

Electronic Supplementary Information

Synthesis, molecular dynamics simulations, and biology of a carba-analogue of the trisaccharide repeating unit of *Streptococcus pneumoniae* 19F capsular polysaccharide[†]

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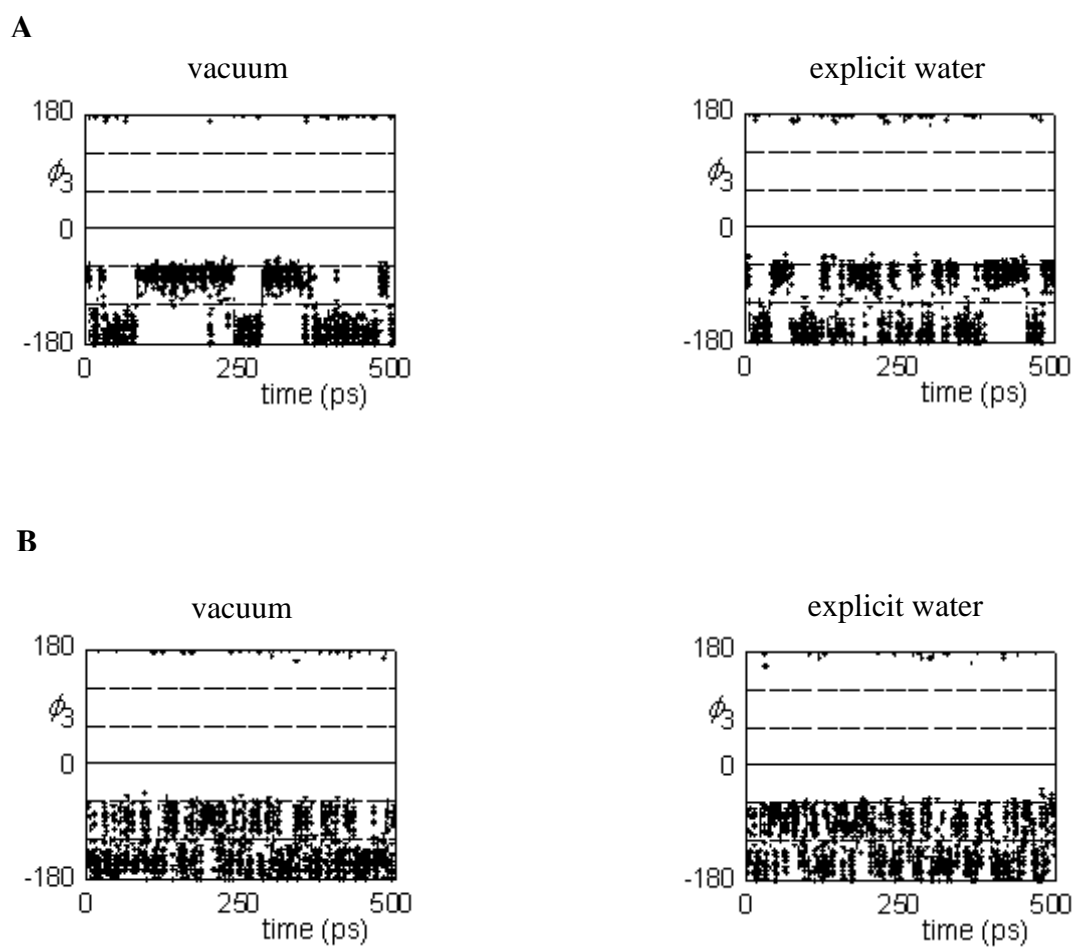


Figure S1 History of ϕ_3 from the MD simulations of the monosaccharide substructures, α -L-Rhap-1-OPO₃H₂ (**A**) and the corresponding carba analogue (**B**), in vacuum (left) and using explicit water as solvent (right).

