RAMAIAH UNIVERSITY OF APPLIED SCIENCES | Faculty of Pharmacy

CHEMID

E-Newsletter

Volume II Issue I March - 2023

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

100th Birth Anniversary of Dr. MS Ramaiah

1922-2022

By Legendries about Karmayogi Dr. MS Ramiaiah on his Birth Anniversary

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Editorial Note

Dear Readers,

CHEMID Volume II, Issue I, at the outset signifies the centenary birth celebration of Karmayogi Mathikere Sampige Ramaiah, a renowned educationist, philanthropist, infrastructure visionary, industrialist, and a pioneer in creating several landmark infrastructure projects in India. We would like to honor his immense contributions to Organisational development and express our gratitude for his inspiring vision and tireless dedication.

We welcome the new appointments of the Pharmaceutical Chemistry department, Mrs. Vijayalakshmi S and Mr. Rajdeep Ray. We are excited to have them onboard and look forward to their contributions.

We'd also like to express our appreciation to all our students who achieved outstanding results in the semester end examination. Your hard work and dedication are admirable.

We are grateful to the college authorities for their support and trust in us and hope to continue to live up to their expectations. We, at the Department of Pharmaceutical Chemistry, are committed to the holistic development of our students and we strive to make them industry-ready professionals.

Finally, we'd like to commend our staff and students for their contributions in publications and presentations in the last quarter. Your efforts are greatly appreciated.

We look forward to a successful future with all of you!

Editor in Chief
Dr. Harish Kumar DR

Contents

Welcoming New Departmental Faculty

Mrs. Vijayalakshmi S is an Assistant Professor at the Department of Pharmaceutical Chemistry under the Faculty of Pharmacy at RUAS. She is an alumni of the institute having completed her B.Pharm and M.Pharm here. She also holds a PG Diploma in Patents law from NALSAR University, Hyderabad and is currently working on completing her Ph.D. from KLE University with a research focus mainly on synthetic chemistry.

Mrs. Vijayalakshmi S
Assistant Professor

Her experience includes working as a Research associate with Analytica Chemie Inc, Bangalore in Scientific Support Division of R & D and as an Assistant professor in East West college of Pharmacy. She has expertise in preparation of schemes by searching literature in Sci-finder, Reaxys, Patent search for Active Pharmaceutical Intermediates or impurities as reference standards. She also has hands on experience of in-vitro anticancer studies (cell line studies) related to Ph.D. from IBAB, Bengaluru. Her research interests are varied in nature and include AI based drug discovery, computer aided drug design and synthesis and evaluation of new chemical entities. She is also a Registered Pharmacist under Karnataka State Pharmacy Council.

Mr. Rajdeep Ray
Assistant Professor

Mr. Rajdeep Ray is currently working as an Assistant Professor for the Department of Pharmaceutical Chemistry in Faculty of Pharmacy, Ramaiah University of Applied Sciences. He has completed M. Pharm from Manipal College of Pharmaceutical Sciences in 2015. He has also worked in synthetic R&D lab in the industry. His research interests lie in Antitubercular Drug Discovery, Antiviral Drug Discovery, Synthetic Chemistry, and Computational Chemistry. He is proficient in multi-step drug synthesis and purification techniques like column chromatography, crystallization etc. He is also adept in using computational packages like Schrodinger Suite, Gromacs, Autodock, Sybyl, Pymol etc. He has published several articles in Scopus-indexed journals of high reputation.

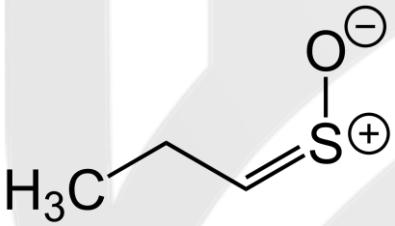
Chemistry In Everyday Life

Tanya, I M.Pharm

Whatever we do, starting from morning to evening we all are surrounded by chemistry. Chemistry is not limited to labs and laboratories, it's more than that.
Rising the question from why we get tears while cutting onions to why the octopus's blood is blue everything consists of chemistry. And many more examples in our day-to-day work which comprises of chemicals.

Why do you cry while cutting onions?

The tears roll out while chopping onions is due to the chemical irritant present known as syn- Propanethial-S-oxide.

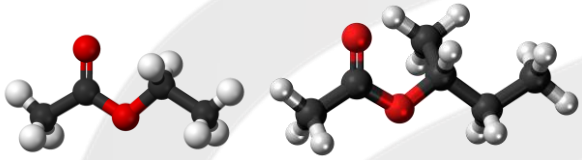


Tooth paste contains…..

The toothpaste we use for cleansing teeth mostly consist of Fluorides. The most common form is Sodium Fluoride, but mono-fluoro-phosphate and stannous fluoride are used.

Nail Polish contains…..

The most common cosmetics the women or girls fond of i.e., Nail Polish comprises of Ethyl acetate and Butyl acetate which gives nail polish its characteristics smell.



Emotions

All Human Beings are made of different types of emotions. Whether love, hate, envy, jealousy are mixed emotions present in humans. These all also arise in the body due to different chemicals present.

GABA(Gamma amnio Butyric acid)has the ability to calm us down.

Endorphins-Helps to relieve pain and also stimulated by Laughter.

Hair Dyes

Hair dyes which help to make our hair beautiful consist of different chemicals which gives them the vibrant colours. The chemicals include Hydrogen peroxide, Ammonia, Parabens, Lead acetate, Resorcinol.

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Green Chemistry: Microwave Assisted Organic Synthesis

B. Sunil Kumar, III M.Pharm

Green chemistry is an operation which is used to reduce or eliminate the generation or usage of hazardous substances in the manufacturing, and application in chemical products. Green chemistry is a set of 12 principles that helps in eliminates the hazardous substance in the chemical produce. The principle of green chemistry as follows.

1) Prevention of waste that is development of zero waste technology in the chemical manufacturing, it is beer to prevent waste in designing than the curing of waste.

2) Atom economy in synthetic method should be designed in such a way that 100% incorporation of starting materials in the final product.

3) The synthetic method can be developed to generate less/nontoxic substance.

4) The final product from the synthesis should have maximum functionality and less toxicity.

5) The use of auxiliary solvent should be made unnecessary wherever possible and harmless when used.

6) The use of energy in the synthetic should be minimum it should consider a environment and economic contact.

7) Raw material should be renewable wherever possible.

8) Unnecessary derivatization should be minimized as possible as it should cause the addition steps (protection and deprotection) in the process and also cause waste.

9) Use of catalytic reagent instead of stoichiometric reagent.

10) The product should fulfill the activity and later it should be degraded into harmless and no effect on the environment.

11) In the development of chemical products, the continuous process monitoring and control the formation of harmless substance.

12) Safer chemistry where in usage of raw materials should not cause any chemical accident, explosion, and fire attacks.[1-4]

Large scale organic synthesis which utilizes basic chemical ingredients and some catalysts, and later reaction complete, separation, purification, storage, packaging and distribution. In the convention method which is used in organic synthesis which cause increase in the heating time, difficultly in operation setup, excess utilization of solvents and cost efficient. During this process additional caring and safety towards workers and also cause the environmental damage due to explosion of waste (byproducts). Green chemistry has ability to increase the efficiency of synthesis method mainly helps in use of less toxic solvents, decrease in steps in synthesis routes and reduce the waste in synthesis.

Microwave is a very important technique in green chemistry, and it is eco-friendly. Because microwaves

cause direct impact on the reactant molecules and cause thermal conductivity which leads to rapid increase in the temperature, microwave radiation is utilized to work on organic synthesis. Microwave heating the molecule should be dipole in nature. The dipoles exert the electric field by aligning the dipoles with the field by rotation. The electric field which inverses each altered and therefore the dipoles move and cause inverse electric field. Characteristics induce rotation and friction between the diploes which produce homogenous heating. Microwave radiation i.e., 300-3000000 mHZ. MW is proportional to the dielectric properties of substance, dielectric constant (ε') and dielectric loss (ε"). The conversion of electromagnetic energy to heat energy at frequency is given by formula: ε'' / ε' = tan δ

Where δ=dissipate, ε'=dielectric constant, ε" =dielectric loss

Mechanism of Microwave

Since different materials respond differently to microwave radiation, not all materials are vulnerable to microwave heating. Materials can respond based on the approach of microwave radiation on the molecules.

1) Material which transparent the MW, e.g. sulphur
2) Material which reflect MW, e.g. copper
3) Material which absorb MW, e.g. water

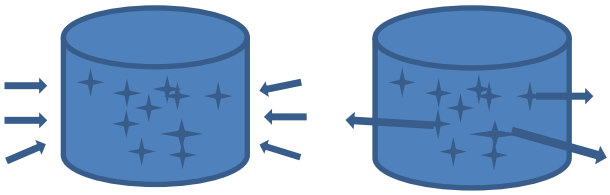
The heating of microwave absorbing materials involves two primary distinct mechanisms: dipolar polarization, conduction mechanism. Microwave absorbing materials are of the utmost importance for microwave chemistry.

Dipolar Polarization: MW irradiation of a molecule which generates the heat by possessing a dipole-moment of the molecules. When a dipole tries to reposition itself in relation to an alternating electric field, it heats up due to the electric field component of the microwave radiation rather than the magnetic field component; and loses energy in the form of heat by molecular friction. Dipolar polarization can produce heat either by the interaction of polar solute molecules like ammonia and formic acid, or through the interaction of polar solvent molecules like water, methanol, and ethanol. A crucial prerequisite for dipolar polarization is that the oscillating field's frequency range be suitable for enabling sufficient inter-particle interaction. A polar molecule's motion will be stopped by intermolecular forces if the frequency range is too high, preventing it from trying to follow the field and leading to insufficient inter-particle interaction. The polar molecule has enough time to align itself in phase with the field, however, if the frequency range is low. Microwave radiation oscillates polar particles and allows for sufficient inter-particle interaction at the right frequency (0.3–30 GHz). As a result, it is the best option for warming polar solutions.

