Supplementary Material

Central-to-Helical-to-Axial Chirality Transfer in Chiroptical Sensing with Ferrocene Chromophore

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Contents

1. NMR spectroscopy

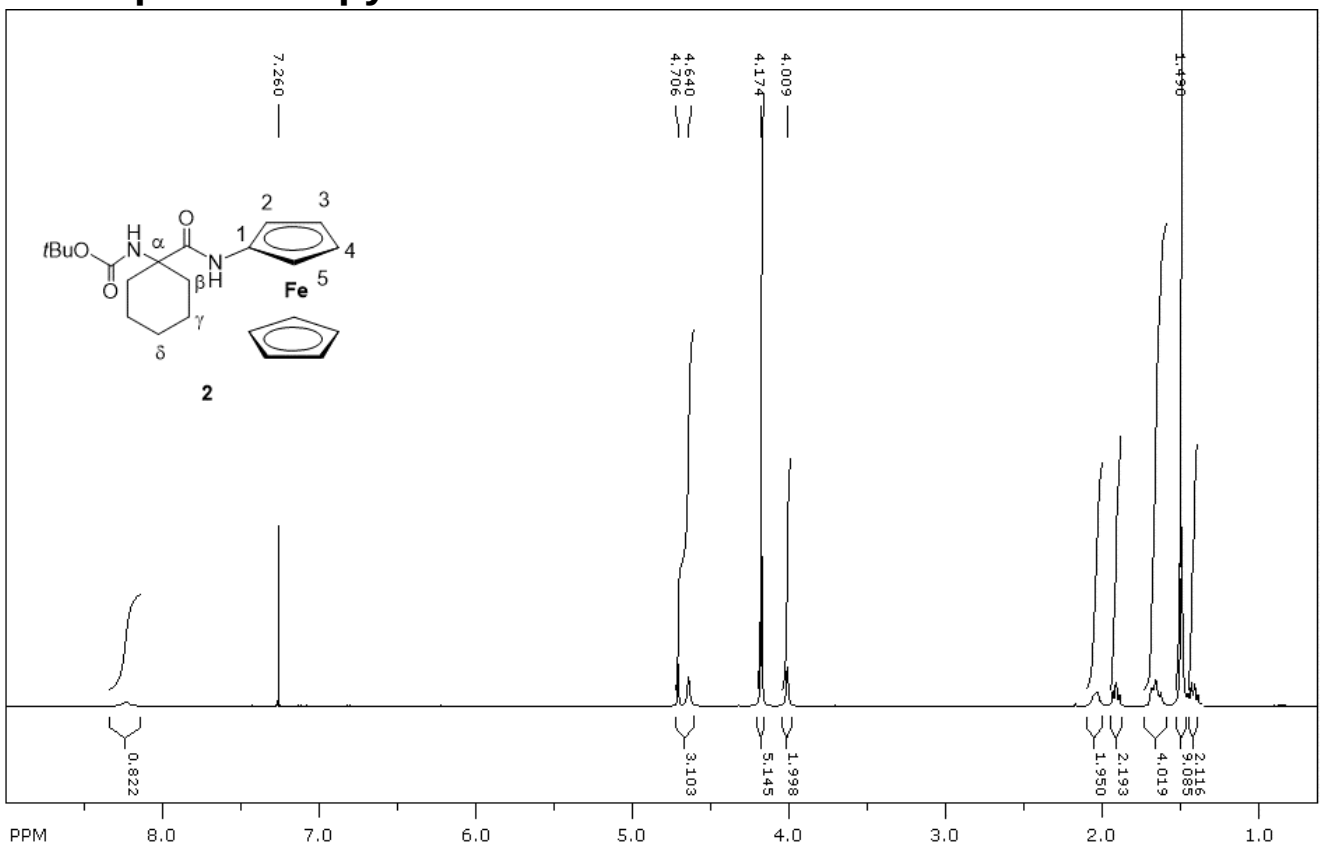

Figure S1. ^{1}H NMR spectrum of **2**, full range

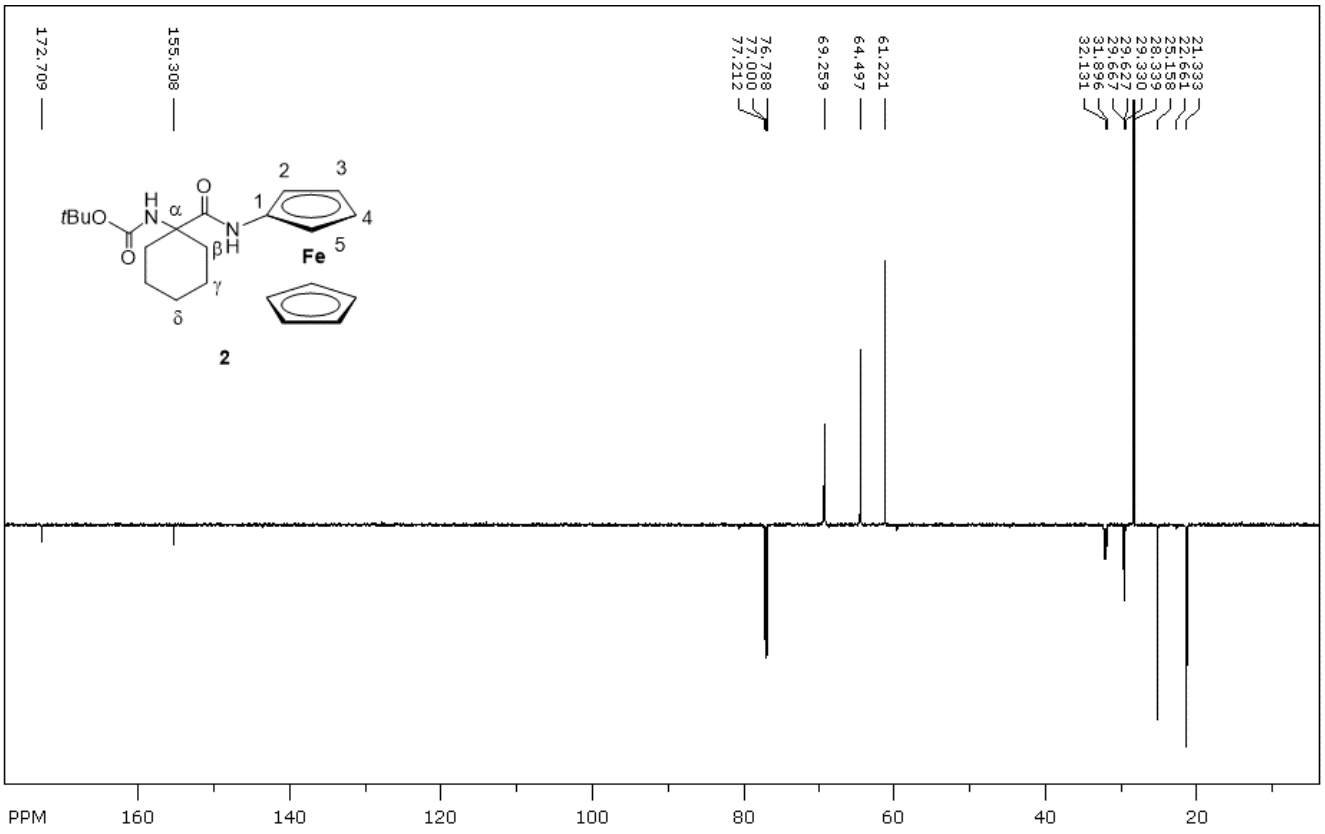

Figure S2. ^{13}C NMR spectrum of **2**, full range

