Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPORTING INFORMATION

Intermolecular Interactions in Electron Transfer through Stretched Helical Peptides

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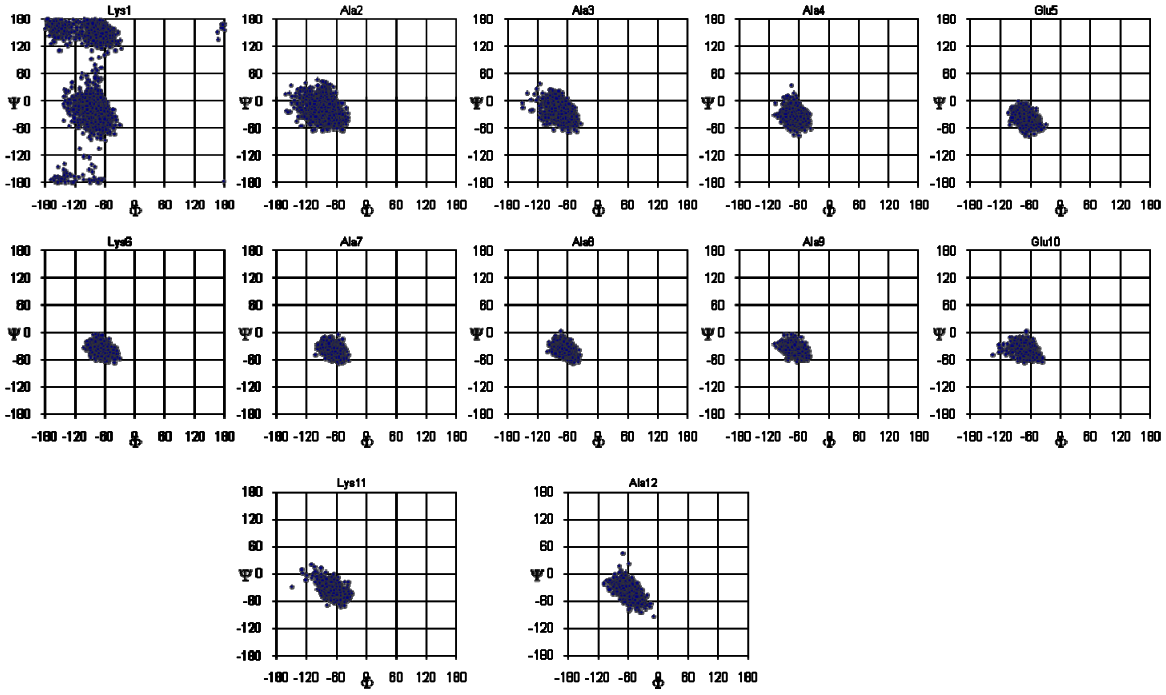

Figure S1. Comparison of the accumulated Ramachandran maps derived from the simulation of the ionized PI peptide in diluted aqueous solution. The maps show the backbone dihedral angles (Φ,Ψ) distribution of the 12 central residues.

