Topics include:

- Target Structure-Guided Drug Discovery
- Feeding SBDD with Biochemical and Biophysical Information
- Ligand-Based Predictions Applied to Drug Design
- SBDD and Computational Chemistry Methods: A Marriage of Innovation
- SBDD of Pharmacological Chaperons

Hear from thought leaders including:

Structure and Function of the G-Protein Coupled Receptor Family
Raymond C. Stevens, Ph.D., Professor, Departments of Molecular Biology and Chemistry, Scripps Research Institute

Structure-Based and Ligand-Based Computational Modeling of Pharmacological Profiles
Ajay N. Jain, Ph.D., Professor, Cancer Research Institute & Department of Lab Medicine, University of California San Francisco

Discovery of Novel Cyclin-Dependent Kinase Inhibitors: A CDK2 Case Study in Structure-Based Drug Design
José Duca, Ph.D., Senior Principal Scientist, 3D-Drug Design Department, Schering Plough Research Institute

The Race for Chemical and Biological Space: A Drug Design Perspective
Tomi Sawyer, Ph.D., Chief Scientific Officer, AILERON Therapeutics; Editor-in-Chief, Chemical Biology & Drug Design

Predicting the Activity of Congeneric Series
W. Patrick Walters, Ph.D., Senior Research Fellow, Computational Chemistry and Molecular Modeling, Vertex Pharmaceuticals, Inc.

Towards Rational Drug Design for Intrinsically Unstructured Proteins - Small Molecules Mediated Inhibition of α-Synuclein Aggregation
Gergely Toth, Ph.D., Scientist, Computational Chemistry and Biology, Chemistry, Elan Pharmaceuticals

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PRE-CONFERENCE WORKSHOP*

WEDNESDAY, JUNE 3

1:10 pm  Chairperson’s Remarks
David Borhani, Ph.D., D.E. Shaw Research, LLC

1:15 pm  The DFG Motif – a Protonation-Dependent Conformational Switch in Protein Kinases
Yibing Shan, Ph.D., D.E. Shaw Research, LLC

Conformations of the conserved DFG motif is well known to be crucial for selective binding of many kinase inhibitors—including the cancer drug imatinib. Using long molecular dynamics simulations of the Abi kinase, we visualized the DFG flip in atomic-level detail and formulated an energetic model predicting that protonation of the DFG apparate controls the flip. Consistent with our model’s predictions, we demonstrated experimentally that the kinetics of imatinib binding to Abi kinase have a pH dependence. Our model suggests a role of the DFG motif as a conformational switch in kinase catalytic cycles. In addition, our experimental results on imatinib suggest a convenient assay to identify DFG-out kinase inhibitors in the absence of structural data.

1:45 pm  Selective Rho Kinase (ROCK) Inhibitors: Design and Synthesis
Hartmut Schirok, Ph.D., Senior Scientist, Bayer Schering Pharma AG

Rho kinase plays a pivotal role in vasoregulation, making it a suitable target for the treatment of hypertension and related disorders. The discovery of Bayer Schering’s azaindole-based ROCK inhibitor will be presented. The structure-activity relationships will be disclosed, elucidated through biochemical, functional, and in vivo assays.

2:15 pm  Aggregating Knowledge to Enhance Kinase Drug Discovery
Natasja Brooijmans, Ph.D., Principal Research Scientist, Pharmaceutical Chemistry, Wyeth

The amount of structural and pharmacological information about kinases and their inhibitors has increased significantly over the years thanks to significant efforts from both public and private institutions. While a number of kinase inhibitors have been approved for use in the clinic, kinases as drug targets still form a significant challenge due to protein flexibility in the kinase catalytic domain and issues with selectivity over related and unrelated kinases.’ We’ll describe our efforts to take advantage of the aggregate of information that is available to enhance kinase drug discovery efforts. Prospective & retrospective virtual screens utilizing multiple crystal structures will be discussed. In addition, we’ll highlight large-scale ligand-based modeling efforts to extract knowledge hidden in databases such as the GVK biodata database.

2:45 pm  Networking Refreshment Break

3:15 pm  Cross-Docking to CDK2: A Virtual Screening Study
Johannes Vogt, Ph.D., Senior Principal Scientist, Schering-Plough Research Institute

Conformations of the conserved DFG motif is well known to be crucial for selective binding of many kinase inhibitors—including the cancer drug imatinib. Using long molecular dynamics simulations of the Abi kinase, we visualized the DFG flip in atomic-level detail and formulated an energetic model predicting that protonation of the DFG apparate controls the flip. Consistent with our model’s predictions, we demonstrated experimentally that the kinetics of imatinib binding to Abi kinase have a pH dependence. Our model suggests a role of the DFG motif as a conformational switch in kinase catalytic cycles. In addition, our experimental results on imatinib suggest a convenient assay to identify DFG-out kinase inhibitors in the absence of structural data.

