



# FRAGMENT-BASED LEAD DISCOVERY CONFERENCE

George Sherman Union, Boston University, Boston  
22 to 25 September 2024

## Sunday, 22 September 2024

- 1:30 PM **Registration opens**
- 2:00 PM **Workshop**  
**Introduction to Fragment-Based Design**  
Dr. Dan Erlanson, Frontier Medicines & Dr. Ben Davis, Vernalis Research
- 5:00 PM **Exhibition opens**
- 6:00 PM **Networking Welcome Reception**

We are delighted to invite you to join us for our Networking Welcome Reception in the Ziskind Lounge. This reception will be an excellent opportunity to mingle with fellow attendees, speakers, and industry leaders in a relaxed and informal setting. Please come and enjoy an evening of networking, drinks, and finger food as we kick off what promises to be an exciting conference.

**8:30 PM End Day 1**

## Monday, 23 September 2024

**8:00 AM Registration Opens & Poster Breakfast**

**Session 1 – Fragments Past and Present**  
**8:30 AM to 10:30 AM**

Chair: Dr. Joe Patel, Nexo Therapeutics

8:30 AM Welcome Note  
Dr. Joe Patel, Nexo Therapeutics

8:45 AM **Opening Keynote**  
*25 Years of Thinking Small*  
Dr. David Rees, Astex Pharmaceuticals

9:30 AM **Invited Speaker**  
*Using Fragments to Answer Questions in Exploratory Drug Discovery*  
Prof. Rod Hubbard, University of York and Vernalis Research

10:00 AM *FBDD Approaches to Tackle Emerging Multi-Component Therapeutic Targets*  
Dr. Juliet Morgan, Sygnature Discovery



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10:30 AM

Networking Break

## Session 2 – Methods

Chair: Dr. Tony Giannetti, Carterra

11:00 AM to 12:15 PM

11:00 AM *Photoactivated Covalent Capture of DNA-Encoded Fragments to Identify Ligands for Challenging Targets*  
Dr. Ben Davis, Vernalis Research

11:30 PM *Expanding Chemical Diversity in Drug Discovery Through Novel Amine-Acid Coupling*  
Ruheng Zhao, University of Michigan

12:00 PM *Biophysical and Structural Biology Methods Enable Fragment-Based Ligand Discovery*  
Dr. Moran Jerabek-Willemsen, WuXi AppTec



12:15 PM

Networking Lunch

12:30 PM Lunchtime Workshop:  
*Fragment-based Design: Scaffold Hopping, Fragment Growing and Bioisosteric Replacements*  
Dr. Michael Drummond, Chemical Computing Group



## Session 3 – Crystallography

Chair: Dr. Ben Davis, Vernalis Research

2:00 PM to 3:45 PM

2:00 PM **Invited Speaker**  
*High-Quality Hits from Xchem with Fast-Forward Fragments Combining HT Crystallography, Fragment Merging and Low-Cost Robotics*  
Prof. Frank von Delft, Oxford University/Diamond Lightsource

2:30 PM *Fast fragment hit-to-lead in drug discovery for novel drug targets*  
Dr. Debanu Das, Xpose Therapeutics

3:00 PM *Crystallographic fragment screening identifies diverse chemical scaffolds for Zika virus NS2B-NS3 protease inhibitor development*  
Dr. Xiaomin Ni, Oxford University

3:30 PM *Accelerating Drug Discovery: Advanced Structural Biology Solutions at ALPX*  
Dr. Andrea Pica, ALPX





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**3:45 PM**

**Networking Break**

**Session 4 – Computational I**  
**4:15 PM to 5:45 PM**

Chair: Prof. Rod Hubbard, University of York

4:15 PM *Invited Speaker*

*AI-First Fragment-Based Drug Discovery at Isomorphic Labs*  
Dr. Rebecca Paul, Isomorphic Labs

4:45 PM *Computational Hot Spot Mapping for Fragment-Based Lead Discovery*  
Prof. Diane Joseph-McCarthy, Boston University

5:15 PM *High-Throughput Activity-Based Fragment Screening with Ulysses™:*  
*Generating Robust Datasets for Machine Learning-Driven Drug Discovery*  
Thomas Fleming, Spirochem/Actoris



**5:30 PM**

**Poster Session**

5:30 PM *Poster Flash Talks*

Join us for a drink and finger food during our poster and networking session. Make the most of the chance to talk to the speakers and fellow delegates. Discover more collaboration opportunities or get answers to your burning questions on fragment-based lead discovery that go beyond the topics discussed today.

