

Supplementary Materials

Functionalization of Rhodamine Platform with 3-Hydroxy-4-pyridinone Chelating Units and Its Fluorescence Behavior towards Fe(III)

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S1. NMR spectra of rosamine 1

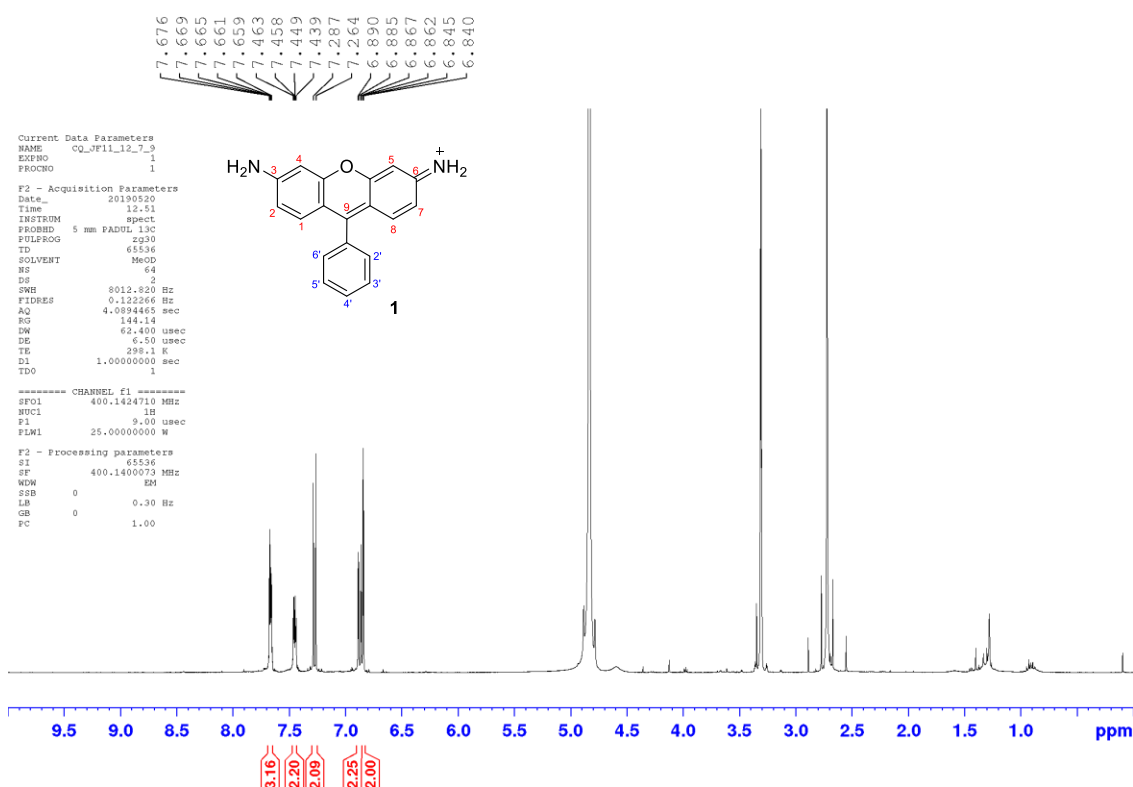


Figure S1. ^1H NMR spectrum (400.15 MHz, CD_3OD) of **1**.

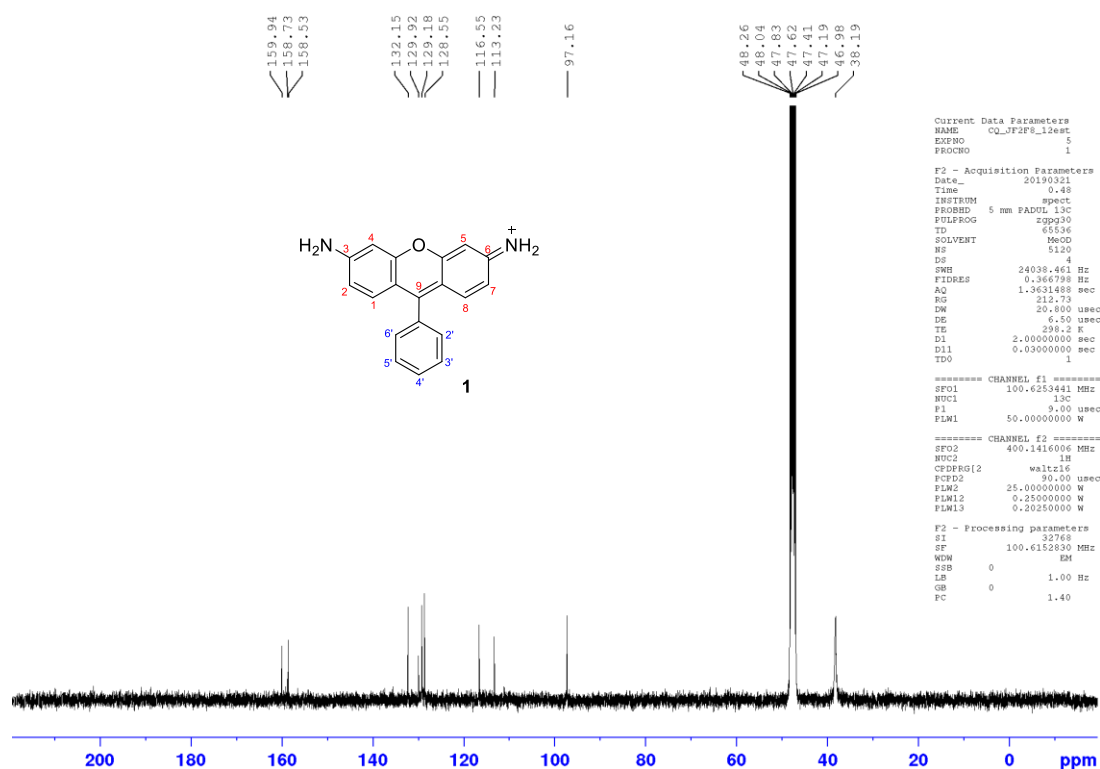


Figure S2. ^{13}C NMR spectrum (100.15 MHz, CD_3OD) of **1**.

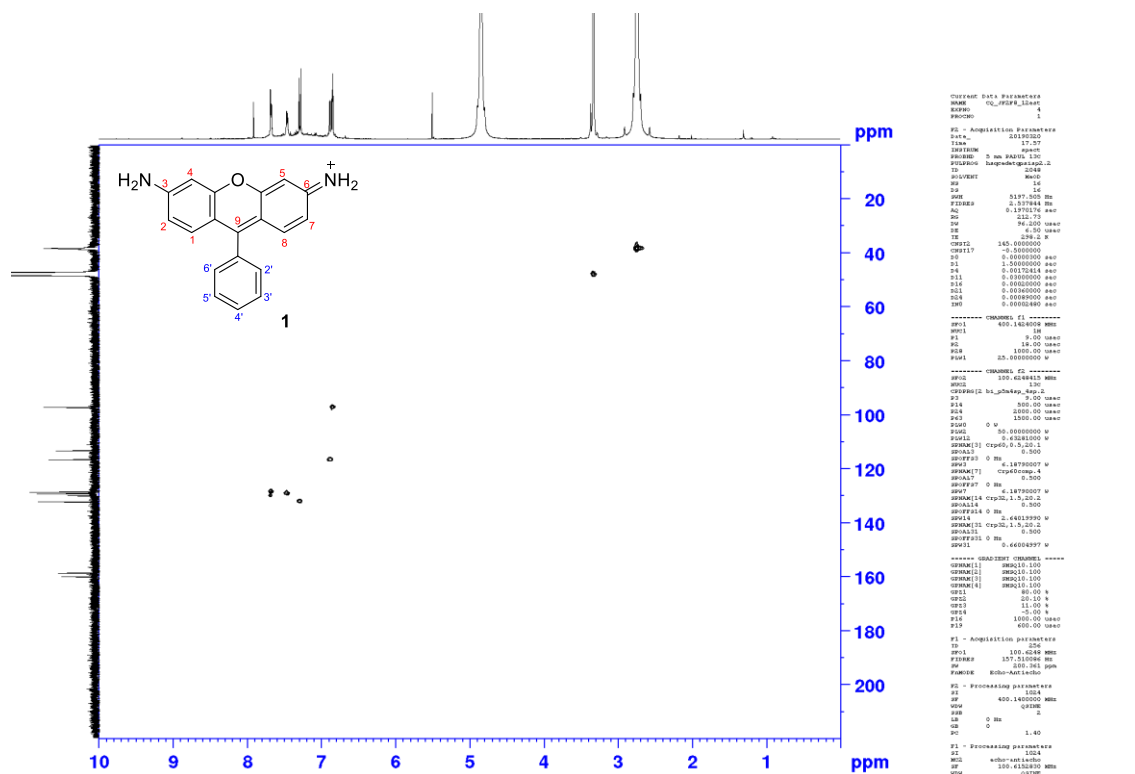


Figure S3. HSQC (^1H , ^{13}C) spectrum of **1**.

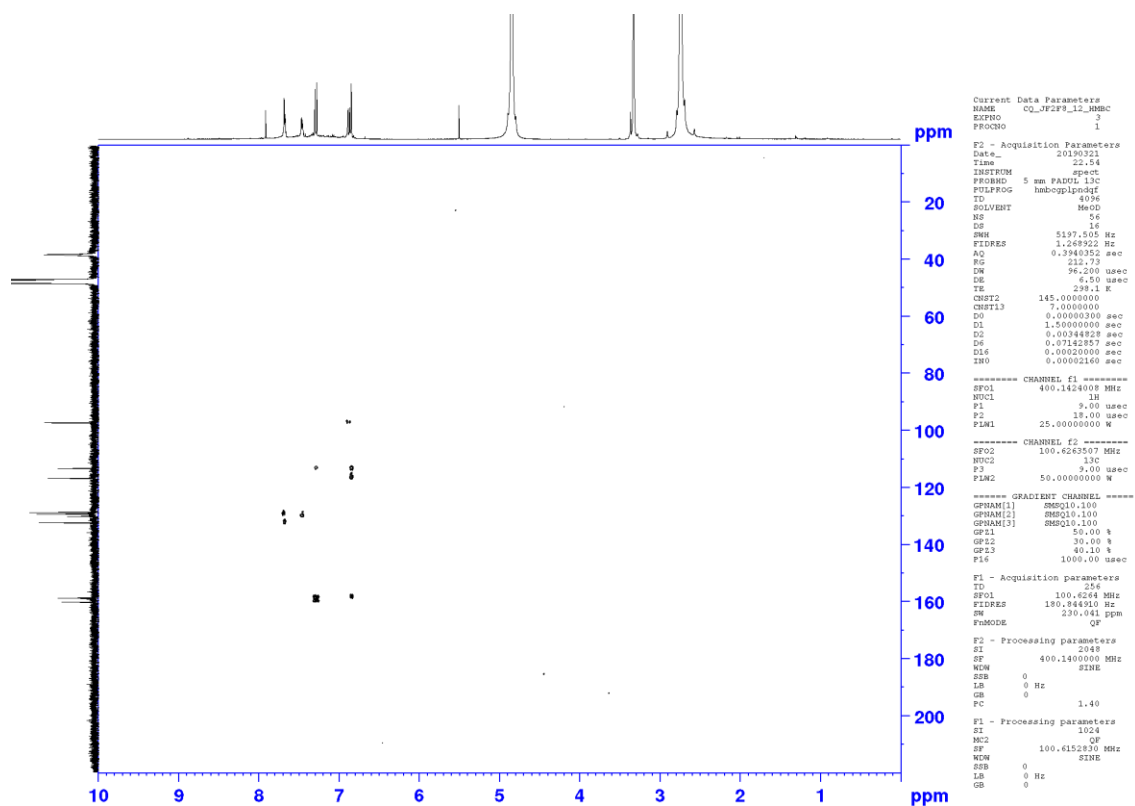


Figure S4. HMBC (^1H , ^{13}C) spectrum of **1**.

