

The PyRosetta Interactive Platform for Protein Structure Prediction and Design: A Set of Educational Modules

Jeffrey J. Gray

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TALARIS UPDATE INCLUDED ... This book contains a set of workshops which teach the PyRosetta program for computational protein structure prediction and design. PyRosetta (http://www.pyrosetta.org) is a Python-based interactive platform for accessing the objects and algorithms within the Rosetta protein structure prediction suite. Rosetta, developed by a consortium of laboratories in the Rosetta Commons, has an unmatched variety of functionalities and is one of the most accurate protein structure prediction and design approaches. The workshops teach how to measure and manipulate protein conformations, calculate energies in low- and high-resolution representations, fold proteins from sequence, model variable regions of proteins (loops), dock proteins or small molecules, design protein sequences, and build custom protocols for operations tailored to particular biomolecular applications.



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