



Tenth Annual

Mastering Medicinal Chemistry

In an Era of Tough Targets

February 13-15, 2013

Moscone North Convention Center
San Francisco, CA

Featured Presentation:



**Using Synthetic Chemistry
to Answer the Challenge
of Increasing Molecular
Complexity in Small
Molecule Drug Discovery**

Simon Bailey, Ph.D., Senior Director,
Worldwide Medicinal Chemistry
Oncology, Pfizer

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Cambridge Healthtech Institute

Cutting Edge Chemistry Case Studies:

- Macrocycles
- Payload Linker and Conjugation Technologies
- Epigenetic Targets
- GPCRs
- Protein-Protein Interactions
- Phenotypic Screening

Novel Approaches to Medicinal Chemistry:

- Novel Technologies for Synthesis
- Medicinal Chemistry Design
- Matched Pairs as a Med Chem Tool
- Flow in Medicinal Chemistry



Molecular Med
TRI-CON 2013

February 11-15 • Moscone North Convention Center • San Francisco, CA

TriConference.com/Medicinal-Chemistry

Conference Programs:

Feb 13-15

Diagnostics Channel

Molecular Diagnostics
Personalized Diagnostics
Cancer Molecular Markers
Circulating Tumor Cells
Digital Pathology – NEW
Companion Diagnostics – NEW

Therapeutics Channel

Mastering Medicinal Chemistry

Cancer Biologics
Clinical and Translational Science

Clinical Channel

Oncology Clinical Trials
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Informatics Channel

Bioinformatics in the Genome Era
Integrated R&D Informatics and Knowledge Management

Cancer Channel

Cancer Molecular Markers
Circulating Tumor Cells
Predictive Pre-Clinical Models in Oncology – NEW
Oncology Clinical Trials
Cancer Biologics

Co-located Event



BAYBIO

Entrepreneur & Investor Roundtables

February 14, 2013, 4:00-7:00 pm
Connect with corporate venture, angel investors and VCs
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Symposia*:

Feb 11-12

Targeting Cancer Stem Cells
Genomics in Medicine – NEW
Point-of-Care Diagnostics
Quantitative Real-Time PCR – NEW
Next Generation Pathology

Partnering Forum*:

Feb 11-12

Emerging Molecular Diagnostics

Short Courses*:

Feb 12

1:30-4:30pm

SC1 Identification & Characterization of Cancer Stem Cells
SC2 Commercialization Boot Camp: Manual for Success in the Molecular Diagnostics Marketplace
SC3 NGS Data and the Cloud
SC4 Best Practices in Personalized and Translational Medicine
SC5 Latest Advances in Molecular Pathology
SC6 Regulatory Approval of a Therapeutic & Companion Diagnostic: Nuts & Bolts
SC7 PCR Part I: qPCR in Molecular Diagnostics
SC8 Data Visualization
SC9 Methods for Synthesis & Screening of Macrocyclic Compound Libraries

5:00-8:00pm (Dinner)

SC10 PCR Part II: Digital PCR Applications and Advances
SC11 Sample Prep and Biorepositories for Cancer Research
SC12 Next-Generation Sequencing in Molecular Pathology: Challenges and Applications
SC13 Strategies for Companion Diagnostics Development
SC14 Patient-Derived Cancer Tissue Xenograph Models
SC16 Microfluidics Technology and Market Trends
SC17 Open Cloud & Data Science

**Separate reg required with a la carte pricing*



TRI-CON All Access Package

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Recommended Short Course*:

1:30 - 4:30 on Tuesday, February 12

SC9 Methods for Synthesis and Screening of Macrocytic Compound Libraries

Macrocytic 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, including current methods for synthesizing and screening macrocytic compound libraries, pros, cons and challenges of different methodologies, and examples of successful macrocytic inhibitors.

