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ABSTRACTS

PLENARY SESSIONS

SEPARATION OF ENANTIOMERS OF NOVEL CHIRAL SULFOXIDES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

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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 pharmacology and toxicology. That is why, enantiomerically pure drug forms are more safe and efficient [1].

The main goal of the present study was to determine relationships between chemical structure of chiral compound and enantioselectivity in high-performance liquid chromatography. For this purpose, novel chiral sulfoxides were synthesized. In addition, their chiral separation was studied with polar organic (methanol, ethanol, 2-propanol, acetonitrile) and normal-phase mobile phases (n-hexane in combination with various alcohols) using variety of cellulose based chiral selectors. Factors determining retention and separation factors in terms of structural variations of analyte molecules were established and are discussed.

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SELF-ASSEMBLED BIODEGRADABLE MICELLAR DRUG CARRIERS MADE OF AMPHIPHILIC PSEUDO-PROTEINS FOR BIOMEDICAL APPLICATIONS

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Biodegradable nanoparticles have gained tremendous attraction as carriers for controlled drug delivery systems. Despite numerous advances in the field of development of suitable methods for administration of various drug and therapeutic agents as well as drug release in a controlled fashion remain considerable challenges. In recent years, polymeric micelles have attracted a lot of attention in terms of their specific properties including delivering of hydrophobic cargo to the target site. They are considered more stable than their surfactant counterparts and can prolong circulation times in vivo and their specific accumulation in the diseased tissues [1]. They can effectively solubilize small hydrophobic drugs in their inner most hydrophobic core while their outer hydrophilic shell can afford protection against any kind of scavenging by the mononuclear phagocytic system [2]. Micelles often display a great resemblance in their comparison to viruses or lipoproteins as carriers of required payload, whether it is DNA for viruses or hydrophobic drugs for lipoproteins [3]. However, both lipoproteins and viruses have their own limitations in delivering their respective payloads to the target sites. Lipoproteins have a greater propensity of being recognized by healthy cells too apart from competing with natural lipoproteins on tumor sites [4]. Viral carriers can be recognized by immune systems, which in turn can elicit an immune response. In contrast, polymeric micelles do afford significant advantages over the above mentioned two carriers in terms of delivery of a hydrophobic payload. Physical stability and chemical stability in plasma, however, still remain the major concerns for polymeric micelles [5]. A variety of PMs drug delivery systems including charged and neutral polymers of both natural and synthetic origin have been developed [6, 7, 8]. However, quite a few polymers capable to form stable micelles with good solubilizing properties and releasing non-toxic and easily metabolizable products upon biodegradation were reported. Therefore, the search for new and more universal micelle-forming polymers is still topical. While the poly(ethylene glycol) (PEG) still represents the most popular biocompatible hydrophilic block, various hydrophobic polymeric blocks can be attached to it. Among the hydrophobic blocks the most promising look nontoxic and biodegradable ones. The biodegradation of the block-copolymers is highly desirable to provide the clearance of nano-carriers from the body after their function is fulfilled. In our previous study [9] we reported on micelle-forming ABA triblock-copolymer in which the biodegradable pseudo-protein - poly(ester amide) (PEA) composed of α-amino acid L-leucine, 1,6- hexane diol and sebacic acid (Mw ca. 4000 Da) was used as a hydrophobic block "B" and H_2N-PEG (Mw 2000 Da) as a hydrophilic block "A". The present paper deals with micelle-forming ABA triblock copolymer in which biodegradable pseudo-protein - PEA composed of more hydrophobic α-amino acid L-phenylalanine, 1,6-hexane diol and sebacic acid is used as a block "B", and H_2N-PEG-2000 as a block "A". We assumed that increased hydrophobicity of the block "B" (i.e. more hydrophobic core of the micelles) can improve the solubilizing potential of the nanoparticulates. It has to be note here that pseudo-protein - PEA composed of the hydrophobic amino acids, fatty diols and dicarboxylic acids showed reasonable biodegradation rates and excellent biocompatibility [10,11].

The synthesis of the goal unsaturated triblock-copolymers *via* the one pot/two-step method was carried out. The obtained ABA triblock-copolymer was tested for the micelle-forming property. This study showed that the tri-blockcopolymer formed stable micelles 100±7 nm in size at 10mg/mL concentration which is considered as an optimal range for pharmaceutical micelles [12].

The obtained preliminary data allow concluding that the ABA triblock-copolymer we have obtained is promising for constructing biodegradable micellar nanocarriers suitable for delivering poorly water-soluble drugs and therapeutic agents. More detailed studies of the obtained micelles including the interaction with hydrophobic drugs are in progress now. These studies shall lead to the development of further improved micellar systems to advance the treatment of numerous diseases.

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SYNTHESIS OF NEW “CLICK” POLYESTERS BEARING 1,2,3-TRIAZOLE RINGS IN THE MAIN CHAIN

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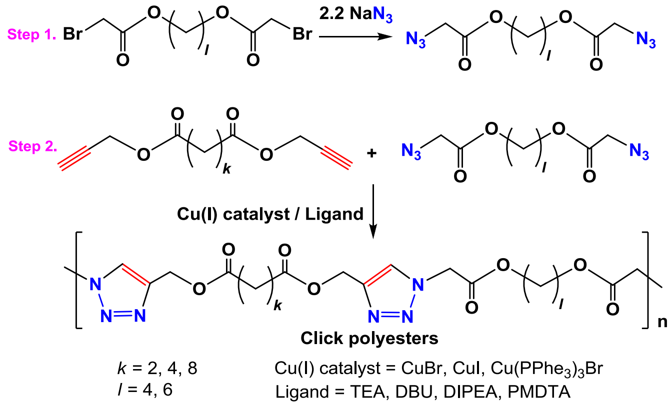
In this work high-molecular-weight AA-BB-type aliphatic polyesters (PEs) were synthesized *via* Cu(I)-catalyzed click step-growth polymerization (SGP) following a new synthetic strategy. The synthesis was performed between diyne and diazide monomers in an organic solvent as one pot process using three components and two stages. The di-propargyl esters of dicarboxylic acids (component 1) were used as diyne monomers, di-(bromoacetic acid)-alkylene diesters (component 2) were used as precursors of diazide monomers, and sodium azide (component 3) was used for generating diazide monomers. The SGP was carried out in two steps: at the Step-1 di-bromoacetates interacted with two moles of sodium azide resulting in diazide monomers which interacted *in situ* with diyne monomers at the Step-2 in the presence of Cu(I) catalyst (Scheme 1).



Scheme 1. Synthesis of click polyesters

A systematic study was done for optimizing the multiparameter click SGP in terms of the solvent, duration of the both Step-1 and Step-2, solution concentration, catalyst concentration, catalyst and ligand nature, catalyst/ligand mole ratio, temperature of the both steps of the click SGP. As a result, high-molecular-weight (MW up to 74 kDa) elastic film-forming click PEs was obtained [1]. These polymers contain 1,4-disubtituted 1,2,3-triazoles in the backbones. The presence of the main-chain triazoles significantly improved the thermal properties of the PEs. Elastic films and nanoparticles made of the new PEs are suitable as biodegradable biomaterials for biomedical applications. Our work should encourage the synthesis of novel heterochain polymers of various types and classes with 1,4-disubtituted 1,2,3-triazoles by applying the new synthetic strategy to both Cu(I)-catalyzed and copper-free click SGP. It should be noted that the possibility of quaternization of 1,2,3-triazole rings of the click polymers using halo-alkyls or bromo-PEG derivatives opens a way to positively charged systems - either water soluble polymers or cross-linked hydrogels both promising for various biomedical applications.

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Teng. Kantaria, Tem. Kantaria, G.Titvinidze, G.Otinashvili, N.Kupatadze, N. Zavradashvili, D. Tugushi, R. Katsarava. Int. J. Polym. Sci, 2018, 14 pages, 2018. https://doi.org/10.1155/2018/6798258

STEPWISE EXTRACTION AND HPLC ANALYSIS OF VALUABLE NATURAL COLORANTS – CAROTENOIDS AND ANTHOCYANINS

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The manufacture of food products and dietary supplements using natural food colorants has been attracted attention in modern food industry. Agro-industrial waste materials and their complex organic contents constitute a significant source of different valuable natural products. Carotenoids and anthocyanins as natural colorants show strong antioxidant and immunomodulation activities and may prevent degenerative diseases. The challenge of extraction of natural product in the twenty-first century is to achieve high selectivity of the desired product and develop energy-saving or renewable energy-based processes. Modern concept of utilization of agro-industrial wastes focuses on complete utilization and use of eco-friendly separation methods that require standard technological equipment for industrial application.

The present research concerns the development of stepwise extraction procedures and HPLC analysis of carotenoids and anthocyanins containing agro-industrial waste materials (tangerine, orange peel and grape skin).

Extractions were carried out in a dynamic supercritical fluid - carbon dioxide (SC-CO_2) and ultrasound assisted extraction systems. The effects of operating pressure and temperature, extraction time, pH, flow rate of the SC-CO_2, sample size and solvent nature used were investigated. The optimal conditions for extraction were found. The drying process and stability of samples obtained from agro-industrial waste materials was studied as well. The main carotenoids - beta-carotene, lycopene and total anthocyanins obtained in organic extracts were quantified using new, rapid, effective and selective developed and validated HPLC methods. The HPLC methods were validated with respect to system suitability test, specificity, linearity-range, accuracy, precision, limit of detection (LOD) and quantitation (LOQ) according to the ICH Q2 guideline. The stability of solutions and dried powder form target compounds were studied as well.

The calibration curves of developed HPLC methods are linear over a concentration range 0.08-6.50 µg/mL for beta-carotene (r^2=0.9992), 0.34-200.20 µg/mL for lycopene (r^2=0.9999); 0.04-80.50 µg/mL and 0.12-80.50 µg/mL for total anthocyanins expressed as cyanidine chloride (r^2=0.9999) and kuromanine chloride (r^2=0.9999); The average recovery equals to 106.8 % for beta-carotene, 101.4 % for lycopene, 95.62 % for cyanidine chloride and 94.9 % for kuromanine chloride.

Hence, the developed stepwise extraction procedures with the optimal parameters can easily be adapted to industrial conditions for the manufacturing processes and the proposed validated HPLC quantitative analytical methods can be used to determine quantitatively the major carotenoids and total anthocyanins in organic solvents solutions.

SYNTHESIS AND BIOLOGICAL ACTIVITY OF NEW 2-PHENYLINDOLES (REVIEW)

Armaz Tsutskiridze (Bachalor’s student), **Mariam Turiashvili, Ioseb Chikvaidze, Shota Samsoniya**

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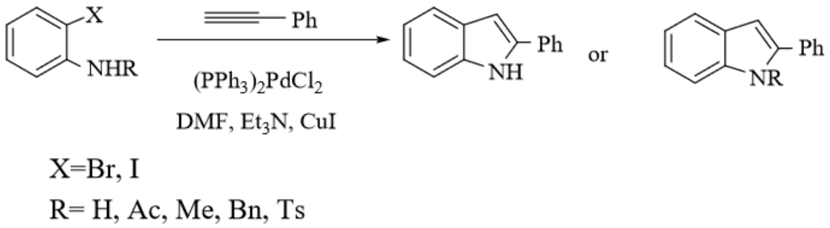
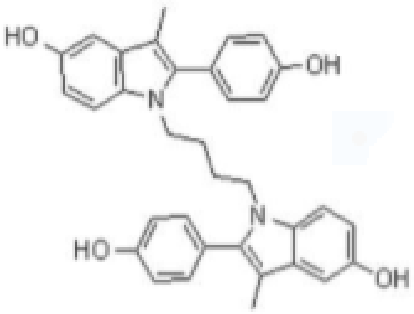
The 2-phenylindole nucleus is an important substructure of numerous natural and pharmacologically active compounds. So it is important to study of new synthesis routes. At this review are displayed facile, mild and efficient synthesis of 2-substituted indole derivatives catalyzed by $Pd(PPh_3)_2Cl_2$Presence of weak Lewis acids.

Scheme 1.



Review describes the design and synthesis of novel SERM type ligands based on the 2-arylindole scaffold to selectively target the estrogen receptor in hormone dependent breast cancers. Some of these novel compounds are designed as bisindole type structures, while others are conjugated to a cytotoxic agent based on combretastatin A4 (CA4) which is a potent inhibitor of tubulin polymerization. The indole compounds 1 and 2 demonstrate estrogen receptor (ER) binding and strong antiproliferative activity in the ER positive MCF-7 breast cancer cell line with IC50 values of 2.71 microM and 1.86 microM respectively. These active compounds induce apoptotic activity in MCF-7 cells.



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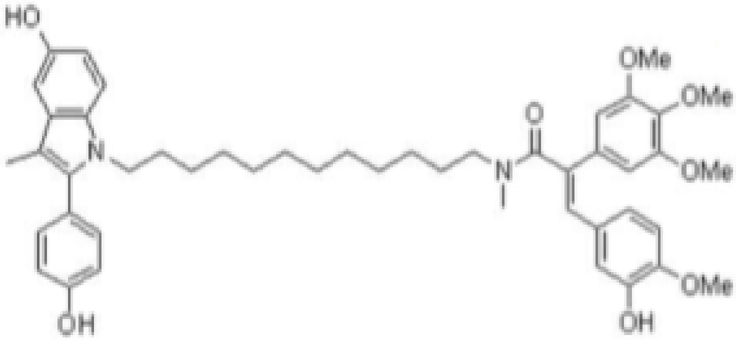
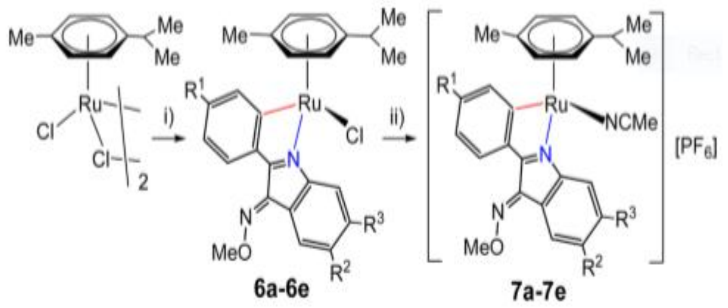


2

The novel ruthenacycles show a remarkable cytotoxic activity in MCF7 and MDA-MB231 breast cancer cell lines, which clearly exceeds those of the trans and cis isomers of [PtCl2(L)(DMSO)] derived from the same ligands and even that of cisplatin.



