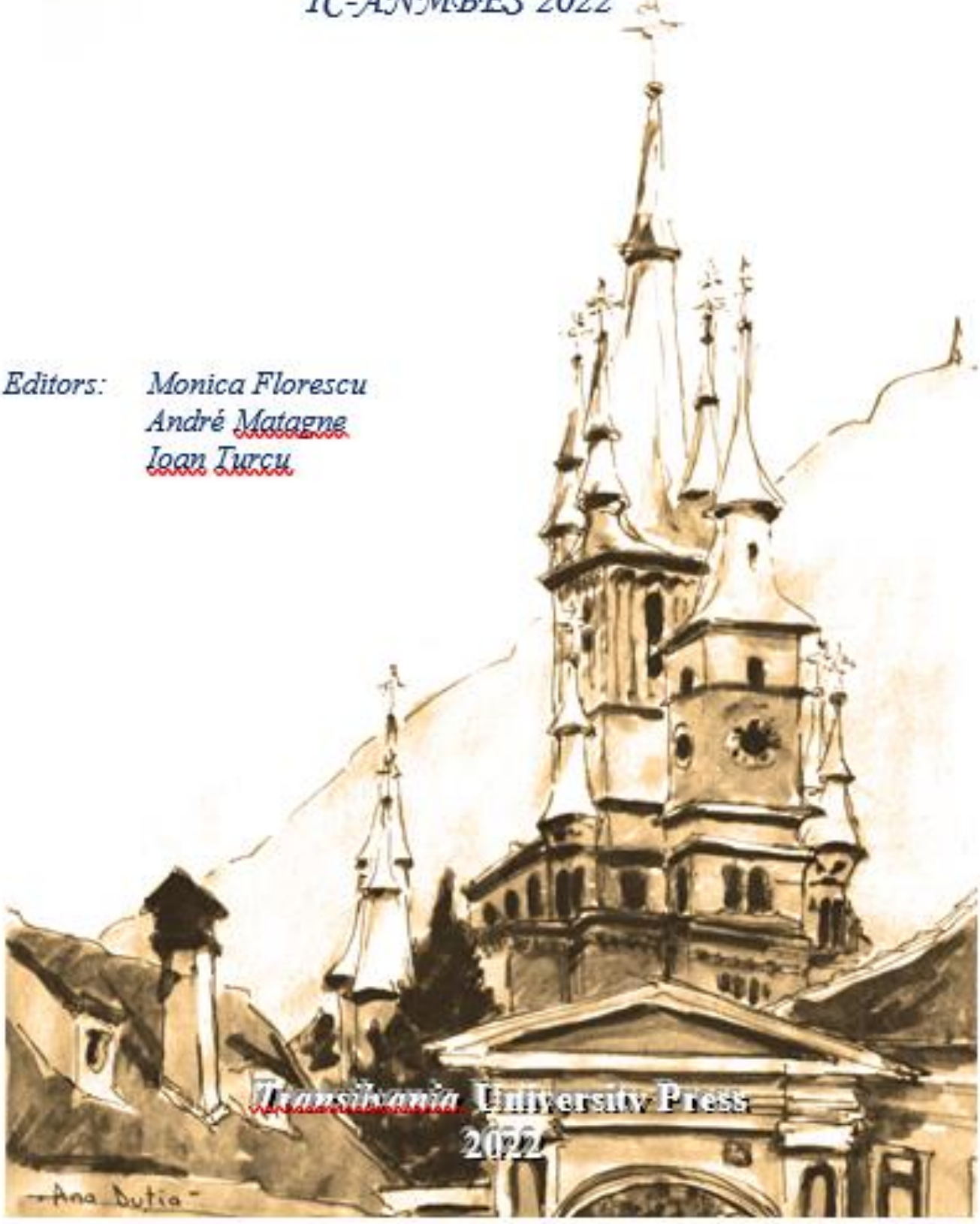
Analytical and Nanoanalytical Methods for Biomedical and Environmental Sciences

IC-ANMBES 2022

Editors: Monica Florescu
André Matagne
Ioan Turcu



Transilvania University Press
2022

***TRANSILVANIA* UNIVERSITY OF BRAŞOV**

International Conference on Analytical and Nanoanalytical Methods for Biomedical and Environmental Sciences

IC-ANMBES 2022

BOOK OF ABSTRACTS

Braşov, 8th -10th June, 2022

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EDITURA UNIVERSITĂŢII TRANSILVANIA DIN BRAŞOV

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B-dul. Iuliu Maniu 41A
Tel: 0268-476050
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Editură acreditată de CNCSIS
Adresa nr. 1615 din 29 mai 2002

ISSN 2360-3461

ISSN-L 2360-3461

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SCIENTIFIC PROGRAMME

ORAL COMMUNICATIONS

June 8th 2022	**Building *Aula Magna* of Transilvania University of Brasov. 41 A Iuliu Maniu Street, Brasov, 500091, Romania.**			
	Room Aula Magna, Chairperson: Monica Florescu, André Matagne, Ioan Turcu			
15.00-16.20			**Registration**	
16.20-16.30			**Opening Ceremony**	
16.30-17.00	Invited talk	I1	Dana Alina Magdas, Maria David, Ariana Raluca Hategan, Romulus Puscas, Adriana Dehelean, Gabriela Cristea, Camelia Berghian-Grosan	Application of acknowledged and emerging approaches for food authentication. Honey – a case study
17.00-17.30	Invited talk	I2	Sorin David, Raluca-Elena Munteanu, Mihaela Gheorghiu, Dumitru Bratu, Ionela-Cristina Petcu, Ioana-Cristina Cernat, Daniela Tudor, Eugen Gheorghiu	Towards a Point of Care System for Rapid, Phenotypic Antimicrobial Susceptibility Testing
17.30-18.00	Affinité Instruments	SI	Sandy Zhao	Democratizing SPR: Bringing the gold standard into your everyday lab
18.15-18.45			**Poster Session (P3, P5, P6 and P7 session numbers)**	
18.45-20.30			**Welcome Party**	
June 9th 2022	**Building *Aula Magna* of Transilvania University of Brasov. 41 A Iuliu Maniu Street, Brasov, 500091, Romania.**			
8.30 - 9.00	**Registration**			
	Room UI6, **Biophysical methods for protein science Chairperson: André Matagne**			
9.00 - 9.30	Invited talk	I3	Jacqueline Cherfils	Membranes prime the RapGEF EPAC1 to transduce cAMP signalling
9.30-10.00	Invited talk	I4	Mauro Dalla Serra	Pore-forming proteins
10.00-10.30	Invited talk	I5	Ana-Nicoleta Bondar	Dynamic interaction networks for conformational couplings of G-Protein Coupled Receptors
10.30-10.50	Contributed talk	O1	Moran Elias-Mordechai, Neta Sal-Man, Ronen Berkovich	Biomechanics of Type III Secretion System
	Room UI7, **Interfaces and biosensing, Chairperson: Eugen Gheorghiu**			
9.00- 9.30	Invited talk	I6	Danny O'Hare	Minimally invasive biosensors for clinical and biomedical applications
9.30- 10.00	Invited talk	I7	Liviu Movileanu	Single-molecule stochastic sensing of proteins in a complex biofluid: finding the needle in a haystack

10.00-10.30	Contributed talk	O2	Mihaela Gheorghiu, Cristina Polonschii, Szilveszter Gaspar, Sorin David, Raluca Munteanu, Eugen Gheorghiu	High-resolution electro-optical mapping of living cells for (bio)sensing: case studies on eukaryotic and prokaryotic (bacterial) cells
10.30-11.00	Contributed talk	O3	Monica Florescu, Melinda David, Claudia Chilom, Adrian Enache, Nicoleta Cazacu	Quantification of levothyroxine: choosing between detection methods
11.00-11.30	**Coffee Break and Poster Session (P3, P5, P6 and P7 session numbers)**			
	Room UI6, Biophysical methods for protein science **Chairperson: Jacqueline Cherfils**			
11.30-12.00	Invited talk	I8	Charly Robert, Maxime Gavage, Frédéric Kerff, Fabrice Bouillenne, Marylène Vandevenne, Julie Lecomte, Patrice Filée, André Matagne	Functional and structural characterization of Bone Morphogenetic Protein 2 and the antagonist Noggin
12.00-12.30	Invited talk	I9	Maximiliano Figueroa, Cristina Martina, André Matagne	Artificial protein design as a tool to study stability and folding in natural proteins
12.30-13.00	Invited talk	I10	Claudiu Gradinaru	Force Without Form: A Disordered Protein Complex Examined with Single-Molecule and Computational Tools
	Room UI7, Interfaces and biosensing, **Chairperson: Danny O'Hare**			
11.30-12.00	Invited talk	I11	Madalina Barsan, Caroline Sanz, Melania Onea, Victor Diculescu	Electrochemical investigations into protein degradation and inhibition
12.00-12.30	Invited talk	I12	Camelia Bala	Affinity-based biosensors as promising tools in doping control
12.30-12.50	Contributed talk	O4	Andra-Sorina Tatar, Cosmin Farcau, Simion Astilean, Sanda Boca	Plasmonic immunosensors based on gold nanourchins for biomarker detection
13.00-14.00	**Lunch**			
	Room UI6, **(Nano)biotechnology,** **Chairperson: Liviu Movileanu**			
14.00-14.30	Invited talk	I13	Zexi Xu, John Seddon, Paul Beales, Michael Rappolt, Arwen Tyler	Lipid nanoparticles with pH-triggered change in their internal connectivity
14.30-14.50	Contributed talk	O5	Szilveszter Gaspar	Electrochemically synthesized nanorods for the optical stimulation of neurons
14.50-15.10	Contributed talk	O6	Anda Les, Helmina Ardeleanu, Nicoleta Melniciuc Puica, Iuliana Motrescu, Dorina Creanga	Quantum-chemical and experimental study on the interactions between the magnetic core and the molecular shell of iron oxide nanoparticles in aqueous suspensions for biomedical applications

15.10-15.30	Contributed talk	O7	Anca Minuti, Dumitru Herea, Luminita Labusca, George Stoian, Horia Chiriac, Nicoleta Lupu	A straightforward method for cell sample preparation to allow a reliable image of the nanomaterials adhering to the surface, using scanning electron microscopy
15.30-15.50	Contributed talk	O8	Luminita C. Miclea, Mona Mihailescu, Nicolae Tarba, Ana-Maria Brezoiu, Ana Maria Sandu, Raul-Augustin Mitran, Daniela Berger, Cristian Matei, Mihaela G. Moisescu, Tudor Savopol	3D reconstructions of intracellular distribution of folate functionalized silica nanoparticles using combined microscopy techniques (fluorescence, dark field and hyperspectral microscopy)
	Room UI7, **(Micro)spectroscopy** **Chairperson: Claudiu Gradinaru**			
14.00-14.30	Invited talk	I14	Pierre-Emmanuel Milhiet	Membrane Organization and Remodelling probed by Atomic Force Microscopy
14.30-14.50	Contributed talk	O9	Alia Colnita, Daniel Marconi, Ioana Brezestean, Nicoleta Dina, Lucian Barbu-Tudoran, Ioan Turcu	Ultrasensitive SERS detection of biomolecules on nanoimprinted substrate
14.50-15.10	Contributed talk	O10	Claudia Stihi, Antoaneta Ene	Romanian moss surveys for temporal trends assessment of heavy metals atmospheric deposition
15.10-15.30	Contributed talk	O11	Arkadiusz Matwijczuk, Lidia Ślusarczyk, Grzegorz Czernel, Iwona Budziak-Wieczorek, Dariusz Karcz, Beata Myśliwa-Kurdziel, Monika Serbo-Hooper, Gotard Burdziński, Andrzej Niewiadomy	Spectroscopic and Theoretical Studies on the Effects of Excited State Intramolecular Proton Transfer in 4-[5-(naphthalen-1-ylmethyl)-1,3,4-thiadiazol-2-yl]benzene-1,3-diol
15.30-15.50	Contributed talk	O12	Lidia Ślusarczyk, Arkadiusz Matwijczuk, Grzegorz Czernel, Dariusz Karcz, Mariusz Gagoś, Jose Chavez, Joseph Kimball, Luca Ceresa, Zygmunt Gryczyński, Ignacy Gryczyński, James Hooper	Studies on mode of action of the synergistic systems incorporating 1,3,4-thiadiazole derivatives and polyene-based antibiotics against selected fungal species
15.50-16.20	**Coffee Break and Poster Session (P1, P2, P4 and P8 session numbers)**			
	Room UI6, Novel materials and biomaterials **Chairperson: Pierre-Emmanuel Milhiet**			
16.20-16.50	Invited talk - online	I15	Edmond Magner	Electrochemical Immobilisation of Enzymes for Biocatalysis
16.50-17.20	Invited talk,	I16	Oana Hosu, Andreea Cernat, Mihaela Tertis, Bogdan Feier, Cecilia Cristea	Functionalized materials as versatile tools for advanced (bio)sensing systems
17.20-17.40	Contributed talk	O13	Alina Vasilescu, Roberta Banciu, Victoria Paun, Valentina Dinca, Anca Bonciu, Petru Epure, Cristina Purcarea	Enzymatic inks based on aldehyde dehydrogenases for the electrochemical detection of aldehydes in a wide temperature range

17.40-18.00	Contributed talk	O14	Mihaela Deaconu, Ana-Maria Prelipcean, Ana-Maria Brezoiu, Mioara Prundeanu, Daniel Lincu, Raul-Augustin Mitran, Grădișteanu Pîrcălăbioru Grațiela, Cristian Matei, Daniela Berger	Novel composites based on natural compounds for topical applications
19.00-23.00	**Gala Dinner (Restaurant Platinum, Brasov – Romania)**			
June 10th 2022	**Building *Aula Magna* of Transilvania University of Brasov. 41 A Iuliu Maniu Street, Brasov, 500091, Romania.**			
	Room Aula Magna, **Innovation in Environmental Monitoring, Chairperson: Camelia Bala**			
9.30-10.00	**Poster Session (even numbers)**			
10.00-10.30	Invited talk	I17	George Ivanov, Petar Ivanov, Velichka Strijkova, Evgenija Bogdanova, Todor Vlakhov, Anna Amova	Chemical sensors for volatile organic compounds for ecological monitoring based on nano-thin organized organic films
10.30-10.50	Contributed talk	O15	Anda Gabriela Tenea, Gabriela Vasile, George Buica, Cristina Dinu, Mihaela Mureseanu	Electrochemical method for mercury detection in wastewater samples using a portable device
10.50-11.10	Contributed talk	O16	Petru Epure, Ana-Maria Gurban, Mihaela Doni	Innovative 3d suction lysimeter and portable detector for on-field monitoring of pollutants directly in soil
11.10-11.30	**Coffee Break**			
	Room Aula Magna, **Food production and authentication, Chairperson: Victor Diculescu**			
11.30-11.50	Contributed talk	O17	Rebeca Moldovan, Karolina Milenko, Elizaveta Vereshchagina, Bogdan Iacob, Kenneth Schneider, Cosmin Farcău, Ede Bodoki	Spectroelectrochemical Detection of Thiabendazole Residues in Fruit Juice
11.50-12.10	Contributed talk	O18	Camelia Berghian-Grosan, Maria David, Alina Magdas	Raman spectroscopy and Machine Learning – a new methodology for fruit spirits authentication
12.10-12.30	Contributed talk	O19	Adriana Dehelean, Alina Magdas, Gabriela Cristea, Ioana Feher, Ariana Hategan	The differentiation of Transylvanian fruit distillates using supervised statistical tools based on isotopic and multi-elemental fingerprint
12.30-12.50	Contributed talk	O20	Gabriela Ioana Cristea, Cezara Voica, Romulus Puscas, Ioana Feher, Dana Alina Magdas, Adriana Dehelean	Pork meat authenticity – from stable isotopes and elemental fingerprint to table…
12.50-13.15	**Closing Ceremony**			
14.00-22.00	**Social Program – Visit and Dinner at Cantacuzino Castle, Busteni, Romania**			

POSTER COMMUNICATIONS

Number	Authors	Title
P1. Biophysical methods for protein science & Biomembranes and model membranes		
P 1.1	Lorant Janosi, George Necula, Alexandra Farcas, Ioan Turcu	*In Silico* Modeling of a Short Arginine and Tryptophan-based Antimicrobial Peptide's Interaction with Bacterial and Mammalian Membranes
P 1.2	Claudia Gabriela Chilom, Nicoleta Cazacu	A pharmacological and molecular docking approach of polyphenolic compounds and outer membrane protein TolC from *E. Coli*
P 1.3	Bogdan Zorila	Components of (hydro)alcoholic extracts from propolis affects the order of bilayer and microenvironment in model lipid membranes
P 1.4	Niculina Sonia Suvar, Paula Podea, Eliza Mateh Eszter, Andreea Maria Iordache, Razvan Dragoescu	Nutritional chemical evaluation and antioxidant capacity of spices
P2. Interfaces and biosensing		
P 2.1	George R. Ivanov	A high surface-to-volume ratio monolayer nano-thin organic film for chemical sensor applications
P 2.2	Vlad-Andrei Moldovan, Alexandru-Milentie Hada, Sorina Suarasan, Timea Nagy-Simon, Adriana Vulpoi, Simion Astilean, Monica Potara	Aptamer-modified citrate-capped gold nanoparticles for sensitive visual detection of C-reactive protein
P 2.3	Teodora Lupoi, Denisa Capatana, Bogdan George Feier, Cecilia Cristea	Aptasensors for the detection of molecules involved in QS and biofilm formation
P 2.4	Andra-Sorina Tatar, Sanda Boca, Alexandra Falamas, Lucian Barbu-Tudoran, Cosmin Farcau	Self-assembled gold nanostar films as substrates for surface-enhanced optical spectroscopy
P 2.5	Cristian Mușuroi, Marius Volmer, Elena Helerea, Mihai Oproiu	An analytical approach for magnetoresistive sensor performance on magnetic nanoparticles detection for biosensing systems
P3. Early diagnosis and precision medicine & Clinical diagnosis and therapy		
P 3.1	Alexandra Pusta, Mihaela Tertis, Rodica Turcu, Ladislau Vekas, Cecilia Cristea	Targeted drug delivery systems based on magnetic and gold nanoparticles for the treatment of hepatocellular carcinoma
P 3.2	Alina Tantau, Alina Mandrutiu, Mihaela Laszlo, Vasile Negrean, Cristian Tefas, Carmen Preda, Dan Vodnar, Ciprian Brisc, Marcel Tantau	Viability and clinical effects of Lactobacillus Plantarum ATCC 8014 using an innovative probiotic drink in human being
P 3.3	Ana Maria Raluca Gherman, Vasile Chiș, Nicoleta Elena Dina	Can molecular docking solely predict antibiotics' bactericidal activity?

