Thermodynamic, kinetic, and structural parameterization of human carbonic anhydrase interactions toward enhanced inhibitor design

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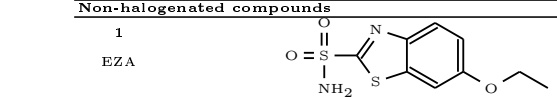
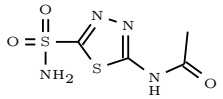
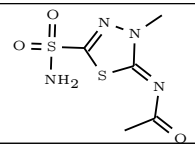
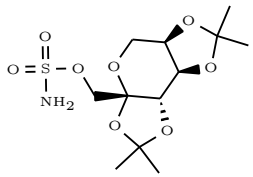
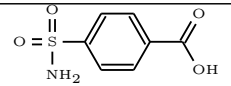
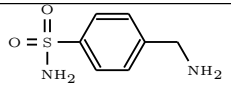
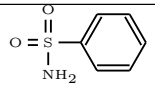
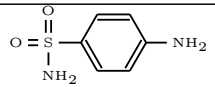
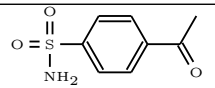
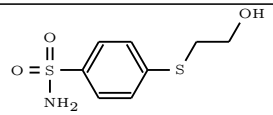
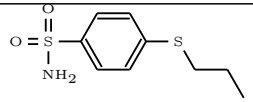
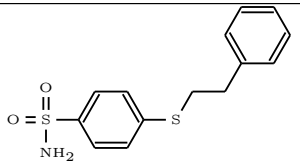
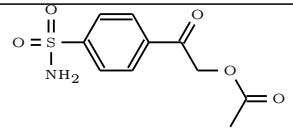
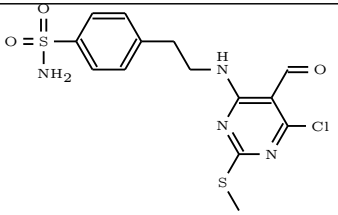
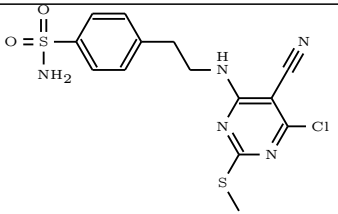
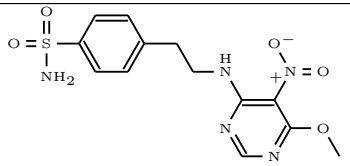
Contents

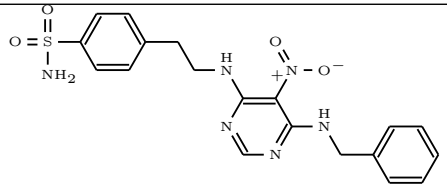
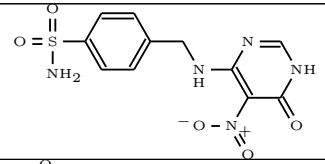
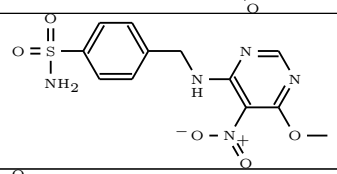
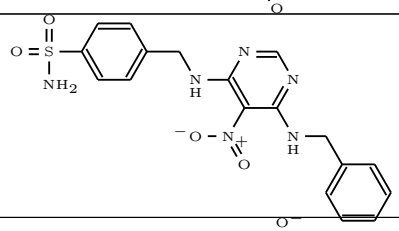
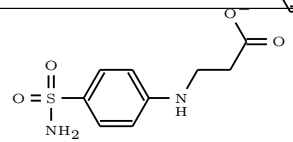
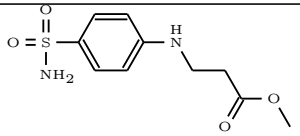
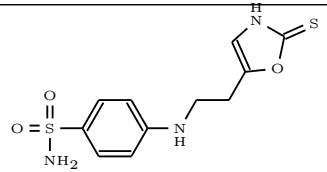
1 Supplementary tables

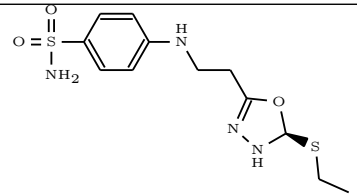
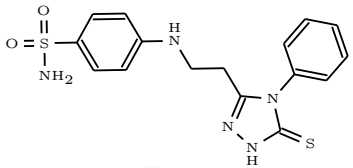
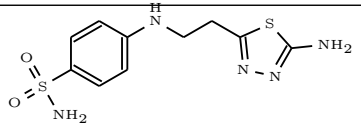
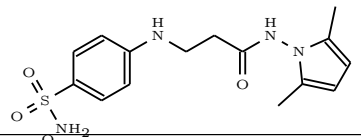
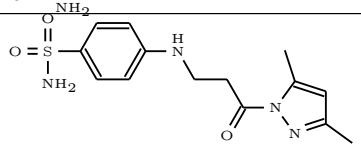
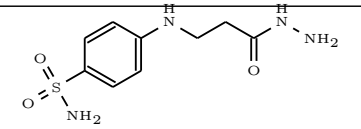
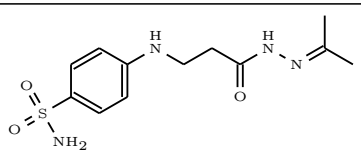
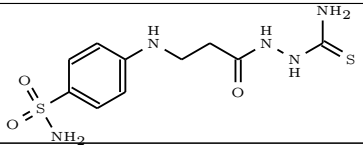
1.1 Table 1

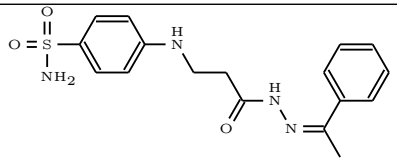
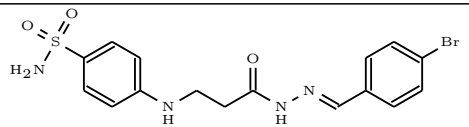
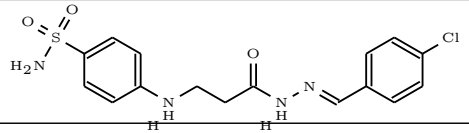
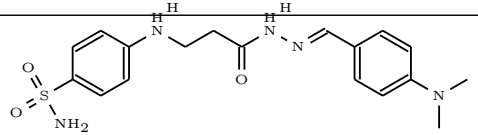
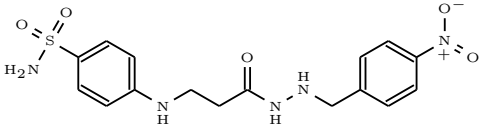
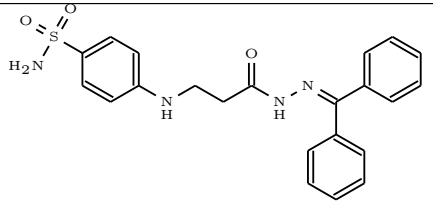
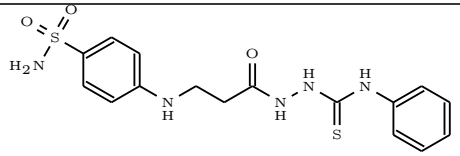
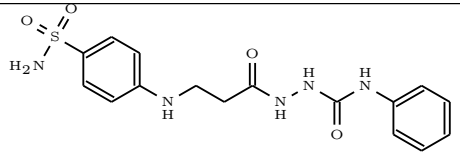
Table 1: Observed (pH 7.0) and intrinsic dissociation constants (nM) and observed (pH 7.0) and intrinsic Gibbs energies ($kJ\,mol^{-1}$) of compound binding to recombinant 12 human catalytically active CAs at 37 °C

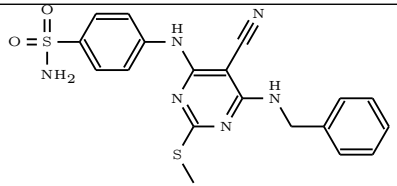
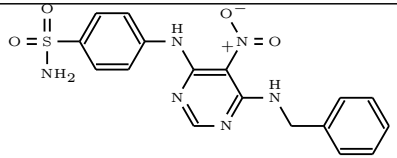
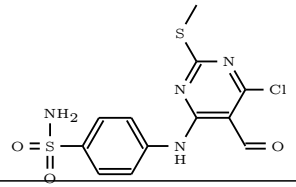
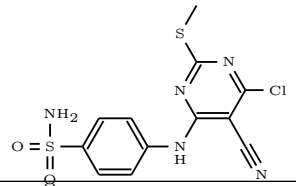
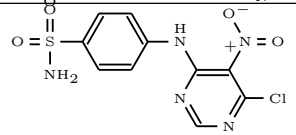
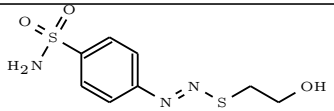
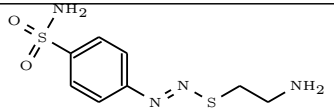
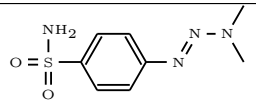
			Thermodynamic binding parameters											
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
Non-halogenated compounds														
1		$K_{d,obs}$ (nM)	17	1.3	5200	82	26	8.6	33	0.61	1.9	71	19	10
		ΔG_{obs} ($kJ\,mol^{-1}$)	-46.2	-52.8	-31.4	-42.1	-45.0	-47.9	-44.4	-54.7	-51.8	-42.4	-45.8	-47.5
EZA		$K_{d,int}$ (nM)	2.0	0.073	160	3.1	2.3	0.57	0.40	0.031	0.071	3.6	2.3	0.51
		ΔG_{int} ($kJ\,mol^{-1}$)	-51.6	-60.1	-40.3	-50.5	-51.3	-54.9	-55.8	-62.4	-60.2	-50.1	-51.3	-55.2
2		$K_{d,obs}$ (nM)	2400	46	40 000	87	840	140	220	13	21	130	79	63
		ΔG_{obs} ($kJ\,mol^{-1}$)	-33.4	-43.5	-26.1	-41.9	-36.1	-40.6	-39.5	-46.8	-45.5	-40.9	-42.1	-42.8
AZM		$K_{d,int}$ (nM)	1100	9.8	4600	12	270	34	9.8	2.4	2.9	24	35	12
		ΔG_{int} ($kJ\,mol^{-1}$)	-35.5	-47.5	-31.7	-47.0	-39.0	-44.3	-47.5	-51.1	-50.6	-45.2	-44.3	-47.1
3		$K_{d,obs}$ (nM)	200	100	40 000	250	ND	67	830	50	36	500	200	110
		ΔG_{obs} ($kJ\,mol^{-1}$)	-39.8	-41.4	-26.1	-39.2	ND	-42.6	-36.1	-43.3	-44.2	-37.4	-39.8	-41.3
MZM		$K_{d,int}$ (nM)	110	27	5600	41	ND	19	44	11	6.0	110	110	25
		ΔG_{int} ($kJ\,mol^{-1}$)	-41.4	-44.9	-31.2	-43.8	ND	-45.8	-43.7	-47.2	-48.8	-41.2	-41.4	-45.1
4		$K_{d,obs}$ (nM)	34 000	110	≥200 000	67	≥200 000	2.5	13 000	25	34	82	240	20
		ΔG_{obs} ($kJ\,mol^{-1}$)	-26.5	-41.4	≥-22.0	-42.6	≥-22.0	-51.0	-29.1	-45.1	-44.3	-42.1	-39.2	-45.7
TPM		$K_{d,int}$ (nM)	970	1.4	1500	0.58	20 000	0.038	35	0.30	0.30	0.97	6.8	0.24
		ΔG_{int} ($kJ\,mol^{-1}$)	-35.7	-52.5	-34.6	-54.8	-27.8	-61.8	-44.3	-56.5	-56.6	-53.5	-48.5	-57.1
5		$K_{d,obs}$ (nM)	11 000	4000	≥200 000	3300	3100	20 000	11 000	4000	1800	3300	5800	4000
		ΔG_{obs} ($kJ\,mol^{-1}$)	-29.3	-32.0	≥-22.0	-32.5	-32.7	-27.9	-29.4	-32.0	-34.1	-32.5	-31.1	-32.0
CARBS		$K_{d,int}$ (nM)	61	10	270	5.4	12	57	5.8	8.9	3.0	7.4	30	8.9
		ΔG_{int} ($kJ\,mol^{-1}$)	-42.8	-47.4	-38.9	-49.1	-47.0	-43.0	-48.9	-47.8	-50.6	-48.3	-44.6	-47.8
6		$K_{d,obs}$ (nM)	83 000	17 000	≥200 000	17 000	ND	41 000	21 000	28 000	18 000	34 000	≥200 000	≥200 000
		ΔG_{obs} ($kJ\,mol^{-1}$)	-24.2	-28.3	≥-22.0	-28.4	ND	-26.1	-27.7	-27.0	-28.2	-26.5	≥-22.0	≥-22.0
PAMBS		$K_{d,int}$ (nM)	150	14	110	9.0	ND	39	3.7	21	9.7	25	690	290
		ΔG_{int} ($kJ\,mol^{-1}$)	-40.6	-46.5	-41.3	-47.7	ND	-44.0	-50.0	-45.6	-47.6	-45.1	-36.6	-38.8
7		$K_{d,obs}$ (nM)	7700	1900	≥200 000	17 000	6700	33 000	13 000	7200	1500	12 000	7500	5100
		ΔG_{obs} ($kJ\,mol^{-1}$)	-30.3	-33.9	≥-22.0	-28.4	-30.7	-26.6	-29.0	-30.5	-34.5	-29.1	-30.4	-31.4
BSA		$K_{d,int}$ (nM)	6.5	0.78	44	4.3	4.0	15	1.1	2.5	0.40	4.4	6.2	1.8
		ΔG_{int} ($kJ\,mol^{-1}$)	-48.6	-54.0	-43.7	-49.6	-49.8	-46.4	-53.2	-51.0	-55.8	-49.6	-48.7	-51.9
8		$K_{d,obs}$ (nM)	85 000	13 000	≥200 000	13 000	36 000	≥200 000	68 000	62 000	15 000	82 000	150 000	29 000
		ΔG_{obs} ($kJ\,mol^{-1}$)	-24.2	-29.1	≥-22.0	-29.0	-26.4	≥-22.0	-24.7	-24.9	-28.6	-24.3	-22.7	-27.0
SULFA		$K_{d,int}$ (nM)	150	11	180	7.0	45	190	12	46	8.3	60	260	21
		ΔG_{int} ($kJ\,mol^{-1}$)	-40.5	-47.3	-40.0	-48.4	-43.6	-39.9	-47.1	-43.5	-47.9	-42.9	-39.1	-45.6

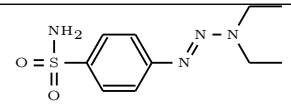
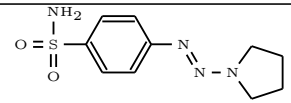
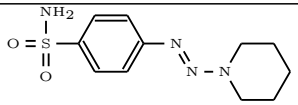
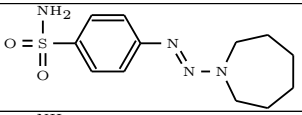
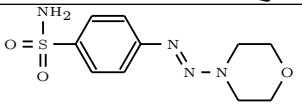
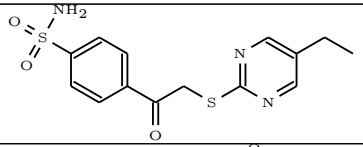
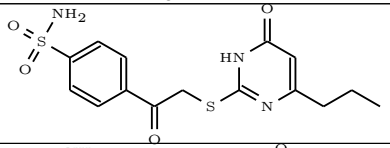
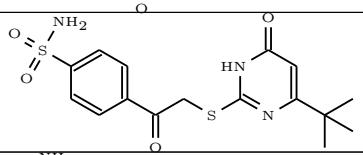
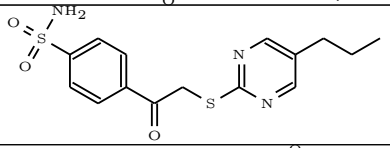
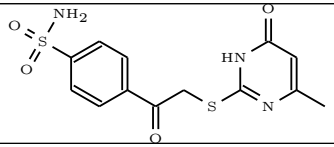
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
9		$K_{d,obs}$ (nM)	670	430	ND	ND	770	ND	ND	250	ND	2900	2900	ND
		ΔG_{obs} (kJ mol^{-1})	-36.7	-37.8	ND	ND	-36.3	ND	ND	-39.2	ND	-32.9	-32.9	ND
E11-0		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
10		$K_{d,obs}$ (nM)	110	140	ND	3900	5800	10 000	5000	200	850	2900	1400	250
		ΔG_{obs} (kJ mol^{-1})	-41.3	-40.6	ND	-32.1	-31.1	-29.7	-31.5	-39.7	-36.0	-32.9	-34.7	-39.2
VD11-31		$K_{d,int}$ (nM)	0.11	0.070	ND	1.2	4.2	5.5	0.50	0.086	0.26	1.2	1.4	0.11
		ΔG_{int} (kJ mol^{-1})	-59.0	-60.3	ND	-52.9	-49.7	-49.0	-55.2	-59.7	-56.8	-52.9	-52.5	-59.2
11		$K_{d,obs}$ (nM)	5.0	25	ND	1700	3700	67	830	40	100	330	290	26
		ΔG_{obs} (kJ mol^{-1})	-49.3	-45.1	ND	-34.2	-32.3	-42.6	-36.1	-43.9	-41.5	-38.4	-38.8	-45.0
VD12-10		$K_{d,int}$ (nM)	0.0029	0.0070	ND	0.30	1.5	0.021	0.048	0.0098	0.018	0.081	0.16	0.0063
		ΔG_{int} (kJ mol^{-1})	-68.5	-66.2	ND	-56.5	-52.3	-63.4	-61.2	-65.3	-63.8	-59.9	-58.1	-66.5
12		$K_{d,obs}$ (nM)	4.5	12	≥200 000	ND	1300	14	1100	17	77	220	50	19
		ΔG_{obs} (kJ mol^{-1})	-49.5	-47.1	≥-22.0	ND	-34.9	-46.6	-35.3	-46.2	-42.2	-39.6	-43.3	-45.8
VD11-36		$K_{d,int}$ (nM)	0.0032	0.0039	36	ND	0.65	0.0054	0.077	0.0049	0.017	0.063	0.034	0.0055
		ΔG_{int} (kJ mol^{-1})	-68.2	-67.7	-44.1	ND	-54.5	-66.9	-60.0	-67.1	-64.0	-60.5	-62.1	-66.8
13		$K_{d,obs}$ (nM)	100	100	ND	ND	ND	ND	ND	100	ND	1200	1400	ND
		ΔG_{obs} (kJ mol^{-1})	-41.5	-41.5	ND	ND	ND	ND	ND	-41.5	ND	-35.0	-34.7	ND
E84x		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
14		$K_{d,obs}$ (nM)	490	110	≥200 000	2900	ND	200	13 000	860	33	1000	140	500
		ΔG_{obs} (kJ mol^{-1})	-37.5	-41.3	≥-22.0	-32.9	ND	-39.8	-29.1	-36.0	-44.4	-35.6	-40.6	-37.4
JS69		$K_{d,int}$ (nM)	0.28	0.031	30	0.51	ND	0.063	0.72	0.21	0.0060	0.24	0.082	0.12
		ΔG_{int} (kJ mol^{-1})	-56.6	-62.4	-44.6	-55.1	ND	-60.5	-54.3	-57.4	-66.6	-57.0	-59.9	-58.8
15		$K_{d,obs}$ (nM)	160 000	420	ND	ND	ND	ND	ND	100	ND	ND	100	ND
		ΔG_{obs} (kJ mol^{-1})	-22.5	-37.9	ND	ND	ND	ND	ND	-41.5	ND	ND	-41.5	ND
JS68		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
16		$K_{d,obs}$ (nM)	67	71	≥200 000	2500	ND	1100	3300	130	180	1000	280	220
		ΔG_{obs} (kJ mol^{-1})	-42.6	-42.4	≥-22.0	-33.2	ND	-35.3	-32.5	-40.8	-40.0	-35.6	-38.9	-39.5
JS72		$K_{d,int}$ (nM)	0.049	0.025	38	0.57	ND	0.44	0.24	0.041	0.041	0.31	0.20	0.068
		ΔG_{int} (kJ mol^{-1})	-61.2	-62.9	-44.0	-54.9	ND	-55.5	-57.1	-61.6	-61.6	-56.5	-57.5	-60.3

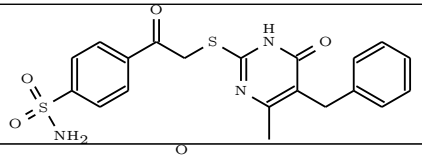
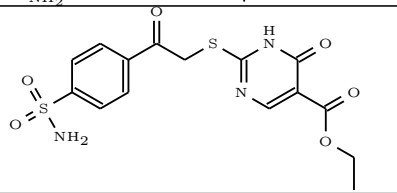
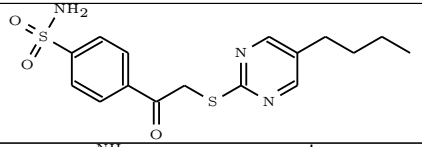
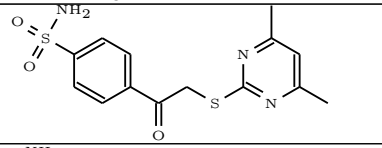
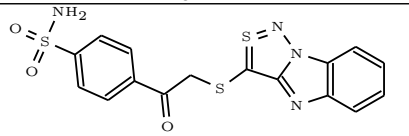
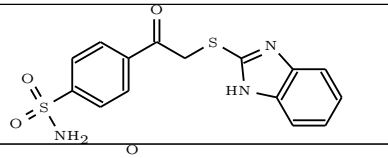
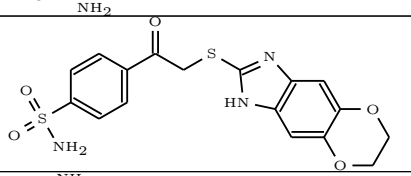
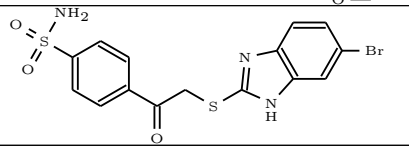
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
17 JS76		$K_{d,obs}$ (nM)	620	16	≥200 000	20 000	ND	4000	25 000	710	500	ND	1700	500
		ΔG_{obs} (kJ mol^{-1})	-36.8	-46.3	≥-22.0	-27.9	ND	-32.0	-27.3	-36.5	-37.4	ND	-34.3	-37.4
		$K_{d,int}$ (nM)	0.46	0.0056	38	4.5	ND	1.6	1.8	0.22	0.11	ND	1.2	0.15
		ΔG_{int} (kJ mol^{-1})	-55.4	-66.8	-44.0	-49.5	ND	-52.2	-51.9	-57.3	-59.0	ND	-52.9	-58.2
18 JS80		$K_{d,obs}$ (nM)	170	170	ND	ND	ND	ND	ND	250	ND	ND	20	ND
		ΔG_{obs} (kJ mol^{-1})	-40.2	-40.2	ND	ND	ND	ND	ND	-39.2	ND	ND	-45.7	ND
		$K_{d,int}$ (nM)	0.13	0.059	ND	ND	ND	ND	ND	0.077	ND	ND	0.014	ND
		ΔG_{int} (kJ mol^{-1})	-58.8	-60.7	ND	ND	ND	ND	ND	-60.0	ND	ND	-64.3	ND
19 JS71		$K_{d,obs}$ (nM)	36	53	ND	ND	ND	ND	ND	830	ND	ND	240	ND
		ΔG_{obs} (kJ mol^{-1})	-44.1	-43.2	ND	ND	ND	ND	ND	-36.1	ND	ND	-39.2	ND
		$K_{d,int}$ (nM)	0.027	0.019	ND	ND	ND	ND	ND	0.26	ND	ND	0.18	ND
		ΔG_{int} (kJ mol^{-1})	-62.7	-63.7	ND	ND	ND	ND	ND	-56.9	ND	ND	-57.9	ND
20 JS75		$K_{d,obs}$ (nM)	25	100	≥200 000	5000	ND	10 000	25 000	4200	400	ND	1200	1000
		ΔG_{obs} (kJ mol^{-1})	-45.1	-41.5	≥-22.0	-31.5	ND	-29.7	-27.3	-31.9	-38.0	ND	-35.0	-35.6
		$K_{d,int}$ (nM)	0.018	0.035	38	1.1	ND	4.0	1.8	1.3	0.090	ND	0.90	0.31
		ΔG_{int} (kJ mol^{-1})	-63.7	-62.0	-44.0	-53.1	ND	-49.9	-51.9	-52.8	-59.6	ND	-53.7	-56.5
21 KR50-1		$K_{d,obs}$ (nM)	40 000	13 000	≥200 000	ND	ND	ND	62 000	22 000	ND	9500	33 000	ND
		ΔG_{obs} (kJ mol^{-1})	-26.1	-29.1	≥-22.0	ND	ND	ND	-24.9	-27.6	ND	-29.8	-26.6	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
22 KR50-2		$K_{d,obs}$ (nM)	36 000	9100	≥200 000	ND	ND	ND	71 000	36 000	ND	33 000	59 000	ND
		ΔG_{obs} (kJ mol^{-1})	-26.4	-29.9	≥-22.0	ND	ND	ND	-24.6	-26.4	ND	-26.6	-25.1	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
23 KR50-14		$K_{d,obs}$ (nM)	13 000	4500	≥200 000	ND	ND	ND	33 000	4500	ND	5900	26 000	ND
		ΔG_{obs} (kJ mol^{-1})	-29.1	-31.7	≥-22.0	ND	ND	ND	-26.6	-31.7	ND	-31.0	-27.2	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

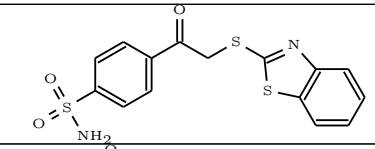
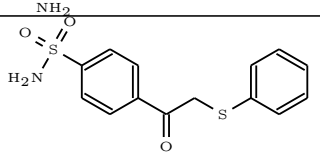
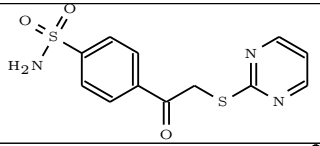
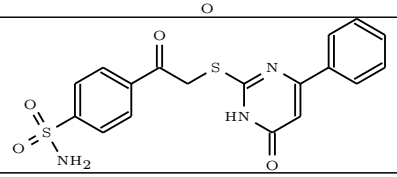
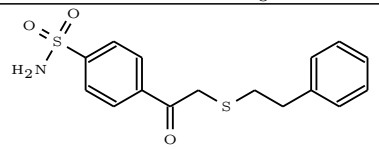
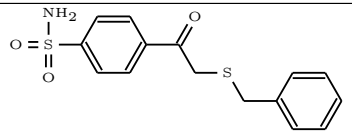
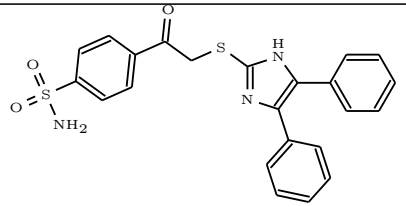
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
24		$K_{d,obs}$ (nM)	5900	1200	≥200 000	ND	ND	ND	29 000	5600	ND	11 000	3300	ND
		ΔG_{obs} (kJ mol^{-1})	-31.0	-35.2	≥-22.0	ND	ND	ND	-27.0	-31.2	ND	-29.5	-32.5	ND
KR50-15		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
25		$K_{d,obs}$ (nM)	10 000	2000	ND	ND	ND	ND	11 000	6700	ND	6700	10 000	ND
		ΔG_{obs} (kJ mol^{-1})	-29.7	-33.8	ND	ND	ND	ND	-29.4	-30.7	ND	-30.7	-29.7	ND
KR50-17b		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
26		$K_{d,obs}$ (nM)	170 000	20 000	ND	ND	ND	ND	140 000	100 000	ND	130 000	83 000	ND
		ΔG_{obs} (kJ mol^{-1})	-22.4	-27.9	ND	ND	ND	ND	-22.8	-23.7	ND	-23.2	-24.2	ND
KTU10		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
27		$K_{d,obs}$ (nM)	17 000	2000	≥200 000	ND	ND	ND	25 000	11 000	ND	29 000	6300	ND
		ΔG_{obs} (kJ mol^{-1})	-28.4	-33.8	≥-22.0	ND	ND	ND	-27.3	-29.4	ND	-27.0	-30.9	ND
KR50-13		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
28		$K_{d,obs}$ (nM)	1700	670	≥200 000	ND	ND	ND	27 000	3300	ND	14 000	4000	ND
		ΔG_{obs} (kJ mol^{-1})	-34.3	-36.7	≥-22.0	ND	ND	ND	-27.1	-32.5	ND	-28.8	-32.0	ND
KR50-12		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
29		$K_{d,obs}$ (nM)	56 000	11 000	≥200 000	ND	ND	ND	62 000	29 000	ND	33 000	77 000	ND
		ΔG_{obs} (kJ mol^{-1})	-25.3	-29.5	≥-22.0	ND	ND	ND	-24.9	-27.0	ND	-26.6	-24.4	ND
KR50-3		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
30		$K_{d,obs}$ (nM)	45 000	7100	≥200 000	ND	ND	ND	71 000	29 000	ND	33 000	50 000	ND
		ΔG_{obs} (kJ mol^{-1})	-25.8	-30.5	≥-22.0	ND	ND	ND	-24.6	-27.0	ND	-26.6	-25.5	ND
KR50-4		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
31		$K_{d,obs}$ (nM)	59 000	10 000	ND	ND	ND	ND	50 000	29 000	ND	33 000	77 000	ND
		ΔG_{obs} (kJ mol^{-1})	-25.1	-29.7	ND	ND	ND	ND	-25.5	-27.0	ND	-26.6	-24.4	ND
KR50-21		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

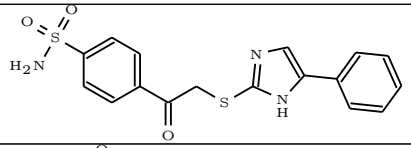
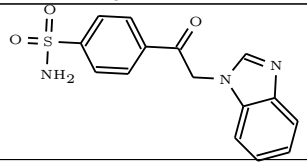
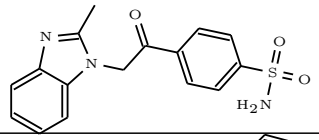
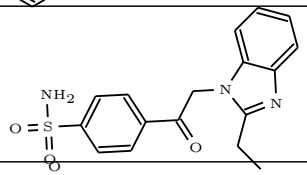
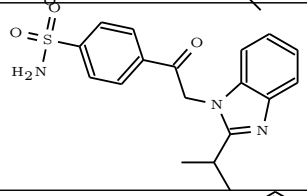
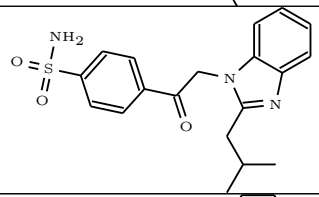
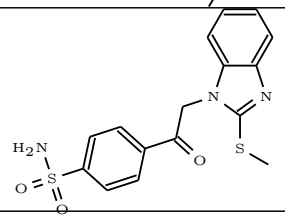
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
32 KR50-5		$K_{d,obs}$ (nM)	15 000	1900	≥200 000	ND	ND	ND	25 000	13 000	ND	33 000	5600	ND
		ΔG_{obs} (kJ mol^{-1})	-28.6	-34.0	≥-22.0	ND	ND	ND	-27.3	-29.1	ND	-26.6	-31.2	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
33 KR50-10		$K_{d,obs}$ (nM)	13 000	1800	≥200 000	ND	ND	ND	7100	5900	ND	31 000	7100	ND
		ΔG_{obs} (kJ mol^{-1})	-29.1	-34.1	≥-22.0	ND	ND	ND	-30.5	-31.0	ND	-26.7	-30.5	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
34 KR50-9		$K_{d,obs}$ (nM)	13 000	2000	ND	ND	ND	ND	6700	13 000	ND	33 000	8300	ND
		ΔG_{obs} (kJ mol^{-1})	-29.1	-33.8	ND	ND	ND	ND	-30.7	-29.1	ND	-26.6	-30.1	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
35 KR50-11		$K_{d,obs}$ (nM)	37 000	8300	≥200 000	ND	ND	ND	50 000	25 000	ND	33 000	56 000	ND
		ΔG_{obs} (kJ mol^{-1})	-26.3	-30.1	≥-22.0	ND	ND	ND	-25.5	-27.3	ND	-26.6	-25.3	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
36 KTU17		$K_{d,obs}$ (nM)	20 000	3600	ND	ND	ND	ND	25 000	25 000	ND	67 000	50 000	ND
		ΔG_{obs} (kJ mol^{-1})	-27.9	-32.3	ND	ND	ND	ND	-27.3	-27.3	ND	-24.8	-25.5	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
37 KR50-6		$K_{d,obs}$ (nM)	11 000	1400	≥200 000	ND	ND	ND	25 000	17 000	ND	50 000	4300	ND
		ΔG_{obs} (kJ mol^{-1})	-29.4	-34.7	≥-22.0	ND	ND	ND	-27.3	-28.4	ND	-25.5	-31.8	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
38 KR50-16b		$K_{d,obs}$ (nM)	9100	4000	ND	ND	ND	ND	8300	5600	ND	5600	9100	ND
		ΔG_{obs} (kJ mol^{-1})	-29.9	-32.0	ND	ND	ND	ND	-30.1	-31.2	ND	-31.2	-29.9	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
39 KR50-16a		$K_{d,obs}$ (nM)	29 000	4000	≥200 000	ND	ND	ND	7100	13 000	ND	1900	19 000	ND
		ΔG_{obs} (kJ mol^{-1})	-27.0	-32.0	≥-22.0	ND	ND	ND	-30.5	-29.1	ND	-34.0	-28.1	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

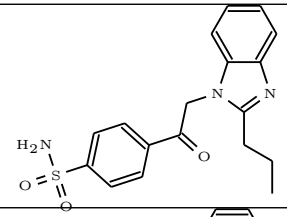
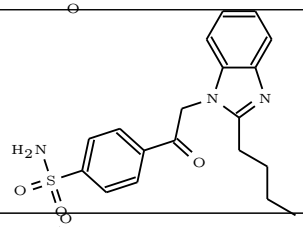
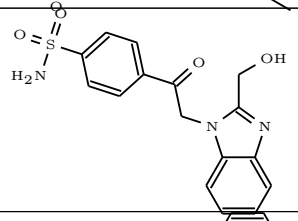
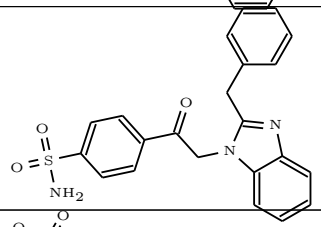
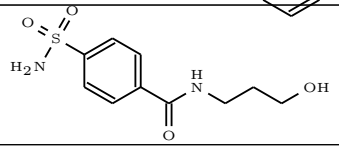
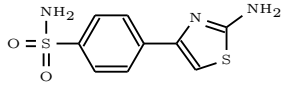
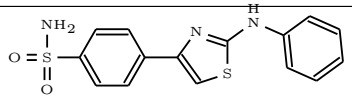
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
40		$K_{d,obs}$ (nM)	100 000	100 000	≥200 000	50 000	ND	≥200 000	≥200 000	≥200 000	330	≥200 000	100 000	33 000
		ΔG_{obs} (kJ mol^{-1})	-23.7	-23.7	≥-22.0	-25.5	ND	≥-22.0	≥-22.0	≥-22.0	-38.4	≥-22.0	-23.7	-26.6
JS46		$K_{d,int}$ (nM)	74	35	38	11	ND	79	14	61	0.075	310	72	10
		ΔG_{int} (kJ mol^{-1})	-42.3	-44.2	-44.0	-47.2	ND	-42.1	-46.5	-42.8	-60.1	-38.7	-42.4	-47.4
41		$K_{d,obs}$ (nM)	71	170	≥200 000	10 000	ND	670	17 000	10 000	50	29 000	1400	290
		ΔG_{obs} (kJ mol^{-1})	-42.4	-40.2	≥-22.0	-29.7	ND	-36.7	-28.4	-29.7	-43.3	-26.9	-34.7	-38.8
JS48		$K_{d,int}$ (nM)	0.053	0.059	38	2.3	ND	0.26	1.2	3.1	0.011	9.0	1.0	0.088
		ΔG_{int} (kJ mol^{-1})	-61.0	-60.7	-44.0	-51.3	ND	-56.8	-52.9	-50.5	-65.0	-47.7	-53.3	-59.7
42		$K_{d,obs}$ (nM)	830	350	ND	ND	ND	ND	ND	1900	ND	8300	610	ND
		ΔG_{obs} (kJ mol^{-1})	-36.1	-38.3	ND	ND	ND	ND	ND	-33.9	ND	-30.1	-36.9	ND
JS43		$K_{d,int}$ (nM)	0.61	0.12	ND	ND	ND	ND	ND	0.44	ND	2.6	0.44	ND
		ΔG_{int} (kJ mol^{-1})	-54.7	-58.8	ND	ND	ND	ND	ND	-55.5	ND	-51.0	-55.5	ND
43		$K_{d,obs}$ (nM)	1200	130	ND	ND	ND	ND	ND	2300	ND	2500	310	ND
		ΔG_{obs} (kJ mol^{-1})	-35.1	-40.8	ND	ND	ND	ND	ND	-33.5	ND	-33.2	-38.6	ND
JS44		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
44		$K_{d,obs}$ (nM)	560	91	10 000	5000	ND	3300	13 000	130	67	1700	2.0	250
		ΔG_{obs} (kJ mol^{-1})	-37.1	-41.8	-29.7	-31.5	ND	-32.5	-29.1	-40.8	-42.6	-34.3	-51.6	-39.2
JS45		$K_{d,int}$ (nM)	0.41	0.032	1.9	1.1	ND	1.3	0.90	0.041	0.015	0.51	0.0014	0.077
		ΔG_{int} (kJ mol^{-1})	-55.7	-62.3	-51.7	-53.1	ND	-52.7	-53.7	-61.6	-64.2	-55.1	-70.3	-60.0
45		$K_{d,obs}$ (nM)	33	67	ND	ND	ND	ND	3200	290	ND	2000	2000	ND
		ΔG_{obs} (kJ mol^{-1})	-44.4	-42.6	ND	ND	ND	ND	-32.6	-38.8	ND	-33.8	-33.8	ND
MK8		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
46		$K_{d,obs}$ (nM)	500	280	ND	ND	ND	ND	8300	1000	ND	6300	7700	ND
		ΔG_{obs} (kJ mol^{-1})	-37.4	-38.9	ND	ND	ND	ND	-30.1	-35.6	ND	-30.9	-30.3	ND
MK9		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
47		$K_{d,obs}$ (nM)	100	180	ND	ND	ND	ND	13 000	770	ND	4000	1700	ND
		ΔG_{obs} (kJ mol^{-1})	-41.5	-40.0	ND	ND	ND	ND	-28.9	-36.3	ND	-32.0	-34.2	ND
MK5		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

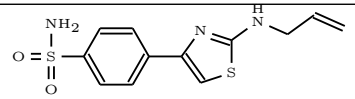
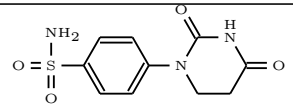
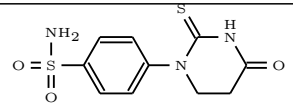
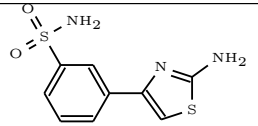
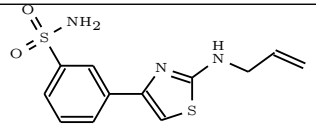
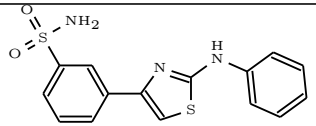
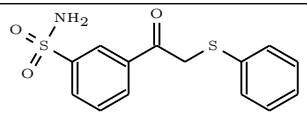
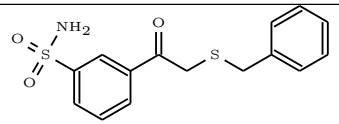
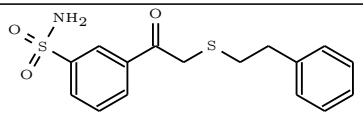
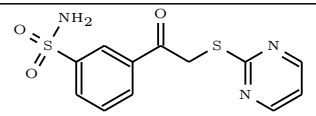
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
48		$K_{d,obs}$ (nM)	13	71	ND	ND	ND	ND	13 000	200	ND	590	500	ND
		ΔG_{obs} (kJ mol^{-1})	-46.7	-42.4	ND	ND	ND	ND	-28.9	-39.8	ND	-37.0	-37.4	ND
MK6		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
49		$K_{d,obs}$ (nM)	33	130	ND	ND	ND	ND	13 000	450	ND	1800	830	ND
		ΔG_{obs} (kJ mol^{-1})	-44.4	-40.8	ND	ND	ND	ND	-28.9	-37.6	ND	-34.1	-36.1	ND
MK2		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
50		$K_{d,obs}$ (nM)	6.7	63	ND	ND	ND	ND	10 000	120	ND	770	330	ND
		ΔG_{obs} (kJ mol^{-1})	-48.5	-42.8	ND	ND	ND	ND	-29.7	-41.1	ND	-36.3	-38.4	ND
MK1		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
51		$K_{d,obs}$ (nM)	3.8	43	ND	ND	ND	ND	14 000	130	ND	770	170	ND
		ΔG_{obs} (kJ mol^{-1})	-49.9	-43.7	ND	ND	ND	ND	-28.8	-41.0	ND	-36.3	-40.2	ND
MK3		$K_{d,int}$ (nM)	0.0093	0.050	ND	ND	ND	ND	3.4	0.13	ND	0.78	0.40	ND
		ΔG_{int} (kJ mol^{-1})	-65.5	-61.1	ND	ND	ND	ND	-50.3	-58.7	ND	-54.0	-55.8	ND
52		$K_{d,obs}$ (nM)	40	100	ND	ND	ND	ND	12 000	400	ND	4000	1100	ND
		ΔG_{obs} (kJ mol^{-1})	-43.9	-41.5	ND	ND	ND	ND	-29.3	-38.0	ND	-32.0	-35.3	ND
MK4		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
53		$K_{d,obs}$ (nM)	25	13	ND	360	1400	4000	5000	56	ND	1000	29	ND
		ΔG_{obs} (kJ mol^{-1})	-45.2	-46.9	ND	-38.2	-34.7	-32.0	-31.5	-43.1	ND	-35.6	-44.8	ND
E63		$K_{d,int}$ (nM)	0.090	0.022	ND	0.41	3.8	7.9	1.8	0.085	ND	1.5	0.10	ND
		ΔG_{int} (kJ mol^{-1})	-59.6	-63.3	ND	-55.7	-50.0	-48.1	-51.9	-59.8	ND	-52.3	-59.3	ND
54		$K_{d,obs}$ (nM)	15	83	ND	200	670	1000	1200	250	ND	91	63	ND
		ΔG_{obs} (kJ mol^{-1})	-46.5	-42.0	ND	-39.7	-36.7	-35.6	-35.0	-39.2	ND	-41.8	-42.8	ND
E66		$K_{d,int}$ (nM)	0.054	0.15	ND	0.23	1.8	2.0	0.45	0.38	ND	0.14	0.23	ND
		ΔG_{int} (kJ mol^{-1})	-60.9	-58.4	ND	-57.2	-52.0	-51.6	-55.5	-55.9	ND	-58.5	-57.3	ND
55		$K_{d,obs}$ (nM)	1.7	67	ND	390	1600	2000	5000	48	32	170	4.9	ND
		ΔG_{obs} (kJ mol^{-1})	-52.0	-42.6	ND	-38.0	-34.5	-33.8	-31.5	-43.4	-44.5	-40.2	-49.3	ND
E67		$K_{d,int}$ (nM)	0.0063	0.12	ND	0.44	4.1	4.0	1.8	0.074	0.036	0.26	0.018	ND
		ΔG_{int} (kJ mol^{-1})	-66.5	-58.9	ND	-55.5	-49.8	-49.9	-51.9	-60.1	-62.0	-56.9	-63.8	ND
56		$K_{d,obs}$ (nM)	22	13	ND	200	1500	6300	5000	67	ND	1400	23	ND
		ΔG_{obs} (kJ mol^{-1})	-45.5	-46.9	ND	-39.7	-34.5	-30.9	-31.5	-42.6	ND	-34.7	-45.4	ND
E61		$K_{d,int}$ (nM)	0.080	0.022	ND	0.23	4.1	12	1.8	0.10	ND	2.2	0.082	ND
		ΔG_{int} (kJ mol^{-1})	-59.9	-63.3	ND	-57.2	-49.8	-46.9	-51.9	-59.3	ND	-51.4	-59.9	ND
57		$K_{d,obs}$ (nM)	67	67	ND	380	500	2500	3700	170	ND	560	360	ND
		ΔG_{obs} (kJ mol^{-1})	-42.6	-42.6	ND	-38.1	-37.4	-33.2	-32.2	-40.2	ND	-37.1	-38.3	ND
E59		$K_{d,int}$ (nM)	0.24	0.12	ND	0.43	1.3	5.0	1.3	0.26	ND	0.85	1.3	ND
		ΔG_{int} (kJ mol^{-1})	-57.0	-58.9	ND	-55.6	-52.7	-49.3	-52.7	-56.9	ND	-53.8	-52.8	ND

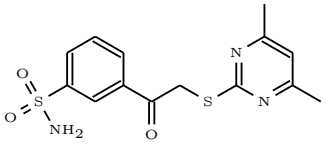
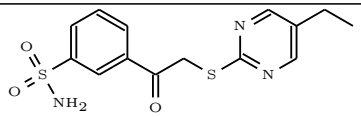
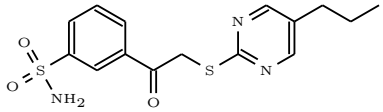
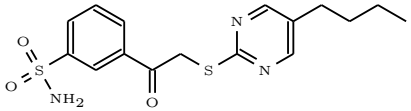
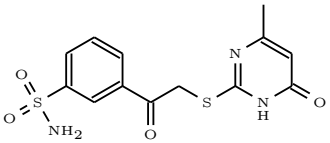
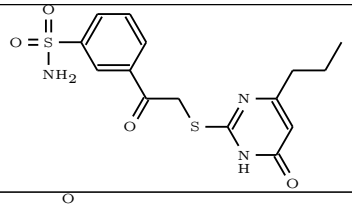
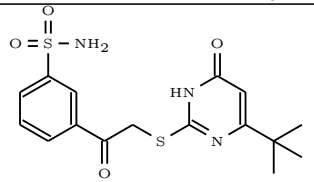
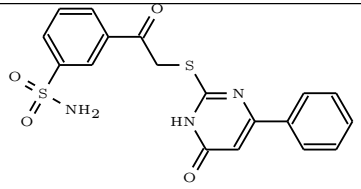
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
58		$K_{d,obs}$ (nM)	33	22	ND	290	1100	4000	1200	140	ND	710	8.3	ND
		ΔG_{obs} (kJ mol^{-1})	-44.4	-45.4	ND	-38.8	-35.3	-32.0	-35.0	-40.6	ND	-36.5	-47.9	ND
E60		$K_{d,int}$ (nM)	0.12	0.039	ND	0.33	2.9	7.9	0.45	0.22	ND	1.1	0.030	ND
		ΔG_{int} (kJ mol^{-1})	-58.8	-61.8	ND	-56.3	-50.6	-48.1	-55.5	-57.3	ND	-53.2	-62.4	ND
59		$K_{d,obs}$ (nM)	26	18	ND	75	330	4500	2500	200	ND	370	290	ND
		ΔG_{obs} (kJ mol^{-1})	-45.0	-45.9	ND	-42.3	-38.4	-31.7	-33.2	-39.8	ND	-38.2	-38.8	ND
E62		$K_{d,int}$ (nM)	0.095	0.032	ND	0.085	0.88	9.0	0.90	0.31	ND	0.57	1.0	ND
		ΔG_{int} (kJ mol^{-1})	-59.5	-62.3	ND	-59.8	-53.7	-47.7	-53.7	-56.5	ND	-54.9	-53.3	ND
60		$K_{d,obs}$ (nM)	24	14	ND	320	710	1800	5000	100	ND	1400	29	ND
		ΔG_{obs} (kJ mol^{-1})	-45.2	-46.6	ND	-38.5	-36.5	-34.1	-31.5	-41.5	ND	-34.7	-44.8	ND
E64		$K_{d,int}$ (nM)	0.090	0.025	ND	0.36	1.9	3.6	1.8	0.15	ND	2.2	0.10	ND
		ΔG_{int} (kJ mol^{-1})	-59.6	-62.9	ND	-56.0	-51.8	-50.1	-51.9	-58.2	ND	-51.4	-59.3	ND
61		$K_{d,obs}$ (nM)	19	33	ND	610	1400	1000	2500	130	ND	910	83	ND
		ΔG_{obs} (kJ mol^{-1})	-45.8	-44.4	ND	-36.9	-34.7	-35.6	-33.2	-41.0	ND	-35.9	-42.0	ND
E65		$K_{d,int}$ (nM)	0.071	0.059	ND	0.69	3.8	2.0	0.90	0.19	ND	1.4	0.30	ND
		ΔG_{int} (kJ mol^{-1})	-60.2	-60.7	ND	-54.4	-50.0	-51.6	-53.7	-57.7	ND	-52.6	-56.5	ND
62		$K_{d,obs}$ (nM)	20	20	ND	1500	1100	1700	ND	170	ND	1100	330	ND
		ΔG_{obs} (kJ mol^{-1})	-45.7	-45.7	ND	-34.5	-35.3	-34.3	ND	-40.2	ND	-35.3	-38.4	ND
E69		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
63		$K_{d,obs}$ (nM)	38	33	ND	250	670	2500	ND	200	ND	330	67	ND
		ΔG_{obs} (kJ mol^{-1})	-44.0	-44.4	ND	-39.2	-36.7	-33.2	ND	-39.8	ND	-38.4	-42.6	ND
E70		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
64		$K_{d,obs}$ (nM)	50	40	ND	1400	400	13 000	ND	150	ND	1700	67	ND
		ΔG_{obs} (kJ mol^{-1})	-43.3	-43.9	ND	-34.7	-38.0	-29.1	ND	-40.4	ND	-34.3	-42.6	ND
E71		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
65		$K_{d,obs}$ (nM)	63	31	ND	290	400	670	ND	100	ND	330	33	ND
		ΔG_{obs} (kJ mol^{-1})	-42.8	-44.5	ND	-38.8	-38.0	-36.7	ND	-41.5	ND	-38.4	-44.4	ND
E72		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

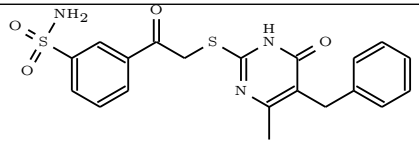
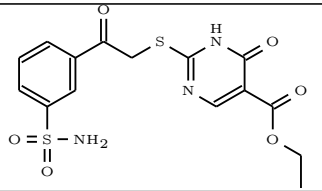
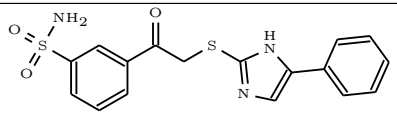
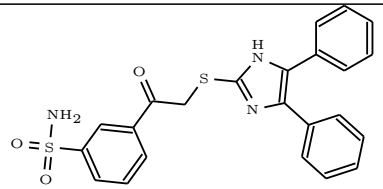
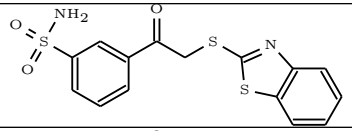
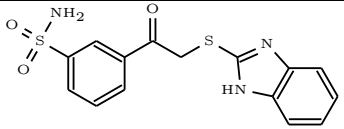
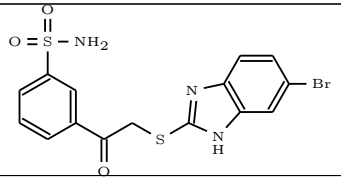
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
66		$K_{d,obs}$ (nM)	13	5.0	ND	50	330	330	ND	29	ND	500	15	ND
		ΔG_{obs} (kJ mol^{-1})	-46.9	-49.3	ND	-43.3	-38.4	-38.4	ND	-44.8	ND	-37.4	-46.4	ND
E73		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
67		$K_{d,obs}$ (nM)	3.7	6.0	ND	380	1000	ND	ND	50	ND	290	33	ND
		ΔG_{obs} (kJ mol^{-1})	-50.1	-48.8	ND	-38.1	-35.6	ND	ND	-43.3	ND	-38.8	-44.4	ND
E88		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
68		$K_{d,obs}$ (nM)	41	17	ND	1100	2500	ND	910	67	220	560	290	ND
		ΔG_{obs} (kJ mol^{-1})	-43.9	-46.2	ND	-35.4	-33.2	ND	-35.9	-42.6	-39.5	-37.1	-38.8	ND
E90		$K_{d,int}$ (nM)	0.15	0.029	ND	1.2	6.6	ND	0.33	0.10	0.25	0.85	1.0	ND
		ΔG_{int} (kJ mol^{-1})	-58.3	-62.5	ND	-52.9	-48.5	ND	-56.3	-59.3	-57.0	-53.8	-53.3	ND
69		$K_{d,obs}$ (nM)	200	50	ND	ND	3300	ND	ND	14	ND	38	50	ND
		ΔG_{obs} (kJ mol^{-1})	-39.8	-43.3	ND	ND	-32.5	ND	ND	-46.6	ND	-44.0	-43.3	ND
E95		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
70		$K_{d,obs}$ (nM)	2.3	5.0	ND	220	220	670	ND	6.7	ND	200	10	ND
		ΔG_{obs} (kJ mol^{-1})	-51.2	-49.3	ND	-39.5	-39.5	-36.7	ND	-48.5	ND	-39.8	-47.5	ND
E97		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
71		$K_{d,obs}$ (nM)	2.0	10	ND	40	400	500	ND	7.1	ND	100	38	ND
		ΔG_{obs} (kJ mol^{-1})	-51.6	-47.5	ND	-43.9	-38.0	-37.4	ND	-48.3	ND	-41.5	-44.0	ND
E99		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
72		$K_{d,obs}$ (nM)	330	170	ND	ND	ND	ND	ND	120	ND	4000	77	ND
		ΔG_{obs} (kJ mol^{-1})	-38.4	-40.2	ND	ND	ND	ND	ND	-41.1	ND	-32.0	-42.2	ND
AR6		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

