

**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**

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**Monday Morning, 3 May**

09:00	McBride, Lincoln	Fluidigm
09:20	Durst, Roger	Bruker
09:40	Ferrara, Joseph	Rigaku
10:00	<b>Break</b>	

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/MSC

**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	<b>Break</b>	

**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	<b>Break</b>	

10:30	David, Nathaniel	Versant
10:50	<b>Panel Discussion</b>	

**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**

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**Tuesday Afternoon**

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	<b>Break</b>		
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

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

**Wednesday Morning, 5 May**

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	<b>Break</b>		
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

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