

SCHEDULE

World Molecular Engineering Network Seventeenth Annual Meeting on Structural Biology

30 April – 4 May 2006, San Jose del Cabo, Baja, Mexico

Sunday Evening, 30 April

San Jose Conference Room

17:30 – 17:45 Dan Santi and Ian Wilson

Introduction and Welcome

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

Darcy, Maureen Fluidigm
Barbas, Carlos TSRI

Short Presentations (5 min.) by TSRI and UCSF Graduate Students, Postdoctoral Fellows, and Others

Apriletti, James	UCSF	Structural Determinants for Selective Thyroid Hormone Receptor Antagonists
Chandonia, John-Marc	UCBerkeley	The Impact of Structural Genomics
Chen, Yu	UCSF	Sub-Angstrom Resolution Protein Crystal Structure: WYSIWYG
Deu Sandoval, Edgar	UCBerkeley	Engineering of an obligate homodimeric enzyme into a heterodimeric hybrid with dual specificity
Egea, Pascal	UCSF	Targeting Proteins to and across Membranes
Friedland, Gregory	UCSF	Using computational models to interpret NMR experiments of protein dynamics
Ghosh, Kingshuk	UCSF	Small Numbers Fluctuations in Biology
Howard, Rebecca	UCSF	A C-Terminal Coiled-Coil Domain Drives Assembly and Specificity in KCNQ Channels
Ivanetich, Kathryn	UCSF	Application of DNA sequencing & quantitative PCR microbial source tracking assays to identify host sources of fecal pollution in watersheds
Lang, Paula Theresa	UCSF	Computational Method Development for Targeting RNA: Applications to HIV TAR
Scheer, Justin	UCSF	A conserved allosteric site and mechanism in caspases identified by disulfide-trapping
Topf, Maya	UCSF	Combining Comparative Modeling and CryoEM Density Fitting
Barglow, Katy	TSRI	Discovering disease associated enzymes by proteome reactivity profiling
Chappie, Joshua	TSRI	Towards the structural understanding of dynamin GTPase
Debler, Erik	TSRI	Crystal structure of the IL-2 signaling complex
Evans, Michael	TSRI	Preparation and reactivity of a natural product-like library of activity-based probes
Grbic, Jovana	TSRI	Investigating the regulatory role of BMI-1 in hematopoietic stem cell regulation and cancer
Hills, Ron	TSRI	Cooperative self-association in amyloidogenic peptides
Kerkow, Don	TSRI	Characterization of a potentially novel RNA binding motif found within the <i>C. elegans</i> protein NSF-2
Lander, Gabriel	TSRI	CryoEM reconstruction reveals key insights into viral DNA packaging machinery
Manuell, Andrea	TSRI	Structure of the chloroplast ribosome and implications for light-regulated translation
Ward, Andrew	TSRI	Structural and functional analysis of the ABC transporter MsbA
Yoshioka, Craig	TSRI	Automating random conical data collection

20:15 – 21:00 **Reception**

In the Main Garden

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Monday Morning, 1 May

09:00	Brenner, Steven	UCBerkeley
09:20	Sjolander, Kimmen	UCBerkeley
09:40	Sali, Andrej	UCSF
10:00	Yeates, Todd	UCLA
10:20	Break	
10:50	Nollert, Peter	deCODE
11:10	Williamson, Jamie	TSRI
11:30	Byram, Susan	Bruker AXS
11:50	Ruth, Ronald	Lyncean Tech

Advances in Structural Biology & Proteomics (Chair: Brian Shoichet)

Phylogenomics and Metagenomics
New algorithms for phylogenomic inference of protein function
Modeling the structures of proteins and macromolecular assemblies
Do thermophiles stabilize their protein complexes by entangling them in links and knots?
Going the extra mile: Rational surface mutagenesis
Postproteomic approach to ribosome assembly
Latest equipment and crystallographic results from Bruker
Recent tests of the compact light source

Monday Afternoon

16:30	Wells, James	UCSF
16:50	Shoichet, Brian	UCSF
17:10	Kortemme, Tanja	UCSF
17:30	Abagyan, Ruben	TSRI
17:50	Break	
18:05	Paulson, James	TSRI
18:25	Stroud, Robert	UCSF
18:45	Minor, Dan	UCSF
19:05	Stout, Dave	TSRI

Protein Engineering and Drug Discovery (Chair: Jack Kirsch)

Site-directed ligand discovery
Relating proteins by their ligands
Reengineering specificity in signaling domains
Advances in virtual lead discovery and structure annotation

Immune System and Membrane Proteins (Chair: Todd Yeates)

Sweet spots in B cell signaling
Membranes 4 billion years - What's new?
Ion channels in pieces: Structural dissection of channel action and regulation
Experiments toward crystallization of transhydrogenase

Tuesday Morning, 2 May

09:00	Santi, Dan	UCSF
09:20	Vieth, Michel	Eli Lilly
09:40	Muskal, Steven	Eidogen-Sertanty
10:00	McRee, Duncan	ActiveSight
10:20	Break	
10:50	Syed, Rashid	Amgen
11:10	He, Molly-Min	Sunesis
11:30	May, Andy	Fluidigm

SPONSORS (Chair: James Wells)

Synthetic biology approaches to polyketide bio-synthesis
Advancing drug discovery with computational chemistry - from docking to chemogenomics
Broader visibility after proliferating the structural proteome – Are promiscuous drugs inevitable?
Fishing for fragments with the ACTOR Robot
P38 MAP kinase inhibitors: Discovery and selection of drug candidates
A novel mechanism for small molecule inhibition of TNF-alpha
Aspects of crystallization using free interface diffusion

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Tuesday Afternoon

Nucleic Acids & Viruses (Chair: Jamie Williamson)

16:30	Gottesfeld, Joel	TSRI	DNA and chromatin therapeutics for triplet repeat diseases
16:50	Millar, David	TSRI	Nucleic acid-protein complexes as therapeutic drug targets
17:10	James, Thomas	UCSF	Interactions of Poly(C) binding protein with telomeric DNA and telomerase RNA
17:30	Baxter, John	UCSF	Selective modulation of the thyroid hormone receptor
17:50	Break		
18:05	Yang, Xiang-Lei	TSRI	Two conformations of a crystalline human tRNA synthetase – tRNA complex: Implications for protein synthesis
18:25	Johnson, Jack	TSRI	An asymmetric CryoEM reconstruction of infectious P22 virus shows that a component of the DNA packaging motor is also a sensor for chromosome condensation density
18:45	Yeager, Mark	TSRI	Native hepatitis B virions and capsids visualized by electron cryomicroscopy
19:05	Finn, M.G.	TSRI	Viruses and click chemistry: polyvalent platforms and connectivity tools of use in structural and functional biology

Wednesday Morning, 3 May

Assemblies and Computation (Chair: Andrej Sali)

08:30	Dill, Kenneth	UCSF	Using folding physics for protein structure prediction
08:50	Kirsch, Jack	UCBerkeley	Protein/protein interactions in the gas phase
09:10	Sanner, Michel	TSRI	Computational representation of protein flexibility: Applications to automated docking
09:30	Finer-Moore, Janet	UCSF	The structure of the ER-luminal domain of Ire1, a sensor for unfolded protein
09:50	Break		
10:20	Deniz, Ashok	TSRI	Shedding light on protein aggregation using fluorescence
10:40	Milligan, Ronald	TSRI	Structural studies on microtubule binding proteins
11:00	Balch, William	TSRI	Structural and functional design of cargo nanocages
11:20	Olson, Arthur	TSRI	Computational biology from atoms to cells