Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Effect of Puckering Motion and Hydrogen Bond Formation on the Vibrational Circular Dichroism Spectrum of a Flexible Molecule: the case of (S)-1-Indanol

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Supplementary Information

Table S1 Energetic and structural parameters of the most stable conformers of (S)-1-indanol in a CCl_4 continuum calculated at the BLYP/6-31G++(d,p) level

Geometry	Gibbs free energy (kcal/mol)	Boltzmann population (%)	$C_9C_4C_3C_2$ angle (°)	C_9C_1OH angle (°)
1eq	0.00	28	16.4	55.1
1ax	0.16	22	-12.7	44.9
2ax	0.64	10	-14.2	-54.6
3eq	0.56	11	16.0	-167.4
2eq	0.21	20	15.7	-77.4
3ax	0.67	9	-14.7	-176.0

Table S2 Energetic and structural parameters of the most stable conformers of (S)-1-indanol in a DMSO continuum calculated at the B3LYP-D3/6-31G++(d,p) level

Geometry	Gibbs free energy (kcal/mol)	Boltzmann population (%)	$C_9C_4C_3C_2$ angle (°)	C_9C_1OH angle (°)
1eq	0.00	35	17.4	54.9
1ax-a	0.05	31	-13.7	54.6
1ax-b	0.46	16	-15.5	48.7
1ax-c	0.57	13	-16.8	55.0
2ax	1.16	5	-15.6	-44.9

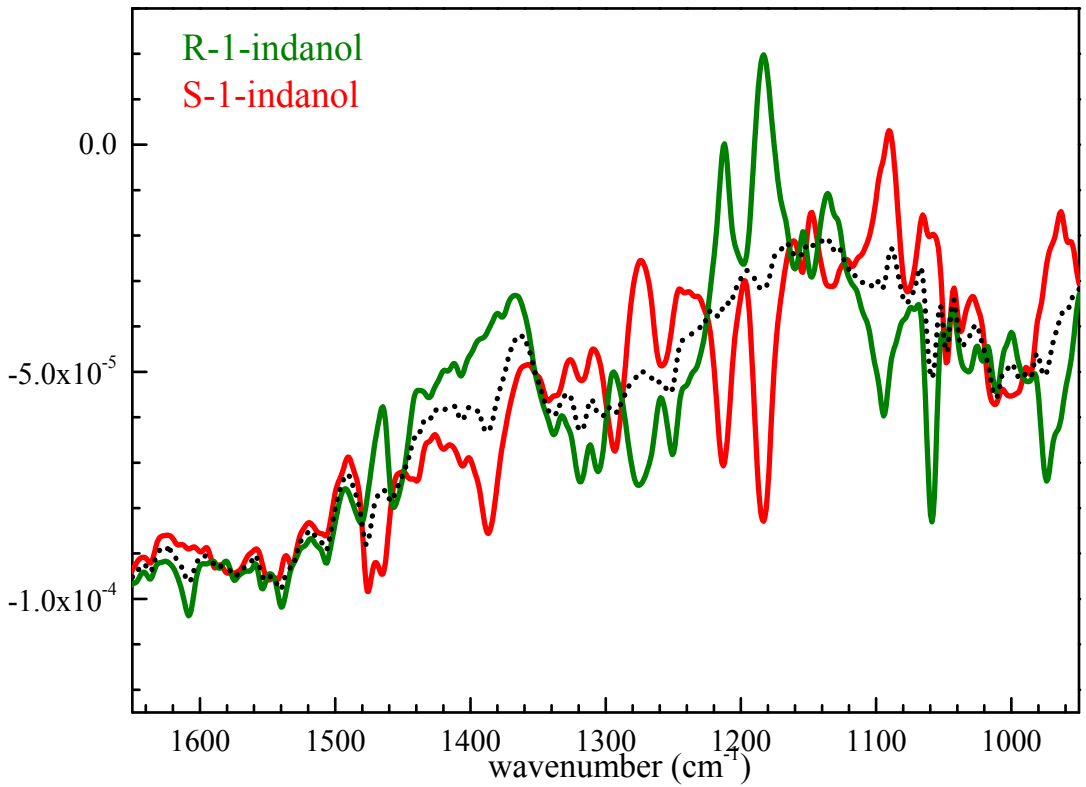

Figure S1: Raw experimental VCD spectra of R and S-1-Indanol together with the baseline (dotted line).

