Cambridge Healthtech Institute’s 6th Annual
Structure-Based Drug Design
June 14-16, 2006 • World Trade Center • Boston, Massachusetts

Conference Highlights:

• Pre-Conference Short Course: Designing Structure-Based Kinase Inhibitors
• Cutting-Edge Sessions from Industry Leaders
• Hot Topic Sessions on Fragment-Based Drug Discovery
• Panel Discussion: How Much More Effective will Drug Discovery Become in the Next 10 Years?
• Case Studies from Abbott Laboratories and Wyeth Research
• And much more!

Hear from Industry Leaders Including:

• Peter Fedichev, Ph.D., Corporate Scientific Officer, Quantum Pharmaceuticals
• William L. Jorgensen, Ph.D., Whitehead Professor of Chemistry, Department of Chemistry, Yale University
• Dr. Mario Lobell, Computational Chemistry, Bayer HealthCare, Germany
• Klaus Müller, Ph.D., Pharmaceutical Research-Head of Science & Technology Relations, F. Hoffmann-La Roche Ltd.
• Mark Murcko, Ph.D., Vice President and Chief Technology Officer, Vertex Pharmaceuticals, Inc.
• Christopher Murray, Ph.D., Director, Computational Chemistry and Informatics, Astex Therapeutics
• Leszek Poppe, Ph.D., Principle Scientist, Molecular Structure Department, Amgen, Inc.
• Tomi K. Sawyer, Ph.D., Senior Vice President, Drug Discovery, ARIAD Pharmaceuticals
• Robert A. Volkmann, Ph.D., Senior Research Fellow, Pfizer Global Research and Development
• And many more!

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2:15 Determinants of Selectivity in Targeting the JAK Family of Kinases for Treatment of Cancer and Inflammatory Disease

Dr. Andrew Wilks, Corporate Scientific Officer, R&D, Cytopia Research Pty, Ltd., Australia

The JAK family of PTKs has four members in the human genome (JAK1, JAK2, JAK3 and TYK2) each of which plays an important role in the intracellular signaling downstream of particular cytokines. A single point mutation in the kinase like domain of JAK2 has recently been linked to a significant proportion of cases of Myeloproliferative Disorders, including Polycythemia Vera (PCV) and Essential Thrombocytemia. Parallel computational approaches to molecular modeling, drug design and in silico screening are being explored to generate potent and highly specific small molecule inhibitors of a number of the JAK family of PTKs. Co-crystallography of these potent and specific JAK inhibitors with the JAK2 kinase domain provides important insights into the feasibility of generating drugs against these important targets.

2:45 Refreshment Break

3:15 In silico ADMET Traffic Lights and PhysChem Scores and their Application to Kinase Inhibitors

Dr. Mario Lobell, Computational Chemistry, Bayer HealthCare, Germany

The need for in silico characterization of HTS hit structures as part of a data driven hit selection process is demonstrated. A solution is described in form of the in silico ADMET Traffic Light and PhysChem scoring system. The described in silico system has been extensively validated with Bayer in-house data, literature data and a collection of launched small molecule drugs. The system is applied to examples of kinase inhibitor drugs and drug candidates.

3:45 Structural Basis for the Non-Competitive Inhibition of Human MEK1

Dr. Jeffrey Ohren, Senior Scientist, Structural Biology Group, Department of Chemistry, Pfizer Global Research & Development

MAP kinase 1 (MEK1) plays an integral role in the formation, progression and survival of tumors, in addition to mediating many inflammatory processes. As a result, MEK1 represents an attractive target for pharmacological intervention in both proliferative and inflammatory diseases. The recent X-ray structure of human MEK1 in a complex with ATP and a non-competitive, small molecule inhibitor provides structural insight into a unique mode of kinase inhibition and may provide a platform for the structure-based design of the next generation of protein kinase inhibitors.

