

Supporting Information

Synthesis, characterization and biological evaluation of cationic porphyrin-terpyridine derivatives

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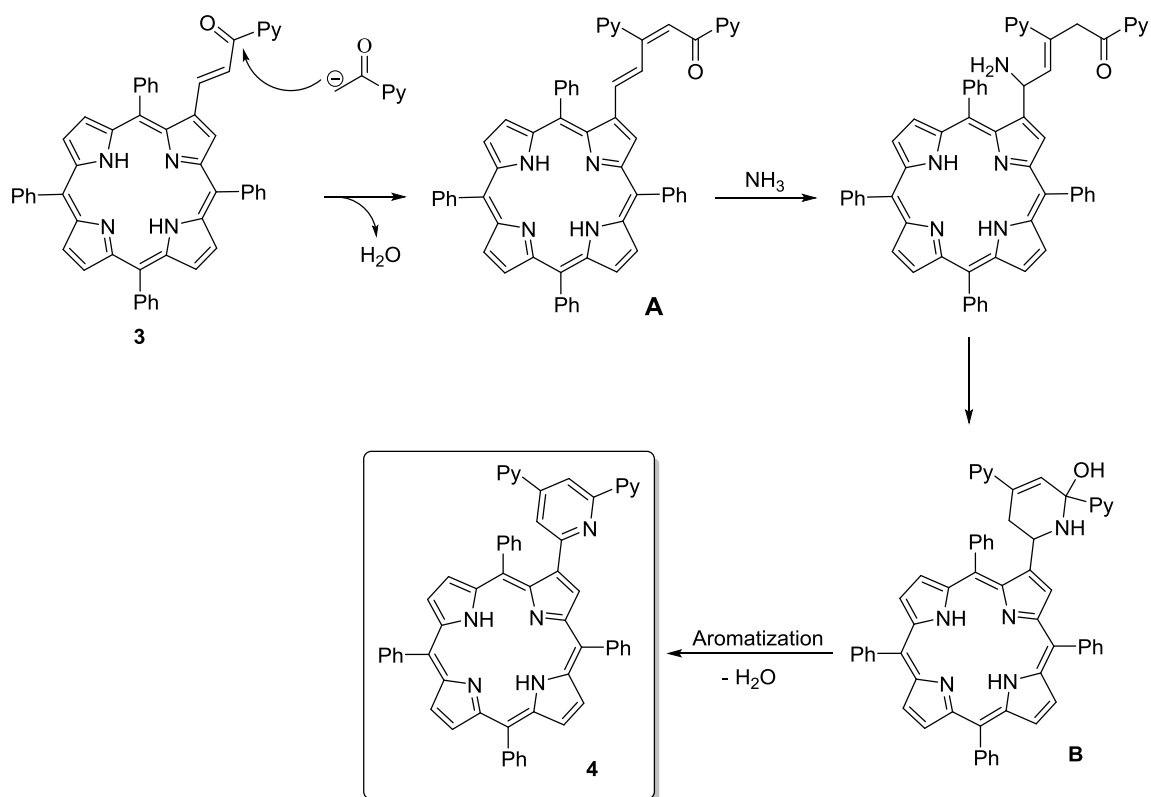
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I - Mechanistic pathway for the synthesis of compound 4.



Scheme S1. Mechanistic pathway for the synthesis of compound 4.

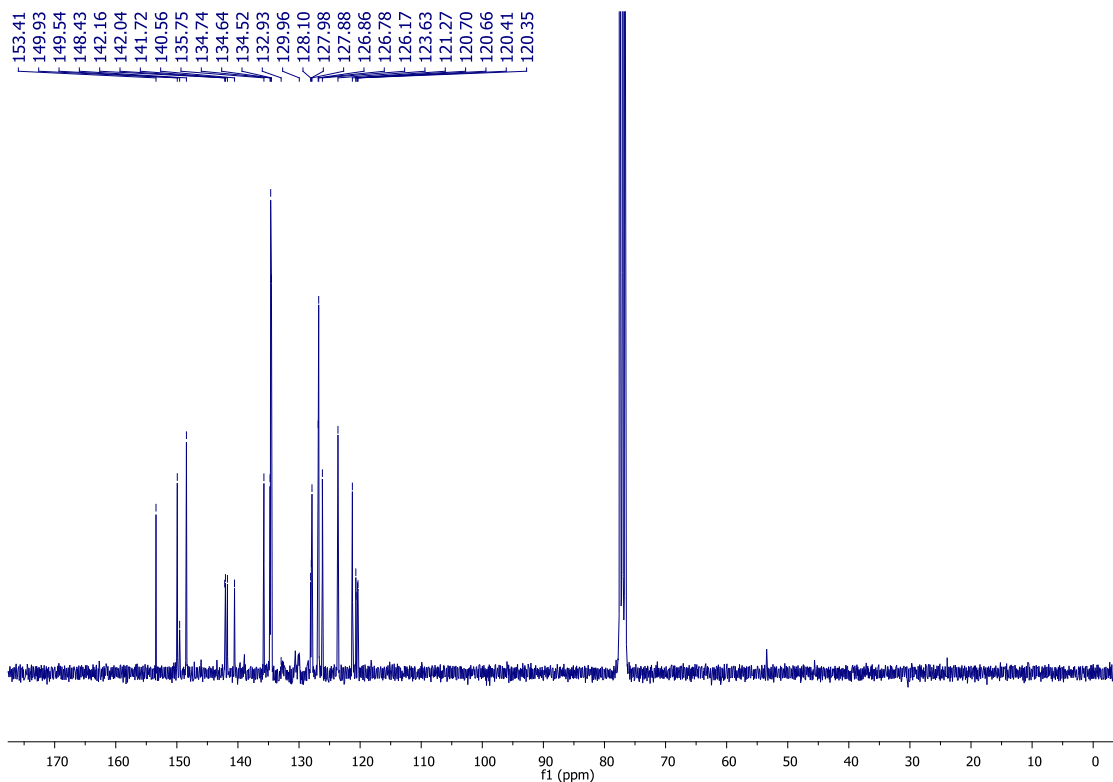


Figure S3. ^{13}C NMR spectrum of compound **1b** in CDCl_3 .

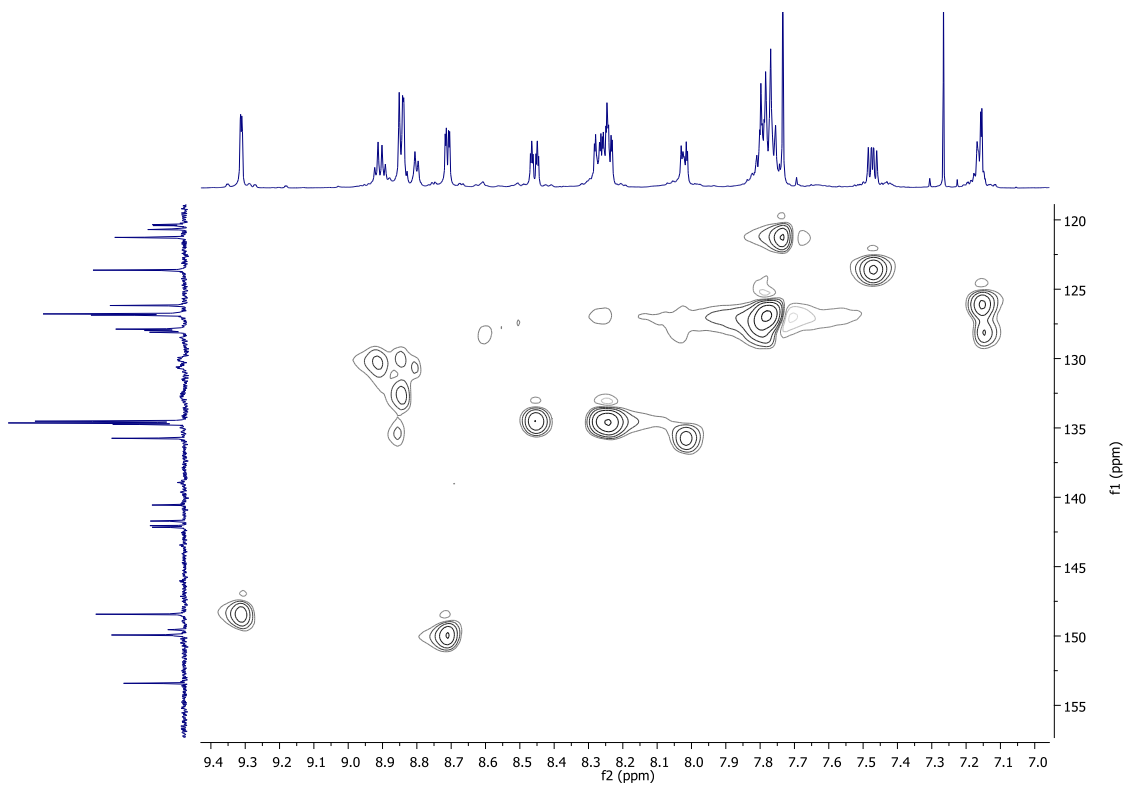


Figure S4. Partial HSQC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **1b** in CDCl_3 .

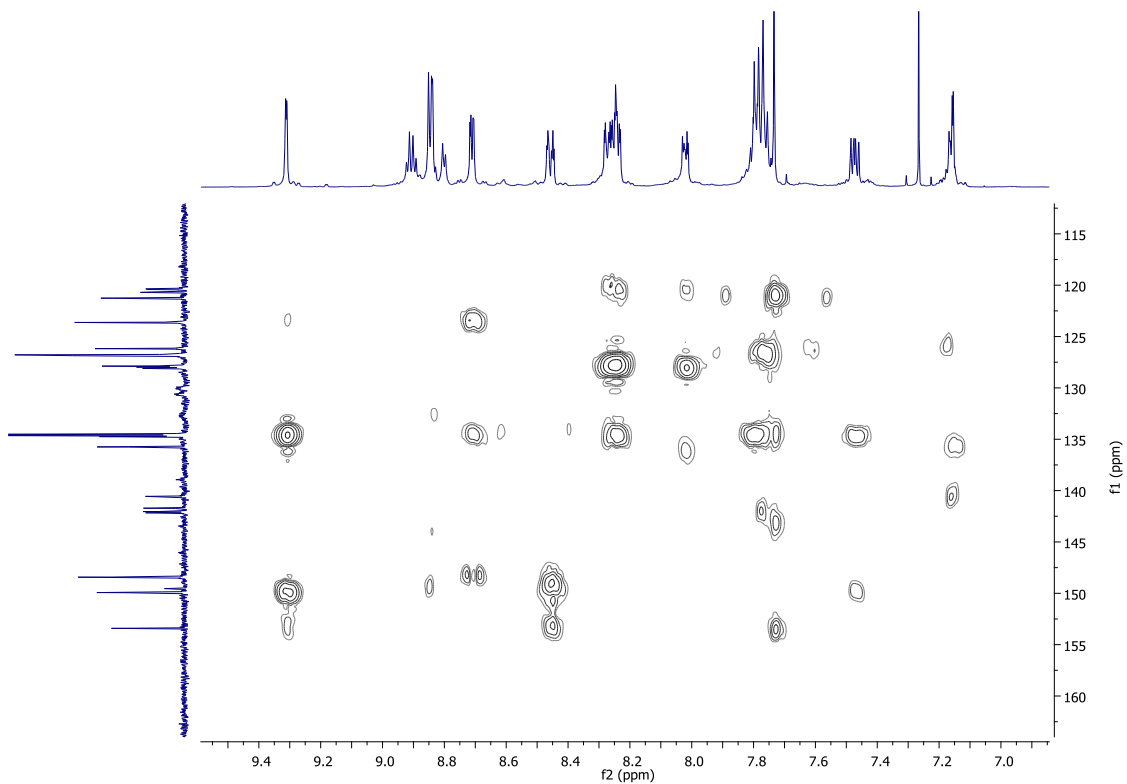


Figure S5. Partial HMBC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **1b** in CDCl_3 .