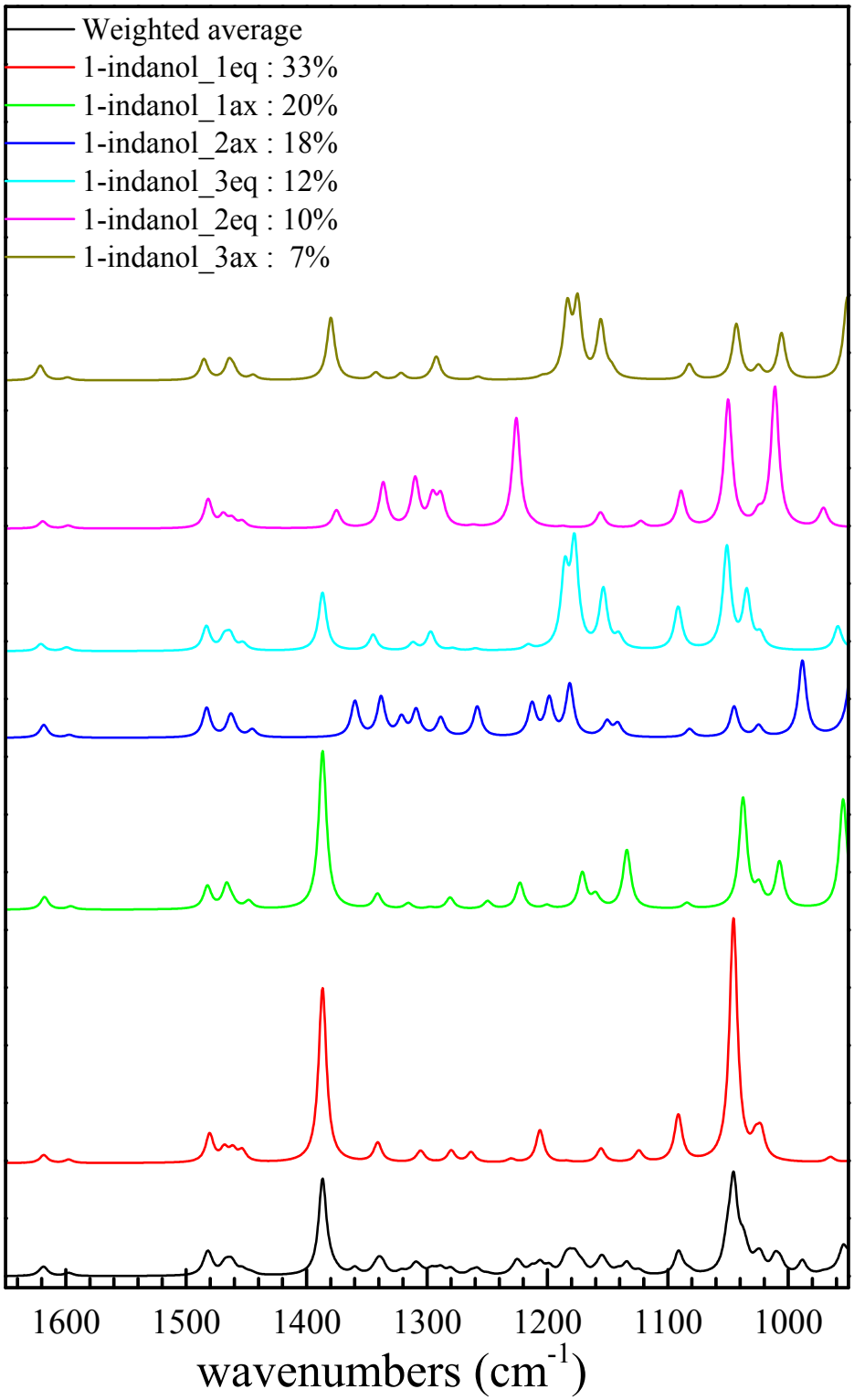

Figure S2: Simulated IR spectrum obtained from the weighted IR spectra of the most stable (S)-1-indanol structures in a CCl_4 continuum together with individual contributions, calculated at the B3LYP/6-31G++(d, p) level

