

SUPPORTING INFORMATION

The Cation Effect on the Solubility of Glycylglycine and N-Acetylglycine in Aqueous Solution: Experimental and Molecular Dynamic Studies

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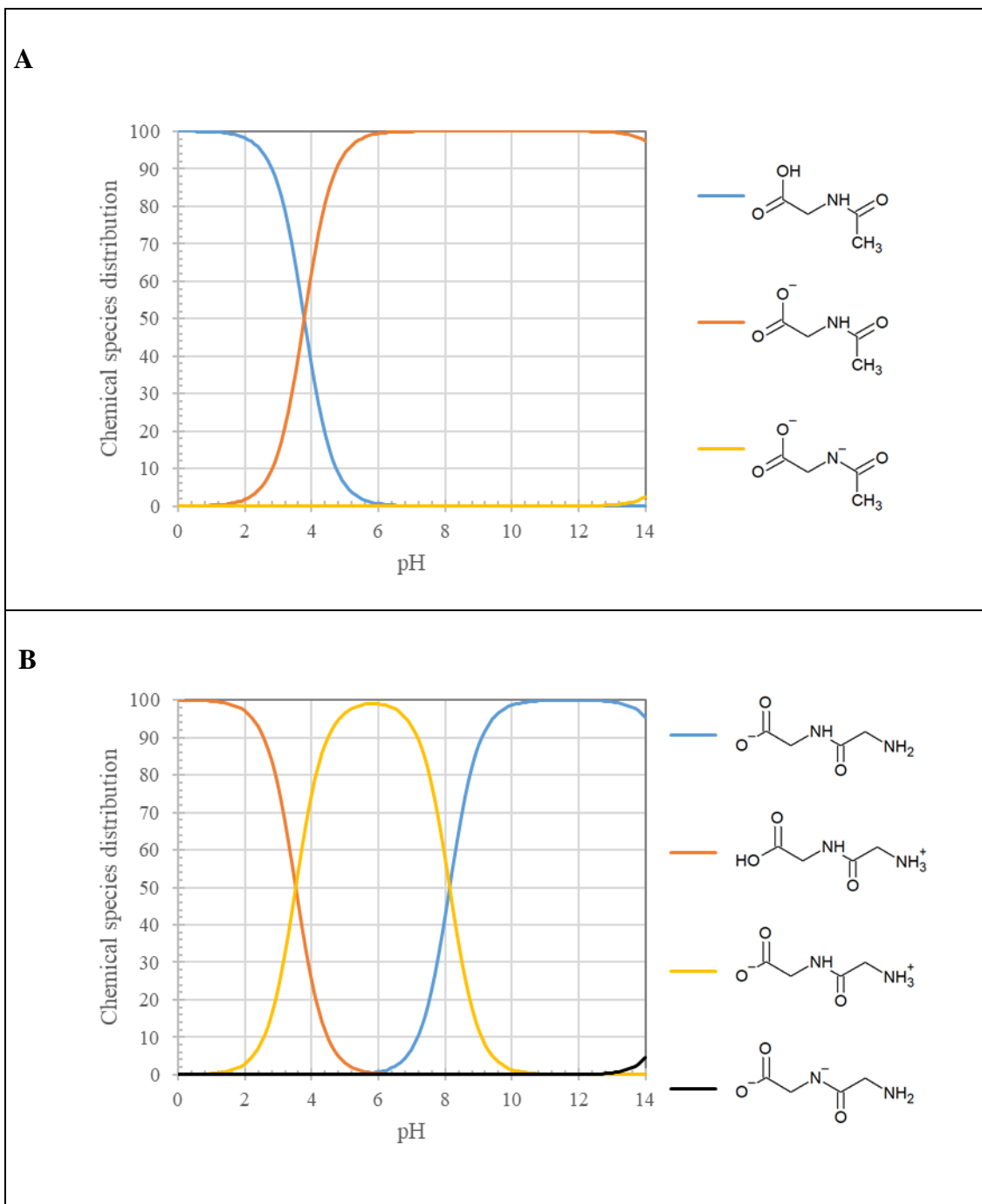


Figure S1. Chemical species distribution as a function of pH of N-acetyl glycine (A) and diglycine (B). Calculations performed using the Software Chemicalize, ChemAxon Ltd, 1998-2019 (<https://chemicalize.com/>).

