RAMAIAH UNIVERSITY OF APPLIED SCIENCES | Faculty of Pharmacy

Volume II Issue III December - 2023

CHEMID

E-Newsletter

Department of Pharmaceutical Chemistry

New BEL Rd, M S R Nagar, Mathikere, Bengaluru, Karnataka 560054

DR. M.S. RAMAIAH CENTENARY YEAR CELEBRATIONS 1922-2022

RAMAIAH Group of Institutions

26th Anniversary of

KARMA YOGI DR. M S RAMAIAH, FIAE

Founder Chairman
(1922-1997)

A great visionary
who inspired us to create a better future.

A great philosopher & guide
who enlightened us.

A great leader and renowned educationist
who motivated us to build a better society for all.

A great philanthropist
And above all a "true" human being.

Today, 25th December 2023, on 26th Anniversary of our beloved Founder Chairman 'Karma Yogi', Dr. M. S. Ramaiah we redeem to follow his footsteps in maintaining the tradition envisioned by him.

RAMAIAH INSTITUTIONS *for* Health *and* Education

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Ramaiah Group of Institutions
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Editorial Note

Dear Readers,

Welcome to the latest edition of CHEMID, where we delve into an array of intriguing topics within the realm of chemistry and its diverse applications. In this issue, we bring you a rich tapestry of articles, departmental updates, and noteworthy achievements that highlight the vibrancy of our academic community.

Our featured articles open new windows into the historical landscape of Indian healthcare, chronicling the extraordinary journey of Acharya Prafulla Chandra Ray—a true trailblazer in the field. Additionally, we address contemporary concerns with an insightful exploration of the threat posed by nitrosamines to drug products. Shifting our focus, we uncover the potential of 3,3'-Diindolylmethane (DIM) in preventing dental caries, adding a novel dimension to our understanding of preventive dentistry.

The academic prowess of our department is underscored by an impressive array of publications, with 25 noteworthy contributions from July to November 2023. This diverse collection of research mirrors the commitment of our faculty and students to advancing the frontiers of chemical knowledge.

Our departmental presentations, numbering 25 in this issue, showcase the dedication and expertise of our academic community in disseminating knowledge. Moreover, we take pride in the recognition received by our staff, who have been invited as resource persons in various conferences, seminars, guest lectures, and faculty development programs.

The highlight of this edition is the comprehensive coverage of the "International E-Conference on Exploring the Frontiers of In-silico Drug Discovery." This event stands as a testament to our commitment to staying at the forefront of scientific inquiry, providing a global platform for the exchange of ideas and advancements in the field.

In the realm of accomplishments, we celebrate the successful completion of Dr. Vijayabanu P's PhD journey—an achievement that reflects the dedication and scholarly pursuit within our academic community.

However, our joy is tempered by the somber note of the condolence section, where we mourn the untimely demise of our beloved student, Mr. Tagore. His presence will be deeply missed, and our thoughts go out to his family and friends during this difficult time.

We also invite you to exercise your mental faculties with the challenging crossword puzzle, a delightful addition for those who enjoy a cerebral challenge.

As we navigate through the diverse content of this issue, we hope you find inspiration, knowledge, and a renewed sense of curiosity. Your continued support and engagement fuel the vitality of CHEMID, and we look forward to bringing you more enlightening content in future editions.

Editor-in-Chief
Dr. DR Harish Kumar

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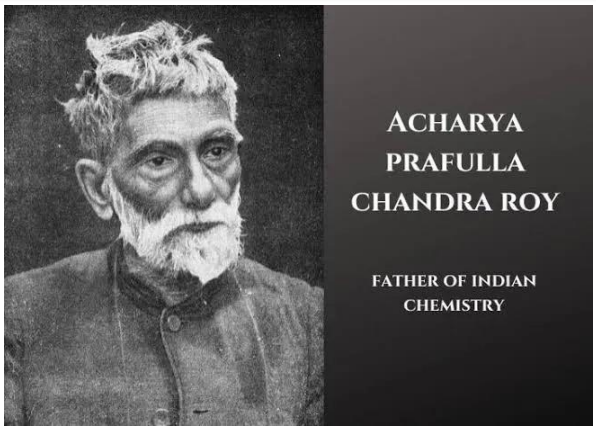
The Trailblazer of Indian Healthcare: The Inspiring Odyssey of Acharya Prafulla Chandra Ray



Acharya Prafulla Chandra Ray was not just a name but an embodiment of unyielding determination and relentless vision. His journey, born in the colorful landscape of rural Bengal in 1861, sculpted the foundation of the Indian pharmaceutical industry. Ray's tale was one of resilience, fueled by the unquenchable thirst for knowledge and a heart pulsating with the desire to transform India's healthcare landscape.

In the serene ambiance of his village, Ray's inquisitive mind, ignited by the flickering flames of education, burgeoned. A fervent learner, he embarked on an academic expedition that ultimately led him to the venerable halls of the University of Edinburgh. It was here, amid the scholarly conversations and rigorous academic pursuits, that he adorned himself with the mantle of knowledge, earning a doctorate in chemistry.

Armed with his profound understanding of chemical science, Ray returned to his homeland. In 1901, against the backdrop of the majestic river Hooghly, Bengal Chemical and Pharmaceutical Works, Ltd., emerged as a beacon of hope in the realm of healthcare. It was not merely an enterprise but a crusade to democratize access to essential medications for the people of India.

The genesis of the company was mired in adversity. Ray faced financial constraints and logistical impediments, yet his resolute spirit fortified his journey. Drawing from the reservoir of knowledge amassed during his academic pursuits, he spearheaded the indigenous production of vital pharmaceuticals and chemicals within the country.

The company's inception marked a turning point in the annals of Indian healthcare. Bengal Chemical and Pharmaceutical Works, Ltd., led the charge in developing indigenous pharmaceutical capabilities, emancipating India from the shackles of imported medicines. Ray's visionary initiatives cast a profound and lasting impact on the nascent Indian pharmaceutical industry.

Acharya Prafulla Chandra Ray's odyssey isn't merely history confined to books; it's a living testament to the confluence of knowledge and unwavering determination. His story continues to echo through time, resonating as an inspiration for aspiring individuals, urging them to dream and toil indefatigably towards manifesting their visions.

Dr. AR Mahesh
Asst. Prof

Nitrosamine- threat to drug products?

Nitrosamines are a class of chemical compounds in which the nitroso group is attached to the amine group. In vivo studies have proven that nitrosamines can produce a carcinogenic effect in rats and mice. Valsartan a drug used in combination with other medication for the treatment of hypertension was found to be contaminated with impurity nitrosamines by the EU in the year 2018. Further, many other drugs like metformin, rifampicin, and ranitidine have also been found to have unacceptable levels of nitrosamines. Due to the potent carcinogenic effect of nitrosamines FDA, EMA, and other regulatory agencies have made it mandatory to check for the presence of nitrosamines.

