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Advances and Progress in Drug Design

15 - 16 FEB 2016

Holiday Inn Kensington Forum, London, UK

Optimising protein-based drug discovery and biophysical tools to prioritise novel drug candidates and protein-ligand structures.

CHAIR FOR 2016:


Gregg Seigal, Chief Executive Officer, **ZoBio**

FEATURED SPEAKERS:


Doug Johnson, Research Fellow, **Pfizer**


Tove Sjögren, Associate Director, **AstraZeneca**


Herman van Vlijmen, Senior Director, **Janssen**


Armin Ruf, Section Head, Biostructure, **Roche**


Gianni Chessari, Director, **Astex Pharmaceuticals**


Hans Matter, Senior Scientist, **Sanofi-Aventis**


Jordi Munoz Muriedas, Investigator, **GSK**


Manuel Francisco Molina-Martin, Research Scientist, **Eli Lilly**


Howard Feldman, Principal Scientist, **Chemical Computing Group**

WHY YOU SHOULD ATTEND:

- Understand key developments in **protein-based drug design**
- Optimise **biophysical** tools for compound **validation** and **high resolution screening**
- **Learn** unique benefits of **small molecule covalent drug design**
- Efficiently prosecute protein-protein interactions through **fragment-based** approaches
- Gain new insights in organised dynamic structures on a 3D project database using **novel algorithms** to determine specific subunits
- Understand data mining workflows and the **IMI Open PHACTS** project

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PLUS TWO INTERACTIVE HALF-DAY POST-CONFERENCE WORKSHOPS

Wednesday 17th February 2016, Holiday Inn Kensington Forum, London, UK

WORKSHOP A

A Fresh View on Molecular Recognition: The Dynamic Perspective

Workshop Leader: **Dr. Xavier Barril**, ICREA Research Professor, School of Pharmacy, **Barcelona University**

8.30am - 12.30pm

WORKSHOP B

Analysis and Application of Ligand Conformation in Drug Design

Workshop Leaders: **Dr. Emma Blaney**, Senior Programme Manager, and **Dr. Martin Watson**, Head of NMR, **C4X Discovery**

1.30pm – 5.30pm

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Advances and Progress in Drug Design

Day One | Monday 15th February 2016

8.30 **Registration & Coffee**

9.00 **Chairman's Opening Remarks**
Gregg Seigal, Chief Executive Officer, **ZoBio**

Enabling Biophysical Assays with Key Therapeutic Applications

9.10 **OPENING ADDRESS: Driving biophysics in drug discovery**

- Enabling proteins for biophysics and structural biology
- Detecting and characterising small molecule-target interactions with biophysics
- The complementarity of NMR and X-ray for structural information

Gregg Seigal, Chief Executive Officer, **ZoBio**

9.50 **Small molecules in drug design**

- Are all protein-fragment interactions favourable?
- Is the bound conformation a low energy geometry?
- Where do I grow my fragment?

Gianni Chessari, Director, **Astex Pharmaceuticals**

10.30 **Morning Coffee**

11.00 **Structure-based drug design within the lipid bilayer**

- Optimisation of protein and lipid interactions
- The role of solvent in the protein-lipid interface
- Ligand efficiency metrics in the context of membrane embedded binding sites

Tove Sjögren, Associate Director, **AstraZeneca**

11.40 **Organising 3D project data for structure-based drug design**

- It is often desirable to organize disparate crystallographic project data into a common homogeneous format, ready to use for modelling. Thus, we present a web-based application that permits users to specify numerous options controlling superposition and alignment of structures in a family or project, ligand specification, and whether electron densities or other grids are to be included.
- The final result is a project database containing superposed structures all in the same frame of reference. From here, structures can be dynamical regrouped, e.g. by scaffold class, for easy management, and can be easily browsed and used as a starting point for further research.
- The system is able to handle multi-subunit complexes, including structures which may be missing subunits, by using a novel algorithm to determine which subunits of each complex correspond to each other.
- Specific applications of the output database files include family-based homology modeling, which benefit from a highly enriched source for templates and loop conformations; and family-specific searching and further filtering of structures.

