

# BOOK OF ABSTRACTS



**National Conference of Chemistry**  
**XXXVII Edition**

**The Conference is jointly organized by:**



**Romanian Chemical Society**



**Romanian Academy**



**Valahia University of Targoviste**

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Thanks to our sponsors for accepting the invitation to be close to the CNCHIM2024 Conference and supporting this event.

It is always important to have reliable partners who share common interests with ours.

Together maybe we will not build the future but, for sure, we will try on making this world a better place for everyone.



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*"Help others achieve their dreams and you will achieve yours"*

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Les Brown



## SCHEDULE

Wednesday, September 25<sup>th</sup>, 2024

International Conference Center - Valahia University of Targoviste

8 <sup>00</sup> – 10 <sup>00</sup>	<b>Registration</b>
10 <sup>00</sup> – 11 <sup>20</sup>	<b>Red Hall</b> <b>Opening Ceremony</b> <b>Awarding the prizes of the Romanian Chemical Society</b>
11 <sup>20</sup> – 11 <sup>30</sup>	<b>Coffee Break</b>
11 <sup>30</sup> – 13 <sup>00</sup>	<b>Red Hall</b> <b>Plenary Session</b> Chairpersons: Marius Andruh & Edouard Badarau
11 <sup>30</sup> – 12 <sup>15</sup>	<b>Plenary Lecture: Ion Tiginyanu</b> – Bio-inspired hybrid 3D nanoarchitectures for multifunctional applications
12 <sup>15</sup> – 13 <sup>00</sup>	<b>Plenary Lecture: Dumitru Coman</b> – Reindustrialization / Renaissance of the chemical industry in Romania
13 <sup>00</sup> – 14 <sup>30</sup>	<b>Lunch</b>
14 <sup>30</sup> – 15 <sup>40</sup>	<b>Parallel Session</b>
14 <sup>30</sup> – 15 <sup>40</sup>	<b>Red Hall</b> <i>Organic, Bioorganic, and Food Chemistry</i> Chairpersons: Valeria Harabagiu & Adrian Someșan
14 <sup>30</sup> – 14 <sup>55</sup>	<b>Conference: Philipp Sulzer, Markus Müller, Tobias Reinecke, Stefan Feil, Andreas Mauracher, Rene Gutmann, Alfons Jordan</b> - PTR-MS: Basics, applications, and recent technological advancements
14 <sup>55</sup> – 15 <sup>10</sup>	<i>Darin Hariz, David Chen, Catalin Duduianu, Mihaela Balan-Porcarasu, Ana Maria Macsim, Gabriela Liliana Ailiesei, Mihaela Cristea, Cristina Stavarache, Raluca Stan, Natalia Usurelu, Veaceslav Kulcitki, Alina Nicolescu, Calin Deleanu</i> - Assessment of reproducibility in NMR metabolomics
15 <sup>10</sup> – 15 <sup>25</sup>	<i>David Chen, Darin Hariz, Catalin Duduianu, Mara Anastasia Isvoranu, Natalia Usurelu, Alina Nicolescu, Calin Deleanu</i> - Magnesium supplements and the body clearance of their organic ligands. The magnerot case

15 <sup>25</sup> – 15 <sup>40</sup>	<i>Maria Alexandra Baicus, Ion Grosu, Niculina D. Hadade, Mihail Barboiu</i> - Water permeation across a series of imines - Potential artificial water channels
14 <sup>30</sup> – 15 <sup>35</sup>	<b>Blue Hall</b> <i>New Materials and Nanomaterials</i> Chairperson: Radu Silaghi-Dumitrescu & Radu Lucian Olteanu
14 <sup>30</sup> – 14 <sup>55</sup>	<b>Conference:</b> <i>Isabela C. Man, R. Jalba, D. L. Isac, Yuheng Zhao, Ionut Tranca</i> – Exploring the activity of the graphene quantum dots (GQDS) for the electrochemical oxygen reduction reaction using DFT
14 <sup>55</sup> – 15 <sup>20</sup>	<b>Conference:</b> <i>Andrei Honciuc</i> – Fundamentals and applications of <i>Amphiphilic Janus</i> nanoparticles
15 <sup>20</sup> – 15 <sup>35</sup>	<i>George Mihail Teodorescu, Zina Vuluga, Rodica Mariana Ion, Marius Ghiurea, Cristian Andi Nicolae, Augusta Raluca Gabor</i> – Influence of surface treated ash powder on the properties of glass fiber reinforced polypropylene
15 <sup>40</sup> – 16 <sup>00</sup>	<b>Coffee Break</b>
16 <sup>00</sup> – 16 <sup>55</sup>	<b>Parallel Session</b>
16 <sup>00</sup> – 16 <sup>55</sup>	<b>Red Hall</b> <i>Organic, Bioorganic, and Food Chemistry</i> Chairpersons: Anca Silvestru & Cristiana Rădulescu
16 <sup>00</sup> – 16 <sup>25</sup>	<b>Conference:</b> <i>Robert I. Botea, Ionuț Melinte, Irina Scarlat</i> – Rapid determination of acrylamide in processed foods using advanced LC-MS/MS techniques
16 <sup>25</sup> – 16 <sup>40</sup>	<i>Cristina Stoian</i> - Study of the impact of nitrites from meat preparations on health
16 <sup>40</sup> – 16 <sup>55</sup>	<i>Andreea Oanea, Niculina D. Hadade, Mihail Barboiu</i> - Creating bilayer membrane channels with responsive macrocycles
16 <sup>00</sup> – 16 <sup>40</sup>	<b>Blue Hall</b> <i>New Materials and Nanomaterials</i> Chairperson: Laura Monica Gorghiu & Rodica Olar
16 <sup>00</sup> – 16 <sup>15</sup>	<i>Mirela Honciuc, Andrei Honciuc, Ana Maria Solonaru</i> – Polyphenols encapsulated in polymeric microparticles: Absorption and release properties
16 <sup>15</sup> – 16 <sup>30</sup>	<i>Adriana Petronela Chiriac, M. D. Damaceanu</i> – Electrogenerated ProDOT-based polymers for energy storage smart window applications
16 <sup>30</sup> – 16 <sup>45</sup>	<i>Ana Maria Solonaru, Andrei Honciuc, Mirela Honciuc, Oana Iuliana Negru</i> – Microspheres obtained from pickering emulsion stabilized by <i>Janus</i> nanoparticles as adsorbents of metal ions from water
17 <sup>00</sup> – 18 <sup>00</sup>	<b>Poster Session 1</b> Chairpersons: Marius Andruh & Cristian Silvestru & Marcela Mihai & Mihaela Doni
19 <sup>30</sup>	<b>Welcome Reception</b>

Thursday, September 26<sup>th</sup>, 2024

International Conference Center - Valahia University of Targoviste

8 <sup>00</sup> – 10 <sup>00</sup>	<b>Registration</b>
10 <sup>00</sup> – 11 <sup>30</sup>	<b>Red Hall</b> <b>Plenary Session</b> Chairperson: Ecaterina Andronescu & Mihaela Doni
10 <sup>00</sup> – 10 <sup>45</sup>	<b>Plenary Lecture:</b> Lilian Saryeddine, Axelle Grelard, Estelle Morvan, Bruno Aliès, Corinne Bure, Isabelle Bestel, Edouard Badarau – Design of a new generation of photosensitive liposomes for therapeutic applications
10 <sup>45</sup> – 11 <sup>30</sup>	<b>Plenary Lecture:</b> Michaela Dina Stănescu – Valorization of the grape seeds resulted in the wine production process
11 <sup>30</sup> – 12 <sup>00</sup>	<b>Coffee Break</b>
12 <sup>00</sup> – 13 <sup>05</sup>	<b>Parallel Session</b>
12 <sup>00</sup> – 13 <sup>05</sup>	<b>Red Hall</b> <i>Inorganic chemistry physical and analytical chemistry</i> Chairpersons: Andrei Honciuc & Rodica Mihaela Dinică
12 <sup>00</sup> – 12 <sup>25</sup>	<b>Conference:</b> Anca Silvestru - Organochalcogen compounds and their metal complexes. Synthesis, structure, and potential applications
12 <sup>25</sup> – 12 <sup>50</sup>	<b>Conference:</b> Radu Silaghi Dumitrescu - Synergy between computations and experiments on transition metal complexes: Challenges with isomerism, spin states and spectroscopy
12 <sup>50</sup> – 13 <sup>05</sup>	Stefan Dimitriu, Sergiu Shova, Mihai Raduca, Marius Andruh – Design of an organic cage using Mannich and Schiff reactions
12 <sup>00</sup> – 13 <sup>05</sup>	<b>Blue Hall</b> <i>Macromolecular and Supramolecular Chemistry</i> Chairpersons: Aurel Tăbăcaru & Cristina Stoian
12 <sup>00</sup> – 12 <sup>25</sup>	<b>Conference:</b> Aurica Farcas - Supramolecular organic semiconductors: recent advances and perspectives for optoelectronics
12 <sup>25</sup> – 12 <sup>50</sup>	<b>Conference:</b> Maria Cazacu - Approaches towards smart and sustainable silicones
12 <sup>50</sup> – 13 <sup>05</sup>	Tamas Melinda, Anca Silvestru – Di- and triorganotin(IV) complexes with organoselenolato ligands
13 <sup>05</sup> – 14 <sup>30</sup>	<b>Lunch</b>
14 <sup>30</sup> – 15 <sup>45</sup>	<b>Parallel Session</b>
14 <sup>30</sup> – 15 <sup>45</sup>	<b>Red Hall</b> <i>Inorganic chemistry physical and analytical chemistry</i> Chairpersons: Mihaela Badea & Radu Claudiu Fierăscu
14 <sup>30</sup> – 14 <sup>55</sup>	<b>Conference:</b> Vlad Penciu, Adrian Alexandru Somesan, Richard A. Varga – Novel organotin(IV) alkoxides – from synthesis to reactivity

14 <sup>55</sup> – 15 <sup>20</sup>	<b>Conference:</b> <i>Mihai Raduca, Marius Andruh</i> – From nitronyl nitroxides towards homo- and hetero-di-radicals used as ligands for the synthesis of 3d and 4f complexes
15 <sup>20</sup> – 15 <sup>45</sup>	<b>Conference:</b> <i>Claudiu Roman, Cecilia Arsene, Iustinian Gabriel Bejan, Romeo Iulian Olariu</i> - Multi-referential relative kinetic methods versus pseudo-first method for assessing of the gas-phase ozonolysis of unsaturated volatiles in environmental sciences
14 <sup>30</sup> – 15 <sup>15</sup>	<b>Blue Hall</b> <i>Macromolecular and Supramolecular Chemistry</i> Chairpersons: Ioan Cezar Marcu & Lidia Lungu
14 <sup>30</sup> – 14 <sup>45</sup>	<i>Melinda-Maria Bazarghideanu, Marius-Mihai Zaharia, Camelia-Georgiana Marandis, Stergios Pispas, Marcela Mihai</i> – Graft copolymers derived from amylopectin and synthetic homopolymers
14 <sup>45</sup> – 15 <sup>00</sup>	<i>Maria Medrihan, Andrei Honciuc, Valeria Harabagiu, Mirela Honciuc, Ana-Maria Solonaru, Oana Negru</i> – Polymeric microspheres obtained from Pickering Emulsion Polymerization Technology (PEmPTech) for colorimetric recognition of metal ions
15 <sup>00</sup> – 15 <sup>15</sup>	<i>Marius-Mihai Zaharia, Elena-Daniela Lotos, Florin Bucatariu, Melinda-Maria Bazarghideanu, Stergios Pispas, Marcela Mihai</i> - In-situ synthesis of gold nanoparticles mediated by chitosan-g-poly(N-isopropylacrylamide)
15 <sup>45</sup> – 16 <sup>00</sup>	<b>Coffee Break</b>
16 <sup>00</sup> – 17 <sup>30</sup>	<b>Parallel Session</b>
16 <sup>00</sup> – 17 <sup>30</sup>	<b>Red Hall</b> <i>Inorganic chemistry physical and analytical chemistry</i> Chairpersons: Claudiu Roman & Crinela Dumitrescu
16 <sup>00</sup> – 16 <sup>15</sup>	<i>Cosmina Bohan, Alexandra Pop</i> – Silver(i) complexes of diorganosulfur ligands based on oxazol-5(4h)-one moiety
16 <sup>15</sup> – 16 <sup>30</sup>	<i>Laurentiu Valentin Soroaga, Giorgiana Alina Negru, Cecilia Arsene, Romeo Iulian Olariu</i> – The rare earth elements distribution in atmospheric particles as tracers for source apportionment
16 <sup>30</sup> – 16 <sup>45</sup>	<i>Raffaele Fontana, Cristian Silvestru</i> - Study on the oxidative addition of different substrates to N,C-chelated cyclobismuthane
16 <sup>45</sup> – 17 <sup>00</sup>	<i>Catalin Eduard Salgau, Anca Silvestru</i> - Silver(I) complexes of pyridine-based ligands
17 <sup>00</sup> – 17 <sup>15</sup>	<i>Alexandru Sonica, Jozsef Simon, Maria Lehene, Radu Silaghi-Dumitrescu</i> - Binding biomedically relevant agents to hemoglobin
17 <sup>15</sup> – 17 <sup>30</sup>	<i>Toma Galaon</i> - Detection of Over 1000 Pesticides as Food Contaminants according to European Regulations
17 <sup>30</sup> – 18 <sup>30</sup>	<b>Poster Session 2</b> Chairpersons: Marius Andruh & Cristian Silvestru & Marcela Mihai & Mihaela Doni
19 <sup>30</sup>	<b>Diner</b>



Friday, September 27<sup>th</sup>, 2024

International Conference Center - Valahia University of Targoviste

8 <sup>00</sup> – 10 <sup>00</sup>	<b>Registration</b>
10 <sup>00</sup> – 14 <sup>00</sup>	<b>Red Hall</b> <b>Plenary Session:</b> Chairpersons: Marcela Mihai & Corneliu Radu
10 <sup>00</sup> – 10 <sup>45</sup>	<b>Plenary Lecture:</b> Ioan-Cezar Marcu – Catalytic applications of multicationic layered double hydroxide-based materials
10 <sup>45</sup> – 11 <sup>30</sup>	<b>Plenary Lecture:</b> Valeria Harabagiu – Role of Models and Challenges in the Institutional Development
11 <sup>30</sup> – 12 <sup>00</sup>	<b>Conference:</b> Denisa Valentina Negreanu, Teodora Staicu, Maria Alexandra Nacu, Maria Larisa Alexandru, Bogdan Zorila – Indoor radon measurement in laboratories of a university
12 <sup>00</sup> – 12 <sup>30</sup>	<b>Conference:</b> Mihaela Apostol – New Technologies for Environmental Monitoring
12 <sup>30</sup> – 13 <sup>30</sup>	<b>Workshop Reaxys:</b> Piotr Golkiewicz, Beata Fidzinska - Research enhancement in organic chemistry, inorganic chemistry, and life sciences
13 <sup>30</sup> – 14 <sup>00</sup>	<b>Award Ceremony</b> <b>Closing Ceremony</b>

**POSTER SESSION 1**

***Inorganic Chemistry, Physical and Analytical Chemistry***

- ICPAC\_P1.** *Cornelia Amarandei, Alina Giorgiana Negru, Cristina Iancu, Romeo Iulian Olariu, Cecilia Arsene* – Analysis of size-segregated particle-bound polycyclic aromatic hydrocarbons in Iasi urban area
- ICPAC\_P2.** *Nicoleta Andrian, Radu Silaghi-Dumitrescu, Maria Lehne, Bianca Vasile (Stoean), Emese Gál* – Candidates and precursors for anticancer drug
- ICPAC\_P3.** *Alexandra Virginia Bounegru, Constantin Apetrei* – Electrochemical biosensitive detection of tyrosol in olive oils
- ICPAC\_P4.** *Andreea Dogaru, Adrian E. Ion, Catalin Maxim, Sergiu Shova, Simona Nica, Marius Andruh* – Crystal engineering of azulene-based imine cages
- ICPAC\_P5.** *Adrian E. Ion, Andreea Dogaru, Anamaria Hanganu, Catalin Maxim, Sergiu Shova, Simona Nica, Marius Andruh* – Self-assembly of azulene-based bis tren cages. Structural and electrochemical investigations
- ICPAC\_P6.** *Alina Giorgiana Negru, Claudiu Roman, Cornelia Amarandei, Cecilia Arsene, Romeo Iulian Olariu* – Insights into the characterization of the aerosol-phase of limonene photooxidation products under nox and nox-free simulated conditions
- ICPAC\_P7.** *Aurel Tăbăcaru* – Detection of tetracycline and diclofenac by a photoluminescent copper(I) coordination compound
- ICPAC\_P8.** *Maria Lehene, Cezara Zagrean-Tuza, Stefania D. Iancu, Sergiu-Raul Cosma, Adrian M.V. Brânzanic, Radu Silaghi-Dumitrescu* – The chlorite adduct of aquacobalamin: Contrast with chlorite dismutase
- ICPAC\_P9.** *Tudor Jula, Cătălin Maxim, Arpad Rostas, Maria Suci, Mihaela Badea, Rodica Olar* – Biologically active species based on copper(II) complexes with heterocyclic n-based donor ligands
- ICPAC\_P10.** *Rodica Olar, Cătălin Maxim, Mariana Carmen Chifiriuc, Mihaela Badea* – New complexes with nicotinamide exhibiting antimicrobial properties

***New Materials and Nanomaterials***

- NMN\_P1.** *Denisse Iulia Bostiog, Bogdan Florin Craciun, Dragos Peptanariu, Mariana Pinteala* – Development and in vitro evaluation of customizable gold nanoparticle-based non-viral vectors for targeted gene therapy in breast cancer
- NMN\_P2.** *Stefania Eliza Tanasie, Emilia Amzoiu, Adina Segneanu, Manuel Ovidiu Amzoiu, Gabriela Rau, Felicia Ciulu-Costinescu, Denisa Constantina Amzoiu, Maria Viorica Ciocilteu* - *Armoracia rusticana*: from physicochemical research on the species to the development of some pharmaceutical applications
- NMN\_P3.** *Ana Lorena Neagu, Ana Mihaela Gavrilă, Andreea Miron, Iulia Elena Neblea, Catalin Zaharia, Petru Epure, Hugues Brisset, Horia Iovu, Andrei Sarbu, Tanta Verona Iordache* – Carbon electrodes modified with molecularly imprinted polymers for lipopolysaccharides sensing

- NMN\_P4.** *Iulia Elena Neblea, Tanta Verona Iordache, Andrei Sarbu, Anita Laura Chiriac, Ana Mihaela Gavrilă, Bogdan Trica, Mircea Teodorescu, François-Xavier Perrin, Iuliana Caras, Anamaria Zaharia* – Molecularly imprinted nanogels for targeted recognition of spike protein from SARS-COV-2
- NMN\_P5.** *Raluca Ioana Jalba, I.C. Man, D.L. Isac, S.G. Soriga* – N-doped GQDS for ORR – A theoretical approach
- NMN\_P6.** *Alexandru Anghel, Alexandra Burdusel, Ecaterina Andronescu* - Bioglass-based nanohybrids
- NMN\_P7.** *Alexandra Claudia Birca, Bogdan Dimitrie Carp, Ecaterina Andronescu* - Assessing the influence of hydrothermal synthesis temperature on rosmarinic acid loaded silica nanoparticles
- NMN\_P8.** *Delia Stefania Motoroiu, Alexandra Burdusel, Ecaterina Andronescu* - Controlled release systems based on montmorillonite
- NMN\_P9.** *Delia Stefania Motoroiu, Alexandra Burdusel, Ecaterina Andronescu* - Controlled release systems loaded with biologically active molecules

### ***Environmental Protection and Monitoring***

- EPM\_P1.** *Elena Petronela Bran, Daniela Nicuta, Luminita Grosu, Irina Claudia Alexa, Adriana Luminita Finaru* – Regional food by-products and waste as a potential source of bioactive compounds - *in vivo* and *in vitro* evaluation
- EPM\_P2.** *Magdalena Simona Fogorasi, Mihaela Dochia, Dorina Rodica Chambre, Michaela Dina Stanescu* – The influence of different enzymatic treatments on cotton dyeing
- EPM\_P3.** *Marinela Gancea, Mioara Costache, Cristiana Radulescu, Mariana Cristina Arcade, Alin Constantin Barbu, Sorin Marian Dragut, Ioana Daniela Dulama, Andreea Laura Banica, Ioan Alin Bucurica* – Climate change implication on fish habitats in ponds and risk related to ecosystem health
- EPM\_P4.** *Roxana Ioana Matei, Irina Fierascu, Anda Maria Baroi, Toma Fistos, Ioana Silvia Hosu, Radu Claudiu Fierascu* – Evaluation of phosphatic materials efficiency for water remediation
- EPM\_P5.** *Maria Raluca Bucur (Popa), Cristiana Radulescu, Raluca Maria Stirbescu, Ioana Daniela Dulama, Ioan Alin Bucurica, Sorina Geanina Stanescu* – Isolation and identification of microplastics in daily skin cream and lotion
- EPM\_P6.** *Anca Sandu Balan (Tabacariu), Oana Irina Patriciu, Ioana Adriana Stefanescu, Irina Loredana Ifrim, Adriana Luminita Finaru* – *Sambucus nigra* L.: A source of bioactive compounds with antifungal effects
- EPM\_P7.** *Cristiana Radulescu, Ioana Daniela Dulama, Claudia Stihă, Andreea Laura Banica* – Impact of past mining activity on the quality of surface and groundwater resources