**7:00 PM**      **End Day 2**



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**Tuesday, 24 September 2024**

**8:00 AM Poster Breakfast**

**Session 5 – Success Stories**  
**8:45 AM to 10:15 AM**

Chair: Dr. Dan Erlansson, Frontier Medicines

**8:45 AM Invited Speaker**

*Fragment-Based Discovery of Novel and Potent STING Agonist*  
Dr. Chaohong Sun, Abbvie

**9:15 AM** *Fragment-Based Discovery of Allosteric Modulators of  $\beta$ -Glucocerebrosidase*  
Dr. Puja Pathuri, Astex Pharmaceuticals

**9:45 AM** *Identification and Development of Fragment-Derived Chemical Matter in Previously Unknown Allosteric Sites of WRN*  
Dr. Daniel Wyss, Merck & Co.

**10:15 AM**

**Networking Break**

**Session 6 – Computational II**  
**11:00 AM to 12:30 PM**

Chair: Prof. Diane Joseph-McCarthy, Boston University

**11:00 AM Invited Speaker**

*Combining Active Learning, Synthesis on Demand Libraries, and Fragment Screening in Early Drug Discovery*  
Dr. Pat Walters, Relay Therapeutics

**11:30 AM** *Marrying Structures with Computation for Augmented Fragment-Based Drug Discovery*  
Dr. Paul Mortenson, Astex Pharmaceuticals

**12:00 PM** *Fragment-Based Identification and Analysis of Cryptic Ligand Binding Sites*  
Dr. Sandor Vajda, Boston University



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**12:30 PM**

**Networking Lunch**

**Session 7 – Fragments Against SARS-CoV-2**  
**1:45 PM to 3:15 PM**

Chair: Dr. Daniel Wyss, Merck & Co.

**1:45 PM Invited Speaker**

*The SARS-CoV-2 Macrodomein and How to Inhibit it*

Prof. James Fraser, University of California, San Francisco

**2:15 PM** *Utilizing FBDD Screening to Develop a Novel Class of Inhibitors for SARS-Cov-2  
Papain-Like Protease*

Dr. Ashley Taylor, Vanderbilt University

**2:45 PM** *Fragment-Based Lead Discovery Against SARS-CoV-2 nsp3 Macrodomein*

Dr. Thomas Vargo, PostEra

**3:15 PM**

**Networking Break**

**Session 8 – SARS-CoV-2 and Beyond**  
**3:45 PM to 5:30 PM**

Chair: Prof. Martin Scanlon, Monash University

**3:45 PM** *From Fragments to In-Vivo Optimized Leads for the SARS-CoV2 Nsp3 Macrodomein  
Mac1 – An Emerging Target in Antiviral Therapy*

Prof. Adam Renslo, University of California, San Francisco

**4:15 PM** *Development of EcDsbA Inhibitors as Antivirulence Agents*

Dr. Yildiz Tasdan, Monash University

**4:45 PM** *Accelerating Structure Enabled Antiviral Discovery Through Crystallographic Fragment  
Screening with The Xchem Platform*

Dr. Blake Balcomb, Oxford University/Diamond Lightsource

**5:15 PM** *Every Crystal Matters*

Holger von Möller, Molox GmbH

**5:30 PM End Day 2**

**7:00 Conference Dinner at Nightshift Brewing**

Join us for an unforgettable evening of networking and dinner at Night Shift Brewing at Boston's Lovejoy Wharf. Overlooking the Boston Harbour, this venue provides an excellent opportunity to delve further into today's topics. Savour delicious local brews and gourmet bites while fostering your network.



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**Wednesday, 25 September 2024**

**8:00 AM Poster Breakfast**

**Session 9 – Finding New Sites with Fragments**  
**9:00 AM to 10:15 AM**

Chair: Dr. Heike Schönherr, Relay Tx

9:00 AM *Biological Validation of a Novel eIF4E Binding Site Identified by Fragment Screening Using Mutational Analysis and Targeted Protein Degradation*  
Andrew Woodhead, Astex Pharmaceuticals

9:30 AM *Enabling NMR Fragment Screening and Hit-to-Lead Medicinal Chemistry via NMR for SAR*  
Prof. Steven LaPlante, NMX Research and Solutions Inc

10:00 AM *Exploring the Power of Structural Biology on Degradation Discovery*  
Larry Jin, Biortus Biosciences Co. Ltd.

BIORTUS

10:15 AM *Award Ceremony & Announcements*  
Dr. Heike Schönherr, Relay Therapeutics

**10:30 AM**

**Networking Break**

**Session 10 – Fragments in the Future**  
**11:00 AM to 12:45 PM**

Chair:

11:00 AM **Invited Speaker**  
*Sample multiplexing combined with profiling covalent cysteine libraries for FBDD*  
Prof. Steven Gygi, Harvard University

11:30 AM *Fragment Screening of Adenosine A2a Receptor Using Native Lipid Nanodiscs*  
Philip Rawlins, Domainex

12:00 PM **Closing Keynote**  
*Prospective Discovery of Molecular Glues Using Site-Directed Fragments*  
Prof. Michelle Arkin, University of California, San Francisco

12:45 PM *Closing remarks*  
Joe Patel, Nexo Therapeutics

**1:00 PM End FBLD 2024**