SMi present their 2nd annual conference...

Drug Design

24th & 25th February 2003,
Radisson Edwardian Marlborough Hotel, London

A unique opportunity to learn from leading industry experts including:

- Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca
- Dr Serge Halazy, Worldwide Head of Chemistry, Serono
- Dr Vincent Mikol, Head, Structural Biology & Molecular Modelling, Aventis
- Dr David Manallack, Head, Applied Design, De Novo Pharmaceuticals
- Dr Daniel Wyss, Associate Director, Macromolecular NMR, Structural Chemistry, Schering-Plough
- Dr Bernd Kuhn, Scientist, Molecular Design, Hoffman-La Roche
- Dr Daniel Robertson, Research Scientist, Eli Lilly
- Dr Siegfried Reich, Vice President & Head, Viral & Ophthalmic Diseases Zone, Pfizer

Benefits of Attending:

- MEET KEY EXPERTS at the cutting edge of new techniques for optimising the drug design process
- DE NOVO DESIGN: keep up to date with the developments
- COMPUTATIONAL TECHNIQUES: familiarise yourself with novel computational solutions to drug design
- EXPLOITING PROTEIN STRUCTURES: learn how to make good use of available structural information
- FOCUSED LIBRARIES: maximise the efficiency of identifying quality leads
- INTEGRATED PROCESSES FOR DRUG DESIGN: discover how to use different methods to deliver the best results

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Chairman's Opening Remarks
Dr Philip Dean, Chief Scientific Officer, De Novo Pharmaceuticals

OPENING ADDRESS

ADVANCES IN 3D STRUCTURE FOR DRUG DESIGN

Lead finding and optimisation
- Advances in 3D structure determination technologies
- Role of structural data in drug discovery
- Multiparametric optimization will be exemplified by in-house programmes
- Has 3D-based virtual screening delivered on its promise?

Dr Vincent Mihalik, Head, Structural Biology & Molecular Modelling, Aventis

LIBRARY DESIGN AND SCREENING TECHNIQUES

HIGH-THROUGHPUT CONFORMATIONAL SEARCH

A novel approach to a familiar step in identifying potential hits in large databases
- Requirements for efficiently screening databases containing large numbers of compounds
- A new, fragment-based method for efficiently generating low energy conformers for compounds in such databases
- Applications in pharmacophore refinement and searching
- Implementation within the Molecular Operating Environment (MOE)

Dr Steve Maginn, Director, Scientific Services, Chemical Computing Group

STRUCTURE-DRIVEN LEAD DISCOVERY AND OPTIMISATION

High-throughput virtual screening and binding free energy calculations
- High-throughput virtual screening for lead discovery
- Advanced binding free energy calculations
- High-throughput co-crystallization for lead discovery and optimisation
- SGx drug discovery strategy
- Structure-driven selectivity design, not just affinity

Dr Jeff Blaney, Vice President, Computational Chemistry, Structural GenomiX

VIRTUAL SCREENING AND DE NOVO DESIGN

Key issues of two complementary techniques in drug design
- Pros and cons of some current structure-based docking tools
- Inclusion of pharmacophores in docking
- Protein flexibility addressed by MM-PBSA
- de novo design as a neglected technique
- Examples of the usefulness of structure based de novo design
- Clustering structures generated by de novo design

Dr Bernd Kuhn, Scientist, Molecular Design, Hoffman-La Roche

Networking Lunch

Chairman's Opening Remarks
Dr Bill Primrose, Director, Structural Biology, PanTherix

REVOLUTIONARY NEW COMPUTATIONAL SCREENING TECHNIQUES

Case study: Quasi2
- Traditional pharmacophore models define the minimum requirements for activity but not necessarily for optimum conditions
- Optimising molecular similarity within a set of ligands with respect to binding characteristics
- Use of virtual site models in database searching
- Bridging the gap between pharmacophore screening and HTP docking
- Experimental validation of Quasi2
- Designing active compounds 'tailored' to virtual site features

Dr David Manallack, Head, Applied Design, De Novo Pharmaceuticals

Day One
24th February 2003

Morning Coffee

2.00 Case study: Quasi2

2.40 COMBINING PHARMACOPHORE AND DE NOVO COMPOUND GENERATION FOR VIRTUAL SCREENING INTO ONE COMPUTATIONAL METHOD

Case study: AutoPhore
- Natural ligands or xenobiotics are used to generate multiple pharmacophore and/or molecular shape models on the fly
- Novel drug-like molecules are generated from a set of chemical reactions and starting materials using genetic algorithms
- Each compound is probed, weighted and prioritised against the set multiple pharmacophores providing feedback to the genetic algorithm
- Most promising 3D similar compounds are finally synthesised and tested
- Biological feedback on the synthesised compounds allows selection of the best pharmacophores from the set and their refinement

