Amit Sharma, Ph.D.

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An enthusiastic pharmaceutical scientist driven by a relentless pursuit to discover better ways of healing and healthcare outcomes. Interested in a career as a Medicinal/Organic/Computational Chemist, drug design and discovery. Previous academic and research experience in medicinal chemistry and drug design with in-depth knowledge of:

- Alzheimer's Disease drug development
- Anti-Infective drug discovery
- Targeted small molecule/peptides/polymer synthesis (Hit-to-Lead optimization)
- Computer aided drug design

Available to relocate worldwide

Education

Ph.D. – Medicinal Chemistry 2019-2024
Birla Institute of Technology and Science (BITS), Pilani, India

Master in Pharmacy (M.Pharm.)- Pharmaceutical Chemistry 2017-2019
Birla Institute of Technology (BIT), Mesra, Ranchi, Jharkhand, India

Bachelor in Pharmacy (B.Pharm.)- Pharmaceutical Sciences 2013-2017
Dr. A.P.J. Abdul Kalam Technical University, Lucknow, Uttar Pradesh, India

Experience

July 2025- Present — **Scientific Researcher (R1) at National Institute for Research and Development of Isotopic and Molecular Technologies (INCDTIM), Cluj-Napoca, Romania (EU)**

Feb 2025- July 2025 — **Assistant Professor at Manipal Academy of Higher Education (MAHE), Manipal College of Pharmaceutical Sciences (MCOPS), India**

Aug 2019- May 2024 — **Graduate Teaching Assistant at Birla Institute of Technology and Science (BITS), Pilani, Pilani Campus, India**

- Tutorial Instructor of Undergrad and Postgrad students in various pharmaceutical subjects, including Biological Chemistry (PHA F242), Advanced Pharmaceutical Chemistry (PHA G544), Advanced Medicinal Chemistry (PHA G621), Instrumental Methods of Analysis (PHA F313), Computer Aided Drug Design (PHA G541), Natural Drugs (PHA F344), Pharmaceutical Chemistry (PHA F241), Medicinal Chemistry I (PHA F312) Medicinal Chemistry II (PHA F342).

Technical Skills and Core Competencies

In-silico Drug Design
- Computer Aided Drug Design tools such as Schrödinger (Glide), Molegro Virtual Docker, Homology/Pharmacophore modeling, High-throughput virtual screening (HTVS), AutoDock, AutoDock Vina, PyRx, SeeSAR, Qik Prop, Swiss ADME, Protox, DruLiTo, OSIRIS Data Warrior, PyMOL 3.0, Desmond, UCSF Chimera 1.10.2, VMD 1.9.2.
- Proficient in SBDD/LBDD/Fragment based drug design, Molecular dynamics simulation (protein-ligand)

Grant Writing
- Academia Sinica postdoc. grant**,** DST-CRG, CSIR, ICMR, DBT

Synthetic Organic/ Medicinal Chemistry
- Design and synthesis of novel heterocyclic derivatives as AChE/BACE-1 dual inhibitors for the treatment of Alzheimer's disease.
- Harnessing the antimicrobial potential of pyrrole- and indole-derived allylidene hydrazine carboximidamides: From bench to bioactivity evaluation.
- Proficient in conventional as well as microwave assisted and ultra-sonication induced organic synthesis.
- Multi-step organic synthesis, optimizing chemical process and scale-up synthetic methods
- Purification techniques: Column chromatography, Preparative TLC, Recrystallization, Fractional Distillation, Flash chromatography.
- Handling of different metal catalyst such as palladium, copper, rhodium, iridium, cobalt etc. with proper care and safety precautions.
- Skilled in Peptide synthesis via couplings reagents like DCC, HOBt, EDCl.HCl, HATU and HBTU etc. with proper care and at most efficiency.

Analytical Evaluation
- Characterization of organic compounds using NMR (^{1}H, ^{13}C), ATR, LC-MS/MS, HRMS, HPLC, GC, Fluorescence Spectroscopy, UV Spectroscopy, Polarimetry, DSC, TGA.

***In-vitro* Studies**
- *In-vitro* primary and secondary human and mice cell lines culture, bacterial cell culture (BSL-1/2) & biological evaluation of various cells using techniques such as cytotoxicity (MTT), apoptosis, cellular uptake assay using multicolor flow cytometry, confocal, and fluorescence microscopy.

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- Skillful in *In-vitro* enzyme inhibition assays (ELISA based FRET, ELLMAN).
- Proficient in performing *In-vitro* antimicrobial activity of test compounds.

Software's

Data handling and interpretation interface such as-

- MestReNova, ACD Chemsketch, Chemdraw, Marvin Sketch, Top Spin for structural analysis.
- Graphpad Prism, Origin for data analysis & statistics.

