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Barbosa S C et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

The importance of cyclic structure on labaditin activity against a gram-positive bacteria

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Antimicrobial resistance has reached alarming levels in many countries, thus leading to a search for new classes of antibiotics, such as antimicrobial peptides whose activity is exerted by interacting specifically with the microorganism membrane. In this study, we investigated the molecular-level mechanism of action for Labaditin (Lo), a 10-amino acid residue cyclic peptide from Jatropha multifida with known bactericidal activity against *Streptococcus mutans.* Lo showed be also effective against *Staphylococcus aureus (S. aureus)* but this does not apply to its linear analogue (L1). Using polarization-modulated infrared reflection absorption spectroscopy (PM-IRRAS), the secondary structure of Lo has shown to be preserved upon interacting with Langmuir monolayers containing a phospholipid mixture mimicking *S. aureus* membrane, in contrast to L1. This structure preservation is key for the Lo self-assembly forming peptide nanotubes that induce pore formation (unimeric) in large unilamellar vesicles (LUVs), according to permeability assays and dynamic light scattering measurements. Therefore, the comparison between Labaditin (Lo) and its linear analogue L1 allowed us to infer that the bactericidal activity of Lo is more related to its interaction with the membrane. It does not require specific metabolic targets, which makes cyclic peptides promising for antibiotics without bacteria resistance.

Biography

Simone Cristina Barbosa has completed her PhD at University of Sao Paulo/Brazil focusing in antimicrobial peptides. The postdoctoral studies was done at the UBC – Canada, and now a days at the University of Sao Paulo. The present results are related her last research performed in her postdoc in Brazil.

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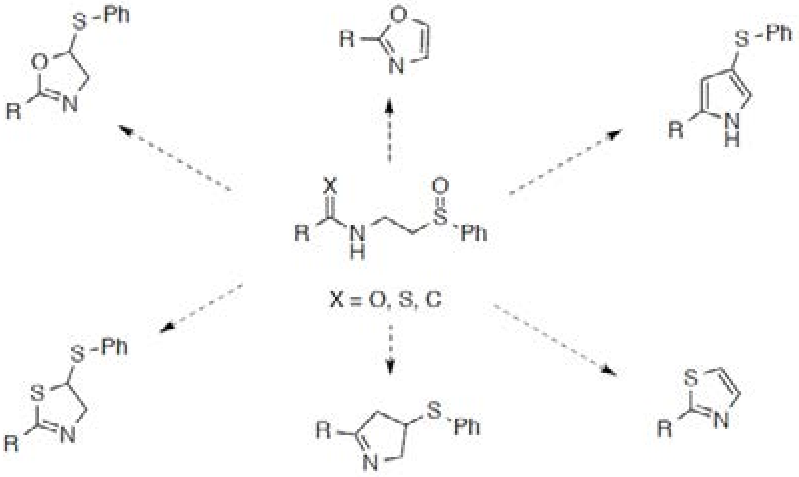
Notes:

Diego Gamba-Sanchez et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Synthesis of 5-membered heterocyclic systems by the pummerer reaction

Diego Gamba-Sanchez, **Juan Rueda-Espinosa** and **Andres Gomez-Angel**
University of Los Andes, Colombia

The Pummerer reaction has been studied for many years as a powerful methot to form C-Nu bonds, its aplications in total synthesis of natural products has been recently reviewed showing its grate potential. We recently publised a new method to obtain oxaxolines by Pummerer chemistry, and the goal of the current study is to extend the scope of this methodology to the synthesis of other heterocylcic systems. The results include approaches to pyrroles, ozaxoles, thiazoles and the application of the methodology to the total synthesis of siphonazole and muscoride A.



Biography

Diego Gamba-Sanchez obtained his PhD in 2010 from the Ecole Polytechnique at Palaiseau. After one year as a postdoctoral associate in the laboratory of Prof. Thorsten Bach, e moved back to Colombia ans started his independent carrier at the Universidad de los Andes in Bogotá. His research focused on new methodologies using Pummerer chemistry and the development of synthetic routes to natural products.

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Notes:

Melitta Patricia Kiss et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Kinetic investigation of the formation of neodymium(III) porphyrin complexes

Melitta Patricia Kiss, **Zsolt Valicsek** and **Ottó Horváth**
University of Pannonia, Hungary

Lanthanide(III) ions offer good opportunities to examine the special properties of out-of-plane (OOP or sitting-atop=SAT) metalloporphyrins, utilizing the well-known lanthanide contraction. Their insertion into the coordination cavity of porphyrin ligand is a slow and complicated process in aqueous solution, originating from the high stability of their aqua complexes and oligomer forms. As a consequence of the lanthanide(III) ions' Pearson-type hard character, they can coordinate rather to the peripheral substituent of porphyrin, if it possesses similarly hard O-donor atom (e.g. carboxy-, sulfonato-phenyl). Only under thermodynamic control, at higher temperatures, can coordinate the metal ion also, or rather, to the four pyrrolic nitrogens; resulting in the formation of typical metalloporphyrin complexes. SAT complexes can be used as photocatalysts in redox reactions, as photosensors in the medical science in luminescence imaging and as polymer diodes in cancer treatment. We investigated the reaction between the 5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin and the neodymium(III) ion, as well as the effect of the ionic strenght, the temperature and the potential axial ligands on these processes. The structures of different complexes were identified on the basis of their UV-Vis absorption spectra. The bidentate O-donor acetate and glycol, as well as the monodentate ethanol and chloride don't dissociate from the metal ion, only monoporphyrin can form. In the presence of non-coordinating perchlorate anion, bisporphyrins can form, too. At lower temperatures, the lanthanide(III) ions were not able to coordinate into the cavity of the macrocycle, to the softer pyrrolic nitrogens, rather to the sulfonato groups, resulting in the formation of the free-base ligands' tail-to-tail dimer. So the coordination position of metal ion can be influenced by temperature.

Biography

Melitta Patricia Kiss got her MSc degree in chemistry at University of Pannonia, Veszprém, Hungary. Now she is a PhD student at the Department of General and Inorganic Chemistry at the same university. In her research work she studies the formation of lanthanide porphyrin complexes from equilibrial and kinetic aspects since 7 years.

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Notes:

Facile synthesis of polyindole via emulsion polymerization: Effects of oxidant and surfactant types and doping

Katesara Phasuksom and **Anuvat Sirivat**
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Conductive polyindole (PIn) was synthesized by emulsion polymerization at room temperature under various synthesis conditions. The effects of oxidizing agents ($FeCl_3$, $(NH_4)S2O_8$) and surfactant types (cationic; cetyltrimethylammonium bromide (CTAB), anionic; sodium dodecylsulfate (SDS) and non-ionic; polysorbate 80 (TW80)) were investigated systematically. The PIn synthesized without surfactant was investigated and compared. The PIn/FeCl3 showed higher electrical conductivity by one order of magnitude compared to $(NH_4)S_2O_8$ due to a lower over-oxidation level as verified by X-ray photoelectron spectroscopy. Synthesis of PIn in the presence of a surfactant was determined by using difference of surfactant/monomer mole ratio, suitable ratio for the obtained smallest particle size was 1:0.05 for SDS and CTAB and 1:0.1 for TW80. In this work, the PIn with the nano-scaled size of 60.3 ± 10.8 nm in diameter was found in the emulsion system of SDS. Moreover, the SDS system provided higher electrical conductivity than the PIn synthesized with CTAB and TW80 since the anionic surfactant was an efficient dopant. To improve the electrical conductivity of PIn, $HClO_4$ was utilized as a doping agent for the doping process. The electrical conductivity of PIn clearly depends on doping mole ratio of dopant/indole, it was dramatically increased by 4-5 orders of magnitude with respect to PIn before doping. The highest electrical conductivity in this work obtained of the PIn after doping at 25:1 of doping mole ratio was as high as 14.56 ± 2.39 S/cm which has never been reported previously.

Biography

Katesara Phasuksom completed her B.Sc. with first class honours in Industrial Chemistry from King Mongkut's University of Technology North Bangkok (KMUTNB), Thailand in 2010 and her M.S. in Material Science from KMUTNB in 2013. She is received a PhD scholarship from the Royal Thai Government through the Royal Golden Jubilee Ph.D Program in 2015 and now is studying at Chulalongkorn University in Polymer Science.

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Sirivipa Mongkolkitikul et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

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May 11-13, 2017 Barcelona, Spain

Electrically controlled release of ibuprofen from pectin hydrogel in transdermal drug delivery

Sirivipa Mongkolkitikul and **Anuvat Sirivat**
Chulalongkorn University, Thailand

Transdermal drug delivery system (TDDS) is the alternative route to transport drug molecule to a systematic circulation through the human skin. The major advantage of TDDS is the ability to avoid the first-pass metabolism. However, TDDS has certain limitations: the level of drug permeated across the skin is low and the drug size has an adverse effect on the permeation. To improve those limitations, the electrical potential and conductive polymer were utilized. This work attempted to design a transdermal patch consisting of ibuprofen as a model drug and pectin hydrogel as a drug matrix. The effects of the crosslinking agent type, crosslinking ratio (the mole of the crosslinking agent to the mole of the pectin monomer), mesh size, and electric potential were investigated. The diffusion coefficients and the release mechanism of the ibuprofen on the pectin hydrogels were determined and investigated using a modified Franz-Diffusion cell in an MES buffer solution of pH 5.5, at a temperature of 37 °C, for 48 h. The amount of drug release was analyzed by UV-Visible spectrophotometry. The result showed the drug diffusion coefficient increased with increasing mesh size and electric potential.

Biography

Sirivipa Mongkolkitikul completed her B. Eng. with a second-class honour in Petrochemical and Polymeric Materials from Silpakorn University, Thailand in 2014, and now she is studying for a Master degree in Polymer Science at the Petroleum and Petrochemical College, Chulalongkorn University, Thailand.

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Nophawan Paradee et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Porous zeolite y-alginate hydrogel composites for electrically controlled transdermal drug delivery

Nophawan Paradee and **Anuvat Sirivat**
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The electrical current is used to enhance drug permeation in transdermal drug delivery (TDD) via iontophoresis. However, the effective transport of the drug ions is decreased via the ion transport competition between buffer ions and drug ions. This limitation is eliminated by encapsulating the drug ions in the porous zeolite. In this work, folic acid (FA) as the cationic model drug was loaded into the zeolite Y by an ion-exchange process before embedding in a Ca-alginate matrix in order to study the release mechanism under applied electrical potential. The FA was released from the zeolite/Ca-alginate composite hydrogel through the diffusion controlled mechanism (Fickian diffusion) in two steps: i) the FA release from the zeolite via the ion-exchange process; and ii) the enhanced diffusion transport through hydrogel. The amount of FA release depended on the electrical potential and Si/Al ratio of zeolite. The higher Si/Al ratio (lower aluminum content) provided the higher amount of FA release due to a lower hydrogen bonding interaction from aluminum. Moreover, the electrical potential applied with the anode on the matrix effectively increased the diffusion of drug resulting from the electro-repulsive force between the positively charged FA and the charged electrode. Therefore, the fabricated zeolite/hydrogel is of a potential material to be used in electrically controlled TDD.

Biography

Nophawan Paradee completed her B.Sc. with a first class honour in Industrial Chemistry from King Mongkut's University of Technology North Bangkok, Thailand in 2008, and a PhD in Polymer Science from the Petroleum and Petrochemical College, Chulalongkorn University, Thailand in 2016. She has published 15 papers in reputed journals.

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Rong-Xin Yuan, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Two cobalt-dicarboxylate metal-organic frameworks with photo-catalytic property

Rong-Xin Yuan
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Because of the high costs and secondary pollutants generating from traditional biological and physical treatment methods, scientists have focused on the exploitations of new catalysts recently. Here, two cobalt-dicarboxylate photo-catalysts $[Co(4\text{-}pysmia)(H_2O)_2]_n$ (1) and $[Co_3(\mu\text{-}OH)(H_2O)(pysmiaH)(pysmia)_2]_n$ (2) have been hydrothermally synthesized from the reactions of 5-((pyridin-4-ylthio)methyl)isophthalic acid (H_2pysmia) with $CoSO_4$. 1 represents a 2D network with a Schläfli symbol of 6^3. 2 is an unprecedented (3,3,7)-connected network with the Schläfli symbol of $(4^3)(4{\cdot}8^2)(4^5 6^{11} 8^5)$. Both 1 and 2 manifest photocatalytic activities for degradation of methylene blue (MB) under UV light irradiation and show good stabilities toward UV-light photocatalysis. Remarkably, the degradation rate of 2 towards MB can reach 91.4%.

Biography

Rong-Xin Yuan has completed his PhD in 2002 at Nanjing University. From 2002 to 2004, he worked at University of Bielefeld and University of Nottingham as postdoctoral fellow. Now he is the director of Jiangsu Provincial Key Laboratory of Advanced Functional Materials. He has published more than 60 papers in reputed journals and has been serving as an editorial board member of the Journal of Soochow University (Natural Science Edition).

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Min Ji Park et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

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Continuous glucose monitoring sensors modified with nitric oxide-releasing nanofiber for improving biocompatibility: A freely-moving rat model

Min Ji Park[1], **Min Heo**[2], **Yeong Rim Kim**[2], **Gi Ja Lee**[3] and **Jae Ho Shin**[1,2*]
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The blood glucose levels of patients with diabetes mellitus should be tightly monitored. In general, diabetic patients have used the strip-type glucose sensors. Because such strip-type sensors provide the instantaneous value, however, patients cannot immediately respond to hyperglycemic or hypoglycemic events. On the other hand, *in vivo* glucose biosensors are able to determine the glucose levels in real-time, allowing to effectively warn hyperglycemic or hypoglycemic conditions. Indeed, a continuous glucose monitoring sensor provides maximal information about varying blood glucose levels throughout the day, and is able to facilitate the making of optimal treatment decisions for diabetic patients. However, upon implantation of a sensor into a body, a cascade of inflammatory response is initiated, ultimately making *in vivo* glucose measurement erratic. Therefore, the appropriate fusion of biocompatible coating materials and glucose sensing devices has been one of the most critical issues. With discovery of nitric oxide (NO) as a potent antithrombotic and anti-inflammatory agent, a variety of NO storage/release nanomaterials have been reported to improve the biocompatibility of indwelled medical devices, including metal/metal oxide clusters, silica nanoparticles, dendrimers, and polymeric nanofibers. Herein an implantable glucose microsensor modified with NO-releasing silica/polymer *hybrid* nanofibers is demonstrated. By controlling NO release properties (e.g., total NO storage amount, half-life time of NO release, and maximum flux), the sensor performance *in vivo* (using a freely-moving rat model equipped with a wireless signal transmitter/receiver device) will is evaluated, in terms of sensor lifetime, accuracy, and stability.

