Supporting Information

Cationic pyrrolidine/pyrroline-substituted porphyrins as efficient photosensitizers against *E. coli*

Bruno M. L. Ladeira ¹, Cristina J. Dias ¹, Ana T. P. C. Gomes ², Augusto C. Tomé ¹, Maria G. P. M.S. Neves ¹, Nuno M. M. Moura ^{1,*}, A. Almeida ^{2,*} and M. Amparo F. Faustino ^{1,*}

- ¹ LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193, Aveiro, Portugal; brunoladeira@ua.pt (B.L.); cristina.jesus.dias@ua.pt (C.J.D.); gneves@ua.pt (M.G.P.M.S.N.)
- ² CESAM, Department of Chemistry, University of Aveiro, 3810-193, Aveiro, Portugal; ana.peixoto@ua.pt (A.T.P.C.G.)

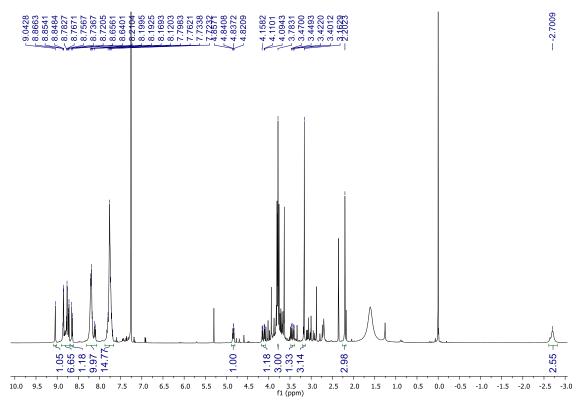


Figure S1. ¹H NMR spectrum of compound 2 in CDCl₃.

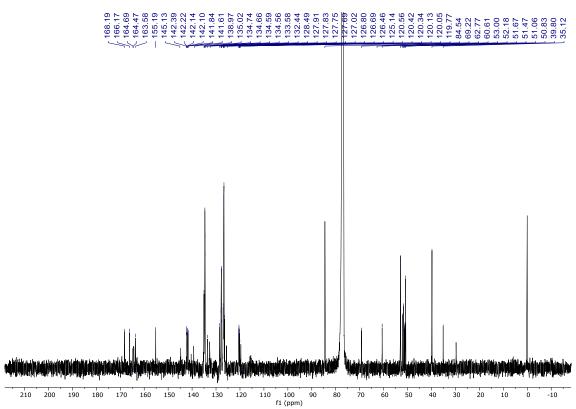


Figure S2. ¹³C NMR spectrum of compound 2 in CDCl₃.

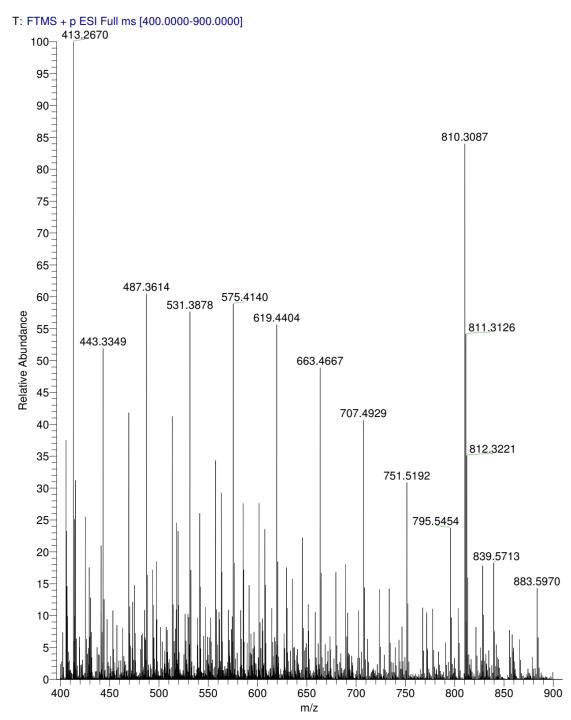


Figure S3. HRMS-ESI(+) spectrum of compound 2.

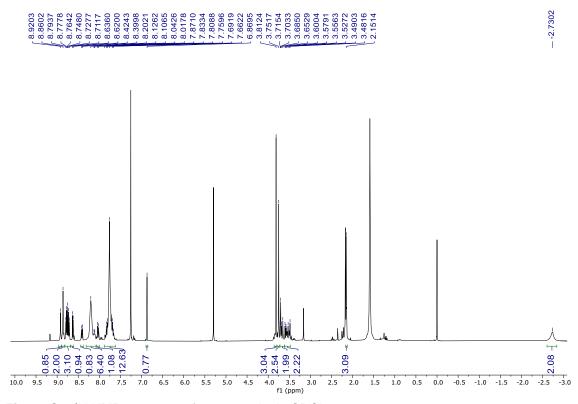


Figure S4. ¹H NMR spectrum of compound 3 in CDCl₃.

