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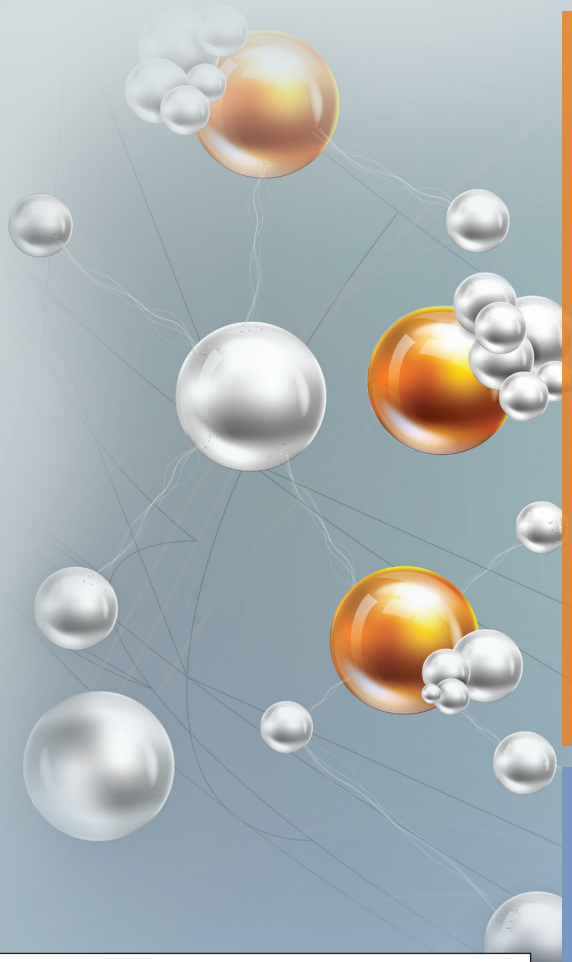
Advances and Progress in Drug Design

16th -17th FEB 2015

Marriott Regents Park Hotel, London, UK



CHAIRS FOR 2015:

Andreas Bender, Lecturer for Molecular Informatics, **University of Cambridge**

Dr Hugo Gutierrez de Teran, Senior Researcher, Division of Computational and Systems Biology, **Uppsala University**

KEY SPEAKERS INCLUDE:

- **Gary Tresadern,** Principal Scientist, Computational Chemistry, Lead Discovery, **Janssen Research and Development**
- **Henrik Moebitz,** Investigator, **Novartis**
- **Sudharsan Sridharan,** Scientist, **MedImmune Ltd**
- **Gianni Chessari,** Director, Computational Chemistry, **Astex Pharmaceuticals**
- **Oliver Plettenburg,** Head of Biosensors & Chemical Probes, **Sanofi**
- **Michael Overduin,** Professor of Structural Biology, **University of Birmingham**
- **Dr Zara Sands,** Principal Scientist, Medicinal Chemistry, **UCB BioPharma**
- **Richard Lewis,** Executive Director, Computer-Aided Drug Design, **Novartis**

BUSINESS BENEFITS FOR 2015:

- **DISCUSS** the application of computational based drug design with five presentations focusing on modelling and engineering
- **JOIN** the panel discussion on computational and predictive tools for the application of drug discovery
- **ENHANCE** your understanding of fragment-based drug design by listening to presentations led by UCB Pharmaceuticals, Astex Pharmaceuticals, ZoBio and the University of Birmingham
- **LISTEN** to talks on structure-based drug design from Lead Pharma, Sanofi, Novartis and Heptares Therapeutics

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PLUS AN INTERACTIVE HALF-DAY POST-CONFERENCE WORKSHOP

Wednesday 18th February 2015, Marriott Regents Park Hotel, London, UK

Fragment-Based Lead Discovery: Issues and Applications

Workshop Leader: **Dr Stephen Roughley,** Principal Scientist, Medicinal Chemistry, **Vernalis (R&D) Ltd.**

