***TRANSILVANIA* UNIVERSITY OF BRAŞOV**

International Conference on

Analytical and Nanoanalytical Methods

for

Biomedical and Environmental Sciences

IC-ANMBES 2016

BOOK OF ABSTRACTS

Braşov, June 29th-July 1st, 2016

Editors: *Monica Florescu*
Séverine Le Gac
Valerică Raicu
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Transilvania University Press

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SCIENTIFIC PROGRAMME

ORAL COMMUNICATIONS

June 29th 2016	**Building *Aula Magna* of Transilvania University of Brasov. 41 A Iuliu Maniu Street, Brasov, 500091, Romania.**			
	Room UI7, Chairperson: Monica Florescu			
15.30-17.30			**Registration**	
17.30-17.40			**Opening Ceremony**	
17.40-18.20	Plenary Lecture	P1	Kalina Hristova,	Probing the Early Stages of Receptor Signalling with Quantitative Fluorescence Techniques
18.20-19.00	Plenary Lecture	P2	Caroline Montagner , Michaël Nigen , Olivier Jacquin , Gordon C.K. Roberts , Christian Damblon , Christina Redfield , André Matagne*	The Role of Active Site Flexible Loops in Catalysis and of Zinc in Conformational Stability of Bacillus cereus 569/H/9 β-lactamase
19.00-20.00			**Welcome Party and Poster Session (odd numbers)**	

June 30th, 2016	**Building *Aula Magna* of Transilvania University of Brasov. 41 A Iuliu Maniu Street, Brasov, 500091, Romania.**			
	Room UI2, **Chairperson: Kalina Hristova,**			
9.00-9.40	Plenary Lecture	P3	Leon WMM Terstappen*	Interrogation of Circulating Tumor Cells a tool towards personalized medicine
	Room UI2, Nanobiotechnology, Chairperson: Leon WMM Terstappen,			
9.40-10.10	Keynote,	K1	Rodica-Mariana Ion	Bio-Nanotechnology SS Enhancer in Photodynamic Therapy
10.10-10.40	Keynote,	K2	Aram J Krauson , Morgan Hall , Charles G Starr , Taylor Fuselier , W. Berkeley Kauffman , William C Wimley*	Conformational Fine-tuning of the Membrane Selectivity of Pore-forming Peptides.
10.40-11.05	Invited talk	O1	Ionel Popa	The Nano-Mechanics of Single Proteins
	Room UI3, Spectroscopy, Chairperson: Kalina Hristova			
9.40-10.10	Keynote,	K3	Valerică Raicu	Probing Association and Dissociation of Proteins in Living Cells: Toward Multi-Dimensional FRET Spectrometry
10.10-10.35	Invited talk	I1	Ronen Berkovich	Reconstruction Surface Potential from Atomic Friction Measurements

10.35-10.55	Contributed talk	O2	Violeta L. Calin*, Mona Mihailescu , Nicolae Mihale , Eugenia Kovacs , Tudor Savopol , Mihaela G. Moisescu	Optical and Electrical Biophysical Methods for Identification of Cellular Malignancy
11.00-11.30	**Coffee Break and Poster Session (odd numbers)**			
	Room UI2, Analytical methods for medical physics, Chairperson: Ioan Turcu,			
11.30-12.00	Keynote,	K4	Yuri Feldman	Unexplored Avenues of Human Skin: Reading Personal Stress in the Sub-THz Frequency Range
12.00-12.25	Invited talk	I2	Horia I. Petrache*, Merrell A. Johnson , Stephen R. Wassall , Bruce D. Ray	Interactions of Amino Acids with Lipid Membranes
12.25-12.45	Contributed talk	O3	Mihaela Georgeta Moisescu*, Bogdan Mircea Matei , Fawzia Sha'at , Luminita Claudia Miclea , Andreea Iulia Iorgu , Laura Georgiana Bajenaru , Lucia Pirvu , Cristina Hlevca , Cristian Matei , Dana Berger , Ramona Daniela Pavaloiu , Tudor Savopol	Impedance-based Real-time Monitoring of Cellular Growth for Phytotherapeutic Extracts and Porous Artificial Drug Carriers
12.45-13.05	Contributed talk	O4	Eugen Gheorghiu*, Cristina Polonschii , Sorin Mihai David, Mihaela Gheorghiu , Mihnea Rosu-Hamzescu , Dumitru Bratu	Plasmonic based EIS: towards a sensitive analytical method gathering the virtues of both SPR and EIS
	Room UI3, Microfluidics and point-of-care microdevices, Chairperson: Séverine Le Gac,			
11.30-12.00	Keynote	K5	Holger Becker	Microfluidics – 25 Years of Hype, Hope and Hubris
12.00-12.25	Invited talk	I3	Davide Ferraro , Jerome Champ , Bruno Teste , Marco Serra , Laurent Malaquin , Jean-Louis Viovy , Patricia DeCremoux , Stephanie Descroix*	Droplet Microfluidics Applied to HER2 Gene Expression in Breast Cancer
12.25-12.45	Contributed talk	O5	Wayne Francis , Colm Delaney*, Larisa Florea , Dermot Diamond	Chemotactic Ionic Liquid Droplets: Striving to Mimic Nature
12.45-13.05	Contributed talk	O6	Jennifer Deignan*, Larisa Florea , Shirley Coyle , Dermot Diamond	Contactless Conductivity Sensor for Wearable Sweat Monitoring
13.00-14.00	**Lunch**			
	Room UI2, **Chairperson: Valerică Raicu**			

14.00-14.40	**Plenary Lecture**	**P4**	Marius Schmidt	Ultrafast Dynamics in Proteins Investigated by Time-Resolved Serial Femtosecond Crystallography
	Room UI2, **Analytical methods for medical physics, Chairperson: Valerică Raicu**			
14.40-15.10	Keynote	K6	Paul Shin-Hyun Park*	Atomic Force Microscopy-Based Approaches to Probe the Structure of Membrane Proteins
15.10-15.35	Invited talk	I4	Raluca Ioana Stefan-van Staden	A New Approach on Biomedical Analysis
15.35-15.55	Contributed talk	O7	Diana David-Rus*, Afrodita Liliana Boldea	Data mining and statistical methods that might help in understanding fluorescence experiments
15.55-16.15	Contributed talk	O8	Laura Zelencova , Raminta Rodaitė-Riševičienė , Viktorija Skaidrutė Dainauskaitė , Simona Kalibataitė , Gintautas Saulis*	The Influence of Medium on Amplex Red as Indicator for Fluorescent Hydrogen Peroxide during High-Voltage Electric Impulses
	Room UI3, **Medical analysis and diagnosis, Chairperson: Séverine Le Gac,**			
14.40-15.10	Keynote	K7	Lourdes Basabe-Desmonts	Self-powered Microfluidics for Point of Care Analysis
15.10-15.35	Invited talk	I5	Valérie Taly	Microfluidics for cancer research
15.35-16.00	Invited talk	I6	Govind Kaigala	Hydrodynamic Shaping of Sub-Nanoliter Volumes of Liquids at Biological Interfaces for Tissue Microprocesing and Biopatterning
16.00-16.45	**Coffee Break and Poster Session (even numbers)**			
	Room UI2, **Sensors and biosensors, Chairperson: Raluca Ioana Stefan-van Staden**			
16.45-17.15	Keynote	K8	Amina Rhouati , Akhtar Hayat , Gaelle Catanante , Jean Louis Marty*	Are Biosensors Right Tools For Food Contaminants Monitoring
17.15-17.35	Contributed talk	O9	Danielle Bruen*, Larisa Florea , Colm Delaney , Dermot Diamond	Two-Component Fluorescent Sensing of Saccharides
17.35-17.55	Contributed talk	O10	Sandra A.V. Eremia , Iuliana Mihalache , Mihaela Kusko , Eugeniu Vasile , Antonio Radoi*	Molybdenum Disulfide and Graphene Quantum Dots as Electrode Modifiers for Laccase Biosensor
17.55-18.15	Contributed talk	O11	Bogdan Feier*, Cecilia Cristea , Robert Sandulescu	Electrochemical Methods for the Detection of β-Lactam Antibiotics
19.30-23.00	**Gala Dinner (Aro Palace Club, Eroilor Blvd., no. 27-29, Brasov – Romania)**			
	Room UI3, **Novel materials and biomaterials for analytical methods,**			

	Chairperson: Rodica-Mariana Ion			
16.45-17.05	Contributed talk	O12	Rodica Turcu*, Alexandrina Nan , Teodora Radu , Anca Petran , Alexander Bunge , Monica Circu , Izabell Craciunescu	Novel Functionalized Magnetic Nanosystems with Tailored Properties for Biomedical Applications
17.05-17.25	Contributed talk	O13	Luiza Buimaga-Iarinca*, Cristian Morari , Ioan Turcu	Organic Molecules - Metallic System Interaction: A DFT Approach
17.25-17.45	Contributed talk	O14	Eugenia Eftimie Totu*, Corina Marilena Cristache , Ibrahim Isildak	Improving Poly(methyl methacrylate) Properties for Dental Aplication by Adding Titanium Oxide Nanoparticles
17.45-18.05	Contributed talk	O15	Nicoleta Tosa*, Alexandra Falamas , Cristian Tudoran , Lucian Barbu , Valer Tosa	Metallic Micro- and Nanostructured Materials as Supporting Electrodes for Biomolecular Spectroscopy
19.30-23.00	**Gala Dinner (Aro Palace Club, Eroilor Blvd., no. 27-29, Brasov – Romania)**			

July 1st, 2016	**Building *Aula Magna* of Transilvania University of Brasov. 41 A Iuliu Maniu Street, Brasov, 500091, Romania.**			
	Room UI2, **Chairperson: Otilia Ana Culicov**			
9.30-10.10	**Plenary Lecture**	**P5**	Vidmantas Ulevicius	Development and Application of Innovative Techniques for Atmospheric Organic Aerosol Composition Measurement
	Room UI2, **Atomic and nuclear methods, Chairperson: Vidmantas Ulevicius**			
10.10-10.40	Keynote	K9	Otilia Ana Culicov*, Valery Shvetsov*	The Neutrons: A Powerful Tool in Environmental and Biological Studies
10.40-11.05	Invited talk	I7	Claudia Stihi*, Ion V. Popescu , Marina Frontasyeva , Cristiana Radulescu , Antoaneta Ene , Otilia Culicov , Inga Zinicovscaia , Ioana Daniela Dulama , Simona Cucu-Man , Radu Todoran , Anca Gheboianu , Iulian Bancuta , Gabriel Dima , Alin Bucurica	Heavy Metal Air Pollution Study in Romania Using Moss Biomonitoring together with NAA and AAS Analytical Techniques
11.05-11.25	Contributed talk	O16	Antoaneta Ene*, Marina V. Frontasyeva	Neutron Activation Analysis as a Tool for Environmental and Materials Research
	Room UI3, **Sensors and biosensors, Chairperson: Jean Louis Marty**			
10.10-10.40	Keynote	K10	Andrei Florin Danet*, Carmen Simona Litescu , Claudia Valentina Popa	Nanomaterials And Chemiluminescence Based Method for the Determination of Antioxidant Capacity
10.40-11.05	Invited talk	I8	Jacobus (Koos) Frederick van Staden	The Potential of Sensor Platforms for Dynamic Integrated Process

				Control in Real-Time. Are they Suitable to Function Properly in the Environment?
11.05-11.25	Contributed talk	O17	Sorin Mihai David , Eugen Gheorghiu*, Cristina Polonschii , Mihaela Gheorghiu , Dumitru Bratu	Advancing Magneto-Optical Surface Plasmon Resonance For Biosensing
11.25-12.00	**Coffee Break and Poster Session (even numbers)**			
	Room UI2, **Novel materials and biomaterials for analytical methods, Chairperson: Marius Schmidt**			
12.00-12.20	Contributed talk	O18	Aishling C Dunne*, Joseph Hennessy , Síobhan MacArdle , Larisa Florea , Dermot Diamond	Photo-Responsive Hydrogels with Enhanced Volume Changes due to Local pH alterations
12.20-12.40	Contributed talk	O19	Alexandru Tudor*, Colm Delaney , Wayne Francis , Larisa Florea , Dermot Diamond	Solvent Sensing Fluorescent poly(Ionic Liquid) Ionogels
12.40-13.00	Contributed talk	O20	Larisa Florea*, Aishling Dunne , Wayne Francis , Danielle Bruen , Alexandru Tudor , Dermot Diamond	Stimuli-responsive Materials for Self-reporting Micro-fluidic Devices
13.00-13.20	Contributed talk	O21	Tugce Akyazi , Janire Saez , Lourdes Basabe-Desmonts , Fernando Benito-Lopez*	When Microfluidics met Smart Materials
	Room UI3, **Sensors and biosensors, Chairperson: Andrei Florin Danet**			
12.00-12.20	Contributed talk	O22	Mihaela Gheorghiu*, Luciana Stanica , Cristina Polonschii , Dumitru Bratu , Octavian Popescu , Eugen Gheorghiu	A New Twist for Optogenetics: Light Driven Dynamics for Cell Based Sensing
12.20-12.40	Contributed talk	O23	Anca Florea , Cecilia Cristea , Nicole Jaffrezic Renault , Robert Sandulescu*	Molecularly Imprinted Electrochemical Sensors for Detection of Drugs and Pollutants
12.40-13.00	Contributed talk	O24	Yawar Abbas*, Fleur van Rossem , Séverine Le Gac	Oxygen Sensing using an Ultra-microelectrode array at the millisecond time-scale
13.00-13.20	Contributed talk	O25	María Virumbrales-Muñoz *, Adithya Sridhar*, Rosa Monge , Jose María Ayuso , Guillermo Llamazares , Ignacio Ochoa , Albert Ruggi , Luis Fernández , Séverine Le Gac *	Oxygen Sensitive Hydrogel Matrix for 3D Cell Culture and 3D Oxygen Concentration Mapping
13.20-13.40	**Closing Ceremony**			
13.40-14.30	**Lunch**			

POSTER COMMUNICATIONS

	Chairpersons: Séverine Le Gac, Jean Louis Marty, Valerică Raicu, Ioan Turcu	
Number	**Authors**	**Title**
Nanobiotechnology		
PNb1	Manuela Stan*, Ildiko Lung , Maria-Loredana Soran , Cristian Leostean , Teofil-Danut Silipas , Sebastian Alin Porav	Magnetic Iron Oxide (Fe_3O_4) Nanoparticles From Agro-Wastes For Removal Of Antibiotic Pollutants From Waters
PNb2	Ildiko Lung , Manuela Stan*, Ocsana Opris , Maria-Loredana Soran , Cristian Leostean , Florina Copaciu , Sebastian Alin Porav	Application Of Magnetite Nanoparticles Synthesized Using Agricultural Sources For Removal Of Lanasyn Red Dye
PNb3	Daniel Marconi*, Alia Colniţă , Bogdan Cozar, Ioan Turcu	Highly ordered Iron Phthalocyanine (FePc) Nanometer-Sized Layers Deposited on Si (111) 7x7 by Molecular Beam Epitaxy
PNb4	Haitham Al Keline , Livia Petrescu*, Dan Florin Mihailescu	ZnO Nanoparticles for Biosensing Applications
PNb5	Aurelia Apetrei *, Tudor Luchian	Indirect Assessment of Antimicrobial Peptides Binding Affinity to Lipid Bilayers via a Single Nanopore Sensing Technique
PNb6	Aurelia Apetrei*, Andrei Ciuca*, Jong-kook Lee , Chang Ho Seo , Yoonkyung Park , Tudor Luchian	Tuning the Interaction Environment for Single Nanopore-based Sensing of Gram-negative Bacterial Cells
PNb7	Sumayah Ibraheem , Livia Petrescu*, Dan Florin Mihailescu	Interaction of Silver Nanoparticles with Lipid Monolayer as a Model of Biological Membranes
PNb8	Olteanu Radu Lucian , Nicolescu Cristina-Mihaela*, Bumbac Marius	Characterization of Silver and Copper Nanoparticles Synthesized by Bottom-Up Approach Using Plant Extracts
PNb9	Olteanu Radu Lucian , Nicolescu Cristina-Mihaela*, Bumbac Marius	Study on the Synthesis Process of Silver Nanoparticles in Salvia Officinalis Extract Using UV-VIS Spectroscopy
PNb10	Livia Neagu*, Ioan Dorobantu	Kynetic and Thermodynamic Properties of the System Nanoimmunosorbent- Analyte (2,4-D) in the Presence of Enzymatic Label Used in Homogenous Elisa Technique for Detection Of 2,4-D from Environmental and Alimentary Samples
PNb11	Marcela-Corina Rosu*, Crina Socaci , Lidia Magerusan , Florina Pogacean , Maria Coros , Emoke Pall , Stela Pruneanu	Pectin-based Composites containing Graphene as Substrates for Cells Growth
Spectroscopy		
PSp1	Alia Colnita*, Daniel Marconi , Nicoleta Elena Dina , Ionut Bogdan Cozar , Nicolae Leopold , Ioan Turcu	Fabrication of Nanostructured Au Films as Promising SERS Substrates for the Detection of Pathogenic Bacteria
PSp2	Andreea Antonia Georgescu*, Andrei Florin Danet , Claudia Stihi , Cristiana Radulescu , Ioana Daniela Dulama	Evaluation of the Chemical Compositon and Micronutrients of Wild and Commercial Mushrooms of Dambovita
PSp3	Claudia Gabriela Chilom*, Bogdan Zorilă , Doina Gazdaru , Aurel I Popescu	Characterization of Some Physico-chemical Properties and Interactions of Human and Bovine Serum Albumin with Mitomycin C
PSp4	Cristina M. Muntean*, Ioan Bratu	(Sub)Picosecond Dynamics in LacDNA Molecules as Probed with UV Resonance Raman Spectroscopy

PSp5	Cristina M. Muntean*, Ioan Bratu , Carmen Tripon , Nicoleta Dina	(Sub)Picosecond Relaxation Processes in Nucleic Acids Constituents and in DNA Molecules: a Raman and Surface-Enhanced Raman Spectroscopy Assessment
PSp6	Mircea Bogdan*, Adrian Pirnau , Silvia Neamtu , Calin G Floare	1H NMR Characterization of the Host – Guest Inclusion Complex between β – Cyclodextrin and Tolmetin
PSp7	Adrian Pirnau*, Mircea Bogdan , Calin G Floare , Mihaela Mic , Silvia Neamtu	NMR study on the Low-Affinity Interaction of Human Serum Albumin with Zidovudine
PSp8	Ionut Bogdan Cozar*, Daniel Marconi , Alia Colniţă , Ioan Turcu	Spectroscopic Investigation Of Iron Phthalocyanine (FePc) Molecular Layers Deposited On Au/Si
PSp9	Ahmed Kareem Hammood Jaberi , Maria Mernea , Octavian Calborean , Dan Florin Mihailescu*	Lipopolysaccharide Association with Allantoin Crystals Addressed through THz and FTIR Spectroscopy
PSp10	Bogdan Zorila*, Mihaela Bacalum	Study of the Interaction Between Antimicrobial Peptides and Model Cell Membranes by Steady State and Time Resolved Fluorescence
PSp11	Adina Elena Scripa (Tudose) , Dan Gheorghe Dimitriu , Dana Ortansa Dorohoi*	Dispersion Of Vizible Rotatory Power For Aqueous Glucose Solutions
PSp12	Cezarina Ana Morosanu , Andreea Celia Benchea , Daniela - Babusca , Dan Gheorghe Dimitriu , Dana Ortansa Dorohoi*	Quantum Mechanical Characterization And Solvatochromic Study Of Quercetine
PSp13	Andreea Celia Benchea*, Daniela - Babusca , Dan Gheorghe Dimitriu , Crtomir - Podlipnik	Solvatochromic Study And Quantum-mechanical Characterization Of Methyl Red
PSp14	Daniela - Babusca , Andreea Celia Benchea , Dan Gheorghe Dimitriu , Dana Ortansa Dorohoi*	Spectral And Quantum Mechanical Study of 3-(2-Benzothiazolyl)-7-(Diethylamino)-Coumarin In Binary Solutions
PSp15	Cristiana Rădulescu , Claudia Stihi , Dumitru Lazurcă , Oana Bute , Romulus Gruia , Mihaela Ilie , Octavian Olaru , Ioana-Daniela Dulamă , Raluca Știrbescu , Sofia Teodorescu , Monica Florescu *	Characterization of Phenolic Constituents of Lavandula Angustifolia Mill. Extracts
Microfluidics and point-of-care microdevices		
PMp1	Mihai Lungu*, Adrian Neculae , Antoanetta Lungu , Nicolae Strambeanu	Investigations Regarding Possibility on Flue Gas Filtration by Selective Retaining of Nanoparticles using Positive Dielectrophoresis
PMp2	Mihăiță Nicolae Ardeleanu*, Emil Lungu , Ioan Tivig , Tudor Savopol , Mihaela G. Moisescu *	Innovative Integrated System for Sorting and Extraction of Adherent Cells
PMp3	Mihăiță Nicolae Ardeleanu*, Florina Violeta Anghelina , Simona Mihai , Vasile Bratu , Ileana Nicoleta Popescu *	Design of Microfluidic Device and Measurement of MPWM for Single Cell/Particle Manipulation
Analytical methods for medical physics		
PMf1	Alina Giorgiana Galon (Negru) , Romeo Iulian Olariu , Cecilia Arsene *	Ion Chromatographic Analysis of Atmospheric Particles with Potential Impact on Human Health
PMf2	Viktorija Skaidrutė Dainauskaitė*, Raminta Rodaitė-Riševičienė , Gintautas Saulis	Generation of Hydrogen Peroxide by High-Voltage Pulses in Cell-Free Media
PMf3	Florina Dorina Covaciu*, Olivian Ciprian Marincas , Alina Dana Magdas , Zaharie Moldovan	Determination of trace pesticides in carrot samples having different origin by chromatography and mass-spectrometry

		methods
PMf4	Cezara Voica*, Ioana Feher , Dana Alina Magdas , Gabriela Cristea	Metal Content in Selected Vegetables from the Romanian Market and Estimation of the Daily Intake
PMf5	Anca Daniela Farcas*, Augustin Mot , Vlad Toma , Laurian Vlase , Silvia Neamtu , Marcel Parvu	Comparative Antioxidant and Prooxidant Activities of Five Plantago Species
PMf6	Georgiana Mardare (Balusescu) , Romeo Iulian Olariu , Cecilia Arsene*	Gas Chromatography/Mass Spectrometry (GC/MS) as Challenging Problems Solving Microanalytical Tools
PMf7	Mihaela Streza*, Bogdan Belean , Maria Miclaus	On the Improvement of Lock-in Thermography Detection of Microgaps Located at the Tooth-filling Interface
PMf8	Lorant Janosi*, Mihaela Bacalum , Mihai Radu , Florina Zorila , Ioan Turcu	The Effect of the 3D Hydrophobic Moment of Short ARG- and TRP-Based Peptides on Charged Membranes
PMf9	Alexandra Farcaş, Luiza Buimagă-Iarinca, Calin Floare, Lorant Janosi*	Plasma Membrane Model Dynamics in the Presence of Ras Protein Nanoclusters
PMf10	Lucia Elena Enciu*, Madalina Croitoriu , Gabriel Baranga , Alexandru Mihail Oprea , Amalia Constantinescu , Claudia Gabriela Chilom	Retrospective Analysis of Cases Treated in HDR Brachytherapy Compartment, of Patients with Neoplastic Diseases in Gynecological Area
PMf11	Mihaela Bacalum	Antimicrobial Peptides Show Antitumor Activity Against SH-SY-5Y Human Neuroblastoma Cells
PMf12	Yassine Kadmi , Lidia Favier*, Mariana Liliana Pacala , Dominique Wolbert	A Sensitive Analytical Approach for the Screening of a Toxic Chlorinated Aromatic Compound at Ultra-Trace Levels in Water Samples
Medical analysis and diagnosis		
PMa1	Avgustina Krasimirova Danailova*, Svetla Jeliazkova Todinova , Lidia Gartcheva , Sashka Boichova Krumova , Stefka Germanova Taneva	Calorimetric Monitoring of Patients with Multiple Myeloma after Autologous Stem-Cells Transplantation
PMa2	Elisabeta Antonescu*, Felicia Gabriela Gligor , Maria Totan	Quantitative Determination of Fe 3+ in Pharmaceutical Forms by Means of UV-VIS Spectrophotometry
PMa3	Livia Chilug*, Radu A. Leonte , Alina Raicu , Marcela E. Barbinta Patrascu , Alexandru C. Ion , Catalin Tuta , Dana Niculae	Improving Tumor Uptake and Retention of 68Ga Radiolabeled Compounds Using Gold Nanoparticles as Intracellular Delivery System
Sensors and biosensors		
PSb1	Andrei Florin Danet*, Liliana Parcalabu , Claudia Valentina Popa , Roxana Porumb , Elena Branduse , Alina Vasilescu *	Antioxidant Potential of Aronia-Enriched Wines Assessed by Chemiluminometric, Spectrophotometric and Electrochemical Methods
PSb2	Luiza Buimaga-Iarinca , Cristian Morari*	DFT investigation of SubPC migration on metallic surface
PSb3	Sarmad Al Hadeethi , Catalin Dumitru Petrescu *, Livia Petrescu , Dan Florin Mihailescu	Conductance Recorder for Biomedical Applications
PSb4	Lidia Magerusan*, Crina Socaci , Florina Pogacean , Maria Coros , Marcela-Corina Rosu , Alexandru Turza , Stela Pruneanu	N-doped Graphene Nanomaterial for Chemical/Electrochemical Detection of H2O2

