RAMAIAH UNIVERSITY OF APPLIED SCIENCES | Faculty of Pharmacy

CHEMID

E-Newsletter

Volume II Issue II July-2023

Department of Pharmaceutical Chemistry
New BEL Rd, M S R Nagar, Mathikere, Bengaluru, Karnataka 560054

101st Birth Anniversary of Dr. M S Ramaiah

1922-2023

Editorial Team

Chief Patron
Dr. Kuldeep K Raina
Hon'ble Vice Chancellor

Patron
Dr. Govind R Kadambi
Pro- Vice Chancellor
Research

Patron
Dr. O P Kharbanda
Pro- Vice Chancellor
Health Sciences

Patron
Dr. G S Venkatesh
Registrar

Advisory
Dr. Bharath Srinivasan
Dean, FPH

Editor in Chief
Dr. Harish Kumar D R

Managing Editor
Dr. Lakshmi M Sundar

Managing Editor
Dr. A R Mahesh

Associate Editor
Prof. M Narayan Babu

Associate Editor
Dr. Judy Jays

Associate Editor
Dr. BV Suma

Associate Editor
Mrs. Knolin K Thatchil

Associate Editor
Mrs. Vijayabhanu P

Associate Editor
Dr. Yuvapriya M K

Associate Editor &
Social Media Coordinator
Dr. Parasuraman P

Associate Editor
Mrs. Vijayalakshmi S

Associate Editor
Mr. Rajdeep Ray

Editorial Note

Dear Readers,

I am delighted to present the latest edition of our department's newsletter, 'CHEMID.' As we continue to progress in the field of Pharmaceutical Chemistry, this newsletter serves as a platform to showcase the accomplishments, research, and events that have shaped our journey. In this issue, we have included a wide array of articles, publications, and oral presentations, highlighting the impressive research efforts undertaken by our faculty and students. The dedication and hard work put into these contributions are commendable.

Our faculty and students have been actively involved in groundbreaking research, and this section showcases some of the most notable publications and studies carried out within the Department of Pharmaceutical Chemistry. Their innovative work has significantly contributed to the advancement of pharmaceutical sciences. We take great pride in the number of research papers published by our department members in esteemed journals. These publications reflect our commitment to producing high-quality research that contributes to the global scientific community.

Our esteemed faculty members have been invited as resource persons to various academic and industry events. This section acknowledges their contributions in sharing knowledge and expertise beyond our institution providing insights into the workshops attended, helping us stay up-to-date with the latest advancements in the field.

The students of the department have been actively participating in conferences and symposiums, presenting their research findings to a wider audience. The oral presentations section highlights their efforts to disseminate knowledge and gain valuable feedback from peers and experts. We extend our heartfelt congratulations to all our students who successfully qualified in the Graduate Pharmacy Aptitude Test (GPAT). Your achievements bring pride to our department, and we wish you the best for your future endeavours. The hard work and dedication of our M.Pharm students have borne fruit, and this section celebrates their successful completion of the program. We wish them success in their careers and hope they continue to contribute to the pharmaceutical field.

The Department of Pharmaceutical Chemistry has been active in organizing events that promote scientific inquiry and collaboration. This section highlights the successful events we have conducted, bringing together academia, industry, and students. We also look forward to an exciting upcoming event, International E-conference on Exploring the Frontiers of Insilico Drug Discovery: Trends, Challenges and Opportunities, details of which

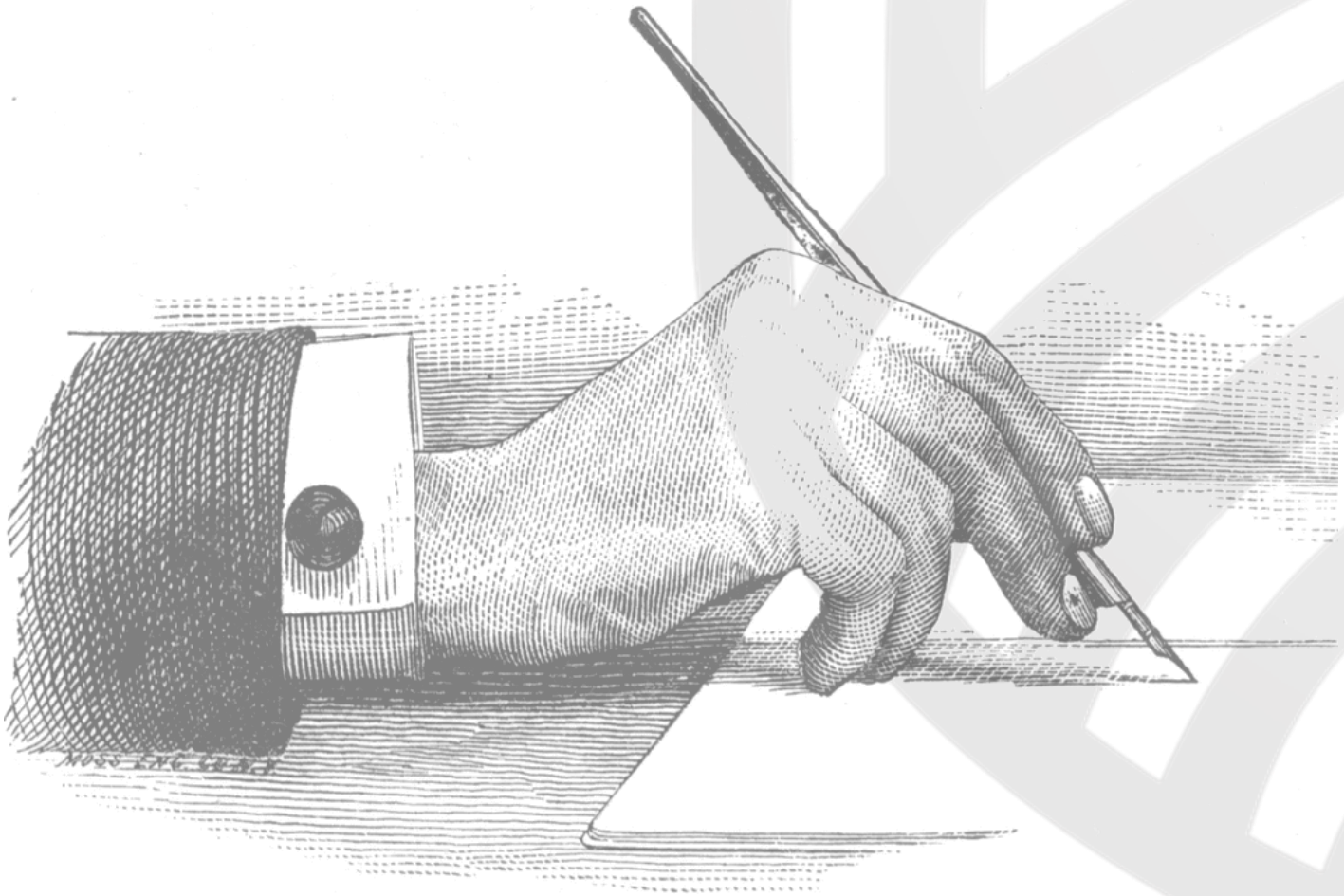
are provided in this section. Your active participation and engagement are crucial in making it a grand success.

I want to express my gratitude to all the contributors and the newsletter team for their hard work in putting together this edition of 'CHEMID.' It is through your collective efforts that we can showcase the achievements and advancements of our department.

I hope you find this newsletter informative and inspiring. As we move forward, let us continue to uphold the values of excellence, innovation, and collaboration that define our department.

Editor in Chief

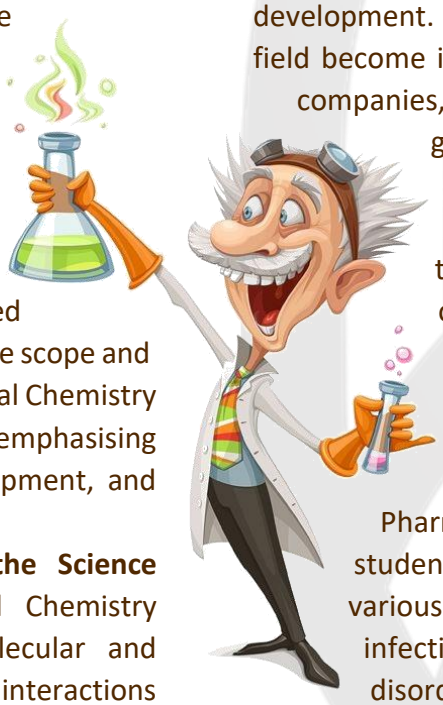
Dr. Harish Kumar DR



Contents

Perceiving the Significance of M.Pharm/Ph.D Pharmaceutical Chemistry as an indispensable need for thriving Pharmaceutical Industry

Pharmaceutical/Medicinal Chemistry is an interdisciplinary field that plays a pivotal role in the development of life-saving drugs and medicines. It provides a comprehensive study of chemical principles applied to the design, synthesis, and optimization of pharmaceutical agents as a Master's specialisation. This article delves into the scope of Pharmaceutical/Medicinal Chemistry as a Master's specialisation, emphasising its significance, potential career opportunities, and impact on the healthcare industry. The Indian pharmaceutical industry is one of the fastest-growing in the world, with significant advances in R&D and manufacturing. The Master of Pharmacy (M.Pharm) in Pharmaceutical Chemistry is critical to fueling this growth and meeting the ever-increasing demand for skilled professionals. This section discusses the scope and importance of M.Pharm Pharmaceutical Chemistry in the Indian pharmaceutical industry, emphasising its impact on drug discovery, development, and production..



Medicinal Chemistry: Unravelling the Science Behind Life-saving Drugs: Medicinal Chemistry focuses on understanding the molecular and chemical aspects of drugs and their interactions with biological systems. Students pursuing this Master's specialization delve into topics such as drug design, mechanism of action, structure-activity relationships, and drug metabolism. This knowledge equips them to contribute significantly to the development of novel therapeutic agents and the enhancement of existing drugs.

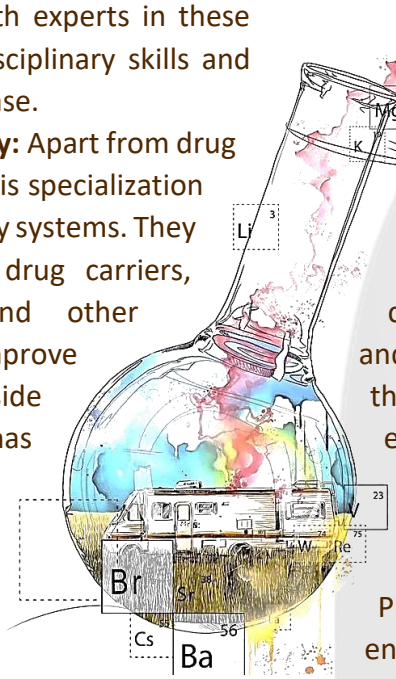
Drug Discovery and Development: The pharmaceutical industry's primary objective is to discover and develop new, safe, and effective drugs to address various medical needs. M.Pharm Pharmaceutical Chemistry graduates play a pivotal role in this process, utilizing their expertise in medicinal chemistry to design and synthesize potential drug candidates. They identify new molecular entities with desirable properties and optimize them for therapeutic efficacy, making them an indispensable driving force for drug discovery in India. Pharmaceutical/Medicinal Chemistry is at the forefront of drug discovery and development. Graduates with expertise in this field become invaluable assets in pharmaceutical companies, research institutions, and government agencies involved in the process of bringing new drugs to the market. They participate in target identification, hit-to-lead optimization, and preclinical studies, leading to potential drug candidates.

