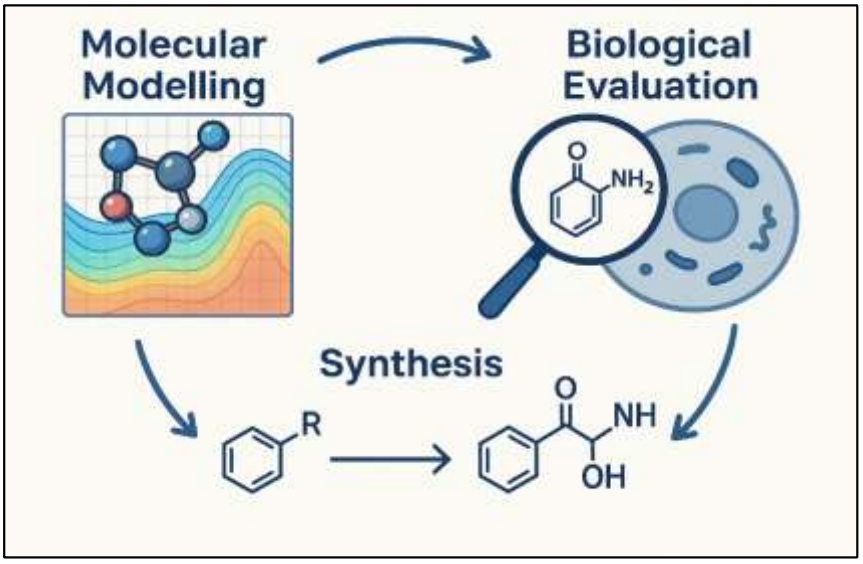
Research Group- Medicinal Chemistry Group

- **Name of Principal Investigator/ Group Leader**: **Dr. Swastika Ganguly**
- **Research Theme**: Design, synthesis and evaluation of novel heterocyclic analogs for various biological activities

- **Broad Area of Research and Scope:**
  - Medicinal Chemistry
  - Computer Aided Drug Design
- **Scope:**

Medicinal chemistry is a dynamic and interdisciplinary field that lies at the intersection of chemistry, biology, pharmacology, and computational sciences. It focuses on the design, synthesis, and development of pharmaceutical agents to improve human health. The scope of medicinal chemistry is vast, encompassing various stages of drug discovery and development, as well as integrating emerging technologies and methodologies.



Total Number of Publications by the group: 50

Top 5 Article with impact factor: (Vancouver Style)

1. Sony J. K, Swastika G., Pravin K., Raju P., and Anoop K., Homology modeling, molecular dynamics simulation, and novel pyrazole analog design of Candida albicans lanosterol 14α-demethylase, a target enzyme for antifungal therapy, J. Biomol. Str. Dyn. 2017; 35(7):1446–1463. Impact factor: 5.3
2. Geeta Y. and Swastika G**.**, Structure activity relationship (SAR) study of benzimidazole scaffold for different biological activities: a mini-revie . Eur. J. Med. Chem, 2015; 97: 419- 443.Impact factor:11.7
3. Nigam J. M. , Swastika G**.** , Kiattawee C. , Supaphorn S., Siriwan S.and Thitinan A.,Synthesis, *in vitro* Anti-HIV-1RT evaluation, molecular modeling, DFT and acute oral toxicity studies of some benzotriazole derivatives. Journal of Structural Biology.
   DOI: https://doi.org/10.1016/j.jsb.2024.108094. Impact factor 3.0
4. Rahul G. and Swastika G**.**, An Integrative Computational Approach for Design and Evaluation of Novel [1,2,4]triazolo[3,4-b][1,3,4]thiadiazole Analogues as Dual-Action Anti-Retroviral and Anti-Bacterial Agents: Insights into Rational Drug Design Strategies. J. Comput. Biophy. Chem.,

https://doi.org/10.1142/S2737416524500418 Impact factor: 2.44

5. Krishnan S. K., **Swastika G.**, Ravichandran V. and Erik D. C., Synthesis, Antiviral activity and Cytotoxicity Evaluation of Schiff bases of some 2-PhenylQuinazoline-4(3)H-ones, Eur. J. Med. Chem. 2010; 45 :,5474-5479. Impact factor:11.7

