

# CytoCell: A Computational Study in Aqueous Solution and an Infrared Spectroscopic Structural Characterization

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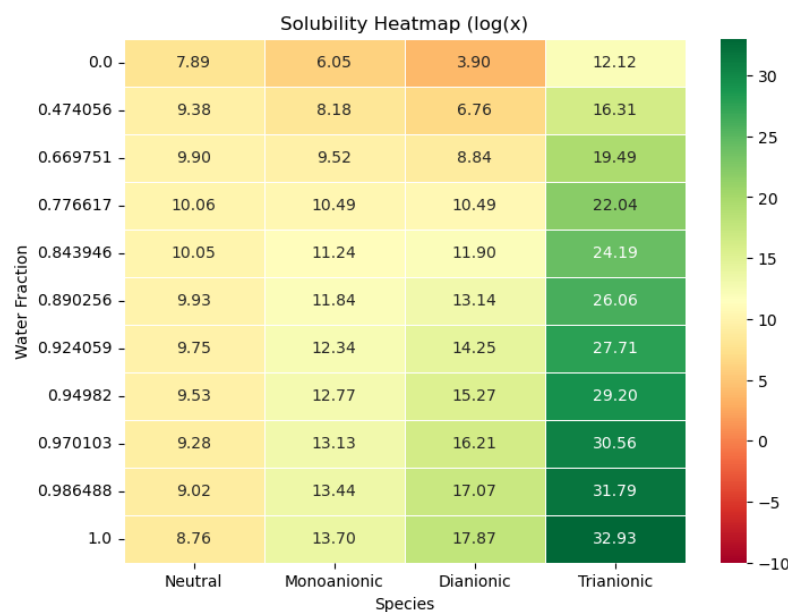
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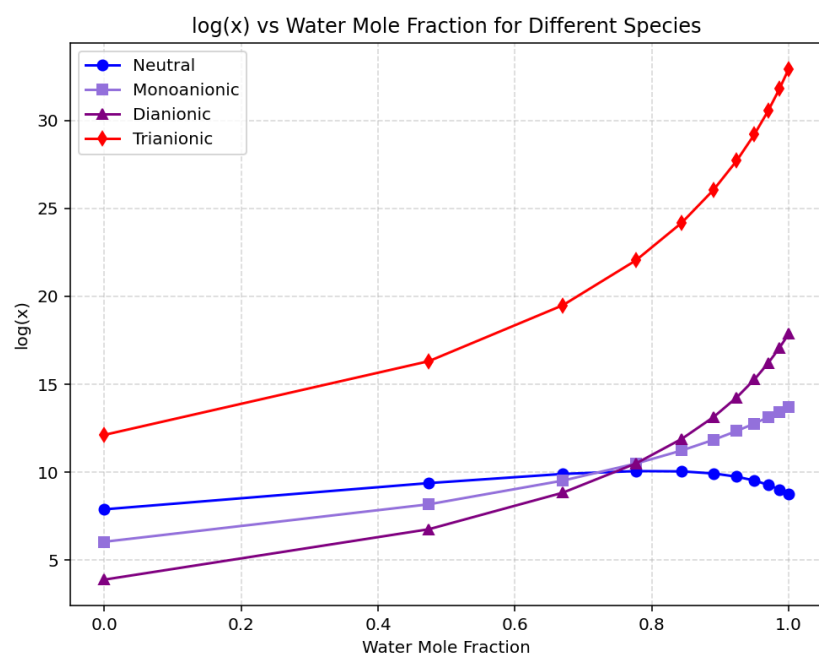
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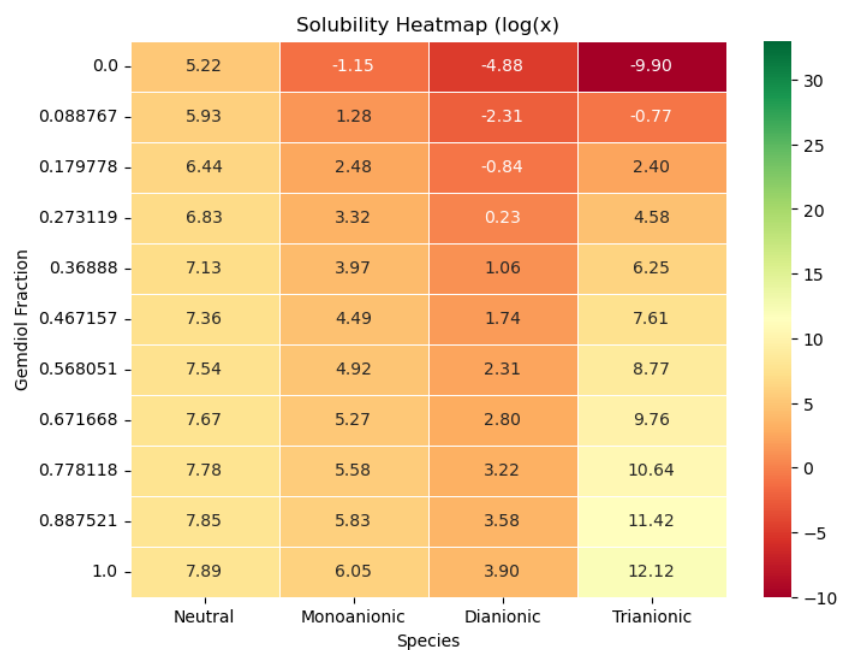
## Supplementary Information



