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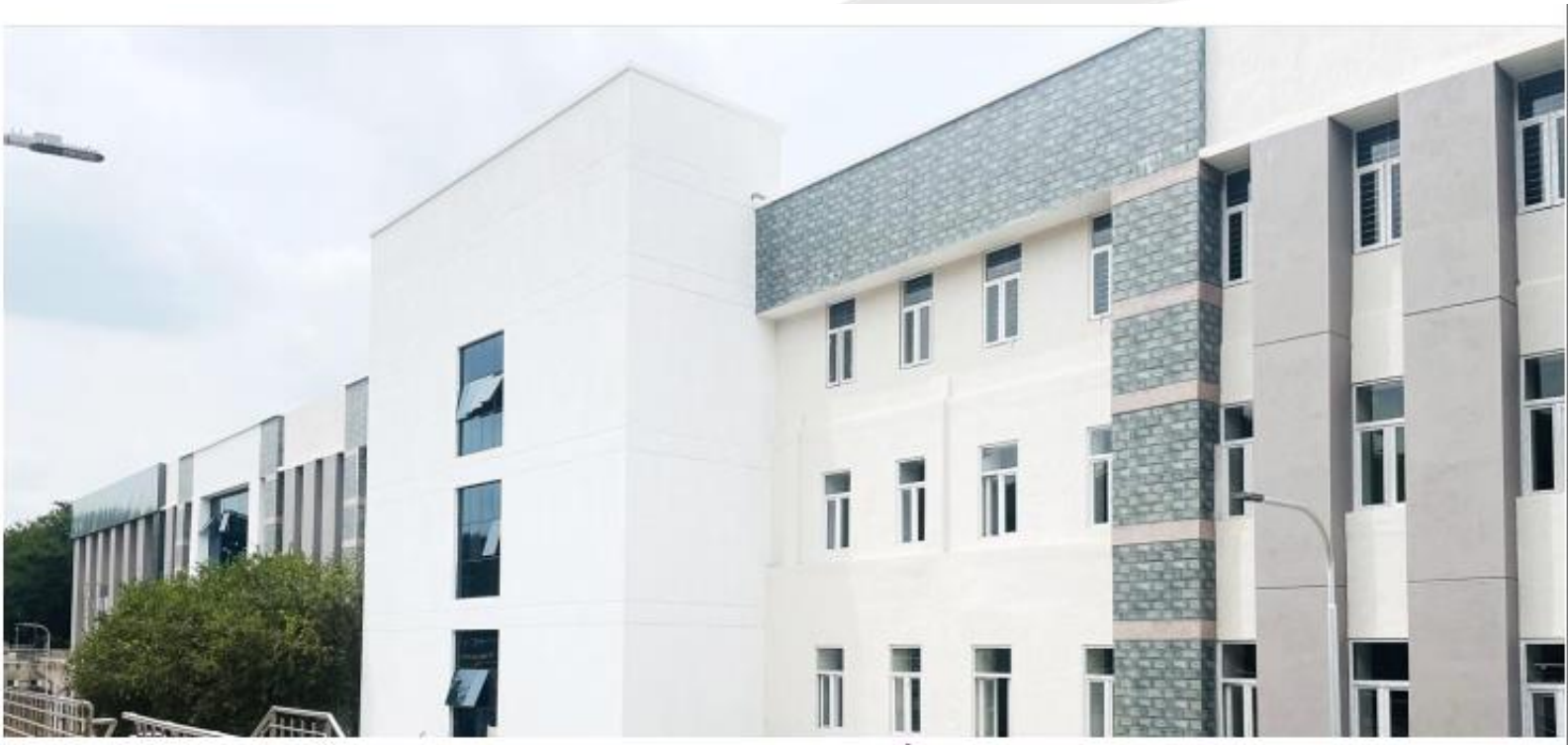
Celebrating 100 Years of Karmayogi



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Contents

Education- My View point

Education is a continuous process, which involves many small (may not be recognizable) steps to be taken by the facilitators including teachers, mentors in shaping an individual to become a cultured and a responsible citizen of the Nation.

Education is not limited to just getting a diploma / UG degree / PG degree / PhD degree, but a medium to understand and differentiate the good versus bad aspects relating to our society as a whole.

In achieving this goal, one has to have a lot of perseverance keeping in mind that achieving the target is important but the path chosen to achieve the target is even more important and essential. When a person, as I perceive, tries to tread the right path even though he faces many hurdles will achieve the targeted goals of life. Further, while treading this path, the individual will be learning various techniques, strategies, capabilities in achieving the right goal.

Lately, we are getting confused between the two terms 'educated' and 'literate', thinking that they both are synonyms and sometimes may be true. People may be literate but may not be educated. An illiterate may be considered as educated if the individual thinks about the welfare of the society and many times the reverse may not be true.

Presently, our society is facing a lot of problems basically due to, in my opinion, lack of values or values influenced by external dynamics and also the way we impart education - concentrating more on the goal rather than the path we tread to achieve it.

Hope the new education policy proposed by the Government may set right certain existing anomalies / shortcomings.

Nevertheless, we as a society have to be more enlightened, vigilant and work to facilitate our young minds in achieving new pinnacles to lead and show the right path to the whole world and fly our tricolor even higher among those of various other nations of the world.

Jai Hind

Prof. M. Narayana Babu,
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Research & Reviews

IBUPROFEN: ACTUAL VERSUS GREEN SYNTHESIS

Genne Soujanya, M.Pharm 2nd Semester

Introduction

Ibuprofen is a FDA- approved drug, widely used to treat inflammatory diseases. It is also approved to treat mild to moderate pain and readily accessible as a non-prescription drug for pain. It's chemical formula $C_{13}H_{18}O$ (Ngo, V.T. & Bajaj, T., 2022, Fig-1).

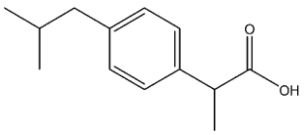


Figure 1 *Structure of Ibuprofen*

Ibuprofen is a non-selective inhibitor of an enzyme cyclooxygenase (COX). This enzyme is essential for the prostaglandin's (PG) synthesis through the arachidonic acid pathway. The COX is required for the conversion of arachidonic acid to PG in the human body. Ibuprofen restricts the COX enzyme, which is used to prepare the PGs, thus it decreases the level of PGs (ibuprofen/ mechanism of action [Accessed 24 Oct.2022])

Synthesis of Ibuprofen: The synthetic method created by Boots pure drug Company-UK contained six stages for Ibuprofen synthesis with stoichiometric reagents, moderately low atom efficiency and significant inorganic salt arrangement (Muresan, A., 2018)

Steps involved in the synthesis of Ibuprofen are shown in figure 2

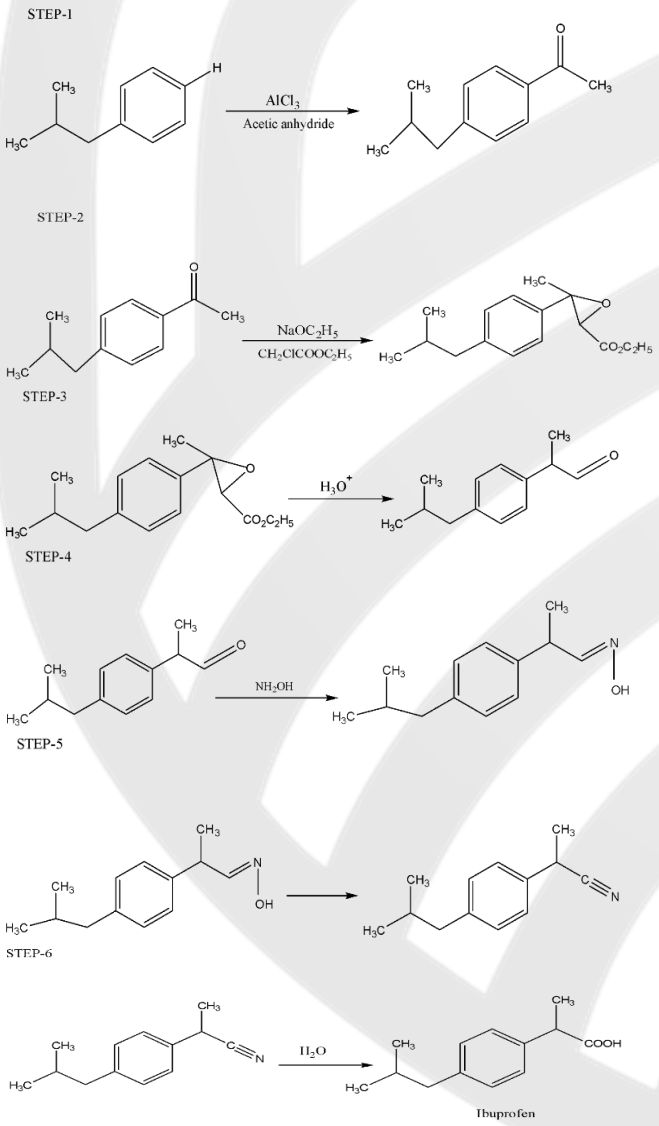


Figure 2 *Steps involved in the synthesis of Ibuprofen*

In step-1 isobutyl benzene undergoes acetylation by acetic anhydride presence of aluminium chloride and by product as acetic acid and atom economy is 74.58% which is calculated by the given formula

Atom economy (%) = mass of atoms in desired product/ mass of atoms in reactants X 100

Atom Economy: The number of atoms from the starting material that are still present in the useful products after a chemical reaction is complete is known as the atom economy. Unnecessary side products from reactions might result in less efficient atom utilization and higher waste. Atom economy, which compares the amount of useful product obtained to the amount calculated theoretically is often a better indicator of reaction efficiency than yield. So, it makes sense to choose processes that maximize atom economy (Twelve Principles of Green Chemistry, Compound interest [2015])

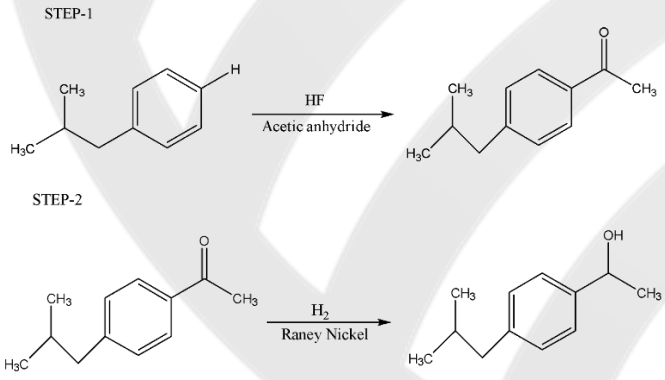
In step 2, three reactants are involved and shows atom economy of 71.49%. In original pathway of synthesis every step shows less atom economy as shown in the table 1

Green Synthesis: A new route was developed for Ibuprofen synthesis in 1980's called green synthesis which involves only three steps and shows high atom economy. This new route was created by Boots-Hoechst-Celanese (BHC) Company (USA). Green chemistry is to diminish the chemical related influence on humans and also on environment. C.Warner and T. Anastas developed twelve principles for green chemistry in 1991. They are 1) Waste prevention 2) Atom economy 3) Less hazardous chemical synthesis 4) Designing safer chemicals 5) Safer solvents and Auxiliaries 6) Design Energy Efficiency 7) Use of Renewable feedstock 8) Reduce derivatives 9) Catalysis 10) Design for degradation 11) Real time analysis for pollution prevention 12) Inherently safer chemicals for accident prevention.

