REGISTER BY MARCH 15
FOR MAXIMUM SAVINGS!

CLICK HERE TO REGISTER ONLINE!

Organized by
Cambridge Healthtech Institute

CAMBRIDGE HEALTHTECH INSTITUTE'S EIGHTH ANNUAL

Drug Discovery Chemistry

REGISTER BY MARCH 15 FOR MAXIMUM SAVINGS!

APRIL 16-18, 2013
HILTON SAN DIEGO RESORT & SPA · SAN DIEGO, CA

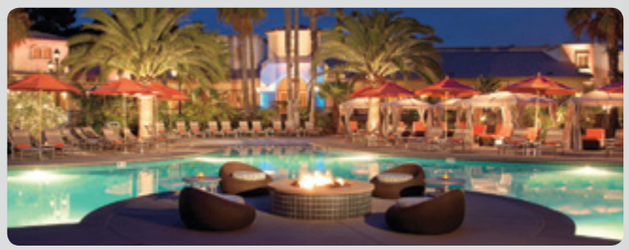
OPTIMIZING SMALL MOLECULES FOR TOMORROW'S THERAPEUTICS

NOBEL LAUREATE PLENARY KEYNOTE
APRIL 16 • 4:30PM
Jack W. Szostak, Ph.D.,
Investigator, Howard Hughes Medical Institute;
Professor of Genetics, Harvard Medical School

SYMPOSIA
Antiviral Drug Discovery
Small Molecule Candidates to Combat Human Viral Infections

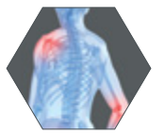
Property-Based Drug Design
Improving the Drug Discovery Process by Optimizing Bio-Physical Properties

EVENT FEATURES
More than 100 Technical Presentations
10 Short Courses
Exclusive Exhibit & Poster Viewing Hours
Interactive Roundtable, Breakout & Panel Discussions
30+ Scientific Posters
400 High-Level Participants
Dedicated Networking Opportunities

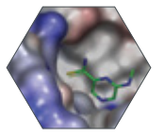


HILTON SAN DIEGO RESORT & SPA • SAN DIEGO, CA

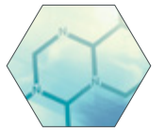
APRIL 16-17



4TH ANNUAL
Anti-Inflammatories

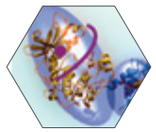


8TH ANNUAL
Fragment-Based Drug Discovery

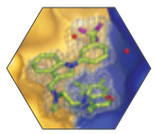


INAUGURAL
Constrained Peptides and Macrocyclics Drug Discovery

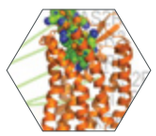
APRIL 17-18



4TH ANNUAL
Kinase Inhibitor Chemistry



6TH ANNUAL
Protein-Protein Interactions



INAUGURAL
GPCR-Based Drug Design

DrugDiscoveryChemistry.com

REGISTER BY MARCH 15 FOR MAXIMUM SAVINGS!

CLICK HERE TO REGISTER ONLINE!

Organized by Cambridge Healthtech Institute

CONFERENCE-AT-A-GLANCE

MONDAY, APRIL 15	SYMPOSIA: ANTI-VIRAL DRUG DISCOVERY	SYMPOSIA: PROPERTY-BASED DRUG DESIGN	SHORT COURSES
TUESDAY, APRIL 16	ANTI-INFLAMMATORIES	FRAGMENT-BASED DRUG DISCOVERY	CONSTRAINED PEPTIDES AND MACROCYCLICS DRUG DISCOVERY
	COMBINED PLENARY SESSION		
	WELCOME RECEPTION IN THE EXHIBIT HALL WITH POSTER VIEWING		
WEDNESDAY, APRIL 17	CONTINENTAL BREAKFAST & BREAKOUT DISCUSSIONS (IN SESSION ROOMS)		
	ANTI-INFLAMMATORIES	FRAGMENT-BASED DRUG DISCOVERY	CONSTRAINED PEPTIDES AND MACROCYCLICS DRUG DISCOVERY
	KINASE INHIBITOR CHEMISTRY	PROTEIN-PROTEIN INTERACTIONS	GPCR-BASED DRUG DESIGN
	DINNER SHORT COURSES		
THURSDAY, APRIL 18	KINASE INHIBITOR CHEMISTRY	PROTEIN-PROTEIN INTERACTIONS	GPCR-BASED DRUG DESIGN
	WALK AND TALK LUNCHEON IN THE EXHIBIT HALL WITH POSTER VIEWING		

CORPORATE SPONSORS

Chemical Computing Group · LipoScience · Schrödinger · selcia

For sponsorship and exhibit information, please contact:
Suzanne Carroll, Senior Business Development Manager • 781-972-5452 • scarroll@healthtech.com

LEAD SPONSORING PUBLICATIONS:

Bio-IT World · nature · The Scientist · Science AAAS · GEN Genetic Engineering & Biotechnology News

ADDITIONAL MEDIA PARTNERS:

Bentham Science · BioSpace.com · Combinatorial Chemistry & High Throughput Screening www.bscipubl.demon.co.uk/cchts · Current Medicinal Chemistry · ddn · pharmaphorum · PharmaVOICE · www.PharmCast.com – Pharmaceutical Internet – · San Jose biocenter · SelectScience · SYNFACTS · SYNLETT · SYNTHESIS · Thieme Chemistry

REGISTER BY MARCH 15 FOR MAXIMUM SAVINGS!

CLICK HERE TO REGISTER ONLINE!

Organized by Cambridge Healthtech Institute

WELCOME
TO DRUG DISCOVERY CHEMISTRY

Cambridge Healthtech Institute's Drug Discovery Chemistry, now in its eighth year, is one of the few conferences geared towards medicinal chemists working in pharma and biotech. This four day event, focused on discovery and optimization challenges of small molecule drug candidates, offers many exciting opportunities for scientists to create a unique program according to personal interests.

New this year are two meeting tracks ("Constrained Peptides and Macrocyclics" and "GPCR-Based Drug Design") that represent areas of chemistry where new advances and technologies are leading to renewed interest. They nicely complement our most popular meetings from the past few years (Anti-Inflammatories, Fragment Based Drug Design, Kinase Inhibitor Chemistry and Protein-Protein Interactions).

To make the event even more cohesive but without leaving anyone's core focus out, we are offering two full day pre-conference symposia (Property-Based Drug Design and Antivirals). We have also expanded our scope by including more short courses to cover the specific therapeutic areas and approaches that many chemists find themselves moving towards or needing updated knowledge about.

We invite you to peruse this brochure to see for yourself the exciting science that is in store for you. Attendees' learning opportunities are not limited to the scientific and technology talks. Our audience and speakers participate in informal roundtable breakout sessions and expert panel discussions as part of the regular meeting tracks and discovery scientists at all levels and from different types of settings are able to interact with each other when the individual tracks join for poster and coffee breaks in the exhibit hall.

We look forward to meeting you in San Diego,

Margit Eder, Ph.D.
Conference Director

Anjani Shah, Ph.D.
Conference Director

NOBEL LAUREATE PLENARY KEYNOTE:

mRNA Display: From Basic Principles to Macrocycle Drug Discovery

Jack W. Szostak, Ph.D., Investigator, Howard Hughes Medical Institute; Professor of Genetics, Harvard Medical School; Alex Rich Distinguished Investigator, Department of Molecular Biology and the Center for Computational and Integrative Biology, Massachusetts General Hospital.

Dr. Szostak received the 2009 Nobel Prize in Physiology or Medicine for his fundamental contributions to our understanding of telomere structure and function, and the role of telomere maintenance in preventing cellular senescence. Dr. Szostak's early research on the genetics and biochemistry of DNA recombination led to the double-strand-break repair model for meiotic recombination. In the 1990s, Dr. Szostak and colleagues developed in vitro selection as a tool for the isolation of functional RNA, DNA and protein molecules from large pools of random sequences. His laboratory has used in vitro selection and directed evolution to isolate and characterize numerous nucleic acid sequences with specific ligand binding and catalytic properties.

Dr. Szostak is a member of the National Academy of Sciences and a Fellow of the New York Academy of Sciences, the American Academy of Arts and Sciences, and the American Association for the Advancement of Science. Dr. Szostak has published over 200 scientific papers and has been awarded 15 US patents.

REGISTER BY MARCH 15 FOR MAXIMUM SAVINGS!

CLICK HERE TO REGISTER ONLINE!

Organized by
Cambridge Healthtech Institute

One-Day Symposia*

April 15

INAUGURAL SYMPOSIUM • APRIL 15, 2013 - APRIL 15 - 8:30 AM-4:30 PM

Antiviral Drug Discovery

This one-day symposium will bring together medicinal chemists who discover and develop new antiviral therapies. With the world becoming a smaller place, viral infections once contained to specific areas are now more wide-spread, increasing the need for novel therapies to combat once-rare viral infections. Thus, in addition to following the promising progress of new all-oral combination therapies to combat HCV, the meeting will also focus on treatments for human-targeted viruses that represent emerging unmet medical needs.

Discovery of GS-9620, an Oral TLR-7 Agonist for the Treatment of Hepatitis B Infection
Randall Halcomb, Ph.D., Director, Medicinal Chemistry, Gilead Sciences

Hepatitis C Anti-virals (tentative talk title)
John Howe, Ph.D., Senior Scientist, Anti-virals, Merck Research Laboratories

Developing Antivirals for Emerging Disease
Dennis E. Hruby, Ph.D., CSO, Siga Technologies

Development of Smallpox Antiviral Drugs in the Post-Eradication Era
Robert Jordan, Ph.D., Director, Biology, Gilead Sciences

Challenges in RSV Drug Discovery
(tentative talk title)
Kelli Kuhen, Ph.D., Senior Research Investigator, Antivirals, Novartis

Panel Discussion: Future Directions in Antiviral Research
Moderator: Christy Hebner, Ph.D., Research Scientist II, HCV Clinical Virology, Gilead Sciences, Inc.

