Rajendra KRISTAM

Flat 201, DAISY Block
Pavani Residency, Puttenahalli, Yelahanka,
BANGALORE, 560064, India
E-mail: rajkristam11@gmail.com,
Mobile: 0091-9880138932

***Summary**: Leading the computational chemistry team for support of drug discovery projects. Leading an academic collaboration/project for a novel immuno-oncology target and coordinating the efforts towards development of hits-to-candidates. Supervising development of machine-learning/Artificial Intelligence platform with tools for targets and key ADMET end-points. Having worked in both ligand-based drug design (LBDD) and structure-guided drug design (SGDD) teams, I am familiar with the drug discovery research processes, well versed in chemical information concepts, a few programming languages, and machine-learning/AI techniques. Have prior experience in a top class paint company, a world-class pharmaceutical company and founded an educational start-up along with two classmates. Working in contract research organizations (CROs) ever since. Communication, creativity, self-motivation and diligence are key personal characteristics. Published eleven research articles in reputed journals and co-inventor in fifteen patents.*

WORK EXPERIENCE

January 2022 – Present**:** **Jubilant Biosys Ltd,** Bangalore, India.
Jubilant is a contract research organization
http://www.jubilantbiosys.com
Associate Director (In Silico), Drug Discovery group.

Role highlights

- Involved in Artificial Intelligence/Deep Learning efforts of the company
- Leading a project for an academic collaboration drug discovery project, working on a novel immune-oncology target towards hit-to-candidate development.
- Managing the computational chemistry team support for drug discovery programs of the company with various clients.
- Involved in drafting proposals for prospective drug discovery projects with new clients.
- Managing software for the group. Evaluating other software, esp., for structure-based drug discovery projects.

July 2014 – January 2022**: Jubilant Biosys Ltd,** Bangalore, India.
Jubilant is a contract research organization
http://www.jubilantbiosys.com
Principal Scientist (In Silico), Drug Discovery group.

Role highlights

- Project leader for an academic collaboration drug discovery project, working on a novel immune-oncology target towards hit-to-candidate development.
- Manage the computational chemistry team support for drug discovery programs of the company with various clients.
- Involved in drafting proposals for prospective drug discovery projects with new clients.
- Manage software for the group. Evaluating other software, esp., for structure-based drug discovery projects.

Oct 2007 – June 2014**:** **Jubilant Biosys Ltd,** Bangalore, India.
Jubilant is an pioneering informatics and a drug discovery company
http://www.jubilantbiosys.com
Project Manager (In Silico), Drug Discovery group.

Role highlights

- Project leader, virtual lab for computational/collaborative support (VLCS). Under the project, I supervised the team to provide computational support (models and reports) to client's programs.
- Under the VLCS project for Eli Lilly, the team helped in assessing more than 140 biological targets for the client.
- Computational support for discovery programs of the company with various clients.
- Conceive and execute technological increments to existing in-house software programs

June 2006 – Sept 2007t**:** **Jubilant Biosys Ltd,** Bangalore, India.
Jubilant is an pioneering informatics and a drug discovery company
http://www.jubilantbiosys.com
Senior Research Scientist (In Silico), Drug Discovery group.

Role highlights

- Working with external clients on collaborative target-to-hit and hit-to-lead projects.
- Supervising technological development aimed at extending functionality of existing software
- Conceptualizing and development of software for use in in-house and external projects.
- Building of ADMET models that aid in drug discovery process.
- Training new recruits & juniors in various computational chemistry techniques and build a cohesive and effective team.
- Supervising summer project trainees.

April 2006 – June 2006**:** **Aurigene Discovery Technologies Ltd,** Bangalore, India.
Aurigene is a pioneer in new drug discovery research in India.
http://www.aurigene.com
Associate Scientist (Compchem), SGDD group.

Role highlights

- Optimizing lead series of a project.
- Recruiting quality computational chemists and building an effective team.
- Established docking/screening procedure for a project that led to hit generation.
- Modeling CYP inhibition and hERG inhibition for ADME support of a project early on
- Using Fragment-Based Drug Design methodology *in silico* for a project.
- Worked/working on diverse targets

Oct 2005 – April 2006**:** **Aurigene Discovery Technologies Ltd,** Bangalore, India.
Senior Research Associate (Compchem), SGDD group.

