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Structural and spectroscopy investigation of lanthanide complexes with bioligands derivatives of 1,2,3-triazol"

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With the focus on the design of new lanthanide complexes with better properties, the effect of La, Ce, Pr and Nd ions on four $Ln(ligand)_3$ complexes and at three DFT levels of calculation was analyzed. Three of the ligands chosen were based on the 1,2,3-triazole ring. The molecular structure, lanthanide-ligand binding mode, and spatial arrangement of the ligands in these complexes was found to depend on the theoretical method, the basis set used and lanthanide. This arrangement was nearly symmetric by CAM-B3LYP and M06-2X methods and Lanl2dz basis set, but deformed by B3LYP and the Cep-4g and Lanl2mb basis sets. Due to the spatial arrangement of the ligands, hydrated water molecules appeared in the structure of the largest complex by the appearance of a broad ν(O-H) band in the experimental IR spectrum. The arrangement of these water molecules little changed with the lanthanide ion, but their amount especially increases in the Ho and Er complexes.

Among the geometric parameters, atomic charges, HOMO-LUMO energies and other molecular properties obtained, new relationships and trends were established that can be extrapolated to other complexes and may facilitate the synthesis of new complexes by selecting the ligand and lanthanide ion most suitable to the desired property of complex. Therefore, it was found that as much the ligand size increased, the dipole moment incremented, and a reduction of the Ln atomic charge led to a lengthening of the La-O bonds. As the ligand became larger and more complex, the Ln charge is increased,

and this effect was more pronounced in Ln ions with large positive charge. Increasing in the ligand size significantly reduced the HOMO energy, and led to very low Eg values, indicating that they have high chemical reactivity and small excitation energies to the manifold of excited states.

Keywords: DFT methods; 1,2,3-triazols; Lanthanide complexes; Vibrational spectroscopy.

Biography

Mauricio Alcolea Palafox is a doctor of quantum chemistry and vibrational spectroscopy and professor of Physical Chemistry department, Complutense University, Spain. His main investigation is “DFT research of anticancer and antiviral prodrugs” for the design of new compounds with higher activity and lower side effects. Using several high-level DFT methods together with infrared, Raman and NMR spectra, as well as accurate scaling procedures, structure-activity and structure-property relationships were established that facilitate the synthesis of novel prodrugs. Interactions of them with different DNA:DNA and RNA:RNA microhelices or through molecular docking calculations of how they bind to few aminoacids of the receptor target protein, allow us to have a first idea of whether the selected molecule could act as an effective anticancer/antiviral prodrug. Prof. Palafox is a leading scientist of the scientific program 3.2.2 “Biologically Active Heterocyclic Ligands and Metal Complexes with Antioxidant Activity”, part of the project BG-RRP-2.004-0004-C01

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Design and study of the properties of novel systems based on metallodrugs for various therapeutic applications

Santiago Gómez-Ruiz

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The burgeoning field of theranostics, a fusion of therapy and diagnosis, is revolutionizing biomedicine. It leverages the synergistic effects of therapeutic treatments and early diagnosis, opening up exciting avenues in medicinal applications. In the context of drug delivery, theranostics is driving the creation of multifunctional nanoplatforms. These innovative systems integrate molecular imaging fragments with therapeutic compounds, demonstrating impressive efficacy in both preclinical and clinical trials.

Our research group has been at the forefront of this revolution, developing theranostic systems to combat cancer and bacterial infections. We have successfully combined potent therapeutic metallodrugs with imaging agents based on luminescent ligands within nanostructured materials. Our portfolio includes a diverse range of theranostic systems, from mesoporous silica nanoparticles (MSNs) and fibrous silica particles (FSPs) to N-functionalized graphene quantum dots (NGQDs), among others. These systems, loaded with tin, copper, ruthenium, or silver agents and co-functionalized with targeting agents, have shown promising results against cancer and bacterial models in both in vitro and in vivo tests and are now under study against some neurodegenerative diseases.