^{a}Legend: (i) Ag[PF_6] in acetone, removal of AgCl, treatment with the corresponding ligand **3** and SiO_2 column chromatography; (ii) Ag[PF_6] in MeCN.

SECTIONS

BIOMATERIALS WITH SUFFICIENT BIOCOMPATIBILITY

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Materials that do *not* come in contact with human bodies have to fulfill certain mechanical, thermophysical and/or tribological requirements in function of an application. Materials that do come in such contact have an extra set of requirements that need to be reckoned with. A human body can consider a material coming from outside as an intruder and will try to destroy it. Thus, 'persuading' the human organism that there is no attack - only an attempt to help - becomes the first task.

These issues are typically *not* covered in the study programs of Materials Science and Engineering (MSE) or Mechanical Engineering nor in the respective textbooks. There is only one exception, a textbook with a chapter on Biomaterials: W. Brostow & H.E. Hagg Lobland, Materials: Introduction and Applications, John Wiley & Sons 2017.

We discuss uses of biomaterials in a variety of applications, including joint replacements, scaffolds and obturation materials. Scaffolds are frameworks or structural elements that hold cells or tissues together maintaining their shape. Artificial scaffolds are often porous - allowing in-growth of the natural cells - an example of 'cooperation' between the human organism and the intervention from outside.

SYNTHESIS AND STUDY OF [4-(IMIDAZOLE-1-YL)THIAZOLE-2-YL)]NAPHTHYLAMINES

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Search for new biologically active compounds is still urgent problem for chemists and pharmacologists. New heterocyclic systems are being created and already known heterocycles are being deeply studied in order to their versatile use.

Synthesis of therapeutic agents, which significantly increase duration of the life at various cancer deseases, is an urgent problem of Experimental and Clinical Pharmacology.

It is known that important for human compounds, such as nitrogen bases, vitamins, enzymes, amino acids contain imidazole ring. Thiazole structure is found in biologically active compounds (e.g. Vitamin B) and in medications (penicillines, sulphanidamide agents). Some therapeutic preparations that contain thiazole ring, are capable slow down or completely stop multiplication of cancer cells in the diseased organs. In this regard the compounds, which contain thiazole ring condensed with benzene ring and having inhibition capacity, are notable [1-6].

On the other hand, a number of naphthaline ring-containing compounds reveal biological activity. They are intermediate products in the production of various medications, organic dyes, surfactants and polymeric materials. Some naphtalene derivatives have physiological activity similar to narcotic and psychotropic substance activities.

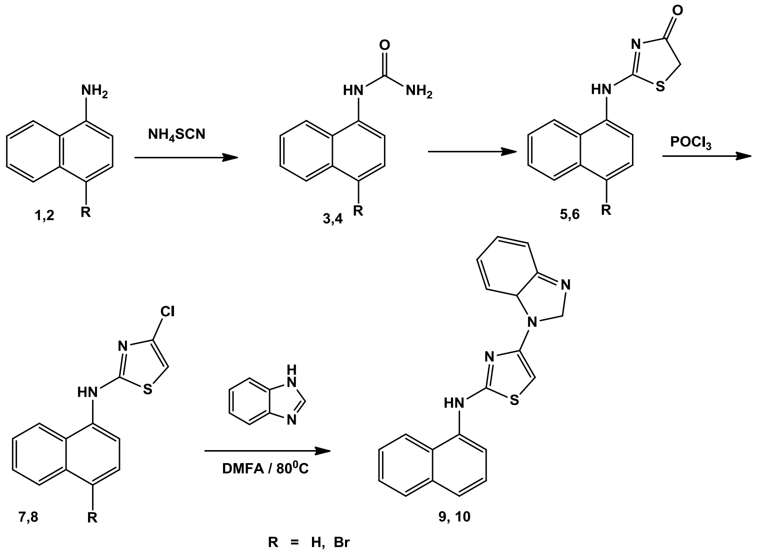
Consequently, condensation of naphthaline ring with thiazole and imidazole rings makes it possible obtaining a wide range of new heterocyclic compounds revealing feasible inhibitory and intercalation activity. Therefore we believe it is reasonable to carry out synthesis of new derivatives of the mentioned systems, as well as transformation of earlier obtained compounds in order to reveal valuable substances.

New diheterocyclic thiazole containing system, [4-(imidazol-1-yl)thiazole-2-il)]-naphtylamine, was synthesized by 4 steps.

Firstly, synthesis of 1-naphtalylthiourea was carried out by using two different methods to establish optimal conditions. Cyclisation of synthesized thiourea was realized by using ethylbromoacetate in ethanol. The favorable conditions (increasing of yield) waschosen for desoxychlorynation of 2-(naphtalen-1-ylamino)thiazole-4(5H)-one. The target product was obtained by condensation of 4-chloro-N(naphtalen-1-yl)thiazol-2-amine and benzimidazole in DMF.

This synthesis was processed within the fund of Shota Rustaveli National Science Foundation of Georgia.

Scheme



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THERMODYNAMIC CHARACTERIZATION OF SEPARATION OF FENOPROFEN ENANTIOMERS USING AMYLOSE TRIS(3,5-DIMETHYLCARBAMATE) COATED ON SILICA GEL STATIONARY PHASE IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

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This study represents thermodynamic characterization of separation of fenoprofen enantiomers inHPLC. Silicagel coated with amylose tris(3,5-dimethylcarbamate) was used as a stationary phase. Mixture of n-hexane/2-propanol was used as a mobile phase with flow rate of 2 ml per min. The experiment was conducted in the temperature range of 15–75 ºC with 5 ºC steps. The Gibbs´s free energy(ΔG^o), the molar enthalpy (ΔH^o) and the molar entropy (ΔS^o) of the analyte transfer from the mobile to the stationary phase were calculated using the plot of natural logarithm of the separation factor versus the reciprocal of the absolute temperature and according to the Gibbs-Helmholtz equation: $\Delta G^o = \Delta H^o - T\Delta S^o = -RT\ln K$.

From the results of this study it is clearly shown that increasing of temperature causes decrease of retention times of enantiomers, as well as values of resolution. At 45 ºC co-elution of both enantiomers and at 55ºC temperature reversal of elution order of enantiomers was observed.

Results of the study show that at low temperatures molar Gibbs’s free energy is mainly influenced by enthalpic term, but at high temperatures the enthalpic term is more and more compensated by entropic term and the isoenantioselective temperature, $\Delta_{S,R}\Delta G^o$ equals to zero and the enantiomers are no longer separated. Above the isoenantioselective temperature reversal of elution order of the enantiomers is occurred. Separation of enantiomers is now dominated by the entropic term [1].

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1. Chankvetadze, B., Recent developments on polysaccharide-based chiral stationary phases for liquid-phase separation of enantiomers, J. Chromatogr. A, 1269 (2012) 26-51.

THERMODYNAMICAL CHARACTERIZATION OF SEPARATION OF FENOPROFEN ENANTIOMERS USING AMYLOSETRIS (3,5-DIMETHYLCARBAMATE)IMMOBILIZED ON SILICA GEL STATIONARY PHASES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

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This study represents thermodynamic characterization of separation of enantiomers of fenoprofen in HPLC. Silicagel coated with amylose tris(3,5-dimethylcarbamate) was used as stationary phase, Mixture of n-hexane/ethanol-98:2+0.1% formic acid was used as a mobile phase, with flow rate of 2 ml per min. The experiment was conducted at the temperature range of 10 – 60ºC with 5ºCsteps.The Gibbs´s free energy(ΔG^o), the molar enthalpy (ΔH^o) and the molar entropy (ΔS^o) of the analyte transfer from the mobile to the stationary phase were calculated using the plot of natural logarithm of the separation factor versus the reciprocal of the absolute temperature and according to the Gibbs-Helmholtz equation: $\Delta G^o=\Delta H^o-T\Delta S^o=-RTlnK$.

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References:

1. Chankvetadze, B., Recent developments on polysaccharide-based chiral stationary phases for liquid-phase separation of enantiomers, J. Chromatogr. A, 1269 (2012) 26-51.

THERMODYNAMICAL CHARACTERIZATION OF SEPARATION OF IBUPROFEN ENANTIOMERS USING AMYLOSE TRIS-(3,5-DIMETHYLCARBAMATE)IMMOBILIZED ON SILICA GEL STATIONARY PHASES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

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This study represents thermodynamical characterization of separation of ibuprofen enantiomers in HPLC. Silicagel coated with amylose tris(3,5-dimethylcarbamate) was used as a stationary phase. Mixture of n-hexane/ethanol-98:2+0.1% formic acid was used as a mobile phase, with flow rate of 2 ml per min. The experiment was conducted at the temperature range of 10–75 ºC with 5 ºC steps. The Gibbs´s free energy(ΔG^o), the molar enthalpy (ΔH^o) and the molar entropy (ΔS^o) of the analyte transfer from the mobile to the stationary phase were calculated using the plot of natural logarithm of the separation factor versus the reciprocal of the absolute temperature and according to the Gibbs-Helmholtz equation: $\Delta G^o = \Delta H^o - T\Delta S^o = -RT\ln K$.

From the results of this study it is clearly shown that increasing of temperature causes decrease of retention times of enantiomers, as well as values of resolution. At 55ºCco-elution of both enantiomers and at 65ºC temperature reversal of elution order of enantiomers was occurred.

Results of the study show that at low temperatures molar Gibbs's free energy is mainly influenced by enthalpic term, but at high temperatures the enthalpic term is more and more compensated by entropic term and the isoenantioselective temperature, $\Delta_{S,R}\Delta G^o$ equals to zero and the enantiomers are no longer separated. Above the isoenantioselective temperature reversal of elution order of the enantiomers is occurred. Separation of enantiomers is now dominated by the entropic term [1].

References:

1. Chankvetadze, B., Recent developments on polysaccharide-based chiral stationary phases for liquid-phase separation of enantiomers, J. Chromatogr. A, 1269 (2012) 26-51.

SYNTHESIS OF NEW ADAMANTANE AND INDOLE CONTAINING DIPEPTIDES VIA UGI REACTION

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Adamantane derivatives are known to have a broad spectrum of biological activity including antiviral, antimicrobial, anticarcinogenic, anticataleptic, immunotropic, neuro-psychotropic and other effects. The wide spectrum of pharmacological activities of adamantane line derivatives are conditioned by the structure of their molecules. The diamond-like firm cyclic structure determines their unique physical, chemical and biological properties. The incorporation of an adamantyl moiety into several molecules results in compounds with relatively high lipophilicity, which in turn can modify the biological availability of these molecules. The adamantyl-bearing compound is more lipophilic than their des-adamantyl analogues. The high lipophilicity and unique geometry of the adamantane skeleton enhances considerably the permeability and adsorption of this type of compounds with respect to cell membranes This property of adamantane became of a great interest of scientists to use adamantane fragment for delivering the medicin alremedies inside cells and enhancing their pharmacological properties [1,2].

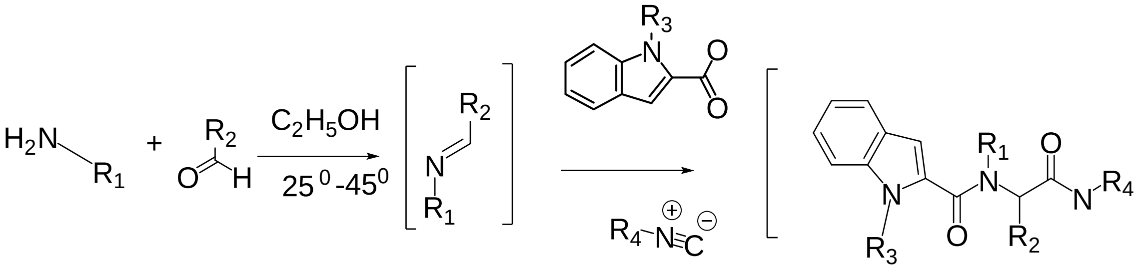
The Adamantane and Indole containing Peptide Selection Strategy is based on the following objectives: It is known that indoles are one of the most important alkaloids molecules found extensively in biological systems, which play vital role in many of the biochemical process [3]. Indole derivatives found to possess high which includes antibacterial, analgesic, antipyretic, antifungal, anti-inflammatory, anthelmintic, cardiovascular, anti-convulsant and selective COX-2 inhibitory activities. There are also amazing numbers of indole containing drugs in the market as well as compounds in clinical evaluation [3].

As it is known, peptides are biologically active substances. As therapeutic agents are widely manufactured in the modern pharmaceutical industry and synthesized compounds on their base are effectively used in neurology, endocrinology and hematology.

On the one hand, the interesting properties of Peptides, and on the other hand, the high biological activity of adamantane and indole containing compounds have become a cause to choose synthesis of Adamantane and Indole ring containing Dipeptides via multicomponent Ugi reaction as a research object, where reacting components are isocyanides, carbonic acids, amines and oxo-derivatives.

