

FBLD 2010 Agenda



Sunday, 10th October

Noon - Registration opens

13:00 - 14:30 CCG Workshop "Free MOE Workshop"

14:30 - 15:30 CCG + BioSolveIT "Synergies for FBLD"

15.30 - 17:00 BioSolveIT Workshop "Fragment-Based Ligand Design in Teams"

17:30 - 19:00 Mixer with food and drink

Monday 11th October

Fragment Libraries and Chemical Space
(Andrew Leach & Mike Hann, GlaxoSmithKline, co-chairs)

8:00 - 8:45 Plenary Introduction: "Current Perspectives in Fragment-Based Discovery"
Rod Hubbard, Vernalis & University of York

8:45 - 9:25 "Enumeration, Mapping and Scoring of Chemical Space",
Jean-Louis Reymond, Department of Chemistry and Biochemistry, University of Berne, Berne
Switzerland

9:25 - 9:55 "From Druggability, to Ligand Efficiency, to the Universe of Heterocyclic Rings",
Colin Groom, Cambridge Crystallographic Data Centre

9:55 - 10:25 Coffee & Tea

10:25 - 10:55 "Design and Application of LEF, a Library of Chemical Fragments with Different Local
Environment of Fluorine",
Anna Vulpetti, Novartis

10:55 - 11:25 "Shape Diversity in Fragment Library Design: Theory and Practice",
Ken Brameld, Roche

11:25 - 11:55 "Fragment Based Druggability Screening to Predict Lead Discovery Success",
Fredrik Edfeldt, AstraZeneca R&D

11:55 - 12:25 Three - Four 10 minute poster/vendor talks to be selected in August 2010

12:30 - 13:30 Lunch, Posters & Vendors

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Biophysics A: Hit Identification
(Don Huddler, GlaxoSmithKline, Chair)

13:30 - 14:10 “NMR and Computational Approaches to Fragment Hit ID”
Maurizio Pellecchia, Burnham Institute for Medical Research

14:10 - 14:40 “Ligand-Detected NMR Fragment Screening”,
Ben Davis, Vernalis

14:40 - 15:10 “Fragment Library Screening with SPR”,
Tony Giannetti, Genentech

15:10 - 15:40 “Automated SPR Data Processing and Sensogram Classification”,
Constantine Kreatsoulas, Merck

15:40 - 16:10 Coffee & Tea

16:10 - 16:40 “Biophysical Ligand Screening of Soluble and Membrane-Bound Targets”,
Gregg Siegal, ZoBio & Universiteit Leiden

16:40 - 17:10 "Small Molecule Fragment Screening with Biolayer Interferometry on the ForteBio
Octet Red Instruments,
Charles A. Wartchow, Hoffman La Roche

17:10 - 17:40 Round Table Q&A

18:00 - Food, Drink, Posters & Vendors

Tuesday 12th October

Biophysics B: Screening and Characterization Technologies
(Tony Giannetti, Genentech, Chair)

8:30 - 9:15 “Overview of Biophysics for Fragment Discovery and Characterization”,
Glynn Williams, Astex Therapeutics

9:15 - 9:45 “Developments in fragment screening for GPCRs”,
Rebecca Rich, University of Utah

9:45 - 10:15 “Comparison of plate-based biophysical binding assay methods for fragment library
screening”,
Kartik Narayan, Merck

10:15 - 10:45 Coffee & Tea

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10:45 - 11:15 “Predicting success from X-ray Crystallographic Screening of Fragments”,
Doug Davies, Emerald BioStructures

11:15 - 11:45 “Culling Through Fragment Hits with Biophysical Approaches”,
Bill Metzler, Bristol-Myers Squibb

11:45 - 12:15 "Fragment-based screening for inhibitors of PDE4A using enthalpy arrays and X-ray crystallography",
Michael Recht, Palo Alto Research Centre

12:15 - 12:30 Round Table Q&A

12:30 - 13:30 Lunch, Posters & Vendors

Chemistry Follow-up Strategies
(Dan Erlanson, Carmot Therapeutics, Chair)

13:30 - 14:00 “From Weak NMR-Detected Fragment Hits to First-in-class Recommendation Candidates for BACE-1”,
Dan Wyss, Merck

14:00 - 14:30 "Ups and downs of structurally un-enabled fragment optimization",
Adam Renslo, University of California, San Francisco

14:30 - 15:00 “Targeting Protein-Protein Interactions via Kinetic Target-Guided Synthesis “,
Roman Manetsch, University of South Florida

15:00 - 15:30 Coffee & Tea

15:30 - 16:00 “Shortening the Time to a Successful Fragment HTL Campaign”,
Sandy Farmer, Boehringer Ingelheim Pharmaceuticals, Inc

16:00 - 16:30 "Discovery of new high-affinity PDE10 inhibitors using fragment based lead generation and knowledge-based design",
Jeffrey S. Albert, AstraZeneca

16:30 - 16:50 "Novel PDK1 Inhibitors Discovered through FBLD",
M. Catherine Johnson, Pfizer

16:50 - 17:10 "FBLD: A PDK1 Case Study",
Jeffrey M. Axten, GlaxoSmithKline

18:00 - Conference Banquet

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Wednesday 13th

Success Stories and Chemical Biology
(Rod Hubbard, Vernalis & The University of York, Chair)

8:30 - 9:10 "Fragment-Based Ligand Discovery : New Opportunities with Well-Known Targets",
Wolfgang Jahnke, Novartis

9:10 - 9:50 "Targeting the Intractable",
Chaohong Sun, Abbott Labs

9:50 - 10:30 "Beyond Growing and Linking: Impact of Fragments on the Discovery of Kinase
Inhibitors",
Andreas Kuglstatter, Roche

10:30 - 11:00 Coffee & Tea

11:00 - 11:30 "Fragment based drug discovery of selective inhibitors of Fibroblast Growth Factor
Receptor (FGFr)",
Gordon Saxty, Astex Therapeutics

11:30 - 12:15 "Fragments - a Story That Will Run and Run".
Chris Abell, University of Cambridge

12:30 - Close of Conference