AutoDock Vina Binding Energies (Local Minimization)
(Gold = Cognate substrate)

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	-3.0	-3.0	-2.3	-2.7	-1.4	-3.2	-3.7	-2.7	-3.3	-2.7	-3.6	-3.1	-4.9	-1.3	-2.0	-2.2	-2.2	-3.7	-3.6	-3.6
anc_prors_edit	-2.7	-4.5	-1.8	-1.8	-2.1	-4.3	-3.5	-3.0	-4.0	-1.1	-3.4	-2.8	-2.8	-1.8	-1.2	-2.6	-1.1	-1.3	-1.7	-2.0
modern_prors	-4.2	-4.5	-4.1	-3.8	-3.1	-3.6	-3.3	-3.8	-2.2	-3.3	-4.9	-4.1	-5.3	-5.0	-4.1	-2.8	-4.0	-3.8	-4.6	-4.6
anc_thrrs_cat	-4.1	-4.3	-3.3	-2.2	-3.1	-3.7	-4.9	-3.7	-2.5	-1.1	-2.0	-3.8	-2.5	-3.3	-3.6	-3.2	-3.8	-2.0	-2.6	-2.5
anc_thrrs_cat_zn	-2.5	-3.9	-3.5	-3.8	-2.9	-3.3	-2.4	-3.0	-2.5	-2.5	-1.6	-2.7	-2.9	-3.1	-3.4	-3.4	-3.7	-2.5	-2.9	-3.4
modern_thrrs	-3.0	-3.8	-2.8	-2.8	-2.6	-2.6	-3.4	+5	-2.0	-1.6	-3.0	-3.1	+6	-4.0	-2.2	-2.9	-4.9	-2.2	-3.0	-0.2
modern_thrrs_ecoli_zn	-3.1	-4.0	-3.2	-3.1	-2.7	-3.6	-3.8	-3.2	-2.8	-2.2	-4.8	-4.3	-3.7	-4.0	-2.1	-4.1	-3.1	-4.0	-3.4	-4.2

Vina Score (kcal/mol)
Blue=Binding | Red=Rejection