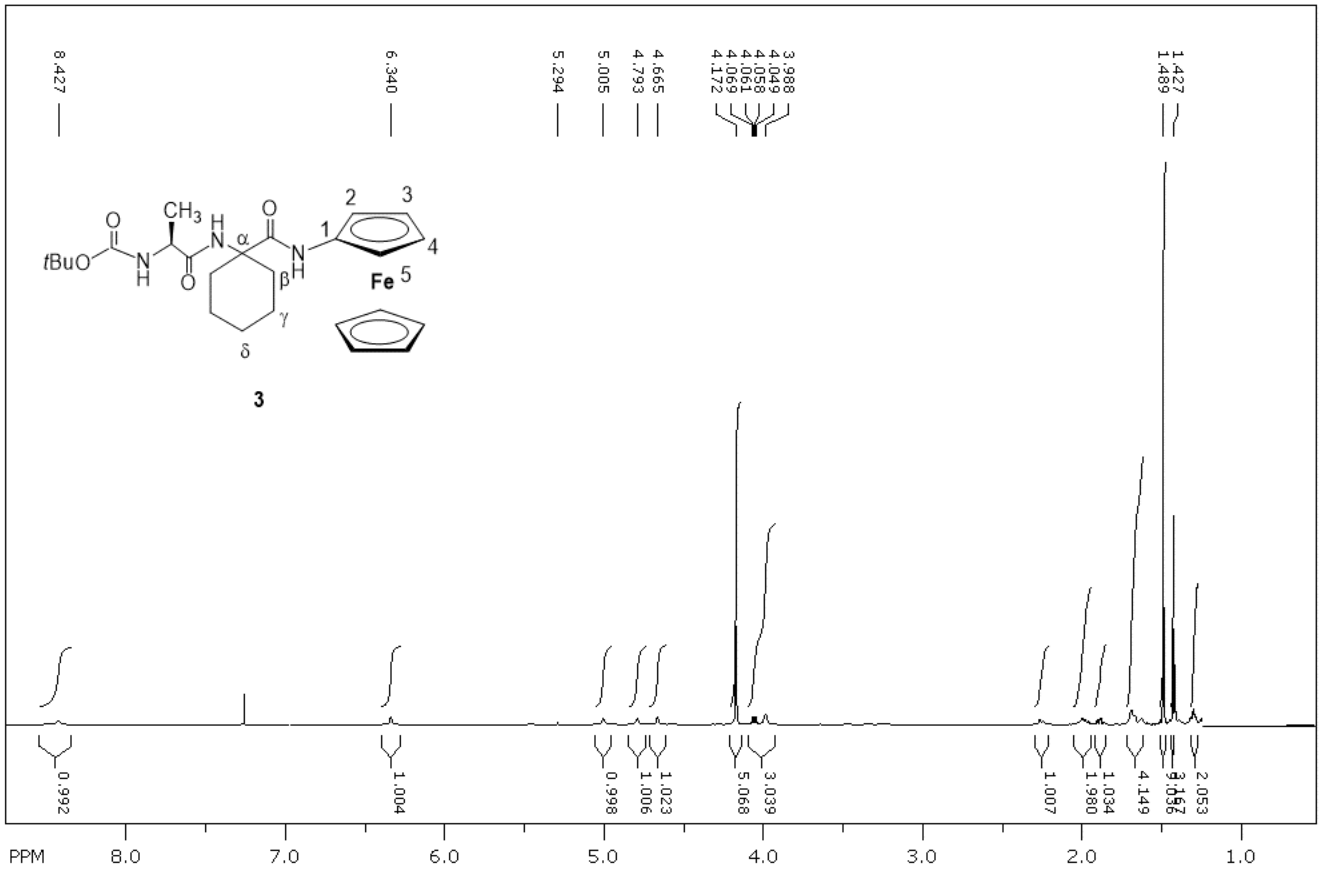

Figure S3. ^{1}H NMR spectrum of **3**, full range

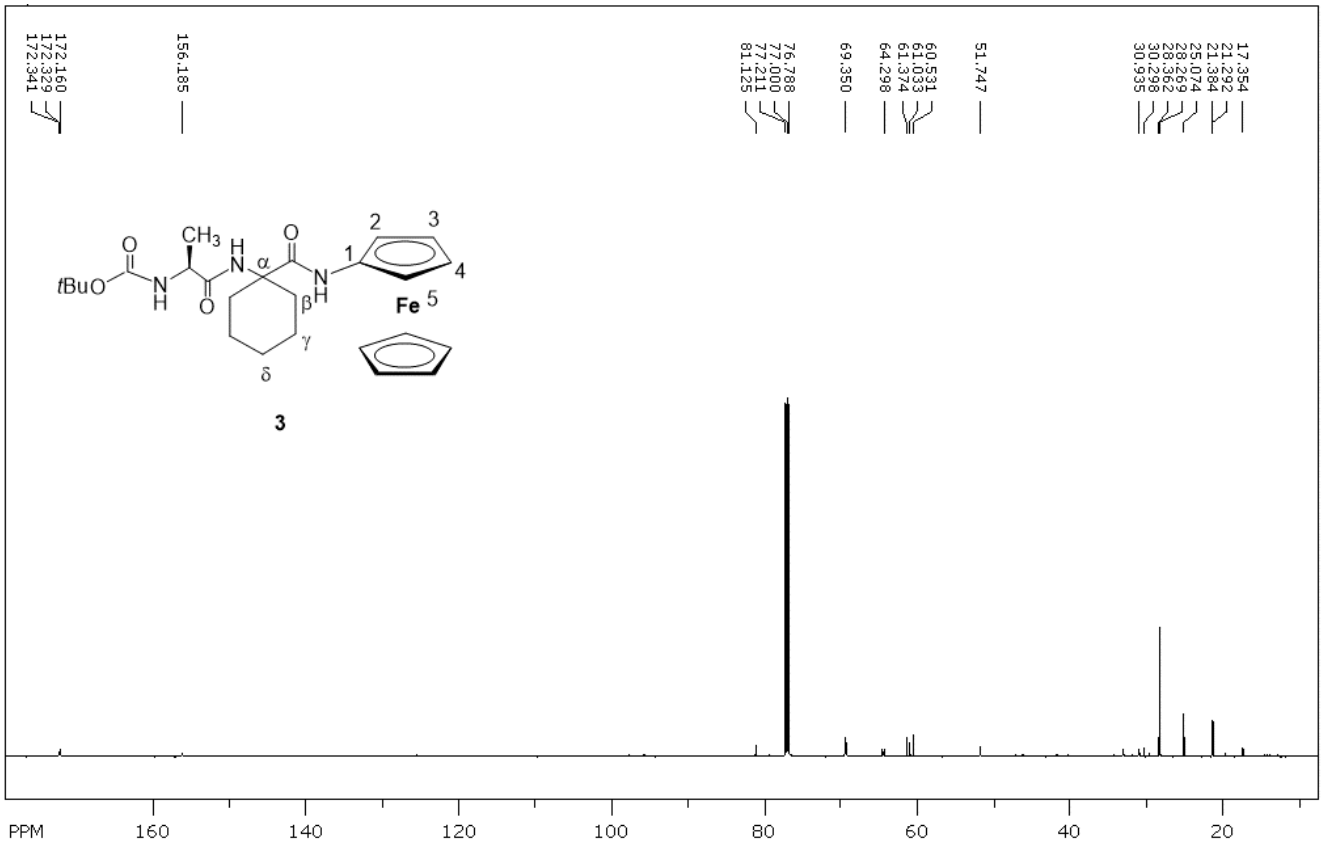

Figure S4. ^{13}C NMR spectrum of **3**, full range

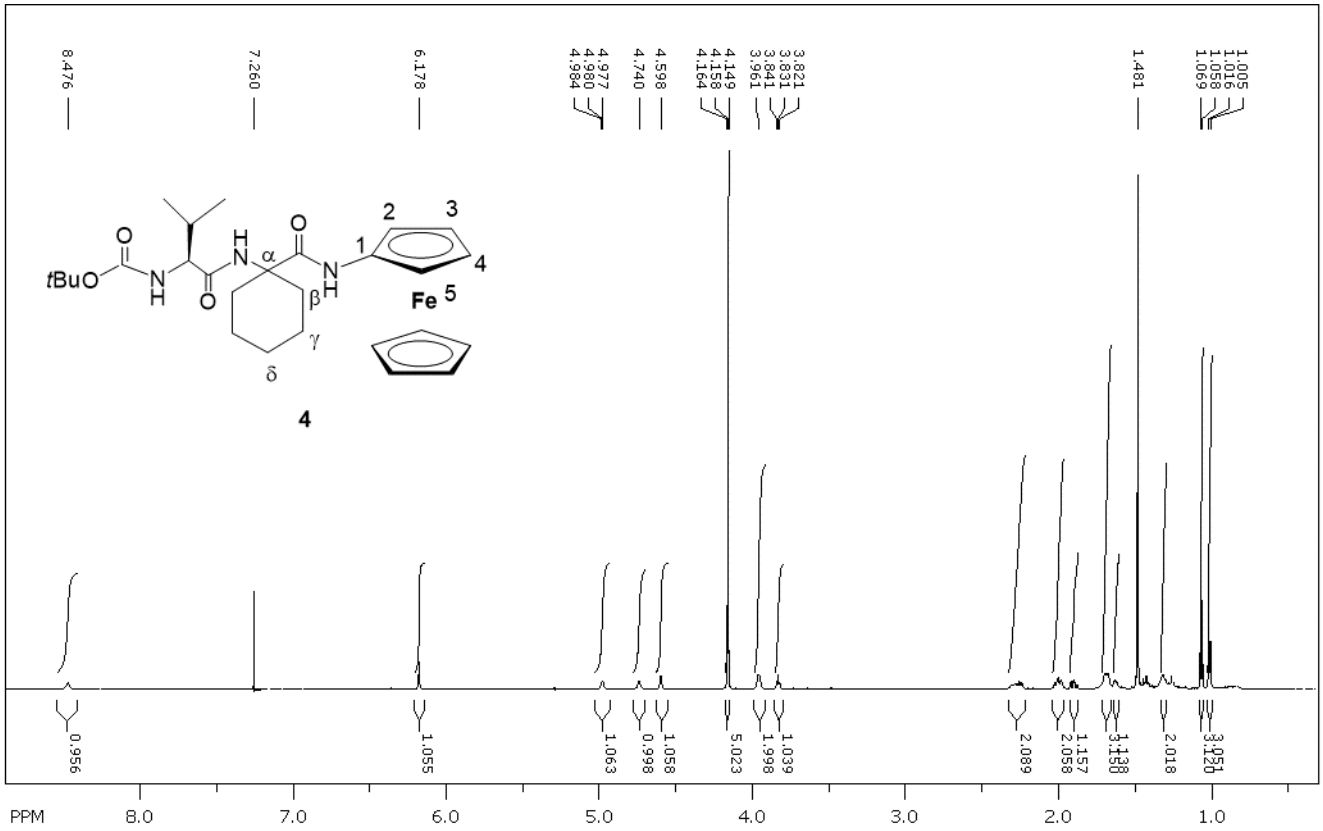

Figure S5. ^{1}H NMR spectrum of **4**, full range

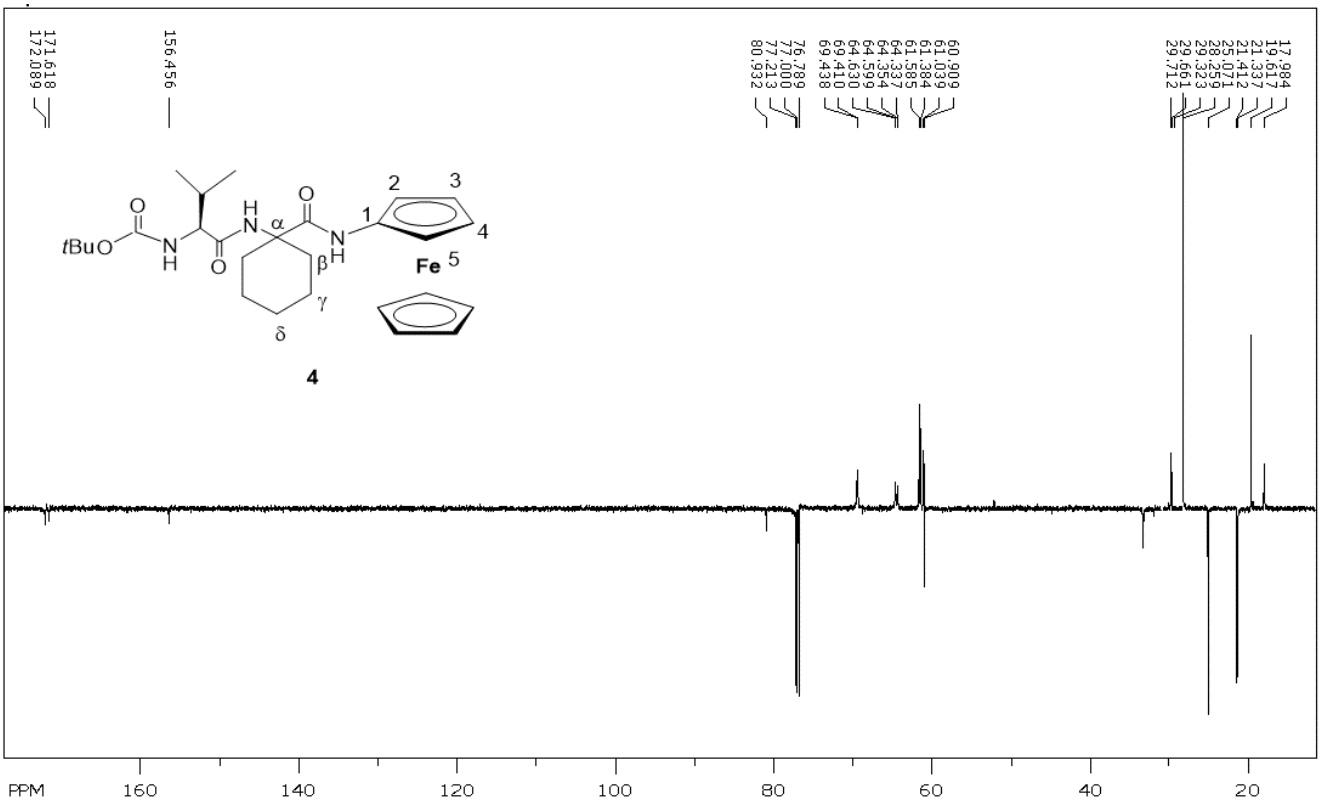

