

# Supporting Information for “On Choosing the Optimal Rigid Receptor for Docking and Scoring in the CSAR 2013/2014 Experiment”

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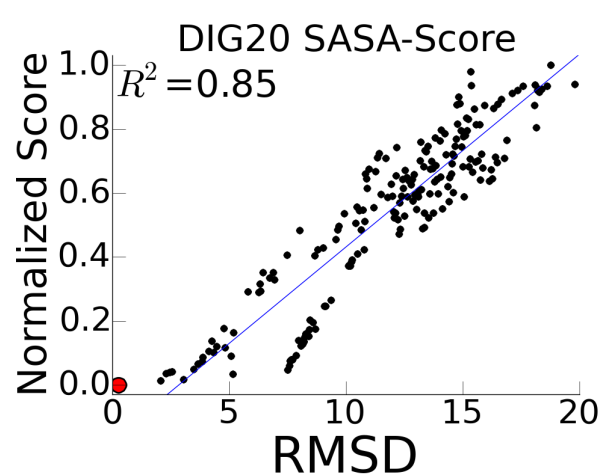
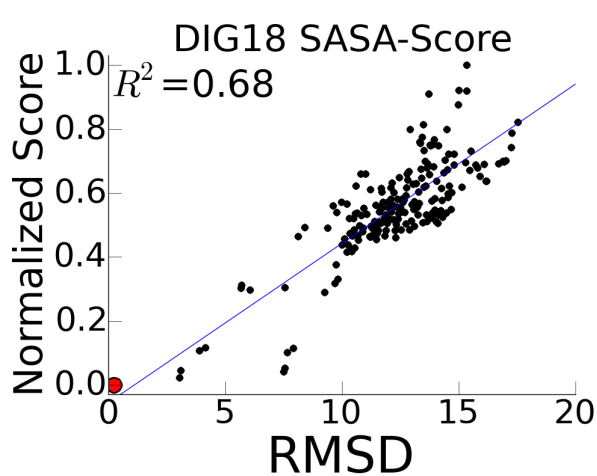
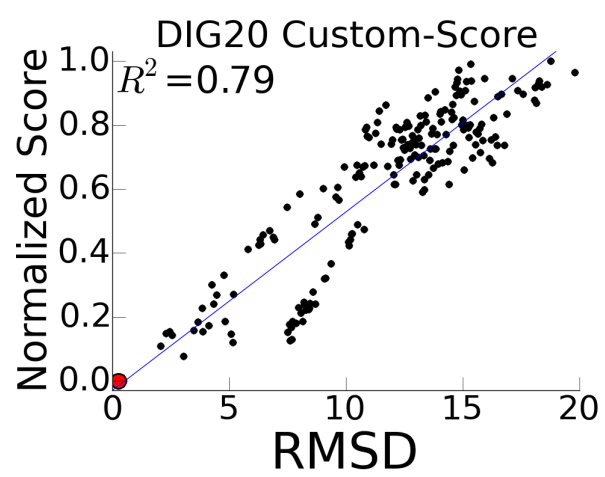