This lecture will delve into our group's significant contributions, spotlighting our latest breakthroughs. We will discuss the synthesis and characterization methods, as well as the biological studies that have underscored the influence of the structural features and composition of the drug-delivery systems on their therapeutic activity. Our findings have paved the way for the design of innovative multifunctional nanomaterials, which hold great promise for future clinical trials.

Keywords: Theranosis; Nanomaterials; Metallodrugs; Therapy.

Biography

Prof. Santiago Gómez-Ruiz is Full Professor of Inorganic Chemistry at URJC, Spain and is renowned for his pioneering work in the field of theranostics. With over 190 publications of high impact, he leads the high-output research group "COMET-NANO". His research focuses on the design of metallodrug-functionalized nanomaterials and advanced materials with photocatalytic applications. Recognized internationally, he has been listed among the Top 2% researchers by Stanford University in 2021. Prof. Gómez-Ruiz has made significant contributions to the treatment of diseases like cancer, bacteria and ALS through his innovative theranostic systems. His work in photocatalysis has led to the development of versatile ultrareactive photocatalytic materials with industrial, environmental, energy and chips applications. He has collaborated with companies like Chevron Phillips and holds two patents on nanomaterials. Committed to societal impact, he has been awarded a grant for the development of photocatalytic selective sprays against SARS-CoV-2. As a dedicated mentor, he has supervised numerous PhD students and posdocs. He serves as an associate editor of Environmental Chemistry Letters and is reviewer for prestigious journals. His expertise is sought after by various research agencies for proposal evaluations including Marie

Sklodowska Curie Fellowships. Prof. Santiago Gómez-Ruiz is a team member of the scientific program 3.2.2 "Biologically Active Heterocyclic Ligands and Metal Complexes with Antioxidant Activity", part of the project BG-RRP-2.004-0004-C01.

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Fabrication of Chitosan/PVA enriched MgO nanocomposite and its applications towards environment and medicine

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In this work, Chitosan (CS) and Poly vinyl alcohol (PVA) were tethered with Magnesium oxide (MgO) to synthesize nanocomposite (CS/PVA/MgO) through green chemical method. Magnesium oxide nanoparticles is synthesized via green chemical method using *Moringa oleifera* bark extract which is non-toxic in nature, environmentally friendly and also inexpensive mode of preparation. The nanocomposites were Characterized by Fourier Transform – Infra red spectroscopy (FT-IR), X-Ray diffraction (XRD), Scanning Electron Microscopy (SEM). The Elemental composition of the nanocomposite is studied by Energy Dispersive X-Ray (EDAX) analysis technique which confirms the successful formation of the (CS/PVA/MgO) nanocomposite. In this work, the synthesized nanocomposite has an excellent degrading activity on dyes like crystal violet, Methylene blue, Methyl Orange under direct sunlight. Further, in vitro studies clearly demonstrate that this nanocomposite shows maximum zone of inhibition (ZOI) on

bacteria like staphylococcus aureus, Escherichia coli etc., Chitosan based nanocomposites also indicates the improved activity for the wound healing processes. Thus, the present investigation target photodegradation of dyes and antibacterial activity.

Keywords: Green chemical method; Moringa oleifera; CS/PVA/MgO nanocomposite; Antibacterial activity.

Biography

R. Rajavel is working as a Professor in Department of Chemistry, Periyar University, Salem, Tamilnadu. His current research expertise on Decorated Schiff base metal complexes for enzyme mimicking activity and catechol oxidation, Mesoporous metal complexes for heterogeneous Catalytic activity on organic synthesis, Photocatalytic activity for dye degradation and Biomaterials for antibacterial activity.