Role in Combating Diseases: With a Master's specialization in Pharmaceutical/Medicinal Chemistry, students can contribute to the fight against various diseases, including cancer, infectious diseases, neurological disorders, and more. They work on designing specific molecules that target disease-causing agents or regulate biological processes to achieve therapeutic outcomes. India is often referred to as the "pharmacy of the world" due to its prominence in the production of generic drugs. M.Pharm Pharmaceutical Chemistry graduates contribute significantly to this aspect of the industry. They work on reverse-engineering brand-name drugs to develop affordable, high-quality

generic versions, making essential medicines accessible to a vast population.

Collaborative Research Opportunities: Pharmaceutical/Medicinal Chemistry is highly collaborative, often involving researchers from diverse fields such as pharmacology, biochemistry, and molecular biology. Master's students have the opportunity to collaborate with experts in these areas, enhancing their interdisciplinary skills and broadening their knowledge base.

Advancements in Drug Delivery: Apart from drug design, Master's students in this specialization explore innovative drug delivery systems. They study nanotechnology-based drug carriers, targeted drug delivery, and other advanced techniques that improve drug efficacy and minimize side effects. This area of research has tremendous potential to revolutionize healthcare practices.



Regulatory Affairs and Quality Control: Pharmaceutical/Medicinal Chemistry graduates are also well-suited for roles in regulatory affairs and quality control. They can work with regulatory agencies to ensure that new drugs meet safety and efficacy standards, and contribute to quality control processes to maintain the integrity of pharmaceutical products. Navigating complex regulatory frameworks is a significant challenge for the pharmaceutical industry. M.Pharm Pharmaceutical Chemistry professionals are well-versed in regulatory requirements and contribute to the compilation of documentation for drug approval. Their expertise expedites the regulatory process and helps companies launch new products more efficiently.

Academic and Research Opportunities: Completing a Master's in Pharmaceutical/Medicinal Chemistry opens doors to further academic pursuits, such as pursuing a Ph.D. or engaging in postdoctoral research. These opportunities allow individuals to delve deeper into specialized areas of drug development and make significant contributions to scientific knowledge.

Quality Control and Assurance: The Indian pharmaceutical industry faces strict regulations and international standards concerning drug quality and safety. M.Pharm Pharmaceutical Chemistry professionals are equipped with the necessary skills to conduct rigorous quality control tests on raw materials, intermediates, and finished products. Their expertise ensures that drugs meet the required standards, enhancing the reputation of Indian pharmaceutical companies in the global market.

Collaboration with Academia: M.Pharm Pharmaceutical Chemistry programs often encourage collaborations with academic institutions, fostering a synergistic relationship between industry and academia. Such collaborations facilitate joint research projects, knowledge exchange, and access to state-of-the-art facilities, nurturing a skilled workforce and accelerating the pace of drug discovery.

Research and Development: Research and development (R&D) is the backbone of the pharmaceutical industry. M.Pharm Pharmaceutical Chemistry graduates are involved in cutting-edge research to explore new therapeutic avenues and develop innovative drug delivery systems. Their contributions drive advancements in pharmaceutical technology, leading to novel drug formulations and treatment modalities.

Patent and Intellectual Property: Intellectual property plays a critical role in the pharmaceutical industry, safeguarding innovations and promoting

further investments in research. M.Pharm Pharmaceutical Chemistry professionals actively contribute to patent applications for novel drug molecules and delivery systems. This not only protects the interests of the industry but also encourages inventiveness and competitiveness in the market.

Pharmacovigilance: Pharmacovigilance is essential for monitoring and evaluating drug safety throughout its lifecycle. M.Pharm Pharmaceutical Chemistry graduates contribute to pharmacovigilance activities by assessing adverse drug reactions, conducting post-marketing surveillance, and ensuring patient safety through continuous monitoring of drug profiles.

Drug Formulation: M. Pharm Pharmaceutical Chemistry graduates also work on drug formulation, ensuring that the final product has the desired stability, bioavailability, and therapeutic effect. They collaborate with other professionals, such as pharmacists and formulation scientists, to optimize drug delivery systems and dosage forms.

Clinical Research: Clinical trials are an integral part of drug development, evaluating the safety and efficacy of new medications. M.Pharm Pharmaceutical Chemistry professionals often participate in clinical research, contributing their expertise to ensure the smooth conduct of trials and accurate data analysis.

Career Opportunities as M.Pharm/ PhD (Pharmaceutical Chemistry)

A career as a Master's graduate in Pharmaceutical Chemistry offers a wide range of exciting and rewarding opportunities in the pharmaceutical and related industries. The knowledge and skills acquired during the program equip graduates to contribute to drug discovery, development, quality control, research, and innovation. Here are some potential career paths and opportunities for individuals with a Masters's degree in Pharmaceutical Chemistry:

Medicinal Chemist: As a medicinal chemist, you will be at the forefront of drug discovery and development. You will design and synthesize new molecules to target specific diseases, optimizing their pharmacological properties and ensuring their safety and efficacy.

Pharmaceutical Research Scientist: Pharmaceutical research scientists are involved in cutting-edge research to explore new therapeutic avenues, drug delivery systems, and advanced technologies. You may work in both academic and industrial research settings, contributing to scientific advancements in the field.

Computational Chemist: The role of a person with an M.Pharm degree in Pharmaceutical Chemistry as a computational chemist can be crucial and multi-faceted. Computational chemistry is a field that utilizes computer simulations and modelling to study chemical structures, properties, and interactions. It plays an increasingly important role in drug discovery, development, and optimization processes within the pharmaceutical industry. Here's how an M.Pharm graduate in Pharmaceutical Chemistry can contribute as a computational chemist: Drug Design and Discovery, Lead Optimization, ADME-Tox Prediction, Molecular Modelling, Quantitative Structure-Activity Relationship (QSAR) Analysis,

Virtual Screening and High-Throughput Computing, Biological Simulations, Data Analysis and Bioinformatics, Collaboration with Experimental Scientists: Computational chemists collaborate with experimental scientists, such as medicinal chemists, biologists, and pharmacologists, to guide and support their research efforts. They help in the interpretation of experimental results and offer suggestions for further investigations. The role of an M.Pharm in Pharmaceutical Chemistry as a computational chemist is instrumental in driving drug discovery and development processes by integrating computational techniques with experimental methodologies. Their contributions aid in identifying potential drug candidates, optimizing lead compounds, and gaining a deeper understanding of drug-receptor interactions.

Quality Control/Quality Assurance Specialist: Quality control and assurance are critical aspects of the pharmaceutical industry. Graduates in Pharmaceutical Chemistry play an essential role in ensuring the quality, safety, and compliance of pharmaceutical products through rigorous testing and adherence to regulations.

Formulation Scientist: Formulation scientists are involved in developing drug formulations that optimize drug delivery, stability, and bioavailability. Your knowledge of Pharmaceutical Chemistry will be invaluable in formulating drugs in various dosage forms, such as tablets, capsules, and injectables.

Analytical Chemist: Analytical chemists play a crucial role in the pharmaceutical industry by developing and validating analytical methods to analyse drugs and pharmaceutical products. Your expertise in Pharmaceutical Chemistry will be essential in ensuring accurate and reliable results.

Regulatory Affairs Specialist: Regulatory affairs professionals are responsible for navigating complex regulatory frameworks and ensuring that pharmaceutical products meet all necessary requirements for approval and commercialization. Your understanding of drug development and regulations will be highly sought after in this role.

Pharmacovigilance Specialist: Pharmacovigilance professionals monitor and evaluate the safety of drugs throughout their lifecycle, identifying and assessing adverse drug reactions. As a Pharmaceutical Chemistry graduate, you will have the expertise to contribute effectively to pharmacovigilance activities.

Intellectual Property/Patent Specialist: With your knowledge of drug molecules and formulations, you can work in intellectual property and patent-related roles, helping pharmaceutical companies protect their innovations and navigate legal aspects of drug development.

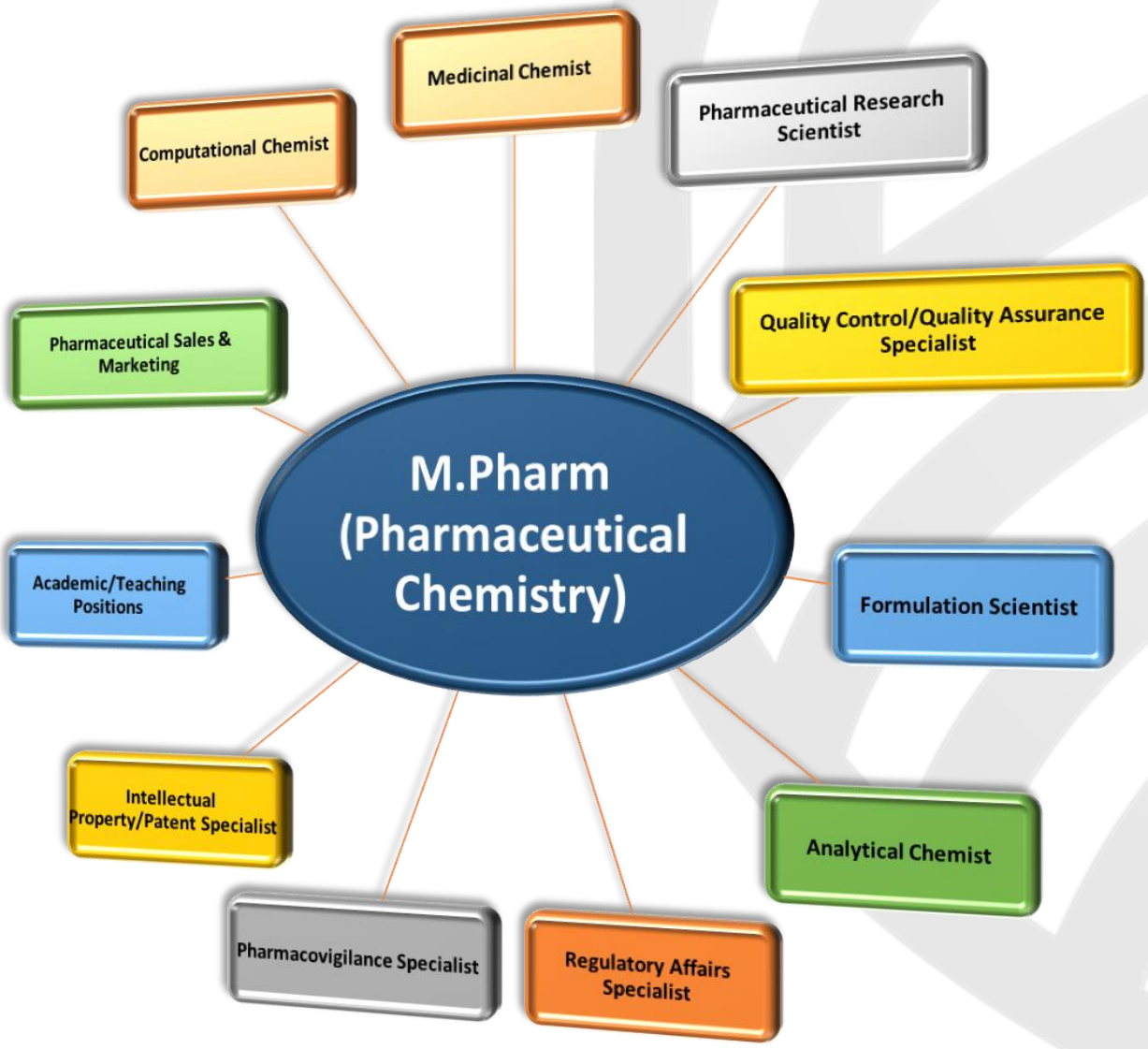
Academic/Teaching Positions: If you have a passion for education and research, you can pursue academic or teaching positions in universities, colleges, or research institutions. This will allow you to share your knowledge with the next generation of scientists and contribute to the growth of the field.