Conduction Mechanism: Heat is produced by the conduction mechanism through resistance to an electric current. Electrons or ions in a conductor oscillate as a result of the fluctuating electromagnetic field, creating an electric current. There is internal opposition to this current, which heat the conductor. Because of the ability to believe that the more polar the solvent, the more readily the microwave irradiation is absorbed and the higher the temperature obtained, a solution containing ions, or even a single isolated ion with a hydrogen bonded cluster, will move through the solution under the influence of an electric field, resulting in energy expenditure. When the irradiated sample is an electrical conductor, the charge carriers (electron, ions, etc) move through the material under the influence of the electric field, producing polarization. Any electrical resistance will result in heating from these induced currents in the sample. The method's main drawback is that it cannot be used with materials

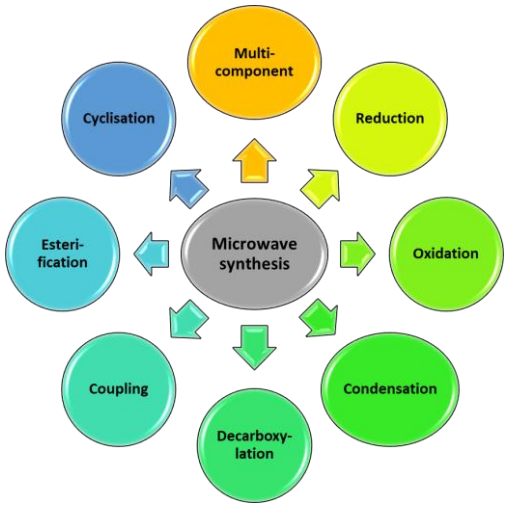
with high conductivities, so these materials reflect the majority of incident energy.5-6

Microwave Versus Conventional Synthesis: In conventional synthesis method he furnaces, or oil bath are used to produce heat to the vessel and later transfer into the reactant molecule. To achieve the required temperature for the synthesis by conventional method it takes much longer time. And in microwave assisted synthesis the radiation penetrates inside the reactant and produces heat by interacting with microwave radiation and the reactant molecule. MW has more advantages than the conventional method in increasing the rate reaction, high yield, solvent free, less time consuming. Specifically, lead creation, hit-to-lead efforts, and lead optimization are three main steps of the drug development process where microwave synthesis has the potential to influence medicinal chemistry activities.[7-8]



CONVENTIONAL METHOD MICROWAVE METHOD

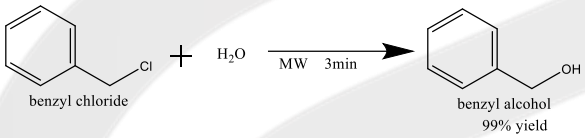
Applications of Microwave Synthesis:



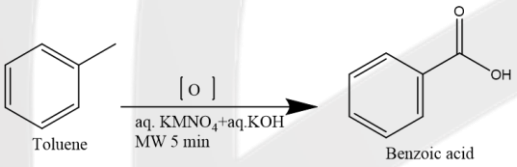
1) Using solvents 2) Solvent free conditions

Using solvents[9]

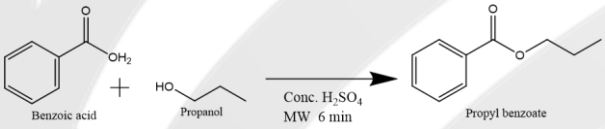
a. Hydrolysis: Benzyl chloride undergoes hydrolysis in presence of water which gives benzyl alcohol where conventional heating it requires 35 min to complete the reaction in microwave oven, I completes in 3 min and 97% of yield.



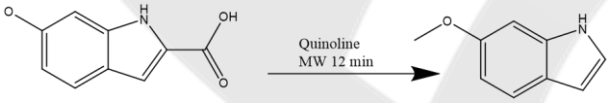
b. Toluene undergoes oxidation in presence of KMnO4 in normal condition it requires 10-12 hr of reflux for completing the reaction, where in microwave condition it requires just 5 min, and the yield is 40%.



c. The combination of benzoic acid and n- propanol on heating in a microwave oven for 6 min in presence of catalytic amount of conc. Sulfuric acid gives propylbenzoate



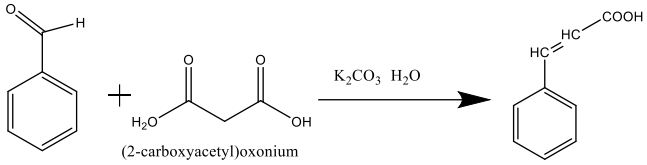
d. The decarboxylation of carboxylic acids involves refluxing in quinoline and in presence of copper chromate and the yields is low. However, in the presence of microwaves decarboxylation takes place in much shorter time.



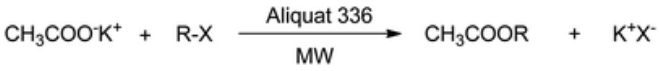
Solvent free condition:

a. Using solid liquid phase: in knoevenagel condensation between carbonyl compounds and active methylene

compounds, such as malonic acid, using tetrabutylammonium bromide, potassium carbonate in water forming unsaturated acids in excellent yield and purity under microwave irradiation.



b. Using equal amounts of salt and alkylating agent in presence of methyltrioctylammonium chloride (10% mol), Loupy reported that potassium acetate may be alkylated in the absence of a solvent in a conveyor oven in 1993. No matter the chain length, kind of halide leaving group, or scale, yields are nearly quantifiable in 1-2 min (up to 500 mmol).[10]



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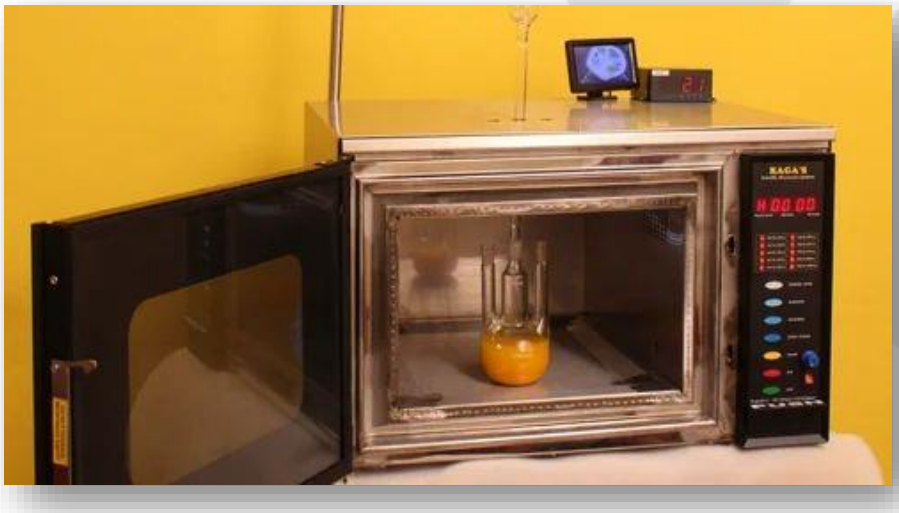
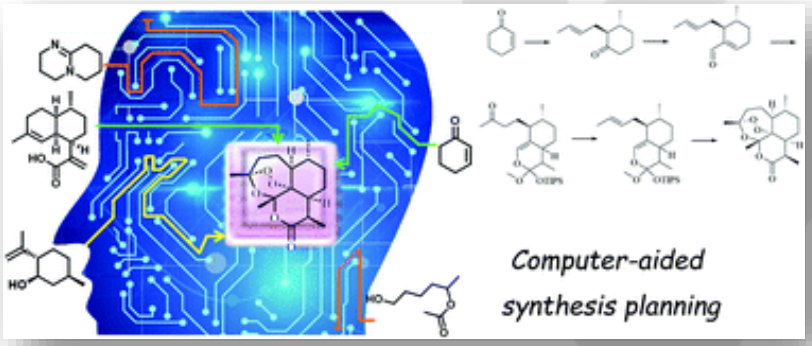


Essentials of Computer–Aided Synthesis Planning (CASP)

Shreya Shet, I M.Pharm

As we all know, the development of new drugs is a tedious and expensive process, spanning numerous years and costing billions of dollars. As of now, on an average, up to half of the cost is being spent in the pre–clinical phase. Moreover, there is an omnipresent and urgent need to come up with new therapeutics to resolve the quagmire of dreadful diseases that have been afflicting humanity for long. Therefore to solve such an issue as early as possible, there is a need to reduce the vast timeline of drug development; this is where automation and computerization play a major role. They ensure the reduction of the time taken to complete major tasks in drug discovery as well as ensure better accuracy and precision of the results, which is also necessary to avoid loss of time, effort and money spent in research due to failure from errors in the results.



In this aspect, Computer Aided Drug Design (CADD) is a technique, very familiar to us. This assists us in performing hit–to–lead discovery and lead modification with maximum precision and accuracy and within the shortest time possible. But that same drug must be readily available for testing and actual administration to the users. For that, there must be a synthetic route for the drug which is feasible, quick, and safe. Therefore, there is another computer–aided technique, which is 'Computer Aided Synthesis Planning (CASP)' which is a blooming and increasingly popular technique, besides CADD.

CASP involves an automated retrosynthetic analysis of a drug molecule, essentially with the help of machine learning algorithms. An ideal CASP program takes a molecular structure as the input and displays a sorted list of detailed reaction schemes, each of which connects that molecule all the way back to purchasable starting materials via a series of chemically feasible reaction steps. These schemes are arranged according to various criteria such as complexity, feasibility, eco-friendliness, cost–effectiveness, the yield of the molecule etc. There is more than one approach to derive the most suitable synthetic pathway for the molecule: that is conducting molecular similarity studies, application of transition-state theory, usage of artificial neural networks etc. The usage of artificial neural networks is the most popular approach. It enables the user to predict which transformations a given molecule can undergo. Similarly, to the retrosynthetic analysis step, a distinction can be made between the older rule–based or heuristic methods of synthesis planning and more fuzzy methods, usually based on these neural networks. Irrespective of the approach, reactions that cannot be performed in practice or that lead away from the target molecule are eliminated. Again, the machine learning approach can be based on template-based models or

template–free models. Template–based approaches match the input molecules to the entire template library by solving a subgraph isomorphism problem to obtain candidate reactants. On the other hand, template-free approaches utilize text representation of molecules (SMILES or InChI) to cast the retrosynthesis problem as a sequence-to-sequence prediction problem. Transforming target molecules to reactants becomes a translation task that converts the SMILES string of a product to that of reactants.

As of 2023 numerous CASP platforms have been launched. The most popular ones are SYNTHIA, AiZynthFinder, ICSYNTH and ASKCOS.

Therefore, computer-aided synthesis planning has the potential to revolutionize and maybe even redefine a scientist's approach towards synthetic chemistry and even significantly accelerate the discovery of new molecules. This makes CASP a promising area of research to expand the capabilities of this technique as much as possible to further speed up the drug development process.

