Supporting Information

Construction and test of ligand decoy sets using MDock: CSAR benchmarks for binding mode prediction

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Figure S1

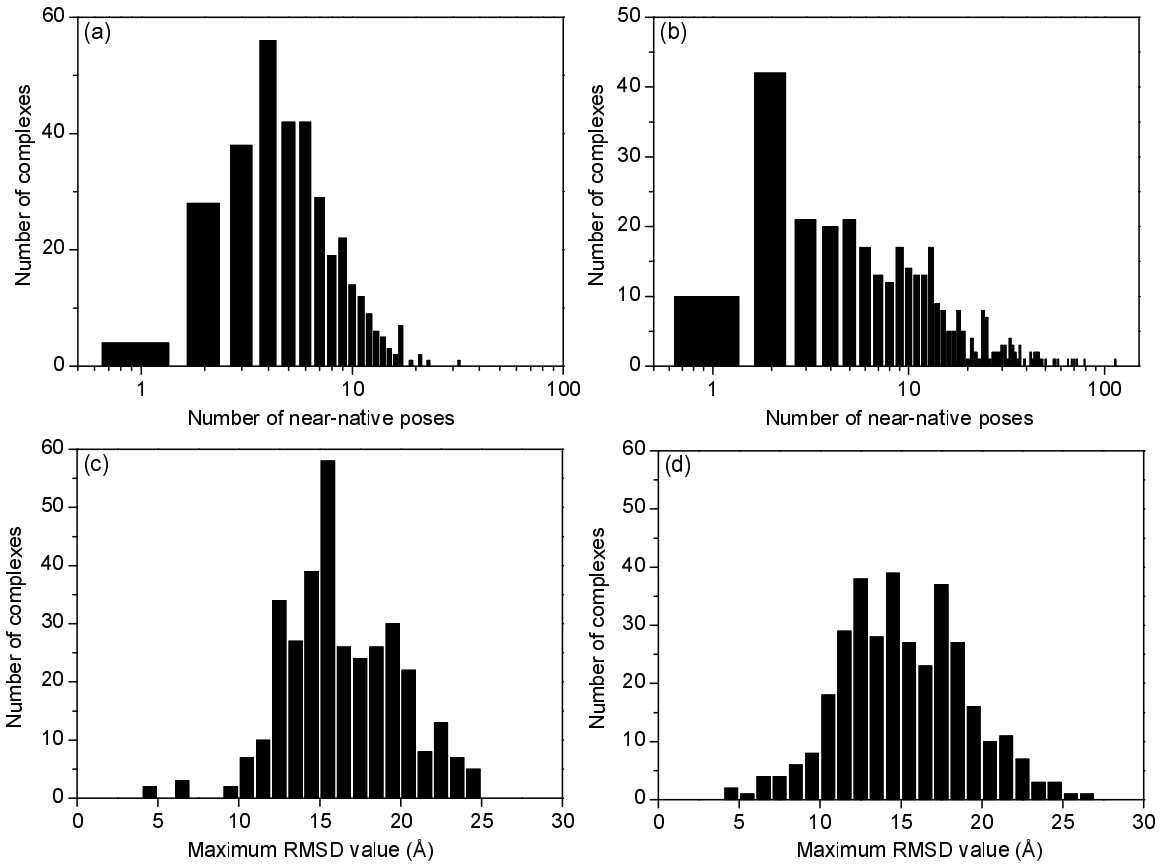

Figure S1: The statistics of the ligand binding decoys for the CSAR-NRC HiQ benchmark: The number distribution of the near-native binding modes (RMSD<2.0 Å) in the (a) rigid-ligand and (b) flexible-ligand decoys of a complex; The maximum RMSD distribution in the (c) rigid-ligand and (d) flexible-ligand decoys of a complex. Notice that the horizontal axes in Panel (a) and Panel (b) are in logarithmic scales.

