

Additional Materials

Aggregation patterns of curcumin and piperine mixtures in different polar media

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1. Atom-atom RDFs

1.1. Water

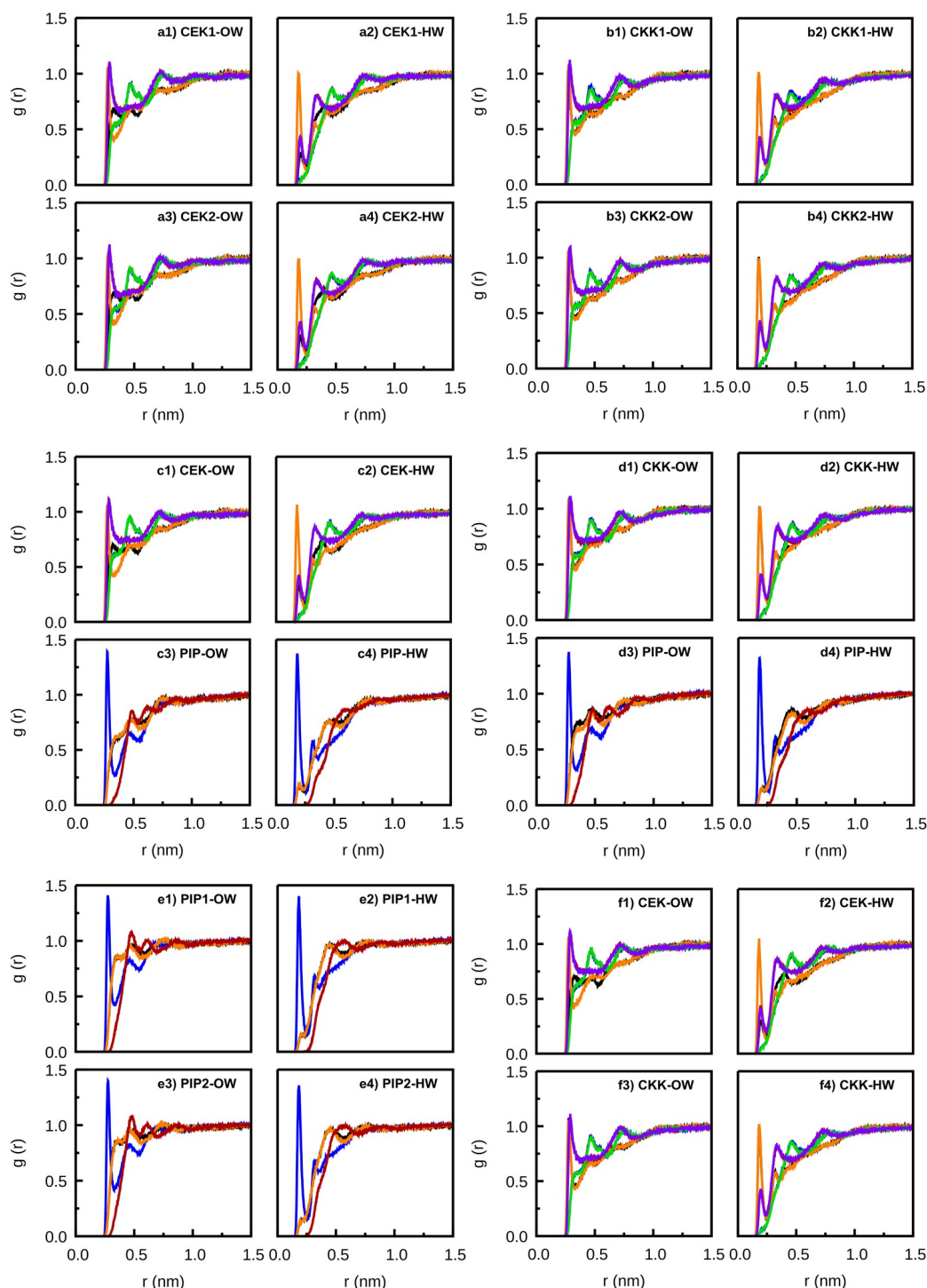


Figure 8. Solute-solvent atom-atom RDFs between the oxygens of the solute molecules and the hydrogen or oxygen (HW or OW) of water for six simulations of distinct pairs of solute molecules in water: a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK. Key for colors of CEK and CKK: 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.

