

## **Computational and Experimental Methods for High Confidence Protein Structure Prediction**

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Computational modeling of protein structure can provide a fast and relatively inexpensive alternative to direct structure determination via X-ray crystallography or nuclear magnetic resonance. A rather recent trend in the prediction of polypeptide conformation is the use of experimental results from reactions such as proteolytic digestion, chemical modification, and cross-linking. Incorporation of these results into the modeling process introduces a number of computational challenges. For chemical modification reactions, some of the challenges include identification (and even quantitation) of reaction products from experimental results, estimation of reaction rates, correlation of reaction rates with structural, sequence, physical and chemical properties of reactive residues, and estimation of model quality. We have developed a suite of software tools that facilitate these and other steps on the pathway to reliable structure prediction. Here we will discuss several of the tools and techniques involved in the context of their contribution to the process of deriving a high quality structural model.