Biography

Minji Park received her B.S. degree in Department of Chemistry at Kwangwoon University in 2015. Currently, she is studying for her M.S. degree in analytical chemistry at the same University. Her research interest is mainly in the develpoment of glucose biosensor using electrochemical methods.

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Notes:

Rashed Alremeithi et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Development and validation of an analytical methodology for the simultaneous quantitative determination of synthetic cathinones in urine and plasma using GC-NCI-MS

Rashed Alremeithi[1, 2], **Mohammed A Meetani**[1*], **Anas A Alaidaros**[1], **Adnan S Lanjawi**[2] and **Khaled T Alsumaiti**[2]
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Development and validation of sensitive and selective method for enantioseparation and quantitation of synthetic cathinones "bath salts" has been done by using GC-MS with chemical ionization source in negative mode (NCI). Indirect chiral separation of thirty six synthetic cathinone compounds have been achieved by using optically pure chiral derivatizing agent (CDA) called (S)-(−)-N- (trifluoroacetyl)pyrrolidine-2-carbonyl chloride (L-TPC) which converts cathinone enantiomers into diastereoisomers that can be separated on achiral columns. As a result of using Ultra inert 60 m column and performing slow heating rate (2 °C/min) on the GC oven, an observed enhancement in enantiomer peaks resolution have been achieved. An internal standard, (+)-cathinone, was used for quantitation of synthetic cathinone. Method validation in terms of linearities, limits of detection (LOD), limits of quantitation (LOQ), recoveries and reproducibilities have been obtained for fourteen selected compounds that ran simultaneously as a mixture after being spiked in urine and plasma. It was found that the LOD's of the fourteen synthetic cathinones in urine was in the range of 0.02 -0.76 ppb and in plasma it was in the range of 0.02 - 0.34 ppb. While the LOQ's of the mixture in urine was in the range of 0.07 - 2.31 ppb and in plasma it was in the range of 0.07 – 1.03 ppb. Unlike the Electron Impact ion source (EI), NCI showed higher sensitivity by three orders of magnitude by comparing with the previous results. The correlation coefficient (R^2) values for the mixture components was found to be higher than 0.99.

Biography

Rashed Humaid Alremeithi has completed his PhD at the age of 28 years from United Arab Emirates University. He is working at Dubai Police forensic labortory. He has published 2 papers in reputed journals.

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Notes:

Synthesis of 1, 2, 3-triazole-linked salicylamide analogs as potent aurora kinase inhibitors

Jae-Sang Ryu
Ewha Womans University, Republic of Korea

The Aurora family is a member of the Ser/Thr protein kinases regulating mitosis. They includes Aurora A, B and C possessing individual function and different cellular localization during cell cycle. An overexpression of Aurora A and B, which has been observed in various tumor types, is known to connect to chromosomal instability, oncogenic transformation, and tumor progression. Although Aurora kinase is considered as a promising therapeutic target in cancer and several Aurora inhibitors have currently reached the clinical evaluation stage, Aurora-selective drug is not yet approved by FDA. Previously, we identified a potent antiproliferative substance by constructing a small molecule library that mimics lavendustin, a natural kinase inhibitor, using a rapid 'click-fragment assembly' and screening method. Based on this lead compound, various 1,2,3-triazolylsalicylamide analogs were designed, synthesized via Cu(I)-catalyzed azide–alkyne 1,3-dipolar cycloaddition (CuAAC) and evaluated biochemically for the Aurora kinase inhibitory activities. Among twenty-four membered 1,2,3-triazole library, compound **8a** exhibited much lower IC_{50} values against Aurora A kinase than the lead compound, and compound **8m** showed a nanomolar IC_{50} value against Aurora B. In this presentation, we describe the design, synthesis, and biochemical evaluation of 1,2,3-Triazole-linked Salicylamide Analogs.

Biography

Jae-Sang Ryu has completed his PhD from Northwestern University, IL, USA and postdoctoral studies from Memorial Sloan-Kettering Cancer Center, NY, USA. He is a profssor of college of Pharmacy & Graduate School of Pharmaceutical Sciences, Ewha Womans University, Seoul, Korea. He has been searching for new drug candidates based on disease mechanisms and combinatorial approaches. His lab is currently working on the development of allergic/anticancer drugs using peptide libraries and natural compound-like compound libraries. He has published many papers in SCI international journals and applied for patents related to the development of antiallergic drugs and anti-cancer drugs.

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Notes:

Jung-Mi Hah, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Targeting CNS protein kinase as therapeutics for neurodegenerative diseases

Jung-Mi Hah
Hanyang University, Republic of Korea

The development of protein kinase inhibitors is becoming increasingly important in the development of drugs for peripheral diseases, while protein kinase targets in CNS diseases are rarely developed due to the difficulties of common CNS drug discovery. However, a number of protein kinases are being studied as targets for brain diseases. When developing them, the nature of low-molecular inhibitors - the molecular design that considers cytochrome P450-mediated metabolism, must be accompanied by blood. brain barrier permeability. Degenerative brain diseases and ischemic brain diseases, which are typical brain diseases, are directly caused by brain cell death, but they are recognized as a result of intracellular signal transduction. Therefore, protein kinase Has begun to be studied. The c-Jun N-terminal kinase (JNK) pathway in the MAPK pathway, which is a representative cell signaling system that regulates cell death, has been verified as a target in relation to many diseases. In particular, JNK3 isoform is expressed in brain tissue The distribution is concentrated, and the connection with neuronal death has been studied extensively.In this study, we have developed a low-molecular-weight inhibitor that can regulate its function by molecular targeting of JNK3 (c-Jun N-terminal kinase), which is considered to play a key role in the brain cell death mechanism of degenerative brain disease , And to conduct a study on structural optimization focusing on improvement of BBB permeation structure of existing lead material.

Biography

Jung-Mi Hah has completed her PhD at the age of 32 years from Northwestern University and postdoctoral studies from Albert Einstein College of Medicine. She is the director of graduate school of Pharmacy at Hanyang University. She has published more than 40 papers in reputed bioorganic and medicinal chemistry journals.

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Jiwon Lee et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Study of electrochemical performance: Olivine-monoclinic complexes of cathode material for Li-ion batteries

Jiwon Lee and **Youngil Lee**
University of Ulsan, Korea

Olivine LiMPO4 (M=Fe, Mn, Co, Ni, etc.) structured cathode materials for lithium ion battery enabling use in individual IT device, electric vehicles, and high energy storage systems have been investigated due to low cost and structural stability. However, olivine materials have lower electronic conductivity and discharge capacity compared to other structure of cathode materials. Herein, we present the preparation and characterization of olivine-monoclinic structured material without using external carbon source to improve specific discharge capacity with wide operating voltage range (1.0 - 4.5 V) having high electronic conductivity as a cathode material. X-ray diffraction powder pattern of pristine shows complex of olivine, monoclinic, and vonsenite structures. The disordered vonsenite structure can be changed to active ordered monoclinic structure after the first cycle. Cycle voltammetry analysis confirms the activation of both the olivine and the monoclinic after the first cycle.

Biography

Youngil Lee has completed his Ph.D. at the age of 27 years from Louisiana State University and is currently professor of department of chemistry at University of Ulsan from 2005. He has been studied characterization and synthesis of cathode materials for lithium ion battery and published more than 90 papers in reputed journals. Especially, he is interesting to study of solid-state NMR spectroscopy on the relationship between the microstructure and electrochemical properties for energy materials.

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Pervin Unal Civcir, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

A Theoretical Calculations of Band Gaps of conducting polymers with electron donor–acceptor unit

Pervin Unal Civcir
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The interaction between alternating donors and acceptors results in a diminished band gap. With determining the proper donor (D) and acceptor (A) groups, it is possible to decrease the band gap (<1.8 eV) as much as possible or to adjust HOMO (highest occupied molecular orbital)-LUMO (lowest unoccupied molecular orbital) levels. Therefore, in this study the theoretical methods were used for the modelling of the donor–acceptor type conjugated polymers. Quantum chemical calculations were performed using density functional theory (DFT) to investigate the HOMO–LUMO energy gap of benzothiadiazole based donor–acceptor type conjugated polymers: poly{4,7-bis(3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6-yl)benzo[c][1,2,5]thiadiazole} (P1), poly{4,7-bis(3,3-dimethyl-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6-yl)benzo[c][1,2,5]thiadiazole} (P2), poly{4,7-bis(3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6-yl)-5,6-diphenylbenzo [c][1,2,5]thiadiazole} (P3) and poly{4,7-bis(3,3-dimethyl-3,4-dihydro-2H-thieno[3,4-b][1,4]dioxepin-6-yl)-5,6-diphenyl-benzo[c][1,2,5] thiadiazole} (P4). DFT is one of the most successful quantum chemistry tools for the description of ground-state properties of metals, semiconductors and insulators. Compared to other quantum chemistry methods, the DFT approach gives low computational cost and accurate results. The geometries of the monomers and oligomers were optimized using semi-empirical PM6 method in the gas phase. The band gaps of the polymers were performed by the B3LYP level of theory (Becke three-parameter hybrid correlation functional combined with Lee–Yang–Parr correlation functional) with 6-31G(d) basis set. Band gaps of the studied polymers were obtained by extrapolating oligomers gaps to infinite chain lengths. The results indicate that calculated band gaps are in good agreement with the experimental values in the literature. The theoretical methods used in this study are promising for the modelling of similar donor–acceptor type novel conjugated polymers.

Biography

Civcir completed her PhD at the University of East Anglia, UK in 1992 and became a professor in Ankara University in 2009. She is a lecturer in Ankara University, Faculty of Science, Chemistry Department. She works in the field of Organic and Computational Chemistry and has published more than15 papers in reputed journal. She has written a Chemistry book in Turkish. She was involved in translating the five Chemistry books from English to Turkish.

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Ulku Dilek Uysal et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Newly synthesized schiff bases: Structure analysis, theoretical IR, UV, ^{1}H, ^{13}C-NMR spectra and structure-activity relationship

Ulku Dilek Uysal[1], **Ayşe Aydogdu**[2] and **Halil Berber**[1]
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Schiff bases are most widely used organic compounds. They are used as pigments and dyes, catalyst, intermediates and polymer stabilizer. They exhibit a biological activities, including antifungal, antibacterial, antimalarial, antiproliferative, anti-inflammatory, antiviral, antipyretic,and herbicide properties. Furthermore, they have anti-tumor activity. These are widely applicable in analytical determination, using complex formation reactions, utilizing the variation in their spectroscopic characteristics following changes in pH and solvent. They have been used for manufacturing organic light emitting diodes having significant applications in night-vision readable displays, optical communications, laser technology and optical sensors recently [1]. To understand the mechanism of these properties, we need to some physicochemical properties of the five Schiff bases (Figure 1) synthesized by our group. Their structures were elucidated by ^{1}H-NMR, ^{13}C-NMR. Two out of the Schiff bases are original. Their properties have been searched DFT method with Gaussian 09 [2] program (B3LYP/6-311++G(d,p)) and compared with experimental values.

Biography

Ulku Dilek Uysal has completed her PhD in 2001 from Gazi University and postdoctoral studies from Intitute of Chemical Technologies of Italian National Council of Research (CNR). She is proffessor of Anadolu University at Chemistry Department. She has published more than 25 papers.

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Ayse Aydogdu et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Newly synthesized Schiff bases: Structure analysis, theoretical IR, UV, ^{1}H, ^{13}C-NMR spectra and structure-activity relationship

Ayse Aydogdu[1], **Ulku Dilek Uysal**[2] and **Halil Berber**[2]
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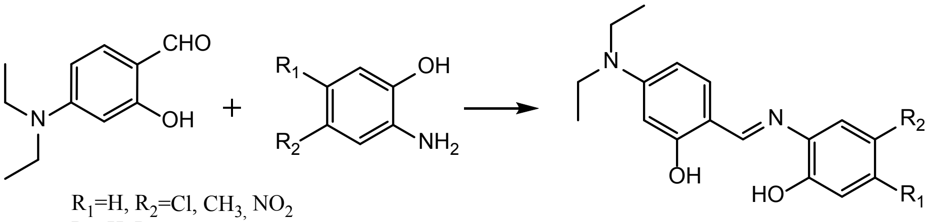
Schiff bases are most widely used organic compounds. They are used as pigments and dyes, catalyst, intermediates and polymer stabilizer. They exhibit a biological activities, including antifungal, antibacterial, antimalarial, antiproliferative, anti-inflammatory, antiviral, antipyretic,and herbicide properties. Furthermore, they have anti-tumor activity. These are widely applicable in analytical determination, using complex formation reactions, utilizing the variation in their spectroscopic characteristics following changes in pH and solvent. They have been used for manufacturing organic light emitting diodes having significant applications in night-vision readable displays, optical communications, laser technology and optical sensors recently [1]. To understand the mechanism of these properties, we need to some physicochemical properties of the five Schiff bases (Figure 1) synthesized by our group. Their structures were elucidated by 1H-NMR, 13C-NMR. Two out of the Schiff bases are original. Their properties have been searched DFT method



R_1=H, R_2=Cl, CH_3, NO_2
R_2=H, R_2=Cl, CH_3,

Biography

Ayse Aydogdu has taken her Bachelor's degree in 2015 from Anadolu University. She is student of Anadolu University at Graduate School of Sciences.

