



● Charged (negative)
 ● Glycine
 ● Hydrophobic

● Polar
 → H-bond
 ● Pi-cation
 ○ Solvent exposure

C

Ligand	R	ΔG CDK2 (kcal/mol)	ΔG ERK2 (kcal/mol)	S_i (kcal/mol)	Ligand	R	ΔG CDK2 (kcal/mol)	ΔG ERK2 (kcal/mol)	S_i (kcal/mol)
6		-10.57	-12.21	-1.64	18		-8.28	-9.03	-0.75
10		-9.87	-11.44	-1.57	21		-7.82	-10.13	-2.31
11		-8.71	-10.28	-1.57	22		-9.69	-11.6	-1.91
12		-8.86	-11.22	-2.36	23		-7.86	-10.63	-2.77
13		-8.44	-10.41	-1.97	24		-8.98	-10.75	-1.77
14		-8.69	-11.06	-2.37	25		-7.87	-9.61	-1.74
15		-10.36	-11.92	-1.56	26		-8.92	-10.59	-1.67
16		-9.57	-10.91	-1.34	27		-8.01	-8.6	-0.59
17		-9.86	-12.33	-2.47	28		-8.76	-9.93	-1.17