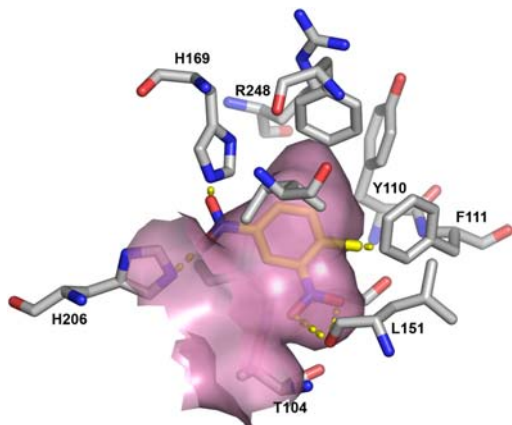


PSDI XV 2007 Workshop

Autrans, France
28-30 October 2007



Programme

Sunday 28 October

12h onwards **Arrivals during afternoon & evening**
19h00 *Welcome Cocktail*
20h until late *Buffet dinner*

Monday 29 October

08h30-08h45 **Research Director's Introduction** **S. Larsen**
ESRF

The Drug Discovery Process

Chair: *M. Hann (GlaxoSmithKline)*

08h45-09h20 **Current status & future prospects of structural Biology in drug discovery** **M. Hennig**
Hoffmann-La Roche

09h20-09h55 **Drug discovery for neglected diseases in an academic setting** **R. Brenk**
University of Dundee

09h55-10h30 **Academics messing with Drugs – Structural Biology at the Institute of Cancer Research** **L. Pearl**
ICR

10h30-11h00 *Coffee break*

Challenging Targets

Chair: H. Käck (AstraZeneca)

11h00-11h35	Crystal structure of human leukotriene C4 synthase – an integral membrane protein in the biosynthesis of inflammatory mediators	P. Nordlund SGC/Karolinska
11h35-11h55	Structure & Function of <i>human</i> ECE	C. Oefner Arpida
11h55-12h15	Structure-based approaches to PKB inhibitor design	T. Davies Astex
12h15-12h35	Structural description of a novel inhibition mechanism of aurora kinases by the MK-0457 (VX-680)	K. Brown Vertex

12h35-14h30

Lunch

Breakout Sessions – in parallel

NMR

Chair: T. Maurer (Böhringer Ingelheim)

14h30-16h30	Speaker 1: A. Ross, Hoffmann-La Roche Speaker 2: R. Weisemann, Bruker Speaker 3: R. Meinecke, Böhringer Ingelheim Speaker 4: G. Williams, Astex
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Protein Production / Crystallisation

Chair: D. Hart (EMBL) / A. Ruf (Hoffmann-La Roche)

Library screening strategies for soluble protein expression	
14h30-16h30	Speaker 1: S. Hörer, Böhringer Ingelheim Speaker 2: L. Pearl, Domainex Speaker 2: D. Hart, EMBL Speaker 3: P. Nordlund, Evitra

Crystallography

Chair: M. Mathieu (Sanofi-Aventis)

Automatic ligand fitting	
14h30-16h30	Speaker 1: G. Warren, OpenEye Speaker 2: JC Mozziconacci, Schrödinger Speaker 3: J. Patel & T. Davies, Astex Speaker 4: T. Womack, Global Phasing

16h30-17h00

Coffee break

Exhibitor Clips

Chair: A. D'Arcy (Novartis)

17h00-17h10	Speaker 1: C. Sterling, Rigaku
17h10-17h20	Speaker 2: E. Marquis, Fluidigm
17h20-17h30	Speaker 3: E. Boronowsky, Qiagen
17h30-17h40	Speaker 4: J. Duncan, Oxford Diffraction
17h40-17h50	Speaker 5: L. Damian, MicroCal
17h50-18h00	Speaker 6: G. Warren, OpenEye
18h00-18h10	Speaker 7: A. Coetzee, Bruker
18h10-18h20	Speaker 8: A. Sparkes, Schrödinger
18h20-18h30	Speaker 9: S. Newstead, Molecular Dimensions

Poster Session

19h00-20h00 Cocktail and Poster Session

20h00

Gala Dinner

Tuesday 30 October

New Techniques and Strategies

Chair: G. Williams (Astex)

09h00-09h20	APSY and NOEXRY: Fully automated assignment of NMR resonances of proteins	G. Wider ETH Zürich
09h20-09h40	High-quality, novel inhibitors through fragment-based lead generation	R. Folmer AstraZeneca
09h40-10h00	Fragment-based lead discovery: beta secretase 1	J. Patel Astex
10h00-10h20	Simplifying screening for protein crystals	A. Tucker Pfizer

10h20-11h00

Coffee Break

Biophysical Techniques: Complementary Approaches

Chair: B. Schoot (Galderma)

11h00-11h20	Rapid, label-free screening and affinity ranking of fragment libraries binding selectively to drug targets	S. Löfas Biacore
11h20-11h40	Biophysical methods to give insight and enhance crystallisation success	C.W. Chung GlaxoSmithKline
11h40-12h00	The high attrition rate of co-crystallisation experiments	J-M. Rondeau Novartis

<i>12h00-13h30</i>	<i>Lunch</i>
14h00-17h30	Free time & leisure activities (dairy, caves, walk)
17h30-18h00	Return and coffee/tea

Collaborations and News

Chair: D. Brown (Pfizer)

18h00-18h30	An introduction to and demonstration of PIMS, a flexible laboratory information management system for protein production	R. Esnouf OPPF
18h30-18h50	ISpyB: a web-based laboratory information system for crystal analysis with X-rays	S. Monaco ESRF
18h50-19h10	Remote control of MX experiments at the ESRF	G. Leonard ESRF
19h10-19h40	Round up from breakout sessions	

20h00 *Dinner*

For those interested, there is also a Visit to the ESRF in Grenoble:

Wednesday 31 October

08h00 Coach service from L'Escandille to the ESRF, site entrance, deposit luggage

Visit of the ESRF

Chair: S. Larsen (ESRF)

09h30-09h50	Director General's Introduction	W.G. Stirling ESRF
09h50-10h20	Automation on ESRF MX beamlines	G. Leonard ESRF

10h20-10h45 *Coffee break*

10h45-12h30 a) General visit of the ESRF
b) General visit to the PSB (Partnership in Structural Biology)
c) Visit of the MX beamlines – overview of the automation of the MX beamlines
d) Visit of the MX beamlines – troubleshooting of MX beamlines (reserved for regular users of the ESRF)

12h00-14h00 *Lunch*

14h00 Departure