRUIT POWDER FORTIFICATION ON THE VOLATILE PROFILE OF CONFECTIONERY PRODUCTS

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Volatile compounds play an important role in the quality assessment and consumer acceptance of foods since they are majorly responsible for the development of sensory properties[1]. Confectionery products are consumed mainly for their hedonic value, nevertheless, an increasing consumer demand can be observed for value-added products containing functional ingredients[2]. The aim of our research was to investigate the addition of antioxidant-rich fruit powders on the aroma profile of biscuits and white chocolates. Powders of sea buckthorn (*Hippophae rhamnoides*), rose hip (*Rosa canina*), black chokeberry (*Aronia melanocarpa*), acerola cherry (*Malpighia emarginata*) and goji berry (*Lycii fructus*) were involved in the experiment. Biscuits were prepared according to the recipe proposed by the American Association of Cereal Chemists (AACC-approved method 10-50D)[3] by substituting wheat flour with 10% fruit powder. Chocolates were created by enriching conventional white chocolates melted at 45±2 °C with 10% of fruit powder. Qualitative analysis of volatile compounds of the powders, biscuits and chocolates was conducted by using a headspace-solid-phase microextraction-gas chromatography-mass spectrometry (HS-SPME-GC-MS) method. Based on prior experiments, divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) fiber coating was chosen to extract volatiles at 40 °C. In the case of fruit powders, potential markers of botanical origin were identified. Rose hip powder was rich in volatile compounds, especially in terpenes and terpenoids. Other fruit powders contained fewer volatiles belonging to diverse chemical classes, such as aldehydes, ketones, alcohols, esters and acids. The number of the volatile constituents was higher in white chocolates – including the control sample – compared to biscuits. Thermal decomposition contributes to this observation, although, some aroma compounds are formed during the heat treatment of biscuits. Certain volatiles of fruit powders were also detected in the enriched biscuits and chocolates, which indicates that these products are applicable to modify the aroma profile, and potentially to improve the sensory acceptance of confectionery products. Our further objective is to investigate the relationship between the volatile composition and consumer preference of the fruit powder-enriched biscuits and chocolates.

*Acknowledgements:* This research was supported by the New National Excellence Program of the Ministry for Innovation and Technology (ÚNKP-22-3-II-MATE-23). Rita Végh acknowledges the support of the Doctoral School of Food Sciences, Hungarian University of Agriculture and Life Sciences.

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# $[Ln_2(hfac)_4(ac)_2(OH_2)_2(OMe)_2]$ – VERSATILE PRECURSOR FOR OPTICAL ACTIVE D-F METAL-COMPLEXES

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The dinuclear precursor $[Ln_2(hfac)_4(ac)_2(OH_2)_2(OMe)_2]$, synthesised in a quite simple way, has the potential to be an important precursor for the synthesis of coordination compounds with various properties.[1] By reacting a [3d(valen)-type complexes with this precursor, we can obtain dinuclear 3d-4f compounds with an additional *syn*-*syn* acetato bridge between the two metal ions.[2] Our perspective is, by using this synthetic pathway to achieve optical active, luminescent and magnetic materials. For this purpose, we replaced the 1,3- propanediamine in the starting $H_2$valen-ligand with a chiral diamine[3] in order to obtain 3d-4f, chiral, acetato-bridged complexes. Subsequently, we want to change the acetato-bridge with optically active carboxylato ligands for a more intense transfer of the optical information to the metal ions. The preliminary synthetic results will be presented, consisting in the synthesis and single-crystal X-ray diffraction investigations of dinuclear d-f complexes with racemic mixtures of diamines.

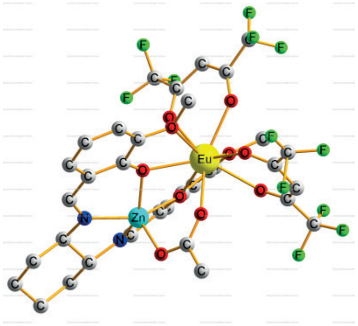

**Figure 1**-Perspective view of the crystal structure of the complex [ZnEuL[1]].
The hydrogen atoms were omitted for clarity

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# NOVEL CERIUM OXIDE-TYPE HIGH ENTROPY RARE EARTH OXIDES FOR PHOTOCATALYTIC $CO_2$ HYDROGENATION

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Carbon dioxide ($CO_2$) is a double-edged sword. Although it helps create a warm environment on Earth, the excessive burning of fossil fuels has led to a continuous rise in $CO_2$ concentration in the atmosphere, resulting in irreversible climate changes [1, 2]. High entropy materials, which consist of various elements in single-phase compounds, are known for their unique properties and crystal structures due to their high configurational entropy. The recent research trend has focused on utilizing nanostructured ceria ($CeO_2$) in various applications due to its availability, affordability, and stability. It has been found that this rare earth oxide has the potential to be used in photocatalytic applications, including energy production, hydrogen generation, oxygen evolution, and storage capacity enhancement [3, 4].