In the present study, we synthesized a series of novel indole- and adamantane moiety containing peptides by an Ugi-4CR by using N-methyl-indole-2-carboxylic acid and 1H-indole-2-carboxylic acid as an acid, Glycine ethyl ester and amino-1-adamantane as an amine, butyraldehyde, isobutyraldehyde and benzaldehyde as oxo compound, as an izonitrile we chose adamantine-1-isocyanoacetate and ethylisocyanoacetate. The reaction was carried out according to Scheme 1, among the equimolar ratio of the reacting components in the ethanol area, in different temperatures. After reaction is completed, the reaction mixtures were diluted with dichloromethane. Organic phase was washed withsaturated $NaHCO_3$ solution, followed by a 1M $KHSO_4$ solution. It was dried on Na_2SO_4 and concentrated on rotary evaporator. After the complete removal of the solvent, peptides (1-14) were separated by column chromatography with a standard method (SiO_2, Petroline Ether / Ethylacetate). The yield of obtained dipeptides (1-14) was 32-60%.

Scheme 1



1-14

R_1= (**1-6**)-$CH_2COOC_2H_5$, (**7-14**) -Ad;
R_2 =(**1,4, 7,10,13, 14**)-i-C_3H_7,(**2,5,7,10,13,14**)-C_3H_7 , (**3,6,9,12**)-C_6H_5;
R_3= (**1-7**)-H; (**4-6,10-14**)-CH_3 ;
R_4=(**1- 10**)-$CH_2COOC_2H_5$, (**12-14**)-Ad;

The structures of obtained new compounds (1-14) are determined by IR and NMR spectrum.

Acknowledgment: The designated project has been fulfilled by financial support of the Shota Rustaveli National Science Foundation (Grant YS-2016/71).

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SEPARATION OF TERBUTALINE ENANTIOMERS IN CAPILLARY ELECTROPHORESIS WITH CYCLODEXTRIN-TYPE CHIRAL SELECTORS AND INVESTIGATION OF STRUCTURE OF SELECTOR-SELECTAND COMPLEXES

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The affinity pattern of terbutaline enantiomers towards various cyclodextrins was studied using capillary electrophoresis. The affinity pattern of terbutaline enantiomers was the same towards all studied cyclodextrins except heptakis(2-O-methyl-3,6-di-O-sulfo)-β-CD. Nuclear magnetic resonance spectroscopy was used for understanding of fine structural mechanisms of interactions of β-cyclodextrin and its two sulfated derivatives with the enantiomers of terbutaline. The structure of terbutaline complexes with all 3 cyclodextrins studied was different from each other. In confirmation with our earlier studies it was shown again that capillary electrophoresis represents very sensitive technique for studies of affinity patterns in cyclodextrin complexes with chiral guests. Other instrumental (e.g. NMR spectroscopy and X-ray diffraction analysis) and theoretical techniques, although very useful for obtaining the information regarding the stoichiometry, binding constants and structure of intermolecular complexes, as well as about the forces involved in selector-select and binding and chiral recognition, may sometimes fail to properly sense those fine differences in the affinity patterns. Therefore, it is recommended to use capillary electrophoresis in order to examine correctness of affinity pattern determined for intermolecular complexes of cyclodextrins with guest molecules by other.

Capillary electrophoresis (CE) has been established as useful technique for analytical scale separation of enantiomers. To the major advantages of CE belong high plate numbers, operation in a single phase and advantages associated to this, easy adjustment of enantiomer migration order (EMO), possibility of generation of high separation selectivity from rather low thermodynamic selectivity of recognition, fast screening of chiral selectors, short method development time, easy combination of chiral selectors, etc. Until now still less recognized, and as the consequence less employed, remains high potential of this technique for sensing very weak effects in intermolecular interactions. High sensitivity of CE for detection of weak intermolecular recognition relies on high separation efficiency (theoretical plate numbers) of this technique. Thus, for instance, the thermodynamic selectivity of recognition 1.01 is sufficient for observing baseline resolved peaks in CE while this is not the case in chromatographic techniques even with the most advanced packing materials, column technologies and instrumentation. In addition to this, no immobilization of receptor/selector is required in CE and real physiological conditions can be mimicked easier compared to chromatographic techniques.

Other instrumental techniques, such as nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry, as well as molecular modeling calculations can provide invaluable information regarding the stoichiometry, structure and binding constants of selector-select and complexes but may not be as accurate and sensitive as CE is from the viewpoint of detection of selector-select and affinity pattern.

The affinity pattern of TBT enantiomers towards cyclodextrins (CD) was studied by using CE. Further, for selected TBT-CD complexes the structure in solution was studied by using 1D- and 2D rotating frame nuclear Over hauser enhancement spectroscopy (ROESY), atomistic models build, selector-select and interactions visualized and binding energies and partial contributions to them computed based on molecular mechanics (MM) calculations.

THERMODYNAMIC CHARACTERIZATION OF SEPARATION OF NAPROXEN ENANTIOMERS USING AMYLOSE TRIS (3-CHLORO-5-METHYL- PHENYLCARBAMATE) COATED OR COVALENTLY IMMOBILIZED ON SILICA GEL STATIONARY PHASES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

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The goal of our research was the calculation of thermodynamic parameters of separation of naproxen enantiomers in high-performance liquid chromatography. This can help to predict the suitable conditions of the analysis for the given compound and given column and to achieve the desired selectivity and elution order of enantiomers.

For the experiment arylpropionic acid derivative particularly naproxen, was chosen. This analyte was selected based on screening of 28 arylpropionic acid derivatives. These substances are non-steroidal anti-inflammatory drugs (NSIDs). It is important to separate their enantiomers, as frequently only one enantiomer has pharmacological activity and the other is inactive or even toxic.

Amylose tris(3-chloro-5-methylcarbamate) coated or covalently immobilized on silicagel was used as a stationary phase in this study. We have compared thermodynamic parameters of enantiomeric separation using coated and immobilized columns. Experiment was held at different temperatures and different mobile phases. We have studied if the enantioseparation is controlled by enthalpic or entropic term and what is the effect of temperature on values of retention and separation factor.

THERMODYNAMIC CHARACTERIZATION OF SEPARATION OF KETOPROFEN ENANTIOMERS USING AMYLOSETRIS (3-CHLORO-5-METHYLPHENYLCARBAMATE) COATED AND COVALENTLY IMMOBILIZED ON SILICA GEL STATIONARY PHASES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

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Arylpropionic acid derivatives are widely used chiral drugs. They belong to non-steroidal anti-inflammatory drugs group and are used as painkillers. Enantioseparation of chiral drugs is very important as their enantiomers commonly exhibit different pharmacological and toxicological properties. For this experiment ketoprofen was used as an analyte.

The goal of our research was the calculation of thermodynamic parameters of enantioseperation in high-performance liquid chromatography. The study can help to predict the right conditions for the analysis of given compounds and given columns and to achieve the desired selectivity and elution order of enantiomers.

Amylose tris(3-chloro-5-methylcarbamate) coated or covalently immobilized on silicagel was used as stationary phases in this experiment. We have compared thermodynamic parameters of enantiomeric separation using coated and immobilized columns. Experiment was performed at different temperatures using different mobile phases: mixture of n-hexane and polar organic solvents (2-propanol or ethanol) with the different volume ratios.

SEPARATION OF CHIRAL SULFOXIDES WITH CHLORO-SUBSTITUTED PHENYLCARBAMATES IN HIGH- PERFORMANCE LIQUID CHROMATOGRAPHY

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The goal of the present project was to synthesize and analyze newly synthesized chiral sulfoxides on their chiral recognition ability with different chloro-substituted cellulose phenylcarbamate-based chiral selectors in high-performance liquid chromatography using different polar organic mobile phase. By systematic variation of the chemistry and structure of chiral selectors and selectands those structural features were revealed which are the most critical for selector-selectand binding and chiral recognition ability.

It is very important to understand interactions between chiral compound and chiral center of the selector. These effects were observed in 2-propanol, methanol, ethanol as mobile phases and hexane as a non-polar component. This study illustrates that the additives to the mobile phase can be used for the adjustment of separation selectivity, not only mobile phase has significant influence, but also chemical structure of compounds has big role, as the group with donor or acceptor ability can change separation factor. It is important also for study of chiral recognition mechanisms with polysaccharide-based chiral stationary phases. The most likely structural elements responsible for chiral recognition were revealed.

SYNTHESIS OF ISOMERIC PYRROLOINDOLO[2,3-B]-QUINOXALINES AS APOTENTIONAL DNA INTERCALATORS

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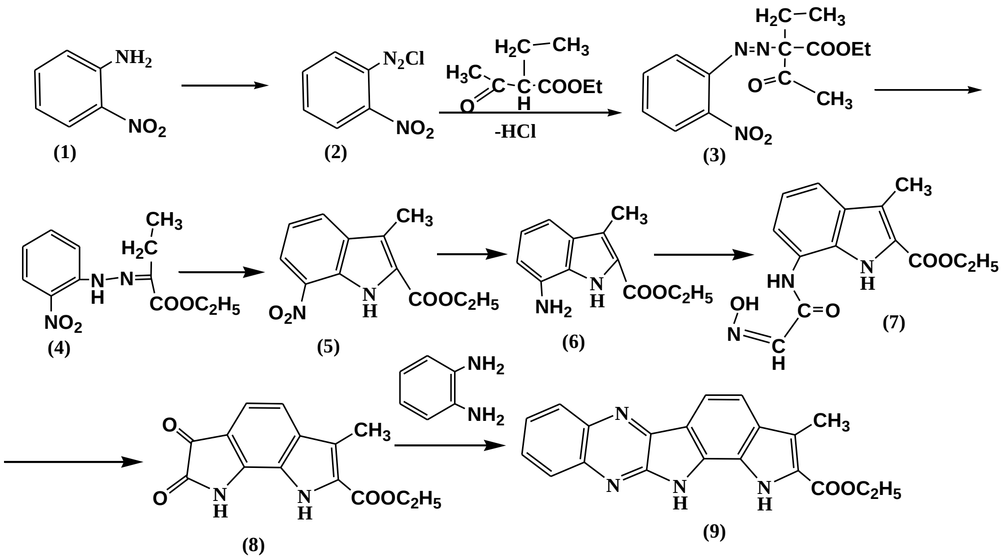
Heterocyclic compounds containing quinoxaline and/or indole rings have attracted considerable attention as a consequence of their diverse biological activities. Quinoxalines play an important role as a basic skeleton for the design of a number of antibiotics such as Echinomycin, Levomycin and Actinoleucin. In particular, 6H-Indolo[2,3-b]quinoxaline, a planar fused heterocyclic compound exhibits a wide variety of pharmacological activities. They are characterized by high antiviral, antifungal, cytotoxic, antimutagenic, anticancerogenic, herpes and other activity. Some 6H-indolo[2,3-b]quinoxaline derivatives, such as B-220 and 9-OH-B-220 have shown good binding affinity to DNA. In our opinion, it is interesting to build a new five ring containing condensed heterocyclic system by condensation of pyrroloindole and quinoxaline rings. It is possible to have 12 isomeric pyrroloindoloquinoxaline. It was successful to integrate indole and pyrrole nucleis in the trycyclic pyrroloindole condensed nucleous systems.

The basic compound was 3-methyl-2-etoxycarbonyl-7-nitroindole. (5) Reduction of nitro group of 3-methyl-2-etoxycarbonyl-7-nitroindole carried out in classical condition in area of $SnCl_{2,}$ ethanol and hydrochloric acid. Synthesis of isatin (8) is based on Sandmeier’s classical method. To transform 7-amino-2etoxycarbonylindole into isonitroso compound is carried out in room temperature in chloralhydrate and hydroxylamine. The last stage is the condensation reaction with o-phenylendiamine. It carried out in glacial acid.

Scheme



ENANTIOSEPARATION OF CHIRAL SULFOXIDES IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY WITH POLYSACCHARIDE-BASED CHIRAL SELECTORS AND AQUEOUS-ORGANIC MOBILE PHASES

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This study presents the results on separation of enantiomers in high-performance liquid chromatography (HPLC) with polysaccharide-based chiral selectors and aqueous-organic mobile phases. The factors responsible for a reversal of elution order have also been studied.

Separation of enantiomers of 14 chiral sulfoxides was studied on 17 chiral stationary phases based on polysaccharide trisphenylcarbamate derivatives. The mixtures of methanol-water and acetonitrile-water were used as mobile phases. This study showed that separations with methanol-water mobile phases follows typical reverse-phase behavior, namely, increasing of water content in mobile phase increased the retention time. However, in case of acetonitrile-water mixtures the behavior was a combination of hydrophilic and hydrophobic interaction chromatography. In some cases, reversal of enantiomer elution order was observed based on the content of water in the mobile phase. Column efficiency, resolution and selectivity varied depending on chiral selector and chiral analyte.

PHYSICAL AND CHEMICAL CHARACTERISTICS OF TUNG OIL OBTAINED BY VARIOUS METHODS

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Tung (Aleurites Fordii), as initial material in the production of high-quality technical oil, has great industrial importance. By the degree of drying capacity, Tung oilis far beyond the well-known vegetable oils, creatinggreat prospects for for its practical application. Tunglaquer-dyes protect metals against corrosion. It is the best in shipbuilding, aviation, mostly due to its small density, it is also used in electrical engineering. Tung oil is also widely used in the textile industry.

In the production field, there is well-known tung-aluminium, a waterproof material made of tung oil and aluminum rust that does not burn in the fire.

The subject of our research was the tung oil spread in Georgia, which was obtained in three different ways: direct extraction, squeezing out and combined method.

We were experimenting with the same raw materials and compared the results obtained.