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Facile synthesis of egg shell derived hydroxyapatite/chitosan enriched with CuO derived from *C. dactylon* extracts for wound healing applications

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This study presents a novel approach to the synthesis of hydroxyapatite (HAp) derived from eggshells, combined with

chitosan and enriched with copper oxide (CuO) nanoparticles, derived from *Cynodon dactylon* extracts, for potential wound healing applications. The biocomposite was synthesized through a facile method, capitalizing on the natural abundance and bioactivity of the components. The physicochemical properties of the synthesized biocomposite were characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM), confirming the successful incorporation of CuO into the HAp/chitosan matrix. The in-silico studies, including molecular docking and dynamics simulations, were conducted to predict the interaction of the biocomposite with key proteins involved in the wound healing process, revealing strong binding affinities and potential mechanisms of action. In vitro assays were performed to evaluate the cytocompatibility, antibacterial activity and wound healing efficacy of the biocomposite. The results demonstrated significant antibacterial effects against common wound pathogens and promoted cell proliferation, indicating its suitability for wound healing applications. This study highlights the potential of using environmentally sustainable materials and green synthesis methods in the development of advanced biomaterials for medical applications.

Keywords: Hydroxyapatite; Wound healing; Biocomposite; Antibacterial activity.

Biography

Prof. V. Raj is currently working as the Professor and Head in the Department of Chemistry, Periyar University, Salem, Tamil Nadu, India. His current research expertise is synthesis of novel composites using advanced materials and their applications in the field of medicine, energy and environment.

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Lanthanide complexes with biologically active ligands – interactions with free radical-generating model systems

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Lanthanide coordination complexes, incorporating 1,2,3-triazoles and coumarins, have emerged as promising candidates in the exploration of novel antioxidant agents due to their unique electronic structures, luminescent properties, and versatile coordination chemistry. The Authors' work aims to elucidate the antioxidant properties of such complexes, exploring the potential synergistic effects of lanthanoid ions with 1,2,3-triazole-bearing and coumarin ligands, which are known for their radical scavenging abilities. Several different lanthanoid cations were utilized as coordination centers. UV-VIS spectroscopy was applied in a number of *in vitro* antioxidant assays that include 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging, 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) radical cation decolorization, Fenton-generated hydroxyl radical scavenging and impact on UV-induced 2-deoxyribose degradation. Luminol-dependent chemiluminescence (LDCL) was additionally applied to elucidate *in vitro* the potential scavenging effect of the novel complexes on hypochlorite and superoxide ions. The activities of the ligands are compared to those

of the respective complexes. The impact of the type of lanthanoid ion on the complexes' behavior was also investigated.

Our experiments yielded a number of interesting results. As expected, the scavenging properties of the ligands were improved by coordination with the lanthanoid ions in presence of some of the radical-generating model systems utilized. On the other hand, ligands and complexes that scavenged DPPH, ABTS and suppressed UV-induced 2-deoxyribose degradation behaved as strong pro-oxidants in presence of the physiologically significant Fenton reaction. Some of the ligands investigated behaved as scavengers of hypochlorite and superoxide, but after coordination with lanthanoids the observed concentration-dependent effect was not only nullified, but completely reversed. The type of lanthanoid coordination center also had a significant impact on the properties observed.

The results reported herein present the impact of lanthanoid complexation on the radical-scavenging properties of 1,2,3-triazole-bearing and coumarin ligands and reveal some interesting opportunities for potential medicinal applications.

Keywords: Lanthanides; 1,2,3-triazoles; Coumarins; Radical Scavengers.

Biography

Dr Lozan Todorov, PhD currently serves as a Senior Assistant Professor at the Department of Chemistry at the Faculty of Pharmacy in Medical University – Sofia, Bulgaria. His PhD thesis, under the scientific supervision of Professor Irena Kostova, deals with antioxidant properties of gallium and lanthanum complexes with 5-aminoorotic acid. He has participated in and overseen a number of university-level projects in close collaboration with Dr Hristova-Avakoumova at the Department of Medical Physics and Biophysics

at the Faculty of Medicine, Medical University-Sofia. Dr Todorov's research experience includes a variety of antioxidant assays, involving disparate reactive species, derived from various model systems. His current research interests are associated with the promising field of lanthanoid coordination chemistry and its potential applications in biomedical sciences. To that effect, together with Professor Kostova, Dr Hristova-Avakoumova and in collaboration with a multinational research team, including prominent scientists from Spain, India and Italy, Dr Todorov is participating in a new project "Biologically Active Heterocyclic Ligands and Metal Complexes with Antioxidant Activity", part of the Research Universities program, financed by the European Union, the Bulgarian Ministry of Education and the Bulgarian National Sciences Fund.