Table 1 *Atom economy of each step involved in the synthesis of ibuprofen*

Reactions steps	Reagent chemical - formula	Relative molecular mass of used Reagents	Relative molecular mass of used Products	Relative molecular mass of by-products/waste	Atom economy (%)
Step 1	$C_{10}H_{14}$	134.0	176.0	60.0	74.58
	$C_4H_6O_3$	102.0			
Step 2	$C_{12}H_{16}O$	176.0	366.5	104.5	71.49
	$C_4H_7O_2Cl$	122.5			
	C_2H_5ONa	68.0			
Step 3	$C_{16}H_{22}O_3$	262.0	281.0	91.0	67.61
	H_3O	19.0			
Step 4	$C_{13}H_{18}O$	190.0	223.0	18.0	91.93
	NH_3O	33.0			
Step 5	$C_{13}H_{19}NO$	205.0	187.0	18.0	91.22
Step 6	$C_{13}H_{17}NH_4O_2$	187.0	182.0	17.0	92.38
		36.0			

Here also same starting materials like original synthesis i.e., isobutyl benzene and acetic anhydride but the catalyst used in green route was Hydrogen fluoride, because this solvent is non-toxic to humans and produce less waste and more atom economy. The by-products formed in first step was utilized in another reaction. In second step Raney nickel and hydrogen was used as catalysts and this reaction was carried out at normal room pressure and temperature. In step-3 CO and Pd catalysts are used and all these catalysts can be recycled and reused. By-products formed in green route was less compare to original synthesis. (Muresan, A.., 2018). Steps involved in the green synthesis of Ibuprofen as shown in the below figure-3



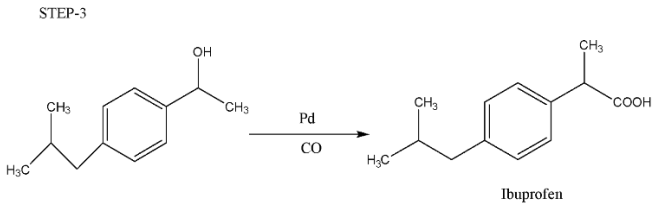


Figure 3 *Steps involved in green synthesis of Ibuprofen*

The atom economy was 74.58% in the first step of green route, the second step has atom economy of 100.0% and in the last step also atom efficiency was 100.0% (Table -2). In green route, atom efficiency was maximum due to the usage of safer solvents and catalyst and this route is eco-friendly and can complete the synthesis within three steps and waste production is minimum.

Table 2 *Atom economy in the green synthesis of ibuprofen*

Reactions steps	Reagents chemical formula	Relative molecular mass of used Reagents	Relative molecular mass of Products	Relative molecular mass of by-products or waste	Atom Economy, (%)
Step 1	$C_{10}H_{14}$	134.0	176.0	60.0	74.58
	$C_4H_6O_3$	102.0			
Step 2	$C_{12}H_{16}O$	176.0	178.0	0.0	100.0
	H_2	2.0			
Step 3	$C_{12}H_{18}O$	178.0	206.0	0.0	100.0
	CO	28.0			

Conclusion

In the synthesis of Ibuprofen using two routes, it could be observed that the conventional method has six steps and formed more by-products, lots of waste and low energy efficiency. Atom efficiency for entire original synthesis of Ibuprofen was only 40.48%. Whereas, in green synthesis of Ibuprofen only three steps are involved; solvents and reagents used in this pathway were easily recyclable. By products formation was minimum with more atom efficiency (77.44%). This green synthetic route was environmentally friendly and non-toxic to human beings, nowadays this route is preferred compare to original Ibuprofen synthesis.

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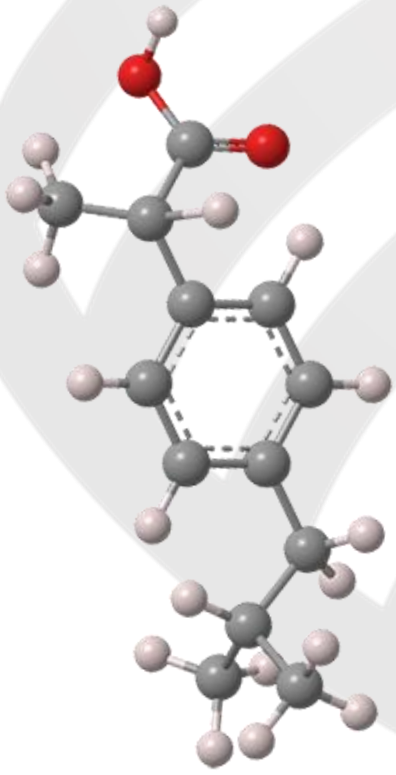

CURRENT TRENDS IN DEVELOPMENT OF ANTI-TB DRUGS

SRINIVAS G, M.Pharm 2nd Semester

Introduction:

Robert Koch discovered *Mycobacterium tuberculosis*, the organism that causes tuberculosis (TB) infection, in 1882. TB medications is the typical four-drug combination which is moderately priced and effective in drug-sensitive (DS) TB patients.

Isoniazid, rifampin, pyrazinamide, and ethambutol are administered daily over a period of 6 to 9 months as part of the four-drug regimen. However, soon after the first medication, TB drug resistance started to develop. The development of genetic resistance to an antibacterial medication is made possible by chromosomal alterations that take place between 10^{-6} to 10^{-8} times for every mycobacterial replication. Finding and creating a unique antibiotic is a very challenging task, and it is one that is shared with general, broad-spectrum antibacterial medication development. It has been widely reported on the need for new antibiotics and the rarity of such species. Just two novel antibiotic series have been released in the previous 40 years. The current method of antibiotic discovery and development is inherently challenging due to the difficulty in advancing target-based hits and lack of well-established PK-pharmacodynamic paradigms.

Additional obstacles on the TB field include:

Absence of validated and human-like pathophysiology in animal models currently used for drug development, insufficient clinical labs for clinical trials, and insufficient funding for research are all factors adding to the hindrances in the anti-TB drug discovery. According to the World Health Organization (WHO), latent tuberculosis infection (LTBI) is a condition in which the immune system continues to respond to *Mycobacterium tuberculosis* antigens stimulation without showing signs of clinically manifested active TB and with bacillary replication absent or below some unspecified threshold due to immunological control. In around 5–15% of people with pulmonary TB infection during the course of their lifetime, active TB illness either manifests within 1-2 years of infection or when latent infection is reactivated. Three axes, including disease pathophysiology and severity, bacterial persistence and treatment tolerance, and genetic resistance, are present in the spectrum of tuberculosis (TB). The pathology of TB disease is a dynamic continuum that progresses from a wholly latent, asymptomatic infection to an active disease with a large

bacterial burden in open cavities, which promotes transmission and more frequent treatment failure. People who have LTBI and are developing incipient TB are at a high risk of becoming active and would benefit from therapy and risk assessment for reactivation. The variety of microenvironments produced by the spectrum of immunopathology allow the pathogen to respond with metabolic and physiological changes that result in drug tolerance or phenotypic drug resistance and persistent disease.

In terms of the number of medications a bacterium is resistant to as well as the degree of resistance to each drug, drug tolerance as well as additional patient and pathogen characteristics cause a spectrum of genetic resistance. Such variation along three dimensions hampers clinical trials and produces a gradient of reduced treatment efficacy and lesion sterilisation both within and across patients. It also presents a multifaceted problem for healthcare programmes.

It takes several months to treat all active TB disease forms with a variety of medications

Although the heterogeneity of disease development, host response and drug resistance profiles makes drug discovery and therapy more challenging, it also offers opportunity to stratify patient populations and improve therapeutic and preventive measures. Due to the fact that TB is primarily a disease of resource-poor nations, current infrastructure barely allows for relatively sophisticated interventions.

This increases the already challenging research mandate's operational and implementation issues significantly.

Diabetes is known to triple the chance of acquiring active TB and, like HIV, is linked to the suppression of cell-mediated immunity.

Each diabetes-related TB case could potentially result in the infection of more people, increasing the overall TB burden in the community. It is unclear what biological factors contribute to diabetics' reduced ability to respond to anti-TB drugs and to their higher risk of MDR-TB development. However, it's likely that diabetes suppresses cell-mediated immunity, which leads to greater rates of tuberculosis infection.

TABLE 1 *Unique targets that have been crystallized for anti-TB drug discovery*

TARGET	TARGET PROTIEN	FUNCTION	PDB-ID
Cell-wall	Alanine racemase	Peptidoglycan biosynthesis	6SCZ
	L,D-transpeptidase (LdtMt1)	Peptidoglycan biosynthesis	4JMN-100, 4JMX-100
	Galactofuranosyltransferase	Arabinogalactan and lipoarabinomannan biosynthesis	4FIX-101, 4FIY-101
	Pks13	Mycolic acid biosynthesis	3TZW, 3TZX, 3TZY, 3TZZ-102
Amino acids and co-factors	AroC	Shikamate pathway	2O11, 2O12-118
	Pantothenate kinase	Vitamin B5 synthesis	3AVP, 3AVQ, 3AEZ, 3AFO, 3AF1, 3AF2, AF3, AF4-119
Targets in DNA Metabolism	Class1b ribonucleotide reductase (NrdF)	Ribonucleotide reduction	1UZR-123
	DnaN	DNA metabolism	4TR7-126
Recent targets	alkylhydroperoxide reductase E (AhpE)	Scavenges peroxides	5ID2 96
	biliverdin reductase Rv2074	Protects against oxidative stress	5JAB 95
	acetyltransferase Eis	Inactivation of kanamycin	5EBV, 5EC4 98

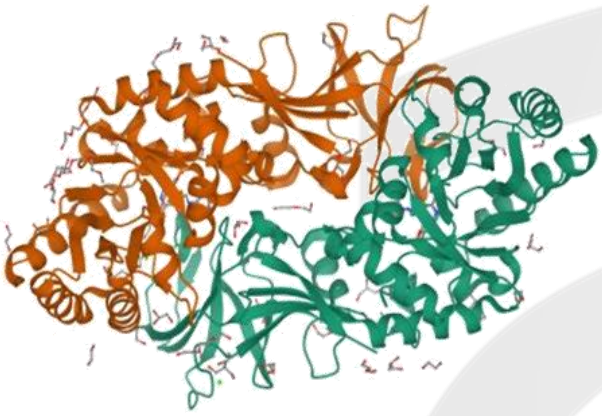

Fig- 1: 3D structure of the target Alanine racemase **(PDB ID: 6SCZ)**

TABLE – 2: Compounds with anti-TB activity currently in the lead optimization stage

