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About the Conference

For the second consecutive year, the American Chemical Society Georgia Student Chapter in collaboration with San Diego State University Georgia, Tbilisi State University, and Georgian Chemical Society are proud to provide a unique opportunity for young scientists and senior researchers in the region to come together and promote innovation and development in the field of Chemistry.

The main objective of this symposium is to establish a platform for scientists in the Caucasus region to come together and discuss advancements in the field. We aim to expand the American Chemical Society network and provide networking and professional development opportunities to professionals, scientists and students.

This symposium will represent a wide variety of topics in Chemistry. Lectures and posters will cover a range of different topics of chemistry listed below.

TOPICS

Analytical Chemistry

Physical Chemistry

Theoretical Chemistry

Organic Chemistry

Biochemistry

Inorganic Chemistry

Environmental Chemistry

Ecology

Welcome Message from the Conference Chair

Welcome to our 2019 Annual American Chemical Society (ACS) Georgia Student Chapter International Symposium. In collaboration with San Diego State University, San Diego State University-Georgia, Tbilisi State University, Georgian Chemical Society and SDSU-Georgia International Student Chapter, we are proud to provide an international platform for sharing research advances in the field of Chemistry and Biochemistry.

The aim of this symposium is to promote collaboration and networking and to share research highlights among our professors, students and professionals from different universities and research institutions not only in Georgia but also from the Caucasus Region. We encourage you to join our annual symposium and share your latest research highlights with fellow scientists from the region. SDSU-Georgia is grateful for the support from the United States Millennium Challenge Corporation and the Georgian Government.

William G. Tong, Ph.D.

Chair, American Chemical Society Georgia Student Chapter 2nd Annual International Symposium, Tbilisi Georgia May 31 - June 01, 2019

Chair, Department of Chemistry and Biochemistry, San Diego State University, San Diego, California.

Committees

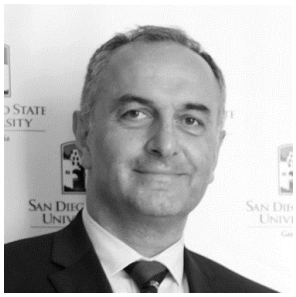
Chair of the Conference

Dr. William Tong

Distinguished Professor

Chair of Department of Chemistry and Biochemistry San Diego State University

Co-Chair of the Symposium



Dr. Nugzar Davitashvili

Vice-Dean, SDSU-G

Co-Chair of the Symposium

Dr. Nino Kokiashvili

Senior Researcher, TSU, SDSU-G

Co-Chair of the Symposium

Dr. Giorgi Jibuti

Assistant Professor, TSU, SDSU-G

Co-Chair of the Symposium

Tamar Basiashvili

Senior Student, SDSU-G

Scientific Committee

Dr. William Tong – Chair of the Symposium, Distinguished Professor, Chair of the Department of Chemistry and Biochemistry, SDSU
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Dr. Shota Samsoniya – Professor, Doct.Chem.Sci., Academician, Chair of the Chemistry Department, TSU
Dr. Bezhan Chankvetadze – Professor, Doct.Chem.Sci., Academician, Chair of Physical and Analytical Chemistry Department, TSU
Dr. Nodar Lekishvili - Professor Emeritus, Doct.Chem.Sci., President of the Chemical Society of Georgian, TSU
Dr. Nino Kokiashvili - Senior Researcher, Invited Professor, TSU, SDSU-G
Dr. Giorgi Jibuti - Assistant Professor, TSU, SDSU-G
Dr. Magda Alania - Associate Professor, TSU, SDSU -G
Dr. Giorgi Burjanadze - Assistant Professor, TSU, SDSU-G
Dr. Ana Goletiani - Associate Professor, GTU, SDSU-G
Dr. Nikoloz Nioradze - Associate Professor, TSU, SDSU-G
Dr. Giorgi Dalakishvili - Associate Professor, ILIAUNI, SDSU-G

Organizing Committee

Dr. William Tong - Chair of the Symposium, Distinguished Professor, Chair of the Department of Chemistry and Biochemistry, SDSU
Dr. Halil Guven - Dean, SDSU Georgia
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Tamar Maisuradze - Senior Student, SDSU-G
Magda Aptsiauri - Senior Student, SDSU-G
Mariam Basilaia - Senior Student, SDSU-G
Giorgi Meshvildishvili - President-Elect of ACS Georgia Student Chapter, SDSU-G
Ani Rukhadze - Vice President-Elect of ACS GSC, SDSU-G
Sandro Gogia – Secretary-Elect Junior Student, SDSU – G

Conference Program

Day 1

DAY 1 – TSU Building 1, Concert Hall			
TIME	Presenter	Affiliation	Presentation Title
08:30 – 09:30	Registration – Welcome Coffee and Tea		
09:30 – 10:00	Opening Remarks – Moderator – Dr. Nugzar Davitashvili		
09:30 – 09:35	Dr. Nugzar Davitashvili – Vice-Dean, SDSU-Georgia		
09:35 - 09:40	Dr. William Tong – Distinguished Professor, Chair, SDSU		
09:40 - 09:45	Dr. Nodar Surguladze - Tertiary Education Project Director, MCA-Georgia		
09:45 - 09:50	Dr. Ramaz Khomeriki – Prof. Dean of Exact and Natural Sciences, TSU		
10:00 – 13:00	Keynote Address – Session Chair – Dr. William Tong		
10:00 – 10:30	Dr. Jeffrey Roberts	Dean, College of Sciences, Professor of Chemistry, San Diego State University	Surface Modification of Aerosol Nanoparticles for Materials Applications
10:30 – 11:00	Dr. Bezhan Chankvetadze	Professor, Academician, Chair of Institute of Physical and Analytical Chemistry, Tbilisi State University	Our Recent Studies on Thermodynamics of Enantioseparations with Polysaccharide-Based Chiral Selectors in High-Performance Liquid Chromatography
11:00 – 11:30	Dr. William Tong	Distinguished Professor, Chair of Department of Chemistry and Biochemistry, San Diego State University	Zeptomole-Level Detection Methods for Biomarkers Using Multi-Photon Nonlinear Laser Wave-Mixing Spectroscopy
11:30 – 12:00	Dr. Thomas Beattie	Chair, ACS National Senior Chemists Committee	50+ YEARS OF DRUG DEVELOPMENT: Wow, How Things Have Changed!
12:00 – 12:30	Dr. Omar Mukbaniani	Professor, Chair of Macromolecular Chemistry, Tbilisi State University	Fluorine Containing Solid Polymer Electrolyte Membranes
12:30 – 13:00	Dr. Ramaz Katsarava	Professor, Academician, Institute of Chemistry and Molecular Engineering, Agricultural University of Georgia	Pseudo-Proteins – A New Family of Biodegradable Polymers

13:00 – 15:00	Poster Session		
13:00 – 14:00	Lunch		
13:30 – 14:00	NMR Lab Tour		
15:00 – 16:30	Plenary Session 1 – Session Chair – Dr. Nino Kokiashvili		
15:00 – 15:20	Dr. Giorgi Jibuti	Assistant Professor, Chair of English Language Chemistry Program, TSU & SDSU-Georgia	SMART | AtmoSim_Lab: Air Contamination Research at Tbilisi State University
15:20 – 15:40	Dr. Peter van der Geer	Associate Professor, Biochemistry, SDSU	Signal Transduction by Receptor Protein-Tyrosine Kinases
15:40 – 16:00	Dr. Ramaz Gakhokidze	Professor, Chair of Department of Bioorganic Chemistry, TSU	Way to Reduce Global Warming with Bioenergy Activators
16:00 – 16:20	Dr. Rusudan Kakava	PhD in Chemistry, TSU Instructor, SDSU-G	Synthesis of Novel Chiral Sulfoxides and Study of Their Enantioseparation Using HPLC
16:20 – 16:30	Ana Shalamberidze	President ACS-GSC, 4th year BSc student, SDSU- G	Introduction to ACS Georgia Student Chapter
16:30 – 18:00	Plenary Session 2 – Session Chair – Dr. Giorgi Jibuti		
16:30-16:45	Givi Kalandia	Vice-President ACS-GSC, 4th year BSc student, SDSU-G	West Georgian Chromatography Center and Determination of Stilbenes in Several Georgian Wines
16:45 – 17:00	Elguja Gojiashvili	Treasurer, ACS-GSC, 4th year BSc student, SDSU- G	Making Ligands for the General Catalyst Control of the Monoisomerization of 1-Alkenes to cis-2-Alkenes
17:00 – 17:15	Elene Aslanikashvili	3rd year BSc student, SDSU-G	Using Differential Scanning Calorimetry to Study the Thermal Properties of Semicrystalline Polymers
17:15 – 17:30	Ana Kutchuashvili	3rd year BSc student, SDSU-G	Analysis of Sulfoxides Using High Performance Liquid Chromatography
17:30 – 17:45	Sandro Gogia[1], Mariam Khvichia	[1]Treasurer-elect ACS-GSC 3rd year BSc students, SDSU-G	Characterization of Hardness in Pencil Leads and Analyzation of Cosmetic Products Using Differential Scanning Calorimetry
17:45 – 18:00	Mariam Abramishvili	3rd year BSc student, SDSU-G	Synthesis and Transformation of Adamantane-Containing Some Schiff Bases

Day 2

DAY 2 – TSU, Building I, Auditorium 115			
TIME	Presenter	Affiliation	Presentation Title
08:30 – 09:30	Registration – Welcome Coffee and Tea		
09:30 – 12:00	Plenary Session 3 – Session Chair – Dr. Nikoloz Nioradze		
09:30 – 09:50	Dr. Nikoloz Nioradze	Professor, R. Agladze Institute of Inorganic Chemistry and Electrochemistry, TSU	Nanogap Scanning Electrochemical Microscopy
09:50 - 10:10	Dr. Khatuna Barbakadze	Assistant Professor, Tbilisi State Medical University	High-Performance Fluorinated Hybrid Materials
10:10 – 10:25	Ann Gogolashvili	PhD Student, TSU Instructor, SDSU-G	Chiral Separation in Capillary Electrophoresis with Cyclodextrin-Type Chiral Selectors and Investigation of Structure of Selector-Selectant Complexes by Using Nuclear Magnetic Resonance Spectroscopy
10:25 – 10:40	Ketevan Kharaishvili	PhD Student, TSU	Optimization of Average Sampling
10:40 – 10:55	Elene Gvazava	PhD Student, TSU	Evaluation of the Air Pollution and Comparison of Pollutants' Concentrations in Heavy and Light Traffic Hours
10:55 – 11:10	Salome Pantsulaia	MS Student, TSU	Overview of the Current Experiments on Air Pollution Control in Tbilisi
11:10 – 11:25	Rukhadze Ani[1], Sandro Mestvirishvili	[1]Vice-president elect ACS-GSC, 3rd year BSc students, SDSU-G	Effect of Extraction Methods on Yield, Structural and Thermal Properties of Pectin Samples
11:25 – 11:40	Nino Mamasakhlisi	3rd year BSc student, SDSU-G	Synthesis and Some Transformations of Adamantane-1-Carboxylic Acid Derivatives
11:40 – 11:55	Nino Nikolaishvili, Nika Asatiani	3rd year BSc student, SDSU-G	DSC Characterization of Inulin/Coenzyme Q10 Sample and its Potential Application in Drug Delivery Systems
12:00 – 13:00	Lunch Break		
13:00 – 14:15	Plenary Session 4 - Session Chair – Dr. Ana Goletiani		
13:00 – 13:15	Ani Chakhrakia	3rd year BSc student, SDSU-G	Synthesis and Application of Amino-1-Adamantane Containing Dipeptides via Multicomponent Reaction
13:15 – 13:30	Tamar Kerdikoshvili	3rd year BSc student, SDSU-G	Synthesis of Some Schiff Bases and Dipeptides from N-(1-Adamantyl carbonyl)o-Phenylenediamine

13:30 – 13:45	Nino Gavashelishvili	3rd year BSc student, SDSU-G	Thermal Properties of Green and Roasted Coffee
13:45 – 14:00	Sergi Betkhoshvili	2nd year BSc student, SDSU-G	Synthesis of Suprofen S-oxide from Suprofen Using mCPBA and Comparison to the Clopidogrel Oxidation Results Regarding the Substituent Effects
14:00 – 14:15	Natia Inadze	2nd year BSc student, SDSU-G	Oxidation of Thiophene Group in Tioconazole to Tioconazole S-oxide Using mCPBA
14:15 – 14:30	Nika Kutalia, Khatia Merabishvili	2nd year BSc students, SDSU-G	Investigation of Thermal Stability of B-Group Vitamins
14:30 – 15:00	Award Ceremony		
15:00 - 15:15	Group Photo		