The highest yield capacity was observed when processing tung oil by combined method (94,29% of existing in raw material), followed by processing by method of direct extraction (89,16%) and then by method of squeezing out (34,53%).

To compare tung oils obtained by different methods, we studied its major physical-chemical characteristics. Density, refraction index, acidity index, the values of soap solution bubble test and ester numbers. The squeezed-out and extractive tung oils are essentially the same. The maximum difference between these characteristics is not greater than 0,1%.

The study of fatty acids included in the tung oil by method of air-liquid chromatography has shown that in all cases, there are dominated 18 carbon atomic fatty acids, small-molecular fatty acids from C_2 (vinegar)to C_{14}(trimyristin). They change to 0.1% of the total composition. In most cases they are represented as mark.

The dominant compound in tung oil is $C18:3$-α-eleostearic acid,followed by $C18:2$–linoleic and $C16:0$ palmitin acid.

PRECURSOR EFFECTS ON SUPERCONDUCTIVITY PROPERTIES OF TL-1223 HTS

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Formation of the Tl-based superconducting materials critically depends on the used precursor and synthesis conditions. Using the wet chemistry offers some advantages in comparison with the classical solid-state ceramics processing, especially, better chemical homogeneity and higher reactivity of the precursor powder. On this basis the influence of $Ba_2Ca_2Cu_3O_y$ precursor on the synthesis and properties of $TlBa_2Ca_2Cu_3O_y$ has been examined.

$TlBa_2Ca_2Cu_3O_y$ superconducting samples were prepared by a two-step method. In the first step, was prepared Ba:Ca:Cu = 2:2:3 multiphase ceramic precursors, for comparisons two methods we synthesized precursors by sol-gel method using polymerization (SGMP) and as well as ordinary solid-state reaction method (SSRM). In second step on both samples Tl_2O_3 was added and finale synthesis of $TlBa_2Ca_2Cu_3O_y$ was carried out in a sealed quartz tube.

We note that for both methods, starting materials was used powders materials (Sigma-Aldrich) of BaO (99.98%), $CaCO_3$ (99.0%) and CuO (99.999%). The synthesis of a precursor by the sol-gel method was used acetic and nitric acid for dissolved oxide and EDTA acid (≥ 99%) as a complex-forming agent. For polymerization we used Acrylamide monomers (≥ 99%); N,N' – Methylenebis(acrylamide) (99%); 2,2-Diethoxyacetophenone (>95%).

The X-ray diffraction pattern of $Ba_2Ca_2Cu_3O_y$ precursor powder showed that, the samples consists only two phases of $BaCuO_2$ and Ca_2CuO_3. The existence of $BaCuO_2$ and Ca_2CuO_3 phases only is a good indicator for qualitative preparation precursor powder with Ba:Ca:Cu = 2:2:3 cation ration.

The sensitivity of X-ray diffraction to carbonate might be not sufficient, therefore we used IR spectroscopy for fixed anything remain CO_3^{2-} impurity species. Absorption spectra of the precursors, with annealed in different temperature, are shown in fig. 1 for the range 400-4000 cm^{-1}. The signature of carbonate is clear for SSR-precursor annealed at 900°C. The CO_3^{2-} ion which occurs at 692 cm^{-1}, at 855 cm^{-1}, at 1,058 cm^{-1}, and at 1,440 cm^{-1}.

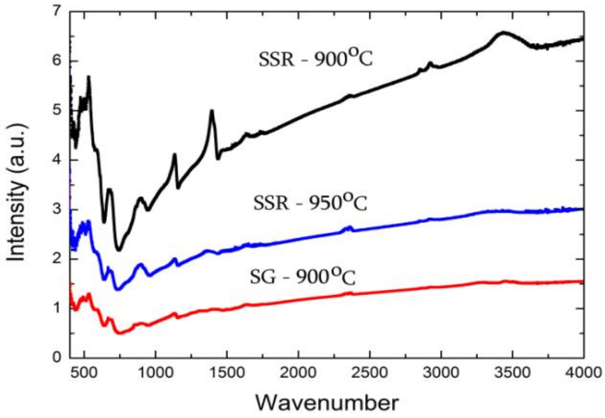

Figure 1: IR spectral analysis of $Ba_2Ca_2Cu_3O_y$ after annealing in flowing oxygen partial pressure of 0.3 BAR: For SG-precursor at 900 °C and for SSR-precursor at 900°C and at 950°C

By contrast, for SG-precursor annealed at 900°C remain CO_3^{2-} impurity species are not observed and also for SSR-precursor annealed at 950°C. Barium crystalline oxide BaO presents an intense band at ~483 cm^{-1} and a low one at ~503 cm^{-1}. The appearance of strong IR absorption band at 424 cm^{-1} may be attributed to the lattice vibrations of CaO. According to McDevitt and Baun, there are two IR absorptions characterizing Ca–O lattice vibrations of pure CaO, a broad, strong absorption centered around 400 cm^{-1} and a medium strong band at 290 cm^{-1}, which, if present, are involved in the blackout absorption displayed in the present spectrum at <600 cm^{-1}. For CuO quantum dots, three main vibrational modes are observed at 468, 529, and 590 cm^{-1}. As a result, we could conclude that, in comparison with SSRM in SGMP sample we found highest value of the transport critical current densities J_c.

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THE EVALUATIN OF SOME QUALITATIVE PARAMETERS OF VEGETABLES AND THE PRODUCTS PRODUCED FROM THEM

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The vegetables represent important source of vitamins, phytoncides, microelements and nutritious fibers for a human. Despite the difference between the vegetables they all have the following common qualities: carbohydrates, vitamins, great amount of biologically active admixtures on the basis of low consistency of proteins and fats, great consistency of water; great amount of vitamins and minerals; support the activity of food digestion ferments; the possibility of using them in the form of raw [1]. In 2005 Georgian parliament has adopted a law about “Food Safety and Quality” according to which the basic principles for food safety are the following: risk analysis, warning, transparency and protection of customers' interests.” The main goal of the law is: “protection of customers' health, life and economic interests regarding to the grocery for the Customer, foreseeing effective functioning of inside market and the diversity of it” [2, 3].

Taking into account great importance of vegetables in food ratio of a human our goal was to provide evaluation of some qualitative parameters of vegetables (potato, onion, tomato) and the product received from them (tomato-pasta) being realized at local Georgian market. For examination potato (Khulo, Akhalkalaki, Turkish), onion (Gori, Turkish), tomato (Marneuli, Turkish), tomato-pasta (Marneuli and Turkish - “Kingtom”) were selected.

Maximum permissible concentration of nitrates in potato equals to 20 mg/kg. This parameter was minimal in Akhalkalaki potato (95,7 mg/kg) and it was maximal in Turkish one (240,5 mg/kg). The consistency of nitrates in Khulo potato was 148 mg/kg. According to the mentioned parameter the priority was given to Akhalkalaki potato. The starch is one of the main consisting parts of potato (25%), the calorific value of it equals to 4 kcal/g. the high concentration of starch was fixed Akhalkalaki potato (23%) compared to Khulo potato (21%). The concentration of starch in Turkish potato was lower by 6% to the set norms, though it is notable that no samples were satisfying the desirable results by the concentration of starch [4].

The onion is distinguished from the vegetable crops with the lowest concentration of nitrates. The maximal permissible concentration of nitrates in onion equals to 80 mg/kg. In examination samples of Gori and Turkish onions the concentration of nitrates was lower by 3-4 times to maximal permissible concentration norm. Herewith, according to the mentioned parameter, Gori Onion was distinguished with the better quality (19, 5 mg/kg) compared to the Turkish (23,8 mg/kg) onion [5, 6].

The maximum permissible concentration of nitrates in tomato equals to 250 – 300 mg/kg. The concentration of nitrates in the samples of Marneuli and Turkish tomato is in the limits of maximal permissible concentration 250-267 mg/kg. The concentration of nitrates in Turkish tomato is 1,1 times more rather than Marneuli tomato [7].

Titric acidity of Marneuli tomato-pasta was less by 3% from Turkish tomato-pasta “Kingtom” [8]. According to the soluble dry substance, Marneuli tomato-pasta had insignificant priority [9,10].

Hence, the best physical-chemical parameters of Akhalkalaki potato, Gori onion, Marneuli tomato and Marneuli tomato-pasta were distinguished among the vegetable samples taken for examination.

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STUDY THE LEVEL OF TOXICITY AND POSSIBILITIES OF REMEDIATION OF ARABLE SOILS CONTAMINATED WITH HEAVY METALS IN IMERETI REGION (CHIATURA-ZESTAFONI)

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Soil is a complex and diverse changing according to climatic-landscape territories. Plants can maximally accumulate toxic substances from soil with their further migration in transfer to the human body. For this purpose, a natural migratory soil-plant-man relationship is used.

Much importance is given to ecotoxicology, where the bio-indication and chemical and biological monitoring operations of environmental protection are combined. The consumer attitude toward soil and their improper use contributed to the development of negative processes. Almost all soil types in Georgia experience a shortage of necessary nutrient elements. Any agriculture production should be considered as circulation of substances, implying the management and maintenance of ecological balance. Unless soil fertility is constantly increased, the growth of agricultural production could hardly be retained. The detrimental effect of industrial waste on bio-systems and generally on the ecological situation belongs to the series of problematic issues. An important place is occupied by reintroduction of industrial waste into the production circle by using cost-effective and efficient technologies and the obtaining of worthy products there from [1].

The object of the present research is Chiatura-Zestafoni arable soils of Imereti industrial region. The level of heavy-metal contamination and toxicity of the soils under study was studied using modern test methods. In particular, TCLP (toxic Hazardous Characteristic Leaching Procedure) test method implies the soil leaching process over 24 hours under conditions of continuous agitation using a magnetic stirrer. It enables to identify the active water-soluble forms, toxicity characteristic, valence, pH and range of heavy metal from leached soils.

According to the WET test method, soil leaching procedure takes place over 48 hours under conditions of continuous agitation using a magnetic stirrer. In the view of error, the results of the both methods were compared.

For soil restoration and remediation an organic fertilizer and plant growth stimulant K3 was used, the technology of which had been developed by us. Pilot research was carried out in different regions. The results are positive and the organic fertilizer/stimulant is being now certified for its future production and marketing on noth the local and international market. The fertilizer can be applied to fertilize and remediate all types of soil. For microorganisms available in soil it represents a vitally important nutrient medium, both in the liquid and solid form. It regulates the redox process in soil, improves soil porosity, increases the content of general organics and humus which, in turn, tells upon quality and quantity of the final product. It production is simple, non-waste, quality and cost-effective. In case the soil type and suitability factor are correctly identified, the favorable results will not tackle long the product`s quality and yield will correspondingly grow. [2] [3].

The visual image of the fertilizer is given below:

Figure 1. Fertilizer-stimulant K3

Production of organic/non-chemical fertilizers is effective and profitable both in Georgia as well as in the European Union countries, where soil degradation also represents a serious problem. We should not make soils dependent solely on chemical fertilizers. To guarantee a good yield, soil should be regularly fertilized and subjected to a follow-up remediation. The proper management in farming means the growing of safe agricultural products and upgrading their quality which, in turn, will contribute to the development of a competitive production.

The level of toxicity of soils contaminated with heavy metals, their active/soluble forms, valency, pH and range/prevalence in one of the industrial regions of Georgia (Chiatura-Zestafoni) were studied using the EPA test-methods. For less fertile and barren soils a new method of producing an organic fertilizer and plant growth stimulant K3 was developed, which can be applied in both the liquid and solid form. The fertilizer is distinguished by the simplicity of technology, ecological safety and a wide range of application.

The technologies developed and applied by us are up-to-date and with good prospects for a wide application in agriculture as well as in the identification of the toxicity level of any industrial waste and conditions for their further remediation. By our calculations, it will highly compete with the fertilizers and plant growth of agricultural production could hardly be retained. The detrimental effect of industrial west on bio-systems and generally on the ecological situation belongs to the series of problematic issues.

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IMPACT OF MODIFICATION ON THE THERMAL AND MECHANICAL BEHAVIOR OF ANTIMICROBIAL HYBRID COMPOSITES

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Hybrid binder systems have been attracting much attention recently for the purpose of the creation of high-performance or high-functional polymeric composite materials. The versatility of the inorganic-organic hybrids offers polymers that improve the durability, the mechanical, thermal, chemical and heat resistance, the weatherability, gloss and color retention and adhesion of composites, coatings, adhesives, paints, medical and dental products etc.

The use of coatings as a method to protect microbiologically-influenced corrosion is focused on the application of non-toxic products based on polymer matrix (silicones, polyurethanes, epoxy resins and fluorinated compounds etc.); modifiers of polymer networks;

bioactive additives (inorganic, organic& organometallic compounds, bio-molecules, clusters, etc.); curing agents.

Thermophysical investigations of control and modified polymer composites and hybrid materials based on polyfunctional hetero-chained organic polymers have been carried out.

Differential Scanning Calorimetry (DSC) monitors heat effects associated with phase transitions and chemical reactions as a function of temperature and it was used to characterize the important properties of the researched materials, such as the crystallinity, thermal transition and the melting temperatures. Tests were performed on DSC 200 apparatus (Netzsch, Germany) in N_2 atmosphere at the heating rate of 5◦C/min from -100 to +300◦C region. Endothermic picks on DSC curves corresponded to the glass transition temperatures (T_g) of tested samples are shown in the range from +38.8^{o}C to +59.7^{o}C. Doping of nano ATO as bioactive component into basic polymer has no significant influence on the value of T_g. Glass transition temperature regions are more sensitive towards siloxane modifiers. In particular, their incorporation provokes a decrease of T_g from 58.7-56^{o}C to 38.8-44.3^{o}C.