Pharmaceutical Sales and Marketing: As a Master's graduate in Pharmaceutical Chemistry, you can explore opportunities in sales and marketing roles, promoting pharmaceutical products to healthcare professionals and

consumers while utilizing your technical knowledge to communicate the product's features and benefits effectively.

A Master's degree in Pharmaceutical Chemistry opens up a plethora of career opportunities in the pharmaceutical and related industries. Whether you choose to contribute to drug discovery, research, quality control, regulatory affairs, or education, your expertise will be highly valued and can make a significant impact on the development and improvement of life-saving medications. As the pharmaceutical industry continues to grow and evolve, your specialized skills will remain in demand, offering you a promising and fulfilling career path. The scope of Pharmaceutical/ Medicinal Chemistry as a Master's specialization is vast and impactful. Graduates play a crucial role in drug discovery, development, and delivery, contributing to advancements in healthcare and the treatment of various diseases. This interdisciplinary field offers a dynamic and rewarding career path with numerous opportunities for research, innovation, and collaboration. As the demand for effective medications continues to grow, the role of these specialized chemists becomes increasingly vital in shaping the future of medicine.

- ***Dr. AR Mahesh***



Unveiling the Molecular Architecture: Isolation and Spectral Analysis of Colchicine

Colchicine is a naturally occurring alkaloid that has attracted significant attention in the fields of chemistry and pharmacology. It is derived from the plant species Colchicum autumnale (Fig-1), commonly known as autumn crocus or meadow saffron. This compound has a complex molecular structure and exhibits intriguing chemical properties, making it a subject of great interest for researchers.

Fig-1: *Colchicum autumnale*

Chemically, colchicine belongs to the category of phenanthrene alkaloids and possesses a tricyclic structure (Fig-2). Its core structure consists of a pentacyclic framework, composed of three rings: a phenanthrene ring, a heptane ring, and a tetrahydrofuran ring. The presence of these fused rings contributes to the unique properties and biological activities of colchicine.

The molecular formula of colchicine is $C_{22}H_{25}NO_6$, indicating its composition of carbon, hydrogen, nitrogen, and oxygen atoms. It possesses a molecular weight of approximately 399.44 g/mol.

Colchicine is N - (5, 6, 7, 9 - tetrahydro - 1, 2, 3, 10 - tetramethoxy - 9 - oxobenzo [a] heptalen -7-yl)- ,(S)-acetamide.It is obtained from corms which are bulb shaped of autumn crocus plant , Colchicum autumnale. Primarily used to treat gout.

Colchicine is pale yellow in colour, amorphous scales, or powder, odorless and darkens on exposure to light.

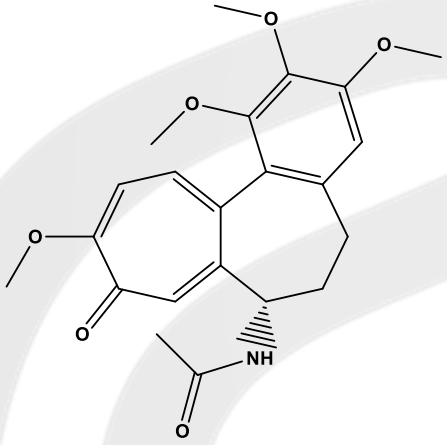


Fig-2: Chemical Structure of Colchicine

One of the remarkable features of colchicine is its ability to bind to tubulin, a protein involved in cell division. By binding to tubulin, colchicine disrupts the assembly of microtubules, which are essential for various cellular processes, including mitosis and cell motility. This mechanism of action makes colchicine a valuable tool in studying the dynamics of microtubules and their role in cellular functions.

The chemical synthesis of colchicine is challenging due to its intricate structure and complex stereochemistry. Therefore, isolation from natural sources remains the primary method of obtaining colchicine for research and pharmaceutical purposes. However, advances in synthetic methodologies have enabled the production of colchicine analogs and derivatives, facilitating investigations into their structure-activity relationships and potential therapeutic applications.

Structural elucidation plays a crucial role in understanding the chemical properties and biological activities of colchicine. Various spectroscopic techniques, such as nuclear

magnetic resonance (NMR) spectroscopy, mass spectrometry (MS), and X-ray crystallography, have been employed to determine the exact arrangement of atoms within the colchicine molecule. These studies have provided valuable insights into its three-dimensional structure and have contributed to our understanding of its interactions with biological targets.

Colchicine is a fascinating compound with a complex chemical structure that holds significant importance in the field of chemistry. Its ability to disrupt microtubule assembly and its potential therapeutic applications make it an intriguing subject for further research. The elucidation of its molecular structure has been instrumental in unraveling its mechanism of action and exploring its potential in various biomedical contexts

Isolation of colchicine

Alcoholic extraction: Alcohol was used to extract the corm or seed, followed by alcohol distillation in order to remove insoluble fat and resins. The syrupy residue is mixed with more water and then filtration takes place. Chloroform is used to continuously extract the aqueous extract. It can also be triturated with $PbCO_3$ and when it is filtered again, small volume evaporates and then extraction with chloroform is done. A crystalline complex of colchicine is obtained with chloroform. Steam is used to distil the chloroform. Alcohol can also be used for this purpose. When the residual solution evaporates, amorphous colchicine is produced. It may crystallize as pale-yellow needles from ethyl acetate.

Spectral Analysis of Colchicine

UV Spectrum: The UV spectrum of cochicine shows two absorption maxima at 351 and 243 nm with absorptivity values of 45 and 81 (Fig-3).

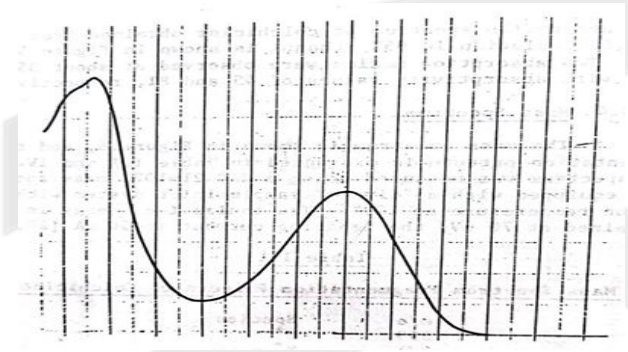


Fig-3: UV spectrum of Colchicine

Infrared Spectrum

Using a Beckman 5260 grating infrared spectrophotometer, IR spectrum (Fig-4) was obtained by using KBr dispersion of the material (dried) [105 degrees,3 hours]. Principal bands are 1248, 1566,1589 cm^{-1}.

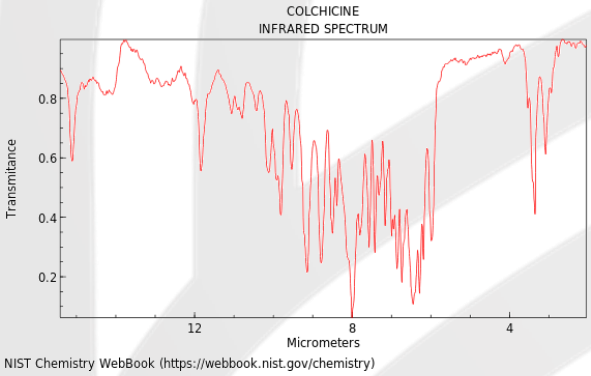


Fig -4: Infrared Spectrum of Colchicine

Reference:

Klaus Florey and Brittain, H.G. (1972) Analytical profiles of drug substances and excipients, Volume 10, pp 153 - 217.

-Nandini MS
II Sem M.Pharm

Isolation And Structural Elucidation of An Antimalarial: Betulinic Acid

Betulinic acid (3-hydroxy-3β-lup-20(29)-en-28-oic acid) is one of the leading phytoconstituents possessing anti-malarial activity.

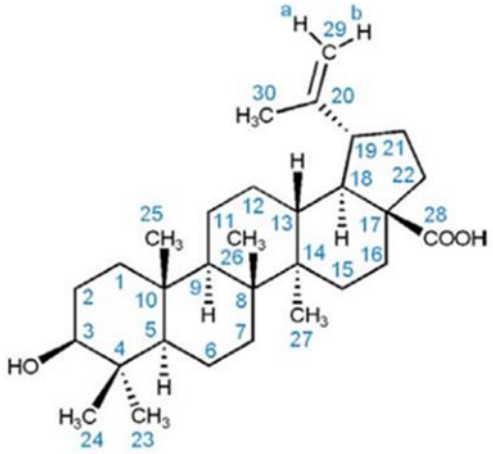


Fig-1: Structure of Betulinic acid

The recognition of betulinic acid (Fig-1) as an anti – malarial agent all started with the urgent need to come up with newer anti -malarials since there had been many cases of emerging drug resistance of the plasmodial parasites to the common antimalarial like chloroquine, quinine, primaquine, mefloquine etc. Through extensive research, it was found that in Tanzania, an ethanolic infusion of the root bark of Uapaca nitida Mu¨ll-Arg. (Euphorbiaceae) had been used at the Peramiho Mission, Tanzania, as a treatment for malaria back in the 1980s when malaria was rampant in the region as this formula had been in use by the indigenous people since time immemorial. (Costa et al., 2009). In the 1990s various studies on the phytoconstituents of this extract for anti -malarial activity was carried out and it was found that mainly betulinic acid was responsible for the activity as it displayed the best *in vitro* antiplasmodial activity against K1 P. falciparum (Kirby et al., 1993). The ethanol extract also displayed *in vivo* activity (NK65 P. berghei in mice). Betulinic acid mainly acts by schizont growth inhibition and their premature death, but the mechanism leading to such an event is yet to be deduced. Also, betulinic acid was found to possess only moderate lipophilicity (Innocente et al., 2012). Therefore, the acetyl derivative of betulinic acid (Fig-2) was introduced to increase the lipophilicity and hence enhance the penetration of betulinic acid into the erythrocytes for exhibition of its activity.

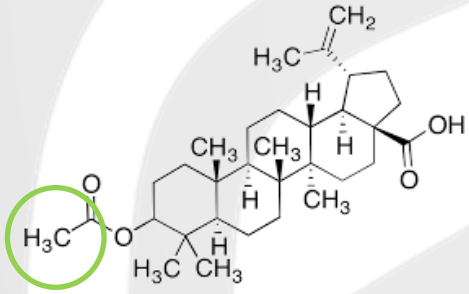


Fig-2: Acetyl betulinic acid

Later piperazinyl derivatives of acetyl betulinic acid (Fig-3) were found to possess even more enhanced activity against *P. falciparum* schizonts in erythrocytes *in vitro*.

