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

All quantities are reported as point estimate +- 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}.