

## Program for Day 1, August 4th 2006 Room A, Fortaleza Convention Center

9:00 *Opening remarks*

### Session 1: **Evolution** (Chair - [Ilan Samish](#))

9:05 [Nick V. Grishin](#). **Dramatic Evolutionary Changes in Protein Structures.**

9:35 Sandra Maguid, Gustavo Parisi, [Sebastian Fernandez-Alberti](#), Julian Echave. **Sequence-structure-flexibility relationship in protein evolution.**

9:55 Maria S. Fornasari, [Gustavo Parisi](#). **Protein Structure Diversity and Sequence Divergence in Evolution.**

10:15 [Diana K Ekman](#), Åsa K Björklund, Arne Elofsson. **Evolutionary History of Multi-Domain Proteins.**

10:35 *Coffee Break*

11:05 Christopher Dupont, Song Yang, Brian Palenik, [Philip E. Bourne](#). **Modern Proteomes Contain Imprints of Ancient Shifts in Environmental Chemistry.**

### Session 2: **Homology Modeling** (Chair – [Nick Grishin](#))

11:35 Francisco Melo, Alejandro Panjkovich, Andrej Sali, Marc A. Marti-Renom. **Structure Specific Statistical Potentials for Protein Structure Prediction.**

11:55 [Iris Antes](#), Thomas Lengauer. **DynaDock: Inhibitor based Refinement of Homology Modeled Protein Structures for Molecular Docking.**

12:15 *Lunch and Laptop Session 1*

15:00 **Discussion 1: The roles of Evolution, physics and informatics** (Chair - [Phil Bourne](#)).

### Session 3: **Ligand Binding** (Chair - [Phil Bourne](#))

15:45 [Rafael J. Najmanovich](#), Richard J. Morris, Janet M. Thornton. **Single-Family Analysis of Binding Site Structural Similarities.**

16:05 [Thomas Funkhouser](#), Roman Laskowski, Janet Thornton. **Matching Volumetric Models of Protein Active Sites.**

16:25 [Melissa R. Landon](#), Spencer C. Thiel, David R. Lancia Jr., Sandor Vajda. **Identification of Druggable "Hot Spots" in Ligand Binding Pockets by Computational Solvent Mapping of Proteins.**

16:45 *Coffee Break*

### Session 4: **Model Quality** (Chair - [John Moult](#))

17:15 Michal J. Gajda, Marta Kaczor, [Janusz M. Bujnicki](#), Anastasia Bakulina, Andrzej Kasparski, Alan M. Friedman, Chris Bailey-Kellogg. **FILTREST3D: a Simple Method for Discrimination of Multiple Structural Models Against Spatial Restraints.**

17:35 [Marcin Pawlowski](#), Janusz Bujnicki, Ryszard Matlak. **Meta-MQAP: an SVM-based meta-server for the quality assessment of protein models.**

17:55 [Wah Chiu](#), Matthew L Baker. **Modeling Protein Components of Biological Nano-Machines in Subnanometer Resolution CryoEM Density Maps.**

18:25 *Break: Busses to evening session*

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| 20:00 | <i>Get-together Dinner</i> at main headquarters hotel (Oasis Atlantic Imperial)                           |
| 21:00 | <u>John Moult</u> . <b>CASP: Progress, Bottlenecks, Prognosis, and Messages for Computational Biology</b> |
| 23:00 | <i>Lights out...</i>                                                                                      |

## Program for Day 2, August 5th 2006

### Session 5: **Physics and Folding** (Chair - Goran Neshich)

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| 9:00  | <u>Jeffery G. Saven</u> . <b>Theoretical Methods for the Design and Engineering of Proteins.</b>                                                                                                                                                                                       |
| 9:30  | <u>Ilan Samish</u> , Oksana Kerner, David Kaftan, Eran Goldberg, Avigdor Scherz. <b>Datamining the Fourth Dimension from Crystal Structures: Structure-Function-Entropy Relationships in Membrane Proteins.</b>                                                                        |
| 9:50  | <u>Anna C.V. Johansson</u> , Erik Lindahl. <b>Simulation of Amino Acid Solvation Structure in Transmembrane Helices and Implications for Membrane Protein Folding.</b>                                                                                                                 |
| 10:10 | <u>Ingo Ruczinski</u> , Kevin W. Plaxco, Tobin R. Sosnick. <b>On the Precision of Experimentally Determined Protein Folding Rates and [Phi]-Values.</b>                                                                                                                                |
| 10:30 | <i>Coffee Break</i>                                                                                                                                                                                                                                                                    |
| 11:00 | <u>Janet M. Thornton</u> , Gemma L. Holliday, Alex Gutteridge, James Torrance, Gail J. Bartlett, Daniel E. Almonacid, Noel M.O'Boyle, Peter Murray-Rust, John B. O. Mitchell. <b>Using the Three Dimensional Structures of Enzymes to Understand Catalysis.</b> (invited presentation) |

### Session 6: **Disorder** (Chair - Thomas Lengauer)

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| 11:30 | <u>Zsuzsanna Dosztányi</u> , Márk Sándor, István Simon. <b>Prediction of Order and Disorder at the Domain Level.</b>                                                                      |
| 11:50 | <u>Avner Schlessinger</u> , Marco Punta, Burkhard Rost. <b>Identifying Natively Unstructured Proteins Using Residue Contact Predictions.</b>                                              |
| 12:10 | <i>Lunch and Laptop Session 2</i>                                                                                                                                                         |
| 15:00 | <b>Discussion 2:</b> What are the greatest overlooked challenges in computational structural biology and what are the most over-studied low impact areas? (Chair: <u>Steven Brenner</u> ) |

### Session 7: **Protein-Protein Interactions and Domains** (Chair – Steven Brenner).

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| 15:45 | <u>Bingding Huang</u> , Michael Schroeder. <b>Integrate the Degree of Burial and Conservation of Surface Residues into Protein-protein Docking.</b>     |
| 16:05 | <u>Stefano Lise</u> , David T Jones, Alice Walker-Taylor. <b>Docking protein domains in contact space.</b>                                              |
| 16:25 | <u>Scooter Willis</u> . <b>Predicting Co-evolving Pairs in Pfam Based on Mutual Information of Mutation Events Measured Along the Phylogenetic Tree</b> |
| 16:45 | <i>Coffee Break</i>                                                                                                                                     |

### Session 8: **Networks and Graphs** (Chair - Rafael Najmanovich)

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| 17:15 | <u>Frank P DiMaio</u> , Jude W Shavlik, George N. Phillips <b>A Probabilistic Approach to Protein Backbone Tracing in Electron Density Maps.</b> |
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| 17:35 | <u>Antonio del Sol</u> , Marcos J. Arauzo-Bravo, Dolors Amoros, Ruth Nussinov. <b>Network Robustness and Modularity of Protein Structures in the Identification of Key Residues for the Allosteric Communications.</b> |
| 17:55 | <u>Steven Brenner</u> . <b>The RNA Structural World.</b>                                                                                                                                                               |
| 18:25 | Closing remarks                                                                                                                                                                                                        |
| 18:30 | <i>The End: Shuttle back to Hotels.</i>                                                                                                                                                                                |