Drug (Chemical class)	Developer/Sponsor	Mechanism of action and target.
Arylsulfonamides	TB Alliance, GSK,	Inhibits tryptophan biosynthesis
Bortezomid	SPRINT-TB (National University of Singapore)	Mtb proteasome inhibitor
Cyclopeptides	TB Alliance, Sanofi	Unknown
Diarylquinolones	TB Alliance, Janssen	ATP Synthase
DprE Inhibitors (Azaindoles)	TB Alliance, Calibr	Affects cell-wall biosynthesis by DprE1 inhibition
Indazoles	TB Alliance, GSK	Affects cell-wall biosynthesis by Enoyl acyl reductase (InhA) inhibition
Indoles	SPRINT-TB (National University of Singapore)	Inhibit the ZipA-FtsZ interaction
Oxazolidinones	Sanofi, TB Alliance	Protein synthesis inhibitors by binding to the 50s ribosomal subunit of the 23S rRNA
MmpL3 Inhibitors (Indolcarboxamide)	TB Alliance	Inhibits transportation of metabolites from the cytosol of Mtb and ATP synthesis
PKS-13	Dundee, Texas A & M University	Polyketide synthase inhibitor
Thiadiazole	GSK, ORCHID	Affects cell-wall biosynthesis by Enoyl acyl reductase (InhA) inhibition
Oxaboroles	Anacor Pharmaceuticals, GSK	Inhibits protein synthesis by LeuRS inhibition
Macrolides	TB Alliance, Sanofi	Inhibits protein synthesis by 30S Ribosomal subunit inhibition
Pyrazinamide/Nicotinamide Analogues	TB Alliance, Yonsei University	Inhibits membrane energetics
Pyridomycin (Natural product of Dactylosporangium fulvum or Streptomyces pyridomyceticus)	Ecole Polytechnique Federale de Lausanne	Directly targets NADH- dependent enoyl ACP-reductase (InhA)F by competing for the NADH-binding site
Pyrimidines	AstraZeneca	Inhibitors of NDH-2
Ruthenium (II) phosphine/diamine/picolinate complexes	UNESP/School of Pharmaceutical Sciences	Unknown
SPR-113	Kanury Rao, Sundeep Duggar	Inhibits the anti-lipolytic G protein-coupled receptor, GPR109A
Spectinamides (SPR10199)	St Jude Children's Research Hospital, University of Tennesse Health Centre, Colorado State University, University of Zurich, Microbiotix	Inhibits protein synthesis by 16s Ribosomal subunit inhibition
Squaramides	TB Alliance	Blocks endocytic receptor-mediated mechanisms
TL1 Inhibitors (Capurmycins)	Sequella	Inhibits cell wall peptidoglycan biosynthesis by Translocase 1 inhibition
Xanthones	SPRINT-TB (National University of Singapore)	ATPase Interferes with the bacterial cell membrane

TABLE 3 *Drugs in pre-clinical and clinical development in the TB pipeline*

Drug	Developer/Sponsor	Stage of clinical development	Chemical class	Mechanism of action and target
		Pre-clinical development		
CPZEN-45	Lilly TB Drug Discovery initiative	Early-stage development	Caprazamycin derivative (Nucleoside antibiotic)	Inhibition of cell-wall biosynthesis through decaprenyl-phosphate- GlcNAc-1-phosphate transferase, WecA (Rv1302) inhibition
SQ-609	Sequella Inc.	Early stage	Dipiperidine	Inhibition of cell-wall biosynthesis
TBI-166	TB Alliance Institute of Materia Medica (IMM)	Early stage	Riminophenazine	Accumulation of lysophospholipids, through phospholipase A 2 (PLA 2) activity stimulation

Spectinamide 1599	St Jude Children's Research Hospital, University of Tennessee, Colorado State University, University of Zurich and Microbiotix	Early stage	Spectinomycin analogues	Inhibits protein synthesis by 16s Ribosomal subunit inhibition
BTZ-043	University of Munich, Hans-Knöll-Institut (HKI), German Center for Infection Research (DZIF)	GLP Toxicity	Benzothiazinone	Inhibits Mtb cell wall synthesis by blocking the decaprenyl- phosphoribose-2'-epimerase (DprE1)
PBTZ-169	Innovative Medicine for Tuberculosis (iM4TB)	GLP Toxicity	Benzothiazine	Inhibits cell-wall biosynthesis through DprE1 inhibition.
TBA-7371	AstraZeneca	GLP Toxicity	Benzothiazinone	Inhibitor of DprE1, disrupting cell-wall biosynthesis
GSK-070	Anacor Pharmaceuticals, GSK, TB Alliance	GLP Toxicity	Oxaborole	Leucyl-tRNA synthetase inhibitor
		Clinical development		
Q203	Qurient Co. Ltd	Phase I	Imidazopyridine	Inhibits mycobacterial growth through Cytochrome bc1 complex inhibition
Sutezolid (PNU-100480)	Sequella	Phase II	Oxazolidinones	Bacterial ribosome
SQ-109	Sequella, NIH	Phase II	Ethylenediamine	MmpL3
High Dose Rifampicin	CDC, Sanofi-aventis	Phase II (DS-TB), Phase III (LBTI)	Rifamycin	Inhibits transcription through RNA polymerase inhibition
AZD5847	AstraZeneca	Phase II	Oxazolidinone	Inhibits protein synthesis through 50s ribosomal subunit inhibition
Levofloxacin	CDC, NIAID	Phase II	Fluoroquinolone	Inhibits enzymes necessary to separate DNA, thus inhibiting cell replication
Pretomanid (PA-824)	TB Alliance	Phase III (Bedaquiline-Pretomanid- Pyrazinamide regimen)	Nitroimidazole	Inhibits cell-wall mycolic acid biosynthesis through of ketomycolates inhibition
Bedaquiline (TMC-207) for MDR-TB	TB Alliance Janssen	Phase II (Bedaquiline-Pretomanid-Pyrazinamide regimen), Phase III (MDR-TB)	Diarylquinoline	Inhibit ATP synthesis through ATP synthase inhibition
Bedaquiline-Pretomanid-Linezolid	TB Alliance, Janssen	Phase III	New Investigational Drugs	Treatment of patients with XDR-TB

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SEROTONIN HYPOTHESIS FOR DEPRESSION

Divya B, M.Pharm 2nd Semester

Introduction

Depression is considered as the most common and serious mental disorder globally. It is a leading cause for disability. According to WHO, India is considered as the most depressed country in the world.

How depression differ from sadness?

Sadness is a situation of being emotionally upset or in pain. It is referred to a natural human emotion that people feel at certain times in their lives. It fades away as the time passes. But depression is a long-term metal illness which impairs social, occupational and other important areas of functioning

Different causes triggers depression

• Stressful events like bereavement or relationship breakdown there is risk of depression may occur

• Low self-esteem or overly self-critical - These personality traits which are due to the gene which is inherited from parents or early life experience can cause depression

• Family history like if any of the family had depression in the past such as parents or siblings, it's more likely that you'll also develop it

• Some women are very vulnerable to depression after pregnancy, this is due the hormonal changes and physical changes can lead to postnatal depression

• Loneliness caused by becoming cut off from family and friends can increase the risk of depression

• Taking too much of alcohol or drugs that results in spiral depression.

• There is high risk of depression when there is life long life threating illness like heart disease, cancer, severe head injury, hypothyroidism etc.

Types of Depression

- Mild, moderate and severe depression
- Bipolar disorder
- Dysthymia
- Atypical depression
- Postnatal depression (PND)
- Seasonal affective disorder (SAD)
- Psychotic depression
- Mixed depression with anxiety disorder

Hypothesis of serotonin imbalance leading to depression. Serotonin is a biochemical which act as a neurotransmitter that helps in relay messages. Serotonin is also considered as the natural mood

stabilizers. They include brain cells involved in mood, memory, sleep, sexual desire and function, learning, temperature regulation and some social behaviour.

The widely believed theory proposed decades ago that the imbalance in the level of serotonin influences the mood which leads to depression. The researchers believed that due to the low production od serotonin by brain cells, lack in receptor sites to receive the serotonin or if there is inability of serotonin to reach the receptor or shortage in tryptophan, the chemical which is used in making serotonin leading to depression (Fig 01)

Fig 1: Serotonin imbalance and depression

A recent analysis has shown that there is no evidence found that low levels or reduced activity of serotonin in brain causes depression. Large amount of people take antidepressant because they have led to the believe there is biochemical cause, but the new analysis has reported that there is no clear grounded evidence. There are also studies comparing the level of serotonin in depression and healthy control participants. It was found that higher level of serotonin activity in people with depression. They also tried lowering the serotonin level in people through diet reported that lowering the serotonin level this way did not cause depression.

People with stressful events, illness, low self-esteem, taking too much alcohols and drugs can trigger the cause of depression and even supressing of new braincells by stress and other events causes depression. It is also believed that taking of common antidepressant medication which is known as SSRIs (selective serotonin reuptake inhibitor) which is designed to boost serotonin levels, helps in production of new brain cells which allows the depression to lift.

Conclusion:

Depression is a group of condition which is associated with the elevation or lowering the persons mood.

Decades ago, it has been proposed that low levels of serotonin levels in a person leads to depression. But the recent survey reports show there is no clear evidences that depression is caused due to low levels or low activity of serotonin. Some study shows the depression is caused due to some stressful events and other conditions or due to stress there is suppression of new brain cells leading to depression. The use of common antidepressants helps in production of new brain cells which uplifts from depression.

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CAN MACHINE LEARNING HELP US TO REPURPOSE DRUGS FOR ALZHEIMER'S DISEASE:

Madhushree.K, M.Pharm 2nd Semester

Introduction

The most prevalent form of dementia, known as Alzheimer's disease, is an irreversible neurological condition that affects more than 5.1 million persons over the age of 65 and is the sixth largest cause of death in the US. Alzheimer's disease affects 5% of people over 65, 20% of people over 85, and more than one-third of people over 90. It is a typical age-dependent neurodegenerative illness. Because of this, its prevalence will continue to rise as life expectancy rises in the absence of effective prevention and therapeutic measures. The processes behind the Alzheimer's disease pathogenesis are still unclear. The hallmarks of the condition and the subject of several investigations are the accumulation of the proteins tau and Amyloid beta (Ab), as well as a reduction in acetylcholine. Four cholinesterase inhibitors (tacrine, rivastigmine, donepezil, and galantamine) and one N-methyl-D-aspartate receptor inhibitor (memantine), the only treatments available for Alzheimer's disease, are only symptomatic and do not affect the underlying disease mechanisms or change the course of the disease. As a result, drug repurposing might present a chance to find more clinical stage molecules.

Repurposing Of Drug By Machine Learning

A recent study described a method using 80 kinase inhibitor-treated neuronal cell lines to access the gene expression profile using machine learning to estimate the pathology and severity of Alzheimer's disease. Ruxolitinib and regorafenib, which were investigated for mechanism, were among the top-scoring drugs; nevertheless, neither in vitro nor in vivo experimental validation against Alzheimer's disease was done. Brains with Alzheimer's disease had higher amounts of active Glycogen Synthase Kinase 3 (GSK3), according to post-mortem investigation. The pharmaceutical industry is interested in GSK3 inhibitors because they may be used to treat diabetes, cancer, Parkinson's disease, psychiatric disorders, and stem cell proliferation in addition to Alzheimer's disease. With almost 2300 molecules (from ChEMBL) and a fivefold cross-validation receiver operating characteristic (ROC) > 0.90, are assembled and validated a Bayesian machine learning model for inhibiting GSK3β. To determine which commercial chemicals should be tested first, a computational model was employed. GSK3 inhibitor ruboxistaurin, a therapeutic candidate,

was discovered. The Z'LYTE Kinase Experiment, a secondary in vitro assay, revealed an IC_{50} (drug dose necessary for 90% inhibition) of 155 nM. The IC_{50} of ruboxistaurin for GSK3 was higher than that of its initial target protein kinase (PKC) (6 nM), but it was lower than that of PKC, a protein kinase that is closely related to GSK3 (360 nM). As an independent GSK3 inhibitor for the treatment of neurological or psychiatric disorders, ruboxistaurin has been granted a patent. For 10 Alzheimer's disease targets, Bayesian machine learning models was curated and validated. Generally, ROC > 0.8 and Matthews correlation coefficient (MCC) > 0.5 are the fivefold cross-validation statistics. Even though some datasets are modest, those containing thousands of molecules appear to have the best potential. Then, new modulators of these proteins that may be employed alone or in combination to treat Alzheimer's disease could be discovered using these computational models.