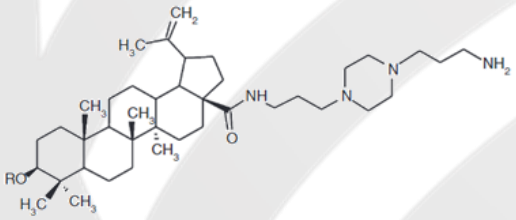


Fig-3: Piperazine derivative where R = acyl or 2-methyl propane

Moreover, their mechanism of action had also been deduced; the inhibition of schizont growth and premature death is brought about by disturbance in the calcium homeostasis in the schizonts (Silva et al., 2015).

Extraction and Isolation of Betulinic Acid

Betulinic acid is usually obtained from the bark of birch (Betula sp.) and plane trees (Platanus sp.) (Fig-4).

Since a typical plane tree of 15 m height drops several kilograms of bark on the ground by simply following its biological rhythm, the bark can be just picked up from the ground. Whereas in the case of birch trees, the white bark must be stripped from the trunk.

Fig-4: (A) Birch tree and (B) Plane tree

To extract and isolate betulinic acid:

1. The collected bark is air - dried and ground using a grinder.
2. Then 70 g of the rather coarse powder is extracted with 700 ml of dichloromethane for 6 hours via Soxhlet extraction.
3. Then the yellow extract obtained is filtered and filtrate is concentrated to half of its initial volume and is chilled under -18°C for crystallization.
4. On filtration, yellow crystals of crude betulinic acid are obtained. Then on work-up of the mother liquor, another 100 mg of betulinic acid can be obtained.
5. To isolate the crude product, it is recrystallized by using 100 mL boiling methanol wherein, the filtrate obtained must be chilled under -18 °C for the colourless crystals of pure betulinic acid to separate out.
6. The crystals are rinsed with 5 mL of ice-cold methanol and dried.

Spectroscopic Data of Betulinic Acid

IR Spectroscopy: In this IR spectrum (Fig-5), OH stretch of the carboxylic acid at 3050 cm^{-1}, the sp^2 and sp^3 CH stretching vibrations at near 3000 cm-1 and just above 3000 cm^{-1} respectively, the C=O double bond close to 1700 cm^{-1} and the aliphatic C=C double bond near 1600 cm^{-1} can be clearly identified and so is the typical wavenumber of about 3100 cm^{-1} for a terminal $=CH_2$ group.

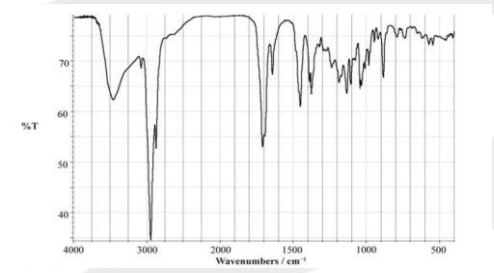


Fig-5: IR spectrum of betulinic acid

Proton NMR

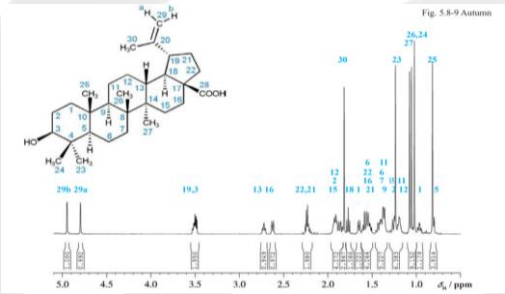


Fig-6: Proton NMR spectrum of betulinic acid at 700 MHz in pyridine-d5

For this NMR (Fig-6), a 700 MHz spectrometer was applied. The two olefinic protons i.e., H-29a and H-29b are found to resonate at δH = 4.80 and 4.95 ppm. The next signal in the proton spectrum which is at 3.5 ppm integrates for two protons, which from their chemical shifts are assigned to H-19 and H-3.; the signal of the methyl group C-30 which is attached to a sp2 center can be identified from its chemical shift of 1.82 ppm.

Carbon -13 NMR

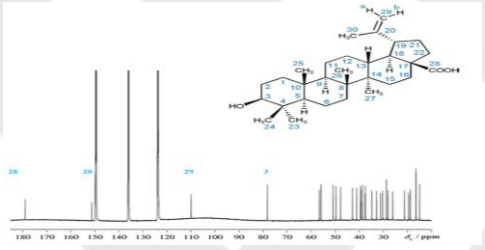


Fig-7: ^{13}C NMR spectrum of betulinic acid at 175 MHz in pyridine-d5

In this ^{13}C NMR spectrum (Fig-7, Table-1) 4 signals can be identified from their typical chemical shifts, that is C-28 at 179.1, C-20 at 151.3, C-29 at 111.0 and C-3 at 78.2 ppm. The group of signals

between 60 and 10 ppm is magnified, so as to clearly identify the signals for the remaining carbon atoms.

Mass Spectroscopy:

The mass spectrum of betulininc acid (Fig-8) depicts the typical pattern of a polycyclic compound having many CH_2 and CH groups which leads to an array of signals separated by 13 and 14 mass units. The M-18 peaks at 438 m/z suggests the elimination of water and the M-45 peak at 411 m/z, the elimination of a carboxyl group. Characteristic is the m/z value of 248, which gives an indication that after ionization maybe at C-28 or C-20, the molecule has been cleaved by breaking the two bonds between C-8 and C-14 and between C-9 and C-11.

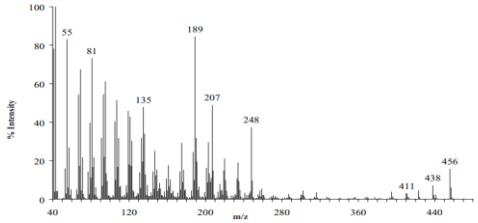


Fig-8: Mass spectrum (EI) of betulinic acid

This can be formulated, in detail, by ionization at the isopropenyl group and a hydrogen transfer leading to ion 'a' which then undergoes a second hydrogen shift leading to 'b'. From 'b', a retro-Diels - Alder reaction forms the radical, ion 'c' with m/z = 248 (Fig-9).

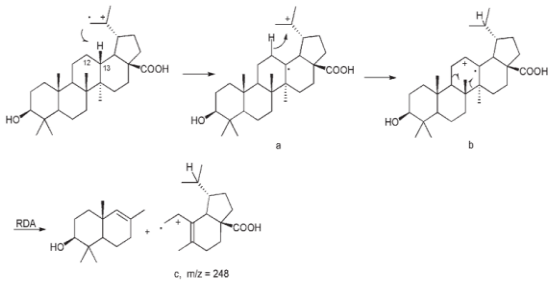


Fig-9: The first possible of fragmentation sequence of betulinic acid

Another possible fragmentation begins by ionization at the carboxyl group (Fig-10); two McLafferty rearrangements lead to ions 'd' and then 'e', which is finally cleaved to the radical ion 'f', again with m/z = 248.

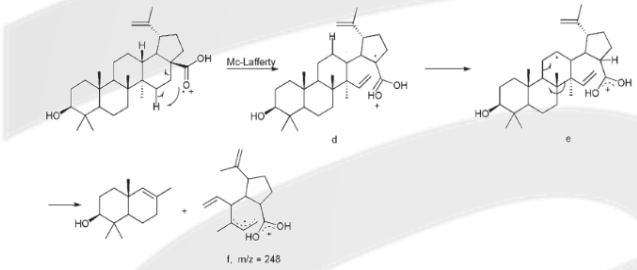


Fig-10: The second possible of fragmentation sequence of betulinic acid

References:

1. de Sá, M. S., Costa, J. F., Krettli, A. U., et al., (2009) Antimalarial activity of betulinic acid and derivatives *in vitro* against Plasmodium falciparum and *in vivo* in *P. berghei* infected mice, Parasitology research, 105(1), pp. 275–279.

2. Innocente, A. M., Silva, G. N., Cruz, L. N., at al., (2012) Synthesis and antiplasmodial activity of betulinic acid and ursolic acid analogues, Molecules (Basel, Switzerland), 17(10), pp. 12003–12014.

3. Silva, G.N.S., Schuck, D.C., Cruz, L.N., et al., (2015) Investigation of antimalarial activity, cytotoxicity and action mechanism of piperazine derivatives of betulinic acid., Trop Med Int Health, 20, pp. 29-39.

4. Chatwal, GR., Anand, SK. (2015) Instrumental Methods of Chemical Analysis, Mumbai: Himalaya Publishing House, pp. 2.345 – 2.346, 2.355 – 2.356.

5. Berger, S., Sicker, D., (2009) Classics in Spectroscopy, Weinheim: Verlag GmbH & Co.KGaA, pp. 153 – 167.

- Shreya Shet
II Sem M.Pharm

In-Silico Evaluation of Phytochemicals from *Phyllanthus Niruri*: As Potential HER-2 Inhibitors

Introduction

Breast cancer accounts for more than one in ten new cancer diagnoses in women, making it the most prevalent type of cancer. HER-2 (Human epidermal growth factor receptor) is considered as an effective target for breast cancer. The present study focuses on the HER-2 inhibition potential of flavonoids from *Phyllanthus niruri* (Fig-1) by *in vitro* studies.

Fig-1: Leaves of *Phyllanthus niruri*

Experimental methods:

Identification of drug molecules

Based on the literature research of HER-2 inhibitors, the currently used medications identified were lapatinib (Fig2), trastuzumab, pertuzumab.

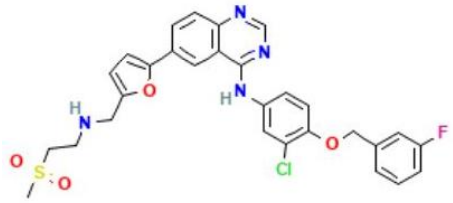


Fig-2: Chemical Structure of the standard drug Lapatinib

Molecular docking study:

Molecular entities were downloaded from 0050UBCHEM and the target structure from PDB, further purified using SPDB viewer. Molecular docking was carried out using PyRx software, and the docking scores were analyzed.

Table-1: docking score of the ligands with the HER-2 target

SL.NO.	COMPOUND NAME	PUBCHEM ID	BINDING AFFINITY
1	Nirurin	125896	-9
2	Quercetol A	44257151	-8.5
3	Rutin	5280805	-8.1
4	Niruriflavone	11494293	-8
5	Quercetin	5280343	-8
6	Quercitrin	5280459	-7.9
7	Gallocatechin	65084	-7.9
8	Astragalin	5282102	-7.6
9	Lapatinib	208908	-8.8

Results and discussions:

The docking results (Table-1) showed that phytochemicals Nirurin (Fig-3), Quercetol A, Rutin had better binding to HER-2 when compared to standard drug. It was also noted that Astragalin had less binding affinity to HER-2 in comparison.