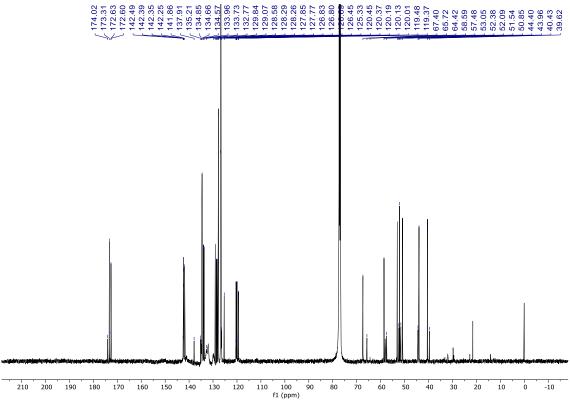


Figure S5. ¹³C NMR spectrum of compound 3 in CDCl₃.

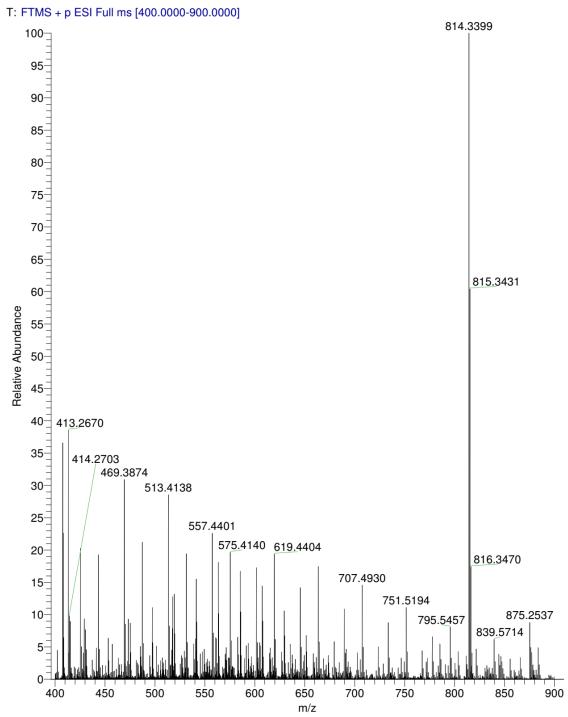


Figure S6. HRMS-ESI(+) spectrum of compound 3.

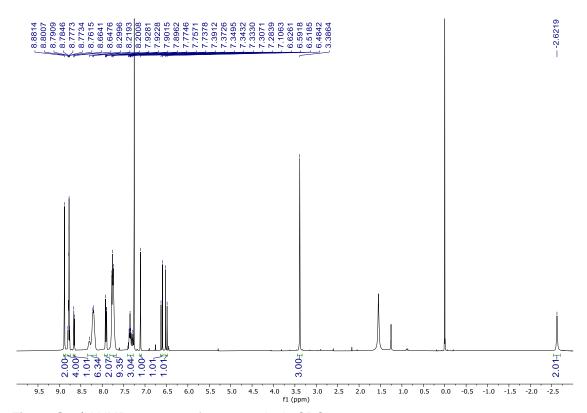


Figure S7. ¹H NMR spectrum of compound 4 in CDCl₃.

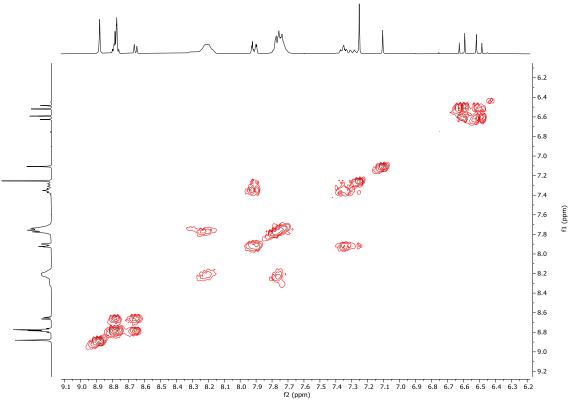
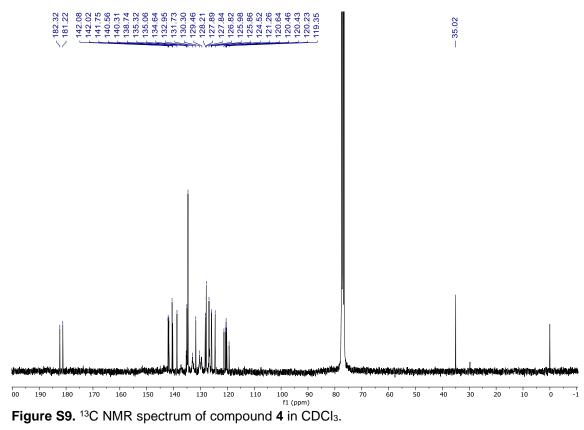


Figure S8. Partial COSY ¹H/¹H NMR spectrum of compound 4 in CDCl₃.