	P4. Innovation in Environmental Monitoring	
P 4.1	Lucian-Gabriel Zamfir, Petru Epure, Cristina Mitrea, Mariana Constantin, Iuliana Raut, Maria-Luiza Jecu, Mihaela Doni, Ana-Maria Gurban	A comparative study of different nanomaterials used in the development of sensitive electrochemical sensors for nitrite determination and monitoring in soil
P 4.2	Cristina Dinu, Anda Gabriela Tenea, Gabriela Geanina Vasile, Ecaterina Anca Serban	Bioaccumulation of toxic metals in two different thymus species
P 4.3	Abdulhusein Jawdhari, Dan Mihăilescu, Cristian-Emilian Pop	Microplastics induced toxicity on Oreochromis niloticus (Nile tilapia)
P 4.4	Valentina Andreea Petre, Ionut Nicolae Cristea, Ecaterina Anca Serban, Florentina Laura Chiriac	Bioaccumulation and translocation factors of synthetic auxins in aromatic plants (Basil)
P 4.5	Markus Zetes, Alexandru Milentie Hada, Monica Focsan, Timea Nagy-Simon, Simion Astilean, Ana Maria Craciun	Synthesis and characterization of novel histidine-stabilized gold nanoclusters for the sensitive and selective detection of Fe from water samples
P 4.6	Florinela Pirvu, Cristina Ileana Covaliu, Iuliana Paun, Vasile Ion Iancu, Florentina Laura Chiriac	Development and Validation of new HPLC-DAD method for detection of anti-inflammatory drugs in surface water samples
P 4.7	Ionuț Nicolae Cristea, Alina Tătăruş, Andreea Valentina Petre, Laura Florentina Chiriac	Novel method for assessment of various herbicides in soil and surface water from agricultural areas
P 4.8	Maria – Loredana Soran, Otilia Ana Culicov, Ildiko Lung, Adina Stegarescu, Ocsana Opriș	The impact assessment of metal/metal salts on onion
P 4.9	Florentina Laura Chiriac, Valentina Andreea Petre, Iuliana Paun, Florinela Pirvu, Ionut Nicolae Cristea, Vasile Ion Iancu	Ultra-trace LC-MS/MS method for detection and quantification of perfluoroalkyl substances (PFAS) in Romanian surface waters
P 4.10	Ecaterina Anca Serban, Gabriela-Geanina Vasile, Cristina Dinu, Anda-Gabriela Tenea, Daniela Simina Stefan, Ileana Rau	Ultrasensitive method for quantification of tin in water samples using new HG-ICP-EOS equipment
P 4.11	Gyorgy Deak, Răzvan Matache, Tiberius Dănălache, Marius Raischi, Raluca Prangate	Pilot validation system of breeding habitats of sturgeon species
	P5. Novel materials and biomaterials	
P 5.1	Manuela Stan, Adriana Popa, Dana Toloman, Dan Vodnar, Gheorghe Borodi, Lucian Barbu-Tudoran, Sergiu Macavei, Ovidiu Pana	Nickel oxide-silver-antibiotic nanocomposites for antimicrobial applications
P 5.2	Melinda David, Teodor Adrian Enache, Lucian Barbu-Tudoran, Monica Florescu, Camelia Bala	Biologically synthesized gold nanoparticles for the detection of reactive oxygen species
P 5.3	Anca Andreea Turcanu, Ecaterina Matei, Maria Rapa, Andra Mihaela Predescu, Andrei Constantin Berbecaru, George Coman, Cristian Predescu	Biowaste valorization via HTC process for the retention of some emerging pharmaceutical pollutants from aqueous solutions
P 5.4	Maria Coroş, Florina Pogăcean, Codruța Varodi, Stela Pruneanu	Effect of hydrothermal doping on the morphology, structure and composition of sulphur, boron-co-doped graphene
P 5.5	Codruta Varodi, Maria Coros, Florina Pogacean, Alexandra Ciorita, Alexandru Turza, Stela Pruneanu	Electrochemical Detection of Piroxicam with Nitrogen-Doped Graphene-Based Sensor

P 5.6	Maria Rapa, Anca Andreea Turcanu, Carmen Gaidau, Mariana Daniela Berechet, Anamaria Mosutiu, Andrei Constantin Berbecaru, Mirela Sohaciu, Cristian Predescu	Exploring of hydrolysate keratin and biopolymers spinnable properties to fabricate nanofibers for wound healing management
P 5.7	Violeta-Carolina Niculescu, Amalia Soare, Irina Petreanu	Facile synthesis of raspberry-like mesoporous silica nanomaterial
P 5.8	Codrut Costinas, Catalin Alexandru Salagean, Liviu Cosmin Cotet, Monica Baia, Klara Magyari, Lucian Baia	Investigations on the stability of graphene oxide dispersions
P 5.9	Christina Zalaru, Rodica Tatia, Ioan Calinescu, Lucia Moldovan	Mathematical modeling by Response Surface Method of a triterpene saponins mixturewith a raised antiproliferative effect
P 5.10	Christina Zalaru, Diana Pricope, Florea Dumitrascu, Constantin Draghici, Ludmila Otilia Cinteza, Maria Marinescu, Isabela Ana Tarcomnicu, Carmen Mariana Chifiriuc, Marcela Popa	Novel azopyrazole compoundswith antibacterial activitiy
P 5.11	Alexandra Falamas, Maria Stefan, Cosmin Farcau, Ioana Marica, Fran Nekvapil	Photophysical and vibrational spectroscopic behavior of Rhodamine 6G deposited on ZnO and gold decorated ZnO nanoparticles thin films
P 5.12	Ovidiu Pana, Sergiu Macavei, Maria Stefan, Dana Toloman, Adriana Popa, Cristian Leostean, Lucian Barbu-Tudoran, Manuela Stan	PLD deposition of FePt-BaTiO3 thin films heterostructures
P 5.13	Maria – Loredana Soran, Ildiko Lung, Adina Stegarescu, Ocsana Opriș, Otilia Ana Culicov, Alexandra Ciorîță	The antibacterial properties of nanocomposites based on antibiotic association with carbon nanotubes and metal oxides
P 5.14	Daniel Marconi, Alia Colniţă, Ioana Brezestean, Lucian Barbu-Tudoran, Ioan Turcu	Tunable anti-counterfeit labels based on Ag coated nanotrenches arrays
P 5.15	Maria Marinescu, Ludmila Otilia Cinteză, Iulian Ioniţă, Christina Marie Zălaru	Synthesis and characterization of some azo-compounds as nonlinear optical materials
P 5.16	Maria Marinescu, Ludmila Otilia Cinteză, Iulian Ioniţă, Maria Antonia Tanase, Andreia Cristina Soare, Christina Marie Zălaru	Synthesis, NLO properties and DFT studies of some heterocyclic compounds
P6. (Micro)spectroscopy		
P 6.1	Daniel Marconi, Alia Colniţă, Nicoleta Elena Dina, Ioana Brezestean, Diana Bogdan, Lucian Barbu-Tudoran, Ioan Turcu	High quality, 3D silver nanotrenches fabricated by nanoimprint lithography as flexible SERS detection platform
P 6.2	Andreea Ioana Brezestean, Elena Nicoleta Dina, Maria Raluca Ana Gherman, Alia Colniță, Daniel Marconi	SERS-based smart antibiogram: from concept to routine analysis
P 6.3	Andreea Ioana Brezestean, Maricel Bocăneală, Ana Maria Raluca Gherman Sebastian Alin Porav, Irina Kacsó, Elena Rakosy Tican, Elena Nicoleta Dina	Spectroscopic investigation of exopolysaccharides purified from Arthrospira platensis cultures as potential bioresources
P 6.4	Alexandru Cătălin Sălăgean, Liviu Cosmin Coteț, Monica Baia, Klara Magyari, Lucian Barbu, Lucian Baia	The study of molybdenum disulfide phase changes and its stability by micro-Raman spectroscopy

P7. (Nano)biotechnology		
P 7.1	Mihaela Mic, Adrian Pirnau, Calin G. Floare, Gabriel Marc, Ovidiu Oniga, Laurian Vlase, Mircea Bogdan, Bianca-Maria Tihăuan	Synthesis and molecular interaction between drugs with strong antioxidant and antiradical activity and macromolecular receptors
P 7.2	Isabela S. Dragomir, Alina Asandei, Irina Schiopu, Ioana C. Bucataru, Loredana Mereuta, Tudor Luchian	Detection of nucleobases on short functionalized peptide-nucleic acid sequences using nanopore-tweezing method
P 7.3	Alexandra Farcas, Lorant Janosi, Simion Astilean	DNA-conjugated gold nanoparticles as key components in the design of non-viral CRISPR/Cas9-Gold-based delivery vehicles
P 7.4	Daria Stoia, Madalina Nistor, Dumitrita Rugina, Monica Focsan	Polymeric microcapsules for targeted and controlled delivery of therapeutic molecules at human retina level
P 7.5	Ioana Cezara Bucataru, Loredana Mereuta, Alina Asandei, Isabela Dragomir, Tudor Luchian	Protein nanopore-based method for sequence specific detection of single-stranded DNA using gold nanoparticles and peptide nucleic acids
P 7.6	Alexandru Stefan Chis, Ștefania Dana Iancu, Oana Maria Biro, Andrei Ștefancu, Nicolae Leopold	Silver nanogrid substrates for accurate SERS analysis
P 7.7	Adrian Pirnau, Mihaela Mic, Calin G Floare, Maria Miclăuș, Irina Kacso, Mariana Palage, Mircea Bogdan, Bianca-Maria Tihăuan	Spectroscopic, calorimetric and molecular modeling approaches of the interaction of quaternary ammonium compound with β-CD
P8. Food production and authentication		
P 8.1	Florina-Dorina Covaciu, Zaharie Moldovan, Gabriela Cristea	Determination of the fatty acids, cholesterol and glycerides in pork meat fat using the GC-FID and GC-MS system
P 8.2	Roberta Banciu, Alina Vasilescu, Victoria Ioana Paun, Pablo Fanjul-Bolado, Cristina Purcarea, Andreea Catalina Lulea	Electrochemical assay of acetaldehyde in wines based on novel a cold–active aldehyde dehydrogenase: comparison of mediated versus non mediated detection
P 8.3	Andreea Catalina Lulea, Robert Ruginescu, Roberta Maria Banciu, Elena Brinduse, Petru Epure, Cristina Purcarea, Alina Vasilescu	Fast electrochemical measurement of laccase activity for monitoring grapes' infection with Botrytis cinerea
P 8.4	Florina-Dorina Covaciu, Camelia Bergian-Grosan, Ioana Feher, Dana-Alina Magdas	Fatty acid profile analysis in sunflower oils by GC-FID and vibrational spectroscopic methods
P 8.5	Dana Alina Magdas, Maria David, Ariana Raluca Hategan, Camelia Berghian-Grosan	Fruit spirits authentication based on Raman spectroscopy in corroboration with advanced statistical tools
P 8.6	Camelia Berghian-Grosan, Csilla Muller Molnar, Alina Magdas	Honey – a food matrix case for authenticity evaluation by Raman spectroscopy and Machine Learning algorithms
P 8.7	Adriana Dehelean, Gabriela Cristea, Alina Dana Magdas, Ioana Feher, Romulus Puscas, Valentin Mirel	Isotopic and elemental composition of meat and their differentiation according to geographical area via multivariate chemometric analysis
P 8.8	Csilla Molnar, Simona Cinta Pinzaru	Quantitative SERS Analysis of Cylindrospermopsin Cyanotoxin in Solution and in Fish Tissue
P 8.9	Csilla Molnar, Berghian-Grosan Camelia, Cinta Pinzaru Simona, Magdas Alina	Rapid detection of Thiabendazole pesticide in frozen fruits and vegetables commercialized in Romanian stores

Oral Communications

Invited Talks

I1. Application of acknowledged and emerging approaches for food authentication. Honey – a case study

Dana Alina Magdas, Maria David, Ariana Raluca Hategan, Romulus Puscas, Adriana Dehelean, Gabriela Cristea, Camelia Berghian-Grosan

[1] National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, 400293, Romania

The development of new analytical approaches, able to properly address food and beverages authenticity issues, represents nowadays a constant preoccupation among research and control laboratories. Among the most falsified food commodities, honey has a special place due to the limited available quantities corroborated with high market demand, especially in regard to some varieties. The most appreciated honey features, either in terms of taste or medicinal effects, are directly related to the botanical and geographical origin and consequently directly reflected in its commercial value. For these reasons, the development of easy-to-use but also reliable tools for rapid honey authenticity detection needs to be developed. In this light, a comparison between the efficiency of acknowledged markers (stable isotope composition and elemental profile) for the honey differentiation and discrimination potential of vibrational spectroscopy (IR and Raman) is presented and discussed in the present work. Each method is treated in terms of both positive results and limitations; particular consideration is paid to the current challenges and further perspectives. For the development of the honey recognition models, advanced chemometric tools were used and special attention was given to the experimental data pre-processing step, in order to increase the accuracy rates of the developed models. Moreover, the relationship between the markers based on which the models were constructed and each specific classification was investigated.

Acknowledgement:
This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS–UEFISCDI, project number PN-III-P4-ID-PCE-2020-0644 (Contract no. 7PCE/2021), within PNCDI III.

I2. Towards a Point of Care System for Rapid, Phenotypic Antimicrobial Susceptibility Testing

Sorin David[1], Raluca-Elena Munteanu[1, 2], Mihaela Gheorghiu[1, 2], Dumitru Bratu[1], Ionela-Cristina Petcu[1], Ioana-Cristina Cernat[1], Daniela Tudor[1, 2], Eugen Gheorghiu[1, 2]

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Assessing the amount & viability of bacteria without calibration curves, is an unmet capability for point-of-care instrumentation. Advancing our innovative approach[1, 2], we demonstrate rapid, accurate, direct assessment of target bacteria in a label-free, lab-on-a-chip platform.

The talk will bestow conceptual and experimental advances to enable microbial capturing using a novel magnetophoretic setup, formation of aggregates comprising bioaffine Magnetic Beads (MB) and bacterial cells. Their analysis allows dynamic quantitation of markers of cell Viability and bacterial concentration.

Electrical impedance spectroscopy (EIS) & periodic magnetic actuation are deployed for dynamic EIS fingerprinting of the magnetophoresis of affinity bound bacteria- MB aggregates.

Magnetophoresis enabling measurement cells with custom designed two micro electrodes addressed by EIS at two frequencies are optimized to provide a direct measure of: (1) cell Capacitance, hence of membrane integrity as marker of cell Viability, and (2) cell Concentration, consistent with: microscopic modeling[3] and complementary EIS & optical assays[4,5]. Case studies for rapid phenotypic assessment of bactericidal antibiotics effect will address cell membrane capacitance variations consistent with viability loss.

The simplicity of design and operation to assess the amount and the viability of target bacteria provides unique capabilities for an easy adaptation for point-of-care/ in field use. The approach is also suitable for other applications i.e., to quantitate live or dead cells (including non-culturable) from various biomedical and environmental samples.

Acknowledgements:
Support of PNIII projects P4-ID-PCE-2020-2432 and -1433 as well as P2-2.1-PED-2019-5155, -5185, -4932 is gratefully acknowledged.

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SI. Democratizing SPR: Bringing the gold standard into your everyday lab

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Surface plasmon resonance (SPR) is considered a gold standard technique for drug screening but instruments are traditionally only found in large pharmaceutical companies with high-throughput and automation design in mind. As a result, SPR is seen as an inaccessible option, being complex and costly to operate. However, SPR can and should be available for multi-faceted biosensing applications as it is inherently a sensitive, real-time, and label-free technique.

Affinité Instruments has made it its mission to offer portable, affordable and easy-to-use SPR to enable all researchers to use it as an analytical tool in diverse fields. Applications can expand from life sciences to material and environmental sciences. It can be employed as an analytical tool for rapid biomarker detection, quick binding and surface material characterization, as well as environmental monitoring. Example applications as well as latest work using portable SPR such as development of saliva-based point of care tests to detect SARS-CoV-2 will be presented. Plus, hear from an Affinité application scientist, who will explain what it really means to have a portable SPR in your lab and how it can act as a ‘swiss army knife’ in any research lab to be used anytime, anywhere.

I3. Membranes prime the RapGEF EPAC1 to transduce cAMP signaling

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EPAC1 is a guanine nucleotide exchangefactor for small GTPases of the Rap family. It is a major transducer of cAMP signaling in cells and a therapeutic target in cardiac diseases. However, how its very low affinity for cAMP allows it to respond to physiological cAMP fluxes has remained a conundrum. Here, we identify anionic membranes as the missing component of EPAC1 activation. We find that membranes increase the affinity of EPAC1 for cAMP by 2 orders of magnitude, bringing it to the same range as that reported for the other major cAMP transducer, protein kinase A. Furthermore, EPAC1 is partially activated by anionic membranes in the absence of cAMP, and anionic membranes and cAMP synergize to yield a dramatic increase of its GEF activity . Our results indicate that under physiological conditions, EPAC1 must be primed by membranes to respond to cAMP. We analyzed the mechanism of action of the chemical inhibitor CE3F4 in this activation framework, revealing that in cells EPAC1 must be fully activated by both cAMP and the membrane to be inhibited by CE3F4. Together, our findings reformulate previous concepts of cAMP signaling to include a hitherto overlooked role of membranes through EPAC proteins, with important implications for drug discovery.

I4. Pore-forming proteins

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Pore-forming toxins (PFT) constitute the largest and best characterized class of protein toxins, accounting for more than 30% of all known bacterial protein toxins. They are potent virulence factors evolved during ancient competition among organisms for defense and/or attack purposes. Interestingly, similar structures and modes of action are also adopted by components of the immune system, like perforin and complement, and by antimicrobial peptides.

PFT are normally able to drill poorly selective nanometer-sized holes into the target cell membranes, causing cell death through osmotic imbalance.

Regarding the pore structure, two conformations have been described: a purely proteinic channel or a protein-lipid mixed arrangement. This second case is characterized by the co-presence of lipid and protein elements in the pore walls. Lipid heads could either intercalate between protein monomers or constitute the chord of arc shaped pores. In both cases the lipid lamellar structure is destroyed and lipids should bend, assuming a toroidal shape.

Here I will shortly discuss examples of both classes of functional pores formed by bacterial an animal toxins, investigated by biophysical techniques, like electrophysiology, AFM, fluorescence. Experimental evidences supporting the ability to punch proteolipidic nanopores into lipid membranes will be presented.

I5. Dynamic interaction networks for conformational couplings of G-Protein Coupled Receptors

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G-Protein Coupled Receptors (GPCRs) are membrane proteins which recognise and bind extracellular ligands to initiate cell signalling pathways of major interest to human health and disease. The molecular mechanisms by which GPCRs couple ligand binding to large-scale protein conformational change are essential to understand, because description of these mechanisms could guide the development of GPCR-targeted drugs. To this aim, we have developed graph-based algorithms that facilitate efficient analyses of large data sets of GPCR structures from structural biology and numerical simulations, and derived accurate force-field parameters of opioid drugs. From analyses of a large set of static GPCR structures, and from numerical simulations of opioid receptors, we identify internal hydrogen-bond networks whose dynamics could be used to characterise conformational intermediates of GPCRs. The accurate force-field parameters we derived for opioid drugs enable accurate atomistic simulations for probing drug-receptor interactions.

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I6. Minimally-invasive biosensors for clinical and biomedical applications

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Biosensors present difficulties associated with *in vivo* implementation. Implantation in tissue can cause foreign body responses that affect both sides of the interface: protein adsorption can interfere with molecular recognition chemistry, affect mass transport and lead to partitioning of the analyte. Inflammation leads to entrainment of low molecular weight species and the mere presence of the sensor compresses capillaries. Finally, surgical implementation presents considerable ethical barriers for device development.

Alternative approaches include the use of microneedle sensors to sample interstitial fluid in viable epidermis, avoiding exposure to blood and nerve endings and enabling facile device recovery in the case of failure. I shall present the use of microneedle enzyme-based biosensors for therapeutic drug monitoring and closed-loop dosing for antimicrobial drugs[1] , [2]and for the measurement of tissue lactate concentrations as a biomarker for sepsis.

Similarly, the analysis of exhaled condensed breath is relatively non-invasive and, with appropriate control of the device's thermofluid characteristics, can be used to quantify hydrogen peroxide as a biomarker for inflammation associated with chronic obstructive pulmonary disease[3]. We have also been able to determine lactate concentrations in EBC and shown good agreement in healthy volunteers in comparison with LC-MS reference methods based on venous blood.[4]

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I7. Single-molecule stochastic sensing of proteins in a complex biofluid: finding the needle in a haystack

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A protein-selective biological nanopore has been used for identifying individual proteins in a complex biological fluid. Our approach thwarted traditional nanopore techniques of protein detection that rely on the analysis of current blockages. On the contrary, we engineered a protein bait at the tip of the nanopore, so the protein detection occurred on its extramembranous side.[1, 2] A key player in this approach was a polypeptide extension on the protein bait that facilitated the single-molecule detection of proteins in real time. Then, we optimized electrical recordings of this modular nanopore, so that we extended our method in a biofluid. Because protein captures outside the nanopore were noted as pore openings, these events were also unambiguously separated from current blockages produced by the biofluid constituents.[3] Finally, our strategy can provide a quantitative assessment of a given protein in challenging conditions of complex biofluids.

Acknowledgments.
I am thankful to my recently graduated PhD students, Avi Thakur and Lauren Ashley Mayse, as well as others in my laboratory and funding agency (The U.S. National Institutes of Health, grants R01 GM088403 and R01 GM129429).

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I8. Functional and structural characterization of Bone Morphogenetic Protein 2 and the antagonist Noggin

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Bone morphogenetic proteins (BMPs) belongs to the transforming growth factor-β superfamily of multifunctional cytokines. They induce a broad set of different cellular effects, including stem cell maintenance, migration, differentiation, arrest of maturation, proliferation, and apoptosis. These findings have opened stimulating opportunities towards new therapeutic approaches for the treatment of many diseases and/or metabolic disorders. Thus, BMP-2 and BMP-7 have been approved by the U.S. Food and Drug Administration for clinical application in the context of bone repair. Unfortunately, the lack of knowledge concerning BMP interaction pathways has been responsible for a misunderstanding and an underappreciation of the side effects associated with BMP-based therapeutic approaches. Therefore, the high degree of interest in BMPs as potential biopharmaceuticals is now mitigated by some unresolved issues.

In this study, we used BMP-2 as a model system to gain insight into both the relationship between structure and function in BMPs and the principles that govern affinity for their cognate antagonist Noggin. Both proteins were produced and characterized with the help of complementary biophysical techniques, including optical spectroscopies, mass spectrometry, multi-angle light scattering coupled with size exclusion chromatography, and X-ray crystallography. Furthermore, a series of *in vitro* cell-based assays were performed, in combination with enzymatic measurements, RT-qPCR and matrix staining, which allowed monitoring of differentiation. Finally, we developed efficient live-imaging assays to follow in real-time the sequential passage of stem cells into mature chondrocytes, and then into hypertrophied chondrocytes.

I9. Artificial protein design as a tool to study stability and folding in natural proteins

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The central dogma in structural biology is: the tertiary structure of a protein is defined by its primary structure. Determining the fold of a protein from its sequence is called the protein folding problem. The “inverse” protein folding problem rises then as given a tertiary structure, defining a sequence(s) that folds into this given structure. Solving the inverse protein folding problem has a huge impact in protein engineering, because it represents, first, a demonstration of a full knowledge about protein structure and its interpretation through physical and mathematical models; and second, using this information we can create new proteins, exploring new folds and define synthetic enzymatic reactions. This fascinating statement, however, is far to be achieved. Several groups around the world are trying to solve the inverse protein folding problem, with only few examples of success.

The Octarellin project born in the 90s with the final goal of solve the inverse protein folding problem using as target the $(ba)_8$ fold, or better known as Tim-barrel. This fold is widely found in nature: 10% of the proteins are able to adopt it, harvesting 5 of the 6 biochemical reactions. Then, the TIM-barrel fold is an ideal scaffold to try to define artificial sequences able to fold as it. This lecture will summarize our different approaches to design our Octarellin proteins, and how these have led to create different protein generations, to finally discuss what we have learned from our still increasing experience and how this knowledge can be extrapolated to design different proteins. Moreover, we will discuss how different approaches, theoretical and experimental, may be used to discriminate between protein models designed from scratch.

