Supporting Information

The effects of self-aggregation on the vibrational circular dichroism and optical rotation measurements of glycidol

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TABLE S1. The relative Gibbs free energies Δ*G* (kcal/mol) and the normalized Boltzmann factor B_f at 298.15K based on the relative Gibbs free energy of the ternary glycidol conformers at the B3LYP/6-31G* level of theory.

Trimer	ΔG (kcal/mol)	B_f (%)
T1	0	81.07
T2	1.128	12.07
T3	1.867	3.47
T4	2.082	2.41
T5	2.972	0.54
T6	3.074	0.45

Fig. S1 Optimized geometries of the six lowest energy conformers of the glycidol trimer at the B3LYP/6-31G* level of theory.

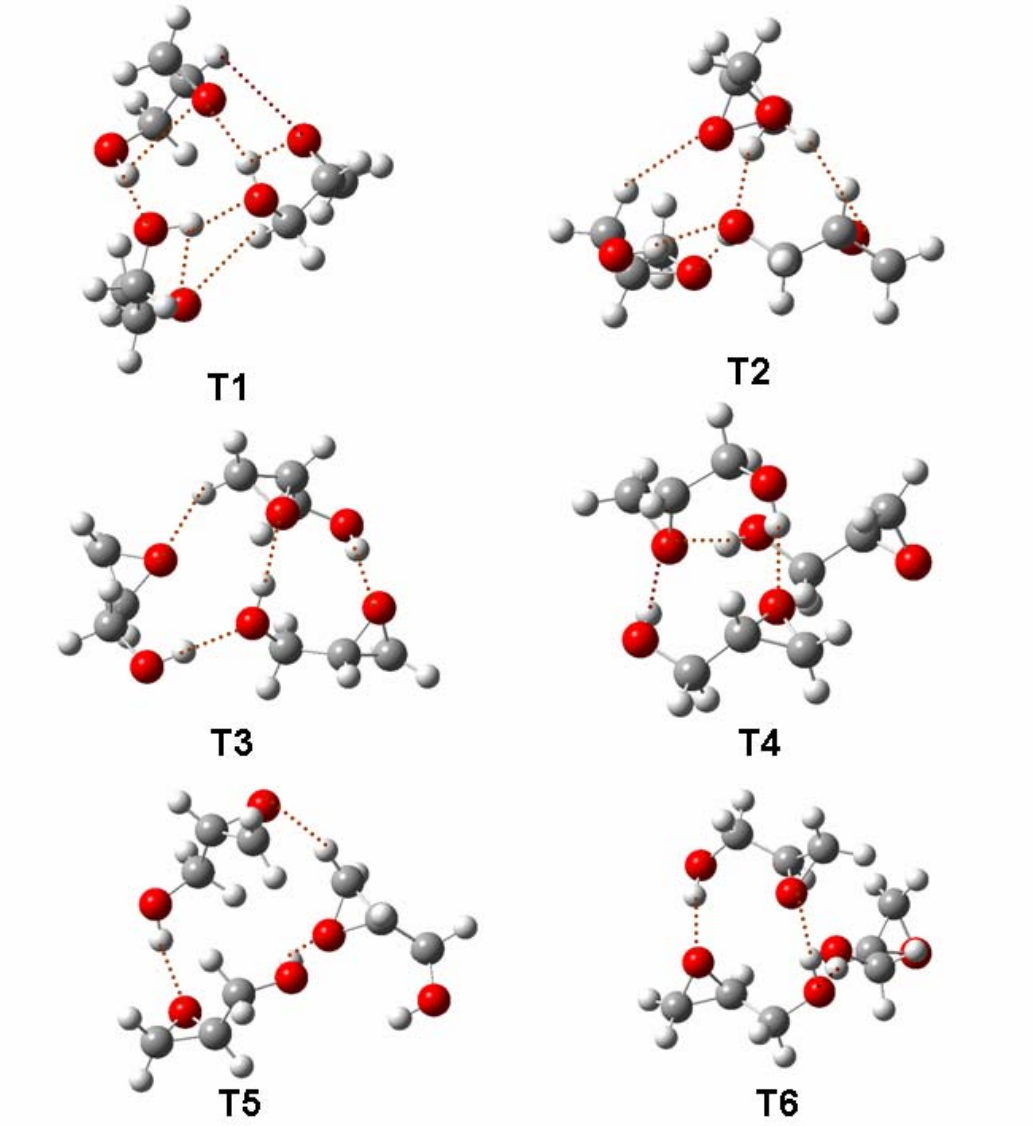

Fig. S2 Calculated VA and VCD spectra of the conformers of the glycidol monomer and dimer, that are not included in the text, at the B3LYP/6-311++G** level of theory.

