Abstract Submitted
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Harnessing uncertain data for structure prediction of proteins and peptide binding[1] ALBERTO PEREZ, SBU — Physics based simulations based on Molecular Dynamics have long held the promise to produce accurate free energies, pathways, mechanisms and structures by filling in the Ångstrom by Ångstrom and picosecond-to-picosecond details that cannot be observed experimentally. In practice, such calculations have been too computationally expensive but for the smallest systems . We have developed an advanced sampling technique called MELD (Modeling Employing Limited Data) that can harness problematic data (noisy, ambiguous or sparse) coming from different sources (experiment or general knowledge). We have used it to accurately predict the structures of several proteins in a blind test event called CASP and to predict binding poses and relative binding free energies of p53 derived peptides to the proteins MDM2 and MDMX. During this talk I will present an overview of the methodology and its applications.

[1]NIH

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