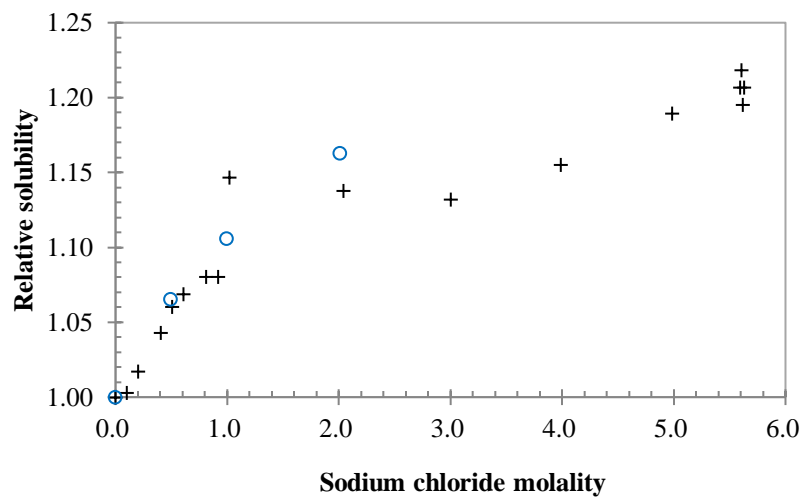


Figure S2. Relative solubility of diglycine in aqueous solutions of NaCl: this work (○), Breil et al.[1] (+).

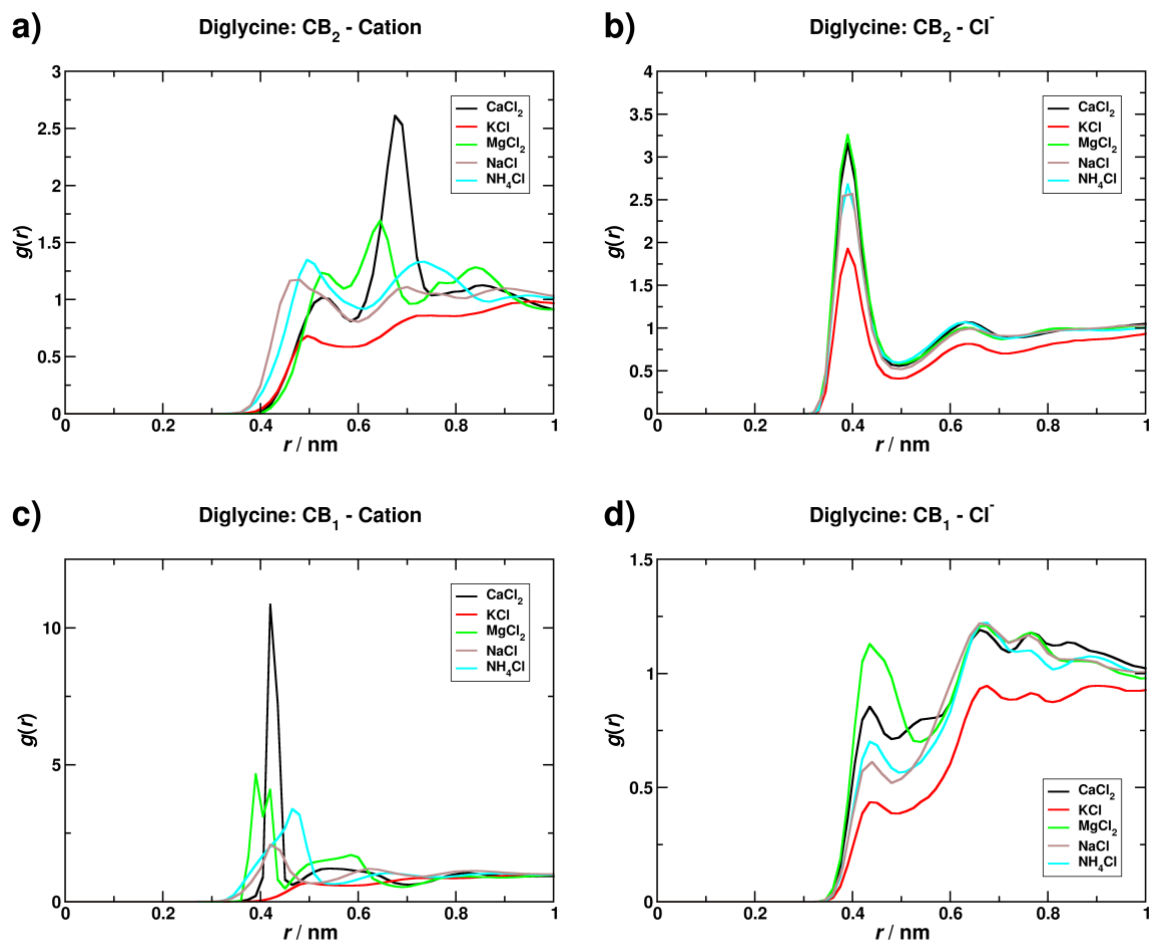


Figure S3. Radial distribution functions of the cations (left) and the chloride anion (right) of the NaCl, KCl, NH₄Cl, CaCl₂ and MgCl₂ salts around the alpha carbons of diglycine.