- With effective antivirals on the market for management of HIV and HBV and additional promising treatments to cure HCV likely to hit the market soon, what do you foresee as the next major target(s) for antiviral research?
- Does pursuing viruses affecting smaller populations or the third-world change the way we perform antiviral drug discovery research? If so, how?
- What do you foresee as the role of small molecules, biologics, and vaccines in the future of antiviral therapies?
- Predictions—the next big antiviral breakthrough?

SECOND ANNUAL SYMPOSIUM • APRIL 15 • 8:30 AM - 4:30 PM

Property-Based Drug Design

Hybrid Inverse-QSAR: A Novel Approach for Determination of Optimum Values of Descriptors
Vijay Masand, Ph.D., Assistant Professor, Department of Chemistry, Vidya Bharati College

A Rationally-Designed Polypharmacy Drug Discovery Project in Schizophrenia Using a Quantitative Systems Pharmacology Approach
Hugo Geerts, Ph.D., CSO, Computational Neuropharmacology, In Silico Biosciences

***In silico* Method for Predicting Ames Activities**
Jörg Bentzien, Ph.D., Scientist, Boehringer Ingelheim Pharmaceuticals, Inc.

Interpreting Data
Terry Stouch, Ph.D., President, R&D, Science for Solutions, LLC

Panel Discussion: Considering Physicochemical Properties

- What drug properties are essential and when should they be determined?
- *In silico* vs experiment – is one set of data sufficient?
- Hydrophobicity in drug discovery – measurement or calculation?
- What's next for predictive methods?

**Separate registration is required*

Symposia and Pre-Conference Workshops
Sponsorship Opportunity

Includes 15-minute or 30-minute podium presentation during the symposia or pre-conference workshop, as well as your company logo displayed on marketing materials and on-site signage. Please contact Suzanne Carroll at 781-972-5452 or at scarroll@healthtech.com for details.

REGISTER BY MARCH 15 FOR MAXIMUM SAVINGS!

CLICK HERE TO REGISTER ONLINE!

Organized by Cambridge Healthtech Institute

Short Courses*

**Separate registration is required*

MONDAY, APRIL 15 • 8:00-11:00 AM

Molecular Interactions and Drug Design

Tutor: Kent Stewart, Ph.D., Senior Research Fellow, Abbott Laboratories

This course provides an overview of protein-ligand interactions and drug design principles. The presentation is targeted to medicinal chemists. Part 1 covers hydrophobic, H-bonding and electrostatic interactions; Part 2 covers specialized topics such as conformation analysis, pi-stack, cation-pi, halogen bonding, protein-protein interface, and covalent inhibition. Medchem case studies are incorporated.

- Learn drug design principles generally applicable to all medchem programs.
- Interpret atomic-level protein X-ray and modeled structures of binding modes.
- Understand the relative amounts of potency gain from different interactions.
- Case studies illustrate all of the design strategies.

An Intro to the Field of Antibody-Drug Conjugates

Tutor: Ho Sung Cho, Ph.D., Chief Technical Officer, Ambrx

ADCs are an emerging modality in cancer. This course will give you an overview of the current advances being made in the clinic, review the design of novel payloads and linkers, and discuss some of the challenges being faced in developing future linkers and cytoxic drugs.

- Design of novel linkers, payloads and ADC's for Cancer
- Innovative chemistry strategies for ADC discovery
- Design, synthesis, and characterization of small molecule antibody therapeutics

MONDAY, APRIL 15 • 12:00 - 3:00 PM

Advancing Tools and Technologies for Fragment-Based Design

Tutor: Daniel A. Erlanson, Ph.D., Co-Founder, Carmot Therapeutics, Inc.

This short course will cover the basic ideas behind fragment discovery, outline the major tools for discovering fragments and provide case studies in the optimization of fragments to drug leads.

Immunology Basics for Chemists

Tutor to be Announced

- Review of inflammatory process and significant cellular and molecular players
  - cytokine biology
  - receptor pathways
- Autoimmune and Inflammation-related diseases
  - Which are most prevalent? Which have the greatest need for new therapies?
  - Underlying biologic defects
  - Associated targets and their place in signal transduction pathways
- Current treatment landscape
  - Review of current state of anti-cytokine therapies (mostly biologics)
  - Biologics v. Small Molecules
  - What's on the Horizon
  - What is needed

MONDAY, APRIL 15 • 3:30 - 6:30 PM

Enabling Macrocyclic Compounds for Drug Discovery: Opportunities, Challenges and Strategies

Tutor: Mark L. Peterson, Ph.D., Vice President, Operations, Tranzyme Pharma

Macrocyclic compounds fill an important chemical space between small molecules and biologics. This course will discuss the recent developments in the field of macrocycle synthesis and screening, as well as specific aspects of these compounds for drug discovery and development purposes. Topics to be Covered:

- Unique characteristics of macrocycles
- The challenges of macrocycle synthesis and screening
- Current methods for synthesizing and screening macrocyclic compound libraries
- Pros and cons of each methodology
- Drug discovery and development considerations for macrocyclic molecules
- Examples in the discovery of bioactive synthetic macrocycles
- Remaining challenges and possible solutions

Influencing Stem Cell Differentiation

Tutor to be Announced

Topics to be Covered:

- High-throughput screening
- Screening for compounds that allow stem cells to grow
- The physical and chemical influence of compound structures on stem cell differentiation
- Identifying small molecules that selectively promote ESC differentiation

Introduction to Allosteric Modulation of GPCRs

Tutor: Karen J. Gregory, Ph.D., Post-Doctoral Fellow, Jeffrey Conn Laboratory, Pharmacology, Vanderbilt University

Quantifying allosteric modulation

- Binding vs functional assays
- HTS and *in vitro* strategies
- *In vivo* experimental design

Complexities and challenges

- What to optimize for?
- Molecular switches and flat/steep SAR
- Modulation bias & context dependent pharmacology
- Multiple allosteric sites
- Probe dependence
- Some GPCRs are functional heterodimers

How can structural information aid modulator drug discovery?

- Mechanism validation (orthosteric, allosteric or bitopic?)
- Inform SAR
- Identify novel binding sites
- Virtual ligand screening

WEDNESDAY, APRIL 17 DINNER COURSES • 6:30 - 9:00 PM

Practical Aspects of Structure-Based Drug Discovery with GPCRs

Tutors: Robert Cooke, Ph.D., Head, Biomolecular Structure Department, Heptares
Michael Hanson, Ph.D., Director, Structural Biology, Receptos

- The quality of structures that can be expected and what can be done with the data.
- Expected throughput and turnaround times
- Working with fragments
- Dealing with conformational states
- Impact on modeling activities
- Comparison with more established SBDD efforts (eg kinases)
- Incorporating data from purified protein assays
- A couple of case studies covering the process

Epigenetic Targets: Chemical Tools

Tutors to be Announced

This course will focus on what a chemist needs to know regarding epigenetic targets. It will start with a biology review of epigenetic modifications and then address challenges in designing probes and inhibitors for various EPG modifiers. Issues such as optimizing compounds for selectivity, potency and avoidance of toxicity will also be covered.

- Targeting Histone Methyl Transferases (HMTs)
- Inhibiting Demethylases (DMTs)
- Designing Histone Deacetylase Inhibitors (HDACi)
- Bromodomain and extra-terminal (BET) proteins

TUESDAY, APRIL 16

Scientific Advisor: Martin Braddock, Ph.D., Senior Principal Scientist, Inflammation, Neuroscience and Respiratory Global Medicines Development, AstraZeneca

7:00 am Registration and Morning Coffee

BTK and JAK Inhibitors for Inflammation

8:00 Chairperson's Opening Remarks

» 8:10 FEATURED PRESENTATION

Targeted Covalent-Reversible Inhibitors for Bruton's Tyrosine Kinase

Suvit Thaisrivongs, Ph.D., Executive Director, Chemistry, Pfizer

One strategy for optimizing pharmacological potency and selectivity for a number of challenging targets is to engage the non-catalytic cysteine residues with covalent inhibitors. Moreover, the utilization of a covalent inhibitor that reversibly forms an adduct is attractive as it may provide the pharmacodynamic benefit with reduced liability of long-lived irreversible protein adducts. Structure-based design led to the discovery of such a class of inhibitors for BTK. The optimized compound has been shown to be efficacious in several pre-clinical animal models of arthritis and autoimmune diseases. This offers promise as a therapeutic candidate for the treatment of autoimmune and inflammatory diseases.

8:50 Design and Characterization of Targeted Covalent Inhibitors of BTK

C. Eric Schwartz, Ph.D., Senior Director, Chemistry, Celgene Avilomics Research

One strategy for optimizing pharmacological potency and selectivity for a number of challenging targets is to engage the non-catalytic cysteine residues with covalent inhibitors. Moreover, the utilization of a covalent inhibitor that reversibly forms an adduct is attractive as it may provide the pharmacodynamic benefit with reduced liability of long-lived irreversible protein adducts. Structure-based design led to the discovery of such a class of inhibitors for BTK. The optimized compound has been shown to be efficacious in several pre-clinical animal models of arthritis and autoimmune diseases. This offers promise as a therapeutic candidate for the treatment of autoimmune and inflammatory diseases.

9:20 Potential of Selective BTK Inhibitors for Treating Autoimmune Diseases

Daigen Xu, M.D., Ph.D., Research Leader, Inflammation Discovery, Hoffman La-Roche

BTK may contribute to the development of autoimmune diseases by mediating the production and effector function of (auto)antibodies. Consistently, a selective and reversible BTK inhibitor produces efficacy in models of rheumatoid arthritis and systemic lupus erythematosus. The data provide a proof-of-concept for developing BTK inhibitors as therapeutics for these diseases.

9:50 Networking Coffee Break

10:15 BTK Inhibitor

Longcheng Wang, Ph.D., Pharmacyclics

10:45 Discovery and Optimization of Selective JAK1 Inhibitors as Potential Treatments for Rheumatoid Arthritis

Mark Zak, Ph.D., Scientist, Discovery Chemistry, Genentech

JAK1 inhibitors exhibiting selectivity over JAK2 may hold the potential to maximize therapeutic efficacy against RA and other immune disorders, while minimizing unwanted anemia. Our strategies to identify selective and orally bioavailable JAK1 inhibitors will be presented, and the preclinical characterization of the lead molecule will be described.