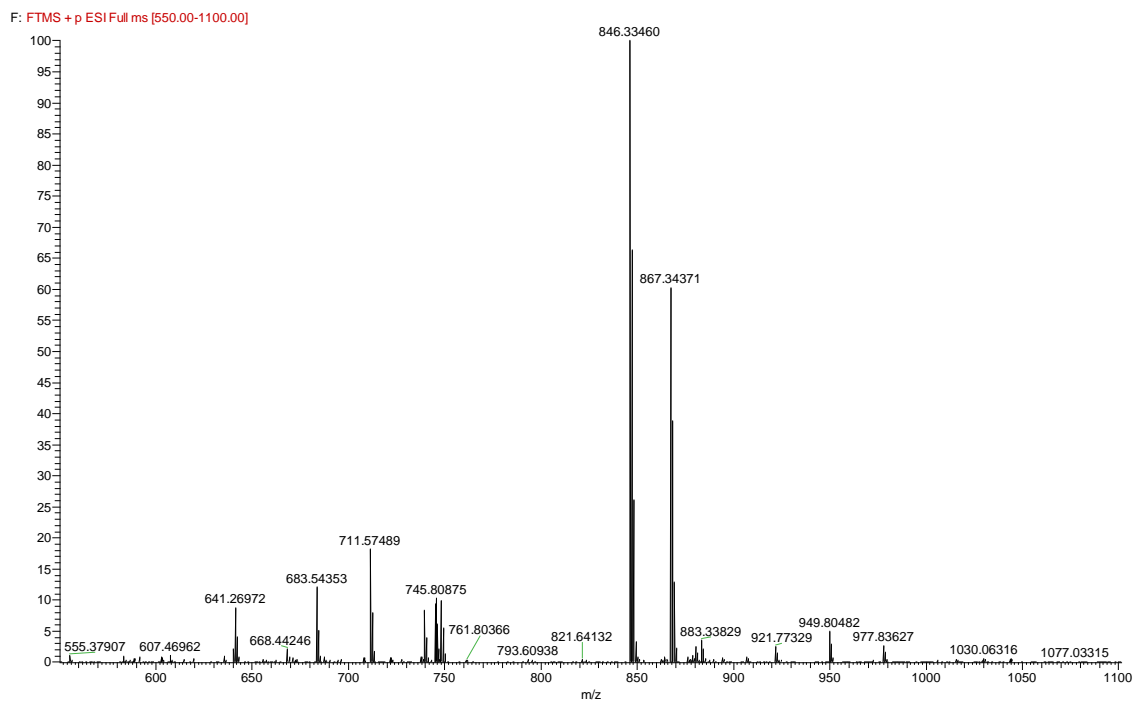
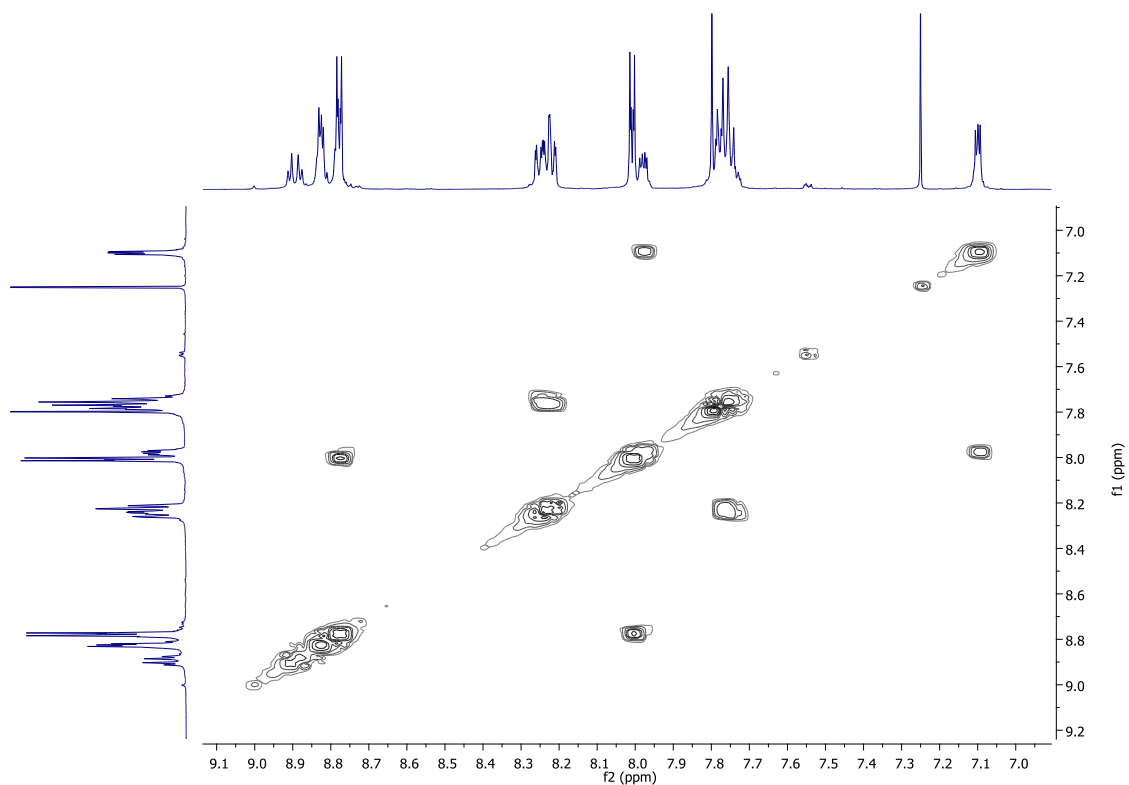
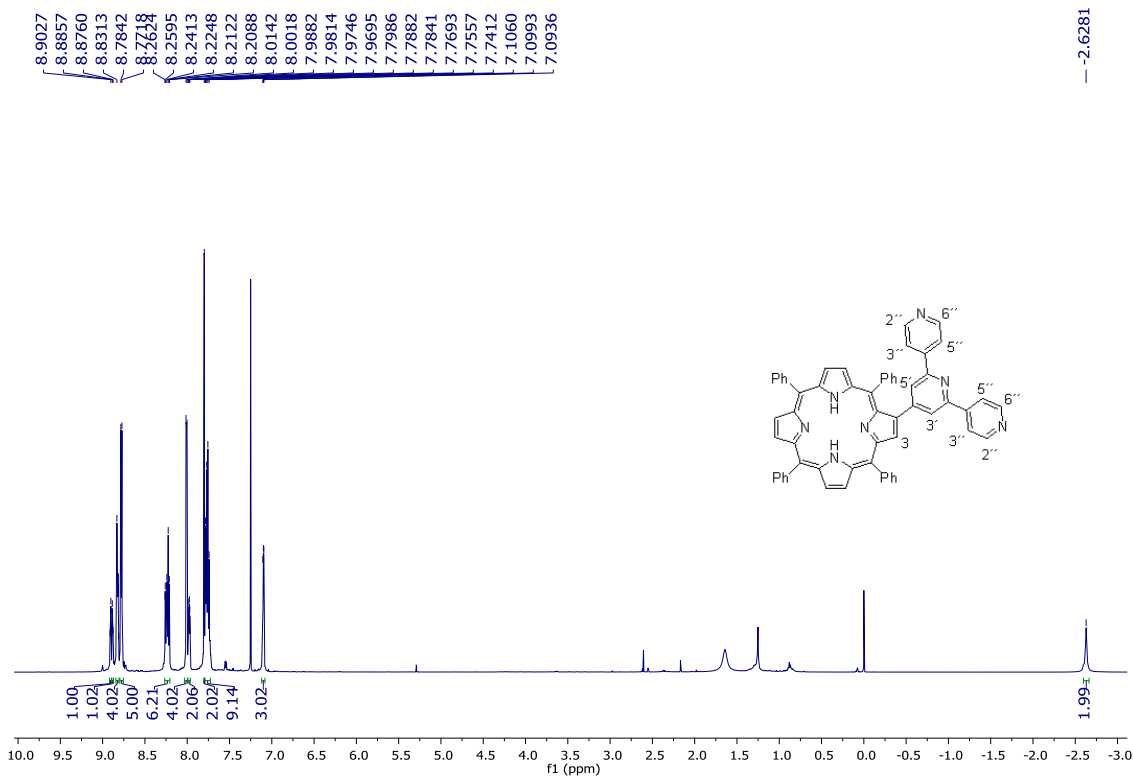


Figure S6. HRMS spectrum of compound **1b**.



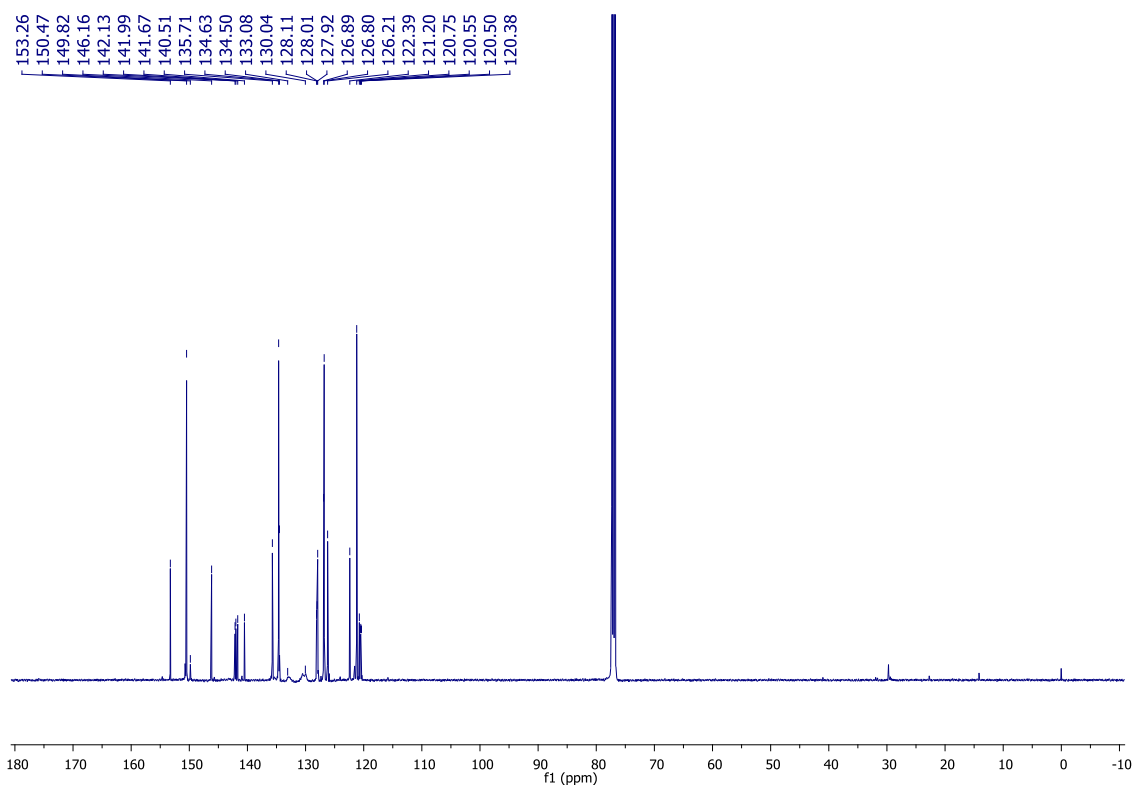


Figure S9. ^{13}C NMR spectrum of compound **1c** in CDCl_3 .

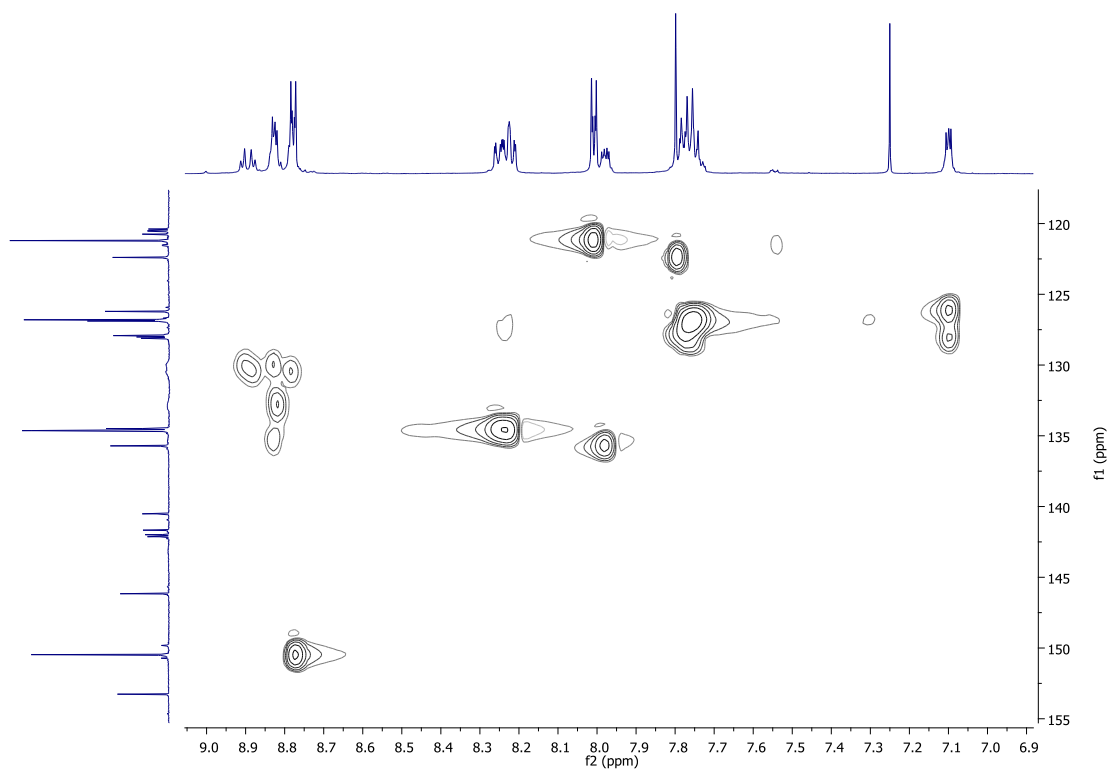


Figure S10. Partial HSQC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **1c** in CDCl_3 .

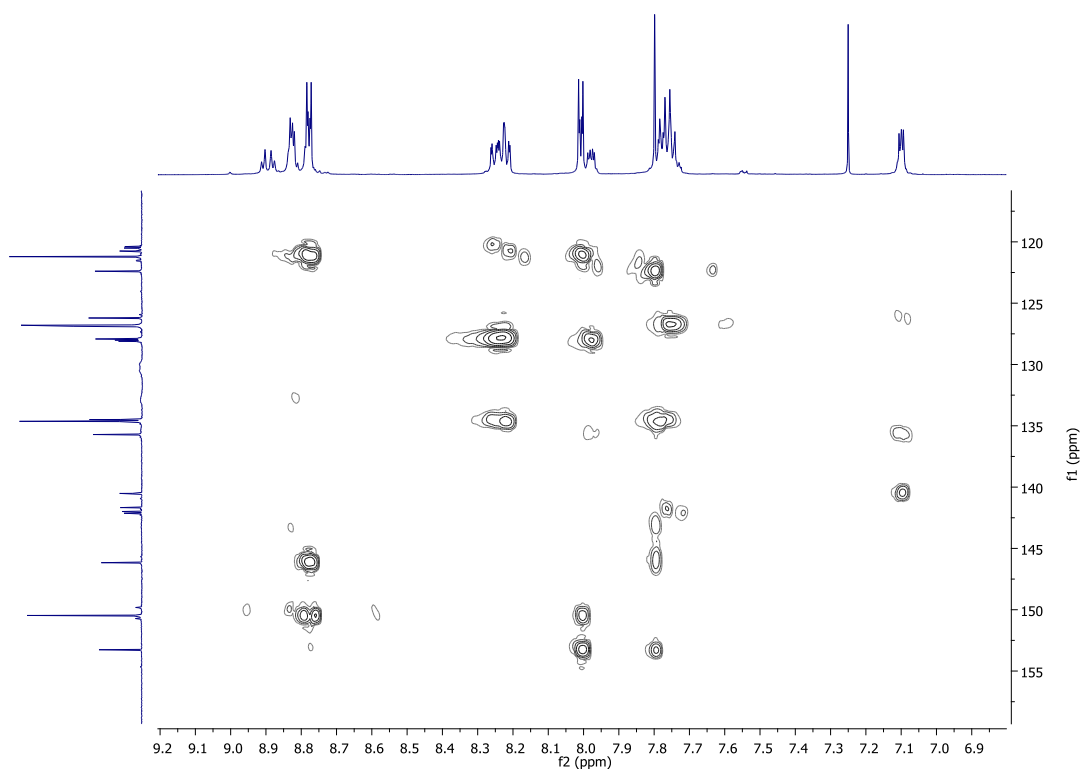


Figure S11. Partial HMBC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **1c** in CDCl_3 .