Figure S2

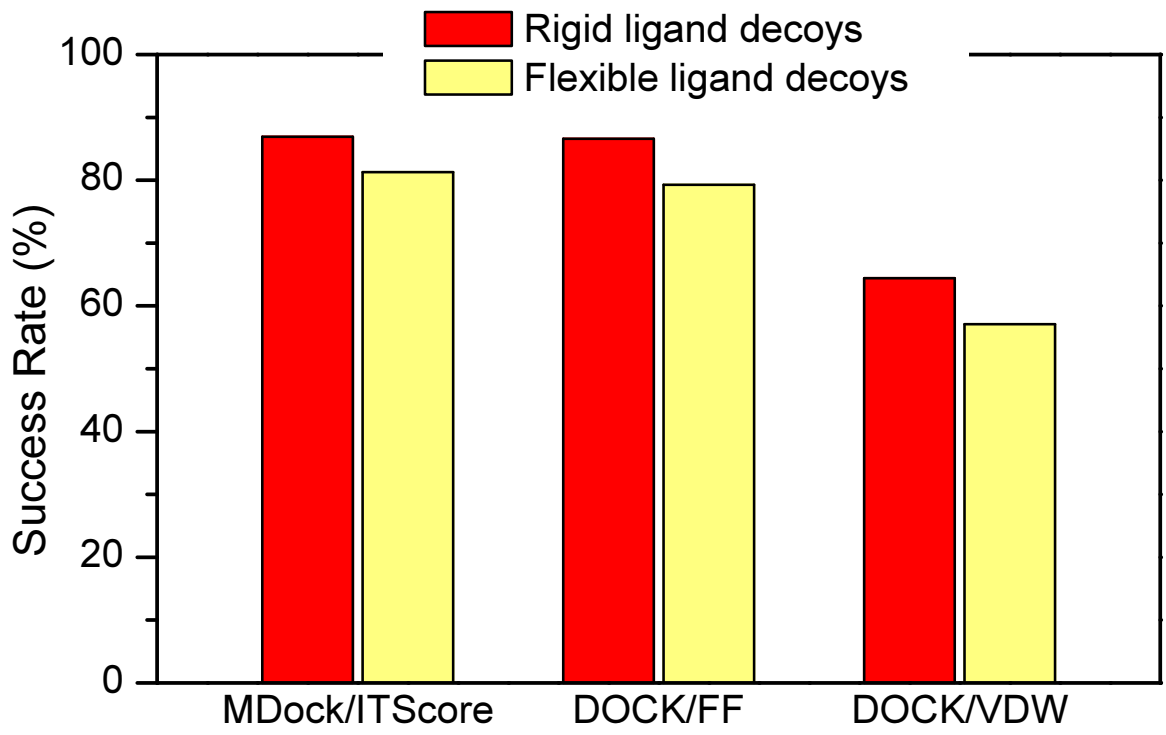

Figure S2: The success rates of ITScore, DOCK/FF, and DOCK/VDW on identifying native binding modes with the ligand decoys constructed for the CSAR-NRC HiQ benchmark using the criterion of RMSD < 2.0 Å from the native structure if the top-scored pose was considered.