Howard Feldman, Principal Scientist, **Chemical Computing Group**

12.20 **Networking Lunch**

1.30 **KEYNOTE ADDRESS: Reviving covalent drug design: Discovery of PF-04457845, an irreversible FAAH inhibitor with exquisite selectivity**

- The unique benefits of small molecule covalent drug candidates
- Activity-based protein profiling and clickable probes to evaluate selectivity of covalent binding
- Biomarkers and PET ligand to determine target engagement in humans

Doug Johnson, Research Fellow, **Pfizer**

Protein-Based Drug Discovery and Structural Screening

2.10 **KEYNOTE ADDRESS: Quality control of misfolded protein response- via PPP1R15A inhibition by the highly selective first-in-class IFB-088 to treat protein misfolding diseases**

- Case study: Mode of action of IFB-088 small molecule drug in inhibiting PPP1R15A a regulatory subunit of PP1c
- Prevent challenges of the specificity needed to target the molecular chaperones
- Selective inhibition of phosphatase complex through its regulatory subunit represent a novel avenue for therapeutic interventions

Philippe Guedat, CEO, **InFlectis BioScience**

2.50 **Design Strategies for compound libraries in High Throughput Screening (HTS)**

- Generation and implementation of chemoinformatic tools for the design and production of high throughput chemical libraries
- DOE tools for reaction "scouting" on a flow-based library production platform

Stevan Djuric, Senior Director, **Abbvie**

3.30 **Afternoon Tea**

4.00 **eHOMO calculations as a predictor for mutagenesis propensity of compounds**

- "HOMOlogate" your compounds to understand their mutagenic risk
- Use it as a tool to improve interpretation of mechanisms driving mutagenicity
- Use it as a tool improve communication between safety and lead optimisation

Jordi Munoz-Muriedas, Investigator, **GSK**

4.40 **Linked open data in drug discovery: Where are we?**

- The IMI Open PHACTS project: status and outlook
- Data mining workflows using linked open data
- A pharma challenge: merging public and private data

Herman van Vlijmen, Senior Director, **Janssen**

5.20 **Early prediction and large scale analysis of binding sites**

- Prioritizing kinase structures for drug discovery efforts
- Dealing with protein flexibility
- Mining selectivity determining features in binding sites

Simone Fulle, Research Group Leader,
BioMedX Innovation Centre

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

6.00 - 7.00 **Drinks Reception sponsored by Chemical Computing Group**

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Advances and Progress in Drug Design

Day Two | Tuesday 16th February 2016

8.30 **Registration & Coffee**

9.00 **Chairman's Opening Remarks**
Gregg Seigal, Chief Executive Officer, **ZoBio**

Enabling Progress and Reviving Opportunities in Drug Development

9.10 **OPENING ADDRESS: Structure-based drug discovery inspired by fragments: Methods, design and binding affinity**

- Fragments combined with structure-based design play an important role in today's drug discovery. The use of fragment-derived building blocks as seeds for further design will be illustrated in this contribution.
- A fragment deconstruction approach will be presented to explore the super-additivity of fragment linking in protein-ligand complexes. By connecting two fragments with a single bond for serine protease inhibitors, a high linker contribution with significant improvement in affinity was observed.
- Scoring functions are models for estimating the strength of non-covalent interaction. Key is a fundamental understanding of favourable and unfavourable protein-ligand interactions. Some tailoring towards fragments and lead-series will be shown.
- Interaction of halogen atoms to binding sites has also consequences for affinity. Some interaction components of fragment contacts to aryl-rings, halogen-bonding and binding-site desolvation will be discussed. As classical force-fields cannot account for halogen-mediated interactions due to missing treatment of the "sigma"-hole, local properties from quantum-mechanical techniques that do not suffer from these limitations, will be presented.

Hans Matter, Senior Scientist, **Sanofi-Aventis**

9.50 **Water mapping on drug design**

- Computational analyses of water and drugability implications
- Probing drug-binding pathways and to deduce rank-order of binding affinities
- Predicting thermodynamic contributions of the water framework surrounding protein binding pockets

Ben Tehan, Principle Computational Chemist, **Heptares Therapeutics**

10.30 **Morning Coffee**

11.00 **Structure-based drug design of the first known inhibitors of PHGDH**

- Multiple hit finding strategies conducted in parallel including directed libraries, HTS and fragment based lead generation for this challenging target
- X-ray structures give unique insight to the binding mode and enable structure based design
- Application of biophysical methods - NMR, biocore and ITC to aid prioritisation and characterisation of hits and lead to delivery of first known PHGDH inhibitors

Attilla Ting, Computational Chemist, **AstraZeneca**

11.40 **Growing a baby: Identifying and optimising quality leads and overcoming restraints in drug discovery**