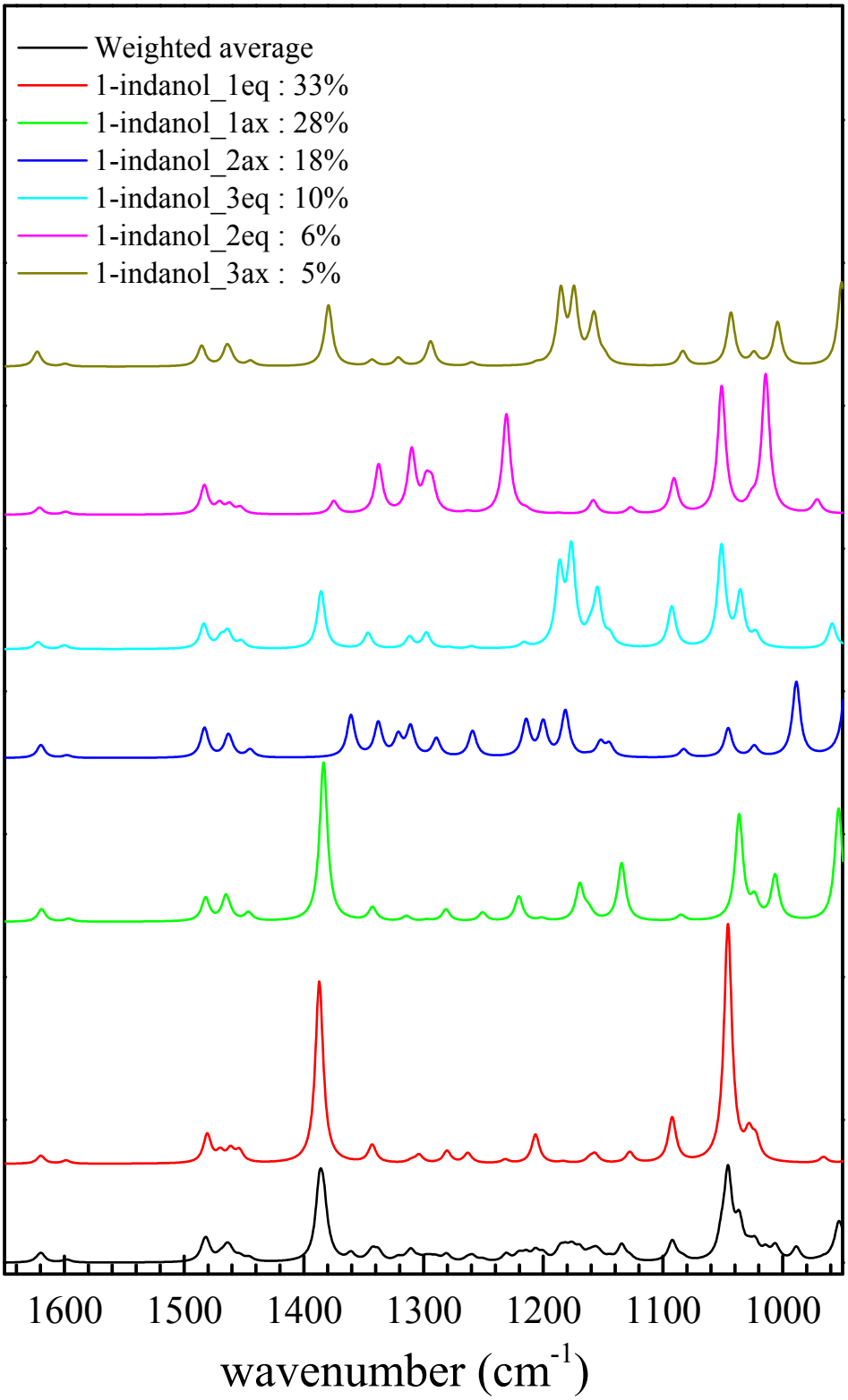

Figure S3: Simulated IR spectrum obtained from the weighted IR spectra of the most stable 1(S)-1-indanol structures in a CCl_4 continuum together with individual contributions, calculated at the B3LYP-D3/6-31G++(d, p) level

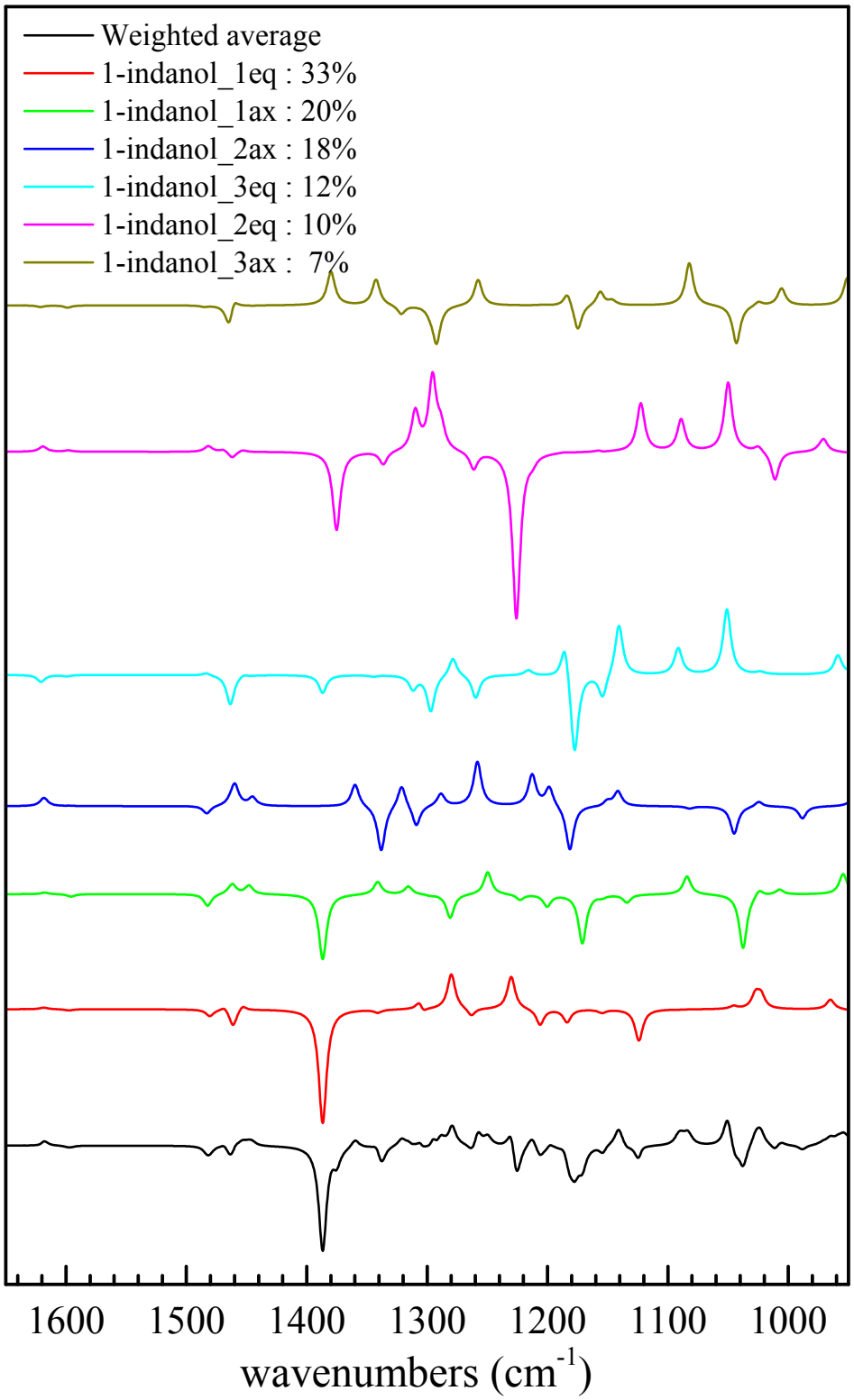

Figure S4: Simulated VCD spectrum obtained from the weighted VCD spectra of the most stable (S)-1-indanol structures in a CCl_4 continuum together with individual contributions, calculated at the B3LYP/6-31G++(d, p) level