11:15 Sponsored Presentation *(Opportunity Available)*

11:45 Luncheon Presentation *(Sponsorship Opportunity Available)* **or Lunch on Your Own**

1:00 pm Session Break

Macrocyclics (Mostly) and Inflammation

1:25 Chairperson's Remarks

1:30 Discovery and Characterization of JAK1 Selective Macrocycles from a Cell-Based HTS Campaign

Jennifer Venable, Ph.D., Principal Scientist, Immunology Chemistry, Janssen Research & Development, LLC

2:00 Apremilast, a Targeted PDE4 Inhibitor in Development for Psoriatic Arthritis, Psoriasis, and Other Inflammatory Conditions

Peter H. Schafer, Ph.D., Senior Principal Investigator, Translational Development, Celgene Corporation

A premilast is an oral small molecule specific inhibitor of PDE4 with promising clinical efficacy in psoriasis and psoriatic arthritis. The expression of PDE4 in psoriatic skin and arthritic synovium, and the effects of apremilast on synovial fibroblasts, osteoclasts, osteoblasts, and osteocytes will be presented.

2:30 Nanocyclix: Potent and Selective Inhibitors for Novel Kinases in Cancer, CNS, Inflammation and Metabolic Diseases

Jan Hoflack, Ph.D., Head, Drug Discovery, ONCODESIGN Biotechnology

The Nanocyclix platform consists of low molecular weight macrocyclic kinase inhibitors that are exquisitely selective due to a high degree of shape complementarity with the ATP binding pocket. Multiple "First in Class" opportunities will be described in different therapeutic areas and will include detailed structural information on binding modes and selectivity generation.

3:00 Sponsored Presentation *(Opportunity Available)*

3:15 Refreshment Break in the Exhibit Hall with Poster Viewing

4:00 Macrocycles for Drug Discovery - Identification of Small Molecule Synthetic Macrocycle Antagonists of Human IL17A

Nick Terrett, Ph.D., CSO, Ensemble Therapeutics Corporation

Ensemble Therapeutics has developed a DNA-programmed chemistry platform for the rapid synthesis and screening of macrocycles (Ensemblins™). Using this platform, small molecule macrocyclic

NEXT

compounds have been discovered that are nanomolar inhibitors of the interaction of the IL17A cytokine with its receptor. These compounds are anti-inflammatory in IL17-dependent animal inflammatory models and optimized for oral bioavailability.

» 4:30 PLENARY KEYNOTE

mRNA Display: From Basic Principles to Macrocycle Drug Discovery

Jack W. Szostak, Ph.D., Investigator, Howard Hughes Medical Institute; Professor of Genetics, Harvard Medical School; Nobel Laureate

The covalent attachment of a nascent protein or peptide to its own mRNA allows the *in vitro* selection of functional proteins and peptides from large libraries. This approach has recently been extended to the *in vitro* selection of highly modified cyclic peptides, a promising class of therapeutic agents.

5:30 Welcome Reception in the Exhibit Hall with Poster Viewing

6:30 End of Day

7:00 - 10:00 Complimentary Shuttle Bus Roundtrips to Downtown San Diego, Courtesy of Hilton San Diego Resort & Spa

WEDNESDAY, APRIL 17

7:45 am Continental Breakfast Breakout Discussions

In this interactive session, several topics will be offered for discussions and delegates are invited to choose a topic of interest and join the moderated discussion at hand. In this informal setting, participants are encouraged to share examples from their work, vet ideas with peers and be part of a group problem-solving endeavor. We emphasize that this is an informal exchange amongst scientists and is not meant to be, in any way, a product promoting session.

New Targets and Approaches for Inflammation

8:55 Chairperson's Opening Remarks

9:00 Anti-Chemokine Neutraligands as Potential Anti-inflammatory Drugs: From *in vitro* to *in vivo* Studies

Jean-Luc Galzi, Ph.D., Professor, Biotechnology and Cellular Signaling, University of Strasbourg

The discovery and use of small chemical compounds targeting chemokines -or neutraligands- will be described within the scope of anti-inflammatory therapeutic research. The potency of these chemokine neutralizing compounds in airway inflammation will be presented, illustrating new concepts in allergic disease treatment. The generality of the concept will be discussed.

9:30 Restoration of Phagocytic Function in Gaucher Macrophages by Non-Inhibitory Small Molecule Chaperones

Samarjit Patnaik, Ph.D., Research Scientist, National Center for Advancing Translational Sciences, NIH

Gaucher disease is a rare genetic disorder caused by lack of glucocerebrosidase enzymatic activity. This leads to pronounced lysosomal substrate storage and impaired function in macrophages, the crucial sentinel cells that initiate acute inflammation. We demonstrate effective reversal of disease phenotypes in advanced cellular models with non-inhibitory small molecule chaperones.

10:00 Coffee Break in the Exhibit Hall with Poster Viewing

10:45 Discovery of Lesinurad, a URAT1 Inhibitor in Clinical Development for the Treatment of Gout

Jean-Luc Girardet, Ph.D., Vice President, Chemistry & Development Support, Ardea Biosciences, Inc.

Lesinurad is currently being developed for the treatment of hyperuricemia in gout patients. This molecule acts by inhibiting the reabsorption of uric acid in the kidney. It is being studied in phase 3 as combination therapy with xanthine oxidase inhibitors which reduce the production of serum uric acid.

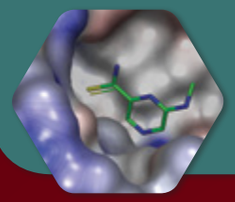
11:15 Targeted Peptide Nanomedicine for Rheumatoid Arthritis

Hayat Onyuksel, Ph.D., Professor, Biopharmaceutical Sciences, University of Illinois at Chicago

Vasoactive intestinal peptide (VIP) is an endogenous neuropeptide with demonstrated anti-inflammatory activity. However, its intravenous use is limited due to its very short half life. We have developed a targeted, stable and safe nanomedicine of VIP using phospholipid micelles, and showed its high activity with no side effects on an animal model of RA.

11:45 End of Conference

BACK



TUESDAY, APRIL, 16

7:00 am Registration and Morning Coffee

8:00 Chairperson's Opening Remarks

Roderick E. Hubbard, Ph.D., Senior Fellow, Vernalis (R&D) Ltd.; Professor, University of York, UK

» 8:10 KEYNOTE PRESENTATION

Alex MacKerell, Ph.D., Grollman-Glick Professor of Pharmaceutical Sciences; Director, Computer-Aided Drug Design Center School of Pharmacy University of Maryland

Using FBDD for Protein-Protein Interactions

8:50 Fragment-Based Approaches Targeting Protein-Protein Interactions

Richard Taylor, Ph.D., Principal Scientist, CADD, UCB

We will demonstrate an analysis of fragment hit rates against a range of novel Protein-Protein Interaction targets, using one of the largest fragment collections in the industry. We will show how this information can be used to guide the library design and the overlap with drug-like properties. Furthermore, some of the common problems associated with PPI targets and fragments will be discussed, and how the use of antibodies can overcome some of these issues.

9:20 Strategies for Fragment Evolution

Roderick E. Hubbard, Ph.D., Senior Fellow, Vernalis (R&D) Ltd.; Professor, University of York, UK

It is relatively straightforward to find fragments that bind to most proteins. The challenge is what to do with them, which to choose and how to evolve to higher affinity hits. I will discuss some new ideas which allow rapid and efficient exploration of the SAR attainable from fragment starting points and also summarise some recent experiences in using these and other techniques for developing leads against challenging targets.

9:50 Networking Coffee Break

Optimizing Hit-to-Leads

10:15 Fragment-Based Drug Design Using Molecular Dynamics

David Soriano del Amo, Ph.D., Head, Med. Chemistry, Acelelra Ltd.

Fragment-based drug design (FBDD) is an established method in drug discovery. *In silico* methods are a natural complement for biophysical assays and a variety of different approaches have been explored. In this study we apply recent advances in high-throughput molecular dynamics to assess the effectiveness of this simulation technique in selecting hits from a fragment library and predicting binding modes and affinities. A small 34-element fragment library was screened for binding to human factor Xa, using unbiased all-atom molecular dynamics simulations (Amber 99SB force field and ACEMD) performed at high ligand concentration and physiological conditions. The resultant trajectories were analyzed for fragment-protein interaction. Predicted hits compared favorably with a prior experimental assay using saturation transfer difference NMR spectroscopy.

10:45 19F NMR Spectroscopy as a General Approach for Fragment Screening

Brad Jordan, Ph.D., Senior Scientist, Molecular Structure and Characterization, Amgen

Most NMR-based fragment screening methods make use of 1H NMR. Here, a more general use of 19F NMR-based fragment screening will be demonstrated in several areas: as a key tool for rapid and sensitive detection of fragment hits, as a method for the rapid development of SAR on the hit-to-lead path using in-house libraries and/or commercially available compounds, and as a quick and efficient means of assessing target druggability.

11:15 Rationalizing Non-Standard Interactions in Ligand Design: The Duality of Halogens

Sponsored by CHEMICAL COMPUTING GROUP

Chris Williams, Ph.D., Principal Scientist, Chemical Computing Group

Non-standard intermolecular interactions have been recognized as significant factors in protein-ligand binding, but their exploitation in ligand design can been difficult, because they are inadequately modeled using molecular mechanics based methods. Here we propose a model of intermolecular interactions based on Extended Hückel Theory (EHT), which accounts for electronic effects on interaction strength. The qualitative and semi-quantitative accuracy of the model is demonstrated using case studies that highlight the importance of these interactions.

11:45 Luncheon Presentation *(Sponsorship Opportunity Available)* **or Lunch on Your Own**

1:00 pm Session Break

Computational Approaches and Library Design

1:25 Chairperson's Remarks

Edward T. Zartler, PhD, President & CSO, Quantum Tessera Consulting

1:30 "Fat, Drunk, and Stupid is No Way to Go through Life": (Re)Thinking Fragment Libraries

Edward T. Zartler, Ph.D., President, CSO, Quantum Tessera Consulting

Conventional thinking about fragment libraries tends to focus on size, partitioning in alcohol (clogP), and exploring a small portion of chemical space. This talk will present new points of view in regards to the size of molecules, solubility, and how best to interrogate 2D and 3D space.