I10. Force Without Form: A Disordered Protein Complex Examined with Single-Molecule and Computational Tools

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Intrinsically disordered proteins (IDPs) are an extreme case of fluctuating 3D conformations, which makes their characterization challenging. However, IDPs play critical roles in regulatory protein interactions, such as mRNA cap-dependent translation initiation, which is regulated by the interaction of the folded eukaryotic initiation factor 4E (eIF4E) with the disordered eIF4E binding proteins (4E-BPs) in a phosphorylation-dependent manner. The Gradinaru lab at University of Toronto specializes in multidimensional single-molecule fluorescence (SMF) spectroscopy, a uniquely suited technique to resolve microscopic distributions of states and dynamics. In this talk, I will share our recent SMF results on the 4E-BP2 protein, which paint a paint a sequence-level rigidity map of three states of this disordered protein differing in phosphorylation or binding status and distinguish regions that form contacts with eIF4E. Our new SMF data was used in conjunction with preexisting nuclear magnetic resonance, small-angle X-ray scattering data to calculate conformational ensembles of 4E-BP2 using a Bayesian method of structural refinement Applying clustering algorithms to these optimized ensembles reveals distinct structural states that delineate the extended dynamic interaction interface between 4E-BP2 and eIF4E. An integrative use of multiple biophysical experiments probing disparate scales, computational modelling and polymer physics provides valuable insights into IDPs and their diverse biological functions.

I11. Electrochemical investigations into protein degradation and inhibition

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The 20S proteasome is a protein complex involved in the proteolysis of damaged proteins. In some medical anomalies, the proteasome is synthesized in abnormally high concentrations, turning this enzymatic complex into a: *i*) target for drug development; and *ii*) biomarker of medical conditions. The objectives of this work intends to answer these two characteristics of the 20S proteasome through the development of electrochemical biosensor for: *i*) investigating the 20S proteasome activity, an essential step for drug screening strategies; and *ii*) quantification of the 20S proteasome biomarker in body fluids.

To answer the first objective, different immobilization procedures of the 20S proteasome were tested, including bio-affinity interactions with monoclonal and polyclonal antibodies. The influence of the antibody–proteasome interactions towards the enzymatic activity was investigated using electroactive substrates specific for each caspase-, trypsin- and chymotrypsin-like activity[1]. The efficiency of this assay for screening compounds with pharmaceutical properties was demonstrated for naturally occurring compounds, and for synthetic drugs.

For the second objective, different immobilization strategies of the antibody layer were tested. These includes oriented immobilization of a capture monoclonal antibody on a self-assembled monolayer of 4-mercaptophenylboronic acid[2], or immobilization through a mixt layer of conductive polymers functionalized with aminophenylboronic acid[3]. The construction of the immunosensor was evaluated by surface plasmon resonance and gravimetric analysis. The implication of the electrode architecture on the device performance are discussed and the detection of the 20S proteasome in serum samples performed.

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Acknowledgements

Financial support from UEFISCDI project PN-III-P4-ID-PCE-2020-1403, and CNCS the Core Program 2019–2022 (contract 21N/2019).

I12. Affinity-based biosensors as promising tools in doping control

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Innovative bioanalytical approaches can be foreseen as interesting means for solving relevant emerging problems in anti-doping control. Recently, affinity-based biosensors have started to be considered in sport medicine and doping control analysis because they are cheap, easy to use and sufficiently selective analytical devices, characterized by a reversible interaction with the analyte under investigation allowing the use of the same sensor for multiple analyses. The current diagnostic methods such as enzyme-linked immunosorbent assay (ELISA) and polymerase chain reaction require skilled personnel and expensive equipment that are not available in resource-limited settings.

The lecture intends to be an overview on the research activity developed by our group in the affinity sensing, especially the design of the interface between the physical transducer and the biological recognition elements. We report a proof-of-concept based an affinity format for early detection of cannabinoids in urine samples, designated for doping control. The method was able to detect cannabidiol (CBD) and the main metabolite 11-nor-Δ9-tetrahydrocannabinol-9-carboxylic acid (carboxy-THC) in diluted urine samples.

Acknowledgement:
This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P4-ID-PCE-2020-0998, within PNCDI II

I13. Lipid nanoparticles with pH-triggered change in their internal connectivity

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Under various conditions of temperature, pressure and hydration, certain lipids or lipid mixtures can adopt inverse cubic phases: either *bicontinuous* ones based on underlying periodic minimal surfaces, or *discontinuous* ones based on packings of discrete inverse micelles. The latter structures are of particular interest for very slow release of encapsulated drugs or other active substances.

We have previously shown that addition of weakly-polar amphiphiles such as diacylglycerols to phospholipids leads to the formation of a discontinuous cubic phase of spacegroup Fd3m, with a structure based upon a complex close packing of two types of quasi-spherical inverse micelles. We have also studied the structure of this phase by contrast variation neutron scattering, and have shown that the more weakly amphiphilic diacylglycerol component is preferentially located in the smaller, more highly curved inverse micelles (A.I.I. Tyler, unpublished data).

We have dispersed this bulk Fd3m phase into ‘micellosomes’ by sonication in the presence of the amphiphilic block copolymer F127, and have used x-ray diffraction to compare their structure to that of the bulk Fd3m cubic phase. We have recently demonstrated that Fd3m micellosomes can be formed in buffer at pH 7.4 by mixtures of monoolein and oleyl alcohol, containing a small amount of an ionizable lipid. By lowering the pH to below pH 6, the zwitterionic lipid becomes cationic, triggering a phase transition within the lipid nanoparticle from an internally-confined Fd3m structure (micellosome), to a porous inverse hexagonal H_{II} phase (hexosome), favouring release of any encapsulated contents. We have used a combination of small-angle x-ray scattering and cryo-TEM to determine the detailed internal structure within the Fd3m micellosomes.

I14. Membrane Organization and Remodeling probed by Atomic Force Microscopy

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Atomic Force Microscopy (AFM) is a technique that involves raster scanning of the sample with a sharp tip. It is a very powerful tool to probe the topography of biological samples under physiological conditions with a vertical and lateral resolution in the nanometer range. In particular, AFM is an exceptional technique to probe the architecture and dynamics of biological membranes.

I will illustrate the exceptional ability of AFM to analyze, at the nanoscale, the organization of membrane components as well as membrane remodeling through recent studies that took advantage of advanced high-speed imaging and AFM-fluorescence correlative microscopy.

I15. Electrochemical Immobilisation of Enzymes for Biocatalysis

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Electrochemical based enzyme immobilisation techniques can enable surface control that allows for surface modification at the micron scale. Enzyme immobilisation can be performed using a wide range of approaches that include alkanethiol, diazonium and a large range of polymer modified surfaces. Self-assembly of thiols has been widely used for the surface modification of electrodes and is an attractive method for the immobilisation of enzymes for use in biosensors and biocatalysis. We have described the electrochemical deposition of SAMs for the spatial and sequential immobilisation of the redox protein cytochrome c (cyt c) [1] and have now extended this process, employing the same approach of blocking and unblocking of electrodes surfaces, to successfully immobilise a sequence of three separate enzymes in a sequential manner in aqueous solution. The enzymes selected were alcohol dehydrogenase (ADH) (EC 1.1.1.1), formaldehyde dehydrogenase (FLDH) (EC 1.2.1.46) and formate dehydrogenase (FoDH) (EC 1.2.1.2). Recent work on the use of electrochemical deposition to immobilize *Candida antartica* lipase B for use in a flow system [2] has been extended to the immobilization of a cascade system. A range of electrodes modified with redox polymers (polypyrrole, polyaniline and polythiophene), silicates, and diazonium salts were evaluated as supports with polypyrrole providing the optimal catalytic activity and stability. Three enzyme cascade systems based on glucose oxidase, horseradish (or chloro) peroxidase and catalase have been developed as model reactors together with enzymatic systems for the regeneration of NADH (3, 4).

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I16. Functionalized materials as versatile tools for advanced (bio)sensing systems

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The surface of electrodes modified with nanostructured or composite materials can increase the analytical performance of (bio)sensors and open the way for sensors miniaturization and portability. These modifiers can also contribute to the stability and improvement in the immobilization of bioreceptors, enhancing the overall analytical performance of the sensors in terms of sensitivity and electro-conductivity. The latest discoveries in the field of nanomaterials have been introducing a wide range of electrode materials that could be further modified with bioelements or biomimetic receptors, assuring highly sensitive and selective (bio)sensors. Carbon-based materials and nanocomposites have become attractive materials for electrochemical (bio)sensors development and are widely used as modifiers for electrode surfaces to expand the active surface area and to increase the number of immobilized biological entities. Other modifiers frequently used in sensors design, metallic nanoparticles have attracted increased attention in the biosensing area due to their advantageous properties. For instance, Au and Pt nanoparticles are maybe the most used NPs in biological and sensing applications. Their excellent conductivity, good biocompatibility, and large surface area lead to higher loading of biological elements on the sensing platform. Some immuno- and bio-assays are commercially available today to a wide audience. By simply changing the bioelement type, other biosensors were developed, for instance, those based on affinity or immunological recognition (antibody-antigen). The requirements of nowadays analytical analysis such as rapidity, low cost, high specificity and sensitivity, stability, and long shelf-life are connected with the involvement of a wide plethora of nanomaterials in the development of advanced sensing devices. Several examples of such sensing assays will be discussed with a focus on the nanomaterials used that greatly influence the analytical parameters.

I17. Chemical sensors for volatile organic compounds for ecological monitoring based on nano-thin organized organic films

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Volatile organic compounds (VOCs) are men-made liquid chemicals used in the manufacturing process of paints, pharmaceuticals, refrigerants. They are with a low boiling point, which easily evaporates them into gas that can be harmful to humans. They can also contaminate water sources. VOCs are inert, highly dilute and volatile, their sticking affinity to various types of surfaces is low and this makes their detection very difficult. Currently, the most precise detection methods use a combination of gas chromatography and mass spectroscopy that are not suitable for in-field real-time monitoring. We have developed an alternative approach based on portable chemical sensors with nano-thin sensing layer coating prepared by the Langmuir-Blodgett method. Different materials were tested, among them phospholipids, a fluorescently labeled phospholipid, the fatty acid Arachidic acid, and Cadmium Arachidate. Coating thickness, density, and packing of molecules were optimized for maximum sensitivity. Very fast detection and reversibility of the sensor for multiple uses are obtained. The major transduction method was gravimetric with the use of very sensitive Surface Acoustic Wave resonators. In some cases electrical impedance spectroscopy and fluorescence measurements were used for additional identification. Sensors for both high and low VOC concentrations were tested.

Oral Communications

Contributed talks

O1. Biomechanics of Type III Secretion System

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The type III secretion system (T3SS), which is found almost exclusively in pathogenic bacteria, is used for establishing contact with the host cell and deliver effector proteins in to infected cells. For instance, in the case of intestinal diseases, the T3SS “syringe-like” filament penetrates the thick mucus barrier that protects epithelial cells in the intestinal tract to facilitate the attachment in order to transmit the bacterial pathogens into them. Considering the mechanical shear stresses induced by the mucosal flow within the intestinal tract, it is reasonable to assume that the T3SS filament possess noteworthy elastic resilience. Yet, the mechanical nature that enables the unique performance of this filament remain unknown. With the intention of unraveling the origin of the T3SS filament, we use Atomic Force Microscopy (AFM) to study the conformational structure of single T3SS filaments. We first study its mechanical properties by excreting direct force on filaments that extends from a living bacterium and then perform nano-indentation in order to investigate the filament’s viscoelastic response and most importantly, the internal interactions between its constituting protein. Pulling filaments from bacterium surface reveals that although being relatively soft materials, they are more rigid than expected from hollow filament model (which may indicate the presence of biological substance within them). The indentation measurements on wild type and mutated filaments displayed that removal of a small segment considerably lowers the structural elasticity of the filament. Beyond the insights provided here, the modifications in the T3SS protein can pave a way for design of tunable bioinspired materials.

O2. High-resolution electro-optical mapping of living cells for (bio)sensing: case studies on eukaryotic and prokaryotic (bacterial) cells

Mihaela Gheorghiu[1, 2], Cristina Polonschii[1], Szilveszter Gaspar[1], Sorin M. David[1], Raluca Elena Munteanu[1, 2], Eugen Gheorghiu[1, 2]

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Mapping the impedance of bio-electrified interfaces is critical for developing biosensing platforms for chemical, biomedical or environmental applications. We demonstrate a multimodal, label-free, high spatial resolution and low temporal noise functional imaging instrument enabling impedance mapping - beyond the limitations of standard electrode-based technologies (surface or scanning ones) and of quantitative phase microscopy. The findings are consistent with a comprehensive theoretical model and ground a wider range of electrically-modulated optical assays for measuring the electric field locally and achieving electro-optical maps with high spatial and temporal resolutions.

In a step forward, we exploit the electrical modulation of the refractive index of a tailored (sensing) interface, via an externally applied AC voltage and use the label-free, real-time features of the reflectance microscopy to provide label-free contrast of the impedance of the cellular and sub-cellular architectures in the vicinity of an electrified interface.

We demonstrate high-resolution electro-optical mapping of biosystems and bio-interfaces allowing access to dynamics of single cells, either eukaryotic or prokaryotic (bacterial) cells, to reveal the response (both on cell cycle progression and on cellular viability/integrity/homeostasy [2]) to stimuli of biomedical relevance at the cellular level.

The virtues and challenges of the novel opto-electrochemical method as an enabling tool to monitor charged intracellular trafficking and impedance contrasts in living cells are highlighted, together with proof of concepts of fast bacterial detection, antimicrobial susceptibility testing and cytopathic effect evaluation of relevance for viral infection.

Acknowledgments
Support of PNIII projects P4-ID-PCE-2020-2432 and -1433 as well as P2-2.1-PED-2019-5155, -5185, -4932 is gratefully acknowledged.

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O3. Quantification of LT4: choosing between detection methods

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Many drugs, as well as food supplements (e.g. vitamins), are transported by serum albumin and influence the transport of thyroid hormones in the blood and their binding to protein receptors on the surface of cell membranes. The synthetic form of the thyroxine hormone (T4), levothyroxine (LT4) is used as medication in pathologies of the thyroid gland, like hypothyroidism. The mechanism of the interaction of LT4 with albumins [1] or the influence of vitamins on their binding [2] was studied using spectrometry measurements. The induction of conformational changes in the structure of these proteins was observed, which leads to the increased structural stability of the protein complexed with LT4 under the action of denaturing factors and shortening or prolonging the storage time of LT4 in blood plasma. Further, the BSA-LT4 interaction can be used to develop spectroscopic biosensors for LT4 detection with a limit of detection of 230 nM.

To improve the sensitivity, nanoparticle-based electrochemical sensors were implemented as simple and reliable methods to monitor the effect of administration of LT4, which is currently done mainly through clinical observations. Carbon nanotubes [3] and bimetallic nanoparticles on graphene oxide sheets [4] were used to develop label-free sensors for LT4 with detection limits starting with 30 nM, and decreasing to 6 pM. Electrochemistry was used to characterize, compare, and optimize the most suitable nanoparticle-based sensors, as well as for the analytical detection of LT4.

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Acknowledgments:
This work was supported by a Romanian Ministry of Research and Innovation grant, CCCDI - UEFISCDI, Project number PN-III-P1-1.2-PCCDI-2017-0062, contract no. 58, within PNCDI III.

O4. Plasmonic immunosensors based on gold nanourchins for biomarker detection

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A highly sensitive and specific detection of biomarkers can be achieved using immunosensors based on plasmonic nanoparticles (NPs). The detected signal can be enhanced by optimizing the physical properties of the NPs *via* tuning particle morphology and surface chemistry. In this regard, spiked NPs such as gold nanourchins (GNUs) show tremendous promise due to the high electromagnetic fields generated at their tips. This particular feature endorses them as feasible Surface-Enhanced Raman Scattering (SERS) sensor components.

Herein we propose an in-liquid sandwich-type SERS immuno-nanosensor that can be applied for the rapid detection of protein biomarkers. The sensing unit consists of biomarker-bridged gold nanourchin-gold nanosphere (GNU-GNS) or gold nanourchin-gold nanourchin (GNU-GNU) pairs. The generated interparticle hot-spots are responsible for the additional increase in SERS signal intensity of the reporter molecule. Formation of interparticle pairs was confirmed by UV-Vis-NIR extinction and DLS measurements, and explored by FDTD theoretical modelling. Our results show that particle conjugation with polymers provides chemical stability while antibody-biofunctionalization favors an immunological-grade detection of the targeted analyte.

The use of an easy-to-handle, cost- and time-effective portable Raman device makes this sensing technique promising in terms of feasibility, rapidness and sensitivity. Moreover, the design of such nano-based architectures aims to function as an essential step toward the development of an innovative sandwich-layout microfluidic SERS immuno-nanosensor. The targeted applications envisage the early detection of relevant biomarkers for neurodegenerative diseases, malignant afflictions, metabolic disorders or other imbalanced physiological conditions.

Acknowledgement:
A-S.T. would like to acknowledge the financial support through the Core Program, Project No. PN.19.35.02.01. This work was partially supported by a grant of Ministry of Research and Innovation, CNCS-UEFISCDI, project number PN-III-P1-1.1-TE-2021-0234, within PNCDI III.

O5. Electrochemically synthesized nanorods for the optical stimulation of neurons

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Retina neurons lose their sensitivity to light in a number of eye diseases such as Retinitis Pigmentosa (RP) and age-related macular degeneration (ARMD). Using nanomaterials to re-establish the light-sensitivity of these neurons is an approach that has recently gained considerable attention (see, for example, [1]). In line with this approach, we have used template-assisted electrochemical depositions to build light-sensitive nanorods (with diameter around 260 nm and length in between 1.5 µm and 16 µm, depending on the experimental conditions). The nanorods were either made entirely of poly(3-hexylthiophene) (P3HT) or bi-segmented, made half of P3HT and half of Au. The nanorods were characterized with UV-Vis spectrometry, atomic force microscopy (AFM), Kelvin probe force microscopy (KPFM) and regarding the photocurrents they generate. Moreover, their biocompatibility and their ability to optically modulate the firing activity of primary neurons was also investigated. The results obtained up to now (some of which are presented in one of our recent publications [2]) show that the P3HT nanorods made with our electrochemical approach are promising when it comes to the optical stimulation of neurons.

Acknowledgement:
The financial support from the Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI) through ERA-Net project nanoLight (https://nanolight-project.eu/) is greatly acknowledged.

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O6. Quantum-chemical and experimental study on the interactions between the magnetic core and the molecular shell of iron oxide nanoparticles in aqueous suspensions for biomedical applications

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During the last decades iron oxide nanoparticles are widely studied due to their various applications in biomedical fields: contrast agents in the magnetic resonance imagistic, magnetically targeting of drug carriers and experimental tumor hyperthermia (1-3). This research was focused on the theoretical and experimental study of the interactions between various molecules and the surface of iron oxide nanoparticles prepared by co-precipitation method. Following the surface modification of magnetic nanoparticles (MNP) the stability of their dispersion in aqueous medium could be ensured based on the predominant electric repulsive forces that balance the magnetic dipole-dipole attraction. Quantum chemical modeling carried out by us has revealed some physical-chemical properties of coating molecules (dipole moment, energies of frontier orbitals, etc.) that suggest their suitability for the interaction with both MNP iron cations and surrounding water. Microstructural investigations (Scanning electron microscopy, X-ray diffractometry, FTIR spectroscopy) have shown that good crystallinity and granulation of the suspension ferrophase was obtained while FTIR recordings confirmed the molecule interactions with MNP surface. The nanotoxicity study was carried out on agro-industrial plantlets in early ontogenetic stages with focus on the photosynthesis efficacy.

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O7. A straightforward method for cell sample preparation to allow a reliable image of the nanomaterials adhering to the surface, using scanning electron microscopy

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The interactions between diverse nanomaterials and biological cells are typically validated and further examined by specific imaging methods such as transmission and/or scanning electron microscopy (TEM and/ or SEM) in order to properly investigate the effects of the nanomaterial delivered into the cell or bound on the cell membrane. The process of preparing biological samples for scanning electron microscopy usually entails the so-named critical point drying process, which is not only expensive, but needs to be carefully implemented to prevent damage of the sample. On the other hand, drying the specimen directly in vacuum can incur other disadvantages such as cell deflation with consequent loss of specific morphology. In this paper, we present the results obtained in our cell culture laboratory for samples which have been dried in a controlled manner in the biological safety hood followed by vacuum.

We have tested the method using osteosarcoma cells and adipose derived stem cells. The aim was to observe if nanomaterials such as nanowires (NW) (diameter 200 nm, length 2 μm) or magnetic nanoparticles (MNP) (diameter under 100 nm) were present on the cell surface after 24h of incubation with the cells.

The procedure assumed a standard growth of the cell culture, followed by direct fixation on sterilized silicon wafers. Subsequently, the cells were dehydrated using ethanol solutions in increasing concentrations, followed by air drying in the biological safety hood and in vacuum. The silicon wafers were then sputter coated with a 5 nm gold layer and imaged with a scanning electron microscope. The obtained images pointed out an excellent efficiency of the method utilized that succeeded to preserve cell morphology within biological samples while highlighting the presence of NW/MNP on the cell surface.

