Fourth Annual
PROPERTY-BASED
DRUG DESIGN
IN MEDICINAL CHEMISTRY

Driving Drug Discovery Success by Designing Right Physicochemical and Biophysical Properties

June 11-12, 2015
Westin Boston Waterfront, Boston, MA

EVENT FEATURES:
• 2015 discussion topics include: Design Consideration for New & Non-Traditional Molecules, Designing Molecules with Better Deliverability, Evaluation of Drug Properties, Overcoming Challenges in Discovery, Development & Clinic
• 65+ Exhibitors in a Shared Exhibit Hall
• Network with 950+ Attendees during Networking Breaks and Poster Session in Exhibit Hall

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WorldPrem Clinical Congress
Tackling Translational Challenges

Featured Speakers
Nick Terrett, Ph.D.
CSO, Ensemble Therapeutics Corp.

Peter Kenny, Ph.D.
Visiting Scientist, NEQUIMED-IQSC, University of São
Conference-at-a-Glance

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<tr>
<th>Tuesday, June 9</th>
<th>Pre-Conference Short Courses*</th>
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<td>Novel Preclinical Models in Oncology</td>
<td>Translational Imaging in Cancer Drug Development</td>
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<th>Wednesday, June 10</th>
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Property-Based Drug Design in Medicinal Chemistry

The drug discovery landscape is rapidly changing and with it comes the need to generate leads with lower attrition rate. Property-based drug design approach is guiding researchers in designing candidates with the right balance of physicochemical properties - safety and absorption, distribution, metabolism, and excretion (ADME) profiles. 4th Annual Property-Based Drug Design in Medicinal Chemistry conference will bring together experts and leaders from industry and academia to share strategies and case studies for new and non-traditional molecules, how computational modeling and data management can be used effectively, and to discuss novel ways to measure or predict properties to make molecules more drug-like and overcome challenges in discovery, development, and the clinic.

Plenary Keynote Panel

Wednesday, June 10 | 5:00 pm

Our Plenary Keynote Panel this year features senior executives from pharma/biotech who have played an important role in bringing to market some of the most innovative drugs in recent years. They are here to share their stories on what transpired behind-the-scenes, how they could overcome the translational challenges, and what they see as key drivers in making similar breakthroughs going forward.

Plenary Keynote Panelists:

- **Clinical Development of Keytruda**
  - David Kaufman, M.D., Ph.D., Director/Senior Principal Scientist, Oncology/Immunotherapy, Clinical Research, Merck

- **Discovery of Ivacaftor, an Orally Bioavailable CFTR Potentiator**
  - Peter Groutterhuis, Ph.D., Senior Director, Chemistry, Vertex Pharmaceuticals

- **Harvoni Drug Development Challenges: The Role of Risk in Rapid Development**
  - Phillip Pang, M.D., Ph.D., Director, Clinical Research, Gilead Sciences

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molecular properties. We will present BROOD v 2.1 a fragment-based R-group

Lead optimization is not a simple one-dimensional optimization of affinity

Gregory L. Warren, Ph.D., Senior Applications Scientist, OpenEye Scientific

Filtering to Fragment Replacement in BROOD

3:35 A Delicate Balancing Act: Applying Property

variety of interesting macrocyclic chemotypes.

Here we present computational approaches and property/ADME trends seen in a

Macrocycles are found widely in nature and several are marketed as

A great deal of progress has been made in recent years in elucidating design

Pfizer, Inc.

Alan M. Mathiowetz, Ph.D., Director, Worldwide Medicinal Chemistry,

Protein-Protein Interaction Targets, a Case Study

Christopher N. Johnson, Ph.D., CChem FRSC, Director, Medicinal Chemistry,

Astex has successfully applied fragment-based drug design to protein-protein

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

Macrocycles can rapidly generate millions of synthetic macrocycles using
dNA-programmed chemistry, and how they are efficiently screened

against protein-protein interaction targets to identify hit compounds and

SAR. The novel approach will be illustrated with successful examples of

2:05 KEYNOTE PRESENTATION: EXPLORING MACROCYCLES FOR DRUG

CHALLENGING PROTEIN-PROTEIN INTERACTIONS

of lead discovery programs, including the discovery of novel XIAP and

IL17A antagonists.

2:35 Property- and Fragment-Based Design Considerations for

Protein-Protein Interaction Targets, a Case Study

Christopher N. Johnson, Ph.D., CCChem FRSC, Director, Medicinal Chemistry,

Astex Pharmaceuticals

Designing compounds with suitable properties for inhalation present unique

challenges to the medicinal chemist. This talk will discuss a number of

programs from within Pfizer that have addressed this issue, across numerous

target classes, to produce inhaled candidate drug molecules for the treatment

of various lung diseases – Inhibition of GPCRs, PDEs and Kinases have been

targeted successfully via this approach.

