

Figure S1: Water Surface Accessible Area for AA3 plotted against the Ramachandran angles  $\Phi$  and  $\Psi$ ,  $\text{nm}^3$

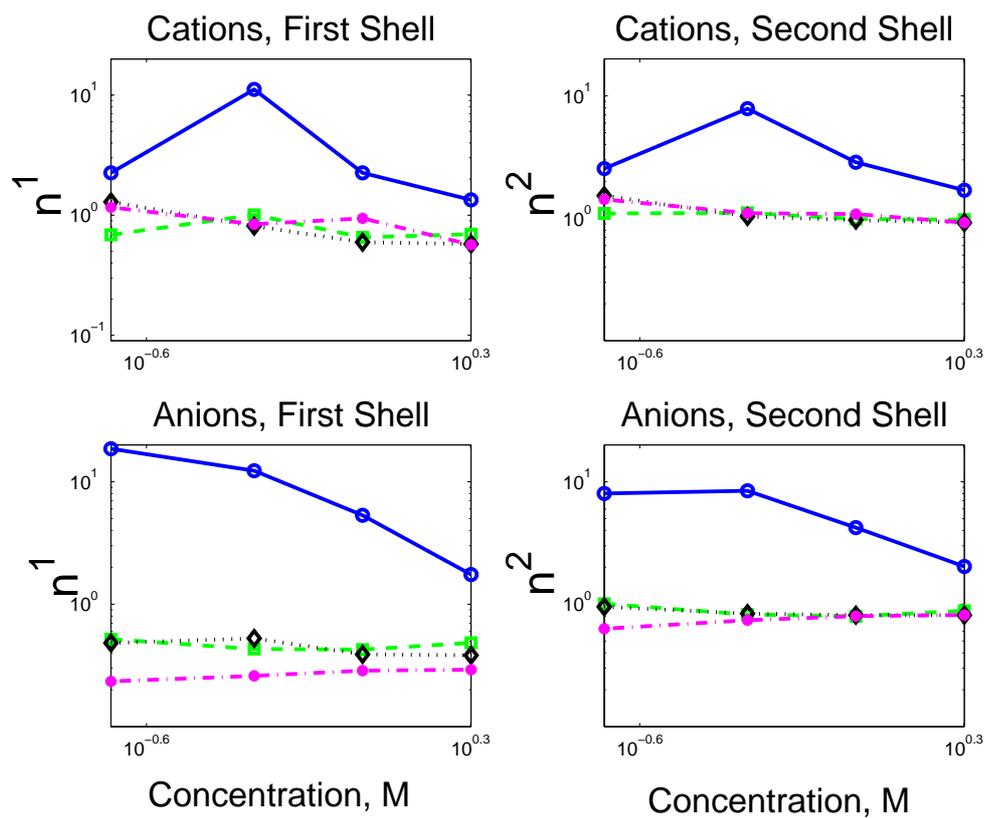


Figure S2: Relative 'local' density of sodium **cations** (top) and **anions** (bottom) in the **first** (left) and **second** solvation shell of the **whole** tripeptide plotted against the molar concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line ( $\circ$ ) -  $F^-$ ; green dashed line ( $\square$ ) -  $Cl^-$ ; black dotted line ( $\diamond$ ) -  $Br^-$ ; purple dash-dotted line ( $\bullet$ ) -  $I^-$ .