4:15 Insights for Design: Differential Binding of Inhibitors to Active and Inactive CDK2

Dr. Campbell McInnes, Head, Structure-Based Drug Group, Cyclacel Ltd., Scotland

The cyclin-dependent kinases (CDKs) are important anti-cancer targets and despite having been characterized in complex with a wide variety of inhibitors, the majority of CDK2 structures solved are of the inactive enzyme. Crystalllographic data exists for only one ATP-competitive inhibitor in both the active cyclin-bound and inactive CDK2 forms. We have solved the structures of six inhibitors in both the monomeric CDK2 and binary CDK2/cyclin A complexes and demonstrate for the first time that significant differences in binding of CDK2 ligands occur depending on the activation state. The binding mode of two ligands varies substantially as a result of binding site differences induced upon CDK2 activation. Furthermore, an energetic analysis of CDK2/cyclin complexes demonstrates that a good correlation exists between the in vitro potency and calculated energies of interaction, while indicating that no such relationship exists for monomeric CDK2-inhibitor structures. These results confirm that structures solved in complex with the monomeric CDK2 do not fully reflect the active conformation of bound inhibitors. This analysis reveals significant implications for inhibitor design towards active structures since these are distinct from the inactive CDK2 and also suggests that the monomeric CDK2 conformation could be selectively inhibited.

4:45 End of Short Course

4:45-5:30 Main Conference Early Evening

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predict the affinity for large and diverse ligand sets binding to a common target protein and suggest a potential to predict adverse effects triggered by drugs and chemicals [6].

11:25 Case Study of Structure-Based Design for DPP-IV Inhibition
Kenton Longenecker, Ph.D., Protein Crystallographer, Structural Biology Department, Abbott Laboratories
Pharmacological inhibition of dipeptidyl peptidase IV (DPP-IV) is a recently explored strategy aimed to benefit patients with type-II diabetes by regulating plasma glucose levels. X-ray crystallographic studies of DPP-IV in complex with inhibitors aided drug candidate discovery through structure-based evaluation and design. This presentation will highlight contributions of structural biology to these efforts at Abbott Laboratories.

11:55 An Integrated Approach to Library Design
W. Pat Walters, Ph.D., Senior Research Fellow, Computational Chemistry and Molecular Modeling, Vertex Pharmaceuticals, Inc.
A chemist designing a combinatorial library must consider many criteria when selecting reagents for synthesis. Factors such as target potency, physical properties, metabolic stability, and off-target activity are among many parameters that must be optimized. Although computational models exist to aid the chemist, these models are often poorly validated and are not easily integrated into the drug discovery process. As part of a continuing effort to provide library design tools for medicinal chemists, we have created a software tool known as MedChem2. This software provides an easy means of linking a virtual combinatorial library with a well-validated set of computational models. The application of these models can dramatically reduce the size of a virtual library, and help to focus a chemistry effort on the most relevant compounds. Models in MedChem2 are constructed using NOMAD, an internally developed software platform that allows computational chemists to identify optimal combinations of molecular descriptors and machine learning methods. Models generated using NOMAD can then be published to MedChem2 where they become part of the medicinal chemistry workflow. This presentation will provide an overview of NOMAD and MedChem2, as well as example applications of both programs.

12:25pm Lunch on Your Own

Experimental Approaches

1:35 Chairperson's Remarks

1:45 Biospectra Analysis: Model Proteome Characterizations for Linking Molecular Structure and Biological Response
Robert A. Vollmann, Ph.D., Senior Research Fellow, Pfizer Global Research and Development
Establishing quantitative relationships between molecular structure and biological effects has been a long-standing goal in drug discovery. An operationally simple probabilistic structure-activity relationship (SAR) approach, termed biospectra analysis, which uses pattern similarity between biospectra of molecules as determinant, will be described. Comparison of biospectra derived from in vitro assays yields precise chemical structure information and is useful for identifying pharmacology and side effect similarities between medicines. Specific examples will be provided.

2:15 Discovery of Ligands for Nurr1 by Combined Use of NMR Screening with Different Isotopic and Spin-Labeling Strategies
Laszek Poppe, Ph.D., Principle Scientist, Molecular Structure Department, Amgen, Inc.
A comprehensive approach to target screening, hit validation and binding site determination by nuclear magnetic resonance spectroscopy (NMR) is presented. Screening by 19F NMR signal perturbation, followed up by magnetization transfer experiments and second-site screening with spin-labeled ligands, led to discovery of a molecule which binds to the Ligand Binding Domain of Nurr1 with dissociation constant ∼ 20 μM. With the help of uniform and residue specific 15N isotope labeling and derivatization of Cys residues with 2-mercaptoethylamine-1,13C we were able to determine the binding site location with knowledge of the APO coordinates.