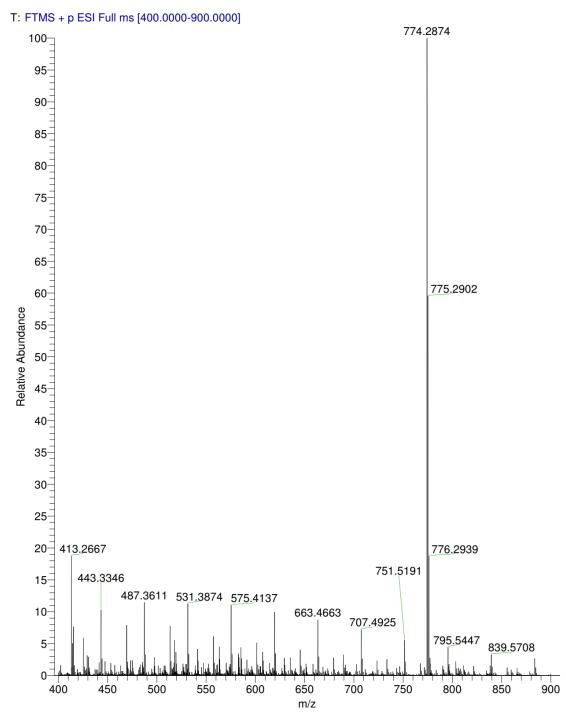


Figure S10. HRMS-ESI(+) spectrum of compound 4.

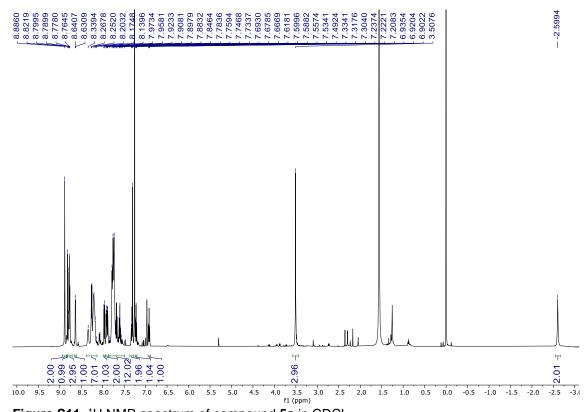


Figure S11. ¹H NMR spectrum of compound 5a in CDCl₃.

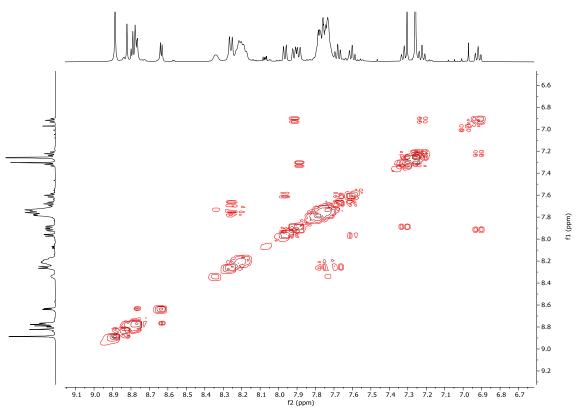
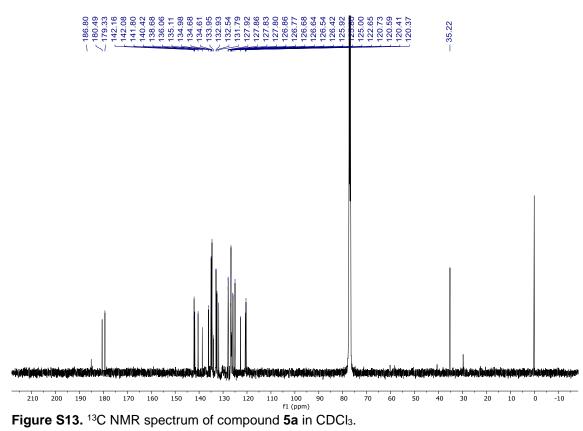


Figure S12. Partial COSY ¹H/¹H NMR spectrum of compound 5a in CDCl₃.



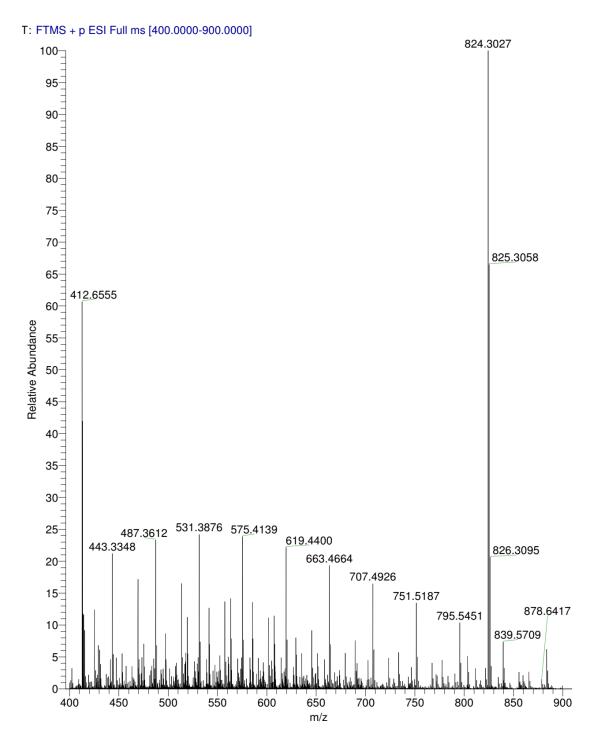


Figure S14. HRMS-ESI(+) spectrum of compound **5a**.