Types of nitrosamines

TABLE 1: TYPE AND CLASSIFICATION OF NITROSAMINES

TYPES	FULL FORM	CLASSIFICATION AS PER IARC
NDMA	N- nitroso dimethylamine	2A
NDEA	N- nitroso diethylamine	2A
NDBA	N- nitrosobutylamine	2B
NPIP	N- nitrosopiperidine	2B
NPYR	N- nitrosopyrrolidine	2B
NMOR	N- nitrosomorpholine	2B
NDPhA	N- nitrosodipheylamine	3
NPRO	N- nitrosoproline	3
NSAR	N- nitrososcarosine	3

2A- probably carcinogenic to humans; 2B- possibly carcinogenic to humans; 3- not carcinogenic to humans

The carcinogenic effect of these nitrosamine impurities is due to the biotransformation of these drugs in the liver by microsomal enzymes like CYP2E1. This enzyme converts the nitrosamines impurity to alkyl diazonium ions, which causes damage to DNA.

- The drugs from which nitrosamines impurity was derived include
  a. Sartan
  b. Metformin
  c. Rifamapcin
  d. Ranitidine
  e. Champix

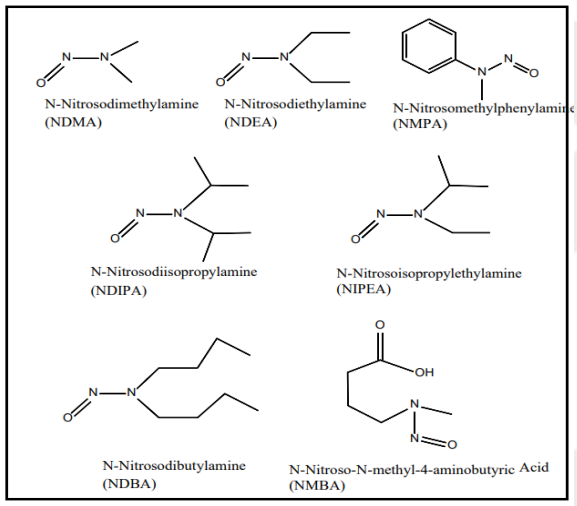


FIGURE 1: STRUCTURE OF DIFFERENT TYPES OF NITROSAMINES

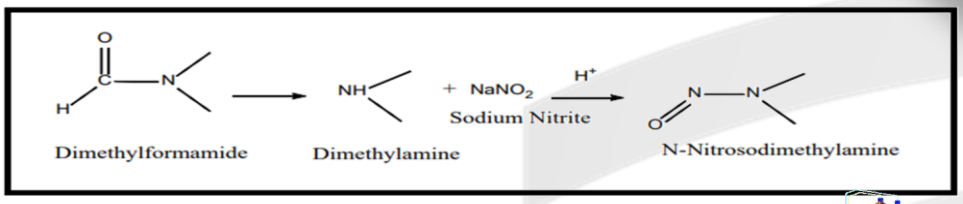
Potential Sources of Nitrosamines

a. Formation during API processing
b. Use of sodium nitrite and secondary or tertiary amine
c. Recycled solvents, catalyst and reagents
d. Packaging components
e. Water, third party recycled solvents and cross contamination

Causes for the formation of nitrosamines

1. The reaction between secondary and tertiary amine with nitrosating agents like nitrite salts under acidic conditions leads to the formation of nitrosamines. In the case of valsartan, during the final stage of manufacturing i.e., the synthesis of tetrazole ring led to high levels of nitrosamine impurity.
2. Nitrosamines can be produced when contaminated reagents or solvents are used
3. In the case of ranitidine, self-degradation leads to the formation of nitrosamine impurity
4. In the case of metformin, the reaction of residual amines with nitrosating agents during primary packaging leads to the formation of nitrosamines

Formation of NMDA



Analytical methodology for identifying nitrosamines

For the assessment of nitrosamines in API and other drug products, the analytical methodology used is reversed-phase liquid chromatography or Gas chromatography combined with mass spectroscopy or nitrogen chemiluminescence. The reference standard is prepared by using a ready-to-use methanol solution thereby limiting the analyst from exposure to carcinogenic effects. Nitrosamines being light-sensitive, requires the preparation of fresh sample or the use of amber-colored containers or light-sensitive containers. since they can degrade at higher temperatures column temperature must be taken care.

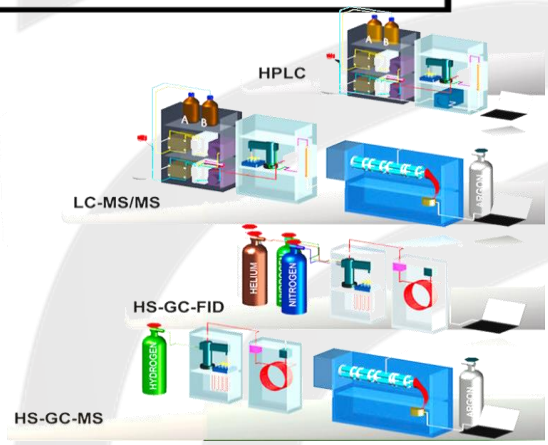


FIGURE 2: VARIOUS DETECTION TECHNIQUES

According to ICH guidelines, the permissible amount of different nitrosamines are discussed below in the table

TABLE 2: DIFFERENT ANALYTICAL TECHNIQUES

GAS CHROMATAGRAPHIC TECHNIQUES	LIQUID CHROMATOGRAPHIC TECHNIQUES	NON CHROMATOGRAPHIC TECHNIQUES
a.GC-FID/GC-ECD is used for the detection of nitrosamines that are oxidized to their corresponding nitramines and also for the detection of heptafluorobutyryl derivatives. b.GC with MS is used for the detection of nitrosamines in drinking water c.GC with NPD (nitrogen phosphorus detector) or NCD (nitrogen chemiluminescence detector) is used where the nitrosamines are pyrolyzed, this liberates NO that is oxidized to NO2 which is then detected d.Other methods like PCI-MS/MS with methanol or ammonia or methane, EI-MS/MS, and high-resolution mass spectroscopy (HRMS) are reported	a.Reversed-phase high-performance liquid chromatography followed by UV detection at wavelength 230-233 nm is used for detecting NDMA impurities b.LC with tandem mass spectroscopy, LC-HRMS, or ion mobility is used with HPLC c.Electrospray ionization or atmospheric pressure chemical ionization is also used d.Liquid chromatographic techniques are more advantageous when compared to other techniques because they can detect both thermally stable and unstable nitrosamines	a.Polarography, direct electrochemical detection with molecularly imprinted polymers, UV photolysis, and chemiluminescence detection is also other non-chromatographic methods used for detecting nitrosamines impurity

TABLE 3: LIMIT OF NITROSAMINES IN DRUG PRODUCTS

NITROSAMINES	LIMIT (ng/day)
NDMA	96
NDEA	26.5
NMBA	96
NMPA	26.5
NIPEA	26.5
NDIPA	26.5

The above limits are accepted if the drug product contains only any nitrosamine. If more than one nitrosamine impurity is present then the limit depends on the maximum daily dose of the drug.

1. If the maximum daily dose is less than 880mg/day, the limit of nitrosamines should not be more than 30ng/day.
2. If the maximum daily dose is more than 880mg/day, the limit of nitrosamine should not exceed 26.5mg/day.

