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Combining Consensus and Ensemble Docking Methods to Improve Molecular Docking CONNOR MORRIS, DENNIS DELLA CORTE, Brigham Young University — Molecular docking programs are computational tools used to predict protein-ligand binding poses and energy. They are widely used in drug discovery to filter binding ligands from nonbinding ones in the search for potential drug candidates. However, they suffer from two main weaknesses: inaccurate scoring functions and rigid protein receptors. Two distinct methods, consensus docking and ensemble docking, are used to account for these problems separately. Consensus docking uses multiple docking scoring functions to evaluate docking poses, mitigating the weaknesses of each individual scoring function. Ensemble docking uses molecular dynamics (MD) to incorporate protein flexibility into docking simulations. Combining consensus docking and ensemble docking methods into a single docking protocol leads to improved docking results.

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