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for
Biomedical and Environmental Sciences

IC-ANMBES 2018

BOOK OF ABSTRACTS

Braşov, 23rd -25th May, 2018

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SCIENTIFIC PROGRAMME

ORAL COMMUNICATIONS

May 23th 2018	**Building *Aula Magna* of Transilvania University of Brasov. 41 A Iuliu Maniu Street, Brasov, 500091, Romania.**			
	Room Aula Magna, Chairperson: Monica Florescu, Valerică Raicu, Ioan Turcu			
15.00-16.30			**Registration**	
16.30-16.40			**Opening Ceremony**	
16.40-17.20	Plenary Lecture	P1	Graeme Milligan University of Glasgow, UK	GPCR Quaternary Structure and Possible Implications for Drug Discovery
17.20-18.00	Plenary Lecture	P2	Marius Schmidt University of Wisconsin-Milwaukee, USA	Mix-And-Inject at Free Electron Lasers
18.00-20.00			**Welcome Party and Poster Session (odd numbers)**	

May 24th 2018	**Building *Aula Magna* of Transilvania University of Brasov. 41 A Iuliu Maniu Street, Brasov, 500091, Romania.**			
	Room UI6, Chairperson: André Matagne			
9.00-9.40	Plenary Lecture	P3	Jochen Balbach Martin-Luther-University Halle-Wittenberg, Germany	Conformational Protein Plasticity Studied by NMR Spectroscopy
	Room UI6, Biophysical methods in the study of protein folding, misfolding and assembly, Chairperson: André Matagne			
9.40-10.10	Keynote,	K1	Charlotte Vendrely University of Cergy-Pontoise, France	Weighting Amyloid Fibers
10.10-10.40	Keynote,	K2	Francisco Conejero-Lara Universidad de Granada, Spain	Using Multidisciplinary Biophysical Techniques to Unveil Protein Aggregation Mechanisms
10.40-10.55	Contributed talk	O1	Paulina Komorek Polish Academy of Sciences, Poland	Changes in Lysozyme's II-Structure as a Result of its Interaction with a Gold Surface – A Crucial Step for Alzheimer's Disease Mystery Solving
	Room UI7, Electrified interfaces and biosensing, Chairperson: Pankaj Vadgama,			
9.40-10.10	Keynote	K3	Camelia Bala University of Bucharest, Romania	Molecular Recognition - Versatility and Challenges in the Design of Biosensor
10.10-10.25	Contributed talk	O2	Ana Maria Titoiu International Centre of Biodynamics, Romania	Flow Injection Analysis System Integrating Electrochemical Sensors for Monitoring the Alcoholic Fermentation of Wines
10.25-10.40	Contributed talk	O3	Raluca-Elena Munteanu International Centre of Biodynamics, Romania	Extracellular pH of Cancer Cells and Normal Cells as Revealed with a Voltammetric pH Microsensor
10.40-10.55	Contributed talk	O4	Melinda David Transilvania University of Brasov, Romania	Characterization and Evaluation of Biosensor Architectures Incorporating Nanomaterials as Sensitive Tools for Analytical Detection of Glucose
11.00-11.30	**Coffee Break and Poster Session (odd numbers)**			
	Room UI6, Biophysical methods in the study of protein folding, misfolding and assembly, Chairperson: Francesco Conejero-Lara			
11.30-12.00	Keynote	K4	Vincent Forge Biosciences and Biotechnology Institute of Grenoble, France	Amyloidosis: Taking Advantage of the Specific Structural Features of Amyloid Fibbers for the Design of Diagnostic
12.00-12.30	EBSA-sponsored speaker	K5	André Matagne University of Liège, Belgium	Improving the Quality of Protein Samples for Higher Quality Results
12.30-12.55	Invited talk	I1	Claudiu Gradinaru University of Toronto, Canada	Signalling via Oligomeric Receptors and G proteins Detected by Single-Molecule Fluorescence
	Room UI7, Electrified interfaces and biosensing Chairperson: Fred Lisdat,			

11.30-12.00	Keynote	K6	Pankaj Vadgama Queen Mary University of London, UK	Bioelectrochemical Monitoring: The Challenges of Clinical Adaptation
12.00-12.25	Invited talk	I2	Tudor Luchian „Alexandru Ioan Cuza" University, Romania	Interrogation of Biomolecular Structure at Nanoscale
12.25-12.40	Contributed talk	O5	Alina Vasilescu International Centre of Biodynamics, Romania	Stable NADH Detection with Carbon Nanofibers and Meldola Blue-Modified Electrodes
12.40-12.55	Contributed talk	O6	Monica Florescu Transilvania University of Brasov, Romania	Performance Evaluation of Nanozyme Sensors Towards Antioxidant Capacity Detection
13.00-14.00	**Lunch**			
	Room UI6 **Chairperson: Valerică Raicu**			
14.00-14.40	**Plenary Lecture**	P4	Anne K. Kenworthy Vanderbilt School of Medicine, USA	Altering Protein Function by Pharmacologically Targeting Membrane Domains
	Room UI6, **Novel materials and biomaterials for analytical methods** **Chairperson: Marius Schmidt**			
14.40-15.10	Keynote	K7	Simion Astilean, Monica Potara , Monica Focsan , Timea Simon , Ana Gabudean - Craciun , Sorina Suarasan , Sanda Boca-Farcau , Andreea Campu , Dana Maniu , Cosmin Farcau	Designing multifunctional plasmonic nanoplatforms for applications in nanomedicine
15.10-15.25	Invited talk	I3	Robert Sandulescu „Iuliu Hatieganu" University of Medicine and Pharmacy Cluj-Napoca, Romania	Graphene Based Electrochemical Sensors for Biomedical Applications
15.25-15.40	Contributed talk	O7	Victor Diculescu National Institute of Materials Physics, Romania	High Surface Area Flexible Electrodes for Wearable Devices and Actuators
15.40-15.55	Contributed talk	O8	Andreea-Maria Campu Babes-Bolyai University, Romania	Microfluidic Platform for Integrated Plasmonic Dual Detection
	Room UI7, **Medical analysis and diagnosis,** **Chairperson: Graeme Milligan**			
14.40-15.10	Keynote	K8	Kalina Hristova Johns Hopkins University, USA	The Delta Peptide from Ebola
15.10-15.35	Contributed talk	O9	Adrian Enache National Institute of Materials Physics, Romania	Protein Carbonyl Electrochemical Detection
15.35-15.50	Contributed talk	O10	Mihaela Bacalum Horia Hulubei National Institute for Physics and Nuclear Engineering, Romania	Antimicrobial Effects of Short Tryptophan-and Arginine-Rich Peptide On Methicillin-Resistant Staphylococcus Aureus
15.50-16.45	**Coffee Break and Poster Session (even numbers)**			

	Room UI6, Microspectroscopy **Chairperson: Kalina Hristova**			
16.45-17.15	Keynote,	K9	Valerică Raicu University of Wisconsin-Milwaukee, USA	Fluorescence micro-spectroscopy techniques and approaches for characterization of protein association in living cells
17.15-17.40	Invited talk	I4	Ronen Berkovich Ben-Gurion University of the Negev, Israel	Near-wall hydrodynamic effects on tethered DNA under shear flow
17.40-17.55	Contributed talk	O11	Fran Nekvapil Babes-Bolyai University, Romania	Translation of SERS Technique to Hydrobiology: Use of Metallic Plasmonic Nanoparticles to Quench Fluorescence in Raman Spectroscopy Analysis of Natural Fluids
19.00-23.00	**Gala Dinner (Restaurant Aro, Brasov – Romania)**			
	Room UI7, Analytical methods for (nano)biotechnology **Chairperson: Robert Sandulescu**			
16.45-17.00	Contributed talk	O12	Ileana Cristina Covaliu University Politehnica of Bucharest, Romania	Synthesis And Technological Innovation of Fe_3O_4 Nanomaterial Applied in Wastewater Treatment by Flotation
17.00-17.15	Contributed talk	O13	Luminita C. Miclea „Carol Davila" University of Medicine and Pharmacy, Romania	Multiparameter Study of Cultured Cell Behaviour Modified by Nanoparticles
17.15-17.30	Contributed talk	O14	Costinela Valerica Georgescu „Dunarea de Jos"University of Galati, Romania	Volumetric Quantitative Analysis of Pure Ascorbic Acid in Tablets
17.30-17.45	Contributed talk	O15	Elena-Ines Adam-Dima „Carol Davila" University of Medicine and Pharmacy, Romania	Selenium Nanoparticles – Premises for Their Therapeutic Use in Pathologies Related to Oxidative Stress
19.00-23.00	**Gala Dinner (Restaurant Aro-Palace, Brasov – Romania)**			

May 25th 2018	**Building *Aula Magna* of Transilvania University of Brasov. 41 A Iuliu Maniu Street, Brasov, 500091, Romania.**			
	Room Aula Magna, **Chairperson: Jochen Balbach**			
9.30-10.10	**Plenary Lecture**	**P5**	Fred Lisdat Technical University Wildau, Germany	Label-Free Sensing Strategies Using Impedance Spectroscopy, SPR and Photoelectrochemistry
	Room UI6, **Medical analysis and diagnosis** **Chairperson: Jochen Balbach**			
10.10-10.40	Contributed talk	O16	Luiza Buimaga-Iarinca National Institute for Research and Development of Isotopic and Molecular Technologies, Romania	IMAGCELL – Assessing Living Cells Natural Features by Employing Optical Microscopy and Statistical Analysis
10.40-11.05	Contributed talk	O17	Ion Hurjui „Grigore T. Popa" University of Medicine and Pharmacy, Romania	Human Serum Expression Levels of Monocyte Chemoattractant Protein-1 in Type 2 Diabetic Subjects
11.05-11.20	Contributed talk	O18	Ecaterina Radu National Institute of R&D for Technical Physics, Romania	Magneto-Mechanical Actuation of Fe-Cr-Nb-B Magnetic Particles for Destruction of Osteosarcoma Cells
11.20-11.35	Contributed talk	O19	Alexandra Farcas Babeş-Bolyai University, Romania	Cationic Polymers as Drug Delivery Systems
	Room UI7, Analytical methods for medical physics **Chairperson: Tudor Luchian**			
10.10-10.35	Invited talk	I5	Alexey Zhemchugov Joint Institute for Nuclear Research, Russia	Spectral CT with a Medipix Detector for Biomedical Applications
10.35-10.50	Contributed talk	O20	Violeta L. Calin „Carol Davila" University of Medicine and Pharmacy, Romania	Potential of Non-Invasive Quantitative Holographic Imaging in Evaluation of Malignancy and Treatment Efficiency of Melanoma Cells
10.50-11.05	Contributed talk	O21	Tomas Kondela Comenius University UK in Bratislava, Slovakia	The Effect of Cholesterol and/or Melatonin on the Amyloid-B Peptides Loaded Model Membranes
11.05-11.20	Contributed talk	O22	Radu – Dan Necula Transilvania University of Brasov, Romania	Low Cost Electrical Muscle Stimulator (EMS) Tested with Biopac
11.20-11.35	Contributed talk	O23	Ileana-Constanta Rosca Transilvania University of Brasov, Romania	Static Analysis of the Human Body Balance Following an Induced Vertigo
11.35-12.00	**Coffee Break and Poster Session (even numbers)**			
	Room UI6, **Novel materials and biomaterials for analytical methods** **Chairperson: Simion Astilean**			
12.00-12.30	Keynote	K10	George Stan National Institute of Materials Physics, Romania	Comparative in Vitro Behaviour of Bioglass Coatings in Simulated Body Media with Improved Biomimicry: Challenging a Paradigm

12.30-12.45	Contributed talk	O24	Larisa Florea Dublin City University, Ireland	Novel Photo-responsive Structures for microSensors and microActuators
12.45-13.00	Contributed talk	O25	Colm Delaney Dublin City University, Ireland	Boronic Acids for the Generation of Responsive Hydrogels
	Room UI7, Atomic and nuclear methods **Chairperson: Alexey Zhemchugov**			
12.00-12.25	Invited talk	I6	Chudoba Dorota Joint Institute for Nuclear Research, Russia	Neutron Scattering Methods in Characterization of Pharmacological Systems
12.25-12.50	Contributed talk	O26	Claudia Stihi Valahia University of Targoviste, Romania	Investigation of Spatio-Temporal Atmospheric Deposition of Cd and Pb in Romania Using Moss Biomonitoring
13.05-13.40	**Closing Ceremony**			
14.00-22.00	**Social Program**			

POSTER COMMUNICATIONS

	Chairpersons: André Matagne, Pankaj Vadgama, Valerică Raicu, Ioan Turcu	
Number	**Authors**	**Title**
Biophysical methods in the study of protein folding, misfolding and assembly		
P Bp 1	Niculina-Sonia Suvar, Ramona Bleiziffer, Paula Podea, Andreea Maria Iordache, Monica Culea	Characterization of Some Seed Extracts by Using Isotopic Dilution-Gas Chromatography-Mass Spectrometry
P Bp 2	Georgiana Petrareanu, Antonio Mondini, Paris Lavin, Alina Vasilescu, Cristina Purcarea	Molecular Adaptations to Low Temperatures of Cold-Active Microbial Catalysts
P Bp 3	Alina Asandei, Isabela Stefania Dragomir, Tudor Luchian, Aldo E Rossini, Mauro Chinappi, Yoonkyung Park	Readout of Small Peptides Primary Structure, with a Protein Nanopore
P Bp 4	Ana-Maria Raicu, David N. Arnosti	Adaptation of a CRISPR Interference Method for Probing Chromatin Properties of Repressor Domains
P Bp 5	Alexandra Farcas, Luiza Buimagă-Iarinca, Porav Sebastian, Lorant Janosi, Calin Floare	Structural Features and Aggregation of NRas Proteins and it's Oncogenic Mutations
In-silico methods		
P Si 1	Luiza Buimaga-Iarinca, Alexandra Farcas, Lorant Janosi	Use of Molecular Docking as a Tool for Comparative Binding Analysis of Large Peptides to Ras Wild Type and Oncogenic Proteins
P Si 2	Lorant Janosi, George Necula, Mihaela Bacalum, Mihai Radu, Ioan Turcu	In silico studies on the dynamics and energetics of histidine-modulated arginine- and tryptophan-based peptides in membrane models
Analytical methods for medical physics		
P Mf 1	Andreea Celia Benchea, Dana Ortansa Dorohoi, Ion Hurjui, Loredana Liliana Hurjui	Solvatochromism and Quantum-mechanical Study of 8-Hydroxyquinoline: Comparison of Solvent Scales
P Mf 2	Costinela Valerica Georgescu, Cristian Catalin Gavat, Doina Carina Voinescu	Spectrophotometric UV analysis method of acetylsalicylic acid in tablets
P Mf 3	Andreea Celia Benchea, Dana Ortansa Dorohoi, Loredana Liliana Hurjui, Ion Hurjui	The Computed Parameters and Solvatochromic Study of Two Fluorescent Molecules
P Mf 4	Radu Dan Necula, Corneliu Drugă, Ionel Serban, Angela Repanovici, Diana Cotoros	Tribological modelling of the hip joint
P Mf 5	Ioana Andreea Brezestean, Alina Tantau, Maria Gorea, Nicolae Har, Leontin David, Simona Cinta Pinzaru	New Data on Growing Mechanism of Human Gallstones from Transylvania, Romania: A joint Confocal Micro-Raman, Polarized Light Microscopy, X-Ray Diffraction and Thermal Analysis Study
P Mf 6	Carmen-Elisabeta Manea, Mirela Mihon, Dana Niculae, Catalin Stelian Tuta	Quality control of radiopharmaceuticals

P Mf 7	Mirela Mihon, Carmen Elisabeta Manea, Dana Niculae	Validation of a color spot test for determination of Kryptofix 2.2.2 in radiopharmaceuticals production
P Mf 8	Cristina Alexandra Constantin, Claudia Chilom, Mihaela Bacalum	Anticancer activity of Luteolin studied in carcinoma and sarcoma cells
P Mf 9	Diana Cotoros, Corneliu Druga, Ionel Serban, Angela Repanovici, Radu Dan Necula	Biomechanical and thermographic study of syndromes induced by human body vibrations
P Mf 10	Diana Cotoros, Ionel Serban, Corneliu Druga, Anca Stanciu, Radu Dan Necula	Influence of variable frequency noise upon the human factor stability
P Mf 11	Ileana-Constanta Rosca, Ionel Serban, Corneliu Nicolae Druga, Dan Radu Necula	LabVIEW routine for encephalographic signal processingLabVIEW routine for encephalographic signal processing
P Mf 12	Adrian Serban, Sebastian Toma, Marius Moga, Monica Florescu	The prevalence of cancers and hormone replacement therapy
Novel materials and biomaterials for analytical methods		
P Bm 1	Manuela Stan, Ildiko Lung, Adina Stegarescu , Ocsana Opris, Simona Gutoiu, Maria-Loredana Soran, Teofil-Danut Silipas, Cristian Leostean, Ovidiu Pana, Mihaela Diana Lazar, Alin Sebastian Porav	Preparation of MnO_2/Carbon Nanotubes with Sorption Properties
P Bm 2	Maria Coros, Florina Pogacean, Lidia Magerusan, Marcela-Corina Rosu, Valentin Mirel, Stela Pruneanu	A New Approach Towards the Synthesis of Graphene Based Materials
P Bm 3	Lidia Magerusan, Stefan Gergely, Stela Pruneanu, Florina Pogacean, Maria Coros	Electronic Portable Device for Selective Lead Ion Detection from Different Water Sources
P Bm 4	Stela Pruneanu, Florina Pogacean, Lidia Magerusan, Maria Coros, Marcela-Corina Rosu, Valentin Mirel	Graphene Synthesis by Exfoliation of Graphite Rod via Pulses of Current
P Bm 5	Lidia Magerusan, Florina Pogacean, Maria Coros, Alexandru Turza, Stela Pruneanu	Green Methodology for Chitosan/Carbon Base Nanomaterial Preparation and its Applicability in Sunset Yellow Detection
P Bm 6	Florina Pogacean , Lidia Magerusan, Maria Coros, Valentin Mirel, Stela Pruneanu	Electrochemical Detection of 8-Hydroxy-2'-deoxyguanosine Using Graphene Modified Electrodes
P Bm 7	Laurentiu Susu, Andreea Campu, Simion Astilean, Monica Focsan	Designing Efficient Low Cost Paper-based Sensing Nanoplatforms
P Bm 8	Maria Stefan, Ovidiu Pana, Adriana Popa , Dana Toloman, Teofil-Danut Silipas, Cristian Leostean, Sergiu Macavei, Lucian Barbu-Tudoran, Manuela Stan	Synthesis and Characterization of $CoFe_2O_4$@TiO_2:Tb Magnetic Recoverable Photocatalyst
P Bm 9	Cristina M. Muntean, Nicoleta E. Dina, Maria Coros, Nicoleta Tosa, Alexandru Turza, Monica Dan, Ioan Turcu	Graphene-Based SERS Platforms for Molecular Diagnosis
P Bm 10	Rodica-Mariana Ion	Microcapsules as Carrier Systems in Photodynamic Therapy
P Bm 11	Marcela-Corina Rosu, Maria Coros, Florina Pogacean, Alexandru Turza, Doina Prodan, Stela Pruneanu	Photocatalytic Ability of Cotton Pads Modified with TiO_2-Pt/Reduced Graphene Oxide and SiO_2-Pt/Reduced Graphene Oxide Composites

P Bm 12	Lacramioara Oprica, Larisa Popescu, Maria Balasoiu, Alexander Kuklin, Dorina Creanga	Silver nanoparticles synthesized by green chemistry method and their bioimpact on environmental microorganisms
P Bm 13	Sourav Das, Zoltán Gazdag, Lajos Szente, Mátyás Meggyes, Györgyi Horváth, Tamás Kőszegi	Antioxidant and Antimicrobial properties of Randomly Methylated β Cyclodextrin complexed Essential Oils
P Bm 14	Ceren Durmus, Eda Aydındogan, Zinar Pinar Gumus, Takeshi Endo, Shuhei Yamada, Suna Timur, Yusuf Yagci	Catechol-attached Polypeptide with Functional Groups as Electrochemical Sensing Platform for K2-Spice
P Bm 15	Eda Aydindogan, Takeshi Endo, Shuhei Yamada, Suna Timur, Yusuf Yagci	Catechol-bearing Polypeptide Modified Gold Nanoparticles for Point-of-Care Detection of Immunoglubulin G as a Cancer Biomarker
P Bm 16	Melinda David, Hugo C. Novais, Christopher M.A. Brett	Deep Eutectic Solvents as Ecological Media for the Development of Novel Redox Polymer-Film Modified Electrochemical Sensors
P Bm 17	Adrian Blidar, Bogdan Feier, Robert Săndulescu, Cecilia Cristea	Electrochemical Behaviour Of Vancomycin And Its Direct Detection On A Graphene Based Electrochemical Sensor
P Bm 18	Andra Mihaela Predescu, Ecaterina Matei, Maria Râpă, Cristian Pantilimon, George Coman, Cătălin Gradinaru, Cristian Predescu	Formulations and investigations of chitosan/polyvinyl alcohol blends for various applications
P Bm 19	Violeta-Carolina Niculescu, Nadia Paun, Marius Miricioiu, Mihaela Iordache	Highly efficient, rapid, and simultaneous removal of dyes from wastewater using mesoporous silica
P Bm 20	Rita Csepregi, Viktória Temesfői, Tamás Kőszegi	Multiparametric Green Fluorescent Protein-Based Microplate Cell Viability Assay
P Bm 21	Ecaterina Matei, Andra Predescu, Maria Rapa, Andrei Berbecaru, Claudia Dragan, Mirela Sohaciu, Cristian Predescu	Novel bio-composite used for Cr(VI) removal from effluents
P Bm 22	Maria Mihăilescu, Adina Negrea, Mihaela Ciopec, Petru Negrea, Gerlinde Rusu, Narcis Duteanu, Alina Barbulescu	Palladium Retrieval From Residual Waters Resulted From Galvanotechnique Industry
P Bm 23	Nadia Paun, Violeta Carolina Niculescu, Marius Gheorghe Miricioiu	Mesoporous silica-media for natural anthocyanins dye adsorption
P Bm 24	Ioan Milosan , Monica Florescu, Daniel Cristea, Mihai-Alin Pop, Tibor Bedo	Electrochemical Evaluation of Heat-Treated AISI 316 Stainless Steel in Solar Furnaces to be used as possible implant material
Medical analysis and diagnosis		
P Ma 1	Cristina Surdu-Bob, Cristin Coman, Ene Vlase, Florica Barbuceanu, Daniela Ionita, Marius Badulescu	Copper Toxicity Of Metallic Bone Implants – A Pilot Study
P Ma 2	Cristin Coman, Ene Vlase, Cristina Surdu-Bob, Florica Barbuceanu, Mihaela Ene, Florina Zorila, Danut Turcu, Alexandru Anghel	Preliminary Studies On The Effectiveness Of Targeted Copper And Silver Therapy Against Established Osteomyelitis
P Ma 3	Bianca Elena Popovici, Maria Mitrica, Ioana Nitu, Flaviu Moldovan	Variation of Blood Pressure in Adolescents Population in Brasov District
P Ma 4	George Madalin Danila, Mihaela Puiu, Lucian Gabriel Zamfir, Camelia Bala	Development of an Enzyme-Linked Immunosorbent Assay to Ghrelin Agonists and Antagonists Detection

P Ma 5	Christina Zalaru, Veronica Georgiana Preda, Marianta Alexandra Strinoiu, Bianca Georgiana Patrascu, Florea Dumitrascu, Constantin Draghici, Isabela Ana Tarcomnicu, Maria Marinescu, Marilena Ferbinteanu, Andrei Juncu	Synthesis and cytotoxicity of new aminopyrazolo-benzimidazoles derivatives
P Ma 6	Christina Zalaru, Cristina Croitoru, Georgiana Adriana Popa, Luisa Gabriela Ilie, Florea Dumitrascu, Constantin Draghici, Rodica Tatia, Lucia Moldovan, Marilena Ferbinteanu	Synthesis, cytotoxicity and antitumor activity of new halogenoaminopyrazoles derivatives
P Ma 7	Alexandru Milentie Hada, Monica Potara, Sorina Suarasan, Adriana Vulpoi, Emilia Licarete, Simion Astilean	4MBA Labeled Chitosan Coated Gold-Silver Core-Shell Nanoparticles as In Vitro SERS Traceable pH Sensors
P Ma 8	Monica Florescu, Melinda David	Development and Evaluation of Novel Polymer-Based Tyrosinase Biosensor for Selective Dopamine Detection
Microspectroscopy		
P Sp 1	Cristina Balan, Monica Baia	Experimental Micro-Raman and IR spectroscopic analysis of amikacin combined with DFT-based calculations
P Sp 2	Alia Colnita, Ana Maria Raluca Gherman, Tiberiu Szoke-Nagy, Ionut Bogdan Cozar, Nicoleta Elena Dina	The Use of In situ Surface Enhanced Raman Spectroscopy Technique for Antibiotic Resistance Determination of Pathogenic Microorganisms
P Sp 3	Nelya V. Doroshkevich, Grigory M. Arzumanyan, Kahramon Z. Mamatkulov, Hanna V. Bandarenka	Detection of DNA molecules by SERS spectroscopy with silvered porous silicon as an active substrate
P Sp 4	Ioana Andreea Brezestean, Fran Nekvapil, Leontin David, Simona Cinta Pinzaru	Microbial Community From Cojocna Balneary Lakes: Rich Resource Of Carotenoids Ascertained By Resonance Raman Micro-Spectroscopy
Analytical methods for (nano)biotechnology		
P Nb 1	Claudia Maria Gutu, Octavian Tudorel Olaru, Anca Ungurianu, Denisa Marilena Margina, Mihaela Ilie, Dumitru Lazurca, Monica Florescu	Berries Buckthorn Oil - Subcritical Fluid Extraction, Chemical Characterization And Biological Efficacy Of A Potential Food Supplement
P Nb 2	Claudia Maria Gutu, Octavian Tudorel Olaru, Anca Ungurianu, Mihaela Ilie, Denisa Marilena Margina, Dumitru Lazurca, Monica Florescu	Lavandula Oil – extraction, chemical characterization and potential biological effects
P Nb 3	Alina Vasilescu, Claudia Valentina Popa, Simona-Carmen Litescu, Andrei Florin Danet	Antioxidant Capacity Determination by Using Nano-Oxides of MoO_3 and CeO_2
P Nb 4	Adrian Pirnau, Mircea Bogdan, Calin G Floare , Mihaela Mic, Silvia Neamtu	Competitive Binding of Tolmetin to b-CD and HSA
P Nb 5	Alia Colnita, Daniel Marconi, Maria Suciu, Lucian Barbu-Tudoran, Ioan Turcu	Fabrication of Nanotrenches and Microfluidic Channels for Biomolecular Detection

