



CHEM MASTERY



DEPARTMENT OF PHARMACEUTICAL CHEMISTRY - NEWS LETTER

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DEVAKI AMMA MEMORIAL COLLEGE OF PHARMACY

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INSTITUTION VISION

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To provide state-of-art infrastructure, research facilities with eminent faculties to disseminate advanced knowledge in pharmacy education through innovative teaching- learning process with human and ethical values.

ISSUE HIGHLIGHTS

- ☞ Quantum chemistry in drug design
- ☞ Robotics revolutionizing drug development: Accelerating innovation and efficiency.
- ☞ Department activities.



Princy C.

QUANTUM CHEMISTRY IN DRUG DESIGN

Quantum chemistry in drug design is a rapidly developing area that leverages the principles of quantum mechanics to study the behavior of molecules at the atomic and subatomic levels. This approach allows pharmaceutical chemists to gain deeper insights into molecular interactions, which can significantly enhance the drug discovery and design process. Quantum mechanics provides detailed predictions of how molecules interact at the electronic level. By

calculating the electronic structure of molecules, quantum chemistry can predict how a drug candidate will bind to its target protein, enzyme, or receptor. This is far more accurate than traditional methods like molecular docking, which often rely on approximations. Understanding these interactions allows chemists to optimize drug candidates for stronger binding affinity, which can lead to more potent and selective drugs. Virtual screening using quantum chemistry methods allows researchers to predict how a large library of molecules will interact with a target protein, without the need for physical experimentation. This helps prioritize which compounds to synthesize and test in the lab. Quantum calculations can also assess the stability of drug-protein complexes and predict how changes in the drug structure might affect its binding efficiency or pharmacological activity. Quantum chemistry provides a highly detailed understanding of molecular properties like charge distribution, polarity, and dipole moments, which can influence a drug's absorption, distribution, metabolism, excretion, and toxicity (ADMET profile). By using quantum mechanical methods to predict these properties early in the design process, researchers can avoid costly failures in later stages of drug development and tailor compounds for better pharmacokinetics.

The interaction between a drug (ligand) and its protein target is at the core of drug efficacy. Quantum chemistry can model these interactions at a very high level of detail, including non-covalent interactions like hydrogen bonding, van der Waals forces, and electrostatic forces. Quantum calculations can help identify the best binding sites on proteins and refine ligands to bind more effectively, enhancing the drug's activity and specificity. Quantum chemistry methods can be used to predict potential toxicity by analyzing how a drug might interact with off-target proteins or other biological molecules. By modelling



In the remembrance of
Shri. K. V. Sankaranarayanan
(01.01.1948 - 12.07.2013)
Founder, Devaki Amma Memorial Institutions

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the behaviour of drug candidates at the quantum level, scientists can identify reactive sites that could lead to adverse effects. This early prediction of side effects can help minimize the risk of developing harmful drugs and refine the molecular structure to avoid these issues.

Quantum chemistry is increasingly used to study how drugs are metabolized in the liver by enzymes like cytochrome P450. These enzymes play a crucial role in breaking down drugs and can influence their effectiveness and potential for side effects. Understanding how drugs interact with these enzymes at the quantum level can help design compounds that are more stable, have fewer metabolic by-products, or are less likely to interact with enzymes that cause unwanted side effects.

Advances in computational chemistry software, powered by quantum chemistry methods, have made these techniques more accessible and practical for drug design. Quantum chemistry packages like Gaussian, ORCA, and Q-Chem allow researchers to perform calculations that would otherwise be impractical or too time-consuming. In recent years, these tools have become more efficient, enabling the study of increasingly complex biological systems, such as protein-ligand complexes, even at the quantum level. Quantum dots, which are tiny nanoparticles with quantum mechanical properties, are being explored in drug delivery systems. These particles can be used to improve the targeting, imaging, and controlled release of drugs within the body. Understanding their behaviour and interaction with biological molecules using quantum chemistry is helping to develop more effective nanomedicines for specific diseases, such as cancer.

