

Predicting Structure: Current Techniques and Challenges

By Arun Arjunakani and Joseph Jagusah

TASSER Techniques	QUARK	Challenges (cont.)
<ul style="list-style-type: none"> ● This is a family of structure prediction techniques. ● I-TASSER is a server based program. <ul style="list-style-type: none"> ○ User submits an amino acid ○ Program returns several possible structures based on known ones. ● M-TASSER is a program specifically designed for tertiary structure prediction and is more accurate 	<ul style="list-style-type: none"> ● QUARK is a program attempting to fold small proteins ab initio. ● QUARK represents proteins by their side-chain center of mass and peptide backbone.. ● QUARK does not fix bond lengths and angles. ● Searches through conformational space allow one-third of short proteins (<100 residues) with TM-ratios of >.5 to be successfully folded 	<ul style="list-style-type: none"> ● Analysis is generally done on fragments instead of the whole protein. ● Larger proteins (120 amino acids or more) are hard to accurately predict.
Fold-It	Challenges	Bibliography
<ul style="list-style-type: none"> ● Fold-It is a game designed to teach people about protein structure ● This online game uses rosetta structure prediction methodology ● This is an example of crowdsourcing scientific research. 	<ul style="list-style-type: none"> ● Most accurate programs require template structures to predict protein folding. ● Knowledge of the temperature and other thermodynamic properties of a protein-solution system is difficult to predict. ● The ‘Search Space’ of all possible conformations of a protein is large when not constraining the search. 	<p>Bioinformatic Tools. (n.d.). Retrieved November 5, 2015, from https://bioinformatictools.wordpress.com/tag/i-tasser/</p> <p>I-TASSER server for protein structure and function prediction. (n.d.). Retrieved November 2, 2015, from http://zhanglab.ccmb.med.umich.edu/I-TASSER/about.html</p> <p>Popović, Z., & Baker, D. (n.d.). Predicting protein structures with a multiplayer online game. <i>Nature</i>, 466, 756–760. Retrieved November 1, 2015, from http://www.nature.com/nature/journal/v466/n7307/full/nature09304.html</p> <p>Xu, Dong, and Yang Zhang. "Ab Initio Protein Structure Assembly Using Continuous Structure Fragments and Optimized Knowledge-based Force Field." <i>Proteins: Structure, Function, and Bioinformatics</i>. Web. 1 Nov. 2015.</p>

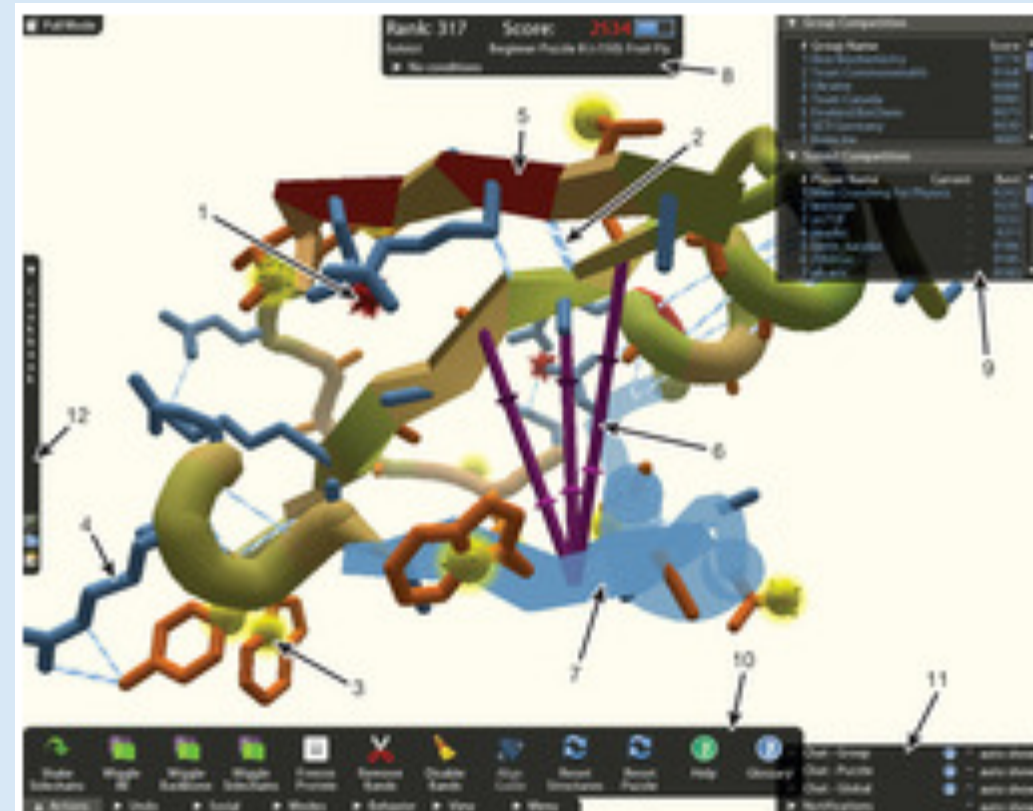


Figure 1: This is a screenshot of the Foldit game.