Dr. SUMAN SINHA

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EDUCATION

2011-2017:	Doctorate of Philosophy, Pharmaceutical Technology, Universiti Sains Malaysia
2004-2006:	Master of Technology, Pharmaceutical Chemistry, Vellore Institute of Technology
1997-2001:	Bachelor of Pharmacy, Berhampur University.

WORK EXPERIENCE

May 2017–present	Post-Doctoral Fellow, Tata Institute of Fundamental Research, Hyderabad
June 2011–April2017	Research Assistant, Department of Pharmaceutical Technology, School of Pharmaceutical Sciences, Universiti Sains Malaysia, Penang, Malaysia
June 2009-June 2011	Assistant Professor, Department of Chemistry, Karunya University, Tamil Nadu, India
Aug 2007-May 2009	Senior Lecturer, Department of Pharmacy, Lovely Professional University, Punjab, India
Sept 2006-July 2007	Lecturer, Roorkee College of Pharmacy and Allied Sciences, Uttarakhand, India
April 2002-Feb 2004	Medical Representative with Nicolas Piramal India Ltd.

CURRENT RESEARCH

- Development of competitive protein inhibitors against therapeutic targets in malarial invasion.
- Development of peptide inhibitors against AMA1-RON2 interaction.
- Computational structural biology using atomistic molecular simulations. I apply both equilibrium dynamics as well as enhanced sampling techniques to understand free energy surfaces pertaining to molecular recognition.
- Elucidation of binding pathways for drug like molecules into therapeutic targets like proteins and DNA and RNA.

RESEARCH PROJECTS UNDERTAKEN

- M.Tech dissertation on peptide synthesis and small molecule crystallography.

- Synthesis and biological evaluation of natural and synthetic naphthoquinonoids on leishmanial and colon cancer cell lines.

- Synthesis and biological evaluation of natural and synthetic naphthoquinonoids on colon cancer cell lines.

- Computer aided design of dual inhibitors of H1N1 and H5N1 neuraminidase towards the development of anti-swine flu drugs.

ACADEMIC COURSES TAUGHT

- Medicinal chemistry

- Computer aided drug design

- Organic chemistry

SPECIALIZED TRAINING (DRUG DISCOVERY)

- Participated in hands on training on different techniques in drug discovery with Aurigene Discovery Technologies, Bangalore, India, Aug-Sept, 2013.

- Participated in short term research project on molecular dynamics simulation as a visiting student with Dr.Jagannath Mondal at Tata Institute of Fundamental Research, Centre for Interdisciplinary Sciences at Hyderabad, India, Aug-Sept, 2016.

TECHNICAL EXPERTISE (softwares)

Schrodinger Suite (Glide, Phase, Pymol, etc), Autodock, Genetic Optimisation for Ligand Docking (GOLD), Vina, VLife Molecular Design Suite (VLife Sciences), Gromacs and Plumed.

WORKSHOPS ATTENDED

- Workshop on Structure Based Drug Design, March 13-15, 2008, conducted by National Institute of Pharmaceutical Education and Research (NIPER)
- Workshop on Cheminformatics and Approaches in Drug design, 11-13th December, 2009, conducted by Vellore Institute of Technology and Schrodinger Inc.
- Workshop on Free Energy Calculations for Chemical and Biological Systems, 17-22 March 2019 conducted by Indian Institute of Technology Kanpur.

ACADEMIC PRESENTATIONS

- Poster titled "Effects of branched Beta-carbon dehydro residues on peptide conformation in 'International symposium on Green and Sustainable Chemistry' jointly organized by Delhi University and New Jersey Institute of Technology, 2006.

- Poster titled "Structure based drug design using alpha, beta, dehydro residues" in International symposium on Green and Sustainable chemistry' jointly organized by Delhi University and New Jersey Institute of Technology, 2006.

- Poster titled "A synthetic and molecular simulation approach to understand the chemical basis of Plasmodium falciparum AMA1-RON2 Interaction" in in-house symposium organized by Tata Institute of Fundamental Research Hyderabad, 2018.