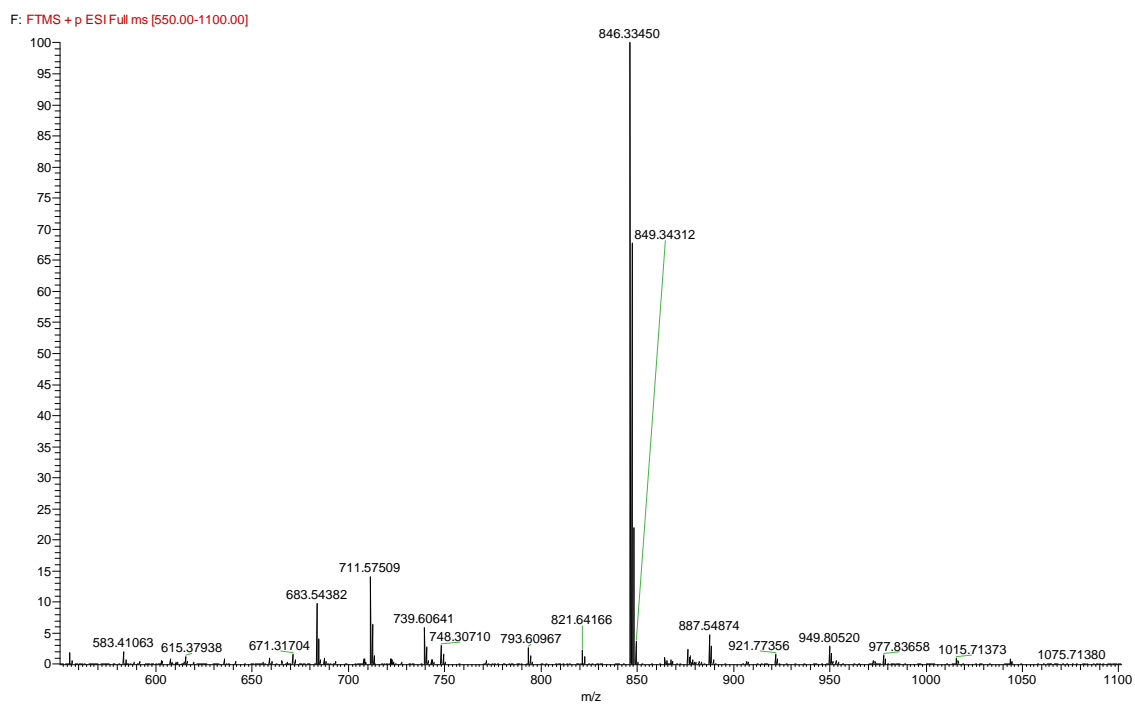
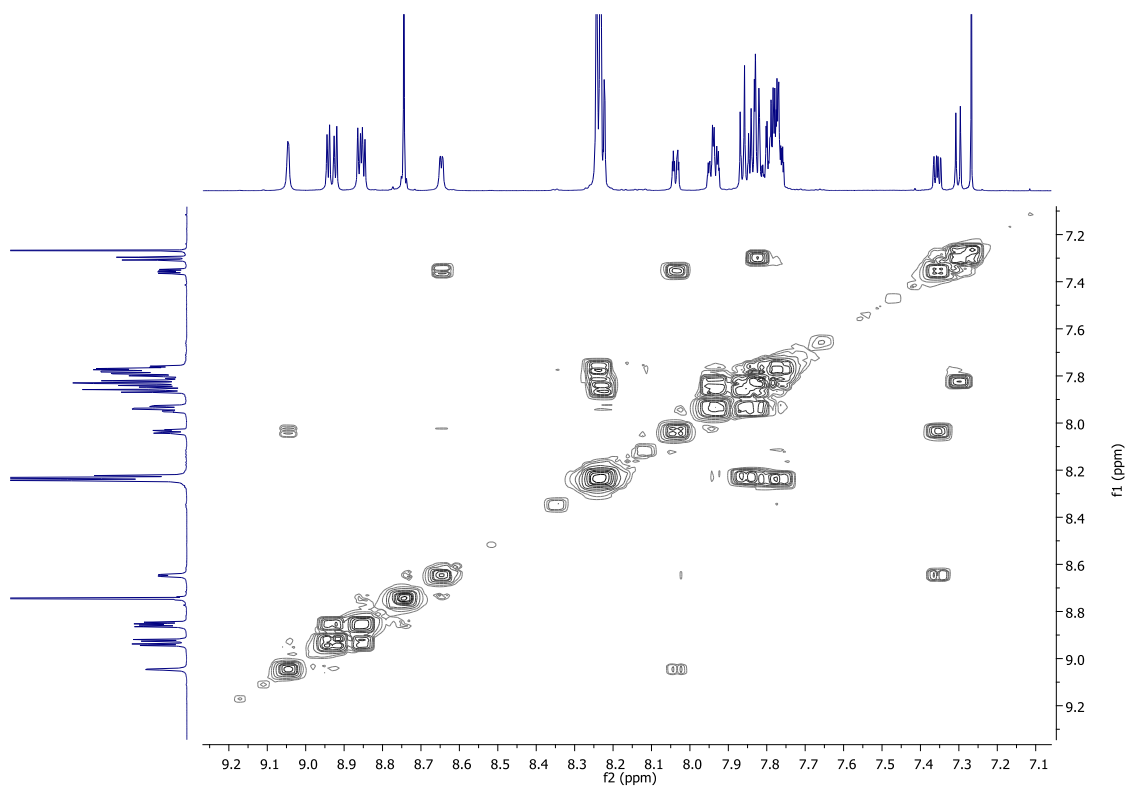
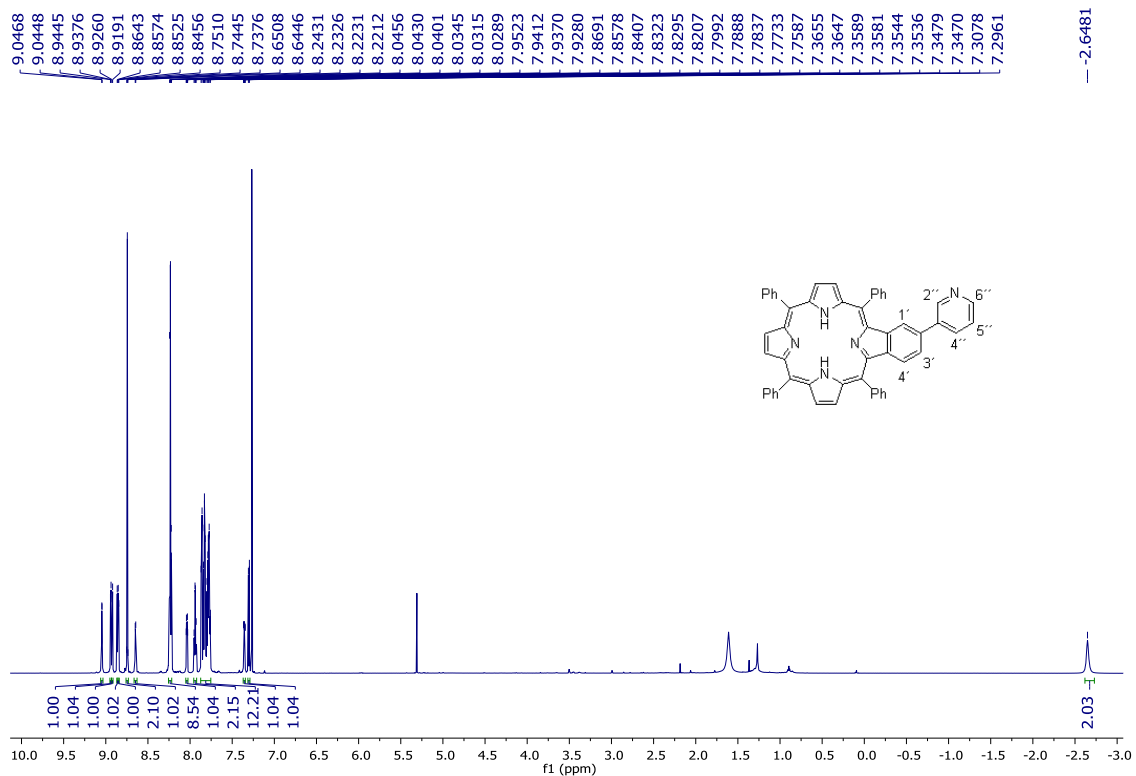


Figure S12. HRMS spectrum of compound **1c**.



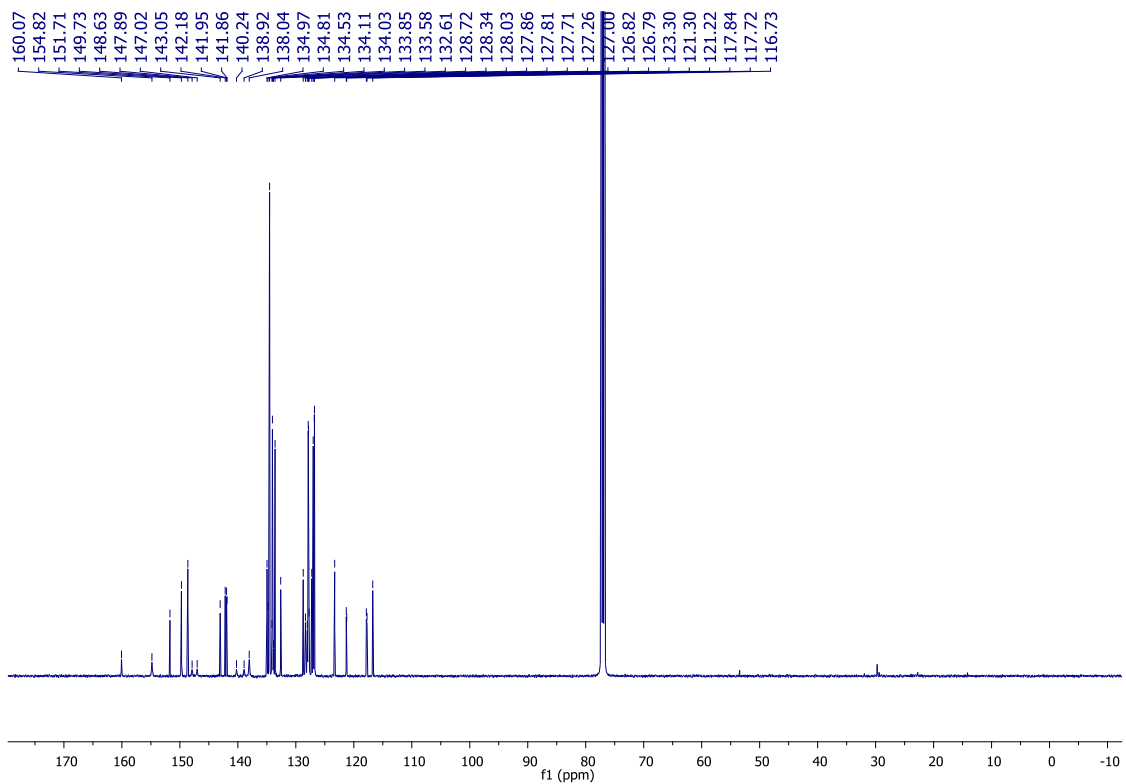


Figure S15. ^{13}C NMR spectrum of compound **2b** in CDCl_3 .

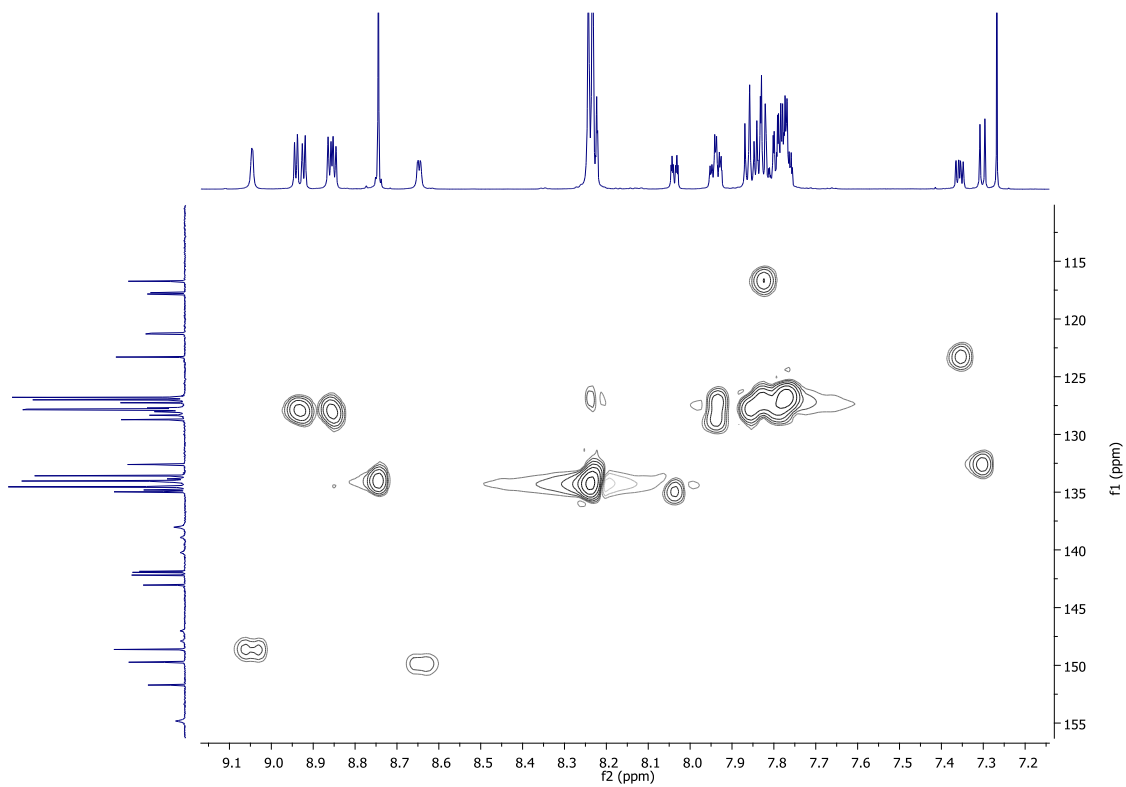


Figure S16. Partial HSQC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **2b** in CDCl_3 .

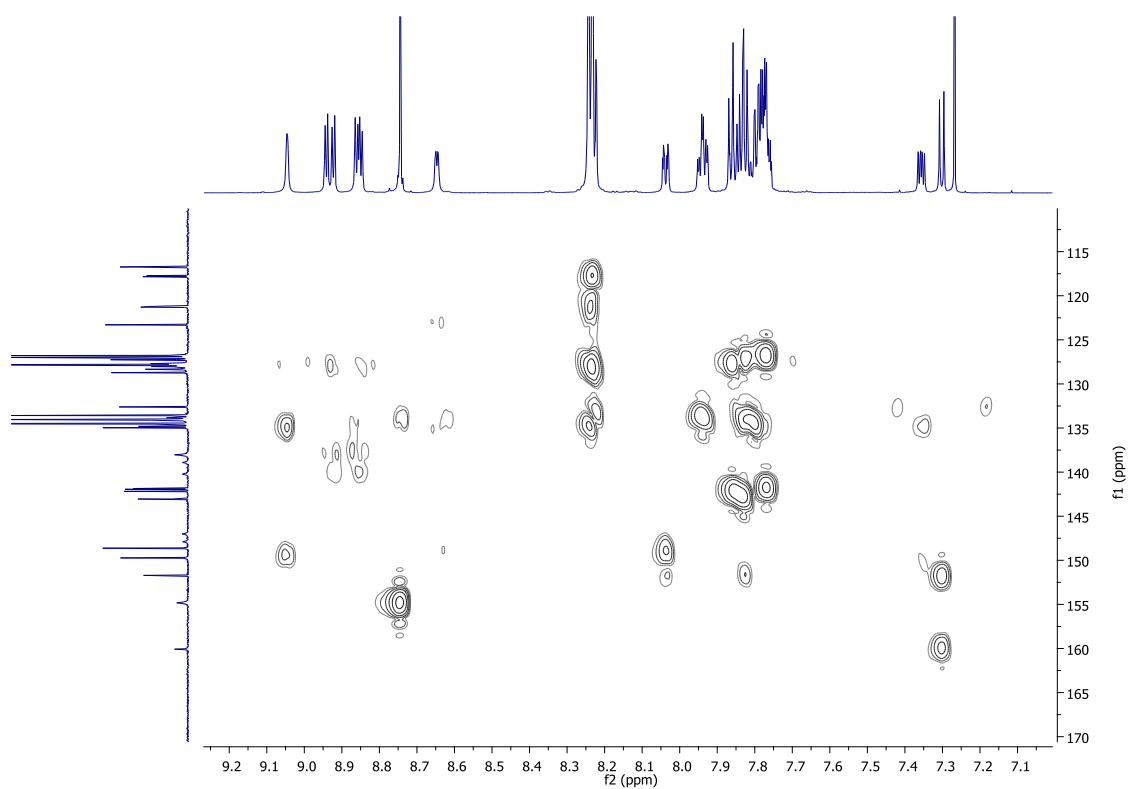


Figure S17. Partial HMBC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **2b** in CDCl_3 .