P Nb 6	Mihaela Mic, Adrian Pirnau , Maria Miclaus, Calin G. Floare, Iren Kasco, Mariana Palage, Mircea Bogdan	Molecular Interaction between Drugs with Antimicrobial Activity and Macromolecular Receptor
P Nb 7	Livia Neagu, Ioan Dorobantu	Nanoimmunosorbents based on functionalized SiO_2 nanoparticles used in affinity chromatography techniques to separate antibodies from complex biological mixtures (antisera)
P Nb 8	Daniel Marconi, Alia Colniţă, Radu Tiberiu Brătfălean, Ioan Turcu	Single-step Fabrication Of Silicon Nanocones For Biosensing Applications
P Nb 9	Zagrai Mioara, Dehelean Adriana, Rada Simona, Pica Maria, Culea Eugen	Structural and optical properties of the gadolinium-lead-borate glasses and vitroceramics
P Nb 10	Simona-Carmen Litescu, Andrei-Florin Danet, Claudia Valentina Popa, Georgiana Badea, Viorica Tamas, Alexandru Suciu	Valorization of By-Product Rezulted in Processing of Milk Thistle Oil by Cold Pressing. Recovery of Silymarin
P Nb 11	Irina Schiopu, Andrei Ciuca, Alina Asandei, Aurelia Apetrei, Chang Ho Seo, Yoonkyung Park, Tudor Luchian	Exploring PNA-DNA Hybrids with a Nanopore-Based Technique
P Nb 12	Ana Maria Raluca Gherman, Daniel Marconi, Alia Colniță, Laszlo Szabo, Nicolae Leopold, Tiberiu Szoke-Nagy, Nicoleta Elena Dina	Microfluidic Portable Device for Pathogens' Rapid SERS Detection
P Nb 13	Alina Asandei, Andrei Ciuca, Irina Schiopu, Aurelia Apetrei, Loredana Mereuta, Chang Ho Seo, Yoonkyung Park, Tudor Luchian	Single-Molecule Study of pH- and Salt-Induced Conformational Changes of PAMAM-G1 and -G1.5 Dendrimers, with Protein Nanopores
P Nb 14	Cristina Ileana Covaliu, Ecaterina Matei, Iosif Hulka, Gigel Paraschiv	Study of Activated Carbon Performance For Depollution of Wastewater Containing Organic (C_6H_6 and C_6H_5-CH_3) And Inorganic (Pb^{+2} and Zn^{+2}) Pollutants
P Nb 15	Fran Nekvapil, I Brezestean, B Glamuzina, S Tomšić, L Barbu-Tudoran, V Chis, S Cinta Pinzaru	Natural Biocomposite Material with Antioxidant Properties and a Source of Valuable Compounds: the Cuticle of Squilla mantis Shrimp
P Nb 16	Ecaterina Matei, Cristina Covaliu, Andra Predescu, Andrei Berbecaru, Claudia Dragan, Cristian Predescu	Depollution of wastewaters using nanobiotechnology based on new TiO2 photocatalyst
P Nb 17	Lavinia Gabriela Carpen, Tomy Acsente, Diana Iulia Savu, Maria Adriana Acasandrei, Elena Matei, Claudia Gabriela Chilom, Gheorghe Dinescu	Influence of Nanometric Tungsten Dust on Fibroblasts Cells
P Nb 18	Paulina Komorek, Robert Stokłosa, Joanna Zemła, Małgorzata Lekka, Barbara Jachimska	Physicochemical characterization of poly-L-lysine and its interactions with globular proteins
P Nb 19	Larisa Popescu, Dorina Creanga, Liviu Sacarescu, Marian Grigoras, Nicoleta Lupu	The magnetic contamination of Fe_3O_4@GA against some biotic components of the environment
P Nb 20	Diana Stegarus , Constantin Paladi , Ecaterina Lengyel , Roxana Ionete	Bacteria Involvement in Biodegradation of Chlorinated Organic Compounds in Ground Water
P Nb 21	Diana Stegarus , Ramona Cristea , Roxana Ionete , Ecaterina Lengyel , Mircia Toderici	PCB and Pesticides Monitoring and its Implications to Food Quality Assessment - Case Study on Milk

P Nb 22	Leopold Tie, Monica Focsan, Cristian Tira, Andreea Campu, Adriana Vulpoi, Jocelyne Bosson, Simion Astilean	Controlling the End-to-End Assembly of Gold Nanorods to Enhance the Plasmonic Response in Near Infrared (NIR)
Atomic and nuclear methods		
P Na 1	Afag Madadzada, Marina V. Frontasyeva, Sevinj R. Hajiyeva, Margarita S. Shvetsova, Zarifa T. Veliyeva, Orxan B. Hajiyev	Assessment of Atmospheric Deposition of Trace Elements in Baku (Azerbaijan) Using Moss Bags
P Na 2	Irina Fierascu, Valentin Raditoiu, Cristian Andi Nicolae, Alina Raditoiu, Raluca Somoghi, Monica Raduly, Bogdan Trica, Radu Claudiu Fierascu, Lia Mara Ditu	Analytical Characterization and Potential Applications of Metal-Substituted Apatitic Materials
P Na 3	Gabriela Ioana Cristea, Cezara Voica, Adriana Dehelean, Dana Alina Magdas, Ioana Feher, Romulus Puscas, Florina Covaciu	Application of Isotopic and Elemental Profiling in Food Products and Beverages
P Na 4	Dehelean Adriana, Kovacs Melinda, Magdas Dana Alina, Cristea Gabriela, Feher Ioana	Baby food supplements quality evaluation through different analytical methods
P Na 5	Afag Madadzada, Jalal A. Nagiyev, Aydan A. Garibli, Marina V. Frontasyeva, Adil A. Garibov	ENAA of Soil Samples from Small District of Azerbaijan: Search for Actinides
P Na 6	Radulescu Cristiana, Claudia Stihi, Monica Florescu, Dumitru Lazurca, Ioana Daniela Dulama, Sofia Teodorescu, Radu Lucian Olteanu, Raluca Maria Stirbescu	Bioactive Properties and Chemical Composition of Juglans Regia L. Extracts
P Na 7	Gabriela Ioana Cristea, Dana Alina Magdas, Cezara Voica, Ioana Feher, Romulus Puscas, Stelian Radu, Valentin Mirel	Isotopic and Elemental Fingerprint of Transylvanian Pork Meat
P Na 8	Radulescu Cristiana, Alina Bintintan, Mihai Gligor, Rodica Mariana Ion, Ioana Daniela Dulama, Claudia Stihi, Sofia Teodorescu, Raluca Maria Stirbescu, Radu Lucian Olteanu, Ioan Alin Bucurica	Pollution Effects on Painted Pottery of Romanian Cultural Heritage
P Na 9	Margarita Shvetsova, Marina Frontasyeva , Inna Kamanina , Sergey Pavlov , Afag Madadzada , Konstantin Vergel	Active Moss Biomonitoring With Moss Sphagnum Girgensohnii in the Park of Moscow
Biomembranes and model membranes		
P Mm 1	Corina Ciobanasu, Isabela Dragomir, Aurelia Apetrei, Tudor Luchian	Penetrating Properties of LyP-1 Homing Peptides in Giant Unilamellar Vesicles
P Mm 2	Alexandra Besleaga, Aurelia Apetrei, Lucel Sirghi	Investigation of molecular interactions between antimicrobial peptides and biomimetic lipid membranes
P Mm 3	Ion Hurjui, Dana Ortansa Dorohoi, Ionela Lacramioara Serban Andreea Celia Benchea, Irina Gradinaru, Loredana Liliana Hurjui,	Spectral study of model membrane fluidity using a fluorescent marker
P Mm 4	Bogdan Zorila, Mihaela Bacalum, Mihai Radu	Evaluation of Lipid Membrane Tryptophan Rich Peptides Bound Fraction by Fluorescence Spectrum Deconvolution

Oral Communications

Plenaries

P1. Applications of Spatial Intensity Distribution Analysis (SpIDA) to interrogate the quaternary structure of G protein-coupled receptors

Graeme Milligan[1], John Pediani[2], Richard J Ward[2], Sara Marsango[2]

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Spatial Intensity Distribution Analysis (SpIDA) allows use of super-Poissonian distribution functions to obtain density maps and quantal brightness values from pixel-integrated fluorescence intensity histograms created from confocal images containing appropriate fluorophores. Following stable expression in HEK293 cells of G protein-coupled receptors (GPCRs) of interest linked to monomeric enhanced green fluorescent protein (mEGFP) we have analysed regions of interest on the baso-lateral surface of the cells to establish, relative to well defined monomeric controls, the steady state proportions of monomeric and dimeric forms of mEGFP-tagged GPCRs and how this may be regulated by ligands that bind the receptors. In the case of the dopamine D_3-receptor subtype then, with expression levels in the region of 60 receptor per mm^2, some 60% of the receptor is present as dimeric forms. Addition of either of the anti-psychotic drugs haloperidol or spiperone resulted in rapid transformation to predominantly monomeric forms of the receptor. Such an effect was not produced, however, by concentrations of other D_3 receptor antagonist ligands including eticlopride, nemonapride and clozapine. To explore potential mechanisms responsible for these differences we have applied molecular dynamics simulations to potential binding poses of these ligands. We observed that by distinct means, spiperone and haloperidol alter the positions of key regions of the transmembrane domains that form interfaces of dimerisation whilst the other ligands do not.

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P2. Mix-and-inject at free electron lasers

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X-ray Free Electron Lasers (XFELs) are the hottest X-ray sources of the world. Currently, there are 4 XFELs operational, in the US, Japan, Germany, and South Korea. The Swiss XFEL is about to get online. These machines deliver femtosecond X-ray pulses with between 10^9 to 5 x 10^{12} quasi-monochromatic X-ray photons per pulse in a small (0.1%) bandwidth. Pulse repetition rates vary from 30 Hz to 5 Mhz. These machines offer unprecedented opportunities for structure determination of biological macromolecules. Tiny nano and microcrystals, down to the single particle level can be used in diffraction experiments. Radiation damage due to the ionizing X-rays is not an issue, since the diffraction patterns are collected faster than the damage of the sample. This is called the “diffraction-before-destruction” principle. I review recent advances in the field and outline opportunities for the understanding of structure function relationships in biologically and bio-medically interesting proteins and enzymes.

P3. Conformational plasticity of the GPCR activating parathyroid hormone

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The parathyroid hormone (PTH) from glands controls the blood calcium and phosphate level via its G-protein coupled receptors (GPCR). PTH, a 84 residue peptide, is intrinsically disordered and adopts an a-helical conformation for N-terminal residues 15-34 upon binding to the extra cellular domain of the receptor [1]. These residues form the core cross-b structure in fast forming amyloid fibrils, which is possibly a storage form of the PTH hormone and thus a functional amyloid conformation [2]. NMR-detected phosphorylation at the N-terminus of PTH by cell-lysate of parathyroid glands still allows hormone binding to the ectodomain but abolishes GPCR activation *in vivo* [3]. The same inhibition can be achieved by a Zn^{2+} anthracenyl-terpyridine complex binding to the N-terminus of PTH [4]. PTH(1-34) is already an approved drug against osteoporosis, where this Zn^{2+} coordination complex now allows to control receptor activation not by targeting the receptor itself but at the level of its agonist. The N-terminal residues of PTH thus can adopt various functional conformations depending on the local environment including binding partners, posttranslational modifications, or amyloid fibrils, and we found a conformation selective metal coordination complex to inhibit receptor activation.

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P4. Altering protein function by pharmacologically targeting membrane domains

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A key mechanism that regulates the function of a wide range of membrane proteins is their association with cholesterol- and sphingolipid-enriched membrane nanodomains known as membrane rafts. Rafts are thought to co-exist in biological membranes with surrounding disordered phase domains, and the movement of specific proteins into or out of rafts has been linked to a number of diseases. However, rafts have proven to be notoriously difficult to study in intact cells, and we still lack a clear understanding of the mechanisms that selectively target membrane proteins to rafts. How the specialized environment of lipid rafts influences protein function is also still nebulous. To address these questions, we are utilizing giant plasma membrane vesicles (GPMVs) as a model system. GPMVs can phase separate into a mixture of raft and non-raft domains and are readily isolated from a variety of cell types, making them an ideal system to study mechanisms underlying raft association and function. I will summarize recent work from our group using GPMVs to examine how several different bacterial toxins are targeted to rafts. I will also discuss our ongoing efforts to perform high throughput screens using GPMVs to identify new pharmacological approaches to manipulate raft structure and function.

P5. Label-free sensing strategies using impedance spectroscopy, SPR and photoelectrochemistry

Fred Lisdat[1]

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Label- free methods are valuable tools during the development of sensors and biosensors since they allow to optimize the conditions for surface modifications and biomolecule binding. However, these methods have also increasingly be used as transduction methods in the sensing process itself. The analytical potential results mainly from the fact that the labelling process of biomolecules can be avoided. Furthermore, these techniques can help to understand the behaviour of molecules on surfaces.

The presentation will address three different examples demonstrating the potential but also drawbacks of label-free techniques. The focus is here on impedance spectroscopy (EIS), surface plasmon resonance (SPR) and photoelectrochemistry (PE). EIS can be used for the detection of nucleic acids exploiting their highly charged character [1,2]. This can be applied for concentration analysis, mismatch detection or the analysis of binding events of molecules to nucleic acids. A recent interest can be seen in abasic DNA Here a different behaviour after hybridisation can be found on electrodes compared to fully complementary strands.

SPR exploits changes on the optical density near the surface. Limitations occur when only small changes happen. It can be shown however, that even conformational changes such as the formation of G quadruplex structures can be detected when a proper capture strand design is used. Furthermore, the potential of online binding detection can be used for the discrimination of structural similar proteins [3].

The use of light in combination with electrodes allows a spatial control of the read-out and thus, has potential for multianalyte detection. Other attractive features result from the energy input in the system, which can change the potential behaviour compared to non-illuminated electrodes [4,5].

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Oral Communications

Biophysical methods in the study of protein folding, misfolding and assembly

K1. Weighting Amyloid Fibers

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Amyloid fibers are self-assembled protein structures associated to both pathological and physiological processes. They possess a high aspect ratio with diameters around 2-20 nm, lengths of a few microns, and a high molecular weight. Fiber samples often contain a mix of different morphologies. Such features challenge the measurement of their accurate mass (the total amount of proteins within the fibers) as well as the identification of the populations present in the sample. Classical mass spectrometry methods are a powerful tool to investigate protein structure but, in the case of amyloids, they are limited to the study of the early steps of the protein self-assembly mechanisms. We show here that charge detection mass spectrometry (CDMS), recently developed for large self-assembled system like viruses, can be used to precisely determine the mass of individual amyloid fibers made of pathological and physiological proteins. The characterization of the heterogeneity of the population is also possible. This method will allow the investigation of the mechanisms of formation of amyloid fibers and could help to get insight into some pathological processes like the strain phenomenon described in the prion-related diseases.

K2. Using multidisciplinary biophysical techniques to unveil protein aggregation mechanisms

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Protein misfolding and aggregation are associated to a variety of diseases, including several neurodegenerative disorders, such as Alzheimer's or Parkinson's diseases. Formation of fibrillar amyloid aggregates is a hallmark of these pathologies. Unveiling the mechanistic details of amyloid formation is crucial to design therapeutic strategies against these disorders and the earliest molecular events occurring during the amyloid aggregation cascade are of very high. Here we show how several biophysical techniques can be combined with a kinetic analysis of initial aggregation rates to decipher the earliest molecular events that lead to nucleation of amyloid structure. We describe the experimental kinetics of aggregation of an SH3 domain, used as a model, as well as aggregation kinetics of amyloid-beta peptides. We analyze how experimental conditions influence the aggregation rates and use simple kinetic models to extract kinetic and thermodynamic parameters characterizing the initial molecular events. Our results indicate that rapid formation of dynamic oligomers seems to be a common seminal event in the formation of more stable oligomers and aggregates that can nucleate amyloid fibrils and may also be responsible for the generation of cytotoxic species observed early during the fibrillation process. Targeting these initial oligomerization events may be an interesting approach to treat or prevent amyloidosis.

K4. Amyloidosis: taking advantage of the specific structural features of amyloid fibers for the design of diagnostic

Jonathan Pansieri[1], Christel Marquette[1], Vincent Forge[1]

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Amyloidosis' diseases remain a considerable clinical challenge due to their variable existing forms and involvement in different organs and tissues, and therefore they are often misdiagnosed or diagnosed very late. However, recent advances on important aspects of amyloid-related pathogenesis, and developments in their diagnosis, monitoring, and treatment, have greatly improved outcomes. A hallmark of these diseases is the accumulation of amyloid deposits due to the self-aggregation of misfolded proteins into amyloid fibers. Each disease is associated to particular proteins: the Alzheimer disease to Aβ(1-42) and tau, the Parkinson disease to α-synuclein, the type II diabetes mellitus to amylin, the familial polyneuropathy to Val30Met mutated transthyretin for instance. We propose a new strategy for the early diagnostic of amyloidosis based on multimodal nanoparticles targeted toward amyloid deposits. The multimodal nanoparticles allow various sensitive imaging technics (fluorescence, PET or MRI). Two types of targeting have been investigated: i) generic ones using either the Pittsburgh compound B or a nanobody, and ii) specific ones with peptides whose design is based on amyloid fiber structures. The last type should allow to identify the protein involved in the amyloid deposits and, hence, to identify the disease. These nanoparticles have been tested on three different amyloid fibrils, made of Aβ(1-42) (Alzheimer's disease), amylin (type II diabetes mellitus), or mutated Val30Met transthyretin (familial polyneuropathy). The amyloid recognition properties of these targeted nanoparticles have been investigated both in vitro on amyloid fibers prepared with recombinant proteins and ex vivo on pathological tissues from mice models.

K5. Quality control of purified proteins to improve research data reproducibility: improving the time-efficiency and quality of your results

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In this presentation I will introduce the ARBRE (Association of Resources for Biophysical Research in Europe) network and the associated COST Action CA15126, termed MOBIEU (Molecular Biophysics in Europe). ARBRE was launched in June 2014 as on open pan-European initiative to gather scientists active in the field of molecular-scale biophysics. This has been consolidated in 2016 with a successful COST application dedicated to “Integrating Molecular Biophysics Approaches for Biology and Healthcare”. In particular, I will focus on the activities of WG 4, which is dedicated to optimization of the data quality. As reported recently in Nature [1], there is a real concern in the scientific community about the problem of irreproducible results. In this context, the objective of WG4 is to establish good laboratory practices and improved standard operation procedures (SOPs), which can be applied within and beyond the MOBIEU community. Thus, in close collaboration with members of another informal network, i.e. Protein Production and Purification Partnership in Europe (P4EU), ARBRE-MOBIEU has produced a joint initiative on recombinant protein quality. We aim to develop a minimal reporting standard/best practice for the quality control of recombinant proteins to ensure that the input material used in biological, biophysical and biochemical research is of high quality. This condition, in turn, will result in more reliable and reproducible final data. The prescribed tests must be simple to perform using standard laboratory equipment, while still producing data acceptable as admission criteria for biophysical or structural biology labs. We have listed some recommendations for what we propose as (i) minimal information, (ii) minimal quality control parameters and (iii) extended quality control parameters/standards.

I1. Signaling via Oligomers of Receptors and G Proteins Detected by Single-Molecule Fluorescence

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Uncertainty over the mechanism of signaling via G protein-coupled receptors (GPCRs) relates in part to questions regarding their supramolecular structure. GPCRs and heterotrimeric G proteins are known to couple as monomers under various conditions. Many GPCRs are known to form oligomers under many of the same conditions, however, and the biological role of those complexes is unclear. We have used dual-color fluorescence spectroscopy (dcFCS) and single-particle photobleaching to identify and characterize oligomers of the M_2 muscarinic receptor and of G_{i1} in purified preparations and live CHO cells. The photobleaching patterns of eGFP-M_2 were indicative of a tetramer and unaffected by muscarinic ligands; those of eGFP-G_{i1} were indicative of a hexamer and unaffected by GTP. A complex of M_2R and G_{i1} was tetrameric in both, and activation by a full agonist plus GTP reduced the oligomeric size of G_{i1} without affecting that of the receptor.

Measurements on differently tagged receptors and G proteins (M_2-mCherry and eGFP-G_{i1}) in live cells detected significant cross-correlations only in the presence of an agonist, which therefore promoted coupling of the receptor and G protein. The agonist-promoted coupling was retained when a fluorophore-tagged receptor lacking the ligand-binding site was co-expressed with the wild-type receptor and tagged G_{i1} (M_2(D103A)-mCherry, wt-M_2, and eGFP-G_{i1}), indicating that the ligand acted via an oligomeric receptor. Our results point to a model in which an agonist promotes transient coupling of otherwise independent oligomers of the M_2 receptor on the one hand and of G_{i1} on the other, and that an activated complex leads to a reduction in the oligomeric size of the G protein. They suggest that GPCR-mediated signaling proceeds, at least in part, via oligomers.

O1. Changes In Lysozyme's II-Structure As A Result Of Its Interaction With A Gold Surface – A Crucial Step For Alzheimer's Disease Mystery Solving

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The causes of neurodegenerative diseases like Alzheimer and Parkinson are still unknown. One of the hypothesis combines the development of the Alzheimer's disease with formation of lysozyme's aggregates. In this work, the adsorption of lysozyme onto the gold surface under different conditions of pH, ionic strength and concentration was investigated using optical method – Multi Parameter Surface Plasmon Resonance (MP-SPR) and mechanical method – Quartz Crystal Microbalance (QCM-D). Experimental data shows that maximum adsorption efficiency was obtained at the pH=10, which corresponds to lysozyme's isoelectric point. Comparing results from MP-SPR and QCM-D methods allow to calculate the hydration level of lysozyme's layer. Structure of lysozyme's layer onto the gold surface was estimated according to Random Sequential Adsorption (RSA) model. The hydrophilic nature of lysozyme was assessed by contact angle measurements (CA). They show that lysozyme's hydrophilicity increases with surface coverage and ionic strength of solutions. The stability of lysozyme's conformation was examined using Polarization-Modulation Infrared Reflection Absorption-Spectroscopy (PM-IRRAS) method. Analysis of the PM-IRRAS data shows that the interaction between lysozyme and the gold surface caused changes in its II-structure in comparison with conformation in solution obtained from Circular Dichroism measurements. Strong misfolding of lysozyme's structure was observed in extreme pH conditions (4 and 9). This strong changes in lysozyme's II-structure are linked to formation of aggregates, which are directly connected with Alzheimer's disease.

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Oral Communications

Electrified interfaces and biosensing

K3. Molecular Recognition - Versatility and Challenges in the Design of Biosensors

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The lecture will illustrates the practical applications of surface modification of electrochemical and SAW sensors, focusing on layer-by-layer assembly and thiol-driven self-assembly and sol-gel chemistry, grafting chemistries including click chemistry and practical applications from environmental and biomedical analysis areas.

Biosensor technology represents an extremely wide field with an increased interest for application in food and agriculture industries. The aim of our work is to emphasis the biosensing methods as emerging analytical tools for detecting mycotoxins in food matrices, as feasible and promising alternatives to classical analytical methods [1]. Affinity sensors built-up on gold surfaces are probably the most versatile platforms for real time monitoring of biomolecular events and detection of structurally complex analytes through molecular recognition. Due to their inherent properties, thin gold films uphold tunable 1D, 2D and 3D scaffolds of alkylthiols or peptides in a variety of immobilization formats. Our research group has focused on developing multifunctional supports for a mycotoxins detection which can be used with electrochemical [2], SPR [3] and SAW [4] transducers. In this context, we optimized alkylthiolated supports for SPR and SAW transducers for the direct detection Aflatoxin B1-protein bioconjugates in serum samples and redox peptide SAMs for direct antibody detection through voltammetric measurements. The achievements were extending for developing affinity formats for the indirect detection of low molecular weight analytes.

K6. Bioelectrochemical Monitoring: The Challenges of Clinical Adaptation

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Bioelectrochemical sensors have secured an exceptional niche in Medical Point of Care testing. However, there is a critical need to secure controlling interfaces that facilitate a chemistry transduction sequence that is neither affected by cellular and colloid/protein deposition nor by diffusible molecules able to create an additional background responses or to passivate the working electrode surface. Our materials approach for such surface stabilisation has derived mainly from the use of polymeric membranes. These are typically microporoous or homogeneous and designed variously to improve tissue and blood compatibility and to serve as low molecular weight cut-off/ionomeric barriers to reject interferent microsolutes. For continuous operation, surface fouling is a cumulative problem, recalibration difficult and in the case of tissue deployment a serious challenge, given that there is no independent means of verifying tissue concentration. Our barrier membranes include polyurethane, modified polycarbonate and PVC. We have also designed recessed devices to impose additional diffusional restrictions on macromolecules. Monitoring of glucose, lactate and O_2 will be presented, and a planar system for sweat ions and lactate described based on PEDOT:PSS as solid electrolyte, together with a smart textile ISE variant. More generally, the mix of polymeric materials and bioelectrochemical sensors is set to enhance clinical care through more reliable patient surveillance but requires materials science input.

I2. Interrogation of biomolecular structure at nanoscale

Tudor Luchian[1], Alina Asandei[1], Irina Schiopu[1], Andrei Ciuca[1], Loredana Mereuta[1], Aurelia Apetrei[1], Corina Ciobanasu[1]

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The nanoscale description of individual biomolecules interaction with, and movement through nanopores, reveals unique physical properties of it, unseen in macroscopic recordings. The working principle of the approach is deceptively simple: biomolecules are driven to (and through) the nanopore by an applied potential difference, and once inside the nanopore they displace a roughly equivalent volume of solvent. Consequently, they induce a reversible change in the ionic electrical current measured across the nanopore. The statistical analysis of such volumetric blockade events in terms of duration and magnitude, provides information regarding the physical and chemical properties of the biomolecules under investigation. In this review we outline several results obtained in our lab, in the attempt to shed light into the physical description of certain biopolymers (e.g., peptides, DNA, PNA, dendrimers), with the a-hemolysin (a-HL) nanopore. We describe an approach to control analyte residence times in a single nanopore, whose proof-of-principle strategy resorted to using polypeptides whose C- and N-termini contained distinct patches of basic and acidic amino acids. With this approach, dubbed by us 'nanopore tweezer', and by employing custom-designed, polycationic peptide-functionalized PNAs, we utilized the a-HL isolated in a lipid membrane as a single-molecule sensor, to detect and investigate the voltage-dependent unzipping of the PNA-DNA duplex. The nanopore tweezer has proven also useful to demonstrate the proof-of-concept enabling primary structure exploration of custom-engineered polypeptides, via discrimination between selected neutral amino acid residues. We investigated the movement of confined dendrimers in nano-spaces smaller than the diameter of dendrimers. The electric force acting on the dendrimer impels the dendrimer to stretch within the nanopore, and beyond a certain threshold, it drives the analyte across the nanopore through regions with smaller physical diameter than the dendrimer, making the approach useful to probe their elastic properties of biomolecules at uni-molecular level.

O2. Flow Injection Analysis System Integrating Electrochemical Sensors For Monitoring The Alcoholic Fermentation Of Wines

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The aim of the study was to develop a flow injection analysis (FIA) system, for monitoring the evolution of glucose and total phenols concentrations during the alcoholic fermentation of wines. A commercial biosensor consisting in a screen-printed carbon electrode (SPCE) modified with glucose oxidase and $[Fe(CN)_6]^{4-}$ was optimised for glucose detection. The total phenolic concentration (TFC) was measured with a SPCE modified with multi walled carbon nanotubes (MWCNTs). The sensors were integrated in an experimental set-up consisting of a flow-through cell, a peristaltic pump, an injection valve, and a computer-controlled potentiostat. The glucose biosensor was polarised at -0.025 V (vs. Ag/AgCl) and required a running buffer enriched with $[Fe(CN)_6]^{4-}$ to ensure stable and interference free measurements. In these conditions, the glucose sensor was usable for up to 5 days and had a linear range from 0.06 to 1 mM. Moreover, the determined glucose concentrations were similar to those obtained by the official method of the International Vine and Wine Organisation. The electrode for TFC was polarized at 1.0 V and required an acid running buffer. In these conditions, the MWCNT-modified electrode reported TFC values which were highly correlated but smaller that the TFC values obtained by the Folin Ciocalteu test. The FIA system was successfully applied for monitoring the fermentation of red wines, moreover the concept was also transferred into an automated system for monitoring an industrial fermentation process. While the SPCE-based sensors have adequate analytical characteristics and stability, further optimization is ongoing to eliminate the need of added mediator in glucose sensing, and to determine the origin of the differences between the electrochemical detection of TFC and the classic Folin Ciocalteu method.

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O3. Extracellular pH of cancer cells and normal cells as revealed with a voltammetric pH microsensor

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While it is known that the extracellular pH (pH_e) of cancer cells is different from the pH_e of normal cells, there are not many tools to investigate this difference with high spatial resolution (that is required for revealing cellular heterogeneity). Therefore, we built a voltammetric pH microsensor and then used it to reveal the pH_e gradients developed by adherently growing human colorectal adenocarcinoma cells (HT-29) and human embryonic kidney cells (HEK-293).

The voltammetric pH microsensor was built using a novel graphene-syringaldazine composite as pH-sensitive layer. The small size of the sensor (diameter of the active area of 37 μm) facilitated measuring the pH_e of as few as 4-6 cells. The pH_e gradient developed by these few cells was calculated using a pH value measured close to the cells (~ 28 μm) and a pH value measured far from the cells (~ 528 μm).

It was observed that HT-29 cells develop a wide range of pH gradients (from 0.1 to 0.8 pH units) while HEK-293 cells never develop pH gradients larger than 0.4 pH units. Therefore, the investigated cancer cells are characterized by a metabolic heterogeneity that exceeds that displayed by the investigated normal cells.

O4. Characterization and Evaluation of Biosensor Architectures Incorporating Nanomaterials as Sensitive Tools for Analytical Detection of Glucose

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Nanoparticles based on carbon materials, offer the advantage of an enhanced surface area, increased sensitivity, stability and biocompatibility. They considerably improve the conducting properties of an electrochemical sensing platform, and can lead to real-time response with high selectivity for bioactive compounds detection in medical, food or environmental monitoring. Alongside nanoparticle integration, polymers provide increased sensitivity and specificity.

