FBLD
Fragment-based Lead Discovery Conference 2009

Draft timetable - FBLD2009

THE FOLLOWING PROGRAMME IS DRAFT ONLY.

THE TIMING OF ALL SESSIONS AND TALKS IS SUBJECT TO CHANGE.

Sunday 20th September 2009

Pre-Conference Workshop. See website for further details. **Separate registration is required**

Monday 21st September 2009

09.00 – 11.00	Coffee and Registration (Tea and Coffee from 10:30)
11.00 – 11.20	Introduction – Rod Hubbard
Fragment library design	
11.20 – 12.00	Chris Murray, Astex "Screening sets for fragment-based drug discovery"
12.00 – 12.30	Ijen Chen, Vernalis "Fragment libraries: analysis of output from 8 years of screening"
12.30 – 12.50	Contributed Talk: Doug Davies, Decode "Fragments of Life"
12:50 – 14:00	**Lunch**
Detecting fragment binding	
14:00 - 14:40	Tony Giannetti, Genentech "Recent Developments in SPR-Based Fragment Discovery"
14:40 – 15.10	James Murray, Vernalis "Experiences in the identification and characterisation of fragments that bind"
15.10 – 15.40	Tea and posters
15.40 – 16.00	Contributed talk: NovAlix "Native Mass Spectrometry: An ESI Tool for Fragment Library Screening"
16.00 – 16.30	Gregg Siegal, ZoBio "Into the great unknown: Fragment Based Drug Discovery on Membrane Proteins"
Round table - practical issues in fragment based discovery	
16.30 – 17.30	Chair - Jeff Blaney, Genentech
17.30 – 19.00	Posters with drinks reception in the Atrium of the Centre

Dinner
(a pre-paid meal is available at a number of restaurants in York city centre. Sign up at registration. A York student will act as host and guide for each venue)

Tuesday 22nd September 2009

Fragments, scoring functions and docking

09.00 – 09.50	Gerhard Klebe, Univ Marburg “Mapping Protein-Binding Sites: Where Fragments Go and Where They Grow”
09.50 – 10.30	Marcel Verdonk, Astex
10.30 – 11.00	Tea/Coffee
11.00 – 11.50	Brian Shoichet, UCSF "Docking for fragments: hit-rates, structures and chemical space"
11.50 – 12.10	Contributed talk: Daniel Robinson, Schrodinger "Energetic analysis of fragment docking and application to structure-based pharmacophore hypothesis generation"
12.10 – 13.30	**Lunch and posters**

Design from fragments

13.30 – 14.00	Diane Joseph-McCarthy, Astra Zeneca, Waltham, MA “Fragment based de novo design: Past to Present”
13.45 – 14.25	Andreas Bender, University of Leiden
14.25 – 15.00	Peter Johnson, University of Leeds
15.00 – 15.30	Tea/Coffee
15.30 – 15.50	Contributed talk: John van Drie "Ligand design using DOS chemistry plus computational fragment mapping "
15.50 – 16.10	Contributed talk: Marcus Gastreich, BioSolveIT "Interactive Fragment Growing, Linking, and Merging"
16.10 – 16.30	Contributed talk: Fabrice Moriaut, Medit "Computational Fragment-Based Approach at PDB Scale by Protein Local Similarity"
16.30 – 17.30	Round Table discussion Chemistry challenging modelling
17.45 – 18.30	**MGMS AGM**
	Conference dinner at the National Railway Museum

Wednesday 23rd September 2009

Implementing fragments in big pharma

09.00 – 09.40 Sam Hughes, Pfizer, UK
"Implementing fragment approaches at Pfizer"

Case histories and success stories

Series of short presentations on success stories - 15 mins describing fragment evolution story published or disclosed in 2009 - with structures

09.40 - 10:00 Daniel Wyss – Schering Plough, Cambridge, MA
"SbN / FBDD Yields Highly Potent and Selective BACE Inhibitors"

10.00 – 10.20 Igor Mochalkin, Merck Serono, MA

10.20 – 10.50 Tea/Coffee

10.50 – 11.10 Robert Godemann, Evotec
"Application of functional assays to fragment screening as a hit-finding strategy for □-secretase"

11.10 – 11.30 Lee Walmsley, Vernalis
"From fragments to candidates in 2009"

11.30 – 11.50 Gordon Saxty, Astex
"Fragment-Based Discovery of AT9283; A Multi-Targeted Kinase Inhibitor with Potent Aurora, JAK and Abl Activity"

Plenary lecture

11.50 – 12.40 Phil Hajduk, Abbott
"A potpourri of fragmented things..."

