Supporting information

Table SI1 Boltzmann weights (%) for B3LYP/6-31G* and B3LYP/cc-pVDZ for 3*S*1'***R-1***.

Conformer	W (cc-pVDZ)	W (6-31G*)
1	4.062	1.848
2	10.042	3.527
3	10.042	6.733
4	4.932	2.724
5	2.756	1.427
6	2.584	1.254
7	5.987	2.244
8	5.987	2.244
9	5.261	3.527
10	4.932	3.527
11	2.271	1.848
12	5.613	3.763
13	3.137	1.732
14	5.613	1.522
15	2.94	1.732
16	5.613	6.733
17	1.643	1.522
18	3.137	3.1
19	4.062	20.205
20	2.756	1.427

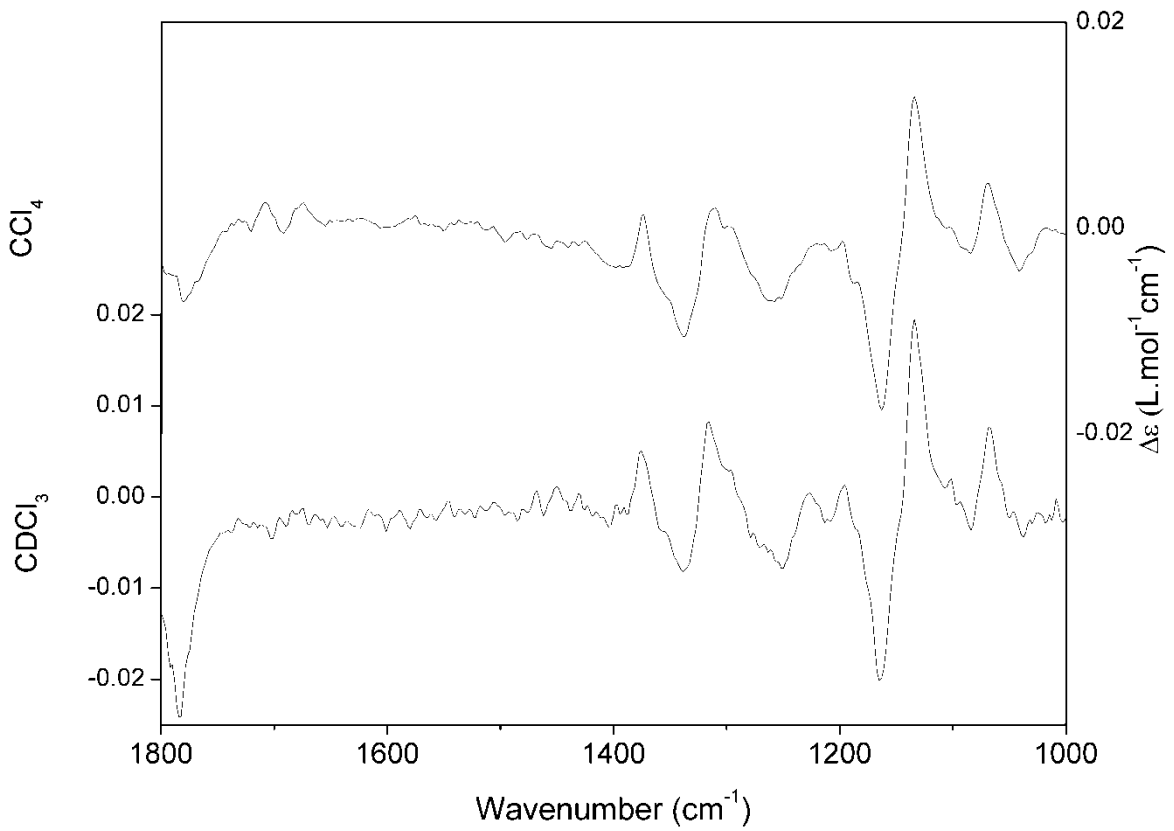

Fig. SI1 Experimental spectra for ***1*** in $CDCl_3$ and CCl_4. Apart from some details and baseline position no differences can be seen, showing that solvent effects are of minor importance for the molecule under study.

Table SI2 Similarity measure $\sum_{fg}$ of the VCD-spectra of 6 conformers of 3*S*1'*S*-***1***, in %, for the region 1000cm^{-1} to 1500 cm^{-1}. Conformers of the same class have a fairly large similarity index, whereas conformers of different classes show less similarity. This proves that the spectral features in this region are also dependent on the hydroxyethyl dihedral angle, although to a lesser extent than for 3*S*1'*R*-***1***.