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PG/UG Projects Submitted

LEAD IDENTIFICATION FOR ALDOSE REDUCTASE ENZYME: A COMPUTATIONAL AND EXPERIMENTAL APPROACH

Student: Jeevitha Lokesh
Research Supervisor: Mr. Damodar Nayak A, Dr. Parasuraman Pavadai

Abstract:

Aldose reductase is a vital enzyme involved in the polyol pathway responsible for the development and progression of diabetic cataract by accumulation of excess of sorbitol. It is one of the leading causes of visual impairment and blindness globally. Despite variety of drugs have been developed to inhibit the aldose reductase enzyme; however, they are associated with numerous adverse effect and poor pharmacokinetics. Thus, there is a need for new drug to inhibit aldose reductase enzyme to treat diabetic cataract. Drug repurposing is a method used for identifying new therapeutic use for already existing drugs that have been approved for other diseases. Hence, the present study focuses on repurpose the FDA approved drugs for their inhibitory action on ALR enzyme by using in silico and in vitro approach to treat cataract. Docking was performed using Autodock vina. ADMET and drug likeness properties was predicted by 'pkCSM'. Molecular dynamics simulation is carried out for top most complex using DESMOND software. Anti-Cataract activity was evaluated by estimating the Bio-chemical parameters such as MDA, Total protein content, Aldose reductase, Catalase, GSH, and sorbitol level in the goat eye lenses. Molecular docking results indicated Lipoic acid, Caffeine and Torsemide have good binding affinity towards aldose reductase enzyme -11.6Kcal/mol- 11.2 kcal/mol like that of standard drug Liderostat. These drugs showed acceptable ADMET Properties and satisfied Lipinski rules of five. MD analysis showed better stability with the target protein and produced the significant results in the in vitro analysis by inhibiting the aldose reductase enzyme. Among them Torsemide shows higher percentage of inhibition than Lipoic acid and Caffeine.

Keywords: Drug repurposing; Aldose reductase; Molecular docking; Molecular Dynamics.

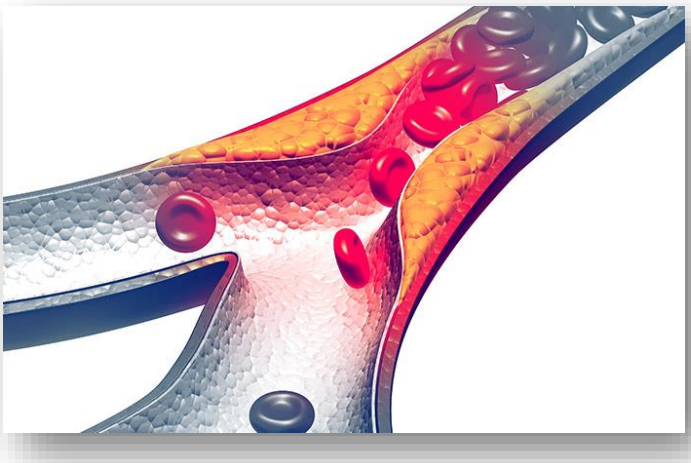
EXPLORING THE ANTI-INFLAMMATORY ACTIVITY OF LP-PLA2 INHIBITORS BY IN-SILICO METHOD

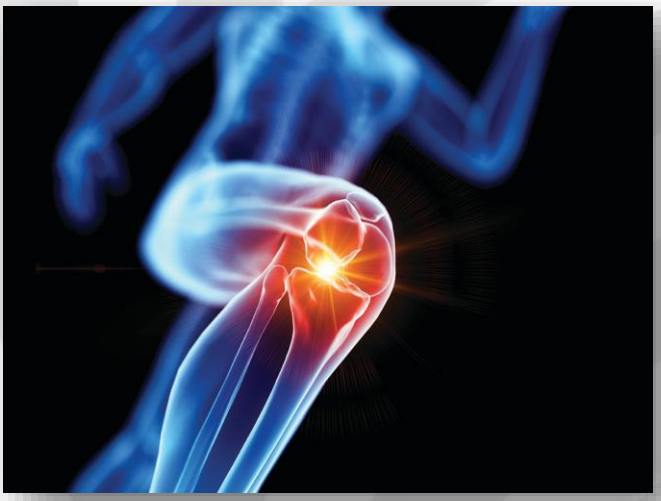
Students: Jhansi Laxmi, Kirthi Bhushan, Manasa Kuruba, Merina Elizabeth Mathew, Sahana H U and Shraddha Hegde
Research Supervisor: Dr. Lakshmi M Sundar

Abstract:

Lipoprotein-associated phospholipase A2(Lp-PLA2) enzyme is one such specific target which is produced by the inflammatory cell and is associated with the proinflammatory mediators of the atherogenic process Computational methods could be one of the best alternate approaches to identify novel compounds due to its easy and broader applications. Thus, the present study focuses on the In-Silico methods to explore inhibitors of LP-PLA2 for anti-inflammatory activity.

Keywords: Chronic inflammation, Human LP-PLA2, In-silico, anti-inflammatory, Darapladib.





Anjana Vidya Srivathsa, I Sem M.Pharm

MACHINE LEARNING APPROACH ON LEAD IDENTIFICATION FOR POTENT ANTI-CYSTIC FIBROSIS MOLECULES

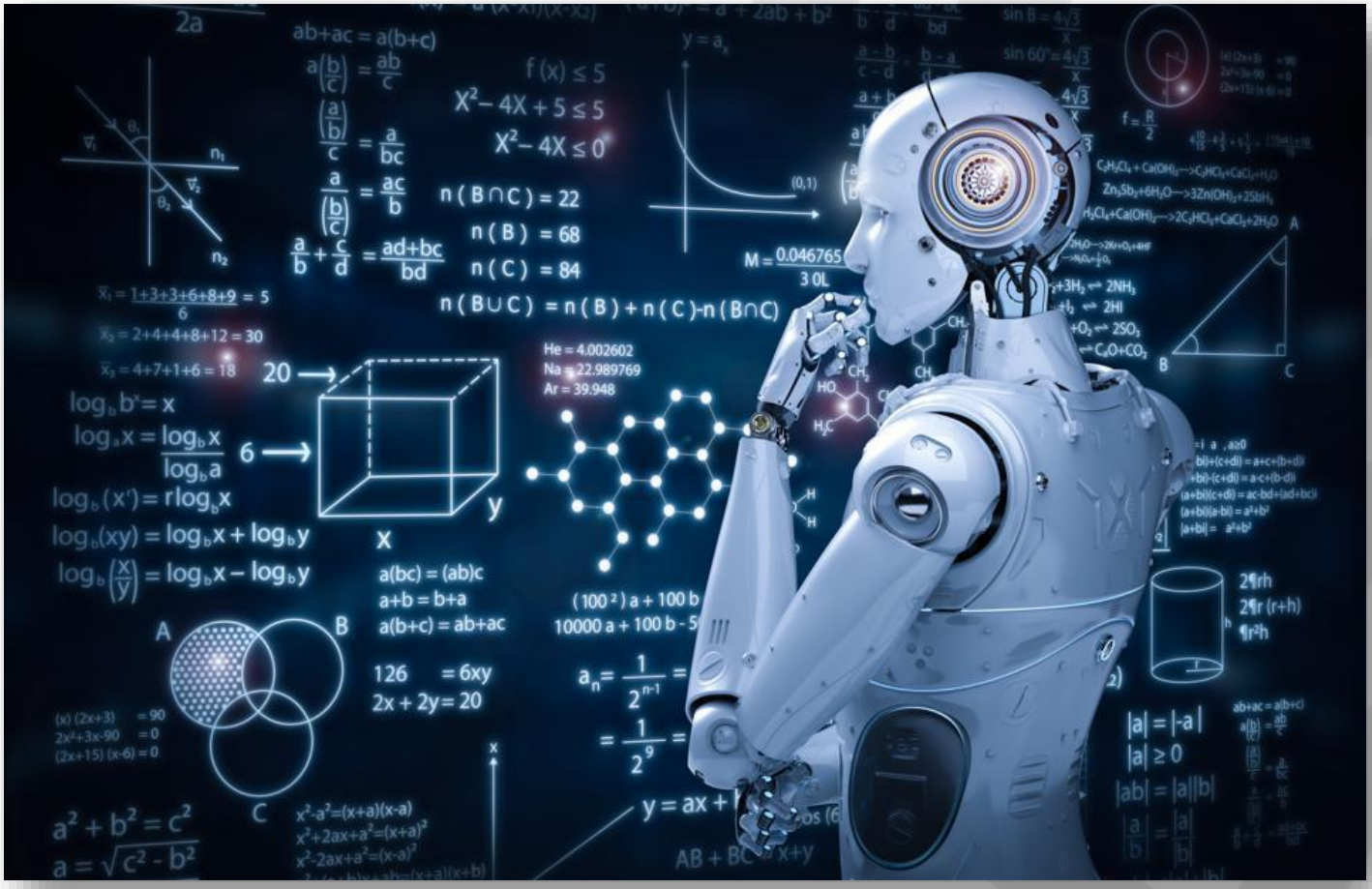
Student: Shraddha Prabhakar Hegde
Research Supervisor: Mrs. Vijaybhanu P & Dr. Girinath G. Pillai

Abstract:

Cystic fibrosis is the most common life-limiting disease which is inherited genetically. It affects multiple organs including lungs, kidney, liver, intestine, pancreas etc leading to the life-threatening complications like bronchitis, osteoporosis, infertility, frequent infections and diabetes. management of cystic fibrosis is very complex and there is no permanent cure till date. Few FDA approved drugs are available for the management of the disease but they were reported to be showing no promising improvement in the disease condition. Many research studies suggested that it is much more difficult to find the drug molecules for the cystic fibrosis due to its complexity. Based on these issues, the present study focuses on designing potent molecules against cystic fibrosis using machine learning approaches. F508del-CFTR was identified as the potential target and 864 associated ligands were selected as the initial data set. Docking based virtual screening and ML based model development was carried out for the purpose of multi-arameter optimization. Based on the pharmacokinetic profile of the template molecule,90 novel molecules were designed applying pre-determined chemical transformations. Top 5 molecules were selected based on the molecular docking results and retrosynthetic pathway was determined accordingly. ADME and activity of best 5 molecules were determined using machine learning methods. All the 90 newly designed molecules were considered for the molecular docking against delF508-CFTR protein among which 5 hit molecules were identified namely ACF-1, ACF-2, ACF-3,ACF-4 and ACF-5 with docking scores of -18.29, -15.2,-15.0,-13.14, and -12.52 respectively. All 5 molecules were considered for the

retrosynthetic planning from AIzynthfinder. Pharmacokinetic properties of these molecules were determined using StarDrop software and they were found to be within the range. Biological activity of the molecules was determined using the AdaBoost ML model and predicted IC50 were found to have the value range from 15.8 to 63.0 µM. Since the molecules have shown promising results, they could be promising lead candidates in the future perspective against cystic fibrosis.