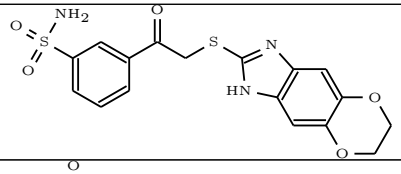
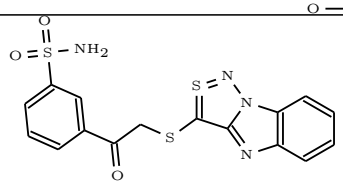
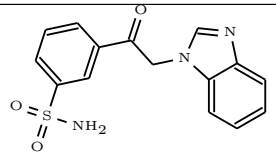
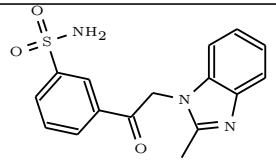
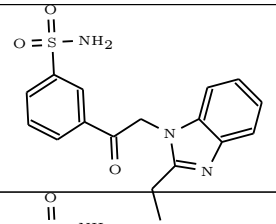
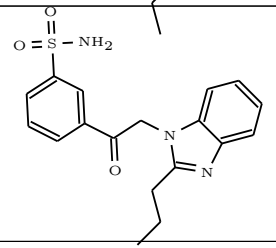
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
73		$K_{d,obs}$ (nM)	100	20	ND	ND	ND	ND	ND	25	ND	400	67	ND
		ΔG_{obs} (kJ mol^{-1})	-41.5	-45.7	ND	ND	ND	ND	ND	-45.1	ND	-38.0	-42.6	ND
AR7		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
74		$K_{d,obs}$ (nM)	33	4.0	28 000	1600	2500	310	3800	20	67	910	83	16
		ΔG_{obs} (kJ mol^{-1})	-44.4	-49.8	-27.1	-34.4	-33.2	-38.6	-32.2	-45.7	-42.6	-35.9	-42.0	-46.3
E79		$K_{d,int}$ (nM)	0.37	0.021	79	5.4	20	1.9	4.1	0.092	0.23	4.2	0.90	0.073
		ΔG_{int} (kJ mol^{-1})	-56.0	-63.4	-42.2	-49.0	-45.7	-51.8	-49.8	-59.6	-57.2	-49.7	-53.7	-60.2
75		$K_{d,obs}$ (nM)	10	6.2	33 000	2200	2500	420	3900	29	66	720	77	9.1
		ΔG_{obs} (kJ mol^{-1})	-47.5	-48.7	-26.6	-33.6	-33.2	-37.9	-32.1	-44.8	-42.6	-36.5	-42.2	-47.7
E80		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
76		$K_{d,obs}$ (nM)	8.3	5.0	59 000	1900	1100	330	3400	20	35	400	50	10
		ΔG_{obs} (kJ mol^{-1})	-47.9	-49.3	-25.1	-33.9	-35.3	-38.4	-32.4	-45.7	-44.2	-38.0	-43.3	-47.5
E81		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
77		$K_{d,obs}$ (nM)	4.0	5.6	≥200 000	860	710	500	4000	20	27	480	33	10
		ΔG_{obs} (kJ mol^{-1})	-49.8	-49.0	≥-22.0	-36.0	-36.5	-37.4	-32.0	-45.7	-44.9	-37.5	-44.4	-47.5
E82		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
78		$K_{d,obs}$ (nM)	8.3	5.6	160 000	970	830	330	5000	17	24	830	33	6.2
		ΔG_{obs} (kJ mol^{-1})	-47.9	-49.0	-22.6	-35.7	-36.1	-38.4	-31.5	-46.2	-45.2	-36.1	-44.4	-48.7
E83		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
79		$K_{d,obs}$ (nM)	3.6	4.0	22 000	980	500	250	1500	18	12	2000	38	8.1
		ΔG_{obs} (kJ mol^{-1})	-50.1	-49.8	-27.7	-35.7	-37.4	-39.2	-34.6	-45.9	-47.0	-33.8	-44.0	-48.0
E84		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

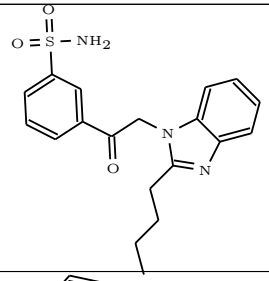
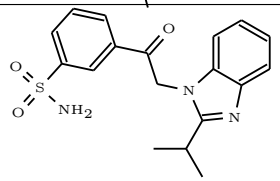
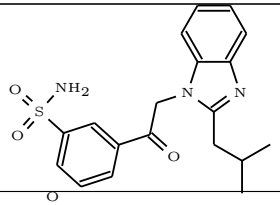
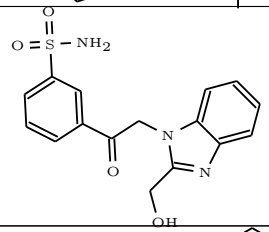
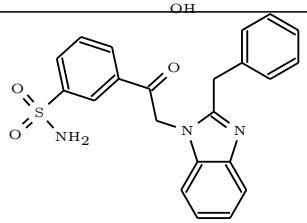
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
80		$K_{d,obs}$ (nM)	7.1	5.6	56 000	1700	1000	290	4000	17	24	670	29	7.9
		ΔG_{obs} (kJ mol^{-1})	-48.3	-49.0	-25.3	-34.2	-35.6	-38.8	-32.0	-46.1	-45.3	-36.7	-44.8	-48.1
E85		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
81		$K_{d,obs}$ (nM)	11	4.2	≥200 000	1800	1200	710	2500	20	25	1000	50	7.1
		ΔG_{obs} (kJ mol^{-1})	-47.2	-49.7	≥-22.0	-34.2	-35.0	-36.5	-33.2	-45.7	-45.1	-35.6	-43.3	-48.3
E93		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
82		$K_{d,obs}$ (nM)	8.3	4.2	21 000	1700	770	110	2900	20	36	1100	63	7.7
		ΔG_{obs} (kJ mol^{-1})	-47.9	-49.7	-27.8	-34.2	-36.3	-41.2	-32.9	-45.7	-44.2	-35.5	-42.8	-48.2
E86		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
83		$K_{d,obs}$ (nM)	140	100	≥200 000	1400	14 000	1000	6700	20	360	8300	290	150
		ΔG_{obs} (kJ mol^{-1})	-40.6	-41.5	≥-22.0	-34.7	-28.8	-35.6	-30.7	-45.7	-38.2	-30.1	-38.8	-40.4
E87		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
84		$K_{d,obs}$ (nM)	2500	250	ND	2600	3300	10 000	ND	500	ND	4000	4500	ND
		ΔG_{obs} (kJ mol^{-1})	-33.2	-39.2	ND	-33.2	-32.5	-29.7	ND	-37.4	ND	-32.1	-31.7	ND
E10-4		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
85		$K_{d,obs}$ (nM)	130	180	≥200 000	5000	2000	5000	10 000	830	67	2500	2200	130
		ΔG_{obs} (kJ mol^{-1})	-41.0	-40.0	≥-22.0	-31.5	-33.8	-31.5	-29.7	-36.1	-42.6	-33.2	-33.5	-41.0
E74		$K_{d,int}$ (nM)	0.15	0.11	63	1.9	1.8	3.3	1.2	0.42	0.025	1.3	2.7	0.064
		ΔG_{int} (kJ mol^{-1})	-58.3	-59.2	-42.7	-51.8	-52.0	-50.3	-52.9	-55.6	-62.9	-52.8	-50.9	-60.5
86		$K_{d,obs}$ (nM)	50	200	≥200 000	10 000	3300	2500	100 000	1400	67	8300	330	290
		ΔG_{obs} (kJ mol^{-1})	-43.3	-39.8	≥-22.0	-29.7	-32.5	-33.2	-23.7	-34.7	-42.6	-30.1	-38.4	-38.8
E75		$K_{d,int}$ (nM)	0.061	0.12	63	3.7	2.9	1.6	12	0.73	0.025	4.2	0.40	0.15
		ΔG_{int} (kJ mol^{-1})	-60.6	-59.0	-42.7	-50.0	-50.6	-52.1	-47.0	-54.2	-62.9	-49.7	-55.8	-58.3

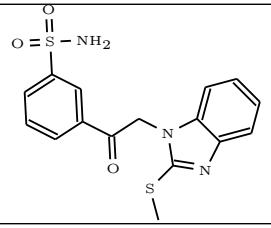
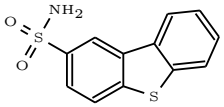
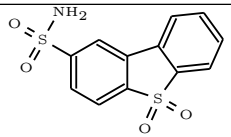
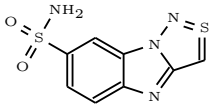
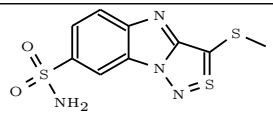
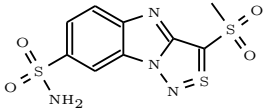
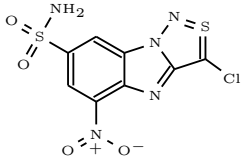
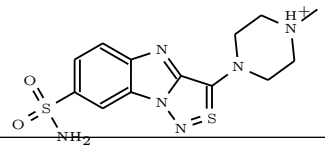
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
87		$K_{d,obs}$ (nM)	25	71	≥200 000	1100	1100	2900	5300	560	83	1100	620	40
		ΔG_{obs} (kJ mol^{-1})	-45.1	-42.4	≥-22.0	-35.3	-35.3	-32.9	-31.3	-37.1	-42.0	-35.3	-36.8	-43.9
E76		$K_{d,int}$ (nM)	0.030	0.042	63	0.42	0.97	1.9	0.63	0.28	0.031	0.57	0.75	0.020
		ΔG_{int} (kJ mol^{-1})	-62.4	-61.6	-42.7	-55.7	-53.5	-51.8	-54.6	-56.7	-62.3	-54.9	-54.2	-63.4
88		$K_{d,obs}$ (nM)	3800	830	ND	ND	ND	ND	13 000	1500	ND	5600	8300	ND
		ΔG_{obs} (kJ mol^{-1})	-32.1	-36.1	ND	ND	ND	ND	-29.1	-34.5	ND	-31.2	-30.1	ND
KR50-18a		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
89		$K_{d,obs}$ (nM)	1100	670	ND	ND	ND	ND	8300	1600	ND	5600	2900	ND
		ΔG_{obs} (kJ mol^{-1})	-35.3	-36.7	ND	ND	ND	ND	-30.1	-34.4	ND	-31.2	-32.9	ND
KR50-18b		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
90		$K_{d,obs}$ (nM)	33 000	5000	≥200 000	5600	17 000	25 000	7900	8300	830	10 000	6700	2500
		ΔG_{obs} (kJ mol^{-1})	-26.6	-31.5	≥-22.0	-31.2	-28.4	-27.3	-30.3	-30.1	-36.1	-29.7	-30.7	-33.2
E11-63		$K_{d,int}$ (nM)	38	2.7	59	1.9	14	15	0.88	4.0	0.29	4.8	7.4	1.2
		ΔG_{int} (kJ mol^{-1})	-44.0	-50.8	-42.9	-51.7	-46.7	-46.4	-53.7	-49.9	-56.6	-49.4	-48.2	-53.0
91		$K_{d,obs}$ (nM)	5900	1800	≥200 000	9600	17 000	8300	20 000	6700	220	10 000	670	1000
		ΔG_{obs} (kJ mol^{-1})	-31.0	-34.1	≥-22.0	-29.8	-28.4	-30.1	-27.9	-30.7	-39.5	-29.7	-36.7	-35.6
E11-65		$K_{d,int}$ (nM)	6.7	0.99	59	3.4	14	5.1	2.2	3.2	0.078	4.8	0.74	0.48
		ΔG_{int} (kJ mol^{-1})	-48.5	-53.4	-42.9	-50.3	-46.7	-49.2	-51.3	-50.4	-60.0	-49.4	-54.2	-55.3
92		$K_{d,obs}$ (nM)	1200	670	≥200 000	420	17 000	6700	7100	5000	140	17 000	670	1100
		ΔG_{obs} (kJ mol^{-1})	-35.0	-36.7	≥-22.0	-37.9	-28.4	-30.7	-30.5	-31.5	-40.6	-28.4	-36.7	-35.5
E11-67		$K_{d,int}$ (nM)	1.4	0.36	59	0.15	14	4.1	0.80	2.4	0.050	7.9	0.74	0.50
		ΔG_{int} (kJ mol^{-1})	-52.5	-56.0	-42.9	-58.4	-46.7	-49.8	-54.0	-51.2	-61.1	-48.1	-54.2	-55.2
93		$K_{d,obs}$ (nM)	100	560	ND	4500	1700	ND	ND	1400	ND	1200	290	ND
		ΔG_{obs} (kJ mol^{-1})	-41.5	-37.1	ND	-31.7	-34.3	ND	ND	-34.7	ND	-35.0	-38.8	ND
E11-7		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
94		$K_{d,obs}$ (nM)	260	560	ND	1800	6700	5000	ND	1500	ND	430	200	ND
		ΔG_{obs} (kJ mol^{-1})	-39.0	-37.1	ND	-34.1	-30.7	-31.5	ND	-34.5	ND	-37.8	-39.8	ND
E11-71		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
95		$K_{d,obs}$ (nM)	230	710	ND	5000	5900	3300	ND	4000	ND	1400	170	ND
		ΔG_{obs} (kJ mol^{-1})	-39.4	-36.5	ND	-31.5	-31.0	-32.5	ND	-32.0	ND	-34.7	-40.1	ND
E11-69		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
96		$K_{d,obs}$ (nM)	770	1100	ND	3400	420	15 000	1900	4000	690	3300	1300	ND
		ΔG_{obs} (kJ mol^{-1})	-36.3	-35.3	ND	-32.4	-37.9	-28.6	-33.9	-32.0	-36.6	-32.5	-34.9	ND
E11-9		$K_{d,int}$ (nM)	2.8	2.0	ND	3.9	1.1	31	0.69	6.1	0.78	5.1	4.8	ND
		ΔG_{int} (kJ mol^{-1})	-50.7	-51.7	ND	-49.9	-53.2	-44.6	-54.4	-48.7	-54.1	-49.2	-49.4	ND

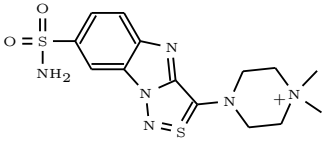
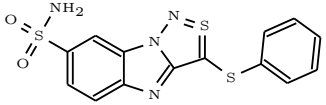
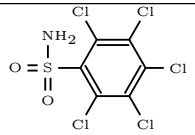
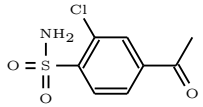
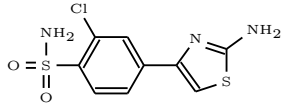
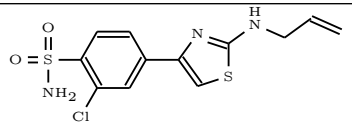
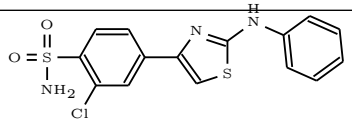
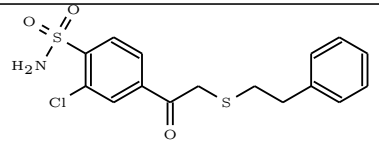
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
97		$K_{d,obs}$ (nM)	370	1000	ND	2500	2000	ND	13 000	6700	ND	3300	1000	ND
		ΔG_{obs} (kJ mol^{-1})	-38.2	-35.6	ND	-33.2	-33.8	ND	-29.1	-30.7	ND	-32.5	-35.6	ND
E11-11		$K_{d,int}$ (nM)	1.4	1.8	ND	2.8	5.3	ND	4.5	10	ND	5.1	3.6	ND
		ΔG_{int} (kJ mol^{-1})	-52.6	-52.0	ND	-50.7	-49.1	ND	-49.5	-47.4	ND	-49.2	-50.1	ND
98		$K_{d,obs}$ (nM)	500	670	ND	5000	130	10 000	8300	2500	ND	3800	560	ND
		ΔG_{obs} (kJ mol^{-1})	-37.4	-36.7	ND	-31.5	-41.0	-29.7	-30.1	-33.2	ND	-32.1	-37.1	ND
E11-13		$K_{d,int}$ (nM)	1.8	1.2	ND	5.6	0.33	20	3.0	3.8	ND	5.9	2.0	ND
		ΔG_{int} (kJ mol^{-1})	-51.8	-53.0	ND	-49.0	-56.3	-45.7	-50.6	-49.9	ND	-48.8	-51.6	ND
99		$K_{d,obs}$ (nM)	370	560	ND	3700	110	5600	5000	3300	ND	4200	330	ND
		ΔG_{obs} (kJ mol^{-1})	-38.2	-37.1	ND	-32.3	-41.3	-31.2	-31.5	-32.5	ND	-31.9	-38.4	ND
E11-15		$K_{d,int}$ (nM)	1.4	0.98	ND	4.1	0.29	11	1.8	5.1	ND	6.4	1.2	ND
		ΔG_{int} (kJ mol^{-1})	-52.6	-53.5	ND	-49.8	-56.6	-47.2	-51.9	-49.2	ND	-48.6	-52.9	ND
100		$K_{d,obs}$ (nM)	500	310	ND	4200	33	2000	4300	2200	ND	1800	280	ND
		ΔG_{obs} (kJ mol^{-1})	-37.4	-38.6	ND	-31.9	-44.4	-33.8	-31.8	-33.5	ND	-34.1	-38.9	ND
E11-17		$K_{d,int}$ (nM)	1.8	0.55	ND	4.7	0.088	4.0	1.6	3.4	ND	2.8	1.0	ND
		ΔG_{int} (kJ mol^{-1})	-51.8	-55.0	ND	-49.4	-59.7	-49.9	-52.3	-50.3	ND	-50.8	-53.4	ND
101		$K_{d,obs}$ (nM)	830	1200	ND	3600	5000	13 000	11 000	4000	ND	3700	1500	ND
		ΔG_{obs} (kJ mol^{-1})	-36.1	-35.0	ND	-32.3	-31.5	-29.0	-29.4	-32.0	ND	-32.2	-34.5	ND
E11-19		$K_{d,int}$ (nM)	3.1	2.2	ND	4.0	13	26	4.0	6.1	ND	5.7	5.5	ND
		ΔG_{int} (kJ mol^{-1})	-50.5	-51.4	ND	-49.8	-46.8	-45.1	-49.8	-48.7	ND	-48.9	-49.0	ND
102		$K_{d,obs}$ (nM)	500	500	ND	5000	3300	33 000	17 000	3300	ND	1700	830	ND
		ΔG_{obs} (kJ mol^{-1})	-37.4	-37.4	ND	-31.5	-32.5	-26.6	-28.4	-32.5	ND	-34.3	-36.1	ND
E11-25		$K_{d,int}$ (nM)	1.8	0.88	ND	5.6	8.8	66	6.0	5.1	ND	2.6	3.0	ND
		ΔG_{int} (kJ mol^{-1})	-51.8	-53.7	ND	-49.0	-47.8	-42.6	-48.8	-49.2	ND	-51.0	-50.6	ND
103		$K_{d,obs}$ (nM)	100	500	ND	20 000	10 000	17 000	45 000	500	ND	1200	170	ND
		ΔG_{obs} (kJ mol^{-1})	-41.5	-37.4	ND	-27.9	-29.7	-28.4	-25.8	-37.4	ND	-35.0	-40.2	ND
E11-27		$K_{d,int}$ (nM)	0.37	0.88	ND	23	26	33	16	0.77	ND	1.9	0.60	ND
		ΔG_{int} (kJ mol^{-1})	-56.0	-53.7	ND	-45.4	-45.0	-44.4	-46.2	-54.1	ND	-51.7	-54.7	ND
104		$K_{d,obs}$ (nM)	71 000	1300	ND	14 000	100 000	≥200 000	≥200 000	≥200 000	ND	58 000	9400	ND
		ΔG_{obs} (kJ mol^{-1})	-24.6	-34.9	ND	-28.8	-23.7	≥-22.0	≥-22.0	≥-22.0	ND	-25.2	-29.8	ND
E11-29		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

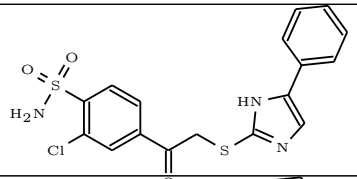
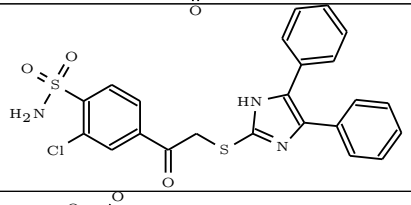
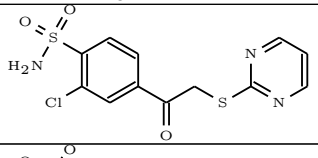
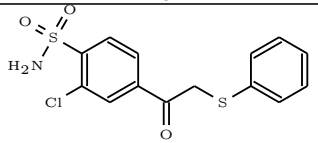
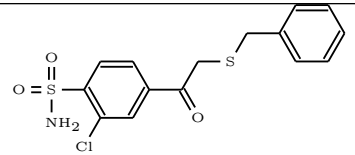
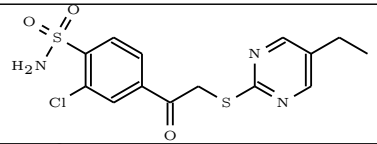
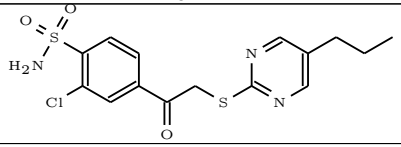
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
105		$K_{d,obs}$ (nM)	2200	1100	ND	6700	1000	1700	3300	13 000	ND	6700	1400	ND
		ΔG_{obs} (kJ mol^{-1})	-33.5	-35.3	ND	-30.7	-35.6	-34.3	-32.5	-29.1	ND	-30.7	-34.7	ND
E11-21		$K_{d,int}$ (nM)	8.2	2.0	ND	7.5	2.6	3.3	1.2	19	ND	10	5.1	ND
		ΔG_{int} (kJ mol^{-1})	-48.0	-51.7	ND	-48.2	-50.9	-50.3	-52.9	-45.8	ND	-47.4	-49.2	ND
106		$K_{d,obs}$ (nM)	1200	670	ND	1400	1400	ND	2100	1000	ND	1000	2200	ND
		ΔG_{obs} (kJ mol^{-1})	-35.0	-36.7	ND	-34.7	-34.7	ND	-33.7	-35.6	ND	-35.6	-33.5	ND
E11-23		$K_{d,int}$ (nM)	4.6	1.2	ND	1.6	3.8	ND	0.75	1.5	ND	1.5	8.0	ND
		ΔG_{int} (kJ mol^{-1})	-49.5	-53.0	ND	-52.2	-50.0	ND	-54.1	-52.3	ND	-52.3	-48.0	ND
107		$K_{d,obs}$ (nM)	6700	1700	ND	5000	1100	6700	ND	4000	ND	3300	1400	ND
		ΔG_{obs} (kJ mol^{-1})	-30.7	-34.3	ND	-31.5	-35.3	-30.7	ND	-32.0	ND	-32.5	-34.7	ND
E11-75		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
108		$K_{d,obs}$ (nM)	5000	1000	ND	6700	2500	6700	ND	1700	ND	5900	770	ND
		ΔG_{obs} (kJ mol^{-1})	-31.5	-35.6	ND	-30.7	-33.2	-30.7	ND	-34.3	ND	-31.0	-36.3	ND
E11-73		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
109		$K_{d,obs}$ (nM)	71	140	ND	2500	670	4000	3300	560	ND	710	190	ND
		ΔG_{obs} (kJ mol^{-1})	-42.4	-40.6	ND	-33.2	-36.7	-32.0	-32.5	-37.1	ND	-36.5	-40.0	ND
E11-57		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
110		$K_{d,obs}$ (nM)	590	910	ND	830	400	5000	ND	3300	ND	910	2000	ND
		ΔG_{obs} (kJ mol^{-1})	-37.0	-35.9	ND	-36.1	-38.0	-31.5	ND	-32.5	ND	-35.9	-33.8	ND
E11-31		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
111		$K_{d,obs}$ (nM)	3300	1100	ND	1700	170	5000	ND	1400	ND	3300	2900	ND
		ΔG_{obs} (kJ mol^{-1})	-32.5	-35.3	ND	-34.3	-40.2	-31.5	ND	-34.7	ND	-32.5	-32.9	ND
E11-33		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

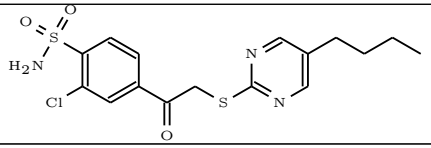
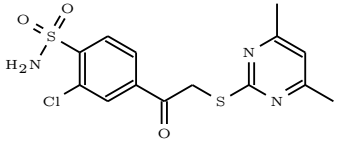
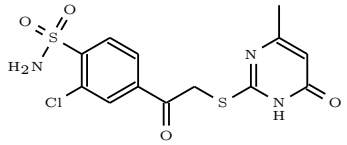
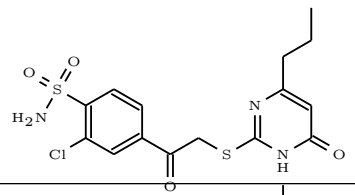
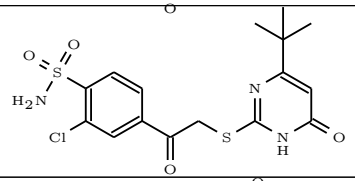
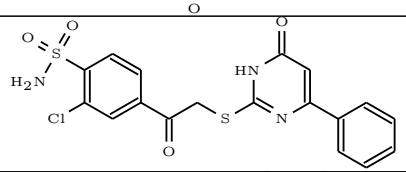
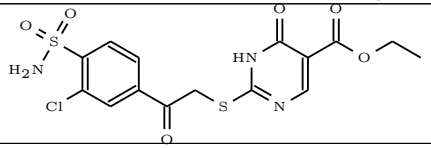
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
112		$K_{d,obs}$ (nM)	2500	1000	ND	3300	1000	20 000	ND	2900	ND	2500	1400	ND
		ΔG_{obs} (kJ mol^{-1})	-33.2	-35.6	ND	-32.5	-35.6	-27.9	ND	-32.9	ND	-33.2	-34.7	ND
E11-35		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
113		$K_{d,obs}$ (nM)	2000	1000	ND	2300	290	6700	ND	3000	ND	1000	670	ND
		ΔG_{obs} (kJ mol^{-1})	-33.8	-35.6	ND	-33.5	-38.8	-30.7	ND	-32.7	ND	-35.6	-36.7	ND
E11-61		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
114		$K_{d,obs}$ (nM)	4300	3600	≥200 000	1600	25	10 000	6700	6700	670	13 000	2400	1700
		ΔG_{obs} (kJ mol^{-1})	-31.8	-32.3	≥-22.0	-34.4	-45.1	-29.7	-30.7	-30.7	-36.7	-29.1	-33.4	-34.3
E11-37		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
115		$K_{d,obs}$ (nM)	9100	7700	≥200 000	13 000	100 000	2800	67 000	17 000	230	17 000	2000	2000
		ΔG_{obs} (kJ mol^{-1})	-29.9	-30.3	≥-22.0	-29.1	-23.7	-33.0	-24.8	-28.4	-39.4	-28.4	-33.8	-33.8
E11-39		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
116		$K_{d,obs}$ (nM)	4800	7700	≥200 000	1500	100 000	≥200 000	≥200 000	25 000	310	14 000	3300	2000
		ΔG_{obs} (kJ mol^{-1})	-31.6	-30.3	≥-22.0	-34.5	-23.7	≥-22.0	≥-22.0	-27.3	-38.6	-28.8	-32.5	-33.8
E11-41		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
117		$K_{d,obs}$ (nM)	1000	6700	≥200 000	37 000	100 000	≥200 000	25 000	25 000	120	11 000	1000	1200
		ΔG_{obs} (kJ mol^{-1})	-35.6	-30.7	≥-22.0	-26.3	-23.7	≥-22.0	-27.3	-27.3	-41.0	-29.4	-35.6	-35.0
E11-43		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

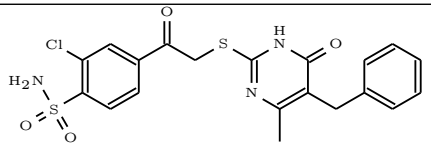
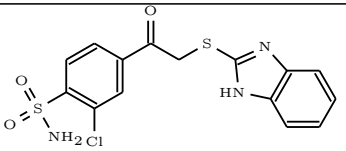
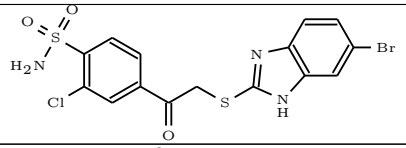
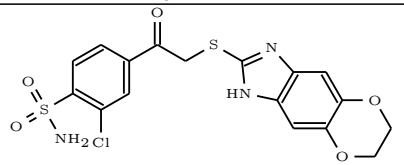
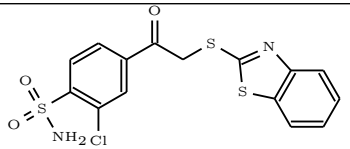
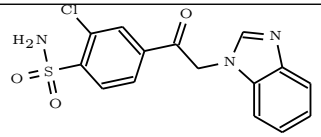
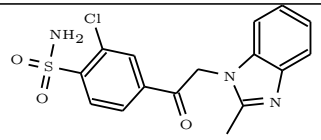
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
118		$K_{d,obs}$ (nM)	670	2900	≥200 000	1700	100 000	100 000	100 000	25 000	500	11 000	670	1000
		ΔG_{obs} (kJ mol^{-1})	-36.7	-32.9	≥-22.0	-34.3	-23.7	-23.7	-23.7	-27.3	-37.4	-29.4	-36.7	-35.6
E11-45		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
119		$K_{d,obs}$ (nM)	2500	17 000	≥200 000	720	100 000	6700	30 000	100 000	190	20 000	1600	1300
		ΔG_{obs} (kJ mol^{-1})	-33.2	-28.4	≥-22.0	-36.5	-23.7	-30.7	-26.8	-23.7	-39.9	-27.9	-34.4	-35.0
E11-47		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
120		$K_{d,obs}$ (nM)	130	5000	≥200 000	500	100 000	6700	ND	25 000	160	8300	1400	770
		ΔG_{obs} (kJ mol^{-1})	-41.0	-31.5	≥-22.0	-37.4	-23.7	-30.7	ND	-27.3	-40.3	-30.1	-34.7	-36.3
E11-49		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
121		$K_{d,obs}$ (nM)	5000	4000	≥200 000	1000	830	6700	25 000	5700	380	13 000	2000	1900
		ΔG_{obs} (kJ mol^{-1})	-31.5	-32.0	≥-22.0	-35.6	-36.1	-30.7	-27.3	-31.1	-38.1	-29.1	-33.8	-33.9
E11-51		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
122		$K_{d,obs}$ (nM)	2500	1700	≥200 000	2200	5900	5000	10 000	13 000	120	5000	1100	910
		ΔG_{obs} (kJ mol^{-1})	-33.2	-34.3	≥-22.0	-33.5	-31.0	-31.5	-29.7	-29.1	-41.1	-31.5	-35.3	-35.9
E11-53		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

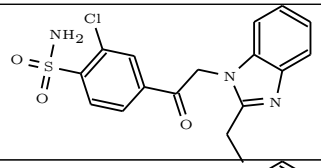
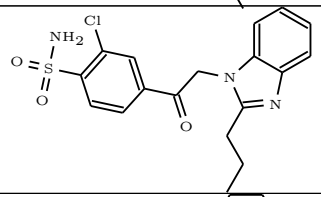
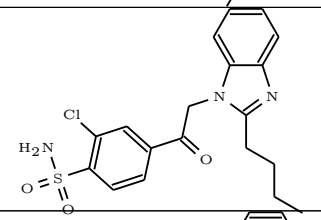
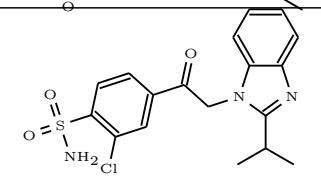
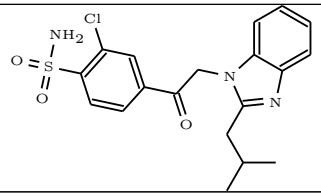
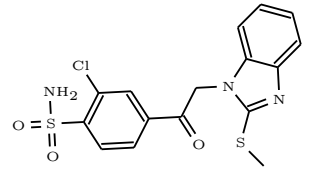
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
123		$K_{d,obs}$ (nM)	1700	3400	≥200 000	960	100 000	3300	22 000	25 000	91	5000	830	1100
		ΔG_{obs} (kJ mol^{-1})	-34.3	-32.4	≥-22.0	-35.7	-23.7	-32.5	-27.6	-27.3	-41.8	-31.5	-36.1	-35.3
E11-55		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
124		$K_{d,obs}$ (nM)	580	640	ND	ND	ND	ND	ND	6500	ND	2400	1100	ND
		ΔG_{obs} (kJ mol^{-1})	-37.0	-36.8	ND	ND	ND	ND	ND	-30.8	ND	-33.4	-35.5	ND
VD90		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
125		$K_{d,obs}$ (nM)	190	88	ND	ND	ND	ND	ND	1300	ND	910	260	ND
		ΔG_{obs} (kJ mol^{-1})	-39.9	-41.9	ND	ND	ND	ND	ND	-34.9	ND	-35.9	-39.1	ND
VD94		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
126		$K_{d,obs}$ (nM)	1400	380	ND	ND	ND	ND	ND	2400	ND	3600	1400	ND
		ΔG_{obs} (kJ mol^{-1})	-34.7	-38.1	ND	ND	ND	ND	ND	-33.3	ND	-32.3	-34.8	ND
VD65		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
127		$K_{d,obs}$ (nM)	150	1300	ND	ND	ND	ND	ND	8500	ND	3200	2700	ND
		ΔG_{obs} (kJ mol^{-1})	-40.6	-34.8	ND	ND	ND	ND	ND	-30.1	ND	-32.6	-33.1	ND
VD20		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
128		$K_{d,obs}$ (nM)	240	470	ND	ND	ND	ND	ND	2400	ND	ND	3500	ND
		ΔG_{obs} (kJ mol^{-1})	-39.2	-37.6	ND	ND	ND	ND	ND	-33.3	ND	ND	-32.4	ND
VD70		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
129		$K_{d,obs}$ (nM)	3100	110	ND	ND	ND	ND	ND	350	ND	2300	400	ND
		ΔG_{obs} (kJ mol^{-1})	-32.7	-41.2	ND	ND	ND	ND	ND	-38.3	ND	-33.4	-38.0	ND
VD78		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
130		$K_{d,obs}$ (nM)	420	1500	ND	ND	ND	ND	ND	6700	ND	50 000	1100	ND
		ΔG_{obs} (kJ mol^{-1})	-37.8	-34.6	ND	ND	ND	ND	ND	-30.7	ND	-25.5	-35.4	ND
VD80		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

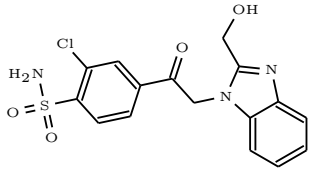
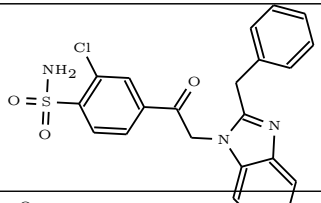
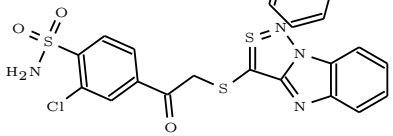
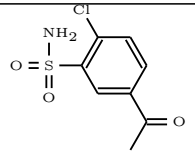
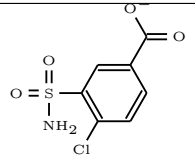
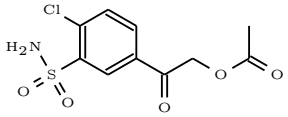
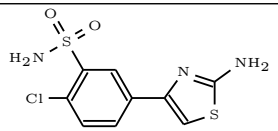
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
131		$K_{d,obs}$ (nM)	8800	8200	ND	ND	ND	ND	ND	≥200 000	ND	25 000	110 000	ND
		ΔG_{obs} (kJ mol^{-1})	-30.0	-30.2	ND	ND	ND	ND	ND	≥-22.0	ND	-27.3	-23.5	ND
VD81		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
132		$K_{d,obs}$ (nM)	100	50	ND	ND	ND	ND	ND	410	ND	2000	360	ND
		ΔG_{obs} (kJ mol^{-1})	-41.5	-43.3	ND	ND	ND	ND	ND	-37.9	ND	-33.8	-38.3	ND
VD9		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
Chlorinated compounds														
133		$K_{d,obs}$ (nM)	33	100	ND	ND	200	ND	1000	22	130	560	17	29
		ΔG_{obs} (kJ mol^{-1})	-44.4	-41.5	ND	ND	-39.8	ND	-35.6	-45.4	-40.9	-37.1	-46.2	-44.7
VD13-03		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
134		$K_{d,obs}$ (nM)	100	170	ND	1900	1100	ND	ND	170	ND	1700	200	ND
		ΔG_{obs} (kJ mol^{-1})	-41.5	-40.2	ND	-34.0	-35.3	ND	ND	-40.2	ND	-34.3	-39.8	ND
E11-2		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
135		$K_{d,obs}$ (nM)	100	290	≥200 000	1200	3300	4200	11 000	670	560	2000	530	180
		ΔG_{obs} (kJ mol^{-1})	-41.5	-38.8	≥-22.0	-35.0	-32.5	-31.9	-29.4	-36.7	-37.1	-33.8	-37.3	-40.0
E11-62		$K_{d,int}$ (nM)	0.34	0.46	170	1.3	8.0	7.5	3.7	0.93	0.57	2.8	1.7	0.25
		ΔG_{int} (kJ mol^{-1})	-56.2	-55.4	-40.1	-52.8	-48.0	-48.2	-50.1	-53.6	-54.8	-50.8	-52.0	-56.9
136		$K_{d,obs}$ (nM)	17	100	≥200 000	1400	1200	1400	17 000	150	250	500	77	91
		ΔG_{obs} (kJ mol^{-1})	-46.2	-41.5	≥-22.0	-34.7	-35.0	-34.7	-28.4	-40.4	-39.2	-37.4	-42.2	-41.8
E11-64		$K_{d,int}$ (nM)	0.056	0.16	170	1.5	3.0	2.6	5.5	0.22	0.26	0.70	0.25	0.13
		ΔG_{int} (kJ mol^{-1})	-60.8	-58.1	-40.1	-52.4	-50.6	-51.0	-49.0	-57.4	-56.9	-54.3	-57.0	-58.7
137		$K_{d,obs}$ (nM)	50	250	170 000	1100	3300	1200	50 000	250	140	2000	33	130
		ΔG_{obs} (kJ mol^{-1})	-43.3	-39.2	-22.4	-35.3	-32.5	-35.0	-25.5	-39.2	-40.6	-33.8	-44.4	-41.0
E11-66		$K_{d,int}$ (nM)	0.17	0.40	140	1.1	8.0	2.3	16	0.35	0.15	2.8	0.11	0.17
		ΔG_{int} (kJ mol^{-1})	-58.0	-55.8	-40.6	-53.1	-48.0	-51.3	-46.2	-56.1	-58.3	-50.8	-59.1	-57.9
138		$K_{d,obs}$ (nM)	1.8	8.3	ND	420	130	2000	ND	7.7	ND	230	1.9	ND
		ΔG_{obs} (kJ mol^{-1})	-51.9	-47.9	ND	-37.9	-40.8	-33.8	ND	-48.2	ND	-39.4	-51.8	ND
E11-68		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

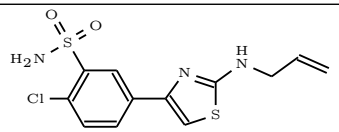
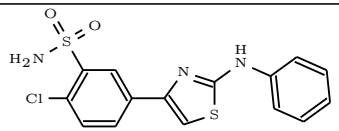
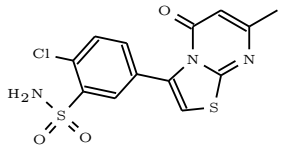
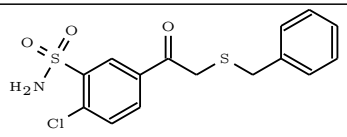
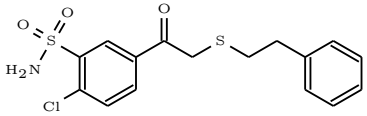
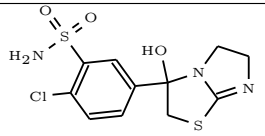
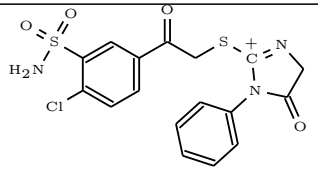
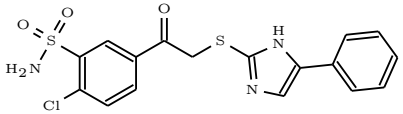
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
139		$K_{d,obs}$ (nM)	33	13	ND	670	770	1000	ND	11	ND	250	6.7	ND
		ΔG_{obs} (kJ mol^{-1})	-44.4	-46.9	ND	-36.7	-36.3	-35.6	ND	-47.2	ND	-39.2	-48.5	ND
E11-74		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
140		$K_{d,obs}$ (nM)	67	33	ND	1700	290	2500	ND	25	ND	3300	10	ND
		ΔG_{obs} (kJ mol^{-1})	-42.6	-44.4	ND	-34.2	-38.8	-33.2	ND	-45.1	ND	-32.5	-47.5	ND
E11-72		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
141		$K_{d,obs}$ (nM)	10	11	ND	910	360	ND	2500	5.0	200	830	17	ND
		ΔG_{obs} (kJ mol^{-1})	-47.5	-47.2	ND	-35.8	-38.3	ND	-33.2	-49.3	-39.8	-36.1	-46.2	ND
E11-8		$K_{d,int}$ (nM)	0.12	0.061	ND	3.2	3.0	ND	2.8	0.024	0.70	4.0	0.19	ND
		ΔG_{int} (kJ mol^{-1})	-59.0	-60.6	ND	-50.4	-50.6	ND	-50.7	-63.0	-54.3	-49.8	-57.7	ND
142		$K_{d,obs}$ (nM)	1.0	5.6	ND	38	130	ND	1100	2.9	ND	71	5.0	ND
		ΔG_{obs} (kJ mol^{-1})	-53.4	-49.0	ND	-44.0	-41.0	ND	-35.3	-50.7	ND	-42.4	-49.3	ND
E11-6		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
143		$K_{d,obs}$ (nM)	1.4	10	ND	130	250	500	ND	7.7	ND	130	7.7	ND
		ΔG_{obs} (kJ mol^{-1})	-52.5	-47.5	ND	-41.0	-39.2	-37.4	ND	-48.2	ND	-40.8	-48.2	ND
E11-70		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
144		$K_{d,obs}$ (nM)	6.7	8.5	ND	620	400	1500	5000	10	ND	440	2.1	ND
		ΔG_{obs} (kJ mol^{-1})	-48.5	-47.9	ND	-36.8	-38.0	-34.5	-31.5	-47.5	ND	-37.7	-51.5	ND
E11-12		$K_{d,int}$ (nM)	0.077	0.047	ND	2.2	3.3	9.6	5.7	0.048	ND	2.1	0.024	ND
		ΔG_{int} (kJ mol^{-1})	-60.0	-61.3	ND	-51.4	-50.3	-47.6	-48.9	-61.2	ND	-51.5	-63.1	ND
145		$K_{d,obs}$ (nM)	5.3	7.1	ND	480	330	1800	3300	17	ND	590	1.2	ND
		ΔG_{obs} (kJ mol^{-1})	-49.1	-48.3	ND	-37.5	-38.4	-34.1	-32.5	-46.2	ND	-37.0	-52.8	ND
E11-14		$K_{d,int}$ (nM)	0.061	0.039	ND	1.7	2.8	11	3.8	0.080	ND	2.8	0.014	ND
		ΔG_{int} (kJ mol^{-1})	-60.6	-61.8	ND	-52.1	-50.8	-47.2	-50.0	-59.9	ND	-50.7	-64.4	ND

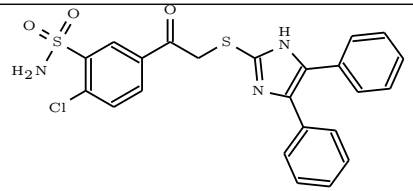
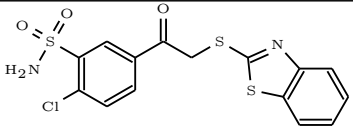
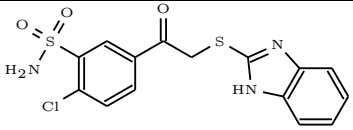
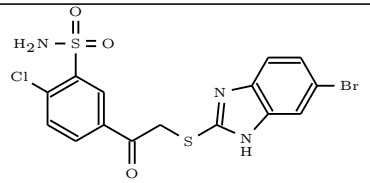
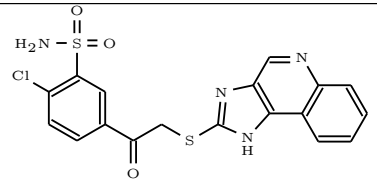
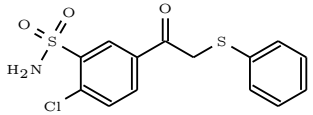
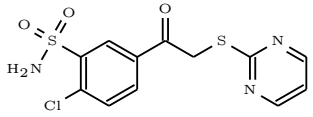
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
146		$K_{d,obs}$ (nM)	6.2	7.7	ND	400	330	1700	3300	11	ND	360	1.8	ND
		ΔG_{obs} (kJ mol^{-1})	-48.7	-48.2	ND	-38.0	-38.4	-34.3	-32.5	-47.2	ND	-38.3	-51.9	ND
E11-16		$K_{d,int}$ (nM)	0.072	0.042	ND	1.4	2.8	10	3.8	0.053	ND	1.7	0.021	ND
		ΔG_{int} (kJ mol^{-1})	-60.2	-61.6	ND	-52.5	-50.8	-47.4	-50.0	-61.0	ND	-52.0	-63.4	ND
147		$K_{d,obs}$ (nM)	5.0	17	ND	1300	770	ND	2900	13	ND	910	10	ND
		ΔG_{obs} (kJ mol^{-1})	-49.3	-46.2	ND	-34.9	-36.3	ND	-32.9	-46.9	ND	-35.9	-47.5	ND
E11-10		$K_{d,int}$ (nM)	0.058	0.092	ND	4.7	6.4	ND	3.2	0.060	ND	4.4	0.11	ND
		ΔG_{int} (kJ mol^{-1})	-60.8	-59.6	ND	-49.4	-48.6	ND	-50.4	-60.7	ND	-49.6	-59.0	ND
148		$K_{d,obs}$ (nM)	6.7	28	ND	560	200	3300	2500	36	ND	330	33	ND
		ΔG_{obs} (kJ mol^{-1})	-48.5	-44.9	ND	-37.1	-39.8	-32.5	-33.2	-44.2	ND	-38.4	-44.4	ND
E11-18		$K_{d,int}$ (nM)	0.077	0.15	ND	2.0	1.7	21	2.8	0.17	ND	1.6	0.38	ND
		ΔG_{int} (kJ mol^{-1})	-60.0	-58.3	ND	-51.7	-52.1	-45.6	-50.7	-58.0	ND	-52.2	-55.9	ND
149		$K_{d,obs}$ (nM)	10	110	ND	1200	290	5000	4500	50	ND	200	83	ND
		ΔG_{obs} (kJ mol^{-1})	-47.5	-41.3	ND	-35.0	-38.8	-31.5	-31.7	-43.3	ND	-39.8	-42.0	ND
E11-24		$K_{d,int}$ (nM)	0.12	0.61	ND	4.4	2.4	31	5.1	0.24	ND	0.96	0.94	ND
		ΔG_{int} (kJ mol^{-1})	-59.0	-54.7	ND	-49.6	-51.2	-44.6	-49.2	-57.1	ND	-53.5	-53.6	ND
150		$K_{d,obs}$ (nM)	0.35	26	ND	1200	50	250	9100	7.5	ND	250	1.2	ND
		ΔG_{obs} (kJ mol^{-1})	-56.1	-45.0	ND	-35.0	-43.3	-39.2	-29.9	-48.2	ND	-39.2	-53.0	ND
E11-26		$K_{d,int}$ (nM)	0.0041	0.15	ND	4.4	0.41	1.6	10	0.036	ND	1.2	0.013	ND
		ΔG_{int} (kJ mol^{-1})	-67.6	-58.4	ND	-49.6	-55.7	-52.3	-47.4	-62.0	ND	-52.9	-64.5	ND
151		$K_{d,obs}$ (nM)	98	110	ND	18 000	7700	100 000	ND	22	ND	320	15	ND
		ΔG_{obs} (kJ mol^{-1})	-41.6	-41.3	ND	-28.2	-30.3	-23.7	ND	-45.4	ND	-38.6	-46.4	ND
E11-28		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
152		$K_{d,obs}$ (nM)	14	20	ND	590	170	ND	2900	25	ND	250	77	ND
		ΔG_{obs} (kJ mol^{-1})	-46.6	-45.7	ND	-37.0	-40.2	ND	-32.9	-45.1	ND	-39.2	-42.2	ND
E11-22		$K_{d,int}$ (nM)	0.16	0.11	ND	2.1	1.4	ND	3.2	0.12	ND	1.2	0.87	ND
		ΔG_{int} (kJ mol^{-1})	-58.1	-59.1	ND	-51.5	-52.6	ND	-50.4	-58.9	ND	-52.9	-53.8	ND

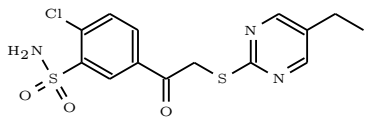
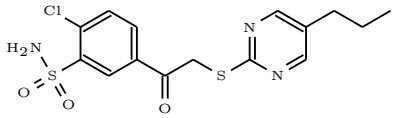
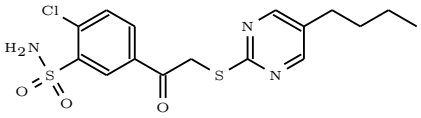
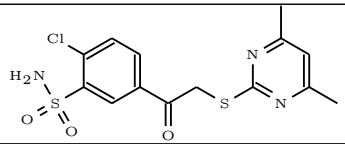
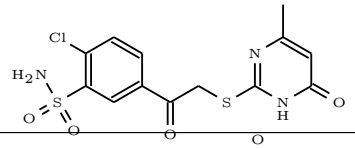
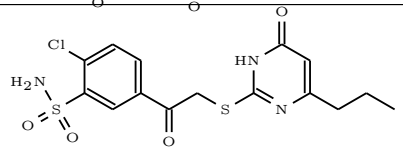
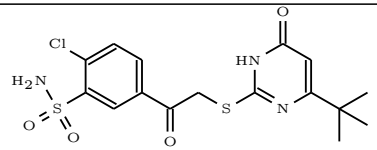
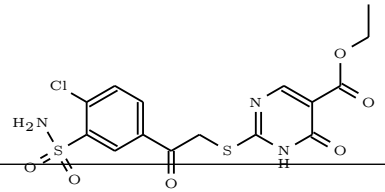
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
153		$K_{d,obs}$ (nM)	20	67	ND	710	200	500	1900	100	ND	910	25	ND
		ΔG_{obs} (kJ mol^{-1})	-45.7	-42.6	ND	-36.5	-39.8	-37.4	-34.0	-41.5	ND	-35.9	-45.1	ND
E11-20		$K_{d,int}$ (nM)	0.23	0.37	ND	2.5	1.7	3.1	2.1	0.48	ND	4.4	0.28	ND
		ΔG_{int} (kJ mol^{-1})	-57.2	-56.0	ND	-51.0	-52.1	-50.5	-51.5	-55.3	ND	-49.6	-56.7	ND
154		$K_{d,obs}$ (nM)	6.7	33	ND	150	1000	ND	ND	11	ND	330	27	ND
		ΔG_{obs} (kJ mol^{-1})	-48.5	-44.4	ND	-40.4	-35.6	ND	ND	-47.2	ND	-38.4	-44.9	ND
E11-30		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
155		$K_{d,obs}$ (nM)	17	20	ND	370	400	ND	ND	5.0	ND	380	11	ND
		ΔG_{obs} (kJ mol^{-1})	-46.2	-45.7	ND	-38.2	-38.0	ND	ND	-49.3	ND	-38.1	-47.2	ND
E11-32		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
156		$K_{d,obs}$ (nM)	33	33	ND	1000	500	3300	ND	14	ND	1000	33	ND
		ΔG_{obs} (kJ mol^{-1})	-44.4	-44.4	ND	-35.6	-37.4	-32.5	ND	-46.6	ND	-35.6	-44.4	ND
E11-34		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
157		$K_{d,obs}$ (nM)	4.5	3.3	ND	710	2500	1000	ND	2.5	ND	500	2.0	ND
		ΔG_{obs} (kJ mol^{-1})	-49.5	-50.3	ND	-36.5	-33.2	-35.6	ND	-51.0	ND	-37.4	-51.6	ND
E11-56		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
158		$K_{d,obs}$ (nM)	12	8.3	25 000	1700	1000	1200	3300	4.0	59	830	19	14
		ΔG_{obs} (kJ mol^{-1})	-47.1	-47.9	-27.3	-34.3	-35.6	-35.0	-32.5	-49.8	-42.9	-36.1	-45.8	-46.6
E11-36		$K_{d,int}$ (nM)	0.49	0.16	270	21	30	28	14	0.069	0.75	14	0.78	0.25
		ΔG_{int} (kJ mol^{-1})	-55.3	-58.1	-39.0	-45.5	-44.7	-44.8	-46.7	-60.3	-54.2	-46.5	-54.0	-57.0
159		$K_{d,obs}$ (nM)	5.9	11	110 000	1100	1400	770	2800	11	63	200	23	24
		ΔG_{obs} (kJ mol^{-1})	-48.8	-47.3	-23.5	-35.3	-34.7	-36.3	-33.0	-47.2	-42.8	-39.8	-45.3	-45.2
E11-38		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