S2. NMR spectra of dihydrorosamine 2

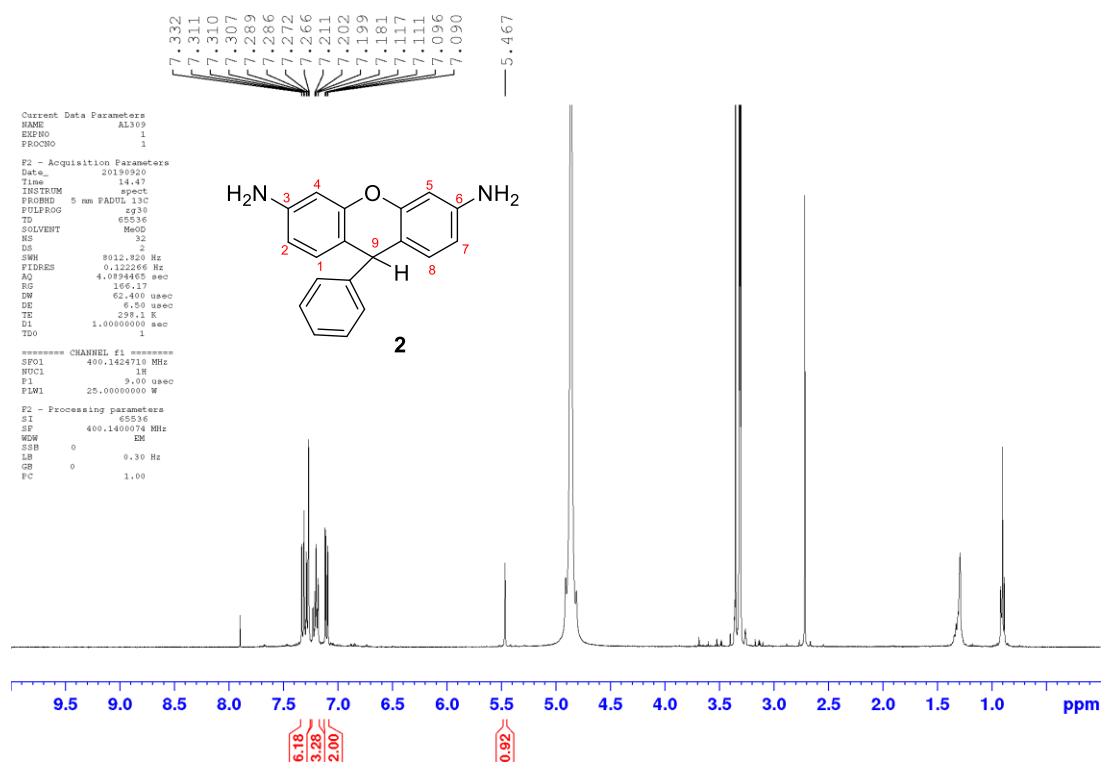


Figure S5. ¹H NMR spectrum (400.15 MHz, CD₃OD) of 2.

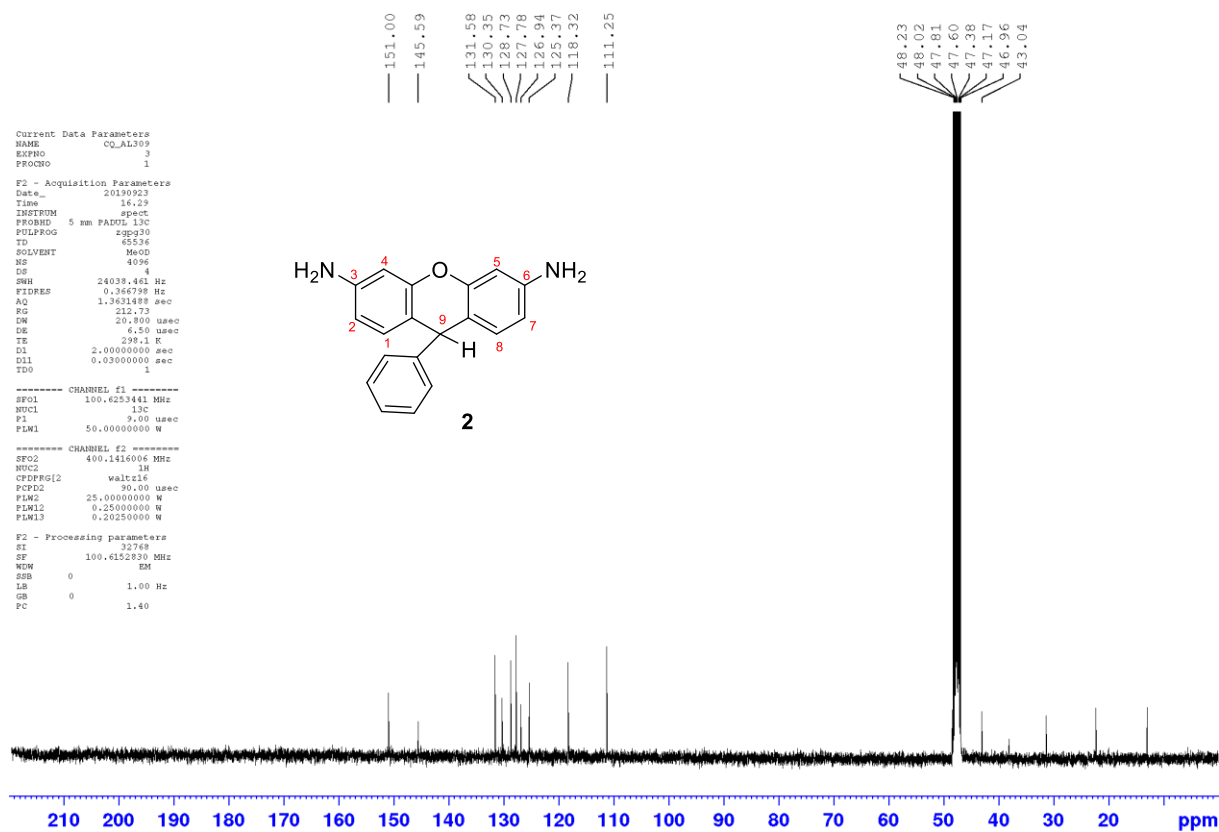


Figure S6. ¹³C NMR spectrum (100.15 MHz, CD₃OD) of 2.

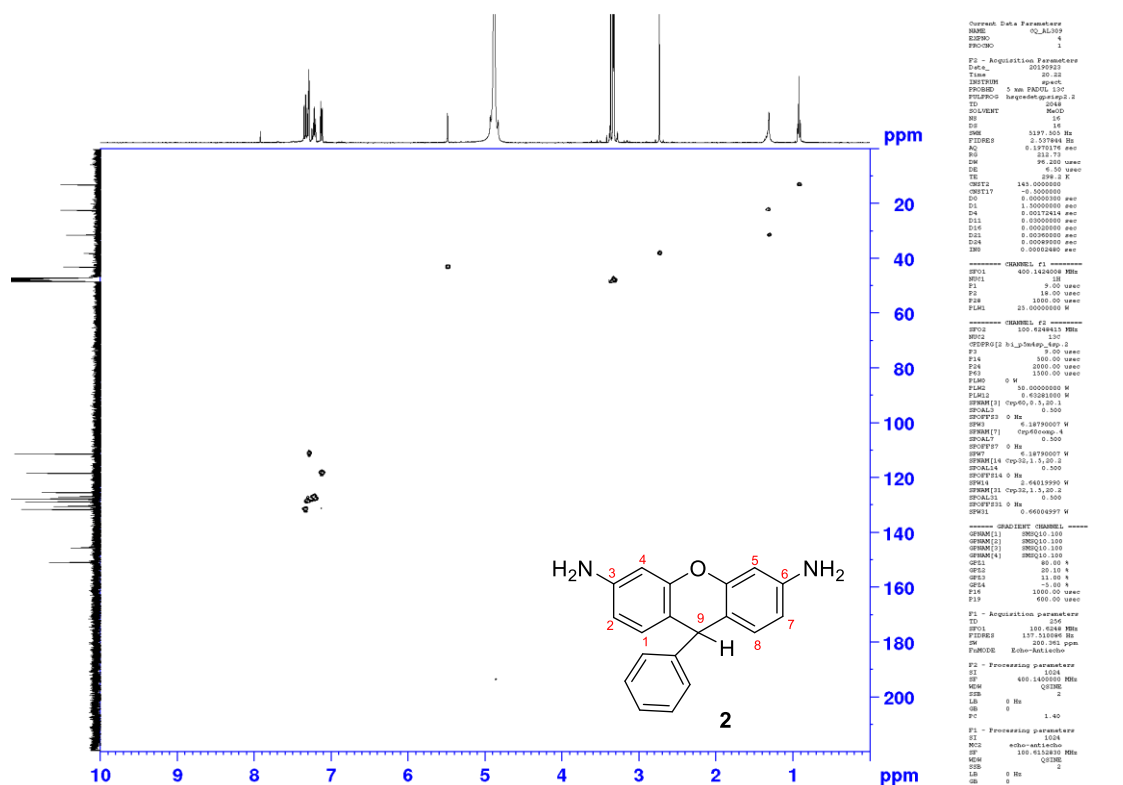


Figure S7. HSQC (^1H , ^{13}C) spectrum of **2**.

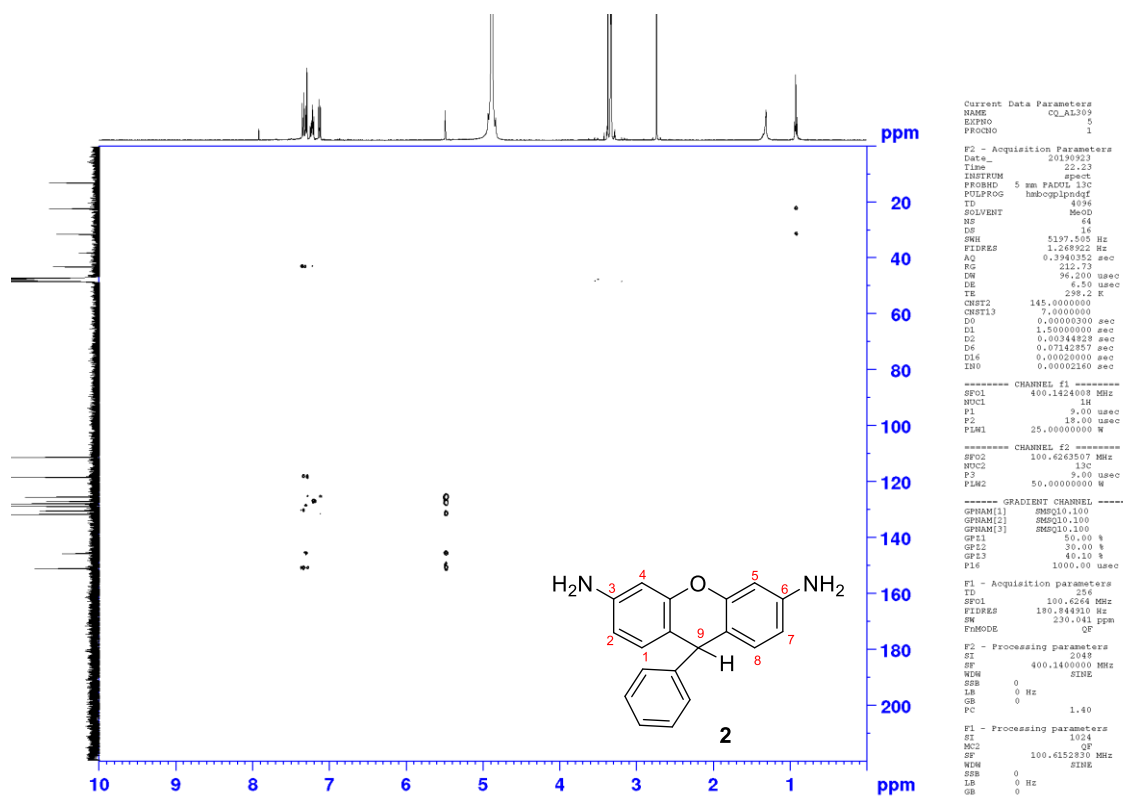


Figure S8. HMBC (^1H , ^{13}C) spectrum of **2**.