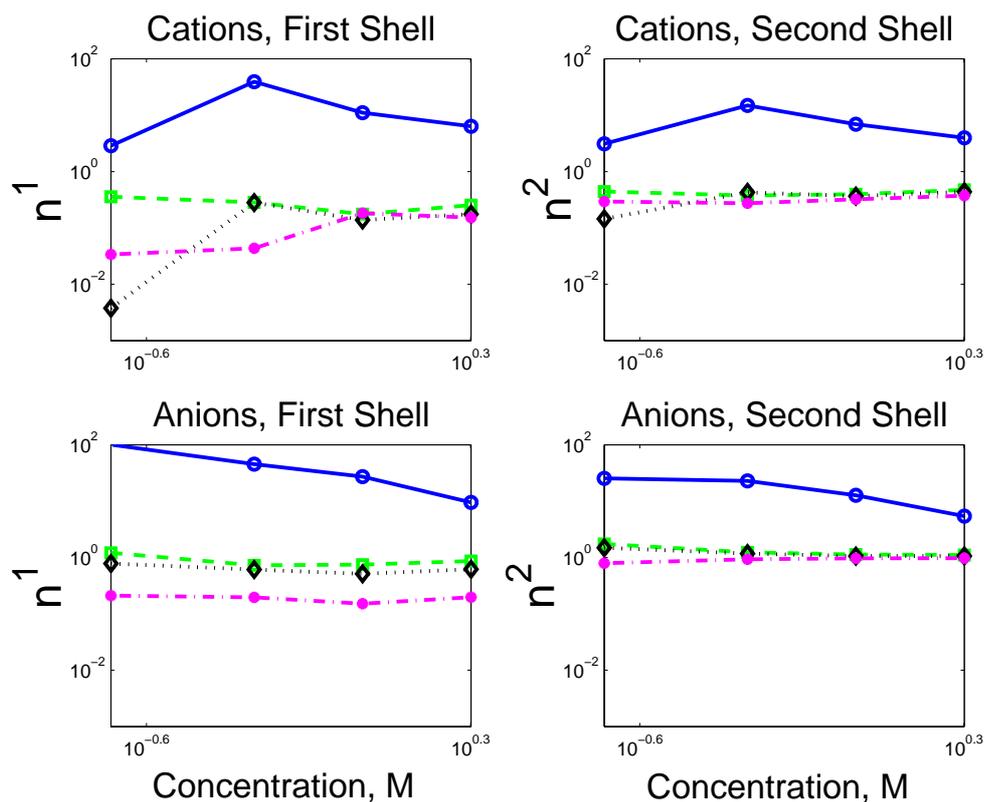


Figure S3: Relative 'local' density of sodium **cations** (top) and **anions** (bottom) in the **first** (left) and **second** solvation shell of the tripeptide **amino terminus** plotted against the concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line ( $\circ$ ) -  $F^-$ ; green dashed line ( $\square$ ) -  $Cl^-$ ; black dotted line ( $\diamond$ ) -  $Br^-$ ; purple dash-dotted line ( $\bullet$ ) -  $I^-$ .

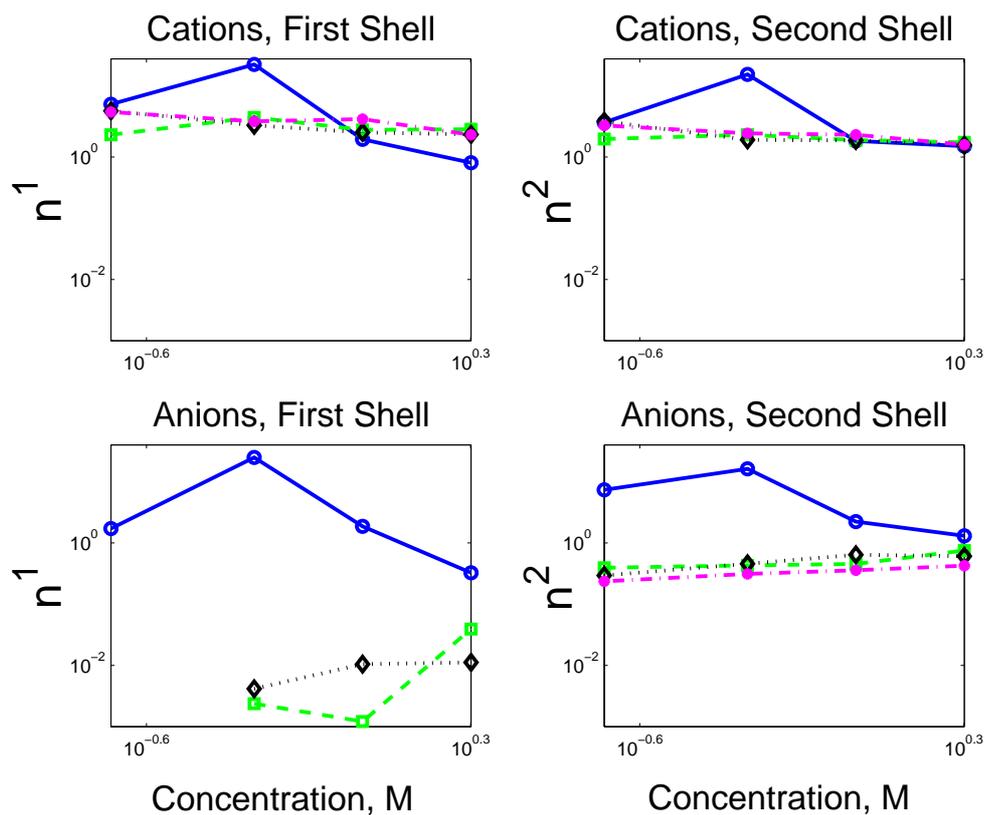


Figure S4: Relative 'local' density of sodium **cations** (top) and **anions** (bottom) in the **first** (left) and **second** solvation shell of the tripeptide **carboxyl terminus** group plotted against the concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line ( $\circ$ ) -  $F^-$ ; green dashed line ( $\square$ ) -  $Cl^-$ ; black dotted line ( $\diamond$ ) -  $Br^-$ ; purple dash-dotted line ( $\bullet$ ) -  $I^-$ .

