Additional Materials

Aggregation patterns of curcumin and piperine mixtures in different polar media

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1. Energetic perspective of aggregation

1.1. Water

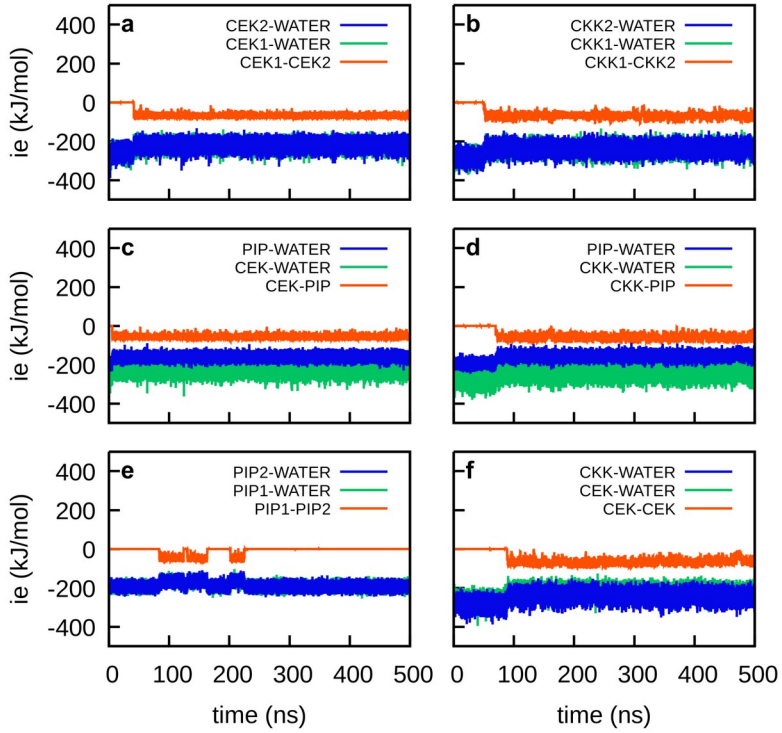

Figure 1. Solute-solute and solute-solvent pairwise interaction energies plots for six simulations of distinct pairs of solute molecules in water: a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK.

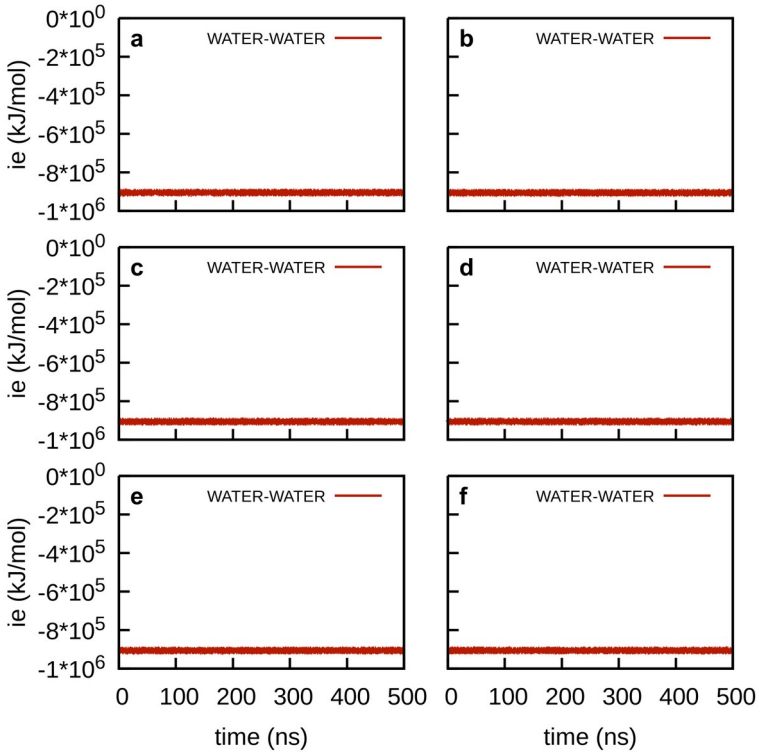

Figure 2. Solvent-solvent pairwise interaction energies plots for six simulations of distinct pairs of solute molecules in water: a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK.