Acknowledgements:
Work supported by (UEFISCDI) Contract no. PCE20/2021 (PN-III-P4-ID-PCE-2020-2381).

O8. 3D reconstructions of intracellular distribution of folate functionalized silica nanoparticles using combined microscopy techniques (fluorescence, dark field and hyperspectral microscopy)

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Drug delivery systems represent a topic of a wide scientific interest, being used in therapeutics and diagnostics. The cytotoxicity and intracellular distribution of non-fluorescent mesoporous silica nanoparticles (MSNs) functionalized with folate and loaded with cytotoxic Irinotecan (Iri), were evaluated on cultured cells. Folate played the role of MSNs uptake enhancer since cancer cells present high expression of folate receptors on the membrane.
We employed enhanced dark field microscopy (eDFM) from CytovivaR working in two modes: hyperspectral imaging (HSI) and fluorescence imaging, the latter benefitting from cell 3D reconstruction.
After 24h from seeding, we incubated Caco-2 and NIH3T3 cells with MSNs for another 24h or 48h. Cells viability was assessed using colorimetric formazan-based assay (MTS). Caco-2 cells were prepared separately for HSI (non-stained) and for fluorescence eDFM (cytoskeletal actin: AlexaFluor488 Phalloidin and nucleus: DAPI). Images were processed using CytovivaR and lab-made routines implemented in MATLAB and the following have been obtained: spectral profiles at pixel level, cells 3D reconstructions, MSNs counting in areas corresponding to nucleus and cytoplasm. The presence of folate on MSNs increased statistically significant the cytotoxicity of Iri for all incubation times, more on Caco-2 than on NIH3T3 (which aligns with data about higher expression of membrane folate receptor on cancer cells).
The microscopy evaluations revealed that the folate linked on MSNs enhanced their uptake and determined a preferential MSNs localization in the close vicinity of the nucleus.
Our study combines microscopy techniques to quantitively evaluate the cellular penetration of non-fluorescent MSNs. An original post processing procedure of serial Z-stack fluorescent images was developed to highlight the MSNs localization in 3D reconstructions of cellular compartments.

O9. Ultrasensitive SERS detection of biomolecules on nanoimprinted substrate

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Recently, surface-enhanced Raman scattering (SERS) has become a frequently used ultrasensitive tool able to provide in-situ mechanistic and dynamic information of metallic/solution interfaces, at the molecular/atomic level. Since the enhanced Raman signal is mainly assigned to the plasmonic effect in metallic nanostructures, the local architecture of signal-enhancing surfaces need to be accurately controlled and thus a significant amplification could be acquired [1]. Consequently, nanofabrication techniques have been intensively employed to get well defined SERS-active nanopatterns, providing multiple hotspots, highly suitable for real-time monitoring [2]. Using an emerging nanoimprint lithographic technique (NIL), we successfully fabricated flexible and tunable SERS-active nanosurfaces. Networks of nanotrenches and nanopillars with 300 nm height and 400 nm and 1 μm periods, respectively, were imprinted in thermoplastic polymers, metalized with Ag/Au and characterized by SEM and AFM microscopic techniques [3]. The nanofabricated substrates were used for the detection of 2 test biomolecules: i) crystal violet, a well-known recalcitrant and toxic dye and ii) nodularin, a potent toxin produced by cyanobacteria *Nodularia spumigena*. The nanostructures are very suitable for SERS detection of crystal violet for example, reaching a limit of detection of 10 pM for Ag nanotrenches and of 1 μM in case of the Au nanopillars.

Acknowledgements:
The authors would like to acknowledge the financial support through the Core Program, Project No. PN 19 35 02 01.This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS – UEFISCDI, project number PN-III-P1-1.1-TE-2021-0753.

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O10. Romanian moss surveys for temporal trends assessment of heavy metals atmospheric deposition

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Through the Romanian moss surveys, data on the levels of heavy metals in naturally growing mosses were provided. The surveys have been repeated at five-year intervals in 2010, 2015, and 2020 in the framework of the *International Cooperative Programme on Effects of Air Pollution on Natural Vegetation and Crops*. The analytical techniques used for the quantification of heavy metals (V, Cr, Fe, Ni, Cu, Zn, As, Cd, and Pb) in moss samples were: atomic absorption spectrometry (2010), inductively coupled plasma mass spectrometry (2015, 2020) and instrumental neutron activation analysis (2010, 2015, 2020). Based on the reported concentrations of metals in moss samples collected from each survey, statistical analysis of the temporal trends (2010 – 2020) of atmospheric deposition across Romania was performed by calculating the geometric mean and median values per metal and per survey year. The changes in heavy metals concentration in mosses were mapped. A significant decrease in Cd and Pb concentrations has been detected in the northern and western parts of Romania.

O11. Spectroscopic and Theoretical Studies on the Effects of Excited State Intramolecular Proton Transfer in 4-[5-(naphthalen-1-ylmethyl)-1,3,4-thiadiazol-2-yl]benzene-1,3-diol

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This work deals with an advanced spectroscopic and theoretical studies on *4-[5-(naphthalen-1-ylmethyl)-1,3,4-thiadiazol-2-yl]benzene-1,3-diol* (NTBD). The spectroscopic measurements were carried out in the range of solvents with varied polarity, as well as in their selected mixtures. An interesting effects related to the excited state intermolecular proton transfer (ESIPT) were observed in the analysed 1,3,4-thiadiazole derivative dissolved solvent systems mentioned. In few cases the effect of dual fluorescence related to the ESIPT phenomenon was noticed. Also, the effect observed may be enhanced/induced, and the energy barrier between *keto** and *enol** forms may be reduced most likely due to a molecular aggregation processes related to AIE fluorescence (Aggregation-Induced Emission). Only a single emission band was observed in polar solvents such as methanol, though the ESIPT-related effect of dual fluorescence emerged in solvent mixtures, e.g. methanol:water. Measurements with the use of transient absorption spectroscopy confirmed that the primary effect in the phenomenon studied was excited state electron transfer, and its its dynamics was very clearly revealed. The subsequent [TD]DFT quantum-mechanical calculations corroborated the spectroscopic observations and underscored the impact of aggregation in terms of inducing/enhancing ESIPT – i.e. the contribution of AIE processes. Therefore, in our study, we were able to comprehensively examine the dynamics of proton transfer occurring in a biologically interesting molecule from the group of 1,3,4-thiadiazoles - NTBD.

O12. Studies on mode of action of the synergistic systems incorporating 1,3,4-thiadiazole derivatives and polyene-based antibiotics against selected fungal species

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Derivatives of 1,3,4-thiadiazole are well known for their broad array of biological activity, some of which may be of therapeutic interest. In particular, compounds from this group often demonstrate a strong antifungal properties which may additionally be enhanced upon their concomitant action with commercially available antibiotics such as amphotericin B (AmB). Example of such synergistic effects was reported by our group for mixtures of 4-(5-methyl-1,3,4-thiadiazole-2-yl) benzene-1,3-diol (C1) and AmB, though the detailed mechanistic studies were omitted. Therefore the current study aims at more detailed examination of the mode of action of the synergistic system mentioned.

The electronic absorption and stationary fluorescence data suggest that the synergistic system C1-AmB causes a disaggregation of AmB micelles. This effect is evidenced by a notable positioning change of the AmB absorption maximum in PBS. In more detail, the band at 345 nm characteristic of the AmB aggregate shifts to approximately 335 nm as result of addition of the C1 aliquot. These results are well-correlated with the fluorescence data, wherein the emission band characteristic of the aggregate disappeared upon the C1 addition. Also, the TCSPC data obtained are in-line with the steady state fluorescence and electronic absorption results, and suggested that the active form of AnB-C1 tandem is characteristic of a particular fluorescence lifetime. Furthermore, the additional stationary and time resolved fluorescence anisotropy studies gave evidence for the aggregation-dependence of the synergistic action of C1-AmB system. The experimental data were additionally backed up with a number of theoretical methods including quantum chemistry calculations

O13. Enzymatic inks based on aldehyde dehydrogenases for the electrochemical detection of aldehydes in a wide temperature range

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Aldehydes are relevant markers in the assessment of human health, for the quality of food quality and environmental air. Enzymatic biosensors hold much promise for the specific and sensitive detection of aldehydes in various matrices. Yet, the low stability of enzymes and the necessity to function adequately in wide ranges of conditions hampered the development of such promising tools.

Motivated by this, we developed enzymatic preparations of aldehyde dehydrogenases from Flavobacterium Pl002 (F-ALDH) and from Sulfolobus tokadaii (ST-ALDH) immobilized on magnetic particles functionalized with nickel nitrilotriacetic acid. The particles were mixed with different additives- bovine serum albumin, glycerol, polyethyleneglycol, carboxymethylcellulose, Brij and Tween 20- to ensure adequate stability and viscosity. The stability of the inks at 4° C was assessed by spectrophotometric tests of enzymatic activity. The inks were deposited on screen printed electrodes, filter paper and glass slides. Besides dropcasting, the surface modification with magnetic beads functionalized with F-ALDH was also performed by Matrix Assisted Pulsed Laser Evaporation (MAPLE). The dried enzyme-coated interfaces were characterized by Atomic Force Microscopy and Scanning Electron Microscopy. The enzymatic activity was determined spectrophotometrically (enzyme coated paper and glass slides) or by amperometry (screen-printed electrodes). Calibration plots for acetaldehyde were acquired with the screen printed electrodes modified with F-ALDH and ST-ALDH at different temperatures in the 17° C- 80° C range.

The main results of the study are: preparations containing F-AlDH immobilized on magnetic beads maintain enzymatic activity for more than 4 months; some inks prepared by the addition of viscosity and surfactant agents were active for more than 2 weeks at 4° C; the surfaces coated with these inks displayed enzymatic activity; MAPLE proved to be suitable for obtaining homogeneous enzymatic coatings; the feasibility of using enzyme coated interfaces for the determination of aldehydes at different temperatures relevant for practical applications was proven.

O14. Novel composites based on natural compounds for topical applications

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Skin is a vital organ that serves as a barrier to protect against external factors. Its functions are impaired by injuries that can give rise to serious complications, which subsequently require immediate intervention to restore the functions of damaged skin. Through strategies of tissue engineering, new materials are developed that not only offer structural support, but also provide functionality. In this work, matrices that combine synthetic and naturally derived materials were employed for the development of novel advanced materials designed for topical applications to aid wound healing. These novel composite materials consist of a collagen porous scaffold and an herbal polyphenolic extract embedded in mesoporous silica nanoparticles. Thus, the final composite material mimics the structural characteristics of skin conferred by the collagen component and, at the same time proving functionality regarding antibacterial activity provided by the herbal polyphenolic extract. The polyphenolic extract showed good activity against *P. aeruginosa* biofilm formation, while its embedding in mesoporous silica nanoparticles with a diameter of approximately 100 nm diameter proved good protection against degradation in time of natural compounds.

O15. Electrochemical method for mercury detection in wastewater samples using a portable device

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The aim of the study was to verify the performance parameters of the proposed method for the determination of Hg(II) in wastewater. The method using screen-printed carbon electrodes modified (ECS) with poly L films (ECS-poly**L**) was validated in-house following the standard procedure for analytical methods.

ECS containing carbon working electrode (2 mm diameter), carbon auxiliary electrode and Ag/AgCl reference electrode (BVT Technologies, Czech Republic) were used. An organic ligand (poly**L**) capable of complexing Hg(II) ions was deposited on the carbon working electrode surface. The potentiostat used was a portable PalmSens 4 type, coupled to a laptop and equipped with a PSTrace Software. The method consisted in three steps. First step was to apply Cyclic Voltammetry (CV) and Differential Pulse Voltammetry (DPV) on the modified electrode in acetate buffer solution at pH = 3 for 5 minutes. Second stage was deposition of Hg(II) ions on the electrode for 20 minutes in a solution of Hg(II) with same acetate buffer. The last stage consisted in insertion of the electrode after washing with ultrapure water in acetate buffer at pH = 3 and performing the DPV procedure for 10 minutes.

The maximum admissible value in wastewater according to Romanian legislation is 50 µg/L. At this value, the measurement accuracy (14%) and uncertainty (18%) were determined, as well as the tests to verify the robustness of the method.

The robustness tests indicate that ± 10% variation of pH and acetate buffer concentration does not significantly affect the method, while reaction time has a strong effect on the procedure and makes the method less robust from this point of view. The advantages of the method are inexpensive equipment, portable, suitable for field determination; small size of the electrodes used; simplified procedure; reaction medium does not require controlled atmosphere.

Acknowledgements:
This research was funded by Romanian National Authority for Scientific Research, UEFISCDI, under grant PN-III-P2-2.1-PED-2019-0730, contract no. 293PED/2020.

O16. Innovative 3D suction lysimeter and portable detector for on-field monitoring of pollutants directly in soil

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A 3D printed soil solution extractor system has been developed for monitoring and control of different nitrogen-based compounds in soil. This soil extractor integrates electrochemical sensors developed by our partner ICECHIM for sensitive detection and continuous monitoring of nitrogen-based compounds in soil.

An innovative wireless portable detector has been designed and developed to have multiple channels available for several sensors that may be employed for the nitrogen-based compounds determination. Employment of the wireless system for controlling the detector and data acquisition allows to control several detectors in the same time increasing the number of data collected during the soil pollutants monitoring.

The manufacturing of the 3D lysimeter was done using different materials and different configurations, in order to ensure a high degree of portability and mobility, being able to facilitate the installation in the ground at a shallower depth than those commercially available.

For designing the wireless system for controlling a portable detector connected to the electrochemical sensors integrated in the suction lysimeter a target architecture has been developed for a portable amperometric detector. Preliminary measurement applications based on microcontrollers have been developed. This device benefits from existence of a smart touch control and a graphical interface that provide the user the possibility to connect with the electrochemical interface, to choose the working protocol, to establish the duration between the set methods, to choose the name of the sample and the file name where the data will be saved. After setting the parameters, the method can be started manually or automatically at preset intervals.

The 3D based suction lysimeter and the portable wireless detector developed for on-field monitoring of different pollutants in soil responds to the need of a tool for soil contaminants monitoring and controlling in real-time.

O17. Spectroelectrochemical Detection of Thiabendazole Residues in Fruit Juice

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The discovery of surface enhanced Raman scattering (SERS) from an electrochemical (EC)-SERS experiment is known as a historic breakthrough [1]. Since then, great progress has been made in using this technique for various analytical purposes, Raman spectroelectrochemistry representing now a promising alternative to conventional analytical methods.

By manipulating the surface charge through polarization, the physico-chemical interaction between the substrate and the target molecule can be controlled and facilitated. As a result, a higher enhancement of the Raman signal is observed. The EC modulation of substrate potentials during SERS analysis brings a series of other benefits, such as higher selectivity, possibility of preconcentration, reusability and improved reproducibility [2]. Furthermore, the electrochemical methods for "roughening" (activation) of the low-cost screen-printed electrodes offer a convenient, accessible, and ready-to-use alternative to commercially available SERS substrates that are expensive and sometimes irreproducible.

In this work we report the first EC-SERS detection of thiabendazole, a systemic fungicide used in agriculture that can be found as a contaminant in various foods, including fruit juices. Commercially available gold SPEs were used after an optimized EC activation procedure. An applied potential to the substrate (-0.8V vs. Ag/AgCl) further increases the SERS signal of thiabendazole allowing its detection down to 0.06 ppm (0.3 μM), with a relatively wide linear range (0.5 - 10 μM) and good intermediate precision (RSD% 10). As acidity of juice has a high variability, the pH-dependence of the SERS response was also investigated. The recovery of thiabendazole from unprocessed, spiked juice samples was found to be more than 80%. Furthermore, the possible integration of the developed EC-SERS sensor in a microfluidic chip was successfully demonstrated, suggesting a feasible implementation of miniaturized systems for real-time detection.

Acknowledgement:
The research leading to these results has received funding from the NO Grants 2014-2021, under Project contract no. 32/2020.

O18. Raman spectroscopy and Machine Learning – a new methodology for fruit spirits authentication

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In the light of the necessity for rapid methods development to investigate the authenticity of foods and beverages, Raman spectroscopy can be seen as a cost-effective, accessible and non-destructive tool for these matrices' investigation. However, the authenticity assessment as well as the adulteration detection are sensitive subjects and of crucial significance, both for the producers and consumers entities. A Raman database contains large amounts of data, which are very difficult to handle and interpret without the involvement of the chemometric methods. To this impediment, the complexity of the fruit distillates must be considered, both in terms of the vast number of substances containing in the beverage and the low concentration of some constituents. The application of Machine Learning approach to the Raman data demonstrated the applicability of this methodology for the fruit spirits investigation. Thus, the prediction models for the matrix trademark fingerprint or botanical and geographical origin have been constructed and discussed in relation with their efficiency. The proposed approach proved to be very efficient for the trademark fingerprint identification, a predictive model with a 95.5% accuracy being obtained in this case. The geographical discrimination of the fruit spirits was also possible (best model accuracy 90.9%), while for botanical origin, it was proved, for the first time, that the fruit variety differentiation is possible, using this approach, only inside each producer products. This observation can be explained by the fact that these beverages are obtained through several processing steps (i.e. most of the time after two distillation processes) that affect the initial fingerprint of the raw materials.

Acknowledgement
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P2-2.1-PED-2019-1699 (contract no. 260PED/ 2020) within PNCDI III.

O19. The differentiation of Transylvanian fruit distillates using supervised statistical tools based on isotopic and multi-elemental fingerprint

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In this study, 46 fruit spirits (plums, apples, grapes, quinces, apricots, pears and cherries) from different Transylvanian regions were investigated from isotopic and elemental content point of view. Two advanced supervised statistical techniques (LDA and PLS-DA) were applied in order to identify the optimum chemometric model for distillate samples differentiation according to their *geographical region*, *producer* and *fruit varieties.* For geographical origin, the correct discrimination rate were 91.2% using PLS DA and 88.2% using LDA. The distillate samples were successfully classified in accordance with their trademark fingerprint in a percentage of 93.5% by LDA, and 89.1% by PLS DA. The effectiveness of PLS DA was proved for the discrimination of plum spirits from the others distillates, which was achieved in a percentage of 84.2%, compared to 63% for LDA. To sum up, PLS DA vs. LDA can be used as the optimum models for the geographical origin vs. producers differentiation of Transylvanian fruit distillates.

Acknowledgements:
This work was supported by a grant of the Ministry of Research, Innovation and Digitalization, CNCS/CCCDI–UEFISCDI, project number 260PED/2020, within PNCDI III.

O20. Pork meat authenticity – from stable isotopes and elemental fingerprint to table…

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Pigs red meat is consumed worldwide, representing around 40 % from world meat production. Romanians are important pork meat consumers, the annual mean quantity consumed per capita being about 35 kg. In the last years, consumer interest in the origin of the food they consume has increased, with a willingness to pay a higher price for food from a certain geographical region that is usually associated with either a quality given by the lack of pollution in that region, either with a different growth regime, such as food without feed concentrates/ pasture breeding. In this work**,** the isotopic fingerprint and elemental profiles of pork meat samples in corroboration with linear discriminant analysis (LDA) and artificial neural networks (ANNs) were used in order to evaluate the geographical provenance and animal diet. LDA attributed the geographical origin of meat samples in a percentage of 91.4 % for initial and 90.3 % for cross-validation classification, respectively. Using ANNs procedure, the overall precents of geographical classification for training, testing and validation steps were 94.7%, 80.0 % and 90.9%, respectively. To distinguish the feeding regime, LDA was applies also, resulting a percentage of 97.8 % in the initial classification, and 94.6 % in cross-validation step.

Poster Communications

P1. Biophysical methods for protein science & Biomembranes and model membranes

P1.1 *In Silico* Modeling of a Short Arginine and Tryptophan-based Antimicrobial Peptide's Interaction with Bacterial and Mammalian Membranes

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The interaction of the HRWWRWWRR short arginine(R) and tryptophan(W)-based antimicrobial peptide (RW-AMP) with bacterial and mammalian membranes is characterized *in silico* by means of peptide-lipid interactions (molecular dynamics simulations) and potential of mean force calculations (non-equilibrium PMF calculations) along the normal to the lipid bilayer. Membrane models compared are DOPC for mammalian membrane, and DOPC+DPPG 85:15 and DOPC+DOPG 85:15 for bacterial membrane models, respectively.

The PMFs indicate a ~ 20% stronger adhesion of RW-AMP for DOPC+DOPG bilayer compared to DOPC, combined with ~ 1 A closer binding of the peptide to the membrane surface. The slightly increased proximity of RW-AMP to the bilayer with 15% PGs is also reflected in the smaller number of hydrogen bonds the peptide forms with water in the case of bacterial membrane binding. Moreover, MD simulations show enhanced interaction of RW-AMP peptides with DOPC lipids in the presence of PG charged headgroups.

In conclusion, the 4 positively charged arginine aminoacids bring the RW-AMP peptide somewhat closer to the negatively charged PG headgroups of the bacterial membrane models than in the simple PC mammalian membrane models. The increased proximity leads to enhanced interaction with the DOPC headgroups in presence of the PGs and slightly higher water exclusion.

Acknowledgements:
INCDTIM authors would like to acknowledge the financial support through the Core Program, Project No. PN19-35 02 01. IFIN-HH author would like to acknowledge funding from the ERDF co-financed project CECBID-EOSC (Grant no. POC/397/1/1-24405).

