

ID	name	K_a (M ⁻¹)	ΔG (kcal/mol) ^(a)	ΔH (kcal/mol)	$T\Delta S$ (kcal/mol) ^(b)	n
OA-G0	cyclopentyl acetic acid	$(147.0 \pm 7.0) \times 10^2$	-5.68 \pm 0.03	-4.8 \pm 0.2	0.8 \pm 0.2	1
OA-G1	trans-2-hexenoic acid	$(26.0 \pm 1.0) \times 10^2$	-4.65 \pm 0.02	-5.5 \pm 0.2	-0.9 \pm 0.2	1
OA-G2	(s)-(-)-perillic acid	$(140.0 \pm 6.0) \times 10^4$	-8.38 \pm 0.02	-12.1 \pm 0.5	-3.7 \pm 0.5	1
OA-G3	5-hexenoic acid	$(62.0 \pm 2.0) \times 10^2$	-5.18 \pm 0.02	-7.5 \pm 0.3	-2.4 \pm 0.3	1
OA-G4	(s)-(-)-citronellic acid	$(164.0 \pm 7.0) \times 10^3$	-7.11 \pm 0.02	-6.9 \pm 0.3	0.2 \pm 0.3	1
OA-G5	2-methyl-4-pentenoic acid	$(233.0 \pm 9.0) \times 10$	-4.59 \pm 0.02	-5.3 \pm 0.2	-0.7 \pm 0.2	1
OA-G6	4-methylpentanoic acid	$(44.0 \pm 2.0) \times 10^2$	-4.97 \pm 0.02	-5.3 \pm 0.2	-0.3 \pm 0.2	1
OA-G7	2,2-dimethyl-4-pentenoic acid	$(36.0 \pm 1.0) \times 10^3$	-6.22 \pm 0.02	-7.4 \pm 0.3	-1.2 \pm 0.3	1
TEMOA-G0	cyclopentyl acetic acid	$(28.0 \pm 1.0) \times 10^3$	-6.06 \pm 0.02	-7.8 \pm 0.4	-1.8 \pm 0.4	1
TEMOA-G1	trans-2-hexenoic acid	$(24.0 \pm 2.0) \times 10^3$	-5.97 \pm 0.04	-8.2 \pm 0.6	-2.3 \pm 0.6	1
TEMOA-G2	(s)-(-)-perillic acid	$(98.0 \pm 4.0) \times 10^3$	-6.81 \pm 0.02	-9.3 \pm 0.4	-2.5 \pm 0.4	1
TEMOA-G3	5-hexenoic acid	$(128.0 \pm 9.0) \times 10^2$	-5.6 \pm 0.04	-8.9 \pm 0.4	-3.2 \pm 0.4	1
TEMOA-G4	(s)-(-)-citronellic acid	$(51.0 \pm 2.0) \times 10^4$	-7.79 \pm 0.02	-8.9 \pm 0.4	-1.1 \pm 0.4	1
TEMOA-G5	2-methyl-4-pentenoic acid	$(113.0 \pm 5.0) \times 10$	-4.16 \pm 0.02	-8.0 \pm 0.3	-3.8 \pm 0.3	1
TEMOA-G6	4-methylpentanoic acid	$(91.0 \pm 5.0) \times 10^2$	-5.4 \pm 0.03	-6.2 \pm 0.2	-0.8 \pm 0.2	1
TEMOA-G7	2,2-dimethyl-4-pentenoic acid	$(107.0 \pm 4.0) \times 10$	-4.13 \pm 0.02	-8.3 \pm 0.3	-4.2 \pm 0.3	1
CB8-G0	lexapro	$(81.0 \pm 6.0) \times 10^3$	-6.69 \pm 0.05	-4.2 \pm 0.2	2.5 \pm 0.2	1
CB8-G1	detrol	$(40.0 \pm 3.0) \times 10^4$ ^(c)	-7.65 \pm 0.04	-5.0 \pm 0.2	2.6 \pm 0.2	0.5
CB8-G2	palonosetron	$(41.0 \pm 4.0) \times 10^4$	-7.66 \pm 0.05	-6.5 \pm 0.3	1.2 \pm 0.3	1
CB8-G3	quinine	$(53.0 \pm 5.0) \times 10^3$	-6.45 \pm 0.06	-2.5 \pm 0.1	4.0 \pm 0.2	1
CB8-G4	gallamine triethiodate	$(51.0 \pm 4.0) \times 10^4$ ^(d)	-7.8 \pm 0.04	-9.8 \pm 0.4	-2.0 \pm 0.4	0.33
CB8-G5	(1R,2S,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-amine	$(99.0 \pm 9.0) \times 10^4$	-8.18 \pm 0.05	-3.2 \pm 0.1	5.0 \pm 0.1	1
CB8-G6	cycloheptanamine	$(13.0 \pm 1.0) \times 10^5$	-8.34 \pm 0.05	-5.7 \pm 0.2	2.6 \pm 0.2	1
CB8-G7	cyclooctanamine	$(21.0 \pm 4.0) \times 10^6$	-10.0 \pm 0.1	-6.5 \pm 0.3	3.5 \pm 0.3	1
CB8-G8	cyclododecanamine	$(83.0 \pm 6.0) \times 10^8$	-13.5 \pm 0.04	-14.4 \pm 0.6	-0.9 \pm 0.6	1
CB8-G9	(2R,3as,5S,6as)-hexahydro-2,5-methanopentalen-3a(1H)-amine	$(23.0 \pm 3.0) \times 10^5$	-8.68 \pm 0.08	-4.6 \pm 0.2	4.0 \pm 0.2	1
CB8-G10	(1s,3r,5R,7S)-3-aminoadamantan-1-ol	$(10.0 \pm 1.0) \times 10^5$	-8.22 \pm 0.07	-2.0 \pm 0.08	6.2 \pm 0.1	1
CB8-G11	cyclohexane diamine	$(50.0 \pm 4.0) \times 10^4$	-7.77 \pm 0.05	-2.11 \pm 0.08	5.67 \pm 0.1	1
CB8-G12a	aricept	$(167.0 \pm 9.0) \times 10^5$	-9.86 \pm 0.03	-9.2 \pm 0.4	0.7 \pm 0.4	1
CB8-G12b	aricept	$(146.0 \pm 6.0) \times 10^3$ ^(c)	-7.05 \pm 0.02	-4.8 \pm 0.2	2.2 \pm 0.2	2
CB8-G13	oxaliplatin	$(161.0 \pm 8.0) \times 10^3$	-7.11 \pm 0.03	-6.8 \pm 0.3	0.3 \pm 0.3	1

All quantities are reported as point estimate \pm statistical error from the ITC data fitting procedure. The upper bound (1%) was used for errors reported to be $< 1\%$. We also included a 3% relative uncertainty in the titrant concentration assuming the stoichiometry coefficient to be fitted to the ITC data [1]. This is exact only for the OA/TEMOA sets (with the exception of OA-G5, TEMOA-G5, and TEMOA G7). For the other guests, we may expand the error analysis to include also the effect of the uncertainties in titrand concentration and cell volume.

^(a) Statistical errors were propagated from the K_a measurements.

^(b) All experiments were performed at 298 K.

^(c) Units of M⁻².

^(d) Units of M⁻³.