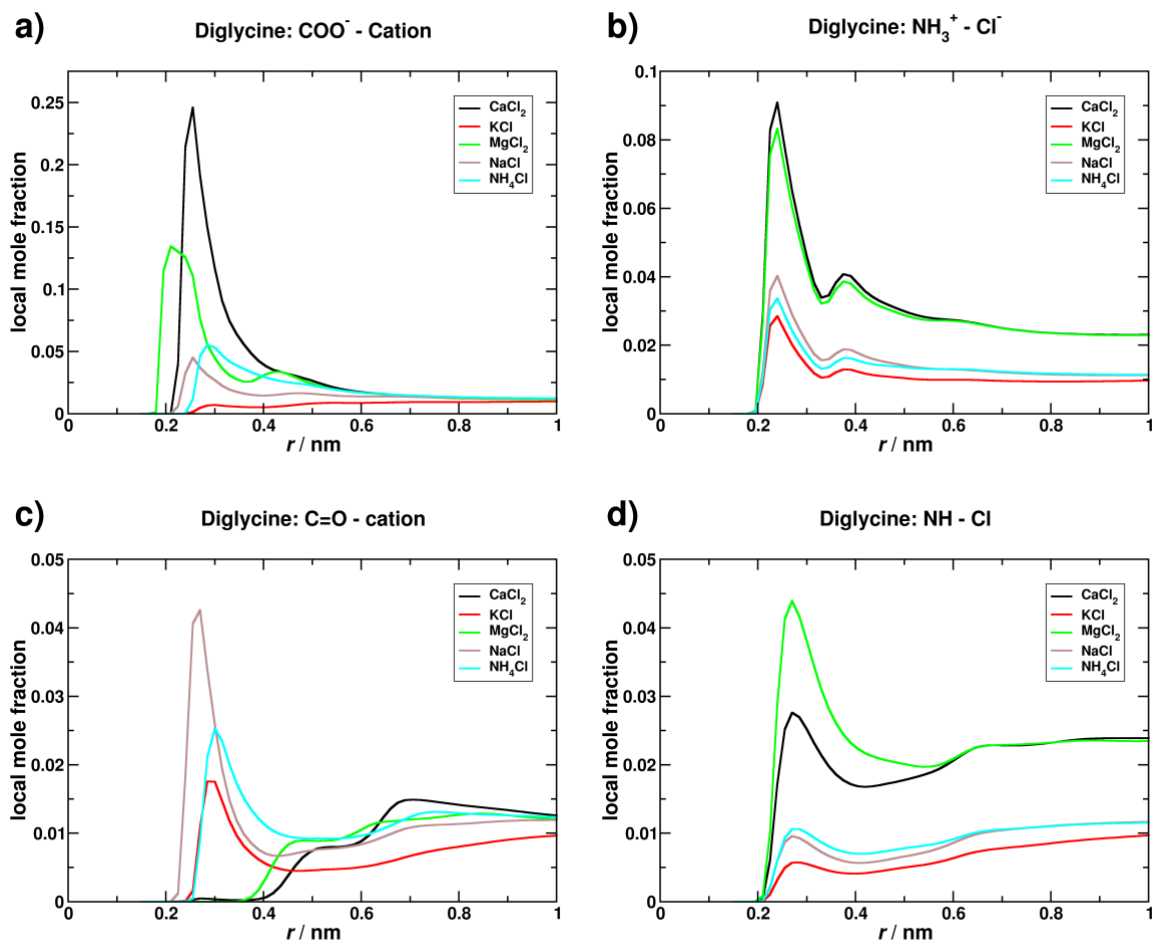


Figure S4. Local mole fractions of the cations (left) and the chloride anion (right) of the NaCl, KCl, NH₄Cl, CaCl₂ and MgCl₂ salts around selected groups of diglycine. The local mole fractions were calculated as in ref. [2].