1.2. Ethanol

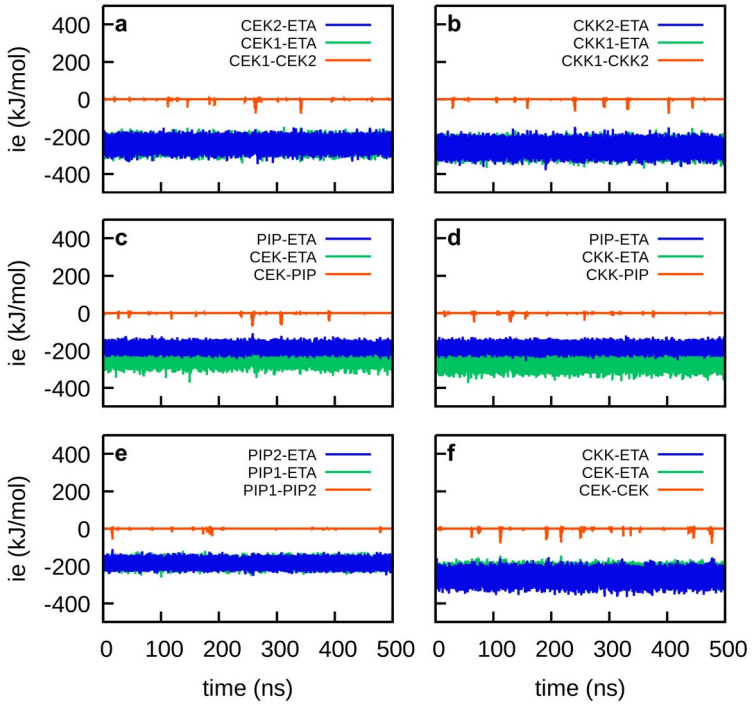

Figure 3. Solute-solute and solute-solvent pairwise interaction energies plots for six simulations of distinct pairs of solute molecules in ethanol: a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK.

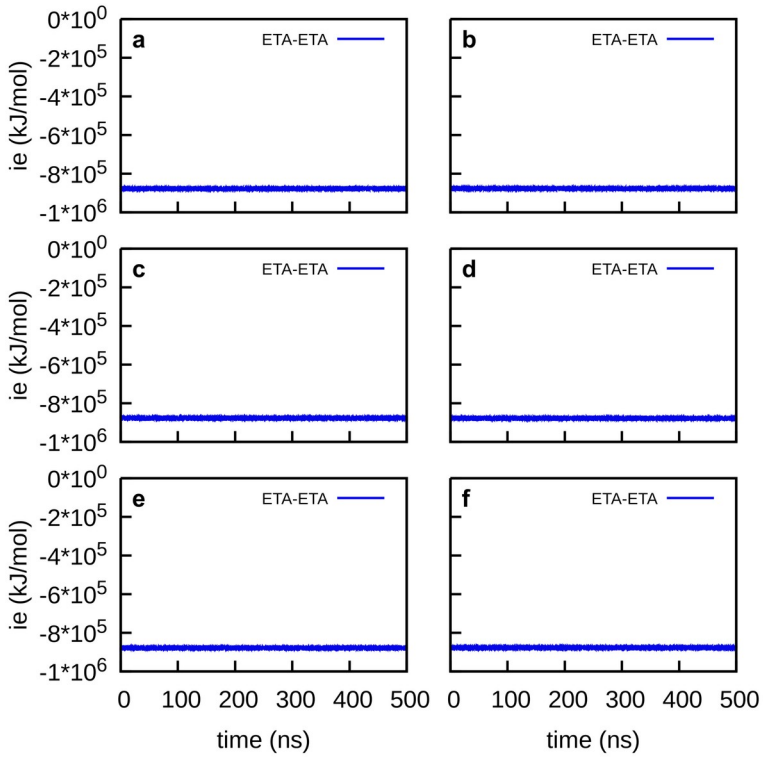

Figure 4. Solvent-solvent pairwise interaction energies plots for six simulations of distinct pairs of solute molecules in ethanol: a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK.