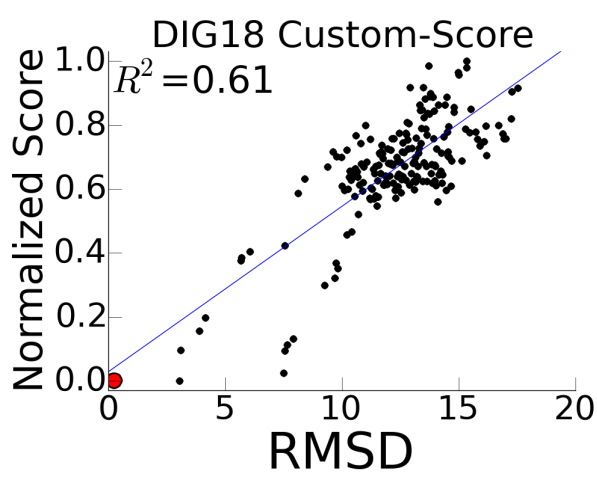
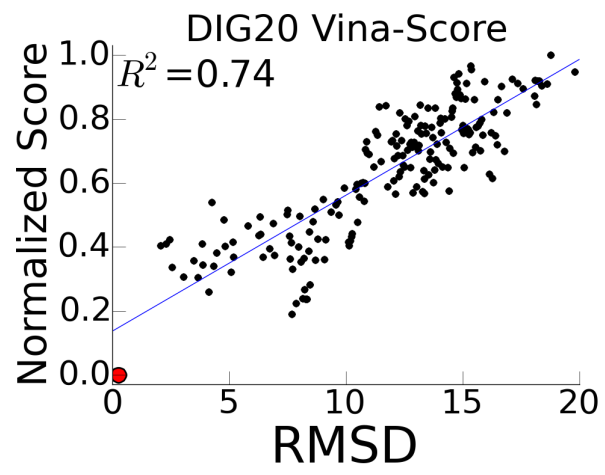
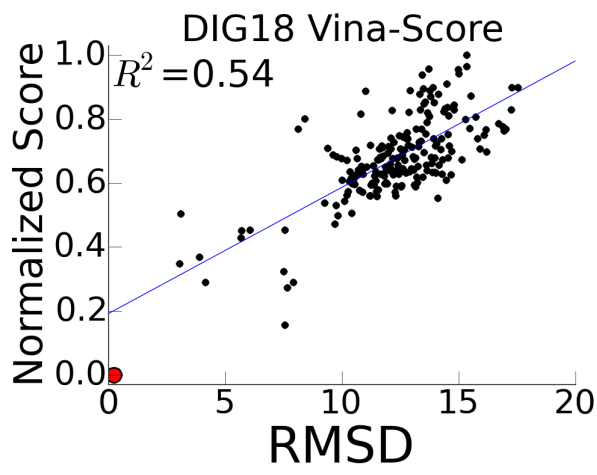
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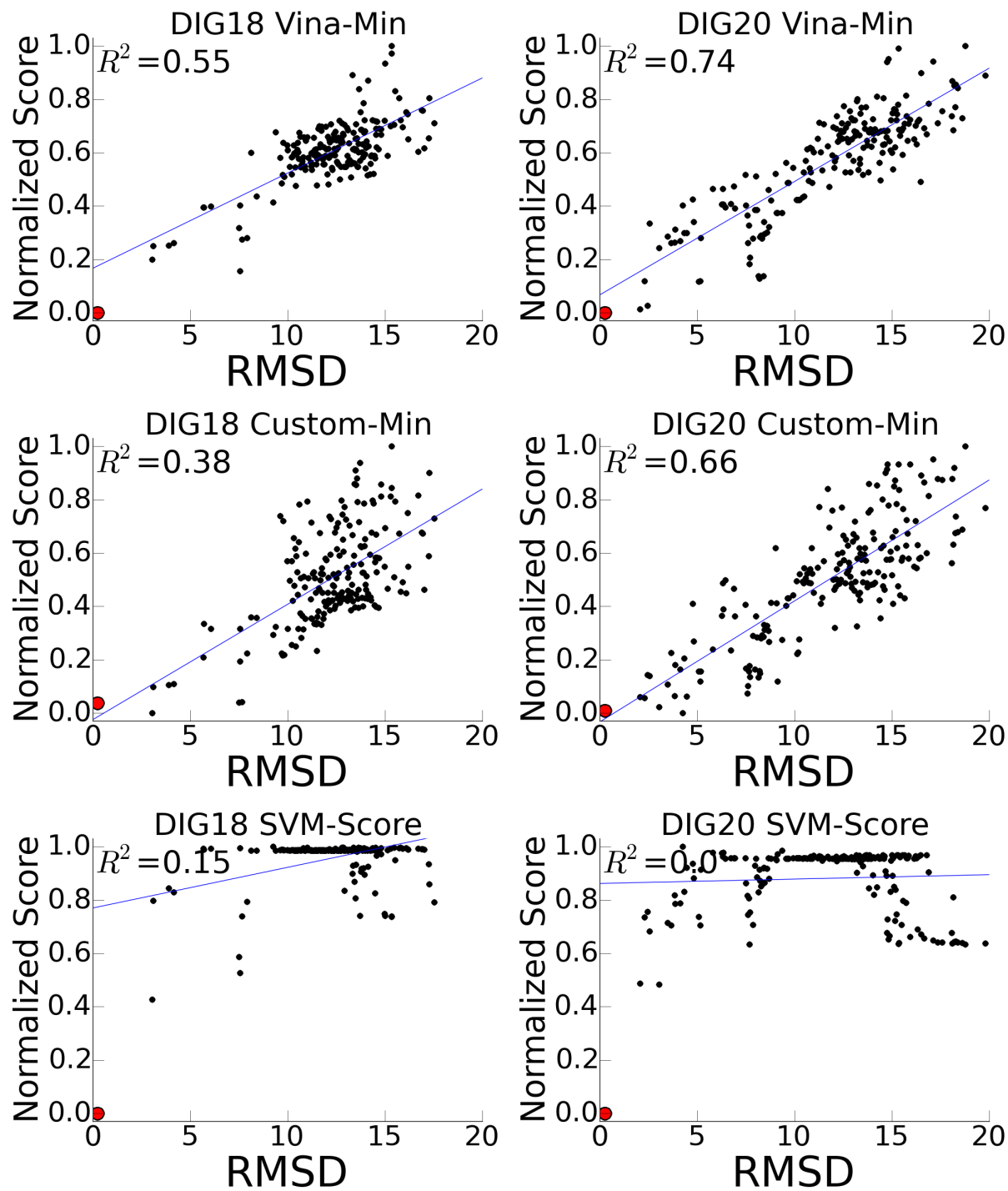
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## Table S1

