

ST1. GScore and BFE values of structurally distinct HDACi against HDAC2

HDAC Inhibitor	Target HDAC	GScore	$\Delta G_{\text{binding}}$ (kcal/mol)
LAQ824	HDAC2	-10.74	-67.7911
CRA-024781		-9.88	-53.2132
LBH-589		-9.88	-55.6214
HC-toxin		-6.64	-79.5371
Valproic acid		-3.61	-9.09224