ID	name	K_a (M^{-1})	ΔG (kcal/mol) [a]	ΔH (kcal/mol)	$T\Delta S$ (kcal/mol) [b]	n
clip-g1	4-azaniumylbutylammonium	31000.0 +- 9000.0	-6.1 +- 0.2	-6.1 +- 0.8	0.0 +- 0.8	0.86
clip-g2	5-azaniumylpentylammonium	1270000.0 +- 80000.0	-8.32 +- 0.04	-8.8 +- 0.3	-0.4 +- 0.3	1.00
clip-g3	6-azaniumylhexylammonium	24000000.0 +- 3000000.0	-10.05 +- 0.07	-10.9 +- 0.3	-0.8 +- 0.3	0.90
clip-g15	trimethyl-[6-(trimethylammonio)hexyl]ammonium	52000000.0 +- 4000000.0	-10.52 +- 0.05	-12.8 +- 0.4	-2.2 +- 0.4	0.97
clip-g12	hexyl(trimethyl)ammonium	1210000.0 +- 70000.0	-8.29 +- 0.03	-8.4 +- 0.3	-0.1 +- 0.3	0.94
clip-g5	8-azaniumyloctylammonium	150000000.0 +- 30000000.0	-11.1 +- 0.1	-11.4 +- 0.4	-0.3 +- 0.4	0.89
clip-g16	10-azaniumyldecylammonium	300000000.0 +- 100000000.0	-11.5 +- 0.2	-11.2 +- 0.4	0.3 +- 0.4	0.89
clip-g17	12-azaniumyldodecylammonium	500000000.0 +- 300000000.0	-11.8 +- 0.4	-10.4 +- 0.3	1.4 +- 0.5	0.97
clip-g9	1-adamantylammonium	360000.0 +- 30000.0	-7.57 +- 0.05	-4.8 +- 0.2	2.8 +- 0.2	0.95
clip-g6	1-adamantyl(trimethyl)ammonium	11000000.0 +- 2000000.0	-9.6 +- 0.1	-10.2 +- 0.4	-0.6 +- 0.4	0.83
clip-g11	1-(1-adamantyl)ethanamine	4100000.0 +- 600000.0	-9.02 +- 0.08	-7.4 +- 0.3	1.6 +- 0.3	0.85
clip-g10	Can't format in LaTeX	1000000.0 +- 100000.0	-8.17 +- 0.08	-5.8 +- 0.2	2.3 +- 0.2	0.99
clip-g8	[4-(azaniumylmethyl)phenyl]methylammonium	8500000.0 +- 700000.0	-9.45 +- 0.05	-10.6 +- 0.3	-1.1 +- 0.3	0.90
clip-g18	1-methyl-4-(1-methylpyridin-1-ium-4-yl)pyridin-1-ium	54000000.0 +- 8000000.0	-10.55 +- 0.09	-12.4 +- 0.4	-1.8 +- 0.4	0.95
clip-g19	4-(1,1-dimethylpiperidin-1-ium-4-yl)-1,1-dimethyl-piperidin-1-ium	360000000.0 +- 80000000.0	-11.7 +- 0.1	-13.6 +- 0.4	-2.0 +- 0.5	0.79
clip-g7	(4-azaniumylcyclohexyl)ammonium	59000.0 +- 5000.0	-6.5 +- 0.05	-6.7 +- 0.3	-0.2 +- 0.3	0.83
OA-g1	hexanoate	4400.0 +- 200.0	-4.97 +- 0.02	-5.54 +- 0.1	-0.6 +- 0.1	1.00
OA-g2	4-chlorobenzoate	116000.0 +- 5000.0	-6.91 +- 0.02	-9.6 +- 0.2	-2.6 +- 0.2	1.00
OA-g3	(4 S)-4-isopropenylcyclohexene-1-carboxylate	870000.0 +- 70000.0	-8.1 +- 0.05	-12.0 +- 0.02	-3.9 +- 0.02	1.00
OA-g4	(3 S)-3,7-dimethyloct-6-enoate	95000.0 +- 8000.0	-6.79 +- 0.05	-6.7 +- 0.1	0.07 +- 0.02	1.00
OA-g5	Can't format in LaTeX	3000.0 +- 100.0	-4.73 +- 0.02	-7.48 +- 0.05	-2.75 +- 0.05	1.00
OA-g7	trimethyl-(4-methylcyclohexyl)ammonium	28000.0 +- 2000.0	-6.07 +- 0.05	-5.7 +- 0.1	0.3 +- 0.1	1.00
OA-g8	1-adamantyl(trimethyl)ammonium	900000.0 +- 700000.0	-8.1 +- 0.5	-7.8 +- 0.2	0.4 +- 0.2	1.00