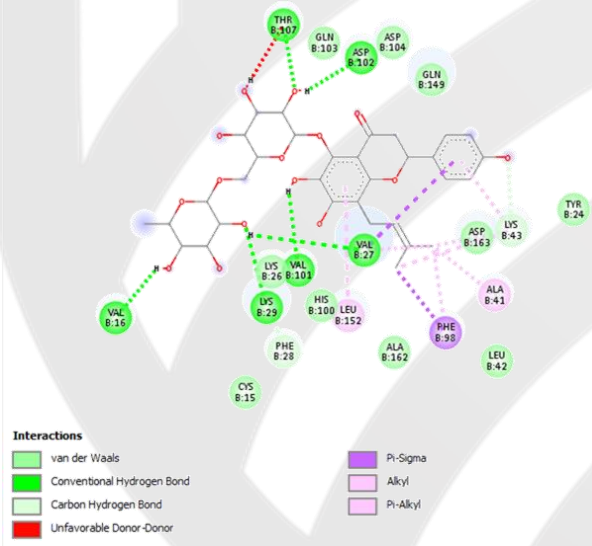


Fig-3: 2D-interactions of HER-2 - nirurin

Conclusion:

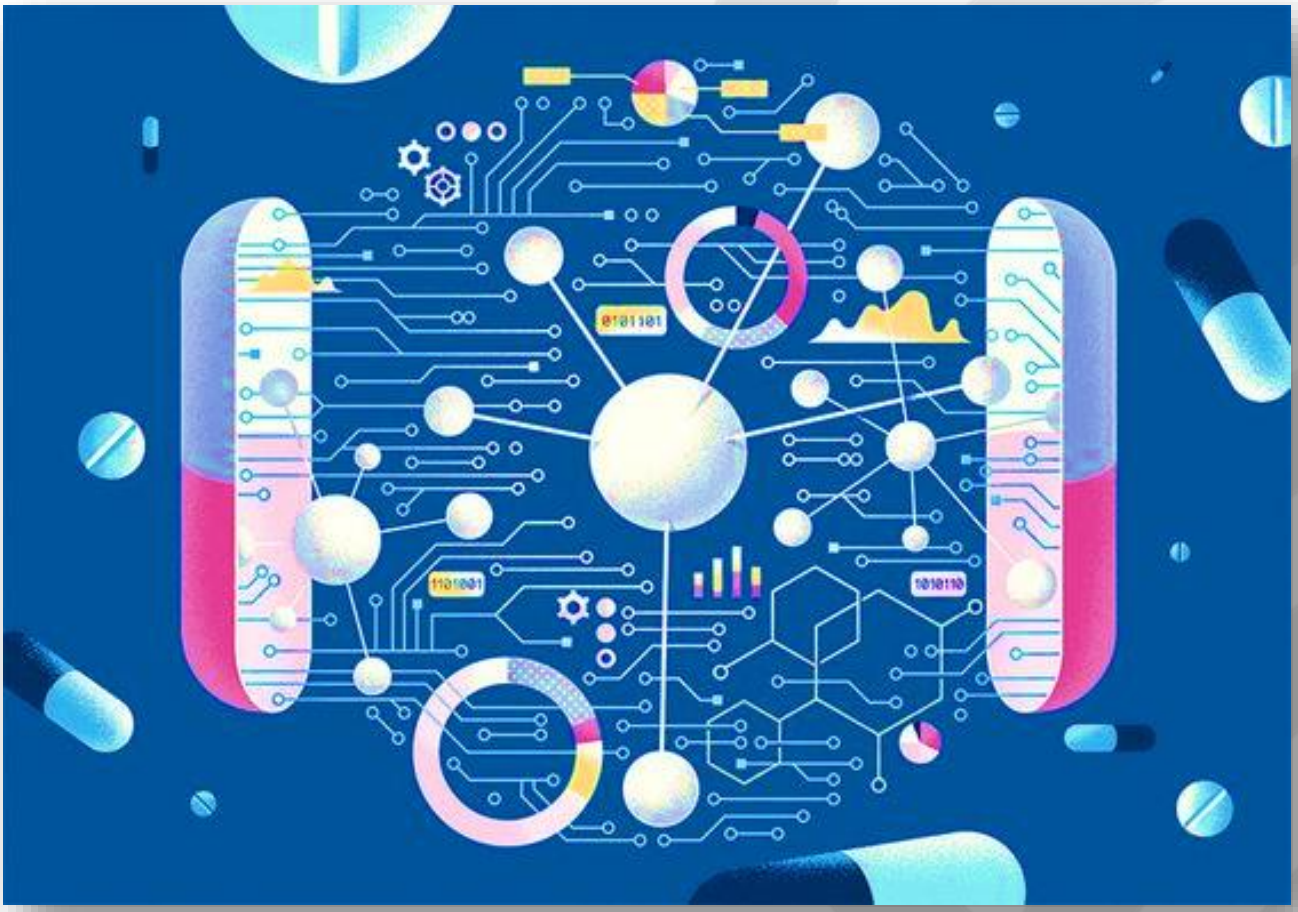
Based on molecular docking studies Nirurin showed high binding affinity with HER-2 as a target, with a docking score of -9. Further its

ADMET properties should be evaluated and *in-vitro, in-vivo* studies to be carried out.

Reference:

1. Bagalkotkar. G., Sagineedu. S. R., Saad. M. S and Stanslas. J (2006) Phytochemicals from Phyllanthus niruri Linn. And their pharmacological properties: a review, Journal of Pharmacy and Pharmacology, 58(12):pp1559-15570.
https://doi.org/10.1211/jpp.58.12.0001

- Tejas and Harshith
VIII Semester, B. Pharm



PG Group Project Submited

Identification and validation of novel MAO-B inhibitors through ligand based Pharmacophore Modelling for the Management of Parkinson's Disease

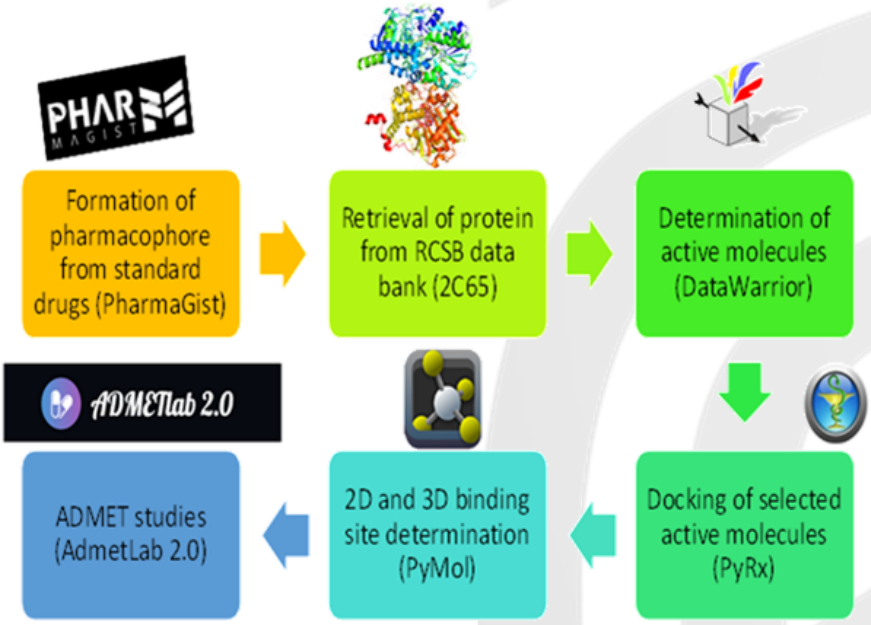
Students: Jyothi S, Megha N, Shannon D Almeida, Sharath S Holalkere, Sharon Esther Samuel

Research Supervisor: Prof. M Narayana Babu

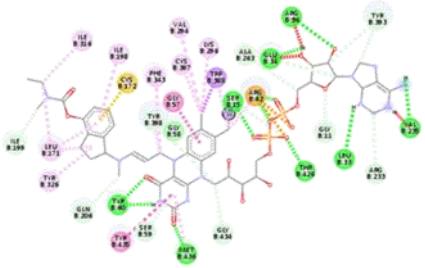
Abstract: Monoamine oxidase B (MAO-B) is a protein that is involved in metabolism of dopamine. Inhibition of this enzyme can thus increase dopamine levels, thus alleviating symptoms of parkinsonism. Parkinsonism is a chronic disorder which involves low concentration of dopamine in critical areas of the brain. Several selective and non-selective antagonists are currently in clinical trial phases or in the market, which work based on this method of action. The objective of this study was to determine a pharmacophore based on standard drugs and then evaluate its efficacy using in silico docking method. This work deals with the identification and validation of novel MAO-B inhibitors through ligand-based pharmacophore modelling for the management of Parkinson's disease. The pharmacophore was obtained using PharmaGist software. The reference ligands chosen were selective and non-selective MAO-B inhibitors which are already in the market. The obtained pharmacophore was then uploaded on ZincPharmer, and a thousand hits were selected, with the best energy conformation. The data was then screened using DataWarrior software based on selected parameters. Forty-six unique ligands were obtained. These were docked using PyRx software to validate the generated ligands using MAO-B protein, obtained from RCSB protein databank. The protein-ligand complexes are then analysed for 2D and 3D interactions using Biovia Discovery Studio and PyMol. Several of the ligands showed better binding affinity when compared to the standard drugs. Finally, ADMET studies were carried out from the SMILES string, using the online webserver AdmetLab 2.0. All the ligands conformed to drug-likeliness guidelines and their predictive bioavailability was found to be good. Drug identification was carried out to find novel MAO-B inhibitors for the treatment of Parkinson's disease, we used ligand-based pharmacophore modelling. Based on the preliminary studies 49 hits was found to be show high binding affinity with MAO-B. Top 10 ligands were obtained from

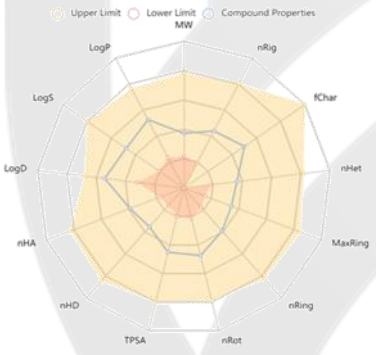
pharmacophore modelling subsequently evaluated for ADMET properties using ADMET lab 2.0 web server. The Zinc data base molecule ZINC74691584 will obey the Lipinski rule of five, by this the molecule can observe well by orally and it pass BBB and CNS to show its activity.