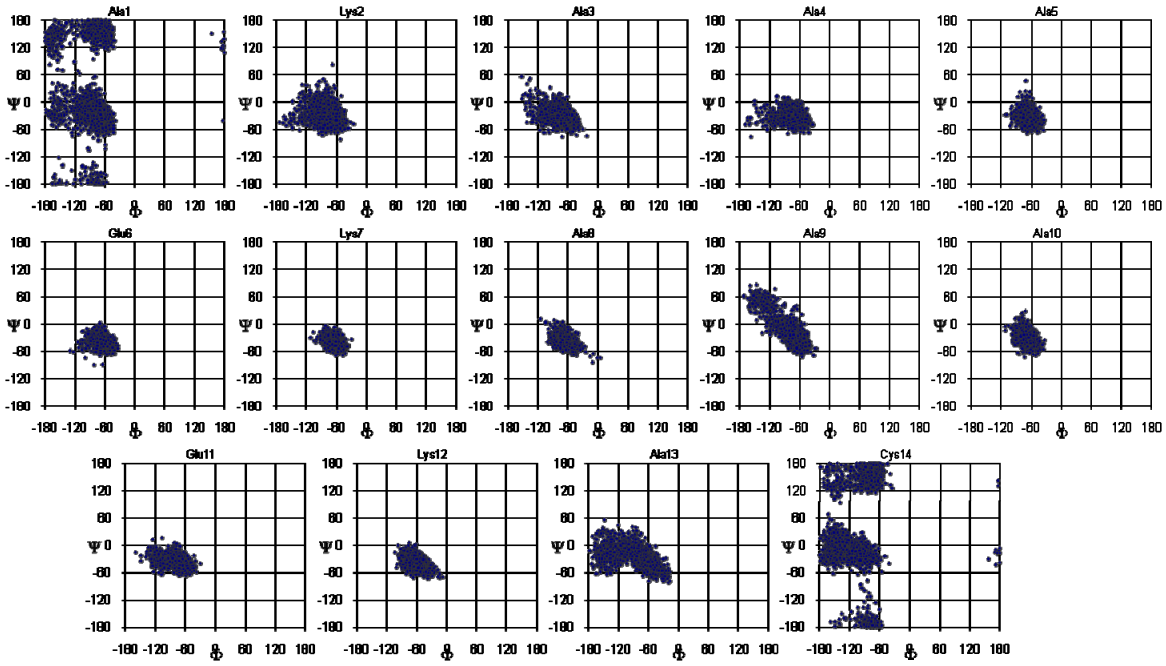

Figure S2. Comparison of the accumulated Ramachandran maps derived from the simulation of the blocked PI peptide in diluted aqueous solution. The maps show the backbone dihedral angles (Φ,Ψ) distribution for all residues.