8.30am – 12.30pm

www.drug-design.co.uk

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8.30 **Registration & Coffee**

9.00 **Chairman's Opening Remarks**
Dr Hugo Gutierrez de Teran, Senior Researcher, Division of Computational and Systems Biology, **Uppsala University**

COMPUTATIONAL BASED DRUG DESIGN

OPENING ADDRESS

9.10 **Compound Design and Analysis Using Integrated Chemical and Biological Information**

- How to use integrate bioactivity information and gene expression data for mode-of-action analysis
- How to use integrated biological and chemical data for compound selection and drug repurposing
- How to use integrated data sources for safety assessment and scaffold prioritization

Andreas Bender, Lecturer for Molecular Informatics, **University of Cambridge**

9.50 **Structure based design of PDE2 inhibitors**

- Potent and selective PDE2 inhibitors have been identified
- Structure based design was crucial for their identification
- Modelling approaches of increasing sophistication will be discussed

Gary Tresadern, Principal Scientist, Computational Chemistry, Lead Discovery, **Janssen Research and Development**

10.30 **Morning Coffee**

11.00 **Creating Focused Mutant Libraries for Protein Engineering**

- Computational approach for calculating mutation frequencies and predicting mutation probabilities for sequence residue sites
- Apply mutation probabilities to efficiently sample and reduce the sequence search space
- Enrich the number of actives by generating virtual focused protein and antibody libraries for rational biologics design

Paul Labute, President and CEO, **Chemical Computing Group**

11.40 **Application of computational structural biology tools in biotherapeutics discovery**

- Key challenges in biotherapeutics discovery
- How is structural information useful in facing these challenges
- Case studies in applying structural bioinformatics to these challenges
- Future perspective

Sudharsan Sridharan, Scientist, **MedImmune Ltd**

12.20 **Networking Lunch**

KEYNOTE ADDRESS

1.20 **The ABC of kinase conformations – Interplay of conformation, sequence and ligand binding**

- On the basis of a structure based sequence alignment a universal residue nomenclature is proposed. In this talk a comprehensive classification of kinase domain conformations with a small set of clusters is presented.
- Stabilization of the active conformation, as well as inactivation by displacement of helix-C or the activation loop is linked to the interaction between helix-C and the DFG motif.
- We show that the conformation of the DFG motif is tightly correlated with the propensity of helix-C displacement

Henrik Moebitz, Investigator, **Novartis**

PHARMACOKINETICS, POLYPHARMACOLOGY & METABOLISM IN DESIGN

2.00 **Predicting protein structure, ligand binding and receptor selectivity on GPCRs**

- The GPCR-ModSim web server has been recently upgraded to account for novel templates and modelling strategies, which will be here presented and discussed
- Our computational protocols to investigate GPCRs include a new method to predict site-directed mutagenesis effects on ligand binding, based on free energy calculations
- We will show recent applications on the adenosine receptors family: successful prediction of mutagenesis effects on the A2A adenosine receptor, as well as on the design of adaptive scaffolds for each of the four members of this family of GPCRs

Dr Hugo Gutierrez de Teran, Senior Researcher, Division of Computational and Systems Biology, **Uppsala University**

2.40 **Afternoon Tea**

3.10 **Identification of drug candidates using network pharmacology based computational modelling**

- Biology and disease are complex systems that can be modelled as networks of interacting proteins.
- Network science allows the identification of key proteins that can be perturbed for maximum system level effects.
- Proprietary chemoinformatics tools allow e-Therapeutics to identify compounds that interact with those sets of key proteins, and hence which are likely to show phenotypic activity

Ben Allen, Computational Research Scientist, **e-Therapeutics**

3.50 **PANEL DISCUSSION**

How have computational and predictive tools matured for the application of drug discovery?