The layer-by-layer (LbL) method was used to incorporate polymers and carbon based nanoparticles onto electrode surfaces for glucose detection while dispersing glucose oxidase and carbon nanomaterials in the positively-charged chitosan polymer. Bilayer self-assembly was obtained by alternating chitosan with the negatively charged poly(styrene sulfonate). Electrodeposition of PEDOT (poly(3,4-ethylenedioxythiophene)) onto the bare electrode surface, further improved its sensitivity towards glucose detection in wine samples.

Characterization and optimization studies using electrochemical techniques were carried out in order to evaluate biosensor performance. Voltammetry and electrochemical impedance spectroscopy were employed for characterization of the nanostructured architectures, while the analytical properties of the biosensors were determined by fixed potential amperometry. LbL film growth was monitored by surface plasmon resonance and quartz crystal microbalance, in order to evaluate the interactions involved in the assembly of the biomolecules. Scanning electron microscopy revealed the morphological structure.

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O5. Stable NADH Detection with Carbon Nanofibers and Meldola Blue-Modified Electrodes

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The electrochemical detection of NADH provides a sensitive and easy way to determine various substrates of the reactions catalysed by NAD^+- dependent dehydrogenases. Nanomaterial-modified electrodes have advanced the electrochemical oxidation of NADH, furthermore, their combination with electrochemical mediators on screen-printed electrodes enables sensitive, low cost detection of NADH with minimal interferences in real-world samples. In this work we studied several combinations of efficient NADH mediators (Meldola Blue, Methylene Blue, Toluidine Blue O) with commercial screen-printed carbon electrodes, i.e. with mesoporous carbon, modified with single or multi wall carbon nanotubes or modified with carbon nanofibers. The sensors were compared with bare carbon electrodes and with commercial Meldola Blue-modified electrodes. The best sensitivity for NADH detection by amperometry was observed for Meldola Blue/carbon nanofibers electrodes, for which a detection limit of 1.0 μM, a linear range of 5-500 μM and a sensitivity of 13.8 ±1.1 $\mu A.Lmmol^{-1}$ were determined. While this sensitivity was much higher than of corresponding commercial sensors, the mediator gradually desorbed from the electrodes. To enhance sensor stability, Meldola Blue was precipitated by complexing with $[Ni(NH_3)_6]Cl_2$. The sensor was characterized by XPS, SEM and cyclic voltammetry and its stability upon repetitive calibrations by amperometry was checked both in batch and in flow injection analysis setups. Furthermore, the NADH detector was coupled with a new NAD^+-dependent aldehyde dehydrogenase from a psychrophile bacteria for the analysis of aliphatic and aromatic aldehydes, i.e. acetaldehyde and benzaldehyde.

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O6. Evaluation of Nanozyme Sensors for the Detection of Antioxidant Capacity

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Oxidative stress due to free radicals, which are formed in large quantities in living organisms under certain conditions, plays a major role in many chronic and degenerative disorders. There are plants that contain many antioxidant compounds that can inhibit the oxidation of biomolecules under oxidative stress. The main goal is to allow a quick access to the global antioxidant activity of real samples such as plant extracts. The present study investigates the total antioxidant capacity of hydro-soluble plant extracts having medical properties which were prepared in different forms using two extraction methods and a variety of solvents, each of them having an influence upon the antioxidant capacity of the extract. Nanozyme modified electrochemical sensors, as rapid screening tools, were evaluated and optimized for this purpose. Electrochemical measurements such as cyclic voltammetry, differential pulse voltammetry and amperometric detection were used to evaluate the total antioxidant capacity (TAC) and electrochemical index (EI) of the plant extracts. The results were correlated those obtained with classical and sensitive method of chemiluminescence.

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Oral Communications

Novel materials and biomaterials for analytical methods

K7. Designing multifunctional plasmonic nanoplatforms for applications in nanomedicine

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In this presentation we give an overview of the current approaches in our laboratory to fabricate and functionalize a large variety of plasmonic and hybrid nanostructures with the aim to integrate their spectroscopic, therapeutic and imaging capabilities in nanomedicine. From nanostructured films fabricated using self- or template-assisted assembling methods to chemically synthesized gold or silver nanoparticles of various size and shape (rods, prisms, stars-shaped), we provide both the right optical response for sensing and required biocompatibility to translate them into specific in vitro and in vivo studies. Scanning confocal Raman microscopy combined with dark-field and fluorescence microscopy (manly FLIM) were used to record relevant information about nanoparticle localization, chemical composition and intracellular pH mapping. For instance, a class of biocompatible "optically hot" nanoparticles stabilized by biopolymer coating (chitosan, poly(ethylene) glycol, pluronic, gelatine) were efficiently used for both spectroscopic intracellular imaging via SERS and FLIM and to demonstrate their multimodal activity as nanoprobes, drug delivery carriers and plasmonic-induced hyperthermia agents. In recent years, our research group has provided several "proofs of concept" of therapeutic mechanisms based on plasmon-induced phothotermal therapy (PTT), photodynamic therapy (PDT) and nanochemotherapy. Currently we focus on development of nanoplatforms for enhanced treatment of cancer by synergistically combined multiple NIR light-activated nanotherapies.

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K10. Comparative In Vitro Behaviour of Bioglass Coatings in Simulated Body Media with Improved Biomimicry: Challenging a Paradigm

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Synthetic physiological fluids are currently used as a first in vitro bioactivity assessment for bone grafts. Our understanding about the interactions taking place at the fluid/implant interface has evolved remarkably along the last decade and does not complies with the traditional ISO/FDIS 23317 protocol in purely inorganic simulated body fluid (SBF). The advances in our knowledge point out to the need of a true paradigm shift towards testing physiological fluids with enhanced biomimicry and a better understanding of the materials structure-dissolution behavior. This will contribute to “upgrade” our vision about entire cascade of events taking place at the implant surfaces upon immersion in the testing media or after implantation. Starting from an osteoinductive bioglass (BG) composition with the ability to alleviate the oxidative stress, thin BG films with different degrees of polymerization were deposited onto titanium substrates. Their biomineralization activity in SBF and in a series of new inorganic-organic media with increasing biomimicry that more closely simulate the human intercellular environment was compared. A comprehensive range of advanced characterization tools (scanning electron microscopy; grazing incidence X-ray diffraction; Fourier Transform Infra-red, micro-Raman, energy dispersive, X-ray photoelectron and surface enhanced laser desorption/ionization–time of flight mass spectroscopies; plus, cytocompatibility assays using mesenchymal stem cells) was used. The information gathered can be very useful to biologists, biophysicists, clinicians and material scientists with special interest in teaching and research. By combining all the analyses, we propose herein a step forward towards establishing an improved unified protocol for testing bioactivity of implant materials.

I3. Design of graphene based electrochemical biosensors for biomedical applications

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Among the two-dimensional nanomaterial, graphene has emerged as the most used material for electrode surface modification aiming the elaboration of (bio)sensors for the detection of relevant molecules for biomedical applications. The interest for graphene is mainly due to its special mechanical, optical and electronic properties. Moreover, the arrangement of the sp^2-type carbon atoms in a rigid honeycomb in graphene sheets determines the achievement of a material presenting excellent thermal conductivity and electron transfer capability together with the highest mechanical strength among all materials. The increasingly use of graphene for the development of electrochemical (bio)sensors is due to its high specific surface area and to the ease of its covalent and/or non-covalent functionalization with a wide range of materials, allowing thus the immobilization of a higher number of biomolecules and a remarkable increase of the sensitivity. Several examples of the latest approaches regarding the elaboration and application of the graphene-based electrochemical biosensors in the analysis of drugs and other relevant targets for clinical interest have been summarized and will be presented.

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O7. High Surface Area Flexible Electrodes for Wearable Devices and Actuators

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Flexible electrodes for continuous monitoring possess physiological and biochemical sensing properties, as well as motion sensing capabilities. The field of flexible electrodes is continuously investigated and devices such as flexible printed circuit boards, polymer foils, meshes of microscopic metallic fibers and nanowire networks are currently developed. Such electrode systems are excellent candidates for skin patch sensors for the quantification of biomarkers in biological fluids and can be combined with conductive polymers conferring actuating properties.

In this context, polymeric microscopic meshes and nanowires were obtained by electrospinning. In order to insure a highly conductive path, these nano and microscopic structures were metallized by magnetron sputtering, thermal evaporation or by electrochemical deposition. Two configuration of these conductive fibers are depicted. In the first configuration, the metallized fibers were attached on a flexible support, in order to increase their mechanical strength while maintain flexibility and tested for their capabilities in detecting electrolytes and biomarkers in sweat. In the second configuration, the actuating properties of the free standing metallized fibers coated with a layer of polypyrrole was investigated and their ability to manipulate micro-spheres, as well as to hold and release a piece of copper wire was described.

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O8. Microfluidic Platform for Integrated Plasmonic Dual Detection

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Currently, efficient high-throughput and affordable plasmonic lab-on-chip devices have gathered a lot of attention in the biosensing field of application. Anisotropic gold nanoparticles are known for their unique optical properties[1], which ensure an ultrasensitive and specific detection, and therefore, their controlled integration into microfluidic channels takes the development of such devices one step forward by overcoming significant challenges like sample volume, delivery and alteration[2]. Moreover, the synergy of Localized Surface Plasmon Resonance (LSPR) and Surface Enhanced Raman Spectroscopy (SERS) techniques to detect and identify the analyte of interest inside of a single plasmonic-microfluidic chip, allows the successful implementation of a miniaturized-portable system for real-time biodetection.

Herein, we propose a novel approach to fabricate microfluidic devices with integrated plasmonic transducers to obtain miniaturization, portability and minimizing the analysis time. Specifically, the strategy we apply involves two steps: i) the deposition of gold bipyramid nanoparticles (AuBP) onto a functionalized solid substrate and ii) the integration of the as-fabricated plasmonic substrate into a polydimethylsiloxane microfluidic circuit. The presence of isolated and end-to-end linked AuNP on the substrate was confirmed by SEM and AFM investigations. Then, the LSPR sensitivity of the plasmonic-microfluidic device was evaluated by monitoring the optical responses at refractive index changes proving a bulk sensitivity of 449 RIU/nm for the longitudinal LSPR band and 629 RIU/nm for the band assigned to end-to-end linked nanoparticles. Finally, a much higher electric field generated in the gaps between linked AuBP was subsequently proved by the SERS detection of molecules in continuous flow conditions by loading the analyte into the microfluidic channel *via* syringe pump. In conclusion, our miniaturized portable microfluidic system aims to detect and identify with high specificity and accuracy analyte molecules in laminal flow, providing thus a groundwork for further biosensing applications.

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O24. Novel Photo-responsive Structures for microSensors and microActuators

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The continuing interest in stimuli-responsive materials has yielded quite an expansive variety of smart materials that respond to a wide range of stimuli such as electrical current, pH and light, among others [1]. A subclass of this family is comprised of stimuli-responsive hydrogels that are three-dimensional, hydrophilic, polymer networks capable of large water intake. Incorporation of responsive units in such polymeric networks allows for their use as micro-machines capable of doing mechanical work in response to the chosen stimulus. The application of smart materials offers tangible solutions in the field of actuators for microfluidic valves, artificial muscles and biomimetic robots [2-5].

Moreover, new capabilities such as motility, switchable selective uptake and release of molecular agents, sensing, signalling and seeking, will enable microstructures and micro-vehicles to manifest many of the features of biological entities.

Herein we explore several bioinspired stimuli-responsive microstructures for actuation and sensing. A particular focus will be the emphasis on the important role of light as a means to enable control and interrogate stimuli-responsive materials, and exploration on how these might provide initial building blocks for creating futuristic microsystems.

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O25. Boronic Acids for the Generation of Responsive Hydrogels

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Several approaches currently exist for continuous monitoring of saccharides, however, to this point most sensors have involved the use of electrochemical approaches based on enzymes, such as glucose oxidase.[1] It is widely accepted that a method of continuous monitoring of glucose would prove highly beneficial for diabetes sufferers. The use of boronic acids to bind saccharides has been investigated for many years as a facile means to monitor the concentration of sacharrides in solution [2]. Successful means of translating such optimised responses to complex polymeric matrices have proved significantly more difficult. Such a feat would prove invaluable for diagnostic and self-regulating systems.

Herein we present a family of novel boronic acid derivatives, using an easily-adaptable synthesis. We demonstrate a suite of applications, encompassing self-assembling gels and cross-linked hydrogels, which can bind saccharides and modulate a range of chosen responses. This binding has been probed using a series of different techniques, including optical and impedance spectroscopy. This effect can be exploited within a miniaturised device and monitored using a low-cost photodetector.

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Oral Communications

Medical analysis and diagnosis

K8. Ebola Virus Delta Peptide is a Viroporin

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The Ebola virus (EBOV) genome encodes for a partly conserved, 40-residue, nonstructural polypeptide, called the delta peptide, which is produced in abundance during Ebola virus disease. The function of the delta peptide is unknown, but sequence analysis has suggested that delta peptide could be a viroporin, belonging to a diverse family of membrane-permeabilizing small polypeptides involved in replication and pathogenesis of numerous viruses. Full length and conserved C-terminal delta peptide fragments permeabilize the plasma membranes of nucleated cells of rodent, dog, monkey and human origin, increase ion permeability across confluent cell monolayers and permeabilize synthetic lipid bilayers. Permeabilization activity is completely dependent on the disulfide bond between the two conserved cysteines. The conserved C-terminal portion of the peptide is biochemically stable in human serum, and most serum-stable fragments have full activity. Taken together, the evidence strongly suggests that Ebola virus delta peptide is a viroporin, and may be a novel, targetable aspect of Ebola virus disease pathology.

O9. Protein Carbonyl Electrochemical Detection

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In the past decade, the development of sensor platforms as alternative candidates to classical devices has enabled rapid advances in many analytical fields. Although the biological effects of oxidative stress on living organism it is known for many years there is a high demand on the development of new devices able for fast determination and quantification of these effects [1, 2].

The main lesions induced in proteins by oxidative stress are represented by the chemical modification of oxidizable amino acids residues tyrosine, triptophan, histidine, cysteine and methionine, as well as the formation of carbonyl groups at threonine, proline, arginine and lysine side chain residues.

The electrochemical determination of the protein carbonyl (PC) fraction was performed at a sensor based on immobilization of 2,4 - dinitrophenol hydrazine (DNPH), which covalently binds the carbonyl groups, as the molecular recognition layer. The PC fraction was obtained from the interaction of BSA (bovine serum albumin) with Fenton reagents and the reaction of conjugation with DNPH took place at the room temperature and at the physiological pH.

The voltammetric results showed that the oxidation current of DNPH decreased with the increase of the incubation time due to the formation of the covalent linkage between hydrazine group of DNPH and CP, leading to an electrochemically inactive complex. A detection limit of 126 µg/mL was obtained for an incubation time of 20 s.

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O10. Antimicrobial effects of short tryptophan-and arginine-rich peptide on methicillin-resistant Staphylococcus aureus

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Methicillin-resistant Staphylococcus aureus (MRSA) infections represent the most significant challenge encountered in the management of skin and soft-tissue infections both in hospitals and in community settings [1, 2]. Combined with the lack of new efficient antibiotics, this issue has led to the use of alternative classes of antimicrobial agents like antimicrobial peptides [3, 4].

This study investigated the antibacterial activity of one short tryptophan-and arginine-rich peptide (reported previously in [5]) against 1 Methicillin susceptible Staphylococcus aureus (MSSA) and 9 MRSA strains isolated from skin and soft tissues infections. The peptide exhibited potent antimicrobial activity against Staphylococcus aureus ATCC 25923 reference strain and the 10 clinical isolates at a concentration of 16 µg/mL. The cytotoxicity of the peptide against human skin fibroblast cells was evaluated and half viability concentration (IC_{50}) was found at ~ 520 µg/mL. The therapeutic index was found to be ~32. Atomic force microscopy was used to analyze the effect of peptides on bacterial membrane and biofilm formation. The results show that the peptide has the potential to become a good candidate for topic applications against Staphylococcus aureus, including MRSA.

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O16. IMAGCELL – Assessing living cells natural features by employing optical microscopy and statistical analysis

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The living cells have an intrinsic dynamical behavior. Their surrounding membranes perform correlated movements, even if they are free cells - like bacteria, floating cells – like erythrocytes, or building blocks in living tissues.

To analyze and discriminate the unique features of each living cell, we designed and implemented a protocol which includes a complex statistical analysis of living cells images. In this respect, sequences of optical-microscopy images are processed to assess their “dynamical fingerprints”, and by this to discriminate between normal and affected state.

In this presentation we will show that our method allows the discrimination between normal cells and those affected by variations of the suspension media parameters (temperature, presence/absence of glucose, drugs), assess the effect of antibiotics on pathogenic bacteria, and allows the discrimination between different types of tumoral cells.

Although these investigations are still in the beginning, we think that our protocol holds future promises to make the tissue diagnosis more reliable, cheaper, and most important – faster.

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O17. Human serum expression levels of monocyte chemoattractant protein-1 in type 2 diabetic subjects

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Background - Type 2 diabetes mellitus (T2DM) and obesity are major risk factors for cardiovascular disease. Monocyte chemoattractant protein-1 (MCP-1/CCL2) is one of the chemokine implicated in the etiologies of pathogenesis of cardiovascular disease, obesity and diabetes-related diseases wich have increased a lot during the past years. The enzyme-linked Immunosorbent Assay (ELISA) is one of the used clinical diagnostic tool for the detection and quantification of protein biomarkers.

Objective - The highlights of this paper include the evaluation of MCP-1/CCL2 levels using enzyme-linked immunosorbent assay. The method applies absorption spectrophotometry to measure the absorbance (optical density) of the sample using a monochromatic light source and optical sensor. Methods - We examined three groups: patients with T2DM, T2DM and obesity and healthy volunteers group. Fasting blood samples were collected from each. We designed the study for comparisons between the mentioned groups regarding blood serum MCP-1/CCL2. Thus we also determined glycemia and the blood levels of the following: cholesterol, low-density lipoprotein cholesterol, and triglycerides. Blood serum MCP-1/CCL2 was measured using a commercially available ELISA kit. Results – Compared to the healthy control group MCP-1/CCL2 was elevated in both study groups (T2DM, T2DM and obesity). Moreover, levels of serum glucose, MCP-1/CCL2 and lipid abnormalities were the highest in the T2DM+obesity group. Conclusions – We used the system for MCP1/CCL2 ELISA detection in human serum. The device performs automated analysis of the results and presents absorbance values and diagnostic test results. The present work brings evidence that patients with established T2DM have a different cytokine profile compared to healthy controls and this could indicate changes in the immune function for T2DM patients.

O18. Magneto-mechanical actuation of Fe-Cr-Nb-B magnetic particles for destruction of osteosarcoma cells

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Magnetic particles (MPs) have been lately used in biomedicine as magnetic carriers for drug delivery, thermoseeds for magnetic hyperthermia and, more recently, for their capability to induce apoptosis by mechanical forces [1]. In this work we have studied the effect of mechanical oscillations generated by Fe-Cr-Nb-B MPs introduced in variable magnetic fields (MFs) on osteosarcoma cells. The particles exhibit large magnetic induction, high magnetic susceptibility, and adjustable Curie temperature determined by Cr content [2]. MPs of 40÷200 nm were dispersed in cell culture medium and exposed to a variable MF generated through a special laboratory-made coil system powered by an electronic system which allows application of a time and amplitude variable MF. The results have shown that cellular viability decreases with 25% after the exposure of cells loaded with MPs for 10 min to a 10 Oe MF. Our experiments have shown that cellular viability is influenced by the concentration of MPs in cell culture media, by the time of exposure and by frequency and intensity of the MF applied. When hyperthermia is applied simultaneous with the exposure to MF, the effect of cellular death is amplified. The results highlight the perspective of using magneto-mechanically induced force to selectively kill cancerous cells by itself or associated with hyperthermia.

O19. Cationic Polymers as Drug Delivery Systems

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Gene therapy, which implies the delivery of nucleic acids into cells, has attracted a great interest for more than a decade. Cationic polymers, such as polyethylenimine (PEI), are among the most commonly used non-viral vectors and provide a highly efficient therapeutic method for the transfer of genomic material. This study presents all-atom molecular dynamics simulations of PEI/DNA complexes in explicit solvent. The simulations show the PEI ability to effectively neutralize the charge of the phosphate groups in nucleic acids. This is important in reducing the interactions of the resulting PEI/DNA complexes with the nontarget cells.

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Oral Communications

Microspectroscopy

K9. Fluorescence Micro-spectroscopy Techniques for Probing Protein Association in Living Cells

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Investigations of static or dynamic interactions between proteins or other biological macromolecules in living cells commonly rely on the use of fluorescent tags with one or more colors (or spectral properties). One such method is Förster Resonance Energy Transfer (FRET) Spectrometry, which allows determination of the quaternary structure of biomolecules from cell-level distributions, or spectra of occurrence frequency of FRET efficiencies. Another family of fluorescence-based methods, grouped under the name of fluorescence fluctuation spectroscopy (FFS), includes number and brightness analysis (N&B), fluorescence correlation spectroscopy (FCS) and spatial intensity distribution analysis (SpIDA).

Many investigators often face the dilemma of choosing between simple but rather qualitative analysis of their samples, as provided by FFS, and fully quantitative approaches, such as FRET spectrometry, that may seem too complex either technologically or mathematically. Building on our experience in the development and use of such methods, here we introduce using theoretical arguments and simulations, a new class of micro-spectroscopic techniques. These methods rely on statistical analysis of color mixing in subpopulations of molecules attached to fluorescent tags with different colors to extract association stoichiometry and quaternary structure of macromolecular complexes in living cells.

One of these methods, termed Color-Contrast (CoCo) Spectrometry, relies on statistical analysis of color mixing in subpopulations of fluorescently tagged molecules to probe molecular association stoichiometry. The second method, called FRET-induced Contrast Shift (FiCoS) Spectrometry, exploits the color change induced by FRET to also derive geometric information in addition to stoichiometry. The main appeal of the first method is its simplicity, while that of the second is its ability to provide structural information. These methods are designed to reduce both instrumental and mathematical complexity without sacrificing analytical power.

I4. Near-wall hydrodynamic effects on tethered DNA under shear flow

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We utilized single-molecule tethered particle motion (TPM) spectroscopy, optimized for studying the behavior of short (0.922 mm) dsDNA molecules under shear flow conditions, in the proximity of a wall (surface). These experiments track the individual trajectories through a gold nanobead (40 nm in radius), attached to the loose end of the DNA molecules. Under such circumstances, local interactions with the wall become more pronounced, manifested through hydrodynamic interactions. To elucidate the mechanical mechanism that affects the statistics of the molecular trajectories of the tethered molecules, we estimate the resting diffusion coefficient of our system. Using this value and our measured data, we calculate the orthogonal distance of the extended DNA molecules from the surface. This calculation considers the hydrodynamic drag effect that emerges from the proximity of the molecule to the surface, using the Faxén correction factors. Our finding enables the construction of a scenario according to which the tension along the chain builds up with the applied shear force, driving the loose end of the DNA molecule away from the wall. With the extension from the wall, the characteristic times of the system decrease by three orders of magnitude, while the drag coefficients decay to a plateau value that indicates that the molecule still experiences hydrodynamic effects due to its proximity to the wall.

O11. Translation of SERS Technique to Hydrobiology: Use of Metallic Plasmonic Nanoparticles to Quench Fluorescence in Raman Spectroscopy Analysis of Natural Fluids

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Raw hydrobiological samples, especially fluids and liquids coming from nature exhibit a nuisance fluorescing effect when excited with visible laser lines in blue-green range of the electromagnetic spectrum. This effect may arise from a wide variety of molecules contained in natural aquatic ecosystems, and can be so pronounced, that it effectively covers actual Raman spectroscopy signal. Here we present several examples of quenching the fluorescence effect by silver nanoparticles (AgNPs) in three kinds of natural liquid samples, which allowed recording of meaningful surface enhanced Raman scattering (SERS) spectra. (1) The coelomic fluid of sea urchins represents a very complex bodily fluid. We recently suggested that coelomic fluid could be an important indicator for tracking changes in the marine ecosystem of the sea urchin (Nekvapil et al., 2018). (2) Ethanol extract of green algae contains mainly chlorophylls and carotenoid pigments, and finally, (3) we consider natural spring mineral waters. All these kinds of samples exhibit strong fluorescence when conventional Raman spectroscopy of them is aimed. Upon addition of these samples to AgNPs in certain, well investigated ratios, fluorescence is quenched, and Raman bands are enhanced through SERS effect. As a result, clear bands assigned to chlorophyll, carotenoid or quinone pigments are observed, respectively. These examples extend the applications of Raman spectroscopy to in basic and applied aquatic biology and ecology research.

Reference:

Nekvapil, F., Tomšić, S., Cintă Pinzaru, S. Comparative Raman spectroscopy study of the coelomic fluid of grazing sea urchins and their native seawater: prospect for a potential indicator of environmental aggression. In: Şerban, G. et al. (Eds.) Air and water components of the environment. Babeș-Bolyai University, 2018, ISSN: 2067-743, p. 27 – 34.

Oral Communications

Analytical methods for (nano)biotechnology

O12. Synthesis and technological innovation of Fe_3O_4 nanomaterial applied in wastewater treatment by flotation

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In the wastewater treatment by flotation technique, nanoparticles may act as surfactant molecules, being incorporated into surfactant-stabililised foams for several years. In the scientific literature exist studies which present the capacity of nanoparticles to act as foams/emulsion stabilizers. The stability and the formation of foams are dependent of the particles size, surfactant type and concentration.

In this study was investigated the application of magnetite (Fe_3O_4) nanomaterial in flotation and the experiments consisted in testing it for the removal of pollutants such as oil from wastewater. Fe_3O_4 nanomaterials were prepared by coprecipitation and, respectively, forced hydrolysis method. Before testing their application in wastewater treatment by flotation, both oxides nanomaterials were structural and morphological characterized by XRD, SEM and TEM analyses. In order to evaluate their potential of application in oil removal from wastewater by flotation were studied the following parameters: repartition coefficient, purification factor and separation efficiency. Moreover, the flotation efficiency was investigated by measuring the maximum froth height at equilibrium.

O13. Multiparameter Study of Cultured Cell Behavior Modified by Nanoparticles

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There is a continuous interest in nanoparticle-based bio-compatible materials as efficient vehicles for drug delivery systems and their interactions with live organisms at cellular level. To mimique live conditions without interfering with the cells, label-free techniques were paired with standard tests for evaluating the cellular proliferation. Real-time impedance based assay is a non-invasive method of quantification of cultured cells growth in an adherent physiological state using dedicated plates with gold electrodes embedded in well's bottom. We correlated xCELLigence RTCA system with microscopic imaging, formazan-based metabolic and endocytosis assays to evaluate the effects of several categories of inorganic nanoparticles (NPs) (MCM-41and SBA 15 mesostructured silica and six samples of mesoporous titania) on culture cells (NIH 3T3 murine fibroblasts, CaCo2 human adenocarcinoma, B16F10 murine melanoma). To indicate the molecular pathway used by NPs to access the cell cytoplasm, two endocytosis inhibitors (filipin III and chlorpromazine) were used. The cytotoxic effect of NPs was evaluated by continuous monitoring (days) of the cells incubated with various concentrations of NPs in the presence or absence of endocytosis inhibitors. Data analysis depended on the cell line and NPs-type. RTCA helped differentiate between concentrations of filipin III/chlorpromazine, which do not harm the cells, but exert an inhibitory effect on endocytosis. Their addition improved the cell proliferation despite de NPs high concentration, which was a direct proof of their endocytotic uptake mechanism. An apparent stimulating effect of titania NPs, showed by the metabolic viability tests, has been discussed differently when RTCA method has been employed. The functionalized NPs had various effects on benign versus malign cells. Impedance-based method provides an advantage over standard end-point methods for studying cellular viability offering the possibility of direct analysis of the interaction between NPs with various cells.

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O14. Volumetric Quantitative Analysis of Pure Ascorbic Acid in Tablets

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Ascorbic acid is a water soluble vitamin with significant antioxidant action, that plays an important role in protecting human body from infection and disease. It is acquired from dietary sources only, primarily fresh fruits and vegetables. The main goal of this study was to exactly quantify pure ascorbic acid in tablets of two pharmaceuticals. Proposed objective consisted in improvement and application of a iodometric titration method for ascorbic acid quantitative analysis. Following the appropriate standardization of the iodine (I_2) 0.1 N solution by titration on a calibrated 0.1 N sodium thiosulphate ($Na_2S_2O_3$), the volumetric quantitative determination of ascorbic acid coming from two different pharmaceutical products was performed. Obtained results, which were the same for both pharmaceuticals, showed that average percentage concentration of pure ascorbic acid calculated in vitamin C tablet was 96.58%. Ascorbic acid content per tablet in both pharmaceuticals was 173.84 mg, very close to stated amount of active substance (180 mg). Permissible percentage deviation from declared content of pure active substance was only 3.42%, below maximum of ± 5% imposed by Romanian Pharmacopoeia, 10-th Edition and European Pharmacopoeia, 9-th Edition. Statistical analysis confirmed experimental results and contained very small Standard Error values SE = 0.214476, Confidence Level (95.0 %) = 0.551328, Standard Deviation SD = 0.525357 and P value = 7.44×10^{-6} , ranging from normal limits. Relative Standard Deviation (Coefficient of variation or homogeneity) RSD = 26.268% was situated below maximum permissible value of 30-35%. The iodometric performed method can be successfully applied in quantitative pure ascorbic acid analysis from different types of fruits, vegetables, juices. and various brands of vitamin tablets samples.