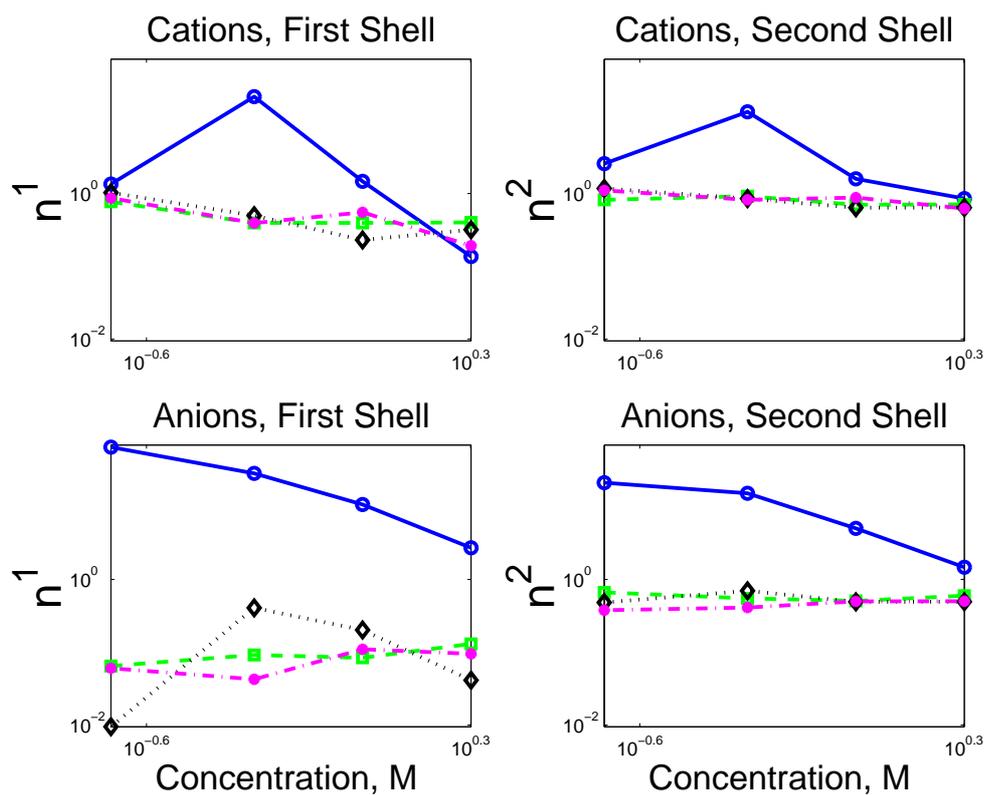


Figure S5: Relative 'local' density of sodium **cations** (top) and **anions** (bottom) in the **first** (left) and **second** solvation shell of the tripeptide **backbone** groups plotted against the concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line ( $\circ$ ) -  $F^-$ ; green dashed line ( $\square$ ) -  $Cl^-$ ; black dotted line ( $\diamond$ ) -  $Br^-$ ; purple dash-dotted line ( $\bullet$ ) -  $I^-$ .

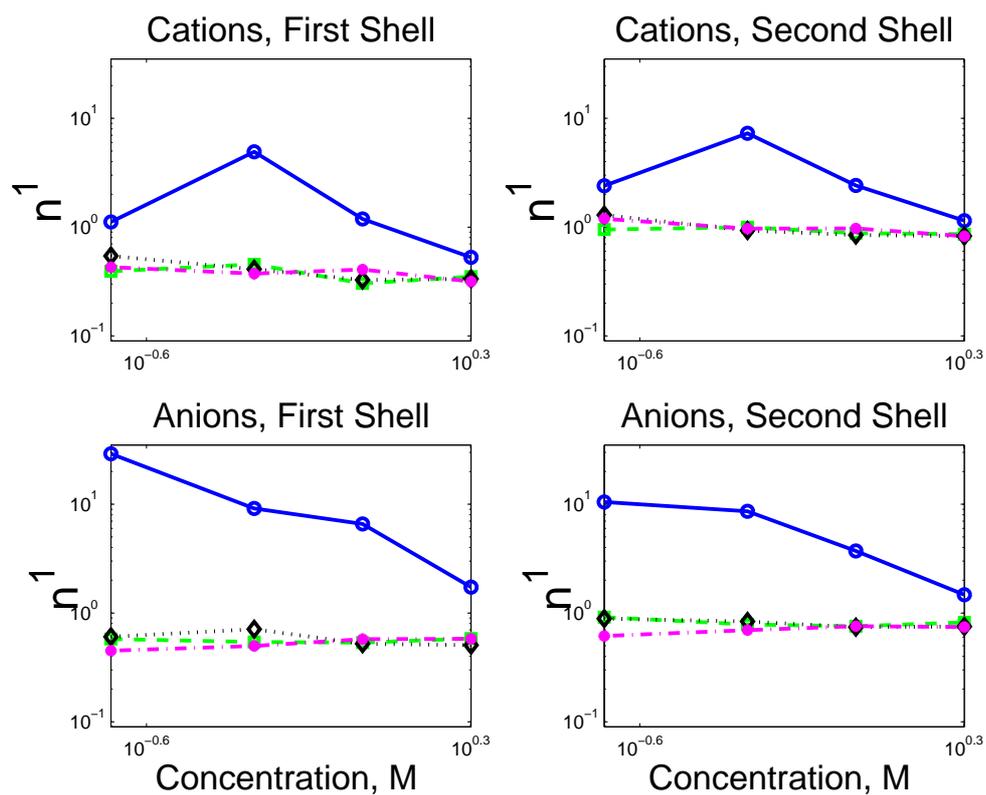


Figure S6: Relative 'local' density of sodium **cations** (top) and **anions** (bottom) in the **first** (left) and **second** solvation shell of the tripeptide **side** groups plotted against the concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line (○) - F<sup>-</sup>; green dashed line (□) - Cl<sup>-</sup>; black dotted line (◇) - Br<sup>-</sup>; purple dash-dotted line (●) - I<sup>-</sup>.