Keywords: Cystic fibrosis, CFTR, F508Delta, Machine learning, AdaBoost



HIT-TO-LEAD IDENTIFICATION OF THERAPEUTIC AGENTS FOR RHEUMATOID ARTHRITIS - HIF-1 ALPHA

Student: Shruthika R
Research Supervisor: Dr. Girinath G Pillai, Dr. Parasuraman Pavadai

Abstract:

Rheumatoid arthritis (RA) is a chronic, progressive and disabling autoimmune inflammatory condition, characterized by pain, stiffness, inflammation of the synovium and destruction of cartilage which ultimately results in substantial disability. HIF-1α expression is strongest in the sub-lining layer of RA synovium and is related to both angiogenesis and inflammation in synovium from RA patients. HIF-1α contributes to the pathogenesis of RA by increasing the generation of autoimmune-related components, such as proinflammatory cytokines. We aimed to generate a validated QSAR model with a data consisting of experimental dataset of different molecules against HIF-1 alpha to determine the physicochemical properties of compounds essential for HIF-1 α inhibition and to identify novel lead molecules with HIF 1-α inhibitory activity and bioavailability. Lead optimization and in-silico approaches were employed in this research work. QSAR model was generated and validated by using ORANGE-Random Forest method algorithm. Molecular descriptors explained the significance of chemical properties essential to determine the physicochemical properties available within the chemical structures. 110 hit molecules were designed based on their ADMET properties; Molecular docking of the hit molecules indicated that the compound CHEMBL2323957 was found to have the best score of -20.16 in comparison to the reference molecule CHEMBL2323956 which showed the score -12.85. Retrosynthetic pathway was developed for top 5 compounds. Docking was performed for all the 110 molecules and the ADMET evaluation indicated the compounds has good pharmacokinetic properties. The research work resulted in the generation of a validated QSAR model with higher degree of external predictive ability and significance to inhibitory activity against RA. We propose novel compounds with enhanced RA inhibitory activity and bioavailability with their retrosynthetic pathways.

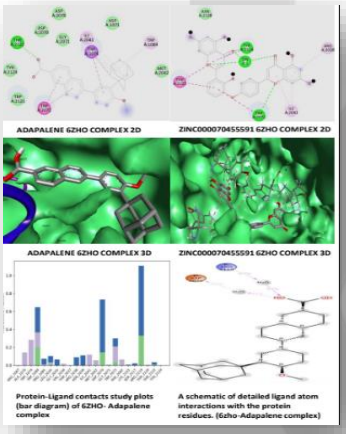
Keywords: Rheumatoid Arthritis, HIF-1α, Machine Learning, Drug design.

REPURPOSING OF NATURAL AND FDA APPROVED DRUG TO TREAT MIGRAINE: A COMPUTATIONAL APPROACH

Students: Sankhasubhra Jana, Koushal V Gowda, Shreyas K S, Sri Raksha L, Sushmitha N, Sushma H S
Research Supervisor: Dr. Parasuraman Pavadai

Abstract:

"Migraine" is a complex neurologic disorder characterized by recurrent moderate to severe headache. Though migraine causes aren't fully understood, genetics and environmental factors play a role. Mostly multi - purpose drugs like antidepressants, antiseizure, antihypertensive drugs and Botox injections are being used to prevent Migraine. From the study conducted, we have found that two drugs namely, "Adapalene" and "Trospium" have proved to be more potent drug candidates from the selected test drugs for the treatment of Migraine. To support this claim, we employed a drug repurposing strategy with the known, approved FDA and natural drugs available on the ZINC database. We performed molecular docking with the selected ligand and target protein 6zho – which is a crystal structure of a CGRP receptor ectodomain heterodimer with bound high affinity inhibitor.



The binding affinity scores of Adapalene and Trospium were the preferred ones. Moreover, we assessed the 2D and 3D molecular interaction to identify the common hydrophobic interactions of each drug candidate with the target protein 6zho.

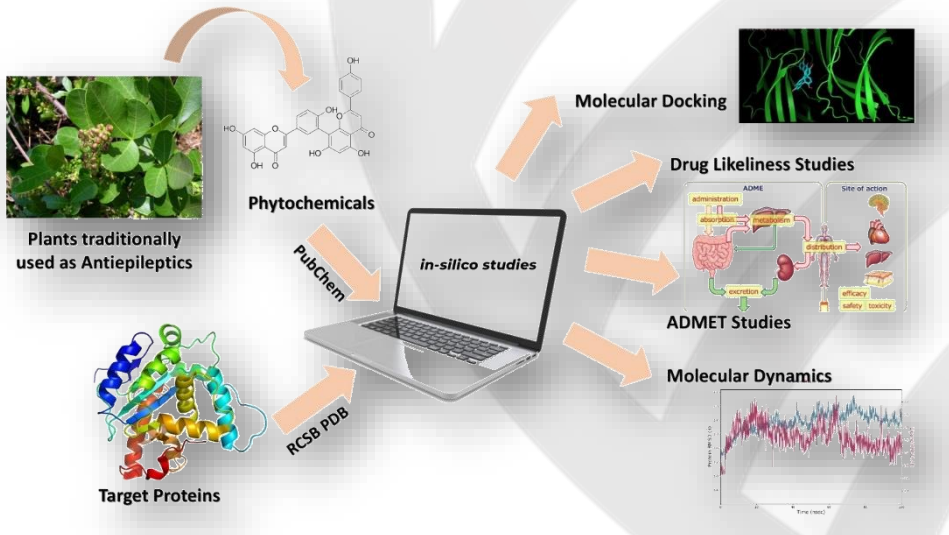
Furthermore, we also conducted dynamic studies to understand the dynamic, structural aspects and properties of the ligand (Adapalene and Trospium) and the selected protein 6zho.To conclude, we have found out two newer drugs that can be employed for further drug and formulation development process. Hence, we can therefore say that, Adapalene and Trospium can successfully join the army of drugs in order to treat Migraine.

IN-SILICO EVALUATION OF PHYTOCHEMICALS AS POTENTIAL ANTIEPILEPTIC DRUGS

Students: Akilan.M, Harshini Anand, Ritrick Dey, Shiva.S, Sushmitha.B
Research Supervisor: Dr. AR Mahesh

Abstract:

Numerous phytochemical substances have been used therapeutically to treat epileptic conditions. The antiepileptic properties of isolated phytochemicals from various natural medicinal sources are well documented. The underlying mechanisms behind how these isolated elements exhibit their anticonvulsant 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 Amentoflavone with GABA B 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 antiepileptic agent.



IN-SILICO STUDIES OF HER2 INHIBITORS FOR TREATMENT OF BREAST CANCER

Students: Jishnu Prakash P, Aravind T, Kavya Salvankar, Sanjana Shetty, Shreya K

Research Supervisor: Dr. MK Yuvapriya

Abstract:

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 approach is to identify new leads by combining Pharmacophore modelling & Molecular Docking studies and ADMET Analysis. This study focuses on ligand-based Pharmacophore Modelling of HER2 inhibitors for breast cancer with six marketed drugs using online tool Pharmagist. 3353 hits were generated for the appropriate pharmacophore alignment by using Zinc Pharmer. These hits were filtered employing Data warrior software. Filtered 230 compounds were subjected to Molecular Docking. Molecular docking studies were carried out using Autodock software. Docking studies gives information of binding affinity of the ligands to the target in terms of docking score and binding interaction with the amino acids residues of the target which were compared with that of standard drugs. Pharmacokinetic and Toxicity prediction of the ligands were done using free software pkSCM. Five compounds possess greater binding affinity to human HER2 in comparison with standard drug Neratinib. ADMET studies revealed that these molecules were safe, non-toxic, and optimum according to Lipinski's rule of five. Hence these Five lead compounds can be investigated further by Molecular Dynamic studies and then it can be optimized further with knowledge of medicinal chemistry and assessed for their potential using *in-vitro* and *in-vivo* studies as HER2 inhibitors for the treatment of Breast Cancer.

Keywords: Breast Cancer, Human Epidermal Growth Factor Receptor, Pharmacophore modelling, Molecular docking, ADMET Analysis.