Course Instructors:

Dehua Pei, Ph.D., Professor of Chemistry and Biochemistry, The Ohio State University

Mark L. Peterson, Ph.D., Vice President, Operations, Transzyme Pharma

* Separate Registration Required

WEDNESDAY, FEBRUARY 13

7:00 am Registration and Morning Coffee

Plenary Keynote Session

8:00 Plenary Keynote Presentation (See web for details)

9:40 Refreshment Break in the Exhibit Hall with Poster Viewing

Increasing Complexity, Macrocycles, 3-D Structure, Shape & Chirality

11:00 Chair's Remarks: Nick Terrett, Ph.D., CSO, Ensemble Therapeutics Corp.

11:10 Opening Address: Using Synthetic Chemistry to Answer the Challenge of Increasing Molecular Complexity in Small Molecule Drug Discovery

Simon Bailey, Ph.D., Senior Director, Worldwide Medicinal Chemistry Oncology, Pfizer

This presentation will provide examples of the positive benefits of increased molecular complexity in small molecule drug candidates and illustrate how medicinal chemists can adopt new synthetic chemistry strategies to access molecularly complex compounds.

11:40 Beyond the Rule of Five – Novel Strategies for Accessing Macrocytic Chemical Space

Keith James, President, Ferring Research Institute; Visiting Investigator, The Scripps Research Institute

Macrocycle-based drug design represents a compelling strategy for addressing challenging molecular targets, and an exciting new frontier in drug discovery. This presentation will describe both novel strategies for accessing this intriguing region of chemical space, and some unique properties of macrocytic systems.

12:10 pm Moving in New Circles – An Introduction to Macrocycles in Drug Discovery

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

Recently there has been a rapid growth in interest in small molecules outside of Lipinski 'Rule of 5' space. Macrocytes can bind to challenging protein targets and maintain good drug-like properties offering a new fertile direction for drug discovery.

12:40 Exploiting the Chemical Space of Macrolides as Promising Templates for New Drugs

Sponsored by



Vesna Gabelica Markovic, Ph.D., Senior Director, Chemistry, Fidelita

Macrolides are stereospecific macrolactones with drug-like physicochemical properties. This will be demonstrated in the presentation with examples which describe the design and evaluation of novel classes of anti-infective and anti-inflammatory macrolides.

1:45 20th Anniversary Cake in the Exhibit Hall with Poster Viewing

Payload Linker and Conjugation Technologies

2:15 Chairperson's Remarks

2:20 Design of Novel Linkers, Payloads & Antibody-Drug Conjugates for the Treatment of Cancer

Christopher J. O'Donnell, Ph.D., Senior Director, Oncology Medicinal Chemistry, Pfizer

ADCs are an emerging modality for the treatment of cancer. This talk will focus on Pfizer's innovative chemistry strategy to discover and develop new linker-payload classes that will yield more efficacious and potentially better tolerated conjugates to advance this area of research.

2:50 ADCs for the Treatment of Cancer

John Flygare, Ph.D., Sr. Scientist, Discovery Chemistry, Genentech

Combining the specificity of a monoclonal antibody with the cell killing ability of a cytotoxic agent is an outstanding method for treating cancer. This presentation will review successful applications of this technology and discuss future directions of linkers and cytotoxic drugs used in this approach.

3:20 Using Small Molecules to Engineer and Explore Human Immunity

David A. Spiegel, Ph.D., Associate Professor of Chemistry, Yale

This talk describes research efforts in our laboratories toward the design, synthesis, and characterization of small molecule antibody recruiting therapeutics. It is our hope that this strategy will serve as a starting point toward entirely novel scientific insights and therapeutic approaches.

Lead Sponsoring Publications:

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3:50 Rationalization and Visualization of Non-Standard Interactions: The Effect of Thyronine Halogen Substituents on Thyroid Hormone Receptor Binding

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

4:20 Networking Reception in the Exhibit Hall with Poster Viewing (Sponsorship Opportunities Available)

5:20 Breakout Discussions in the Exhibit Hall

- Macrocycles & Exploring the Middle Space
- Payloads, Linkers and Conjugates
- Epigenetic Targets – The Way Forward
- Protein-Protein Interactions

6:20 Close of Day

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12:15 pm Knowledge Mining by Structure Search

Jinbo Lee, Ph.D., CSO, Scilligence Corporation

With prevalence of cross-organization collaborations and R&D reorganizations, knowledge can be easily lost in a large pile of unstructured data such as PPT, Word, Excel and PDF. Through a case study example, knowledge mining and preservation by structure searching makes possible by Chawler/Chem4Sharepoint.