Role highlights

- Computational chemist for the company's first project with an external partner.
- Optimize the several lead series of a project. Build a SAR/QSAR for each lead series.
- Virtual screening of focused libraries by docking and pharmacophore-based screening.
- Evolve new leads based on existing leads, pharmacophore, patentability, and synthetic feasibility in consultation with medicinal chemists.
- Evaluate new software to assess its suitability for the company.
- Do the initial groundwork for any new target before a project based on the target starts.
- Actively support and contribute in the company's foray into Fragment-Based Drug Design methodology.

Mar 2004 – Sept 2005**:** **Aurigene Discovery Technologies Ltd,** Bangalore, India.
Research Associate (Compchem), SGDD group.

Role highlights

- Generate virtual combinatorial libraries for scaffolds.
- Select a diverse compound set from a library by diversity analysis and clustering.
- Virtual screening of libraries by docking and/or pharmacophore-based screening.
- Building up a SAR/QSAR using various assay results.
- Training medicinal chemists in the use of computational chemistry software.
- Suggest new scaffolds based on pharmacophore, validate its FTO (freedom to operate) and synthetic feasibility in consultation with medicinal chemists.

Oct 2003 – Jan 2004**:** **Lilly Research Centre, Eli Lilly & Company Ltd,** Surrey, UK.
Chemist, CADD group.

Role highlights

- QSAR modelling.
- Pharmacophore modelling.
- Database building and database searching by various modes (pharmacophore, 2D, 3D, flexible, similarity etc.)
- Homology modelling when crystal structural data is unavailable.

June 2003 – Aug 2003**:** **Lilly Research Centre, Eli Lilly & Company Ltd,** Windlesham, Surrey, UK.
Summer Placement, CADD.

Role highlights

- Worked on project, titled "***Comparison of conformational analysis techniques to generate pharmacophores using Catalyst***". Published as a research article.
- Used conformational analysis software (Catalyst, OMEGA, Chem-X, MacroModel), Corina, Isis/Draw and Isis/Base.
- Used Catalyst for pharmacophore modelling and QSAR.

June 1999 – Jan 2002**:** **Founded a start-up in education sector, along with a couple of classmates.**

Role highlights

- Attempted setting up examination services, content and website development
- Coordinated and interfaced with a few venture capitalists, content providers, and other professionals in the education sector.

June 1996 – Dec 1998: **Asian Paints (India) Ltd.,** Patancheru, Hyderabad, India.
Asian Paints is the 6th largest paint company in Asia.
Supervisor-Chemist, Quality Assurance Department

Role highlights

- Supervised the Effluent Treatment Plant of the entire company.
- Supervised quality control activities in water-based and solvent-based paint processing.
- Oversaw ISO 9001 implementation in ETP and later in Quality Assurance Department.

EDUCATION

2011 – present: **PhD** from the ***SASTRA University***, Thanjavur, Tamil Nadu. Thesis title: *A ligand-based computational paradigm for development of inhibitors of enzymes and its application to the analysis of TRPV1 inhibitors as drug candidates for the treatment of chronic and nociceptive pain.*

2002 – 2003: **MSc in Chemoinformatics** from the ***University of Sheffield***, Sheffield, United Kingdom. Notable courses in the program include: *Chemoinformatics, Molecular Modelling, Database Design, Information Storage and Retrieval, Object-Oriented Programming (Java) and Information Systems Modelling.*

1998 - 2000: **Advanced Diploma in Software Technology** in *ECIL – Software Training Unit*, Secunderabad, India.

1998 - 2000: **MBA** (**Marketing)** from ***Osmania University***, Hyderabad, India.

1994 - 1996: **MSc** with **Chemistry** as major from the ***University of Hyderabad***, Hyderabad, India.

ACADEMIC PROJECTS

1. Title: ***"A comparison of 2D fragment bit strings and physicochemical property data in the selection of diverse subsets"*;** MSc Chemoinformatics. Duration: 4 months.

