MANVI

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ABOUT ME

Highly motivated and dedicated computational chemist with over 13 years of experience providing high level support to various projects. Skilled in managing multiple projects and possessing exceptional communication and interpersonal skills, with a proven ability to work both independently and as part of a team. Currently seeking a new role to leverage my expertise and expand my skills to effectively lead and manage scientific initiatives.

PROFESSIONAL EXPERIENCE

Aurigene Pharmaceutical Services Limited, Bengaluru **March 2022 - Present**
Scientist

- Supporting various projects aiming to identify novel small molecules targeting different protein targets.
- Successfully delivered various projects on/before time.
- Supported internal project with POC study. Contributed towards project planning, design prioritization and compound selection. Team successfully identified 6 active compounds, where 2 compounds were novel.
- Supported reaction-based compound library enumeration.
- Supported in generating various high quality project proposals. Few of the projects are onboarded.
- Proposed new core along with various other designs for one of the projects. Few of the compounds generated with this core showed one-digit micromolar activity.
- Worked on predicting putative binding poses for partner peptides to target proteins.
- PROTAC platform: Helping in setting up the PROTAC pipeline which includes ternary complex prediction, PROTAC degradation prediction and PROTAC design. Supported ideating and prioritizing selected PROTAC designs for synthesis and testing which resulted in notable success.
- Conducted extensive Free Energy Perturbation (FEP) calculations to provide insights into the effects of molecular modifications of binding free energy aiding in compound optimization.

Centre for Chemical Biology and Therapeutics **September 2018 - March 2022**
, InStem, NCBS, Bengaluru

Project Scientist I

- Supported various projects to create small molecule probe that modulate novel classes of targets.
- Supported design of partner peptide constructs based on experimental data along with the help of In-silico tools. For one of the projects, out of three peptide constructs one showed affinity in single digit micromolar and another in two-digit micromolar.
- Predicted putative binding poses for partner peptides in couple of projects.
- Predicted possible binding poses for small molecules targeting PPIs based on experimental data and was able to explain the SAR. Also worked on binding pose prediction for experimentally obtained fragment hits for one of the PPI targets.
- Worked on fragment to lead identification using fragment growing and fragment linking approach. Experimental evidence was pending.

- Done MD simulation to support the observation of experimental crystal structure data. Work is published.
- Used Ligand- and Structure-based Virtual Screening followed by MD simulation for one of the microbial targets to identify novel inhibitors. Work is published.
- For one of the client projects, predicted small molecules binding poses and suggested pocket mutations to validate the pose. Experimental evidence was pending.
- Provided inputs for various targets ideation.

Jubilant Biosys Limited, Bengaluru **August 2010 - August 2018**
Sr. Research Associate

- Published a work on building a classification model for blood brain barrier penetration.
- Built homology model of kinase DFG-out state and one of the GPCRs. The putative binding mode was predicted based on extensive docking and QM calculations. Compounds were evaluated and prioritized for the synthesis. Model was quite well in differentiating active and inactive molecules.
- For one of the client projects, predicted binding mode for the reference molecule was in very good agreement to the X-ray binding mode.
- For various drug discovery projects, suggested molecules based on protein active site were actives.
- Both ligand- and structure-based virtual screening was used in drug discovery projects to identify drug-like molecules. Ligand-based approaches included shape screening, similarity search, Pharmacophore screening and core-hopping, whereas structure-based screening included docking, ensemble docking, E-pharmacophore model and core hopping. The selected compounds were purchased, and 12% compounds showed >35% inhibition at 10μM. For one of the projects, the iterative process of ligand-based virtual screening led to the identification of novel scaffolds as well as the ideas for modifications to the core for improved activity.
- Theoretical study using quantum calculations was conducted to study the reaction mechanisms.
- Also worked on PPIs. Suggested one of the peptide constructs showed >30% inhibition.

EDUCATION

SASTRA University - Thanjavur, India

M.Tech Bioinformatics
June 2010

Banaras Hindu University - Varanasi, India

M.Sc. Bioinformatics
June 2007

COMPUTATIONAL SKILLS

- CompChem suite: Schrodinger, ICMPro, Cresset
- Chemoinformatics: Chemaxon (IJC), Chemoffice, ISIS/MDL, MarvinView
- Molecular dynamics: GROMACS, Desmond
- FEP: Schrodinger
- Protein-protein docking: Hex, Z-dock, PatchDock, ClusPro, FlexPepdock, HADDOCK:
- Protein sequence analysis: EMBOSS, Clustal W, T-Coffee, TMCoffee, PROMALS3D & other Sequence-structures based analysis tools

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PUBLICATIONS

- Singh M., Divakaran R., Konda LSK., Kristam R., A classification model for blood brain barrier penetration. J Mol Graph Model. 2020 May;96:107516. doi: 10.1016/j.jmgm.2019.107516. Epub 2019 Dec 20. PMID: 31940508.
- Kannt, A. et al., A small molecule inhibitor of Nicotinamide N-methyltransferase for the treatment of metabolic disorders. Sci Rep 8, 3660 (2018).
- Ruf S et al., Novel nicotinamide analog as inhibitor of nicotinamide N-methyltransferase. Bioorg Med Chem Lett. 2018 Mar 1;28(5):922-925.
- Mathivanan, S.; Chunchagatta L., Puneeth Kumar ; Singh, M.; Giridharan, S.; Sathish, K.; Bharatham, K.; Kamariah, N., Structure of a 14-3-3 : FOXO3a phosphopeptide complex reveals 14-3-3 isoform specific binding of FOXO phosphoproteins. ACS Omega. 2022 Jul 5;7(28):24344-24352.
- Singh, M.; Kempanna, P.; Bharatham, K. Identification of Mtb GlmU Uridyltransferase Domain Inhibitors by Ligand-Based and Structure-Based Drug Design Approaches. Molecules 2022, 27, 2805.

ACHIEVEMENTS

- Received "Individual Excellence Award" (2022) at APSL for successfully completing and delivering various client-based projects.
- Received "Team Excellence Award (2023)" at APSL for contributing towards various CADD projects.
- Received "Team Excellence Award (2024)" at APSL for contributing towards AILDD platform.
- Topper in M.Tech (2010).
- Received “Spot award” in Jubilant Biosys (2011) for consistent & effective support for client- based and internal discovery projects.
- Received “Most Engaged Associate” award in Jubilant Biosys (2014) for consistent & effective support for client-based and internal discovery projects.
- Been part of the “Best team award (2015)” for the contributions made to the internal project.
- Been part of two “Best team awards” (2016) in recognition of the contribution towards client projects.
- Been part of the “BRD4” project which has been out-licensed to Checkpoint Therapeutics.
- Delivered guest lecture at “Symbiot, 2023”, national conference conducted by Manipal Institute of Technology, Manipal
- Delivered a webinar on “Application of Bioinformatics in Drug Discovery” at Karapagam university (2020).

ORGANIZATIONAL SKILLS

- Handling client based as well as internal projects independently.
- Ability to adapt quickly to new environments and technologies.
- Innovative thinking in applying analysis and creativity to problem solving.
- Ability to work with team and support the team members effectively.
- Project delivery always on/before time.

References are available on request.