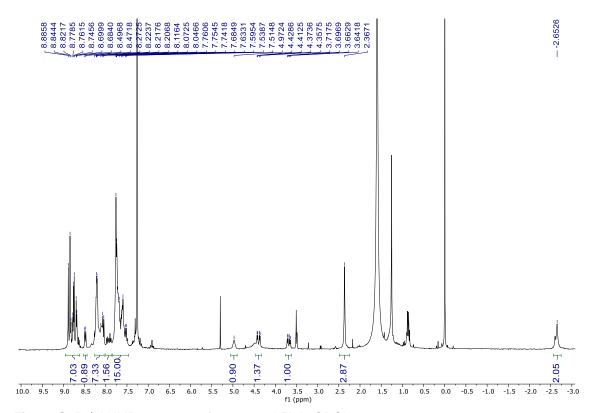


Figure S15. ¹H NMR spectrum of compound 5b in CDCl₃.

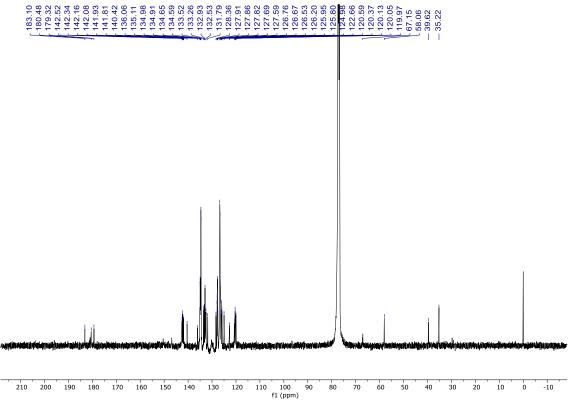


Figure S16. ¹³C NMR spectrum of compound 5b in CDCl₃.

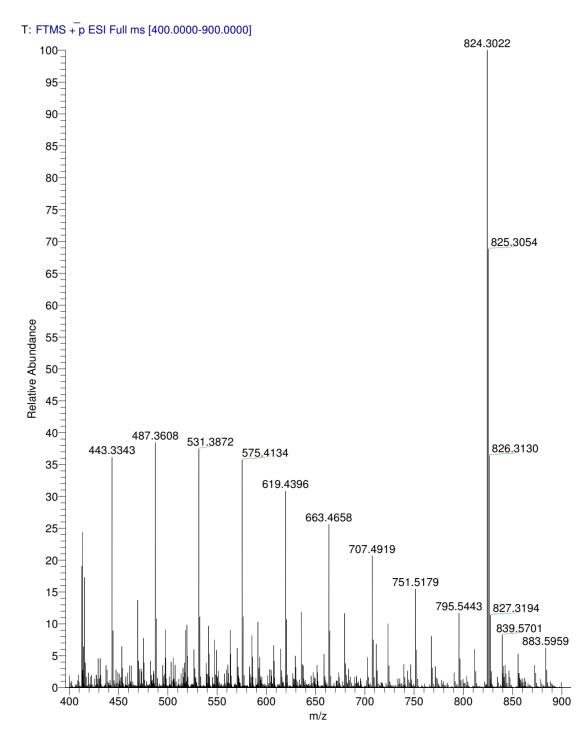


Figure S17. MS-ESI(+) spectrum of compound 5b.

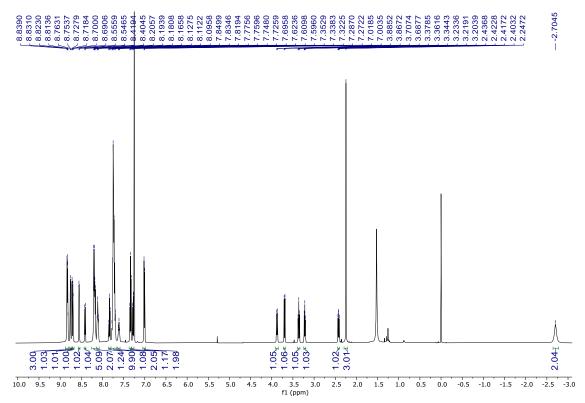


Figure \$18. ¹H NMR spectrum of compound 6a in CDCl₃.

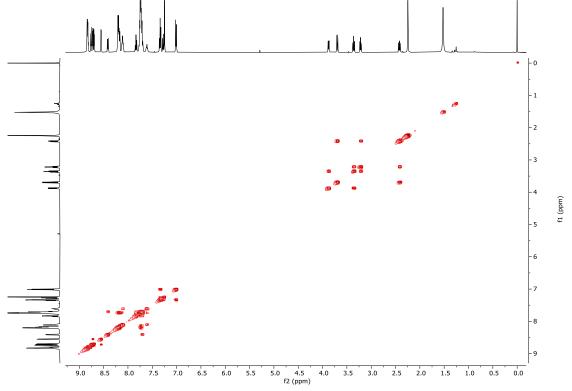


Figure S19. Partial COSY ¹H/¹H NMR spectrum of compound 6a in CDCl₃.

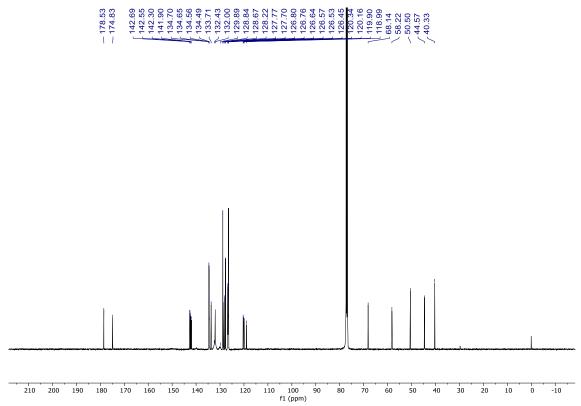


Figure S20. ¹³C NMR spectrum of compound 6a in CDCl₃.

