Supplementary Information: The influence of solvent representation on nuclear shielding calculations of protonation states of small biological molecules

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Table T1: Comparison of aug-pc-2 vs. aug-pcS-2

	aug-pc-2		*aug-pcS-2*	
Nucleus	Accuracy	R^2	Accuracy	R^2
^{13}C	± 2.9	1.0	± 4.0	1.0
^{1}H	± 1.1	0.2	± 2.2	0.16

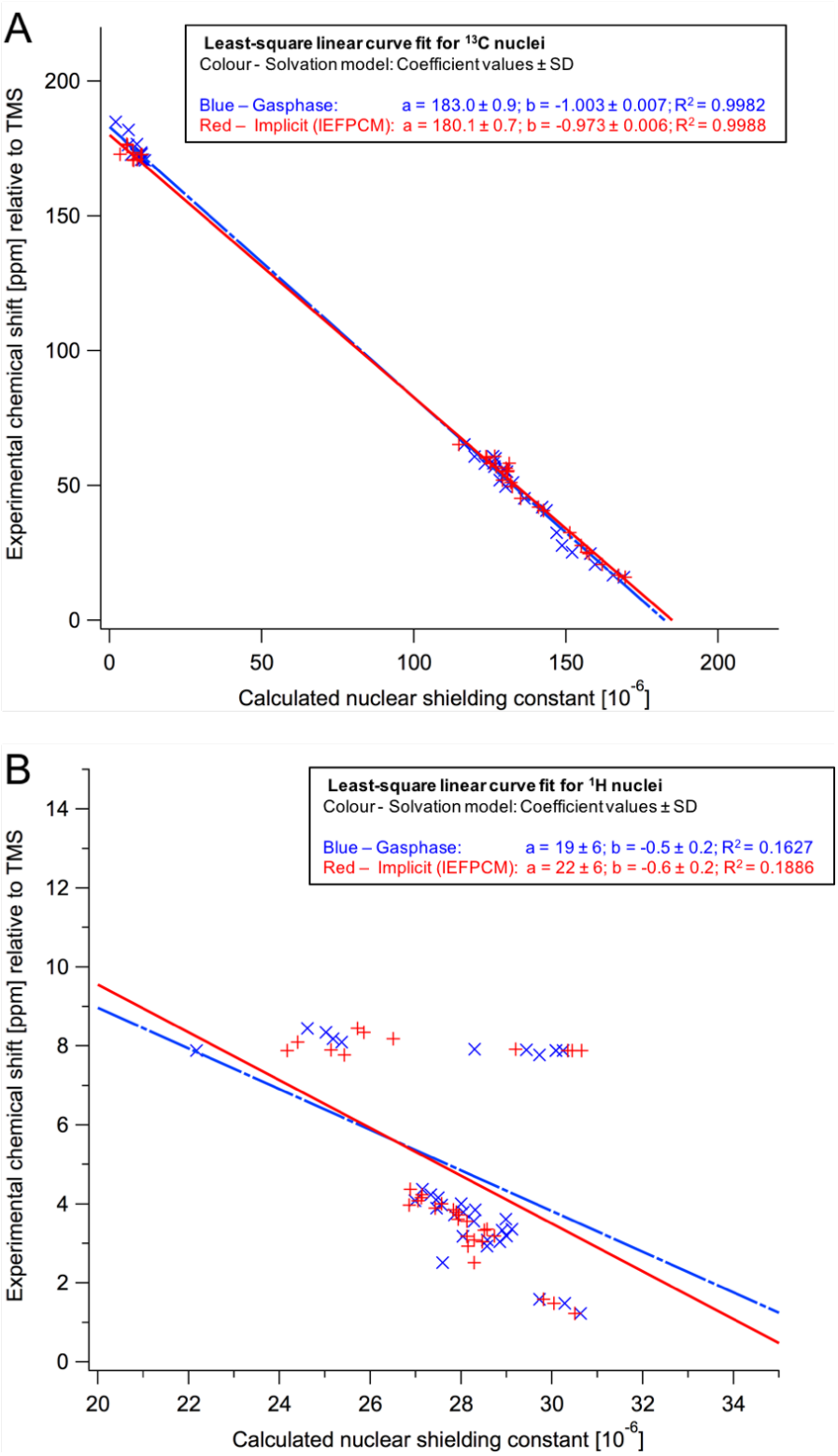

Fig. S2: Correlation between nuclear shielding values calculated in gas phase or IEFPCM and experimental