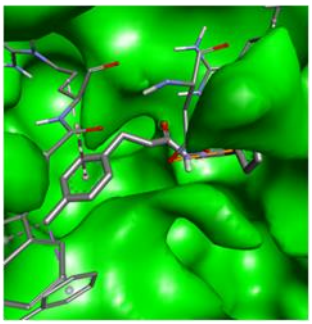
Schematic representation of work

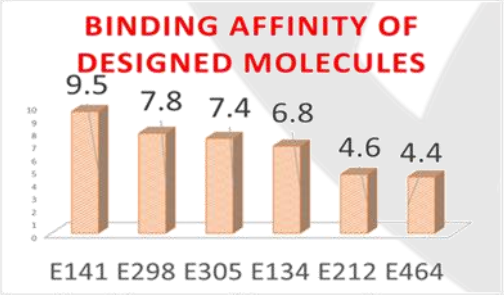


Results: 2D, 3D interactions, bioavailability net









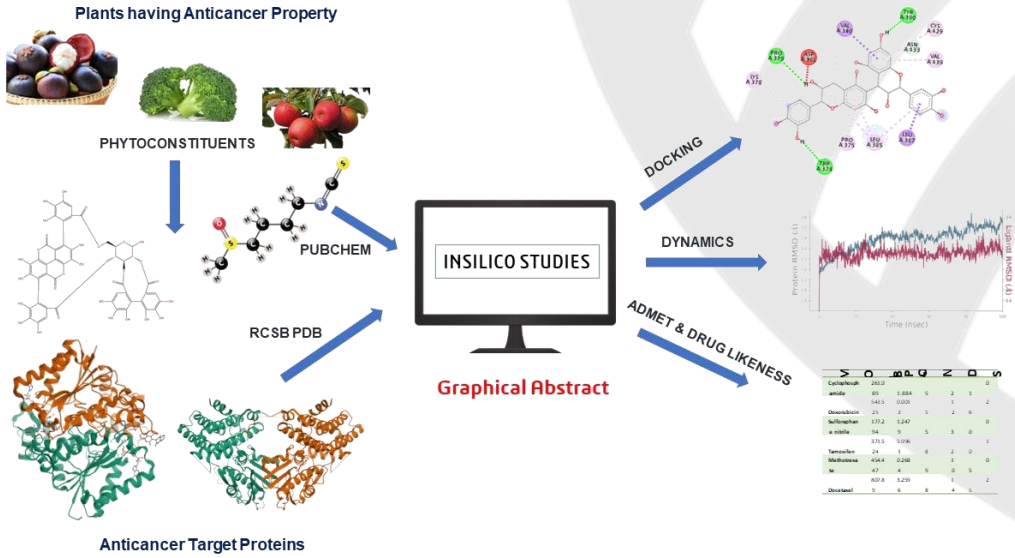
Docking studies: results

Screening of Phytochemicals as Potential Breast Cancer Inhibitors – A Multi-Targeted Computational Study

Students: Adrija Chowdhury, Farseena M, Govardhan K R, Mamillapalli Annapoorna, Nikita Singh, Rajenderaa S
Research Supervisor: Dr. AR Mahesh

Abstract: Numerous phytochemical substances have been used therapeutically to treat cancer conditions. The anticancer properties of isolated phytochemicals from various natural medicinal sources are well documented. The underlying mechanisms behind how these isolated elements exhibit their anticancer effects is particularly unknown. The goal of the current investigation is to suggest potential receptors for these phytoconstituents' binding. We investigated the molecular interactions utilizing *in-silico* molecular docking research with verified docking techniques to determine their potential binding mechanisms, in-silico ADME/T studies and validation of the hit compound with receptor through molecular dynamics studies. Further, validation of the identified hit molecules of this hypothesis by pharmacological evaluation would provide their effectiveness as a potential anticancer agent.

-



Graphical Abstract

Publications

1. Vellur, Senthilkumar, **Parasuraman Pavadai**, Ewa Babkiewicz, Sureshbabu Ram Kumar Pandian, Piotr Maszczyk, and Selvaraj Kunjiappan. 2023. "An In Silico Molecular Modelling-Based Prediction of Potential Keap1 Inhibitors from Hemidesmus indicus (L.) R.Br. against Oxidative-Stress-Induced Diseases" Molecules 28, no. 11: 4541. https://doi.org/10.3390/molecules28114541

2. Gade, Anushree Chandrashekhar, Manikanta Murahari, **Parasuraman Pavadai,** and Maushmi Shailesh Kumar. 2023. "Virtual Screening of a Marine Natural Product Database for In Silico Identification of a Potential Acetylcholinesterase Inhibitor" Life 13, no. 6: 1298. https://doi.org/10.3390/life13061298

3. Srivathsa Vidya Anjana, Sadashivappa Markuli Nandini, Hegde Krishnamurthy Apeksha, Radha Srimathi, **Mahesh Ramu Agasa**, Ammunje Nayak Damodar, Sen Debanjan, Theivendren Panneerselvam, Govindaraj Saravanan, Kunjiappan Selvaraj, **Pavadai Parasuraman**, A Review on Artificial Intelligence Approaches and Rational Approaches in Drug Discovery, Current Pharmaceutical Design 2023; 29(15) . https://dx.doi.org/10.2174/1381612829666230428110542

4. Arumugam, M., Shanmugavel, B., Sellppan, M., & **Pavadai Parasuraman**. (2023). In silico evaluation of some commercially available terpenoids as spike glycoprotein of SARS-CoV-2 - inhibitors using molecular dynamic approach. Journal of biomolecular structure & dynamics, 1–7. Advance online publication. https://doi.org/10.1080/07391102.2023.2201848

5. Rajeshkumar, R. R., **Pavadai Parasuraman**., Panneerselvam, T., Deepak, V., Pandian, S. R. K., Kabilan, S. J., Vellaichamy, S., Jeyaraman, A., Kumar, A. S. K., Sundar, K., & Kunjiappan, S. (2023). Glucose-conjugated glutenin nanoparticles for selective targeting and delivery of camptothecin into breast cancer cells. Naunyn-Schmiedeberg's archives of pharmacology, 10.1007/s00210-023-02480-y. Advance online publication. https://doi.org/10.1007/s00210-023-02480-y

6. Kabilan, S. J., Kunjiappan, S., Sundar, K., **Pavadai Parasuraman**., Sathishkumar, N., & Velayuthaperumal, H. (2023). Pharmacoinformatics-based screening of active compounds from Vitex negundo against lymphatic filariasis by targeting asparaginyl-tRNA synthetase.

Journal of molecular modeling, 29(4), 87. https://doi.org/10.1007/s00894-023-05488-6

7. Devi RN, Pounraj P, Kumar SB, Saral A, Vinnarasi JK, Vivek C, **Parasuraman P**, Irfan A, Muthu S. Electronic, intermolecular, quantum computational investigations, molecular docking and simulation studies of the potent antiviral drug EIDD-2801. Journal of the Indian Chemical Society. 2023 Mar 1;100(3):100953.

8. Vellur, S., **Pavadai Parasuraman**., Pandian, S.R.K. et al. Optimization of ultrasound-assisted extraction of bioactive chemicals from Hemidesmus indicus (L.) R.Br. using response surface methodology and adaptive neuro-fuzzy inference system. Food Sci Biotechnol (2023). https://doi.org/10.1007/s10068-023-01351

9. Chaitra R, Gandhi R, Jayanna N, Satyanath S, **Pavadai Parasuraman**, Murahari M. Computational design of MmpL3 inhibitors for tuberculosis therapy. Molecular Diversity. 2023 Feb;27(1):357-69.

10. Jabeen, **BV Suma.** Stability indicating UPLC-MS/MS method for quantification and identification of cefepime and its degradants in API. Journal of Applied Pharmaceutical Sciences. 2023; 13(5):199-207.

11. Kunjiappan S, Panneerselvam T, Pandian SR, **Pavadai Parasuraman**, Govindaraj S, Ravishankar V, Arunachalam S, Murugesan S. Nanoparticles for diagnosis and treatment of renal diseases. InEmerging Nanotechnologies for Medical Applications 2023 Jan 1 (pp. 95-130). Elsevier.

12. **Agasa Ramu Mahesh,** Josephine Leno Jenita. Designing multi-epitope vaccine for SARS-COV-2 through in-silico techniques. International Journal of Biology, Pharmacy, and Allied Sciences 12 (03) 2023

13. Somashekar M Metri, Maharani Bhandarakavathe, Shivanand Kolageri, Vishal Babar, Pratik P Maske, Prashant P Chavan, **Agasa Ramu Mahesh**. Novel Benzopyrole Derivatives: Design, Synthesis, and Molecular Docking Study as Potent Anti-Inflammatory Agents. **Eur. Chem. Bull. 2023**, 12(10), 1061-1077

Oral Presentations

1. **B V Suma** , Nayana J, Identification of Novel 2-mercapto benzimidazole Derivatives for the treatment of Breast Cancer: A Computational Approach, at International Conference on Latest Trends and Innovations in Pharmaceutical and Biosciences, Career Point School of Pharmacy, Career Point University, Kota Rajasthan on 18.03.2023

2. Nayana J **B V Suma** , Design of Novel 2-mercaptobenzimidazole Derivatives for the treatment of Prostate Cancer: An In-silico Approach at International Conference on Latest Trends and Innovations in Pharmaceutical and Biosciences, Career Point School of Pharmacy, Career Point University, Kota Rajasthan on 18.03.2023

3. Brundha SN, **B V Suma** In silico study on 1,3,4 thiadiazole derivatives tethered with isoniazid on her2 for anti-breast cancer activity at International Conference on Latest Trends and Innovations in Pharmaceutical and Biosciences, Career Point School of Pharmacy, Career Point University, Kota Rajasthan on 18.03.2023

4. Govardhan K R, Adrija Chowdhury, Farseena M, Mamillapalli Annapoorna, Nikita Singh, Rajenderaa S, **Agasa Ramu Mahesh**, Screening of phytochemicals as potential breast cancer inhibitors – A multi-targeted computational study., International Conference on "Multidisciplinary Approaches in Engineering, Science, Agriculture & Social Studies" (MAESASS-2023) 27 - 28 May, 2023

5. **Mahesh AR,** Sunil Kumar B. Aurones as an important scaffold for anticancer research - a computational approach. National Conference on "Drug Delivery and Translational Research, College of Pharmaceutical Sciences, DSU, Bengaluru on 17th March 2023.

6. Soundarya R , Shannon D Almeida , H R Sameera , Govardan , Golla Sireesha, Damodar Nayak A , **Parasuraman Pavadai.** Identification of Poly ADH-Ribose Polymerase-1 (PARP-1) inhibitors: An AI based Computational approach. 3rd International Congress on Biological and Health Sciences. 14th - 16th April 2023

7. Golla Sireesha, Soundarya R, H R Sameera, Govardhan K R, Shannon D Almeida, Damodar Nayak A, **Parasuraman Pavadai.** Identification of Carbonic Anhydrase IX Selective inhibitors: An AI based Computational approach. 3rd International Congress on Biological and Health Sciences. 14th - 16th April 2023

8. Srinivas G, Jeevitha Lokesh, Harish Kumar D R, Damodar Nayak A, **Parasuraman Pavadai.**

Identification Of Potential Lead for Aldose Reductase Enzyme in The Treatment of Cataract: A Computational and Experimental Approach. 3rd International Congress on Biological and Health Sciences. 14th - 16th April 2023

9. Govardhan K R, Golla Sireesha, Soundarya R, Shannon D Almeida, H R Sameera, Damodar Nayak A, **Parasuraman Pavadai.** Exploring the possible mechanism of Capsaicin in the Treatment of Breast Cancer: A Computational Approach. 3rd International Congress on Biological and Health Sciences. 14th - 16th April 2023

10. Shannon D Almeida, H R Sameera, Govardhan K R, Golla Sireesha, Soundarya R, Damodar Nayak A, **Parasuraman Pavadai.** Exploring the possible mechanism of a cystine moiety in the treatment of Parkinson's Disease – A Computational Approach. 3rd International Congress on Biological and Health Sciences. 14th - 16th April 2023

11. H R Sameera, Govardhan K R, Golla Sireesha, Soundarya R, Shannon D Almeida, Anbu J, Damodar Nayak A, **Parasuraman Pavadai.** Screening of Dunaliella salina moieties for Myocardial Infarction: A computational study. 3rd International Congress on Biological and Health Sciences. 14th - 16th April 2023

Workshop Attended

1. **Dr. Suma B V**, completed 10 days National workshop on Research Methodology in online mode from 04th June to 13th June 2023 conducted by Uudaan Educational Services

Invited Lectures

1. **Dr. Judy Jays** presented as a resource person in a National level Faculty development programme on “Mentor-mentee system – The current need” Positioning of essentials for perception on inspirational teaching and research for Novice Faculty in Pharmacy” organised by School of Pharmacy, Sri Balaji Vidyapeeth, Puducherry and Mother Theresa Post Graduate & Research Institute of Health Sciences, Puducherry in association with APTI, Tamilnadu branch from 4th to 25th April 2023.