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Hulya Ayar Kayali et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Synthesis, characterization and anticancer activity of new organometallic ruthenium(II/III) complexes

Hulya Ayar Kayali[b,d], **Zehra Tavşan**[a], **Pelin Köse Yaman**[b], **BetUl Şen**[c], **Cansu Sonay Karagöz**[a] and **Elif Subaşı**[b]
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Novel organo ruthenium (II/III) complexes ([(η^6-p-cymene)Ru(η^1-S-TSC)Cl2], (1); and *trans*-[RuCl$_2$(PPh$_3$)$_2$(η^2-N,S-TSC)], (2) have been synthesized from the reflux reaction of [{(η^6-p-cymene)RuCl}$_2$(μ-Cl)$_2$] and [RuCl$_3$(PPh$_3$)$_3$] with a new TSC (2-acetyl-5-chloro-thiophene thiosemicarbazone) in methanol and benzene, respectively. TSC and both of the complexes have been characterized by elemental analysis, UV–Vis, FT-IR and ^{1}H NMR spectroscopy. The single crystal structure of TSC has been determined by X-ray crystallography revealing that TSC crystallized in the monoclinic space group P2$_{1/c}$. The spectroscopic studies showed that TSC is coordinated to the central metal as a neutral monodentate ligand coordinating via its thiocarbonyl sulfur atom (C=S) in (1), whereas TSC acts as a bidentate anionic chelating ligand with azomethine nitrogen (C=N) and thiol sulfur atom in (2). Both ruthenium complexes displayed higher antiproliferative activities against selected tumor cell lines than TSC ligand, and significantly lower cytotoxic dose towards cancer cell lines and normal colon cell compared to cisplatin. (1) was more active against the colon cancer while (2) was highly cytotoxic towards ovarian carcinoma cells. However, DNA and BSA binding studies for the characterization of antitumor mechanism of ruthenium complexes indicated that these complexes interacted weakly with DNA and BSA, as quantified by K$_b$ in contrast with the importing into cell and accumulation in cytoplasm and then nucleus. These results showed that the mechanism of action may be different from DNA intercalation mechanism. Also, spectral evidences showed these complexes may prefer different transport system instead of binding with albumin. It has been observed that the complexes exhibited different cell cycle arrest on cell lines. Furthermore, our results demonstrated that these newly synthesized ruthenium complexes appear to be as a good antitumor drug candidate. This project has been supported by TUBITAK 215Z663.

Biography

Hulya Ayar Kayali has completed her MSc and PhD from University of Dokuz Eylul in 1997 and 2005, respectively in 2003 and postdoctoral studies from McGill University, Canada, 2011. She works at Dokuz Eylul University from 1998 and she is a professor from 2014. She has published more than 35 papers in reputed journals.

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Notes:

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Min-Young Lyu et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Comparison of thermal and physical properties of fossil and bio-based polycarbonates

Min-Young Lyu[1], **Jung Hyun Park**[1], **Hyung Jin Nho**[2], **Myung Sool Koo**[2] and **Sung Hwan Cho**[2]
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[2]Samyang Central R & D Center, South Korea

Bio-based polymer has advantages as an environmentally friendly material. It is obtained from corn or other plants. Fossil-based polycarbonate (PC) is polymerized using bisphenol-A (BPA), whereas bio-based PC is polymerized using isosorbide monomer. The thermal and physical properties have been studied for bio-based and fossil-based PC. The thermal properties were measured by differential scanning calorimetry, differential thermal analysis, and thermal gravimetric analysis. Bio-based PC showed a low glass transition temperature and weak thermal resistance compared with those characteristics of fossil-based PC. Bio-based PC exhibited a higher optical property, which was verified by transmittance, haze, and birefringence. Bio-based PC showed higher transmittance and lower haze than those characteristics of fossil-based PC. The birefringence of injection molded specimens of bio-based and fossil-based PC were also compared and the bio-based PC showed lower birefringence. Bio-based PC shows weak thermal resistance than that of fossil-based PC, whereas bio-based PC shows higher optical characteristics than those of fossil-based PC.

Biography

Min-Young Lyu has completed his PhD at the age of 33 years from The University of Akron, Ohio, USA. He is the professor in the Department of Mechanical System Design Engineering at the Seoul National Univiersity of Science and Technology. He was a chief researcher in Samyang Central R&D Center and a associate engineer in LG Production Research Center. He has published more than 90 papers in the world and has been serving as an editorial board member of Polymer(Korea) and Elastomers & Composites.

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conferenceseries.com

A Szyszkowska et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

Structure characterization of 2,6-bis(2-hydroxyethyl)-1-phenylimidazo[1,5-c]-quinazoline-3,5-dione

A Szyszkowska[a], **I Zarzyka**[a], **S Pawlędzio**[b], **D Trzybiński**[b] and **K Woźniak**[b]
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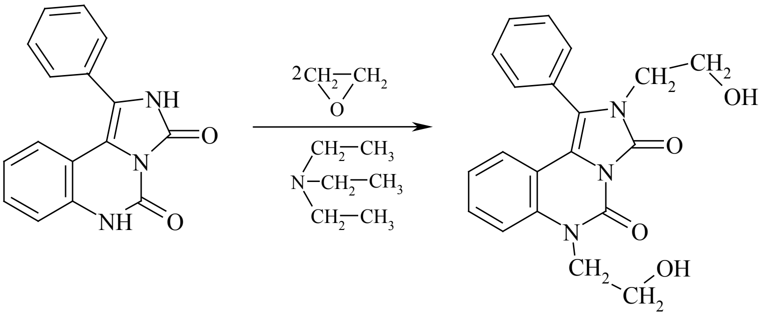
[b]University of Warsaw, Poland

The work presents the results of reaction product of 1-phenyl-2H,6H-imidazo[1,5-c]quinazoline-3,5-dione with 2 molar excess ethylene oxide.



1 -phenyl-2,6-bis(2-hydroxyethyl)imidazo[1,5-c]quinazoline-3,5-dione was isolated at high yield from the reaction mixtures and identified based on the IR, 1H-and 13C-NMR spectroscopies. X-Ray diffraction measurement was also performed for the single-crystals obtained by crystallization of crude product from ethanol. It was indicated that 1-phenyl-2,6-bis(2-hydroxyethyl) imidazo[1,5-c]quinazoline-3,5-dione crystallizes in the monoclinic P21/n space group with two molecules of compound in the asymmetric unit of the crystal lattice. The crystal analysis revealed various types of molecular interactions in the crystal lattice of investigated compound. To understand better the nature of packing of molecules in the crystal lattice of investigated compound the Hirshfeld surface analysis was performed.

Biography

Agnieszka Szyszkowska graduated MA in 2014 at the University of Jan Kochanowski. She completed two courses of study: chemistry and biology. She started PhD at the Rzeszów University of Technology in 2014.

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Dila Ercengiz et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Theoretical IR, UV, ^{1}H and ^{13}C-NMR spectra of certain Schiff bases derived substituted-2-aminophenol and hydroxyl benzaldehyde

Dila Ercengiz[1], **Halil Berber**[2] and **Ulku Dilek Uysal**[2]
Anadolu University, Turkey

Schiff bases are compounds formed by the condensation of an active carbonyl group with primary amine or N-substituted imine containing an imino group (R-C=N-). They have been used as ligands, liquid crystals, heterogeneous catalysts, high-performance organic light emitting diodes (OLED), and to design molecular ferromagnet, in catalysis and biological applications [1]. In this study, five Schiff bases (Figure 1) have been synthesized and characterized with ^{1}H and ^{13}C-NMR. These Schiff bases' Gibbs Free Energies, Dipole moments, HOMO-LUMO values, theoretical IR, UV, ^{1}H and ^{13}C-NMR spectra have been researched by DFT method with Gaussian09 program (B3LYP/6-311++G(d,p)) [2] and compared than those with experimental values. Structure- reactivity relationship for these molecules was also searched.

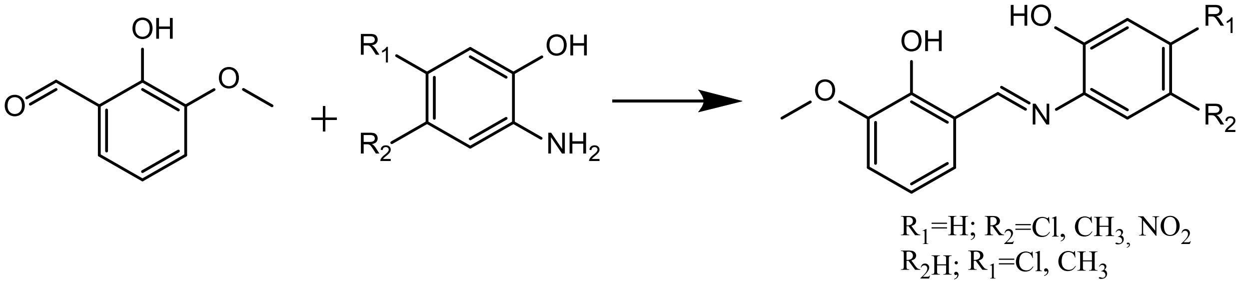

Figure 1. The studied Schiff bases.

Biography

Dila Ercengiz has completed her Bachelor's degree in 2015 from Anadolu University. She is student of Anadolu University at Graduate School of Sciences.

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Elif Subaşı et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Half-sandwich ruthenium-arene complex containing heterocyclic thiosemicarbazone: The X-ray crystal structures and DNA interactions

Elif Subaşı[a], **Pelin Köse Yaman**[a], **Birgul Kehlibar**[d], **Betul Şenc**, **Cansu Sonay Karagöz**[b] and **Hulya Ayar Kayali**[a,d]
[a,b,c,d]Dokuz Eylul University, Turkey

The organoruthenium complex [(η6-p-cym)Ru(η1-S-TSC)Cl2], (1) and (2-acetyl-5-methyl-thiophene thiosemicarbazone) TSC ligand were investigated *in vitro* for their properties as prospective anti-tumour agents. The complex and TSC have been characterized by elemental analysis, UV–Vis, FT-IR and ^{1}H NMR spectroscopy. The crystal structures of TSC and (1) have been determined by X-ray crystallography and (1) represented as the first structurally characterized arene–ruthenium half-sandwich complex with a monodentate S coordinated TSC ligand. It is revealed that TSC, crystallized in the monoclinic space group P21/c and complex (1) shows a distorted octahedral geometry around the Ru centre. The mononuclear complex adopts a typical three legged piano-stool geometry with the metal centre coordinated by two chlorides and a TSC ligand. The cytotoxic activity of the complex against human ovarian (A2780, SKOV-3 and OVCAR-3) and colon (DLD, CCD-18Co, Caco-2) cell lines was investigated. The complex exhibit higher cytotoxicity in three cancer cell lines than in normal cell (CCD-18Co). The Caco-2 cell was especially susceptible to the complex, with an IC50 value (0.18 μM) lower than cisplatin (64.72 μM). The cytotoxic values of (1) treated A2780 cells (1.15 μM) was also lower than cisplatin treated (10.08 μM). The results showed that the complex exhibits the higher cytotoxicity against colon cell lines than ovarian cell lines. The cellular uptake and localization suggest that (1) can be successfully taken up by the all studied cells, and the complex can enter into the cytoplasm and accumulate in the cell nuclei. The cell cycle distribution shows that the complex inhibits the cell growth in the generally G0/G1 and/or G2/M phases arrest. These results show that the complex may be a potential anticancer drug.

Biography

Elif Subaşı has completed her MSc from University of Reading, England in 1996 and PhD from Ege University, Turkey in 2003 and postdoctoral studies from University College London, England. She works at Dokuz Eylul University from 2003 and she is a professor from 2012. She has published more than 25 papers in reputed journals.

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conferenceseries.com

Goncagul Serdaroglu, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

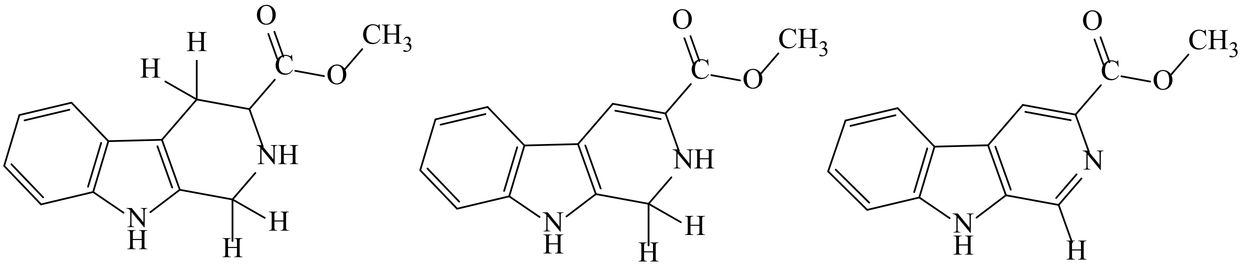
4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

The DFT Calculations on relationship between Solvation Energies and aromaticity of THβC, DHβC, βC

Goncagul Serdaroglu
Cumhuriyet University, Turkey

The βC, which are naturally extracted from plants and obtained as secondary metabolism products from human tissues and marine organisms, have a very important place in many research fields because of their pharmacological properties such as inhibition activity against to the human cancer cell lines, antimalarial, fungicidal, convulsant, and so on. Here, this study used computational chemistry tools to predict the possible chemical behavior of these non-aromatic, half-aromatic and full aromatic compounds in the living body. Geometry optimization and frequency calculations have been performed in the three basis set levels, both in the gas and in the aqueous phases. The stabilization free energies increase in the following order as 0 (9.32 kcal) < 1 (9.50 kcal) < 2 (10.18 kcal) with B3LYP/6311++G** basis set in water phases. The electron density on molecular surface have changed in the following order: 2 (0.128) < 1 (0.123) < 0 (0.114) with the B3LYP/6-311++G** level of theory in water phase. It seems to be the structure 2 is the most reactive structure because it has the lowest negative and the highest positive charge centers and it seems to be the most reactive and most aromatic and less stable structure.



0 1 2

Figure 1. The β-Carbolines given as 0 (THβC-3-carboxylic acid methyl ester), 1 (DHβC-3-carboxylic acid methyl ester), 2 (βC-3-carboxylic acid methyl ester)

Biography

Goncagul Serdaroğlu has completed his PhD from Cumhuriyet University (2008) and postdoctoral studies from Auburn University (2013). She works on the structural properties and chemical behavior of biologically and pharmacologically important molecules by using computational tools.