Acknowledgments. This study is simply a scientific research paper that does not aim to confirm or deny the official results of pharmaceutical manufacturing companies nor to cause any image damage.

O15. Selenium Nanoparticles – Premises For Their Therapeutic Use In Pathologies Related To Oxidative Stress

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Pathologies are usually associated with an increase of the oxidative stress status. Oxidative stress results as an imbalance between pro oxidants and antioxidants favouring the first. Oxidative stress may be a triggering cause for certain diseases, but it can also set as a consequence that brings numerous physiological and particularly biochemical damage. Thus, reducing the oxidative stress represents a chronic disease prevention strategy as well as a limitative one if referring to its harmfulness. There are several techniques and compounds that may diminish free radicals generation and impact, the responsible chemical species for altering most of the biomolecules when oxidative stress occurs. Among these, nanoparticles are an intensively studied field. Most of the nanoparticles are used as carriers for antioxidants, but selenium nanoparticles (SeNPs) stand out for being antioxidants themselves. The synthesis material and method put an important fingerprint on the dynamics of these entities inside the animal and human body. Their antioxidant behaviour is correlated with an antidiabetic and anti-inflammatory effect as well. Interestingly, in certain cancer cells (HEP G2, HMC, HDF, HNSCC), SeNPs exhibit specific antitumour properties. Apart from these benefits, studies also showed antimicrobial features for these particles, such as antiviral, antibacterial, antifungal and several applications are already available for use. Their toxicological profile did not gather data that would hinder the use as a drug treatment. This study presents the in vivo and *in vitr*o beneficial effects of the SeNPs, that encourage the hypothesis of their multipurpose therapeutic use. Despite these, our experiments didn't confirm the antioxidant effect. SeNPs resulted from a chemogenic synthesis, with 100-140 nm diameter proved no antioxidant or protective effect on MRC-5 and HPF cells. Yet, other methods should be explored (e.g.: biogenic) in order to obtain SeNPs with antioxidant effect and consequently therapeutically active in metabolic diseases.

Oral Communications

Analytical methods for medical physics

I5. Spectral CT with a Medipix detector for Biomedical Applications

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The hybrid pixel detectors based on a Medipix readout chip have revolutionized the radiation imaging during the last decade. They possess a number of novel features, like single photon counting, photon energy resolution and possibility to use high-Z sensor materials. These features allow not only to obtain the low noise X-ray image of excellent quality, but also to use spectral information for material decomposition. A review of the method of spectral CT using a Medipix detector will be given. The results obtained by the JINR group in the field of spectral CT using a Medipix detector with GaAs:Cr sensor will be presented. The possibility of material decomposition based on the dependence of the linear attenuation coefficient on energy will be demonstrated. It will be shown that pre-segmentation of reconstructed data allows improving the quality and accuracy of quantitative measurements. The possible use of spectral CT technique for biomedical applications will be discussed.

O20. Potential of non-invasive quantitative holographic imaging in evaluation of malignancy and treatment efficiency of melanoma cells

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Digital Holographic Microscopy (DHM) offers the possibility of real time visualisation of living cells, allowing to monitor the cell status during dynamic processes like cell cycle or following the action of various stimuli, such as electric fields. Cellular refractive index and shape related characteristics may be recorded with high resolution from a single exposure without chemical staining, revealing subtle dissimilarities between cells with different pathological status.

We used a DHM experimental set-up in off-axis configuration to study the metastatic potential (MP) of B16F10 cells (a murine cellular model of melanoma) and their behaviour under the action of a train of electric pulses specific for electrochemotherapy (ECT).

Cell response was monitored seconds and minutes after electric pulse application with two types of cell parameters: those addressing a specifically defined area of the cell (refractive index and cell height) and global parameters (projected area, optical phase shift profile and dry mass). Both categories of parameters showed biphasic behaviour related to the transmembranar water dynamics and membrane resealing after the application of electric pulses.

The B16F10 cells were compared to B16F1 subline, characterized by a lower MP. The optical characteristics (refractive index, dry mass density and distribution of phase shift in reconstructed quantitative phase images analyzed with Sarle's bimodality coefficient) were found statistically different for the two sublines. F10 have higher refractive index and lower dry mass density than F1 cells. Histograms of phase shift distribution were unimodal for F10 and bimodal for F1 cells. We propose this optical signature as a label-free complex of biomarkers for estimation of cells MP.

O21. The effect of cholesterol and/or melatonin on the amyloid-β peptidesloaded model membranes

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Alzheimer's disease (AD) is a devastating neurodegenerative disease characterized by dementia and memory loss for which no cure or effective prevention is currently available. One of the hallmarks of AD is the formation of senile plaques, primarily consisting of amyloid-beta (Ab) peptides. The crucial role in this process is thought to be imparted by peptide-membrane interactions, modulated by membrane composition. Changes to the structural properties of membrane are known to be accompanied also by the changes in membrane physico-chemical properties. The cholesterol increases the order of lipid hydrocarbon chains and increases the stiffness of membrane. On the other hand, melatonin was found to increase the fluidity of membrane and counteracted the effect of cholesterol. Our previous experiments [1] revealed the counteracting effect of melatonin to that of cholesterol in neat lipid membranes. We have extended our investigations recently by including transmembrane Ab peptide in these model membranes. Small angle neutron diffraction measured at four different contrast conditions was utilized for a determination of structure in transversal direction. The obtained bilayer structure reflected the elevated amounts of cholesterol by its thickening, while the fluidizing effect of melatonin evoked the membrane thinning. However, the resulting effects on the overall thickness of membrane in the case of both cholesterol and/or melatonin seem to be suppressed in the presence of peptide. This confirm the crucial role of Ab in the onset of Alzheimer's disease [2].

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2. A. Martel, et al. JACS 139, 137-148 (2017).

O22. Low Cost Electrical Muscle Stimulator (EMS) Tested with Biopac

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The present paper is aimed towards creating a low-cost electrical muscle stimulation device and monitoring the muscle activity using high performance electromyography device, BIOPAC.

The electrical muscle stimulator is essentially an electronic device which has the ability to contract the muscles via electrical current sent to the electrodes. The power of the device is provided by a 9 V battery, which ensures the portability of the device. The electrical muscle stimulation is provided mainly by two timers that are designed to carry electrical impulses and count them, a transformer, a LED that monitors the transmission of the impulse and three potentiometers which are used to change the length, the duration and the amplitude of the impulse that will be sent to the muscle via electrodes. This type of electronic device addresses patients with cervical spine pain, to increase muscle strength, warming and relaxation. By using this EMS device in certain pathologies of the neck, the patients are able to relieve neck pain without using medication.

Biopac is used for monitoring differences between a natural and an electrical stimulated contraction.

O23. Static Analysis of the human body balance following an induced vertigo

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This paper is aimed towards a static evaluation of the human body balance, on a force platform such as Kistler platform, following an induced vertigo by spinning the subject.

Vertigo is the feeling of spinning even when the person stays in place. The environment seems to move vertically or horizontally. Some people feel like they're spinning. The effect may be easy or hardly noticeable, or it may be so severe that the subject may fall to the ground.

Vertigo is more severe than dizziness, described as a slight uncertainty in orthostatic position.

Dizziness can make the movement difficult, as the feeling of rotation affects the balance.

The recorded values were acquired at a frequency of 100Hz for 30 seconds, which led to the recording of 3000 values for every different parameter.

A specialized numerical analysis software, IDL (Interactive Data Language), was used for the realization of the graphs and the statistical analysis of the results obtained on the Kistler force platform.

Oral Communications

Atomic and nuclear methods

I6. Neutron Scattering Methods in Characterization of Pharmacological Systems

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The dual properties of particle and wave, zero electric charge, magnetic dipole moment, large rest mass, and isotope - specific scattering, make neutrons very attractive and effective tool for determining the structure and dynamics of condensed matter. In the addition to typical utilization of neutron scattering in hard condensed matter studies, it finds its special role also in soft matter investigations, and those of pharmacological systems in particular. One of the underlying reasons is a unique ability of neutron to be scattered by the objects of interest in both the elastic and inelastic way.

The elastic neutron scattering covers a process in which the energy, or equivalently the wavelength of neutron does not change as a result of its interaction with the target nuclei. Neutron techniques in this category comprise small-angle scattering (SANS), ultra-SANS, reflectometry, and powder diffraction. These techniques provide information about structures ranging from the sub-Angstrom (<10-10m) to supra-micron sizes (>10-5 m).

Inelastic neutron scattering, on the other hand, involves the energy change as a result of scattering event in which the neutron may lose or gain energy by imparting energy to or from the sample, respectively. These techniques provide information on dynamics spanning a broad temporal range that is covered by vibrational spectroscopy (~10-14s), quasielastic neutron scattering (~10-13-~10-9 s), and spin echo spectroscopy (down to ~10-7 s).

In the lecture, I will present main neutron scattering methods used in the investigations of pharmacological systems. Some examples of scientific results achieved on facilities of the IBR-2 reactor will be discussed in more details.

O26. Investigation of Spatio-Temporal Atmospheric Deposition of Cd and Pb in Romania Using Moss Biomonitoring

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In this investigation, data derived from moss surveys conducted in Romania in 2010 and 2015 about concentrations of Cd and Pb in moss samples, were compiled. The obtained data in both surveys were statistically processed and the spatial distribution maps of factor scores based on elemental concentrations together with the spatial distribution maps of heavy metals in moss were drawn. The site specific temporal trends for Cd and Pb were observed between the two moss surveys. The data sets from both moss surveys indicate, in the case of mean concentration, a decrease of concentrations in moss: from 2 mg/kg to 0.48 mg/kg for Cd and from 30.63 mg/kg to 5.51 mg/kg for Pb.

Poster Communications

Biophysical methods in the study of protein folding, misfolding and assembly

P Bp 1. Characterization of Some Seed Extracts by Using Isotopic Dilution-Gas Chromatography-Mass Spectrometry

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The phytochemicals from fruis and vegetables have health benefits to lower the risk for the development of health problems. Their contribution is of interest for protection against cardiovascular diseases, cancer, diabetes, obesity, constipation. The aim of this study was to compare the content of amino acids and metals and the antioxidant activity of different seeds used as food supplements. Isotopic dilution -gas chromatography coupled with mass spectrometry (ID-GC-MS) was applied for quantitative determination of free amino acids of some seed extracts (e.g. linseed, poppy, grape, hemp, nuts, pumpkin, sesame, watermelon, chia, etc). Good linearity results for amino acids were found, the regression coefficient beeing over 0.99 for the majority of analyzed amino acids.

The antioxidant attributes of the seed's extracts were evaluated using DPPH (1,1-diphenyl-2-picrylhydrazyl) free radical scavenging antioxidant assays. The study characterized the variation of the free amino acids and essential amino acids within the different samples associated with their essential and toxic elements content and antioxidant capacity. The amino acids, minerals and metals content and antioxidant properties proved their nutritional quality to be used as food supplements.

P Bp 2. Molecular Adaptations to Low Temperatures of Cold-Active Microbial Catalysts

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Psychrophilic bacteria, extremophiles that thrive at low temperatures, contain enzymes adapted to function in cold environments. NAD^+-dependent aldehyde dehydrogenase (F-ALDH) from Flavobacterium PL02, an Antarctic isolated bacterial strain, and the aspartate transcarbamoylase (ATC) from Glaciibacter superstes originating from an Alaska ice brine were investigated as catalyst in biosensing and cold adaptation biomarker, respectively. The protein sequence of these cold-active enzymes is homologous to corresponding proteins from other psychrophlic and psychrotrophic bacteria. Structural analysis revealed in both cases a specific aminoacid composition favouring the protein flexibility under low temperatures such as the reduced number of cysteine residues. 3D modelling indicated insertions of loop-motifs both at subunit interfaces and at the C-terminus, providing enzyme flexibility to performed catalysis at near freezing temperatures. Hydrophobic core analysis revealed the distribution of reduced hydrophobic cores as compared to mesophilic and thermophilic counterparts related to protein stability. Cloning and functional characterization of F-ALDH expressed in E. coli provided a stable and active catalyst for aldehyde oxidation at temperatures as low as 4ºC, capable of using a series of aliphatic and aromatic substrates, providing a valuable biocomponent for cold-active biosensors for wine, cosmetics and food industries. The quantitative response of G. superstes ATC exposed to heat-shock cycles as a model experiment for microbial response to environmental changes indicated this cold-adapted enzyme as a valuable marker for bacterial resilience.

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P Bp 3. Readout of Small Peptides Primary Structure, with a Protein Nanopore

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One of the current challenges in modern proteomics is the application of nanopore technology to peptides and proteins identification and sequencing. To date, protein nanopores were successfully used to studying conformational changes of proteins, DNA sequencing, reveal post-translational modification of proteins, and to estimate the shape, volume, charge, rotational diffusion coefficient and dipole moment of individual proteins. Herein, we set to investigate the possibility of discrimination between neutral amino acid residues from the primary structure of 30 amino acids long, custom-engineered peptides, through the analysis of ionic current fluctuations ensued by pepide’s slowed-down translocation across a single α-hemolysin (α-HL) nanopore. We found that the transient presence inside the α-HL of alanine, tryptophan or serine residues from the primary sequence of peptides, resulted in distinct features of the fluctuations associated to the peptide-induced, reversible blockade of the ionic current through nanopore. We proposed that the α-HL sensitivity to the molecular exclusion at the most constricted region mediates ionic current blockade events correlated with the volumes that are occluded by at least three alanine or serine or tryptophan residues, and provides the specificity needed to discriminate between groups of neutral amino acids.

Reference:

Alina Asandei, Aldo E. Rossini, Mauro Chinappi, Yoonkyung Park, Tudor Luchian, Protein Nanopore-Based Discrimination between Selected Neutral Amino Acids from Polypeptides, **Langmuir**, 2017, 33 (50), 14451–14459

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P Bp 4. Adaptation of a CRISPR Interference Method for Probing Chromatin Properties of Repressor Domains

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Transcriptional repressors are involved in chromatin modification through binding to cofactors and modifiers and in this way regulate gene expression and cell differentiation. These regulatory mechanisms early in eukaryotic development are critical for the maturation of the embryo, yet the mechanism of action of many repressors remains to be fully elucidated. Taking a genome-wide approach to studying repressor activity sheds light on the large body of binding sites of corepressors such as Retinoblastoma, Groucho, and CtBP, as well as DNA binding repressors such as Knirps and Hairy. However, binding events seen in Chromatin Immunoprecipitation (ChIP) and other genome-wide studies do not always correlate with direct transcriptional repression by these corepressors. Repressors and corepressors often bind thousands of sites but only induce transcriptional effects at a small fraction of associated genes. The specific developmental stage, chromatin environment, or associated basal transcription machinery can influence the effectiveness of repressors and corepressors in ways that still need to be further explored. In order to uncover the mechanisms of transcriptional control and the physiological importance of repressor binding to DNA in the context of development, we are engineering a vector fusing a nuclease dead Cas9 enzyme to a repressor domain to direct it to various genomic targets via the recruitment of gene-specific single guide RNAs. We will couple dCas9 repression with RNA-seq data to identify relevant and specific targets - a method that can help us interpret the many binding events seen in ChIP-seq experiments. This adapted CRISPR interference method will allow for comparative analysis of repression pathways in eukaryotes and show how genomic, temporal, and tissue-specific contexts impact corepressors. Furthermore, it will give us insight into the progression of cancers arising from the misregulation of these fundamental pathways.

P Bp 5. Structural Features and Aggregation of NRas Proteins and it's Oncogenic Mutations

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Ras proteins (HRas, NRas and KRas) belong to a class of GTPase proteins that are expressed in all mammalian cells. These switch proteins constitute essential components of the signal transduction processes. Hence, normal cycle between an inactive GDP-bound state and an active GTP-bound state is highly affected by the presence of oncogenic mutations. Permanent alterations in Ras genes of the nucleotide sequence are detected in ∼25% of human cancers.

The role of cancer-associated point mutations in NRas was studied using molecular dynamics simulations. Atomistic models were used to study the wild-type and mutated (G12V) protein interaction with cellular membrane. In order to characterize the mechanism of aggregation, semi-atomistic coarse-grained simulations were performed.

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Poster Communications

In-silico methods

P Si 1. Use of Molecular Docking as a Tool for Comparative Binding Analysis of Large Peptides to Ras Wild Type and Oncogenic Proteins

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Ras proteins are key factors in the signal transduction pathway which regulates cell growth and proliferation. In order to such a signal to be sent, a Ras protein cluster formation is necessary, usually including a small number of proteins. Their mutations are responsible for the formation of much larger – and sometimes permanent - clusters, which may be associated with a continuous signal for cell proliferation. In fact, their mutations are responsible for over 85% of specific cancers, and occur in 15-30% of all cancers.

Although several approaches were tested to date, only little success in Ras-caused cancer therapeutics was attained. Here we propose an alternative computer-based approach to find peptides that would disrupt oncogenic Ras association.

In this respect, we performed molecular docking analysis to find possible specific interactions of peptides to Ras. We selected over 400 peptides from PepBank with sizes between five and fifteen amino-acids. Evaluating parameters such as: (i) peptide-protein complex geometry, (ii) binding strength and (iii) peptide binding site, we identified a few peptides that bind differently to specific sites in wild type and oncogenic mutated protein.

We consider that these peptides hold high promises in disrupting large Ras clusters formation. However, the molecular docking method only refers to interactions that occur in vacuum. In this respect, the peptides need to be further subjected to other computational methods to assess their effect in more complex systems, i.e. with membrane, water and ions found in the live cell environment.

Acknowledgments: We would like to acknowledge the financial support from UEFISCDI grant PN-II-RU-TE-2014-4-2418.

P Si 2. In silico studies on the dynamics and energetics of histidine-modulated arginine- and tryptophan-based peptides in membrane models

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Antimicrobial peptides (AMPs) are short sequences of aminoacids used as defense mechanism against foreign bodies. The selectivity of interaction with bacterial cells over mammalian cells underlines their significant potential in developing AMP-based drugs.

Starting from a highly efficient tryptophan- and arginine-rich AMP (RRWWRWWRR) new analogs were designed by substitution of tryptophans or arginines with histidines. Here we performed molecular dynamics simulations showing that their antimicrobial activity can be correlated to the 3D-hydrophobic moment and to a simple structure-based packing parameter. The presence of histidine enhances the aggregation of cationic AMPs around anionic lipids. Hence, the position of the histidine within the peptide sequence can be linked with AMP's mechanism of interaction with the membrane surface.

We used non-equilibrium potential of mean force calculations (by means of the FR method) reveal the energetics and potential mechanism of highly efficient AMP's binding to bacterial membrane models.

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Poster Communications

Analytical methods for medical physics

P Mf 1. Solvatochromism and Quantum-mechanical Study of 8-Hydroxyquinoline: Comparison of Solvent Scales

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The solvatochromism study of electronic absorption spectra of 8-HQ was investigated in polar and non-polar solvents. Some electro-optical parameters of the studied molecule was performed with Spartan'14 software using DFT method. The contribution of the intermolecular interactions to the spectral shifts in the binary solutions of the studied compound was established. A comparison of solvent polarity scales of Kamlet-Taft and Catalan attempt to evaluate behavior of solute-solvent interactions.

P Mf 2. Spectrophotometric UV analysis method of acetylsalicylic acid in tablets

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Acetylsalicylic acid is a most common non-steroidal anti-inflammatory drug, the main component of pharmaceutical aspirin tablets that suppresses inflammation, relieves mild and moderate pain. Due to its efficient anti-platelet antiaggregant function, it is always used to prevent a number of serious heart disease including heart attack and stroke To exactly quantify pure acetylsalicylic acid in pharmaceutical tablets, a spectrophotometric UV method was developed and proposed to be applied. 100 µg/mL working solution was prepared by acetonitrile p.a. 1:10 dilution from stock solution 1000 µg/mL A series of eight standard solutions (1.2 µg/mL– 6 µg/mL) were obtained from working solution 100 µg/mL.. Standard solutions absorbances were read out at $\lambda_{max.}$ = 226 nm. Five measurements were made for each concentration. Calibration graph of spectrophotometer was plotted. Similarly, acetylsalicylic acid analysis sample was prepared from tablets of a pharmaceutical product and average absorbance was measured. The amount of pure acetylsalicylic acid per pharmaceutical tablet was 497.474 mg, close enough of active substance content declared by pharmaceutical manufacturer (500 mg), with a average permissible deviation of only 0.505%, below maximum of ± 5% indicated by Romanian and European Pharmacopoeia. Statistic analysis revealed that spectrophotometric UV method was linear in the range of 1.2-16.0 µg / mL; the linear regression coefficient was: R^2 = 0.99914 and the coefficient of correlation R = 0.99957, R > 0.999 were located within the normal range. Standard error of linear regression was SE = 0.009726. Detection limit, LD = 0.509 µg / mL and Quantification Limit, LQ = 1.697 µg / mL were within normal range of values. Spectrophotometric analysis method can be successfully applied in quantitative pure acetylsalicylic acid analysis from different brands of pharmaceuticals.

Acknowledgments . This study is simply a scientific research paper that does not aim to confirm or deny the official results of pharmaceutical manufacturing company nor to cause any image damage.

P Mf 3. The Computed Parameters and Solvatochromic Study of Two Fluorescent Molecules

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A quantum-mechanical characterization and the some electro-optical parameters of the studied molecule were evaluated using Spartan'14 program. Absorption spectra of two molecules with various substituents and molecular size were studied in different solvents. The contribution of each type of interactions to the total spectral shift are studied usingthe solvent multiple parameters empirical scale defined by Kamlet and Taft.

P Mf 4. Tribological modelling of the hip joint

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The paper presents a series of aspects regarding the main bio-tribological phenomena (lubrication, wear, friction) occurring in the synovial joints. It should be emphasized once again that rubbing and wear are different phenomena. Thus, certain components of the synovial fluid (e.g. glycoprotein lubricant - LGP) can act to reduce friction in synovial joints while other constituents (e.g. protein complex or hyaluronic acid) can act to reduce cartilage wear. Although a great deal of research has been carried out around the world about the bio-tribological processes in the human body's synovial joints, due to their complexity they have not yet been fully understood and could not establish a unique model of lubrication mechanism in these joints. The problem is complicated by the fact that in reality the cartilage is neither homogeneous nor isotropic and undergoes a large deformation during loading. According to several researchers, implantation and expulsion of synovial fluid in cartilage is not a simple phenomenon, although the boosted or weeping type of lubrication suggests this. The self-generating lubrication mechanism postulated by Mow et al. (1987) takes into account the biphasic nature of cartilage and is based on the load-dividing factor between the solid phase and the liquid.

In recent years, studies have also been carried out to explore possible links between synovial joint lubrication mechanisms and degeneration processes (e.g. osteoarthritis).

Tribological modelling is based on a number of parameters, such as: lubricant film thickness (or synovial fluid), maximum physiological load, articular cartilage surface roughness, friction coefficient, surface roughness and lubrication regime.

P Mf 5. New Data on Growing Mechanism of Human Gallstones from Transylvania, Romania: A joint Confocal Micro-Raman, Polarized Light Microscopy, X-Ray Diffraction and Thermal Analysis Study

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Recent review on gallstones investigation [1] showed effervescent research continuously conducted to find proper treatment on biliary lithiasis.

We report the here new data on gallstone chemical composition and formation in patients from Romania. Among 93 sample previously studied [2], a set of 9 freshly collected gallstones from one volunteer patient, was selected to get insight into the growing mechanism of gallstones. The gallstones were of particular interest, because of their morphology suggesting adjacent mutual obstruction of growth directions and their great agglomeration (a total of 58 pieces). Using polarized light microscopy, X-ray diffraction (XRD) and vibrational micro-Raman spectroscopy techniques we were able to elucidate the layered micro-structure the chemical composition as well as the nucleation and growing mechanism of gallstones. Spotted inclusions of Cl- or F-apatite were also detected. Inorganic matter resulted after gallstones thermal treatment revealed a carbonate and phosphate content after organic counterpart fired. Polarized microscopy clearly showed the concentric growing cholesterol crystals in consecutive layers. Valuable information on their development could suggest necessary mechanism for their inhibition.

References:

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2. I. Brezestean, N. Har, A. Tantau, M.Gorea, M. M. Venter, S. Cinta Pinzaru*, Analytical study of gallstones in patients from Transylvania, Romania,* 2015 Studia Chemia, LX, pp 29-43

P Mf 6. Quality control of radiopharmaceuticals

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Radiopharmaceuticals are radioactive preparations used in nuclear medicine as tracers in diagnostic imaging and for the treatment of certain diseases.

The aim of this work was to describe quality control (QC) testing for PET radiopharmaceuticals. Quality control procedures were performed according to the European Pharmacopeia analytical methods which are described in monograph: appearance, pH, half-life, radionuclidic identity, radiochemical and chemical purity, bacterial endotoxins and osmolality. The chromatographic methods used in determining chemical and radiochemical purity are high performance liquid chromatography (HPLC), thin layer chromatography (TLC) and gas chromatography (GC). The instruments which are used to detect radiation in measuring radiochemical purity are dose calibrators and scintillation detectors.

P Mf 7. Validation of a color spot test for determination of Kryptofix 2.2.2 in radiopharmaceuticals production

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The aim of this work was to validate a fast method to determine the Kryptofix 2.2.2 content in ^{18}F-radiopharmaceutical products.

Kryptofix 2.2.2 (4,7,13,16,21,24-hexaoxo-1,5-10-diazabicyclo-[8.8.8]-hexacosane) is used as phase transfer catalyst in preparation of ^{18}F-labeled compound and is a critical impurity. It is necessary to determine accurate, reliable and efficient way the concentration level of the impurity because can have toxic effect. Therefore, the determination of Kryptofix 2.2.2 is essential for quality control of radiopharmaceuticals, as emphasized by European Pharmacopoeia (EurPh 9.0, 2017).

The spot test method described for analysis of K2.2.2 proved to be linear and specific. The limit of detection for method was 6µg/mL. The method was validated for specificity according to the International Conference on Harmonization guidelines.

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P Mf 8. Anticancer activity of Luteolin studied in carcinoma and sarcoma cells

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Luteolin, a flavonoid which is part of our daily nutrition, shows anti-oxidant, anti-inflammatory and anti-carcinogenic effects [1, 2]. Previous studies reported that Lutelolin alters the expression of key components in the tumor cell metabolism pathways, thus inducing cell cycle inhibition and apoptosis [2, 3]. The main mechanism of the anticancer effects of luteolin is apoptosis, but other mechanisms, such as cell cycle inhibition and antiangiogenesis were also reported [4, 5].

The aim of this study was to determine the mechanism of the anticancer effect of Luteolin against carcinoma and sarcoma cells. Five cell lines: two normal cell line (L929 – mouse fibroblasts and BJ – human fibroblasts) and three cancer cell lines (Hep G2 – human hepatocellular carcinoma, HT-29 – human colorectal adenocarcinoma and MG-63 – human osteosarcoma) were investigated in vitro. First we evaluated cells viability using the MTS assay, for cells treated with different concentration of Luteolin (0 - 250 μM) for 24 h. The test showed that HT-29 cells were the most resistant to Luteolin treatment. Finally, the mechanism of death was investigated for two concentrations (10 and 100 μM). The results showed that Luteolin induces apoptosis in both carcinoma and sarcoma cells.

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P Mf 9. Biomechanical and thermographic study of syndromes induced by human body vibrations

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There is a multitude of working activities that subject the human body to oscillations of low amplitude and high frequency, which may influence the health of the body structure (bones, muscles, nervous system). Some of the most common problems that may affect health due to vibrations occurrence are the White Fingers Disease (Raynaud's Syndrome), Carpal Tunnel Syndrome, joints lesions or muscular fatigue. These are mostly the results of using vibratory tools or working with hard massive equipment.

The early discovery of these syndromes may lead to preventing more serious symptoms which could impede upon the future activities of the working person. The paper aims at proposing a methodology for the study of human subjects by biomechanical and thermographic analysis in order to early determine any changes in their motion ability and blood circulation following the influence of different types of vibrations.