DSC study show also phase transition in the glassy state, so called β-transitions (T_β). The addition of bioactive additive into modified polymer composites reduces absolute value of T_β from –56^{o}C to –(48-51)^{o}C. Thus, adding of 3 wt.% ATO to PU, results in lowering of the β-transition temperature centered around the regions from –43.6^{o}C to –37^{o}C correspondingly. Thus, addition of BCs enhances the stability of the low temperature amorphous phase.

Decomposition behavior and thermal stability was determined using Perkin Elmer TGA-7. Cured samples were studied at the heating rate of 20°C/ min in the temperature range of 50°C-800°C. All results from thermal studies has shown a high influence of the modifiers and bioactive additives on the thermal stability of the basic polymer matrices under investigation. The modified materials presented decomposition temperature higher than those of the non-modified materials. Namely, intensive destruction process of pure PU matrix occurred at 290-460^{o}C with a large weight loss of 81.3% of the original weight. The second stage of decomposition commenced at 460-570^{o}C with drop of remaining weight. The thermal stability of modified PU-composites shown improvement, - both $T_{\mathrm{st.dec}}$ and T_{max} are shifted to higher temperatures with respect to pure PU. This effect enhances as the amount of modifier increases. Further addition of BC shifts $T_{\mathrm{In.dec.}}$ to the higher temperatures with significantly reduced weight loss. The full thermal degradation of modified hybrid composites was observed in the range of 580-685^{o}C.

By performed studies the improvement with thermal stability and with T_g compared to the non-modified firms for high temperature applications of obtained mechanically and photochemically stable composites has been shown.

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TRIBOLOGICAL CHARACTERISTICS OF FLUORINE CONTAINING FUNCTIONALIZED POLYMER HYBRID COMPOSITES

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Fluorine-containing polymers are widely used in material science because of their unique properties including high thermal, chemical, aging, and weather resistance; They are well known as extremely low surface energy materials, which have low dielectric constants, and flammability; excellent inertness to solvents and moisture adsorption, as well as interesting oil and water repellent surface. Materials on their basis have been achieved the transition from fundamental researches to practical applications and have been proposed for the development of advanced hybrid organic-inorganic coatings of various substrates (textiles, papers, leather, wood, etc.).

The tribological properties (adhesion, scratch and wear resistance, friction) and morphology of the hybrid coating materials based on fluorine containing functionalized polymer composites and bioactive additives have been investigated. Infrared spectroscopy (IR) analysis was performed to determine the eventual curing extent of the systems studied. Micro Scratch tester [CSEM, Neufchatel] and Nanovea pin-on-disk tribometer was applied to study tribological behavior and long-term performance of researched materials. Penetration and residual depths as a function of the scratch number at the constant force (5.0N) was measured during scratch tests to determine sliding wear (SWD) and scratch resistance. Progressive scratch testing with linearly increased load 1.0N-30.0N was performed to study resistance to the instantaneous penetration. The average dynamic friction values and dependence of the dynamic friction on the sliding distance of non-modified and modified matrices and corresponding hybrid coatings were determined as well.

Results of testing of laboratory patterns have shown improved features by modification depending on the type and ratio of hybrid components. In particular, good adhesion on various surfaces, high scratch resistance, lowered dynamic friction coefficient, increased viscoelastic recovery, increased wear resistance and lower values of wear rate at room temperature even after thermal aging. Scanning electron microscopy observations [(SEM), Nicon Eclipse ME 600] before and after testing and aging (50 and 500 μm) have shown significant amounts of wear debris and crack formation for non-modified polymer composites while insignificant wear tracks, more ductile behavior and no phase separation are seen for modified hybrid systems.

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STUDIES OF ARSENIC CONTAMINATION OF RIVERS AND SOILS IN SOME REGIONS OF GEORGIA

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In Georgia there are many sources, whether natural or anthropogenic, which causes environmental pollution by arsenic compounds. Arsenic sulfide ore mining, processing and production of arsenic-containing drugs was carried out for decades (Racha-Lechkhumi and lower Svaneti). In the Article is presented studies of eco-chemical conditions for soils contaminated areas with arsenic industrial wastes (in the village Uravi - Ambrolauri Municipality, village Tsana - Lentekhi Municipality) and surface water (River Tskhenistskali and Lukhuni) 2014-2016years.

The sampling of the soil and water, conservation, labeling, storage and transportation were produced in the accordance with the International Standard Organization (ISO) standard methodology. The study was conducted in laboratory by the ISO standards and USEPA methods in soil samples arsenic will be determined by plasma–emission spectrometer.

The survey results shows that the arsenic maximum content in 2014 were observed in the vicinity of Uravi white arsenic treatment plant, where the arsenic maximum concentration was 61814.9 mg/kg and in the settling of the surrounding area - 36373.7 mg/kg; According to the 2015 data a high value was observed only in the samples from the 3rd site and settling in the village Tsana. The results were the following 59025.0 mg/kg and 55795.0mg/kg. Ecologically most polluted rivers are: Tskhenistskali and Lukhuni.River Tskhenistskali (upper Tsana) arsenic concentracion in 2014 exceeded the MPC. While in 2016 the concentrations were in the norms and in most cases it has been a declining trend.

REACTION CONDENSATION OF P-AMINOBENZOIC ACID ETHYL ESTERS WITH D-GLUCOSE AND D-GALACTOZE AND THEIR BIOLOGICAL ACTIVITY

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Synthesis of carbohydrate derivative and study of their biological activities an important process for disease prevention. Especially, carbohydrate containing nitroso group, because they have an effect of vasodilator. They play an important role in the process of apoptosis and cell- proliferation. Also, carbohydrate derivatives containing nitroso group participates in the functioning of the immune system and nervous system.

The goal of present investigation consists in synthesis of N-glycosilamines containing in a Molecule nitroso group (N=O). As an initial substance in the given work has been used the products of condensation of D-glucose (1) and D-galactose (2) from p-aminobenzoic acids ethyl esters - β– N-p-aminobenzoic acids ethyl esters-D–glucopyranozylamine and β– N-p-amino-benzoic acids ethyl esters- D–galactopyranozylamine (4).

By interaction of compounds (3,4) with sodium nitrite corresponding nitroso-derivatives (5,6) has been received. Reaction proceeds according to the following scheme: The structures of obtained compounds were established by physical-chemical methods of analysis.

Investigation of biological activity potential of synthesized substances will be carried out by the of “PASS Online” computer application.

The effect of nitroso (-N-N=O) group on the biological activity spectrum of synthesized N-glycosides will be revealed by assessment of structure-activity relationship. The investigation result enables selection of the most prospective compounds from the set of synthesized substances.

PREPARATION OF RESORBABLE POLY(ESTER AMIDE) NANOPARTICLES FOR OCULAR DRUG DELIVERY

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The elaboration of nano- and microscale drug delivery systems is very actual nowadays since the selective (targeted) drug delivery is one of the important problems of modern pharmacotherapy. Most of the eye diseases are related to visual impairment and blindness. Treatment of these pathologies is one of the major challenges of modern ophthalmology.The eye is well protected by efficient mechanisms that rapidly remove drugs after instillation on the eye surface. Physical-biological barriers such as the cornea prevent drugs from intraocular penetration. Hence, eye drops are less effective for the treatment of various diseases, which necessitates a risk-containing procedure of intravitreal injection. One of the rational ways to overcome the problem is the application of drug-loaded polymeric nanoparticles (NPs) that are able to penetrate through the ocular barriers when administered topically. Amino acid-based biodegradable poly(ester amide)s (PEAs) are one of the most promising for the design of NPs.

We have elaborated biodegradable NPs of various types by nanoprecipitation of the PEA composed of L-leucine, 1,6-hexanediol and sebacic acid (8L6). The originally designed arginine-based cationic PEA and comb-like PEA containing lateral PEG-2000 chains along with 8L6 anchoring fragments in the backbones were used to construct positively charged and PEGylated NPs. The NPs were loaded with fluorescein diacetate (FDA) as a fluorescent probe to detect if the NP penetrated into the cells. A preliminary in vivo study on intraocular infiltration of the NPs has been done using wild-type C57BL/6 mice. After penetrating into the cellular lysosomes, FDA probes became visible due to the hydrolysis of the diacetate groups, thus allowing for the detection of the NPs as tiny fluorescent spots inside the tissues. One day after administration, fluorescent dots were found at various sites - always in the peripheral cornea and the sclera, and in different layers of the outer retina depending on the type of NPs used. Four days after administration, fluorescent dots were still visible in the peripheral cornea and the sclera with some of the NPs. These results show that the new type of NPs infiltrate the ocular tissues after topical administration and are taken up by the cells. This raises hope that the NPs may be useful for ocular delivery of therapeutic agents.

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ATMOSPHERIC MEASUREMENTS AND MONITORING IN TBILISI

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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 O_3 41 M for ozone measurement.

For our analysis we also used oxygen and argon pressurized cylinders. Argon was used for sample dilution prior to analysis and for washing out cylinders and oxygen was used for ozone generation and purge gas for NOx chemiluminescence instrument.

As mentioned above, measurement of nitrogen oxides is conducted via ozone chemiluminescence.

$$\boldsymbol{NO} + \boldsymbol{O}_3 \rightarrow \boldsymbol{NO}_2 + \boldsymbol{O}_2$$

$$\boldsymbol{NO} + \boldsymbol{O}_3 \rightarrow \boldsymbol{NO}_2{}^* + \boldsymbol{O}_2$$

$$\boldsymbol{NO}_2{}^* \rightarrow \boldsymbol{NO}_2 + \boldsymbol{h\nu}$$

$$\boldsymbol{NO}_2{}^* + \boldsymbol{M} \rightarrow \boldsymbol{NO}_2 + \boldsymbol{M}$$

$\boldsymbol{NO}$ react with ozone to form some amount of exited $\boldsymbol{NO}_2$ molecule, which returns to ground state and emits photon, which is detected by photomultiplier tube.

Together with the online sampling we also perform cylinder sampling. We choose 3 points for sampling at the same time, with 2 cylinders at each place in order to measure the inaccuracy between the measurements. We took samples at different times during a day, to determine air contamination gradients for air pollution in time.

As a result of our measurements, most of them nitrous oxides were higher than the concentration limit. The high concentration of air pollution is indicated during the rush hour.

CONTAMINATION GRADIENT FOR AIR POLLUTANTS IN SPACE

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Climate change and its impact on ecosystem is one of the main problems of 21st century. Increase of greenhouse gases in the atmosphere was regarded as an important cause. Atmospheric composition has significantly changed due to intensive technogenic pollution.

Atmospheric pollution due to dust, carbon, sulfur and nitrogen oxides, ground ozone quantity in Georgia and especially in Tbilisi significantly exceeded maximum permissible level, that effected human health.

In Georgia the public transport system is not sufficiently developed.Most vehicles on Tbilisi's roads are old and run on diesel.

Thus, the main purpose of our study was to assess the level of pollution in Tbilisi's atmospheric air. Namely the determination of air pollutants concentrations and their monitoring in the air.

The work was performed on the basis of SMART | AtmoSim_LAB. The laboratory investigates air pollution in Tbilisi.

NO and NO2 was measured using ECOPHYSICS CLD 780 TR Ozone chemiluminescence instrument, CO/CO_2 and CH_4 was measured by PICARO CRDS cavity ringdown spectroscope.

During the experiment we observe the level of air pollution in different districts of Tbilisi. In this particular case we took samples at different places and different time of the day - in the morning, afternoon and evening.

NITROGEN OXIDES POLLUTION IN TBILISI

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

$$\boldsymbol{NO}_2^* \rightarrow \boldsymbol{NO}_2 + \boldsymbol{h\nu}$$

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

$$\boldsymbol{NO} + \boldsymbol{O}_3 \rightarrow \boldsymbol{NO}_2^* + \boldsymbol{O}_2$$

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

$$\boldsymbol{NO}_2^* \rightarrow \boldsymbol{NO}_2 + \boldsymbol{h\nu} \text{ (radiating)}$$

$$\boldsymbol{NO}_2^* + \boldsymbol{M} \rightarrow \boldsymbol{NO}_2 + \boldsymbol{M} \text{ (quenching)}$$

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

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

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 $\mu g/m^3$ and for NO is 40 $\mu g/m^3$ (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 are 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.

DEVELOPING THE ALOE PULP SUPPOSITORY FOR TREATING INFLAMMATORY AND HEMIC DISEASES

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The paper dwells on the aloe as the properties of medicinal plant. The examples of using the aloe for treatment of many diseases are given. The paper also justifies the possibility of developing the medicinal herbal remedies containing the candle-shape aloe pulp. For the preparation of the suppository, there has been selected the diphilic basis in the form of goat’s fat, which is a natural, less allergic product and is melting easily for the release of medicinal substances at a body temperature. Goat's fat belongs to the bases of a diphilic emulsion nature and receives the liquid component equally, without adding the emulsion. Using the appropriate technology, there has been developed greenish colored suppository of the uniform consistency. The weight of the finished medicinal candle is 2 g, and it contains 1,2 g of goat’s fat and 0,8 g of the aloe pulp. The melting temperature is 370^0C. At a room and temperature, it retains its shape and stability. It is kept in the refrigerator, and shelf life is 1 week. Antiseptic, anti-inflammatory, wound-healing, blood-stopping in the medicinal candles are in a unique combination with softening and regenerative properties of goat’s fat. It can be used for treating proctitis, paraproctitis, hemorrhoid and other straight intestine diseases.

HYDROCHEMICAL STUDY OF WATER FROM TENGIZI SPRING OF NAKHUNAO COMMUNITY OF MARTVILI MUNICIPALITY

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Chemically clean water does not exist in nature. When moving through the earth's crust, water comes in contact with many minerals, solves them, and carries throughout its entire journey. Natural water is a solution containing substances of various character and condition [1].

