

Protein	UniProt ID	Active Site Structure	Active Site Substrate	Active Site Annotation	Allosteric Site Structure	Allosteric Modulator	Allosteric Site Annotation	Type	Size	Slope	t-value	P-value	R2	Half Distance
GCK	P35557	1V4S, 3FGU	ANP,BGC, GLC	from 1V4S	1V4S,3ID8	MRK (activator)	literature (Kamata et al., 2004) (Larion & Miller, 2009)	kinase	465	-0.043143	-9.147	< 2.2e-16	0.1654	15.73543
PTP1B	P18031	1PTY	PTR	from 1PTY	1T48,1T49, 1T4J	892,BB3,FRJ (inhibitor)	consensus	phosphatase	435	-0.02548	-4.191	3.71E-05	0.05474	19.73865
PDK1	O15530	4RQK, 5LVM	ADE,ATP	consensus	3ORZ,4RQK	2A2 (activator), R1S (inhibitor)	from 4RQK	kinase	556	-0.048941	-7.152	7.56E-12	0.1519	12.28401
CHK1	O14757	2E9N, 5OOP	76A,ANP	consensus	3F9N	38M (inhibitor)	from 3F9N	kinase	476	-0.039685	-6.378	8.00E-10	0.1302	15.89498
CASP1	P29466	2HBQ, 6BZ9	C,PHQ	consensus	2FQQ	F1G (inhibitor)	from 2FQQ	protease	404	-0.024747	-3.794	0.000188	0.05308	22.64102
IDH	O75874	5YFN, 6ADG, 6B0Z, 6BKZ, 6IO0	FLC,ICT,MG, NAP,NDP	consensus from 6B0Z, 6BKZ, 6IO0	5SUN,6B0Z, 6BKZ,6BL2, 6IO0	70Q, AOU, C81, CIT, DWM, DWS (inhibitor)	consensus from 6B0Z, 6BKZ, 6IO0	oxidoreductase	414	-0.036131	-6.531	2.26E-10	0.1042	15.36862