## POSTER SESSION 2

### Organic, Bioorganic, and Food Chemistry

- OBFC\_P1.** *Mihaela Balan-Porcarasu* – NMR strategies for elucidating chemical modification mechanisms of cyclodextrins
- OBFC\_P2.** *Andreea Laura Banica, Cristiana Radulescu, Raluca Maria Stirbescu, Ioana Daniela Dulama, Ioan Alin Bucurica, Sorina Geanina Stanescu* – Isolation and identification of microplastics in milk – a potential health risk for children
- OBFC\_P3.** *Mariana Deleanu, Laura Toma, Gabriela Sanda, Anca V. Sima, Justinian Tomescu, Georgeta Alexandru, Camelia S. Stancu* – Preparation and characterization of hawthorn berries and grapes skin extracts; antioxidant and anti-inflammatory effects in endothelial cells
- OBFC\_P4.** *Mihai Deleanu, Mona Irina Doana, Alina Nicolescu, Petru Filip* - Generation of tert-butylcyanoketene from 2,5-diazido-3,6-di-tert-butyl-1,4-benzoquinone. The old story reinvestigated
- OBFC\_P5.** *Alina Nicolescu, Florentina Georgescu, Emilian Georgescu, Florea Dumitrascu, Marcel M. Popa, Calin Deleanu* – Synthesis of new potentially bioactive carbamoyl substituted pyrrolo [2,1-a]isoquinolines
- OBFC\_P6.** *Svetlana Blaja, Crina Vicol, Lidia Lungu, Alexandru Ciocarlan, Aculina Aricu* – Antioxidant activity of local lavender, clary sage and coriander essential oils
- OBFC\_P7.** *Bradut – Bogdan Minea, Cristiana Radulescu* – Quantitative screening method for pesticide residues in citrus using gas chromatography-tandem mass spectrometry
- OBFC\_P8.** *Ana-Maria Mocanu, Marius Sorin Avramescu, Andreea Veronica Botezatu, Bianca Furdui, Rodica Mihaela Dinica, Geta Cârâc* – Electrochemical evaluation of antioxidant capacity of *Perrilla* extracts
- OBFC\_P9.** *Alina Nicolescu, Natalia Usurelu, Daniela Blanița, Mihaela Balan-Porcarasu, Sergiu Gladun, Calin Deleanu* – Methylmalonic aciduria diagnosed by NMR spectroscopy
- OBFC\_P10.** *Alina Nicolescu, Natalia Usurelu, Victoria Hlistun, Gabriela Liliana Ailiesei, Calin Deleanu* – Galactosemia monitored by NMR spectroscopy
- OBFC\_P11.** *Ana-Maria Mocanu, Marius Sorin Avramescu, Andreea Veronica Botezatu, Bianca Furdui, Rodica Mihaela Dinică, Geta Cârâc* – Electrochemical evaluation of antioxidant capacity of *Perilla* extracts
- OBFC\_P12.** *Natalia Birca, Adina Organ, Vladilena Girbu, Alic Barba, Alina Nicolescu, Calin Deleanu, Veaceslav Kulciti* – Simultaneous quantitative determination of rosmarinic, oleanolic and ursolic acids in *Salvia glutinosa* extracts by QNMR spectroscopy
- OBFC\_P13.** *Mihaela Nechifor (Tudorache), Cristiana Radulescu, Radu Lucian Olteanu, Claudia Lavinia Buruleanu* – Phenolic profiles and antioxidant activity of grape pomaces from Fetească Albă and Tămâioasă Românească varieties
- OBFC\_P14.** *Maria Daniela (Ionica) Mihaila, Fănică Bălănescu, Andreea-Veronica Botezatu, Marius Vasile Bardan, Bianca Furdui, Rodica-Mihaela Dinica* – Phytochemical investigation of *Iris pseudacorus* extracts by HPTLC

- OBFC\_P15.** *Alexandru Ciocarlan, Lidia Lungu, Svetlana Blaja, Ion Dragalin, Lucian Lupascu, Tatiana Calugaru-Spataru, Zinaida Balmus, Violeta Popescu, Aculina Aricu* – Chemical composition and antimicrobial activity assessment of absolute from different rose (*Rosa damascena* mill.) cultivars
- OBFC\_P16.** *Alexandra-Mariana Ionescu, Rodica-Mihaela Dinica, Andreea-Veronica Botezatu, Bianca Furdui, Alina-Viorica Iancu, Costel Vinatoru, Fernanda Marujo Marques, Maria Paula Cabral Campello* – Evaluation of the biological activity of some vegetable extracts containing neuroprotective chemical compounds
- OBFC\_P17.** *Alina Nicolescu, Natalia Usurelu, Chiril Boiciuc, Ana-Maria Macsim, Calin Deleanu* – Glutaric aciduria diagnosed by NMR spectroscopy
- OBFC\_P18.** *Ana-Maria Mocanu, Andreea Veronica Botezatu-Dediu, Alexandra Mariana Ionescu, Bianca Furdui, Fernanda Marujo Marques, Maria Paula Cabral Campello, Sorin Marius Avramescu, Rodica Mihaela Dinica* – Deep eutectic solvents as advantageous extractants for enhancement of antimicrobial activity and anti-inflammatory potential of *Perilla frutescens* L. britt. extracts
- OBFC\_P19.** *Cyril Nicolay, Ion Grosu, Niculina D. Hadade* – New ethidium bromide based ruberry organic frameworks as anion exchange membranes
- OBFC\_P20.** *Elena-Mirela Suceveanu, Irina-Loredana Ifrim* - Strategies to improve Melomel production
- OBFC\_P21.** *Bianca Vasile (Stoean), Maria Lehene, Radu Silaghi-Dumitrescu, Luiza Gaina* – Development and characterization of new platinum(IV) complexes with carboxylic or phenolic ligands: Synthesis, structural insights, and computational studies

## BIO-INSPIRED HYBRID 3D NANOARCHITECTURES FOR MULTIFUNCTIONAL APPLICATIONS

ION TIGINYANU<sup>1</sup>

Nowadays there is a strong demand for new multifunctional materials compatible with both electronics and living organisms. The main focus in this lecture will be on novel bioinspired hybrid nanomaterials characterized by high-surface-to-volume ratio – the so-called aeromaterials based on semiconductor compounds. In particular, we report on a novel three-dimensional nanoarchitecture of gallium nitride, called aero-GaN or Aerogalnite, which represents the first artificial material exhibiting dual hydrophobic-hydrophilic behavior (<https://en.wikipedia.org/wiki/Aerogalnite>). The 3D nanoarchitecture is based on GaN micro-tubular structures with nanoscopic thin walls, the inner surface being covered by an ultrathin film of zinc oxide. The micro-tubular structures are shown to self-organize when interacting with water, forming self-healing membranes characterized by high elasticity and cargo capabilities. The characteristics of the membranes resemble those inherent to a biological cell membrane. Aerogalnite-based self-propelled liquid marbles exhibiting rectilinear movement as well as stationary and pulsed rotations will be demonstrated. The properties of aero-GaN and liquid marbles will be presented in the context of prospects for their applications in photocatalysis, microfluidics, microelectronics, and biomedicine.

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## DESIGN OF A NEW GENERATION OF PHOTOSENSITIVE LIPOSOMES FOR THERAPEUTIC APPLICATIONS

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The clinical solutions involving light-triggered drug delivery systems (DDS) require the use of photosensitive chemicals that should be at least: (i) biocompatible; (ii) chemically and biologically stable and (iii) easy to integrate in the desired delivery system. If the general approach is to reprogram the “original role” of natural photosensitizers, our approach was different: to use a minimalist photosensitizer in the structure of phospholipids which could be transformed by light into natural molecules. Diazirine is one the smallest photosensitive moiety discovered to date, never exploited as a release trigger.

Guided by molecular dynamics, a photosensitive phospholipid was designed to mimic the self-assembling abilities of natural phospholipids. The diazirine-conjugated amphiphile was efficiently accessed in 5 steps by hem<sup>4</sup>i-synthesis from lyso-phospholipids coupled with a judiciously functionalized fatty acid. The nanoparticles obtained after formulation were characterized for their physico-chemical and biological properties, and investigated for their light-triggered cargo release abilities.

DLS, cryo-TEM, and solid-state NMR showed that this minimalist photosensitive moiety was successfully incorporated into the structure of photosensitive liposomes. In the absence of light: (i) diazirine blocks the diffusion of the cargo over at least 20 days (ii) decreases the transition temperature of the control phospholipids by 20°C. The release rate of the cargo can be easily modulated by light, from slow to fast release [1]. The diazirine-conjugated phospholipid has the same toxicity profile as the natural control phospholipid (DMPC) in the absence of light and generates natural phospholipids by light irradiation.

This new class of photosensitive phospholipids has great potential in drug delivery [2] as it solves many issues related to the current photosensitive DDS used in clinics today.

**Keywords:** liposomes; diazirine; triggered release.

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## VALORIZATION OF THE GRAPE SEEDS RESULTED IN THE WINE PRODUCTION PROCESS

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Climate changes imposed a new development policy. The UN Commission report “*Our Common Future*” emphasized the obligation to preserve the reserves of raw materials and fossil fuels for the next generations. The concept of sustainable development started to be implemented, and the Sustainable Development Goals (SDGs) were adopted by the member states of the UN for “*achieving peace and prosperity for both people and the planet*” [1]. A special concern was directed to waste valorization. Waste is now considered a source of energy and raw material, and the target is “*zero waste*”. Such policy ensures not only the sources for raw materials and energy but also pollution reduction [2]. The waste hierarchy was established, and its application was imposed by the legislation.



Waste is to be avoided wherever possible and unavoidable waste should be reused rather than landfilled or incinerated.

The wine production generates waste, such as grape seeds (~ 22%) which contain: oil, antioxidants, and cellulosic materials. Thus, extraction and valorization of these components are mandatory. The results obtained in this respect are presented [3-5]. These results confirm the necessity to treat the grape seeds not as a disposable waste but as a source of valuable products.

**Keywords:** sustainable development; waste valorization; grape seeds.

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## CATALYTIC APPLICATIONS OF MULTICATIONIC LAYERED DOUBLE HYDROXIDE-BASED MATERIALS

IOAN CEZAR MARCU<sup>1</sup>

Layered double hydroxides (LDH) are anionic clays having the general formula  $[(M^{2+})_{1-x}(M^{3+})_x(OH)_2]^{x+}(A^{n-})_{x/n} \cdot mH_2O$  with  $0.2 \leq x \leq 0.4$ .<sup>[1]</sup>  $M^{2+}$  and  $M^{3+}$  are bivalent and trivalent cations, respectively, with ionic radii not too different from that of  $Mg^{2+}$  [2]. They are hexa-coordinated to hydroxyl groups forming two-dimensional sheets of edge-sharing octahedra, which stack to generate a layered structure. Various inorganic or organic anions  $A^{n-}$  can be inserted between the layers to compensate the positive charge brought by the  $M^{3+}$  cations partially replacing  $M^{2+}$  cations in the brucite-like sheets [2]. Several cations can enter simultaneously in the layers, where they are homogeneously distributed and intimately mixed together, leading to multicationic LDH. Due to their structure, together with their compositional flexibility, the LDH possess versatile physicochemical properties, which make them excellent candidates as multifunctional nanostructured catalysts and catalyst precursors [1, 3].

A large variety of variable-valence cations can be introduced into the LDH structure, not only into the brucite-like layers but also into the inter-layer region as heteropolyanions and metal complexes [3]. Their redox properties, which can be enhanced in multicationic LDH via a synergistic interaction, determine the catalytic behavior of these materials in reactions involving redox mechanisms. They can be used as such, particularly in low-temperature liquid-phase organic transformations [1], or as mixed oxides obtained by their controlled calcination in high-temperature gas-phase processes [4]. Indeed, the thermal decomposition of the multicationic LDH leads to homogeneous mixed oxide structures with relatively high surface areas, good thermal stabilities, and tunable acid-base and redox properties, which make them very attractive catalytic materials [3,4].

Based on a number of selected examples from our research work, the remarkable behavior of transition-metal-containing multicationic ex-LDH mixed oxide catalysts in different processes such as bio-oil hydrodeoxygenation, ethanol conversion, light alkanes oxydehydrogenation, and methane total oxidation, will be highlighted and explained in correlation with their peculiar physicochemical characteristics.

**Keywords:** layered double hydroxides; multicationic mixed oxides; catalytic materials.

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## ROLE OF MODELS AND CHALLENGES IN THE INSTITUTIONAL DEVELOPMENT

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"Petru Poni" Institute of Macromolecular Chemistry was born on paper [1] in the difficult years after the Second World War (1948), under a mobilizing motto - *PER ASPERA AD ASTRUM* - at the initiative of the Romanian Academy and a group of chemists - university professors. Since its beginnings, the Institute has benefited from the leadership of outstanding personalities, characterized by a deep sense of humanity associated with managerial talent.

Starting with topics on coordination chemistry and valorization of some vegetable raw materials, the Institute's research interests evolved along the years towards macromolecular chemistry, polymer technology, and material science, following "hot" international trends and balancing basic and applied research activity [2]. Today, polymeric (nano)(bio)materials (dielectric elastomers, metal-organic frameworks, porous functional composites, self-healing, self-cleaning, superhydrophobic, multistimuli responsive materials, nonviral vectors, drug delivery systems, sorbents, coatings, membranes) with properties, tailored by design are studied, benefiting of the modern infrastructure recently secured by several dedicated projects. With a highly qualified, hard-working, and equilibrated on age and experienced staff, an exceptional research infrastructure, a last five years portfolio of more than 1340 papers (85% in Q1/Q2 journals) internationally cited research papers, 17 books/118 book chapters, over 38 patents, the Institute is proud to announce its classification in 2023 by international evaluation [3] on the second position as a research institute in Romania and in category I, following the institutional evaluation realized by the Romanian Academy. The Doctoral School of Chemical Science of SCOSAAR is specializing yearly around 40 young people especially in the synthesis, and characterization of new macromolecular compounds, aiming to obtain advanced materials for different applications.

The presentation deals with the development of the Institute over the years, as influenced by our mentors and by the historical or actual challenges the Institute was/is facing, as well as with its answers to socio-economic demands.

**Keywords:** guidance/mentoring; tradition/modernism; challenges; institutional development.

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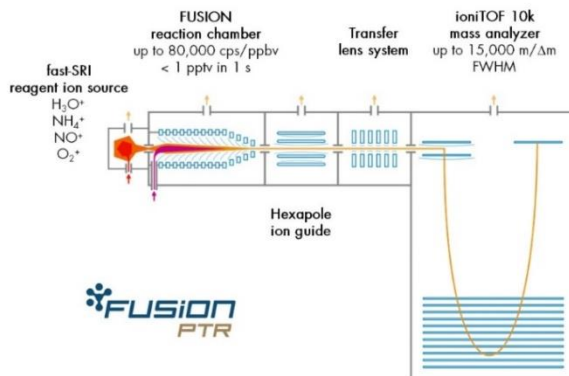
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## PTR-MS: BASICS, APPLICATIONS, AND RECENT TECHNOLOGICAL ADVANCEMENTS

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ANDREAS MAURACHER<sup>1</sup>, RENE GUTMANN<sup>1</sup>, ALFONS JORDAN<sup>1</sup>

Proton-Transfer-Reaction - Mass Spectrometry (PTR-MS) is a well-established real-time trace gas analysis technology utilized in environmental research, atmospheric chemistry, food and flavor research, medical sciences, cleanroom monitoring, etc. [1].

Here, we present the scientific basics of PTR-MS, give an overview of exciting fields of application, and introduce some of the latest technological advances. One example of the latter is the FUSION PTR-TOF 10k [2]; compare figure) equipped with a novel reagent ion source enabling reagent ion switching in 1-2 s and a redesigned reaction chamber for the highest sensitivities and sub-pptv detection limits within 1 s. To demonstrate that these performance values are not just numbers in a spec-sheet but open up new analytical worlds that were previously inaccessible, we present, results of nose-space measurements during the consumption of food. For this highly complex matrix (mixture of endogenous compounds + room air + food constituents and metabolites) common PTR-MS devices often fail because of limited selectivity and sensitivity. With the FUSION PTR-TOF 10k up to 9 isobaric molecules can be clearly separated for one nominal  $m/z$ , e.g. during the consumption of chocolate or truffle products, and compounds can still be detected in the nose-space after 20 exhalations, e.g. onion aroma after the consumption of only one sip of chicken soup.



**Keywords:** PTR-MS; real-time; VOCs; PTR-TOF; high sensitivity.

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## RAPID DETERMINATION OF ACRYLAMIDE IN PROCESSED FOODS USING ADVANCED LC-MS/MS TECHNIQUES

ROBERT I. BOTE<sup>1</sup>, IONUT MELINTE<sup>1</sup>, IRINA SCARLAT<sup>1</sup>

Acrylamide is a highly polar, water-soluble compound that forms during high-temperature cooking and is present in many everyday foodstuffs. It has been classified as a Group 2A carcinogen by the International Agency for Research on Cancer (IARC) [1]. As a result, there is a significant health concern, particularly for children who are more exposed to acrylamide on a body weight basis [2]. This study aims to develop and validate a rapid and cost-effective LC-MS/MS method for quantifying acrylamide in various processed foods.

The study utilized the ACQUITY UPLC I-Class System coupled with the Xevo TQ-S micro Tandem Quadrupole Mass Spectrometer. Homogenized food samples were extracted using a modified QuEChERS Acrylamide Starter Kit. An isotopically labeled internal standard (Acrylamide-d<sub>3</sub>) was added to correct for variability during extraction, clean-up, and analysis. Performance was assessed using the criteria from Commission Regulation (EU) 2017/2158, evaluating trueness and precision with spiked samples and FAPAS test materials as reference materials.

The method demonstrated excellent performance, with trueness and precision meeting the required standards. Calibration standards prepared over a range of 0.5 to 2500 ng/mL showed coefficients of determination ( $r^2 > 0.999$ ) and residuals (<10%), confirming the method's accuracy. The use of acrylamide-d<sub>3</sub> as an internal standard improved the method's accuracy and repeatability, with measured recoveries within the 86%-107% range and repeatability between 1.6% and 5.5%.

The ACQUITY UPLC HSS C18 SB Column provided excellent retention and peak shape for acrylamide, with optimized LC-MS/MS conditions offering superior sensitivity and selectivity. The method also proved to be effective across various matrices, including challenging ones like potato chips and coffee, with minimal interference. The method is applicable for checking compliance with EU benchmark levels and has potential for due diligence testing at lower concentrations.

The study successfully developed a robust, sensitive, and reproducible LC-MS/MS method for determining acrylamide in processed foods, meeting all performance criteria outlined by EU regulations. This method can be a valuable tool for food safety management and regulatory compliance.

**Keywords:** Acrylamide; LC-MS/MS; food safety; method validation; UPLC.

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## FUNDAMENTALS AND APPLICATIONS OF AMPHIPHILIC JANUS NANOPARTICLES

ANDREI HONCIUC<sup>1</sup>

Janus nanoparticles (JNPs), named after the two-faced Roman deity Janus, are a class of nanomaterials characterized by their dual-faced structure, where each side possesses distinct physical or chemical properties. A typical Janus nanoparticle consists of two distinct lobes resembling a snowman or a dumbbell shape. This unique asymmetry allows JNPs to be multifunctional, making them highly versatile for a wide range of applications. Typically, polymeric JNPs can be synthesized via seeded emulsion polymerization.

This work highlights the ability of JNPs to self-assemble into supra-structures, such as micelles, capsules, and giant vesicles, demonstrating that amphiphilicity is a scalable property. A further consequence of amphiphilicity is that JNPs can stabilize foams and Pickering emulsions. In foam lamellae, the JNPs self-assemble into double-layered highly organized membranes. Their ability to self-assemble makes them useful in designing advanced reconfigurable materials [1].

Thanks to their architecture, JNPs possess the unique ability to couple form and function. By adjusting the relative ratio between the Janus lobes with distinct compositions, the overall particle properties can be gradually varied. This is particularly useful because the properties can be tuned without chemical modifications but rather through changes in particle morphology. This is especially advantageous in electronics. For example, JNPs that are semiconducting on one lobe and electrically insulating on the other lobe [1, 2] have been obtained. Further, by varying the relative lobe sizes, the overall conductivity and dielectric properties of the JNPs can be tuned without altering the molecular structure, which makes them extremely valuable as pigments for printed circuits. This work highlights several major avenues in which JNPs can be applied as truly innovative materials, showcasing their versatile potential across various fields.

**Keywords:** Janus nanoparticles; amphiphiles; self-assembly; Pickering emulsions; organic electronics.

**Acknowledgements:** *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, project number PN-III-P4-PCE-2021-0306 (Contract Nr. PCE62/2022).*

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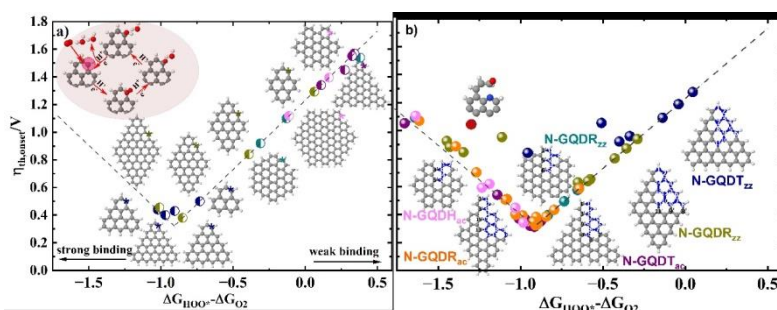
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## EXPLORING THE ACTIVITY OF THE GRAPHENE QUANTUM DOTS (GQDs) FOR THE ELECTROCHEMICAL OXYGEN REDUCTION REACTION USING DFT

ISABELA COSTINELA MAN<sup>1\*</sup>, RALUCA IOANA JALBA<sup>1</sup>, DRAGOS LUCIAN ISAC<sup>1,2</sup>, YUHENG ZHAO<sup>3</sup>, IONUT TRANCA<sup>3</sup>

The study was carried out in the context of ongoing research aimed at discovering more effective catalysts for the oxygen reduction reaction (ORR) in PEM fuel cells such as to replace the best-performing one, Pt which is scarce and expensive. Graphene quantum dots (GQDs) are gaining attention for this application, due to low dimensionality, abundance in edge sites, and quantum confinement [1]. In this study we investigate at the theoretical level using density functional theory (DFT), the possible activities towards ORR of undoped and N-doped GQDs of various shapes (triangular, rhombohedral, hexagonal) and sizes (C13-C114) with zigzag and armchair terminations under the effect of the implicit water model as implemented in GPAW software. For the undoped ones, the edges of the triangular and the largest rhombohedral shapes with zigzag terminations present the highest potential activities (predicted low onset overpotentials ( $\eta_{th,onset}$ ) blue and dark yellow points in Figure 1a) [2]. For the other shapes, we predict low activities, especially for the armchair terminated ones (purple, pink, cyan points – Figure 1a). For the N-doped structures, an inversion of the activity is observed (Figure 1b). Structural changes in some of the N-doped structures take place when O\* moiety is formed during the reaction (red point in Figure 1a). A correlation between the strength of adsorption and the p electronic states of the carbon sites was established.



**Figure 1** Theoretical onset overpotential ( $\eta_{th,onset}$ ) on a) edges of undoped-GQDs b) N-GQDs

**Keywords:** DFT; ORR; GQD; N-GQD; fuel cell.

**Acknowledgements:** This work is supported by UEFISCDI, the project PN-III-P1-1.1-TE-2021-0931 and by L'Oréal Women in Science fellowship.

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## ORGANOCHALCOGEN COMPOUNDS AND THEIR METAL COMPLEXES. SYNTHESIS, STRUCTURE AND POTENTIAL APPLICATIONS

ANCA SILVESTRU<sup>1</sup>

Organoselenium compounds continue to attract a significant interest as valuable candidates in medicinal chemistry [1], catalysis and organic synthesis [2], or as key species for optoelectronic devices [3]. A special attention was paid during last years to derivatives bearing organic groups with nitrogen or oxygen donor atoms, showing an increased thermal and hydrolytic stability and enhanced specific properties.

Our recent studies were focused on new classes of diorganodichalcogenides or homo- and heteroleptic diorganochalcogen(II) compounds bearing organic groups with N or O donor atoms, as well as on their main group or late *d* metal complexes [4, 5].

We report here about compounds of type  $R_2Se_2$  and  $R^1R^2E$  ( $E = S, Se$ ), where  $R^1, R^2 = 2-XC_6H_4CH_2$  ( $X = Br, Me, Ph_2Sb$ ),  $2-(R_2NCH_2)C_6H_4$  [ $R = Me, Et; R_2 = (CH_2CH_2)_2O$ ],  $CH_2CH_2pz$  ( $pz = pyrazole$ ),  $CH_2Phtz$  ( $Phtz = phenylthiazole$ ), as well as upon several pyridine based derivatives bearing pendant arms with donor atoms.