2:00 DNA-Encoded Chemical Libraries for Fragment-Based Drug Discovery

Joerg Scheuermann, Ph.D., Senior Scientist, MoB, Pharmaceutical Sciences, ETH Zurich

In the implementation of Encoded Self-Assembling Chemical ("ESAC")-libraries, low-molecular weight compounds (fragments) are displayed on the 5′ and 3′ ends of DNA heteroduplexes which are formed upon hybridization of two small sized complementary DNA-encoded fragment sublibraries, thus yielding a large combinatorial library. Using these libraries for affinity-based selections enables the discovery of pairs of simultaneously binding fragments, which can subsequently be tested on DNA using standard techniques (e.g. SPR) and converted to high-affinity binders without DNA. The technology is perfectly suited for fragment-based lead-discovery and lead expansion (affinity maturation) of existing leads and case stories will be described.

2:30 Chemistry is the Key: Expanding the Diversity of Fragment Screening Libraries

Justin Bower, Ph.D., Head, Chemistry, Drug Discovery Programme, The Beatson Institute for Cancer Research

The target agnostic design of fragment libraries lends itself to screening against a range of potential targets and the gain in understanding of

NEXT

Organized by
Cambridge Healthtech Institute

how PPI's exert their biological effects coupled with developments in structural biology, biophysical screening technologies and computational disciplines is increasingly bringing this class of target within the range of Fragment-Based Drug Design. This talk will explore the potential of using fragment -based methods to unearth hits against PPI's, detailing a discussion on fragment library composition along with suggestions of how future, more structurally diverse fragments which occupy different regions of chemical space to the vast majority of current fragment libraries can be designed and selected.

Sponsored by selcia

3:00 Successful Identification of Validated Fragment Hits Using Affinity Capillary Electrophoresis (ACE)

Carol Austin, Ph.D., Biology Group Leader, Selcia Ltd

ACE, in combination with the Selcia's fragment library, has been successfully used to identify fragment hits from different targets. The majority of hits have been validated using orthogonal techniques indicating a low false positive rate. The microscale technique does not require tethering of the target and is not dependent on protein size or high purity.

3:15 Refreshment Break in the Exhibit Hall with Poster Viewing

4:00 Impact of Novel Computational Approaches on Prospective FBDD Projects: From Screening Campaigns to *de novo* Design

Julen Oyarzabal, Ph.D., Director, Small Molecule Discovery Platform, Ctr for Applied Medical Research (CIMA), University of Navarra

I will present the impact of three novel computational approaches on prospective fragment-based drug discovery case studies: i.- Building a focused fragments library for screening campaign ii.- Fragment-hopping strategy to discover novel and chemically feasible scaffolds. iii.- Data mining and visualization tool to identify key fragments (R-groups) as well as ligand-receptor interactions from proprietary DBs, patents, … and transfer this knowledge to novel chemical series.

» 4:30 PLENARY KEYNOTE

mRNA Display: From Basic Principles to Macrocycle Drug Discovery

Jack W. Szostak, Ph.D., Investigator, Howard Hughes Medical Institute; Professor of Genetics, Harvard Medical School; Nobel Laureate

The covalent attachment of a nascent protein or peptide to its own mRNA allows the *in vitro* selection of functional proteins and peptides from large libraries. This approach has recently been extended to the *in vitro* selection of highly modified cyclic peptides, a promising class of therapeutic agents.

5:30 - 6:30 Welcome Reception in the Exhibit Hall and Poster Viewing

7:00 - 10:00 Complimentary Shuttle-Bus Roundtrips to Downtown San Diego, courtesy of Hilton San Diego Resort & Spa

WEDNESDAY, APRIL 17

7:45 am Continental Breakfast Breakout Discussions

In this interactive session, several topics will be offered for discussions and delegates are invited to join the moderated discussion at hand. In this informal setting, participants are encouraged to share examples from their work, vet ideas with peers and be part of a group problem-solving endeavor. We emphasize that this is an informal exchange amongst scientists and is not meant to be, in any way, a product promoting session.

Case Studies

8:55 Chairperson's Opening Remarks

9:00 Talk Title to be Announced

Rommie E. Amaro, Ph.D., Assistant Professor, Department of Chemistry, University of California, San Diego

9:30 Fragment-Based Discovery of Novel, Selective PI3Kβ Inhibitors as Anti-Thrombotic Agents

Fabrizio Giordanetto, Ph.D., Project Leader, Principal Scientist, Medicinal Chemistry, CVGI iMed, AstraZeneca R&D

Structure-based evolution of the original fragment hits coupled with property-based design resulted in the identification of potent, selective Phosphoinositide 3-kinases (PI3K) p110β isoform inhibitors with favourable *in vivo* antiplatelet effect. Despite the antiplatelet action, no significantly increase in bleeding time was observed. Additionally, due to the engineered selectivity over p110β, no insulin resistance was induced.

10:00 Coffee Break in the Exhibit Hall with Poster Viewing

10:45 The *de novo* Fragment-Based Drug Discovery of ITK Inhibitors

Heather Twin, Ph.D., Research Scientist, Vertex Pharmaceuticals

Interleukin-2 inducible T-cell kinase (Itk) is a member of the Tec family of non-receptor protein kinases which plays a central role in T-cell signalling. Inhibition of Itk presents an attractive approach for the treatment of autoimmune and allergic diseases. X-ray crystallography was used to aid the design of a series of potent and selective Itk inhibitors.

11:15 Chiral Amine Fragments for ALS Treatments

Joe Sweeney, Ph.D., Professor of Catalysis and Chemical Biology, Department of Chemistry, University of Huddsfield

This presentation will describe the preparation and screening of chiral amine-containing small molecules with relevance for hypothesis-validation and therapy in amyotrophic lateral sclerosis.

11:45 End of Conference

BACK

Organized by Cambridge Healthtech Institute

TUESDAY, APRIL, 16

Scientific Advisor: Dinesh Patel, Ph.D., CEO, Protagonist Therapeutics

7:00 am Registration and Morning Coffee

Creating Constrained Peptides

8:00 Chairperson's Opening Remarks
Dinesh Patel, Ph.D., CEO, Protagonist Therapeutics

» 8:10 FEATURED PRESENTATION

A Renaissance of Constrained and Macrocyclic Peptide Drug Discovery: Transforming Nature's alpha-Helix into Breakthrough Medicines
Tomi Sawyer, Ph.D., CSO, Aileron Therapeutics

A renaissance of peptide drug discovery is leveraging innovative approaches to create constrained and macrocyclic analogs as novel modulators of extracellular and intracellular targets as well as tackle complex disease mechanisms. As a case study, advancements in stapled peptide technology to transform Nature's alpha-helix into breakthrough medicines will be presented.

8:50 Engineered Knottin Peptides: A New Class of Tumor Targeting and Molecular Imaging Agents
Jennifer Cochran, Ph.D., Associate Professor, Bioengineering, Stanford University

Cystine knot peptides (also known as knottins) are constrained by three interwoven disulfide bonds that confer high chemical, thermal, and proteolytic stability ideal for *in vivo* applications. We used rational and combinatorial methods to engineer knottin peptides that bind with low to sub-nanomolar affinity to tumor-associated receptors. In this talk, the evaluation of engineered knottin peptides in preclinical tumor models and their promise as diagnostic and therapeutic agents will be discussed.

9:20 Constrained Opioid Peptides
Steven Ballet, Ph.D., Research Group of Organic Chemistry, Departments of Bio-Engineering Sciences and Chemistry, Vrije Universiteit Brussel

9:50 Networking Coffee Break

10:15 Oral Disulfide Rich Peptide (DRP) Therapeutics
Dinesh Patel, Ph.D., CEO, Protagonist Therapeutics

10:45 Using Disulfide-Constrained Peptides as Novel Agonists in Protein-Protein Interactions
Sarah Dong, Ph.D., Senior Scientist II, Chemistry Department, Affymax, Inc.

Peptides containing constrained disulfide bonds can display unique conformations allowing them to bind and activate target receptors similar to natural ligands. Examples of novel synthetic peptides that serve as effective agonists of the respective receptors despite having no sequence homology to EPO or G-CSF receptors will be discussed.

11:15 Sponsored Presentation *(Opportunity Available)*

11:45 Luncheon Presentation *(Sponsorship Opportunity Available)* **or Lunch on Your Own**

1:00 pm Session Break

Macrocyclic-Based Drug Candidates

1:25 Chairperson's Remarks

1:30 SOM230: A New Therapeutic Modality for Cushing's Disease
Ian Lewis, Ph.D., Research Chemist, Global Discovery Chemistry, Novartis

SOM230 has recently shown promise as the first effective pituitary directed medical treatment for Cushing's disease. Indeed, the multiple high affinity binding of SOM230 to somatostatin receptor subtypes enables much more effective inhibition of ACTH release *in vitro* and *in vivo*. Recent clinical studies involving treatment of Cushing's disease with SOM230 have demonstrated that SOM230 produced a decrease in urinary free cortisol (UFC) levels in 76% of patients during 15 days, with direct effects on ACTH release, establishing a new therapeutic modality for Cushing's disease.

2:00 Discovery of Stereochemically Complex Macrocyclic Hsp90 Inhibitors
Christoph Zapf, Ph.D., Principal Scientist, Worldwide Medicinal Chemistry, Pfizer

We wish to disclose the design and synthesis of a series of stereochemically complex, rule-of-five compliant small molecule macrocycles that were fine-tuned to be metabolically stable and devoid of hERG activity. The compounds showed impressive biomarker activity 24 hours post dosing in different cell lines. When studied in a lung cancer xenograft model, the macrocycles demonstrated prolonged exposure in tumors and significant tumor size reduction.

2:30 Discovery of TZP-102, a Macrocycle-Based Oral Ghrelin Receptor Agonist and GI Prokinetic Agent for the Treatment of Diabetic Gastroparesis
Helmut Thomas, Ph.D., Senior Vice President, Research and Preclinical Development, Tranzyme Pharma

3:00 Sponsored Presentation *(Opportunity Available)*

3:15 Refreshment Break in the Exhibit Hall with Poster Viewing

4:00 Macrocycles for Drug Discovery - Identification of Small Molecule Synthetic Macrocycle Antagonists of Human IL17A
Nick Terrett, Ph.D., CSO, Ensemble Therapeutics Corp.

