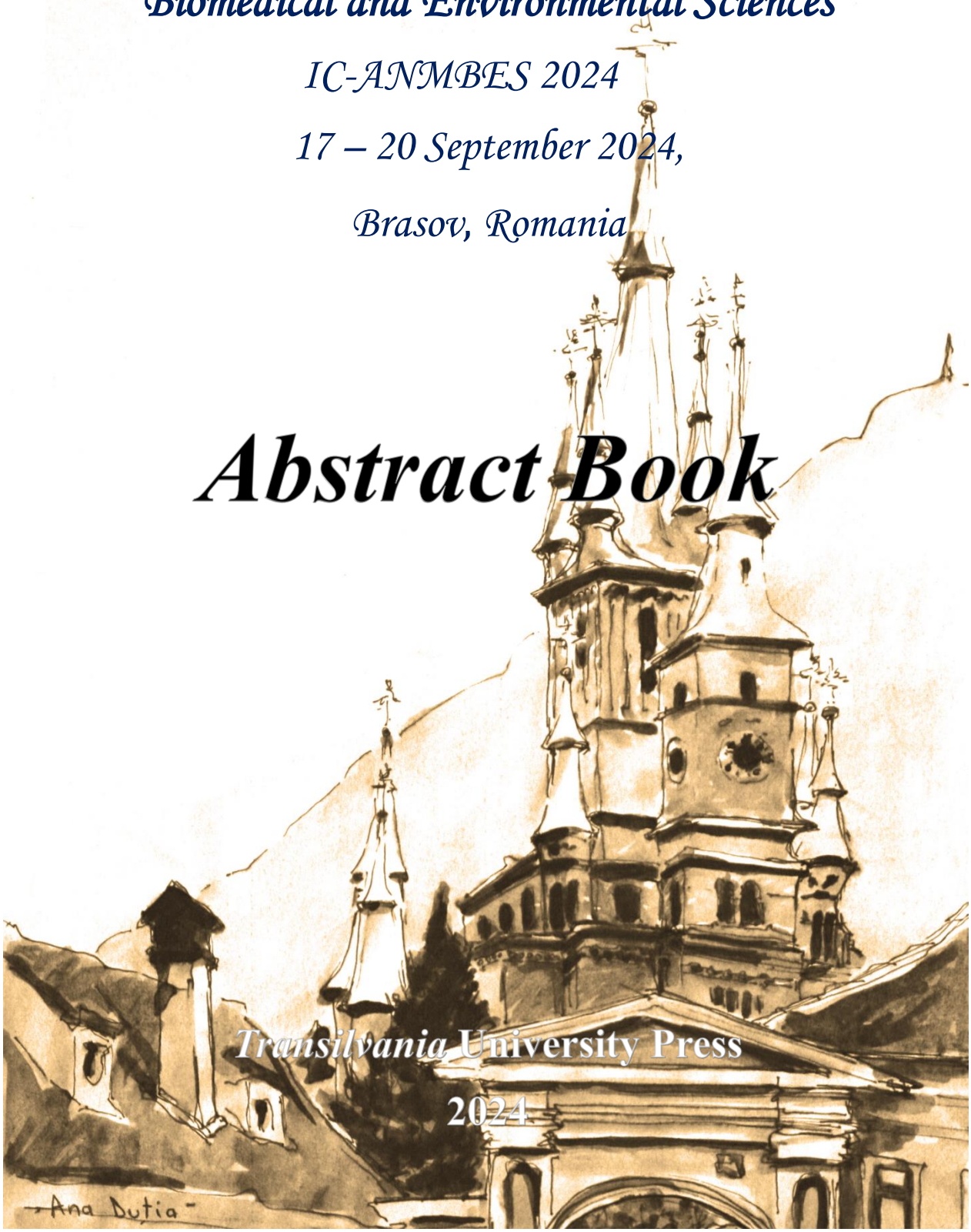
Analytical and Nanoanalytical Methods for Biomedical and Environmental Sciences

IC-ANMBES 2024

17 – 20 September 2024,

Brasov, Romania



Abstract Book

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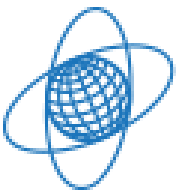

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***TRANSILVANIA* UNIVERSITY OF BRAŞOV**

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

IC-ANMBES 2024

BOOK OF ABSTRACTS

Braşov, 17th -20th September, 2024

Editors: Monica Florescu
André Matagne
Ioan Turcu

Transilvania University Press

2024

EDITURA UNIVERSITĂŢII TRANSILVANIA DIN BRAŞOV

Adresa: 500091 Braşov
B-dul. Iuliu Maniu 41A
Tel: 0268-476050
Fax: 0268-476051
Email: editura@unitbv.ro

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

17th September 2024

14:30 – 16:45	**Registration**	
16:45 – 17:00	**Opening Ceremony**	
	Chairs: Monica Florescu, André Matagne, Ioan Turcu	
17:00 – 17:40	**Plenary P1**	
	Aitziber L. Cortajarena	Engineering protein-based assemblies and hybrid tools for biomedicine and technology
17:40 – 18:10	**Invited talk I1**	
	John Michael Seddon, Colin P Pilkington, Claudia Contini, Joseph D Barritt, Paul A Simpson, Ignacio Gispert, Suet Y Chui, Yuval Elani	Engineering Cubosomes and Liposomes using Microfluidics
18:10 – 18:40	**Invited talk I1**	
	Arkadiusz Matwijczuk, Lidia Ślusarczyk, Klaudia Rząd, Mariusz Gagoś, James Hooper	Advanced spectroscopic and theoretical research into a synergistic composition containing a selected 1,3,4-thiadiazole derivatives and a polyene antibiotics
18:40 – 20:30	**Welcome Party**	

18th September 2024

08:30 – 09:00	**Registration**	
	Biophysical methods for protein science	
	Chair: Ioan Turcu	
09:00 – 09:30	**Invited talk I3**	
	André Matagne	Enhancing Research Data Reproducibility Through Protein Quality Control
09:30 – 10:00	**Invited talk I4**	
	Julien Mignon, Tanguy Leyder, Denis Mottet, Catherine Michaux	Revealing Intrinsic Disorder and Aggregation Properties of The DPF3 Zinc Finger Protein
10:00 – 10:20	**Contributed talk O1**	
	Ziv Klausner, Ionel Valentin Popa, Ronen Berkovich	*History dependent kinetics (aging) in sequential unfolding of polyproteins under tension*
10:20 – 10:40	**Contributed talk O2**	
	Romain Malempré	*Unravelling The High-Resolution Folding Pathway of a Large Monomeric Protein Reveals a Conserved Mechanism In β-Lactamases*
10:40 – 11:10	**Coffee Break and Poster Session**	
	Food production and authentication	
	Chair: Dana Alina Magdas	
11:10 – 11:40	**Invited talk I5**	
	Tina Kosjek, Rui FM Silva, Dušan Žigon, Lea Pogačnik da Silva	Exploring Polyphenolic Composition and Neuroprotective Potential of Invasive Knotweeds

11:40 – 12:00	**Contributed talk O3**	
	Maria David, Camelia Berghian-Grosan, Dana Alina Magdas	ATR-IR and FT-Raman Analysis Employed for the Authentication of Transylvanian Honey
12:00 – 12:20	**Contributed talk O4**	
	Adriana Dehelean, Florina-Dorina Covaciu, Gabriela Cristea, Alina Dana Magdas, Ioana Feher	The Quality and Safety Evaluation of Infants Foods from Romanian Market
12:20 – 12:40	**Contributed talk O5**	
	Gabriela Cristea, Cezara Voica, Romulus Puscas, Ioana Feher, Dana Alina Magdas	From Field to Plate, Potatoes Meet Mass Spectrometry
12:40 – 13:00	**Photo session (inside stairs)**	
13:00 – 14:00	**Lunch**	
14:00 – 15:00	**Poster Presentation Session**	
	Chair: Manuel Dauchez	
15:00 – 15:40	**Plenary P2**	
	Jose Luis Capelo Martinez	The Journey from Urine Proteome to Personalized Medicine
	Artificial Intelligence in analytical methods	
	Chair: Manuel Dauchez	
15:40 – 16:10	**Invited talk I6**	
	Minnatallah Al-Yozbaki, Ellie Giles, Benjamin M Samudio, Lee J Byrne, Cornelia M Wilson	Lung cancer crosstalk and the identification of small molecule stabilizers of the NF-kB complex.
16:10 – 16:30	**Coffee Break and Poster Session**	

16:30 – 17:00	**Invited talk I7**	
	Alessandro Chiolerio	Colloid Intelligence
17:00 – 17:30	**Invited talk I8**	
	Dana Alina Magdas, Ariana Raluca Hategan, Maria David, Camelia Berghian-Grosan	Uncovering subtle honey adulteration through the corroboration of green analytical methods and machine learning
17:30 – 17:50	**Contributed talk O6**	
	Ariana Raluca Hategan, Adriana Dehelean, Romulus Puscas, Gabriela Cristea, Dana Alina Magdas	The Development of Food Authentication Models with a High Generalizability Power Using Artificial Neural Networks
17:50 – 18:10	**Contributed talk O7**	
	Marius Dobinda Albu	Improving Gait Analysis with Advanced Data Collection: A Basis for AI
19:30 – 23:00	**Gala Dinner at *PLATINUM Restaurant*, Brasov**	

19th September 2024

09:00 – 09:30	**Registration**	
	Innovation in Environmental Analysis	
	Chair: Liviu Movileanu	
09:30 – 10:00	**Invited talk I9**	
	Claudia Stihi, Antoaneta Ene, Marina Frontasyeva, Cristiana Radulescu, Inga Zinicovscaia, Otilia Culicov	Multi-Elements Atmospheric Deposition Studies in Romania Using Combined Analytical and Moss Biomonitoring Techniques
10:00 – 10:30	**Invited talk I10**	
	Antoaneta Ene, Ana Pantelică, Florin Sloată, Claudia Stihi, Oleg Bogdevich, Elena Culighin	Nuclear and Atomic Techniques for the Determination of Microcomposition of Industrial Soils
10:30 – 10:50	**Contributed talk O8**	
	Bianca Linca, Andrei Borsos, Ileana Radulescu, Dragos Mirea	Assesment of soil radioactivity in Romania using Gamma Spectroscopy and XRF Analysis
10:50 – 11:10	**Contributed talk O9**	
	Andrei Paul Borsos, Bianca Linca, Ileana Radulescu, Andrei Emanuel Turturica, Constantin Mihai	Evaluation of scintillation detectors used for internal contamination dosimetry measurements
11:10 – 11:30	**Coffee Break and Poster Session**	
	Innovative Methods and Technology for Bioanalysis	
	Chair: Carlos Lodeiro	
11:30 – 12:00	**Invited talk I11**	
	Suzana Ferreira-Dias, Fátima Peres	Do all Virgin Olive Oils meet the Health Claim "Olive Oil polyphenols"?

12:00 – 12:30	**Invited talk I12**	
	Margarida Moldão-Martins, Tiago Vieira, Luisa Brito, Vitor Delgado Alves	Sustainable Packaging for Post-harvest Preservation of Highly Perishable Fresh Fruits
12:30 – 12:50	**Contributed talk O10**	
	Ramona Mirela Plesnicute, Lacramioara Oprica, Cristina Rimbu, Iuliana Motrescu, Daniel Herea, Dorina Creanga	Silver Nanoparticles Synthesized with Vegetal Antioxidants and Their Antimicrobial Properties
12:50 – 13:05	**Sponsor: Carl Zeiss Instruments SRL**	
	Radu Hogas (Regional Sales Manager Microscopy Romania)	ZEISS Microscopy - the Solution for Materials Research
13:05 – 14:00	**Lunch**	
	Chair: André Matagne	
14:00 – 14:40	**Plenary P3**	
	Carlos Lodeiro	Silver Nanoparticles: Revolutionizing Antimicrobial Tactics, Proteomics and as Drug Delivery Systems
	Biophysical methods for protein science	
	Chair: André Matagne	
14:40 – 15:10	**Invited talk I13**	
	Manuel Dauchez	Modeling and simulations of the extracellular matrix in a multiscale level
15:10 – 15:40	**Invited talk I14**	
	Liviu Movileanu	Bioinpired Nanopore Sensors Using Antibody Mimetic Technologies
15:40 – 16:10	**Invited talk I15**	

	Guillaume Roussel	Bacterial protein export: dynamic machines for dynamic clients.
16:10 – 16:30	**Contributed talk O11**	
	Alexandra Farcas, Lorant Janosi	N-Ras Conformational States and Substates are Modulated by Membrane and Point Mutation
16:30 – 16:50	**Coffee Break and Poster Session**	
	Innovation in Diagnosis and Therapy	
	Chair: Jose Luis Capelo Martinez	
16:50 – 17:20	**Invited talk I16**	
	Nuno C. Santos	Atomic Force Microscopy-Based Force Spectroscopy Assessment of Cardiovascular Patients' Risk
17:20 – 17:40	**Contributed talk O12**	
	Violeta L. Calin, Mona Mihailescu, George E. D. Petrescu, Mihai Gheorghe Lisievici, Nicolae Tarba, Daniel Calin, Victor Gabriel Ungureanu, Diana Pasov, Felix M. Brehar, Radu M. Gorgan, Mihaela G. Moisescu, Tudor Savopol	Grading of Gliomas using Digital Holographic Microscopy - A Supervised Machine-Learning Approach
17:40 – 18:00	**Contributed talk O13**	
	Adrian Serban, Monica Florescu, Jean-Benjamin Murat, Lorena Dima	Current Analytical Methods of Vancomycin Assays and New Perspectives

20th September 2024

08:45 – 09:00	**Registration**	
	Novel materials and biomaterials	
	Chair: Victor Diculescu	
09:00 – 09:30	**Invited talk I17**	
	Andreea-Isabela Lazar, Denisa Ficai, Anton Ficai	Innovations in Nerve Regeneration
09:30 – 09:50	**Contributed talk O14**	
	Netta Vidavsky	Analytical Exploration of the Link Between Thyroid Cancer and the Composition and Crystal Properties of Microcalcifications
09:50 – 10:10	**Contributed talk O15**	
	Florina-Lucica Zorilă, Daria Stoia, Roberta Moisa (Stoica), Mioara Alexandru, Monica Focșan, Mihaela Bacalum	Smart plasmonic dressings with synergistic photothermal and antimicrobial activity
10:10 – 10:30	**Contributed talk O16**	
	Dragos Viorel Brezoi, Simona Mihai, Anca Irina Gheboianu	Ferrofluids Based on Magnetite Nanoparticles for Biomedical Applications
10:30 – 11:00	**Coffee Break**	
	Interfaces, Sensing and Smart Devices	
	Chair: Anton Ficai	
11:00 – 11:30	**Invited talk I18**	
	Victor Diculescu	Electrospun Fibers and Paper-Based Biosensors: An Approach for Point-of-Care Diagnostics

11:30 – 12:00	**Invited talk I19**	
	Teodor Adrian Enache	Advanced functional materials and cell cultures applications – from (bio)sensing to cell differentiation
12:00 – 12:20	**Contributed talk O17**	
	Mihai Costache	Neuro Modulation by Applying Low Frequency Trans Cutaneous Electrical Impulses on The Skin Close to the Vagus Nerve
12:20 – 13:00	**Awards and Closing Ceremony**	
14:00 – 22:00	**Social Program – Visit at Făgăraș Fortress and Dinner at *La Promenada* Restaurant, Râșnov**	

POSTER COMMUNICATIONS

Number	Authors	Title
P1. (Nano)biotechnology		
P 1.1	Brezestean Andreea Ioana, Marconi Daniel, Dina Elena Nicoleta, Maria Suciu, Colniță Alia	Flexible ZnO@Ag hybrid thin films synthesized by Magnetron Sputtering technique for SERS detection
P 1.2	Brezestean Andreea Ioana, Marconi Daniel, Sanda Boca, Colniță Alia, Andra-Sorina Tatar	Gold nanourchins for trace-level SERS detection of analytes
P 1.3	Daniel Marconi, Alia Colniţă, Ioana Brezestean, Maria Suciu	High-throughput tunable 3D nanostructured surfaces fabricated by nanoimprint lithography
P 1.4	Mihaela Mic, Adrian Pirnau, Ioana Grosu, Călin G. Floare, Xenia Filip	Systematic study of the conjugation of hyaluronic acid, native or oxidized, with dopamine
P 1.5	Adrian Pîrnău, Mihaela Mic, Călin G. Floare, Bianca M. Tihăuan, Mădălina Axinie (Bucos), Gabriel Marc, Ovidiu Oniga, Ovidiu Crișan	Synthesis and Evaluation of the Binding Affinity of a new Polyphenolic Thiazole with strong antioxidant activity to macromolecules: Computational and Experimental Investigations
P 1.6	Isabela Dragomir, Irina Schiopu, Loredana Mereuta, Alina Asandei, Tudor Luchian	How Much is Too Much: a Study on the Influence of Copper Ions Concentration on DNA Structure
P 1.7	Andreea Balmus, Radu Lapusan, Raluca Borlan, Mara Muntean, Olga Soritau, Monica Focsan	Magnetic Nanoparticles Coated with Bovine Serum Albumin and Grafted with Curcumin as Innovative Theranostic Agents
P 1.8	Alia Colniță, Daniel Marconi, Nicoleta Elena Dina, Ioana Andreea Brezestean, Vlad Alexandru Toma, Claudia Andreea Moldoveanu, Maria Suciu, Alexandra Ciorita	Label-free SERS detection of Parkinson's Disease biomarkers using a hybrid, 3D architecture platform
P 1.9	Adina - Elena Segneanu, Ionela-Amalia Bradu, Crina Sicoe, Gabriela Vlase, Titus Vlase	Micro-spray formulation of new microcarriers based on Romanian Wild-Growing Inonotus obliquus-Physicochemical Properties, In vitro evaluation
P2. Novel materials and biomaterials		
P 2.1	Roberta Moisă, Claudia Ioana Drăghici, Bogdan Zorilă, Mihaela Bacalum	Using Nanoparticles as Carriers For Anticancer Peptides In Two Cancerous Cell Lines
P 2.2	Iulia Teodora Varga-Kocsis, Ioana Georgeta Grosu, Xenia Filip, Bianca Maria Tihăuan, Claudiu Filip	Biocompatible Hyaluronic Acid@Polydopamine Hydrogels with Improved Bacterial Inhibition
P 2.3	Maria O. Miclăuș, Ioana Georgeta Grosu, Iulia Teodora Varga Kocsis, Xenia Filip, Ana Maria Raluca Gherman, Irina Kacso, Flavia Adina Martin	Development and Characterization of Hyaluronic Acid@Polydopamine@Gelatin Hydrogels

