

## SREE DATTHA INSTITUTE OF PHARMACY

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Nagarjuna Sagar Road, Sheriguda (V), Ibrahimpatnam (M), R.R.Dist., Greater Hyderabad-501510. T.S

Ph.:+91-8801099936/35, 9393808082,

Email: principalsdip@sreedattha.ac.in,www.sreedattha.ac.in

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Sr.No	NAME OF THE TEACHER	TITILE OF THE BOOK / CHAPTER PUBLISHED	ISBN/ISSN NUMBER	NAME OF THE PUBLISHER
1.	Dr.U. Sambamoorthy	Computation al modelling of drug disposition	978-81- 954048-4-1	WPI Publishers- Elsevier index
2.	Mrs.Syeda Hina Naaz	Unfolding the potential of Benzothiazole derivatives As bioactive agents: Recent advances	ISBN:978-81- 958789	Innovare academic sciences pvt ltd
3.	Mrs. G. Deepthi Reddy	Unfolding the potential of Benzothiazole derivatives As bioactive agents: Recent advances	ISBN:978-81- 958789	Innovare academic sciences pvt ltd
4.	Mrs. J. Prathyusha	Molecular docking, synt hesis, charact erization of Sulfamethoxa zole Schiff base metal complex and its anti bacterial, Anti inflammatory,	978-81- 19761-40-1	Advanced concepts in pharmaceuti cal research

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		Anti- depressant activity		
5.	Dr. Yamjala Ganesh	Combatting Antibiotic Resistance: Leveraging Fecal Microbial Transplantati on for Gut Health	ISSN: 0967- 0912	Springer Nature Singapore Pte Ltd.



## Computational modelling of drug disposition

Unnam Sambamoorthy<sup>1</sup>', Sandip Prasad Tiwari<sup>2\*</sup>, Lagnajit Mahapatra<sup>3</sup>,

Bikash RanjanJena4, Suryakanta Swain 5, SK Abdul Rahaman6

- <sup>1</sup>Department of Pharmaceutics, Sree Dattha Institute of Pharmacy, Rangareddy District, Sheriguda, Ibrahimpatnam, Telangana- 501510, India
- Faculty of Pharmacy, Kalinga University, Naya Raipur, Chhattisgarh- 492101, India
- <sup>3</sup>Sri Sivani College of Pharmacy, Srikakulam, Chilakpalem, Pin-532402, Andhra Pradesh, India
- <sup>4</sup>School of Pharmacy and Life Sciences, Centurion University of Technology and
- Management, Jatni, Khurda-752050, Odisha, India School of Pharmacy and Paramedical Sciences, K.K. University, Berauti, Nepura,
- School of Pharmacy and Paramedical Sciences, K.K. University, Beradit, Repara,
  Biharsharif, Nalanda-803115, Bihar, India
- Department of Pharmaceutical Chemistry, Nirmala College of Pharmacy, Atmakur Village, Mangalagiri Mandal, Guntur-522 503, Andhra Pradesh, India

#### 2.1 Introduction

In olden days, drug discovery had the focal point enormously on its effectiveness and selectivity in opposition to the biological target. As a consequence, virtually half of the drug components are unsuccessful at research investigations through clinical trials of phase II and III, due to the unwanted drug pharmacokinetics characteristics such as ADME as well as the toxicity (ADMET). The demands to organize the rising cost of novel drug development have altered the pattern since the mid-nineteenth century (Bergstrom, 2005). Especially, in-vitro evaluation of the disposition in the early segment of drug innovation has broadly been adopted to lessen the attrition rate at further superior stages. A lot of, in-vitro ADMET property associated high-throughput screening (HTS) techniques, have been originated and implemented effectively. The rapid boom of computational power, historic advancement of in-silico modeling algorithms, and copious computational programs have also been developed, which focus on modeling the ADMET distinctiveness. An extensive list of available lucrative ADMET modeling software has been developed until the date for drug innovations and research (Slavica, Marko, 2010). The computational model explication for the solubility forecast might afford the collections of chemical compounds, macro, and micro molecules screenings. These combinatorial libraries become supportive of distinguishing the substances which are potentially difficult to eradicate with inadequate solubility (Slavica, Marko, 2010). Further-more solubility forecast from chemical structure, such model's execution often can present an imminent into structure-solubility co-relationships and can