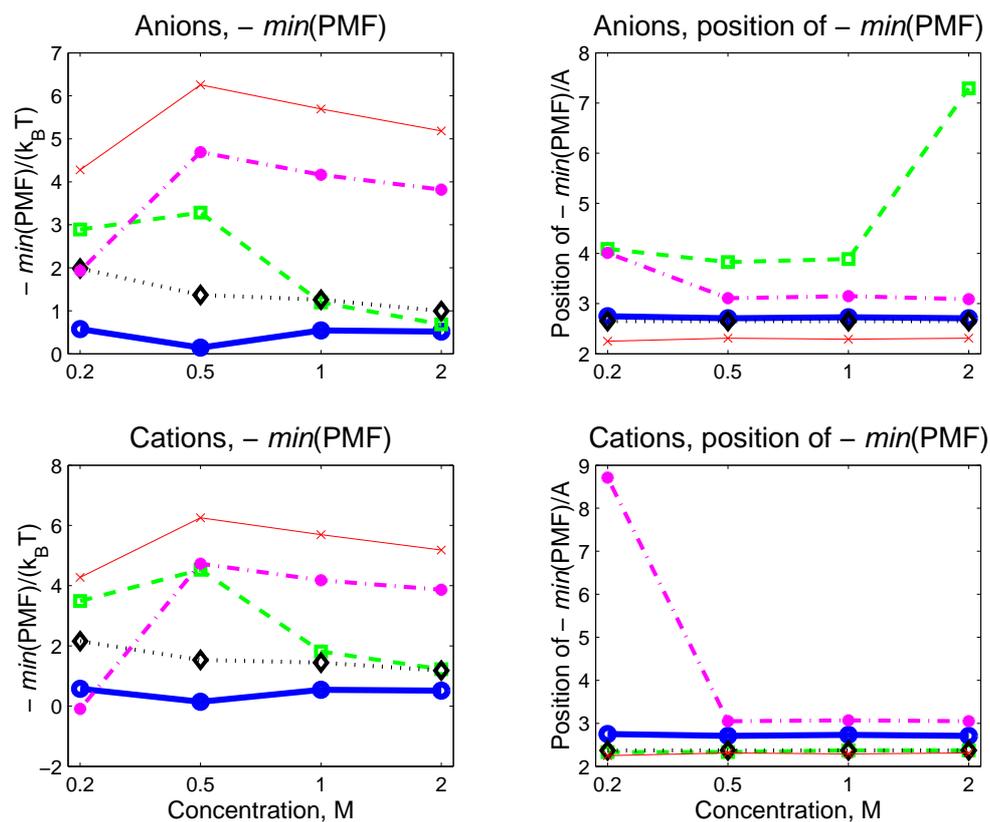


Figure S7: Depth (left side) and position (right side) of the PMF minima between the **carboxyl terminus**,  $F^-$  anions (top) and  $Na^+$  cations (bottom) in  $NaF$  solution. The data are shown as functions of salt concentration. Different lines correspond to different PMFs: tripeptide group - water oxygen PMF corresponds to the solid blue line (thick,  $\circ$ ); tripeptide group - ion PMF corresponds to the green dashed line ( $\square$ ); ion - water PMF corresponds to the black dotted line ( $\diamond$ ), ion - ion PMF corresponds to the purple dash-dotted line ( $\bullet$ ) -  $I^-$  and ion - counterion PMF corresponds to the red solid line (thin, crosses). The values for the minima depths are shown in  $k_B T$  units and the minima positions are shown in Angstroms.