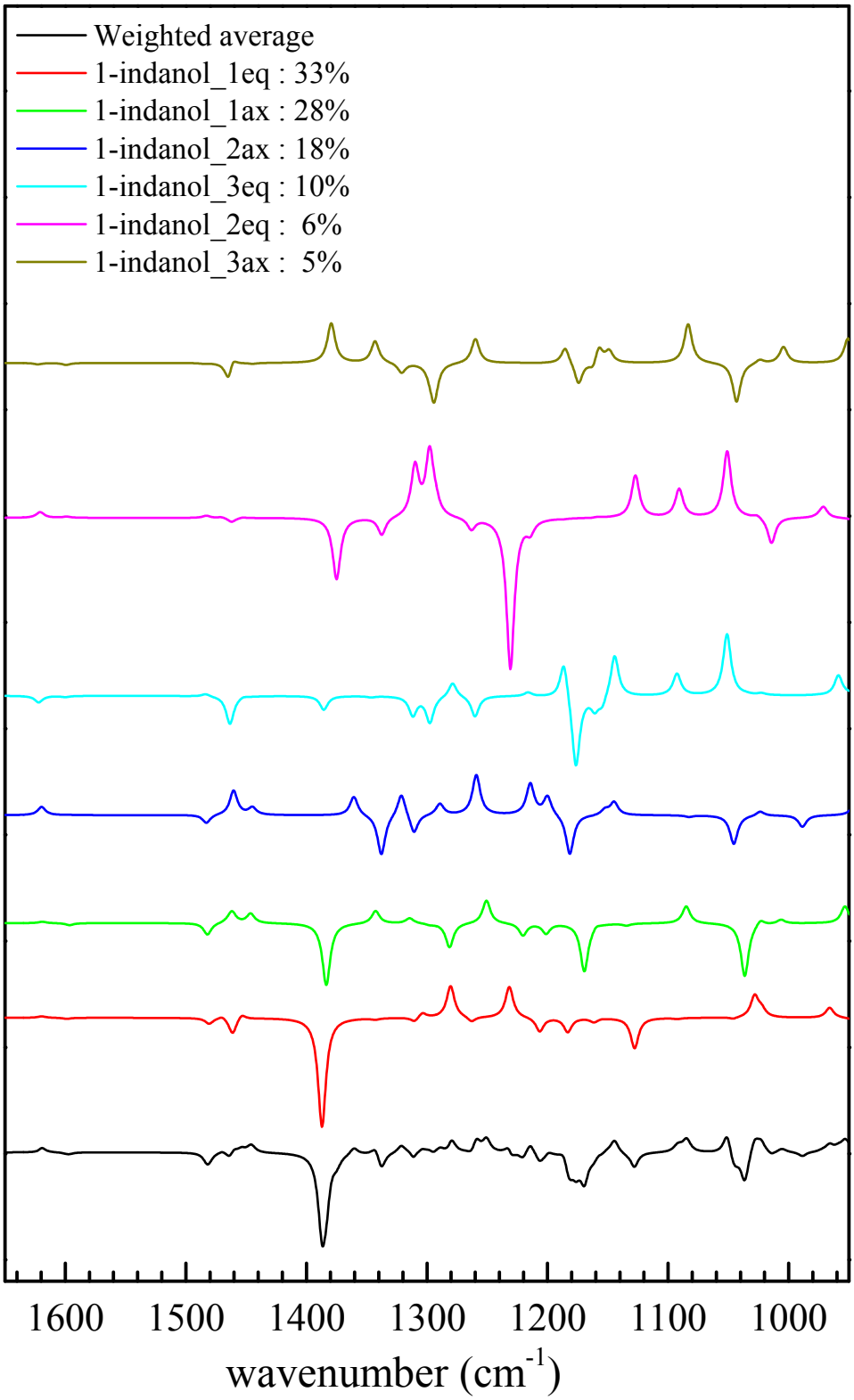

Figure S5: Simulated VCD spectrum obtained from the weighted VCD spectra of the most stable (S)-1-indanol structures in a CCl_4 continuum together with individual contributions, calculated at the B3LYP-D3/6-31G++(d, p) level