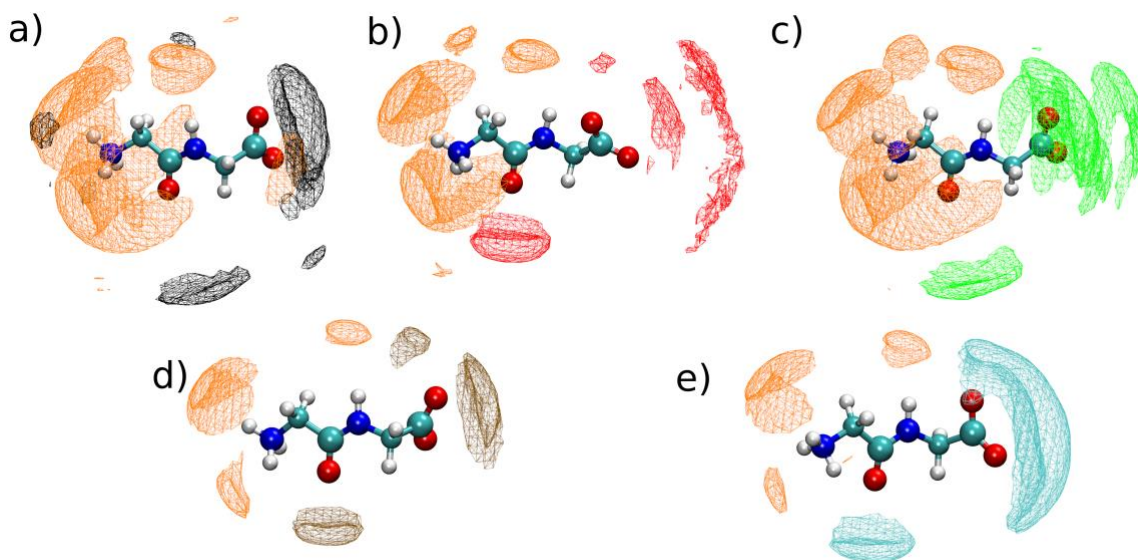


Figure S5. Spatial distribution functions (SDFs) of the cations and the chloride anion of the a) CaCl_2 , b) KCl , c) MgCl_2 , d) NaCl and e) NH_4Cl salts around selected groups of diglycine. Color code for spheres: white, H; cyan, C; blue, N; and red, O. Color code for isosurfaces: orange, Cl^- ; black, Ca^{2+} ; red, K^+ ; green, Mg^{2+} ; brown, Na^+ ; and cyan, NH_4^+ . Isodensity values are 5 particles/ nm^3 for both the anion and the cations. The SDFs were obtained with the TRAVIS code.[3]