P1.2 A pharmacological and molecular docking approach of polyphenolic compounds and outer membrane protein TolC from *E. Coli*

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The protein TolC from E. coli acts as a tunnel in the transport of molecules across the outer membrane of bacteria and is involved in the export of many molecules such as antibiotics, organic solvents colicin V and α-hemolysin. Drugs whose active ingredients are plant molecules can be used as alternatives to antibiotics against bacterial strains. The antimicrobial potential of some polyphenolic compounds with phytoalexin properties - apigenin, baicalin, daidzein, genistein, luteolin, and resveratrol against TolC protein in the bacterium E. Coli was monitored by investigating the pharmacological properties, bioactivity, and oral toxicity of polyphenolic compounds. For fulfilling these objectives, in silico methodology was applied. PyRx tool was used to prepare dock file and docking analysis done by AutoDock Vina. Based on ADME properties selected molecules were further analyzed by molecular docking to find the safe and effective drug-like compounds. The interaction studies were done by using Discovery Studio visualizer. his study could help in the design of compounds that can bind to TolC protein in bacteria E. Coli and to influence the interaction of TolC to proteins from the membrane of bacteria, and implicitly, to influence the resistance of bacteria to polyphenolic drugs.

Keywords:
TolC, polyphenolic compounds, ADMET, pharmacokinetics, phytoalexins, pharmacological properties

P1.3 Components of (hydro)alcoholic extracts from propolis affects the order of bilayer and microenvironment in model lipid membranes

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Propolis is the most heterogeneous product that can be obtained from the growth of honey bees (*Apis mellifera*), more than 300 types of molecules being identified in his composition. Propolis is produced by honey bees from resins, collected from plants, especially trees, mixed in turn with various substances (for example enzymes, especially from the salivary glands) secreted by them and with beeswax.

In this study were evaluated the effects of (hidro)alcoholic propolis extracts on two types of model lipid membranes (POPC, 1–palmitoyl–2–oleoyl–glycerol–3–phosphocholine lipids, which mimic mammalian cell membrane and a mixture of POPE – 1–palmitoyl–2–oleoyl–sn–glycerol–3–phosphoethanolamine and POPG – 1–palmitoyl–2–oleoyl–sn–glycerol–3–phosphor–(1'–rac– glycerol) (sodium salt) lipids, in a ratio of 75:25 w/w, which mimic bacterial cell wall) using different fluorescence spectroscopy techniques. In order to assess the effects of propolis extracts on model membranes, the steady state fluorescence, time resolved fluorescence and fluorescence anisotropy techniques were used. As fluorescent markers for lipid bilayers DPH, TMA-DPH and Laurdan were used.

Using the fluorescence spectroscopy techniques mentioned above, the interactions between the soluble (hydroalcoholic) components of propolis and the two types of lipid bilayers used were highlighted. The differences that appear at the interaction between the two types of lipid membranes and propolis are due to the constituents of the latter (different proportions of hydrophobic molecules and / or that have electric charge).

Acknowledgements:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-PD-2019-0778, within PNCDI III, and through the National Core Program No. PN 19 06 02 03/2019.

P1.4 Nutritional chemical evaluation and antioxidant capacity of spices

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In the food industry, the availability of natural extracts with a pleasant taste or smell, combined with a preservative action, is a common need. Spices are used in the food industry as significant elements in improving the flavor of food. Plants used as spices usually contain a large number of essential oils and are known for their antioxidant capacity, which plays an essential role in maintaining health, protection against coronary heart disease and cancer. Their nutritional quality is often ignored. They are a good source of polyphenols and flavonoids and also an important source of amino acids having an important involvement in stabilizing lipid peroxidation and inhibiting various types of oxidizing enzymes.

This study aims to perform a chemical nutritional evaluation of some plants used as flavoring compounds in food (black and white piper, cardamom, nutmeg, ginger, oregano, turmeric, basil, dill, thyme and allspice), using modern analytical techniques: gas chromatography coupled with mass spectrometry - GC-MS, optical emission spectrometry with inductively coupled plasma - ICPOS, spectrometry in UV-VIS, etc.

Poster Communications

P2. Interfaces and biosensing

P2.1 A high surface-to-volume ratio monolayer nano-thin organic film for chemical sensor applications

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For chemical sensors it is important to obtain fast detection times which requires a thin sensing layer coating to eliminate long volume diffusion times. However, this decreases sensitivity. The best way to increase sensitivity and level of detection is to increase the surface-to-volume ratio of a thin film. In our research we use the best method to prepare organized organic nano-thin films – the Langmuir-Blodgett (LB) method. The task of increasing the surface-to-volume is currently achieved by others by incorporating in the LB films coated nanoparticles, carbon nanotubes, or quantum dots. We propose a simpler method to achieve this task. We use the fluorescently head labeled phospholipid DPPE-NBD. By depositing an LB monolayer under special conditions we obtain 3D pyramids. Depending on the deposition surface pressure we can vary the height of these pyramids from 6 to 50 nm. Their diameter in the base is in the range from 50 to 400 nm. Thus a well-developed surface is obtained. In order to verify the increased sensitivity of this structure, we tested it as a gas sensor to saturated vapors of some organic solvents. An LB monolayer was deposited on a surface acoustic wave resonator which measures the mass of the layer and adsorbed mass of the gas. The sensor shows some selectivity between polar and non-polar solvents. It has extreme sensitivity to non-polar solvents e.g. chloroform, adsorbing more mass than the mass of the layer itself. Sorption and desorption occur within seconds and there is complete recovery to baseline. Also, the sensor shows minimum sorption of water vapors, which usually interfere with such measurements. All these make this coating an easy to prepare, promising sensing layer for low gas concentrations.

P2.2 Aptamer-modified citrate-capped gold nanoparticles for sensitive visual detection of C-reactive protein

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Human C-reactive protein (CRP) is a sensitive biomarker of inflammation and tissue damage which is associated with various diseases and pathological conditions, such as cardiovascular diseases, sepsis, viral infections, and recently was identified as an early clinical indicator of the development of coronavirus disease [1]. Normal CRP levels for humans are between 8-10 mg/l, but chronic low levels of CRP (5 mg/l) indicate the risk of developing cardiovascular diseases. Therefore, rapid, reliable, high-sensitivity CRP assays are necessary to detect small variations in CRP levels in order to timely predict such diseases. Herein, we validate a CRP colorimetric assay based on the aggregation of colloidal citrate-capped gold nanoparticles (AuNPs) functionalized with a CRP-specific aptamer (apt-AuNPs). First, the spherical structure of the AuNPs is revealed by transmission electron microscopy and confirmed by the presence of one localized surface plasmon resonance (LSPR) mode in the UV-Vis extinction spectrum. Next, the AuNPs are functionalized with a CRP-specific aptamer and their behavior in the presence of CRP was studied. The interaction of apt-AuNPs with different CRP concentrations resulted in color-changes of the colloidal solution recognized even by the naked-eye. Moreover, UV-Vis spectroscopy is used to evaluate the performance of the sensing method and the appearance of a new plasmonic band attributed to aggregated NPs was observed, which represents the detection mechanism of this work. A linear dynamic range was obtained by monitoring the ratio between the LSPR bands of aggregated and individual NPs. Thus, the proposed apt-AuNPs based sensing platform brings new horizons in the rapid, selective, and highly sensitive detection of CRP.

Acknowledgement
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-1592, within PNCDI III.

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P2.3 Aptasensors for the detection of molecules involved in QS and biofilm formation

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An important medical concern is represented by the failure of antibiotics to treat bacterial infections, which leads to high mortality rates. *P. aeruginosa* is among the most highly virulent and antibiotic-resistant bacteria, its virulence is owned to the ability to form an adherent biofilm on the affected surfaces that increases the resistance to disinfectants, UV light, and antibiotics. The bacteria communicate through a system called quorum sensing (QS) by producing molecules like N-3-oxo-dodecanoyl L-homoserine lactone (3O-C_{12}-HSL) and cyclic dimeric guanosine monophosphate (c-di-GMP). When a threshold of population density is achieved, it triggers the switch from planktonic form to biofilm and the production of virulence factors (1).

To increase the chances of survival of a *P. aeruginosa* infection, early diagnosis is required. The main diagnosis technique is by laboratory growth (culture), however, this is a time-consuming method that needs specialized personnel.

In this study, new electrochemical biosensors were developed as a diagnosis tool for the selective and sensitive detection of molecules involved in QS (3O-C_{12}-HSL) and biofilm formation (c-di-GMP). The support electrode used was a portable and easy to use carbon screen printed electrode (C-SPE) that was then modified with gold nanoparticles (AuNPs). Biomimetic elements represented by thiol functionalized aptamers were integrated into the AuNPs-based sensing platform to increase the specificity of the method. In order to avoid nonspecific adsorption, the remaining unoccupied AuNPs were blocked with 6-mercapto-1-hexanol. After every modification step, the electrode was characterized by differential pulse voltammetry (DPV) and electrochemical impedance spectroscopy (EIS) using $[Fe(CN)_6]^{3-/4-}$ as a redox probe. This method showed good sensibility and specificity and can act as a promising tool in detecting healthcare associated infections.

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P2.4 Self-assembled gold nanostar films as substrates for surface-enhanced optical spectroscopy

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Star-like gold nano-objects such as nanostars and nanourchins possess remarkable optical properties due to their highly anisotropic shape. Specifically, their sharp tips can act as antennae for capturing and amplifying incident light, as well as for enhancing the light emitted by nearby fluorophores or the scattering efficiency of Raman reporters. At the same time, their optical response, dominated by surface plasmon resonances, is highly tunable by the dimensions and shape of the particle's core and tips.

The main goal of this work is to obtain self-assembled gold nanostar films as plasmonic substrates for surface-enhanced optical spectroscopy. Gold nanostars obtained using a two-step seed mediated synthesis protocol were further stabilised with polyvinylpyrrolidone (PVP) of different molecular weights. The colloidal nanoparticles were characterised by UV-Vis-NIR extinction spectroscopy, Dynamic Light Scattering, and Transmission Electron Microscopy. Gold nanostars were assembled into films by convective self-assembly on solid substrates. The obtained plasmonic films were characterised by UV-Vis-NIR extinction spectroscopy, and Scanning Electron Microscopy. The efficacy of the plasmonic films as Surface Enhanced Fluorescence (SEF) or Surface Enhanced Raman Scattering (SERS) substrates was assessed by the use of several molecular fluorophores / Raman reporters (e.g. Nile Blue A, Crystal violet, Rhodamine 800). Steady-state and time-resolved fluorescence investigations were performed in order to highlight fluorescence intensity enhancement and fluorescence lifetime modification effects. The SERS signal was also spectroscopically assessed. The experimental results are corroborated with theoretical modelling by FDTD simulations.

The developed innovative platform based on gold nanostar films holds promising potential for fabricating biosensors based on plasmon-enhanced optical spectroscopy.

Acknowledgement.
This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS-UEFISCDI, project number PN-III-P4-ID-PCE-2020-1607, within PNCDI III. Author L. B.-T. acknowledges support from the Nucleu Programme, supported by MCID, project no. PN 19.35.02.01.

P2.5 An analytical approach for magnetoresistive sensor performance on magnetic nanoparticles detection for biosensing systems

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Magnetic micro-devices are an essential part in developing highly sensitive and low-cost methods for clinical testing and diagnosis. The intrinsic characteristics of magnetic field sensors (high scalability, sensitivity and integrability with semiconductor integrated circuits) make them a great choice for detecting magnetic nanoparticles (MNPs). The development of magnetic field biosensors primarily focuses on equivalent magnetic noise reduction or overall design improvements in order reduce costs or physical size while also keeping the desired detection characteristics. Current demands of biological systems diagnostics are for low-cost fabrication methods, scalability, integrability, and ease of use.

The central point of this review is on the theoretical and operational basis for developing a state-of-the-art magnetoresistive biosensor system for detecting labeled magnetic nanoparticles. A classification of magnetoresistive biosensors is performed as well as some of the steps for the biofunctionalization process. An analysis is carried out in terms of practical solutions to improve sensor characteristics (signal to noise ratio, sensitivity, detection limits etc.). Less common approaches such as analyzing the derivative of the output signal and spectral analysis for detection in AC magnetic fields are considered.
Sensor placement, configuration, operational principles and approaches for MNPs sensing processes are targeted. A utilitarian approach to micromagnetic simulations for magnetic nanoparticles and evaluating sensor performance is also discussed. Methods suitability is evaluated based on references or experimental results.
The described theoretical and practical methods can be applied for integrating novel advancements into a lab-on-a-chip device for biomedical diagnosis applications.

Acknowledgments:
This work was supported by a grant of the Romanian Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2019-3514, within PNCDI III.

Poster Communications

P3. Early diagnosis and precision medicine & Clinical diagnosis and therapy

P3.1 Targeted drug delivery systems based on magnetic and gold nanoparticles for the treatment of hepatocellular carcinoma

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Hepatocellular carcinoma (HCC) is the most common type of liver cancer and is ranked among the most common causes of cancer-related mortality worldwide. Despite its many benefits, sorafenib (SOR), the treatment of choice for advanced-stage HCC, presents several limitations, such as poor water solubility, low bioavailability and systemic adverse reactions. These limitations can be overcome by encapsulating SOR into different drug carriers whose specificity can be enhanced by functionalizing them with tumor cell-specific aptamers.

In this study, four types of carriers were used for the encapsulation of SOR. Two types of gold-based carriers: simple gold nanoparticles (AuNP) and PEGylated gold nanoparticles (AuNP-PEG) were employed, as well as two different types of magnetic carriers: azelaic acid functionalized magnetic nanoparticles (MNP) and poly-tartaric acid functionalized magnetic nanoclusters (MNC). The tumor cell specific aptamer TLS11a was used to functionalize the carriers in order to ensure their selectivity towards tumor cells. The carboxyl-functionalized carriers (AuNP-PEG, MNP and MNC) were functionalized with amino-terminated aptamer TLS11a via NHS/EDC coupling and amide bond formation, while in the case of AuNPs, the thiolated TLS11a aptamer was linked via Au-S bond. Aptamer coupling was confirmed by UV-Vis spectrophotometry, as well as by Raman spectroscopy and FT-IR spectroscopy in the case of gold-based carriers. Electrochemical impedance spectroscopy was also used to confirm aptamer immobilization onto the MNPs. The aptamer-functionalized carriers were then loaded with SOR and loading was confirmed by UV-Vis spectrophotometry, as well as by Raman spectroscopy and FT-IR spectroscopy in the case of gold-based carriers. Finally, SOR release studies were performed using UV-Vis spectrophotometry.

Acknowledgement:
A.Pusta acknowledge UMF Internal Grant Nr. 882/52/12.01.2022

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P3.2 Viability and clinical effects of *Lactobacillus Plantarum* ATCC 8014 using an innovative probiotic drink in human being

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Background. Clinical trials are based on probiotics containing Lactobacillus Plantarum 299v. Studies on probiotics containing Lactobacillus Plantarum ATCC 8014 are few. Probiotics with Lactobacillus Plantarum ATCC 8014 have not yet been tested on human subjects. The aim of this study was to assessment of the effect of a probiotic vegetal fermented beverage with Lactobacillus Plantarum ATCC 8014 on the feces bacterial composition and on the consistency and frequency of defecations in healthy volunteers.

Method: Twenty healthy volunteers ingested a daily dose of Lactobacillus plantarum ATCC 8014 (7.5-8 g/L equivalent to 2x 10^{10}CFU / day) for 7 days. Stool samples were collected before and after consumption. The fecal bacterial concentration of Lactobacillus plantarum ATCC 8014 was measured. The frequency and consistency of the stool after consumption was evaluated. **Results:** Lactobacillus plantarum ATCC 8014 crossed the gastrointestinal barrier. Fecal concentrations of Lactobacillus plantarum ATCC 8014 significantly increased by an average of 220% compared to the initial percentage (p 0.05), from 3,52 x10^5CFU to 7,75 x 10^7CFU after consumption. Half of the subjects experienced a change in stool consistency and frequency. **Conclusions:** After the consumption of the probiotic drink, the fecal concentration of Lactobacillus plantarum ATCC 8014 significantly increases in healthy volunteers. Half of the subjects experienced a change in stool consistency and frequency.

P3.3 Can molecular docking solely predict antibiotics' bactericidal activity?

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Molecular docking is a computational tool used for virtual screening of active compounds in order to identify the hits from the leads when searching for a new drug. It is said to be a more accessible, cheaper, faster, and a more user friendly version of high-throughput assays – a complex technology performed at multidisciplinary level, in general available only to big pharmaceutical companies.

In this study we aim to identify the antibiotic(s) with the best bactericidal activity on different Gram-positive and negative species. For prevailing the classification, we take into account the highest binding energies, geometric specificity, and, if present, other interactions with the receptor such as hydrogen bonds. The considered antibiotics belong to two different classes of beta-lactams – penicillins and cephalosporins.

Antibiotics' reactivity is also described by Frontier Molecular Orbital studies and Electrostatic Potential Surfaces based on Density Functional Theory calculations.

After ranking the antibiotics from the most to the least bactericidal compound, a comparison with experimental disk diffusion tests on both Gram-positive and negative bacteria were made in order to draw the conclusions – can molecular docking solely predict antibiotics' bactericidal activity?

Acknowledgment:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, through CNCS/CCCDI – UEFISCDI, grant number PN-III-P1–1.1-TE-2019–0910 within PNCDI III.

Poster Communications

P4. Innovation in Environmental Monitoring

P4.1 A comparative study of different nanomaterials used in the development of sensitive electrochemical sensors for nitrite determination and monitoring in soil

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Sensitive electrochemical sensors for the detection of nitrite in soil were developed using screen-printed carbon electrodes (SPEs) modified with different nanocomposite materials based on carbon nanotubes, metallic nanoparticles and polymers.

The use of nitrogen-based fertilizers is very important for plant growth, thus the conversion of ammonium via nitrite to nitrate by microorganisms leads to nitrate leaching and decreases the availability of nitrogen for plant growth. Nitrate excess in the environment also results in the eutrophication of various bodies of water and growth of toxic algae. Thus, the detection of nitrite, as an indicator of the nitrification process, is of great importance for environmental and agricultural applications.

Commercially available SPEs were modified using 2D based carbon nanomaterials (nanotubes) and metallic/metallic alloy nanoparticles (e.g., Au, Pt, Ag, Au-Ag) in order to increase the analytical performances for sensitive and selective determination of nitrite.

The oxidation of nitrites at the carbon-based electrodes occurs at high values of applied potential, increasing also the effect of potential interfering compounds and decreasing in the same time the selectivity of nitrite detection. Thus, the use of conductive nanomaterials was approached in order to improve the sensitivity of the sensors towards the oxidation of nitrite and to decrease the applied over-voltage.

Various polymers (e.g., 2,6-dihydroxynapthtalene; 4-2-aminoethyl-aniline, chitosan) were used in order to enhance the stability of the nanomaterial at the sensor's surface and to improve the selectivity of the developed sensors. Thus, electrodeposition or drop casting of the polymers on the previously functionalized electrode surfaces were performed.

The ratios between carbon nanomaterials and metallic nanoparticles used for functionalization of SPEs and the method for polymer deposition were optimised. Developed sensors were characterised using electrochemical techniques.

Acknowledgements:
This work was supported by Ministry of Research, Innovation and Digitization through International Program PNIII-ERANET-MANUNET-NITRISENS no 216/2020

P4.2 Bioaccumulation of toxic metals in two different thymus species

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Satureja hortensis and ***Thymus serpyllum*** are two aromatic plants of the Laminaceae family often used both as spices and for medicinal purposes. The aim of this study was to evaluate the bioaccumulation of As, Cd, Ni and Pb in the root, stem, leaves and flowers of plants grown on a polluted soil. To carry out the experiments, the seeds were planted in a greenhouse using universal soil and watered with tap water. The physical-chemical characterization of seeds, soil and tap water was done. The seedlings were planted in pots that contained polluted soil collected from the vicinity of a pyrite waste dump (Valea Calugareasca, Romania). Both experiments (***Satureja hortensis*** and ***Thymus serpyllum***) were performed in three different pots in which 15-20 seedlings were planted. In order to compare the results, control experiments using universal soil and seedlings were carried out. Every month from June to August, thyme plants were collected and the metal content (As, Cd, Ni, Pb) in different parts of the plant (root, stem, leaves and flowers) was determined using inductively coupled plasma optical emission spectrometry (ICP-OES).

Metal transfer from root to aerial parts (TF) and translocation from soil to root (BCF) were calculated. Although the experiments were carried out in the same environmental conditions (greenhouse with controlled temperature and light intensity), it was observed that the thyme species developed different. While ***Satureja hortensis*** reach flowers stage, in the case of ***Thymus serpyllum*** the flowering did not take place. While ***Satureja hortensis*** root accumulates arsenic, ***Thymus serpyllum*** root accumulates nickel in the first months of the experiment. The obtained results show that both thyme species accumulate lead in the root. An accumulation of cadmium in the stem was observed in both plants, and none of the metals accumulates in the leaves.

Acknowledgements:
This research was funded by the Ministry of Research, Innovation and Digitization of Romania, National Research Program “Nucleu”, contract no. 20N/2019, Project code PN 19 04 01 01.

P4.3 Microplastics induced toxicity on *Oreochromis niloticus* (Nile tilapia)

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Microplastics are considered emergent pollutants as an increasingly number of reports are indicating aquatic environment contamination with such agents.