1:15 Refreshment Break in the Exhibit Hall with Poster Viewing

Hot Targets to Watch: Epigenetic Targets

1:40 Chairperson's Remarks: Ed Olhava, Epizyme, Inc.

1:45 Chemically Targeting the Histone Lysine Methyltransferase EZH2 (Enhancer of Zeste Homolog 2)

Sharad K. Verma, Ph.D., Investigator, Medicinal Chemistry, GlaxoSmithKline

The histone lysine methyltransferase EZH2 is frequently over-expressed in a variety of cancerous tissues. The synthesis and development of highly potent and selective small molecule inhibitors of EZH2 will be described from a medicinal chemistry perspective.

2:15 Inhibition of BET Bromodomains for the Treatment of Cancer

Brian K. Albrecht, Ph.D., Senior Director, Medicinal Chemistry, Constellation Pharmaceuticals

Inhibition of the BET bromodomain family of chromatin readers leads to effective tumor growth inhibition in xenograft models. The discovery and optimization of a series of potent and selective isoxazoloazepine BET inhibitors will be presented.

2:45 Discovery of EPZ-5676, A Potent and Selective Inhibitor of the Histone Methyltransferase DOT1L

Ed Olhava, Ph.D., Assoc. Dir., Pre-Clinical Development, Epizyme, Inc.

The clinical candidate EPZ-5676, a DOT1L inhibitor for treatment of MLL-rearranged leukemia, is described. The lead series was discovered via structure guided design. Crystallography aided optimization of the pharmacokinetic properties and potency of this series led to EPZ-5676.

3:15 Advances in the Treatment of Water Molecules for Assessing Druggability, Understanding SAR, and Computing Binding Energies

Chris Higgs, Senior Applications Scientist, Schrödinger

Significant progress has recently been made in the treatment of water molecules in drug design. Specifically, the ability to compute the thermodynamic properties of individual waters has allowed researchers to gain insights into the biomolecular recognition process that was not previously possible. Here, we present the latest advances in the WaterMap method and applications to assessing druggability, SAR, affinity, and selectivity. We highlight examples where knowledge of explicit water thermodynamics is essential in understanding the molecular recognition process.

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THURSDAY, FEBRUARY 14

7:00 am Breakfast Presentation (Sponsorship Opportunity Available) or Morning Coffee

8:00 Plenary Keynote Panel (See Web for Details)

9:40 Refreshment Break in the Exhibit Hall with Poster Viewing

Increasing Complexity (Continued)

10:40 Chair's Remarks: Michael Foley, Broad Institute

10:45 Membrane Permeability and Oral Bioavailability of Macrocycles

Matthew P. Jacobson, Ph.D., Professor, Pharmaceutical Chemistry, Department of Bioengineering and Therapeutic Science, University of California San Francisco

I will discuss the emerging understanding of how synthetic and natural product macrocycles achieve membrane permeability and oral bioavailability, despite not being considered drug-like by many simple criteria. Examples will include cyclic peptides and polyketides, emphasizing design strategies.

11:15 Synthetic Macrocycles: Leveraging Natures Design Strategy

Michael Foley, Ph.D., Director, Chemical Biology, Broad Institute

This presentation will describe progress towards creating a macrocycle collection at the Broad Institute using the build-couple-pair strategy for diversity-oriented synthesis. Case studies of several DOS-derived macrocycles will be presented as an example of the utility of this screening collection against 'undruggable' targets.