S3. NMR spectra of conjugate **3**

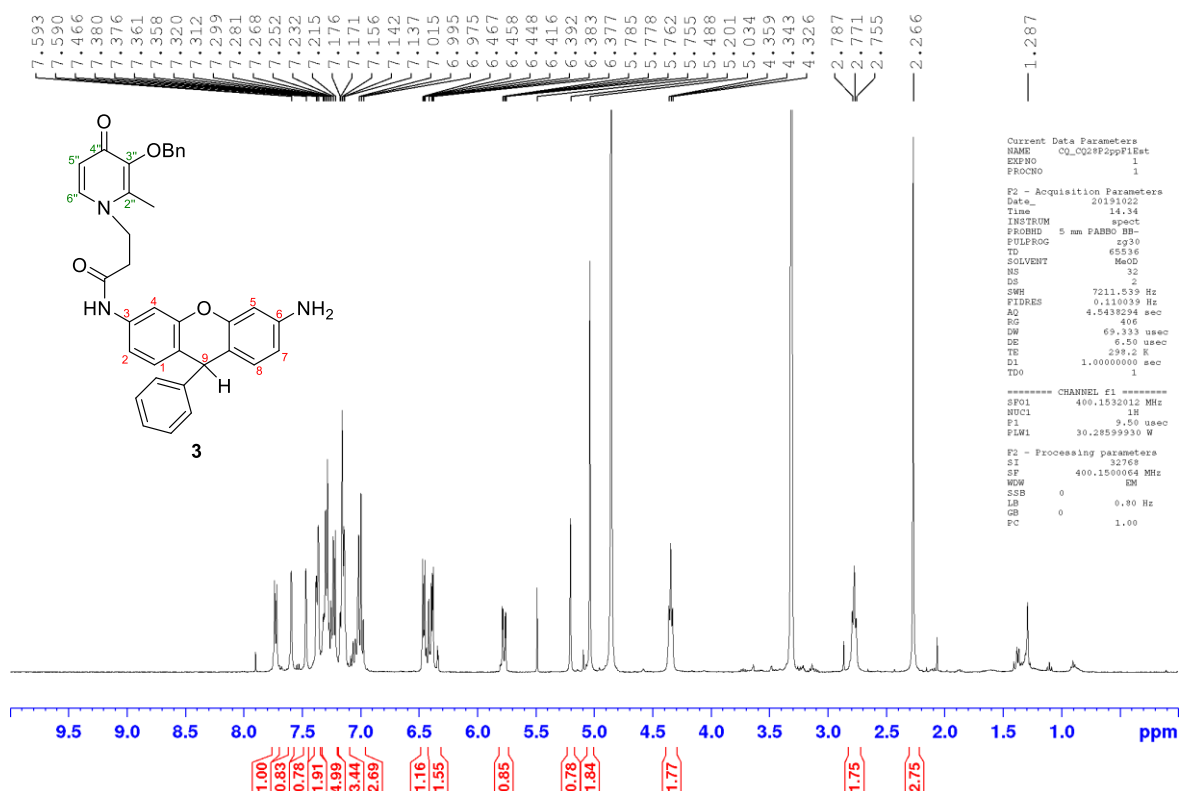


Figure S9. ¹H NMR spectrum (400.15 MHz, CD₃OD) of **3**.

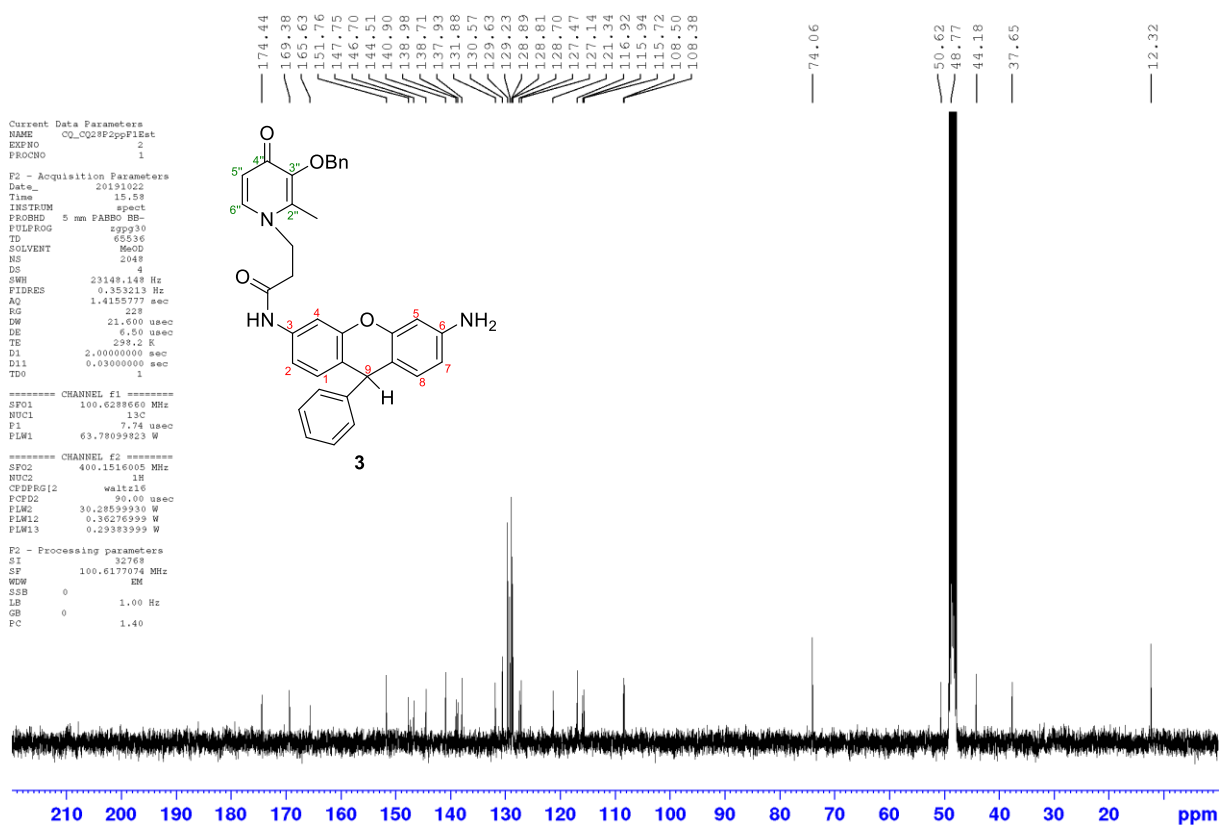


Figure S10. ¹³C NMR spectrum (100.15 MHz, CD₃OD) of **3**.

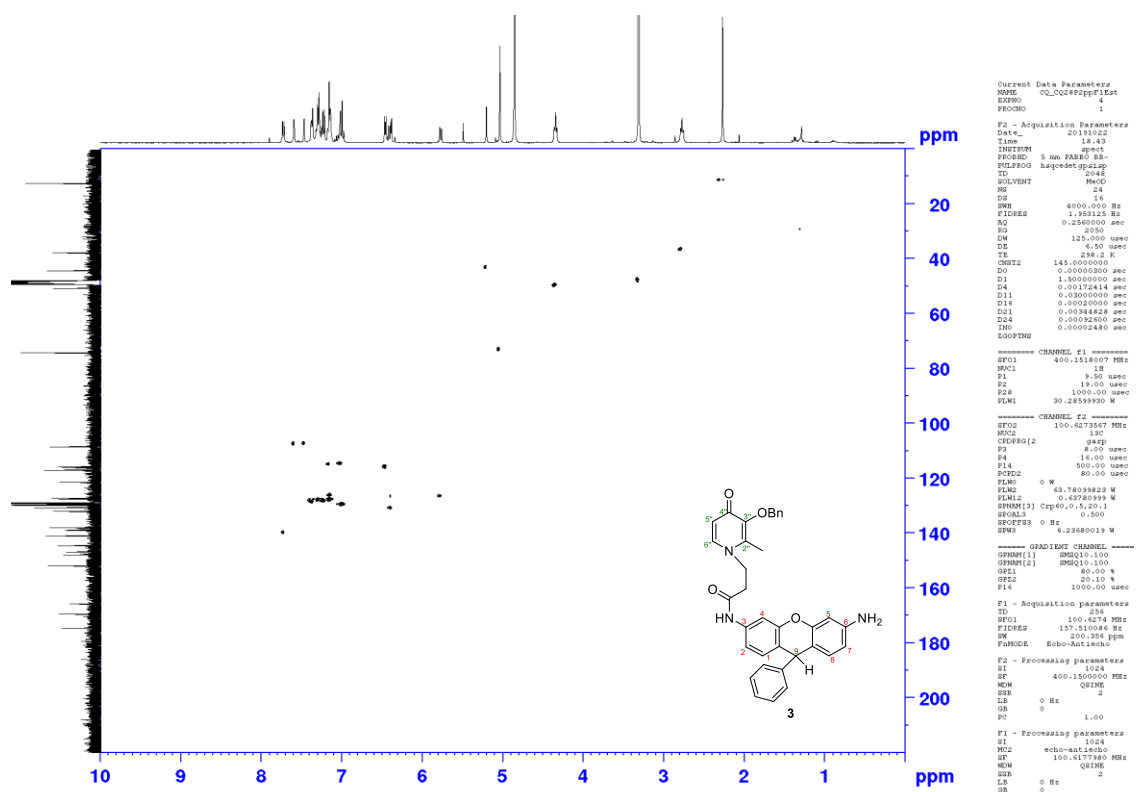


Figure S11. HSQC (^1H , ^{13}C) spectrum of **3**.

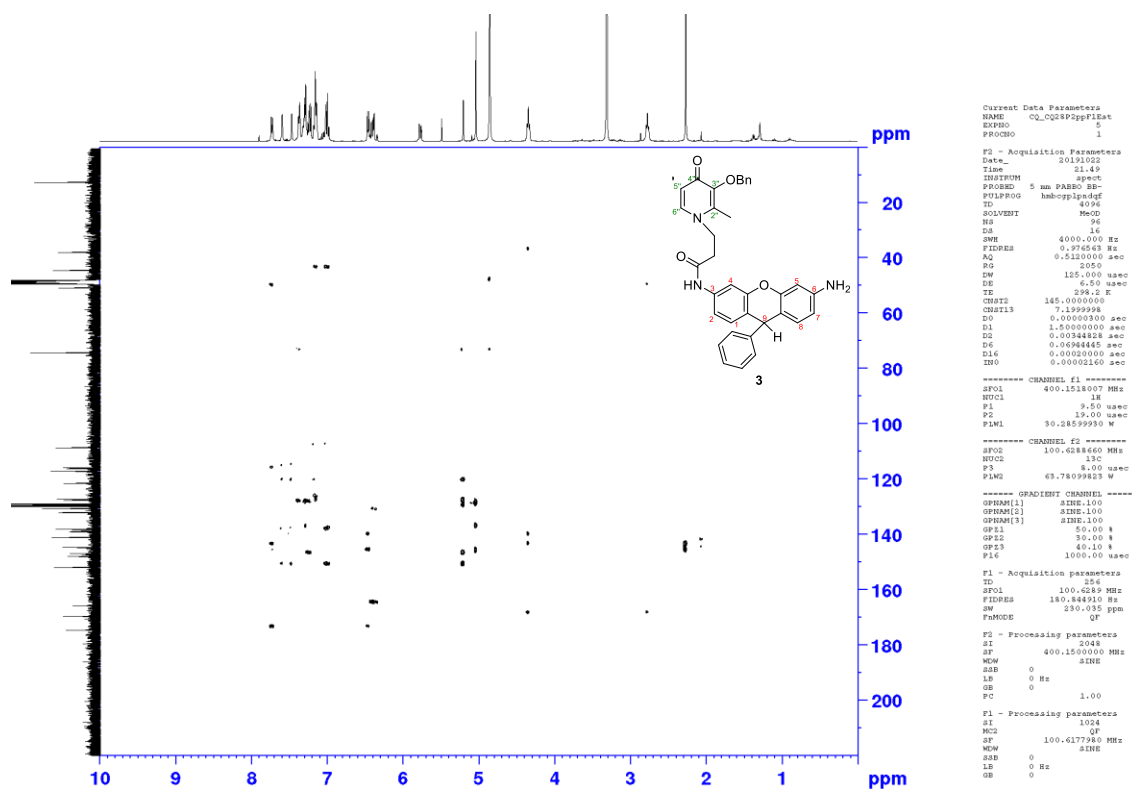


Figure S12. HMBC (^1H , ^{13}C) spectrum of **3**.

