Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

The systematic influence of solvent on the conformational features of furanosides

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Supporting Information

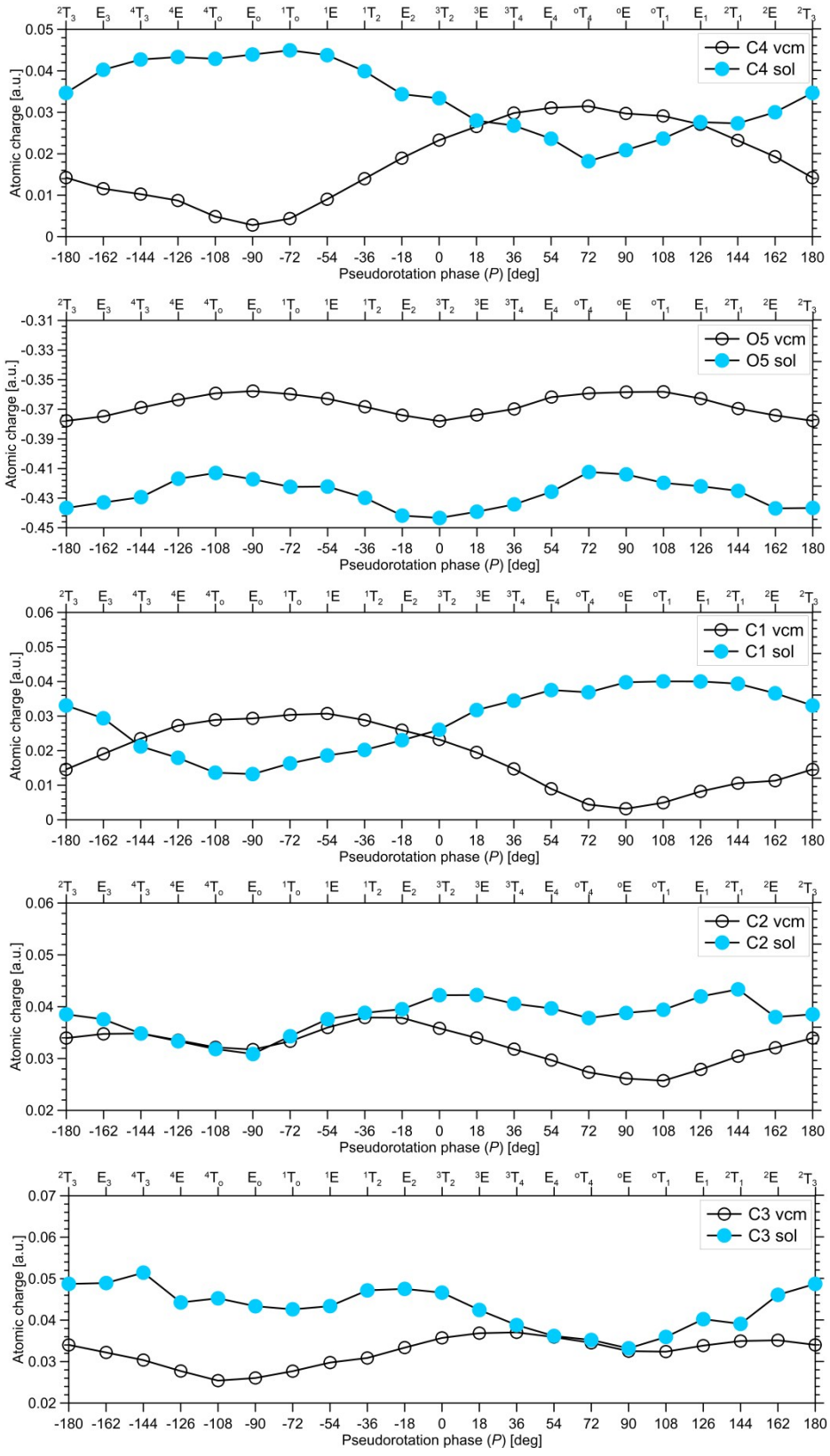

Fig. S1. The average atomic charges calculated for all heavy atoms in the THF molecule by using the Mulliken method [(Mulliken 1955)] in vacuum (white dots) or in aqueous solvent (blue dots). The structures used for calculations included all frames of the unbiased MD trajectories generated within the BP86/def2-SVP potential (see main manuscript for details).