Figure S6. ^{13}C NMR spectrum of **4**, full range

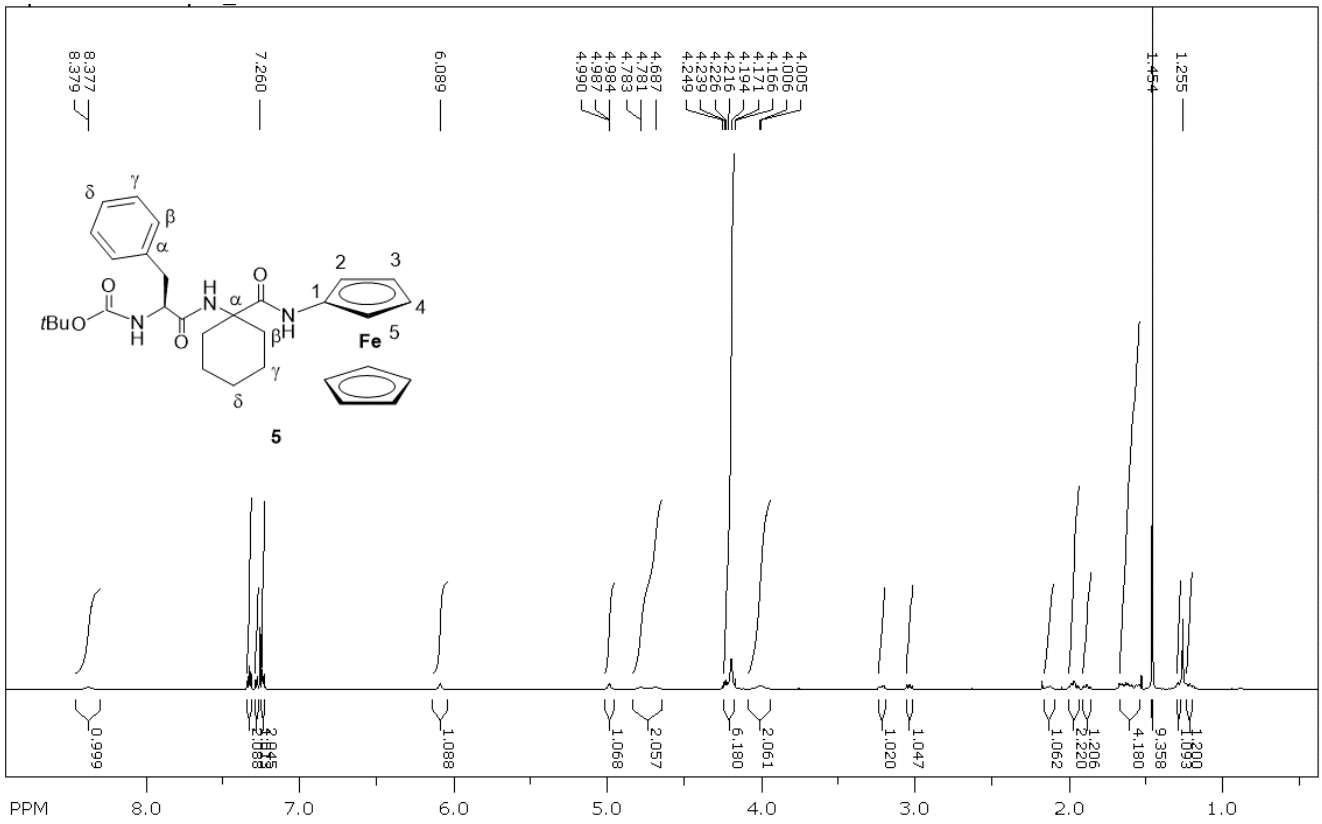

Figure S7. ^{1}H NMR spectrum of **5**, full range

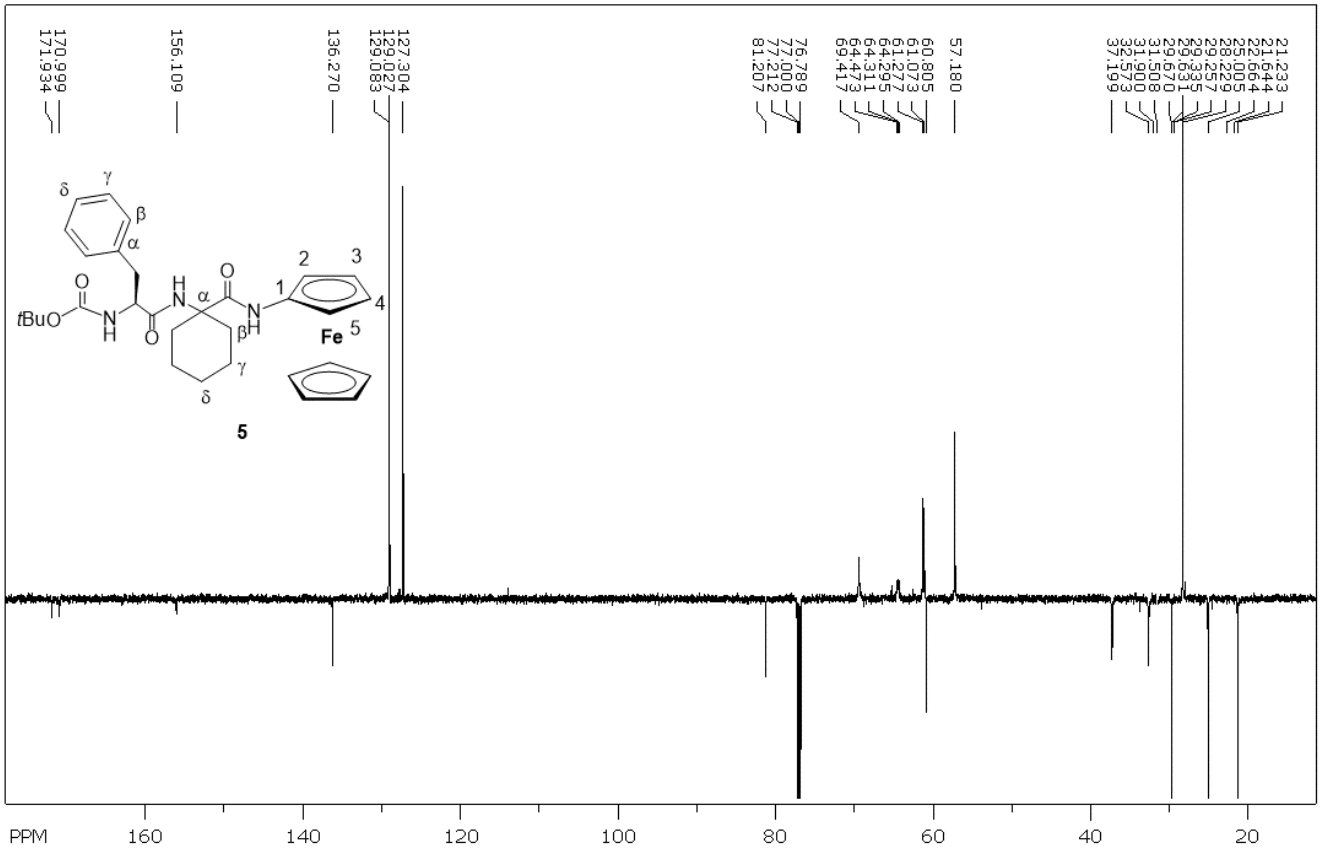

Figure S8. ^{13}C NMR spectrum of **5**, full range

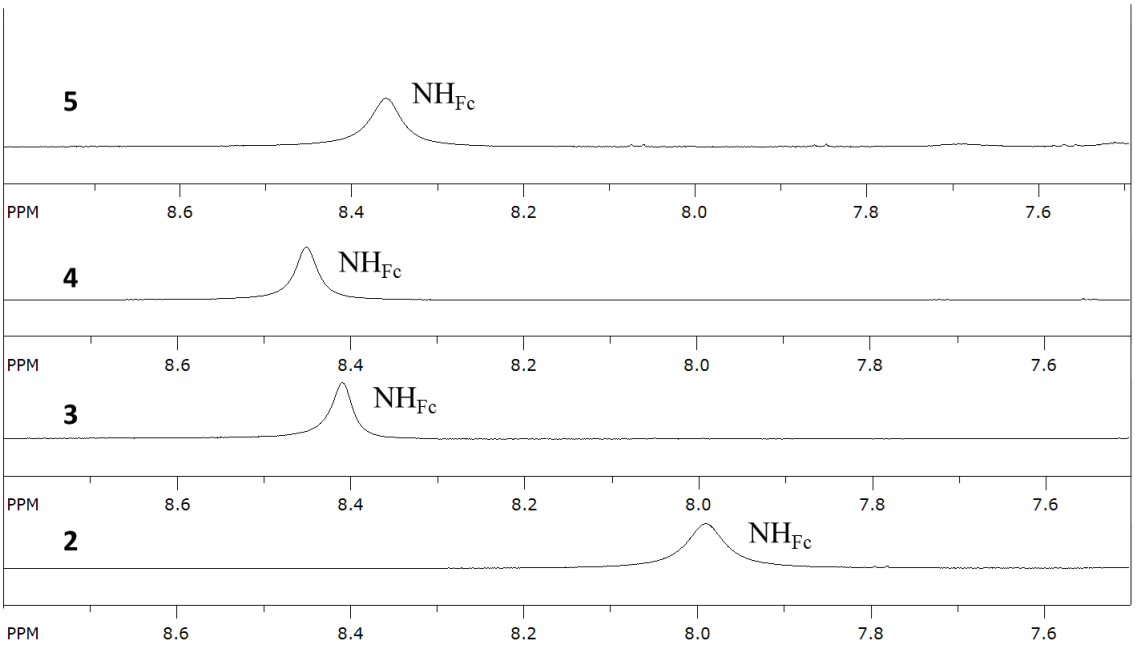

Figure S9. NH_{Fc} resonances in the NMR spectra of dilute solutions of **2**-**5** (*c* = 2 mmol dm^{-3})