The project involved an attempt to assess and compare diversity of compound sets selected by different bases, like, 2D fragment bit strings, physicochemical properties and Molconn Z properties. The software project involved extensive programming in Java and usage of Sybyl molecular modelling package. It was observed that compound set selected on different bases yielded nearly similar diversity in each case, although, 2D fragment-based selection seemed to result in slightly better diversity.

2. Title: ***"Doped Organic Semiconductors of Hexacyanotrimethylenecyclopropane (HCTMCP))"*;** MSc Chemistry. Duration: 10 months.

The project was a part of the curriculum and involved an investigation into organic extrinsic n-type semi-conductivity of HCTMCP. An attempt was made to observe, assess and ascertain partial ionicity or mixed valence in this molecular material by doping the monovalent of HCTMCP with its divalent. This project entailed synthesis and analysis of the organic solid, HCTMCP, and literary survey of electrical properties in organic solid-state chemistry.

TECHNICAL SKILLS

Computational chemistry suites: Sybyl, Schrodinger and a few modules in Discovery Studio
Molecular Modelling: Sybyl, Schrodinger, Spartan
Pharmacophore Modelling: Catalyst, GASP & Phase
Conformational Analysis: Catalyst, MacroModel, OMEGA, Chem-X, Confort
Homology Modelling: Insight II, Sybyl/Composer, SwissPDB-Viewer, Prime
Docking: Sybyl/FlexX/FlexiDock, Shrodinger/Glide/CombiGlide, MOE/Dock, GOLD
Other: Corina, Concord, ISIS/Draw, ISIS/Base, ChemOffice, UNIX/IRIX/HP-UX/Linux
Programming: Java, Basic knowledge of Fortran77 & Python
Molecular Dynamics: AMBER, Desmond
Machine-Learning / Deep-Learning: Basic foundational knowledge

PUBLICATIONS

Khalifa N, Kumar Konda LS, **Kristam R**, **Machine learning-based QSAR models to predict sodium ion channel (Nav 1.5) blockers**, Future Med Chem. **2020**, 12(20), 1829-1843.

Tamizharasan N, Gajendran C, **Kristam R**, Sulochana SP, Sivanandhan D, Mullangi R, Mathivathanan L, Hallur G, Suresh P, **Discovery and optimization of novel phenyldiazepine and pyridodiazepine based Aurora kinase inhibitors**, Bioorg Chem. **2020**; 99, 103800.

Singh M, Divakaran R, Konda LSK, **Kristam R**, **A classification model for blood brain barrier penetration**, J Mol Graph Model. **2020,** 96, 107516.

Kannt A, Rajagopal S, Kadnur SV, Suresh J, Bhamidipati RK, Swaminathan S, Hallur MS, **Kristam R**, Elvert R, Czech J, Pfenninger A, Rudolph C, Schreuder H, Chandrasekar DV, Mane VS, Birudukota S, Shaik S, Zope BR, Burri RR, Anand NN, Thakur MK, Singh M, Parveen R, Kandan S, Mullangi R, Yura T, Gosu R, Ruf S, Dhakshinamoorthy S, **A small molecule inhibitor of Nicotinamide N-methyltransferase for the treatment of metabolic disorders**, Sci Rep. **2018,** 8(1), 3660.

Ruf S, Hallur MS, Anchan NK, Swamy IN, Murugesan KR, Sarkar S, Narasimhulu LK, Putta VPRK, Shaik S, Chandrasekar DV, Mane VS, Kadnur SV, Suresh J, Bhamidipati RK, Singh M, Burri RR, **Kristam R**, Schreuder H, Czech J, Rudolph C, Marker A, Langer T, Mullangi R, Yura T, Gosu R, Kannt A, Dhakshinamoorthy S, Rajagopal S, **Novel nicotinamide analog as inhibitor of nicotinamide N-methyltransferase**, Bioorg Med Chem Lett. **2018**, 28(5), 922-925.

Swaminathan S, Birudukota S, Thakur MK, Parveen R, Kandan S, Juluri S, Shaik S, Anand NN, Burri RR, **Kristam R**, Hallur MS, Rajagopal S, Schreuder H, Langer T, Rudolph C, Ruf S, Dhakshinamoorthy S, Gosu R, Kannt A, **Crystal structures of monkey and mouse nicotinamide N-methyltransferase (NNMT) bound with end product, 1-methyl nicotinamide**, Biochem Biophys Res Commun. **2017**, 491(2), 416-422

Kristam R, Rao SN, D'Cruz AS, Mahadevan V, Viswanadhan VN, **TRPV1 antagonism by piperazinyl-aryl compounds: A Topomer-CoMFA study and its use in virtual screening for identification of novel antagonists**, J Mol Graph Model. **2017**, 72,112-128.