PUBLICATIONS

- Molecular Dynamics Simulation Elucidates Oligosaccharide Recognition Pathways by Galectin-3 at Atomic Resolution, Jaya Krishna Koneru, **Suman Sinha**, Jagannath Mondal, Journal of Biological Chemistry DOI: https://doi.org/10.1016/j.jbc.2021.101271, (In Press Accepted Manuscript Published online: October 4, 2021)

- Computational and experimental studies of plasmodium falciparum protein PfAMA1 domain-II loop dynamics: implications in PfAMA1-PfRON2 binding event, **Suman Sinha**, Anamika Biswas, Jagannath Mondal, and Kalyaneswar Mandal, bioRxiv:doi: https://doi.org/10.1101/2021.10.10.463826, (**manuscript submitted**)

- A Chimeric Peptide Inhibits Red Blood Cell Invasion by Malaria Parasites with Two Orders of Magnitude Increased Efficacy, Jamsad Mannuthodikayil, **Suman Sinha**, Sameer Singh, Anamika Biswas, Irshad Ali, Purna Chandra Mashurabad, Wahida Tabassum, Pratap Vydyam, Mrinal Kanti Bhattacharyya, Kalyaneswar Mandal
  bioRxiv: https://www.biorxiv.org/content/10.1101/2021.09.28.462119v1
  (**manuscript submitted**)

- Role of Molecular Dynamics in Optimizing Ligand Discovery: Case study with Novel Inhibitor Search for Peptidyl t-RNA Hydrolase, Bhupendra Dandekar, **Suman Sinha**, Jagannath Mondal, (https://doi.org/10.1016/j.chphi.2021.100048).

- In Silico Reoptimization of Binding Affinity and Drug-Resistance Circumvention Ability in Kinase Inhibitors: A Case Study with RL-45 and Src Kinase Jaya Krishna Koneru, **Suman Sinha**, Jagannath Mondal, *J. Phys. Chem. B* 2019.

- Application of Non-Affine parameter (NAP) in binding site detection for novel inhibitors of *Leishmania donovani* DNA topoisomerase-1, Dheeraj Dube, **Suman Sinha**, Jagannath Mondal, Surajit Sengupta (**manuscript under preparation**).

- Antileishmanial activity evaluation of bis-lawsone analogs and DNA topoisomerase-I inhibition studies. Sharma G, Chowdhury S, **Sinha S**, Majumder HK, Kumar SV. J Enzyme Inhib Med Chem. 2014 Apr;29(2):185-9.

- 4-Methyl-2-oxo-2*H*-chromen-7-yl 4-fluorobenzenesulfonate. **S. Sinha**, H. Osman, H. A. Wahab, M. Hemamalini and H.-K. Fun,Acta Cryst. (2012). E68, o641-o642

- 3-Hydroxy-2-(4-methoxybenzenesulfonamido) butanoic acid. **S. Sinha**, H. Osman, H. A. Wahab, M. Hemamalini and H.-K. Fun, Acta Cryst. (2011). E67, o3275.

- 4-Methyl-2-oxo-2*H*-chromen-7-yl 4-methoxybenzenesulfonate. **S. Sinha**, H. Osman, H. A. Wahab, M. Hemamalini and H.-K. Fun, Acta Cryst. (2011). E67, o3457
- Ethyl 2-acetyl-3-anilinobutanoate. S. Priya, **S. Sinha**, V. Vijayakumar, T. Narasimhamurthy, T. Vijay and R. S. Rathore, Acta Cryst. (2006). E62, o5367- o5368.

RESEARCH REVIEWING EXPERIENCE

Reviewer, Scientific Reports, https://www.nature.com/srep/

REFEREES

- Dr.Kalyaneswar Mandal, Tata Institute of Fundamental Research, Hyderabad (https://www.tifrh.res.in/~kmandal/); Ph: +91 40 20203092
- Dr.Jagannath Mondal, Tata Institute of Fundamental Research, Hyderabad (https://www.tifrh.res.in/~jmondal/); Ph: +91 40 20203091
- Dr. Aneesh Tazhe Veetil, Tata Institute of Fundamental Research, Hyderabad (https://www.veetil-lab.com/); Ph: +91 40 20203071
- Dr.Sharmistha Dey, All India Institute of Medical Sciences, New Delhi (https://www.aiims.edu/en/notices/126-biophysics/720-dr-sharmistha-dey.html); Ph:+91-11-26546435

Suman Sinha.

Date: 18.02.2022
Place: Hyderabad, India.