S4. NMR spectra of conjugate 4

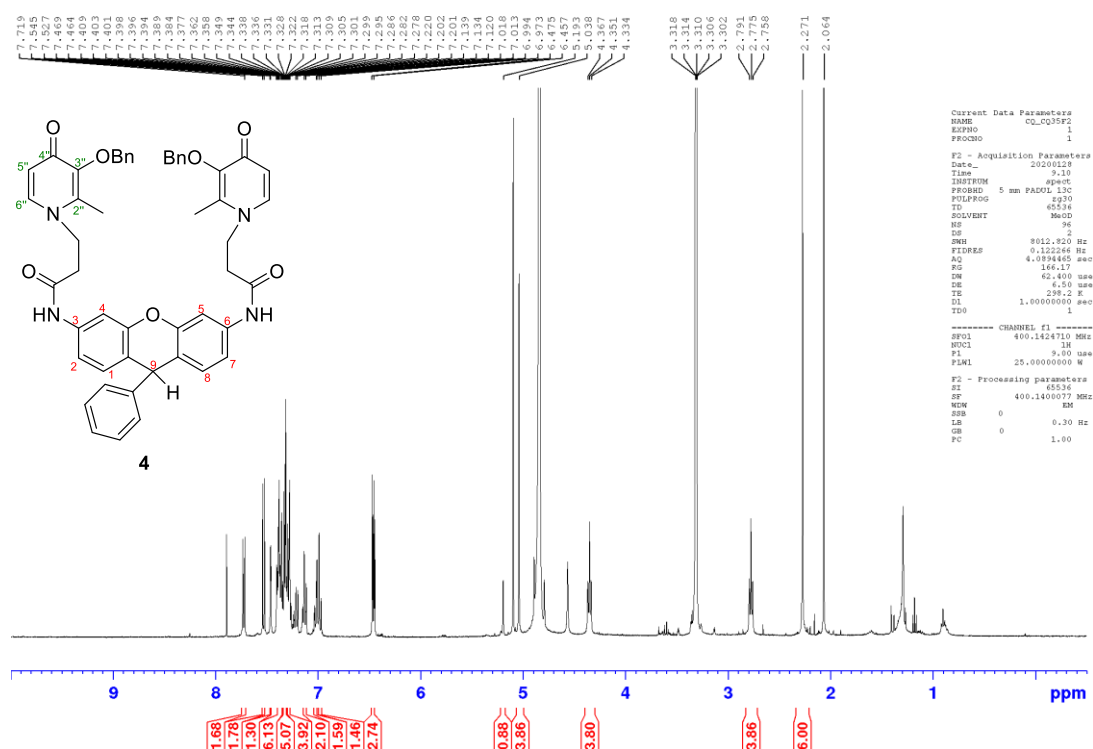


Figure S13. ¹H NMR spectrum (400.15 MHz, CD₃OD) of 4.

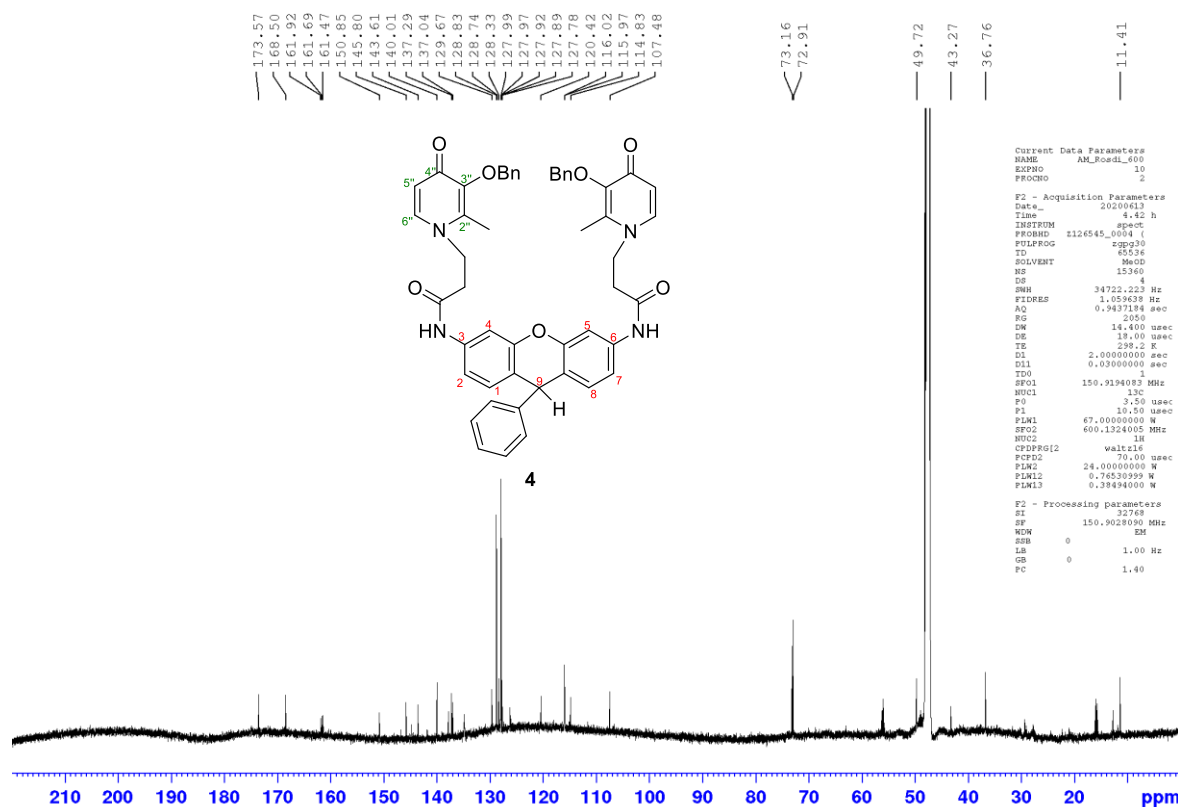


Figure S14. ¹³C NMR spectrum (150.92 MHz, CD₃OD) of 4.

S5. NMR spectra of conjugate 5

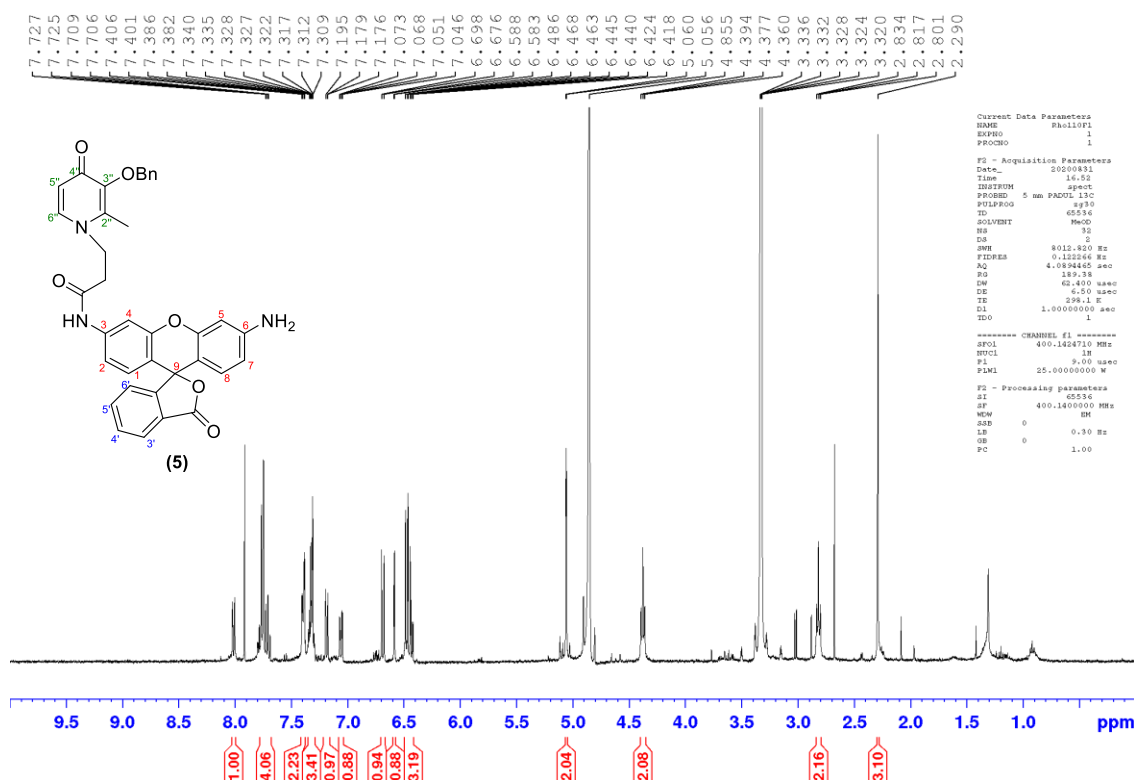


Figure S15. ¹H NMR spectrum (400.15 MHz, CD₃OD) of 5.

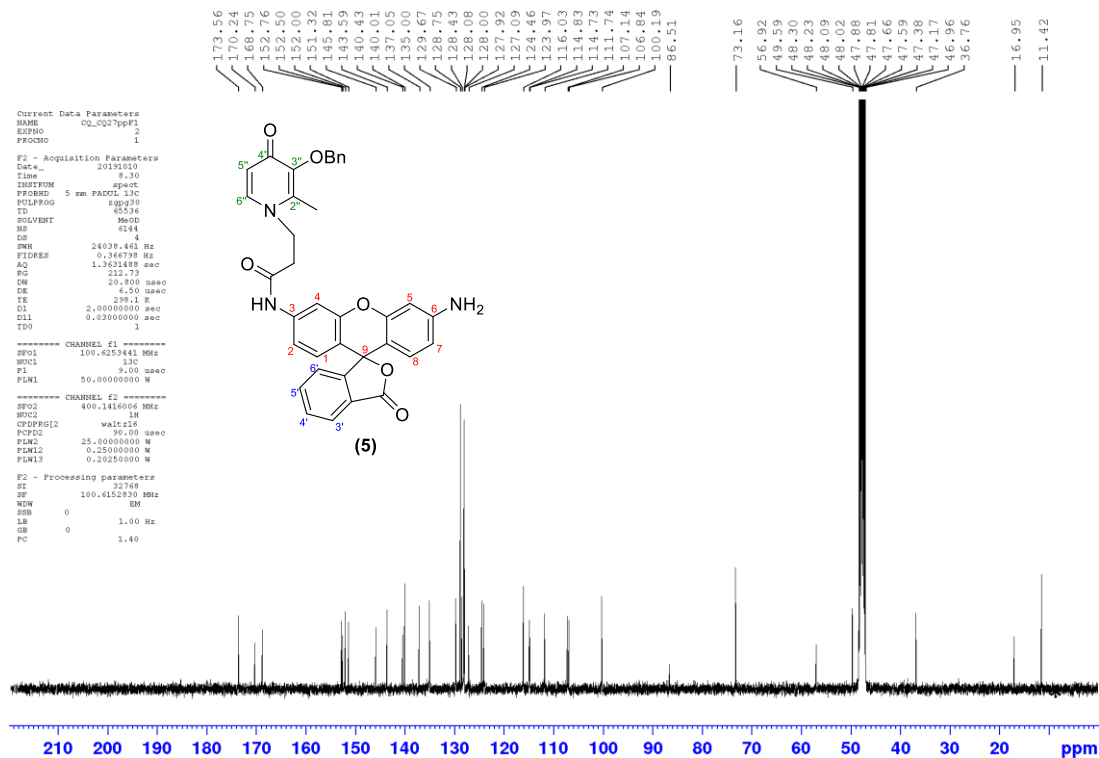


Figure S16. ¹³C NMR spectrum (100.15 MHz, CD₃OD) of 5; * denote residual solvent (ethanol).