The integration of quantum chemistry with machine learning (ML) and artificial intelligence (AI) is a hot trend in drug design. Quantum calculations provide the detailed, high-level data needed to train machine learning models, which can then predict drug properties and behaviour with greater accuracy. AI-powered models trained on quantum mechanical data can expedite the discovery of novel drug candidates by predicting the activity and toxicity of new compounds before they are synthesized. Despite its potential, the application of quantum chemistry in drug design does have challenges such as Computational cost and Complexity of biological systems. However, as computational power increases and algorithms improve, quantum chemistry is expected to become an even more integral part of drug design, offering highly precise insights that can accelerate the development of safer, more effective drugs. Quantum chemistry is transforming drug design by providing detailed, accurate models of molecular interactions and properties. This allows researchers to optimize drug candidates for potency, specificity, and safety, ultimately leading to faster and more successful drug development. While still evolving, it promises to revolutionize the way pharmaceutical chemistry is practiced in the future.

HYPERSPECTRAL IMAGING IN DRUG IDENTIFICATION



Aiswarya G. K.

Hyperspectral imaging (HSI) is an advanced analytical technique that combines imaging and spectroscopy to capture a wide spectrum of light across multiple wavelengths. Unlike traditional imaging, which uses only three colour bands (red, green, and blue), HSI collects hundreds of narrow spectral bands, allowing for detailed chemical analysis of substances. This technology is widely applied in pharmaceutical quality control, forensic investigations, and environmental monitoring. In forensic drug detection, HSI enables rapid identification of illicit substances such as cocaine, heroin, and fentanyl in powders, tablets, or liquids without requiring physical contact or chemical reagents. It is also valuable in pharmaceutical manufacturing, ensuring uniformity in drug

formulations and detecting counterfeit medications.

The mechanism of Hyperspectral Imaging (HSI) involves the collection of both spatial and spectral information from a sample to create detailed images that reflect the chemical composition of the material. In HSI, a sample is illuminated with light, typically from a broad spectrum, and the reflected or transmitted light is captured by a sensor. This sensor is equipped with a spectrometer that divides the light into many narrow bands across a wide range of wavelengths, usually from ultraviolet through visible to infrared. Each pixel in the captured image represents not only the spatial position of the sample but also the intensity of light at each specific wavelength, creating a spectral signature for that point. The result is a "hyperspectral cube" where the third dimension is the spectral data for each spatial location. By analyzing these spectral signatures with advanced software and algorithms, distinct chemical compounds within the sample can be identified and quantified based on their unique absorption and reflection characteristics at specific wavelengths. This ability to differentiate materials based on their molecular structure enables precise identification of

drugs, contaminants, and other substances in a variety of fields, from pharmaceuticals to environmental monitoring.

Hyperspectral Imaging (HSI) offers several significant advantages in drug detection and analysis. One of its key benefits is that it is non-destructive, allowing for the examination of samples without altering or damaging them, which is particularly valuable in fields like forensic science and pharmaceutical quality control. HSI also provides high sensitivity, capable of detecting trace amounts of substances, including illicit drugs or contaminants, that might not be identified by other techniques. The ability to capture both spatial and spectral information simultaneously enables a thorough and accurate analysis of complex samples, making it ideal for identifying counterfeit drugs or verifying the consistency of drug formulations. Furthermore, HSI is rapid, providing real-time data that speeds up the analysis process, which is crucial in fast-paced environments such as law enforcement or emergency toxicology. Additionally, it can be integrated with AI and machine learning algorithms to further enhance its capabilities, automating the detection and classification of substances with high accuracy. Its portability, particularly with the development of handheld systems, also makes HSI suitable for on-site drug testing and monitoring in various environments, including fieldwork and point-of-care applications. Overall, HSI represents a versatile, fast, and accurate method for drug detection and analysis.