Their coordination behavior towards Sn, Cu and Ag was investigated both in solution and in solid state. Selected compounds were studied for their antiproliferative activity or for their optical properties.

**Keywords:** diorganochalcogenides; metal complexes; solution behaviour; solid-state structure.

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**SYNERGY BETWEEN COMPUTATIONS AND EXPERIMENTS ON  
TRANSITION METAL COMPLEXES: CHALLENGES WITH  
ISOMERISM, SPIN STATES AND SPECTROSCOPY**

RADU SILAGHI-DUMITRESCU<sup>1</sup>

For relatively large bioinorganic centers, such as hemes, vitamin B<sub>12</sub>, or the FeMoCo iron-sulfur-molybdenum cluster of nitrogenase, computational chemistry may be an obligate addition to experimental methods – especially when investigating short-lived species such as catalytic cycle intermediates. However, the large size of these systems, together with the gaps in experimental knowledge regarding their structure/purity/properties, make it particularly challenging to (1) apply accurate computational methods and (2) expect an accurate experimental benchmark. Nevertheless, a good number of reports will still claim excellent experiment-theory agreement and will thereby confuse anyone approaching the field from the outside.

Case studies will be presented, all centered around efforts to unravel the reactivity of bioinorganic transition metal centers towards small molecules, such as the non-heme iron enzyme superoxide reductase, the ferryl Compound II species of heme proteins (globins, peroxidases, cytochromes P450, catalase etc), the heme-iron-sulfur center of sulfite reductase, and the peroxide complex of cobalamin (vitamin B<sub>12</sub>).

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## NOVEL ORGANOTIN(IV) ALKOXIDES – FROM SYNTHESIS TO REACTIVITY

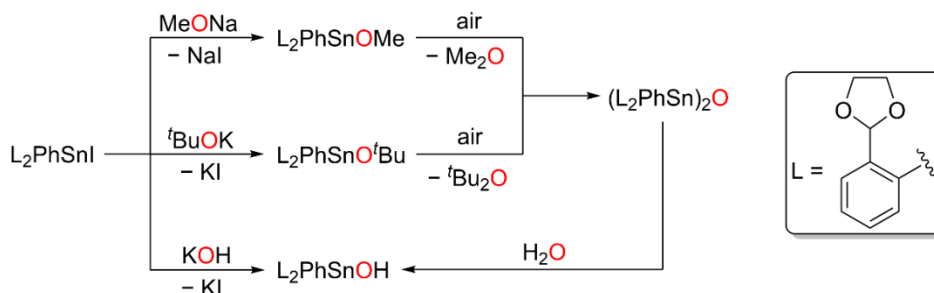
VLAD PENCIU<sup>1</sup>, ADRIAN ALEXANDRU SOMESAN<sup>1</sup>, RICHARD A. VARGA<sup>1</sup>

Organotin(IV) compounds containing Sn-OR bonds (alkoxides) or Sn-OSiR<sub>3</sub> bonds (siloxides) have mostly been studied in the last decades, and they are known for their biological activity [1], as well as precursors for hybrid organic-inorganic materials [2]. Examples of such derivatives are scarce, and their reactivity was less investigated compared to that of their Sn(II) analogs.

Organotin(IV) alkoxides and/or siloxides are generally obtained reacting an organotin(IV) halide with an alkali-metal alkoxide. Other procedures describe trans-alcoholysis reactions[3] or the reaction of tin(IV) amides with lactides, following a ring opening mechanism [4].

Our group developed a series of organotin(IV) species starting from the 2-[(CH<sub>2</sub>O)<sub>2</sub>CH]C<sub>6</sub>H<sub>4</sub> moiety, with a protected carbonyl function that could be easily converted into a Schiff base or a carboxylic acid. Additionally, this also acts as a C, O-chelating ligand increasing the coordination number of the tin center and the stability of the final complex.

In this work we present the results obtained on the synthesis, characterization, and reactivity of different organotin(IV) alkoxides and siloxides towards CO<sub>2</sub>, as well as their hydrolysis products.



**Figure 1.** Synthesis of organotin(IV) alkoxides and their decomposition products.

**Keywords:** organotin(IV) alkoxides; <sup>119</sup>Sn NMR; siloxides; CO<sub>2</sub> activation.

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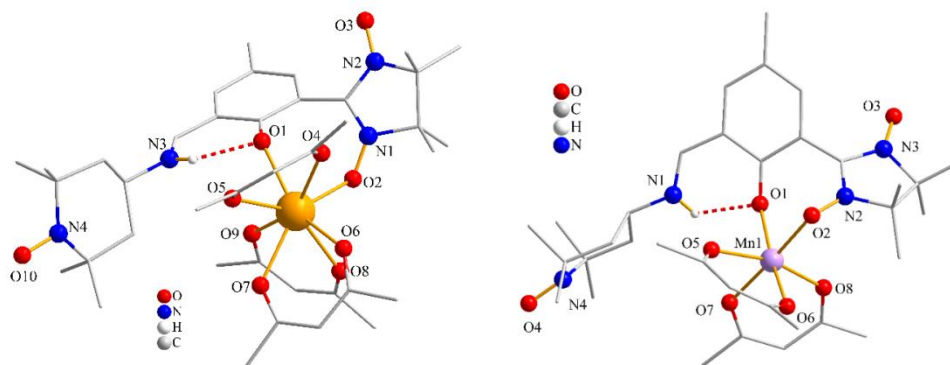
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## FROM NITRONYL NITROXIDES TOWARDS HOMO- AND HETERO-DI-RADICALS USED AS LIGANDS FOR THE SYNTHESIS OF 3d AND 4f COMPLEXES

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Paramagnetic ligands containing two identical or different radical moieties ( $S = 1$ ) play an important role in molecular magnetism [1-3]. The nitronyl nitroxide, 2-(2-hydroxy-3-formyl-5-methylphenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-oxyl 3-oxide (HL), due to its available carbonyl unit, was used to generate homo- and hetero-di-radicals via Schiff condensation. For example, HL was condensed with 1,3-diaminopropane and 4-amino-TEMPO to generate the paramagnetic ligands  $H_2L^1$  and  $HL^2$ . Both ligands have been reacted with hexafluoroacetylacetonato complexes of 3d and 4f metal ions generating mono- (Figure 1), and dinuclear complexes with different spin topologies. Their similarities and differences have been investigated. The (pseudo-)polymorphism is present in the case of  $[M(HL^2)(hfac)_2]$ , where  $M = Mn, Co, Ni, Zn$ , and  $[Yb_2(H_2L^1)(hfac)_6]$ . The crystal structure of  $[Ni(HL^2)(hfac)_2]$  presents channels with a 1 nm diameter.



**Figure 1** Perspective views of the crystal structures of  $[Gd(HL^2)(hfac)_3]$  (left) and  $[Mn(HL^2)(hfac)_2]$  (right). A part of the hydrogen atoms and all fluorine atoms were removed for clarity.

**Keywords:** nitronyl nitroxide; paramagnetic ligand; magnetism; organic radical.

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## MULTI-REFERENTIAL RELATIVE KINETIC METHODS VERSUS PSEUDO-FIRST METHOD FOR ASSESSING THE GAS-PHASE OZONOLYSIS OF UNSATURATED VOLATILES IN ENVIRONMENTAL SCIENCES

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ROMEO IULIAN OLARIU<sup>1,2,3\*</sup>

Ozonolysis plays a significant role in the removal of anthropogenic and biogenic unsaturated volatile compounds from the atmosphere. The accurate measurement of the gas-phase reaction rate coefficients of ozone with such compounds is crucial for quantifying the products and secondary organic aerosol precursors, assessing the atmospheric global budget and distribution of OH radicals, and evaluating the tropospheric photochemical ozone production [1]. The current kinetic databases exhibit high uncertainties in the reaction rate coefficients due to a lack of data regarding ozonolysis reactions [2]. The objective of this study is to present, compare, and discuss the advantages and disadvantages of employing the multi-referential relative kinetic methods in experimental settings, in contrast to the absolute pseudo-first order method. This study emphasizes the various methods for mitigating interferences resulting from the secondary chemistry of the OH radicals generated during ozonolysis. Experimental laboratory investigations were performed using the 760 L Environmental Simulation Chamber made of quartz from the "Alexandru Ioan Cuza" University of Iasi (ESC-Q-UAIC) and the long-path absorption FTIR spectroscopy technique. The findings presented in this study will enhance our comprehension of the physicochemical processes of unsaturated volatiles within the lower atmospheric system.

**Keywords:** ozonolysis, OH interferences, FTIR spectroscopy, atmospheric chemistry.

**Acknowledgments:** The authors acknowledge the PN-III-P4-PCE2021-0673 (ATMO-SOS) and PN-III-P2-2.1-PED2021-4119 (SOA-REACTOR) UEFISCDI project. The authors UEFISCDI project, MySMIS no. 127324 grant - RECENT AIR and the European Commission under the Horizon 2020 – Research and Innovation Framework Programme, H2020-INFRAIA-2020-1, ATMO-ACCESS Grant Agreement number: 101008004 for their support.

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## SUPRAMOLECULAR ORGANIC SEMICONDUCTORS: RECENT ADVANCES AND PERSPECTIVES FOR OPTOELECTRONICS

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Organic semiconducting materials have attracted considerable interest, owing to their potential as next-generation organic electronic devices [1]. Despite the great potential of these materials, many aspects remain poorly understood, especially their strong tendency to aggregate which results in diminished photophysical and transport properties. In the past decade, the field of polymer science has witnessed remarkable innovations and progress, alongside major advances in the complementary field of supramolecular science, which has produced a variety of supramolecular architectures with unprecedented properties and performance [2]. The threading of macrocyclic molecules (hosts) onto the conjugated chains (guests) does not disrupt the  $\pi$ -conjugation and can additionally improve the solubility, as well as the photophysical and transport properties of these encapsulated semiconductor materials [2-4].

Recently published supramolecular compounds obtained by our research group based on polyfluorene, polyazomethines, and poly(3,4-ethylenedioxythiophene) that have been included into cucurbit[7]uril, native and permofified  $\beta$ - or  $\gamma$ -cyclodextrins host molecules will be discussed. These results have shown the beneficial effect of encapsulation resulting in diminished interchain interactions and packing in insulated molecular wires. Subsequently, recent achievements obtained by exploiting these supramolecular materials in optoelectronics will be highlighted. These findings will provide clear information about improvements of the photophysical and transport properties of such encapsulated compounds, relevant to applications where the prevention of luminescence quenching without hindering charge transport is essential.

**Keywords:** Host-guest complexes; luminescence; energy gaps; photovoltaic; biomimetic ionic channels.

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## APPROACHES TOWARDS SMART AND SUSTAINABLE SILICONES

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The versatility of silicone materials makes them valuable across diverse applications, ranging from medicine and healthcare to the food industry, textiles, construction, electrical and electronics, as well as automotive and aerospace. Their chemical stability, resistance to environmental conditions, and extreme temperatures, along with exceptional mechanical and dielectric properties, enhance both their performance and that of integrated products. Traditionally, silicones, whether in the form of rubbers, resins, oils, or greases, have played passive roles such as support, protection, sealing, bonding, lubrication, and electrical insulation.

Recent research has expanded the potential of silicones by exploring them as active, smart materials capable of responding to mechanical and electrical stimuli. They are now being investigated as dielectric elastomers for electromechanical transducers, including sensors, actuators, and capacitors. These properties can be tailored through chemical modifications, such as introducing suitable polar or functional groups, utilizing both silicone-specific and organic chemistry reactions, or through physical modifications like incorporating active nanofillers or interpenetrating with other polymers. Additionally, responsiveness to other stimuli (optical, magnetic, thermal, etc.) is feasible in fully silicone-based materials or those where silicone functions as a matrix or structural motif.

Furthermore, in response to the growing demand for reducing the environmental impact of synthetic polymers, new solutions are being developed that incorporate the principles of sustainability and the circular economy, including in silicone technology. These innovations include supramolecular cross-linked silicone materials that are thermoplastic or solvent-processable. They offer adjustable properties, dynamic responses to environmental changes, and self-healing capabilities. Consequently, they not only provide a more eco-friendly alternative to traditional methods of recycling thermosetting silicones but also ensure superior performance in critical applications.

Several initiatives and achievements in these areas are presented and critically analyzed.

**Keywords:** silicones; dielectric elastomers; supramolecular crosslinking; self-healing; sustainability.

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## INDOOR RADON MEASUREMENT IN LABORATORIES OF A UNIVERSITY

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Indoor air quality in public buildings is of particular importance, especially in homes, offices, schools or universities, where people spend more than half of their time. Therefore, the measurement of radon, a noble indoor radioactive gas, is crucial, as both the World Health Organization and the International Agency for Research on Cancer have identified radon as a first-order human carcinogen. This work aims to monitor radon concentration in five laboratories of a university in Romania. In the rooms selected for this study, both professors and students work, and some of them store ionizing radiation sources. The main source of radon inside the buildings is the soil from which radon is constantly released. Building materials are also an important source of radon. Radon concentrations inside buildings are measured using Airthings Wave smart detectors measurements were carried out between October 2020 and April 2021 and show that radon concentrations range between 28 Bq/m<sup>3</sup> and 120 Bq/m<sup>3</sup>, with an average of 40 Bq/m<sup>3</sup>. The imposed maximum level of 300 Bq/m<sup>3</sup> was never exceeded. In one laboratory the radon activity concentration reached higher values up to 120 Bq/m<sup>3</sup>. The obtained data revealed a low risk in terms of radon exposure for students, while for teachers, who spend significantly more time inside the laboratories, it is recommended to wear a respiratory protection mask and to limit the exposure time when handling neutron-irradiated samples.

**Keywords:** radon, radioactivity, air quality, monitoring.

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## NEW TECHNOLOGIES FOR ENVIRONMENTAL MONITORING

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Nowadays Environmental Monitoring became an important tool to study environmental conditions and trends, offering information to explain climate changes, to develop government policies as support of health people. As technology is evolving very fast, it allows us to gather accurate information, very useful for more and more pollutants detection and further to allow taking the proper steps to decrease the concentration of specific pollutants and at the end to improve the life quality.

Tehnoinstrument is an engineering company with significant experience in the market (since 1997) offering equipment and solutions for Environmental Monitoring. The presentation will contain a few technologies, and the latest innovations developed by our partners such as:

- Integrated systems for air quality monitoring- mobile and stationary stations containing pollutants analyzers: PM<sub>10</sub>, PM<sub>2.5</sub>, NO<sub>2</sub>, O<sub>3</sub>, NH<sub>3</sub>, CO, CO<sub>2</sub>, SO<sub>2</sub>, H<sub>2</sub>S, ultrafine particles (UFP), portable chromatographs, and so on;
- Greenhouse gases analyser: CO<sub>2</sub>, CH<sub>4</sub>, O<sub>3</sub>, N<sub>2</sub>O; next generation of mobile survey of CH<sub>4</sub> emissions;
- Last Technologies for Elemental Black-Carbon-Monitoring – Per unit of mass, black carbon has a warming impact on climate that is 460-1500 times stronger than that of CO<sub>2</sub>, which makes its monitoring and mitigation important for early reductions in current global warming predictions;
- Water analyzer and remote sensing networks – new technologies dedicated to research studies for chemical, physical, and biological parameters in rivers, lakes, and groundwater;
- Sampling systems for air and water quality measurements.

**Keywords:** environmental monitoring; analytical technologies; integrated systems for air and water monitoring.

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**ASSESSMENT OF REPRODUCIBILITY IN NMR METABOLOMICS**

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Metabolomics has become an important topic in a wide range of scientific areas, including medicine, pharmacology, nutrition and metabolism, food sciences, and environmental research. As metabolomics requires the processing of large numbers of multiple parameters, the reproducibility of data for statistical purposes is a key issue. Recent studies have shown impressive interlaboratory reproducibility of NMR spectra, but such studies involved trained personnel and standardized solutions [1, 2]. The present study aims to expand our preliminary study [3], to evaluate the NMR reproducibility for metabolomics when combining both dedicated NMR solutions and multipurpose NMR equipment and to compare the reliability of NMR metabolomics data when involving both specialized NMR operators and chemistry users from outside the NMR group (including researchers and students). The present study expands the previous preliminary results with additional data and additional parameters, including the evaluation of a recently introduced Biobanking QC Package. The new study for interlaboratory assessment of NMR reproducibility involves two NMR instruments and is currently testing operators having different backgrounds and metabolomics expertise, belonging to several laboratories from both Romania and the Republic of Moldova. The results aim to estimate the expected reproducibility of data for our ongoing metabolomics research.

**Keywords:** NMR; metabolomics; reproducibility; quantitation.

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## MAGNESIUM SUPPLEMENTS AND THE BODY CLEARANCE OF THEIR ORGANIC LIGANDS. THE MAGNEROT CASE

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Magnesium is important in maintaining the healthy state of the organism as it contributes to keeping the heart rhythm and blood pressure in normal ranges as well as maintaining the bones strong. Recommended magnesium doses for adults are ranging between 300-450 mg/day [1]. There are currently several magnesium products available as food supplements or over-the-counter pharmaceuticals. These products include either magnesium alone as a metallic ion, or in combination with other ions like calcium and zinc. For human use, magnesium is conditioned either as inorganic salt (e.g. oxide, chloride, hydroxide, carbonate) or organic salts (e.g., citrate, orotate, lactate, aspartate) the organic ligands presumably enhancing the body's absorption. NMR metabolomics is an emerging field allowing the simultaneous identification and quantitation of several metabolites in biological fluids. We have previously applied this technique for both pharmacokinetic studies [2] and medical diagnosis [3, 4]. The present study describes pharmacokinetic results on the Magnerot supplement as followed by NMR metabolomics. Magnerot is a human dietary supplement in which the magnesium ion is bonded as orotate. Our findings show a total clearance of the organic ligand in 26 hours after a single dose of 1/3 of the daily recommended quantity of the medicine. We report on several pharmacokinetic studies with follow-up of orotate clearance after single doses of 33, 67, 100, and 133% of the daily recommended dose of Magnerot.

**Keywords:** NMR; metabolomics; orotate; magnesium; pharmacokinetics.

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## WATER PERMEATION ACROSS A SERIES OF IMINES - POTENTIAL ARTIFICIAL WATER CHANNELS

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MIHAIL BARBOIU<sup>1,2</sup>

Artificial water channels (AWCs) are synthetic transmembrane molecules developed based on the properties of Aquaporin proteins, designed to selectively and efficiently transport water across lipid bilayers [1-3]. AWCs commonly feature a core cavity that incorporates both hydrophilic and hydrophobic groups and has varying diameters that facilitate the passage of water. Additionally, they possess a hydrophobic shell that enables their insertion into lipid membranes and facilitate subsequent analysis of water transport [3]. When discussing the structure of channels, there are two main approaches to designing these systems: supramolecular channels, which can self-assemble from multiple molecular components to form AWC architectures spanning the bilayer, and unimolecular channels, which consist of a single molecular entity that can span the entire length of the bilayer [2-4]. Figure 1 illustrates an AWC, selectively transporting water over hydrated metal ions across lipid bilayers.

This study focuses on mechanochemical synthesis, structural characterization, and channel-like self-assembly within lipid bilayers of several imidazole-based imines featuring various alkyl chains. The investigation of their ability to transport water was assessed by the stopped-flow method to measure the compounds' net permeability in a lipid bilayer. Water and proton transport activities of the reported compounds through bilayer membranes were found to correlate with the length of the grafted alkyl chain. Enhanced water permeability observed for compounds with longer hydrophobic tails is most probable due to their favorable interaction with the bilayer membrane.

**Keywords:** artificial water channels; imines; water permeability; water transport.

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**Figure 1.** Representation of a self-assembled AWC selectively transporting water across a lipid bilayer.

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## STUDY OF THE IMPACT OF NITRITES FROM MEAT PREPARATIONS ON HEALTH

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Nitrites are added to the production of meat preparations to give them a red color or to preserve their red color. Nitrites can become toxic to the human body because they form nitrosamines with primary and secondary amines; nitrosamines have a known carcinogenic action. Nitrites are potentially toxic, especially for children, because they produce methemoglobin. An undesirable effect of nitrites is a vasodilator, with the release of blood pressure. This research aims to determine the nitrite content in 12 meat products (i.e., 3 pates, 6 salami, and 3 semi-preserved meat). The nitrites determination was performed with Peter-Griess reagent, by spectrophotometric method [1]. For this purpose, an aqueous extract from the studied meat preparations was used. The determinations were made in relation to a calibration line. It was found that all of them have a residual nitrite level higher than the maximum level allowed by the European legislative norms [2]. It has been noted that a quantity of meat preparations used at a meal, of 250 g, has a higher intake of nitrites than the recommended daily intake for an adult. It has been observed that if only these meat preparations were used in the case of a ketogenic diet, the maximum level of nitrites allowed daily for an adult would be greatly exceeded. In conclusion, it is necessary to monitor more closely the meat preparations in the trade in terms of nitrites content. Obviously, is necessary to explain to the population the issues regarding the consumption of these products.

**Keywords:** nitrites; meat preparations; health.

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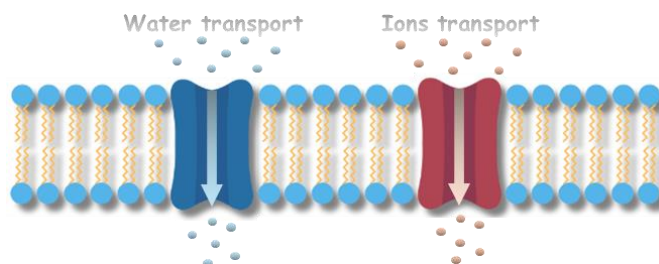
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## CREATING BILAYER MEMBRANE CHANNELS WITH RESPONSIVE MACROCYCLES

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One of the most challenging issues humanity faces nowadays is the lack of clean, potable water, a problem that worsens as the population grows [1]. In the last few years, membrane filtration processes such as reverse osmoses (RO) and nanofiltration (NF) have been intensively explored for water and waste-water treatment, nevertheless, this type of system remains rather expensive [2]. This determined researchers to focus on developing more efficient filtration membranes, by incorporating artificial water channels (AWC) in order to create low-energy process [3]. Artificial water channels are organic, self-assembled structures that mimic the function of aquaporins [4]. Moreover, similar structures can work selectively as ionophores, facilitating selective transport of ions through cell membranes, and can be used in technological and biomedical fields [5].

This work deals with the synthesis, structural characterization, and investigation of a series of organic macrocycles and cages used as transporters for water or selective ion transport. For the water transport experiments, we determined the net permeability of the compounds in a lipid bilayer by the stopped-flow method. In the case of ion transport we measured their activity intensity into the monodisperse unilamellar vesicles (LUVs) expressed as half maximal effective concentration ( $EC_{50}$ ) and Hill number.



