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Final Agenda

Organized by Cambridge Healthtech Institute

Twelfth Annual

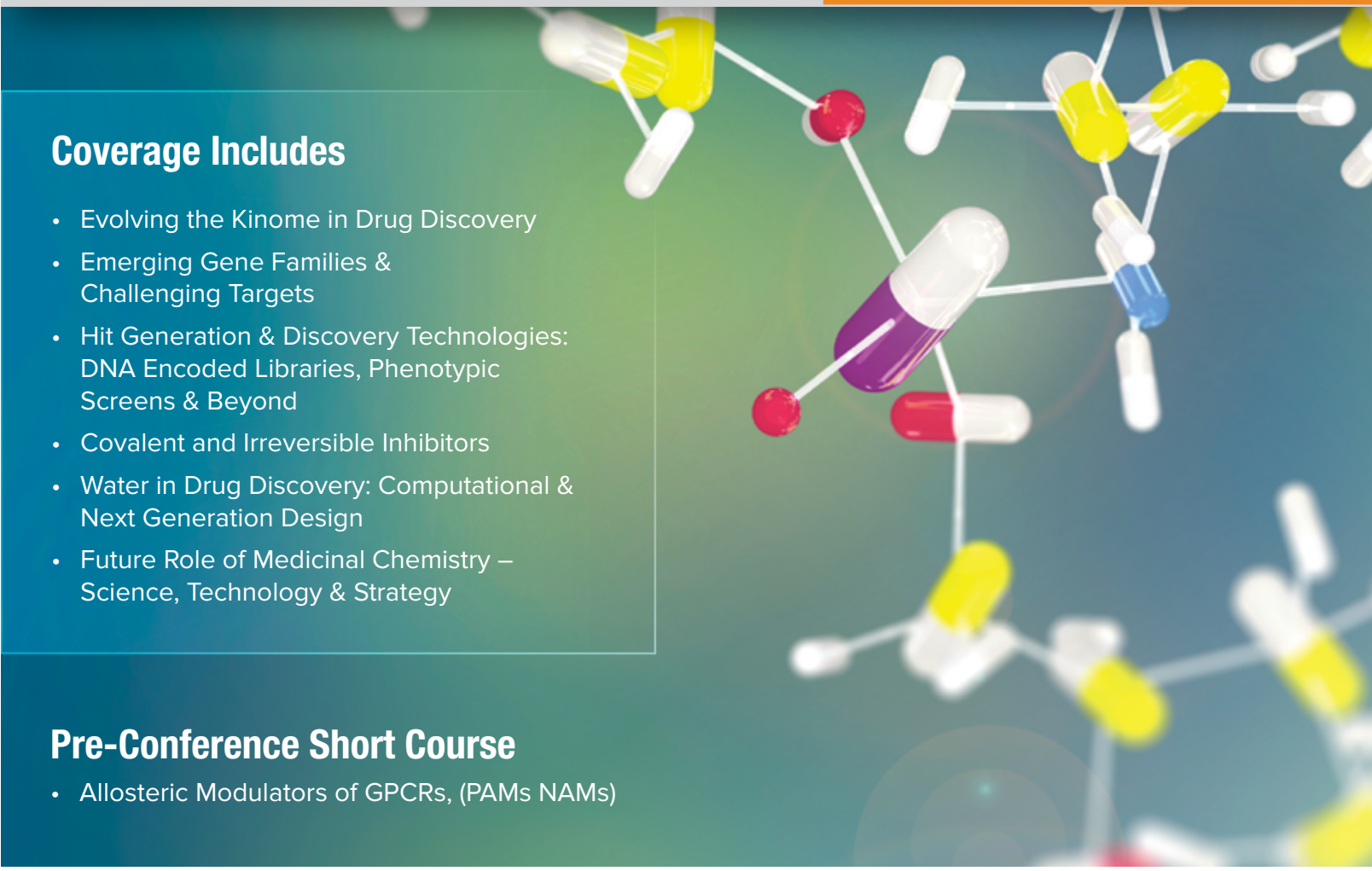
MASTERING MEDICINAL CHEMISTRY

Case Studies, Hot Topics & Med Chem Strategy

JUNE 10-11, 2015

Westin Waterfront
Boston, MA

Part of: WPC WORLD PRECLINICAL CONGRESS



Coverage Includes

- Evolving the Kinome in Drug Discovery
- Emerging Gene Families & Challenging Targets
- Hit Generation & Discovery Technologies: DNA Encoded Libraries, Phenotypic Screens & Beyond
- Covalent and Irreversible Inhibitors
- Water in Drug Discovery: Computational & Next Generation Design
- Future Role of Medicinal Chemistry – Science, Technology & Strategy

Pre-Conference Short Course

- Allosteric Modulators of GPCRs, (PAMs NAMs)

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PRE-CONFERENCE SHORT COURSE

TUESDAY, JUNE 9 | 2:00 – 5:00 PM

Allosteric Modulators of GPCRs, (PAMs NAMs)

The course will provide an overview on allosteric modulation of class A, B and C GPCRs: screening, molecular pharmacology, signal bias, medicinal chemistry and development challenges. For each of these areas, we will cover the theory and best practices while delving into case studies to highlight key challenges and caveats.

Instructors:

Corey Hopkins, M.D., Research Assistant Professor, Vanderbilt Center for Neuroscience Drug Discovery

Cody J. Wenthur, Pharm. D., Graduate Student, Department of Pharmacology, Vanderbilt University Medical Center

Suggested Event Package:

June 9 Short Course*: **Allosteric Modulators of GPCRs, (PAMs NAMs)**

June 10-11: **Mastering Medicinal Chemistry Conference**

June 11-12: **Property-Based Drug Design in Medicinal Chemistry Conference**

June 11 Dinner Short Course*: **Optimizing Physical Properties of Molecules to Achieve High-Quality Clinical Candidates**

** Separate registration required.*

WEDNESDAY, JUNE 10

7:00 am Registration and Morning Coffee

EXECUTIVE PANEL: FUTURE ROLE OF MEDICINAL CHEMISTRY – SCIENCE, TECHNOLOGY & STRATEGY