Calcium and magnesium ions are the leading ions of low-mineralized waters. [2]. The calcium content in the waters of the rivers does not exceed 250 mg/l. The content of magnesium and calcium is much higher in the underground waters [3]. The content of magnesium, calcium and iron in fresh waters depends on soil type, water season and the period of the day [4].

The aim of our study was to study the content of magnesium, calcium, iron, HCO_3^-, SO_4^{2-}, Cl^-, I^-, CO_2, oxygen, BOD$_5$ and biogenic elements in Waters of Tengizi Spring of the village Nakhunao in Martvili Region.

The relevance of the issue' is conditioned by the fact that the content of the above-mentioned ions in the water will be analyzed for the first time. Highly sensitive methods were selected for this reason.

Analyzes were conducted in the Analytical Chemistry Laboratory at Akaki Tsereteli State University. The methods approved in hydrochemical practice were used for the analysis [5].

The acidity rate was measured by a potentiometric method (Potentiometer pH 673-M).

Chlorides were determined through the mercurymetric method (titrant 0,01 $Hg(NO_3)_2$. indicator diphenyl (carbazole).

Hydrocarbonates were determined through the acidimetric method (titrant 0,1-0.011 N HCl indicator methyl orange).

The content of calcium and magnesium, as well as general hardness of waters are determined by a complexonometric method (titrant 0,01N, complexon III. Eriochrome Blackwas used for the determination of magnetic ion content, a recommended range was created through ammonia buffers; Murexide was used as an indicator to determine calcium ion. Alkaline environment was created through 2N sodium alkali).

Sulfate ions were determined by the classical gravimetric method, the precipitation form is $BaSO_4$.

General iron in waters is determined through photometric method after pre-oxidation in the alkaline area (photometric reagent sulfosalicylic acid) (photoelectric colorimeter).

Carbon dioxide was determined through alkalimetric method. Titrant 0,1-0.011N $NaOH$. Indicator phenophtalein.

We have observed oxidation by means of permanganometric method (oxidizer 0,01N $KMnO_4$, in acidic area. Titrant 0,01 N $H_2C_2O_4$)

Oxygen content and BOD$_5$ were determined through the iodometric method (titrant 0,01 N $Na_2S_2O_3$. In alkaline environments $Mn(OH)_2$ is oxidized through the oxygen dissolved in water and is transformed into the four-valence manganese compound, which during the acidation in case of excessive KI produces I_2).

The amount of dry residue is determined through classical gravimetric method.

Iodide ion was determined through Reznikov method [6] (titrant 0,01N $Na_2S_2O_3$). Oxidizer - bromine water).

Biogenic substances were determined by a photometric method: NO_2^- shell reagent, NO_3^- sodium salicylate, NH_3 Nesler's reagent, PO_4^{3-} ammonium phosphormolibdate.

Table 1. The Results of Hydrochemical Study of Water from Tengizi Spring of Nakhunao Community of Martvili Municipality

pH	**Mg^{2+}**	**Ca^{2+}**	**General iron**	**HCO_3^-**	**SO_4^{2-}**	**Cl^-**	**CO_2^-**	**Oxidability**	**Oxygen content**	**BOD_5**	**Dry residue**	**NO_2^-**	**NO_3^-**	**NH_3**	**PO_4^{3-}**	**I^-**
	Mg/l															Mkg/l
6,28	0,1000	0,0074	0,02	0,0060	0,0206	0,0005	0,0118	2,16	9,79	8,16	0,33	-	-	-	-	2,538

The content of the above-mentioned ions in the studied waters is within the scope of the norm and can be used for drinking and agricultural purposes.

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ECOLOGICAL CATASTROPHES ON OUR PLANET

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Air pollution of the atmosphere is considered a major problem of mankind. As modern civilization continues developing, the environment becomes more damaged. As technology progresses, we must use more energy. The main resources used for energy are oil, gas and raw minerals. Using fossil fuels for energy results in emissions, that are harmful to the atmosphere. For example, carbon dioxide, sulfur and nitric oxides, and other dangerous gases which violate the thermodynamic balance between the earth and space. As we know, 70% of radiation is absorbed by our planet and the remaining 30% is reflected. When a concentration of carbon dioxide hits its maximum, it obstructs the process of energy exchange, which causes a global process called the “Greenhouse Effect”

In general, the “Greenhouse Effect” is the process by which radiation warms the planet’s surface to a temperature higher than it would be without its atmosphere. Contribution to the greenhouse effect on the earth looks like: water vapor (36-70%), carbon dioxide (9-26%), methane (4-9%), ozone (3-7%). When the temperature increases, many unpleasant processes happen such as: landslides, avalanches, and an uneven distribution of rain which leads to flooding. It’s known that every year approximately 150,000 people are killed by these negative consequences.

Another significant problem which influences the earth is the depletion of the ozone layer. The Ozone Shield is the region in the atmosphere which absorbs most of the sun’s ultraviolet radiation and protects our population. In 1976 researchers revealed that the ozone layer was more depleted by chemicals called chlorofluorocarbons which were released in the atmosphere. With the reduction of the Ozone Shield, radiation enters the atmosphere and threatens world life, increases the risk of skin cancer for human beings and other ecological problems. The destruction caused by chlorofluorocarbons is due to interaction with electromagnetic radiation and releases halogen’s radicals, therefore destroying ozone molecules.

The depletion of the ozonosphere by anthropogenic factors is an unfortunate reality which remains a main problem of humanity. The Vienna Convention was negotiated in 1985 in order to protect the environment and therefore society. Twenty countries signed on for protection of the Ozone layer. After a short time, 43 countries agreed on this protocol. Today almost every country in the world prohibits using hazardous chlorofluorocarbons.

Annual events are held all over the world for the protection of nature. In order to solve the problem of the “Greenhouse Effect”, it is recommended to find a new way to produce electricity instead of using fossil fuels. We must plant more trees, referred to as “Green Gold”. Unsuitable ecological conditions influence not only the environment, but society as well. It is every person’s duty to care for our planet and make advantageous conditions for the following generations.

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NATURAL AND SYNTHETIC NON-SUGAR SWEETS

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Fighting to obesity and diabetes is importance and actual issues today. Both problems are duo of irregular eating carbohydrates and other organic compounds.

Solutions of those problems are balanced and exact planed diet.

To control and prevent excess weight and diabetes, it needs to low of level carbohydrates and use less calories products such as sugar substitutes and as known artificial sweeteners.

There are many varieties use of them like in cooking, sometimes they are main compound of tooth paste and most important is beverages, like calories free drinks.

There are many advantages of use sugar substitutes like they do not cause caries which lead to tooth decay, they do not or little contain calories and can be used during diabetes, because they do not increase level of glucose.

Sugar (sucrose)'s substitutes history started in the end of nineteenth century, exact in 1879 when first artificial sweetener-saccharine was accidentally created.

After decades many theories were created which correlate organic molecule structure and their organoleptic properties each theory made little efforttodevelopto synthetic sugar substitutes. However today there is huge use of natural sugar substitutes such as mono carbohydrates' derivatives and other compounds.

Even though there are more and more people who use these food additives, there is always doubt that they cause some diseases like cancers or increase chances to it. This doubt based on lack of researches, but this does not mean that every sugar substitute is good to use. There are some which are banned because they toxicity action in human body. FDA (American food and drug administration) defines which sugar substitutes can be used in USA and do limit how much they can be consumed each day for one person.

At last it is importance for chemist to study for analysis used compounds to prevent ourselves from danger use of them and most importance finds new ones to they will be better for use to our hearth.

For report were used the data from internet:

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CRYSTAL FIELD THEORY FOR COMLEX COMPOUNDS: MAIN ASPECTS

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Theory of bonding in coordination compounds must account for properties such as color and magnetism, as well as stereochemistry and bond strength. No single theory as yet does all this for us. Several different approaches have been applied to transition metal complexes. We will consider only one of them – crystal field theory – because it accounts for both the color and magnetic properties of many coordination compounds.

Crystal field theory explains the bonding in complex ions purely in terms of electrostatic forces. In a complex ion, two types of electrostatic interaction come into play. One is the attraction between the positive metal ion and the negatively charged ligand or the negatively charged end of a polar ligand. This is the force that binds the ligands to the metal. The second type of interaction is electrostatic repulsion between the lone pairs on the ligands and the electrons in the *d* orbitals of the metals.

d-Orbitals have different orientations, but in the absence of external disturbance they all have the same energy. In an octahedral complex, central metal atom is surrounded by six lone pairs of electrons (on the six ligands). So, all five *d*-orbitals experience electrostatic repulsion. The magnitude of this repulsion depends on the orientation of the *d*-orbitals.

As a result of these metal-ligand interactions, the five *d*-orbitals in an octahedral complex are split between two sets of energy levels: a higher level with two orbitals($d_{x^2-y^2}$andd_{z^2}), having the same energy and a lower level with three equal-energy orbitals (d_{xy}, d_{yz}დაd_{xz}).The crystal field splitting(Δ) is the energy difference between two sets of *d*-orbitals in a metal atom when ligands are present. The magnitude of Δ depends on the metal and the nature of the ligands: it has a direct effect on the color and magnetic properties of complex ions.

The best way to measure crystal field splitting is to use spectroscopy to determine the wavelength at which light is absorbed. This information enables us to calculate the crystal field splitting.

Based on spectroscopic data for a number of complexes, all having the same metal ion but different ligands, chemists calculated the crystal splitting for each ligand and established a spectrochemical series, which is a list of ligands arranged in increasing order of their abilities to split the d-orbital energy levels.

The magnitude of the crystal field splitting also determines the magnetic properties of a complex ion.

The actual number of unpaired electrons (or spins) in a complex ion can be found by magnetic measurements. In general, experimental data support predictions based on crystal field splitting. However, classification to low- and high-spin complexes can be made only if the metal ion contains more than three and fewer than eight *d* electrons.

The splitting of d-orbital energy levels in two other types of complexes – tetrahedral and square-planar, is also considered in the crystal field theory. In fact, the splitting pattern for a tetrahedral ion is just the reverse of that for octahedral complexes.

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THE ESSENCE ON ADDITIVE METHOD OF STRUCTURAL INGREDIENTS AND THE ANALYSIS OF THE OBTAINED RESULTS

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In order to determine thermal constants of hard silicates, the paper suggests the basic essence on “additive method of structural ingredients” and the short analysis of results obtained from the realization of this method.

It is shown that, unlike the existing calculation methods of thermal constants of these compounds, the proposed method is based on the data in thermodynamic basins itself.

It is noted that this method of silicates is based on the information existed in physical chemistry. It is subject to the principle that the quality of each new body structural organization is determined by combining elements with a lower and higher structural arrangement of quality in the energy units.

The essence of the concepts used in the proposed method, the calculation and the assessment of the received assignments are given. The idea is that this method belongs to the so-called " the number of "approximations." It is possible to estimate obscure experimental data for assessing a solid, anhydrous substance (reaction).

ASSESSMENT OF INDOOR AIR QUALITY OF KUTAISI PUBLIC BUILDINGS

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The issues of air pollution in Georgia is problematic. According to the Ministry of Environment Protection and Agriculture, in four cities - Tbilisi, Kutaisi, Batumi and Rustavi air pollution level is very high. At the same time, indoor air quality deserves considerable attention from healthcare and labour safety.

The goal of our research was to study how outdoor air quality affects the quality of the indoor air and what factors affect the indoor air quality. The presented information reflects the results of the study, which was performed In Kutaisi, in terms of indoor air quality study of public buildings.

Based on desk review, the Ilia Chavchavadze Avenue was selected as the most loaded and "hot point" in case of air quality. The concentration of contaminant agents in the air was determined by using two portable multi-function testing devices - Air Detector DT-35789 and TemTop LKC-1000E Professional Air Quality Detector, which allow to define the concentrations of fine particulate dust matter (PM2.5 and PM10), Formaldehyde (CHCO) and Total Volatile Organic Compounds (TVOC, including benzene). In fact, the widespread use of new products and materials in our days has resulted in increased concentrations of indoor pollutants, especially of volatile organic compounds (VOCs), which pollute indoor air and affect human health. As a result, the air of all kinds of indoor spaces is frequently analyzed for VOCs.

A high level of Air Quality Index as measured as "contaminated air" was calculated for 23 cases resulting from 72 measurements conducted at various times. Particular contamination was observed in shops of furniture, paint and footwear sections, with CHCO (0,472÷0,719 mg/m^3) and TVOC (0.431÷9.999 mg/m^3) concentrations. Limited value of CHCO on the national level is 0.3 mg/m^3 and according to WHO recommendation – 0.15 mg/m^3. Based on the analysis of the cases, the outdoor air quality on Chavchavadze's Avenue effects on the indoor air quality of the buildings, but in case of cooling and air conditioning system, absorption system and interior greenery there was no undesirable quality of indoor

ON THE POSSIBILITY TO PREDICT THE RANGE OF FEATURES OF SILICATE ENAMEL

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Traditionally, in the creation of new enamel composition, general information about the effects of enamel properties of various oxides is used. The source of this information is mainly the experiment, which is quite laborious and requires significant material costs. This is caused by the fact that it is more often used to calculate the enamel qualities for reporting methods because they are able to bring the experiment's share to a minimum by predicting a certain event.

One of the most important factors can become a silicate, like enamel glass as a factor of hindering the overall achievement of this goal. Despite the fact that it does not belong to the rank of material - it is an integral part of the composition derived from the naturally formed bodies. It belongs to the variety of amorphous solid bodies, the structure which is still at the hypothetical level. In spite of this, a number of possibilities have already been developed, which have been suggested to offer projection methods that are closer to the realities of glass and enamel properties. Exactly that information is included in our work.