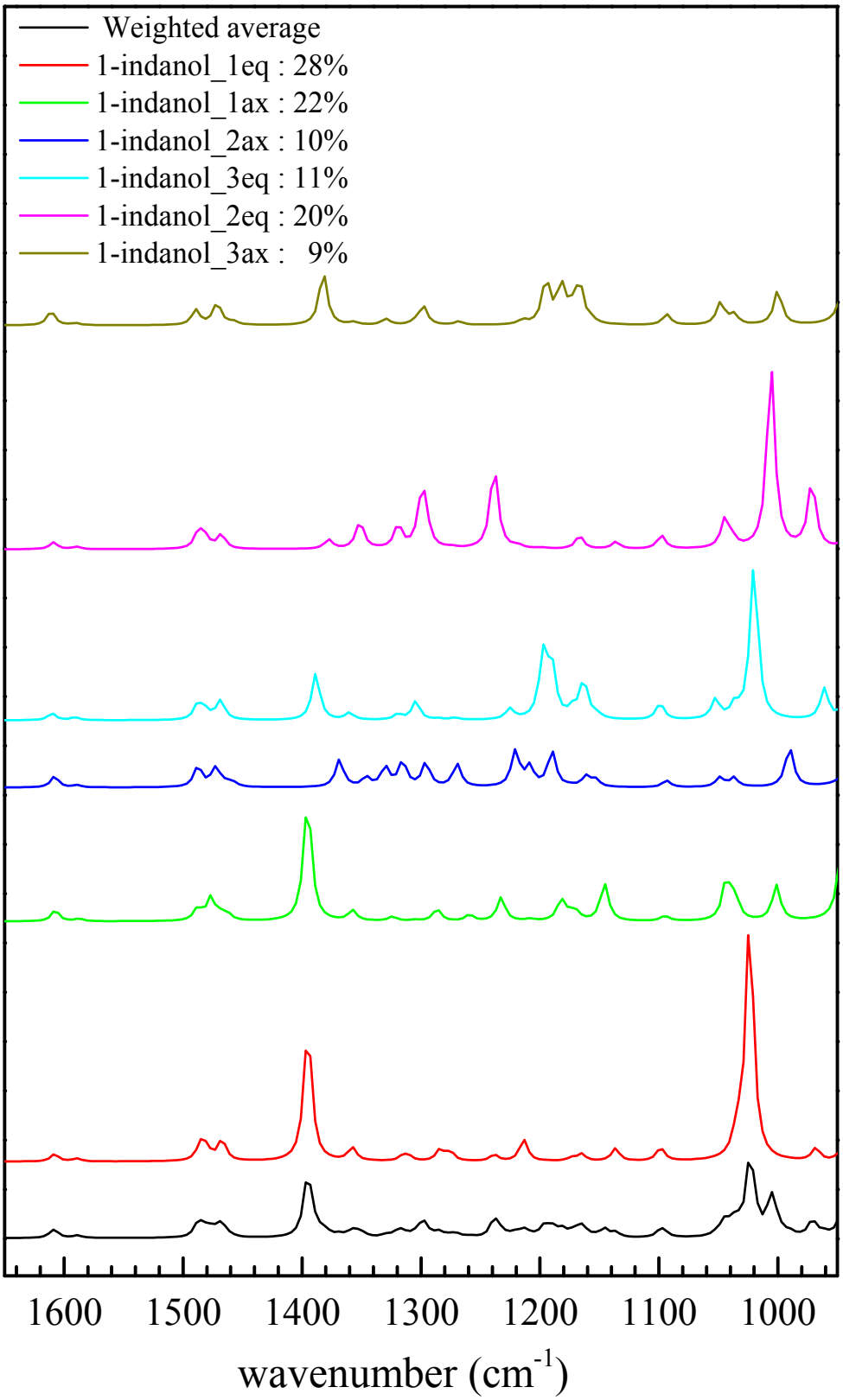

Figure S6: Simulated IR spectrum obtained from the weighted IR spectra of the most stable (S)-1-indanol structures in a CCl_4 continuum together with individual contributions, calculated at the BLYP/6-31G++(d, p) level.

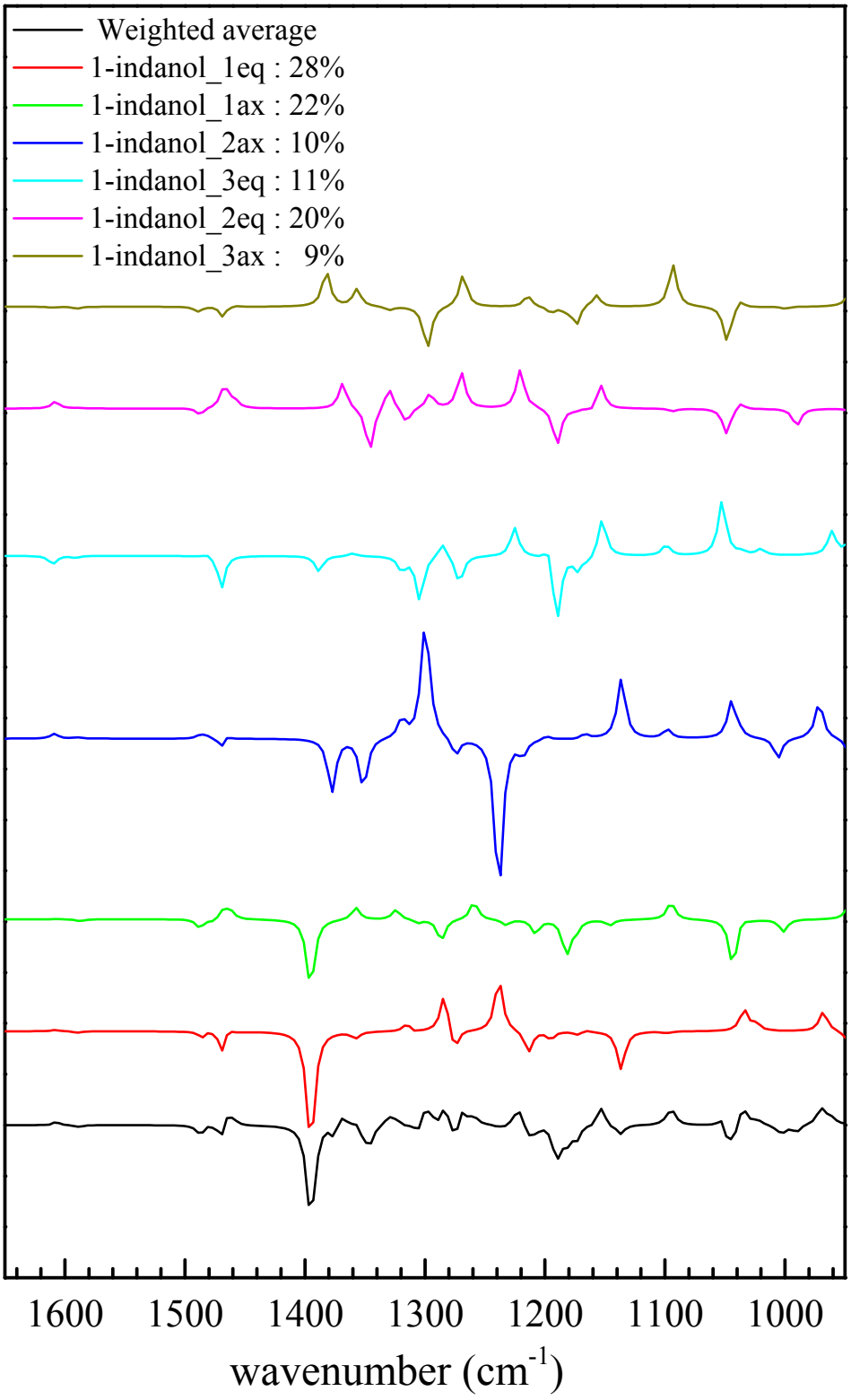

Figure S7: Simulated VCD spectrum obtained from the weighted VCD spectra of the most stable (S)-1-indanol structures in a CCl_4 continuum together with individual contributions, calculated at the BLYP/6-31G++(d, p) level.