chemical shift values for ^{13}C (A) and ^{1}H (B) nuclei. *For both nuclei types, calculations were performed in gas phase (blue, intermitted line) and implicit solvation (IEFPCM) (red, continuous line).*

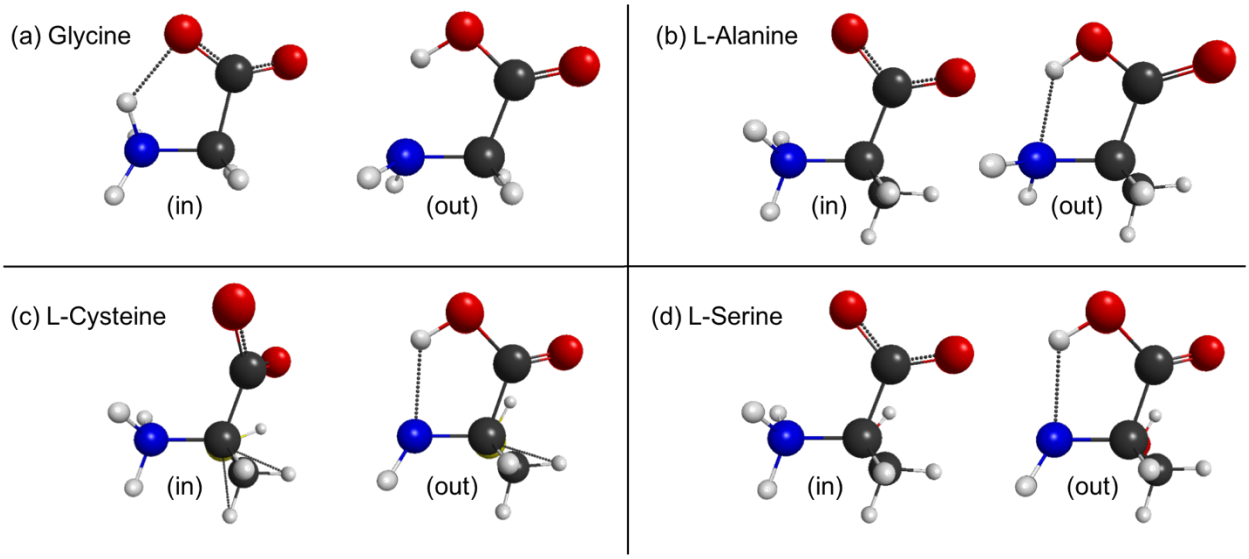

Fig. S3 Relocation of a proton in the zwitterionic state *between starting conformation (in) and conformation optimized in gas phase (out). Atom types are coded by colour: carbon – black, hydrogen – white, oxygen – red, nitrogen – blue, sulfur – yellow.*