TABLE 4: LIMIT OF NDMA AND NDEA IN DIFFERENT DRUG PRODUCTS

API NAME	NDMA INTERIM LIMITS (PPM)	NDEA INTERIM LIMITS (PPM)
VALSARTAN	0.3	0.083
LOSARTAN	0.96	0.27
OLMESARTAN	2.4	0.66
IRBESARTAN	0.32	0.088
CANDESARTAN	3.0	0.83

Different methods to control nitrosamines in drugs

1. **Use high-quality raw materials:** Ensure that raw materials used in the manufacturing process are of high quality and free from N-nitrosamine impurities. Establish a reliable supplier qualification process and conduct regular audits to ensure the quality of raw materials.
2. **Conduct risk assessments:** Identify potential sources of N-nitrosamine impurities in the manufacturing process and perform risk assessments to evaluate their likelihood and severity. Develop strategies and controls to mitigate the identified risks.
3. **Implement good manufacturing practices (GMP):** Adhere to GMP guidelines to ensure consistent and high-quality manufacturing processes. GMP provides a set of standards and controls that help prevent contamination and ensure product safety.
4. **Monitor and test products:** Regularly monitor and test finished products for the presence of N-nitrosamine impurities. Implement a robust sampling and testing plan to detect any contamination and take appropriate corrective actions.
5. **Use validated analytical methods:** Utilize validated analytical methods that are specific and sensitive to detect and quantify N-nitrosamine impurities accurately. Ensure that the analytical methods are appropriately validated and verified for their intended use.
6. **Implement appropriate cleaning procedures:** Establish and follow appropriate cleaning procedures to prevent cross-contamination between batches. Use cleaning agents and methods that are effective in removing N-nitrosamine residues.

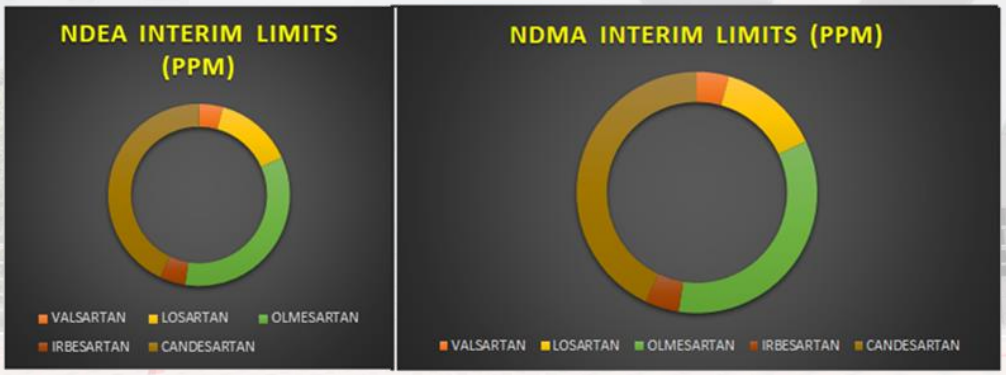


FIGURE 3: GRAPHICAL REPRESENTATION OF THE ABOVE TABLE

6. **Implement appropriate cleaning procedures:** Establish and follow appropriate cleaning procedures to prevent cross-contamination between batches. Use cleaning agents and methods that are effective in removing N-nitrosamine residues.
7. **Control process parameters:** Optimize and control process parameters such as temperature, pH, reaction time, and intermediates to minimize the formation of N-nitrosamines during the manufacturing process. Conduct process validation studies to ensure the effectiveness of the control measures.
8. **Train personnel:** Provide comprehensive training to all personnel involved in the manufacturing process, emphasizing the importance of controlling Nnitrosamine impurities. Train them on proper handling of raw materials, equipment, and finished products to prevent contamination.
9. **Collaborate with suppliers:** Establish a collaborative relationship with suppliers and communicate the importance of N-nitrosamine control. Work closely with them to ensure that raw materials are tested and meet the required quality standards before being used in the manufacturing process.
10. **Stay up-to-date with regulatory requirements:** Continuously monitor and stay informed about the latest regulatory requirements related to N-nitrosamine impurities. Regularly review and update procedures and processes to ensure compliance with regulatory guidelines and expectations.

Implementing these best practices can help pharmaceutical manufacturers effectively control N-nitrosamine impurities, ensuring the safety and quality of their products.

Conclusion

Many agencies around the globe are working on the effects of nitrosamines on humans. The in-vivo studies on rats and mice were found to be positive for hepatic and renal cancer but the same studies on humans are found to be positive for hepatic cancer and negative for renal cancer.

Further studies are still going on and we can not affirmatively conclude any results on the effects of nitrosamines. The root cause for the production of nitrosamine impurity is not known and in the future other causes can be discovered for the production of nitrosamine as an impurity. FDA, EMA, and other regulatory agencies have partnered together and agreed to share all the information on nitrosamine as an impurity in drug products.

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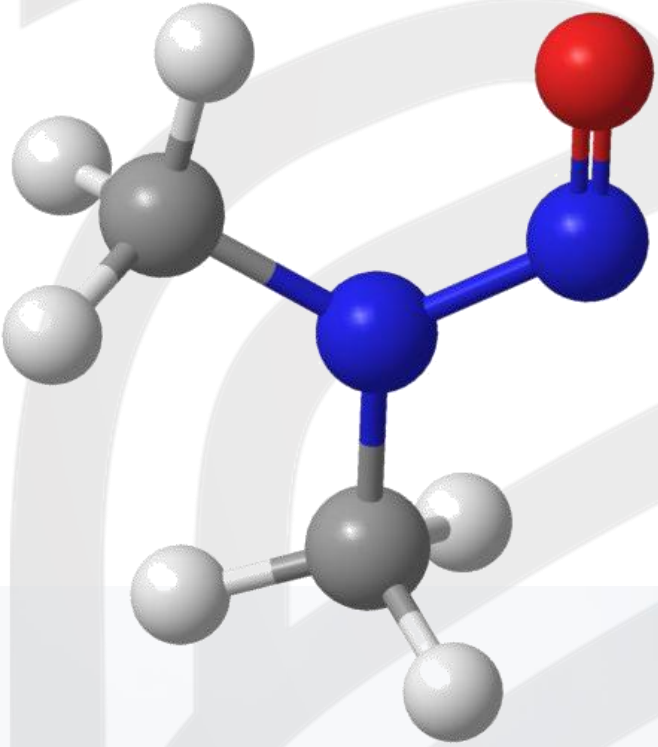

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Harnessing the power of 3,3'-Diindolylmethane (DIM) for Dental Caries Prevention

Abstract

Dental Caries, commonly called as tooth decay is a prevailing cause of concern among children and adults. Streptococcus mutans, an oral bacterium plays an important role in the development of tooth decay. This article explores the wonders of 3'3 Diindolylmethane (DIM) a compound found in cruciferous vegetables, as a natural molecule that prevents dental caries.

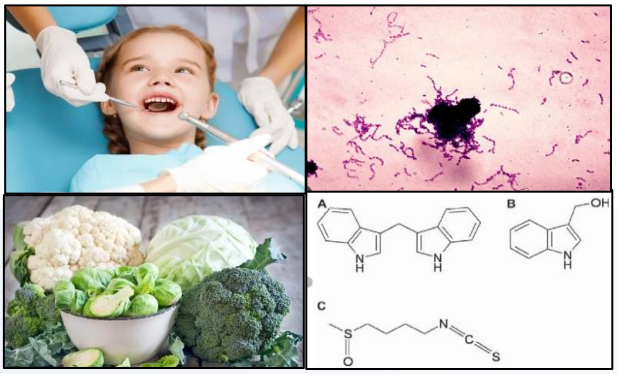

FIGURE 1: Dental Check up and Dental Caries discovery, Streptococcus mutans (Bacteria associated with Dental Caries), DIM is derived from cruciferous vegetables, DIM Molecular structure

Introduction

What is a cavity?