Poster Session

Day 1 – TSU Building , Concert Hall			
Poster Session Presentations			
Poster Number	Presenter	Affiliation	Name of Presentation
1	Dr. Marina Gakhutishvili	Lecturer, Tbilisi State University	Arsenic (III) Oxide in poly(Vinyl Chloride) PVC
2	Magda Aptsiauri	4th year BSc student, SDSU-G	Investigation of Thermal Properties of New Semicrystalline Polymers
3	Nikoloz Kvinikadze	4th year BSc Student, TSU	Synthesis of Some New Derivatives of Pyridazino[4,5-b]Indoles
4	Ana Shalamberidze	President ACS- GSC, 4th year BSc student, SDSU-G	Design and Synthesis of New Fluorescent Thymidine Analogues
5	Davit Khutsishvili	2nd year BSc student, SDSU-G	Enantioseparation of Brompheniramine, Chlorpheniramine and Dimethindene Maleate in Capillary Electrophoresis Using Cyclodextrins as Chiral Selectors
6	Giorgi Meshveldishvili	President elect ACS-GSC, s3rd year BSc student, SDSU-G	Synthesis of 5(6)-Nitro-[2-(3-Acetamido-Adamantyl-1)]-1H-Benzimidazole Derivatives
7	Ana Tavartkiladze	3rd year BSc student, SDSU-G	Thermal Properties of Fresh and Roasted Coffee Beans
8	Nikoloz Shurgaia	3rd year BSc student, SDSU-G	Synthesis and Some of Transformation 2(1-Adamantyl)-1H-Benzimidazole
9	Tamar Khatiashvili	MS student, TSU	Nitrogen Oxides Pollution in Tbilisi
10	Sofiko Maglakelidze	2nd year BSc student, SDSU-G	Synthesis of Chiral Sulfoxides and Separation of Enantiomers by HPLC Method
11	Mariam Basilaia, Tamar Maisuradze	4th year BSc student, SDSU-G	Using Protein Design to Engineer a Scaffold for Regio-Selective C-H Functionalization
12	Luka Tatarashvili	4th year BSc student, SDSU-G	Ultrasensitive Detection of Cancer Biomarker CEA Using Multi-Photon Non-Linear Laser Wave-Mixing Spectroscopy
13	Salome Dushashvili	2nd year BSc student, SDSU-G	Thermal Stability of Folic Acid and its Deficiency in Humans
14	Asmat Kontselidze	2nd year BSc student, SDSU-G	Study of Toxicity of Heavy Metal Ions Using Algae Model
15	Mariam Vardiashvili	3rd year BSc student, SDSU-G	Thermal Property of Pencil Leads and Various Cosmetic Products. Resistivity of Graphite Pencils.

16	Nino Shatirishvili	4th year BSc student, SDSU-G	Novel Detection of Biomarkers of Pancreatic Cancer Using Microfluidics and Nonlinear Multi-Photon Laser Wave-Mixing Detector
17	Sopho Khokhonishvili	3th year BSc student, SDSU-G	Thermal Properties of Georgian Nuts
18	Veronica Coen	2nd year BSc student, SDSU	Synthesis Some of 5(6)-Nitro-2-(1-Adamantylmethyl)-1H-Benzymidazole and its Derivatives
19	Tamara Gabour Sad	PhD Student, Saarland University, Batumi Shota Rustaveli State University	Identification of Phenolic Compounds in Endemic Species in Georgia

Keynote Speakers

SESSION CHAIR – Dr. William Tong

Dr. Jeffrey Roberts - Surface Modification of Aerosol Nanoparticles for Materials Applications

Dr. Bezhan Chankvetadze - Our Recent Studies on Thermodynamics of Enantioseparations with Polysaccharide-Based Chiral Selectors in High-Performance Liquid Chromatography

Dr. William Tong - Zeptomole-Level Detection Methods for Biomarkers Using Multi-Photon Nonlinear Laser Wave-Mixing Spectroscopy

Dr. Tom Beattie - 50+ YEARS OF DRUG DEVELOPMENT: Wow, How Things Have Changed!

Dr. Omar Mukbaniani – Fluorine Containing Solid Polymer Electrolyte Membranes

Dr. Ramaz Katsarava – Pseudo-Proteins – A New Family of Biodegradable Polymers

Surface Modification of Aerosol Nanoparticles for Materials Applications

Jeffrey Thomas Roberts
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e-mail: jtroberts@sdsu.edu

The surfaces of aerosol particles, especially nanometer-sized aerosol particles, present a fascinating and compelling challenge to the materials scientist. Aerosols have become increasingly important in the synthesis of certain nanostructured materials. At the same time, recent advances in instrumentation have created new opportunities for studying chemical processing. It is now possible, for instance, to monitor adsorption or desorption of monolayer quantities of material on an authentic aerosol. This presentation will describe the potential use of aerosols for high-yield synthesis of nanoparticles for materials, explored through examples out of our laboratory. In one example, self-assembled amine monolayers are grown pm Si nanoparticles as small as 6 nm diameter. In another, polymethylmethacrylate shells are grown deposited on nanoparticle Al. The strategies described in this work are potentially generalizable as new platforms for creating functionalized nanoparticles and nanocomposite materials, using only simple starting materials in a single pass reactor and under low temperature conditions.

Our Recent Studies on Thermodynamics of Enantioseparations with Polysaccharide-Based Chiral Selectors in High-Performance Liquid Chromatography

Bezhan Chankvetadze
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Polysaccharide-based chiral columns and materials are the most widely used ones for the separation of enantiomers of chiral compounds in liquid-phase techniques such as high-performance liquid chromatography (HPLC), nano liquid chromatography (nano-LC), supercritical fluid chromatography (SFC) and capillary electrochromatography (CEC). In recent years we have succeeded in obtaining with these materials very high separation factor [1], extremely high separation efficiency [2] and baseline separation of enantiomers on the scale of few seconds [3]. In addition, in SFC quite unusual enantioseparations of underivatized amino acids with polysaccharide-based chiral columns was achieved [4]. In last two years our efforts are focused mostly on the understanding the role of the temperature in chromatographic enantioseparations. In this presentation thermodynamic characteristics of enantioseparation process is discussed and some hidden effects of temperature on the separation process are highlighted.

References:

1. T. Khatiashvili, R. Kakava, I. Matarashvili, H. Tabani, C. Fanali, A. Volonterio, T. Farkas, B. Chankvetadze, Separation of enantiomers of selected chiral sulfoxides with cellulose tris(4-

chloro-3-methylphenylcarbamate)-based chiral columns in high-performance liquid chromatography with very high separation factor, J. Chromatogr. A, 1545 (2018) 59-66.
2. Q. Kharaishvili, G. Jibuti, T. Farkas, B. Chankvetadze, Further proof to the utility of polysaccharide-based chiral selectors in combination with superficially porous silica particles as effective chiral stationary phases for separation of enantiomers in high-performance liquid chromatography J. Chromatogr. A, 1467 (2016) 163-168
3. N. Khundadze, S. Pantsulaia, C. Fanali, T. Farkas, B. Chankvetadze, On our way to sub-second separations of enantiomers in high-performance liquid chromatography, J. Chromatogr. A 1572 (2018) 37-43.
4. E. Lipka, A-E. Dascalu, Y. Messara, E. Tsutsqiridze, T. Farkas, B. Chankvetadze, Separation of enantiomers of native amino acids with polysaccharide-based chiral columns in supercritical fluid chromatography, J. Chromatogr. A 1585 (2019) 207–212.

Zeptomole-Level Detection Methods for Biomarkers Using Multi-Photon Nonlinear Laser Wave-Mixing Spectroscopy

William Tong

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Multi-photon nonlinear laser wave-mixing methods with zeptomole (10^{-21} mole) or sub-parts-per-quadrillion-level detection sensitivity are presented for a wide range of biomedical and environmental applications. Laser wave mixing offers better detection sensitivity levels as compared to fluorescence-based methods and yet our wave-mixing methods can detect both fluorescing and nonfluorescing molecules, i.e., labeled and native biomolecules without using tags or labels. The detector probe volume is very small (picolitre), and hence, it offers high spatial resolution for 2D or 3D mapping of single cells. Picolitre-level probe volumes also offer effective interfacing to microarrays, lab-on-a-chip, chip-based electrophoresis systems and microfluidics. Unlike fluorescence methods, our laser methods produce a strong coherent laser-like signal beam with its own propagation direction, and hence, it is easy to detect with excellent signal-to-noise ratios. We use a wide range of lasers with wavelengths from UV (solid-state lasers) and visible (tunable external cavity diode lasers) to mid-IR (tunable quantum cascade lasers). We have demonstrated ultrasensitive detection levels for a range of applications including biomarkers for Parkinson's, Alzheimer's, multiple sclerosis, cancer cells, heart-failure biomarkers, and viruses (HPV, HIV). We will also discuss MCC SDSU-G Post-Compact collaborations between SDSU and TSU faculty colleagues and students.

50+ YEARS OF DRUG DEVELOPMENT: Wow, How Things Have Changed!

Thomas R. Beattie
American Chemical Society Fellow, Independent Consultant, San Diego, CA 92122, USA

The author travels through 50+ years of drug development history in the U.S., and, based on his own experiences in big pharma, small biotech, and biopharmaceutical consulting, highlights some changes which have occurred in the biotech industry. The workforce trained by the SDSU-Georgia Chemistry Degree Program will have the opportunity to contribute in the future innovation economy of Georgia, especially in building the new biotech industry.

Fluorine Containing Solid Polymer Electrolyte Membranes

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The wide application of organosilicon polymers in many fields of techniques pushed the development of organosilicon chemistry and increased application-oriented researches in above mentioned field. Nowadays, development of new and more efficient methods of energy storage and conversion is one of the major problems facing scientists. This includes the efficient storage of electricity. Therefore, development of batteries and other energy storage devices with high energy density, low energy losses during operation, low cost and long lifetime is one of the most important challenges.

The aim of our work is synthesis of siloxane-based polymer electrolytes with pendant propyl trifluoroacetate side groups; Investigation of sol-gel reaction of this polymers for obtaining of new solid polymer electrolyte membranes on the base of Lithium trifluoromethylsulfonate (triflat) and Lithium bis(trifluoromethanesulfonyl)imide and study their electro physical properties.

The hydrosilylation reaction of 2.4.6.8-tetrahydro-2.4.6.8-tetramethylcyclotetrasiloxane (D_4^H) with allyl trifluoroacetate and vinyltriethoxysilane at 1:4.2 and 1:3:1 ratio of initial compounds in the presence of Platinum catalysts, at 60^0C temperature corresponding new D_4^R and $D_4^{R,R'}$ type adduct have been obtained.

Via ring opening copolymerization reaction of D_4^R and $D_4^{R,R'}$ in solution, in the presence of anhydrous powder-like potassium hydroxide and tetramethyl ammonium fluoride, at various temperatures range 60-80^0C, new comb-type methylsiloxane polymers with pendant allyl trifluoroacetate side groups have been obtained.

Synthesized comb-type polymers were analyzed by FTIR, ^{1}H, ^{13}C, and ^{29}Si NMR spectroscopy, DSC and GPC methods.

Sol-gel reactions of polymers doped with Lithium trifluoromethylsulfonate (triflat) and Lithium bis(trifluoromethanesulfonyl)imide have been studied and solid polymer electrolyte membranes have been obtained. The ion-conductivity of the membranes was determined via electrical impedance spectroscopy.

Acknowledgments:

The financial support of the Georgian National Science Foundation and Science and Technology Centre in Ukraine STCU-2016-16 (6301), is gratefully acknowledged.

Pseudo-Proteins – A New Family of Biodegradable Polymers

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Proteins are one of the most appropriate biomaterials for a variety of biomedical applications including resorbable surgical and pharmaceutical devices owing to their innate affinity to tissues, enzymatic biodegradability with releasing a-amino acids (a-AAs) which could be assimilated by the organism promoting in that way tissue regeneration. However, the proteins have some serious shortcomings among which one of the most important is immunogenicity that is attributed to their molecular architecture. We have developed a new generation of a-AA based biodegradable (AABB) polymers having non-proteinaceous macromolecular architecture less recognizable by the immune system of the living organism. The key monomers to build up the macromolecules of the new architecture are diamine-diester monomers made of a-AAs and diols. Several classes of AABB polymers – poly(ester amide)s (PEA), poly(ester urea)s (PEU) and poly(ester urethane)s (PEUR), both regular and functional ones, having the widest range of material properties have been designed. The AABB polymers, similar to proteins, show a high tissue affinity/compatibility and release a-AAs upon the biodegradation, therefore they can be considered as pseudo-proteins suitable for numerous biomedical applications in regenerative medicine, pharmacy, etc. [1-4].

References:

1. R. Katsarava, Z. Gomurashvili. Biodegradable Polymers Composed of Naturally Occurring a-Amino Acids. Handbook of Biodegradable Polymers - Isolation, Synthesis, Characterization and Applications, Lendlein, A. and Sisson, A., Eds., Wiley-VCH, Verlag GmbH & Co. KGaA, 2011, pp 107-131.
2. R. Katsarava, N. Kulikova, J. Puiggalí. Amino Acid Based Biodegradable Polymers – promising materials for the applications in regenerative medicine (Review). J. J. Regener. Med., 1, 2016, 012.
3. N. Zavradashvili, G. Jokhadze, M. Gverdtsiteli, D. Tugushi, R. Katsarava. Biodegradable functional polymers composed of naturally occurring amino acids (Review)., Res. Rev. Polym., 8, 2017, 105-128.
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Plenary Session 1

SESSION CHAIR – Dr. Nino Kokiashvili

Dr. Peter van der Geer – Signal Transduction by Receptor Protein-Tyrosine Kinases

Dr. Ramaz Gakhokidze – Way to Reduce Global Warming with Bioenergy Activators

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Ana Shalamberidze - Introduction to ACS Georgia Student Chapter

SMART | Atmosim_Lab: Air Contamination Research at Tbilisi State University

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SMART | AtmoSim_LAB was opened in the framework of Georgian German Science Bridge (GGSB) by collaboration between Chair of Physical and Analytical Chemistry and Institute of Energy and Climate-Troposphere (IEK-8, Forschungszentrum Jülich) and with support of Tbilisi City Hall and National Environmental Agency. SMART | AtmoSim_LAB was opened on September 29, 2017 at TSU Building 2, room 353.