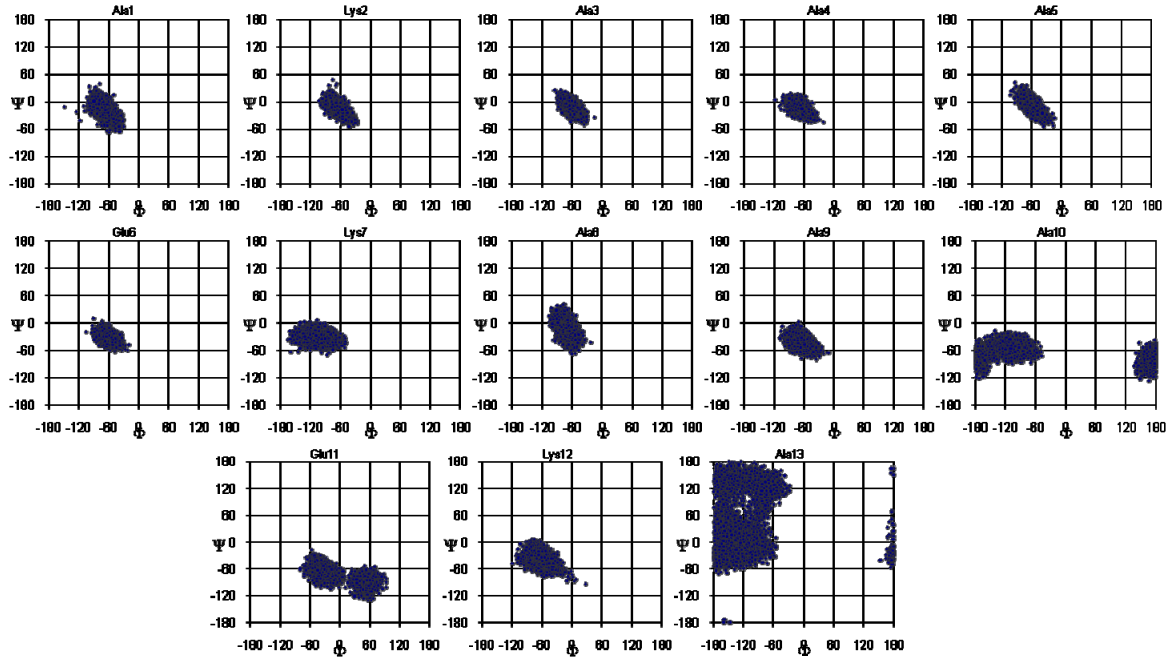

Figure S3. Comparison of the accumulated Ramachandran maps derived from the simulation of the PAuS-I peptide in water/TFE solution. The maps show the backbone dihedral angles (Φ,Ψ) distribution for all residues.

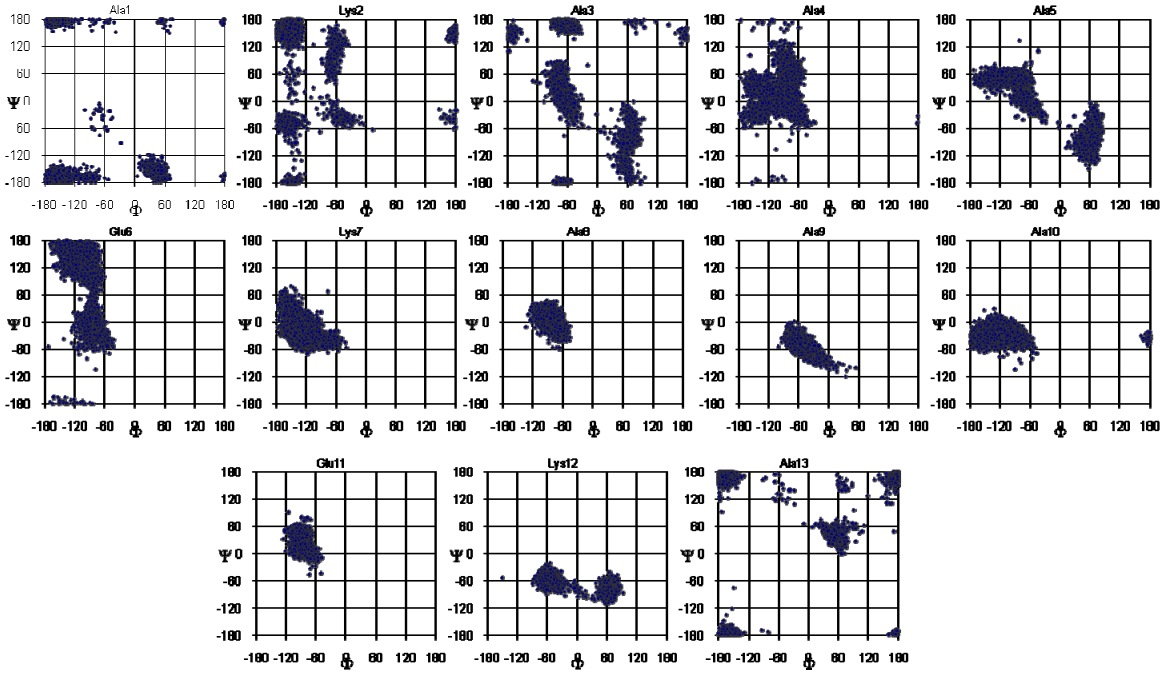

Figure S4. Comparison of the accumulated Ramachandran maps derived from the simulation of the PAuS-I peptide in the gas phase. The maps show the backbone dihedral angles (Φ,Ψ) distribution for all residues.