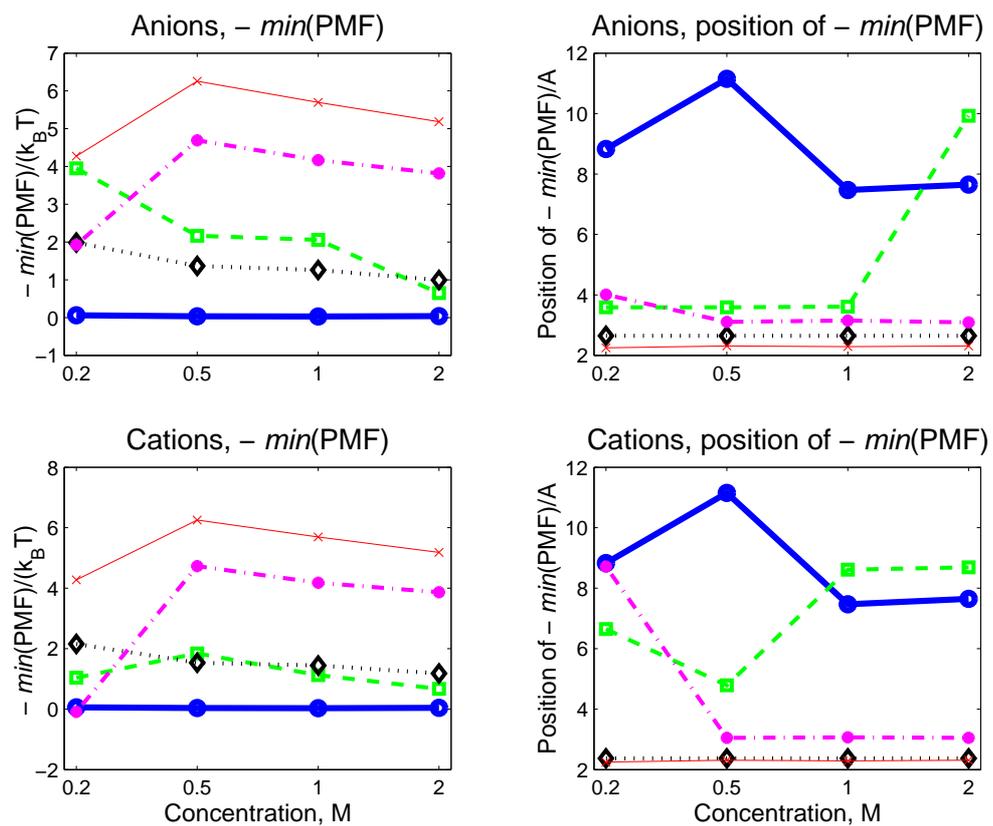


Figure S8: The same data as on the Fig. 7 for the second side chain group and  $NaF$  solution.

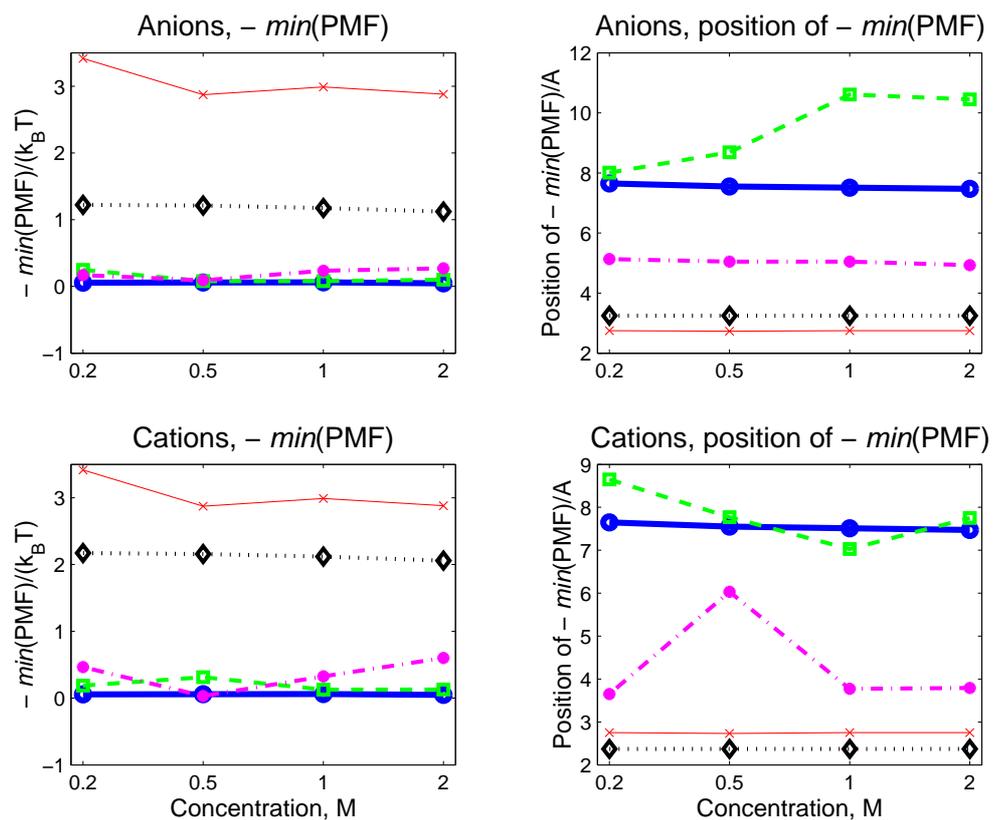


Figure S9: The same data as on the Fig. 7 for the **second side chain group** and *NaCl* solution.