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Ulku Dilek Uysal, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

Theoretical study on a newly approved pharmaceutical formulation active components-Indacaterol and Roflumilast

Ulku Dilek Uysal and **Halil Berber**
Anadolu University, Turkey

Indacaterol (In) is 5-{(1R)-2-[(5,6-diethyl-2,3-dihydro-1H-inden-2-yl)amino]-1-hydroxyethyl}-8-hydroxy-2(1H)-quinolinone maleate. Roflumilast (Ro) (3-cyclopropylmethoxy-4-difluoromethoxy-N-[3,5-dichloropyridyl-4]- benzamide) (Fig. 1). They have been approved for chronic obstructive pulmonary disease (COPD) [1]. According to the World Health Organization (WHO), more than 200 million people have moderate-to- severe COPD worldwide [2]. It is in urgent need of the theoratical properties and structure-activity relationship information for Indacaterol and Roflumilast. These are searched by DFT method with Gaussian09 program (B3LYP/6-311++G(d,p)).

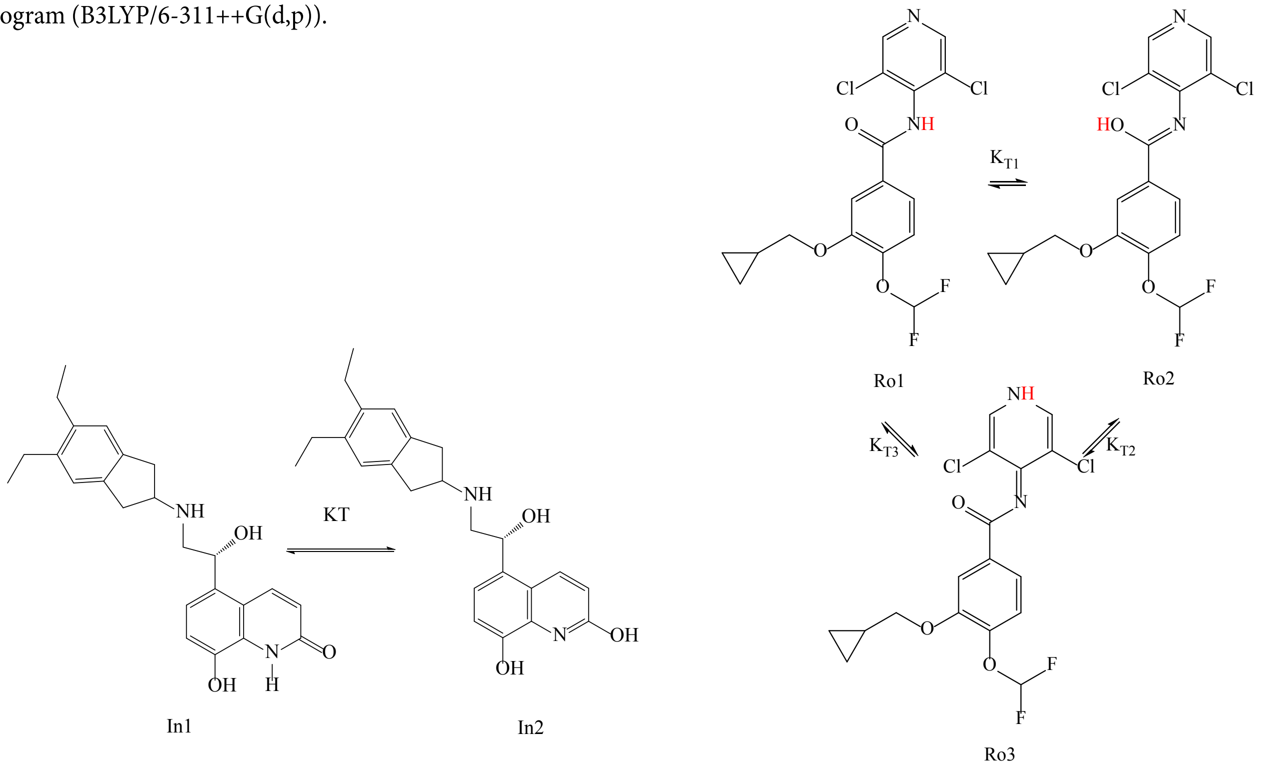

Fig. 1. Chemical structure of Indacaterol (In), Roflumilast (Ro) and their tautomers.

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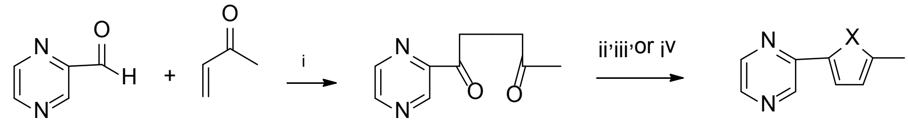
Pervin Unal Civcir, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Computational study of the synthesis of pyrrole-pyrazines

Pervin Unal Civcir
Ankara University, Turkey

In continuation of our studies of extended heterocyclic systems with potential semi-conductivity and nonlinear optical properties, we have synthesized and studied theoretically some pyrazine derivatives possessing a pyrrole (or thiophene, or furan) ring systems. Extension of the Stetter protocol used in the previous work 1-4 was unsuccessful for the pyrazine analogues because of the poor accessibility of formylpyrazine only gave a complex mixture of products from which the pyrazine could not be isolated.5 We have tried to obtain pyrrolylpyrazine, furylpyridazines, and thienylpyridines from formylpyridazines, via the Paal-Knorr reaction on the intermediary pyrazinyl- 1,4-diketones, using ammonium acetate, polyphosphoric acid or Lawesson's reagent 14, respectively (Scheme 1). The intermediate 1,4-diketone was synthesized via the Stetter reaction in the presence of thiazolium salt as a catalyst. Therefore, we aimed to study theoretically in detail the mechanism of the synthesis for the pyrazine derivatives. In this work, the experimentally suggested mechanisms of Stteter6 and Paal-Knorr7,8 reactions for only pyrrolypyrazine have been modelled with density functional theory (DFT)9, which gives low computational cost and accurate results. Geometries of stationary points along the reaction coordinate have been optimized at BP3LYP10,11 (the hybrid gradient-corrected exchange functional, proposed by Becke, combined with the gradient-corrected correlation functional of Lee, Yang, and Parr) levels of theory using 6-31G* and 6-31G** basis sets12 without any symmetry consideration. Vibrational frequency calculations were used to characterize all stationary points as either minima (no imaginary frequencies) or transition states (with only one imaginary frequency). Vibrational frequencies were also used to evaluate zero point energies and the thermodynamic data. Intrinsic reaction coordinate (IRC) calculations were traced to ensure that the transition states connect the proper minima.13 Mechanisms of the reactions are explained in the potential energy diagrams.



i: Thiazolium chloride, triethylamine, dioxane
ii:Ammonium acetate,
II: Polyphosphoric acid
III:Lawesson's reagent

X=NH, O, S

This study was supported by Ankara University BAP Project Coordinator by code number 12A4240001.

Biography

Civcir completed her PhD at the University of East Anglia, UK in 1992 and became a professor in Ankara University in 2009. She is a lecturer in Ankara University, Faculty of Science, Chemistry Department. She works in the field of Organic and Computational Chemistry and has published more than15 papers in reputed journal. She has written a Chemistry book in Turkish. She was involved in translating the five Chemistry books from English to Turkish.

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Hulya Ayar Kayali et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Synthesis, characterization and anticancer activity of new organometallic ruthenium(II/III) complexes

Hulya Ayar Kayali[b,d], **Zehra Tavşan**[a], **Pelin Köse Yaman**[b], **Betül Şen**[c], **Cansu Sonay Karagöz**[a] and **Elif Subaşı**[b]
Dokuz Eylül University, Turkey

Novel organo ruthenium (II/III) complexes ([(η6-p-cymene)Ru(η1-S-TSC)Cl2], (1); and trans-[RuCl2(PPh3)2(η2-N,S-TSC)], (2) have been synthesized from the reflux reaction of [{(η6-p-cymene)RuCl}2(μ-Cl)2] and [RuCl3(PPh3)3] with a new TSC (2-acetyl-5-chloro-thiophene thiosemicarbazone) in methanol and benzene, respectively. TSC and both of the complexes have been characterized by elemental analysis, UV–Vis, FT-IR and 1H NMR spectroscopy. The single crystal structure of TSC has been determined by X-ray crystallography revealing that TSC crystallized in the monoclinic space group P21/c. The spectroscopic studies showed that TSC is coordinated to the central metal as a neutral monodentate ligand coordinating via its thiocarbonyl sulfur atom (C=S) in (1), whereas TSC acts as a bidentate anionic chelating ligand with azomethine nitrogen (C=N) and thiol sulfur atom in (2). Both ruthenium complexes displayed higher antiproliferative activities against selected tumor cell lines than TSC ligand, and significantly lower cytotoxic dose towards cancer cell lines and normal colon cell compared to cisplatin. (1) was more active against the colon cancer while (2) was highly cytotoxic towards ovarian carcinoma cells. However, DNA and BSA binding studies for the characterization of antitumor mechanism of ruthenium complexes indicated that these complexes interacted weakly with DNA and BSA, as quantified by Kb in contrast with the importing into cell and accumulation in cytoplasm and then nucleus. These results showed that the mechanism of action may be different from DNA intercalation mechanism. Also, spectral evidences showed these complexes may prefer different transport system instead of binding with albumin. It has been observed that the complexes exhibited different cell cycle arrest on cell lines. Furthermore, our results demonstrated that these newly synthesized ruthenium complexes appear to be as a good antitumor drug candidate. This project has been supported by TUBITAK 215Z663.

Biography

Hulya Ayar Kayali has completed her MSc and PhD from University of Dokuz Eylul in 1997 and 2005, respectively in 2003 and postdoctoral studies from McGill University, Canada, 2011. She works at Dokuz Eylul University from 1998 and she is a professor from 2014. She has published more than 35 papers in reputed journals.

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A Szyszkowska et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Structure characterization of 2,6-bis(2-hydroxyethyl)-1-phenylimidazo[1,5-c]-quinazoline-3,5-dione

A Szyszkowska[a], **I Zarzyka**[a], **S Pawlędzio**[b], **D Trzybińskib** and **K Woźniak**[b]
[a]The Rzeszów University of Technology, Poland
[b]University of Warsaw, Poland

The work presents the results of reaction product of 1-phenyl-2H,6H-imidazo[1,5-c]quinazoline-3,5-dione with 2 molar excess ethylene oxide.

1-phenyl-2,6-bis(2-hydroxyethyl)imidazo[1,5-*c*]quinazoline-3,5-dione was isolated at high yield from the reaction mixtures and identified based on the IR, ^{1}H-and ^{13}C-NMR spectroscopies. X-Ray diffraction measurement was also performed for the single-crystals obtained by crystallization of crude product from ethanol. It was indicated that 1-phenyl-2,6-bis(2-hydroxyethyl)imidazo[1,5-c]quinazoline-3,5-dione crystallizes in the monoclinic $P2_{1/n}$ space group with two molecules of compound in the asymmetric unit of the crystal lattice. The crystal analysis revealed various types of molecular interactions in the crystal lattice of investigated compound. To understand better the nature of packing of molecules in the crystal lattice of investigated compound the Hirshfeld surface analysis was performed.

Biography

Agnieszka Szyszkowska graduated MA in 2014 at the University of Jan Kochanowski. She completed two courses of study: chemistry and biology. She started PhD at the Rzeszów University of Technology in 2014.

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Dila Ercengiz et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

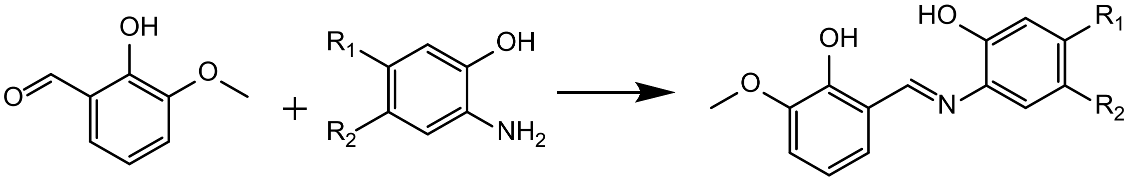
4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

Theoretical IR, UV, ^{1}H and ^{13}C-NMR spectra of certain Schiff bases derived substituted-2-aminophenol and hydroxyl benzaldehyde

Dila Ercengiz[1], **Halil Berber**[2] and **Ulku Dilek Uysal**[2]
[1,2]Anadolu University,Turkey

Schiff bases are compounds formed by the condensation of an active carbonyl group with primary amine or N-substituted imine containing an imino group (R-C=N-). They have been used as ligands, liquid crystals, heterogeneous catalysts, high-performance organic light emitting diodes (OLED), and to design molecular ferromagnet, in catalysis and biological applications [1]. In this study, five Schiff bases (Figure 1) have been synthesized and characterized with ^{1}H and ^{13}C-NMR. These Schiff bases' Gibbs Free Energies, Dipole moments, HOMO-LUMO values, theoretical IR, UV, ^{1}H and ^{13}C-NMR spectra have been researched by DFT method with Gaussian09 program (B3LYP/6-311++G(d,p)) [2] and compared than those with experimental values. Structure- reactivity relationship for these molecules was also searched.



R_1=H; R_2=Cl, CH_3, NO_2
R_2H; R_1=Cl, CH_3

Figure 1. The studied Schiff bases.

Biography

Dila Ercengiz has completed her Bachelor's degree in 2015 from Anadolu University. She is student of Anadolu University at Graduate School of Sciences.

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Nirnay Samanta et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Collective hydration dynamics in some amino acid solutions: A combined GHz-THz spectroscopic study

Nirnay Samanta[1], **Debasish Das Mahanta**[1], **Samiran Choudhury**[2], **Anjan Barman**[2] and **Rajib Kumar Mitra**[1]
[1,2]S N Bose National Centre for Basic Sciences, India

A detailed understanding of hydration of amino acids, the building units of protein, is a key step to realize the overall solvation processes in proteins. In the present contribution we have made a combined GHz (0.2-50) to THz (0.3-2.0) experimental spectroscopic study to investigate the dynamics of water at room temperature in presence of different amino acids (Glycine, L-Serine, L-Lysine, L-Tryptophan, L-Arginine and L-Aspartic acid). The THz absorption coefficient, $\alpha(\nu)$ of amino acids follows a trend defined by their solvent accessible surface area (SASA). The imaginary and real dielectric constants obtained in GHz and THz regions are fitted into multiple Debye model to obtain various relaxation times. The ~100 ps time scale obtained in the GHz frequency region is attributed to the rotational motion of the amino acids. In the THz region we obtain ~8 ps and ~200 fs time scales which are related to the cooperative dynamics of H-bond network and partial rotation or sudden jump of the under-coordinated water molecules. These timescales are found to be dependent on the amino acid type and the cooperative motion if found to be dependent on both the hydrophobic as well as the hydrophilic residue of amino acids.

