**Simulation of Raman optical activity**

of multi-component monosaccharide samples

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**Fig. S1.** Relative potential energy distributions

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**Fig. S1.** Calculated (B3LYP/6-311++G***/CPCM) relative potential energy distributions (PED) of selected stretching (ν), bending (δ), and torsion (τ) coordinates in DG vibrations.
Fig. S2. Example of a cluster of α-D-glucose with water molecules, and dependence of ROA spectral error (in %) on the number of averaged snapshots, preselected from 1000 ones by the parallel variable selection approach (J. Kessler, M. Dračínský and P. Bouř, J. Comput. Chem., 2012, 34, 366-371).
Fig. S3. Comparison of selected torsional angles as obtained by MD and DFT computations, for $\alpha$-DM (left) and $\beta$-DM (right). MD probability histograms (black line) were obtained during 10 ns simulations with the GLYCAM06 force field. The DFT distribution bars (red, in arbitrary scale) were obtained from the B3LYP/6-311++G**/CPCM conformational scan and Boltzmann weighting.
Fig. S4. Experimental Raman and ROA spectra of DG and DM mixtures.