

**FINAL SCHEDULE**  
**World Molecular Engineering Network Fourteenth Annual Meeting on Structural Biology**  
4-8 May 2003, San Jose del Cabo, Baja, Mexico

**Sunday Evening, 4 May**

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

**Introduction**

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

Peter Domaille	GeneFormatics
Tim Harris	Structural GenomiX
Kirk Clark	Novartis
Tom Pelton	Aventis
Dirk Bussiere	Chiron
David Weaver	SPRL

**Introductory Talk**

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

**TSRI Students**

Calarese, Dan	TSRI	Domain exchange in a human antibody promotes multivalent recognition of HIV-1
Chapados, Brian	TSRI	Structural basis for FEN-1 substrate specificity and PCNA-mediated activation
Craighead, John	TSRI	Structure of the RNA polymerase II/TFIIF complex
Kelker, Matt	TSRI	Purification and crystallization of human TREM-1
Manuell, Andrea	TSRI	mRNA-protein interactions in translation
Shore, David	TSRI	Structure of the CD3 signaling complex
Wolan, Dennis	TSRI	Structural insights into the mechanisms of both the transformylase and cyclohydrolase reaction of avian ATIC
Zhang, Jessie	TSRI	Structural studies and inhibitor design for human GAR Tfase

**UCSF, UCB Post-docs , Graduate students, and Others**

Alber, Frank	UCSF	Modeling the 3D-structure of the yeast nuclear pore complex
Anderson, Marc	UCSF	Progression in the synthesis of phalloidin
Chodera, John	UCSF	Do proteins fold by zipping? A perspective from atomistic simulations
Finer-Moore, Janet	UCSF	Structural correlates of drug resistance in variants of a dynamic enzyme
Ivanetich, Kathy	UCSF	Research projects at the Biomolecular Resource Center
Jouravel, Natalia	UCSF	Structure and dynamics of Thyroid Hormone Receptor: the interactions of ligand binding domains of TR and RXR
Mayer, Moriz	UCSF	Screening for small molecules binding to RNA
Ng, Ho-Leung	UCB	Structural polymorphism of calmodulin
Togashi, Marie	UCSF	Effect of a surface charge cluster in TR function
Walkup, Ward	UCSF	Isolation and characterization of single stranded binding protein from Arthrobacter Aurestens TW17

20:15 – 21:00 **Reception**

**In the Main Garden**

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### Monday Morning, 5 May

09:00	Burley, Steve	Structural GenomiX
09:20	McRee, Duncan	Syrrx
09:40	Stevens, Ray	TSRI
10:00	Abdel-Meguid, Sherin	SPRL
10:20	<b>Break</b>	

### Drug Discovery & Disease (Chair: I. Wilson)

09:00	Burley, Steve	Structural GenomiX	Structure-based drug discovery for protein kinase targets in human cancers
09:20	McRee, Duncan	Syrrx	DPP-IV = A target for type II diabetes
09:40	Stevens, Ray	TSRI	Structure based design of PKU therapeutics
10:00	Abdel-Meguid, Sherin	SPRL	Drug Discovery at SPRL
10:20	<b>Break</b>		
10:50	Betz, Steve	GeneFormatics	Discovery informatics drives efficient lead identification: Application to PIPs
11:10	Thanos, Chris	Sunesis	High affinity small molecule binding at a protein hot spot
11:30	Kelly, Jeff	TSRI	Understanding the energetics of amyloidosis and manipulating the landscape with small molecules and trans-suppression to prevent disease
11:50	Kuhn, Peter	TSRI	Detection of biomolecular interactions

### Monday Afternoon

16:30	Alber, Tom	UCB
16:50	Taunton, Jack	UCSF
17:10	Berger, James	UCB
17:30	Stout, Dave	TSRI
17:50	<b>Break</b>	

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

16:30	Alber, Tom	UCB	Mechanistic conservation in eukaryotic and prokaryotic Ser/Thr protein kinases
16:50	Taunton, Jack	UCSF	Rational discovery of electrophilic protein kinase inhibitors
17:10	Berger, James	UCB	Structural mechanism of topoisomerase II inhibition by the chemotherapeutic, ICRF-187
17:30	Stout, Dave	TSRI	Conformational diversity in crystal structures of four mammalian cytochrome P450s
17:50	<b>Break</b>		

### Immune System (Chair: R. Stevens)

18:10	Wilson, Ian	TSRI	Glycolipid binding by CD1
18:30	Paulson, Jim	TSRI	The ying and yang of sialic acid function
18:50	Wentworth, Paul	TSRI	Chemistry and biology of antibody-catalyzed water oxidation
19:10	Romesberg, Floyd	TSRI	Immunological evolution of protein dynamics

### SPONSORS (Chair: D. Santi)

09:00	Santi, Dan	Kosan
09:20	Spataro, Kristin	Fluidigm
09:40	Byram, Sue	Bruker AXS
10:00	<b>Break</b>	
10:30	Mack, David	Alta Partners
10:50	Nathaniel David	Versant Ventures
11:10	Round Table	

09:00	Santi, Dan	Kosan	Polyketide synthases
09:20	Spataro, Kristin	Fluidigm	A novel method for protein crystallization: Fluidigm's TOPAZ protein crystallization system
09:40	Byram, Sue	Bruker AXS	Crystallographic instrumentation developments for structural biology
10:00	<b>Break</b>		

10:30	Mack, David	Alta Partners	Life sciences company formation - The Alta perspective
10:50	Nathaniel David	Versant Ventures	Entrepreneurship in the best of times, the worst of times
11:10	Round Table		Industrializing drug discovery – fact or fantasy in today's financial and scientific world
			(Discussion Leader: C. Samuels-Pearson)

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**Tuesday Afternoon**

			<b>Nucleic Acids / Nucleic Acid-Proteins/Receptors (Chair: S. Burley)</b>
16:30	James, Tom	UCSF	The importance of being RNA
16:50	Millar, David	TSRI	Single-molecule fluorescence studies of RNA conformation and folding
17:10	Gottesfeld, Joel	TSRI	Chemical probes of nucleosome structure and dynamics
17:30	Asturias, Francisco	TSRI	Electron microscopy studies of eukaryotic transcription machinery
17:50	<b>Break</b>		
18:10	Roberts, Vickie	TSRI	Predicting DNA/protein interactions
18:30	Fletterick, Robert	UCSF	LRH1 nuclear receptor
18:50	Webb, Paul	UCSF	Use of structure to analyze TR interactions with coregulators and dimer partners
19:10	Baxter, John	UCSF	Using structure to develop selective thyroid hormone receptor modulators

**Wednesday Morning, 7 May**

			<b>Computational Chemistry, Folding, Design and Molecular Assemblies (Chair: R. Fletterick)</b>
08:30	Dawson, Phil	TSRI	Topological engineering of proteins
08:50	Dill, Ken	UCSF	Protein folding: A twist on the transition state idea
09:10	Sali, Andrej	UCSF	Modeling of 3D structures of proteins and macromolecular assemblies
09:30	Olson, Art	TSRI	Current challenges in protein docking
09:50	<b>Break</b>		
10:10	Stroud, Bob	UCSF	Selectivity in a transmembrane channel family
10:30	Minor, Dan	UCSF	Ion channel structure and function
10:50	Guy, Kip	UCSF	Engineering an orthogonal actin-phalloidin pair for <i>in situ</i> control of actin polymerization
11:10	Yeager, Mark	TSRI	Three-dimensional model of the human platelet integrin $\alpha_{IIb}\beta_3$ based on electron cryo-microscopy and x-ray crystallography