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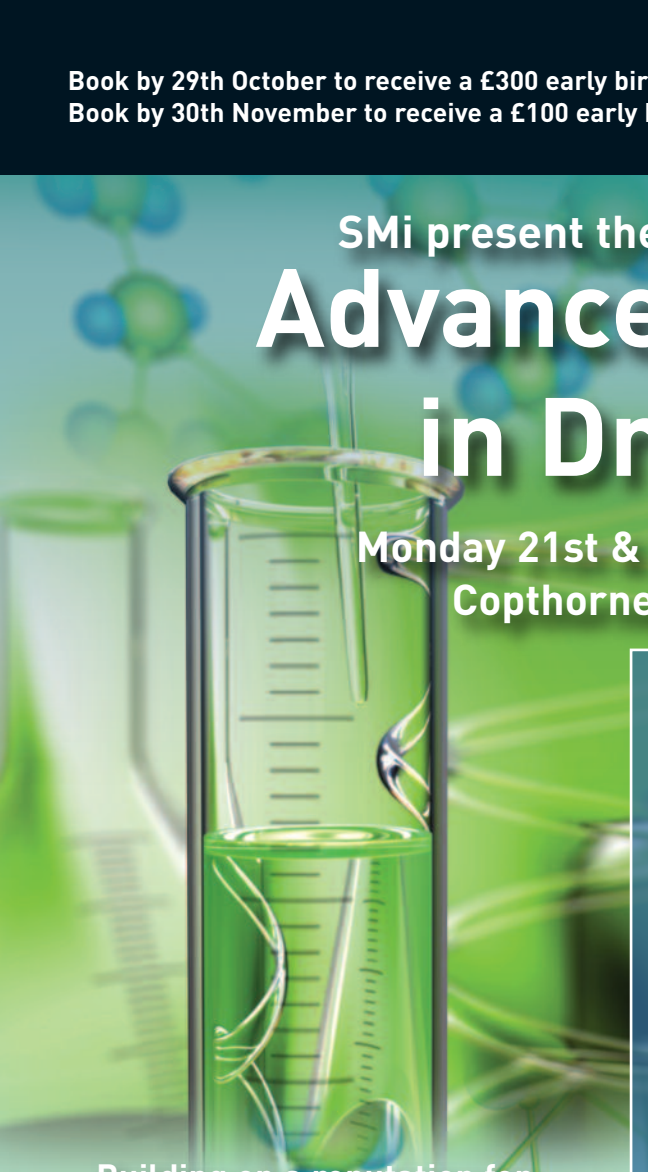
SMi present their 10th annual conference...

Advances & Progress in Drug Design

Monday 21st & Tuesday 22nd February 2011
Copthorne Tara Hotel, London, UK



Building on a reputation for strong scientific content, SMi is proud to present its historic 10th annual Advances & Progress in Drug Design conference. Attend this event to examine the latest groundbreaking research and technologies in a practically focused, networking friendly environment.

KEY SPEAKERS INCLUDE:

José Duca
Head, Computer-Aided Drug Discovery
Novartis

György Keserü
Head of Discovery Chemistry
Gedeon Richter

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

Hans-Joachim Boehm
Global Head of Chemistry
Roche

Martha Head,
Director, Computational Chemistry US
GlaxoSmithKline

Chris Murray
VP of Discovery Technologies
Astex Therapeutics

KEY TOPICS INCLUDE:

- **Examine** the latest developments and advancements in drug design
- **Discover** innovative research and technologies
- **Case studies** demonstrating both successes and failures
- **Network** and benchmark against the most efficient and cost effective approaches

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PLUS AN INTERACTIVE POST-CONFERENCE WORKSHOP
Wednesday 23rd February 2011

Addressing & Overcoming the Challenges of Fragment-Based Drug Design

Hosted by **Steve Swann,** Senior Research Chemist - Fragment-Based Drug Design, **Abbott**
8.30am - 1.00pm

To attend, contact Billy Roden on Tel +44 (0) 20 7827 6186, Fax +44 (0) 20 7827 6187, email broden@smi-online.co.uk or visit www.smi-online.co.uk/ts05.asp to register online
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Advances & Progress in Drug Design

Day One | Monday 21st February 2011

www.smi-online.co.uk/ts05.asp

8.30 Registration & coffee

9.00 **Chairman's opening remarks**
Chris Phillips, Senior Principal Scientist, **Pfizer**