Biography

Nirnay Samanta is a Senior Research Fellow (PhD scholar) in Physical Chemistry under the supervision of Dr. Rajib Kumar Mitra in S.N. Bose National Centre for Basic Sciences, India. He is working on biophysical Chemistry and uses THz spectroscopy, GHz spectroscopy, steady state as well as time resolved fluorescence spectroscopy etc. He has published 8 papers in reputed journals.

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Krishnendu Pal, Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Biophysical characterization of dynamic hysteresis and energetics of the gating processes of the voltage gated sodium ion channel using nonequilibrium response spectroscopy

Krishnendu Pal
S N Bose National Centre for Basic Sciences, India

Here we have studied the dynamic as well as the non-equilibrium thermodynamic response properties of voltage-gated Na-ion channel. Using sinusoidally oscillating external voltage protocol as Nonequilbrium Response Spectroscopic tool, we have both kinetically and energetically studied the non-equilibrium steady state properties of dynamic hysteresis in det ails. We have estimated the work done associated with the dynamic memory due to a cycle of oscillating voltage. We have quantitatively characterised the loop area of ionic current which gives information about the work done to sustain the dynamic memory only for ion conduction, while the loop area of total entropy production rate gives the estimate of work done for overall gating dynamics. The maximum dynamic memory of Na-channel not only depends on the frequency and amplitude but it also depends sensitively on the mean of the oscillating voltage and here we have shown how the system optimize the dynamic memory itself in the biophysical range of field parameters. The relation between the average ionic current with increasing frequency corresponds to the nature of the average dissipative work done at steady state. It is also important to understand that the utilization of the energy from the external field can not be directly obtained only from the measurement of ionic current but also requires nonequilibrium thermodynamic study.

Biography

Krishnendu Pal, 27 years, is doing PhD in S.N. Bose National Centre For Basic Sciences, Kolkata-106, India. His area of research includes theoretical and computational investigation of kinetics and nonequilibrium thermodynamics of Dynamic hysteresis, Drug bindings(Local Anesthetics), Inactivation process of voltage gated sodium ion channel and study of stochastic resonance in neurons.

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Ozge Yuksel Orhan et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Utilization of CO_2 in petrochemical plants

Ozge Yuksel Orhan and **Erdogan Alper**
Hacettepe University, Turkey

Good quality CO_2 is produced and currently discharged to atmosphere in majority of integrated petrochemical sites. For instance, ethylene oxide facilities alone discharge more than 3 millions tons CO_2 annually (Both, 1.5 millions and 6.2millions tons annual production is reported for this CO_2 source indicating also lack of information). Urea production is a clear example of CO_2 conversion where produced ammonia is reacted with CO_2 from the same facility. Several other processes can be identified, such as polycarbonate productions in ethylene and/or propylene oxide plants which are recently implemented. Two cheap chemicals, namely methane and CO_2, can be turned to acetic acid. Production of benzoic acid from CO_2 and benzene is an alternative feasible route and could well be implemented. In this paper, manufacture of selected number of value-added products (acrylic acid, electrochemical ethylene, electrochemical mono-ethylene glycol, polyols and isocyanate or equivalent) will be reviewed briefly. The choice is somehow arbitrary since there are gigantic numbers of possibilities which can be envisaged by employing products of a large integrated complex.

Biography

Ozge Yuksel Orhan obtained her Ph.D. in Chemical Engineering from Hacettepe University, Turkey, in December 2014. Her thesis is entitled "The Absorption Kinetics of CO_2 into Ionic Liquid-CO_2 Binding Organic Liquid Hybrid Solvents". Currently, she is a Research and Teaching Assistant at Chemical Engineering Department of Hacettepe University. Her research topics have dealt with the study of carbon dioxide capture by novel solvents. Erdogan Alper is a Professor at the Chemical Engineering Department of Hacettepe University in Ankara, Turkey. He obtained his BSc (Honours) (First Class) from Birmingham University, England (1968), and earned his PhD from Cambridge University (1972). In 1977–1978, he was an Alexander von Humboldt fellow at Hannover University, Germany, and received Turkish Scientific and Technological Research Council prize in Engineering in 1982. His research areas include carbon dioxide capture by innovative solvents, fuel cell modelling by CFD, petroleum refining and petrochemical technologies. He published 4 books and around 150 research papers in cited journals.

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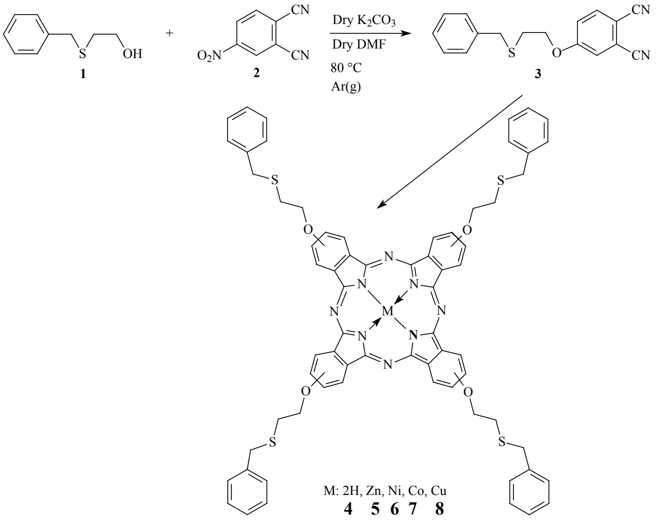
Cigdem Yagci et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Novel organosoluble phthalocyanines bearing 2-(Benzylthio)ethoxy units: synthesis and characterization

Cigdem Yagci[1]**,Bilgin, Ahmet** [1], **Acıerik, Nagihan** [2] and **Kadi, Cigdem**[2]
[1]Kocaeli University, Faculty of Education, Kocaeli, Turkey
[2]Karabük University, Faculty of Scienc, Karabük, Turkey

Phthalocyanines have been employed extensively as subunits for the construction of functional materials since they exhibit special optical and electronic properties and self-organizing abilities to form columnar mesophases, Langmuir–Blodgett (LB) multilayers and aggregates in solution, or in the solid state.1,2 Applications of peripherally unsubstituted phthalocyanines are restricted because of their insolubility in common solvents. Phthalocyanines own an extended π-conjugated electron system which allows π stacking between planar macrocycles, provided the distance between the macrocycles is small. By the peripheral attachment of alkyl, alkoxy or alkylthio groups to the macrocycle, metal phthalocyanine complexes can be made soluble in common organic solvents.3 Heteroatom-functionalized substituents can be introduced onto the periphery of the phthalocyanine nucleus. These peripheral groups are capable of binding soft or hard metal cations and provide donor sites for binding different metal ions. We presented synthesis and characterization of new organosoluble phthalocyanines bearing 2-(benzylthio)ethoxy units in this work. For this purpose 4-[2-(benzylthio)ethoxy]phthalonitrile was prepared with the reaction of 4-nitrophthalonitrile with the hydoxyl end group of 2-(benzylthio)ethanol. Metal-free and metallo phthalocyanines (4-8) were synthesized by cyclotetramerization reaction of the novel phthalonitrile derivative under suitable conditions. Aggregation and metal binding properties of ZnPc (5) was investigated. All the novel compounds have been characterized by FT-IR, NMR, DSC, TGA techniques.



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Fereniki Perperopoulou et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Characterization of the pesticide detoxifying enzyme C*d*GSTM1-1 by kinetic analysis and differential scanning fluorimetry

Fereniki Perperopoulou[1], **Farid Ataya**[2] and **Nikolaos E Labrou**[1]
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[2]College of Science King Saud University, Saudi Arabia

Glutathione transferases (GSTs, EC. 2.5.1.18) form a large group of multifunctional enzymes, best known for their involvement in the metabolism and inactivation of a wide range of xenobiotic compounds. GSTs catalyze the nucleophilic attack of the reduced form of glutathione (γ-L-Glu-L-Cys-Gly, GSH) on the electrophilic center of a variety of compounds such as pesticides, herbicides etc. The conjugation of GSH to such molecules results in the increase of their solubility and the reduction of their toxicity. GSTs are useful tools with a variety of biotechnological applications in many fields. The natural ability of the GSTs to interact with xenobiotic compounds gives the opportunity to develop enzyme biosensors for the simple and direct monitoring of environmental pollutants. In the present work we report the cloning, kinetic and structural characterization of the GSTM1-1 from camel (*Camelus dromedarius*) as well as a screening method to identify ligands that bind the protein. The C*d*GSTM1-1 enzyme was expressed in *E. coli* and purified by affinity chromatography. The ligandin function of the enzyme was evaluated by measuring the ability of forty seven xenobiotic compounds to bind and inhibit enzyme activity. The inhibition potency was measured with the CDNB/GSH assay system. The IC_{50} value and the kinetic analysis of the compound that showed the highest inhibition were determined. The results showed that the enzyme exhibits high selectivity towards the fungicide zoxium zoxamide. The thermodynamic stability of C*d*GSTM1-1 and the influence of zoxium zoxamide were investigated using the differential scanning fluorimetry (DSF). The results are explored for the development of an optical biosensor for the determination of zoxium zoxamide in environmental samples.

Biography

Fereniki Perperopoulou studied Agricultural Biotechnology at the Agricultural University of Athens. She remained at the Agricultural Biotechnology Department of the Agricultural University of Athens, where she earned a master's degree on "Bioactive Protein Products & Technology". From 2014 to date she is a PhD candidate at the Department of Biotechnology (Agricultural University of Athens), working on the subject "Protein engineering and molecular study of transferase glutathione", for which she has been awarded a scholarship under the scheme research projects for excellence iky/siemens.

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Foteini M Pouliou et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Investigation of the interaction of the tau class glutathione tranferase with pesticides by differential scanning fluorimetry

Foteini M Pouliou and **Nikolaos E Labrou**
Agricultural University of Athens, Greece

Glutathione transferases (GSTs, EC 2.5.1.18) constitute one of the most important families of detoxifying enzymes in nature with multiple biotechnological applications. GSTs contribute to the phase II biotransformation of xenobiotics in a variety of organisms, with members of the family being involved in both the metabolism and transportation of potentially toxic ligands (e.g. pesticides). The goal of this study was to apply GST as a model in order to investigate whether ligands' mode of inhibition could be discerned through thermal denaturation profiles. A library of Tau class GSTs was constructed by DNA shuffling using the DNA encoding the *Glycine max* GSTs G*m*GSTU2-2, G*m*GSTU4-4 and G*m*GSTU10-10. The DNA library contained chimeric structures of alternated segments of the parental sequences and point mutations. Chimeric GST sequences were expressed in *Escherichia coli*, purified by affinity chromatography and their enzymatic activities towards CDNB (1-chloro-2,4-dinitrobenzene) were determined. A selected chimeric enzyme which exhibited high catalytic activity and stability was used as a model for the assessment of the GST-pesticide interaction with a differential scanning fluorimetry (DSF). DSF signatures were obtained and analysed in the absence and in the presence of different concentrations of the substrate GSH, the inhibitor S-hexyl GSH and a range of different pesticides. The results of the study are explored for the development of a DSF-based assay for the direct determination of pesticides in environmental samples.

Biography

Foteini Pouliou is a PhD candidate at the Agricultural University of Athens since 2014. She majored in biotechnology at the department of biotechnology of the same university in 2012 and enrolled in her Master of Science (MSc) studies in 2013 focusing on bioactive products and protein technology. Her research interests include protein engineering, enzyme and environmental biotechnology. She has been working on Glutathione Transferases (GSTs), a group of detoxification enzymes. She has been awarded a grant by the State Scholarships Foundation under the scheme research projects for excellence iky/siemens.

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Thanyathon Niyomthai et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Effect of hydrogen on catalytic activity of ziegler-natta catalysts prepared by different methods in ethylene polymerization

Thanyathon Niyomthai, Bunjerd Jongsomjit and **Piyasan Praserthdam**
Chulalongkorn University, Thailand

Ethylene homopolymerization by two types of Ziegler-Natta catalysts including none-THF and none-EtOH catalysts was compared. The influences of hydrogen concentrations on surface active sites of these catalysts were investigated based on catalytic activity. From the results, the EDX analysis and surface area measurement confirmed that none-EtOH catalyst had better active center distribution than that of none-THF. Thus, the none-EtOH catalyst could retard the hydrogen effect on surface active sites and show higher activity with increased hydrogen pressures1. However, catalytic activity was lower with high hydrogen pressure. In addition, to study for more detail about the hydrogen effect, none-THFs were modified with different metal halide additives ($AlCl_3$ and $FeCl_2$). Lewis acid modification can improve activity because it can remove the remaining THF in the final catalyst, which can poison the catalyst active sites via the ring-opening of THF[2] which was confirmed by FT-IR and XRD measurements. Moreover, the activity enhancement was due to the formation of acidic sites by modifying the catalysts with Lewis acids. Thus, $FeCl_2$ doped catalyst (Fe-THF) exhibited the highest activity followed by $AlCl_3$ doped catalyst (Al-THF) and undoped catalyst (ZN-THF). In the H_2/C_2H_4 molar ratio of 0.08, Fe-THF showed a better hydrogen response on the surface active sites than Al-THF due to more titanium clustered distribution. Fe-THF is considered to have more clustered Ti species than Al-THF[3]. As a consequence, it led to obtain more possible chances to proceed chain transfer reaction by hydrogen.

Biography

Thanyathon studies the doctoral degree of chemical engineering at chulalongkorn university and joined catalysis and catalytic reaction engineering research group with the Royal Golden Jubilee program of Thailand Research Fund (TRF).

