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| **Event name (Dates, Hotel name)** |
| ***Time*** | ***ID*** | ***Title*** | ***Author*** | ***Page*** |
| 9:00 | **Opening remarks, Chair name**, Chair Affiliation |
| **Session 1: Computational Protein Design (chair: John Moult, U. Maryland)** |
| 9:10 | **K** | **Keynote presentation title** | **Bruce Donald**, Duke |  |
| 9:40 | 8 | Presentation title | Presenter name |  |
| 10:00 | 23 | Presentation title | Presenter name |  |
| 10:20 | Coffee |
| **Session 2: Local Interactions (chair: Guido Capitani, Paul Scherrer Institute)** |
| 10:50 | **K** | **Polypharmacology of Drugs and Metabolites** |  |  |
| 11:20 | 24 |  |  |  |
| 11:40 | 4 |  |  |  |
| 12:00 | 6 |  |  |  |
| 12:20 | Lunch & Poster/Laptop session (Swan Ballroom) |
| **Session 3: Crystal Clear Interactions (chair: Matthieu Chartier, U. Sherbrooke)** |
| 14:50 | **K** |  |  |  |
| 15:30 | 26 |  |  |  |
| 15:50 | 22 |  |  |  |
| 16:10 | 10 |  |  |  |
| 16:30 | *Coffee* |
| **Session 4: Integrative Assembly and Modeling (chair: Dmitrij Frishman, Technishce U., Munich)**  |
| 17:00 | **K** |  |  |  |
| 17:30 | 33 |  |  |  |
| 17:50 | 38 |  |  |  |
| 18:30 | Pre-dinner reception (Osprey terrace, Swan Hotel) |
| 19:30 | Dinner (Osprey 1/2, Swan Hotel) |
| **After dinner Warren DeLano session (chair: Philip Bourne, NIH)** |
| 20:30 |  | Introduction | Ilan Samish & Philp Bourne | 12 |
| 20:40 |  | Very Long Molecular Dynamics Simulations: Progress, Problems, and Promise | David E. Shaw, D. E. Shaw Research | 12 |
| **3Dsig: Day 2** (July 9th, Osprey 1/2, Swan Hotel) |
| ***Time*** | ***ID*** | ***Title*** | ***Author*** | ***Page*** |
| **Session 5: Structural flexibility (chair: Ilan Samish, Weizmann Institute)** |
| 9:00 | **K** | **Changes in Ligand Binding in Enzyme Families during Evolution** | **Janet Thornton**, European Bioinformatics Institute | 13 |
| 9:30 | 29 | A Two-step Random Forest Approach for the Identification of the Structural Features of Ligand:Receptor Complexes that are Characteristic of Functional Selectivity. | Michael LeVine, Cornell | 38 |
| 9:50 | 34 | Tertiary Structural Propensities Reveal Fundamental Sequence/Structure Relationships | Gevorg Grigoryan, Dartmouth | 40 |
| 10:10 | 47 | Ordering the Disordered Proteins | Shula Shazman, Open U. Israel | 42 |
| 10:30 | Coffee |
| **Session 6: Couples theory: what makes it work? (chair: Andras Fiser, Albert Einstein College of Medicine)** |
| 11:00 | **K** | **The Landscape of Intertwined Associations in Homo-Oligomeric Proteins** | **Shoshana J. Wodak**, U. Toronto | 15 |
| 11:30 | 12 | Computational Methods to Predict Allosteric Sites on Proteins: a New Route to Drug Discovery? | Joe Greener, Imperial College London | 44 |
| 11:50 | 15 | Prediction of Compensatory Sites through Force Application | Matteo Tiberti, Queen Mary U. London | 46 |
| 12:10 | Lunch & Poster/Laptop session (Swan Ballroom) |
| **Session 7: Making order in a wild world (chair: Rafael Najmanovich, U. Sherbrooke)** |
| 15:00 | **K** | **From Genomes to small-molecules** | **Rafael Najmanovich**, U. Sherbrooke | 16 |
| 15:30 | 44 | Frustration-Guided Motion Planning Reveals Conformational Transitions In Proteins | Dominik Budday, U. Erlangen-Nuremberg | 48 |
| 15:50 | 17 | Capturing and Modeling Structural Flexibility | Thomas Hrabe, Sanford Burnham Prebys Medical Discovery Institute | 50 |
| 16:10 | 14 | Considering Chain Flexibility in Protein Structure Model Evaluation | Daisuke Kihara, Purdue U. | 52 |
| 16:30 | Coffee |
| **Session 8: Recognizing protein folding beyond the hydrophobic core (chair: Ruth Nussinov, National Cancer Institute, NIH)** |
| 17:00 | **K** | **Molecular Principles for Optimizing Protein-DNA Interactions** | **Yaakov (Koby) Levy**, Warren DeLano Keynote, Weizmann Institute | 17 |
| 17:30 | 35 | Unexpected Features of the 'Dark' Proteome of Structural Biology | Sean O'Donoghue, CSIRO & Garvan Institute | 54 |
| 17:50 | 11 | Latest Developments of the Protein Fold Recognition Method ORION  | Jean-Christophe Gelly, U. Paris Diderot | 56 |
| 18:10 | Closing remarks & Award ceremony (Warren DeLano award & best poster awards), Philip Bourne |
| 18:20 | End of 3DSIG 2016 |