Electronic Supplementary Material (ESI) for Molecular BioSystems

Supporting Materials

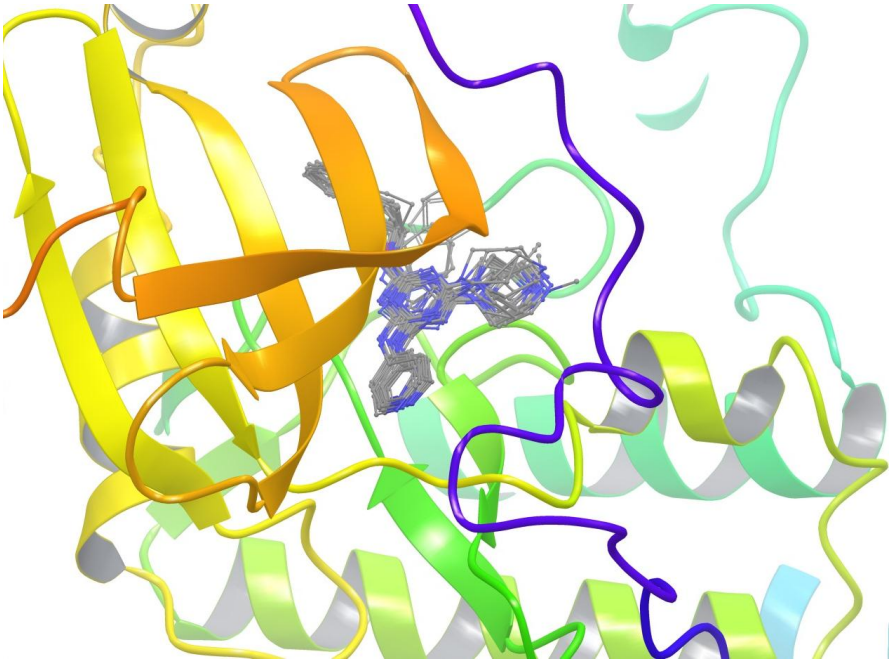

Figure S1. The alignments of 21 docked structures in the binding site of ROCK1.

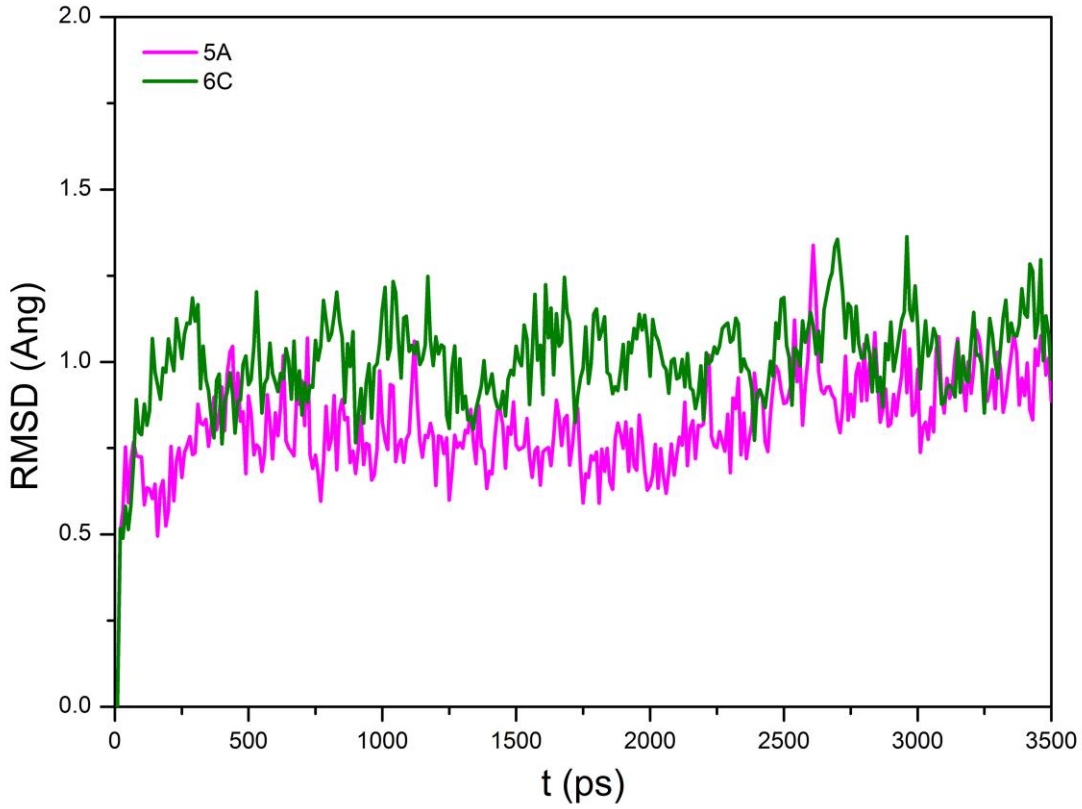

Figure S2. Root-mean-square displacement (RMSD) of the backbone C_α atoms of the binding pocket residues for the ROCK1/inhibitor complexes (5A and 6C) with respect to the first snapshot as a function of time.