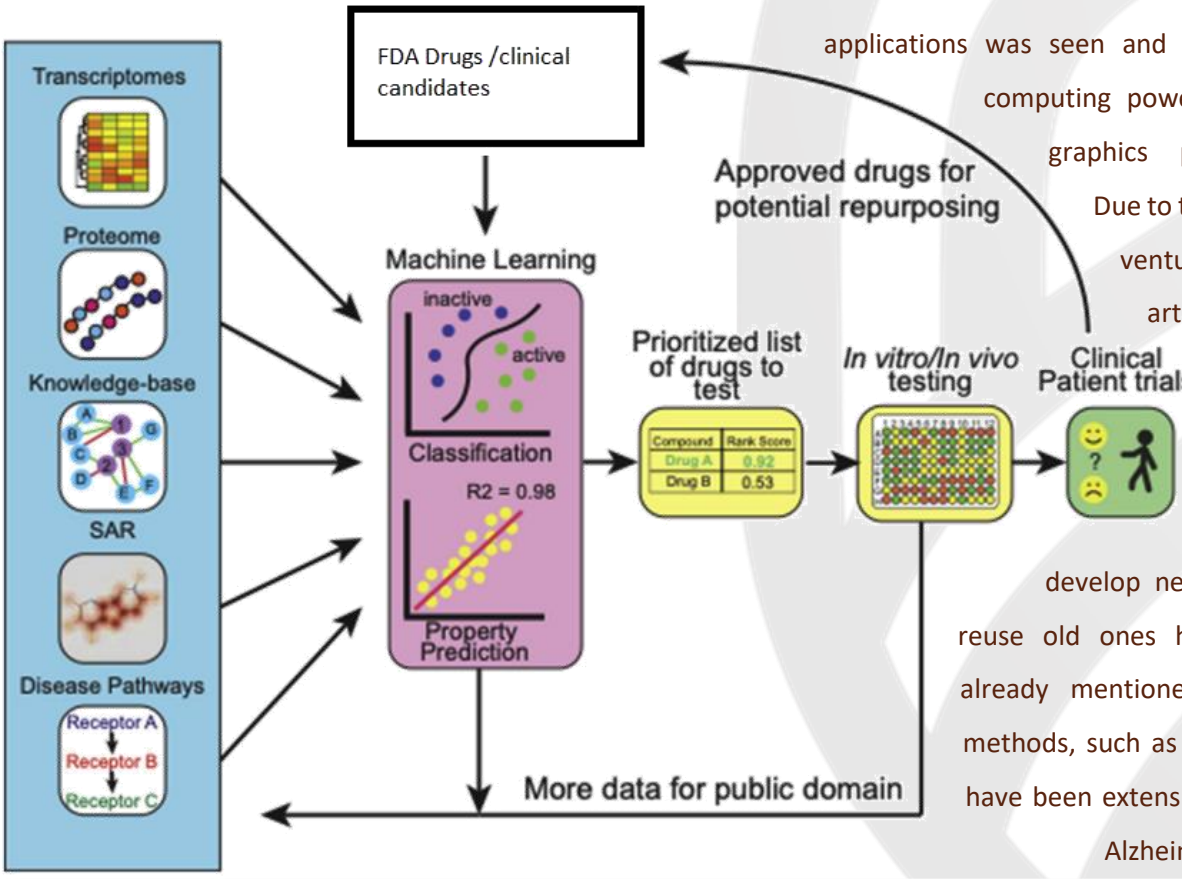

Fig 01: Overview of computational machine learning approaches for drug repurposing.

Conclusion

The use of machine learning for drug repurposing has increased gradually over the past ten years as its applications was seen and the revolution in computing power brought on by graphics processing units. Due to this, the number of venture capital-backed artificial intelligence drug discovery firms using just computational methods to develop new medications or reuse old ones has increased. As already mentioned, computational methods, such as machine learning, have been extensively used to treat Alzheimer's disease. Although it is still in its infancy in terms of development and applications, some of the rewards has already begun to reap, such as discovering new applications for these already-approved pharmaceuticals by utilising the vast volumes of publicly available data. This may

allow speedier identification of medications for novel disease applications in a manner that may also be more cost effective. In conclusion, the final test of this strategy's effectiveness will be if repurposed medications really reach patients.

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EFFECT OF TATTOOS AND IMMUNE RESPONSE IN OUR BODY

RADHIKA N, M.Pharm 2nd Semester

Fig 1 Art of making tatoos

Introduction

Tatoo a mark, figure, design or word intentionally fixed or placed on the skin. It can be done by using coloured ink, dyes and pigments. the art of making tattoos is called as Tattooing (Fig-1).

Tattoos can be decorative, symbolic or pictorial. Around the globe, the practice of tattooing is seen and well documented since ancient times in humans. ex: Tribal tattoos, cultural tattoos, mummified preserved skin tattoos etc.

Role of Immune System In Tattoo:

A Tattoo is a form of body modification where designs are made by inserting ink, dyes and/ or pigments, either indelible or temporary into the layers of skin especially dermis layer. In case of Permanent tattoos: the ink or dye directly injected in the skin, which results in the stimulation of immune system that leads to excess proliferation of immune cells such as macrophages and movement of these cells towards the site of tattoo. These immune cells absorb the ink or dye as part of pinocytosis or phagocytic process and stays at the site holding the dye/ink, this led to fixation of tattoo in our body (Fig-2). If immune cells are matured and dies, the ink will be released which is then again hold up by newer macrophages which are produced in our body.

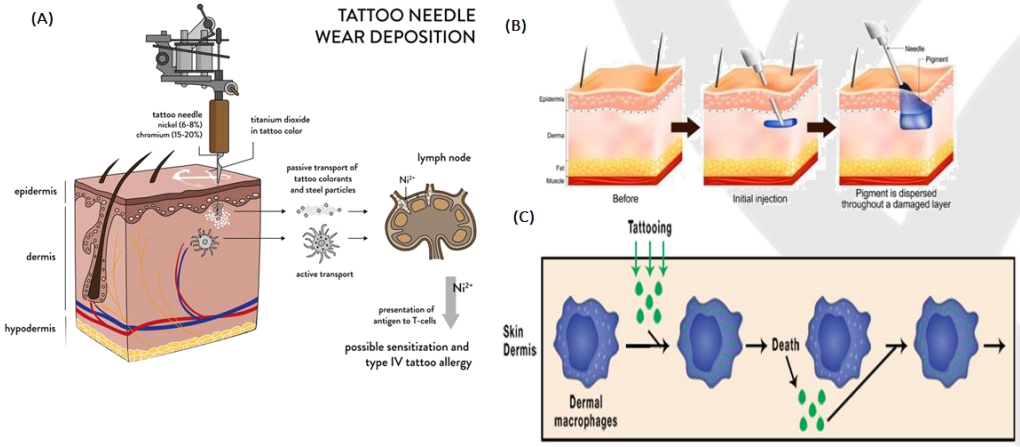

Fig 2 (A) Injection of tattoo inks in the dermis layer of skin (B) Release of dye or ink from tattoo injection (C) Proliferation of immune cells at the site of tattoo injection

Effects of Tattoos On Body:

Now-a-days, there is a considerable increase in the number of people, especially youngsters prefer to get multiple tattoos on their body. As the number of tattoos increase on body, it increases the risk of various infections, because sufficient number of immune cells won't be there to fight against the infection as immune cells were assigned to hold ink/ dye. So immune deficient or immunocompromised patient should not prefer tattoos. In the process of tattooing, the use of artificial ink, dye or pigment ingredients and the excess proliferation of immune cells, sometimes leads to hypersensitive allergic reactions such as redness, granuloma, swelling, scars and various skin disorders. If the tattoo making equipment are not cleaned and sterilized or contaminated with infected person's blood, it will lead to various blood borne diseases and skin infections

Preventive Measures:

- Don't get unnecessary tattoos on your body
- Don't use low quality, adulterated inks, dye or pigments for tattooing process
- During healing to tattoo, keep the skin clean, don't rub the skin and don't swim in water
- Apply moisturizers, sun screen as recommended, wash gently with non-irritating soap

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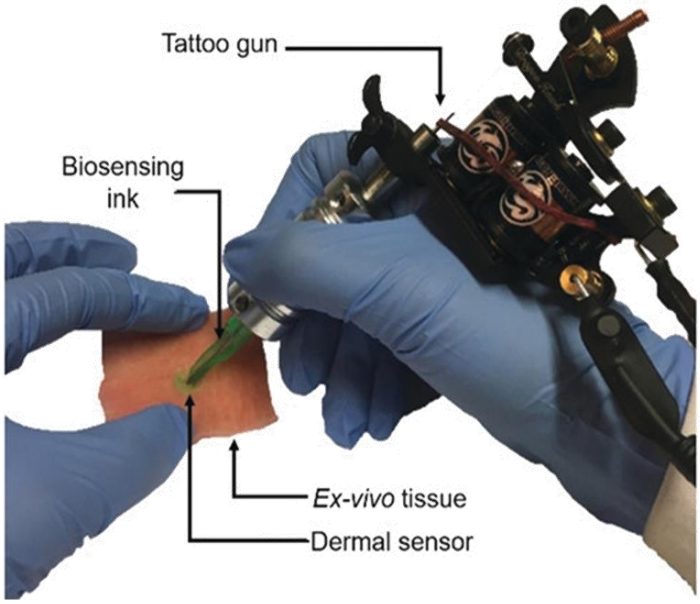
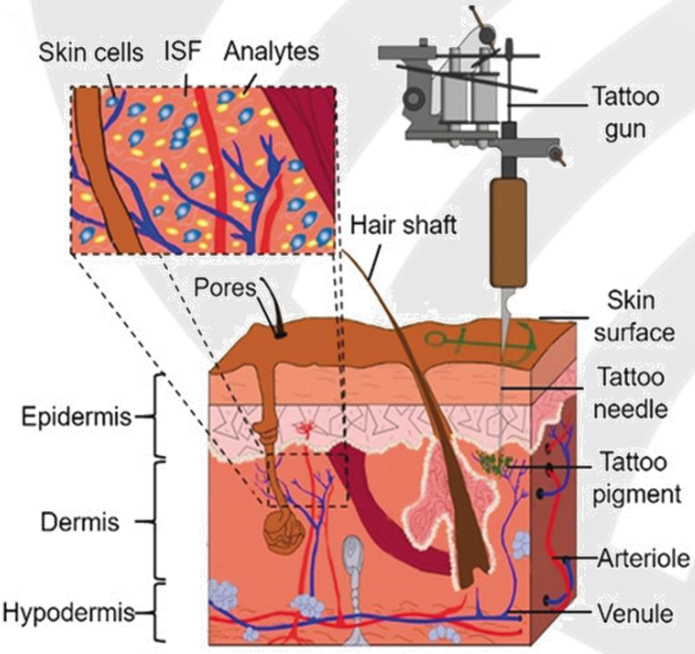
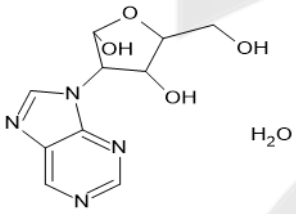




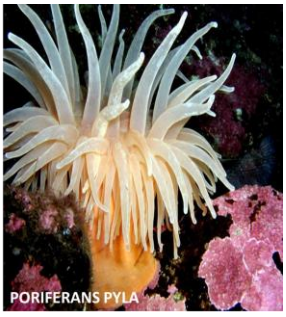
MARINE IN MEDICINAL CHEMISTRY

DEVIKA MURALEEDHARAN, M.Pharm 1st Semester

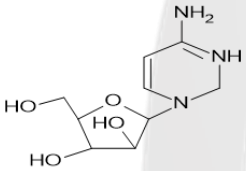


Vidarabine

The contribution of natural products has shown the importance of drug discovery in present-day development. The chemical diversity of natural products is aligned closely with the synthetic library of drug discovery projects.