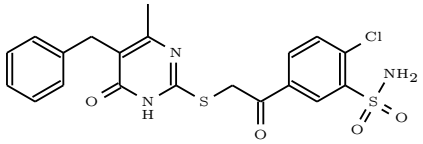
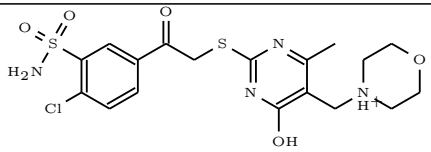
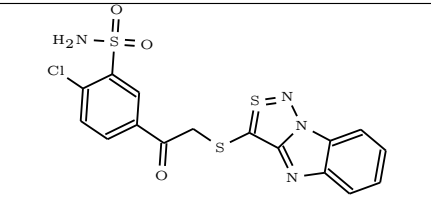
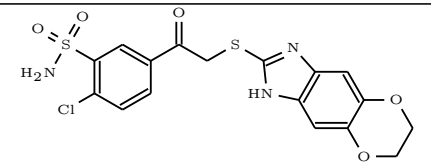
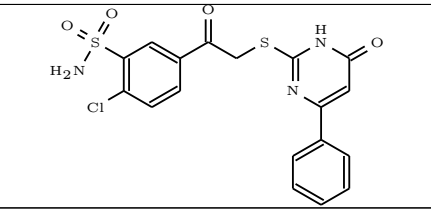
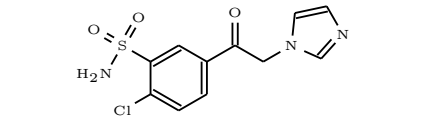
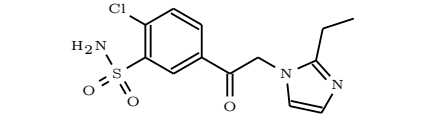
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
160		$K_{d,obs}$ (nM)	4.8	6.2	≥200 000	930	500	1000	2300	7.7	8.3	67	11	7.7
		ΔG_{obs} (kJ mol^{-1})	-49.4	-48.7	≥-22.0	-35.8	-37.4	-35.6	-33.5	-48.2	-47.9	-42.6	-47.1	-48.2
E11-40		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
161		$K_{d,obs}$ (nM)	2.9	3.6	≥200 000	1400	1700	1200	22 000	4.2	14	63	5.6	5.6
		ΔG_{obs} (kJ mol^{-1})	-50.7	-50.1	≥-22.0	-34.7	-34.3	-35.0	-27.6	-49.7	-46.6	-42.8	-49.0	-49.0
E11-42		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
162		$K_{d,obs}$ (nM)	3.3	2.7	130 000	1100	830	670	5000	3.3	10	110	2.5	5.0
		ΔG_{obs} (kJ mol^{-1})	-50.3	-50.8	-23.2	-35.3	-36.1	-36.7	-31.5	-50.3	-47.4	-41.2	-51.0	-49.3
E11-44		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
163		$K_{d,obs}$ (nM)	5.0	14	≥200 000	960	670	1100	5600	5.0	9.1	330	40	5.0
		ΔG_{obs} (kJ mol^{-1})	-49.3	-46.6	≥-22.0	-35.7	-36.7	-35.3	-31.2	-49.3	-47.7	-38.4	-43.9	-49.3
E11-46		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
164		$K_{d,obs}$ (nM)	6.7	14	≥200 000	1000	1000	710	4000	5.0	3.9	500	40	2.4
		ΔG_{obs} (kJ mol^{-1})	-48.5	-46.6	≥-22.0	-35.5	-35.6	-36.5	-32.0	-49.3	-49.9	-37.4	-43.9	-51.2
E11-48		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
165		$K_{d,obs}$ (nM)	1.7	3.3	≥200 000	950	500	500	23 000	4.5	13	67	9.1	12
		ΔG_{obs} (kJ mol^{-1})	-52.1	-50.3	≥-22.0	-35.7	-37.4	-37.4	-27.6	-49.5	-46.9	-42.6	-47.7	-47.1
E11-54		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

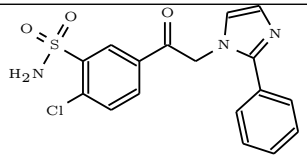
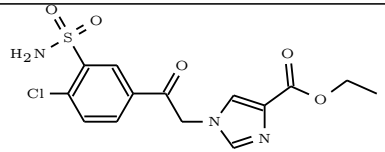
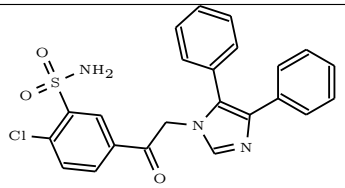
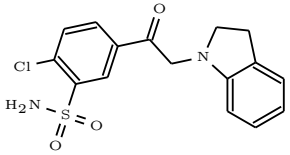
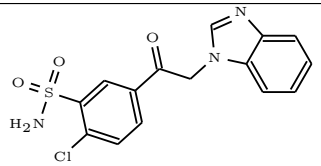
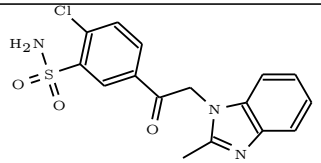
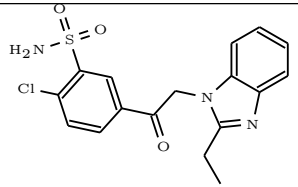
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
166		$K_{d,obs}$ (nM)	10	14	33 000	1300	250	670	3100	5.0	25	1000	67	22
		ΔG_{obs} (kJ mol^{-1})	-47.5	-46.6	-26.6	-34.9	-39.2	-36.7	-32.7	-49.3	-45.1	-35.6	-42.6	-45.4
E11-50		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
167		$K_{d,obs}$ (nM)	8.3	2.9	≥200 000	980	1000	5000	1400	8.3	71	170	6.7	10
		ΔG_{obs} (kJ mol^{-1})	-47.9	-50.7	≥-22.0	-35.7	-35.6	-31.5	-34.7	-47.9	-42.4	-40.2	-48.5	-47.4
E11-52		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
168		$K_{d,obs}$ (nM)	67	250	ND	180	1000	13 000	3300	650	ND	3000	500	ND
		ΔG_{obs} (kJ mol^{-1})	-42.6	-39.2	ND	-40.0	-35.6	-29.1	-32.5	-36.7	ND	-32.7	-37.4	ND
E11-60		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
169		$K_{d,obs}$ (nM)	17 000	710	ND	360	770	100	ND	830	ND	ND	200	ND
		ΔG_{obs} (kJ mol^{-1})	-28.4	-36.5	ND	-38.3	-36.3	-41.5	ND	-36.1	ND	ND	-39.8	ND
E16		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
170		$K_{d,obs}$ (nM)	20 000	1200	ND	1000	ND	ND	ND	1000	ND	1200	280	ND
		ΔG_{obs} (kJ mol^{-1})	-27.9	-35.0	ND	-35.6	ND	ND	ND	-35.6	ND	-35.0	-38.9	ND
E17		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
171		$K_{d,obs}$ (nM)	10 000	500	ND	670	140	3300	67 000	330	ND	ND	220	ND
		ΔG_{obs} (kJ mol^{-1})	-29.7	-37.4	ND	-36.7	-40.6	-32.5	-24.8	-38.4	ND	ND	-39.5	ND
E39		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
172		$K_{d,obs}$ (nM)	17 000	670	≥200 000	670	5000	2000	1400	200	710	1100	560	220
		ΔG_{obs} (kJ mol^{-1})	-28.4	-36.7	≥-22.0	-36.7	-31.5	-33.8	-34.7	-39.8	-36.5	-35.3	-37.1	-39.5
E35		$K_{d,int}$ (nM)	72	1.4	220	0.88	16	4.7	0.60	0.36	0.95	2.0	2.4	0.40
		ΔG_{int} (kJ mol^{-1})	-42.4	-52.6	-39.5	-53.7	-46.3	-49.4	-54.7	-56.0	-53.6	-51.6	-51.2	-55.8

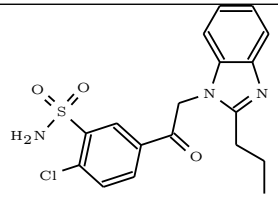
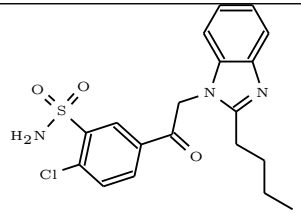
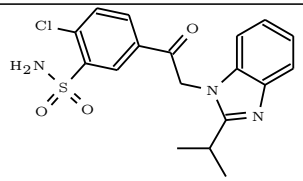
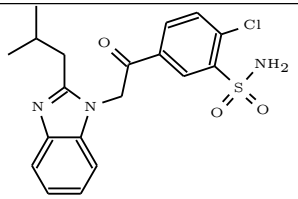
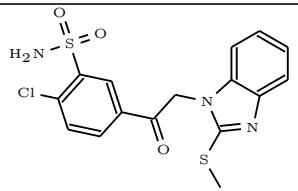
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
173		$K_{d,obs}$ (nM)	2200	670	170 000	200	1000	1700	22 000	170	360	1700	200	150
		ΔG_{obs} (kJ mol^{-1})	-33.5	-36.7	-22.4	-39.8	-35.6	-34.3	-27.6	-40.2	-38.3	-34.3	-39.8	-40.4
E42		$K_{d,int}$ (nM)	9.6	1.4	190	0.27	3.1	3.9	9.4	0.30	0.47	3.0	0.85	0.28
		ΔG_{int} (kJ mol^{-1})	-47.6	-52.6	-39.9	-56.8	-50.5	-49.9	-47.6	-56.5	-55.3	-50.6	-53.8	-56.7
174		$K_{d,obs}$ (nM)	1400	670	≥200 000	500	20 000	1800	25 000	1400	2200	5800	250	1200
		ΔG_{obs} (kJ mol^{-1})	-34.7	-36.7	≥-22.0	-37.4	-27.9	-34.1	-27.3	-34.7	-33.5	-31.1	-39.2	-35.0
E43		$K_{d,int}$ (nM)	6.2	1.4	220	0.66	62	4.2	11	2.6	2.9	10	1.1	2.3
		ΔG_{int} (kJ mol^{-1})	-48.7	-52.6	-39.5	-54.5	-42.8	-49.7	-47.3	-51.0	-50.6	-47.4	-53.3	-51.3
175		$K_{d,obs}$ (nM)	14 000	1800	ND	ND	ND	ND	ND	3300	ND	4000	4000	ND
		ΔG_{obs} (kJ mol^{-1})	-28.8	-34.1	ND	ND	ND	ND	ND	-32.5	ND	-32.0	-32.0	ND
E32C		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
176		$K_{d,obs}$ (nM)	500	130	ND	670	220	500	ND	150	ND	830	150	ND
		ΔG_{obs} (kJ mol^{-1})	-37.4	-40.8	ND	-36.7	-39.5	-37.4	ND	-40.5	ND	-36.1	-40.5	ND
E98		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
177		$K_{d,obs}$ (nM)	400	180	ND	1000	130	500	ND	170	ND	1200	71	ND
		ΔG_{obs} (kJ mol^{-1})	-38.0	-40.0	ND	-35.6	-41.0	-37.4	ND	-40.2	ND	-35.0	-42.4	ND
E96		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
178		$K_{d,obs}$ (nM)	2000	130	ND	100	1100	2200	2300	170	ND	290	260	ND
		ΔG_{obs} (kJ mol^{-1})	-33.8	-41.0	ND	-41.5	-35.3	-33.5	-33.5	-40.2	ND	-38.8	-39.0	ND
E40		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
179		$K_{d,obs}$ (nM)	12	170	ND	2200	500	4000	ND	400	ND	ND	710	ND
		ΔG_{obs} (kJ mol^{-1})	-47.1	-40.2	ND	-33.5	-37.4	-32.0	ND	-38.0	ND	ND	-36.5	ND
E58		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
180		$K_{d,obs}$ (nM)	11 000	3300	ND	ND	ND	ND	ND	10 000	ND	1000	91	ND
		ΔG_{obs} (kJ mol^{-1})	-29.4	-32.5	ND	ND	ND	ND	ND	-29.7	ND	-35.6	-41.8	ND
AR2		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

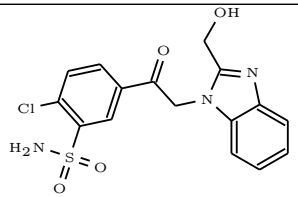
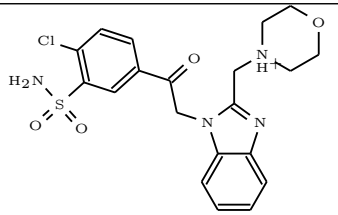
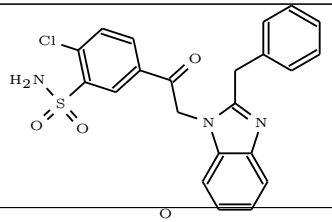
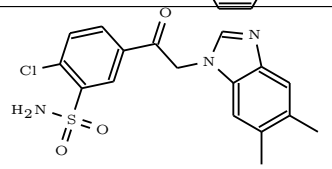
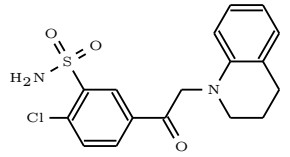
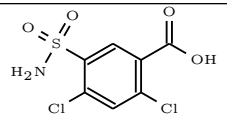
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
181		$K_{d,obs}$ (nM)	6700	67	ND	ND	ND	ND	ND	91	ND	1800	140	ND
		ΔG_{obs} (kJ mol^{-1})	-30.7	-42.6	ND	ND	ND	ND	ND	-41.8	ND	-34.1	-40.6	ND
AR1		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
182		$K_{d,obs}$ (nM)	1200	290	ND	2900	42	13 000	ND	4100	ND	1400	10 000	ND
		ΔG_{obs} (kJ mol^{-1})	-35.1	-38.8	ND	-32.9	-43.8	-29.1	ND	-32.0	ND	-34.7	-29.7	ND
E31		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
183		$K_{d,obs}$ (nM)	1000	130	ND	560	13	400	ND	53	ND	500	170	ND
		ΔG_{obs} (kJ mol^{-1})	-35.6	-40.8	ND	-37.1	-46.9	-38.0	ND	-43.2	ND	-37.4	-40.2	ND
E21		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
184		$K_{d,obs}$ (nM)	1200	63	ND	ND	6.7	ND	2800	130	ND	580	56	ND
		ΔG_{obs} (kJ mol^{-1})	-35.0	-42.8	ND	ND	-48.5	ND	-33.0	-41.0	ND	-37.0	-43.0	ND
E38		$K_{d,int}$ (nM)	14	0.34	ND	ND	0.055	ND	3.1	0.60	ND	2.8	0.63	ND
		ΔG_{int} (kJ mol^{-1})	-46.5	-56.2	ND	ND	-60.9	ND	-50.5	-54.7	ND	-50.8	-54.6	ND
185		$K_{d,obs}$ (nM)	1200	33	ND	910	170	ND	ND	ND	ND	1000	33	ND
		ΔG_{obs} (kJ mol^{-1})	-35.0	-44.4	ND	-35.8	-40.2	ND	ND	ND	ND	-35.6	-44.4	ND
E27		$K_{d,int}$ (nM)	14	0.18	ND	3.2	1.4	ND	ND	ND	ND	4.8	0.38	ND
		ΔG_{int} (kJ mol^{-1})	-46.5	-57.8	ND	-50.4	-52.6	ND	ND	ND	ND	-49.4	-55.9	ND
186		$K_{d,obs}$ (nM)	830	250	ND	670	330	1400	23 000	710	ND	400	250	ND
		ΔG_{obs} (kJ mol^{-1})	-36.1	-39.2	ND	-36.7	-38.4	-34.7	-27.6	-36.5	ND	-38.0	-39.2	ND
E54		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
187		$K_{d,obs}$ (nM)	4300	330	ND	590	67	ND	560	710	ND	1400	330	ND
		ΔG_{obs} (kJ mol^{-1})	-31.9	-38.4	ND	-37.0	-42.6	ND	-37.1	-36.5	ND	-34.7	-38.4	ND
E89		$K_{d,int}$ (nM)	55	2.1	ND	2.3	0.62	ND	0.70	3.8	ND	7.8	4.2	ND
		ΔG_{int} (kJ mol^{-1})	-43.1	-51.6	ND	-51.2	-54.6	ND	-54.3	-49.9	ND	-48.1	-49.7	ND

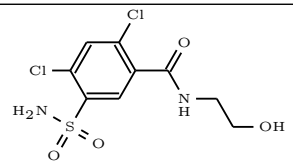
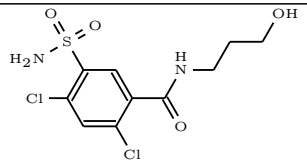
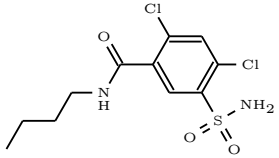
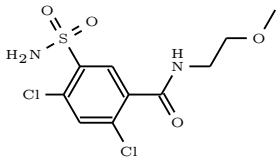
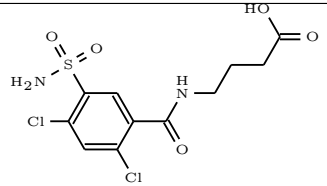
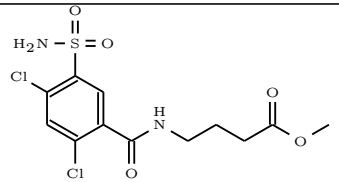
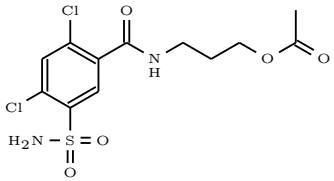
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
188		$K_{d,obs}$ (nM)	1800	140	ND	400	6.2	ND	670	330	ND	1200	110	ND
		ΔG_{obs} (kJ mol^{-1})	-34.1	-40.6	ND	-38.0	-48.7	ND	-36.7	-38.4	ND	-35.0	-41.3	ND
E50		$K_{d,int}$ (nM)	21	0.79	ND	1.4	0.052	ND	0.75	1.6	ND	6.0	1.3	ND
		ΔG_{int} (kJ mol^{-1})	-45.6	-54.0	ND	-52.5	-61.0	ND	-54.1	-52.2	ND	-48.8	-52.8	ND
189		$K_{d,obs}$ (nM)	1300	120	ND	290	5.0	560	1100	220	ND	1100	37	ND
		ΔG_{obs} (kJ mol^{-1})	-34.9	-41.1	ND	-38.8	-49.3	-37.1	-35.3	-39.5	ND	-35.5	-44.1	ND
E45		$K_{d,int}$ (nM)	15	0.66	ND	1.0	0.041	3.5	1.3	1.1	ND	5.1	0.41	ND
		ΔG_{int} (kJ mol^{-1})	-46.5	-54.5	ND	-53.4	-61.6	-50.2	-52.8	-53.2	ND	-49.2	-55.7	ND
190		$K_{d,obs}$ (nM)	1400	67	ND	250	4.0	ND	500	200	ND	1100	67	ND
		ΔG_{obs} (kJ mol^{-1})	-34.7	-42.6	ND	-39.2	-49.8	ND	-37.4	-39.8	ND	-35.3	-42.6	ND
E53		$K_{d,int}$ (nM)	16	0.37	ND	0.89	0.033	ND	0.57	0.96	ND	5.3	0.75	ND
		ΔG_{int} (kJ mol^{-1})	-46.2	-56.0	ND	-53.7	-62.2	ND	-54.9	-53.5	ND	-49.1	-54.1	ND
191		$K_{d,obs}$ (nM)	1000	220	ND	1200	130	1700	1000	330	ND	1400	330	ND
		ΔG_{obs} (kJ mol^{-1})	-35.6	-39.5	ND	-35.0	-41.0	-34.3	-35.6	-38.4	ND	-34.7	-38.4	ND
E49		$K_{d,int}$ (nM)	12	1.2	ND	4.4	1.0	10	1.1	1.6	ND	6.9	3.8	ND
		ΔG_{int} (kJ mol^{-1})	-47.1	-52.9	ND	-49.6	-53.3	-47.4	-53.1	-52.2	ND	-48.4	-50.0	ND
192		$K_{d,obs}$ (nM)	830	200	ND	600	400	2500	1000	180	ND	320	200	ND
		ΔG_{obs} (kJ mol^{-1})	-36.1	-39.8	ND	-36.9	-38.0	-33.2	-35.6	-40.1	ND	-38.6	-39.8	ND
E32		$K_{d,int}$ (nM)	9.6	1.1	ND	2.1	3.3	16	1.1	0.86	ND	1.5	2.3	ND
		ΔG_{int} (kJ mol^{-1})	-47.6	-53.2	ND	-51.5	-50.3	-46.3	-53.1	-53.8	ND	-52.3	-51.3	ND
193		$K_{d,obs}$ (nM)	670	67	ND	170	250	670	830	56	ND	100	56	ND
		ΔG_{obs} (kJ mol^{-1})	-36.7	-42.6	ND	-40.2	-39.2	-36.7	-36.1	-43.1	ND	-41.5	-43.1	ND
E57		$K_{d,int}$ (nM)	7.7	0.37	ND	0.59	2.1	4.1	0.94	0.27	ND	0.48	0.63	ND
		ΔG_{int} (kJ mol^{-1})	-48.2	-56.0	ND	-54.8	-51.5	-49.7	-53.6	-56.8	ND	-55.3	-54.6	ND
194		$K_{d,obs}$ (nM)	100	50	ND	330	290	1800	2000	28	ND	43	25	ND
		ΔG_{obs} (kJ mol^{-1})	-41.5	-43.3	ND	-38.4	-38.8	-34.1	-33.8	-44.8	ND	-43.7	-45.1	ND
E52		$K_{d,int}$ (nM)	1.2	0.28	ND	1.2	2.4	11	2.3	0.14	ND	0.21	0.28	ND
		ΔG_{int} (kJ mol^{-1})	-53.0	-56.7	ND	-53.0	-51.1	-47.2	-51.3	-58.6	ND	-57.4	-56.7	ND
195		$K_{d,obs}$ (nM)	1200	50	ND	ND	100	1200	200	38	ND	200	130	ND
		ΔG_{obs} (kJ mol^{-1})	-35.0	-43.3	ND	ND	-41.5	-35.0	-39.8	-44.0	ND	-39.8	-41.0	ND
E46		$K_{d,int}$ (nM)	14	0.28	ND	ND	0.83	7.8	0.23	0.18	ND	0.96	1.4	ND
		ΔG_{int} (kJ mol^{-1})	-46.5	-56.7	ND	ND	-53.9	-48.1	-57.2	-57.8	ND	-53.5	-52.5	ND

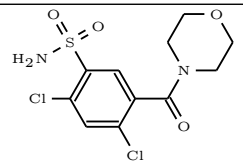
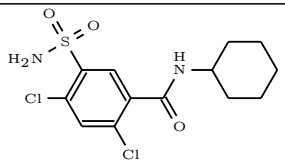
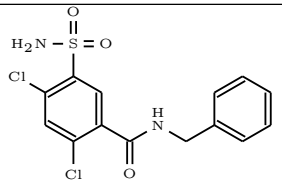
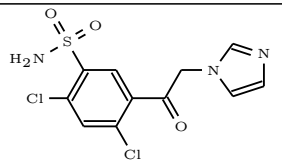
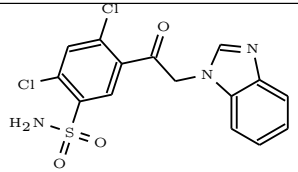
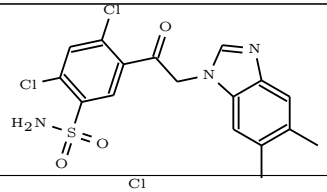
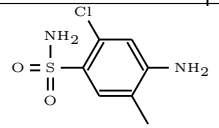
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
196		$K_{d,obs}$ (nM)	450	26	ND	140	110	330	290	130	ND	230	42	ND
		ΔG_{obs} (kJ mol^{-1})	-37.6	-45.0	ND	-40.6	-41.3	-38.4	-38.8	-40.8	ND	-39.4	-43.8	ND
E33		$K_{d,int}$ (nM)	5.2	0.15	ND	0.50	0.92	2.1	0.32	0.64	ND	1.1	0.47	ND
		ΔG_{int} (kJ mol^{-1})	-49.1	-58.4	ND	-55.2	-53.6	-51.5	-56.3	-54.6	ND	-53.2	-55.4	ND
197		$K_{d,obs}$ (nM)	2000	200	ND	120	250	3300	5000	500	ND	1000	330	ND
		ΔG_{obs} (kJ mol^{-1})	-33.8	-39.8	ND	-41.1	-39.2	-32.5	-31.5	-37.4	ND	-35.6	-38.4	ND
E44		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
198		$K_{d,obs}$ (nM)	2700	1200	ND	400	2.5	1200	ND	580	ND	1400	630	ND
		ΔG_{obs} (kJ mol^{-1})	-33.1	-35.2	ND	-38.0	-51.0	-35.0	ND	-37.0	ND	-34.8	-36.8	ND
E56		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
199		$K_{d,obs}$ (nM)	3100	170	ND	ND	6.7	ND	ND	110	ND	910	41	ND
		ΔG_{obs} (kJ mol^{-1})	-32.7	-40.2	ND	ND	-48.5	ND	ND	-41.3	ND	-35.8	-43.9	ND
E36		$K_{d,int}$ (nM)	36	0.92	ND	ND	0.055	ND	ND	0.54	ND	4.4	0.46	ND
		ΔG_{int} (kJ mol^{-1})	-44.2	-53.6	ND	ND	-60.9	ND	ND	-55.0	ND	-49.6	-55.4	ND
200		$K_{d,obs}$ (nM)	5000	26	ND	3300	33 000	ND	ND	170	ND	290	100	ND
		ΔG_{obs} (kJ mol^{-1})	-31.5	-45.0	ND	-32.5	-26.6	ND	ND	-40.2	ND	-38.8	-41.5	ND
E94		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
201		$K_{d,obs}$ (nM)	110 000	1500	≥200 000	83	13	10 000	1200	1200	2000	3000	1300	590
		ΔG_{obs} (kJ mol^{-1})	-23.5	-34.5	≥-22.0	-42.0	-46.7	-29.7	-35.0	-35.2	-33.8	-32.7	-35.0	-37.0
E14-1		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
202		$K_{d,obs}$ (nM)	26 000	1700	≥200 000	11 000	450	3700	4300	2600	1200	2900	620	530
		ΔG_{obs} (kJ mol^{-1})	-27.2	-34.2	≥-22.0	-29.4	-37.6	-32.2	-31.8	-33.1	-35.0	-32.9	-36.8	-37.3
VR15-3		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

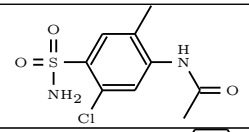
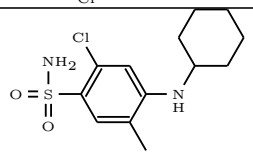
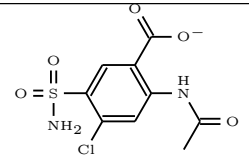
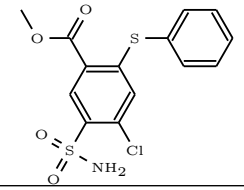
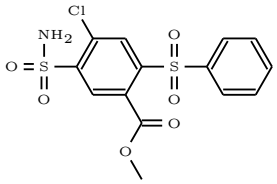
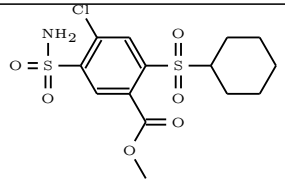
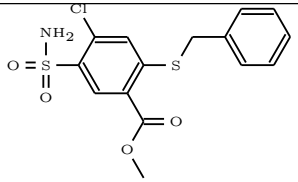
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
203		$K_{d,obs}$ (nM)	ND	ND	50 000	ND	ND	310	ND	ND	670	ND	ND	150
		ΔG_{obs} (kJ mol^{-1})	ND	ND	-25.5	ND	ND	-38.6	ND	ND	-36.7	ND	ND	-40.4
VR15-5		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
204		$K_{d,obs}$ (nM)	31 000	1100	170 000	1400	33	1000	2100	2100	1600	2800	1700	480
		ΔG_{obs} (kJ mol^{-1})	-26.7	-35.3	-22.4	-34.7	-44.4	-35.6	-33.7	-33.7	-34.4	-33.0	-34.2	-37.5
VR15-4		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
205		$K_{d,obs}$ (nM)	≥200 000	20 000	≥200 000	≥200 000	≥200 000	≥200 000	≥200 000	≥200 000	15 000	≥200 000	34 000	17 000
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-27.9	≥-22.0	≥-22.0	≥-22.0	≥-22.0	≥-22.0	≥-22.0	-28.6	≥-22.0	-26.5	-28.4
VR15-6		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
206		$K_{d,obs}$ (nM)	5000	1000	≥200 000	150	1200	830	3800	4200	1000	1700	620	250
		ΔG_{obs} (kJ mol^{-1})	-31.5	-35.6	≥-22.0	-40.4	-35.0	-36.1	-32.1	-31.9	-35.6	-34.3	-36.8	-39.2
AZ15-15		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
207		$K_{d,obs}$ (nM)	11 000	1600	≥200 000	640	0.25	3300	720	1000	770	3100	360	300
		ΔG_{obs} (kJ mol^{-1})	-29.4	-34.5	≥-22.0	-36.8	-57.0	-32.5	-36.5	-35.6	-36.3	-32.7	-38.3	-38.7
E2		$K_{d,int}$ (nM)	130	8.6	600	2.3	0.0021	21	0.81	4.8	2.7	15	4.0	1.5
		ΔG_{int} (kJ mol^{-1})	-40.9	-47.9	-36.9	-51.3	-69.3	-45.6	-54.0	-49.4	-50.8	-46.4	-49.8	-52.4
208		$K_{d,obs}$ (nM)	10 000	2000	≥200 000	1200	330	4000	5000	2500	1000	6100	200	260
		ΔG_{obs} (kJ mol^{-1})	-29.7	-33.8	≥-22.0	-35.2	-38.4	-32.0	-31.5	-33.2	-35.6	-31.0	-39.8	-39.1
E3		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
209		$K_{d,obs}$ (nM)	7100	560	130 000	1400	670	1700	2500	1700	580	2500	200	210
		ΔG_{obs} (kJ mol^{-1})	-30.5	-37.1	-23.2	-34.7	-36.7	-34.3	-33.2	-34.3	-37.0	-33.3	-39.8	-39.6
E12		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

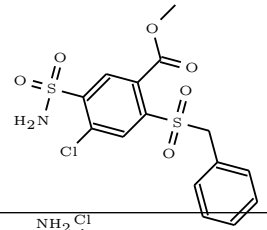
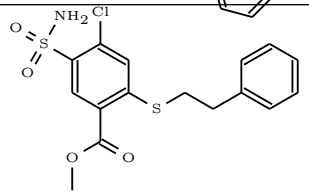
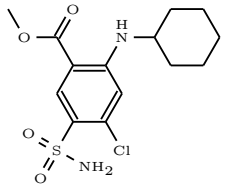
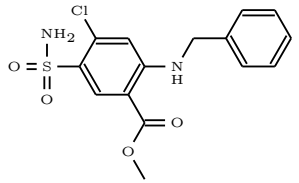
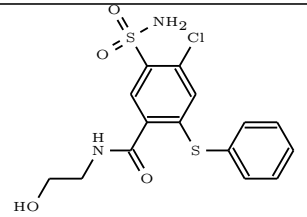
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
210		$K_{d,obs}$ (nM)	10 000	830	≥200 000	6400	14 000	2000	3300	2500	1100	1400	710	130
		ΔG_{obs} (kJ mol^{-1})	-29.7	-36.1	≥-22.0	-30.8	-28.8	-33.8	-32.5	-33.2	-35.4	-34.7	-36.5	-41.0
E18		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
211		$K_{d,obs}$ (nM)	10 000	450	≥200 000	2300	3300	5000	4500	3300	1100	2900	200	100
		ΔG_{obs} (kJ mol^{-1})	-29.7	-37.6	≥-22.0	-33.5	-32.5	-31.5	-31.7	-32.5	-35.3	-32.9	-39.8	-41.5
E14		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
212		$K_{d,obs}$ (nM)	4500	670	≥200 000	800	3300	1200	6700	3300	380	810	190	180
		ΔG_{obs} (kJ mol^{-1})	-31.7	-36.7	≥-22.0	-36.2	-32.5	-35.0	-30.7	-32.5	-38.1	-36.2	-40.0	-40.0
E13		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
213		$K_{d,obs}$ (nM)	3300	480	≥200 000	5800	5900	2400	9100	1000	400	2000	1400	130
		ΔG_{obs} (kJ mol^{-1})	-32.5	-37.5	≥-22.0	-31.1	-31.0	-33.4	-29.9	-35.6	-38.0	-33.8	-34.7	-41.0
E19		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
214		$K_{d,obs}$ (nM)	5000	1000	≥200 000	1500	670	3300	560	1700	530	1400	560	130
		ΔG_{obs} (kJ mol^{-1})	-31.5	-35.6	≥-22.0	-34.5	-36.7	-32.5	-37.1	-34.3	-37.2	-34.7	-37.1	-41.0
E22		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

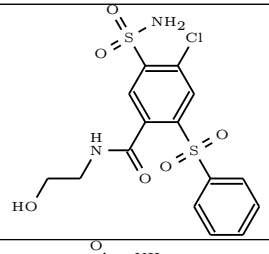
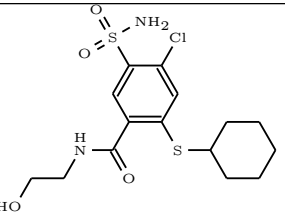
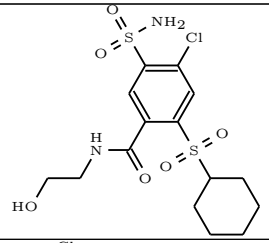
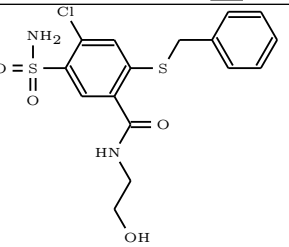
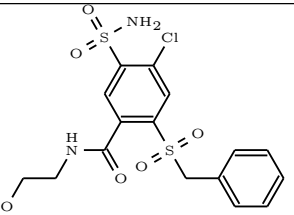
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
215		$K_{d,obs}$ (nM)	ND	1000	≥200 000	1400	19	1800	2200	400	470	6100	380	250
		ΔG_{obs} (kJ mol^{-1})	ND	-35.6	≥-22.0	-34.7	-45.9	-34.1	-33.5	-38.0	-37.6	-31.0	-38.1	-39.2
E6		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
216		$K_{d,obs}$ (nM)	40 000	4200	ND	100 000	11 000	17 000	ND	10 000	ND	20 000	6300	ND
		ΔG_{obs} (kJ mol^{-1})	-26.1	-31.9	ND	-23.7	-29.4	-28.4	ND	-29.7	ND	-27.9	-30.9	ND
E20		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
217		$K_{d,obs}$ (nM)	7200	1600	≥200 000	1500	1000	1200	1200	2400	660	980	490	150
		ΔG_{obs} (kJ mol^{-1})	-30.5	-34.5	≥-22.0	-34.6	-35.6	-35.0	-35.0	-33.4	-36.7	-35.7	-37.5	-40.5
E7		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
218		$K_{d,obs}$ (nM)	7100	590	80 000	3300	0.77	500	2000	1700	620	3100	770	190
		ΔG_{obs} (kJ mol^{-1})	-30.5	-37.0	-24.3	-32.5	-54.1	-37.4	-33.8	-34.3	-36.8	-32.7	-36.3	-39.9
VR15-1		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
219		$K_{d,obs}$ (nM)	2700	1200	≥200 000	3300	400	220	10 000	3300	400	2500	530	330
		ΔG_{obs} (kJ mol^{-1})	-33.0	-35.0	≥-22.0	-32.5	-38.0	-39.5	-29.7	-32.5	-38.0	-33.2	-37.3	-38.4
AZ15-16		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
220		$K_{d,obs}$ (nM)	50 000	330	11 000	1500	20 000	2500	4000	110	670	620	330	440
		ΔG_{obs} (kJ mol^{-1})	-25.5	-38.4	-29.4	-34.6	-27.9	-33.2	-32.0	-41.3	-36.7	-36.8	-38.4	-37.7
EA1-1		$K_{d,int}$ (nM)	150	0.47	8.4	1.3	42	3.9	1.1	0.14	0.60	0.76	0.96	0.54
		ΔG_{int} (kJ mol^{-1})	-40.6	-55.4	-47.9	-52.6	-43.8	-49.9	-53.1	-58.6	-54.7	-54.1	-53.5	-55.0

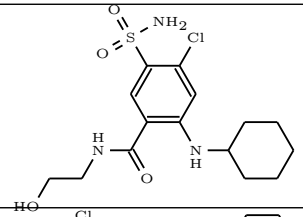
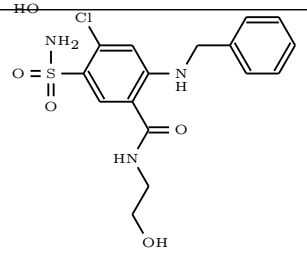
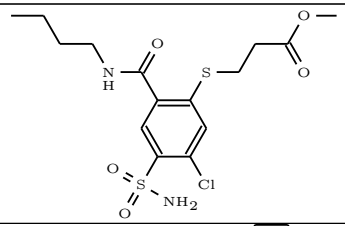
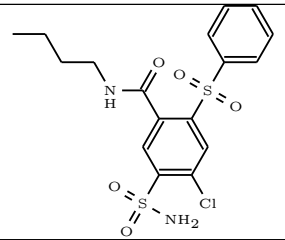
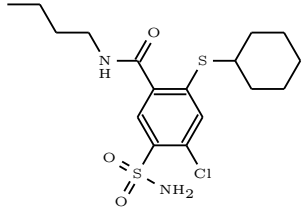
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
221		$K_{d,obs}$ (nM)	100 000	83	8300	400	5000	400	620	10	170	130	560	67
		ΔG_{obs} (kJ mol^{-1})	-23.7	-42.0	-30.1	-38.0	-31.5	-38.0	-36.8	-47.5	-40.2	-41.0	-37.1	-42.6
EA3-1		$K_{d,int}$ (nM)	1400	0.58	31	1.8	52	3.1	0.89	0.060	0.74	0.75	7.9	0.40
		ΔG_{int} (kJ mol^{-1})	-34.7	-54.8	-44.5	-51.9	-43.2	-50.5	-53.7	-60.6	-54.2	-54.1	-48.1	-55.8
222		$K_{d,obs}$ (nM)	≥200 000	10	25 000	7.1	8300	770	1000	10	50	170	620	63
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-47.5	-27.3	-48.3	-30.1	-36.3	-35.6	-47.5	-43.3	-40.2	-36.8	-42.8
EA4-1		$K_{d,int}$ (nM)	2900	0.069	94	0.032	87	6.0	1.4	0.060	0.22	1.0	8.9	0.38
		ΔG_{int} (kJ mol^{-1})	-32.9	-60.3	-41.7	-62.3	-41.9	-48.8	-52.5	-60.6	-57.3	-53.4	-47.8	-55.9
223		$K_{d,obs}$ (nM)	33 000	20	7100	83	5000	83	170	5.0	50	50	400	50
		ΔG_{obs} (kJ mol^{-1})	-26.6	-45.7	-30.5	-42.0	-31.5	-42.0	-40.2	-49.3	-43.3	-43.3	-38.0	-43.3
EA5-1		$K_{d,int}$ (nM)	540	0.15	30	0.41	58	0.73	0.26	0.034	0.25	0.34	6.3	0.34
		ΔG_{int} (kJ mol^{-1})	-37.2	-58.2	-44.6	-55.7	-42.9	-54.2	-56.8	-62.1	-57.0	-56.2	-48.7	-56.2
224		$K_{d,obs}$ (nM)	50 000	63	12 000	10	3400	250	590	11	71	200	710	40
		ΔG_{obs} (kJ mol^{-1})	-25.5	-42.8	-29.2	-47.5	-32.4	-39.2	-37.0	-47.2	-42.4	-39.8	-36.5	-43.9
EA8-1		$K_{d,int}$ (nM)	810	0.48	51	0.050	40	2.2	0.93	0.075	0.36	1.4	11	0.27
		ΔG_{int} (kJ mol^{-1})	-36.2	-55.3	-43.3	-61.1	-43.9	-51.4	-53.6	-60.1	-56.1	-52.6	-47.2	-56.8
225		$K_{d,obs}$ (nM)	≥200 000	140	45 000	280	2000	2300	1400	67	290	40	670	87
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-40.6	-25.8	-38.9	-33.8	-33.4	-34.7	-42.6	-38.8	-43.9	-36.7	-41.9
EA12-1		$K_{d,int}$ (nM)	2500	0.84	150	1.1	18	15	1.7	0.34	1.1	0.21	8.1	0.45
		ΔG_{int} (kJ mol^{-1})	-33.3	-53.9	-40.6	-53.3	-46.0	-46.4	-52.0	-56.2	-53.2	-57.5	-48.0	-55.5
226		$K_{d,obs}$ (nM)	100 000	50	50 000	110	1200	67	1000	20	140	130	500	59
		ΔG_{obs} (kJ mol^{-1})	-23.7	-43.3	-25.5	-41.3	-35.0	-42.6	-35.6	-45.7	-40.7	-41.0	-37.4	-42.9
EA11-1		$K_{d,int}$ (nM)	1600	0.39	210	0.55	15	0.58	1.6	0.14	0.69	0.84	7.9	0.40
		ΔG_{int} (kJ mol^{-1})	-34.4	-55.9	-39.6	-54.9	-46.5	-54.8	-52.2	-58.6	-54.4	-53.8	-48.1	-55.8
227		$K_{d,obs}$ (nM)	100 000	63	50 000	50	17 000	670	1200	17	130	330	830	100
		ΔG_{obs} (kJ mol^{-1})	-23.7	-42.8	-25.5	-43.3	-28.4	-36.7	-35.2	-46.2	-41.0	-38.4	-36.1	-41.5
EA4-1-2		$K_{d,int}$ (nM)	1700	0.51	220	0.26	200	6.1	2.0	0.12	0.65	2.4	14	0.71
		ΔG_{int} (kJ mol^{-1})	-34.2	-55.2	-39.5	-56.9	-39.7	-48.8	-51.7	-58.9	-54.5	-51.2	-46.6	-54.3

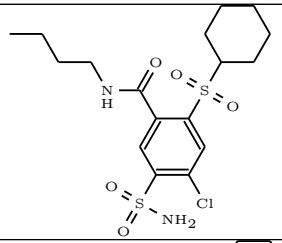
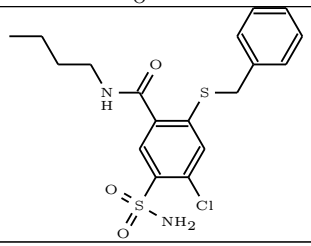
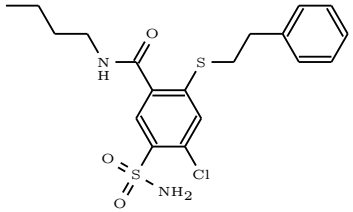
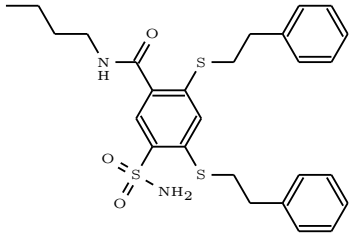
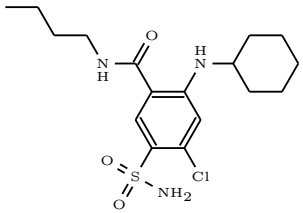
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
228		$K_{d,obs}$ (nM)	≥200 000	200	100 000	330	≥200 000	4000	1400	33	150	400	1200	170
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-39.8	-23.7	-38.4	≥-22.0	-32.0	-34.7	-44.4	-40.4	-38.0	-35.2	-40.2
EA7-1		$K_{d,int}$ (nM)	3200	1.5	420	1.7	2300	35	2.3	0.23	0.77	2.7	19	1.1
		ΔG_{int} (kJ mol^{-1})	-32.6	-52.3	-37.8	-52.1	-33.4	-44.3	-51.3	-57.3	-54.1	-50.8	-45.9	-53.1
229		$K_{d,obs}$ (nM)	71 000	170	≥200 000	170	2500	77	1400	29	250	1700	180	67
		ΔG_{obs} (kJ mol^{-1})	-24.6	-40.2	≥-22.0	-40.2	-33.2	-42.2	-34.7	-44.8	-39.2	-34.3	-40.0	-42.6
EA9-1		$K_{d,int}$ (nM)	1000	1.2	750	0.74	26	0.60	2.0	0.17	1.1	10	2.6	0.40
		ΔG_{int} (kJ mol^{-1})	-35.5	-53.0	-36.3	-54.2	-45.0	-54.7	-51.6	-57.9	-53.1	-47.5	-51.0	-55.8
230		$K_{d,obs}$ (nM)	25 000	20	2000	22	670	7.7	140	5.0	91	130	330	13
		ΔG_{obs} (kJ mol^{-1})	-27.3	-45.7	-33.8	-45.4	-36.7	-48.2	-40.6	-49.3	-41.8	-41.0	-38.4	-46.7
EA10-1		$K_{d,int}$ (nM)	360	0.14	7.5	0.099	6.9	0.060	0.20	0.030	0.40	0.75	4.7	0.080
		ΔG_{int} (kJ mol^{-1})	-38.2	-58.5	-48.2	-59.4	-48.4	-60.7	-57.5	-62.4	-55.7	-54.1	-49.4	-59.9
231		$K_{d,obs}$ (nM)	29 000	420	10 000	1600	28	2600	2000	130	400	1100	260	130
		ΔG_{obs} (kJ mol^{-1})	-27.0	-37.9	-29.7	-34.5	-44.8	-33.1	-33.8	-41.0	-38.0	-35.5	-39.0	-41.0
AZ15-10		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
232		$K_{d,obs}$ (nM)	5000	300	17 000	1100	1.8	1000	1400	140	370	3300	710	130
		ΔG_{obs} (kJ mol^{-1})	-31.5	-38.7	-28.4	-35.3	-51.9	-35.6	-34.7	-40.6	-38.2	-32.5	-36.5	-41.0
AZ15-9		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
233		$K_{d,obs}$ (nM)	7700	530	22 000	2900	4.5	2500	4000	710	1100	4000	1100	830
		ΔG_{obs} (kJ mol^{-1})	-30.3	-37.3	-27.6	-32.9	-49.5	-33.2	-32.0	-36.5	-35.3	-32.0	-35.4	-36.1
AZ15-12		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
234		$K_{d,obs}$ (nM)	50 000	29 000	ND	ND	ND	ND	ND	100 000	ND	50 000	17 000	ND
		ΔG_{obs} (kJ mol^{-1})	-25.5	-27.0	ND	ND	ND	ND	ND	-23.7	ND	-25.5	-28.4	ND
E13-1a		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

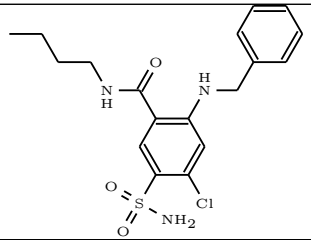
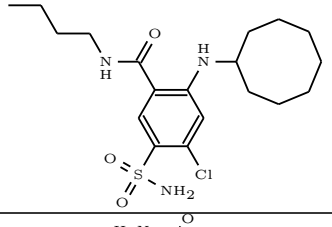
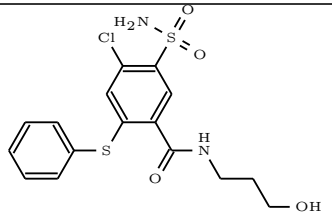
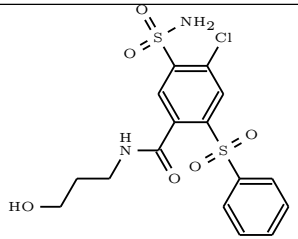
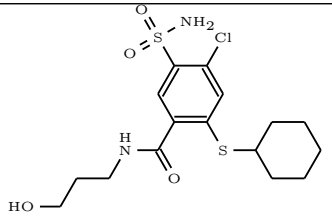
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
235		$K_{d,obs}$ (nM)	6300	6700	ND	17 000	25 000	3300	ND	4000	ND	12 000	2000	ND
		ΔG_{obs} (kJ mol^{-1})	-30.9	-30.7	ND	-28.4	-27.3	-32.5	ND	-32.0	ND	-29.3	-33.8	ND
E13-1		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
236		$K_{d,obs}$ (nM)	290	5000	ND	≥200 000	100 000	25 000	ND	100 000	ND	420	590	ND
		ΔG_{obs} (kJ mol^{-1})	-38.8	-31.5	ND	≥-22.0	-23.7	-27.3	ND	-23.7	ND	-37.9	-37.0	ND
E13-4		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
237		$K_{d,obs}$ (nM)	10 000	2200	ND	560	100 000	67 000	ND	670	ND	2500	1100	ND
		ΔG_{obs} (kJ mol^{-1})	-29.7	-33.5	ND	-37.1	-23.7	-24.8	ND	-36.7	ND	-33.2	-35.3	ND
E13-2		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
238		$K_{d,obs}$ (nM)	10 000	36	25 000	33	100 000	290	200	50	2.5	6.7	17	11
		ΔG_{obs} (kJ mol^{-1})	-29.7	-44.2	-27.3	-44.4	-23.7	-38.8	-39.8	-43.3	-51.0	-48.5	-46.2	-47.2
EA2-2		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
239		$K_{d,obs}$ (nM)	140	0.91	3300	25	770	13	56	0.45	3.3	22	5.6	0.86
		ΔG_{obs} (kJ mol^{-1})	-40.6	-53.7	-32.5	-45.1	-36.3	-46.7	-43.1	-55.4	-50.3	-45.4	-49.0	-53.8
EA2-2o		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
240		$K_{d,obs}$ (nM)	≥200 000	50 000	≥200 000	46 000	≥200 000	20 000	≥200 000	≥200 000	9600	82 000	69 000	100 000
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-25.5	≥-22.0	-25.8	≥-22.0	-27.9	≥-22.0	≥-22.0	-29.8	-24.2	-24.7	-23.7
EA2-3o		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
241		$K_{d,obs}$ (nM)	6900	110	50 000	100	100 000	5000	360	150	2.9	22	38	40
		ΔG_{obs} (kJ mol^{-1})	-30.6	-41.3	-25.5	-41.5	-23.7	-31.5	-38.3	-40.4	-50.7	-45.4	-44.0	-43.9
EA2-4		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

