Supporting Information

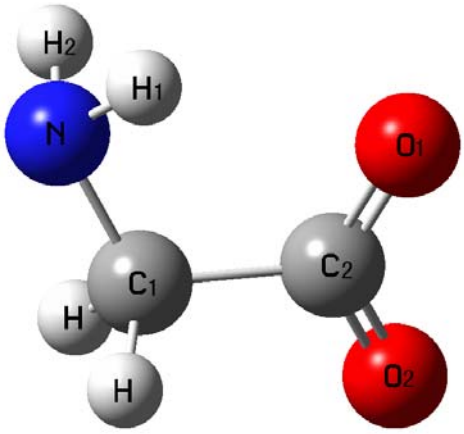

Figure S1. Computed conformer of deprotonated glycine. We labled the atoms in order to mark intra- and inter-hydrogen bonds, angles and dihedrals.

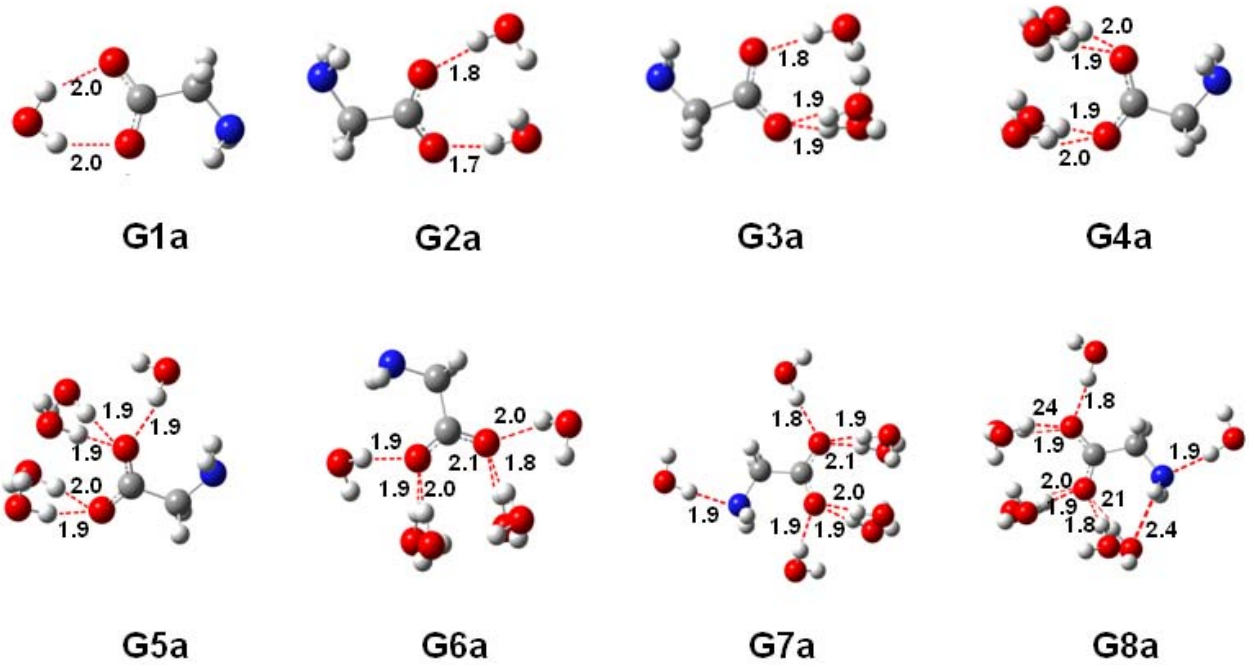

Figure S2. The lengths (Å) of inter-hydrogen bonds for all the most stable the hydration of the deprotonated glycine.

Table S1. Some basic geometric parameters for all the most stable structures with each particular hydration number.

Conformer	$H_1 \ldots O_1$ distance (Å)	$H_2 \ldots O_1$ distance (Å)	$N-C_1-C_2$ angle (°)	$C_1-C_2-O_1$ angle (°)	$N-C_1-C_2-O_1$ dihedral (°)
G1a	2.3	2.9	115.7	116.0	17.0
G2a	2.4	2.9	115.9	116.6	16.9
G3a	2.5	2.8	116.4	117.4	9.1
G4a	2.6	2.6	116.9	117.5	0.1
G5a	2.8	2.6	117.7	117.6	-6.0
G6a	2.8	2.6	117.5	118.4	-7.2
G7a	2.8	2.6	117.0	118.2	-5.1
G8a	2.8	2.7	118.1	118.5	-10.3