P 2.4	Ioana-Georgeta Grosu, Adrian Pirnau, Iulia Teodora Varga-Kocsis, Xenia Filip, Ana Maria Raluca Gherman, Irina Elisabeta Kacso, Andrea Simion, Flavia Adina Martin, Claudiu Filip	Innovative Hydrogels from Hyaluronic Acid-Dopamine Conjugates: Structural, Thermal and Mechanical Properties
P 2.5	Claudia Lar, Stelian Radu, Jozsef-Zsolt Szücs-Balázs, Ancuța Balla, Cristina Marcu, Codruța Varodi, Ștefan Bugeac	Hydrophilic coated materials with polydopamine to be used in the 18O separation plant through H_2O distillation
P 2.6	Cristina Marcu, Jozsef-Zsolt Szücs-Balázs, Ancuța Balla, Ștefan Bugeac, Claudia Lar, Stelian Radu, Codruta Varodi	Theoretical Design of a Combined Separation Cascade for Oxygen Isotope Separation
P 2.7	Florina Pogacean, Lidia Magerusan, Stela Pruneanu	Enhanced Sulfamethoxazole Assay Based on Selective Graphene Sensing Platform
P 2.8	Lidia Magerusan, Florina Pogacean, Stela Pruneanu	Rapid And Selective Ferulic Acid Quantification Based on Sulphur-Doped Graphene
P 2.9	Christina Marie Zălaru, Andreea Elena Aloman, Valentina Claudia Popa, Petruta Oancea, Maria Marinescu	Identification, Determination of the Content of Bioactive Compounds from Gerbera X Hybrid Extracts
P 2.10	Alexandru Pahomi, Ionela Amalia Bradu, Gabriela Vlase, Mihaela Budiul, Mădălin Bunoiu, Titus Vlase	The influence of the polymer matrix on the size of the hydroxyapatite particles
P 2.11	Alexandru Pahomi, Ionela-Amalia Bradu, Gabriela Vlase, Mădălin Bunoiu, Mihaela Budiul, Vlase Titus	Synthesis and characterization of some metals doped hydroxyapatite with different applications
P 2.12	Maria Marinescu, Christina Marie Zălaru, Claudia Valentina Popa, Marcela Popa	Synthesis, Antibacterial Properties and ADME Studies of Pyrazolone Derivatives
P 2.13	Klaudia Rząd, Bożena Gładyszewska, Lidia Ślusarczyk, Anita Kwaśniewska, Grzegorz Gładyszewski, Wiktor Drwal, Arkadiusz Matwijczuk	Photophysical properties of the selected 1,3,4-thiadiazole derivatives investigated in gel, polymer matrix and isopropanol
P 2.14	Melinda David, Teodor A. Enache, Lucian Barbu-Tudoran, Monica Florescu, Camelia Bala	Biologically Synthesized Gold Nanoparticles for the Detection of Water Contaminants
P 2.15	Ioan Turcu, Simion Astilean, Alina Vasilescu, Monica Focsan, Ana-Maria Craciun, Daniel Marconi, Alia Colnita, Monica Potara	A SERS sensor based on an aptamer functionalized nanoplasmonic platform for ultrasensitive and selective detection of biomarkers
P 2.16	Robert Wolff	The Yellow Pigments in Trichonephila Spider Silks: A Spectroscopic Study
P 2.17	Cornelia M Wilson, Jess Holder, Carlos Lodeiro, Elisabete Oliveira, Lee J Byrne, Carol Trim, Emilia Bertolo	Investigating the effect of silica nanoparticles as a drug delivery system for Doxorubicin in the treatment of Breast and Lung Cancer.
P3. Early diagnosis and precision medicine		
P 3.1	Andra-Sorina Tatar, Ioana-Andreea Brezestean, Daniel Marconi, Alia Colnita, Sanda Boca	Aptamer-conjugated gold nanourchins: promising microfluidic SERS-detection tools for early diagnosis of Alzheimer's Disease

P 3.2	Dragos-Ioan Olariu, Ciprian-Paul Mairean, Magdalena Aflori, Brindusa Dragoi, Rares-Ionut Stiufiuc	Plasmonic substrates based on gold nanoparticles for cancer detection by means of SERS analysis of biofluids
P 3.3	Claudia Teodora Dinca, Anca Maria Ilea	Thrombotic Thrombocytopenic Purpura (TTP): Diagnostic Challenges and Case Study
P 3.4	Claudia Ioana Draghici, Mihaela Bacalum, Maria Mernea	The Effect Of Hesperidin On Neuronal Cell Membranes
P 3.5	Horia Buzduga, Teodor Bucur, Monica Florescu	Nanofibers and Electrospinning: Methods of Fabrication, Properties, and Applications in Medicine through Drug Delivery
P4. Innovation in Environmental and Pharmaceutical Analysis		
P 4.1	Alexandru Pahomi, Ionela Amalia Bradu, Mădălin Bunoiu, Gabriela Vlase, Titus Vlase	Desorption profile of local hemostatic carbazochrome loaded on chitosan-HA scaffolds
P 4.2	Ionela-Amalia Bradu, Camelia-Daniela Ionas, Mihaela Budiul, Gabriela Vlase, Titus Vlase	Physicochemical characterization of polymeric membranes with Riluzole for amyotrophic lateral sclerosis treatment
P 4.3	Ionela Amalia Bradu, Mihaela Simona Călinescu, Dorinel Okolisan, Mădălina Grădinaru, Gabriela Vlase, Titus Vlase	Absorption of phosphorus from water using hydrogels based on biopolymers
P 4.4	Ionela Amalia Bradu, Alexandra Tășală, Gabriela Vlase, Titus Vlase	Compatibility study for leflunomide delivery systems
P 4.5	Eugen Nicolae Traista, Camelia Traista, Niculina Sonia Suvar, Maria Prodan, Andrei Szollosi-Mota, Irina Nalboc, Gheorghe Daniel Florea	Procedure for the Determination of Alluvial Gold in Gravel Pit Products
P 4.6	Eugen Nicolae Traista, Camelia Traista, Niculina Sonia Suvar, Maria Prodan, Andrei Szollosi-Mota, Irina Nalboc, Gheorghe Daniel Florea	Process for Concentrating and Determining the Content of Rare Metals in Gravel Pit Products
P 4.7	Irina Schiopu, Isabela Dragomir, Alina Asandei	Stability of DNA-gp32 Binding Protein Molecular Complex: The Influence of Electrostatic Interactions
P 4.8	Niculina Sonia Suvar, Paula Podea, Diana Cristina Covaciu, Alina Filip, Diana Elena Muntea, Adrian Matei	Evaluation of the Chemical Composition, Antioxidant and Antibacterial Activity of Different Hop Varieties
P 4.9	Budiul Mihaela Maria, Vlase Gabriela, Bradu Ionela–Amalia, Grădinaru Mădălina, Pahomi Alexandru, Vlase Titus	Preformulation Studies Regarding Membranes Containing Active Pharmaceutical Ingredients with Analgesic and Antipyretic Activity
P 4.10	Antoaneta Ene, Elena Zubcov, Oleg Bogdevich, Svitlana Kovalyshyna	Heavy Metals and Persistent Organic Pollutants in Wetland Soils and Sediments from Lower Danube-Prut River Region

P5. Innovative Methods and Technology for Bioanalysis		
P 5.1	Ionela Nicoleta Irimescu, Nicolae Tarba, Roxana Popescu, Simona Ionita, Mihaela Deaconu, Cosmin Mustaciosu, Eugen Scarlat, Ana-Maria Pleava, Daniela Berger, Diana Savu, Mona Mihailescu	Quantitative Evaluation of Codelivery Nanoparticles Incorporation in Cultured Cells
P 5.2	Cristian Emilian Pop, Robert Wolff, Dan Florin Mihăilescu	Bisphenol A analyses and quantification inconsistencies via HPLC-UV
P 5.3	Rabha Ayad, Nadia Amessis-Ouchemoukh, Salim Ouchemoukh, Rita Pacheco, Wided Fersi, Monica Florescu	Electrochemical Determination, Antioxidant Activity, FTIR-ATR Spectroscopy and Anticancer Effect of Honey Extract Collected from Jijel City (Algeria)
P 5.4	Wided Fersi, Melinda David, Noureddine Baaka, Hatem Dhaouadi, Rabha Ayed, Sonia Dridi, Monica Florescu	Electrochemical Approaches for Evaluating Antioxidant Properties of Hypericum Triquetrifolium Turra Extracts
P 5.5	Vlase Titus, Ionela-Amalia Bradu, Mădălin Bunoiu, Gabriela Vlase	Microscopic (SEM, IR, Raman), spectroscopic and thermal methods for Micro and Nanoplastics characterization.
P 5.6	Călin Gabriel Floare, Radu Mărginean, Mihaela Mic, Liviu Zârbo, Adrian Pîrnău	Generation and detection of non-classical correlations using nuclear magnetic resonance
P6. Food production and authentication		
P 6.1	Cezara Voica, Gabriela Cristea, Andreea Iordache, Carmen Roba	Health Risk Assessment of Heavy Metals in Selected Root Vegetables
P 6.2	Cezara Voica, Andreea Iordache, Constantin Nechita, Carmen Roba	Occurrence And Health Risk Assessment of Alkali Metals and Macronutrients in Potable Waters
P 6.3	Florina-Dorina Covaciu, Melinda Haydee Kovacs, Veronica Floare Avram, Adriana Dehelean	Nutritional Profiling of Fatty Acids and Metals in Cookies and Biscuits for Children
P 6.4	Gabriela Cristea, Adriana Dehelean, Romulus Puscas, Cezara Voica, Ariana Raluca Hategan	Hen Egg Characterisation Based on Isotopic and Elemental Fingerprints
P 6.5	Florina-Dorina Covaciu, Veronica Cornelia Floare-Avram, Ioana Feher	Comprehensive Analysis of Pesticide Residues in Potato Tubers: A GC-FID Approach
P 6.6	Florina-Dorina Covaciu, Gabriela Cristea, Veronica Cornelia Floare-Avram, Ioana Feher	Egg Yolk Fatty Acids: GC-FID Differentiation of Backyard and Barn Hen Eggs

Oral Communications

Plenary

P1. Engineering protein-based assemblies and hybrid tools for biomedicine and technology

Aitziber L. Cortajarena

[1] Center for Cooperative Research in Biomaterials (CIC biomaGUNE), Basque Research and Technology Alliance (BRTA), Donostia-San Sebastián 20014, Spain
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Inspired by nature, we explore biomolecules and their derivatives as novel biomedical and technological tools. Among biomolecules, proteins rise huge interest due to their high structural and functional versatility, biocompatibility, and biodegradability. In particular, we mainly focus on a class of engineered repeat proteins, due to their stability and robustness as a base scaffold that can be easily tailored to endow desired functions to the protein and to encode defined supramolecular assembly properties. On the one hand, we have developed strategies to create ordered protein-based biomaterials by re-engineering protein-protein interactions.[1] On the other hand, the introduction of metal-binding residues (e.g., histidines, cysteines) drives the coordination of metal ions and the subsequent formation of tailored nanomaterials.[2,3] Additionally, new binding capabilities can be encoded within the CTPR unit or this can be conjugated with other peptides/proteins.[3] These properties allow the development of protein-nanomaterial composites.[4,5] Generally, the fusion of two distinct materials exploits the best properties of each, however, in protein-nanomaterial composites, the fusion takes on a new dimension as new properties arise. These composites have ushered the use of protein-based nanomaterials as biopharmaceuticals beyond their original therapeutic scope and paved the way for their use as theranostic agents, as demonstrated in our pioneering in vitro and in vivo examples.[3,4] In addition, these protein hybrids can be also implemented in technological applications, towards protein-based bioelectronic materials. [6]

References

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P2.The Journey From Urine Proteome to Personalized Medicine

Jose Luis Capelo Martinez

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Bladder cancer (BC) is the most prevalent malignancy of the urinary system, posing a significant global health issue with approximately 600,000 new cases diagnosed annually. This study addresses the urgent need for minimally invasive and cost-effective diagnostic technologies that enhance patient outcomes and reduce treatment morbidity.

Our research has refined BC diagnosis and improved prognosis through a tailored treatment approach, drawing on various advancements in urine sample processing, proteome analysis, and mass spectrometry data interpretation.

This comprehensive work advances the understanding of BC and supports the development of personalized treatment strategies. The findings also suggest potential improvements for various other conditions and cancers.

Acknowledgements

PROTEOMASS Scientific Society is acknowledged by the funding provided to the Laboratory for Biological Mass Spectrometry Isabel Moura (#PM001/2019 and #PM003/ 2016). This work received support from Fundação para a Ciência e a Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior (FCT/MCTES) through the projects LA/P/0008/2020 DOI 10.54499/LA/P/0008/2020, UIDP/50006/2020 DOI 10.54499/UIDP/50006/2020 and UIDB/50006/2020 DOI 10.54499/UIDB/50006/2020. H.M.S. acknowledges the Associate Laboratory for Green Chemistry-LAQV (LA/P/0008/2020) DOI 10.54499/LA/P/0008/2020 funded by FCT/MCTES for his research contract. L.B.C. are supported by the FCT/MCTES PhD grant 2019 (SFRH/BD/144222/2019) and (2023.00528.BD).

P3. Silver Nanoparticles: Revolutionizing Antimicrobial Tactics, Proteomics and as Drug Delivery Systems

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Silver nanoparticles stand at the forefront of biomedical and analytical research, boasting versatile applications across various domains. Our recent endeavours focus on pioneering sustainable approaches for synthesizing silver and silver@silica-based nanoparticles. These nanoparticles are invaluable tools in biomarker discovery within Proteomics, combating antibiotic resistance in microbial studies, and advancing optical detection. In proteomics, gold, silver and iron magnetic nanoparticles have been ingeniously employed to unravel intricate protein structures and interactions. We've tailored their physical properties through meticulous engineering to selectively capture and analyze proteins with unprecedented precision, shedding light on disease mechanisms and facilitating biomarker discovery.[1-8]

With a keen awareness of the global challenge of antimicrobial resistance, we've delved into utilizing silver and gold nanomaterials as novel antimicrobial agents. Incorporated into polymers or solution-based formulations, these nanoparticles exhibit potent antimicrobial properties, disrupting bacterial cell membranes and interfering with essential cellular processes. Additionally, our exploration of monometallic or bimetallic alloy nanoparticles has led to breakthroughs in optical sensing technologies. These functionalized nanoparticles exhibit high sensitivity and real-time detection capabilities, responding specifically to target molecules and generating measurable signals. Such optical sensors hold immense promise for monitoring drug delivery, ensuring food safety, and controlling water quality.

These transformative solutions offer innovative analytical strategies with far-reaching implications, paving the way for advancements in diverse fields, including biomedical sciences.

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Oral Communications

Invited Talks

I1. Engineering Cubosomes and Liposomes using Microfluidics

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Lyotropic liquid crystals of 1-, 2-, or 3-dimensional periodicity spontaneously assemble when lipids are mixed with aqueous solvent under various conditions of temperature and hydration. The most relevant non-lamellar phases from a biological perspective are the inverse hexagonal HII phase, and the inverse cubic phases, which can either be bicontinuous, based on underlying periodic mininal surfaces, or discontinouous, based on packings of discrete inverse micelles.

For potential medical applications, bulk lipid phases can be dispersed into lipid nanoparticles of the order of 100 – 200 nm in diameter. These are named hexosomes when formed from the HII phase, cubosomes when based on inverse bicontinuous cubic phases, and micellosomes when based on discontinuous cubic phases.

We have developed a microfluidic hydrodynamic focussing technology for the production of relatively monodisperse cubosomes and hexosomes, whose size is relatively monodisperse and can be controlled by varying the flow rate ratio between the aqueous buffer and ethanolic streams [1]. We have also reviewed this field [2].

We have now extended this approach, combining microfluidics with conjugation chemistry, to synthesise nano-sized liposomes having two discrete bilayer compartments, one inside the other, which we term centrisomes [3]. We can control the composition of each bilayer, as well as the separation between the bilayers, opening up many possibilities for functionality.

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I2. Advanced spectroscopic and theoretical research into a synergistic composition containing a selected 1,3,4-thiadiazole derivatives and a polyene antibiotics

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Fungal diseases have been killing more than a million people annually for many years. Patients are given increasingly higher doses of drugs, making the fungi more and more resistant, and patients with additional medical conditions are particularly vulnerable [1]. The gold standard among the drugs known today is Amphotericin B, but unfortunately it causes a vat array of side effects. In our research group, we have been looking for solutions to this problem for many years. Thus, we combined a compound from the 1,3,4-thiadiazole group (of 4-(5-methyl-1,3,4-thiadiazole-2-yl) benzene-1,3-diol C1) with Amphotericin B, achieving a great result. Compounds from the 1,3,4-thiadiazole group are known for their excellent biological properties such as anti-cancer, anti-inflammatory and neuroprotective effects [2]. The biological results prompted us to study the mechanism of action of this synergistic system in more detail. To this end, our research group performed a series of spectroscopic studies including UV-Vis measurements, fluorescence emission, fluorescence lifetimes, circular dichroism (CD) and fluorescence anisotropy. Our preliminary hypothesis suggests that the addition of compound C1 causes disaggregation of AmB molecules. Upon addition C1 to the AmB solution, we can notice a change in the position at the absorption maximum of the characteristic band of the AmB aggregate from 345 nm to 335 nm, and this result is also confirmed by the results of the fluorescence spectroscopy, where we can observe the disappearance of the emission band of the AmB aggregate. The experimental data obtained by TCSPC methods were also confirmed by quantum chemical calculations.

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I3. Enhancing Research Data Reproducibility Through Protein Quality Control

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The scientific community aims to enhance transparency and reliability in published research, with a specific focus on the quality of biological reagents, notably recombinant proteins. Concerns have been raised regarding irreproducible results, prompting discussions on common quality issues associated with recombinant proteins and their impact on downstream applications. In response, professionals in protein purification and characterization have collaboratively developed guidelines [1] for improved quality control.

These guidelines include minimal information requirements for protein identity, production parameters, and long-term stability, as well as a minimal set of quality tests for purity, homogeneity, and identity. Additional recommendations cover DNA contamination, “spectral and thermal denaturation signatures”, homogeneity, “competent fraction”, storage conditions, batch-to-batch reproducibility, and other factors based on intended applications. Evaluation [2] of these guidelines over a one-year period suggests that their implementation can enhance experimental reliability and optimize protein quality. Investing in protein QC benefits all stakeholders in life sciences, including researchers, editors, and funding agencies, by improving data veracity and minimizing resource wastage.

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I4. Revealing Intrinsic Disorder And Aggregation Properties Of The DPF3 Zinc Finger Protein

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Double PHD fingers 3 (DPF3) is a zinc finger protein, found in the BRG1-associated factors (BAF) chromatin remodelling complex, and is involved in the regulation of gene expression.[1] Very recently, it was found involved in mitosis, supporting a previously unknown role in various cancers.[2] Two DPF3 isoforms have been identified, respectively named DPF3b and DPF3a.[3] Very few structural data are available for these isoforms, and their specific functionality remains unclear.

