DR. SHAILENDRA S. CHAUDHAERY

Sr. Scientist, Medicinal Chemistry Division
INCOZEN Pvt. Ltd
Address: 450 MN Park, Genome Valley, Turkapally, Telangana 500078
Phone No, ; (+91) 6201980672 , 8002834999 ,
E-mail: shailendrac@incozen.com , shail12cdri@gmail.com
Bachupally, Hyderabad, Telangana

CAREER OBJECTIVE

- As a Computational Chemist, Computer-Assisted Drug Design (CADD), Cheminformatics scientist, interested in multi-disciplinary research area in Drug discovery, which involved in projects, collaboration and help in solving challenging problems, from hit to lead identification across all biological target classes and major therapeutic indications.

PROFESSIONAL EXPERIENCE SUMMARY

- Total 13 years of experience in the area of Computer-Assisted Drug Design (CADD), Molecular modelling and Drug design, Computational Chemist.
- Currently, Working as Sr. Scientist, Medicinal Chemistry Division, INCOZEN Pvt. Ltd. Genome Valley, Turkapally, Telangana.
- Earlier, Research Scientist, CADD Lab, INDRAS Pvt. Ltd. Support Medicinal Chemistry.

RESEARCH SKILLS & EXPERTISE

- Excellent work knowledge of modern computational techniques, conducted, managed, and to support of computer aided drug design (CADD) research.
- Apply a wide variety of drug design and computational chemistry methods to improve potency, selectivity, and ADME properties while minimizing toxicological risk.
- Applying computational chemistry tools and approaches for the identification and evaluation of binding sites on proteins. Evaluating, benchmarking and developing methodology for structure-based drug design.
- Experience in Structure-Based Virtual Screenings, Library Designing, filtering, Development of Disease specific drug database and fragment-based drug discovery.
- Proficiency in MD simulation program: Desmond.
- Estimate the Binding Affinity/Free energy, docking scores of various novel targets using Docking software etc.
- Fragment based optimization, Shape-based screening, Scaffold Hopping, Bio-isosteric replacement.
- Fingerprint generation and diversity analysis, ADME & PK predictions.

- ❖ Toxicity alert assessment, WaterMap based analysis, Denovo design
- ❖ Development of Quantitative/Qualitative Pharmacophore Models QSAR, Machine Learning and Virtual Screening.
- ❖ Good knowledge of statistics: descriptive statistics, regression analysis, clustering and model building.
- ❖ Understanding of SAR interpreting data using modeling and data-mining technologies.
- ❖ Experience with machine learning (supervised and unsupervised), active learning, statistical design of experiments, multi-objective modeling.
- ❖ knowledge of programming language (such as Python).
- ❖ Proficiency in commercial computational chemistry packages (examples include Maestro/Schrodinger, MOE/Chemical Computing Group, OpenEye, Cresset, Biovia discovery studio).

PROFESSIONAL EXPERIENCE SUMMARY

From	To	Designation	Organization	Role
June 2021	Till date	Sr. Scientist,	INCOZEN Pvt. Ltd. Genome Valley, Turkapally, Telangana.	• Support Medicinal chemist for lead identification and optimization.
July 2o2o	May 2o21	Research Scientist-I, CADD Lab,	INDRAS Pvt. Ltd. & INCOZEN Pvt. Ltd.	• Support Medicinal chemist for lead identification and optimization.
May 2012	Feb 2019	Lecturer	Department, National Institute of Pharmaceutical Education and Research (NIPER), Hajipur, India.	• Teaching course to M.S.(Pharm) and PhD students about various aspects of molecular modelling. • Nodal officer
Mar 2012	May 2012	Research Associate / (Postdoc)	University of Hyderabad, Hyderabad, India.	
Nov 2011	Feb 2012	Research Associate / (Postdoc)	Dr. B.R. Ambedkar centre for Biomedical Research (ACBR), New Delhi, India	Project entitled: “Bio-informatics infrastructure facility”.

Nov 2010	Aug 2011	Research Associate / (Postdoc)	Jawaharlal Nehru University (JNU), New Delhi, India.	Project entitled: "Pharmacophore model development, validation, virtual screening, lead identification and optimization for Plasmodium Falciparum".