## Chapter-

## UNFOLDING THE POTENTIAL OF BENZOTHIAZOLE DERIVATIVES AS BIOACTIVE AGENTS: RECENT ADVANCES

Sayeda hinanaaz<sup>1</sup>, Laxmi Devi BN<sup>2</sup>, Deepthi Gudigopuram<sup>3</sup>, Gayatri Devi<sup>4</sup>, Krishna Komaragiri<sup>5</sup>, Harsha Sri Kamma<sup>6</sup>, Naresh Podila<sup>7\*</sup> <sup>1</sup>Department of Pharmaceutical Chemistry, Assistant professor, Sreedattha institute of pharmacy, Sheriguda, Ibrahimpatnam, R.R. District, Hyderabad, Telangana, India, <sup>2</sup>Department of Pharmaceutical Chemistry, Joginapally B.R. Pharmacy college, Yenkapally, Moinabad. Hyderabad, Telangana, <sup>3</sup>Department of Pharmaceutical Chemistry, Assistant professor, Sreedattha institute of pharmacy, Sheriguda, Ibrahimpatnam, R.R. District, Hyderabad, Telangana, India, <sup>4</sup>Department of Pharmaceutics, NRI College of Pharmacy, Pothavarapadu, Agripalli, Eluru District, A.P., India, <sup>6</sup>Department of Pharmaceutical Sciences, Vignan Pharmacy College, Vadlamudi, Guntur, A.P., Inida, 5.7 Department of Pharmaceutical Sciences, School of Biotechnology and Pharmaceutical Sciences, Vignan's Foundation for Science, Technology and Research, Vadlamudi, Guntur, A.P., India

ABSTRACT: Because of their wide spectrum of pharmacological properties, benzothiazole derivatives have attracted a lot of attention in recent years for study and development. It has been discovered that substances based on benzothiazoles are useful in the treatment of a number of illnesses, such as cancer, microbial infections, and cardiovascular conditions. Research on the synthesis of benzothiazole derivatives has been ongoing, and many synthetic techniques have been devised to get these molecules, the creation of something new limproved biological characteristics and specificity of novel sentfolds.

## **Combatting Antibiotic Resistance:** Leveraging Fecal Microbial Transplantation for Gut Health

Prashasti Upreti, Lalchand D. Devhare, Lara Hashim Abdulmageed, Yamjala Ganesh Kumar, Rajesh Kumar, and G. Dharmamoorthy

Abstract

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This chapter provides a comprehensive exploration of the relationship between gut microbes and human health. It explores the pivotal roles gut microbiota play in maintaining homeostasis, influencing metabolism, modulating the immune system, and even impacting neurological functions. The disruptive phenomenon of dysbiosis, characterized by an imbalance in the gut microbial community, is thoroughly examined, highlighting its association with various diseases, including inflammatory bowel diseases and antibiotic-resistant infections. Fecal microbiota transplantation emerges as a revolutionary therapy that seeks to restore healthy microbial balance in the gut along with addressing various gastrointestinal disorders and MDRO, presenting key insights from existing studies and case

P. Upreti (>1)

Department of Microbiology, Graphic Era Deemed to be University, Dehradun, Uttarakhand, India

L. D. Devhare

Manwatkar College of Pharmacy, Chandrapur, Maharashtra, India

L. H. Abdulmageed

University of Anbar, Ramadi, Anbar, Iraq

Department of Pharmacognosy and Phytochemistry, Sree Dattha Institute of I Hyderabad, Telangana, India

Maharaja Agrasen School of Pharmacy, Maharaja Agrasen University, Solan, Himachal Pradesh, India

G. Dharmamoorthy

Department of Pharmaceutical Analysis, MB School of Pharmaceutical Sciences (Erstwhile SreeVidyanikethan College of Pharmacy), Mohan Babu University,

Tirupati, Andhra Pradesh, India

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Corresponding Author	Family Name Upreti		
· ·	Particle		
	Given Name	Prashasti	
	Suffix		
	Division	Department of Microbiology	
	Organization/University	Graphic Era Deemed to be University	
	Address	Dehradun, Uttarakhand, India	
Author	Family Name	Devhare	
	Particle		
	Given Name	Lalchand D.	
	Suffix		
	Division		
	Organization/University	Manwatkar College of Pharmacy	
	Address	Chandrapur, Maharashtra, India	
Author	Family Name	Abdulmageed	
	Particle		
	Given Name Lara Hashim		
	Suffix		
	Division		
	Organization/University	University of Anbar	
	Address	Ramadi, Anbar, Iraq	
Author	Family Name	Kumar	
	Particle		
	Given Name	Yamjala Ganesh	
	Suffix		
	Division	Department of Pharmacognosy and Phytochemistry	
	Organization/University	Sree Dattha Institute of Pharmacy	
	Address	Hyderabad, Telmana Index	

Particle		
i unitiele		
Given Name	Rajesh	
Suffix		
Division		
Organization/University	Maharaja Agrasen School of Pharmacy, Maharaja Agrasen University	
Address	Solan, Himachal Pradesh, India	
Family Name	Dharmamoorthy	
Particle		
Given Name	G.	
Suffix		
Division	Department of Pharmaceutical Analysis	
Organization/University	MB School of Pharmaceutical Sciences (Erstwhile SreeVidyanikethan College of Pharmacy), Mohan Babu University	
Address	· Tirupati, Andhra Pradesh, India	
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	Suffix Division Organization/University  Address Family Name Particle Given Name Suffix Division Organization/University  Address This chapter provides a compreh gut microbes and human health play in maintaining homeostas immune system, and even impaphenomenon of dysbiosis, chara community, is thoroughly examidiseases, including inflammate infections. Fecal microbiota tranthat seeks to restore healthy microarious gastrointestinal disorder existing studies and case repeantibiotic-resistant infections, Fedecolonization but also holds furprotocols.	