**Keywords:** artificial water channels; ion transport; water transport; macrocycle; cage.

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## INFLUENCE OF SURFACE TREATED ASH POWDER ON THE PROPERTIES OF GLASS FIBER REINFORCED POLYPROPYLENE

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Glass fiber reinforced polypropylene is a regularly used composite in various industries due to its dimensional stability and increased stiffness [1]. To achieve the required mechanical properties high amounts of glass fibers are used (30-50%) which makes the recycling process more difficult. Studies evolved to reduce the glass fiber concentration in polymer composites and incorporate cheaper, low concentration nanofillers without affecting the general mechanical properties of the composites [2]. This research aims to investigate the effect of ash powder treated with three different agents on the properties of glass fiber-reinforced polypropylene. 30% glass fiber-reinforced polypropylene (PP-F) was used as the composite matrix. 3 treatment agents: a polyol (P), a fatty acid amide (S), and a silane (O) were used to treat the surface of ash powder (C) in dynamic conditions. Samples, with 25% glass fiber and 5% surface-treated ash, obtained through extrusion and injection molding were used for dynamic-mechanical (DMA), thermal (TGA and DSC), and nanomechanical characterization. Nanoindentation results show an increase in reduced modulus and hardness of 44-52% and 47-60%, respectively, for the ash-treated composites compared to PP-F. TGA analysis shows a higher weight loss for PP-F at the temperature of a maximum decomposition rate compared to PP-F-CP and PP-F-CS indicating better thermal stability for the ash-treated composites.

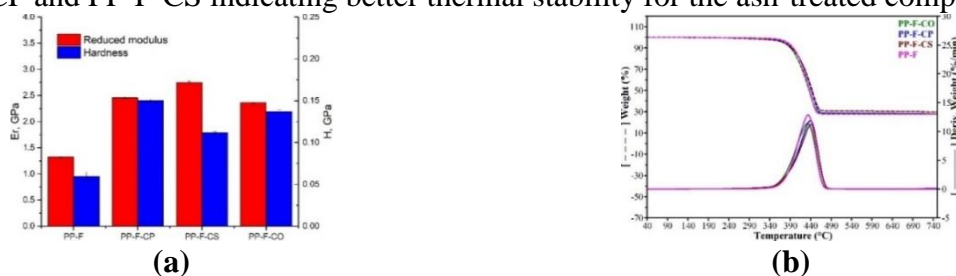


Figure 1. Properties of PP composites (a) Nanomechanical; (b) TGA and DTGA curves.

DSC analysis showed similar melting and crystallization temperatures between all samples. DMA analysis showed a slight decrease in storage modulus for PP-F-CP and PP-F-CS (0.03-1.5%) and higher for PP-F-CO (7%) compared to PP-F. In conclusion, composites based on PP reinforced with 25% glass fiber and 5% treated ash present improved properties being a viable alternative to composites based on PP reinforced with 30% glass fiber.

**Keywords:** polypropylene; glass fiber; treated ash powder; nanoindentation.

**Acknowledgments:** The authors gratefully acknowledge Core Program AQUAMAT no.23.06.01.01.03.

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## POLYPHENOLS ENCAPSULATED IN POLYMERIC MICROPARTICLES: ABSORPTION AND RELEASE PROPERTIES

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Polymeric microparticles obtained through Pickering emulsion polymerization technology (PEmPTech) [1] have unique structural and functional properties, which makes them suitable for use in applications across various fields. PEmPTech involves the stabilization of emulsions using Janus nanoparticles or pseudo-amphiphilic spherical nanoparticles [2], instead of traditional surfactants. The process begins with the creation of an oil-in-water emulsion, where the dispersed phase contains polymerizable monomers. Nanoparticles adsorb at the interface, providing stability and preventing coalescence. Polymerization of the monomers results in solid microspheres with a nanostructured surface due to the trapping of emulsion-stabilizing nanoparticles.

One of the primary applications of these polymeric microspheres is in the food industry and nutraceuticals as carriers for flavors, vitamins, and probiotics, and in the biomedical field can be utilized as drug delivery systems. The stability provided by nanoparticle-stabilized emulsions ensures prolonged shelf life and controlled release of encapsulated substances, enhancing the quality and nutritional value of food products and treatments.

In this work, novel polymeric microspheres were synthesized via the Pickering Emulsion Polymerization Technology (PEmPTech) method. Further, these microspheres were used for encapsulation of a natural polyphenolic compound extracted from *Brassica oleracea* L. var. *Capitata* f. *rubra*. Polyphenols are known for their important health benefits, such as antioxidant and antitumoral activity, protection against various diseases like diabetes, cardiovascular, or neurodegenerative illnesses [3]. However, their properties are often compromised by various environmental factors that lead to their degradation. Thus, it is crucial to encapsulate them in appropriate carriers to improve their photochemical, thermal, and oxidative stability. The newly designed microparticles have been studied in terms of their absorption/release properties for further applications in the human health industry.

**Keywords:** Pickering emulsions; microparticles; polyphenols.

**Acknowledgements:** *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, project number PN-III-P4-PCE-2021-0306 (Contract Nr. PCE62/2022).*

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## ELECTROGENERATED ProDOT-BASED POLYMERS FOR ENERGY STORAGE SMART WINDOW APPLICATIONS

ADRIANA PETRONELA CHIRIAC<sup>1</sup>, MARIANA DANA DAMACEANU<sup>1</sup>

Conducting polymers are studied as electrode material for electrochemical sensors and energy storage devices due to their excellent properties such as structure-driven conductivity, molecular flexibility, and easy coating. Among various conducting polymers, those based on 3,4-propylenedioxythiophene (ProDOT) have emerged as polymers with improved optoelectronic properties suitable for use in electrochromic devices, as well as electrode materials in supercapacitors [1], due to their ability to store electrical charges. Since derivatives based on thiophene have been scarcely studied as both electrochromic and capacitive materials [2], we considered of particular interest to focus on the development of two ProDOT-based polymers for use as electrode materials in energy storage smart window applications.

Among diverse synthetic strategies that are presently used to obtain polythiophenes, electrochemical polymerization is highly preferred due to some advantages, such as short reaction time and, simple, practical, and inexpensive way to generate desired surface structures on different substrates. To electrogenerate the polymers, a classical three-electrode electrochemical cell consisting of indium tin oxide-coated glass (ITO) as the working electrode, platinum wire as the auxiliary electrode, and Ag/AgCl as the reference electrode was used. The electropolymerization processes were performed with monomer solutions of 10 mM concentration, in different electrolyte systems.

Two polymers functionalized with hydroxy or aromatic ester group have been synthesized by electropolymerization reactions. The polymer structures were confirmed by ATR-FTIR spectroscopy and investigated by AFM to evaluate the film morphologies. A detailed study concerning their electrochromic properties and capacitive behavior was accomplished by cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), spectroelectrochemistry, and chronoamperometry measurements, to evidence their potential for use as active materials in energy storage smart windows. In the three-electrode cell configuration, these ProDOT-based polymers revealed the highest specific areal capacitance of 7.063 mF/cm<sup>2</sup> at a scan rate of 20 mV/s and 4.29 mF/cm<sup>2</sup> at 0.01 mA/cm<sup>2</sup>, in CV and GCD measurements, respectively. Meanwhile, they change the colour when pass from charge to discharge states.

Two ProDOT-based polymers were successfully prepared by electrochemical polymerization. Both polymers showed electrochromic behavior, with color change from purple or deep blue to highly transmissive blue/grey, being a promising material for use in energy storage smart window applications.

**Keywords:** conjugated polymers; ProDOT; electrochromism; energy storage.

**Acknowledgments:** *This work was supported by a grant of the Ministry of Research, Innovation, and Digitization, CNCS/CCCDI – UEFISCDI Romania, project no. PN-III-P4-PCE-2021-1728, contract no. 46/2022.*

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## MICROSPHERES OBTAINED FROM PICKERING EMULSION STABILIZED BY JANUS NANOPARTICLES AS ADSORBENTS OF METAL IONS FROM WATER

ANA MARIA SOLONARU<sup>1</sup>, ANDREI HONCIUC<sup>1</sup>, MIRELA HONCIUC<sup>1</sup>, OANA IULIANA NEGRU<sup>1</sup>

With the fast industrialization, agricultural expansion, and urban development, discharge pollution of water with heavy metals such as Cu(II), Cd(II), Hg(II), and Pb(II), poses a significant threat to terrestrial and aquatic environments, as well as for the human health. For these reasons, in this work, we employ the Pickering Emulsion Polymerization Technology (PEmPTech) [1, 2] which is a facile method for obtaining polymeric microsphere adsorbents, stabilized by different types of nanoparticles [3]. The adsorption capacity of these polymeric microspheres can be tuned by the type of nanoparticles used for stabilization of the emulsion. For this purpose, we emulsify a mixture of monomers containing vinyl groups in the presence of an initiator and in the presence of homogeneous or Janus nanoparticles to obtain Pickering emulsions, which can be polymerized. We obtain polymeric microspheres that exhibit a good adsorption capacity for various metal ions. Further, perform asymmetric chemical modifications and we explore the effect of different functional group on the surface of the Janus lobes on the adsorption capacity of the obtained microspheres. We thus demonstrate that the obtained materials can be employed as promising adsorbents for the removal of heavy metals from contaminated waters.

**Keywords:** nanoparticles; microspheres; Pickering Emulsion Polymerization; metal ion recovery; adsorption capacity.

**Acknowledgments:** *This work was supported by a grant of the Ministry of Research, Innovation, and Digitization of Romania, CNCS/CCCDI-UEFISCDI, project number PN-III-P4-PCE-2021-0306 (Contract Nr. PCE62/2022).*

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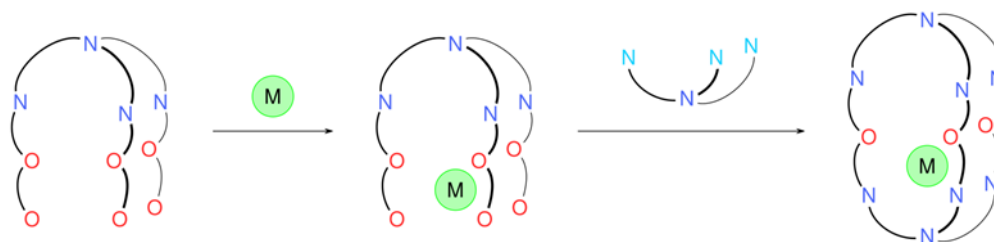


## DESIGN OF AN ORGANIC CAGE USING MANNICH AND SCHIFF REACTIONS

STEFAN DIMITRIU<sup>1,2</sup>, SERGIU SHOVA<sup>3</sup>, MIHAI RADUCA<sup>1,2</sup>, MARIUS ANDRUH<sup>1,2</sup>

Cage compounds feature captivating structures, considering their symmetry and complexity. They also present important applications, such as the template synthesis of nanoparticles, the stabilization of reactive molecules, molecular separations, and drug delivery systems. To synthesize an organic cage, rigid precursors, template agents or high dilutions can be employed.

An organic cage was obtained following two successive organic reactions - Mannich and Schiff. To prevent the formation of polymeric species, transition metal ions were involved as templates in the cage-closing Schiff step (Figure 1). This strategy was used in the literature for the synthesis of a macrocycle [1]. The structures of the new complexes were determined by single crystal X-ray diffraction measurements. The synthesis was successful with Mn<sup>2+</sup>, Co<sup>2+</sup>, and Ni<sup>2+</sup> ions, due to the octahedral geometry acquired, which locked the molecule in the tripod-like conformation. Cu<sup>2+</sup> ions couldn't be used to obtain the cage, due to their preference for a coordination number of 5.



**Figure 1.** The synthesis strategy of the cage compounds.

**Keywords:** transition metal complexes; organic cage; template synthesis.

**References:**

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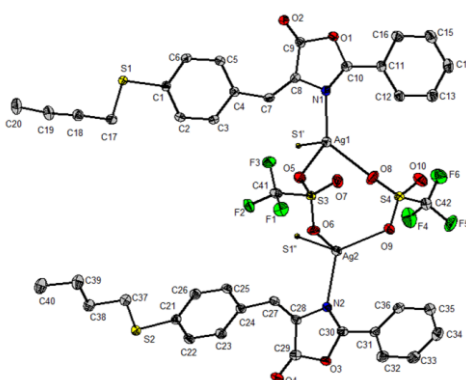
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## SILVER(I) COMPLEXES OF DIORGANOSULFUR LIGANDS BASED ON OXAZOL-5(4H)-ONE MOIETY

COSMINA BOHAN<sup>1</sup>, ALEXANDRA POP<sup>1</sup>

The coordination chemistry of potentially multidentate ligands drew an increased attention during the last years in relation with their transition metal complexes. The combination of *soft* (chalcogen) and *hard* (nitrogen, oxygen) donors leads to complexes with improved properties which make them appropriate for applications in materials science or biology [1]. Incorporating different donor atoms within the same ligand represents a challenge since various coordination patterns can be achieved.

In this context, we report the synthesis and structural characterization of several new heteroleptic diorganosulfur(II) species. The coordination behavior of (*n*-Bu) [4-{2-C<sub>6</sub>H<sub>5</sub>-(4*H*)-oxazol-5-one}CHC<sub>6</sub>H<sub>4</sub>]S was investigated towards silver(I) salts (Figure 1). The obtained silver complexes were characterized in solution by multinuclear (<sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F, <sup>31</sup>P), 2D and VT NMR experiments, and mass spectrometry. Several compounds were investigated by single-crystal X-ray diffraction. The optical properties of the compounds were studied by fluorescence spectroscopy.



**Figure 1.** Thermal ellipsoids representation at 50% probability for the asymmetric unit in [Ag{(n-Bu)[4-{2-C<sub>6</sub>H<sub>5</sub>-(4*H*)-oxazol-5-one}CHC<sub>6</sub>H<sub>4</sub>]S}][OTf]

**Keywords:** organosulfur ligands, structural investigation, group 11 metal complexes, optical properties

**References:**

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## THE RARE EARTH ELEMENTS DISTRIBUTION IN ATMOSPHERIC PARTICLES AS TRACERS FOR SOURCE APPORTIONMENT

LAURENTIU VALENTIN SOROAGA<sup>1,2</sup>, GIORGIANA ALINA NEGRU<sup>1,2</sup>,  
CECILIA ARSENE<sup>1,2,3</sup>, ROMEO IULIAN OLARIU<sup>1,2,3</sup>

Rare Earth Elements (REEs) are known tracers for the natural and anthropogenic sources' contribution to various natural environments, including lake, river, and ocean water, sediment, and soil [1]. This is possible due to the REEs unique and extremely similar physical and chemical behavior, which marks any geochemical anomaly as a strong indicator of additional sources for these elements in the investigated environment. In more recent times, as a consequence of technological advances and in particular concerning sensitivity, the distribution of REEs in atmospheric particles can also be employed for the identification of potential sources, both natural and anthropogenic in origin [2, 3]. This study presents data on the development of the Inductively Coupled Plasma–Mass Spectrometry (ICP-MS) method for the analysis of REEs in atmospheric particles. The sample preparation was performed by microwave-assisted wet digestion with HNO<sub>3</sub> 65%. The specific tuning and calibration conditions that enable the quantification of the REEs at the sub-ppb level of concentration are discussed. Results for the NIST 1649b Urban Dust certified reference material (CRM) are presented. While for this CRM CRM-certified values of REEs concentration are not available, the evaluation of the mineralization process efficiency and the overall analytical performance of the investigated method can still be under scrutiny. The impact of collision gas flow on the analytes was evaluated by comparing the influence of using a He flow of 80 mL/min with that of no collision gas. It was determined that the use of a collision gas flow had minimal to no effect on some analytes. In addition, the values for the limit of quantification (LOQ) were sufficiently high to allow for accurate quantification. However, for some analytes, the use of the collision gas was not favorable for their quantification at the level of concentrations expected to be found in this specific matrix.

**Keywords:** Rare Earth Elements; atmospheric particulate matter; source appointment.

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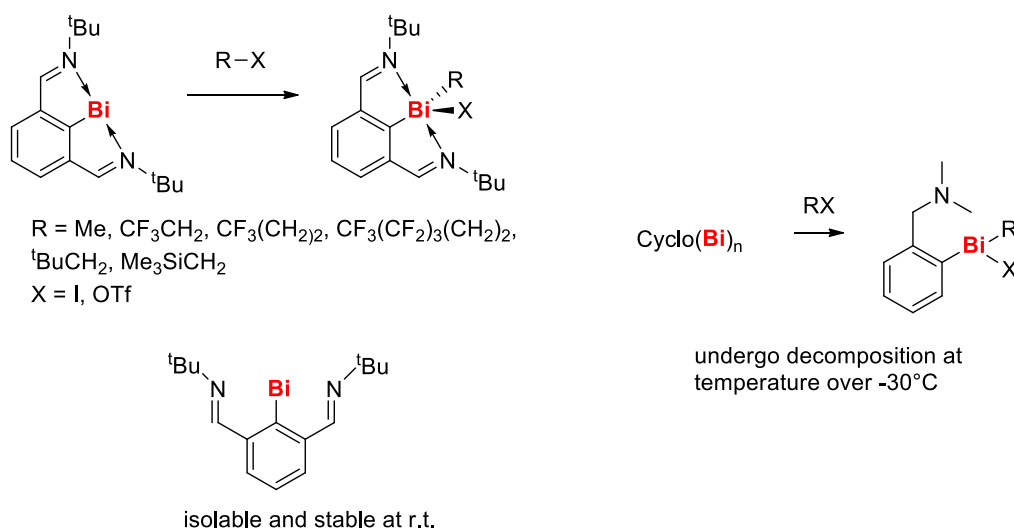
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## STUDY ON THE OXIDATIVE ADDITION OF DIFFERENT SUBSTRATES TO N,C-CHELATED CYCLOBISMUTHANE

RAFFAELE FONTANA<sup>1</sup>, CRISTIAN SILVESTRU<sup>1</sup>

Bismuthinidenes are a class of organobismuth compounds analog to carbenes, due to their unusual oxidation state of bismuth they are reactive and unstable. Polydentate chelating Lewis-base ligands, or sterically hindered ligands are required to stabilize the monomeric species, that will otherwise undergo dimerization or cyclization [1].

Bismuthinidenes, recently, have displayed interesting applications as redox catalysts due to their transition metal-like behavior and the possibility to access the Bi(I)/Bi(III) oxidation states, an example of this is the transfer-hydrogenation of azo compounds by amino-borane complex reported by Wang et al. (2019) [2] which is catalyzed by a monomeric bismuthinidene. The main objective of this work is to probe the limit of oxidative addition to cyclobismuthanes, a class of non-stabilized bismuth(I) compounds, toward different substrates compared with the reactivity of monomeric bismuth(I) species.



**Keywords:** Bismuth(I); oxidative addition; pnictinidenes; organobismuth; metal-metal bond reactivity.

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## SILVER(I) COMPLEXES OF PYRIDINE-BASED LIGANDS

CATALIN EDUARD SALGAU<sup>1</sup>, ANCA SILVESTRU<sup>1</sup>

Organochalcogen compounds have attracted an increasing interest in the last years due to their valuable use in various fields, including synthetic chemistry, catalysis, materials science, and biochemistry [1].

Recently, the synthesis of new selenium compounds has attracted considerable attention with regard to their potential applications in Organic Light-Emitting diodes, preparation of metal chalcogenide nanoparticles, or synthesis of antitumor agents [2]. Notably, the pyridine group is recognized to have an important role in many derivatives with proven biological or catalytic properties [3].

In this research, a new organochalcogen compound, containing pyridine and hydroxo functionalities, has been synthesized by the reduction of di(2-pyridil) diselenide with sodium borohydride, followed by the reaction of the as-formed sodium organoselenolate with 1-chloro-2-methyl-2-propanol. The compound 1,1'-selenobis(2-methyl-1-(pyridin-2-yl)propan-2-ol) (**L**) was further used in complexation reactions with AgOTf (**1**) and AgNO<sub>3</sub> (**2**). The compounds were characterized in solution by multinuclear NMR spectroscopy (<sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F, <sup>77</sup>Se, as appropriate) and mass spectrometry. The crystal and molecular structures of the silver complexes were determined by single-crystal X-ray diffraction.

In solid state, both Ag(I) complexes exhibit dimeric associations formed by intermolecular Se...Ag interactions.

**Keywords:** diorganoselenides; silver(I) complexes; structural characterization.

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## BINDING BIOMEDICALLY RELEVANT AGENTS TO HEMOGLOBIN

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We divide the interactions of hemoglobin (Hb) with small molecules into five types. Type 1 would involve direct interaction with the heme. Within this category, one may further define three different interactions involving the coordination of the iron (e.g., O<sub>2</sub>, NO, CN<sup>-</sup>, nitrite, sulfide, peroxides, etc.), the interaction of small molecules with the iron-bound ligands (e.g., nitric oxide or nitrite vs. oxyhemoglobin) or covalently attaching small molecules/ions to the iron-bound porphyrin (e.g., sulfide, reactive oxygen species, etc.) Type 2 includes carbon dioxide and other physiological allosteric effectors binding to the center of the Hb tetramer. Type 3 involves hydrophobic pockets within the protein, probed with inert gases such as xenon. Type 4 is associated with binding at locations other than the heme or the central intersubunit cavity. Within Type 4, two sub-types may be defined. Type 4a involves sites that affect heme reactivity. Due to the involvement of redox-active amino acids, Type 4a sites have been shown to harbor covalent modifications especially from ROS and/or to act as entry points for electrons towards the rest of the protein, with final targets identified including other redox-active amino acids ( $\alpha$  Trp14,  $\beta$  Trp15,  $\beta$  Trp37, Cys93, Y145, Y35, Y24, Y42, Y130 or Y140). Type 4b sites would involve no redox-active amino acids – which importantly includes Trp and Tyr, thus implying that such sites are likely to be silent in terms of the protein's intrinsic fluorescence and hence distinctly more difficult to probe. Type 5 interactions would involve small molecules that interact with each other outside Hb, but still affect Hb indirectly, for instance leading to apparent autocatalytic processes (e.g., superoxide, from Hb's autooxidation reaction). We explore here the Type 4 interactions with biomedically relevant ligands in Hb as well as, for comparison, serum albumin, using docking calculations as well as experiments [1–3].

**Keywords:** hemoglobin interactions; redox-active sites; therapeutic agents.

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## **DETECTION OF OVER 1000 PESTICIDES AS FOOD CONTAMINANTS ACCORDING TO EUROPEAN REGULATIONS**

TOMA GALAON<sup>1</sup>

A high-performance multiresidue workflow was developed and validated for the simultaneous quantitation of over 1,000 pesticide compounds in tomato samples to accelerate and simplify routine laboratory food testing. The workflow quantitates the most utilized pesticide residues simultaneously in 20 minutes runs using a single sample preparation method (QUECHERS) for both LC/MS/MS and GC/MS/MS analyses, which leads to high-throughput, simplified analysis, and lower laboratory costs. The workflow includes sample preparation, chromatographic separation, mass spectrometric (MS) detection, data analysis, and data interpretation using Agilent LC/MS/MS and GC/MS/MS systems. Workflow performance was evaluated and verified according to the SANTE 11312/2021 guideline based on instrument limit of detection (LOD), calibration curve linearity, and recovery.

