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SMi presents their 9th annual...

Advances & Progress in Drug Design

Novel Technologies & Techniques

22nd & 23rd February, 2010, Crowne Plaza, St. James, London

KEY SPEAKERS INCLUDE:

Romano Kroemer
Head, Drug Design
Sanofi-Aventis

Paul Leeson
Director of Medicinal Chemistry
AstraZeneca

Chris Murray
VP, Discovery Technology
Astex Therapeutics

Paul Bamborough
Section Head: Computational Chemistry
GlaxoSmithKline

Jonathan Mason
Chief Scientist
Chief Scientist, Lundbeck Research

Robert Glen
Director of Chemistry, Unilever Centre for Molecular Informatics
Cambridge University

SMi's 9th annual Advances in Drug Design Conference aims to address the latest developments in drug design and offer tangible examples of these processes in practice

KEY BENEFITS OF ATTENDING:

- **Hear** the latest developments in computational drug design
- **Discover** structure and fragment based techniques for compound design
- **Case studies** with real life data and a strong take home message
- **Learn** from your peers the methods that work, and those that don't

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PLUS A HALF DAY POST-CONFERENCE WORKSHOP

WEDNESDAY 24TH OF FEBRUARY 2010

Efficient Optimisation Procedures for a Drug Candidate Molecule

8.30am – 1pm

In association with: Muscagen

www.smi-online.co.uk/2010drugdesign.asp

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CPD CERTIFIED

Advances & Progress in Drug Design

Day One | Monday 22nd February 2010

www.smi-online.co.uk/

8.30 Registration & coffee

9.00 **Chairman's Opening Remarks**
Chris Phillips, Senior Principal Scientist, **Pfizer Global Research and Development**

9.10 **KEYNOTE ADDRESS:**
Challenges in Drug Design
- Impact of drug-like properties
- Addressing pipeline attrition
- Use of ligand efficiency metrics

Paul Leeson, Director of Medicinal Chemistry, **AstraZeneca**

STRUCTURE BASED DRUG DESIGN

9.50 **NNRTI Design: Structure-Based Approaches**
Successful application in the development of non-nucleoside reverse transcriptase inhibitors
- Structure Based Molecular Hybridization
- Design strategies for drug-resistant viral strains
- Structures in lead selection

Chris Phillips, Senior Principle Scientist, **Pfizer Global Research and Development**

10.30 Morning Coffee

11.00 **Hybrid Docking**
Combining ligand and protein structure information for enhanced virtual screening performance
- Use of the structure of a bound ligand to enhance molecular docking performance
- Docking by smart overlay of ligand structure, scoring against the protein structure
- Overlay process that only takes account of relevant chemical interactions
- **Case study:** DUD dataset results

Mark McGann, Principal Developer, **OpenEye Scientific Software**

11.40 **GPCR Drug Design by Ligand Based NMR**
Innovative applications of NMR methods to intact biological membranes
- Non-radioactive NMR binding assay for a G-protein coupled receptor (GPCR)
- Method development on PKA
- Qualitative and fast analysis of INPHARMA data: cross-chemotype alignments
- **Case study:** GPR40

Stefan Bartoschek, Senior Scientist, **Sanofi-Aventis**

12.20 Networking Lunch

1.20 **Transforming GPCR Drug Discovery**
Expediting the study of GPCRs
- Dramatically stabilising receptors
- The isolation of purified, stabilized and functional GPCRs
- Case study: the StaR technology and its uses in drug discovery programmes

Benjamin Tehan, Senior Computational Chemist, **Heptares Therapeutics**

2.00 **GPCR Models as Tools for Structure-Based Design**
Construction, validation and use of GPCR models in project work
- New trends in GPCR model construction
- Model validation by single point mutagenesis and employment of various biological assays
- Typical drawbacks and obstacles in GPCR modelling
- Application of GPCR models in agonist and antagonist lead optimization

Christofer Tautermann, Computational Chemistry, Department of Lead Discovery, **Boehringer Ingelheim Pharma**

FRAGMENT BASED DRUG DESIGN

2.40 **KEYNOTE ADDRESS:**
Better Leads with Fragment-Based Discovery/Design?
What's needed & how do we get there
- A target perspective: kinases, proteases, phosphodiesterases - and now GPCRs
- An in silico perspective: what can be done, and how does it perform?
- A property and polypharmacological perspective

Jonathan Mason, Chief Scientist, **Lundbeck Research &** Head, Computational Chemistry, **Heptares Therapeutics**

3.20 **Fragment Optimisation**
Experiences in progressing fragment hits to in-vivo leads
- Selecting fragments for progression
- Scaffold hopping and scaffold novelty
- Addressing selectivity and pharmacokinetic properties
- **Case history:** elaborating fragments hits to in vivo kinase inhibitors