Summary and Future perspectives

12.40 – 12.50 Rod Hubbard

Close of main conference

12.50 – 14.00 **Lunch**

END

14.00 – 16.00 Accelrys workshop in TR1 – see below
14.00 – 17.00 BioSolveIT workshop in TR3 – see below

The organisers of FBLD2009 are extremely grateful to the following for their generous sponsorship for this meeting. The funds have helped to keep the registration costs down for all participants:

MGMS
CCG
ZoBio
FujiFilm
Accelrys
Corning
Schrodinger
Tripos

The following companies have reserved breakout rooms in the Centre during the meeting, where further details about their products and services can be discussed:

Corning
CCG
BioSolveIT
Fuji
Schrodinger
Accelrys

Accelrys and BioSolveIT will be holding workshops / user meetings from 14:00 – 16:00 on the Wednesday afternoon after the conference. See (web sites to be provided)

Other companies will be presenting posters and will be able to discuss their products and services in the poster Atrium.

Fragment-based lead design with Multiple Copy Simultaneous Search (MCSS)

Hugues-Olivier BERTRAND, Fellow, LS Modeling and Simulations, Accelrys

Fragment-based methods are increasingly becoming popular for lead design and scaffold-hopping in drug discovery. In this workshop we will provide an overview of all the fragment based design methods in Discovery Studio, and highlight the well-published and validated MCSS methodology as well as some MCSS applications. MCSS is a powerful CHARMm-based method for docking small fragments within a protein binding site. This scientific functionality can be accessed through a fully automated workflow with associated analysis and visualization tools.

The presentation will be followed by a Discovery Studio 2.5 demonstration.

Free BioSolveIT Workshop on Fragment-Based Ligand Design

Presenters: Marcus Gastreich, Christian Lemmen and Peter Oledzki

Time and Place: 14:00-17:00 - Fabrication Teaching Room 3 (TR3)

Keywords: fragments, growing, merging, linking, de novo, synthesizable, scaffold hopping, free

Have you ever thought to yourself you would like to minimize the number of experiments you do? Ever wondered about how computation could help you?

Are you interested in fragment-based design? Excited about what the potential future might hold as this methodology is maturing? Ever thought it would be great to play with computation to perform fragment-based design to compliment what you do, but don't trust the results from computation?

To merge, or not to merge, to grow, or to link? There are many questions out there!

Or maybe the question that needs answering is somewhat different for you? After all there are many ways to approach a problem with different people living differing philosophies and perspectives!

Maybe you think: Why oh why do our medicinal chemists never want to talk to me? Bribe them to possibly make the molecules you predict? Why doesn't software produce the molecules that they would consider making? Alternatively, why can't my results stimulate them to make that killer compound? If only I could give him a molecule with a recipe for cooking it up!

Well, in this post-conference interactive workshop BioSolveIT will present its approach to computational Fragment-Based Ligand Design. An overview of our industry proven fragment-based design technology will be presented and discussed. Examples of BioSolveIT tools success will be explained with application studies and successful real life industry prospective test cases will be presented.

The interactive workshop will address four main areas:

1) The BioSolveIT Fragment Spaces concept: combining fragments together using known experimental protocols to design synthesizable molecules with a recipe for a medicinal chemist to create them with!

2) The ability to merge, grow, and link fragments utilizing 3D information will be addressed, showing you how using a few simple clicks can produce an on-the-fly computed slide show of results that can be seen in seconds.

3) The power of creating and searching your own company or project dependent fragment space to optimize the content of IP and chemical diversity in the design of ligands.

4) The utility of growing ligands in a structure-based fashion from a fragment-based hit found in a crystallographic screen or a docked fragment pose.

Please sign up for this FREE interactive workshop where you can play with BioSolveIT tools to perform a multitude of fragment based design tasks computationally. All you need to do is bring a laptop and administrator rights (Windows) along with you, and register for the workshop on the BioSolveIT registration page! (link - http://www.biosolveit.de/workshops/2009/02/)