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**DI- AND TRIORGANOTIN(IV) COMPLEXES  
WITH ORGANOSELENOLATO LIGANDS****MELINDA TAMAS<sup>1</sup>, ANCA SILVESTRU<sup>1</sup>**

Organotin(IV) compounds have attracted considerably increased interest over the last years due to their potential biological properties (antibacterial or antitumor agents) and their applications as precursors for nanomaterials for optoelectronics. On the other hand, various organoselenium compounds were intensively studied for their antioxidant and antiproliferative properties, or they were used as immunomodulators and anti-inflammatory or antidepressant drugs [1, 2]. Our recent research interest was focused on the synthesis and structural characterization of organotin compounds with organoselenolato ligands with potential for biological applications. 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-(Me<sub>2</sub>NCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>.

We report here on the synthesis and structural characterization of several homo- and heteroleptic diorganotin(IV) and triorganotin(IV) complexes with organoselenolato ligands of type pzCH<sub>2</sub>CH<sub>2</sub>Se<sup>-</sup> (pz = pyrazole). Compounds of type RR'Sn(SeCH<sub>2</sub>CH<sub>2</sub>pz)<sub>2</sub> (R = 2-(Me<sub>2</sub>NCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>; R' = Me, <sup>n</sup>Bu, Ph) were prepared by reacting RR'SnCl<sub>2</sub> with Na[SeCH<sub>2</sub>CH<sub>2</sub>pz] in a 1:2 molar ratio. Similarly were prepared compounds of type RR'<sub>2</sub>Sn(SeCH<sub>2</sub>CH<sub>2</sub>pz) and R<sub>2</sub>R'Sn(SeCH<sub>2</sub>CH<sub>2</sub>pz) (R = 2-(Me<sub>2</sub>NCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>; R' = Me, <sup>n</sup>Bu, Ph), when a 1:1 molar ratio was used in the reaction of Na[SeCH<sub>2</sub>CH<sub>2</sub>pz] with the heteroleptic triorganotin chloride. The homoleptic compounds of type R<sub>3</sub>Sn(SeCH<sub>2</sub>CH<sub>2</sub>pz) (R = Me, Bu, Ph, Bn) were obtained by reacting R<sub>3</sub>SnCl with Na[SeCH<sub>2</sub>CH<sub>2</sub>pz]. All compounds were characterized by multinuclear (<sup>1</sup>H, <sup>13</sup>C{<sup>1</sup>H}, <sup>77</sup>Se{<sup>1</sup>H}, <sup>119</sup>Sn{<sup>1</sup>H}) NMR experiments and mass spectrometry.

**Keywords:** organoselenolato ligands; organotin(IV) complexes; structural characterization.

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## GRAFT COPOLYMERS DERIVED FROM AMYLOPECTIN AND SYNTHETIC HOMOPOLYMERS

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The "grafting to" technique is one of the methods used for the synthesis of functionalized polysaccharides with synthetic polymers [1]. Amylopectin (AMP) is a natural biopolymer, one of the major components found in starch granules, and consists of  $\alpha$ -D-glucopyranose residues linked by  $\alpha$ -(1,4) and  $\alpha$ -(1,6)-glycosidic bonds. Due to its low cost, high biocompatibility, and biodegradability, AMP is widely used in various applications [1,2]. Over the years, synthetic polymers have been grafted onto different polysaccharides for the development of suitable materials for wastewater treatment and biomedical applications. Poly(*N*-isopropylacrylamide) (PNIPAM) and poly(2-(dimethylamino) ethyl methacrylate) (PDMAEMA) are water-soluble and thermoresponsive polymers, PDMAEMA being also known as pH-responsive. Both are promising polymers for the medical field due to their low biodegradability and considerable biocompatibility [2,3]. The aim of this study was the synthesis and characterization of the new AMP-*g*-PNIPAM and AMP-*g*-PDMAEMA copolymers, applying the "grafting to" technique. PNIPAM and PDMAEMA were obtained in our laboratory via reversible addition-fragmentation chain transfer (RAFT) polymerization which is a versatile radical polymerization method used for the generation of molecular weight-controlled polymers. FTIR spectroscopy, <sup>1</sup>H-NMR spectrometry, and TGA analysis were used to confirm the successful synthesis of the grafted copolymers. According to the performed characterization, the grafting of PNIPAM and PDMAEMA chains onto AMP was successfully achieved. Also, the self-assembly of the graft copolymers in an aqueous solution was investigated by dynamic and electrophoretic light scattering measurements indicating the formation of environmentally responsive nanostructures.

**Keywords:** polysaccharides; poly(*N*-Isopropylacrylamide); poly(2-(dimethylamino) ethyl methacrylate); amylopectin; grafting.

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## POLYMERIC MICROSPHERES OBTAINED FROM PICKERING EMULSION POLYMERIZATION TECHNOLOGY (PEMPTech) FOR COLORIMETRIC RECOGNITION OF METAL IONS

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Environmental and especially water pollution represents an important problem concerning the well-being of all organisms. Metal ion pollution has notably increased in recent years due to various industrial activities, chemical manufacturing, etc. While current technologies address this issue, they often come with several drawbacks, limiting their effectiveness in pollution control. In this work, we developed an innovative method for producing green and sustainable materials capable of colorimetric recognition of several metal ions, including Cu<sup>2+</sup>, Co<sup>2+</sup>, and Ni<sup>2+</sup>. These materials were synthesized using Pickering emulsion polymerization technology (PemPTech)[1–3], a technique that involves the stabilization of two immiscible phases by a non-polluting stabilizing agent, specifically silica nanoparticles. PemPTech is an aqueous-based and surfactant-free synthesis method<sup>[1]</sup> that offers a cost-effective, sustainable, and environmentally friendly alternative to conventional methods, providing a robust solution for monitoring and controlling metal ion pollution. This method not only enhances the environmental compatibility of the process but also improves the efficiency of metal ion detection. The resulting polymeric microspheres exhibit high sensitivity for metal ion recognition, facilitated by the incorporation of specific ligands known for their strong/specific metal-binding capabilities. Our study highlights the potential of Pickering emulsion polymerization as a versatile platform for developing advanced materials for environmental remediation applications.

**Keywords:** Pickering emulsion polymerization; polymer microspheres; metal ion adsorbents; environmental remediation; water pollution.

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**IN-SITU SYNTHESIS OF GOLD NANOPARTICLES MEDIATED BY CHITOSAN-g-POLY(N-ISOPROPYLACRYLAMIDE)**

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Gold nanoparticles (AuNPs) have been already used in a wide range of applications, including catalysis, sensing, medicine, pharmaceuticals, environment, electronics, and optics [1]. As a result, numerous synthetic approaches have been used to achieve the appropriate AuNP size and form. Using polymer chains as reducing and stabilizing agents simplifies AuNPs production, allowing for one-pot synthesis in aqueous or organic conditions with minimal post-synthesis work-up [2]. One of the most intriguing characteristics is that certain parts of copolymer chains can play an important role in the *in-situ* synthesis of AuNPs, by ionic exchange/chelate formation and Au<sup>3+</sup> subsequent reduction and offering the desired colloidal stabilization. Furthermore, the thermoresponsive properties of some macromolecular chains can be exploited to create enhanced smart/responsive hybrid nanomaterials.

The novelty of this study is the one-pot synthesis of AuNPs mediated by aqueous chitosan-g-poly(*N*-isopropylacrylamide) (Chit-g-PNIPAM) copolymer solution without the aid of any reducing agent. The synthesis of the Chit-g-PNIPAM biological-synthetic hybrid copolymer was made in our laboratory [3], by a two-step process: first, the homopolymer was synthesized by reversible addition-fragmentation chain transfer (RAFT) polymerization of *N*-isopropylacrylamide, and then it is attached to the backbone of chitosan via a radical-mediated coupling reaction, following the "grafting to" technique. The kinetics of Chit-g-PNIPAM/AuNPs hybrid nanostructures formation have been studied, related to the reaction temperature and [N]/[Au] molar ratio, by dynamic light scattering (DLS), UV-Vis spectroscopy and scanning transmission electron microscopy (STEM). Summarizing, the synthesis of AuNPs, without the need for additional reducing agents, was successfully obtained in the presence of Chit-g-PNIPAM copolymer in aqueous solution at elevated temperature, 60°C, and at the optimum [N]/[Au] = 2.05 molar ratio.

**Keywords:** RAFT polymerization; AuNPs; Chitosan-g-PNIPAM; thermal response.

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## RESEARCH ENHANCEMENT IN ORGANIC CHEMISTRY, INORGANIC CHEMISTRY, AND LIFE SCIENCES

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Reaxys, a premier chemistry database, has introduced a suite of new features designed to enhance the efficiency, accuracy, and depth of chemical research. This workshop aims to provide an in-depth exploration of these innovative tools and functionalities, illustrating how they can significantly benefit researchers in academia and industry alike. Key highlights include an advanced search algorithm that streamlines the retrieval of complex chemical information, a revamped user interface for improved navigation and user experience, and enhanced data analytics capabilities that facilitate the interpretation of vast datasets. Additionally, the integration of cutting-edge machine learning models offers predictive insights, aiding in the discovery of novel compounds and reactions. Attendees will gain hands-on knowledge of these features through live demonstrations, practical examples, and case studies showcasing real-world applications. By leveraging the new capabilities of Reaxys, researchers can accelerate their workflows, achieve more accurate results, and push the boundaries of chemical science. This workshop is essential for anyone looking to stay at the forefront of chemical research and innovation regardless of experience in using Reaxys.

**Keywords:** Reaxys; database; literature; patents; bibliographic search; Elsevier.

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**ANALYSIS OF SIZE-SEGREGATED PARTICLE-BOUND  
POLYCYCLIC AROMATIC HYDROCARBONS IN IASI URBAN AREA**

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Polycyclic aromatic hydrocarbons (PAHs) are atmospheric pollutants with a significant level of interest due to their toxicity and implications in atmospheric chemistry [1]. The present work reports the development of a high-performance liquid chromatography with fluorescence detection (HPLC-FLD, Agilent Technologies) method for determining PAHs in particulate matter (PM) and its application on the field samples. The chromatographic and detection parameters were optimized. The best separation of PAHs was achieved on a Hypersil Green PAH (2.1×150 mm, 3 µm; Thermo Fisher Scientific) analytical column, with gradient elution using acetonitrile and water as mobile phases at a 0.35 mL min<sup>-1</sup> flow rate. The extraction process was optimized using acetonitrile and hexane:acetone mixture (1/1, v/v), respectively, and a vortex (Biosan) system. The hexane:acetone extracts were evaporated under a nitrogen stream and reconstituted in 250 µL acetonitrile. The quality control of the analytical method was assessed using the NIST standard reference material SRM 1649b (urban dust). The recovery efficiencies were in the 60%-106% range for PAHs with more than 3 rings, except benzo[*a*]anthracene (126%). Aerosol samples used in the present study were collected in November 2023 (4 sampling events) from a sampling site located in Iasi, at 35 m above the ground level, for 72 hours using a 13 stages cascade Dekati Low-Pressure Impactor (DLPI) (0.0276-9.94 µm size range). Extraction of PAHs from aerosol samples with hexane:acetone mixture followed by evaporation to dryness under a nitrogen stream and reconstitution with acetonitrile indicated a significant loss of PAHs with less than 3 rings in the structure. A bimodal size distribution was observed for the investigated PAHs, with the major peak in the accumulation mode (0.1-1.0 µm). The concentration of benzo[*a*]pyrene, presenting the highest toxicity reported by the Environmental Protection Agency (EPA), in the PM<sub>10</sub> fraction (PM with aerodynamic diameter <10 µm) was 0.57±0.48 ng m<sup>-3</sup>, while the values for Σ<sub>14</sub>PAHs was 3.72±1.03 ng m<sup>-3</sup>. Source apportionment and health risk evaluation will be assessed in future research.

**Keywords:** PAHs; UHPLC-FLD; size distribution; atmospheric aerosols

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**CANDIDATES AND PRECURSORS FOR ANTICANCER DRUG**

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Cisplatin is a Pt(II) drug commonly used in anticancer treatments. The efficacy of cisplatin is hampered by side effects, resistance, and limited targeting of cellular mechanisms. The research presented here explores the behavior of Pt(IV) complexes in biologically relevant interactions with the aim of developing new selective anticancer drugs. Ligands bearing carboxyl groups (trigonelline, formononetin) or hydroxyl groups (chrysin and derivatives of chrysin) were used for coordination.

The above-mentioned interactions were monitored using spectroscopy – primarily UV-Vis and fluorescence, but also NMR and EPR. A major component of blood, to which any therapeutic agent would be exposed, is hemoglobin (Hb). A range of compounds with therapeutic action/potential (anticancer and beyond), including Pt(II)-based compounds, have been shown to affect the oxidative reactivity of Hb – either by acting as antioxidants or as agents of oxidative stress that promote Hb autoxidation<sup>[1]</sup>. Thus, the oxy-Hb autoxidation reaction was studied, in the presence of Pt(IV) hexacoordinated complexes and also of ligands.

The peroxidase reactivity of Pt(IV) complexes and ligands was assayed with ferryl-Hb. Ligands bearing aromatic hydroxyl groups showed high activities, reducing ferryl-Hb to met-Hb as expected. Binding of complexes to albumin as well as to Hb was confirmed by fluorescence measurements. Pt(IV) drug candidates are generally expected to be reduced to Pt(II) by thiol pools inside living cells<sup>[2]</sup>, so the reaction between glutathione (GSH) and Pt(IV) complexes was spectrophotometrically followed. A decrease in absorbance was found, indicating a reduction to Pt(II) – as also confirmed by TD-DFT calculations.

Such bifunctional assemblies can act as pro-drugs, as the cellular environment reduces platinum(IV) to platinum(II), thus liberating in situ cisplatin (or variations thereof) and the additional drug. Studying the interactions of potential drugs with proteins provides us with information regarding mechanisms of action, side effects, and selectivity.

**Keywords:** hemoglobin; Pt(IV) drugs, albumin; UV-Vis spectroscopy, oxidative stress.

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## ELECTROCHEMICAL BIOSENSITIVE DETECTION OF TYROSOL IN OLIVE OILS

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Tyrosol, a phenolic compound found in olive oils, is valued for its antioxidant properties and health benefits, including anti-inflammatory effects and protection against cardiovascular diseases [1]. Accurate detection of tyrosol is essential for assessing the quality and authenticity of olive oil [2]. In this context, the new study aimed to develop a biosensor using a screen-printed electrode modified with carbon nanotubes (CNT) and tyrosinase (Tyr). CNTs were chosen for their large surface area and excellent conductivity, facilitating efficient electron transfer. Tyrosinase catalyzes the oxidation of tyrosol, generating a detectable electrochemical signal. Electrochemical characterization of the biosensor was performed using cyclic voltammetry (CV) and square wave voltammetry (SWV). CV revealed clear redox reactions for tyrosol, confirming the enzymatic activity of Tyr on the electrode surface. SWV demonstrated increased sensitivity, showing a robust and reproducible signal.

Calibration was carried out in a concentration range from 0.1  $\mu\text{M}$  to 20  $\mu\text{M}$ , showing linearity between the biosensor current and tyrosol concentration, with a detection limit in the nanomolar range. The practical application of the biosensor was tested on olive oil samples, using a simplified extraction method for isolating the phenolic compounds. Analyses showed accurate and reproducible detection of tyrosol. Validation of the results by the standard addition method confirmed the precision and reproducibility of the biosensor, with excellent recovery values (in the range of 97.83-101.08 %) for tyrosol added to the olive oil sample extracts.

In conclusion, this carbon nanotube and tyrosinase-based biosensor provide a rapid, sensitive, and accurate method for detecting tyrosol in olive oils, making it a valuable tool for quality control and authenticity certification of food products.

**Keywords:** tyrosol; electrochemical detection; biosensor; olive oil.

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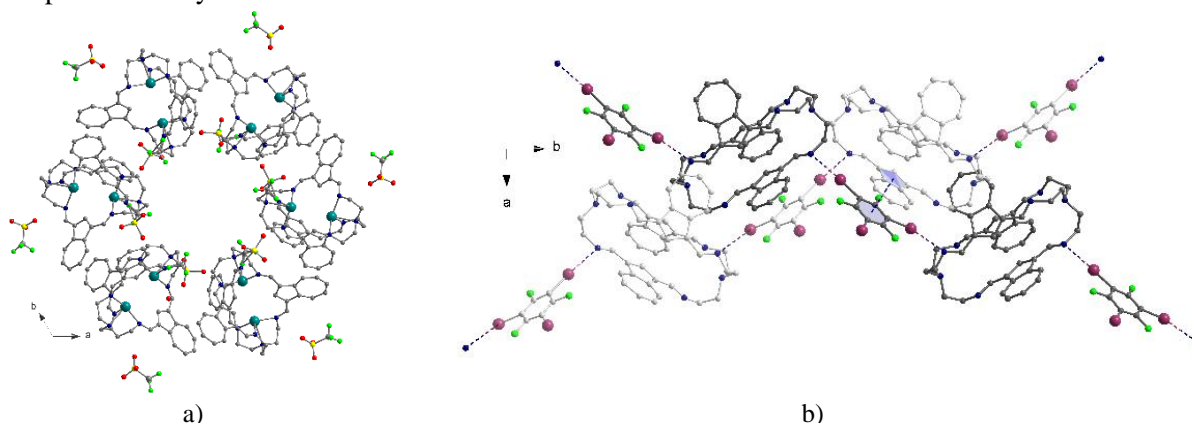
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## CRYSTAL ENGINEERING OF AZULENE-BASED IMINE CAGES

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Molecular self-assembly of organic and metal-organic cages is of high research interest, owing to their exciting properties and relevance in supramolecular chemistry and materials science [1]. The first example of a cage-like molecule was reported by Dietrich et al. (1969), a compound termed cryptands, that display three-dimensional cavities with strong binding anion affinity [2].

We recently synthesized *bistren* discrete [2+3] organic cages using azulene-1,3-carboxaldehyde and tris(2-aminoethyl)amine or 2,4,6-trimethyl-1,3,5-benzenetriamine. In the presence of a cationic guest (silver triflate), the molecular cage forms  $\pi$ - $\pi$  stacked porous supramolecular network (Figure 1a). Moreover, the discrete organic cages can act as halogen bond acceptors. As such, using 1,3,5-trifluoro-2,4,6-triiodobenzene, one-dimensional *zig-zag* chains are assembled *via* N $\cdots$ I interactions (Figure 1b). The chains are further connected through C-H $\cdots$ F contacts and  $\pi$ - $\pi$  stacking interactions forming 2D interpenetrated layers.



**Keywords:** self-assembly, azulene derivatives, organic cages, metal-organic cages.

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## SELF-ASSEMBLY OF AZULENE-BASED BIS TREN CAGES. STRUCTURAL AND ELECTROCHEMICAL INVESTIGATIONS

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Organic cages are self-assembled molecules that are typically formed from two distinct multifunctionalised components using reversible dynamic covalent chemistry [1]. We investigated the self-assembly process of tris(2-aminoethyl) amine (tren) with azulene-1,3-dicarboxaldehyde, through [1+1] and [2+3] imine condensation reactions. The interest of this research is oriented towards the understanding of the role of the azulene-1,3-dialdehyde in molecular organic cage assembling and in the crystal packing of the resulting solids. The new compounds were characterized both in solution and solid state, to confirm their stability. The conformational flexibility was investigated by variable temperature <sup>1</sup>H NMR spectroscopy. The presence of the azulene moieties provides the resulting material with multifunctionality in terms of redox and fluorescence properties.

**Keywords:** self-assembly, azulene derivatives, bis tren cages, electrochemical investigations.

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## INSIGHTS INTO THE CHARACTERIZATION OF THE AEROSOL-PHASE OF LIMONENE PHOTOOXIDATION PRODUCTS UNDER NO<sub>x</sub> AND NO<sub>x</sub>-FREE SIMULATED CONDITIONS

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Highly oxygenated organic molecules, generated mainly through the oxidation of monoterpenes, play a crucial role in secondary organic aerosols (SOA) formation due to their low volatility [1]. Among monoterpenes, limonene is of particular interest for its high global emission rates and SOA formation yields [2]. The present study aimed to investigate the SOA formation process through the OH radicals-initiated photooxidation of limonene under NO<sub>x</sub> (NO<sub>x</sub> = NO + NO<sub>2</sub>) and NO<sub>x</sub>-free conditions. The experiments were performed using facilities provided by the 760 L Environmental Simulation Chamber made of Quartz (ESC-Q-UAIC) together with state-of-the-art instruments such as scanning mobility particle sizer spectrometer (SMPS, model 3936, TSI), and proton-transfer-reaction time-of-flight mass spectrometer (PTR-ToF-MS, model 6000 X2, IONICON) coupled with aerosol chemical composition analyzer (CHARON). The obtained size-dependent aerosol number and mass concentrations in the 10.2 - 414.5 nm size range revealed the prompt formation of SOA during the oxidation of limonene in the absence of NO<sub>x</sub>. The mass concentration of SOA was significantly reduced under high NO<sub>x</sub> conditions, reaching a maximum of 3.0 µg·m<sup>-3</sup>, in contrast to the maximum concentration of 2.6·10<sup>3</sup> µg·m<sup>-3</sup> measured in the NO<sub>x</sub>-free experiments. Observed differences between NO<sub>x</sub> and NO<sub>x</sub>-free simulated conditions highlight the strong suppression of NO<sub>x</sub> upon the nucleation processes during limonene photooxidation, and selectively favor the formation of oxidation products.

**Keywords:** limonene; OH radicals; secondary organic aerosols; oxidation products.

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## DETECTION OF TETRACYCLINE AND DICLOFENAC BY A PHOTOLUMINESCENT COPPER(I) COORDINATION COMPOUND

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Copper(I) coordination compounds have attracted considerable attention during the last decades, due to their great potential in displaying favorable and largely tunable redox and luminescence properties. In many examples, the applicability of Cu(I) coordination compounds could be demonstrated as photosensitizers in hydrogen evolution reaction schemes and dye-sensitized solar cells, or as emitters in organic light-emitting diodes (OLEDs) and light-emitting electrochemical cells (LECs), or as sensors for oxygen as well as photoredoxcatalysts in various organic reactions. Significant improvements in the design of homoleptic and heteroleptic Cu(I) coordination compounds resulted in promising photophysical properties, such as highly luminescent complexes with long-lived excited states [1, 2]. The present work presents the synthesis and characterization of a heteroleptic coordination compound based on copper(I) thiocyanate in combination with phosphorus- and nitrogen-donor ligands, along with its evaluation of photoluminescent properties, which shall be used in the fluorescent detection study of some pharmaceutical substances, such as tetracycline and diclofenac.