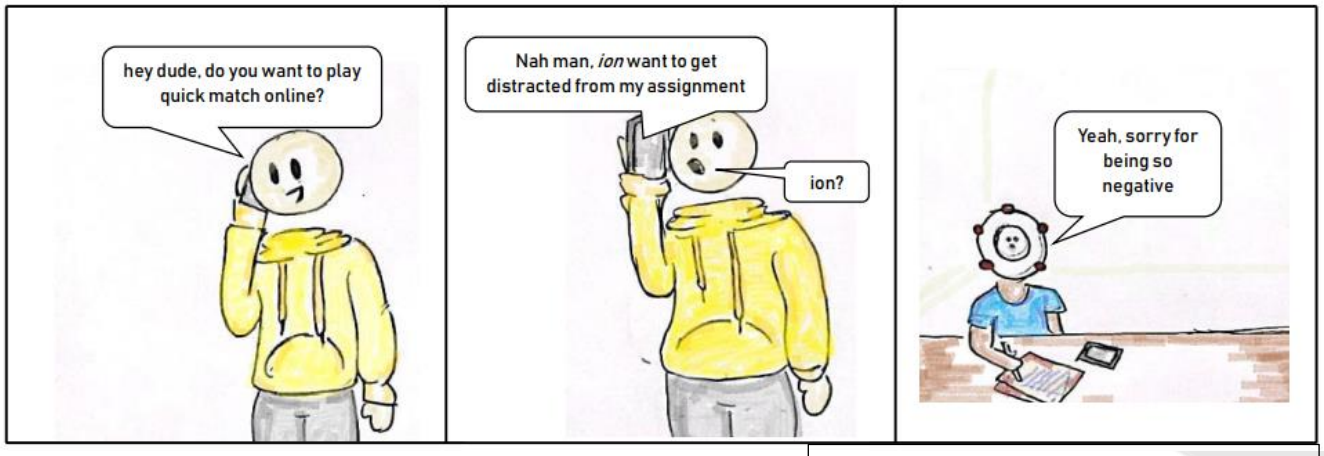
Publications

1. Shanmugampillai Jeyarajaguru Kabilan, Selvaraj Kunjiappan, Krishnan Sundar, **Parasuraman Pavadai**, Nivethitha Sathishkumar & Haritha Velayuthaperumal. Pharmacoinformatics-based screening of active compounds from Vitex negundo against lymphatic filariasis by targeting asparaginyl-tRNA synthetase. Journal of Molecular Modeling. 2023; 29:87. https://doi.org/10.1007/s00894-023-05488-6. (Springer Nature- IF: 2.172).
2. R. Niranjana Devi, P. Pounraj, S Birendra Kumar, A. Saral, J. Kileyoba Vinnarasi, C. Vivek, **P. Parasuraman**, Ahmad Irfan, S. Muthu. Electronic, intermolecular, quantum computational investigations, molecular docking and simulation studies of the potent antiviral drug EIDD-2801. Journal of the Indian Chemical Society. 2023; 100(3): 100953. https://doi.org/10.1016/j.jics.2023.100953.(Elsevier publisher - IF: 0.243)
3. Manisha Devi, **G Chaitanya Sai**, Damodar Nayak A, **Parasuraman Pavadai**, Selvaraj Kunjiappan, Anbu Jayaraman. Identification of Lead Moiety to Treat Polycystic Ovarian Syndrome from Ganoderma lucidum: A Computational Approach. Biointerface Research in Applied Chemistry. 2022;13(5):1-20. https://doi.org/10.33263/BRIAC135.461. (SCOPUS INDEXED)
4. Arjun Kumar Kalimuthu, **Parasuraman Pavadai**, Theivendren Panneerselvam, Ewa Babkiewicz, Joanna Pijanowska, Piotr Mrowka, Gopalan Rajagopal, Venkataraman Deepak, Krishnan Sundar, Piotr Maszczyk, Selvaraj Kunjiappan. Cytotoxic Potential of Bioactive Compounds from Aspergillus flavus, an Endophytic Fungus Isolated from Cynodon dactylon, against Breast Cancer: Experimental and Computational Approach. Molecules. 2022;27:8814. https://doi.org/10.3390/molecules27248814. (MDPI- IF: 4.927)
5. Nausheen Ahmed, R Deveswaran, **P Parasuraman**, S Bharath, C Priyanka, PS Santosh. Topical delivery of natural extract for accelerated wound healing. Materials Today: Proceedings. 2022. https://doi.org/10.1016/j.matpr.2022.10.200. (SCOPUS INDEXED)
6. Leno Jenita J, **Mahesh AR**, Sah P, Rathore SS. Optimization of parameters for the design and evaluation of fenofibrate loaded floating microspheres by Taguchi method. J Res Pharm. 2023; 27(1): 130-144 (SCOPUS INDEXED)

7. Jenita JJL, **Mahesh AR**, Sudarshan BP, Rathore SS, Banu S. Development and evaluation of capecitabine loaded human serum albumin nanoparticles for breast cancer. CTBP [Internet];16(3s):40-9.
8. **Mahesh AR**, Jenita JL. Designing multi-epitope vaccine for SARS-COV-2 through in-silico techniques. International Journal of Biology, Pharmacy, and Allied Sciences, 12(3): 1041-1051.
9. Jabeen, **Suma BV**. Stability indicating UPLC-MS/MS method for quantification and identification of cefepime and its degradants in API. J Appl Pharm Sci, 2023. https://doi.org/10.7324/JAPS.2023.118104
10. **Vijaybhanu, P., Harish Kumar, D.R.,** Sarasija, S. (2023) Conjugation of Curcumin and Metformin for Improved Pharmacological Profile in Cancer Therapy: An In-Silico Approach. Biointerface Research in Applied Chemistry, 13(2), p. 101.

Book Chapter

1. Selvaraj Kunjiappan, Theivendren Panneerselvam, Sureshbabu Ram Kumar Pandian**, Parasuraman Pavadai**, Saravanan Govindaraj, Vigneshwaran Ravishankar, Sankarganesh Arunachalam, Sankaranarayanan Murugesan. Nanoparticles for diagnosis and treatment of renal diseases. Emerging Nanotechnologies for Medical Applications. Elsevier Book Chapter Pages 95-130, 2023. https://doi.org/10.1016/B978-0-323-91182-5.00009-7
2. **Burhanuddin Madriwala, Judy Jays**. Developing an Analytical Method and Validation for Estimation of Residual Solvents in Gliclazide Using Gas Chromatography. Challenges and Advances in Pharmaceutical Research. 0(11), page 54-67 https://doi.org/10.9734/bpi/capr/v9/3756C



Anjana Vidya Srivathsa, I Sem M.Pharm

Poster & Oral Presentation

1. Nayana J, Suma B.V. Identification of Novel 2-mercaptobenzimidazole derivatives for the treatment of tuberculosis: A computational approach. International conference on Innovation and advances in pharmaceutical Sciences ACU Karnataka India on 10th and 11th February 2023.
2. Akshith R, Brundha SN, Suma B.V. In-silico Evaluation Studies on Quinazoline Analogues as an Antifungal agent. International conference on Innovation and advances in pharmaceutical Sciences ACU Karnataka India on 10th and 11th February 2023.
3. Madhushree K, Judy Jays. Design of Novel Amino=pyrimidines as GABA Amino Transferase Inhibitors to Treat Convulsions: A Computational Approach. International conference on Innovation and advances in pharmaceutical Sciences ACU Karnataka India on 10th and 11th February 2023.
4. Anjana Vidya Srivathsa, Suma B.V. Anti-cancer activity of 1,3,4 thiadiazole derivatives based on molecular docking and ADMET studies. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences, November 2022 on 29/11/2022
5. Apeksha K Hegde, Suma B.V. Anti-Tubercular activity of 1,3,4 thiadiazole derivatives on in-silico method. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences, November 2022 on 29/11/2022
6. Devika Muraleedharan, Suma B.V. Molecular docking and ADMET studies of thiadiazole derivatives for antibacterial activity. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences, November 2022 on 29/11/2022
7. Nandini M S, Suma B.V, Anti-Bacterial activity of 1,3,4 thiadiazole derivatives on in-silico method. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences. November 2022 on 29/11/2022
8. Protyusha Maji, Suma B.V. Molecular Docking and ADMET studies of Thiadiazole derivatives for anti-fungal activity, New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences, November 2022 on 29/11/2022

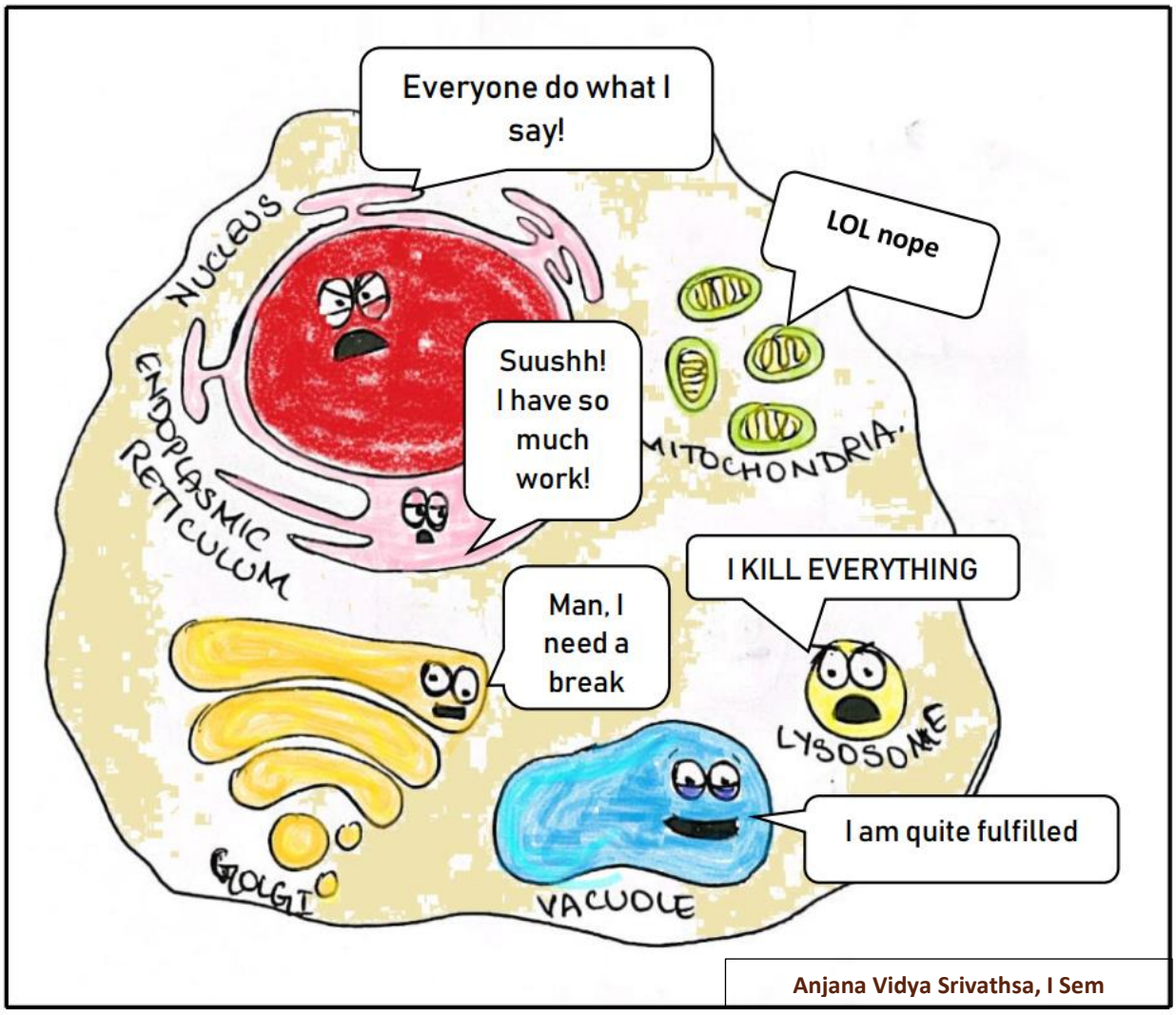
9. Shreya Shet, Suma B.V. Molecular docking and ADMET studies of pyrimidine derivatives for anti-inflammatory activity. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences. November 2022 on 29/11/2022
10. Tanya Maheshwari, Suma B.V. Molecular docking and ADMET studies of thiadiazole derivatives for anti-inflammatory activity. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences. November 2022 on 29/11/2022
11. Brundha S N, B V Suma. In-silico study on 1,3,4 thiadiazole derivatives with isoniazid for anti-tuberculosis activity. 4th International Conference on to Foster the Drug Development Strategies in Novel Pharmaceutical and Its Global Challenges, organized by Krupanidhi College of Pharmaceutical Sciences. December 2022 on 16th -17th December
12. Basavana Gowda, Parsuraman. P and Lakshmi M. Sundar. Potent lead identification for the treatment of depression: A Computational Approach. Drug Discovery and *In-silico* Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (online)
13. B Sunil Kumar, Agasa Ramu Mahesh, Parasuraman Padavai. Identification of Potent Lead to Inhibit DHFR for the Treatment of Cancer: A Computational Approach. Drug Discovery and In-silico Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (online)
14. Divya B, Agasa Ramu Mahesh, Vijaybhanu P, Parasuraman Pavadai. Pharmacophore Identification of Alternative HMG-COA Reductase Inhibitor: A Computational Approach. Drug Discovery and In-silico Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (Online)
15. Genne Soujanya, Knolin K Thachil, Parasuraman Padavai. Identification of Novel Lead to Inhibit HIV Protease: A Computational Approach. Drug Discovery and In-silico Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (online)
16. Golla Sireesha, Damodar Nayak A, Parasuraman Padavai. Discovery of Novel Lead Moieties as Anti-Cholinesterase Agents: A Computational Approach. Drug Discovery and In-silico Drug Design, November 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (online)