	1 (b)	**2 (b)**	**3 (b)**	**4 (a)**	**7 (a)**	**8 (a)**
1 (b)	100	72	76	40	47	47
2 (b)	72	100	54	21	43	23
3 (b)	76	54	100	33	32	56
4 (a)	40	21	33	100	77	73
7 (a)	47	43	32	77	100	74
8 (a)	47	23	56	73	74	100

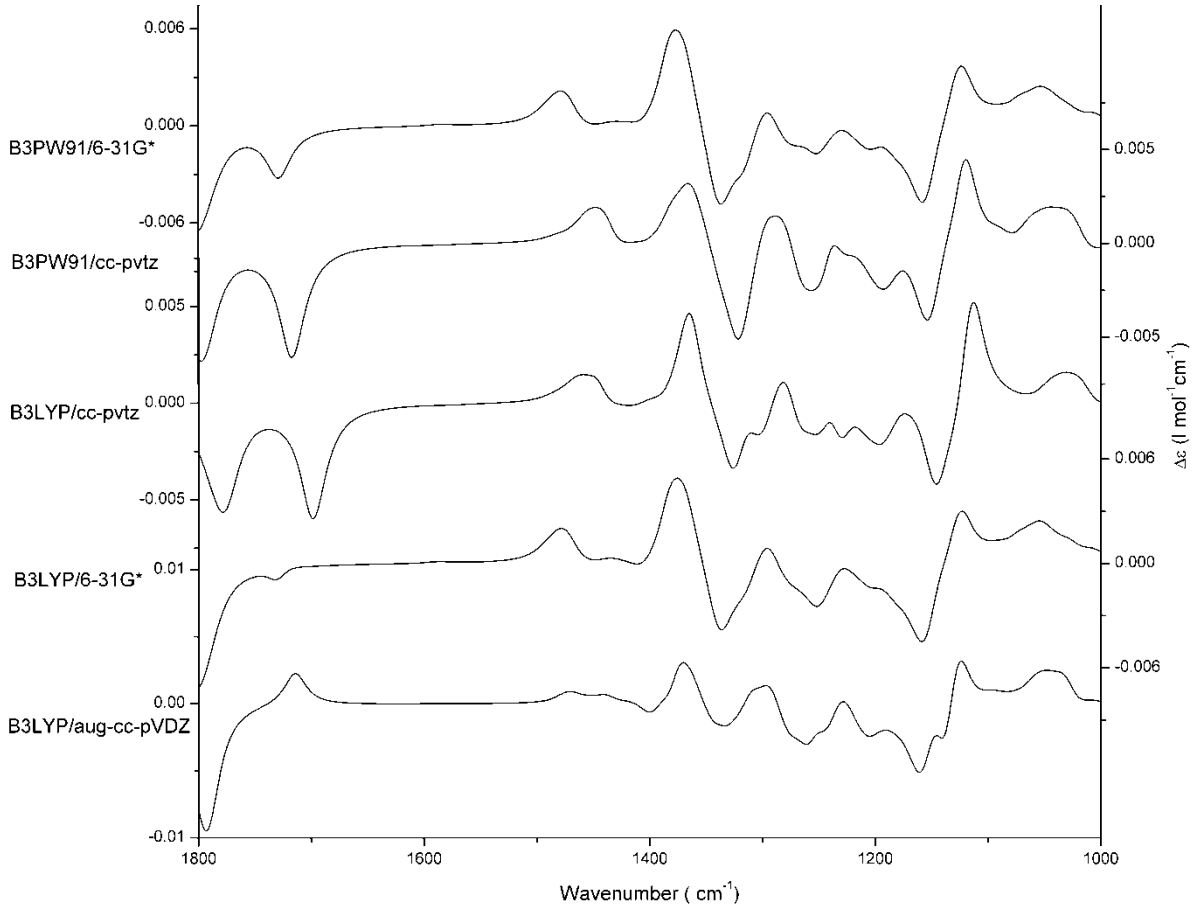

Fig. SI2 Boltzmann weighted, Lorentzian broadened VCD spectra for 3*S*1'*R*-1 on 5 different levels of theory. Visual inspection as well as numerical data (Table SI3) suggest that little to no sign changes occur when going from one level of theory to another.

Table SI3 Similarity of the calculated VCD-spectra on different levels of theory compared to the B3LYP/aug-cc-pVDZ/PCM level of theory used in the article. The data show a very high similarity between levels of theory.

Functional	Basis set	Σ_{max}
B3LYP	6-31G*	85.1
	cc-pVTZ	73.2
	aug-cc-pVDZ	90.6
B3PW91	6-31G*	79.8
	cc-pVTZ	76.4