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Environmentally derived bacteriophages and their lytic proteins: An alternative to mitigate drug resistance

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Bacteriologically confirmed treatment failures are now widely reported owing to an increase in resistance to numerous drug classes, including commonly used β-lactams, macrolides and fluoroquinolones. Bacteriophages (phages) are viruses that specifically target bacteria, offering a targeted approach to bacterial infections. Phage therapy, which uses these natural bacterial predators, is gaining traction due to its specificity and ability to combat multidrug-resistant (MDR) bacteria. Many recent studies

have highlighted the potential of environmentally derived bacteriophages and their proteins as promising alternatives to combat drug-resistant pathogens (https://doi.org/10.2147/IDR.S348700; https://doi.org/10.1002/cbf.4022). Phages and their derived proteins, such as endolysins and depolymerases, have been shown to effectively target and lyse MDR pathogens (https://doi.org/10.1007/s11356-023-28081-z). For instance, phage-derived enzymes have demonstrated significant efficacy against drug-resistant *Acinetobacter baumannii* and *Pseudomonas aeruginosa*, common culprits in hospital-acquired infections (https://doi.org/10.3389/fmed.2022.1047752; https://doi.org/10.1186/s12941-020-00389-5). There have been successful clinical cases and trials demonstrating the effectiveness of phage therapy. For example, personalized phage therapy has been used to treat carbapenem-resistant *A. baumannii* lung infections, showing promising results in patients with chronic obstructive pulmonary disease (COPD) (https://doi.org/10.1007/s00705-023-05910-7).

Additionally, phage therapy is not limited to clinical settings. It has potential applications in agriculture, food safety, and environmental decontamination, providing a versatile tool in the fight against bacterial contamination and resistance. Advances in genetic engineering have enhanced the efficacy and host range of bacteriophages. By modifying phages, researchers can create tailored therapies to target specific bacterial strains, thus overcoming limitations of traditional antibiotics (https://doi.org/10.1007/s00449-023-02938-6). Staphefekt SA.100, Exebacase (CF-301), and N-Rephasin®SAL200 are some commercially available phage protein – endolysin to treat plant diseases.

Overall, the use of environmentally derived bacteriophages and their proteins offers a viable and effective alternative to traditional antibiotics, especially in the context of increasing antimicrobial

resistance. Further research and clinical trials are essential to fully integrate phage therapy into mainstream medical practice.

Keywords: Phage therapy; Phage; Endolysins; MDR.

Biography

Dr. Aditi Singh has a Doctorate degree with specialization in Medical Microbiology. Her thesis work was on pathogenesis of Japanese encephalitis virus, a cause of high mortality and morbidity in developing countries. At present she is working as Professor in Amity University, Lucknow (INDIA) - a leading private university in India. Dr. Singh has over 23 years of research and teaching experience and has published >60 research papers. She also has three edited Books and fourteen book chapters to her credit. Dr. Singh is the Editorial board member or Peer-reviewer of many reputed international journals. Her research interest majorly focuses on various approaches to combat antibiotic resistance in drug resistant common pathogens. In one of her previous studies, they have shown two novel coliphages from sewage water and these phages were found to be effective against drug resistant E. coli. Whole genome sequencing was done and analysis of that has shown presence of three novel endolysin sequences.