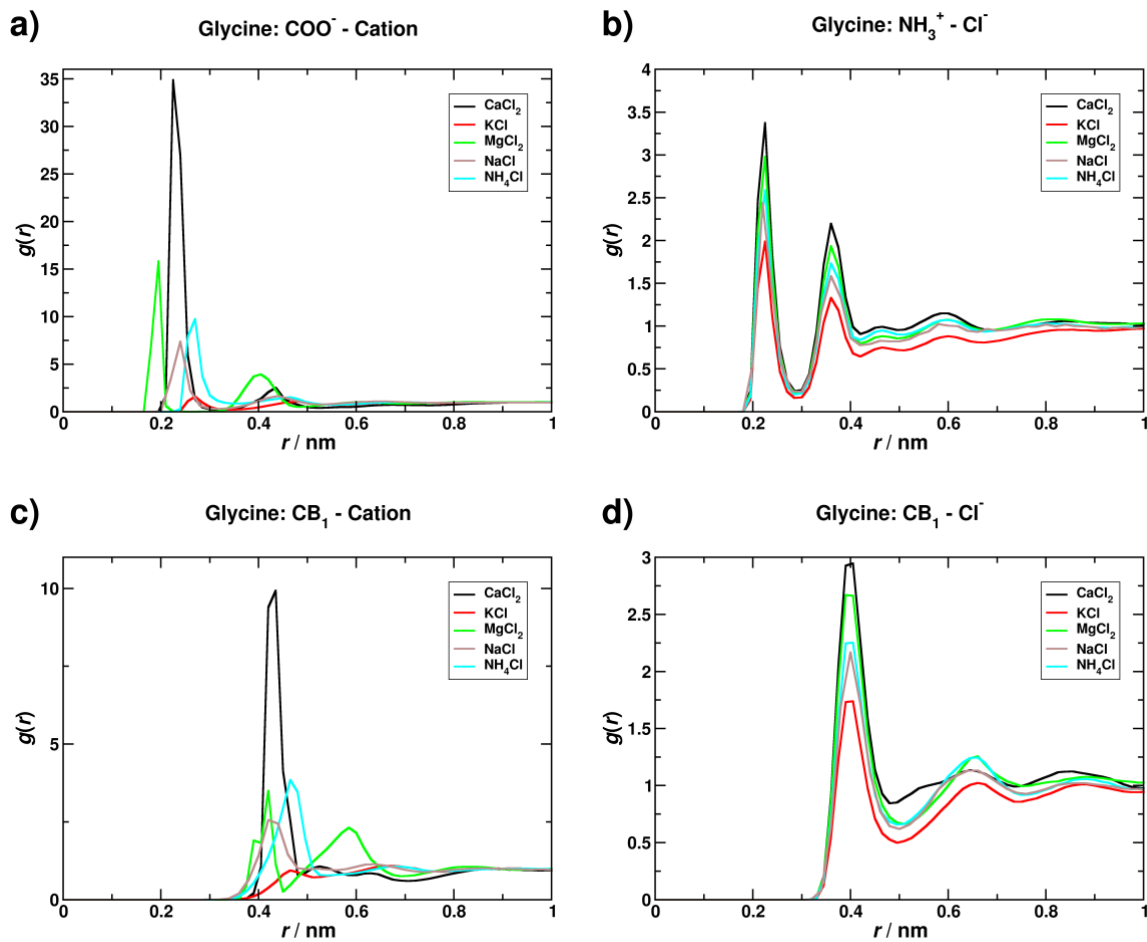


Figure S6. Radial distribution functions of the cations (left) and the chloride anion (right) of the NaCl, KCl, NH₄Cl, CaCl₂ and MgCl₂ salts around selected groups of glycine.