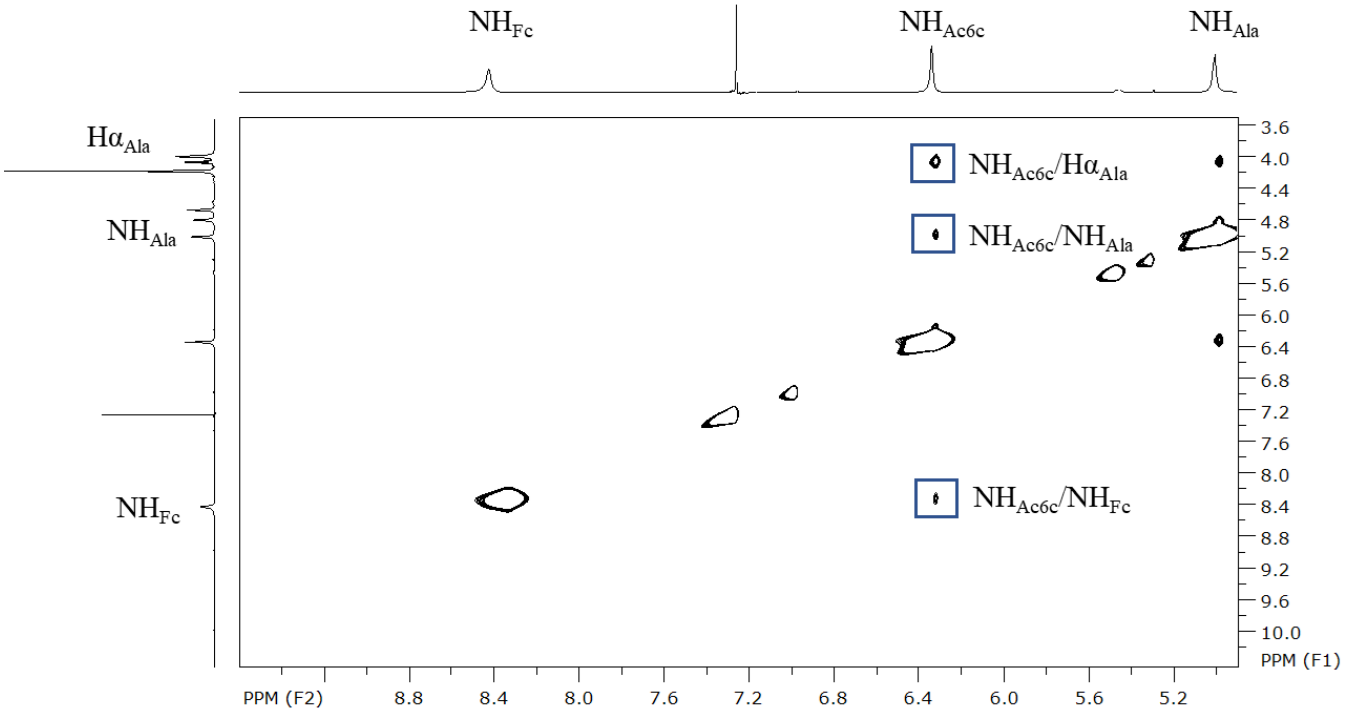

Figure S10. Sequential interactions in the NOESY spectrum of **3**

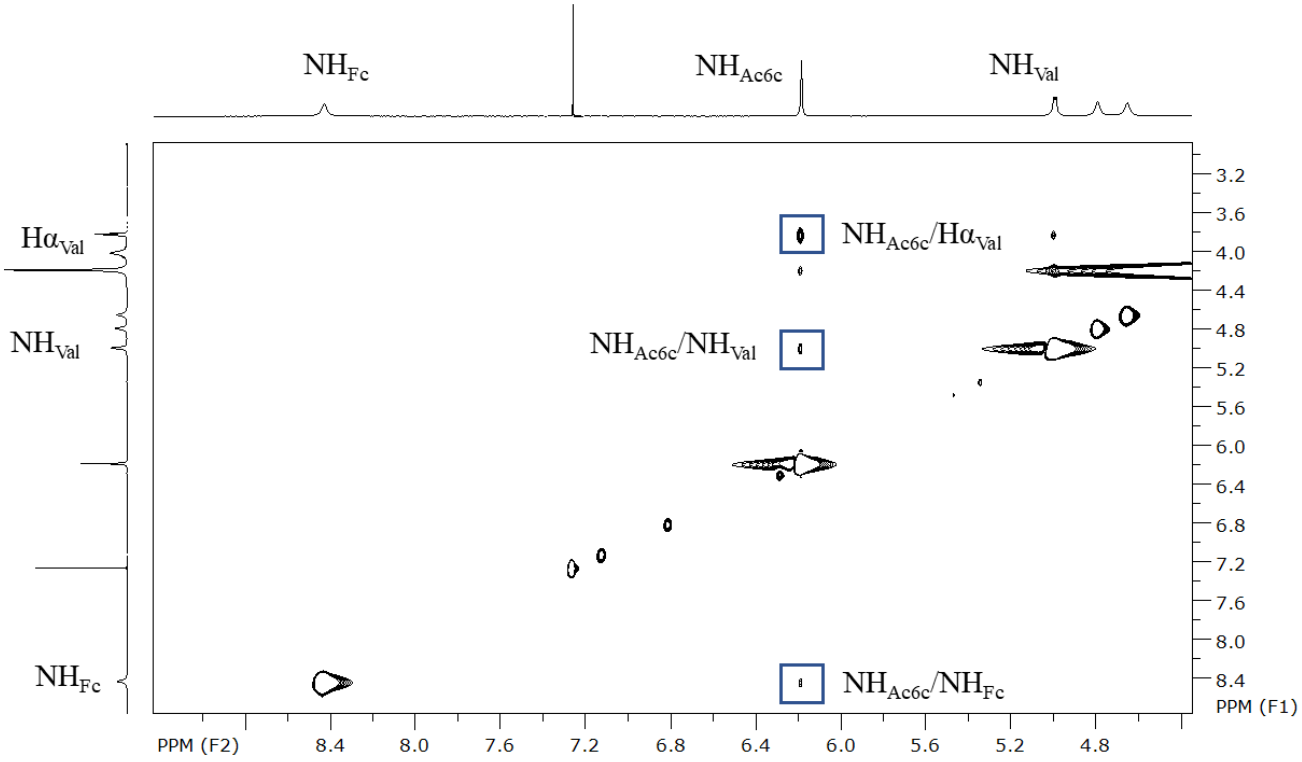

Figure S11. Sequential interactions in the NOESY spectrum of **4**

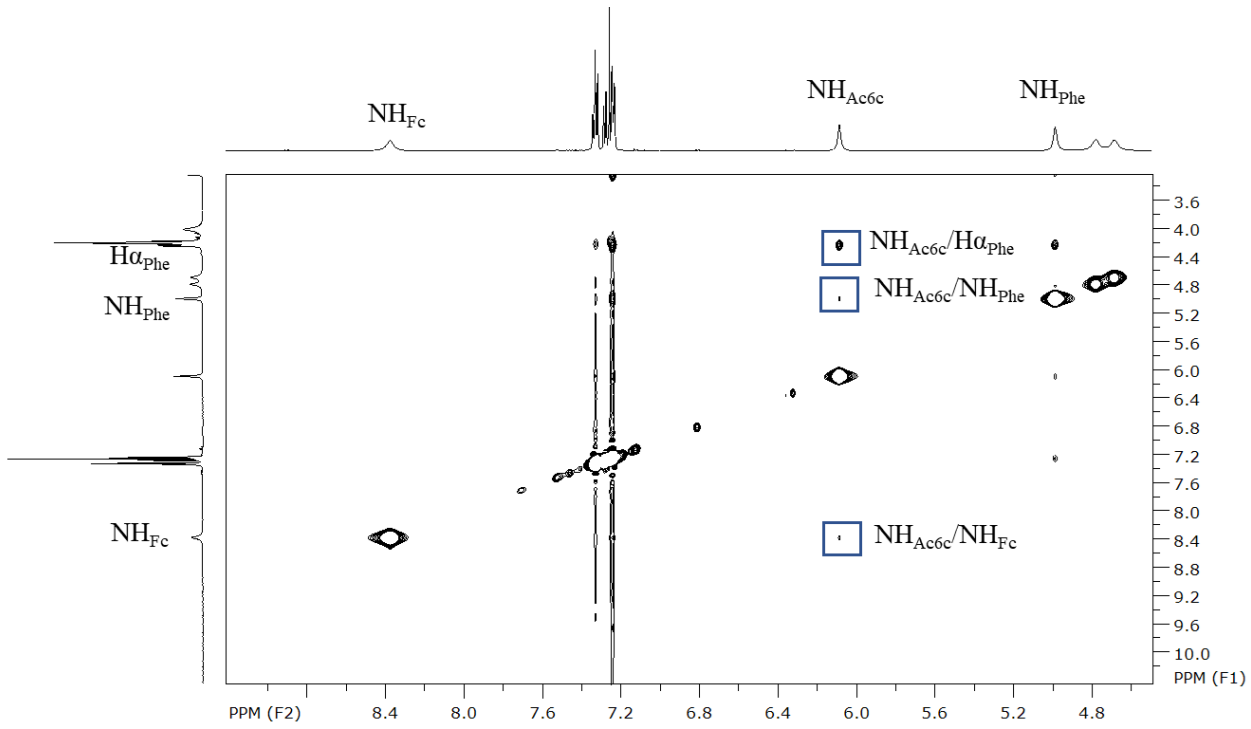

Figure S12. Sequential interactions in the NOESY spectrum of **5**

2. DFT study

2.1. Conformational Study

Table S1. Relative energies (in kJ mol^{-1}) of the most stable conformers (< 10 kJ mol^{-1}) of compounds **3–5** optimized in chloroform at 298 K. Optimizations performed at the B3LYP-D3/6-311+G(d,p), LanL2DZ for Fe level of theory, SMD model for solvent effects. Value of the χ angle (in deg), X–Y distances (in Å) of the selected X–H···Y hydrogen bonds connecting the *n*-membered rings.