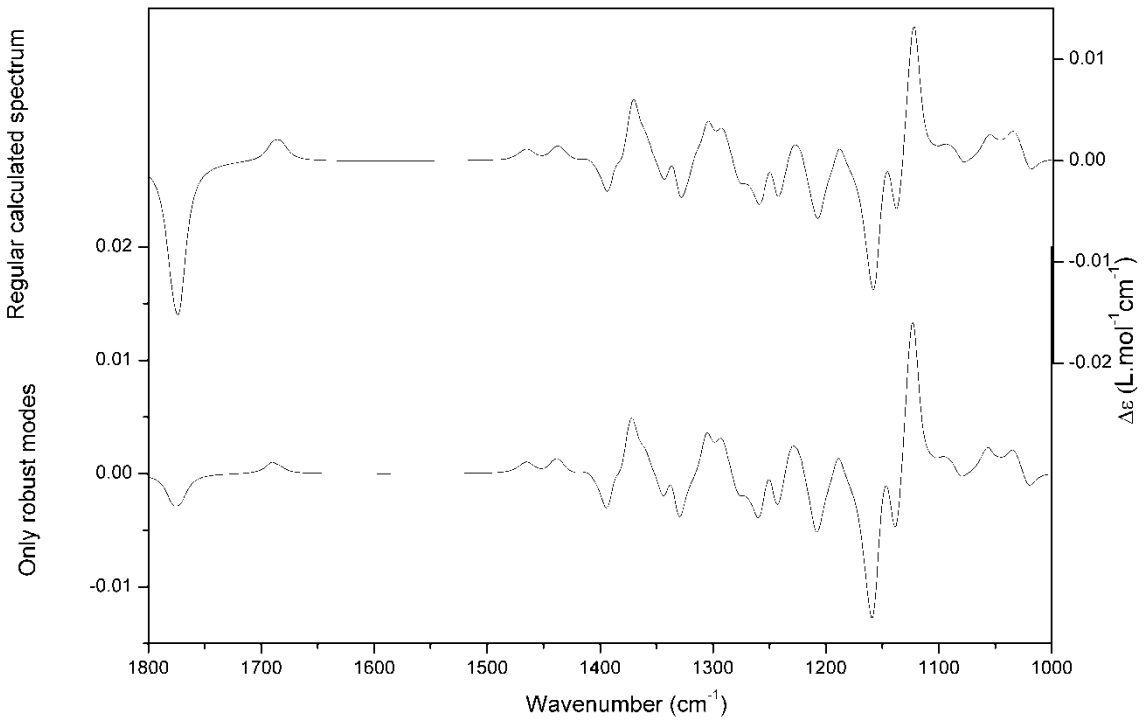

Fig. SI3 VCD spectra for 3S1'R-***1*** generated as usual (upper) and with non-robust modes left out (lower).

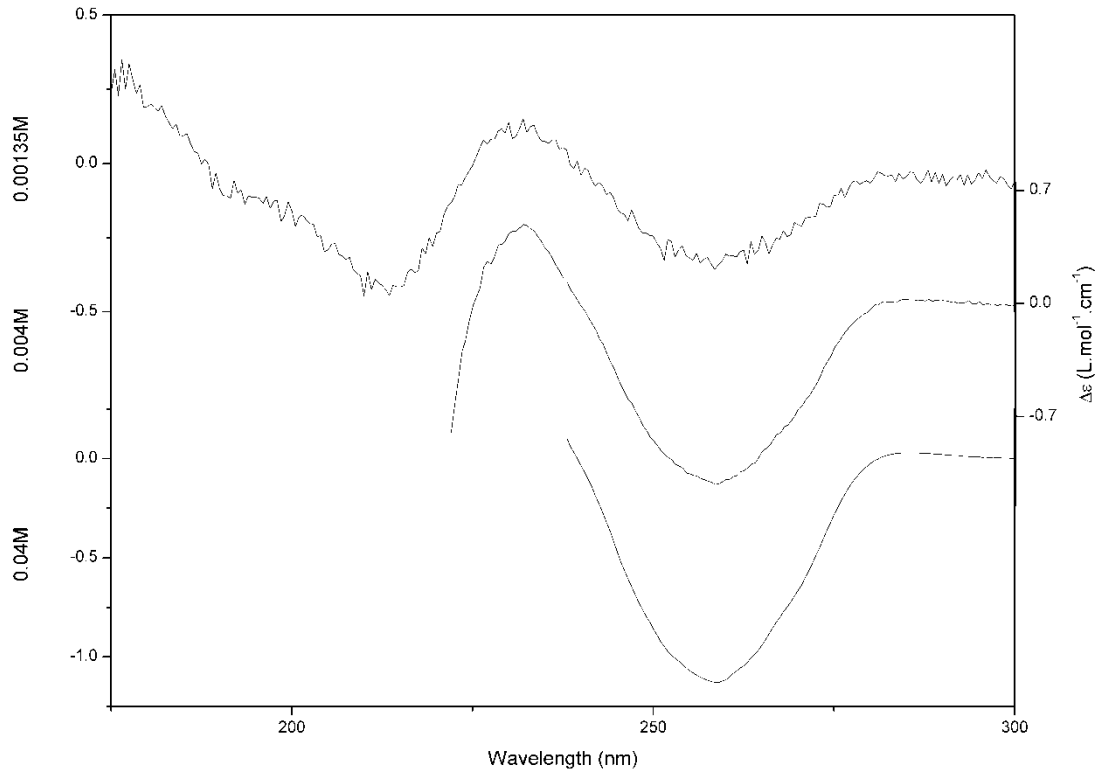

Fig. SI4 ECD-spectra measured for low (top), medium (middle) and high (bottom) concentration. Increasing the concentration vastly improves S/N but yields spectra in a limited spectral range.