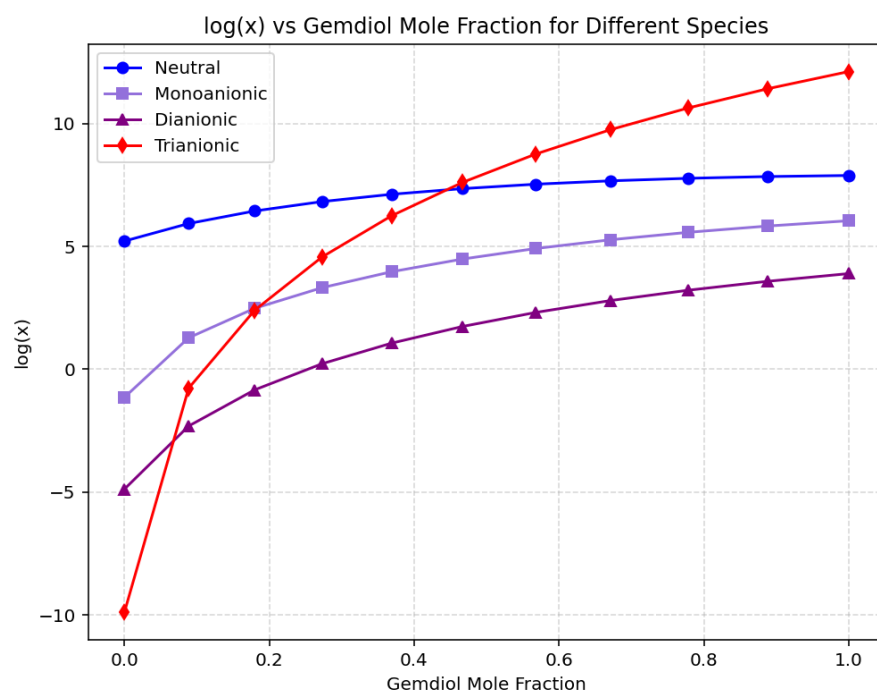
**Figure S1.** Heatmap of solubility vs. water fraction for the neutral, monoanionic, dianionic and trianionic structures in a Water-Gemdiol mixture.



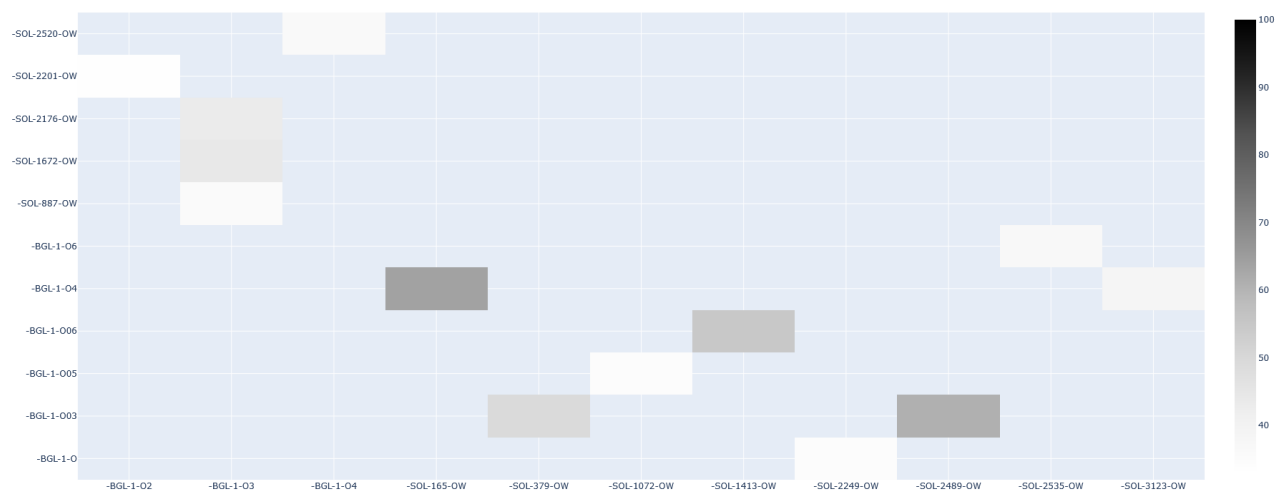
**Figure S2.** Evolution of solubility as a function of water mole fraction for the neutral, monoanionic, dianionic and trianionic structures in a Water-Gemdiol mixture.