According to disorder predictors, both isoforms present disordered structures. While DPF3b shows scores of a moderately disordered protein, DPF3a is a highly disordered protein with scores comparable to those of α-synuclein or tau, two very well-known intrinsically disordered proteins.[4,5]

The characterization of DPF3s disordered nature is therefore fully pertinent for a better understanding of their functionality. Furthermore, the identification of specific aggregation properties can also reveal new DPF3 functions, making it a new drug targetable amyloidogenic protein. By combining predictive disorder algorithms, as well as spectroscopic, microscopic, and scattering techniques, we report the intrinsically disordered character and prone-to-aggregate *in vitro* behaviour of DPF3a. Complementarily, its structural properties are shown by molecular dynamics simulation.

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I5. Exploring Polyphenolic Composition and Neuroprotective Potential of Invasive Knotweeds

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Japanese knotweed (*Fallopia japonica*), Giant knotweed (*Fallopia sachalinensis*), and their hybrid, Bohemian knotweed (*Fallopia* × *bohemica*), are recognized as highly invasive plant species globally. Initially introduced for ornamental purposes, these plants have rapidly spread throughout Europe, posing significant ecological and economic challenges over the past two centuries due to their adverse effects on biodiversity and infrastructure.

This study investigates the presence of various bioactive secondary metabolites, including stilbenes, flavonoids, phenolic acids, carotenoids, chlorophylls, and triterpenic acids, in these knotweeds. Ethanolic extracts were obtained from freeze-dried samples of shoots and root peels of all three species, and their total phenolic content was assessed using the Folin-Ciocalteu method. Further analysis involved ultra-high-performance liquid chromatography coupled with a hybrid quadrupole-ion trap mass detector (UHPLC-MS/MS), employing reversed-phase chromatography and tandem mass spectrometry for quantification. Additionally, the extracts were evaluated for their neuroprotective potential against oxidative stress-induced neuronal cell damage.

Results showed the highest total polyphenolic content in the root peels of Giant knotweed using the Folin-Ciocalteu method, while the shoots of Bohemian knotweed exhibited the highest concentration of polyphenolic compounds via UHPLC-MS/MS, identifying eight polyphenolic compounds in at least one sample. These findings underscore the reliability of the Folin-Ciocalteu and UHPLC-MS/MS methods in assessing polyphenolic compounds in knotweeds, albeit with potential variations in results.

Furthermore, all tested extracts demonstrated effective inhibition of apoptotic and necrotic-like neuronal cell death induced by oxidative stress, highlighting their potential as neuroprotective agents in the context of neurodegenerative diseases.

I6. Lung cancer crosstalk and the identification of small molecule stabilizers of the NF-kB complex

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Non-small cell lung cancer (NSCLC) is a devastating cancer with poor prognosis, no effective treatment and understanding of disease progression. Sortilin levels are deregulated in a number of human diseases, including neurological disorders and lung cancers. Sortilin has recently been identified as a critical regulator of the inflammatory response. The inflammatory response coordinates various signalling pathways and is mediated by the transcription factor nuclear factor kappa-light-chain enhancer (NF-κB) of resident tissue cells and immune cells. Inflammatory responses play a crucial role in the immune system, autoimmune diseases, and cancer. NF-κB is directly regulated through protein−protein interactions, including those with p50:p65/RelA dimer and IκBa to form a trimeric complex in the cytoplasm. IkBa serves to sequesters the p50:p65/RelA dimer in an inactive state. IkBa becomes phosphorylated and subsequently degraded. This liberates the p50:p65/RelA dimer, which is its active form that moves to the nucleus to act as a transcription factor. These pathways are often deregulated in a number of cancers. In this study, we used artificial intelligence molecular screening to obtain a set of small molecule compounds predicted to target a binding site within the p50:p65/RelA:IκBa trimer complex. These compounds were screened on lung cancer cell lines using a luciferase assay, and the function of positive hits was further evaluated and validated using an assay to assess for small molecules acting as 'Molecular glues'. Our study identified a novel strategy to potentially stabilise the p50:p65/RelA:IκBa trimer complex with the potential to reduce the inflammatory pathway which is deregulated in cancer.

I7. Colloid Intelligence

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Intelligence, understood as cognitive process, can be described both through a symbolic approach, which couples itself well with the adoption of technological elements such as the digital world, and through a continuum approach, more familiar with biology. Current experiments performed with functional liquids will be discussed, with a reference to holonomic machines and to the achievement of liquid state analogue memories, artificial neural networks and reservoir computers, where the continuum approach is more appropriate. Recent results about the first liquid state, electrically programmable, in memory computing system will be discussed, highlighting novelties, opportunities and drawbacks of using liquid reservoirs for calculus. In particular their massively parallel structure, resilience towards fluid loss, electrostatic discharges and mechanical vibrations, and most importantly their infinite endurance suggest several advantages. Pavlovian learning in colloids and related effects will also be discussed.

I8. Uncovering subtle honey adulteration through the corroboration of green analytical methods and machine learning

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Recently, the rapid advancements in the development of portable analytical equipment have uncovered new possibilities in the field of food and beverage authentication and control. Against this background, special attention has been given to the employment of green analytical techniques like IR and Raman spectroscopies, which possess important advantages such as minimal to no preparation, rapid analysis, non-destructive characteristics, and low analysis costs.

Honey represents one of the top counterfeit food products worldwide, being counterfeit not only through the addition of sugar-based adulterants but also through the false declaration of its origin (i.e. botanical source, geographical origin). Therefore, in order to ensure quality and traceability for consumers, reliable, cheap, and easy-to-use control tools are needed. In this context, the present work proposes the association of two green analytical techniques, IR and Raman spectroscopies, with advanced data processing tools based on machine learning algorithms in order to develop new recognition models for detecting one of the finest forms of honey adulteration, namely the presence of lower-value honey in more expensive varieties. For this purpose, two high-monetary value honey types, acacia and linden, have been mixed in different ratios with cheaper varieties, which, in the frame of the present study, were represented by colza and sunflower. The obtained results have highlighted that highly effective machine learning recognition models can be constructed based on the acquired IR and Raman spectra in order to detect subtle honey adulterations, leading to accuracy scores greater than 88% after the cross-validation procedure.

Acknowledgments:
This work was supported by the MCID through the “Nucleu” Program within the National Plan for Research, Development, and Innovation 2022–2027, contract no. 27N/2023, PN 23 24 03 01.

I9. Multi-Elements Atmospheric Deposition Studies in Romania Using Combined Analytical and Moss Biomonitoring Techniques

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Combined analytical and moss biomonitoring techniques were applied to study the multi-element atmospheric deposition in Romania.

Moss samples collected during three sampling campaigns in the summers of 2010, 2015 and 2020 were analysed using combined analytical techniques: Flame/Graphite furnace Atomic Absorption Spectrometry in 2010, Inductively Coupled Plasma–Mass Spectrometry in 2015 and 2020, and Instrumental Neutron Activation Analysis in 2010 and 2015.

The concentrations of 30 elements, including key toxic metals such as Pb, Cd, were quantified. The distribution patterns indicate a decreasing trend of toxic metals concentrations and different pollution sources were identified and characterized using principal component analysis (PCA). The contamination factors, pollution load index and geo-accumulation index were calculated to assess the air pollution levels in the country.

I10. Nuclear and Atomic Techniques for the Determination of Microcomposition of Industrial Soils

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Industrial activities release toxic elements into the environment, posing a severe risk to ecosystems and human health. The aim of the study was to investigate soil contamination patterns in areas affected by the chemical and steel industries in Romania, by using advanced complementary atomic and nuclear methods, such as Proton-induced X-ray emission (PIXE), and Particle-induced gamma-ray emission (PIGE), X-ray Fluorescence (XRF) and Atomic Absorption Spectrometry (AAS).

The concentration of most of the investigated potential toxic elements and heavy metals were found to exceed the world averages for the crustal elements content or the legislated normal values and alert/intervention thresholds, being a cause for concern of industrial emissions and disposal of industrial wastes.

High values of the single and multiple complex contamination indices indicate a moderate pollution of industrial soils in the studied areas around the steel and chemical industry and a high pollution degree of the waste soils originated from chlor-alkali production, emphasizing the need for further research, establishing a risk assessment framework of soil heavy metals pollution and regular monitoring of environmental compartments impacted by anthropogenic activities.

Acknowledgments:
This research was funded by EC through JOP Black Sea Basin 2014-2020, project code BSB27-MONITOX.

I11. Do all Virgin Olive Oils meet the Health Claim "Olive Oil polyphenols"?

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Virgin olive oil (VOO) is the main source of fat in in the Mediterranean diet, which has been related to longevity and reduced risk of morbidity and mortality of the population of Mediterranean region. Health benefits of VOO have been ascribed to its high content in monounsaturated fatty acids (oleic acid content: 55.00-83.00%) and linoleic acid content (C18:2: 2.50- 21.00%). Moreover, VOO health benefits must also be ascribed to the presence of phenolic compounds with different biologic activities, like antioxidant, anti-inflammatory and anti-microbial effects. The evidence that "olive oil polyphenols contribute to the protection of blood lipids from oxidative stress" is already strong enough to enable the legal use of the health claim "Olive oil polyphenols", recognized by the Commission Regulation ((EU) No 432/2012 of 16 May 2012).

However, this health claim "Olive oil polyphenols" can only be applied if the "olive oil contains more than 5 mg of hydroxytyrosol and its derivatives (e.g. tyrosol) per 20 g of oil". Total phenolic content of VOO may vary from around 50-800 mg/kg, which means 1-20 mg/20 g (two table spoons). Since not all the phenolic compounds correspond to hydroxytyrosol and its derivatives, most of commercial VOO do not fil the requirements of this health claim.

The presence and content of these polyphenols strongly depend on olive cultivar, ripening, fruit damage caused by pests and diseases, agronomic practices, geographical location, post-harvest, olive oil extraction and storage. These aspects, together with positive impact of phenolics on sensory properties of VOO, will be addressed.

I12. Sustainable Packaging for Post-harvest Preservation of Highly Perishable Fresh Fruits

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The food packaging material is an important factor in the fresh fruit industry, and it is dominated by petroleum-based polymers. The interest in minimizing harmful effects on the environment has led to a significant growth in the production of bio-based packaging materials. Raspberries are fruits that have a high level of appreciation from consumers due to their sensory, nutritional, and functional qualities. However, they are highly perishable fruits and always need to be packed. The goal of this study was to extend the shelf-life of fresh red raspberries (Rubus idaeus. L. cv. 'Kweli') by introducing film pads (chitosan) with active ingredients (green tea and rosemary ethanolic extracts) into commercial compostable packages. Pads were placed under the fruits in fruit trays, and then they were heat sealed with a polyacid lactic film. Preservation studies were carried out at refrigeration conditions (4 ºC) for 14 days. Raspberry samples were analysed over time (0, 3, 7, 14 days) for: fungal decay, weight loss, firmness, surface colour (CIE Lab), total solid soluble content (0Brix), volatile acidity, total phenolic content, and antioxidant activity. The results allow to conclude that green tea and rosemary extracts, incorporated in the chitosan pads, were highly effective in reducing fungal growth and decay of raspberry during storage. Fruits preserved using packages with active film-pads of rosemary extracts showed the lower weight loss (5.6%), firmness decrease (3.7%) and antioxidant activity reduction. This sustainable packaging system could be advantageous for other soft fruits to enhance their marketability during extended periods or distances.

I13. Modeling and simulations of the extracellular matrix in a multiscale level

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The extracellular matrix ECM is composed of very large extracellular molecules and macromolecules secreted by cells; it is a biochemical reservoir and it provides structural supports to the surrounding cells. The composition of ECM varies according to multicellular structures and cellular types. Macromolecules of the ECM are often huge macromolecules constituted of numerous multi-globular domains, with fibrous structures and/or glycosylated molecules. These domains and patterns could adopt numerous structures and have a fabulous adaptability and most of the time a large flexibility to perform their functions. Most of the three-dimensional structures at the atomic and molecular levels are provided by experimental data from crystallographic and NMR experiments.

Far from the static and blocked structures, idealized conformations deposited into structural databases, proteins are highly dynamic molecules. These multidomain macromolecules undergo conformational changes on temporal and spatial scales over several orders of magnitude. Over the past decades, molecular dynamics (MD) simulations have demonstrated atomistic details that underlie protein dynamics in conjunction with biophysical experiments when available. If simulations of matrikines (components from the degradation of ECM), proteins and some of their interactions are performed quite easily with MD, there are limitations of the degree to which molecular simulations accurately and quantitatively describe protein motions. Using derived video games, we have developed a demonstrator using physical engines that allows us to evaluate different scenarii of interactions of dozen to hundreds of proteins in a ECM environments. From a dedicated configuration, it is then possible to extract specific interactions to perform classical MD.

I14. Bioinpired Nanopore Sensors Using Antibody Mimetic Technologies

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In this talk, I will dwell on recent developments in nanopore technologies that impact molecular biomedical diagnostics. Significant progress has been accomplished in protein analytics using nanopore-based techniques. However, creating generalizable nanopore sensors to detect proteins at a single-molecule level without the confinement of the pore interior remains challenging.1, 2 We addresses this long-standing technological difficulty by formulating, developing, and validating a new class of sensing elements in single-molecule protein detection. The key ingredient of this technology is fusing an external programmable antibody-mimetic binder with a monomeric protein nanopore.3, 4 This strategy drastically expands the spectrum of applications of nanopore sensors to a broad range of proteins and biomarkers without altering their modular architecture, high specificity, and sensitivity. Notably, these nanopores operate in biofluids at clinically relevant concentration ranges of protein biomarkers and with an extended time bandwidth. In this case, the reporting signal unambiguously distinguishes protein recognition events at single-molecule precision without the requirement of utilizing complex analysis algorithms.

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Acknowledgements.
This work was funded by the CUSE Initiative of the Syracuse BioInspired Institute at Syracuse University, and the US National Institutes of Health, grants R01 EB033412 and R01 GM151299 (all to L.M.).

I15. Bacterial protein export: dynamic machines for dynamic clients.

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About a third of the bacterial proteome is exported outside the cytoplasm. The vast majority is exported by the evolutionary conserved Sec translocase. However, this membrane-embedded channel allows the secretion of non-folded clients exclusively, meaning that secretory clients that evolutionary know how to fold, need to remain unfolded in the cytoplasm until their final delivery the translocon.

In that context, we are focusing on the role of cytoplasmic chaperones to maintain a secretory client non-folded by combining single-molecule Forster Resonance Energy Transfer (smFRET) to monitor the folding of the client, and local hydrogen-deuterium exchange (HDX-MS) to describe the intrinsic dynamics of folding intermediates.

Using this unique combination, we demonstrated that chaperones involved in the secretory pathway have some effect on the folding kinetics of the client, with SecB being the ideal chaperone for our model client. Indeed, SecB acts as (i) a holdase, keeping unfolded protein in an expanded and dynamic state, competent for secretion; (ii) a denaturase by bringing folding intermediates to the expanded state; and finally (iii) a foldase, releasing a different folding intermediate that seems to reach the native state via a different pathway.

I16. Atomic Force Microscopy-Based Force Spectroscopy Assessment of Cardiovascular Patients' Risk

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Erythrocytes are deformable cells that undergo progressive biophysical and biochemical changes affecting normal blood flow. Fibrinogen, one of the most abundant blood plasma proteins, is a primary determinant for changes in hemorheological properties, and a major independent risk factor for cardiovascular diseases. We have previously demonstrated the biomedical relevance of the measurement of single-molecule fibrinogen-erythrocyte receptor binding and erythrocyte-erythrocyte adhesion, using atomic force microscopy (AFM)-based force spectroscopy, at the level of clinical prognosis in heart failure and essential arterial hypertension patients. Recently, the adhesion between human erythrocytes was further assessed by comparing AFM-based force spectroscopy measurements with micropipette aspiration technique, in the absence and presence of fibrinogen. These experimental data were used for the development of a mathematical model to examine the biomedical relevant interaction between two erythrocytes. More recently, we evaluated changes in fibrinogen-erythrocyte and erythrocyte-erythrocyte interactions in carotid artery disease (CAD) patients, and characterized the biomechanical properties of carotid atherosclerotic plaques from CAD patients. Blood samples collected from CAD patients, before and after endarterectomy surgery (including a 3-year follow up) were analyzed and compared to a control group of healthy blood donors. This study comprising hemorheological parameters and AFM measurements of fibrinogen-erythrocyte and erythrocyte-erythrocyte interactions, as well as cell biomechanical properties, provided clinically-relevant data on the post-surgery improvement of the patients and on the evolution as a function of time of the restenosis process.

I17. Innovations in Nerve Regeneration

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In this presentation, we will focus our attention to the materials used in nerve grafting, especially composite materials based on graphene-related materials. Graphene-related materials are increasingly used in many medical and non-medical applications. Their use is justified especially considering the special biological, chemical, mechanical and electric properties. In nerve regeneration, all these properties are essential and, especially grapheneoxide can fulfil all the requested characteristics, including the electric stimulation for the regeneration purpose or the electric triggering capacity for controlling the release rate of the biological active agents loaded into these grafts; the tuneable hydrophil/ hydrophobe ratio, which is especially important in the delivery but also in the biocompatibility; etc.

Acknowledgments:
The authors are acknowledging the support of the project ERANET-FLAG-ERA-Smart2Graph-1: “Smart nerve grafts based on graphene-related composite materials with electric-triggering capability for central and peripheral nervous system regeneration”.

I18. Electrospun Fibers and Paper-Based Biosensors: An Approach for Point-of-Care Diagnostics

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The development of point-of-care (POC) diagnostic tools has become crucial for timely and accurate disease detection. This study explores the integration of electrospun fibers and paper-fluidic substrates as a novel approach for POC diagnostics. Electrospun fibers, with high surface area and tunable properties, provide an excellent platform for flexible electrodes development. When combined with the simplicity and cost-effectiveness of paper-fluidic substrates, this hybrid system offers significant advantages in developing biosensing systems. The fabrication process, characterization, and application of these biosensors in detecting various biomarkers in body fluids and for detection of PCR amplified nucleic acids, are discussed. The results indicate that this approach holds great potential for enhancing the accessibility and efficiency of diagnostic tests.

I19. Advanced functional materials and cell cultures applications – from biosensing to cell differentiation

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The most amazing biological structure is the living cell, a dynamic machine that integrates a wide variety of biochemical structures, continuously adapting and responding to the local environment. The cellular systems produce and transform signaling biomarker molecules to inter-communicate, and their integration in biosensing devices became an important tool to understand the underlying mechanisms of different diseases, as well as to perfect timely disease diagnosis and personalized therapeutic approaches. As in any scientific field, the optimum experimental conditions in terms of sensitivity and minimization of undesirable effects requires the appropriate model. Thus, the electrochemical sensing of cells biomarkers requires the cultivation of the cells at/near the (bio)sensor surface, maintaining an appropriate electroactive available surface, and avoiding the passivation. This can be achieved using electrospun nanofibers polymer scaffolds, which allow the cell cultivation in desired condition. These scaffolds have a dual-role, serving as polymeric support for cell culture and as an electrochemical transducer, the later requiring their metallization and/or functionalization with specific components. Based on this, the screening of cellular stress has been achieved integrating the cells and the biosensor components on the transducer whereas the melanin exocytosis was successfully quantified using a commercial electrode. Either directly on the surface of the (bio)sensor or spatially detached from it, the integration of cell cultures in (bio)sensing platforms based on electrospun polymeric nanofibers represents a powerful bioanalytical tool able to provide real-time information about the biomarkers release, enzyme activity or enzyme inhibition effects on cells, as well as monitoring of different cellular events.