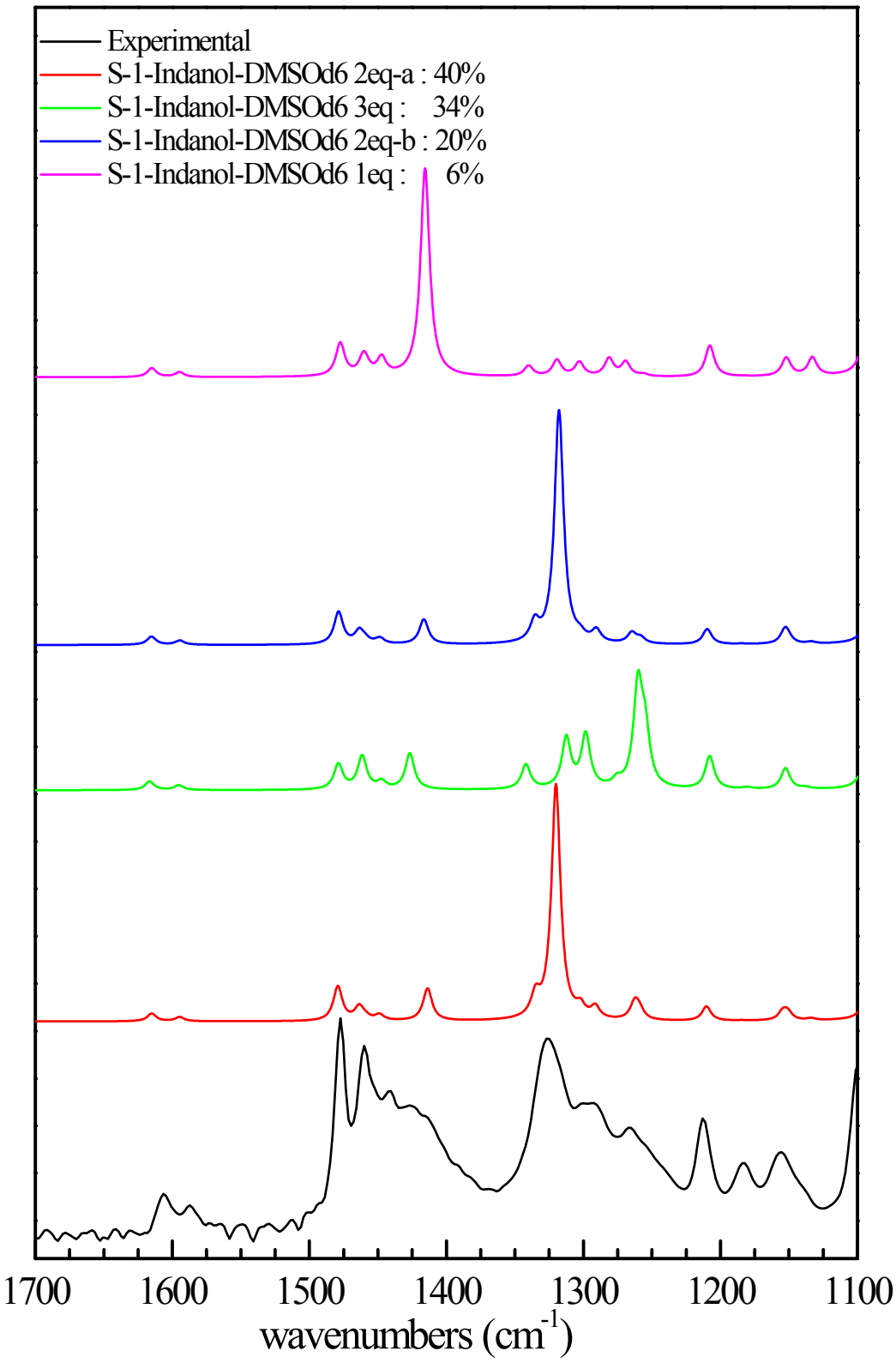

Figure S8: Simulated IR spectra of the most stable (S)-1-indanol:DMSO-d6 complexes in a DMSO continuum, calculated at the B3LYP/6-31G++(d, p) level, together with experimental spectrum.