- Clinical evaluation of fragment-derived chemical leads in comparison to alternative methods
- Enabling biophysical technologies in drug discovery
- Bridging different approaches in drug design to identify and optimise meaningful drug lead compounds.
- Opportunities in biophysical screening to catch up with FBDD techniques

Manuel Molina, Research Scientist, **Eli Lilly**

12.20 **Networking Lunch**

Biophysical Tools and ADME

1.30 **High resolution for drug discovery**

- X-Ray crystallographic follow up of hits from high throughput or fragment screening
- The advantages of obtaining X-ray complex structures early and at high resolution
- Strategies to increase the success rate in co-crystallization and soaking

Armin Ruf, Section Head Biostructure, **Roche**

2.10 **Optimising ADME properties**

- Assessing the binding kinetics of the protein-drug fragment relative to elimination kinetics
- Optimising ADME models through computational techniques
- In Silico metabolite prediction of hERG toxicity and associated challenges

Alexander Hillisch, Director, Medicinal Chemistry, **Bayer**

2.50 **CASE STUDY: Fragment-based approach at UCB**

- Targeting Protein-Protein Interactions (PPIs): Challenges
- Prosecuting PPI using fragment-based approach
  - Choosing targets for NCE programmes
  - Fragments at UCB
  - Fragment screening capacity at UCB - fragment screen of 12 PPI targets
  - Identifying reliable chemical starting points-screening cascade triage
- Antibodies as tools to find new chemical matter

Marta Westwood, Senior Scientist, **UCB Pharma**

3.30 **Afternoon Tea**

4.00 **Biophysical screening tools for compound validation**

- Small molecule probes to elucidate structural information and early validation
- Tackling sensitivity issues in small-molecule ligand screening to generate lead hits
- Integrated approaches for fragment screening to increase robustness

Alexey Rak, Head of Bio Structure and Biophysics, **Sanofi**

4.40 **Assessment of binding kinetics and "slow-off" rates**

- Optimisation of factors that control K_{ass} and K_{diss} rates
- Assessing the effects of receptor binding kinetics on drug efficacy an duplications of side effects

Matthias Frech, Director, Molecular Interactions & Biophysics, **Merck KGaA**

5.20 **Enabling biophysical tools for hit lead generation**

Molecular Dynamics (MD) simulations are becoming the workhorse of routine drug design applications.

- Solvent and dynamic effects bring about a major improvement in the quality of the predictions
- Real applications of drugability assessment, binding site mapping and virtual screening will be presented

Xavier Barrill, ICREA Research Professor, **Barcelona University**

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

Supported by

HALF-DAY POST-CONFERENCE WORKSHOP A
Wednesday 17th February 2016
8.30am – 12.30pm
Holiday Inn Kensington Forum, London, UK

A Fresh View on Molecular Recognition: The Dynamic Perspective

Workshop Host:
Dr. Xavier Barril, ICREA Research Professor,
School of Pharmacy, **Barcelona University**

Overview of the workshop

The introduction of dynamic information has changed our perspective on molecular recognition. The processes of ligand association and dissociation, the flexibility of the protein or the role of water, are all critical aspects that are increasingly appreciated. This workshop will discuss how such changes in perspective provides new insights for structure-based drug design and to what extend these aspects can be investigated in practice.

Why you should attend:

Molecular dynamics (MD) is a well-established technique, but the drug discovery community has embraced it only recently. Here we will discuss some of the new venues that MD has open, how it has changed our view of protein-ligand complexes but also what are the limits and what MD can and cannot do for you.

Programme

8.30 **Registration and Coffee**

9.00 **Opening remarks and introductions**

9.10 **Session 1: Kinetics vs thermodynamics: a question of perspective**
- Importance of kinetics
- Association/dissociation pathways
- Structural factors that affect the kinetic behaviour

9.50 **Session 2: Water molecules and binding hot spot**
- The dynamic behavior of solvent molecules
- Identification of binding hot spots using dynamic information

10.30 **Morning Tea**

11.00 **Session 3: Practical aspects of MD simulations**
- Introduction to MD
- Real time, simulated time, computing time
- Examples of reliable MD applications for drug design

12.20 **Closing remarks**

12.30 **End of Workshop**

About the workshop host:

Dr. Xavier Barril, ICREA Research Professor,
School of Pharmacy, **Barcelona University**