**Keywords:** copper(I) thiocyanate; coordination compound; P,N-donor ligands; fluorescent detection.

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## THE CHLORITE ADDUCT OF AQUACOBALAMIN: CONTRAST WITH CHLORITE DISMUTASE

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In the reaction of aquacobalamin (aquaCbl) with chlorite, a stable species are detected and assigned as a Co(III)-chlorite. Its UV-vis spectrum is almost identical to that of aquaCbl, except for some minor differences at ~430 nm; cyanide can eliminate and prevent these changes. The <sup>1</sup>H-NMR spectra reveal strong influences of chlorite on the B2 and B4 protons of the cobalt-bound dimethyl benzimidazole ligand. Together, the UV-vis and NMR titrations suggest a K<sub>d</sub> of 10 mM or higher for chlorite on Cbl. Resonance Raman spectra reveal minor changes in the spectrum of aquaCbl to chlorite – as well as a disappearance of the free chlorite signals, consistent with Cbl-chlorite complex formation. Corroboration for these interpretations is also offered from mass spectrometry and DFT calculations. This Co(III)-OCIO<sup>-</sup> complex would be a stable analog of the first reaction intermediate in the catalytic cycle of chlorite dismutase or in the reaction of chlorite with a number of other heme proteins. The differences in reactivity between Co(III) cobalamin and Fe(III) heme towards chlorite are analyzed and rationalized, leading to a reconciliation of experimental and computational data for the latter.

**Keywords:** chlorite; cobalamin; UV-Vis; NMR; DFT; chlorite dismutase.

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**BIOLOGICALLY ACTIVE SPECIES BASED ON COPPER(II)  
COMPLEXES WITH N-BASED DONOR LIGANDS**TUDOR JULA<sup>1</sup>, CATALIN MAXIM<sup>1</sup>, ARPAD ROSTAS<sup>2</sup>, MARIA SUCIU<sup>2</sup>,  
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As an essential biocation, copper is usually involved in biologically active complexes design based on its lower systemic toxicity, accompanied by other useful properties such as acid borderline character and both stereochemical and oxidation state versatility. All these allow the interaction with a wide range of target biomolecules such as DNA and cytosolic enzymes [1]. As a result, several complexes that exhibit antimicrobial, antitumor, or anti-inflammatory activities were reported for this ion. Many species are based on ligands with chelating properties and intercalative ability, such as N-heterocycles derived from bipyridine and triazolopyrimidine [2]. To modulate biological activity, we extended this field in the synthesis of new series of complexes of type  $[\text{Cu}(\text{N-N})_2(\text{tp})](\text{ClO}_4)_2$  (N-N = 2,2'-bipyridine/ 1,10-phenantroline and tp = 5,7-dimethyl-1,2,4-triazolo[1,5-a]pyrimidine). The compounds were characterized based on data provided by elemental analyses, IR, UV-Vis, and EPR spectroscopy, as well as single-crystal X-ray diffraction. The tp ligand behaves as unidentate, while N-N ones act as chelate in a distorted penta-coordinate stereochemistry. Both complexes crystallize in the triclinic system, space group P (2), with two moieties in the unit cell. The complexes exhibit the selective ability to scavenge  $\text{O}_2^-$  reactive oxygen species but show no sensitivity towards OH. The complex with 1,10-phenantroline was more active against Gram-negative (*Pseudomonas aeruginosa*, *Escherichia coli*), Gram-positive (*Staphylococcus aureus*, MRSA) bacterial strains and fungus *Candida albicans*, both planktonic and biofilm embedded lifestyles. The activity for some strains falls in the micromolar range. The assays were performed *in vitro* on murine melanoma (B16), human colorectal (Caco-2), and human lung adenocarcinoma (A549) cell lines.

**Keywords:** biofilm; copper complex; molecular structure; 1,2,4-triazolo[1,5-a]pyrimidine; tumor cell.

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## NEW COMPLEXES WITH NICOTINAMIDE EXHIBITING ANTIMICROBIAL PROPERTIES

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Nicotinamide is used clinically in the treatment of pellagra, as a radiosensitizer in radiotherapy treatment of tumors, in the treatment of type I diabetes, and in neurodegenerative diseases such as Parkinson's and Alzheimer's [1, 2]. Also, nicotinamide possesses anti-inflammatory and antioxidant characteristics. Complex combinations containing biologically active molecules as ligands can exhibit enhanced biological activity compared to their constituents. The literature review indicates that there are very few examples of complexes with nicotinamide as the sole ligand. Combinations with mixed ligands are much more numerous and can be mononuclear or polynuclear. However, there are few reports on their biological activity. Taking these considerations into account, four new cobalt (II) and nickel (II) complexes containing nicotinamide have been synthesized. These have been formulated as mononuclear,  $[M(NCA)_2(H_2O)_4](Macr)_2$  (M: Co, Ni) and dinuclear,  $[Co_2(NCA)_4(Macr)_4] \cdot 2NCA$ ,  $[Ni_2(NCA)_4(acr)_3(acrpr)]$ , where NCA represents nicotinamide, acr/Macr denotes the acrylate/methacrylate anion, and acrpr represents the ester of propionic acid with acrylic acid. All compounds were characterized by elemental analyses, IR, UV-Vis spectra as well by single crystal X-ray diffraction. The compounds exhibit good antibacterial activity against various types of bacteria and fungi.

**Keywords:** complexes; cobalt; nickel; nicotinamide; antimicrobial properties.

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## DEVELOPMENT AND *IN VITRO* EVALUATION OF CUSTOMIZABLE GOLD NANOPARTICLE-BASED NON-VIRAL VECTORS FOR TARGETED GENE THERAPY IN BREAST CANCER

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Current therapeutic options for genetic and acquired disorders are limited and outdated. Gene therapy, an increasingly advanced field, offers significant potential to meet the urgent need for new and targeted treatments [1]. Gene therapy for different melanoma types utilizes both non-viral and viral vectors, demonstrating promising outcomes [2]. Non-viral methods present benefits such as reduced cytotoxicity, although the vector components significantly influence transfection efficiency, as evidenced by *in vitro* evaluations [3].

This study presents the development and *in vitro* evaluation of gold nanoparticle-based non-viral gene carriers (AuNPs) with customizable properties. These carriers were engineered by creating supramolecular "host-guest" inclusion complexes of  $\beta$ -cyclodextrin ( $\beta$ -CD) attached to a branched polyethyleneimine (*b*PEI) layer with varying molecular weights on the surface of AuNPs. An innovative and less common approach involving microwave irradiation was used to prepare the *b*PEI- $\beta$ -CD functionalized AuNPs. The  $\beta$ -CD units on the vector formed an inclusion complex with an adamantane-polyethylene glycol conjugate featuring the WXEAAYQRFL decapeptide, which selectively targets the MCF-7 breast cancer cell line.

When evaluating transfection capabilities, the resulting AuNP-based polyplexes incorporating *b*PEI with a molecular weight of 25kDa and carrying pCS2 plasmid DNA demonstrated higher transfection efficiency in MCF-7 cells compared to HOS cells, indicating a specific affinity for MCF-7. These results underscore the potential of this adaptable system as a promising platform for future *in vivo* applications using AuNP-based non-viral vectors.

**Keywords:** *gold nanoparticles; non-viral vector; gene delivery; MCF-7 cells; transfection.*

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## **ARMORACIA RUSTICANA: FROM PHYSICOCHEMICAL RESEARCH ON THE SPECIES TO THE DEVELOPMENT OF SOME PHARMACEUTICAL APPLICATIONS**

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The traditions of using *A Armoracia rusticana* for medicinal purposes are still applied in many countries. However, the dominance of synthetic drugs by companies has led to the insufficient use of medicinal plants that have been used for centuries in natural treatments [1]. *A Armoracia rusticana* has remarkable effects in treating various ailments and is cheap but extremely effective [2]. This paper explores the process of obtaining and preparing some products developed by us. An initial hybrid system with horseradish and kaolinite was formulated, aiming to investigate the benefits of the *A Armoracia rusticana* synergistically with kaolinite. Additionally, another potential product (toothpaste enriched with horseradish extract) was investigated for its potential teeth-whitening effects. A series of modern techniques were used to characterize *A Armoracia rusticana* and the kaolinite-*A Armoracia rusticana* hybrid system, including ultra-high performance liquid chromatographic with ultraviolet detection and mass spectrometry (UHPLC-UV-MS), electrospray ionization quadrupole time-of-flight mass spectrometry (ESI-QTOF-MS), X-ray diffraction (XRD), scanning electron microscopy and energy-dispersive X-ray spectroscopy (SEM-EDX), dynamic light scattering (DLS), Fourier-transform infrared spectroscopy (FTIR). This research showed that horseradish peroxidase (HRP), present in horseradish roots, enhances whitening effects, and toothpastes with horseradish extract act through this enzyme, similar to the whitening processes with hydrogen peroxide used in dental offices.

**Keywords:** system hybrid; whitening effect; *A Armoracia rusticana*.

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## CARBON ELECTRODES MODIFIED WITH MOLECULARLY IMPRINTED POLYMERS FOR LIPOPOLYSACCHARIDES SENSING

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Gram-negative Bacteria (GNB) such as *Pseudomonas aeruginosa*, *Salmonella enterica*, and *Escherichia coli* are considered significant threats to human health, particularly due to the continuous shed of endotoxins (namely, lipopolysaccharides LPS) during their lifetime. LPS is the main constituent of the outer layer of GNBs (LPS) [1]. Although individuals tolerate a certain level of endotoxins in the organism, high levels of LPS can lead to serious heart diseases, disorders affecting the liver, and thyroid, or even contribute to Parkinson's disease [2]. Therefore, this study presents an innovative method for developing cheap and stable electrochemical sensors for detecting LPS on site. In this respect, the electrodes were modified with molecularly imprinted polymer (MIPs) microparticles, by inserting them in the formulations of hybrid inks. MIPs are obtained by polymerization/crosslinking of functional monomer(s) around the target molecule called template (herein, LPS). Extraction of the template molecule leads to specific binding sites that allow the recognition and the rebinding of the same or structural-resembling molecules. Sensors were prepared by combined 3D inkjet printing, as it was found to be more economical and efficient for small-medium series of sensors. MIP microparticles were synthesized by sol-gel and extensively characterized by FTIR, SEM, DLS, BET, TGA/DTG, and UV-Vis analyses, while the thereof hybrid inks were investigated to determine their physical properties before printing (e.g., viscosity). The final sensors were analyzed morphologically and electrochemically (by CV/DPV).

Following physicochemical characterization, a homogenous incorporation of MIPs in the conductive layer was confirmed. The developed LPS-imprinted sensing device exhibited excellent analytical performances, enabling a limit of detection (LoD) of 0.058  $\mu\text{M}$  and a fast response time in aqueous media (less than 1 minute). The present discoveries are highly promising, especially considering the cost-effectiveness of the ink formulations and of the printing method.

**Keywords:** modified electrodes; molecular imprinting; 3D inkjet printing; bacteria endotoxin.

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## MOLECULARLY IMPRINTED NANOGELS FOR TARGETED RECOGNITION OF SPIKE PROTEIN FROM SARS-COV-2

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The recent global outbreak of COVID-19 has driven an increase in research focused on developing new methods for detection and treatment. One promising method involves creating synthetic antibodies that can specifically target the Spike S1 protein, the component of the virus responsible for transmitting the viral entity into host cells [1]. Nanogels (NGs), which are particles consisting of a 3D network of crosslinked polymer chains with a size of 10 to 300 nm, can be engineered to exhibit various properties, such as high-water content, biocompatibility, and responsiveness to stimuli [2]. Molecularly imprinted polymers (MIPs) represent a promising class of synthetic materials, designed to offer high specificity and sensitivity towards their target molecules [3]. Therefore, this study focuses on the synthesis of MIP nanogels (MIP-NGs), which involves imprinting the 3D structure of the Spike S1 RBD template molecule in a nanohydrogel matrix. The resulting imprints in the MIP-NGs serve as affinity hot-spots for Spike S1 protein rebinding; thus, acting as synthetic antibodies.

The MIP-NGs were obtained by reverse miniemulsion polymerization of polyethylene glycol diacrylate as a macromonomer in the presence of SARS-CoV-2 Spike S1 protein RBD (PSS1) as a template molecule. Control NGs were prepared without PSS1.

Characterization of NGs was carried out using different techniques such as FTIR, TGA/DTG, DLS, TEM, and SEM. FTIR and TGA/DTG analyses confirmed the extraction of both emulsifiers and templates from the MIP-NGs, while DLS and SEM/TEM images highlighted the individual spherical structures of the synthesized NGs. The binding affinity of PSS1 was studied using UV-Vis (Bradford method) and SDS-PAGE, while the cytotoxicity was evidenced by MTT assays. These analyses indicated that the MIP-NGs exhibited higher binding affinity for PSS1 compared to the control NGs, as well as high cellular viability in 72 hours at various dilutions.

In summary, MIP-NGs exhibited high specificity and binding affinity for PSS1, making them promising candidates for synthetic antibody development. Additionally, MIP demonstrated excellent biocompatibility, making them suitable for potential in vivo applications.

**Keywords:** molecularly imprinted nanogels; protein recognition; affinity; cytotoxicity

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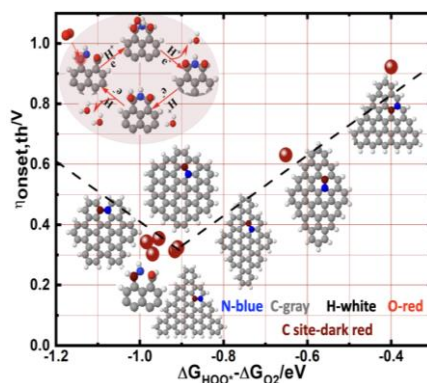
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## N-DOPED GQDs FOR ORR – A THEORETICAL APPROACH

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Oxygen reduction reaction (ORR) plays a key role in controlling the performance PEM-fuel cells. Efficient electrocatalysts should have low overpotentials, rich catalytic sites, and low cost [1]. Metal-free-graphene-based are considered promising alternatives to state-of-the-art precious Pt catalysts [2]. Factors like size, doping, surface functionalization, and regulation of the number of available active sites in graphene quantum dots (GQDs)s play an important role in ORR efficient control. By N-doping, these drastically alter their electronic characteristics, offering more electrocatalyzing active sites [3]. We investigate, using DFT, the thermodynamic ORR activity of N-doped GQDs of various shapes (triangle, rhombohedral, hexagonal), having zigzag/armchair terminations and N-located in all inequivalent positions, by following the  $4e^-$  pathway mechanism. The most active sites are placed closer to the edges than to the basal plane of the quantum dots (Fig. 1). Also, the most active sites are placed on the armchair terminated shapes and on the zigzag hexagonal one, while on the triangular and rhombohedral with zigzag terminations, no activity is predicted. By correlating ORR intermediates adsorption energies to the corresponding PDOS of each closest N-doping carbon neighbour, all sites of weakest adsorption present band gaps, comparing to much stronger adsorption sites having semi-metallic/metallic behaviour. After N-doping, O adsorption makes structural changes in several triangle structures, e.g. C-N breaking bond, creating other possible active sites within the zigzag structures (Figure 1).



**Figure 1.** Best active sites on volcano plot by fitting theoretical onset overpotential to  $O_2$  protonation free energy. Top-view pictures are illustrated of each structure.

**Keywords:** DFT; ORR; N-GQD; active sites; PDOS.

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## BIOGLASS-BASED NANOHYBRIDS

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Every year, millions of people suffer considerable loss of bone tissue due to various traumas or diseases that result in disability and reduced quality of life. In recent years, intensive scientific research has been done to find biomaterials with improved properties and applicability in the orthopedic field.

Silica-based bioglasses are of particular importance in the medical field. This importance is provided by their unique properties: osteoconductivity, osteoprodutivity, and osteoinductivity.

This work aimed to synthesize a bioglass composition as follows: 50%SiO<sub>2</sub>-45%CaO-5%P<sub>2</sub>O<sub>5</sub>-x%CeO<sub>2</sub>-y%SrO molar percentages where x and y take the values of 2.5, 5, and 10.

The sol-gel method was used to prepare bioglass samples in an acidic environment. Afterward, the samples were analyzed by multiple physicochemical characterization methods such as X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS), and thermal analysis.

**Keywords:** bioglass; sol-gel method; FTIR; XRD; SEM-EDS, thermal analysis.

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## ASSESSING THE INFLUENCE OF HYDROTHERMAL SYNTHESIS TEMPERATURE ON ROSMARINIC ACID-LOADED SILICA NANOPARTICLES

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Silica nanoparticles modified with the addition of rosmarinic acid have emerged as a promising combination in medical applications, particularly in the fields of drug delivery systems. Rosmarinic acid, a natural polyphenolic compound known for its anti-inflammatory, antioxidant, and antimicrobial properties, is effectively encapsulated within silica nanoparticles to enhance its bioavailability and therapeutic efficacy. This innovative approach not only facilitates targeted delivery to affected tissues but also improves the stability of rosmarinic acid, thereby prolonging its therapeutic effects. Moreover, the unique surface properties of silica nanoparticles allow for functionalization, enabling further modifications that can enhance drug loading capacity and release profiles. This study focuses on the synthesis of silica nanoparticles using the hydrothermal method, with variations in synthesis temperature to thoroughly analyze and discuss their resultant physicochemical properties. Additionally, mesoporous silica samples are functionalized with rosmarinic acid to create controlled-release systems tailored for medical applications. By understanding how synthesis conditions affect these nanoparticles, the research aims to optimize their performance in drug delivery, enabling more effective and targeted therapeutic strategies in the medical field.

**Keywords:** Rosmarinic acid; silica nanoparticle; hydrothermal method.

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## CONTROLLED RELEASE SYSTEMS BASED ON MONTMORILLONITE

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Montmorillonite is a layered clay with excellent absorption and intercalation properties, providing an ideal support for cerium oxide and Paclitaxel. Its structural properties allow for the controlled loading and release of therapeutic agents. In this work's context, MMT will support the uniform distribution of cerium oxide nanoparticles and Paclitaxel, ensuring the stability and efficacy of the powder. The implementation of this powder in clinical practice can significantly reduce the incidence of restenosis and other post-angioplasty complications, improving the prognosis of patients with atherosclerosis and reducing the costs associated with repeated medical treatments. This will lead to an improvement in the quality of life of patients and a reduction in the economic burden on the health system.

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## CONTROLLED RELEASE SYSTEMS LOADED WITH BIOLOGICALLY ACTIVE MOLECULES

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Conventional treatment of atherosclerosis often involves the use of stents to maintain vascular patency and prevent arterial occlusion. However, this approach carries significant risks of recurrence and complications, such as restenosis (narrowing of the artery) and thrombosis (formation of blood clots). These complications can lead to the need for repeated interventions and increase medical costs, negatively affecting the quality of life of patients. The aim of this work is the development of an innovative powder based on montmorillonite (MMT) and cerium oxide ( $\text{CeO}_2/\text{Ce}_2\text{O}_3$ ), loaded with Paclitaxel, a chemotherapeutic agent known for its antiproliferative properties. This powder will be intended for fixation on stenting balloons to allow application to the vascular endothelium, facilitating the controlled release of Paclitaxel in the area affected by atheroma. This controlled release will help reduce inflammation and prevent restenosis post-angioplasty.

**Keywords:** Montmorillonite; Paclitaxel; controlled release system.

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## REGIONAL FOOD BY-PRODUCTS AND WASTE AS A POTENTIAL SOURCE OF BIOACTIVE COMPOUNDS - *IN VIVO* AND *IN VITRO* EVALUATION

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Numerous types of food waste or by-products, such as eggshell, whey or pomaces contain important bioactive compounds (vitamins, minerals, proteins, lipids, fiber, organic acid, polyphenols, etc.), some found in large quantities. These bioactive compounds offer the potential to convert food by-products and waste into valuable products, in areas such as biofertilizers, bioenergy, biosurfactants, nutritional foods, etc. [1].

Our research team has expressed its interest in investigations concerning the reuse of local food by-products and waste, with the aim of finding innovative solutions to valorize them especially in regard to their fertilizing potential. Following the promising results of our previous study, it has been shown that grape pomace extract can have a stimulating effect on the *in vitro* development of plants if it is added in a certain proportion to the basal medium [2]. The extrapolation of the *in vitro* results to the *in vivo* investigation represents an important step. In this view, an *in vivo* plant-growth experiment was set up to investigate the separated or joined effect of some by-products and waste such as eggshell powder, whey, sea buckthorn pomace powder, and grape pomace extract on *Phaseolus vulgaris* and *Brassica oleracea* var. *italica* growth and development. The visual observation and preliminary biometric measurements showed that the high nutrient content of these food by-products and waste fertilizers promoted favorable soil conditions for the growth and development of plants. The use of food by-products and waste as biofertilizers can represent a sustainable alternative solution for both agriculture and waste management.

**Keywords:** local food waste; valorization; *Phaseolus vulgaris*; *Brassica oleracea* var. *italica*

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## THE INFLUENCE OF DIFFERENT ENZYMATIC TREATMENTS ON COTTON DYEING

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Textile finishing procedures produce new fabrics with improved features such as appearance, comfort, and fastness. One downside of traditional chemical techniques is the pollution produced during these processes.

A novel clean one-stage finishing and dyeing treatment for cotton by using Cellulases and reactive dyes is proposed. The use of enzymes to obtain the desired qualities of textile materials, rather than the polluting chemicals frequently used results in numerous benefits that cannot be attained by typical chemical treatment. These benefits include improved product quality, lower energy use, and less wastewater, the enzymatic treatment being a sustainable procedure [1, 2].

The study describes the effect of Cellulases treatment on a cotton knitted fabric to determine the enzyme's influence on the fabric's colour. The colour attributes brightness, chroma, and hue were investigated by using a Datacolor 500 spectrophotometer equipped with Datacolor Tools 2.0 software based on the CIELAB equation.

The study aimed to establish a correlation between the type of enzyme, the dye structure, and the colour differences. Thus, various enzyme concentrations and treatment times have been experimented and the optimal conditions have been proposed. Enzymatic treatments exert different influences on colour attributes. These changes may be ascribed to the uneven fuzziness of textile material. The experimental results demonstrated the potential of dyeing and finishing knitted cotton in a single step. Since the colour differences are within the tolerance limit.

**Keywords:** biofinishing; cellulases; cotton knitted fabric; reactive dyes; colour measurement.

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## CLIMATE CHANGE IMPLICATION ON FISH HABITATS IN PONDS AND RISK RELATED TO ECOSYSTEM HEALTH

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MARIAN DRAGUT<sup>1,2</sup>, IOANA DANIELA DULAMA<sup>5</sup>, ANDREEA LAURA  
BANICA<sup>2,5</sup>, IOAN ALIN BUCURICA<sup>5</sup>

Climate change represents one of the most important drivers of freshwater transformation, and the effects include changes in the structure and composition of biodiversity and its functioning. In the last years, the effect of climate change has been felt in Romania through the increase in air temperature and extreme weather phenomena (prolonged drought, heat waves, storms, floods, tornadoes, etc.). Temperature plays a critical role in the growth and development of aquatic animals. In Romania, fish production is carried out in ponds and reservoirs, through the extensive and semi-intensive growth of cyprinids in polyculture with other species. These systems are very vulnerable and strongly affected by climate change, both directly through problems related to water availability, ensuring the necessary levels in the conditions of increasing water and air temperatures, prolonged drought, evaporation, and extreme weather phenomena, but also indirectly through the physiological stress induced on fish populations, as a result of the increase in temperature, the lack of oxygen, the decrease in the metabolic rate and feeding, the increased incidence of diseases. This study aims to investigate the aquatic environmental conditions monitoring in terms of the last two years of climate change (i.e., 2022 and 2023, from May to September), in artificial ponds of Nucet Research and Development Institute for Fish Farming, Romania. The parameters of the pond water (i.e., dissolved oxygen and temperature) were associated with weather data (temperature, pressure, wind speed and direction, dew point) during two years of monitoring campaigns (for each year from May to September), correlated with recorded climate change data, showed a decrease in dissolved oxygen amount in the water drops considerably, sometimes below the limit of 4 mg/L. In this case, the feeling of hunger is stopped, and the fish begin to stop consuming the additional food, directly influencing the decrease in the growth rate of the specimens.