For this purpose, the team will use an experimental setup consisting of a thermovision camera and a Kistler platform force, whose data will be acquired by a dedicated laptop. The analysis of the experimental results leads to conclusions related to the manner of early detection of vibrations related syndromes and propose methods of monitoring the staff involved in such activities.

P Mf 10. Influence of variable frequency noise upon the human factor stability

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Our modern world is inevitably a permanent source of sounds of different physical characteristics, some of them beneficial for the human factor, even with healing properties and some becoming part of the growing environmental stress, better known as noise pollution. Besides the usual negative effects like hearing problems, neurological diseases or psychological issues, some types of noise may lead to sudden loss of stability according to their wave length, frequency, distance from the human factor, location, etc.

The present paper aims at illustrating by practical experiments using healthy subjects in a controlled environment the influence of variable frequency sounds, occurred in different locations in a random manner upon the stability of human factor. Loss of stability during various activities interrupted by random and variable noise may endanger the health or even the life of the affected person.

In order to determine the degree of stability loss and the types of sounds inducing a higher influence upon the human body, an experimental setup was accomplished at the Advanced Mechatronic Systems Laboratory, consisting mainly of a Kistler force platform, laptop for data acquisition, sound generator with speakers.

The acquired data were analyzed and conclusions drawn to be able to prevent work accidents or other unfortunate situations that might lead to health endangerment.

P Mf 11. LabVIEW routine for encephalographic signal processingLabVIEW routine for encephalographic signal processing

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The research presented in the present paper concern the treatment of signals obtained from monitoring the encephalic function through electroencephalogram. The signal processing is based on the creation of a routine in named Labview software, which allow analyzing both electrocardiographic and electroencephalographic (EEG) signals.

Automatic interpretation of an EEG implies analyzing a large diversity of normal and abnormal wave forms on a great number of channels. EEG monitoring aims the detection of significant changes either for slow and fast waves (spikes).

A routine was created in LabVIEW software for processing the EEG signal and to indicate anesthesia degree (cerebral state index). After caption and filtering, the signal is distributed through four channels corresponding the electroencephalographic frequencies. Further, the signal was transformed as to be possible its graphic representation and, the Cerebral state index was estimated by implementing its specific formula and expressed by a numerical value.

This application has the advantage to save data in in different formats as to be visualized and interpreted by other software giving the graphic representations (Excel, Origin etc.). It also allows to be used for a great number of subjects, depending on PC memory, and it is easy and friendly to use for persons that have no specific IT education. The last but not the least, it is very low cost: LabVIEW license and low cost for acquisition board and two black boxes.

P Mf 12. The prevalence of cancers and hormone replacement therapy

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In pathologies where the glandular secretion is affected, and the normal concentration of a specific hormone is lower than the normal level, a hormonal deficit is appearing. The best therapy in this situation is the hormone replacement which ensures exogenous intake of hormones and consists in administration of synthetic hormones to adjust the concentration to a physiological level. However, recently, clinical trials suggest that a high dose of exogenous hormones may increase the cancer risks.

This work presents the outcomes of the study obtained by a thorough and disciplined literature search over the last five years of the prevalence of different types of cancers at patients with hormone replacement therapy. The search engines used were PubMed and Scopus, and the search was focused on thyroid hormones, cortisol and sexual hormones.

In this study, we concluded that the incidence of cancer is higher in patients with high levels of thyroid hormones, especially for high-substituted FT4 cases, as evidenced by a large number of cell line and patient studies. In order to analyze the role of cortisol and sex hormones, it should be taken into account that their chemical structure is based on thyroid hormone structures.

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Poster Communications

Novel materials and biomaterials for analytical methods

P Bm 1. Preparation of MnO_2/carbon nanotubes with sorption properties

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Magnetic nanocomposites based on carbon nanotubes are a high interest due to their potential applications in various fields such as: water decontamination, sensors for improved detection and tracking of contaminants, biomedicine, etc. Thus CNTs decorated with different types of nanoparticles may be used for removal of various pollutants (e.g. drugs, metals, pesticides and germs from contaminated water). Nanoparticles have two key properties that make them particularly attractive as sorbents: larger surface area than bulk particles and can be functionalized with various chemical groups to increase their affinity towards target compounds. The second property improves the selectivity of nanoparticles for specific pollutants. Good results were obtained by using CNTs decorated with magnetic nanoparticles (magnetite, iron zero valent) especially in case of dyes and heavy metals removal.

In this study, the preparation and characterization (XRD, BET, TEM) of multi-walled carbon nanotubes containing MnO_2 nanoparticles are presented. Water decontamination tests regarding dyes removal are also described.

Acknowledgments: This work was carried out through the Core Programme, developed with the support of MCI, project no. PN18-03 02 03.

P Bm 2. A New Approach Towards the Synthesis of Graphene Based Materials

Maria Coros, Florina Pogacean, Lidia Magerusan, Marcela-Corina Rosu, Valentin Mirel, Stela Pruneanu

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The synthesis of graphene with controllable characteristics is of significant importance for its application in various fields ranging from drug delivery to energy storage. The electrochemical exfoliation of graphite is a promising approach to produce graphene and graphene-related materials due to its easy, fast, and environmentally friendly nature. Currently, the limited understanding of the exfoliation process obstructs targeted modification of graphene properties. The purpose of our work was to establish the possibility of electrochemical production of graphene with small amounts of defects via pulse exfoliation of graphite rods in acidic solutions. We investigated the process of pulse electrochemical exfoliation and the impact of its parameters on the produced graphene.

Acknowledgments: This work was financially supported by the Ministry of Research and Innovation (MCI), Core Program, Project PN 18 03 02 02.

P Bm 3. Electronic Portable Device for Selective Lead Ion Detection from Different Water Sources

Lidia Magerusan, Stefan Gergely, Stela Pruneanu, Florina Pogacean, Maria Coros

[1] INCDTIM

The altering of living environment is one of the most complex problems of mankind due to its repercussions, in most cases irreversible and chronic, with negative impact on human health. Through industrial pollution some metal ions reach water sources. These ions are considered particularly dangerous pollutants due to the imbalances and diseases that they can cause (even at low concentrations) and because of their cumulative effect in the body. Hence, heavy metal ions severely harm human health, and for this reason, it has become a critical and necessary issue to accurately detect and quantify them by developing simple, fast and sensitive methods. The aim of the present study was to develop a modern electrochemical platform in order to provide a portable solution for the selective, facile and rapid identification and quantification of lead ions from different water sources. The electronic device was designed and made in the form of an experimental model. The instrument includes a hardware interface connected to the PC using an USB port and LabView software dedicated to this tool. The application allows setting the measurement parameters, developing the algorithm for processing the acquired signal, viewing the data and the obtained voltammograms. The instrument was designed and fabricated as a mini-potentiostat for on-site detection of pollutants.

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P Bm 4. Graphene Synthesis by Exfoliation of Graphite Rod via Pulses of Current

Stela Pruneanu, Florina Pogacean, Lidia Magerusan, Maria Coros, Marcela-Corina Rosu, Valentin Mirel

[1] INCDTIM

Graphene was prepared by exfoliation of graphite rod via pulses of current in solution containing a mixture of boric acid and sodium chloride. The pulse exfoliation method prevents the over-heating of the solution which has a negative impact on the quality of the exfoliated material. The material was morphologically and structurally characterized by TEM and XRD. The performances of a glassy carbon (GC) electrode modified with graphene (GC/EGr) were tested towards Sunset Yellow (SY) detection and compared with those of bare GC. As expected, the graphene-modified electrodes have a high sensitivity (0.8 $A \cdot M^{-1} \cdot cm^{-2}$), a wide linear range (6 x 10^{-7} - 10^{-4} M) and low detection limit (LOD = 2 x 10^{-7} M). In contrast, the bare GC electrode has higher detection limit (LOD = 10^{-6} M) and considerably lower sensitivity towards SY (0.02 $A \cdot M^{-1} \cdot cm^{-2}$).

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P Bm 5. Green Methodology for Chitosan/Carbon Base Nanomaterial Preparation and its Applicability in Sunset Yellow Detection

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Synthetic colorants containing azo functional groups (-N=N-) and aromatic ring structures have been widely used to replace natural food color in food industry due to the many advantages they offer: low production costs, excellent color uniformity as well as high stability during preparation processes. However, it is necessary to note that such synthetic colorants are able to affect human health being pathogenic, particularly when they are excessively consumed. Carbon-based materials are currently at the forefront of materials research due to their outstanding physical, mechanical and electrical properties and exceptional catalytic/electrocatalytic activity. The ability to be dispersed in various polymer matrix leads to a new class of polymer nanocomposites with a wide range of applicability (e.g. food packaging, biosensors, water treatment or drug delivery). The main goal of this study was to provide a facile, rapid, inexpensive way for the green, one-step and large-scale preparation of chitosan/carbon base nanomaterial, trough electrochemical exfoliation of graphite rods, without the use of any organic solvent. The obtained nanocomposite was characterized from morphological and structural point of view. Furthermore, the applicability of chitosan/carbon based-glassy carbon modified electrodes for accurate detection and quantification of sunset yellow was also reported.

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P Bm 6. Electrochemical Detection of 8-Hydroxy-2'-deoxyguanosine Using Graphene Modified Electrodes

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8-Hydroxy-2'-deoxyguanosine (8-OHdG) is a biomarker of DNA oxidative stress and a risk factor for a variety of diseases including cancer, diabetes, and neurological disorders. This work presents a novel approach for the synthesis of graphene nanosheets through pulse exfoliation of graphite rods. Two graphene based materials were prepared via pulse exfoliation method. The first material (denoted EGr-A) was prepared by exfoliation of the graphite rod in acidic solution (mixture of H_2SO_4:HNO_3) and the second material (denoted EGr-S) was prepared by exfoliation of the graphite rod in a salt solution of ammonium sulfate.

The performances of the electrochemically exfoliated graphene (EGr-A and EGr-S) attached to the glassy carbon (GC) surface were evaluated in pH 6 PBS solution, containing different concentrations of 8-OHdG. It was found that the redox process was highly accelerated when EGr-A or EGr-S modified GC electrode was used. In addition, the peak currents were significantly higher than those obtained with bare GC substrate. The calibration plots of the graphene-modified electrodes have a high sensitivity (0.53 $A \cdot M^{-1} \cdot cm^{-2}$ for GC/EGr-A and 0.67 $A \cdot M^{-1} \cdot cm^{-2}$ for GC/EGr-S), a wide linear range (3 x 10^{-7} - 10^{-4} M) and low detection limit (LOD = 10^{-7} M). In contrast, the bare GC electrode has higher detection limit (LOD = 3 x 10^{-7} M) and considerably lower sensitivity (0.22 $A \cdot M^{-1} \cdot cm^{-2}$). The same measurements were performed in artificial urine solution.

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P Bm 7. Designing Efficient Low Cost Paper-based Sensing Nanoplatforms

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Over the past few years, there has been an increase in developing new biosensing devices since the diagnosis of a disease in an incipient stage can lead to a more efficient treatment. Therefore, it is necessary to develop simple, affordable and accurate point-of-care tools for direct biodiagnostics. Paper-based nanosensors can be a promising choice due to their low-cost and facile fabrication, ease of use, high sensitivity, specificity and flexibility[1]. In this context, the quality of these nanoplatforms can be improved by making use of the optical properties of gold nanoparticles[2], which are well-suited for Localized Surface Plasmon Resonance (LSPR) and Surface Enhanced Raman Scattering (SERS).

In this work, we propose a new plasmonic paper-based dual LSPR-SERS nanoplatform with improved detection abilities in terms of high sensitivity and reproducibility. Firstly, the synthesized colloidal gold nanorods (GNRs) with well-controlled plasmonic response obtained by tuning the nanoparticles' aspect ratio were validated as efficient dual modal LSPR-SERS nanosensor in solution using the p-Aminothiophenol (p-ATP) analyte. Then the GNRs were efficiently immobilized onto the paper via the immersion approach, obtaining thus nanoplatforms with modulated LSPR response. The successful deposition was confirmed by both LSPR measurements, demonstrating the preserved LSPR response and the homogeneity of the paper nanoplatform, and SEM images identify the nanoparticles onto the cellulose fibers. Finally, the LSPR and SERS performances of the as designed paper plasmonic nanoplatforms were evaluated by determining the limit of detection (LOD). In conclusion, our optimized plasmonic paper-based biosensing design could be further considered as an excellent candidate for miniaturized biomedical applications.

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P Bm 8. Synthesis and Characterization of CoFe2O4@TiO2:Tb Magnetic Recoverable Photocatalyst

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Photocatalytic technology offers a facile and cheap method for removing organic pollutants from wastewater. Additionally, the magnetic separation provides a suitable solution for wastewater depollution by applying external magnetic field. The aim of this paper is to prepare and characterize new core-shell composite nanoparticles of $CoFe_2O_4$@TiO_2:Tb type with controlled morpho-structural, optical and magnetic properties and increased magnetic separation efficiency.

The $CoFe_2O_4$@TiO_2:Tb core-shell nanoparticles were prepared by a two-stage process: first $CoFe_2O_4$ nanoparticles were obtained by chemical coprecipitation method and then the coating by terbium doped TiO_2 nanocrystallites was realized by a sol-gel process. The as-prepared nanoparticles were calcined at high temperature in order to transform the initially amorphous titanium dioxide into a crystalline phase.

XPS investigations evidenced the qualitative composition of samples and the presence of Tb dopant at the expected concentrations. The transmission electron microscopy (TEM) and high resolution TEM (HRTEM) evidenced that the $CoFe_2O_4$@TiO_2:Tb nanoparticles have a polyhedral shapes with mean sizes at about 10 nm. The analysis of magnetic properties showed that all the samples show superparamagnetic behavior. The photocatalytic tests demonstrated that the composite nanoparticles exhibit good photocatalytic activity toward the degradation of RhB solution.

This work offers a route for the improvements of photocatalytic systems which integrates magnetic-semiconductor nanoparticles with effective doping and recoverability by a magnetic field.

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P Bm 9. Graphene-Based SERS Platforms for Molecular Diagnosis

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We have developed surface-enhanced Raman spectroscopy (SERS)-activ substrates based on mixtures of graphene/Ag nanocomposites, and a silver colloid, respectively, for biomedical applications. We have succeeded to assemble Ag nanoparticles onto the graphene sheets for SERS studies. The mixture with the best SERS enhancement properties was selected for the analysis of a biopolymer at low pHs. Chemical stabiliy under acidic conditions has been found for this system.

Our results might have possible future applications in sensor technology.

Acknowledgments: We acknowledge help with TEM images to Prof. Dr. Gabriel Katona. The authors wish to thank to Prof. Dr. Nicolae Leopold for facilitating the surface-enhanced Raman spectroscopic measurements at “Babeş-Bolyai” University, Cluj-Napoca, Romania, to Eng. Sorina Niţu for providing the leaf tissues from a medicinal plant and to Drs. Ana Coste and Adela Halmagyi for extracting the DNA sample from leaves. This work was supported by a grant of the Romanian Ministery of Research and Innovation, Core Programme, Project nr. PN 18 03 02 01.

P Bm 10. Microcapsules as Carrier Systems in Photodynamic Therapy

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The application of micro/nanotechnology for treatment, diagnosis, and control of biological systems is now often referred to nanomedicine. The use of various nanomaterials as pharmaceutical delivery systems for drugs, DNA, and imaging agents has gained an increasing attention. Cancer nanotechnology is an interdisciplinary research, cutting across the disciplines of biology, chemistry, engineering, physics & medicine with superior effects to traditional methods: surgery, radiation treatments, chemotherapeutic agents and hormonal treatments [1]. Photodynamic therapy (PDT) is a treatment modality for cancer and various other diseases. In photodynamic therapy (PDT) the incorporation of photosensitizers (PSs) in nanostructured drug delivery systems, such as polymeric microcapsules (PNPs) is a potential strategy for medical applications. These systems have the ability to explain and to modify each of the critical steps of PDT, particularly photosensitizer design and delivery, interaction with different biological/ cellular targets, offering a greater insight into mechanisms of action: photosensitizer application, light activation and singlet oxygen generation for good outcomes [2]. Photodynamic therapy itself occurs via activated photosensitizer (triplet state), resulting in the production of various reactive oxygen species, amongst them singlet oxygen as the primary photochemical product. The aim of this paper is to review system-based drug delivery systems for photodynamic therapy of cancer, with some tested natural drugs (capsaicine, colchicine) examplified in medicine.

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P Bm 11. Photocatalytic Ability of Cotton Pads Modified with TiO_2-Pt/Reduced Graphene Oxide and SiO_2-Pt/Reduced Graphene Oxide Composites

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Nowadays, high quality fabrics having self-cleaning, antimicrobial and UV blocking characteristics can be developed by modifying textile materials with different nanomaterials. The purpose of this work was to obtain photocatalytic textiles by deposition of TiO_2-Pt/reduced graphene oxide and SiO_2-Pt/reduced graphene oxide composites onto cotton pads. The morfo-structural and optical characteristics of powders were investigated by SEM, X-ray diffraction, FTIR and UV-VIS spectroscopy. The photocatalytic activity of treated textiles was evaluated by degradation of methyl red aqueous solution under ultraviolet (UV) light irradiation. The photodegradation efficiency of the treated cotton pads with TiO_2-Pt/reduced graphene oxide composite was clearly superior to that of similar textiles containing SiO_2-based materials. It is expected that TiO_2/graphene-based nanocomposites might be used to introduce high performance *characteristics* of various textile products.

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P Bm 12. Silver nanoparticles synthesized by green chemistry method and their bioimpact on environmental microorganisms

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Nowaday, the advanced research on silver nanoparticles (AgNPs) is motivated by their various and interesting applications. Our research was focused on the bioeffects of AgNPs on Phanerochaete chrysosporium (able to degrade wood cellulose from wood waste). The silver nanoparticles were eco-synthesized using an aqueous extract of celandine (Chelidonium majus). Green synthesis of AgNPs was monitored by absorption spectroscopy, visible range (Shimadzu Pharma Spec device).

AgNPs suspension was supplied in different concentrations (40µl, 60µl, 80µl, 100µl) in the same volume (100 ml) of culture medium inoculated with cellulolytic fungi *Phanerochaete chrysosporium*.

We assayed the activity of antioxidant enzymes - superoxide dismutase (SOD, EC 1.15.1.1) and catalase (CAT, EC 1.11.1.6). The response of fungus was different depending on the AgNPs concentrations and the age of culture (7 and respectively 14 days after inoculation). Thus, the activity of the defensive antioxidant SOD enzyme was stimulated at both time intervals (7 days and 14 days after inoculation) with increasing AgNP concentration. On the other hand, the same trend of increase of enzymes activity was observed at CAT - the activity of catalase in the experimental variants of 80 and 100 µl AgNPs being significantly higher than the control samples.

This could be taken as proof that catalytic action of silver nanoparticles has generated free radicals in the cells while the cellular defence mechanisms were able to enhance the biosynthesis of antioxidant enzymes. Thus, the delivery of AgNPs in the biosphere, after utilization, is capable to influence cellulolytic fungi which, in turn, are able to balance silver polluting effect.

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P Bm 13. Antioxidant and Antimicrobial properties of Randomly Methylated β Cyclodextrin complexed Essential Oils

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Essential oils (EOs) have been in a major research focus for years to eliminate the use of toxic synthetic food preservatives. They are widely applied in food packaging because of their potency in antioxidant and antifungal activities to improve food quality and extending shelf life. EOs are highly hydrophobic in nature therefore they maybe entrapped/encapsulated by randomly methylated ß cyclodextrins (RAMEBs) to ensure the preservation of antioxidant and antimicrobial properties of EOs. In our present study, we evaluated the total antioxidant capacity of nine RAMEB encapsulated essential oils/pure components by three different assays. A simple, reliable microplate fluorescence viability test for rapid assessment of live/dead microbes for RAMEB-essential oil complexes on Gram-negative, Gram-positive test bacteria and on *Schizosaccharomyces pombe* fungus have also been done in our present study. The microplate assay was validated by flow cytometry. The antioxidant activity of RAMEB encapsulated thyme oil and its component thymol was found to be the highest followed by lemon balm oil, lavender oil and peppermint oil. RAMEB-thyme oil showed highest MIC (MIC_{80} = 0.125 – 0.25 mg/ml, 0.156 – 0.312 mg/ml, 0.5 - 1 mg/ml) against *S. pombe*, *E. coli* and *S. aureus* respectively, followed by lemon balm oil, peppermint oil and lavender oil. In antifungal and antimicrobial testings, RAMEB-citral (MIC_{80} = 0.0078 – 0.156 mg/ml, 0.125 – 0.25 mg/ml, 0.078 – 0.156 mg/ml) which is close to RAMEB-thymol (MIC_{80}= 0.078 – 0.156 mg/ml, 0.125 -0.5 mg/ml, 0.25 – 0.5 mg/ml) showed high antifungal and antimicrobial activity against the tested microbes. Our data suggests that RAMEB complexation of EOs could eliminate the limitations of volatility and losses of essential oils during food processing or storage. Complexation enhances the antioxidant capacity, microbial termination abilities of EOs encouraging food industry to use them as a controlled release system in varoius applications in food industry and aroma science.

P Bm 14. Catechol-attached Polypeptide with Functional Groups as Electrochemical Sensing Platform for K2-Spice

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Compounds which have similar psychoactive properties to tetrahydrocannabinoyl (THC) are found in cannabis and obtained by using various chemicals in the laboratory environment called "Synthetic Cannabinoids". The common feature of all synthetic cannabinoids is that they act on the cannabinoid receptors in the body and mimic the effects of Δ9-THC, which is the active chemical at various levels. JWH-018 is the first synthetic cannabinoid to be found in plant products since it is easily synthesized and has a high pharmacological effect. Various studies have been done on the electrochemical detection of these synthetic cannabinoid compounds. In this study, an electrochemical biosensor is developed by using K2 antibody for the selective detection of JWH-018. For detection, a glassy carbon electrode was coated with catechol-attached polypeptide (CtP). Afterwards, K2 antibody was immobilized on the polypeptide chains with glutaraldehyde as a cross-linker. Modification of the surface is monitored with various electrochemical techniques such as differential pulse voltammetry (DPV), cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). Furthermore, analytical parameters such as limit of detection, repeatability were calculated. In the final part of the work, the GCE/CtP/Antibody/JWH-018 electrode is tested with synthetic saliva and urine samples which contained a known concentration of JWH-018. Confirmatory analysis is done with chromatographic measurements.

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P Bm 15. Catechol-bearing Polypeptide Modified Gold Nanoparticles for Point-of-Care Detection of Immunoglubulin G as a Cancer Biomarker

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Increasing evidence in the last decade proved that various cancel cells can produce IgG, though the exact function of cancer-derived IgG has not been discovered yet. The over-expression of IgG in cancer cells is claimed to be associated with poor prognosis. It also is found that cancer-derived IgG is involved in proliferation of various cancer cells. Additionally, differentiation in glycosylation processes of serum IgG is found to be a potential identification of patients with cancer.

Herein, we present a proof-of-concept study, a novel synthesis of catechol-bearing polypeptide (CtP) coated gold nanoparticles (AuNPs) by simultaneous photoinduced electron transfer and free radical polymerization processes and its application on a point-of-care, paper-based, colorimetric immunoassay to detect IgG as a cancer biomarker. Antibody-antigen affinity-based sensor system is established with AuNP-CtP-Anti-IgG bioconjugate and IgG as an analyte. Sandwich type immunoassay principles are applied. Colorimetric analysis of the results is conducted via a smartphone, capturing the image of the results and analysing these data on ImageJ software. Results holds promise to be used on other cancer biomarkers and become a point-of-care test system to be used practically.

P Bm 16. Deep Eutectic Solvents as Ecological Media for the Development of Novel Redox Polymer-Film Modified Electrochemical Sensors

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Deep eutectic solvents (DES) are a new class of “green” solvents and have been successfully used in the preparation of advanced materials, as an alternative to ionic liquids. DES are composed of a mixture of hydrogen bond donors and acceptors, which self-associate to form a new eutectic phase [1]. Recent applications have included their use as media for the formation of conducting polymer films [2] and redox polymer films [3] for sensing applications.

In this work, the phenazine dyes methylene green (MG) and thionine as well as the azine dye neutral red (NR) were electropolymerized in DES to form a redox polymer film on glassy carbon electrodes. In order to obtain good performance, the best DES composition and polymerization conditions were established. The DES ethaline was formed from a 1:2 ratio of choline chloride and ethylene glycol mixing during heating and allowing to cool. A small amount of strong acid was then added to improve the conductivity. The redox polymer-film modified electrodes obtained with this new approach were electrochemically characterized by voltammetric measurements and by electrochemical impedance spectroscopy. The analytical parameters for the electrochemical sensing of ascorbate were determined by fixed potential amperometry and showed good results.

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P Bm 17. Electrochemical Behaviour Of Vancomycin And Its Direct Detection On A Graphene Based Electrochemical Sensor

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Vancomycin is a glycopeptide antibiotic, indicated for the treatment and prophylaxis of severe infections caused by Gram-positive bacteria by parenteral administration. The main drawback of the treatment with vancomycin is the relative high occurrence of nephrotoxicity, ototoxicity and the spread of bacterial resistance to antibiotics.

Therefore, there is an increasing need of analytical tools for the therapeutic drug monitoring of vancomycin, in order to maximize efficacy and improve the clinical outcome for the patients and to minimize the emergence of antibiotic resistance [1]. The purpose of this study was the development of a fast and sensitive electrochemical method for the analysis of vancomycin.

The electrochemical behaviour of vancomycin was studied using different techniques, like cyclic voltammetry and differential pulse voltammetry and different electrodes: glassy carbon electrode, boron-doped diamond electrode, bare carbon-based screen printed electrode (SPE) or modified with carbon nanotubes or graphene.

Vancomycin presents one irreversible electrochemical oxidation peak. The electrochemical oxidation of vancomycin is influenced by the pH of the electrolyte, the electrode material and by electrochemical parameters. A low pH combined with the graphene modified SPE yielded the best results. The method allows quantitative analysis of low amounts of vancomycin, presenting good selectivity.

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P Bm 18. Formulations and investigations of chitosan/polyvinyl alcohol blends for various applications

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The aim of the present paper is to explore the properties of medium molecular-weight chitosan/polyvinyl alcohol blends as films and cross-linked microparticles for different applications. Chitosan/poly(vinyl alcohol) cross-linked films were obtained by using aqueous solution of polyvinyl alcohol mixed with aqueous solution of chitosan salt in a mixing ratio of 3:1; 1:1; 1:3 in the presence of 5 % v/v glutaraldehyde. New reticulated materials have spheres shapes and were tested for Pb (II) removal capacity from waters. The results pointed out a good efficiency (almost 84%) of these materials as potential adsorbent materials. For comparison purpose, thin thickness films from the same quantities of the mixed solution were obtained by solution casting method in glass plates and dried at room temperature. Surface morphology (AFM), molecular interactions of the samples, atomic force microscopy and ATR-FTIR spectroscopy were studied. The surface morphology of the cross-linked films exhibits a nanoparticle aggregation structure. ATR-FTIR results indicated the strong interactions between chitosan/PVA films before and after cross-linked treatment.

P Bm 19. Highly efficient, rapid, and simultaneous removal of dyes from wastewater using mesoporous silica

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Dyes are widely used in food technology, leather tanning, photoelectrochemical cells, paints, textile dyes, paper, etc, these industries producing large amount of so-called coloured wastewater. Many of these dyes have toxic or carcinogenic effects, causing serious damages on aquatic organisms and human being as well. Due to the increasingly stringent restrictions on the organic contents in the industrial effluents, it will be necessary to remove them before wastewater is discharged. However, the treatment of dye-containing effluents is difficult. At this moment, the adsorption method is considered the most suitable for removing and recycling the dyes in wastewater. The mesoporous materials have become effective adsorbents own to their unique structures and characteristics such as huge surface areas, high pore volumes, relatively even distributions of pore sizes, surfaces enriched with unsaturated groups and orderly long-range structures. The mesoporous silica nanoparticles were prepared by a facile hydrothermal method and characterized by scanning electron microscopy, Fourier-transform infrared spectroscopy, and Brunauer-Emmett-Teller. The materials showed highly efficient and rapid adsorption properties for dyes such as rhodamine, crystal violet, or Nile blue. It could be stated that the adsorption is mainly controlled by electrostatic interactions and hydrogen bonding between the dyes and the mesoporous silica. As a low-cost, biocompatible, and environmentally friendly material, mesoporous silica has a potential application in wastewater treatment for removing some environmental cationic contaminants.