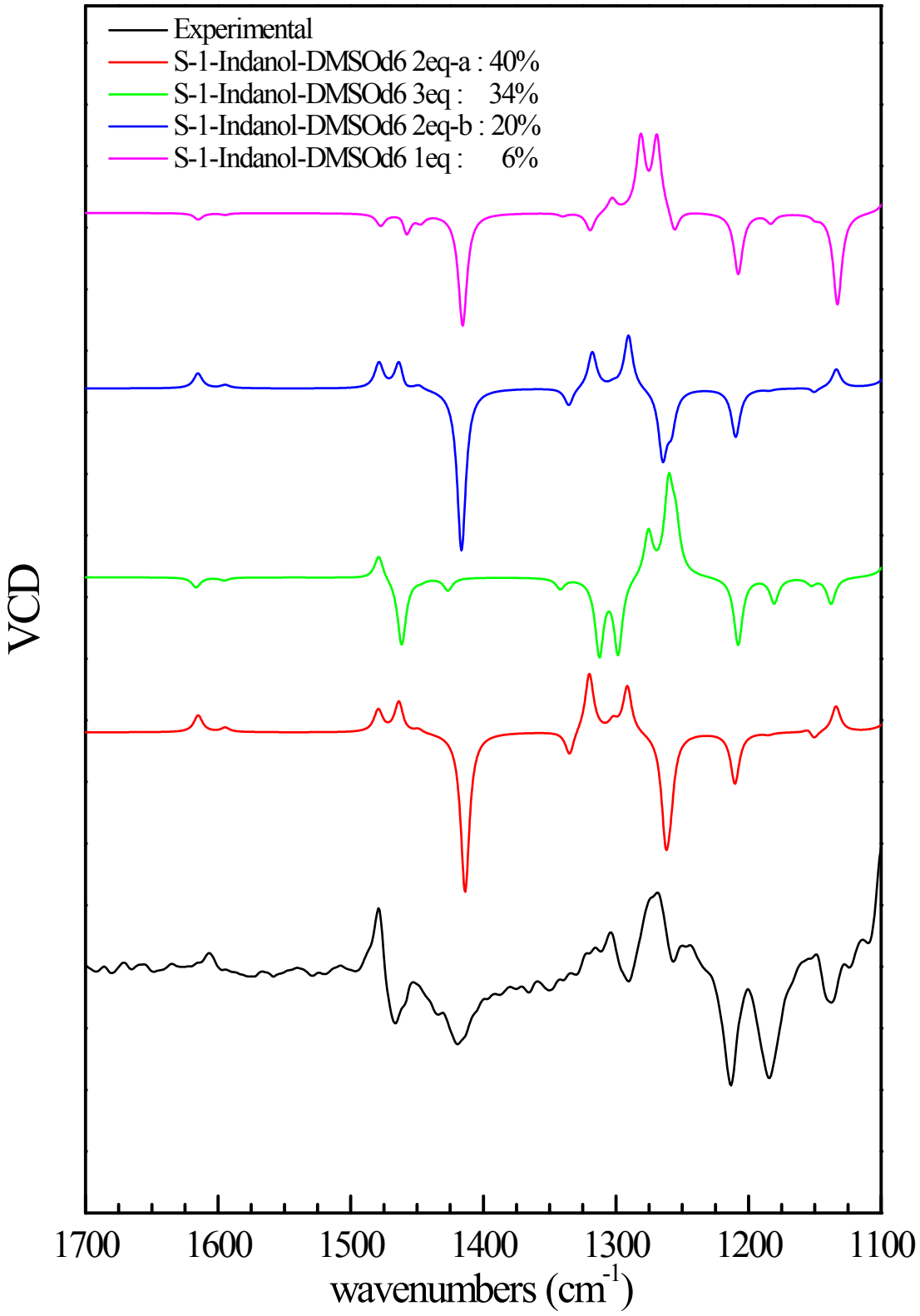

Figure S9: Simulated VCD spectra of the most stable (S)-1-indanol:DMSO-d6 complexes in a DMSO continuum, calculated at the B3LYP/6-31G++(d, p) level, together with experimental spectrum