1.3. Solvent Mixture (30:70)

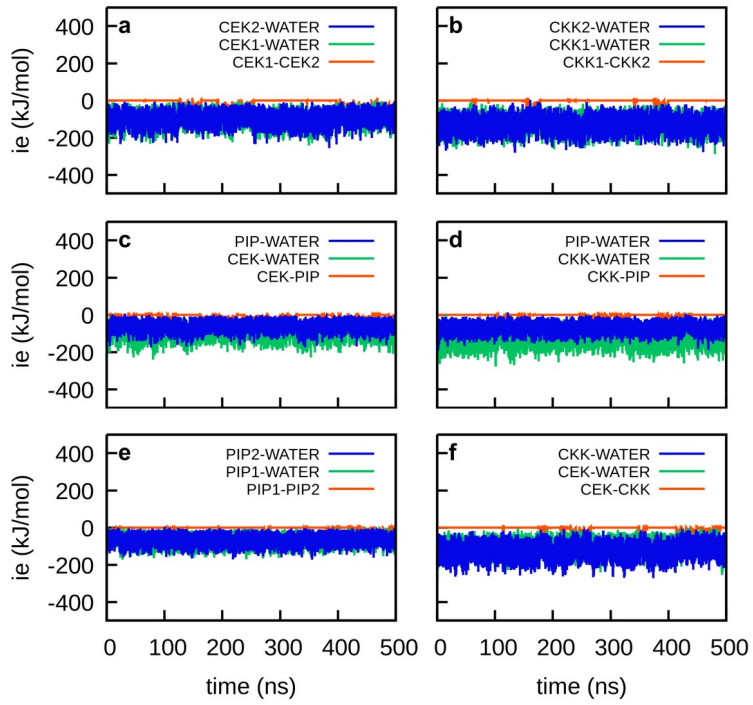

Figure 5. Solute-solute and solute-solvent pairwise interaction energies plots for six simulations of distinct pairs of solute molecules in solvent mixture (30:70): a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK.

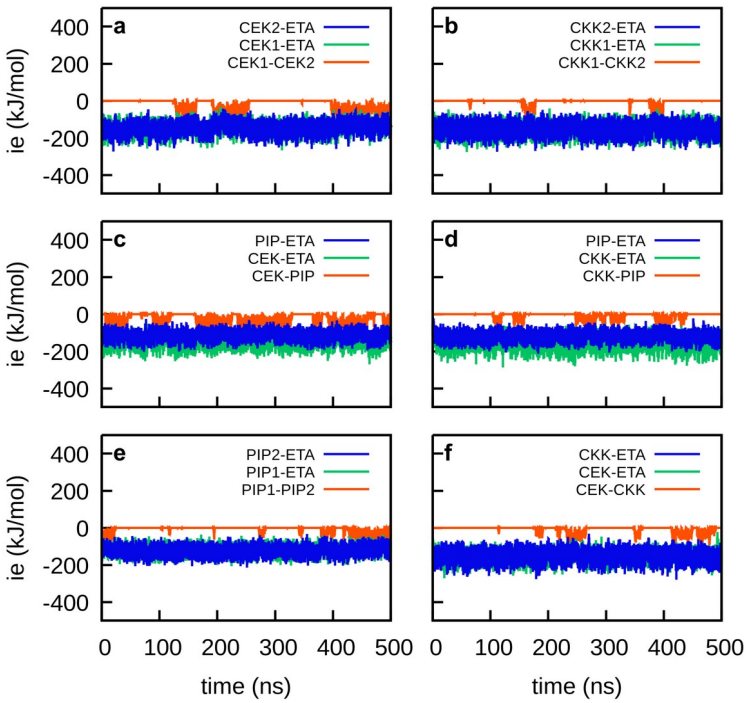

Figure 6. Solute-solute and solute-solvent pairwise interaction energies plots for six simulations of distinct pairs of solute molecules in solvent mixture (30:70): a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK.

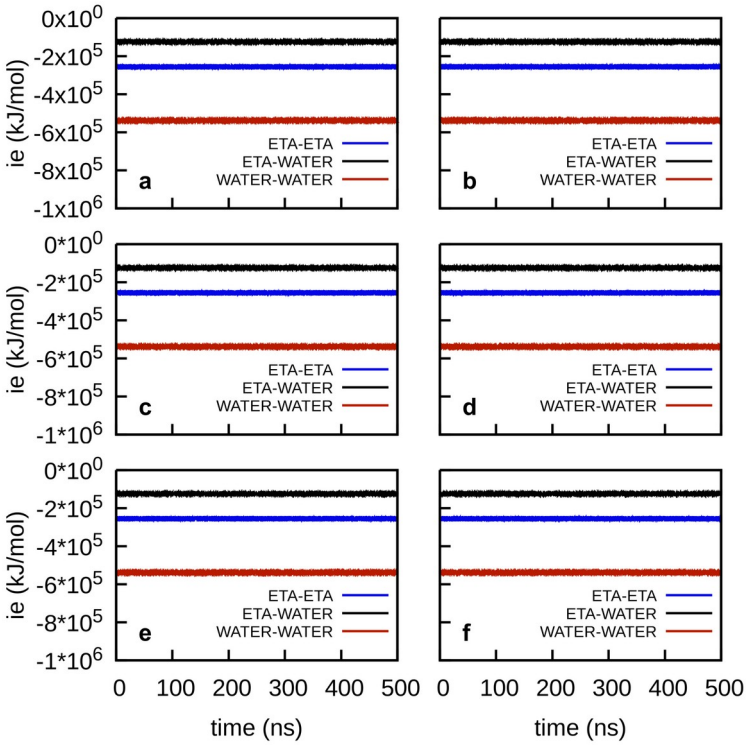

Figure 7. Solvent-solvent pairwise interaction energies plots for six simulations of distinct pairs of solute molecules in solvent mixture (30:70): a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK.