P Bm 20. Multiparametric Green Fluorescent Protein-Based Microplate Cell Viability Assay

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Cell-based viability assays play an essential role in testing the toxicological effect of any substance in tissue cultures. Instead of using a single viability parameter, it is strongly suggested to perform as many different approaches as possible to get valid information on the viability of the treated cells. In our work, a novel multiparametric technique was worked out using one-step extraction for measuring ATP, green fluorescent protein (GFP) content, nucleic acid level (propidium-iodide, (PI) signal)) and intracellular protein content on a microplate reader. Dose response analyses were done by treatment of GFP-transfected A-549 mouse lung cancer cell line with metabolic poisons (sodium fluoride (NaF), cycloheximide (CHX) and ochratoxin A (OTA)). After treatments, for quantitative evaluation, cells were lysed with 0.1% Triton X-100 containing borate buffer (0.2 M, pH 9.2) supplemented with 20 mM EDTA-Na_2. This one-step extraction released the intracellular components without loss or degradation. ATP was measured from the extracts with bioluminescence method. Lysates were stained with PI for 5 min. Fluorescence of PI and GFP was detected at 530/620 nm and 480/510 nm excitation/emission wavelengths, respectively. Intracellular proteins were quantified by fluorescent derivatization with fluorescamine. The results were compared with apoptosis/necrosis analysis by flow cytometry. Our results showed a dose-dependent decrease of GFP/PI/total protein levels in the treated cells. Cycloheximide proved to be the most effective in decreasing all measured intracellular parameters (40-60% of the control samples). GFP expression, together with ATP/PI/total protein data makes our model to be a simple and reliable method for assessment of viable cell population in toxicology assays.

P Bm 21. Novel bio-composite used for Cr(VI) removal from effluents

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A composite (Fe3O4-CS) consisting of magnetite nanoparticles (Fe3O4) entrapped into chitosan (CS) was “green synthesized” in order to investigate the adsorption of hexavalent chromium Cr(VI) from aqueous solutions. X-ray diffraction (XRD), scanning electron microscopy (SEM), and atomic force microscopy (AFM) were used to characterize the Fe3O4-CS nanomaterial in comparison with uncoated magnetite. Fourier transform infrared spectroscopy (FTIR), Uv-Vis spectroscopy, absorption spectroscopy and equilibrium sorption of Cr(VI) described by the Langmuir and Freundlich isotherm models were investigated. The results revealed that the magnetite nanoparticles entrapped into chitosan matrix exposed an average particle size of 15 nm with high efficiency for Cr(VI) removal. Finally, the reusability of the Fe3O4-CS as bio-composite with nano-size dimensions was investigated by successive three sorption/desorption cycles. The remarkable sorption capacities, and high reusability and stability of the Fe3O4-CS suggest the promising potential of this novel bio-composite in the removal of Cr(VI).

P Bm 22. Palladium Retrieval From Residual Waters Resulted From Galvanotechnique Industry

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Effective recovery of palladium ions from acidic waste solutions is really important due to his intensive usage as a catalyst for different industrial processes, and due to high price paid for his production from natural resources. The present paper aims to test the ability of new natural adsorbent for palladium ions removal. Being know that adsorption capacity of natural silicates (florisil) for metallic ions, new adsorbents were obtained by florisil modification with two amino acids (L glutamic acid and L cysteine). EDX and FTIR spectra have been recorded for proving the modification of florisil with these aminoacids.

Firstly, the maximum adsorption capacity of new obtained materials was studied. To establish the adsorption mechanism, the obtained experimental data were fitted using Langmuir, Freundlich and Sips adsorption isotherms in order.

A mathematical model of the absorption capacity function of the initial concentration of the absorbent material is also provided.

P Bm 23. Mesoporous silica-media for natural anthocyanins dye adsorption

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Anthocyanins are naturally occurring dyes found in many flowers, vegetables and fruits. Natural occurring anthocyanins are potentially suitable as dyes in food and cosmetic industry, due to their non-toxicity property. In order to be widely used, the anthocyanins must be immobilized on an inorganic host, improving also their stability. The aim of this study was the adsorption of some significant amount of natural anthocyanin dye onto mesoporous silica, highlighting its stability enhancement by the complexation. Since mesoporous silica is known to have a large surface area, it expectedly has potential to adsorb enough amounts of various organic molecules, including dyes. The anthocyanin dye has successfully been adsorbed on the mesoporous silica containing small amount of magnesium. The amount of the adsorbed anthocyanin has been increased by modifying the pore wall with amino groups. The light stability of the adsorbed anthocyanins has been improved by making the composite with the samples containing magnesium. Photo-fading of the samples was measured under visible light irradiation to check whether the stability of the dye was influenced by the modification of the silica.

P Bm 24. Electrochemical Evaluation of Heat-Treated AISI 316 Stainless Steel in Solar Furnaces to be used as possible implant material

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Appropriate selection of implant material is very important for the long-term success of implants. To optimize biological performance, implants should be tested to reduce the negative biological response, while maintaining an appropriate function. The paper presents a study concerning the electrochemical characterization of the AISI 316 stainless steels to determine their corrosion resistance in environments that simulate biological fluids. This material was treated by means of solar energy in the Vertical Solar Furnace (VSF) - CIEMAT-PSA, Tabernas, Almería (Spain). AISI 316 stainless steel was subjected to a hyper-hardening treatment at 1050°C austenitizing temperature with a rapid cooling in cold water following by 3 variants of tempering (150, 250 and 350°C). After heat treatment in the solar furnace, the specimens were analyzed to determine their corrosion resistance by potentiodynamic and electrochemical impedance spectroscopy measurements in environments that simulate fluids (NaCl 0.9% and Ringer solution). Based on the collected data, conclusions could be drawn on the electrochemical characteristics of this thermally treated steel with solar energy and the possibility of applying this unconventional heat treatment for the processing of biocompatible materials.

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Poster Communications

Medical analysis and diagnosis

P Ma 1. Copper Toxicity Of Metallic Bone Implants – A Pilot Study

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Targeted delivery of antibacterial materials represents a new hope in the treatment of osteomyelitis, as systemic antibiotics were found not to be fully successful. In this respect, copper and silver materials introduced either as implants or nanoparticles are currently under assessment by the scientific community. Concern related to their toxicity hinder their clinical use, in spite of demonstrated efficiency. As dose is the key factor in any treatment, be it based on antimicrobial metals or antibiotics, the challenge now is to finely "tune" metallic exposure to obtain the maximum benefit to risk ratio.

In the quest to assess antibacterial-metal toxicity of metallic bone implants, we inoculated copper and silver ½ mm particles in healthy rabbit tibia using an experimental model. In this pilot test, the animals were clinically monitored over 30 days. Histological and radiological investigations were undertaken 30 days after inoculation.

Copper corrosion behaviour in physiological saline solution and in human blood plasma was also studied. For this purpose, electrochemical analytical tools such as potentiodynamic test, electrochemical impedance spectroscopy, open circuit potential as well as in vivo analysis were undertaken.

Ion release in corrosive media followed a decline with time, most probably due to formation of chemical deposits via surface interaction with the respective media. The reduced copper bioavailability has as direct consequence a decrease in toxicity at the level of inoculation, a hypothesis confirmed by histology.

These results suggest that, with a further increase in metal implant surface, only a temporary higher copper release rate may be obtained. In the long term, copper corrosion in biological media does not depend on the initial surface area.

Acknowledgments: This work was supported by a grant of UEFISCDI, No. PN-III-P1-1.2-PCCDI-2017-0728.

P Ma 2. Preliminary Studies On The Effectiveness Of Targeted Copper And Silver Therapy Against Established Osteomyelitis

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We evaluated here the antibacterial effectiveness of copper and silver ½ mm particles as potential treatment of acute and chronic osteomyelitis. For this purpose, a rabbit tibial model was used.

Acute and chronic osteomyelitis was obtained by inoculation of $5x10^6$CFU/ml bacterial suspension in two trepanations per rabbit tibia, 30 and 60 days after inoculation, respectively. Cotton meshes were also used as foreign bodies. Then, the particle treatment was inserted into the infected trepanations. The animals were clinically monitored over 30 more days after treatment. Histological and radiological investigations were also undertaken.

Evidence of bone regeneration was found in bone marrow. Regenerative processes suggested by the presence of osteoclasts, osteoblasts and conjunctive tissue were also identified in the compact bone of treated rabbits. It should also be mentioned here that the meshes were not removed before inoculation of treatment particles, this showing good effectiveness of proposed treatment.

In vitro studies were also undertaken. A modified antibiotic assay was used. A lysis zone was observed around each particle.

The results demonstrated that copper and silver ½ mm particles are promising candidates for the treatment of osteomyelitis. Further studies aiming at establishing doses and improved treatment procedures will be undertaken.

Acknowledgments: This work was supported by a grant of UEFISCDI, No. PN-III-P1-1.2-PCCDI-2017-0728.

P Ma 3. Variation of Blood Pressure in Adolescents Population in Brasov District

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Introduction: The increasing prevalence of hypertension in childhood population during last years justify the interes of paediatricians in determination of the evolution trend of bloo pressure in children.

Objective: Our aim was to analize the antropometrical parameters and the value of blood pressure in adolescents.

Material and method: we had performed a prospective study in 2017 (March – June) during adolescent population in Brasov district, aged between 14-18 years with measurement of weight, hight, body mass index and blod pressure.

Results: Our study group consists 398 children, 173 girls and 225 boys; 10,15% of girls had hypertension and 89,85% had normal BP; 13,5% of boys had hypertension, 3,5% had “high normal”BP and 83% had normal BP. Regarding BMI: 16,18 % of girls were overweight and 9,24% were obese; 21,77% of boys were overweight and 9,33% were obese.

Conclusions: both in boys and girls the BMI tends to be higer then 50^{th} percentile; regarding BP also the values both in boys and girls tend to be higher then 50^{th} percentiles, boys had more often “high normal” BP then girls.

P Ma 4. Development of an Enzyme-Linked Immunosorbent Assay to Ghrelin Agonists and Antagonists Detection

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Ghrelin, the "hunger hormone" is a 28-aminoacid peptide hormone produced in the gastrointestinal tract[1]. Besides regulating appetite, distribution and rate of energy use[2], ghrelin and synthetic ghrelin mimetics are responsible for triggering the endogenous production of growth hormone, reducing body weight and fat mass[3]. Enzyme-linked immunosorbent assay (ELISA) is one of the most reliable method for point of care diagnostic and is also an important tool to characterize new proteins and their interactions with receptors and antibodies. ELISA kits for ghrelin quantification are commercially available, but those for ghrelin agonists (important for promotion of growth hormone synthesis) and antagonists (used for treatment of obesity) are not yet developed. Therefore, our study focuses on direct competitive format ELISA for the detection of synthetic mimetics (agonists and antagonists). Firstly, ELISA microplates were coated with streptavidin and biotinylated polyclonal antibody against ghrelin receptor (Growth Hormone Secretatgoue Receptor, GHSR-1a), a 7-transmembrane domain, G-protein coupled receptor. Next, human recombinant GHSR-1a was incubated and a competition step was established between the ghrelin-biotin conjugate and ghrelin agonists (GHRP-5) and antagonists (D-Lys^3-GHRP-6). For the quantitative purposes, a bio-conjugate streptavidin - horseradish peroxidase (STR-HRP) was used and the detection was carried out at 450nm using 3,3',5,5'-tetramethylbenzidine (TMB) as HRP chromogen substrate.

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P Ma 5. Synthesis and cytotoxicity of new aminopyrazolo-benzimidazoles derivatives

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Pyrazole derivatives develop a considerable interest in the medical field due to their therapeutic action as anti-tumor, antibacterial, anti-inflammatory, tyrosinase inhibitors.

A new series of substituted N-[(1H-pyrazol-1-yl)methyl]-aminobenzimidazole Mannich bases were synthesized, characterized by IR, ^{1}H-NMR, ^{13}C-NMR, UV-Vis, MS. *In vitro* cytotoxicity of the new compounds was studied using MTS assay.

The cell viability was analyzed quantitatively by MTT assay and cell morphology was observed on the culture stained with Hematoxylin-Eosin, after the direct contact of the cells with solutions of the new compounds at concentration ranges between 1-20µg/mL.

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P Ma 6. Synthesis, cytotoxicity and antitumor activity of new halogenoaminopyrazoles derivatives

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Studies have also described that some Mannich bases possess anti-inflammatory, antibacterial, antimicrobial, antifungal, antihistaminic and anti-tumor activities

A new series of substituted N-[(1H-pyrazol-1-yl)methyl]-halogenoaminopyrazole Mannich bases were synthesized, characterized by IR, ^{1}H-NMR, ^{13}C-NMR, UV-Vis, MS and tested for their antitumor activity. All the synthesized compounds were tested *in vitro* on NCTC normal cells and Hep-2 tumor cells. These tests were performed by MTT method for the determination of the compounds cytotoxicity and antitumor effect.

The cell viability was analyzed quantitatively by MTT assay and cell morphology was observed on the culture stained with Hematoxylin-Eosin, after the direct contact of the cells with solutions of the new compounds at concentration ranges between 1-20µg/mL.

P Ma 7. 4MBA Labeled Chitosan Coated Gold-Silver Core-Shell Nanoparticles as In Vitro SERS Traceable pH Sensors

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As intracellular pH is one of the key parameters in many biological events, the measurement of cellular pH is highly informative to understand how cells function [1]. In this work, we developed a biocompatible and optically stable nanocomplex for in vitro pH monitoring via surface-enhanced Raman scattering (SERS) spectrum of specific molecular tag. Our nanocomplex consists of chitosan coated gold-silver core-shell nanoparticles (chit-Au-AgNPs) labelled with para-mercaptobenzoic acid molecules (4MBA). Zeta potential measurements were made on different pH values of the colloidal solution to verify the optical stability. Its sensitivity toward pH modifications was firstly confirmed in aqueous solutions by SERS measurements under 533 nm and 632 nm excitation laser lines from the modifications of vibrational bands assigned to carboxyl group of 4MBA as function of various pH from acid to alkaline. The internalization of 4MBA-chit-Au-AgNPs in ovarian cancer cells was assessed using dark-field microscopy. Furthermore, the cellular viability in the presence of labelled core-shell nanoparticles was appraised through MTT assays. The ability of 4MBA-chit-Au-AgNPs to operate as in vitro contrast agents and pH sensors was validated using Confocal Raman Microscopy (CRM). The precise localization of the nanocomplex inside cells and the intracellular pH around them was provided by multivariate analysis of Raman spectra collected by the CRM scanning. Due to its properties of pH sensing and SERS traceability, the reported nanocomplex hold great promise for application in cancer diagnosis.

P Ma 8. Development and Evaluation of Novel Polymer-Based Tyrosinase Biosensor for Selective Dopamine Detection

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Dopamine (DA) is an important neurotransmitter, linked to a large variety of medical conditions, such as Parkinson, Alzheimer, attention deficit hyperactivity disorder or schizophrenia. Its detection still lacks a simple, reliable diagnosing tool for early detection. A novel tyrosinase-based biosensor was developed and evaluated for simple, rapid, inexpensive, sensitive and selective detection of DA in the presence of its main interfering, ascorbic acid (AA) [1]. Gold electrodes were previously modified with cobalt (II)-porphyrin (CoP) film with electrocatalytic activity, which acts both as electrochemical mediator and enzyme support. Electrochemistry was mainly used for biosensor optimization and characterization. Electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) were employed to identify interfacial changes of the gold electrodes after CoP film deposition and enzyme entrapment. All detection measurements were carried out by differential pulse voltammetry (DPV). By optimizing conditioning parameters, in the DPV plot a separation of 130 mV between the oxidation peak potentials for AA and DA was obtain to clearly discriminate between the two substances. The tyrosinase-based biosensor reached a sensitivity of 1.22 ± 0.02 μA cm^{-2} μM^{-1} and a detection limit of 0.43 μM with a linear range up to 30 μM. Due to its good reproducibility and stability, the biosensor performances were tested in the presence of real dopamine medication, with satisfactory results in terms of recovery and relative standard deviation values. These results determine the biosensors applicability in real samples such as blood serum.

Acknowledgments: We hereby acknowledge the structural funds project PRO-DD (POS-CCE, O.2.2.1., ID 123, SMIS 2637, No 11/2009 for providing the infrastructure used in this work.

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Poster Communications

Microspectroscopy

P Sp 1. Experimental Micro-Raman and IR spectroscopic analysis of amikacin combined with DFT-based calculations

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Amikacin, with the chemical formula $C_{22}H_{43}N_5O_{13}$, is an antibiotic often used in treatments of bacteraemia or septicaemia, also in respiratory tract infections or intra-abdominal infections. In some cases, the physicians administrate amikacin in post-operative infections either in complicated and recurrent urinary tract [1,2].

In spite of its large applicability area and the frequent use in clinics there are no studies reporting about a complete vibrational analysis of the amikacin molecule. Therefore, the aim of this study was to obtain a comprehensive vibrational investigation of amikacin both from an experimental and theoretical point of view. In this respect micro-Raman and IR absorption spectra were recorded and the assignment of the vibrational modes was performed by using the theoretical data of the density functional theory (DFT) based simulations carried out at B3LYP/6-311+G* and BPW91/6-311+G* theoretical levels.

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P Sp 2. The Use of *In situ* Surface Enhanced Raman Spectroscopy Technique for Antibiotic Resistance Determination of Pathogenic Microorganisms

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Although antibiotics have been used for decades to treat various bacterial diseases, their inappropriate use led to an increasing trend in the antibiotic- resistant bacterial infections. The disk diffusion assay is the most popular method used to determine bacterial susceptibility to antibiotics, even if it is very time-consuming, while polymerase chain reaction (PCR) and mass-spectrometry based techniques are expensive and cannot be applied to living bacteria or to monitor the response of a single bacterial cell to antibiotic treatment [1]. Surface Enhanced Raman Scattering (SERS) combines the advantages of Raman spectroscopy and nanotechnology and provide information on the chemical components in bacterial cells. SERS-based biosensors hold great promise as a platform for rapid and sensitive detection of bacterial pathogens by decreasing time of diagnosis and preventing infection-related morbidity and mortality. We monitored using SERS several scenarios: antibiotic free bacterial culture, bacterial culture treated with a class of antibiotic to which the bacteria showed sensitivity and when the bacterial culture was treated with a resistant bacterial antibiotic. Their SERS signatures were compared and the spectral results were analyzed using the Principal Component Analysis (PCA) statistical method for a rapid grouping and discrimination.

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P Sp 3. Detection of DNA molecules by SERS spectroscopy with silvered porous silicon as an active substrate

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Progress in an engineering of the SERS substrates has driven a tremendous interest to study DNA by the SERS spectroscopy. However, the practical application of this method is still in its infancy comparing to the traditional techniques of the DNA detection. In this work, we investigate the effect of such substrates on the spectra of the herring sperm DNA to choose optimal conditions of the SERS measurements resulting in a reliable DNA study.

The spectra were measured with a 3D laser scanning confocal CARS microscope SOL Instruments. An adsorption of analyte molecules was realized by a drop deposition of herring sperm DNA in 0.01M NaCl water solution on the silvered porous silicon (PS).

The results on the DNA study by the SERS spectroscopy with the silvered PS presented here were partially similar to those with solid SERS substrates that gave surface enhancement from DNA but weak reproducibility of the spectra. This was typical for the measurements in random points on the SERS substrate. However, from the results of this article it is likely that the classical spectra of the DNA molecules can be found by the SERS substrate mapping. Moreover, the prospects for the DNA detection by the SERS spectroscopy with lasers of 473, 633, and 785 nm wavelengths are very encouraging. The most promising result is in the detection of the DNA molecules at very low concentration (10^{-10} M) with the silvered PS. According to our knowledge, detection of such a small amount of DNA has not been reported elsewhere. It shows an advantage of the developed silvered PS compared to other solid SERS active substrates. Although in a competitive field, the SERS substrate based on PS is a very unusual material that can help to overcome some of the existing problems in the DNA study by SERS spectroscopy.

P Sp 4. Microbial Community From Cojocna Balneary Lakes: Rich Resource Of Carotenoids Ascertained By Resonance Raman Micro-Spectroscopy

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Resonance Raman (RR) spectroscopy of microbial community from two salt lakes known for their therapeutic benefits are reported. Our previous raw water study showed spectroscopic characteristic of the lakes, probing several water samples collected in two consecutive years. Among the two lakes, Torok Lake showed 1.1449 times higher sulfate concentration than the Grate lake in 2016 and 0.737 in 2017 respectively, according to the calculated ratio of the Raman band of sulfate at 979 cm^{-1} relative to water band which suggested different nutrients balance in the two lakes (Brezestean, et al) [1].

Here we extended the study at single microorganism's level. Microbial investigation has been achieved directly from the raw water samples collected in summer 2017, without separation or processing steps.

Microorganisms ranging in 1 to 5 μm diameter showed distinct RR spectra of carotenoids under 532 nm excitation. Analysis of the RR spectra indicated multiple deconvoluted Lorentzian components which resembled the main RR band of carotenoid attributable to the C=C stretching in the 1512-1528 cm^{-1} range. Larger microalgae, documented as Dunalliella salina [2] showed bands at 1002, 1154 and 1516 cm^{-1}, resembling the β-carotene dominant carotenoid along with lutein and zeaxanthin [2], while smaller microbial community of about 1 μm size characteristic to cyanobacteria showed bands at 1003, 1150 and 1506 cm^{-1}. Crystallized salts resulted after water evaporation showed gypsum formation as identified by Raman microspectroscopy. Raman data illustrates valuable carotenoids available in raw waters and suggests the capability to constant monitor their level and species along the seasonal variation induced by temperature and fluctuant nutrients level.

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Poster Communications

Analytical methods for (nano)biotechnology

P Nb 1. Berries Buckthorn Oil - Subcritical Fluid Extraction, Chemical Characterization And Biological Efficacy Of A Potential Food Supplement

Claudia Maria Gutu[1], Octavian Tudorel Olaru[2], Anca Ungurianu[3], Denisa Marilena Margina[3], Mihaela Ilie[1], Dumitru Lazurca[4], Monica Florescu[5]

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Sea-buckthorn has been widely used both as food and in traditional therapy. Subcritical fluid extraction (SFE) is a novel technique which provides good extraction yields and preserves the biological activity of the phytochemicals. The present study aims at the evaluation of the chemical composition of a SFE buckthorn oil and its antioxidant activity.

In order to be analyzed for the fatty acids composition by GC-MS the oil underwent a saponification process. The identification of the compounds was performed using NIST mass spectrum library. The HPTLC analysis was performed on the oil dissolved in chloroform and on the saponificated sample.

The 2, 2-diphenyl-1-picrylhydrazyl (DPPH) free radical was used to assess the free radical scavenging activity. The antioxidant activity was also evaluated with $ABTS^{\cdot+}$ and FOX-PCA assays, using standard curves obtained with ascorbic acid for DPPH and $ABTS^{\cdot+}$ and with cumene hydroperoxide for FOX-PCA.

The GC-MS analysis allowed the identification of palmitic and oleic acids as major components, followed by stearic acid. As for the phytosterols, stigmasterol was identified. The presence of beta-sitosterol was uncertain, as for neither of the three mobile phases it could not be separated from stigmasterol.

The scavenging effect of the oil against DPPH decreased with the increase of the oil dilution from 1:10 to $1:10^6$, maintaining a dose-dependency. The ABTS assay did not vary in a dose dependent manner.

In conclusion, the oil extracted from sea buckthorn berries by SFE preserves its main components (fatty acids and phytosterols), and also a high antioxidant effect.

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P Nb 2. Lavandula Oil – extraction, chemical characterization and potential biological effects

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Lavandula species and their by-products have been used in therapy since antiquity. The subcritical fluid extraction (SFE) is a new technique capable to ensure good extraction yields and also to preserve the biological activity of the extracted fraction from the vegetal product.

The aim of our study was to assess the chemical composition of an oily SFE extract from Lavandula angustifolia and to evaluate its antioxidant activity in order to extrapolate the results to clinical use.

We developed a GC-MS method as well as a TLC one that allowed us to identify and evaluate the SFE extract. The oil was rather rich in components with known beneficial biological activity having as major compounds linalyl acetate, linalool, cineole and caryophyllene oxide. The stable 2, 2-diphenyl-1-picrylhydrazyl (DPPH) free radical was used to assess the free radical scavenging activity of different dilutions of the oil in ethanol. Results indicate a good activity even at a dilution of 10^{-6} (v/v), comparable with that of 3.9 μM ascorbic acid. The antioxidant activity was also evaluated $ABTS^{\cdot+}$ and FOX-PCA assays, as compared to ascorbic acid and cumene hydroperoxide, respectively. Both indicated a pronounced antioxidant activity of the oil, even at high dilutions.

In conclusion, SFE oil extracted from Lavandula angustifolia flos provides a good product, with satisfactory antioxidant activity, which cloud be used as a herbal supplement in various diseases characterized by redox imbalance.

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P Nb 3. Antioxidant Capacity Determination by Using Nano-Oxides of MoO_3 and CeO_2

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An innovative nano-oxides based method for rapid determination of antioxidants and antioxidant capacity of food, teas, non-carbonated beverages and biological samples was studied.

The method is based on immobilization of nano-oxides of CeO_2 and MoO_3 on filter paper. The oxide nano-particle changes colour after interaction with an antioxidant by means of redox and surface chemistry reactions. The obtained sensors are scanned by a conventional office scanner and the blue colour intensity (BCI) of colour is determined. By plotting the inverse of BCI as a function of log of standard antioxidants concentration, calibration curves are obtained. The following antioxidants were studied: caffeic, chlorogenic, gallic, ellagic, tanic, rosmarinic acids, quercetin, kaempherol, apigenin, luteolin and rutin. A comparison of calibration curves for studied antioxidants by using nano-oxides of CeO_2 and MoO_3 has been made. The developed method was applied for antioxidant determination of different plant extracts.

The assay is very fast, it could be easily automated, portable, and the required instrumentation is inexpensive.

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P Nb 4. Competitive Binding of Tolmetin to b-CD and HSA

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The host–guest interaction of tolmetin (TOL) with b-cyclodextrin (b-CD) and the influence of human serum albumin (HSA) on the formation of the inclusion complex were studied by 1D and 2D NMR spectroscopy. The TOL/b-CD inclusion complex formed at a molar ratio of 1:1 with a binding constant value of 2164.5 $L \cdot mol^{-1}$. Data analysis showed that the addition of 10 $\mu mol \cdot L^{-1}$ of HSA weakened the strength of TOL binding to b-CD (K_a = 1493 $L \cdot mol^{-1}$). The interaction of TOL with HSA in the absence and presence of b-CD was studied by analyzing the fluorescence quenching data. The Stern– Volmer quenching constants and the binding constants are found to be smaller in the presence of b-CD, suggesting that b-CD hinders the strong interaction of TOL with HSA by complex formation. Additionally, the presence of b-CD does not induce conformational and microenvironmental changes on HSA.

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P Nb 5. Fabrication of Nanotrenches and Microfluidic Channels for Biomolecular Detection

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Nanoimprint lithography (NIL) is an emerging and compelling lithographic technique, which relies on the mechanical deformation of a wide range of materials (imprint resists), by using a hard mold with 3D high-resolution nanoscale features. Since its appearance, NIL has been used not only to create isolated nanopatterns, but also to fabricate unique nanoscale devices for a variety of applications including bionanotechnology, optics, and plasmonics [1]. Our aim is to develop new nanostructured devices with high resolution architecture suitable for ultrasensitive biomolecular detection. Two types of 3D, micro/nanostructures (microfluidic channels and nanotrenches) were fabricated using NIL and assessed by Scanning Electron Microscopy (SEM) technique. The protocol consisted in the identical replication of the micro/nanomotifs from a Silicon mold on flexible, transparent substrates. The single high resolution patterning step in the NIL process provides a precise and repeatable replication of the micro/nanoscale patterns, making the NIL technique much more versatile than other expensive techniques such as e-beam lithography.

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P Nb 6. Molecular Interaction between Drugs with Antimicrobial Activity and Macromolecular Receptor

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Spectroscopic investigation supported by molecular modeling methods has been used to describe the inclusion complex of β-cyclodextrin (β-CD) with 1-Methyl-1-({2-[4-(trifluoromethyl) phenyl]-1,3-thiazol-4yl}methyl)piperidinium chloride (1MPTMPC) in solution and in solid state. Solution-state complexation between the 1MPTMPC and β-CD was established using ^{1}H NMR spectroscopy and isothermal titration calorimetry (ITC). The details of β–CD/1MPTMPC molecular interaction was analyzed by ^{1}H 2D NMR allowing the proposition of an inclusion model for 1MPTMPC into β–CD. Rotating frame NOE spectroscopy (ROESY) was used to certain the solution geometry host – guest complex. The results reveal that the 1MPTMPC molecule penetrates into β–CD cavity with both aromatic and thiazol rings. From the ^{1}H NMR spectroscopic studies 1:1 complex stoichiometry was indicated and association constant value (K) was determined as 925 M^{-1}. Thermodynamic analysis using ITC revealed that the association constant was 808.8 M^{-1} with favorable enthalpy and entropy changes. These thermodynamic parameters indicate that the binding is dominated by hydrophobic interactions, which is in agreement with inclusion complex formation. Powder X-ray diffraction and DSC method were used to confirm complexation between β-CD and 1MPTMPC in the solid state. Computational molecular investigation to obtain the most probable confomation of the inclusion compound was performed using AutoDock and AutoDock Vina.

