

Preferential solvation of glucose and talose in water/acetonitrile mixtures: a molecular dynamics simulation study

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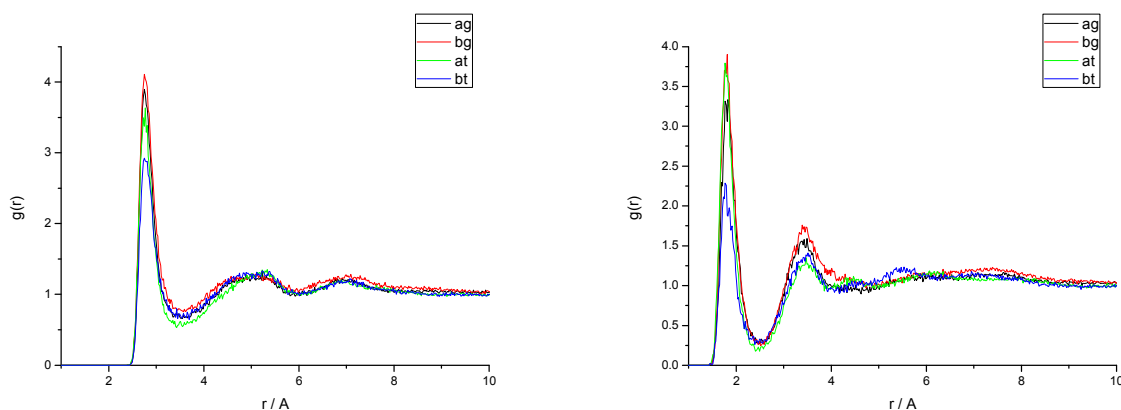


Figure S1. 1:1 H₂O/ACN mixture. (Left): Average radial distribution function, $g(r_{OwOs})$, of the distance between water oxygen and hydroxyl sugar oxygens. (Right): Average radial distribution function, $g(r_{OwHs})$, of the distance between water oxygen and hydroxyl sugar hydrogens. (black) α -glucose; (red) β -glucose; (green) α -talose; (blue) β -talose.

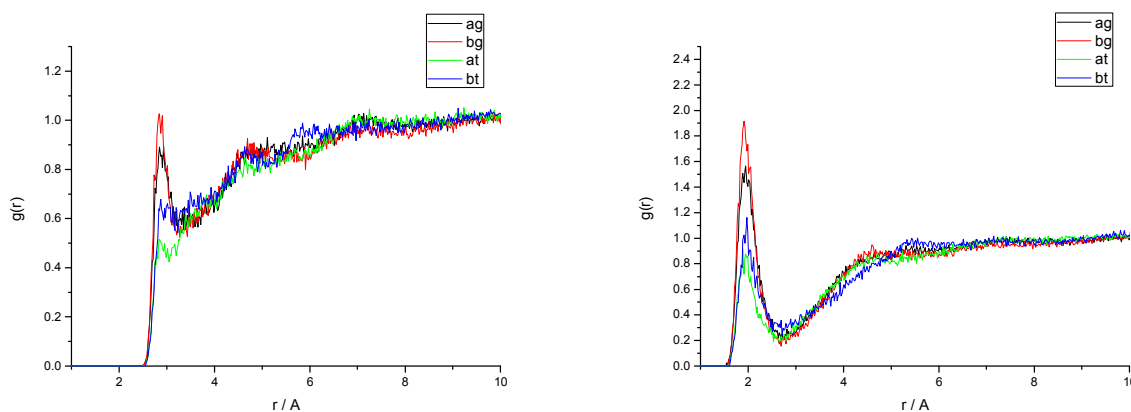


Figure S2. 1:1 H₂O/ACN mixture. (Left) Average radial distribution function, $g(r_{NaOs})$, of the distance between ACN nitrogen and hydroxyl sugar oxygens. (Right) Average radial distribution function, $g(r_{NaHs})$, of the distance between ACN nitrogen and hydroxyl sugar hydrogens. (black) α -glucose; (red) β -glucose; (green) α -talose; (blue) β -talose.