PSb5	Irina Schiopu*, Sorana Iftemi , Tudor Luchian	Probing The Key Metal Binding Residues In Mutant Amyloid Peptides
PSb6	Pavel Barko, Adrian Șerban, Monica Florescu*	Sensors for lipo- and hidrosoluble antioxidant compounds in vegetal resources extracts
Novel materials and biomaterials for analytical methods		
PBm1	Claudiu Filip , Crina Anca Socaci , Flavia Adina Martin , Ioana Georgeta Grosu *, Irina Elisabeta Kacso , Maria Olimpia Miclăuş , Mirabela Ligia Golban , Xenia Filip	Supramolecular Systems for Drug Delivery Applications
PBm2	Flavia Adina Martin , Monica Florescu , Teodora Radu , Rodica Turcu , Claudia Lar , Niculina Hadade , Ion Grosu , Ioan Turcu *	Terpyridine-Terminated Self-Assembled Monolayers on Gold Substrate for Metal Ions Sensing
PBm3	Camelia Berghian-Grosan *, Alexandru Radu Biris , Fumiya Watanabe , Alexandru Sorin Biris	Graphene-Bimetallic Nanoparticles Hybrid Materials for DNA Bases Detection
PBm4	Silvia Neamtu*, Daniel Marconi , Flavia Adina Martin , Ioan Turcu	Fe Ions Caption by Terpyridine Functionalized Au Substrate Analyzed by Impedance Spectroscopy
PBm5	Lidia Magerusan*, Crina Socaci , Florina Pogacean , Maria Coros , Marcela-Corina Rosu , Stela Pruneanu	Graphene-Porphyrin Based Electrodes for H_2O_2 Electrochemical Detection
PBm6	Ecaterina Matei , Andra Predescu*, Claudia Dragan , Cristian Pantilimon , Cristian Predescu	Methods for Assessment of Two Promising Nano-hybrids Materials used for Metallic Ions Removal
PBm7	Cristian Predescu , Sorin Ciuca , Ecaterina Matei*, Andra Predescu , Mirela Sohaciu , Andrei Berbecaru	Structure and Properties of some Metallic Biomaterials from system Ti-Nb-Fe used in Implantology
PBm8	Elena Bacalum, Edina Rusen, Florentina Rizea, Aurel Diacon, Mihaela Cheregi, Adriana Gheorghe, Bogdan Bucur, Victor David	Optimization of Solid Phase Extraction Based On Molecular Imprinted Adsorbents for Furaltadone
PBm9	Melinda David, Christopher Brett*, Monica Florescu*,	Evaluation of Conductor Polymer with Layer-by-Layer based Architecture for Glucose Biosensing
PBm1	Claudiu Filip , Crina Anca Socaci , Flavia Adina Martin , Ioana Georgeta Grosu *, Irina Elisabeta Kacso , Maria Olimpia Miclăuş , Mirabela Ligia Golban , Xenia Filip	Supramolecular Systems for Drug Delivery Applications
Atomic and nuclear methods		
PNa1	Dana Alina Magdas , Gabriela Ioana Cristea*, Cezara Voica	Stable Isotope Fingerprinting In Pharmaceuticals Authentication
PNa2	Elena Zubcov , Antoaneta Ene*, Victor Ciornea , Lucia Bileţchi , Natalia Zubcov	The Study of Metal Migration in the Aquatic Environment
PNa3	Mirela Mihon*, Dana Niculae , Alina Catrinel Ion , Catalin Stelian Tuta , Vasile Lavric	Improved method for determination of identity and chemical purity of [18F]FLT
PNa4	Florina Dorina Covaciu *, Alina Dana Magdas , Adriana Dehelean , Gabriela Ioana Cristea , Ioana Coralia Feher , Romulus Horatiu Puscas	Multi-elemental, isotopic and trace pesticides analysis of wild and cultivated berries species
PNa5	Gabriela Ioana Cristea*, Dana Alina Magdas , Cezara Voica , Romulus Puscas	Vegetable Characterization Using Stable Isotope And Elemental Signature

PNa6	Cezara Voica *, Diana Lazar , Gabriela Blanita , Dana Alina Magdas	Wastewater decontamination using highly porous Metal Organic Framework (MOF) and nanostructured carbon materials
PNa7	Diana Costinel*, Roxana Elena Ionete , Oana Romina Botoran , Raluca Popescu , Elisabeta Irina Geana	Oxygen isotope ratios in the ethanol and water of Romanian wines as approach in improving the assessment of ethanol origin and illegal watering
PNa8	Roxana Elena Ionete*, Diana Costinel , Diana Ionela Stegarus , Oana Romina Botoran , Claudia Sandru , Elisabeta Irina Geana	Characterisation and Classification of Wines from Some Grape Varieties Grown in Romania: An Approach Based on Metals and Phenolic Compounds

Oral Communications

Plenaries

P1. Probing the Early Stages of Receptor Signaling with Quantitative Fluorescence Techniques

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We have developed Quantitative Imaging FRET methodologies to study the interactions between membrane receptors in biological membranes. The methods yield association constants, and allow us to follow structural changes in response to ligand binding to the receptors, or due to pathogenic mutations. We have used these methods to examine how VEGFR-2, the primary regulator of new blood vessels development, is activated in the plasma membrane by its ligands. VEGFR-2 has been hypothesized to be monomeric in the absence of bound ligand, and to undergo dimerization and activation only upon ligand binding. We have shown, however, that VEGFR-2 forms dimers in the absence of ligand when expressed at physiological levels, and that these dimers are active. Ligand binding leads to a change in the TM domain conformation, resulting in increased kinase domain activation. We further show that the pathogenic C482R VEGFR-2 mutant, linked to infantile hemangioma, is constitutively active because it mimics the structure of the ligand-bound wild-type dimer. This work demonstrates that the current models of VEGFR2 signal transduction across the plasma membrane are over-simplified and need to be amended.

P2. The Role of Active Site Flexible Loops in Catalysis and of Zinc in Conformational Stability of *Bacillus cereus* 569/H/9 β-lactamase

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Metallo-β-lactamases catalyse the hydrolysis of most β-lactam antibiotics and hence represent a major clinical concern. The conformational properties of the BcII β-lactamase have been studied in the presence of chemical denaturants, using a variety of techniques, including enzymatic activity measurement and fluorescence, circular dichroism, and 2D NMR spectroscopies. The data from the various experiments provide evidence that binding of two zinc ions not only increases the conformational stability of the BcII metallo-β-lactamase, but also restores the 3D structural organization that is lost for apoBcII unfolding in the presence denaturant. Moreover the results highlight the importance of a relatively well-defined conformation for two loops that border the active site in order to maintain enzymatic activity.

P3. Interrogation of Circulating Tumor Cells a tool towards personalized medicine

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Circulating tumor cells (CTC) are cancer cells disseminated into the blood from primary or metastatic sites. The presence of CTC is predictive of relatively short survival in metastatic carcinomas, and the more CTC are present the worse the outcome (1). The promise of CTC as a real time liquid biopsy to guide therapy can only be met when CTC are present in the blood volume analyzed, can be detected and isolated from this blood and the information needed for treatment choice can be extracted and is representative of the tumor. To increase the likelihood of isolating tumor cells technologies are being developed that examine up to 5 liters of blood (2). To extract treatment relevant information analysis at the single cell level is needed, as tumor cells are heterogeneous. Preferably all treatment relevant molecular pathways need to be identified at the protein, RNA and DNA level. Microfluidic devices can play an important role in extracting treatment relevant information from individual cancer cells and have the potential to be used in personalized medicine (3).

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P4. Ultrafast Dynamics in Proteins Investigated by Time-Resolved Serial Femtosecond Crystallography

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High impact (large scale) scientific projects are conducted by multi-institutional collaborations at high end, large scale facilities financed and supported by multinational funds. The United States National Science Foundation (NSF) funds Science and Technology Centers (STCs) that *"conduct world-class research through partnerships among academic institutions, national laboratories, industrial organizations, and/or other public/private entities, and via international collaborations, as appropriate"*. The BioXFEL STC was established in 2013 with the following mission: *"Using a pulsed hard X-ray laser, our researchers can image biological molecules in atomic detail, view their functional motions by taking brief snapshots, and observe interactions in their native environment. This opens up a new world to biology, to science, and to human health"* (see https://www.bioxfel.org/**).** Serial Femtosecond Crystallography (SFX) is an emerging technique performed at ultra-brilliant and ultra-shortly pulsed X-ray sources. The Linac Coherent Light Source (LCLS) at SLAC in Stanford, U.S.A., is a Free Electron Laser for Hard X-rays (X-ray FEL) which produces ultra-short (~40 femtosecond, 40 x 10^{-15} s) X-ray pulses with 10^{12} X-ray photons in each pulse. The X-ray beam can be focused to spots smaller than 1 micormeter which is exquisitely suited to investigate tiny specimen such as nano- and micro crystals down to the single molecule level. The tiny crystals are injected into the X-ray beam one by one, in a serial fashion, each crystal in random orientation. When a crystal in flight is hit by the intense 40 femtosecond X-ray pulse, it disintegrates. However, before it is destroyed, it scatters and a diffraction pattern with Bragg spots is recorded on a specially designed detector with fast readout times. This is called the diffraction-before-destruction principle and lies at the heart of SFX. From tens of thousands of these diffraction patterns complete crystallographic datasets with accurate intensities can be collected. If a reaction can be initiated in the crystal for example with an ultrashort optical laser pulse a time-delay delta-t before it is probed by the X-ray pulse, the reaction can be structurally investigated. The time-resolution is essentially given by the 40 femtosecond duration of the X-ray pulse. The tiny crystals are intercepted twice in flight, first by the optical pump laser, and then by the probe X-ray pulse. SFX becomes time-resolved (TR-SFX). Here, TR-SFX results are presented on a time-scale from 100 femtoseconds to 1 microsecond. We[1,2] show the earliest events of a photo-activated reaction in a protein and gain unprecedented insight into the chemistry and the mechanism of the reaction.

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2.Collaboration of 45 scientists from 3 countries and 13 institutions led by the BioXFEL Science and Technology Center (NSF-1231306).

P5. Development and Application of Innovative Techniques for Atmospheric Organic Aerosol Composition Measurement

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The widespread of Aerosol Mass Spectrometers (AMS) greatly improved the real-time organic aerosol (OA) monitoring, providing OA mass spectra which contain sufficient information for quantitative apportionment of OA sources. In early spring the Baltic region is frequently affected by high pollution events due to biomass burning in that area. Here is presented a comprehensive study to investigate the impact of biomass/grass burning (BB) on the evolution and composition of aerosol in Preila, Lithuania, during springtime open fires. Long term OA monitoring is fundamental for elaboration of appropriate mitigation strategies, and development of more accurate climate models. Non-refractory submicron particulate matter (NR-PM_1) was measured by an Aerodyne Aerosol Chemical Speciation Monitor (ACSM) and a source apportionment with the Multilinear Engine (ME-2) running the Positive Matrix Factorization (PMF) model was applied to the OA fraction to investigate the impact of biomass/grass burning. Satellite observations over regions of biomass burning activity supported the results and identification of air mass transport to the area of investigation. Sharp increases in biomass burning tracers, such as levoglucosan up to 683 $ng \cdot m^{-3}$ and black carbon up to 17 $\mu g \cdot m^{-3}$ were observed during this period. A further separation between fossil and non-fossil primary and secondary contributions was obtained by coupling ACSM PMF results and radiocarbon (^{14}C) measurements of the elemental (EC) and organic (OC) carbon fractions. Non-fossil organic carbon was the dominant fraction of PM_1, with the primary and secondary fractions contributing 26 – 44% and 13 – 23% to the total carbon (TC), respectively. 5 – 8% of the TC had a primary fossil origin, whereas the contribution of fossil secondary organic carbon was 4 – 13%. Non-fossil EC and fossil EC ranged from 13 – 24% and 7 – 12%, respectively. Isotope ratio of stable carbon and nitrogen isotopes were used to distinguish aerosol particles associated with solid and liquid fossil fuel burning.

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Oral Communications

Nanobiotechnology

K1. Bio-Nanotechnology SS Enhancer in Photodynamic Therapy

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Photodynamic therapy (PDT) and bio-nanotechnology show striking similarities in clinical design and mechanistics. Photodynamic therapy (PDT) is an alternative approach for improved cancer treatment. In PDT, the administered photosensitizer (PS) is subsequently activated by light with a specific wavelength, causing selective damage of the tumor and its surrounding vasculature [1]. The success of PDT is limited by the low water solubility and photobleaching of the administed photosensitizers (PSs), which compromises the clinical use of several molecules. Nanoparticles (NT) exhibit an “Velcro effect” to the tumor cells and based on this concept, the application of nanotechnology in medicine could offer many exciting possibilities in cancer treatment. NT has the ability to explain each of the critical steps of PDT particularly photosensitizer design and delivery, light source, the photodynamic mechanisms of action. Incorporation of PSs (porphyrins and phthalocyanines) in nanostructured drug delivery systems, such as polymeric nanoparticles (PNPs), gold or silver nanoparticles (AuNPs or AgNPs), hydrogels, liposomes, or nanocarbons as fullerenes [2] is a potential strategy to improve PDT efficiency. The aim of this paper is to review photodynamic therapy of cancer by using nanomaterials for the enhancement of photodynamic activity. Some eloquent examples revealed from the personal research are shown and discussed, too.

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K2. Conformational Fine-tuning of the Membrane Selectivity of Pore-forming Peptides.

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To better understand the sequence-structure-function relationships that control the activity and selectivity of membrane-permeabilizing peptides, we screened a peptide library, based on the archetypal pore-former melittin, for loss-of-function variants. This was accomplished by assaying library members for failure to cause leakage of entrapped contents from synthetic lipid vesicles at a peptide-to-lipid ratio of 1:20, 10-fold higher than the concentration at which melittin efficiently permeabilizes the same vesicles. Surprisingly, about one-third of the library members are inactive under these conditions. In the negative peptides, two changes of hydrophobic residues to glycine were especially abundant. We show that loss-of-function activity can be completely recapitulated by a single-residue change of the leucine at position 16 to glycine. Unlike the potently cytolytic melittin, the loss-of-function peptides, including the single-site variant, are essentially inactive against phosphatidylcholine vesicles and multiple types of eukaryotic cells. Loss of function is shown to result from a shift in the binding-folding equilibrium away from the active, bound, α-helical state toward the inactive, unbound, random-coil state. Accordingly, the addition of anionic lipids to synthetic lipid vesicles restored binding, α-helical secondary structure, and potent activity of the "negative" peptides. While nontoxic to mammalian cells, the single-site variant has potent bactericidal activity, consistent with the anionic nature of bacterial membranes. The results show that conformational fine-tuning of helical pore-forming peptides is a powerful way to modulate their activity and selectivity.

O1. The Nano-Mechanics of Single Proteins

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Proteins are the work-horse of our body and force is a natural perturbation with a major role in numerous processes, such as muscle contraction or cellular interactions. Recently, it was found that domain unfolding occurs over extended time scales and can trigger a change in the elasticity of a tissue or can be involved in recruiting other binding partners. However, the folding dynamics of a protein over these human time scales is unknown. Here I will present a system based on a new single molecule to study the folding of single proteins under force over the course of several days, a time comparable to the turnover of proteins in the human body. This new single molecule technique combines the strength of HaloTag covalent attachment with the stability of magnetic tweezers and can expose single protein constructs to forces similar to those experienced by proteins *in vivo*. Using this new technique, we found that immunoglobulin domains (Ig) from titin, a protein that gives muscles their elasticity, continuously undergo unfolding/folding transitions at physiological sarcomere lengths and forces of 6–8 pN. While current theories of muscle contraction take into account only the power stroke of the myosin motors, our measurements suggest a new mechanism where domain refolding under force is inextricably linked to the myosin cycle. Based on our measurements, we find that the contractile energy delivered by titin folding is comparable to the energy produced by myosin motors. These findings place protein folding as an important mechanism where tandem multidomain proteins can adjust the elasticity of tissue and deliver or store energy based on changes in the experienced force.

Oral Communications

Spectroscopy

K3. Probing Association and Dissociation of Proteins in Living Cells: Toward Multi-Dimensional FRET Spectrometry

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When an excited fluorescent molecule, called a ‘donor,’ is located within a few nanometers of an unexcited molecule, i.e., an ‘acceptor,’ part of the donor’s energy may be transferred to the acceptor. This quantum mechanical effect, known as Förster (or Fluorescence) Resonance Energy Transfer (FRET), causes the acceptor molecule to emit light with red-shifted wavelengths compared to the excitation wavelength. Detection of such spectral shifts helps determine whether two or more fluorescent molecules interact with one another thereby allowing one to extract quantitative information regarding supra-molecular arrangements of biological macromolecules. This talk will begin with an overview of the main theoretical and technological advances that led to the introduction of *FRET spectrometry*, a method relying on acquiring Forster resonance energy transfer (FRET) histograms (or spectrograms) from fluorescence images to extract the stoichiometry and quaternary structure of protein complexes in living cells. Our method relies on a novel two-photon microscope with spectral resolution (called an Optical Micro-Spectroscope, or OptiMiS) and a competent theory of FRET in oligomeric complexes of arbitrary geometry. The second part of the talk will present recent results obtained by us and our collaborators from studies of oligomeric complexes of membrane proteins in living cells in the presence and absence of their natural ligands.

I1. Reconstruction Surface Potential from Atomic Friction Measurements

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Friction is a phenomenon encountered in everyday life , ranging from the macro- (earthquakes, violin playing, machinery, etc.) to the nano-scales (electronic devices, biological machinery etc.), where two surfaces come into contact and move with respect to each other, resulting with an irreversibly energy dissipation. One of the key features that characterize friction is the underlying interfacial interaction potential. Understanding the role of dissipation energy and surface potential in frictional mechanisms is essential for tribology, nanoscale fabrication, catalysis, adhesion and so on. To get an adequate estimation of the free energy landscape of an experimental system, high quality data is required. This necessity is met in measurements performed with Atomic Force Microscope (AFM). The AFM enables probing nanoscale frictional forces due to its ability to approach the 'single-asperity' level, and measure the dynamical interaction between a cantilever tip and the surface of interest, resulting with atomic stick-slip force pattern. In such experiments, estimation of the surface energy corrugation is typically carried out within the phenomenological framework of the Prandtl-Tomlinson model, which does not provide comprehensive information on the surface potential. Here we face such inverse problem and reconstruct physically meaningful potential maps out of the recorded friction signals by applying a different approach to calculate the surface potential. Through the application of the nonequilibrium work relation, or more specifically, the *Jarzynski* equality, we can directly reconstruct the underlying interaction potential of the surface combining simulations and AFM measurements. Unlike the previous methodology, the latter is model-free, and enables the calculation of the surface interaction potential directly from the measured force and position time series. Such implementation is beneficial to technological applications as molecular optimization of catalysts, and additionally to micro- and nano-electro-mechanical systems (MEMS and NEMS), where high surface-to-volume ratio amplifies damages and energetic inefficiency caused friction.

O2. Optical and Electrical Biophysical Methods for Identification of Cellular Malignancy

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Early cancer detection as well as accurate cellular diagnostic represents major challenges for the biomedical research. In various *in vitro* conditions the cell malignancy may be correlated with morphological characteristics, optical properties, strength of attachment, growth rate, etc.

There are reports about the great potential of the cellular (mainly nuclear) refractive index (RI) in the diagnosis and treatment of cancer cells providing static and dynamic information about composition and organizational structure of the cell (protein content, dry mass, etc.). Various microscopic-based methods are used to explore RI (quantitative phase and interference microscopy, confocal and scattering spectroscopic microscopy).

Real Time Cell-based Assay (RTCA), used mainly for screening cytotoxicity and drug design, can be also exploited to obtain data about cell adhesion, spreading and proliferation. The technique is based on the impedance response of microelectrodes covered with cells when low voltage alternating currents are applied.

The clonogenic tests are standards in biology studies for quantifying the cellular proliferation capacity in various physical and chemical conditions.

In this work we compared the RIs of two sub-lines of the B16-melanoma murine cultures. Digital Holographic Microscopy was employed to quantify the RIs of living cells. The data were correlated with the cellular proliferation capacity when evaluated by RTCA and clonogenic tests. The RIs were higher for the more metastatic sub-line. Our results may contribute to the developing of clinically oriented applications in cancer diagnosis using non-invasive and free-labelling methods.

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Oral Communications

Analytical methods for medical physics

K4. Unexplored Avenues of Human Skin: Reading Personal Stress in the Sub-THz Frequency Range

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The coiled structure of the tips of the sweat ducts embedded in the epidermis of human skin has given rise to the supposition that at sub-THz frequencies the response of the ducts should be similar to low Q helical antennas. As such, this response should reflect the activity of the perspiration system, governed by the Sympathetic Nerve System. We show that indeed the temporal behavior of the reflection coefficient at sub THz frequencies is highly correlated to the temporal behavior of the blood pressure, the pulse rate and other physiological parameters in response to physical, mental and emotional stresses imposed on the subject. Although correlation between changes in the reactance spectrum in this frequency range and physiological activities has been shown, a direct link between the electromagnetic reflection and the helical structure itself has remained to be established. The fact that the sweat ducts manifest natural homochirality is hence forth used to produce this link. We report the detection of circular polarization asymmetry in the electromagnetic reflection from the human skin at sub-THz frequencies in vivo. We argue that the observed circular dichroism can be interpreted uniquely as the signature of the helical structure itself.

I2. Interactions of Amino Acids with Lipid Membranes

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Physical measurements of amino acid interactions with lipid membranes are of interest not only for a quantitative description of cellular signalling processes but also for the development of new materials. Using small-angle x-ray scattering we show that amino acids modify the attractive van der Waals interaction between lipid membranes in proportion to their electrical polarizability. Amino acids also bind to lipid membranes inducing changes in membrane surface properties. We investigate this binding for the case of aromatic amino acids using conventional 1H NMR spectroscopy. In this method, we first generate reference spectra in isopropanol-d8/D2O solutions and then determine an equivalent isopropanol concentration (EIC) for hydrogen sites of aromatic groups, in essence constructing a map of their hydrophobic environment. The EIC maps provide information on relative affinities of aromatic side chains for various lipid types and also inform on amino acid orientation preference when bound to membranes.

O3. Impedance-based Real-time Monitoring of Cellular Growth for Phytotherapeutic Extracts and Porous Artificial Drug Carriers

Mihaela Georgeta Moisescu[1], Bogdan Mircea Matei[1], Fawzia Sha'at[1, 2], Luminita Claudia Miclea[1], Andreea Iulia Iorgu[3], Laura Georgiana Bajenaru[3], Lucia Pirvu[2], Cristina Hlevca[2], Cristian Matei[3], Dana Berger[3], Ramona Daniela Pavaloiu[2], Tudor Savopol[1]

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In the last decade the cell-based label-free technologies received an increasing attention in preclinical drug development studies. These technologies provide information about cellular status in the early stages of drug development process. Such m odern biomedical research is based upon fundamental studies before advancing towards clinical stage.