2. Atom-atom RDFs

2.1. Water

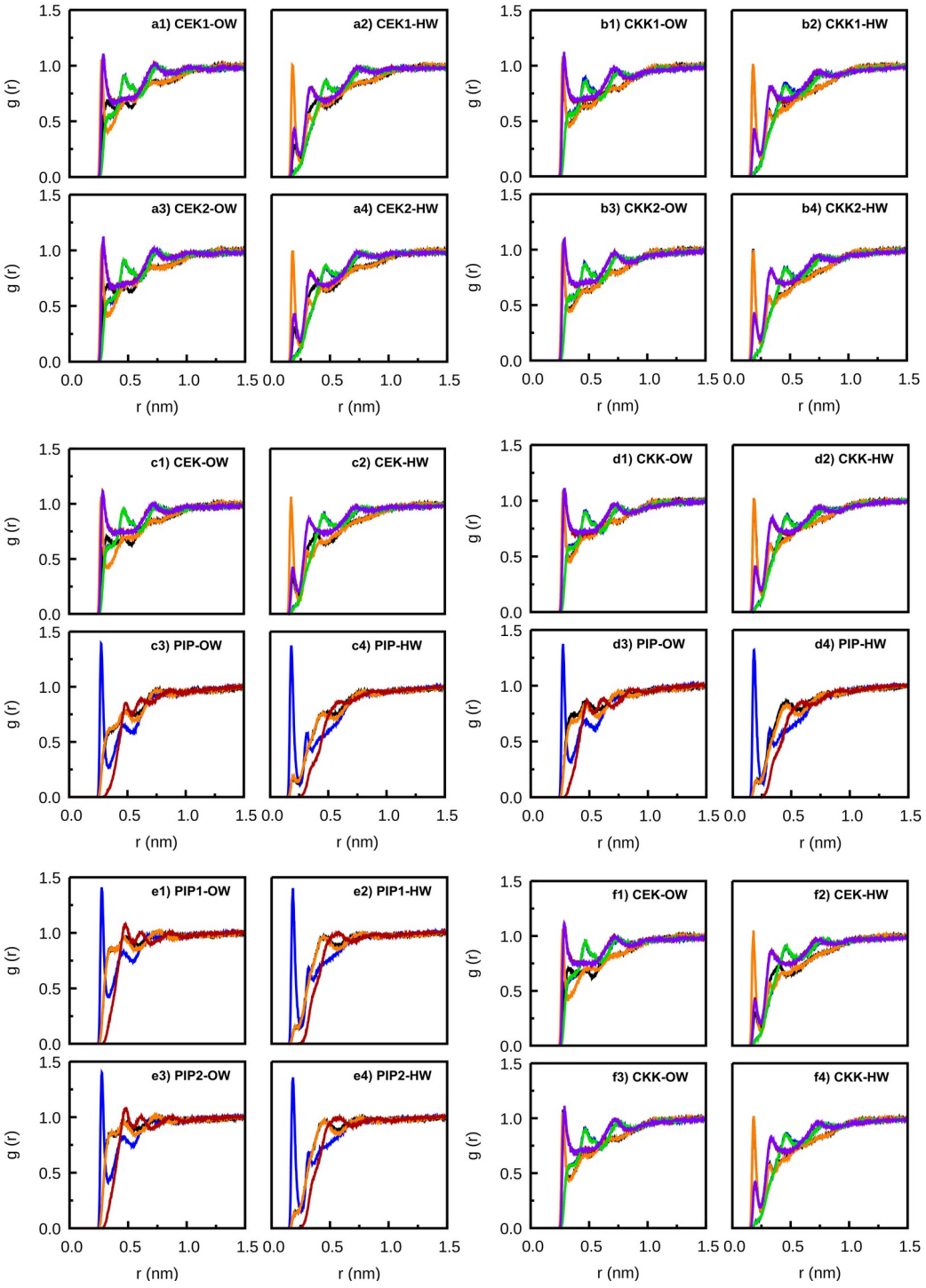

Figure 8. Solute-solvent atom-atom RDFs between the oxygens of the solute molecules and the hydrogen or oxygen (HW or OW) of water for six simulations of distinct pairs of solute molecules in water: a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK. Key for colors of CEK and CKK: O1 (blue), O10 (black) O12 (yellow), O18 (red), O19 (green), O7 (purple); Key for colors of PIP: O1 (blue), O2 (black), O3 (yellow), N1 (red). The represented oxygens are identified in Figure S1. Note in that panels b and e, O10 line is not visible due to the overlap with the O12 line.