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## Molecular Docking, Synthesis, Characterization of Sulphamethoxazole Schiff Base Metal Complexes and its Antibacterial, Anti-Inflammatory and Anti **Depressant Activity**

Mugdivari Sangeetha a+++, R. Gandhimathi a#, Shushma Voggu att and Jammula Prathyusha att

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#### **ABSTRACT**

The goal of the study is to create metal complexes that are higher than schiff's base using metals like copper, metal, and metallic element, as well as to synthesis schiff's base, an antibacterial medication, using aromatic organic compounds like p-diethyl amino benzyldehyde and p-dimethyl amino benzyldehyde. Schiff bases are versatile organic compounds which are widely used and synthesized by condensation reaction of different amino compound with aldehydes or ketones known as imine. Schiff base ligands are considered as privileged ligands as they are simply synthesized by condensation. The synthesized schiff's bases were regenerate to its ion Schiff bases by treating with methyl group halide. The ion Schiff bases were regenerate to metal complexes by treating with metals like CuCl2, ZnCl2 and CdCl2. All the synthesized compounds were characterised by Elemental analysis, IR and 1H proton magnetic resonance. Docking study was performed to know the interaction of binding sites with protein receptor using MAO-B enzymes (PDB ID: 2BK5) and COX-2 enzyme (PDB ID: 5IKR) by Virtual Screening software for Computational Drug Discovery. Synthesized metal complexes were evaluated for antibacterial, anti inflammatory and antidepressant activity. Copper metal complexes showed potent antibacterial and anti-inflammatory activity. Significant anti-depressant activity was shown for 2A2 and 2B2 zinc metal complexes.

Keywords: Sulphamethoxazole; antibacterial; anti-inflammatory; antidepressant activity.

<sup>&</sup>lt;sup>a</sup> Department of Pharmaceutical Chemistry and Analysis, School of Pharmaceutical Sciences Institute of Science, Technology and Advanced Studies (VISTAS), Pallavaram, Tamilnadu, India.

<sup>\*\*</sup> Research scholar;

<sup>\*</sup>Corresponding author: E-mail: gandhimathi.sps@velsuniv.ac.in;

have been made possible through the use of synthetic methodologies and improvements to existing technologies. Numerous biological actions, such as anticancer, antibiotic, antifungal, antimicrobial, HIV–I protease inhibition, and antiarteriosclerosis properties, have been demonstrated by benzothiazole derivatives. Research on the pharmacological characteristics of benzothiazole derivatives is still an intriguing field with the possibility of finding novel medications and treatments. The current overview of benzothiazole and its derivatives gives a thorough rundown of their biological activity and production. In addition to being a helpful resource for scientists engaged in synthetic chemistry and drug discovery, this review is anticipated to stimulate additional study and creation of benzothiazole-based molecules with improved pharmacological characteristics.

#### INTRODUCTION

Because of their many physiological roles, heterocyclic molecules like benzothiazole are particularly important in organic chemistry and drug discovery<sup>1</sup>. The possible biological actions of benzothiazole and its derivatives have been the subject of much research. Benzothiazole derivatives, especially 2-aminobenzothiazoles, were studied in the 1950s for their potential muscle relaxant effects. Since then, a variety of pharmacological effects, such as those that are antibacterial, anti-inflammatory, analgesic, anticonvulsant, antiviral, anthelmintic, antioxidant, and anticancer, have been discovered in benzothiazole analogues <sup>2,3</sup>.

One type of heterocycle that contains sulfur is called benzothiazole, which is made up of a thiazole ring fused to a benzene ring. Due to its strong pharmacological and biological activity, the benzothiazole ring system was first discovered in a variety of marine and terrestrial natural compounds. Today, it is widely employed as an enzyme inhibitor, vulcanization accelerator, antioxidant, plant growth regulator, antifluorescence material, inflammatory, imaging reagent, electroluminescent device<sup>4-7</sup>. In particular, benzothiazole is a key compound in medicinal chemistry and has a wide range of biological activities, such as anti-cancer<sup>8, 9</sup>, anti-bacterial<sup>10</sup>, <sup>11</sup>, anti-tuberculosis <sup>12</sup>, <sup>13</sup>, anti-diabetic<sup>14</sup>, anthelmintic<sup>15</sup>, anti-tumor<sup>16–18</sup>, anti-viral<sup>19, 20</sup>, anti-oxidant<sup>21</sup>, anti-inflammatory<sup>22</sup>, <sup>23</sup>, anti-glutamate and antianticonvulsant<sup>25</sup>, muscle parkinsonism<sup>24</sup>, activities relaxant neuroprotective<sup>27</sup>, and inhibitors of multiple enzymes <sup>28</sup>. As a result, the synthesis of benzothiazoles is very desirable due to their strong biological activity and high therapeutic potential. Benzothiazote