AKSHAY RAUL

COMPCHEM RESEARCHER



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EDUCATION

M.S. in Medicinal Chemistry, 2020

National Institute of Pharmaceutical Education and Research (NIPER), S.A.S Nagar, India

- Graded 8.6/10 CGPA
- Thesis submission "Design and Synthesis of Phenyl linked quinazolinone amidines as trypanothion reductase inhibitors "

Bachelore of Pharmacy, 2018

KLE College of Pharmacy, Belagavi, Karnataka, India

Graduated with Percentage: 72.64%

PUBLICATION

 Review article "Biguanides: Species with versatile therapeutic applications" in European Journal of Medicinal Chemistry.

DOI: 10.1016/j.ejmech.2021.113378

AREAS OF EXPERTISE

to promote health care system.

- Structure and ligand-based drug design, virtual screening,
- Molecular docking (Rigid, IFD and covalent docking) ,Free energy calculation (MMGBSA/PBSA)

Aspiring for a job which enables me to showcase my technical and professional knowledge and to contribute to drive the

standard, quality and value of the organization in the endeavour

- Scaffold hopping, shape-based screening and bioisosteric replacement
- Pharmacophore modeling, Similarity/Near neighbor search/Clustering
- Homology modeling, Molecular dynamics simulation.
- PROTAC design
- De-novo Drug design and Fragment based drug design
- Basic quantum mechanics and Energy calcualtions (DFT/HF)
- Library Enumeration, calculating molecular properties

Software exposure: Schrodinger suits, ICM Molsoft, Knime workflows,

Cresset's Flare and Spark, Guassian, RDkit, Gromacs,

Programming languages known: C++ and Basic Python

EXPERIENCE

- Senior Research Associate Syngene International Ltd |
 Oct 2020 Present
- Supporting Medchem projects, CADD projects, Database curation and handling

CO-CURRICULAR

 Poster presentation (Title: Green chemistry: Solvents and Catalysts a Greener Approach) In APPI-17 National seminar on "Environmental Physiology- High Altitude and Space"

LANGUAGES KNOWN

- English
- Hindi
- Kannad
- Marathi

HOBBIES

- · Trekking and Travelling
- Yoga
- Numismatics

REFERENCE

Prof. P.V. Bharatam

Professor & Head Dept. of Medicinal Chemistry, NIPER, Sector-67, SAS Nagar (Mohali), Punjab, IN - 160062 Ph: +91-172-2292018 pvbharatam@niper.ac.in

ACADEMIC ACHIVEMENTS

- Qualified NIPER Ph.D-JEE, 2022 (For Ph.D in Pharmacoinformatics) -All India Rank 2
- NIPER masters entrance exam 2018 with All India Rank 173
- Qualified AICTE Graduate Pharmacy Aptitude Test (GPAT), 2018
- Awarded NIPER fellowship for 2 years by Ministry of Chemicals and Fertilizers, Govt. of India, to pursue M.S. (Pharm.) in Medicinal Chemistry
- Awarded with Sir Ratan Tata Scholarship for being meritorious in 2nd and 3rd year B.Pharm respectively
- Honored with Best Student Award in Bachelor of Pharmacy, 2018

EXTRA-CURRICULAR

- Active member of National Service Scheme (NSS) in KLE College of Pharmacy and NIPER, Mohali: Responsible for various volunteering social activities like blood donation camp, cleanliness campaigns, awareness events in nearby elementary and middle schools
- Placement Coordinator of the Department of Medicinal Chemistry,
 2019-20: Responsible for organizing placement drives and acts as an interface between the employing organization and the students