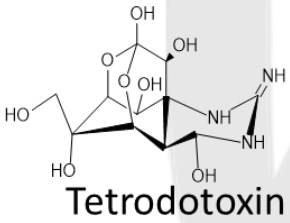


Marine organisms are considered the most relevant source of bio-active natural products than terrestrial plants and non-marine microorganisms. Approximately 29,500 natural marine products have been identified by the end of 2018, anticancer and cytotoxic activities was the major reports. Oceans cover 70% of the earth's surface with huge diversity. Supply of material is the only drawback of marine natural products because as it is naturally obtained the amount is very less. Synthesis and semi-synthesis are the only way to solve this problem of supply. There are mainly 6 types of therapeutic agents that are considered marine natural product derivatives. Anti-cancer Cytarabine (ara-C) and antiviral vidarabine (ara-A) were the first drugs approved by US Food and Drug Association in (1969 and 1976). Cytarabine is still used.



Cytarabine

Aspergillus sp. An isolated marine fungus, this antimicrobial agent inhibits tubulin polymerization. Tectin a tetrodotoxin alkaloid isolated from puffer fish liver is in phase III clinical trial on its analgesic effects. ω-3fatty acids from krill is in phase II clinical trials of CaPre.



Tetrodotoxin

Although majority of bio active medicinal natural products are a source of marine invertebrates, porifera (sponges) and cnidaria phyla are the true origin of various marine natural products. Most invertebrates are sessile.

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PG/UG Projects Submitted

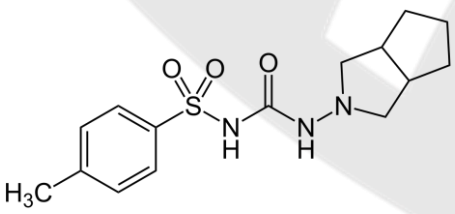
ANALYTICAL METHOD VALIDATION OF GLICLAZIDE RELATED SUBSTANCES BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY METHOD

Student: Sabhyatha T.S
Research Supervisor: Prof. Narayanababu

Abstract:

The present study was undertaken with an objective of method validation a rapid, simple, cost effective HPLC method for the determination of related substances of Gliclazide. A simple, rapid and specific method for analysis of gliclazide by a sensitive high-performance liquid chromatographic method is described. Validation of method is carried out in accordance with USP guidelines. The method was validated for parameters like accuracy, precision, linearity, specificity, robustness and system suitability. These proposed methods are suitable for the determination of title drugs in quality control laboratories in pharmaceutical industries. The mobile phase used for the chromatographic runs consisted of (450ml) acetonitrile and (550ml) water. The separation was achieved on LiChroCART Supersher RP-8 column, (250 mm × 4.0 mm, 5µm), using isocratic mode. Drug peaks were well separated and were detected by a UV detector at 235 nm, the method was linear at the concentration range. Gliclazide limit of detection (LOD) and limit of quantification (LOQ) was 0.003 and 0.01 while LOD and LOQ for Impurity-F was 0.003 and 0.01 respectively. The presented validated method is rapid, economic, simple, accurate, sensitive, robust, specific and linear. It can be used for routine analysis of gliclazide.

Keywords: Method Validation, Relative Standard Deviation, System suitability, Limit of detection, Limit of quantitation, Impurity-F, Gliclazide, RS-HPLC.



ENRICHMENT OF G2019S-LRRK2 KINASE INHIBITORS USING MACHINE LEARNING TECHNIQUES

Student: Jhansi Laxmi CH
Research Supervisor: Prof. M. Narayana Babu

Abstract:

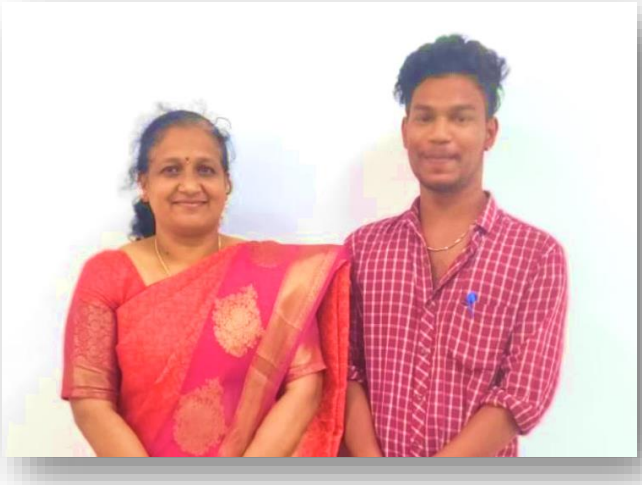
Motivation: Parkinson's disease is a chronic, progressive neurodegenerative disorder. The disease is characterized by the loss of dopaminergic neurons with a consequent decrease in dopamine levels in the brain. The Symptoms include tremor, rigidity, postural instability, impaired speech, bradykinesia, cognitive impairment, mental illness, and olfactory dysfunction. FDA approved therapies for Parkinson's disease, are intended to manage a patient's symptoms, however, these treatments are often associated with adverse events. Currently, there are no disease-modifying therapies that slow or stop the progression of this devastating neurodegenerative disorder. Thus, present study focuses on designing potent molecules against G2019S-LRRK2 using Machine learning techniques. Method: G2019S-LRRK2 was identified as the potential target and Homology modelling was used for protein preparation 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-parameter optimization. Based on the pharmacokinetic profile of the template molecule,97 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.

Conclusion: In this study, the 3D structure of LRRK2 kinase domain was built based on homology modelling and refined by MD simulations. Molecular docking-based virtual screening was employed as multi parameter optimization. 97 molecules were designed. retrosynthetic pathway was proposed and ADME properties were determined for the top five molecules, they were found to be within the range. Biological activity of the molecules was determined using Random Forest ML model and predicted IC50. Since the molecules have shown promising results, they could be potential lead compounds for therapeutic agents in Parkinson's disease.

Keywords: Parkinson's disease, SeeSAR, Homology modelling, Machine learning, molecular dynamics simulations.

SYNTHESIS OF NOVEL BENZIMIDAZOLE DERIVATIVES TETHERED WITH ISONIAZID FOR BIOLOGICAL ACTIVITY

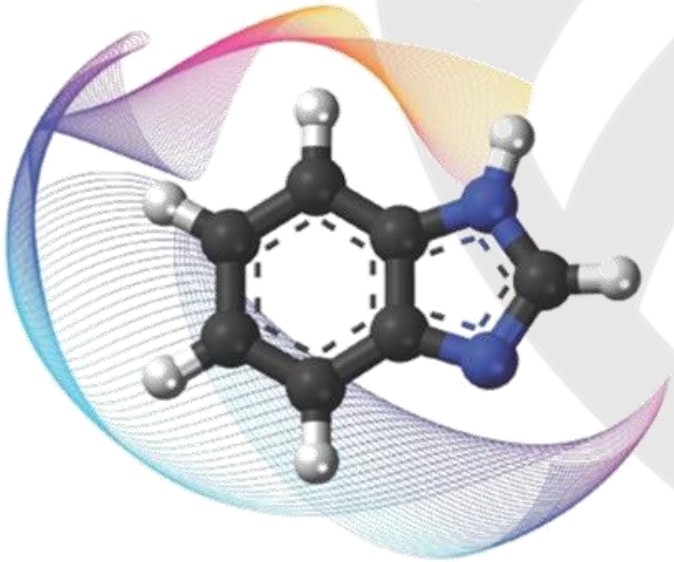
Student: Medicharla Sri Dathya
Research Supervisor: Dr. BV Suma



Abstract:

Benzimidazole is a prominent nucleus with different biological activities. Isoniazid is the first line drug used in the treatment of Tuberculosis. Henceforth tethering these two molecules may show better therapeutic activity. Molecular docking studies for the designed molecules has shown prominent results for different biological activities. All the designed molecules were synthesized and in vitro studies were carried out for antimicrobial, anti inflammatory, anti cancer, anti-tubercular activites.

Keywords: Benzimidazole, Isoniazid, Molecular docking, Anti-cancer, Anti-TB, Anti-microbial, Anti-inflammatory, Synthesis



SYNTHESIS OF NOVEL BENZOTRIAZOLE DERIVATIVE TETHERED WITH ISONIAZID FOR BIOLOGICAL ACTIVITY

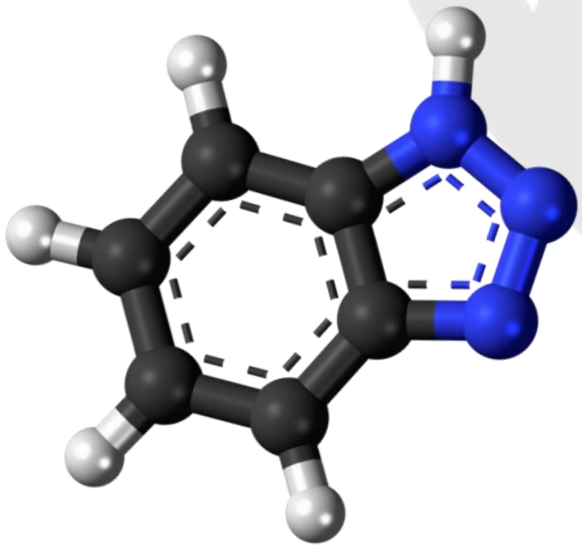
Student: Aishwariya
Research Supervisor: Dr. BV Suma

Abstract:

The potential of bacteria to acquire resistance to antimicrobial drugs is complicating the treatment of various microbial diseases. The need for potent antimicrobial drug for the treatment of wide range of infections has become the need of the hour. The incorporation of two potent antimicrobial nucluei has proved the enhancement in the potency of its activity. The research work mainly focusses on two nucleus ie; Benzotriazole and Isoniazid which has shown good activity against various antibacterial, antifungal, antiviral targets and Isoniazid which is a first line anti-TB drug. Benzotriazole is of enormous pharmaceutical importance due to its powerful and significant biological activity; thus, the synthesis of derivatives is of major interest. Computational simulation has shown the affinity of the ligand molecules designed for various anti-microbial targets.

The characterization data and microbial assays have proven that the synthesized compound BVSA1C as a promising novel derivative. BVSA1C has shown potent activity against anti-cancer estrogen receptor.BVSA1C has more activity compared to standard anti-TB drug lie Pyrazinamide .

Keywords: Anti-TB, Anti-microbial, Anti-fungal, Benzotriazole, Isoniazid, Antimicrobial resistance, Computational chemistry, Synthetic chemistry



DESIGN, SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL EVALUATION OF SUBSTITUTED BENZENE TETHERED WITH AZOLE DERIVATIVES

Student: Gandaboyana Chaitanya Sai
Research Supervisor: Dr. Judy Jays

Abstract:

Pyrazole derivatives have been reported to possess various pharmacological activities along with anti-microbial and anti- cancer activity. Increasing antimicrobial resistance to the existing drugs has dictated the need to develop novel effective agents. With the perspective of synthesizing a new pyrazole derivative. Based on molecular docking studies ten promising pyrazole derivatives were selected and synthesized. The ligands were drawn in chemdraw Professional 15.0 in SDF format and docking was performed using autodock vina4. The 2D interaction was obtained using 'Pymol 2.4' and 'BIOVIA Discovery Studio Visualizer 4.5'. The ADMET and drug likeness properties was predicted by 'pkcsm'. The pyrazole derivatives were synthesized from intermediates 'chalcones' by cyclo condensation reaction in presence of alcohol. Anti-microbial studies was carried out by using cup plate method and anti-cancer was carried by using MTT assay.