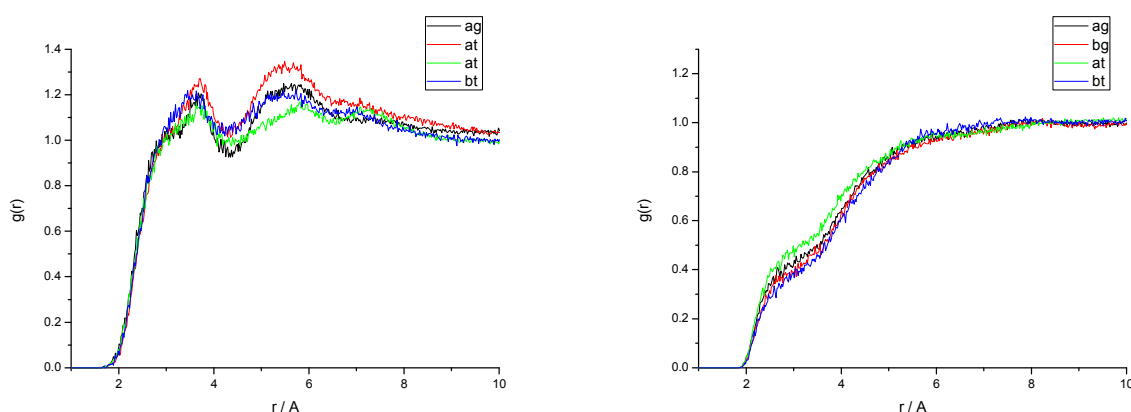


Figure S3. 1:1 H₂O/ACN mixture. (Left): Average radial distribution function of the distance between water hydrogens and alkyl sugar hydrogens $g(r_{HwCHs})$. (Right): Average radial distribution function, $g(r)$, of the distance between ACN hydrogens and alkyl sugar hydrogens $g(r_{HaCHs})$. (black) α -glucose; (red) β -glucose; (green) α -talose; (blue) β -talose.

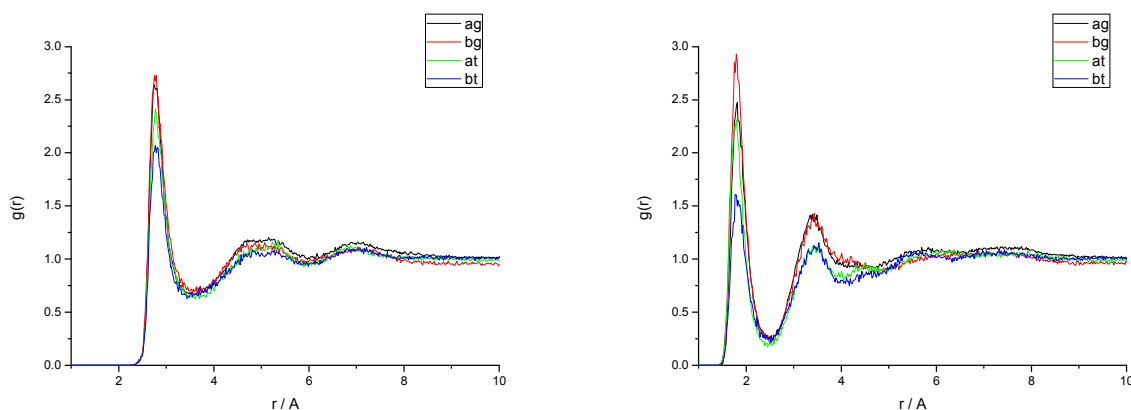


Figure S4. 2:1 H₂O/ACN mixture. (Left) Average radial distribution function, $g(r_{\text{OwOs}})$, of the distance between water oxygen and hydroxyl sugar oxygens. (Right): Average radial distribution function, $g(r_{\text{OwHs}})$, of the distance between water oxygen and hydroxyl sugar hydrogens. (black) α -glucose; (red) β -glucose; (green) α -talose; (blue) β -talose.