11:45 Molecular Complexity and Promiscuity

Frank Lovering, Ph.D., Principle Scientist II, Computational Chemistry, Pfizer

Complexity, as measured by fraction sp3 and the presence of chiral centers, impacts success in the clinic. We illustrate the relationship between complexity and promiscuity as well as Cyp450 inhibition - factors that are critical to success in drug discovery.

3:45 Valentine's Day Celebration and Poster Competition Winner Announced in the Exhibit Hall
(Last Chance to View Posters)

Hot Targets To Watch: GPCRs

4:30 Chair's Remarks: *Graeme Semple, Arena Pharmaceuticals*

4:35 Discovery of APD811: An Orally Available Prostacyclin Receptor Agonist for the Treatment of Pulmonary Arterial Hypertension

Graeme Semple, Ph.D., Vice President, Discovery Chemistry, Arena Pharmaceuticals, Inc.

Our design and SAR of new prostacyclin receptor agonists for PAH will be described. Special attention was paid to pharmacokinetic behavior and pharmaceutical properties of prospective candidates.

5:05 The New Era of Structure-Based Drug Design GPCRs

Jonathan S. Mason, Ph.D., Drug Design & Computational Chemistry, Heptares Therapeutics Ltd.

The wealth of new GPCR structures enables full SBDD for this important target class. Druggability analyses will be presented, and multiple structure-based candidate designs from the mutationally stabilized receptors (StaRs) used at Heptares that uniquely exist in precisely defined biologically-relevant conformations.

Hot Targets to Watch: PPI

5:35 Has Fragment Discovery Helped Us Solve the Protein-Protein Interactions Challenge?

Michelle R. Arkin, Ph.D., Associate Adjunct Professor, Pharmaceutical Chemistry, UCSF School of Pharmacy

We will describe some of the issues and advances in tackling protein-protein interactions by fragment-based lead discovery. We utilize a range of approaches to understand molecular recognition features that lead to binding to protein interfaces and to develop inhibitors of these challenging targets.

6:05 Sponsored Presentations (Opportunities Available)

6:35 Close of Day

FRIDAY, FEBRUARY 15

8:00 am Morning Coffee

Hot Targets to Watch: PPI (Continued)

8:30 Chair's Remarks: *Stephen Hale, Ensemble Therapeutics*

8:35 Monomeric and Dimeric SMAC Mimetics as Pro-Apoptotic Agents in Anticancer Therapy

Pierfausto Seneci, Ph.D., Professor, Chemistry, University of Milan

This talk will include details of a rational design, synthesis, *in vitro* and *in vivo* biological profiling of potent oncology candidates. An integrated approach was employed using X-ray, NMR, computational chemistry, medicinal chemistry, *in vitro* biology and pharmacology among others.

9:05 The Solution to "Tough-to-Drug" Targets: An Integrated Discovery Engine Leveraging the Unique Properties of Synthetic Macrocycles

Stephen Hale, Ph.D., Vice President, Drug Discovery, Ensemble Therapeutics

Many high-value targets have proven to be intractable to traditional "small-molecule" discovery efforts. Ensemble has a discovery platform that allows for the rapid identification of novel macrocyclic compounds active against challenging targets, including protein:protein interaction targets.

Novel Approaches to Medicinal Chemistry

9:35 Technologies for Synthesis: Development of Macrocyclic Inhibitors against K-Ras Protein

Speaker to be Announced

Developing small-molecule inhibitors against Ras has met with many challenges. A high-throughput method has been developed to synthesize, screen, and decode macrocyclic compound libraries of 107 diversity. Screening of such libraries has identified compounds that disrupt Ras-effector complexes at high nanomolar to low micromolar concentrations.