conformer	Δ*E* / kJ mol^{-1}	χ angle / °	$NH_{Fc}\cdots OC_{Boc}$ 10-membered	$NH_{Fc}\cdots OC_{AA}$ 7-membered	$NH_{Ac6c}\cdots OC_{Boc}$ 7-membered
3-1	0.00	−82.4	2.99		
3-2	4.67	90.2	2.94		
3-3	5.93	77.7			3.02
3-4	8.83	−86.8	2.98		
3-5	9.48	−81.3		2.84	
3-6	9.72	−74.8		2.82	2.94
4-1	0.00	−83.4	2.98		
4-2	3.25	−78.9	2.99		
4-3	9.67	−71.0		2.80	
5-1	0.00	−84.5	3.00		
5-2	4.84	83.9		2.81	
5-3	8.62	−68.5		2.84	2.95
5-4	8.80	69.2		2.84	2.85
5-5	9.31	−144.6		2.85	
5-6	9.39	−81.6		2.82	

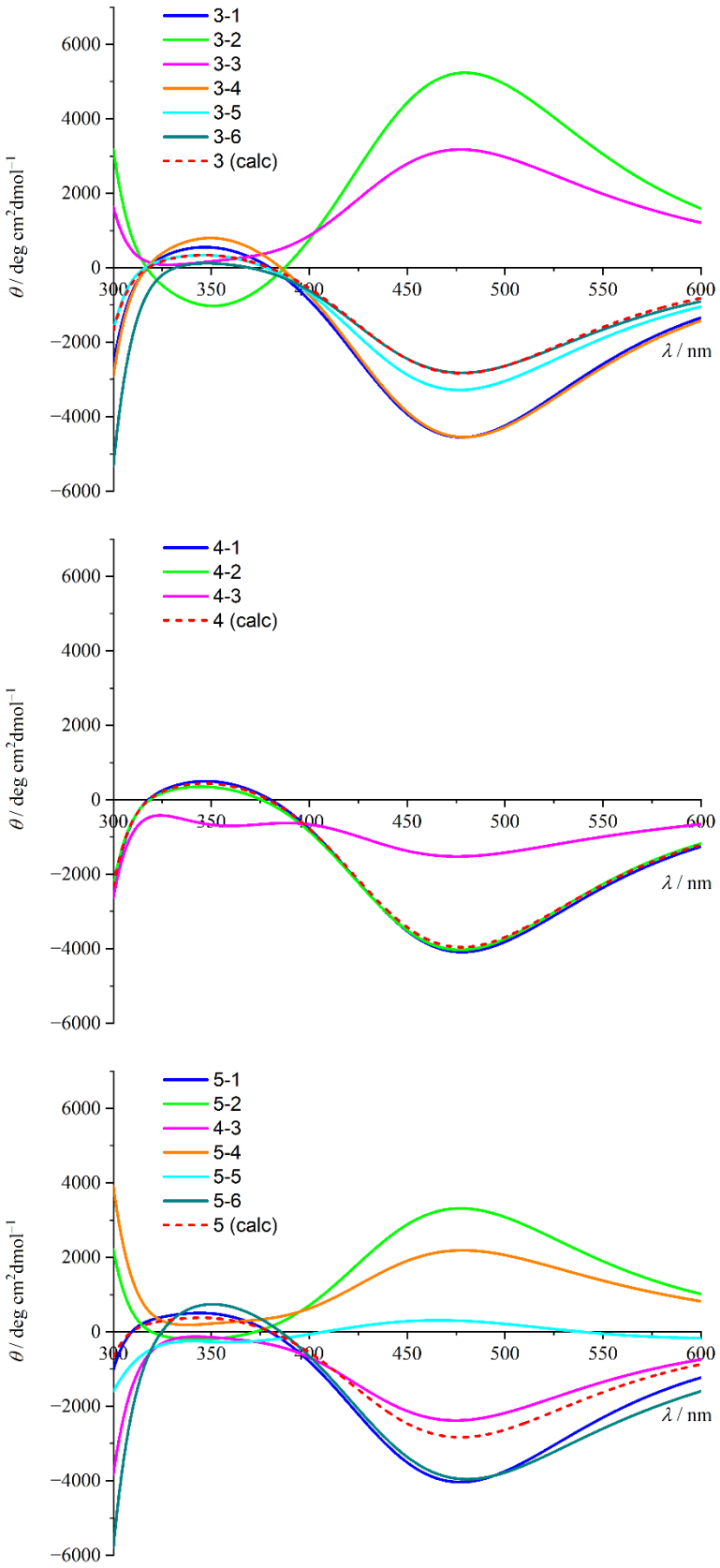

Figure S13. TD-DFT calculated ECD spectra of **3**, **4** and **5**. The final Boltzmann-averaged spectrum at 298 K (red dashed line) is obtained by weighting each conformer spectrum (colored solid lines) with the appropriate conformer Boltzmann weight factor for the final set of structures as named in Table S1.

2.1. Excited states

Conformer **3-1**

Excited states 1 to 6 of the conformer **3-1**. The left side displays pairs of natural transition orbitals and occupation numbers (above arrows) particular to the states of interests. The right side shows a density difference plot for each transition, with regions of increased (violet) and decreased (cyan) electron density.

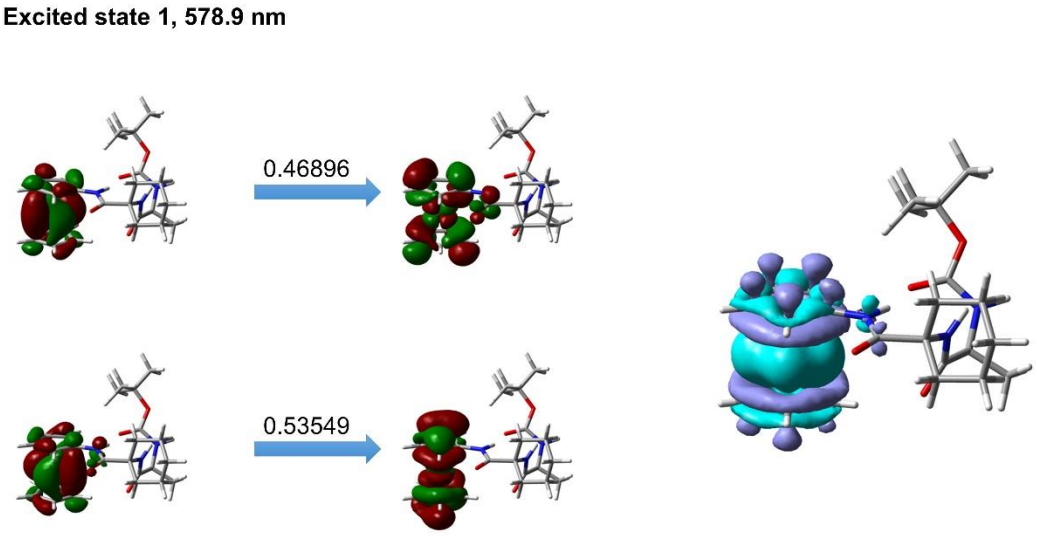

Figure S14. Excited state 1 of the conformer **3-1**.

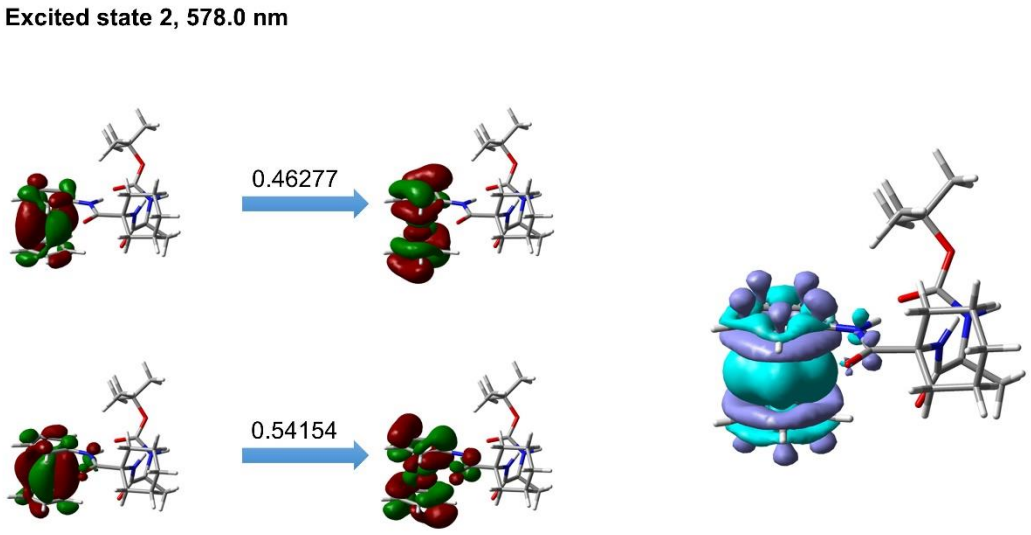

Figure S15. Excited state 2 of the conformer **3-1**.

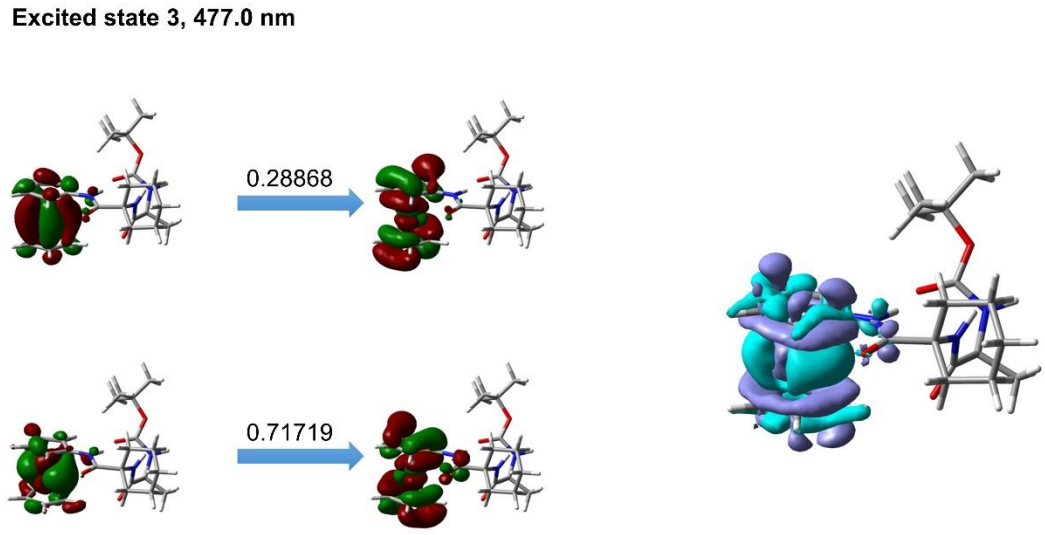

Figure S16. Excited state 3 of the conformer **3**-**1**.