Homology, Modeling, and Ligand-Based Design

2:45 Success and Lessons from 11 betaHSD1 Homology Models: Using Models of Very Low Homology in Docking and Design
Ying-Duo Gao, Ph.D., Senior Research Fellow, Molecular Systems, Merck & Co. Inc.
11beta-hydroxysteroid dehydrogenase type1 (11beta-HSD1) is a potential target for treatment of some of the health problems associated with Metabolic Syndrome. In assisting medicinal chemistry in lead optimization, we generated homology models of human and mouse 11betaHSD1 enzymes based on 17betaHSD1 and 17alphaHSD1 structures. These models were used extensively in the program. In this presentation we demonstrate that models with very low homology (<25%), that may only partly present the active site correctly, can be highly valuable for understanding SAR of the ligands and suggesting new
design. In addition, the recently available crystal structures of human and mouse 1betaHSD1 allowed us to assess the homology models and discuss how to improve this type of modeling.

3:15 Technology Watch (Sponsorship Available)
Beyond Scoring Functions: Fast First-Principles Quantum and Molecular Physics Tools for Structure-Based Drug Design
Kay Denis, MBA., Postion TBA, Tintarc, Inc., Business Partner/distributor of Quantum Pharmaceuticals; On behave Peter Fedichev, Ph.D., CSO, Quantum.Corporate Scientific Officer, Quantum Pharmaceuticals
Quantum is a computational platform aimed at direct predictions of powerful quantum and molecular modeling structure based tools for fast and accurate predictions of protein-ligand binding affinities. The ingredients are: a good, polarizable force field based on quantum mechanics, a solvation energy model; and statistical physics for entropy change calculations. The transferability of the vacuum force field for aqueous calculations is ensured by its polarizability and the quality of the water model, but not by the excessive parametrization. This ideology provides a solid and physically motivated ground for the free binding energy calculations. The software has been extensively tested against all available experimental data and has been recently released. Possible areas of application: High Throughput Virtual Screening, Computer Aided Drug Design, Cheminformatics, Computational Chemistry and Biology, ADMET prediction. An unprecedented level of accuracy together with a simple and efficient user interface allows for in silico lead optimization. The technology is expected to speed up drug R&D radically and irrevocably change the computational chemistry and drug discovery.

3:30 Networking Refreshment Break, Poster and Exhibit Viewing

4:00 Docking Studies of A3 Agonists and Antagonists: Suggest Activation Mechanism of Adenosine Receptor
Soo-Kyoung Kim, Ph.D., Senior Research Associate, Beckman Institute, Molecular Simulation Center, California Institute of Technology
To determine the different binding modes of agonist and antagonist to A3 adenosine receptor (AR), the docking studies of A3 selective nucleoside agonists and non-nucleoside antagonists were compared by using the FlexX and the FlexDock automated docking procedure. There are common binding regions for the exocyclic amino groups of each 9H-purine ring in agonist CI-IB-MECA and the H1[1,2,4]triazolo[1,5-c]quinazoline ring in non-nucleoside antagonist CGS19941 through H-bonding to the side chain of N6.55. In addition, hydrophobic interactions of 6-N-aryl groups were overlapped, interacting with F168 in EL2. For binding domains of agonist, additional H-bonding of the ribose 3'- and 5'-substituents with the hydrophilic amino acids T3.36, S7.42, and H7.43 and hydrophobic interaction of the terminal methyl group of the 56c61602-2,4-aminonaphthalene interacted with the hydrophobic side chain of F6.44 required for the characteristic side chain movements of TM6 and TM7. Here we present the novel insights in the putative activation mechanism of AR1. The fact that agonist binding disrupts the intramolecular H-bonding network through W8.48 and H7.42 and occurs the rotation of TM6 suggests that these activation mechanisms might be extended to other members of the AR family. Collaboration with Kenneth A. Jacobson, Ph.D., Section Chief.

