

SUPPORTING INFORMATION

Rapid Decomposition and Visualisation of Protein-Ligand Binding Free Energies by Residue and by Water

Christopher J. Woods, Maturios Malaisree, Julien Michel, Ben Long,
Simon McIntosh-Smith and Adrian J. Mulholland

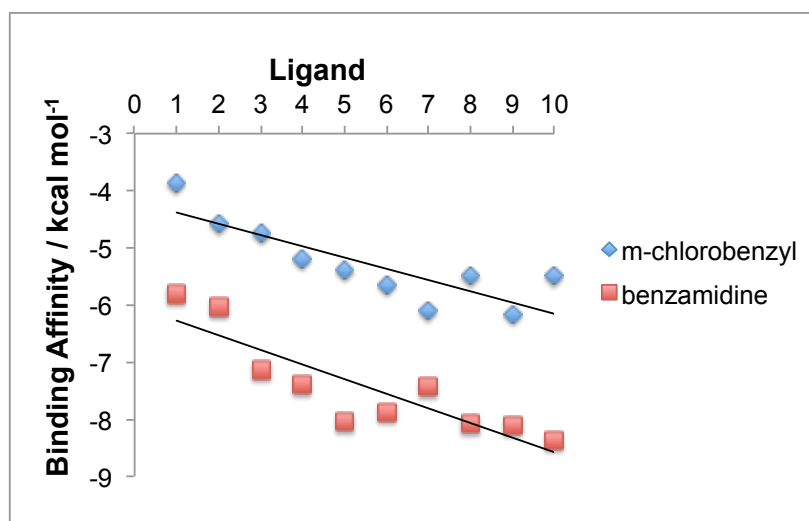


Figure S1. Experimentally measured binding affinities for the 10 ligands studied in this work (m-chlorobenzyl) and for the ten benzamidine analogs. Binding affinities are taken from Muley et al., doi: 10.1021/jm9016416 (reference 32 in our paper).

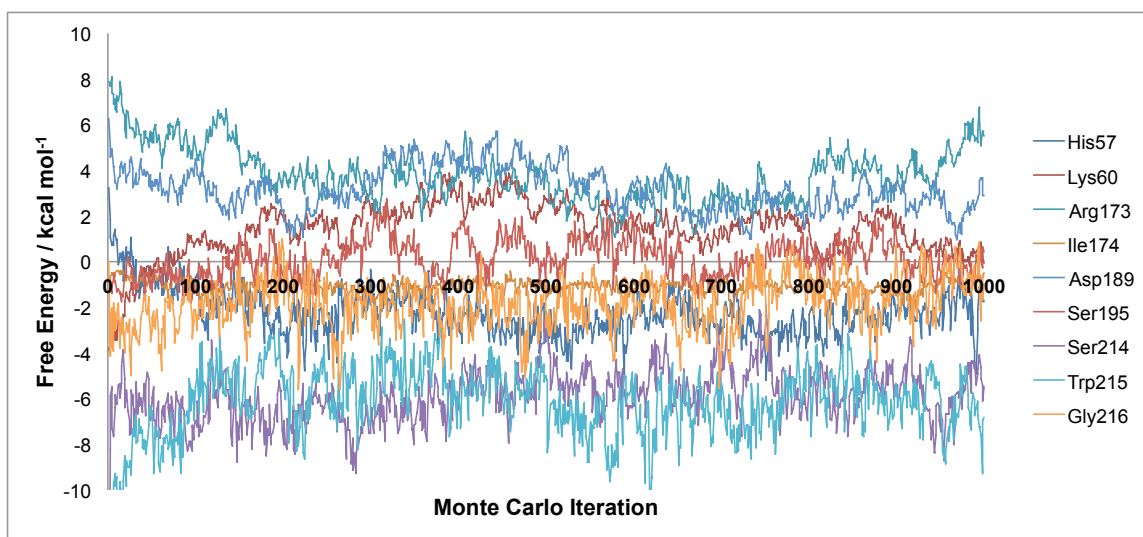


Figure S2. Components of the waterswap free energy for selected residues as calculated using averages calculated over individual Monte Carlo iterations for the 20 ns snapshot of ligand 9 bound to thrombin.