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	Michael LeVine, Cornell	38

		of Ligand:Receptor Complexes that are Characteristic of Functional Selectivity.		
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			