Revealing the binding modes and the unbinding of 14-3-3σ proteins and inhibitors by computational methods

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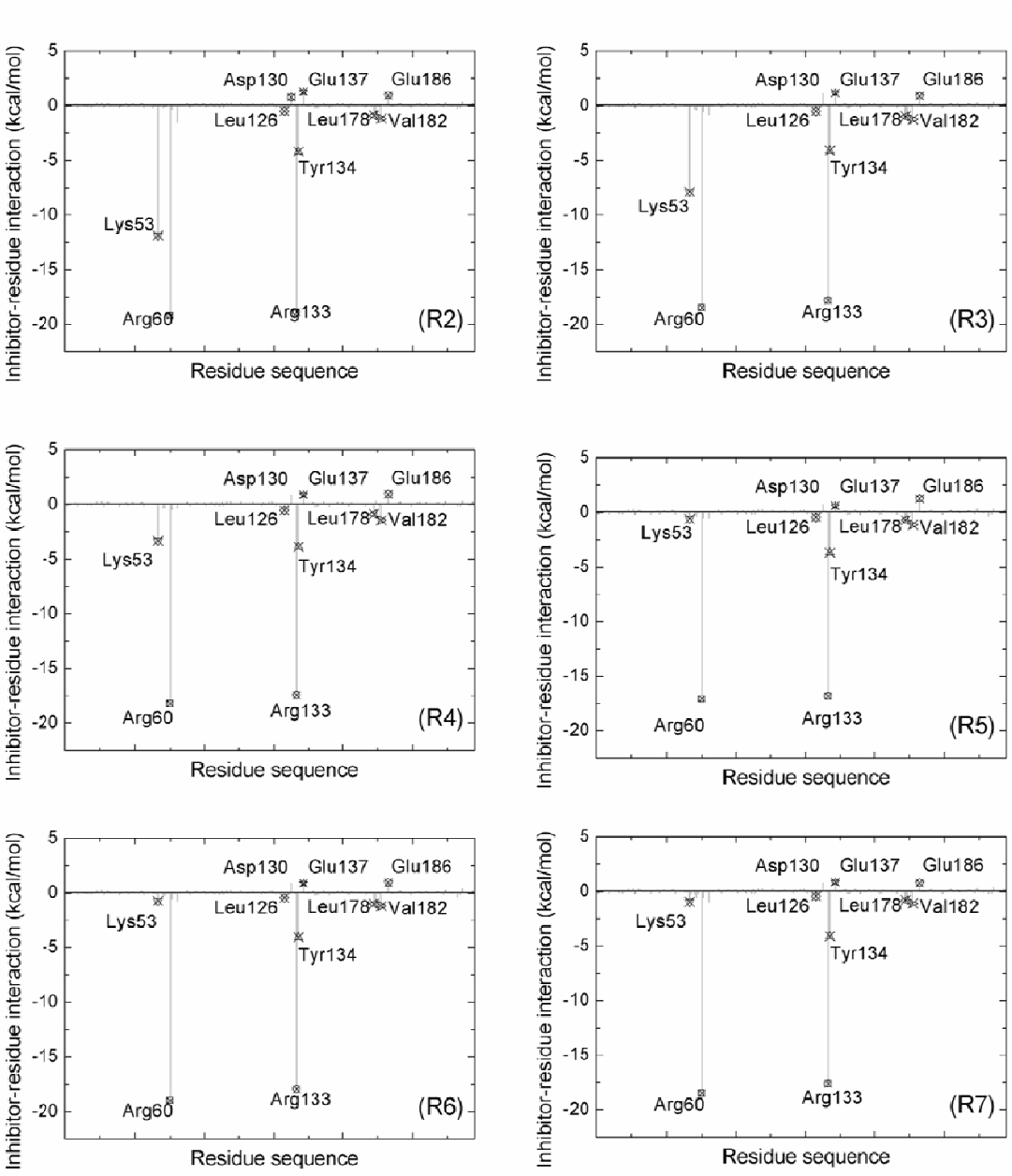

Figure S1. Decomposition of on a per-residue basis for the compounds R2- R7.

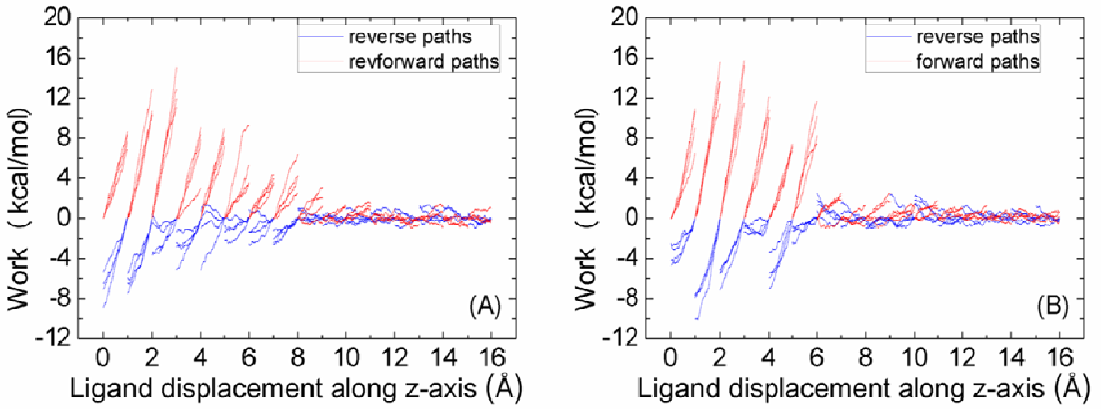

Figure S2. Plots A and B are the work done along the forward and reverse pulling paths for compound R1 and R8, respectively. In the forward direction, the atoms of a inhibitor were pulled away from the binding site. In the reverse direction, the atoms of a inhibitor were pulled back to the binding site.