Professional Training

- FTIR and 2D NMR techniques, Pharmacophore modeling and protein-ligand interaction using SeeSAR Workstation, Schrödinger modules, Biosafety and Biohazards (BSL-1/2)

Projects

1. **Synthesis of dendrimers containing sulfonium ions in the backbone for anti-bacterial applications (PNRR Project- Next Gen. EU Program).**
2. **Design, synthesis and biological evaluation of β-secretase and acetylcholinesterase as dual inhibitors for the development of anti-Alzheimer's agents.**
3. **Harnessing the antimicrobial potential of pyrrole- and indole-derived allylidene hydrazine carboximidamides: From bench to bioactivity evaluation.**
4. **Butadiene sulfone catalyzed monobromination of arenes and hetero-arenes with NBS as the bromination source: A simple, mild, efficient and chemoselective protocol. (New method development)**
5. **Design, synthesis and studies of novel 1,2,3-trisubstituted tetrahydroimidazoles as anti-infective agents.**

Publications

1. Dash S, Kini SG, **Sharma A***. MraY: An Emerging Therapeutic Target in Bacterial Peptidoglycan Biosynthesis for The Discovery of Novel Antibiotics from Natural and Synthetic Origin. *European Journal of Medicinal Chemistry*. **2025** (Accepted on 01-10-2025). (*****corresponding author)
2. Dash S, Kini SG, **Sharma A***. Bisquinoline as a Promising Scaffold in Anti-Infective Drug Discovery: The Current State of the Art and Future Prospects. *Expert Opinion on Drug* Discovery. **2025** July, 1–28. (*****corresponding author)
3. **Sharma A**, Jain SJ, Jha PN, Rudrawar S, Bharate SB, Jadhav HR. Unfolding the Potential of Pyrrole- and Indole-Based Allylidene Hydrazine Carboximidamides as Antimicrobial Agents. *ACS Infectious Diseases.* **2025** Feb 14;11(2):493-505.
4. **Sharma A,** Rudrawar S, Bharate SB, Jadhav HR. Recent advancements in the therapeutic approaches for Alzheimer's disease treatment: current and future perspective. *RSC Medicinal Chemistry.* **2024** Dec 6;16(2):652-693.
5. **Sharma A**, Rudrawar S, Sharma A, Bharate SB, Jadhav HR. Design, synthesis, *in silico*, and *in vitro* evaluation of pyrrol-2-yl-phenyl allylidene hydrazine carboximidamide derivatives as AChE/BACE 1 dual inhibitors. *RSC Advances*. **2024** Aug 23;14(37):26703-26722.
6. **Sharma A**, Rudrawar S, Sharma A, Bharate SB, Jadhav HR. Unveiling the potential of novel indol-3-yl-phenyl allylidene hydrazine carboximidamide derivatives as AChE/BACE 1 dual inhibitors: a combined *in silico*, synthesis and *in vitro* study. *RSC Advances*, **2024** Jul 30;14(33):23853-23872.
7. **Sharma A,** Jadhav HR, Anubhav Rai, Naga R. Lakkaniga, Harish C. Chandramoorthy, Hossam Mohammed Kamli, Mohammad Y. Alshahrani, and Prasanna Rajagopalan. A Comprehensive Review of Systemic Targeted Therapies in Cancer Treatment. *Current Cancer Therapy Reviews*. **2024**: 461-480.
8. **Sharma A**, Rudrawar S, and Jadhav HR. Butadiene Sulfone-catalyzed Monobromination of Arenes with NBS as the Bromination Source: A Simple, Mild, Efficient, and Chemoselective Protocol. *Letters in Organic Chemistry*. **2024**: 201-208.
9. Chattaraj B, Khanal P, Nandi A, Das A, **Sharma A**, Mitra S, Dey YN. Network pharmacology and molecular modelling study of *Enhydra fluctuans* for the prediction of the molecular mechanisms involved in the amelioration of nephrolithiasis. *Journal of Biomolecular Structure and Dynamics*. **2023**;41(24):15400-15410.
10. Chattaraj B, Nandi A, Das A, **Sharma A**, Dey YN, Kumar D, R M. Inhibitory activity of *Enhydra fluctuans Lour*. on calcium oxalate crystallisation through *in silico* and *in vitro* studies. *Frontiers in Pharmacology*. **2023** Jan 20;13:982419.

Grants & Awards

- NSTC (MOST) Postdoc. Research Fellowship, Taiwan (Host: GRC, Academia Sinica) 2025
- Institute Research Fellowship: BITS, Pilani, India 2019-2024
- AICTE-NDF: Qualified 2019
- Qualified GPAT: 96.93 % with 165 score 2018
- Qualified NIPER-JEE: AIR 545 2018

Reference list

1. Prof. Swastika Ganguly Email: swastikaganguly@bitmesra.ac.in
2. Prof. Prabhat Nath Jha Email: prabhatjha@pilani.bits-pilani.ac.in
3. Dr. Saurabh Sharma Email: ssharma6@stanford.edu