**Keywords:** climate change; fish; monitoring, risk.

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## EVALUATION OF PHOSPHATIC MATERIALS EFFICIENCY FOR WATER REMEDIATION

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The presence of pollutants in water bodies poses significant environmental and health challenges, increasing the necessity of effective and sustainable remediation technologies. Adsorption has emerged as a highly effective method for removing organic contaminants due to its simplicity, cost-effectiveness, and high efficiency [1]. This study demonstrates the efficiency of two metal-substituted phosphatic materials, BaHAP and MnHAP, regarding the adsorption of ibuprofen and phenol from aqueous solutions.

The materials' synthesis process involved a combination of co-precipitation and sol-gel methods, using calcium nitrate and diammonium phosphate as precursors, while salts of barium and manganese were chosen for the metal-substitution stage [2]. The materials were used as prepared or calcined at 300 °C, to increase the crystallinity degree and, also, the crystallite size. The prepared adsorbents were characterized through various analytical techniques, such as X-ray diffraction, X-ray fluorescence, FTIR spectroscopy, thermal analysis, and scanning electron microscopy, respectively.

The results obtained revealed an optimal adsorbent dosage for the adsorption processes of ibuprofen and phenol of 5 mg/L. A greater amount of ibuprofen was adsorbed by calcined MnHAP, whereas BaHAP demonstrated the highest efficiency for phenol adsorption. Also, the results presented statistical differences between the calcined and uncalcined samples. For ibuprofen adsorption, the calcined sample provided the most favorable results.

In conclusion, the phosphatic materials proposed in this paper represent potential candidates as adsorption materials for environmental decontamination.

**Keywords:** organic pollutants; adsorption; phosphatic materials; ibuprofen; phenol.

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## ISOLATION AND IDENTIFICATION OF MICROPLASTICS IN DAILY SKIN CREAM AND LOTION

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The cosmetics sector in the dermato-cosmetics category represents an enormous international market, worth several billions of dollars, which in recent years has faced major adaptations due to the current health crisis. There is a growing consumer awareness of their health, thus increasing the demand for truly effective, sensory, and safe cosmetic products. When it comes to skincare products, consumers these days are looking for customized, highly effective cosmetics tailored to their skin concerns. Several active cosmetic molecules are already in use and provide different benefits to the skin (UV protection, anti-aging, antioxidant, anti-acne, skin lightening, skin hydration, etc.). The skin, as the interface between the body and the external environment, is continuously exposed to numerous factors (physical, chemical, and biological) that can often lead to skin damage, such as sunburn, skin cancers, premature skin aging, skin inflammation, hyperpigmentation, and acne. To prevent and/or treat these skin lesions, the use of active ingredients in skin care formulations is of great interest.

Starting from the structure of the skin and products with topical application, as well as from the category of age and sex (i.e., children, adults, elderly, women, men), in this research microplastics, which are in the category of contaminants of emerging concern, were investigated, from products with daily application on the skin, creams and lotions. On the other hand, skin health depends a lot on lifestyle, a balanced diet, organized exercise, both quantitative and qualitative rest, and good stress management. Several dermato-cosmetics (i.e., external care and treatment), products (e.g., facial creams, lotion for skin, micellar waters, body creams, and perfumed body lotions) from 15 brands (125 samples analyzed) randomly collected often used by the humans, were studied. Optical microscopy corroborated with the micro-FTIR technique recorded/identified the presence of 43 fragments and 162 fibers, mostly with polymeric structures (i.e., polypropylene, polyethylene, polyacrylic, cellulose acetate, polyester, elastane).

**Keywords:** skin; topical application; microplastic; micro-FTIR; optical microscopy.

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## **SAMBUCUS NIGRA L.: A SOURCE OF BIOACTIVE COMPOUNDS WITH ANTIFUNGAL EFFECTS**

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The replacement of artificial compounds with natural ones through the superior usage of natural resources is a contemporary alternative with respect to the principles of sustainable chemistry. Natural resources have diverse applications in various disciplines. Since bioactive chemicals derived from plants have minimal environmental impact, their application as biopesticides is becoming more widespread. Black elder (*Sambucus nigra*) contains a variety of phytochemicals, including flavonoids, polyphenols, alkaloids, anthocyanins, hydroxycinnamic acids, and hydroxybenzoic acids. Antibacterial, antioxidant, anti-inflammatory, analgesic, cicatrizing, antidiabetic, antihypertensive, and other biological activities of black elder (*Sambucus nigra*) bioactive compounds are widely recognized. These compounds also possess important phytosanitary properties, including insecticidal, antifungal, and antibacterial effects. As eco-friendly biopesticides, their extracts can be applied. In the present study, the aqueous and hydroalcoholic extracts of dried elder leaves and flowers, obtained by the modern method of extraction assisted by ultrasound and maceration, were subjected to microbiological testing by the diffusimetric method. This aimed to evaluate the antifungal potential of the microorganisms *Alternaria* spp. and *Aspergillus* spp. isolated from the cucumber leaves in PDA and Sabouraud medium of both fresh extracts and those stored for some time. Compared to *Aspergillus* species, elderberry extracts suppress the growth of *Alternaria* spp. at a higher rate. The extracts have a stronger antifungal action in the PDA culture medium than in the Sabouraud medium. Regarding the extracts that were kept for three months, no antifungal activity against *Aspergillus* species was detected, irrespective of the culture medium.

**Keywords:** elderberry; extracts; antifungal activity; *Alternaria* spp.; *Aspergillus* spp.

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## IMPACT OF PAST MINING ACTIVITY ON THE QUALITY OF SURFACE AND GROUNDWATER RESOURCES

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This study focused on the potential threat of former uranium, copper, and charcoal mines from two areas containing former extraction uranium ore sites, Ciudanovita and Lisava, as well as copper ore from Moldova Noua and charcoal mines from Anina, Banat Region, Romania. This study highlighted the correlation between heavy metal concentrations and physicochemical indicators of surface and groundwater water (*i.e.*, EC, DO, pH, resistivity, salinity, and ORP), by using multivariate analysis, to shape a regional-based model on spatial distributions and variability of toxic contaminants from the hydrographic basin of Banat, Romania, as a consequence of former uranium, copper and charcoal mines. Although the actions were less visible on a high scale and the studies barely existed, the awareness of the risk must be present among the population. Therefore, it was required a complex study to assess the state of the facts of those areas and how much will anthropogenically impact the region. In this regard, eleven metals including Al, Cr, Mn, Fe, Ni, Co, Cu, Zn, Sr, Cd, and Pb from different water samples (well, spring, river, and lake), collected from three mining areas (uranium, copper, and coal mines) were investigated. Non-carcinogenic and carcinogenic health risks of seven heavy metals were assessed using the estimated daily intake (EID), daily intake metals (DIM), and target hazard quotient (THQ). The obtained THQ values were within the acceptable limits for cancer risks for adults, but for children's are toxic, eight samples out of eighteen. However, the HRI and THQ values for Cd and Pb for children were three times higher than those for adults. This is a source of concern as their prevalence in well water exposes children and residents in the Banat Region to the risk of various types of cancers. The data provided by this research can be used to develop a framework for quantifying some of the physicochemical indicators that stakeholders and authorities use when preparing guidelines for water quality (GWQ) taking into consideration these mining areas which cause strong pollution of the environment and pose risks to human health.

**Keywords:** mining area; health risk; water resources; physicochemical indicators.

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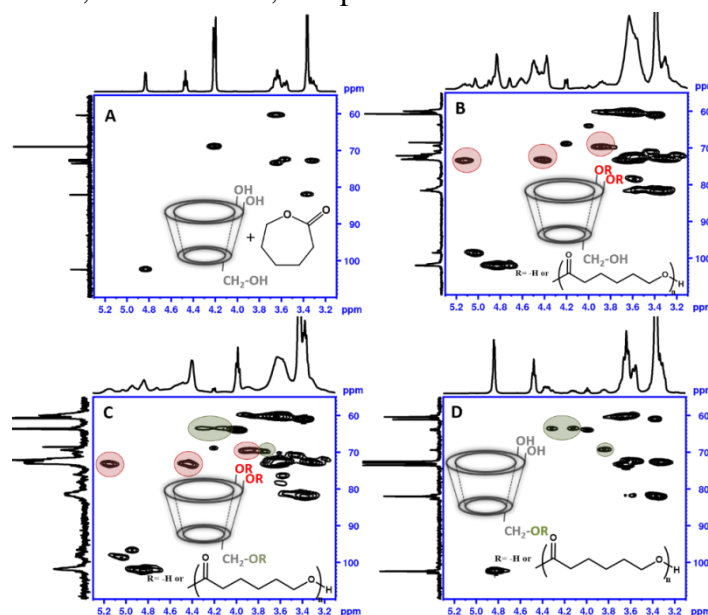
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## NMR STRATEGIES FOR ELUCIDATING CHEMICAL MODIFICATION MECHANISMS OF CYCLODEXTRINS

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NMR spectroscopy is an invaluable tool for elucidating reaction mechanisms, offering detailed structural, dynamic, and kinetic information. Its ability to provide real-time monitoring and in-depth analysis of molecular interactions makes it indispensable in both academic research and industrial applications.

The present paper describes the NMR study of the reaction mechanism of  $\beta$ -cyclodextrin with  $\epsilon$ -caprolactone in presence of basic organocatalysts [1]. Key intermediates were characterized (Fig. 1) to confirm the proposed reaction pathways. The complex spectra were carefully deciphered and mechanistic details were extracted. In situ NMR allowed the continuous monitoring of the reaction mixtures over time, providing real-time data on the formation and consumption of reactants, intermediates, and products.



**Figure 1.**  $^1\text{H}$ ,  $^{13}\text{C}$ -HSQC spectra for A) initial reaction mixture, and products with: B) large rim substitution, C) random substitution, D) small rim substitution.

**Keywords:** NMR spectroscopy; cyclodextrins;  $\epsilon$ -caprolactone.

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## ISOLATION AND IDENTIFICATION OF MICROPLASTICS IN MILK – A POTENTIAL HEALTH RISK FOR CHILDREN

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Recently, microplastics (MPs) contamination of food products has gained a special interest, both for government agencies around the world and the scientific community. Humans come into direct contact with plastics and their breakdown by-products globally, especially nano- and micro-plastics. Microplastics can hurt human health due to their complex physical and chemical characteristics (polymer type, size, shape, charge, number, etc.). Still, the scale of these exposures and the resulting health effects are either largely unknown or unstudied. MPs concentration, duration of exposure, presence of additives used during plastic processing, particle surface modification and hydrophobicity are all essential in determining toxicity. The toxicity of microplastics includes monomers i.e., vinyl chloride, ethenylbenzene, and chemicals produced from phenolic compounds i.e., alkylphenols, brominated flame retardants, and bisphenol A. One of the main goals of MPs toxicity assessment should be to detect the presence of these compounds. The current study is intended to be a first step in elucidating the risk generated by microplastics in branded milk, in terms of chemical composition and toxic effects on humans, especially on pregnant women and children. An absolute novelty of this study consisted in the development of a method for isolating the microplastics from the matrix of the branded milk samples using ultrasound technique at constant temperature and pressure, high-performance vacuum filtration method with various high-purity filtration membranes. On the other hand, the combined application of the structure-sensitive technique Fourier transform infrared micro-spectroscopy in conjunction with different approaches of optical microscopy and scanning electron microscopy - energy dispersive spectroscopy (SEM-EDS), as preliminary physicochemical investigations carried out on MPs from branded milk samples, was a significant objective of this study, to elucidate their type, structure, and chemical composition. In this respect, analyzing the MPs sizes, it was observed that length varied from tens of micrometers to a few centimeters in some cases and the thickness reached 15  $\mu\text{m}$  and even more for various samples. From a visual and chemical point of view, the microparticles identified in the analyzed samples presented a fibrous structure (polypropylene), with a glossy, matte or transparent appearance. Black was the predominant color and other colors identified were: blue, yellow, brown and/or red.

**Keywords:** MPs; milk isolation process; micro-FTIR; optical microscopy; SEM-EDS.

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## PREPARATION AND CHARACTERIZATION OF HAWTHORN BERRIES AND GRAPES SKIN EXTRACTS; ANTIOXIDANT AND ANTI-INFLAMMATORY EFFECTS IN ENDOTHELIAL CELLS

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The berries, flowers, and leaves of hawthorn (*Crataegus m.*) are well known for the treatment of hypertension, digestive illnesses and as hepatoprotective remedy. The skin of grapes (*Vitis v.*) is an important source of biologically active compounds, in particular resveratrol, procyanidins, and polyphenols. This study aimed to prepare, characterize, and evaluate the antioxidant and anti-inflammatory potential of the combined extracts from hawthorn (Hex) and grapes skin (Gex) to generate a new formulation for human health care.

Hawthorn berries and grapes skin were dried and grounded into fine powder and extracted with 70% ethanol for 2 h, and 80% ethanol for ½ h respectively, at 60°C, under magnetic stirring, followed by filtration, ethanol evaporation and freeze-drying, resulting the lyophilized Hex and Gex. Total polyphenols (TP) of the extracts were determined by the Folin-Ciocalteu method, total flavonoids (TF) by AlCl<sub>3</sub> method <sup>[1]</sup>, flavonoids and polyphenols profile by UHPLC and total procyanidins by European Pharmacopoeia 10.0 method. To determine the cytotoxic effects of the extracts, human endothelial cells (HEC, EA.hy926 cell line) were incubated with different concentrations of Hex and/or Gex (5 and 10 µg/ml equivalent procyanidins). To evaluate the beneficial effects of the extracts in HEC, the cells were first preincubated with the concentration of Hex and/or Gex for 2h, followed by their exposure to tumor necrosis factor α (TNFα, 10 ng/ml), in the presence of Hex and/or Gex for another 24h. Gene expression of the pro-inflammatory molecule monocyte chemoattractant protein-1 (MCP-1) and the antioxidant enzyme superoxide dismutase-1 (SOD-1) were evaluated <sup>[2]</sup>. Hyperoside and catechin are the main flavonoids present in Hex, while the Gex is rich in catechin, trans-resveratrol, myricetin, rutin, and quercetin. The TP content was 3 times higher and procyanidins concentration 6 times greater in Gex compared to Hex. We established that the equivalent of 5µg procyanidins/mL for each extract (apart and together) preserves the cells viability, and demonstrated that their combination exerts significantly increased antioxidant and anti-inflammatory effects by up-regulating SOD-1 and down-regulating MCP-1 gene expressions in HEC exposed to TNFα, compared to Hex or Gex alone. Formulating the hawthorn and grapes skin extracts together might be successfully used to ameliorate disorders affected by increased inflammation and oxidative stress.

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**Keywords:** hawthorn; skin grapes; procyanidins; MCP-1; SOD-1.

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## GENERATION OF TERT-BUTYLCYANOKETENE FROM 2,5-DIAZIDO-3,6-DI-TERT-BUTYL-1,4-BENZOQUINONE. THE OLD STORY REINVESTIGATED

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The thermal cleavage of 2,5-diazido-3,6-di-tert-butyl-1,4-benzoquinone (DADtBuBQ) leading to tert-butylcyanoketene (TBCK), published in 1970 by Moore and Weyler, opened a fertile research domain: the chemistry of cyanoketenes [1, 2]. DADtBuBQ can be converted to 2-cyano-4-azido-2,5-di-tert-butyl-1,3-cyclopentadienone through photolysis with 3600-Å light. Cyclopentadienone, on thermal decomposition in refluxing benzene quantitatively yields TBCK. According to the authors, two pathways would be possible: either a concerted ring contraction to the ketene dimer which then dissociates to a ketene, or an electrocyclic ring opening to a zwitterionic intermediate cleaving to the cumulene [3].

Our study aimed to investigate the kinetics of TBCK formation via azide cleavage starting from DADtBuBQ but this time observing the changes in the molecule's structure revealed by solution and solid-state NMR spectrometry. Kinetic experiments have been done at 50, 55, 60, and 65°C in C<sub>6</sub>D<sub>6</sub>, recording spectra every 15 minutes at the first 2 temperatures and every 5 minutes for the last two at the start of the experiments.

According to our results, the formation of TBCK from the DADtBuBQ starting material undergoes through a TBCK dimer.

**Keywords:** tert-butylcyanoketene; NMR; thermal azide cleavage.

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## SYNTHESIS OF NEW POTENTIALLY BIOACTIVE CARBAMOYL SUBSTITUTED PYRROLO [2,1-a]ISOQUINOLINES

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Pyrrrolo[2,1-*a*]isoquinoline is a privileged framework present in many natural alkaloids. The interest in synthetic approaches toward novel synthetic pyrrrolo[2,1-*a*]isoquinolines increased in time due to the discovery of important biological activities of pyrrrolo[2,1-*a*]isoquinoline compounds [1-3].

We present here novel carbamoyl-substituted pyrrrolo[2,1-*a*]isoquinoline derivatives synthesized by the one-pot three-component synthetic protocol starting from isoquinoline, substituted 2-chloro/bromo-*N*-phenylacetamides and symmetrical and non-symmetrical acetylenic dipolarophiles in 1,2-epoxypropane used as acid scavenger and reaction solvent in moderate to good yields. The multicomponent reactions were carried out by simply mixing all reaction components in 1,2-epoxybutane and heating the reaction mixture at reflux temperature. A slightly modified procedure was applied when symmetrical-disubstituted highly active dimethyl acetylenedicarboxylate was used as dipolarophyle.

All synthesized carbamoyl-substituted pyrrrolo[2,1-*a*]isoquinoline derivatives were characterized by chemical and spectral analyses. The structure-activity relationship data calculated by the SwissADME methodology shows that many of the synthesized compounds have drug-likeness physicochemical properties.

**Keywords:** one-pot multicomponent reaction; pyrrrolo[2,1-*a*]isoquinoline; bioactive compounds.

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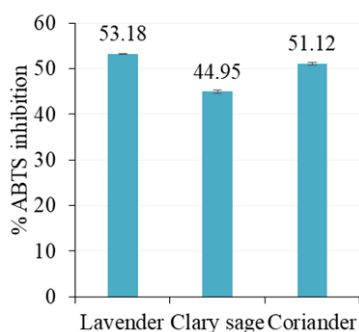
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## ANTIOXIDANT ACTIVITY OF LOCAL LAVENDER, CLARY SAGE, AND CORIANDER ESSENTIAL OILS

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Industrially produced Lavender (*Lavandula angustifolia* Mill.), Clary sage (*Salvia sclarea* L.), and Coriander (*Coriandrum sativum* L.) essential oils are widely used in cosmetic, food, and beverage industries [1]. Due to the abundance of bioactive compounds like unsaturated sesquiterpenic hydrocarbons and their oxygenated derivatives [2], these oils show various biological properties. Recent findings demonstrated a good correlation between the chemical composition and the antimicrobial activity of Lavender essential oil and its by-products [2]. The present study aims to enrich the data on the antioxidant activity of local essential oils. For this, the well-known ABTS<sup>+</sup> antioxidant assay was used as reported previously [3], and the comparative data on the antioxidant activity of tested oils were obtained for the concentration of 30 mg/mL (Fig. 1).



**Figure 1.** ABTS<sup>+</sup> inhibition by local Lavender, Clary sage, and Coriander essential oils at a concentration of 30 mg/mL

According to the results depicted in the Figure, all three essential oils possess antioxidant activity against ABTS<sup>+</sup>. The lavender essential oil shows the most efficient result, being able to inhibit 53.18% of ABTS<sup>+</sup>, followed by Coriander essential oil which inhibits 51.12% of free radical species, and Clary sage essential oil which has a free radical scavenging activity equivalent to 44.95% of ABTS<sup>+</sup> inhibition. These findings are promising and encourage further investigations on this subject.

**Keywords:** lavender; clary sage; coriander; essential oils; antioxidant activity.

**Acknowledgments:** This research was supported by the institutional research program of the State University of Moldova, subprogram code 010601

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## QUANTITATIVE SCREENING METHOD FOR PESTICIDE RESIDUES IN CITRUS USING GAS CHROMATOGRAPHY-TANDEM MASS SPECTROMETRY

BRADUT BOGDAN MINEA<sup>1</sup>, CRISTIANA RADULESCU<sup>1,2,3</sup>

Citrus fruits, with their role as a valuable functional food and health-beneficial effect for humans, are included in the current diet of all age groups (from children to the elderly), due to their high content of flavonoids, vitamins, carbohydrates, phenolic acids, and microelements. Considering the real health benefits of citrus bioactive compounds, it is understandable that any substance that can modify/destroy their structure and properties (mainly with the formation of stable clusters) represents a major risk for humans. The pesticides from citrus, regardless of the structure/class/dose, harm their functional properties.

This research highlighted the constant presence of pesticide residues in citrus fruits, and this fact is mainly due to the phytosanitary treatments carried out both on the crops in the development phase and on the fruits in the storage phase (e.g. insecticides, fungicides, etc.). The results obtained by gas chromatography-tandem mass spectrometry (GC-MS/MS) showed that from 21 lemon samples, 18 samples (85.71%) contained pesticide residues with values between 0.005 and 2.700 mg/kg. In addition, several samples contained unauthorized active substances, i.e., spirodiclofen and o-phenylphenol (ones from non-EU area), and the most dangerous sample turned out to contain a mixture of both pesticides - unauthorized by the Romanian rules - together with another dangerous pesticide, i.e., malathion. The most frequently quantified pesticides in analyzed citrus samples were imazalil, thiabendazole, pyrimethanil, pyraclostrobin, and fludioxonil. As a brief mention, fruit samples have been collected randomly from the Romanian markets and 85.7% of the total samples analyzed contained pesticide residues in variable quantities, but in a very high percentage. The samples with the most detected pesticides were in citrus imported from outside the European Union.

**Keywords:** pesticide residue; citrus; maximum residue limit; GS-MS/MS.

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## ELECTROCHEMICAL EVALUATION OF ANTIOXIDANT CAPACITY OF PERILLA EXTRACTS

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Medicinal plants are used worldwide to treat and prevent a variety of ailments, the interest in their uses being current due to their therapeutic potential and reduced side effects compared to antibiotics and synthetic drugs.

This study followed the extraction of some active chemical and biological compounds with the help of solvents with different polarities. Following the chemical tests, these extracts were subjected to various biochemical methods to reveal possible biological activities. It was wanted to highlight activities such as the anti-inflammatory effect, the antimicrobial and antitumor activity.

