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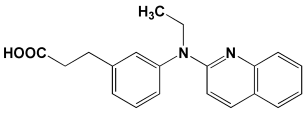
Supplementary file 1

AutoDock4.2 validation results for different 3D holo RhoA-ligand complexes retrieved from PDB

Target	PDB code	Resolution (Å)	Structures of Co-crystallographic inhibitors	ΔG_b (kcal/mol)	Top-ranked population (Out of 50)	RMSD from reference (Å)
RhoA	5JHH	2.30		-7.37	28	1.64