8:00 Chairperson's Opening Remarks

Stewart L. Fisher, Ph.D., Principal, SL Fisher Consulting, LLC

8:05 Target Validation and Reproducibility - A Chemistry Perspective

Mark Bunnage, Ph.D., Vice President, Worldwide Medicinal Chemistry, Pfizer

Reproducibility of the scientific literature is a topic of significant current interest. This discussion will focus on irreproducibility issues in target validation and what it means for medicinal chemistry.

8:12 So You Want to Improve Your Medicinal Chemistry?

Jeremy J. Edmunds, Ph.D., Director, Immunology Medicinal Chemistry, Abbvie

Once a compound has been made by a medicinal chemist all that remains is to reveal the properties associated with that compound. When one considers the considerable expense that is associated with developing a drug, it is clearly the responsibility of the chemist to ensure that they are preparing the most optimal compound. To achieve this we have focused our efforts within Abbvie medicinal chemistry toward excellence in design and excellence in synthesis. Here we will describe the trials and tribulations of this approach.

8:19 Outsourcing of Medicinal Chemistry

David Bauer, Principal Scientist, Head of Medicinal Chemistry Outsourcing, Amgen

The presentation will give an overview of how leveraging external partnerships is being used at Amgen to support our Medicinal Chemistry organization. The key components of our outsourcing strategy will be discussed.

8:26 Pre-Competitive Collaboration – How AstraZeneca's Open Innovation Program is Changing the Way We Deliver Medicine to Patients

Pamela Hill, Open Innovation Program Manager, Emerging Innovations, AstraZeneca, R&D Boston

The AstraZeneca Open Innovation platform has been created to help us identify and establish mutually beneficial collaborations that will lead to the discovery and development of new medicines. We provide collaborators with access to late-stage compounds, our compound collection as well as our cheminformatics and screening technologies to validate and publish novel science.