3:45 pm  Kino-Pocketome: The Structural Classification and Targeting of Non-Traditional Kinase Binding Sites
Ruben Abagyan, Ph.D, Professor, Department of Molecular Biology, The Scripps Research Institute Adjunct Professor, University of California, San Diego, School of Pharmacy

A comprehensive structural set of kinases and their complexes with inhibitors and peptides has been collected and classified in terms of multi-conformational (flexible) pockets of various types. An application of the flexible pocketome approach to kinase modeling, virtual ligand screening and ligand specificity profiling is also presented. We applied the method to two types of pockets, the type II inhibitor binding pocket (the DOLPHIN method) and a pocket at the protein-protein interaction interface exemplified by CK2 alpha/beta interactions.

4:15 pm  Panel Discussion: Structuring the Road to Success

4:45 pm  End of Workshop

*Separate registration is required.
Virtual Screening in SYBYL provides a unique means of selecting the most promising R-group candidates, all presumably synthesizable. R-Group Description: A larger variety of R-group candidates is described, based on objective and relatively accurate pIC50 predictions using Topomer CoMFA, with remarkable ease and speed. Validation studies continue to strongly confirm these apparent benefits.

Success in lead optimization requires discovery of one or more R-groups that confer the desired properties on a clinical candidate. Large compound collections implicitly describe a larger variety of R-group candidates, all presumably synthesizable. R-Group Virtual Screening in SYBYL provides a unique means of selecting the most promising of these, based on objective and relatively accurate pIC50 predictions using Topomer CoMFA, with remarkable ease and speed. Validation studies continue to strongly confirm these apparent benefits.

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10:00
Virtual Screening for R-Groups
Richard Cramer, Ph.D., Senior Vice President, Science & Chief Scientific Officer, Tripos
Success in lead optimization requires discovery of one or more R-groups that confer the desired properties on a clinical candidate. Large compound collections implicitly describe a larger variety of R-group candidates, all presumably synthesizable. R-Group Virtual Screening in SYBYL provides a unique means of selecting the most promising of these, based on objective and relatively accurate pIC50 predictions using Topomer CoMFA, with remarkable ease and speed. Validation studies continue to strongly confirm these apparent benefits.

10:30
Networking Coffee Break, Poster and Exhibit Viewing

11:00
Discovery of Novel Cyclin-Dependent Kinases Inhibitors: A CDK2 Case Study in Structure-Based Drug Design
José Duca, Ph.D., Senior Principal Scientist, 3D-Drug Design Department, Schering Plough Research Institute

11:30
Special Co-Presentation
A Flexible Approach to Induced Fit Docking
Sander B. Nabuurs, Ph.D., Group Leader, Computational Drug Discovery, Center for Molecular and Biomolecular Informatics, Radboud University Nijmegen Medical Centre
Markus Wagener, Ph.D., Project Leader, Cheminformatics, Molecular Design & Informatics, Schering-Plough Research Institute
Reliably predicting the binding modes of a set of (proposed) compounds, taking both receptor and ligand flexibility into account, and subsequently ranking these compounds by their binding affinity remains a tremendous challenge. First, we will present the methodology behind and recent developments in our induced fit docking tool Flexy. The second part of our contribution will focus on realistic large-scale induced fit cross-docking studies using sets of receptor-ligand complexes with known affinity. Our progress towards an affinity prediction model based on obtained docking results will be presented and potential pitfalls and requirements to arrive at accurate predictions will be discussed.