A cavity is a small hole or a hollow space that forms on the surface of the tooth due to the decay of the tooth. This decay is predominantly caused due to the acid-producing bacteria present in the mouth, which demineralizes the enamel (the outermost protective layer of the tooth) and causes damage to the subsequent layers. This dental caries needs to be treated at the earliest. If not, they grow larger causing immense damage and pain to the tooth.

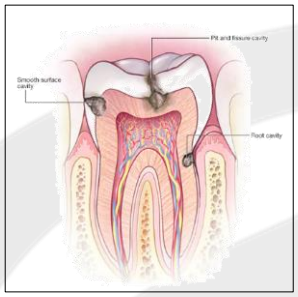

Figure 2: Cavity formation in the tooth

How do cavities develop?

Cavities develop through a process known as Dental Caries. The steps involved are: -

1. Plaque Formation:

Plaque is a sticky colorless film of bacteria that forms a layer on the surface of the tooth. These bacteria consume sugars in the form of glucose, fructose and sucrose from the food and beverages we consume and release acid by the process of fermentation as a byproduct.

2. Acid Attack:

The acid released in the above process erodes the enamel which is the hard, outer protective layer of the tooth

3. Cavity formation:

If demineralization continues for a long period of time it leads to the formation of a small hole called as Dental Cavity. If the decay or cavity is not treated immediately, it can progress deeper in the tooth reaching the soft inner layers such as the pulp.

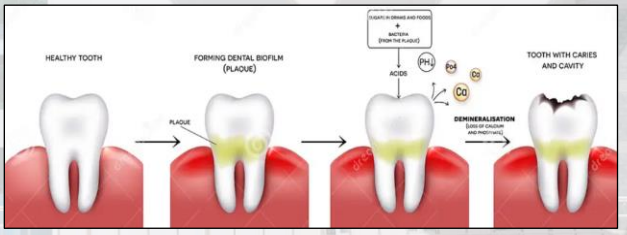

Figure 3: Stages of tooth decay

Methods to prevent tooth decay

1. One must have a good Oral hygiene routine which must include brushing the teeth twice a day with fluoride toothpaste. Fluoride, a mineral prevents the tooth decay from progression and even reverse the effects of early tooth decay. The interdental parts of the mouth must also be cleaned using floss or cleaners.
2. Making healthy food choices, eating a balanced diet filled with nutritious vegetables and fruits. Avoiding snacking and sugary foods and beverages on a daily basis.
3. See a Dentist for regular oral check-ups and professional cleaning.

FIGURE 4: Methods to prevent tooth decay

How to cure tooth decay?

Regular dental checkups can help identify the severity of the cavity. The following are the methods of treatment.

Fluoride Treatments

• If the cavity has just begun, a fluoride treatment may help restore the enamel and has the ability to reverse the cavity in its early stages.

Fillings

• Fillings also called as restorations are done when the decay has progressed beyond the early stage. These are made of various materials such as dental amalgam, tooth colored composite resins

Crowns

• For a weakened tooth, a custom fitted covering that replaces the tooth's entire natural crown is needed.

The dentist's drill all the way down to the decayed part and clean the area. Once the cleaning of the tooth is done, the artificial crown is fitted on to the original tooth.

Root canals

• If the decay reaches the innermost areas of the tooth such as the pulp, a root canal is a must. This treatment method involves removal of the decayed pulp instead of removing the entire tooth

Tooth extractions

• In extreme case of tooth decay, the tooth is extracted and an artificial tooth is implanted.

DID YOU KNOW?

A new and innovative discovery has been made by the Researchers from Ben-Gurion University of the Negev, in collaboration with teams from Sichuan University and the National University of Singapore, that 3,3'-Diindolylmethane (DIM) – a naturally occurring molecule also referred to as bisindole – can reduce biofilms responsible for plaque and cavities by a remarkable 90%.

What is DIM?

3'3 Diindolylmethane is a biologically active dimer derived from the endogenous conversion of indolent-3-carbinol (I3C), a naturally occurring glucosinolate which is found in many cruciferous vegetables.

Most crucifers biosynthesize, the breakdown product of which is Indol-3-carbinol.It is structurally and chemically liable to aqueous acidic media. Mammals secrete gastric juice such as HCL (acidic media) and their gastrointestinal tract is home to a variety of microbes. Once the Indol-3-carbinol comes in contact with this acid in the stomach it gets converted into 3'3 Diindolylmethane commonly called as DIM.

DIM's Mode of Action

The DIM formed in the stomach degrades the biofilms present on the surface of the tooth. Thus, reducing the tooth decay by 90%(as per National Library for Medicine)

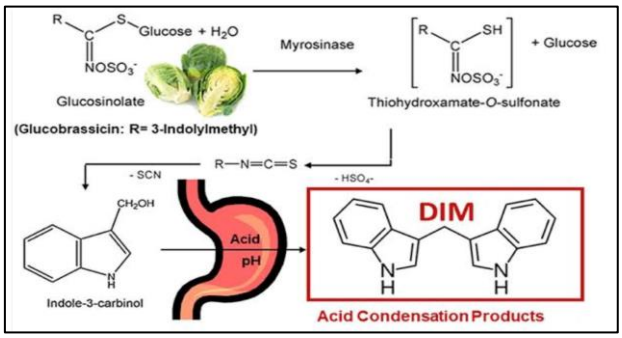

FIGURE 5: Formation of 3'3 Diindolylmethane

Ms. Ananya Krishnamurthy B.Pharm

Dr. BV Suma Asso. Prof

What is a Biofilm?

A biofilm is a community of microorganisms (such as bacteria, fungi, and algae) that adhere to a surface and are encased in a protective matrix of extracellular polymeric substances (EPS). It is a complex, three-dimensional structure that develops on the surface of teeth via the attachment of primary microbial colonizers. They are notoriously difficult to eradicate and can cause many dental complications.

A study published in the National Library of Medicine showed that DIM attenuated the growth of Streptococcus mutans by 92%.

Conclusion

Furthermore, treatment with DIM lowered extracellular polymeric substance (EPS) production and decreased its durability significantly under acidic conditions. Therefore, the anti-biofilm and anti-virulence properties of DIM against Streptococcus mutans bacteria in an "oral setting" provides evidence for its usefulness in reducing biofilm formation and potentially for caries attenuation.