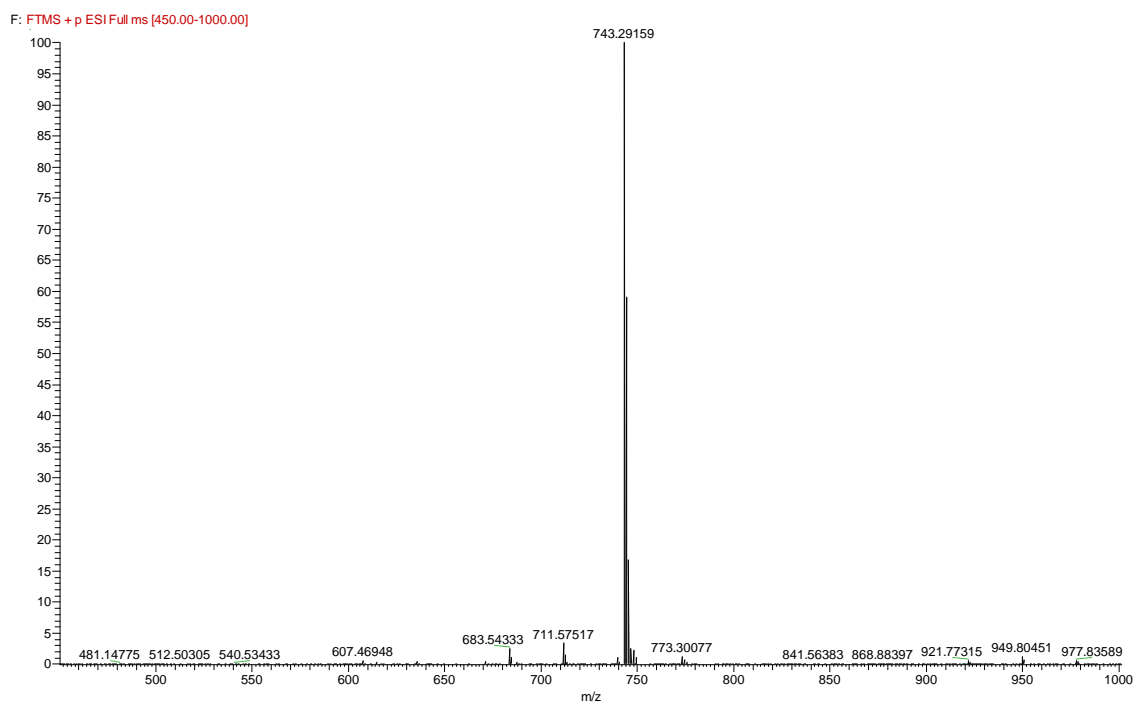


Figure S18. HRMS spectrum of compound **2b**.

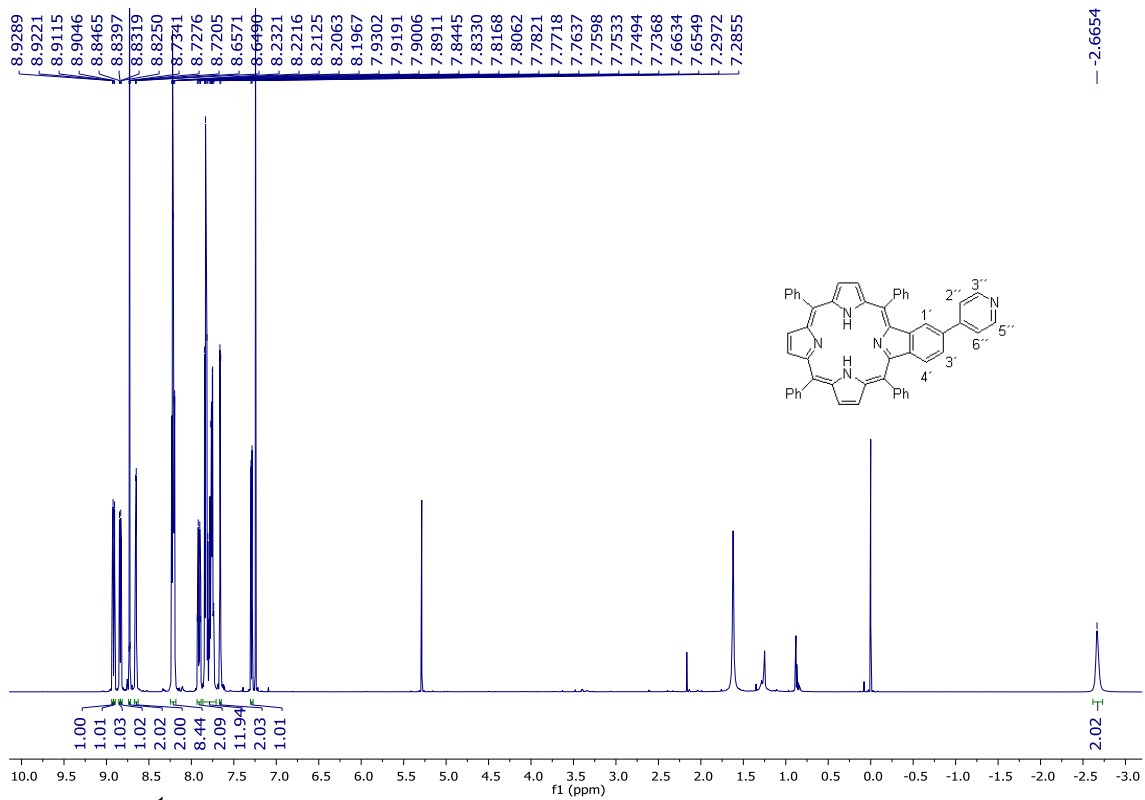


Figure S19. ^1H NMR spectrum of compound **2c** in CDCl_3 .

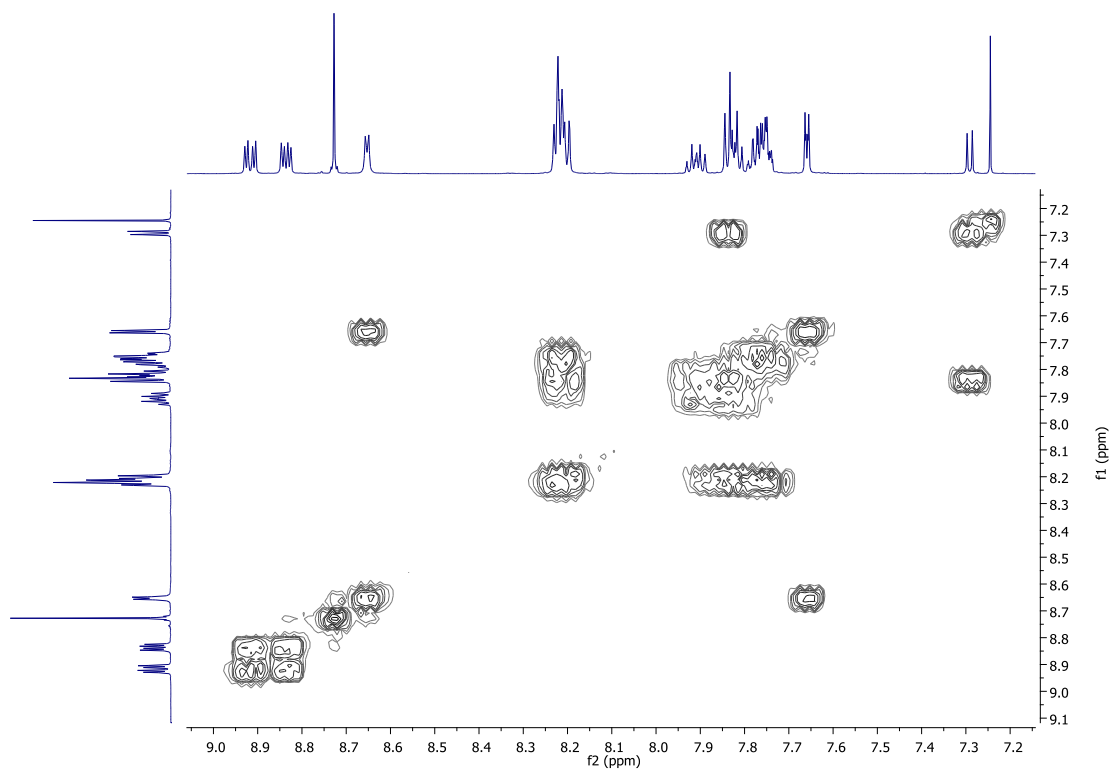


Figure S20. Partial COSY ($^1\text{H}/^1\text{H}$) spectrum of compound **2c** in CDCl_3 .

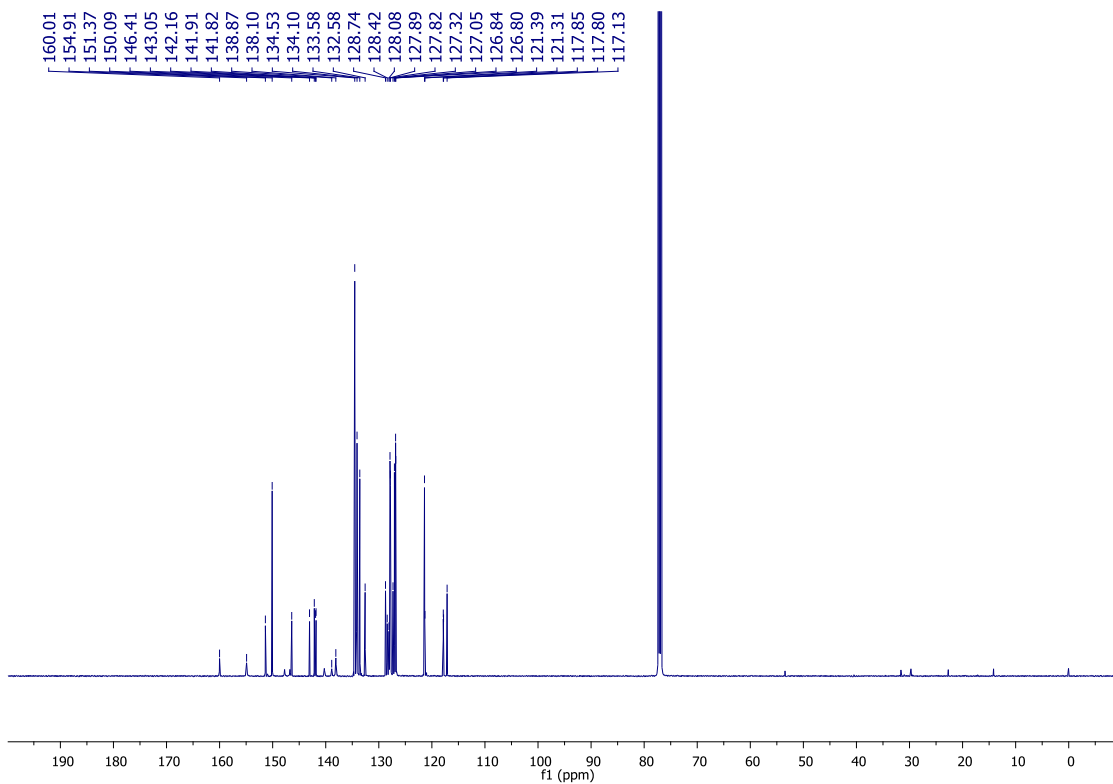


Figure S21. ^{13}C -NMR spectrum of compound **2c** in CDCl_3 .

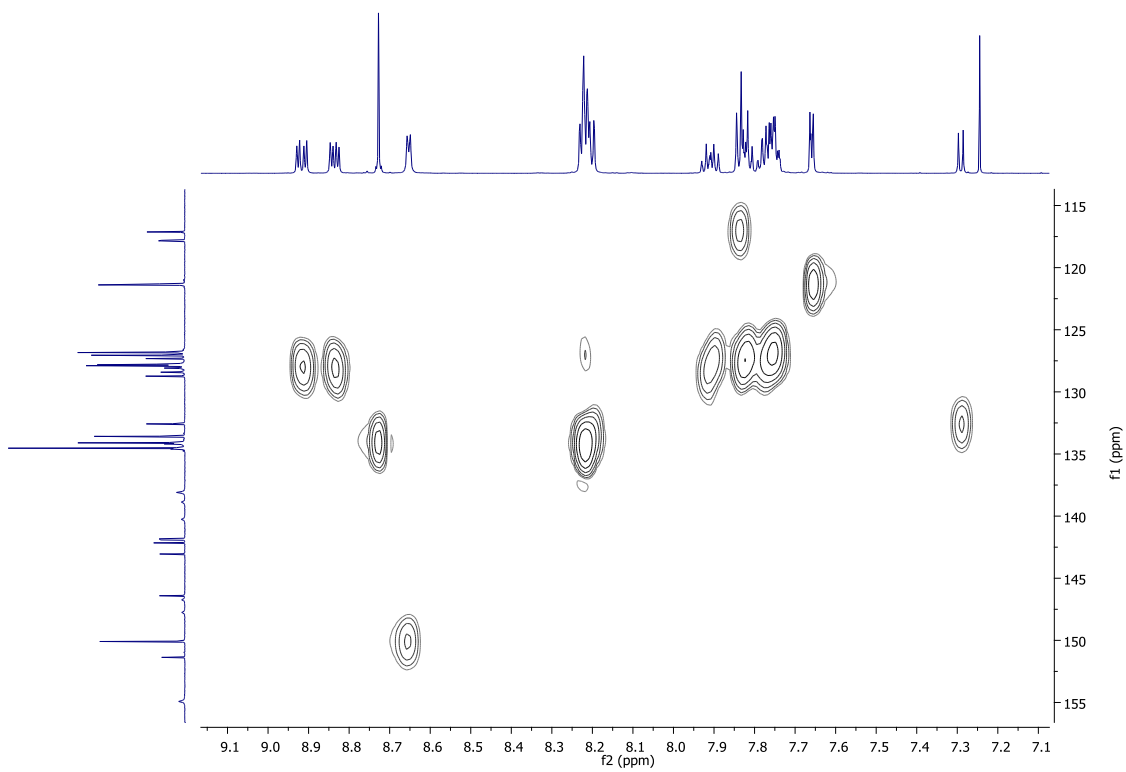


Figure S22. Partial HSQC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **2c** in CDCl_3 .

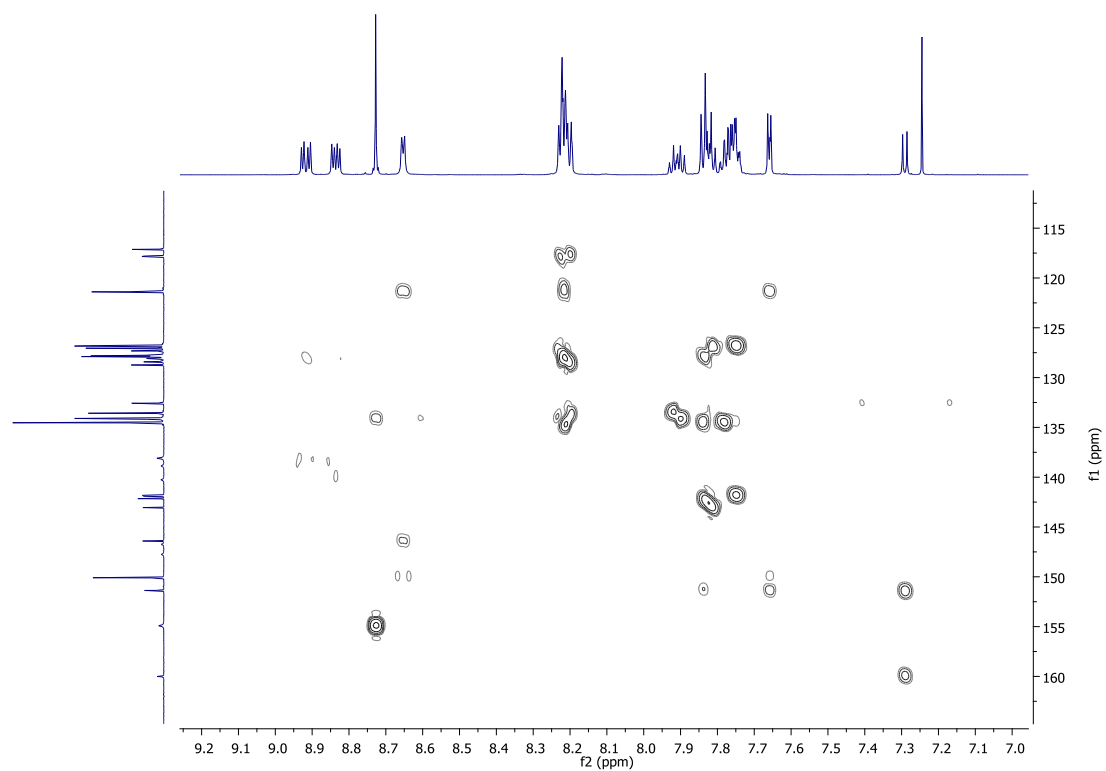


Figure S23. Partial HMBC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **2c** in CDCl_3 .