In this study, we exposed juvenile specimens of *Oreochromis niloticus* to 500 and 1000 ppm concentrations of polyvinyl chloride microplastics (PVC MPs), the worlds third most widely produced plastic polymer. PVC is also one of the most widely used plastic materials in medical applications, being considered safe and with a low cost of ownership. Although considered biologically inert under optimal usage conditions, PVC can be mixed with additives sometimes up to 50% by weight, in order to obtaining special characteristics. Such additives additions (e.g., Bisphenols) are not required by law to be made knowable to the consumer per product/quantity. These additives can give an additional ecotoxicological effect as they are being released under UV light, salinity and temperature and can have cancerogenic and endocrine disruptive activities.

If not properly managed, PVC waste is inevitably getting fragmented and consequently such fragments end up in the aquatic ecosystems as microplastics (5 mm –1000 nm).

During our study, the specimens and water parameters (pH, temperature, Oxygen saturation) were closely monitored for 40 days before the sacrifice of the specimens took place. Liver tissue samples were collected for histological and biochemical analyses. Low catalase activity was observed in the 1000 ppm exposed group as well as high malondialdehyde (MDA) levels, indicating oxidative stress. Glutathione peroxidase was significantly less in the 500 and 1000 ppm groups in contrast to the control group. These findings were correlated with liver and intestinal histopathological modifications, which were absent in the control group.

In conclusion, although considered biologically inert, PVC MPs affects the enzymatic activity in fish organisms as well as it leads to tissue alterations, therefore it can be considered an important ecotoxicological marker in aquatic environments.

P4.4 Bioaccumulation and translocation factors of synthetic auxins in aromatic plants (Basil)

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The aim of this activity was to identify synthetic auxins (Picloram and Clopyralid) in aromatic plats (basil) in order to determine their accumulation degree in plant organs in a study carried out over 15 days. During the experiment, a substrate consisting of peat and humus, without auxin content, controlled contaminated with a concentration of 100 ng/g d.w. was used. Auxins were identified using an Agilent 1260 liquid chromatograph coupled with an Agilent 6410B triple quadrupole mass spectrometer (LC-MS/MS) with positive electrospray ionization source. Experiments showed that basil was able to accumulate about half the amount of Clopyralid from the soil, while the amount of Picloram determined was less than 10 ng/g. Clopyralid was determined in all plant tissues, while Picloram was mostly found in the root and only in a single sample in the stem. Calculating the bio-concentration factors, the determined values were subunit, which means that neither of the two compounds is bioaccumulative. The values of the root concentration factor were also sub-unitary in all cases. Calculating the ability of translocating organic compounds from root to stem also obtained subunit values, suggesting inefficient translocation of Clopyralid and Picloram from root to stem and the tendency to accumulate in the root. Therefore, the basil showed a preferential accumulation of Clopyralid in the leaves rather than in the stem, the value of its ability to move from the stem to the leaves being higher than 1.

Acknowledgements:
This research was funded by the Ministry of Research, Innovation and Digitization of Romania, National Research Program “Nucleu”, contract no. 20N/2019, Project code PN 19 04 01 01.

P4.5 Synthesis and characterization of novel histidine-stabilized gold nanoclusters for the sensitive and selective detection of Fe from water samples

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Iron (Fe) is an indispensable micronutrient that participates in many physiological and pathological processes. However, high concentrations of Fe can induce a variety of serious diseases, such as low blood pressure, Parkinson, Alzheimer, etc [1]. Therefore, it is absolutely necessary to develop fast, accessible and reliable sensing methods for the detection of Fe. Having remarkable features regarding sensitivity and selectivity, gold nanoclusters (AuNCs) are extensively used to develop photoluminescent sensors for the detection of different chemical and biological analytes. Therefore, within this study, we fabricated a cheap, fast and simple sensing platform based on the quenching effect of novel synthesized histidine stabilized AuNCs (His-AuNCs) photoluminescence (PL) when interacting with Fe from water samples. Preliminary to this, we performed a thorough characterization of the synthesized His-AuNCs, which presented a strong 470 nm emission under 380 nm excitation with great photostability. Furthermore, we demonstrated the PL “turn-off” selectiveness of His-AuNCs against Fe and, afterwards, quantified the PL quenching effect at different concentrations of Fe ions in solution using a portable fluorescence spectrometer. The triplicated experiments presented a limit of detection (LOD) lower than the limit of Fe in drinking water admitted by the World Health Organization (35 μM). The obtained results prove that the synthesized His-AuNCs, performing as a fast, selective, accessible and cheap sensing platform, represent promising candidates in environmental applications, for the monitoring of Fe levels in water samples.

Funding:
This research was funded by the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project PN-III-P1-1.1-TE-2019-0700. The present work has received financial support through the Special Scholarship for Scientific Activity, contract number 36.606/02.12.2021

Reference
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P4.6 Development and Validation of new HPLC-DAD method for detection of anti-inflammatory drugs in surface water samples

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The main purpose of this paper was to develop and validate an HPLC-DAD chromatographic method for the detection and quantification of nonsteroidal anti-inflammatory drugs, namely: acetaminophen (ACF), diclofenac (DCF), ibuprofen (IBF) and ketoprofen (KTF) in surface waters. Following the LC detection optimization procedure, the parameters that generated the maximum sensitivity (minimum peak width, maximum efficiency, maximum signal-to-noise ratio) were chosen for all compounds analyzed together with a minimum chromatographic separation time. The optimal HPLC separation parameters for experimentally established non-steroidal anti-inflammatory drugs are as follows: Eclipse C18 chromatographic column 15 mm x 4.6 mm, 5 µm; column temperature: 20 ° C; injection volume: 10 µL; mobile phase: 20 mM phosphate buffer in ultrapure water (brought to pH = 3.3): acetonitrile; mobile phase flow: 1 mL / min; gradient elution mode; UV detection: λ = 248 nm for acetaminophen, 255 nm for ketoprofen, and 280 nm for diclofenac and 220 nm for ibuprofen, separation time: 10 minutes. After acidification to pH 2, the surface water samples were extracted using polymeric Strata X cartridges. The limit of quantification (LOQ) of the method was 0.3 µg/L for ACF, 0.6 µg/L for KTF, 0.65 µg/L for IBF and 0.15 µg/L for DCF. Recovery ranged from 81% to 96% for KTF, DCF, IBF, and ACF. Nine surface water samples taken from several areas in Romania were analyzed. The highest concentration determined for ACF was 21.25 µg/L, for KTF was 0.89 µg/L, and for DCF anti-inflammatory drugs; ibuprofen; acetaminophen; diclofenac; ketoprofen and IBU the determined concentrations values were situated below the quantification limit of the method.

Acknowledgements:
This research was funded by the Ministry of Research, Innovation and Digitization of Romania, National Research Program “Nucleu”, contract no. 20N/2019, Project code PN 19 04 01 01.

P4.7 Novel method for assessment of various herbicides in soil and surface water from agricultural areas

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Herbicides used in agriculture can be partially assimilated by plants, but most of the active compounds remain in the soil or are washed, easily reaching the adjacent surface waters, where the maximum allowable amount for each herbicide is set at 0.1 µg /L. A method developed and validated for simultaneous determination of various carbamate and biphenyl ethers herbicides using solvent extraction and tandem mass spectrometry (GC 1310 TSQ 8000 Evo, Thermo Scientific) is described in the current paper. For chromatographic separation, a TG-5MS, 60m x 0.25 mm x 0.25 µm column with helium as carrier gas was used. SRM mode using nitrogen as collision gas and two specific transitions were used for each compound, one for quantification and the second for qualification. Ethyl acetate was used for extraction, with sonication for soil samples. For Chlorpropham, Triallat, Prosulfocarb, Oxyfluorfen, Aclonifen and Bifenox, good linearity was obtained in the 10-500 µg/L range (R^2 from 0.993 to 0.997). LOD varied between 2.5-9.0 ng / L (water) and 0.1-0.4 ug/Kg dry weight (soil). All samples had been collected at the end of autumn. Farmland soil used for sunflower crops southwest to Bucharest and surface water close to sampling areas were evaluated with the described method. In soil samples, concentrations from 6.5 to 17.8 µg/Kg were founded for Prosulfocarb and Aclonifen in less than half of the samples. Prosulfocarb, Aclonifen and Bifenox were identified in most of the surface water with concentrations from 6.2 to 21 ng/L. Chlorpropham, Triallat and Oxyfluorfen were not been identified in the studied samples.

Acknowledgements:
This research was funded by the Ministry of Research, Innovation and Digitization of Romania, National Research Program “Nucleu”, contract no. 20N/2019, Project code PN 19 04 01 01.

P4.8 The impact assessment of metal/metal salts on onion

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Heavy metals (*e.g.* Cu, Mn, Pb, Cd, Ni, Zn) due to the rapid industrialization became an important problem in the entire world and can imbalance the whole ecosystem by their cumulative effects or long-term interactions. These actions affects in the negatively way the crops yield and its consumers. Food security became thus a high-priority concern for sustainable global development. Onion (*Allium cepa L.*) is the most commonly used vegetable in the entire world and it is known to accumulate high concentration of Pb and Cd, while it shows growth inhibition at higher concentration of Cu. The impact of these heavy metals and also Mn on the bioactive compounds is not yet elucidates. The soluble salts from soil, transferred to vegetables became an important source of contamination for humans when consuming them increasing the interests regarding the effect of heavy metals on plants.

The growth of plants in the presence of different concentrations of the heavy metals salts was compared with those grown in the absence of salts. The influence of heavy metals salts on bioactive compounds of onion were investigated by UV-Vis spectrophotometry. The correlation between these has also been traced.

Acknowledgments:
This work was carried out in the framework of Romanian-JINR cooperation (Order 365/11.05.2021; 366/11.05.2021 and 367/11.05.2021).

P4.9 Ultra-trace LC-MS/MS method for detection and quantification of perfluoroalkyl substances (PFAS) in Romanian surface waters

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Per- and polyfluoroalkylated substances (PFAS) are bioaccumulative, toxic and, most importantly, ubiquitous in both the environment and humans. Wastewater treatment and discharge of wastewater treatment plant effluents into natural emissaries is representing the main aquatic environment contamination source with PFAS compounds. The detection and quantification of these compounds (perfluorobutanoic acid - PFBA, perfluoropentanoic acid - PFPeA, perfluorohexanoic acid - PFHxA, perfluoroheptanoic acid - PFHpA, perfluorooctanoic acid - PFOA, perfluorooctansulfonate acid - PFOS, perfluorononanoic acid - PFNA, perfluoroundecanoic acid - PFNuDA and isotopically labeled perfluorooctanoic acid $^{13}C_8$) in surface water samples involves the use of highly sensitive and accurate analytical methods. For this purpose, a new analytical method for the quantification of PFAS compounds at the ultra-trace level has been developed and validated, using liquid chromatography coupled with mass spectrometry (LC-MS/MS). The experiments for determining the optimal chromatographic separation and mass-spectrometric detection conditions were performed on an Agilent 1260 series liquid chromatograph system coupled with an Agilent 6410B triple quadrupole mass spectrometer equipped with an electrospray ionization source, in negative mode. Separation of the compounds was performed using a Zorbax Eclipse C18 chromatographic column (2.1 x 100 mm, 3.5 µm), maintained at a temperature of 30°C. The injection volume was 10 µL, the elution of the compounds being performed using a mobile phase Aq 5mM ammonium acetate/MeOH, at a flow rate of 0.2 mL/min, in isocratic regime. The obtained results indicate the recovery rates were between 82 and 110%, while the relative standard deviations (RSDs) values obtained for intra-day and inter-day precision parameters were situated between 3.7–6.2% and 7.8–10.4%, respectively. The matrix effects were also evaluated and the obtained values ranged from 84 to 102%. The new LC-MS/MS method proved to be accurate and sensitive, with very low quantification limits in surface water (0.13 and 0.80 ng/L).

Acknowledgements:
This research was funded by the Ministry of Research, Innovation and Digitization of Romania, National Research Program “Nucleu”, contract no. 20N/2019, Project code PN 19 04 01 01.

P4.10 Ultrasensitive method for quantification of tin in water samples using new HG-ICP-EOS equipment

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Tin (Sn) is widely used in industry, being a potentially important pollutant of environmental contamination. Although inorganic Sn is relatively non-toxic, organotin compounds represent a significant environmental problem. Inorganic salt can also be converted to organic tin compounds by methylation. Due to its potential impact on the environment, the determination of Sn trace levels is important. The principle of the Sn determination from water samples using HG-ICP-EOS technique consist in the instant reduction of Sn^{4+} ions to Sn^{2+} ions in reaction with 5 mL of saturated boric acid (50 g/L) in 1% (v/v) HCl. Hydride generation was performed in the FIAS 400 equipment cell after the reaction between the Sn^{2+} solution and the reducing agent (0.4% NaBH4 in 0.05% NaOH) in the presence of a saturated solution of boric acid (50 g/L) in 1% (v/v) HCl. Tin detection was performed using an ICP-EOS AVIO 500 at λ = 189.923 nm after volatile hydride transport by the argon to the spray chamber and then to plasma.

The maximum admissible value (MAV) allowed in surface water quality in the national legislation is 2.2 µg/L (OMMGA 161/2006). The calibration curve was set in the range 2 µg/L to 10 µg/L (y = 2279.8x + 1940.9, R = 0.999). In terms of performance characteristics, the method has low detection limit (0.3 µg/L) and quantification limit (1.0 µg/L). Precision data at MAV indicated 0.4 µg/L (7.4%) for repeatability, 0.5 µg/L (8.6%) for intermediate precision, respectively 0.2 µg/L (20%) for measurement uncertainty. The developed method is suitable for Sn detection in surface water.

P4.11 Pilot validation system of breeding habitats of sturgeon species

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This research is a necessity given the importance of conserving and protecting aquatic ecosystems, as well as declining species, especially sturgeon species. Given that these species are considered vulnerable and critically endangered according to IUCN Red List rules and because there is currently insufficient data to prove their possible breeding habitats, the main purpose of this research on the invention is to obtain a data volume of the utmost importance with regard to the areas meeting the breeding criteria of these species. Thus, it describes a pilot installation for validating the breeding habitats of sturgeon species located on the Lower Danube. At the same time, this invention has the following aims: to identify and validate possible breeding habitats, to facilitate the collection of biological material in order to verify the risk of infection with AcIV-E or other viruses, and to validate the fact that sturgeons perform their reproductive cycle within their natural habitats.

Poster Communications

P5. Novel materials and biomaterials

P5.1 Nickel oxide-silver-antibiotic nanocomposites for antimicrobial applications

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In the last years, the antimicrobial effect of metal and metal oxide nanoparticles in combination with antibiotics has attracted an increasing interest from the scientific community. Nanoparticles combined with optimal antibiotics have been shown to provide excellent synergistic properties. Likewise, silver-antibiotic combination demonstrated their efficiency against various pathogenic microorganisms. In this work, NiO-Ag-antibiotic (sulfamethoxazole, norfloxacin) composite materials were prepared with the aim to evaluate their antimicrobial potential. The nanocomposites were characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), scanning electron microscopy (SEM). The antimicrobial activity of the prepared composites was tested against several pathogenic strains including *Staphylococcus aureus* ATCC 49444, *Escherichia coli* ATCC 8739, *Pseudomonas aeruginosa* ATCC 24853, *Salmonella typhimurium* ATCC 14028, *Candida parapsilosis* ATCC 22019, *Candida albicans* ATCC 10231. The minimum inhibitory concentration (MIC) values demonstrated the antimicrobial efficacy of the NiO-Ag-antibiotic nanocomposites.

Acknowledgments:
This research work was financially supported by the Romanian Ministry of Research, Innovation and Digitization (MCID) within Core Programme, project PN19 35.

P5.2 Biologically synthesized gold nanoparticles for the detection of reactive oxygen species

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Metallic nanoparticles offer the advantage of an enhanced surface area, increased sensitivity, stability, and biocompatibility and considerably improve the conducting properties of an electrochemical sensing platform. They offer real-time response with high selectivity for bioactive compounds relevant in biomedical or environmental applications. Hence, gold nanoparticles (AuNP) are excellent candidates for the development of label-free sensors as rapid screening tools for specific biomolecules, such as reactive oxygen species (e.g., hydrogen peroxide (H_2O_2)).

Biologically synthesized AuNPs were obtained by reducing chloroauric acid ($HAuCl_4$) using various plant extracts. The reduction process and variation of parameters such as plant extract and metallic salt concentration were monitored using UV-Vis spectrophotometry. The synthesized AuNPs have different shapes, sized and functional groups, depending on the biomolecules present in the plant extracts: proteins, sugars, enzymes, amino acids and other metal traces, highlighted by Transmission Electron Microscopy (TEM) and Fourier-transform infrared spectra (FTIR). Cyclic Voltammetry and electrochemical impedance spectroscopy were also used for the characterization of the AuNPs.

An application for the use of biologically synthesized AuNPs is also presented by modifying the surface of a screen-printed carbon-based electrode with the newly synthesized AuNPs, for the sensitive and selective detection of H_2O_2. Using fixed potential amperometry, high sensitivities and low detection limits were obtained.

Acknowledgments:
This work was supported by a grant of the Romanian Ministry of Research and Innovation, CNCS - UEFISCDI, project number PN-III-P1-1.1-PD-2019-1285, contract no. 123 within PNCDI III.

P5.3 Biowaste valorization via HTC process for the retention of some emerging pharmaceutical pollutants from aqueous solutions

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In today's world, due to population increase, there are many alarming and potential catastrophic problems like climate changes, environmental pollution and enormous mass of wastes produced constantly, thus leading mankind to find innovative solutions for the management, recycling and valorization of biomass from by-products of agricultural production, food processing and organic household residues [1]. Biomass is the raw material of the bioeconomy, and researchers believe the future will bring many biomass-derived products such as biofuels, 'green chemicals' and biomaterials [2].

In this research biomass waste consisting of walnut shells (WS) was treated via hydrothermal carbonization process (HTC) to obtain eco-friendly materials that can be used for environmental applications like pollutant retention from water sources. Three materials (HTCWS1, HTCWS2, HTCWS3) were obtained using a dynamic autoclave at 220°C, autogenous pressure, 1:10 biomass-water weight ratio, and 3 different reaction times: 1h, 6h and 12h. The eco-materials were characterized by means of ATR-FTIR analyses, SEM-EDS, pHpzc, and to determine the removal efficiencies of some emerging pharmaceutical pollutants (methylene blue - MB and paracetamol - PRM), a UV-VIS spectrophotometer was used.

The results obtained suggest that the materials were efficient in the retention of MB and PRM from water solutions, thus making them suitable for environmental applications.

Acknowledgments:
The authors would like to express appreciation for the support of the Romanian Ministry of Research, Innovation and Digitalization, CCCDI - UEFISCDI, project number PN-III-P3-3.5-EUK-2019-0237, within PNCDI III (NonActivPans), under the Contract No 219/2020.

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P5.4 Effect of hydrothermal doping on the morphology, structure and composition of sulphur, boron-co-doped graphene

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Heteroatom doping can effectively tailor the local structures and electronic states of intrinsic two-dimensional materials such as graphene, and enhance their optical, electrical, and mechanical properties. Heteroatom co-doped high-quality graphene has been taken into account as a promising host material to enhance conductivity and improve electrochemical performances. In this work, an easy hydrothermal method was employed to prepare sulphur, boron co-doped graphene. The doping process was performed at 120°C for 3 hours. The morphology, structure and composition were studied. The obtained materials were thoroughly investigated by SEM, X-Ray powder diffraction, Raman and XPS. As indicated by XPS, the concentration in the sample may reach 13.5 at% for sulphur and 1.6 at% for boron. Such large difference may be due to the fact that doping by boron atoms can be regarded as hole doping; doping by sulfur atoms in graphene can be viewed as electron doping. Our work offers a simple and relatively low-cost approach to increase the amount of doped heteroatom.

Acknowledgments:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI–UEFISCDI, Project Number PN-III-P4-ID-PCCF-2016-0006, within the PNCDI III.

P5.5 Electrochemical Detection of Piroxicam with Nitrogen-Doped Graphene-Based Sensor

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Heteroatom-doped graphene has applications in electroanalysis due to its unique electronic structure and stable chemical properties. In the present work, a nitrogen-doped graphene-modified glassy carbon electrode NGr/GC was developed for the investigation of the electrochemical behavior of piroxicam in pharmaceutical samples. Nitrogen-doped graphene (NGr) was synthesized by the hydrothermal method using urea as reducing and doping agent for graphene oxide (GO). The morphological and structural characteristics of GO and NGr samples were investigated by scanning electron microscopy (SEM) and X-ray diffraction (XRD). As indicated by elemental analysis, the concentration of nitrogen in the NGr sample was 6 wt%.

Next, the electrochemical detection of piroxicam (PIR) was tested with both bare GC and the graphene-modified electrode (NGr/GC). A considerable enhancement in the response of piroxicam on the surface of the modified electrode was observed compared with the unmodified electrode. In the case of bare GC, the oxidation signal of PIR in pH 5 acetate bufffer was very broad and appeared at high potential (+0.7 V). In contrast, the signal recorded with the NGr/GC electrode was significantly higher (four times) and shifted towards lower potentials (+0.54 V), proving the electro-catalytic effect of nitrogen-doped graphene. The NGr/GC electrode was also tested for its ability to detect piroxicam in pharmaceutical drugs (Flamexin) and the results proved the performance of the NGr electrode and its applicability in real sample detection.

Acknowledgments:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI–UEFISCDI, Project Number PN-III-P4-ID-PCCF-2016-0006, within the PNCDI III.