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Departmental Publications

10. Divya B, Mahasin K, Madhushree K, Devika M, Agasa Ramu Mahesh, Saravanan G, Suresh R, R. Sathish Adithya**, Parasuraman P.** Pharmacophore Identification of Alternative HMG-CoA Reductase Inhibitor: A Computational Approach. Bull. Env. Pharmacol. Life Sci., Vol 12[7] June 2023: 186-190
11. Nayana R J, Bandral S K, Genne S, Golla S, Agasa Ramu Mahesh, Selvaraj K, Theivendren P, R. Sathish Adithya, Parasuraman P. Identification of Novel GABA-A Inhibitor For The Treatment Of Epilepsy: A Computational Approach. Bull. Env. Pharmacol. Life Sci., Vol 12[7] June 2023: 180-185.
12. Golla S, Nayana R J, Bandral S K, Genne S, Agasa Ramu Mahesh, Selvaraj K, Theivendren P, R. Sathish Adithya, Parasuraman P. Identification of Novel Lead Moieties as Anti-Cholinesterase Agents: A Computational Approach. Bull. Env. Pharmacol. Life Sci., Vol 12[7] June 2023: 175-179.
13. Vimal John Samuel, Agasa Ramu Mahesh, Sagar Panagante. In Silico Investigation of Mode of Action of Certain Isolated Compounds of Tephrosia Species as Antihyperlipidemic Agents. Bulletin of Environment, Pharmacology and Life Sciences, 12(6); 2023:
14. Soundarya R, Basavana Gowda H D, Brunha S N, Srinivas G, Agasa Ramu Mahesh, Debanjan Sen, Veerasamy Ravichandran, M Aynul Rifaya, Parasuraman Pavadai. Discovering New Lead Moieties as Ace Inhibitors: A Computational Approach. Bulletin Of Environment, Pharmacology and Life Sciences, 12(6); 2023:
15. Srinivas G, Soundarya R, Basavanagowda H D, Brundha S N, Agasa Ramu Mahesh, Debanjan Sen, Veerasamy Ravichandran, M Aynul Rifaya, Parasuraman Pavadai. Identification of Lead Moiety To Inhibit Catechol- O-Methyl Transferase In The Treatment of Parkinson's Disease: A Computational Approach. Bulletin Of Environment, Pharmacology and Life Sciences, 12(6); 2023:
16. Brundha. S N, Soundarya G, Srinivas. G, Basavana Gowda. H D, Agasa Ramu Mahesh, Veerasamy Ravichandran, Debanjan Sen, Deepa R, Parasuraman Pavadai. Evalution of Potential Histamine H2 Receptor Antagonist: A Computational Approach. Bulletin of Environment, Pharmacology and Life Sciences, 12(6); 2023:
17. Basavana Gowda H D, Brunha S N, Srinivas G, Soundarya R, Agasa Ramu Mahesh, Debanjan Sen, Veerasamy Ravichandran, Deepa R, Parasuraman Pavadai. Potent Lead Identification for The Treatment of Depression: A Computational Approach, Bulletin Of Environment, Pharmacology And Life Sciences, 12(6); 2023:
18. Devika Muraleedharan, Divya B, Mahasin Khan, Madhushree K, Agasa Ramu Mahesh, Saravanan Govindaraj, Suresh R, Goutam Hanje, Parasuraman Pavadai, Potent Lead Identification for Cox-2 Enzyme: A Computational Approach, Bulletin of Environment, Pharmacology And Life Sciences, 12(6); 2023:
19. Madhushree K, Devika M, Divya B, Mahasin Khan, Radhika N, Agasa Ramu Mahesh, Saravanan Govindaraj, Suresh R, Goutam Hanje, Parasuraman Pavadai, Potent Lead Identification Against Xanthine Oxidase for The Treatment of Gout: A Computational Approach. Bulletin of Environment, Pharmacology and Life Sciences, 12(6); 2023:

Departmental Publications

20. Bandral Sunil Kumar, Genne Soujanya, Golla Sireesha, Nayana Ravindra Jawale, Agasa Ramu Mahesh, Selvaraj Kunjiappan, Theivendren Panneerselvam, S. Kanimozhi, Parasuraman Pavadai. Identification of Potent Lead to Inhibit DHFR for The Treatment of Cancer: A Computational Approach. Bulletin Of Environment, Pharmacology and Life Sciences, 12(6); 2023:

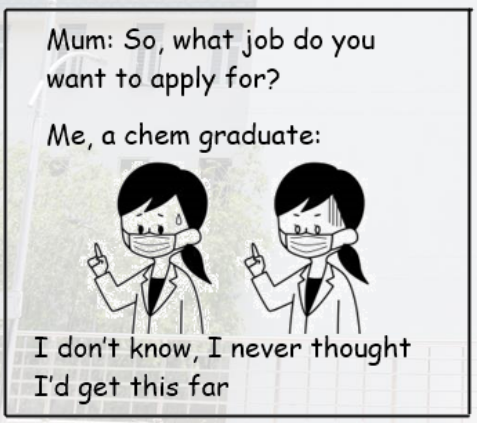
21. Genne Soujanya, Golla Sireesha, Nayana Ravindra Jawale, Bandral Sunil Kumar, Agasa Ramu Mahesh, Selvaraj Kunjiappan, Theivendren Panneerselvam, R. Sathish Adithya, Parasuraman Pavadai. Identification of Novel Lead to Inhibit HIV Protease: A Computational Approach. Bulletin of Environment, Pharmacology and Life Sciences, 12(6); 2023:

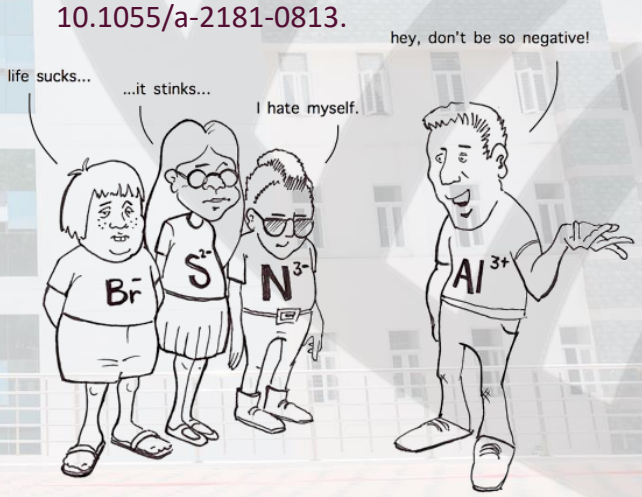
22. Richa Sood, Darshitha, Agasa Ramu Mahesh, Seema S. Rathore, Josephine Leno Jenita. Synthesis of Zinc Oxide Nanoparticles using Centella asiatica. Advances in Pharmacology and Pharmacy 11(4): 270-278, 2023. DOI: www. 10.13189/app.2023.110404

23. Ruthu V, Sadath Abdulla, Nikitha GR, Sagar DLN, Agasa Ramu Mahesh, Rekha S. Phytochemical Screening of Oils from Gossypium Barbadense and Nelumbo Nucifera on Human Lung Fibroblast Shows Free Radical Scavenging Activity. Eur. Chem. Bull. 2023, 12(Special Issue 5), 01 - 09

24. 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

25. Ramesh S, Almeida SD, Hammigi S, Radhakrishna GK, Sireesha G, Panneerselvam T, Vellingiri S, Kunjiappan S, Ammunje DN, Pavadai P. A Review of PARP-1 Inhibitors: Assessing Emerging Prospects and Tailoring Therapeutic Strategies. Drug Res. 2023. Advance online publication. doi: 10.1055/a-2181-0813.





Departmental Presentations

1. Aleesha, AR Mahesh presented a Poster on topic Isolation and characterisation of phytochemicals from roots and aerial parts of Boerhaavia Diffusa in Convention on drug discovery and development 2023 organised by College of Pharmaceutical Sciences, Dayananda Sagar University Bengaluru on 18th & 19th October 2023.

2. Dr. Yuvapriya presented a Poster on topic Insilico studies of HER 2 inhibitors for treatment of breast cancer in Convention on drug discovery and development 2023 organised by College of Pharmaceutical Sciences, Dayananda Sagar University Bengaluru on 18th & 19th October 2023.