The future of Hyperspectral Imaging (HSI) in drug detection and analysis is poised for significant advancements driven by emerging technologies. One of the most promising trends is the integration of artificial intelligence (AI) and machine learning, which will further enhance HSI's ability to automatically analyze complex spectral data and improve the accuracy of drug identification. These AI-driven systems can accelerate decision-making processes by quickly classifying and identifying substances in real-time, reducing the need for manual interpretation. Another trend is the development of miniaturized and portable HSI systems, making it easier to conduct on-site drug testing in field settings, such as border control, law enforcement, and emergency response. Additionally, as hyperspectral sensors become more affordable and accessible, there is potential for widespread use in everyday applications, including healthcare, environmental monitoring, and counterfeiting prevention. Advances in data processing algorithms will also contribute to more efficient and faster analysis, allowing for more dynamic real-time drug surveillance. The growing interest in personalized medicine could lead to the application of HSI in monitoring individual drug responses and metabolism. Overall, the future of HSI in drug detection is marked by increased automation, accessibility, and real-time, high-precision capabilities, paving the way for more efficient and widespread use across various industries. One major issue is the high cost of hyperspectral sensors and processing equipment, making it less accessible for many industries. Additionally, HSI generates vast amounts of data, leading to storage and computational challenges, as processing and analyzing such high-dimensional data require advanced algorithms and significant computing power. Another challenge is the complexity of image interpretation, as distinguishing between similar spectral signatures can be difficult and often requires expert knowledge. Furthermore, environmental factors such as atmospheric interference, lighting conditions, and sensor noise can affect the accuracy of hyperspectral images. Lastly, real-time processing remains a challenge, as HSI systems often require long processing times, limiting their effectiveness in time-sensitive applications like disaster response or surveillance.

DEPARTMENT ACTIVITIES

Ph. D. SCHOLARS IN DEPARTMENT

NAME	UNIVERSITY	REG. No.
Mrs. Ayswarya K.	MAHE, Manipal	230600125
Mrs. Shalima N. K.	Vinayaka Mission University	23PH01AP10
Mrs. Nimmi. M.	Vinayaka Mission University	23PH01AP06

DEPARTMENT PROJECTS IN PROGRESS

1	Unraveling the regulatory role of (p)ppGpp in bacterial persistence: Targeting (p)ppGpp hydrolase in Escherichia coli for novel potent inhibitors
2	Isolation, characterization and pharmacological evaluation of biomolecules from medicinal plants
3	Bioprospecting and Analysis of phytoconstituents for therapeutic potential

SEMINAR ORGANIZED

Department of Pharmaceutical Chemistry has organized one day seminar on 'strategic steps for securing government funding and launching research activities' for the faculties of Devaki Amma Memorial College of Pharmacy on 20.12.2024.



CONFERENCES / WORKSHOPS ATTENDED

Dr. Arunlal V. B., Mrs. Ayswarya K., Mrs. Ayisha Nitha and Mrs. Aparna P. have participated in 'National Level Workshop on Interpretation of Various Analytical Techniques & Design of Experiments' at Moulana College of Pharmacy on 31.08.2024.

Mrs. Ayswarya K., Mr. Syamjith P. and Mrs. Anjana K. have participated in 'Workshop on Cardiopulmonary Resuscitation (CPR) and First Aid Management' at Academic Staff College, KUHS on 27.09.2024.



Ms. Aiswarya G. K., Mrs. Neethu Dasan, Mrs. Athira M. A, and Mrs. Anjana K. along with 5th Semester B. Pharm Students have participated in 'One day seminar on Emerging Trends in Pharmacy: A Glimpse into The Future' at National College of Pharmacy on 18.10.2024



Mrs. Ayswarya K., Dr. Shaimol T., Mrs. Nimmi M., Mrs. Shantiya K., Mr. Syamjith P. & Mr. Mridhul Mohan along with 3rd Year Pharm. D. and 6th Semester B. Pharm students have participated in '3rd International Scientific Symposium' organized by KSPC and APTI held at Nayanar Academy, Kannur on 19.10.2024. Mrs. Nimmi M. has presented a poster in the symposium.



Mrs. Ayswarya K. along with 4th Semester B. Pharm students has participated in 'Malappuram IEDC Cluster Meet-up' at MES College of Engineering, Kuttippuram on 19.11.2024.



Dr. Anson S. Maroky, Dr. E. Tamil Jothi E., Mrs. Neethu Dasan, Mrs. Anjana P. & Ms. Athulya Dileep T. D. have accompanied 8th Semester B. Pharm students for industrial visit at 'Belco Pharma', New Delhi on 29.11.2024.