10:05 Sponsored Presentations (Opportunities Available)

10:35 Coffee Break

11:00 Phenotypic Screening & Chemical Biology: Development of Isoform Selective Inhibitors of Class I and Class II HDACs for CNS and Metabolic Disorders

Edward, Holson, Ph.D., Director, Stanley Center for Psychiatric Research, Broad Institute of MIT and Harvard

Taking a chemical genetics approach, we have developed a "toolkit" of HDAC inhibitors which includes a variety of highly potent and selective inhibitors. These novel inhibitors include HDAC 1: HDAC1,2: HDAC 3: HDAC 1,2,3: HDAC 6: and the first demonstration of HDAC 6,8 inhibitors.

11:30 Medicinal Chemistry Design: Delta-Selective Opioid Agonists for the Treatment of Chronic Pain

Robin Polt, Ph.D., Professor of Chemistry & Biochemistry, BIO5, University of Arizona

Here we report the synthesis of a series of glycosylated deltorphin-based peptides that possess selectivity and efficacy for the delta opioid receptor (DOR). From this series, a lead candidate compound (BBI 11008) was identified.

12:00 pm Discovery and Optimization of Selective JAK1 Inhibitors as Potential Treatments for Rheumatoid Arthritis

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

We wished to identify JAK1 inhibitors as prospective therapeutics for rheumatoid arthritis (RA) and other immunologic disorders. Details of the design and optimization efforts, as well as the biological characterization and chemical structure of the lead compound will be presented.

12:30 Luncheon Presentations (*Sponsorship Opportunities Available*) or **Lunch on Your Own**

1:45 Chairperson's Remarks: *Elizabeth Farrant, Cyclofluidic Ltd*

1:50 Matched Pairs: Mastering Medicinal Chemistry with Molecular Matched-Pairs

Jonas Boström, Ph.D., Computational Chemist, Medicinal Chemistry, AstraZeneca

We will present novel and efficient matched-pair approaches, combined with important medicinal chemistry data, and demonstrate use in drug design. Observations affecting lipophilicity will be given extra attention.

2:20 Flow Chemistry: Generation of Kinase Structure Activity Data Using Integrated Microfluidic Synthesis, Screen and Design

Elizabeth Farrant, Ph.D., Chief Business Officer, Cyclofluidic Ltd

This presentation describes the application of an integrated microfluidic platform where potential lead molecules are designed, synthesized, purified and screened in fast serial mode.

2:50 Flow Chemistry: Integrating Flow Chemistry in Drug Discovery

Noel S. Wilson, Ph.D., Senior Scientist I, Global Pharmaceutical Discovery, Hit to Lead, Abbott Laboratories

3:20 Close of Conference

Hotel Information

Reserve your hotel and save \$100 off your conference registration*

*You must book your reservation under the Tri-Conference room block for a minimum of 4 nights at the Marriott or the Intercontinental Hotel. One discount per hotel room.

Conference Venue:

The Moscone North Convention Center
747 Howard Street
San Francisco, CA 94103
www.moscone.com



Host Hotel:

San Francisco Marriott Marquis
55 Fourth Street
San Francisco, CA 94103
(T) 415-896-1600
Reservations: 888-575-8934

Discounted Group Rate: \$229 s/d*
Cutoff Date: January 14, 2013

* Room Rate includes complimentary internet access in your guestroom

Additional Recommended Hotel:

InterContinental San Francisco Hotel
888 Howard Street
San Francisco, CA 94103
(T) 415-616-6500

Discounted Group Rate: \$235 s/d
Cut Off Date: January 14, 2013

Please visit TriConference.com to make your reservations online or call the hotel directly to reserve your sleeping accommodations. You will need to identify yourself as a Molecular Med Tri-Con 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.

Sponsorship & Exhibit 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. Signing on early will allow you to maximize exposure to hard-to-reach decision makers.

Breakfast & Luncheon Presentations

Opportunities may include a 15 or 30-minute podium presentation during the main agenda. Boxed lunches are delivered into the main session room, which guarantees audience attendance and participation. Packages include: exhibit space, on-site branding, and more.

Invitation-Only VIP Dinner/Private Receptions

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.