In our research, we prepared six ceria-based rare earth high-entropy oxides (HEOs) with fluorite structure and examined their photocatalytic behavior toward $CO_2$ hydrogenation. The cationic site in the fluorite lattice consists of five equimolar elements, including Sm, Ce, Pr, La, and Nd (rare earth elements) and Y and Zr (transition metals). The HEOs exhibit band gaps ranging from 2.65 to 3.37 eV and appropriate valence and conduction band positions for $CO_2$ reduction. The samples possess high photocatalytic activity, which can be attributed predominantly to the accessibility of more active sites, resulting in more photogenerated electrons. The materials produced carbon monoxide as the main product, but some methane and methanol were also generated. The photocatalytic performance of all studied HEOs surpasses single fluorite oxides or equivalent mixed oxides. The $Ce_{0.2}Zr_{0.2}La_{0.2}Nd_{0.2}Sm_{0.2}O_2$ (CZLNS) showed the highest photocatalytic conversion of $CO_2$ (29.7 %) and formation rate for CO (1256.1 nmol) among the HEO samples and its pristine $CeO_2$ counterpart (6.6 %). The best-performing photocatalyst was investigated further by theoretical modeling using density functional theory.

*Acknowledgements:* AS gratefully acknowledges the support of the Bolyai Janos Research Fellowship of the Hungarian Academy of Science and the " ÚNKP-22-5 -SZTE-587" New National Excellence Program as well as the funding provided by the Indo-Hungarian TÉT project (2019-2.1.13-TÉT_IN-2020-00015) and FK 143583 of NKFIH and Project no. TKP2021-NVA-19 under the TKP2021-NVA funding scheme of the Ministry for Innovation and Technology and ZK is grateful for K_21 138714 and SNN_135918 project from the source of the National Research, Development and Innovation Fund. The Ministry of Human Capacities through the EFOP-3.6.1-16-2016-00014 project and the 20391-3/2018/FEKUSTRAT are acknowledged. Project no. RRF-2.3.1-21-2022-00009, titled National Laboratory for Renewable Energy has been implemented with the support provided by the Recovery and Resilience Facility of the European Union within the framework of Programme Széchenyi Plan Plus.

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# PROSPECTIVE STUDIES ON THE DEVELOPMENT OF NANOCOMPOSITE BASED ELECTROCHEMICAL SENSORS FOR THE DETECTION OF CLINICALLY RELEVANT MOLECULES

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The monitoring of clinically relevant compounds such as hydrogen peroxide, glucose, lactate and cortisol is of great importance for evaluation of the human health status. These represent markers of various medical conditions such as inflammation, diabetes and sepsis. Among various sensing methods used for the detection of such compounds, the electrochemical sensors and the advance of nanotechnology offer the advantages of miniaturization and integration into portable detection systems, with low costs for clinical applications[1,2].

The present study proposes the development of innovative electrochemical (bio)sensors based on modification of flexible screen-printed carbon paste electrodes (SPEs) with different nanocomposite materials, possessing flexible and enhanced electrochemical, optical and resistant properties. Thus, a hydrated agarose-polyaniline based polymer network has been doped with conductive carbon-based nanomaterials (e.g., carbon nanotubes, polyhydroxylated fullerene), allowing the polymerization and gelation of the hydrogel precursors solutions with the conductive nanomaterials[3]. The conditions of the polymerization (pH medium, temperature, time), the reticulation and swelling degrees were optimized. Specific bioreceptors (glucose and lactate oxidases) were used for dedicated functionalization and further entrapment in the hydrogel network structure for the sensitive and selective detection of some biological analytes (e.g., hydrogen peroxide, glucose and lactate).

In order to confirm the development of the interpenetrated agarose-polyaniline network, the obtained films were characterized by FTIR spectroscopy, SEM and TGA analyses. The electrocatalytic properties of the biocomposite films were studied by cyclic voltammetry (CV), amperometry and electrochemical impedance spectroscopy (EIS).

The performance of the developed (bio)sensors for the detection of specific analytes showed a synergistic combination of the benefits offered by the hydrogel-nanomaterial and specific bioreceptors (enzymes) for the design of new versatile (bio)sensors.

*Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project M-ERANET-3-FULSENS-GEL within PNCDI III, Contract no. 318/2022 and within Program 1 - Development of the national research and development system, Subprogram 1.2 -Institutional performance- Projects to finance excellence in RDI, Contract no. 15PFE /2021*

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# DETERMINATION OF FATTY ACID COMPOSITION IN BREAST MILK

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Lipids provide the majority of energy for developing infants in human milk (HM), as well as essential fatty acids (FA). The FA composition of HM is highly variable because it is influenced by many factors, such as maternal diet and health, feeding duration, and lactation satges. Changes can be observed in specific FA classes according to distinct patterns over the time of lactation[1,2]. FA composition of HM derived from different stages of lactation was ivestigated in this study.The mothers were all healthy owing normal BMI indexes. Neonates were born on time. Fifteen mothers provided HMs during their lactation period. Sample preparation was conducted based on ISO 16958:2015 reference method with slight modifications. Different dilution factors were tested on the final solution. FA compositions were analyzed by GC-FID. Fatty acid results were calculated as a proportion of total fatty acids. The changes in the FA composition of breast milk during the lactational period were demonstrated by grouping the compounds based on their chemical structure (SFA: saturated FA; MUFA: mono unsaturated FA; PUFA: polyunsaturated FA; **Fig 1.** A,B,C).

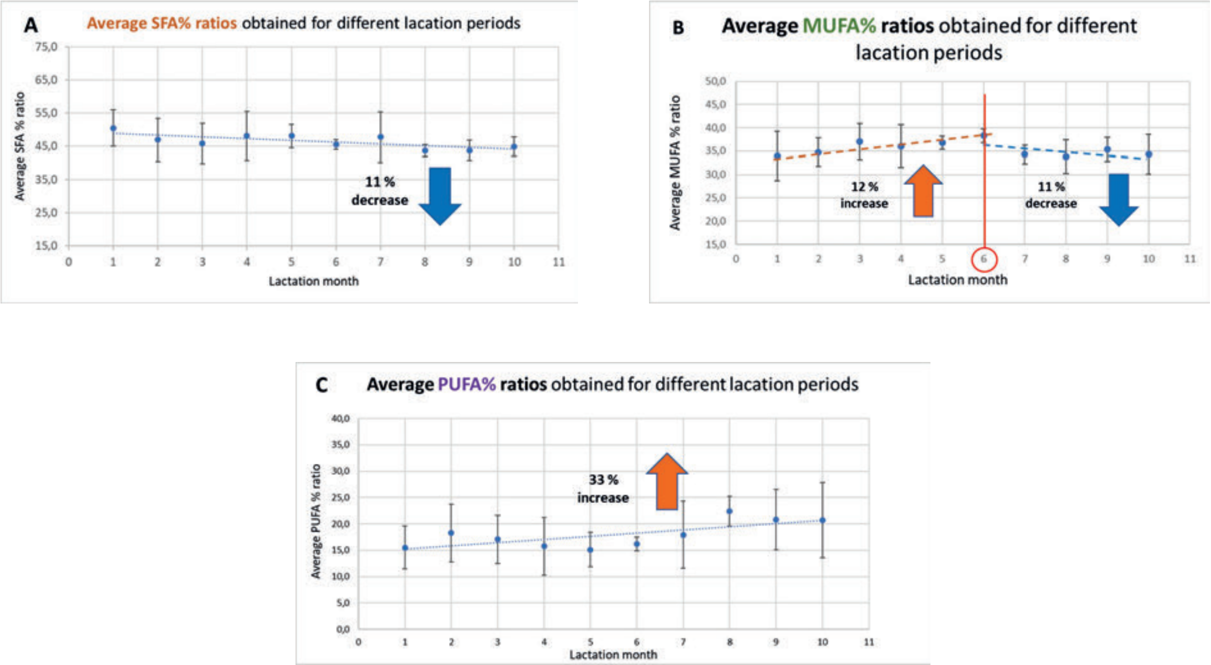

**Figure 1.** Tendencies of average fatty acid ration in the SFA% group (A), MUFA% group (B) and PUFA% group (C) in human milk samples deriving from different lactation periods

*Acknowledgement:* The research was funded by RECOOP Grant # 016 Pregnant Obesity and GDM changing human milk secretory cytokines and altering IgG - IgA N-glycans and fatty acids. We are also grateful for the Stipendium Hungaricum scholarship provided to the PhD student.

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