Mrs. Shantiya K., Mrs. Shalima N. K. and Mr. Mridhul Mohan along with 3rd Semester B. Pharm students have participated in '36th IPGA Conference' at Amrita School of Pharmacy on 07.12.2024.



Mrs. Ayswarya K., Mrs. Shalima N. K. and Ms. Aiswarya G. K. have participated in 'Interactive Workshop on Revolutionizing Drug Design: Hands-on Training with AutoDock' at National College of Pharmacy on 25.01.2025.



Mrs. Neethu Dasan, Mrs. Shitha G. and Mrs. Princy C. along with 1st Semester M. Pharm. (Pharmaceutical Chemistry) students have participated in workshop on 'Synergistic Spectroscopic Techniques: Leveraging IR, NMR and Mass Spectra for Structural Elucidation' at National College of Pharmacy on 19.02.2025.



Mrs. Aparna P. and Mrs. Jeena Chandran have participated in 'Pharmanecia 4.E International Research Conference' conducted by JSS Academy of Higher Education and Research, Ooty from 07.03.2025 to 08.03.2025. Both have presented e-posters in the conference.



RESEARCH PUBLICATIONS

1. **Byju K., Arunlal V. B., Ayisha Nitha P. and Princy C.***, Studies on Isolated Constituents of *Hemigraphis alternata* (Burm. F.) T. Anders and In Vitro Evaluation of Anticancer Activity, *ijons*, 2024, 15 (86), 8041-8047.
2. **Aparna P.*, Biju C. R., Arun Lal V. B., Princy C., Ayisha Nitha P., Shalima N. K. and Babu G.**, Recent Synthetic Approaches to Oxadiazole and Thiadiazole Derivatives as Biologically Potent Anti-Inflammatory Agents, *wjpls*, 2024, 10 (11), 340-344.
3. **Shalima N. K.*, Ayswarya K., Shitha G., Ayisha Nitha P., Aiswarya G. K., Aparna P., Dr. Biju C. R., Dr. Byju K., Dr. G. Babu and Nimmi M.**, Evaluation of Hepatoprotective Activity of Seeds of *Prunus Dulcis*, *wjpls*, 2025, 11(2), 130-133.
4. **Shalima N. K.*, Nimmi M., Dr. Biju C. R., Dr. Byju K., Neethu Dasan M., Princy C. and Dr. G. Babu**, Antioxidant Activity of The Seeds of *Prunus Dulcis* Using DPPH Assay, *wjpls*, 2025, 11(2), 94-97.

ACHIEVEMENTS

B. Pharm. (2019 batch) students have secured 100% results in their elective subjects 'Advanced Instrumental Techniques' in KUHS 8th semester B. Pharm. Degree Regular Examinations held in July 2024.



M. Pharm. Pharmaceutical Analysis students (2021 batch) have successfully completed the thesis presentation in KUHS 4th Semester M. Pharm. Degree Regular Examinations held in June 2024.



SOCIAL ACTIVITIES

Staff and students of the department have participated and donated blood in blood donation camp organized by NSS Unit of Devaki Amma Memorial College of Pharmacy on 19.06.2024



Mrs. Nimmi M. and Mrs. Shitha G. along with non-teaching Staff And 8th Semester B. Pharm. students have participated in medical camp jointly organized by NSS Unit of Devaki Amma Memorial College of Pharmacy and lions club, Calicut university at Elambulassery ALP School on 01.07.2024



Mrs. Shalima N. K. and Mrs. Shantiya K. along with 6th Semester B. Pharm. students have participated in medical camp organized by NSS Unit of Devaki Amma Memorial College of Pharmacy at ALP School, Pullikkunnu on 30.08.2024.

Mrs. Ayisha Nitha P., Ms. Arathi T. P., Mr. Mridhul Mohan and Mr. Shijin M. S. along with 6th Semester B. Pharm. and 4th Year Pharm. D. students have participated in NSS special camp organized by NSS Unit of Devaki Amma Memorial College of Pharmacy at Wayand from 27.02.2025 to 02.03.2025





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