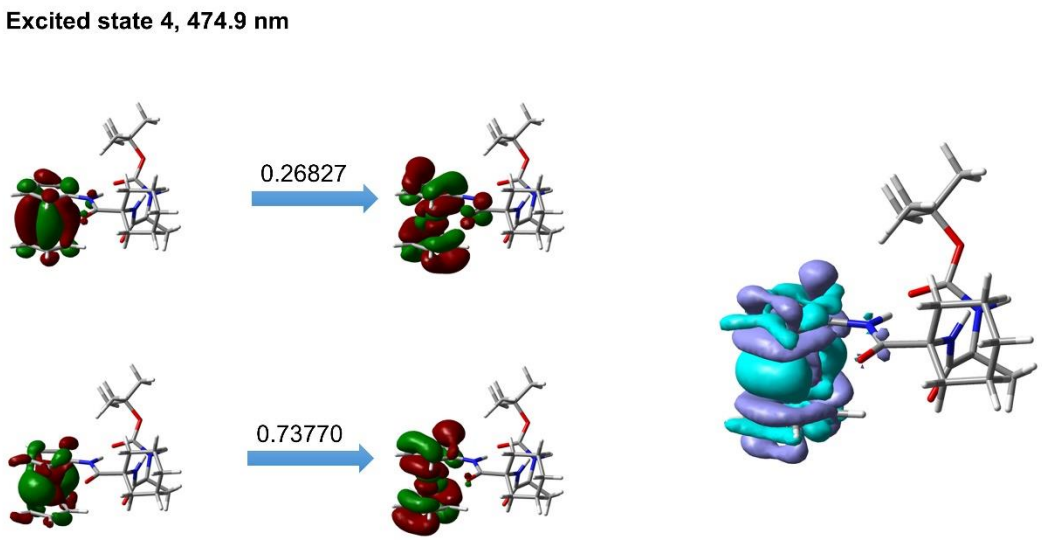

Figure S17. Excited state 4 of the conformer **3**-**1**.

Excited state 5, 355.4 nm

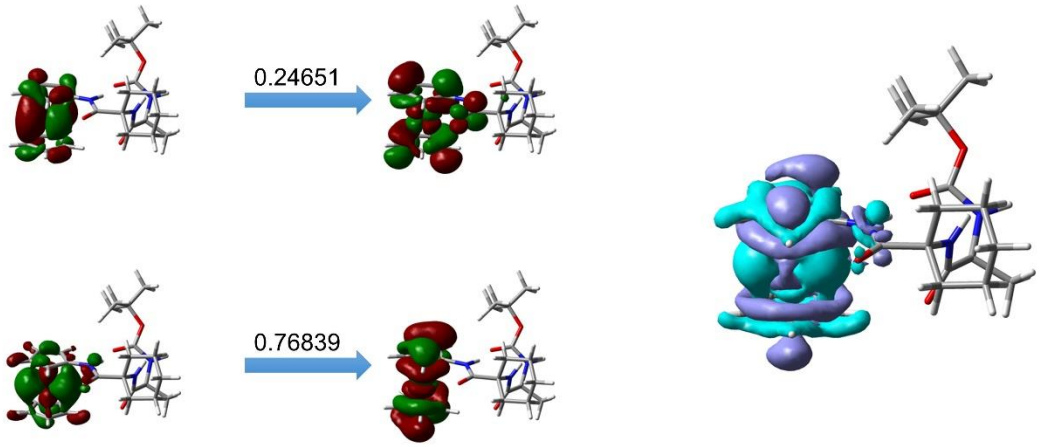

Figure S18. Excited state 5 of the conformer **3**-**1**.

Excited state 6, 352.6 nm

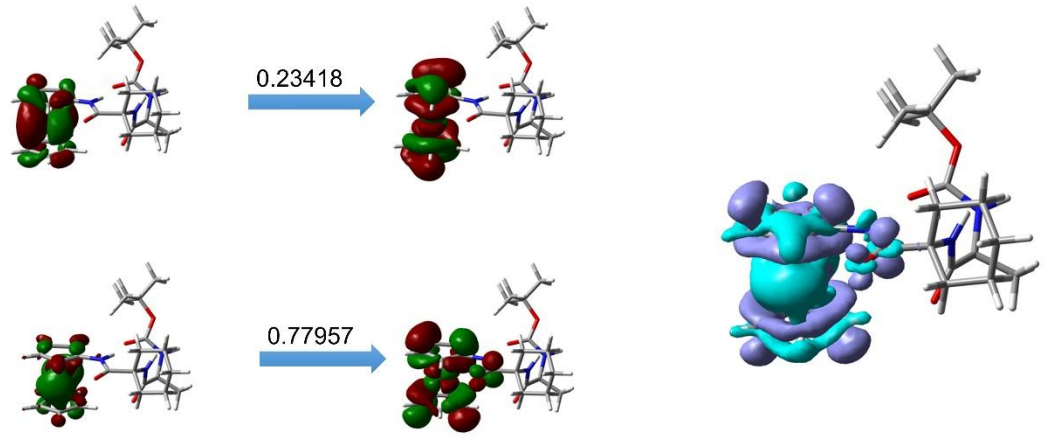

Figure S19. Excited state 6 of the conformer **3**-**1**.

Conformer **4-1**

Excited states 1 to 6 of the conformer **4-1**. The left side displays pairs of natural transition orbitals and occupation numbers (above arrows) particular to the states of interests. The right side shows a density difference plot for each transition, with regions of increased (violet) and decreased (cyan) electron density.

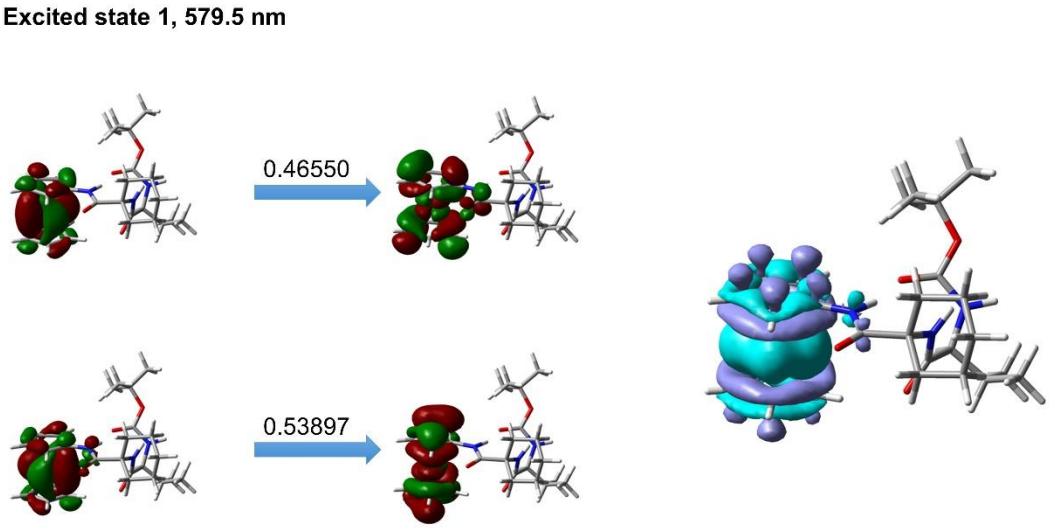

Figure 20. Excited states 1 of the conformer **4-1**.

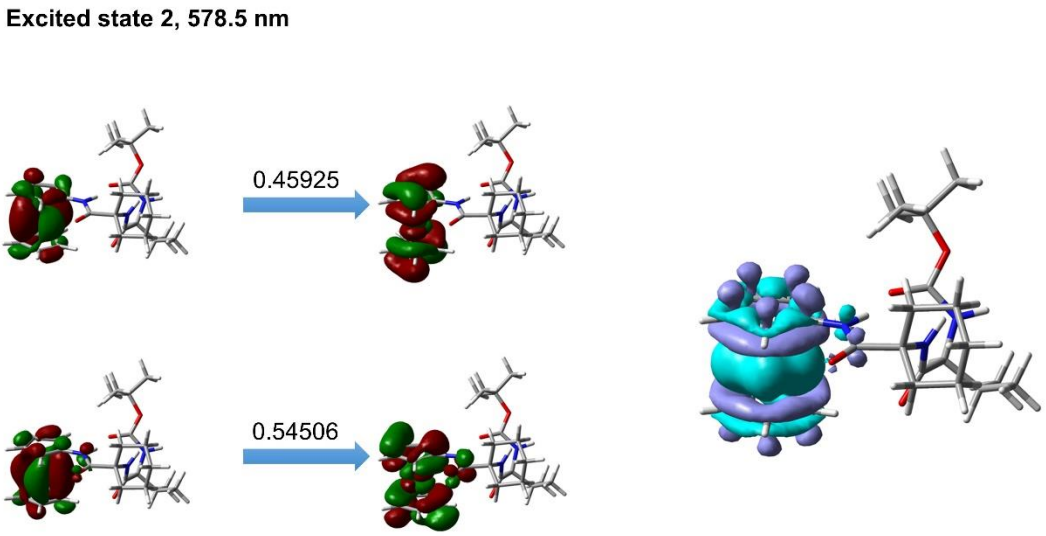

Figure S21. Excited states 2 of the conformer **4-1**.