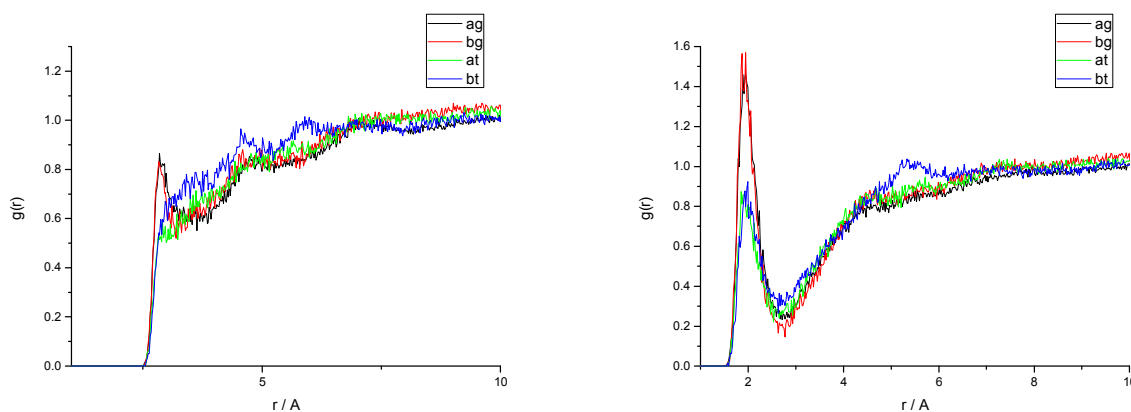


Figure S5. 2:1 H₂O/ACN mixture. (Left) Average radial distribution function, $g(r_{\text{NaOs}})$, of the distance between ACN nitrogen and hydroxyl sugar oxygens, (Right) Average radial distribution function, $g(r_{\text{NaHs}})$, of the distance between ACN nitrogen and hydroxyl sugar hydrogens. (black) α -glucose; (red) β -glucose; (green) α -talose; (blue) β -talose.