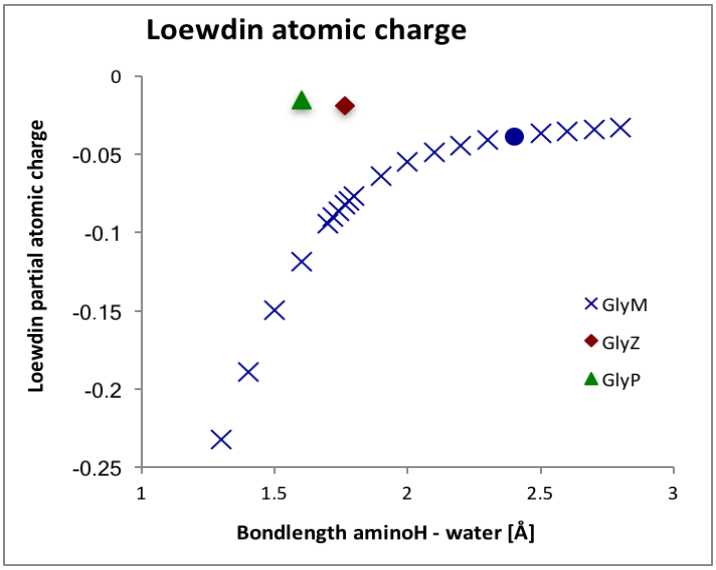

Fig. S4: Partial charge *of the H_N of the glycine anion (blue) with varying bond length. Blue dot indicates energy lowest conformer. Partial charge for H_N of the optimised glycine zwitterion and protonated form are also shown (red and green, respectively).*

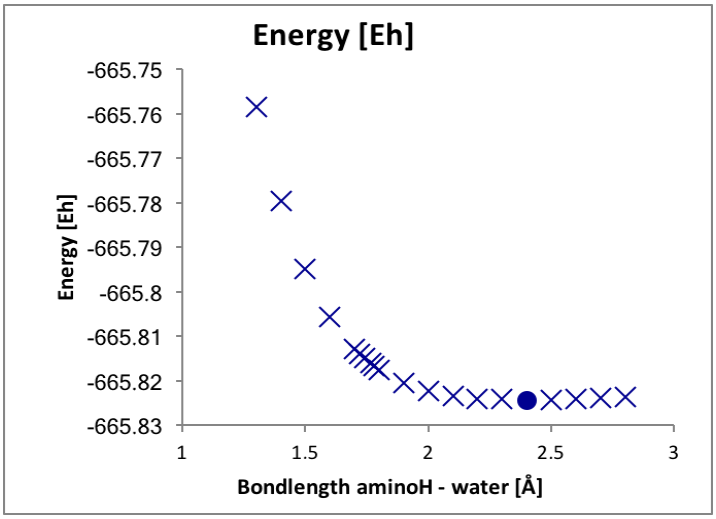

Fig. S5: Energy *of the glycine anion (blue) with varying bond length. Blue dot indicates energy lowest conformer.*

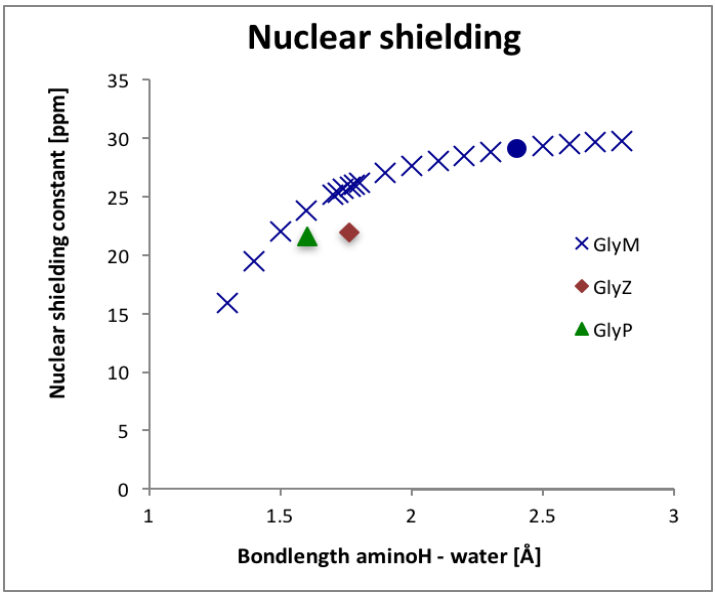

Fig. S6: Nuclear shielding *of the H_N of the glycine anion (blue) with varying bond length. Blue dot indicates energy lowest conformer. Partial charge for H_N of the optimised glycine zwitterion and protonated form are also shown (red and green, respectively).*