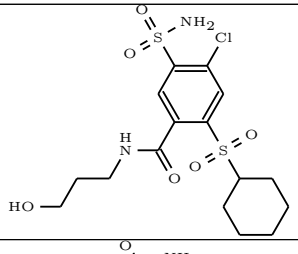
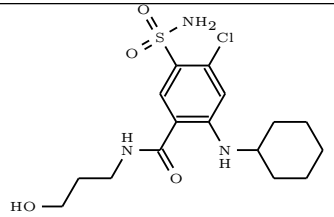
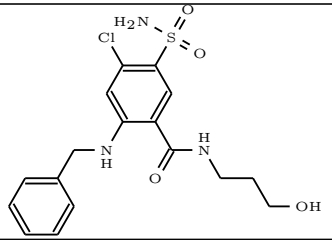
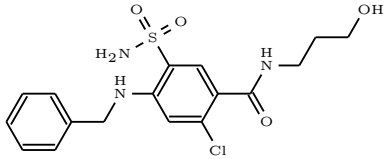
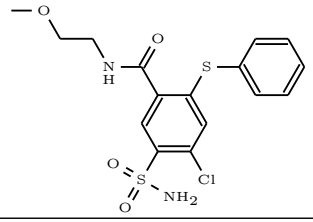
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
242		$K_{d,obs}$ (nM)	≥200 000	≥200 000	≥200 000	9100	≥200 000	100 000	100 000	≥200 000	3300	10 000	110 000	6700
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	≥-22.0	≥-22.0	-29.9	≥-22.0	-23.7	-23.7	≥-22.0	-32.5	-29.7	-23.5	-30.7
EA2-4o		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
243		$K_{d,obs}$ (nM)	13 000	170	15 000	290	100 000	1800	620	110	13	53	36	8.3
		ΔG_{obs} (kJ mol^{-1})	-29.0	-40.2	-28.6	-38.8	-23.7	-34.1	-36.8	-41.3	-46.9	-43.2	-44.2	-47.9
EA2-5		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
244		$K_{d,obs}$ (nM)	14 000	910	33 000	ND	≥200 000	ND	5600	10 000	ND	ND	ND	ND
		ΔG_{obs} (kJ mol^{-1})	-28.8	-35.9	-26.6	ND	≥-22.0	ND	-31.2	-29.7	ND	ND	ND	ND
EA2-7		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
245		$K_{d,obs}$ (nM)	50 000	ND	≥200 000	ND	ND	ND	3300	2900	ND	ND	ND	ND
		ΔG_{obs} (kJ mol^{-1})	-25.5	ND	≥-22.0	ND	ND	ND	-32.5	-32.9	ND	ND	ND	ND
EA2-8		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
246		$K_{d,obs}$ (nM)	10 000	31	15 000	1.4	5600	330	1400	11	4.0	6.2	100	3.0
		ΔG_{obs} (kJ mol^{-1})	-29.7	-44.5	-28.6	-52.5	-31.2	-38.4	-34.7	-47.2	-49.8	-48.7	-41.5	-50.6
EA3-2		$K_{d,int}$ (nM)	96	0.14	38	0.0042	38	1.7	1.3	0.045	0.012	0.025	0.94	0.012
		ΔG_{int} (kJ mol^{-1})	-41.6	-58.4	-44.0	-67.5	-44.0	-52.0	-52.6	-61.4	-64.9	-62.9	-53.6	-64.8

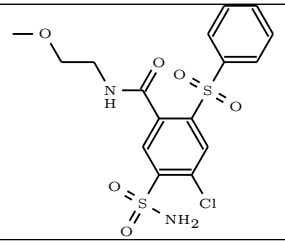
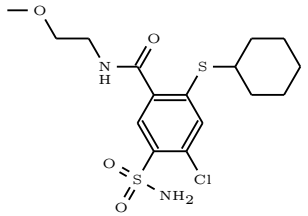
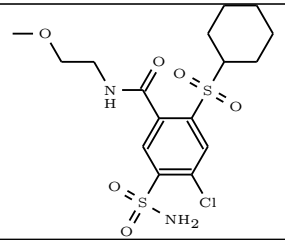
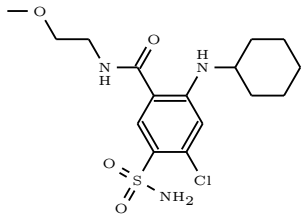
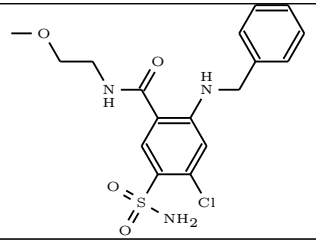
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
247		$K_{d,obs}$ (nM)	2000	5.0	8300	ND	1000	17	910	1.2	3.0	5.6	17	3.0
		ΔG_{obs} (kJ mol^{-1})	-33.8	-49.3	-30.1	ND	-35.6	-46.2	-35.9	-52.8	-50.6	-49.0	-46.2	-50.6
EA3-2o		$K_{d,int}$ (nM)	99	0.12	110	ND	35	0.44	4.4	0.026	0.046	0.11	0.81	0.062
		ΔG_{int} (kJ mol^{-1})	-41.6	-58.9	-41.4	ND	-44.2	-55.5	-49.6	-62.8	-61.4	-59.0	-54.0	-60.6
248		$K_{d,obs}$ (nM)	1000	10	13 000	10	590	77	1200	2.5	1.2	2.0	29	1.1
		ΔG_{obs} (kJ mol^{-1})	-35.6	-47.5	-29.1	-47.5	-37.0	-42.2	-35.0	-51.0	-52.8	-51.6	-44.8	-53.2
EA3-3		$K_{d,int}$ (nM)	9.2	0.044	30	0.028	3.9	0.38	1.1	0.0096	0.0035	0.0077	0.26	0.0042
		ΔG_{int} (kJ mol^{-1})	-47.7	-61.5	-44.7	-62.6	-49.9	-55.9	-53.1	-65.4	-68.0	-66.0	-56.9	-67.5
249		$K_{d,obs}$ (nM)	1400	3.3	25 000	33	330	10	1200	4.0	3.1	20	25	1.8
		ΔG_{obs} (kJ mol^{-1})	-34.7	-50.3	-27.3	-44.4	-38.4	-47.5	-35.0	-49.8	-50.5	-45.7	-45.1	-51.9
EA3-3o		$K_{d,int}$ (nM)	75	0.084	340	0.54	13	0.28	6.5	0.088	0.051	0.44	1.3	0.040
		ΔG_{int} (kJ mol^{-1})	-42.3	-59.8	-38.4	-55.0	-46.9	-56.7	-48.6	-59.7	-61.1	-55.5	-52.8	-61.7
250		$K_{d,obs}$ (nM)	2100	13	50 000	33	500	150	1600	3.3	15	10	91	13
		ΔG_{obs} (kJ mol^{-1})	-33.7	-46.8	-25.5	-44.4	-37.4	-40.4	-34.5	-50.3	-46.5	-47.5	-41.8	-46.9
EA3-4		$K_{d,int}$ (nM)	14	0.040	84	0.067	2.3	0.54	1.0	0.0091	0.029	0.027	0.58	0.034
		ΔG_{int} (kJ mol^{-1})	-46.6	-61.7	-42.0	-60.4	-51.2	-55.0	-53.4	-65.5	-62.5	-62.7	-54.8	-62.1
251		$K_{d,obs}$ (nM)	6300	36	14 000	250	710	77	2400	9.1	45	83	130	20
		ΔG_{obs} (kJ mol^{-1})	-30.9	-44.2	-28.9	-39.2	-36.5	-42.2	-33.4	-47.7	-43.6	-42.0	-41.0	-45.7
EA3-4o		$K_{d,int}$ (nM)	340	0.94	200	4.2	28	2.3	13	0.21	0.77	1.9	6.7	0.46
		ΔG_{int} (kJ mol^{-1})	-38.4	-53.6	-39.8	-49.7	-44.8	-51.3	-46.8	-57.4	-54.1	-51.7	-48.5	-55.4

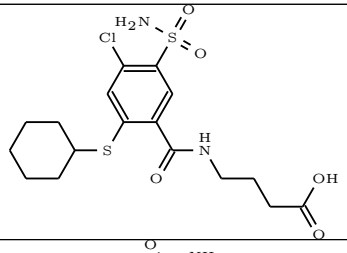
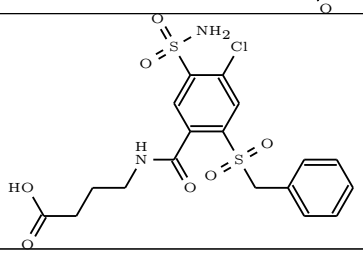
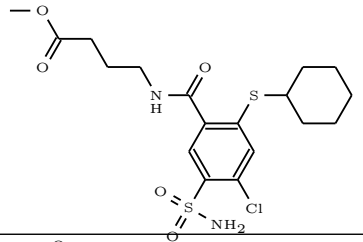
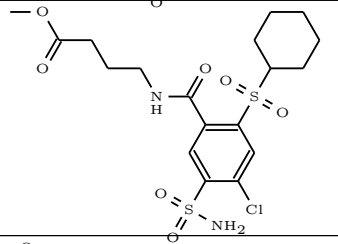
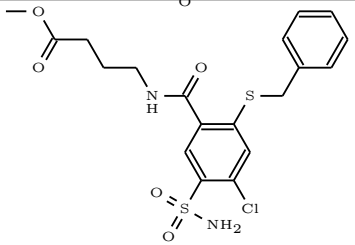
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
252		$K_{d,obs}$ (nM)	14 000	420	≥200 000	ND	50 000	50 000	33 000	3300	20	ND	670	ND
		ΔG_{obs} (kJ mol^{-1})	-28.8	-37.9	≥-22.0	ND	-25.5	-25.5	-26.6	-32.5	-45.7	ND	-36.7	ND
EA3-7		$K_{d,int}$ (nM)	26	0.37	240	ND	66	50	6.0	2.6	0.011	ND	1.2	ND
		ΔG_{int} (kJ mol^{-1})	-45.0	-56.0	-39.3	ND	-42.6	-43.3	-48.8	-51.0	-65.0	ND	-52.9	ND
253		$K_{d,obs}$ (nM)	6300	77	≥200 000	ND	ND	2000	6700	230	40	170	400	20
		ΔG_{obs} (kJ mol^{-1})	-30.9	-42.2	≥-22.0	ND	ND	-33.8	-30.7	-39.4	-43.9	-40.2	-38.0	-45.7
EA3-8		$K_{d,int}$ (nM)	3.7	0.021	30	ND	ND	0.63	0.38	0.055	0.0072	0.041	0.23	0.0049
		ΔG_{int} (kJ mol^{-1})	-50.1	-63.3	-44.6	ND	ND	-54.6	-55.9	-60.9	-66.1	-61.7	-57.2	-67.1
254		$K_{d,obs}$ (nM)	13 000	10	13 000	ND	ND	ND	560	2.5	5.0	14	200	ND
		ΔG_{obs} (kJ mol^{-1})	-29.1	-47.5	-28.9	ND	ND	ND	-37.1	-51.0	-49.3	-46.6	-39.8	ND
AZ14-2		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
255		$K_{d,obs}$ (nM)	670	3.3	3300	ND	4500	3.7	240	0.25	0.67	2.9	11	1.1
		ΔG_{obs} (kJ mol^{-1})	-36.7	-50.3	-32.5	ND	-31.7	-50.0	-39.3	-57.0	-54.5	-50.7	-47.2	-53.1
EA5-2o		$K_{d,int}$ (nM)	33	0.079	43	ND	160	0.099	1.2	0.0051	0.010	0.059	0.54	0.023
		ΔG_{int} (kJ mol^{-1})	-44.4	-60.0	-43.7	ND	-40.3	-59.4	-53.0	-67.0	-65.3	-60.7	-55.0	-63.1
256		$K_{d,obs}$ (nM)	400	2.5	10 000	5.0	400	8.3	500	0.53	0.83	0.50	25	2.0
		ΔG_{obs} (kJ mol^{-1})	-38.0	-51.0	-29.7	-49.3	-38.0	-47.9	-37.4	-55.1	-53.9	-55.2	-45.1	-51.6
EA5-3		$K_{d,int}$ (nM)	3.7	0.011	24	0.014	2.6	0.041	0.45	0.0020	0.0023	0.0019	0.23	0.0077
		ΔG_{int} (kJ mol^{-1})	-50.1	-65.0	-45.2	-64.4	-50.9	-61.6	-55.5	-69.4	-69.0	-69.5	-57.3	-66.0

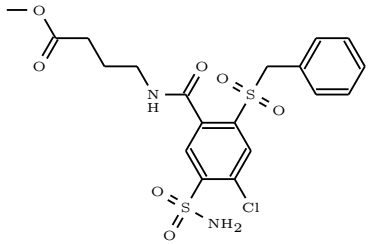
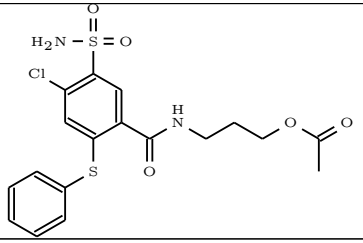
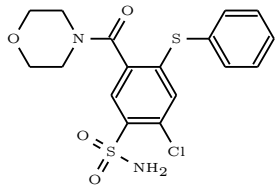
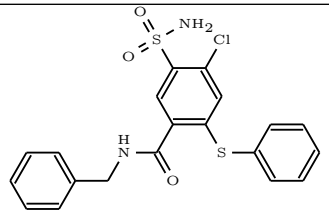
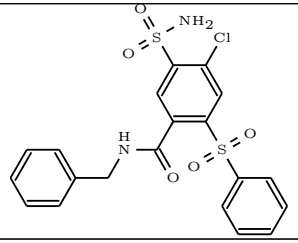
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
257		$K_{d,obs}$ (nM)	1100	1.4	8300	29	1500	1.1	310	0.63	0.43	2.5	7.1	1.1
		ΔG_{obs} (kJ mol^{-1})	-35.3	-52.5	-30.1	-44.8	-34.5	-53.1	-38.6	-54.6	-55.6	-51.0	-48.3	-53.1
EA5-3o		$K_{d,int}$ (nM)	55	0.034	110	0.43	55	0.030	1.5	0.013	0.0066	0.051	0.35	0.023
		ΔG_{int} (kJ mol^{-1})	-43.1	-62.2	-41.4	-55.6	-43.1	-62.5	-52.4	-64.6	-66.4	-61.1	-56.1	-63.1
258		$K_{d,obs}$ (nM)	1800	2.9	≥200 000	ND	400	11	560	5.3	3.3	2.4	71	11
		ΔG_{obs} (kJ mol^{-1})	-34.1	-50.7	≥-22.0	ND	-38.0	-47.2	-37.1	-49.1	-50.3	-51.2	-42.4	-47.3
EA5-4		$K_{d,int}$ (nM)	11	0.0079	300	ND	1.7	0.035	0.32	0.013	0.0060	0.0058	0.41	0.026
		ΔG_{int} (kJ mol^{-1})	-47.3	-65.9	-38.7	ND	-52.1	-62.1	-56.4	-64.7	-66.6	-66.7	-55.7	-62.9
259		$K_{d,obs}$ (nM)	1500	2.0	20 000	ND	320	2.7	670	4.0	1.2	1.4	20	7.1
		ΔG_{obs} (kJ mol^{-1})	-34.6	-51.6	-27.9	ND	-38.5	-50.8	-36.7	-49.8	-52.8	-52.5	-45.7	-48.3
EA5-5		$K_{d,int}$ (nM)	7.6	0.0050	27	ND	1.2	0.0076	0.34	0.0087	0.0020	0.0031	0.10	0.015
		ΔG_{int} (kJ mol^{-1})	-48.2	-67.1	-44.9	ND	-52.9	-66.0	-56.2	-65.7	-69.4	-68.3	-59.3	-64.2
260		$K_{d,obs}$ (nM)	40 000	40 000	40 000	ND	40 000	ND	≥200 000	40 000	40 000	40 000	40 000	ND
		ΔG_{obs} (kJ mol^{-1})	-26.1	-26.1	-26.1	ND	-26.1	ND	≥-22.0	-26.1	-26.1	-26.1	-26.1	ND
EA5-5-1		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
261		$K_{d,obs}$ (nM)	≥200 000	910	≥200 000	ND	100 000	1200	17 000	17 000	20	ND	ND	140
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-35.9	≥-22.0	ND	-23.7	-35.0	-28.4	-28.4	-45.7	ND	ND	-40.6
EA5-7		$K_{d,int}$ (nM)	370	0.80	96	ND	130	1.2	3.0	13	0.011	ND	ND	0.11
		ΔG_{int} (kJ mol^{-1})	-38.2	-54.0	-41.7	ND	-40.8	-52.8	-50.6	-46.8	-65.0	ND	ND	-59.1

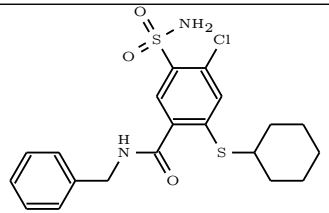
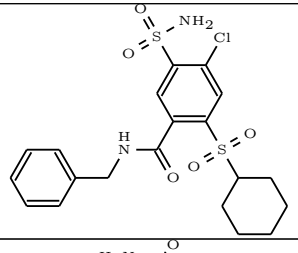
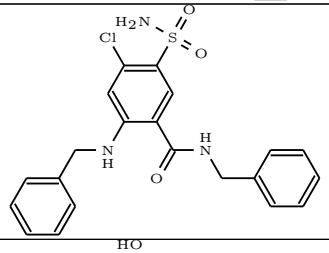
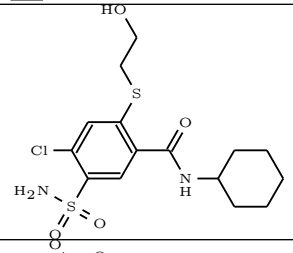
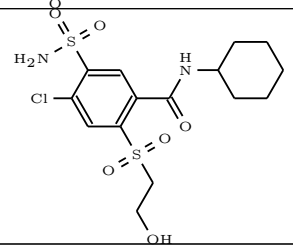
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
262		$K_{d,obs}$ (nM)	33 000	130	≥200 000	ND	≥200 000	7700	20 000	500	40	330	2000	140
		ΔG_{obs} (kJ mol^{-1})	-26.6	-41.0	≥-22.0	ND	≥-22.0	-30.3	-27.9	-37.4	-43.9	-38.4	-33.8	-40.6
EA5-8		$K_{d,int}$ (nM)	19	0.035	30	ND	84	2.4	1.1	0.12	0.0072	0.081	1.1	0.035
		ΔG_{int} (kJ mol^{-1})	-45.8	-62.1	-44.6	ND	-42.0	-51.1	-53.1	-58.8	-66.1	-59.9	-53.1	-62.1
263		$K_{d,obs}$ (nM)	≥200 000	130	≥200 000	ND	≥200 000	6700	20 000	2000	10	670	ND	12
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-41.0	≥-22.0	ND	≥-22.0	-30.7	-27.9	-33.8	-47.5	-36.7	ND	-47.0
EA5-9		$K_{d,int}$ (nM)	370	0.11	96	ND	270	6.6	3.6	1.5	0.0057	0.51	ND	0.0094
		ΔG_{int} (kJ mol^{-1})	-38.2	-59.1	-41.7	ND	-39.0	-48.5	-50.1	-52.3	-66.7	-55.1	ND	-65.4
264		$K_{d,obs}$ (nM)	6700	5.0	33 000	1.7	4500	130	830	1.2	2.0	0.83	180	5.6
		ΔG_{obs} (kJ mol^{-1})	-30.7	-49.3	-26.6	-52.1	-31.7	-41.0	-36.1	-52.8	-51.6	-53.9	-40.0	-49.0
EA4-2		$K_{d,int}$ (nM)	69	0.025	89	0.0053	34	0.69	0.84	0.0054	0.0063	0.0036	1.8	0.024
		ΔG_{int} (kJ mol^{-1})	-42.5	-63.0	-41.8	-66.9	-44.4	-54.4	-53.9	-66.9	-66.5	-67.9	-51.8	-63.0
265		$K_{d,obs}$ (nM)	1400	3.3	17 000	28	5600	19	1400	0.33	1.5	3.1	67	4.0
		ΔG_{obs} (kJ mol^{-1})	-34.7	-50.3	-28.4	-44.9	-31.2	-45.8	-34.7	-56.2	-52.3	-50.5	-42.6	-49.8
EA4-2o		$K_{d,int}$ (nM)	70	0.079	210	0.42	200	0.50	6.9	0.0069	0.023	0.064	3.2	0.082
		ΔG_{int} (kJ mol^{-1})	-42.4	-60.0	-39.6	-55.7	-39.8	-55.2	-48.4	-66.2	-63.1	-60.5	-50.4	-59.8
266		$K_{d,obs}$ (nM)	1200	3.7	25 000	33	430	29	1700	0.67	0.71	1.0	67	2.0
		ΔG_{obs} (kJ mol^{-1})	-35.0	-50.0	-27.3	-44.4	-37.8	-44.8	-34.3	-54.5	-54.3	-53.4	-42.6	-51.6
EA4-3		$K_{d,int}$ (nM)	16	0.023	84	0.13	4.0	0.20	2.1	0.0036	0.0028	0.0054	0.84	0.011
		ΔG_{int} (kJ mol^{-1})	-46.2	-63.2	-42.0	-58.6	-49.8	-57.6	-51.5	-67.9	-68.5	-66.9	-53.8	-65.1

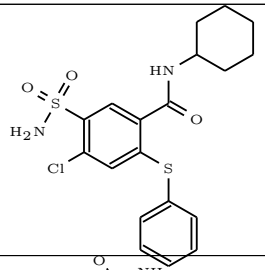
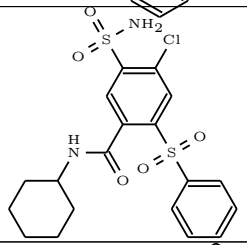
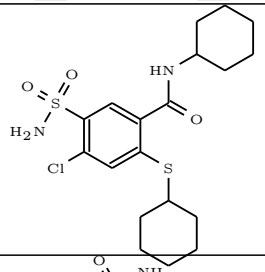
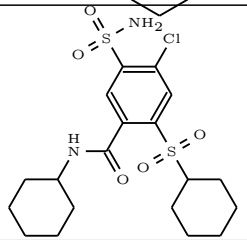
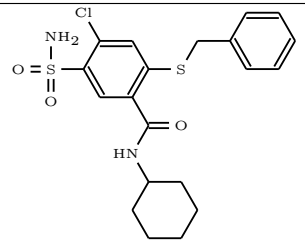
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
267		$K_{d,obs}$ (nM)	1000	1.1	33 000	ND	1400	11	1200	1.4	0.67	8.3	50	5.0
		ΔG_{obs} (kJ mol^{-1})	-35.6	-53.3	-26.6	ND	-34.7	-47.2	-35.0	-52.5	-54.5	-47.9	-43.3	-49.3
EA4-3o		$K_{d,int}$ (nM)	44	0.022	380	ND	45	0.27	5.4	0.026	0.0091	0.15	2.2	0.092
		ΔG_{int} (kJ mol^{-1})	-43.6	-63.2	-38.1	ND	-43.6	-56.8	-49.1	-62.8	-65.5	-58.2	-51.4	-59.6
268		$K_{d,obs}$ (nM)	33 000	190	160 000	ND	160 000	25 000	25 000	1400	8.3	21	ND	77
		ΔG_{obs} (kJ mol^{-1})	-26.6	-39.9	-22.5	ND	-22.5	-27.3	-27.3	-34.7	-47.9	-45.6	ND	-42.2
EA4-7		$K_{d,int}$ (nM)	49	0.13	60	ND	170	20	3.6	0.87	0.0038	0.013	ND	0.047
		ΔG_{int} (kJ mol^{-1})	-43.4	-58.6	-42.8	ND	-40.2	-45.7	-50.1	-53.8	-67.8	-64.7	ND	-61.3
269		$K_{d,obs}$ (nM)	25 000	20	50 000	ND	48 000	7700	13 000	67	31	130	1100	48
		ΔG_{obs} (kJ mol^{-1})	-27.3	-45.7	-25.5	ND	-25.7	-30.3	-29.1	-42.6	-44.6	-41.0	-35.3	-43.5
EA4-8		$K_{d,int}$ (nM)	15	0.0056	7.6	ND	20	2.4	0.72	0.016	0.0056	0.030	0.64	0.012
		ΔG_{int} (kJ mol^{-1})	-46.5	-66.8	-48.2	ND	-45.7	-51.1	-54.3	-64.0	-66.8	-62.4	-54.6	-64.9
270		$K_{d,obs}$ (nM)	25 000	10 000	50 000	ND	140 000	100 000	100 000	100 000	ND	20 000	25 000	6700
		ΔG_{obs} (kJ mol^{-1})	-27.3	-29.7	-25.5	ND	-22.8	-23.7	-23.7	-23.7	ND	-27.9	-27.3	-30.7
EA4-8b		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
271		$K_{d,obs}$ (nM)	5000	8.3	10 000	1.4	4500	40	670	2.5	1.7	2.5	140	2.5
		ΔG_{obs} (kJ mol^{-1})	-31.5	-47.9	-29.7	-52.5	-31.7	-43.9	-36.7	-51.0	-52.1	-51.0	-40.6	-51.0
EA8-2		$K_{d,int}$ (nM)	46	0.037	24	0.0040	30	0.20	0.60	0.0096	0.0047	0.0096	1.3	0.0096
		ΔG_{int} (kJ mol^{-1})	-43.6	-61.9	-45.2	-67.6	-44.6	-57.6	-54.7	-65.4	-67.2	-65.4	-52.8	-65.4

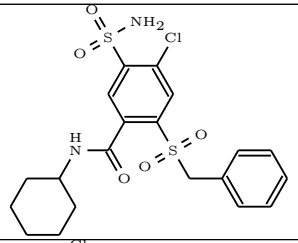
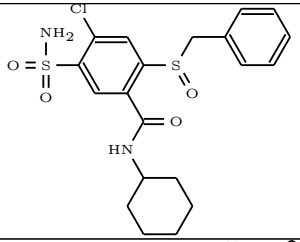
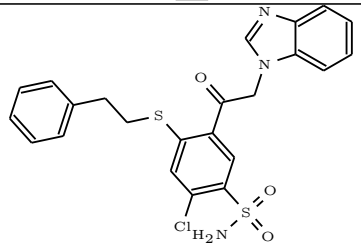
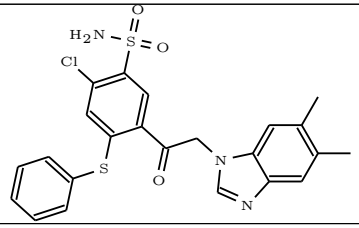
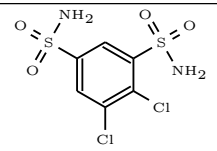
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
272		$K_{d,obs}$ (nM)	3300	3.3	6700	10	2000	7.7	770	0.50	1.6	5.6	36	1.0
		ΔG_{obs} (kJ mol^{-1})	-32.5	-50.3	-30.7	-47.5	-33.8	-48.2	-36.3	-55.2	-52.3	-49.0	-44.2	-53.4
EA8-2o		$K_{d,int}$ (nM)	160	0.079	85	0.15	71	0.20	3.7	0.010	0.024	0.11	1.7	0.021
		ΔG_{int} (kJ mol^{-1})	-40.3	-60.0	-42.0	-58.3	-42.4	-57.5	-50.0	-65.2	-63.1	-59.0	-52.0	-63.4
273		$K_{d,obs}$ (nM)	670	4.0	20 000	10	140	13	670	0.67	1.4	1.7	33	1.7
		ΔG_{obs} (kJ mol^{-1})	-36.7	-49.8	-27.9	-47.5	-40.6	-46.7	-36.7	-54.5	-52.5	-52.1	-44.4	-52.1
EA8-3		$K_{d,int}$ (nM)	6.1	0.018	48	0.028	0.94	0.066	0.60	0.0026	0.0040	0.0064	0.30	0.0064
		ΔG_{int} (kJ mol^{-1})	-48.7	-63.8	-43.5	-62.6	-53.6	-60.4	-54.7	-68.8	-67.6	-66.4	-56.5	-66.4
274		$K_{d,obs}$ (nM)	2500	2.6	20 000	50	330	22	670	2.5	1.0	20	50	2.9
		ΔG_{obs} (kJ mol^{-1})	-33.2	-50.9	-27.9	-43.3	-38.4	-45.4	-36.7	-51.0	-53.4	-45.7	-43.3	-50.7
EA8-3o		$K_{d,int}$ (nM)	120	0.062	260	0.76	12	0.59	3.2	0.051	0.015	0.41	2.4	0.059
		ΔG_{int} (kJ mol^{-1})	-41.0	-60.6	-39.1	-54.1	-47.0	-54.8	-50.4	-61.1	-64.2	-55.7	-51.1	-60.7
275		$K_{d,obs}$ (nM)	20 000	330	100 000	ND	100 000	13 000	10 000	2900	ND	ND	ND	67
		ΔG_{obs} (kJ mol^{-1})	-27.9	-38.4	-23.7	ND	-23.7	-29.1	-29.7	-32.9	ND	ND	ND	-42.6
EA8-7		$K_{d,int}$ (nM)	37	0.29	48	ND	130	12	1.8	2.2	ND	ND	ND	0.051
		ΔG_{int} (kJ mol^{-1})	-44.1	-56.6	-43.4	ND	-40.8	-46.9	-51.9	-51.4	ND	ND	ND	-61.1
276		$K_{d,obs}$ (nM)	20 000	50	≥200 000	ND	14 000	3600	5600	130	33	250	1000	33
		ΔG_{obs} (kJ mol^{-1})	-27.9	-43.3	≥-22.0	ND	-28.8	-32.3	-31.2	-41.0	-44.4	-39.2	-35.6	-44.4
EA8-8		$K_{d,int}$ (nM)	15	0.018	38	ND	7.6	1.4	0.40	0.038	0.0075	0.077	0.72	0.010
		ΔG_{int} (kJ mol^{-1})	-46.5	-63.8	-44.0	ND	-48.2	-52.5	-55.8	-61.8	-66.0	-60.0	-54.3	-65.2

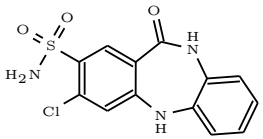
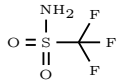
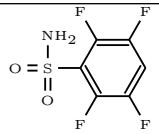
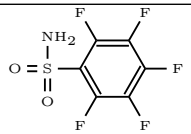
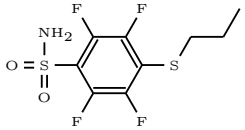
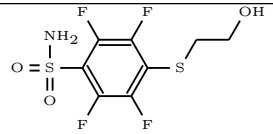
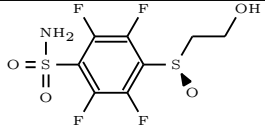
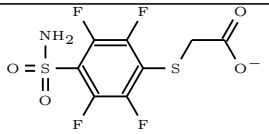
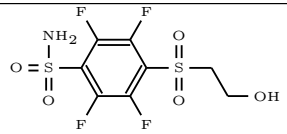
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
277		$K_{d,obs}$ (nM)	3300	13	≥200 000	130	250	33	2200	9.1	2.2	0.40	130	1.8
		ΔG_{obs} (kJ mol^{-1})	-32.5	-46.9	≥-22.0	-40.9	-39.2	-44.4	-33.5	-47.7	-51.4	-55.8	-41.0	-51.9
EA12-3		$K_{d,int}$ (nM)	31	0.055	480	0.36	1.6	0.17	2.0	0.035	0.0063	0.0015	1.1	0.0070
		ΔG_{int} (kJ mol^{-1})	-44.6	-60.9	-37.5	-56.1	-52.1	-58.1	-51.6	-62.1	-66.5	-70.1	-53.1	-66.2
278		$K_{d,obs}$ (nM)	34 000	100	33 000	ND	5600	400	9100	29	300	40	830	50
		ΔG_{obs} (kJ mol^{-1})	-26.5	-41.5	-26.6	ND	-31.2	-38.0	-29.9	-44.7	-38.7	-43.9	-36.1	-43.3
EA12-4o		$K_{d,int}$ (nM)	1900	2.6	480	ND	220	12	49	0.68	5.1	0.92	45	1.1
		ΔG_{int} (kJ mol^{-1})	-34.0	-50.9	-37.5	ND	-39.5	-47.0	-43.4	-54.4	-49.2	-53.6	-43.6	-53.1
279		$K_{d,obs}$ (nM)	2000	10	≥200 000	96	250	6.7	1700	3.3	2.0	1.2	100	2.0
		ΔG_{obs} (kJ mol^{-1})	-33.8	-47.5	≥-22.0	-41.6	-39.2	-48.5	-34.3	-50.3	-51.6	-52.8	-41.5	-51.6
EA11-3		$K_{d,int}$ (nM)	18	0.044	480	0.27	1.6	0.033	1.5	0.013	0.0056	0.0048	0.90	0.0077
		ΔG_{int} (kJ mol^{-1})	-45.9	-61.5	-37.5	-56.8	-52.1	-62.2	-52.4	-64.7	-66.8	-67.2	-53.7	-66.0
280		$K_{d,obs}$ (nM)	2000	4.3	71 000	110	1600	14	1100	20	1.0	12	50	3.0
		ΔG_{obs} (kJ mol^{-1})	-33.8	-49.6	-24.6	-41.2	-34.4	-46.6	-35.3	-45.7	-53.4	-47.1	-43.3	-50.6
EA11-3o		$K_{d,int}$ (nM)	99	0.10	910	1.7	57	0.38	5.4	0.41	0.015	0.24	2.4	0.062
		ΔG_{int} (kJ mol^{-1})	-41.6	-59.3	-35.8	-52.0	-43.0	-55.9	-49.1	-55.7	-64.2	-57.1	-51.1	-60.6
281		$K_{d,obs}$ (nM)	3200	7.8	≥200 000	11	670	43	1700	4.3	46	7.3	180	5.9
		ΔG_{obs} (kJ mol^{-1})	-32.6	-48.1	≥-22.0	-47.2	-36.6	-43.7	-34.3	-49.7	-43.6	-48.3	-40.1	-48.8
EA11-4		$K_{d,int}$ (nM)	19	0.022	300	0.020	2.8	0.14	0.95	0.010	0.081	0.018	1.0	0.014
		ΔG_{int} (kJ mol^{-1})	-45.9	-63.3	-38.7	-63.5	-50.8	-58.5	-53.5	-65.2	-59.9	-63.8	-53.4	-64.4

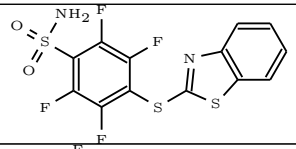
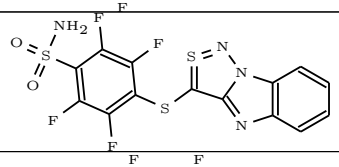
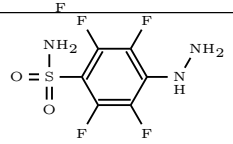
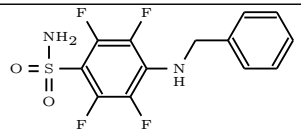
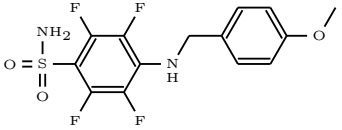
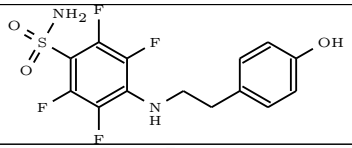
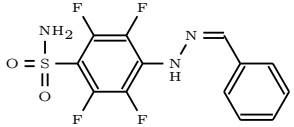
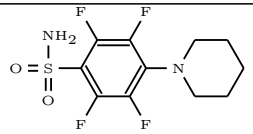
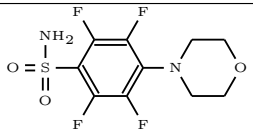
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
282		$K_{d,obs}$ (nM)	15 000	50	67 000	560	5000	140	3300	12	29	120	310	30
		ΔG_{obs} (kJ mol^{-1})	-28.7	-43.3	-24.8	-37.1	-31.5	-40.6	-32.5	-47.1	-44.8	-41.1	-38.6	-44.6
EA11-4o		$K_{d,int}$ (nM)	810	1.3	950	9.4	200	4.2	18	0.27	0.48	2.7	17	0.70
		ΔG_{int} (kJ mol^{-1})	-36.2	-52.7	-35.7	-47.6	-39.8	-49.7	-46.0	-56.8	-55.3	-50.8	-46.1	-54.3
283		$K_{d,obs}$ (nM)	10 000	25	77 000	2.9	2200	100	1400	7.7	5.0	10	330	6.2
		ΔG_{obs} (kJ mol^{-1})	-29.7	-45.1	-24.4	-50.7	-33.5	-41.5	-34.7	-48.2	-49.3	-47.5	-38.4	-48.7
EA4-2c		$K_{d,int}$ (nM)	86	0.10	170	0.0076	14	0.46	1.2	0.028	0.013	0.036	2.8	0.022
		ΔG_{int} (kJ mol^{-1})	-41.9	-59.3	-40.2	-66.0	-46.7	-55.4	-52.9	-62.7	-64.6	-62.0	-50.8	-63.2
284		$K_{d,obs}$ (nM)	≥200 000	1000	≥200 000	2900	≥200 000	12 000	14 000	670	ND	3300	7700	670
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-35.6	≥-22.0	-32.9	≥-22.0	-29.3	-28.8	-36.7	ND	-32.5	-30.3	-36.7
EA7-2		$K_{d,int}$ (nM)	1800	4.4	480	8.1	1300	58	13	2.6	ND	13	69	2.6
		ΔG_{int} (kJ mol^{-1})	-34.0	-49.6	-37.5	-48.0	-34.9	-42.9	-46.8	-51.0	ND	-46.8	-42.5	-51.0
285		$K_{d,obs}$ (nM)	330	4.5	2800	9.1	1800	10	190	9.1	7.7	1.7	150	2.9
		ΔG_{obs} (kJ mol^{-1})	-38.4	-49.5	-33.0	-47.7	-34.1	-47.4	-39.9	-47.7	-48.2	-52.1	-40.4	-50.7
EA10-2		$K_{d,int}$ (nM)	3.1	0.020	6.6	0.026	12	0.051	0.17	0.035	0.022	0.0064	1.4	0.011
		ΔG_{int} (kJ mol^{-1})	-50.5	-63.5	-48.5	-62.9	-47.1	-61.1	-58.0	-62.1	-63.3	-66.4	-52.6	-65.0
286		$K_{d,obs}$ (nM)	91	1.2	1600	32	11 000	9.1	91	0.22	1.2	5.6	16	1.4
		ΔG_{obs} (kJ mol^{-1})	-41.8	-52.9	-34.4	-44.5	-29.5	-47.7	-41.8	-57.3	-53.0	-49.0	-46.2	-52.5
EA10-2o		$K_{d,int}$ (nM)	4.5	0.029	20	0.49	370	0.24	0.44	0.0046	0.018	0.11	0.79	0.029
		ΔG_{int} (kJ mol^{-1})	-49.5	-62.6	-45.7	-55.3	-38.1	-57.1	-55.5	-67.3	-63.8	-59.0	-54.0	-62.5

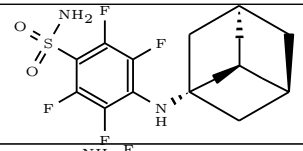
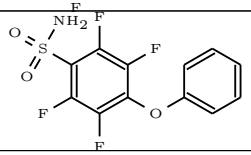
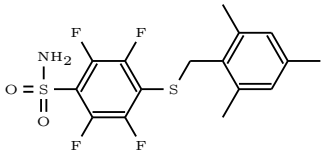
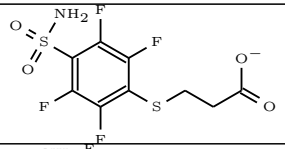
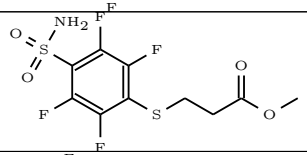
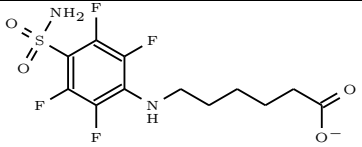
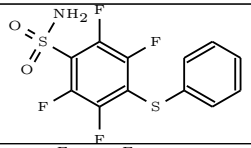
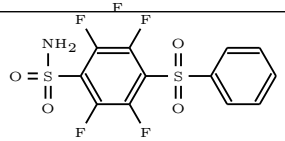
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
287		$K_{d,obs}$ (nM)	83	1.4	4300	86	170	1.4	220	2.6	1.1	1.0	50	1.2
		ΔG_{obs} (kJ mol^{-1})	-42.0	-52.5	-31.8	-41.9	-40.1	-52.5	-39.5	-50.9	-53.1	-53.4	-43.3	-52.8
EA10-3		$K_{d,int}$ (nM)	0.76	0.0063	10	0.24	1.1	0.0071	0.20	0.010	0.0031	0.0038	0.45	0.0048
		ΔG_{int} (kJ mol^{-1})	-54.1	-66.5	-47.4	-57.1	-53.1	-66.2	-57.6	-65.3	-68.3	-67.8	-55.5	-67.2
288		$K_{d,obs}$ (nM)	200	1.0	4000	220	500	1.9	110	1.1	0.83	7.7	14	2.3
		ΔG_{obs} (kJ mol^{-1})	-39.8	-53.4	-32.0	-39.5	-37.4	-51.8	-41.4	-53.1	-53.9	-48.2	-46.6	-51.3
EA10-3o		$K_{d,int}$ (nM)	9.9	0.024	51	3.3	18	0.050	0.51	0.023	0.013	0.16	0.69	0.047
		ΔG_{int} (kJ mol^{-1})	-47.5	-63.1	-43.3	-50.3	-46.0	-61.1	-55.1	-63.1	-64.7	-58.2	-54.4	-61.3
289		$K_{d,obs}$ (nM)	4000	40	≥200 000	ND	100 000	1200	3300	130	25	330	2000	15
		ΔG_{obs} (kJ mol^{-1})	-32.0	-43.9	≥-22.0	ND	-23.7	-35.2	-32.5	-41.0	-45.1	-38.4	-33.8	-46.4
EA10-8		$K_{d,int}$ (nM)	2.3	0.011	30	ND	42	0.37	0.19	0.030	0.0045	0.081	1.1	0.0038
		ΔG_{int} (kJ mol^{-1})	-51.2	-65.0	-44.6	ND	-43.8	-56.0	-57.7	-62.4	-67.3	-59.9	-53.1	-67.8
290		$K_{d,obs}$ (nM)	45 000	420	≥200 000	330	5600	360	5000	110	91	180	710	110
		ΔG_{obs} (kJ mol^{-1})	-25.8	-37.9	≥-22.0	-38.4	-31.2	-38.3	-31.5	-41.3	-41.8	-40.0	-36.5	-41.3
EA9-11		$K_{d,int}$ (nM)	260	1.2	300	0.60	23	1.1	2.9	0.27	0.16	0.44	4.1	0.27
		ΔG_{int} (kJ mol^{-1})	-39.0	-53.0	-38.7	-54.7	-45.3	-53.1	-50.7	-56.8	-58.1	-55.5	-49.8	-56.8
291		$K_{d,obs}$ (nM)	50 000	330	≥200 000	1100	4800	140	4800	140	130	360	910	130
		ΔG_{obs} (kJ mol^{-1})	-25.5	-38.4	≥-22.0	-35.4	-31.6	-40.6	-31.6	-40.6	-41.0	-38.3	-35.9	-41.0
EA9-11o		$K_{d,int}$ (nM)	1600	5.1	1600	11	110	2.4	15	1.9	1.2	4.7	28	1.7
		ΔG_{int} (kJ mol^{-1})	-34.4	-49.2	-34.3	-47.3	-41.3	-51.1	-46.5	-51.8	-52.9	-49.4	-44.8	-52.1

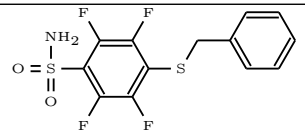
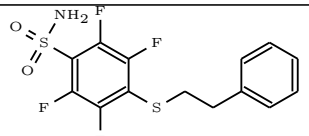
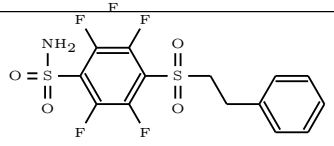
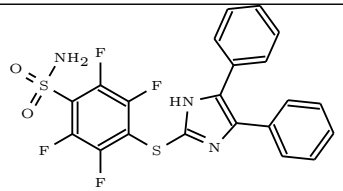
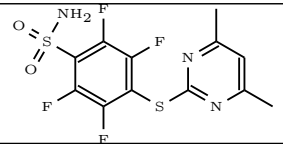
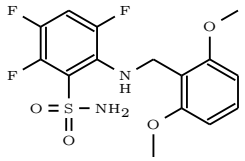
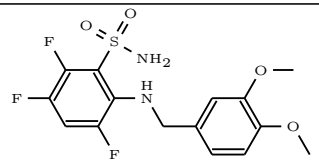
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
292		$K_{d,obs}$ (nM)	2000	130	≥200 000	56	6700	110	5000	63	77	130	360	130
		ΔG_{obs} (kJ mol^{-1})	-33.8	-41.0	≥-22.0	-43.1	-30.7	-41.3	-31.5	-42.8	-42.2	-41.0	-38.3	-41.0
EA9-2		$K_{d,int}$ (nM)	18	0.55	480	0.16	44	0.55	4.5	0.24	0.22	0.48	3.2	0.48
		ΔG_{int} (kJ mol^{-1})	-45.9	-55.0	-37.5	-58.2	-43.7	-55.0	-49.5	-57.1	-57.4	-55.3	-50.4	-55.3
293		$K_{d,obs}$ (nM)	1200	20	≥200 000	ND	10 000	ND	1700	11	ND	91	67	5.0
		ΔG_{obs} (kJ mol^{-1})	-35.0	-45.7	≥-22.0	ND	-29.7	ND	-34.3	-47.2	ND	-41.8	-42.6	-49.3
EA9-2o		$K_{d,int}$ (nM)	62	0.47	2600	ND	350	ND	8.1	0.23	ND	1.9	3.2	0.10
		ΔG_{int} (kJ mol^{-1})	-42.8	-55.3	-33.2	ND	-38.3	ND	-48.0	-57.2	ND	-51.8	-50.4	-59.3
294		$K_{d,obs}$ (nM)	560	50	≥200 000	100	2000	4.0	5600	20	3.3	33	130	8.3
		ΔG_{obs} (kJ mol^{-1})	-37.1	-43.3	≥-22.0	-41.5	-33.8	-49.8	-31.2	-45.7	-50.3	-44.4	-41.0	-47.9
EA9-3		$K_{d,int}$ (nM)	5.1	0.22	480	0.28	13	0.020	5.0	0.077	0.0094	0.13	1.1	0.032
		ΔG_{int} (kJ mol^{-1})	-49.2	-57.3	-37.5	-56.7	-46.8	-63.5	-49.3	-60.0	-65.4	-58.7	-53.1	-62.3
295		$K_{d,obs}$ (nM)	2000	22	≥200 000	400	13 000	7.7	3300	17	2.0	33	56	4.0
		ΔG_{obs} (kJ mol^{-1})	-33.8	-45.4	≥-22.0	-38.0	-29.1	-48.2	-32.5	-46.2	-51.6	-44.4	-43.1	-49.8
EA9-3o		$K_{d,int}$ (nM)	99	0.52	2600	6.1	440	0.20	16	0.34	0.030	0.69	2.7	0.082
		ΔG_{int} (kJ mol^{-1})	-41.6	-55.1	-33.2	-48.8	-37.7	-57.5	-46.2	-56.2	-62.4	-54.4	-50.9	-59.8
296		$K_{d,obs}$ (nM)	1900	59	≥200 000	180	180	ND	2500	11	29	83	110	13
		ΔG_{obs} (kJ mol^{-1})	-33.9	-42.9	≥-22.0	-40.0	-40.0	ND	-33.2	-47.2	-44.8	-42.0	-41.3	-46.7
EA9-4		$K_{d,int}$ (nM)	11	0.16	300	0.32	0.76	ND	1.4	0.027	0.051	0.20	0.63	0.032
		ΔG_{int} (kJ mol^{-1})	-47.2	-58.1	-38.7	-56.3	-54.1	ND	-52.5	-62.7	-61.1	-57.5	-54.6	-62.3

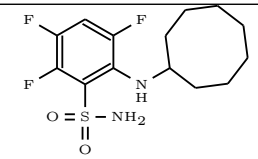
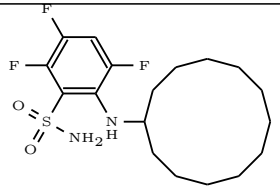
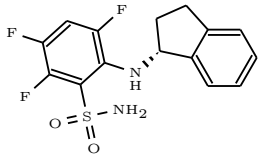
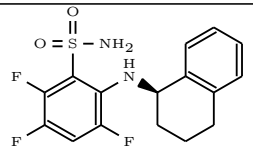
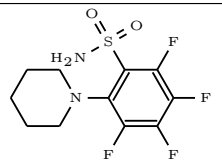
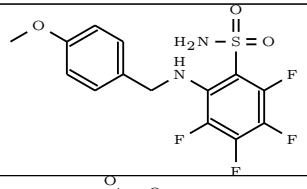
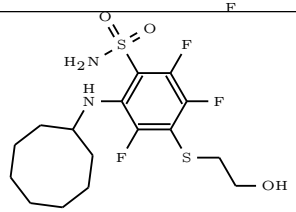
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
297		$K_{d,obs}$ (nM)	18 000	220	≥200 000	2100	12 000	16	4000	53	91	430	430	50
		ΔG_{obs} (kJ mol^{-1})	-28.1	-39.5	≥-22.0	-33.7	-29.3	-46.3	-32.0	-43.2	-41.8	-37.8	-37.8	-43.3
EA9-4o		$K_{d,int}$ (nM)	1000	5.7	2900	36	470	0.47	22	1.2	1.5	10	23	1.1
		ΔG_{int} (kJ mol^{-1})	-35.6	-48.9	-32.9	-44.2	-37.6	-55.4	-45.5	-52.9	-52.3	-47.5	-45.3	-53.1
298		$K_{d,obs}$ (nM)	≥200 000	1700	≥200 000	ND	≥200 000	≥200 000	4800	1700	2200	7100	1200	≥200 000
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-34.3	≥-22.0	ND	≥-22.0	≥-22.0	-31.6	-34.3	-33.5	-30.5	-35.0	≥-22.0
EA9-4o1		$K_{d,int}$ (nM)	20 000	12	5300	ND	2100	1600	6.8	10	9.9	43	18	1200
		ΔG_{int} (kJ mol^{-1})	-27.8	-47.1	-31.3	ND	-33.7	-34.5	-48.5	-47.5	-47.5	-43.7	-46.0	-35.1
299		$K_{d,obs}$ (nM)	1900	500	91 000	2500	7.1	2000	11 000	1700	26	290	290	20
		ΔG_{obs} (kJ mol^{-1})	-33.9	-37.4	-24.0	-33.2	-48.3	-33.8	-29.4	-34.3	-45.0	-38.8	-38.8	-45.7
AZ15-13		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
300		$K_{d,obs}$ (nM)	17 000	2400	≥200 000	≥200 000	45	25 000	59 000	10 000	710	14 000	6700	620
		ΔG_{obs} (kJ mol^{-1})	-28.3	-33.4	≥-22.0	≥-22.0	-43.6	-27.3	-25.1	-29.7	-36.5	-28.8	-30.7	-36.8
E15-1		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
301		$K_{d,obs}$ (nM)	1000	5.6	ND	13	33	0.50	63	1.0	13	17	6.2	2.5
		ΔG_{obs} (kJ mol^{-1})	-35.6	-49.0	ND	-46.9	-44.4	-55.2	-42.8	-53.4	-46.9	-46.2	-48.7	-51.0
DCP		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