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Role of reflectance spectroscopy for diagnosing thyroid disorders and assessing the effectiveness of an ayurvedic medication in thyroid treatment

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Fourier transform infrared-attenuated total reflectance (FTIR-ATR) spectroscopy has been found useful for monitoring the efficacy of the Ayurvedic drug Thyronil during the treatment of hypothyroidism in women. In the present work, the lipid-to-protein ratios of hypothyroid patients increased immediately after treatment and then decreased to the levels observed in a healthy group. These parameters can serve as potential biomarkers to indicate successful remission and suggest that FTIR-ATR spectroscopy may provide a rapid optical method for continuous monitoring or evaluation of hypothyroid disorders. This technique's ability to provide real-time feedback on biochemical changes makes it a valuable tool in personalized medicine.

The work also focuses on identifying the active component, ethyl hexadecanoate, responsible for the anti-thyroid properties of the seeds of *Commiphora Mukul* (Guggulu) using Gas Chromatography Mass Spectrometry (GCMS). More than 190 active components were obtained from the seeds of *Commiphora Mukul*, each responsible for different medicinal uses. One significant medicinal use is in treating thyroid disorders (both hypothyroidism and hyperthyroidism). The crystal structure of lactoperoxidase obtained from the protein data bank was docked against all the phytochemicals obtained from GCMS. The docking scores and glide energies were determined using Schrödinger Maestro software (version 2013.1). The results of molecular docking showed that ten bioactive compounds, including tetradecanoic acid, ethyl tridecanoate, pentadecanoic acid, linoleic acid, 9-octadecynoic acid, ethyl hexadecanoate, linolelaidic acid, methyl linolelaidate, oxacycloheptadec-8-en-2-one (8Z), and 18-

octadec-9-enolide, effectively inhibit the lactoperoxidase protein. The ADME properties of the compounds were analyzed using Qikprop version 3.6 software from the Schrödinger suite, and the results showed that all the compounds were biologically active, with scores within the acceptable range.

This study revealed the potential of using these ten phytochemicals against lactoperoxidase to treat thyroid disorders, highlighting ethyl hexadecanoate, which exhibited a gliding energy of -33.074 kcal/mol and a docking score of -5.396, as the most promising lead target against thyroid issues. The results suggest that ethyl hexadecanoate acts against thyroid disorders by blocking lactoperoxidase (LPO) and can be further developed into a potent Ayurvedic drug, Thyronil, for anti-thyroid treatment.

In addition to these findings, current research is exploring the application of nanoparticles to enhance the delivery and efficacy of Thyronil and other phytochemicals identified in this study. Nanoparticles can improve the bioavailability and targeted delivery of these compounds, potentially increasing their therapeutic effects while reducing side effects. The use of nanotechnology in this context represents a cutting-edge approach to traditional medicine, merging modern scientific techniques with ancient herbal remedies to develop more effective treatments for thyroid disorders. This interdisciplinary research could pave the way for new advancements in both nanomedicine and Ayurvedic drug development, offering promising prospects for the treatment of thyroid-related health issues.

Keywords: Ayurveda, Thyronil, Ethyl hexadecanoate, Glide score, Glide Energy, Thyroid

Biography

Dr. Janani Panneer Selvam, Ph.D. in Physics from St. Peter's Institute of Higher Education and Research, Chennai, is a distinguished researcher with a strong focus on the application of spectroscopic techniques in medical research. Her work has significantly contributed to the field, particularly in analyzing the active components of guggulu seed (Commiphora mukul) to identify compounds responsible for thyroid disorders. This groundbreaking research led to a national patent and established her as a leader in the use of docking methods to explore the efficacy of Ayurvedic drugs like Thyronil. Her pioneering work in Fourier Transform InfraredAttenuated Total Reflectance (FTIR-ATR) spectroscopy has paved the way for innovative diagnostic techniques. She has used this method to screen biomolecular levels in biological tissues such as skin, hair, and nails, offering a non-invasive alternative to traditional blood tests for diagnosing thyroid disorders.