S6. NMR spectra of conjugate 6

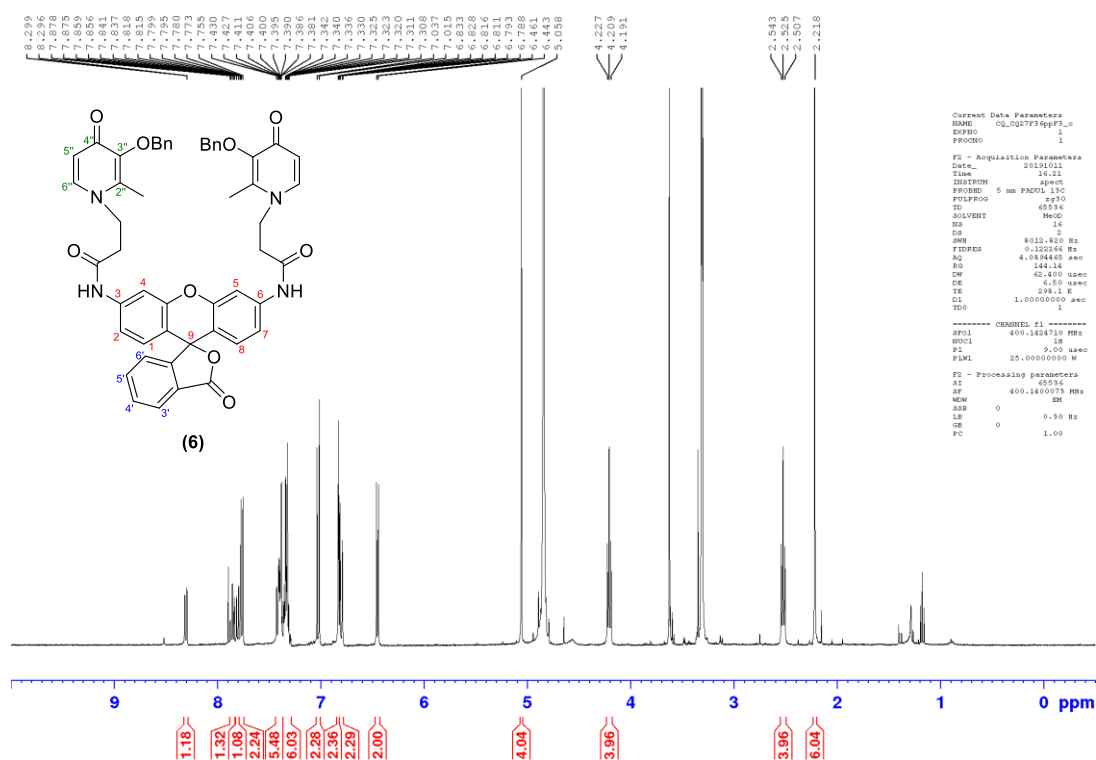


Figure S19. ¹H NMR spectrum (400.15 MHz, CD₃OD) of 6.

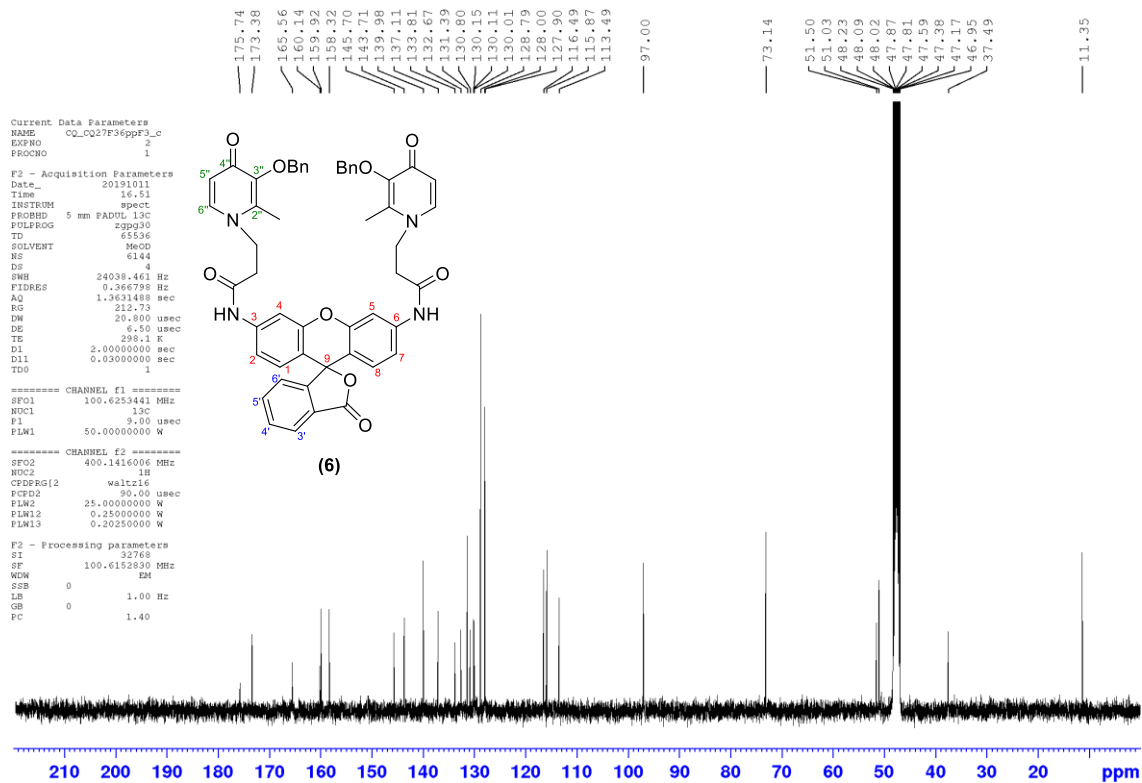


Figure S20. ¹³C NMR spectrum (100.15 MHz, CD₃OD) of 6.

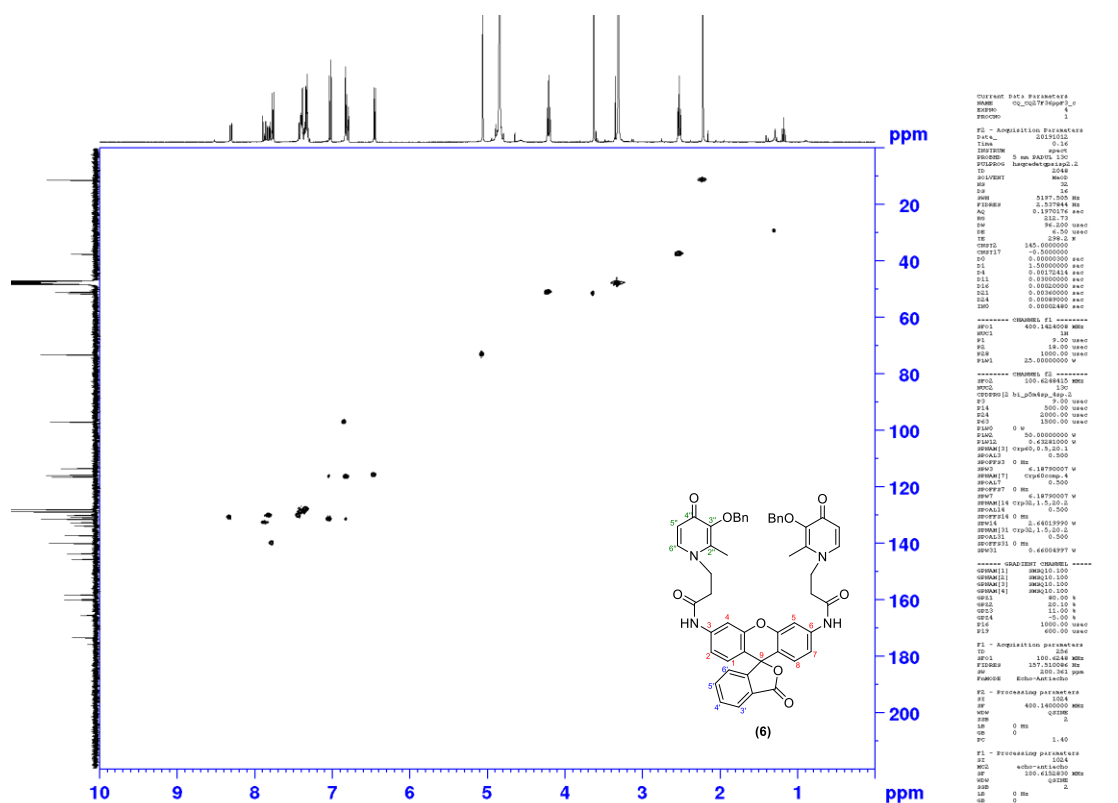


Figure S21. HSQC (^1H , ^{13}C) spectrum of **6**.

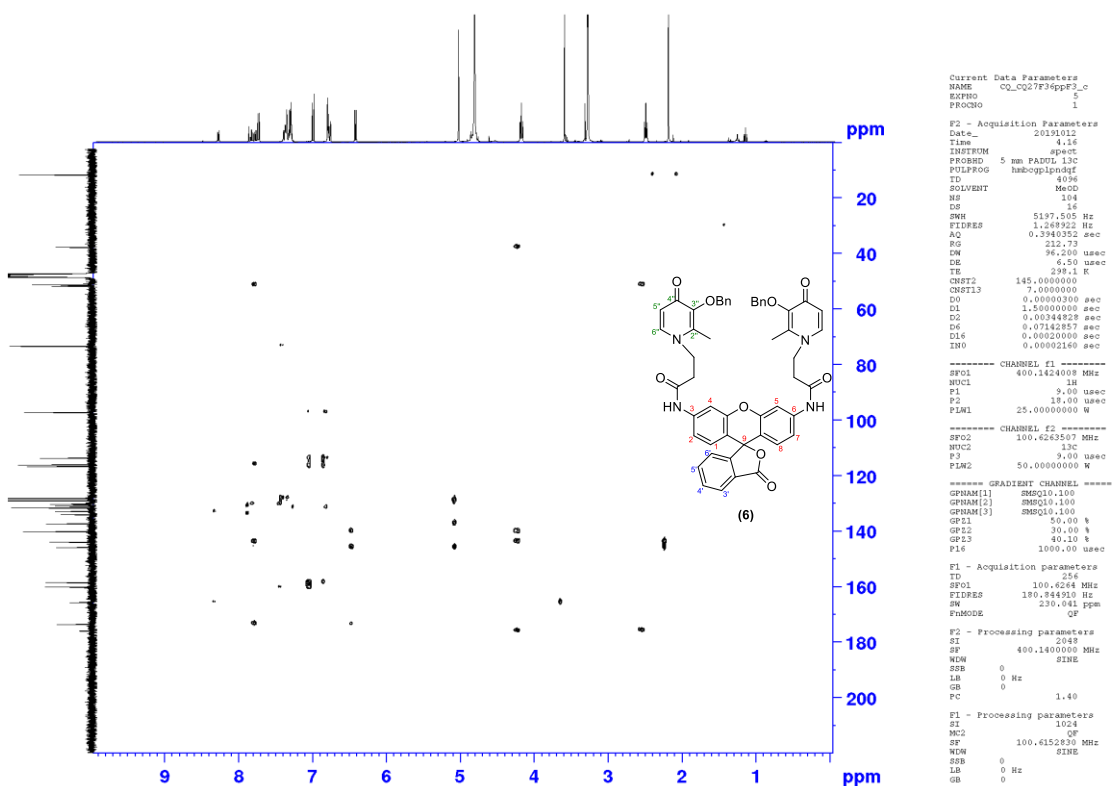


Figure S22. HMBC (^1H , ^{13}C) spectrum of **6**.