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Includes 1 Symposium or Partnering Forum, 2 Short Courses, and 1 Conference Program.	Commercial	Academic, Government, Hospital-affiliated
Advance Registration until January 18, 2013	\$3195	\$1845
Registration after January 18, 2013	\$3250	\$1930

Regular Pricing – A La Carte Options

PARTNERING FORUM (Monday, Feb 11 – Tuesday, Feb 12)

Emerging Molecular Diagnostics	\$1450
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SYMPOSIA (Monday, Feb 11 – Tuesday, Feb 12)

	\$1450	\$1025
S1 Targeting Cancer Stem Cells	S2 Genomics in Medicine	S3 Point-of-Care Diagnostics
S4 Quantitative Real-Time PCR	S5 Next Generation Pathology	

SHORT COURSES (Tuesday, Feb 12)

1 Short Course	\$695	\$395
2 Short Courses	\$995	\$695

Afternoon

- SC1 Identification & Characterization of Cancer Stem Cells
- SC2 Commercialization Boot Camp: Manual for Success in the Molecular Diagnostics Marketplace
- SC3 NGS Data and the Cloud
- SC4 Best Practices in Personalized and Translational Medicine
- SC5 Latest Advances in Molecular Pathology
- SC6 Regulatory Approval of a Therapeutic & Companion Diagnostic: Nuts & Bolts
- SC7 PCR Part I: qPCR in Molecular Diagnostics
- SC8 Data Visualization
- SC9 Methods for Synthesis & Screening of Macrocyclic Compound Libraries

Dinner

- SC10 PCR Part II: Digital PCR Applications and Advances
- SC11 Sample Prep and Biorepositories for Cancer Research
- SC12 Next-Generation Sequencing in Molecular Pathology: Challenges and Applications
- SC13 Strategies for Companion Diagnostics Development
- SC14 Patient-Derived Cancer Tissue Xenograph Models
- SC16 Microfluidics Technology and Market Trends
- SC17 Open Cloud & Data Science

CONFERENCE PROGRAMS (Wednesday, Feb 13- Friday, Feb 15)

Advance Registration until January 18, 2013	\$2145	\$1195
Registration after January 18, 2013	\$2345	\$1245

Diagnostics Channel

- P1 Molecular Diagnostics
- P2 Personalized Diagnostics
- P3 Cancer Molecular Markers
- P4 Circulating Tumor Cells
- P5 Digital Pathology– NEW
- P6 Companion Diagnostics– NEW

Therapeutics Channel

- P7 Mastering Medicinal Chemistry Summit
- P9 Cancer Biologics
- P11 Clinical and Translational Science

Clinical Channel

- P10 Oncology Clinical Trials
- P11 Clinical and Translational Science
- P12 Clinical Sequencing– NEW

Informatics Channel

- P13 Bioinformatics
- P14 Integrated R&D Informatics & Knowledge Management

Cancer Channel

- P3 Cancer Molecular Markers
- P4 Circulating Tumor Cells
- P15 Predictive Pre-Clinical Models in Oncology – NEW
- P10 Oncology Clinical Trials
- P9 Cancer Biologics

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Poster (\$50 Off) Alumni (20% Off) BayBio (20% Off)

*Alumni and BayBio Discount cannot be combined. Discounts not applicable on Event Short Courses

Alumni Discount SAVE 20%: We appreciate your past participation at the Molecular Med TRI-CON. Through loyalty like yours, this event has become a must-attend for senior level decision makers. As a result of your great loyalty, we are pleased to extend this exclusive opportunity to save an additional 20% off the registration rate.

Hotel Discount (\$100 Off): Reserve your hotel and save \$100 OFF your conference registration *you must book your reservation under the Tri-Conference room block for a minimum of 4 nights.

Poster Submission: Discount (\$50 Off) Dedicated poster sessions for Symposia and Conference Programs. Present your poster at both! ** Poster abstracts are due by **December 21, 2012**. 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.

* CH reserves the right to publish your poster title and abstract in various marketing materials and products. ** One poster discount per registration.

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

How to Register: **TriConference.com/therapeutics**
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Please use
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