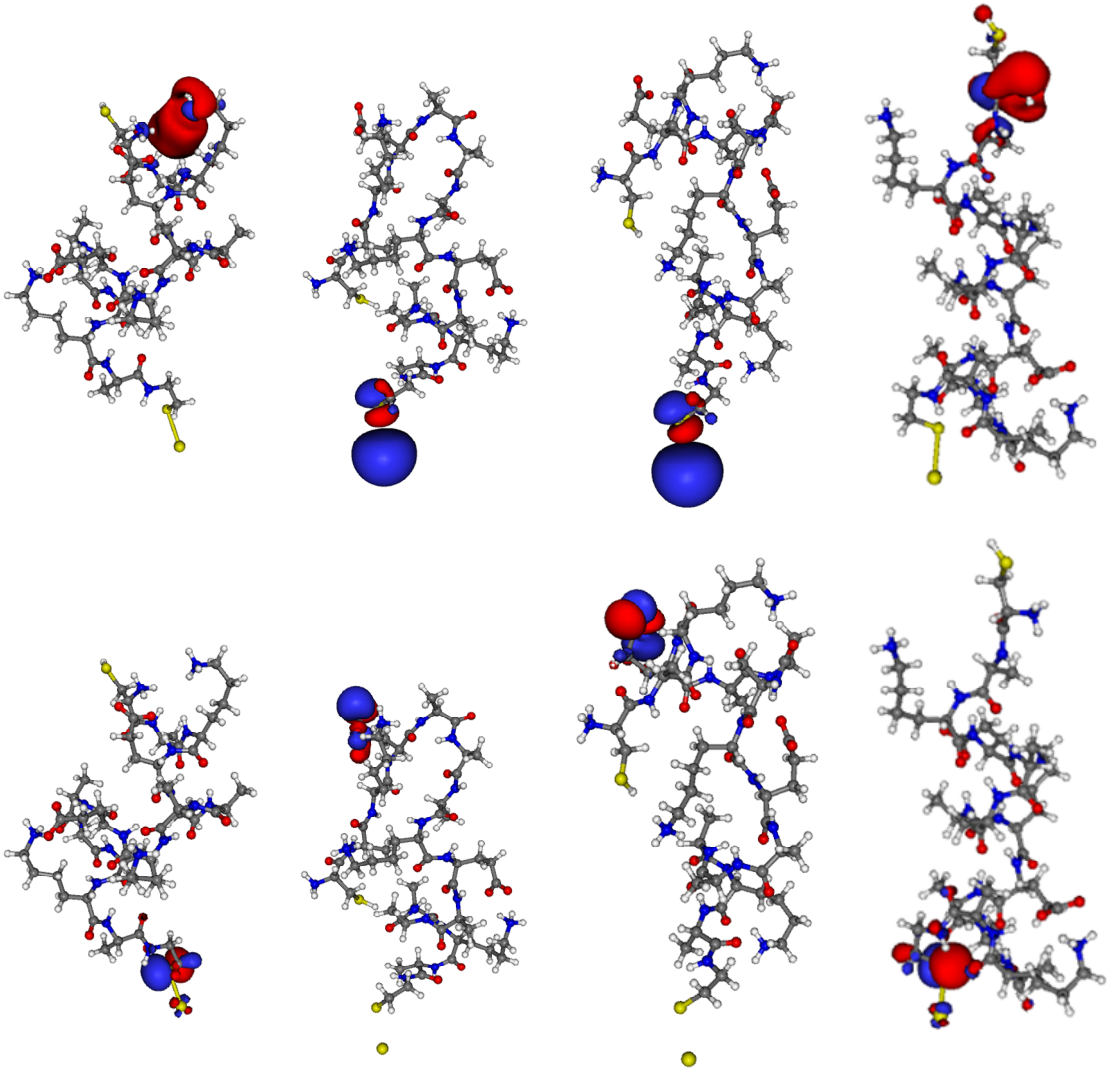

Figure S5. Representation of frontier orbitals (HOMO at the bottom, LUMO at the top) for typical snapshots of the (from left to right) unconstrained, $d_{S\text{-}S}$=1.00 nm, $d_{S\text{-}S}$= 1.50 nm and $d_{S\text{-}S}$= 2.75 nm PAuS-I peptide.