2. **Dr. Judy Jays** presented as a resource person in an interactive session on Gender Sensitivity organised by Faculty of Physiotherapy, MS Ramaiah University of Applied Sciences, Bengaluru on 9th May 2023.

3. **Dr. Parasuraman P** presented as a resource person in One day workshop on "Computer Aided Drug Design" organised by Faculty of Pharmaceutical Sciences, PES University on 10.03.2023.

4. **Dr. AR Mahesh** presented as a resource person in One day workshop on "Computer Aided Drug Design" organised by Faculty of Pharmaceutical Sciences, PES University on 10.03.2023.

5. **Dr. AR Mahesh** presented as a resource person in webinar on "Basics of Computational Drug Design & QSAR-Bridging the Gap Between Molecules & Therapeutics" organized by Altem Technologies Pvt., Ltd., on 23rd June 2023

6. **Dr. Parasuraman P** presented as a resource person in One day workshop on "National Conference on “Emerging Trends in Biotechnology” organised by Mary Matha College of Arts and Science, Periyakulam, Theni, Tamil Nadu on 17.03.2023.

Awards

Congratulating Dr. Rajdeep Ray on successful Defence of PhD
A Visionary Thesis: "Development of Novel Indoles as Antitubercular Agents"

We are delighted to extend our warmest congratulations to Dr. Rajdeep for successfully defending his PhD thesis titled "Development of Novel Indoles as Antitubercular Agents." The remarkable achievement took place on the 3rd of April, 2023, marking a significant milestone in Dr. Rajdeep's academic journey.

Dr. Rajdeep's research work focused on exploring novel indole derivatives with potential antitubercular properties. His dedication to the field of pharmaceutical chemistry and tuberculosis research has brought new perspectives to the fight against this global health challenge. Guided by Experts: Dr. Gautham G. Shenoy and Dr. Raghu Chandrashekar H. The success of Dr. Rajdeep's PhD journey is a testament to the exceptional guidance he received from his esteemed mentors. Dr. Gautham G. Shenoy, Professor in the Department of Pharmaceutical Chemistry, Manipal College of Pharmaceutical Sciences, and Dr. Raghu Chandrashekar H., Professor and Head of the Department of Pharmaceutical Biotechnology, played instrumental roles in shaping Dr. Rajdeep's research and academic pursuits.Dr. Rajdeep's successful defense of his PhD thesis stands as a shining example of dedication, perseverance, and scholarly excellence. The findings from Dr. Rajdeep's research hold the promise of contributing to the development of effective antitubercular agents, addressing a pressing global health concern. His work showcases the potential of pharmaceutical research in combatting infectious diseases.

As Dr. Rajdeep embarks on the next chapter of his academic and professional journey, we are confident that his accomplishments will continue to inspire and lead to further advancements in the field of pharmaceutical research. The entire faculty and student community of the Department of Pharmaceutical Chemistry join hands in celebrating Dr. Rajdeep's success and wishing him a bright and prosperous future.

Congratulations, Dr. Rajdeep! Your achievement is a source of pride for us all.

Congratulating Dr. Parasuraman P for his Recognition as a Prominent Young Scientist

We are thrilled to extend our warmest congratulations to Dr. Parasuraman P, our esteemed Assistant Professor in the Department of Pharmaceutical Chemistry, for being honored with the Young Scientist Award at the International Conference on Multidisciplinary Approaches in Engineering, Science, Agriculture, and Social Studies.


Organized By — In Collaboration With

International Conference on
Multidisciplinary Approaches in Engineering, Science, Agriculture & Social Studies
(MAESASS-2023)

-: Organized By :-
Council of Research & Sustainable Development, India
Society of Education, India
Deptt. of Biochemistry, SLS, Dr. Bhimrao Ambedkar University, Agra
European Laser Academy, Germany

03rd- 04th June, 2023

The executive committee of conference bestow its

Young Scientist Award

presented to

Dr. Parasuraman. P
Assistant Professor, Department of Pharmaceutical Chemistry
Faculty of Pharmacy, M.S Ramaiah University of Applied Sciences

for outstanding contribution in the field of
"Pharmaceutical Chemistry"
on the occasion of International Conference held at
J. P. Sabhagar, Khandari Campus,
Dr. B.R. Ambedkar University, Agra

Dr. Manish Kumar, Convener, MAESASS-2023 | Dr. Deepmala Verma, Secretary, SOE-India | Dr. Mahesh Chandra, Managing Trustee, MAESASS-2023 | Dr. Michael Weber, Patron, MAESASS-2023

In Association with — In Collaboration with
College of Medicine, University of Hail, KSA
University of Agricultural Sciences, Raichur, Karnataka
Quantum University, Roorkee, Uttarakhand
School of Studies in Environmental Science, Jiwaji University, Gwalior, M.P.
Maharishi University of Information Technology, Lucknow, U.P.

Organized collaboratively by the Council of Research and Sustainable Development, India, the Department of Biotechnology at SLS Bhimrao Ambedkar University, Agra, and the European Laser Academy, Germany, the conference took place on 3rd and 4th June 2023. This prestigious recognition is a testament to Dr. Parasuraman's exceptional contributions and groundbreaking research in the field.

His innovative work in pharmaceutical chemistry has demonstrated a profound impact on the broader scientific community, and this award serves as validation of his dedication to advancing knowledge and addressing real-world challenges.

Dr. Parasuraman's passion for multidisciplinary approaches has enabled him to explore new horizons in various areas, including engineering, science, agriculture, and social studies. His collaborative spirit and commitment to excellence have undoubtedly set him apart as an outstanding young scientist.

As a department, we take immense pride in Dr. Parasuraman's accomplishments and are excited about the promising future his research holds. We congratulate him once again on this well-deserved recognition and look forward to witnessing more remarkable achievements in his career.

Please join us in celebrating Dr. Parasuraman P for his outstanding achievement and inspiring dedication to the field of pharmaceutical chemistry. We wish him continued success in his pursuit of knowledge and excellence.

Congratulations, Dr. Parasuraman P!

Departmental Events

"Recent Developments in Pharmaceutical Analysis (RDPA)"

The Department of Pharmaceutical Chemistry at the Faculty of Pharmacy hosted a highly enlightening and insightful one-day seminar on "Recent Developments in Pharmaceutical Analysis (RDPA)" on the 28th of April, 2023. The seminar was held in a hybrid mode, blending the best of both onsite and online participation, and it left a lasting impression on attendees from various colleges across India. Renowned experts from diverse pharmaceutical industries graced the occasion, adding a wealth of knowledge and experience to the event. The distinguished lineup of speakers included:

Dr. Prabhakran. D, Vice-President, *In Vitro* Research Solutions Pvt Ltd., Dr. Kumaravel. S, Head, Analytical Department, Bioplus Life Sciences Ltd., Dr. Syed Salman Lateef, Head, Testing and Services Lab, Wipro Life Sciences Ltd., Mr. Ashwani Gaur, Senior Principal Scientist - DMPK, Syngene International Ltd.,

The primary focus of the seminar was to delve into the applications of cutting-edge technologies in pharmaceutical analysis. The speakers shared valuable insights, highlighting the current trends and advancements in the drug discovery and development process. This emphasis on technological advancements aimed to foster innovation and shape the future of pharmaceutical analysis in the industry.

As a Guiding Light in the Journey of Innovation, the seminar was honored to welcome Dr. J. Narshima Murthy, Director of Scinva

Chemicals and Pharmaceuticals Pvt Ltd, as the esteemed Chief Guest. Dr. Murthy delivered an inspiring keynote address, illuminating the path towards progress in pharmaceutical analysis. His invaluable expertise and vision provided a significant impetus to the discussions during the seminar.

Adding further weight to the event, Dr. Kuldeep K Raina, Vice-Chancellor of RUAS, graced the occasion with his presence and delivered a special address. His encouragement and support bolstered the spirit of collaboration and learning. Dr. S. Bharath, Dean of FPH, extended a warm welcome to all the delegates, acknowledging their active participation both onsite and online.

The success of the seminar would not have been possible without the dedication and efforts of Dr. Harish Kumar, Head of the Department of Pharmaceutical Chemistry. He expressed his sincere gratitude to all participants, speakers, and organizers in a heartfelt vote of thanks, truly encapsulating the spirit of appreciation and camaraderie.

The response to the seminar was overwhelming, with a total of 160 registrations from students, faculty members, and professionals representing various colleges across India. The sheer enthusiasm and engagement of the participants underscored the importance and relevance of the topic, further igniting the flame of curiosity and passion for advancement in pharmaceutical analysis.

The One-Day Seminar on "Recent Developments in Pharmaceutical Analysis (RDPA)" marked a momentous occasion in the academic calendar. The insights shared, discussions held, and connections made during this event will undoubtedly propel the future of pharmaceutical analysis in drug discovery and development. As the Faculty of Pharmacy, we are immensely proud to have hosted such an enlightening seminar, and we look forward to bringing more enriching experiences in the pursuit of knowledge and innovation.

The Department of Pharmaceutical Chemistry Congratulate Dr. Lakshmi Sundar and Dr. Parasuraman P for their effort in organizing such an astonishing event.

"FROM DISTRESS TO DE-STRESS"

The Department of Pharmaceutical Chemistry, in association with esteemed guest speaker Smt. Anusuya R Kashi, organized an enlightening guest lecture on "FROM DISTRESS TO DE-STRESS." The event took place on the 3rd of May, 2023, at the SS Block, attracting 60 students and staff members from the college.

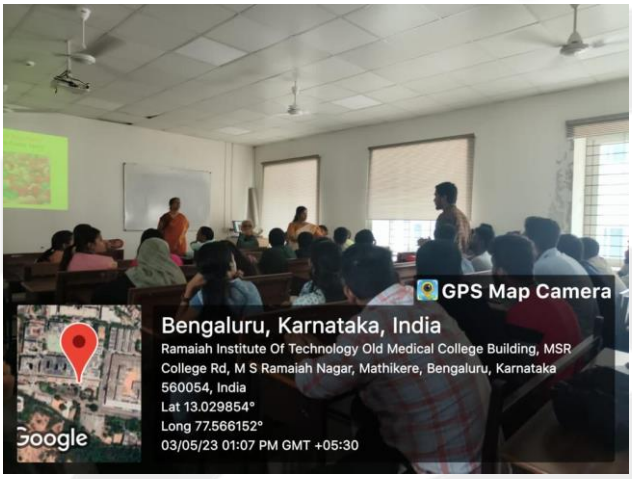
A Remarkable Speaker with a Wealth of Experience Smt. Anusuya R Kashi is an Assistant Professor at Vivekananda College of Pharmacy, Bengaluru, where she has dedicated 23 years to shaping young minds through her passion for teaching. In addition to her academic achievements, she holds an M S in Counselling and Psychotherapy from Kuvempu University, Shivamogga, a testament to her commitment to helping others through counselling.