12:15 pm
Structure-Guided Design of Potent and Selective ERK inhibitors – A Kinase Selectivity Case Study
Alex Aronov, Ph.D., Research Fellow, Medicinal Chemistry and Project Leader, Inflammation, Vertex Pharmaceuticals, Inc.
The Ras/Raf/MEK/ERK signal transduction is a key oncogenic pathway implicated in a variety of human cancers. A number of steps in the pathway have been targeted in anticancer drug design. The presentation will describe the discovery of two distinct chemical series of ERK inhibitors starting with a micromolar lead, with a particular focus on structure-based selectivity design. The following aspects of kinase selectivity design will be highlighted:
• Utility of gene family-based structural lead profiling
• Leveraging differences in inhibitor orientation within the active site for selectivity design
• Leveraging target-specific ligand conformational preferences for selectivity design
• Concept of kinase-likeness and its implications for kinase selectivity

12:45 Structure Based Design of PDE4 Allosteric Modulators
Alex Burgin, Ph.D., Chief Operating Officer, deCODE Biostuctures
Phosphodiesterase 4 (PDE4) is the primary cAMP hydrolysing family of enzymes in human cells. PDE4 inhibitors have been developed for multiple clinical indications; however, no PDE4 inhibitor has been approved because of dose limiting side effects. We have obtained the first crystal structures of the regulatory domains of PDE4B and PDE4D interacting with the catalytic domain and have used these structures to develop allosteric modulators of PDE4 activity. We will describe the development of these unique allosteric modulators and how the crystal structures enabled the development of highly selective modulators with significantly improved safety profiles.
There has been considerable interest in PDE4 as a therapeutic target and structure based drug design has been widely used to develop PDE4 active site inhibitors. We have focused on the development of non-active site inhibitors and created the first PDE4 allosteric modulators that activate the activity of PDE4 enzymes by interacting directly with the regulatory domain.
• We will describe the technologies and approaches that enabled this discovery and how this new approach may be applicable to other phosphodiesterases.
• Demonstration of how PDE4 enzymatic activity is controlled and explanation for how partner proteins may alter PDE4 activity.
• Demonstration of how novel structures can enable the discovery and development of the first allosteric modulators of PDE4 activity.

1:15 Luncheon Technology Presentation (Opportunity Available) or Lunch on Your Own
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FEEDING SBDD WITH BIOCHEMICAL AND BIOPHYSICAL INFORMATION

2:10 Chairperson’s Remarks
Gergely Toth, Ph.D., Scientist, Computational Chemistry and Biology, Chemistry, Elan Pharmaceuticals

2:15 Supplementing Structural Information with Biophysical Data: Adding Value and Understanding in Lead Generation
Stefan Geschwindner, Ph.D., Principal Scientist, Cell, Protein and Structural Sciences, AstraZeneca R&D Mölndal
The provision of structural information in the drug discovery process has proven to be of high value in the past and continues to be highly valued in the future. In the last couple of years the field of label-free assay technologies has seen a dramatic development both in expanding its range with emerging technologies as well as reducing reagent consumption and increasing throughput such that those have and will become very attractive tools in the drug discovery process. The presentation is focusing on what information can be gained from assessing kinetic and thermodynamic parameters and how this can be linked with structural data in order to provide an information-rich package to medicinal chemists that can facilitate their decision-making in the lead generation process. Some examples will be discussed that highlight the power of combining structural information with biophysical data.

2:45 Using Thermodynamic Information to Enhance Quality of Design in Lead Generation
Andrew D. Scott, Ph.D., Senior Scientist, Structural Biology and Biophysics Group, Pfizer Global Research and Development

The process of advancing screening hits to lead compounds and ultimately to clinical candidates requires extensive decision-making based on experimental data. Early-Stage drug development is mostly based on finding the highest affinity compounds. Numerous assays give accurate affinity measurements but as Ka is composed of multiple components, some of which favor the ability of a molecule to act as a potent and selective drug, and some which do not, measuring affinity alone gives limited insight into the mechanism of binding. Isothermal Titration Calorimetry (ITC) can give a full thermodynamic signature (ΔGobs, ΔHobs, ΔSobs and KB, obs) as well as stoichiometry of binding from a single experiment. The optimal use of ITC and how thermodynamic parameters can drive hit selection and optimization towards higher affinity leads will be discussed.

- How to use thermodynamic data to drive hit selection and optimization
- How to run ITC experiments to monitor small enthalpic and entropic changes
- Examples where thermodynamic data has proved valuable for hit selection and optimization
- Recent advances in ITC technology

3:15 Networking Refreshment Break, Poster and Exhibit Viewing

SBDD OF PHARMACOLOGICAL CHAPERONS
4:00 Towards Rational Drug Design for Intrinsically Unstructured Proteins - Small Molecules Mediated Inhibition of α-Synuclein Aggregation
Gergely Toth, Ph.D., Scientist, Computational Chemistry and Biology, Chemistry, Eli Lilly and Company

Increasing evidence indicates that the self-assembly of proteins is often associated with the molecular events leading to neuronal death in a range of neurodegenerative diseases. Since many of these proteins are intrinsically disordered it has been particularly challenging to develop effective strategies for discovering small molecules inhibitors of their aggregation. We present here an approach that combines biophysical techniques with a rational computer-aided discovery procedure based on an ensemble of NMR structures and their abilities of self-association. These results suggest that targeting monomeric proteins with small molecules is a viable drug discovery strategy towards the identification and rational design of aggregation inhibitors of intrinsically disordered proteins.