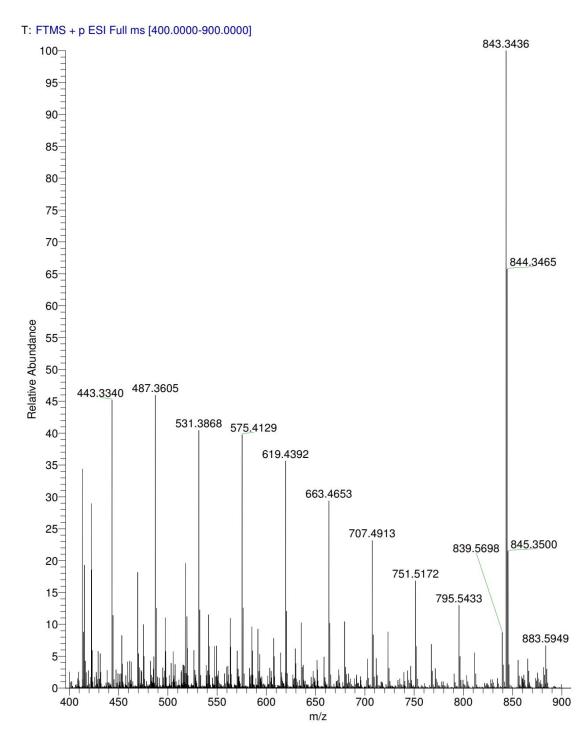


Figure S21. HRMS-ESI(+) spectrum of compound 6a.

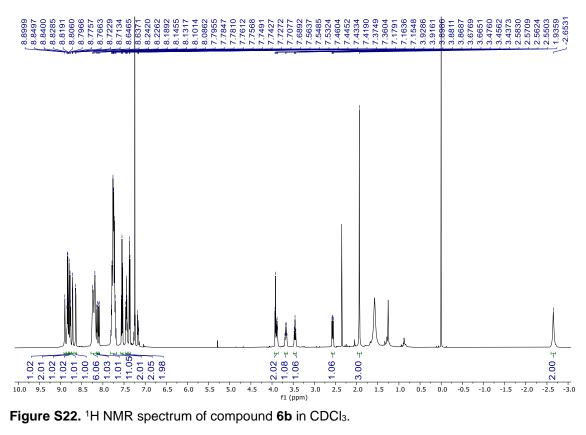


Figure S22. ¹H NMR spectrum of compound **6b** in CDCI₃.

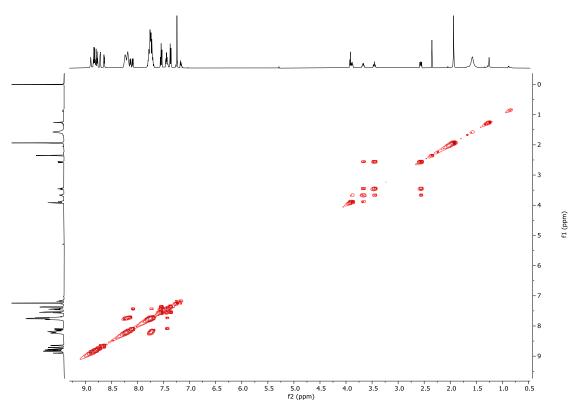
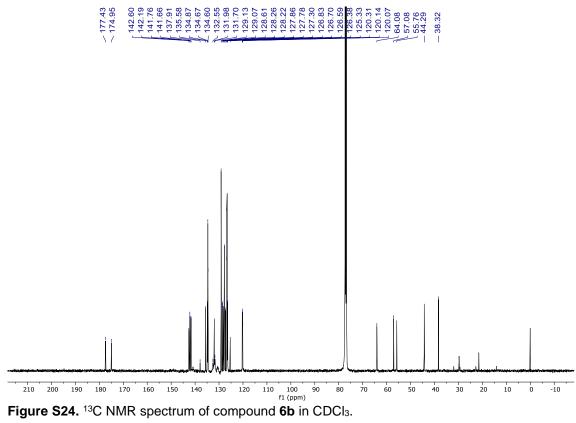


Figure S23. Partial COSY ¹H/¹H NMR spectrum of compound 6b in CDCl₃.