Investigation of in- vitro anti-microbial activity of compounds JJC3 (A-J) has been performed by using cup-plate method against two bacterial and one fungal species. Some of synthesized compounds showed good antibacterial activity and compared with Ciprofloxacin. Some of the compounds exhibited good anti-fungal activity comparable to ketoconazole. Compounds JJC3 H, I and J has showed promising activity in both anti-bacterial and anti-fungal activities. Compound JJC3E has exhibited potent activity in anti-cancer activity.

Keywords: Pyrazole, Molecular Docking, ADMET, Anti-Microbial, Anti-Cancer.

ANALYTICAL METHOD VALIDATION FOR ESTIMATION OF RESIDUAL SOLVENTS IN GLICLAZIDE USING GAS CHROMATOGRAPHY

Student: Burhanuddin Madriwala
Research Supervisor: Dr. Judy Jays & Mr. B. Srinivasa Rao

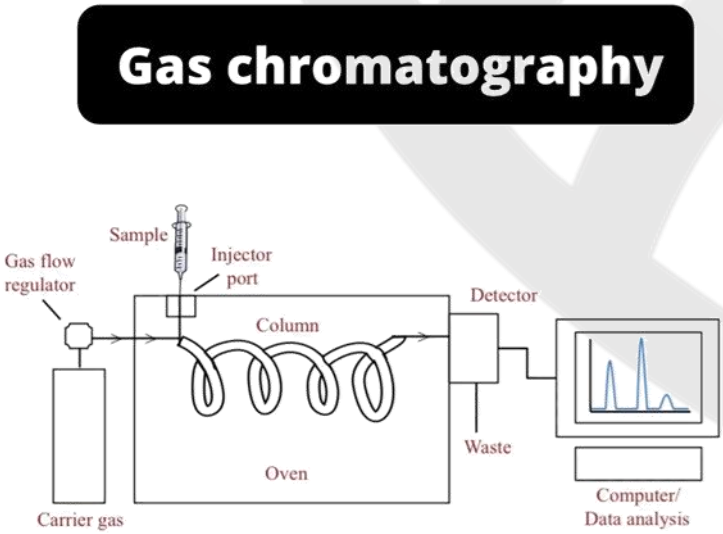
Abstract:

Analytical method validation is a process of providing documented evidence that claims reliability, consistency and reproducibility of a newly developed method. Gas Chromatography is a widely used technique for analysing a variety of samples like biological samples, separation of volatile components in plants, impurity profiling, determination of the chemical composition of formulations, etc. The present work involves determining the consistency, reliability and reproducibility of a newly developed method for estimating residual solvents in Gliclazide using Gas chromatography by performing its validation. The validation is performed as per the validation protocol designed based on ICH Guidelines Q2(R1). The solutions are prepared using N-Methyl-2-Pyrrolidone diluent as per the procedure given in protocol and appropriately injected as per the sequence. The parameters checked were System suitability, Specificity, Linearity and Range, Accuracy, Precision, Limit of detection, Limit of quantitation, Ruggedness and Robustness.

The data for each parameter tested is compiled and documented. It was found that the results obtained for each parameter were in compliance with their given acceptance criteria.

The method of analysis complies with all the parameters tested and it was found to be reliable, consistent and reproducible.

Keywords: Gas chromatography, Method validation, Residual solvents, System suitability, Specificity, Linearity, Range, Accuracy, Limit of Detection, Limit of Quantitation, Precision, Ruggedness, Robustness.



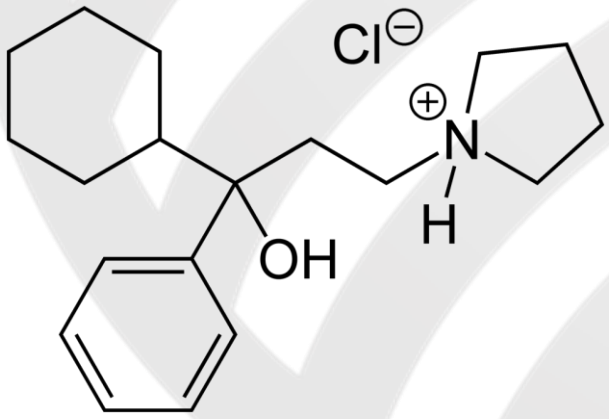
NOVEL ANALYTICAL METHOD DEVELOPMENT AND VALIDATION OF RP-HPLC METHOD FOR ASSAY AND DISSOLUTION OF PROCYCLIDINE HYDROCHLORIDE TABLETS

Student: Mallepalle Srividya
Research Supervisor: Dr. Lakshmi M Sundar & Dr. S. Kumaravel

Abstract:

Procyclidine belongs to a class of medication called anti-cholinergics that work by blocking acetylcholine. Procyclidine is used in the treatment of Parkinson's disease drug-induced extrapyramidal disorders. Simple,rapid, accurate and precise RP-HPLC method for the estimation, dissolution profile and stability studies of procyclidine hydrochloride in pharmaceutical dosage form was developed and validated. The validation parameters of RP-HPLC methods for the % content of assay, dissolution, and short term stability studies of the procyclidine hydrochloride were within the range. Theoretical plates for procyclidine hydrochloride were 8277. Tailing factor for procyclidine hydrochloride was 1.7. The correlation coefficient is 0.999.The retention time for the procyclidine hydrochloride peak is around 8 minutes. The relative standard deviation of peak area for six measurements is less than 2%. The retention time for the procyclidine peak eluted in the dissolution method is around 3 minutes. The release of the drug is in the range of 99-103%.

Keywords: HPLC, Procyclidine hydrochloride, Method development, Method validation, Dissolution, Assay



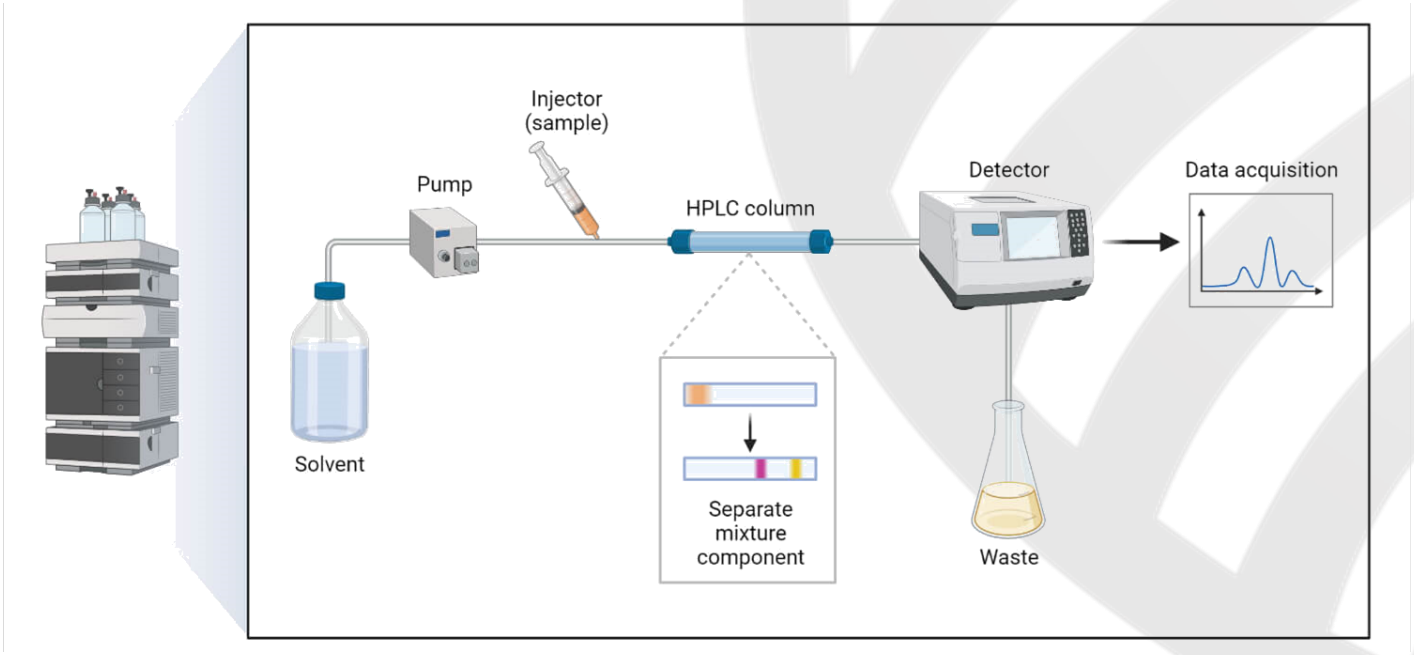
Analytical Method Development and Validation for Assay of Furosemide Liquid Injection by RP-HPLC Method

Student: Poornima
Research Supervisor: Mrs. Knolin K Thachil

Abstract: The developed RP-HPLC method includes isocratic elution with potassium dihydrogen ortho phosphate buffer with a pH of 5.5 and acetonitrile was used in the ratio of 75:25. The C18 (Waters) 10µm, 125A0, 3.9mm X 300mm column with a detection wave length of 270nm. Furosemide was eluted as a sharp peak at 5.1 minutes and analysis were run at a flow rate I mL/min. Furosemide was further subjected to stress conditions (hydrolysis, oxidation, and thermal degradation) and the stressed samples were analysed by use of the RP-HPLC method.

The developed method was found to be linear in the concentration range of 0.05µg/ml to 5.0µg/ml. The limit of detection (LOD) and limit of quantification (LOQ) were 0.01µg/mL and 0.03µg/mL respectively. The method was robust and reproducible and the mean recoveries were in the range of 98.0% to 102.0%. The developed method was found to be simple, accurate, cost effective, rugged and robust.

