

S1 Table

CID	structure derivation	EC50						
		Rab7	H-Ras	H-Ras G12V	Cdc42	Cdc42 Q61L	RhoA	Rac1
1067700	X=O;R <sub>1</sub> =Me;R <sub>2</sub> =Me;R <sub>3</sub> =OH;R <sub>4</sub> =CS-NH-CO; R <sub>5</sub> =phenyl	0.12 ± 0.055	0.16 ± 0.16	0.052 ± 0.044	1.09 ± 1.62	0.047 ± 0.038	0.062 ± 0.049	0.062 ± 0.049
1251121	R <sub>3</sub> =OMe	>1000	>1000	>1000	>1000	>1000	NA	NA
46916263	R <sub>1</sub> =H	0.14 ± 0.11	0.13 ± 0.10	0.13 ± 0.12	9.09 ± 12.28	4.04 ± 5.58	0.12 ± 0.07	0.08 ± 0.03
46916266	R <sub>1</sub> =H;R <sub>2</sub> =H	0.16 ± 0.067	0.17 ± 0.094	0.12 ± 0.12	0.11 ± 0.064	0.13 ± 0.078	0.23 ± 0.21	0.18 ± 0.13
53377401	R <sub>2</sub> =Et	0.032 ± 0.0073	0.028 ± 0.011	0.035	2.2 ± 3.7	0.077 ± 0.087	0.046	0.053
53377399	R <sub>1</sub> =H;R <sub>2</sub> =t-butyl	0.47	0.14	0.13	1.57	0.94	0.20	0.14
53377403	R <sub>1</sub> -R <sub>2</sub> =(CH <sub>2</sub> ) <sub>4</sub> -	0.04	0.03	0.03	NA	NA	0.10	0.06
740871	R <sub>4</sub> =CO-CH <sub>2</sub>	>1000	>1000	>1000	>1000	>1000	NA	NA
1280844	R <sub>4</sub> =CS-NH	NA	NA	3.55	391.00	125.70	1.39	4.06
46916265	R <sub>4</sub> =CO-NH-CO	0.31 ± 0.09	0.44 ± 0.41	0.49 ± 0.48	17.00	0.47	0.33 ± 0.03	0.35 ± 0.05
53377397	R <sub>5</sub> =2-MeO-phenyl	1.12	1.32	0.81	20.77	2.35	NA	NA
53301934	R <sub>5</sub> =3-MeO-phenyl	0.15 ± 0.13	0.13 ± 0.13	0.12 ± 0.12	0.58 ± 0.83	0.50 ± 0.71	0.20 ± 0.13	0.19 ± 0.06
53301932	R <sub>5</sub> =4-MeO-phenyl	0.14 ± 0.07	0.14 ± 0.09	0.17 ± 0.10	1.2 ± 1.0	0.23 ± 0.039	0.15 ± 0.06	0.13 ± 0.06
53301935	R <sub>5</sub> =2-F-phenyl	0.14 ± 0.16	0.15 ± 0.18	0.12 ± 0.14	3.72 ± 5.15	0.79 ± 1.13	0.18 ± 0.22	0.18 ± 0.24
53301930	R <sub>5</sub> =3-F-phenyl	0.32 ± 0.09	0.33 ± 0.09	0.38 ± 0.14	21.17 ± 35.48	2.20 ± 3.14	0.47 ± 0.14	0.48 ± 0.01
53377405	R <sub>5</sub> =4-F-phenyl	0.41 ± 0.19	0.33 ± 0.22	0.091	1.0 ± 1.2	0.88 ± 0.47	0.11	0.15
53301931	R <sub>5</sub> =2-Br-phenyl	0.43 ± 0.68	0.62 ± 1.00	0.43 ± 0.68	46.77 ± 66.01	14.76 ± 20.80	0.48 ± 0.74	0.60 ± 0.80
53301936	R <sub>5</sub> =3-Br-phenyl	2.51 ± 2.10	1.72	1.08	191.81 ± 243.66	23.67 ± 23.88	>1000	31.06
53301933	R <sub>5</sub> =4-Br-phenyl	0.30 ± 0.18	0.33 ± 0.24	0.32 ± 0.22	25.86 ± 44.07	10.89 ± 18.37	0.32 ± 0.13	0.26 ± 0.11
53377404	R <sub>5</sub> =2-Me-phenyl	0.41	0.44	0.38	2.66	1.35	0.49	0.44
53377400	R <sub>5</sub> =3-Me-phenyl	1.16	1.39	0.85	5.87	1.83	1.45	1.51
53377395	R <sub>5</sub> =4-Me-phenyl	0.14	0.19	0.18	0.53	0.43	0.13	0.15
53377402	R <sub>5</sub> =2-furyl	0.074	0.079	0.065	16.17	0.33	0.092	0.059
