ID	name	K_a (M^{-1})	ΔG (kcal/mol)	ΔH (kcal/mol)	$T\Delta S$ (kcal/mol) [b]	n
CB8-G1	Methamphetamine[a] [c]	150000.0 +- 10000.0	-7.05 +- 0.04	-7.8 +- 0.3	-0.8 +- 0.3	1.00
CB8-G2	Fentanyl[a] [c]	19000000.0 +- 1000000.0	-9.93 +- 0.03	-10.8 +- 0.3	-0.9 +- 0.3	1.00
CB8-G3	Morphine[a] [d]	340000000.0 +- 20000000.0	-11.63 +- 0.03	-13.6 +- 0.4	-2.0 +- 0.4	1.00
CB8-G4	Hydromorphone[a] [d]	170000000.0 +- 10000000.0	-11.22 +- 0.04	-15.8 +- 0.5	-4.6 +- 0.5	1.00
CB8-G5	Ketamine[a] [e]	1090000000.0 +- 80000000.0	-12.32 +- 0.04	-17.3 +- 0.5	-5.0 +- 0.5	1.00
CB8-G6	PhenylCyclohexylPiperidine(PCP)[a] [e]	21000000000.0 +- 2000000000.0	-14.07 +- 0.06	-14.9 +- 0.4	-0.8 +- 0.5	1.00
CB8-G7	Cocaine[a] [c]	640000.0 +- 50000.0	-7.92 +- 0.04	-8.3 +- 0.3	-0.3 +- 0.3	1.00
TEMOA-G1	3-hydroxy-2-napththoic acid	130000.0 +- 10000.0	-6.96 +- 0.05	-17.0 +- 1.0	10.0 +- 1.0	1.00
TEMOA-G2	p-bromophenol	1480000.0 +- 60000.0	-8.41 +- 0.02	-15.7 +- 0.2	7.2 +- 0.2	1.00
TEMOA-G3	cyclopentylacetic acid	17400.0 +- 700.0	-5.78 +- 0.02	-7.9 +- 0.2	2.2 +- 0.2	1.00
TEMOA-G4	piperonylic acid	460000.0 +- 20000.0	-7.72 +- 0.02	-17.7 +- 0.3	10.0 +- 0.3	1.00
TEMOA-G5	p-toluic acid	78000.0 +- 3000.0	-6.67 +- 0.02	-14.2 +- 0.8	7.6 +- 0.7	1.00
TEETOA-G1	3-hydroxy-2-napththoic acid	2000.0 +- 200.0	-4.49 +- 0.05	-13.6 +- 0.2	9.2 +- 0.1	1.00
TEETOA-G2	p-bromophenol	6100.0 +- 200.0	-5.16 +- 0.02	-11.6 +- 0.3	6.5 +- 0.3	1.00
TEETOA-G3	cyclopentylacetic acid[f]	NaN +- NaN	NaN +- NaN	NaN +- NaN	NaN +- NaN	1.00
TEETOA-G4	piperonylic acid	1900.0 +- 200.0	-4.47 +- 0.05	-13.0 +- 0.9	8.5 +- 0.8	1.00
TEETOA-G5	p-toluic acid[g]	270.0 +- 10.0	-3.32 +- 0.02	NaN +- NaN	NaN +- NaN	1.00

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 for the Isaacs (CB8) dataset, where concentration error had not been factored in to the original error estimates. For the TEMOA/TEETOA sets, provided uncertainties already include concentration error. ΔG was obtained from K_a via the standard thermodynamic equation. The average ΔH and ΔG values were then used to calculate an average -T, and the corresponding standard deviations calculated using the standard equation for the propagation of uncertainties for subtraction. The deviations in log K_a and ΔG were obtained by using the standard equation for the propagation of uncertainties for logarithms.

([a]) Statistical errors were propagated from the K_a measurements.
([b]) All experiments were performed at 298 K.
([c]) Direct ITC titration.
([d]) Competitive ITC titration with C1.
([e]) Competitive ITC titration with C2.
([f]) Binding is too weak to be observed by 1H-NMR or ITC.
([g]) Determined by 1H-NMR spectroscopy.