Figure S3

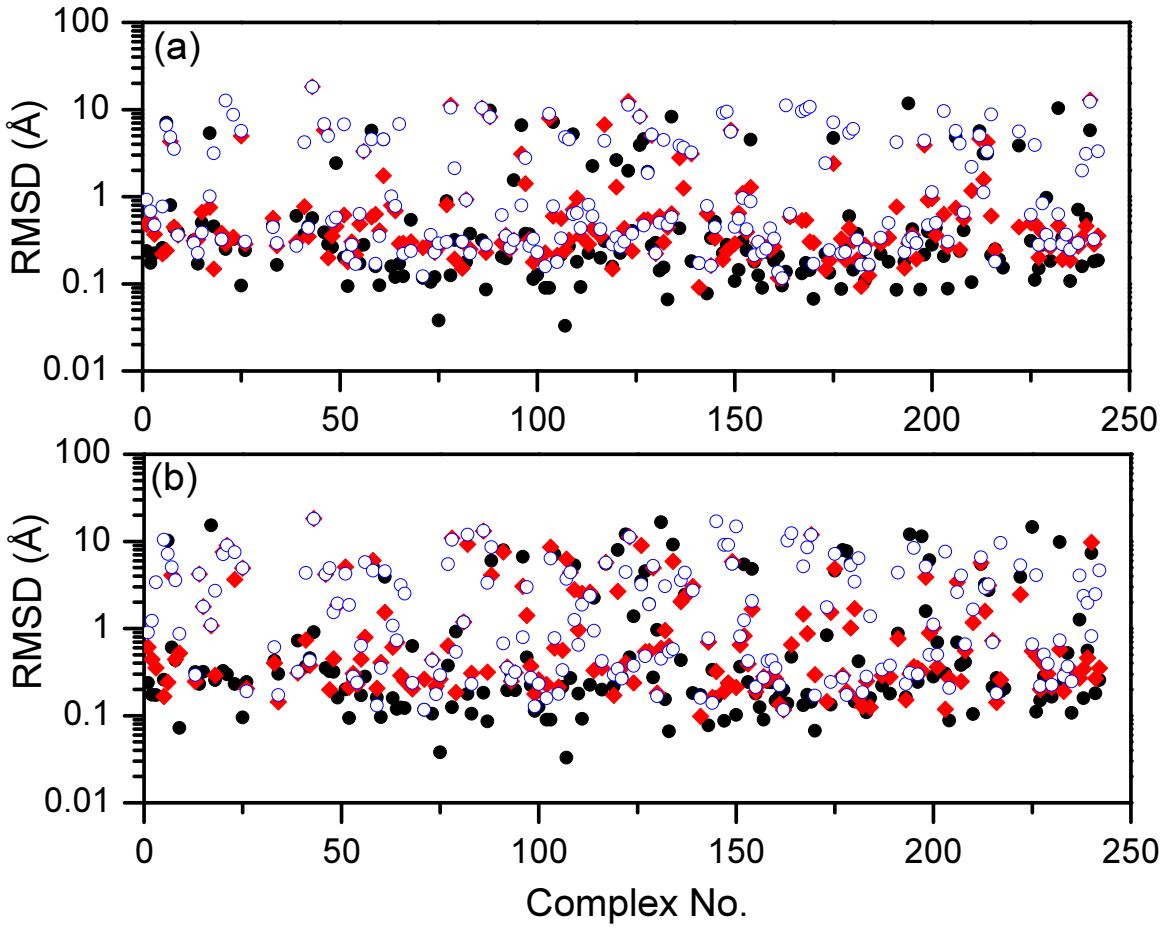

Figure S3: The RMSD values of the top binding modes predicted by ITScore (black, filled circle), DOCK/FF (red, filled diamond), and DOCK/VDW (blue, open circle) with set 1 of the CSAR-NRC HiQ benchmark: (a) rigid ligand decoys; (b) flexible ligand decoys. Notice that the CSAR-NRC HiQ ID numbers of the complexes are not sequential, and therefore the x axes extend up to 250, which is more than the total number of complexes.

Figure S4

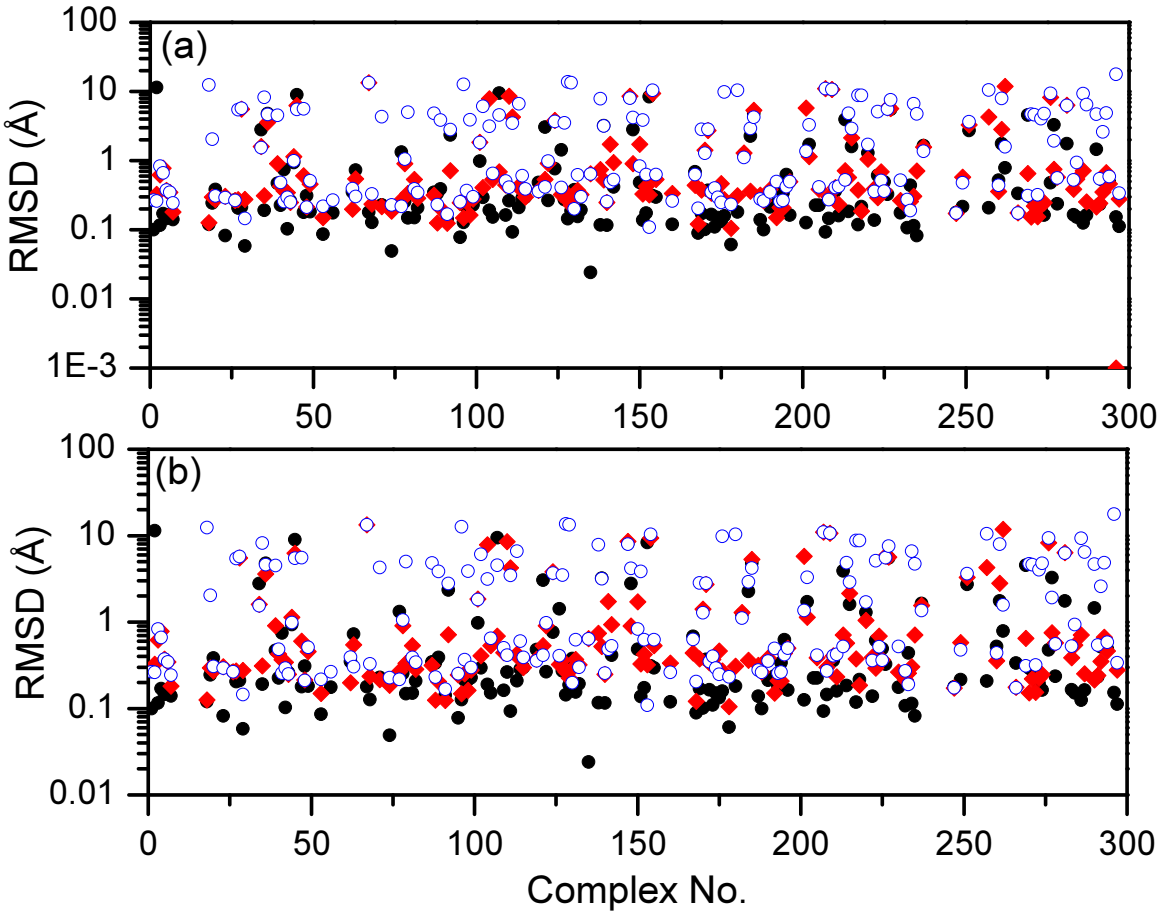

Figure S4: The RMSD values of the top binding modes predicted by ITScore (black, filled circle), DOCK/FF (red, filled diamond), and DOCK/VDW (blue, open circle) with set 2 of the CSAR-NRC HiQ benchmark: (a) rigid ligand decoys; (b) flexible ligand decoys. Notice that the CSAR-NRC HiQ ID numbers of the complexes are not sequential, and therefore the x axes extend up to 300, which is more than the total number of complexes.