Xavier Barril is an ICREA Research Professor at Barcelona University's School of Pharmacy. His research focuses on the discovery of bioactive molecules exploiting unusual mechanisms of action through a combined use of computational and experimental techniques. In parallel, his group develops new computational tools to tackle such tough targets (e.g. drugability, docking, hot spot characterization) and strives to improve our understanding of molecular events of biological and pharmacological importance (e.g. binding kinetics, allosterism). Prof. Barril received his Ph.D. from the University of Barcelona in 2001 for theoretical studies on the ligand-receptor molecular recognition process. He then joined the Applications Modelling team at Vernalis (Cambridge, UK) where he was involved in a range of projects, from target identification to preclinical studies. In 2005 he was appointed ICREA Research Professor and joined Barcelona University's School of Pharmacy. He has co-authored more than 60 scientific publications, including research papers, reviews and book chapters. With a strong focus on translational research, Prof. Barril is co-author of 7 patents and co-founder of Minoryx Therapeutics, a company focusing in the development of new treatments for rare diseases.

About the organisation:

ICREA, Catalan Institution for Research and Advanced Studies, is a foundation supported by the Catalan Government and guided by a Board of Trustees. It was created in response to the need to seek new hiring formulas that would make it possible to compete with other research systems on a similar footing by focusing on hiring only the most talented and extraordinary scientists and academics. ICREA offers permanent, tenured positions to researchers from all over the world to come and work in Catalonia. Over the years these positions have become a synonym of global academic excellence.

Offering new research positions every year and promoting research in Catalonia, Cooperation, international openness and excellence are ICREA's hallmarks.

HALF-DAY POST-CONFERENCE WORKSHOP B
Wednesday 17th February 2016
1.30pm – 5.30pm
Holiday Inn Kensington Forum, London, UK

Analysis and Application of Ligand Conformation in Drug Design

Workshop Host:
Dr. Emma Blaney, Senior Programme Manager, and
Dr. Martin Watson, Head of NMR, **C4X Discovery**

Overview of the workshop

With the expertise of the team from C4X Discovery, this unique workshop will explore how conformational insights can impact rational design in drug discovery. The leaders will discuss the range of techniques available to experimentally determine molecular conformations, and their associated advantages and limitations. The case studies and discussion session will explore the principles of conformational design, and how such knowledge can be used to complement alternative design strategies and technologies.

Key Benefits of Attending:

- Consider the techniques available to quantify free ligand conformations
- Understand and predict the impact of conformational change on binding affinity
- Use this knowledge to improve properties such as selectivity
- Network with key industry professionals

Programme

1.30 **Registration and Coffee**

2.00 **Opening remarks and introductions**

2.10 **Conformational design in drug discovery:**
- Introduction to molecular conformation
- Principles and objectives of conformational design

2.50 **C4X NMR analysis:**
- Outline of data collection and analysis
- Conformational model and descriptions
- Example structural analyses

3.30 **Afternoon Tea**

4.00 **Case studies and discussion session:**
- Interrogate how conformational insight can improve pharmacophore models
- Investigate how conformational design can improve selectivity profiles

5.20 **Closing remarks**

5.30 **End of Workshop**

About the workshop hosts:

Emma Blaney, Senior Programme Manager, **C4X Discovery**
Dr Emma Blaney has been active in medicinal chemistry design since her PhD research at the University of Leeds. Since graduating in 2003 she has worked at GSK (Harlow) in Lead Optimisation and was more recently Section Head at Peakdale Molecular. Her ongoing interest in molecular design led her to join C4X Discovery as Senior Programme Manager. Her role is to lead the internal drug discovery programmes using the insights from the conformational design expertise of the company.

Martin Watson, Head of NMR, **C4X Discovery**
Dr Martin Watson is an experienced NMR spectroscopist gaining his PhD from the University of Sheffield in 2006 specialising in biomolecular NMR. Since then he has worked on applications of NMR in drug discovery. He worked first at AstraZeneca and in 2011 joined C4X Discovery where he now leads the NMR team. The team deliver conformational information for internal drug discovery programmes and to external collaborators in the industry.

About the organisation:

C4X Discovery is a Manchester-based company focused on optimising drug discovery and design. The company uses its NMR-based technology to solve the dynamic 3D structures of a broad range of biomolecules. C4X Discovery's NMR technology shows what shapes active molecules prefer to adopt, providing high-quality templates for drug discovery and design. C4X Discovery is using its technology in collaboration with the pharmaceutical industry and to build its own proprietary pipeline of high-value therapeutic candidates.

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