List of features considered for training the SVM-Score ranking method for CSAR 2013 Phase 2. The bolded terms were used in the final model.

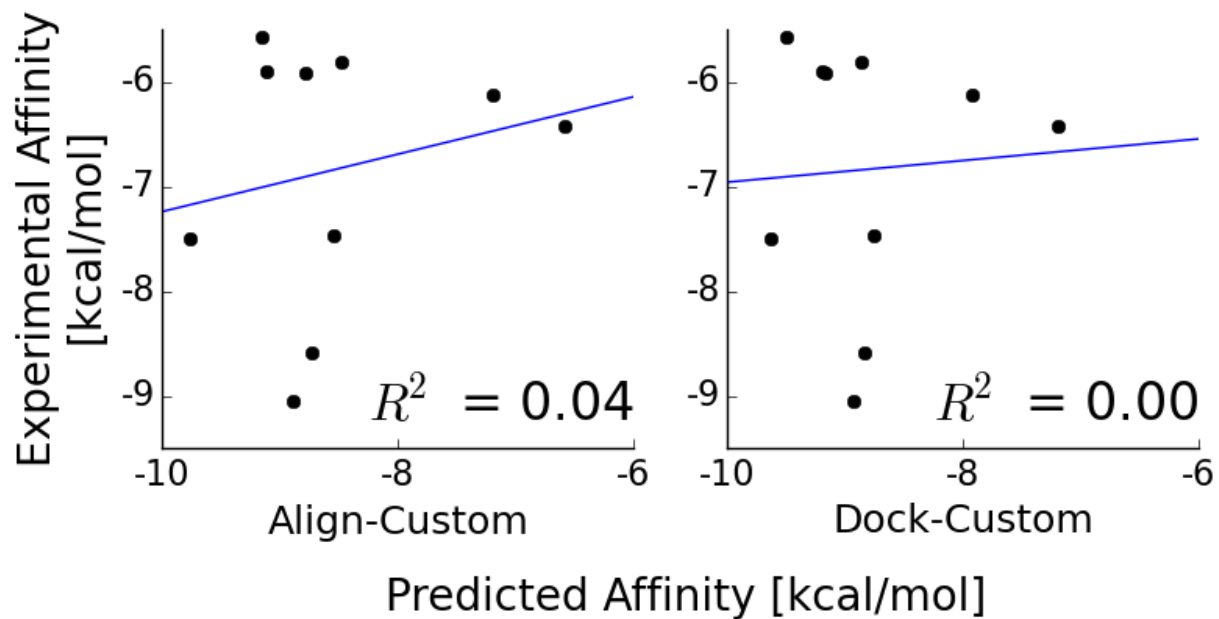
Source	Term
	<b>Vina Score</b> <b>Custom Score</b> <b>Total SASA</b> Hydrophobic SASA
Unweighted Vina Scoring Terms	gauss(o=0,_w=0.5,_c=8) gauss(o=3,_w=2,_c=8) repulsion(o=0,_c=8) hydrophobic(g=0.5,_b=1.5,_c=8) non_dir_h_bond(g=-0.7,_b=0,_c=8)
Unweighted Custom Scoring Terms	vdw(i=4,_j=8,_s=0,_^=100,_c=8) non_dir_h_bond(g=-0.7,_b=0,_c=8) ad4_solvation(d-sigma=3.6,_s/q=0.01097,_c=8)





**Figure S1**

The RMSD of the decoy poses from CSAR 2013 Phase 2 plotted against their normalized scores using the six methods used. The red circle indicates the near-native pose and the blue line indicates the best-fit curve and the  $R^2$  is shown in each of the plots.



**Figure S2**

The Custom scoring function provides poor affinity predictions. (left) Pre-generated conformers are aligned to a co-crystallized ligand and energy minimized with the Custom scoring functions, or (right) compounds are docked with the Custom scoring function. The blue line shows the linear fit and the  $R^2$  value is shown in each subplot.