Keywords: Method Development, validation, LOD, LOQ, Furosemide, RP-HPLC



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

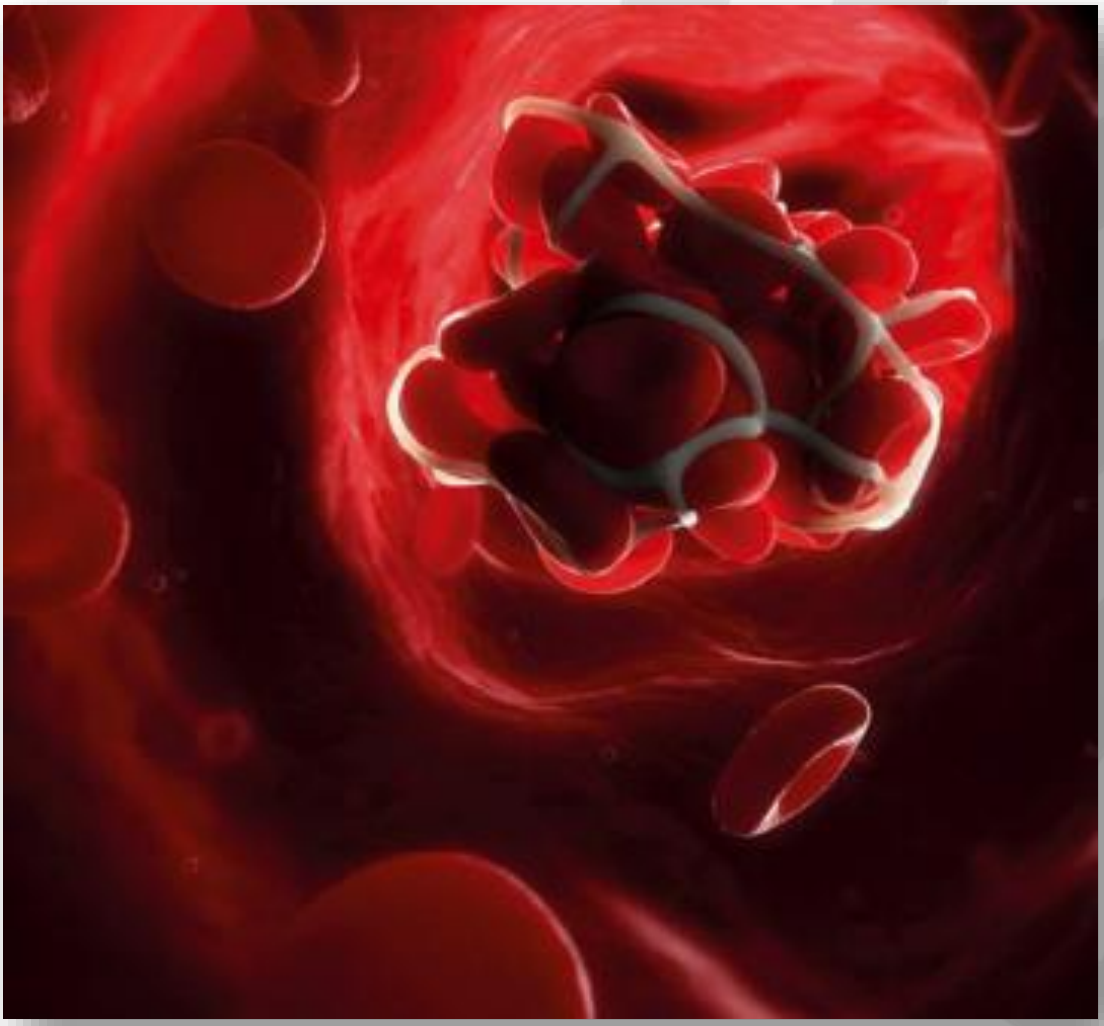
Abstract:

Currently, 350 million individuals worldwide suffer from one of the prevalent illness disorders known as chronic inflammation. 80 percent of other chronic diseases, including diabetes, kidney disease, cancer, depression, Parkinson's disease, Alzheimer's disease, cardiovascular disease, and arterial diseases including atherosclerosis, are mediated by it. Despite the fact that there are many compounds with highly effective activity, the non-specific inhibition of the majority of the compounds and their negative effects have necessitated the development of alternative ways to locate novel compounds that precisely inhibit chronic inflammation. One such target is the lipoprotein-associated phospholipaseA2 (Lp-PLA2) enzyme, which is connected to proinflammatory mediators of the atherogenic process. Computational techniques may be the best alternative.

The selection of medicinal plants and identification of phytochemicals having reported anti-

inflammatory activity was carried out using the online tool IMPPAT 2.0. (Indian Medicinal Plant Phytochemistry and Therapeutics) database. The drug likeliness and ADMET properties of the identified phytochemicals were downloaded from the IMPPAT database. Molecular docking was carried out to determine the binding affinity of the compounds with the target protein Lp-PLA2. Among them, the phytochemicals Silibinnin and Quercetin were considered as the best with a better dockingscore in comparison with the reference molecule Darapladib. ADMET properties of the phytochemicals silibinnin, berberine and quercetin showed excellent $CaCO_2$ permeability, and no toxicity related to hERG blockers and AMES test for the mutagenicity.

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



International Workshop

Click here to watch the glimpse of the workshop

Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ramaiah University of Applied Sciences, Bengaluru organized the 3rd International Workshop on *"Computational Tools in Drug Design - CTDD"* on 22nd and 23rd September 2022. Over 40 delegates from 11 universities across the country were part of this workshop and gained knowledge & hands-on experience with respect to *In silico* tools used in Drug Design

Webinar

Department of Pharmaceutical Chemistry Organized a webinar on

"SMART TOOLS FOR EFFECTIVE RESEARCH" on 14th May 2022.

RAMAIAH UNIVERSITY OF APPLIED SCIENCES | Faculty of Pharmacy

FPH

Department of Pharmaceutical Chemistry

Invites for a webinar

on

SMART TOOLS FOR EFFECTIVE RESEARCH

Webinar highlight

Research is undoubtedly one of the most painstaking and thorough process. Irrespective of discipline, stage of work and career, research can be an arduous and time-consuming task. Right from browsing the library shelves and internet for literature, performing experiments, writing papers, to publishing it, researchers are always running with the clock's hands. Regardless of research domain, there's an online tool help researchers organize notes, cite sources, find important articles, connect with peers in the field, and much more. However, with so many options available at a click, search for reliable resources can be frustrating at times; it gets difficult to find a tool that delivers best results. This webinar features some of the most recommended online tools available for researchers.

Resource Person

Dr. K. Selvaraj

Associate Professor

Department of Biotechnology,
Kalasalingam Academy of Research and Education
(Deemed to be University), Krishnankoil

Speaker profile

Dr. K. Selvaraj pursued his Post-Doctoral Research Fellowship from the University of Warsaw, Poland and Ph. D from Jadavpur University, Kolkata. His latest accolades include a Project fund of INR 25,00,000/- from Department of Biotechnology, Government of India 2020-2022 and INSA Visiting Scientist Fellowship for two months, at Indian Institute of Technology, Roorkee, India, 2020. He has 80 scholarly publications to his credit in peer reviewed journals.

Convener
Dr. S. Bharath
Dean

Co-Ordinators
Dr. Harish Kumar D R
Dr. Parasuraman P

Date: 14/MAY/2022
Time: 11:00 AM – 12:30 PM IST

Registration & Event Link:
Microsoft Teams

For Queries: fph_pharmachem@msruas.ac.in +91-9629396767

Publications

1. Jaikanth Chandrasekaran, Senthilkumar Elumalai, Vidya Murugesan, Selvaraj Kunjiappan, **Parasuraman Pavadai** and Panneerselvam Theivendren. Computational design of PD-L1 small molecule inhibitors for cancer therapy. Molecular Diversity. 2022. https://doi.org/10.1007/s11030-022-10516-3. **(Springer Nature- IF: 3.364**)
2. Dessai PG, Dessai SP, Dabholkar R, Pednekar P, Naik S, Mamledesai S, Gopal M, **Pavadai P**, Kumar BK, Murugesan S, Chandavarkar S, Theivendren P, Selvaraj K. Design, synthesis, graph theoretical analysis and molecular modelling studies of novel substituted quinoline analogues as promising anti-breast cancer agents. Molecular Diversity. 2022. https://doi.org/10.1007/s11030-022-10512-7. **(Springer Nature- IF: 3.364**)
3. Palanichamy, Chandrasekar, **Parasuraman Pavadai**, Theivendren Panneerselvam, Sankarganesh Arunachalam, Ewa Babkiewicz, Sureshbabu Ram Kumar Pandian, Kabilan Shanmugampillai Jeyarajaguru, Damodar Nayak Ammunje, Suthendran Kannan, Jaikanth Chandrasekaran, Krishnan Sundar, Piotr Maszczyk, and Selvaraj Kunjiappan. *Aphrodisiac Performance of Bioactive Compounds from Mimosa pudica Linn.: In Silico Molecular Docking and Dynamics Simulation Approach*. Molecules 2022;27:3799. https://doi.org/10.3390/molecules27123799. (**MDPI- IF: 4.927**)
4. MADRIWALA, B., **Suma B.V.**, and J. JAYS. "Molecular Docking Study of Hentriacontane for Anticancer and Antitubercular Activity". International Journal of Chemistry Research, vol. 6, no. 4, Oct. 2022, pp. 1-4, doi:10.22159/ijcr.2022v6i4.208. **(SCOPUS INDEXED)**
5. AISWARIYA, **Suma. B. V.**, and M. S. SATYA. "Molecular Docking and ADMET Studies of Benzotriazole Derivatives Tethered with Isoniazid for Antifungal Activity". International Journal of Current Pharmaceutical Research, vol. 14, no. 4, July 2022, pp. 78-80, doi:10.22159/ijcpr.2022v14i4.2004. **(SCOPUS INDEXED)**
6. M. S. SATYA, **Suma. B. V**, AISWARIYA. Molecular Docking and ADMET Studies Of Ethanone, 1-(2-Hydroxy-5-Methyl Phenyl) for Anti-Microbial Properties. International Journal of Current Pharmaceutical Research, Vol 14, Issue 6, 24-27. **(SCOPUS INDEXED)**
7. Jabeen, **Bangalore Venkatappa Suma**. Newly validated stability-indicating ultra-performance liquid chromatography-tandem mass spectrometry method for the estimation of Ceftaroline Fosamil by using a quadrupole mass detector. Journal of Applied Pharmaceutical Science Vol. 12(06), pp 215-223, June, 2022. **(SCOPUS INDEXED)**
8. Aiswarya Raju and **Judy Jays.** In-Silico Molecular Docking Studies, Synthesis and Biological Evaluation Of Novel Furan-Azetidinone Hybrids As Potential Anticancer Agents. IJPSR, 2022; Vol. 13(7): 2759-2764. **(SCOPUS INDEXED)**

9. Burhanuddin Madriwala, **Judy Jays, G.** Chaitanya Sai. Molecular Docking and Computational Pharmacokinetic Study of Some Novel Coumarin–Benzothiazole Schiff's Base for Antimicrobial Activity. Int J Pharm Pharm Sci, Vol 14, Issue 8, 16-21. **(SCOPUS INDEXED)**
10. G. Chaitanya Sai, **Judy Jays,** Burhanuddin Madriwala. Design, Binding Affinity Studies and In Silico ADMET Predictions of Novel Isoxazoles as Potential Anti-Bacterial. Int J Curr Pharm Res, Vol 14, Issue 4, 74-77. **(SCOPUS INDEXED)**
11. Jayashree A. Heremath, Harish Kumar DR. A Novel RP-HPLC Method Development and Validation for the Quantification of a Potential Anti-Diabetic Drug Metformin Hydrochloride in Tablet Dosage Form. Int J Curr Pharm Res, Vol 14, Issue 5 (Accepted). **(SCOPUS INDEXED)**
12. J. Josephine Leno Jenita, Jahnavi Kulkarni, **Agasa Ramu Mahesh**, Shanaz Banu, Seema S. Rathore, Manjula D. Exposition of Protein Kinase Targeted Nanoplatforms: An Extensive Review. Advances in Pharmacology and Pharmacy 10(2): 128-137, 2022 **(SCOPUS INDEXED)**

Poster Presentations

1. Shraddha Prabhakar Hegde, Sahana H.U, Jhansi Laxmi C H, Kirthi Bhushan A, Manasa Kuruba, Merina Elizhabeth Mathew and **Lakshmi M. Sundar**. Exploring the anti-inflammatory activity of Lp-PLA2 inhibitors by *In-silico* method, National Conference on Clinical Pharmacology: Drug Re-purposing: A New Ray to Overcome COVID-19 Disaster, K R Mangalam University, Gurugram. April 29, 2022.
2. Mallepalle Srividya, **Lakshmi. M. Sundar** and Kumaravel. S. Novel Analytical Method Development of RP-HPLC Method For Assay and Dissolution of Procyclidine Hydrochloride, National Conference on Recent Advancement and Challenges in Analytical Chemistry, JSS Academy of Higher Education and Research, -Mysuru. May 20, 2022.
3. Burhaniddin Madriwala, **Judy Jays.** Molecular docking and computational Pharmacokinetic study of flavonoid analogues tethred with Isoniazid for antitubercular activity. National conference on Multi-disciplinary research in Pharmaceutical sciences from 9-11th February, 2022
4. G Chaitanys Sai, **Judy Jays.** Molecular Docking and ADMET studies of Pyrazole derivatives. 2nd World congress of Pharmacology-Drug Discovery and development on 30th January, 2022
5. **Judy Jays, Parashuram P**, Saravanan J. Screening of some novel isoxazoles against c.albicans for their potential use asantifungals: a computational approach. International Conference on Current Trends in Drug Discovery Development & Delivery organized by KL University, on 21st and 22nd October 2022