Oral Communications

Contributed talks

O1. History dependent kinetics (aging) in sequential unfolding of polyproteins under tension

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Polyproteins, composed of tandemly arrayed proteins, perform specific physiological functions under mechanical loads through partial unfolding and extension, such as in muscle activity and cellular signaling. Single molecule force spectroscopy (SMFS) studies suggest that the sequential unfolding times of N proteins within a polyprotein are independent and identically distributed (iid). According to this assumption, the unfolding kinetics of a polyprotein should follow an exponential distribution. However, they are reported to display non-exponential behavior. Various interpretations and statistical methods have been proposed to explain this deviation, all based on the iid assumption. We demonstrate that applying external tension as an unfolding agent introduces correlations between sequential events during the poly-protein unfolding, challenging the iid assumption. Using a continuous time random walk approach, we show that polyprotein unfolding exhibits anomalous subdiffusive transport, indicative of aging. Combining this with free-energy landscape reconstruction, we provide a physical explanation: each unfolding event elongates the chain, altering unfolding probabilities as chain stiffness decreases. We further explore this by investigating sequential unfolding at decreasing forces. Statistical order analysis reveals that even under the lowest load, sequential unfolding does not follow the iid model, consistent with a power law distribution. Free energy analysis shows that the elasticity of the unfolded segments affects the overall one-dimensional energy landscape and uncovers the hierarchical nature of activation barriers during sequential unfolding, explaining the observed non-exponential behavior.

O2. Unravelling The High-Resolution Folding Pathway Of A Large Monomeric Protein Reveals A Conserved Mechanism In β-Lactamases

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The detailed characterization of the folding of a large protein is conducted on a model enzyme, the BS3 class A β-lactamase. The principal goal is to determine the order of formation of its secondary structure elements using quenched-flow HDX pulse-labelling experiments, combined with both NMR and mass spectrometry (MS) measurements. Class A β-lactamases (Mr ca. 29000) are among the largest proteins studied for their folding properties. As observed with most large proteins, folding is not kinetically two-state, and intermediate partially folded species are observed. The highly conserved cis peptide bond between residues 166 and 167, in a long Ω-loop at the active site of these enzymes, controls important steps in the refolding reaction. The sequence of the two structural domains implies a substantial movement of the polypeptide chain during the folding process. One domain (composed of both α-helices and β-sheet) is made up of the N- and C-terminal parts of the protein, whereas the other domain (all α) is formed by the central part of the polypeptide chain.

HDX-MS experiments revealed the initial formation of molecules with native-like protection against exchange (EX1) in the secondary structural elements closest to the N- and C-terminal parts of the sequence, then propagating to the core of the protein. These results suggest an intermediate species with a folding nucleus allowing a productive process toward forming fully active enzyme molecules.

Additionally, molecular dynamics (MD) simulations and machine learning-based folding prediction algorithms explored the very first folding steps, providing complementary insights and highlighting a common pathway for other serine β-lactamases

O3. ATR-IR and FT-Raman Analysis Employed for the Authentication of Transylvanian Honey

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Honey represents a desired food commodity, not only due to its delightful taste and particular aroma but also for the beneficial health effects induced. As important honey quantities are imported and exported onto the market, the issue of adulteration by sugar addition or substitution of special monofloral honey with cheaper varieties is threatening the consumers. As a result, many researchers are focusing on discouraging these unfair practices by developing honey authentication models capable of differentiating between honey botanical and geographical origins.

In this regard, the present study uses the ATR-IR and FT-Raman spectroscopy analysis in order to detect differences in the vibrational spectra of the most common honey varieties produced in Transylvania, Romania, represented by acacia, honeydew, and rapeseed. The determined spectral variances were explained in terms of the chemical composition, which is dependent on the varietal source of the investigated honey. Moreover, a pilot study that follows the development of authentication models capable of differentiating honey samples' botanical and geographical origins was conducted in order to control honey labeling. The proposed methodology, which involved the processing of the fused IR and Raman vibrational data with machine learning tools, obtained efficient classification models able to correctly discriminate acacia honey from lots of other varieties and to distinguish honey produced in a restricted geographical area of Romania, from that produced in other EU countries.

Acknowledgments:
This work was supported by the MCID through the “Nucleu” Program within the National Plan for Research, Development, and Innovation 2022–2027, contract no. 27N/2023, PN 23 24 03 01.

O4. The Quality and Safety Evaluation of Infants Foods from Romanian Market

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Because the first year of a child's life is a particularly vulnerable and sensitive period in human development, it is crucial that food products intended for this age group meet high quality and safety standards. Complementary feeding is a vital step in an infant's development, transitioning them from breast milk or formula to a more diverse diet. It involves the introduction of purees and other foods that provide essential nutrients, support growth, and encourage healthy eating habits. Ensuring the quality and safety of these foods, while gradually introducing a variety of textures and flavors, helps promote optimal health and development during this critical period. In this context, the present study aimed to evaluate: 1) the content of macro/micro minerals and potentially toxic elements; 2) the fatty acid profile and nutritional indices of ready-to-use food, targeted toward infants, containing one or more of ingredients: fruits, vegetables or meat, commercially available in Romania. The methodology included inductively coupled plasma mass spectrometry (ICP-MS) for elemental profile analysis and gas chromatography with flame ionization detection (GC-FID) for lipid profile analysis. Furthermore, this pilot study aimed to assess the potential health risks to infants from food consumption by evaluating the estimated daily intake (EDI), target hazard quotient (THQ), and hazard index (HI).

Acknowledgments:
This work was supported by the MCID through the “Nucleu” Program within the National Plan for Research, Development, and Innovation 2022–2027, contract no. 27N/2023, PN 23 24 03 01.

O5. From Field to Plate, Potatoes Meet Mass Spectrometry

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Globally, there are more than 4000 potato varieties, each with its own unique size, colour and shape. After corn, wheat and rice, potatoes are the fourth largest crop in the world. The potato (Solanum tuberosum) is a staple food source for many people around the world. Many consumers prefer to pay a higher price for a traditional cultivation regime of a certain product (potato, in this case), without fertilizers, and which comes from a certain region, appreciating the taste of that product. Investigated samples from this work are coming from different countries, Romania vs. abroad. The isotopic fingerprint and elemental profiles of potato samples in corroboration with linear discriminant analysis (LDA) were used in order to evaluate the geographical provenance of potato.

The percent obtained for initial classification was 84.3%, while for cross-validation was 80.4%, respectively. Significant differentiation markers were: $\delta^{13}C$, $\delta^{18}O$ and Sr.

Acknowledgments.
The financial support for this work was provided by the National Authority for Scientific Research and Innovation, Program NUCLEU, contract no. PN 23 24 03 01.

O6. The Development of Food Authentication Models with a High Generalizability Power Using Artificial Neural Networks

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Food authentication represents a global concern, necessitating the development of reliable recognition tools with large-scale applicability. This is particularly crucial for honey, one of the most commonly falsified food commodities, where robust authentication models are essential to certify its origin. In this regard, the present study proposes the development of new honey authentication models concerning the botanical origin and harvesting year based on the application of Artificial Neural Networks (ANNs). As input data, the association between stable isotope ratios and elemental profile has been used. In order to construct recognition tools having broad applicability, a diverse data set has been employed, comprising more than 200 honey samples belonging to 26 botanical sources, produced in six different countries, and collected across various seasons and two harvesting years. By reducing the dimensionality of the input data to the most significant features and by conducting an in-depth optimization procedure, highly efficient classification models have been constructed, having accuracy scores greater than 86% on an independent test set, which proved the suitability of the proposed solution for a large-scale application in the field of honey authenticity control.

Acknowledgments:
This work was supported by the MCID through the "Nucleu" Program within the National Plan for Research, Development, and Innovation 2022–2027, contract no. 27N/2023, PN 23 24 03 01.

O7. Improving Gait Analysis with Advanced Data Collection: A Basis for AI

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The purpose of this research was to develop a framework for contrasting normal and abnormal gait patterns using two variables: acceleration and the force the foot applies to the ground.

The components used were: a development board Arduino MKR1000 Wi-Fi, an ADXL345 accelerometer module, a USB 5V step-up module, a switch, three RFP602 (5Kg) pressure sensors (which convert pressure into an electric signal), three 10kΩ resistors to increase the measured value of ground pressure, three 1.2V rechargeable batteries mounted on a holder. The application used to write the code was Arduino IDE, and the system was programmed in a derivative of C++. Data was transmitted to a PC via the open-source platform thinger.io.

The device was positioned at the ankle level of the plegic limb of the affected subject and on the same side of a healthy subject (both of approximately the same weight). Data was collected in three scenarios:

- transition from sitting to standing.
- maintaining orthostatic position with bilateral support.
- physiological and pathological gait

The accelerometer captures changes in speed and direction, the pressure sensors provide insights into foot-ground contact and pressure distribution. The data variability suggests the need for more refined data processing techniques. Considering the limits in the accuracy of the data gathered, the integration of AI technology is proposed as a future enhancement. AI algorithms could refine data accuracy, interpretation, provide predictive analytics, offering more detailed and objective gait analysis.

O8. Assesment of soil radioactivity in Romania using Gamma Spectroscopy and XRF Analysis

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Understanding the distribution and effects of radionuclides in various ecosystems depends on the study of environmental radioactivity. The main objective of this study is to evaluate the radiation levels identified in soil samples collected from different regions across Romania. It was performed a thorough analysis of soil samples to identify radionuclides using High Purity Germanium (HPGe) gamma spectroscopy and X-ray Fluorescence (XRF) analysis. This two approaches makes the study more robust. Furthermore, controlled settings were maintained during the measurement process in order to reduce external influences and guarantee data integrity. After assessing the gamma spectra and considering the detector efficiency and background radiation, the activity concentrations for the identified radionuclides were determined by data analysis. After that, the statistical examination was performed on the activity concentrations to evaluate regional variability and quantify uncertainty. The distribution of radioactivity was mapped using geospatial tools, which additionally helped to identify hotspots and possible sources associated with anthropogenic activity.

Specific identification of gamma-emmiting radionuclides, such as Uranium-238, Thorium-232, Potassium-40, is made possible by the excellent resolution and efficiency of HPGe detector, enhanced by XRF analysis which provides extensive elemental composition data that improves the comprehension of the geological background of possible radioactive sources from anthropogenic influences. The methods used, such as sample collection and preparation , as well as the dual analytical techniques of gamma spectroscopy and XRF analysis, will be covered in detail in this presentation. The statistical evaluation of the data, the interpretation of the results, and the comparison with global safety standards will also be discussed.

O9. Evaluation of scintillation detectors used for internal contamination dosimetry measurements

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This study showcases the measurements and efficiencies of different scintillator detectors: NaI(Tl), LaBr3(Ce) and CeBr3, used for internal contamination dosimetry measurements, which is important for occupational and environmental radiation protection, uses whole-body counting to measure radionuclide radiation within the human body. This method has evolved alongside advancements in radiation detection technologies, improving the accuracy and sensitivity of measurements. The research highlights the progression from traditional NaI(Tl) to modern high-resolution HPGe both being more common than the newer LaBr3(Ce) and CeBr3 detectors, which are a middle ground.

The study addresses the performance comparison of these detectors based on energy resolution, efficiency, and minimum detectable activity, employing certified gamma sources for calibration. NaI(Tl) detectors, while commonly used, exhibit lower energy resolution compared to LaBr3(Ce) and CeBr3 detectors. LaBr3(Ce) detectors, despite their superior resolution, have high intrinsic radioactivity, limiting their minimum detection limits. Conversely, CeBr3 detectors offer a balanced performance with good energy resolution and lower intrinsic radioactivity, making them promising for internal dosimetry.

Experimental results show CeBr3 detectors at a 3.6% resolution at 662 keV, present a feasible alternative to the traditional NaI(Tl) detectors, overcoming some of the limitations posed by LaBr3(Ce) detectors and don´t require cooling unlike the HPGe detectors . The study concludes that integrating CeBr3 detectors in whole-body counting systems could enhance the accuracy and reliability of internal contamination measurements, thus representing a possible advancement in radiation dosimetry technologies.

O10. Silver Nanoparticles Synthesized with Vegetal Antioxidants and Their Antimicrobial Properties

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Due to their antimicrobial activity silver nanoparticles (AgNPs) are widely used in sanitation, cosmetics, textiles and medical domains. Vegetal extracts of lemon and berry fruits as well as of green tea dry leaves were used to conduct silver reduction according to adapted Turkevich technique.

The synthesis protocols were based on the reduction of Ag+ from the same amount of AgNO3 with the natural reducing agents from the vegetal sources. The antioxidant activity of the vegetal extracts was assayed as total phenol content, total flavone content and DPPH radical scavenging activity. The synthesized AgNP microstructural and optic properties were investigated by suitable methods like X-ray diffraction, dynamic light scattering, dark field optical microscopy, and UV-Vis spectrophotometry. Antimicrobial activity of colloidal AgNPs was assayed by agar diffusion and by time-kill kinetics methods against ATCC bacterial strains of S. aureus and E. coli and on a fungus strain of C. albicans.

All four AgNP samples exhibited typical crystallization properties in fcc cubic system, characteristic spectral band, tens of nm size in optical visualization and 60-120 nm hydrodynamic diameters, presenting several months stability in refrigerator. Agar diffusion assay revealed best antimicrobial and antifungal activity for AgNPs synthesized with lemon fruit extract. Time-kill kinetics carried out for the incubation times of 6-12-24-48-72 hours evidenced remarkable antimicrobial activity of AgNPs synthesized with lemon and green tea against S. aureus and for blackberry synthesized AgNPs against E. coli, recommending those AgNPs for practical uses. New tests are planned for the viability of AgNP-treated cells.

O11. N-Ras Conformational States and Substates are Modulated by Membrane and Point Mutation

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Ras proteins are oncogenic GTPases known to present multiple conformational states, as reported by a variety of crystallographic structures. GTP-bound states are grouped into two main states: the "inactive" state 1 and the "active" state 2. Recently, it was shown that the H-Ras isomer's state 2 exhibits two substates that are directly related to the orientation of Tyr32 towards the GTP-bound pocket or outwards. We showed that N-Ras isomer exhibits another substate of state 2 related to a third orientation of Tyr32, parallel to the GTP-bound pocket. We further showed that this substate is highly populated in the G12V (oncogenic) mutation of N-Ras and barely present in its wildtype form. We also explored the importance of membrane in the conformational states and protein stability, and highlighted its significant influence on the conformational sampling of NRas' (sub)states, which is crucial in the activation/deactivation cycle of Ras.

Acknowledgments:
This research was funded by the Ministry of Research, Innovation and Digitization through the “Nucleu” Program within the National Plan for Research, Development and Innovation 2022-2027, project PN23-24-01-02.
The authors would like to acknowledge the National Institute for Research and Development of Isotopic and Molecular Technologies’ “DataCenter” for the computational resources.

O12. Grading of Gliomas using Digital Holographic Microscopy - A Supervised Machine-Learning Approach

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Gliomas, the most prevalent type of brain cancer, have rising incidence and high mortality rates. They are classified into grades (I-IV) and sub-types (astrocytoma, ependymoma, oligodendroglioma) based on histological and molecular characteristics, with grade IV glioblastoma being the most aggressive. Accurate grading is essential for treatment planning and prognosis, but current methods - based on (immuno)histopathological diagnosis - rely on complex, costly, and subjective immunohistopathological analysis.

Digital Holographic Microscopy (DHM), an interferometric technique, offers a quantitative phase image (QPI) that maps the optical phase delay caused by the sample's refractive index and thickness. DHM has shown promise in differentiating between healthy and cancerous tissues. This study introduces a glioma grading method using QPIs of unstained tissues and machine-learning models. A transmission DHM setup in off-axis configuration captured QPIs, from which custom algorithms extracted numerous statistical, textural, and morphological parameters for each grade.

These parameters were used to train and test multi-class classifiers for automatic glioma grading. The algorithms distinguished six classes (normal tissue and five glioma subtypes) and effectively differentiated glioma grades II to IV. The highest sensitivity and specificity were achieved for grade II astrocytoma and grade III oligodendroglioma, with strong performance also in recognizing grade III anaplastic astrocytoma and grade IV glioblastoma.

DHM was confirmed as a valuable complement to traditional methods, providing objective, quantitative phase parameters that reflect the morphological and biochemical changes in malignancy. This method enhances clinical diagnostics by offering a quantitative assessment of pathological indicators, aiding in more accurate clinical decisions.

O13. Current Analytical Methods of Vancomycin Assays and New Perspectives

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Vancomycin is a glycopeptide antibiotic administered intravenous to treat severe systemic infections. Serum vancomycin levels monitoring allow early posology corrections to a specific therapeutic range, improving treatment efficiency and avoiding toxicity.

The present study regroup results of Vancomycin external quality controls obtained from 310 medical laboratories in France in mars 2024. This database contains equally the devices and method used to perform the analysis. The advantages, limits and choice criteria for each method has been analysed, together with method distribution and current clinical needs.

Turbidimetry represents the widest measurement technique with 83,54% from all laboratories, followed by EMIT (enzyme multiplied immunoassay technique) with 15,48% and 0,98% for chemiluminescence methods. The most used reaction principle is KIMS (kinetic interaction of microparticles in a solution) with 41,93% from all laboratories. All methods use antigen antibody reactions, none of the laboratories do not use the reference technique (mass spectrometry).

Results revealed that vancomycin monitoring (VM) is current available in medium and big hospitals centres due to current available methods, sample cadence, convenience, completion time, automation and price. The vancomycin dosage devices for medium laboratories are oversized and can be inexistent for the small ones. Rare cases were reported with important bias probably because of a reduced antibody specificity.

In conclusion, the vancomycin assays in France are based on antigen antibody reactions, KIMS being the most used technique. New dosage methods suitable for point of care (POC) devices may fit better in some medium/small laboratories.

O14. Analytical Exploration of the Link Between Thyroid Cancer and the Composition and Crystal Properties of Microcalcifications

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One of the key challenges in diagnosing thyroid cancer lies in the substantial percentage of indeterminate diagnoses of thyroid nodules that have undergone fine-needle aspiration biopsy for cytological evaluation. To address this challenge, we isolated microcalcifications (MCs) from the material remaining at the end of the cytology procedure. We characterized their morphology, elemental composition, and crystal phases using SEM-EDS, FTIR, and ICP-OES according to the nodule malignancy. We demonstrated that hydroxyapatite MCs may aid nodule diagnosis based on their composition. In particular, Zn-enriched MCs have emerged as potential cancer biomarkers. To better understand if the elevated Zn fraction within MCs is a consequence of cancer or if the Zn-enriched MCs encourage tumorigenesis, we developed an in vitro model system. We treated the human thyroid cancer cell line MDA-T32 with synthetic MC analogs comprising hydroxyapatite crystals with varied pathologically relevant Zn fractions and assessed the cellular response.