17. Mahasin Khan, Agasa Ramu Mahesh, Harish Kumar D R, Parasuraman Padavai. Discovery of Novel AKT2 Inhibitors for The Treatment of Breast Cancer: A Computational Approach. Drug Discovery and In-silico Drug Design Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (Online)
18. Nayana J, B V Suma, Parasuraman Pavadai. Identification of Novel Gaba-A Inhibitor for the Treatment of Epilepsy: A Computational Approach. Drug Discovery and In-silico Drug Design Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (Online)
19. Basavana Gowda H D, Lakshmi M Sundar, Parasuraman Pavadai. Potent Lead Identification for The Treatment of Depression: A Computational Approach. Drug Discovery and In-silico Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (Online)
20. Radhika N, Agasa Ramu Mahesh, M K Yuvapriya, Parasuraman Pavadai. Potent Lead Identification for COX-2 Enzyme: A Computational Approach. Drug Discovery and In-silico Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (Online)
21. Brundha S N, Agasa Ramu Mahesh, B V Suma, Parasuraman Pavadai. Evaluation of Potential Histamine H2 Receptor Antagonist: A Computational Approach. Drug Discovery and In-silico Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (Online)
22. Madhushree K, Judy Jays, Parasuraman Pavadai. Potent Lead Identification Against Xanthine Oxidase for The Treatment of Gout: A Computational Approach. Drug Discovery and In-silico Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (Online)
23. Soundarya R, Damodar Nayak A, Parasuraman Padavai. Discovering New Lead Moieties as Ace Inhibitors: A Computational Approach. Drug Discovery and In-silico Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (Online)
24. Srinivas G, Agasa Ramu Mahesh, Harish Kumar D R, Parasuraman Pavadai. Identification of Lead Moiety to Inhibit Catechol-O-Methyl Transferase: A Computational Approach. Drug Discovery and In-silico Drug Design. Nov 2022 on 18.11.2022 in Royal School of Pharmacy, Guwahati, Assam (Online)
25. Tejas Kumar A, B Sunil Kumar, Agasa Ramu Mahesh, Parasuraman Padavai. Identification of Potent Lead to Inhibit DHFR For the Treatment of Cancer: A Computational Approach. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences in November 2022 on 29/11/2022

26. M Rashikamani, Divya B, Agasa Ramu Mahesh, Parasuraman Pavadai. Identification of Potent Lead to Inhibit HMG-COA Reductase: A Computational Approach. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences in November 2022 on 29/11/2022

27. Bhumika. M, Golla Sireesha, Parasuraman Padavai. Identification of Lead Moieties to Inhibit Cholinesterase Enzyme: A Computational Approach. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences in November 2022 on 29/11/2022

28. Vikas Manu, Srinivas G, M Narayana Babu, Parasuraman Pavadai. Potent Lead Identification Against Catechol-O-Methyl Transferase: A Computational Approach. New horizons for drug discovery and Innovation in Health care and Pharmaceutical Research, Dayananda Sagar College of Pharmaceutical Sciences in November 2022 on 29/11/2022



Awards

Best Innovative Project on RUAS Innovation Day, 18 Nov 2022, RUAS Peenya, Bangalore

EXPLORING THE ANTI-INFLAMMATORY ACTIVITY OF THE INDIAN MEDICINAL PLANT CONSTITUENTS TO INHIBIT LP-PLA2 BY IN SILICO AND IN VITRO METHODS

Students: Dilip Chekuri, Bindushree G, Cerin Sarah Reji, Richu Siby Jude and Shamil Siraj

Research Supervisor: Dr. Lakshmi M Sundar

Best Oral Presentation Award

EVALUATION OF QUINAZOLINE DERIVATIVES ON BREAST CANCER BY IN-SILICO METHOD

Student: Mr. Koushal V Gowda I M.Pharm

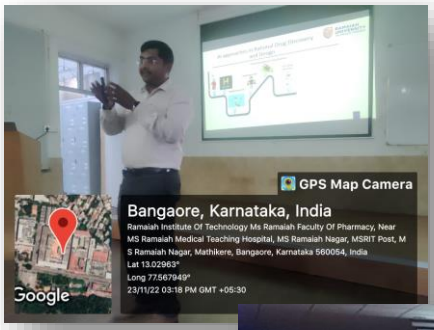
Research Supervisor: Dr. Suma BV

Conference: International Conference on Innovation And Advances In Pharmaceutical Sciences Held At Acu Karnataka India On 10th And 11th Feburary 2023

Co-Author: Ms. Brundha Sn

Invited Lectures

1. **Dr. Parasuraman Pavadai** has delivered invited lecture on "Artificial Intelligence in Drug Discovery and Development for infectious Diseases" in 6th National Symposium on "Emerging Infectious Diseases and Novel Drug Development" at Swamy Vivekananda College of Pharmacy, Elayampalayam, Tiruchengode, Namakkal on 2nd and 3rd December 2022.
2. **Dr. Parasuraman Pavadai** was invited as a resource person in a 5-day weekend workshop on "Finishing School – Pharmaceutical Industry Orientation" Organised by Drug Design and Development Centre, FPH, RUAS during October -November 2022.
3. **Dr. Parasuraman Pavadai** has delivered invited lecture on "Teaching and Learning Computational Drug Design: The Road Ahead" in Faculty Development program organised by Literary Committee, Faculty of Pharmacy, RUAS during 23rd – 26th November 2022.
4. **Dr. AR Mahesh** was invited as a resource person in a 5-day weekend workshop on "Finishing School – Pharmaceutical Industry Orientation" Organised by Drug Design and Development Centre, FPH, RUAS during October -November 2022.
5. **Dr. AR Mahesh** has delivered invited lecture on "Teaching and Learning Computational Drug Design: The Road Ahead" in Faculty Development program organised by Literary Committee, Faculty of Pharmacy, RUAS during 23rd – 26th November 2022.



Student Achievements

Toppers in the Department of Pharmaceutical Chemistry
Even Semester Examination November 2022

B.Pharm II Semester

BP202T	Pharmaceutical Organic Chemistry I- Theory	Anuhya B Bhavana B Renee Rebecca Cherian Susheela Veerappayyanavaramath
BP203T	Biochemistry- Theory	Renee Rebecca Cherian
BP208P	Pharmaceutical Organic Chemistry I – Practical	Mohitosh Bera
BP209P	Biochemistry- Practical	Anuhya B

Student Achievements

Toppers in the Department of Pharmaceutical Chemistry
Even Semester Examination November 2022

B.Pharm IV Semester

BP401T	Pharmaceutical Organic Chemistry III– Theory	Arunkumar C Nandita Ravi
BP402T	Medicinal Chemistry I– Theory	Arunkumar C
BP406P	Medicinal Chemistry I – Practical	Arunkumar C

Student Achievements

Toppers in the Department of Pharmaceutical Chemistry
Even Semester Examination November 2022

B.Pharm VI Semester

BP601T	Medicinal Chemistry III –Theory	Tejas Kumar A
BP606T	Quality Assurance –Theory	Sudatt Dixit
BP607P	Medicinal chemistry III –Practical	Sudatt Dixit Amulya Sharon C Payal

Student Achievements

Toppers in the Department of Pharmaceutical Chemistry
Even Semester Examination November 2022