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Thanyathon Niyomthai et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

Theoretical study: Non-small cell lung cancer drugs

Ulku Dilek Uysal and **Halil Berber**
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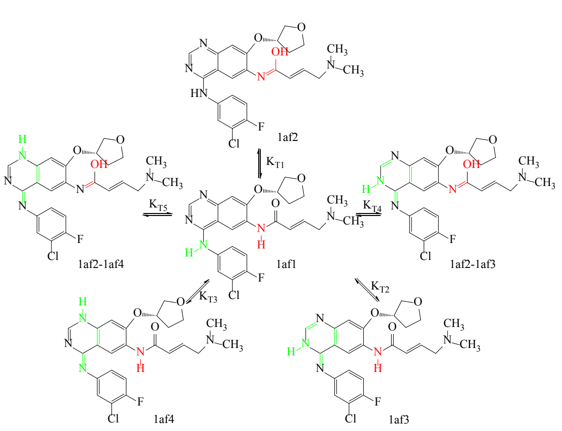
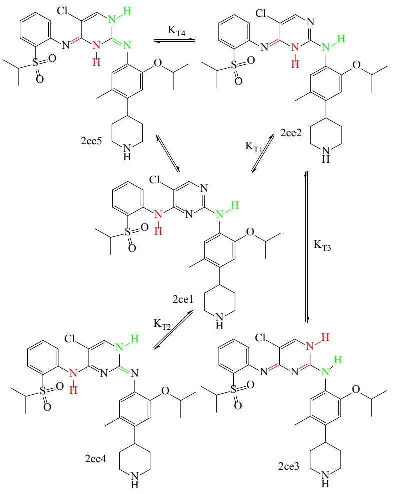
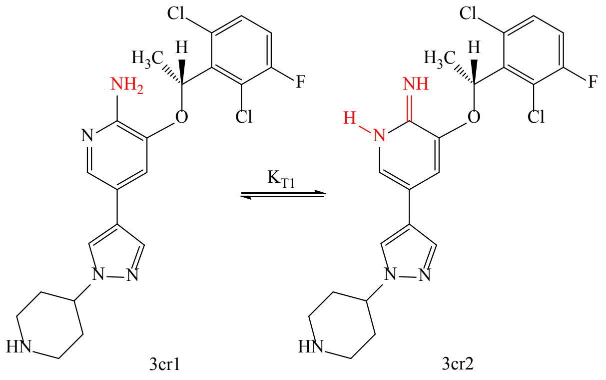
Afatinib, crizotinib and ceritinib (Figure 1) have been used as a treatment for non-small lung cancer in recent years [1]. To the best of our knowledge; there has been no theoretical research about these three non-small cell lung cancer drugs in the literature. The theoretical investigation of these molecules is an urgent need to understand the residance mechanism of these drug active components.







Biography

Ulku Dilek Uysal has completed her PhD in 2001 from Gazi University and postdoctoral studies from Intitute of Chemical Technologies of Italian National Council of Research (CNR). She is proffessor of Anadolu University at Chemistry Department. She has published more than 25 papers.

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May 11-13, 2017 Barcelona, Spain

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A Szyszkowska et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Structure characterization of 2,6-bis(2-hydroxyethyl)-1-phenylimidazo[1,5-c]-quinazoline-3,5-dione

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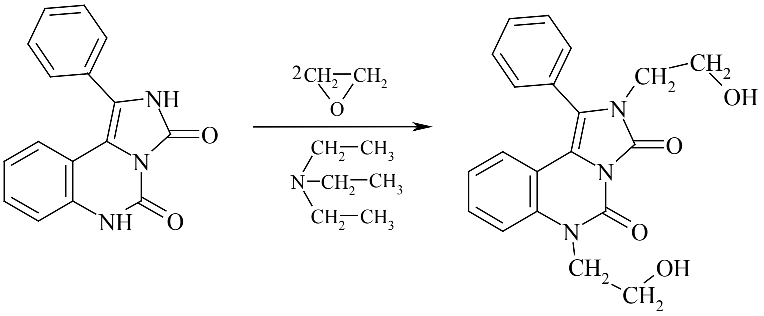
The work presents the results of reaction product of 1-phenyl-2H,6H-imidazo[1,5-c]quinazoline-3,5-dione with 2 molar excess ethylene oxide.



1-phenyl-2,6-bis(2-hydroxyethyl)imidazo[1,5-*c*]quinazoline-3,5-dione was isolated at high yield from the reaction mixtures and identified based on the IR, ^{1}H-and ^{13}C-NMR spectroscopies. X-Ray diffraction measurement was also performed for the single-crystals obtained by crystallization of crude product from ethanol. It was indicated that 1-phenyl-2,6-bis(2-hydroxyethyl)imidazo[1,5-c] quinazoline-3,5-dione crystallizes in the monoclinic $P2_{1/n}$ space group with two molecules of compound in the asymmetric unit of the crystal lattice. The crystal analysis revealed various types of molecular interactions in the crystal lattice of investigated compound. To understand better the nature of packing of molecules in the crystal lattice of investigated compound the Hirshfeld surface analysis was performed.

Biography

Agnieszka Szyszkowska graduated MA in 2014 at the University of Jan Kochanowski. She completed two courses of study: chemistry and biology. She started PhD at the Rzeszów University of Technology in 2014.

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E J Llorent-Martinez et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Phytochemical composition, antioxidant activity and enzyme inhibitory properties of *Lathyrus* species: Potential sources of bioactive compounds

E J Llorent-Martinez[1], **G Zengin**[2], **L Molina-Garcia**[1] and **M L Fernández-de Córdova**[1]
Jaen University, Spain
[2] Selcuk University, Turkey

Many wild plants commonly used in folk medicine, such as different species from the genus *Lathyrus*, may represent new sources of biologically active compounds. Therefore, the study of the composition and (bio)chemical behaviour of extracts from these plants may provide valuable information. Several *Lathyrus* species have been studied: *L. aureus, L. pratensis, L. czeczottianus* and *L. nissolia*. Extracts from these plants were analyzed by high-performance liquid chromatography with electrospray ionization mass spectrometric detection (HPLC-ESI-MSn) to determine their phenolic profile. The *in vitro* antioxidant activity and enzyme inhibitory evaluation were also investigated. The main phenolic compounds (flavonoids and saponins, mainly) and the antioxidant and enzyme inhibition results are here reported. The phenolic contents and the (bio)chemical properties of the analyzed extracts presented significant variations in the different *Lathyrus* species. However, the high number of phenolic compounds and the antioxidant and enzyme assays suggest that these plants may be further used in phytopharmaceutical or food industry applications.

Biography

E J Llorent-Martinez completed his PhD studies in Analytical Chemistry at the University of Jaén, and continued his research in the University of Madeira, University of Castilla-La Mancha and University of Jaén. He has published more than 60 papers in reputed journals and has been serving as an editorial board member of two scientific journals for several years. His main research involves the analysis of the (bio)chemical composition of plants and food.

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Zehra Tavşan et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Synthesis, characterization and anticancer activity of new organometallic ruthenium(II/III) complexes

Zehra Tavşan[a], **Pelin Köse Yaman**[b] , **BetUl Şen**[c], **Cansu Sonay Karagöz**[a] and **Elif Subaşıb Hulya Ayar Kayali**[b,d]
[a,b,c,d]Dokuz Eylul University, Turkey

Novel organo ruthenium (II/III) complexes ([$(\eta^6$-p-cymene)Ru(η^1-S-TSC)Cl_2], (1); and trans-[$RuCl_2(PPh_3)$2(η^2-N,S-TSC)], (2) have been synthesized from the reflux reaction of [{(η^6-p-cymene)RuCl}$_2$(μ-Cl)$_2$] and [$RuCl_3(PPh_3)_3$] with a new TSC (2-acetyl-5-chloro-thiophene thiosemicarbazone) in methanol and benzene, respectively. TSC and both of the complexes have been characterized by elemental analysis, UV–Vis, FT-IR and 1H NMR spectroscopy. The single crystal structure of TSC has been determined by X-ray crystallography revealing that TSC crystallized in the monoclinic space group P21/c. The spectroscopic studies showed that TSC is coordinated to the central metal as a neutral monodentate ligand coordinating via its thiocarbonyl sulfur atom (C=S) in (1), whereas TSC acts as a bidentate anionic chelating ligand with azomethine nitrogen (C=N) and thiol sulfur atom in (2). Both ruthenium complexes displayed higher antiproliferative activities against selected tumor cell lines than TSC ligand, and significantly lower cytotoxic dose towards cancer cell lines and normal colon cell compared to cisplatin. (1) was more active against the colon cancer while (2) was highly cytotoxic towards ovarian carcinoma cells. However, DNA and BSA binding studies for the characterization of antitumor mechanism of ruthenium complexes indicated that these complexes interacted weakly with DNA and BSA, as quantified by Kb in contrast with the importing into cell and accumulation in cytoplasm and then nucleus. These results showed that the mechanism of action may be different from DNA intercalation mechanism. Also, spectral evidences showed these complexes may prefer different transport system instead of binding with albumin. It has been observed that the complexes exhibited different cell cycle arrest on cell lines. Furthermore, our results demonstrated that these newly synthesized ruthenium complexes appear to be as a good antitumor drug candidate. This project has been supported by TUBITAK 215Z663.

Biography

Hulya Ayar Kayali has completed her MSc and PhD from University of Dokuz Eylul in 1997 and 2005, respectively in 2003 and postdoctoral studies from McGill University, Canada, 2011. She works at Dokuz Eylul University from 1998 and she is a professor from 2014. She has published more than 35 papers in reputed journals.

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J Jiménez-López et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Rosa rubiginosa and *Fraxinus oxycarpa* herbal teas: study of their phytochemical profiles and antioxidant activities

J Jiménez-López[1], **E J Llorent-Martinez**[2], **P Ortega-Barrales**[1] and **A Ruiz-Medina**[1]
[1]Jean University, Spain
[2]University of Castilla-La Mancha, Spain

The consumption of infusions and herbal teas has always been an important part of folk medicine. As a result, the study of their (bio)chemical properties and composition is important. In this work, the phytochemical profile and antioxidant activity of *Rosa rubiginosa* and *Fraxinus oxycarpa* herbal teas are reported for the first time. The chemical profiles were evaluated by high-performance liquid chromatography with electrospray ionization mass spectrometric detection (HPLC-ESI-MS^n), as well as by their total phenolic and flavonoid content. The highest percentage of compounds in the extracts of *Rosa rubiginosa* corresponded to phenolic acids and flavonoids, whereas coumarins and secoiridoids were dominant in *Fraxynus oxycarpa* extracts. The antioxidant activities were evaluated by the *in vitro* antioxidant assays DPPH and ABTS. Comparing both samples, *Fraxinus oxycarpa* presented the highest antioxidant activity. This study can contribute to a better understanding of the nutritional and health-promoting properties of uncommon herbal teas.

Biography

J Jiménez-López is developing her PhD since 2014 at University of Jaén (Spain). She has published seven papers in reputed journals. E. J. Llorent-Martinez has completed his PhD from University of Jaén and is developing postdoctoral studies at IRICA. He has published more than 60 papers in reputed journals and has been serving as an editorial board member in different international journals. P. Ortega-Barrales and A. Ruiz-Medina, both full professors at University of Jaén, have published more than 70 and 90 papers cited in the *JCR*, respectively, and more than 20 book or book chapters. Moreover, they hold different positions in university management.

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J Jiménez-López et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

A new approach for the determination of nitenpyram and pyraclostrobin in food samples through a sensitive photochemically induced fluorescence sensor

J Jiménez-López, E J Llorent-Martinez, P Ortega-Barrales and **A Ruiz-Medina**
Jean University, Spain

Pesticides, one of the major classes of environmental pollutants, are widely used throughout the world. Due to their toxicity, it is important to develop analytical methods for the accurate determination of pesticides in a wide range of samples, specially in food samples. Although most methods make use of chromatographic techniques, other alternatives may provide interesting advantages, such as low-cost or simplicity. In this sense, the aim of the work here presented is to use automated luminescent sensors for the analysis of specific analytes. Two widely used pesticides, nitenpyram (NTP) and pyraclostrobin (PRCL), have been selected as target compounds. The system was automatized, making use of Multicommutated Flow Injection Analysis (MCFIA). Photochemically Induced Fluorescence (PIF) was used as detection technique. Hence, the first step consisted in the on-line UV irradiation of sample or standard solutions to generate the corresponding fluorophores. Then, the on-line separation and pre-concentration of the analytes was carried out on the surface of C_{18} silica gel beads placed inside the flow-cell, recording the analytical signal with the analytes sorbed on the C18 microbeads. The use of 3-way solenoid valves in the system allowed an easy handling of solutions, requiring minimum volumes for each analysis, hence minimizing wastes generation. The proposed analytical method presents detection limits of 9 and 5 $\mu g\ L^{-1}$ for NTP and PRCL, respectively. Recovery experiments were carried out in different kinds of food samples: wine, table grapes and wine grapes, obtaining satisfactory results in all cases. Spiking levels were selected according to the legislated maximum residue limit (MRL). The simplicity, low-cost, high sensitivity and high selectivity of the proposed method makes it an interesting alternative for the analysis of these two pesticides, as the method complies with the current MRLs in these samples.

Biography

J Jiménez-López is developing her PhD since 2014 at University of Jaén (Spain). She has published seven papers in reputed journals. E.J. Llorent-Martinez completed his PhD in the University of Jaén and is developing postdoctoral studies at IRICA; he has published more than 60 papers in reputed journals and has been serving as an editorial board member in different international journals. P. Ortega-Barrales and A. Ruiz-Medina, both full professors at University of Jaén, have published more than 70 and 90 papers cited in the JCR, respectively, and more than 20 book or book chapters. Moreover, they hold different positions in university management.