These MC analogs displayed an inverse relationship between Zn fraction and crystallinity, as shown by X-ray diffractometry, and their zeta potential decreased once Zn was incorporated into the crystal. The cellular response was evaluated in terms of cell migration, proliferation, the tendency of the cells to form multicellular spheroids, and the expression of cancer markers. Our findings suggest that if thyroid MCs play a role in promoting cancerous behavior in vivo, it is likely a result of the interplay of crystallinity with Zn and carbonate fractions in MCs.

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O15. Smart plasmonic dressings with synergistic photothermal and antimicrobial activity

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Skin and soft tissue infections (SSTIs) represent an important portion of entire classes of infection diseases. Both Gram negative and positive bacteria can lead to SSTIs, however S. aureus sums up the highest percentage of the SSTIs with evidence suggesting that methicillin-resistant S. aureus (MRSA) represent between 30-40%. The inappropriate or excessive use of conventional antibiotics in medicine, agriculture or food industry has led to today's alarming increase in multidrug resistant bacteria. In an attempt to address this problem, we manufactured innovative and original smart plasmonic dressing with application for SSTIs. The smart plasmonic dressing were obtained functionalization of spherical shaped gold nanoparticles (AuNPs) on cotton fibers together with the antimicrobial peptide Cecropin A, thus obtaining a dual treatment effect: thermic and antimicrobial. The thermoplasmonic effect of AuNPs in control conditions was showed following its exposure to the flash of a phone. The smart plasmonic dressing obtained in this way shows no toxicity for BJ epithelial cells when are exposed to it for 24 hours. The growth of S. aureus suspensions exposed to the action of the smart plasmonic dressing is inhibited, the most pronounced effect being observed after illuminating the dressing for 5 min with the phone's flash. An amplified effect is also observed in the case of the application of the smart plasmonic dressing in combination with the flash on the S. aureus biofilm, the treatment leading to the destabilization of the biofilm and the modification of the bacteria's morphology.

Acknowledgments:
This work was supported by a grant of the Ministry of Research, Innovation and Digitalization, CCCDI-UEFISCDI, project number PN-III-P2-2.1-PED-2021-3342. M.R. and M.B. acknowledge financial support from the MCID through the "Nucleu" Program within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 21 02 02.

O16. Ferrofluids Based on Magnetite Nanoparticles for Biomedical Applications

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This paper presents experimental research on the connection between the magnetic properties and the viscosity of ferrofluid based on magnetite nanoparticles, for the study of capillary motion (micro-channels). The magnetite nanoparticles have been obtained by chemical coprecipitation. Some examination methods as X-ray diffraction, atomic force microscopy, and vibrating sample magnetometer have been used to characterize the magnetite nanoparticles. The variation on the viscosity in the magnetic field of ferrofluids based on superparamagnetic magnetite has parabolic allure and in the absence of the magnetic field has a linear allure. Also, the movement of ferrofluids in capillaries made inside the transparent polydimethylsiloxane (PDMS) matrix was observed under the microscope. The experiment helps in the detailed study of the possibility to trap ferrofluids based on magnetite nanoparticles loaded with drug through bio capillaries.

O17. Neuro Modulation by Applying Low Frequency Trans Cutaneous Electrical Impulses on The Skin Close to the Vagus Nerve

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Transcutaneous low frequency electrical nerve stimulation is an electrotherapy method, with multiple health benefits, with non-invasively applying electrodes on the skin. Depending on the frequency, type of electrical impulses and amplitude/intensity, this therapy can reduce chronic and acute pain by blocking pain signals to the brain, also determining the release of endorphins (natural pain killers) and improving the blood flow to the target area or can achieve neuro modulation by stimulating the vagus nerve tone. It can be used to reduce the high blood pressure and the high cardiac pulse (tachycardia) caused by heart malfunction. I constructed an electrical impulse generator of variable frequency and amplitude using a STM32 microcontroller, programmed in the C/C^{++} which generates trains of impulses with frequency between 5 Hz and 45 Hz. The shape of the impulses is “spike”, simulating very well the impulses generated by the neurons i.e. the action potentials. When I measured the brain waves with the help of an electronic encephalograph, I could see an improvement in the gamma brain waves, interpreted by the software as an increase of focus factor. When I disconnected the generator, the focus factor returned to its initial value.

After reconnection, the focus factor increased again at 100%. This demonstrates that the neuro modulation increased as a result of the therapy of the generator, and not by chance.

Poster Communications

P1. (Nano)biotechnology

P1.1 Flexible ZnO@Ag hybrid thin films synthesized by Magnetron Sputtering technique for SERS detection

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Latest developments in the field of surface-enhanced Raman scattering (SERS) trace-level detection rely mainly on flexible substrates based on irregularly shaped structures designed in order to enhance the hot-spots. In this context, we report the in-house fabrication and characterization of flexible, easy-to-use and affordable nanostructured SERS substrates based on hybrid ZnO@Ag thin films. The ZnO-based interlayer and the Ag layer on top were deposited by magnetron sputtering (MS) on three types of commercially available thermoplastic substrates.

By varying the thickness of the deposited thin films, we assessed the influence of their topography and roughness on the Raman signal amplification. We investigated the growth mode of the Ag nanoclusters with or without the ZnO interlayer. From the scanning electron microscopy (SEM) analysis, it was concluded that the Ag atoms covered the entire surface of the film, uniformly filling the area of ZnO grains, forming ziolate Ag clusters. From the SERS analysis performed on the ZnO@Ag hybrid substrates, a limit of detection (LOD) of 10-7 M was reached for the crystal violet (CV) molecule. The highest performance regarding the Raman signal amplification was demonstrated for a Ag film thickness of 15 nm Ag deposited on Zeonor® with a relative standard deviation (RSD) below 10%.

Acknowledgements:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2021-0753 and and through the "Nucleu" Program within the National Plan for Research, Development and Innovation 2022-2027, project PN.23.24.01.02.

P1.2 Gold nanourchins for trace-level SERS detection of analytes

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Gold nanourchins (GNUs) are star-like anisotropic nanoparticles, characterised by a multitude of sharp spikes emerging from a cvasi-spherical core. Their geometry and composition render them excellent signal enhancers for techniques such as Surface Enhanced Raman Spectroscopy (SERS). Under laser excitation, the electromagnetic field enhancement located at their tips and vertices is increased by 8-10 orders of magnitude, while hot-spot formation between tips of closely adjacent particles boosts this effect an additional 100 times. Hot-spots appear through controlled particle aggregation, which can be induced by either reducing the surface charge of the particles (hence the repulsive forces), or by conjugating recognition elements (polyclonal antibodies or aptamers) which result in particle-target-particle sandwich structures. Thus, the signal of Raman-active molecules from the particle vicinity is further intensified when sandwich structures occur via target analytes, allowing GNUs to function as SERS detection tools.

Raman-active molecules such as para-aminothiophenol (pATP), 4-Mercaptobenzoic acid (4MBA), and Nile Blue A (NB) were detected by SERS at trace-level concentrations. Moreover, nanocomplexes composed of GNUs tagged with a Raman-active molecule and biofunctionalized with molecular recognition moieties were employed for the detection of disease biomarkers. A microfluidic system was designed, allowing cost-effective measurements on low-volume samples. The implementation of such a syringe-pump – microfluidic SERS detection platform allows for controlled and reproducible interactions and more reliable results.

Acknowledgements:
This work was supported by MCID, CNCS-UEFISCDI, through project number PN-III-P1-1.1-TE-2021-0234 within PNCDI-III, and through the "Nucleu" Program within the National Plan for Research, Development and Innovation 2022-2027, project PN.23.24.01.02.

P1.3 High-throughput tunable 3D nanostructured surfaces fabricated by nanoimprint lithography

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Transparent and flexible polymeric materials used as substrate have been used to develop new optical devices with improved performances, due to their easily processing at the nanoscale level. Nanostructured surfaces coated with metals have a huge potential for the development of efficient and tunable optical devices. Nanoimprint lithography (NIL) is a modern yet simple and scalable method to fabricate highly-ordered flexible three dimensional (3D) nanostructured surfaces over large areas with high reproducibility. It consists in the mechanical deformation of a thermoplastic or UV-cured polymeric substrate by using a hard mold with 3D architecture.

This work shows the fabrication of high-quality grating-type nanostructured surfaces with variable pitch using NIL technique which will serve as substrates in specialized sensors with improved properties for the detection of molecular analytes. To obtain a high resolution in replication of the mold into the substrate, we optimized the experimental parameters such as the substrate temperature, pressure and imprinting time in correlation with the chosen thermoplastic polymer (Zeonor, Topas.). The morphotopographic characteristics of the metalized nanotrenches were assessed by scanning electron microscopy (SEM) technique.

Acknowledgements:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2021-0753 and by MCID through the "Nucleu" Program within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 01 02.

P1.4 Systematic study of the conjugation of hyaluronic acid, native or oxidized, with dopamine

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The aim of our research was the development of new functional hydrogel matrices based on hyaluronic acid and dopamine (DA). In order to improve the mechanical properties of the hydrogels, the third component, X (X = collagen and methocel), was introduced.

For the use of hydrogels as surgical adhesives and regenerative dressings, hyaluronic acid fulfills all the biomedical characteristics, but to improve the adhesion of the hydrogel, which is a determining factor for this type of applications, the preparation of hyaluronic acid@dopamine gels is considered. The X component can act as a thickening agent, optimizing the mechanical properties of the hydrogels, or it can induce a greater variation in the dimensions characteristic of the microporous structure of the resulting material, in this way facilitating the transport of regeneration factors to the tissues with which it comes into contact.

Starting from fundamental studies on the nature of interactions in HA-DA and HA-X conjugates, the experimental conditions for their formation were first identified. These conjugates are the basis for obtaining bi- and tri-component hydrogels (HA@DA, respectively HA@DA@X), optimized from the point of view of the physico-chemical and structural characteristics required in applications such as regenerative skin dressings and surgical bioadhesives.

The thermodynamic characterization of the interactions between the two components was carried out by Isothermal titration calorimetry (ITC), and the HA-DA conjugates were investigated by liquid NMR spectroscopy in order to introduce a method to quantify the degree of conjugation.

Acknowledgments.
This research was funded and by MCID through the "Nucleu" Programme within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 01 05 and Installations and Special Objectives of National Interest (IOSIN), IZOSTAB.

P1.5 Synthesis and Evaluation of the Binding Affinity of a new Polyphenolic Thiazole with strong antioxidant activity to macromolecules: Computational and Experimental Investigations

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In this study, we designed, synthesized and analyzed a water-soluble molecule presenting a good antioxidant activity, namely N'-(4-(3,4-dihydroxyphenyl)-3-methyl-2,3-dihydrothiazol-2-yl)-4 hydroxybenzohydrazide hydrochloride. The formation of the inclusion complex of the studied compound and β - CD in aqueous solution has been investigated using isothermal titration calorimetry (ITC), spectroscopic and theoretical methods. An estimation of the thermodynamic parameters of the inclusion complex showed that it is an enthalpy - driven process. Our observations also show that hydrophobic interactions are the key interactions that prevail in the complex. ^{1}H NMR measurements were applied to study the interaction with βCD by changing the studied compound concentration in the solution. A molecular docking study added an additional insight to the experimental ITC and NMR analysis regarding the binding conformation of the new polyphenolic compound to βCD.

Acknowledgments:
This research was funded by and by MCID through the "Nucleu" Programme within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 01 05, Installations and Special Objectives of National Interest (IOSIN), IZOSTAB and through the project PN-III-P2-2.1-PTE-2021-0303.

P1.6 How Much is Too Much: a Study on the Influence of Copper Ions Concentration on DNA Structure

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Metal ions are crucial for biological systems, working as cofactors in numerous biochemical reactions. However, when situated above optimal concentration levels, these metals become toxic to cells. Copper, for example, is an essential metal for humans, necessary for enzymes activity in human biological systems. When present at elevated concentrations, copper ions bind to specific sites and can alter the conformational structures of proteins, polynucleotides, DNA, and biomembranes, causing neurodegenerative disorderes, cancer and other diseases.

In this study we analyzed the impact of the Cu2+ concentration on the interaction with a short single-stranded DNA sequence (ssDNA) consisting of fifteen nucleobases, using the alpha-hemolysin (α-HL) nanopore as a sensing platform. The Cu2+-induced conformational changes on the ssDNA structure were characterized by stochastic analysis of ionic current fluctuations and interaction kinetics of these complexes with the nanopore. Our data suggest that Cu2+ binds to ssDNA molecules with high affinity and induces significant secondary structure changes, in a concentration-dependent manner.

By examining the effects of varying Cu2+ concentration, we revealed novel insights into the conformational changes induced by these ions on the ssDNA structure. Our findings have potential implications in understanding copper-related pathologies and biological consequences of copper exposure, particularly in environments with heavy metal contamination.

Acknowledgments:
This work was supported by a grant of the "Alexandru Ioan Cuza" University of Iasi, within the Research Grants program, Grant UAIC, GI-UAIC-2023-01 and was conducted in a facility hosted by the Laboratory of Molecular Biophysics and Medical Physics, Faculty of Physics, "Alexandru Ioan Cuza" University, Iasi.

P1.7 Magnetic Nanoparticles Coated with Bovine Serum Albumin and Grafted with Curcumin as Innovative Theranostic Agents

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Over the last years, magnetic nanoparticles (MNPs) received an increasing interest from scientists due to their unique qualities. They are promising candidates for various medical applications, including magnetic resonance imaging contrast agents, photothermal therapy, and after functionalization, they gain new capabilities as theranostic agents to be used in either treatment or diagnosis. In this study, we developed MNPs with a mean diameter of 6.3±1.4 nm and a zeta potential of 31.6±2.6 mV, using an adapted coprecipitation method. Interestingly, the as-synthesized MNPs also showed photothermal properties after irradiation with NIR wavelengths. For biomedical applications and future functionalization, we biocompatibilized the MNPs with bovine serum albumin (BSA) protein, revealing an increased mean diameter of 66.8±9.2 nm, confirmed both by TEM and DLS measurements, and a zeta potential of 63.7±1.8 mV, which indicates the formation of the BSA corona on MNPs surface. Furthermore, we successfully functionalized the biocompatible MNPs with curcumin, a natural compound acting as both an antioxidant and a fluorophore. The curcumin grafting was confirmed through several spectroscopic techniques, exhibiting a 78% loading efficiency of the fluorophore. Finally, to assess the viability of the designed MNPs, in vitro assays were conducted on melanoma cells, which showed an improved biocompatibility of the MNPs following the coating with BSA and the grafting with curcumin. Moreover, using confocal fluorescence microscopy, we confirmed the good internalization of the MNPs within living melanoma cells.

Acknowledgments:
'Grant for Young scientists', awarded by Babes-Bolyai University, contract number SRG-UBB 32995/23.06.2023.

P1.8 Label-free SERS detection of Parkinson's Disease biomarkers using a hybrid, 3D architecture platform

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Surface-enhanced Raman scattering (SERS) technique has proven a reliable diagnosis tool to detect biomarkers for neurodegenerative diseases. We report herein an innovative and hybrid SERS sensing platform based on ZnO and Ag thin films fabricated using modern "top-down" and "bottom-up" approaches, for the detection of dopamine (DA), as a relevant biomarker in case of Parkinson's disease (PD). A network of periodical nanotrenches and nanogaps with equal width (400 nm) and depth (300 nm) were fabricated on Zeonor™ flexible substrate using nanoimprint lithography technique. The ZnO and Ag films were deposited by pulsed laser deposition in a controlled oxygen atmosphere.

Our sensing and affordable sensor based on the joint use of ZnO/Ag thin films on a thermoplastic substrate greatly benefits from the enlarged contact area between the analyte and enhancing layers, with a high influence on the overall electromagnetic field intensity distribution around the nanotrenches. As a clinically relevant direct application, we investigated spiked, artificial cerebrospinal fluid (aCSF) samples with physiologically identical salts concentrations in order to detect low DA concentrations in simulated biological fluids. Furthermore, experimental samples from healthy and PD's induced- mouse striatum and cortical were investigated for ELISA-based estimation of α-synuclein and DA levels, in combination with a SERS/PCA assessment.

Acknowledgements:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2021-0753 and by MCID through the "Nucleu" Program within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 01 02.

P1.9 Micro-spray formulation of new microcarriers based on Romanian Wild-Growing Inonotus obliquus- Physicochemical Properties, In vitro evaluation

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Chaga mushroom (*Inonotus obliquus*) is a fungus known for its therapeutic properties in traditional medicine. Recent research has been focusing on its chemical composition and biological activity. The proportion of phytoconstituents varies due to various endo and exogenic factors, including the host tree (birch), as it is a pathogenic plant. The maltodextrin microencapsulation of bioactive compounds is a popular method to enhance their stability and release mechanism. This study presents the comprehensive identification of metabolite profiles using gas chromatography-mass spectrometry (GC-MS) and quadrupole ionization time-of-flight mass spectrometry (ESI-QTOF-MS) of wild Romanian Chaga mushrooms.

In addition, two spray-dried maltodextrin microcarriers based on Chaga were developed.

The first microcarrier emerges from Chaga microencapsulation in maltodextrin. The second carrier was prepared in two successive stages, namely Chaga-AgNPs complex formation and accompanied by the new complex microencapsulation in maltodextrin. The morpho-structural and thermal behavior of the newly prepared microcarriers were analyzed using several techniques, including FT-IR, XRD, DLS, SEM, EDS, Raman, and thermogravimetric analysis.

Furthermore, the study investigated encapsulation yield, encapsulation efficiency, and encapsulation content. Antioxidant screening employed four in vitro, non-competitive methods: total phenolic assay, 2,2-Diphenyl-1-picrylhydrazyl (DPPH) radical-scavenging assay, phosphomolybdate (total antioxidant capacity), and iron(III)-phenanthroline antioxidant assay. The collective results suggest the potential application as promising new antioxidant vehicle candidates with versatile applications, ranging from target delivery systems to nutraceuticals.

Poster Communications

P2. Novel materials and biomaterials

P2.1 Using Nanoparticles As Carriers For Anticancer Peptides In Two Cancerous Cell Lines

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There exists a sub-class of antimicrobial peptides with anticancer properties (ACPs), which have a high affinity for the anionic lipid membrane components of the cancer cells. In order to increase the efficiency of these molecules, we use organically modified silica nanoparticles as drug carriers for them, particularly for Gramicidin A (GA). Also, the composition of the nanoparticles was varied depending on surface functionality, by obtaining Ormosil NP using ammonia and Ormosil NP using APTES. These peptide delivery systems can be seen as potential drug releasers which will reduce the present limitations (cytotoxicity, degradation or delivery problems).