S7. NMR spectra of Rho110_monoHPO

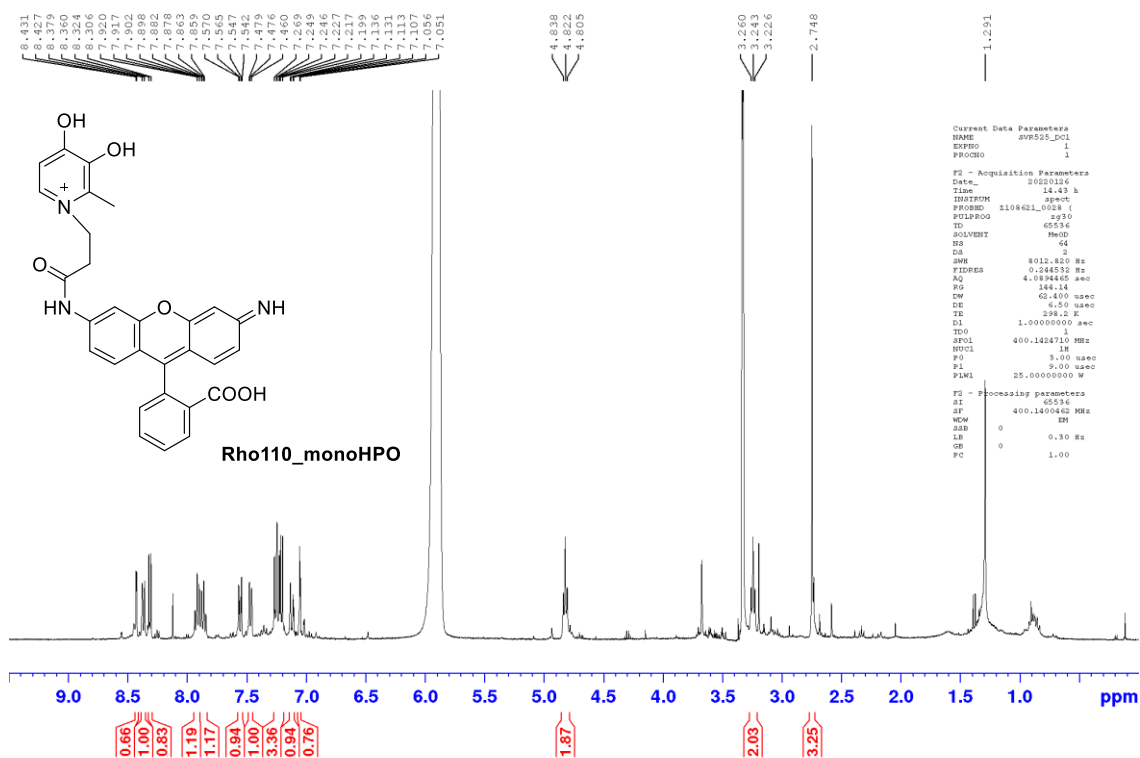


Figure S23. ¹H NMR spectrum (400.15 MHz, CD₃OD+DCI) of Rho110-monoHPO.

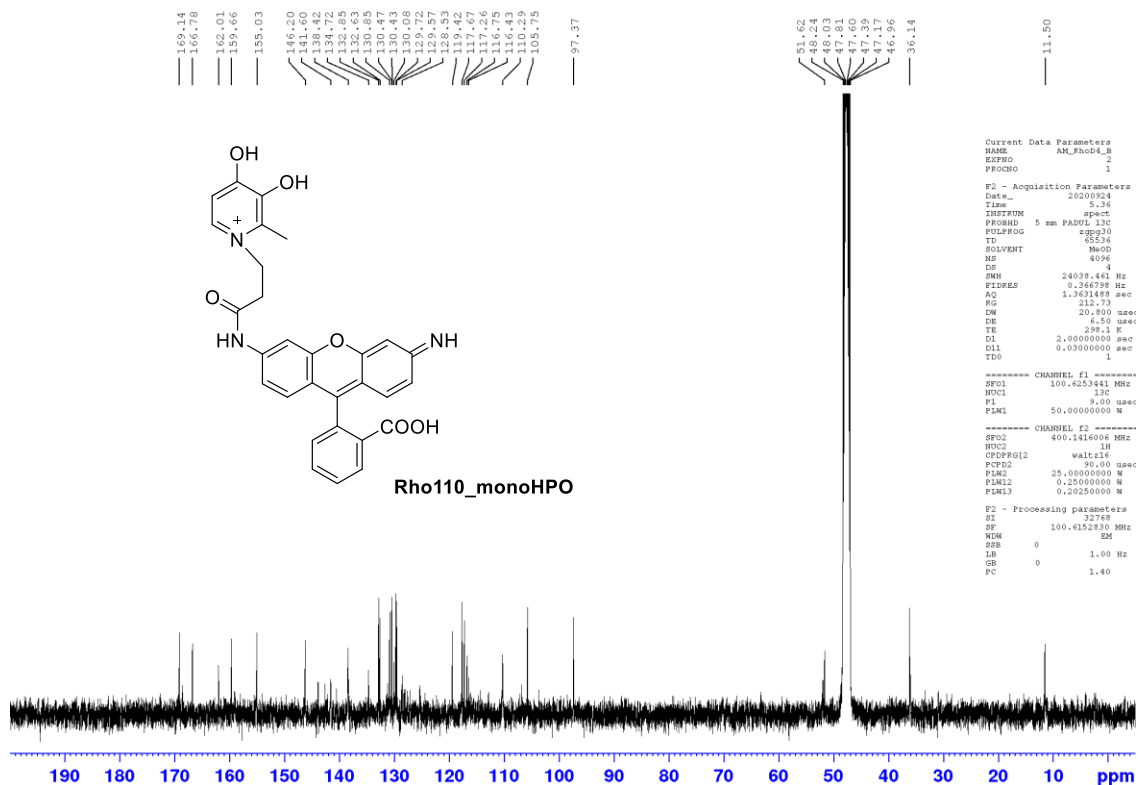


Figure S24. ¹³C NMR spectrum (100.15 MHz, CD₃OD) of Rho110-monoHPO.

S8. Comparison of the ^1H NMR spectra of rosamine **1** and dihydrorosamine **2**

According to Figure S25, the ^1H NMR spectrum of rosamine **1** shows three signals at 6.84-7.28 ppm, that are typical of the xanthene scaffold and two signals at 7.44-7.68 ppm, attributed to the phenyl ring. After hydrogenation, the ^1H NMR spectrum of the resulting dihydrorosamine **2** shows an additional singlet at 5.48 ppm corresponding to the resonance of 9-H proton, together with slight changes in the chemical shifts of the remaining aromatic signals, due to the interruption of π -conjugation of the xanthene core.

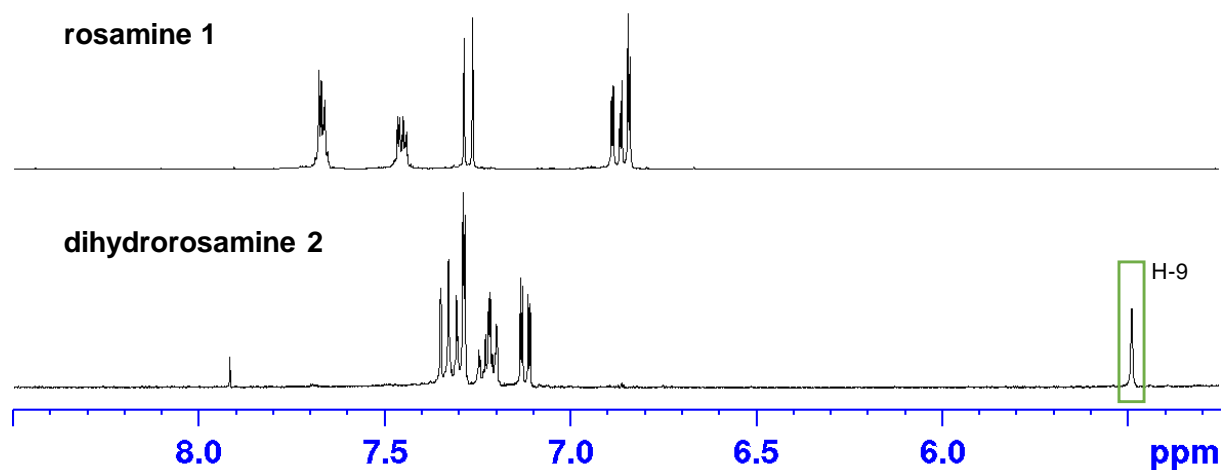


Figure S25. Comparison of the ^1H NMR spectra of **1** and **2**.

S9. Comparison of the ^1H NMR spectra of mono- and disubstituted derivatives
3 and 4

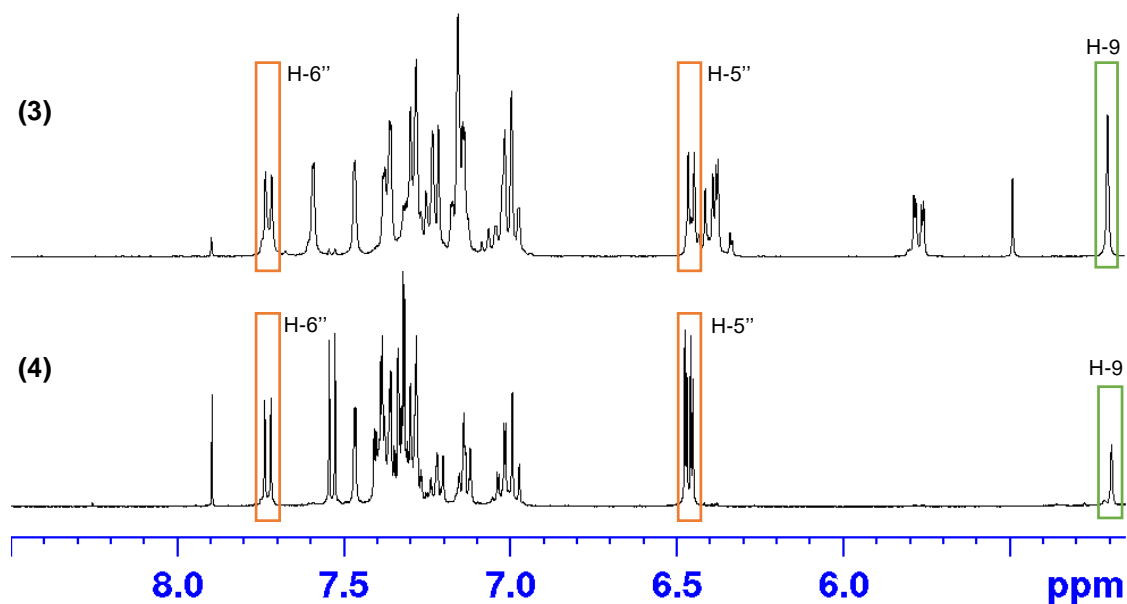


Figure S26. Aromatic region of the ^1H NMR spectrum of mono- and disubstituted derivatives 3 and 4, in CD_3OD .

S10. Comparison of the ^1H NMR spectra of mono- and disubstituted derivatives
5 and 6

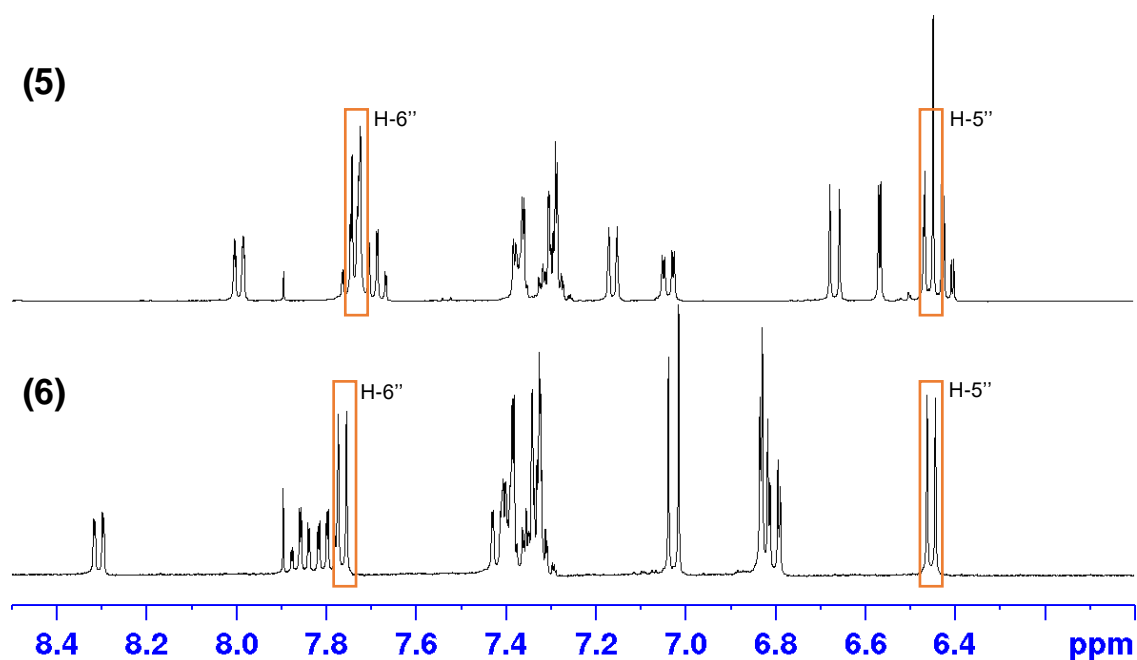


Figure S27. Aromatic region of the ^1H NMR spectrum of mono- and disubstituted derivatives 5 and 6, in CD_3OD .