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Probing the influence of FTIR spectroscopy using ATR technique for materials characterization in the field of medicine

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Spectroscopy is a major tool in analyzing many physical, chemical and biological phenomena and it is being used widely in various laboratories. Mid-Infrared (IR) spectroscopy is an extremely reliable

and well recognized fingerprinting method. Many substances can be characterized, identified and also quantified. The technique of Attenuated Total Reflectance (ATR) has in recent years revolutionized solid and liquid sample analyses because it combats the most challenging aspects of infrared analyses, namely sample preparation and spectral reproducibility. Overall, sample preparation is easier for liquid transmission studies when compared to solid transmission sampling, but both suffer from inevitable reproducibility issues, given the complexity of the sample preparation methods. In addition, preparation can be very messy and time consuming and is further complicated by difficulties is getting sample to matrix ratios correct and homogenous throughout the sample. The materials involved are fragile and hydroscopic and the quality of measurements can be adversely affected if handled or stored incorrectly. The technique of Attenuated Total Reflectance addresses these issues.

An attenuated total reflection accessory operates by measuring the changes that occur in a totally internally reflected infrared beam when the beam comes into contact with a sample. An infrared beam is directed onto an optically dense crystal with a high refractive index at certain angle. This internal reflectance creates an evanescent wave that extends beyond the surface of the crystal into the sample held in contact with the crystal. It can be easier to think of this evanescent wave as a bubble of infrared that sits on the surface of the crystal. This evanescent wave protrudes only a few microns (0.5 μ - 5 μ) beyond the crystal surface and into the sample. Consequently, there must be good contact between the sample and the crystal surface. In regions of the infrared spectrum where the sample absorbs energy, the evanescent wave will be attenuated or altered. The attenuated energy from each evanescent wave is passed back to the IR beam, which then exits the opposite end of the crystal and is passed to the detector in the IR spectrometer. The system then generates an infrared spectrum.

ATR spectroscopy is a dynamic technique for materials characterization. But the better utilization of science gives an opportunity to use FTIR – ATR in the advanced materials characterization. Spectroscopy is a major tool in analyzing many physical, chemical, and biological phenomena and is widely used in various laboratories. Mid-Infrared (IR) spectroscopy is a reliable and well-recognized fingerprinting method, allowing for the characterization, identification, and quantification of many substances. Recently, the technique of Attenuated Total Reflectance (ATR) has revolutionized solid and liquid sample analyses by addressing the challenging aspects of infrared analyses, particularly sample preparation and spectral reproducibility.

An ATR accessory measures changes in a totally internally reflected infrared beam when it comes into contact with a sample. An infrared beam is directed onto a high refractive index crystal at a certain angle, creating an evanescent wave that extends into the sample. This wave protrudes only a few microns beyond the crystal surface, requiring good contact between the sample and the crystal. The attenuated energy from the evanescent wave is then passed back to the IR beam, which exits the crystal and is detected, generating an infrared spectrum.

ATR spectroscopy is a dynamic technique for materials characterization. Advanced applications of FTIR-ATR include studying the sensitivity of Fourth Derivative FTIR-ATR spectroscopy with bulk fill composites used in dentistry and Nanocellulosic Fibrils extracted from natural fibers. Changes in crystallinity of fill composites and Nanocellulose are manipulated with the internal absorption ratio in the zeroth order FTIR-ATR spectra, while the spectral difference is highlighted in the Fourth Derivative FTIR-ATR spectra. The average and Difference FTIR spectra are also obtained and deployed for materials characterization.

Moreover, FTIR-ATR spectroscopy has shown promising results in various medicinal and diagnostic applications. It has been used to study bulk fill composites (dentin) in dentistry, where it helps in analyzing the materials used for dental restorations. The efficacy of medicines for acne has been explored using Density Functional Theory (DFT) studies, providing insights into the molecular interactions and effectiveness of acne treatments. FTIR-ATR has also been employed to identify diabetes mellitus through hair and skin analysis, offering a non-invasive method for early detection and monitoring of the disease. Additionally, the efficacy of the Ayurvedic drug Thyronil for hypothyroid women patients has been evaluated using FTIR-ATR, demonstrating its potential in monitoring treatment effectiveness and patient response.