Ensemble Therapeutics has developed a DNA-programmed chemistry platform for the rapid synthesis and screening of macrocycles (Ensemblins™). Using this platform, small molecule macrocyclic compounds have been discovered that are nanomolar inhibitors of the interaction of the IL17A cytokine with its receptor. These compounds are anti-inflammatory in IL17-dependent animal inflammatory models and optimized for oral bioavailability.

NEXT

Organized by
Cambridge Healthtech Institute

» 4:30 PLENARY KEYNOTE

mRNA Display: From Basic Principles to Macrocycle Drug Discovery

Jack W. Szostak, Ph.D., Investigator, Howard Hughes Medical Institute; Professor of Genetics, Harvard Medical School; Nobel Laureate

The covalent attachment of a nascent protein or peptide to its own mRNA allows the *in vitro* selection of functional proteins and peptides from large libraries. This approach has recently been extended to the *in vitro* selection of highly modified cyclic peptides, a promising class of therapeutic agents.

5:30 Welcome Reception in the Exhibit Hall with Poster Viewing

6:30 End of Day

7:00 - 10:00 Complimentary Shuttle Bus Roundtrips to Downtown San Diego, Courtesy of Hilton San Diego Resort & Spa

WEDNESDAY, APRIL 17

7:45 am Continental Breakfast Breakout Discussions

In this interactive session, several topics will be offered for discussions and delegates are invited to choose a topic of interest and join the moderated discussion at hand. In this informal setting, participants are encouraged to share examples from their work, vet ideas with peers and be part of a group problem-solving endeavor. We emphasize that this is an informal exchange amongst scientists and is not meant to be, in any way, a product promoting session.

Macrocyclics

8:55 Chairperson's Opening Remarks

9:00 Direct Selection of CyclomimeticsTM from mRNA Display Libraries

Douglas A. Treco, Ph.D., President and CEO, Ra Pharmaceuticals

9:30 Successful Application of Novel Constrained Macrocycles in Drug Discovery

Daniel Obrecht, Ph.D., CSO, Polyphor, Ltd.

PEMfinder® (PEM=Protein Epitope Mimetics) and MacroFinder® are two complementary macrocycle-based platforms (MW= 400-2000) that have been developed by Polyphor as powerful tools to identify potent and selective modulators of intra- and extracellular protein-protein interactions (PPIs).This presentation will describe successful drug discovery case studies of applying PEMfinder® and MacroFinder® from discovery to the clinic.

10:00 Coffee Break in the Exhibit Hall with Poster Viewing

10:45 Targeting Protein-Protein Interactions with Engineered Cyclotides

Julio Camarero, Ph.D., Associate Professor, Pharmacology and Chemistry, University of Southern California

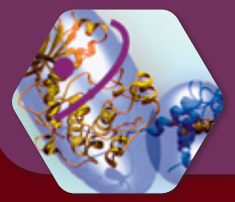
I will present new data on the biosynthesis of cyclotides using bacterial and yeast expression systems for the generation of large genetically-encoded cyclotide-based libraries for high throughput cell-based screening and selection of cyclotides with novel biological activities. We will also report the design and biosynthesis of a MCoTI-grafted cyclotide with the ability to target intracellular and extracellular protein-protein interactions.

11:15 Bi-Cyclic Peptides to Target Endopeptidases

Christophe Bonny, Ph.D., CSO, Bicycle Therapeutics Limited

The Bicycle technology is based on repertoires of peptides displayed on the surface of bacteriophages which can be modified with an organochemical scaffold to create a diverse array of constrained peptides. These repertoires have been extensively used for iterative selections to identify high affinity binding peptides for a wide array of proteases. Results will be presented that exemplify the potential of the technology and its application to animal models of diseases.

11:45 End of Conference



WEDNESDAY, APRIL 17

12:30 pm Registration

Optimizing Selectivity

1:30 Chairperson's Opening Remarks

1:40 Discovery of Highly Potent, Selective and Brain-Penetrable LRRK2 Inhibitors

Anthony Estrada, Ph.D., Scientist, Medicinal Chemistry, Genentech, Inc.

There is a high demand for potent, selective and brain-penetrable LRRK2 inhibitors to test whether inhibition of LRRK2 kinase activity will reduce the rate of disease progression in Parkinson's disease patients (PD) or animal models of PD. Starting from ligand efficient aminopyrimidine LRRK2 inhibitors, a thorough lead optimization process using property and structure-based drug design was executed. High throughput *in vivo* pharmacokinetic profiling enabled rapid validation of *in vitro* permeability and metabolic stability predictions. This resulted in the rapid discovery of inhibitors possessing an ideal balance of LRRK2 cellular potency, broad kinase selectivity, metabolic stability, and brain penetration across multiple species.

2:10 Talk Title to be Announced

Ann Aulabaugh, Ph.D., Senior Scientist, Structural Biology and Biophysics, Pfizer

2:40 Type II Protein Kinase Inhibitors for Increased Biochemical Efficiency and Kinome Selectivity: Experiences with PYK2 and SYK

Seungil Han, Ph.D., Senior Principal Scientist, Pfizer

In our pursuit to develop highly selective protein kinase inhibitors with increased biochemical efficiency in a cellular environment, we embarked on a systematic program to identify and characterize Type II inhibitors for two protein kinases, PYK2 and SYK. Application of different structural biology techniques along with sophisticated computational approaches have led to the identification of 'DFG-out' or 'C-helix-out' inhibitors of PYK2 and SYK. Crystal structures of these kinases with Type II inhibitors reveal the inherent dynamics within the kinase module of PYK2 and SYK that result in novel druggable binding sites outside of their adenine site. I will discuss our experiences in developing selective Type II inhibitors of protein kinases.

3:10 Sponsored Presentation *(Opportunity Available)*

3:40 Refreshment Break in the Exhibit Hall with Poster Viewing

4:20 Cell-Based Kinase Assays in Drug Discovery: Application to Selectivity Analysis and Personalized Medicine

Deborah J. Moshinsky, Ph.D., Founder and President, Cell Assay Innovations, LLC

This talk will focus on specific cellular model systems utilized in kinase drug discovery for potency, selectivity, and mechanism of action analyses. Examples of how these cell-based systems enable more physiologically relevant selectivity assessments will be given. Additionally, application of cellular kinase assays to personalized medicine will be outlined, with a particular emphasis on screening for inhibitors of drug-resistant mutant kinases.

4:50 TRK Selectivity

Thomas Bertrand, Ph.D., LG-CR / Structure Design & Informatics, Sanofi Pasteur (tentative)

5:20 Moderated Breakout Discussions

In this interactive session, several topics will be offered for discussions and delegates are invited to choose a topic of interest and join the moderated discussion at hand. In this informal setting, participants are encouraged to share examples from their work, vet ideas with peers and be part of a group problem-solving endeavor. We emphasize that this is an informal exchange amongst scientists and is not meant to be, in any way, a product promoting session.

6:20 End of Day

6:30 - 9:00 pm Dinner Short Courses *(Separate registration required, see page 3 for details.)*

THURSDAY, APRIL 18

7:45 am Breakfast Workshop Presentation *(Sponsorship Opportunity Available)* **or Morning Coffee**

Exploring the Chemical Space

8:15 Chairperson's Opening Remarks

» 8:20 FEATURED PRESENTATION

The Catalytic Domain of NF-kB Inducing Kinase Adopts an Active Conformation in the Absence of Phosphorylation

Sarah G. Hymowitz, Ph.D., Director, Department of Structural Biology, Genentech, Inc.

To better understand molecular basis of NF-kB inducing kinase (NIK) activity, we undertook a systematic expression and cloning effort to produce soluble and crystallizable NIK protein. This effort yielded crystal structures of apo human and murine NIK kinase domain as well as several structures of NIK bound to ATP-competitive inhibitors. These structures reveal the NIK kinase domain has an active-like conformation in the absence of phosphorylation and displays significant conformational variability.

9:00 Talk Title to be Announced

Zhulun Wang, Ph.D., Scientific Director, Amgen

9:30 Suitable Affinity Reagents for PAKs: Tight and Specific Binders from Rational Approaches

Ramesh Jha, Ph.D., Scientist, Bioscience Division, B10, MS M888, Los Alamos National Laboratory

PAKs are full of 'hotspot' regions for protein-protein interactions and play roles in several pathological conditions. This provides opportunities for design of affinity reagents and blockers. Using existing 3D structures of PAK1, specific binders that could distinguish 'open' and 'closed ' states were designed. The rational approaches used to design these affinityreagents will be discussed. Finally insights will be offered for targeting the regions on PAKs with unknown structure.

10:00 Coffee Break in the Exhibit Hall with Poster Viewing

NEXT

Organized by
Cambridge Healthtech Institute

10:45 *In silico* Fragment-Based Discovery of Novel Classes of Potent and Selective Tyrosine Kinase Inhibitors

Hongtao Zhao, Ph.D., Scientist, Biochemistry, University of Zurich

We have developed an efficient *in silico* procedure called ALTA, which stays for anchor-based library tailoring approach, to interrogate a library of compounds for high throughput screening. First, small and mainly rigid virtual fragments are docked in the binding site. The fragments with most favorable calculated binding free energy (anchors) are used to identify the compounds with 2D structure containing one of these anchors, which are then submitted to flexible ligand docking. The essential of this ALTA approach is the novel fragmentation algorithm, which can generate fragments with high chemical richness that can serve as a starting point either directly for hit optimization or for identification of their "parent" compounds. This approach has led to identification of two novel classes of tyrosine kinase inhibitors, and the straightforward hit-to-lead optimization by addition of just one or two heavy atoms leads to two series of potent and selective inhibitors. The predicted binding modes were further confirmed by X-ray crystallography.

