

Supporting Information

S1 Table 1. Boltzmann Distributions of the hydrated GA conformers and relative Gibbs free energies (kJ mol⁻¹)

Calculated conformer	ΔG^a	%	ΔG^b	%
CC-W-1	0	72.5	0	72.9
CC-W-2	1.18	15.1	1.26	14.8
CC-W-3	2.93	8.3	3.12	8.4
CC-W-4	4.21	4.0	4.96	3.9
TG-W-5	10.8	0.9	11.32	0.8
TG-W-6	12.9	0	12.83	0
TT-W-7	13.2	0	13.4	0
TT-W-8	19.3	0	18.86	0
CT-W-9	25.3	0	24.2	0

Gibbs free energy values were estimated according to $\Delta G = -RT \ln K$. Calculated from ΔG with a temperature of 298 K. ΔG^a obtained at ω B97X-D/cc-pVTZ and ΔG^b calculated at MP2/6-311+g(d,p) level with the G09W program package.