Enamel production requires number of requests. Among them the most important attention is paid to the selection of the material from the draft compositions that is predisposed to form the condition of glass in the given conditions. Just as great attention is paid to time-temperature setting for selected composition of enamel and to determine the temperature coefficient of the enamel linear thermal expansion because its magnitude is much more precisely based on the properties of the "metal-enamel" composite.

The ability to determine the tendency for glass formation is based on imagination. According to this imagination silicate enamel [SiO_4] creates a spatial frame of tetrahedra. Other cations in the enamel will be placed in the inanities of carcass. Then the relation of other oxides in the SiO2 enamel can be determined by determining the quality of the frame (fSi) and its size shows the tendency for glass formation. It is considered that the glass can be obtained fSi = 0.500-0.333- S.

A lot of methods, which mainly base on the information existing in thermodynamics, are offered because of current processes in the search system and to predict the resulting products. Most of them are based on different ways of the jibs-free energy minimization method and the thermodynamic coefficient of system equilibrium so called "Isotherm" method.

PRODUCTION OF SORBENTS WITH DIFFERENT SPECIFIC SURFACES FROM SECONDARY RAW MATERIALS (NUTSHELL, SAWDUST) BY THERMAL CONVERSION

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Creation of new materials is one of the basic problems on the path of development of mankind. Obtaining of various new materials with previously specified properties in order to overcome new challenges in different spheres of technology and industry is permanently essential.

From this point of view, obtaining of new carbonaceous materials from cheap secondary raw material, particularly, from domestic waste, containing cellulose fibre (sawdust, nutshell, hazelnut shell, etc.) is quite interesting.

The goal of the research is obtaining of high-quality carbonic material with specified and unique properties from secondary raw materials by an essentially new method - conversion process with the help of relatively cheap technologies.

Secondary raw materials (nutshell, sawdust) are processed at 850^0C, for 2 hours, using water vapor (with the calculation of 1 ml of water per 1gr of raw material) in a special reactor. The resulting carbonaceous material is grinded in a special mill, sieved and divided into different fractions (700 µm, 315 µm, 40 µm).

The specific surface of the obtained carbonaceous materials of different fractions was determined on a special equipment (Gemini VII), which determines the specific surface of the material. The results are shown in Table 1.

Table 1. Specific surface of different fractions

#	Raw material	Specific surface of different fractions, m^2/g		
		700 mkm	315mkm	40 mkm
1	Sawdust	492.95 m^2/g	470.64 m^2/g	476.35 m^2/g
2	Nutshell	637.33 m^2/g	599.87 m^2/g	526.387 m^2/g

According to the measurement results, the 700 µm fraction of the obtained carbon materials has a large specific surface. In case of nutshell, the specific surface area is larger than that of sawdust. The obtained carbon materials due to their high specific surface can be used as sorbents.

STUDY OF THE SORPTION ACTIVITY OF MATERIALS OBTAINED BY THERMAL CONVERSION OF CELLULOSE-CONTAINING WASTE

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As a result of human activity, huge amounts of heavy metal ions flow into above-ground waters and underground water. The main sources of pollution are enterprises of the fuel and energy complex, non-ferrous metallurgy, and motor transport. The presence of heavy and non-ferrous metals in water and food harms health of population.

Economically, the purification process is one of the expensive processes. As a rule, most of the known methods require considerable time, reagent and energy resources to achieve a high level of purification.

The search for materials that would allow purification of the environment, various objects used by humans, fluids, and air from contaminants, is becoming an increasingly urgent task. One of the most effective methods for purifying the environment are adsorption methods, which are widely used for the deep purification of water from dissolved ions of heavy and non-ferrous metals, using various sorbents. The efficiency of adsorption cleaning can reach 85-95% and depends on the chemical nature of the adsorbent, the size of the adsorption surface, the chemical structure of the substance and its state in solution.

Activated carbons, mineral sorbents and sometimes production wastes (ashes, slags, sawdust, etc.) are often used as a sorbent.

The purpose of this work is to study the properties of various sorbents obtained from sawdust of various trees, from hazelnut shells, from polymers by thermal conversion at different temperatures using a reagent. For possible widespread use of the obtained sorbents, special attention is paid to the specific surface area of these sorbents.

The study of the specific surface of the obtained sorbents was carried out on a Gemini VII instrument. Measurement results:

1. For the sorbent obtained from the hazelnut shell, the specific surface area was 400.5 m^2 / g.
2. For the sorbent obtained from sawdust, the specific surface was 50.9 m^2 / g.
3. For the sorbent obtained from polymers, the specific surface area was 187.3 m^2 / g.

As shown by previous results during the study of various sorbents, materials obtained by processing polymers can be competitive, in comparison with sorbents, specially obtained from various materials. The size of the surface of the particles is ambiguously correlated with the adsorption capacity of the sorbent.

We have conducted research on the use of a sorbent obtained from recycled shell of hazelnuts. Sorption properties with respect to bivalent copper ions were studied. Studies were carried out on a model solution of copper (II) sulfate (Ccu ++ = 0.64 mg / ml), simulating natural and waste water. All experiments were performed at room temperature.

The results of the study of the sorption capacity of the material are given in the tables and figures 1,2,3,4:

Table 1. The adsorption capacity of the sorbent obtained from walnut

Fraction size (μm)	Initial concentration Cu^{++}, (mg/ml)	The adsorption capacity of the sorbent,(mg/g)			
		Sorption time (hour)			
		2	20	26	45
40	0,640	*38.7*	*42.4*	*43.2*	*43.6*
315		*21.4*	*29.6*	*31.3*	*29.8*
400		*18.8*	*24.4*	*27.6*	*27.6*
700		*13.1*	*15.7*	*16.2*	*16.9*
1200		*12.8*	*14.2*	*15.3*	*15.3*

Table 2. Adsorption value (mg/g) Cu^{++}

Fraction size (μm)	Equilibrium concentration after adsorption (mg / ml)			
	Sorption time (hour)			
	2	20	26	45
40	*0.253*	*0.208*	*0.216*	*0.206*
315	*0.426*	*0.327*	*0.344*	*0.342*
400	*0.452*	*0.396*	*0.364*	*0.364*
700	*0.509*	*0.483*	*0.478*	*0.471*
1200	*0.512*	*0.498*	*0.487*	*0.487*

It can be seen from these tables that the maximum sorption occurs at a fraction size of 40 μm, where the sorbent capacity with respect to copper ions ranges from 38.7 to 43.6 mg / g. According to the results, it is also observed that equilibrium adsorption is achieved within 20 hours.

SYNTHESIS OF COORDINATION COMPOUNDS OF SOME BIOLOGICALLY ACTIVE d-METALS

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The subject of our research is the synthesis of complex compounds of manganese chloride and nickel with N, N-dimethylformamide (DMF).

Manganese is important for healthy plant growth, as are all trace elements. It plays a significant role in the process of photosynthesis.

Manganese is characterized by a coordination number of 4 or 6.

Table 1.

Oxidation number	Coordination number	Structure of compounds	Compounds
0	6	octahedron	$Mn_2 (CO)_{10}$
+2	4 6	tetrahedron octahedron	$[MnCl_4]^{2-}$, $MnF_6]^{4-,}$ $[Mn (OH_2)_6]^{2+}$
+3	6	octahedron	Mn_2O_3
+4	6	octahedron	MnO_2
+6	4	tetrahedron	$[MnO_4]^{2-}$

Research data shows that nickel is important for animals and plants, but its function is not defined.

N, N-dimethylformamide (DMF) is an important polar aprotic solvent. It has a relatively high melting point.

N, N-dimethylformamide (DMF) is a ligand in coordination chemistry.

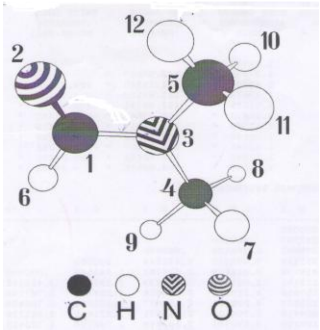

Figure 1. The molecule of DMF

The energy, geometric, and structural features of DMF are calculated by the quantum-chemical method AM1.

Compounds of manganese (II) and nickel (II) chlorides with DMF were obtained. Chlorides of Manganese (II) and nickel (II) were used as basic salts. Synthesis was carried out in hot alcohol solutions.

New coordination compounds were obtained in the solid state. Their composition is determined using elemental analysis, and individuality is determined by determining the melting point. Solubility in various inorganic and organic solvents was determined. Synthesized compounds are studied using the method of infrared absorption spectroscopy.

The rule of coordination of DMF with metals has been established. In the synthesized complexes, the DMF molecule is coordinated with the metal through an oxygen atom.

QUANTUM-CHEMICAL STUDY OF THE COORDINATION COMPOUNDS OF NITRATE, SULFATE, CHLORIDE AND ZINC BROMIDE WITH DIMETHYL SULFOXIDE

Zurab Gogberashvili[1], Maia Tsintsadze[1, 2], Nana Gegeshidze[1, 2]

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[2]R. Agladze Institute of Inorganic Chemistry and Electrochemistry, 0186, Tbilisi, Georgia
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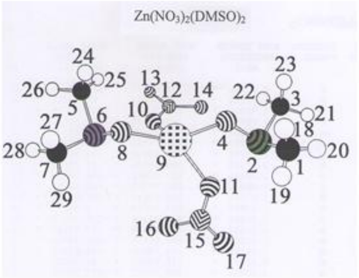
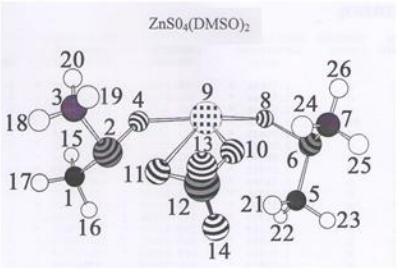
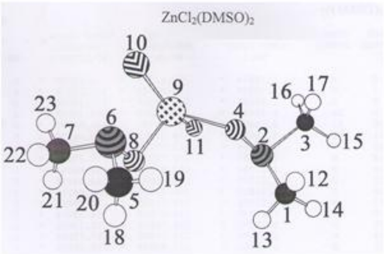
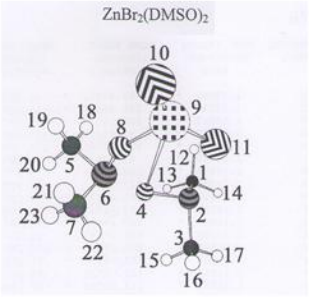
The aim of our study was to study the properties of the complex formation of transition metals with dimethyl sulfoxide (DMSO).

Based on the quantum-chemical method AM1, the energy, geometric and structural characteristics of complex molecules of dimethyl sulfoxide with sulphate, nitrate, chloride and zinc bromide have been studied of the general formula ZnX_2 $(DMSO)_2$, where X = SO_4^{2-}, NO_3^-, Cl^-, Br^-, DMSO - dimethyl sulfoxide. These quantum chemical calculations are shown in table 1.









The dimethyl sulfoxide molecule contains two donor atoms capable of forming chemical bonds with the complexing metal: it is the oxygen and sulfur atoms. But analysis of electron density and effective charges on atoms in ZnX_2 $(DMSO)_2$ molecules, where X = SO_4^{2-}, NO_3^-, Cl^-, Br^- (Table 1), also studying the population of atomic orbitals on atoms, showed that the formation of a chemical bond with the metal is carried by the oxygen atoms O (4) and O (8) of the molecule of dimethyl sulfoxide.

Based on the data of quantum-chemical calculations, it can be argued that the coordination of dimethyl sulfoxide molecule with the zinc atom through sulfur atoms is not carried out.

In this case, on the basis of calculations, one cannot unambiguously assert about the influence of the nature of the anion on the complexation process.