11:15 Discovery of AS1940477, a Highly Potent p38 MAPK Inhibitor

Toru Asano, Ph.D., Scientist, Drug Discovery Research, Astellas Pharma, Inc.

p38 mitogen-activated protein kinase (MAPK) plays a key role in immune responses through the production of cytokines such as TNF-alpha and IL-6. p38 MAPK is an attractive target for drugs to treat autoimmune diseases, although development of many p38 MAPK inhibitors have discontinued due to low efficacy and the need for high dosing. We have identified AS1940477 a highly potent p38 MAPK inhibitor with a novel tetrahydropyrazolopyrimidine structure. Data will be presented on the discovery and optimization of tetrahydropyrazolo-pyrimidine derivatives, including a favorable PK profile, and animal studies.

11:45 Kinase-Directed Phenotypic Screening: Identification of a Novel Target for Inflammatory Disease

David Chantry, Ph.D., Senior Director, Translational and Cellular Biology, Array BioPharma

12:15 Sponsored Presentation *(Opportunity Available)*

12:30 Walk and Talk Luncheon in the Exhibit Hall (Last Chance for Poster and Exhibit Viewing)

Case Studies

1:55 Chairperson's Remarks

2:00 Talk Title to be Announced

Leyi Gong, Ph.D., Scientist, SRI International (tentative)

2:30 Small Molecule Inhibitors of the c-Fes Tyrosine Kinase: Potential Applications in Myeloid Leukemia and Myeloma

Tom Smithgall, Ph.D., William S. McEllroy Professor of Biochemistry; Chairman, Microbiology and Molecular Genetics, University of Pittsburgh School of Medicine

c-Fes is a cytoplasmic protein-tyrosine kinase that regulates normal cellular differentiation, the innate immune response, and vasculogenesis. Elevated c-Fes kinase activity is associated with Flt3+ AML and multiple myeloma. This talk will address the discovery and characterization of several classes of potent c-Fes inhibitors as well as their activity against these forms of cancer.

3:00 Chemistry to Unlock ROCK in Clinic

Olivier Defert, Ph.D., Amakem NV

Two case studies will be discussed in this lecture. First, we will focus on the design and the evaluation of a locally acting ROCK inhibitor as drug candidate for the treatment of glaucoma, AMA0076, which is currently in Phase 2 clinical development. Finally, the profile of the preclinical candidate for the treatment of respiratory diseases, AMA0247, will be shown. This compound showed efficacy in a variety of relevant *in vivo* models for asthma and COPD, with at least 500-fold lower exposure in the blood versus the lung tissues.

3:30 Presentation to be Announced

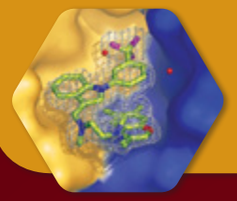
4:00 End of Conference

BACK

REGISTER BY MARCH 15 FOR MAXIMUM SAVINGS!

CLICK HERE TO REGISTER ONLINE!

Organized by Cambridge Healthtech Institute



WEDNESDAY, APRIL 17

12:30 pm Registration

PPI Drug Discovery - Novel Approaches

1:30 Chairperson's Opening Remarks

1:40 Systems and Network Pharmacology to Target Protein-Protein Interaction Networks in Cancer

Asfar Azmi, Ph.D., Research Scientist, Pathology and Oncology, Karmanos Cancer Institute, Wayne State University

To have an impact, interventions within a PPI network need to be multiple but highly selective. The major challenge is to design a promiscuous strategy that hits multiple weak nodes in cancer cell PPI without invoking undesirable side effects to normal cell network. The emergence of systems and network biology has enhanced our knowledge of PPIs and has allowed deeper evaluations of drug induced perturbations that has helped to decode the complex mechanisms of drug action. Emerging concepts such as 'Network Pharmacology' and 'Systems Pharmacology' are solidifying their position in cancer medicine.

2:10 PPI Drug Discovery - Peptide Mimicry and Fragment Approaches

David Fry, Ph.D., Head, Biostructural Research, Hoffman-La Roche

Modulating protein-protein interactions (PPIs) with small molecules is a difficult objective, but could potentially lead to a wide variety of novel and important therapeutics. PPI systems represent a unique class of drug target, and it has been shown that successful modulators of PPIs tend to have certain properties that distinguish them from drugs that act against more conventional target classes. One way toward understanding these key properties is to carefully study successful examples of PPI modulators and, at an atomic level, compare their binding strategies to those employed by the natural protein partners. Further, with regard to the fragment-based approach, we can learn by performing retrospective analyses of completed, successful programs - that is, deconstruct known PPI modulators into successively smaller fragments, and survey their potency and binding locations, and then compare these attributes to those of the parent compounds.

2:40 Bimolecular Fluorescence Complementation (Bifc) as a Novel Imaging-Based Screening for Inhibitors of Protein-Protein Interactions

Chang-Deng Hu, M.D., Ph.D., Associate Professor, Medicinal Chemistry and Molecular Pharmacology, Purdue University

Since the original report of BiFC in 2002, it has become a widely accepted method to study PPIs in various model organisms. Many critical PPIs have also been identified by the use of BiFC in living cells and animals. Further, recent improvements in the technology have also increased signal-to-noise ratio dramatically. Compared to other methods such as FRET, its higher signal-to-noise ratio (20 fold) is the most attractive feature for BiFC-based high throughput screening.

3:10 Sponsored Presentation

Sponsored by SCHRÖDINGER.

Speaker to be Announced

3:40 Refreshment Break in the Exhibit Hall with Poster Viewing

Computational Methods

4:20 PocketQuery: Protein-Protein Interaction Inhibitor Starting Points from Protein-Protein Interaction Structure

David Koes, Ph.D., Research Assistant Professor, Computational and Systems Biology, University of Pittsburgh

PocketQuery is a web interface for exploring the properties of protein-protein interaction (PPI) interfaces with a focus on the discovery of promising starting points for small-molecule design. PocketQuery rapidly focuses attention on the key interacting residues of an interaction using a 'druggability' score that provides an estimate of how likely the chemical mimicry of a cluster of interface residues would result in a small-molecule inhibitor of an interaction. These residue clusters are chemical starting points that can be seamlessly exported to a pharmacophore-based drug discovery workflow.

4:50 Recent Advances in the Prediction of Protein Interaction Interfaces

Jarek Meller, Ph.D., Associate Professor, Environmental Health, University of Cincinnati

Computational methods to predict interaction sites using protein structure and sequence information are coming out of age. Recent developments in this field, accuracy of current prediction methods, inherent limitations and challenges are presented. Prediction of hot spots and druggable sites within interaction interfaces are also discussed.

5:20 - 6:20 Moderated Breakout Discussions

In this interactive session, several topics will be offered for discussions and delegates are invited to choose a topic of interest and join the moderated discussion at hand. In this informal setting, participants are encouraged to share examples from their work, vet ideas with peers and be part of a group problem-solving endeavor. We emphasize that this is an informal exchange amongst scientists and is not meant to be, in any way, a product promoting session.

6:30 - 9:00 Dinner Short Courses *(separate registration required, see page 3 for details)*

THURSDAY, APRIL 18

7:45 am Breakfast Workshop Presentation *(Sponsorship Opportunity Available)* **or Morning Coffee**

8:15 Chairperson's Opening Remarks

» 8:20 FEATURED PRESENTATION

Protein-Protein Interaction Drug Space: Stapled Peptide Drug Development

Tomi K. Sawyer, Ph.D., CSO, Aileron Therapeutics

Protein-protein interaction (PPI) drug space has become recognized as a promising new opportunity to advance a new modality of therapeutics for numerous diseases. The preponderance of such PPIs involve alpha-helical intermolecular recognition. This presentation will highlight recent advances in stapled peptide drug development.

Rational Design

9:00 pH-Dependent Regulation of Cytokine-Receptor Interactions

Michael Hodsdon, M.D., Ph.D., Associate Professor, Laboratory Medicine, Yale University

Recognition of prolactin, a protein hormone and cytokine, by its receptor demonstrates a dramatic dependence on solution acidity across a physiologic range, such that acidification from pH 7.5 to 6.0 results in an approximately 500-fold decrease in affinity. This phenomenon has important implications for intracellular

NEXT

trafficking of endocytosed cytokine-receptor complexes. Biophysically, the pH-dependent behavior depends on a highly cooperative set of four histidine residues within the receptor-binding interface. A survey of cytokine-receptor complex tertiary structures reveals similar histidine-rich interfaces, which would be predicted to display similar pH dependence, along with histidine-free interfaces, expected to be pH independent. Site-directed mutagenesis can be used to rationally engineer pH-dependent behavior to both experimentally investigate its physiologic importance and also to potentially manipulate receptor trafficking.

9:30 Selective Protein-Protein Interactions Inhibition Result in Protection from Cardiac Ischemia and Reperfusion Injury

Nir Qvit, Ph.D., Research Associate, Chemical and Systems Biology, Stanford University

We rationally identified a peptide inhibitor of one of several functions mediated by delta-PKC. Our inhibitor is an allosteric inhibitor of the kinase and therefore, unlike inhibitors of the catalytic site, unlikely to affect other kinases. This peptide is an inhibitor of protein-protein interaction, thus a member of a novel family of pharmacological agents with therapeutic promise.

10:00 Coffee Break in the Exhibit Hall with Poster Viewing

Strategies to Regulate PPIs

10:45 What Compounds for what PPI Target?

Olivier Sperandio, Ph.D., Drug Designer - CDithem Platform, Senior Research Associate, Inserm

I will describe our new iPPI-DB database that contains more than 1600 inhibitors of protein-protein interactions (iPPI) on about 15 classes of PPI targets with information on pharmacological activities, physico-chemical properties for the compounds, and biological descriptions about the PPI targets. The database was used to get some insight into the chemical space of iPPI with the ultimate aim of selecting PPI-friendly compounds to modulate PPI targets.

11:15 2P2I3D: A Focused Chemical Library Dedicated to Protein-Protein Interactions

Xavier Morelli, Ph.D., Group Leader & Principal Investigator, CRCM, CNRS

This talk will address some challenging questions: biological and chemical spaces of PPI with known orthosteric inhibitors, druggability assessment of protein-protein interactions, design and validation of chemical libraries dedicated to PPI.

