

	Template Finding	Assembling/ Sampling	Loop Modeling	Scoring	Refinement	Model Quality Assessmt
J. Fernando Bazan NeuroScience	Find good templates, fold recognition, family assembly.					
Gaurav Chopra Levitt Group Samudrala Group Stanford					Refinement	
Rodrigo Faccioli & Leandro Bortot University of Sao Paulo, Brazil		Conformational sampling using evolutionary computing-based approaches as implemented in our framework, which can handle multiple combinations of fitness functions and evolutionary algorithms. It will be possible to implement suggestions made during the upcoming discussions.		Perform some energy and structure-related calculations of the predicted structures with GROMACS. These include, but are not limited to: solvation energy, protein potential energy, flexibility, solvent accessible surface area and number of intraprotein hydrogen bonds.	Perform different kinds of molecular dynamics simulations such as simulated annealing or replica exchange molecular dynamics of the predicted structures.	
Firas Khatib & FoldIt Baker Lab University of Washington	Participate in specific components of the protein structure prediction pipeline where game playing humans could help.					
Narcis Fernandez-Fuentes Aberystwyth University, UK		Fragment-based assembling of protein structures using a supersecondary library.	Loop modeling			
Chen Keasar Ben Gurion University					Automation of an aspect of refinement, which is the decision of which parts of the model need not be	

					refined. For example, highly conserved catalytic residues are practically identical in all template residues and thus are most likely to be structurally conserved in the target. Generate lists of structurally conserved residues.	
Andrzej Kloczkowski Nationwide Children's Hospital						Yes
Justin MacCallum Ken Dill's Lab Stony Brook University	Integrate different sorts of information. These methods would generally come towards the end of the pipeline after all of the alignments, etc have been completed.					
Harold Scheraga & Adam Liwo Scheraga Group Cornell		Sampling. Will use coarse-grained UNRES force field with the multiplexed replica exchange method.				
Hongyi Zhou Skolnick Lab Georgia Tech					Refinement	