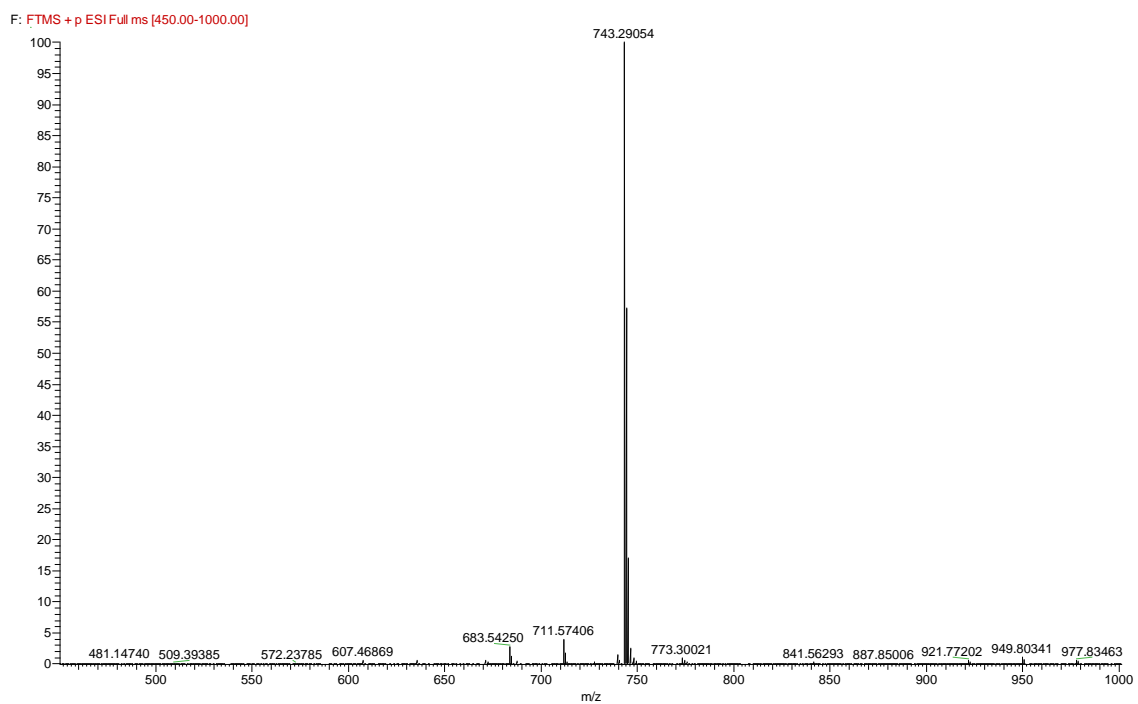


Figure S24. HRMS spectrum of compound **2c**.

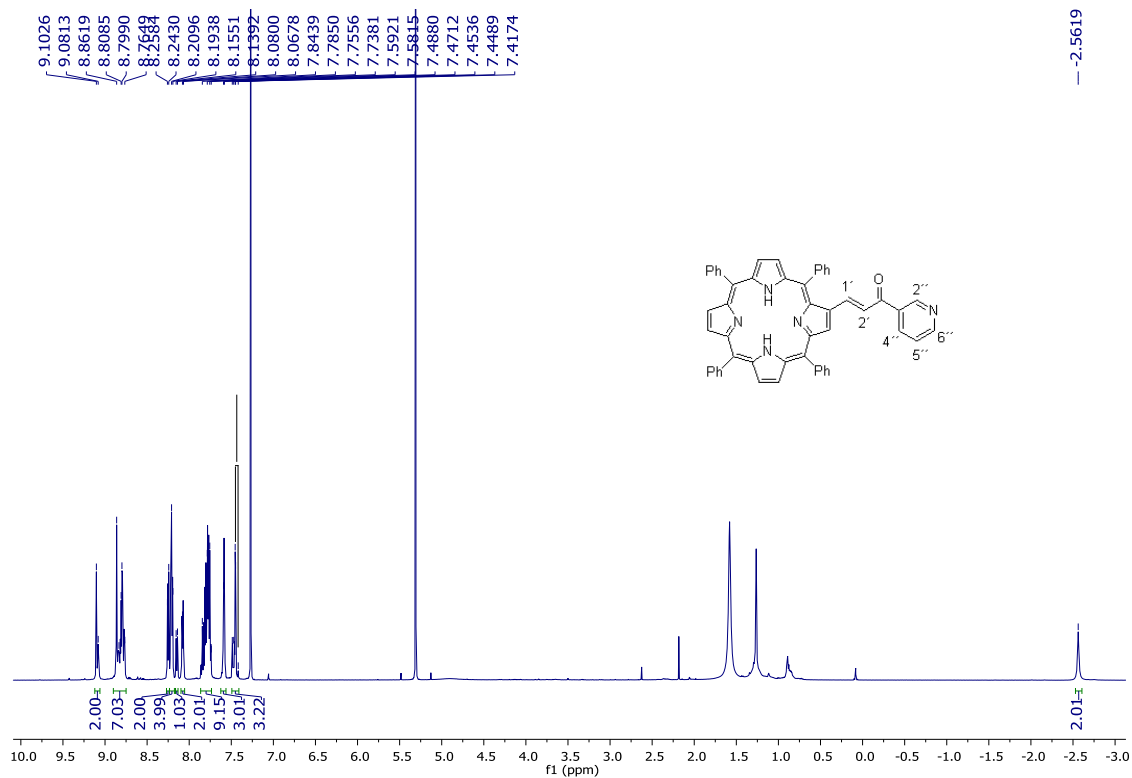


Figure S25. ^1H NMR spectrum of compound **3b** in CDCl_3 .

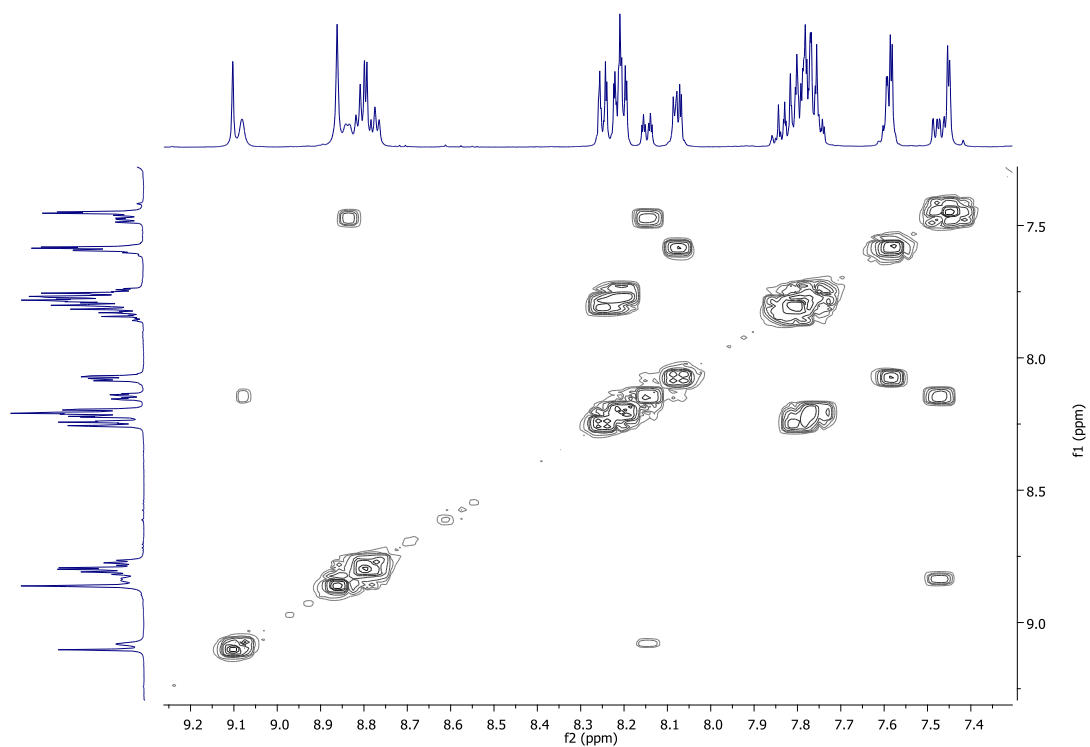


Figure S26. Partial COSY ($^1\text{H}/^1\text{H}$) spectrum of compound **3b** in CDCl_3 .

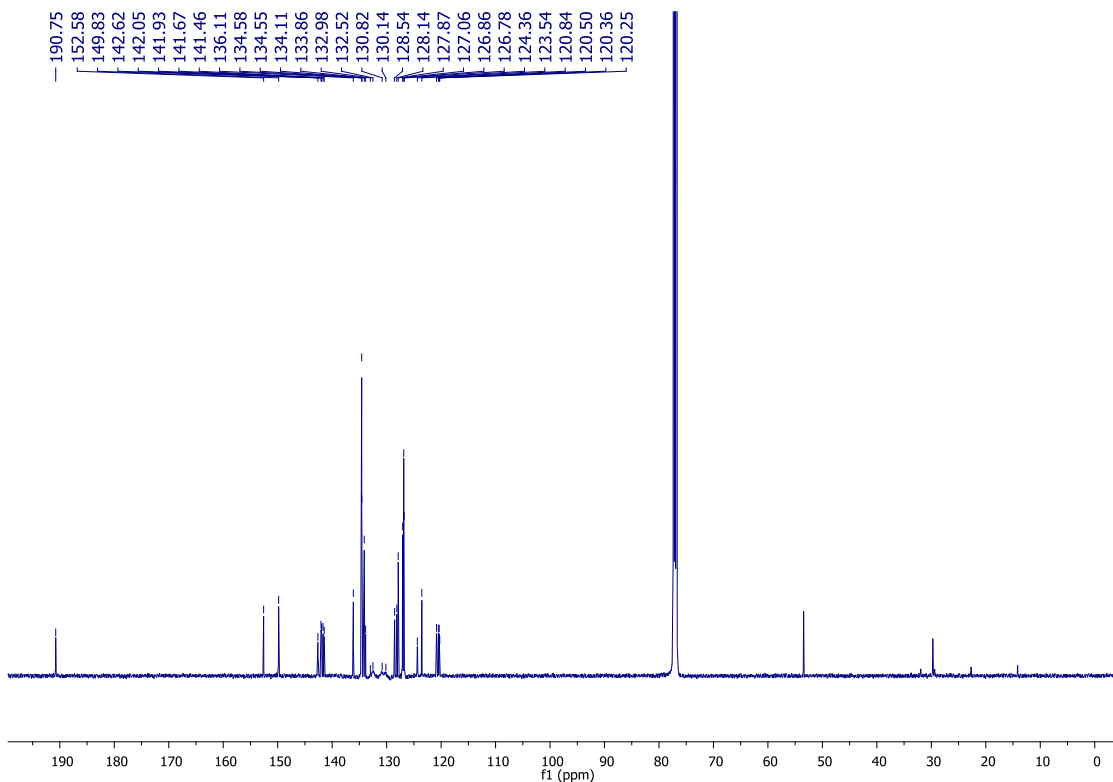


Figure S27. ^{13}C NMR spectrum of compound **3b** in CDCl_3 .

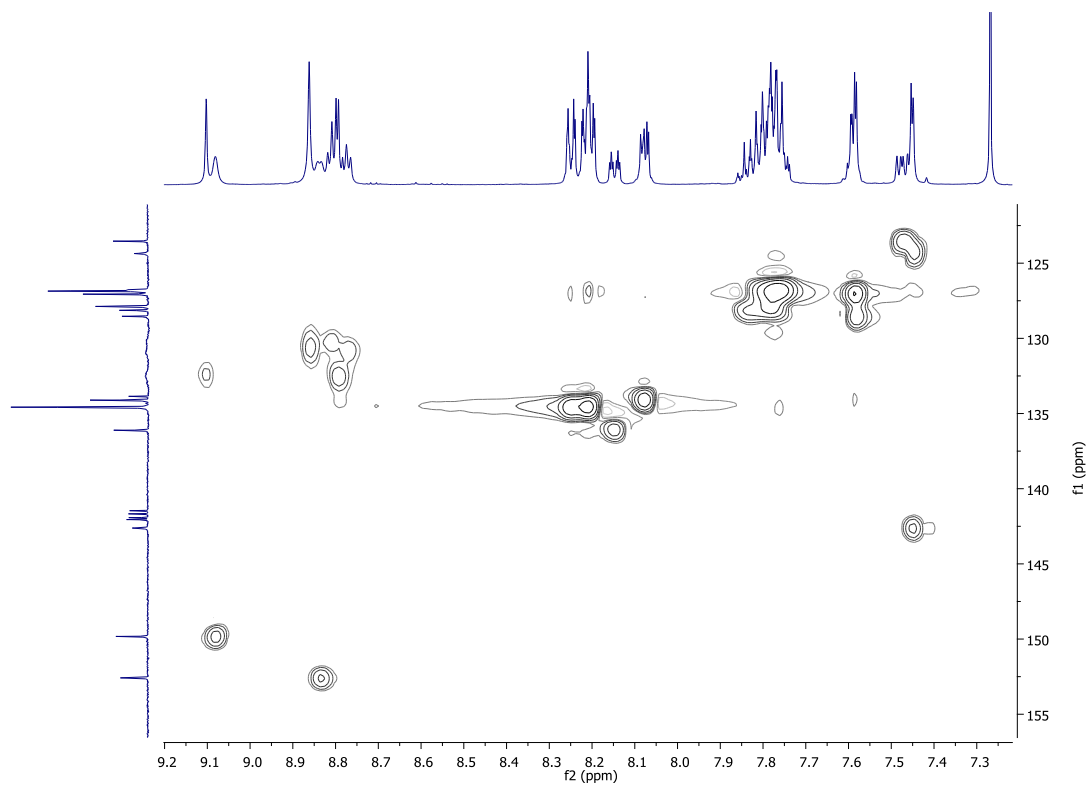


Figure S28. Partial HSQC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **3b** in CDCl_3 .