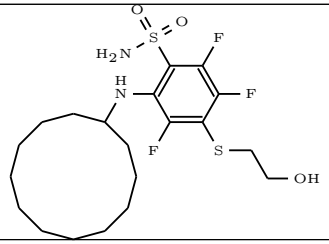
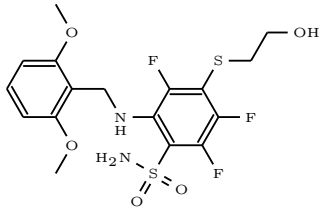
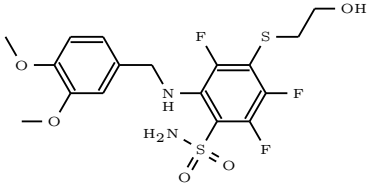
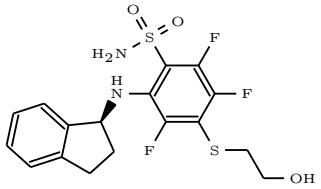
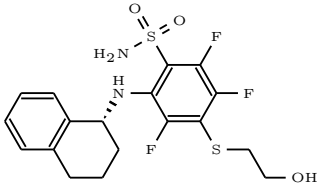
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
302		$K_{d,obs}$ (nM)	56 000	5300	100 000	4500	4000	13 000	5900	13 000	5000	2200	2600	1700
		ΔG_{obs} (kJ mol^{-1})	-25.3	-31.3	-23.7	-31.7	-32.0	-29.0	-31.0	-29.1	-31.5	-33.5	-33.2	-34.3
VR14-1		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
Fluorinated compounds														
303		$K_{d,obs}$ (nM)	61	21	1000	65	39	ND	14	8.3	43	110	40	43
		ΔG_{obs} (kJ mol^{-1})	-42.8	-45.6	-35.6	-42.7	-44.0	ND	-46.6	-47.9	-43.7	-41.3	-43.9	-43.7
TFMSA		$K_{d,int}$ (nM)	51	8.4	220	17	24	ND	1.2	2.9	11	38	33	15
		ΔG_{int} (kJ mol^{-1})	-43.3	-47.9	-39.5	-46.2	-45.3	ND	-53.0	-50.7	-47.2	-44.0	-44.4	-46.4
304		$K_{d,obs}$ (nM)	4.1	29	29 000	560	290	1.8	670	11	150	330	20	56
		ΔG_{obs} (kJ mol^{-1})	-49.8	-44.8	-26.9	-37.1	-38.8	-51.9	-36.7	-47.2	-40.5	-38.4	-45.7	-43.1
VD12-22		$K_{d,int}$ (nM)	0.22	0.73	400	9.2	11	0.053	3.5	0.25	2.5	7.5	1.1	1.2
		ΔG_{int} (kJ mol^{-1})	-57.3	-54.2	-38.0	-47.7	-47.2	-61.0	-50.2	-57.0	-51.1	-48.2	-53.3	-52.8
305		$K_{d,obs}$ (nM)	3.3	46	ND	740	450	38	430	56	150	780	76	35
		ΔG_{obs} (kJ mol^{-1})	-50.3	-43.6	ND	-36.4	-37.7	-44.0	-37.8	-43.0	-40.5	-36.3	-42.2	-44.2
VD10-9		$K_{d,int}$ (nM)	0.22	1.4	ND	15	21	1.3	2.7	1.5	3.0	21	4.9	0.96
		ΔG_{int} (kJ mol^{-1})	-57.3	-52.5	ND	-46.4	-45.6	-52.7	-50.8	-52.3	-50.6	-45.5	-49.3	-53.5
306		$K_{d,obs}$ (nM)	0.058	2.2	3800	100	200	0.050	140	1.1	5.4	37	2.4	3.6
		ΔG_{obs} (kJ mol^{-1})	-60.8	-51.3	-32.2	-41.4	-39.8	-61.1	-40.6	-53.1	-49.1	-44.1	-51.2	-50.1
VD12-05		$K_{d,int}$ (nM)	0.0035	0.065	60	2.0	8.8	0.0017	0.86	0.028	0.10	0.93	0.14	0.093
		ΔG_{int} (kJ mol^{-1})	-68.0	-60.4	-42.9	-51.7	-47.8	-69.9	-53.8	-62.6	-59.3	-53.6	-58.4	-59.5
307		$K_{d,obs}$ (nM)	0.15	11	29 000	440	400	1.7	200	13	32	220	11	5.0
		ΔG_{obs} (kJ mol^{-1})	-58.3	-47.3	-26.9	-37.7	-38.0	-52.1	-39.8	-46.8	-44.5	-39.5	-47.2	-49.3
VD10-13		$K_{d,int}$ (nM)	0.0094	0.32	480	8.5	18	0.056	1.2	0.34	0.61	5.8	0.68	0.13
		ΔG_{int} (kJ mol^{-1})	-65.4	-56.4	-37.5	-47.9	-46.0	-60.8	-52.9	-56.2	-54.7	-48.9	-54.4	-58.7
308		$K_{d,obs}$ (nM)	0.88	20	33 000	2000	200	40	500	14	29	250	50	29
		ΔG_{obs} (kJ mol^{-1})	-53.7	-45.7	-26.6	-33.8	-39.8	-43.9	-37.4	-46.6	-44.7	-39.2	-43.3	-44.8
AZ13-1		$K_{d,int}$ (nM)	0.22	2.4	2200	150	36	5.4	12	1.5	2.3	26	12	3.0
		ΔG_{int} (kJ mol^{-1})	-57.3	-51.2	-33.6	-40.4	-44.2	-49.1	-46.9	-52.4	-51.3	-45.0	-46.9	-50.6
309		$K_{d,obs}$ (nM)	0.32	15	ND	290	330	17	1000	5.0	67	50	6.7	83
		ΔG_{obs} (kJ mol^{-1})	-56.4	-46.4	ND	-38.8	-38.4	-46.2	-35.6	-49.3	-42.6	-43.3	-48.5	-42.0
VD12-01		$K_{d,int}$ (nM)	0.020	0.45	ND	5.5	15	0.56	6.1	0.13	1.3	1.3	0.41	2.2
		ΔG_{int} (kJ mol^{-1})	-63.5	-55.5	ND	-49.0	-46.4	-54.9	-48.7	-58.7	-52.8	-52.7	-55.7	-51.4
310		$K_{d,obs}$ (nM)	0.20	17	20 000	510	310	22	67	7.1	41	250	29	33
		ΔG_{obs} (kJ mol^{-1})	-57.6	-46.2	-27.9	-37.3	-38.6	-45.4	-42.6	-48.3	-43.9	-39.2	-44.8	-44.4
VD10-35		$K_{d,int}$ (nM)	0.064	2.5	1700	50	71	3.8	2.1	0.95	4.0	33	8.9	4.4
		ΔG_{int} (kJ mol^{-1})	-60.5	-51.0	-34.3	-43.3	-42.4	-50.0	-51.5	-53.5	-49.8	-44.4	-47.8	-49.6

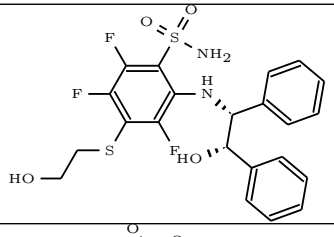
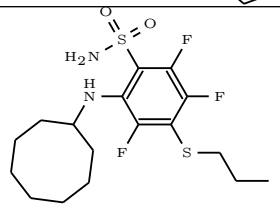
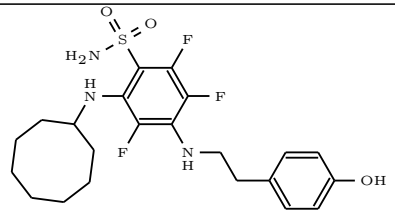
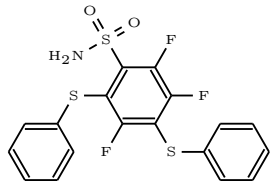
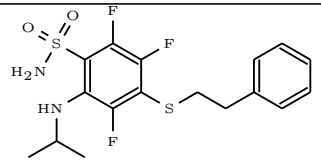
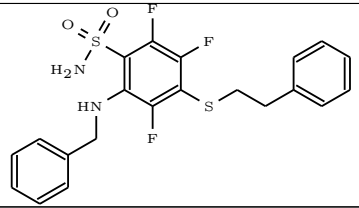
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
311		$K_{d,obs}$ (nM)	1.1	0.65	ND	730	200	2.0	200	0.22	5.1	120	0.32	0.50
		ΔG_{obs} (kJ mol^{-1})	-53.3	-54.5	ND	-36.4	-39.8	-51.6	-39.8	-57.3	-49.2	-41.1	-56.4	-55.2
VD10-49		$K_{d,int}$ (nM)	0.13	0.037	ND	27	17	0.13	2.3	0.011	0.19	5.9	0.037	0.025
		ΔG_{int} (kJ mol^{-1})	-58.8	-61.9	ND	-44.9	-46.1	-58.7	-51.2	-65.0	-57.7	-48.8	-61.9	-62.9
312		$K_{d,obs}$ (nM)	0.40	6.7	ND	87	25	5.0	220	13	8.3	110	2.5	5.0
		ΔG_{obs} (kJ mol^{-1})	-55.8	-48.5	ND	-41.9	-45.1	-49.3	-39.5	-46.9	-47.9	-41.3	-51.0	-49.3
VD10-28		$K_{d,int}$ (nM)	0.063	0.50	ND	4.2	2.8	0.42	3.4	0.82	0.40	7.3	0.39	0.33
		ΔG_{int} (kJ mol^{-1})	-60.5	-55.2	ND	-49.7	-50.7	-55.6	-50.2	-53.9	-55.8	-48.3	-55.9	-56.3
313		$K_{d,obs}$ (nM)	13	91	ND	1200	1100	1000	1000	300	710	1100	140	170
		ΔG_{obs} (kJ mol^{-1})	-46.7	-41.8	ND	-35.2	-35.4	-35.6	-35.6	-38.7	-36.5	-35.3	-40.6	-40.2
VD10-14		$K_{d,int}$ (nM)	0.18	0.57	ND	4.8	10	7.1	1.3	1.7	2.9	6.2	1.9	0.92
		ΔG_{int} (kJ mol^{-1})	-57.9	-54.8	ND	-49.4	-47.4	-48.4	-52.7	-52.1	-50.7	-48.7	-51.8	-53.6
314		$K_{d,obs}$ (nM)	0.20	9.1	ND	800	1000	8.3	1200	44	25	330	5.0	3.8
		ΔG_{obs} (kJ mol^{-1})	-57.6	-47.7	ND	-36.2	-35.6	-47.9	-35.0	-43.7	-45.1	-38.4	-49.3	-50.0
VD10-16		$K_{d,int}$ (nM)	0.0061	0.13	ND	7.5	22	0.14	3.7	0.55	0.23	4.2	0.15	0.048
		ΔG_{int} (kJ mol^{-1})	-66.6	-58.6	ND	-48.2	-45.5	-58.5	-50.0	-54.9	-57.2	-49.7	-58.3	-61.2
315		$K_{d,obs}$ (nM)	0.17	10	ND	67 000	500	ND	1800	20	18	330	2.5	6.7
		ΔG_{obs} (kJ mol^{-1})	-58.0	-47.5	ND	-24.8	-37.4	ND	-34.1	-45.7	-45.9	-38.4	-51.0	-48.5
VD12-70		$K_{d,int}$ (nM)	0.0048	0.14	ND	580	10	ND	5.1	0.24	0.16	4.0	0.070	0.079
		ΔG_{int} (kJ mol^{-1})	-67.2	-58.6	ND	-37.0	-47.4	ND	-49.2	-57.1	-58.1	-49.9	-60.3	-60.0
316		$K_{d,obs}$ (nM)	0.50	1.7	ND	360	330	1.9	ND	0.50	11	150	0.40	6.7
		ΔG_{obs} (kJ mol^{-1})	-55.2	-52.1	ND	-38.3	-38.4	-51.7	ND	-55.2	-47.2	-40.4	-55.8	-48.5
VD12-13		$K_{d,int}$ (nM)	0.011	0.018	ND	2.4	5.3	0.023	ND	0.0046	0.076	1.4	0.0087	0.062
		ΔG_{int} (kJ mol^{-1})	-65.0	-63.8	ND	-51.1	-49.1	-63.1	ND	-67.3	-60.1	-52.5	-65.6	-60.6
317		$K_{d,obs}$ (nM)	2.0	3.5	ND	300	2000	5.0	25 000	43	50	5000	2.2	50
		ΔG_{obs} (kJ mol^{-1})	-51.6	-50.2	ND	-38.7	-33.8	-49.3	-27.3	-43.7	-43.3	-31.5	-51.4	-43.3
VD10-20		$K_{d,int}$ (nM)	0.028	0.023	ND	1.3	20	0.037	34	0.25	0.21	29	0.030	0.29
		ΔG_{int} (kJ mol^{-1})	-62.7	-63.1	ND	-52.8	-45.7	-61.9	-44.3	-57.0	-57.4	-44.7	-62.4	-56.6
318		$K_{d,obs}$ (nM)	0.053	13	ND	3600	520	25	1700	14	15	100	13	8.3
		ΔG_{obs} (kJ mol^{-1})	-61.0	-46.9	ND	-32.3	-37.3	-45.1	-34.3	-46.6	-46.4	-41.5	-46.9	-47.9
VD12-63		$K_{d,int}$ (nM)	0.0026	0.29	ND	53	18	0.65	7.9	0.29	0.22	2.0	0.59	0.17
		ΔG_{int} (kJ mol^{-1})	-68.8	-56.6	ND	-43.2	-46.0	-54.5	-48.1	-56.6	-57.3	-51.6	-54.8	-58.0
319		$K_{d,obs}$ (nM)	0.098	18	ND	1600	1200	1000	1100	46	50	500	28	14
		ΔG_{obs} (kJ mol^{-1})	-59.4	-45.9	ND	-34.3	-35.0	-35.6	-35.3	-43.6	-43.3	-37.4	-44.9	-46.6
VD10-12		$K_{d,int}$ (nM)	0.0022	0.19	ND	11	20	12	2.4	0.42	0.34	4.6	0.60	0.13
		ΔG_{int} (kJ mol^{-1})	-69.2	-57.7	ND	-47.2	-45.7	-47.0	-51.1	-55.6	-56.2	-49.5	-54.7	-58.6

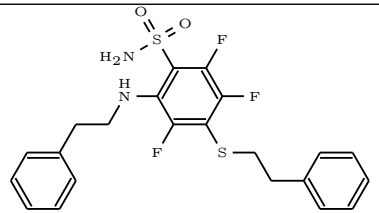
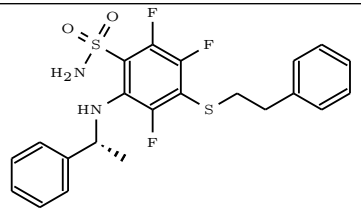
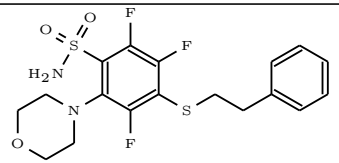
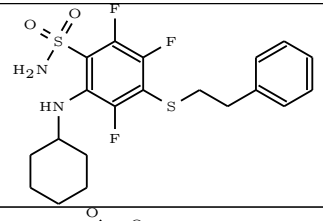
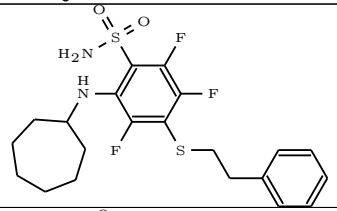
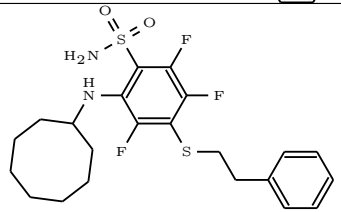
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
320		$K_{d,obs}$ (nM)	0.050	5.0	ND	450	250	5.0	500	1.0	3.3	17	0.50	0.67
		ΔG_{obs} (kJ mol^{-1})	-61.1	-49.3	ND	-37.7	-39.2	-49.3	-37.4	-53.4	-50.3	-46.2	-55.2	-54.5
VD10-51		$K_{d,int}$ (nM)	0.0012	0.057	ND	3.3	4.3	0.064	1.2	0.0099	0.024	0.17	0.012	0.0066
		ΔG_{int} (kJ mol^{-1})	-70.8	-60.8	ND	-50.4	-49.7	-60.5	-53.0	-65.3	-63.0	-58.1	-64.9	-66.3
321		$K_{d,obs}$ (nM)	0.10	1.6	ND	830	130	1.0	400	1.0	17	50	1.0	3.3
		ΔG_{obs} (kJ mol^{-1})	-59.3	-52.2	ND	-36.1	-40.8	-53.4	-38.0	-53.4	-46.2	-43.3	-53.4	-50.3
VD12-47		$K_{d,int}$ (nM)	0.011	0.085	ND	29	11	0.061	4.4	0.047	0.58	2.3	0.11	0.16
		ΔG_{int} (kJ mol^{-1})	-65.0	-59.8	ND	-44.8	-47.3	-60.6	-49.6	-61.3	-54.8	-51.2	-59.1	-58.2
322		$K_{d,obs}$ (nM)	0.067	3.3	ND	20 000	3300	3.3	20 000	2.5	7.7	100	3.3	1.7
		ΔG_{obs} (kJ mol^{-1})	-60.4	-50.3	ND	-27.9	-32.5	-50.3	-27.9	-51.0	-48.2	-41.5	-50.3	-52.1
VD11-49		$K_{d,int}$ (nM)	0.0044	0.10	ND	400	160	0.12	130	0.068	0.15	2.7	0.21	0.045
		ΔG_{int} (kJ mol^{-1})	-67.4	-59.2	ND	-38.0	-40.4	-58.9	-40.9	-60.3	-58.2	-50.8	-57.4	-61.4
323		$K_{d,obs}$ (nM)	0.40	20	ND	400	290	67	500	10	50	91	20	33
		ΔG_{obs} (kJ mol^{-1})	-55.8	-45.7	ND	-38.0	-38.8	-42.6	-37.4	-47.5	-43.3	-41.8	-45.7	-44.4
VD11-56		$K_{d,int}$ (nM)	0.036	0.86	ND	11	18	3.2	4.4	0.37	1.4	3.4	1.8	1.2
		ΔG_{int} (kJ mol^{-1})	-62.0	-53.8	ND	-47.2	-45.9	-50.4	-49.6	-55.9	-52.6	-50.3	-52.0	-52.8
324		$K_{d,obs}$ (nM)	0.33	5.0	20 000	ND	ND	ND	500	1.7	20	150	3.3	ND
		ΔG_{obs} (kJ mol^{-1})	-56.2	-49.3	-27.9	ND	ND	ND	-37.4	-52.1	-45.7	-40.4	-50.3	ND
AZ14-1		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
325		$K_{d,obs}$ (nM)	0.14	67	ND	570	400	200	2900	150	77	170	14	10
		ΔG_{obs} (kJ mol^{-1})	-58.5	-42.6	ND	-37.1	-38.0	-39.8	-32.8	-40.5	-42.2	-40.2	-46.6	-47.5
VD10-21a		$K_{d,int}$ (nM)	0.0040	0.93	ND	5.1	8.4	3.1	8.4	1.8	0.69	2.0	0.41	0.12
		ΔG_{int} (kJ mol^{-1})	-67.6	-53.6	ND	-49.2	-47.9	-50.5	-47.9	-51.9	-54.4	-51.6	-55.7	-58.8
326		$K_{d,obs}$ (nM)	0.094	3.4	ND	240	500	1.0	200	6.3	11	18	1.3	100 000
		ΔG_{obs} (kJ mol^{-1})	-59.5	-50.3	ND	-39.3	-37.4	-53.4	-39.8	-48.7	-47.3	-45.9	-52.6	-23.7
VD10-18		$K_{d,int}$ (nM)	0.012	0.20	ND	9.5	46	0.068	2.5	0.33	0.41	0.97	0.17	5300
		ΔG_{int} (kJ mol^{-1})	-64.8	-57.5	ND	-47.6	-43.6	-60.3	-51.1	-56.3	-55.7	-53.5	-58.0	-31.3
327		$K_{d,obs}$ (nM)	0.050	3.3	ND	290	ND	5.0	160	0.67	0.77	17	2.5	0.67
		ΔG_{obs} (kJ mol^{-1})	-61.1	-50.3	ND	-38.8	ND	-49.3	-40.4	-54.5	-54.1	-46.2	-51.0	-54.5
VD11-51		$K_{d,int}$ (nM)	0.021	0.68	ND	38	ND	1.1	6.6	0.12	0.10	3.0	1.0	0.12
		ΔG_{int} (kJ mol^{-1})	-63.3	-54.4	ND	-44.0	ND	-53.1	-48.5	-58.9	-59.3	-50.6	-53.3	-58.9

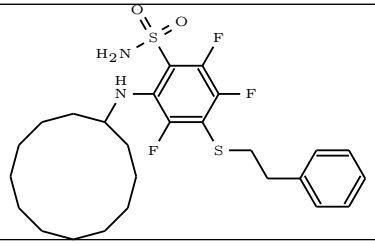
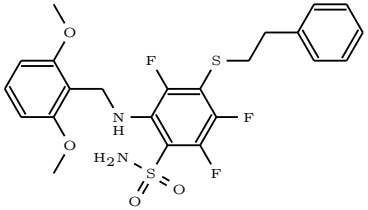
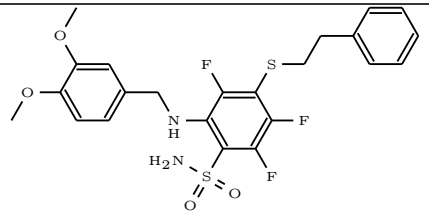
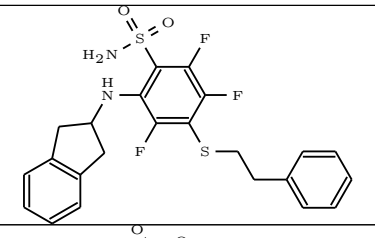
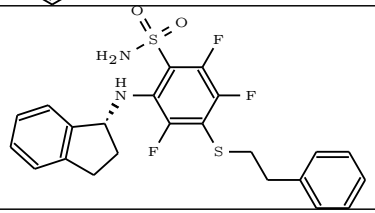
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
328		$K_{d,obs}$ (nM)	0.025	3.3	ND	1200	430	5.0	330	2.5	5.0	140	2.0	6.7
		ΔG_{obs} (kJ mol^{-1})	-62.9	-50.3	ND	-35.0	-37.8	-49.3	-38.4	-51.0	-49.3	-40.6	-51.6	-48.5
VD11-61		$K_{d,int}$ (nM)	0.000 66	0.042	ND	10	8.3	0.072	0.87	0.028	0.041	1.6	0.052	0.074
		ΔG_{int} (kJ mol^{-1})	-72.3	-61.6	ND	-47.4	-48.0	-60.2	-53.8	-62.7	-61.7	-52.2	-61.0	-60.1
329		$K_{d,obs}$ (nM)	0.32	1.7	ND	810	200	0.56	400	0.83	5.8	76	0.27	1.4
		ΔG_{obs} (kJ mol^{-1})	-56.4	-52.1	ND	-36.1	-39.8	-54.9	-38.0	-53.9	-48.9	-42.2	-56.8	-52.5
VD11-9		$K_{d,int}$ (nM)	0.024	0.061	ND	19	11	0.023	3.0	0.026	0.13	2.4	0.020	0.045
		ΔG_{int} (kJ mol^{-1})	-63.0	-60.6	ND	-45.8	-47.3	-63.1	-50.6	-62.8	-58.6	-51.1	-63.5	-61.4
330		$K_{d,obs}$ (nM)	0.25	1.2	ND	2500	140	ND	140	1.2	22	77	0.40	13
		ΔG_{obs} (kJ mol^{-1})	-57.0	-52.8	ND	-33.2	-40.6	ND	-40.6	-52.8	-45.4	-42.2	-55.8	-46.9
VD11-10		$K_{d,int}$ (nM)	0.087	0.21	ND	270	36	ND	4.8	0.18	2.4	11	0.14	1.8
		ΔG_{int} (kJ mol^{-1})	-59.7	-57.5	ND	-39.0	-44.2	ND	-49.3	-57.8	-51.2	-47.2	-58.5	-51.9
331		$K_{d,obs}$ (nM)	14	5.8	ND	83	330	6.7	140	1.7	1.0	540	2.0	40
		ΔG_{obs} (kJ mol^{-1})	-46.6	-48.9	ND	-42.0	-38.4	-48.5	-40.6	-52.1	-53.4	-37.2	-51.6	-43.9
VD10-45		$K_{d,int}$ (nM)	2.2	0.43	ND	4.0	38	0.57	2.2	0.11	0.048	35	0.31	2.6
		ΔG_{int} (kJ mol^{-1})	-51.3	-55.6	ND	-49.8	-44.1	-54.9	-51.4	-59.1	-61.2	-44.2	-56.4	-50.9
332		$K_{d,obs}$ (nM)	2.9	9.6	ND	1800	2000	1.4	1000	10	18	280	2.9	1.7
		ΔG_{obs} (kJ mol^{-1})	-50.7	-47.6	ND	-34.1	-33.8	-52.5	-35.6	-47.5	-46.0	-38.8	-50.7	-52.1
VD10-50		$K_{d,int}$ (nM)	0.23	0.37	ND	44	120	0.062	7.9	0.34	0.44	9.6	0.23	0.056
		ΔG_{int} (kJ mol^{-1})	-57.2	-56.0	ND	-43.7	-41.2	-60.6	-48.1	-56.2	-55.5	-47.6	-57.2	-60.8
333		$K_{d,obs}$ (nM)	1000	4000	ND	ND	20 000	ND	11 000	33 000	670	20 000	5000	2900
		ΔG_{obs} (kJ mol^{-1})	-35.6	-32.0	ND	ND	-27.9	ND	-29.4	-26.6	-36.7	-27.9	-31.5	-32.9
VD12-31		$K_{d,int}$ (nM)	19	37	ND	ND	280	ND	21	270	4.0	160	95	23
		ΔG_{int} (kJ mol^{-1})	-45.8	-44.1	ND	ND	-38.9	ND	-45.5	-39.0	-49.9	-40.3	-41.7	-45.3
334		$K_{d,obs}$ (nM)	560	670	ND	13 000	5000	610	13 000	6700	250	5000	140	500
		ΔG_{obs} (kJ mol^{-1})	-37.1	-36.7	ND	-29.1	-31.5	-36.9	-29.1	-30.7	-39.2	-31.5	-40.6	-37.4
VD12-37		$K_{d,int}$ (nM)	12	6.9	ND	83	78	7.1	27	60	1.7	45	3.0	4.5
		ΔG_{int} (kJ mol^{-1})	-47.0	-48.4	ND	-42.0	-42.2	-48.3	-45.0	-42.8	-52.1	-43.6	-50.5	-49.5

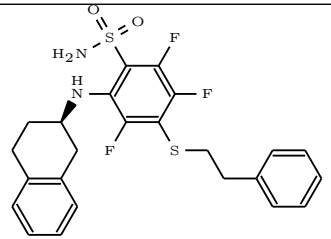
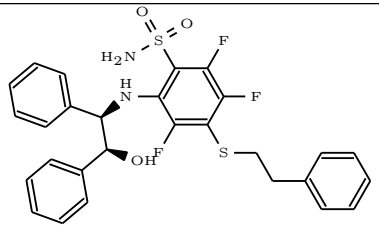
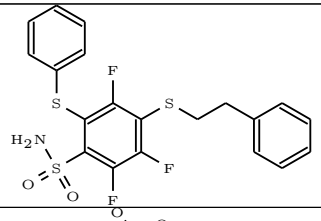
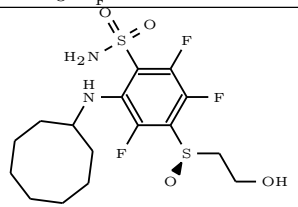
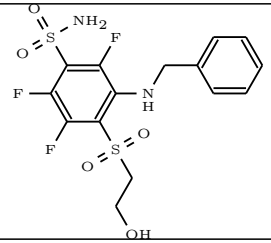
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
335		$K_{d,obs}$ (nM)	610	230	ND	1500	1200	20	4000	290	10	720	140	83
		ΔG_{obs} (kJ mol^{-1})	-36.9	-39.4	ND	-34.6	-35.2	-45.7	-32.0	-38.8	-47.5	-36.4	-40.7	-42.0
VD12-36		$K_{d,int}$ (nM)	9.3	1.7	ND	6.8	13	0.16	5.9	1.8	0.047	4.6	2.1	0.53
		ΔG_{int} (kJ mol^{-1})	-47.7	-52.1	ND	-48.5	-46.9	-58.1	-48.8	-51.9	-61.3	-49.5	-51.5	-55.1
336		$K_{d,obs}$ (nM)	2200	5200	≥200 000	1200	14 000	2500	≥200 000	56 000	7.1	8200	1000	500
		ΔG_{obs} (kJ mol^{-1})	-33.6	-31.4	≥-22.0	-35.0	-28.8	-33.2	≥-22.0	-25.2	-48.4	-30.2	-35.5	-37.4
VD12-35		$K_{d,int}$ (nM)	42	48	1000	7.5	200	26	1900	460	0.042	66	20	4.0
		ΔG_{int} (kJ mol^{-1})	-43.8	-43.4	-35.6	-48.2	-39.8	-45.0	-33.9	-37.6	-61.6	-42.6	-45.7	-49.8
337		$K_{d,obs}$ (nM)	12 000	3000	ND	40 000	10 000	67	3600	15 000	59	2500	380	330
		ΔG_{obs} (kJ mol^{-1})	-29.2	-32.7	ND	-26.1	-29.7	-42.6	-32.3	-28.7	-42.9	-33.2	-38.1	-38.4
VD12-38		$K_{d,int}$ (nM)	260	32	ND	270	160	0.78	7.6	130	0.39	23	8.2	3.0
		ΔG_{int} (kJ mol^{-1})	-39.1	-44.5	ND	-39.0	-40.4	-54.0	-48.2	-40.8	-55.8	-45.4	-48.0	-50.6
338		$K_{d,obs}$ (nM)	10 000	2200	ND	100 000	20 000	3300	7700	21 000	65	10 000	450	330
		ΔG_{obs} (kJ mol^{-1})	-29.7	-33.5	ND	-23.7	-27.9	-32.5	-30.3	-27.7	-42.7	-29.7	-37.6	-38.4
VD12-29-2		$K_{d,int}$ (nM)	160	17	ND	500	230	29	12	140	0.32	68	7.2	2.3
		ΔG_{int} (kJ mol^{-1})	-40.3	-46.1	ND	-37.4	-39.4	-44.7	-47.0	-40.6	-56.3	-42.6	-48.3	-51.3
339		$K_{d,obs}$ (nM)	130 000	29 000	ND	50 000	14 000	ND	≥200 000	≥200 000	3500	≥200 000	14 000	10 000
		ΔG_{obs} (kJ mol^{-1})	-23.0	-26.9	ND	-25.5	-28.8	ND	≥-22.0	≥-22.0	-32.4	≥-22.0	-28.8	-29.7
VD12-67-1		$K_{d,int}$ (nM)	680	71	ND	78	52	ND	500	2100	5.4	2100	71	21
		ΔG_{int} (kJ mol^{-1})	-36.6	-42.4	ND	-42.2	-43.2	ND	-37.4	-33.7	-49.1	-33.7	-42.4	-45.5
340		$K_{d,obs}$ (nM)	67	200	ND	ND	4000	4.3	710	560	50	1000	140	63
		ΔG_{obs} (kJ mol^{-1})	-42.6	-39.8	ND	ND	-32.0	-49.6	-36.5	-37.1	-43.3	-35.6	-40.6	-42.8
VD12-69-1		$K_{d,int}$ (nM)	1.6	2.3	ND	ND	70	0.057	1.7	5.6	0.37	10	3.4	0.63
		ΔG_{int} (kJ mol^{-1})	-52.2	-51.2	ND	ND	-42.5	-60.8	-52.0	-49.0	-56.0	-47.4	-50.3	-54.6
341		$K_{d,obs}$ (nM)	24 000	1000	≥200 000	1500	3300	100	5000	200	0.77	240	98	140
		ΔG_{obs} (kJ mol^{-1})	-27.4	-35.6	≥-22.0	-34.5	-32.5	-41.5	-31.5	-39.7	-54.1	-39.3	-41.6	-40.6
VD12-09		$K_{d,int}$ (nM)	460	9.1	980	8.9	45	1.0	9.3	1.6	0.0045	1.9	1.8	1.1
		ΔG_{int} (kJ mol^{-1})	-37.6	-47.7	-35.7	-47.8	-43.6	-53.4	-47.7	-52.2	-67.4	-51.8	-51.9	-53.1

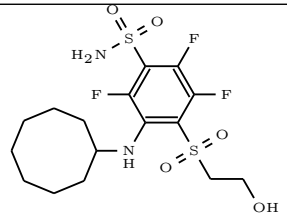
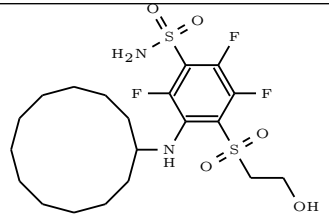
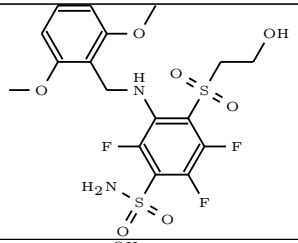
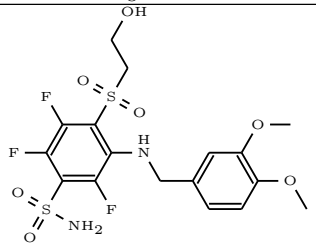
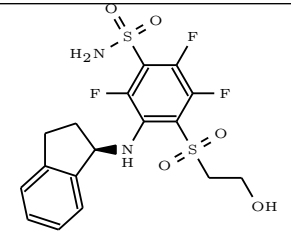
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
342		$K_{d,obs}$ (nM)	20 000	1700	ND	100 000	ND	50	33 000	3300	0.25	330	11	50
		ΔG_{obs} (kJ mol^{-1})	-27.9	-34.3	ND	-23.7	ND	-43.3	-26.6	-32.5	-57.0	-38.4	-47.2	-43.3
VD12-19		$K_{d,int}$ (nM)	390	15	ND	600	ND	0.52	63	27	0.0015	2.7	0.21	0.40
		ΔG_{int} (kJ mol^{-1})	-38.0	-46.4	ND	-36.9	ND	-55.1	-42.7	-44.9	-70.2	-50.9	-57.4	-55.7
343		$K_{d,obs}$ (nM)	20 000	20 000	ND	ND	33 000	1200	58 000	20 000	250	20 000	20 000	100
		ΔG_{obs} (kJ mol^{-1})	-27.9	-27.9	ND	ND	-26.6	-35.0	-25.2	-27.9	-39.2	-27.9	-27.9	-41.5
VD12-16		$K_{d,int}$ (nM)	430	210	ND	ND	520	15	120	180	1.7	180	430	0.91
		ΔG_{int} (kJ mol^{-1})	-37.8	-39.7	ND	ND	-37.3	-46.5	-41.0	-40.0	-52.1	-40.0	-37.8	-53.7
344		$K_{d,obs}$ (nM)	13 000	1300	ND	8300	670	50	11 000	750	110	4700	47	200
		ΔG_{obs} (kJ mol^{-1})	-28.9	-35.0	ND	-30.1	-36.7	-43.3	-29.4	-36.4	-41.3	-31.6	-43.5	-39.8
VD12-17		$K_{d,int}$ (nM)	260	12	ND	50	9.3	0.52	21	6.0	0.66	38	0.89	1.6
		ΔG_{int} (kJ mol^{-1})	-39.1	-47.1	ND	-43.3	-47.7	-55.1	-45.5	-48.8	-54.5	-44.0	-53.7	-52.2
345		$K_{d,obs}$ (nM)	8300	2800	ND	6700	10 000	330	3300	1700	7.4	1200	33	170
		ΔG_{obs} (kJ mol^{-1})	-30.1	-33.0	ND	-30.7	-29.7	-38.4	-32.5	-34.3	-48.2	-35.0	-44.4	-40.2
VD12-15		$K_{d,int}$ (nM)	180	29	ND	45	160	4.0	7.3	15	0.051	12	0.73	1.5
		ΔG_{int} (kJ mol^{-1})	-40.0	-44.7	ND	-43.6	-40.3	-49.8	-48.3	-46.4	-61.1	-47.1	-54.2	-52.3
346		$K_{d,obs}$ (nM)	20 000	10 000	ND	33 000	13 000	2500	25 000	12 000	10	2000	100	200
		ΔG_{obs} (kJ mol^{-1})	-27.9	-29.7	ND	-26.6	-29.0	-33.2	-27.3	-29.3	-47.5	-33.8	-41.5	-39.8
VD12-18		$K_{d,int}$ (nM)	390	93	ND	200	180	26	48	95	0.060	16	1.9	1.6
		ΔG_{int} (kJ mol^{-1})	-38.0	-41.7	ND	-39.8	-40.0	-45.0	-43.5	-41.7	-60.7	-46.2	-51.8	-52.2

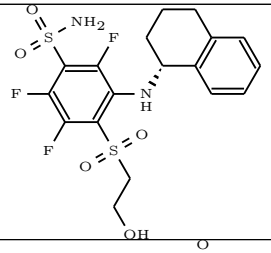
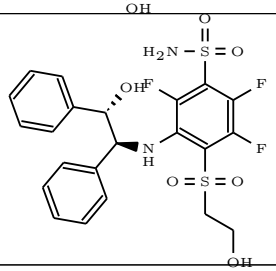
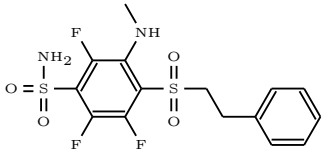
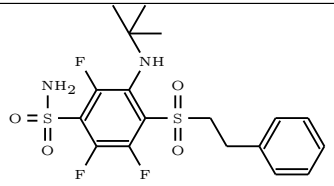
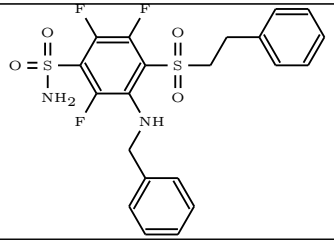
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
347		$K_{d,obs}$ (nM)	≥200 000	≥200 000	ND	100 000	ND	≥200 000	33 000	≥200 000	50	6700	5600	670
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	≥-22.0	ND	-23.7	ND	≥-22.0	-26.6	≥-22.0	-43.3	-30.7	-31.2	-36.7
VD12-11		$K_{d,int}$ (nM)	19 000	8900	ND	570	ND	10 000	61	7700	0.28	52	100	5.2
		ΔG_{int} (kJ mol^{-1})	-28.1	-30.0	ND	-37.1	ND	-29.7	-42.8	-30.3	-56.6	-43.2	-41.5	-49.2
348		$K_{d,obs}$ (nM)	≥200 000	3300	ND	17 000	25 000	1400	20 000	1400	1.7	1000	670	350
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-32.5	ND	-28.4	-27.3	-34.7	-27.9	-34.7	-52.1	-35.6	-36.7	-38.3
VD12-08		$K_{d,int}$ (nM)	19 000	31	ND	99	350	15	38	12	0.010	8.1	13	2.9
		ΔG_{int} (kJ mol^{-1})	-28.0	-44.6	ND	-41.6	-38.3	-46.4	-44.0	-47.1	-65.3	-48.0	-46.9	-50.7
349		$K_{d,obs}$ (nM)	100 000	10 000	ND	2200	ND	≥200 000	100 000	1700	14	1400	770	170
		ΔG_{obs} (kJ mol^{-1})	-23.7	-29.7	ND	-33.5	ND	≥-22.0	-23.7	-34.3	-46.6	-34.7	-36.3	-40.2
VD12-14		$K_{d,int}$ (nM)	61	2.9	ND	0.42	ND	330	6.0	0.43	0.0027	0.36	0.46	0.043
		ΔG_{int} (kJ mol^{-1})	-42.8	-50.6	ND	-55.7	ND	-38.5	-48.8	-55.6	-68.7	-56.0	-55.4	-61.5
350		$K_{d,obs}$ (nM)	41 000	2000	ND	100 000	33 000	40	560	56	0.35	1000	20	620
		ΔG_{obs} (kJ mol^{-1})	-26.0	-33.8	ND	-23.7	-26.6	-43.9	-37.1	-43.1	-56.1	-35.6	-45.7	-36.8
VD10-27		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
351		$K_{d,obs}$ (nM)	3300	500	ND	10 000	670	ND	3300	130	50	2900	67	43
		ΔG_{obs} (kJ mol^{-1})	-32.5	-37.4	ND	-29.7	-36.7	ND	-32.5	-41.0	-43.3	-32.9	-42.6	-43.7
VD11-71		$K_{d,int}$ (nM)	65	4.6	ND	60	9.3	ND	6.3	1.0	0.30	23	1.3	0.35
		ΔG_{int} (kJ mol^{-1})	-42.7	-49.5	ND	-42.9	-47.7	ND	-48.6	-53.4	-56.5	-45.3	-52.8	-56.1
352		$K_{d,obs}$ (nM)	5000	2500	ND	ND	1000	5.0	3300	1700	8.2	2900	110	67
		ΔG_{obs} (kJ mol^{-1})	-31.5	-33.2	ND	ND	-35.6	-49.3	-32.5	-34.3	-48.0	-32.9	-41.3	-42.6
VD11-53-2		$K_{d,int}$ (nM)	97	23	ND	ND	14	0.052	6.3	13	0.049	23	2.1	0.54
		ΔG_{int} (kJ mol^{-1})	-41.6	-45.3	ND	ND	-46.6	-61.0	-48.6	-46.7	-61.2	-45.3	-51.5	-55.0

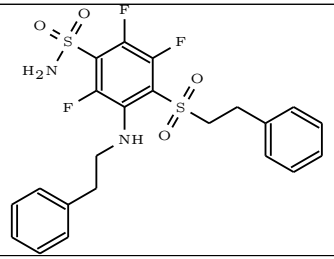
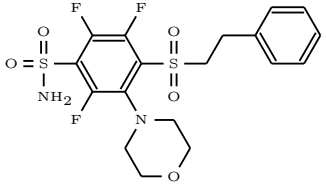
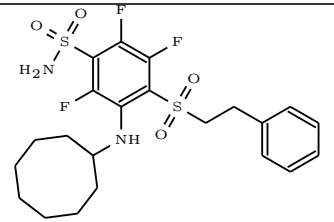
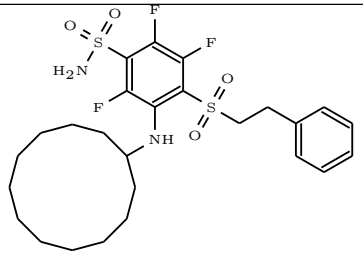
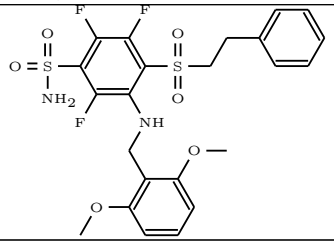
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
353		$K_{d,obs}$ (nM)	7100	2200	ND	≥200 000	5000	50	≥200 000	14 000	17	1000	330	50
		ΔG_{obs} (kJ mol^{-1})	-30.6	-33.5	ND	≥-22.0	-31.5	-43.3	≥-22.0	-28.8	-46.2	-35.6	-38.4	-43.3
VD11-65		$K_{d,int}$ (nM)	140	21	ND	6000	70	0.52	1900	120	0.099	8.1	6.3	0.40
		ΔG_{int} (kJ mol^{-1})	-40.7	-45.6	ND	-31.0	-42.5	-55.1	-33.9	-41.2	-59.4	-48.0	-48.6	-55.7
354		$K_{d,obs}$ (nM)	1700	3300	≥200 000	2000	200	17	1600	4000	29	5000	40	500
		ΔG_{obs} (kJ mol^{-1})	-34.3	-32.5	≥-22.0	-33.8	-39.8	-46.2	-34.4	-32.0	-44.7	-31.5	-43.9	-37.4
VD12-07		$K_{d,int}$ (nM)	32	31	1000	12	2.8	0.17	3.1	32	0.17	40	0.76	4.0
		ΔG_{int} (kJ mol^{-1})	-44.5	-44.6	-35.6	-47.0	-50.8	-57.9	-50.5	-44.4	-57.9	-43.9	-54.1	-49.8
355		$K_{d,obs}$ (nM)	29 000	5900	ND	170 000	33 000	≥200 000	100 000	≥200 000	20 000	100 000	100 000	11 000
		ΔG_{obs} (kJ mol^{-1})	-27.0	-31.0	ND	-22.4	-26.6	≥-22.0	-23.7	≥-22.0	-27.9	-23.7	-23.7	-29.4
VD11-67		$K_{d,int}$ (nM)	550	55	ND	990	460	3200	190	8100	120	810	1900	90
		ΔG_{int} (kJ mol^{-1})	-37.1	-43.1	ND	-35.6	-37.6	-32.6	-39.9	-30.2	-41.1	-36.2	-33.9	-41.8
356		$K_{d,obs}$ (nM)	11 000	250	ND	2000	20 000	100 000	50 000	170	3.8	500	500	ND
		ΔG_{obs} (kJ mol^{-1})	-29.5	-39.2	ND	-33.8	-27.9	-23.7	-25.5	-40.2	-49.9	-37.4	-37.4	ND
VD11-62		$K_{d,int}$ (nM)	210	2.3	ND	12	280	1000	95	1.3	0.023	4.0	9.5	ND
		ΔG_{int} (kJ mol^{-1})	-39.7	-51.2	ND	-47.0	-38.9	-35.5	-41.7	-52.6	-63.1	-49.8	-47.6	ND
357		$K_{d,obs}$ (nM)	≥200 000	1400	ND	ND	ND	170	14 000	1000	11	1200	500	500
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-34.7	ND	ND	ND	-40.2	-28.8	-35.6	-47.2	-35.0	-37.4	-37.4
VD12-06		$K_{d,int}$ (nM)	19 000	13	ND	ND	ND	1.7	27	8.1	0.066	10	9.5	4.0
		ΔG_{int} (kJ mol^{-1})	-28.0	-46.8	ND	ND	ND	-52.0	-44.9	-48.0	-60.4	-47.4	-47.6	-49.8
358		$K_{d,obs}$ (nM)	≥200 000	≥200 000	ND	100 000	ND	5000	≥200 000	≥200 000	6.8	4000	710	330
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	≥-22.0	ND	-23.7	ND	-31.5	≥-22.0	≥-22.0	-48.5	-32.0	-36.5	-38.4
VD11-59		$K_{d,int}$ (nM)	19 000	9300	ND	600	ND	52	1900	8100	0.041	32	14	2.7
		ΔG_{int} (kJ mol^{-1})	-28.0	-29.9	ND	-36.9	ND	-43.2	-33.9	-30.2	-61.7	-44.4	-46.7	-50.9

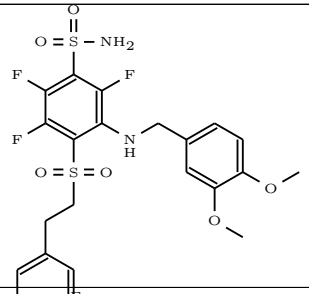
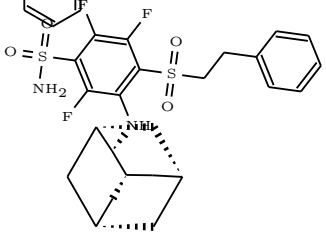
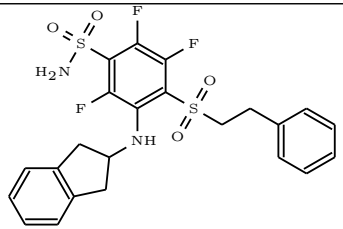
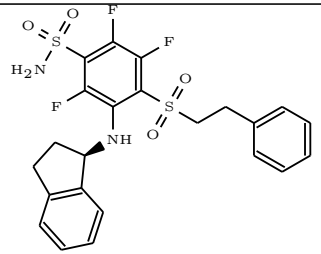
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
359		$K_{d,obs}$ (nM)	≥200 000	≥200 000	≥200 000	≥200 000	25 000	≥200 000	≥200 000	≥200 000	7.8	≥200 000	1700	4300
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	≥-22.0	≥-22.0	≥-22.0	-27.3	≥-22.0	≥-22.0	≥-22.0	-48.1	≥-22.0	-34.3	-31.8
PG7		$K_{d,int}$ (nM)	19 000	9300	1000	6000	350	2100	1900	8100	0.046	8100	32	35
		ΔG_{int} (kJ mol^{-1})	-28.0	-29.9	-35.6	-31.0	-38.3	-33.7	-33.9	-30.2	-61.3	-30.2	-44.5	-44.2
360		$K_{d,obs}$ (nM)	6700	≥200 000	ND	ND	ND	≥200 000	≥200 000	≥200 000	330	≥200 000	3300	1800
		ΔG_{obs} (kJ mol^{-1})	-30.7	≥-22.0	ND	ND	ND	≥-22.0	≥-22.0	≥-22.0	-38.4	≥-22.0	-32.5	-34.1
VD12-03		$K_{d,int}$ (nM)	130	9300	ND	ND	ND	10 000	1900	8100	2.0	8100	63	15
		ΔG_{int} (kJ mol^{-1})	-40.9	-29.9	ND	ND	ND	-29.6	-33.9	-30.2	-51.6	-30.2	-42.7	-46.5
361		$K_{d,obs}$ (nM)	350	1800	ND	ND	910	ND	20 000	3100	52	10 000	16	400
		ΔG_{obs} (kJ mol^{-1})	-38.3	-34.1	ND	ND	-35.8	ND	-27.9	-32.7	-43.2	-29.7	-46.2	-38.0
VD12-04		$K_{d,int}$ (nM)	6.8	17	ND	ND	13	ND	38	26	0.31	81	0.31	3.2
		ΔG_{int} (kJ mol^{-1})	-48.5	-46.1	ND	ND	-46.9	ND	-44.0	-45.1	-56.4	-42.1	-56.4	-50.4
362		$K_{d,obs}$ (nM)	5800	3300	ND	110 000	ND	250	6700	4000	3.3	1700	100	200
		ΔG_{obs} (kJ mol^{-1})	-31.1	-32.5	ND	-23.5	ND	-39.2	-30.7	-32.0	-50.3	-34.3	-41.5	-39.8
VD11-64		$K_{d,int}$ (nM)	110	31	ND	660	ND	2.6	13	32	0.020	13	1.9	1.6
		ΔG_{int} (kJ mol^{-1})	-41.3	-44.6	ND	-36.7	ND	-50.9	-46.9	-44.4	-63.5	-46.7	-51.8	-52.2
363		$K_{d,obs}$ (nM)	≥200 000	≥200 000	ND	100 000	ND	ND	≥200 000	≥200 000	ND	≥200 000	1000	170
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	≥-22.0	ND	-23.7	ND	ND	≥-22.0	≥-22.0	ND	≥-22.0	-35.6	-40.2
VD11-74		$K_{d,int}$ (nM)	19 000	9300	ND	600	ND	ND	1900	8100	ND	8100	19	1.3
		ΔG_{int} (kJ mol^{-1})	-28.0	-29.9	ND	-36.9	ND	ND	-33.9	-30.2	ND	-30.2	-45.8	-52.6

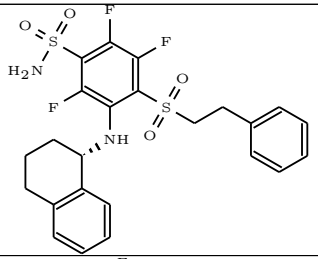
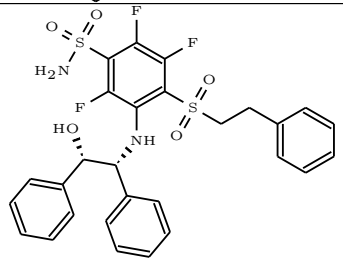
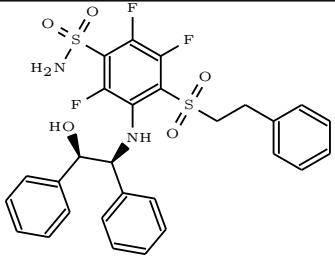
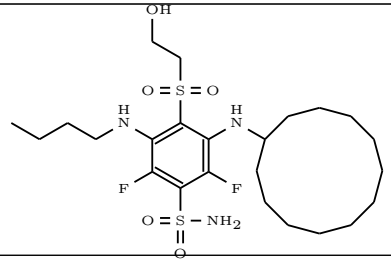
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
364		$K_{d,obs}$ (nM)	3500	≥200 000	ND	100 000	ND	≥200 000	≥200 000	≥200 000	31	≥200 000	330	500
		ΔG_{obs} (kJ mol^{-1})	-32.4	≥-22.0	ND	-23.7	ND	≥-22.0	≥-22.0	≥-22.0	-44.6	≥-22.0	-38.4	-37.4
VD11-75		$K_{d,int}$ (nM)	69	9300	ND	600	ND	2100	1900	8100	0.18	8100	6.3	4.0
		ΔG_{int} (kJ mol^{-1})	-42.5	-29.9	ND	-36.9	ND	-33.7	-33.9	-30.2	-57.8	-30.2	-48.6	-49.8
365		$K_{d,obs}$ (nM)	≥200 000	≥200 000	ND	≥200 000	ND	67 000	100 000	≥200 000	71	≥200 000	≥200 000	2500
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	≥-22.0	ND	≥-22.0	ND	-24.8	-23.7	≥-22.0	-42.4	≥-22.0	≥-22.0	-33.2
VD11-63		$K_{d,int}$ (nM)	19 000	9300	ND	6000	ND	700	190	8100	0.42	8100	19 000	20
		ΔG_{int} (kJ mol^{-1})	-28.0	-29.9	ND	-31.0	ND	-36.5	-39.9	-30.2	-55.6	-30.2	-28.0	-45.7
366		$K_{d,obs}$ (nM)	67 000	1100	ND	ND	33 000	ND	6300	2500	0.39	4000	50	ND
		ΔG_{obs} (kJ mol^{-1})	-24.8	-35.3	ND	ND	-26.6	ND	-30.9	-33.2	-55.8	-32.0	-43.3	ND
VD12-57		$K_{d,int}$ (nM)	1300	10	ND	ND	460	ND	12	20	0.0023	32	0.95	ND
		ΔG_{int} (kJ mol^{-1})	-34.9	-47.4	ND	ND	-37.6	ND	-47.0	-45.7	-69.0	-44.4	-53.5	ND
367		$K_{d,obs}$ (nM)	58 000	2200	≥200 000	13 000	1700	1800	3900	500	0.40	250	170	240
		ΔG_{obs} (kJ mol^{-1})	-25.2	-33.5	≥-22.0	-29.1	-34.3	-34.1	-32.1	-37.4	-55.8	-39.2	-40.2	-39.3
AZ13-2-2		$K_{d,int}$ (nM)	3300	61	3000	220	69	57	22	12	0.0071	6.0	9.4	5.7
		ΔG_{int} (kJ mol^{-1})	-32.5	-42.8	-32.8	-39.5	-42.5	-43.0	-45.5	-47.0	-66.2	-48.8	-47.6	-48.9
368		$K_{d,obs}$ (nM)	200	83	ND	90	330	3.3	130	130	0.63	25	14	13
		ΔG_{obs} (kJ mol^{-1})	-39.8	-42.0	ND	-41.8	-38.4	-50.3	-40.8	-41.0	-54.6	-45.1	-46.6	-46.9
VD10-39b		$K_{d,int}$ (nM)	23	4.6	ND	3.2	27	0.21	1.5	6.0	0.022	1.2	1.6	0.60
		ΔG_{int} (kJ mol^{-1})	-45.3	-49.5	ND	-50.4	-44.9	-57.5	-52.3	-48.8	-63.2	-52.9	-52.2	-54.7