2.2. Ethanol

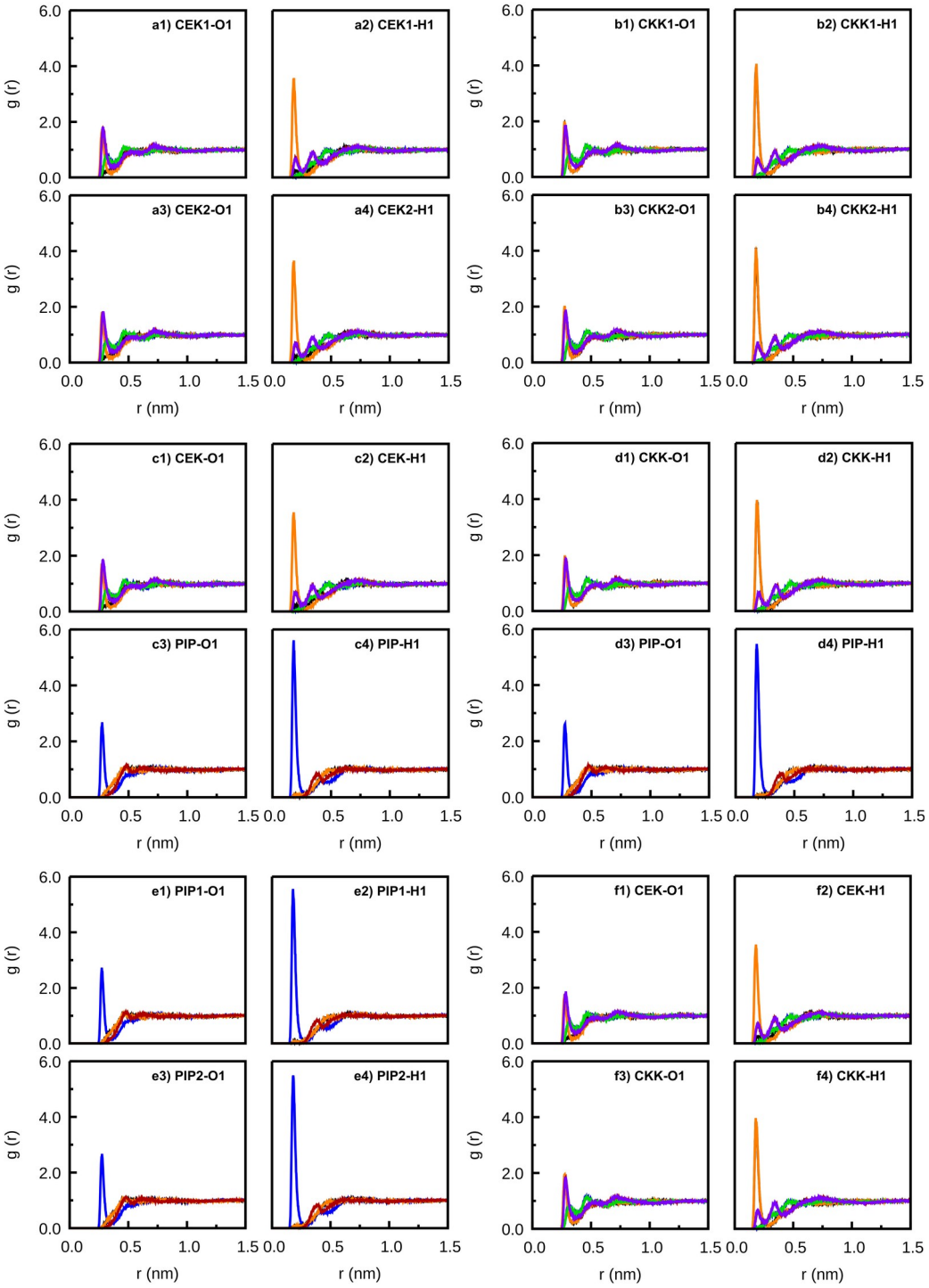

Figure 9. Solute-solvent atom-atom RDFs between the oxygens of the solute molecules and the hydrogen or oxygen (H1 or O1) of ethanol for six simulations of distinct pairs of solute molecules in water: a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK. The represented oxygens are identified in Figure S1. Key for colors of CEK and CKK: O1 (blue), O10 (black) O12 (yellow), O18 (red), O19 (green), O7 (purple); Key for colors of PIP: O1 (blue), O2 (black), O3 (yellow), N1 (red). Note in that panels b and e, O10 line is not visible due to the overlap with the O12 line.