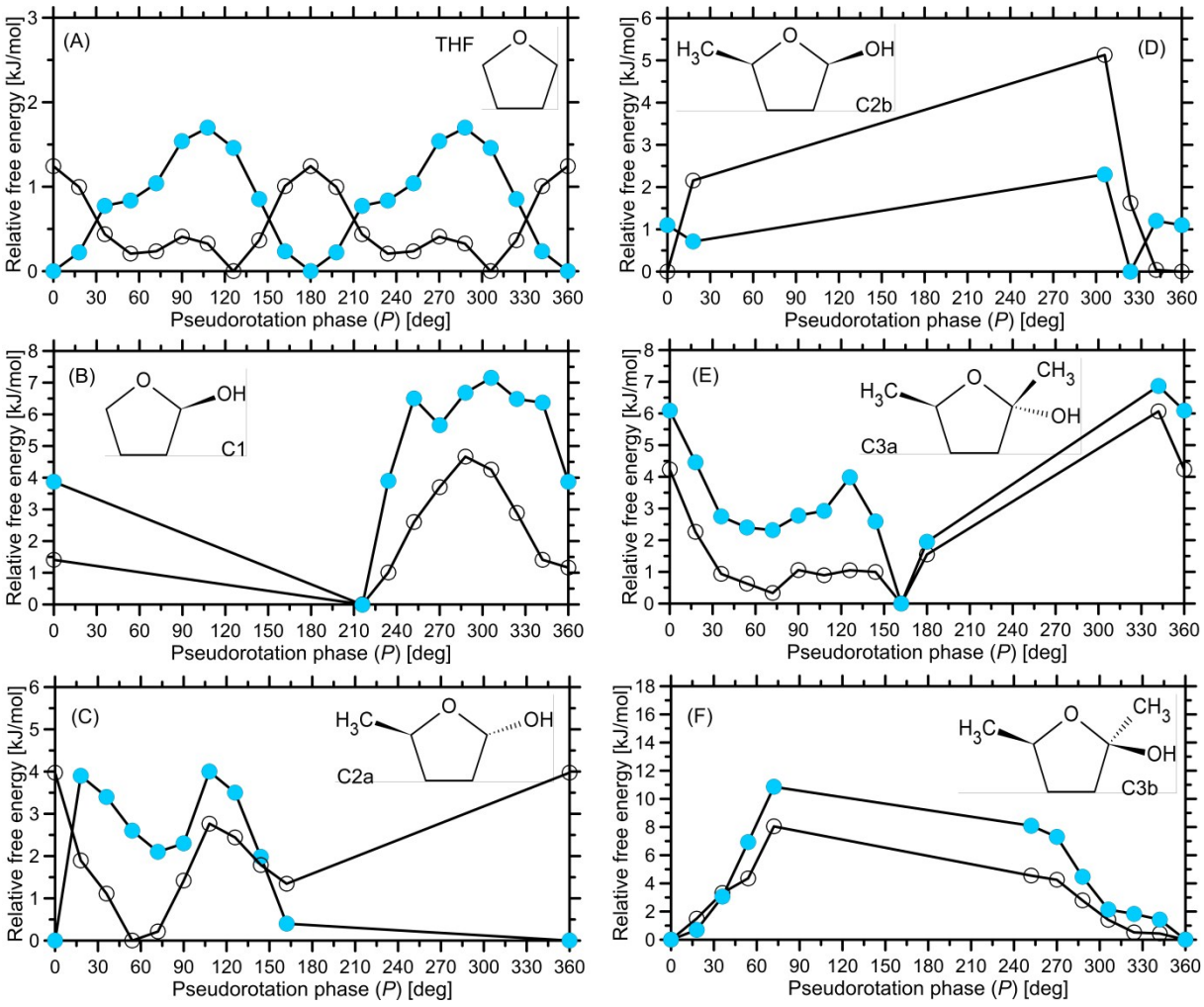

Fig. S2. The comparison of the pseudorotation-characteristic free energies calculated from QM/MM-MD simulations for different furanosides in vacuum (white dots) or in aqueous solvent (blue dots). The calculations relied on the BP86/def2-SVP potential (see details in the main manuscript). The energies are scaled to zero according to their lowest value.

