

JASMIT KAUR PhD

PROFILE

- Twelve years industrial experience in the application of computational chemistry tools (protein modelling, small molecule modelling, virtual screening and property prediction) to projects at different stages of the drug discovery pipeline.
 - Extensive knowledge of commercial computational chemistry software.
 - Effective time management, planning and organisation of my work to successfully deliver high quality data on a multitude of research projects at any one time.
 - Contributed to a range of multidisciplinary strategic initiatives within the drug discovery research process. A key member of both technology and project steering committees and instrumental in assessment and implementation of automated processes which improved productivity.
 - Significant experience in working in target classes such as GPCRs, kinases and proteases across a variety of therapeutic areas including cardiovascular, CNS, oncology and analgesia.
 - Good communication skills. Regular oral and written presentations to Senior Management, external collaborators and at project team and departmental meetings.
 - An outstanding team player with good networking skills. A natural ability for and enjoyment of interacting, sharing and developing ideas with colleagues from all disciplines and at all levels.
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EMPLOYMENT HISTORY

Senior Computational Chemist, Piramed

Jan 2007- Nov 2007

- Implemented a functional and effective computational chemistry platform (both software and hardware) to support drug discovery portfolio at Piramed.
- Provided project support for a range of targets in different phases of the oncology portfolio. Close interaction with medicinal chemists. Regular presentations at multidisciplinary project meetings. Contributed to quarterly reports.
 - Provided hypothesis relating to PI3K selectivity using sequence alignments and homology models and prioritised chemical targets suggested for synthesis by medicinal chemists on a lead optimization project.
 - Worked on collaborative projects and successfully influenced the strategy for lead finding projects which led to identification small lead-like μM compounds using virtual screening methods.
 - Analysed proprietary crystal structures and utilized structure-based design to design libraries for synthesis.
 - Used Pipeline Pilot to evaluate SAR data and implemented and deployed web based tools such as property calculations for medicinal chemists in conjunction with an external consultant.
- Responsible for defining and implementing a strategy for broadening the lipid kinase franchise. A detailed analysis and recommendations was presented to the Scientific Advisory Board meeting.
- Delivered hands-on training of DS Visualiser 7.0 accompanied with tutorials to medicinal chemists.
- Critically evaluated the scientific and strategic merits of potential new targets for the portfolio as part of multidisciplinary team.

Senior Molecular Modeller, Inpharmatica Ltd

December 2004 – August 2006

- Provided computational support on a diverse range of external collaborative projects. Used a range of computational tools (virtual screening, SBDD, pharmacophore generation and 2/3D similarity searches) and chemical/biological databases. Collated and interpreted scientific data to perform in depth analysis and design of validated computational models to meet project objectives with available resources within specified timelines. Communicated results through a combination of written reports and oral presentations to clients by face-to-face meetings or teleconference.
- As part of a multidisciplinary team, contributed to the enhancement and validation of proprietary computational tools for Chematica™, one of the company's software platforms. Successfully developed and implemented property based methods to analysis compound databases, scaffold generation and analysis tools, a new scoring scheme for ligand-based druggability. These tools were distributed to a range of clients within the pharmaceutical research sector and used on collaborative projects.

- Developed commercial skills through participation (product demonstrations, presentations) in early discussions with potential collaborators alongside colleagues in Business Development.

Research Investigator, OSI Pharmaceuticals UK

September 2002 – November 2004

- Provided project support for a range of targets in different phases of the oncology portfolio. Close interaction with medicinal chemists. Regular presentations at multidisciplinary project meetings.
 - Successfully applied virtual screening approaches using combination of protein homology and ligand-based models to identify several novel chemical series for a kinase target.
 - Utilising proprietary crystal structures of kinase co-complexes to guide medicinal chemist strategies to achieve desired biological profile of lead series.
 - Application of small molecule methods (biostere/molecular superposition analysis) to discover a novel chemotype as part of a fast follower program for a kinase.
 - Identified μM hits for an acetyltransferase using sequential screening approaches for an external collaboration.
 - Analysed HTS data of corporate collection against targets to prioritise further compounds for testing using similarity searches, establish SAR trends and perform property profiling.
- A key role within computational chemistry group
 - Responsible for acquisition, implementation and maintenance of CCDC suite of tools.
 - Involved in defining global software/hardware strategy, objectives and in staff recruitment.
 - Led initiative in the implementation of an automated and integrated platform of HTS data analysis tools in collaboration with Informatics team.
- Computational representative on a number of multidisciplinary steering groups and committees
 - Member of Structure-Based Steering Group which assessed targets amenable to crystallography, established and monitored a network of collaborations in the field.
 - Defined and implemented strategic initiatives to improve the process of HTS data analysis as part of the HTS Review Team.
 - Critically evaluated the scientific and strategic merits of potential new targets for oncology portfolio as part of multidisciplinary team.