Impedance-based techniques for real-time monitoring of cellular growth are such a label-free efficient method for screening cytotoxicity, obtaining data on cell adhesion and proliferation or cell migration in the presence of various substances. The electric cell-substrate impedance system works with life cells adherent on gold electrodes. Harmless AC signals of few μA are applied leading to the generation of an electric field which is impeded by the presence of the cells. Impedance changes will thus reflect the overall interaction of the cells with the electrodes when various compounds modify the cellular features.

We exploited the xCELLingence system from Roche to quantify the cell viability when either several phytotherapeutic extracts or porous artificial drug carriers interacted with human and non-human cell cultures (several cell lines with different histological origins). The effect of cytotoxic Irinotecan was studied either loaded on the drug carriers or directly incubated with the cells simultaneous to several phytotherapeutic extracts (*Asperula O.*, *Geranium R.*, *Epilobium H.*, *Fagus S.*, *Juglans R.*). We found cellular responses significantly variant with respect to the cell line or compound nature, or to the simultaneity of exposure.

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O4. Plasmonic based EIS: towards a sensitive analytical method gathering the virtues of both SPR and EIS

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The quest for impedance assays with increased spatial resolution led to development of a new technique, Plasmonic based Electrical-Impedance-Spectroscopy, P-EIS [1,2]. P-EIS combines EIS and Surface Plasmon Resonance, SPR, capabilities by deploying an electrode exhibiting plasmonic properties in a set-up combining an AC signal generator (as the ones used for EIS) and a SPR module. When performing P-EIS, the whole sensing area is accessible with exquisite spatial resolution which is not limited by the size or distribution of the electrodes (as in the case of EIS) but solely by the (lateral) propagation length of the surface plasmons. Depending on sensor structure and incident light wavelength, this spatial resolution could reach sub-micrometer range suitable for multiplexed and in cell analyses.

We present an advanced EIS and P-EIS experimental set-up [3], the biosensing results and the theoretical framework behind P-EIS enabling reconstruction of the impedance and surface charge density maps from SPR data acquired when applying an AC potential modulation to an electrode (with plasmonic properties).

We highlight the actual conditions allowing assessment of the amplitude and phase of the impedance from the P-EIS signal and provide a thorough comparison between classical EIS and P-EIS measurement, with emphasis on experimental limitations, in the context of a novel plasmonic EIS microscopy system which is currently developed within ICB.

P-EIS outstanding applicative potential that spans from biosensing to analysis of living cells will be outlined.

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Oral Communications

Microfluidics and point-of-care microdevices

K5. Microfluidics – 25 Years of Hype, Hope and Hubris

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More than 25 years after the introduction of the concept of the “miniaturized total chemical analysis system (μTAS)” and about 20 years after the gold digger`s frenzy about how this technology would revolutionize all aspects of chemical, biological or diagnostic applications, it is worth to have a look how this technology has matured (or at what places it might have made a wrong turn). We see nowadays a significant part of the early day’s promises being fulfilled and a rapidly growing range of applications and products. This addresses especially the full functional integration of complex analytical or diagnostic workflows as well as the ability to reduce complexity, cost and size of the accompanying instrument, leading to systems which can be applied at the point-of-interest. A review on technical roadblocks and challenges as well as success factors for the commercialization of microfluidic devices will be presented as well as an overview on commercially available manufacturing routes with their specific application to microfluidics.

I3. Droplet Microfluidics Applied to HER2 Gene Expression in Breast Cancer

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The development of precision medicine and the multiplication of targeted therapies and associated molecular biomarkers, call for major progress in genetic analysis methods, allowing increased multiplexing and the implementation of more complex decision trees, without cost increase or loss of robustness. Here we report on a miniaturized platform that combines droplet microfluidics and magnetic tweezers. This platforms integrates: mRNA purification, reverse transcription and amplification in a fully automated and programmable way, in droplets of 250nL directly sampled from a microtiter-plate.

This platform decreases sample consumption about 100 fold as compared to conventional platforms used in clinics, as well as it reduces drastically human manipulations and contamination risk. The performance of this microfluidics approach was first evaluated with cell lines, showing robust operation on RNA quantities corresponding to less than one cell, and then clinically validated with a cohort of 21 breast cancer samples, for the determination of their HER2 expression status, in a blind comparison with an established routine clinical analysis.

O5. Chemotactic Ionic Liquid Droplets: Striving to Mimic Nature

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Chemotaxis, the ability of cells to move in response to certain stimuli, forms the basis for a family of signalling proteins, known as Chemokines. Their ability to control immune responses and cell migrations has proven a fascinating topic for chemists who try to find synthetic analogues to mimic this behaviour.

Herein we report the movement of ionic liquid (IL) droplets, based on trihexyl(tetradecyl)phosphonium chloride ($[P_{6,6,6,14}]Cl$), which exhibit chemotactic behaviour. These IL droplets can be moved spontaneously and guided to specific destinations in the presence of ionic strength gradients.[1] In addition, signalling and seeking $[P_{6,6,6,14}]^+$ droplets can also be developed which chemotactically find each other in open fluidic networks. The signal droplet releases a chemical signal that creates a gradient inside the fluidic channel. In response to this signal, the seeker droplet is enabled to chemotactically find the signal droplet and merge with it at its stationary location, in a manner similar to the triggered cell-migration seen in chemokine proteins.

The movement of the droplet is due to the diffusion of $[P_{6,6,6,14}]^+$ surfactant, which causes Marangoni-like flows and is modulated by the solubility of the anion in the aqueous solution. For the seeker droplet ($[P_{6,6,6,14}]Cl$), the high solubility of the Cl^- is reliant on the local ionic strength. When placed in an ionic strength gradient, there is an asymmetrical release of the surfactant from the droplet which results in unidirectional movement towards the ionic source. The signal droplet ($[P_{6,6,6,14}]DCA$), which releases the ionic chemoattractant, remains stationary due to poor solubility of DCA^- anion. Therefore, when both signal and seeker droplets are placed in a fluidic network, the seeker droplet autonomously seeks out the signal.

We propose these droplets as micro-vessels for chemical reactions at pre-determined locations, cargo carriers and possible drug-delivery systems.

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O6. Contactless Conductivity Sensor for Wearable Sweat Monitoring

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Analysis of sweat offers a wealth of information related to hydration, nutrition, and athletic performance. The conductivity of sweat can be directly related to sodium chloride concentration, as these are the most abundant electrolyte ions present in sweat [1]. Individuals affected by cystic fibrosis contain a higher concentration of Cl^- ions in their sweat. Prescription medications for the disease reduce Cl^- concentrations in sweat, and as a result, the efficacy of these medications can be monitored non-invasively with sweat collection.

In previous work, we have demonstrated the use of capacitively coupled contactless conductivity detection (C^4D) for testing the response of commercial gold microelectrodes to NaCl solutions using multiple sampling platforms [2]. This work presents the optimization of channel and sampling volumes to calculate and minimize the sensor's response time for applications in wearable sweat sensing. In preparation for on-body testing, the functionality of the chip was optimized for relevant flow rates of sweat. Sweat rate can vary drastically depending upon the subject and body part. Additionally, those affected by cystic fibrosis have difficulty exercising for extended periods of time. Due to these restrictions, the volume of sweat needed to produce a signal is of critical importance. In this work, PDMS microchannels were created which minimized platform volume for on-body analysis. Using varying concentrations of NaCl solutions (10 mM - 130 mM) and the average flow rates for the arm (730 g/m^2h), back (797 g/m^2h) and forehead (894 g/m^2h), a calibration curve was created and the average response time was calculated for each body location. Finally, tests were completed with artificial sweat and compared to the calibration curves.

Oral Communications

Analytical methods for medical physics

K6. Atomic Force Microscopy-Based Approaches to Probe the Structure of Membrane Proteins

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Membrane proteins are embedded in a lipid bilayer, which presents a barrier to the molecular and structural study of these biologically important molecules under physiologically relevant conditions. Atomic force microscopy (AFM) is a nanotechnology that overcomes some of the intrinsic limitations in the study of membrane proteins and provides high-resolution observations and manipulations of biological samples in a near-native environment. AFM studies on the membrane protein rhodopsin will be the subject matter for this presentation. Rhodopsin is the dim light receptor, and a prototypical G protein-coupled receptor, present in the photoreceptor cells of the retina. Upon photon capture, rhodopsin initiates vision by setting in motion a series of biochemical events termed phototransduction. Rhodopsin is embedded in disc membranes of rod photoreceptor cells. Apart from its central role in vision, rhodopsin also plays a structural role in maintaining the health of photoreceptor cells. There are over 100 mutations in rhodopsin that have been identified to cause a variety of inherited retinal disorders ranging from night blindness to retinal degeneration. Currently, we have applied two AFM methodologies to probe the structure of rhodopsin in native membranes. AFM imaging has been used to visualize the organization of rhodopsin in native disc membranes. I will present what we have learned so far about the native organization of rhodopsin and the factors that contribute to this organization. AFM-based single-molecule force spectroscopy (SMFS) has been used to probe the molecular interactions stabilizing receptor structure. I will present what SMFS studies have revealed about constitutively active forms of rhodopsin that cause congenital night blindness or Leber congenital amaurosis. Based on findings from SMFS studies, we have begun to develop an AFM-based method to image rhodopsin based on its functional state.

I4. A New Approach on Biomedical Analysis

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New tools and methods were developed for the assay of specific cancer biomarkers, neurotransmitters, citokines, and adipokines. The new tools are based on stochastic sensors – the only type of sensors that can perform qualitative and quantitative analysis. The advantages of these tools and methods are: the matrix is not influencing the response of the sensor; there is possible to determine very small amounts of biomarker in complex matrices; the limits of determination are low enough to determine specific biomarkers even in children saliva; no processing of the sample is required for the assay of the biomarkers.

Screening tests for whole blood and saliva samples were developed for breast, ovarian, colon, and lung cancers. Seven neurotransmitters were determined from zebrafish, and from different biological fluids: cerebrospinal liquid, whole blood, cord blood, serum, plasma, urine. Adipokines, citokines were determined from whole blood and saliva samples..

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O7. Data Mining and Statistical Methods for Data Analysis of Fluorescence Experiments

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The aim of this work is to present the main statistical issues and data mining methods used to understand fluorescence experiments. Microarray and *Förster resonance energy transfer (*FRET) type of fluorescence experiments will be presented to examine whether statistical and data mining methods that traditionally are used for microarray experiments can be used to shed light on FRET type of experiments. We address and emphasize some central issues of statistical methods which are highly relevant to microarray experiments and we consider that have much to offer for FRET type of experiments as well. Some concrete examples will be presented.

Acknowledgments: the first author acknowledge the support from project: PN-II-PT-PCCA-2013-4-0930 that made this work possible.

O8. The Influence of Medium on *Amplex Red* as Indicator for Fluorescent Hydrogen Peroxide during High-Voltage Electric Impulses

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Fluorescent dyes often use to study cell membrane electropermeabilization. When a high-voltage pulse is applied to the electrolyte solution, a variety of electrolysis reactions occur at the metal-electrolyte interfaces. Metal ions that released from the electrodes can react with the fluorescent dyes and quench their fluorescence. This may have an impact when estimating the efficiency of electropermeabilization. In this study, the influence of the medium treated by high-voltage pulse and Al^{3+}, Fe^{2+}, Fe^{3+}, Cr^{6+}, Ni^{2+} and Mn^{7+} ions on the fluorescence of fluorescent tracer molecules, including fluorescent indicator for hydrogen peroxide, in various solutions was studied.

Cell culture medium consisted of Dulbecco's modified Eagle's medium supplemented with 9 % fetal bovine serum and 1 % L-glutamine solution (all Sigma–Aldrich Chemie, Steinheim, Germany). 50 µl of the culture medium or a solution of a fluorescent dye was treated with a square-wave electric pulse with the duration of 0,1–2 ms and the amplitude 0,2–2,4 kV/cm. The fluorescence of calcein, meso-tetrakis (4-sulfonatophenyl) porphyrin (TPPS4), doxorubicin (Adriamycin) and H_2O_2 indicator *Amplex Red* was studied. The fluorescence was measured at room temperature using Tecan spectrofluorimeter (Tecan Group, Männedorf, Switzerland).

The medium which was treated by the electric pulse with the amplitude of 1,2 kV/cm and the duration of 500 and 2000 µs can almost completely quench calcein fluorescence. When the concentration of the metal ions increase in solution, the intensity of the fluorescence of calcein, TPPS4, Adriamycin and *Amplex Red* decrease. For example, 1 mM of Fe^{3+} or Ni^{2+} ions suppressed fluorescence of calcein by 15 and 79 % respectively. Fe^{3+} at the concentration of 1 mM totally suppressed the fluorescence of porphyrin-sulphonate, by 30 % – the fluorescence of Adriamycin, and by 30–50 % the fluorescence of *Amplex Red*.

It can be summarized that the cell culture medium pretreated by high-voltage pulse quenches the fluorescence of various fluorescent molecules, mainly due to the metal ions released from the stainless-steel and aluminum electrodes.

The results of the current study can be useful for optimizing the electroporation method as well as for introducing it to medicine or industry.

Oral Communications

Medical analysis and diagnosis

K7. Self-powered Microfluidics for Point of Care Analysis

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Point of care is a global market constantly increasing. It is expected to grow over the 27.5 billion € by 2018. Point of care testing has applications in many different segments, such as medical diagnostics environmental analysis and sport sciences. And different end users, from self to professional and industrial monitoring, benefit from these developments.

The list of analytical targets is extensive from biomolecules, small organic and inorganic compounds, to cells or particles. And the samples to analyse may vary from physiological fluids, like blood, saliva, urine, sweat, to waters or air samples.

Microfluidic devices appear as the main platform to provide the means to analyze only small sample volume in a semi or fully automated way. The main objective is to provide the simplest devices, able to deliver accurate analytical measurements, but easy to use by not trained personnel.

Ideal POC analytical devices, should be low cost to make them disposable, but should integrate a number of functions to make them efficient. This functions are, sample preparation, and sensing capabilities. Features such as flow and shear forces control, besides material compatibility with the samples, are strict requirements in the design of new devices.

In our lab we work on the development of self-powered microfluidic platforms for POC testing. For this purpose we use polymeric materials to define both, microfluidic integrated architectures, and modular detachable and tuneable micropumps for flow control. Several examples of self-powered microfluidic analytical devices will be showed. [1,2]

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I5. Microfluidics for Cancer Research

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Droplet based digital PCR represents a highly efficient tool for cancer research allowing to reach unprecedented sensitivity and accuracy for single molecule and single cell analysis. We will first illustrate its pertinence for overcoming actual clinical oncology challenges by presenting the results of different retrospective and prospective studies. In particular, the detection of circulating tumor DNA and its potential use for patient treatment management will be demonstrated. Finally we will also illustrate the pertinence of droplet based digital PCR for single cell analysis in cancer research.

I6. Hydrodynamic Shaping of Sub-Nanoliter Volumes of Liquids at Biological Interfaces for Tissue Microprocesing and Biopatterning

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In contrast to standard microfluidics, which are typically closed, we developed a scanning, non-contact microfluidic technology that can shape liquids in the "open space" over surfaces. This technology utilizes a microfluidic probe inspired by the invention of scanning probe technologies in IBM Research – Zurich. The MFP has microfabricated structures for localizing as little as 100 picoliters of a liquid of interest on immersed surfaces using a hydrodynamic flow confinement. With flow confinement operating at volumes smaller than 1 nanoliter, a few tumor cells can be targeted in a human tissue section for the specific staining of disease markers. Such flow confinement and efficient use of chemicals can be further optimized using a new concept called "hierarchical" hydrodynamic flow confinement. The MFP also permits patterning surfaces with proteins in an additive and subtractive manner, forming gradients of proteins on surfaces, and interacting with cells on surfaces. For high-quality biopatterning of receptors on surfaces, we study the interplay between diffusion, advection and surface chemistry overcoming limitations of existing biopatterning, such as passive diffusion, uncontrolled wetting and drying artefacts. I will show how the hydrodynamics-based locations of liquids on surfaces and new concepts pertaining to tissue microprocessing and convection enhanced biopatterning may contribute to the analysis of critical samples in the context of next generation pathology and precision diagnostics.

Oral Communications

Sensors and biosensors

K8. Are Biosensors Right Tools For Food Contaminants Monitoring

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In recent years, the number of food contaminants continues to increase, threatening food safety and leading to a serious risk of foodborne illness. Food contamination can arise from environment (organic chemicals, metals and their complexes), or from a microbiological origin (harmful bacteria, bacterial and fungal toxins). Aiming to provide safe food to consumers, food safety authorities set maximum levels for certain contaminants in food. Therefore, it is of great importance to develop high-performing methods for the determination of these molecules in food matrices at trace levels.

The current tendency has driven the development of biosensors as new analytical tools able to provide fast, reliable, and sensitive measurements with low cost; many of them aimed for on-site analysis. Biosensors may not completely replace the official analytical methods, but can be used both by regulatory authorities and by industry to add up the information for routine testing and screening of samples. Biosensors are defined as analytical devices incorporating a biological material, or biomimic, intimately associated with or integrated within a physicochemical transducer or transducing microsystem. The main advantages of biosensors are short times of analysis, low cost of assays, portable equipment, real-time measurements, and suitability as remote devices. These new technologies have been applied in quantitative analysis of various target analytes.

Our objective is to present a survey of these methodologies. We will highlight the different biosensors developed by various research groups in many laboratories all over the world. Recently, a new class of bioreceptors namely aptamers have been emerged as promising alternative to replace the antibody in the design of biosensors . An aptamer is a sequence of single or double stranded DNA or RNA, selected from a random library according to its ability to bind a target molecules. A special emphasis is given to design and development of aptamer based biosensors

O9. Two-Component Fluorescent Sensing of Saccharides

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Boronic acid (BA) derivatives are capable of strong, but reversible interactions with diol-containing compounds like sugars, due to the Lewis acidic properties of the BA moiety[1]. Incorporation of a BA component into charged molecules, can be used to induce quenching in the emission of a fluorescent molecule, thereby creating a two-component sensing system[2]. The change in fluorescent intensity of the system is achieved *via* the formation of a ground-state complex, through electrostatic interactions between the fluorophore and BA-quencher. In the presence of saccharides, the formation of a boronate diester results in the dissociation of BA-quencher and fluorophore ground-state complex and leads to a sequential recovery of fluorescence[2].

In this work, the synthesis of a novel BA-quencher is presented, which contains a positively charged N atom, to promote the electrostatic interactions with the fluorophore, 7-hydroxycoumarin (7HC). As expected, photophysical characterisation shows that upon increased BA-quencher concentrations an extremely efficient and sequential decrease in the fluorescence intensity is observed. The introduction of glucose to this two-component system allows for a recovery in fluorescence and can be used to indirectly quantify glucose concentrations. In addition, the inclusion of anchoring moieties to the BA-quencher shows wonderful potential for the incorporation of these molecules into porous hydrogel platforms. To conclude, this glucose-sensing switch shows a high sensitivity for sugar detection, where on incremental additions of glucose, an increase in fluorescence can be observed.

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O10. Molybdenum Disulfide and Graphene Quantum Dots as Electrode Modifiers for Laccase Biosensor

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Nowadays, graphene quantum dots (GQDs) generate increasing interest for their potential applications, due to their extraordinary optical and electrical properties [1]. Few papers reports on GQDs-based electrochemical biosensors. Zhao et al. have designed an electrochemical biosensor based on the interaction between GQDs and single-stranded DNA [2], Muthurasu and Ganesh have also developed an enzymatic biosensor by anchoring horseradish peroxidase on GQDs for the detection of H_2O_2 [3], Razmi and Mohammad-Rezaei have immobilised glucose oxidase on GQDs and have obtained a performant platform for sensitive detection of glucose [4].

In this work the possibility of using molybdenum disulfide (MoS_2) and GQDs as electrode modifiers for constructing a sensitive and reusable laccase based biosensor will be described. The developed laccase biosensor has responded efficiently to caffeic acid over a concentration range of 0.38-100 μM, had a detection limit of 0.32 μM and a sensitivity of 17.92 nA μM^{-1}. The proposed analytical tool was successfully applied for the determination of total polyphenolic content from red wine samples.

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O11. Electrochemical Methods for the Detection of β-Lactam Antibiotics

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Antibacterial drugs have revolutionized the treatment of infectious diseases, but there are different problems associated with the use of antibiotics; the use and misuse have resulted in the development and spread of antibiotic resistance. Thus, there is a need for developing new analytical sensors, able to detect selectively low concentrations of antibiotics from different matrices.

The purpose of this study was to develop a fast and sensitive electrochemical method for the analysis of different penicillins and cephalosporins.

One research direction for the detection of these β-lactam antibiotics was the employment of their electrochemical oxidation using boron-doped diamond working electrodes. The analytical method was optimised for the detection of oxacillin and cephalexin in terms of analysis conditions, selectivity and sensitivity and it was applied to real samples.

Aptamers are a suitable option for assuring a good selectivity and sensitivity to electrochemical analyses of antibiotics. Thus, another research direction of this study was the development of an electrochemical aptasensor for the detection of ampicillin from environmental and pharmaceuticals samples, using carbon or gold electrodes modified with an aptamer selective to ampicillin. Several experimental parameters were optimized and the method was evaluated in terms of selectivity and sensitivity toward the ampicillin detection. The detection of ampicillin with the developed aptasensors is a label-free method, using the variation of the charge transfer resistance in the Nyquist plots of EIS signals to quantify the ampicillin concentration in the sample.

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Oral Communications

Novel materials and biomaterials for analytical methods

O12. Novel Functionalized Magnetic Nanosystems with Tailored Properties for Biomedical Applications

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Biomedical nanomagnetics, i.e. magnetic nanoparticles based techniques used in medicine, is a multi-disciplinary research area unifying efforts in science, nanotechnology and know-how from nanomaterials engineering and medicine, a hot topic of the rapidly developing field of nanomedicine. Among the magnetic carriers for medical use, magnetic iron oxide nanoparticles and their nanocomposites engineered with a large variety of functional coatings are among the most promising materials for applications in magnetic hyperthermia, magnetic resonance imaging (MRI) contrast enhancement, magnetically targeted and triggered drug delivery in cancer treatments.

We report a comparative study of magnetic nanosystems with tunable size, morphology, magnetic and surface properties designed for biomedical applications. Different synthesis methods, such as coprecipitation, thermal decomposition, solvothermal and polyol method have been used for the preparation of magnetic single-core and multi-core nanoparticles with controlled size, shape and composition. Magnetic fluorescent nanosystems were obtained by the rare earth complexation of magnetic nanoparticles functionalized with chelating agents. The correlation between synthesis parameters and the properties of magnetic nanosystems have been determined by advanced characterization methods such as electron microscopies (TEM, HRTEM, SEM), X-ray photoelectron spectroscopy, X-ray diffraction, vibrating sample magnetometry.

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O13. Organic Molecules – Metallic System Interaction: A DFT Approach

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We present a theoretical investigation that addresses the most important aspects of the interaction between α-glycero-phosphatidyl-choline and Au(111) surface. For the density functional calculations we employed both traditional exchange-correlation functionals and newly developed vdW-D2 corrected one. The comparison between these functionals allows us to spot the role of van der Waals effects into the molecule-surface interaction.

The effect of an external field applied to the molecule-surface system was also explicitly investigated. Our results reveal a complex picture where the molecular adsorption is dominated by the interplay between a weak molecule-surface interaction and a rather important deformation energy of the adsorbed molecule. In the presence of an external electric field, the choline moiety provided the strongest response in terms of binding energy as well as geometric configuration of the adsorbate.

The purpose of our investigation is to provide a model allowing understanding of the atomic details of the interactions between phospholipids and metallic surfaces, which is relevant for biosensor development.