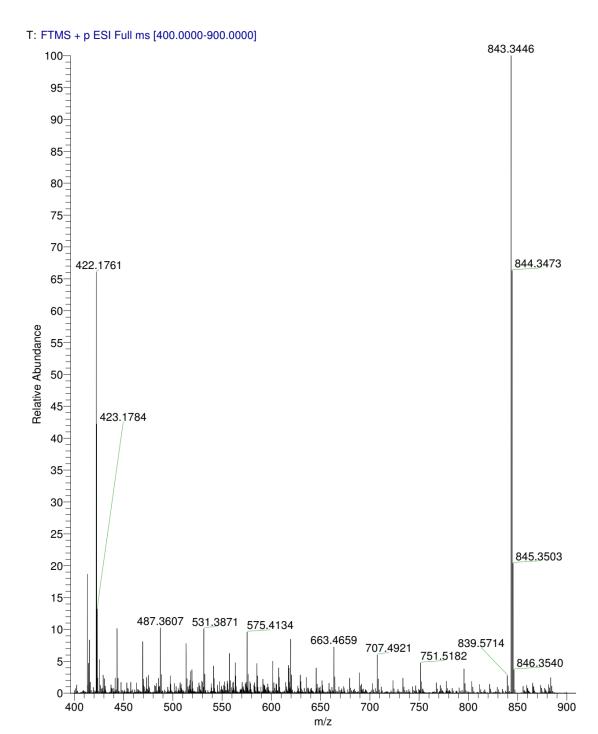


Figure S25. HRMS-ESI(+) spectrum of compound 6b.

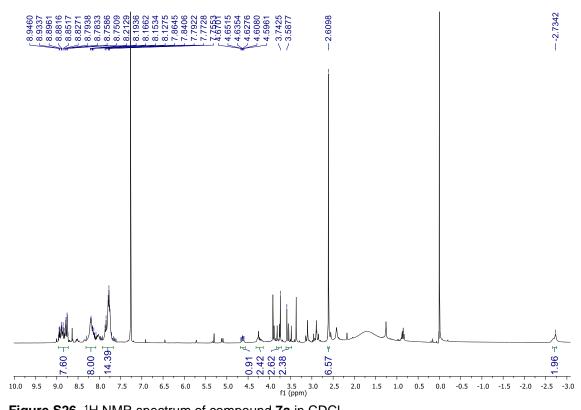


Figure S26. ¹H NMR spectrum of compound 7a in CDCI₃.

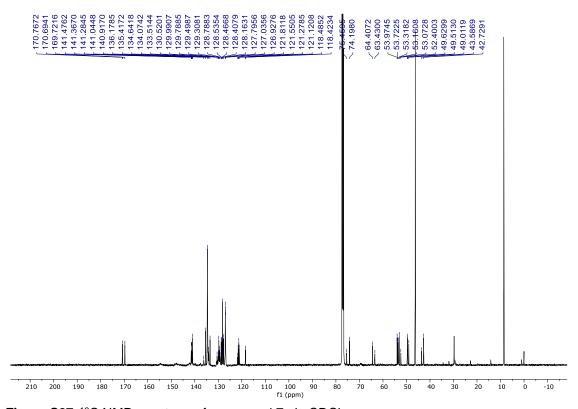


Figure S27. ¹³C NMR spectrum of compound 7a in CDCl₃.

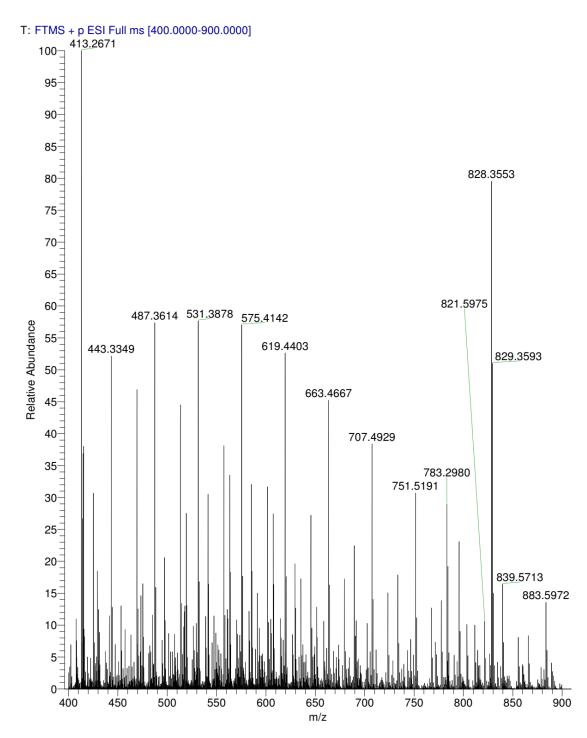


Figure S28. HRMS-ESI(+) spectrum of compound **7a**.

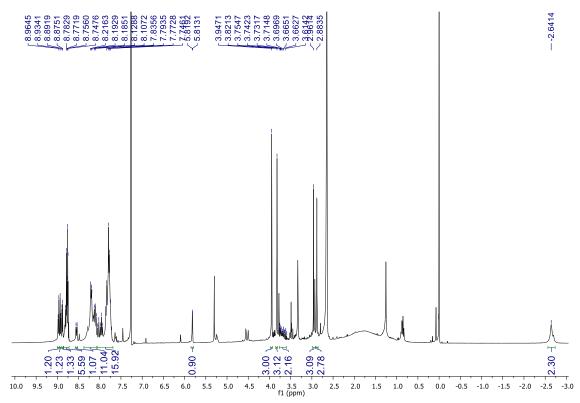


Figure S29. ¹H NMR spectrum of compound 7b in CDCl₃.

