**SUMAN SINHA**

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**EDUCATIONAL QUALIFICATIONS**

PhD, Pharmaceutical technology (computer aided drug design), Universiti Sains Malaysia (USM), 2017.

M.Tech, Pharmaceutical Chemistry, Vellore Institute of Technology (VIT), July 2006.

B.Pharm, Berhampur University, Feb 2001.

**PROFESSIONAL EXPERIENCE**

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| May 2017 – present | Post Doctoral Fellow, Tata Institute of Fundamental Research, Hyderabad |
| June 2011 – April 2017 | 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. |

**COURSES TAUGHT**

* Medicinal chemistry
* Computer aided drug design
* Organic chemistry

**CURRENT RESEARCH**

* Design of competitive protein inhibitors against therapeutic targets in malarial invasion.
* Design of peptide inhibitors against AMA1-RON2 interaction.
* Establish structure activity relationships (QSAR) on wild and mutant type kinases, acetylcholinesterase, and H1N1 and H5N1 neuraminidases for novel inhibitor design.
* Design of combinatorial libraries based on natural scaffolds with inputs from QSAR.

**RESEARCH PROJECTS UNDERTAKEN**

* M.Tech dissertation on peptide synthesis and small molecule crystallography from the Department of Biophysics, All India Institute of Medical Sciences (AIIMS), New Delhi.Primary work was to design and synthesize novel peptides against enzymes responsible for inflammation and confirm the structures by X-ray 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.
* Computer aided design of novel inhibitors of acetylcholinesterase.
* Molecular dynamics simulation analysis of protein-small molecules/protein/peptide/DNA.

**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.

**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**

* 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.
* Potential Novel Dengue Virus NS2B-NS3 Protease Inhibitors From Natural Scaffolds: A Preliminary Study, **S. Sinha**, Nadhirah Tahir, H. Osman, H. A. Wahab, (**manuscript submitted**).
* Application of non-affinity parameters (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**).
* 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 (**manuscript submitted**).
* Understanding the role of PfAMA1 Domain II loop towards stabilization of RON2: Perspectives from enhanced sampling dynamics. **Suman Sinha**, Jagannath Mondal and Kalyaneswar Mandal (**manuscript under preparation**).
* Computational insights into native and designed ligand binding to galectin-3 using atomistic molecular dynamics and markov state modeling, Jaya Krishna Koneru, **Suman Sinha**, Jagannath Mondal ((**manuscript under preparation**)

# Antileishmanial activity evaluation of bis-lawsone analogs and DNA topoisomerase-I inhibition studies. [Sharma G](http://www.ncbi.nlm.nih.gov/pubmed?term=Sharma G%5BAuthor%5D&cauthor=true&cauthor_uid=23534930), [Chowdhury S](http://www.ncbi.nlm.nih.gov/pubmed?term=Chowdhury S%5BAuthor%5D&cauthor=true&cauthor_uid=23534930), [Sinha S](http://www.ncbi.nlm.nih.gov/pubmed?term=Sinha S%5BAuthor%5D&cauthor=true&cauthor_uid=23534930), [Majumder HK](http://www.ncbi.nlm.nih.gov/pubmed?term=Majumder HK%5BAuthor%5D&cauthor=true&cauthor_uid=23534930), [Kumar SV](http://www.ncbi.nlm.nih.gov/pubmed?term=Kumar SV%5BAuthor%5D&cauthor=true&cauthor_uid=23534930). [J Enzyme Inhib Med Chem.](http://www.ncbi.nlm.nih.gov/pubmed/23534930) 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.](http://journals.iucr.org/e) (2011). [E67](http://journals.iucr.org/e/contents/backissues.html), 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/

**PERSONAL PROFILE**

* Date of Birth : 19.03.1978
* Gender : Male
* Nationality : Indian
* Languages Known : English, Hindi, Bengali

**REFEREES**

1] Dr.Kalyaneswar Mandal, Tata Institute of Fundamental Research, Hyderabad

(https://www.tifrh.res.in/~kmandal/); Ph: +91 40 2020 3092

2] Dr. Jagannath Mondal, Tata Institute of Fundamental Research, Hyderabad

(https://www.tifrh.res.in/~jmondal/); Ph:  +91 40 2020 3091

3] 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

Date: 04.04.2021

Place: Hyderabad, India.