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O14. Improving Poly(methyl methacrylate) Properties for Dental Aplication by Adding Titanium Oxide Nanoparticles

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Although removable dentures are usually less appreciated due to concerns regarding their comfort, aesthetics, masticatory function, occlusal stability and maintenance of oral hygiene, it still remains a viable and predictable treatment choice in clinical dentistry. Real obstacles still remain in designing an optimal complete denture due to their poor thermal conduc-tivity, effect on taste, resistance and bacterial contamination.The biocompatible polymer poly(methyl methacrylate) (PMMA) is widely used for complete denture manufacturing due to its important advantages: non-irritating, tasteless, odourless, with affordable cost and good aesthetic aspect. Unfortunately, there are several drawbacks mainly regarding mechanical resistance, bacterial contamination and thermal perception. Significant PMMA characteristics improvements were obtained by introducing nano fillers onto polymeric matrix with strong impact on the macroscopic properties of the polymer even though the filler content is hardly few weight percent. The present work outlines the characteristics and future trend for development of PMMA/TiO_2 for complete dentures fabrication. Some of the new trends includes PMMA denture base improvement by using various additives/filler, especially TiO_2 based leading to better recorded performance. Not only dental materials need to be improved but also the manufacturing technique and the use of computer-aided design/computer-aided manufacturing (CAD/CAM) technology which will lead to simplification of the laboratory work, shorten chair times and increases treatment's quality. The fabrication of complete dentures using improved PMMA especially by addingTiO_2 nanoparticles is considered a promising field. When using newly improved materials, wear behaviour and frictional force were analysed thoroughly with respect to size of the additive/ filler, their dispersion and percentage in the composite. The 5% TiO_2 nanoparticles reinforced PMMA composite has an optimum dispersion in the matrix with lowest particles agglomeration. When a PMMA sample coated with TiO_2 was studied, it was noticed a good performance related to the natural light-induced photo catalytic inactivation and anti-adhesion of bacteria.

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O13. Metallic Micro- and Nanostructured Materials as Supporting Electrodes for Biomolecular Spectroscopy

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The aim of this work was to develop new metallic micro- and nanostructured materials as supporting electrodes for molecular and biomolecular spectroscopy. These novel materials are made of metallic nanoparticles generated by direct laser writing and anchored on active surfaces in controlled patterns. SEM images of the metallic patterns display a uniform distribution as size and shape of the inner nanostructures. UV-Vis spectra of these structured materials functionalized with biomolecules indicate the lack of nanoparticle aggregation, meanwhile SERS investigations evidenced the attachment of the biomolecules on the metallic nanostructures.

The control over the patterns generation as well as the spectroscopic behavior of these novel metallic nanostructured materials make them good candidates for fabrication of supporting electrodes with applications in biomolecular spectroscopy.

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Oral Communications

Atomic and nuclear methods

K9. The Neutrons: A Powerful Tool In Environmental And Biological Studies

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The modern science demands complementary approaches in investigation of environmental and biological objects. Together with protons, neutrons form the nucleus of most atoms. Neutrons are therefore part of all the matter that surrounds us. When are released from the nucleus, the neutrons can be a scientific probe in investigating condensed and soft matter. Neutrons provide structural and elemental information of relevance to drug delivery systems, various diseases, intrinsic nature of pollutants and many other tasks to be solved in health, life and environmental studies. Few examples of the scientific research results obtained with neutrons at IBR-2 reactor of the Joint Institute for Nuclear Research are presented. The opportunities for obtaining beam time at IBR-2 fast pulsed reactor are also described.

I7. Heavy Metal Air Pollution Study in Romania Using Moss Biomonitoring together with NAA and AAS Analytical Techniques

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The heavy metal air pollution in Romania was investigated by using moss species as bioindicators. The research is a part of international programme UNECE ICP Vegetation program-moss surveys.A total of 330 moss samples, *Pleurozium schreberi*, *Hylocomium splendens*, *Hypnum cupressiforme* and other species were collected during the dry seasons of summer and autumn of 2010. The content of 34 elements: Na, Mg, Al, Cl, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu*, Zn, As, Br, Rb, Sr, Cd*, Sb, Ba, Cs, La, Ce, Sm, Tb, Hf, Ta, W, Pb*, Th, and U was determined in the large-scale concentration range — from 10000 mg/kg for Al and K to 0.001 mg/kg for some rare earths by two complementary methods: instrumental epithermal neutron activation analysis (INAA) and graphite furnace/flame atomic absorption spectrometry (GFAAS /FAAS)*. The obtained data 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 realized. Median values for some heavy metals in moss samples collected in Romania, such as Cd (1.20 mg/kg dw) and Pb (30.8 mg/kg dw) are high compared to other European countries. The results revealed that the atmospheric deposition of these metals is a considerable problem in the northern and north-western parts of Romania.

O16. Neutron Activation Analysis as a Tool for Environmental and Materials Research

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Some applications in metallurgical industry of instrumental neutron activation analysis (INAA), using both thermal (reactor) neutrons and fast (14 MeV) neutrons obtained from industrial neutron generators based on D-T $^{3}H(d,n)^{4}He$ nuclear reaction are presented. Analytical applications of reactor INAA in the environmental studies (soil, mosses, vegetation, air filters, etc.) are reviewed.

Thermal INAA was applied at Horia Hulubei Institute of Physics and Nuclear Engineering (IFIN-HH), Bucharest-Magurele, Romania, and Frank Laboratory of Neutron Physics (FLNP) of Joint Institute of Nuclear Research (JINR), Dubna, Russia, to investigate the trace element content of raw materials (iron ores), final products (pig iron, deoxidized steel) and by-products (slag) of metallurgical industry at Iron and Steel Works at Galati (Romania) and to assess the transfer efficiency of some elements from input to output materials in blast furnace and Linz-Donawitz (*LD*) converters.

A study of the capabilities of 14 MeV INAA used in extraction metallurgical industry for alkali metal determination in raw materials for iron and steel industry, and for gold in auriferous sands and rocks in respect to the interferences of all useful nuclear reactions has been accomplished using the neutron generator facility from Activation Laboratory, Nuclear Unit, Iron and Steel Works of Galati.

The INAA technique is particularly effective in solving environmental problems where multi-element analysis of a great number of samples is required. It proves its contribution in elucidating the major problems in the studies of the chemical composition of objects in the biosphere with a view to understanding the role of various elements in the functioning of living organisms and ecosystems under anthropogenic impact.

The perspectives of applying INAA for characterization of high purity materials such as synthesized diamonds, lithium and boron nitrides in combination with characterization of their structure using imaging techniques are described.

Oral Communications

Sensors and biosensors

K10. Nanomaterials And Chemiluminescence Based Method For The Determination Of Antioxidant Capacity

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We shall refer only to the food non-enzymatic antioxidants which have the capacity to scavenge the reactive oxygen species such as: $^{\bullet}OH$, $O_2^{\bullet-}$, H_2O_2, $^1O_2$, $ROO^{\bullet}$ or reactive nitrogen species such as: $ONOO^-$. The food antioxidants belongs to many classes of compounds: carotenoids, vitamine E and derivatives, phenols, phenolic acids, flavonoids, etc. There are many methods for the determination of the total antioxidant capacity (TAC) of different food products: spectrophotometric, fluorimetric, amperometric, potentiometric, voltammeric, etc. In the following we shall discuss only about recent methods based on the use of nanomaterials and on chemiluminescence for antioxidant capacity determination.

It was proposed a ceria nanoparticle-based assay for rapid detection of food antioxidants. The assay is based on the use of immoblized ceria nanoparticle (or other nanoparticle) on paper, which changes color after interaction with antioxidants by means of redox and surface chemistry reactions. The sensors are scanned by using a conventional office scanner, and the red, green, blue (RGB) color breakdown is analyzed. By plotting the inverse of blue color intensity versus log of concentration are obtained calibration curves for different standard antioxidants. The method allow the assay of antioxidant capacity of different types of sample very fast. The assay is very cheap and portable and it could be easily automated.

Luminol is the most used reagent for chemiluminescence assays. Among many proposed methods for chemiluminescence TAC determination we shall focus on several recent assays such as the determination based on the use of luminol/Co(II)EDTA/H_2O_2 system in a batch and in a flow injection configuration; the assay based on the gallic acid enhancement effect for luminol-$AgNO_3^-$ silver nanoparticles chemiluminescence system; and the assay based on the amplification with several order of magnitude by trihydroxybenzoate derivatives of the light emission of alkaline luminol when it is oxidised by gold ions.

I8. The Potential of Sensor Platforms for Dynamic Integrated Process Control in Real-Time. Are they Suitable to Function Properly in the Environment?

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The industry of tomorrow places a heavy demand on more efficient processes that performs in a more fluent cost-saving and sustainable way throughout the whole process production system. These industries need improvements in process monitoring and measurement that is the key for delivering better process control and therefore more sustainable processes. Innovations in process measurement are therefore needed to relate more closely to the full stream process environment to deliver better higher final quality products by allowing better process control and hence substantial cost reduction and a friendlier environment.

This will need a complete new approach for the different scenarios regarding the innovation, development, design, behaviour, implementation and application of sensor (electrochemical and optical) systems. These type of measuring devices and probes should functioned in temperatures on a continuous basis for extended periods ranging from temperatures around 1000 ºC to room temperature and even below and from high pressures to normal pressures depending on the process production system. This talk will look and outlined different types of electrochemical and optical devices currently available and the potential to function reliable and sustainable in the environment of integrated process control in real-time.

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O17. Advancing Magneto-Optical Surface Plasmon Resonance for Biosensing

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In spite of the exquisite analytic potential of Magneto Optical Surface Plasmon Resonance (MOSPR) assays revealed in detection of various gases, their applicability to biosensing has been limited due to major issues concerning chip stability.

We advance solutions to surpass current limitations of MOSPR sensing assays based on innovative chip structure, tailored measurement, and improved methods for data analysis.

The structure of the chip is adjusted to contain an optimized Co-Au alloy layer instead of successive thin layers of homogenous metals with magnetic and plasmonic properties, as currently used. Moreover, using a custom designed measurement configuration that allows fast acquisition of the whole SPR curve, i.e. the reflectivity is measured at multiple angles of incidence as opposed to single incidence angle reflectivity analyses, a high signal to noise ratio is achieved, suitable for detection of minute variations of refractive indices hence providing increased analytic sensitivity.

The proposed approach presents improved magneto-plasmonic properties, and a structural stability similar to standard Au-SPR chips allowing for flow-through high sensitivity bioaffinity assays in saline solutions.

The proposed structure of the MOSPR sensing chip and the procedure of data analysis allow for long time assessment in liquid media, a significant advancement over existing MOSPR chips, and confirm the MOSPR increased sensitivity over standard SPR analyses opening new applicative domains.

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Oral Communications

Novel materials and biomaterials for analytical methods

O18. Photo-Responsive Hydrogels with Enhanced Volume Changes due to Local pH alterations

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Photo-responsive hydrogels of varying compositions containing spiropyran photochromic units have been widely studied in recent years due to their many potential applications, including photo-actuated micro-valves for microfluidic devices [1,2].

In this study two hydrogel formulations were employed to produce reversible photo-responsive hydrogel actuators operative in neutral pH. Both compositions contain the photochromic unit spiropyran acrylate (SP) and acrylic acid (AA) copolymerised in the main polymer backbone, together with *N*-isopropylacrylamide (NIPAAm) or acrylamide (AAm), respectively. At neutral pH, the AA comonomer dissociates to the acrylate anion (A^-) and the proton transfers to the SP unit to give the more hydrophilic protonated merocyanine (MC-H^+) form, which triggers water uptake and hydrogel expansion. Under white light irradiation, the MC-H^+ reverts to the more hydrophobic SP isomer, with simultaneous reformation of acrylic acid, and hydrogel contraction.

In the case of p(NIPAAm-*co*-AA-*co*-SP) hydrogel, an area contraction of up to 45% of its fully hydrated size was achieved after 4 min of white light exposure followed by reswelling to up to 85% of the initial size after 11 min in the dark.

In the case of p(AAm-*co*-AA-*co*-SP) hydrogel, the SP unit serves also as a reversible photo-acid generator changing the local pH which in turn determines the ratio of AA/A^-, and therefore the hydrophilic character of the polymer backbone. In this case, photo-contraction of ~15% in diameter is achieved within 90 seconds of white light irradiation followed by reswelling to ~95% of its fully hydrated size after further ~30 seconds in the dark.

In both cases the photo-induced contraction/reswelling processes were reversible and repeatable over at least 3 cycles with no detectable hysteresis.

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O19. Solvent Sensing Fluorescent poly(Ionic Liquid) Ionogels

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Ionic liquids (ILs) have gathered a lot interest in recent years, due to their properties, such as high electrochemical and thermal stability, good solvation properties, negligible vapour pressure and general high versatility due to their tuneable structure [1]. Owing to this versatility, a multitude of IL subclasses were synthesized, including poly(ionic liquid)s (PILs) and fluorescent ionic liquids [2]. Poly(ionic liquid)s are ILs that feature polymerizable groups in either the cation, the anion, or both, and have similar properties to the ILs from which they are synthesized. Fluorescent ILs possess a fluorescent moiety in their structure. Herein we describe the synthesis and purification of a trihexyltetradecyl phosphonium fluorescein ($P_{6,6,6,14}Fl$) ionic liquid, followed by its incorporation in a crosslinked poly(tetrabutyl sulfopropylmethacrylate) ($pP_{4,4,4,4}SPMA$) matrix, to create fluorescent PIL ionogels for solvent sensing. The ionogels were polymerised in circular moulds with a diameter of 3 mm and a height of 1mm. Following this, the PIL ionogels were swollen in several different solvents, namely hexane, toluene, acetone, acetonitrile, dichloromethane, methanol and deionized water, were characterised using optical microscopy, UV-Vis and Fluorescence Spectroscopy. The results indicate a significant difference in the swelling behaviour of the $P_{6,6,6,14}Fl$ ionogels in different solvents, coupled with different photophysical properties. In conclusion, an ionic liquid containing a fluorescein moiety was synthesised and used together with a polymerizable ionic liquid to produce ionogels with solvent sensing capabilities.

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O20. Stimuli-responsive Materials for Self-reporting Micro-fluidic Devices

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The integration of stimuli-responsive materials into microfluidic systems can provide a means for external control over fluid flow along with inherent sensing capabilities, which can reduce the overall complexity of microfluidic devices. Herein we present several approaches for introducing fluid movement and sensing using stimuli-responsive materials. The first approach comprises the use of adaptive nanostructured coatings for direct sensing of flow in continuous flow mode. For this, the inner walls of micro-capillaries and micro-channels were coated with polymeric materials that can be used to detect a variety of target species. Two types of adaptive coatings will be discussed. The first one is based on the conductive polymer polyaniline (PAni)[1,2] while the second consists of polymeric brushes based on spiropyran[3,4]. Using the "grafting" approach homogeneous coatings were obtained on the micro-channel/micro-capillary surface that retained their inherent nano-morphology. The optical proprieties of these coatings change in response to a variety of target analytical species (divalent metal ions, solvents of different polarities, ammonia, H^+) passing through the microfluidic device in continuous flow mode. The grafting approach can provide nanostructured to microstructured coatings that combine small diffusion paths with relatively thick optical path lengths, thereby providing sensitive and fast optical responses to the target analytes.

The second approach comprises the use of porous photo-actuated hydrogels as photo-controlled micro-valves in microfluidic systems for repeatable ON/OFF flow modulation in flowing streams over a wide pH range.

Incorporation of such stimuli-controlled structures in microfluidic devices offers unprecedented versatility and external flow control. We envision using these systems to create a new generation of sustainable, low-cost, photonically-controlled and self-reporting fluidic systems.

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O21. When Microfluidics met Smart Materials

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The integration of chemo/biosensors[1] and reagents for long term storage[2] in the microchannels of a microfluidic device using smart materials has several technological advantages compared to bench based technology, such as reduction of the volume that is needed to monitor certain analytes, minimisation of cross-contamination from the surrounding environment, continuous flow operation and long life storage, among others. Moreover, the incorporation of stimuli responsive materials in microfluidics is enabling new ways of fluidic control and manipulation that overpasses existing technology, opening new avenues for the commercialisation of these devices.[3]

As in the movie “When Harry met Sally...” where the two main characters were meant for each other, there is pure chemistry between microfluidics and smart materials. Therefore, in this contribution we present our latest advances on the integration of smart materials in microfluidics in order to provide new functionalities to Point of Need Microfluidic Platforms.[4] We make use of UV-photoprintable ionogel materials, polymer gels that incorporate ionic liquids, as building blocks to produce reagent storage arrays in microfluidic devices as well as microvalves and micropumps for fluid manipulation and control.

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Oral Communications

Sensors and biosensors

O22. A New Twist for Optogenetics: Light Driven Dynamics for Cell Based Sensing

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Biosensing cellular platforms involving adherent cells and electric cell-substrate impedance sensing (ECIS) are a matter of intense scrutiny. Electrogenic cell cultures (neurons, cardiomyocytes) traditionally used for functional assays demonstrate a high analytic potential but also a detrimental sensitivity to environmental conditions and high biological variability.

We hereby demonstrate a novel cellular sensing concept based on real time electrical assessment of light responsive, non-excitable cells upon recurring illumination modulated by extracellular stressors/stimuli, including effect of various analytes. Cell impedance, governed by exogenous (light driven) cellular processes, such as dynamics of cell membrane and cell-surface adhesion during illumination and recovery phases depends on cells' ability to restore membrane parameters towards the resting levels and enables assessment of analytes' effect, hence their quantitation.

To this effect, both a dedicated cell line custom modified to express light-sensitive ion channel proteins and an analytical platform for inducing and monitoring cell responses upon illumination were respectively advanced.

This novel sensing concept has been applied to reveal cellular effect of model analytes, highlighting specific evolutions of impedance data characteristic for cellular status and the nature of extracellular stimulus, dramatically decreasing the classical ECIS analysis time and being amenable to high parallelization. The applicative potential in cell based biosensing will be discussed.

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O23. Molecularly Imprinted Electrochemical Sensors for Detection of Drugs and Pollutants

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Molecular imprinting is a versatile technique for the fabrication of artificial receptors, with a wide range of applications in chromatographic separation, solid phase extraction and chemosensors. The imprinting process produces synthetic polymers with cavities complementary in size, shape and chemical functionality with the analyte of interest, which are able to recognize and bind the analyte from complex matrices with high selectivity. MIPs have the advantages over their biological counterparts of ease of synthesis, low cost, high thermal and chemical stability and long storage life.

The integration of MIPs in chemical sensors has received increased attention lately. MIP based electrochemical sensors have been applied with promising results in various fields, such as clinical, bioanalytical and environmental analysis.

Several studies have been proposed for the development of electrochemical MIP-sensors for the sensitive and selective detection of various target analytes, such as drugs and pollutants. TNT, gemcitabine, tetracycline, estradiol and glyphosate have been investigated as template molecules. A generic protocol for the fabrication of MIP was developed based on electropolymerization of *p*-aminothiophenol functionalized-gold nanoparticles. In order to obtain imprinted films, the electropolymerization process was performed in the presence of the target analyte which serves as template molecule, the subsequent removal of the template leaving cavities that serve as specific recognition sites. Combining the advantages of molecular imprinting and electrodeposition with those conferred by gold nanoparticles, the developed sensors exhibited good sensitivity and high selectivity. Several parameters influencing the performance of the sensors have been optimized and the resulted sensing materials have been successfully applied for the analysis of real samples.

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O24. Oxygen Sensing using an Ultra-microelectrode Array at the Millisecond Time-scale

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A short pulse choronoamperometric technique using an ultra-microelectrode array (UMEA) (36-UME array, UME dimensions: 2 µm Ø ; 20 µm spacing; and 390 ± 20 nm recess) is presented. The UMEAs are fabricated from sputtered platinum in an oxide-nitride-oxide insulating layer on a glass substrate using standard cleanroom processes. The oxygen concentration is determined by reducing oxygen at the UMEAs and measuring the slope of the corresponding current at short time-scale within 5 ms. Using this short time-scale measurements the amount of oxygen consumed is dramatically low as compared to the conventional chronoamperometric technique. Therefore, this sensing technique is suitable for measuring *in situ* the respiratory activity of biological substrates such as microtissues in nL volumes with minimal disturbance to their environment.

O25. Oxygen Sensitive Hydrogel Matrix for 3D Cell Culture and 3D Oxygen Concentration Mapping

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Oxygen is a vital marker in cell biology and local variations in its concentration are associated to complex phenomena such as metastasis. Therefore, studying oxygen and its variations is of importance when using *in vitro* models, as for instance in microfluidic devices. However, currently available sensors provide local information on the oxygen concentration only in their direct vicinity. Ideally, 3D information on the oxygen levels will help design and exploit complex *in vitro* models. To achieve this, we propose a novel approach using a ruthenium-based dye that is covalently coupled to a hydrogel.

The oxygen-sensitive matrix is prepared by covalently coupling a Ru-based dye to primary amine groups in collagen using NHS/EDC chemistry. The conjugated matrix exhibit similar properties to native collagen as assessed using SEM and AFM. Stern-Volmer plots for different initial dye concentrations (10-100 µM) in MES buffer show linear relationship. The presence of the dye in the collagen matrix does not have any adverse effects on cell viability. Finally, after embedding of HCT-116 spheroids in the oxygen-sensitive matrix in a microdevice, changes in oxygen concentration are recorded in the direct vicinity of the spheroid after 24h.

In the future, we aim to employ this oxygen-sensitive matrix for correlating local oxygen tension and metastatic cancer cell migration in a microfluidic platform.

Poster Communications

Nanobiotechnology

PNb1. Magnetic Iron Oxide (Fe_3O_4) Nanoparticles From Agro-Wastes For Removal Of Antibiotic Pollutants From Waters

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In this work, magnetite nanoparticles (Fe_3O_4 NPs) were successfully synthesized using extracts from three abundantly found agricultural wastes, namely peels of black grapes (*Vitis vinifera* L.), lemon (*Citrus limon*) and cucumber (*Cucumis sativus*). The use of agro-wastes for nanoparticle synthesis serves dual purpose of using this inexpensive, easily available source of active biochemical components, and also helps in the prevention of pollution resulting in the case of its improper disposal. The biosynthesized Fe_3O_4 NPs have been characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), X-ray photoelectron spectrometry (XPS), FTIR (Fourier Transform Infrared spectroscopy), and Vibrating sample magnetometer (VSM) studies. The magnetic nanoparticles were further tested for the removal of various antibiotics from liquid matrices. A Box-Behnken experimental design by combination of investigated parameters was employed to obtain a high efficiency in the removal of antibiotics. The effect of pH, volume of antibiotic and temperature on the retention of selected antibiotics (piperacillin, tazobactam, sulfamethoxazole, tetracycline, trimethoprim, ampicillin and erythromycin) using the magnetite nanoparticles was investigated. The analyses of the studied pharmaceuticals were carried out on a Shimadzu 2010 liquid chromatograph and the separation was performed using a Grace Alltima RP-18 (3 µm, 10x0.3 cm, Merck, Germany) column thermostated at 40°C. The mobile phase consisted of acetonitrile-ultrapure water (90:10, v/v) (A) and ultrapure water with 0.1% formic acid (B). Except sulfamethoxazole and trimethoprim, a high degree of removal (over 90%) for all the other studied antibiotics was obtained. It was concluded that Fe_3O_4 NPs synthesized with cucumber peel extract were most efficient for retention of antibiotics, followed by Fe_3O_4 NPs obtained with lemon peel extract.

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PNb2. Application Of Magnetite Nanoparticles Synthesized Using Agricultural Sources For Removal Of Lanasyn Red Dye

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The green method for synthesis of nanoparticles using plant extracts is easy, efficient, and eco-friendly, thus gaining increasing interest for the field of nanotechnology in the last years. The studies performed showed that phytochemicals present in the plant extracts may act both as a reducing as well as stabilizing agents in the synthesis process. In the present work, magnetite nanoparticles (Fe_3O_4 NPs) were synthesized using extracts from pale green kohlrabi (*Brassica oleracea var. gongylodes*) leaves and pink grapefruit (*Citrus paradise* Macf.) peel. The as-synthesized Fe_3O_4 NPs have been characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), X-ray photoelectron spectrometry (XPS), FTIR (Fourier Transform Infrared spectroscopy), and Vibrating sample magnetometer (VSM) studies. A large number of research papers have been focused on the multiple applications of magnetite nanoparticles, including investigations on their dye removal efficiency from wastewaters. Textile manufacturing is one of the largest industrial sources generating wastewater that contains a large number of water-soluble chemical pollutants, thus causing toxicological problems to the aquatic environment. Azo dyes, along with anthraquinone dyes, are the textile colorants most commonly used in textile industry. In this study, the synthesized magnetic nanoparticles were further tested for the removal of Lanasyn Red (an azo dye) from liquid matrices. The studies of dye adsorption were performed within experiments conducted by varying initial concentration of dye, adjustment of the pH solution, dosage of Fe_3O_4 and contact time, etc.