Ian Collins, Reader in Medicinal Chemistry, **The Institute of Cancer Research**

4.00 Afternoon Tea

4.30 **Optimising Fragments Using Structure-Based Drug Design**
Case studies from many fragment to lead campaigns
- Application of fragment screening to hsp90
- The production of clinical candidates from fragment screening
- Stabilising the bound conformation - a secure way to affinity optimisation
- Strategies for maintaining ligand efficiency

Chris Murray, VP, Discovery Technology, **Astex Therapeutics**

5.10 **Fragment-Based Discovery of a Potent Inhibitor of the Antiapoptotic Protein Bcl-x_L**
- "SAR by NMR" approach to fragment-based screening
- First and second site screen following by linking and HTOS
- Optimization of "linked" molecule driven by structure
- **Case Study:** discovery of ABT-737 for treatment of cancer

Andrew Petros, Associate Research Fellow, Fragment Screening and Lead Characterization, **Abbott**

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

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Advances & Progress in Drug Design

Day Two | Tuesday 23rd February 2010

8.30 Re-registration & coffee

9.00 **Chairman's opening remarks**
Roderick E. Hubbard, Professor, University of York & Senior Fellow, **Vernalis**

FRAGMENT BASED DRUG DESIGN

9.10 **Experiences in Structure and Fragment-Based Discovery**
Experiences in fragment-based discovery of lead series of compounds
- Working with fragments in biotech and academia
- What works and doesn't work in structure-based design
- The importance of integration across structure, modelling and chemistry

Roderick E. Hubbard, Professor, University of York & Senior Fellow, **Vernalis**

9.50 **Docking of Fragments into Receptor Structures**
Evaluation of different methods and comparison with experimental data
- Evaluation of pose prediction and enrichment
- Effect of re-scoring
- Influence of receptor structures and characteristics
- On improving structure-based virtual screening

Romano Kroemer, Head, **Drug Design, Sanofi-Aventis**

10.30 Morning Coffee

11.00 **Growing Fragments at UCB**
Successes and challenges in growing a fragment-based capability in a Biopharma company
- Application to novel protein-protein interaction targets
- Exploiting the synergies between high affinity antibodies and small molecules
- Using biologicals to help evolve fragments

Richard Taylor, Principal Scientist, Computer-Assisted Drug Discovery, **UCB Celltech**

COMPUTER AIDED DRUG DESIGN

1140 **'Fuzzy' Ligand- and Receptor-Based Virtual Screening Techniques for Rapid Hit and Lead Finding**
- 2D and 3D Pharmachophores
- De-Orphanization of Protein Targets
- Pseudoreceptors
- **Case study:** histamine H4 Receptor, APOBEC, PPAR

Gisbert Schneider, Chair for Computer-Assisted Drug Design, **Eidgenössische Technische Hochschule Zürich**

12.20 **Lead Optimisation Technologies**
- Virtual screening with Topomer Search
- De-Novo Design

Senior Representative, Tripos
Speaker TBC

1.00 Networking Lunch

2.00 **ROW - Reaction Oriented Workflows**
Creating lead libraries by virtual synthesis based on the retrosynthetic analysis of hit structures
- Structurally diverse libraries
- Synthetically feasible lead structures
- High optimization potential

Guido Kirsten, Application Scientist, **Chemical Computing Group**

2.40 **Combining Simulation and Drug Design in GPCRS**
- Large scale simulation of complex biomolecules is now possible over significant time intervals
- Combining ligand-based and phenomenological models leads to better compound selection
- Introducing clinical tissue samples at an early stage can clarify target selection
- **Case study:** GPCRs APJ (Apelin) & 5HT1B

Robert Glen, Director of Chemistry, Unilever Centre for Molecular Informatics, **Cambridge University**

3.20 Afternoon Tea

KEYNOTE ADDRESS:

3.50 **System-Based Drug Discovery for Non-Oncology Kinase Targets**
- Kinase affinity profiling and selectivity
- **Case study:** the contribution of rational design to the discovery of kinase inhibitors for the treatment of inflammatory diseases

Paul Bamborough, Section Head: Computational Chemistry, **GlaxoSmithKline**

4.30 **Challenges of Kinase Inhibitors in Lead Optimisation**
Approaches used to tackle selectivity issues in recent kinase lead optimisation programmes
- Exploitation of structural information
- Review of computational approaches
- Challenges for the future

David Buttar, Associate Principal Scientist, **AstraZeneca**

4.50 **ChEMBL: Open Source Chemogenomics Data**
Data-mining and KDD approaches to make drug discovery and lead optimisation easier
- Overview of ChEMBL tools and databases
- Applications of chemogenomic data in aiding drug design
- **Case study:** successes using ChEMBL

Anna Gaulton, Senior Data Integration and Development Officer, **European Bioinformatics Institute**

5.50 **Chairman's Closing Remarks and Close of Conference**

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WHO SHOULD ATTEND:

Chief Executives, Vice Presidents, Heads, Directors, Scientists and Project Leaders of:

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- Formulation/Pre-formulation
- Cheminformatics
- Computer Assisted Drug Design
- Drug Development
- Technology Assessment
- Business Development
- Discovery Chemistry
- Computational Biology
- Licensing Managers/Patent Officers
- Life Cycle Management
- Global Alliances
- Regulatory and Technical Affairs
- Product Development
- Business Development
- R&D, Strategic Planning and Development

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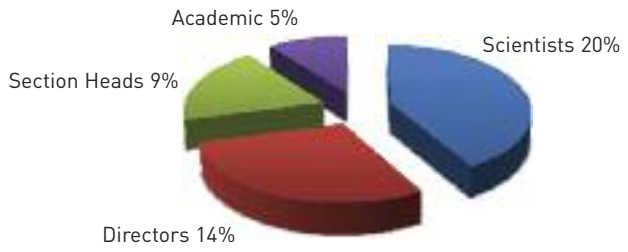

HALF DAY POST-CONFERENCE WORKSHOP
Wednesday 24th February 2010
Crowne Plaza, St. James, London
8.30am – 1pm

Efficient Optimisation Procedures for a Drug Candidate Molecule

In association with:

Muscagen

Overview:
The workshop will focus on economic and highly efficient optimisation procedures for a drug candidate molecule. It will be taken for granted that early metabolic studies involving liver microsomes and Ames tests have been carried out. The programme concentrates on a number of case studies demonstrating, accurate quantitative models involving simple equilibria (binding constants from membrane binding on receptors), steady state equilibria (ligand-receptor interactions involving agonism) and rate processes (ligand-receptor interactions 'in vivo', enzyme inhibition involving the b-lactam potencies of penicillins, cephalosporins,). Are there simple accurate transport models for determining drug half-lives where kidney elimination is rate dependent? The availability of X-ray data, species amino acid differences, sub–receptor variations and simple homology modelling is now extensive. The development of sub-receptor selectivity becomes obvious, in principle. Is random screening a largely irrelevant exercise? How do we bring X-ray structures to life using ligand data? Is 'loose' binding a prerequisite of antagonism? What use are X-ray structures when favourable entropy of antagonist binding contributes 10,000-fold to the potency?

Programme:

8.30 Registration and coffee

9.00 Welcome and Introductions:

9.10 Partition, Conformation, Interaction

9.30 Case Study I Guanine-Nucleotide-coupled receptors

10.30 Morning Tea Break

11.30 Case Study II Enzyme Inhibition
12.00 b-lactam antibiotics

12.45 Discussion session

1.00 Close of workshop

About the workshop leader:
Robin Davies has published some 35 papers encompassing drug design and is the founder and CEO of Muscagen, founded in 2000. Muscagen is a computation based, rational drug discovery company. It uses analysis of 3D protein structures, a proprietary model of receptor action, and state-of-the-art software, to design molecules which interact with receptors on the surface of human cells in specific ways.

The objective is to produce candidate drugs for valuable target markets from limited numbers of these molecules. Its approach is potentially cost-effective, efficient, reduces animal testing, and avoids likely side effects. The company's core activity is the design and structural optimisation of potent molecules that show highly selective receptor action. The synthesis and testing of these molecules are not core activities of Muscagen, and will be done in close collaboration with industry partners.

PHARMACEUTICAL FORWARD PLANNER

OCTOBER 2009

30Sep/01	KOL Knowledge Leaders
05/06	Partnerships with CRO's
12/13	Conducting Clinical Trials in Europe
21/22	Nutraceuticals & Functional Foods
26/27	Point of Care Diagnostics
28/29	European Pharmaceutical Pricing and Reimbursement*

NOVEMBER 2009

16/17	COPD: Novel Therapeutics and Management Strategies*
18/19	Cell Based Assays
25/26	Clinical Trials in CNS

DECEMBER 2009

02/03	Cold Chain Distribution

JANUARY 2010

18/19	Paediatric Clinical Trials
18/19	KOL Nordics*
20/21	Pre-filled Syringes
27/28	Electronic Laboratory Notebooks

FEBRUARY 2010

01/02	Biomarkers Summit
03/04	Adaptive Designs in Clinical Drug Development
10/11	Parallel Trade
15/16	Stem Cells
22/23	Drug Design

MARCH 2010

10/11	Imaging in Oncology
15/16	Pharmacovigilance
17/18	Superbugs & Superdrugs
24/25	Accelerating Patient Recruitment in Clinical Trials

APRIL 2010

19/20	Asthma & COPD
21/22	Computer Systems Validation
26/27	High Throughput Screening
28/29	Controlled Release

MAY 2010

10/11	Generics, Supergenerics & Patient Strategies
17/18	Clinical Trial Logistics

JUNE 2010

07/08	Pain Therapeutics
14/15	KOL Europe*
17/18	Global Protein Summit
28/29	RNAi, siRNA & miRNA
28/29	Pharmaceutical Portfolio & Product Lifecycle Management

*These conferences will take place in mainland Europe.

ADVANCES & PROGRESS IN DRUG DESIGN

Conference: 22nd & 23rd February, 2010, Crowne Plaza St James, London Workshops: Wednesday 24th February 2010, London

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