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P Nb 7. Nanoimmunosorbents based on functionalized SiO2 nanoparticles used in affinity chromatography techniques to separate antibodies from complex biological mixtures (antisera)

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The paper presents the process for the obtainment of SiO_2 (Ø=15 nm) based nanoimmunosorbents used in affinity chromatography techniques for the separation of antibodies from complex biological mixtures (antisera). The nanoimmunosorbents consists of SiO_2 nanoparticles, to which the specific antigen is covalently coupled and has the advantage of a large specific surface (> 200 m^2/g) compared to the classical affinity chromatography method. For example, using as the solid phase 1 g of nanoimmunosorbent in affinity chromatography, about 200 mg of specific antibodies can be separated in a single step. The separation operation consists in the slow passage of the complex mixture of antiserum proteins through the affinity column, where the specific antiserum antibody binds to the antigen coupled covalently to the solid phase (nanoimmunosorbent) leading to its retention, and the protein of the mixture is removed by eluting the column with an eluent (a buffer). Finally, by using an acidic eluent (e.g. glycine-HCl pH 2.8) or basic (e.g. triethylamine pH 11.5), the immune complex is dissociated and the specific antibody is collected by a fraction collector and analyzed spectrophotometrically for identification. Antibodies thus purified are used in immunochemical assays techniques like ELISA (Enzyme Linked Immunosorbent Assay), RIA (Radioimmunoassay), FIA (Fluorescent immunoassay).

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P Nb 8. Single-step Fabrication Of Silicon Nanocones For Biosensing Applications

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The fabrication of well-defined nanostructures leads to different and unique properties compared to those of the bulk material, showing high promise in the development of very versatile biosensing platforms. During the recent years, the nanostructured silicon (Si) surfaces have been successfully used as multiplexed platforms for biomedical applications. Nanostructured surfaces are of particular interest in the field of medicine, especially in various areas of healthcare: biosensing, drug delivery, biomaterials, implants therapeutics and medical devices and instruments. The purpose of this work is to optimize a single-step fabrication process of Si cones-like nanostructures on Si(111) reconstructed substrates. The substrate temperature is the most important parameter in the Si/Si growth, allowing the control of the surface nanostructuration and the occurrence of well defined nanocones. We investigate the effect of different substrate temperatures on the density and size distributions of Si nanocones formed during the molecular beam epitaxy (MBE) deposition of Si/Si(111) 7 × 7 reconstructed surfaces. The nanocones were characterized using scanning tunnelling microscopy (STM) and the height and the bottom area distributions of the Si nanocones were assessed. The obtained distributions are interrelated suggesting the self-similarity of the nanostructures grown during the deposition protocol. Moreover, depending on the envisioned application, the fabricated Si nanocones morphology can be tuned for optimal detection of low signals, in the development of molecular and biological sensors, lab-on-a-chip devices or/and point-of-care applications.

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P Nb 9. Structural and optical properties of the gadolinium-lead-borate glasses and vitroceramics

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This paper presents a study, performed by X-ray diffraction (XRD), infrared (IR) spectroscopy, ultraviolet-visible (UV-VIS) spectroscopy, electron paramagnetic resonance (EPR) spectroscopy of glasses of the general compositions $xGd_2O_3 \cdot (100-x)[4B_2O_3 \cdot Pb]$, where x=0-50 mol % Gd_2O_3, prepared by melt quenching method. IR data show that by the addition of Gd_2O_3 concentrations, oxygen atoms can accommodate by transforming some structural units $[BO_3]$ from the conversion of boroxol units into structural units $[BO_4]$, and the gadolinium ions prefer to occupy positions near the $[BO_3]$ units useful for load compensation. The ability of gadolinium ions to attract $[BO_3]$ units leads to a decrease in the degree of polymerization of the host matrix and the formation of the crystalline phases of Pb and Pb_2O in agreement with XRD data. With the addition of dopant contents in the vitroceramic matrix, an increasing tendency is observed in the intensity of UV-Vis bands centered at 245 nm. The UV-Vis band at 310 nm and attributed to Pb^{+2} ions increases in intensity with the addition of high concentrations of Gd_2O_3. The EPR spectra of Gd^{+3} ions in glasses exhibit four resonance lines situated at about g≈2, 2.8, 4.8 şi 6. The resonance signal at g≈6 suggests the presence of isolated Gd^{+3} ions in the absence of clustering, while g≈2 indicates the formation of gadolinium ion clusters. The intensity of the resonance line at g≈6 increases with the addition of gadolinium trioxide to x = 40 mol % Gd_2O_3, then for higher concentrations it decreases.

P Nb 10. Valorization of By-Product Rezulted in Processing of Milk Thistle Oil by Cold Pressing. Recovery of Silymarin

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Milk thistle (Silybum marianum (L.) Gaertneri) fruits are used in alternative *and conventional medicine*, largely for treatment of liver disorders. The main active component of this plant fruits is silymarin, a mixture of lignano-flavonoids including: silychristin, silydianin, silybin A, silybin B, isosilybin A and isosilybin B. From milk thistle fruits it is obtained a precious oil by cold-pressing and a by-product reach in silymarin (1.5 - 4.0 %).

The aim of this work was to develop a method for recovery of silymarin from the by-product resulted from processing of milk thistle oil by cold-pressing of fruits. It were used different extraction methods with common solvents and mixture of them. The main extraction conditions were studied. Silymarin content of by-product and of the obtained silymarin concentrates were evaluated by different HPLC methods. The obtained extracts and silymarin concentrates were characterized also in terms of total phenols and antioxidant capacity.

By using the developed procedure for silymarin recovery from the by-product it was obtained a silymarin concentrate with a content of silymarin more than 50%.

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P Nb 11. Exploring PNA-DNA Hybrids with a Nanopore-Based Technique

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Nanopores are considered to provide a useful, versatile, label-free technique for resolving the kinetics, sequence, structure and other molecular properties of nucleic acids, natural (DNA, RNA) or artificial (PNA). Peptide nucleic acids (PNAs) are DNA mimicking molecules, in which the deoxyribose sugar backbone is replaced with repeating uncharged N-(2-aminoethyl)-glycine units linked by peptide bonds. Herein, we designed a 10-mer PNA sequence conjugated with a polycationic peptide, used to target complementary and non-complementary DNA molecules. Upon hybridization a stable PNA-DNA duplex is obtained, with the positively charged peptide and the negatively charged DNA forming a dipole. An electric field applied across an α-hemolysin (α-HL) protein nanopore drives the PNA-DNA hybrid towards the nanopore's lumen and electrophoretically threads the positively charged PNA through the nanopore, separating it from the negatively charged DNA. Four distinct sub-states were identified along the molecular pathway of the hybrid: the capture of the hybrid by the nanopore; the escape of the hybrid without unzipping; the unzipping state, followed by the translocation of the PNA. Unhybridized PNA was still detectable, but with a very distinct signal in the ionic current through the nanopore, as confirmed by the single PNA control electrophysiology experiments. In this work we show and describe the accurate detection and the irreversible unzipping process of a PNA-DNA duplex using a single-molecule nanopore-based technique. Based on the obtained data, we proposed a kinetic model that allowed us to calculate the thermodynamic properties of the molecules, such as the unzipping reaction rate constants and the free energy barrier height for the unzipping process.

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P Nb 12. Microfluidic Portable Device for Pathogens' Rapid SERS Detection

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Label-free Surfaced-Enhanced Raman Scattering (SERS) - based detection is a very promising alternative for rapid monitoring real samples, offering single-cell sensitivity[1, 2], with no contribution from the aqueous environment and a high precision classification of bacteria, at strain level[2, 3].

Here we present a microfluidic cell design and setup for alternative pathogens' detection based on SERS technique. The innovative approach consists in the *in situ* silver nanoparticles (AgNPs) synthesis inside the microfluidic flow-cell and the signal detection by using a portable, Raman spectrometer as detector.

The proposed alternative detection method is rapid (in less than 15 minutes), highly sensitive, and culture and label-free. A microfluidic flow-cell, a flow system, and a handheld Raman spectrometer are the main components of the device. The detection protocol was optimized by testing the SERS detection of several well known pathogens, such as *Escherichia coli* (*E. coli*).

We expect that this approach will be a ready-to-use detection tool with high sensitivity (single-cell level) for the culture-free analysis of real biological samples, and high precision classification of pathogens, at strain level.

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P Nb 13. Single-Molecule Study of pH- and Salt-Induced Conformational Changes of PAMAM-G1 and -G1.5 Dendrimers, with Protein Nanopores

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Physical features of generations 1 and 1.5 poly(amidoamine) (PAMAM) dendrimers were studied at different pH's and salt concentrations, by employing the stochastic analysis of ionic current fluctuations induced by their interaction with a single α-hemolysin (α-HL) nanopore, clamped at distinct electric potentials. A change in the dendrimer's net charge, as induced by pH changes, was shown to affect the kinetics of their interaction with the nanopore, which occurred faster at acidic as compared to neutral pH's. Further to this, ionic strength- and pH-induced conformational changes in the dendrimer's structure were assessed from the analysis of dwell-times associated with dendrimers transient residence inside the nanopore. Quite unexpectedly, the PAMAM-G1.5 dendrimer, which is larger (~ 2.5 nm diameter) than the α-HL's constriction region (1.5 nm diameter), was demonstrated to squeeze through and move across the nanopore above a certain threshold of the applied electric potential, whose value was found sensitive to pH and ionic strength. We posit that the interplay between electrophoretic and electro-osmotic forces acting on the dendrimer, as well as the changes in flexibility between dendrimer's branches, strongly dictate the behavior of the PAMAM-G1 and -G1.5 in nano-confined volumes.

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P Nb 14. Study of Activated Carbon Performance For Depollution of Wastewater Containing Organic (C_6H_6 and C_6H_5-CH_3) And Inorganic (Pb^{+2} and Zn^{+2}) Pollutants

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Many heavy metals, such as lead and zinc, have been found in high concentrations in surface waters and underground water due to pollution resulting from industrial activities. The removal of toxic heavy metal ions such as lead and zinc from industrial and mining wastewaters has been widely studied because their are responsible for several types of health problems caused to animals and human beings. Also, there are many organic compounds, which must be prevented from reaching in drinking water from various sources of pollution. Between all the wastewater treatment techniquies, adsorption has multiple advantages (easy to use, cost effective and so one).

For these reasons in this paper the experiments were conducted to study the capacity of our prepared activated carbon for removal of Zn(II), Pb(II), toluene and benzene from water.

The as-prepared activated carbon samples were characterized using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX). The adsorption of Zn(II) and Pb(II) were investigated by using atomic adsorption spectroscopy (AAS) technique. The results were compared and presented in more details in the present paper.

P Nb 15. Natural Biocomposite Material with Antioxidant Properties and a Source of Valuable Compounds: the Cuticle of *Squilla mantis* Shrimp

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Bio-inspired materials are an emerging field of research and have received increasing scientific interest. Such materials have superior mechanical, optical or other advantageous properties, aimed for various biocomposite applications. Among promising candidates are the cuticles of insects and crustaceans. In this paper we present a comprehensive structural study of marine crustacean *Squilla mantis* cuticle. Molecular information on the cuticle composition was obtained using Raman spectroscopy (RS), ultrastructure was imaged using high resolution scanning electron microscopy (HR-SEM), and elemental spectroscopy and mapping was achieved using electron diffraction x-ray spectroscopy (EDX). Telson cuticle is composed mainly of amorphous calcium carbonate (ACC), with inclusions of magnesian ACC and calcium phosphate. Claw has similar composition, however, it is reinforced with higher levels of phosphates and fluoride. Cross-section of the telson cuticle exhibits a sandwich-like structure: outermost and innermost layers are hardened by calcite and phosphate, while the middle part is hollow and criss-crossed with organic fibers. The claw featured mineralised cuticle rich in P and F with organic matrix filling the space inside the conical shell. Additionally, we investigated and identified carotenoid pigment and carotenoid-protein complexes on the surface of the telson cuticle. We propose *S. mantis* cuticle as a novel biocomposite with embedded antioxidant capacity via carotenoids as well as a source of valuable compounds like chitin and carotenoids.

P Nb 16. Depollution of watewaters using nanobiotechnology based on new TiO_2 photocatalyst

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Photocatalysis has become a common word and various nanomaterials having photocatalytic functions are widely studied. Among many candidates for photocatalysis, TiO_2 is almost the only material suitable for industrial use at present. In this paper, we present the TiO2 synthesis starting from Ti sheets putted into contact with a mixture of NaOH 0.1 N and acetone for 72 hours under ambient conditions. The finally obtained sheets were washed with distilled water and ethanol and the surface was analyzed by microscopy and diffraction in order to evaluate the composition of the surface layer and the morphology. Thus, SEM and EDS results and XRD indicated the formation of TiO_2 on the edges of nanometer circles onto the surface of Ti sheets. For testing of photocatalytic capacity for wastewater treatment an amount of 1 g containing two Ti sheets having TiO_2 on the surface were contacted with a methylene blue solution of at room temperature and under UV light. The decreasing of methylene blue concentrations was investigated by Uv-Vis spectroscopy indicating the obtaining of 100% of eficiency for removing of methylene blue from wastewaters.

P Nb 17. Influence of Nanometric Tungsten Dust on Fibroblasts Cells

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In future fusion devices, like ITER, expected power and temperature of plasma that is facing the tungsten components can trigger the formation of tungsten dust in the plasma chamber. This dust, composed of tungsten particles of nanometric size (WNPs), can present safety issues in case of failure of confinement during a loss of vacuum accident (LOVA) [1] [2]. Accidental interaction of tungsten nanoparticles can be harmful for fusion workers.

In order to undertake the cytotoxicity studies, fusion devices relevant dust has been produced on purpose using MS-GAS technique [3], [4]. After that, BJ human skin fibroblast cells were treated with different concentrations of WNPs and the cytotoxicity was observed by using MTS viability assay and scanning electron microscopy (SEM). Up to 100 µg/ml WNPs, the viability of BJ cells was not significantly affected after 24h exposure to WNPs. At concentrations higher than 100 µg/ml (up to 2 mg/ml), where WNPs seem to interfere with MTS assay readings, the visualization of cells by SEM revealed that the treatment with metal nanoparticles at concentrations higher than 100 µg/ml (up to 2 mg/ml) induced the decrease of the cell proliferation (density), while the cell morphology is preserved.

In addition, the SEM imaging technique enabled visualization of nanoparticle internalization into cells exposed to high WNPs concentrations.

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P Nb 18. Physicochemical characterization of poly-L-lysine and its interactions with globular proteins

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In this research, physicochemical properties of PLL have been deeply investigated by Dynamic Light Scattering (DLS) and electrophoretic mobility. PLL monolayers onto Au surfaces in various conditions of ionic strength has been performed by Multi-Parameter Surface Plasmon Resonance (MP-SPR) and Quartz Crystal Microbalance with Dissipation Monitoring (QCM-D). The association (ka), dissociation (kd) rate constants and the affinity constant (Kd) of PLL molecules onto Au were calculated. These parameters indicate that the PLL monolayers remain irreversible adsorbed onto Au surface. Combine of results obtained by this two methods allows to determine the degree of hydration of PLL monolayers depending on pH and ionic strength. The hydrophobicity of PLL monolayers was analyse by contact angle measurements (CA). The PLL molecules have tendency to conformational changes from a random-coil to a α-helix or a β-sheet structure type. Poly-L-lysine conformation in solution and on Au surface depending on pH was studied by Circular Dichroism (CD) and Fourier Transform Infrared Spectroscopy (FTIR). Conformation changes of PLL molecules was additionally confirmed by Atomic Force Microscopy (AFM). What is more, interactions between PLL and globular proteins on Au surface was investigated by QCM-D and MP-SPR methods. The mechanisms of interaction of PLL with globular protein together with the analysis of conformational changes and reorganization of molecule structures have great cognitive value. It will also contribute to a better understanding of the physicochemical mechanisms of creating polyelectrolyte layers with controlled architecture and functionality.

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P Nb 19. The magnetic contamination of Fe_3O_4@GA against some biotic components of the environment

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This study was planned to reveal the impact of Fe_3O_4@GA NPs (suspension dilutions of 20µl/l, 40µl/l, 60µl/l, 80µl/l and 100µl/l) on the biotic components of the environment. The particles magnetic core was yielded by chemical co-precipitation method[1] and stabilized in water with Gallic acid shell[2]. The nanometric size and quasi spherical shape of synthesized particles was evidenced by TEM; crystallinity i.e. spinel structure was revealed by XRD while magnetizability, mainly superparamagnetic properties were emphasized by VSM. MNP suspensions were supplied for seven days to freshly germinated sunflower seedlings grown on watered porous paper support in Petri dishes at room temperature. The seeds were chosen from single mother plant in order to avoid genetic variability. Green tissue samples were used to extract assimilatory pigments: chlorophyll A, chlorophyll B and carotenes in acetone 90%[3]. Spectral investigation was carried out to estimate the content of each pigment type in sunflower seedling tissue for five replicates in the case of each NP suspension dilution. The noticeable effect of NPs could be related to their ability of circulate through the vascular system by means of the *plasmodesmata* channels[4], which have average diameter of 50 nm varying between 20 and 200 nm. Some NPs, with larger size, could still remain embedded in bio-membranes or in the cell cellulose wall, the local magnetic field disturbing transmembrane ion channels with influence on cell biochemistry including assimilatory pigment synthesis; the NPs that entered the green tissue cells could affect the cell biochemistry due to the catalytic effects of iron ions released from their surface.

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P Nb 20. Bacteria Involvement in Biodegradation of Chlorinated Organic Compounds in Ground Water

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Decontamination of soil and groundwater has always been a major environmentally and economically issue, being a complex process involving massive financial spendings. Considering this, the use of bacteria with in situ biodegradation capabilities of chlorinated compounds could potentially be an effective approach as long as the availability of bacterial strains and the facility of their introduction conduct to a reasonable working environment both ecologically and financially. Microbial degradation is considered a perspective solution in the elimination of micropollutant organic compounds from the environment, and can subsequently be improved by creating genetically modified or isolated bacteria by various selection methods. These processes can greatly influence the decontamination process of soils in various industrial regions of the world. According to various studies the *Pseudomonas* species enable the aerobic biodegradation of a numerous organic compounds, including chlorinated aromatic compounds. In this respect, the present study focuses on the peculiarities of the *Pseudomonas* bacterium, that demonstrates the ability to grow on various organic substrates, and thus becomes a possible candidate for dehalogenation of various types of chlorinated organic compounds. Our results showed the reduction of some compounds such as trichloroethane, tetrachloroethane, trichloromethane, and tetrachloromethane, with values ranging from 19% to 37%, over a time period of 120 days.

P Nb 21. PCB and Pesticides Monitoring and its Implications to Food Quality Assessment - Case Study on Milk

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Considering the consumer awareness for high quality and safe agro-food products, including of animal origin, this research was aimed to highlight the impact of the provenance of cow milk to its quality. Therefore, an investigation of the polychlorinated biphenyls (PCB) and pesticides (α – HCH, β-HCH, δ-HCH, Aldrin, Dieldrin, Endrin, DDE, DDD, DDT and Endosulfan) on cow milk samples collected from four different areas around Sibiu (Romania) was performed. Results showed that the minimum content of PCB and pesticides were registered in samples collected from Rasinari area, a mountain area favourable for animal breeding. The milk samples were collected during two months, in 2017, from different farmers. The statistical analysis showed that the PCB and pesticides parameters of these milk samples were significantly different (p0.05).

P Nb 22. Controlling the End-to-End Assembly of Gold Nanorods to Enhance the Plasmonic Response in Near Infrared (NIR)

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Over the past decades, there has been tremendous interest in the development of strategies to confine and enhance light at nanoscale in targeted locations ("hot-spots"). The so-called hot spots can address a large variety of applications from surface-enhanced Raman spectroscopy (SERS), plasmon-enhanced fluorescence, nanophotochemistry and nanophototherapy[1]. Their generation can result from the near-field coupling between the surface plasmon modes of the individual particles. Due to their anisotropic shape, gold nanorods (AuNRs) are well suited to yield strong field enhancements in NIR by end-to-end assembling.

Here, we report a direct approach to produce and stabilize linear assemblies of AuNRs in aqueous solution at pH=3.1 by adsorption of cysteine at the end of AuNRs. The time evolution of successively recorded extinction spectra exhibits well-definited isosbestic point at 834 nm which is consistent with a “first-order like reaction” between isolated AuNRs and end-to-end assembled nanorods as “final-products”. Interestingly, the kinetic process of the plasmonic assembly can be stopped at any moment, depending of the desired plasmonic response, by enveloping the already arranged AuNRs in poly (sodium-p-styrenesulfonate) polyelectrolyte. The formation of linear end-to-end assemblies via interparticle hydrogen bonding between cysteine linkers was confirmed not only experimentally by the occurrence of the specific NIR plasmonic band and by TEM examination, but also theoretically by finite-difference time-domain numerical simulations. Finally, a much higher electric field in the gaps between linked nanoparticles was subsequently demonstrated by SERS detection of molecules with enhancement factor better than of individual AuNRs. The development of such controllable plasmonic assemblies could benefit to the fabrication of novel optically enhanced nanodevices.

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Poster Communications

Atomic and nuclear methods

P Na 1. Assessment of Atmospheric Deposition of Trace Elements in Baku (Azerbaijan) Using Moss Bags

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In urban areas, air quality is strongly influenced by numerous anthropogenic activities. High population density, heavy traffic and domestic heating in winters in the centre, and various industrial activities at the outskirts, influence atmospheric concentrations of trace elements. For the first time the moss *Sphagnum girgensohnii* (in bags) as a biomonitor species was used to characterize different pollution sources at a local scale and long-range transport of air pollutants in Baku, the capital of Azerbaijan. Moss bags were exposed at twenty-one urban sites in the city of Baku for 3 and 6 months starting from December 2016. For elemental determination, two complementary analytical techniques were used: neutron activation analysis (NAA) and atomic absorption spectrometry (AAS)*. A total of 38 elements were determined: Na, Mg, Al, Cl, K, Ca, Sc, Ti, V, Cr, Mn, Ni, Cu*, Co, Fe, Zn, As, Se, Br, Sr, Cd,* Rb, Mo, Sb, I, Ba, Cs, La, Ce, Sm, Tb, Hf, Ta, W, Au, Pb*, Th, and U. NAA allowed determination of a large set of elements, previously not assessed in air pollution of the study area. Multivariate Statistical Analysis (Factor Analysis) was applied to characterize the potential pollution sources. For the some elements, notably Mg, Fe, Ni and Sb, higher concentrations for the six month exposure relative to the three month exposure were observed during the period December-May. Distribution maps of element-pollutants were created using modern GIS technologies.

P Na 2. Analytical Characterization and Potential Applications of Metal-Substituted Apatitic Materials

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Four types of metal substituted hydroxyapatite were obtained and characterized using Energy-dispersive X-ray fluorescence, X-ray diffraction, thermal analysis and transmission electron microscopy. From the evaluation of the potential applications (evaluation of the antimicrobial properties and the photodegradation of Methylene Blue) it can be concluded that the two applications seem to be competing. Thus, MnHAP, that showed the best degradation efficiency of MB from the substituted materials has poor antimicrobial potential against most of the studied lines, in the experimental protocols followed. Again, CoHAP, that showed antimicrobial properties against all the studied lines, in all the experimental protocols, exhibited a low degradation efficiency of MB. This can be explained by the properties of the pure material: HAP, the best studied materials for the degradation of Methylene Blue has no antimicrobial efficiency against the studied lines. Thus, from the performed experiments, it cannot be proposed a single material to be used in both applications, but rather specific materials for each targeted potential use (HAP, MnHAP or SnHAP for photodegradation experiments, respectively CoHAP for antimicrobial applications).

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P Na 3. Application of Isotopic and Elemental Profiling in Food Products and Beverages

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Isotope Ratio Mass Spectrometry (IRMS) and Inductively Coupled Mass Spectrometry (ICP-MS) are two specialized analytical techniques used in food authenticity and quality control. In the food industry, it is necessary to determine whether or not a product's actual contents agree with the labeled contents. We studied different matrices from isotopic and elemental point of view: vegetable (commercial and organic), fruits, vegetable oils, fruit juices, beverages (wines, ciders, and beers), meat, milk and dairy products. For instance, for investigated fruit juices, the results shown that most of the commercial fruit juices were made from concentrates by re-dilution with water and some of them contain corn or cane sugar. Differences between concentrations of macronutrients in juices samples indicated that fertilization or soil characteristics, as well as addition of preservative or adulterant, influence the quality and nutritional values of the product. In addition, by corroborating these two methods with chemometrics, supplementary information might be provided.

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P Na 4. Baby food supplements quality evaluation through different analytical methods

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Aroma and benefic organic compounds content give the essential character of food and provides variety and interest to what we consume. For infant baby foods are often the first complementary weaning foods; therefore, their high quality are necessary, in order to satisfy the baby's special growing needs. In present work, the contents of metals, aroma and organic compounds were investigated in different baby food supplements available in supermarkets from Romania and other countries. Volatile compounds as esters, ketones, aldehydes, alcohols, benzenic derivatives and fatty acid methyl esters content were evaluated qualitatively and quantitatively through GC-MS and GC-FID. From a totally of 37 monitored fatty acid methyl esters (FAMEs) only fifteen fatty acids were identified and quantified in baby foods, where from unsaturated fatty acids linoleic acid (C18:2n6c) was determined in higher percent (85.6 %) while from saturated fatty acids the palmitic acid (C16:0) was the most prevalent (37.1 %). Considering volatile organic aroma compounds, differences between food ingredients was also evidenced. Different chemometric methods were used for the statistical interpretation of experimental data: ANOVA test, Pearson correlation, Principal Component Analysis, and Linear Discriminant Analysis.

P Na 5. ENAA of Soil Samples from Small District of Azerbaijan: Search for Actinides

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For the first time epithermal neutron activation analysis (ENAA) at the reactor IBR-2 of FLNP JINR was applied to study elemental content of soil samples collected in Azerbaijan. Sampling sites were chosen in five different locations characterized in the interval of altitudes of 200-650 meters above the sea level, at depth of 20-30 cm in the area not affected by any mining and industrial activity. Tungsten carbide vibratory disc mill was used for grinding the samples. Thus, tungstem was excluded from the determined elements. Then samples were sieved with Retsch AS -200 sieve shaker. Triplicates of each sample (~100 mg) were subject to short (60 s) and long (3 d) irradiation in cadmium-screened channel of installation REGATA at the reactor IBR-2 [1]. A total of 48 elemental concentrations (Na, Mg, Al, S, Cl, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Zn, As, Se, Br, Rb, Sr, Zr, Nb, Mo, Ag, In, Sb, I, Cs, Ba, La, Ce, Nd, Sm, Eu, Gd Tb, Dy, Tm, Yb, Lu, Hf, Ta, W, Au, Hg, Th, and U) were determined. Quality control was provided by using NIST Standard Reference Materials (San Joaquin Soil 2709; Trace elements in Coal (Bituminous) 1632c) and IRMM (EU) BRC 667. Advantages of applying epithermal NAA are demonstrated. The results obtained were compared with the Upper Continental Core (UCC), regarding the Normal Mid Ocean Ridge Basalt (N MORB) [2].