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PNb3. **Highly ordered Iron Phthalocyanine (FePc) Nanometer-Sized Layers Deposited On Si (111) 7×7 By Molecular Beam Epitaxy**

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In recent years, there has been an increasing interest in organic semiconductor thin layers due to their important role in the fabrication of new materials for optoelectronic applications and photovoltaic devices. In particular, metallophthalocyanines on solid state substrates based compounds have attracted great attention to applications such as organic light emitting diodes, organic solar cells, field-effect transistors, molecular gas sensors, memories and optoelectronic devices.

Molecular beam epitaxy (MBE) is a well-known technique used to grow organic semiconductor nanometer-sized layers on various substrates. Iron phthalocyanine (FePc) nanostructurated films were grown on Si (111) 7×7 substrates at temperature on 300K by MBE under ultra-high vacuum (UHV) of 2×10^{-10} mbar.

The spatial orientation of the thin layers of FePc was assessed by Raman spectroscopy, and demonstrates the presence of the molecules on the Si (111) 7×7 surface. The fingerprint band of the compound is located at 1558 cm^{-1} and is linked to the influence of the Fe ion on the initial vibrational structure of the Pc molecule.

Scanning Tunneling Microscopy (STM) measurements were performed in UHV at room temperature and suggested the in-plane orientation of the FePc molecules on the Si substrate.

Acknowledgments: Financial support from the National Authority for Scientific Research and Innovation - ANCSI, Core Programme, Project PN16-30 02 01, "Tehnici de micro- și nano-fabricație dedicate dezvoltării de dispozitive moleculare respective termoelectrice și a senzorilor pe bază de grafene", is gratefully acknowledged.

PNb4. **ZnO Nanoparticles for Biosensing Applications**

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The biocompatibility and low toxicity of ZnO nanoparticles are optimal properties for their application in biomedical environment. Nanostructured ZnO is a compound easy to manufacture and a suitable candidate for producing of biosensors with enhanced performances.

The **goal** of our research was to obtain ZnO nanoparticles and improve the properties of their surface in order to developing biosensors for biomedical applications.

Synthesis: ZnO nanoparticles were synthesized by hydrothermal method using zinc nitrate as a precursor.

Nanoparticles **characterization**: Phase identification and average size of crystallites were determined by X-ray diffraction. The morphological characteristics of nanoparticles were observed using scanning electronic microscopy; their optical properties were characterized using UV-visible spectroscopy. We obtained Fourier transform infrared (FT-IR) spectra to see the absorption bands and we measured the electrical conductivity of the nanoparticles.

Conclusions: Morphology and properties of ZnO nanoparticles are suitable for future testing in biomedical applications.

Acknowledgments: This study was financially supported by Romanian National Authority for Scientific Research (grants PNII PCCA-16/2012, PNII PCCA-89/2012, and EraNet 4-004/2013).

PNb5. Indirect Assessment of Antimicrobial Peptides Binding Affinity to Lipid Bilayers via a Single Nanopore Sensing Technique

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Antimicrobial peptides (AMPs) are short, positively charged peptides that are part of the innate immune system of many organisms, contributing to their protection against microbial infections. A key feature of cationic peptides is their capability to distinguish bacterial from mammalian cells based on their different lipid composition. The net positive charge of AMPs is very important for their selectivity, as they target bacteria by a non-specific mechanism of binding to the negatively charged moieties of the outer membrane of bacterial cells. In this work we propose a nanopore-based sensing technique able to assess the binding affinity of selected cationic AMPs to small unilamellar vesicles (SUVs) of different lipid composition. AMP molecules were added to one side of a planar lipid membrane spanned by a single α-hemolysin (α-HL) protein pore and were allowed to reversibly interact with the lumen of the nanopore causing reversible blockage events in the ionic current flow through the channel under an applied transmembrane voltage. Statistical analysis of these blockage events generated the kinetic description of the interaction between free peptides in solution and α-HL, corresponding to a simple bimolecular reaction with a linear dependence of the onward reaction rate on the concentration of peptide. We further added a third participant to the aqueous environment (SUVs consisting of DOPC and DOPC:DOPG 4:1, respectively, in different incremental concentrations), which competitively interacts and binds peptide monomers in solution, shifting the equilibrium of the peptide-pore reaction to the left. Our single-channel ion current recordings allowed us to indirectly monitor the adsorption of AMPs to negatively charged and zwitterionic lipid vesicles, and the results showed that the binding affinity of cationic peptides is higher for negatively charged membranes (containing DOPG).

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PNb6. **Tuning the Interaction Environment for Single Nanopore-based Sensing of Gram-negative Bacterial Cells**

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The development of miniaturized devices able to sense and detect pathogens with high speed and sensitivity represents an important topic in biotechnology and safety-monitoring activities. In this work we present a first proof of concept demonstrating the potential of a biological nanopore-based technique for real time detection of selected Gram-negative bacteria (i.e.: Pseudomonas aeruginosa and Escherichia coli). Bacterial cells bear a net negative charge on their surface which promotes their reversible capture by a single α-hemolysin (α-HL) protein pore embedded in a reconstituted planar lipid membrane. Our results show that the biological nanopore sensor is able to detect individual bacterial cells and assess the selective binding of antimicrobial peptides (AMPs) to bacterial membranes via electrophysiology recordings of current blockages induced upon electrophoretically-driven bacteria-nanopore interaction. The addition of CMA3 peptides in the bacterial suspension altered the association kinetics of bacterial cells with the α-HL pore. The cationic peptides adsorb at the interface of bacteria, decreasing the net negative surface charge and thereby lowering the strength of the interaction with the electric field created by the external applied voltage. Despite this, data show that the presence of CMA3 peptides in the system led to an increase in the frequency of interaction between bacteria and the protein pore, due to additional repulsive electrostatic interactions between negative charges on the bacterial surface and the ring of net negative electric charge present at the entrance of the α-HL lumen, at neutral pH. By conducting experiments in an acidic environment (pH=4), we were able to fine-tune the negative electric charge at the entrance of the protein lumen and thereby increase the frequency of bacteria-nanopore interactions.

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PNb7. **Interaction of Silver Nanoparticles with Lipid Monolayer as a Model of Biological Membranes**

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The most important arsenal in the fight against pathogens is the antibiotics. They bring great therapeutic benefit and this medication is the most commonly prescribed and used. Nevertheless, bacterial resistance has become an alarming phenomenon in our days, the bacterial evolution keeping up with development of the new generation of antibiotics.

An alternative to antibiotics is the silver nanoparticles (AgNPs), whose antimicrobial activity is well known since ancient times, but the mechanism of action is not fully understood. There are proposed three paths of action for AgNPs: i) damage of the cell membrane and complexing of intracellular components with nanoparticles; ii) disruption of ATP synthesis and DNA replication; iii) formation of reactive oxygen species and DNA damage.

The aim of this study is to decipher the intimate mechanism of action of AgNPs on prokaryotes and eukaryotes cell membranes.

Our hypothesis is that the AgNPs destabilizing the cell membrane by the action on the lipids.

Researches have focused on using Langmuir Blodgett technique for making lipid monolayers as model for an artificial cell membrane, followed by characterization of the interaction that occurs at the interface lipid/AgNP.

In the experiments, were recorded two-dimensional pressure isotherms for different lipid monolayers (phosphatidylcholine - PC, bacterian lypopolysaccharides - LPS) deposited on a subphase of pure (distilled water) in the presence and absence of silver nanoparticles synthesized and stabilized with citrate.

Conclusions: At concentrations above 35 g / ml we found an fluidifiant effect of AgNPs on lipid monolayer (PC or LPS). In these conditions, the membrane can display pores that may affect the viability of the cells.

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PNb8. **Characterization of Silver and Copper Nanoparticles Synthesized by Bottom-Up Approach Using Plant Extracts**

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In this study we report a “green” approach for the synthesis of silver and copper nanoparticles (NPs), in which the rosemary (*Rosmarinus Officinalis), sage (Salvia Officinalis), oregano (Origanum Vulgare), lavender (Lavandula), elderberries (Sambucus), Saint John’s wort (Hypericum Perforatum)* extracts were applied for the reduction of silver and copper ions and the stabilization of the formed nanostructures.

The obtained extracts have different content of reductive organic species that produce NPs with various shapes (nano cube, semi round and triangular nano plate) and different sizes. At the same time, the reaction conditions (pH, temperature, concentration of the ionic solution, type of the extraction solvent, the extraction procedure) were monitored.

The synthesized NPs were characterized by UV-VIS, IR spectroscopy and x-ray diffraction in order to establish the correlation between the reaction conditions and the NPs size. The prepared solutions showed an absorption band at about 400 nm, for the silver NPs and at 600 nm, approximately, for the copper NPs due to surface plasmon resonance (SPR).

Consequently, optimal parameters for the tuning of the NPs formation process were proposed.

PNb9. **Study on the Synthesis Process of Silver Nanoparticles in *Salvia Officinalis* Extract Using UV-VIS Spectroscopy**

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Silver nanoparticles (AgNPs) were synthesized by bottom-up approach using *Salvia Officinalis* extract. AgNPs are products of Ag^{+} reaction with organic compounds from plant extract, such as polyphenols and flavonoids. Presence of AgNPs, their particle size range and stoichiometric ratio were evaluated by UV-VIS spectroscopy. Scans performed in various reaction mixtures showed an absorption maximum at 430 nm, indicating a size of AgNPs around 50 nm. Job's Method and experimental setup were used to study the equilibrium involved in the process. Stoichiometric ratios were determined by following the changes of absorbance maximum values versus silver / plant extract ratio, for experiments performed at different temperatures and pH values. Conclusions on synthesis parameters influence on process equilibrium were drawn.

PNb10. **Kynetic and Thermodynamic Properties of the System Nanoimmunosorbent- Analyte (2,4-D) in the Presence of Enzymatic Label Used in Homogenous Elisa Technique for Detection Of 2,4-D from Environmental and Alimentary Samples**

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The paper presents kinetics and thermodynamic of the immune systems antibody (anti 2,4-dichlorophenoxyacetic acid)-antigen (2,4-dichlorophenoxyacetic acid) in the presence of the enzymatic label used in homogenous ELISA (Enzyme Linked Immunosorbent Assay) technique based on the use of the nanoimmunosorbents made of nanoparticles of silicon dioxide functionalized by covalent binding of the antibody anti 2,4-dichlorophenoxyacetic acid on the surface of the nanoparticles. 2,4-dichlorophenoxyacetic acid is used as a pesticide in agriculture to control and destroy of the weeds.

The purpose of the kinetic studies of the binary system: solid phase-anti 2,4-D antibody (nanoimmunosorbent)- 2,4-D in the presence of enzymatic label is to determine the immune complex forming rate constant (direct reaction), the dissociation of the complex rate constant and equilibrium constant K for different temperatures.

In order to established the thermodynamics properties of the immune systems: antibody-antigen in the presence of enzymatic label were determined the values of the equilibrium constants at the two temperatures, variation of the Gibbs energy, variation of the reaction enthalpy and the variation of the standard entrophy.

The homogenous ELISA technique is applied for detection of the residual pesticide 2,4-dichlorophenoxyacetic acid from alimentary and environmental samples.

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PNb11. **Pectin-based Composites containing Graphene as Substrates for Cells Growth**

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Graphene-like materials possess a wide range of unique properties and show a huge potential for various biomedical applications. As substrates for cells proliferation and differentiation, graphene can be used by itself or in combination with other types of materials, like nanoparticles or polymers. In this study, graphene oxide (GO) was obtained from graphite by a chemical oxidation process (a modified Hummer's method). Thermally reduced graphene oxide (rGO) was formed as a result of annealing treatment of GO under argon atmosphere. Both GO and rGO were embedded into pectin (a natural and biocompatible polymer) matrix. Since the physico-chemical characteristics of obtained materials have significant effects on the cells metabolic activity, the composites were evaluated by means of Infrared Spectroscopy (FTIR), X-ray powder Diffraction (XRD) and Scanning Electron Microscopy (SEM). The colorimetric MTT metabolic activity assay was used to compare the biological responses of stabilized human palatal mesenchymal stem cells after their interaction with each composite. The cytotoxicity studies results showed that pectin-GO composite has low cytotoxicity (under 2 %), while pectin-rGO composite presents harmful effect for the same cells (above 52%). Fluorescence microscopy experiments confirmed the presence of living cells that were uniformly distributed in the culture medium, with several colony-forming cells. However, the molecular interaction between the composite materials and human cells is not yet elucidated.

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Poster Communications

Spectroscopy

PSp1. **Fabrication of Nanostructured Au Films as Promising SERS Substrates for the Detection of Pathogenic Bacteria**

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As there is a continuous emerging of new and multidrug-resistant pathogens, the need to develop faster, more accurate and multiplex detection methods is crucial. Having several unique characteristics, such as the ability to provide molecule-specific fingerprint-like spectra and the non-destructive, label-free, and highly sensitive nature of the measurement, SERS (Surface-Enhanced Raman Scattering) spectroscopy gain more and more popularity in problems related to ultrasenzitive detection. Our aim is to fabricate nanostructured metallic films for SERS-based, whole-bacteria detection applications. Thin Au/Si(111) films were deposited by molecular beam epitaxy under ultra-high vacuum (UHV) environment. The nanostructured surface topography, growth mode and controlled roughness of the Au films were assessed using Scanning Tunneling Microscopy (STM). The deposition process of the Au-coated Si substrates was optimized in order to exhibit a high SERS signal of the investigated bacteria. High resolution and reproducible SERS spectra of *Rosetta* strain of the Gram-negative bacteria *Escherichia coli* (*E. coli*) were obtained using the 632.8 nm laser line with a power in the μW range, in order to avoid sample degradation. The spectra are comparable to those obtained using Ag-based SERS active substrates and opens an avenue for nanostructured films SERS-based biosensors.

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PSp2. Evaluation of the Chemical Compositon and Micronutrients of Wild and Commercial Mushrooms of Dambovita

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The mushrooms present an interest for consumption as food, for traditional medicine as drug or in bioremediation, due to their nutritional, antioxidant, antimicrobial and therapeutic values. In this paper a comparative study, between some wild-growing mushrooms species and some commercial cultivated mushrooms species, was made. Three species of edible wild-growing mushrooms (*Pleurotus ostreatus, Cantharellus cibarius* and *Agaricus campestris*) and four species of cultivated mushrooms (*Pleurotus ostreatus, Cantharellus cibarius, Agaricus bisporus white* and *Agaricus bisporus brown*) were selected to determine the chemical composition (crude protein, crude fat, total carbohydrates and ash), total phenols, total amino acids, acid ascorbic and elemental contents (Fe, Zn, Cu, Mn, Cr, Ni, Cd, Co, Pb, Ca, Mg, Na and K). All investigated mushrooms were found to be good sources of proteins and total carbohydrates. The highest protein content was found in the wild *Cantharellus cibarius* (32.55 g/100g), while the total carbohydrate content was higher in the commercial *Pleurotus ostreatus* species (72.8 g/100g). The wild species revealed a higher content in phenols and total amino acids and a lower content in ascorbic acid than commercial mushrooms. For the both types of fungi, the trend of macro elements concentrations was K > Mg > Ca > Na while the trend of heavy metals concentrations was Fe > Zn > Mg > Cu > Cr > Pb > Ni > Cd > Co.

PSp3. **Characterization of Some Physico-chemical Properties and Interactions of Human and Bovine Serum Albumin with Mitomycin C**

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A special interest in the medical field is paid to the interaction and transport mechanisms of cytostatics by serum albumins. This work aims to investigate some of the physico-chemical propreties and the molecular interactions of human and bovine serum albumins with mitomycin C cytostatic, and also to study the thermodynamic stability of the complexes of these proteins with mitomycin C. The pH and temperature influence on serum albumins propreties and the binding mechanism of mitomycin C to these proteins have been followed by UV absorbtion spectroscopy, seady-state fluorescence, and time-resolved fluorescence.

The binding propreties of mitomycin C drug to bovin and human serum albumins show that the fluorescence of serum proteins were quenched by MMC, through a static quenching mechanism. MMC spontaneously binds to one site of BSA and HSA, respectively, with very similar and moderate affinity constants. The thermodynamic parameters suggest that the main role in the binding of MMC to serum proteins belongs to the hydrophobic interactions and hydrogen bonding. This study may contribute to a better understanding of the binding mechanism of anti-tumour drugs to serum albumins that are important carriers for the drugs and other substances.

PSp4. **(Sub)Picosecond Dynamics in LacDNA Molecules as Probed with UV Resonance Raman Spectroscopy**

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In this work, we report an UV Resonance Raman (UVRR) spectroscopic study on double-stranded and single-stranded DNA oligomers. Investigation of (sub)picosecond dynamical changes induced in a natural DNA recognition site, in the presence and absence of divalent metal ions (Mn^{2+}, Ca^{2+}) at two pH values (6.4 and 3.45), respectively, providing data about changes in half bandwidths and in the global relaxation times of LacDNA subgroups UVRR vibrations, are of interest. The targeted DNA is a non-palindromic 22-mer duplex representing the primary cyclic AMP receptor protein (CRP) binding site of the *E. coli* lac promoter.

Resonance Raman scattering simplifies the highly complex and congested vibrational pattern of DNA as exclusively vibrations coupling to the electronic transition are resonantly enhanced.

The full-widths at half-maximum (FWHM) of the UVRR bands studied in this work are in the wavenumber range 13.5-39.5 cm^{-1} for double-stranded DNA and between 14-55 cm^{-1} for single-stranded DNA, respectively. The molecular relaxation processes corresponding to double-stranded DNA have a global relaxation time smaller than 0.786 ps and larger than 0.269 ps. For single-stranded oligonucleotides, a global relaxation time between 0.193-0.758 ps has been found.

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PSp5. **(Sub)Picosecond Relaxation Processes in Nucleic Acids Constituents and in DNA Molecules: a Raman and Surface-Enhanced Raman Spectroscopy Assessment**

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Raman scattering can be used to study the fast (sub)picosecond relaxation processes in nucleic acids and their components.

In the present work, Raman total half band widths of seven nucleic acids constituents (adenosine, guanosine hydrate, cytidine, thymidine, uridine, adenosine 5′-monophosphate disodium salt and 2’ - deoxyadenosine - 5’ - monophosphate) have been measured, respectively. In our study, we have established that the full widths at half-maximum (FWHMs) for the Raman bands of the investigated nucleic acids constituents are typically in the wavenumber range from 9 to 27 cm^{-1}. Moreover, the molecular relaxation processes studied in this work are characterized by global relaxation times with values smaller than 1.18 ps and larger than 0.39 ps.

Besides, the surface molecular dynamics parameters are indicated for several protonated genomic DNAs, using surface-enhanced Raman spectroscopy.

The dependencies of the total half bandwidths and of the corresponding global relaxation times, on molecular fragments and on the type of nucleic acids subgroups are reported.

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PSp6. ^{1}H NMR Characterization of the Host – Guest Inclusion Complex between β – Cyclodextrin and Tolmetin

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Nonsteroidal antiinflamatory drugs (NSAIDs) are common analgesics and antiinflamatory agents, which inhibit the cyclooxygenase enzyme. Although highly effective for these purposes, they usually cause a high incidence of gastrointestinal ulcerative lesions. The use of cyclodextrins (CDs), as a family of pharmaceutical excipients and drug carriers has become an increasingly successful method to improve the general bioavailability of drugs. Tolmetin is a NSAI drug belonging to the family of arylalkanoic acid. This drug is used to decrease the level of hormones that cause pain, swelling, tenderness and stiffness that results from muscle skeletal and bone related diseases. Cyclodextrins are naturally occurring cyclic oligosaccharides known for their effect on stability, solubility and bioavailability of various drugs. The shape of naturally occurring cyclodextrins can be represented as a toroidal hollow truncated cone having many primary and secondary hydroxyl groups crowning the narrower and wider rims of the hollow cone, respectively. CDs are capable of forming inclusion complexes with many drugs by taking up a whole drug molecule, or some part of it, into the cavity. The interaction between β – cyclodextrin with tolmetin was investigated using NMR analysis of complexation – induced chemical shifts, the method of continuous variation (Job's analysis), and analysis of ROESY spectrum. The Job's plot confirms that the complex formed has 1 : 1 stoichiometry. The association constant, K_a of the obtained complex was calculated and found to be 2164,5 M^{-1}. The ROESY spectrum was used to ascertain the solution geometry of the host – guest complex.

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PSp7. **NMR study on the Low-Affinity Interaction of Human Serum Albumin with Zidovudine**

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The extent of protein binding is important to know for both pharmacokinetic and pharmacodynamic reasons. E.g. a high protein binding of a drug allows a transport in plasma at concentrations higher than expected from the drug's water solubility and thus, a greater plasma-to-tissue gradient. According to the current knowledge only the free, i.e. the unbound, fraction of a drug is able to bind to a receptor or an enzyme and along with this to induce a pharmacological effect.

Typically, processes such as the immune response, ion transport, and gene transcription and translation do not occur until ligands are recognized and bound specifically by a certain protein. Among investigated proteins, a special attention was paid to human serum albumin (HSA), the principal extracellular protein in blood plasma.

Zidovudine (ZDV), also known as azidothymidine (AZT), is an antiretroviral medication used to prevent and treat HIV/AIDS. Zidovudine was the first drug approved for the treatment of HIV. It is a nucleoside analog reverse transcriptase inhibitor, or nuke. These drugs block the reverse transcriptase enzyme.

Besides these classical techniques (dialysis, ultrafiltration, ultracentrifugation and different electrophoresis techniques) used in many laboratories of the pharmaceutical industries, NMR experiments can also be used for the characterization of the drug–protein interactions, especially the measurement of the selective relaxation time T_1.

The purpose of this study was the characterization of the protein binding of Zidovudine, by means of NMR spectroscopic method. Via T_1 selective relaxation measurements the extent of the protein binding and locus of drug–protein interaction was determined as dissociation constants K_D.

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PSp8. **Spectroscopic Investigation Of Iron Phthalocyanine (FePc) Molecular Layers Deposited On Au/Si**

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The organic semiconductor thin layers have received significant interest nowadays because of their important role in the fabrication of new materials. Phthalocyanines (Pc) and their metal complexes (MPc) have attracted considerable interest and have been found to be highly promising candidates for a variety of applications such as liquid crystals, organic light emitting diodes, photosensitizers, memories and optoelectronic devices. The different chemical structures allowing the design of compounds capable of meeting certain needs make Pc/MPc particularly attractive.

Gold has an important role in thin films biosensors, optoelectronics, electronics and electromagnetic sensors. Molecular beam epitaxy (MBE) is a well-known technique used to grow Au nanometer-sized films on various substrates. The Si(111) – (7×7) surface reconstruction is a very good template for the growth of metallic nanoscale films.

The 100 nm thick gold films were deposited using molecular beam epitaxy technique onto Si(111) 7×7 substrates. Iron phthalocyanine (FePc) nanostructurated films were grown on Si (111) 7×7 substrates at temperature on 300K by MBE under ultra-high vacuum (UHV) of 2×10^{-10} mbar.

Aiming to elucidate their molecular structures and the spatial orientation Raman and the ultrasensitive surface enhanced Raman spectroscopic methods were used. The molecular vibrations of FePc molecules deposited on the Au/Si substrate were investigated by Raman and SERS spectroscopies. The spectra were recorded using 532 nm and a 633 nm laser lines with a power in the μW range, in order to avoid sample degradation. The band assigned to the FePc compound is located at 1558 cm^{-1}.