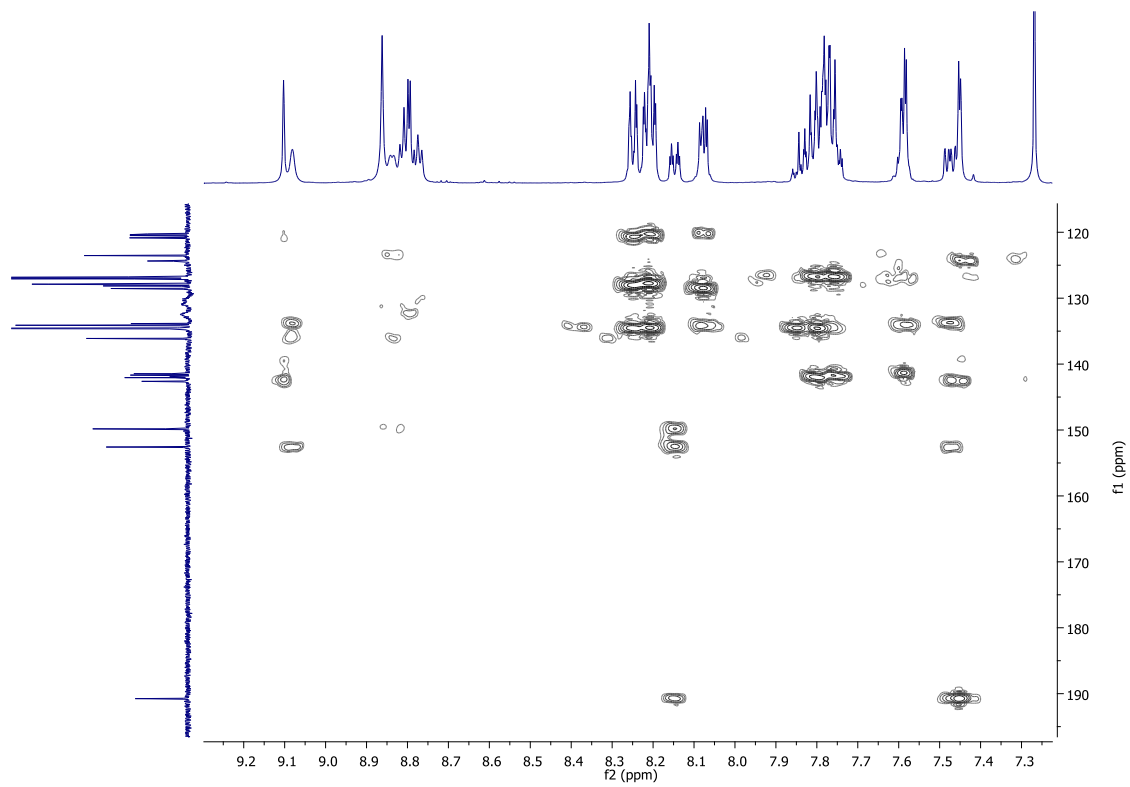


Figure S29. Partial HMBC (¹H/¹³C) spectrum of compound **3b** in CDCl₃.

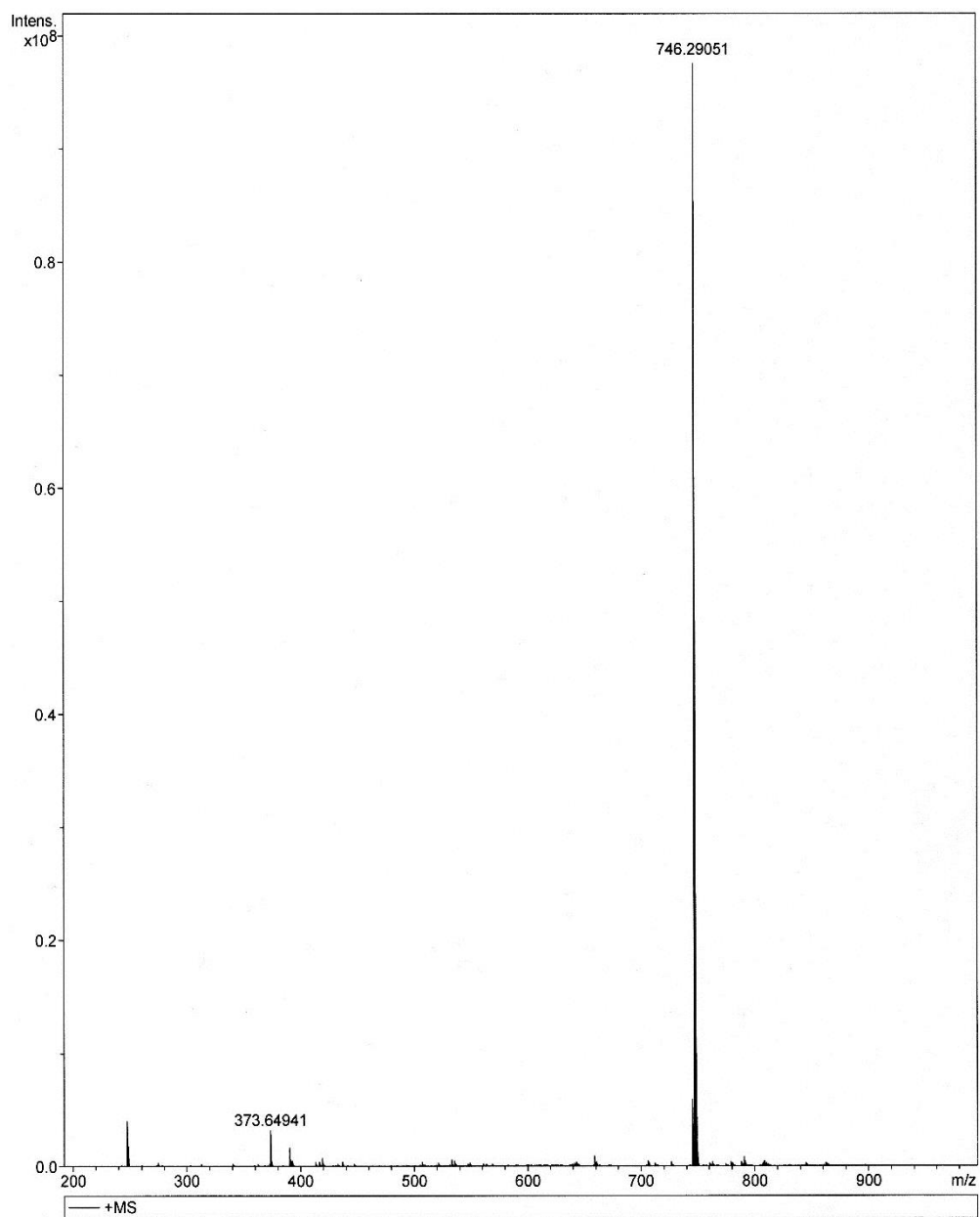


Figure S30. HRMS spectrum of compound **3b**.

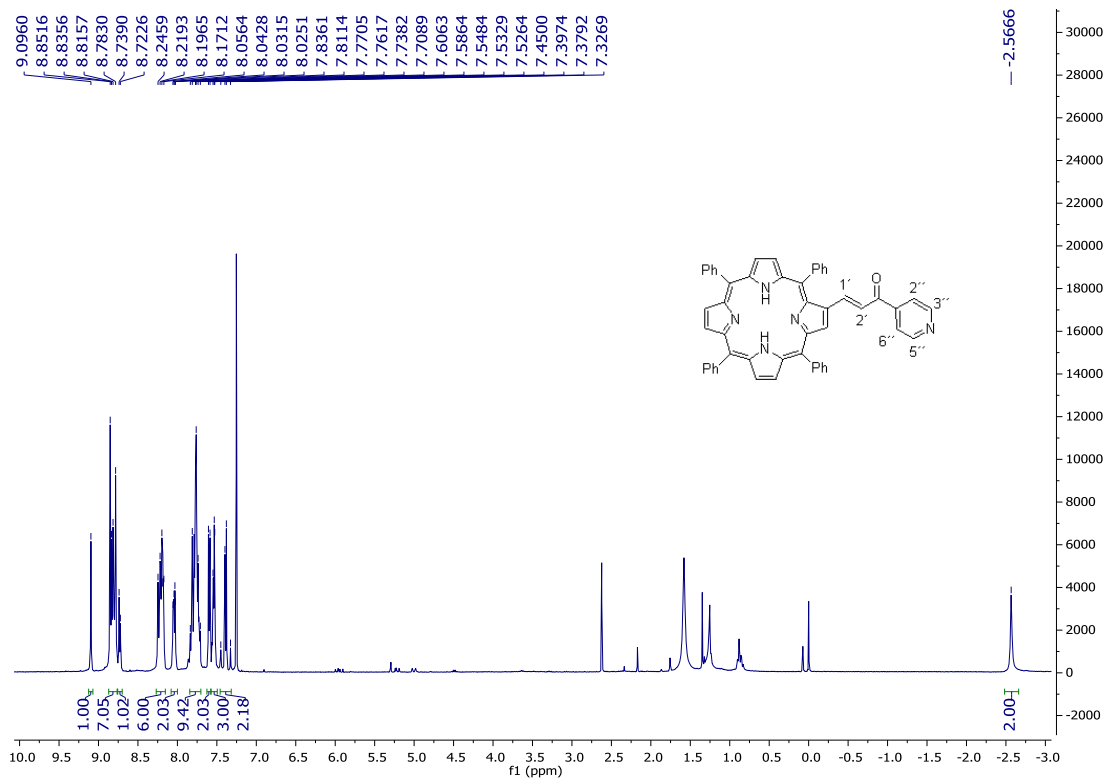


Figure S31. ^1H NMR spectrum of compound **3c** in CDCl_3 .

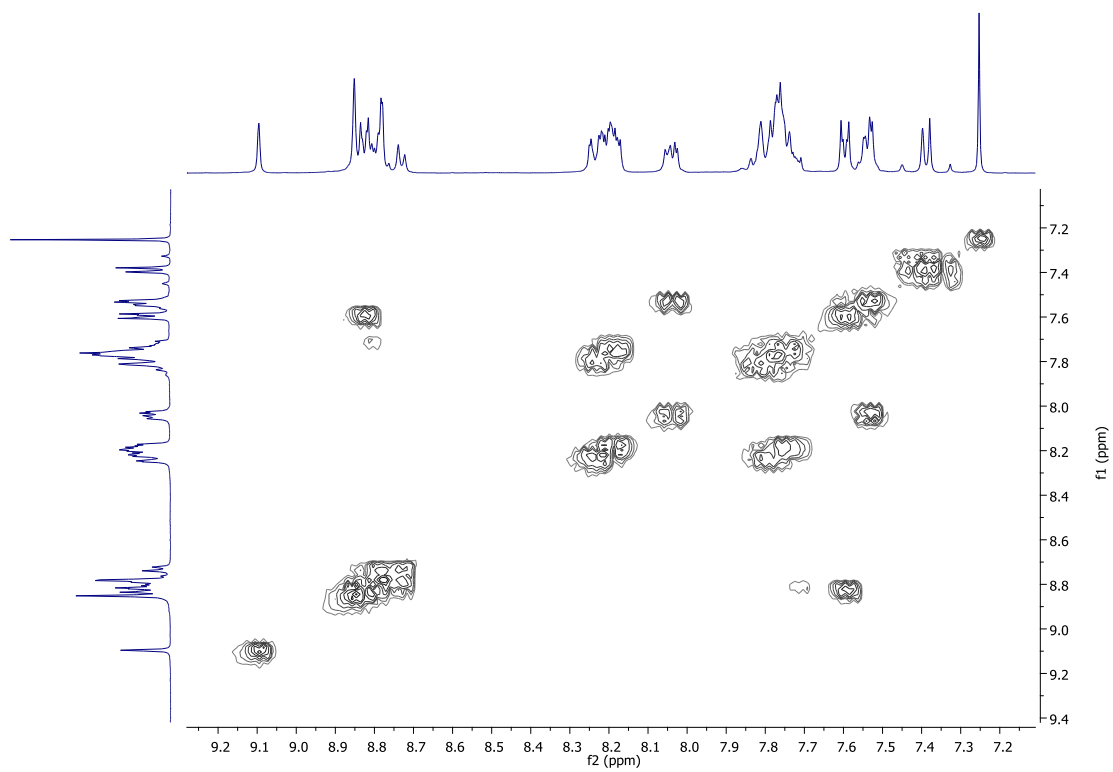


Figure S32. Partial COSY ($^1\text{H}/^1\text{H}$) spectrum of compound **3c** in CDCl_3 .

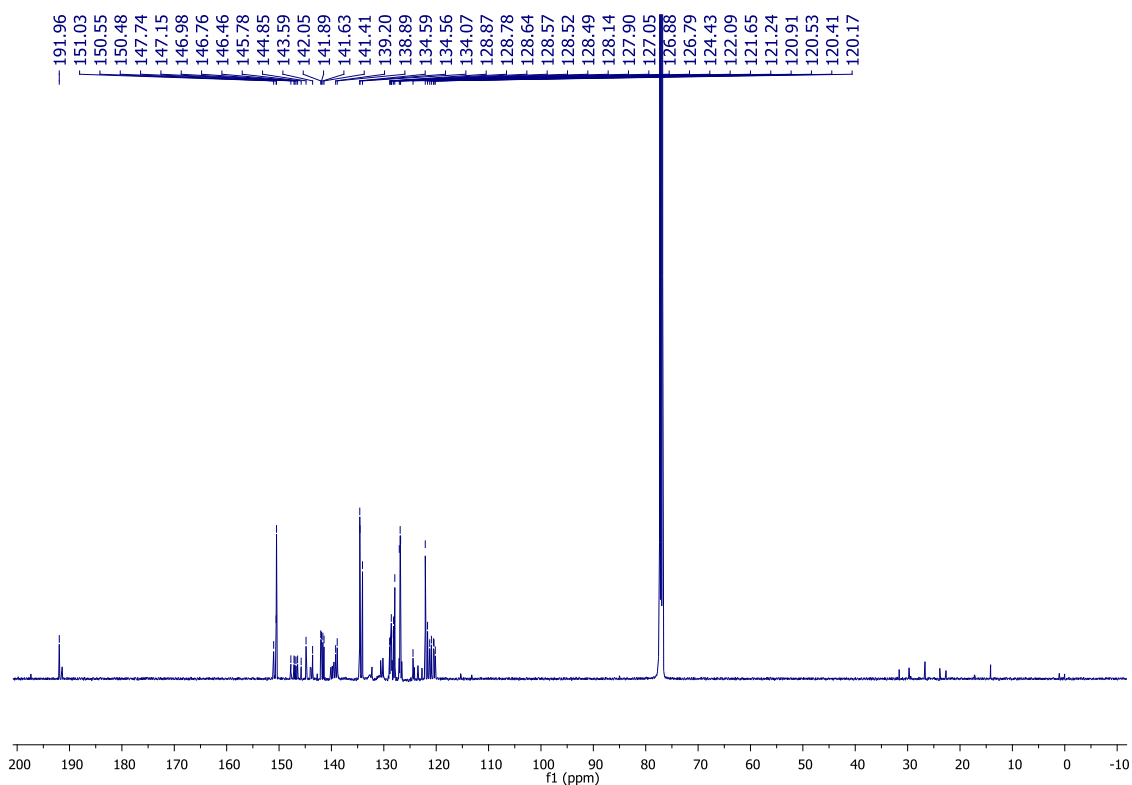


Figure S33. ^{13}C NMR spectrum of compound **3c** in CDCl_3 .

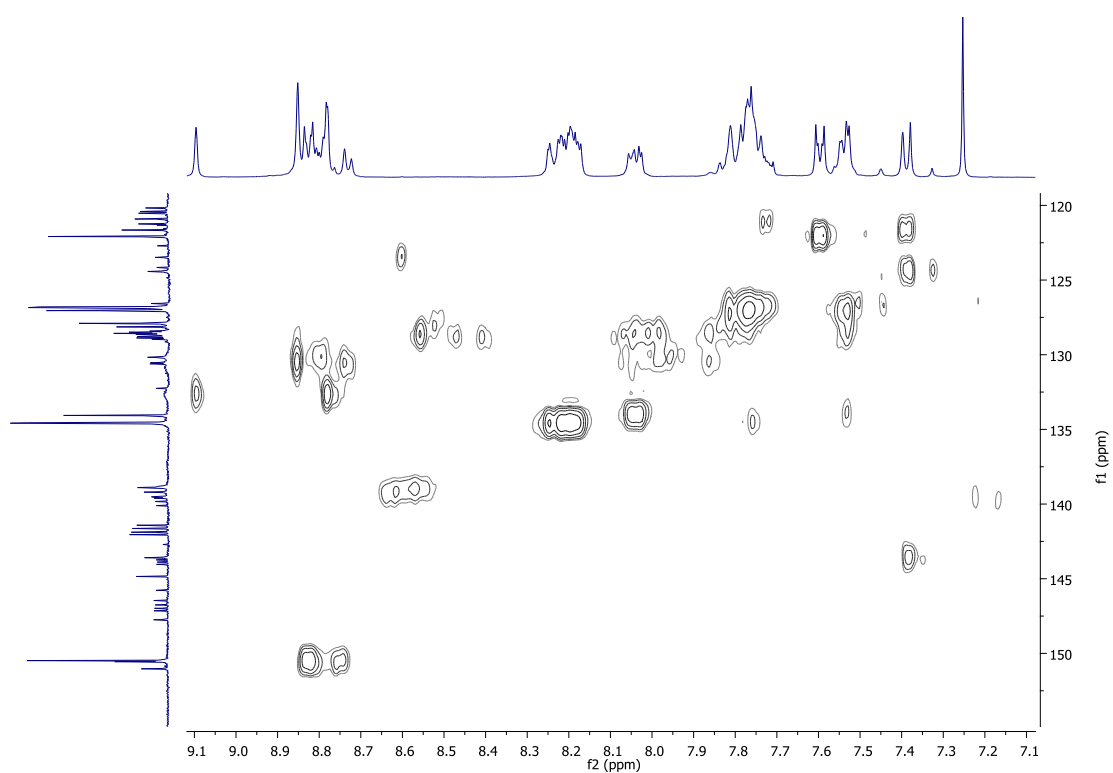


Figure S34. Partial HSQC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **3c** in CDCl_3 .