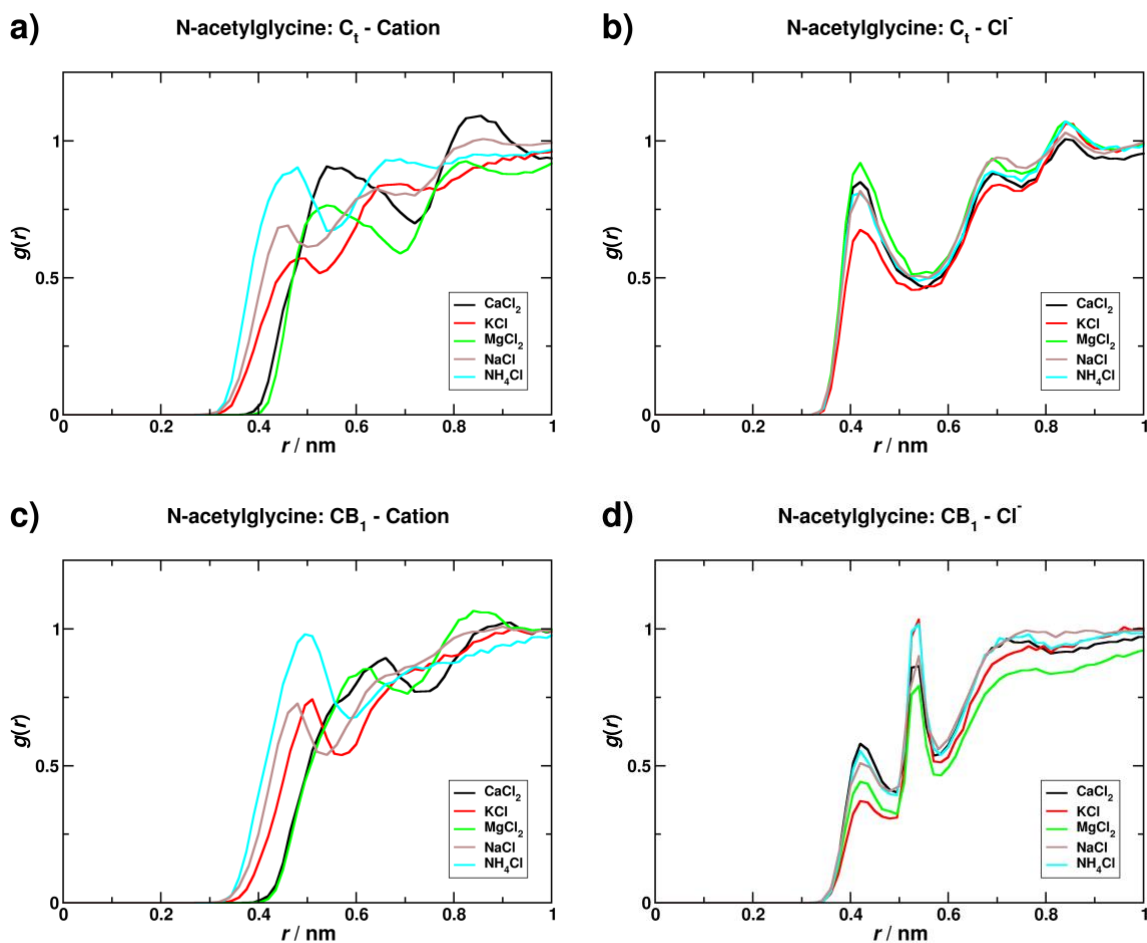


Figure S7. Radial distribution functions of the cations (left) and the chloride anion (right) of the NaCl, KCl, NH_4Cl , $CaCl_2$ and $MgCl_2$ salts around the terminal and the alpha carbons of N-acetylglycine.