P5.6 Exploring of hydrolysate keratin and biopolymers spinnable properties to fabricate nanofibers for wound healing management

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Traditional wound dressing management includes materials such as cotton gauze dressings, hydrogels and foams, in form of bandages, cohesive wrap, impregnated gauze, or natural materials like leaves, cobwebs, and honey extracts [1]. The drawbacks of these materials are referring to loading them with exudates, degradation of the skin of the wound, frequent dressing changes, non-biomimicry, difficulty in loading with suitable drugs, and the delay to wound healing leading to a high cost of wound management.

Among all natural polymers, keratin prepared by solubilization of sheepskin wool is a promising protein for wound regeneration proved by a good cytocompatibility and partially preserved secondary structure after electrospinning process [2].

In this paper, keratin hydrolysate was extracted in an alkaline medium and further investigated for its ability to form nanofibers in combination with chitosan, poly(ethylene oxide) (PEO), and poly(hydroxybutyrate-co-valerate (PHBV) biopolymers, respectively. Structural functional groups for each keratin – biopolymer nanofibers evaluated from attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR) as well as thermal stability performed by differential scanning calorimetry (DSC) were performed.

Results show that the keratin/PEO and keratin/PHBV nanofibers are easy to process and their thermal stability recommend them as possible biomaterials for wound treatment.

Acknowledgments:
The authors would like to express appreciation for the support of the Romanian Ministry of Research, Innovation and Digitalization, CCCDI - UEFISCDI, project number PN-III-P3-3.5-EUK-2019-0237, within PNCDI III (NonActivPans), under the Contract No 219/2020.

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P5.7 Facile synthesis of raspberry-like mesoporous silica nanomaterial

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Raspberry-like hierarchical structured nanocomposites have recently gained attention due to their structural versatility for various applications such as adsorption, catalysis, energy storage, or nanomedicine. They consist of small corona particles placed over large core particles with impressive properties, such as unique morphology, high specific surface area, or high surface roughness. In this respect, targeted research projects must result in the facile controllable synthesis of these mesoporous particles, obtaining materials with tunable surface properties and oriented hierarchical structures. This study presents the one-pot synthesis method for raspberry-like mesoporous silica with particle size of around 400 nm. Raspberry-like mesoporous silica was synthesized using a modified Stöber method. Briefly, 0.004 moles hexadecyltrimethylammonium bromide was dissolved into a solution containing 100 mL absolute ethanol and 167 mL ultrapure water, then, 5 mL ammonia aqueous solution was added. After stirring for 2 h at 35 °C, 2.4 mL tetraethyl orthosilicate was added to the solution and stirred for another 24 h. Then, the mixture was transferred to a Teflon-lined autoclave and heated for 24 h at 100 °C. The solid was collected by vacuum filtration and washed with ethanol and water, respectively. The surfactant was removed by calcination at 550 °C for 6 h. The nanomaterials were characterized by scanning electron microscopy, specific surface area, pores diameters, Fourier-transformed infrared spectroscopy, and thermos-gravimetric analysis. The results indicated that the raspberry-like silica had a specific surface area of around 1250 m^2/g and average pores diameters of 2.96 nm. This method allows the generation of hierarchical nanostructured silica by mimicking the diatom cells structures. Further studies are currently in progress in order to evaluate the efficiency in adsorption and catalysis.

P5.8 Investigations on the stability of graphene oxide dispersions

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As an oxidized form of graphene, graphene oxide (GO) has a lot of potential applications in the electronic, sensing, environmental and medical fields. The structural features of GO that govern its stability in different solvents are not well known and remain a source of controversy among scientists. Understanding its stability (or lack thereof) in liquid solvents is critical for fine-tuning the material's characteristics and its potential involvement in future applications.

Taking the aforementioned considerations into account, the present work provides a study of the alteration of the structural and edge-surface characteristics of 2D GO nanosheets, as well as their stability, during dispersion in various solvents, through the use of Dynamic Light Scattering (DLS), Zeta Potential, X-Ray Diffraction (XRD), Raman and FT-IR Spectroscopy measurements. The samples were synthesized through an original modified Marcano-Tour method and were examined for several weeks after the synthesis. Based on the obtained experimental results and literature information, a new structural dynamic model is proposed, which is accurately outlined by the experimental data. It is based on the cleavage of the carbon bonds acting in the first weeks, while the bonding of oxygen functional groups on the carbon lattice occurs, and the transformation of epoxide and hydroxyl groups into adsorbed water molecules in a process driven by the availability of hydrogen in GO nanosheets. In addition to this, the stability of the GO dispersions in different solvents was also assessed, based on the measured values of the zeta potential.

P5.9 Mathematical modeling by Response Surface Method of a triterpene saponins mixturewith a raised antiproliferative effect

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In our study, three saponins present in *Hedera helix* L. were tested by determining cytotoxicity and antiproliferative effect. The saponins of interest were *in vitro* analyzed at different concentrations on normal fibroblasts and cervix ephitelial tumor cells.

The obtained results were analyzed by mathematical modeling with RSM (Response Surface Method) using Design Expert 11 software, correlating mixtures composition of the three saponins in different proportions with their cytotoxic properties, in order to optimize the saponins mixture to obtain a maximum antiproliferative effect [1, 2].

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P5.10 Novel azopyrazole compoundswith antibacterial activitiy

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The pyrazole nucleus shows considerable attention due to their excellent bioactivity [1]. These heterocyclic compounds and their derivatives have been evaluated as a source of therapeutic agents [2]. The development of new antimicrobial drugs is one of the most important health problems in the world, justifying the need to identify innovative antimicrobial agents. [3-5]. A number of new azopyrazole compounds have been synthesized and characterized by IR spectroscopic mats, 1 H-13 C-NMR, UV-Vis, MS. The compounds were tested in vitro for their antibacterial activity.

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P5.11 Photophysical and vibrational spectroscopic behavior of Rhodamine 6G deposited on ZnO and gold decorated ZnO nanoparticles thin films

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In this study we investigated the photophysical and vibrational spectroscopic behavior of Rhodamine 6G (R6G) on zinc oxide (ZnO) and gold (Au) decorated ZnO nanoparticles thin films. ZnO is a versatile semiconductor with applications ranging from optical devices to biomedical. Here we explored its potential as substrate for surface enhanced Raman scattering (SERS), as well as its effect on the fluorescence properties of a common dye. ZnO nanoparticles [1] of about 15 nm diameters were obtained using polyol method and were decorated with Au nanoparticles following a controlled chemical synthesis. R6G was incorporated in a polyvinyl alcohol (PVA) matrix to allow its deposition as thin films. Additionally, PVA is widely used to protect fluorophores from photobleaching and thermal decomposition and can be of use for photonic devices applications, as well as for biomedical, or environmental monitoring applications [2]. The optical properties of R6G molecules in PVA were investigated and compared to those of the dye deposited on thin films based on ZnO nanoparticles, respectively ZnO-Au nanocomposites. The adsorption of R6G into solid systems showed modifications of its photophysical properties. Time-resolved fluorescence spectroscopy investigations, namely time-correlated single photon counting (TCSPC), were performed and the fluorescence lifetime of R6G was correlated with the effect of ZnO, respectively ZnO-Au nanostructures on its photophysical behavior. Finally, the ZnO nanoparticles and ZnO-Au nanocomposites were used as substrates for SERS and their application for R6G detection was demonstrated [3].

P5.12 PLD deposition of FePt-$BaTiO_3$ thin films heterostructures

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Multiferroic heterostructures with coupled ferroelectric and ferromagnetic elements have attracted an ever-increasing amount of interest recently due to their strong magnetoelectric coupling at room temperature. The magnetoelectric coupling leads to electric field control of magnetism, or magnetic field manipulation of polarization, which provides a wide variety of applications in spintronics and electronic devices. The successful deposition of high- quality films strongly depends on reliable and optimal fabrication techniques. It is known that through the use of PLD technique, even for complex materials, the stoichiometry of the target is preserved within the deposited film. Thus, FePt thin films were grown on Al_2O_3(0001) using PLD technique at 5 Hz laser repetition rate with 370 mJ energy in Ar atmosphere at 700°C. On optimized FePt thin films was deposited $BaTiO_3$ layer with 250 mJ energy, at 5 Hz laser repetition rate in Ar atmosphere at 600°C. Structural, morphological, optical and magnetic properties of the prepared heterostructures were investigated.

Acknowledgments:
This work was supported by the Romanian Ministry of Research, Innovation and Digitization, Core Programme, Project PN19 35.

P5.13 The antibacterial properties of nanocomposites based on antibiotic association with carbon nanotubes and metal oxides

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In the recent years it has been observed that the large numbers of bacteria are becoming resistant to most commonly prescribed antibiotics and the number of resistant strains is significantly growing. The development of new drugs in medicine became very important. Carbon nanotubes (CNTs) due to their ultra-high surface area, high mechanical strength, but ultra-light weight, excellent chemical and thermal stability are considered ideal candidates for drug delivery. In order to improve the properties, metal and metal oxide nanoparticles with magnetic properties are attached to CNTs surface. Magnetic nanoparticles have the advantage that they can be recovered and reused. In order to obtain new drugs delivery system, an antibiotic was retained on nanocomposites based on CNTs and metal oxides. The antibacterial properties were investigated. For these purpose, ciprofloxacin was elected due to well-known antibiotic applied against Gram-positive and Gram-negative bacteria.

Acknowledgments:
This work was carried out through the Core Programme, developed with the support of MCI, project no. PN 19 35 02 03 (36N/13.02.2019).

P5.14 Tunable anti-counterfeit labels based on Ag coated nanotrenches arrays

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Flexible polymeric substrates have been used in recent years for developing new optical devices with improved performance, due to their processability at the nanoscale level. Nanostructured surfaces coated with noble metals have a huge potential for the development of efficient and tunable optical devices. Metallized nanotrenches demonstrate attractive properties being frequently used as optical elements in applications from spectroscopy to metrology and lasers [1]. Here, we focus on the design and fabrication of anti-counterfeit optical labels based on tunable Ag coated nanotrenches. They are able to excite and detect photons in the visible range, which makes them suitable as simple interrogation and authentication techniques. Nanotrenches arrays with 800 nm pitch were fabricated by nanoimprint lithography (NIL) in Zeonor and Topaz flexible and transparent substrates. After that they have been metalized with Ag (thin films of tunable thicknesses) using magnetron sputtering deposition technique [2]. For a uniform array of nanotrenches imprinted in the substrates, the NIL fabrication parameters were optimized. The morphological and structural properties of the metalized nanotrenches were assessed by scanning electron microscopy (SEM) technique. The wavelength dependent absorbance of metalized nanotrenches was assessed by UV-Vis and the measured spectroscopic data have been used as feedback for tuning the architecture of the designed nanostructures.

Acknowledgements:
The authors would like to acknowledge the financial support through the Core Program, Project No. PN 19 35 02 01.

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P5.15 Synthesis and characterization of some azo-compounds as nonlinear optical materials

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Spiranes, alkynes, azo-dyes, heterocycles, ferrocenes, porphyrins, dendrimers, fullerenes, or perylenes, with special geometries and certains electronic molecular parameters, possess nonlinear optical (NLO) properties and have several major advantages over their inorganic counterparts. Azo-dyes are proven to be interesting for their fluorescence properties and also, these compounds have been studied for their nonlinear optical (NLO) response [1,2]. The NLO property occurs mainly due to push−pull systems in D−π−A conjugation which certainly improves the molecular polarizability [3-5].

We report here the synthesis of some azo-dyes by two-steps classical method of diazotation and coupling reactions. The structures of the synthesized compounds were confirmed by ^{1}H-NMR, ^{13}C-NMR, FTIR and elemental analysis. The solvatochromic properties of the compounds were studied. The evaluation of the nonlinear optical properties of these azo-dyes was done by determining the second harmonic generation (SHG) using an experimental setup. It was found that the synthesized azo-dyes were good candidates for NLO properties.

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Acknowledgements:
This work was supported by University of Bucharest, code PN-III-P2-2.1-PED-2019-3009.

P5.16 Synthesis, NLO properties and DFT studies of some heterocyclic compounds

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The discovery of new heterocyclic compounds with nonlinear optical properties (NLO) is a priority research direction in materials chemistry, as the literature reports various heterocyclic, thiophene, benzimidazole, thiazole, pyrimidine compounds with remarkable NLO properties [1-6]. The synthesis of new compounds possessing the second harmonic (SHG) is thus the first step in finding new nonlinear optical materials.

We report here the synthesis and characterization by 1H-NMR, 13C-NMR, FTIR and elemental analysis of a series of heterocyclic compounds. For the synthesized compounds, the second harmonic was determined and DFT calculations were made to correlate the structures of the compounds with the distribution of the HOMO, LUMO orbitals and the Egap energy differences between them, as well as with other geometric or molecular parameters [3,7]. A good correlation was found between the determined NLO properties and the parameters of the studied molecules.

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Acknowledgements:
This work was supported by University of Bucharest, code PN-III-P2-2.1-PED-2019-3009.

Poster Communications

P6. (Micro)spectroscopy

P6.1 High quality, 3D silver nanotrenches fabricated by nanoimprint lithography as flexible SERS detection platform

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Current state-of-the–art detection platforms based on surface-enhanced Raman scattering (SERS) heavy rely on 3-dimensional nanoarrays architectures due to their high reproducibility and uniform density of the hot spots. Moreover, due to their dependence on the optical property of size, shape and periodicity, the periodic nanoarchitectures can be tailored and used in the fabrication of nanodevices with electronical, photonical and biotechnological applications. In this work we present an effective method to fabricate an ultrasensitive detection platform based on reproducible and high resolution, nanostructured SERS substrates. One important advantage is the capability of mass production, which reduces the overall production costs of SERS substrates. We employed nanoimprint lithography technique to fabricate well-controlled periodic nanotrenches on a flexible and transparent substrate. Tunable thickness silver (Ag) films were deposited on the imprinted substrate using direct current magnetron sputtering. Ultralow concentration of crystal violet as analyte sample was detected in case of the Ag film with a thickness of 25 nm [1]. Silver aggregates enabling plasmonic properties were assessed by SEM and AFM measurements. Our final purpose is to use these SERS substrates to develop optical biosensors for the detection of bacterial specific signaling molecules with high impact in quorum sensing.

Acknowledgements:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project numbers PN-III-P1-1.1-TE-2019-0910 and PN-III-P1-1.1- TE-2021-0753, within PNCDI III and Core-Program, Project No. PN 19 35 02 01.

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P6.2 SERS-based smart antibiogram: from concept to routine analysis

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Biological Component Analysis (BCA) is a common strategy to correctly deconvolve Raman spectra when the biochemical components whose major contribution to the spectrum is partially known and their spectral signature is also known. But it is a real challenge to know absolutely all the constituents of a biological sample or to identify them only Raman. That is why such an approach is most often used, by recognizing the marker bands (**Raman Identifying Bands**). The large classes of biological components (proteins, lipids, amino acids, etc.) have specific spectra already known both individually and in collective contribution. The simplest approach is to reduce the number of molecular species that contribute to the Raman signal recorded only to those that have a significant contribution, such as significant spectral band intensity. The rest of the signal is considered a residual signal, which results practically from the difference between the Raman spectrum of the sample and that of the corresponding model, which includes the universal spectral profiles of the biomolecular components. We performed a BCA adapted approach for unravelling the constituents of the bacterial cell wall that are active in **surface-enhanced Raman scattering (SERS)** spectroscopy. For a more clinically relevant response, we investigated control samples, resistant species and susceptible species to latest generation antibiotics. Thus, any small variations in the sample composition, in our case of the bacterial cell wall, will introduce variations in the difference spectrum, which will be highlighted by the chemometric analysis applied automatically later. In this way, the procedure for extracting the difference spectrum between the samples and the model spectra could be used as a decision factor in the clinical routine.

Acknowledgements:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, UEFISCDI, project number PN-III-P1-1.1-TE-2019-0910.

P6.3 Spectroscopic investigation of exopolysaccharides purified from *Arthrospira platensis* cultures as potential bioresources

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Abstract: *Arthrospira platensis* is a cyanobacteria from the Order *Oscilatoriales.* Nicknamed “the food of the future” because its great nutritive properties, it has an estimated production of 20 tons per year, (FAO, 2008) with future prospects of reaching over 90 tons per year by 2028 (Meticulous Research® in collaboration with the European Algae Biomass Association). During its growth, *Arthrospira platensis* releases biopolymers, mostly of carbohydrate nature. The primary roles of these biopolymers, also called exopolysaccharides (EPS), are in helping biofilm development (a structure that helps create an optimal environment for bacterial growth). EPS have the potential of becoming valuable industrial resources. In this study, Raman and Fourier-transform infrared (FTIR) spectroscopies were employed in order to structurally characterize ApEPS50 and ApEPS80 purified from *Arthrospira platensis* AICB49. The biopolymers were obtained by a stepwise ice-cold ethanol purification from the harvested culture media. A three-step process was used for this purification, the final volumes of ethanol for each step being 20% (not enough yield), 50% (ApEPS50) and 80% (ApEPS80). Dextran from VWR Chemicals was also used for comparative spectral profiling. Solid-state ^{13}C NMR (*ss*NMR) analysis was performed for further confirmation of primary component analysis. The aim of this study is to identify and characterize valuable microbial byproducts that are often overlooked by the industry. While “bound” EPS are contained within the biomass and might contribute to the benefic health effects of *spirulina* as a food supplement, the released EPS have the potential of being important bioresources. This work presents the spectral fingerprints of such released EPS, offering insights into the yield and purification process. The tentatively identified saccharide species found in our samples are rhamnose, D(+)-glucose and D(+)-galactose.

Funding:
The authors acknowledge the financial support through the Core Program, Project No. PN 19 35 02 01.

P6.4 The study of molybdenum disulfide phase changes and its stability by micro-Raman spectroscopy

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Two-dimensional (2D) nanostructured materials gained a lot of attention in the past few years. Molybdenum disulfide (MoS_2) is a 2D, graphene like nanostructure with many potential applications such as energy storage, hydrogen and oxygen evolution reaction, photocatalysis and achieved a lot of interest in the scientific community lately [1]. In this study, we are trying to catch a glimpse of phase changes in MoS_2 by using micro-Raman spectroscopy, alongside other characterization techniques such as X-ray diffraction. More precisely the MoS_2 stability towards the changes induced by different laser wavelengths and intensities as well as MoS_2 transition from metallic 1T to semiconducting 2H phase or to MoO_3 are followed [2]. In this respect, we propose the obtaining of a flower-like three-dimensional networked MoS_2 as revealed by scanning electron microscopy, by using different precursors and Mo to S ratios. Two lasers with wavelengths of 532 and 632.8 nm were involved for Raman characterization of molybdenum disulfide. Alongside metallic and semiconducting phases of MoS_2, its transformation to MoO_3 was studied by laser intensity changes at normal atmosphere in the presence of oxygen [2]. Overall, micro-Raman spectroscopy can be a useful tool to study the phase changes and transfer of MoS_2 into MoO_3 nanostructures.

Poster Communications

P7. (Nano)biotechnology

P7.1 Synthesis and molecular interaction between drugs with strong antioxidant and antiradical activity and macromolecular receptors

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Oxidative stress is caused by an imbalance between the action of reactive oxygen species and the ability of the biological system to detoxify rapidly by neutralizing reactive species or repairing any damage to lipids, proteins or DNA. In order to combat oxidative stress, we developed a synthetic molecule which has in its structure the elements strictly necessary for a good antioxidant and antiradical activity, without bulky or inert moieties and to have a good solubility in water, namely dihydroxy-phenyl-thiazole-hydrazinium chloride (DPTH).The present study focuses on the determination of binding and thermodynamic parameters that characterize the DPTH-macromolecules interaction by using modern, specific and complementary techniques, such as isothermal titration calorimetry (ITC) and selective spin-lattice proton NMR experiments. Molecular docking calculations were also performed to characterize DPTH conformations in interaction with macromolecular receptors.

Acknowledgements:
Financial support from the Ministry of Research and Innovation—MCI, Core Programme, Project PN 18 03 02 01 and Project PD75/14.02.2022.

P7.2 Detection of nucleobases on short functionalized peptide-nucleic acid sequences using nanopore-tweezing method

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Nucleic acid sequencing is used for revealing genetic variations at the molecular level and it became undisputed in fundamental and clinical or forensic science, epidemiology, and biotechnology applications.

In this work we used the a-hemolysin (a-HL) nanopore to detect nucleobases from short amino acid-functionalized, peptide-nucleic acids (PNA), in real time, with no biochemical labeling, short sample preparation time and low costs. In order to enhance the time resolution of a-HL-based molecular detection and discrimination on polypeptides, we used "the nanopore-tweezer approach", which is based on the electrostatic tug-of-war between the charges on opposite sides of the model polypeptides and the applied potential.

We employed PNAs engineered with lysine and glutamic acid segments at the N and C-termini and a central sequence of different nucleotides. We extended the a-HL nanopore-tweezer method and assessed the system's ability to discriminate among distinct nucleobases on PNA sequences from ionic current fluctuations measured in a single PNA- a-HL blockade event. [1]

Our findings demonstrate that a-HL sensitivity at the most constricted region provides the specificity needed to recognize bases in homopolymeric PNA.

Acknowledgements.
This work was supported by grants PN-III-P1-1.1-TE-2019-0037, PN-III-P4-ID-PCE-2020-0011.