PSp9. Lipopolysaccharide Association with Allantoin Crystals Addressed through THz and FTIR Spectroscopy

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Lipopolysacchides (LPS) are the endotoxins of Gram-negative bacteria. They represent a high risk for human health, as their toxicity is exhibited even at low concentrations. Selective LPS removal from biological samples can be performed with allantoin. Allantoin crystallizes at concentrations higher than its solubility limit (5 mg/ml) and mostly forms 500 nm crystals. LPS molecules form a monolayer on allantoin crystals, the LPS monolayer adsorption occurring when 3-8 mg of LPS molecules are added to 1 g of allantoin.

Here we addressed the binding of LPS molecules to allantoin crystals by using Terahertz (THz) and Fourier transformed infrared (FTIR) spectroscopy. THz spectroscopy (far infrared radiation with the frequencies 0.3 – 3 THz, 1 THz = ~33.35 cm^{-1}) and reveals high amplitude, low frequency, collective motions of biomolecules associated to their conformational transitions. On the other hand, FTIR (mid-infrared radiation with the frequencies 4000 cm^{-1} – 400 cm^{-1}) measures high frequency, localized motions of biomolecules that show indirect information about their conformational transitions.

THz and FTIR spectra were measured on lyophilized samples comprising different LPS – allantoin ratios (0 mg, 1.5 mg, 3 mg, 6 mg, 8 mg, 10 mg, 12 mg LPS / 1 g of allantoin). LPS and allantoin were solvated in HEPES buffer with 150 mM NaCl and a pH adjusted to 7.5. Samples were centrifuged. The sediment was preserved and it was additionally dried by lyophilisation. Our results show differences in the absorption of samples. In the case of THz results, the spectra present a similar shape, except for the low frequencies where we identified the contribution of increasing LPS concentration. In the case of FTIR data, the overall shape of LPS-allantoin mixtures spectra resembles that of allantoin, except for a change in peaks intensities. The results obtained by both techniques will be interpreted based on molecular modelling results.

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PSp10. **Study of the Interaction between Antimicrobial Peptides and Model Cell Membranes by Steady State and Time Resolved Fluorescence**

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Antimicrobial peptides (AMPs) are the result of the immune system response of organisms to various bacterial or fungal infections. The study of AMPs is a challenging task, due to the fact that the pathogenic microorganisms have gained a great resistance to an increased number of classical antibiotics and other treatments. For this reason a special importance is given to designing new peptide structures with antimicrobial potential.

The aim of this study is to characterize the interactions between new synthesized peptides (P1 - P8) with two types of model membranes, namely, **DOPC** and **DOPC-DOPG (85% / 15%) SUV’s.** The studied peptides, containing at least two tryptophan residue, are: **P1** (RR**WW**RH**W**RR), **P2** (RR**W**HR**WW**RR), **P3** (RRH**W**R**WW**RR), **P4** (RR**W**HRH**W**RR), **P5** (RR**WW**R**WW**RR), **P6** (HR**WW**R**WW**RR), **P7** (RR**WW**H**WW**RR) and **P8** (HR**WW**H**WW**RH).

Using **steady state** and **time resolved fluorescence** techniques, the fluorescence quenching of tryptophan residues by acrylamide was recorded separately for every peptide-lipid combination and, also, for each peptide in PBS. After data processing, quenching data were analyzed by fitting to the Stern-Volmer equation:

where and are the fluorescence intensities in the absence and presence of the quencher, respectively, is the molar quencher concentration and is the Stern-Volmer quenching constant. The constant is equal to where is the bimolecular quenching constant and is the lifetime of the fluorophore in the absence of quencher.

PSp11. **Dispersion Of Vizible Rotatory Power For Aqueous Glucose Solutions**

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In order to determine the dispersion of the visible rotatory power of glucose aqueous solutions, the method of channeled spectra was applied.

The channeled spectra were recorded at a spectrophometer to which a device consisting from two crossed polarizers having a cell containing active solution between them has been attached in the measure beam.

The visible rotatory birefringence of glucose solution is about $[2.75 – 1.3]10^{-6}$ and the dispersive parameter varies in the range $[1.8 – 3.0]10^{-8}$.

In specified rotation of aqueous glucose solution varies in the visible range with about 100 degrees/ dm, decreasing from blue to red.

PSp12. **Quantum Mechanical Characterization And Solvatochromic Study Of Quercetine**

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Quercetin is a flavonol found in many fruits, vegetables, leaves and grains. It can be used as an ingredient in supplements, beverages or foods.

Quercetin is a flavonoid with anticancer activity, strong antioxidant properties and may help protect against heart diseases.

Quercetin is commonly present as a glycoside and is converted to glucuronide/ sulfate conjugates during intestinal absorption and only conjugated metabolites are therefore found in circulating blood.

Quercetin belongs to a group of plant pigments called flavonoids that give many fruits, flowers, and vegetables their colors.

Quercetin can also help stabilize the cells to release histamine in the body and thereby have an anti-inflammatory and antihistamine effect.

A quantum-mechanical characterization and the some properties of quercetine were evaluated using Spartan'14 program.

The solvatochromic studies were done, showing the presence of different types of interactions. The supply of each type of interaction to the total spectral shifts was established.

PSp13. **Solvatochromic Study And Quantum-mechanical Characterization Of Methyl Red**

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Methyl Red is a comonly mono azo dye, used in laboratory assay, as colorant in textile industries and other comercial products.

Methyl Red is an azobenzene organic photocromic material, it is carcinogenic in nature and caused respiratory, skin and digestive problems.

A quantum-mechanical charcterizations for Methyl Red was performed by using Density Function Theory (DFT) method from Spartan'14 program.

Some physical chemical (acid-base equilibrium, dipole moment and polarizability in excited states) properties of the Methyl Red were theoretical calculated.

The contribution of different types of interactions to spectral shifts in homogeneous solutions and the limits in which the excited states dipole moment of the studied molecule can vary were established by solvatochromic study.

PSp14. Spectral And Quantum Mechanical Study of 3-(2-Benzothiazolyl)-7-(Diethylamino)-Coumarin In Binary Solutions

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Coumarine 6 (or 3-(2-Benzothiazolyl)-7-(diethylamino)-coumarin) is a fluorescent substance used as biological and chemical sensor, fluorescent probe and laser dye.

The absorption and the fluorescence spectra of 3-(2-Benzothiazolyl)-7-(diethylamino)-coumarin were studied in order to study the intermolecular interactions based on solvathocromic effect and the contributions of each type of interaction to the total spectral shifts were estimated.

Some physico-chemical properties of Coumarine 6 were calculated using Density Function Theory (DFT) method with the hybrid functional B3LYP level of theory combined with 6-311+G basis set.

The excited state dipole moment was calculated from Stokes shifts expressed by Lippert-Mataga, Bakhsiev and Kawski–Chamma–Viallet equations as functions on solvent macroscopic parameters.

PSp15. **Characterization of Phenolic Constituents of *Lavandula Angustifolia Mill.* Extracts**

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The flowers of lavender and essential oil separately from them are widely used in therapy [1], both Romania and especially in the European Community, where in the last decade were conducted extensive researches that have as result the appearance in the pharmaceutical market of a new drug, Lasea® which containing under the name of silexan, Lavandulae aetheroleum enriched with linalool [2]. Starting from the fact that the European Pharmacopoeia [3] allows the use for medicinal purposes only the flowers of Lavandula sp., the main aim of our research it was to investigate the chemical characterization of Lavandula angustifolia Mill extracts obtained by three extraction methods: ultrasound-assisted extraction (UAE), pressurized liquid extraction (PLE) and extraction in fluid at under-critical pressure and controlled temperature. The vegetal extracts were obtained in different mixture, such as: 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. These extracts were then analyzed for their qualitative composition by high performance thin layer chromatography (HPTLC), FTIR and Raman as well, and total phenolic content by ultraviolet-visible spectrophotometry (UV-VIS). HPTLC analysis revealed the following components in the extracts: caffeic acid, ferulic acid, rosmarinic acid and coumaric acid, as well as the major flavonoid compounds (e.g. rutoside, luteolin and apigenin) and catechin. The obtained extracts had different phenolic contents depending on the type of extract. The greatest amount of phenolics was found in the Lavandula extract obtained by extraction in fluid at under-critical pressure and controlled temperature.

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Poster Communications

Microfluidics and point-of-care microdevices

PMp1. **Investigations Regarding Possibility on Flue Gas Filtration by Selective Retaining of Nanoparticles using Positive Dielectrophoresis**

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The growing number of on-road vehicles, suspension of the dust, and anthropogenic activities from urban areas all over the world exacerbate the levels of ambient air pollution, with dramatic effects on the health of urban dwellers. Fine particulate air pollution from anthropogenic emissions always includes nanoparticles. The intense research work performed during the last decade reveals the harmfulness of nanoparticles as they can penetrate straight into the lungs and blood stream, but, in the same time, the severe technical limitations in the processes of filtration and manipulation of that class of airborne particulate matter. Among the physical methods attempted for manipulating (retaining and separating) nanoparticles from gas suspensions, those based on *dielectrophoresis* (DEP) proved to be the most promising. The paper presents a set of relevant results obtained by our group in the selective retaining of nanoparticles suspended in a gaseous environment using positive dielectrophoresis. Both theoretical and experimental results are outlined. In the first part of the study, model-based computer simulations describing the behavior of nanoparticles with sizes ranging from 50 to 150 nm in a dielectrophoretic micro-system are presented. The second part contains the description of the DEP-based microfluidic device for retaining of nanoparticles from flue gas designed in our laboratory and some experimental results showing the capability of the device to capture the nanoparticles.

PMp2. **Innovative Integrated System for Sorting and Extraction of Adherent Cells**

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The aim of this work is to build a micromanipulation system able to sort cells which are recognized according to their shape (or other morphological parameters observed by visual inspection).

Software for tagging a certain type of cell from a heterogeneous population of adherent or partially adherent cells, recognized by the operator as cells of interest was created; the interesting cells, “soft” labelled, can be traced even if they become mobile in the visual field of microscope and subsequently change their shape.

A microfluidic device designed to detach, transport and sort the tagged cells was built. The system integrates a high accuracy microscopy stage, correlated with one robot for the extractor terminal manipulation, a microfluidic chip and a group of microrobots for trapping of one single cell.

Main advantages of our system compared to other similar devices consist in the following: very well controlled pressure for the suction process, small and precise manipulated volumes (nano- to femtoliters).

The system was tested on murine adherent cells plated for variable durations (to achieve different adherence degrees) and the working parameters (pressure, frequency and pulses number) were optimized.

For further development of the system, we intent to create a software-based method of intelligent recognition and tracing of cells.

Our results may contribute to the developing of clinically oriented applications in cancer diagnosis using non-invasive and free-labelling methods.

PMp3. **Design of Microfluidic Device and Measurement of MPWM for Single Cell/Particle Manipulation**

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A microfluidic device designated for measurement of fluidic flows with different viscosity, necessary within trapping/realising of cells/particles system has been developed. We use a new concept as Microfluidic Pulse Width Modulation (MPWM) for controlling transport of a single cell/particle. The image processing helped the nano-hydraulic volumes/flow rates measurement, through tracking inovative methods with the purpose to build a a flow sensor. The device open an unique opportunitie for single cell study with applications in biomedical devices, tools for biochemistry or analytical systems.

Poster Communications

Analytical methods for medical physics

PMf1. **Ion Chromatographic Analysis of Atmospheric Particles with Potential Impact on Human Health**

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Air pollution, mostly induced by $PM_{2.5}$ fraction (i.e. particulate matter with aerodynamic diameter <2.5 μm), has been recently suggested to lead nowadays to about 3.3 million premature deaths per year worldwide while this could double by 2050 [1]. The water soluble fraction of atmospheric particles is known to contain important chemicals increasing the solubility of some toxic organic compounds [2]. The present work reports about results on the analysis of trace water soluble ions (WSI) in fine atmospheric particles from Iasi, north-eastern Romania. Size resolved particles were collected over a time period of 36-hour on aluminium filters using a 13 stages cascade Dekati Low-Pressure Impactor (DLPI) (0.0276-9.94 μm size range and 29.85 L min^{-1} flow rate). The WSI fraction (*i.e.*, H_3CCOO^-, $HCOO^-$, F^-, Cl^-, NO_2^-, Br^-, NO_3^-, SO_4^{2-}, $C_2O_4^{2-}$, Li^+, Na^+, NH_4^+, K^+, Mg^{2+} and Ca^{2+}) has been investigated by ion chromatography and the concentrations of all analysed species were at nanomolar level. For the NO_3^- ion the concentration varied in the 5.3-187.4 nmol m^{-3} range while for the SO_4^{2-} ion it was in the 5.7-113.5 nmol m^{-3} range. Ammonium ion concentration was the highest in the investigated aerosol samples with levels varying in the 22.4 nmol m^{-3} and 301.0 nmol m^{-3} range (mean of 83.6 nmol m^{-3} and median of 83.1 nmol m^{-3}). Further analysis of the data revealed the completeness of the ionic balance (with a 0.99 value for the ratio between the cations and anions and a 0.97 value for the correlation coefficient), which might represent a quality control step within data investigation process even at such low concentration levels.

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PMf2. **Generation of Hydrogen Peroxide by High-Voltage Pulses in Cell-Free Media**

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Electroporation offers a number of applications in biology, oncology, immunology, and biotechnology. However, when a high-voltage is applied to the electrolyte solution, besides membrane permeabilization, various electrolysis reactions occur at the electrode-solution interfaces. One of the results of these electrochemical reactions is generation of reactive oxygen species (ROS). Although ROS formation following electroporation with long (μs–ms) electric pulses or nsPEF exposure has been reported earlier, no detailed analysis of this process has been carried out yet. In this study, generation of hydrogen peroxide as a result of the exposure of a cell-free media by high-voltage pulses has been studied.

Generation of hydrogen peroxide in hightly buffered solution HB1, Dulbecco's Modified Eagle's medium (DMEM), Phosphate buffered saline (PBS), and distilled water was studied. The cuvette with stainless-steel electrodes was used. Hydrogen peroxide was detected with AmplexRed® (10-Acetyl-3,7-dihydroxyphenoxazine), which has a great specificity, stability, and selectivity. AmplexRed is nonfluorescent until, in the presence of horseradish peroxidase, it reacts with hydrogen peroxide to produce highly fluorescent resorufin. 50 μM of the AmplexRed dye were added to the medium and treated with high-voltage pulses. Fluorescence intensity in a solution was measured using TECAN GeniosPro spectrophotometer (Tecan Group, Männedorf, Switzerland).

Treatment of HB1 medium by a single square-wave electric pulse with the duration of 0.5–2 ms and the amplitude of 100–400 V (0.5-2.0 kV/cm) significantly increased dye emission. The AmplexRed fluorescence intensity was also dependent on the number of pulses, the conductivity, and composition of the medium (PBS, H_2O, DMEM, HB1).

Conclusion: During high–voltage electric pulses, hydrogen peroxide is generated in cell–free media. Pulses of micro–millisecond duration increased fluorescence of hydrogen peroxide indicator AmplexRed depending on the duration, voltage, and/or number pulses. The conductivity and composition of the medium were also important.

PMf3. **Determination of Trace Pesticides in Carrot Samples Having Different Origin by Chromatography and Mass-Spectrometry Methods**

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Carrot is characterized as one of the most important vegetables due to its high consumption worldwide. For the carrot culture, the intensive and constant use of pesticides for the control of pests, diseases, and weeds is necessary in order to minimize losses in addition to increasing productivity and agricultural production quality. Multiple pesticide residues have been observed in some samples of carrot, which put the health of the consumers at risk of adverse effects. It is quite apparent that such a state of affairs calls for the need of more accurate, cost-effective, and rapid analytical techniques capable of detecting the minimum concentrations of the multiple pesticide residues. The aim of the paper is the development of method for high sensitivity and selectivity based on chromatography and mass-spectrometry for the detection of traces of pesticide. The QuEChERS (Quick, Easy, Cheap, Effective, Rugged and Safe) sample preparation method was conducted and shown to have good performance for pesticide extraction in carrot samples. These techniques are accurate, reliable, less time consuming and cost-effective analysis and are recommended for monitoring pesticide contaminants in vegetables. The data will be compared with the accepted maximum residue level.

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PMf4. **Metal content in selected vegetables from the Romanian market and estimation of the daily intake**

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Among other routes, food is one of the main sources of consumer exposure to heavy metals. Chemical analyses constitute an important tool for quality control in the food industry where on-line, fast and simple methods are required.

An Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) based multi-elemental profiling was performed to assess the quantitative complement of toxic metals and essential mineral elements (Zn, Cu, Mn, Ni, Sr, Fe, Ba, Cr, Pb, As, Cd) of 50 vegetables, collected from the Romanian market. The accuracy and precision of the used procedure were determined by analysis of the certified reference material CRM - IAEA-359 Cabbage. The recoveries of the metals were in the range of 79-108 %.

The concentrations of Mn and Cu in the analysed samples were in the range of 7.43-41.80 $mg \cdot kg^{-1}$ and 4.45-25.65 $mg \cdot kg^{-1}$ in tomato samples, 5.65-42.03 $mg \cdot kg^{-1}$ and 4.66-35.12 $mg \cdot kg^{-1}$ in pepper samples and 17.95-97.41 $mg \cdot kg^{-1}$ and 7.71-27.51 $mg \cdot kg^{-1}$ in egg-plant samples, respectively.

For the evaluation of health risk related to the consumption of vegetables, two parameters were calculated**:** daily intake rate (DIR) and target hazard quotient (THQ).

The analysis of variance (ANOVA) successfully highlighted the elements that could distinguish vegetable samples having different origin or elements that could be used as markers for varieties differentiation in the case of pepper. Principal Component Analysis (PCA) extracted five main components which explained a total variance of 78.2 % from the total variance of data.

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PMf5. **Comparative Antioxidant and Prooxidant Activities of Five *Plantago* Species**

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Since ancient times *Plantago* species have been used as herbal remedies to treat a considerable number of diseases. Because of high amounts of polyphenolic compounds, *Plantago* species have become notorious worldwide for their antioxidant potential. In this study, the hydroalcoholic extracts of five *Plantago* species (*P. arenaria*, *P. cornuti*, *P. lanceolata*, *P. major* and *P. media*) were evaluated for their antioxidant activity, but also for their prooxidant reactivity. In order to examine the antioxidant activity, we investigated the free radical scavenging activity by DPPH bleaching assay, Trolox equivalent antioxidant capacity (TEAC) assay and also Folin-Ciolcâlteu method for hydrophilic antioxidants quantification. Moreover, other new physiological methods (Inhibition of hemoglobin ascorbate peroxidase activity and liposome oxidation) have been used for antioxidant activity determination. Among tested species, the extracts of *Plantago arenaria* and *P. media* have shown the strongest antioxidant activity. Besides, the prooxidant activity was determined using a method which involves free radicals generated by laccase and the oxidation of haemoglobin. Surprisingly, even if these species have a strong antioxidant capacity, their prooxidant potential is almost insignificant, which is why these extracts have a great potential for future therapeutic strategies. The antioxidant reactivity was also evaluated by the kinetic profiles of the semiquinone radicals generated by alkaline treatment of the extracts and monitored using EPR. The phytochemical characterization of the extracts was performed by HPLC/MS.

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PMf6. **Gas Chromatography/Mass Spectrometry (GC/MS) as Challenging Problems Solving Microanalytical Tools**

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Gas chromatography/mass spectrometry (GC/MS), as a synergistic combination of two powerful microanalytical techniques, offers an indispensable tool for fields as environmental science, forensics, medical and biological research, human health and food safety, the flavour and fragrances industry, packaging and others [1]. Within medicinal plants known to man those containing tropane alkaloids are among the oldest [2]. In ancient time extracts of various solanaceous plants containing tropane alkaloids were recommended for various curative purposes, nowadays some alkaloids of this genus (e.g., scopolamine) are extracted for the pharmaceutical industry [2], and today many bioactive herbs became actually the most powerful "bio-drugs" abused by younger people [3]. The present work reports about preliminary results on the quantitative assay process of scopolamine in *Datura inoxia*, by using a GC-MS system. Preliminary estimation in methanol extracts allow us to infer levels of scopolamine (extracted by methanol) of ~443.56 µg/g dry weight seeds, ~189.45 µg/g dry weight flowers, and ~44.75 µg/g dry weight leaves. In all other solvents, although the ranked amount of scopolamine in various plants organs followed a similar trend, the extraction efficiency was much diminished. Moreover, peak purity analysis of the recorded chromatogram revealed that the MS could better discriminate/separate between specific fragments of scopolamine and a co-eluting peak. This aspect will be however further investigated.

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PMf7. **On the improvement of lock-in thermography detection of microgaps located at the tooth-filling interface**

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In this paper, the adaptation of some experimental and commercial composite sealants to the tooth are analyzed by optical microscopy and IR lock-in thermography.

This study conducted in vitro on cross section of human teeth shows that a photothermal contrast given by the presence of micro-gaps located at the tooth-dental interface is detected in both amplitude and phase images. The use of the second derivative of the amplitude and phase images improves the quality of the processed images, enhancing the defect signature on the surface. The proposed algorithms lead to a diagnosis of open cracks with a very good contrast. The phase image is more sensitive to the presence of micro-features and discontinuities across the interface than the amplitude image. A combination of amplitude and phase images, together with optical techniques, increases the accuracy in evaluating dental interfaces. Nevertheless, for a proper interpretation of infrared thermograms, a correct excitation frequency must be selected. In order to be detected, the microgap must be located into the heat-diffusion zone. Both scattering and absorption of light in teeth must be taken into account as well.

Due to its non-invasive and non-contact character, lock-in thermography has the potential to become a useful tool for testing the adhesion ability of new dental stuffs and adhesives to the hard dental tissue and different packaging techniques used in dentistry, as well.

PMf8. The Effect of the 3D Hydrophobic Moment of Short ARG- and TRP-Based Peptides on Charged Membranes

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The increasing rates of the reported multidrug-resistant infections recorded in recent years prompted an intense search to discover novel compounds with improved antimicrobial capacity. Due to their properties, AMPs (antimicrobial peptides) drew huge attention as potential source of antimicrobial agents and/or in drug design. Most of these AMPs are small (below 50 aa) cationic peptides, with a net charge ranging from +2 to +7 at physiological pH, due to their high content of positively charged aas like: lysine (K), arginine (R), and histidine (H). Another important property of AMPs is their amphipathic nature, with the most important hydrophobic aa being tryptophan (W). The content of hydrophobic aas can reach up to 50%.We used molecular dynamics simulations to investigate the conformational dynamics of short cationic peptides at the surface of charged model membranes. Four newly synthesized 9-aminoacid sequence peptides were studied: a control peptide, containing only R and W aminoacids, and other three peptides, which replaced an arginine with a histidine, two placed at one end, and another in the middle of the control peptide sequence. Our study shows that the peptide's 3D hydrophobic moment plays an important role in its membrane surface activity, and it could be further correlated with experimental results obtained on their antimicrobial activity.

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PMf9. **Plasma Membrane Model Dynamics in the Presence of Ras Protein Nanoclusters**

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Ras proteins belong to a class of GTPase switch proteins that have an essential role in regulating the behaviour of cells. These intracellular signaling proteins are currently under investigation as possible targets for cancer treatment. Coarse-grained molecular dynamics simulations were performed to investigate the formation and evolution of Ras nanoclusters in mammalian model membranes. Ras proteins were inserted into the cytoplasmic side of the plasma membrane model (di-C16:0- phosphatidylcholine (DPPC) : di-C18:2-phosphatidylcholine (DLiPC) : cholesterol (CHOL) 5:3:2) where they formed highly dynamic nanoclusters, both in size and in composition. Presence of Ras protein nanoclusters has a significant impact on the model membrane behaviour. Properties such as phase behaviour, diffusion coefficient, surface tension and order parameter are also influenced by the temperature variation of the model membrane.

