

ST2. GScore and BFE values of structurally distinct HDACi against HDAC1

HDAC Inhibitor	Target HDAC	GScore	$\Delta G_{\text{binding}}$ (kcal/mol)
LAQ824	HDAC1	-9.4	-63.6098
CRA-024781		-8.7	-40.8433
LBH-589		-9.51	-54.0967
HC-toxin		-6.65	-73.5482
Valproic acid		-2.48	37.09804