These applications highlight the versatility and advanced capabilities of FTIR-ATR spectroscopy in both material science and medical diagnostics, showcasing its role in the evolving landscape of modern scientific research. This shows that the materials characterization technique also grows along with the exploration of Modern materials.

Keywords: DFT methods; FTIR Spectroscopy; ATR Technique; Materials Characterization; Medicine.

Biography

Prof. S. Gunasekaran has completed his Ph.D. in molecular spectroscopy from Anna University and obtained his D.Sc. from University of Madras. Dr. S. Gunasekaran, Dean (R&D) of St. Peter's Institute of Higher Education and Research, Avadi, Chennai, began his teaching career at the Pachaiyappa‟s College, Chennai, and remains a dedicated Teacher to this day. But Dr. Gunasekaran was restless to do more, than just teach a syllabus, so he went about promoting research activities in the department by

garnering funds to equip the Laboratory with instruments for research. As Dean (R&D), he took support from the Management of St. Peter‟s Institute of Higher Education & Research and he has established Sophisticated Analytical Instrumentation Facility (SAIF-SPIHER), housed with advanced spectrophotometers. His area of research is the application of spectroscopy in varied fields that are likely to yield results beneficial to society, like materials science, medical physics, environmental science and molecular dynamics. Till date, Dr. Gunasekaran has successfully guided more than 80 candidates who have obtained their Ph.D. He has to his credit, more than 475 publications in reputed journals and has h-index as 47 and i10- index as 214 with 9300 citations. Dr. Gunasekaran has authored 14 books for Higher Secondary Physics, Secondary Science and Environmental Education, in both Tamil and English medium. His sincere and dedicated hard work fetched him many awards, including the prestigious Tamil Nadu Scientist Award (TANSA) in physical sciences for the year 2013. He is a team member of the scientific program 3.2.2 "Biologically Active Heterocyclic Ligands and Metal Complexes with Antioxidant Activity", part of the project BG-RRP-2.004-0004-C01.

Prof. S. Gunasekaran is the Founder and the President of Indian Spectrophysics Association (ISPA), started in 1998. ISPA through its initiatives provides access not only for quality education in spectroscopy and its applications, enhance innovative researches, but also inculcates values, commitment and dedication to the society, thus helping to build a strong future for every researcher. ISPA has organized 30 international, 35 national and 20 state level conferences, seminars, workshops.

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Theoretical and spectral study of bioactive Ln(III) complexes

Irena Kostova

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Lanthanides and their various organometallic and coordination compounds are widely studied and extensively used in medical practice. They have quickly gained prominence in cancer diagnosis and therapy, owing to their versatile biochemical properties, wide spectrum of biological activity, and low toxicity. Numerous lanthanide(III) complexes have been reported to have exhibited pronounced cytotoxic activity on a wide range of tumor cell populations of different origins, with these complexes always showing a significantly higher inhibition potential than the initial ligands and inorganic salts. This class of tumor-inhibiting metal complexes has been shown to be effective against tumors, resistant to classical Pt complexes. Their influence on the levels of reactive particles generated by various ROS model systems has been studied, confirming the antioxidant capacity of the lanthanide complexes. The information obtained on the interaction of complexes with the model systems studied could serve to clarify the mechanisms of action in future experiments with these compounds *in vitro* and *in vivo*.

Herein, the synthesis, structural and vibrational characterization of the newly synthetized lanthanide(III) coordination complexes through theoretical and spectroscopic results was carried out particularly by means of spectral (FT-IR, FT-Raman, NMR) and elemental analysis. The significant differences observed from the spectral data of the Ln(III) complexes, attributed to the coordination

process with the metal ions, have been confirmed by DFT calculations. The geometry optimization explained the molecular and electronic structures, vibrational assignments, reactive binding sites, H-bonds and other structural properties confirming the structure and the changes in the complex conformation.