Our study aims to evaluate the total antioxidant capacity of some extracts of *Perilla frutescens*, which is known to improve some affections due to its expectorant and anti-inflammatory, antitumor properties, etc. [1]. Methanolic, hydromethanolic (1:1v/v) and in DES (deep eutectic solvents) extracts were prepared from finely chopped, ultrasonicated and filtered leaves.

A comparative electrochemical study was performed for all the extracts obtained (CV- cyclic voltammetry; OCP- open circuit potential). The samples before and after CV experiments were also studied spectrophotometrically (UV-Vis).

The results demonstrated the presence in the extracts of some antioxidant compounds from the class of polyphenols.

**Keywords:** *Perilla spp.*; chemical compounds; biological activities, cyclic voltammetry.

**Acknowledgments:** This work was partially supported by Internal Grant 2024 no. 2487/31.05.2024 of Department of Chemistry, Physics and Environment, Faculty of Sciences and Environment, "Dunarea de Jos" University of Galati, "Evaluation of Natural Organic Compounds with Biologically Active Potential" and ADER grant 5.2.1. – "Conservation and valorization of the genetic heritage of aromatic and medicinal species that can be cultivated on the territory of Romania".

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## METHYLMALONIC ACIDURIA DIAGNOSED BY NMR SPECTROSCOPY

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Methylmalonic aciduria (MMA) is a rare inborn error of metabolism (IEM) disease due to errors in the propionate metabolism. MMA can either be primary (due to an enzyme or cofactor deficiency) or secondary to a vitamin B<sub>12</sub> deficiency. Primary MMA is due to a defect in the methylmalonyl-CoA mutase enzyme (which catalyzes the conversion of methylmalonyl-CoA to succinyl-CoA), leading to the excretion of several compounds like methylmalonic acid, propionylcarnitine, and methylcitric acid in the body's fluids.

For this and other related pathologies, as for most of the IEM, the prognosis of their evolution and their level of irreversible damage to various organs depend on how early the treatment is started and, thus, on how early they are diagnosed. Several guidelines for the diagnosis and management of these pathologies have been published <sup>[1]</sup>.

Current diagnostic standards are based on GC/LC-MS analyses of urine and blood plasma [2]. With the advent of NMR instrumentation, this emerging method became a valuable tool in the diagnosis of MMA and other rare diseases [3].

We are reporting on <sup>1</sup>H NMR monitoring of five MMA patients. A comprehensive set of metabolites have been monitored in their urine. It is shown that, in addition to being a therapy assessment, the levels of methylmalonic acid and glycine in urine can indicate the type of MMA mutation (MMAA *versus* MMUT). Average concentrations and ranges of the following MMA-associated metabolites: glycine, methylmalonic acid, orotic acid, orotidine, L-carnitine, and propionylcarnitine are presented for all monitored patients.

**Keywords:** NMR; rare diseases; methylmalonic aciduria.

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**GALACTOSEMIA MONITORED BY NMR SPECTROSCOPY**

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NMR spectroscopy is a quick and efficient tool for diagnosis and follow-up of several inborn errors of metabolism. In many suspicious cases, particularly in countries where only a few inborn errors are included in national screenings, NMR may provide the first indication for a rare metabolic disease. Galactosemia is an inherited defect of galactose metabolism caused by an enzyme deficiency that prevents the proper metabolism of galactose. This condition occurs in an estimated 1 in 60,000 people. In galactosemia a diet without lactose is mandatory. Infants with galactosemia are started on milk substitute formula, usually a lactose-free soybean protein formula, and are required to keep a lactose-restricted diet for the rest of their lives. Before diagnosis, when normal milk is administered, galactose is building up in the organism as the main metabolite of lactose <sup>[1]</sup>. When the patient is under a specific diet galactose can hardly be detected. However, even when the products based on normal milk are completely excluded, small amounts of galactose are finding their way into organism, e.g. through fruits and vegetables which are allowed in the diet, or through other metabolic pathways.

We report on a case of a five-month-old girl diagnosed with galactosemia which was followed up by NMR to assess the efficiency of the diet. In the absence of galactose as main marker of galactosemia, in order to indirectly follow up its presence in the organism, we have been monitoring by NMR the presence of galactitol. Galactitol proved to be the main marker indicating the efficiency of the specific diet in galactosemia. Assignments of various signals of metabolites in urine and their concentration range over the monitored period are presented.

**Keywords:** NMR; rare diseases; galactosemia; galactose; galactitol.

**Acknowledgments:** *This study was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, contract no. 30ROMD/2024, project PN-IV-P8-8.3-ROMD-2023-0249 (DiMoMeD).*

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A comparative electrochemical study was performed for all the extracts obtained (CV- cyclic voltammetry; OCP- open circuit potential). The samples before and after CV experiments were also studied spectrophotometrically (UV-Vis).

The results demonstrated the presence in the extracts of some antioxidant compounds from the class of polyphenols.

**Keywords:** *Perilla spp.*; chemical compounds; biological activities, cyclic voltammetry

**Acknowledgments:** *This work was partially supported by Internal Grant 2024 no. 2487/31.05.2024 of Department of Chemistry, Physics and Environment, Faculty of Sciences and Environment, “Dunarea de Jos” University of Galati, “Evaluation of Natural Organic Compounds With Biologically Active Potential” and ADER grant 5.2.1. – “Conservation and valorization of the genetic heritage of aromatic and medicinal species that can be cultivated on the territory of Romania”.*

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## SIMULTANEOUS QUANTITATIVE DETERMINATION OF ROSMARINIC, OLEANOLIC AND URSOLIC ACIDS IN *SALVIA GLUTINOSA* EXTRACTS BY QNMR SPECTROSCOPY

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Romanian glutinous sage (*Salvia glutinosa*) came recently into focus as a rich source of valuable phytochemicals [1]. In particular, the antiproliferative,  $\alpha$ -glucosidase inhibitory activity, as well as the *in vivo* anti-inflammatory activity has been demonstrated for *S. glutinosa* extracts [2]. The investigation of the secondary metabolites content in these extracts has been mainly concentrated on phenolic compounds. We present in the current communication our results on the identification of substantial amounts of oleanolic (OA) and ursolic (UA) acids in *S. glutinosa* extracts, prepared from integral plants collected in the Durău area of Neamț County, Romania. The use of qNMR spectroscopy provided to be a convenient tool for the quantitative determination of these triterpenes, along with rosmarinic acid (RA), a known major component of *S. glutinosa* with strong antioxidant properties.

The identification of the diagnostic signals corresponding to OA, UA, and RA and quantitative determination were achieved based on two-dimensional HSQC spectra, calibration curves have been plotted against the signals of the internal standard – methyl 4-nitrobenzoate [3]. The validation of analytical measurement was performed by a parallel HPLC determination of the three acids in the investigated extracts.

The results of the determination provided values from 2.4 to 4.1 mg of each organic acid per 100 mg of extract, which match the literature data on the content of RA in *S. glutinosa*.

The developed qNMR method provides a robust and easily applicable analytical tool for the investigation of *S. glutinosa* plants under a potential valorization scenario.

**Keywords:** qNMR; triterpenic acids; phenolic acids; sage.

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## PHENOLIC PROFILES AND ANTIOXIDANT ACTIVITY OF GRAPE POMACES FROM FETEASCĂ ALBĂ AND TĂMÂIOASĂ ROMÂNEASCĂ VARIETIES

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Grape's pomace is the waste from the pressing process of red and white grapes, with the final goal being to obtain high-quality wine. Usually, grape pomace comprises stalks/clusters, skins, and seeds/kernels, representing approximately 25% of the total weight of the grapes used in the winemaking process. White grape pomace is investigated less in terms of bioactive compounds and antioxidant properties, despite the high demand for food that exhibits good health and prevents diseases caused by oxidative stress. The research for obtaining new natural compounds that can be employed to improve food characteristics for health benefits or medicinal purposes has accelerated research on Green Chemistry.

This study highlighted that grape stem, a serious environmental pollutant, could be valorized to extract phenolic compounds for use as bioactive and/or functional ingredients. The objectives of this study were: (1) to investigate the composition of grape pomace in terms of phenolic and flavonoid content, as well as their antioxidant activities, in relation to grape variety, extraction procedure, and anatomical part of grapes; (2) to evaluate the correlation between the phenolic content, antioxidant activity, grape variety, anatomical part, and extraction procedure. In this respect, the established correlation could be utilized to optimize the extraction of phenolics from grape by-products and for further utilization as functional ingredients. In addition, the findings from this study will be useful for winemaking producers and producers of food ingredients, based on the correlations established by the statistical approach. The performed experimental screening was designed to assess several indices of the polyphenolic composition of grape by-products (pomace, stems, and skin and seeds mixture), such as total polyphenolic content, total flavonoid content, and their antioxidant activity, for two white grape Romanian varieties (i.e., Fetească Albă and Tămâioasă Românească).

**Keywords:** white grape pomace; phenolics; antioxidant activity – IC<sub>50</sub>; principal component analysis; functional food.

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## PHYTOCHEMICAL INVESTIGATION OF *IRIS PSEUDACORUS* EXTRACTS BY HPTLC

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*Iris pseudacorus* L. (Iridaceae) or yellow flag is an herbaceous perennial, native to North America, north Africa, Europe, and Western Asia [1]. Given the current interest in the study of phytochemical compounds that is demonstrated by a large number of scientific studies, our research focused on an aquatic plant from the Danube Delta Biosphere Reserve, Romania [2]. High-performance thin-layer chromatography (HPTLC) has multiple benefits namely providing simultaneous qualitative and quantitative analysis [3].

In the current study, high-performance thin-layer chromatography was used to investigate the profiles of polyphenolic compounds of alcoholic extracts of *Iris pseudacorus*. To determine the level of toxicity of *Iris pseudacorus* extracts, their effects on wheat (*Triticum aestivum* L.) seed germination were tested against control samples. High-performance thin-layer chromatography was performed to identify some phenolic compounds from analyzed extracts. Plants contain a wide range of compounds with important pharmacological actions that can be used in the treatment of both chronic and infectious diseases or in pathologies where modern drugs prove to be ineffective.

In the current study, obtained data revealed that *Iris pseudacorus* extracts exhibit significant potential in terms of antioxidant activity, antibacterial and antifungal activity, or tannins and alkaloids content. In this respect, these extracts can improve the effect of some drugs such as antibiotics and diuretic substances.

**Keywords:** *Iris pseudacorus*.; phytochemical compounds; HPTLC.

**Acknowledgments:** This work was partially supported by Internal Grant 2024 no. 2487/31.05.2024 of Department of Chemistry, Physics, and Environment, Faculty of Sciences and Environment, "Dunarea de Jos" University of Galati, "Evaluation of Natural Organic Compounds with Biologically Active Potential".

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## CHEMICAL COMPOSITION AND ANTIMICROBIAL ACTIVITY ASSESSMENT OF ABSOLUTE FROM DIFFERENT ROSE (*ROSA DAMASCENA* MILL.) CULTIVARS

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A fairly large number of essential oils-producing plant species are known, of which only around 200 are cultivated industrially. From this series, the Damask rose (*Rosa damascena* Mill.) occupies a special place, due to the primary products obtained from petals, like concrete, absolute and rose water or preparations based on them, which are used on a large scale in various industries such as perfumery and cosmetics, but also in food and pharmaceutical products due to their antimicrobial, antioxidant, relaxing, anti-inflammatory, insecticidal, anti-HIV, hypnotic and others properties [1-3]. Compared to the main world producers, Moldova, unlike the recent past, is a modest producer represented by a few growers and rose processing factories, but the great variety of cultivars widespread here is important for the renaissance of this field and this study is a first step. The concrete was obtained from the petals collected from 4 varieties, Lani, Raduga, Ukraina (in the laboratory), and Krimaskaia (industrially), by extracting them with a non-polar solvent and absolute by concrete extraction with polar solvent and subsequent sedimentation of the waxes in a cold. As a result, concrete was obtained within yields ranging from 0.25% to 0.36% in the order of Lani=Krimaskaia<Ucraina<Raduga, and the absolute was obtained within yields ranging from 42.8% up to 72.3% in order Krimaskaia<Raduga<Ucraina<Lani. By GC-MS analysis of the absolute samples, along with other constituents, the major phenyl-ethyl alcohol was quantified in a range of 60.7% to 78.5% (in accordance with the UE standard) in order Raduga<Ucraina<Krimaskaia<Lani. The *in vitro* antimicrobial evaluation of the rose absolute samples was performed against 4 bacterial (*Xanthomonas campestris*, *Erwinia caratovora*, *Bacillus subtilis*, *Pseudomonas fluorescens*) and 2 fungal (*Candida albicans* and *Saccharomyces cerevisiae*) species and showed their moderate activity at MBC/MFC of about 0.06% - 0.03%.

**Keywords:** essential oil; *Rosa damascena* Mill.; chemical composition; antimicrobial activity.

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## EVALUATION OF THE BIOLOGICAL ACTIVITY OF SOME VEGETABLE EXTRACTS CONTAINING NEUROPROTECTIVE CHEMICAL COMPOUNDS

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*Sideritis spp.* is part of the genus *Sideritis*, *Lamiaceae* family, and is often found in Western and Southwestern areas of Europe [1]. *Rumex* is one of the 50 genera of the *Polygonaceae* family, which includes approximately 200 species that can adapt depending on their growth area [2].

This study followed the extraction of some active compounds with the help of solvents with different polarities. These extracts were subjected to various biochemical methods to reveal possible biological activities. It was wanted to highlight activities such as the anti-inflammatory effect, the antimicrobial and antitumor activity.

The results obtained are promising from both a chemical and a bioactive point of view so that *Sideritis spp.* and *Rumex spp.* can be considered for future *in vivo* and *in vitro* testing.

The importance of the obtained results shows that these extracts have a special potential that deserves to be further studied in new directions of chemical and biological research.

In conclusion, these extracts present a potential that can be considered for future research in the medical field, for various chronic or acute conditions.

**Keywords:** *Sideritis spp.*; *Rumex spp.*; chemical compounds; biological activities.

**Acknowledgments:** This work was partially supported by Internal Grant 2024 no. 2487/31.05.2024 of Department of Chemistry, Physics and Environment, Faculty of Sciences and Environment, "Dunarea de Jos" University of Galati, "Evaluation of Natural Organic Compounds With Biologically Active Potential" and ADER grant 5.2.1. – "Conservation and valorization of the genetic heritage of aromatic and medicinal species that can be cultivated on the territory of Romania".

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## GLUTARIC ACIDURIA DIAGNOSED BY NMR SPECTROSCOPY

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Rare diseases are currently defined as diseases affecting less than 1 in 2000 persons. There are over 6000 known rare diseases, and the combined incidence of rare diseases is estimated to affect as much as 4% of the entire population [1]. Most of these diseases are due to inborn errors of metabolism (IEM) and they are also referred to as intoxication-type metabolic disorders due to the fact that deficient enzymes lead to the accumulation of toxic metabolites in the organism [2, 3].

Glutaric aciduria is due to a defect in an enzyme that helps break down lysine, hydroxylysine, and tryptophan, which are building blocks of protein. Excessive levels of these amino acids and their intermediate breakdown products (glutaric acid, glutaconic acid, 3-hydroxyglutaric acid) can accumulate and cause damage to the brain, particularly the basal ganglia, which are regions that help control movement. Intellectual disability may also occur. The incidence of GA is estimated to 1 of every 30,000 to 40,000 births.

We are reporting on 1.5 years old boy suspected of mitochondrial disease, diagnosed by <sup>1</sup>H and COSY NMR as glutaric aciduria (GA), and subsequently confirmed as glutaric aciduria type 1 (GA1) through classical tests.

**Keywords:** NMR; rare diseases; propionic aciduria.

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## DEEP EUTECTIC SOLVENTS AS ADVANTAGEOUS EXTRACTANTS FOR ENHANCEMENT OF ANTIMICROBIAL ACTIVITY AND ANTI-INFLAMMATORY POTENTIAL OF *PERILLA FRUTESCENS* (L.) BRITT. EXTRACTS

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Deep eutectic solvents (DES) are considered potential green media with selective and efficient properties for extracting bioactive ingredients from medicinal plants. *P. frutescens* (L.) Britt. is a common annual plant in the Lamiaceae family, cultivated in the Southeast Asian region [1]. Modern pharmacological studies have shown that *P. frutescens* demonstrate various activities including, anti-inflammatory, anti-allergic, anti-tumor and antibacterial [2]. In this study, extracts of *P. frutescens* obtained with eutectic solvents and with the traditional methanol solvent are compared. The antimicrobial, anti-inflammatory activity and toxicity of these extracts were tested.

Following the use of the human albumin denaturation technique, the anti-inflammatory activity of *P. frutescens* extracts was highlighted. Also, the antimicrobial activity was tested against 3 microorganisms Gram-negative and Gram-positive bacteria. Genotoxicity and cytotoxicity were studied for all DES systems and extracts that showed antimicrobial activity. The analysis of the variation of the hydrogen donor component (HBD) in DES based on choline chloride proved to be an effective strategy for selecting the right solvent according to the target bioactive compounds to improve the biological activity.

Due to their outstanding properties to extract bioactive compounds from *P. frutescens* red leaves, deep eutectic solvents have a high potential to be used as friendly alternatives to conventional solvents, since their polarity is comparable to that of water and methanol.

**Keywords:** deep eutectic solvents; antimicrobial activity; toxicity.

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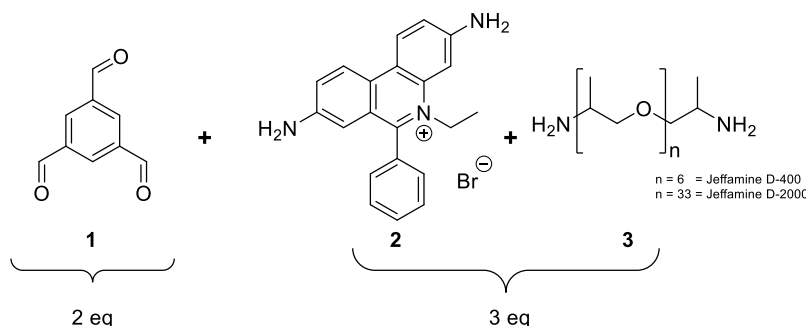
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## NEW ETHIDIUM BROMIDE BASED RUBERRY ORGANIC FRAMEWORKS AS ANION EXCHANGE MEMBRANES

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The anion exchange membranes [1] (AEMs) are a promising candidate for electrochemical application, such as facilitating selective HO<sup>-</sup> ion transport between the air electrode and the zinc electrode in zinc-air batteries. They serve as a physical barrier between the electrodes, preventing electrical short circuits. However, AEMs typically face challenges related to stability in basic solution and low conductivity. Therefore, our focus is on addressing these issues through a new membrane design. We present herein the design and the synthesis series of COF-ROF membranes that are prepared from 1,3,5-benzenetrialdheyde **1**, ethidium bromide **2** and different types Jeffamine **3** (Fig. 1). Ethidium bromide **2** has been previously used as a positively charged monomer in the preparation of covalent organic frameworks [2], which have demonstrated effective conductivity attributed to their porosity and the presence of quaternary amine groups. The membranes were prepared using stoichiometric amounts of tri-aldehyde (2 equivalents) and diamine (3 equivalents). Various ratios of rigid components (ethidium bromide) and flexible components (Jeffamine D-2000 or Jeffamine D-400) were employed to optimize both the COF/ROF ratio and the number of positive charges. All reactions were monitored using <sup>1</sup>H-NMR, and the membranes were characterized by FT-IR, DSC, and TGA. Furthermore, ion exchange capacity and the water uptake were assessed. The most promising membranes will be tested in zinc air battery.



**Figure 1.** Monomers used for membranes synthesis.

**Keywords:** ethidium bromide; covalent organic frameworks; anion exchange membranes; energy storage.

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## STRATEGIES TO IMPROVE MELOMEL PRODUCTION

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The current study recommends developing new melomel types using native bee honey as a starting material and diverse ingredients such as grapefruit, pomegranate, ginger, mint, pollen, and rose syrup. In addition, this study investigated at how additives affected the fermentation process as well as the physicochemical and sensory aspects of the produced beverages. As a control sample, the experiment's material contained meat produced in the laboratory (with honey: water ratio of 1:3) with no additives. Each sample used monofloral linden honey from local producers (Bacău, Romania) as a raw material. Two sets of experiments were carried out: with addition of fruit juice to the honey solution before and after alcoholic fermentation. The samples fermented for 10-16 days before being cooled for at least 10 days. The results demonstrated that diverse fruit juice additions had a substantial impact on the kinetics of the mead fermentation process as well as the sensory and physicochemical properties of the melomel varieties. For example, samples with additional pollen and grapefruit juice showed a significantly faster start of alcoholic fermentation than the control sample. We found that mixed fermentation increases the efficiency of the mead fermentation process while also greatly increasing the ethanol concentration. Our research has revealed that using of different methods of fermentation influences the physical, chemical, and sensory aspects of the final product. However, it was found that samples in which fruit juices were added after the alcoholic fermentation stage had better organoleptic characteristics than those in which a mixed fermentation was carried out.

**Keywords:** Honey fermentation; *Saccharomyces cerevisiae*; sensorial characteristics.

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## DEVELOPMENT AND CHARACTERIZATION OF NEW PLATINUM(IV) COMPLEXES WITH CARBOXYLIC OR PHENOLIC LIGANDS: SYNTHESIS, STRUCTURAL INSIGHTS, AND COMPUTATIONAL STUDIES

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Platinum-based anticancer treatments include side effects, drug efflux transporter resistance, and restricted cellular mechanism targeting [1]. In this study, new platinum(IV) complexes with carboxylic or phenolic ligands were synthesized and characterized in the attempt to overcome these issues. The platinum(IV) complexes were synthesized from platinum(II) cisplatin-type scaffolds by incorporating therapeutic agents as ligands. This made it possible to make multipurpose therapeutic agents that could be used as pro-drugs to improve selectivity while limiting toxicity.

Biological active inhibitors with hydroxyl groups were bound to platinum(IV) by a carbonate bridge, whereas those with carboxyl units were directly inserted as carboxylate ligands. A carbonate bridge is used for incorporating hydroxyl-containing ligands into platinum(IV) complexes by derivatizing the pharmacophore with N,N'-disuccinimidyl carbonate (DSC) and reacting with the hydroxyl group. The temperature and molar ratio control whether platinum(IV) complexes are mono- or dicarbonated [2].

The axial ligand coordination through carbonate or carboxylate units at platinum(IV) (obtained by oxidation of cisplatin raw material) allows intracellular reductants to cleave metal-ligand bonds and release the bioactive inhibitor and cytotoxic platinum(II) species.

DFT calculations assisted the stages preceding the synthesis, leading to the final design of the desired complexes. For all platinum(IV) complexes axially functionalized with carboxylic or phenolic ligands, the structural formula was assigned by <sup>1</sup>H, <sup>13</sup>C, <sup>195</sup>Pt NMR spectroscopy and mass spectrometry (HRMS).

**Keywords:** Pt(IV) prodrugs; carbonate-bridge-platinum(IV); DFT.

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