Laboratory received research instruments to measure major contaminants in air such as nitrogen monoxide, nitrogen dioxide, carbon monoxide, carbon dioxide, methane, particulate matter.

SMART | AtmoSim_LAB received funding from Tbilisi City Hall to investigate air quality in Tbilisi and develop novel methods for air quality monitoring. Laboratory has Georgian and German scientific advisors, academician full professor Bezhan Chankvetadze (TSU) and professor Ramaz Botchorishvili (TSU) are Georgian advisors, Dr. Franz Rohrer, Professor Astrid Kiendler Scharr, Professor Andreas Wahner, Dr. Robert Wegener (IEK-8, Forschungszentrum Jülich) are advisors from German side.

Along with routine analysis and evaluation of contaminants, scientific studies are conducted to develop contamination model and forecast methods, as well as new methods and platforms of analysis. Bachelor, master and doctorate students of TSU are participating in research activities, performing various analysis on contaminants in atmosphere and developing mathematical model of contamination.

In the following presentation, detailed overview of traditional and novel research methods will be presented as well as overview of current and future research plans.

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Signal Transduction by Receptor Protein-Tyrosine Kinases

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Growth and differentiation factors are small proteins that mediate communication between cells and that regulate cell division, differentiation, and survival. These extracellular messengers act by binding to receptor protein-tyrosine kinases. Protein kinases are enzymes that transfer the □-phosphoryl group of ATP to the side chain of the amino acid tyrosine present in proteins. Upon ligand binding receptor protein-tyrosine kinases first autophosphorylate on one or more tyrosine residues present in the activation loop of the kinase domain. This results in

stabilization of the active conformation of the kinase. Subsequently, the receptor autophosphorylates on tyrosine residues that are present outside the kinase domain. These tyrosine residues act as binding sites for proteins that contain phosphotyrosine-binding domains. These proteins are activated or inactivated as a consequence of their interaction with the receptor. In my presentation I will highlight several types of experiments that have been used to further our understanding of receptor-protein-tyrosine kinase signaling.

Way to Reduce Global Warming with Bioenergy Activators

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Global warming or global climate change – the biggest and most serious problem we are facing in this century – is the phenomenon due to which global temperatures are increasing. During the last century the temperature of the Earth increased by one degree. Global warming effects everyone living on the Earth, as it is happening right now all around us. Global warming effect can cause serious damage to cities and towns, as extreme weather is becoming more and more a problem because of strong hurricanes and tornadoes, droughts and floodings occur. The increase in temperature caused the melting of ice and, accordingly, the rise of the level of the world ocean. Together with global warming, the risk of destruction of living organisms sharply increases. Global warming consequences, including the loss of life, economic disruption and population dislocation are growing each year. We can no longer afford to ignore global warming. It is a serious problem that needs to be stopped. One of the reasons for climate changes is the growth of the amount of carbon dioxide causing the so-called greenhouse effect.

Many methods and concepts of dealing with preventing car- bon dioxide from entering the atmosphere have been proposed. The projects for saving the world from global warming are being actively carried out all over the world. According to one of the mentioned projects, the disposition of millions of 60cm diameter lenses around the Earth will cause the reflection of sun rays and, accordingly, the decrease of sun radiation. Pursuant to another project, across the Earth the layer of cosmic vessels or small particles should be created, which should cover the tropics, and this will result in climate softening. But for the realization of this project colossal sums of money are required: 500 billion dollars are needed for the disposition of cosmic spaceships and in the case of small particles from 6 to 200 trillion dollars are required.

Concentartion of carbon dioxide in the atmosphere is naturally regulated by numerous processes. The movement of carbon between the atmosphere and the land is dominated by natural processes such as plant photosynthesis. While these natural processes can absorb some of the net 6,1 billion metric tons of anthropogenic carbon dioxide emission produced each year, an estimated 3,2 billion metric tons is added to the atmosphere annually. The Earth's positive imbalance between emission and absorption results in the accumulation of carbon dioxide in the atmosphere.

Due to the increase of the chlorophyll level and intensification of photosynthetic activity, one of the most effective results of bioenergyactivators use is the acceleration of growth and development of plants (e.g. of wood plant by 4-5 years) and growth of the total size of leaf surface by 482%, whereas, according to the literature data, that parameter is only 15-17%. (see Pic. and Table, p. 89) With the use of bioenergyactivators on 1 million hectares, up to 30 million tons of carbon dioxide will be removed from the atmosphere by

green plants each year. According to the literature data, in the same area the evasion of only 1 million ton of carbon dioxide is possible.

Synthesis of Novel Chiral Sulfoxides and Study of Their Enantioseparation Using HPLC

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Enantiomeric separation of chiral compounds is extremely important because most of the bioorganic molecules, synthetic drugs and agrochemicals are chiral compounds. Enantiomers in racemic drug compounds are characterized with different biological activities, including pharmacodynamics, pharmacokinetics and toxicology. That is why, enantiomerically pure drug forms are safer and more efficient (1-4).

The main goal of the present study was to determine relationships between chemical structure of chiral compound and enantioselectivity in high-performance liquid chromatography. In order to understand the relationships between chemical structure and enantioselectivity, about 50 new chiral sulfoxides were synthezised and their chiral separations were performed with polar organic and normal-phase mobile phases using variety of cellulose based chiral selectors.

The main factors contributing in molecular recognition of macromolecules were revealed. Distribution of electron density and geometry of analyte molecules seem to be the major factors affecting enantioselectivity and molecular recognition ability of chiral molecules.

Acknowledgements:

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Introduction to ACS Georgia Student Chapter

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ACS Georgia student chapter was officially registered as one of the international student chapters of American Chemical Society in December 2015 and since then, the chapter members have demonstrated the enthusiasm and willingness to contribute to the scientific development of Georgia among their peers and new generations. The goals of this Chapter are to afford an opportunity for students of a chemical science to become better acquainted, to secure the intellectual stimulation that arises from professional association, to obtain experience in preparing and presenting technical material before chemical audiences, to foster a professional spirit among the members, to instill a professional pride in the chemical sciences, and to foster an awareness of the responsibilities and challenges of the modern chemist. The activities through which these goals are achieved include but are not limited to planning the field trips to the scientific institutes, having professional speakers deliver lectures to students and providing information about their ongoing research or upcoming conferences for students to participate in, STEM academies, school outreach and lab tours for younger generations, Chemistry festival promoting science from an early age, helping our students attend and present at international conferences, including ACS National meetings or organize one themselves.

Plenary Session 2

SESSION CHAIR – Dr. Giorgi Jibuti

Givi Kalandia – West Georgian Chromatography Center and Determination of Stilbenes in Several Georgian Wines

Elguja Gojiashvili - Making Ligands for the General Catalyst Control of the Monoisomerization of 1-Alkenes to cis-2-Alkenes

Elene Aslanikashvili – Using Differential Scanning Calorimetry to Study the Thermal Properties of Polymers

Ana Kutchuashvili – Analysis of Sulfoxides Using High Performance Liquid Chromatography

Sandro Gogia, Mariam Khvichia – Characterization of Hardness in Pencil Leads and Analyzation of Cosmetic Products using Differential Scanning Calorimetry

West Georgian Chromatography Center and Determination of Stilbenes in Several Georgian Wines

Givi Kalandia[1] , Aleko Kalandia[2] , Maia Vanidze[2]

San Diego State University Georgia[1]

Batumi Shota Rustaveli State University [2]

West Georgia Chromatography Center is part of Batumi Shota Rustaveli State University. In chromatography center the unique and vast biodiversity of western Georgia and the bioresources of black sea are researched for their preservation and rational utilization. This is achieved by identification of bioactive compounds and their structure. The analysis involves determination of alkaloids, phenolic compounds, flavons, anthocyanins, vitamins, organic acids, carbohydrates, pesticides, minerals and other qualitative/quantative analysis. Center is equipped with financing of Shota Rustaveli National Science Foundation of Georgia. Some of the equipment are Acquity UPLC with Single Quadrupole Mass Specrometer and PDA Detector, Waters HPLC system with UV/Vis Detector, Waters HPLC system and Refractive Index Detector, Waters HPLC system with conductivity detector, GC Thermo TRACE 1310, supercritical pressure fluid extraction apparatus SFE 100, also several UV/Vis spectrophotometers, pH-meters, conductometers, and refractometers. One of the projects that I personally took part in was determination of Stilbenes in several Georgian wines. Stilbenes are non-flavonoid phenolic compounds. They protect plants from many diseases and ultraviolet radiation (Alonso-Villaverde et.al, 2011). The recent interest in them is explained by the fact that they are a powerful antioxidant with great activity. Against the backdrop of modern environmental problems, it is important that the human diet includes products with antioxidant properties. Such products are grapes and wine, which contain various types of phenolic compounds. The biological activity of phenolic compounds of the class of stilbenes, as physiologically active compounds, are tested in different directions. After wine making process, the residues are often used to produce dietary supplements (Anastasiadi et.al, 2010). Determination of Stilbenes is conducted by HPLC UV, MS, and PDA (Careri et.al, 2003).

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Making Ligands for the General Catalyst Control of the Monoisomerization of 1-Alkenes to *cis*-2-Alkenes

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Alkenes are fundamental chemical feedstocks and are used on massive industrial scales. Alkene isomerization is simple, and it may seem that all the synthetic problems in this area should have been solved by now. However, there is one problem still yet to be solved. It is the case to control both regio- and stereochemistry, particularly in the case of converting a 1-alkene to *trans*-2-alkene or *cis*-2-alkene. (E)-alkenes are basically more stable than (Z)-alkenes. Many desirable synthesis targets feature (Z)-alkenes, so do many natural feedstocks, thus alkene isomerization catalysts capable of making or processing (Z)-alkenes are of high interest. Our group's goal is to make (Z)-selective catalyst.

The team I am working with now, made (E)-selective catalyst, that has been cited as "being one of the best in terms of catalyst loading, reaction yields, and E-stereoselectivity."[3] In 2014 same team made adjusted catalyst that allowed unprecedented catalyst control of both positional and geometric selectivity in making E-alkenes.[5-6] Understanding the origin of selectivity in the CpRu(PN) family of catalysts through computations and new experimental data, is crucial to guide a rational design of (Z)-selective catalyst candidates.

For the last years, the group has been working to modify the CpRu(PN) platform to promote (Z)-alkene formation. From the computational calculations, placing the pendant base on the Cp ring showed promising results. The research I was involved included analyzing and proposing the correct reaction sequences to synthesize Cp rings with pendant bases. We also calculated number of Cp ring derivatives and using quinoline as a pendant base, decreased the relative energies of Z species, suggesting that the energy barriers for making Z-alkenes could be less than making E-alkene. Reaction syntheses of Cp rings with quinoline are proposed.

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Using Differential Scanning Calorimetry to Study the Thermal Properties of Semicrystalline Polymers

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Semicrystalline polymers are very versatile molecules with a wide spectrum of properties and an also wide range of applications. Because of their versatility, it is very important to evaluate

the newly synthesized polymers' characteristics and study how they react to temperature change or exposure to various chemicals. The aim of this research is to use differential scanning calorimetry in order to study the thermal properties of six newly synthesized polymers, 1L6/8L6 (70/30), 1L6/8L6 (50/50), 1L6/8L6 (40/60), 8F6, 8L6, 8L6/8F6(85/15), prior and after recrystallisation with two different solvents, ethanol and dichloromethane. Using DSC, the polymers were heated to 250°C, cooled to -40°C and then heated again to 250°C, which gave a clear picture of how their thermal properties are changed by high/low temperatures or solvents. The DSC curves showed that 40/60 1L6/8L6 polymer was more thermally stable as its glass transition temperature stayed relatively consistent after the first heating and the change in the specific heat capacity was lower on the heating and cooling stages. As for the solvents, the results indicate that ethanol is a better solvent for both polymers if one is looking to preserve/improve the polymers' thermal properties.

Analysis of Sulfoxides Using High Performance Liquid Chromatography

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High performance liquid chromatography is an effective analytical method for separation, quantification and qualification of substances. Stationary phase is the most important part of HPLC which is characterized with high selectivity. HPLC can also be used to separate enantiomers of chiral substances.