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PMf10. **Retrospective Analysis of Cases Treated in HDR Brachytherapy Compartment, of Patients with Neoplastic Diseases in Gynecological Area**

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This study presents a restrospective analyse of the cases treated with HDR brachytherapy in gynecological area. Brachytherapy, another form of radiotherapy, is an advanced treatment for gynecological diseases. With this approach to treatment, ionizing radiation source is placed near or within the neoplastic tissue. This study was conducted for the treatment given during 2015, on 500 patients treated with internal radiation therapy. The internal radiotherapy was filled with HDR Brachytherapy, with Iridium source, the isotope 192. A number of 1000 applications, 2 for each patient, one per week was made.The treatment prescribed for internal radiotherapy was between 45 Gy and 50.4 Gy, with 2Gy or 1.8Gy per fraction for 5 days per week. The study was done for utero -vaginal and vaginal applications. For the utero-vaginal we used Fletcher-Suit applicators for different histerometry, and for the vaginal applications we used cylindrical applicators of different diameters. 2D required treatment planning images were acquired using simulator Simulix HP 1400 CT. Acquired images were exported in the Treatment Planning System. Planning was conducted using Eclipse BrachyVision software, version 10.0. With this form of brachytherapy, catheters are temporally inserted into a tumor. We check the position of the catheters with millimeter precision, before each treatment. With this technique we give the maximum radiation dose to cancerous tissues, while minimizing the dose to surrounding healthy tissue. Because the cervix is located closed to the bladder and rectum, it is important for radiation treatment to be tightly focused on the cervix to avoid serious side effects. We observe that for each application the doses to organs at risk are very close, arround 2.5Gy. It is important that the applicators to be inserted carrefully for an optim geometry of the source because this can minimise the adverse effects.

PMf11. Antimicrobial Peptides Show Antitumor Activity Against SH-SY-5Y Human Neuroblastoma Cells

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Human neuroblastoma is one of the most frequently diagnosed solid tumors in children and is a cancer derived from the neuronal crest. For patients with late-stage neuroblastoma, one of the main causes, common in neuroblastoma, is their resistance, through different mechanisms, to the cytotoxic drugs used in chemotherapy. In the recent years new treatments, alternative to chemotherapy are explored and one is the use of antimicrobial peptides. Antimicrobial peptides have become recognized as a good candidate in the fight against multi-drug resistant cells. In this study we tested the antitumor activity of 2 antimicrobial peptides (Melittin and Indolicidin) against neuroblastoma SH-SY-5Y cell line. Cell viability against the tumor cells was assessed using MTS assay. The apoptotic/necrotic effects were investigated by immunofluorescence microscopy after double staining with Acridin-orange (AO) and ethidium homodimer –1 (EthD-1). Results showed that both peptides tested can inhibit cell growth and kill the tumoral cells through apoptosis.

PMf12. A Sensitive Analytical Approach For The Screening Of A Toxic Chlorinated Aromatic Compound At Ultra-Trace Levels In Water Samples

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Chlorinated phenols (CPs) are a widespread class of organic pollutants commonly formed during paper and pesticides production or as intermediates during the manufacturing of dyes, plastics and pharmaceuticals. Thus, these kinds of applications commonly lead to wastewater and groundwater contamination. Among these hazardous organic compounds, pentachlorophenol (PCP) is considered as the most toxic and is considered as endocrine disruptor. Hence, there is an increased interest to develop fast and sensitive analytical methods in order to provide a complete overview of their occurrence in aquatic environment. In this context, the purpose of this work was to develop a highly sensitive solid-phase extraction method (SPE) combined with ultra-high performance liquid chromatography coupled with photodiode array detection for the analysis of PCP in water samples at environmentally relevant concentrations. Chromatographic separation was performed using an Acquity BEH C18 column and a mobile phase consisting of acetonitrile/ultra purewater/formic acid (55:45:0.1, v/v/v) at a flow rate of 0.4 mL/min. The performance of the proposed overall method was studied in terms of linearity ($r^2 \geq 0.998$), precision (<5%), accuracy (99%), low limits of detection and quantification (10 and 16 ng/L, respectively). High extraction recoveries (between 98% and 100%) were achieved with the proposed SPE procedure and the RSD was less than 3.1%. In conclusion, the results showed that the developed method is highly sensitive and accurate for the determination of PCP at ultra-traces levels (ng/L) in different types of water samples. Moreover, the obtained data demonstrate that the developed analytical methodology can be applied for the screening of PCP at trace levels in different water samples.

Poster Communications

Medical analysis and diagnosis

PMa1. **Calorimetric Monitoring of Patients with Multiple Myeloma after Autologous Stem-Cells Transplantation**

Avgustina Krasimirova Danailova, Svetla Jeliazkova Todinova, Lidia Gartcheva, Sashka Boichova Krumova, Stefka Germanova Taneva

Recently differential scanning calorimetry (DSC), biophysical technique that directly measures thermally induced conformational transitions of biomolecules in solution, was applied as a novel approach for characterization of the denaturation of the blood plasma/serum proteins in healthy individuals and patients diagnosed with various diseases. We have performed a detailed calorimetric study of the serum proteome of patients with multiple myeloma (MM) with secretion of monoclonal immunoglobulins (IgG, IgM, IgA and Bence Johnes protein) and nonsecretory myeloma, and identified specific thermodynamic features for the different MM types that can well be used for patient's stratification (1-3).

We utilized here the calorimetric approach to monitor myeloma patients after autologous stem cell transplantation. The thermodynamic parameters determined from the calorimetric profiles of blood sera collected at different periods after the transplantation were compared with the variation in the levels of the secreted paraproteins, monoclonal free light and involved heavy/light chains searching for correlations between the calorimetric markers and immunological indicators of prognosis prediction and monitoring response. Data demonstrate the potential of DSC as a non-invasive tool for patients¢ monitoring.

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Pma2. **Quantitative Determination of Fe $^{3+}$ in Pharmaceutical Forms by Means of UV-VIS Spectrophotometry**

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Aim: To develop a new spectrophotometric method allowing quantitative determination of Fe^{3+} in VIS field by complexes formations with *Methylthymol blue* for both the active substance and pharmaceutical forms.

Materials ad methods: There has been conducted a study on the kinetics of forming complex combinations: $^{Fe3+}$ and *Methylthymol blue*. In order to determine the ratio of combination between the metal cation (Fe^{3+}) and the analytical reagent, Job's method was used; then, there took place the validation of the method, both for the active substance and pharmaceutical forms.

Results and discussions: The absorbances were read at a wavelength at which the spectrum showed the maximum absorption level (628 nm). Combination ration between the metal cation (Fe^{3+}) and the analytical reagent was 1: 1. There were determined the method validation parameters (linearity, repeatability, reproducibility, accuracy). Method linearity was checked by the line calibration method (R^2 = 0.9997). The accuracy of the method was tested for the full range of linearity; confidence interval of the mean was 98.79 - 101.13%. Method accuracy was done using the Cohran test ($C_{calculated}<C_{theoretic}$). In this case, $C_{calculated}=0.39<C_{theoretic}=0.68$, intragroup variances were considered homogeneous.

Conclusions: UV-VIS spectrophotometry allowed the quantitative determination of Fe^{3+} in pharmaceutical forms as well. There has been developed a spectrophotometric method in VIS, which allows the quantitative determination of $Fe^{3+,}$ in *iron polymaltose* complexes.

The proposed method is suitable for laboratory and has been successfully used for the quantitative determination of polymaltose iron in commercial pharmaceutical products.

Pma3. **Improving Tumor Uptake and Retention of ^{68}Ga Radiolabeled Compounds Using Gold Nanoparticles as Intracellular Delivery System**

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In the present study we evaluated the ability of gold nanoparticles to increase the available ^{68}Ga positron emitter radioisotope inside tumor cells, using together AuNPs properties to pass cells membrane by endocytosis, and radiolabeled peptides specific tumor targeting properties.

For this purpose we characterized the AuNPs through transmission electron microscopy (TEM) and dynamic light scattering (DLS) techniques, followed by further functionalization with ^{68}Ga radiolabeled somatostatin analogues. After functionalization analysis through UV-Vis spectroscopy, the radiolabeled compounds were incubated on neuroendocrine colorectal cancer cell line HT-29 and pancreatic cell line AR42J. *In vitro* binding kinetics study showed over half of the radioisotope retention inside tumor cells in the presence of AuNP compared with the situation of no nanoparticles added.

This result is attributed to AuNPs possibility to bind several peptides on their surface and further internalize by somatostatin receptors SSTR2, SSTR3 and SSTR5 mediated endocytosis.

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Poster Communications

Sensors and biosensors

PSb1. **Antioxidant Potential of Aronia-Enriched Wines Assessed by Chemiluminometric, Spectrophotometric and Electrochemical Methods**

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Red wines of Negru Aromat variety produced in Valea Calugareasca vineyard have been enriched with antioxidants from aronia. A macerate was obtained by mixing dry aronia fruits with Negru Aromat wine (vintage of 2013), at room temperature for 3 days. The macerate was then mixed with the original wine in different ratios: 10%, 15%, 20% and 25%. Nine months after bottling, the total antioxidant capacity (TAC) of aronia-enriched wines was evaluated by two methods: a chemiluminometric method based on superoxide $O_2^{\bullet -}$ and hydroxyl $HO^{\bullet}$ radicals formed in a Fenton-like reaction (1) and an electrochemical method based on 2,2-diphenyl-1-picrylhydrazyl radical ($DPPH^{\bullet}$). Additional tests included spectrophotometric analysis of chromatic characteristics and phenolic composition as well as electrochemical oxidation profiles achieved by voltammetry of diluted wines using a glassy carbon electrode. The differences between the TAC of wines with different percentages of aronia were found to be insignificant by both methods. Analysis of a larger group of wines, including white, rose and red allowed discussing differences between the two methods for TAC in relation with phenolic composition. Differentiation of various wines, including those with different percentage of aronia could be achieved by chemometric analysis based on all tests described in this study.

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PSb2. DFT investigation of SubPC migration on metallic surface

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We investigated the interaction between the Boron subphthalocyanine chloride molecule (SucPC) and the Ag(111) surface by using Density Functional Theory (DFT) calculations. Our simulations were performed using the Siesta code that uses norm-conserving pseudopotentials in their fully non-local form and expands the wave functions of valence electrons by flexible linear combinations of atomic orbitals (LCAO). As exchange-correlation functional we used the improved version of the RPBE functional developed by Hammer, Hansen and Norskov and the newly developed exchange-correlation functionals including van der Waals corrections of Lee et al.

Our calculations indicate that there is practically no "preferred" position for the adsorbed molecule on the surface. More precisely, a random translation of the molecule on the XoY plane (i.e. parallel to the surface) followed by a structural relaxation leads to a large number of geometric structures that are stable from the energetic point of view. In other words the molecule seems to "migrate" on surface, at room temperature and low coverage. For all these structures only small deformation of the molecule is present. By comparing the results including van der Waals corrections with those produce by classical exchange-correlation functional we found that this trend is independent on the presence of long-range interactions. The total binding energy is close to zero, supporting this dynamical model.

For geometric structures taking into account the bending of the molecule’s symmetry axes with respect to the surface we found a small increase of the binding energy, doubled by an increased selectivity of the adsorption site. This result is consistent with the previous experimental findings and open the way for future applications based on the self-assembly properties generated by the freedom of the SubPC to migrate on the Ag(111) surface.

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PSb3. **Conductance Recorder for Biomedical Applications**

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Tissue conductance measurement has many applications in biomedical research (Electrodermal Activity Recording, Impedance Cardiography, etc.).

Commercially available devices for measuring conductance are either too expensive or have a limited functionality. Therefore we developed a versatile conductance recorder suitable for research and medical applications.

The design has been oriented to provide the following key features: small size, connectivity with a personal computer for downloading data, electrical safety, posibility for adding new functionalities and low cost.

These characteristics were obtained by using of a digital signal processor which performs most functions through software. The hardwired analogic processing was reduced to a minimum to avoid the limitations introduced by this type of implementation. Computer connectivity is made through an USB interface which emulates a standard serial port and therefore do not requires to install a special communication driver. Electrical safety is ensured by optical isolation of the USB interface and powering from low voltage batteries.

Measurements are made by applying an alternating voltage with an amplitude of 0.5 volts and recording current flowing between electrodes. Using of AC eliminates the effects of electrode potential and allows to obtain additional informations about the reactance of the biological material. Alternative excitation voltage is generated using direct digital synthesis which allows a programmable frequency range between 0 and 10 kHz. The current and excitation voltage recording is performed by the analog to digital converter integrated inside the digital signal processor. Electrical characteristics (conductance and susceptance) are obtained as the ratio between current and voltage phasors obtained by applying Discrete Fourier Transform on the recorded signals.

Tests carried on prototype showed that the device has the desired performance and can be used successfully in research and medical applications.

PSb4. **N-doped Graphene Nanomaterial for Chemical/Electrochemical Detection of H_2O_2**

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Graphene-based materials are currently at the forefront of materials research due to their outstanding catalytic/electrocatalytic activity. In particular, nitrogen-doped graphene (N-GR) have attracted much attention because the conjugation between the lone-pair electrons of nitrogen atoms and the graphene *π*-system influences the electrical properties of the material. Hence, electrodes modified with N-GR have been reported to show not only excellent electrocatalytic activity for the detection of various molecules of biological interest (e.g. hydrogen peroxide; NADH) but also to improve the performances of the enzyme-based biosensors.

This work reports the comparison between the chemical and electrochemical detection of H_2O_2, using nitrogen-doped graphene. For the chemical detection, N-doped graphene was used as catalyst for the oxidation of 3,3'-dimethylbenzidine in the presence of hydrogen peroxide. The formation of a blue colored product is dependent on the H_2O_2 concentration and was followed by UV-Vis spectroscopy. Additionally, kinetic data on this process were also obtained.

For electrochemical detection, glassy carbon (GC) electrodes were modified with the desired amount of N-GR, by the drop-casting method. Various electrochemical techniques were used to explore the electrocatalytic effect of GC modified electrodes. Among these, amperometry, cyclic voltammetry and electrochemical impedance spectroscopy are worth mentioning.

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PSb5. **Probing the Key Metal Binding Residues in Mutant Amyloid Peptides**

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Amyloid peptides (Aβ) aggregation is an established pathogenic mechanism of Alzheimer Disease (AD) and its neurotoxic effect is well known. It has been demonstrated that the interactions between Aβ peptides and various metal ions (e.g., Cu^{2+}, Zn^{2+}, Fe^{3+}), when the metal concentration exceeds physiological levels, can promote the aggregation of the Aβ peptides by changing the their normal conformation, acting like seeding factors in the formation of amyloid plaques. Aβ peptides are part of the intrinsically disordered proteins (IDPs) class, which have a highly dynamic and flexible structure, but can adopt a stable conformation in interaction with others molecules (e.g., other proteins, peptides, lipids, metals). Aβ peptide – Cu^{2+} coordination involves three intramolecular histidines (e.i, His-6, His-13 and His-14), with the fourth coordinate being either the amino group of the N-terminus (Asp-1) or the amide group (Ala-2). Here, we systematically examine the Cu^{2+} effect on a set of specially designed amyloid short peptides (Aβ1-16), which display the metal - coordinating main sites. The short Aβ peptides were engineered to contain L- and D- enantiomers of the main Cu^{2+} – coordination residues. By employing single-molecule electrophysiology techniques we monitor the different ionic current blockades, of an α-hemolysin (α-HL) protein nanopore, caused by the capturing of the Aβ1-16 peptides, with and without presence of Cu^{2+} at different concentrations. The specific kinetic characteristics of the peptide-pore and metal-peptide interactions were examined by performing a statistical analysis of the Markov stochastic process. Our data analysis reveals that the replacement of key metal binding residues with their enantiomer can inflict a major change in the Cu^{2+} - binding affinity and provides evidence for the utterly importance of His-6 in the Cu^{2+}-coordination of the short Aβ1-16 peptide.

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PSb6. **Sensors for Lipo- And Hydrosoluble Antioxidant Compounds in Vegetal Resources Extracts**

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Oxidative stress will be manifested in a biological system following either an increased exposure to oxidants or a decrease in antioxidant capacity of the system, or both. These antioxidant defense systems can be categorized into protection via enzymatic activities and protection through lipo- and hydrosoluble low molecular weight antioxidants (LMWA). In human tissues, the cellular LMWA are obtained from various sources: synthesized by the cells, waste products of the cellular metabolism, while ascorbic acid (AA), carotenoids, tocopherols and polyphenols are antioxidants obtained from the diet. As part of the antioxidant reservoir is obtained through the diet, there is a high interest in the assessing of the antioxidant capacity of plasma and the antioxidant capacity of edible plants. In parallel, it is important to evaluate the individual contribution of each of the plant components to the overall (total) antioxidant capacity of the organism.

In this work gold electrodes and gold nanoparticles (AuNP) immobilized on carbon electrode surface were evaluated in the view of their use for label-free electrochemical sensors towards LMWA detection. Cyclic Voltammetry and Differential Pulse Voltammetry methods were employed to characterize the sensors performances in detection of LMWA like beta-carotene and resveratrol from vegetal resources extracts with antioxidant capacities in micromolar range.

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Poster Communications

Novel materials and biomaterials for analytical methods

PBm1. **Supramolecular Systems for Drug Delivery Applications**

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Supramolecular drug-carrier systems present a major interest for the pharmaceutical industry, with a particularly important impact in many therapeutic areas. Obtaining carrier-drug complexes is a viable alternative to increase the therapeutic efficacy of active pharmaceutical ingredients.

Encapsulation of drugs in supramolecular systems (*e.g.*, dendrimers, metal-organic frameworks) presents a number of advantages, including: increasing the bioavailability, stability and solubility of the active substances, reducing their toxicity, improving the metabolism and drug transit through biological barriers. All these lead to the improvement of therapeutic efficacy, in oral, intravenous, topical and transdermal formulations.

The use of dendrimers and metal-organic frameworks (MOFs) in drug-carriers supramolecular systems emerged in the last decade. Dendrimers possess unique properties such as high degree of branching, multivalency, globular architecture while MOFs present highly tunable nature from the point of view of porous size, shape and chemical properties, high surface areas and exposed coordinatively unsaturated metal sites, enabling different kinds of pharmaceuticals to be incorporated.

In this study, PAMAM dendrimers of 5 generation were employed as drug carriers as well as metal-organic frameworks based on non-toxic podands decorated with nucleobases. Their capacity of encapsulating active pharmaceutical ingredients belonging to antibiotics and anti-inflammatory pharmaceutical classes and drug releasing profile were investigated by UV-vis spectroscopy. The newly synthesized MOFs were structurally characterized by X-ray diffraction techniques, FT-IR and NMR spectroscopy.

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PBm2. **Terpyridine-Terminated Self-Assembled Monolayers On Gold Substrate For Metal Ions Sensing**

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Self-assembled monolayers (SAMs) are obtained spontaneously by adsorption of molecular units from solution on the surface of various solid supports. The present contribution is devoted to the development of supramolecular structures on gold substrate involving coordination of suitable metal ions to a terpyridine-terminated SAM.

The fabrication of stable covalently bonded monolayers by specific reactive molecules on Au surface has been investigated with the purpose of developing a stable platform for Fe(II) ions sensing.

For obtaining a chemically stable Au functionalized surface a five steps covalent approach based on suitable reactions was performed: (i) elaboration of an amine-terminated SAM by a functional thiol/amine linker, Cysteamine (Step I); (ii) amide bond formation by aminolysis with a reactive Cyclooctyne with protected acid functions (Step II); (iii) Cu-free click chemistry namely strain-promoted azide-alkyne cycloaddition (SPAAC) with an Azide-functionalized Terpyridine derivative, *via* the 1,2,3-triazole group (Step III). The last two stages are based on complexation reactions of free Terpyridine units with Fe(II) ions, affording a stable Fe(II) bis-Terpyridine complex as the final monolayer.

At each preparation step the obtained molecular layer was characterized by X-ray Phototelectron Spectroscopy (XPS) in order to determine the chemical composition of the resulting SAM and to assess the coverage degree.

Moreover, the molecular interactions occurred on the Au surface at each fabrication step were real-time monitored in terms of Surface Plasmon Resonance (SPR) spectroscopy. SPR is an optoelectronic method through which the binding of ligands is recorded and which is sensitive to the molecular complex permittivity and the electron concentration at or near the metal (Au) surface.

XPS and SPR techniques provided qualitative and quantitative information about each functionalization step showing that Fe(II) ions were coordinated to Terpyridine units.

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PBm3. **Graphene-Bimetallic Nanoparticles Hybrid Materials for DNA Bases Detection**

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Graphene has been widely used in fabrication of modified electrodes for different applications. Electrochemical sensors based on graphene decorated with (bi)metallic nanoparticles owe the capability to solve a lot of analytical problems to their catalytic activity and also to the long term stability.

We investigate the role of cooperative interactions of different bimetallic nanoparticles and graphene in the detection of DNA bases. Thus, a lot of bimetallic nanoparticles supported on graphene have been prepared by radio frequency chemical vapor deposition (RF-cCVD) method using a catalytic system formed of bimetallic nanoparticles supported on MgO and a source of carbon (methane). Different combinations of metallic nanoparticles (gold nanoparticles - AuNs, platinum nanoparticles - PtNs and silver nanoparticles - AgNs) supported on MgO (%), PtNs-AuNs 1:2 and 1.5:1.5 and PtNs-AgNs 1.5:1.5, have been used to prepare the bimetallic nanoparticles supported graphene composites. These nanomaterials have been characterized by Transmission Electron Microscopy, X-ray powder diffraction, Thermogravimetric analysis and Raman Spectroscopy.

The novel hybrid composites have been used to prepare the modified graphene paste electrode (GPE). Different electrochemical techniques (Linear Sweep Voltammetry, Differential Pulse Voltammetry or Square Wave Voltammetry) have been used to evaluate the electrochemical behavior of the DNA bases, under physiological and acidic conditions, at the as-prepared GPE. The results are compared with that obtained, in the same conditions, from the monometallic nanoparticles-graphene composite.

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PBm4. **Fe Ions Caption by Terpyridine Functionalized Au Substrate Analyzed by Impedance Spectroscopy**

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Terpyridine functionalized Au surface offers great advantages for further innovative engineering and developing integrated systems for demanding applications. The present contribution is part of a multifaceted investigation pathways intended to analyze a self-assembled monolayers (SAMs) sensor platform developed for metallic ions sensing. Impedance Spectroscopy (IS) was used to demonstrate the capability of terpyridine units to coordinate Fe ions on functionalized Au substrate. Au InterDigitated microelectrodes (AuIDE) with 5μm spacing were used as substrate for a covalently bonded monolayer based on several molecular moieties: cysteamine, cyclooctine and terpyridine (CIS-OCT-Terpy). IS measurements were performed at room temperature on two frequency ranges: a) 20Hz-10MHz using a Keysight E4990a impedance analyzer and b) in extended ranges to low frequency values (1mHz-1MHz) using a VSP multi-channel BioLogic potentiostat. In both cases the frequency dependence of amplitude and phase were analyzed. The IS response was first tested in KCl solution with an unfunctionalized electrode by the addition of Fe ions. Impedance modification due to the presence of Terpy molecular receptors on functionalized electrode proves the existence of CIS-OCT-Terpy molecular monolayers on Au surface. The presence of Fe ions in small concentrations induces significant changes in the frequency dependence of phase and impedance amplitude figuring out the caption of ions by the Terpy receptors.

Acknowledgments: We acknowledge the financial support provided by the project PN-II-IDPCCE-2011-2-0027

PBm5. **Graphene-Porphyrin Based Electrodes for H_2O_2 Electrochemical Detection**

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The accurate detection of hydrogen peroxide (H_2O_2) is of great interest for scientists since it is one of the products generated during the reactions catalyzed by oxidases. Many techniques have been used to determine H_2O_2, such as UV–Vis spectroscopy, chemiluminescence, or electrochemistry. Recently, amperometric sensors, based on graphene and various types of porphyrins, for H_2O_2 proved to be very promising, due to their simplicity and high sensitivity.

In this work, different composite materials were synthesized by mixing N-doped graphene (N-Gr) with (metallo)tetrapyridylporphyrins (CoTPyP or MnTPyP), and then used to make graphene-porphyrin paste electrodes. The paste electrodes were prepared by adding silicon oil into the composite materials and mixing them into an agate mortar, until a uniformly wetted paste was obtained. The paste was then packed in a PVC tube (3 mm internal diameter and 5 cm long). A copper disk inserted into the graphene-porphyrin paste ensured the electrical contact. Whenever was necessary, a new surface was obtained by pushing out a small amount of the paste from the tube, and polishing with a weighing paper.