S11. MS spectra of rosamines and conjugates

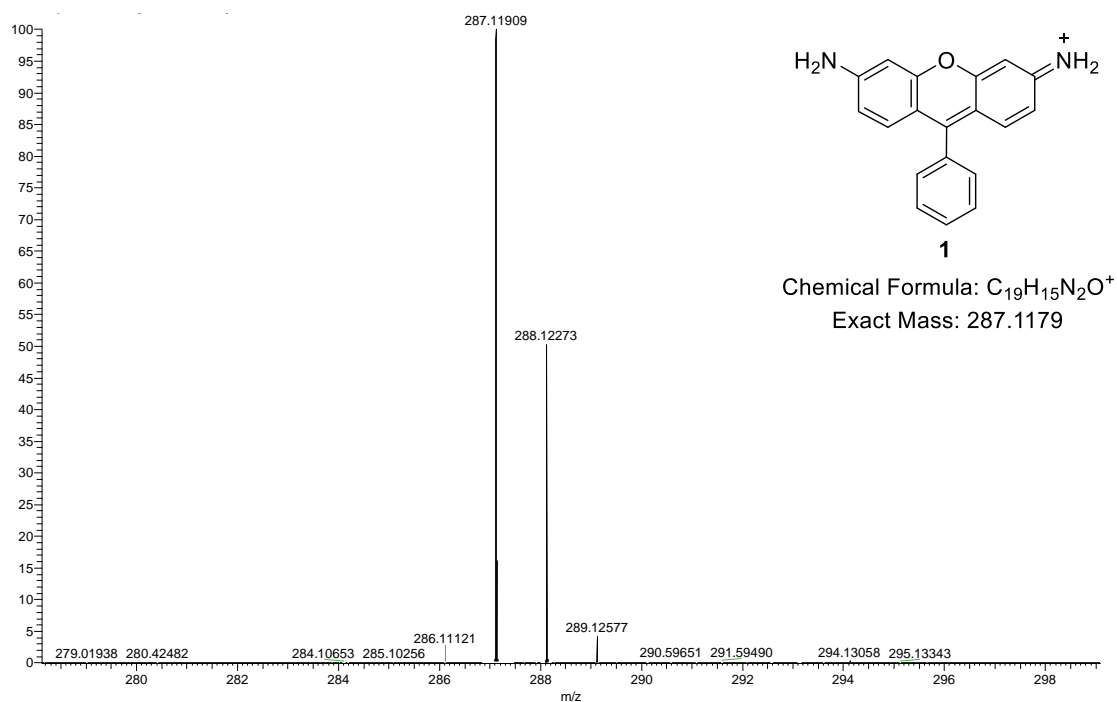


Figure S28. HRMS (ESI) of **1**.

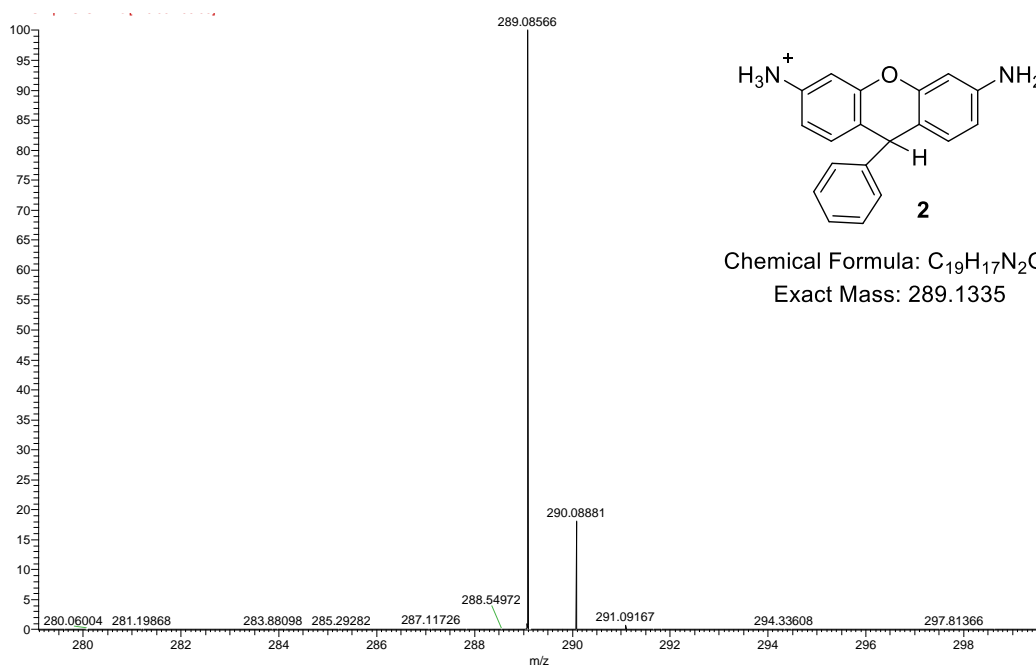


Figure S29. HRMS (ESI) of **2**.

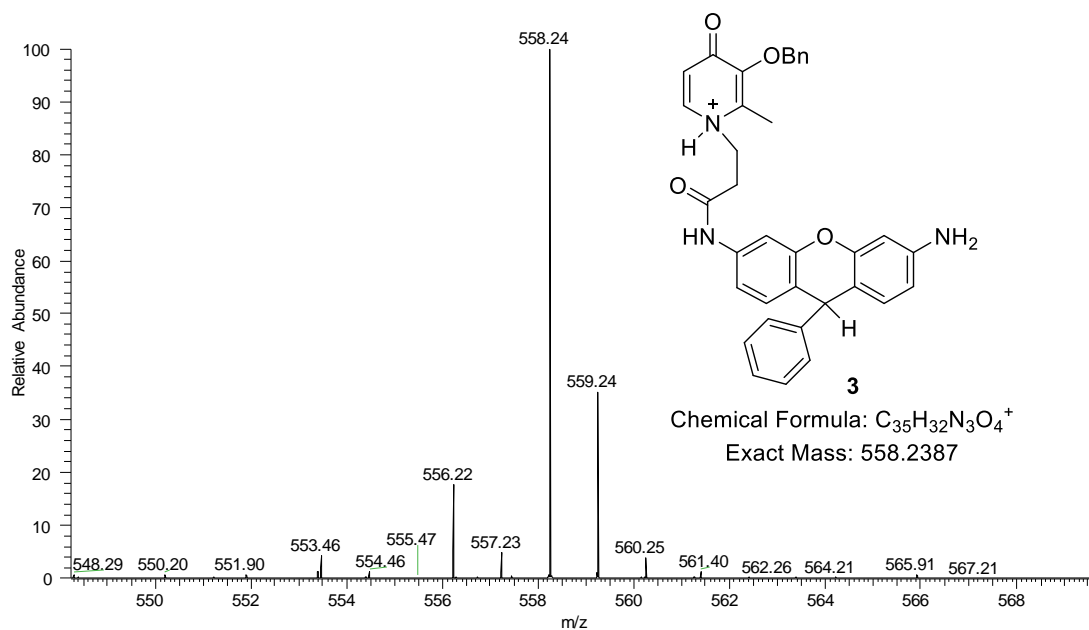


Figure S30. HRMS (ESI) of **3**.

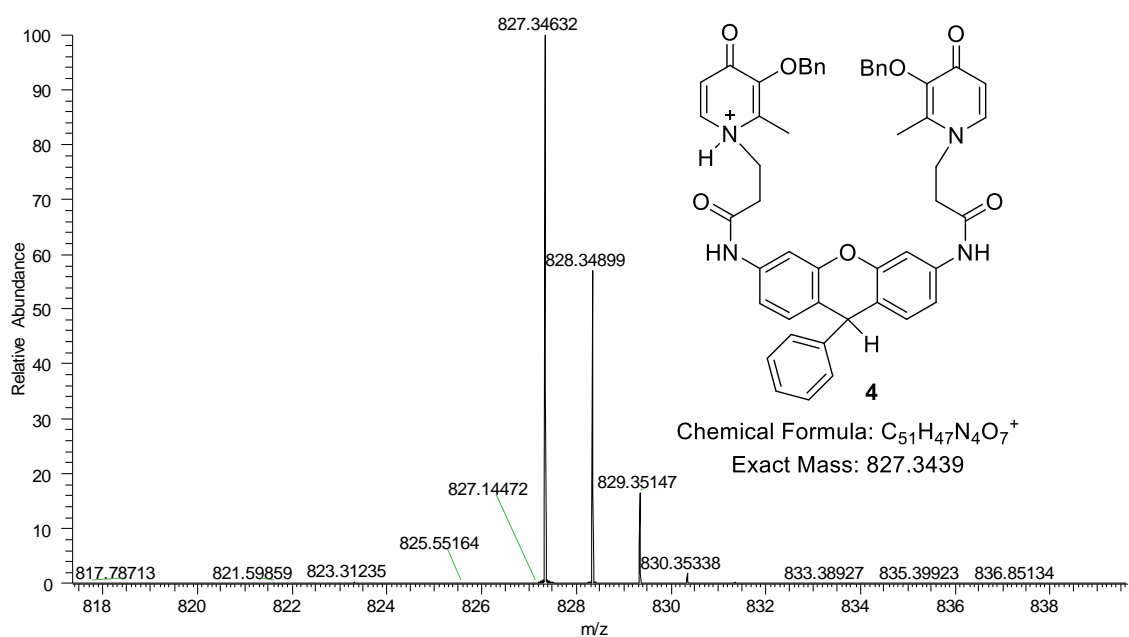


Figure S31. HRMS (ESI) of **4**.

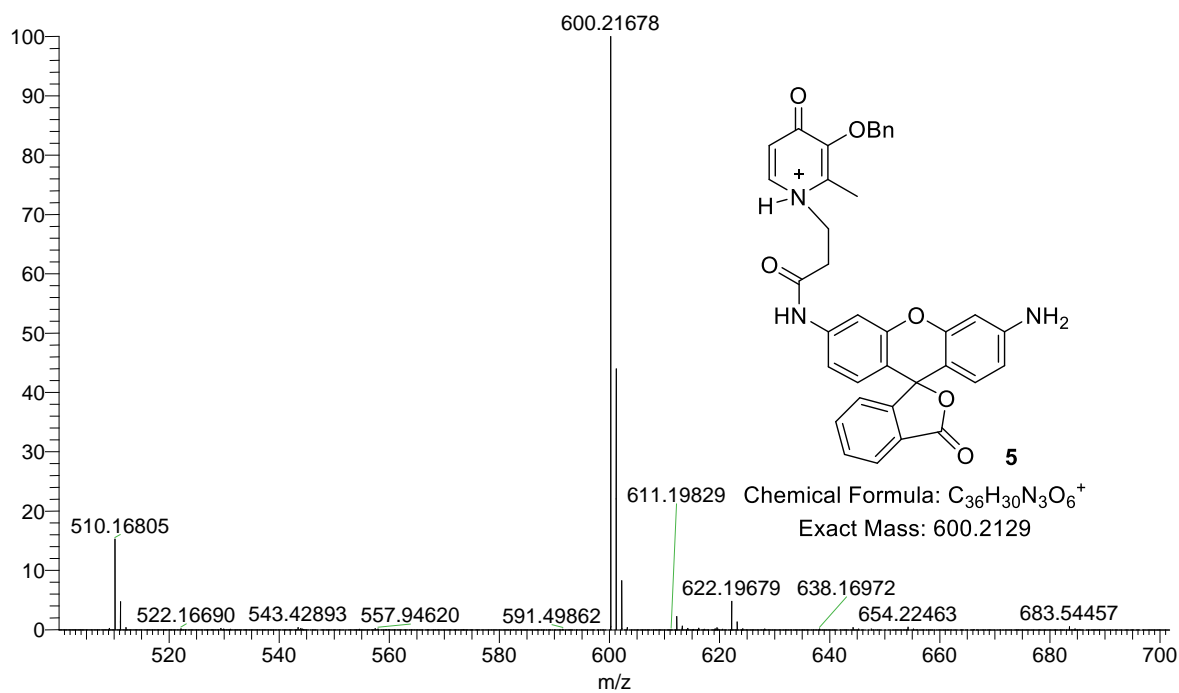


Figure S32. HRMS (ESI) of **5**.