3. Genne Soujanya, Kamatchi Sundara Saravanan and Lakshmi M. Sundar presented a Poster on topic In Silico Analysis of *Carica papya* leaf Chloroform Fraction as Anti-inflammatory agent in Exploring the Frontiers of In Silico Drug Discovery: Trends, Challenges and Opportunities organised by Faculty of Pharmacy, Ramaiah University of Applied Sciences Bengaluru on 28th July 2023.

4. Basavanna Gowda H D, Srinivas G, Girinath G Pillai and Lakshmi M. Sundar presented a Poster on topic Identification and Biological Evaluation of novel Anti-tubercular Agents using Artificial Intelligence based Approach in Exploring the Frontiers of In Silico Drug Discovery: Trends, Challenges and Opportunities organised by Faculty of Pharmacy, Ramaiah University of Applied Sciences Bengaluru on 28th July 2023.

5. Arunkumar. C, Kushboo . B, Nandita Ravi, R. Samyuktha and Lakshmi. M. Sundar presented a Poster on topic In-Silico Prediction of ADMET Properties of Alkaloids and Flavonoids Screened for Anti Dengue Activity in National Conference on Paradigm Shift to AMPs in handling Microbial infection organised by T. John College of Pharmacy Bengaluru on 9th September 2023.

6. Devika Muraleedharan, K Sundara Saravanan and Lakshmi M. Sundar presented a Poster on topic In Silico Exploration of Papaya Leaf Alkaloids as Potential Cytokine Storm Inhibitors in Convention on Drug Discovery and Development 2023 organised by College of Pharmaceutical Sciences, Dayananda Sagar University Bengaluru on 18th October 2023.

7. Dr. Judy Jays presented a Oral presentation on topic Synthesis, in silico molecular docking , ADME prediction and biological evaluation of some novel isoxazoles as plausible inhibitors of S.aureus in International Conference on recent developments on green and sustainable developments organised by Akal University Punjab on 6th -8th September 2023.

8. Shannon D Almeida, H R Sameera, Govardhan K R, Golla Sireesha, Soundarya R, Damodar Nayak A, Parasuraman Pavadai presented on Anti-Parkinsonian Potency of S-Carboxymethyl-L-Cystine Solid Lipid Nanoparticles in Murine and Zebrafish Model in International Conference on Applications of Natural Products Nanomaterials and Nano- pharmaceuticals (ICAN3), School of Life Sciences B.S. Abdur Rahman Crescent Institute of Science and Technology, Chennai, India on 9th and 10th August, 2023.

Departmental Presentations

9. Shannon D Almeida, H R Sameera, Govardhan K R, Golla Sireesha, Soundarya R, Damodar Nayak A, Parasuraman Pavadai presented on Anti-Parkinsonian Potency of S-Carboxymethyl-L-Cystine Solid Lipid Nanoparticles in Murine and Zebrafish Model in International Conference on Applications of Natural Products Nanomaterials and Nano- pharmaceuticals (ICAN3), School of Life Sciences B.S. Abdur Rahman Crescent Institute of Science and Technology, Chennai, India on 9th and 10th August, 2023.

10. H R Sameera, Govardhan K R, Shannon D Almeida, J Anbu, Damodar Nayak A, Parasuraman Pavadai, Golla Sireesha, Soundarya R presented on the topic "Exploring the therapeutic potential of the test formulation against cardiovascular complications using murine and alternative animal model" In the International Conference on Applications of Natural Products Nanomaterials and Nano-pharmaceuticals (ICAN3) at School of Life Sciences, B.S. Abdur Rahman Crescent Institute of Science and Technology, Chennai, India on 9th and 10th August 2023

11. Govardhan K R, H R Sameera, Shannon D Almeida, Golla Sireesha, Soundarya R, J Anbu, Damodar Nayak A, Parasuraman Pavadai presented on the topic "Drug Entangled Carbon Nanotube against breast cancer: A Computational and Pharmacological approach" In the International Conference on Applications of Natural Products Nanomaterials and Nano-pharmaceuticals (ICAN3) at School of Life Sciences, B.S. Abdur Rahman Crescent Institute of Science and Technology, Chennai, India on 9th and 10th August 2023.

12. Damodar Nayak A, Anbu Jayaraman, Parasuraman P, Selvaraj K presented on the topic "Exploring The Possible Mechanisms of Nattokinase in Ameliorating Cardiovascular Diseases: An In-Silico Approach" In the International Conference on Applications of Natural Products Nanomaterials and Nano-pharmaceuticals (ICAN3) at School of Life Sciences, B.S. Abdur Rahman Crescent Institute of Science and Technology, Chennai, India on 9th and 10th August 2023.

13. G Swathi Reddy, Suma B V, Brunda SN presented on the topic "Drug repurposing on epilepsy" in the Convention on drug discovery and development at Dayananda Sagar University, Bangalore on 17th -18th October 2023.

14. A.N.Sneha, Suma B V, Brunda SN presented on the topic "Drug repurposing on fatal familial insomnia" in the Convention on drug discovery and development at Dayananda Sagar University, Bangalore on 17th-18th October 2023

15. Y.A.Srija, Suma B V, Brunda SN presented on the topic "Drug repurposing on emerging liver cirrhosis" in the Convention on drug discovery and development at Dayananda Sagar University, Bangalore on 17th-18th October 2023

16. Janani N, Suma B V, Brunda SN presented on the topic "Drug repurposing on emerging multiple myeloma" In the Convention on drug discovery and development at Dayananda Sagar University, Bangalore on 17th-18th October 2023.

Departmental Presentations

17. Vivan Ranjan Paitpal, Suma B V, Brunda SN presented on the topic "Drug repurposing on emerging nystagmus" In the Convention on drug discovery and development at Dayananda Sagar University, Bangalore on 17th-18th October 2023.

18. Sai Baalaajee, Suma B V, Brunda SN presented on the topic "Drug repurposing on thyroid eye disease" In the Convention on drug discovery and development at Dayananda Sagar University, Bangalore on 17th-18th October 2023.

19. Apeksha K Hegde, Suma B V presented on the topic "Computational Analysis of EFGR Target for treating Paronychia: unveiling Molecular Insights" In the Convention on drug discovery and development at Dayananda Sagar University, Bangalore on 17th-18th October 2023.

20. Shreya Shet, Suma B V presented on the topic "Discovery of Streptococcus mutans Glucosyltransferase -B (GTFB) Inhibitors Using Computational Approaches" In the Convention on drug discovery and development at Dayananda Sagar University, Bangalore on 17th-18th October 2023.

21. Sandra Ross O S, Govardhan K R, H R Sameera, Shannon D Almeida, Golla Sireesha, Soundarya R, J Anbu, Damodar Nayak A, Parasuraman Pavadai presented on the topic "Drug-Entangled Multi-Walled Carbon Nanotubes Against Breast Cancer: A Computational and Pharmacological Approach" In the National Conference on Translational Research in Drug Development TRDDCON – 2023 at Manipal College of Pharmaceutical Sciences, Manipal Academy of Higher Education on 2nd – 4th November 2023.

22. Devika Murileedharan, Parashuram P, Judy Jays. "Unlocking Therapeutic potential: Targeted inhibition of diabetic nephropathy through molecular docking and pharmacophore mapping."4th World Congress on Drug Discovery and Development-2023 by Biogenesis Health Cluster held on 29th October 2023.