The objective of this particular study was to analyze five sulfoxides on different HPLC columns and obtain valuable data due to specificity of enantiomer separation. Analytes were selected to be 2-(benzylsulfinyl)-benzamide, 2-(benzylsulfinyl)-N,N-dimethylbenzamide, 2-(3-bromobenzylsulfinyl)-benzamide, 2-(2-methylbenzylsulfinyl)-benzamide, and 2-(3-methylsulfinyl)-benzamide. Cellulose and amylose derivatives were used as chiral selectors with methanol as a mobile phase. Analysis was performed on Cellulose-4, cellulose-3, cellulose tris(3,5-dimethylphenylcarbamate), amylose-1 and amylose-2 columns.

The research revealed several important details; first, that cellulose-4 is a very useful column to separate enantiomers used during analysis; second, that amylose and cellulose columns release enantiomers with opposite orders. Last, that cellulose-3 with methanol eluent is an ineffective method to qualify given samples.

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Characterization of Hardness in Pencil Leads and Analyzation of Cosmetic Products using Differential Scanning Calorimetry

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Differential scanning calorimetry is a powerful thermo-analytical method that can be used to determine the hardness in pencil leads and analyze the composition of various cosmetic products. The binding agents present in pencil leads, are oil like compounds prone to melting at relative temperatures, and different grade of pencils contain different number of binding agents.

In the present work we investigated the relationship between pencil lead hardness and the amount of binding oils in two graphite pencils 6B and H. Also, we investigated effects of colored pigments of pencil lead structure and effects of different additives in cosmetics.

The data indicates, that lower grade pencils tend to show lower melting peaks, because of the high content of binding agent present, and higher-grade pencil vice-versa. The pigment present in colored pencil increases their melting peaks, by reacting with the binding agent. Low melting organic compounds present in cosmetic compounds, alter the thermal properties of wax, making it more or less spreadable and more or less thermal resistant.

The results illustrate how minor additives, binders and pigments contribute to the whole structure of the sample and alter their thermal properties.

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Plenary Session 3

Dr. Nikoloz Nioradze – Nanogap Scanning Electrochemical Microscopy

Dr. Khatuna Barbakadze – High-performance Fluorinated Hybrid Materials

Ann Gogolashvili – Chiral Separation in Capillary Electrophoresis with Cyclodextrin-Type Chiral Selectors and Investigation of Structure of Selector- Selectand Complexes by using Nuclear Magnetic Resonance Spectroscopy

Ketevan Kharaishvili – Optimization of Average Sampling

Elene Gvazava – Evaluation of the Air Pollution and Comparison of Pollutants' Concentrations in Heavy and Light Traffic Hours

Salome Pantsulaia – Overview of the Current Experiments on Air Pollution Control in Tbilisi

Ani Rukhadze, Sandro Mestvirishvili – Effect of Extraction Methods on Yield, Structural and Thermal Properties of Pectin Samples

Nino Mamasakhlisi – Synthesis and Some Transformations of Adamantane-1-Carboxylic Acid Derivatives

Nino Nikolaishvili, Nika Asatiani – DSC Characterization of Inulin/coenzyme Q10 Sample and its Potential Application in Drug Delivery Systems

Nanogap Scanning Electrochemical Microscopy

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Scanning electrochemical microscopy (SECM)1 is a powerful electroanalytical tool to investigate electron transfer (ET) reactions at heterogeneous interfaces. Herein we demonstrate application of SECM for quantitative electrochemical characterization of graphene grown by chemical vapor deposition (CVD)2, for measurement of permeability of nuclear envelop of nuclear pore complex3 and for study the electrocatalytic activity of individual platinum nanoparticles4.

We found that heterogeneous electron transfer can be remarkably fast at CVD-grown graphene electrodes that are fabricated without using the conventional poly(methyl methacrylate) (PMMA) for graphene transfer from a growth substrate. We used nanogap voltammetry-based scanning electrochemical microscopy to obtain very high standard rate constants k0=25cm/s for ferrocenemethanol oxidation at polystyrene-supported graphene.

We report on a dynamic and spatially resolved mechanism for NPC-mediated molecular transport through nanoscale central and peripheral routes with distinct permeabilities. Specifically, we developed a nanogap-based approach of SECM to precisely measure the extremely high permeability of the nuclear envelope to a small probe molecule, (ferrocenylmethyl) trimethylammonium. Effective medium theories indicate that the passive permeability of 5.9 × 10−2 cm/s corresponds to the free diffusion of the probe molecule through ~22 nanopores with a radius of 24 nm and a length of 35 nm.

Platinum nanoparticles with a few tens to a hundred nm radius were directly electrodeposited on a highly oriented pyrolytic graphite (HOPG) surface via nucleation and growth without the necessity of capping agents or anchoring molecules. A well-defined nanometer-sized tip comparable to the dimensions of the Pt NPs and a stable nanogap between the tip and NPs enabled us to achieve lateral and vertical spatial resolutions at a nanometer-scale and study fast electron-transfer kinetics.

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High-Performance Fluorinated Hybrid Materials

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The successful development of inorganic-organic hybrid materials is linked to the versatility of their processing and to the cost and availability of both precursor species and processing devices. Hybrid materials have brought significant advantages in the coatings performance providing improved corrosion and abrasion resistance, adhesion, mechanical, surface, optical and physico-chemical properties, also enhanced stability towards alkaline medium. Considering the benefits of hybrid coatings, the range of different structures and compositions applied in such coatings continuously increases.

The use of coatings as a method of protection against microbiologically-influenced corrosion is focused on the application of non-toxic products based on: polymer matrix (silicones, polyurethanes, epoxy resins, fluorinated compounds etc.); modifiers of polymer networks; bioactive additives (inorganic, organic and organometallic compounds, bio-molecules, clusters, etc.); curing agents.

Fluorinated hybrid antimicrobial coatings based on functionalized perfluoroalkylmethacrylates, selected bioactive additives and curing agents have been obtained and studied. DSC results allowed identifying glass transition temperatures for the different compositions. Small changes on the mass losses at high temperatures have been investigated by analyzing TGA results. The thermal studies show the possibility of their application at high temperatures. All results from thermal studies have shown a high influence of the modifiers and bioactive additives on the thermal stability of the basic polymer matrices under investigation. The enhanced mechanical strength of obtained hybrid composites is useful for abrasion resistant and protection function necessary for protective and antibiocorrosive coatings. Thus, based on targeted modification the photochemically and mechanically stable, hydrophobic antimicrobial hybrid materials have been elaborated with improved thermal stability, adhesion, and tribological characteristics (wear, scratch resistance, viscosity, dynamic friction) targeted as short-term and long-term active protective coatings.

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Chiral Separation in Capillary Electrophoresis with Cyclodextrin-Type Chiral Selectors and Investigation of Structure of Selector-Selectant Complexes by Using Nuclear Magnetic Resonance Spectroscopy

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Many compounds of biological and pharmacological interest are chiral. The living body with its numerous homochiral compounds being amazingly chiral selector, will interact with enantiomers of chiral drugs commonly differently and metabolize each enantiomer in different extent or by a separate pathway and exabite different pharmacological activity[1]. Thus, one isomer may produce the desired therapeutic activity, while the other one may be inactive or produce undesired or toxic effects. The administration of enantiomerically pure drugs is very important. Thanks to a wide range of modern technologies US Food and Drug Administration (FDA) currently recommends the assessments of activity of each enantiomer of chiral drugs in body and promotes the development of new drugs in enantiomerically pure form.

Capillary electrophoresis is one of the powerful methods for separation of enantiomers, . The major advantage of CE is its own unique mechanism for separation of enantiomers. In addition, CE is highly efficient, very flexible, cost-effective, environmentally friendly miniaturized technique.

Various experimental and theoretical tools can be harnessed for understanding of the nature of those intermolecular forces which are involved in noncovalent selector-select and binding and enantioselective recognition. However, none of these methods alone is able to provide a conclusive (more or less realistic) vision on chiral recognition that would enable to predict the best chiral selector or analyte from the viewpoint of recognition power. Some separation and non-separation methods fit to and extend each other perfectly for chiral analysis. For instance, separations of enantiomers in CE are performed in homogenous solution in a single phase. These conditions can be perfectly mimicked in NMR spectroscopic experiments. Thus, the information gained on stereoselective intermolecular interactions with these two techniques is very complementary and thus, this tandem represents very powerful tool for better understanding of enantioselective recognition mechanisms on the molecular level.

Acknowledgments: Shota Rustaveli National Science Foundation

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Optimization of Average Sampling

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Air pollution occurs when contaminating agents are released into the atmosphere. There are two main types of air pollution, natural and anthropogenic. Some of the pollution come from daily human activities-anthropogenic pollution and natural occurrences-biogenic pollution.

We conducted measurements for nitrous oxides, carbon monoxide and carbon dioxide and methane.

Atmospheric measurements take place online, continuously. We use NOx chemiluminescence instrument ECO PHYSICS CLD 780 TR for measurements of nitrogen oxides and Picarro cavity ringdown spectroscope which we use for measurements of carbon monoxide and carbon dioxide, methane and water concentrations. UV absorption spectroscope Ansyco O3 41 M for ozone measurement.

Together with the online sampling we also perform offline sampling. In this case sampling time was about twenty seconds, but it was not representative of the average samples. In order to increase sampling time, we use different restrictors with various length, but disadvantage of sampling with restrictor was, that filling rate decreases overtime, so when container is full, it contains more air from initial stage, that later stage. To correct for fill rate, plotted container pressure over time.

The pressure gradient depends on the diameter of the restrictor and its length. To verify sampling technique, perform sampling in the laboratory room because the composition of the atmosphere does not change significantly over time. During the sampling using restrictor, we also collected samples without the restrictor: at the start of sampling; t1/2 minutes (half of sampling time) and end of sampling. We use 2 parallel sampling containers at the same time in order to measure the inaccuracy between the measurements.

Similarly, we plan to repeat the analyzes outside the laboratory where the composition of the atmosphere is variable.

Evaluation of the Air Pollution and Comparison of Pollutants' Concentrations in Heavy and Light Traffic Hours

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Bezhan Chankvetadze, Ramaz Botchorisvili, Giorgi Jibuti

Tbilisi State University

Atmospheric studies are important subject in many scientific fields. Study of anthropogenic pollutants is one of the most important subjects. Those pollutants have direct effect on human health and life quality. Measurement of atmospheric composition presents many challenges due to its complex nature, therefore measurement techniques are also complex and diverse.

For exact measurements, it is known, that sampling procedure needs to be correct. Some important variables affecting the sampling manifold design are the diameter, length, flow rate, pressure drop, and materials of construction. Thus, we have studied fill rate dependence on time and the linearity of the graph during sampling using various size restrictors. Time had been chosen from the linear part of the graph for farther analysis.

During our experiment, we have been observing the level of air pollutants on Chavchavadze Ave. (Tbilisi, Georgia) and, also, two points vertical to the road have been chosen. Thus, diffusion of pollutants has been studied during heavy and light traffic hours. Furthermore, different types of cars passing through the road have been counted during sampling and dependence of it on air quality and diffusion of the pollutants has been considered into our evaluation.

This study demonstrates an approach to characterize risks of traffic for on- and near-road populations. In our country, emissions of air pollutants are increasing. Results from near-road monitoring studies show, that air pollutant concentration gradients are quite high. Also, difference in methodology of taking the mean sample has been influenced on accuracy of experiment.

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Overview of the Current Experiments on Air Pollution Control in Tbilisi

Salome Pantsulaia, Elene Gvazava, N. Khundadze, T. Khatiashvili, L. Giunashvili,
N. Kobakhidze, Ketevan Kharaishvili, G. Sheklashvili,
Bezhan Chankvetadze, Ramaz Botchorishvili, Giorgi Jibuti
Tbilisi State University, SMART | AtmoSim_LAB

Air quality in cities is the result of a complex interaction between natural and anthropogenic environmental conditions. Air pollution in cities is a serious environmental problem – especially in the developing countries. The air pollution path of the urban atmosphere consists of emission and transmission of air pollutants resulting in the ambient air pollution. Each part of the path is influenced by different factors. Emission of air pollutants is caused by different anthropogenic processes which can be categorized into the source groups motor traffic, industry, power plants, trade, and domestic fuel. Emissions from motor traffic are very important source group throughout the world.

This study demonstrates an approach to characterize risks of traffic for on- and near-road populations. In our country, emissions of air pollutants are increasing. Especially, this trend is pronounced for nitrogen oxides (NOx). This study suggests that health risks from congestion are potentially significant, and that additional traffic can significantly increase these risks, depending on the type of road and other factors.

During our experiment, we have been observing the level of air pollutants on Pekini Street. 10 locations have been chosen, from which, 5 points are major, and others are variable. Results from near-road monitoring studies show, that air pollutant concentration gradients are quite high. Even though Carbon monoxide is near the permissible norm, according to our experiment NOx concentrations are worthy of attention for all researched locations for almost every day.

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Effect of Extraction Methods on Yield, Structural and Thermal Properties of Pectin Samples

Ani Rukhadze[1], Sandro Mestvirishvili[1], Nino Kokiashvili[1,2]

San Diego State University Georgia[1], Tbilisi State University[2]

Pectin is a natural polysaccharide, present in plant cell walls and mainly used in food industry as a gelling and stabilizing agent [1]. Pectin's ability to bind to heavy metals is remarkable since unlike other chelators, it does not show any side effects on human health and can be used as a medication during heavy metal intoxication [2].

