



Absolute binding energy (local FD ddG minimum)

	Bcl-2	Bcl-xL	Bcl-w	Mcl-1	Bfl-1	Bcl-B
2-CDP06	-76.4	-76.0	-52.8	-70.8	-73.4	-71.5
X-CDP07	-74.7	-97.7	-70.3	-73.6	-65.3	-75.7
W-CDP03	-52.8	-52.8	-106.1	-30.2	-37.6	-46.7
M-CDP04/αMCL1	-47.1	-73.4	-65.0	-89.9	-64.6	-62.5
F-CDP01	-60.6	-90.2	-68.0	-78.6	-90.6	-89.9
B-CDP01	-69.8	-77.9	-74.4	-84.6	-70.9	-86.7

Relative binding energy (local vs. global minima)

	Bcl-2	Bcl-xL	Bcl-w	Mcl-1	Bfl-1	Bcl-B
2-CDP06	-61.5	-59.5	-38.8	-56.2	-59.4	-57.3
X-CDP07	-57.0	-79.4	-52.8	-57.6	-49.9	-59.8
W-CDP03	-38.6	-37.7	-89.8	-16.8	-23.7	-32.0
M-CDP04/αMCL1	-33.3	-58.9	-49.4	-75.7	-51.5	-49.0
F-CDP01	-45.1	-73.7	-52.0	-64.1	-76.3	-73.9
B-CDP01	-54.2	-62.2	-58.1	-69.6	-56.4	-70.6

Dissociation constants (K_d)

	Bcl-2	Bcl-xL	Bcl-w	Mcl-1	Bfl-1	Bcl-B
2-CDP06	9 ± 1	12,000 ± 1,000	1,700 ± 100	> 50,000	> 50,000	> 50,000
X-CDP07	4 ± 1	0.59 ± 0.07	14.9 ± 0.5	17 ± 1	> 50,000	107 ± 9
W-CDP03	30 ± 20	7 ± 1	8 ± 1	57 ± 8	500 ± 300	410 ± 80
M-CDP04/αMCL1	20,000 ± 2,000	340,000 ± 10,000	200,000 ± 200,000	0.15 ± 0.06	200,000 ± 200,000	20,000 ± 10,000
F-CDP01	27 ± 8	11 ± 1	600 ± 80	4.6 ± 0.6	2 ± 2	100,000 ± 100,000
B-CDP01	17 ± 3	20 ± 4	2,000 ± 500	0.46 ± 0.09	520 ± 30	8 ± 1