23. Anjana Srivatsa, Judy Jays. "Bioluminescent algae as potential biomarkers for avoiding subsequent myocardial infarction".4th World Congress on Drug Discovery and Development-2023 by Biogenesis Health Cluster held on 29th October 2023.

24. Protyusha Maji, Judy Jays "Discovering Innovative Cardiovascular Therapies through Molecular Docking and Pharmacophore Mapping. 4th World Congress on Drug Discovery and Development-2023 by Biogenesis Health Cluster held on 29th October 2023.

25. Pradan P Jain, Judy Jays. 'Design, molecular Docking studies, synthesis and characterization of some novel furan derivatives for potential anticancer activity.' Drug Design and evaluation: Current scenario organized by RR College of Pharmacy in association with Karnataka State Pharmacy Council on 30th September 2023

Invited Lectures

The Department of Pharmaceutical Chemistry at MS Ramaiah University of Applied Sciences (RUAS) takes immense pride in acknowledging the notable achievements of our esteemed faculty members who have actively contributed to academic events, sharing their expertise and insights in diverse forums. The following is a staff-wise achievement report based on their engagements:

Dr. Judy Jays

1. Delivered a Guest Lecture on "Interactive Session on Gender Sensitivity" at the College of Physiotherapy, RUAS, on 10th July 2023.

Dr. Parasuraman P

1. Delivered a Guest Lecture on "An Overview of Computer-Aided Drug Design" at RR College of Pharmacy, Bangalore, Karnataka, India, on 22nd July 2023.

2. Participated as a resource person in an e-FDP on "Fostering the Drug Design Via Artificial Intelligence and Sanctifying Molecular Docking Studies" at the School of Pharmaceutical Sciences, Vels Institute of Science, Technology & Advanced Studies, Chennai, Tamil Nadu, India, on 24th July 2023.

3. Conducted a lecture on the "Nitty and Gritty of Computer-Aided Drug Design" at Nargund College of Pharmacy, Bengaluru, on 8th August 2023.

4. Presented a lecture on "An Overview of Computer-Aided Drug Design" at the Department of Biotechnology, MS Ramaiah Institute of Technology, Bengaluru, on 11th August 2023.

5. Participated as a poster evaluator for "Computational Drug Discovery and Development" at Dayanand Sagar University, Bangalore, on 18th-19th October 2023.

6. Conducted a hands-on training cum workshop on "Drug Discovery, Molecular Docking, and Dynamic ADMET Studies" at the Department of Pharmacology, RVS College of Pharmacy, Coimbatore, Tamil Nadu, India, on 3rd November 2023.

7. Engaged in a one-week National Level Faculty Development Program (e-FDP) on "Teaching and Learning Computational Drug Design: The Road Ahead" at "Pharmaceutical Education: Trends & Tools (PET-2023)" on 18th December 2023.

Invited Lectures

Dr. AR Mahesh

1. Delivered a lecture on "Exploring the Power of Computational Drug Design: Revolutionizing Medicinal Discovery" at Nargund College of Pharmacy, Bengaluru, on 8th August 2023.

2. Shared insights on "Applications of QSAR in Drug Design" during a lecture at the Department of Biotechnology, MS Ramaiah Institute of Technology, Bengaluru, on 11th August 2023.

3. Contributed as a Guest Lecturer on "Unleashing the Potential of Computer-Aided Drug Design (CADD) in Drug Discovery" at SET's College of Pharmacy, Dharwad, on 30th September 2023.

4. Contributed to a Faculty Development Program on Education Methodology titled "Empowering Educators: Instruction and Evaluation Methodologies" at Al-Shifa College of Pharmacy, Kerala, from 21st November 2023 to 25th November 2023 where he chaired various sessions across 5 days, covering topics such as Education as a System, Learning Theories and Psychology of Education, Educational Objectives, Microteaching, and Objective-Structured Practical Examination.

•The department extends its sincere congratulations to these accomplished faculty members for their outstanding contributions to academia, enriching the academic and research landscape in pharmaceutical chemistry. Their efforts truly exemplify the commitment to excellence upheld by the Department of Pharmaceutical Chemistry at RUAS.

"International E-Conference on Exploring the Frontiers of In-silico Drug Discovery: Trends, Challenges, and Opportunities"

The International E-Conference on Exploring the Frontiers of Insilico Drug Discovery, hosted by the Department of Pharmaceutical Chemistry at the Faculty of Pharmacy, RUAS, unfolded on the 28th of July 2023, garnering an enthusiastic response with a remarkable 270 registrations. The conference aimed to delve into the contemporary advancements and challenges within insilico drug discovery, with a keen focus on AI & ML in Drug Design Virtual Screening, Pharmacophore Modelling, and QSAR/QSPR Modelling. The event provided a dynamic platform for researchers to present their cutting-edge work, featuring a total of 78 E-Poster presentations in AI & ML in Drug Design Virtual Screening.

The day commenced at 9:30 am with an inaugural function chaired by Dr. Bharath, the Dean of the Faculty of Pharmacy at RUAS. Dr. AR Mahesh, Assistant Professor in the Department of Pharmaceutical Chemistry, provided an overview of the conference, setting the tone for the day. The keynote address, delivered by Dr. Kuldeep Kumar Raina, the Vice Chancellor of RUAS, offered valuable insights into the current trends in drug discovery.

The scientific sessions were enriched by eminent speakers such as Dr. Akshatha Ganne from the University of Arkansas for Medical Science, USA, Prof. Ravichandran from AIMST University, Malaysia, and Dr. Chandrabose Selvaraj from Saveetha University, India. The afternoon session featured 78 E-Poster presentations, showcasing the diverse and innovative research undertaken by participants in the realm of computational drug discovery.

The valedictory session, chaired by Dr. Govind R Kadambi, Pro Vice Chancellor of RUAS, marked the conclusion of the conference. Noteworthy contributions were acknowledged through the announcement of the best poster awards, recognizing outstanding achievements in the field. The event concluded with a vote of thanks by Dr. Parasuraman P, Assistant Professor in the Department of Pharmaceutical Chemistry, FPH. He expressed gratitude to all participants, volunteers, and organizers for their collective efforts in ensuring the success of the conference.

The success of the International E-Conference on Exploring the Frontiers of Insilico Drug Discovery is a testament to the dedication and hard work of Dr. Parasuraman, Dr. AR Mahesh, and the entire faculty and student body of the Department of Pharmaceutical Chemistry. The invaluable contribution of student volunteers played a pivotal role in ensuring a seamless and enriching experience for all attendees.

This e-conference stands as a significant platform for knowledge exchange, collaboration, and the advancement of insilico drug discovery methodologies. It has contributed to the growth of this field, fostering innovation and pushing the boundaries of scientific exploration.

Awards

Congratulating Dr. Vijaybhanu. P on successful Defence of PhD

A Visionary Thesis: "Synthesis, Characterization and In Vitro Evaluation of Anticancer Potential of Curcumin-Drug Conjugate and Pharmacokinetic Studies"

Vijaybhanu. P, currently working as Assistant Professor in the Department of Pharmaceutical Chemistry has successfully defended her Ph. D Thesis titled "Synthesis, Characterization and *In Vitro* Evaluation of Anticancer Potential of Curcumin-Drug Conjugate and Pharmacokinetic Studies" on 17th August 2023. The research work was carried out under the guidance of Dr. D. R. Harish Kumar, Professor and HoD, Department of Pharmaceutical Chemistry, RUAS. The research focused on synthesis of curcumin-metformin conjugate and evaluation of this conjugate for *in vitro* cytotoxic activity. The pharmacokinetic profile of the synthesized conjugate was studied and compared with that of pure curcumin.