1.2. Ethanol

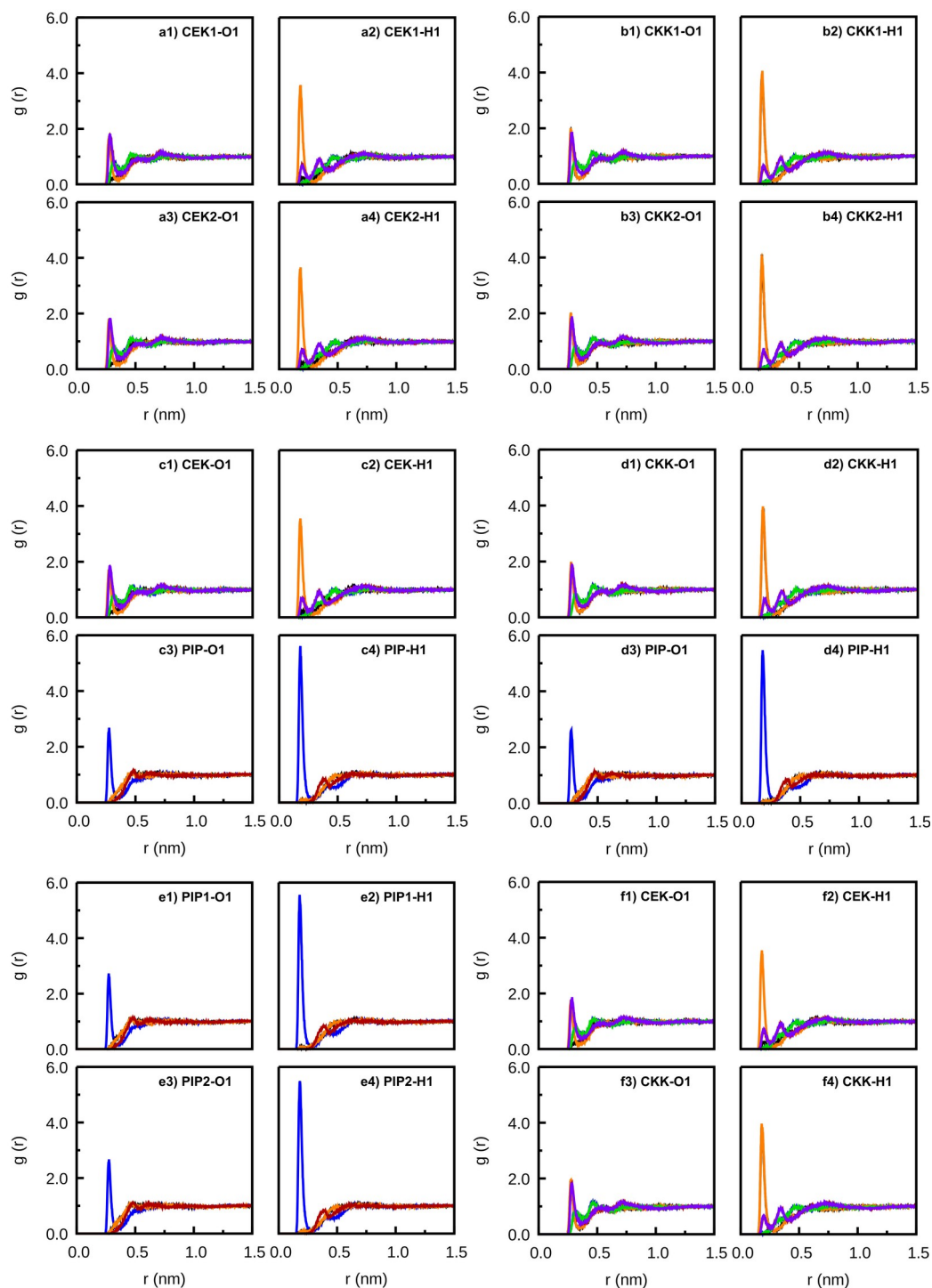


Figure 9. Solute-solvent atom-atom RDFs between the oxygens of the solute molecules and the hydrogen or oxygen (H1 or O1) of ethanol for six simulations of distinct pairs of solute molecules in water: a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK. The represented oxygens are 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.