Patents by the group:

Sl. No	Title and Inventors	Application No. & Date	Status
1	Thiazolidine-2,4-Dione Derivatives,Their Synthesis And Uses, Radhe Shyam Bahare and Swastika Ganguly	Patent No:434035 Application dated 27/01/2012	Granted
2	Novel benzotriazole compounds and their methods of synthesis thereof, Nigam Jyoti Maity and Swastika Ganguly	Application No: 202431017120 A dated 9th March 2024	Published

Research Projects:

Title	Role (PI/ Co-PI)	Funding Agency	Amount (in Lacs)	Duration
In Silico Design, Synthesis and Evaluation of newer azoles as HIV-1-RT inhibitors	PI: Swastika Ganguly CoPI: Abhimanyu Dev	UGC MRP	13.838	3 years (2013-2016)
Design, Synthesis and evaluation of some DAMNI analogs as Novel NNRTIs with broad-spectrum chemotherapeutics	PI: Swastika Ganguly CoPI: Papiya Mitra mazumdar	AICTE-RPS	9.37	2 years (2008-2010)
Synthesis, Evaluation and Molecular Modeling studies of Some Imidazole analogs as potential Non Nucleoside Reverse Transcriptase Inhibitors	PI: Swastika Ganguly CoPI: Papiya Mitra mazumdar	UGC MRP	1.40	2 years (2009-2011)

- **Industry/Academia Collaborations:**
  1. Collaboration with Dr. Mark Ashton and his team, Newcastle University, United Kingdom
  2. Collaboration with Dr. Kiattawee Choowongkomon, Kasetsart University, Bnagkok, Thailand.
  3. Collaboration with Dr. Petrina Kapewangolo,Biochemistry, Microbiology and Biotechnology, University of Namibia, Africa
  4. Collaboration with Dr. Nicholas Cremer,and his team, University of Pittsburgh.
- **Targeted Application Area:** Medicinal Chemistry
- **Achievements:**
  - Development of novel heterocyclic analogs as antimicrobial and antiHIV agents.
  - Patents and publications achieved accordingly.
  - 16 research scholars awarded their Ph.D. degree and more than 30 students awarded their PG degree.

Project 1: In Silico Design, Synthesis and Evaluation of newer azoles as HIV-1-RT inhibitors

Problem Statement

HIV is the pathogenic retrovirus of the lentivirus family and causative agent of AIDS or AIDS Related Complex (ARC). In general, the inhibitors of HIV-1-RT are classified into two main categories: Nucleoside inhibitors (NRTIs) such as AZT, ddI, ddC and 3TC, and Non Nucleoside inhibitors (NNRTIS), like Nevirapine, delaviridine and efavirenz. However, the emergence of resistant viral strains severely impairs the long term efficacy of NNRTIs.

Strategy

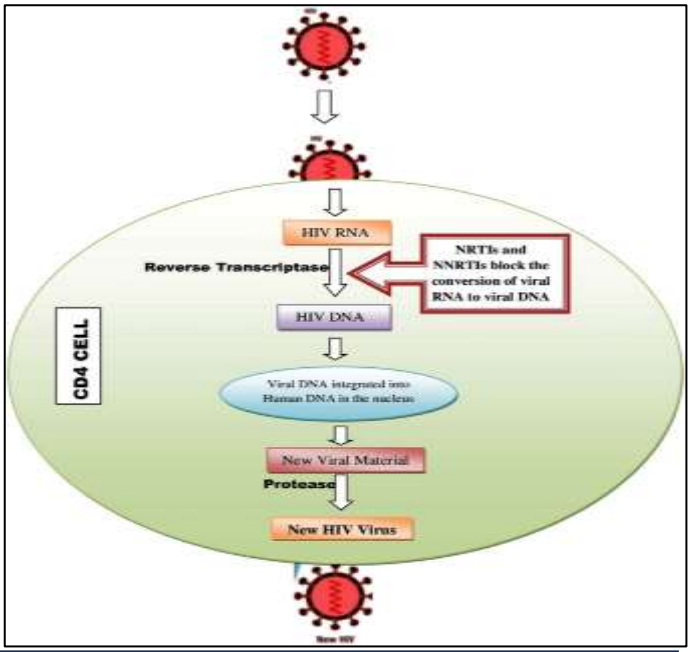
Newer azoles were designed based on the pharmacophoric requirements of NNRTIs, and synthesized. Biological evaluation of the novel heterocycles were carried out in the assay systems of HIV .