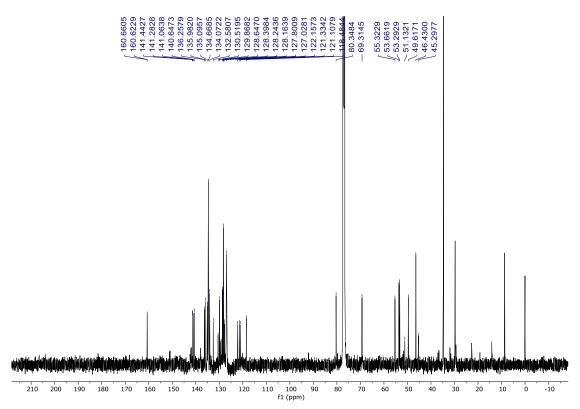


Figure S30. 13C NMR spectrum of compound 7b in CDCl₃.

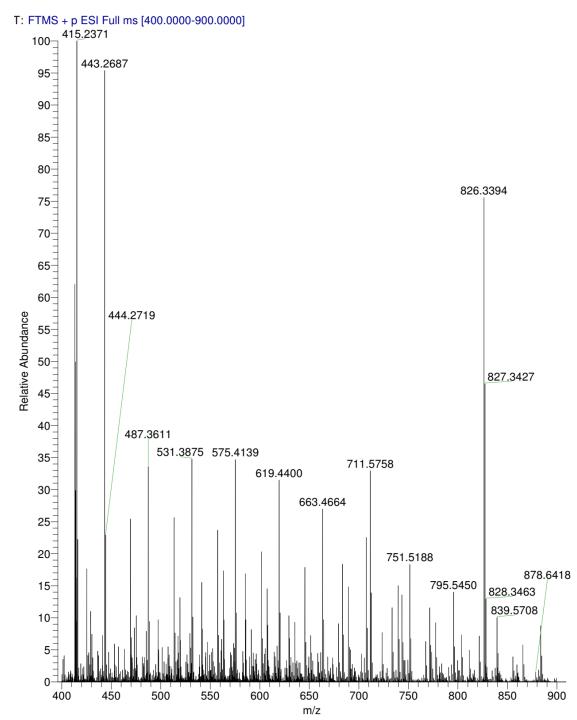


Figure S31. HRMS-ESI(+) spectrum of compound 7b.

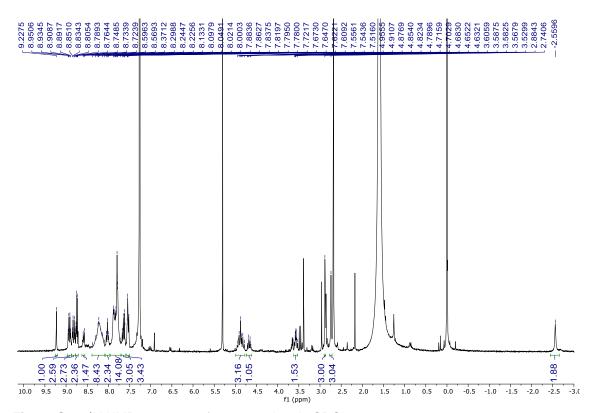


Figure S32. ¹H NMR spectrum of compound 7c in CDCl₃.

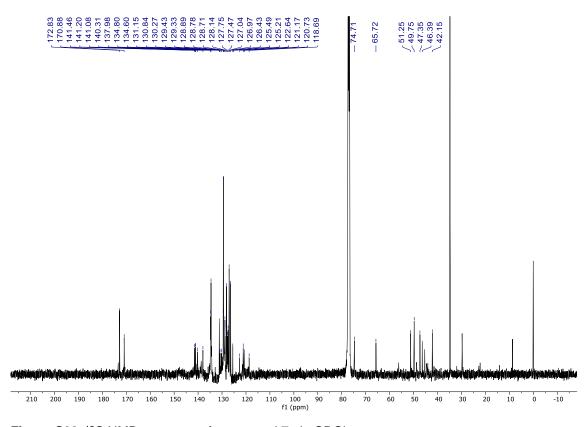


Figure S33. ^{13}C NMR spectrum of compound 7c in CDCl₃.

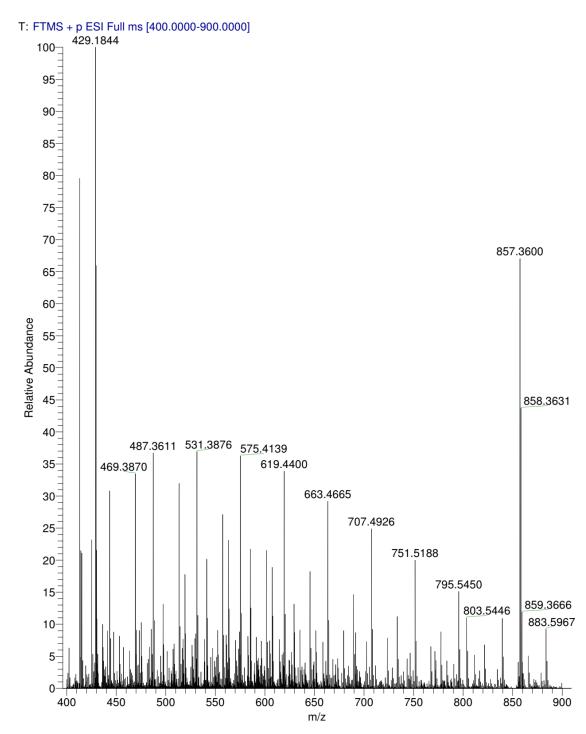


Figure S34. HRMS-ESI(+) spectrum of compound 7c.

