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Informatics scientist with over 15 years of experience in designing, and implementing computational solutions, ranging from large scale infrastructures and algorithm design to predictive model development and project support for small molecule development projects, in a highly collaborative pre-clinical drug discovery setting. My work is supported by over 140 publications (cited more than 6500 times) and multiple public software packages. Having held a variety of leadership roles within Vertex, NCATS as well as in the broader cheminformatics community, my goal is to build a group that will impact therapeutic development, at multiple biological scales, to generate a global picture of the effects of small molecules in biological systems.

Education

2001 – 2005	Ph.D. (Chemistry), Department of Chemistry, The Pennsylvania State University.
1999 – 2001	M.Sc. (Chemistry), Indian Institute of Technology, Kharagpur, India.
1995 – 1998	B.Sc. (Chemistry), Presidency College, Calcutta, India.

Professional Experience

2021 – ... **Director (Data & Computational Sciences), Vertex Pharmaceuticals**

2018 – ... **Associate Director (Computational Chemistry), Vertex Pharmaceuticals**

2017 – ... **Editor-in-Chief, *Journal of Cheminformatics***

Set the topical focus and direction of the journal, with input from the Editorial Board, manage article reviews, editorial policy and decisions

2009 – 2018 **Research Scientist, National Center for Advancing Translational Science, NIH**

Proposed and received approval for a *Research Informatics* group, designed its research agenda and currently managing 1.5 FTEs

Performed research into data mining & visualization methods for high dimensional chemical biology datasets, addressing aspects of polypharmacology, biological network structure and structure-activity relationships

Led the development of Pharos, a platform to explore the dark genome. Responsible for management of NCATS deliverables, interactions with collaborators and renewal of the grant funding this project ($280K/year).

Implemented large scale infrastructure to support two major screening facilities - the NCATS combination screening platform & the Trans-NIH RNAi Screening Facility.

Provided key cheminformatics and computational chemistry support on small molecule development projects across multiple therapeutic areas including infectious disease, oncology and neurodegenerative disease

Professional Experience (continued)

2007 – 2009 **Visiting Assistant Professor, School of Informatics, Indiana University**

Worked on methods to explore high dimensional chemical spaces using a density of space approach to recognize chemical structure clusters

Implementation of a fast 3D searching and pharmacophore matching in very large compound databases

Developed methods for handling large chemical datasets, including predictive modeling of HTS cytotoxicity data, virtual screening and QSAR modeling of large combinatorial libraries for anti-malarial activity

Leadership & Mentoring

Member, Board of Directors, CCDC Inc., 2018 –

Member, Advisory Board, Synthia, 2018 –

Member of the NCATS DPI Strategic Planning group, responsible for developing a long term strategic plan for Informatics research and development.

Co-founder of the Blue Obelisk group, to promote Open Data, Open Source and Open Standards within chemistry. See Guha et al, 2006 & O'Boyle et al, 2011.

Chair (2012), Vice Chair (2011) and Program Chair (2009-2010), ACS Division of Chemical Information

Developed and taught workshops on R for biologists at NCATS and EBI (Hinxton, UK) and involved in scientific mentoring of interns within the Informatics group

Member of the editorial boards of Chemistry Central Journal, Current Computer Aided Drug Design, Journal of Cheminformatics and Synergy