Supporting Information

HybridDock: a hybrid protein-ligand docking protocol integrating protein- and ligand-based approaches

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Figure S1: Binding energy scores vs. experimentally measured affinity data for our hybrid docking protocol and MDock on the 10 ligands against the DIG-binding protein for CSAR 2013 Phase 3.

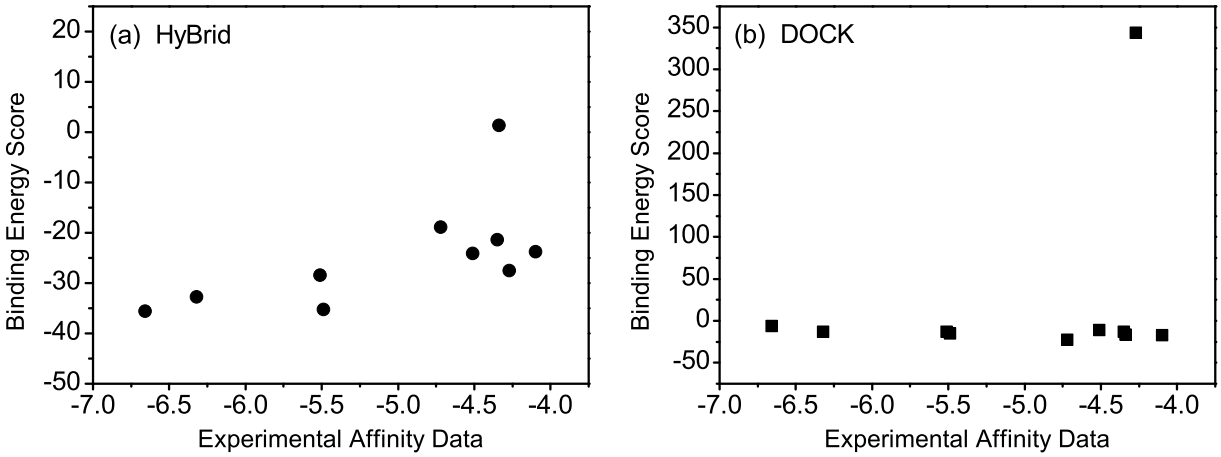

Figure S2: Binding energy scores vs. experimentally measured affinity data for our hybrid docking protocol and MDock for CSAR 2014 Phase 2: A. FXA (163 ligands), B. SYK (276 ligands), and C. TRMD (31 ligands).

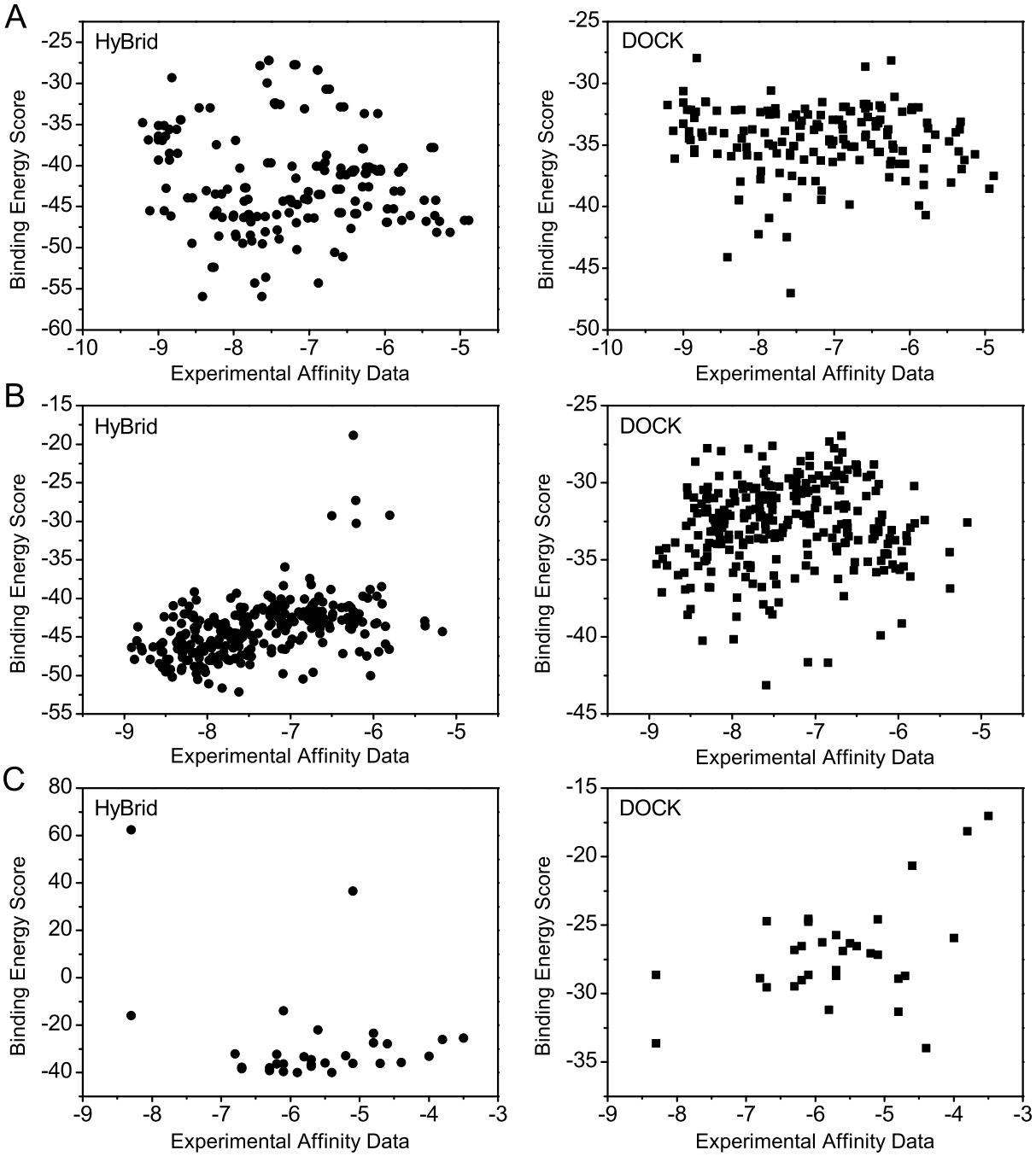

Figure S3: Ligand RMSDs predicted by our hybrid docking protocol and DOCK in binding mode predictions for three FXA (to the left of the blue dashed line), eight SYK (between the blue and green dashed lines), and 31 TRMD (to the right of the green dashed line) protein-ligand complex structures for CSAR 2014 Phase 2.