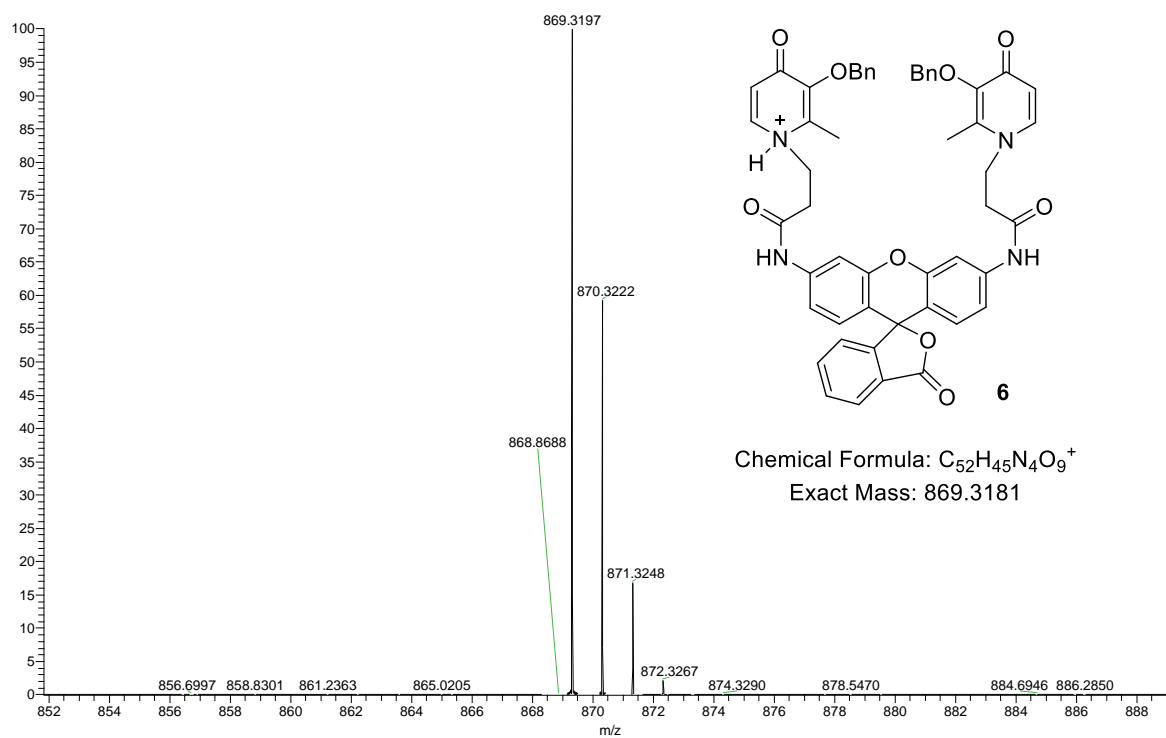


Figure S33. HRMS (ESI) of **6**.

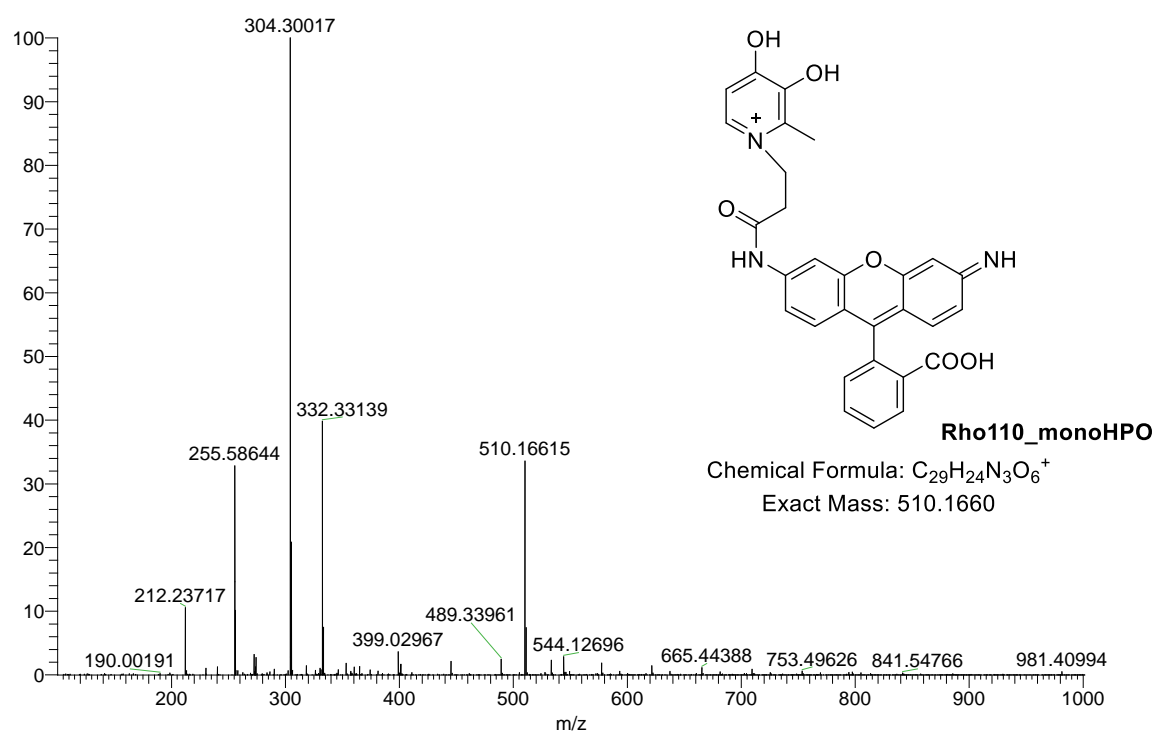


Figure S34. HRMS (ESI) of **Rho110-monoHPO**.

S12. Comparative absorption spectra of **Rho110**, **1**, **2**, **3** and **4**

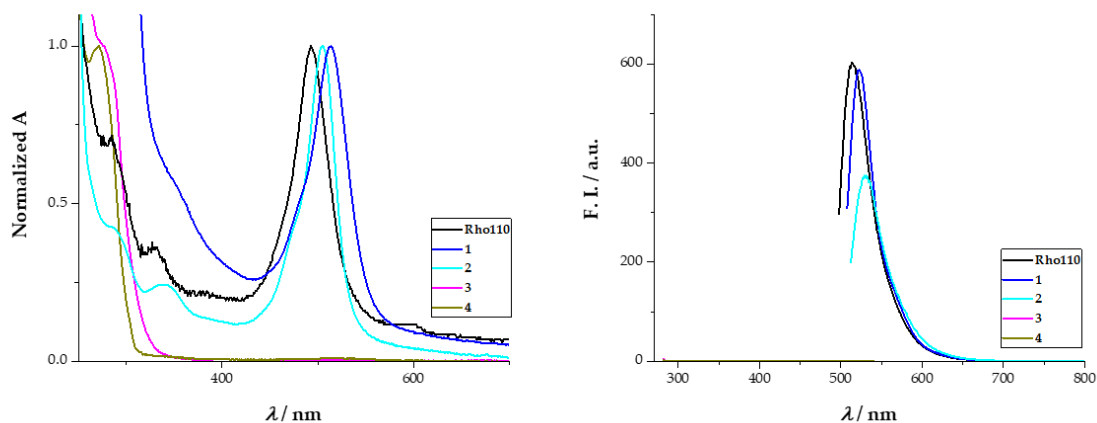


Figure S35. Absorption (normalized) and emission spectra of **Rho110**, **1–4** in CH_2Cl_2 at 25 °C.

S13. Comparative absorption and emission spectra of spirolactone and quinoid forms of **5** and **6**

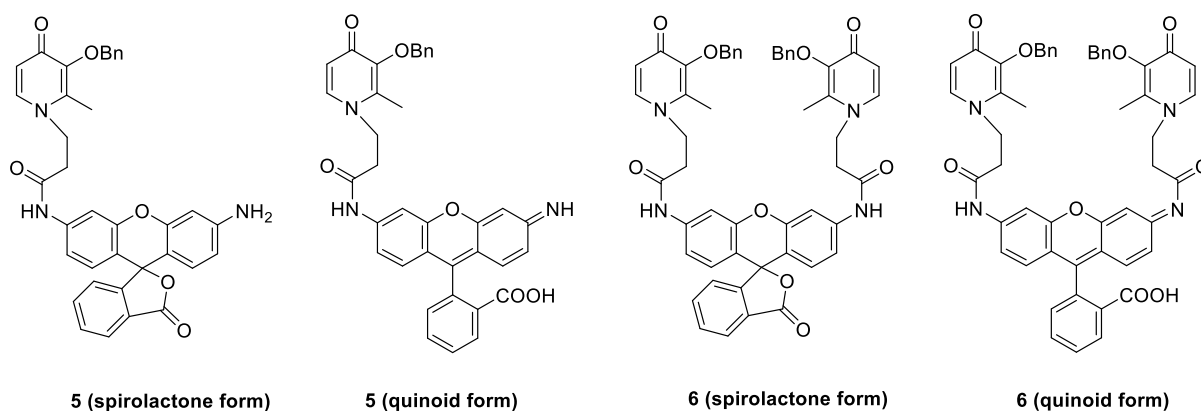
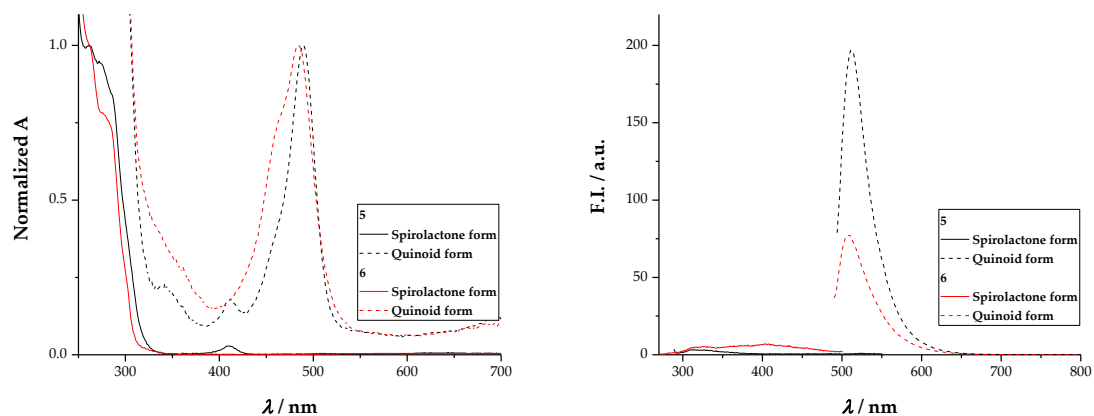


Figure S36. Absorption and emission spectra of **5** and **6** in CH_2Cl_2 before (spirolactone form, full lines) and after an aliquot addition of HCl (37%) (quinoid form, dashed lines) at 25 °C.