Abstract Submitted
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Accessing the limits of ab initio docking methods[1] RADHEY SHYAM, EMIL ALEXOV, Clemson University — Ab initio protein docking is the prediction of the three dimensional structure of a protein-protein complex from the structures of two interacting proteins, receptor and ligand. Here we report our instigation of the performance of several popular ab initio docking algorithms (ZDOCK, GRAMM and 3D-Garden) in a bound test (lock-and-key) on very large set of 2903 cases taken from ProCom database. The bound test was preferred over the unbound because of two reasons (1) to test the performance of docking algorithms without obscuring the results with the effects originating from possible conformational changes and (2) to expand the benchmarking set since we do not need the 3D structures of isolated monomers. The assessment of the predictions was made by computing the ligand RMSD (L_RMSD). The first ten ranked predictions were taken. It was found that, on average, only 28% of the predictions resulted in L_RMSD $<$ 10 A, which is the standard criterion of acceptable models in CAPRI. The performance of the methods was investigated with respect to physical characteristics of the receptor and ligand as well.

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