The study of the biological activity of the studied compounds is a practical upgrade of the applied theoretical approaches and physicochemical methodologies for the characterization of compounds, which enabled the output of useful structure-activity correlations. The cytotoxic effects of the compounds were determined using MTT method on different tumour cell lines. The screening performed revealed that the tested compounds exerted cytotoxic activity upon the evaluated cells which is in line with our preceding studies concerning the activity of lanthanide coordination compounds with diverse biologically active ligands. The results give reason to conclude that lanthanides have proven to be active agents, thus enhancing the potential of Ln(III) complexes as a resource for the discovery of new pharmacologically active agents. The established structure-activity relationship in terms of antitumor, antioxidant properties and enzymatic inhibition can serve as a stable theoretical and practical basis for future rational design of lanthanide complexes with potential biological activity.

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Keywords: Lanthanides; Biologically active ligands; DFT; Vibrational spectroscopy.

Biography

Prof. Irena Kostova is one of the World's Top 1% of scientists according to Stanford University's ranking of scientists with the greatest contribution to the development of modern science. She graduated from Mendeleev University in Moscow with the highest grade. After graduation she has been appointed as a research scientist at the Research Center of the Ministry of Environmental of the Republic of Bulgaria. Defended her PhD and DSc theses at Medical University, Sofia, where she is currently a full professor at Chemistry Department. Graduated her second specialization "Theoretical bases of medical chemistry" at Medical University, Sofia. The main scientific interests and major contributions of Prof. Kostova lie in the field of medicinal chemistry of biologically active organic ligands and their lanthanide complexes with a focus on theoretical and coordination chemistry, vibrational spectroscopy and pharmacology of the studied compounds. Prof. Kostova is an author of about 200 publications with high impact factor and h-index, several textbooks, education book materials and monographs with around 7000 citations in indexed journals. She has been a lecturer at renowned universities in India, Austria, Italy, Romania, Spain, Slovakia etc. Member of the organizing committees of over 30 international conferences. She is an Editor of 7 prestigious international scientific journals, a member of the Editorial Boards of over 25 international journals and a reviewer for numerous high-ranking journals and international projects. Prof. I. Kostova is the Guest Editor of the Special issues of leading international journals, including *International Journal of Molecular Sciences, Molecules, Inorganics, Frontiers in Chemistry, Current Pharmaceutical Design*, etc. and an Editor for the Section "Non-Physiological Metals: Lanthanides, Actinides" in „*Encyclopedia of Metalloproteins*", Springer-Verlag GmbH. She has created and maintains collaborations with a number of European universities in the framework of joint research projects and European programs. She has been a member of the Scientific Experts Panel of Medical and Chemical Sciences of the National Science Fund of the Bulgarian Ministry of Education and Science.

Prof. Irena Kostova, PhD, DSc
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Dear Colleagues,

I take this opportunity to congratulate the participants and the distinguished guests of the *INTERNATIONAL CONFERENCE OF MEDICINAL CHEMISTRY AND DRUG DESIGN*, on September 27-29, 2024 in Sofia, Bulgaria. I have been collaborating closely with you and it is a great honor and pleasure for me to welcome you. This conference intends to present and discuss recent implementations of the scientific program 3.2.2, part of the project BG-RRP-2.004-0004-C01 and to provide opportunities for the presentation of updated research results and development activities related to the joint Project, bringing together the esteemed scientists and promoting professional interactions between them.

My very best wishes for a successful, stimulating and productive conference and my thanks to all the brilliant scientists for participating and sharing the new and exciting results in the field of medicinal chemistry and drug design. In addition to the intellectual pursuits and professional engagements provided by the conference, I hope you will also have time to enjoy the atmosphere in the wonderful city of Sofia during your stay. Enjoy the conference and the beauty of Sofia!

I would like to express my sincere thanks for the financial support, received by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project No. BG-RRP-2.004-0004-C01. The administrative support of the Medical University – Sofia is greatly acknowledged!