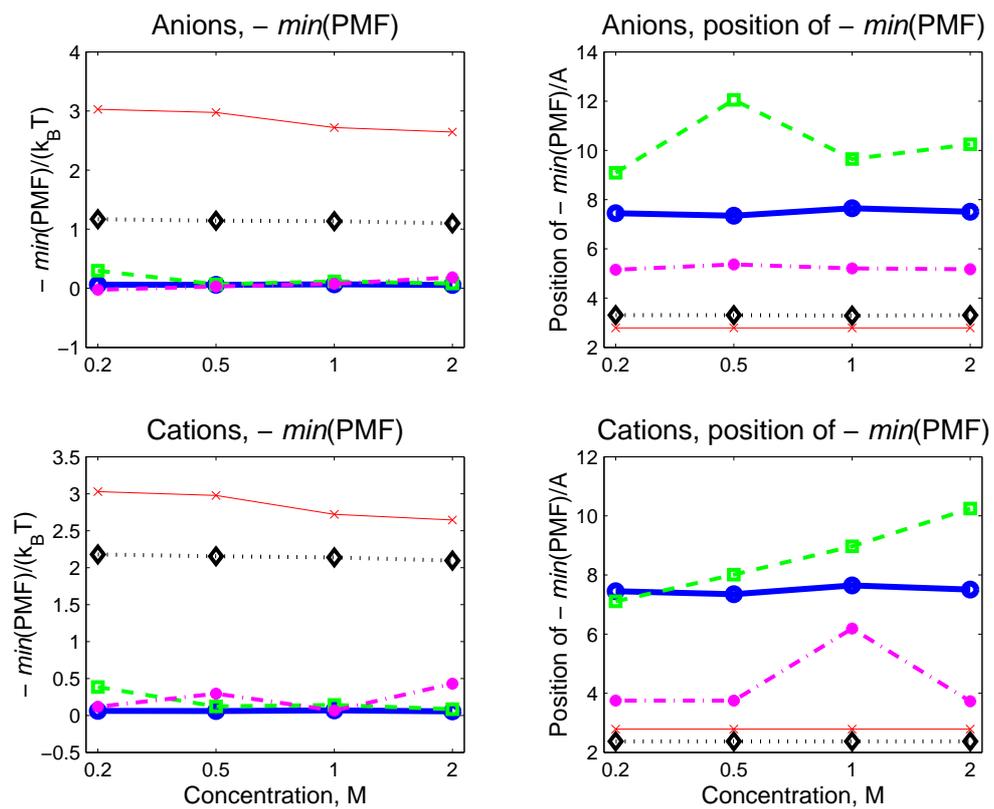


Figure S10: The same data as on the Fig. 7 for the **second side chain group** and *NaBr* solution.

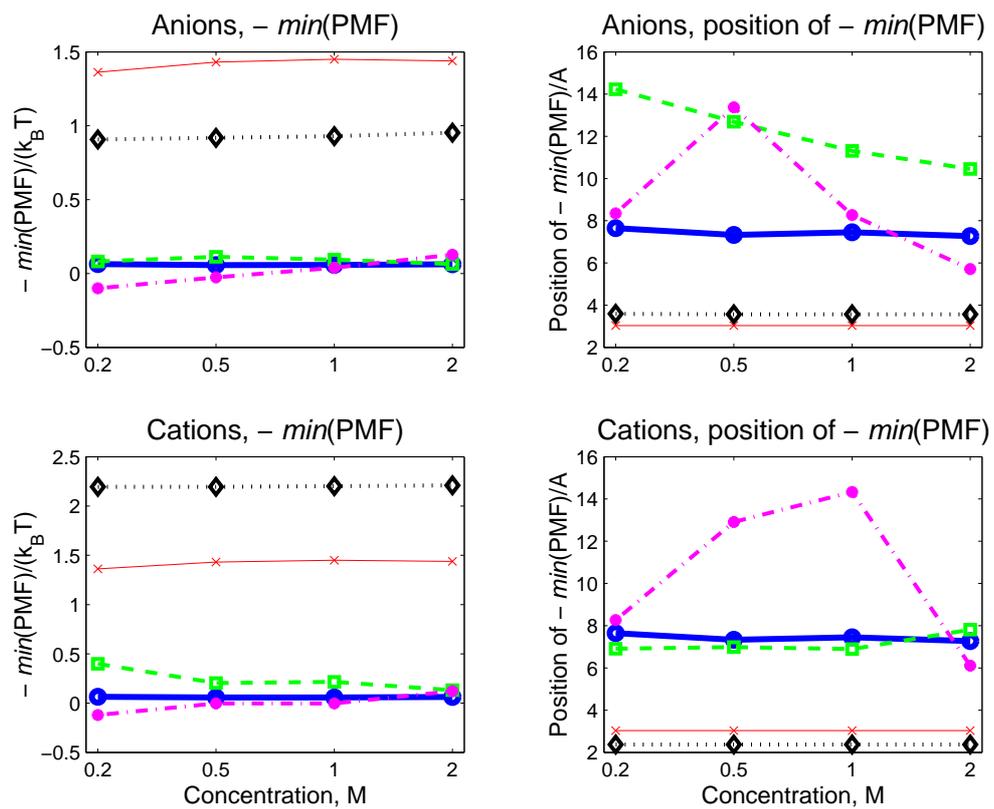


Figure S11: The same data as on the Fig. 7 for the **second side chain group** and *NaI* solution.

