Workshop III: Structural Proteomics

Monday May 10, 2004

8:30–9:15	*Check-In/Light Breakfast (Hosted by IPAM)*
9:15–9:30	*Welcome and Opening Remarks*
9:30–10:30	**Arthur Lesk** (Cambridge University) *Structure and Evolution of the Globins: We thought we understood them*
10:30–11:00	*Break*
11:00–12:00	**Ken Dill** (University of California at San Francisco) *Protein Folding: From physics to conformational searching.*
12:00–2:00	*Lunch (on your own)*
2:00–3:00	**George Rose** (Johns Hopkins University) *Assessing the protein folding problem - theory and simulations*
3:00–3:30	*Break*
3:30–4:30	**Ingo Ruczinski** (Johns Hopkins University) *Protein structure prediction using ROSETTA*
4:30–4:45	*Break*
4:45–5:45	**Steven Brenner** (University of California at Berkeley) *Ancient protein evolutionary relationships inferred from structure*
5:45–12:00	*Wine/Cheese Reception (Hosted by IPAM)*

Tuesday May 11, 2004

8:30–9:30	*Check-In/Light Breakfast (Hosted by IPAM)*
9:30–10:30	**Jose N. Onuchic** (University of California at San Diego) *Exploring the protein funnel energy landscape for folding and function.*
10:30–11:00	*Break*

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11:00–12:00	**Angel Garcia** (Los Alamos National Laboratory) *Simulation of the folding / unfolding thermodynamics of protein A*
12:00–2:00	*Lunch (on your own)*
2:00–3:00	**Scott Schmidler** (Duke University) *Statistical Shape Methods for Datamining in Protein Structure Databases*
3:00–3:30	*Break*
3:30–4:30	**Edward Marcotte** (University of Texas) *Working towards accurate protein interaction maps and the human interactome*
4:30–5:30	**Adam Godzik** (Burnham Institute) *FATCAT : Flexible structure alignment of proteins: lessons for comparative modeling and structural genomics*

Wednesday May 12, 2004

8:30–9:30	*Check-In/Light Breakfast (Hosted by IPAM)*
9:30–10:30	**Patrick Aloy** (European Molecular Biology Laboratory) *Structure-based assembly of protein complexes and networks*
10:30–11:00	*Break*
11:00–12:00	**Ruben Abagyan** (Scripps College) *Predicting induced fit in docking and loop prediction*
12:00–2:00	*Lunch (on your own)*
2:00–3:00	**Jeffrey Skolnick** (State University of New York, Buffalo) *Prediction of Protein Structure and Function on a Proteomic Scale*
3:00–3:30	*Break*
3:30–4:30	**Patricia Babbitt** (University of California at San Francisco) *A Model Linking Structure and Function in Mechanistically Diverse Enzyme Superfamilies*
4:30–4:45	*Break*
4:45–5:45	**John Moult** (University of Maryland) *Annotation of Protein Misfunction: SNPs, Databases and Disease*
5:45–12:00	*Dinner (Hosted by IPAM)*

Thursday May 13, 2004

8:30–9:30	*Check-In/Light Breakfast (Hosted by IPAM)*
9:30–10:30	**Oliver Lichtarge** (Baylor College of Medicine) *Towards Large-Scale Identification and Specific Engineering of Protein Functional Sites*
10:30–11:00	*Break*
11:00–12:00	**Jacque Fetrow** (Wake Forest University) *Synergies of computational and chemical proteomics methods: analysis of yeast serine hydrolases*
12:00–2:00	*Lunch (on your own)*
2:00–3:00	**James Watson** (European Bioinformatics Institute) *Case Studies In Assigning Function From Structure In Structural Genomics*
3:00–3:30	*Break*
3:30–4:30	**Alexander Kister** (Rutgers University) *The common structural and sequence features of the sandwich and barrel proteins. Application to the structural prediction and sequence classification*

Friday May 14, 2004

8:30–9:30	*Check-In/Light Breakfast (Hosted by IPAM)*
9:30–10:30	**Sarah Teichmann** (MRC Laboratory) *Evolution of Multi-Domain Proteins*
10:30–11:00	*Break*
11:00–12:00	**Nick Grishin** (University of Texas, Southwestern Medical Center) *Remote homology inference: what are the limits?*
12:00–1:00	**Mansoor Saqi** (Barts and The London School of Medicine and Dentistry) *Structural diversity within protein superfamilies: implications for remote homolog detection*
1:00–12:00	*Conclusion*