8:33 Talk Title to be Announced

Brian Jones, Head, Discovery Chemistry, Novartis Institute of Biomedical Research

8:40 Panel Q&A with Session Speakers

9:05 The Application of Extended Hückel Theory for Pharmacophore Modeling

Sponsored by CHEMICAL COMPUTING GROUP

Michael Drummond, Ph.D., Applications Scientist, Chemical Computing Group

Pharmacophore models play an essential role in drug discovery. Generating pharmacophore models which encode accurate molecular recognition features are highly dependent on properly defined annotation points. Here we have developed a new approach for pharmacophore modeling which is based on a semi-empirical method using Extended Hückel Theory (EHT). The pharmacophore features generated through the EHT annotation scheme take into account ligand resonance and electron withdrawing effects and are sensitive to non-standard interactions, such as C-H and halogen bond interactions, during pharmacophore screening.

9:35 Small Molecules in Cancer Immunotherapy

Jerry L. Adams, Ph. D., Director, Medicinal Chemistry, Immuno-Oncology & Combinations DPU, GlaxoSmithKline Pharmaceuticals

Immunotherapy for cancer became an effective treatment modality in 2011. The first wave of successful immuno-oncology drugs target T-cell co-receptors by interrupting protein-protein interactions, a mechanism typically unachievable with a small molecule drug. The currently available cancer immunotherapies are biologic in nature, such as antibodies, peptides/proteins and more recently, cells. Nevertheless, modulating the immune system through a small molecule approach offers several advantages which are complimentary and potentially synergistic to biologic modalities. Importantly, the successes of checkpoint inhibition provide direction for further advances in the field of immune-oncology, including what roles small molecule drugs might play. Already clinical trials are underway with small molecule drugs in combination with checkpoint inhibitors. This talk will provide an overview of the strategy for and targets druggable by small molecules.

10:05 Coffee Break in the Exhibit Hall with Poster Viewing

EVOLVING THE KINOME IN DRUG DISCOVERY

10:50 Kinase Drug Discovery Past, Present, and Future

Mark Bunnage, Ph.D., Vice President, Worldwide Medicinal Chemistry, Pfizer

Over recent years there has been remarkable progress in the medicinal chemistry design of selective protein kinase inhibitors. There are now over 20 kinase inhibitor drugs on the market and, with the recent approval of the JAK kinase inhibitor Xeljanz® (tofacitinib citrate), we are now seeing kinase drugs emerge for indications beyond Oncology. This presentation will discuss current approaches to kinase inhibitor drug discovery and share a perspective on future directions in the field.

11:20 Secreted Protein Kinases as Novel Regulators of the Extracellular Environment

Malcolm Whitman, Ph.D., Professor, Department of Developmental Biology, Harvard School of Dental Medicine; Department of Cell Biology, Harvard Medical School

Secreted protein kinases, targeting serine, threonine and tyrosine, have recently been identified and shown to act in the secretory pathway and outside the cell. These novel kinases are divergent from intracellular kinases and represent a new class of drug targets for the modulation of secreted protein and extracellular matrix function.

11:50 Sponsored Presentation *(Opportunity Available)*

12:20 pm Luncheon Presentation *(Sponsorship Opportunity Available)* **or Enjoy Lunch on Your Own**

1:00 Refreshment Break in the Exhibit Hall with Poster Viewing

EVOLVING THE KINOME IN DRUG DISCOVERY (CONT.)

1:30 Chairperson's Remarks

Renato Skerlj, Ph.D., Vice President, Drug Discovery and Preclinical Development, Lysosomal Therapeutics, Inc.

1:35 Akt and RNA Metabolism

Philip N. Tsichlis, M.D., Jane F. Desforges Professor of Medicine, Tufts University School of Medicine

A phosphoproteomics screen of isogenic cell lines expressing different Akt isoforms identified RNA metabolism as an Akt target. The phosphorylation of one of the regulators of RNA metabolism (IWS1) was shown to epigenetically regulate alternative RNA splicing. The role of other Akt targets in RNA processing is under investigation.