Congratulating Dr. Jabeen on successful Defence of PhD

A Visionary Thesis: "Development and Validation of Analytical Method for Determination of Selected Cephalosporin in Active Pharmaceutical Ingredient and its Formulation"

The Faculty of Pharmacy congratulates Ms. Jabeen on completing her Ph.D. under Dr. Suma B.V.'s guidance at M.S. Ramaiah University of Applied Sciences. Dr. Jabeen's research in Pharmaceutical Analytical Chemistry, mentored by Dr. Suma B.V., explores new-generation Cephalosporins and a beta-lactamase inhibitor, utilizing advanced techniques like UPLC-MS/MS for method development and validation. Adhering to ICH guidelines, the study showcases the efficacy of hyphenated analytical techniques. Noteworthy achievements include the first validated UPLC-MS/MS method for Ceftaroline Fosamil estimation and dentification of new Cefepime degradants.

Published articles:

- Jabeen & Suma B.V., (2022). "Newly Validated Stability-Indicating Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry Method for the Estimation of Ceftaroline Fosamil by Using a Quadrupole Mass Detector." J Appl Pharm Sci. 12, 06, 215–223.
- Jabeen, Suma B.V., (2022). "A Critical Review of Analytical Methods for Determination of Ceftaroline Fosamil." J Res Med Dent Sci, 10 (8):91-95.
- Jabeen, Suma B.V., (2023). "Stability Indicating UPLC-MS/MS Method for Quantification and Identification of Cefepime and Its Degradants in API." J Appl Pharm Sci. 2023.
- Suma B.V., (2023). "Simultaneous Determination of Cefepime and Tazobactam by Using Hyphenated Liquid Chromatography (UPLC-MS/MS)." Research Journal of Pharmacy and Technology [Accepted and to be published in the year 2024; vol 17(2)

Additionally, Dr. Jabeen has actively participated in various conferences, presenting both posters and oral presentations. For a comprehensive overview, please refer to the list provided below:

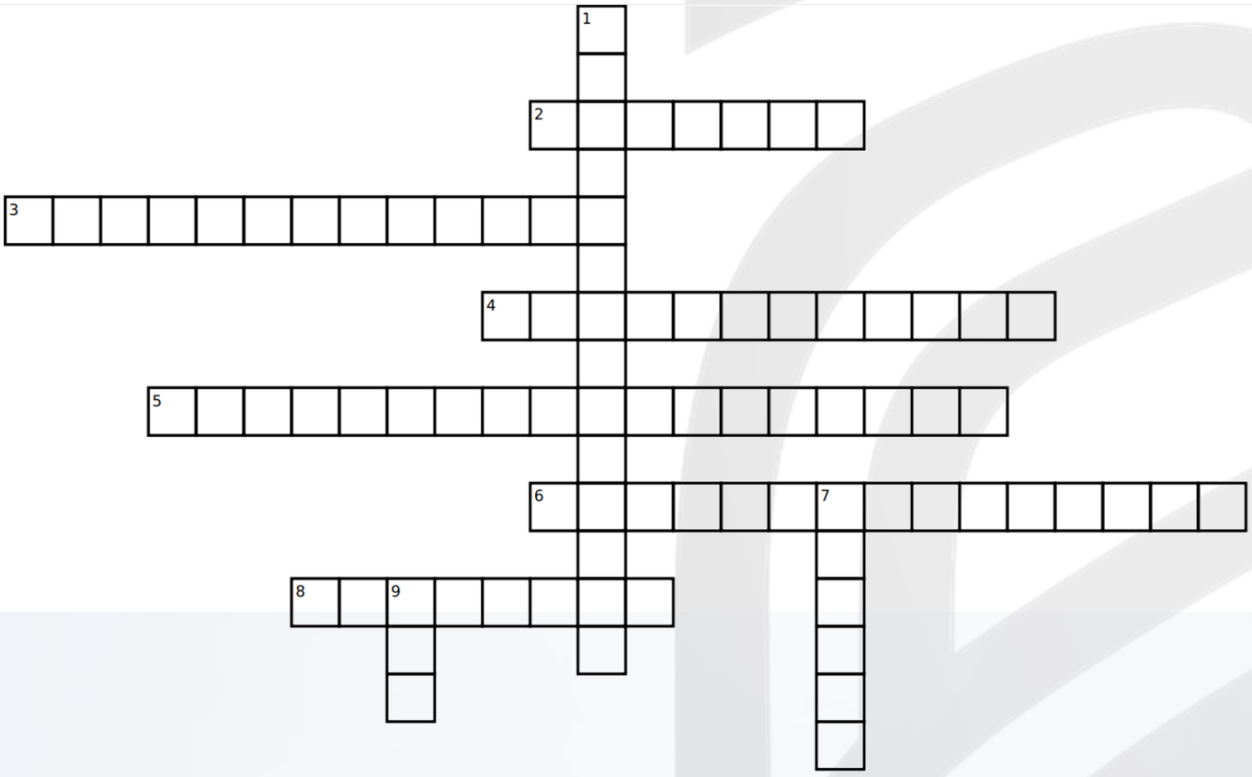
Poster Presentations:

- Jabeen. "Method development and validation of Ceftaroline Fosamil By Using UPLC-MS/TS." Pharmaceutical And Healthcare Challenges In Global Transformation, 11th Apr 2022. VIPER, Narsapur, India.
- Jabeen. "Newly Validated Stability Indicating UPLC–Tandem MS Method for Estimation of Ceftaroline Fosamil by Using Quadrupole Mass Detector." Trending research and innovations in pharmaceutical sciences, 22nd – 23rd Jul 2022. Anurag University (School of Pharmacy), Hyderabad.

Oral Presentation:

- Jabeen. "Simultaneous Determination Of Cefepime And Tazobactam By Using Hyphenated Liquid Chromatography (UPLC-MS/MS)." Challenges and opportunities in pharmaceutical sciences, 29th October 2022. JNTUH University of Pharmaceutical Sciences, Sultanpur, India.

Crossword



Down:

1. The science of predicting the structure and function of biological molecules using computer simulations
7. database of known drugs and their properties used in drug discovery research
9. A common file format for storing molecular structures

Across:

2. A fundamental component of many drug discovery models, representing the specific binding of a molecule to its target
3. Software tools that allow scientists to visualize and analyze molecular structures
4. The branch of biology that focuses on the functions and interactions of biomolecules
5. A type of molecular modeling technique that uses energy minimization to find the stable conformation of a molecule
6. The branch of chemistry that studies the three-dimensional arrangement of atoms in molecules
8. This type of modeling uses mathematical equations to describe the behavior of biological systems

CONDOLENCE

Tagore S

B.Pharm Final Year (2020 Batch)

2002 - 2023

Our hearts are heavy with grief due to the untimely death of our dear student Tagore S on 09th Dec 2023. His family is in our thoughts and prayers.

Faculty of Pharmacy & Management
Ramaiah University of Applied Sciences

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