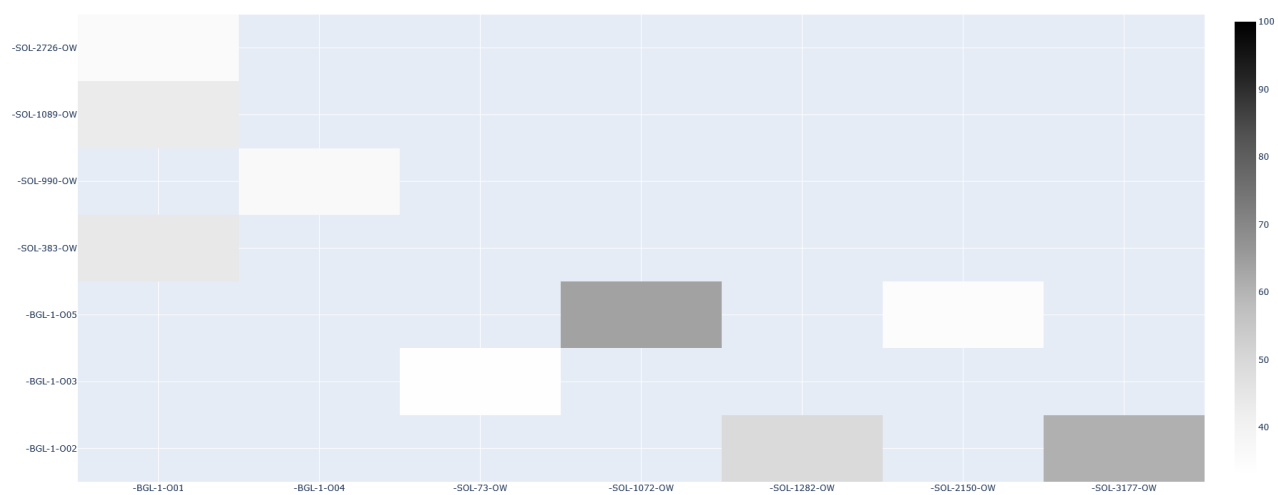
**Figure S3.** Heatmap of solubility vs. Gemdiol fraction for the neutral, monoanionic, dianionic and trianionic structures in a gemdiol-Cyrene mixture.