2:05 Using Ovality to Predict Nonmutagenic, Orally Efficacious Pyridazine Amides as Cell-Specific Spleen Tyrosine Kinase Inhibitors

Matt Lucas, Ph.D., Director, Medicinal Chemistry, Discovery Chemistry and Pharmaceutical Research, Cubist Pharmaceuticals

Tyrosine Kinase Inhibitors' inhibition of spleen tyrosine kinase (SYK) has attracted much attention as a mechanism for the treatment of cancers and autoimmune diseases. The structure-guided optimization of pyridazine amide SYK inhibitors will be presented, along with an approach that led to the successful identification of non-mutagenic examples with reduced cardiovascular liabilities.

EMERGING GENE FAMILIES & CHALLENGING TARGETS

2:35 Solute Carrier Proteins as a Potential Source of New Drug Targets

David Hepworth, Ph.D., Senior Director, Biotherapeutics Chemistry, Worldwide Medicinal Chemistry, Pfizer

Solute carriers (SLCs) are biologically important proteins that control movement of small molecules and ions across membranes. Drug classes that target SLCs include SSRIs and SGLT2 inhibitors. While the SLC family appears to be generally small molecule druggable and is similar in size to the Class A GPCRs, the number drug targets is currently around 10x fewer. The presentation will explore this apparent paradox and provide an overview of the current status of SLC drug discovery.

2:55 Targeting IAP and BCL Protein-Protein Interactions with Small Molecules: Lessons Learned

Brian Aquila, Ph.D., Associate Director, Medicinal Chemistry Oncology Research, AstraZeneca

3:15 Targeting the Arginine Methyltransferases

Kenneth W. Duncan, Ph.D., Associate Director, Molecular Discovery, Epizyme, Inc.

3:35 Modern Drug Research Informatics Applications to CNS, Infectious, Neglected, Rare, and Commercial Diseases

Sponsored by CDD VAULT

Barry Bunin, Ph.D., CEO, Collaborative Drug Discovery (CDD)

A modern approach to drug discovery informatics in 5 collaborative case studies showcasing the CDD Vault will be explored. The CDD Vault manages biological and chemical private data securely with external data.

3:50 Sponsored Presentation *(Opportunity Available)*

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

Plenary Keynote Panel
5:00 pm | Wednesday, June 10

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 Grootenhuis, 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

6:00 Welcome Reception in the Exhibit Hall with Poster Viewing

7:00 Close of Day

THURSDAY, JUNE 11

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.

TABLE 15: Target Vulnerability and Drug:Target Engagement

Moderator: Stewart L. Fisher, Ph.D., Principal, SL Fisher Consulting, LLC

TABLE 16: Blood Brain Barrier Penetrance in Drug Discovery for Med Chemists

Moderator: Byron DeLaBarre, Ph.D., President & Chief Scientist, The Consulting Biochemist, LLC

TABLE 17: Evolving the Kinome in Drug Discovery

Moderator: Renato Skerlj, Ph.D., Vice President, Drug Discovery and Preclinical Development, Lysosomal Therapeutics, Inc.

TABLE 18: Small Molecules and Immunomodulation

Moderator: Jerry L. Adams, Ph. D., Director, Medicinal Chemistry, Immuno-Oncology & Combinations DPU, GlaxoSmithKline Pharmaceuticals

COVALENT AND IRREVERSIBLE INHIBITORS

8:35 Chairperson's Remarks

Byron DeLaBarre, Ph.D., President & Chief Scientist, The Consulting Biochemist LLC

8:45 Covalent Inhibitors as an Approach for Challenging Targets

Atli Thorarensen, Ph.D., Research Fellow, BioTx Medicinal Chemistry, Pfizer

The pharmaceutical industry has in the past decade experienced a decline in innovation of small molecular inhibitors gaining FDA approval. There are many suggestive factors contributing to this decline one of which is that therapeutically important targets are increasingly challenging, preventing the identification of potent and selective chemical modulators. The backdrop to this as a potential solution is the increased focus on design and development of covalent inhibitors. Covalent inhibitors provide potential solutions to this difficult target space but bring additional challenge in medicinal chemistry design due to inhibitors' intrinsic chemical reactivity. This talk will provide an overview of selective covalent drug discovery efforts and what key insights are required for successful covalent drug design.