4:30 SBDD of Pharmacological Chaperons
Dagmar Ringe, Ph.D., Professor of Biochemistry and Chemistry, Rosenstiel Basic Medical Sciences Research Center, Brandeis University

Interactive Panel

5:00 Thinking Out Loud, a Day One Closing Panel: Are we ready for a GPCR structural explosion?
- Raymond C. Stevens, Ph.D., Professor, Departments of Molecular Biology and Chemistry, Scripps Research Institute
- Tomi Sawyer, Ph.D., Chief Scientific Officer, AILERON Therapeutics; Editor-in-Chief, Chemical Biology & Drug Design
- Ajay N. Jain, Ph.D., Professor, Cancer Research Institute & Department of Lab Medicine, University of California San Francisco
- José Duca, Ph.D., Senior Principal Scientist, 3D-Drug Design Department, Schering-Plough Research Institute

5:30 – 6:30 Networking Reception in the Exhibit Hall
11:00 Improving the Quality of Structure-Based Virtual Screen by The Interaction-Focused Post-Docking Analysis
Suo-Bao Rong, Ph.D., Senior Principal Scientist, Medicinal Chemistry – Antibacterials and Neurosciences Computational Chemistry, Pfizer Global R&D
Co-Author: Brian S. Bronk, Ph.D., Senior Director, Medicinal Chemistry – Antibacterials and Neurosciences Computational Chemistry, Pfizer Global R&D
A semi-automatic post-docking protocol, including the key interaction identification, interaction similarity analysis, binding mode clustering, pocket occupancy comparison, and chemotype clustering, has been developed to further improve the hit rate and especially the hit-to-lead success rate for structure-based virtual screens. Key features of the protocol include its flexibility and effectiveness to explore the diversities of both ligand-protein interactions (binding modes) and ligand structures. This method makes it practical for a designer to use experimental SAR to narrow a large number of compounds by visualization as the last step in selecting a small number of representative VS hits for submission to the bioassay. In this way, it is feasible to examine multiple potential directions derived from structure-based virtual screening, thereby increasing the probability of impact on successful hit-to-lead optimization. The protocol has succeeded in several different targets to achieve ~10% hit rate and particularly identify a series of diverse novel scaffolds successful in the hit-to-lead optimization.

11:30 Fragment-Based Drug Discovery (FBDD)
Dr. Richard J. Law, Computational Chemistry Group Leader, Evotec UK Limited
Fragment-based drug discovery (FBDD) represents a change in strategy from the screening of molecules with higher molecular weights and physical properties more akin to fully drug-like compounds, to the screening of smaller, less complex molecules. This is because it has been recognised that fragment hit molecules can be efficiently grown and optimised into leads, particularly after the binding mode to the target protein has been first determined by 3D structural elucidation, e.g., by NMR or x-ray crystallography. Several studies have shown that medicinal chemistry optimisation of an already drug-like lead compound, results in a final compound with increased molecular weight compared to the starting structure. The evolution of a lower molecular weight fragment hit may represent an attractive approach to optimisation. Computational chemistry can play an important role in evolution of a drug-like molecule from a fragment hit, both with and without the available fragment-target co-complex structure.

12:00 pm Entropy, Solvation and Strain Energy – the Stumbling Blocks in Binding Free Energy Calculations
Enrico O. Purisma, Ph.D., Group Leader, Computational Chemistry & Bioinformatics, Biotecnology Research Institute, National Research Council of Canada
An accurate and robust scoring/free energy function is essential for virtual screening and structure-based drug optimization. Entropy, solvation and strain energy are three critical components of binding free energies in protein-ligand complexes. The challenge is to incorporate these terms in an energy function without introducing more noise that drowns out the signal. In this talk, we will examine the magnitude of the contribution of these components to binding free energies. We will describe the use of exhaustive docking to build up a partition function for predominant states. We will illustrate the use of continuum electrostatics and continuum van der Waals methods for solvation contributions.