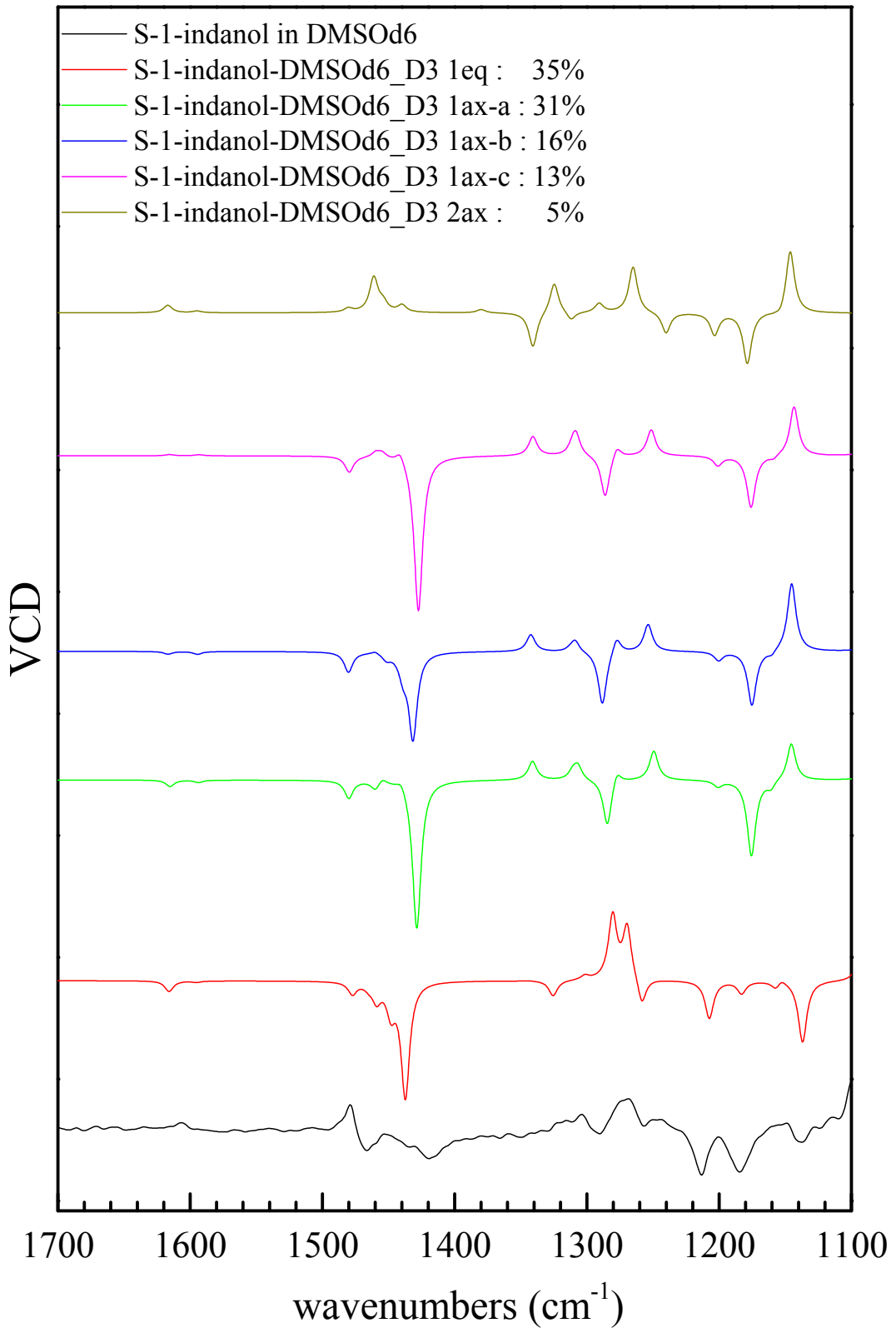

Figure S10: Simulated VCD spectra of the most stable (S)-1-indanol:DMSO-d6 complexes in a DMSO continuum, calculated at the B3LYP-D3/6-31G++(d,p) level, together with experimental spectrum.

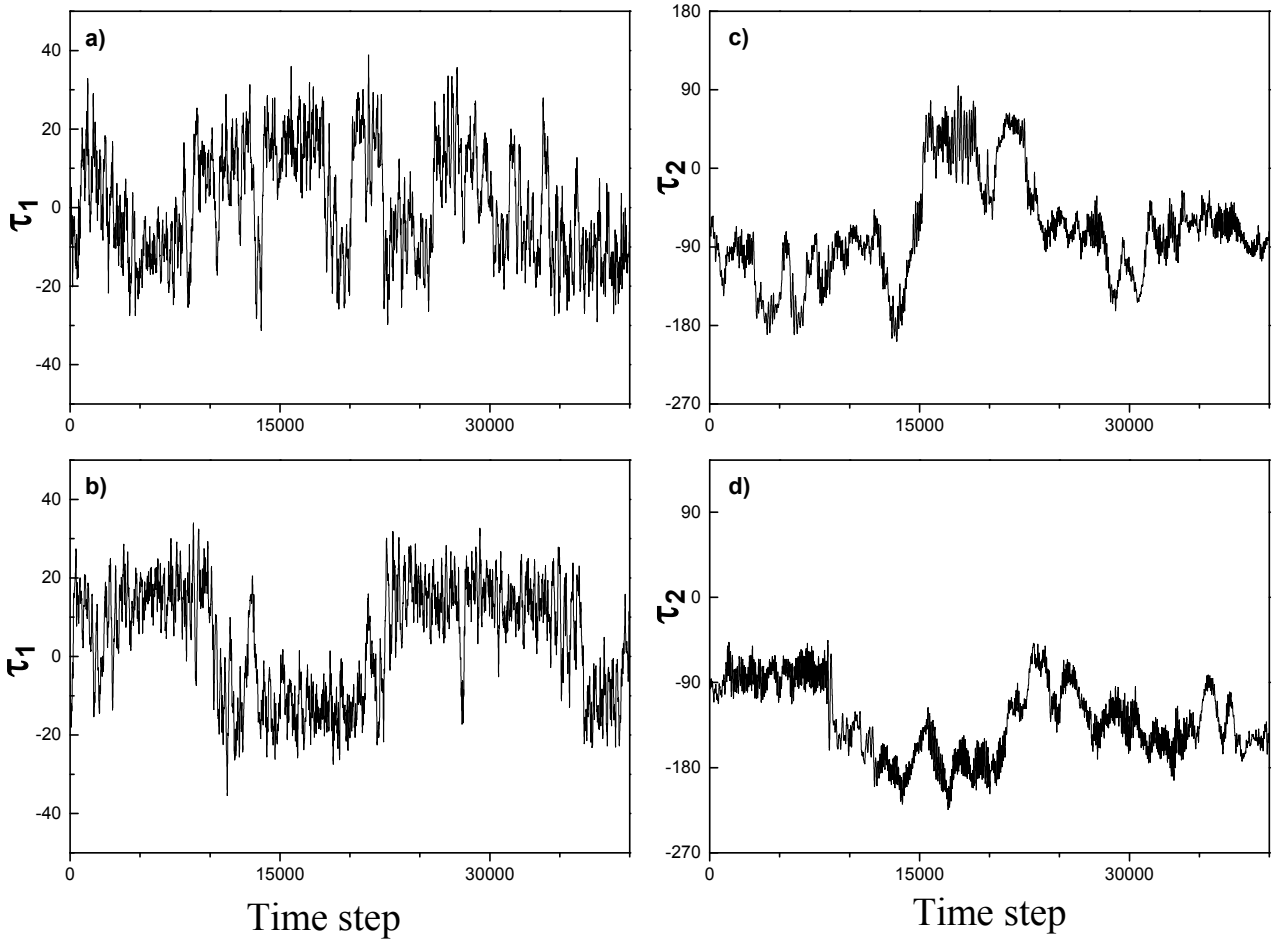

Figure S11. Evolution of the τ_1 and τ_2 angles during the NVE trajectories. a) τ_1 and b) τ_2 angles for the trajectory at 18ps c) τ_1 and d) τ_2 angles for the trajectory at 22ps.