1.3. Solvent Mixture (30_70)

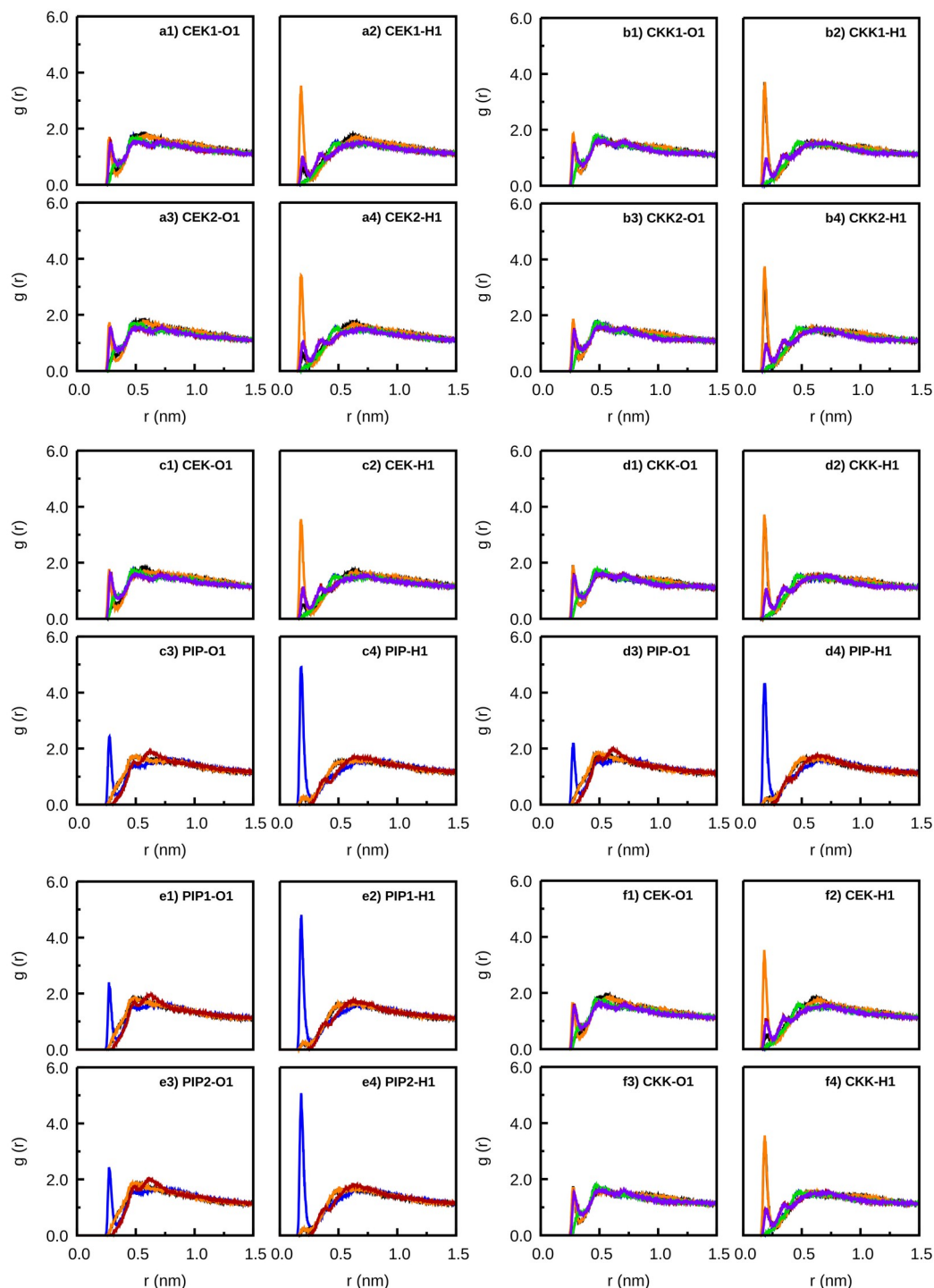


Figure 10. Solute-solvent atom-atom RDFs between the oxygens of the solute molecules and the hydrogen or oxygen of ethanol (H1 or O1) for six simulations of distinct pairs of solute molecules in solvent mixture (30:70): a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK. Key for colors 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.