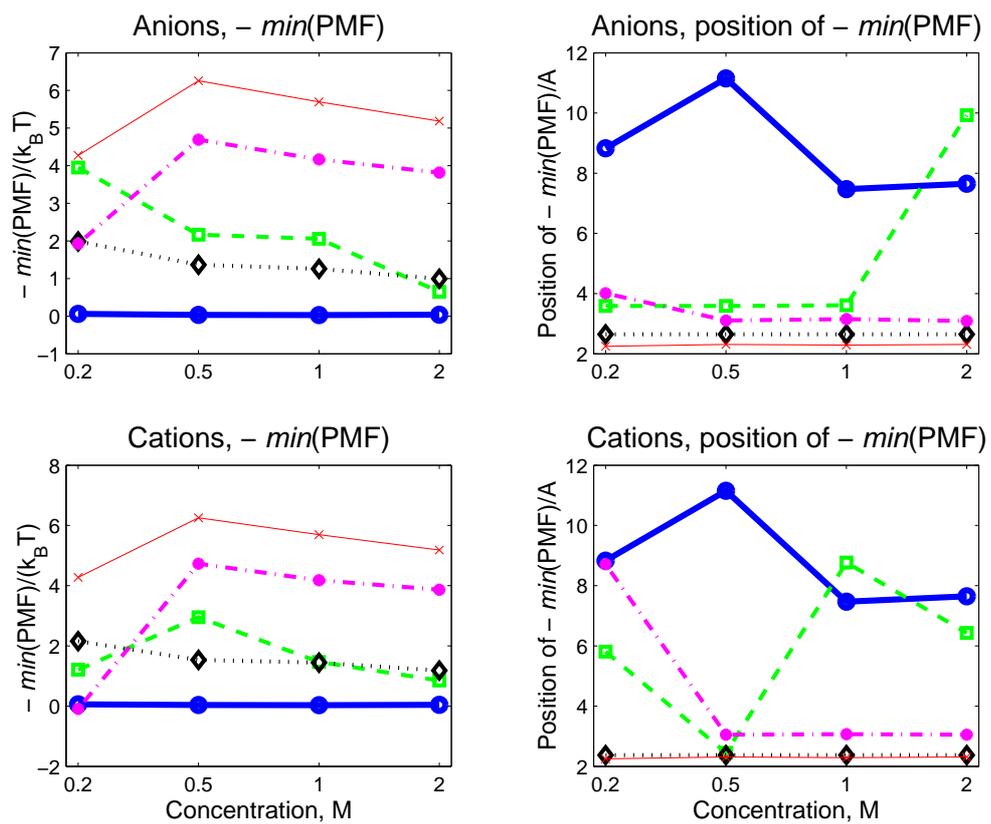


Figure S12: The same data as on the Fig. 7 for the **first backbone group** and  $NaF$  solution.

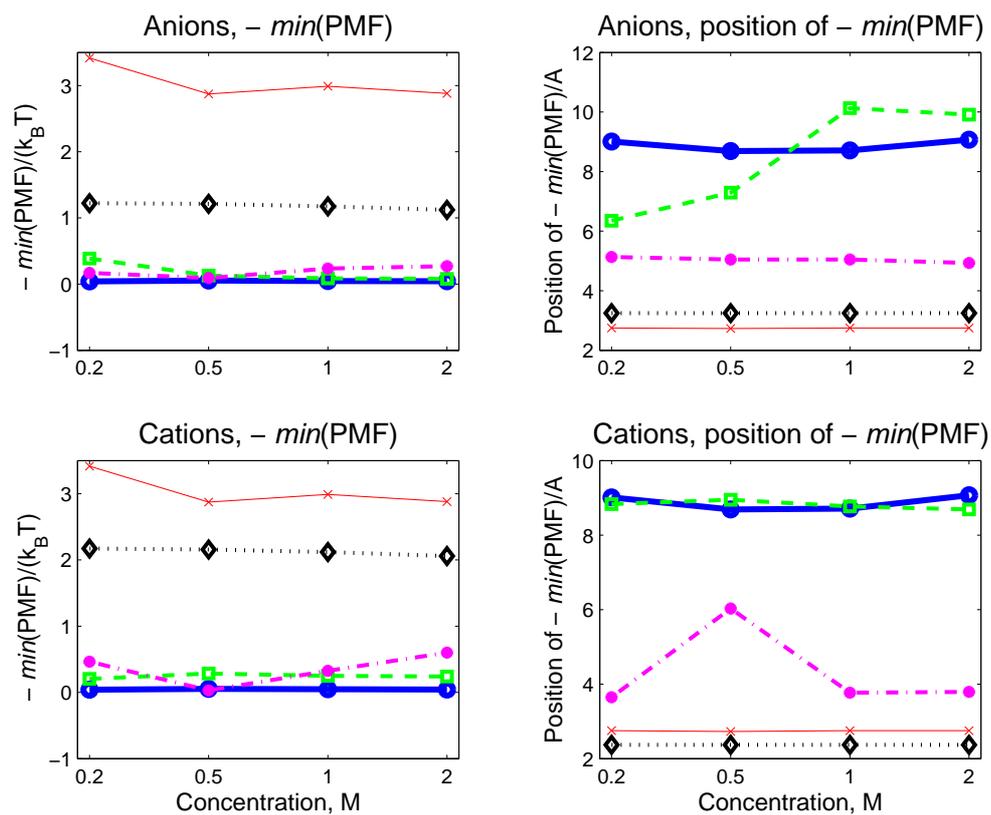


Figure S13: The same data as on the Fig. 7 for the **first backbone group** and *NaCl* solution.