Kalindjian SB, Kadnur SV, Hewson CA, Venkateshappa C, Juluri S, **Kristam R**, Kulkarni B, Mohammed Z, Saxena R, Viswanadhan VN, Aiyar J, McVey D, A **New Series of Orally Bioavailable Chemokine Receptor 9 (CCR9) Antagonists; Possible Agents for the Treatment of Inflammatory Bowel Disease**, J Med Chem. **2016**, 59(7), 3098-111.

Kristam R, Parmar V, Viswanadhan VN, **3D-QSAR analysis of TRPV1 inhibitors reveals a pharmacophore applicable to diverse scaffolds and clinical candidates**, J Mol Graph Model. **2013**, 45, 157-72.

Viney Lather, Jagmohan S. Saini, **Rajendra Kristam**, Narasingapuram Arumugam Karthikeyan, Vitukudi Narayana Balaji, **QSAR Models for Prediction of Glycogen Synthase Kinase-3beta Inhibitory Activity of Indirubin Derivatives,** *QSAR & Combinatorial Science* **, 2008**, 27(6), 718-728.

Rajendra Kristam, Valerie J. Gillet, Richard A. Lewis, and David Thorner. **Comparison of Conformational Analysis Techniques To Generate Pharmacophore Hypotheses Using Catalyst**. *J. Chem. Inf. Model.* **2005,** *45*, 461-476

POSTERS

Rajendra Kristam, S.Kumar, Dhananjay Pendharkar, Jitendra Mohite, Narsimha.S., G.Chandrasekhar, D.Mudignal, G.Mahender Reddy, R.Hegde, Sangeetha Naik, Nandhagopal, D.S.Samiulla, Krishnaprasad, Prasad Shivarudraiah, W.R.Balasubramanian, A.Nandyala, Kavitha Nellore, H.Subramanya and M.Ramachandra. **Discovery of novel PDE4 inhibitors for the treatment of COPD and Asthma.** Drug Discovery Technology, 4-6 Oct 2005, Mumbai, India.

Ruf S, Hallur MS, Anchan NK, Swamy IN, Murugesan KR, Sarkar S, Narasimhulu LK, Putta VPRK, Shaik S, Chandrasekar DV, Mane VS, Kadnur SV, Suresh J, Bhamidipati RK, Singh M, Burri RR, **Kristam R**, Schreuder H, Czech J, Rudolph C, Marker A, Langer T, Mullangi R, Yura T, Gosu R, Kannt A, Dhakshinamoorthy S, Rajagopal S, **Identification and in-vivo efficacy studies of novel NNMT inhibitors**, EFMC, ACSMEDI, Medicinal Chemistry Frontiers 2019, June 10-13, Krakow, Poland

Sameer Mahmood Zaheerbasha, Dhanalakshmi Sivanandhan, Biswajit Kalita, Sowmya Ramaiah, Amir Siddiqui, Bharat R Zope, Sanjay V Kadnur, Madhuri Kanavalli, Krishnakumar V, Srinivasan Swaminathan, Rudresh G, Sunil Mohire, Raghunadha Reddy Burri, **Rajendra Kristam**, Jeyaraj DA, Sriram Rajagopal, and Saravanakumar Dhakshinamoorthy, **Protection Of Beta Cell Mass From Diabetogenic Condition Induced Apoptosis By The Inhibition Of Mammalian Ste20-like Protein Kinase 1 (MST1)**, ADA, June-2019

PERSONAL DETAILS

Date of Birth: 1st January 1972. *Marriage Status*: Married. *Nationality*: INDIAN. *Languages*: English, Hindi and Telugu. Know a bit of Kannada and Spanish. *Interests*: Quizzing, Music, Movies, and Reading. Presently learning Python & Data Science techniques.

REFERENCES

Will be provided on request.