5:45 Discovery of Asunaprevir (BMS-650032): An Approved NS3

Protease Inhibitor for the Treatment of Hepatitis C

Paul Scola, Ph.D., Research Fellow & Group Leader, Department of Virology

Chemistry, Bristol-Myers Squibb Research Co.

Hepatitis C Virus (HCV) infection is an insidious liver disease that affects more

than 170 million people worldwide. The HCV NS3/4A protease is an essential

enzyme for viral replication and, as such, has been validated as a target for

anti-HCV therapy in clinical trials. In this presentation, the discovery of BMS-

650032, a potent and selective inhibitor of the NS3/4A enzyme, recently

approved for treatment of HCV, will be described. Highlights of this discovery

process include the design of the acylsulfonamide chemotype, as well as

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6:15 Close of Day

3:05 Computational Design for Improving ADME Properties of

Peptidic Macrocycles

Alan M. Mathiowetz, Ph.D., Director, Worldwide Medicinal Chemistry,

Pfizer, Inc.

A great deal of progress has been made in recent years in elucidating design

principles for achieving favorable ADME properties in Beyond Rule-of-5

macrocycles. Many of the important principles, such as minimization of exposed

polar surface area to improve permeability, are dependent upon the overall 3D

structure, which can be computationally predicted and confirmed experimentally.

Here we present computational approaches and property/ADME trends seen in a

variety of interesting macrocyclic chemotypes.

3:35 A Delicate Balancing Act: Applying Property

Filtering to Fragment Replacement in BROOD

Gregory L. Warren, Ph.D., Senior Applications Scientist, OpenEye Scientific

Software, Inc.

Lead optimization is not a simple one-dimensional optimization of affinity

and effective computational tools should allow optimization of other

molecular properties. We will present BROOD v 2.1 a fragment-based R-group

and template replacement lead optimization application that can suggest

replacement groups that are simultaneously optimized for many different

properties at once. Several examples to demonstrate this unique ability will

be presented.

4:05 Refreshment Break in the Exhibit Hall with Poster Viewing

DESIGNING MOLECULES WITH BETTER

DELIVERABILITY AND TARGETING

4:45 Optimizing Brain Exposure in CNS Drug Discovery

Ruben Alvarez Sanchez, Ph.D., Head, Pharmaceutical Profiling, Drug

Disposition and Safety, F. Hoffmann-La Roche

For drugs actively transported across the blood-brain barrier, unbound plasma

and unbound brain concentrations differ to an extent that is commonly

unknown. We report on approaches to assess and predict unbound brain

concentration for P-gp substrates and how they can be utilized in early CNS

drug discovery to enhance the understanding of PK/PD relationships and

support a clinically meaningful compound optimization v

5:15 Inhalation by Design: Approaches towards Designing Drug

Candidates for Lung Diseases

Peter Jones, Ph.D., Senior Principal Scientist, Medicinal Chemistry-

Inflammation and Remodelling, Pfizer, Inc.

5:45 Discovery of Asunaprevir (BMS-650032): An Approved NS3

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approved for treatment of HCV, will be described. Highlights of this discovery

process include the design of the acylsulfonamide chemotype, as well as

optimization of ADME and toxicology properties within this chemical series.

6:15 Close of Day

DINNER COURSE* | 7:00 – 10:00 PM

Optimizing Physical Properties of Molecules to

Achieve High-Quality Clinical Candidates

Topics to be discussed:

• Determination, Evaluation and use of physical properties in drug discover

• Discussion of properties such as solubility, ligand efficiency, log P,
crystallizations, and solubility

• Experimental best practices and case studies

Instructor:

Terry Richard Stouch, Ph.D., President, Science for Solutions, LLC

Additional instructors to be Announced

FRIDAY, JUNE 12

7:30 am Interactive Breakout Discussion Groups

Each discussion group in this session is led by a moderator(s) who ensures

focused conversations around key issues. Attendees join a specific group and

the small, informal setting facilitates sharing of ideas and active networking.

Topics for discussion will be made available on the conference website.

PREDICTION AND EVALUATION OF DRUG
Hepatobiliary transport is a major disposition pathway, and estimating its contribution to the total systemic clearance is extremely valuable for predicting clinical pharmacokinetics and understanding the possible mechanisms of hepato-biliary toxicity and potential drug-drug interactions. Furthermore, the clinical importance of hepatic drug transporters has attracted mechanisms of hepato-biliary toxicity and potential drug-drug interactions. Measurements of physicochemical and biomimetic properties in early drug discovery are used for the estimation of in vivo distribution and drug efficiency. The Drug Efficiency Index (DEI) (potency plus drug efficiency) has been shown to be proportional to receptor occupancy. Simultaneous optimization of potency and drug efficiency can help guide candidate selection toward compounds of increased quality and with reduced chance of later stage failures.

Physicochemical and Biomimetic Properties to Guide Lead Optimization

Physicochemical and early ADMET assays guide chemotype evaluation and rational scaffold alteration. This presentation will focus on the integration of these approaches with physiologically based pharmacokinetic modeling (PBPK) to enable the prediction of clinical outcomes and to optimize selection of formulation.

