At physiological conditions, myriads of biomolecules (e.g., amino acids, peptides and proteins) exist predominantly in the zwitterionic structural form and their biological functions will result in these conditions. However, these geometrical structures are inaccessible energetically in the gas phase, and at this point stabilization of amino-acids in physiological conditions is still under debate. In this present work, the electronic properties of the aminoacids molecules in the liquid environment were studied by performing a relaxation of the glycine and alanine geometries in liquid water using the free energy gradient method combined with a Sequential QM/MM approach. Series of Monte Carlo Metropolis simulations of these aminoacids embedded in liquid water followed by only a quantum mechanical calculation in each of them were carried out. Both the local and global liquid environment were emphasized to obtain nuclear magnetic resonance parameters for the molecules in liquid water. The results of the equilibrium structure in solution and the systematic study of the hydrogen bonds were used to discard the direct proton transfer from carboxyl group to the ammonium group of the molecules in water solution. The calculations of the Density Functional Theory (DFT) were performed to study the polarization of the solvent in the parameters of Nuclear Magnetic Resonance (NMR) of the glycine molecule in liquid water. DFT calculations predicted isotropic chemical changes on the H, C, N and O atoms in liquid water solution agree with the available experimental data.