

Supplementary Material: How and How Much Molecular Conformation Affects Electronic Circular Dichroism: the Case of 1,1-Diarylcannabinols

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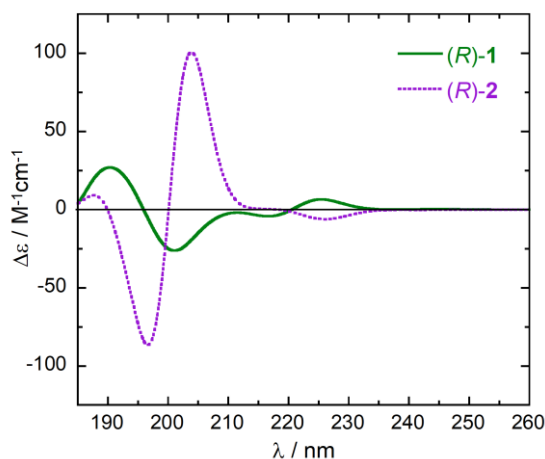


Figure S1. Calculated weighted-average ECD spectra of (R)-1 and (R)-2 at ω B97X-D/def2-TZVP/PCM level. Spectra plotted as sums of Gaussians with 0.15 eV exponential band-width and shifted by +15 nm.

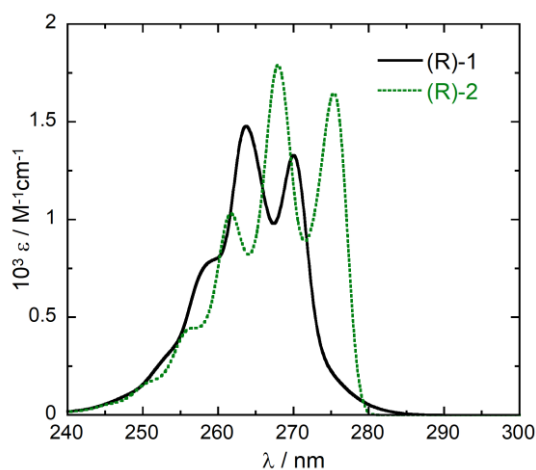


Figure S2. Calculated weighted-average vibronic absorption spectra of (R)-1 and (R)-2 in the 1L_b region. Calculated spectra plotted as sums of Gaussians with 0.025 eV exponential band-width, shifted by +30 nm.

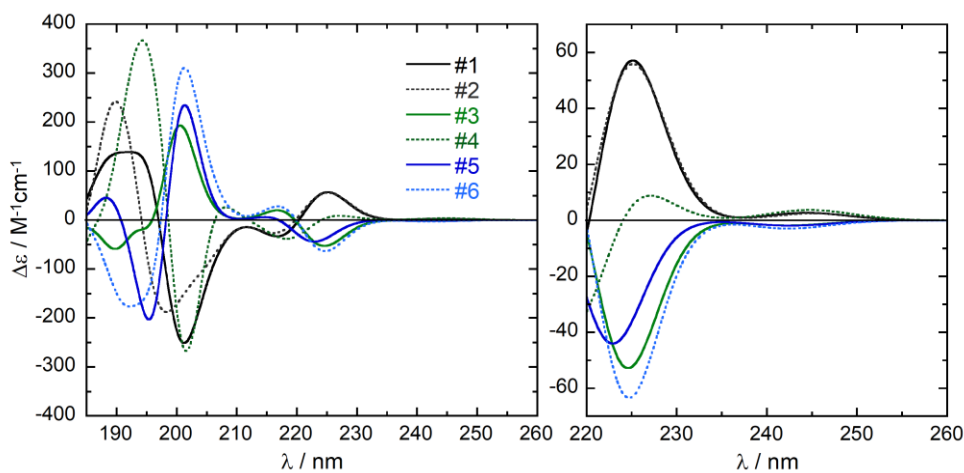


Figure S3. Calculated ECD spectra for conformers #1-#6 of (*R*)-**1** at ω B97X-D/def2-TZVP/PCM level in the 195-260 nm range. The plots on the right show an expansion of the $^1L_a/{}^1L_b$ region. Spectra plotted as sums of Gaussians with 0.15 eV exponential band-width and shifted by +15 nm.

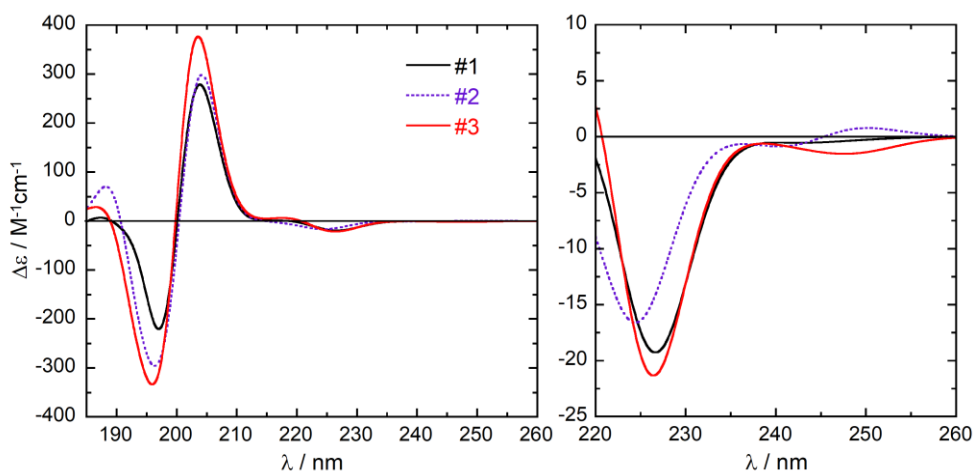


Figure S4. Calculated ECD spectra for conformers #1-#3 of (*R*)-**2** at ω B97X-D/def2-TZVP/PCM level. The plots on the right show an expansion of the $^1L_a/{}^1L_b$ region. Spectra plotted as sums of Gaussians with 0.15 eV exponential band-width and shifted by +15 nm.