

FINAL SCHEDULE

World Molecular Engineering Network Fifteenth Annual Meeting on Structural Biology

2-6 May 2004, San Jose del Cabo, Baja, Mexico

Sunday Evening, 2 May

17:30 – 17:45 R. Fletterick and I. Wilson

Introduction

17:45 – 20:00 **Self-Introductions by Non-Presenting Sponsors**

Byram, Susan K. Bruker AXS Inc.

Colleen Joel Fluidigm Corp.

Stephen Burley SGX

Short Presentations (5 min.) by Postdoctoral Fellows and Graduate Students

UCSF Post-docs, Graduate students, and Others

Anderson, John UCSF Synthetic biology of temporal pathways

Goetz, David UCSF Targeting cysteine proteases of the SARS coronavirus

Karchin, Rachel UCSF Large scale annotation of coding ncSNPs based on structure considerations

Pegg, Scott UCSF The structure-function linkage database

Rice, Luke UCSF Insight into the mechanisms of microtubule nucleation by gamma-tubulin

Rizzo, Robert UCSF Selectivity of thiadiazole urea inhibitors with stromelysin-1 and gelatinase-A from generalized Born molecular dynamics simulations

Borngraeber, Sabine UCSF Androgen receptor associations in vivo

TSRI Students

Bowden, Thomas TSRI Structural studies of CD1 antigens

Chao, Jeff TSRI Joint refinement of L30e-mRNA complex

Chapados, Brian TSRI Substrate recognition by structure-specific nucleases

Debler, Erik TSRI Structural investigation of the blue-fluorescent antibody 19G2

Nelson, Michael TSRI A structure-based study of SARS CoV

Will Placzek TSRI Structural studies of sigma factor regulation

Scanlan, Christopher TSRI Carbohydrate recognition of a broadly neutralizing anti-HIV-1 antibody

Shillington, Edwin TSRI Preliminary studies of an IgG1 (b12):IgA2 chimeric dimer

Shore, David TSRI Towards the structure of TCR co-receptor CD8 $\alpha\beta$

Wolan, Dennis TSRI Structural determination of human ATIC in complex with sulfonyl-containing antifolates and substrate AICAR: Implications for inhibitor design

20:15 – 21:00 **Reception**

In the Main Garden

FINAL SCHEDULE

World Molecular Engineering Network Fifteenth Annual Meeting on Structural Biology

2-6 May 2004, San Jose del Cabo, Baja, Mexico

Monday Morning, 3 May

09:00 McBride, Lincoln Fluidigm
09:20 Durst, Roger Bruker
09:40 Ferrara, Joseph Rigaku
10:00 **Break**

10:50 Shoichet, Brian UCSF
11:10 Jeffrey Blaney SGX
11:30 Buck, Elizabeth Sunesis

Advances in HT Structural Biology (Chair: I. Wilson)

High throughput automation of protein crystallization
Advances in technology and techniques for the structural solution of macromolecules
Recent advances for the home laboratory from Rigaku/MSK

Drug Discovery & Disease

Virtual screening and structure-based inhibitor discovery
Structure-guided drug discovery using fragment based lead identification/lead optimization
Tethering SM to identify small molecule modulators of C5aR activity and to explore mechanisms of receptor activation

Monday Afternoon

16:30 Craik, Charles UCSF
16:50 Dawson, Phil TSRI
17:10 Goodin, David TSRI
17:30 Babbitt, Patricia UCSF
17:50 **Break**

18:10 Wilson, Ian TSRI
18:30 Paulson, James TSRI
18:50 Barbas, Carlos TSRI
19:10 Ivanetich, Kathy UCSF

Enzymes: Structure, Mechanism and Inhibition (Chair: R. Fletterick)

Defining the specificity and function of proteases in complex biological processes
Site specific manipulation of serine protease enzyme-cofactor-substrate complexes
Engineering molecular wires, substrates, and labels in biological structures
Inference of function in enzyme superfamilies

Immune System

1918 Influenza virus hemagglutinin
CD22 glycan interactions in B cell signaling
Chemically-programmed monoclonal antibodies
Advances in bacterial source tracking

Tuesday Morning, 4 May

09:00 Santi, Dan Kosan
09:20 Morize, Isabelle Aventis
09:40 Aszodi, Andras Novartis
10:00 **Break**

10:30 David, Nathaniel Versant
10:50 **Panel Discussion**

SPONSORS (Chair: D. Santi)

Polyketide biosynthesis and pharmaceuticals
Modeling, structural biology and chemical biology at Aventis
In-house scientific software development in Pharma research

Achaogen: The making of a new biology-focused drug company
What is the future of research in big Pharma versus Biotech or Academia?
(Panel Leader: Jean DeLeage)
Panel: David Mack, Stephen Burley, Dan Santi, John Baxter, Isabelle Morize

FINAL SCHEDULE

World Molecular Engineering Network Fifteenth Annual Meeting on Structural Biology

2-6 May 2004, San Jose del Cabo, Baja, Mexico

Tuesday Afternoon

Nucleic Acids / Nucleic Acid-Proteins/Receptors (Chair: S. Burley)

16:30	Millar, David	TSRI	Nucleic acid dynamics and interactions
16:50	Gottesfeld, Joel	TSRI	Sequence-specific DNA alkylators in cancer chemotherapy
17:10	Asturias, Francisco	TSRI	Structural studies of animal fatty acid synthase (FAS)
17:30	Romesberg, Floyd	TSRI	The evolution of biomolecule dynamics
17:50	Break		
18:10	Williamson, Jamie	TSRI	Regulating translation by the STARs
18:30	Fletterick, Robert	UCSF	Androgen receptor antagonists
18:50	Baxter, John	UCSF	Selective modulation of thyroid hormone receptors

Wednesday Morning, 5 May

Computational Chemistry, Folding, Signaling and Molecular Assemblies (Chair: D. Agard)

08:30	Jacobson, Matthew	UCSF	Physics-based modeling of proteins and protein-ligand complexes
08:50	Sali, Andrej	UCSF	Modeling of the structures of proteins and macromolecular assemblies
09:10	Agard, David	UCSF	Intramolecular signal transduction
09:30	Voigt, Christopher	UCSF	Light induction of signaling networks
09:50	Break		
10:10	Yeager, Mark	TSRI	Aquaporins as a novel class of drug targets for treatment of hypertension and congestive heart failure
10:30	Stout, David	TSRI	Structure-conformation and function of transhydrogenase, an integral membrane proton pump
10:50	Johnson, Jack	TSRI	Structure based studies of auto-catalytic chemistry in virus particles: How and why