Oral Presentations

1. **Judy Jays**. Molecular docking studies and *in-silico* pharmacokinetic predictions of some novel amino-pyrimidines as potential inhibitors of E.coli, E-Symposium on Integrated Approaches to Drug Discovery and Development – An Update organized by Department of Pharmaceutical Chemistry, Manipal College of Pharmaceutical Sciences, MAHE, Manipal. July 25 - 27, 2022
2. Medicharla Sri Satya and **Suma B.V**. Molecular Docking and ADMET studies of Benzimidazole derivatives tethered with isoniazid for breast cancer at Ist National Conference on Clinical Pharmacology, Drug Repurposing: A New Ray to overcome COVID 19 disaster organised by DST, SERB, Government of India April 29 2022
3. Aiswariya and **Suma B.V.** Molecular Docking and ADMET studies of Bentriazole derivatives tethered with isoniazid at 1st National Conference on Clinical Pharmacology, Drug Repurposing: A New Ray to overcome COVID 19 disaster organised by DST, SERB, Government of India, April 29, 2022
4. **Suma B.V.** and Medicharla Sri Satya. Molecular docking and ADMET Studies of 2-(1H-Benzotriazoly-1-yl)acetohydrazide containing Isatin Derivatives for Breast cancer, proceedings at 5th Global Cancer Summit, International collaborative conference, BioGensis Helath cluster, Bengaluru, May 22, 2022.
5. Aiswariya and **Suma B.V.** Molecular docking and ADMET Studies of benzotraizole derivatives tethered with Isoniazid, proceedings at 5th Global Cancer Summit, International collaborative conference, BioGensis Helath cluster, Bengaluru, May 22, 2022.
6. Medicharla Sri Satya and **Suma B.V.** Molecular docking and ADMET Studies of benzimidazole derivatives tethered with Isoniazid for Anti-cancer property, proceedings at 5th Global Cancer Summit, International collaborative conference, BioGensis Health cluster, Bengaluru, May 22, 2022.
7. Jhansi Laxmi C H and **Suma B.V.** Molecular Docking and ADMET Studies of Stigmasterol for Anti-microbial Properties proceedings at 5th Global Cancer Summit, International collaborative conference, BioGensis Health cluster, Bengaluru, May 22, 2022.
8. Shraddha Prabhakar Hegde, **Suma B.V.** Molecular DOCKING AND ADMET Studies CHOLESTA-22,24-DIEN-5-OL,4,4-DIMETHYL compound for the antibacterial property proceedings at 5th global cancer summit, International collaborative conference, BioGensis Health cluster, Bengaluru, May 22, 2022.
9. **Judy Jays**, Molecular docking studies and binding site interactions of some novel isoxazoles against the target enzymes of E.coli. E-World Congress On Science, Technology, Engineering & Management "Think

Beyond Covid-19,Non-Communicable Diseases, Biogenesis Health cluster conferences, Bengaluru, on 2nd October 2022

10. **Lakshmi. M. Sundar**, Dilip Chekuri, Bindushree G, Cerin Sarah Reji, Richu Siby Jude and andShamil Siraj. In silico studies on anti-inflammatory activity of Indian medicinal plants. International Conference on Global Trends in Applied Sciences, Medical and Health Science (ICGTASMH 2022), REVA University, Bangalore, October 28, 2022

Awards

Dr. Lakshmi M Sundar received Annual Exemplary Award from RUAS on 12th September 2022 during the Teacher's Day Celebrations at RUAS

Invited Lectures

1. **Dr. Parasuraman** has delivered invited lecture at M S Ramaiah College of Arts Science and commerce, Bengaluru on 1st June 2022.
2. **Dr. Parasuraman** has delivered invited lecture at Erode Sengunthar Engineering College, Tamil Nadu, on 17, September, 2022.
3. **Dr. Parasuraman** has delivered invited lecture at Faculty of Pharmacy, RUAS Bangalore, on 22nd and 23rd September, 2022.
4. **Dr. A R Mahesh** has delivered invited lecture at Faculty of Pharmacy, RUAS Bangalore, on 22nd and 23rd September, 2022.
5. **Dr. Parasuraman** has delivered invited lecture Vinayaka Mission's College of Pharmacy, Salem on 21st October, 2022.
6. **Dr. AR Mahesh** has delivered invited lecture Vinayaka Mission's College of Pharmacy, Salem on 21st October, 2022.

Value Added Course

Department of Pharmaceutical Chemistry conducted Value added course on "Advances in Medicinal Chemistry" from 08-July-2022 to 13-July-2022

Department of Pharmaceutical Chemistry in collaboration with IQAC announces

Value added course

"Advances in Medicinal Chemistry"

08-July-2022 to 13-July-2022
(30 Hours)

COURSE OBJECTIVE

- To provide students with knowledge on the Advances in current Medicinal Chemistry approaches

COURSE OUTCOME

- To design Enzyme inhibitors and Prodrugs
- To understand the basics of Peptide synthesis and Process chemistry
- To introduce environmental friendly Synthetic Techniques

COURSE CONTENTS

- Rational design of enzyme inhibitors
- Peptide chemistry
- Prodrug chemistry
- Process chemistry
- Green chemistry

Student Achievements

M.Pharm (Pharmaceutical Chemistry) students have won the prizes in E-Symposium organized by Manipal Academy of Higher Education.

Ms. Jeevitha Lokesh - 1st Prize and Best Poster in the category of In Silico studies - Guided by Dr. Parasuraman. P, Asst Prof, Department of Pharmaceutical Chemistry and Co-Guided by Mr. Damodar Nayak A, Asst. Prof, Department of Pharmacology.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Certificate of Achievement

This is to certify that

JEEVITHA LOKESH

has won the First Prize for scientific e-poster titled "Lead identification for aldose reductase enzyme to treat cataract: A computational and experimental approach" under the Category-I: *In-Silico* Studies in the *E-Symposium on "Integrated Approaches to Drug Discovery and Development – An Update"* organized by Department of Pharmaceutical Chemistry, Manipal College of Pharmaceutical Sciences, MAHE, Manipal from 25th to 27th July 2022.

Dr. Varadaraj Bhat G, Associate Professor, Coordinator
Dr Suvarna G Kini, Professor and Head, Organizer
Dr C Mallikarjuna Rao, Principal, Convener


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Certificate of Achievement

This is to certify that

VAMSHI R

has won the Third Prize for scientific e-poster titled "Development and validation of novel analytical method for assay of Amphotericin B Liposomal injection formulation" under the Category-III: Analytical Approaches in the *E-Symposium on "Integrated Approaches to Drug Discovery and Development – An Update"* organized by Department of Pharmaceutical Chemistry, Manipal College of Pharmaceutical Sciences, MAHE, Manipal from 25th to 27th July 2022.

Dr. Varadaraj Bhat G, Associate Professor, Coordinator
Dr Suvarna G Kini, Professor and Head, Organizer
Dr C Mallikarjuna Rao, Principal, Convener

Mr. Vamshi R - 3rd Prize in the category of Analytical Approaches - Guided by Dr. D R Harish Kumar, Prof & Head, Department of Pharmaceutical Chemistryand Co-Guided by Dr. Kumaravel, Deputy Manager, Bioplus Ltd.

Ms. Harshini Anand of batch 2018-2022 secured 2nd Place in oral presentation competition in the International Conference on "Current Trends In Drug Discovery, Development & Delivery (CTD-4-2022) held during 21st & 22nd October 2022, organized by KL College of Pharmacy, KL Deemed to be University, Vaddeswaram, AP, India-- Guided by Dr. AR Mahesh, Asst Prof, Department of Pharmaceutical Chemistry.

Student Activities

World Pharmacist's Day

Theme 2022

"Pharmacy united in action for a healthier world"

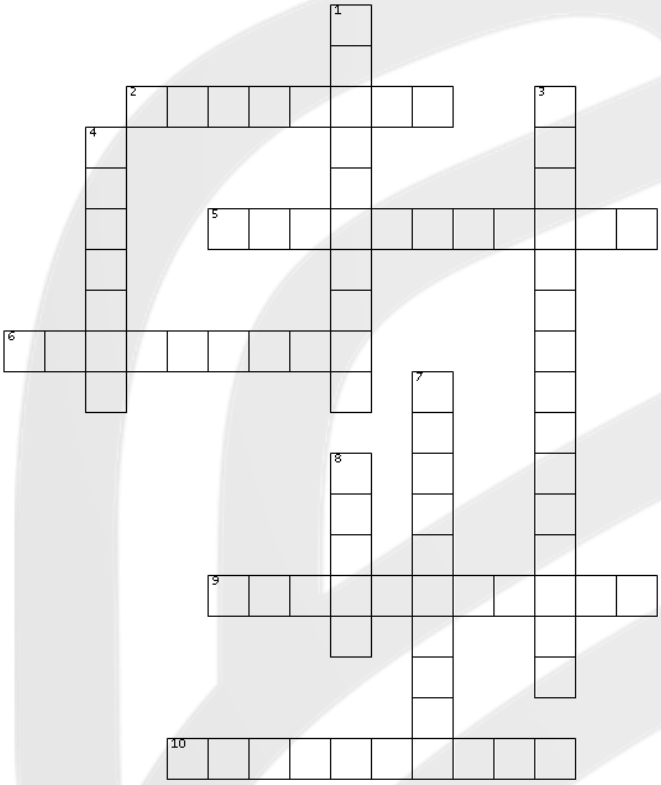
Click on the picture to watch the Video

Cancer Awareness Month

Click on the picture to watch the Video

Cross word

Apeksha K Hegde,Nandini M S and Anjana Vidya Srivathsa, M.Pharm 1st Semester



ACROSS

2. Dye used as photo initiators in preparation of holographic polymers.

5. Antimalarial drug isolated from sweet wormwood which won a Nobel prize in 2015 and was discovered by Tu Youyou.

6. Isonicotinamide with _____ in aqueous medium produces Isoniazid.

9. A potassium sparing diuretic often used in combination with thiazide diuretic for treatment of high blood pressure.

10. A heterocyclic compound that features both amine and ether functional groups and which is completely saturated.

DOWN

1. Reduction of ketones to alkanes using zing amalgam and concentrated hydrochloric acid.

3. An organic compound used as an indicator and can also be used medicinally as a cathartic.

4. Apple seed contains amygdalin, a substance that releases _____ into the bloodstream when chewed and digested.

7. Anticancer drug extracted from pacific yew tree known as the "tree of death".

8. Reagent used in identification of primary, secondary and tertiary alcohols.

Send the Solved Crossword to chemid.fph@gmail.com

COMING SOON

Chemocracy - A Student Club

RAMAIAH UNIVERSITY OF APPLIED SCIENCES | Faculty of Pharmacy

Faculty of Pharmacy
Department of Pharmaceutical Chemistry

CHEMID

A Quarterly E-Newsletter

Volume 1

Issue 2

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