11:45 Multiplex Analysis of Physiologic PPI Networks to Enable Identification of Signaling Signatures and Pharmacologic Targets

Adam G. Schrum, Ph.D., Assistant Professor of Immunology, Mayo Clinic College of Medicine

Physiologic signal transduction is thought to be mediated by sets of PPI that can operate together in modular networks. We present a novel multiplex microsphere based approach to analyze network PPI profiles for the T cell antigen receptor (TCR) signaling pathway. The unique signatures emerging in response to functionally distinct stimuli provide a new perspective on how to approach pharmacologic targeting of this immunologically important pathway.

Sponsored by selcia

12:15 Affinity Capillary Electrophoresis: An ACE method for Monitoring Protein-Protein Interactions (PPIs)

Carol Austin, Ph.D., Biology Group Leader, Selcia Ltd

Affinity Capillary Electrophoresis (ACE) is a high resolution, separation technique capable of readily detecting PPIs in solution. The technique does not require either protein to be immobilised and protein consumption is in the pM-nM range. Inhibitors from a range of starting points can be detected from fragments to natural product extracts.

12:30 Walk and Talk Luncheon in the Exhibit Hall (Last Chance for Poster and Exhibit Viewing)

1:55 Chairperson's Remarks

2:00 Promiscuous Small-Molecule Protein-Protein Interaction Inhibition: Could This Be a Real Concern?

Peter Buchwald, Ph.D., Director, Drug Discovery, Diabetes Research Institute, University of Miami

During our search for costimulatory interaction inhibitors, we have found poly-iodinated xanthene compounds that seem to be nonspecific promiscuous inhibitors of a number of PPIs within the tumor necrosis factor superfamily (e.g., (TNF-R–TNFalaf, CD40–CD154, RANK–RANKL, OX40–OX40L) as well as outside of it. For example, erythrosine B, and FDA-approved food colorant, acts as such an inhibitor with a remarkably consistent median inhibitory concentration (IC50) in the low micro-molar range. (approximately 2–20 mg/L) range.

2:30 Talk Title to be Announced

James Bibb, M.D., Associate Professor, Psychiatry and Neurology and Neurotherapeutics, The University of Texas Southwestern Medical Center

3:00 Compound Combinations for Inhibition of BCL11A

Elmar Nurmemmedov, Ph.D., Scientist, Department of Hematology and Oncology, Harvard Medical School, Children's Hospital Boston

BCL11A is a repressor of fetal hemoglobin (HbF) in adult animals. BCL11A has emerged as an attractive drug target, since its inhibition offers a therapeutic approach for sickle cell disease (SCD) and the b-thalassemias. We have screened for small molecules that can bind at various sites of the target protein. We have developed a model that allows combining these domain-specific compounds for synergistic inhibition of PPIs. We have thus identified several compound groups that can up-regulate HbF to potentially therapeutic levels.

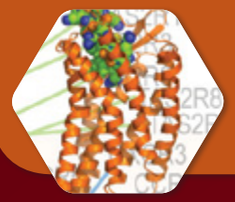
3:30 Talk Title to be Announced

Cheryl Arrowsmith, Ph.D., Professor, Medical Biophysics; Canada Research Chair in Structural Proteomics, University of Toronto

4:00 End of Conference

BACK

Organized by Cambridge Healthtech Institute



WEDNESDAY, APRIL 17

12:30 pm Registration

GPCR Structural Determinants

1:30 Chairperson's Opening Remarks
Scientific Advisor: Michael Hanson, Ph.D., Director, Structural Biology, Receptos

» 1:40 KEYNOTE PRESENTATION

Adventures in S1P Receptor Therapeutics
Hugh Rosen, M.D., Ph.D., Professor, Chemical Physiology, Scripps Research Institute

2:40 Utilizing Structural Insights in GPCR Drug Discovery
Robert Cooke, Ph.D., Head, Biomolecular Structure Department, Heptares
The number of GPCRs for which structural information is available has increased dramatically in recent years, providing valuable insights into ligand recognition and mechanisms of activation, as well as additional starting points for homology modelling. Structure-based drug discovery is now a reality for this family, and the impact of new structures for family A and family B GPCRs will be reviewed.

3:10 Sponsored Presentation *(Opportunity Available)*

3:40 Refreshment Break in the Exhibit Hall with Poster Viewing

4:20 Delineating Determinants of Co-Operativity, Affinity and Bias for Allosteric Modulators of Metabotropic Glutamate Receptor 5
Karen J. Gregory, Ph.D., Post-Doctoral Fellow, Jeffrey Conn Laboratory, Pharmacology, Vanderbilt University; American Australian Association Merck Co. Foundation Fellow 2010; Drug Discovery Biology, MIPS & Department of Pharmacology, Monash University
Comparative modeling combined with the systematic mutagenesis has furthered our understanding of how metabotropic glutamate receptor 5 allosteric modulators exert their effects. We have identified key amino acids within the transmembrane domains that govern modulator affinity and/or cooperativity, as well as mutations that confer molecular switches in modulator pharmacology.

4:50 Mapping Allosteric Sites in GPCRs
Nagarajan Vaidehi, Ph.D., Professor, Immunology, Beckman Research Institute of the City of Hope
GPCRs are allosteric nanomachines that convey the ligand binding information on the extracellular surface to intracellular region. Experiments provide information on which residues are involved in either end of the allosteric communication but no information on the pathway of this communication. We have developed computational methods to map the allosteric pathway in GPCRs. These methods not only provide insights into the mechanism of communication but also provide new approaches to identifying allosteric druggable sites in GPCRs.

5:20 Moderated Breakout Discussions
In this interactive session, several topics will be offered for discussions and delegates are invited to choose a topic of interest and join the moderated discussion at hand. In this informal setting, participants are encouraged to share examples from their work, vet ideas with peers and be part of a group problem-solving endeavor. We emphasize that this is an informal exchange amongst scientists and is not meant to be, in any way, a product promoting session.

6:20 End of Day

6:30 - 9:00 pm Dinner Short Courses *(Separate registration required; see page 3 for details.)*

THURSDAY, APRIL 18

7:30 am Breakfast Workshop Presentation *(Sponsorship Opportunity Available)* **or Morning Coffee**

Probing GPCR Structure

8:15 Chairperson's Opening Remarks

8:20 FEATURED PRESENTATION

Structure of the Agonist-Bound Neurotensin Receptor NTS1
Reinhard Grisshammer, Ph.D., Investigator, National Institute of Neurological Disorders and Stroke (NINDS), NIH
Neurotensin is a peptide that functions as both a neurotransmitter and a hormone through activation of the neurotensin receptor NTS1, a G protein-coupled receptor (GPCR). I will present the structure at 2.8 Å resolution of NTS1 in an active-like state, bound to the peptide agonist. Our findings provide for the first time insight into the binding mode of a peptide agonist to a GPCR.

9:00 High-Resolution Structure of Human Adenosine A2A Receptor Reveals Allosteric Binding Sites for Sodium Ion and Cholesterols
Vadim Cherezov, Ph.D., Assistant Professor, Department of Molecular Biology, The Scripps Research Institute
1.8 A resolution structure of adenosine A2A receptor revealed a Na+ ion, 177 waters, 3 cholesterols and 26 lipids. Such unprecedented high-resolution details help to shed light on the role of waters in ligand binding and receptor activation, and to understand the allosteric effects of sodium, cholesterol and lipids on GPCR function.

9:30 Identifying an Alternate Antagonist Binding Site for a Diabetes Target: A GPCR Case Study
Carleton Sage, Ph.D., Fellow, Computational Systems, Arena

10:00 Coffee Break in the Exhibit Hall with Poster Viewing

10:45 Probing Receptor Signaling Using Genetically-Encoded Unnatural Amino Acids
Thomas P. Sakmar, M.D., Professor, Laboratory of Chemical Biology & Signal Transduction, The Rockefeller University
Recent advances in molecular and structural studies of GPCRs have revolutionized drug discovery. Our aim is to elucidate the principles that underlie ligand recognition in GPCRs and to understand with chemical precision how receptors change conformation in the membrane bilayer when ligands bind. This lecture will describe new interdisciplinary technologies to study receptor dynamics

NEXT

Organized by Cambridge Healthtech Institute

and allosteric mechanisms.

11:15 Nanobodies for the Structural and Functional Investigation of GPCR Transmembrane Signaling

Jan Steyaert, Ph.D., Executive Director and Professor, Molecular and Cellular Interactions, Vrije Univ Brussels

We generated Nanobodies that stabilize transient functional conformations of the human β2 adrenergic receptor. Nanobodies that faithfully mimic G protein binding were used to crystallize active agonist-bound states of this GPCR. Other nanobodies that stabilize the β2AR•Gs complex were instrumental to obtain the crystal structure of this complex, providing the first view of transmembrane signaling by a GPCR.

11:45 Structural Insights into Muscarinic Acetylcholine Receptor Function

Andrew C. Kruse, Graduate Student, Brian Kobilka (2012 Nobel Laureate) Lab, Department of Molecular and Cellular Physiology, Stanford University

I will present the recently determined structures of two muscarinic acetylcholine receptors, which offer new insight into ligand selectivity and allosteric modulation of muscarinic receptors and of GPCRs in general. In addition, I will discuss more recent work toward understanding the ligand binding and activation of these important receptors.

12:15 pm Sponsored Presentation *(Opportunity Available)*

12:30 Walk and Talk Luncheon in the Exhibit Hall (Last Chance for Poster and Exhibit Viewing)

Computational Approaches

1:55 Chairperson's Remarks

2:00 From GPCR Structure to Predictive Models

Ruben Abagyan, Ph.D., Professor, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego

As the number of GPCRs with known crystal structure approaches fifteen, the opportunities for structure based understanding of their function grow dramatically. Here we present the challenges and successes in predicting how orthosteric and allosteric ligands bind to GPCRs, as well as how protein and peptide ligands bind to family A and family B GPCRs.

2:30 Computational Approaches to GPCRs

Christopher A. Reynolds, Ph.D., MRC Fellow, Professor, School of Biological Sciences, University of Essex

Homology models of the calcitonin receptor-like receptor, a medically important class B GPCR; were constructed using a novel approach to the alignment and validated using experiment and theory. Distinct class B motifs and their class A equivalents have been identified. The relevance to drug design is discussed.