- **Dr Hugo Gutierrez de Teran,** Senior Researcher, Division of Computational and Systems Biology, **Uppsala University**
- **Paul Labute,** President and CEO, **Chemical Computing Group**
- **Gary Tresadern,** Principal Scientist, Computational Chemistry, Lead Discovery, **Janssen Research and Development**

4.30 **Chairman's Closing Remarks and Close of Day One**

4.45 **Drinks Reception sponsored by Chemical Computing Group**

6.00 **Close of Drinks Reception**

8.30 **Registration & Coffee**

9.00 **Chairman's Opening Remarks**
Andreas Bender, Lecturer for Molecular Informatics, **University of Cambridge**

FRAGMENT BASED DRUG DESIGN

OPENING ADDRESS

9.10 **Rational GPCR drug discovery?**
- Successful application of ligand-based and structure-based computational approaches for the rational design of novel GPCR antagonists
- Designing novel and improved allosteric GPCR modulators through a computationally integrated design strategy
- Opportunities and challenges that must be addressed to enhance our GPCR rational design capabilities

Dr Zara Sands, Principal Scientist, Medicinal Chemistry, **UCB BioPharma**

9.50 **Fragment Based Design of Protein-Protein Interaction Antagonists**
- X-ray and biophysical fragment screening of protein-protein interaction targets
- Structure based driven optimisation of mM fragment into potent lead molecules
- Development of potent dual antagonist of XIAP and cIAP1

Gianni Chessari, Director, Computational Chemistry, **Astex Pharmaceuticals**

10.30 **Morning Coffee**

KEYNOTE ADDRESS

11.00 **Building a Robust Technology Pipeline for Robust Fragment Based Drug Discovery**
The keys to successful FBDD are:
- Orthogonality
- High quality protein preparations
- Availability of structural information - from multiple methods

Gregg Siegal, Chief Scientific Officer, **ZoBio**

11.40 **NMR-based fragment screening and validation for novel kinase and phosphatase targets**
- Are there novel ways to inhibit kinase targets?
- Could phosphatases become druggable targets?
- Can novel lipid binding sites be identified in targets including proteases?
- Can native membrane:protein targets be isolated?

The methods involved include:
- NMR spectroscopy based fragment screening
- MODA-based prediction of membrane binding sites
- Styrene maleic acid polymer-based protein extraction

Michael Overduin, Professor of Structural Biology, **University of Birmingham**

12.20 **Networking Lunch**

STRUCTURE BASED DRUG DESIGN

CASE STUDY

1.20 **Structure-Based Identification and Optimization of MK2 Inhibitors**
- X-ray crystallography guided the identification of a novel series of MK2 inhibitors
- Optimization of the Lead focused on improvement of DMPK properties
- SBDD drove identification of a sub-series with relatively high cellular activity

Arthur Oubrie, Chief Scientific Officer, **Lead Pharma**

2.00 **Molecular dynamics and drug design**
- Recent applications of endpoint free-energy computational methods such as molecular mechanics Poisson-Boltzmann surface area (MM-PBSA) and generalized Born surface area (MM-GBSA) and linear response methods
- Recent progress in steered molecular dynamics applied to drug design

Francesca Deflorian, Senior Computational Chemist, **Heptares Therapeutics**

2.40 **Afternoon Tea**

3.10 **Structure-based Design of Kinase Inhibitors**
- Kinases represent a target class of high therapeutic interest in oncology and beyond
- The advances of structural biology and the availability of a wide variety of X-ray structures of target and antitarget kinases significantly facilitated the development of new kinase inhibitors
- Fundamentals and structure-based design of various novel kinase inhibitors will be discussed. In addition, a case study on the development of novel, highly selective Rho-kinase inhibitors will be presented

Oliver Plettenburg, Head of Biosensors & Chemical Probes, **Sanofi**

3.50 **Using Chemical and Biological Information for Compound Selection and Prioritization**
- Data-driven discovery - Addressing how modelling can actually impact drug discovery