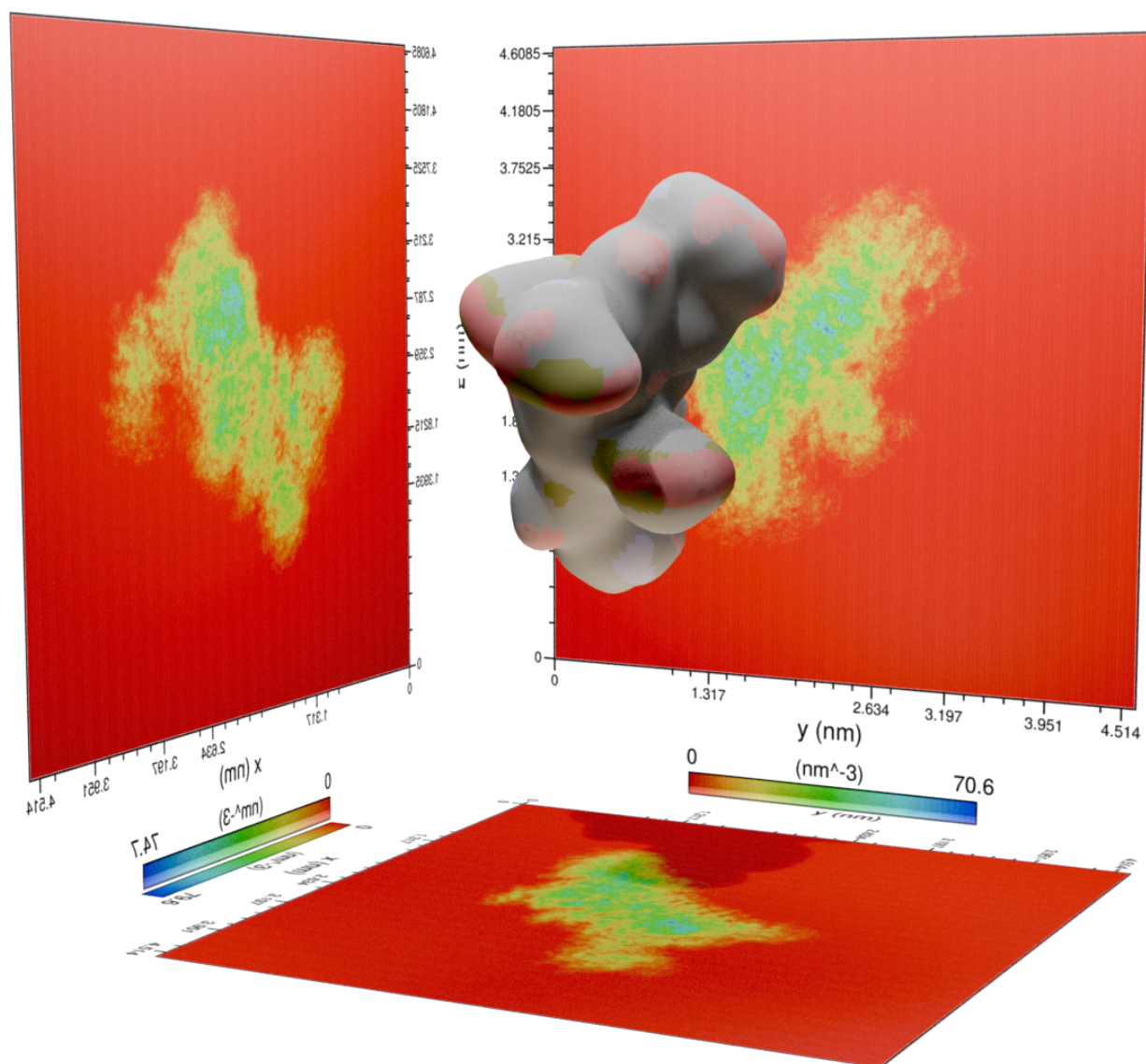
**Figure S4.** Evolution of solubility as a function of Gemdiol mole fraction for the neutral, monoanionic, dianionic and trianionic structures in a Gemdiol-Cyrene mixture.



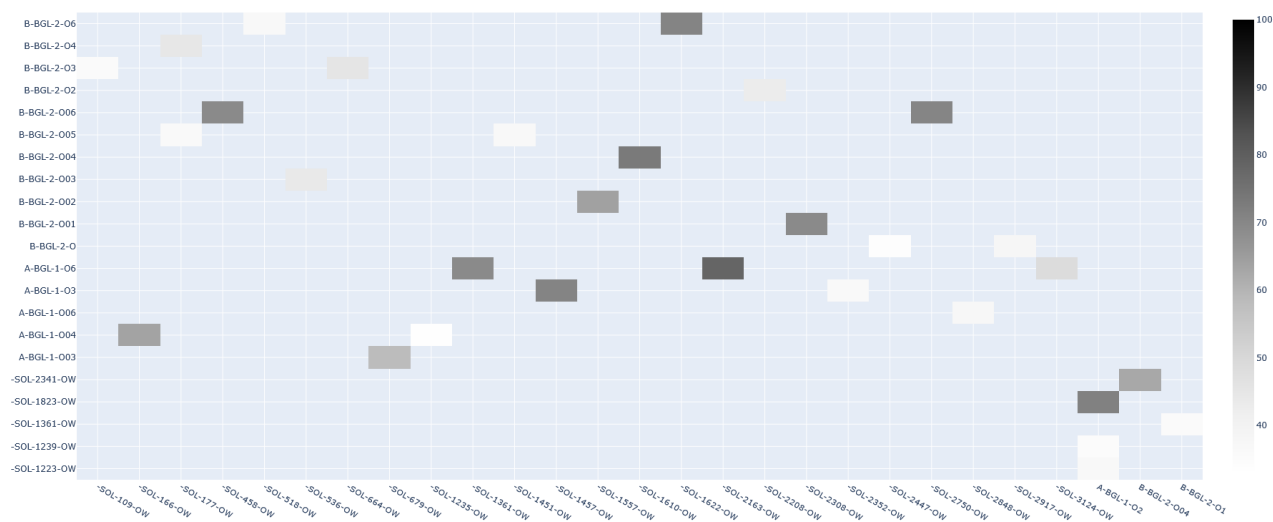
**Figure S5.** Matrix of H-bonds between the oligosaccharide and water molecules.