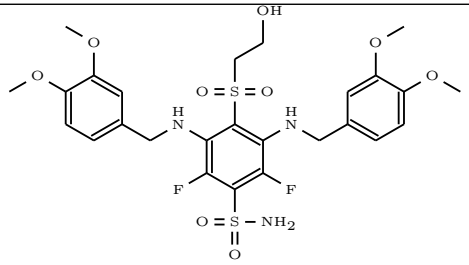
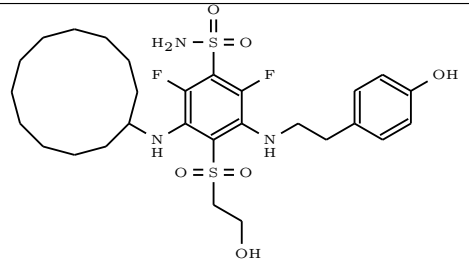
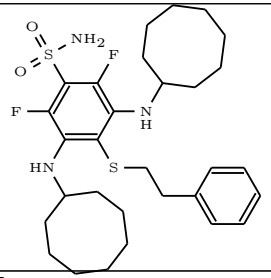
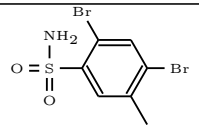
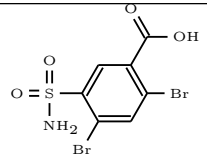
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
369		$K_{d,obs}$ (nM)	830	56	34 000	61	3300	16	67	8.6	0.032	2.9	4.0	4.3
		ΔG_{obs} (kJ mol^{-1})	-36.1	-43.0	-26.5	-42.8	-32.5	-46.3	-42.6	-47.9	-62.3	-50.6	-49.8	-49.6
VD11-4-2		$K_{d,int}$ (nM)	69	2.2	720	1.5	200	0.70	0.54	0.30	0.000 80	0.10	0.33	0.15
		ΔG_{int} (kJ mol^{-1})	-42.5	-51.4	-36.4	-52.3	-39.8	-54.3	-55.0	-56.5	-71.8	-59.3	-56.3	-58.3
370		$K_{d,obs}$ (nM)	520	42	ND	230	3400	200	200	71	52	5.0	0.91	17
		ΔG_{obs} (kJ mol^{-1})	-37.3	-43.8	ND	-39.4	-32.5	-39.8	-39.8	-42.4	-43.3	-49.3	-53.6	-46.2
VD12-30		$K_{d,int}$ (nM)	58	2.2	ND	7.7	270	12	2.2	3.3	1.7	0.23	0.099	0.77
		ΔG_{int} (kJ mol^{-1})	-43.0	-51.4	ND	-48.2	-39.0	-47.0	-51.4	-50.4	-52.0	-57.2	-59.4	-54.1
371		$K_{d,obs}$ (nM)	220	22	≥200 000	140	1000	10	1000	40	0.67	67	25	25
		ΔG_{obs} (kJ mol^{-1})	-39.5	-45.4	≥-22.0	-40.6	-35.6	-47.5	-35.6	-43.9	-54.5	-42.6	-45.1	-45.1
VD12-32		$K_{d,int}$ (nM)	27	1.3	6300	5.3	88	0.66	12	2.0	0.025	3.4	3.0	1.3
		ΔG_{int} (kJ mol^{-1})	-44.9	-52.7	-30.9	-49.1	-41.9	-54.5	-47.0	-51.6	-62.9	-50.3	-50.6	-52.8
372		$K_{d,obs}$ (nM)	83	180	ND	400	67	33	500	14	2.5	83	4.3	500
		ΔG_{obs} (kJ mol^{-1})	-42.0	-40.1	ND	-38.0	-42.6	-44.4	-37.4	-46.6	-51.0	-42.0	-49.6	-37.4
VD12-33		$K_{d,int}$ (nM)	9.2	9.3	ND	14	5.3	2.0	5.4	0.66	0.085	3.8	0.47	23
		ΔG_{int} (kJ mol^{-1})	-47.7	-47.7	ND	-46.7	-49.1	-51.6	-49.1	-54.5	-59.8	-49.9	-55.4	-45.3
373		$K_{d,obs}$ (nM)	1000	17	ND	67	1600	8.3	100	5.0	0.11	8.3	8.3	4.2
		ΔG_{obs} (kJ mol^{-1})	-35.6	-46.2	ND	-42.6	-34.4	-47.9	-41.5	-49.3	-59.1	-47.9	-47.9	-49.7
VD12-34		$K_{d,int}$ (nM)	110	0.91	ND	2.3	130	0.52	1.1	0.24	0.0039	0.40	0.94	0.20
		ΔG_{int} (kJ mol^{-1})	-41.2	-53.6	ND	-51.2	-40.8	-55.1	-53.1	-57.1	-67.7	-55.8	-53.6	-57.5

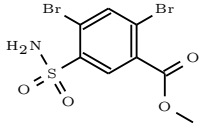
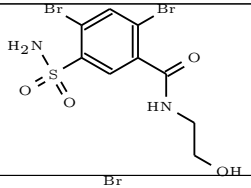
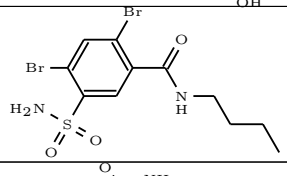
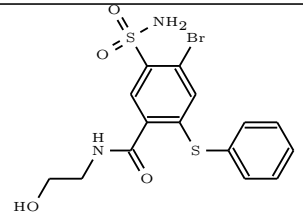
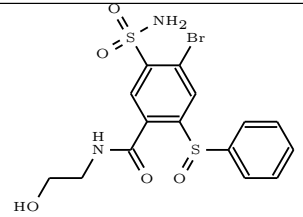
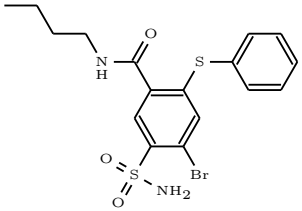
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
374		$K_{d,obs}$ (nM)	1400	61	ND	200	1000	150	450	10	0.050	13	10	6.5
		ΔG_{obs} (kJ mol^{-1})	-34.7	-42.8	ND	-39.8	-35.6	-40.4	-37.6	-47.5	-61.1	-46.8	-47.5	-48.6
VD12-23		$K_{d,int}$ (nM)	160	3.2	ND	6.8	79	9.1	4.9	0.46	0.0017	0.60	1.1	0.30
		ΔG_{int} (kJ mol^{-1})	-40.4	-50.4	ND	-48.5	-42.1	-47.7	-49.3	-55.4	-69.9	-54.7	-53.2	-56.5
375		$K_{d,obs}$ (nM)	22 000	64	ND	ND	5000	10	370	34	ND	16	4.9	ND
		ΔG_{obs} (kJ mol^{-1})	-27.6	-42.7	ND	ND	-31.5	-47.5	-38.2	-44.4	ND	-46.3	-49.3	ND
VD12-25-2		$K_{d,int}$ (nM)	2400	3.3	ND	ND	390	0.58	3.9	1.5	ND	0.71	0.52	ND
		ΔG_{int} (kJ mol^{-1})	-33.3	-50.3	ND	ND	-38.0	-54.8	-49.9	-52.3	ND	-54.3	-55.1	ND
376		$K_{d,obs}$ (nM)	75	5.9	ND	100 000	500	6.7	100	8.3	7.6	290	1.2	5.0
		ΔG_{obs} (kJ mol^{-1})	-42.3	-48.8	ND	-23.7	-37.4	-48.5	-41.5	-47.9	-48.2	-38.8	-52.8	-49.3
VD11-26		$K_{d,int}$ (nM)	8.2	0.31	ND	3400	40	0.40	1.1	0.38	0.26	13	0.14	0.23
		ΔG_{int} (kJ mol^{-1})	-48.0	-56.4	ND	-32.5	-43.9	-55.8	-53.2	-55.9	-56.9	-46.8	-58.6	-57.2
377		$K_{d,obs}$ (nM)	670	1.7	ND	250	720	0.50	50	0.22	0.86	67	5.0	ND
		ΔG_{obs} (kJ mol^{-1})	-36.7	-52.1	ND	-39.2	-36.5	-55.2	-43.3	-57.3	-53.8	-42.6	-49.3	ND
VD11-25		$K_{d,int}$ (nM)	73	0.088	ND	8.3	57	0.030	0.54	0.010	0.029	3.1	0.54	ND
		ΔG_{int} (kJ mol^{-1})	-42.3	-59.7	ND	-47.9	-43.0	-62.5	-55.0	-65.2	-62.5	-50.5	-55.0	ND
378		$K_{d,obs}$ (nM)	53	6.7	ND	910	250	6.7	110	5.0	3.3	40	2.5	ND
		ΔG_{obs} (kJ mol^{-1})	-43.2	-48.5	ND	-35.9	-39.2	-48.5	-41.3	-49.3	-50.3	-43.9	-51.0	ND
VD11-28		$K_{d,int}$ (nM)	5.8	0.35	ND	31	20	0.40	1.2	0.23	0.11	1.8	0.27	ND
		ΔG_{int} (kJ mol^{-1})	-48.9	-56.1	ND	-44.6	-45.7	-55.8	-52.9	-57.2	-59.0	-51.8	-56.8	ND

No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
379		$K_{d,obs}$ (nM)	910	17	ND	2500	500	5.0	330	4.0	3.3	33	6.7	14
		ΔG_{obs} (kJ mol^{-1})	-35.8	-46.2	ND	-33.2	-37.4	-49.3	-38.4	-49.8	-50.3	-44.4	-48.5	-46.6
VD11-54-2		$K_{d,int}$ (nM)	100	0.88	ND	85	40	0.30	3.6	0.18	0.11	1.5	0.72	0.66
		ΔG_{int} (kJ mol^{-1})	-41.5	-53.7	ND	-42.0	-43.9	-56.5	-50.1	-57.8	-59.0	-52.3	-54.3	-54.5
380		$K_{d,obs}$ (nM)	100	1.2	ND	1200	500	4.0	40	2.5	5.6	150	5.0	4.1
		ΔG_{obs} (kJ mol^{-1})	-41.5	-52.8	ND	-35.0	-37.4	-49.8	-43.9	-51.0	-49.0	-40.4	-49.3	-49.8
VD11-15		$K_{d,int}$ (nM)	11	0.066	ND	42	40	0.24	0.43	0.11	0.19	7.1	0.54	0.19
		ΔG_{int} (kJ mol^{-1})	-47.2	-60.4	ND	-43.8	-43.9	-57.1	-55.6	-59.0	-57.7	-48.4	-55.0	-57.7
381		$K_{d,obs}$ (nM)	410	13	ND	1000	2500	10	200	3.3	0.050	6.7	3.3	50
		ΔG_{obs} (kJ mol^{-1})	-37.9	-46.9	ND	-35.6	-33.2	-47.5	-39.8	-50.3	-61.1	-48.5	-50.3	-43.3
VD11-43-2		$K_{d,int}$ (nM)	45	0.66	ND	34	200	0.59	2.2	0.15	0.0017	0.31	0.36	2.3
		ΔG_{int} (kJ mol^{-1})	-43.6	-54.5	ND	-44.3	-39.8	-54.8	-51.4	-58.2	-69.9	-56.5	-56.0	-51.3
382		$K_{d,obs}$ (nM)	2200	710	ND	13 000	6700	610	2500	29 000	0.083	65	1.2	33
		ΔG_{obs} (kJ mol^{-1})	-33.5	-36.5	ND	-29.1	-30.7	-36.9	-33.2	-26.9	-59.8	-42.7	-52.9	-44.4
VD12-39		$K_{d,int}$ (nM)	250	37	ND	420	530	36	27	1300	0.0028	3.0	0.13	1.5
		ΔG_{int} (kJ mol^{-1})	-39.2	-44.1	ND	-37.8	-37.3	-44.2	-44.9	-34.9	-68.5	-50.6	-58.6	-52.3
383		$K_{d,obs}$ (nM)	100	22	≥200 000	1700	1000	4.0	220	670	ND	170	8.3	20
		ΔG_{obs} (kJ mol^{-1})	-41.5	-45.4	≥-22.0	-34.3	-35.6	-49.8	-39.5	-36.7	ND	-40.2	-47.9	-45.7
VD12-41		$K_{d,int}$ (nM)	11	1.1	5600	55	78	0.23	2.4	30	ND	7.5	0.88	0.90
		ΔG_{int} (kJ mol^{-1})	-47.2	-53.1	-31.2	-43.1	-42.2	-57.2	-51.2	-44.6	ND	-48.2	-53.7	-53.7

No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
384		$K_{d,obs}$ (nM)	210	36	110 000	29 000	200	2.5	670	6.7	3.3	250	3.3	33
		ΔG_{obs} (kJ mol^{-1})	-39.6	-44.2	-23.5	-27.0	-39.8	-51.0	-36.7	-48.5	-50.3	-39.2	-50.3	-44.4
VD12-43		$K_{d,int}$ (nM)	23	1.9	3200	970	16	0.15	7.2	0.31	0.11	11	0.36	1.5
		ΔG_{int} (kJ mol^{-1})	-45.3	-51.8	-32.6	-35.7	-46.3	-58.3	-48.3	-56.5	-59.0	-47.1	-56.0	-52.3
385		$K_{d,obs}$ (nM)	650	50	ND	1700	14 000	67	330	5.0	ND	17	5.6	50
		ΔG_{obs} (kJ mol^{-1})	-36.7	-43.3	ND	-34.3	-28.8	-42.6	-38.4	-49.3	ND	-46.2	-49.0	-43.3
VD11-17		$K_{d,int}$ (nM)	71	2.6	ND	56	1100	4.0	3.6	0.23	ND	0.77	0.60	2.3
		ΔG_{int} (kJ mol^{-1})	-42.4	-50.9	ND	-43.0	-35.3	-49.9	-50.1	-57.2	ND	-54.1	-54.7	-51.3
386		$K_{d,obs}$ (nM)	940	35	ND	ND	830	2.0	2000	15	ND	67	1.0	14
		ΔG_{obs} (kJ mol^{-1})	-35.8	-44.2	ND	ND	-36.1	-51.6	-33.8	-46.4	ND	-42.6	-53.4	-46.6
VD11-16		$K_{d,int}$ (nM)	100	1.9	ND	ND	66	0.12	22	0.70	ND	3.1	0.11	0.66
		ΔG_{int} (kJ mol^{-1})	-41.4	-51.8	ND	ND	-42.6	-58.9	-45.5	-54.3	ND	-50.5	-59.1	-54.5
387		$K_{d,obs}$ (nM)	50	2.9	ND	180	3300	1.2	330	1.0	6.7	41	2.0	2.0
		ΔG_{obs} (kJ mol^{-1})	-43.3	-50.7	ND	-40.0	-32.5	-52.8	-38.4	-53.4	-48.5	-43.9	-51.6	-51.6
VD12-42		$K_{d,int}$ (nM)	5.5	0.15	ND	6.0	260	0.074	3.6	0.046	0.23	1.9	0.22	0.092
		ΔG_{int} (kJ mol^{-1})	-49.0	-58.3	ND	-48.8	-39.0	-60.1	-50.1	-61.3	-57.2	-51.8	-57.4	-59.6

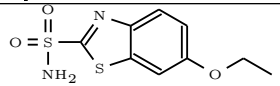
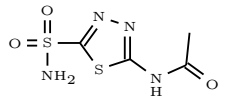
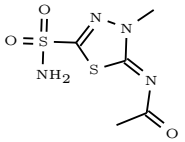
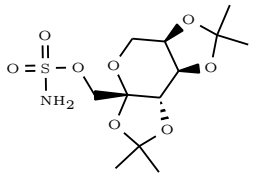
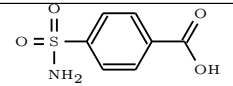
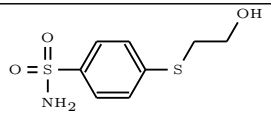
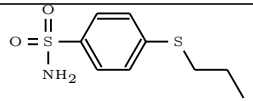
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
388		$K_{d,obs}$ (nM)	1000	6.7	ND	1200	1000	6.7	130	13	ND	50	1.4	100 000
		ΔG_{obs} (kJ mol^{-1})	-35.6	-48.5	ND	-35.0	-35.6	-48.5	-41.0	-46.9	ND	-43.3	-52.5	-23.7
VD12-40		$K_{d,int}$ (nM)	110	0.35	ND	42	79	0.40	1.4	0.57	ND	2.3	0.15	4600
		ΔG_{int} (kJ mol^{-1})	-41.3	-56.1	ND	-43.8	-42.1	-55.8	-52.6	-54.8	ND	-51.3	-58.2	-31.7
389		$K_{d,obs}$ (nM)	580	33	ND	300	2000	20	1000	10	50	250	5.6	100
		ΔG_{obs} (kJ mol^{-1})	-37.0	-44.4	ND	-38.7	-33.8	-45.7	-35.6	-47.5	-43.3	-39.2	-49.0	-41.5
VD11-39		$K_{d,int}$ (nM)	64	1.8	ND	10	160	1.2	11	0.46	1.7	11	0.60	4.6
		ΔG_{int} (kJ mol^{-1})	-42.7	-52.0	ND	-47.4	-40.4	-53.0	-47.3	-55.4	-52.1	-47.1	-54.7	-49.5
390		$K_{d,obs}$ (nM)	1400	91	ND	1400	3300	140	290	40	20	400	6.7	98
		ΔG_{obs} (kJ mol^{-1})	-34.8	-41.8	ND	-34.7	-32.5	-40.6	-38.8	-43.9	-45.7	-38.0	-48.5	-41.6
VD11-33		$K_{d,int}$ (nM)	150	4.8	ND	48	260	8.5	3.1	1.8	0.68	18	0.72	4.5
		ΔG_{int} (kJ mol^{-1})	-40.5	-49.4	ND	-43.4	-39.0	-47.9	-50.5	-51.8	-54.4	-45.9	-54.3	-49.5
391		$K_{d,obs}$ (nM)	17 000	960	≥200 000	17 000	33 000	≥200 000	10 000	≥200 000	0.26	120	260	1200
		ΔG_{obs} (kJ mol^{-1})	-28.3	-35.7	≥-22.0	-28.4	-26.6	≥-22.0	-29.7	≥-22.0	-56.9	-41.1	-39.1	-35.0
VD12-55		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

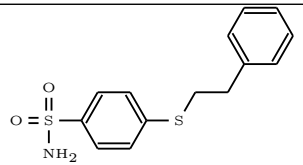
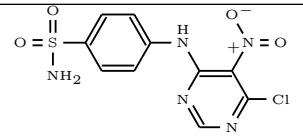
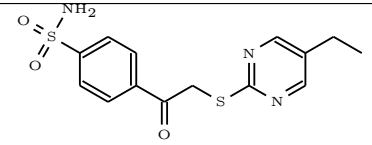
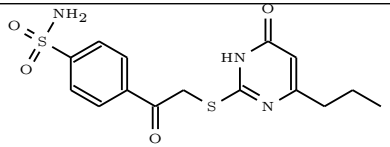
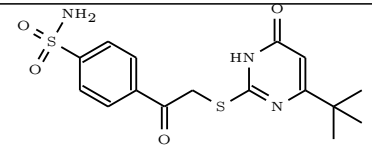
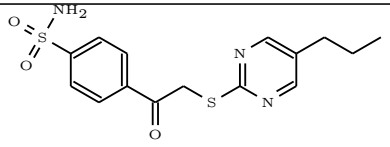
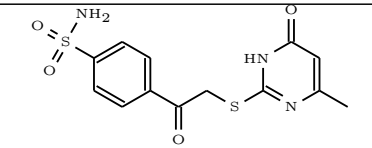
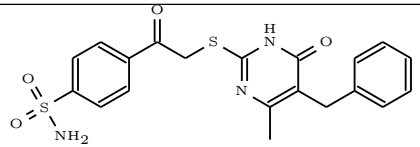
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
392 VD12-33-2		$K_{d,obs}$ (nM)	2000	670	ND	2900	2500	330	17 000	440	43	1000	230	ND
		ΔG_{obs} (kJ mol^{-1})	-33.8	-36.7	ND	-32.8	-33.2	-38.4	-28.4	-37.7	-43.7	-35.6	-39.4	ND
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
393 VD12-65		$K_{d,obs}$ (nM)	20 000	≥200 000	ND	100 000	33 000	≥200 000	5600	≥200 000	1.8	500	330	2000
		ΔG_{obs} (kJ mol^{-1})	-27.8	≥-22.0	ND	-23.7	-26.6	≥-22.0	-31.2	≥-22.0	-51.9	-37.4	-38.4	-33.8
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
394 VD11-57		$K_{d,obs}$ (nM)	≥200 000	≥200 000	≥200 000	≥200 000	ND	≥200 000	≥200 000	≥200 000	330	≥200 000	≥200 000	≥200 000
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	≥-22.0	≥-22.0	≥-22.0	ND	≥-22.0	≥-22.0	≥-22.0	-38.4	≥-22.0	≥-22.0	≥-22.0
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
Brominated compounds														
395 LJ14-2		$K_{d,obs}$ (nM)	1000	620	≥200 000	1300	3400	220	5000	1500	740	2500	240	83
		ΔG_{obs} (kJ mol^{-1})	-35.6	-36.8	≥-22.0	-34.9	-32.4	-39.5	-31.5	-34.5	-36.4	-33.2	-39.3	-42.0
		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
396 LJ14-3		$K_{d,obs}$ (nM)	18 000	420	14 000	1200	27 000	ND	7700	130	620	620	290	510
		ΔG_{obs} (kJ mol^{-1})	-28.1	-37.9	-28.8	-35.2	-27.1	ND	-30.3	-41.0	-36.8	-36.8	-38.8	-37.3
		$K_{d,int}$ (nM)	84	0.92	17	1.7	90	ND	3.5	0.24	0.89	1.2	1.3	0.98
		ΔG_{int} (kJ mol^{-1})	-42.0	-53.6	-46.2	-52.1	-41.8	ND	-50.2	-57.1	-53.7	-52.9	-52.7	-53.5

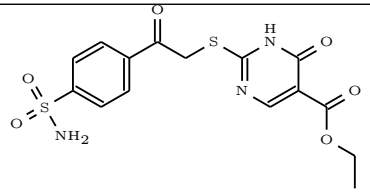
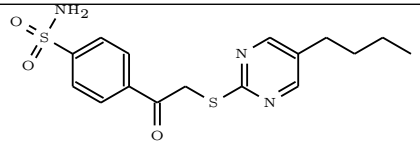
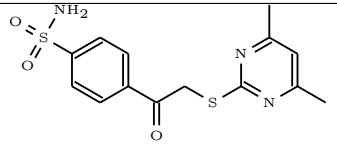
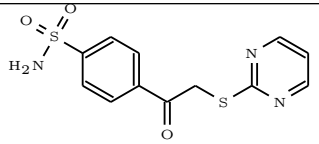
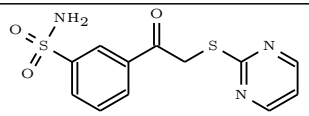
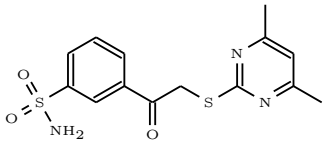
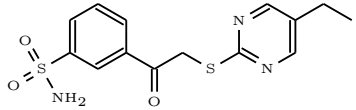
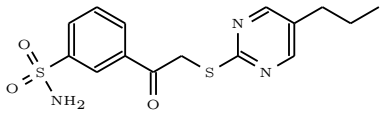
No. Cpd	Structure		CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
397		$K_{d,obs}$ (nM)	20 000	91	≥200 000	140	3700	33	290	56	120	330	63	40
		ΔG_{obs} (kJ mol^{-1})	-27.9	-41.8	≥-22.0	-40.6	-32.2	-44.4	-38.8	-43.1	-41.2	-38.4	-42.8	-43.9
LJ14-4		$K_{d,int}$ (nM)	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		ΔG_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
398		$K_{d,obs}$ (nM)	≥200 000	100	17 000	110	5900	250	1200	17	150	130	530	77
		ΔG_{obs} (kJ mol^{-1})	≥-22.0	-41.5	-28.4	-41.3	-31.0	-39.2	-35.2	-46.2	-40.4	-40.8	-37.3	-42.2
LJ14-5		$K_{d,int}$ (nM)	1800	0.44	40	0.31	39	1.2	1.1	0.064	0.43	0.51	4.7	0.29
		ΔG_{int} (kJ mol^{-1})	-34.0	-55.5	-43.9	-56.4	-44.0	-52.9	-53.3	-60.5	-55.6	-55.1	-49.4	-56.6
399		$K_{d,obs}$ (nM)	110 000	25	13 000	50	4000	18	290	6.7	29	43	370	21
		ΔG_{obs} (kJ mol^{-1})	-23.5	-45.1	-29.1	-43.3	-32.0	-45.9	-38.8	-48.5	-44.8	-43.7	-38.2	-45.6
LJ14-6		$K_{d,int}$ (nM)	1300	0.14	37	0.18	33	0.11	0.32	0.032	0.10	0.21	4.2	0.10
		ΔG_{int} (kJ mol^{-1})	-35.0	-58.5	-44.1	-57.9	-44.4	-59.0	-56.3	-62.3	-59.3	-57.4	-49.7	-59.3
400		$K_{d,obs}$ (nM)	3100	50	22 000	ND	3400	500	1700	13	13	2.0	100	13
		ΔG_{obs} (kJ mol^{-1})	-32.7	-43.3	-27.6	ND	-32.4	-37.4	-34.3	-46.7	-46.9	-51.6	-41.5	-46.9
LJ14-7		$K_{d,int}$ (nM)	29	0.22	53	ND	23	2.5	1.5	0.051	0.035	0.0077	0.90	0.048
		ΔG_{int} (kJ mol^{-1})	-44.8	-57.3	-43.2	ND	-45.4	-51.1	-52.4	-61.1	-62.0	-66.0	-53.7	-61.2
401		$K_{d,obs}$ (nM)	14 000	40	12 000	ND	2500	330	1300	18	17	36	130	14
		ΔG_{obs} (kJ mol^{-1})	-28.9	-43.9	-29.3	ND	-33.2	-38.4	-34.9	-45.9	-46.2	-44.2	-41.0	-46.6
LJ14-10		$K_{d,int}$ (nM)	120	0.18	28	ND	16	1.7	1.2	0.070	0.047	0.14	1.1	0.055
		ΔG_{int} (kJ mol^{-1})	-41.0	-57.9	-44.8	ND	-46.2	-52.1	-52.9	-60.3	-61.3	-58.5	-53.1	-60.9
402		$K_{d,obs}$ (nM)	830	10	6700	3.5	3300	29	830	2.9	2.5	0.80	130	4.0
		ΔG_{obs} (kJ mol^{-1})	-36.1	-47.5	-30.7	-50.2	-32.5	-44.8	-36.1	-50.7	-51.0	-54.0	-41.0	-49.8
LJ14-9		$K_{d,int}$ (nM)	6.1	0.035	13	0.0077	17	0.11	0.60	0.0087	0.0056	0.0024	0.90	0.012
		ΔG_{int} (kJ mol^{-1})	-48.8	-62.1	-46.9	-65.9	-46.0	-59.0	-54.7	-65.6	-66.8	-68.9	-53.7	-64.8

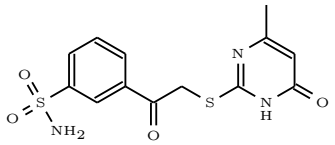
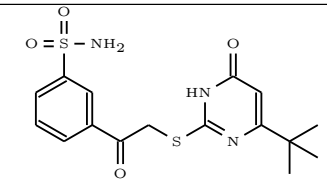
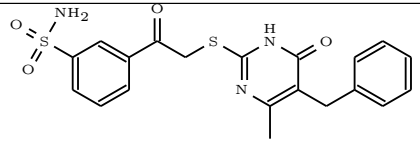
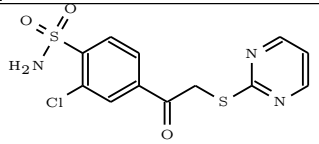
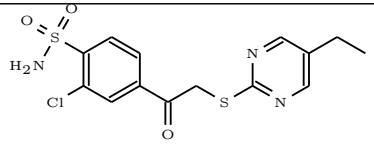
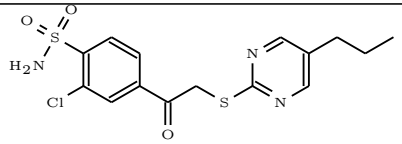
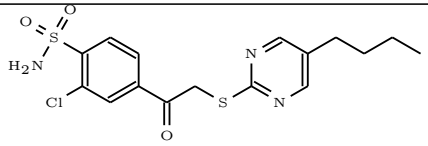
1.2 Table 2

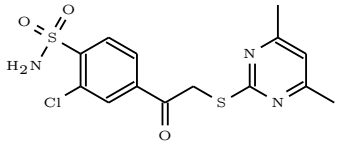
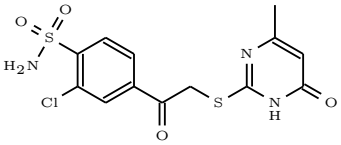
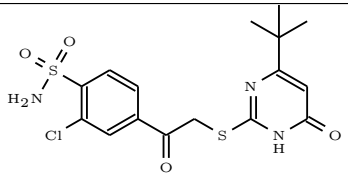
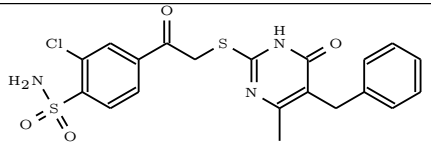
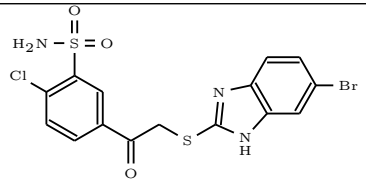
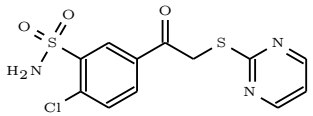
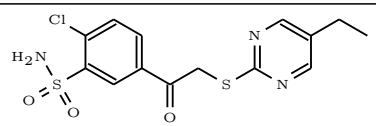
Table 2: Intrinsic thermodynamic parameters of compound binding to CAs at pH7.0 and 37 °C

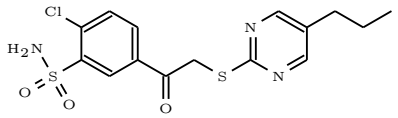
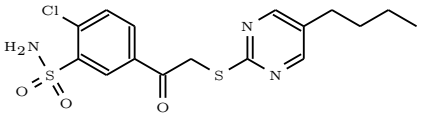
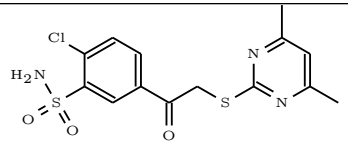
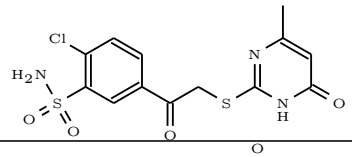
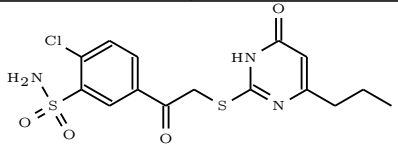
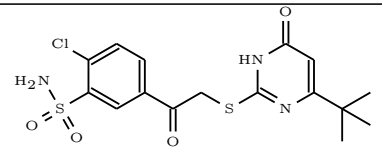
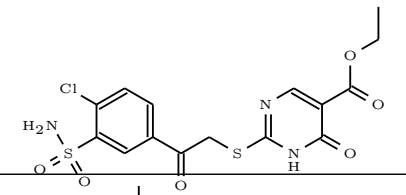
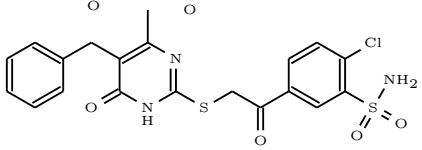
No. Cpd	Structure				Intrinsic thermodynamic binding parameters											
					CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
Non-halogenated compounds																
1		$pK_{a,SA}$	7.82	$K_{d,int}$ (nM)	2.0	0.073	160	3.1	2.3	0.57	0.40	0.031	0.071	3.6	2.3	0.51
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.4	ΔG_{int} (kJ mol^{-1})	-51.6	-60.2	-40.3	-50.6	-51.3	-54.9	-55.8	-62.4	-60.3	-50.1	-51.3	-55.2
EZA		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.9	ΔH_{int} (kJ mol^{-1})	-53.6	-74.9	ND	-48.0	ND	-58.3	-55.2	-56.1	-58.2	-51.9	-50.8	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	19.5	$-T\Delta S_{int}$ (kJ mol^{-1})	2.0	14.7	ND	-2.6	ND	3.4	-0.6	-6.3	-2.1	1.7	-0.5	ND
2		$pK_{a,SA}$	7.03	$K_{d,int}$ (nM)	1100	9.8	4600	12	270	34	9.8	2.4	2.9	24	35	12
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-41.7	ΔG_{int} (kJ mol^{-1})	-35.5	-47.5	-31.7	-47.0	-39.0	-44.3	-47.6	-51.2	-50.7	-45.2	-44.3	-47.1
AZM		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-18.8	ΔH_{int} (kJ mol^{-1})	-50.3	-51.5	ND	-47.1	ND	ND	-35.5	-36.4	-56.1	-47.9	-51.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.9	$-T\Delta S_{int}$ (kJ mol^{-1})	14.8	4.0	ND	0.0	ND	ND	-12.0	-14.8	5.5	2.7	7.3	ND
3		$pK_{a,SA}$	6.86	$K_{d,int}$ (nM)	110	27	5600	41	ND	19	44	11	6.0	110	110	25
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-40.7	ΔG_{int} (kJ mol^{-1})	-41.4	-45.0	-31.2	-43.8	ND	-45.8	-43.7	-47.2	-48.8	-41.3	-41.4	-45.1
MZM		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-20.5	ΔH_{int} (kJ mol^{-1})	-47.6	-45.7	ND	ND	ND	ND	ND	ND	ND	ND	-37.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.2	$-T\Delta S_{int}$ (kJ mol^{-1})	6.3	0.8	ND	ND	ND	ND	ND	ND	ND	ND	-3.8	ND
4		$pK_{a,SA}$	8.50	$K_{d,int}$ (nM)	970	1.4	1500	0.58	20 000	0.038	35	0.30	0.30	0.97	6.8	0.24
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-50.5	ΔG_{int} (kJ mol^{-1})	-35.7	-52.5	-34.6	-54.8	-27.8	-61.9	-44.3	-56.6	-56.6	-53.5	-48.5	-57.2
TPM		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.8	ΔH_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	-25.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	23.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	-23.3	ND
5		$pK_{a,SA}$	9.24	$K_{d,int}$ (nM)	61	10	270	5.4	12	57	5.8	8.9	3.0	7.4	30	8.9
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-54.9	ΔG_{int} (kJ mol^{-1})	-42.8	-47.5	-39.0	-49.1	-47.1	-43.0	-48.9	-47.8	-50.6	-48.3	-44.7	-47.8
CARBS		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-17.1	ΔH_{int} (kJ mol^{-1})	-28.7	-32.1	ND	ND	ND	ND	ND	ND	ND	ND	-33.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	37.7	$-T\Delta S_{int}$ (kJ mol^{-1})	-14.2	-15.4	ND	ND	ND	ND	ND	ND	ND	ND	-11.3	ND
10		$pK_{a,SA}$	9.96	$K_{d,int}$ (nM)	0.11	0.070	ND	1.2	4.2	5.5	0.50	0.086	0.26	1.2	1.4	0.11
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-59.1	ΔG_{int} (kJ mol^{-1})	-59.1	-60.3	ND	-52.9	-49.7	-49.1	-55.2	-59.8	-56.9	-52.9	-52.5	-59.2
VD11-31		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-38.9	ΔH_{int} (kJ mol^{-1})	-55.6	-56.5	ND	ND	ND	ND	ND	-43.2	ND	-41.1	-39.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.2	$-T\Delta S_{int}$ (kJ mol^{-1})	-3.5	-3.8	ND	ND	ND	ND	ND	-16.5	ND	-11.8	-13.0	ND
11		$pK_{a,SA}$	10.2	$K_{d,int}$ (nM)	0.0029	0.0070	ND	0.30	1.5	0.021	0.048	0.0098	0.018	0.081	0.16	0.0063
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-60.6	ΔG_{int} (kJ mol^{-1})	-68.5	-66.2	ND	-56.5	-52.3	-63.4	-61.3	-65.4	-63.8	-59.9	-58.1	-66.5
VD12-10		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-39.3	ΔH_{int} (kJ mol^{-1})	-62.7	-69.0	ND	ND	ND	ND	ND	-45.0	ND	-56.4	-47.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.3	$-T\Delta S_{int}$ (kJ mol^{-1})	-5.8	2.8	ND	ND	ND	ND	ND	-20.3	ND	-3.5	-10.6	ND

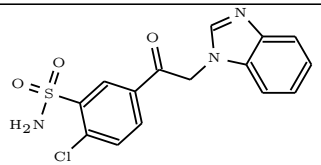
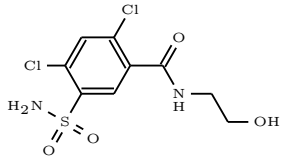
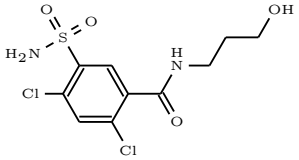
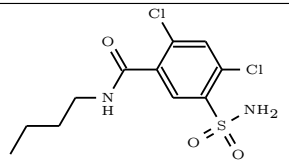
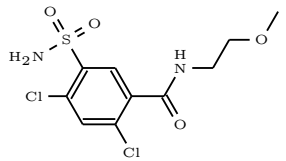
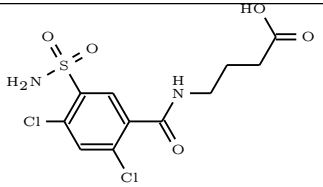
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
12		$pK_{a,SA}$	10.1	$K_{d,int}$ (nM)	0.0032	0.0039	36	ND	0.65	0.0054	0.077	0.0049	0.017	0.063	0.034	0.0055
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-60.1	ΔG_{int} (kJ mol^{-1})	-68.3	-67.8	-44.2	ND	-54.5	-66.9	-60.1	-67.2	-64.0	-60.6	-62.1	-66.8
VD11-36		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-40.2	ΔH_{int} (kJ mol^{-1})	-57.5	-58.4	ND	ND	ND	ND	ND	-45.7	ND	-52.0	-55.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	19.9	$-T\Delta S_{int}$ (kJ mol^{-1})	-10.7	-9.4	ND	ND	ND	ND	ND	-21.4	ND	-8.6	-6.7	ND
44		$pK_{a,SA}$	10.1	$K_{d,int}$ (nM)	0.41	0.032	1.9	1.1	ND	1.3	0.90	0.041	0.015	0.51	0.0014	0.077
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-60.0	ΔG_{int} (kJ mol^{-1})	-55.7	-62.3	-51.8	-53.1	ND	-52.7	-53.7	-61.7	-64.3	-55.2	-70.3	-60.1
JS45		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-21.0	ΔH_{int} (kJ mol^{-1})	-35.0	-49.1	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	39.0	$-T\Delta S_{int}$ (kJ mol^{-1})	-20.7	-13.3	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
53		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.090	0.022	ND	0.41	3.8	7.9	1.8	0.085	ND	1.5	0.10	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-59.6	-63.3	ND	-55.8	-50.0	-48.1	-51.9	-59.8	ND	-52.3	-59.3	ND
E63		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-51.6	-60.6	ND	ND	ND	ND	ND	-60.0	ND	-28.4	-61.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-8.1	-2.6	ND	ND	ND	ND	ND	0.2	ND	-24.0	2.4	ND
54		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.054	0.15	ND	0.23	1.8	2.0	0.45	0.38	ND	0.14	0.23	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-61.0	-58.4	ND	-57.2	-52.0	-51.7	-55.5	-55.9	ND	-58.5	-57.3	ND
E66		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-60.1	-35.5	ND	ND	ND	ND	ND	-33.6	ND	-28.1	-43.9	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-0.9	-22.9	ND	ND	ND	ND	ND	-22.3	ND	-30.4	-13.4	ND
55		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.0063	0.12	ND	0.44	4.1	4.0	1.8	0.074	0.036	0.26	0.018	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-66.5	-59.0	ND	-55.6	-49.8	-49.9	-51.9	-60.1	-62.0	-56.9	-63.9	ND
E67		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-61.5	-34.7	ND	ND	ND	ND	ND	-37.2	ND	-23.5	-48.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-5.0	-24.3	ND	ND	ND	ND	ND	-23.0	ND	-33.4	-15.7	ND
56		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.080	0.022	ND	0.23	4.1	12	1.8	0.10	ND	2.2	0.082	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-59.9	-63.3	ND	-57.2	-49.8	-46.9	-51.9	-59.3	ND	-51.4	-59.9	ND
E61		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-52.6	-41.8	ND	ND	ND	ND	ND	-50.3	ND	-27.3	-58.9	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-7.4	-21.5	ND	ND	ND	ND	ND	-9.0	ND	-24.1	-1.0	ND
57		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.24	0.12	ND	0.43	1.3	5.0	1.3	0.26	ND	0.85	1.3	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-57.1	-59.0	ND	-55.6	-52.7	-49.3	-52.7	-57.0	ND	-53.9	-52.8	ND
E59		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-47.4	-40.2	ND	ND	ND	ND	ND	-64.1	ND	-24.6	-48.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-9.7	-18.7	ND	ND	ND	ND	ND	7.1	ND	-29.2	-4.3	ND
58		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.12	0.039	ND	0.33	2.9	7.9	0.45	0.22	ND	1.1	0.030	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-58.9	-61.8	ND	-56.3	-50.7	-48.1	-55.5	-57.4	ND	-53.2	-62.5	ND
E60		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-47.2	-38.0	ND	ND	ND	ND	ND	-38.3	ND	ND	-48.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-11.6	-23.8	ND	ND	ND	ND	ND	-19.1	ND	ND	-13.9	ND

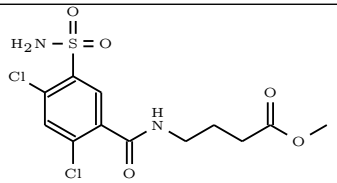
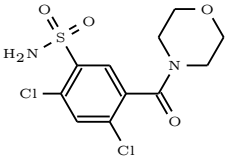
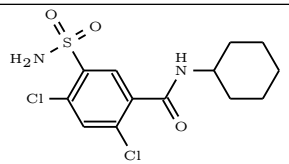
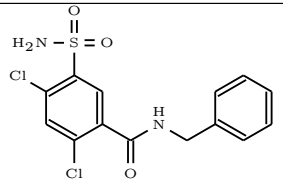
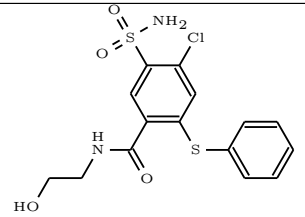
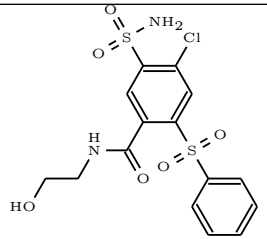
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
59		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.095	0.032	ND	0.085	0.88	9.0	0.90	0.31	ND	0.57	1.0	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-59.5	-62.3	ND	-59.8	-53.8	-47.8	-53.7	-56.5	ND	-54.9	-53.4	ND
E62		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-58.0	-57.7	ND	ND	ND	ND	ND	-55.6	ND	ND	-59.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-1.5	-4.6	ND	ND	ND	ND	ND	-0.9	ND	ND	6.0	ND
60		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.090	0.025	ND	0.36	1.9	3.6	1.8	0.15	ND	2.2	0.10	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-59.7	-62.9	ND	-56.0	-51.8	-50.1	-51.9	-58.3	ND	-51.4	-59.3	ND
E64		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-38.1	-55.3	ND	ND	ND	ND	ND	-59.9	ND	-37.3	-57.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-21.6	-7.7	ND	ND	ND	ND	ND	1.6	ND	-14.1	-2.2	ND
61		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.071	0.059	ND	0.69	3.8	2.0	0.90	0.19	ND	1.4	0.30	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-60.3	-60.8	ND	-54.4	-50.0	-51.7	-53.7	-57.7	ND	-52.6	-56.5	ND
E65		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-54.6	-48.4	ND	ND	ND	ND	ND	-67.3	ND	-36.3	-59.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-5.7	-12.4	ND	ND	ND	ND	ND	9.6	ND	-16.3	2.5	ND
68		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.15	0.029	ND	1.2	6.6	ND	0.33	0.10	0.25	0.85	1.0	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-58.3	-62.5	ND	-52.9	-48.6	ND	-56.3	-59.3	-57.0	-53.9	-53.4	ND
E90		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-52.0	-62.0	ND	ND	ND	ND	ND	-60.4	ND	-43.5	-57.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-6.3	-0.5	ND	ND	ND	ND	ND	1.1	ND	-10.3	3.7	ND
96		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	2.8	2.0	ND	3.9	1.1	31	0.69	6.1	0.78	5.1	4.8	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-50.8	-51.7	ND	-49.9	-53.2	-44.6	-54.4	-48.8	-54.1	-49.2	-49.4	ND
E11-9		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-55.8	-45.3	ND	ND	ND	ND	ND	-19.9	ND	-28.3	-39.3	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	5.1	-6.4	ND	ND	ND	ND	ND	-28.8	ND	-21.0	-10.1	ND
97		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	1.4	1.8	ND	2.8	5.3	ND	4.5	10	ND	5.1	3.6	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-52.6	-52.0	ND	-50.8	-49.1	ND	-49.6	-47.4	ND	-49.2	-50.1	ND
E11-11		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-57.3	-37.8	ND	ND	ND	ND	ND	-20.2	ND	-42.0	-51.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	4.7	-14.2	ND	ND	ND	ND	ND	-27.2	ND	-7.2	1.0	ND
98		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	1.8	1.2	ND	5.6	0.33	20	3.0	3.8	ND	5.9	2.0	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-51.9	-53.0	ND	-49.0	-56.3	-45.7	-50.6	-50.0	ND	-48.9	-51.6	ND
E11-13		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	ND	-35.8	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-17.2	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
99		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	1.4	0.98	ND	4.1	0.29	11	1.8	5.1	ND	6.4	1.2	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-52.6	-53.5	ND	-49.8	-56.6	-47.3	-51.9	-49.2	ND	-48.7	-53.0	ND
E11-15		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	ND	-48.0	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-5.5	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

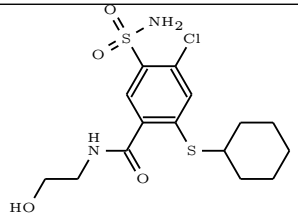
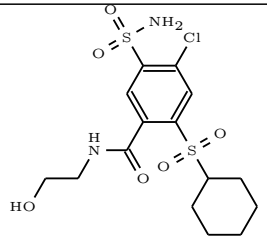
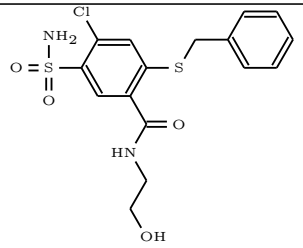
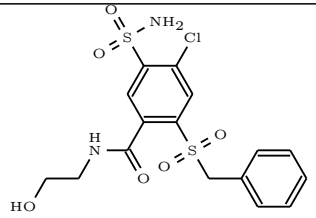
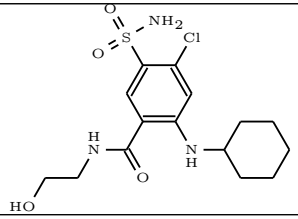
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
101		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	3.1	2.2	ND	4.0	13	26	4.0	6.1	ND	5.7	5.5	ND
E11-19		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-50.6	-51.4	ND	-49.8	-46.8	-45.1	-49.9	-48.8	ND	-49.0	-49.0	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-48.4	-29.5	ND	ND	ND	ND	ND	-28.5	ND	-25.4	-38.0	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-2.2	-22.0	ND	ND	ND	ND	ND	-20.3	ND	-23.5	-11.0	ND
103		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	0.37	0.88	ND	23	26	33	16	0.77	ND	1.9	0.60	ND
E11-27		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-56.0	-53.8	ND	-45.4	-45.0	-44.4	-46.2	-54.1	ND	-51.8	-54.8	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-50.3	-28.8	ND	ND	ND	ND	ND	-14.4	ND	-26.2	-50.9	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	-5.7	-25.0	ND	ND	ND	ND	ND	-39.8	ND	-25.6	-3.9	ND
105		$pK_{a,SA}$	9.40	$K_{d,int}$ (nM)	8.2	2.0	ND	7.5	2.6	3.3	1.2	19	ND	10	5.1	ND
E11-21		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-55.8	ΔG_{int} (kJ mol^{-1})	-48.0	-51.7	ND	-48.2	-50.9	-50.4	-53.0	-45.8	ND	-47.4	-49.2	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	-50.2	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.1	$-T\Delta S_{int}$ (kJ mol^{-1})	2.1	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
Chlorinated compounds																
141		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	0.12	0.061	ND	3.2	3.0	ND	2.8	0.024	0.70	4.0	0.19	ND
E11-8		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-59.0	-60.6	ND	-50.4	-50.6	ND	-50.8	-63.1	-54.4	-49.9	-57.7	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-47.2	-47.6	ND	ND	ND	ND	ND	-35.8	ND	-32.0	-57.9	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-11.8	-13.1	ND	ND	ND	ND	ND	-27.3	ND	-17.9	0.1	ND
144		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	0.077	0.047	ND	2.2	3.3	9.6	5.7	0.048	ND	2.1	0.024	ND
E11-12		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-60.1	-61.4	ND	-51.4	-50.4	-47.6	-49.0	-61.3	ND	-51.5	-63.1	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	ND	-36.0	ND	ND	ND	ND	ND	-24.4	ND	ND	-50.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-25.4	ND	ND	ND	ND	ND	-36.8	ND	ND	-12.4	ND
145		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	0.061	0.039	ND	1.7	2.8	11	3.8	0.080	ND	2.8	0.014	ND
E11-14		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-60.7	-61.8	ND	-52.1	-50.8	-47.2	-50.0	-59.9	ND	-50.8	-64.4	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	ND	-35.3	ND	ND	ND	ND	ND	-25.8	ND	-24.6	-56.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-26.4	ND	ND	ND	ND	ND	-34.1	ND	-26.2	-8.0	ND
146		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	0.072	0.042	ND	1.4	2.8	10	3.8	0.053	ND	1.7	0.021	ND
E11-16		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-60.2	-61.6	ND	-52.5	-50.8	-47.4	-50.0	-61.0	ND	-52.0	-63.5	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-40.6	ND	ND	ND	ND	ND	ND	ND	ND	-39.5	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-19.6	ND	ND	ND	ND	ND	ND	ND	ND	-12.6	ND	ND

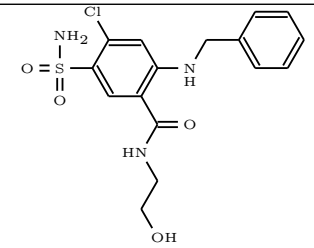
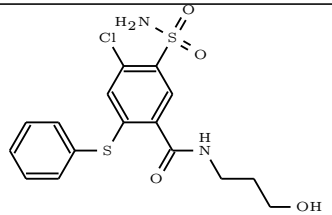
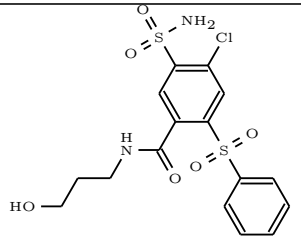
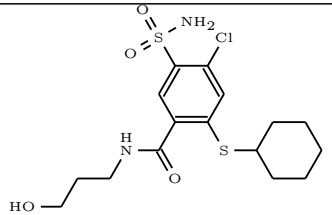
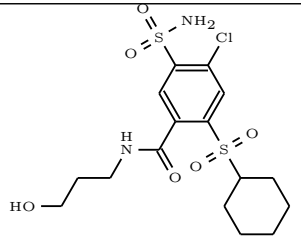
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
147		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	0.058	0.092	ND	4.7	6.4	ND	3.2	0.060	ND	4.4	0.11	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-60.8	-59.6	ND	-49.4	-48.7	ND	-50.4	-60.7	ND	-49.6	-59.1	ND
E11-10		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-46.6	-41.1	ND	ND	ND	ND	ND	-24.6	ND	-36.4	-51.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-14.2	-18.5	ND	ND	ND	ND	ND	-36.1	ND	-13.3	-7.5	ND
148		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	0.077	0.15	ND	2.0	1.7	21	2.8	0.17	ND	1.6	0.38	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-60.1	-58.3	ND	-51.7	-52.1	-45.6	-50.8	-58.0	ND	-52.2	-56.0	ND
E11-18		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-35.6	-30.5	ND	ND	ND	ND	ND	-24.1	ND	-19.1	-41.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-24.5	-27.8	ND	ND	ND	ND	ND	-33.9	ND	-33.2	-14.5	ND
150		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	0.0041	0.15	ND	4.4	0.41	1.6	10	0.036	ND	1.2	0.013	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-67.6	-58.4	ND	-49.6	-55.7	-52.3	-47.4	-62.0	ND	-53.0	-64.6	ND
E11-26		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-44.2	-24.1	ND	ND	ND	ND	ND	-19.9	ND	-49.2	-44.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-23.5	-34.3	ND	ND	ND	ND	ND	-42.1	ND	-3.8	-20.2	ND
153		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	0.23	0.37	ND	2.5	1.7	3.1	2.1	0.48	ND	4.4	0.28	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-57.2	-56.0	ND	-51.0	-52.1	-50.5	-51.5	-55.3	ND	-49.6	-56.7	ND
E11-20		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-50.1	-26.1	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-7.1	-29.9	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
184		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	14	0.34	ND	ND	0.055	ND	3.1	0.60	ND	2.8	0.63	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-46.6	-56.2	ND	ND	-60.9	ND	-50.5	-54.8	ND	-50.8	-54.6	ND
E38		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	ND	-37.3	ND	ND	ND	ND	ND	ND	ND	ND	-40.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-18.9	ND	ND	ND	ND	ND	ND	ND	ND	-14.2	ND
187		$pK_{a,SA}$	8.85	$K_{d,int}$ (nM)	55	2.1	ND	2.3	0.62	ND	0.70	3.8	ND	7.8	4.2	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.5	ΔG_{int} (kJ mol^{-1})	-43.1	-51.6	ND	-51.3	-54.7	ND	-54.3	-50.0	ND	-48.2	-49.7	ND
E89		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-32.1	-32.9	ND	ND	ND	ND	ND	-48.9	ND	-26.6	-33.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.2	$-T\Delta S_{int}$ (kJ mol^{-1})	-11.0	-18.7	ND	ND	ND	ND	ND	-1.1	ND	-21.5	-16.2	ND
188		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	21	0.79	ND	1.4	0.052	ND	0.75	1.6	ND	6.0	1.3	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-45.6	-54.1	ND	-52.5	-61.1	ND	-54.2	-52.2	ND	-48.8	-52.9	ND
E50		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-28.1	-33.9	ND	ND	ND	ND	ND	-32.0	ND	ND	-40.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-17.5	-20.1	ND	ND	ND	ND	ND	-20.2	ND	ND	-12.2	ND