We asked ourselves how these NPs carrying GA will affect 2 colon cancerous cell lines (HT-29 and HCT-116) following a 24h or 48h treatment applied for both 2D and 3D cell cultures. We approached these experiments by analyzing the cytotoxicity, the integrity of the cell membrane (LDH assay), the mitochondrial functioning (ATP measurement), but also the cell cycle modification and ROS formation.

As results, we obtained different response regarding the cytotoxicity between the 2D and 3D cellular culture after 24h and 48h of treatment with nanoparticles with or without GA. It can be observed a significant decrease in the viability of the cancer cells in the case of treatment with higher concentrations of nanoparticles. Also, the cell membrane is affected, the cell cycle suffers modification and also, the reactive-oxygen species formation is increased.

In conclusion, this method of approach in which anticancer peptides are carried by conventional nanoparticles is promising and it represents an important milestone in the cancer treatment.

Supported by:
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS—UEFISCDI, project number PN-III-P1-1.1-TE-2021-1548, within PNCDI III and “Nucleu” Programe within the National Plan for Research, Development, and Innovation 2022-2027, project PN-23-21-02-02.

P2.2 Biocompatible Hyaluronic Acid@Polydopamine Hydrogels with Improved Bacterial Inhibition

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Hyaluronic acid (HA) is a naturally occurring non-sulfated glycosaminoglycan widely utilized in biomedical applications due to its biocompatibility, biodegradability and hydrophilic properties. However, HA-based wound dressings often exhibit inadequate mechanical stability and suboptimal biodegradation profiles, limiting their therapeutic efficacy. This study investigates the enhancement of HA hydrogels through polydopamine (PDA) conjugation, which improves adhesion, biocompatibility, antioxidant properties, and effective cross-linking, thereby reinforcing the hydrogel matrix. HA@PDA hydrogels were synthesized using three distinct experimental conditions.

Cellular proliferation and biocompatibility were evaluated on L929 fibroblasts via MTT assays, indicating excellent biocompatibility. Cytotoxicity was assessed through LDH assays, demonstrating that the hydrogels maintained cellular integrity. Antibacterial efficacy against Escherichia coli and Staphylococcus aureus was examined, revealing significant bacterial growth inhibition by the dopamine-modified HA hydrogels. The incorporation of DA contributed to a more favorable degradation profile, essential for effective wound healing. These findings underscore the potential of HA-DA hydrogels in wound healing applications, characterized by enhanced cell proliferation, superior biocompatibility, and effective antibacterial activity.

Acknowledgments:
This research was funded by MCID through the "Nucleu" Programme 2022-2027, project PN 23 24 01 05.

P2.3 Development and Characterization of Hyaluronic Acid@Polydopamine@Gelatin Hydrogels

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Hyaluronic acid (HA), a high molecular weight polysaccharide (glycosaminoglycan), is successfully used in the treatment of acute or chronic wounds due to its biocompatibility, biodegradability, and physico-chemical properties. The use of hyaluronic acid in its native state for biomedical applications is limited by its weak mechanical properties and the fact that it undergoes rapid degradation processes. Polydopamine (PDA) is a bio-mimetic, biocompatible polymer.

For the use of hydrogels as surgical adhesives and regenerative dressings, hyaluronic acid meets all biomedical characteristics, but to improve the adhesion of the hydrogel, the preparation of hyaluronic acid@polydopamine gels is considered.

To extend the range of physicochemical properties needed for targeted applications, we prepared three-component hydrogels of the type HA@PDA@gelatin. We report the preparation and characterization of a novel HA@PDA@gelatin hydrogels.

The structural characterization of the resulting compounds was performed using ss-NMR, their thermal profile was evaluated by differential scanning calorimetry (DSC) and the morphology of the dried hydrogels was examined using scanning electron microscopy (SEM).

Acknowledgments:
This research was funded by and by MCID through the "Nucleu" Programme within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 01 05.

P2.4 Innovative Hydrogels from Hyaluronic Acid-Dopamine Conjugates: Structural, Thermal and Mechanical Properties

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Hyaluronic acid (HA) has a key role in all stages of wound healing, it modulates processes involved in inflammation moderation, cellular migration and proliferation and angiogenesis. In order to improve the mechanical properties of HA and augment it with new and unique properties, hybrids and conjugates of HA with different molecular systems have been recently developed, finding widespread applications such as bone tissue engineering, wound dressing and drug delivery.

Motivated by the strong and almost substrate-independent adhesion of polydopamine (PDA), the conjugation of HA with dopamine (DA) has attracted interest. Upon subsequent oxidation, these conjugates have been shown to give rise to HA@PDA based hydrogels with improved adhesion and mechanical stability**.**

Herein we report the preparation and characterization of a new HA-DA conjugate and HA@PDA hydrogels starting from the synthesized conjugate. The obtained compounds were structurally characterized by NMR (liquid and solid), the thermal profile was assessed by differential scanning calorimetry (DSC) while the morphology of dried hydrogels was investigated by scanning electron microscopy (SEM). The mechanical properties of the hydrogels were investigated by dynamic mechanical analysis.

Acknowledgments:
This research was funded by MCID: "Nucleu" Programme within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 01 05.

P2.5 Hydrophilic coated materials with polydopamine to be used in the 18O separation plant through H_2O distillation

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Abstract. To develop new functional materials with target applications in the medical field, was proposed the development of materials with a hydrophilic coating for the filling elements in the ^{18}O isotope separation columns to increase the efficiency of the isotope separation processes (through water distillation). The ^{18}O isotope in $H_2{}^{18}O$ is the precursor of the radioactive isotope ^{18}F in ^{18}F-FDG (fluorodeoxyglucose), used as a marker in cancer diagnosis by the PET (Positron Emission Tomography) technique. In order to obtain hydrophilic materials, polydopamine (PDA) coatings were tested on different surfaces, e.g. stainless steel, brass, copper, glass and teflon, and the experimental results confirmed the improvement of the hydrophilicity of the materials by coating with this type of polymer (PDA).

Acknowledgements
.The authors acknowledge financial support from the MCID through the "Nucleu" Programme within the National Plan for Research, Development and Innovation 2023-2026, project PN 23 24 01 05 and through the Installations and Special Objectives of National Interest (IOSIN), IZOSTAB.

P2.6 Theoretical Design of a Combined Separation Cascade for Oxygen Isotope Separation

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Abstract. The theoretical investigation of the possibility of linking two conventional processes for the separation of oxygen stable isotopes, ^{16}O, ^{17}O and ^{18}O, by cryogenic rectification of O_2 and by vacuum rectification of H_2O, was realized, using the general theory of isotope separation in cascades. To achieve the optimum design of a real combined separation cascade, in the first step the external and internal parameters of the individual ideal cascades were determined. In the next step square cascades of countercurrent separation columns were designed followed by their integration in the combined separation cascade.

Acknowledgments.
The authors acknowledge financial support from the MCID through the "Nucleu" Programme within the National Plan for Research, Development and Innovation 2023-2026, project PN 23 24 01 05 and through the Installations and Special Objectives of National Interest (IOSIN), IZOSTAB.

P2.7 Enhanced Sulfamethoxazole Assay Based On Selective Graphene Sensing Platform

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Antibiotics are currently considered as a major source of pollution. Sulfamethoxazole (SFX), an antibacterial sulphonamide drug, commonly prescribed and employed in a variety of bacterial infections, was reported to have a multitude of adverse health reactions, therefore its quantification in pharmaceutical industry, medicine and environment is of great interest. This study reports a novel graphene-based electrochemical sensing platform for enhanced SFX detection. Graphene material was prepared by electrochemical exfoliation at 19 V applied bias, in 0.05 M boric acid/ 0.05 M sodium chloride mixed solution. The performances of the graphene-modified glassy carbon electrode (GR/GCE) were evaluated in terms of selectivity, sensitivity, accuracy, and reproducibility employing cyclic voltammetry, differential pulse voltammetry, and amperometry. Under optimized conditions, at pH 5, the developed sensor shows a remarkable enhancement of the sensing abilities compared to the bare electrode, with a linear response in the 0.009 – 28.8 μM SFX concentration range, and a low limit of detection: 0.00272 μM. Furthermore, the analytical applicability of the modified electrode in real sample analysis was performed on two commercially available pharmaceutical formulations. The results of the study demonstrate that the developed sensing platform is able to achieve high selectivity and sensitivity for SFX detection, thus providing a reliable and cost-effective solution for SFX assay.

Acknowledgments:
This work was supported by the Ministry of Research, Innovation and Digitization through the ‘Nucleu’ Program within the National Plan for Research, Development, and Innovation 2022–2027, project number PN 23 24 03 01.

P2.8 Rapid And Selective Ferulic Acid Quantification Based On Sulphur-Doped Graphene

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Due to the multitude of physiological functions, ferulic acid (FA) has a wide range of applications in the food, cosmetic and pharmaceutical industries. Thus, the development of rapid, sensitive and selective detection tools for its assay is of great interest. This study reports a new electroanalytical approach for the quantification of ferulic acid in commercial pharmaceutical samples using a sulphur doped-graphene based electrochemical sensing platform. The few layer graphene material (exf-SGR) was prepared by electrochemical oxidation of graphite, at low applied bias (5V), in inorganic salt mixture $Na_2S_2O_3/(NH_4)_2SO_4$ (0.3 M each). According to the morpho-structural characterization of the material, it appears to have a high heteroatom doping degree as proved by the presence of sulphur lines in the XRD pattern and the C/S ratio determined from XPS investigations to be 11.57. The electrochemical performances of glassy carbon electrode modified with exf-SGR towards FA detection were tested by cyclic voltammetry in both standard laboratory solutions and real sample analysis. The developed modified electrode shows low limit of detection (30.3 nM), excellent stability and reproducibility proving its potential applicability as a viable solution in FA qualitative and quantitative analysis.

Acknowledgments:
This work was supported by the Ministry of Research, Innovation and Digitization through the ‘Nucleu’ Program within the National Plan for Research, Development, and Innovation 2022–2027, project number PN 23 24 03 01.

P2.9 Identification, Determination of The Content of Bioactive Compounds From Gerbera X Hybrid Extracts

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Gerbera × hybrid is a very popular plant, widely used as a decorative garden plant or cut flower, being the fifth most used cut flower in the world (after rose, carnation, chrysanthemum and tulip). From Gerbera x hybrid extracts, classes of phytocompounds were identified, such as: flavonoids, terpenoids, alkaloids, tannins, anthraquinones, saponins and coumarins.
Among them, flavonoids are present in all parts of the plant, especially in photosynthesis cells, occur abundantly as glycosides and are major coloring components of these flowering plants. Besides flavonoids, coumarins and benzofurans are also present. Due to the very wide spectrum of activities in vivo and in vitro, the phytocompounds present in Gerbera flowers are anticancer, antimicrobial, anti-inflammatory agents. [1-3]
Dry red and yellow petals of Gerbera x hybrid were used to obtain the extracts. The conventional extraction methods approached were refluxing combined with maceration, working in ethanol, in duplicate for each type of plant material.
The obtained extracts were characterized physico-chemically by qualitative analysis for the identification of the phytocompounds present, determination of carbohydrate content, antioxidant activity, UV-Vis spectroscopy.

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P2.10 The influence of the polymer matrix on the size of the hydroxyapatite particles

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The particle size plays an important role in the morphological properties and influences the quality of the fillers used as reinforcing agents. Smaller particles have a larger contact area per unit weight than larger particles, increasing the contact between the polymer and the HA particles, which can lead to better dispersion of the particles in the polymer matrix and avoid the formation of agglomerates. In this study, solutions with different concentrations of chitosan and sodium alginate are used as nucleation media for HA particles. The calcium and phosphate precursor solutions are first adjusted to a pH of 12 and added to the polymer solution at a concentration of 5 % and 10 %, respectively, based on the stoichiometric mass of HA according to the synthesis reaction. After synthesis, a quantity of the resulting powder is calcined at 1000 ˚C. The properties of the particles obtained initially and after calcination are studied comparatively, using the initial synthesis product and the product obtained after dispersion in the polymer matrix. The effects of the polymers on the physicochemical properties of the HA particles are determined using SEM, FT-IR, EDAX, DLS, XRD and TG analysis techniques before and after heat treatment to follow the evolution of the properties

P2.11 Synthesis and characterization of some metals doped hydroxyapatite with different applications

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In recent years, Hydroxyapatite (HA) has seen an increase in popularity primarily due to its presence in human bones. Nevertheless, its popularity was also influenced by its bioactivity and biocompatibility, with different morphologies being studied and leading to various applications, such as nanotubes or coating materials.
Doping the HA with different cations has shown to be a good solution in the past years, due to the biological role of each ion and the enhance of certain properties of HA resulted from doping. In the current study, we decided to dope the HA with Zr, Ba, Ag, Sb, Al, and K, as they have an anti-infectious and antimicrobial effect. The phosphorus source was trimethyl phosphate, and the calcium source was calcium acetate. Most of the added metals have an anti-infectious and antimicrobial role. In order to study the influence of the doped metal nature on the thermal behavior of hydroxyapatite precursors, the samples were examined using thermal analysis, EDAX, RX, ICP-OES, and UATR-FTIR. The change in morphology of the resulted products was studied by SEM. Thus, justified by the ease of doping and the potential biomedical benefits that might result from such scientific efforts, the research presented in this article was dedicated to the cationic doping of HA.
The study presented in this paper proves the synthesis of doped hydroxyapatites with different metals and their different influence on thermal stability and their properties with different effects on the materials with possible medical applications.

P2.12 Synthesis, Antibacterial Properties And ADME Studies Of Pyrazolone Derivatives

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In the last two decades there has been a particular interest in the multicomponent syntheses of various heterocycles. In this study, we proposed the synthesis of substituted pyrazolones by multicomponent reactions [1].
The synthesis of pyrazolones involved four components: β-naphthol, an aromatic hydrazine, ethyl acetoacetate and various aldehydes. Pyrazolones **1**–**5** were obtained in good yields (55–70%) by optimizing the reaction parameters, synthetic method, reaction time, solvent and also catalyst. The reaction was carried out by heating the four reactants to reflux with magnetic stirring and monitoring the reaction by thin layer chromatography. The NMR spectra performed on a Varian Inova-400 (500 MHz), in dimethyl sulfoxide (DMSO-d_6) confirmed the structures of pyrazolones.
All compounds were screened by qualitative and quantitative methods against four bacterial strains [2]. Good and very good antimicrobial activities were found on all tested strains. The antimicrobial activity of pyrazolones **1**–**5** was better than the strains considered as standard, M+ and M-.

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P2.13 Photophysical properties of the selected 1,3,4-thiadiazole derivatives investigated in gel, polymer matrice and isopropanol

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1,3,4-Thiadiazole derivatives exhibit many spectroscopic and surface properties depending on different solvents and in polymer matrices. 1,3,4-thiadiazole derivatives are well known for their wide range of biological activities, including antifungal, anticancer, and neuroprotective activities. The biological activity of these compounds is often defined by spectroscopic techniques. One of the interesting effects exhibited by 1,3,4-thiadiazoles is the ESIPT phenomenon. The literature reports that this phenomenon is closely related to the molecular aggregation of these compounds, which leads to the observation of a double emission band. The paper presents the characteristics of absorption, emission, RLS and fluorescence anisotropy of a selected 1,3,4-thiadiazole derivative in starch-based polysaccharide matrices. The structure of the selected 1,3,4-thiadiazole derivative excludes the possibility of ESIPT processes and therefore only a conventional spectral feature was observed in the solutions. The research carried out in this work aims to determine the potential practical applications of biopolymer films. It is worth emphasizing that the results may indicate a wide range of beneficial applications of the tested biopolymer films, especially those enriched with the addition of 1,3,4-thiadiazole, which has antifungal properties. Additionally, thanks to the presence of highly fluorescent additives, the foil can serve as an innovative biodegradable material for creating environmentally friendly food packaging.

Arkadiusz Matwijczuk gratefully acknowledges the support from Kosciuszko Foundation, The American Centre of Polish Culture

P2.14 Biologically Synthesized Gold Nanoparticles for the Detection of Water Contaminants

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New emerging materials alongside the increasing interest in nanotechnology for various applications from clinical diagnosis to food analysis and environmental monitoring are paving the way for technological advancement. The biological synthesis of metallic nanoparticles using plant extracts with antioxidant properties can offer benefits due to their active compounds. The used walnut extract (Js) contained reducing and stabilizing agents, which were shown to be transferred onto the gold nanoparticles, functionalizing them [1].

The obtained Js-AuNPs were characterized by UV-Vis and FTIR spectroscopies and visualized using TEM. The catalytic effect of the Js-AuNPs was evaluated electrochemically. Electrochemical measurements were also employed for the detection of PFOS (perfluorooctane sulfonate - environmental contaminant from the class of "forever chemicals"). Comparing commercial AuNP to Js-AuNP modified biosensors, the later has a lower LoD (0.64 nM vs. 19.4 nM).

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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 within PNCDI III

P2.15 A SERS sensor based on an aptamer functionalized nanoplasmonic platform for ultrasensitive and selective detection of biomarkers

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The identification and quantification of biomarkers with high specificity and sensitivity is one of the most ambitious goals of modern medical diagnosis. The purpose of this work is to present some results obtained in the design of a plasmonic nanoplatform functionalized with aptamer capable of providing relevant solutions for medical diagnosis. The specificity of the recognition of the target biomarkers is ensured by the aptamers attached to the metal surface and the high sensitivity is achieved by the ultra-sensitive detection of the Surface Enhanced Raman Scattering (SERS) signal.
The fabricated plasmonic nanoplatform is characterized by scanning electron microscopy (SEM), optical reflectivity spectra, SERS measurements and finite-difference time-domain (FDTD) simulations.
The designed SERS-based bioassay enables reproducible, highly sensitive and selective detection of relevant biomarkers.
Considering the versatility of the proposed strategy that can change the molecular target on demand through the use of dedicated molecular bioreceptors, the proposed solution offers an attractive alternative in the design of portable nanosensors for the rapid detection of different disease biomarkers.

Acknowledgements:
The authors acknowledge the financial support from UEFISCDI, Project PN-III-P2-2.1-PED-2021-1998. I.T., A.C. & D.M. acknowledge financial support from the MCID through the "Nucleu" Programe within the National Plan for Research, Development and Innovation 2022-2027, project PN23 24 01 02.

P2.16 The Yellow Pigments in *Trichonephila* Spider Silks: A Spectroscopic Study

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The objective of this project was to determine the chemical composition of the yellow or golden color of the spider silks as well as to differentiate silks between species. The Joro (*Trichonephila* clavate) and Golden Silk Spider (*T. clavipes*) silks were tested for comparison as well as sun exposed vs shade. The primary chemicals focused on were xanthurenic acid and beta carotene (to represent carotene). Fourier Transform Infrared (FTIR) Spectroscopy and Infrared Raman (IR Raman) Spectroscopy were used to determine the chemical differences and detection. FTIR had similar scans for all samples and showed the occurrence of a carotene. IR Raman clearly showed the presence of xanthurenic acid and had a significant number of differences in the samples for carotene. This study confirms both the presence of the two pigments in silk from both species and which analytical method is preferable.