9.10 **Taking advantage of all the tools available to aid rational drug design**
- Challenges in design
- Where the opportunities lie
- Methods to improve drug-like properties
- Lessons learnt and future directions

Hans-Joachim Boehm, Global Head of Chemistry and Centre Manager Pharma Research Basel, **Roche**

9.50 **Shortening the time to a successful fragment HTL campaign**
- Benefit to a parallel application of multiple fragment screening approaches
- Improving the quality of X-ray prioritization by additional and more quantifiable biophysical data
- Identifying the most promising fragment hits for chemical elaboration in FHTL
- Organizational requirements for success in FHTL

Sandy Farmer, Director, Structural Research, **Boehringer Ingelheim**

10.30 Morning coffee

10.55 **Role of waters in structure based design**
To use or not to use... When to target water and the lessons learnt
- Case studies of structure based drug discovery at Pfizer
- Comparison of multiple crystal structures for conserved features
- Targeting the right interactions

David Brown, Head of Crystallography, **Pfizer**

11.35 **SZMAP: Mapping solvent thermodynamics in binding sites**
Semi-continuum theory that captures discrete solvent effects that can be important in enclosed spaces such as binding cavities
- Mapping thermodynamic quantities of a water molecule near protein surfaces employing one explicit water probe
- Use as a correction factor for continuum solvent calculations
- Guiding the design of ligand analogues and optimizing binding affinity

Anthony Nicholls, President and CEO, **OpenEye Scientific Software**

12.15 Networking lunch

1.15 **Rational SBDD for the tough problems: Agonists/antagonists of GPCRs & SAR from indirect interactions**
- Use of stabilised receptors to give new insights into GPCR design from X-ray structures & biophysical screening
- Fragment-based hit identification for several GPCR targets: intra- (GPCR) and inter- (enzyme) target comparisons
- Probing for SAR insights for fragment & ligand binding using GRID and WaterMap

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

1.45 **Approaches for tough targets and SAR: A fragmented but critical voyage using WaterMap**
- Probing the sensitivity of Watermap predicted water energies to the simulation conditions and protein structure
- Probing for SAR insights for fragment & ligand binding to a flexible enzyme binding site using WaterMap & GRID
- Driving the optimisation of fragments - both the core and substitutions - using WaterMap predictions on both apo and liganded structures & GRID hotspots
- Approaching the rationalization of SAR by analysing the whole system, not just the direct ligand-protein interactions - an approach for elusive SAR?

Lena Tagmose, Head of Section, Computational Chemistry, **Lundbeck**

2.15 **PDE4 - beyond the catalytic domain**
Achieving PDE4B subtype selectivity through structure-based design
- Experimental and computational elucidation of subtype selectivity
- Unexpected PDE4 co-crystal structures
- Computational rationalisation of an unprecedented PDE4 ligand binding mode

Michael Kranz, Investigator, **GlaxoSmithKline**

2.55 Afternoon tea

3.20 **Fragment-based drug discovery - does it deliver higher quality leads?**
- Case studies of fragment based drug discovery at Astex
- Comparison of Astex fragment derived leads versus HTS leads
- Methods for prioritising fragment hits and accelerating their progression

Chris Murray, VP of Discovery Technologies, **Astex Therapeutics**

4.00 **Fragment docking by Glide**
Evaluating the docking accuracy of Glide using 16 different docking protocols on 190 protein-fragment complexes
- Identification of the best performing docking protocol for fragments
- The need to develop fragment specific scoring functions
- Cross-docking experiment results
- Lessons learned and illustrative case study examples

György Keserü, Head of Discovery Chemistry, **Gedeon Richter**

4.40 **Progressing fragment hits in the absence of crystal structures**
What to do when things don't crystallise (and why bother?)
- NMR-Guided Models - placing fragments and guiding chemistry
- Validating hits through a suite of biophysical methods
- Rapid chemistry and kinetic prioritisation of productsConfirmed:

James Davidson, Senior Team Leader, Medicinal & Computational Chemistry, **Vernalis**

5.20 **Fragment assisted drug discovery and application to discovery of high affinity PDE10 inhibitors**
- Employing fragment screening information with HTS to evolve a fragment hit from 1 mM to 100 nM potency
- Fragment evolution in the absence of ligand binding structure
- Future applications to targets where structural information is challenging or impossible to obtain

