SUPPORTING INFORMATION

Medusadock 2.0: Efficient and Accurate Protein-Ligand Docking With Constraints

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The relationship between the number of ligand rotatable bonds and RMSD

With an increase in the number of rotatable ligand bonds, the RMSD usually deteriorates. In order to study the relationship between the number of ligand rotatable bonds, constraints and RMSD, we performed dockings for all 4154 complexes in the refined set with MedusaDock 2.0. No constraints are added during the docking. As shown in Figure S3, when the number of rotatable bonds is small, the RMSD increases very rapidly; however, as the number of rotatable bonds increases, the RMSD shows a linear growth trend. We fit the data to Eq. 1:

$$RMSD = NROT^{\alpha} + k \quad (1)$$

where α is 0.543 and *k* is 2.673 when the docking is performed without constraints. When the complexes are subjected to docking with one constraint, α increased slightly to 0.551 and *k* became 1.402. In both cases, the α of less than 1 indicates that the RMSD increases quite slowly with the increase of the number of rotatable bonds. The value of *k* in the one-constraint case (1.271 Å) is less than that in the no-constraint case (2.673 Å), which again highlights the effect of constraints.

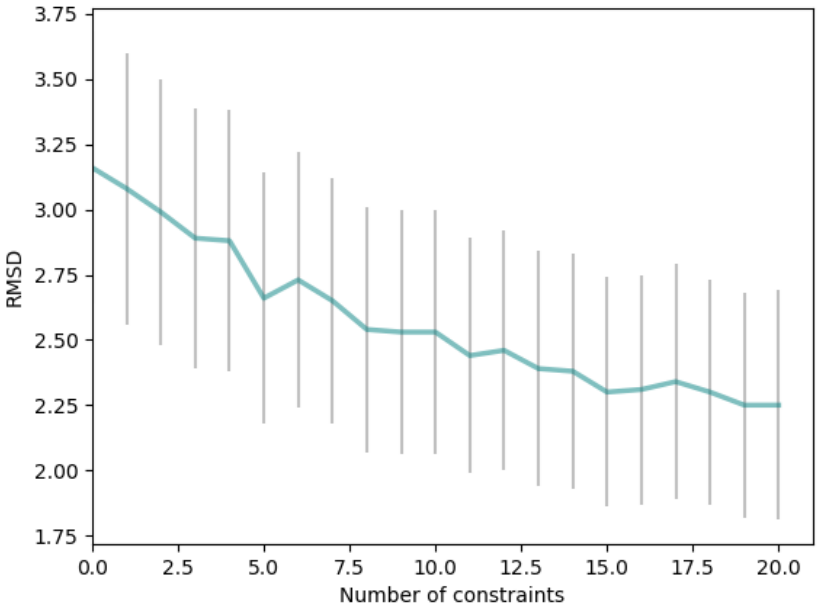

Figure S1. The relationship between RMSD and the number of constraints in the cross-docking test set. The line refers to the average RMSD and the grey bars refer to standard deviations.

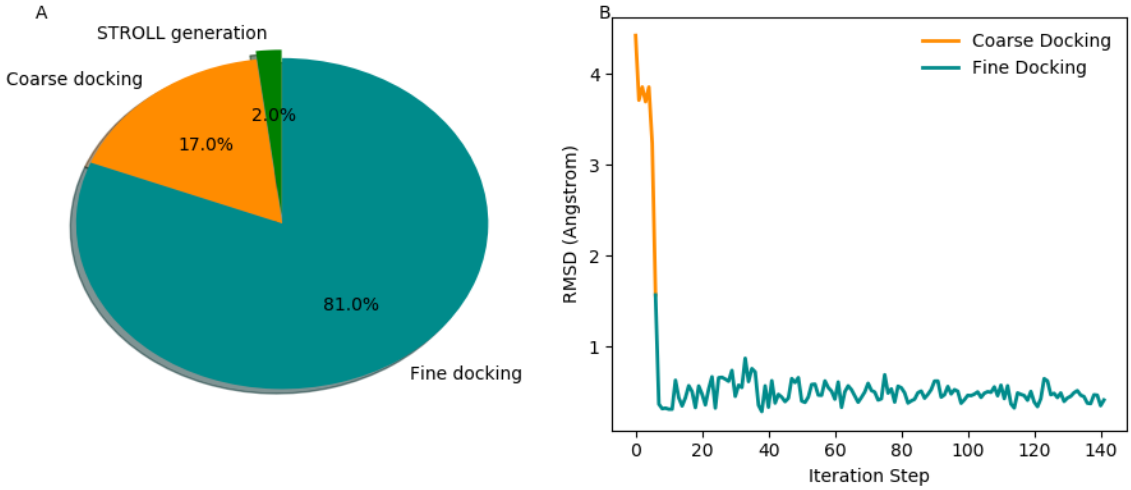

Figure S2. C of the docking time consumed in coarse docking and fine docking. (A) The average percent of time consumed in STROLL generation, the coarse docking, and the fine docking. The average are calculated upon the 100 complexes. (B) RMSD variation during the coarse docking and the fine docking of 2X96.

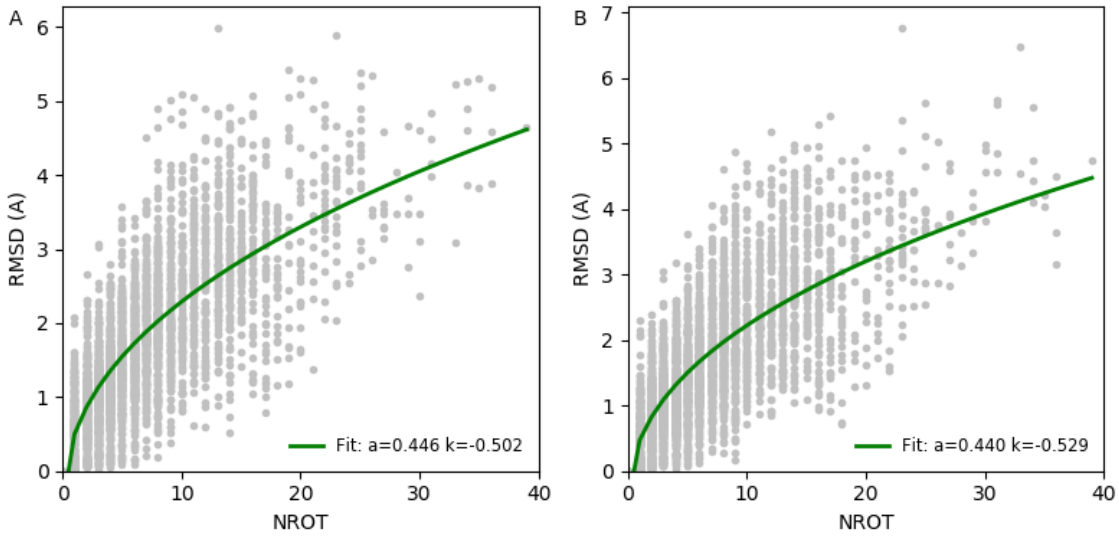

Figure S3. Comparison of the relationship between RMSD and the number of rotatable bonds when using 0 or 1 constraint for all the 4154 complexes. (A) Correlation between RMSD with no constraints and the number of rotatable bonds. (B) Correlation between RMSD with one constraint and the number of rotatable bonds.