Dr Michael Thormann, Research Scientist, Computational Chemistry, Morphochem

INTEGRATED DRUG DESIGN

STRUCTURE-BASED DRUG DISCOVERY FOR GPCRS

An integrated multi-step process
- GPCRs are considered the most important target family for drug discovery
- There are no X-ray structures of GPCRs (except for bovine rhodopsin)
- A novel approach for accurate 3D modelling of GPCRs (PREDICTTM)
- An integrated multi-step drug discovery process: modelling, library preparation, high-throughput screening, multiple scoring, chemical optimisation
- Integrated computational and experimental lead refinement (ICELR™)
- Examples from Predix Pharmaceuticals drug discovery pipeline

Dr Oren Becker, Chief Scientific Officer, Predix Pharmaceuticals

INTEGRATED STRUCTURE-BASED DISCOVERY

Achievements and challenges of a drug discovery engine combining chemoinformatics, virtual screening, NMR and X-ray crystallography
- Design of lead-like screening and fragment libraries
- High-throughput virtual screening of large compound libraries
- Integrated cascade for hit identification and multi-objective lead optimisation
- Integrated cascade that evolves novel hit/lead compounds based on fragments binding to the active site
- Examples from RiboTargets drug discovery pipeline

Dr Mohammad Afshar, Director, IT & Head, Drug Design, RiboTargets

STRUCTURE-BASED AND INFORMATION-DRIVEN DRUG DISCOVERY

Delivering tools to chemists to advance the discovery process
- Evaluating and selecting appropriate computational tools such as 3D conformer generators
- Developing quality, high-throughput docking and scoring solutions and delivering to the bench
- Combining known crystal structures and docking models to assist design of new entities
- Integrating gene family and SAR information into a common interface/portal
- Providing chemogenomics tools to allow the medicinal chemist to explore information in both bio- and chemo- informatics space

Dr Daniel Robertson, Research Scientist, Eli Lilly

Chairman's Closing Remarks followed by DRINKS RECEPTION in association with

Close of Day One

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Day One 24th February 2003
8.30 Re-registration & Coffee

9.00 Chairman’s Opening Remarks
Dr Harren Jhoti, Chief Scientific Officer, Astex Technology

APPLICATION OF PHYSICAL TECHNOLOGIES

9.10 PROTEIN NMR AND LIGAND SCREENING
Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca

Characterising and exploiting protein structural information in support of drug discovery projects
• Screening or structure? A false dichotomy
• Studying the interaction of ligand binding domains and drug scaffolds
• Using NMR with X-ray crystallography and calorimetry to evaluate the binding of existing leads for lead optimisation
• Compositional chemistry and modelling for NMR-based lead generation
• Leading horses to water: new challenges for medicinal chemists
• Exploiting the versatility of NMR: experience in applying different NMR approaches

11.00 Networking Lunch

11.20 PROTEIN NMR AND LIGAND SCREENING
Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca

Using surface plasmon resonance (SPR) and immobilised ligands
• Applications to anti–viral and anti–tumour drug targets
• Structure-based NMR screening (SN)
• Structure-guided lead design based on SN hits
• New tools to determine structures of protein-ligand complexes using NMR data
• Application of SN for discovering lead inhibitors against viral enzymes of the hepatitis C virus (HCV)
• Structure-guided lead optimisation of farnesy I protein transferase (FPT) inhibitors

2.00 PROTEIN NMR AND LIGAND SCREENING
Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca

The application of combinatorial chemistry to DNA sequence recognition
• Introduction to sequence-selective minor groove DNA binding agents
• Development of SP2001 a sequence selective anti-tumour agent
• Applying combinatorial chemistry to sequence recognition
• Early libraries
• Second generation libraries
• Future development of gene targeting

Dr Jennifer Miller, Director, Computer-Aided Drug Design, Signature BioScience

CHALLENGES OF ENABLING A CELL–BASED APPROACH TO DRUG DISCOVERY

2.40 PROTEIN NMR AND LIGAND SCREENING
Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca

Networking Lunch

3.20 PROTEIN NMR AND LIGAND SCREENING
Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca

Networking Lunch

3.40 PROTEIN NMR AND LIGAND SCREENING
Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca

Networking Lunch

4.20 PROTEIN NMR AND LIGAND SCREENING
Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca

Networking Lunch

5.00 PROTEIN NMR AND LIGAND SCREENING
Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca

Networking Lunch

5.40 PROTEIN NMR AND LIGAND SCREENING
Dr Alex Breeze, Head, Protein NMR, Structural Biology Group, AstraZeneca

Networking Lunch

Day Two 25th February 2003

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Drug Design

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