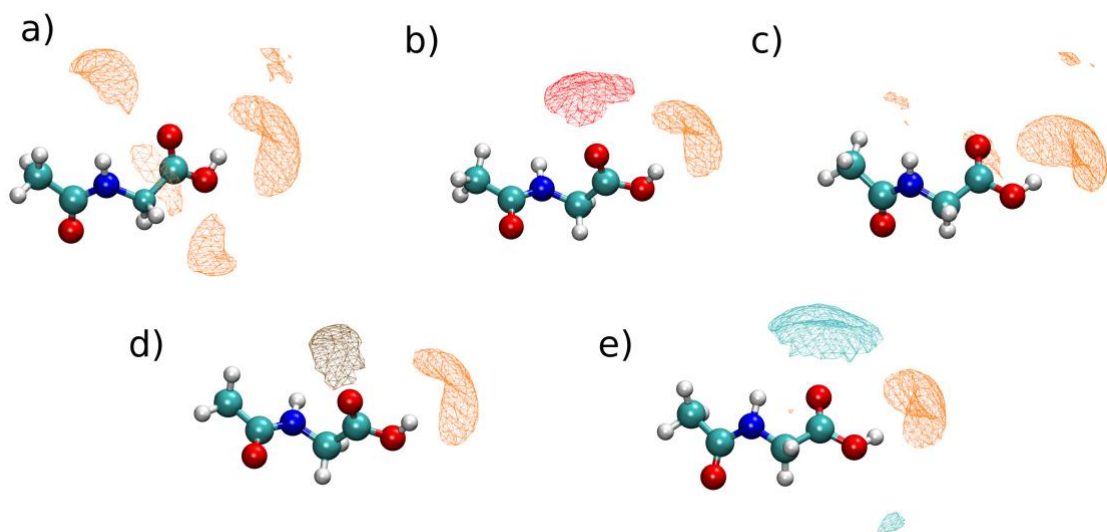
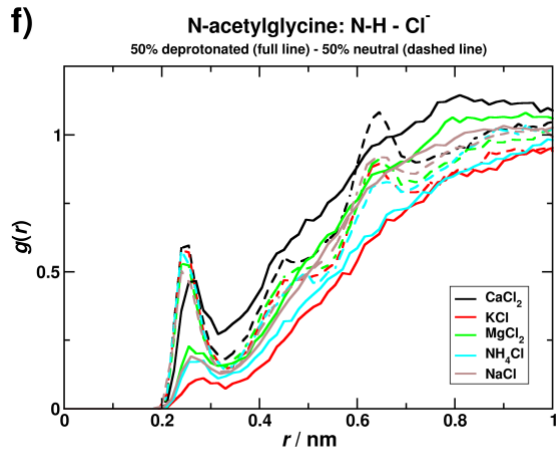
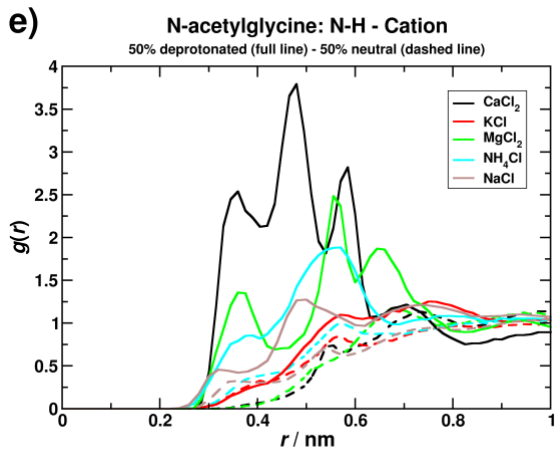
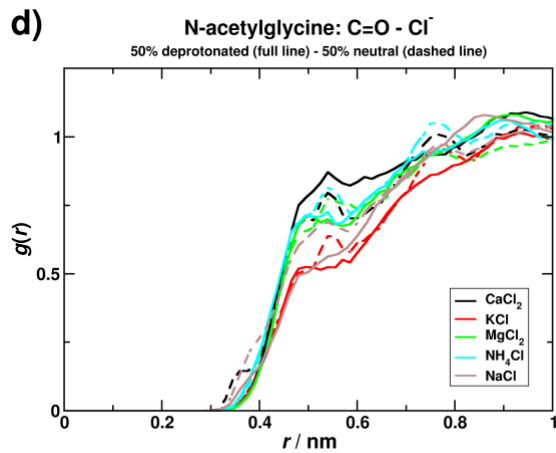
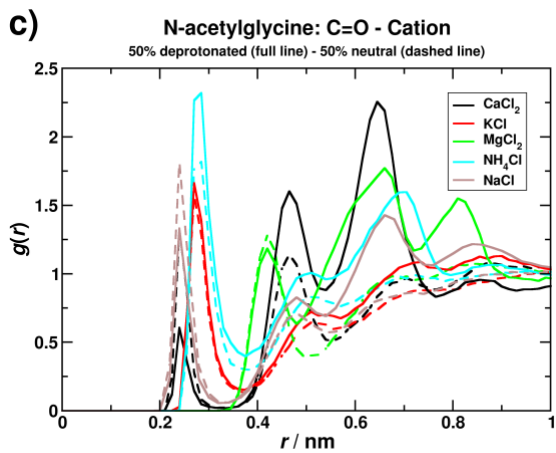
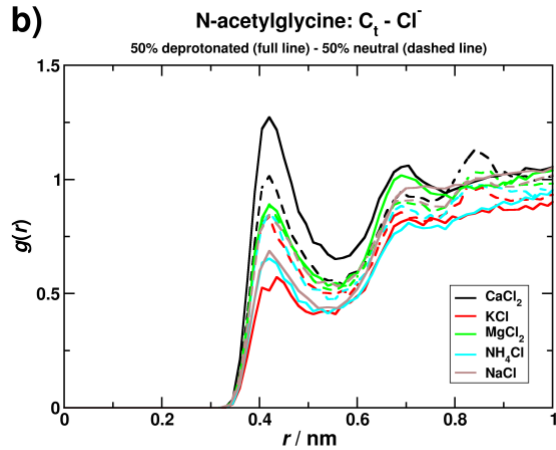
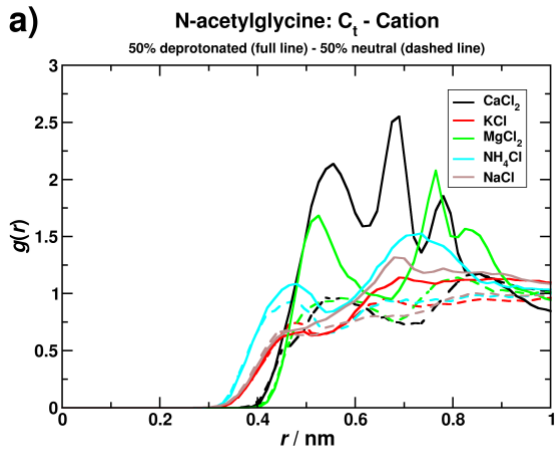


Figure S8. Spatial distribution functions of the cations and the chloride anion of the a) CaCl_2 , b) KCl , c) MgCl_2 , d) NaCl and e) NH_4Cl salts around selected groups of N-acetylglycine. Color code for spheres: white, H; cyan, C; blue, N; and red, O. Color code for isosurfaces: orange, Cl^- ; black, Ca^{2+} ; red, K^+ ; green, Mg^{2+} ; brown, Na^+ ; and cyan, NH_4^+ . Isodensity values for the isosurfaces are 5 particles/nm^3 for both the cations and the chloride anion. The SDFs were obtained with the TRAVIS code.[3]