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M L Fernández-de Córdova et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Assessment of bound 3-monochloropropanediol (3-MCPD) and glycidol content in fats and oils by gas chromatography-ion trap tandem mass spectrometry

M L Fernández-de Córdova, L Molina-Garcia and **E J Llorent-Martinez**
Jean University, Spain

An analytical method for determining bound 3-monochloropropanediol (3-MCPD) and glycidol in fats and oils based on gas chromatography-ion trap mass spectrometry (GC-MS/MS) technique has been developed and applied to the study of concentration levels of these compounds in margarine and olive, palm and sunflower oils. 3-MCPD and glycidol are food contaminants that have been classified as carcinogenic by *the International Agency for Research on Cancer* (IARC). They have been detected in wide range of food such as bread, coffee, pastries, etc., which are produced at high temperatures, as well as in refined animal and vegetable fats and oils, and in foods containing them. In oils and fats, 3-MCPD originates when triglycerides are hydrolyzed to mono- and diglycerides and they then undergo a substitution reaction with chlorine atoms, with temperatures above 140 °C being required. Glycidol was first detected in palm oil due to its high content of diglycerides and the high temperatures used in its refining. In 2014, the European Union (EU) issued a Recommendation to Member States about the need to assess the concentration levels of these contaminants in certain foods, as well as to develop new analytical methods for their determination in order to protect the health of European consumers. The developed method consists of two parallel tests, A and B, which are carried out using basic catalysis. 3-MCPD-d5 is used as internal standard in order to obtain reproducible results. In assay A, both bound 3-MCPD and glycidol are determined. A transesterification of 3-MCPD and glycidol esters is carried out with sodium methoxide in methanol, whereby both compounds are released. The time of this reaction is strictly controlled in order to avoid the conversion of part of 3-MCPD in glycidol. The reaction is stopped by adding an acidic solution of NaCl, which causes the conversion of free glycidol in 3-MCPD. After a clean-up step with isohexane, free 3-MCPD and the internal standard are extracted with ethyl ether:ethyl acetate (6:4, v/v), derivatized with phenylboronic acid (PBA) and determined by GC-MS/MS. The test B is carried out analogously to test A, but in this case the transesterification reaction is stopped by the addition of an acidic solution of a non-chlorinated salt, NaBr. Under these conditions free glycidol reacts to give a product other than 3-MCPD, which does not interfere in its determination. Therefore, in test B only 3-MCPD is determined. The glycidol ester content is determined from the difference between the 3-MCPD ester content calculated in tests A and B. The quantification was performed in MS/MS mode what allowed a significant reduction in the background noise. Ions m/z 91 (147 →91) and m/z 93 (150 93) were selected for the measurement of 3-MCPD phenylboronate and 3-MCPD-d5 phenylboronate, respectively.

Biography

M L Fernández de Córdova is a full professor in Analytical Chemistry at the University of Jaén. She has published more than 75 papers in reputed journals as well as numerous book chapters. Her main researches involve the development of automatic methods of analysis and the determination of contaminants in food.

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L Molina-García et al., Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

Optimization and validation of non-invasive HPLC-MS/MS method for stress quantification in free-living ruminants

L Molina-García[1], **J M Pérez**[1], **M Sarasa**[2], **B Ureña-Gutiérrez**[1], **J Espinosa**[1] and **C Azorit**[1]
University of Jaen, Spain

Wildlife management and conservation can benefit from a quantified understanding of physiological response of free-ranging animals to the various potential stressors. Non-invasive stress monitoring by fecal cortisol metabolites (FCM) determination has proven to be a powerful tool. That is, high performance liquid chromatography coupled to tandem mass spectrometry (HPLC-MS/MS) has emerged as the most accurate method avoiding problems related to the non-specificity and matrix effects of the so-used immunoassays. In this work we have optimized, developed and validated a reliable method for 11-ketoetiocholanolone (11-k), a cortisol metabolite, quantification in ruminant's fecal samples by using and HPLC-MS/MS method. An appropriate extraction and purification procedure was developed to take into account the complex nature of feces. The method consisted in a primary fecal samples extraction with methanol and subsequent clean-up with hexane, followed by purification and pre-concentration of targeted metabolite with solid phase extraction (SPE). The final extract obtained was then analyzed by HPLC-MS/MS making used of a quadrupole-time-of-fly (Q-TOF) tandem mass spectrometer with an electrospray ionization interface operating in positive mode. An isotope internal standard was used in order to minimize matrix effect and to compensate the alterations of the analytical signal. After a rigorous optimization of both sample extraction and HPLC-QTOF parameters, the method was satisfactory validated and the best conditions were stablished. Matrix-matches standards were used for the calibration of the method. The limit of detection and quantification, referred to freeze-dried sample, were 13 and 40 µg kg-1, respectively. Recoveries in the range of 85-110% and RSDs not higher than 15%for the complete analytical procedure, including extraction and analysis, were achieved.

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Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Self-assembled nanomaterials for flexible photo-electronic polymer devices

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Self-assembled nanostructures generated from synthetic polymer systems such as controlled polymer blends, semi-crystalline polymers and block copolymers have gained a great attention not only because of the variety of nanostructures they can evolve but also because of the controllability of these structures by external stimuli. In this presentation, various novel photo-electronic materials and devices are introduced based on the solution-processed nanomaterials such as networked carbon nanotubes (CNTs), reduced graphene oxides (rGOs) and 2 dimensional transition metal dichalcogenides (TMDs) with self assembled polymers including field effect transistor, electroluminescent device, non-volatile memory and photodetector. For instance, a nanocomposite of networked CNTs and a fluorescent polymer turned out an efficient field induced electroluminescent layer under alternating current (AC) as a potential candidate for next generation displays and lightings. Furthermore, scalable and simple strategies employed for fabricating rGO as well as TMD nanohybrid films allowed for high performance and mechanically flexible non-volatile polymer memories and broad band photo-detectors, respectively.

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The sorption material based on ferromanganese nodules for wastewater treatment

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For wastewater treatment of metallurgical plants contaminated with non-ferrous metals and organic substances, it is suggested the use of the sorbent based on ferrous-manganese nodules (FMN). FMN are oceanic mineral associations of hydroxides of iron and manganese. They characterized by high values of porosity and surface area. FMN is a natural cation by dissociating with elimination of H^+ functional groups =Mn-OH on the surface of the manganese dioxide. Cation exchange feature allows you to use such material for the purification of process water from a variety of metals [1].

Water purification based on oxidative function of MnO_2. This material allows no special oxidants needed to convert Fe^{2+} to Fe^{3+}, removed from the cations iron (II).

For the reaction: $2Na^+_{(s)} + Me^{2+}_{(aq)} = 2Na^+_{(aq)} + Me^{2+}_{(s)}$ the thermodynamic description of the exchange ions of various metals, and sodium on the surface of ferrous-manganese nodules, using the law of mass action, the modified ion exchange process. As the basic criterion of sorption abilities cations in the preparation of the lyotropic series was taken decrease the Gibbs energy of ion exchange are shown in table 1.The work is devoted to the study of the sorption capacity and catalytic activity of the FMN in the process of purification of the toxic compounds [2].

Reagentless methods are the most effective and environmentally friendly for wastewater treatment. Their use prevents the secondary pollution of water chemicals. Application of a sorbents with oxidizing function like FMN allows to continuously reduce toxicants from wastewater. FMN could be recommended for use as an oxidant phenol and cyanide in the neutral and weakly alkaline media. Based on the limit values of sorption constants and cations exchange function FMN could be recommended like universal sorbent.

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Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

Evaluation of the coordination of a phosphonic acid-based ligand to the surface of zerovalent iron nanoparticles

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Iron-based nanoparticles are very popular materials due to their interest for biomedical applications such as magnetic resonance imaging, magnetic hyperthermia, drug delivery or in other areas of nanomedicine. However the potential of these nanoparticles is limited by the poor magnetic properties of iron oxides from which they are made of. Zerovalent iron nanoparticles would be more suited given their higher magnetization properties but the synthesis of stable colloidal solutions in water is very challenging due to dipolar interactions and oxidation. Zerovalent iron nanoparticles, with good control of size and cristallinity, are synthetised in non biological media (organic solvants) and present at their surface different coordinated ligands used as stabilizers. Their transfer into water which is mandatory for biomedical applications requires to master the complexity of their surface chemistry in order to avoid their dissolution or total oxidation in aqueous medium.[1] Few work has been done in this direction and only silica coating was succesfully experimented up-to-now,[2] confirming that aggregation of zerovalent iron nanoparticles could be prevented and their oxidation limited in water. As an alternative to silica coating we present here the potential of a poly(ethylene oxide)-phosphonic acid ligand [3] to coordinate onto the surface of zerovalent iron nanoparticles. The anchoring of this ligand allows to passivate the iron nanoparticles and to impart them with water solubility thus affording a well-suited nanomaterial for biomedical applications. The strategy of the synthesis which takes benefit from coordination chemistry concepts [4] and the characterization of the so-obtained nanomaterial will be detailed.

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Carotenoids determination of citruses agro-industrial waste materials using supercritical extraction technique and high performance liquid chromatography

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The present research concerns the extraction of carotenoids from Citruses - tangerine and orange agro-industrial waste materials carried out in a dynamic supercritical fluid - carbon dioxide (SC-CO2) extraction system. The carotenoids - beta-carotene and lycopene obtained in organic extracts were quantified using a new, rapid, effective and selective developed and validated HPLC method. The effects of operating pressure and temperature, extraction time, flow rate of the SC-CO2, sample size and solvent nature used were investigated. The optimal conditions for extraction were found. The method was developed using RP-18 endcapped LiChroCART 4 x 250 mm, 5 µm column with gradient elution of mobile phase A and B;

The method was validated with respect to system suitability test, specificity, linearity-range, accuracy, precision, limit of detection (LOD) and quantitation (LOQ). The stability of solutions were studied as well.

The calibration curve is linear over a concentration range 6.497– 0.081 µg/mL for beta-carotene (r^2=0.99924) and 18.76 – 0.34 µg/mL for lycopene (r^2=0.99990); The LOD and the LOQ are 0.081 µg/mL and 0.041 µg/mL for beta-carotene, 0.034 µg/mL and 0.085 µg/mL for lycopene, respectively; No interference was observed; The main accuracy is 106.8 % for beta-carotene and 101.4 % for lycopene.

The content of each carotenoid per 1 g of dried agro-industrial waste material varies for beta-carotene 0.445 – 3.972 µg (tangerine peel), 0.833 – 2.455 µg (orange peel) and for lycopene 0.051 – 179.988 µg (tangerine peel), 0.091 – 0.114 µg (orange peel).

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Multidisciplinary theoretical studies of small nanostructures of carbon compounds for multiplepurposes

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Carbonaceous materials, based on polyaromatic hydrocarbons (PAH), have multiple applications particularly on: atmospheric chemistry, heavy oil components, interstellar chemistry, liquid crystals, carbonization chemistry, catalysis, electronic components, etc. In this presentation, several interactions between radicals with a PAH (coronene molecule) have being studied: (a) model aging of black carbon (BC) produced in air pollution [1]; (b) formation of molecular species on carbonaceous material of the interstellar medium (ISM) [2]; (c) the metal and metal oxides species formed on pyrolytic graphite platform (PGP), used in electrothermal atomic absorption spectroscopy (ETAAS) [3]; (d) metal supported on graphene for the catalysis of olefin hydrogenation [4]. For modeling the above mentioned systems, quantum chemistry calculations at DFT level, parametric, tight binding, and Monte Carlo techniques were employed.

(a) Potential energy surfaces for •OH reaction with coronene as model of BC were evaluated to explain the aging of BC. It means, BC destruction in atmosphere is simulated by the breaking of C-H and C-C bonds after multiple interactions with •OH with the formation of CO_2 plus H_2O. This aging process goes through on the edge surface oxidation with the formation of OH, C=O, and COOH groups. The increase of the surface hydrophilicity was analyzed by using PM6 and DFT-D, explaining water condensation [1].

(b) Several studies of molecular formation in the ISM were carried out for the formation of H_2, H_2O, CH_4, NH_3 molecules after multiple hydrogenations by (Eley-Rideal (ER) mechanism). Events associated with these processes have been studied with the calculation of chemisorption, diffusion, desorption, and surface reaction barriers [2]. The temperature desorption spectrum (TDS) of H2 on graphite is simulated with a Monte Carlo approach using calculated barriers of each event with DFT. A very good theoretical and experimental matching is obtained. The effect of multiple layers of graphene and ionization (charge effects) were also analyzed.

(c) Comparison between X-ray photoelectron spectra (XPS) and theoretical stability of possible Mo species on a model of pyrolytic graphite at different stages of the ETAAS process was performed [3]. The interpretation of XPS in different regions of the PGP indicates the migration of MoxOy species far from the center region. It was found that very stable oxides on the edges of the graphite are formed, then reductions of these species are feasible because are thermodynamically favored. Carbide formation on the dehydrogenated sites is responsible for observed species at ETAAS.

(d) Highly dispersed nanocatalyst synthetized by metal deposition on small graphenes was theoretically modeled [4]. Metallic nickel chemisorptions on multiple sites yield a very active catalyst for hydrogen activation. The interaction with ethylene is analyzed on different sites. Results show that the activation barrier for ethylene hydrogenation is very low. A novel catalyst is proposed for hydrogenation of hydrocarbons.

One may conclude that carbonaceous surfaces have multivariate technological applications, particularly, for recombination of radical species on their surfaces.

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SAR156497 an exquisitely selective inhibitor of aurora kinases

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The Aurora family of serine/threonine kinases is essential for mitosis. Their crucial role in cell cycle regulation and aberrant expression in a broad range of malignancies have been demonstrated and have prompted intensive search for small molecule Aurora inhibitors. Indeed, over ten of them have reached the clinic as potential anticancer therapies. We will report the discovery and optimization of a novel series of tricyclic molecules that has led to SAR156497, an exquisitely selective Aurora A, -B and -C inhibitor with *in vitro* and *in vivo* efficacy. We will also provide insights into its mode of binding to its target proteins from X-Ray data, which could explain its selectivity.

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Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Catalysis by Copper Derivatives in Substitution and Addition Reactions

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In this presentation two types of processes will be considered.

1. Cross-coupling reactions of carbon-carbon and carbon-heteroatom bond formation (including the reactions of C-H activation)
2. The addition of S-H, Se-H, P-H, H-H bonds to alkynes, alkenes and imines (including asymmetric Friedel-Crafts/Michael addition reactions).

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Surface Derivatization of Zirconium Phosphate Nanoplatelets: Potential Nanocarrier of Doxorubicin Anticancer Drug

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Surface modification of doxorubicin anticancer drug (DOX) intercalated zirconium phosphate (ZrP) nanoparticles (DOX@ZrP) is proposed to improve the potential of this drug delivery system for cancer therapy. The surface of DOX@ZrP nanoparticles was modified with an amorphous layer of Zr(IV) followed by modification with monomethyl-polyethylene glycol-monophosphate (m-PEG-PO3) to increase the DOX@ZrP biocompatibility. $^{31}P\{^1H\}$MAS NMR data shows a new peak at -26 ppm corresponding to the PO_4^{3-} groups coordinated with Zr(IV) on the surface. m-PEG-PO_3/Zr(IV)/DOX@ZrP spectra shows no additional resonance centered at δ of -22.6 ppm generated by proton-phosphorous cross polarization indicating no partial PEG intercalation in the interlaminar space. Simulated body fluid (SBF) was used to determine the *in vitro* release of DOX from DOX@ZrP, Zr(IV)/DOX@ ZrP, and m-PEG-PO_3/ Zr(IV)/DOX@ZrP. MTS cell viability assay reveal that m-PEG-PO_3/ Zr(IV)/DOX@ZrP exhibited a 20% increase in the toxicity comparing with free DOX when PC3 cells are exposed for 48 h. m-PEG-PO3 polymer coating of DOX@ZrP nanoparticles promise to have a strong impact on the targeting, distribution and degradation of the nanoparticles under physiological environment that should result in a more efficient chemotherapy agent than free doxorubicin.