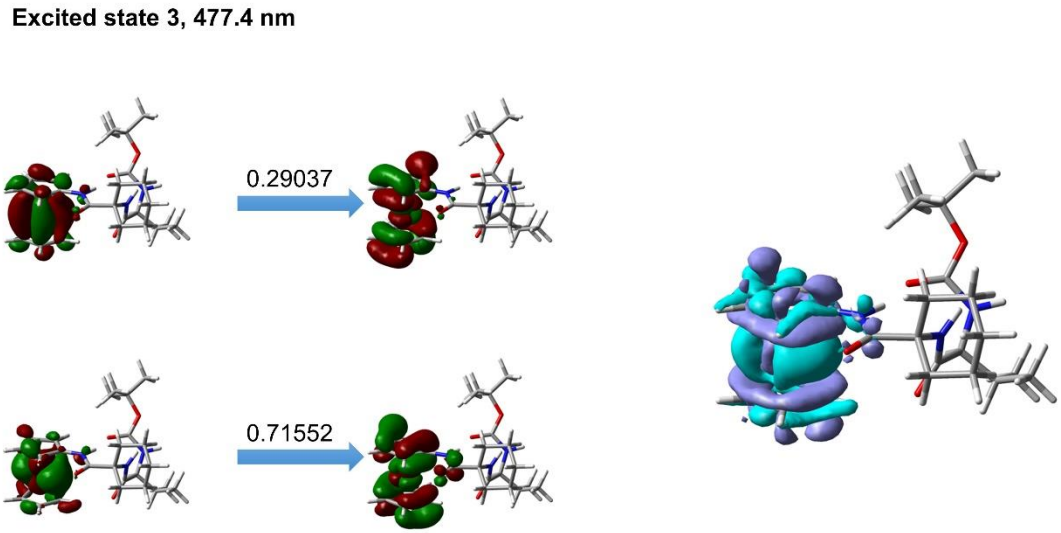

Figure S22. Excited states 3 of the conformer **4**-**1**.

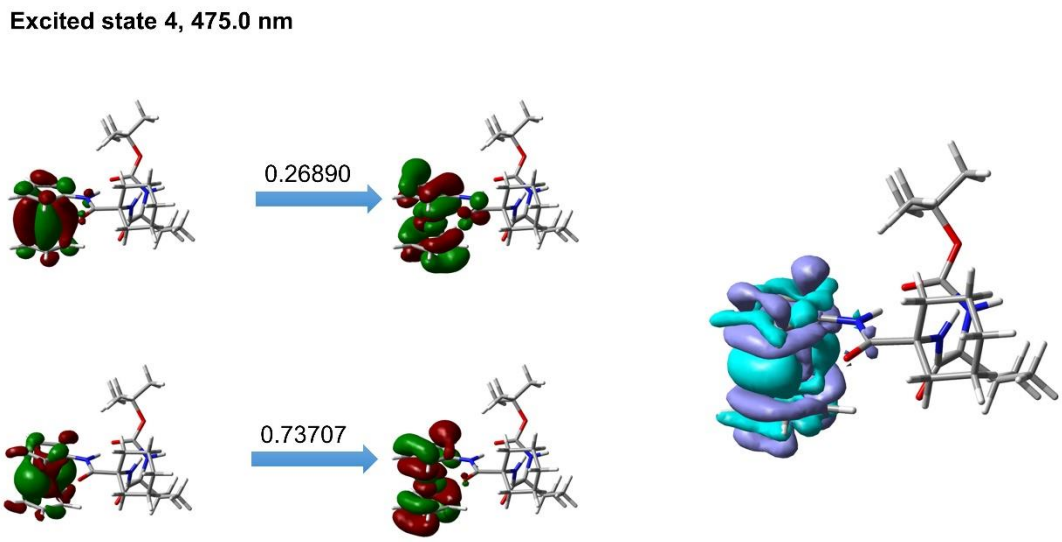

Figure S23. Excited states 4 of the conformer **4**-**1**.

Excited state 5, 355.6 nm

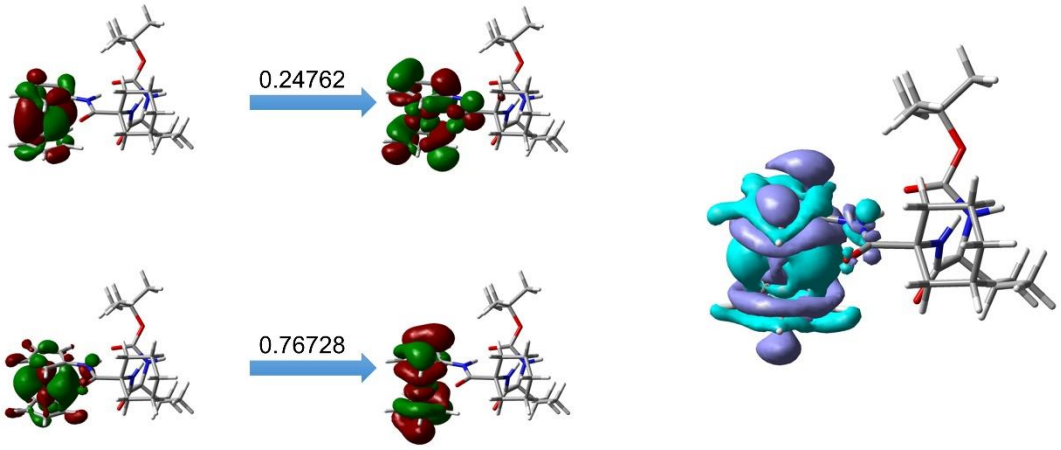

Figure S24. Excited states 5 of the conformer **4**-**1**.

Excited state 6, 352.6 nm

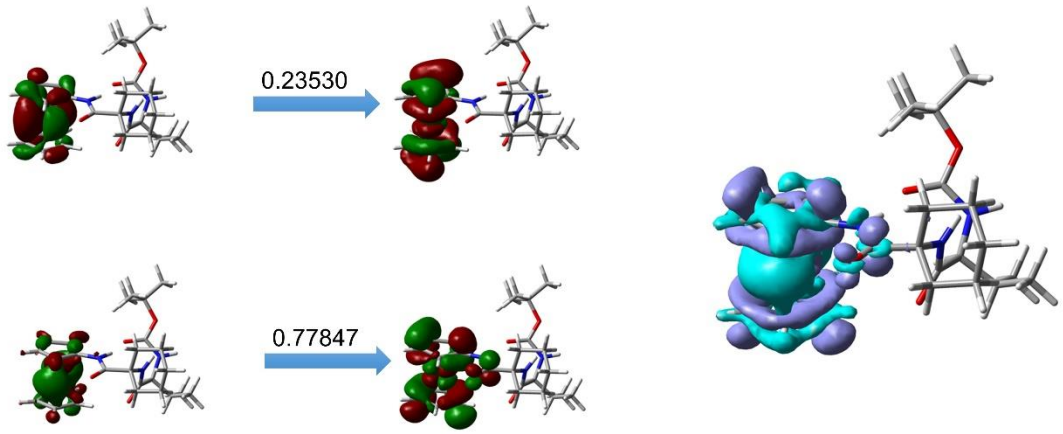

Figure S25. Excited states 6 of the conformer **4**-**1**.

Conformer **5-1**

Excited states 1 to 6 of the conformer **5-1**. The left side displays pairs of natural transition orbitals and occupation numbers (above arrows) particular to the states of interests. The right side shows a density difference plot for each transition, with regions of increased (violet) and decreased (cyan) electron density.

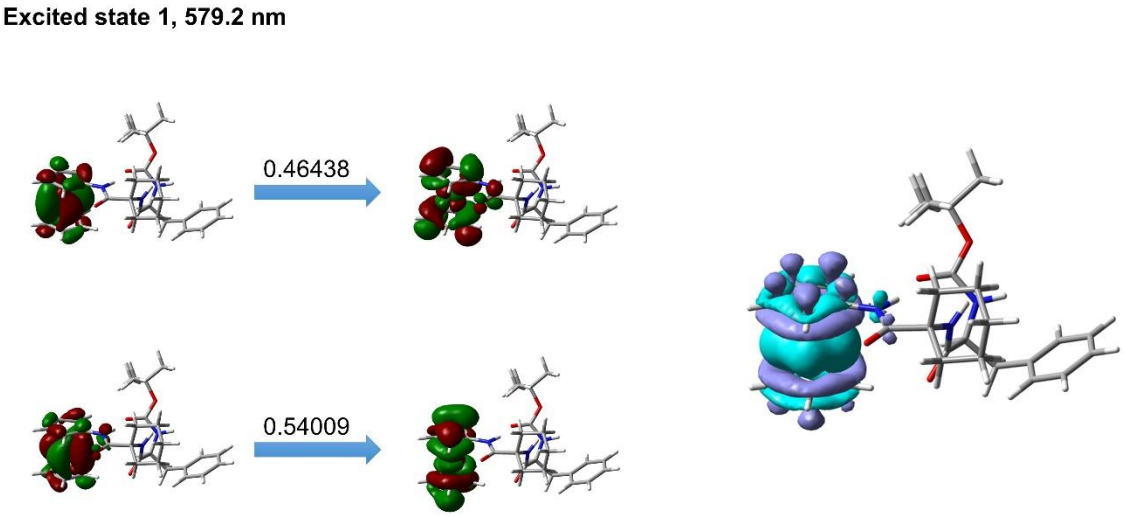

Figure S26. Excited states 1 of the conformer **5-1**.

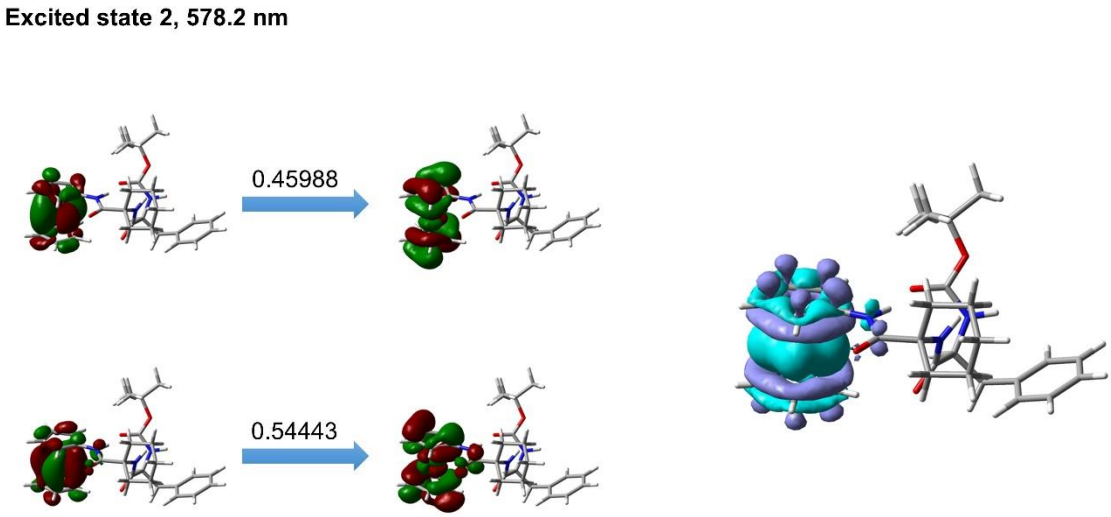

Figure S27. Excited states 2 of the conformer **5-1**.