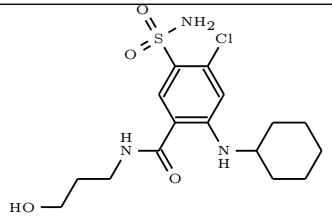
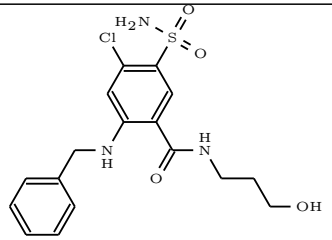
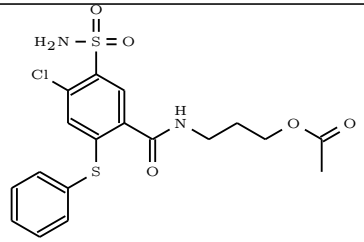
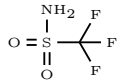
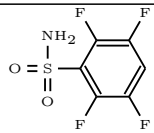
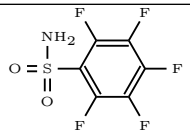
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
189		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	15	0.66	ND	1.0	0.041	3.5	1.3	1.1	ND	5.1	0.41	ND
E45		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-46.5	-54.5	ND	-53.4	-61.7	-50.2	-52.9	-53.3	ND	-49.3	-55.7	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-32.7	-36.0	ND	ND	ND	ND	ND	ND	ND	-19.8	-44.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-13.8	-18.5	ND	ND	ND	ND	ND	ND	ND	-29.5	-11.0	ND
190		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	16	0.37	ND	0.89	0.033	ND	0.57	0.96	ND	5.3	0.75	ND
E53		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-46.2	-56.0	ND	-53.8	-62.2	ND	-54.9	-53.5	ND	-49.1	-54.2	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-28.2	-20.9	ND	ND	ND	ND	ND	-26.8	ND	ND	-40.0	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-18.0	-35.1	ND	ND	ND	ND	ND	-26.7	ND	ND	-14.1	ND
191		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	12	1.2	ND	4.4	1.0	10	1.1	1.6	ND	6.9	3.8	ND
E49		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-47.1	-52.9	ND	-49.6	-53.4	-47.4	-53.1	-52.2	ND	-48.5	-50.0	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-39.4	-23.7	ND	ND	ND	ND	ND	-27.8	ND	-25.5	-29.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-7.8	-29.2	ND	ND	ND	ND	ND	-24.4	ND	-23.0	-20.5	ND
192		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	9.6	1.1	ND	2.1	3.3	16	1.1	0.86	ND	1.5	2.3	ND
E32		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-47.6	-53.2	ND	-51.5	-50.4	-46.4	-53.1	-53.8	ND	-52.4	-51.3	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-36.8	-29.1	ND	ND	ND	ND	ND	-21.2	ND	-13.4	-34.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-10.8	-24.1	ND	ND	ND	ND	ND	-32.7	ND	-38.9	-17.2	ND
193		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	7.7	0.37	ND	0.59	2.1	4.1	0.94	0.27	ND	0.48	0.63	ND
E57		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-48.2	-56.0	ND	-54.8	-51.6	-49.8	-53.6	-56.8	ND	-55.3	-54.6	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-39.5	-24.6	ND	ND	ND	ND	ND	-19.5	ND	-23.8	-39.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-8.7	-31.4	ND	ND	ND	ND	ND	-37.3	ND	-31.5	-15.1	ND
194		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	1.2	0.28	ND	1.2	2.4	11	2.3	0.14	ND	0.21	0.28	ND
E52		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-53.1	-56.8	ND	-53.0	-51.1	-47.2	-51.3	-58.6	ND	-57.5	-56.7	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-44.5	-30.6	ND	ND	ND	ND	ND	-27.9	ND	-16.2	-38.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-8.6	-26.2	ND	ND	ND	ND	ND	-30.7	ND	-41.2	-18.1	ND
195		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	14	0.28	ND	ND	0.83	7.8	0.23	0.18	ND	0.96	1.4	ND
E46		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-46.6	-56.8	ND	ND	-53.9	-48.2	-57.3	-57.8	ND	-53.5	-52.5	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-46.2	-37.8	ND	ND	ND	ND	ND	-42.2	ND	-34.7	-41.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-0.3	-18.9	ND	ND	ND	ND	ND	-15.7	ND	-18.8	-10.9	ND
196		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	5.2	0.15	ND	0.50	0.92	2.1	0.32	0.64	ND	1.1	0.47	ND
E33		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-49.2	-58.4	ND	-55.2	-53.7	-51.6	-56.4	-54.6	ND	-53.2	-55.4	ND
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-34.3	-32.5	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-14.9	-26.0	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

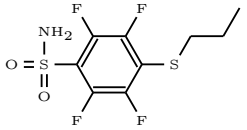
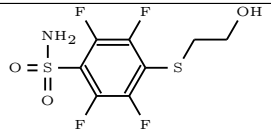
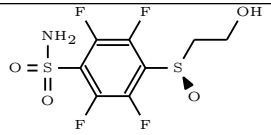
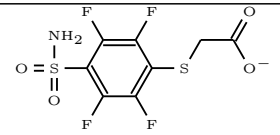
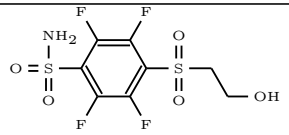
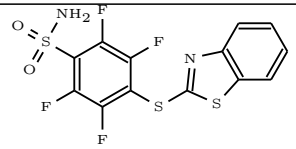
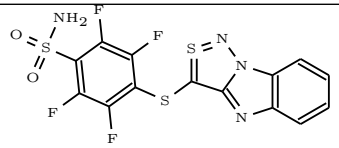
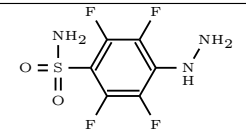
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
207		$pK_{a,SA}$	8.90	$K_{d,int}$ (nM)	130	8.6	600	2.3	0.0021	21	0.81	4.8	2.7	15	4.0	1.5
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.8	ΔG_{int} (kJ mol^{-1})	-40.9	-47.9	-37.0	-51.3	-69.4	-45.6	-54.0	-49.4	-50.8	-46.4	-49.8	-52.5
E2		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-28.0	ΔH_{int} (kJ mol^{-1})	ND	-15.0	ND	ND	ND	ND	ND	ND	ND	ND	-31.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	24.8	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-32.9	ND	ND	ND	ND	ND	ND	ND	ND	-18.8	ND
221		$pK_{a,SA}$	8.80	$K_{d,int}$ (nM)	1400	0.58	31	1.8	52	3.1	0.89	0.060	0.74	0.75	7.9	0.40
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.3	ΔG_{int} (kJ mol^{-1})	-34.7	-54.9	-44.6	-52.0	-43.3	-50.5	-53.8	-60.7	-54.2	-54.2	-48.1	-55.8
EA3-1		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	ND	-32.7	ND	ND	ND	ND	ND	-34.4	ND	-47.9	-45.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.6	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-22.2	ND	ND	ND	ND	ND	-26.2	ND	-6.3	-2.9	ND
222		$pK_{a,SA}$	8.80	$K_{d,int}$ (nM)	2900	0.069	94	0.032	87	6.0	1.4	0.060	0.22	1.0	8.9	0.38
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.3	ΔG_{int} (kJ mol^{-1})	-32.9	-60.3	-41.7	-62.3	-41.9	-48.8	-52.5	-60.7	-57.3	-53.4	-47.8	-56.0
EA4-1		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.3	ΔH_{int} (kJ mol^{-1})	ND	-30.4	ND	ND	ND	ND	ND	-23.1	-25.8	-39.7	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	23.0	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-30.0	ND	ND	ND	ND	ND	-37.6	-31.6	-13.7	ND	ND
223		$pK_{a,SA}$	8.75	$K_{d,int}$ (nM)	540	0.15	30	0.41	58	0.73	0.26	0.034	0.25	0.34	6.3	0.34
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.0	ΔG_{int} (kJ mol^{-1})	-37.2	-58.3	-44.7	-55.7	-43.0	-54.3	-56.9	-62.2	-57.0	-56.2	-48.7	-56.2
EA5-1		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-31.4	ΔH_{int} (kJ mol^{-1})	ND	-35.2	ND	ND	ND	ND	ND	-22.7	ND	-33.2	-32.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.6	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-23.1	ND	ND	ND	ND	ND	-39.4	ND	-23.1	-16.2	ND
224		$pK_{a,SA}$	8.75	$K_{d,int}$ (nM)	810	0.48	51	0.050	40	2.2	0.93	0.075	0.36	1.4	11	0.27
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.0	ΔG_{int} (kJ mol^{-1})	-36.2	-55.3	-43.3	-61.2	-43.9	-51.4	-53.6	-60.1	-56.1	-52.7	-47.2	-56.8
EA8-1		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	ND	-33.3	ND	ND	ND	ND	ND	-29.3	ND	-39.8	-38.8	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.3	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-22.0	ND	ND	ND	ND	ND	-30.8	ND	-12.8	-8.3	ND
225		$pK_{a,SA}$	8.87	$K_{d,int}$ (nM)	2500	0.84	150	1.1	18	15	1.7	0.34	1.1	0.21	8.1	0.45
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.7	ΔG_{int} (kJ mol^{-1})	-33.3	-53.9	-40.6	-53.3	-46.0	-46.4	-52.0	-56.2	-53.2	-57.5	-48.1	-55.5
EA12-1		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.3	ΔH_{int} (kJ mol^{-1})	ND	-37.5	ND	ND	ND	ND	ND	-21.4	ND	-48.2	-59.0	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	23.4	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-16.4	ND	ND	ND	ND	ND	-34.8	ND	-9.3	11.0	ND

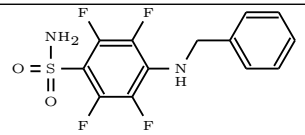
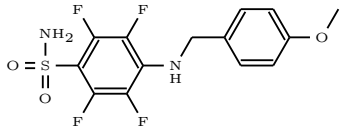
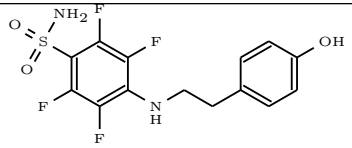
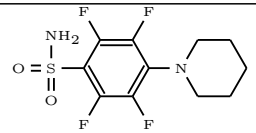
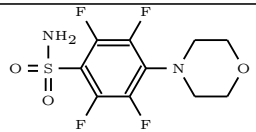
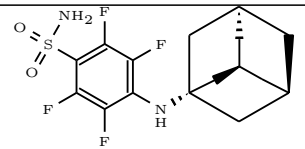
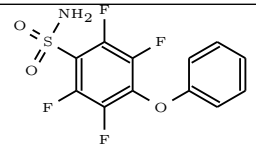
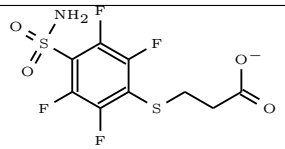
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
226		$pK_{a,SA}$	8.75	$K_{d,int}$ (nM)	1600	0.39	210	0.55	15	0.58	1.6	0.14	0.69	0.84	7.9	0.40
EA11-1		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.0	ΔG_{int} (kJ mol^{-1})	-34.4	-55.9	-39.7	-55.0	-46.5	-54.8	-52.2	-58.6	-54.4	-53.9	-48.1	-55.8
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-31.4	ΔH_{int} (kJ mol^{-1})	ND	-30.0	ND	ND	ND	ND	ND	-26.3	ND	-40.8	-52.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.6	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-25.9	ND	ND	ND	ND	ND	-32.3	ND	-13.1	4.5	ND
228		$pK_{a,SA}$	8.75	$K_{d,int}$ (nM)	3200	1.5	420	1.7	2300	35	2.3	0.23	0.77	2.7	19	1.1
EA7-1		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.0	ΔG_{int} (kJ mol^{-1})	-32.6	-52.3	-37.9	-52.1	-33.4	-44.3	-51.3	-57.3	-54.1	-50.9	-45.9	-53.1
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-31.0	ΔH_{int} (kJ mol^{-1})	ND	-18.9	ND	ND	ND	ND	ND	-23.8	ND	-34.2	-43.9	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.0	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-33.4	ND	ND	ND	ND	ND	-33.5	ND	-16.7	-2.0	ND
229		$pK_{a,SA}$	8.80	$K_{d,int}$ (nM)	1000	1.2	750	0.74	26	0.60	2.0	0.17	1.1	10	2.6	0.40
EA9-1		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.3	ΔG_{int} (kJ mol^{-1})	-35.5	-53.1	-36.4	-54.2	-45.0	-54.8	-51.6	-58.0	-53.2	-47.5	-51.0	-55.8
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.7	ΔH_{int} (kJ mol^{-1})	ND	-28.3	ND	ND	ND	ND	ND	-8.9	ND	-27.1	-48.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.6	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-24.7	ND	ND	ND	ND	ND	-49.1	ND	-20.4	-2.3	ND
230		$pK_{a,SA}$	8.80	$K_{d,int}$ (nM)	360	0.14	7.5	0.099	6.9	0.060	0.20	0.030	0.40	0.75	4.7	0.080
EA10-1		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.3	ΔG_{int} (kJ mol^{-1})	-38.3	-58.5	-48.2	-59.4	-48.4	-60.7	-57.6	-62.5	-55.8	-54.2	-49.4	-59.9
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-27.6	ΔH_{int} (kJ mol^{-1})	ND	-27.4	ND	ND	ND	ND	ND	-26.1	ND	-39.5	-42.8	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	24.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-31.1	ND	ND	ND	ND	ND	-36.4	ND	-14.7	-6.6	ND
246		$pK_{a,SA}$	8.98	$K_{d,int}$ (nM)	96	0.14	38	0.0042	38	1.7	1.3	0.045	0.012	0.025	0.94	0.012
EA3-2		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-53.3	ΔG_{int} (kJ mol^{-1})	-41.7	-58.4	-44.0	-67.5	-44.0	-52.0	-52.7	-61.5	-64.9	-62.9	-53.6	-64.8
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-31.8	ΔH_{int} (kJ mol^{-1})	ND	-38.6	ND	ND	ND	ND	ND	-28.7	ND	-62.4	-40.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.5	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-19.8	ND	ND	ND	ND	ND	-32.8	ND	-0.6	-12.9	ND
247		$pK_{a,SA}$	8.25	$K_{d,int}$ (nM)	99	0.12	110	ND	35	0.44	4.4	0.026	0.046	0.11	0.81	0.062
EA3-2o		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-49.0	ΔG_{int} (kJ mol^{-1})	-41.6	-59.0	-41.4	ND	-44.2	-55.5	-49.6	-62.9	-61.4	-59.0	-54.0	-60.6
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.8	ΔH_{int} (kJ mol^{-1})	ND	-30.2	ND	ND	ND	ND	ND	-31.0	ND	-52.1	-38.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.2	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-28.7	ND	ND	ND	ND	ND	-31.9	ND	-6.9	-15.4	ND

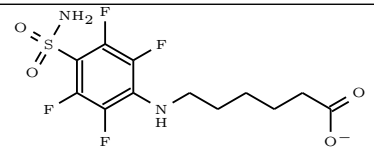
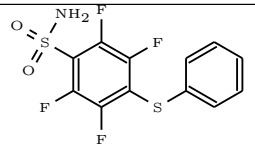
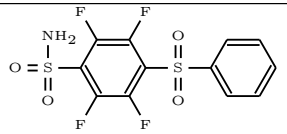
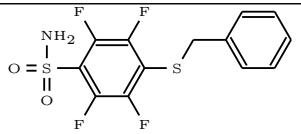
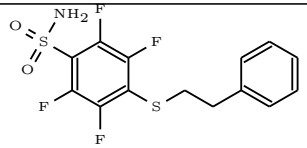
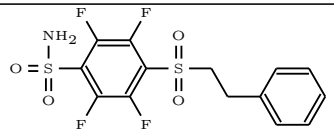
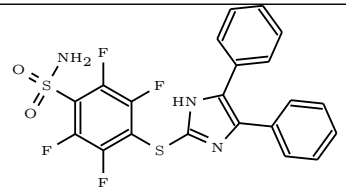
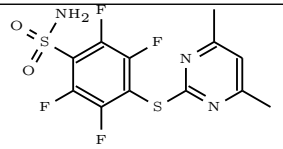
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
248		$pK_{a,SA}$	9.00	$K_{d,int}$ (nM)	9.2	0.044	30	0.028	3.9	0.38	1.1	0.0096	0.0035	0.0077	0.26	0.0042
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-53.4	ΔG_{int} (kJ mol^{-1})	-47.7	-61.5	-44.7	-62.6	-49.9	-55.9	-53.1	-65.4	-68.0	-66.0	-56.9	-67.6
EA3-3		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-32.6	ΔH_{int} (kJ mol^{-1})	ND	-32.9	ND	ND	ND	ND	ND	-21.8	ND	-52.5	-40.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.8	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-28.6	ND	ND	ND	ND	ND	-43.7	ND	-13.5	-16.8	ND
249		$pK_{a,SA}$	8.22	$K_{d,int}$ (nM)	75	0.084	340	0.54	13	0.28	6.5	0.088	0.051	0.44	1.3	0.040
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-48.8	ΔG_{int} (kJ mol^{-1})	-42.3	-59.8	-38.4	-55.0	-46.9	-56.7	-48.6	-59.7	-61.1	-55.6	-52.8	-61.7
EA3-3o		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.4	ΔH_{int} (kJ mol^{-1})	ND	-25.1	ND	ND	ND	ND	ND	-38.1	ND	-41.9	-37.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.4	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-34.7	ND	ND	ND	ND	ND	-21.6	ND	-13.7	-15.1	ND
250		$pK_{a,SA}$	9.15	$K_{d,int}$ (nM)	14	0.040	84	0.067	2.3	0.54	1.0	0.0091	0.029	0.027	0.58	0.034
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-54.3	ΔG_{int} (kJ mol^{-1})	-46.7	-61.7	-42.0	-60.4	-51.2	-55.0	-53.4	-65.6	-62.5	-62.7	-54.8	-62.2
EA3-4		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-31.4	ΔH_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	-33.8	ND	-60.4	-41.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.9	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	-31.8	ND	-2.4	-13.2	ND
251		$pK_{a,SA}$	8.20	$K_{d,int}$ (nM)	340	0.94	200	4.2	28	2.3	13	0.21	0.77	1.9	6.7	0.46
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-48.7	ΔG_{int} (kJ mol^{-1})	-38.4	-53.6	-39.8	-49.7	-44.8	-51.3	-46.9	-57.5	-54.1	-51.8	-48.5	-55.4
EA3-4o		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-25.9	ΔH_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	-24.2	ND	-31.2	-35.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.8	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	-33.3	ND	-20.6	-13.4	ND
252		$pK_{a,SA}$	9.70	$K_{d,int}$ (nM)	26	0.37	240	ND	66	50	6.0	2.6	0.011	ND	1.2	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-57.6	ΔG_{int} (kJ mol^{-1})	-45.0	-56.0	-39.3	ND	-42.6	-43.4	-48.8	-51.0	-65.0	ND	-53.0	ND
EA3-7		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-39.3	ΔH_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	-19.4	-33.0	-53.1	-44.9	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	18.3	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	-31.6	-32.0	ND	-8.1	ND

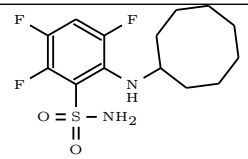
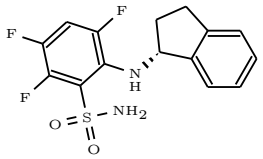
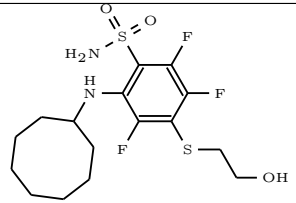
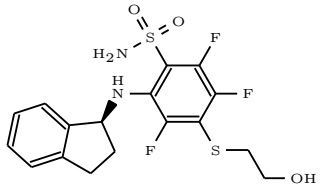
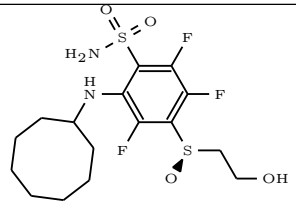
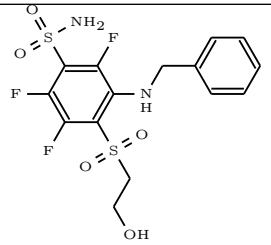
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
253		$pK_{a,SA}$	10.2	$K_{d,int}$ (nM)	3.7	0.021	30	ND	ND	0.63	0.38	0.055	0.0072	0.041	0.23	0.0049
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-60.6	ΔG_{int} (kJ mol^{-1})	-50.1	-63.3	-44.6	ND	ND	-54.6	-55.9	-60.9	-66.2	-61.7	-57.2	-67.2
EA3-8		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-38.1	ΔH_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	-39.7	ND	-53.5	-49.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.5	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	-21.3	ND	-8.2	-7.5	ND
264		$pK_{a,SA}$	8.95	$K_{d,int}$ (nM)	69	0.025	89	0.0053	34	0.69	0.84	0.0054	0.0063	0.0036	1.8	0.024
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-53.1	ΔG_{int} (kJ mol^{-1})	-42.5	-63.0	-41.9	-67.0	-44.4	-54.4	-53.9	-66.9	-66.5	-68.0	-51.9	-63.1
EA4-2		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.3	ΔH_{int} (kJ mol^{-1})	ND	-33.7	ND	ND	ND	ND	ND	-32.4	ND	-52.1	-42.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	23.8	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-29.3	ND	ND	ND	ND	ND	-34.5	ND	-15.9	-9.8	ND
265		$pK_{a,SA}$	8.25	$K_{d,int}$ (nM)	70	0.079	210	0.42	200	0.50	6.9	0.0069	0.023	0.064	3.2	0.082
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-49.0	ΔG_{int} (kJ mol^{-1})	-42.5	-60.0	-39.6	-55.7	-39.8	-55.2	-48.5	-66.3	-63.1	-60.5	-50.4	-59.9
EA4-2o		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	ND	-28.2	ND	ND	ND	ND	ND	-22.9	ND	-25.8	-38.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	24.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-31.8	ND	ND	ND	ND	ND	-43.4	ND	-34.7	-11.7	ND
266		$pK_{a,SA}$	8.85	$K_{d,int}$ (nM)	16	0.023	84	0.13	4.0	0.20	2.1	0.0036	0.0028	0.0054	0.84	0.011
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.5	ΔG_{int} (kJ mol^{-1})	-46.3	-63.2	-42.0	-58.7	-49.8	-57.6	-51.5	-68.0	-68.6	-66.9	-53.9	-65.1
EA4-3		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-31.8	ΔH_{int} (kJ mol^{-1})	ND	-30.1	ND	ND	ND	ND	ND	-25.3	ND	-52.4	-44.9	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-33.1	ND	ND	ND	ND	ND	-42.7	ND	-14.5	-8.9	ND
267		$pK_{a,SA}$	8.30	$K_{d,int}$ (nM)	44	0.022	380	ND	45	0.27	5.4	0.026	0.0091	0.15	2.2	0.092
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-49.3	ΔG_{int} (kJ mol^{-1})	-43.7	-63.3	-38.1	ND	-43.6	-56.9	-49.1	-62.8	-65.6	-58.3	-51.4	-59.6
EA4-3o		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	ND	-20.5	ND	ND	ND	ND	ND	-15.4	ND	-29.6	-34.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	25.0	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-42.7	ND	ND	ND	ND	ND	-47.4	ND	-28.7	-16.8	ND

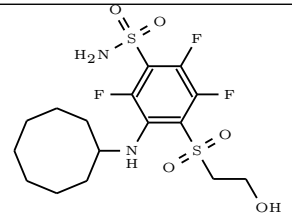
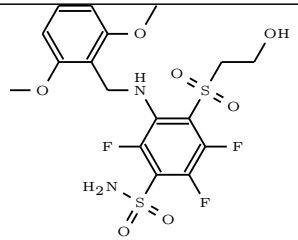
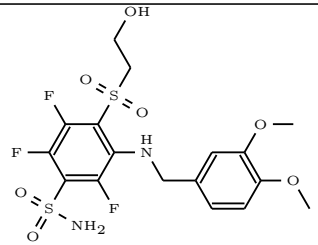
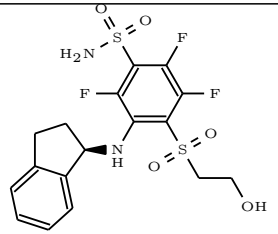
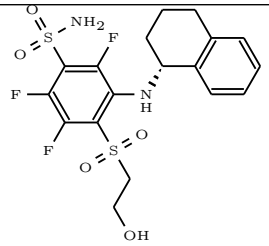
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
268		$pK_{a,SA}$	9.80	$K_{d,int}$ (nM)	49	0.13	60	ND	170	20	3.6	0.87	0.0038	0.013	ND	0.047
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-58.2	ΔG_{int} (kJ mol^{-1})	-43.4	-58.6	-42.9	ND	-40.2	-45.7	-50.1	-53.8	-67.8	-64.7	ND	-61.3
EA4-7		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-39.7	ΔH_{int} (kJ mol^{-1})	ND	-23.9	ND	ND	ND	ND	ND	-16.8	ND	-50.4	-48.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	18.5	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-34.7	ND	ND	ND	ND	ND	-37.0	ND	-14.2	ND	ND
269		$pK_{a,SA}$	10.2	$K_{d,int}$ (nM)	15	0.0056	7.6	ND	20	2.4	0.72	0.016	0.0056	0.030	0.64	0.012
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-60.6	ΔG_{int} (kJ mol^{-1})	-46.5	-66.8	-48.2	ND	-45.7	-51.2	-54.3	-64.1	-66.8	-62.4	-54.6	-64.9
EA4-8		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-36.8	ΔH_{int} (kJ mol^{-1})	ND	-39.3	ND	ND	ND	ND	ND	-28.0	ND	-47.1	-42.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	23.8	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-27.5	ND	ND	ND	ND	ND	-36.0	ND	-15.3	-12.2	ND
283		$pK_{a,SA}$	9.03	$K_{d,int}$ (nM)	86	0.10	170	0.0076	14	0.46	1.2	0.028	0.013	0.036	2.8	0.022
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-53.6	ΔG_{int} (kJ mol^{-1})	-42.0	-59.3	-40.2	-66.0	-46.7	-55.4	-53.0	-62.7	-64.6	-62.0	-50.8	-63.2
EA4-2c		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-28.5	ΔH_{int} (kJ mol^{-1})	ND	-25.1	ND	ND	ND	ND	ND	-17.7	-24.8	-38.5	-35.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	25.1	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-34.3	ND	ND	ND	ND	ND	-45.0	-39.8	-23.5	-15.6	ND
Fluorinated compounds																
303		$pK_{a,SA}$	6.02	$K_{d,int}$ (nM)	51	8.4	220	17	24	ND	1.2	2.9	11	38	33	15
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-35.7	ΔG_{int} (kJ mol^{-1})	-43.3	-47.9	-39.6	-46.2	-45.3	ND	-53.0	-50.7	-47.2	-44.0	-44.4	-46.5
TFMSA		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-16.7	ΔH_{int} (kJ mol^{-1})	-46.5	-36.7	ND	-24.7	ND	ND	ND	-25.5	-31.1	-36.1	-42.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	19.0	$-T\Delta S_{int}$ (kJ mol^{-1})	3.2	-11.3	ND	-21.5	ND	ND	ND	-25.2	-16.1	-7.9	-2.2	ND
304		$pK_{a,SA}$	8.21	$K_{d,int}$ (nM)	0.22	0.73	400	9.2	11	0.053	3.5	0.25	2.5	7.5	1.1	1.2
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-48.7	ΔG_{int} (kJ mol^{-1})	-57.3	-54.2	-38.0	-47.7	-47.2	-61.0	-50.2	-57.0	-51.1	-48.2	-53.3	-52.9
VD12-22		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-25.9	ΔH_{int} (kJ mol^{-1})	-72.5	-42.4	ND	ND	ND	ND	ND	-26.5	-33.5	-31.7	-42.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.8	$-T\Delta S_{int}$ (kJ mol^{-1})	15.2	-11.8	ND	ND	ND	ND	ND	-30.5	-17.6	-16.6	-10.8	ND
305		$pK_{a,SA}$	8.12	$K_{d,int}$ (nM)	0.22	1.4	ND	15	21	1.3	2.7	1.5	3.0	21	4.9	0.96
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-48.2	ΔG_{int} (kJ mol^{-1})	-57.4	-52.5	ND	-46.5	-45.6	-52.7	-50.8	-52.3	-50.6	-45.6	-49.3	-53.5
VD10-9		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.4	ΔH_{int} (kJ mol^{-1})	-69.4	-40.7	ND	ND	ND	ND	ND	-24.7	ND	-32.9	-38.3	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.8	$-T\Delta S_{int}$ (kJ mol^{-1})	12.1	-11.8	ND	ND	ND	ND	ND	-27.6	ND	-12.7	-11.1	ND

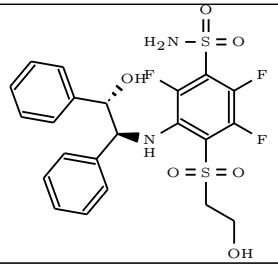
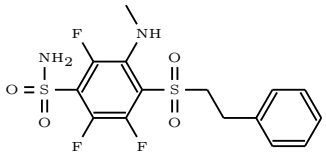
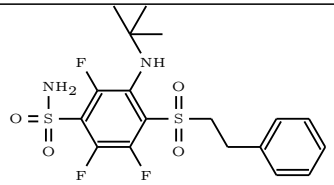
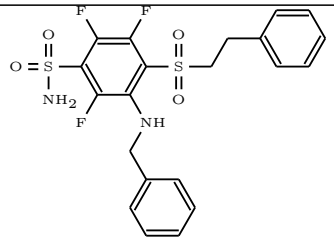
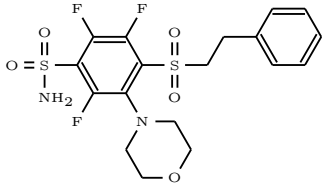
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
306		$pK_{a,SA}$	8.15	$K_{d,int}$ (nM)	0.0035	0.065	60	2.0	8.8	0.0017	0.86	0.028	0.10	0.93	0.14	0.093
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-48.4	ΔG_{int} (kJ mol^{-1})	-68.0	-60.5	-42.9	-51.7	-47.8	-70.0	-53.8	-62.6	-59.4	-53.6	-58.5	-59.6
VD12-05		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.4	ΔH_{int} (kJ mol^{-1})	-74.9	-46.4	ND	ND	ND	ND	ND	-29.8	ND	-30.9	-54.3	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.0	$-T\Delta S_{int}$ (kJ mol^{-1})	6.9	-14.1	ND	ND	ND	ND	ND	-32.8	ND	-22.8	-4.2	ND
307		$pK_{a,SA}$	8.14	$K_{d,int}$ (nM)	0.0094	0.32	480	8.5	18	0.056	1.2	0.34	0.61	5.8	0.68	0.13
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-48.3	ΔG_{int} (kJ mol^{-1})	-65.5	-56.4	-37.5	-47.9	-46.0	-60.9	-52.9	-56.2	-54.7	-48.9	-54.4	-58.7
VD10-13		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.4	ΔH_{int} (kJ mol^{-1})	-84.1	-50.7	ND	ND	ND	ND	ND	-27.8	-43.6	-33.5	-57.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.9	$-T\Delta S_{int}$ (kJ mol^{-1})	18.6	-5.8	ND	ND	ND	ND	ND	-28.4	-11.1	-15.4	2.9	ND
308		$pK_{a,SA}$	7.43	$K_{d,int}$ (nM)	0.22	2.4	2200	150	36	5.4	12	1.5	2.3	26	12	3.0
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-44.1	ΔG_{int} (kJ mol^{-1})	-57.3	-51.2	-33.6	-40.4	-44.2	-49.1	-47.0	-52.4	-51.3	-45.0	-47.0	-50.6
AZ13-1		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-23.4	ΔH_{int} (kJ mol^{-1})	-70.6	-49.3	ND	ND	ND	ND	ND	-29.2	-34.0	-40.7	-48.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.7	$-T\Delta S_{int}$ (kJ mol^{-1})	13.3	-1.8	ND	ND	ND	ND	ND	-23.2	-17.3	-4.3	1.1	ND
309		$pK_{a,SA}$	8.14	$K_{d,int}$ (nM)	0.020	0.45	ND	5.5	15	0.56	6.1	0.13	1.3	1.3	0.41	2.2
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-48.3	ΔG_{int} (kJ mol^{-1})	-63.6	-55.5	ND	-49.0	-46.5	-54.9	-48.8	-58.7	-52.8	-52.8	-55.7	-51.4
VD12-01		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.4	ΔH_{int} (kJ mol^{-1})	-73.7	-53.0	ND	ND	ND	ND	ND	-32.7	ND	-30.5	-63.8	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.9	$-T\Delta S_{int}$ (kJ mol^{-1})	10.1	-2.5	ND	ND	ND	ND	ND	-25.9	ND	-22.2	8.1	ND
310		$pK_{a,SA}$	7.28	$K_{d,int}$ (nM)	0.064	2.5	1700	50	71	3.8	2.1	0.95	4.0	33	8.9	4.4
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-43.2	ΔG_{int} (kJ mol^{-1})	-60.5	-51.0	-34.3	-43.3	-42.5	-50.0	-51.5	-53.6	-49.9	-44.4	-47.8	-49.6
VD10-35		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-23.8	ΔH_{int} (kJ mol^{-1})	-76.8	-45.9	ND	ND	ND	ND	ND	-28.3	-35.5	-24.2	-50.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	19.4	$-T\Delta S_{int}$ (kJ mol^{-1})	16.2	-5.1	ND	ND	ND	ND	ND	-25.3	-14.3	-20.2	2.6	ND
311		$pK_{a,SA}$	7.83	$K_{d,int}$ (nM)	0.13	0.037	ND	27	17	0.13	2.3	0.011	0.19	5.9	0.037	0.025
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.5	ΔG_{int} (kJ mol^{-1})	-58.8	-61.9	ND	-45.0	-46.1	-58.7	-51.2	-65.1	-57.8	-48.9	-61.9	-63.0
VD10-49		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.0	ΔH_{int} (kJ mol^{-1})	-53.0	-37.2	ND	ND	ND	ND	ND	-28.5	ND	-31.5	-43.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-5.8	-24.7	ND	ND	ND	ND	ND	-36.5	ND	-17.3	-18.3	ND
312		$pK_{a,SA}$	7.69	$K_{d,int}$ (nM)	0.063	0.50	ND	4.2	2.8	0.42	3.4	0.82	0.40	7.3	0.39	0.33
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-45.7	ΔG_{int} (kJ mol^{-1})	-60.6	-55.2	ND	-49.7	-50.8	-55.7	-50.3	-54.0	-55.8	-48.3	-55.9	-56.3
VD10-28		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.0	ΔH_{int} (kJ mol^{-1})	-54.6	-34.6	ND	ND	ND	ND	ND	-21.5	ND	-33.1	-43.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	19.7	$-T\Delta S_{int}$ (kJ mol^{-1})	-5.9	-20.7	ND	ND	ND	ND	ND	-32.5	ND	-15.2	-12.2	ND
313		$pK_{a,SA}$	8.84	$K_{d,int}$ (nM)	0.18	0.57	ND	4.8	10	7.1	1.3	1.7	2.9	6.2	1.9	0.92
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.5	ΔG_{int} (kJ mol^{-1})	-57.9	-54.9	ND	-49.4	-47.4	-48.4	-52.8	-52.1	-50.7	-48.7	-51.9	-53.7
VD10-14		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.0	ΔH_{int} (kJ mol^{-1})	-69.6	-43.0	ND	ND	ND	ND	ND	-28.2	ND	-30.3	-48.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	23.5	$-T\Delta S_{int}$ (kJ mol^{-1})	11.6	-11.9	ND	ND	ND	ND	ND	-23.9	ND	-18.4	-3.3	ND

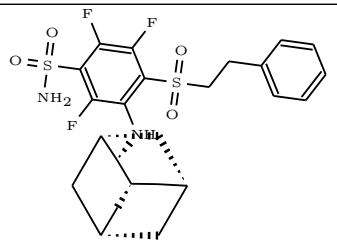
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
314		$pK_{a,SA}$	8.47	$K_{d,int}$ (nM)	0.0061	0.13	ND	7.5	22	0.14	3.7	0.55	0.23	4.2	0.15	0.048
VD10-16		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-50.3	ΔG_{int} (kJ mol^{-1})	-66.6	-58.7	ND	-48.3	-45.5	-58.6	-50.0	-55.0	-57.2	-49.7	-58.3	-61.3
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-31.8	ΔH_{int} (kJ mol^{-1})	-76.4	-55.1	ND	ND	ND	ND	ND	-26.3	ND	-39.2	-52.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	18.5	$-T\Delta S_{int}$ (kJ mol^{-1})	9.8	-3.6	ND	ND	ND	ND	ND	-28.7	ND	-10.5	-6.2	ND
315		$pK_{a,SA}$	8.50	$K_{d,int}$ (nM)	0.0048	0.14	ND	580	10	ND	5.1	0.24	0.16	4.0	0.070	0.079
VD12-70		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-50.5	ΔG_{int} (kJ mol^{-1})	-67.2	-58.6	ND	-37.0	-47.4	ND	-49.3	-57.2	-58.2	-49.9	-60.3	-60.0
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-31.2	ΔH_{int} (kJ mol^{-1})	-76.7	-56.5	ND	ND	ND	ND	ND	-37.1	ND	-43.5	-55.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	19.3	$-T\Delta S_{int}$ (kJ mol^{-1})	9.5	-2.1	ND	ND	ND	ND	ND	-20.1	ND	-6.4	-5.1	ND
316		$pK_{a,SA}$	8.61	$K_{d,int}$ (nM)	0.011	0.018	ND	2.4	5.3	0.023	ND	0.0046	0.076	1.4	0.0087	0.062
VD12-13		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-51.1	ΔG_{int} (kJ mol^{-1})	-65.0	-63.8	ND	-51.1	-49.1	-63.2	ND	-67.3	-60.1	-52.5	-65.7	-60.6
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-30.1	ΔH_{int} (kJ mol^{-1})	-67.9	-46.6	ND	ND	ND	ND	ND	-34.5	ND	-39.6	-69.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.0	$-T\Delta S_{int}$ (kJ mol^{-1})	2.8	-17.3	ND	ND	ND	ND	ND	-32.8	ND	-12.9	3.6	ND
318		$pK_{a,SA}$	8.26	$K_{d,int}$ (nM)	0.0026	0.29	ND	53	18	0.65	7.9	0.29	0.22	2.0	0.59	0.17
VD12-63		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-49.0	ΔG_{int} (kJ mol^{-1})	-68.8	-56.6	ND	-43.2	-46.0	-54.5	-48.1	-56.7	-57.3	-51.6	-54.8	-58.0
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-25.5	ΔH_{int} (kJ mol^{-1})	-59.7	-45.0	ND	ND	ND	ND	ND	-25.6	ND	-31.5	-35.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	23.5	$-T\Delta S_{int}$ (kJ mol^{-1})	-9.1	-11.7	ND	ND	ND	ND	ND	-31.1	ND	-20.2	-19.2	ND
319		$pK_{a,SA}$	8.61	$K_{d,int}$ (nM)	0.0022	0.19	ND	11	20	12	2.4	0.42	0.34	4.6	0.60	0.13
VD10-12		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-51.1	ΔG_{int} (kJ mol^{-1})	-69.3	-57.7	ND	-47.2	-45.7	-47.0	-51.2	-55.7	-56.2	-49.5	-54.8	-58.7
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-29.3	ΔH_{int} (kJ mol^{-1})	-84.8	-51.5	ND	ND	ND	ND	ND	-40.0	ND	-44.7	-49.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.8	$-T\Delta S_{int}$ (kJ mol^{-1})	15.5	-6.2	ND	ND	ND	ND	ND	-15.6	ND	-4.8	-5.6	ND
320		$pK_{a,SA}$	8.58	$K_{d,int}$ (nM)	0.0012	0.057	ND	3.3	4.3	0.064	1.2	0.0099	0.024	0.17	0.012	0.0066
VD10-51		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-50.9	ΔG_{int} (kJ mol^{-1})	-70.8	-60.8	ND	-50.4	-49.7	-60.5	-53.0	-65.3	-63.0	-58.1	-64.9	-66.4
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-25.9	ΔH_{int} (kJ mol^{-1})	-50.2	-24.6	ND	ND	ND	ND	ND	-31.7	ND	-38.2	-30.3	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	25.0	$-T\Delta S_{int}$ (kJ mol^{-1})	-20.6	-36.2	ND	ND	ND	ND	ND	-33.6	ND	-19.9	-34.6	ND
321		$pK_{a,SA}$	7.86	$K_{d,int}$ (nM)	0.011	0.085	ND	29	11	0.061	4.4	0.047	0.58	2.3	0.11	0.16
VD12-47		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.7	ΔG_{int} (kJ mol^{-1})	-65.0	-59.8	ND	-44.8	-47.3	-60.7	-49.6	-61.3	-54.9	-51.2	-59.1	-58.2
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.4	ΔH_{int} (kJ mol^{-1})	-77.5	-57.3	ND	ND	ND	ND	ND	-24.6	ND	-39.5	-43.9	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.3	$-T\Delta S_{int}$ (kJ mol^{-1})	12.4	-2.5	ND	ND	ND	ND	ND	-36.7	ND	-11.8	-15.2	ND
323		$pK_{a,SA}$	7.97	$K_{d,int}$ (nM)	0.036	0.86	ND	11	18	3.2	4.4	0.37	1.4	3.4	1.8	1.2
VD11-56		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-47.3	ΔG_{int} (kJ mol^{-1})	-62.0	-53.8	ND	-47.3	-45.9	-50.4	-49.6	-56.0	-52.6	-50.3	-52.0	-52.9
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-25.5	ΔH_{int} (kJ mol^{-1})	-80.6	-55.2	ND	ND	ND	ND	ND	-32.3	ND	-25.4	-54.3	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.8	$-T\Delta S_{int}$ (kJ mol^{-1})	18.5	1.4	ND	ND	ND	ND	ND	-23.7	ND	-24.9	2.3	ND

No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
325		$pK_{a,SA}$	8.49	$K_{d,int}$ (nM)	0.0040	0.93	ND	5.1	8.4	3.1	8.4	1.8	0.69	2.0	0.41	0.12
VD10-21a		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-50.4	ΔG_{int} (kJ mol^{-1})	-67.7	-53.6	ND	-49.3	-48.0	-50.5	-48.0	-51.9	-54.4	-51.6	-55.8	-58.9
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-32.6	ΔH_{int} (kJ mol^{-1})	-85.9	-59.3	ND	ND	ND	ND	ND	-34.6	ND	-41.3	-67.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	17.8	$-T\Delta S_{int}$ (kJ mol^{-1})	18.2	5.7	ND	ND	ND	ND	ND	-17.3	ND	-10.3	11.8	ND
326		$pK_{a,SA}$	7.80	$K_{d,int}$ (nM)	0.012	0.20	ND	9.5	46	0.068	2.5	0.33	0.41	0.97	0.17	5300
VD10-18		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.3	ΔG_{int} (kJ mol^{-1})	-64.9	-57.5	ND	-47.6	-43.6	-60.4	-51.1	-56.3	-55.7	-53.5	-58.1	-31.3
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-60.2	-41.8	ND	ND	ND	ND	ND	-31.0	ND	-33.3	-42.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.0	$-T\Delta S_{int}$ (kJ mol^{-1})	-4.6	-15.7	ND	ND	ND	ND	ND	-25.2	ND	-20.3	-15.4	ND
327		$pK_{a,SA}$	7.07	$K_{d,int}$ (nM)	0.021	0.68	ND	38	ND	1.1	6.6	0.12	0.10	3.0	1.0	0.12
VD11-51		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-42.0	ΔG_{int} (kJ mol^{-1})	-63.4	-54.4	ND	-44.1	ND	-53.1	-48.6	-58.9	-59.4	-50.6	-53.3	-58.9
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-23.4	ΔH_{int} (kJ mol^{-1})	-40.7	-23.0	ND	ND	ND	ND	ND	-20.0	ND	-31.5	-26.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	18.6	$-T\Delta S_{int}$ (kJ mol^{-1})	-22.7	-31.5	ND	ND	ND	ND	ND	-38.9	ND	-19.2	-27.1	ND
328		$pK_{a,SA}$	8.53	$K_{d,int}$ (nM)	0.000 66	0.042	ND	10	8.3	0.072	0.87	0.028	0.041	1.6	0.052	0.074
VD11-61		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-50.6	ΔG_{int} (kJ mol^{-1})	-72.3	-61.6	ND	-47.5	-48.0	-60.2	-53.8	-62.7	-61.7	-52.3	-61.1	-60.2
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.4	ΔH_{int} (kJ mol^{-1})	-65.3	-42.0	ND	ND	ND	ND	ND	-18.7	ND	-27.6	-42.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	24.2	$-T\Delta S_{int}$ (kJ mol^{-1})	-7.0	-19.6	ND	ND	ND	ND	ND	-44.0	ND	-24.7	-18.4	ND
329		$pK_{a,SA}$	8.05	$K_{d,int}$ (nM)	0.024	0.061	ND	19	11	0.023	3.0	0.026	0.13	2.4	0.020	0.045
VD11-9		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-47.8	ΔG_{int} (kJ mol^{-1})	-63.1	-60.6	ND	-45.9	-47.3	-63.2	-50.6	-62.8	-58.6	-51.2	-63.5	-61.4
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-27.6	ΔH_{int} (kJ mol^{-1})	-61.9	-37.4	ND	ND	ND	ND	ND	-24.8	ND	-30.5	-49.9	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	20.2	$-T\Delta S_{int}$ (kJ mol^{-1})	-1.1	-23.2	ND	ND	ND	ND	ND	-38.0	ND	-20.7	-13.6	ND
330		$pK_{a,SA}$	7.22	$K_{d,int}$ (nM)	0.087	0.21	ND	270	36	ND	4.8	0.18	2.4	11	0.14	1.8
VD11-10		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-42.9	ΔG_{int} (kJ mol^{-1})	-59.7	-57.5	ND	-39.0	-44.2	ND	-49.4	-57.8	-51.2	-47.2	-58.6	-51.9
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-23.4	ΔH_{int} (kJ mol^{-1})	-65.0	-41.8	ND	ND	ND	ND	-31.3	-16.5	ND	-26.1	-55.8	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	19.5	$-T\Delta S_{int}$ (kJ mol^{-1})	5.3	-15.7	ND	ND	ND	ND	-18.1	-41.3	ND	-21.1	-2.8	ND
331		$pK_{a,SA}$	7.69	$K_{d,int}$ (nM)	2.2	0.43	ND	4.0	38	0.57	2.2	0.11	0.048	35	0.31	2.6
VD10-45		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-45.7	ΔG_{int} (kJ mol^{-1})	-51.4	-55.6	ND	-49.9	-44.1	-54.9	-51.4	-59.1	-61.3	-44.2	-56.5	-51.0
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-26.0	ΔH_{int} (kJ mol^{-1})	-27.6	-15.9	ND	ND	ND	ND	ND	-13.9	ND	-17.4	-36.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	19.7	$-T\Delta S_{int}$ (kJ mol^{-1})	-23.8	-39.7	ND	ND	ND	ND	ND	-45.2	ND	-26.9	-20.0	ND
332		$pK_{a,SA}$	8.02	$K_{d,int}$ (nM)	0.23	0.37	ND	44	120	0.062	7.9	0.34	0.44	9.6	0.23	0.056
VD10-50		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-47.6	ΔG_{int} (kJ mol^{-1})	-57.2	-56.0	ND	-43.7	-41.2	-60.6	-48.1	-56.2	-55.6	-47.6	-57.2	-60.9
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.7	ΔH_{int} (kJ mol^{-1})	-53.6	-36.5	ND	ND	ND	ND	ND	-20.6	-33.8	-28.9	-41.0	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.9	$-T\Delta S_{int}$ (kJ mol^{-1})	-3.6	-19.5	ND	ND	ND	ND	ND	-35.6	-21.7	-18.7	-16.2	ND

No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
335		$pK_{a,SA}$	8.78	$K_{d,int}$ (nM)	9.3	1.7	ND	6.8	13	0.16	5.9	1.8	0.047	4.6	2.1	0.53
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-52.1	ΔG_{int} (kJ mol^{-1})	-47.7	-52.1	ND	-48.5	-46.9	-58.1	-48.8	-51.9	-61.3	-49.5	-51.6	-55.1
VD12-36		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-25.5	ΔH_{int} (kJ mol^{-1})	-7.5	-31.6	ND	ND	ND	ND	ND	-5.8	-18.8	-24.4	-9.6	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.6	$-T\Delta S_{int}$ (kJ mol^{-1})	-40.2	-20.6	ND	ND	ND	ND	ND	-46.1	-42.6	-25.2	-41.9	ND
337		$pK_{a,SA}$	8.62	$K_{d,int}$ (nM)	260	32	ND	270	160	0.78	7.6	130	0.39	23	8.2	3.0
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-51.2	ΔG_{int} (kJ mol^{-1})	-39.1	-44.5	ND	-39.0	-40.4	-54.1	-48.2	-40.8	-55.9	-45.4	-48.0	-50.6
VD12-38		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-23.0	ΔH_{int} (kJ mol^{-1})	ND	-5.3	ND	ND	ND	ND	ND	ND	-14.8	-19.3	4.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	28.2	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-39.2	ND	ND	ND	ND	ND	ND	-41.1	-26.1	-52.2	ND
341		$pK_{a,SA}$	8.68	$K_{d,int}$ (nM)	460	9.1	980	8.9	45	1.0	9.3	1.6	0.0045	1.9	1.8	1.1
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-51.5	ΔG_{int} (kJ mol^{-1})	-37.6	-47.7	-35.7	-47.8	-43.6	-53.4	-47.7	-52.2	-67.4	-51.8	-51.9	-53.1
VD12-09		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-25.1	ΔH_{int} (kJ mol^{-1})	ND	-7.3	ND	ND	ND	-50.3	ND	-2.2	-18.8	-24.8	-12.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.4	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-40.4	ND	ND	ND	-3.1	ND	-50.0	-48.6	-27.0	-39.2	ND
345		$pK_{a,SA}$	8.61	$K_{d,int}$ (nM)	180	29	ND	45	160	4.0	7.3	15	0.051	12	0.73	1.5
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-51.1	ΔG_{int} (kJ mol^{-1})	-40.0	-44.7	ND	-43.6	-40.4	-49.9	-48.3	-46.4	-61.1	-47.1	-54.3	-52.3
VD12-15		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-25.1	ΔH_{int} (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	-13.6	-18.1	-11.0	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	26.0	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	ND	ND	ND	ND	ND	ND	ND	-47.5	-29.0	-43.3	ND
367		$pK_{a,SA}$	8.18	$K_{d,int}$ (nM)	3300	61	3000	220	69	57	22	12	0.0071	6.0	9.4	5.7
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-48.6	ΔG_{int} (kJ mol^{-1})	-32.5	-42.8	-32.8	-39.5	-42.5	-43.0	-45.5	-47.0	-66.2	-48.8	-47.7	-49.0
AZ13-2-2		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.5	ΔH_{int} (kJ mol^{-1})	ND	0.9	ND	ND	ND	ND	ND	-1.1	-20.9	-28.6	-2.1	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	24.1	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-43.8	ND	ND	ND	ND	ND	-45.9	-45.3	-20.2	-45.5	ND
368		$pK_{a,SA}$	7.85	$K_{d,int}$ (nM)	23	4.6	ND	3.2	27	0.21	1.5	6.0	0.022	1.2	1.6	0.60
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.6	ΔG_{int} (kJ mol^{-1})	-45.4	-49.5	ND	-50.4	-44.9	-57.5	-52.4	-48.8	-63.3	-53.0	-52.2	-54.8
VD10-39b		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.7	ΔH_{int} (kJ mol^{-1})	-53.7	-22.1	ND	ND	ND	ND	-16.2	-14.7	-25.8	-35.5	-32.4	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.9	$-T\Delta S_{int}$ (kJ mol^{-1})	8.3	-27.4	ND	ND	ND	ND	-36.1	-34.1	-37.5	-17.5	-19.8	ND