2.3. Solvent Mixture (30_70)

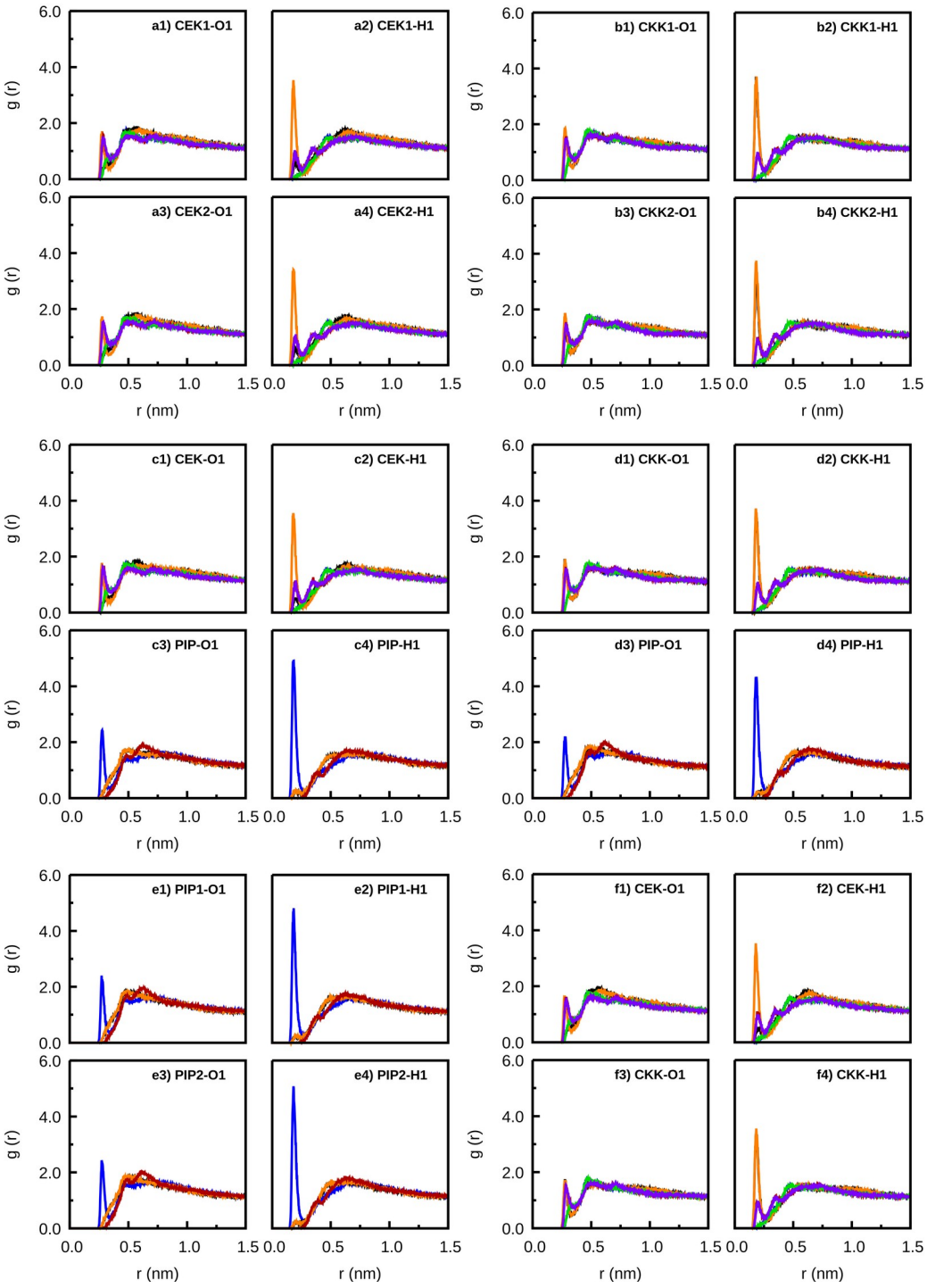

Figure 10. Solute-solvent atom-atom RDFs between the oxygens of the solute molecules and the hydrogen or oxygen of ethanol (H1 or O1) for six simulations of distinct pairs of solute molecules in solvent mixture (30:70): a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK. Key for colors of CEK and CKK: O1 (blue), O10 (black) O12 (yellow), O18 (red), O19 (green), O7 (purple); Key for colors of PIP: O1 (blue), O2 (black), O3 (yellow), N1 (red). The represented oxygens are identified in Figure S1. Note in that panels b and e, O10 line is not visible due to the overlap with the O12 line.