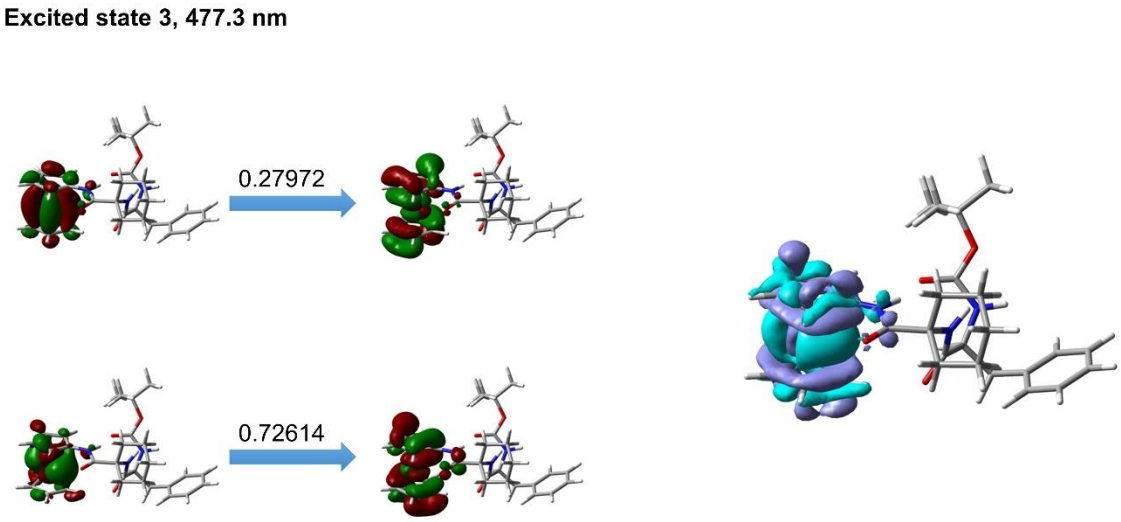

Figure S28. Excited states 3 of the conformer **5**-**1**.

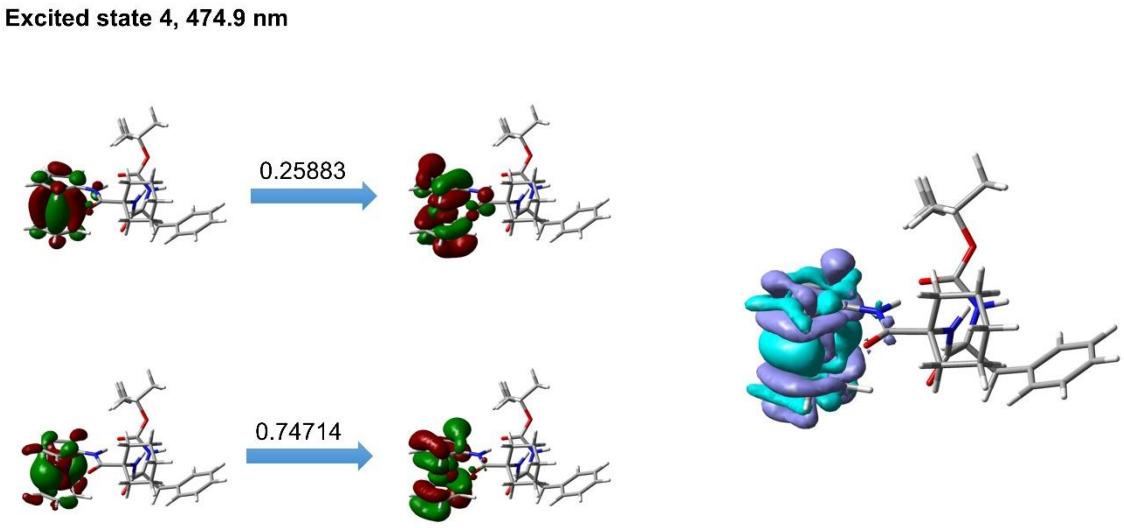

Figure S29. Excited states 4 of the conformer **5**-**1**.

Excited state 5, 355.5 nm

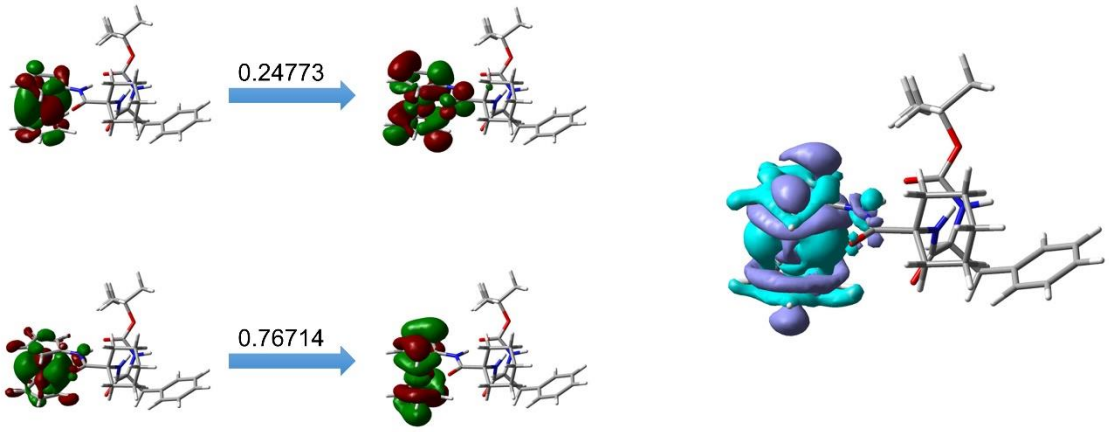

Figure S30. Excited states 5 of the conformer **5**-**1**.

Excited state 6, 352.6 nm

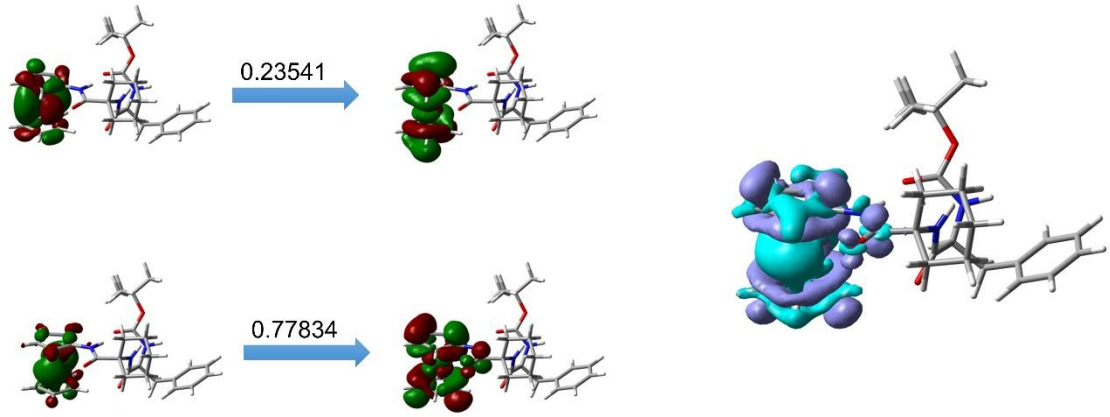

Figure S31. Excited states 6 of the conformer **5**-**1**.

3. UV/Vis spectra

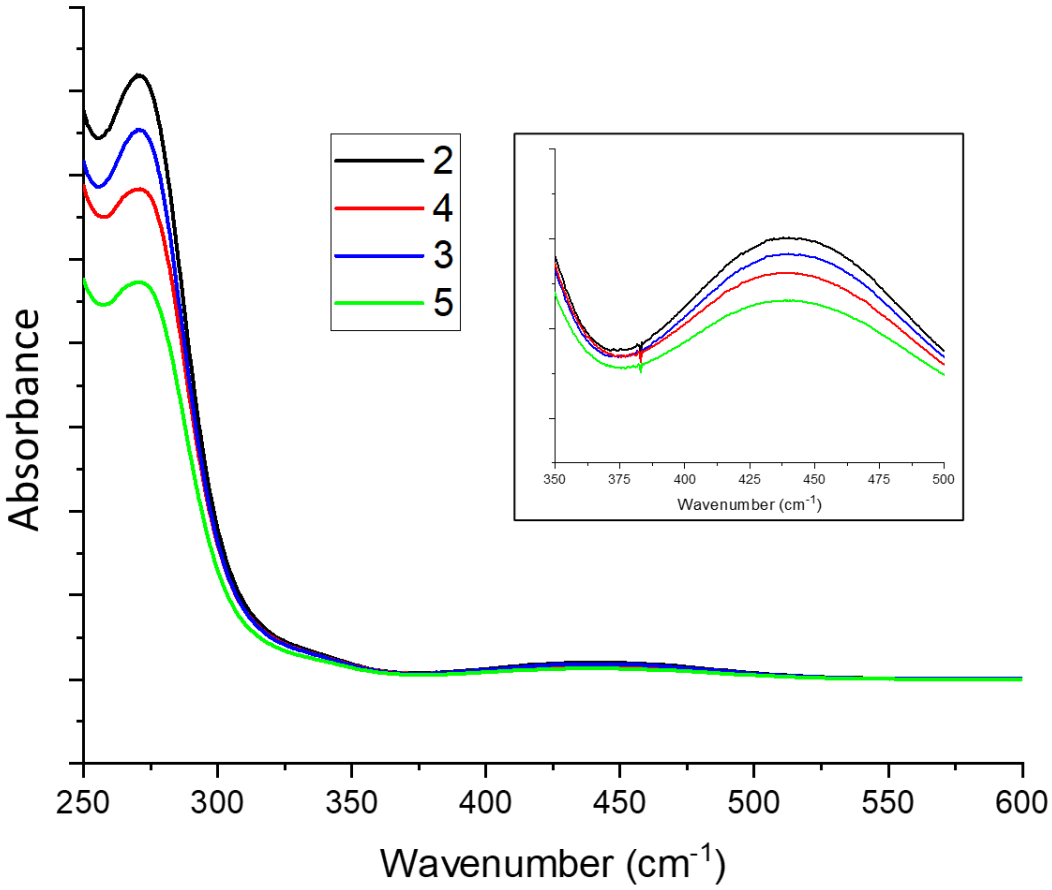

Figure S32. UV/Vis spectra of compounds **2**-**5** in $CHCl_3$.