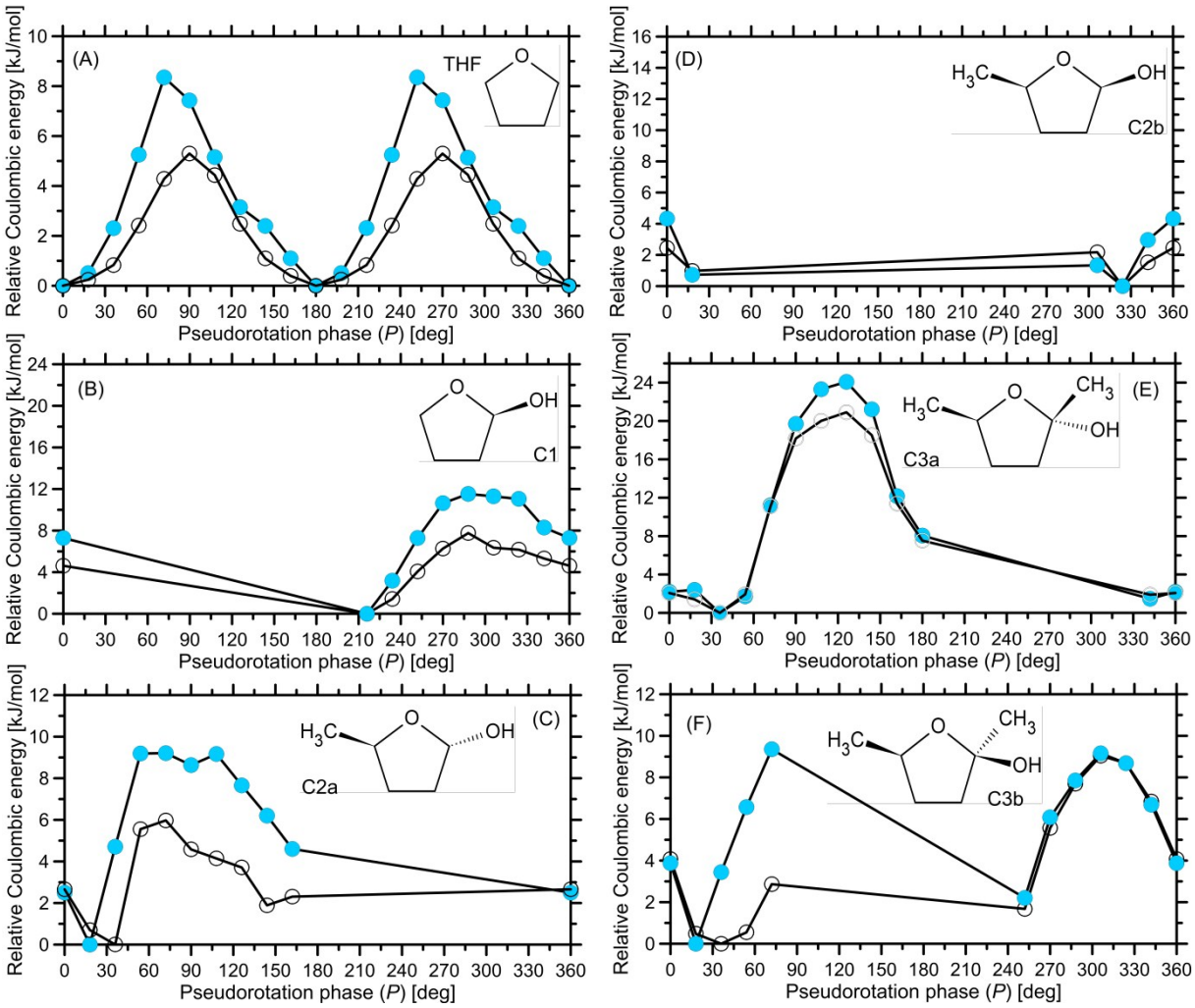

Fig. S3. The comparison of the pseudorotation-characteristic Coulombic energies calculated for all charge-charge interactions that may occur within furanoside ring. The charges used for calculations were obtained by applying the Mulliken method and averaged over all frames of the unbiased QM/MM-MD simulation. They corresponded to the two different cases, i.e. furanosides in vacuum (white dots) or in aqueous solvent (blue dots). The energies are scaled to zero according to their lowest value.

References

Mulliken, R. S., *J. Chem. Phys.***1955**, *23,* 10, 1833–1840.
Wu, A.; Cremer, D. *Int. J. Mol. Sci.* **2003**, 4, 158-192.