The aim of the present study was to investigate the influence of extraction methods on the yield and thermal properties of the pectin samples. We were using simple steps for extraction of pectin from lemon peels. Acid hydrolysis (pH=2-3, temperature 70-80°C) and extraction was done on lemon peels, from which one type of sample was fresh peeled and other two were previously dried at different temperatures, 40°C and 60°C. The most convenient and high yielding way of retrieving pectin was found in the sample of lemon peels dried at 40°C. The least yielding were citrus peels dried at 60°C. The structure of pectin samples was studied by FTIR and "fingerprint" region with other characteristic peaks confirmed the presence of substance [3]. Thermal and structural degradation properties of pectin samples were investigated by using DSC analysis at the temperature range 25°C - 300°C. All samples showed different thermal behavior and state transitions.

The research in combination with other methods will encourage citrus factories to use their waste citrus peels as a raw material for pectin extraction with high yielding method and provide a relatively quick and reproducible characterization of structural changes, occurring during preparation of pectin samples.

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Synthesis and Some Transformations of Adamantane-1-Carboxylic Acid Derivatives

Nino Mamasakhlisi[1], Tinatin Bukia[2]

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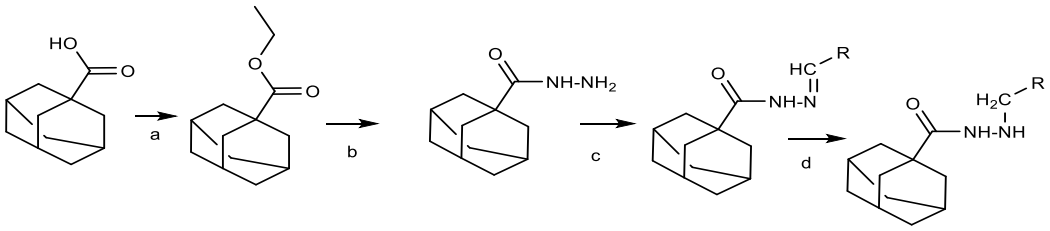
Adamantyl containing compounds have attracted many chemists' attention due to drastic influence on biological processes. They have shown antiviral, antibacterial, antifungal, anti-inflammatory and central nervous and 11b-HSD1inhibitory activities. The lipophilicity of Adamantane changes ADME properties of molecule, binds a hydrophobic site in enzyme and acts as an inhibitor so, they are widely used in drug industry.

These newly synthesized products contain not only Adamantane trace, but also C-N double bond called imine or Schiff base. Schiff bases are active against a wide range of organisms since they play an important role in living organisms, such as decarboxylation, transamination and C-C bond cleavage.

The aim of this research was to synthesize Adamantyl containing drug-like molecules which might have biological activity. Converting Adamantane carboxylic acid to ethyl Adamantane carboxylate was done by solving Adamantane carboxylic acid in absolute ethanol and adding thionyl chloride to the mixture dropwise in stirring condition during 3-4 hours. Secondly, by dropwise adding of hydrazine hydrate pure ester was converted to carbohydrazide. After completion of reaction and washing procedures, white sticky product was left.

The reaction of carbohydrazide and following aromatic aldehydes in ethanol, produced corresponding Schiff bases. All reaction mixtures were washed using hexane through the Schott's funnel. The range of yields of the reactions were between 75-85%. The final step of synthesis was to reduce C-N double bond by reducing agent Sodium borohydride. Two Schiff bases out of three were reduced and collected.



R= -C6H4OH, -C6H5, - C6H4NO3, - C6H4NO2, -C3H7;

The structures were confirmed by IR and 1H NMR spectroscopy.

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DSC Characterization of Inulin/Coenzyme Q10 Sample and its Potential Application in Drug Delivery Systems

Nino Nikolaishvili[1,2], Nika Asatiani[1,2] Nino Kokiashvili[1,2]

San Diego State University Georgia[1], Tbilisi State University[2]

Thermal properties of inulin, Coenzyme Q10, and inulin/Coenzyme Q10 mixture has been studied by differential scanning calorimetry. Inulin and Coenzyme Q10 are often used together where Coenzyme Q10 acts as medium for Inulin and enables its better efficiency. Coenzyme Q10 is supplement which provides energy to cells and is essential for proper function of many organs including heart. Coenzyme Q10 is used to treat diseases, such as high cholesterol, high blood pressure, Alzheimer's disease and dementia, heart failure. Furthermore, new beneficial properties of Inulin are still being discovered, such as drug delivery vehicle, vaccine adjuvant, and immune-stimulator.

The aim of this study was to better understand the thermodynamic interaction between CoQ10 and Inulin. The investigation of the energetic influence of CoQ10 on the Inulin revealed that the addition of CoQ10 causes a significant decrease in the enthalpy and an occurrence of two additional endothermic peaks between 54.4°C and 61.5°C and 142.0°C and 152.2°C respectively. This indicated that the CoQ10 does not considerably perturb the enthalpic stability of the polymer, but instead moderately stabilizes Inulin sample by distributing endothermic peaks over a wide range of temperatures. Furthermore, the impact of CoQ10 on the overall glass transition temperature was considerably small - about 7°C. The second glass transition temperature in the Inulin/CoQ10 was expected because the sample contained copolymer and/or homopolymer.

The study shows that from a thermodynamical point of view there is no disadvantage in using inulin/Coenzyme Q10 mixture in drug delivery applications.

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Plenary Session 4

Ana Chakhrakia – Synthesis and Application of Amino-1-Adamantane Containing Dipeptides via Multicomponent Reaction

Tamar Kerdikoshvili – Synthesis of Some Schiff Bases and Dipeptides from N-(1-Adamantyl-Carbonyl)o-Phenylenediamine

Nino Gavashelishvili – Thermal properties of Green and Roasted Coffee

Sergi Betkhoshvili – Synthesis of Suprofen S-oxide from Suprofen Using mCPBA and Comparison to the Clopidogrel Oxidation Results Regarding the Substituent Effects

Natia Inadze – Oxidation of Thiophene Group in Tioconazole to Tioconazole S-oxide Using mCPBA

Nika Kutalia, Khatia Merabishvili – Investigation of Thermal Stability of B-Group Vitamins

Synthesis and Application of Amino-1-Adamantane Containing Dipeptides via Multicomponent Reaction

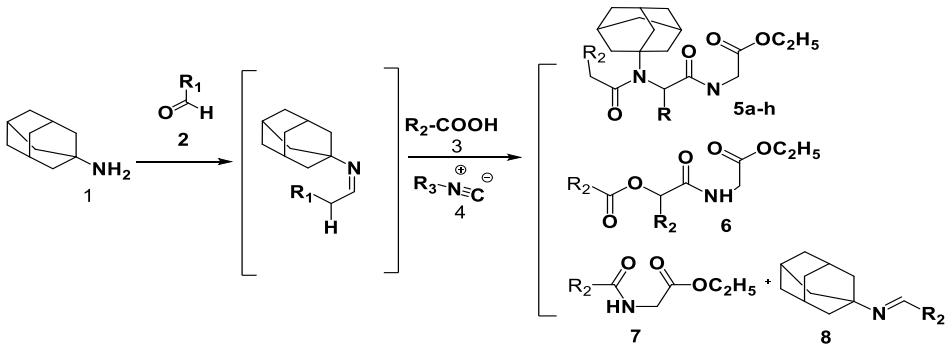
Ani Chakhrakia[1], Tinatin Bukia[2], Shota Samsoniya[2]
San Diego State University Georgia[1], Tbilisi State University[2]

Isocyanide-based Multicomponent Reactions (IMCR) like Ugi Reaction, are the most interesting in order to synthesis biologically active peptides and amides[1]. Ugi reaction involves condensation of four components: An aldehyde, an amine, an isocyanide and an acid are condensed and quickly produce the main product. This 4-component reaction is productive in order to obtain the pseudo peptides, peptides and peptoids.

Adamantine is a widely used compound in synthesis and applications of new drug delivery systems and other numerous transformations [2].

The aim of our research work was to synthesize amino-1-adamantine containing dipeptides via Ugi-4-component reaction. Amino-1-adamantane (1), aldehydes (2), acids (3) and ethylisocya-noacetate (4) were chosen as starting materials of the IMCR (table 1). The reactions were conducted in the ethanol area at 35°C temperature and the mixture were stirred for 32h. Afterwards CH_2Cl_2 was added then quaked with saturated $NaHCO_3$ and 1M $KHSO_4$. The organic phase was concentrated and purified on the column. Dipeptides **5a-h**, Passerini product **6**, amides **7** and shiff bases **8** was obtained according to the scheme **1**.

Scheme 1.



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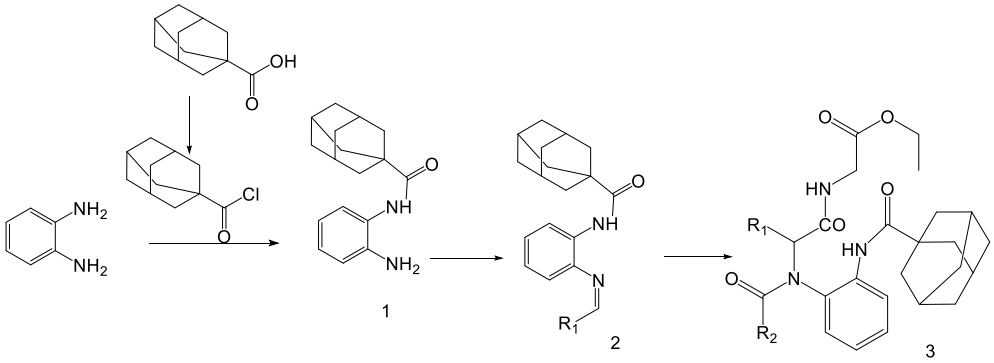
Synthesis of Some Schiff Bases and Dipeptides from N-(1-Adamantyl carbonyl)o-Phenylenediamine

Tamar Kerdikoshvili[1], Ana Goletiani[2], Tinatin Bukia[3]

San Diego State University Georgia[1], Georgian Technical University[2], Tbilisi State University[3]

The remarkable structural and chemical properties of adamantane afford attractive opportunities to design various adamantane-based scaffolds for biomedical applications. Adamantane itself has a great lipophilic property which is greatly beneficial as it enables to its derivatives to hit specific target segments of cells. First of all, this property ensures that the adamantane derived drugs penetrate or bind the lipid bilayer quite well, in some cases incorporating selective binding to certain receptors and ion channels. Also, the lipophilic nature of adamantane prevents the metabolic cleavage of other functional groups which increases the drug's overall activity, making it more effective and long lasting. Moreover, adamantane derivatives are also known for its biocompatibility, meaning they are not toxic. The human liver has the ability to digest these compounds, hence, the chances of drug accumulation in the living organism through the time should be minimal. Considering the activity of N-(1-adamantyl) carboxamides [1 & 2], we aimed to synthesize new derivatives of N-(1-adamantylcarbonyl)-o-phenylenediamine according to the Scheme 1.

Scheme 1



N-(1-adamantyl)carbonyl-o-phenylenediamine (1) was obtained by interaction of adamantane-1-carbonylchloride with o-phenylenediamine with the existence of triethylamine in the absolute ether medium. By condensation of aminoamide **1** with salicyl-, butyl, and iso butyl aldehydes for 5-8 hr heating in the alcohol area was formed corresponding Schiff bases, in which interaction with equimolar ratio of benzoic acid and ethyl isocyanoacetate dipeptide like compound **3** was formed. The structures were confirmed by IR and ^{1}H NMR spectroscopy.

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Thermal Properties of Green and Roasted Coffee

Nino Gavashelishvili[12], Ledi Davitinidze[12], Ana Tavartkiladze[12], Nino Kokiashvili[12]

San Diego State University Georgia[1], Tbilisi State University[2]

Coffee is one of the most appreciated beverages around the world, known with its stimulating and antioxidant properties. The chemical compositions and properties of coffee beans are changing during the roasting process. The aim of the present study was to investigate the influence of high-temperature heating on the composition and thermal behavior of coffee beans roasted on the different temperature and green coffee beans along with determining the moisture content in the samples.

Phase transitions of the nine samples from green and roasted coffee beans were characterized using differential scanning calorimetry (DSC). The beans were randomly picked and grinded, the weight of the samples varied from 10 to 11mg. The measurements were carried out on the temperature range 10-300 °C with a linear increase of 5 K/min, under nitrogen atmosphere.

Using the results from nine different coffees, decomposition temperature and enthalpy were determined for each coffee sample.

Results show a comparison of the DSC curve of nine types of coffee samples. The green coffee sample has the highest endothermic peak at 120 °C associated to the evaporation of water and the melting of some constituents of coffee such as amino acids, lipids and sugars. Green coffee experiments a high and fast decomposition after 200 °C until 290 °C.

We determined various stages of thermal degradation within the coffee beans, along with their thermal transitions. The investigation leads to important information regarding the thermal parameters of chemical compositions in coffee beans, such as initial decomposition temperature.