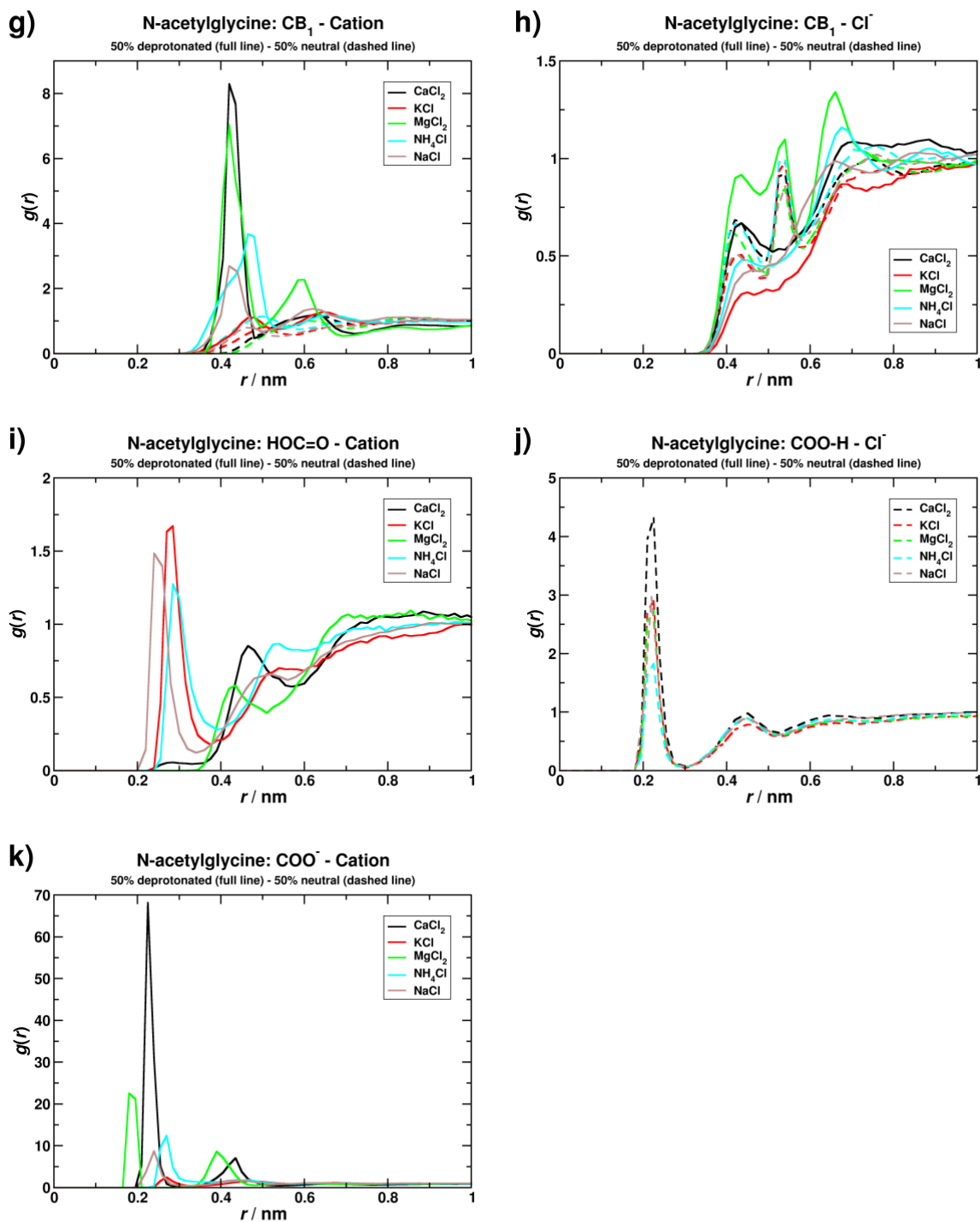


Figure S9. Radial distribution functions of the cations (left) and the chloride anion (right) of the NaCl, KCl, NH_4Cl , CaCl_2 and MgCl_2 salts around selected groups of deprotonated and neutral forms of N-acetylglycine (50-50% mixture).

References:

- [1] M.P. Breil, J.M. Mollerup, E.S.J. Rudolph, M. Ottens, L.A.M. Van Der Wielen, *Fluid Phase Equilib.* 215 (2004) 221–225.
- [2] N. Elpidoforou, I. Skarmoutsos, E. Kainourgiakis, V. Raptis, J. Samios, *J. Mol. Liq.* 226 (2017) 16–27.
- [3] M. Brehm, B. Kirchner, *J. Chem. Inf. Model.* 51 (2011) 2007–2023.