

Sunday 9 October 2016

12:00 - 18:00	REGISTRATION OPEN		
Introductory tutorials - separate registration required			
13:15	Rod Hubbard	Vernalis / University of York	Overview / History / The complete process (to include fragment library design)
	Ben Davis	Vernalis	Finding and characterizing fragments that bind
	Coffee		
	Dan Erlanson	Carmot Therapeutics	What to do with fragments
16:00	END OF TUTORIAL SESSION		
VENDOR WORKSHOPS - FREE TO ALL			
16:00	5 minutes pitch from each of BioSolveIT, CCG, and TBD		
16:20 - 18:00	Parallel sessions in different rooms by each of the vendors: Details at registration		
18:30	OPENING RECEPTION		

Monday 10 October 2016

Session 1: Keynote and Success Stories. CHAIR: TBD			
08:30	Steve Fesik	Vanderbilt	Keynote Lecture: <i>Title TBD</i>
	Izzat Raheem	Merck	Discovery of Pyrazolopyrimidine PDE10A Inhibitors for the Treatment of Schizophrenia Enabled by Fragment Based Lead Discovery
	Heike Schonherr	AstraZeneca	Fragment Assisted Design of Novel PIM Inhibitors Aiming for Inhaled Delivery to Treat Severe Asthma
	Coffee		
Session 2: Success Stories. CHAIR: TBD			
	Wolfgang Jahnke	Novartis	Fragment-based Discovery of ABL001, an allosteric inhibitor of Bcr-Abl
	Bill Marathias	Beryllium	Targeting protein-protein interfaces in Influenza and Ebola viral targets using fragment screening
	Kathy Lee	Pfizer	LEAD GENERATION STRATEGIES: DISCOVERY OF A POTENT, SELECTIVE AND LIPOPHILIC EFFICIENT IRAK4 INHIBITOR, A CLINICAL CANDIDATE FROM FRAGMENT-BASED DRUG DESIGN
	Brad Jordan	Amgen	A fragment linking approach based on 19F-NMR spectroscopy to obtain highly potent and selective inhibitors of beta-secretase
12:10	LUNCH + POSTERS + EXHIBITS		
Session 3: Computational. CHAIR: TBD			
14:00	Sandor Vajda	Boston University	FRAGMENT BASED PREDICTION OF DRUGGABILITY AND FRAGMENT BINDING
	Richard Taylor	UCB	The Next Generation of Fragment Libraries
	John Kulp	MetaLeaps, LLC	Boltzmann Fragment Maps used in Lead Identification and Optimization: A review of diverse applications over 10 years
	Chris Radoux	CCDC	Identifying Interactions that Determine Fragment Binding at Protein Hotspots
	Carsten Detering	BioSolveIT	Inhabiting the chemical compound universe: Virtual chemistry 2.0
	Coffee		
Session 4: Methods. CHAIR: TBD			
	Ali Raja	Nanotemper Technologies	Microscale Thermophoresis: Automated Screening of a Fragment Library against MEK1 Kinase
	Julien Orts	ETH Zurich	NMR Molecular Replacement, NMR ²
17:30	Depending on the number of posters there will be another session for posters and exhibitors - and if enough sponsorship there will be a drinks reception as well		

FREE EVENING

Tuesday 11 October 2016

Session 1: Fragment Chemistry. CHAIR: TBD			
08:30	David Rees	Astex	Opportunity knocks: Organic Chemistry for FBDD
	Prashi Jain	Baylor College of Medicine	The Synthesis and Deployment of Piperazine Scaffolds as Templates for FBLD
	Coffee		
Session 2: Success Stories. CHAIR: TBD			
	Didier ROCHE	Edelris	Could we match Natural Product complexity with 3D-Fragments?
	Catherine Jorand Lebrun	EMD Serono	Three dimensional fragments: a short path from mM to nM potency
	Roxanne Smith	La Trobe University	Development of Antibiotics Targeting MDR Neisserial pathogens using Fragment-Based Drug Design
	Vickie Tsui	Genentech	Diving into the Water: Inducible Binding Conformations for Bromodomains
12:10	LUNCH + POSTERS + EXHIBITS		
Session 3: Success Stories. CHAIR: TBD			
	George Lountos	NIH / NCI	Discovery of an Allosteric Inhibitor of the SUMO-Conjugating E2 Enzyme Ubc9 by Crystallographic Fragment Screening
	Cath Latham	Burnet Institute	NEW DRUG CLASSES FOR HIV: NOVEL ALLOSTERIC INHIBITORS TARGETING HIV-1 REVERSE TRANSCRIPTASE
	Richard Lee	St. Jude	Comparative fragment screening approaches for ClpP activators
	Coffee		
Session 4: Success Stories. CHAIR: TBD			
	Jenny Sandmark	AstraZeneca	Structure based optimisation of fragments to generate selective secreted phospholipase A2 inhibitors.
	Phil Day	Astex	Identification of diverse fragments that bind to lipoprotein-associated phospholipase A2 (Lp-PLA2) and the structure based development of a subset of these fragments into potent and selective lead molecules.
	Fumiaki Yokokawa	Novartis	Discovery of a Potent Non-nucleoside Inhibitor of Dengue RNA-dependent RNA Polymerase using a Fragment-based Lead Generation Approach
19:00	CONFERENCE DINNER		

Wednesday 12 October 2016			
Session 1: Keynote and Success Stories. CHAIR: TBD			
08:30	Mark Sabat	Takeda	Flipped Fragment Poses: Bain or Blessing for Designing Selective Kinase Q Inhibitors?
	John Darby	University of York	Modifying glycoside hydrolase enzyme activity through covalent protein modification with fragments
	Li Xing	Pfizer	A Hinge-hopping Approach to Design of Kinase Inhibitors
	Gregg Siegal	Zobio	Fragments Enable a New Mechanism of Inhibiting Lysine Methyl Transferases.
	Coffee		
	Dan Erlanson	Carmot Therapeutics	Keynote Lecture: TBD
12:00	CONFERENCE CLOSES		