9:05 Discovery of Covalent Inhibitors of Nedd4-1 Ubiquitin Ligase: First-in-Class Covalent Inhibitor of HECT E3s

Alexander Statsyuk, Ph.D., Assistant Professor, Chemistry Department, Northwestern University

We have developed a novel fragment-based drug discovery technology which we call irreversible tethering. We subsequently used this technology and discovered covalent small molecule inhibitor of Nedd4-1 ubiquitin ligase, an enzyme which is a promising drug target to treat Ebola virus infections, IGF-1 driven human cancers, and degrades alpha-synuclein. Remarkably, the developed inhibitor of Nedd4-1 is a first known covalent inhibitor of protein-protein interactions, and is the first known inhibitor of E3 ligase processivity. We will discuss the mechanism of action of Nedd4-1 inhibitor, such as switching Nedd4-1 mediated polyubiquitin chain growth from processive to distributive.

HIT GENERATION & DISCOVERY TECHNOLOGIES: DNA-ENCODED LIBRARIES, PHENOTYPIC SCREENS & BEYOND

9:25 Direct and Synergistic Inhibition of the HCV NS5A Replication Complex

Makonen Belema, Ph.D., Principal Scientist, Discovery Chemistry, Bristol Myers Squibb Co.

The NS5A protein plays multifunctional roles in the hepatitis C virus replication cycle, and its inhibitors are integral components of a promising combination of HCV therapies that secured regulatory approvals recently. Key aspects of the medicinal chemistry effort that optimized a phenotype screen hit to the first-in-class NS5A inhibitor daclatasvir and highlights of mode-of-action studies that revealed considerable synergistic interaction between two distinct classes of NS5A-interacting molecules will be discussed.

9:45 Hit Generation Technologies – From DNA-Encoded Libraries & Phenotypic Screens, to New Chemical Space

Jörg Holenz, Ph.D., Director, Discovery and Preclinical Sciences, Project Leader, AstraZeneca Pharmaceuticals LP

Lead Generation is defining the quality of chemical assets and - given this importance - has undergone significant changes. New hit generation techniques have been added to the pool, and only by cleverly combining these, the challenge to drug novel demanding targets will be met. This lecture will present learnings from successful lead generation case histories.

10:15 Accounting for Water Energetics in Drug Design

Sponsored by SCHRÖDINGER.

Michelle Lynn Hall, Ph.D., Senior Applications Scientist, Schrödinger

Water plays a ubiquitous role in biology and is critical in understanding molecular recognition. While the importance of water is greatly appreciated, a detailed understanding of how to incorporate water into the drug design process has been elusive. For example, crystallography provides the location of a subset of water molecules but cannot place waters throughout the entire binding site. We present strategies for deciding whether it is better to displace, avoid, or bridge a given water molecule once insight into hydration site energetics are in hand.

10:45 Coffee Break in the Exhibit Hall with Poster Viewing

11:30 Triage of High-Throughput Screening Hits: A PAIN in the Assay

Jonathan B. Baell, Ph.D., Director, Australian Translational Medicinal Chemistry Laboratory and Professor, Medicinal Chemistry, Faculty of Pharmacy and Pharmaceutical Science, Monash Institute of Pharmaceutical Sciences

Mathematically, a standard hit rate of say 0.7% necessarily furnishes more false positives from a high throughput screen than the few (if any) real ligands for that target that may lurk within the set of hits identified. Disturbingly, the false positives can appear to be selective and more potent than real and optimizable compounds and are often pursued only to result in inevitable failure and waste of resources. This talk will outline some personal experiences and reflections along with advice on how to efficiently identify problematic screening hits.