Synthesis of Suprofen S-oxide from Suprofen Using *m*CPBA and Comparison to the Clopidogrel Oxidation Results Regarding the Substituent Effects

Sergi Betkhoshvili[1], Bezhan Chankvetadze[2], Rusudan Kakava[2]

San Diego State University Georgia[1], Tbilisi State University[2]

Thiophene S-oxides are important intermediates for synthesis of variety of organic compounds. One of the most reliable ways to produce bicyclic S-oxides is by Diels Alder reactions where thiophene S-oxides act as dienes[1]. The purpose of this study has been to synthesize Suprofen S-oxide from Suprofen, nonsteroidal anti-inflammatory drug. The target compound Suprofen S-oxide isn't well studied currently and further research on this compound might be useful. The reaction conducted was compared to the oxidation of Clopidogrel which also contains thiophene group. The comparison between rates can give us insight into thiophene group reactivity regarding substituent effects.

To avoid possible further oxidation of sulfoxide to sulfone, relatively mild oxidizing agent 77% mCPBA* was used with 1:1 molar equivalence. Generally, oxidation with mCPBA takes place with mechanism of nucleophilic attack (here, by sulfur) on electrophilic oxygen of peroxyacid. Target compound is oxygen addition product to nucleophile. The reaction was conducted in chloroform as a solvent. The reaction rate was quite slow at 0°C (Ice bath), since even after 3

hours from the mixing the reagents no significant change was observed with thin-layer chromatography using moving phases of two mixtures (1 n-hexane: 1 EtOAc, and 9 CH_2Cl_2 : 1 CH_3OH (by volume)). Then reaction mixture was left on room temperature for the next laboratory session and thin-layer chromatography (4 n-Hexane: 1 EtOAc) showed the change had happened. The conclusion of the experiments is that Suprofen was oxidized to Suprofen S-oxide and relatively slow rate was observed due to aromaticity of sulfur cycle that makes sulfur atom weaker nucleophile than in non-aromatic sulfides or thiols. The similar outcome was expected on Clopidogrel oxidation; However, it was faster than Suprofen and this may imply strong effect of substituents. Analysis of after-reaction mixtures was done with HPLC; however, the results aren't obviously conclusive.

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*mCPBA is abbreviation of *meta*-chloro-peroxybenzoic acid, the IUPAC name of the compound is 3-Chlorobenzene-1-carboperoxoic acid

Oxidation of Thiophene Group in Tioconazole to Tioconazole S-oxide Using mCPBA *

Natia Inadze[1], Bezhan Chankvetadze[2], Rusudan Kakava[2]

San Diego State University Georgia[1], Tbilisi State University[2]

Thiophene S-oxides are considerably important organic compounds, especially in medical chemistry and drug metabolism analysis due to their ability to function as key intermediates for synthesis of corresponding thiophenes in biological metabolic pathways in living organisms.[1]The purpose of this study was to synthesize thiophene S-oxides from tioconazole, a synthetic derivative of imidazole, which inhibits the cell-wall synthesis of fungi. The target compound was thought to have somewhat similar biological activity, including reactions with membrane receptors, transporters and other enzymes.[2]

For thiophene group oxidation in the sample compound, 77% m-CPBA was used as an oxidizing agent. In order to have avoided the synthesis of thiophene dioxides and have ensured non-complete oxidation, molar ratio of 1:1 of tioconazole to m-CPBA was mixed. The reaction was carried out at 0^oC, in an ice-bath. Thin-layer chromatography with two kinds of moving phases (9 CH_2Cl_2:1 CH_3OH and 1 C_6H_{14}:1 AcOEt) was utilized for the purpose of observing reaction progress.

As a result of the investigation, it was found that the thiophene group was oxidized under introduced conditions and tioconazole S-oxide was synthesized.

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* m-CPBA – *meta*-Chloroperoxybenzoic acid, common name for 3-Chlorobenzene-1-carboperoxoic acid

Investigation of Thermal Stability of B-Group Vitamins

Nika Kutalia[1], Khatia Merabishvili[1], Luka Simsive[1], George Pkhakadze[1], Nino Kokiashvili[12]
San Diego State University Georgia[1], Tbilisi State University[2]

Food processing can lead to thermal degradation of vitamins due to exposition to high temperature. In our research the thermal stability of the B-group vitamins: Cyanocobalamin (B12), Pyridoxine hydrochloride (B6) and Nicotinic acid (B3) was investigated using differential scanning calorimeter (DSC) on the temperature range 20 -350C with a linear increase of 5K/min, under nitrogen atmosphere. The changes in molecular structure of the analytes were characterized based on FTIR spectrum.

The results showed that cyanocobalamin is more stable than the nicotinic acid and pyridoxine hydrochloride. The decomposition of cyanocobalamin happens by volatilization at 234°C and by thermal degradation at 295°C, while nicotinic acid melts at 239°C and pyridoxine hydrochloride melts and volatilizes at 213°C.

We have investigated the effect of different chemical enhancers (ethanol, methanol) on the thermal properties of cyanocobalamin. The study indicated that ethanol and methanol decreased the thermal stability of cyanocobalamin at different temperature. The changes of DSC curves were confirmed by FTIR spectrum of the analytes.

Poster Session

Dr. Marina Gakhutishvili – Arsenic (III) Oxide in poly(Vinyl Chloride) PVC

Magda Aptsiauri – Investigation of Thermal Properties of New Semicrystalline Polymers

Nikoloz Kvinikadze – Synthesis of Some New Derivatives of Pyridazino[4,5-b]Indoles

Ana Shalamberidze – Design and Synthesis of New Fluorescent Thymidine Analogues

Davit Khutsishvili – Enantioseparation of Brompheniramine, Chlorpheniramine and Dimethindene Maleate in Capillary Electrophoresis Using Cyclodextrins as Chiral Selectors

Giorgi Meshveldishvili – Synthesis of 5(6)-Nitro-[2-(3-Acetamido-Adamantyl-1)]-1H-Benzimidazole Derivatives

Ana Tavartkiladze – Thermal Properties of Fresh and Roasted Coffee Beans

Nikoloz Shurghaia - Adamantane Containing Benzimidazole Derivatives

Tamar Khatiashvili – Nitrogen Oxides Pollution in Tbilisi

Sofiko Maghlakelidze – Synthesis of Chiral Sulfoxides and Separation of Enantiomers by HPLC Method

Mariam Basilaia – Using Protein Design to Engineer a Scaffold for Regio-Selective C-H Functionalization

Luka Tatarashvili – Ultrasensitive Detection of Cancer Biomarker CEA Using Multi-Photon Non-Linear Laser Wave-Mixing Spectroscopy

Salome Dushashvili – Thermal Stability of Folic Acid and its Deficiency in Humans

Asmat Kontselidze – Study of Toxicity of Heavy Metal Ions Using Algae Model

Mariam Vardiashvili – Thermal Property of Pencil Leads and Various Cosmetic Products. Resistivity of Graphite Pencils

Nino Shatirishvili – Novel Detection of Biomarkers of Pancreatic Cancer Using Microfluidics and Non-Linear Multi-Photon. Laser Wave-Mixing Detector

Sopho Khokhonishvili – Synthesis Some of 5(6)-Nitro-2-(1-Amadamntylmethyl)-1H-Benzimidazole and its Derivatives

Veronica Coen – Thermal Properties of Georgian Nuts

Tamara Gabour Sad – Identification of Phenolic Compounds in Endemic Species in Georgia

Arsenic (III) Oxide in poly(Vinyl Chloride) PVC

Marina Gakhutishvili[1], Witold Brostow[2], Stevens Brumbley[2], Nathalie Hnatchuk [2]

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One does not need to argue the importance of providing antibacterial activity to materials. The way it was done earlier was simply using materials which can destroy bacterias. There are immediate problems since some such materials including arsenic are highly toxic; they do destroy bacterias but not only … One option which has been used before our project began was using low molecular weight antibacterial agents. This represents progress as compared to 'nude' arsenic or arsenic oxide; however, toxicity is mitigated.

We put arsenic (III) oxide into poly(vinyl chloride) (PVC). Sufficient antibacterial activity is achieved. The antibacterial material so obtained is non-irritant and non-toxic. At the same time, the PVC-based composite has high thermal stability as demonstrated by thermogravimetric analysis (TGA, PerkinElmer). Thermal transitions have been located by differential scanning calorimetry (DSC, PerkinElmer). Still further, we have determined scratch resistance in a Microscratch Tester from CSM, Peseux, Switzerland. Higher scratch resistance than in neat PVC has been demonstrated, including stronger viscoelastic scratch recovery.

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Investigation of Thermal Properties of New Semicrystalline Polymers

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San Diego State University Georgia[1], Tbilisi State University[2], Agricultural University of Georgia[3]

The thermal characteristics of new semicrystalline polymers and phase transitions were investigated by means of Differential Scanning Calorimetry (DSC).

We have recrystallized semicrystalline polymers with various organic solvents and investigated the effect of recrystallization solvents on the thermal properties of polymers. The thermal characteristics of the crystalline states were found to be strongly influenced by the recrystallization conditions. The influence of different organic solvent in the polymer was determined by the matrix on glass transition (Tg), crystallization, and melting (Tm) processes of the material.

The ability of a polymer to a crystallization process substantially affects its final physical and thermal properties. During the crystallization process, most of semicrystalline polymers, the thickness of which is significantly smaller than other dimensions are being generated.

The thickness of lamellar crystals of a given material is a result of its chemical structure and the kinetics of crystallization more importantly affects selected properties of a given polymer (mechanical, thermal).

Experimental data proved a significant mutual interference between the chemical nature of the monomer and the particularities of the organic solvents which influences the thermal decomposition of the corresponding semicrystalline polymer.

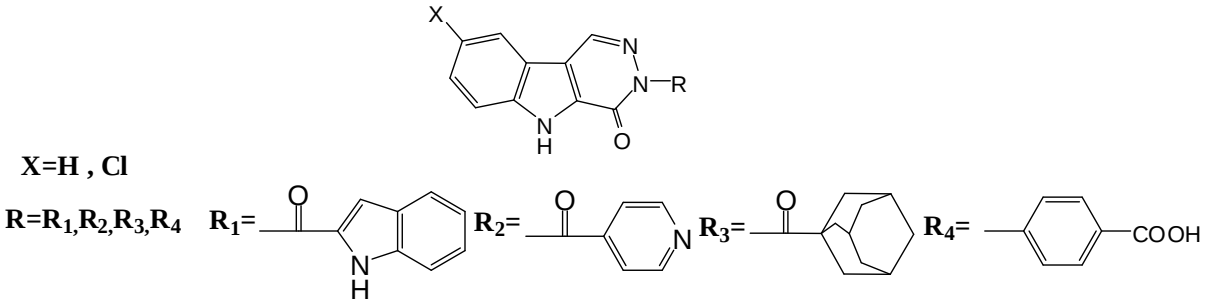
Synthesis of Some New Derivatives of Pyridazino[4,5-b]Indoles

Nikoloz Kvinikadze, Akaki Kalatozishvili, Ioseb Chikvaidze, Shota Samsoniya

Tbilisi State University

Among the isomeric pyridazinoindoles, there are ones that show diverse pharmacological activities against illnesses like Alzheimer, Parkinson, tuberculosis and others. In this work the general method for syntheses of 3-aryl-4-oxo-3H,5H-pyridazino[4,5-b]indoles has been studied. In order to detect new compounds with beneficial properties, new 3-aryl-4-oxo derivatives of 3H,5H-pyridazino[4,5-b]indoles which are heterocycles with three nitrogen atoms and azaanalogue of ß-carbonyl have been synthesized. These compounds are drawn attention from the view of their pharmacological activities or they may be utilized as intermediates for synthesis of new substances with potential physiological activities.

2-Ethoxycarbonylindole has been selected as a key compound for the syntheses. Different groups are contained in the hydrazone fragment of the phenyl core. The optimum conditions have been chosen for cyclization of corresponding aryl hydrazones.



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Design and Synthesis of New Fluorescent Thymidine Analogues

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San Diego State University

While performing their essential functions, nucleic acids encounter a variety of disturbances, such as strand cleavage and ligation, local conformational changes, base damage, flipping and chemical modification. Fluorescent nucleosides continue to play a major role in the biophysical study of these processes. This research aims to add a very important but missing capability to the previously studied fluorescent nucleoside analogues: brightness sufficient to enable single-molecule biophysics and tracking labeled nucleic acids by fluorescence microscopy. These advanced features will give a foundation for future applications of fluorescent nucleosides to the investigation of nucleic acid transport, metabolism, regulatory processes and interactions with potential therapeutic agents in living cells, advance new diagnostic approaches and facilitating drug discovery. The specific aim to pursue this goal is to design, synthesize, and characterize a new emissive fluorescent thymidine analogue designed to maximize brightness red-shift the absorption and emission as compared with existing fluorescent nucleoside analogues. We designed a new tricyclic thymidine analogue with conjugated features expected to maximize fluorescence intensity and to lower the HOMO–LUMO gap, thereby red-shifting absorption and emission. The design and synthesis involve C-riboside formation, which is needed for the desired conjugated system. The main challenge of the 3-step synthesis is regioselectivity of an arene bromination needed for the Heck reaction to produce the C-ribosed. Throughout the research, multiple regioselective director catalysts were used at a high temperature, monitoring by TLC, investigating with NMR, and finally obtaining evidence for the formation of the desired isomer as a minor product. Ongoing work is directed at achieving the desired regioselectivity, which will enable us to complete the synthesis and test this new fluorescent nucleoside analogue.