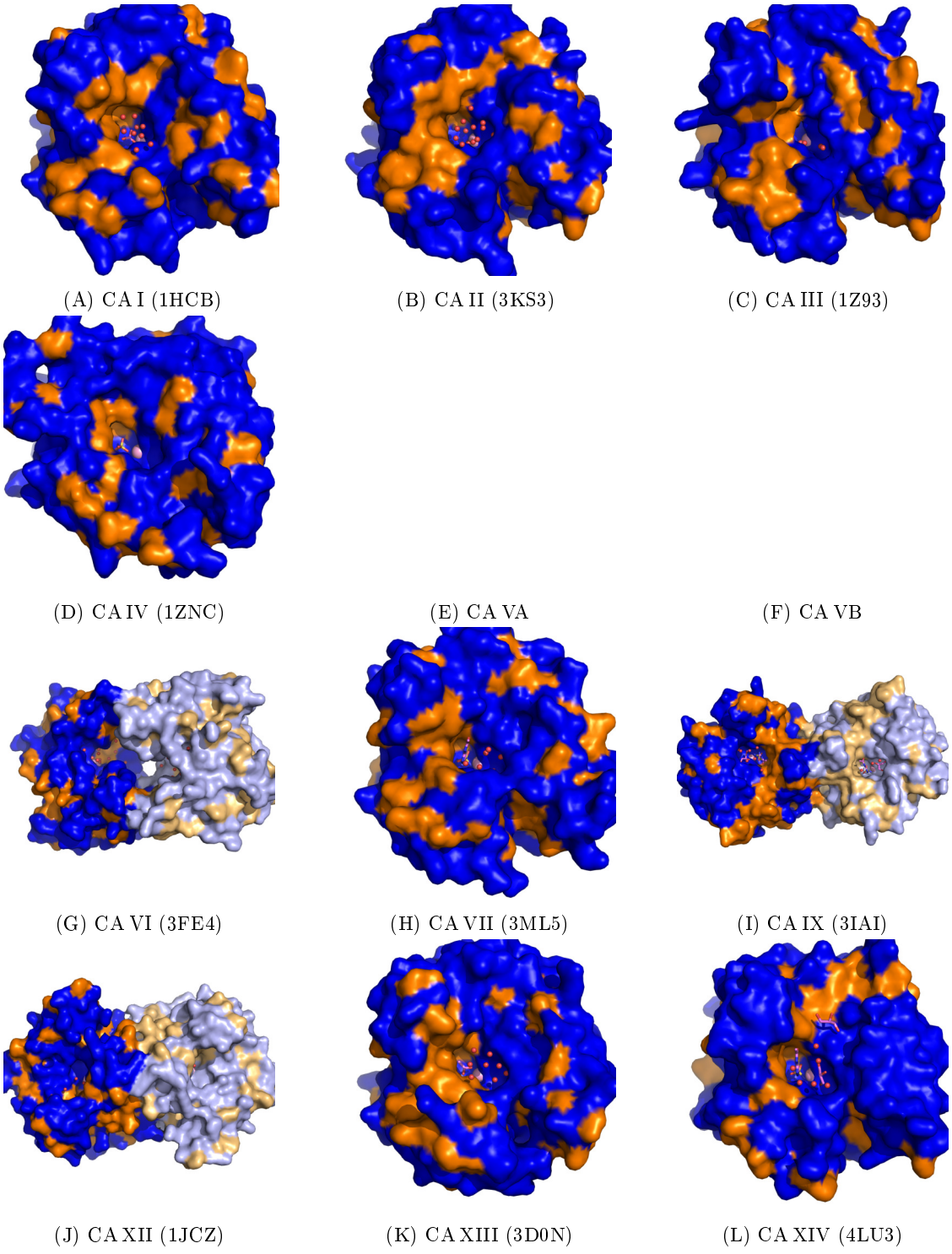
No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
369		$pK_{a,SA}$	8.01	$K_{d,int}$ (nM)	69	2.2	720	1.5	200	0.70	0.54	0.30	0.000 80	0.10	0.33	0.15
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-47.6	ΔG_{int} (kJ mol^{-1})	-42.5	-51.4	-36.5	-52.3	-39.8	-54.3	-55.0	-56.6	-71.8	-59.3	-56.3	-58.4
VD11-4-2		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-25.6	ΔH_{int} (kJ mol^{-1})	0.8	-7.7	ND	ND	ND	ND	ND	-12.2	-24.3	-40.9	-11.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	21.9	$-T\Delta S_{int}$ (kJ mol^{-1})	-43.4	-43.7	ND	ND	ND	ND	ND	-44.4	-47.5	-18.4	-45.1	ND
371		$pK_{a,SA}$	7.82	$K_{d,int}$ (nM)	27	1.3	6300	5.3	88	0.66	12	2.0	0.025	3.4	3.0	1.3
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.4	ΔG_{int} (kJ mol^{-1})	-44.9	-52.8	-30.9	-49.1	-41.9	-54.5	-47.0	-51.6	-63.0	-50.3	-50.6	-52.8
VD12-32		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-22.6	ΔH_{int} (kJ mol^{-1})	-54.8	-51.9	ND	ND	ND	ND	ND	-21.3	-22.9	-17.1	-2.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	23.8	$-T\Delta S_{int}$ (kJ mol^{-1})	9.9	-0.8	ND	ND	ND	ND	ND	-30.3	-40.0	-33.2	-48.2	ND
372		$pK_{a,SA}$	7.87	$K_{d,int}$ (nM)	9.2	9.3	ND	14	5.3	2.0	5.4	0.66	0.085	3.8	0.47	23
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.7	ΔG_{int} (kJ mol^{-1})	-47.7	-47.7	ND	-46.7	-49.1	-51.7	-49.1	-54.5	-59.8	-50.0	-55.4	-45.4
VD12-33		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	ND	-24.1	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.4	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-23.6	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
373		$pK_{a,SA}$	7.85	$K_{d,int}$ (nM)	110	0.91	ND	2.3	130	0.52	1.1	0.24	0.0039	0.40	0.94	0.20
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.6	ΔG_{int} (kJ mol^{-1})	-41.2	-53.7	ND	-51.2	-40.8	-55.1	-53.1	-57.1	-67.7	-55.8	-53.6	-57.6
VD12-34		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	-15.9	-36.4	ND	ND	ND	ND	ND	-12.0	-27.9	-47.0	-21.2	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.3	$-T\Delta S_{int}$ (kJ mol^{-1})	-25.3	-17.3	ND	ND	ND	ND	ND	-45.2	-39.9	-8.8	-32.4	ND
374		$pK_{a,SA}$	7.87	$K_{d,int}$ (nM)	160	3.2	ND	6.8	79	9.1	4.9	0.46	0.0017	0.60	1.1	0.30
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.7	ΔG_{int} (kJ mol^{-1})	-40.4	-50.5	ND	-48.5	-42.2	-47.7	-49.3	-55.4	-69.9	-54.8	-53.2	-56.6
VD12-23		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.0	ΔH_{int} (kJ mol^{-1})	ND	-45.1	ND	ND	ND	ND	ND	-39.1	ND	-29.5	-45.7	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-5.4	ND	ND	ND	ND	ND	-16.3	ND	-25.3	-7.5	ND

No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
375		$pK_{a,SA}$	7.88	$K_{d,int}$ (nM)	2400	3.3	ND	ND	390	0.58	3.9	1.5	ND	0.71	0.52	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.8	ΔG_{int} (kJ mol^{-1})	-33.3	-50.4	ND	ND	-38.1	-54.8	-49.9	-52.4	ND	-54.3	-55.1	ND
VD12-25-2		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.3	ΔH_{int} (kJ mol^{-1})	ND	1.3	ND	ND	ND	ND	ND	-3.4	ND	-24.3	-25.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.5	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-51.7	ND	ND	ND	ND	ND	-49.0	ND	-30.1	-29.6	ND
376		$pK_{a,SA}$	7.87	$K_{d,int}$ (nM)	8.2	0.31	ND	3400	40	0.40	1.1	0.38	0.26	13	0.14	0.23
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.7	ΔG_{int} (kJ mol^{-1})	-48.0	-56.5	ND	-32.5	-44.0	-55.8	-53.2	-55.9	-57.0	-46.8	-58.6	-57.2
VD11-26		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.0	ΔH_{int} (kJ mol^{-1})	ND	-49.0	ND	ND	ND	ND	ND	ND	ND	-27.5	-42.0	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-7.4	ND	ND	ND	ND	ND	ND	ND	-19.2	-16.6	ND
377		$pK_{a,SA}$	7.87	$K_{d,int}$ (nM)	73	0.088	ND	8.3	57	0.030	0.54	0.010	0.029	3.1	0.54	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.7	ΔG_{int} (kJ mol^{-1})	-42.4	-59.7	ND	-48.0	-43.0	-62.5	-55.0	-65.3	-62.6	-50.6	-55.0	ND
VD11-25		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.0	ΔH_{int} (kJ mol^{-1})	ND	-19.6	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-40.1	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
378		$pK_{a,SA}$	7.87	$K_{d,int}$ (nM)	5.8	0.35	ND	31	20	0.40	1.2	0.23	0.11	1.8	0.27	ND
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.7	ΔG_{int} (kJ mol^{-1})	-48.9	-56.1	ND	-44.6	-45.7	-55.8	-53.0	-57.2	-59.1	-51.9	-56.8	ND
VD11-28		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.0	ΔH_{int} (kJ mol^{-1})	ND	-22.9	ND	ND	ND	ND	ND	ND	ND	ND	-17.5	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-33.3	ND	ND	ND	ND	ND	ND	ND	ND	-39.3	ND
380		$pK_{a,SA}$	7.87	$K_{d,int}$ (nM)	11	0.066	ND	42	40	0.24	0.43	0.11	0.19	7.1	0.54	0.19
		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.7	ΔG_{int} (kJ mol^{-1})	-47.3	-60.5	ND	-43.8	-44.0	-57.1	-55.6	-59.0	-57.7	-48.4	-55.0	-57.8
VD11-15		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.0	ΔH_{int} (kJ mol^{-1})	ND	-27.6	ND	ND	ND	ND	ND	ND	ND	-19.0	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-32.9	ND	ND	ND	ND	ND	ND	ND	-29.4	ND	ND

No. Cpd	Structure				CA I	CA II	CA III	CA IV	CA VA	CA VB	CA VI	CA VII	CA IX	CA XII	CA XIII	CA XIV
385		$pK_{a,SA}$	7.87	$K_{d,int}$ (nM)	71	2.6	ND	56	1100	4.0	3.6	0.23	ND	0.77	0.60	2.3
VD11-17		$\Delta G_{pr,SA}$ (kJ mol^{-1})	-46.7	ΔG_{int} (kJ mol^{-1})	-42.4	-50.9	ND	-43.0	-35.3	-49.9	-50.1	-57.2	ND	-54.1	-54.8	-51.3
		$\Delta H_{pr,SA}$ (kJ mol^{-1})	-24.0	ΔH_{int} (kJ mol^{-1})	ND	-19.6	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
		$T\Delta S_{pr,SA}$ (kJ mol^{-1})	22.7	$-T\Delta S_{int}$ (kJ mol^{-1})	ND	-31.3	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

2 Supplementary figures

2.1 X-Ray crystallographic structures of unliganded human CA isoforms



(A) CA I (1HCB) (B) CA II (3KS3) (C) CA III (1Z93)

(D) CA IV (1ZNC) (E) CA VA (F) CA VB

(G) CA VI (3FE4) (H) CA VII (3ML5) (I) CA IX (3IAI)

(J) CA XII (1JCZ) (K) CA XIII (3D0N) (L) CA XIV (4LU3)

Figure 1: X-ray crystallographic structures of 10 catalytically active human CA isoforms, without an inhibitor in the active site. The monomeric ones are oriented in the same orientation with the active site cavities containing Zn^{II} in the front center of each picture. Hydrophobic amino acids are shown in yellow while hydrophilic – in blue. Water molecules in the active site are shown as red spheres while the catalytic Zn^{II} – as a pink sphere. The PDB IDs are listed in the brackets.

2.2 Crystal structure-thermodynamics correlations

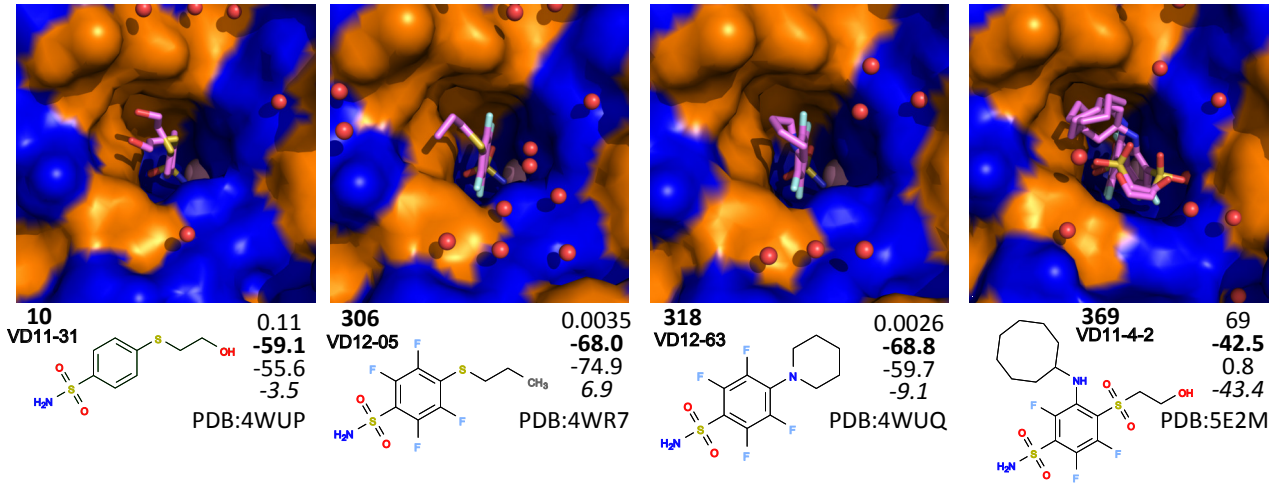


Figure 2: The X-Ray crystallographic structure Pymol renderings of the inhibitors bound in the active site of CA I together with the intrinsic thermodynamic parameters of compound binding. Compound chemical structures are shown below the crystal structures. Compound number and local name is listed on the left, while the numbers on the right show the K_{d_intr} in nM, the intrinsic Gibbs energy of binding in kJ mol^{-1}, the intrinsic enthalpy in kJ mol^{-1}, the intrinsic entropy $-T\Delta S$ in kJ mol^{-1}, and the PDB ID of the crystal structure.

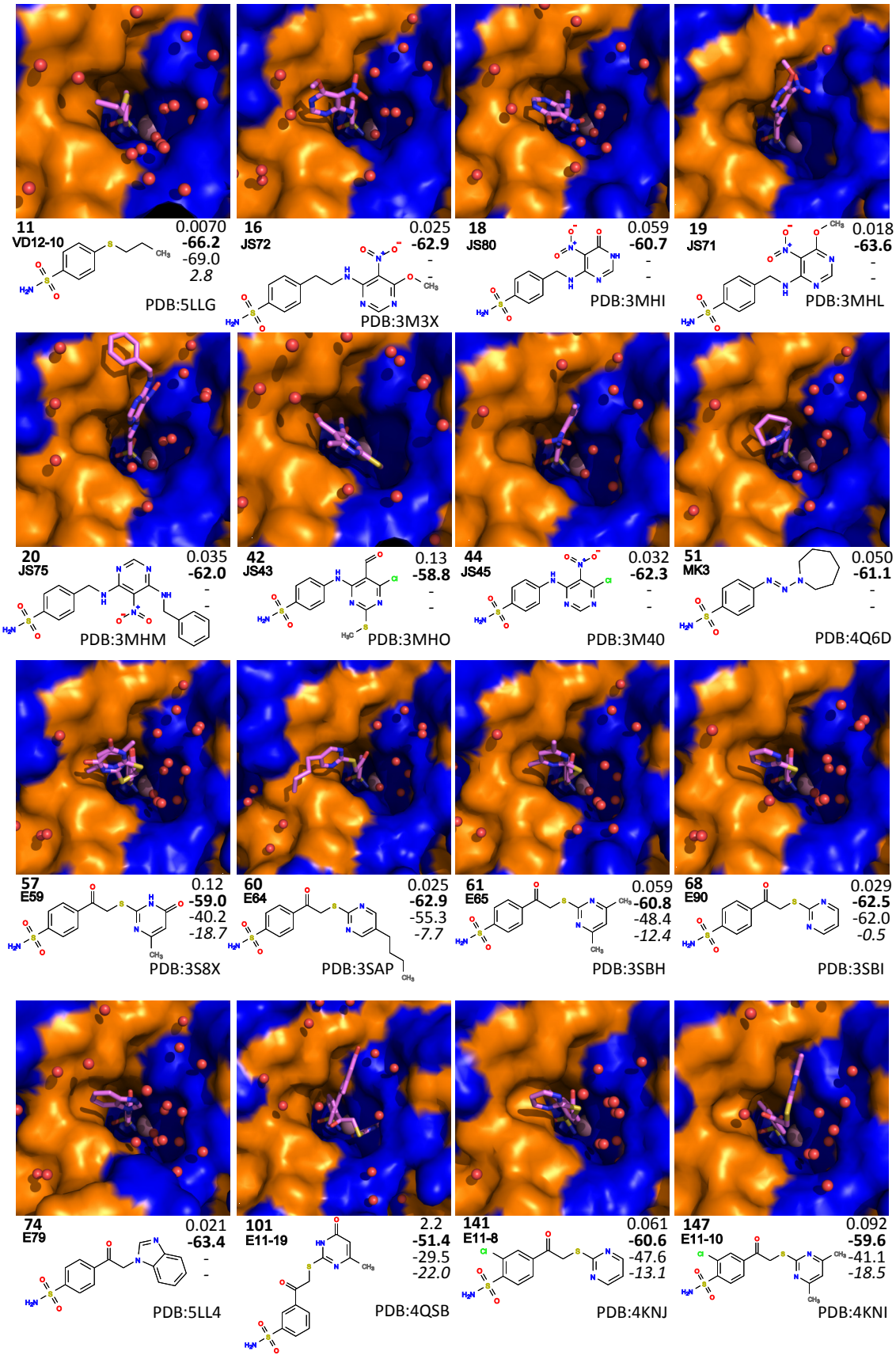


Figure 3: Continuation of the X-Ray crystallographic structure Pymol renderings of the inhibitors bound in the active site of a CA. This page lists inhibitors bound to CAII. See explanation in the legend of Figure 2.

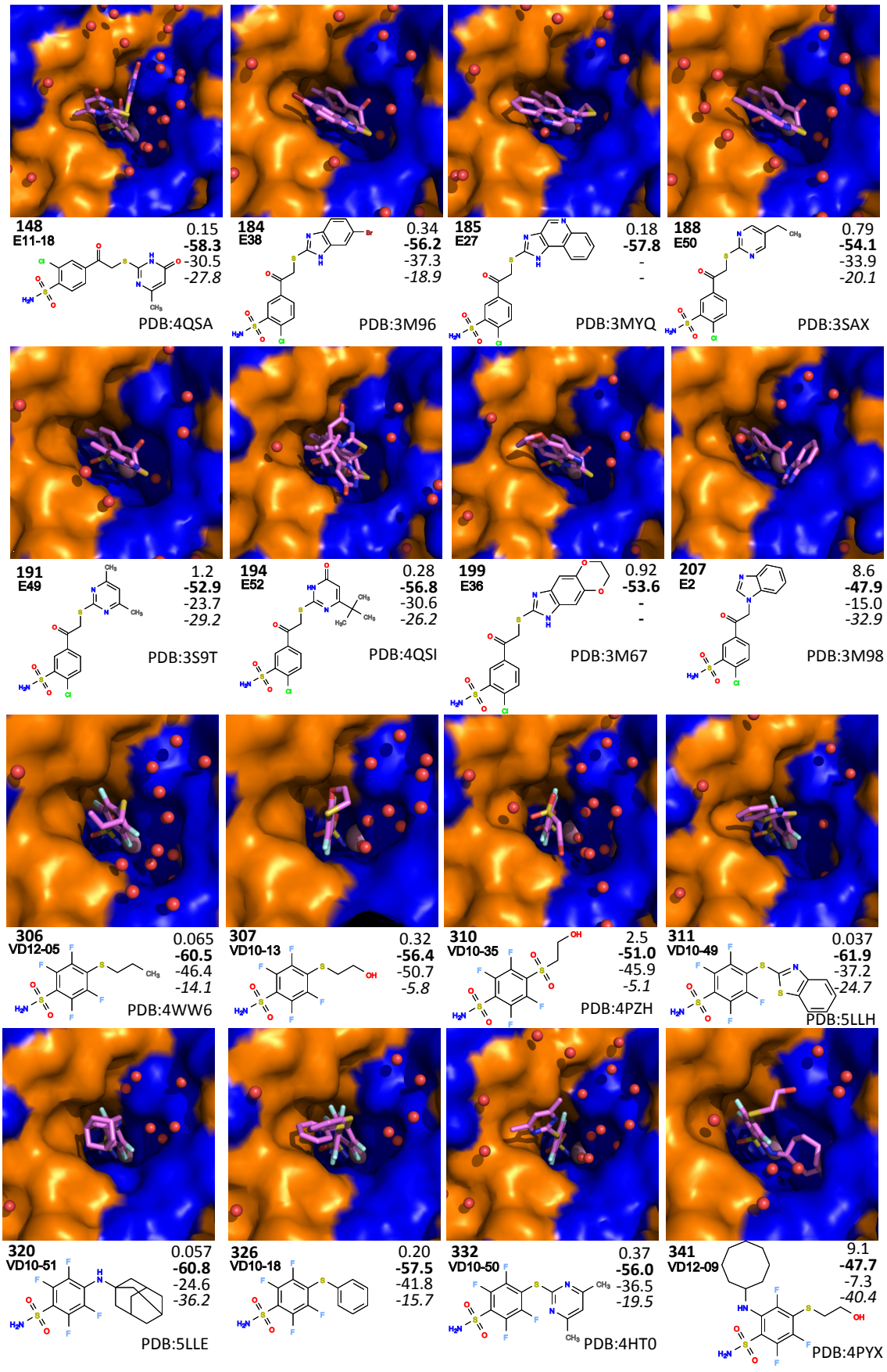


Figure 4: Continuation of the X-Ray crystallographic structure Pymol renderings of the inhibitors bound in the active site of a CA. This page lists inhibitors bound to CAII. See explanation in the legend of Figure 2.

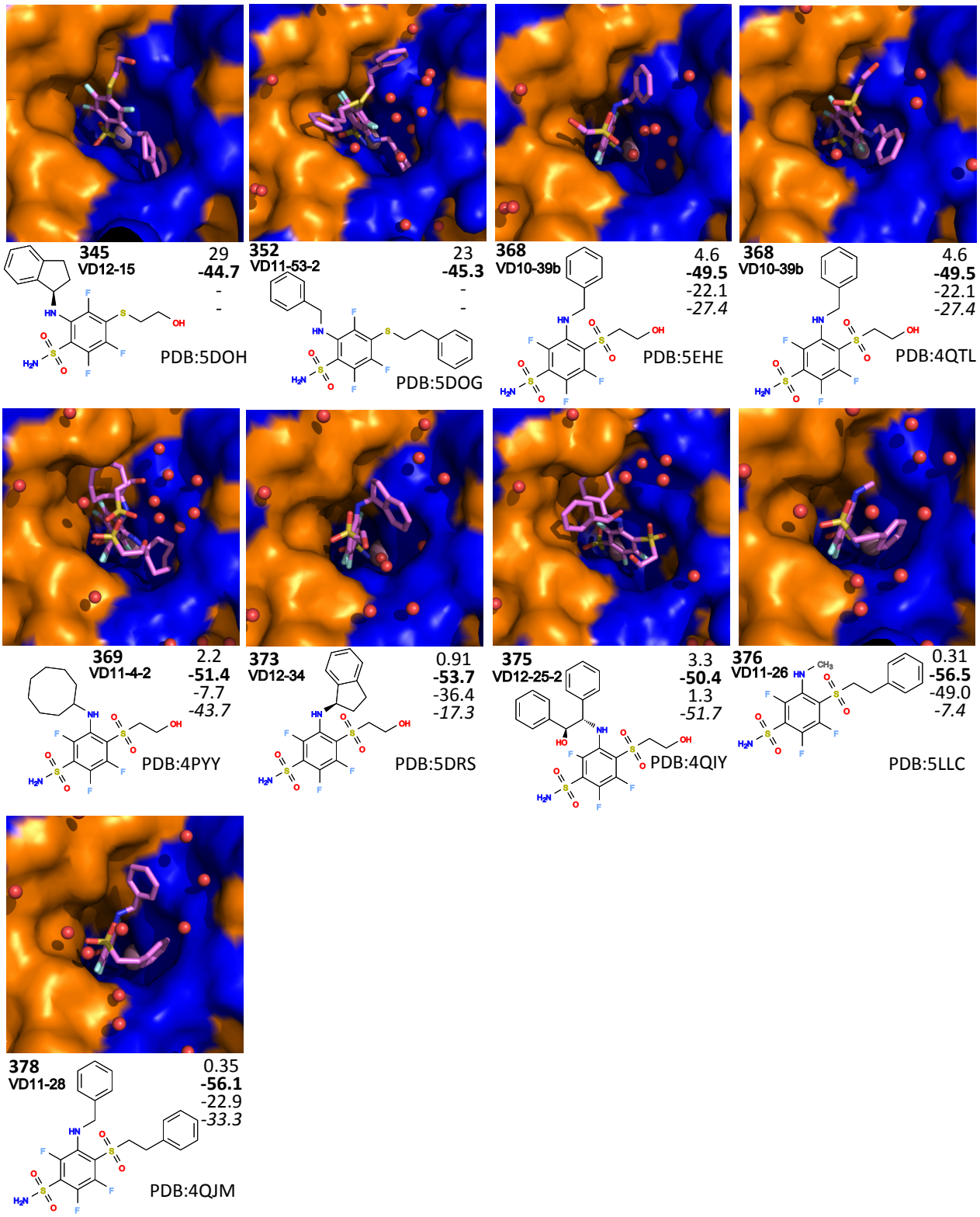


Figure 5: Continuation of the X-Ray crystallographic structure Pymol renderings of the inhibitors bound in the active site of a CA. This page lists inhibitors bound to CAII. See explanation in the legend of Figure 2.

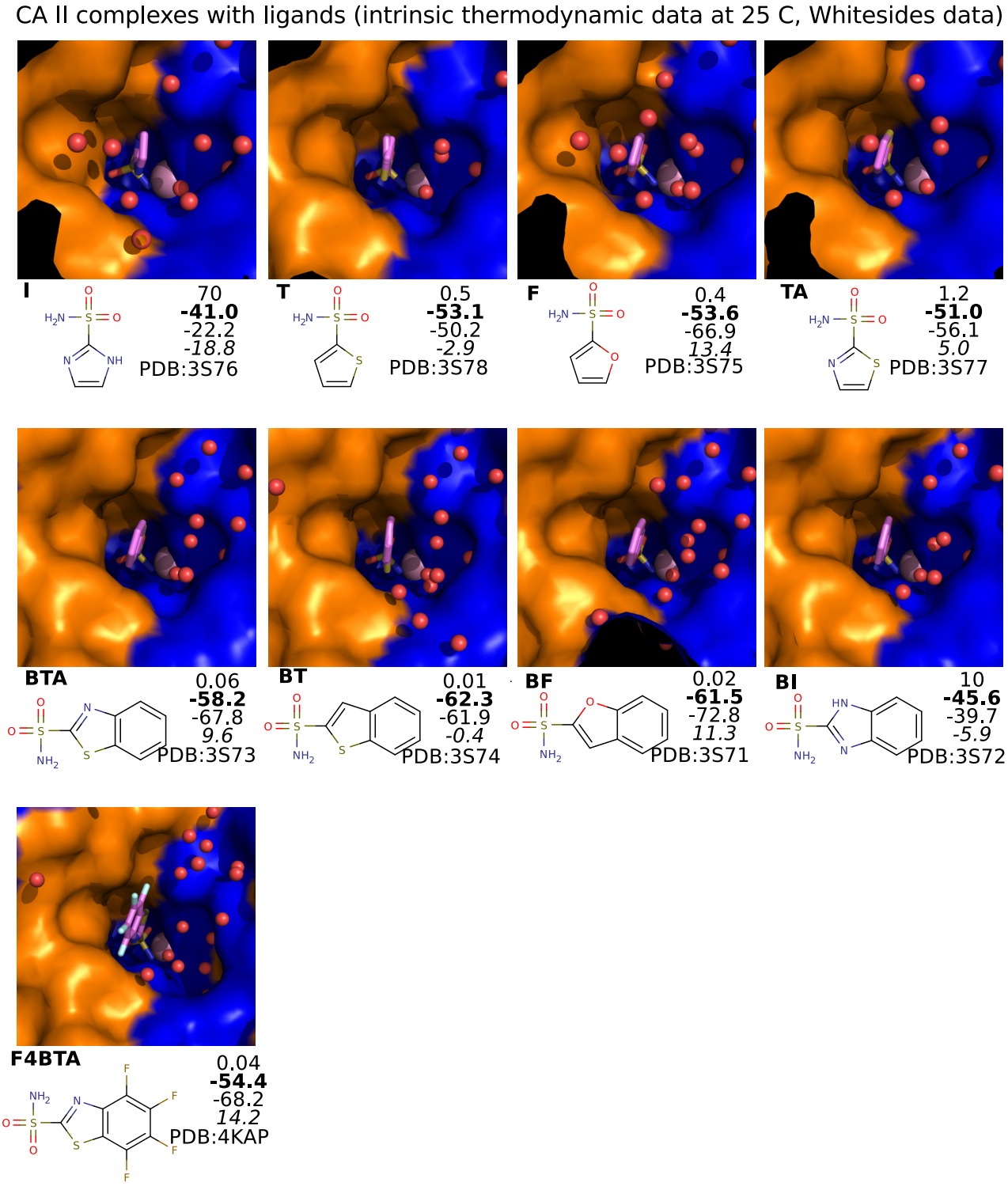


Figure 6: Continuation of the X-Ray crystallographic structure Pymol renderings of the inhibitors bound in the active site of a CA. The structures are taken from the study by Whitesides group (Snyder,2011; Lockett, 2013), the inhibitors are bound in the active site of CA II. See explanation in the legend of Figure 2.

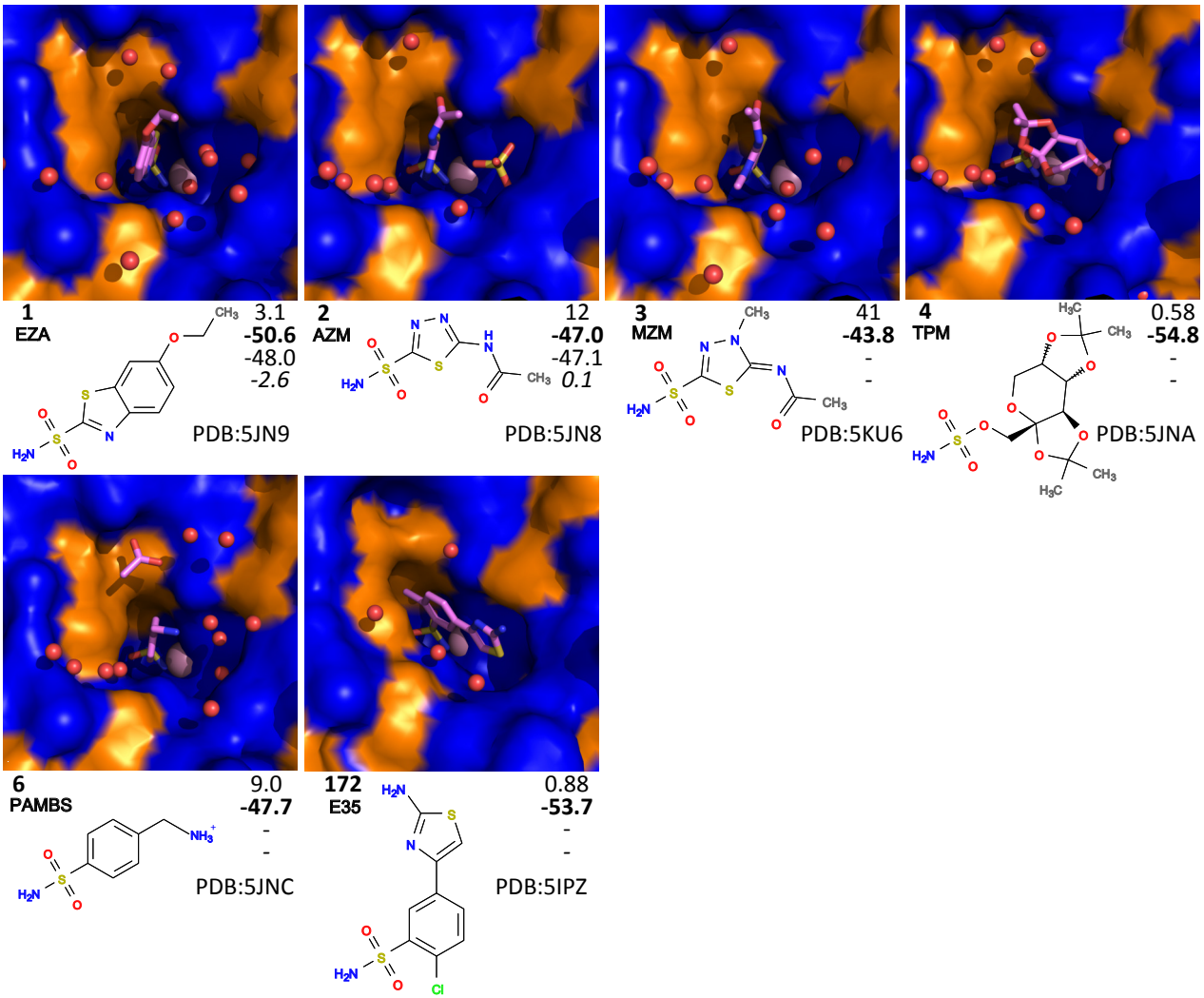


Figure 7: Continuation of the X-Ray crystallographic structure Pymol renderings of the inhibitors bound in the active site of a CA. This page lists inhibitors bound to CAIV. See explanation in the legend of Figure 2.

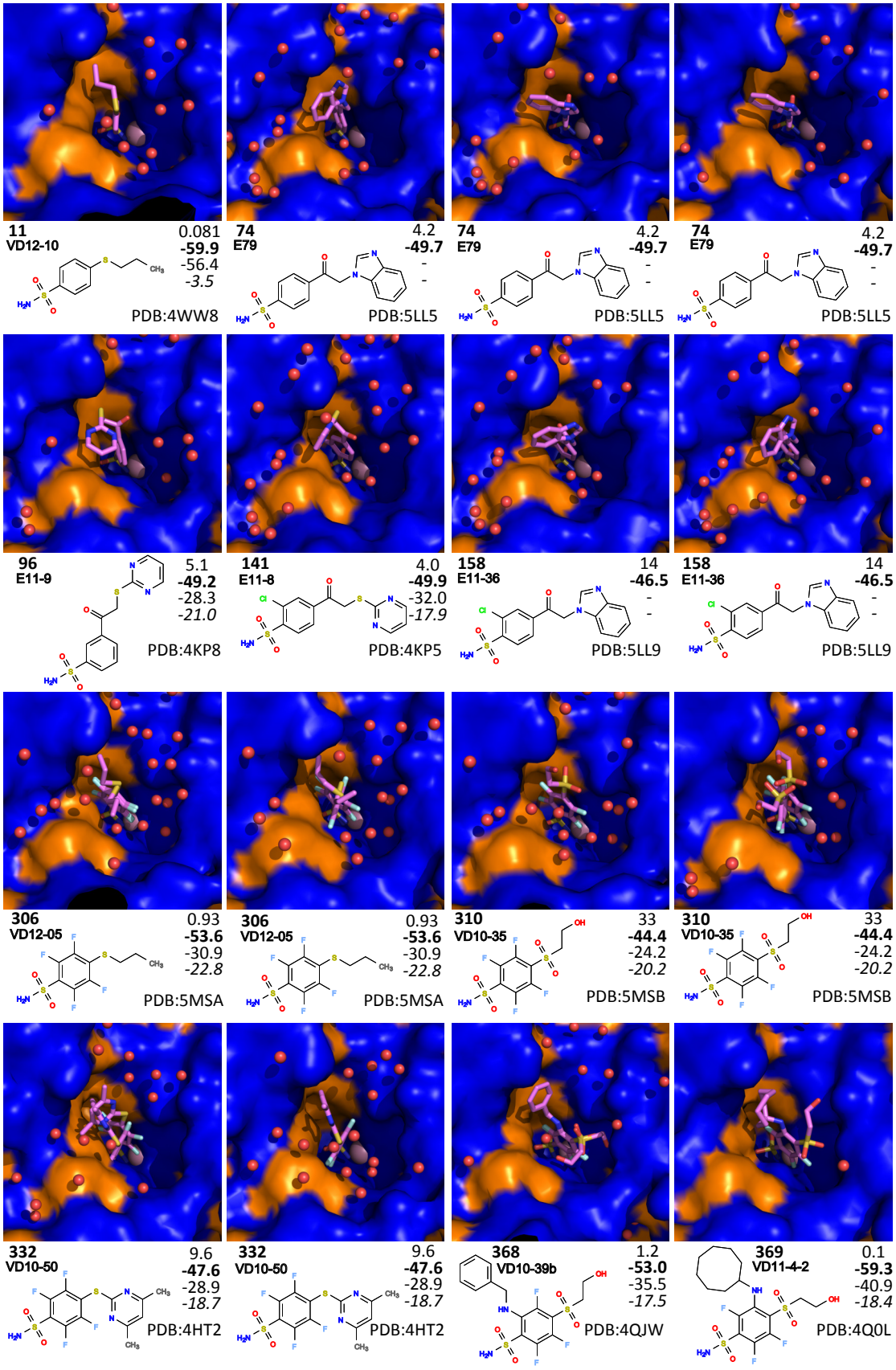


Figure 8: Continuation of the X-Ray crystallographic structure Pymol renderings of the inhibitors bound in the active site of a CA. This page lists inhibitors bound to CA XII. See explanation in the legend of Figure 2.

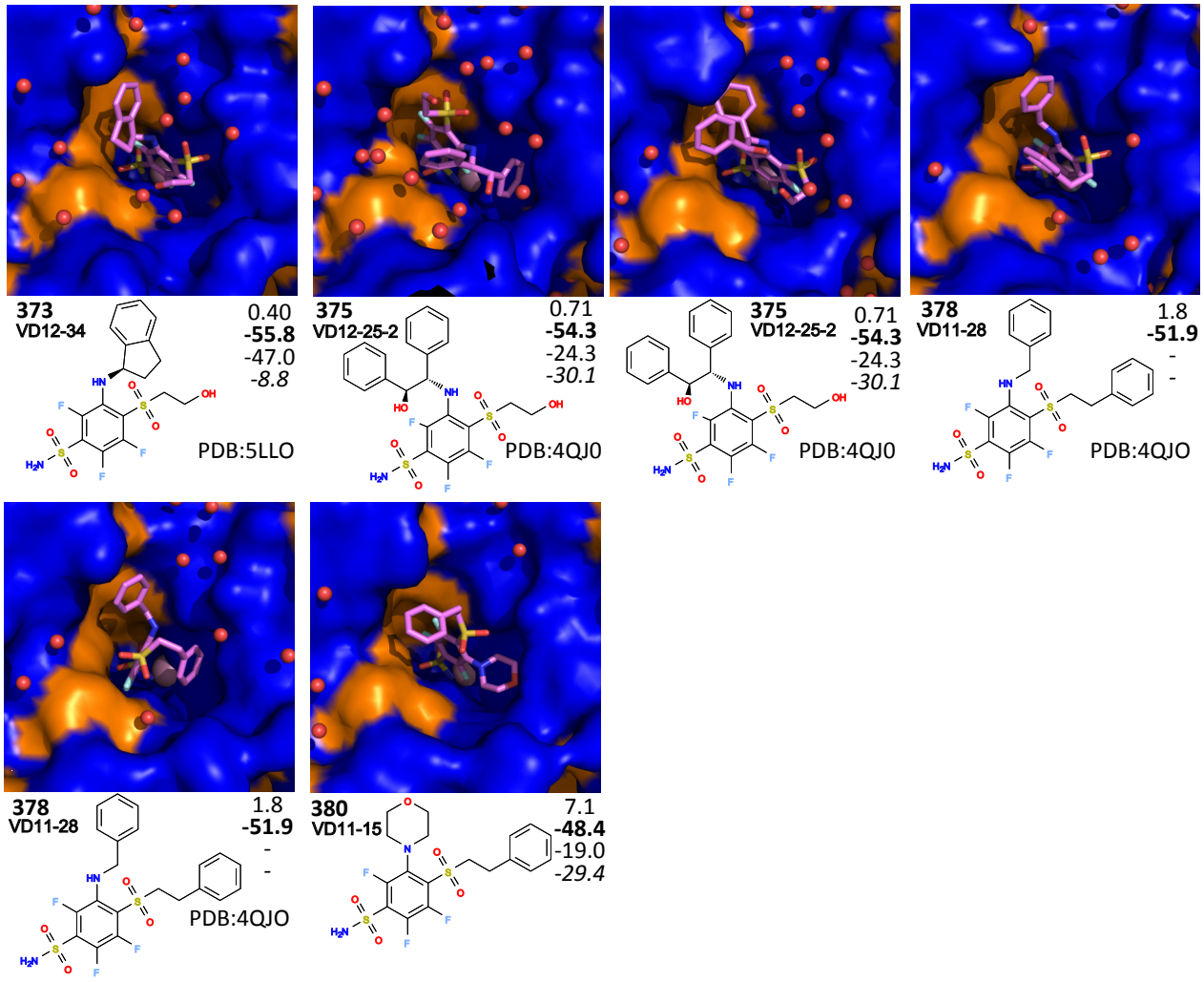


Figure 9: Continuation of the X-Ray crystallographic structure Pymol renderings of the inhibitors bound in the active site of a CA. This page lists inhibitors bound to CA XII. See explanation in the legend of Figure 2.

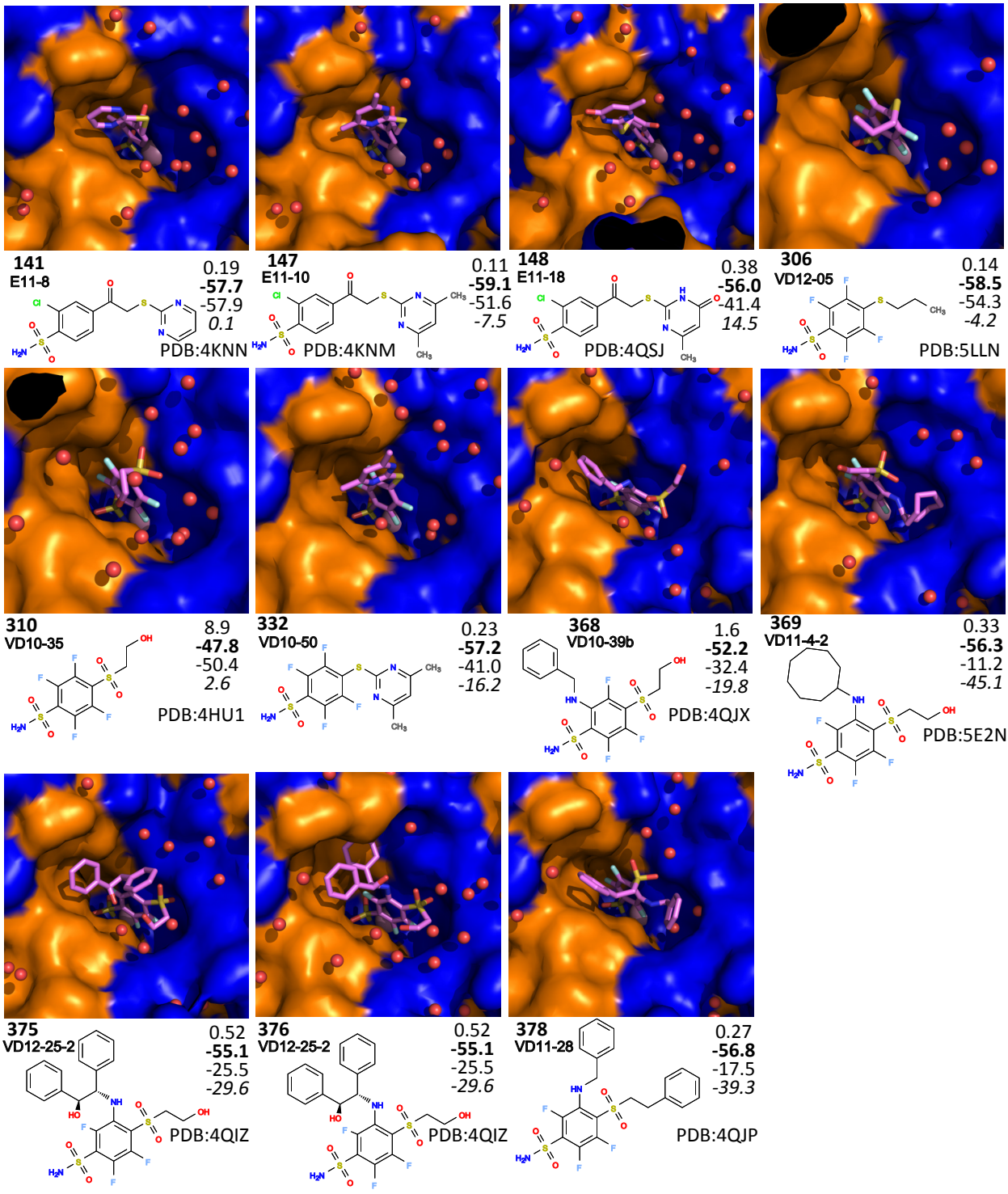


Figure 10: Continuation of the X-Ray crystallographic structure Pymol renderings of the inhibitors bound in the active site of a CA. This page lists inhibitors bound to CA XIII. See explanation in the legend of Figure 2.

2.3 Compound structure-thermodynamics correlation maps

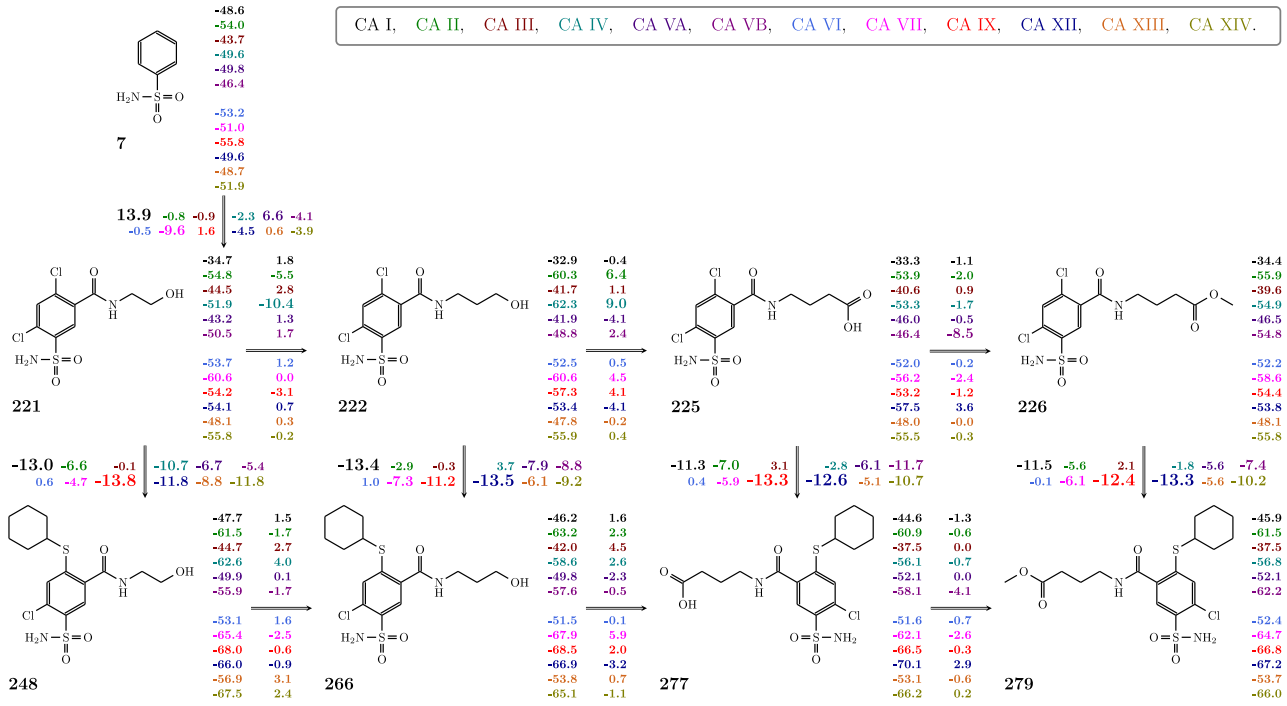


Figure 11: Gibbs energy contributions of compound functional groups in the search of chlorinated compounds that would selectively bind and inhibitCA XII. The map shows a series of compounds connected by arrows beginning with benzenesulfonamide as the weakest inhibitor and ending with the best inhibitors on the right. Numbers next to the structures show the intrinsic Gibbs energies of compound binding to each recombinant human CA isoform. Numbers at the arrows show the differences between the affinities to two connected isoforms. Larger differences are depicted in larger font size to emphasize the largest energy gains upon chemical modifications of the compounds.

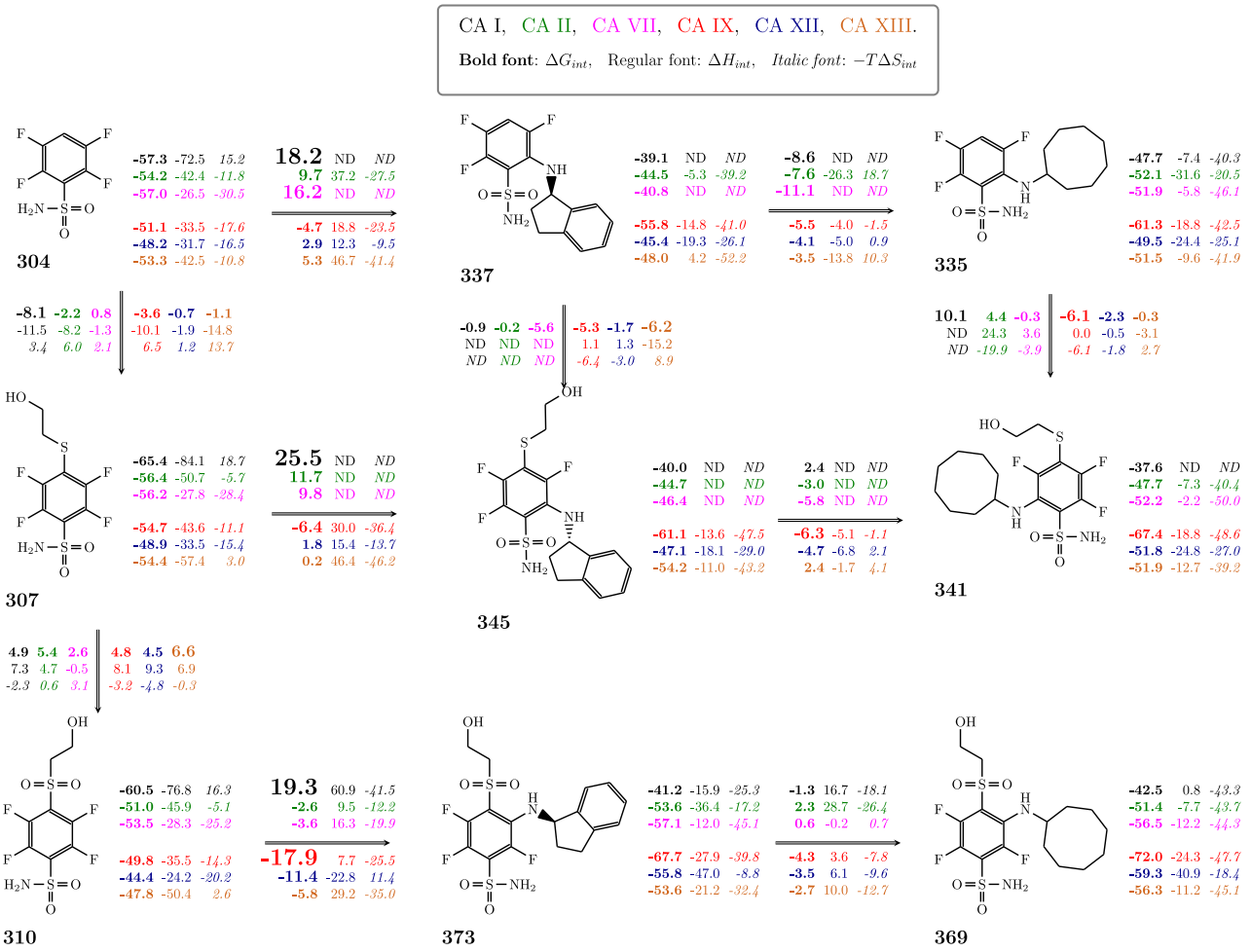


Figure 12: A map of intrinsic Gibbs energy, enthalpy, and entropy gains or loses upon chemical modification of compounds. The map begins with 2,3,5,6-tetrafluoro benzenesulfonamide on the left upper corner as a relatively weak binder and ends with high-affinity and high selectivity CA IX-binding compounds such as **369**. The numbers next to the compounds show the Gibbs energies, enthalpies, and entropies of binding to the tested six CA isoforms, while the numbers on the arrows show the differences in energetic parameters of binding between neighboring compounds. Quite often, the significant gain in affinity was not followed by a gain in exothermic enthalpy.