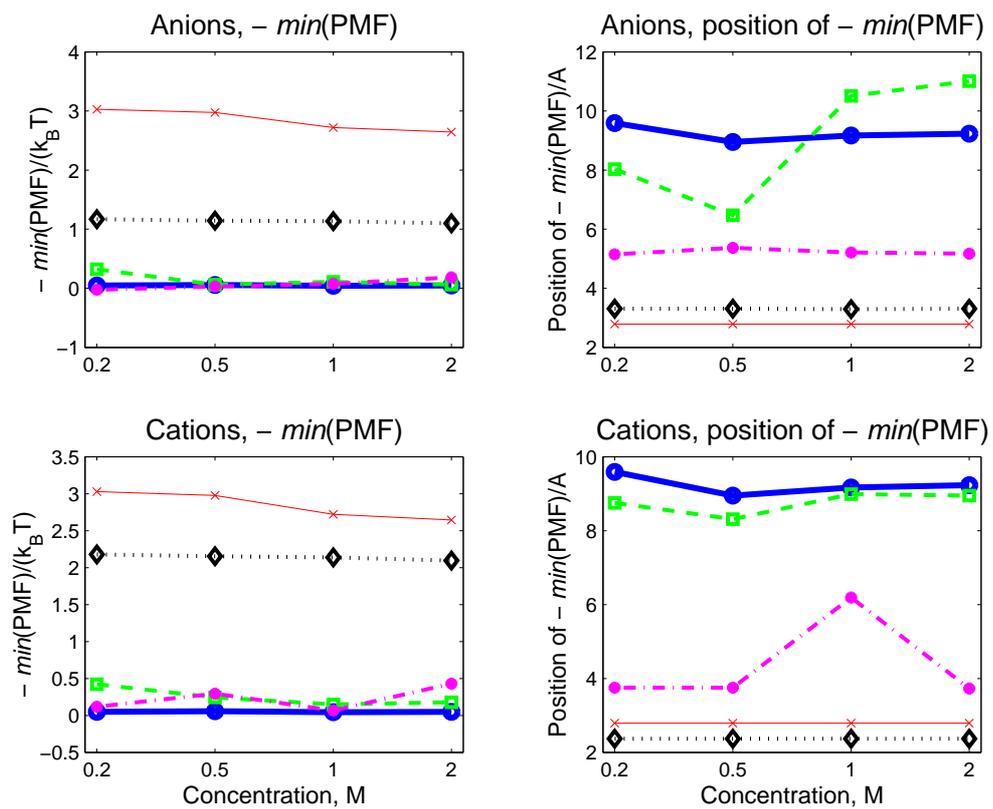


Figure S14: The same data as on the Fig. 7 for the **first backbone group** and *NaBr* solution.

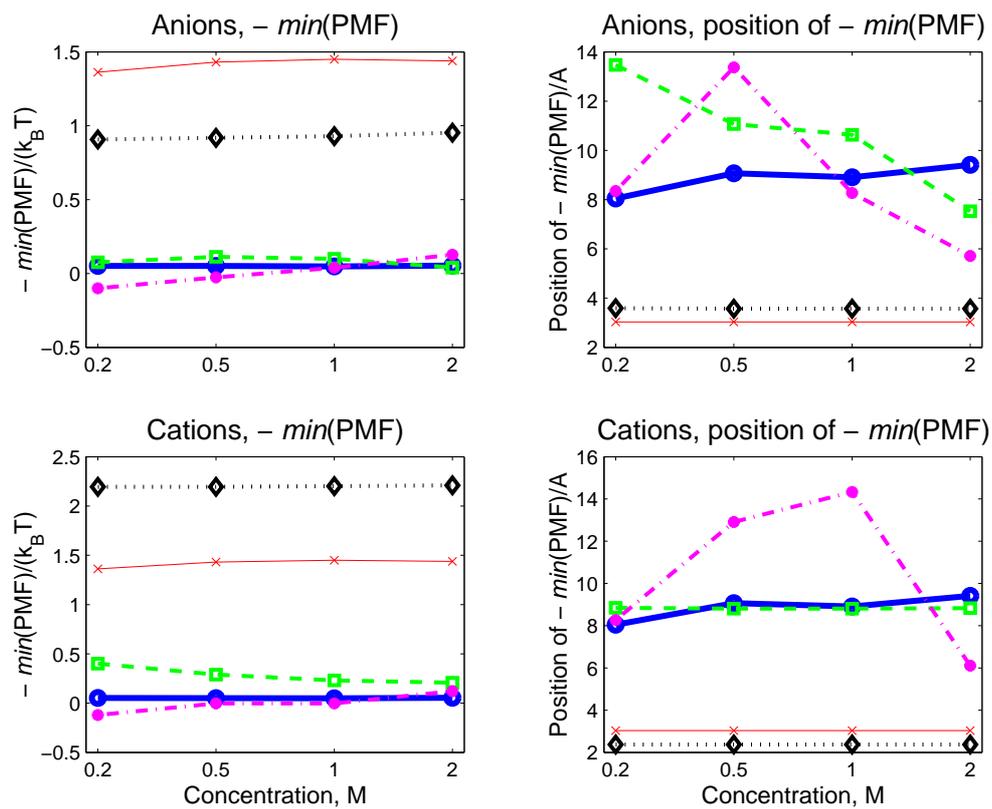


Figure S15: The same data as on the Fig. 7 for the **first backbone group** and *NaI* solution.