M.Pharm II Semester

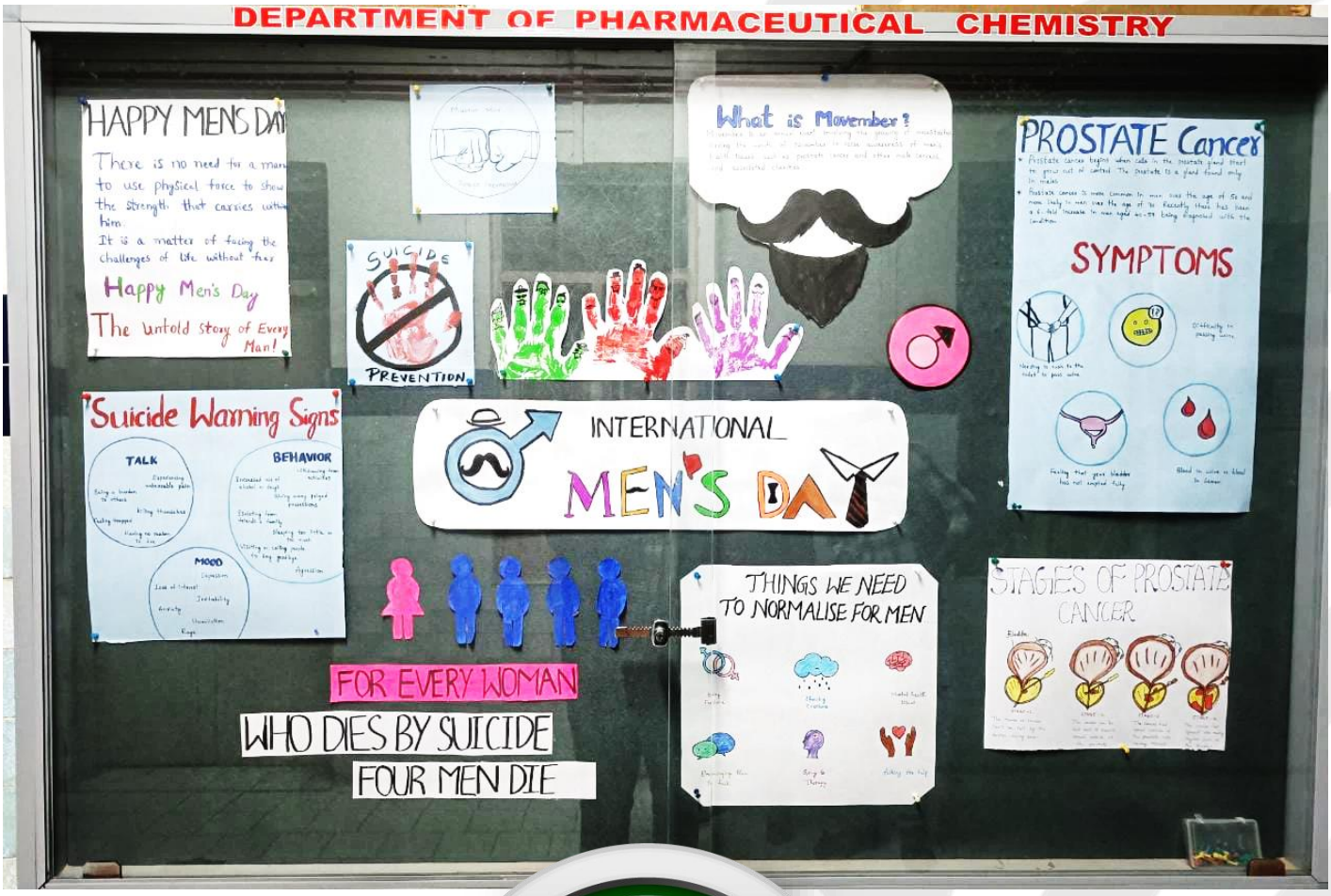
MPC101T	Advanced Spectral Analysis	Mahasin Khan
MPC102T	Advanced Organic Chemistry – II	Bandral Sunil
MPC103T	Computer Aided Drug Design	Mahasin Khan
MPC104T	Pharmaceutical Process Chemistry	Genne Soujanya
MPC105P	Pharmaceutical Chemistry Practical II	Genne Soujanya

Anjana Vidya Srivathsa, I Sem M.Pharm

Student Activities

International Men's Day

International Men's Day (IMD) is a global awareness day for many issues that men face, including parental alienation, abuse, homelessness, suicide, and violence, celebrated annually on November 19.

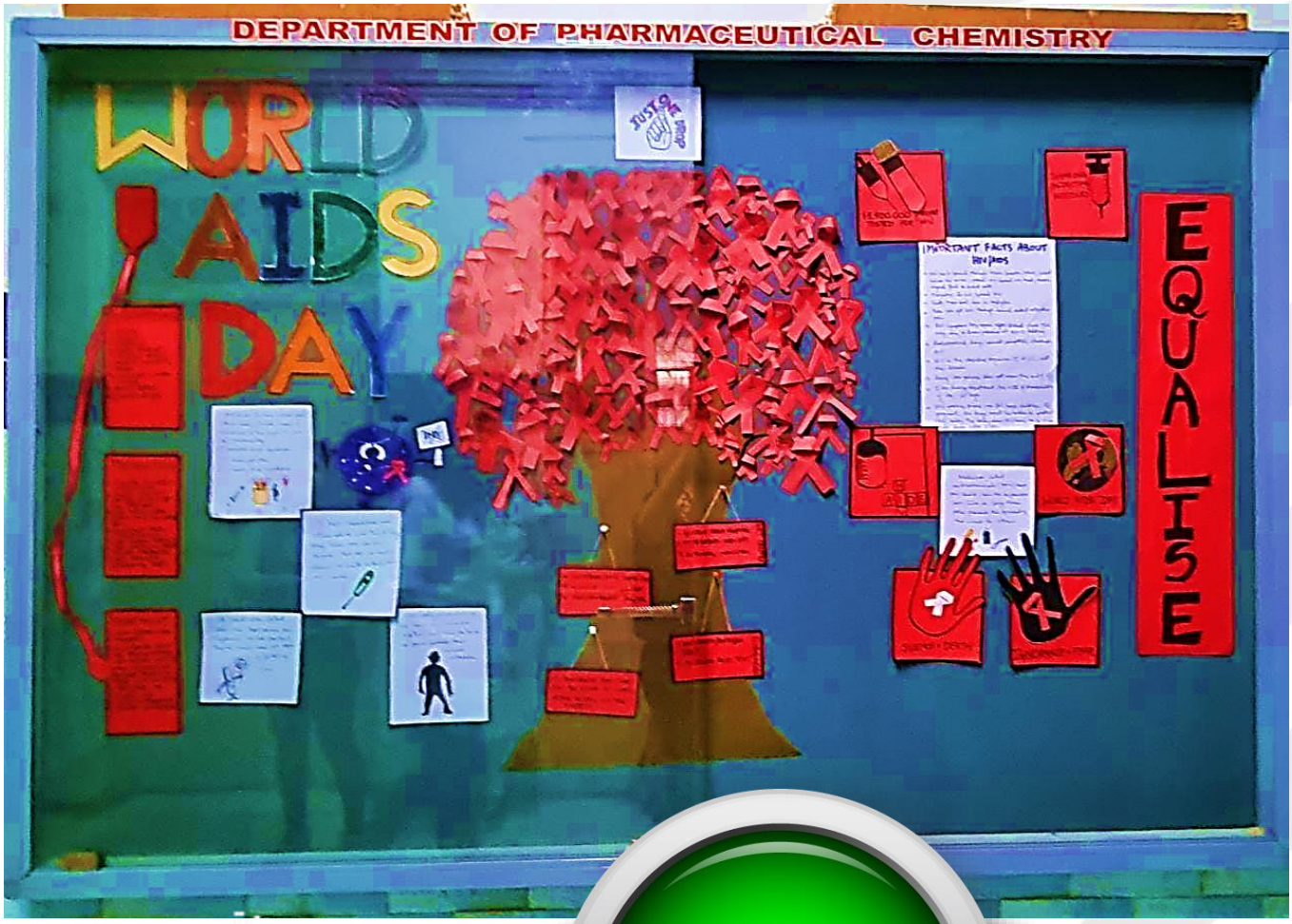


Click Here

World's AIDS Day

Equalize- World AIDS Day 2022

The "Equalize" slogan is a call to action. It is a prompt for all of us to work for the proven practical actions needed to address inequalities and help end AIDS.



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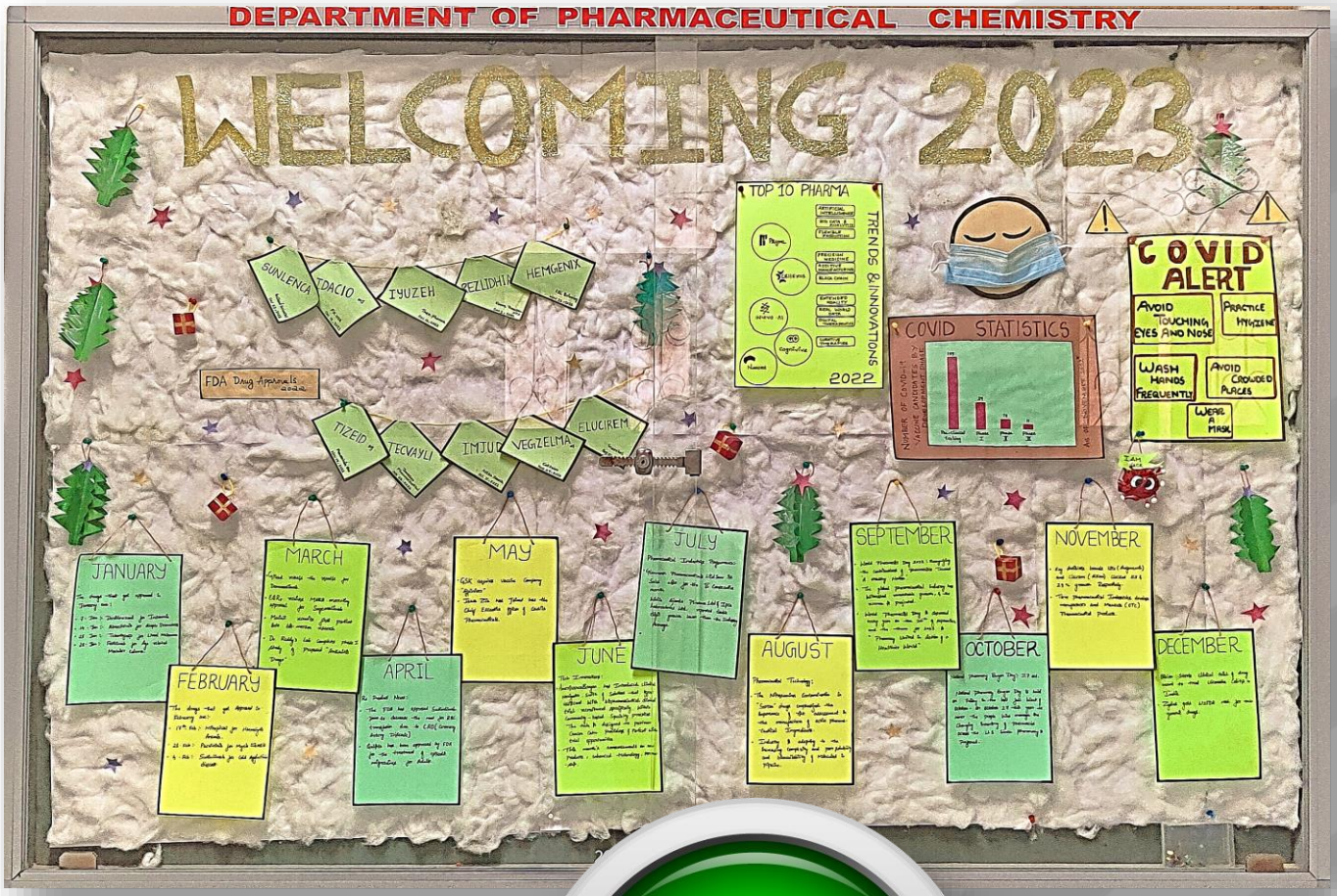
New Year - 2023



