AutoDock Vina Binding Energy Landscape
(Gold boxes = Cognate substrates)

Protein Construct	PRO	THR	SER	ALA	GLY	VAL	ILE	LEU	MET	CYS	TYR	PHE	TRP	ASN	GLN	ASP	GLU	LYS	ARG	HIS
anc_prors_cat	-1.7	-2.0	-1.5	-1.7	+12	-2.3	-3.5	-1.8	-2.8	+20	-1.8	-1.7	-3.6	+3	-1.0	+0.1	+0.9	+0.1	-2.6	-3.0
anc_prors_edit	-0.3	-2.7	-1.2	+0.6	-1.1	-1.5	-1.2	+0.5	-2.5	+1	-2.8	-2.3	-1.9	-1.5	-1.1	-1.5	+2	+2	+3	-0.3
modern_prors	-3.9	-3.0	-3.3	-3.1	-1.8	-2.3	-2.8	-2.6	-0.5	-2.9	-2.8	-2.5	-4.0	-2.2	-3.2	-1.8	-3.0	-2.9	-3.4	-4.4
anc_thrrs_cat	-2.3	-1.9	-0.1	-1.4	+0.9	-2.0	-3.9	-1.3	-0.2	+10	+0.8	+24	-2.7	-2.7	-2.9	+0.6	-3.0	-1.8	+2	+1
anc_thrrs_cat_zn	-2.5	-2.0	-2.5	-3.3	+2	-1.3	+0.2	+3	+0.0	+9	+2	-1.6	-2.7	-1.4	-2.1	-1.4	-1.5	-0.2	-2.3	-2.0
modern_thrrs	-2.1	-0.5	-1.5	+0.6	-0.5	-1.4	-1.9	+12	+11	+5	+1	+4	+86	-1.9	-1.1	-2.1	-1.2	-1.8	-0.1	+3
modern_thrrs_ecoli_zn	-2.5	-3.2	-2.5	-2.8	-1.8	-3.2	-3.1	-2.8	-2.3	-1.3	-3.2	-3.7	-1.8	-2.7	-2.1	-3.2	-2.9	-2.3	-2.7	-2.9

Protein Construct (y-axis) — Amino Acid Ligand (x-axis)

Vina Score (kcal/mol)
Blue=Binding | Red=Rejection
>0 (Steric Rejection) ... 0 ... -2 ... -4 ... -6