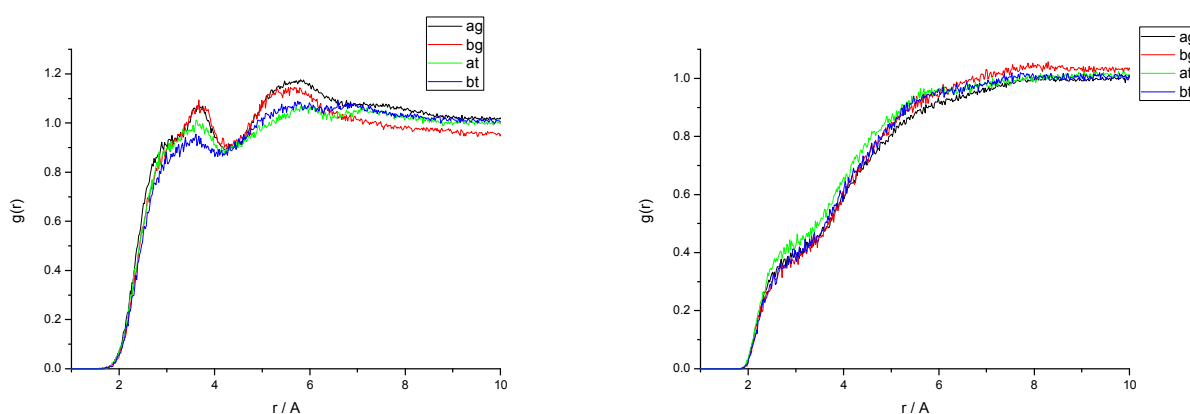
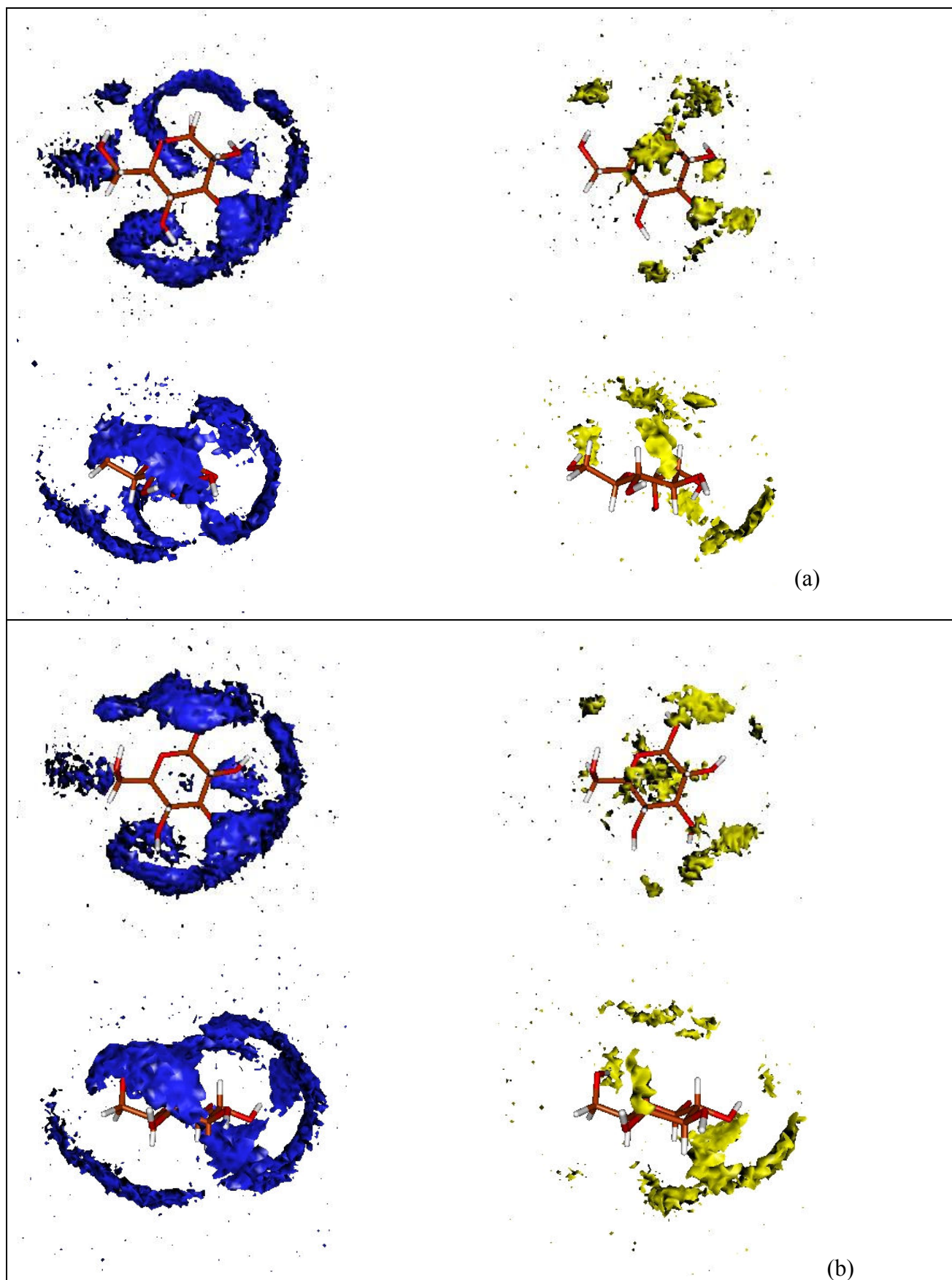


Figure S6. 2:1 H₂O/ACN mixture. Average radial distribution function, $g(r_{\text{HwCHs}})$, of the distance between water hydrogens and alkyl sugar hydrogens. (Right) Average radial distribution function, $g(r_{\text{HaCHs}})$, of the distance between ACN hydrogens and alkyl sugar hydrogens. (black) α -glucose; (red) β -glucose; (green) α -talose; (blue) β -talose.