3:00 Hydrogen/Deuterium Exchange Captures Subtle Conformation Changes to GPCRs Upon Orthosteric Binding

Graham West, Ph.D., Postdoctoral Associate, Molecular Therapeutics, The Scripps Research Institute, Scripps Florida

Using hydrogen/deuterium exchange (HDX) coupled to mass spectrometry, we characterized conformation changes to the beta-2-adrenergic receptor in the presence of orthosteric ligands and absence of allosteric modulators (i.e. G proteins). Shifts to active GPCR conformations by orthosteric ligands alone have not been detected using crystallography. This work provides structural insight into GPCR signaling and presents a potential platform to structurally characterize GPCR-ligand interactions independent of tissue type.

3:30 Presentation to be Announced

4:00 End of Conference

REGISTER BY MARCH 15 FOR MAXIMUM SAVINGS!

CLICK HERE TO REGISTER ONLINE!

Organized by Cambridge Healthtech Institute

Sponsorship, Exhibit, and Lead Generation Opportunities

CHI offers comprehensive sponsorship packages which include presentation opportunities, exhibit space and branding, as well as the use of the pre and post-show delegate lists. Customizable sponsorship packages allow you to achieve your objectives before, during, and long after the event. Signing on early will allow you to maximize exposure to hard-to-reach decision makers!

Agenda Presentations

Showcase your solutions to a guaranteed, highly-targeted audience. Package includes a 15 or 30-minute podium presentation within the scientific agenda, exhibit space, on-site branding and access to cooperative marketing efforts by CHI.

Breakfast & Luncheon Presentations

Opportunity includes a 30-minute podium presentation. Boxed lunches are delivered into the main session room, which guarantees audience attendance and participation. A limited number of presentations are available for sponsorship and they will sell out quickly. Sign on early to secure your talk!

Invitation-Only VIP Dinner/Hospitality Suite

Sponsors will select their top prospects from the conference pre-registration list for an evening of networking at the hotel or at a choice local venue. CHI will extend invitations and deliver prospects. Evening will be customized according to sponsor's objectives i.e.:

- Purely social
- Focus group
- Reception style
- Plated dinner with specific conversation focus

Exhibit

Exhibitors will enjoy facilitated networking opportunities with high-level conference delegates. Speak face-to-face with prospective clients and showcase your latest product, service, or solution.

***Inquire about additional branding opportunities!**

Looking for additional ways to drive leads to your sales team?

Cambridge Healthtech Institute can help!

We offer clients numerous options for custom lead generation programs to address their marketing and sales needs, including:

- **Live Webinars**
- **White Papers**
- **Market Surveys**
- **Podcasts**
- **And More!**

Benefits of working with Cambridge Healthtech Institute for your lead generation needs:

- **Your campaign will receive targeted promotion to Cambridge Healthtech Institute's unparalleled database of over 800,000 individuals, all of which are involved in all sectors of the life sciences – lists can be segmented based on geography, research area, title and industry.**
- **All custom lead generation programs are promoted through our experienced marketing team that will develop and drive targeted campaigns to drive awareness and leads to your lead generation program.**
- **For our webinar programs, we offer assistance in procuring speakers for your web symposia through our extensive roster of industry recognized speakers across multiple disciplines within life sciences, as well as provide an experienced moderator and dedicated operations team to coordinate all efforts.**
- **If choosing a white paper program, we can offer editorial experience and provide an industry recognized author to write your white paper.**

To customize your participation at this event, please contact:

Suzanne Carroll – Senior Business Development Manager

781-972-5452 | scarroll@healthtech.com

Organized by
Cambridge Healthtech Institute

Hotel & Travel Information

Conference Hotel:

Hilton San Diego Resort & Spa
1775 East Mission Bay Drive
San Diego, CA 92109
Phone: 619-276-4010
Discounted Room Rate: $199 s/d
Discounted Cut-off Date: March 15, 2013

Please **click here** or call the hotel directly to make your sleeping accommodations. You will need to identify yourself as a CHI conference attendee to receive the discounted room rate with the host hotel. Reservations made after the cut-off date or after the group room block has been filled (whichever comes first) will be accepted on a space and rate-availability basis. Rooms are limited, so please book early to take advantage of the discount we have negotiated.

We understand that you have many choices when making your travel arrangements, and may ultimately decide to stay at another hotel. Please understand that reserving your room in the CHI room block allows you to take full advantage of the conference sessions, events and networking opportunities, and ensures that our staff will be available to help should you have any issues with your accommodations.

Flight Discounts:

Special discounts have been established with American Airlines for this conference:

- Call 1-800-433-1790 and use Conference code 9243BM
- Go to www.aa.com/group and enter Conference code 9243BM in promotion discount box
- Contact our designated travel agent, Wendy Levine at 1-877-559-5549 or wendy.levine@protravelinc.com

Car Rental Discounts:

Special discount rentals have been established with Hertz for this conference.

- Click here to make your reservation and use our Hertz Convention Number (CV): 04KL0004

Or Call Hertz directly at 800-654-3131 and reference our Discount Number 04KL0004

Visiting San Diego:

With its great weather, miles of sandy beaches, and major attractions, San Diego is known worldwide as one of the best tourist destinations. The San Diego Convention and Visitor's Bureau is the official travel resource for the San Diego region such as maps and directions, visitor safety tips, where to stay, what to do and how to get around. International, and commercial air service for the region is provided by the San Diego International Airport.

- **The San Diego Historical Society connects the past to the future so all generations will understand and appreciate the richness of San Diego's regional history.**
- **The Gaslamp Quarter is Southern California's premier dining, shopping and entertainment district, where you'll find a truly eclectic blend of food, fun and culture all within one of San Diego's most historic areas.**
- **At the world-famous San Diego Zoo, you will see some of the world's rarest wildlife including giant pandas (and Hua Mei, the only panda cub in the U.S.), and koalas.**
- **QUALCOMM Stadium accommodates a variety of events, including major league sports and concerts.**
- **OTIS - The Online Transit Information System lets you find out how to get around San Diego using the Metropolitan Transit System's buses, trolleys, or trains.**
- **A visit to the San Diego Wild Animal Park is like a safari to many of the world's most exotic places.**
- **World-renowned Balboa Park is home to fifteen museums, various arts and international culture associations, as well as the San Diego Zoo, making it one of the nation's largest cultural and entertainment complexes.**
- **SeaWorld San Diego: To entertain, amaze and educate, creating memories that last a lifetime. SeaWorld has hosted more than 100 million guests since opening in 1964.**

REGISTER BY MARCH 15 FOR MAXIMUM SAVINGS!

CLICK HERE TO REGISTER ONLINE!

Organized by Cambridge Healthtech Institute

How to Register: DrugDiscoveryChemistry.com

reg@healthtech.com • P: 781.972.5400 or Toll-free in the U.S. 888.999.6288

Please use keycode DCH F when registering

SHORT COURSES AND SYMPOSIA

	Commercial	Academic, Government, Hospital-affiliated
1 Symposium	$995	$595
1 Symposium + 1 Short Course	$1345	$875
1 Short Course	$695	$395
2 Short Courses	$995	$595
3 Short Courses	$1195	$695
4 Short Courses	$1295	$795

One-Day Symposia (April 15)	Pre-Conference Short Courses (April 15)		Dinner Short Courses (April 17)
Antiviral Drug Discovery	Molecular Interactions and Drug Design	Enabling Macrocyclic Compounds for Drug Discovery	Epigenetic Targets: Chemical Tools
Property-Based Drug Design	Advancing Tools and Technologies for Fragment-Based Design	Influencing Stem Cell Differentiation	Practical Aspects of Structure-Based Drug Discovery with GPCRs
	Immunology Basics for Chemists	Allosteric Modulation of GPCRs	
	An Intro to the Field of Antibody-Drug Conjugates		

CONFERENCE PRICING

STANDARD PACKAGE *(Includes Access to Two Conferences, Excludes Short Courses and Symposia)*

Advance Registration Deadline until March 15, 2013	$2295	$1095
Registrations after March 15, 2013 and on-site	$2395	$1195

BASIC PACKAGE *(Includes Access to One Conference, Excludes Short Courses and Symposia)*

Advance Registration Deadline until March 15, 2013	$1645	$845
Registrations after March 15, 2013 and on-site	$1745	$975

CONFERENCE SELECTIONS:

April 16-17 (Tuesday-Wednesday)	April 17-18 (Wednesday-Thursday)
Track 1: Anti-Inflammatories	Track 4: Kinase Inhibitor Chemistry
Track 2: Fragment-Based Drug Discovery	Track 5: Protein-Protein Interactions
Track 3: Constrained Peptides and Macrocyclics Drug Discovery	Track 6: GPCR Based Drug Design

CONFERENCE DISCOUNTS

POSTER DISCOUNT ($50 Off) Poster abstracts are due by March 15, 2013. Once your registration has been fully processed, we will send an email containing a unique link allowing you to submit your poster abstract. If you do not receive your link within 5 business days, please contact jring@healthtech.com. ** CHI reserves the right to publish your poster title and abstract in various marketing materials and products.*

REGISTER 3 - 4th IS FREE: Individuals must register for the same conference or conference combination and submit completed registration form together for discount to apply.

ALUMNI DISCOUNT: Cambridge Healthtech Institute (CHI) appreciates your past participation at Drug Discovery Chemistry. As a result of the great loyalty you have shown us, we are pleased to extend to you the exclusive opportunity to save an additional 20% off the registration rate. *Please note: Our records must indicate you were an attendee of Drug Discovery Chemistry in the past in order to qualify.*

GROUP DISCOUNTS: Discounts are available for multiple attendees from the same organization. For more information on group rates contact David Cunningham at +1-781-972-5472

Alumni, Group, and 'Register 3 & 4th is Free' discounts cannot be combined.

ADDITIONAL REGISTRATION DETAILS

Each registration includes all conference sessions, posters and exhibits, food functions, and access to the conference proceedings link.

Handicapped Equal Access: In accordance with the ADA, Cambridge Healthtech Institute is pleased to arrange special accommodations for attendees with special needs. All requests for such assistance must be submitted in writing to CHI at least 30 days prior to the start of the meeting.

To view our Substitutions/ Cancellations Policy, go to http://www.healthtech.com/regdetails

Video and or audio recording of any kind is prohibited onsite at all CHI events.