Enantioseparation of Brompheniramine, Chlorpheniramine and Dimethindene Maleate in Capillary Electrophoresis Using Cyclodextrins as Chiral Selectors

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Ann Gogolashvili[1], Bezhan Chankvetadze[1]

Tbilisi State University[1], San Diego State University Georgia[2]

This project deals with enantioseparation of three chiral drugs (brompehiramine, chlorpheniramine and dimethindene) using heptakis 2,6-di-O-methyl-beta-cyclodextrin (DM-□-CD) and heptakis 2,3,6-tri-O-methyl-beta-cyclodextrin (TM-□-CD)as chiral selectors in capillary electrophoresis. The goal was to follow how R and S enantiomers of brompheniramine, chlorpheniramine, and dimethindene interact with the cyclodextrins mentioned above in the presence of monopotassium phosphate buffer (pH 3.0). The research team has run several analyses with decreasing applied pressure from 100 mbar to 0 mbar and 25kV applied voltage. Preferred injection volume for brompheniramine and dimethindene is 50/1, and for chlorpheniramine – 30/1. Chiral selectors and methods used successfully separated the enantiomers of all three compounds with a high number of plates and with sharp, well defined, peaks. The number of plates is following: for brompheniramine: N1≈150696, N2≈45667; chlorpheniramine N1≈73795, N2≈41405 and for dimethindene N1≈106345, N2≈61847. Currently, our

research is focused on increasing the number of plates while decreasing the migration time. In future we plan to follow cyclodextrin – analyte interaction using Nuclear Overhauser Effect (NOE)-based methods in NMR spectroscopy.

Acknowledgments:

The authors want to thank Shota Rustaveli National Science Foundation of Georgia for their financial support (Grant PHDF-18-485).

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Synthesis of 5(6)-Nitro-[2-(3-Acetamido-Adamantyl-1)]-1H-Benzimidazole Derivatives

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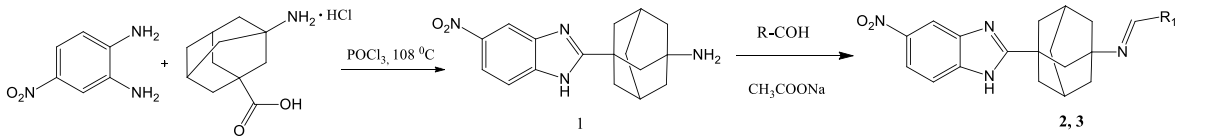
San Diego State University Georgia[1], Tbilisi State University[2], Georgian Technical University[3]

Adamantane is an affordable chemical compound that is used in medicine. Adamantane's derivatives also have big influence on drug development and their bioactivity. Properties of benzimidazole and its derivatives have been studied for over hundred years; special interest of researchers triggered by the fact that 5,6-dimethylbenzimidazole is a component of naturally occurring vitamin B_{12}. Several antihelminthic, antacid and antibacterial drugs are known which have benzimidazole moiety as their essential constituent. Additionally, several bis- and trisbenzimidazole based systems are well-known for their interaction with DNA and interference with several DNA associated processes. This account gives an overview of the benzimidazole based systems and their relevance in medicinal chemistry. Consider the fact that benzimidazoles and adamantanes have high level of bioactivity and are used as a drug against variety of diseases, the synthesis of adamanylated benzimidazoles and study their biological activity is interesting [1]. Previously, we have synthesized 2-(1-adamantyl)benzimidazole derivatives [2].

The aim of the work was to synthesis of 5(6)-nitro-[2-(3-amino-adamantyl-1)]-1*H*-benzimidazole (**4**) and study its interaction with some aromatic aldehydes according to the scheme **1.** Scheme 1.



R_1=$C_6H_4NO_2$, 2-OH-5-$NO_2C_6H_3$

Condensation reaction of 5-nitro-*o*-phenylenediamine with 3-aminoadamantane-1-carboxylic acid hydrochloride in $POCl_3$ produces compound **1**, in which interaction with 5-nitrosalicylaldehyde and 3-nitrobenzaldehyde was conducted in alcohol area by heating at 3-5 h. in presence of equimolar ration sodium acetate. Corresponding Schiff bases **2** and **3** was obtained with 60-64 % yield. The structures were confirmed by IR and ^{1}H NMR spectroscopy.

Acknowledgment:
This work was financially supported by Shota Rustaveli National Science Foundation (SRNSF)

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Thermal Properties of Fresh and Roasted Coffee Beans

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San Diego State University Georgia[1], Tbilisi State University[2]

Coffee is the widely known and consumed beverage all over the world. It is traditional way to energetically start the day for millions of people. The beans of coffee contain a great quantity of chemicals, including caffeine, chlorogenic acid, polyphenols, amino acids and other compounds that also, contribute their aroma and have beneficial influence on human health and decrease the risk of the development of some diseases, including cancer. There are different kind of coffee beans which have different chemical consistence and accordingly, different taste. The degree of roast influences on the chemical composition of coffee.

The aim of the research was to study two most consumed kinds of coffee Arabica and Robusta's roasted and fresh green coffee beans' thermal properties and their comparison in order to determine what differences are there among various types of coffee beans. During the research, moisture content of the milled coffee was determined. Eight differently named coffee samples were analyzed, differential scanning calorimetry DSC 200 F3 Maia was used for study of their thermal properties with the temperature range of 10°C to 300°C, rate of heating 5K/min and flow of liquid nitrogen 40ml/min. Endothermic processes, phase transitions and enthalpy were evaluated. Each types of coffee have different thermal stability and phase transitions. The differences between thermal properties of coffee beans can be caused by their origins, degree of roast and by their chemical compositions. The study showed some similarities between different named coffee beans' thermographs.

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Synthesis and Some of Transformation 2(1-Adamantyl)-1H-Benzimidazole

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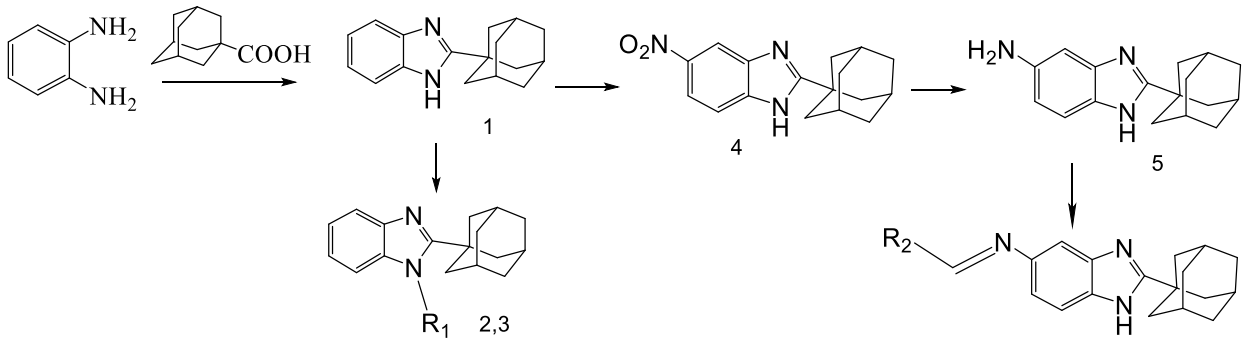
Adamantane active group has proven its high membrane permeability through the path of its lipophilicity and symmetric geometry. Besides, it was shown that in most cases, attachment of adamantane group decreases toxicity and prolongs the activity of substances [1]. On the other hand, Benzimidazole is well-known for anti-viral, antimicrobial and fungicide capabilities. Our research combines the two active group and aims for enhanced biological activity [2].

Previously, we have synthesized 2-(1-adamantyl)-1H-benzimidazole derivatives and studied certain properties of them [3]. The aim of present work was to synthesis of N-alkylated 2-(1-adamantyl)-1H-benzimidazoles, 5(6)-amino-2-(1-adamantyl)-1H-benzimidazole and study some transformations.

2-(1-adamantyl)-1H-benzimidazole (1) in high yield (93%) was obtained by heating a mixture of 1-adamantanecarboxylic acid and o-phenylenediamine in POCl (Scheme 1). By interaction of alkyl halogens with compound 1 in the area of DMF in presence of KOH compound 2 and 3 was synthesized. The nitration reaction of compound 1 was carried out by using at a molar ratio of 1:28 HNO3/H2SO4 and compound 4 was isolated in high yield. 5(6)-amine-2-(1-Adamantyl)-1H-benzimidazole 5 was obtained by reduction of 5(6)-nitro-2-(1-adamantyl)-1H-benzimidazole (4) with molecular hydrogen in the presence of Raney Ni in alcohol area and by interaction of compound 5 with Benz aldehyde and 5-nitrobenzaldehyde corresponding Schiff bases 6 and 7 were isolated in high yields.

Scheme 1



R_1=$CH_2C_6H_5$, C_4H_9

R_2= $C_6H_4NO_2$, C_6H_5

The structures were confirmed by IR and NMR spectroscopy.

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Nitrogen Oxides Pollution in Tbilisi

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Tbilisi State University, SMART | AtmoSim_LAB

The goal of the experiment was to measure NO and NO_2 concentrations in the air of Tbilisi.

Analysis were carried out by the help of NO_x ozone chemiluminescence analyzer. Chemiluminescence is the emission of light, as the result of a chemical reaction. $\boldsymbol{NO_2^* \rightarrow NO_2 + h\nu}$

NO reacts with ozone to produce nitrogen dioxide and oxygen. Some part of NO_2 will be in the excited state.

$$\boldsymbol{NO + O_3 \rightarrow NO_2^* + O_2}$$

There are two ways to return back from the excited state to the ground state: radiating or quenching.

$$\boldsymbol{NO_2^* \rightarrow NO_2 + h\nu}$$ (radiating)

$$\boldsymbol{NO_2^* + M \rightarrow NO_2 + M}$$ (quenching)

As for NO_2 analysis, at first NO_2 is converted to NO. After this blue light converter is used.

$$\boldsymbol{2NO_2 + h\nu \rightarrow 2NO + O_2}$$

NO_2 is harmful for health. Also with sunlight NO_2 can convert back to NO and produce ozone (O_3) as a side pollutant. Because of the potential of NO_2 to produce these "secondary" pollutants, it is important to monitor and regulate NO_2.

Maximum allowed concentration of NO_2 is 60 μg/m^3 and for NO is 40 μg/m^3 (yearly average).

On the first experiment the analysis was carried out in different periods of the day in different areas of Tbilisi: Vake park, Mushthaid garden, Varaziskhevi street, Marjanishvili Square, Didi Dighomi, Saakadze Square, Central Station Square and Freedom Square.

As for the second experiment we measured contamination Gradients for NO_x in Space. We observed: the University area, Varaziskhevi street, Tsereteli avenue, Marjanishvili area.

Vake park and Mushthaid garden are the cleanest places and Varaziskhevi street is the most polluted area in Tbilisi. Traffic is the main reason of NO_x pollution. In areas where road vehicles are the main source of NO_x, there is often higher NO_2 concentrations during rush hour traffic times such as around 7pm weekdays. The ozone concentration increases during the day while the NO_2 concentration decreases. That's because NO_2 transforms to NO in the presence of sunlight. After 6 PM, the NO_2 concentration builds up as there is no sunlight to convert NO_2 back to NO.

Synthesis of Chiral Sulfoxides and Separation of Enantiomers by HPLC Method

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San Diego State University Georgia[1], Tbilisi State University[2]

Chlorpromazine, also known as Largactil and Thorazine, belongs to the class of drugs called phenothiazine antipsychotics. It is used to treat mental illnesses such as schizophrenia, manic phase of bipolar disorder, severe behavioral problems etc. It works by antagonizing dopamine D2 receptors in brain, depressing release of hypothalamic and hypophyseal hormones, may also depress reticular activating system. Despite a lot of advantages this drug has a lot of side effects. Due to this fact we decided to see if its monoxide would have any different effect on the human body. For the oxidation we have used 77% m-CPBA, 1:1 ratio with chlorpromazine to avoid formation of dioxides. For the same reason reaction was carried out in an ice bath at the temperature of 0oC. In order to avoid oxidation of N atom we have preserved it with HCl to decrease nitrogen's reactivity. To check the progress of the reaction we have used TLC (CH2Cl2:CH3OH). Using this method, we also checked the product after its cleaning. To make sure what compound was delivered after the reaction and whether we got enantiomers, we have sent it to IR and NMR and the results were satisfying. We have gotten pair of enantiomers due to oxidizing of sulfur atom. After checking the effect of the new compound on the human body it was revealed that new enzymes were added to the target classes.