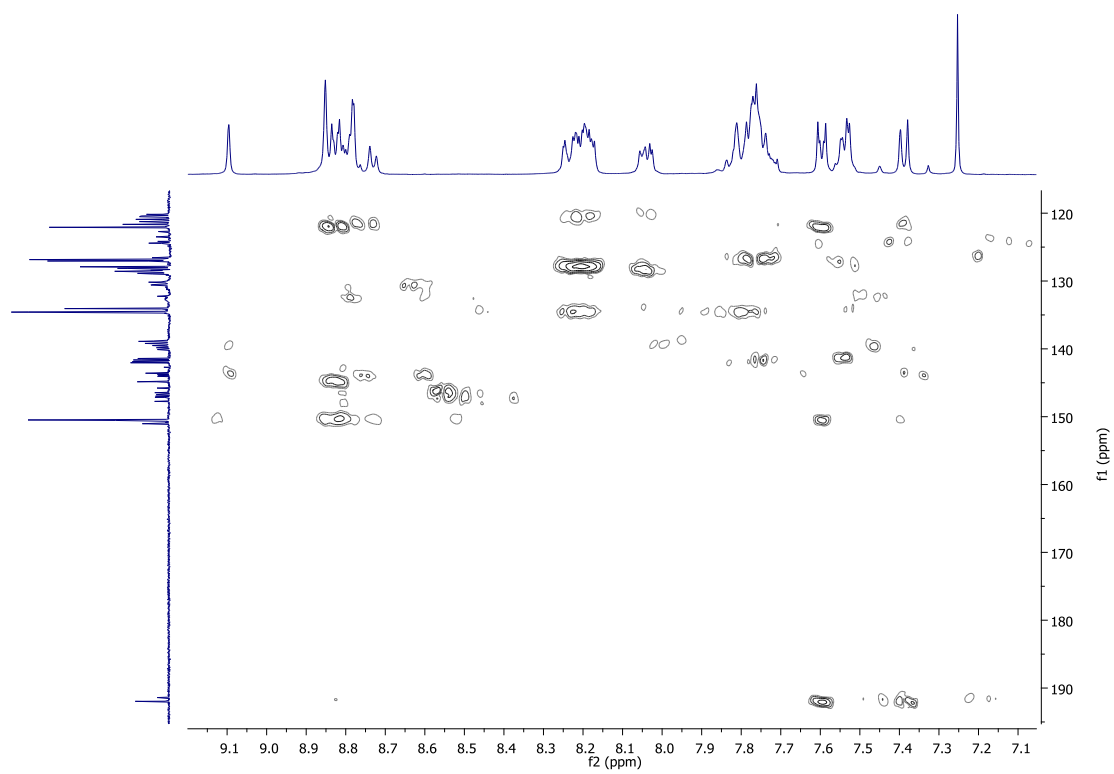


Figure S35. Partial HMBC (¹H/¹³C) spectrum of compound **3c** in CDCl₃.

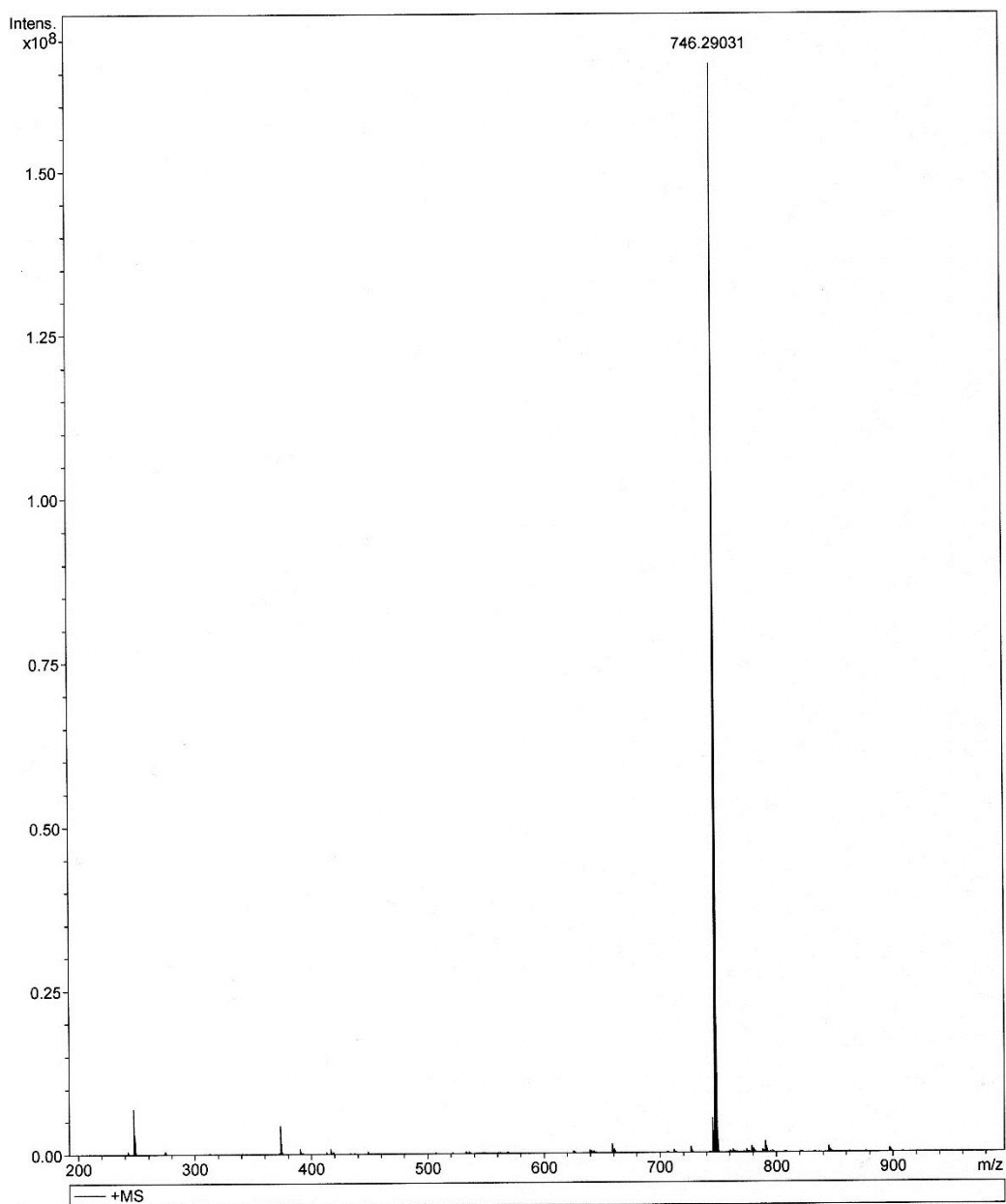


Figure S36. HRMS spectrum of compound **3c**.

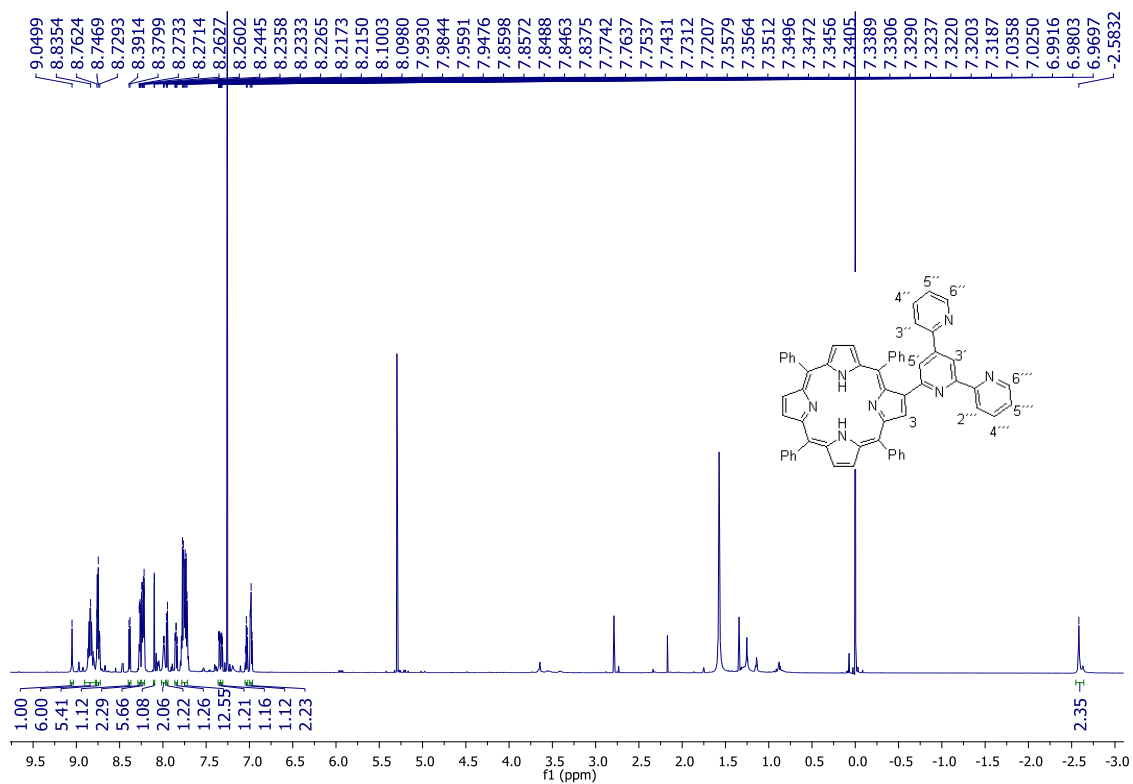


Figure S37. ^1H NMR spectrum of compound **4** in CDCl_3 .

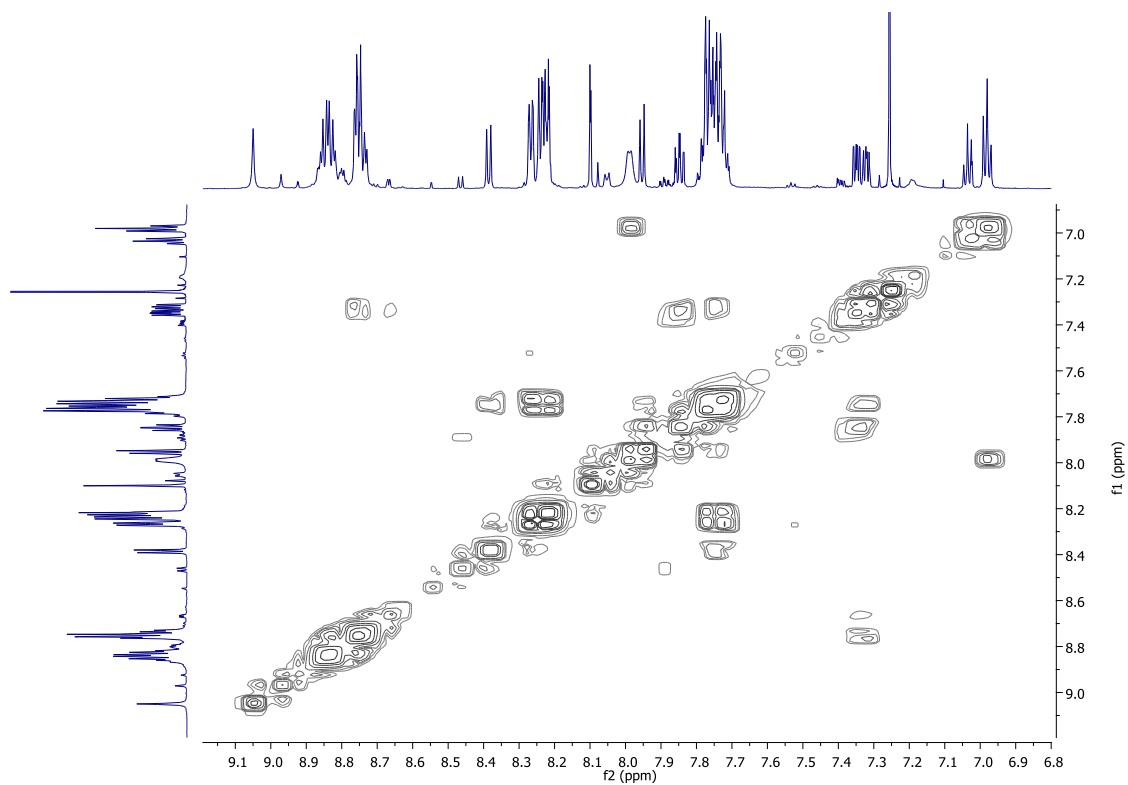


Figure S38. Partial COSY ($^1\text{H}/^1\text{H}$) spectrum of compound **4** in CDCl_3 .

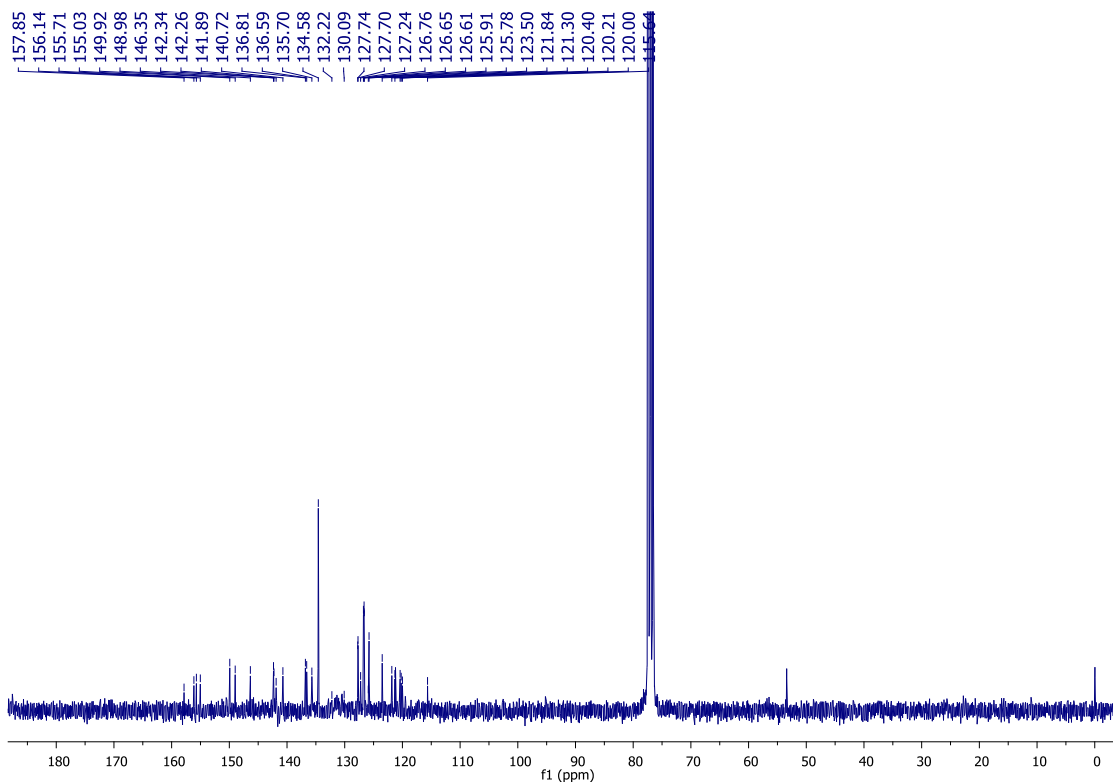


Figure S39. ^{13}C NMR spectrum of compound **4** in CDCl_3 .