EDUCATIONAL QUALIFICATIONS

Degree	Subject	University/ Institute	Year
PhD	Biotechnology	Medicinal and Process Chemistry Division, Central drug research Institute (CDRI) & (Degree awarded from Department of Biotechnology, Integral University, Lucknow, India). Thesis: "Synthesis, QSAR and Molecular Modelling Studies on Anti-Alzheimer's Agents"	2007-2011
MSc	Biotechnology	Kumaun University, Nanital, (Uttaranchal), India.	2002-2004

INTERNATIONAL PUBLICATIONS

- Kant, V., Vijayakumar, S., Sahoo, G. C., Ali, V., Singh, K., ***Chaudhery, S. S***., & Das, P. (2019). In-silico screening and validation of high-affinity tetra-peptide inhibitor of Leishmania donovani O-acetyl serine sulfhydrylase (OASS). ***Journal of Biomolecular Structure and Dynamics***, 37(2), 481-492.
- Sethi, M. K., Singh, D., Murti, K., ***Chaudhaery, S. S***., Pandey, K., & Das, P. (2014) ***World Journal of Pharmaceutical Sciences***, 2(10), 1395-1400.
- Eleftheriou, P., Geronikaki, A., Hadjipavlou-Litina, D., Vicini, P., Filz, O., Filimonov, D., Poroikov V, ***Chaudhaery S. S***., Roy K. K., & Saxena, A. K. (2012). Fragment-based design, docking, synthesis, biological evaluation and structure–activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinonesas cycloxygenase/lipoxygenase inhibitors**.** ***European journal of medicinal chemistry***, 47, 111-124.
- Bennamane, N., Nedjar-Kolli, B., Geronikaki, A. A., & Th, P. (2011). N-Substituted [phenyl-pyrazolo]-oxazin-2-thiones as COX-LOX inhibitors: influence of the replacement of the oxo-group with thioxo-group on the COX inhibition activity of N-substituted pyrazolo-oxazin-2-ones. ***Arkivoc***, 2, 69-82.
- ***Chaudhaery, S. S***., Roy, K. K., Shakya, N., Saxena, G., Sammi, S. R., Nazir, A., ... & Saxena, A. K. (2010). Novel carbamates as orally active acetylcholinesterase inhibitors found to improve scopolamine-induced cognition impairment: pharmacophore-based virtual screening, synthesis, and pharmacology**.** ***Journal of medicinal chemistry***, 53(17), 6490-6505.
- ***Chaudhaery, S. S.,*** Roy, K. K., & Saxena, A. K. (2009). Consensus superiority of the pharmacophore-based alignment, over maximum common substructure (MCS): 3D-QSAR studies on carbamates as acetylcholinesterase inhibitors. ***Journal of chemical information and modeling***, 49(6), 1590-1601.
- Misra, P., Sashidhara, K. V., Singh, S. P., Kumar, A., Gupta, R., ***Chaudhaery, S. S***., ... & Dube, A. (2010). 16α-hydroxycleroda-3, 13 (14) z-dien-15, 16-olide from: a safe and orally active antileishmanial agent Polyalthia longifolia: a safe and orally active antileishmanial agent. ***British Journal of Pharmacology***, 159(5), 1143-1150.
- Saxena, S., ***Chaudhaery, S. S***., Varshney, K., & Saxena, A. K. (2010). Pharmacophore-based virtual screening and docking studies on Hsp90 inhibitors. ***SAR and QSAR in Environmental Research***, 21(5-6), 445-462.
- Saxena, S., ***Chaudhaery, S. S***., Varshney, K., & Saxena, A. K. (2010). Molecular Modelling and Docking Studies on Hsp90 Inhibitors. ***SAR and QSAR in Environmental Research***, 21,1-20.
- Bhargava, P., Kumar, K., ***Chaudhaery, S. S***., Saxena, A. K., & Roy, U. (2010). Cloning, overexpression and characterization of Leishmania donovani squalene synthase. ***FEMS microbiology letters***, 311(1), 82-92.