WATER IN DRUG DISCOVERY: COMPUTATIONAL & NEXT GENERATION DESIGN

11:50 Time-Average Solvation Distributions in Drug Design: A Holistic Approach to Drug Discovery, from Binding Kinetics to Dynamic Modeling

Robert Pearlstein, Ph.D., Senior Investigator, Global Discovery Chemistry, Computer-Aided Drug Discovery, Novartis Institutes for BioMedical Research, Inc.

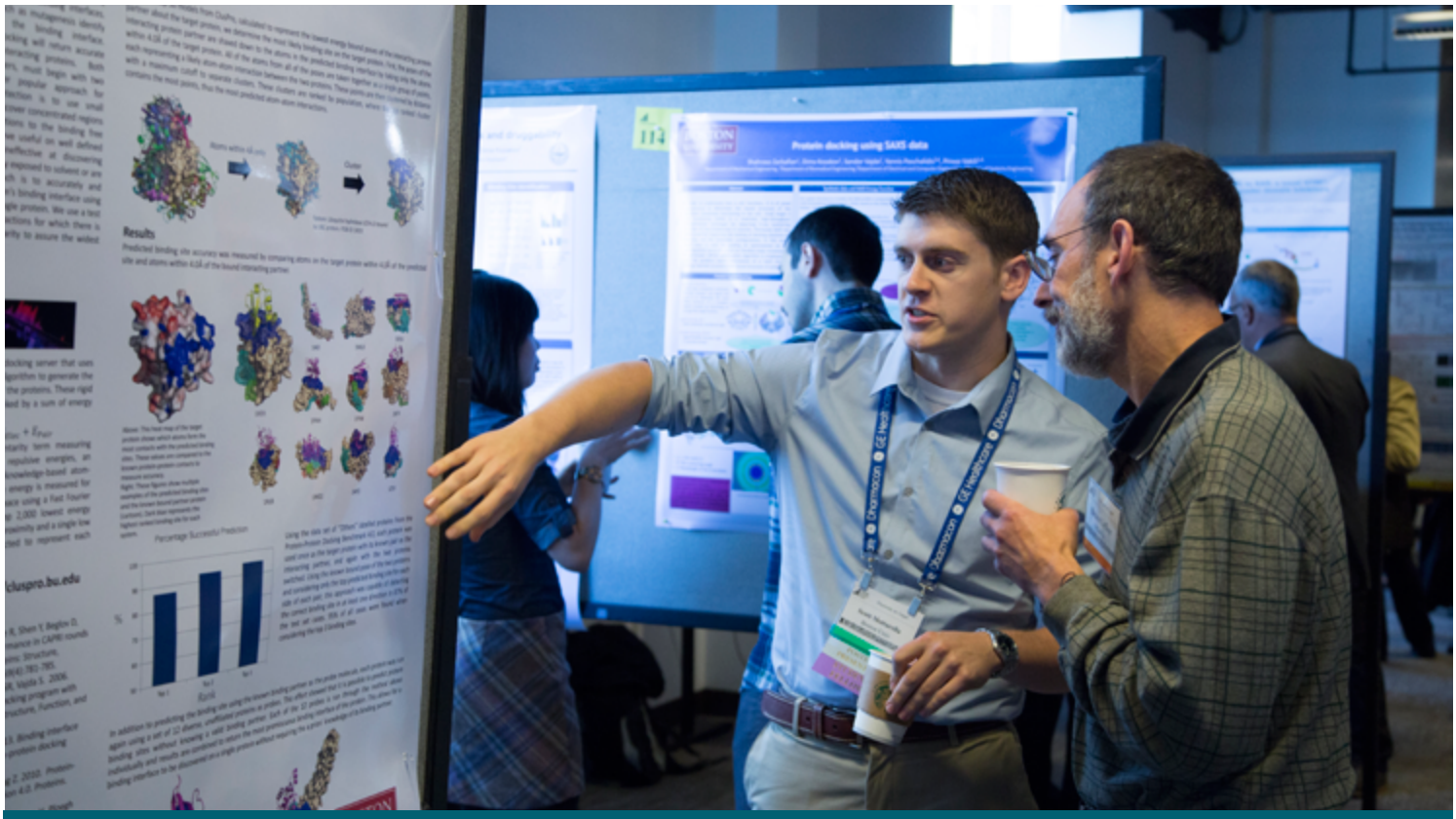
Water is the most important organic molecule in nature and its role in binding processes has been recently made more evident to the computational and medicinal chemistry communities. Our lab has developed a theory from first principles that links solvation to binding kinetics at a molecular level. This allows us to design molecules with desired kinetic profiles, disrupt or enhance specific proton translocation pathways or recapitulate biology from a kinetic viewpoint. We use a comprehensive approach to design chemical matter with optimized pharmaco(binding) kinetics, redefining the role of computational medicinal chemistry in drug discovery.