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Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Allium cepa.L As Acid-Base Indicator

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In this study, a facile and environmentally friendly method was reported for manufacturing of natural acid-base indicator by preparing *Allium cepa. L* juice, which provided the anthocyannins pigment. The anthocyannins pigment was extracted via boiling process. In detailed, the *Allium cepa. L* was cut into small fragments. Then, the small fragments of *Allium cepa. L* was boiled in distilled water in order to extract the anthocyannin pigment. This process was followed by the addition of different solutions, acidic solution, base solution as well as neutral solution were added into separate test tubes filled with extraction of *Allium cepa. L* juices. The obtained *Allium cepa. L* juice was then used as the pigment for the acid-base indicator. The pH of the solution can be determined by observing the colour change in the *Allium cepa. L* juice. The light purplish colour of *Allium cepa. L* juice turned into red colour when added with hydrochloric acid; its purplish colour of the juice turned into yellow when added with sodium hydroxide; the original colour of *Allium cepa. L* did not undergo any observable colour change when distilled water is added into it. The *Allium cepa. L* exhibited excellent colour change property with chemical solutions. These colour changes make the *Allium cepa. L* be attractive for applications in acid-base indicators.

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Optimization and validation of non-invasive HPLC-MS/MS method for free-living ruminants stress quantification

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Wildlife management and conservation can benefit from a quantified understanding of physiological response of free-ranging animals to the various potential stressors. Non-invasive stress monitoring by fecal cortisol metabolites determination has probed to be a powerful tool. That is, high performace liquid chromatography coupled to tandem mass spectrometry (HPLC-MS/MS) has emerged as the most accurate method avoiding problems related to the inespecificity and matrix effects of the so-used immunuassays. In this work we have optimized, developed and validated a reliable method for 11-ketoetiocholanolone (11-k), a cortisol metabolite, quantification in ruminant's fecal samples by using and HPLC-MS/MS method. An appropiate extraction and purification procedure was developed to take into account the complex nature of feces. The method consisted in a primary fecal samples extraction with methanol and subsequently clean-up with hexane, followed by purification and preconcentration of targeted metabolite with solid phase extraction (SPE). The final extract obtained was then anlyzed by HPLC-MS/MS making used of a quadrupole-time-of-fly (Q-TOF) tandem mass spectrometer with an electrospray ionization interface operating in positive mode. An isotope internal standard was used in order to minimize matrix effect and to compensate the alterations of the analytical signal. After a rigurous optimization of both sample extraction and HPLC-QTOF parameters, the method was satisfactory validated and the best conditions were stablished. Matrix-matches standards were used for the calibration of the method. The limit of detection and quantification, refered to freeze-dried sample, were 13 and 40 μg kg-1, respectively. Recoveries in the range of 85-110% and RSDs not higher than 15% for the complete analytical procedure, incluiding extraction and analysis, were achieved. For the best of our knowledge, this is the first time that the hybrid Q-TOF mass detection coupled to HPLC has been employed for the fecal 11-k quantification in ruminants. Due to the high specificity and sensitivity achieved, the method developed could be used as standard technique for unequivocal fecal 11-k quantification not only in ruminants but also in other related species. In addition, the evaluation of inter-individual differences of stress response could be carried out in the future in an accurate manner by using the present method, thus reducing the effects of potential confounding factors.

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Application response surface methodology for determination optimization of trace zinc in environmental samples by adsorptive stripping voltammetry

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Adsorptive stripping voltammetry is one of the stripping voltammetry method that is widely used in the analysis of heavy metals because it has good sensitivity. metals with very small concentrations can be analyzed. The purpose of this study was to obtain the optimum condition of the Zn metal ions simultaneously. To achieve these objectives. required an optimization technique of analytical procedures by using Response Surface Methodology.with Central Composite Design (CCD). The research design was used in this study is a CCD with 4 variables. 3 level and 31 a combination of treatments. The first step of 2k factorial design optimization are: to give the highest level of code values (+1). the lowest level (-1) and code (0) as the center point. Programs that will be used for statistical data processing. namely Mini Tab using RSM. Based on data analysis with response surface method. the obtained optimum conditions for the determination of zinc is: calcon concentration of 0.71 mmol/L; pH = 7.18; accumulation potential -0.56 V and the accumulation time 62.16 s. From the results obtained optimum conditions RSD of 2.5% with a recovery of 98.01%. respectively. Limit of Detection (LOD) for Zn(II) was 1.21 (μg /L). RSM has been successfully applied to the determination of Zn in environmental samples fast and effectively.

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Synthesis of methane-linked *bis*-heterocycles containing the 1,5-disubstituted-tetrazole moiety via Ugi-azide based methodologies

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Bis-heterocycles are structurally complex compounds having two linked, fused, merged or bound heterocyclic frameworks,1 which have attracted much attention of synthetic community due to their potential applications in agrochemistry, optics, material science, and medicinal chemistry.[2] Moreover, 1,5-disubstituted-tetrazoles (1,5-DS-T's) are known as resistant bioisosters of the *cis*-amide bond of peptides,[3] which are present in numerous valuable drugs like the 3rd generation cephalosporin antibiotic Latamoxeb.4 Besides, 1,5-DS-T's are suitable precursors of a plethora of MOF´s and chelating agents.5 Thus, according to our ongoing program to develop short and versatile Ugi-azide based methodologies toward a variety of methane-linked bis-heterocycles containing the 1,5-DS-T moiety, we herein show our most recent published results. In 2013, we described the synthesis of azepino[4,5-b]indol-4-one-1,5-1H-tetrazoles in two steps: i) one pot (Ugi-azide/N-acylation/SN2), and ii) free radical mediated cyclization, as well as in silico studies as 5-Ht6R ligands using docking techniques (Figure 1a).6 In 2014, we reported the synthesis of 2,3,4,9-tetrahydro- -carboline-1,5-1H-tetrazoles by a one pot Ugi-azide / Pictet-Spengler process (Figure 1b).7 In 2014, we reported the synthesis of chromen-4-ones-1,5-1H-tetrazoles via the Ugi-azide reaction and *in vitro* studies of antiparasitic properties against E. histolytica, G. lamblia, and T. vaginalis.8 Then, in 2015 we extended this work synthesizing some fluorinated analogs, which together with the previously synthesized bis-heterocycles were assayed *in vitro* against P. aeruginosa, *S. aureus*, S. schenckii, C. albicans, and C. tropicalis (Figure 1c).9 Finally, just recently in 2016, we reported the synthesis of novel 3-tetrazolyl-tetrazolo[1,5-a]quinolines via a novel one pot Ugi-azide / SNAr / ring-chain azido-tautomerization process (Figure 1d).10 As seen, the Ugi-azide reaction or its combination with further cyclization processes allows the rapid synthesis of a variety of methane-linked bis-heterocycles with potential application mainly in medicinal chemistry because 1,5-DS-T framework has been suitably combined with other heterocyclic systems, which are present in numerous bioactive products, even in drugs.

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Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

4th European Chemistry Congress

May 11-13, 2017 Barcelona, Spain

A new extraction procedure for Bisphenol A (BPA) in canned foods

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A new extraction procedure for the mutagenic BPA in canned food was developed employing an aqueous basic solution of 0.25 M K2CO3 and 0.10 M NaOH after spiking with BPA-d16 as internal standard. The BPA was next extracted into diethyl ether after acidification to pH=4 and centrifugation. Acetylation at dry basic conditions after diethyl ether evaporation was carried out for 30 minutes at 110 0C. Detection of the acetylated BPA was carried out by GC-EI/MS in the SIM mode with pulsed split-less mode. The method was applicable in terms of eliminating the use of solvents like acetonitrile and heptane for the extraction step, where long evaporation times that extend to several hours may have been needed to evaporate acetonitrile. Also removing lipids and precipitating most of the proteins at acidic conditions prior to diethyl ether extraction replacing heptane or hexane use. In addition acetylation is conducted in the absence of water without a freeze-drying step. The method was linear over the range 1μg/L to 460 μg/L with instrument detection limit (IDL) of 0.01 μg/L and a limit of quantitation (LOQ) of 0.034 μg/L. The method detection limit (MDL) ranged from 0.3μg/Kg to 2.0 μg/Kg (wet weight) based on 10 g sample and recovery range from 85% to 94%. BPA concentrations in tested canned foods from outlet stores ranged from < MDL to 57.5 μg/Kg which were below the specific limit of BPA migration in food proposed by the EU and within the food safety and quality criteria.

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Carrier Dynamics in Organolead Halide Perovskites

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Encyclopedia of Bioanalytical Methods for Bioavailability and Bioequivalence Studies of P Two-dimensional (2D) layered perovskites ((A)2(CH3NH3)n−1MnX3n+1, where A is a large aliphatic or aromatic alkylammonium cation working as an insulating layer, M is the metal cation, and X is the halide anion) have already emerged as an attractive material for applications in photovoltaics and other optoelectronic devices. Recent reports have demonstrated that the 2D layered perovskite films actually comprised multiple perovskite phases (with various n values from 1, 2, 3 and 4 to near), even though the films were intended to be prepared as a single-phase. This hybrid feature seems to be ineluctable in fabricating 2D films. However, two important questions remain yet-to-be-answered: first, how the different perovskite phases align in the hybrid films; second, whether the band alignment between different phases induces energy funneling or instead charge separation. The latter is especially important because it dictates the application of these hybrid 2D perovskite films: energy funneling is useful for lightemitting applications, whereas charge separation would be more beneficial for light conversion or detection. Herein, we studied the charge carrier dynamics in 2D multi-layered perovskite films using ultrafast transient absorption and photoluminescence spectroscopy. Researchers found that multiple perovskite phases inside 2D layered perovskite film (including n = 2, 3, 4 and ≈ ∞) naturally align in the order of n along the direction perpendicular to the substrate. Driven by the band alignment between 2D perovskites phases, researchers observed consecutive photoinduced electron transfer from small-n to large-n phases and hole transfer in the opposite direction on hundreds of picoseconds inside the 2D film of ~358 nm thickness. This internal charge transfer efficiently separates electrons and holes to the upper and bottom surfaces of the films, which is a unique property beneficial for applications in photovoltaics and other optoelectronics devices.

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Chem Sci J 2017, 8:2(Suppl)
http://dx.doi.org/10.4172/2150-3494-C1-009

Plant Macromolecule from different species of Boraginaceae family, its synthetic monomer and their anticancer efficacy

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The 13C NMR experiments of water-soluble high-molecular preparations from different species of Boraginaceae family were carried out and simulated 13C NMR spectrum was calculated for 2-hydroxy-3-(3',4'-dihydroxyphenyl)-propionic acid residue (I) of the corresponding polyether using ACD/CNMR Version 1.1 program. Signal positions in the 13C NMR spectrum of this hypothetical structure (I) coincided satisfactory with the experimental values. According to 13C, 1H NMR, APT, 2D heteronuclear 1H/13C HSQC and 2D DOSY experiments the main structural element of these preparations was found to be a regularly substituted by 3,4-dihydroxyphenyl and carboxyl groups polyoxyethylene backbone, namely poly[3-(3,4-dihydroxyphenyl)glyceric acid] (PDPGA) or poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl)ethylene]. The synthesis of racemic monomer of PDPGA 2,3-dihydroxy-3-(3,4-dihydroxyphenyl)propionic acid (DDPPA) and its enantiomers (+)-(2R,3S)-DDPPA and (−)-(2S,3R)-DDPPA was carried out via Sharpless asymmetric dihydroxylation of trans-caffeic acid derivatives using a potassium osmate catalyst and enantiocomplementary catalysts cinchona alkaloid derivatives (DHQ)2-PHAL and (DHQD)2-PHAL as chiral auxiliaries. The opposite configuration of both enantiomers was confirmed by measurements of the optical rotation (+)/(−)-values and circular dichroism spectra. The determination of enantiomeric purity was performed by HPLC analysis. PDPGA and DDPPA exerted anti-cancer efficacy *in vitro* and in vivo against human prostate cancer (PCA) cells via targeting androgen receptor, cell cycle arrest and apoptosis without any toxicity, together with a strong decrease in prostate specific antigen level in plasma. However, our results showed that anticancer efficacy of PDPGA is more effective compared to its synthetic monomer. Overall, this study identifies PDPGA as a potent agent against PCA without any toxicity, and supports its clinical application.

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Synthesis and biological evaluation of BCP derivatives: A steadfast effort towards introducing a contemporary lead optimization tool.

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Potential applications of the bicyclo[1.1.1]pentane (BCP) motif, as a contemporary lead optimization tool, has generated substantial interest in medicinal chemistry.1 However, a realistic introduction of this building-block to the mainstream medicinal chemistry warrants a systematic and steadfast approach towards its development. In 2013, originating from an "out-of-the-box" notion to resolve issues pertaining to an on-going medicinal chemistry study, we recognized the need to resolve the paucity of synthetic access to BCP derivatives.2 Taking cognizance of the non-trivial chemical demeanor of the strained BCP motif, we devised contemporary strategies to secure key BCP derivatives in a scalable fashion. As an outcome, we have now secured a robust and scalable access to a variety of key intermediates such as the BCP amine (1) its 3-fluoro and 3-phenyl substituted counterparts 2 and 3, and 3-pyrazine BCP carboxylic acid (4).3-6 The newly discovered synthetic know-how was deployed to generate a library of BCP-based fragments for an 'in-house' FBDD initiative. Moreover, empowered by our synthetic studies we have also invested efforts to understand the biological behavior of BCP derivatives. In this presentation, I will narrate the background, the progress, and our future objectives related to our work on the BCP derivatives.

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