4:30 Bridging the Gap between Protein Cavities by Virtual Screening
Hans Briem, Ph.D., Senior Scientist, Compound Design and Compound Characterization/Computational Chemistry, Schering AG
One strategy to enhance the binding affinity of protein ligands is to identify sub-pockets on the protein surface to which additional tether groups linked to a given scaffold may bind. We will demonstrate how we used the new module FlexC-Pharm to efficiently dock large combinatorial libraries while simultaneously considering user-defined pharmacophore constraints. This approach allows us to prioritize sets of virtual combinatorial libraries by their ability to bridge the gap between protein cavities of the target of interest.

5:00 Case Presentation of Strategies for High-Throughput Molecular Docking
Diane Joseph-McCarthy, Ph.D., Principal Research Scientist, Chemical and Screening Sciences Department, Wyeth Research
In structure-based design, molecular docking techniques are used to predict the binding of a set of proposed compounds. Accurate molecular docking of small molecules to a target structure requires adequate sampling and accurate scoring of each proposed ligand in the target binding site. The use of our in house pharmacophore-based docking approach on several therapeutic target projects will be presented and compared to the use of commercial software. In addition, the exploration of the inclusion of protein flexibility during docking will be discussed.

5:30-6:30 Networking Reception in the Exhibit Hall

FRED, JUNE 16
NEW TECHNOLOGIES & HOT TOPICS

8:00am Morning Coffee (Sponsorship Available)

8:30 Chairperson’s Remarks
Tom K. Sawyer, Ph.D., Senior Vice President, Drug Discovery, ARIAD Pharmaceuticals

8:40 Structural and Functional Properties of Oncogenic Protein Kinases that Manifest Resistance: Chemical Biology and Drug Design Strategies
Tom K. Sawyer, Ph.D.
Oncogenic protein kinases are key therapeutic targets for drug discovery. X-ray crystallography, biochemical and cellular studies have revealed both structural and mechanistic properties of several oncogenic protein kinases. In increasing number of cases, resistance to current inhibitors has been shown to involve critical amino acid mutations in the ATP or proximate binding sites for small-molecule inhibitors. These challenges are being addressed by both chemical biology and drug design strategies. A case example is T315I mutation of Bcr-Abl kinase.

9:10 Embracing Chemokines: Understanding Specificity and Selectivity of Chemokine Binding Proteins
Joao Dias, Ph.D., Post-doc, Chemistry, Serono Pharmaceutical Research Institute
Chemokines control the migration of leukocytes through interaction with receptors of the seven transmembrane G-protein coupled receptor family. Dysfunction of this system results in excessive cellular recruitment, with dramatic implications in inflammatory and autoimmune diseases. Blocking the receptor-chemokine interaction could thus be therapeutic value, since prevention of this directional migration represents an effective anti-inflammatory strategy. Nature provides efficient strategies, employed by both parasites and viruses, to elude the host’s immune system, and hence avoid an inflammatory response. Ticks can feed from several hours to days or even weeks, evading the host immune response (haemostatic, immune and inflammatory). Tick saliva components include enzymes, enzyme inhibitors, amine binding proteins and cytokine homologues. We have constructed a cDNA library from tick salivary glands, which was screened against several chemokines. We have identified a new chemokine binding protein (ChBP) from tick saliva, which binds to some selected chemokines, and does not share any relevant sequence and structural homology to any other known and available protein. We have solved the crystal structure of the human chemokine MIP-1-alpha in complex with this novel ChBP, and have hence unraveled the specific interactions between these two proteins. Upon complex formation, the N-terminal of the chemokine and the N-terminal and C-terminal of the ChBP are stabilized. The N-terminal of the chemokine plays a major role in this interaction by forming the lid to the pocket that anchors tryptophan 89 from ChBP, which interacts tightly through an aromatic stacking with phenylalanine 29 from MIP-1-alpha. The integration of our current knowledge, combined with protein homology modeling and site directed mutagenesis studies, will provide a consolidated platform for the generation of structure based drug designed chemokine inhibitors.

9:40 Numerical Indices and a Statistical Framework for Structure-Based Drug Design
Cele Abad-Zapatero, Ph.D., Associate Research Fellow, R-46Y Department, Abbott Laboratories
Recently, the concept of ligand efficiency as a measure for lead selection was suggested (Hopkins et al., Drug Discovery Today, 2004, 9:430-431). A more comprehensive analysis of ligand efficiency indicators will be presented, including the concepts of binding efficiency and surface efficiency (Abad-Zapatero and Metz, Drug Discovery Today, 2005, 10:464-469). Their application to guide the process of drug discovery, and specifically its integration into the structure-based drug design methods to make them more efficient and numerically robust.