References:

(1) Dragomir, I. S.; Asandei, A.; Schiopu, I.; Bucataru, I. C.; Mereuta, L.; Luchian, T. The Nanopore-Tweezing-Based, Targeted Detection of Nucleobases on Short Functionalized Peptide Nucleic Acid Sequences. *Polymers* **2021**, *13* (8), 1210. https://doi.org/10.3390/polym13081210.

P7.3 DNA-conjugated gold nanoparticles as key components in the design of non-viral CRISPR/Cas9-Gold-based delivery vehicles

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CRISPR/Cas9 therapy has multiple advantages over traditional gene therapies, being used for effective targeted gene editing. The main challenge in implementing the CRISPR/Cas9-based technology is to design gene delivery vectors that can target more specific mutations in the genome. Hence, DNA-functionalized gold nanoparticles were used to deliver CRISPR/Cas9 in vivo for treatment of inherited disorders, like muscular dystrophy. Because current trials using CRISPR/Cas9-Gold therapy are in the early stages of development, the delivery vectors with less insertional mutagenesis risk should be designed based on molecular-level understanding of the involved systems. To investigate these issues, we computationally optimized such a design in two steps. Firstly, we optimized the DNA loading over a range of nanoparticle sizes in DNA-functionalized gold nanoparticles. In the second stage, we performed molecular dynamics simulations of the Cas9-sgRNA complex. We propose this study as essential in optimizing CRISPR/Cas9-Gold-based delivery vehicles.

P7.4 Polymeric microcapsules for targeted and controlled delivery of therapeutic molecules at human retina level

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Diabetic retinopathy (D.R.) is a serious complication of diabetes, which can lead to blindness. Unfortunately, the drugs used today in the treatment of D.R. have negative side effects, being also difficult to deliver. There is a pressing need to develop an innovative delivery system that has a good loading efficiency of the therapeutic molecule, a controlled and targeted delivery, presenting sensitivity to heat. In this work we propose a novel model of polymeric microcapsules able to encapsulate two FDA approved molecules, a therapeutic molecule (i.e., Avastin) and a NIR fluorophore (i.e., Indocyanine Green – ICG), grafted between the polyelectrolytes layers for intracellular delivery. Precisely, this microsystem was obtained *via* a Layer-by-Layer deposition technique, by adding oppositely charged biocompatible polyelectrolytes on a calcium carbonate core. Subsequently, to make use of its photothermal properties and for localization of the microcapsules within living cells, we interleaved ICG with the polyelectrolytes layers. Finally, we grafted Avastin on the microcapsules, for management of D.R. Hence, microcapsules with a dimension of 1.5 µm were obtained, according to DLS analysis and TEM imaging. The capacity of the microcapsules to operate as effective photo-therapeutic agents was firstly evaluated in solution, following the evaluation in living cells in the near future. The biocompatibility of the Avastin-carrying microcapsules was proven by WST-1 assay. Lastly, cellular internalization and localization of the microcapsules *in vitro* were determined through Confocal Fluorescence Imaging Microscopy technique. Based on the data obtained, this research seeks to implement the microcapsules in the near future as potential intraocular Avastin delivery vehicle for management of D.R.

Funding:
This research was funded by the Romanian National Authority for Scientific Research, CNDI-UEFISCDI, project number PN-III-P2.1-PED-2019-4558. The present work has received financial support through the Special Scholarship for Scientific Activity, contract number 36605/02.12.2021.

P7.5 Protein nanopore-based method for sequence specific detection of single-stranded DNA using gold nanoparticles and peptide nucleic acids

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Conventional approaches for the clinical diagnosis of viral or bacterial infections include: culture and colony counting techniques that require the counting of bacteria, immunological methods based on antigen-antibody interactions and polymerase chain reaction (PCR)-based techniques that involve the analysis of disease-specific nucleic acids. The last mentioned detection methods represent the gold standard for viral detection. Their drawbacks, however, include the expense of equipment, the necessity for qualified personnel, and the time necessary for detection.

In order to overcome these difficulties, we propose a strategy for future easy to use biosensor development that would allow for real-time detection of exogenous short single-stranded DNA sequences (ssDNA) specific for viral infections, while being highly sensitive, as well as cost-effective.

Herein, we used a homo-heptameric α-hemolysin (α-HL) protein nanopore in combination with gold nanoparticles (AuNPs) and a particular class of artificial genetic polymers, namely peptide nucleic acids (PNAs). These synthetic molecular constructs resemble DNA structure, but have an uncharged pseudopeptide backbone rather than the negatively charged sugar-phosphate backbone of DNA. Due to their resistance to enzymatic degradation by nucleases and proteases, as well as their strong hybridization with complementary DNA/RNA targets, PNAs represent potential reagents for detecting nucleic acid targets by hybridization-assisted nanopore sensing.

The fundamental technique in this study was to employ resistive-pulse sensing through a single α -HL nanopore to detect and distinguish AuNPs based on their particular PNA-induced surface property changes and aggregation propensity, both of which are strongly connected to PNA-target ssDNA hybridization, by recording their ionic current blockades signature.

This selective and sensitive ssDNA detection technique could lay the groundwork for next-generation bionanotechnology applications used in clinical diagnosis for the early detection of pathogens, such as influenza virus or coronavirus.

Acknowledgements.
This work was supported by grants PN-III-P1-1.1-TE-2019-0037 and PN-III-P4-ID-PCE-2020-0011.

P7.6 Silver nanogrid substrates for accurate SERS analysis

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Surface-enhance Raman Spectroscopy (SERS) is a sensitive technique for detecting molecules adsorbed to the surface of plasmonic nanoparticles. In order to be used in analytical applications, SERS substrates should ensure reproducibility and should be simple to prepare. Colloidal solutions containing noble metal nanoparticles, such as gold and silver, are the most commonly used substrates. However, for this chemically prepared substrate, deviations in terms of Raman scattering enhancement were reported between laboratories. Therefore, we aimed to develop a metallic substrate of silver nanogrids (AgNg) that is easy to produce, offer high reproducibility and show a high SERS enhancement factor. The substrates were synthesized by Convective Self-Assembling (CSA) method.

The performance of the AgNg was evaluated using Nile Blue test-molecule, the SERS spectra being acquired using a 633 nm laser line, and a limit of detection 10^{-9} M was achieved. The SERS spectra of 10^{-9} M Nile Blue were repeated on five different substrates and a 6.5% relative standard deviation was obtained.

Next, we tested the possibility to use AgNg as enhancement substrate for biological applications of SERS. To this regard, we acquired SERS spectra of a mixture of purine metabolites, creatinine, urea and bovine serum albumin (BSA) samples, simulating the serum composition. The SERS bands of purine metabolites creatinine and urea were observed, without a contribution from BSA. Thus, AgNg can be used as enhancement substrate for biological applications without the need of prior deproteinization of the sample. The SERS spectra of the biological matrix were acquired using a portable Raman spectrometer to be closer to applications in a real-life clinical environment.

To summarize, we optimized AgNg as SERS substrates for clinical application of the SERS in terms of an enhancement factor, ease of use, and reproducibility.

P7.7 Spectroscopic, calorimetric and molecular modeling approaches of the interaction of quaternary ammonium compound with β-CD

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Anticholinergic medicines are a heterogeneous group of substance both from the structural and the therapeutic indications point of view as they can be used in the treatment of many disorders: asthma, gastro-duodenal ulcers, renal/biliary colics, urinary incontinence. In this context, new molecules that contain quaternary ammonium compounds with improved pharmacokinetic and pharmaco-toxicological profile were synthesized. Therefore, encapsulation process of these new compounds synthesized into cyclodextrin could offer the possibility of controlling drug delivery in biological systems, extending the antispasmodic effect and reducing its toxicity and also the increase of the solubility. Spectroscopic investigation supported by molecular modeling methods has been used to describe the inclusion complex of β-cyclodextrin (β-CD) with 1-Methyl-1-({2-[4 (trifluoromethyl)phenyl]-1,3-thiazol-4-yl}methyl) piperidinium chloride (1MPTMPC) in solution and in solid state.

Acknowledgements:
Financial support from the Ministry of Research and Innovation—MCI, Core Programme, Project PN 18 03 02 01 and Project PTE-2021-0303.

Poster Communications

P8. Food production and authentication

P8.1 Determination of the fatty acids, cholesterol and glycerides in pork meat fat using the GC-FID and GC-MS system

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Meat fat is an important structural and functional component of meat and meat products, and its composition in individual fatty acids, cholesterol and glycerides are the main determinant of meat quality. Meat is one of the most nutritious foods which people eat every day. Meat nutrients are essential for our vital functions, they are very important sources of protein, fat, vitamins and minerals. The fat and cholesterol content of pork has been of great interest for research for decades. Cholesterol data are usually accompanied by fat content, fatty acid composition and meat type. Fundamental research on the biological functions and chemical properties of cholesterol has been the driving force behind the development and application of analytical techniques for determining cholesterol. The major source of cholesterol in the human diet is represented by the meat from domestic animals. The cholesterol content of pork is 30 to 81 mg/100 g for raw pork and 56 to 113 mg/100 g for cooked pork. The pork cholesterol is influenced by maturity, fat thickness, animal diet and genetic variation. Meat cholesterol is depending by the presence of triglycerides. Saturated fats contain any animal carcass. Pork has a less beneficial fatty acid profile compared to fish. Saturated fatty acids are considered to be the cause of diseases of the circulatory system, as they increase blood pressure and the concentration of LDL cholesterol which can lead to cardiovascular disease. In this study, two simple, stable and sensitive methods for the simultaneous determination of saturated, monounsaturated and polyunsaturated fatty acids (SFA, MUFA and PUFA), cholesterol and glycerides from meat fat, using gas chromatography with flame ionization detector (GC-FID) and gas chromatography-mass spectrometry (GC-MS), were developed.

Acknowledgments.
The financial support for this work was provided by the Ministry of Research, Innovation and Digitization, UEFISCDI, project number PN-III-P1-1.1-TE-2021-0060.

P8.2 Electrochemical assay of acetaldehyde in wines based on novel a cold–active aldehyde dehydrogenase: comparison of mediated versus non mediated detection

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Electrochemical biosensors and bioassays are fast and easy ways to assess grape and wine's quality. Our study compares two approaches for the electrochemical detection of acetaldehyde, a key compound affecting the organoleptic properties of wine. The measurement of acetaldehyde is based on its conversion to acetic acid in the presence of the enzymatic cofactor nicotinamide adenine dinucleotide NAD^+ and is catalyzed by aldehyde dehydrogenase (ALDH). The amount of acetaldehyde is proportional with the reduced cofactor NADH formed. NADH is detected amperometrically based on its oxidation. A novel cold active aldehyde dehydrogenase, ALDS2, obtained from the arctic microorganism *Flavobacterium PL02* was used in these tests. The first strategy was to measure the amount of NADH using electrodes modified with carbon nanotubes, polarized at 0.5 V. The second approach relied on electrodes modified with the electrochemical mediator Toluidine Blue O and polarized at 0.1 V. The linear range for the detection of NADH was 0.0075-0.125 mM, the sensitivity was 1.15÷0.16 µA.L/mmol and the detection limit was 5.5 µM using CNT-modified electrodes. For TBO-based electrodes, the sensitivity was smaller, 0.32÷0.15 µA.L/mmol. The linear range of the assay using CNT-modified electrodes was 0.1-1 mM acetaldehyde and the sensitivity was 94.5 ÷ 10.6 nA.L $mmol^{-1}$. The accuracy was demonstrated though the analysis of wines spiked with acetaldehyde and by parallel measurements via a spectrophotometric method. Importantly, the results can be extended to other dehydrogenase substrates relevant for quality, such as glycerol, an indicator of grapes' infection with *Botrytis cinerea*.

Acknowledgements:
Financial support by the Romanian Executive Agency for Higher Education, Research, Development and Innovation (UEFISCDI), ERANET-MANUNET-III-WINBIOTOOL-2 (AV), contract 151/9.03.2020 grant, ERANET-M-ENZ4IFACES, contract 166/ 01/05/2020 (for ACL) and PN-III-P2-2.1-PED-2019-2746, contract 266PED/August 03, 2020 (R.MC) is gratefully acknowledged.

P8.3 Fast electrochemical measurement of laccase activity for monitoring grapes' infection with *Botrytis cinerea*

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Botrytis cinerea, the principal pathogen that infects the vine (*Vitis vinifera*), critically affects the quality of wines. Laccase production is part of the pathogenesis of *Botrytis cinerea* infection and its activity in must has been used as an indicator of the degree of infection by this mold.

This work describes a versatile method for fast evaluation of laccase activity, based on dual optical and electrochemical detection that allows quantitative detection in 5 minutes to screen grapes for fungal attack by *Botrytis cinerea*. A paper-assisted electrochemical assay was developed by combining a paper sensor impregnated with the enzymatic substrate dye ABTS with a Au screen-printed electrode.

The method was applied for monitoring the artificial infection of white, rosé, and red grapes with different strains of *Botrytis cinerea*. Amperometric measurements were performed by measuring the cathodic current increase at 0 V vs Ag/AgCl for laccase samples of different activities from 1 to 20 U/mL. A detection limit of 0.26 U/mL was determined. By grouping the grapes according to their degree of infection it was found a good correlation with the laccase activity measured with the sensor. It was also shown the possibility to use the paper sensor independently from the electrochemical assay to screen the laccase activity of musts.

The paper-assisted electrochemical assay was found to be robust, adapted for fast measurements and simple to use by operators with minimum training. On-site tests in the vineyard or at the grape processing points can be performed by making some adaptations such as using a portable potentiostat and a dedicated software platform for data acquisition and interpretation. The optical test can evolve in the direction of smartphone-assisted analytical devices to make it an attractive technology for users.

P8.4 Fatty acid profile analysis in sunflower oils by GC-FID and vibrational spectroscopic methods

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Edible oil is an essential nutrient and an important source of energy. Dietary oils vary in their fatty acid profile (FA), being classified as saturated (SFA), monounsaturated (MUFA), and polyunsaturated (PUFA) fatty acids. A particular interest in the specific fatty acid (FA) composition of oils has been emerging with the growing scientific evidence that the dietary fats are not equivalent in regard to the consumers' health. Generally, for the oils' analysis and fatty acid profile determination, the sample preparation is mandatory, being a laborious task. On the other hand, spectroscopic techniques are widely widespread in the analysis of basic food components, being also popular for the vegetable oils' analysis because of their advantages, which include: rapidity, cost-effectiveness, and, usually, no need for sample preparation. In this regard, two vibrational techniques, Raman and Infrared spectroscopies have been involved for the sunflower oils' characterization. Thus, the spectral profiles of several sunflower oil samples produced under distinct brands have been recorded and compared in order to find the specific spectral features that could help in identifying the differences among the analysed samples. A comparison with the fatty acid profile of sunflower oils acquired by the gas chromatography coupled with flame ionization detector (GC-FID) was also employed and discussed.

Acknowledgments.
The financial support for this work was provided by the Ministry of Research, Innovation and Digitization, UEFISCDI, Programmes: PNCDI III-Programme 2-2.1 PED 2019. Project number 354PED/23.10.2020.

P8.5 Fruit spirits authentication based on Raman spectroscopy in corroboration with advanced statistical tools

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Fruit spirits represent, especially in Eastern Europe, a highly appreciated product being also related to the tradition, and their production 'secret' is left as a legacy from father to sons. The manufacturing process is directly reflected in the final personality of these types of alcoholic drinks therefore, brand protection became a very important issue to be addressed. Authentic fruit spirits are alcoholic drinks with a high commercial value because of the important costs that are involved in their production process. For this reason, the development of analytical tools able to differentiate the fruit distillates, according to some pre-defined criteria as a function of the classification purpose, is necessary. In this light, Raman spectroscopy in corroboration with supervised statistical methods, namely Partial Least Squares Discriminant Analysis (PLS-DA), proved to be very effective for the fruit distillates differentiation with respect to production technology, geographical origin of the raw materials, and also to the fruit variety. The developed recognition models were constructed based on a sample set formed by around 100 samples, having distinct botanical origins (plums, apples, pears, quinces, grapes, cherries, etc.), most of these samples originated from Transylvania, Romania. The practical importance of this proposed approach was mainly related to the application of this rapid, cost-effective, and easy-to-use tool for the fruit distillates trademark fingerprint identification. Besides this, a good sample separation with respect to the geographical origin was possible to be achieved despite the fact that all compared samples belonged to the Transylvania area. The botanical differentiation of the fruit spirits was realized, however, in a modest percentage.

Acknowledgment
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P2-2.1-PED-2019-1699 (contract no. 260PED/ 2020) within PNCDI III.

P8.6 Honey – a food matrix case for authenticity evaluation by Raman spectroscopy and Machine Learning algorithms

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Honey is a complex food matrix possessing about 200 constitutes which concentrations vary in accord with the plant origin, geographical influence or even the year of production. Depending of the time of the year and of the local specificities of regions, different varieties of honeys are produced and commercialized on the market, either monovarietal or polyfloral. These variabilities, especially that associated to the botanical and geographical origin, make difficult the process of honeys investigation and authenticity evaluation. Moreover, the need for rapid and reliable tools for honey matrix analysis is mandatory in order to have high quality products on the market. Raman spectroscopy in combination with Machine Learning algorithms offer a good facility for this matrix investigation. In this regard, the discrimination potential of this methodology based on a vibrational technique and supervised methods is presented and discussed. For this study, authentic honey samples of various botanical origin (acacia, linden, colza, sunflower, coriander, gallium verum, thyme, raspberry, lavender and chestnut) from Romania or France have been analyzed. For the botanical differentiation, the best predictive model was obtained with the SVM – support vector machine algorithm (accuracy of 68.6%). The best result for geographical differentiation of the investigated honeys was achieved using the cubic SVM algorithm (accuracy of 82.7%). The results are discussed in terms of accuracy and different performance parameters such as precision, sensitivity and specificity, insisting on the current challenges and the steps forward in honey classification methods bring by this methodology.

Acknowledgement
This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS–UEFISCDI, project number PN-III-P4-ID-PCE-2020-0644 (Contract no. 7PCE/2021), within PNCDI III.

P8.7 Isotopic and elemental composition of meat and their differentiation according to geographical area via multivariate chemometric analysis

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Meat is a valuable component in people diet. The chemical composition of meat is variable due to the animal species, their diet, age, the tissue type, the geographical region, as well as by the type of animal breeding. The present study analyzed the isotopic content ($^{18}O/^{16}O$, $^{2}H/^{1}H$ and $^{13}C/^{12}C$), macro-, micro- elements and toxic trace elements in different meat cuts of beef (pulp and antricot) and chicken (back, leg, breast and wing) collected from Romanian market and animal farms. Isotopic and elemental profile varied among the species or animal tissues. ANOVA technique was used to find the most representative parameters able to differentiate the animal tissues. Beside this, LDA was performed in order to differentiate meat samples according to geographical origin and identify the best discriminant markers. LDA has allowed obtaining excellent results, both in initially classification and in the cross validation step. The percent of initially classification for chicken meat samples was 98.0% and 95.9% for the cross-validation.

Acknowledgements:
This work was supported by a grant from the MRID, CCDI-UEFISCDI, project number PN-III-P1-1.1-TE-2021-0060, within PNCDI III.

P8.8 Quantitative SERS Analysis of Cylindrospermopsin Cyanotoxin in Solution and in Fish Tissue

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Cylindrospermopsin (CYN), a cyanotoxin occurring in environmental waters as a cyanobacteria metabolite, has recently raised increased interest both in the scientific community and the environment, food control, and health care stakeholders. The primary source of exposure is either drinking water or ingestion of toxin-contaminated food and by inhalation and dermal contact during recreational activities in toxic waterbodies. A tolerable daily intake of 0.02 µg/kg body weight/day for human exposure was calculated based on acute toxicity studies in mice [1]. Here we present a fast and sensitive detection method based on surface-enhanced Raman scattering (SERS) of toxin. Quantitative SERS analysis for concentrations range (Fig. 1) from 2.18 µM to 0.218 nM in aqueous solution and SERS discrimination of artificially intoxicated fish tissue from the normal one, using linear discriminant analysis is achieved, with 100% specificity/sensitivity. The cross-validation procedure provided a 100% clear separation based on the SERS data. The results open reliable perspectives for SERS translation as an effective method for toxin environmental monitoring.

P8.9 Rapid detection of Thiabendazole pesticide in frozen fruits and vegetables commercialized in Romanian stores

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Thiabendazole (TBZ), also known as E233 in Europe, is primarily used to control mold, blight, and other fungal diseases in fruits and vegetables. TBZ is also utilized as a food additive, a preservative, and an antiparasitic. The extensive use of TBZ as a preservative to ensure freshness has resulted in its frequent detection in the water resources of the fruit and vegetable production areas, from where it can be absorbed into the plants, so it directly pollutes the environment and contaminates foods, ultimately being absorbed by the human body. The EU regarding the maximum residue levels for TBZ in or on certain products, defines the pesticide residues and maximum residue levels in mg/kg in fresh or frozen fruits and vegetables. Our previous SERS investigations showed that TBZ could be detected in commercially available citrus fruits and bananas [1]. Here we extend the technique to optimize an algorithm for fast-tracking the TBZ presence in different frozen fruit and vegetable samples, randomly selected from the Romanian markets.

Acknowledgments:
The financial support for this work was provided by the P2.1-PED-2019-3004 Program, Project number 359PED/2020. The project was supported by the UEFISCDI.

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ISSN 2360-3461
ISSN-L 2360-3461