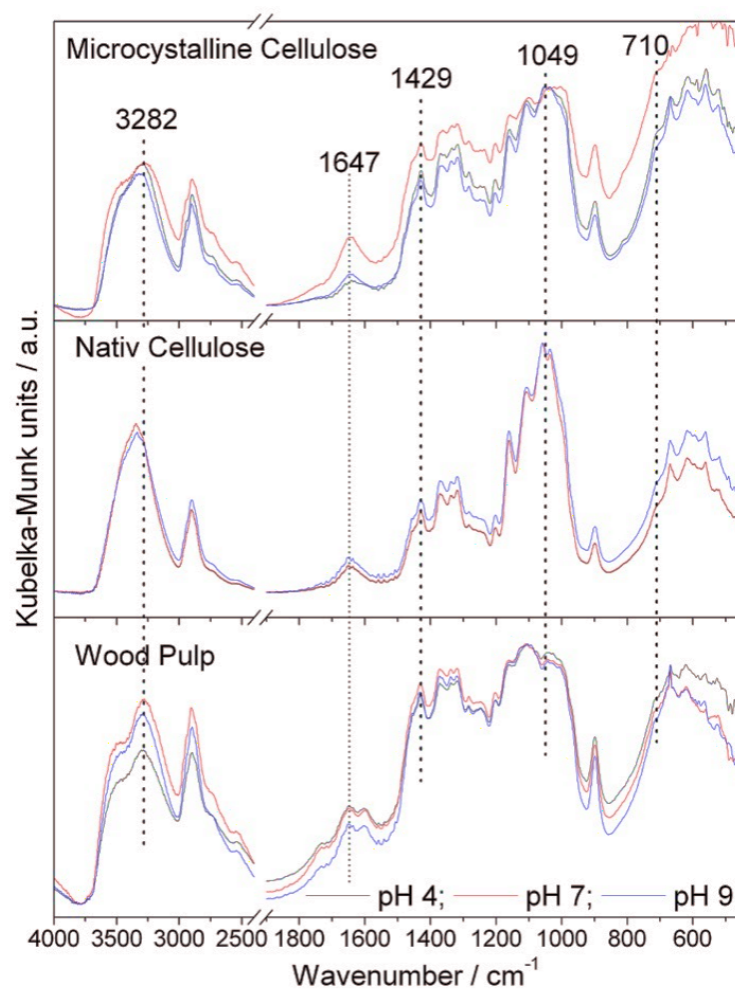
**Figure S6.** Matrix of H-bonds between the citrate groups and water molecules.



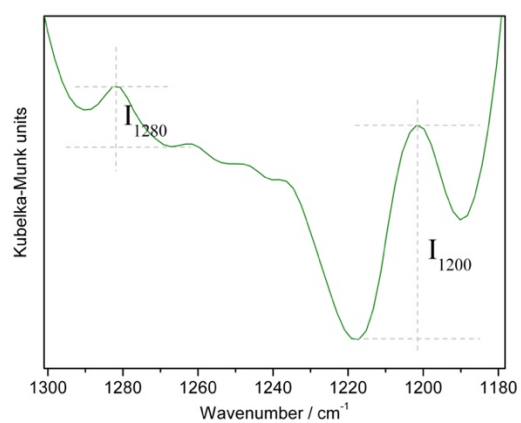
**Figure S7.** 3D representation of the system B suprastructure (Connolly surface).



**Figure S8.** Matrix of H-bonds between the two oligosaccharide and water molecules.



**Figure S9.** DRIFT spectra of cellulose and wood pulp after swelling and solvent evaporation at different pH values. Spectra were normalized to the maxima.



**Figure S10.** Microcrystalline cellulose DRIFT spectra in the region 1300-1180  $\text{cm}^{-1}$ , band intensity used for calculating crystallinity.