10:10 Networking Coffee Break, Poster and Exhibit Viewing

10:55 The Dance of the Molecules: How to Optimize Ligand Alignments in Torsional Space
Robert D. Clark, Ph.D., Senior Director, Software Research Department, Tripos, Inc.
Pharmacophore models have traditionally been limited to features that must be shared by every ligand that binds tightly to the target protein. Most also fail to take steric properties shared among the various known ligands into consideration. ALAHAD is a new fully flexible ligand alignment program that supports multiple partial match feature sets while taking steric overlap into account. Moreover, by separating the problem into torsional and Cartesian components, the program avoids the need to have template molecules.

11:25 High Strain Energies of Bound Ligands - What is Going on?
Paul Labute, President, Chemical Computing Group
The prediction of the bioactive bound conformation of a candidate ligand is important for computational methodologies such as pharmacophore search and docking. The strain energy of a conformation (relative to the global minimum energy) is often used as a criterion for rejection of a conformation from consideration. Recent molecular mechanics studies using ligand-receptor complexes from the PDB have suggested that high strain energies (> 10 kcal/mol) are not only possible but routinely observed. We present the results of computational experiments that attempt to explain these observations and determine their validity.
We have developed new technologies for significantly improving the prediction of binding modes and binding affinities of protein-ligand complexes. Incorporation of polarization of the charges on the ligand, via coupling of mixed quantum mechanics/molecular mechanics methods to docking, enable a dramatic improvement in the robustness of binding mode prediction. Protein structure prediction methods can be used to efficiently model induced fit effects. Finally, a novel scoring function, based on hydrophobic enclosure of the ligand by protein residues, has been developed for assessing binding affinity. Recent results validating this scoring function via explicit molecular dynamics simulations will be presented. Applications to a wide range of pharmacologically interesting targets, such as CDK2 and p38 map kinase, will be discussed.

12:10pm Luncheon Technology Workshop
Sponsored by Schrödinger

Focused Combinatorial Libraries via a Novel Structure-Based Design Methodology

Woody Sherman, Ph.D., Applications Scientist, Department of Applications, Schrödinger

Short Proposal: Combinatorial library design has been evolving toward greater use of small focused libraries that are biased toward a specific target or class of targets and exhibit optimal drug-like physiochemical properties. We will present the application of a novel computational method that performs rapid virtual screening of combinatorial libraries to eliminate unpromising compounds before they are synthesized. This approach is based on new technology that dramatically reduces the combinatorial complexity of the search problem in order to generate an optimized focused library. Furthermore, the program allows for the inclusion of predicted ADMET properties into the overall library selection process. A number of case studies using this methodology will be presented.

12:45 Last Chance to View Posters & Exhibits

1:25 Chairperson’s Remarks

1:30 NMR-Based Discovery of Novel Protein-Protein Interaction Modulators

Markus Schade, Ph.D., Vice President of NMR Drug Discovery, Combinatarie Biopharm AG

By using NMR-based fragment screening, we successfully identified novel, chemically diverse classes of fragment ligands for a demanding protein-protein-interaction (PPI) target, namely the PDZ domain of human A66. We derived a 3D pharmacophore model directly from the NMR binding site information and utilized it for the first round of chemical optimization. For the highest affinity derivative, we determined the 3D protein-fragment complex structure by NMR and used it to guide the second round of fragment-to-lead optimization. This case study demonstrates how NMR-derived structural information supports fast and efficient fragment optimization chemistry.

2:00 Structure-Guided and Property-Guided Design in Drug Discovery

Klaus Müller, Ph.D., Pharmaceutical Research-Head of Science & Technology Relations, F. Hoffmann-La Roche Ltd.

Local bulk increase is a recurrent strategy in drug discovery. However, this is typically accompanied by an undesired increase in lipophilicity. In our search for lipophilic neutral bulk increase, we identified a structural subunit that has been largely overlooked in medicinal chemistry. We find that this unit has the potential to modify compound properties in unique ways and may solve several problems commonly encountered in medicinal chemistry.
Structure-Based Drug Design

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Structure-Based Drug Design

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