Research Scientist, Organon UK

June 1995 – August 2002

- Supported and influenced project lead generation and optimization strategies. Regular presentations at multidisciplinary project meetings. Worked across a range of therapeutic areas including cardiovascular, CNS and analgesia.
 - Identified novel chemotypes using a variety of virtual screening approaches (SBDD, pharmacophore hypothesis) on a number of projects (protease and GPCR).
 - Designed focused libraries and prioritised synthetic proposals by medicinal chemists during lead generation and optimisation phases to improve compound affinity and selectivity.
 - Guided medicinal chemistry strategies to achieve required physical properties and ADME profiles. Successfully deployed a local QSAR model to improve plasma protein binding for a protease target and fragment analysis to improve metabolic stability for GPCR target in lead optimization phase.
- As a member of computational chemistry group
 - Contributed to global and local strategies of computational chemistry within drug discovery.
 - Coordinated, developed and implemented of automated virtual screening platform (software/hardware) within the UK Computational Chemistry Group.
 - Introduced a new methodology to perform automated covalent docking with colleagues.
 - Spent a 2-month secondment in computational chemistry group in the Netherlands.
- Computational representative for multidisciplinary strategic initiatives
 - Managed the Lead Generation Strategy team. Responsibilities included introduction and evaluation of new technologies to ensure optimal application of existing technologies and successful implementation of new technologies within research project teams. Evaluated NMR technologies for drug discovery in collaboration with Analytical Chemistry group.
 - As a member of Cardiovascular Discovery Team, provided scientific and strategic input from a computational perspective in order to advance and maintain the portfolio of research projects within cardiovascular therapeutic field.
 - Analysis of known GPCR ligands and design of GPCR targeted libraries in partnership with medicinal chemists to enhance corporate collection.

TECHNICAL SKILLS

- *Main Programs:* Sybyl (Tripos), InsightII/Cerius2/QUANTA/CHARMm (Accelrys)
- *Protein Modelling:* sequence analysis/alignments (ClustalW, SRS), Homology Modeling (Modeler, WHATIF), molecular simulations (CHARMm), docking algorithms (DOCK4.0, FlexX suite, GOLD), active site analysis (GRID, Superstar, Relibase+, Chematica), de Novo design (Ludi)
- *Ligand-based Modelling:* pharmacophore design (GASP, ChemX, FlexS), conformational analysis (Confort, Rotate, Conquest), QSAR modelling (QSAR+), Library Design/Analysis (Legion, ChemX, Pipeline Pilot), QM (Gaussian98)
- *Data Analysis:* HTS Data-mining (Pipeline Pilot, SAR Navigator, Spotfire)
- *Programming skills:* Awk/Sed, basic PERL and CHARMm scripting language
- *Operating Systems:* SGI, Windows, Linux

TRAINING COURSES

Managerial

- 'Situational Leadership II' The Ken Blanchford Companies, July 2004.
'Selection Interviewing', Communicate, March 2001.
'Team Leadership' Asherman Associates, Inc, Jan 2001.
'Working in R&D Projects: Project Management', PriceWaterhouseCoopers, June 2000.
'Team Player', Asherman Associates, Inc, Oct 1999.

Scientific

- Perl Programming (10 weeks), Chris Carline, Summer 2005.
'Short Course in Drug Metabolism', Patrick J Murphy, April 2004.
'MDL ISIS for Excel, Version2: Participants Guide', MDL, July 2004.
'Pipeline Pilot Basic and Advanced Chemo informatics Training Courses', Scitegic, May 2004.
'Seminars in Oncology for Chemists', University of Hertfordshire, October 2003.
'Docking Workshop FlexX', BioSolveIT, GmbH, October 2003.
'Microsoft FrontPage', Gabriel Scientific Consultancy Ltd, March 2000.

POST-DOCTORAL & EDUCATIONAL HISTORY

<u>DATES</u>	<u>ESTABLISHMENT</u>	<u>INFORMATION SUMMARY</u>
1994 – 1995	University of Surrey Guildford, Surrey, UK	Post-Doctoral Research Fellow with Drs. B. Howlin and G. Webb Protein Modelling of Angiogenin-Inhibitor complexes
1990 – 1993	University of Reading. Berkshire, UK	PhD with Prof. M.G.B Drew, Drs. M. Rodgers and P. Mitchell Thesis: 'A Computational study of Juvenile hormone analogues'. Funded by Ministry of Agriculture, Fisheries and Food (Slough). 3 months work-based placement spent at Slough.
1987 – 1990	University of Reading Berkshire, UK.	B.Sc (Hons): 1 st Class in Chemistry with Subsidiary Mathematics. Awarded the 1990 Year Prize for Inorganic Chemistry.
1980 – 1987	Stroud Girls High School Gloucestershire, UK	3 'A-levels' and 11 'O-levels'

PERSONAL DETAILS

Nationality: British
Marital Status: Single
Sex: Female
Date of Birth: 13th March 1969