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P Na 6. Bioactive Properties and Chemical Composition of *Juglans Regia L.* Extracts

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The chemical composition and antioxidant potential were studied in *Juglans regia* L. extracts obtained by three different methods, such as ultrasound-assisted extraction, rapid pressurized extraction at 6.7 bar, and subcritical fluid extraction (1,1,1,2- tetrafluorethane). The solvents used for the first two methods were mixtures of water and alcohol, glycerine, and propylene glycol, including 50% water *a* (pH = 5)–alcohol; 50% water *b* (pH = 9)–alcohol; 50% water *a* (pH = 5)–glycerol; 50% water *b* (pH = 9)–glycerol; 50% water *a* (pH = 5)–propylene glycol, and 50% water *b* (pH = 9)–propylene glycol. The qualitative composition of *Juglans regia* L. extracts was characterized by attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR) and Raman spectroscopy. The chemical changes induced by extraction techniques, as well as the various functional groups responsible for biological activities were noted in the range of 3600–600 cm^{-1} and also in fingerprint region of the spectra. The antioxidant activity of the extracts was assessed by the reducing power assay, the scavenging effect on DPPH (2,2-diphenyl-1-picrylhydrazyl) radicals. The total phenolics were evaluated with Folin–Ciocalteau reagent using the method described in ISO 14502-1:2005 (2005) slightly modified. The results are expressed as mg of gallic acid equivalent/g of extract (GAEs). The highest yield and most stable isolated total phenolics were obtained by subcritical fluid extraction, followed by extraction at 6.7 bar. The total flavonoid content in all extracts was measured by the aluminium chloride colorimetric assay described by authors.

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P Na 7. Isotopic and Elemental Fingerprint of Transylvanian Pork Meat

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Consumers prefer to pay a higher price for food products from a specific region. Stable isotopes and elemental composition represent powerful tools in the field of food authentication. In this study, $\delta^{13}C$, $\delta^{18}O$, and $\delta^{2}H$ values were determined, alongside with elemental (macro- and microelemental) content from Transylvanian pork meat samples in order to investigate the regional origin of these products and trace pork diet. Chemometric methods were used to highlight significant regional differences among studied parameters and to identify the best discrimination markers for pork meat origin. The isotopic composition of oxygen and hydrogen was determined from the water extracted from meat samples, by cryogenic distillation without isotopic fractionation. The analysis was made by using a Liquid-Water Isotope Analyzer (DLT-100, Los Gatos Research). $\delta^{18}O$ and $\delta^{2}H$ values ranged from -7.3 to -5.4 ‰, and from -54.8 to -33.2 ‰, respectively. The isotopic fingerprint of carbon varied between -24.1 to -20.0 ‰, and the measurements were carried out on an Elemental Analyser, coupled with an isotope ratio mass-spectrometer IRMS (Delta V Advantage, Thermo Scientific). For elemental determinations, a ICP-MS (Elan DRC-e, Perkin Elmer) was used.

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P Na 8. Pollution Effects on Painted Pottery of Romanian Cultural Heritage

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The physical and chemical composition of archaeological ceramics is significantly altered by the life cycle of the artefacts, starting with the production process and use to the post-depositional modification and pollution is a reality. In the Transylvanian Neolithic, the Lumea Nouă communities are considered the creators of an elegant painted pottery. The eponym site is Alba Iulia-*Lumea Nouă*, discovered by chance in 1942, while carrying out some town planning works. From the chronological point of view, the Neolithic communities who have produced this type of pottery are included in the time frame 5200-4900 BC. The origins of this type of painted pottery are still controversial. This study aims to investigate a possible link between the painted pottery from the Alba Iulia-Lumea Nouă settlement and the potential clay sources identified in the proximity of the archaeological site considering the anthropic pollution. In order to establish some correlations between clay source and pottery composition, two analytical techniques (attenuated total reflection - Fourier transform infrared spectrometry and scanning electron microscopy coupled with energy dispersive spectrometry) have been used. The recorded data show similarities for both techniques and give preliminary information regarding the clay composition used for pottery manufacturing in middle Neolithic. Cluster analysis using Average Linkage method correlated the clay sources with the analysed painted pottery. Despite the limited numbers of samples, the archaeometric results indicate that there is an obvious link between the analysed Lumea Nouă painted pottery and two of the selected clay sources from Alba Iulia-*Lumea Nouă* archaeological site. Some of the local clay sources could have been considered the suitable raw material used for the Lumea Nouă pottery type production. However, further determinations performed on a larger set of painted ceramic samples are needed in order to confirm this state of the research.

P Na 9. Active Moss Biomonitoring With Moss *Sphagnum Girgensohnii* in the Park of Moscow

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Quality control of atmospheric air is a priority topic for monitoring the environment [1]. There is a great need for rapid and cost-effective control of atmospheric pollution. The protected and park zones play a recreational role, therefore the assessment of air quality in this area is especially important. For the first time active biomonitoring (moss bags technique) was applied in Moscow, at the state museum-reserve Tsaritsyno. As a bioindicator the moss Sphagnum girgensohnii was chosen. This species was collected in a pristine wetland area Domkino Bay, near Dubna, Russia. S. girgensohnii was bagged and exhibited at 3 locations of Tsaritsyno from June to September of 2017. The goal of this pilot study was to assess air pollution with trace elements from potential pollution sources in Moscow. A total of 34 chemical elements: Na, Mg, Al, Cl, K, Ca, Sc, V, Cr, Mn, Fe, Co, Ni, Zn, Se, As, Br, Rb, Mo, Sr, Sb, I, Ba , Cs, La, Sm, Tb, Ce, Hf, Ta, W, Au, Th, and U were determined in the exposed samples by neutron activation analysis at the reactor IBR-2 of FLNP, JINR, and three environmentally meaningful elements: Pb, Cu, and Cd were determined by atomic absorption spectrometry in the same laboratory. The obtained results were compared with the analogous ones for Belgrade, Serbia, carried out with the same moss and exposure time [2].

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Poster Communications

Biomembranes and model membranes

P Bm 1. Penetrating Properties of LyP-1 Homing Peptides in Giant Unilamellar Vesicles

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Tumor-homing peptides are of particular interest in the development of new drug delivery systems due to their property to specifically bind to tumors. Drugs, fluorophores, nanoparticles or other cargos attached to penetrating homing peptides were successfully delivered into cancer cells. LyP-1 is a 9-amino-acid cyclic peptide that binds specifically to the p32 receptor overexpressed in breast cancer, osteosarcoma, metastatic lymph nodes and atherosclerotic plaques, or prostate cancer, but does not bind to normal cells. Its linear truncated form, tLyP-1 peptide, shows specificity for neuropilin receptors which are overexpressed in tumor vasculature, breast cancer, prostate carcinoma and glioma tumor tissue. Although the receptors for these peptides were identified, the molecular mechanisms involved in ligand recognition and membrane penetration are not fully understood yet.

Herein, we use the well-defined model membranes giant unilamellar vesicles (GUVs) and confocal fluorescence microscopy to study the interaction between fluorescently labeled LyP-1 and tLyp-1 peptides and lipid membranes, in order to prove and understand their direct membrane penetration, in the absence of endocytic entry factors and receptors. GUVs were generated by the electroformation method using lipids that usually compose the cell membrane: phosphatidylcholine (PC), phosphatidylserine (PS), phosphatidylethanolamine (PE) and cholesterol.

Our experimental results reveal that peptides adsorb and translocate across membranes of GUVs with different lipid composition, suggesting that these peptides have also a passive, energy-independent mechanism of uptake. Data showed that the linear form of the peptide, tLyP-1, has an enhanced penetration efficiency compared to the cyclic LyP-1 peptide.

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P Bm 2. Investigation of molecular interactions between antimicrobial peptides and biomimetic lipid membranes

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Antimicrobial peptides (AMPs) are molecules synthesized by living organisms as the first line of defence against bacteria, fungi, parasites, enveloped viruses, or tumor cells. Herein, we use atomic force microscopy (AFM) to probe at single-molecule level the interaction between a selected AMP (magainin II) and supported lipid bilayers (SLBs) of various compositions. Magainin II, a 23-amino-acid, cationic, amphipathic antimicrobial peptide, was chemically bound to an amino-functionalized AFM tip via a flexible bi-functional PEG linker. Investigation of molecular interaction force between one single magainin II peptide attached to the surface of the AFM tip and lipid membranes composed of either neutral phosphatidylcholine (PC), or a mixture of PC and 40 mol% anionic phosphatidylglycerol (PG), was performed via atomic force spectroscopy measurements. Recorded force curves show that magainin II interacts by long range electrostatic attraction forces with negatively charged bilayers (mimicking bacterial membranes), highlighting the role of anionic lipids in the selectivity of AMPs. Statistical analysis of the adhesion force curves recorded upon retraction of the AFM probe allowed us to determine the strength of the binding interaction between a single peptide molecule and the biomimetic membrane, which was found to be approximately 60 pN in the case of negatively charged lipid membranes.

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P Bm 3. Spectral study of model membrane fluidity using a fluorescent marker

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Measuring the spectral characteristics of the fluorophore molecule is a method for obtaining information about the marker location in the cell membrane bilayer. As fluorescent probe is used 1,6-diphenyl-1,3,5-hexatriene (DPH) with special properties depending on the surrounding factors. The spectral modification in the electronic spectra can be correlated with the depth of DPH bounding in bilayer and the environmental factors.

P Bm 4. Evaluation of Lipid Membrane Tryptophan Rich Peptides Bound Fraction by Fluorescence Spectrum Deconvolution

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Most of the fluorophores produce asymmetric emission spectra even in homogenous solution where only one emitting state is expected to be present. This originates from the differences in vibrionic level distributions between ground and excited states (1). An appropriate description of this asymmetric shape in absorption (2) and emission (3) spectra is given by a log-normal function. The aim of this study is to obtain information about the fractions of tryptophan residues populations (bound and unbound to a lipid membrane) by analyzing the emission spectrum from a peptide interacting with lipid membranes.

Fluorescence spectra of tryptophan was deconvoluted as Burstein proposed (4) considering the complex emission spectrum as a superposition of log-normal functions:

$$\begin{cases} I = I_m * \exp\left[-\frac{ln2}{ln^2(\rho)} ln^2\left(\frac{a-\upsilon}{a-\upsilon_m}\right)\right] if\ \upsilon < a \\ I = 0 \qquad\qquad\qquad\qquad\qquad if\ \upsilon \geq a \end{cases} \qquad (1)$$

where: I is the emission intensity, I_m is the maximum of intensity, υ is the wavenumber, υ_m is the position of the peak, $\rho = ((\upsilon_m - \upsilon_{min})/(\upsilon_{max} - \upsilon_m))$ is the asymmetry of the function and $a = \upsilon_m + \frac{(\upsilon_{max} - \upsilon_{min})\rho}{(\rho^2 - 1)}$ is the function limiting-point position.

The peptide used was Indolicidin, a 13-residue antimicrobial peptide containing tryptophan (5 residues). The model membranes consist in liposomes prepared using neutral DOPC and negatively charged DOPC-DPPG (85:15 mol) mixtures.

The results showed that changes in fluorescence spectra of tryptophan can be used to evaluate the relative proportion of fluorophore interacting with the lipid bilayer.

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Index of Authors

Sanda	Boca-Farcau	K7
Mircea	Bogdan	P Nb 4, P Nb 6
Jocelyne	Bosson	P Nb 22
Ioan	Botiz	O8
Izabella	Brand	O1
Radu Tiberiu	Brătfălean	P Nb 8
Christopher	Brett	O4, P Bm 16
Ioana	Brezestean	O11, P Mf 5, P Sp 4, P Nb 15
Elena	Brinduse	O2
Ioan Alin	Bucurica	P Na 8
Luiza	Buimaga-Iarinca	O16, P Bp 5, P Si 1
Oana Catalina	Bute	O26
C		
Violeta	Calin	O20
Andreea	Campu	K7, O8, P Bm 7, P Nb 22
Lavinia	Carpen	P Nb 17
Maria Paz	Carrasco	K2
Einat	Chetrit	I4
Claudia	Chilom	P Mf 8, P Nb 17
Mauro	Chinappi	P Bp 3
Horia	Chiriac	O18
V	Chis	P Nb 15
Dorota	Chudoba	I6.
Simona	Cinta Pinzaru	O11, P Mf 5, P Sp 4, P Nb 15
Corina	Ciobanasu	I2, P Mm 1
Mihaela	Ciopec	P Bm 22
Andrei	Ciuca	I2, P Nb 11, P Nb 13
Irina	Codita	O10
Alia	Colnita	O16, P Sp 2, P Nb 5, P Nb 8, P Nb 12
George	Coman	P Bm 18
Cristin	Coman	P Ma 1, P Ma 2
Francisco	Conejero-Lara	K2
Cristina	Constantin	P Mf 8
Maria	Coros	P Bm 2, P Bm 3, P Bm 4, P Bm 5, P Bm 6, P Bm 9, P Bm 11
Diana	Cotoros	O22, P Mf 4, P Mf 9, P Mf 10
Florina	Covaciu	P Na 3
Cristina	Covaliu	O12, P Nb 14, P Nb 16
Ionut	Cozar	P Sp 2
Dorina	Creanga	P Bm 12, P Nb 19
Cecilia	Cristea	I3, P Bm 17
Gabriela Ioana	Cristea	P Na 3, P Na 4, P Na 7
Daniel	Cristea	P Bm 24
Ramona	Cristea	P Nb 21
Cristina	Croitoru	P Ma 6
Rita	Csepregi	P Bm 20
Monica	Culea	P Bp 1
Eugen	Culea	P Nb 9
D		
Monica	Dan	P Bm 9
Andrei-Florin	Danet	O6, P Nb 3, P Nb 10

George	Danila	P Ma 4
Sourav	Das	P Bm 13
Melinda	David	O4, O6, P Bm 16, P Ma 8
Leontin	David	P Mf 5, P Sp 4
Adriana	Dehelean	P Nb 9, P Na 3, P Na 4
Colm	Delaney	O25
Bruno	Demé	O21
Victor	Diculescu	O7
Nicoleta	Dina	P Bm 9, P Sp 2, P Nb 12
Gheorghe	Dinescu	P Nb 17
Anca	Dinischiotu	O15
Lia Mara	Ditu	P Na 2
Ioan	Dorobantu	P Nb 7
Dana	Dorohoi	O17, P Mf 1, P Mf 3, P Mm 3
Nelya	Doroshkevich	P Sp 3
Tristan	Doussineau	K1
Claudia	Dragan	P Bm 21, P Nb 16
Constantin	Draghici	P Ma 5, P Ma 6
Isabela	Dragomir	P Bp 3, P Mm 1
Elena-Carmina	Dragulescu	O10
Corneliu	Drugă	O22, O23, P Mf 4, P Mf 9, P Mf 10, P Mf 11
Philippe	Dugourd	K1
Ioana Daniela	Dulama	O26, P Na 6, P Na 8
Florea	Dumitrascu	P Ma 5, P Ma 6
Ceren	DURMUS	P Bm 14
Narcis	Duteanu	P Bm 22
E		
Adrian	Enache	O9
Ionut	Enculescu	O7
Takeshi	Endo	P Bm 14, P Bm 15
Antoaneta	Ene	O26
Mihaela	Ene	P Ma 2
Petru	Epure	O2
Alexandru	Evanghelidis	O7
F		
Anca	Farcas	O16, P Si 1
Alexandra	Farcas	O19, P Bp 5
Cosmin	Farcau	K7
Ioana	Feher	P Na 3, P Na 4, P Na 7
Bogdan	Feier	P Bm 17
Marilena	Ferbinteanu	P Ma 5, P Ma 6
José	Ferreira	K9
Radu Claudiu	Fierascu	P Na 2
Irina	Fierascu	P Na 2
Eva	Fischer-Fodor	O16
Calin G.	Floare	P Bp 5, P Nb 4, P Nb 6
Larisa	Florea	O24
Monica	Florescu	O4, O6, P Mf 12, P Bm 24, P Ma 8, P Nb 1, P Nb 2, P Na 6
Monica	Focsan	K7, O8, P Bm 7, P Nb 22
Liliana	Foia	O17

Vincent	Forge	K1, K4
Luminiţa	Fritea	I3
Marina	Frontasyeva	P Na 1, P Na 5, P Na 9
G		
Ana	Gabudean -Craciun	K7
Iulia	Gageanu	O12
Olivier	Gallet	K1
Aydan	Garibli	P Na 5
Adil	Garibov	P Na 5
Yuval	Garini	I4
Szilveszter	Gáspár	O3
Cristian	Gavat	O14, P Mf 2
Zoltán	Gazdag	P Bm 13
Costinela Valerica	Georgescu	O14, P Mf 2
Stefan	Gergely	P Bm 3
Ana	Gherman	P Sp 2, P Nb 12
B.	Glamuzina	P Nb 15
Mihai	Gligor	P Na 8
Maria	Gorea	P Mf 5
Cătălin	Gradinaru	P Bm 18
Irina	Gradinaru	O17, P Mm 3
Claudiu	Gradinaru	I1
Marian	Grigoras	P Nb 19
Zinar	Gumus	P Bm 14
Simona	Gutoiu	P Bm 1
Claudia Maria	Gutu	P Nb 1, P Nb 2
H		
Alexandru	Hada	P Ma 7
Orxan	Hajiyev	P Na 1
Sevinj	Hajiyeva	P Na 1
Nicolae	Har	P Mf 5
Daniel	Herea	O18
Györgyi	Horváth	P Bm 13
Kalina	Hristova	K7
Iosif	Hulka	P Nb 14
Ion	Hurjui	O17, P Mf 1, P Mf 3, P Mm 3
Loredana	Hurjui	O17, P Mf 1, P Mf 3, P Mm 3
I		
Madalina	Ignat-Barsan	O4
Luisa	Ilie	P Ma 6
Mihaela	Ilie	O15, P Nb 1, P Nb 2
Rodica-Mariana	Ion	P Bm 10, P Na 8
Roxana	Ionete	P Nb 21, P Nb 20
Daniela	Ionita	P Ma 1
Andreea	Iordache	P Bp 1
Mihaela	Iordache	P Bm 19
Andreea	Iorgu	O13

J		
Barbara	Jachimska	O1, P Nb 18
Lorant	Janosi	P Bp 5, P Si 1, P Si 2
Andrei	Juncu	P Ma 5
Samuel	Jurado-Urdiales	K2
K		
Inna	Kamanina	P Na 9
Iren	Kasco	P Nb 6
Anne	Kenworthy	P4
Alex	Komin	K7
Paulina	Komorek	O1, P Nb 18
Tomáš	Kondela	O21
Tamás	Kőszegi	P Bm 13, P Bm 20
Eugenia	Kovacs	O20
Melinda	Kovacs	P Na 4
Danila	Kozhevnikov	I5
Norbert	Kučerka	O21
Alexander	Kuklin	P Bm 12
L		
Luminita	Labusca	O18
Paris	Lavin	P Bp 2
Mihaela Diana	Lazar	P Bm 1
Dumitru	Lazurca	P Nb 1, P Nb 2, P Na 6
Małgorzata	Lekka	P Nb 18
Ecaterina	Lengyel	P Nb 20, P Nb 21
Nicolae	Leopold	P Nb 12
Cristian	Leostean	P Bm 1, P Bm 8
Johanne	Leroy-Dudal	K1
Emilia	Licarete	P Ma 7
Fred	Lisdat	P5
Simona-Carmen	Litescu	P Nb 3, P Nb 10
Tudor	Luchian	I2, P Bp 3, P Nb 11, P Nb 13, P Mm 1
Ildiko	Lung	P Bm 1
Nicoleta	Lupu	O18, P Nb 19
M		
Sergiu	Macavei	P Bm 8
Afag	Madadzada	P Na 1, P Na 5, P Na 9
Dana Alina	Magdas	P Na 4, P Na 7
Lidia	Magerusan	P Bm 2, P Bm 3, P Bm 4, P Bm 5, P Bm 6
Kahramon	Mamatkulov	P Sp 3
Carmen	Manea	P Mf 6, P Mf 7
Dana	Maniu	K7
Daniel	Marconi	P Nb 5, P Nb 8, P Nb 12
Denisa Marilena	Margina	P Nb 1, P Nb 2
Maria	Marinescu	P Ma 5
Christel	Marquette	K1, K4
Sara	Marsango	P1
Elisha	Martin	O1
Mihai	Matache	O12

André	Matagne	K5
Ecaterina	Matei	P Bm 18, P Bm 21, P Nb 14, P Nb 16
Cristian	Matei	O13
Elena	Matei	P Nb 17
Carole	Mathevon	K1
Mátyás	Meggyes	P Bm 13
Loredana	Mereuta	I2, P Nb 13
Mihaela	Mic	P Nb 4, P Nb 6
Maria	Miclaus	P Nb 6
Luminita C.	Miclea	O13
Mona	Mihailescu	O20
Maria	Mihăilescu	P Bm 22
Mirela	Mihon	P Mf 6, P Mf 7
Graeme	Milligan	P1
Ioan	Milosan	P Bm 24
Valentin	Mirel	P Bm 2, P Bm 4, P Bm 6, P Na 7
Marius	Miricioiu	P Bm 19, P Bm 23
Maria	Mitrica	P Ma 3
Corina	Moga	O12
Marius	Moga	P Mf 12
Mihaela	Moisescu	O13, O20
Flaviu	Moldovan	P Ma 3
Lucia	Moldovan	P Ma 6
Antonio	Mondini	P Bp 2
Cristian	Morari	O16
Bertrand	Morel	K2
Cristina	Muntean	P Bm 9
Raluca-Elena	Munteanu	O3
Teodora	Murariu	O8
N		
Jalal	Nagiyev	P Na 5
Livia	Neagu	P Nb 7
Silvia	Neamtu	O16, P Nb 4
Radu Dan	Necula	O22, O23, P Mf 4, P Mf 9, P Mf 10, P Mf 11
George	Necula	P Si 2
Adina	Negrea	P Bm 22
Petru	Negrea	P Bm 22
Fran	Nekvapil	O11, P Sp 4, P Nb 15
Cristian Andi	Nicolae	P Na 2
Dana	Niculae	P Mf 6, P Mf 7
Violeta	Niculescu	P Bm 19, P Bm 23
Guy	Nir	I4
Ioana	Nitu	P Ma 3
Hugo	Novais	P Bm 16
O		
Octavian Tudorel	Olaru	P Nb 1, P Nb 2
Radu Lucian	Olteanu	P Na 6, P Na 8
Lacramioara	Oprica	P Bm 12
Ocsana	Opris	P Bm 1
Filip	Orzan	O8

P		
Constantin	Paladi	P Nb 20
Mariana	Palage	P Nb 6
Ovidiu	Pana	P Bm 1, P Bm 8
Jonathan	Pansieri	K1, K4
Cristian	Pantilimon	P Bm 18
Gigel	Paraschiv	O12, P Nb 14
Yoonkyung	Park	P Bp 3, P Nb 11, P Nb 13
Bianca	Patrascu	P Ma 5
Nadia	Paun	P Bm 19, P Bm 23
Sergey	Pavlov	P Na 9
John	Pediani	P1
Georgiana	Petrareanu	O5, P Bp 2
Maria	Pica	P Nb 9
Adrian	Pirnau	P Nb 4, P Nb 6
Paula	Podea	P Bp 1
Florina	Pogacean	P Bm 2, P Bm 3, P Bm 4, P Bm 5, P Bm 6, P Bm 11
Mihai-Alin	Pop	P Bm 24
Georgiana	Popa	P Ma 6
Adrian-Claudiu	Popa	K9
Claudia Valentina	Popa	P Nb 3, P Nb 10
Adriana	Popa	P Bm 8
Larisa	Popescu	P Bm 12, P Nb 19
Bianca Elena	Popovici	P Ma 3
Alin Sebastian	Porav	P Bp 5, P Bm 1
Roxana	Porumb	O2
Monica	Potara	K7, P Ma 7
Veronica	Preda	P Ma 5
Andra	Predescu	P Bm 18, P Bm 21, P Nb 16
Cristian	Predescu	P Bm 18, P Bm 21, P Nb 16
Doina	Prodan	P Bm 11
Stela	Pruneanu	P Bm 2, P Bm 3, P Bm 4, P Bm 5, P Bm 6, P Bm 11
Mihaela	Puiu	P Ma 4
Cristina	Purcarea	O5, P Bp 2
Carmen	Purdel	O15
Romulus	Puscas	P Na 3, P Na 7
R		
Simona	Rada	P Nb 9
Alina	Raditoiu	P Na 2
Valentin	Raditoiu	P Na 2
Ecaterina	Radu	O18
Mihai	Radu	O10, P Si 2, P Mm 4
Stelian	Radu	P Na 7
Cristiana	Radulescu	O26, P Na 6, P Na 8
Monica	Raduly	P Na 2
Ana-Maria	Raicu	P Bp 4
Valerica	Raicu	K8
Maria	Râpă	P Bm 18, P Bm 21
Bertrand	Raynal	K5
Angela	Repanovici	P Mf 4, P Mf 9
Ileana	Roşca	O22, O23, P Mf 11

Aldo	Rossini	P Bp 3
Marcela-Corina	Rosu	P Bm 2, P Bm 4, P Bm 11
Gerlinde	Rusu	P Bm 22
David	Ruzafa	K2
S		
Liviu	Sacarescu	P Nb 19
Robert	Sandulescu	I3, P Bm 17
Tudor	Savopol	O13, O20
Diana	Savu	P Nb 17
Eugen	Scarlat	O20
Irina	Schiopu	I2, P Nb 11, P Nb 13
Marius	Schmidt	P2
Chang Ho	Seo	P Nb 11, P Nb 13
Ionel	Serban	O22, O23, P Mf 4, P Mf 9, P Mf 10, P Mf 11
Adrian	Serban	O6, P Mf 12
Ionela	Serban	O17, P Mm 3
Georgy	Shelkov	I5
Margarita	Shvetsova	P Na 1, P Na 9
Teofil-Danut	Silipas	P Bm 1, P Bm 8
Timea	Simon	K7
Lucel	Sirghi	P Mm 2
Mirela	Sohaciu	P Bm 21
Raluca	Somoghi	P Na 2
Maria-Loredana	Soran	P Bm 1
George	Stan	K10
Manuela	Stan	P Bm 1, P Bm 8
Anca	Stanciu	P Mf 10
Maria	Stefan	P Bm 8
Adina	Stegarescu	P Bm 1
Diana	Stegarus	P Nb 20, P Nb 21
Claudia	Stihi	O26, P Na 6, P Na 8
Raluca Maria	Stirbescu	P Na 6, P Na 8
Robert	Stokłosa	P Nb 18
Michael	Stoneman	K8
Marianta	Strinoiu	P Ma 5
Sorina	Suarasan	K7, P Ma 7
Maria	Suciu	P Nb 5
Alexandru	Suciu	P Nb 10
Cristina	Surdu-Bob	P Ma 1, P Ma 2
Laurentiu	Susu	P Bm 7
Niculina-Sonia	Suvar	P Bp 1
Laszlo	Szabo	P Nb 12
Lajos	Szente	P Bm 13
Tiberiu	Szoke-Nagy	O16, P Sp 2, P Nb 12
T		
Viorica	Tamas	P Nb 10
Alina	Tantau	P Mf 5
Isabela	Tarcomnicu	P Ma 5
Rodica	Tatia	P Ma 6
Viktória	Temesfői	P Bm 20

Sofia	Teodorescu	P Na 6, P Na 8
Mihaela	Tertiş	I3
Mihai	Tibu	O18
Leopold	Tie	P Nb 22
Suna	Timur	P Bm 14, P Bm 15
Cristian	Tira	P Nb 22
Ana Maria	Titoiu	O2, O5
Mircia	Toderici	P Nb 21
Dana	Toloman	P Bm 8
Sebastian	Toma	O11, P Mf 12
S	Tomšić	P Nb 15
Nicoleta	Tosa	P Bm 9
Bogdan	Trica	P Na 2
Cristian	Tudoran	
Ioan	Turcu	O8, O16, P Si 2, P Bm 9, P Nb 5, P Nb 8
Danut	Turcu	P Ma 2
Alexandru	Turza	P Bm 5, P Bm 9, P Bm 11
Catalin	Tuta	P Mf 6
U		
Anca	Ungurianu	P Nb 1, P Nb 2
V		
Pankaj	Vadgama	K6
Eugeniu	Vasile	O12
Alina	Vasilescu	O2, O5, P Bp 2, P Nb 3
Zarifa	Veliyeva	P Na 1
Charlotte	Vendrely	K1
Konstantin	Vergel	P Na 9
Diana	Visinescu	O5
Anat	Vivante	I4
Ene	Vlase	P Ma 1, P Ma 2
Cezara	Voica	P Na 3, P Na 7
Doina	Voinescu	O14, P Mf 2
Adriana	Vulpoi	P Ma 7, P Nb 22
W		
Monika	Wałek	O1
Richard	Ward	P1
Gregory	Wiedman	K8
William	Wimley	K8
Y		
Yusuf	Yagci	P Bm 14, P Bm 15
Shuhei	Yamada	P Bm 14, P Bm 15
Z		
Mioara	Zagrai	P Nb 9
Christina	Zalaru	P Ma 5, P Ma 6
Lucian	Zamfir	P Ma 4
Joanna	Zemła	P Nb 18
Alexey	Zhemchugov	I5
Bogdan	Zorila	P Mm 4
Florina	Zorila	P Ma 2

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