



Ligand	R1	R2	R3	ΔG CDK2 (kcal/mol)	ΔG CDK9 (kcal/mol)	$\Delta\Delta G$ (kcal/mol)
12a	CN	H		-12.27	-11.21	1.06
12b	OH	H		-7.23	-8.22	-0.99
12c	CN	H		-11.45	-11.21	0.24
12e	F	H		-11.62	-11.45	0.17
12f	Cl	H		-10.91	-10.85	0.06
12g	Methyl	H		-10.18	-11.32	-1.14
12h	Ethyl	H		-8.28	-9.56	-1.28
12j	CN	H		-10.04	-11.12	-1.08
12l	CN		H	-10.34	-10.44	-0.1
12n	CN	H		-10.06	-10.97	-0.91
12o	F	H		-10.06	-11.12	-1.06
12q	F	H		-10.91	-11.62	-0.71
12t	CN	H		-9.38	-11.12	-1.74
1a	H	H		-11.62	-11.86	-0.24
1b	H	H		-11.45	-11.86	-0.41