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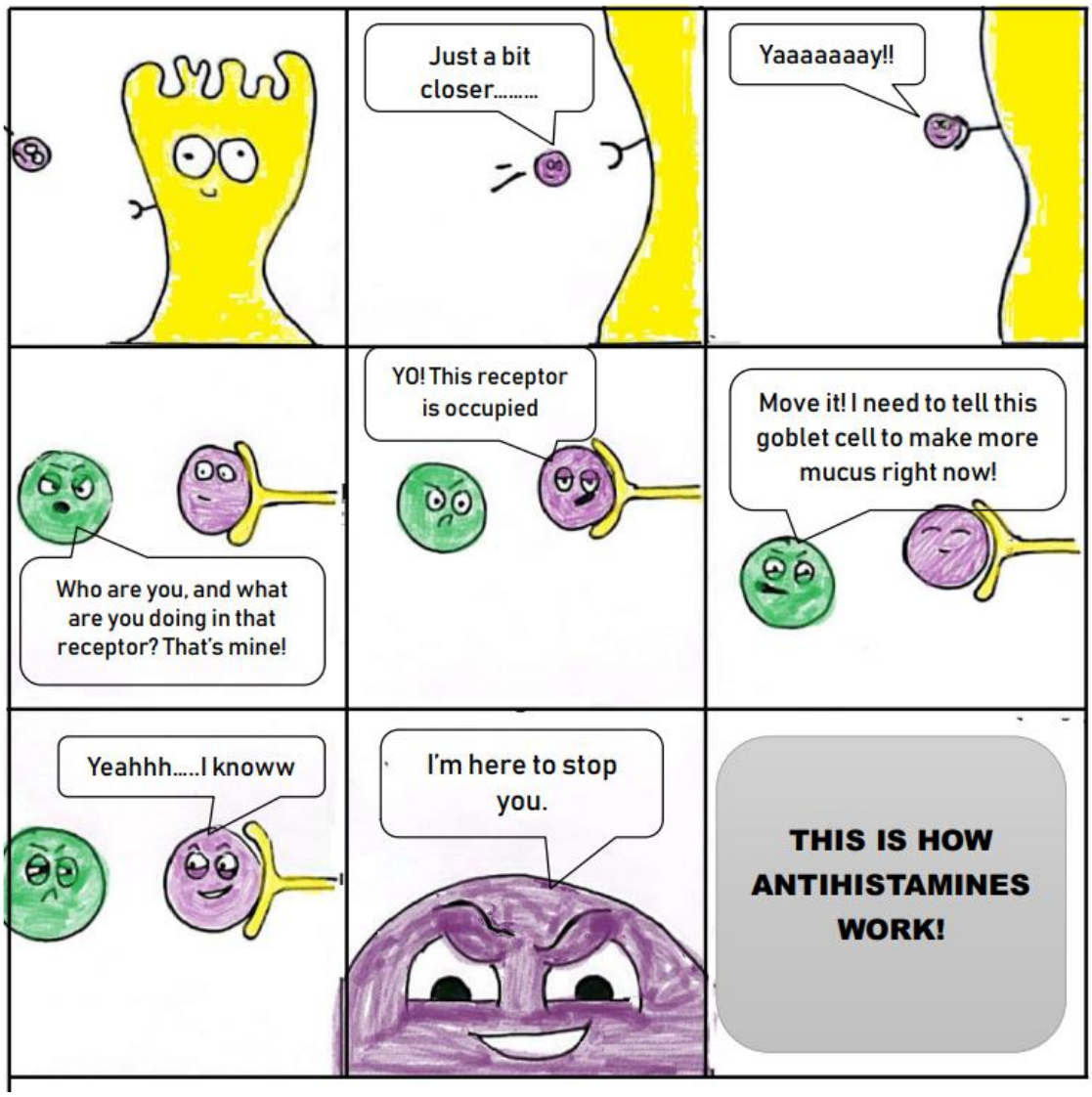
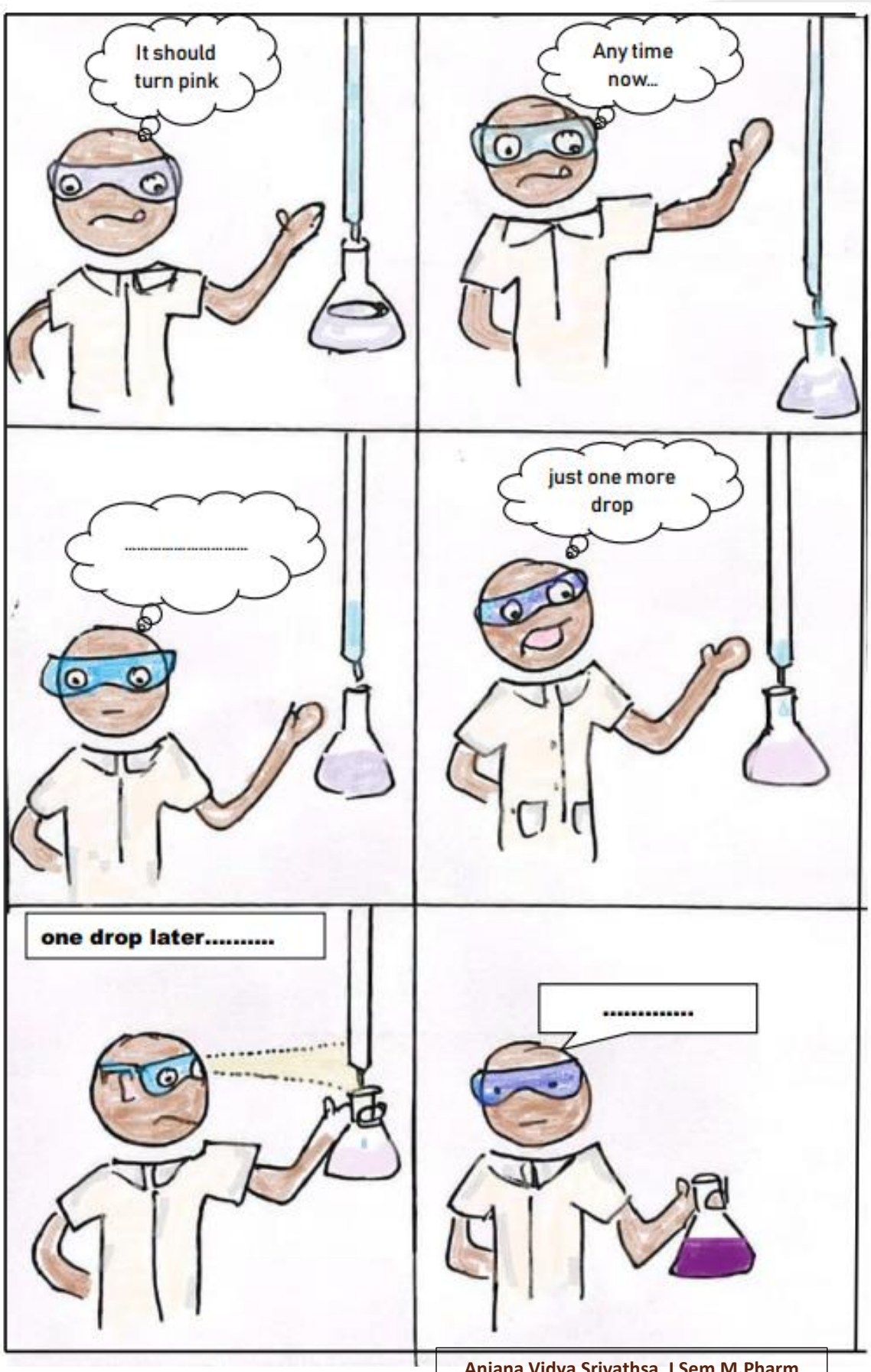
Write it on your heart that every day is the best day in the year.

— Ralph Waldo Emerson

Chemocomics

Anjana Vidya Srivathsa, I Sem M.Pharm





Anjana Vidya Srivathsa, I Sem M.Pharm

Upcoming Event

Patron

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

Co-Patrons

Dr. KULDEEP K RAINA
Vice Chancellor
RUAS

Dr. O. P. KHARBANDA
Pro- Vice Chancellor (Health Sciences)
RUAS

Dr. G. S. VENKATESH
Registrar
RUAS

Convener

Dr. S. BHARATH
Dean, Faculty of Pharmacy

Co-Convener

Dr. HARISH KUMAR. D. R
Professor and Head
Department of Pharmaceutical Chemistry
Faculty of Pharmacy

Organizing Secretaries

Dr. LAKSHMI M. SUNDAR

&

Dr. PARASURAMAN. P
Assistant Professor's
Department of Pharmaceutical Chemistry
Faculty of Pharmacy

About Seminar

Pharmaceutical analysis is an interdisciplinary science comprising various technologies of spectroscopy, chromatography and cell-based assays. The development of robust analytical method is essential for determining the purity of a compound during its synthesis, elucidation of its structure, establishing the stability, pharmacological screening, pharmacokinetics and toxicity studies. Suitable analytical approaches provide accurate and precise data to support the drug discovery and development process. With new technologies emerging in spectroscopic, chromatographic and biological assays, the scope of their applications has widened in the analysis of new drugs, impurities, metabolites and their toxicity studies. This seminar focusses on the applications of latest technologies to highlight current trends and advancements of pharmaceutical analysis in drug discovery and development process.

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.

About Faculty of Pharmacy

Faculty of Pharmacy (FPH), formerly M.S. Ramaiah College of Pharmacy, was established in 1992. The Faculty of Pharmacy, ranked 62nd in the AIR- NIRF 2022, 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 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 and HPLC. Department is equipped with GPU computational facility to help students in developing their skills and knowledge needed to tackle the challenges of drug design and contribute to the development of new and more effective treatments for a variety of diseases.

Invited Speakers

Dr. PRABAKARAN D

Vice President – Operations,
In Vitro Research Solutions Pvt. Ltd,
Bengaluru

EXTRACTABLES AND LEACHABLES IN PHARMACEUTICAL DOSAGE FORMS

Dr. KUMARAVEL S

Head, Analytical Department,
Bioplus Life Sciences Ltd,
Hosur

RECENT INNOVATIONS AND REGULATORY REQUIREMENTS IN PHARMACEUTICAL ANALYSIS

Dr. SYED SALMAN LATEEF

Head, Testing and Services lab,
Wipro Life Sciences Ltd,
Bengaluru

MASS SPEC SOFTWARE IN UNKNOWN STRUCTURE DETERMINATION

Mr. ASHWANI GAUR

Senior Principal Scientist-DMPK,
Discovery Biology,
Syngene International Ltd, Bengaluru

BIOANALYSIS IN DMPK

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Faculty of Pharmacy
Department of Pharmaceutical Chemistry

CHEMID

A Quarterly E-Newsletter

Volume II

Issue I

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