P2.17 Investigating the effect of silica nanoparticles as a drug delivery system for Doxorubicin in the treatment of Breast and Lung Cancer.

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Triple-negative breast cancer (TNBC) and non-small cell lung cancer (NSCLC) have the poorest survival outcomes and progression-free survival of all cancers, with two-thirds of patients being diagnosed at an advanced stage when curative treatments are not viable. Nanotechnology provides tools for cancer detection, monitoring, and treatment, including new imaging agents and targeted drug delivery. Nanoparticles' small size and composition enable them to pass through barriers like the blood-brain barrier while minimizing uptake by healthy cells. This makes them a promising method for delivering anti-cancer drugs, improving drug efficacy, and reducing toxic side effects. Doxorubicin is a widely used chemotherapeutic agent however adverse reactions to the drug such as nausea and fatigue are common. Using nanoparticles as a delivery system for doxorubicin may reduce these side effects. This study aimed to investigate the effects of the anti-cancer drug Doxorubicin on TBNC and NSCLC cell lines to compare the efficacy of this drug when encapsulated in silica nanoparticles with the free drug. Cell assays have been used to determine effects of treatment on cell proliferation, cell migration, apoptosis and 3D spheroid model as well as drug delivery being confirmed by immunofluorescence imaging. The results suggest that by using silica nanoparticles to deliver the drugs to cancer cells, there is a greater response to the Doxorubicin, particularly at lower doses. These results demonstrate that nanoparticles can be a promising way of enhancing cancer treatment using pre-existing drugs and potentially limit harmful side effects.

Poster Communications

P3. Early diagnosis and precision medicine

P3.1 Aptamer-conjugated gold nanourchins: promising microfluidic SERS-detection tools for early diagnosis of Alzheimer's Disease

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Aptamers are short synthetic oligonucleotide sequences, and the latest innovation in targeting molecules. Their small size and easier preparation are major advantages over the formerly employed costly and fragile antibodies. Carefully selected aptamer sequences can offer high selectivity and specificity towards the target, while other functional groups, such as the thiol (-SH), can be easily added for straightforward binding to gold surfaces. Plasmonic gold nanourchins (GNUs) are excellent for Surface Enhanced Raman Spectroscopy (SERS) due to their optical properties, boosted by the anisotropic geometry, resulting in a remarkable electromagnetic field enhancement and thus Raman signal amplification. Combined with aptamers, GNUs may work as promising detection tools for a variety of disease biomarkers.
Currently, after an Alzheimer's disease (AD) diagnosis is made, progression is swift and merciless. However, research shows that even 20 years prior to typical AD symptomatology, AD biomarkers are already altered. Patient screening for an early diagnosis and tracking of disease progression could be performed beginning with middle age, and necessary precautions and measures could be established timely, allowing delayed disease progression.
Herein, early-diagnosis biologically relevant concentrations of the AD biomarker protein-Tau441 are detected via SERS using aptamer-conjugated GNUs. A microfluidic platform is employed for the molecular interaction, allowing the use of small sample volumes and the possibility for portability and ease-of-use of such a detection system.

This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2021-0234 and by MCID through the "Nucleu" Program within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 01 02.

P3.2 Plasmonic substrates based on gold nanoparticles for cancer detection by means of SERS analysis of biofluids

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Given its ultra-sensitivity, surface-enhanced Raman scattering (SERS) analysis of biofluids has gain more attention especially for the development of new cancer diagnostic methods. Many cancer cases are diagnosed after the tumor has spread thus hampering cancer treatment. Therefore, early cancer detection is essential for patient survival since it can considerably improve the efficacy of treatment. Plasmonic nanoparticles (PNPs), usually Ag and Au, play a pivotal role in the development of new cancer detection strategies based on SERS analysis of biofluids due to their capacity to enhance the RAMAN signal of the biomolecules. Rational control of PNPs size, shape and surface charge is crucial as they directly influence the localized surface plasmon resonance properties, thereby affecting SERS signal enhancement. Precise control of these parameters through methods, such as chemical reduction, ensures their optimal performance. The reduction agent plays a key role in the synthesis since its strength controls the size of the final PNPs. Herein, we developed Au-based nanoparticles through Turkevich method and using different reducing agents, i.e., PEG-400, PEG-200, PEI, and citrate, which reducing strength increases from the left to right. They also allowed adjusting the surface charge. By controlling both pH and temperature during synthesis, PNPs' size and surface charge could be tuned. The obtained PNPs were analyzed by DLS, Zeta potential, UV-Vis and TEM to assess hydrodynamic size, surface charge, plasmon resonance, morphology, size and size distribution. The capacity to improve the enhancement factor was evaluated by employing several probe molecules.

Acknowledgments:
H2020–ERA-Chair, no 952390 and PN-III-P3-3.6-H2020-2020-0105/35/2021 (UEFISCDI).

P3.3 Thrombotic Thrombocytopenic Purpura (TTP): Diagnostic Challenges and Case Study

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Thrombotic Thrombocytopenic Purpura (TTP) is a rare, life-threatening hematologic disorder characterized by microangiopathic hemolytic anemia, severe thrombocytopenia, and widespread microvascular thrombosis. The diagnostic challenges associated with TTP arise due to its overlapping clinical presentation with other thrombotic microangiopathies, making early identification critical for patient outcomes. This paper reviews the diagnostic complexities of TTP, emphasizing the importance of prompt recognition and intervention.

A detailed case study is presented, highlighting the clinical presentation, diagnostic process, and treatment outcomes, underscoring the significance of an interdisciplinary approach in managing TTP. The case study illustrates the need for heightened clinical suspicion and the role of ADAMTS13 activity testing in confirming the diagnosis, thus enabling timely therapeutic interventions to reduce morbidity and mortality associated with TTP.

P3.4 The Effect Of Hesperidin On Neuronal Cell Membranes

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Hesperidin, a bioflavonoid found in various Citrus species, is known for its antioxidant, anti-inflammation, anticarcinogen, and antimicrobial properties. Recent studies investigated its interactions with the cell membrane and the activation of different signaling pathways relevant to neurodegenerative diseases, cancer, and cardiovascular diseases.

Our study aimed to characterize the interaction of Hesperidin with the cell membrane to understand the modifications that occur and allow Hesperidin to activate specific signaling pathways against disease. Specifically, we monitored changes in membrane fluidity after treating cells with different concentrations of hesperidin (0-98,28 μM). We used two neuronal cell lines: neuroblastoma (SHSY5Y) and oligodendrocytes (OLN-93). The effect of Hesperidin on membrane fluidity was investigated using Laurdan fluorescence at two different temperatures: 20°C and 37°C. Laurdan, a lipid membrane probe, is sensitive to environmental polarity changes. The fluorescence spectra were interpreted using the generalized polarization parameter (GP).

We have shown that at 20°C, increasing Hesperidin concentrations in both SHSY5Y and OLN-93 cell lines led to a maximum of 440 nm and higher GP values, indicating slight membrane rigidification. At 37°C, both cell lines showed maxima at 440 nm and 490 nm, suggesting slight membrane fluidization. GP values had different trends for each cell line, indicating variations in membrane composition and behavior at 37°C. MTT assay (24h, 48h) showed no effect on cell viability at our used concentrations.

In conclusion, at 37°C, the fluidity of the cell membrane is changed, which can significantly impact cellular responses and the activation of signaling pathways following treatment with Hesperidin.

P3.5 Nanofibers and Electrospinning: Methods of Fabrication, Properties, and Applications in Medicine through Drug Delivery

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Nanofibers produced through electrospinning have emerged as a promising material in biomedical applications due to their high specific surface area, porosity, and ability to deliver active substances in a controlled manner. This study investigates the fabrication and characterization of nanofibers based on polyvinyl alcohol (PVA), chitosan, and distilled water, with vitamin C as the active compound.

The research highlights the potential of these nanofibers in drug delivery systems and wound healing. The electrospun fibers were optimized to achieve a uniform and stable structure capable of incorporating and gradually releasing vitamin C, offering controlled and sustained therapeutic effects. The morphological analysis confirmed the homogeneity and appropriate fiber diameter, crucial for effective biomedical applications.

Furthermore, the release kinetics of vitamin C from the nanofibers showed that these systems could provide a stable and prolonged delivery, which is essential in wound healing and other therapeutic contexts. The study suggests that the incorporation of bioactive compounds like vitamin C into electrospun nanofibers can significantly enhance their functionality, positioning these materials as viable candidates for next-generation wound dressings and targeted drug delivery.

The findings provide a strong foundation for further development and clinical translation of such nanofiber-based systems, offering improved patient outcomes through advanced material design and drug release strategies.

Poster Communications

P4. Innovation in Environmental and Pharmaceutical Analysis

P4.1 Desorption profile of local hemostatic carbazochrome loaded on chitosan-HA scaffolds

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Research suggests that nano- structured composites using biodegradable polymers and bioactive ceramics, such as biphasic calcium phosphates (BCP), possess the ability to simulate the surface and chemical properties of bone. By developing chitosan/BCP composite scaffolds with controlled morphology and rigidity we can increase mechanical properties of the scaffolds due to the fact that chitosan scaffolds alone cannot meet the requirements for hard tissue engineering applications. Also, by incorporation of a local haemostatic drug into the scaffolds we can cease the bleeding that occurs during most of the medical procedures.
This study consists in an initial adsorption of carbazochrome on chitosan scaffolds that contain dispersed hydroxyapatite particles. After the adsorption of the drug, the desorption of it was observed at different pH values depending on the possible applications of the drug-loaded scaffold. The scaffolds used were obtained by lyophilization. Chitosan solutions, with HA particles dispersed in, were froze beforehand lyophilization at -20˚C. At the end of lyophilization, some of the obtained scaffolds were treated with NaOH in order to stabilize the macrostructure.
Characterisation of the scaffolds and HA were done by means of SEM, FT-IR, TGA, EDX and DLS. UV-VIS spectroscopy was used for monitoring the adsorption and desorption of carbazochrome.

P4.2 Physicochemical characterization of polymeric membranes with Riluzole for amyotrophic lateral sclerosis treatment

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Riluzole (Rilu) is a neuroprotective drug that acts as a sodium channel blocker against the pathological influx of sodium to inhibit abnormal glutamatergic neurotransmission in the central nervous system (CNS). This drug is safe and well-tolerated treatment for patients with amyotrophic lateral sclerosis (ALS). Rilu ($C_8H_5F_3N_2OS$) is a drug that falls into the category of benzothiazoles. The average absolute oral bioavailability of Rilu is 60%, while the drug is approximately 90% absorbed. It shows a linear pharmacokinetics over a dose range of 25-100 mg administered every 12 hours.

The topical formulation of Rilu was obtained by immersing the Rilu in the Polylactic acid (PLLA) membrane in the following order: Rilu was dissolved in DMSO or methanol. The PLA membranes were introduced in the Rilu solution, one membrane was kept for 10 minutes in the drug solution and the other membrane for 30 minutes.

TG, DSC and FT-IR studies have been used to highlight the degree of incorporation of the active substance in the membrane and the possible interactions between the drug and the polymer.

The FT-IR spectrums were recorded with a Perkin Elmer Spectrometer 100 with U-ATR technique. This technique allows to record IR spectra of all solid or liquid samples without any preparation beforehand.

The thermal behavior for all of the samples was recorded in air (Lindegas, 5.0) atmosphere with a flow rate of 100 ml·min-1. Samples with mass between 5,0 and 15,0 mg were added to aluminum crucibles.

P4.3 Absorption of phosphorus from water using hydrogels based on biopolymers

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Phosphorus is an element of great economic importance and an essential nutrient for plants and animals. However, an excess of phosphorus in surface waters can cause explosive growth of aquatic plants and algae. This can lead to several water quality problems, including low dissolved oxygen levels, which can cause fish kills and harm other aquatic life. Elevated phosphorus concentrations and associated water quality degradation are a critical water quality problem in many of our nation's rivers and streams. Improving water quality in a lake affected by excessive phosphorus is difficult because phosphorus accumulates not only in the water body, but also in the sediments and biota. Therefore, it can take years for conditions to improve after phosphorus sources have been reduced or removed. It is therefore important to take preventive measures to limit the transfer of phosphorus to surface waters. In this study, we used membrane materials synthesized in various reports including a variety of biopolymers, polysaccharides and/or eggshells. These materials were subjected to thorough characterization before and after the adsorption process. Techniques used included thermogravimetric analysis, Fourier transform infrared spectroscopy (FTIR).

P4.4 Compatibility study for leflunomide delivery systems

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Leflunomide is a synthetic isoxazol or, more specific: 5-methyl-N-[4-(trifluoromethyl)phenyl]-4-isoxazolecarboxamide and it is a crystalline solid. Leflunomide is a drug used for the treatment of rheumatoid arthritis, an illness that affects soft tissues and bones and can cause irreversible joint deformities and functional impairment. Leflunomide has an antiproliferative action. It acts as a dihydroorotate dehydrogenase inhibitor as is has been shown to be selectively inhibited by the active metabolite of leflunomide. This drug is administered orally, and its bioavailability is aprox. 80%. In spite of its rather high bioavailability, leflunomide is practically insoluble in water (less than 40 mg/L), so it belongs to class II of the bio-pharmaceutics classification systems. TG, DSC (figure) and FT-IR studies have been used to highlight the degree of incorporation of the active substance in the membrane and the possible interactions between the drug and the polymer. The paper presents a study by spectroscopic and thermoanalytic techniques of membranes in which Leflulomide was incorporated. The study presents the synthesis and characterization of several types of membranes in order to choose the best membrane for controlled release Leflunomide.The study will be complemented by other techniques that will lead us to the best choice.

P4.5 Procedure for the Determination of Alluvial Gold in Gravel Pit Products

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Gold is one of the most important and sensitive economic resources. The world reserves of this rare metal are limited, in contrast to a steady increase in demand for the metal as a result of the development of the microchip industry. In our country, against the background of a sharp decline in the production of gold extracted from large-scale mining operations, the problem of identifying alternative resources for the production of this metal is being raised. In the context of the development of the recovery economy in our country, more and more emphasis is being placed on the extraction of gold from ballast products. In ballast products, gold is found in the form of native metal particles of different sizes and in different forms. Gold is extracted from these products by simple processes, i.e. by passing the sands over felt mats that retain the high-density minerals. In this context, there is an increasing need to identify specific analytical methods that take into account the specific nature of the activity. As the owners of the ballast plants are not willing to invest in analytical equipment or third party analysis, simple, fast, accurate and cheap methods need to be identified to achieve this. Common methods such as spectral methods such as ICP, atomic absorption, etc., although very sensitive due to the way gold is dispersed in the material, simply turn into a lottery. In this paper, a procedure is presented whereby X-ray fluorescence (XRF) can be used to analyze such materials.

P4.6 Process for Concentrating and Determining the Content of Rare Metals in Gravel Pit Products

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Strategic resources for the development of the economy include titanium, zirconium and rare earths. Diversification of the resources from which these elements can be recovered is of particular importance in order to strengthen import independence. As is known, gold is widely recovered from ballast products, mainly from sands, by passing the material over felt mats, followed by concentration on wobble tables. After gold extraction, the resulting tailings from the concentrating tables are thrown back into the sand. Chemical analysis of these tailings has shown that they contain significant amounts of rare and dispersed metals. The main reason these already concentrated resources are discarded is that their presence was simply not known because the business owners were unwilling to spend the money to carry out this kind of expensive analysis. Also, some of the rare and dispersed metals are present in the sand mass in a non-separable form. In the present work, an analytical procedure for analysing the content of recoverable rare metals in sands is proposed, which consists of two steps: (i) quantitative separation of heavy minerals in a high-density liquid (bromoform), followed by (ii) determination of the rare metal content by X-ray fluorescence spectrography (XRF). The determination of these metals by XRF method, when they are present in the parent material, is affected by large errors due to low concentrations. By concentration with bromoform, the concentration of these elements increases considerably, by one to two orders of magnitude, resulting in well-defined peaks.

P4.7 Stability of DNA-gp32 Binding Protein Molecular Complex: The Influence of Electrostatic Interactions

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Single-stranded DNA (ssDNA) - binding proteins (SSBs) bind to exposed regions of ssDNA, stabilizing them and preventing unfavourable DNA conformations. In the replication process, after the unwinding of the DNA double helix by the helicase enzymes, the gp32 SSB protein, derived from the gene product 32 of the T4 bacteriophage, undergoes continuous binding and unbinding via electrostatic interactions with transiently exposed template strands during DNA synthesis. While strong electrostatic interactions between the gp32-SSB protein and the ssDNA in the replication fork are crucial for stabilizing them, the transient nature of these interactions necessitates the ability to detach and reattach easily to the ssDNA.

To delve deeper into the electrostatic factors influencing the stability of the ssDNA–gp32 molecular complex, such as salt concentration and specific metal ion interactions (e.g., Zn^{2+}), we utilized a rapid measurement technique employing an α-hemolysin (α-HL) protein nanopore. We indirectly evaluated the complex's stability by observing the dissociation process between the gp32 protein and the ssDNA molecular complex through single-molecule electrophysiology experiments and fluorescence spectroscopy techniques.

Our findings reveal, for the first time at the single-molecule level, that the ssDNA-gp32 molecular complex exhibits greater stability at lower ionic strength, and that zinc ions further enhance the stability of the molecular complex across all the salt concentration examined herein. This approach holds great promise in the study of other nucleic acid–protein complexes and in accurately determining drug–protein carrier stability.

Acknowledgments:
This investigation was conducted in a facility hosted by the Laboratory of Molecular Biophysics and Medical Physics, Faculty of Physics, 'Al. I. Cuza' University, Iasi', PN-III-P1-1.1-TE- 2021-0331 and PN-III-P4-ID-PCE-2020-0011 (UEFISCDI-Romania)

P4.8 Evaluation of the Chemical Composition, Antioxidant and Antibacterial Activity of Different Hop Varieties

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Hops (Humulus Lupulus L. - Cannabaceae) is an essential plant in the beer industry, due to the secondary metabolites present in the female inflorescences that give these drinks their bitter taste, aroma, and antiseptic properties. These metabolites have proven particularly important in medicine, through their antimicrobial, antioxidant, anti-inflammatory, anticancer, anti-glycemic, neuroprotective, and sedative properties.

This work evaluated five varieties of hops obtained in Romania to establish the chemical and nutritional composition: Magnum 2017, Perle 2017, Magnum 2018, Perle 2018, and Muller Bitterer 2018.

The method based on the reaction of the stable DPPH radical proved to be the best for determining the antioxidant characteristics of essential oils extracted from hop samples, highlighted using UV/VIS spectrophotometry. The identification of the main compounds contained in the essential oil from the hop cones, respectively the content of amino acids and fatty acids (saturated and unsaturated) were carried out using gas chromatography-mass spectrometry (GC-MS) analysis. To determine the content of essential minerals and microminerals (trace elements), the method of optical emission spectrometry with inductively coupled plasma (ICP-OES) was used. One of the most important characteristics of the volatile oils obtained from hops, namely the antibacterial activity by inhibiting the growth of pathogenic bacteria, is also discussed in the paper, providing complete and detailed coverage of the analyzed subject.