53377398	R <sub>5</sub> =2-thiophene	0.025	0.035	0.024	NA	NA	0.033	0.029
53301937	X=CH <sub>2</sub>	0.066 ± 0.017	0.067 ± 0.024	0.077 ± 0.024	0.28 ± 0.16	0.17 ± 0.086	0.071 ± 0.0096	0.068 ± 0.020
974814	R <sub>3</sub> =OMe; R <sub>4</sub> =none; R <sub>5</sub> =none	>1000	>1000	>1000	>1000	>1000	NA	NA
1097649	R <sub>3</sub> =OEt; R <sub>4</sub> =CS-NH	>1000	>1000	>1000	>1000	>1000	NA	NA
46916262	R <sub>1</sub> =H;R <sub>2</sub> =H;R <sub>3</sub> =OC(CH <sub>3</sub> ) <sub>3</sub>	>1000	>1000	>1000	>1000	>1000	NA	NA
2810966	X=NMe;R <sub>1</sub> =H;R <sub>2</sub> =H;R <sub>3</sub> =OEt; R <sub>4</sub> =CO-NH; R <sub>5</sub> =4-F-phenyl	>1000	>1000	>1000	>1000	>1000	NA	NA
2810963	X=NMe;R <sub>1</sub> =H;R <sub>2</sub> =H;R <sub>3</sub> =OEt; R <sub>4</sub> =CO-NH; R <sub>5</sub> =4-Me-phenyl	>1000	>1000	>1000	>1000	>1000	NA	NA
2810964	X=NMe;R <sub>1</sub> =H;R <sub>2</sub> =H;R <sub>3</sub> =OEt; R <sub>4</sub> =CO-NH-C(CH <sub>3</sub> ) <sub>3</sub> ;R <sub>5</sub> =none	>1000	>1000	>1000	>1000	>1000	NA	NA
46916261	X=NMe;R <sub>1</sub> =H;R <sub>2</sub> =H;R <sub>3</sub> -R <sub>4</sub> =-O-C(=N)-NH-;R <sub>5</sub> =4-F-phenyl	>1000	>1000	>1000	>1000	>1000	NA	NA
46916264	X=NMe;R <sub>1</sub> =H;R <sub>2</sub> =H;R <sub>3</sub> -R <sub>4</sub> =-O-C(=N)-NH-;R <sub>5</sub> =4-Me-phenyl	>1000	>1000	>1000	>1000	>1000	NA	NA
46916260	X=NMe;R <sub>1</sub> =H;R <sub>2</sub> =H;R <sub>4</sub> =CO-NH;R <sub>5</sub> =4-F-phenyl	>1000	>1000	>1000	>1000	>1000	NA	NA
46916259	X=NMe;R <sub>1</sub> =H;R <sub>2</sub> =H;R <sub>4</sub> =CO-NH;R <sub>5</sub> =4-Me-phenyl	49.30	30.20	32.20	26.20	28.00	NA	NA

**S1 Table. Analogues of compound 1 and EC<sub>50</sub> values.** Analogues of compound **1** and EC<sub>50</sub> values. Derivatization sites were indicated as in the main text Figure 1. For EC<sub>50</sub>s with standard deviations, the values were the averages from multiple measurements. It is observed that the standard deviations for compound **1** and some of its analogs against Cdc42 are large. Therefore, the biochemical data for Cdc42 when needed for comparison is from a single set of experiments (Table 2 and Figure 2). For EC<sub>50</sub>s reported without standard deviations, the values were determined from one measurement carried out in duplicate where all the data points were used to fit the sigmoidal dose-response equation. EC<sub>50</sub> values were noted NA when they were not available or data did not give acceptable fit.