The inhibition of the attachment of the HIV-1 viral glycoprotein gp-120 to the host cell receptor CD4 during the first step of the viral entry represents a novel antiretroviral approach. This talk will discuss the modifications made by medicinal chemists based on clinical feedback from multiple compounds, discuss a successful prodrug approach, and describe formulation development leading to a clinical candidate that is currently progressing to Phase III studies.

The current understanding of the physicochemical and structural drivers in order to facilitate rational drug design.
Sponsorship, Exhibit & Lead Generation Opportunities

CHI offers comprehensive sponsorship packages which include presentation opportunities, exhibit space, branding and networking with specific prospects. Sponsorship allows you to achieve your objectives before, during, and long after the event. Any sponsorship can be customized to meet your company’s needs and budget. Signing on early will allow you to maximize exposure to qualified decision makers.

Podium Presentations – Available Within Main Agenda!
Showcase your solutions to a guaranteed, targeted audience through a 15- or 30-minute presentation during a specific conference program, breakfast, lunch, or separate from the main agenda within a pre-conference workshop. Package includes exhibit space, on-site branding, and access to cooperative marketing efforts by CHI. For the luncheon option, lunches are delivered to attendees who are already seated in the main session room. Presentations 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, helping you to make the most out of this invaluable opportunity. 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 qualified delegates. Speak face-to-face with prospective clients and showcase your latest product, service, or solution.

Additional branding and promotional opportunities are available!
Looking for additional ways to drive leads to your sales team? CHI’s Lead Generation Programs will help you obtain more targeted, quality leads throughout the year. We will mine our database of 800,000+ life science professionals to your specific needs. We guarantee a minimum of 100 leads per program! Opportunities include Whitepapers, Web Symposia, Custom Market Research Surveys, and Podcasts.

For sponsorship and exhibit information, please contact:
Joseph Vacca
Associate Director, Business Development
781-972-5431 | jvacca@healthtech.com

2015 Exhibitors & Sponsors (As of January 28, 2015)
AMRI
AntiCancer, Inc.
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ProQinase
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Schro
dinger
SCIVAX Life Sciences, Inc.
Simulations Plus, Inc.
Solid Form Solutions Ltd
Studylog Systems, Inc.
Sygnature Discovery
Synthonyx
Taconic Biosciences
VisualSonics

Hotel & Travel Information

Conference Venue and Hotel:
Westin Boston Waterfront
425 Summer St.
Boston, MA 02210
T: 617-532-4600
Discounted Room Rate: $299 s/d
Discount Cutoff Date: May 13, 2015

Go to the travel page of healthtech.com/Property-Based-Drug-Design for additional info
Pricing and Registration Information

CONFERENCE PRICING
Includes access to 1 conference, excludes short courses

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<td>After May 8, 2015 and on-site</td>
<td>$1,949</td>
<td>$899</td>
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Property-Based Drug Design in Medicinal Chemistry is part of CHI’s World Preclinical Congress 2015
Make the most out of your time in Boston - Add a second event for maximum savings

BEST VALUE! EVENT PRICING
Includes access to 2 conferences, excludes short courses

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<tr>
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<th>$2,999</th>
<th>$1,379</th>
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Program Selection: When registering please indicate the one conference you will attend:

### June 10-11, 2015
- Tumor Models for Targeted Therapy
- Imaging in Oncology
- Mastering Medicinal Chemistry - Recommended Package
- Targeting GPCRs
- Chemical Biology
- Predicting Drug Toxicity
- Blood Brain Barrier

### June 11-12, 2015
- Property Based Drug Design -Recommended Package!

**SHORT COURSE**

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<tr>
<td>Single Short Course</td>
<td>$699</td>
<td>$399</td>
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<td>Two Short Courses</td>
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<td>Three Short Courses</td>
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Please select the short courses you are most likely to attend.

- Drug Metabolism and Its Impact on Decisions in Drug Discovery & Development
- Understanding and Dealing with Drug Disposition in CNS
- Optimizing Physical Properties of Molecules to Achieve High-Quality Clinical Candidates

**CONFERENCE DISCOUNTS**

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<th>Discount Type</th>
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<tr>
<td>Alumni Discount</td>
<td>20%</td>
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<tr>
<td>Drug Safety Executive Council (DSEC) Members</td>
<td>25%</td>
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<tr>
<td>Poster Discount</td>
<td>$50 Off</td>
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**POSTER DISCOUNT ($50 OFF)**

Poster abstracts are due by April 24, 2015. 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.

**ALUMNI DISCOUNT**: Cambridge Healthtech Institute (CHI) appreciates your past participation at Property-Based Drug Design and/or World Pharma Congress. 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 Property-Based Drug Design and/or World Pharma Congress in the past in order to qualify.

**Group Discounts are Available!**
Special rates are available for multiple attendees from the same organization. For more information on group discounts contact David Cunningham at 781-972-5472

**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.

**Please use key code PCM F when registering!**