Cyclic voltammetry and amperometry were used to test the electro-catalytic effect of the paste electrodes, towards the H_2O_2 detection. Calibration curves for H_2O_2 were obtained after optimization of the experimental conditions (type of supporting electrolyte; solution pH) along with the paste composition (graphene:porphyrin ratio).

Acknowledgments: This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation, CNCS – UEFISCDI, project number PN-II-RU-TE-2014-4-0305

PBm6. **Methods for Assessment of Two Promising Nano-hybrids Materials used for Metallic Ions Removal**

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Development of two nanostructured hybrid materials with magnetic core as magnetic nano iron-oxides uncoated (NIOs) and magnetic nano-iron oxides coated with rose leaves extract (NIOEs) are reported here. In order to evaluate the sensitivity of these materials for Cr (VI), Zn(II), Pb(II) and Ca(II) removal from aqueous solutions, before and after treatment with NIO and NIOE, atomic and molecular absorption spectrometry was used. The structure and physicochemical properties of the resulting nano-hybrids were characterized in detail using techniques as scanning electron microscopy (SEM) coupled with energy-dispersive spectra (EDS), IR spectrometry (FTIR) and X-ray diffraction (XRD). According to the experimental results, NIOs present a promising capacity of Cr (VI) removal of approximately 60% and NIOEs at about 89%, after 15 minutes of contact, coupled with an acidic pH, which corresponds to the most industrial waste water conditions. For the removal of Ca(II) and Zn(II) it is necessary to make a pH correction to bring it to neutral values in order to maximize the efficiency. The Pb(II), on the other hand, shows a high removal efficiency when the solution displays a basic pH. The simple rose-extract suspension was also tested for Cr (VI) removal and it indicates approximately 10% capacity of metal removal. The obtained results indicated that the magnetic core of iron-oxides from NIOEs is uniformly distributed into rose leaves extract, this extract acting as a capping agent with a polyphenolic structure. These two nanostructured hybrids are homogeneously dispersed in water due to the stabilization of the polyphenols. Based on the adsorption results, NIOEs combine the unique magnetic properties of NIOs nanoparticles with the excellent adsorption properties and electron transfer ability of polyphenols.

Acknowledgments: This work has been funded by the Sectorial Operational Programme "Increase of Economic Competitiveness", ID 1799/SMIS 48589/2015.

PBm7. **Structure and Properties of some Metallic Biomaterials from system Ti-Nb-Fe used in Implantology**

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Special biomaterials from system Ti-Nb-Fe are obtained in our work by using water cooled crucible levitation melting under an argon atmosphere ensuring a high compositional homogeneity. The motivation of this tendency to realize materials with higher biocompatibility is to replace Al and V, both elements present in classical Ti alloys which exhibit toxicity. From system Ti-Nb-Fe three alloy compositions have been selected and investigated in order to determine the structure and properties. The microstructural evolution of different compositions is investigated in detail using scanning electron microscopy (SEM) coupled with energy-dispersive spectra (EDS) and X-ray diffraction (XRD). As a result of investigations the phasic constitution is predominant β-phase with dendritic distribution and α-phase as traces. The proportion of β phase increase with Nb content. Also, mechanical properties were tested indicate high specific strength, superior corrosion resistance and low modulus of elasticity with increasing of Nb content.

Acknowledgments: This work has been funded by the Sectorial Operational Programme "Increase of Economic Competitiveness", ID 1799/SMIS 48589/2015.

PBm8. **Optimization of Solid Phase Extraction Based On Molecular Imprinted Adsorbents for Furaltadone**

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Molecular imprinted polymers (MIPs) are a modern class of highly cross-linked polymers that can bind certain target compounds (analytes) with high specificity, and have physico-chemical stability, and applicability in harsh chemical media. The MIPs prepared by our team can be optimized for improving their analytical performances (selectivity and adsorption capacity). The characteristics of the prepared MIPs are a result of stronger interactions between the polymeric surface and the template molecule (furaltadone). Analytical procedures based on solid-phase extraction (SPE) and UV spectrometry, liquid-chromatography and cyclic voltametry were developed and optimized for determining low concentration of furaltadone in liquid mixtures. The main experimental parameters for SPE process optimization were: the ratio between loaded sample and re-extraction solvent volumes; the nature of desorption solvent and flow-rate of sample loading. Performance criteria that characterizes the proposed SPE-method such as precision; recovery; enrichment ratio and detection limit were very promising and comparable with those obtained by the analytical techniques commonly used for sample analysis (UV spectrometry, liquid-chromatography and cyclic voltametry).

PBm9. Evaluation of Conductor Polymer with Layer-by-Layer based Architecture for Glucose Biosensing

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Layer-by-layer (LbL) self-assembly is a simple and powerful method, efficient because protein denaturation is minimized since the films are produced under mild conditions, based on the electrostatic adsorption of macromolecules from aqueous solution onto solid supports. Layer-by-layer (LbL) strategies can be effectively used to reduce diffusion time of analytes and improve analyte access to the reaction sites.

In this work, glucose oxidase (GOx) was incorporated in a multilayer film on gold electrode, previously modified with a film of conducting polymer poly(3,4-ethylenedioxythiophene) (PEDOT), by electropolymerization, for a better conductivity of the electrons. Multilayer films containing the enzyme and nitrogen doped graphene (NG) dispersed in the biocompatible positively-charged polymer chitosan {$chit^{+}$(NG+GOx)}, together with the negatively charged polymer poly(styrene sulfonate), PSS^{-}, were assembled.

The LbL film growth was monitored by Surface Plasmon Resonance Spectroscopy (SPR) in order to evaluate the interactions involved in biomolecule immobilization on surfaces. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) also led to identification of the assemblies, confirmed by the analytical properties of the glucose biosensors determined by fixed potential amperometry. The biosensor sensitivity and selectivity, as well as applicability on plant extracts were determined.

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Poster Communications

Atomic and nuclear methods

PNa1. **Stable Isotope Fingerprinting In Pharmaceuticals Authentication**

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Variation in the relative abundance of stable isotope can be a useful tool in the identification and authentication of pharmaceuticals. In this study, a clear differentiation of some common pharmaceutical classes (non-steroidal anti-inflammatory, antitussives and antidepressants drugs) on the basis of their bulk isotopic fingerprints ($\delta^{13}C$ and $\delta^{15}N$) was made. Important differences of carbon isotopic composition ($\delta^{13}C$) of about 7 ‰ between the drugs having the same active substance, but produced by different manufactures were observed. Significant difference, around 3 ‰ between individual batches was also identified. The analyzed samples were purchased directly from pharmacies. The measurements of $\delta^{13}C$ and $\delta^{15}N$ from drug samples were carried out on an Elemental Analyser (Flash EA1112 HT, Thermo Scientific), coupled with an isotope ratio mass-spectrometer IRMS (Delta V Advantage, Thermo Scientific).

Acknowledgments: The financial support for this work was provided by the Program NUCLEU, contract no. PN16-30 01 01.

Pna2. **The Study of Metal Migration in the Aquatic Environment**

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The complexity of study of the trace metal migration in the system water – suspensions – silts – hydrobionts requires the application of validated research methods, and up-to-date techniques and equipment. With reference to hydrobionts of fresh water ecosystems, of most interest is the metal accumulation in higher aquatic plants, aquatic invertebrates (e.g. crustaceans, molluscs, insect larvae), and fish.

In the frame of this study the water samples were filtered *in situ* through membrane filters with pore size of 0.45 μm and preserved with concentrated nitric acid.

Silts and biological materials were transported in boxes with ice to laboratory, dried in oven (105 °C) and grounded. The digestion of samples was undertaken according to EPA 3051A method. In this respect, concentrated acids were used, e.g. nitric, hydrochloric, hydrofluoric, phosphoric and sulphuric acids and their mixtures, and the samples were heated by irradiation with microwaves up to 300 °C, under high pressure of up to 100 bar. The advantages of the sample microwave digestion system are the following: the sample contamination and loss are excluded, the digestion process, depending on the matrix of the analysed sample, lasts from few minutes to several tens of minutes, and the implication of human factor is minimal.

The atomic absorption spectrometry (AAS) was used for determining the content of metals in water samples, and the inductively coupled plasma optical emission spectrometry (ICP-OES) – in water, silt and hydrobiont samples. It is noteworthy that the second has become the most efficient and advantageous method in the study of trace elemental composition of the aquatic environment. The obtain results are of high accuracy, comparable to flame and furnace AAS methods.

Acknowledgments: The work was done in the frame of the EU funded projects MIS ETC 1150 and MIS ETC 1676 (INPOLDE).

Pna3. **Improved Method for Determination of Identity and Chemical Purity of [^{18}F]FLT**

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3′-deoxy-3′-[^{18}F]-Fluorothymidine ([^{18}F]FLT) is seen as a promising positron emitting radiopharmaceutical for clinical use in detecting proliferating cells in various tissues *in vivo*. 3′-Fluoro-thymidine, 2′,3′-Didehydro-3′-deoxythymidine and Kryptofix 2.2.2 are chemical impurities resulting in the [^{18}F]FLT production. Due to their toxic effect, it is mandatory to determine, both accurately and efficiently, the concentration level of these impurities.

The objective of this study was to identify the most suitable method to determin e the identity and chemical purity of [^{18}F]FLT using high performance liquid chromatography (HPLC). The following step was the its optimization, using as operating parameters the chromatographic settings such as the composition and flow rate of the mobile phase, and the column temperature.

For the chemical purity determination, the system of choice was an AgilentBio-inert 1260, equipped with UV and radioactive detectors. Separation was achieved with an analytical reversed phase column (Zorbax SB-C18, 150mm x 2.1 mm, 3.5µm). Excellent repeatability and inter-day precision were obtained. The linearity of the method was proved using five concentration levels. The method was found to be precise, accurate and specific; more, its reproducibility is very good, as the relative standard deviation of the peak area was less than 2%. All these assets recommend its use for determination of identity and chemical purity of [^{18}F]FLT.

Pna4. **Multi-elemental, isotopic and trace pesticides analysis of wild and cultivated berries species**

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The main focus of this study was to investigate differences in isotopic, elemental and trace pesticides content of wild and cultivated berries from some areas of Transylvania. In order to emphasize differences concerning geographical origin of studied berries, stable isotopic ratios of so-called “bio-elements” ($^{2}H/^{1}H$, $^{18}O/^{16}O$, $^{13}C/^{12}C$) were determinal by IRMS. Beside this, determination of elemental fingerprinting profile of berries samples was performed using ICP-MS. For analysis of pesticides at trace level in berries samples a sensitive and selective method, based on gas chromatography and mass-spectrometry was developed. Multivariate statistical analysis was performed in order to evaluate the differences between wild and cultivated fruits. The obtained results suggested that multi-elemental, isotopic and trace pesticides fingerprint techniques are feasible for sample differentiation and comparison.

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Pna5. **Vegetable Characterization Using Stable Isotope And Elemental Signature**

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In this study, samples of vegetables (parsley and celery root, red beet) present on Romanian market were investigated, in order to differentiate, by mean of stable isotopic ($\delta^{13}C$, $\delta^{15}N$, $\delta^{18}O$ and $\delta^{2}H$) fingerprint, the agriculture type (organic versus conventional) that was used for their production. Another aim was to distinguish isotopic and elemental fingerprint of vegetables grown in greenhouses compared to those grown on field (courgettes). The measurements of $\delta^{13}C$ and $\delta^{15}N$ from vegetable samples were carried out on an Elemental Analyser (Flash EA1112 HT, Thermo Scientific), coupled with an isotope ratio mass-spectrometer IRMS (Delta V Advantage, Thermo Scientific). For $\delta^{18}O$ and $\delta^{2}H$ analysis, the equipment used was a Liquid-Water Isotope Analyzer (DLT-100, Los Gatos Research). For elemental determinations, a ICP-MS was used. Some overlap between the $\delta^{15}N$ values of the organic and conventional datasets means that it is necessary to add other markers and also to employ a statistical methodology to try and classify a randomly analyzed "off the shelf" sample as organic/conventional.

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Pna6. **Wastewater decontamination using highly porous Metal Organic Framework (MOF) and nanostructured carbon materials**

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Contamination of water by toxic heavy metals through the discharge of industrial wastewater is a worldwide environmental problem. Heavy metals are nowadays the most important pollutants and becoming a severe public health problem.

The adsorption from aqueous solution of trace amounts of some metals using Metal Organic Framework (MOF) and/or nanostructured carbon materials (ordered carbon, graphene oxide and partially reduced graphene oxide), as highly adsorbent material, has been studied through batch experiments. The choice of these materials was made based on their very particular properties: high surface area, controlled porosity, the possibility to tailor the surface hydrophilicity. The above mentioned materials were prepared by classic methods modified to meet the project requirements. The materials characterization sought to determine some important parameters for adsorption properties such as: (i) surface area and porosity, (ii) surface properties: acidity, degree of oxygenation, (iii) crystalinity, (iv) moisture and temperature stability. The adsorbtion potential of these materials was tested for a large number of metals.

The trace metals determinations were performed by an Inductively Coupled Plasma Mass Spectrometer (ICP-MS), Elan DRC-e Perkin Elmer. For each sample analysis three replicates were measured in order to assure the control quality.

Acknowledgments: The financial support for this work was provided by the National Plan for Research-Development and Innovation PN 16-300204

Pna7. **Oxygen Isotope Ratios in The Ethanol and Water of Romanian Wines as Approach in Improving the Assessment of Ethanol Origin and Illegal Watering**

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Stable isotopes (O-H-C) have been widely used in the last decade to confirm the authenticity and geographical provenance of wines since they do not suffer significant alterations during the winemaking process. The values of $\delta^{18}O$ in wine water and $\delta^{13}C$ in wine ethanol and the deuterium distribution from ethanol molecule registers information on the environmental conditions and photosynthetic pathway, useful for origin (botanical and geographical) assignment of wine and as proof for the addition with non-grape sugar and dilution of wines with water. This work was focused in providing reliable complementary isotopic data to improve the assessment of the ethanol origin and illegal watering of wine. For this purpose wines originated from Romania, harvest years between 2009 and 2015, were analyzed in terms of their $\delta^{18}O$-values in wine water and ethanol. Measurements were performed on an elemental analyzer (EA) coupled with continuous flow – isotope ratio mass spectrometer (CF-IRMS) for $^{18}O/^{16}O$ ratio in water, while $^{18}O/^{16}O$ ratio in ethanol on an EA- pyrolysis interfaced with CF-IRMS. The results showed an improvement in assessing wine in terms of detecting wine watering and assessing ethanol origin.

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Pna8. **Characterisation and Classification of Wines from Some Grape Varieties Grown in Romania: An Approach Based on Metals and Phenolic Compounds**

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There is a growing trend in food industry in combining safety and quality attributes of products with their distinct regional identity. In this study we used data on several elements (Cd, Cu, Cr, Zn, Pb and Ni) and phenolic compounds (gallic, syringic, *p*-coumaric acids, (+)-catechin, (−)-epicatechin, *trans*-resveratrol, rutin, quercetin and vanillin) as complementary markers to characterise and differentiate wines from three wine-growing areas (Murfatlar, Recas and Jidvei) of Romania, according to their geographical and varietal origin. Wines from south-eastern region (Murfatlar) were characterized by their lower content in Cu, Cr and Ni, compared with wines from western (Recas) and central (Jidvei) region, while the content of phenolic compounds in the wine samples showed a visible variation, depending both of the grape variety and geographical origin. The statistical processing tools applied to our results allowed robust differentiation of wines by region, variety, and vintage year. The phenolic compounds (gallic acid, catechin, epicatechin, rutin, quercetin and *trans*-resveratrol) showed the best correlations for the varietal discrimination of wines. Using discriminant analysis, a correct classification of the wines by variety was achieved in a proportion of 88.89% (based only by phenolic compounds) and 96.30 % (based both on phenolic compounds and metals), revealing that elements Cu, Cr and Ni are significant for discrimination. Moreover, a 100% successful classification of wines by region of origin and vintage year was accomplished.

Acknowledgments: This study has been financed by the Romanian Ministry of Education and Research, National Authority for Scientific Research for the financial support, under the NUCLEU Program, project PN 16 36 04 02 Advanced research on the authentication of food origin for implementing innovative fingerprinting methodologies - Emphasis on fruit-based products.

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Kadmi	Yassine	PMf12
Kaigala	Govind-V.	I6
Kalibataitė	Simona	O8
Kauffman	W.-Berkeley	K2
Kovacs	Eugenia	PMa2
Krauson	Aram-J	K2
Krumova	Sashka-Boichova	PMa1
Kusko	Mihaela	O10
L		
Lar	Claudia	PBm2
Lavric	Vasile	PNa3
Lazar	Diana	PMa6
Lazurcă	Dumitru	PSp15
Le Gac	Séverine	O24, O25
Lee	Jong-Kook	PNb6
Leonte	Radu-A.	PMa4
Leopold	Nicolae	PSp1
Leostean	Cristian	PNb1, PNb2
Litescu	Carmen-Simona	K10
Llamazares	Guillermo	O25
Luchian	Tudor	PNb5, PNb6, PSb5
Lung	Ildiko	PNb1, PNb2
Lungu	Emil	PMp2
Lungu	Mihai	PMp1
Lungu	Antoanetta	PMp1
M		
MacArdle	Síobhan	O18
Magdas	Dana-Alina	PMf3, PMf3, PNa1, PNa4, PNa5, PNa6

Magerusan	Lidia	PNb11, PSb4, PBm5
Malaquin	Laurent	I3
Marconi	Daniel	PNb3, PSp1, PSp8, PBm4
Mardare	Georgiana	PMf6
Marincas	Olivian-Ciprian	PMf3
Martin	Flavia-Adina	PBm2, PBm4
Marty	Jean Louis	K8
Matagne	André	P2
Matei	Bogdan-Mircea	O3
Matei	Cristian	O3
Matei	Ecaterina	PBm6, PBm7
Mernea	Maria	PSp9
Merrell	Johnson	I2
Mic	Mihaela	PSp7
Miclăuş	Maria-Olimpia	PMf7, PBm1
Miclea	Luminita-Claudia	O3
Mihai	Simona	PMp3
Mihailescu	Mona	O2
Mihailescu	Dan-Florin	PNb4, PNb7, PSp9, PSb3
Mihalache	Iuliana	O10
Mihale	Nicolae	O2
Mihon	Mirela	PNa3
Moisescu	Mihaela-Georgeta	O2, O3, PMp2
Moldovan	Zaharie	PMf3
Monge	Rosa	O25
Montagner	Caroline	P2
Morari	Cristian	O13, PSb2
Morosanu	Cezarina-Ana	PSp12

Mot	Augustin	PMf5
Muntean	Cristina-M.	PSp4, PSp5
N		
Nan	Alexandrina	O12, PBm2
Neagu	Livia	PNb10
Neamtu	Silvia	PSp6, PSp7, PMf5, PBm4
Neculae	Adrian	PMp1
Nicolescu	Cristina-Mihaela	PNb8, PNb9
Niculae	Dana	PMa4, PNa3
Nigen	Michaël	P2
O		
Ochoa	Ignacio	O25
Olariu	Romeo-Iulian	PMf1, PMf6
Olaru	Octavian	PSp15
Olteanu	Radu-Lucian	PNb8, PNb9
Oprea	Alexandru-Mihail	PMf10
Opris	Ocsana	PNb2
P		
Pacala	Mariana-Liliana	PMf12
Pall	Emoke	PNb11
Pantilimon	Cristian	PBm6
Parcalabu	Liliana	PSb1
Park	Paul-Shin-Hyun	K6
Park	Yoonkyung	PNb6
Parvu	Marcel	PMf5
Pavaloiu	Ramona-Daniela	O3
Petrache	Horia-I.	I2
Petran	Anca	O12

Petrescu	Livia	PNb4, PNb7, PSb3
Pirnau	Adrian	PSp6, PSp7
Pirvu	Lucia	O3
Podlipnik	Crtomir	PSp13
Pogacean	Florina	PNb11, PSb4, PBm5
Polonschii	Cristina	O4, O17, O22
Popa	Ionel	O1
Popa	Claudia-Valentina	K10, PSb1
Popescu	Ion-V.	I7
Popescu	Raluca	PNa7
Popescu	Ileana-Nicoleta	PMp3
Popescu	Octavian	O22
Popescu	Aurel-I	PSp3
Porav	Sebastian-Alin	PNb1, PNb2
Porumb	Roxana	PSb1
Predescu	Andra	PBm6, PBm7
Predescu	Cristian	PBm6, PBm7
Pruneanu	Stela	PNb11, PSb4, PBm5
Puscas	Romulus-Horatiu	PNa4, PNa5
R		
Radoi	Antonio	O10
Radu	Mihai	PMf8
Radu	Teodora	O12, PBm2
Radulescu	Cristiana	I7, PSp2, PSp15
Raicu	Alina	PMa4
Raicu	Valerica	K3
Ray	Bruce-D.	I2
Redfield	Christina	P2

Renault	Nicole Jaffrezic	O23
Rhouati	Amina	K8
Roberts	Gordon-C.K.	P2
Rodaitė-Riševičienė	Raminta	O8, PMf2
Rossem	Fleur van	O24
Rosu	Marcela-Corina	PNb11, PSb4, PBm5
Rosu-Hamzescu	Mihnea	O4
Ruggi	Albert	O25
S		
Saez	Janire	O21
Sandru	Claudia	PNa8
Sandulescu	Robert	O11, O23
Saulis	Gintautas	O8, PMf2
Savopol	Tudor	O2, O3, PMp2
Schiopu	Irina	PSb5
Schmidt	Marius	P4
Scripa-Tudose	Adina-Elena	PSp11
Seo	Chang-Ho	PNb6
Serban	Adrian	PSb6
Serra	Marco	I3
Sha'at	Fawzia	O3
Shvetsov	Valery	K9
Silipas	Teofil-Danut	PNb1
Socaci	Crina-Anca	Pnb11, PSb4, PBm1, PBm5
Sohaciu	Mirela	PBm7
Soran	Maria-Loredana	PNb2
Sridhar	Adithya	O25

Stan	Manuela	PNb1, PNb2
Stanica	Luciana	O22
Starr	Charles-G	K2
Stefan-van-Staden	Raluca-Ioana	I4
Stegarus	Diana-Ionela	PNa8
Stihi	Claudia	I7, PSp2, PSp15
Strambeanu	Nicolae	PMp1
Streza	Mihaela	PMf7
Știrbescu	Raluca	PSp15
T		
Taly	Valérie	I5
Taneva	Stefka-Germanova	PMa1
Teodorescu	Sofia	PSp15
Terstappen	Leon-WMM	P3
Teste	Bruno	I3
Tivig	Ioan	PMp2
Todinova	Svetla-Jeliazkova	PMa1
Todoran	Radu	I7
Toma	Vlad	PMf5
Tosa	Nicoleta	O15
Tosa	Valer	O15
Totan	Maria	PMa3
Tripon	Carmen	PSp5
Tudor	Alexandru	O19, O20
Tudoran	Cristian	O15
Tugce	Akyazi	O21

Turcu	Ioan	O13, PNb3, PSp1, PSp8, PMf8, PBm2, PBm4
Turcu	Rodica	O12, PBm2
Turza	Alexandru	PSb4
Tuta	Catalin-Stelian	PMa4, PNa3
U		
Ulevicius	Vidmantas	P5
V		
Van-Staden	Jacobus-Koos-Frederick	I8
Vasile	Eugeniu	O10
Vasilescu	Alina	PSb1
Viovy	Jean-Louis	I3
Virumbrales-Muñoz	Maria	O25
Vlase	Laurian	PMf5
Voica	Cezara	PMf4, PNa1, PNa5, PNa6
W		
Wassall	Stephen-R.	I2
Watanabe	Fumiya	PBm3
Wimley	William-C	K2
Wolbert	Dominique	PMf12
Zelencova	Laura	O7
Zinicovscaia	Inga	I7
Zorila	Florina	PMf8
Zorilă	Bogdan	PSp3, PSp10
Zubcov	Elena	PNa2
Zubcov	Natalia	PNa2