Richard Lewis, Executive Director, Computer-Aided Drug Design, **Novartis**

4.30 **Chairman's Closing Remarks and Close of Day Two**

HALF-DAY POST-CONFERENCE WORKSHOP
Wednesday 18th February 2015
8.30am – 12.30pm
Marriott Regents Park Hotel, London, UK

Fragment-Based Lead Discovery: Issues and Applications

Workshop Leader:
Dr Stephen Roughley, Principal Scientist, Medicinal Chemistry, **Vernalis (R&D) Ltd.**

Overview of workshop:

This workshop will provide an introduction to Fragment-based Lead Discovery (FBLD), addressing theoretical and practical aspects of the process from library design to screening and low affinity hit elaboration and evolution to high potency hits and leads. The course will cover experimental techniques, target applicability and integration with other hit identification strategies and advice on avoiding the more common pitfalls which may be encountered.

Key Benefits of Attending:

This course is suitable for researchers who are currently using, or who wish to use, Fragment Based Lead Discovery (FBLD) methods to identify and optimise Hits and Leads in a Drug Discovery program. It is also suitable for those who are developing compound libraries for use in FBLD campaigns, and for anyone with an interest in integrating FBLD approaches with existing hit identification and lead optimisation strategies

Agenda:

8.30 **Registration and Coffee**

9.00 **Introduction**

9.10 **Overview & Perspective**

10.00 **Case Studies**

10.30 **Coffee Break**

11.00 **Applications and Issues**

12.00 **Discussion and Q&A**

12.30 **End of Workshop**

About the workshop host:

Stephen D. Roughley obtained his M.A. in 1995 and Ph.D. (with Prof. Andrew B. Holmes, on the modeling and application of nitrone cycloaddition reactions to the synthesis of histrionicotoxin alkaloids) in 1999 from the University of Cambridge, U.K, undertaking placements in Medicinal and Process Chemistry Departments at GlaxoWellcome. In 1999, he joined RiboTargets (later Vernalis) as a medicinal chemist, where he has been involved in drug discovery and technology programs in anti-infective, CNS, and oncology disease areas. Following a secondment in NMR-based fragment screening, he returned to medicinal chemistry as a Principal Scientist and maintains a broad range of interests in drug discovery technologies, medicinal and synthetic chemistry, and cheminformatics.

About the organisation:

Vernalis is a world leader in structure and fragment-based drug discovery, with an excellent track record for innovation and delivery of clinical candidates in a range of therapeutic areas. We have one product on the market, three programmes in Phase II clinical trials and a broad pipeline o(candidates derived from successful collaborations with a number of global pharmaceutical businesses and from our own research activities.

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Drug Design Facts:

Who should attend this conference:
You should attend this event if you work in the Pharmaceutical Industry/Academia with responsibilities in:

- Structural Biology
- Molecular Informatics
- Drug Design
- CADD
- Molecular Science
- Medicinal Chemistry
- Modeling
- Remodeling
- Medicinal Chemistry
- Receptor Biology
- Discovery Chemistry
- Protein Technologies
- Pharmacology
- Molecular Science
- Crystallography
- Structure and Informatics
- Molecular Interaction
- Drug Discovery and Design
- Screening

Job titles include:
- Computational Chemist
- Senior Scientist
- Lead Generation
- Research Scientist
- Research Fellow
- In-silico medicinal chemist
- Research investigator

This year's programme places equal emphasis on CADD, SBDD, FBDD and pharmacokinetics, polypharmacology and metabolism. Pharma industry speakers and leading academics will be sharing their research, challenges and solutions to issues in drug design.

We aim to deliver more diversity this year from big pharma companies to small biotechs, in addition to renowned academics.

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Conference: Monday 16th & Tuesday 17th February 2015, Marriott Hotel Regents Park, London, UK Workshops: Wednesday 18th February 2015, London

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