Applications

- Development of 3 D QSAR model for prediction of unknown compounds for significant activities.
- Development of novel heterocyclic analogs for antimicrobial and antiHIV activities.

Publication

Swastika Ganguly, Sony Jacob K, Therapeutic outlook of pyrazole analogs: A mini review, Mini Reviews in Medicinal Chemistry, 2016, 16, 1-25 DOI: 10.2174/1389557516666151120115302. (SCI)



Project 2: Design, Synthesis and evaluation of some DAMNI analogs as Novel NNRTIs with broad-spectrum chemotherapeutics

Problem Statement:

HIV has been identified as the probable causative agent for AIDS. It targets the monocytes expressing surface CD4 receptors producing profound defects in cell-mediated immunity. Overtime infection leads to severe depletion of CD4 T-lymphocytes (T-cells) resulting in opportunistic infection (OIs) like tuberculosis (TB), fungal, viral, protozoal and neoplastic diseases and ultimately death.

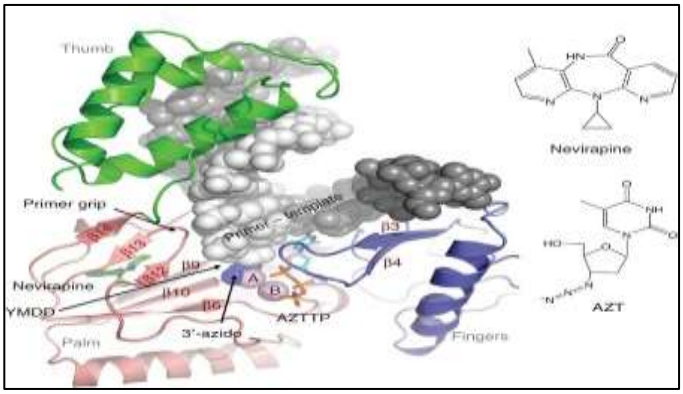
No such drug exists for HIV/AIDS patients which could suppress HIV replication thereby acting as anti-HIV drug and also could treat OIs like TB, hepatitis and other bacterial infections parallely.

Publication & Patents

- S.K. Krishnan, **S. Ganguly**, R. Veerasamy, B. Jan, **,** European Review for Medical and Pharmacological Sciences, 15, 2011, 673-682.. No.: 202331071055 & Date 27.10.23)
- **Swastika Ganguly**, Vatsal Vijay Vithlani, Anup Kr. Kesharwani, Ritu Kuhu, Baskar L, Papiya Mitramazumder, Ashok Sharon and Abhimanyu Dev, Acta Pharm, 2011, 61,187-201.
- S.Murugesan, **S. Ganguly** and G. Maga, , Journal of Chemical Sciences, March 2010, 122(2), 169-176

Strategy

- Newer Dimethoxy nitroimidazoles(DAMNI) were designed based on the pharmacophoric requirements of NNRTIs.
- The designed analogs were synthesized and evaluated for their HIV-1-RT inhibitory activities and antimicrobial activities.



Applications

1.Development of 3 D QSAR model for prediction of unknown imidazoles for significant activities.

2.Development of novel nitroimidazoles for antiHIV activities with broad spectrum chemotherapeutic properties.

Group Members