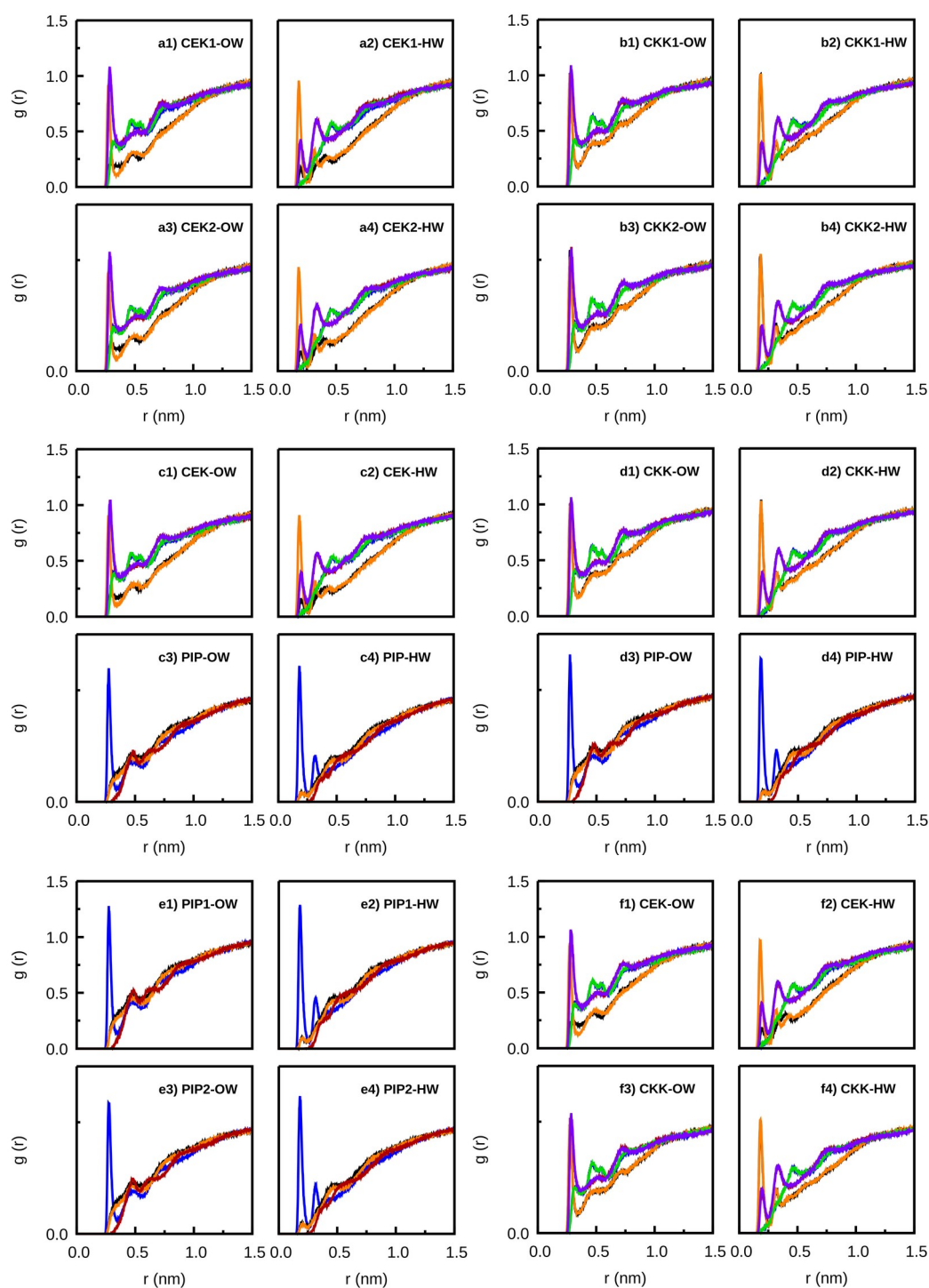


Figure 11. Solute-solvent atom-atom RDFs between the oxygens of the solute molecules and the hydrogen or oxygen of water (HW or OW) for six simulations of distinct pairs of solute molecules in solvent mixture (30:70): a) CEK-CEK; b) CKK-CKK; c) CEK-PIP; d) CKK-PIP; e) PIP-PIP; f) CEK-CKK. Key for colors 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.