

Supplementary Table 1. Potential targets of Cardol

No.	Protein	PDB name	Cardol		Known Inhibitor		Name
			ΔG_{bind} (kcal/mol)	K_i (μM)	ΔG_{bind} (kcal/mol)	K_i (μM)	
1.	AKT	1GZN	-8.10	1.16	-8.55	0.54	Apatinib
2.	ALKR	2XB7	-6.12	32.65	-7.85	1.77	Lorlatinib
3.	AURKA	1MUO	-6.61	14.36	-8.48	0.61	Reversine
4.	B-RAF	6B8U	-6.48	17.92	-9.40	0.13	Regorafenib
5.	B-Catenin	1G3J	-5.25	0.14	-6.54	0.01	ICG001
6.	c-met	5DG5	-7.20	5.26	-8.24	0.91	Tivantinib
7.	CDK2**	1DM2	-7.84	1.78	-6.71	12.07	Roscovitine
8.	CDK5	1H4L	-5.06	194.56	-6.78	10.70	AT7519
9.	CHK1	1NVQ	-6.41	19.94	-7.55	2.92	SRA737
10.	CSF1R	2OGV	-6.64	13.69	-8.00	1.36	Pexidartinib
11.	DYRK1A	4YLL	-7.39	3.83	-8.79	0.36	CHEMBL3589662
12.	FAK1	1MP8	-6.40	20.46	-6.47	18.06	Defactinib
13.	FGFR4	4UXQ	-7.64	2.49	-8.30	0.83	Lenvatinib
14.	GSK-beta	1H8F	-5.81	55.11	-8.11	1.14	Tideglusib
15.	HER2	3PP0	-6.24	26.80	-8.28	0.84	Lapatinib
16.	HSP90alpha	3O0I	-8.26	0.89	-9.85	0.06	EC44
17.	HSP90beta	3NMQ	-8.72	0.41	-10.09	0.04	Sunitinib
18.	IGFR	1K3A	-5.59	79.58	-9.19	0.18	Linsitinib
19.	JAK1	5HX8	-5.53	88.95	-6.87	9.28	Tofacitinib
20.	JAK2	3Q32	-5.63	74.87	-6.98	7.60	Baricitinib
21.	MAPK10	1PMV	-6.61	14.20	-7.04	6.93	Lorlatinib
22.	MAPKp38	1A9U	-6.57	15.35	-9.01	0.25	SB203580
23.	MEK1**	2P55	-7.66	2.44	-5.32	126.32	Refametinib
24.	mTOR	4JSV	-5.06	194.75	-6.40	20.35	AZD-8055
25.	PDK1	2Q8G	-5.80	56.52	-8.01	1.35	AZD-7545
26.	PI3K	3CSF	-6.48	17.64	-6.69	12.48	Buparlisib
27.	RAF1	3OMV	-6.77	10.96	-8.44	0.65	GW5074
28.	ROCK1	Y27632	-4.52	484.34	-7.92	1.58	2ETR
29.	SRC	2BDJ	-6.81	10.24	-9.92	0.05	AP23464
30.	STAT3	6NJS	-4.54	469.10	-6.68	12.61	Napabucasin
31.	STK17beta	3LM0	-6.21	28.26	-9.37	0.13	STK17A/B-IN-1
32.	TGFbR	3TZM	-7.30	4.46	-9.06	0.23	SB431542
33.	TYK2	6OVA	-7.41	3.68	-7.94	1.51	Cerdulatinib
34.	VEGFA	4KZN	-4.85	277.08	-5.26	138.97	Bevacizumab
35.	VEGFR2	4ASE	-7.90	1.63	-10.31	0.02	Sorafenib

“**” indicates the targeted proteins that exhibited more favorable predicted affinities for cardol than their positive inhibitors.