Jeffrey Albert, Principal Scientist, CNS Lead Generation Chemistry, **AstraZeneca**

5.50 **Chairman's closing remarks and close of day one**

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Advances & Progress in Drug Design

Day Two | Tuesday 22nd February 2011

8.30 Re-registration & coffee

9.00 **Chairman's opening remarks**
Martha Head, Director, Computational Chemistry US, **GlaxoSmithKline**

9.10 **Accelerating the lead-to-drug timeline & and reducing compound attrition rates**
- Making the most of structural data of targets to improve hit rate
- Computational methods to aid design and optimisation
- Industrialisation of parallel chemistry
- Case study: In silico structure based design of non-ATP competitive kinase inhibitors

Thomas Chan, Chief Scientific Officer, **ArQule**

9.50 **Generating novel compounds via rule-based molecular transformations**
- Application of customisable, medicinal chemistry inspired transformations to molecules in the 3D context of a binding site
- Filtering of generated compounds by molecular descriptors, QSAR models, pharmacophore queries and synthesisability
- Minimisation of remaining "hits" within a rigid or relaxing binding site, and ranking by binding energy
- Validation examples

Stephen Maginn, Director of Scientific Services, **Chemical Computing Group**

10.30 Morning coffee

10.55 **Perspectives on lead generation at Lilly**
- FBDD and molecular design
- Actives and hit assessment
- Synthetic technologies
- Open innovation

Scott Sheehan, Senior Director - Molecular Design and Lead Generation, **Lilly Research Laboratories**

11.35 **Probabilistic approach to docking and scoring: Belief Docking**
A paradigm shift of how we view docking and scoring results
- Assigning a probability that a molecule will be <1uM based on a docking score
- Development and validation of the approach using different software packages
- Fusion with ligand-based similarity approaches
- Prospective examples
- Present and future additional applications

Steve Swann, Senior Research Chemist - Fragment-Based Drug Design, **Abbott**

12.15 Networking lunch

1.15 **Tailored scoring functions in structure-based design**
Development and applications
- The development and use of tailored scoring functions
- Understanding favourable and unfavourable protein-ligand interactions
- Illustrating the merits and drawbacks in case studies on internal structure-based design case studies
- The integration of functions of different complexity within a design framework for multidimensional compound optimization

Hans Matter, Senior Scientist, Structure, Design & Informatics, **Sanofi-Aventis**

1.55 **Does my raise depend on this?**
Quantifying the role of computational chemistry expertise
- Assertion: Expertise makes a difference in the application of computational technologies for impact on drug discovery
- Experiment: Selection of correct pose from docking decoys in a game-show-like interface
- Is there a measurable difference in expertise? (yes)
- Can we learn (and teach) the components of that expertise? (we think so)

Martha Head, Director, Computational Chemistry US, **GlaxoSmithKline**

2.35 **Getting insights from the voice of protein structures**
Is there enough SBD information?
- A thorough view of available kinase structural information and its hidden messages
- Novel ways to achieve inhibitions in tabu systems
- Tackling Selectivity and Specificity from structurally informed angles

José Duca, Head, Computer-Aided Drug Discovery, **Novartis**

3.15 Afternoon tea

3.40 **Beyond growing and linking: impact of fragments on the discovery of kinase inhibitors**
- At Roche, fragments bound to the protein kinases BTK, IRAK4, SYK, JNK3 and p38 were used to:
- Identify unique protein conformations that allow rational selectivity design
- Create libraries of proprietary kinase inhibitors which serve as high quality "off-the-shelf" hits
- Rapidly discover novel drug candidates by hit expansion and scaffold hopping

Andreas Kuglstatter, Research Scientist II, **Roche**

4.20 **Aromatic ring systems as drug components**
Machine learning, theoretical calculations, and data mining applied to heteroaromatic rings
- Widening the horizons of chemical space by predicting synthetic likelihood
- Not forgetting about tautomers. QM calculations and experimental observations
- Aromatic ring in bioactive molecules: in-house, in nature and in the literature

Will Pitt, Senior Principal Scientist & Visiting Research Associate, **UCB Celltech & University of Cambridge**

5.10 **Chairman's closing remarks and close of day two**

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Who should attend:

Chief Executives, Chief Scientific Officers, Vice Presidents, Heads, Directors, Principal Scientists and Managers in the following areas:

- Drug Design
- Cheminformatics
- Computer Assisted Drug Design
- Drug Development
- Technology Assessment
- Business Development
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- Computational Biology
- Licensing Managers/Patent Officers
- Life Cycle Management
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- Product Development
- Business Development
- R&D, Strategic Planning and Development

Supported by

HALF DAY POST-CONFERENCE WORKSHOP
Wednesday 23rd February 2011
8.30am-1pm

The True Stories of Fragment-Based Drug Design:

A behind-the-scenes look at specific issues, problems and challenges of "building from the ground up"

In association with: Abbott — A Promise for Life

Overview of workshop

The concept of Fragment-based drug discovery has progressively become more prominent in the pharmaceutical industry. Although the execution and success of FBDD continues to grow, there still exist a number of challenges to the approach that continue to affect everyone in the field. This workshop offers the opportunity to present and discuss the issues we are all facing including: general screening tools and approaches, optimization strategies, the role of computational tools, and the general acceptance of the FBDD approach. A series of short vignettes and group discussion will provide additional insight into the challenges we all face and help us create a clearer view of what we can all do to advance the field.

Upon completion of this workshop, you will learn the:

- Shortcomings of various screening methods and biophysical tools
- Challenges in fragment optimization
- Changing the culture: What kind of credibility does FBDD have inside your walls?
- Other "nagging" issues in the field

8:30 Registration & coffee
9:00 Welcome & Introductions
- Experience and backgrounds of participants and hosts
- Purpose and scope of the workshop

9:10 Computational tools
- Are these tools really good enough to help us?

9:50 Biophysical tools and screening methods
- What we love, what we hate and what we actually do routinely

10:30 Morning coffee
11:00 Optimization Strategies:
- Second site screening and linking, growing, cut-and-paste
- Where have we failed and why?

11:40 What can we do better / What is on the horizon for FBDD
- FBDD is still a very small part of the global pharmaceutical industry. What is on the horizon?

12:30 Discussion session
1:00 Close of workshop

About the workshop leader:

Dr. Steve Swann, Research Investigator, Fragment-Based Lead Generation, **Abbott**

Steve began his undergraduate work at St. Francis University in rural Pennsylvania where he received a dual B.S. in Chemistry and Biology. He went on to receive his Ph.D. in Organic Chemistry under John Koh, at the University of Delaware in 2002 where he used molecular modeling to design and synthesize potentially therapeutic vitamin D analogs. After his graduate work he moved onto to Dupont Discovery research where he continued to use computer-aided design to develop novel fungicides and insecticides for an array of protein targets. After 5 years, Steve moved on to Abbott in 2006 where he now uses structure-based design to optimize fragment hits generated from an array of different screening approaches. Steve serves as the head chemist in the fragment screening and lead characterization group and has worked on more than 10 fragment-based projects in the past 12 months, along with several fast-follower programs.

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04/05 Managing Partnerships with CROs
11/12 Personalised Medicine
25/26 Nutraceuticals & Functional Foods
25/26 Point of Care Diagnostics
27/28 European Pharmaceutical Pricing & Reimbursement*

NOVEMBER 2010
10/11 Metabolic Diseases
15/16 Clinical Trials in CNS
17/18 COPD: Novel Therapeutics and Management Strategies*
22/23 Cell-Based Assays

DECEMBER 2010
01/02 Cold Chain Distribution

JANUARY 2011
17/18 Pharmaceutical Microbiology
19/20 Pre-Filled Syringes
24/25 Paediatric Clinical Trials
26/27 Social Media in the Pharmaceutical Industry
31/1 Biomarkers Summit

FEBRUARY 2011
02/03 Adaptive Designs in Clinical Drug Development
07/08 Parallel Trade
21/22 Advances & Progress in Drug Design
23/24 Stem Cells

MARCH 2011
07/08 Imaging in Cancer Drug Development
14/15 Pharmacovigilance
16/17 Superbugs & Superdrugs
23/24 Accelerating patient recruitment & Retention in Clinical Trials
30/31 Controlled Release

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13/14 Asthma & COPD

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11/12 Generics, Supergenerics and Patent Strategies
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