As an expertise in Life Skills Education and Counselling Smt. Anusuya's dedication to helping others extends beyond the classroom. She is a trained Life Skills Educator from NIMHANS, Bangalore, equipping her with the skills to empower individuals with essential life skills. Additionally, her training as a Lay Counsellor at Prasanna Counselling Centre, Bangalore, has honed her ability to offer empathetic and effective counselling to those in need. With a rich history of 15 years of counselling young adults, Smt. Anusuya has positively impacted the lives of many. Her commitment to mental well-being has led her to volunteer as a student counsellor for college students in workshops conducted by the Bengaluru-based NGO, DISHA Charitable Trust for Value Initiatives. Beyond her role as an educator and counselor, Smt. Anusuya is also a freelance writer, delving into topics related to health and wellness, parenting, and spirituality. Her engaging speaking style has made her a sought-after speaker in these domains.

During the guest lecture on "FROM DISTRESS TO DE-STRESS," Smt. Anusuya shared valuable insights on managing stress and promoting mental wellness. The audience, comprising students and staff, benefited greatly from the session, gaining practical ideas on how to navigate through challenging times and find solace in times of distress.

The success of the event was made possible by the able coordination of Dr. Judy Jays, Associate Professor in the Department of Pharmaceutical Chemistry. Her efforts in organizing the guest lecture ensured that students and staff alike could participate and derive maximum value from the session.

We express our gratitude to Smt. Anusuya for sharing her expertise and valuable insights with us. Let us continue to work together towards a mentally resilient and healthier campus.



"Beyond Academics"

The Department of Pharmaceutical Chemistry proudly hosted an inspiring alumni guest lecture on the 8th of April, 2023, featuring the esteemed speaker, Ms. Pretisha Flora Cutinho. Ms. Cutinho, an alumna of the department, has been associated with IQVIA, an American multinational company that specializes in health information technology and clinical research, for the past 3.5 years.

A Journey of Empowerment: Learning from Experience, during the captivating session on "Beyond Academics," Ms. Cutinho shared her remarkable journey, starting from her childhood experiences to her current professional endeavors. Drawing from her own life, she touched upon several invaluable aspects of personal and professional growth.

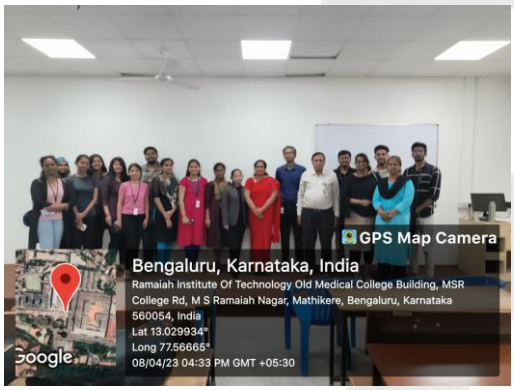
The guest lecture emphasized essential skills and mindsets that transcend academics and contribute to holistic development. Ms. Cutinho shed light on self-learning, problem-solving, cultivating a growth mindset, fostering creative and critical thinking, and recognizing the value of extracurricular activities.

As an insight of Influence and Emotional Intelligence, Ms. Cutinho underscored the significance of influencing with impact, learning from experiences, and nurturing emotional intelligence. These qualities, she highlighted, play a pivotal role in shaping successful careers and building meaningful relationships. Acknowledging the importance of cultural competence and literacy, Ms. Cutinho encouraged students to embrace diversity and expand their knowledge beyond their field of study. Such qualities, she emphasized, not only enrich personal lives but also promote understanding and inclusivity.

The guest lecture witnessed enthusiastic participation and an Interactive Session: Bridging the Gap, with around 90 undergraduate students and 20 postgraduate students attending the session. The interactive nature of the talk allowed students to engage directly with Ms.

Cutinho, seeking insights and advice from her wealth of experience.

The success of this impactful event was made possible by the dedication and coordination of Dr. BV Suma, Associate Professor in the Department of Pharmaceutical Chemistry. Her efforts ensured that students had the opportunity to benefit from the wisdom and experiences shared by the esteemed alumna.



Beyond academic success, the Department of Pharmaceutical Chemistry strives to empower students. Guest lectures from accomplished graduates, such as Ms. Pretisha Flora Cutinho, give essential information and motivation to our aspiring leaders.

We extend our heartfelt thanks to Ms. Cutinho for sharing her journey and wisdom with us. Let us embrace the lessons from this enlightening session and strive to become well-rounded individuals ready to make a positive impact in the world.

Upcoming Event

RAMAIAH UNIVERSITY OF APPLIED SCIENCES | FACULTY OF PHARMACY

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY

Organizes One Day

INTERNATIONAL E-CONFERENCE

on

Exploring the Frontiers of Insilico Drug Discovery: Trends, Challenges and Opportunities

28th July 2023

Core Areas

- AI & ML in Drug Design
- Pharmacophore Modelling
- Virtual Screening
- QSAR/QSPR Modelling

Resource Persons

Prof. Ravichandran V
Head,
Faculty of Pharmacy,
AIMST University, Malaysia

Dr. Chandrabose Selvaraj
Associate Professor
Saveetha University,
Chennai, India

Dr. Akshatha Ganne
Post Doctoral Fellow
University of Arkansas for
Medical Science, USA

RAMAIAH UNIVERSITY OF APPLIED SCIENCES | FACULTY OF PHARMACY

Celebrating 31 Years of Excellence

Patron

Dr. M. R. Jayaram
Hon'ble Chancellor
RUAS

Advisory Committee

Dr Kuldeep Kumar Raina
Vice Chancellor
RUAS

Dr. Om Prakash Kharbanda
Pro- Vice Chancellor
(Health Sciences) RUAS

Dr. G. S. Venkatesh
Registrar
RUAS

Convener

Dr. S. Bharath
Dean, FPH, RUAS

Organizing Secretary

Dr. Harish Kumar D R
Professor and Head
Department of Pharmaceutical Chemistry
FPH, RUAS

Organizing Co-ordinators

Dr. Parasuraman P
Assistant Professor
Dept. of Pharmaceutical Chemistry
FPH, RUAS
+91 9629396767

Dr. A R Mahesh
Assistant Professor
Dept. of Pharmaceutical Chemistry
FPH, RUAS
+91 8892941706

About the Conference

The International e-Conference on Exploring the Frontiers of Insilico Drug Discovery: Trends, Challenges, and Opportunities is a virtual event focused on the latest advancements and challenges in *insilico* drug discovery. This conference brings together researchers, professionals, and experts from around the world to exchange knowledge and insights. With keynote presentations, panel discussions, and research paper presentations, the conference explores cutting-edge trends and technologies in areas like machine learning, molecular docking, and virtual screening. It offers networking opportunities and encourages collaborations among participants. The conference aims to foster innovation and contribute to the progress of in silico drug discovery methodologies and applications.

Scientific Presentations

We invite abstract for E-Poster from research scholars, faculty scientists and industry professionals from India and across the world. Abstracts are invited on following scientific topics for e-poster presentations. Perspective authors are encouraged to present their original, unpublished research work, and the selected abstracts will be called for poster presentations. Abstract up to 300 words in Calibri with font size 12pts, 1.5 line spacing may be submitted in .doc/.docx file with the author's name (presenting author name to be underlined), affiliation and corresponding author email ID.

About Ramaiah University of Applied Sciences

Ramaiah University of Applied Sciences (RUAS) is a private university established by an Act of the State of Karnataka, India, sponsored by the Gokula Education Foundation. Ramaiah University is an innovation university that focuses on academics, research, consultancy, training and leadership development. The university offers outcome-based multidisciplinary education in the domains of medical, paramedical, engineering, life sciences and social sciences. RUAS is oriented towards student-centric professional education and services with applied research whilst maintaining the highest academic and ethical standards in a creative and innovative environment. RUAS inspires critical thinking, personal development, and a passion for lifelong learning. This university has been rated as a "FIVE STAR" Institution by the Karnataka State University Rating Framework (KSURF) – 2019 Government of Karnataka

About Faculty of Pharmacy

Faculty of Pharmacy (FPH), formerly M.S. Ramaiah College of Pharmacy, was established in 1992. The Faculty of Pharmacy, ranked 65 in the AIR-NIRF 2023, is a leading Pharmacy college with 30 years of legacy. It imparts outcome based pharmaceutical education to meet our country's growing demands of well-trained healthcare professionals. The faculty offers a 4-year undergraduate programme - Bachelor of Pharmacy degree (B. Pharm), 2-year Postgraduate programme - Master of Pharmacy degree (M. Pharm) in Pharmaceutics, Pharmacology, Pharmaceutical Chemistry, Pharmacognosy, and Pharmacy Practice, 6-year Doctor of Pharmacy degree (Pharm D), and Doctoral research programme (Ph.D.).

About the Department of Pharmaceutical Chemistry

Department of Pharmaceutical Chemistry was originally established as a part of M S Ramaiah College of Pharmacy. PG program in Pharmaceutical Chemistry was started in the year 2008. The department was integrated into Faculty of Pharmacy in 2014. The department provides outcome-based education and training skills on various aspects of drug design using bioinformatics and computational tools, synthesis by conventional and green chemistry approaches, spectral characterization, and pharmacological evaluation of small molecules. Moreover, students get practical training in handling various analytical instruments including UV-Visible spectrophotometer, FT-IR, Flame photometer, HPLC, HPTLC and GPU Computational Lab.

Student Achievements

Management & Staff, Faculty of Pharmacy
Congratulates All India Rankers in Graduate Aptitude Test (GPAT) 2023

Ankur Shetty
(19PHPH009007)
AIR: 224

Arun Kumar C
(20PHPH009015)
AIR: 250

Rakesha
(19PHPH009057)
AIR: 740

Kushboo. B
(20PHPH009037)
AIR: 921

Abhishek Kumar Mali
(20PHPH009001)
AIR: 2015

Sudatt Dixit
(19PHPH009303)
AIR: 2065

Arun Kumar H S
(19PHPH009011)
AIR: 2152

Ranodeep
(19PHPH009059)
AIR: 2221

M Rashikamani
(19PHPH009032)
AIR: 2771

Tejas Kumar A
(19PHPH009080)
AIR: 3943

Amulya Sharon
(19PHPH009004)
AIR: 4620

Arun Kumar M
(19PHPH009012)
AIR: 9218

Swathi D. N
(19PHPH009077)
AIR: 9331

RAMAIAH UNIVERSITY OF APPLIED SCIENCES | Faculty of Pharmacy

Faculty of Pharmacy
Department of Pharmaceutical Chemistry

CHEMID

A Quarterly E-Newsletter

Volume II

Issue II

Write your feedback & Suggestions to
Editor-in-Chief/ Editors, CHEMID
✉: chemid.fph@gmail.com
Department of Pharmaceutical Chemistry
Faculty of Pharmacy, MSRUAS,
Gnanagangotri Campus, New BEL Road,
Bengaluru-560054