exoOA-g1	hexanoate	ND +- ND	ND +- ND	ND +- ND	ND +- ND	1.00
exoOA-g2	4-chlorobenzoate	40.0 +- 50.0	-2.2 +- 0.7	ND +- ND	ND +- ND	1.00
exoOA-g5	Can't format in LaTeX	12100.0 +- 500.0	-5.57 +- 0.02	-6.17 +- 0.02	-0.6 +- 0.02	1.00
exoOA-g6	hexyl(trimethyl)ammonium	18900.0 +- 800.0	-5.83 +- 0.02	-3.25 +- 0.02	2.58 +- 0.05	1.00
exoOA-g7	trimethyl-(4-methylcyclohexyl)ammonium	130000.0 +- 30000.0	-7.0 +- 0.1	-4.97 +- 0.07	2.0 +- 0.2	1.00
exoOA-g8	1-adamantyl(trimethyl)ammonium	420000.0 +- 70000.0	-7.67 +- 0.1	-5.04 +- 0.05	2.6 +- 0.2	1.00
bCD-g1	trans-4-methylcyclohexanol	2100.0 +- 100.0	-4.52 +- 0.03	-2.6 +- 0.2	2.0 +- 0.2	0.88
bCD-g2	R-rimantadine	35000.0 +- 3000.0	-6.2 +- 0.04	-10.4 +- 0.7	-4.2 +- 0.7	1.00
MGLab_8-g1	trans-4-methylcyclohexanol	260.0 +- 20.0	-3.3 +- 0.05	-1.8 +- 0.4	1.5 +- 0.4	0.89
MGLab_8-g2	R-rimantadine	830.0 +- 50.0	-3.98 +- 0.04	-6.9 +- 0.5	-2.9 +- 0.5	1.03
MGLab_9-g1	trans-4-methylcyclohexanol	210.0 +- 20.0	-3.17 +- 0.05	-2.7 +- 0.8	0.4 +- 0.8	0.88
MGLab_9-g2	R-rimantadine	700.0 +- 40.0	-3.88 +- 0.03	-9.0 +- 0.6	-5.2 +- 0.6	1.00
MGLab_19-g1	trans-4-methylcyclohexanol	210.0 +- 20.0	-3.18 +- 0.04	-2.1 +- 0.2	1.1 +- 0.2	0.83
MGLab_19-g2	R-rimantadine	320.0 +- 20.0	-3.41 +- 0.04	-11.0 +- 1.0	-8.0 +- 1.0	0.94
MGLab_23-g1	trans-4-methylcyclohexanol	220.0 +- 20.0	-3.2 +- 0.05	-3.0 +- 1.0	0.0 +- 1.0	0.76
MGLab_23-g2	R-rimantadine	1510.0 +- 90.0	-4.33 +- 0.04	-7.6 +- 0.5	-3.3 +- 0.5	0.96
MGLab_24-g1	trans-4-methylcyclohexanol	280.0 +- 20.0	-3.34 +- 0.05	-1.6 +- 0.2	1.7 +- 0.2	0.92
MGLab_24-g2	R-rimantadine	1100.0 +- 70.0	-4.15 +- 0.04	-8.6 +- 0.6	-4.5 +- 0.6	1.03
MGLab_34-g1	trans-4-methylcyclohexanol	700.0 +- 100.0	-3.85 +- 0.09	-3.7 +- 0.3	0.1 +- 0.3	0.81
MGLab_34-g2	R-rimantadine	11000.0 +- 7000.0	-5.5 +- 0.4	-9.0 +- 2.0	-3.0 +- 2.0	0.99
MGLab_35-g1	trans-4-methylcyclohexanol	2300.0 +- 200.0	-4.58 +- 0.05	-4.5 +- 0.3	0.1 +- 0.3	0.85
MGLab_35-g2	R-rimantadine	27000.0 +- 2000.0	-6.04 +- 0.04	-7.3 +- 0.5	-1.2 +- 0.5	0.78
MGLab_36-g1	trans-4-methylcyclohexanol	200.0 +- 10.0	-3.15 +- 0.04	-3.0 +- 0.3	0.1 +- 0.3	0.87
MGLab_36-g2	R-rimantadine	100.0 +- 100.0	-2.0 +- 1.0	-11.0 +- 1.0	-8.0 +- 2.0	0.84

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] for the Isaacs (TrimerTrip) and Gilson (cyclodextrin derivatives) datasets, where concentrationerror had not been factored in to the original error estimates. For the OA/exoOA sets, provided uncertaintiesalready included concentration error.

(^{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}.