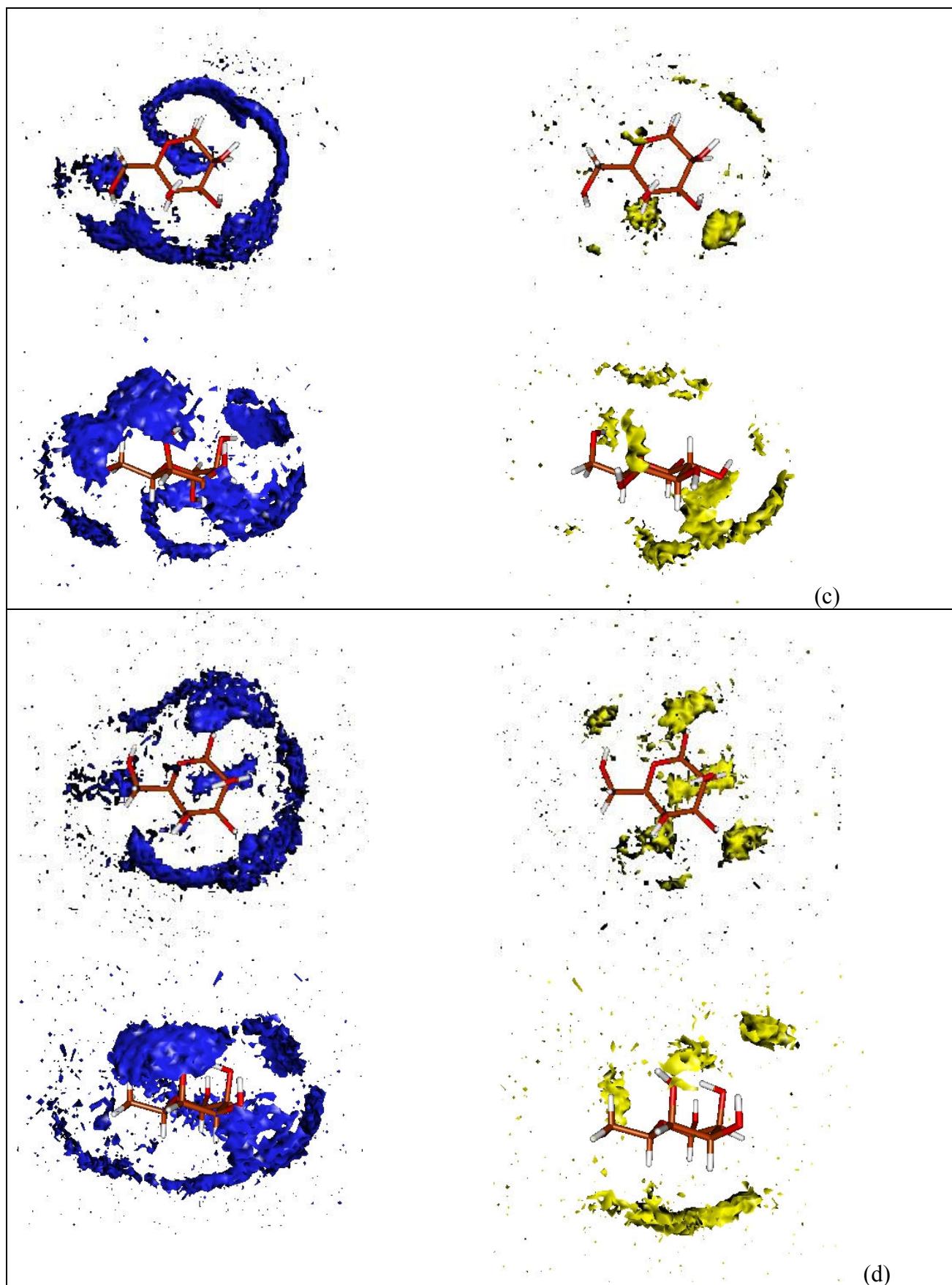


Figure S7. Spatial density functions (isovalue = 8.0) of the probability to find a water oxygen (blue) and ACN nitrogen (yellow) around (a) α -glucose; (b) β -glucose; (c) α -talose; (d) β -talose. For each panel we show the top and the side view.