

ID	name	K_a (M ⁻¹)	ΔG (kcal/mol) ^(a)	ΔH (kcal/mol)	$T\Delta S$ (kcal/mol) ^(b)	
clip-g1	4-azaniumylbutylammonium	31000.0 +- 9000.0	-6.1 +- 0.2	-6.1 +- 0.8	0.0 +- 0.8	
clip-g2	5-azaniumylpentylammonium	1270000.0 +- 80000.0	-8.32 +- 0.04	-8.8 +- 0.3	-0.4 +- 0.3	1.0005
clip-g3	6-azaniumylhexylammonium	24000000.0 +- 3000000.0	-10.05 +- 0.07	-10.9 +- 0.3	-0.8 +- 0.3	
clip-g15	trimethyl-[6-(trimethylammonio)hexyl]ammonium	52000000.0 +- 4000000.0	-10.52 +- 0.05	-12.8 +- 0.4	-2.2 +- 0.4	
clip-g12	hexyl(trimethyl)ammonium	1210000.0 +- 70000.0	-8.29 +- 0.03	-8.4 +- 0.3	-0.1 +- 0.3	
clip-g5	8-azaniumyloctylammonium	150000000.0 +- 30000000.0	-11.1 +- 0.1	-11.4 +- 0.4	-0.3 +- 0.4	
clip-g16	10-azaniumyldecylammonium	300000000.0 +- 100000000.0	-11.5 +- 0.2	-11.2 +- 0.4	0.3 +- 0.4	0.8905
clip-g17	12-azaniumyldodecylammonium	500000000.0 +- 300000000.0	-11.8 +- 0.4	-10.4 +- 0.3	1.4 +- 0.5	
clip-g9	1-adamantylammonium	360000.0 +- 30000.0	-7.57 +- 0.05	-4.8 +- 0.2	2.8 +- 0.2	
clip-g6	1-adamantyl(trimethyl)ammonium	11000000.0 +- 2000000.0	-9.6 +- 0.1	-10.2 +- 0.4	-0.6 +- 0.4	
clip-g11	1-(1-adamantyl)ethanamine	4100000.0 +- 600000.0	-9.02 +- 0.08	-7.4 +- 0.3	1.6 +- 0.3	
clip-g10	Can't format in LaTeX	1000000.0 +- 100000.0	-8.17 +- 0.08	-5.8 +- 0.2	2.3 +- 0.2	
clip-g8	[4-(azaniumylmethyl)phenyl]methylanmonium	8500000.0 +- 700000.0	-9.45 +- 0.05	-10.6 +- 0.3	-1.1 +- 0.3	
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	
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	
clip-g7	(4-azaniumylcyclohexyl)ammonium	59000.0 +- 5000.0	-6.5 +- 0.05	-6.7 +- 0.3	-0.2 +- 0.3	
OA-g1	hexanoate	4400.0 +- 200.0	-4.97 +- 0.02	-5.54 +- 0.1	-0.6 +- 0.1	
OA-g2	4-chlorobenzoate	116000.0 +- 5000.0	-6.91 +- 0.02	-9.6 +- 0.2	-2.6 +- 0.2	
OA-g3	(4 S)-4-isopropenylcyclohexene-1-carboxylate	870000.0 +- 70000.0	-8.1 +- 0.05	-12.0 +- 0.02	-3.9 +- 0.02	
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	
OA-g5	Can't format in LaTeX	3000.0 +- 100.0	-4.73 +- 0.02	-7.48 +- 0.05	-2.75 +- 0.05	
OA-g7	trimethyl-(4-methylcyclohexyl)ammonium	28000.0 +- 2000.0	-6.07 +- 0.05	-5.7 +- 0.1	0.3 +- 0.1	
OA-g8	1-adamantyl(trimethyl)ammonium	900000.0 +- 700000.0	-8.1 +- 0.5	-7.8 +- 0.2	0.4 +- 0.2	
exoOA-g1	hexanoate	ND +- ND	ND +- ND	ND +- ND	ND +- ND	
exoOA-g2	4-chlorobenzoate	40.0 +- 50.0	-2.2 +- 0.7	ND +- ND	ND +- ND	
exoOA-g5	Can't format in LaTeX	12100.0 +- 500.0	-5.57 +- 0.02	-6.17 +- 0.02	-0.6 +- 0.02	
exoOA-g6	hexyl(trimethyl)ammonium	18900.0 +- 800.0	-5.83 +- 0.02	-3.25 +- 0.02	2.58 +- 0.05	
exoOA-g7	trimethyl-(4-methylcyclohexyl)ammonium	130000.0 +- 30000.0	-7.0 +- 0.1	-4.97 +- 0.07	2.0 +- 0.2	
exoOA-g8	1-adamantyl(trimethyl)ammonium	420000.0 +- 70000.0	-7.67 +- 0.1	-5.04 +- 0.05	2.6 +- 0.2	

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].^(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.