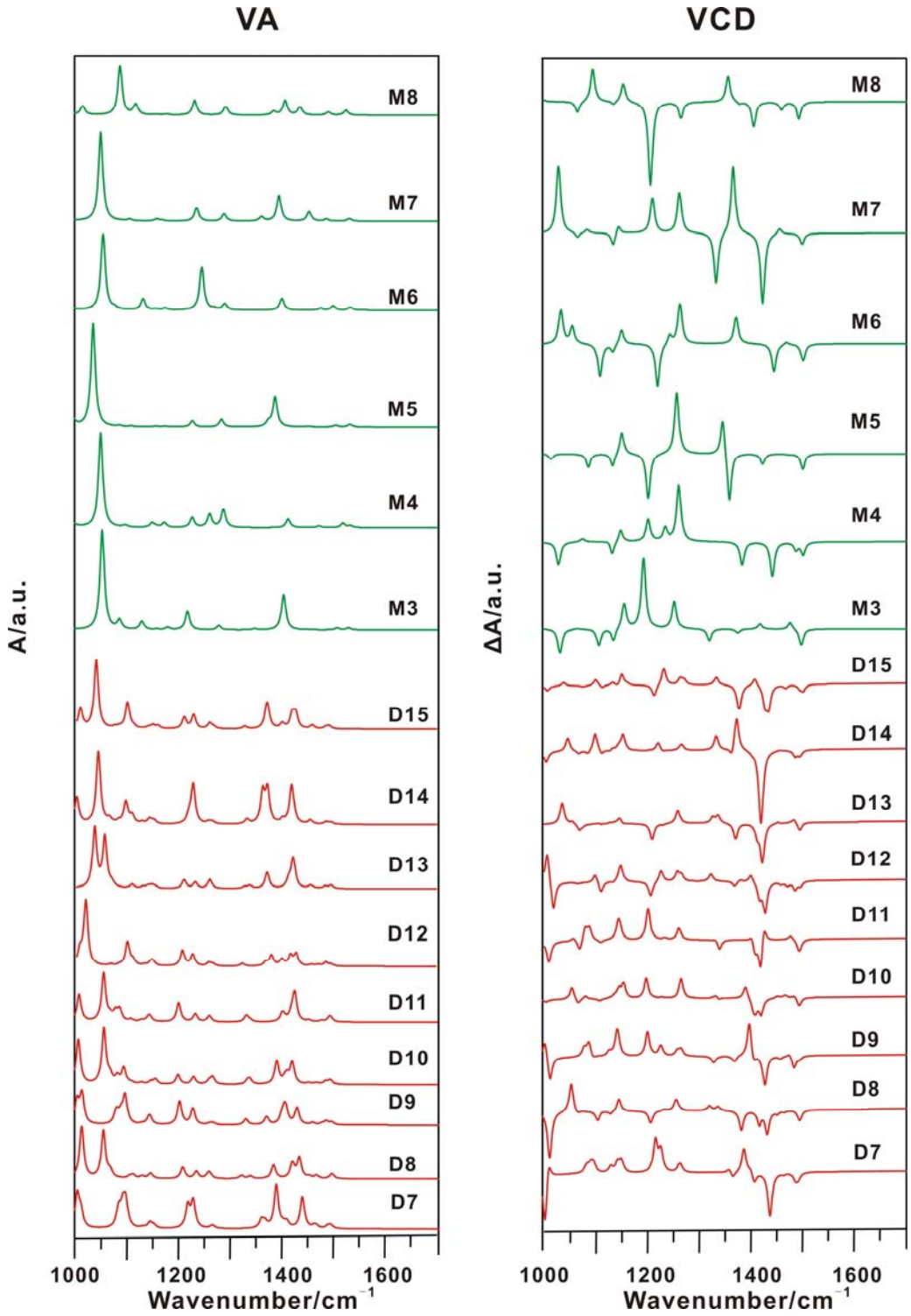

Fig. S3 Calculated VA and VCD spectra of the six lowest energy conformers of the glycidol trimer at the B3LYP/6-31G* level of theory.