12:10 pm Designing Water-Soluble Molecules in Drug Discovery

Michael A. Walker, Ph.D., Principal Scientist, Medicinal Chemistry, Bristol-Myers Squibb Pharmaceutical Research and Development

Aqueous solubility is a major issue in the development of a drug since it plays a central role in bioavailability. A number of strategies have been applied by medicinal chemists in order to rationally design molecules which exhibit appropriate solubility. A majority of these approaches are focused on reducing the hydrophobicity of the molecule. This talk will draw upon the literature and from the presenters own work to provide examples where solubility was increased in unexpected ways.

12:30 Close of Conference



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

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/Medicinal-Chemistry
for additional info

PRICING AND REGISTRATION INFORMATION

	Commercial	Academic, Government, Hospital-affiliated
SINGLE CONFERENCE PRICING (Includes access to **Mastering Medicinal Chemistry** only, excludes short courses)		
Registration after May 8 and on-site	$1,949	$899
EVENT PRICING (Mastering Medicinal Chemistry is part of World Preclinical Conference, Includes access to 2 conferences, excludes short courses)		
Registration after May 8 and on-site	$2,999	$1,399

CONFERENCE SELECTION

June 10-11, 2015	June 11-12, 2015
Mastering Medicinal Chemistry	Property Based Drug Design Tumor Models for Cancer Immunotherapy 3D Cellular Models Targeting Histone Acetylation Chemical Proteomics for Target Validation Functional Genomics Technologies Training Seminar: Applying Pharmacology to New Drug Discovery

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Poster Discount	$50 Off

SHORT COURSES

Single Short Course	$699	$399
Two Short Courses	$999	$699
Three Short Courses	$1,199	$899

SHORT COURSE SELECTIONS

Tuesday, June 9 | 2:00 - 5:00 PM	Thursday, June 11 | 7:00 – 10:00 pm (Dinner provided)
• Allosteric Modulators of GPCRs, (PAMs NAMs)	• ~~Optimizing Physical Properties of Molecules to Achieve High-Quality Clinical Candidates~~ • How to Best Utilize Organotypic 3D Cell Cultures in Oncology • 3D Printing • PDX Models Update
Tuesday, June 9 | 6:00 – 9:00 pm (Dinner provided)	
• ~~Biased GPCR Ligands: Towards Novel Drug Discovery~~ • Understanding and Dealing with Drug Disposition in CNS • Navigating the CiPA Landscape • ~~Imaging in Cancer Research: Modalities, Agents and Strategies~~	

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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.**
* CHI reserves the right to publish your poster title and abstract in various marketing materials and products.

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Alumni Discount: Cambridge Healthtech Institute appreciates your past participation at Mastering Medicinal 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 Mastering Medicinal Chemistry in the past in order to qualify.

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If you are unable to attend but would like to purchase the Mastering Medicinal Chemistry 2015 CD for $350 (plus shipping), please visit healthtech.com/Medicinal-Chemistry. Massachusetts delivery will include sales tax.

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.

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Please use keycode **MCH F** when registering!