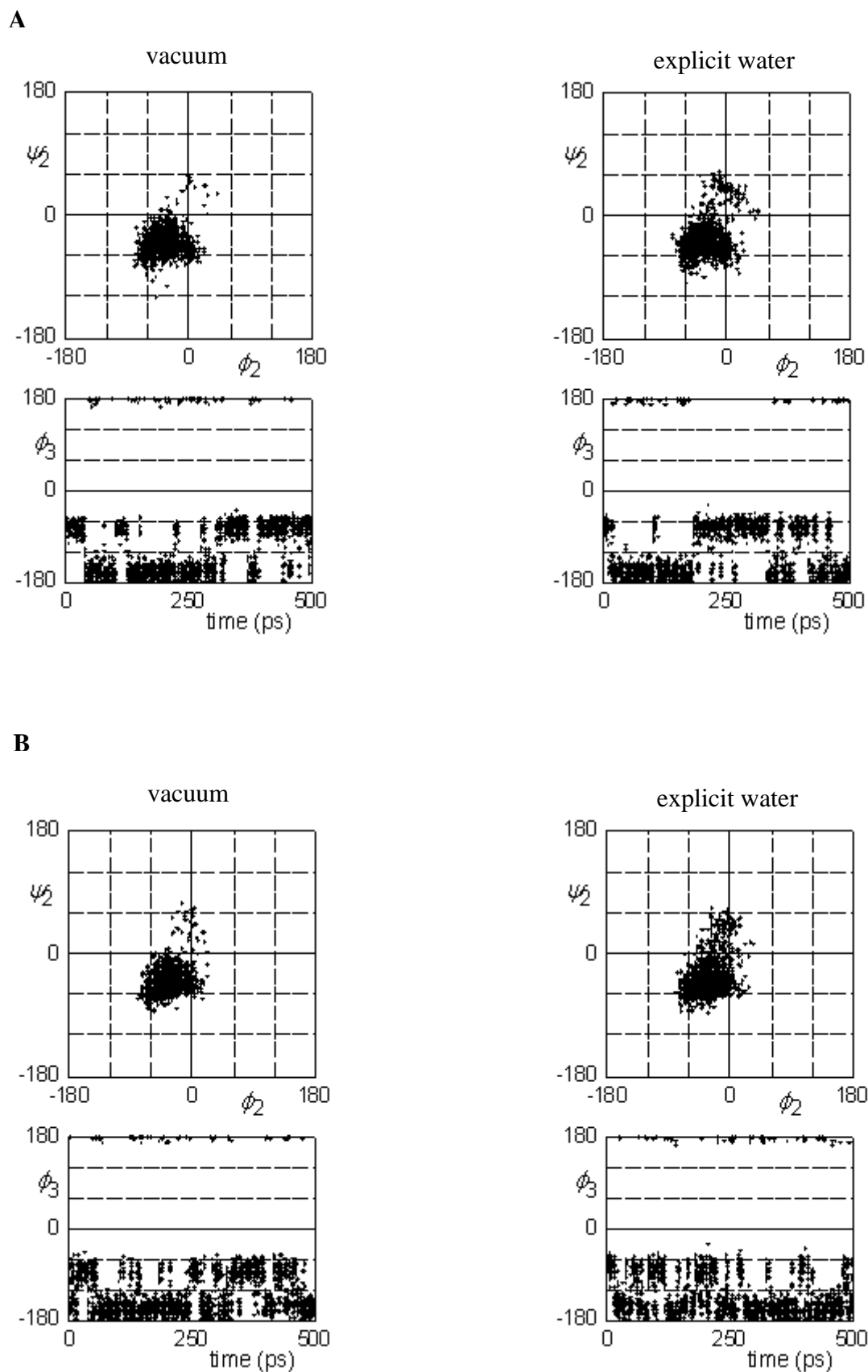


Figure S2 Scatter plots on the ϕ_2/ψ_2 map and history of ϕ_3 from the MD simulations of the disaccharide substructures, α -D-Glcp-(1 \rightarrow 2)- α -L-Rhap-1-OPO₃H₂ (**A**) and the corresponding carba analogue (**B**), in vacuum (left) and using explicit water as solvent (right).