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Using Protein Design to Engineer a Scaffold for Regio-Selective C-H Functionalization

Mariami Basilaia[1], Tamar Maisuradze[1], Caroline Rodrigous[2], Adrian Ramirez[1], Jeffrey Gustafson[1], John J. Love[1]

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The goal of the project is to utilize a well-studied small molecule-protein interaction to replace a C-H bond on the small molecule with a halogen atom (-X). The objective is to use the enzyme - Src protein kinase as a vice to hold a specific organic molecule in active site while subjecting the complex to C-H functionalization. The location(s) of the C-X functionalization will be compared to a control - the unbound small molecule, pyrrolopyrimidine (PPY) which is the strong Src inhibitor. The active site of the enzyme will be re-engineered to promote regio-selective C-X functionalization on a specific aromatic carbon atom. The goal is to exploit a small molecule-protein binding interaction as a template to effect electrophilic aromatic substitution (SEAr). The plan to achieve this is to (1) position a Lewis base moiety (a mutant methionine side-chain) in the Src active site to direct SEAr to a specific position on a bound PPY, and (2) combine in silico and

directed evolution for the rapid discovery of Src mutants. The Src/PPY crystal structure is being assessed in silico for best candidate amino acid positions to mutate to methionine. The resulting library of mutant Src enzymes will be displayed on the surface of bacteria and incubated with fluorescent PPY. Successful binders will be isolated via Fluorescent Activated Cell Sorting. Thus far the gene for the Src kinase was obtained and cloned into Bacterial Surface Display (BSD) system recently developed in the Love Laboratory. PCR-based sub-cloning was verified by standard methods. Polyacrylamide gel electrophoresis was used to demonstrate protein expression. Favorable results from western blot analysis demonstrated that Src still functions as a protein kinase on the surface of E. Coli. Future plans are to incubate BSD Src with PPY and assess the C- H functionalization chemistry on bound and unbound PPY.

Acknowledgements:

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Ultrasensitive Detection of Cancer Biomarker CEA Using Multi-Photon Non-Linear Laser Wave-Mixing Spectroscopy

Luka Tatarashvili[1], William G. Tong[2]

San Diego State University Georgia[1], San Diego State University[2]

Forward-scattering Degenerate Four Wave Mixing (F-DFWM) Laser Spectroscopy is an efficient method of detecting very low concentration of substances. We show an application of this spectroscopic method on the detection of cancer biomarker carcinoembryonic antigen (CEA). Preliminary CEA detection limit is comparable or better than those of ELISA or fluorescence-based techniques. DFWM can be used for both fluorescing (labeled) and non-fluorescing (label-free) samples. All in all, the technique offers enhanced sensitivity if compared to other available methods and at the same time requires no labeling for the sample.

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Thermal Stability of Folic Acid and its Deficiency in Humans

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San Diego State University Georgia[1], Tbilisi State University[2]

Vitamin B-9, folic acid is an essential compound involved in important bio-chemical processes within and relating to living organisms (1). Investigation of the thermal stability of folic acid is very important and useful for a drug storage condition (2).

In this research the thermal stability of folic acid was investigated using differential scanning calorimeter (DSC) at the temperature range 20- 350C. Fourier transform infrared (FTIR) spectroscopy was used for identifying the structural changes in folic acid. The effects caused by folic acid deficiency in humans, especially in infants were reviewed.

DSC thermogram showed that the degradation of folic acid started at 187 °C and the relatively stable temperature for folic acid is lower than 124 °C.

This research attempts to understand correlation between the thermal stability of folic acid and its deficiency in humans.

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Study of Toxicity of Heavy Metal Ions Using Algae Model

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Along with intensification of production, the level of pollution of natural ecosystems with various toxic components increases. This issue is not only for Georgia but for many developed countries [1,2,3]. In this regard, an active study of water ecosystems is required where substances are common in water depths as well as inside the hydrobionts. Some pollutants such as heavy metals, as a result of transformation in chemical and biochemical reactions do not lose the toxicity, which makes them especially dangerous. Nowadays, it is important to find new methods of assessing the influence of heavy metals on water ecosystems and create more operational and reliable information. An important scientific-practical task in this aspect is to study the consistent phases of degradation of fresh water ecosystems to find ways to restore the ecosystem. For this purpose, we have researched on the selection of structurally different algae model. Research modeling materials were: *Miriophylluim hippurides, Vallesneria vallesneria, Cryptocoryne affinis and Lemna minor L.* We used cadmium chloride solution (up to 20 mg / ml concentrations of CdCl2) to study the toxicity effect of heavy metals. Based on the results obtained, the resistance of the organisms included in the model ecosystem against Cd ions distributed as follows - Lemna minor L <Miliophylluim hippurides <Vallesneria vallesneria <Cryptocoryne. Step by step from the

plant's ecosystem, we were able to discern the stabilizing organism of the experimental ecosystem (*Cryptocoryne affinis*). At the expense of this component, over time (on average for 2 months) signs of recovery of ecosystem were observed, which, in the case of *Vallesneria vallesneria* , expressed small size growths. On the basis of our experiment we can conclude that it is necessary to determine the stabilizing organisms of sustainability as result of the study of different types of ecomodels and their use in the planning of restoration of damaged ecosystems.

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Thermal Property of Pencil Leads and Various Cosmetic Products. Resistivity of Graphite Pencils

Mariam Vardiashvili[1,2], Sandro Gogia[1,2], Mariam Khvichia[1,2], Nino Kokiashvili[1,2]

San Diego State University Georgia[1], Tbilisi State University[2]

Differential scanning calorimetry is a thermo-analytical method that can be used to determine the hardness in pencil leads and analyse the composition of various cosmetic products. The relationship between resistivity and pencil grade in graphite was investigated.

This research focused on analysing the thermal factors, which contributed to overall pencil lead structure; hardness and their thermal properties. Upon that, cosmetic products, lipstick and eye pencil, were also investigated and evaluated on their thermal characteristic using thermoanalytical method.

The results illustrate how minor additives, such as binders, low melting organic compounds, and pigments contribute to the whole structure of the sample and alter their thermal properties. This could indicate the importance of differential scanning calorimetry in understanding physical properties of samples, which could be implemented in industries as an additional method for grading, evaluating samples.

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Novel Detection of Biomarkers of Pancreatic Cancer Using Microfluidics and Nonlinear Multi-Photon Laser Wave-Mixing Detector

Nino Shatirishvili, Luka Tatarashvili, Jie Liang, J. Sebastien Pradel, William G. Tong

San Diego State University

We report sensitive detection of carbohydrate antigen 19-9 (CA 19-9) and carbohydrate antigen 242 (CA 242), the biomarkers of pancreatic cancer, using laser wave-mixing spectroscopy. Current detection methods require more time-consuming and complicated labeling steps. Our patented nonlinear laser wave-mixing methods offer significant advantages including label-free native detection, excellent sensitivity, small sample requirements, short optical path length, high spatial resolution and portable detector designs. The wave-mixing signal is generated when the two input beams are mixed inside the analyte and it can be collected with virtually 100% efficiency and maximum signal-to-noise ratio. The signal has a quadratic dependence on analyte concentration, and hence, small changes can be monitored more effectively. Since wave-mixing probe volume is small (nanoliter to picoliter), it is intrinsically suitable for microfluidics or capillary-based electrophoresis systems (e.g., 75 µm i.d. fused silica capillary). Different biomarkers can be immobilized on a custom 3D printed slide. Since wave mixing is an absorption-based method, both fluorophore and chromophore labels could be used, if desired. Excellent sensitivity levels for CA 19-9 are demonstrated using a Chromeo P503 tag and a 473 nm solid-state excitation laser. One can run a standard protein ladder to estimate capillary electrophoresis retention time for CA 19-9. The glass slides and microarrays used in these detection methods for early diagnosis of pancreatic cancer are custom 3D printed in our research lab.

Thermal Properties of Georgian Nuts

Sopho Khokhonishvili[1,2], Makrine Nikolaishvili[1,2], Teona Gvelesiani[1,2] Nino Kokiashvili[1,2]

San Diego State University Georgia[1], Tbilisi State University[2]

Thermal characteristics of various tree nuts and their shells have been extensively investigated and established. Most studies focus on their utility as alternative fuel sources, some others look further into extending shelf life for the seeds. However, there is minimal research about Georgian nuts. Several endemic species have been identified in regions of Georgia and the majority of publicly available information discusses only their physical properties and desirable agricultural conditions. This study aimed to find out more about the thermal properties of 5 different nut seeds by employing differential scanning calorimetry (DSC). The intention was to observe thermal processes and deduce the temperature ranges of stability. The findings can be used and interpreted by business owners and any others who seek to avoid unwanted spoilage by crystallization and other transformations.

Five of the more widely consumed nut seeds were chosen for testing: almond, walnut, peanut, and hazelnuts of eastern and western variety. First, we determined moisture content for each by oven drying cut up pieces at 100℃ for 2 weeks. Next, we performed DSC analysis using Netzsch DSC 200 F3 Maia® on both fresh and dry samples. The thermal properties of nuts seeds were investigated over a temperature from -100°C to 100°C. Thermal conductivity [k] and specific heat capacity [c] of each sample were characterized.

Measured moisture content values fit in the expected range for walnut and peanut, exceeded in almond and hazelnuts. This is likely to be the result of storage without shells which act

as a barrier to excess moisture in the air. Dried samples of all nuts showed significantly lower thermal activity. Based on the prevalence of thermal transformations, most stability is observed on temperatures above 10℃. However, it cannot exceed room temperature (20℃) because many useful nutrients begin to break down and nut seeds may turn rancid. Further research with a more controlled environment could investigate the activity of specific compounds that are in seeds' composition and their effects on taste and shelf life.

Synthesis Some of 5(6)-Nitro-2-(1-Amadamntylmethyl)-1H-Benzimidazole and its Derivatives

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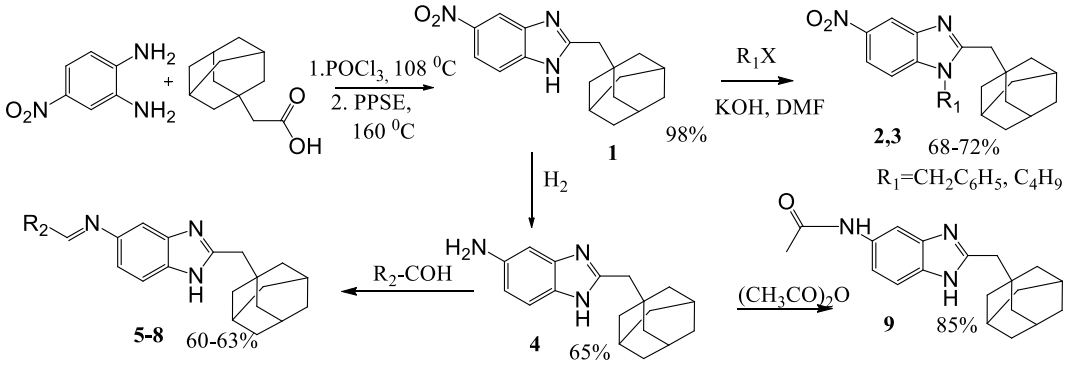
Benzimidazole derivatives are characterized with various types of pharmacokinetic and pharmacodynamic properties. Benzimidazole nucleus is one of the bioactive heterocyclic compounds that exhibit a range of biological activities. The chemistry and pharmacology of adamantane derivatives have been of great interest because of wide range of pharmacological properties. They amplify energy of the human body and significantly improve emotional and physical state in patients.

Previously, we have synthesized 2-(1-adamantyl) benzimidazole derivatives [1]. In the present study the aim of our work was to synthesize a series of novel 5(6)-nitro-2-(1-adamantylmethyl) benzimidazole according to scheme 1.

Scheme 1.



Condensation reaction of 5(6)-nitro-o-phenylenediamine with 1-adamantaneacetic acid was conducted in presence of POCl3 at 1 h heating at 105-108°C temperature and of PPSE at 5 h heating at 160-163 °C. Compound 1 with high yield was obtained. By the interaction of alkyl halogens with 5(6)-nitro-2-(1-adamantylmethyl)-1H-benzimidazole (1) in the area of DMF in presence of KOH compound 2 and 3 was synthesized. The reduction of compound 1 with molecular hydrogen in the presence of Raney Ni was carried out in alcohol area and compound

4 was obtained with 65% yield, in which interaction with 5-bromosalicylic-, 3,5-dibromosalicylic-, 5-nitro-salicylic-, 3-nitrobenzaldehyde in alcohol area by heating at 1-5 h was formed corresponding Schiff bases 5-8. Condensation of amine 4 with acetic anhydride to the formation of the corresponding acyl derivative 9 with a high yield.

The structures were confirmed by IR and 1H NMR spectroscopy.

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Reference:

1. Zurabishvili, D. S.; Bukia T. J., Lomidze, M. O. Trapaidze M. V., Samsoniya, Sh. A. etc., Chem. Heterocycl. Compd. 2015, 51(2), p.139-145. [Khim. Geterotsikl. Soedin. 2015, 51(2), c.139-145].

Identification of Phenolic Compounds in Endemic Species in Georgia

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Endemic pear grows in Adjara, Georgia was collected from three regions in Adjara, including Adjaristskali, Merisi and Dandalo. Each pear fruit was examined and compared by five parts (skin, pulp, fruit, juice and crumbs) to analyze its quantity properties for phenolics. The total amounts of phenols were defined with the help of spectral methods. The highest amount of total phenolic was found in the skin of Adjaristskali which 4500 mg in 1 kg of the skin was around. Previous studies showed that the mountainous areas are rich in biologically active compounds including phenols, flavonols and more other, that's why the study aimed to identify the phenolics content of the pear and which parts of it were the richest with phenol.

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