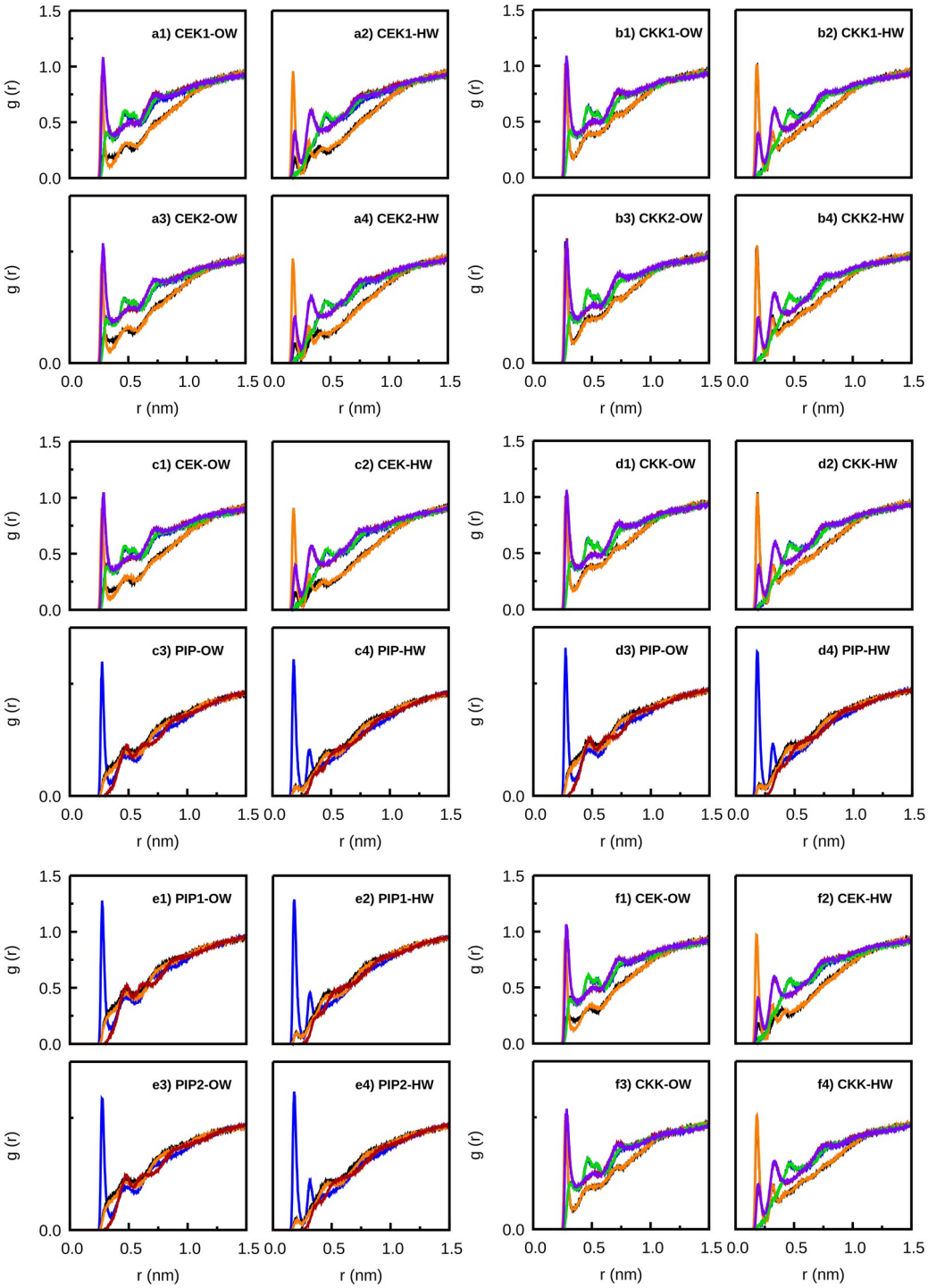

Figure 11. Solute-solvent atom-atom RDFs between the oxygens of the solute molecules and the hydrogen or oxygen of water (HW or OW) for six simulations of distinct pairs of solute molecules in solvent mixture (30:70): a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK. Key for colors of CEK and CKK: O1 (blue), O10 (black) O12 (yellow), O18 (red), O19 (green), O7 (purple); Key for colors of PIP: O1 (blue), O2 (black), O3 (yellow), N1 (red). The represented oxygens are identified in Figure S1. Note in that panels b and e, O10 line is not visible due to the overlap with the O12 line.