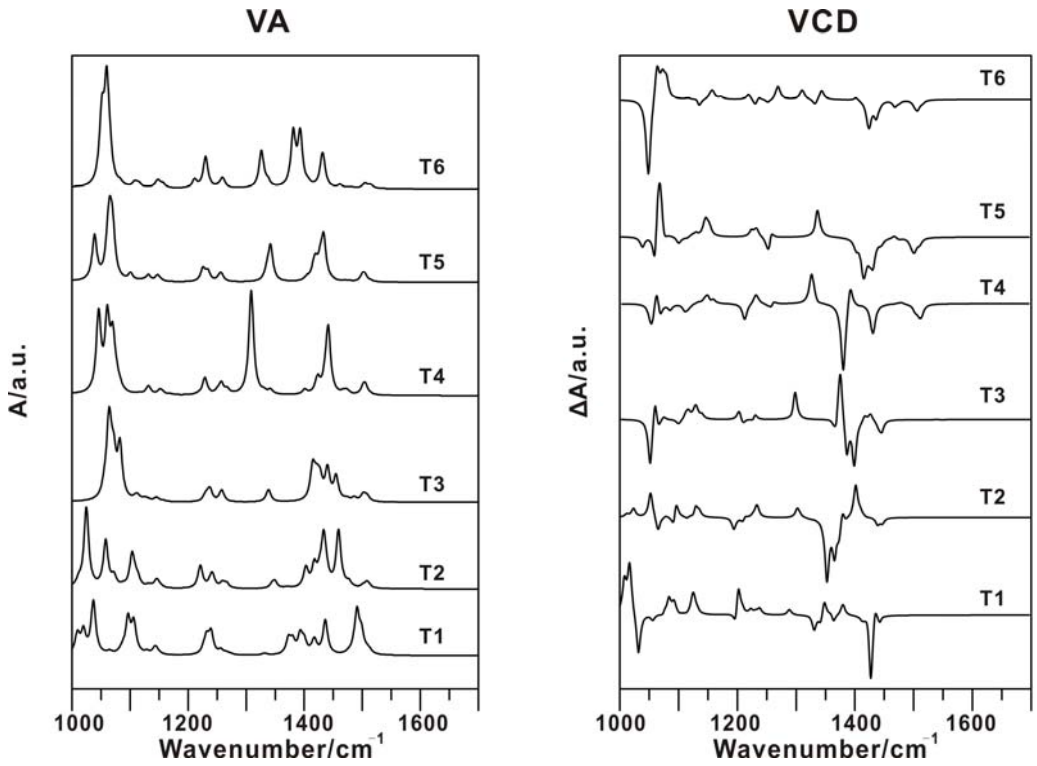

Fig. S4 Calculated VA and VCD (right) spectra for **M1** and **M2** in vacuum (black line) and with IPCM model for $CDCl_3$ (red line) at the B3LYP/6-311++G** level of theory