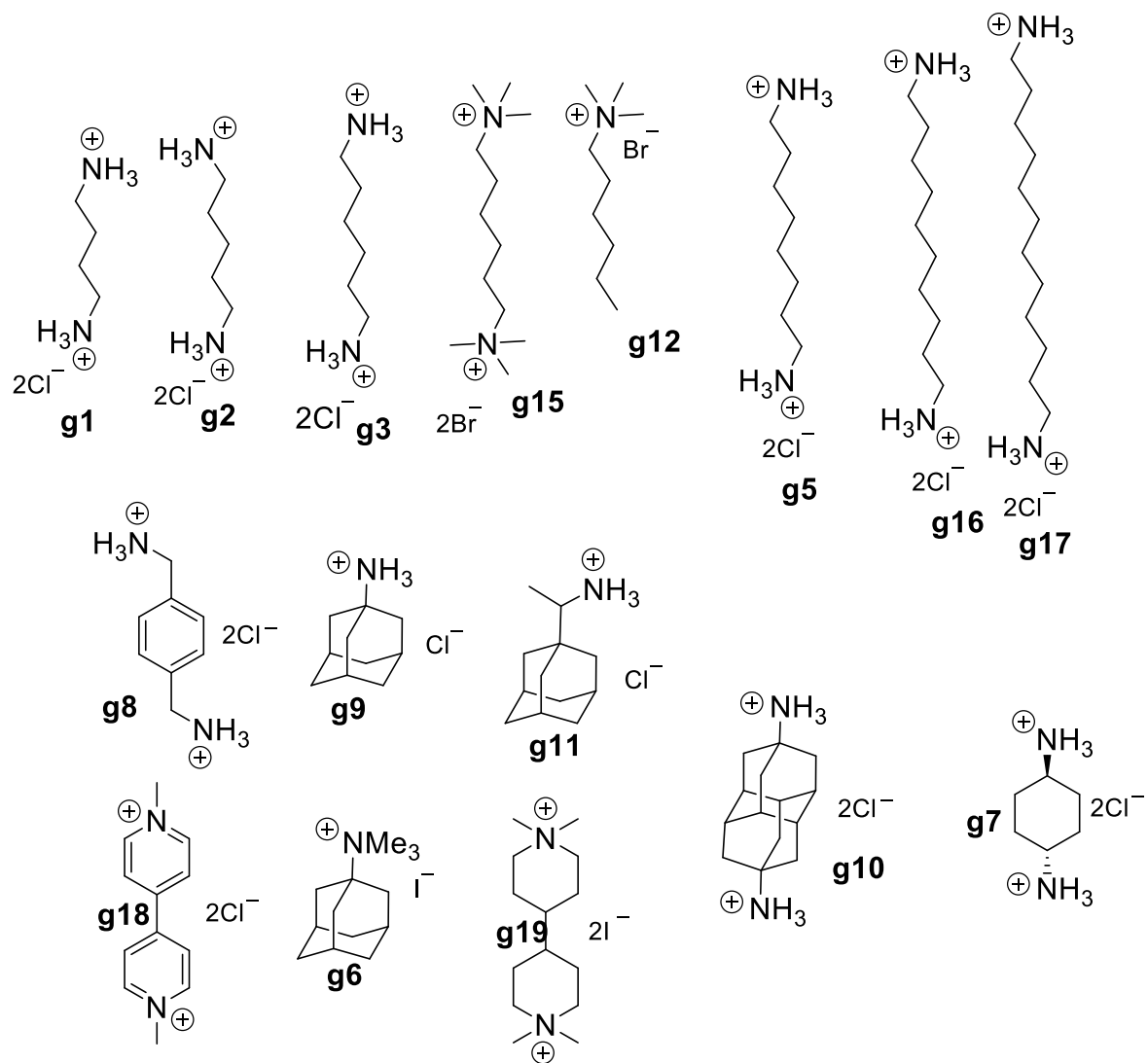


SAMPL7 challenge TrimerTrip data



	Trial 1		Trial 2	
Guests	K_d (M)	ΔH (kcal • mol ⁻¹)	K_d (M)	ΔH (kcal • mol ⁻¹)
g1	$34.2 \times 10^{-6} \pm 3.29\text{e-}6$	-6.03 ± 0.260	$29.6 \times 10^{-6} \pm 7.70\text{e-}6$	-6.14 ± 0.696
g2	$749 \times 10^{-9} \pm 17.7\text{e-}9$	-8.58 ± 0.021	$829 \times 10^{-9} \pm 40.8\text{e-}9$	-8.95 ± 0.053
g3	$43.5 \times 10^{-9} \pm 3.39\text{e-}9$	-10.8 ± 0.044	$41.3 \times 10^{-9} \pm 3.24\text{e-}9$	-10.9 ± 0.043
g15	$18.3 \times 10^{-9} \pm 1.00\text{e-}9$	-12.8 ± 0.033	$20.0 \times 10^{-9} \pm 8.74\text{e-}10$	-12.7 ± 0.028
g12	$830 \times 10^{-9} \pm 23.3\text{e-}9$	-8.54 ± 0.027	$827 \times 10^{-9} \pm 31.0\text{e-}9$	-8.25 ± 0.034
g5	$7.07 \times 10^{-9} \pm 1.13\text{e-}9$	-11.5 ± 0.094	$6.63 \times 10^{-9} \pm 8.99\text{e-}10$	-11.3 ± 0.07
g16	$3.55 \times 10^{-9} \pm 7.80\text{e-}10$	-11.3 ± 0.068	$3.27 \times 10^{-9} \pm 8.48\text{e-}10$	-11.2 ± 0.072
g17	$1.97 \times 10^{-9} \pm 1.06\text{e-}9$	-10.4 ± 0.123	$2.20 \times 10^{-9} \pm 5.76\text{e-}10$	-10.4 ± 0.064
g9	$2.80 \times 10^{-6} \pm 113\text{e-}9$	-4.83 ± 0.036	$2.79 \times 10^{-6} \pm 162\text{e-}9$	-4.72 ± 0.046
g6	$88.3 \times 10^{-9} \pm 9.44\text{e-}9$	-10.1 ± 0.119	$97.0 \times 10^{-9} \pm 13.6\text{e-}9$	-10.3 ± 0.165
g11	$245 \times 10^{-9} \pm 22.3\text{e-}9$	-7.41 ± 0.084	$238 \times 10^{-9} \pm 22.2\text{e-}9$	-7.35 ± 0.084
g10	$902 \times 10^{-9} \pm 64.8\text{e-}9$	-5.88 ± 0.049	$1.17 \times 10^{-6} \pm 72.6\text{e-}9$	-5.80 ± 0.047
g8	$114 \times 10^{-9} \pm 6.79\text{e-}9$	-10.5 ± 0.044	$120 \times 10^{-9} \pm 5.34\text{e-}9$	-10.6 ± 0.033
g18	$17.2 \times 10^{-9} \pm 1.42\text{e-}9$	-12.4 ± 0.045	$19.8 \times 10^{-9} \pm 2.34\text{e-}9$	-12.3 ± 0.069
g19	$2.80 \times 10^{-9} \pm 1.53\text{e-}10$	-13.7 ± 0.039	$2.74 \times 10^{-9} \pm 6.04\text{e-}10$	-13.6 ± 0.144
g7	$16.8 \times 10^{-6} \pm 652\text{e-}9$	-6.61 ± 0.088	$17.2 \times 10^{-6} \pm 1.24\text{e-}6$	-6.80 ± 0.170