The obtained results emphasize the importance of hops not only in the beer industry but also in traditional and modern medicine, offering new perspectives for the exploitation of this valuable ingredient in various fields, including the development of pharmaceutical and nutraceutical products.

P4.9 Preformulation Studies Regarding Membranes Containing Active Pharmaceutical Ingredients with Analgesic and Antipyretic Activity

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Preformulation studies play an important role in the development of new pharmaceutical formulations. Preparations containing paracetamol (Paracet), propyphenazone (Perf) and caffeine (Caff) are used as a combination for pain relief. This combination of active pharmaceutical ingredients causes a reduction in prostaglandin levels, while caffeine is also known to enhance the analgesic effects of paracetamol and propyphenazone.

Paracetamol is a widely used over-the-counter analgesic and antipyretic. Propyphenazone is a non-steroidal anti-inflammatory drug derived from pyrazolone and is found in many over-the-counter analgesic combinations. Caffeine is a xanthine alkaloid used as a psychotropic stimulant and is found in coffee, tea, mate, guarana, cola and cocoa.

In obtaining and developing new pharmaceutical formulations, it is very important to know the physicochemical properties of drugs and pharmaceutical components.

The present study aims to obtain the best pharmaceutical formulation with an alginate-based membrane containing paracetamol, propyphenazone and caffeine for possible transdermal application to eliminate the side effects associated with oral administration.

The new pharmaceutical formulations obtained were analysed by FTIR, thermogravimetric analysis, electron microscopy (SEM) coupled with EDX and UV-Vis.

P4.10 Heavy Metals and Persistent Organic Pollutants in Wetland Soils and Sediments from Lower Danube-Prut River Region

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Heavy metals (HMs), persistent organic pollutants (POPs) such as pesticides, polychlorinated biphenyls (PCBs) and polycyclic aromatic compounds (PAHs) are highly toxic compounds in environment, posing a serious threat to ecosystem state and people's health. The aim of the study was to investigate the soil and sediment contamination levels in aquatic ecosystems of Lower Danube and Lower Prut rivers, including selected transboundary areas at RO-MD and RO-UA borders. Atomic Absorption Spectrometry (AAS) was employed for HMs analysis and GC-ECD and GC-MS for organic pollutants quantification.

The concentration of contaminants and carcinogenic components were found to exceed the legislated values in several sites in Lower Prut floodplain reserve (Beleu Lake, Gotesti, Slobozia Mare), Republic of Moldova, and Lower Danube Chilia branch, being a cause for concern in the river border areas. The obtained results emphasize the need for further research, establishing a risk assessment framework of soil and sediment pollution and regular monitoring of connected aquatic environmental compartments influenced by man-made activities (oil extraction, industrial emissions, old pesticides storage, waste burning, transport in wetland and deltaic areas).

Acknowledgments:
This research was funded by EC through JOP Black Sea Basin 2014-2020, projects BSB27-MONITOX and BSB165-HydroEcoNex.

Poster Communications

P5. Innovative Methods and Technology for Bioanalysis

P5.1 Quantitative Evaluation of Codelivery Nanoparticles Incorporation in Cultured Cells

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Cultured cells (BJ and BT474 lines) incubated with mesoporous silica-based nanoparticles (NPs) functionalized with phenylboronic acid derivative and loaded with doxorubicin and resveratrol were analysed. To establish the incorporation percentage, we designed and developed a digital automated tool starting from experimental hyperspectral images. The tool combines spectral angle mapper with assisted segmentation and counting operations. It is automated and provides the percentage of pixels in which the spectral fingerprint of the NPs is found. The analysis is carried out at the cell level. The projected area of the cells in the BT474 cell line is approx. five times smaller than the projected area of the cells in the BJ line. The incorporation percentage is approx. twice higher for BT474 cell line. The presence of resveratrol in codelivery system favoured the release of Dox from carrier NPs, which contributed to enhance antitumoral effect on BT474 cancer cells after 48 h incubation period with NPs dose 50 μg/mL (3.22±0.63% for D@R@MCM-CPBA versus 8.70±0.20% for Dox alone or 7.07±1.60% for NPs containing only Dox). The breast cancer cells viability decreases directly proportional with D@R@MCM-CPBA concentration, with a maximum cytotoxicity at 150 μg/mL, while the viability of normal fibroblast is maintained above 70%, the threshold for biocompatibility.

Acknowledgments
This work was funded by a grant from the Nat. Program for Res. of the Nat. Assoc. of Technical Univ—GNAC ARUT no. 75/11.10.2023. Hyperspectral imaging due to European Regional Development Fund through Competitiveness Operational Program 2014-2020, Priority axis 1, INOVABIOMED.

P5.2 Bisphenol A analyses and quantification inconsistencies via HPLC-UV

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Bisphenol A (BPA) is a recognized endocrine disruptor commonly found in plastic products, necessitating the development of reliable and convenient detection methods. This study presents a systematic review of existing open-access literature to assess the application of high-performance liquid chromatography coupled with a UV detector (HPLC-UV) for the determination and quantification of BPA, as HPLC-UV is likely the most widely used analytical-grade instrumentation in research facilities.

The review of the literature identified various methodologies for detecting BPA and it was observed that UV detectors were often set to wavelengths that do not correspond to the specific absorption peaks of BPA.

To optimize the detection conditions, we analyzed HPLC-UV data of BPA samples prepared in methanol and acetonitrile. Statistical methods were employed to identify the optimal wavelength and solvent for accurate BPA concentration measurements. Additionally, the consistency of the data was evaluated through correlation analysis, calculation of coefficients of variation, and error estimation for concentration measurements. These analyses were conducted using OriginLab and ChatGPT's Advanced Data Analysis facility.

Analysis performed with AI included linear regressions, T-tests, Analysis of Variance (ANOVA), correlation analysis, and the calculation of coefficients of variation. These tasks were executed using Python and the libraries NumPy, pandas, SciPy, Matplotlib, Seaborn, and scikit-learn.

P5.3 Electrochemical Determination, Antioxidant Activity, FTIR-ATR Spectroscopy and Anticancer Effect of Honey Extract Collected From Jijel City (Algeria)

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Honey is a sweet, tasty animal product derived from nectar and/or honeydew. It is used in various nutritional and therapeutic fields. The aim of this study was to determine the physicochemical characteristics and antioxidant activities of a honey sample from the town of Jijel (Algeria). The honey analyzed complies with Codex Alimentarius Commission standards. Analysis of quality parameters revealed a proline and HMF contents were 435.47 mg/kg and 3.49 mg/kg respectively. Phenolic compounds and flavonoids were found to be higher in honey. In addition, the study of antiradical activity against DPPH and ABTS revealed that honey was able to scavenge DPPH and ABTS radicals with 48.88 and 18.21%, respectively. No cytotoxic effect of honey extract on HepG2 liver cells was observed. The superimposed FTIR spectrum of honey sample observed between 400 and 4000 cm^{-1} is detected, with the 3650-3000 cm^{-1} range corresponding to the stretching vibrations of OH groups in carbohydrates, water and organic acids. For the study of antioxidant capacity by electrochemical generation, the cyclic sweep potential range varies from 0 to about - 1.5V and the cyclic voltammogram is first recorded in the absence of antioxidant additions. Then, microadditions of extract are made, and for each addition the voltammogram is recorded.

This study deserves to be pursued to identify and quantify the biologically active components used in the treatment of several diseases.

Acknowledgments:
As part of the “Eugen Ionescu” doctoral and post-doctoral scholarship program, financed by the Romanian government and provided by the Agence Universitaire de la Francophonie "AUF", I would like to thank all the staff at the University of Brasov, especially the Faculty of Medicine, for their warm welcome.

P5.4 Electrochemical Approaches for Evaluating Antioxidant Properties of Hypericum Triquetrifolium Turra Extracts

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This study focuses on the electrochemical methodologies employed to investigate the antioxidant capacity of natural extracts from **Hypericum Triquetfolium Turra**, a medicinal plant recognized for its antioxidant potential in traditional medicine.

However, this research emphasizes the advantages of electrochemical methods, such as cyclic voltammetry (CV) and differential pulse voltammetry (DPV), which offer enhanced sensitivity and reduced sample preparation time.

The study systematically evaluates the redox properties of various polar extracts derived from the aerial parts of **H. Triquetfolium**, employing electrochemical techniques to identify and quantify its bioactive constituents. Key factors influencing the electrochemical responses, including scan rate, pH, and concentration, were meticulously analysed to establish optimal conditions for antioxidant detection.

The findings reveal that electrochemical methods not only provide a rapid screening approach but also facilitate a detailed characterization of phytochemicals, corroborated by complementary techniques such as FTIR, DPPH, and HPLC/MS.

The results indicate a significant correlation between the anodic area of cyclic voltammograms and the total antioxidant content, allowing for effective discrimination among different extracts.

Acknowledgements:
The authors are grateful to thank the Romanian Government, the University Agency of the Francophonie (AUF) and The Transylvania University of Brasov for the continuous support during the realization of this work

P5.5 Microscopic (SEM, IR, Raman), spectroscopic and thermal methods for Micro and Nanoplastics characterization.

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The present study analyzes the behavior that very small plastic particles adopt when they enter the body of fish and undergo digestion. In order to carry out a more complex analysis, 4 known methods were used, namely: Thermal Analysis, FTIR Spectroscopy, Raman Spectroscopy and Microscopy and Scanning Electron Microscopy (SEM). The samples used were HDPE and PET, and each analysis was performed on the standard samples and on the samples that were previously introduced in a solution that mimics the gastric fluid of fish. After studying the results obtained for each type of method, it was concluded that due to the exposure of these 2 types of nanoplastics to the action of the solution that mimics the digestive fluid, surface damage was highlighted, without structural changes. A structural destabilization was highlighted in the thermogravimetric studies and changes in the diameter of the fibres highlighted in particular by SEM analysis and microscopic techniques. Being a topical and important research topic, this topic is still incompletely elucidated and requires more investigation and analysis.

P5.6 Generation and detection of non-classical correlations using nuclear magnetic resonance

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In this contribution we describe our first attempt to implement optimal pulse sequences to manipulate nuclear spin systems to witness non-classical correlations. We are interested to develop techniques which can be used for the precise and efficient manipulation of thermal spin states of atoms nuclei in organic molecules to implement simple quantum computing experiments. In this study we used a popular heteronuclear spin system consisting of ^{1}H and ^{13}C coupled nuclear spins in chloroform dissolved in acetone with the aim to implement a quantum algorithm.

Acknowledgments
This research was funded by MCID through the "Nucleu" Program within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 01 05, by the Installations and Special Objectives of National Interest (IOSIN), IZOSTAB and by The European Digital Hub from Transylvania (TEDIHT) project 10183508, DIGITAL-2021-EDIH-01.

Poster Communications

P6. Food production and authentication

P6.1 Health Risk Assessment of Heavy Metals in Selected Root Vegetables

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Food safety is an increasing concern, and determining the concentration of heavy metals in vegetables is essential for health risk assessment during consumption.

The main objective of this paper was to estimate the heavy metal concentrations in root vegetables and evaluate human health risks. The concentrations of heavy metals were analysed in over 100 root vegetables (radishes, carrots, and potatoes) collected from the Romanian area. The inductively coupled plasma mass spectrometry technique (ICP-MS) was used for the determinations.

With only a few exceptions, the estimated daily intake of heavy metals associated with vegetable ingestion was within the provisional tolerable daily intake, indicating that the concentration of heavy metals received by the body cannot negatively impact consumers' health. The exceptions are related to soil quality, and the regular consumption of vegetables grown in contaminated soils can harm the human population. As a result, efforts should be made to amend the soil to reduce the uptake of metals in some vegetables.

Heavy metal concentrations in vegetables are strongly dependent on the environmental parameters of the places of their growth; as a result, these data about the heavy metals from vegetables should be supplemented with data about the soil, establishing the transfer characteristics of heavy metals in the body of the vegetable.

This work was supported by the Romanian National Authority for Scientific Research and Innovation, Contract No. 27N/2023, PN 23 24 03 01.

P6.2 Occurrence and Health Risk Assessment of Alkali Metals and Macronutrients in Potable Waters

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Increasing lithium (Li) demand worldwide due to its properties and role in renewable energy will raise water reservoir pollution and side effects on human health.

The present study evaluated the occurrence and human health risks of oral exposure, respectively, and the relationship between alkali metals (Li, Cs) and minerals (Na, Mg, K, Ca) in bottled and spring water. The inductively coupled plasma mass spectrometry technique was used to determine the elements concentrations.

The lithium concentration varied between 0.06–1557 and 0.09–984 µg/L depending on the water sources. The correlation between Li and Na, Mg and K was significant and positive, varying between bottled and spring waters ($p < 0.001$). Lithium exceeded the limit set by the health-based Screening Level (HBSL) in some of the studied water samples. The possible side effects of Li poisoning of water resources on human health have been evaluated using the Estimated Daily Intake Index (EDI) and Total Hazard Quotient (THQ). The oral reference doses (p-RfDs) for the noncancer assessment of daily oral exposure effects for a human lifetime exceeded threshold values for some of the waters, illustrating possible side effects after a long exposure time. The THQ index shows potential adverse health effects, requiring further investigations and remedial actions in 2.38% of spring waters. Further research needs to be continued by analyzing the elemental profile of water and food for chronic diseases.

This work was supported by the Romanian National Authority for Scientific Research and Innovation, Contract No. 27N/2023, PN 23 24 03 01.

P6.3 Nutritional Profiling of Fatty Acids and Metals in Cookies and Biscuits for Children

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Cookies and biscuits are widely favoured for their affordability and long shelf life, making them popular choices among children. These products, deeply rooted in culinary history, are valued for their versatility and convenience. However, they can serve as vectors for metal exposure, either through natural incorporation or contamination during production. Assessing the metal content in foods consumed by children is crucial for understanding potential health risks associated with dietary intake. Despite their widespread consumption, limited data exist on the fatty acid profiles and metal contamination in cookies and biscuits intended for children.

This study addresses this gap by analyzing the fatty acid composition and metal content in various brands of cookies and biscuits available on the Romanian market. Using gas chromatography coupled with flame ionization detection (GC-FID), we quantified the fatty acid profiles across multiple products from different manufacturers.

The findings provide valuable insights into the nutritional quality and safety of these popular snacks, highlighting the importance of monitoring both beneficial nutrients and potential contaminants in foods targeted at young consumers. The results underscore the need for comprehensive evaluation of food products to ensure safe and healthy dietary options for children. By examining the intersection of nutrient composition and contaminant presence, this study contributes to a more informed understanding of the implications of these widely consumed treats on children's health.

This work was supported by the Romanian National Authority for Scientific Research and Innovation, Contract No. 27N/2023, PN 23 24 03 01.

P6.4 Hen Egg Characterisation Based on Isotopic and Elemental Fingerprints

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At global level, in 2022, eggs production was around 87 million tons. The eggs consumption per person continues to rise. The authenticity of food products represents a high priority in today's society as a consequence of globalization and the free trade in goods. For now, the most suitable techniques for tracking the geographical origin of food commodities and the diet of animals are Isotope Ratio Mass Spectrometry (IRMS) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS). The price of foodstuff (eggs, milk, meat, etc) is directly related to the conditions in which the animal was raised. In this respect, using stable carbon isotopes ($^{13}C/^{12}C$) contributes to the identification of corn-based feeding. The egg white and yolk samples coming from different hen's rearing systems (yard and industrial farms) were investigated from isotopic and multi-elemental composition point of view. $\delta^{13}C$ values of potential food sources are discussed versus the dietary intake and contribution to the isotopic fingerprint of the eggs to determine mixing of C3 and C4 diets.

Acknowledgments.
The financial support for this work was supported by the Ministry of Research, Innovation and Digitization, CNS-UEFISCDI, project numbers PN-III-P2-2.1-PED-2021-2406 (contract no. 664PED/2022).

P6.5 Comprehensive Analysis of Pesticide Residues in Potato Tubers: A GC-FID Approach

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The presence of pesticide residues in agricultural produce poses significant health risks, necessitating reliable analytical techniques for detection and quantification. This study presents a comprehensive methodology for analyzing pesticide residues in potato tubers using Gas Chromatography with Flame Ionization Detection (GC-FID).

The approach integrates optimized extraction, efficient separation, and sensitive detection to provide a robust assessment of pesticide contaminants. Potato tubers, a staple crop with extensive agricultural use, were subjected to a meticulous pesticide extraction process using ethyl acetate, following the QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) protocol. The extracts were cleaned up with dispersive solid-phase extraction to remove matrix interferences. GC-FID was employed for the separation and detection of pesticide residues, chosen for its high sensitivity, specificity, and cost-effectiveness.

Method validation included the assessment of linearity, limits of detection (LOD), and quantification (LOQ), precision, and accuracy, achieving recovery rates between 75% and 110% for most target pesticides. The calibration curves exhibited strong linearity ($R^2 > 0.94$), with LODs ranging from 0.01 to 0.05 mg/kg, demonstrating the method's suitability for trace-level analysis. The study successfully identified and quantified multiple pesticide residues in commercial potato samples, highlighting the method's efficacy in routine monitoring and ensuring food safety. This work underscores the critical need for rigorous analytical methods in the detection of pesticide residues, aiming to safeguard consumer health and enhance the integrity of agricultural practices.

This work was supported by the Romanian National Authority for Scientific Research and Innovation, Contract No. 27N/2023, PN 23 24 03 01.

P6.6 Egg Yolk Fatty Acids: GC-FID Differentiation of Backyard and Barn Hen Eggs

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The growing consumer interest in the nutritional quality of eggs has highlighted the need for detailed analyses of eggs produced under different hen-rearing conditions. This study aims to differentiate the fatty acid profiles of egg yolks from backyard and barn hens using Gas Chromatography-Flame Ionization Detection (GC-FID) analysis.

We collected egg samples from both backyard and barn systems and conducted a comprehensive analysis of their fatty acid compositions. The results demonstrated significant differences in the profiles of essential fatty acids, including omega-3 and omega-6 fatty acids, between the two groups. Backyard hen eggs exhibited higher levels of omega-3 fatty acids and a more favorable omega-6 to omega-3 ratio compared to barn hen eggs. These findings suggest that the rearing environment significantly impacts the nutritional quality of egg yolks, providing valuable insights for consumers and producers aiming to optimize dietary benefits. This study underscores the importance of production methods in determining the nutritional profile of eggs and highlights GC-FID analysis as a reliable tool for such differentiation.

This work was supported by the Romanian National Authority for Scientific Research and Innovation, Contract No. 27N/2023, PN 23 24 03 01 and a grant of the Ministry of Research, Innovation and Digitization, CCCDI–UEFISCDI, project number PN-III-P2-2.1-PED-2021-2406 (contract no. 664PED/2022), within PNCDI III.

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