

Ligand	$\Delta G$ solvation	$\Delta E$ interactions	-TAS	$\Delta G$ total	FRET-determined EC50 (3CLpro)
GC376	35.9	-69.3	18.2	-15.2	0.11 $\mu$ M
X77 (docked)	51.1	-88.9	25.6	-12.2	N.A.
X77 (native)	34.4	-62.8	17	-11.4	N.A.
Tipranavir	28.8	-54.4	19.5	-6	47 $\mu$ M
Lopinavir	28.3	-61.9	28.6	-5	219 $\mu$ M
MG-132	19.1	-41.6	18	-4.5	18 $\mu$ M
Darunavir	10.9	-17.8	17.1	10.3	could not be calculated
Cobicistat	82.9	-112.8	44	14.2	could not be calculated
Nelfinavir	112.7	-152.4	81.3	41.6	could not be calculated