

# 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 <i>Arthrobacter Aurestens</i> TW17

20:15 – 21:00

#### Reception

#### In the Main Garden

# FINAL SCHEDULE

## World Molecular Engineering Network Fourteenth Annual Meeting on Structural Biology

4-8 May 2003, San Jose del Cabo, Baja, Mexico

### 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 **Break**

10:50 Betz, Steve GeneFormatics  
11:10 Thanos, Chris Sunesis  
11:30 Kelly, Jeff TSRI  
11:50 Kuhn, Peter TSRI

### Monday Afternoon

16:30 Alber, Tom UCB  
16:50 Taunton, Jack UCSF  
17:10 Berger, James UCB  
17:30 Stout, Dave TSRI  
17:50 **Break**

18:10 Wilson, Ian TSRI  
18:30 Paulson, Jim TSRI  
18:50 Wentworth, Paul TSRI  
19:10 Romesberg, Floyd TSRI

### Tuesday Morning, 6 May

09:00 Santi, Dan Kosan  
09:20 Spataro, Kristin Fluidigm  
09:40 Byram, Sue Bruker AXS  
10:00 **Break**

10:30 Mack, David Alta Partners  
10:50 Nathaniel David Versant Ventures  
11:10 Round Table

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

Structure-based drug discovery for protein kinase targets in human cancers  
DPP-IV = A target for type II diabetes  
Structure based design of PKU therapeutics  
Drug Discovery at SPRL

Discovery informatics drives efficient lead identification: Application to PIPs  
High affinity small molecule binding at a protein hot spot  
Understanding the energetics of amyloidosis and manipulating the landscape with small molecules and trans-suppression to prevent disease  
Detection of biomolecular interactions

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

Mechanistic conservation in eukaryotic and prokaryotic Ser/Thr protein kinases  
Rational discovery of electrophilic protein kinase inhibitors  
Structural mechanism of topoisomerase II inhibition by the chemotherapeutic, ICRF-187  
Conformational diversity in crystal structures of four mammalian cytochrome P450s

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

Glycolipid binding by CD1  
The ying and yang of siglec function  
Chemistry and biology of antibody-catalyzed water oxidation  
Immunological evolution of protein dynamics

### SPONSORS (Chair: D. Santi)

Polyketide synthases  
A novel method for protein crystallization: Fluidigm's TOPAZ protein crystallization system  
Crystallographic instrumentation developments for structural biology

Life sciences company formation - The Alta perspective  
Entrepreneurship in the best of times, the worst of times  
Industrializing drug discovery – fact or fantasy in today's financial and scientific world  
(Discussion Leader: C. Samuels-Pearson)

## FINAL SCHEDULE

### World Molecular Engineering Network Fourteenth Annual Meeting on Structural Biology

4-8 May 2003, San Jose del Cabo, Baja, Mexico

#### Tuesday Afternoon

16:30 James, Tom UCSF  
16:50 Millar, David TSRI  
17:10 Gottesfeld, Joel TSRI  
17:30 Asturias, Francisco TSRI  
1750 **Break**

18:10 Roberts, Vickie TSRI  
18:30 Fletterick, Robert UCSF  
18:50 Webb, Paul UCSF  
19:10 Baxter, John UCSF

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

The importance of being RNA  
Single-molecule fluorescence studies of RNA conformation and folding  
Chemical probes of nucleosome structure and dynamics  
Electron microscopy studies of eukaryotic transcription machinery

Predicting DNA/protein interactions  
LRH1 nuclear receptor  
Use of structure to analyze TR interactions with coregulators and dimer partners  
Using structure to develop selective thyroid hormone receptor modulators

#### Wednesday Morning, 7 May

08:30 Dawson, Phil TSRI  
08:50 Dill, Ken UCSF  
09:10 Sali, Andrej UCSF  
09:30 Olson, Art TSRI  
09:50 **Break**

10:10 Stroud, Bob UCSF  
10:30 Minor, Dan UCSF  
10:50 Guy, Kip UCSF  
11:10 Yeager, Mark TSRI

#### Computational Chemistry, Folding, Design and Molecular Assemblies (Chair: R. Fletterick)

Topological engineering of proteins  
Protein folding: A twist on the transition state idea  
Modeling of 3D structures of proteins and macromolecular assemblies  
Current challenges in protein docking

Selectivity in a transmembrane channel family  
Ion channel structure and function  
Engineering an orthogonal actin-phalloidin pair for in situ control of actin polymerization  
Three-dimensional model of the human platelet integrin  $\alpha_{IIb}\beta_3$  based on electron cryo-microscopy and x-ray crystallography