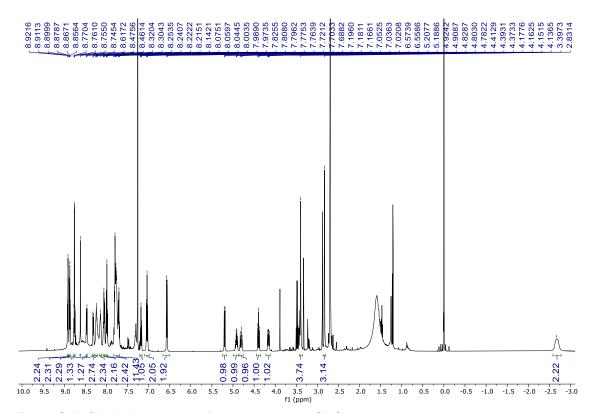


Figure S35. ¹H NMR spectrum of compound 7d in CDCl₃.

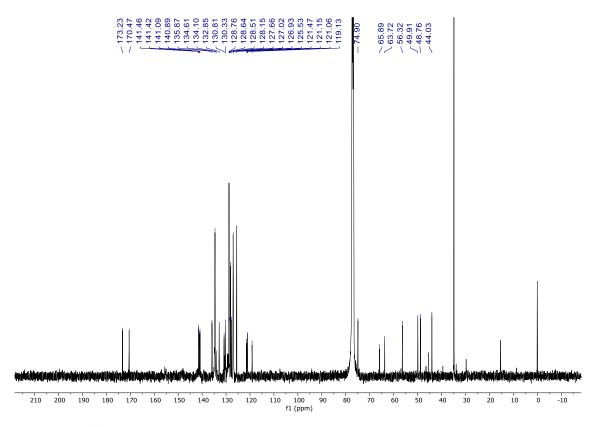


Figure S36. ¹³C NMR spectrum of compound **7d** in CDCl₃.

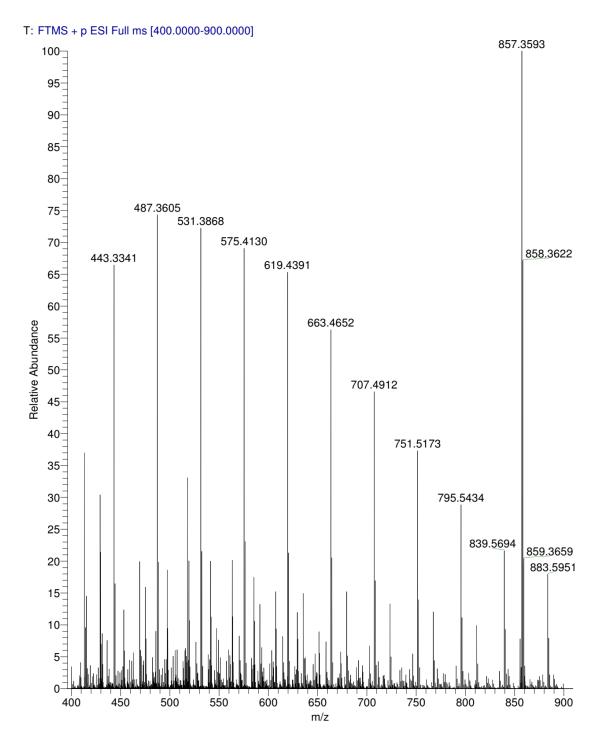


Figure S37. HRMS-ESI(+) spectrum of compound 7d.

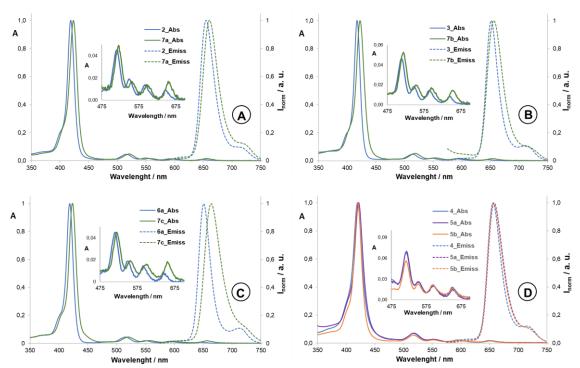


Figure S38. Absorption and normalized emission spectra of compounds **2** and **7a** (A), **3** and **7b** (B), **6a** and **7c** (C) and **4**, **5a** and **5b** in DMF at 298 K ([**2**] = [**3**] = [**4**] = [**5a**] = [**5b**] = [**6a**] = [**6b**] = [**7a**] = [**7b**] = [**7c**] = 2.5μM; λ_{exc2} = 419 nm; λ_{exc7a} = 423 nm; λ_{exc3} = 417 nm; λ_{exc7b} = 423 nm; λ_{exc6a} = 419 nm; λ_{exc7c} = 424 nm; λ_{exc4} = 420 nm; λ_{exc5a} = 422 nm; λ_{exc5b} = 420 nm). in DMF at 298 K. The inset shows the absorption at the Q bands region.