12:30 Luncheon Technology Presentation (Opportunity Available) or Lunch on Your Own
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SBDD and Computational Chemistry Methods: A Marriage of Innovation

1:25 Chairperson’s Remarks
Tomi Sawyer, Ph.D., Chief Scientific Officer, ALLERON Therapeutics; Editor-in-Chief, Chemical Biology & Drug Design

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Methods for Structure-Based Scaffold Replacement
Paul Labute, Ph.D., President, Chemical Computing Group (CCG)
Small molecule scaffold replacement techniques are an important part of drug discovery because of the need to find rapid “follow-on” compounds or alternate series. Fragment-based drug discovery techniques also benefit from scaffold replacement methods because of the need to link fragments that bind to a receptor. We present methods for structure-based scaffold replacement that combine techniques from pharmacophore discovery and ligand-receptor docking. Strategies for the creation of 3D virtual fragment databases are discussed as well as the results of computational experiments.

2:00 Application of Free Energy Perturbation Calculations in Drug Discovery
Woody Sherman, Ph.D., Director Applications Science, Schrodinger Inc.
The accurate prediction of binding free energies has been a primary objective for computational methods since the inception of molecular modeling and computer-aided drug design. In this work we describe a large-scale free energy perturbation (FEP) project designed specifically to make FEP practical in drug discovery. We first describe validation of the methodology using the Desmond molecular dynamics program and the OPLS force field by computing absolute and relative solvation free energies of a diverse set of small molecules. We then present a large set of pharmacologically relevant targets and compounds that are being used for the prediction of relative binding free energies. Finally, we present preliminary results for relative binding free energy predictions and discuss the implications for FEP in drug discovery.

2:15 Networking Refreshment Break, Break and Exhibit Viewing

3:00 Structure-Based and Ligand-Based Computational Modeling of Pharmacological Profiles
Ajay N. Jain, Ph.D., Professor, Cancer Research Institute & Department of Lab Medicine, University of California San Francisco
The current state-of-the-art in drug discovery is largely dominated by incremental advances, with me-too drugs forming a very substantial fraction of the small molecule therapeutics market. Such drugs frequently yield no practical benefits in terms of therapy. Apart from drugs that target rapidly evolving organisms, justification for me-too design is problematic outside of narrow economic grounds. Coupled with a shifting regulatory environment that is changing the economic arguments, the need for truly novel drugs is increasingly apparent. This offers an opportunity for computational methods to have a larger impact than has been the historical norm. A central intellectual challenge is that complex issues involving human inductive bias over the course of drug design history make it difficult to demonstrate the success of computational approaches. Despite the challenges, computational approaches can yield predictive models that support design of novel therapeutics. A unified approach to addressing protein-structure based modeling (docking) as well as ligand-based modeling will be presented.

3:30 Protein-Ligand Docking against Non-Native Protein Conformers
Marcel Verdonk, Ph.D., Director, Computational Chemistry & Informatics, Astex Therapeutics, Ltd.
Docking performance is mostly measured against native protein conformers, i.e., each ligand is docked into the protein conformation from the structure that contained that ligand. In real-life applications, however, ligands are docked against non-native conformations of the protein, i.e., the apo structure or a structure of a different protein-ligand complex. We will present the construction of an extensive test set of non-native protein conformers for a range of drug targets. In addition, we will discuss the effects of docking against non-native protein conformations on docking performance, as well as the usefulness of multiple-conformer docking protocols.
• Definitive insights into
  • Performance of rigid-protein docking against non-native protein conformations
  • Performance of multiple protein conformer docking protocols
• Insights into the unique informatics set-up at Astex

4:00 Binding Site Detection and Druggability Index from First Principles
Xavier Barri, Ph.D., ICREA Research Professor, Fisicoquimica, Facultat de Farmacia, Universitat de Barcelona
Both X-ray crystallography and NMR experiments have demonstrated that small organic solvents can be used to identify specific binding sites on protein surfaces. This effect is reproduced using molecular dynamics with an explicit solvent mixture, which gives us direct access to interaction free energies between the protein and small organic molecules. On a set of proteins of pharmacological interest, we show that the method can detect not only typical small-molecule binding sites, but also protein-protein and low affinity binding sites. Furthermore, by adding the interaction free energy of organic solvent binding sites that cluster together, it is possible to predict the maximal affinity that a drug-like molecule could attain, thus providing a measure of druggability.

4:30 Closing Remarks

4:45 pm Close of Conference

Image Courtesy of: ARIAD Pharmaceuticals and University of Basel/Biographics Laboratory 3R
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