3. Log-scale RDFs plots

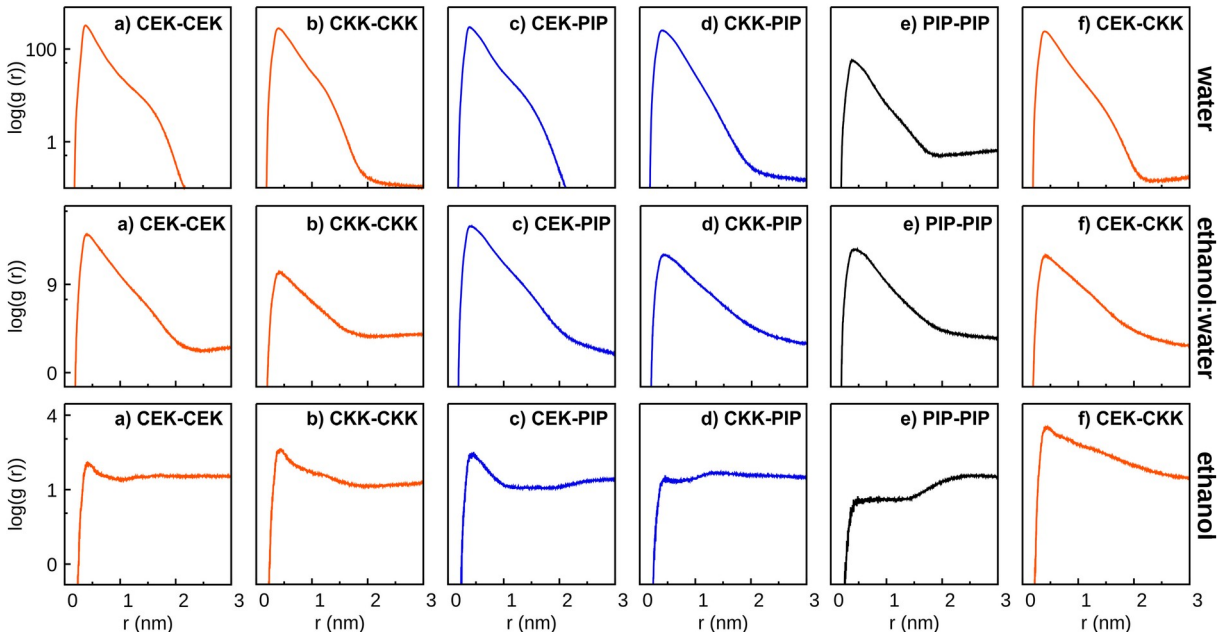

Figure 8. Solute-solute RDFs of six simulations of distinct pairs of solute molecules in water: a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK.;

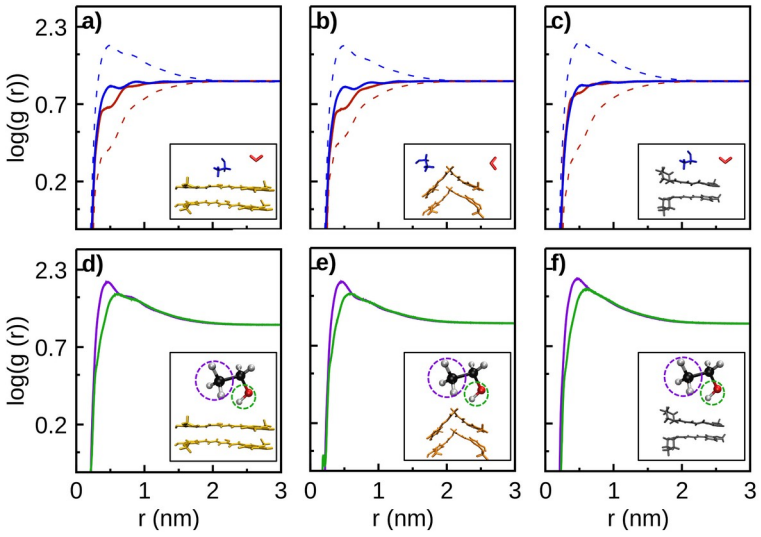

Figure 9. Solute-solvent RDFs for the dimers CEK-CEK (a, d), CKK-CKK (b, e) and PIP-PIP (c, f). Top panels: center-of-mass RDFs related to water (ethanol) are represented by red (blue) lines; solid lines refer to simulations in pure solvents (water or ethanol), while dashed curves are for the (30:70) solvent mixture. The inserts represent the corresponding dimers, as well as one molecule of water (in red) and one molecule of ethanol (in blue). Bottom panels are for simulations with the (30:70) solvent mixture: ethanol-dimer RDFs by taking as reference the -CH3 (purple line) or -OH (green) groups of the ethanol. The inserts represent the corresponding dimers as well as an ethanol molecule with the reference groups marked by a dashed circle.