Table 1. Values of formation heat (ΔH), dipole moments (μ), charges on atoms (q), electron density and distribution of electrons on atomic orbitals (s, p) of molecules of nitrate, sulfate, chloride and zinc bromide with dimethyl sulfoxide (DMSO)

№	Molecule	ΔH, KJ	μ, Д	Atom	Charge, q	Electron density	Atomic orbital electron populations			
							2S	$2P_x$	$2P_y$	$2P_z$
1	$Zn(NO_3)_2(DMSO)_2$	-428.737	4.489	O(4)	-0.715	6.715	1.891	1.794	1.760	1.270
				O(8)	-0.719	6.719	1.889	1.241	1.184	1.746
2	$ZnSO_4(DMSO)_2$	-802.966	8.756	O(4)	-0.792	6.792	1.875	1.808	1.780	1.329
				O(8)	-0.737	6.737	1.883	1.742	1.358	1.755
3	$ZnCl_2(DMSO)_2$	-594.306	6.305	O(4)	-0.760	6.760	1.912	1.801	1.787	1.260
				O(8)	-0.760	6.760	1.012	1.853	1.755	1.240
4	$ZnBr_2(DMSO)_2$	-669.515	8.877	O(4)	-0.858	6.858	1.935	1.832	1.797	1.294
				O(8)	-0.880	6.880	1.880	1.767	1.526	1.707

SYNTHESIS OF COORDINATION COMPOUNDS OF SOME BIOLOGICALLY ACTIVE d-METALS

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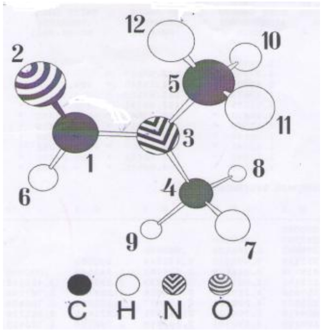

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REDUCTION OF (1,3-DIFORMYLINDENYL)CYCLOPENTA-DIENYLRUTHENIUM DERIVATIVES

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To date, numerous pincer metal complexes with tri-dentate arene, heterocyclic, and other organic ligands have been synthesized. Meanwhile, quite a few complexes with metallocene-based pincer ligands are known. The chemistry of the latter compounds has been rapidly developed since 2002, when rhodium complexes with the 1,3-disubstituted bisphosphine ferrocene ligand were synthesized. The synthesis of pincer complexes of palladium, iridium, and ruthenium with metallocene-based diphosphine ligands was documented. Evidently, appropriate 1,3-disubstituted derivatives are required for the preparation of metallocene-based pincer ligands. Previously, homoannular disubstituted 1,3-bis(hydroxymethyl) derivatives of ferrocene, ruthenocene, and pentamethylruthenocene were used for this purpose. These derivatives can be prepared by the reduction of appropriate 1-formyl-3-ethoxycarbonyl derivatives with lithium aluminum hydride. Now we report the synthesis of new precursors of metallocene-based pincer ligands containing the η^5-coordinated 1,3-bis(hydroxymethyl)-indenyl ligand. We found that the reduction of the (1,3-diformylindenyl)cyclopentadienyl-ruthenium derivatives, $\{\eta^5\text{-1,3-(CHO)}_2C_9H_5\}RuC_p$, (1a, $Cp=C_5H_5$), $\{\eta^5\text{-1,3-(CHO)}_2C_9H_5\}$ RuC_p*, (1b,Cp*=C5Me$_5$), and $\{\eta^5\text{-1,3-(CHO)}_2C_9H_5\}$ $RuCp^f$ (1c,$Cp^F=C_5Me_4CF_3$) with $NaBH_4$ or $LiAlH_4$ under mild conditions affords the corresponding 1,3-bis(hydroxymethyl) derivatives, $\{\eta^5\text{-1,3-(CHO)}_2C_9H_5\}RuCp$ (1a), $\{\eta^5\text{-1,3-(CHO)}_2C_9H_5\}RuC_p$* (2b), and $\{\eta^5\text{-1,3-(CHO)}_2C_9H_5\}RuCp^F$ (2c), in good yields (respectively, 94-97 and 88-90%). Bis (hydroxymethyl) compounds 2a-c are bright-yellow crystalline powders. The structure of diols 2a-c was confirmed by NMR spectroscopy and elemental analysis.

REVIEW OF SYNTHESIS AND BIOLOGICAL ACTIVITY OF RESVERATROL

Lasha Lagvilava

Scientific Supervisors: Ioseb Chikvaidze – Professor, Doctor of Chemical Sciences
Shota Samsoniya – Academician of Georgian National Academy of Sciences, Professor
Ivane Javakhishvili Tbilisi State University
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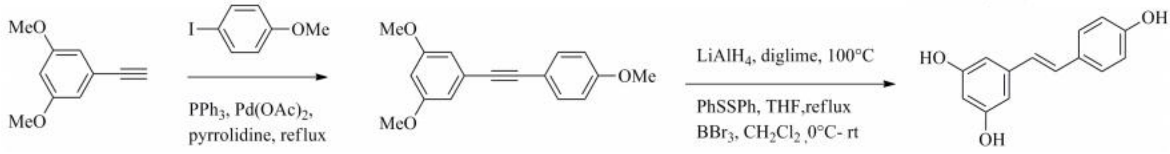
Resveratrol 1, a naturally occurring polyphenolic nonflavonoid antioxidant, is a phytoalexin compound that has been isolated from grape skin, vine bark, nuts, berries and many other plants. This compound has various health benefits, including chemo-preventive effects against cancer, inflammation, aging, obesity, cardiovascular diseases and neuro-degeneration. Antioxidative, antibacterial and antifungal activities have also been attributed to this molecule1, 2. A current area of research is related to synthesis of resveratrol oligomers which present in many cases higher antioxidant properties and better activities for different types of diseases than the same resveratrol. These new results triggered a big interest in the field, which can be appreciated for the great number of research papers and reviews recently published.

Scheme 1

(A new synthesis of resveratrol)



Many synthetic approaches for resveratrol have been reported primarily through Wittig-type reactions3, 4 and Horner–Emmons5, 6, but they usually require relatively long synthetic routes with variable diastereoselectivity. Additionally, approaches involving Pd-catalyzed Heck7-14 or Susuki15 reactions or Ru-catalyzed cross metathesis16,17 have also been published. In most cases using the Heck reaction, preparation of the required precursor takes several steps or it involves the use of expensive catalysts.

We are going to discuss about a simple synthesis of resveratrol (1) with an overall yield of 62% over four steps.

ELECTRONIC STRUCTURE OF COMPLEX COMPOUNDS: VALENCE BOND THEORY

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Valence bond theory is based on the assumption that every two atoms in a molecule are connected to each other by an electron pair, which is localized between these atoms, and therefore the bonds are two-center.

According to this theory, the formation of these complex compounds occurs through donor-acceptor interaction between the complexing agent and the ligand. Bond is forming by overlapping the free acceptor orbitals with the orbitals of the electron pairs of donor atoms.

The free orbitals of the complexing agent (which are involved in the formation of a bond) are mostly nonequivalent energetically and hybridize when a bond is formed. The resulting hybrid orbitals differ from each other only in their spatial orientation. The type of hybridization determines the coordination number of the complexing agent and the geometry of the resulting complex.

Let us explain the formation of some complexes based on the valence bonds theory:

- when hybridization of both the s- and p-orbitals of central atom occurs (sp-hybridization). Coordination number is 2 and complex has linear structure.
- In case of a coordination number 4, complex compound may have tetrahedral or square planar form. Consider $[BF_4]^-$ ion. It has tetrahedral form. Electron pairs are

donated by F^--ions and an acceptor is boron atom in the sp^3-hybridization state. In the same configuration there are some Zinc, Cadmium, Mercury complexes, such as $[Zn(NH_3)_4]^{2+}$, $[Cd(NH_3)_4]^{2+}$, $[Hg(CN)_4]^{2-}$ and so on.

- Consider complexes of d-elements (from all d-orbitals, 4 orbitals are completed with eleqtrons) with coordination number of 4. For the ligand electrons they use (n-1)d, ns-orbitals and from the np-orbitals use 2. Consequently, dsp^2-hybridization of complexing agent takes place. As an example, consider the complex $[Pt(NH_3)_4]^{2+}$.

Complexes with the coordination number of 6 have an octahedral configuration. For octahedral configuration is necessary to release of two orbitals from the d-sublevel. Valence bond method allows predicting the relative reactivity of complex compounds.

It should be noted, that valence bond method can’t explain some properties of complex compounds. It can’t explain the absorption spectra of complex compounds, does not take into account the π-dative interaction between the complexing agent and the ligand and so on.

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1. Raymond Chang. General Chemistry. The essential Concepts. Fifth edition. McGraw Hill Higher Education. New York, 2008.
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ELECTRONIC STRUCTURE OF COMPLEX COMPOUNDS: MOLECULAR ORBITAL METHOD

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Currently, the molecular orbital method (MO) is the most perfect theory for describing the electronic structure of complex compounds. However, its use is associated with sufficient computational difficulties.

When describing coordination compounds, the basic thesis of the MO method (in complex compounds, bonds are carried out by multicenter molecular orbitals, which connect all the atoms that are in the system) is preserved.

The molecular orbital method of a complex compound is written as:

$$\Psi = a\Psi_0 + b\Phi \qquad (1)$$

where Ψ_0 _ is atmic orbital of central ion, Φ _ MO of ligand system (i.e. group orbital). Φ is equal to linear combination of atomic orbitals of ligands:

$$\Phi = \sum_{i=1}^{n} c_i \varphi_i \qquad (2)$$

When building of molecular orbitals, the symmetry of the initial atomic orbitals plays a significant role. Since a detailed analysis of this problem requires the use of the mathematical apparatus of group theory (see Appendix 1), here we present only qualitative representations for the octahedral ML_6 complex (without (π-bond).

In ground state ML_6 octahedral complex (without (π-bond) has 7 energy level: 3 – bonding, 1 – nonbonding and 3 – antibonding.

12 electrons in the complex are located on bonding orbital, 4 _ on nonbonding orbital and 2 – on antibonding orbital.

When π-bonds appear in ML_6 octahedral complex, its diagram has more difficult form.

The theory of molecular orbitals combines both the ideas of the valence bond theory and the crystal field theory. It gives the most common approach to describing the properties of complex compounds. According to the valence bond theory, six σ-bond correspond to six molecular orbitals of the octahedral complex. They are formed by the donor-acceptor interaction of the d^2sp^3 hybrid orbitals of the complexing agent with the electron pairs of six ligands. As for nonbonding π_d and $\sigma_d^{antibonding}$ molecular orbitals, they correspond to d-orbitals of the complexing agent in crystal field theory. They are formed by splitting of d-level in the octahedral field of the ligand.

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1. Raymond Chang. General Chemistry. The essential Concepts. Fifth edition. McGraw Hill Higher Education. New York, 2008.
1. U. Kask; J. D. Rawn; R. A. Delorenzo. General Chemistry. WCB. 1993.
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SAWDUST AND ETHYLSILYCATE BASED COMPOSITES

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Ecologically pure composite materials with new high-technical characteristics have been obtained on the basis of dispersed sawdust (pine) particles (with length less than 50 µm) and ethyl silicate. Composite materials are obtained in different pressure and temperature via simple hot press method. For our composites we have determined bending strength, impact viscosity, and thermal stability by the vicat method and water absorption. Structures were studied using an optical microscope, scanning electron microscopy and energy dispersion micro X-ray spectral analysis.

The optimal conditions for receiving of new, ecologically friendly composites have been established. The obtained composites are characterized by high mechanical characteristics, thermal stability, resistance to microorganisms, ecologic cleansing, low water absorption properties.

Acknowledgments: the financial support of Science & Technology center in Ukraine (Grant №5892 is acknowledged.

ELECTROCHEMICAL INVESTIGATION OF ANTICANCER DRUG GEMCITABINE WITH CALF THYMUS DNA

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Gemicitabine Hydrochloride (GMB) is a synthetic pyrimidine nucleoside and is widely employed in standard treatment for pancreatic cancer, tumours of the bladder, breast, lung, renal cell carcinoma and biliary tract cancer. GMB can be used as both single or in combination with other drugs. GMB presented auspicious response rates in other types of tumour as well, such as lymphomas, ovarian cancer and testicular tumour. As GMB is a pro-drug it follows the pathway of cell processes implying that nucleoside transporters make its entry into the cell possible and an intracellular transformation renders the drug active. The intracellular transformation is catalysed by the enzyme deoxycytidine kinase, in a rate-limiting reaction, to an ultimate triphosphate form (dFdCTP). Lately, the interest in drug-dsDNA electrochemical investigation has gained a lot of momentum. Determining the redox process on the surface of electrode is one of the most applied aspects of electrochemistry. Since electrochemical and biological reactions bear resemblance in more ways than one, it is safe to assume that the electrode oxidation mechanisms and those in the body follow similar principles. The information obtained from the electrochemical response associated with dsDNA–drug interactions is also employed to suggest the interaction mechanism, its type and complex formation, to calculate the binding constant.

AuNPs and AgNPs were used to modify electrode by using layer strategies. SPE/AuNPs/AgNPs/AuNPs/ct-dsDNAnanobiosensor was prepared via layer by layer deposition of silver and gold nanoparticles. Three layers of nanoparticles were deposited and left to air dry. Better results were acquired when ct-dsDNA was immobilized on AuNPs and based on this observation, AgNPs layer was sandwiched between two AuNPs layers. After deciding that these three layers were optimized by trying out different concentrations. Finally, the optimized concentrations for AuNPs/AgNPs/AuNPs were 5 µL/3 µL/5 µL. Later 15 µL of ct-dsDNA was located on modified electrode surface.

A disposablescreenprintedmodifiednanobiosensorwasdevelopedto sense the electro-chemicalresponse of Gemicitabine-DNA interaction. The recommended nanobiosensors SPE/AuNPs/AgNPs/AuNPs/ct-dsDNA was found to be fast, selective and highly sensitive for ct-dsDNA-GMB interaction at very low concentrations. The guanine current signal of ct-dsDNA was decreased to fifty percent of its value when interacted with GMB.

APPLICATION OF CELLULOSE 3,5-DICHLOROPHENYLCARBAMATE COVALENTLY IMMOBILIZED ON SUPERFICIALLY POROUS SILICA FOR THE SEPARATION OF ENANTIOMERS IN HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY

Lia Karadurmus[1], Anna Bardavelidze[1], Antonina Mskhiladze[1], Mehmet Gumustas[2,3], Sibel A. Ozkan[3], Alessandro Volonterio[4,5], Tivadar Farkas[6],
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Our earlier studies have demonstrated the applicability of polysaccharide-based chiral selectors in combination with superficially porous (or core-shell) silica (SPS) particles for the preparation of highly efficient chiral stationary phases (CSP). These materials were successfully applied for the separation of enantiomers in high-performance liquid chromatography (HPLC), nano-liquid chromatography (nano-LC) and also in capillary electrochromatography (CEC). In earlier studies, CSPs were prepared by coating (adsorption) of the chiral selector onto the surface of silica. In this study we report for the first time the CSP obtained by covalent immobilization of a chiral selector onto the surface of SPS particles. The applicability of this CSP for the separation of enantiomers in pure methanol and acetonitrile, as well as in n-hexane/2-propanol mobile phases is shown. The effect of the injected sample amount, mobile phase flow rate and detection frequency on separation performance were studied, as well as high efficiency separation of enantiomers with the analysis time less than15 seconds was attempted.

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