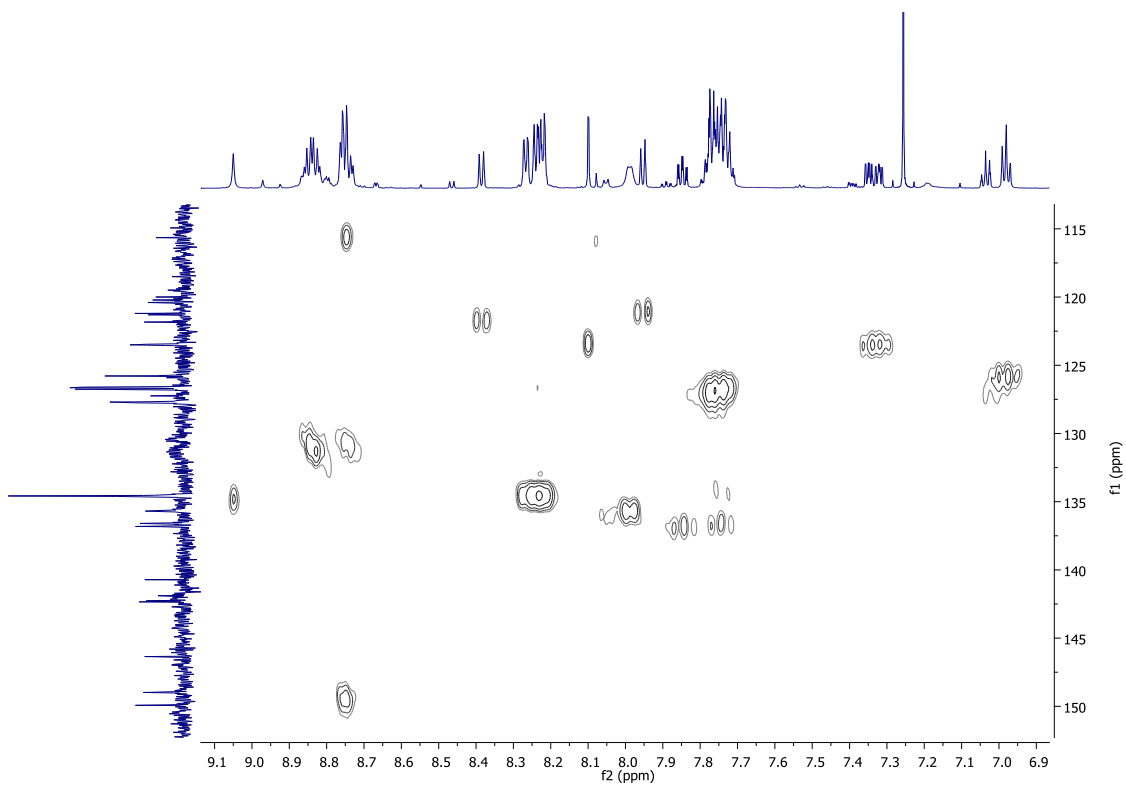


Figure S40. Partial HSQC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **4** in CDCl_3 .

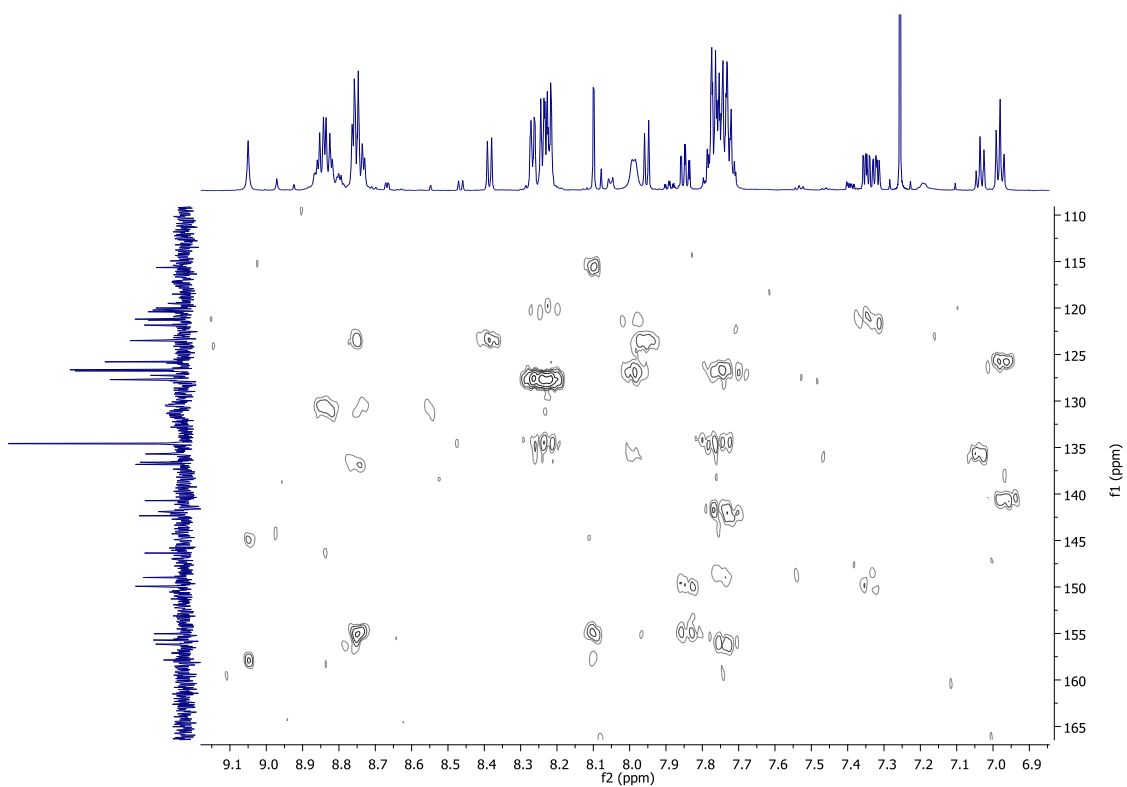


Figure S41. Partial HMBC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **4** in CDCl_3 .

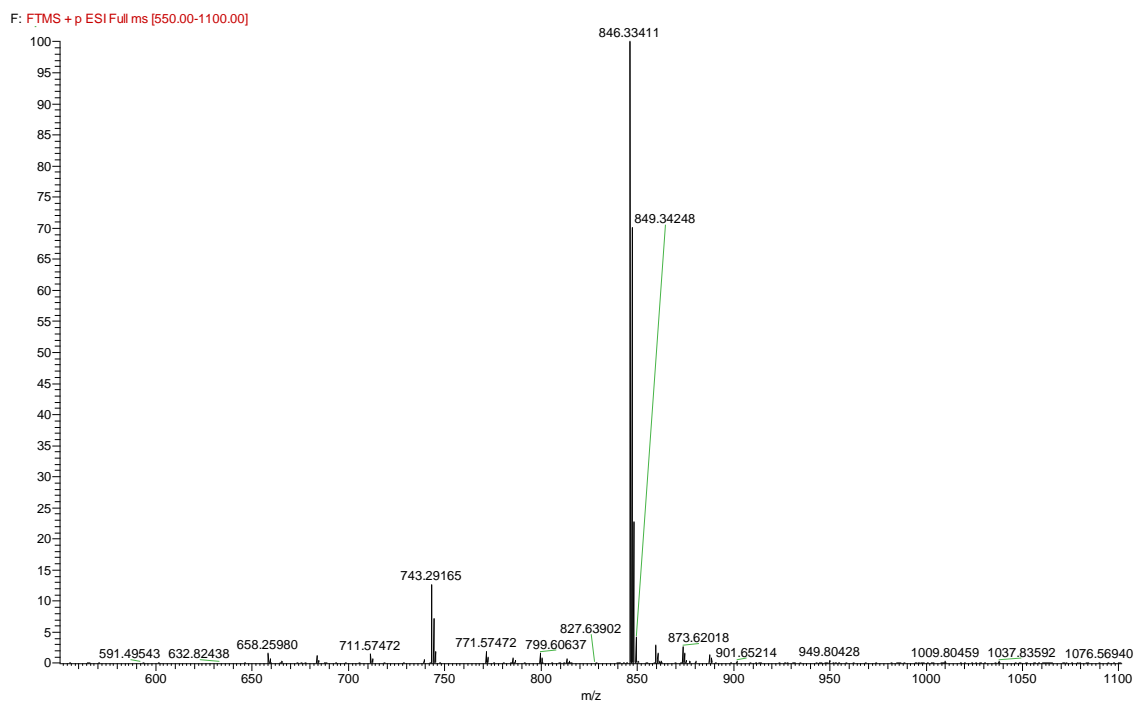


Figure S42. HRMS spectrum of compound **4**.

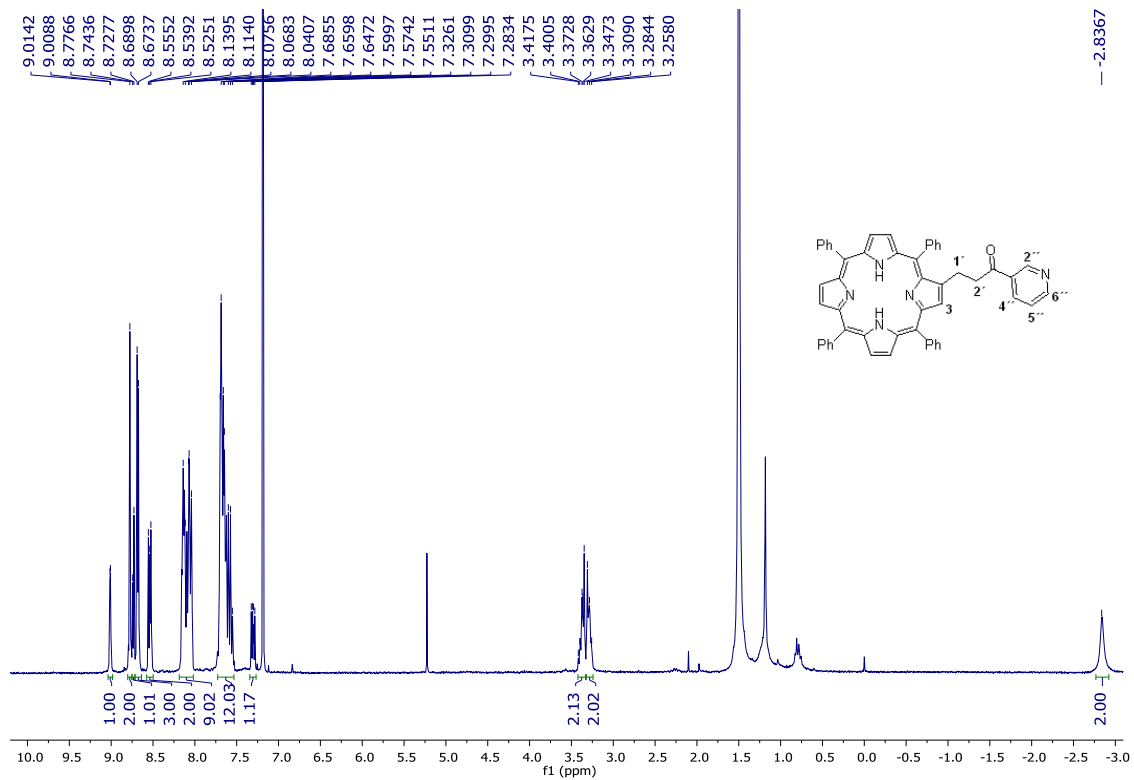


Figure S43. ¹H NMR spectrum of compound **5b** in CDCl₃.

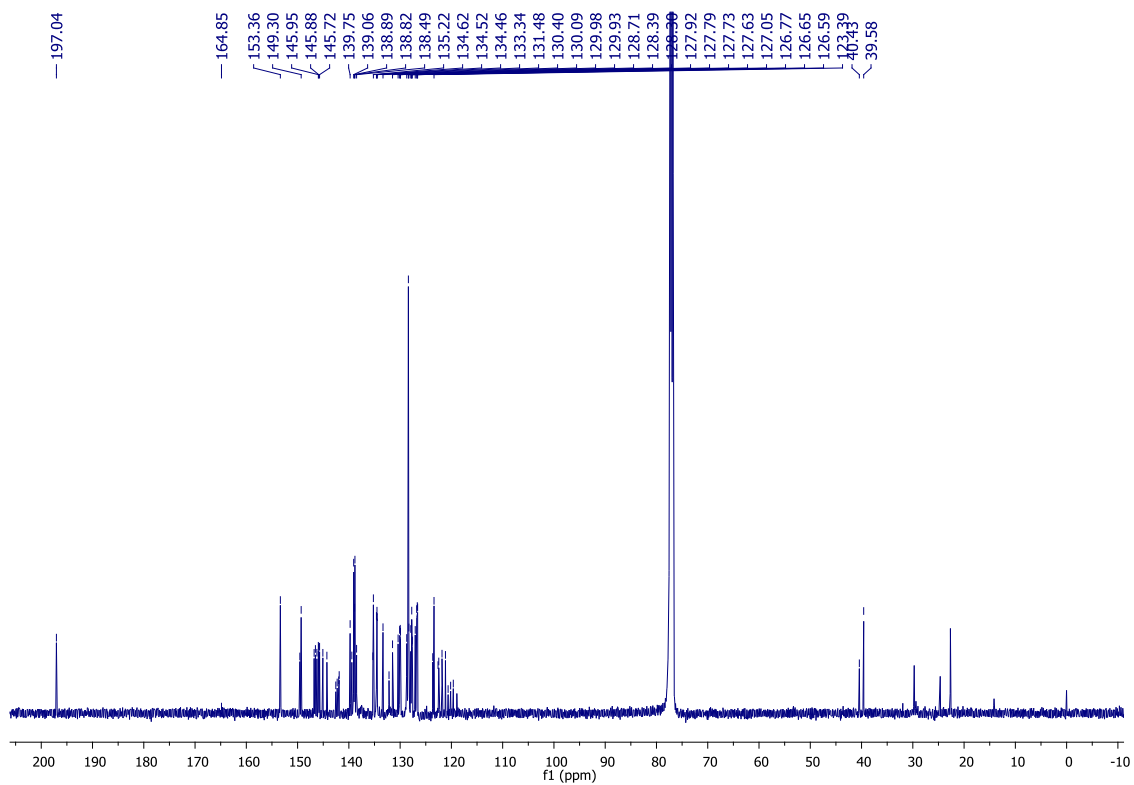


Figure S44. ¹³C NMR spectrum of compound **5b** in CDCl₃.

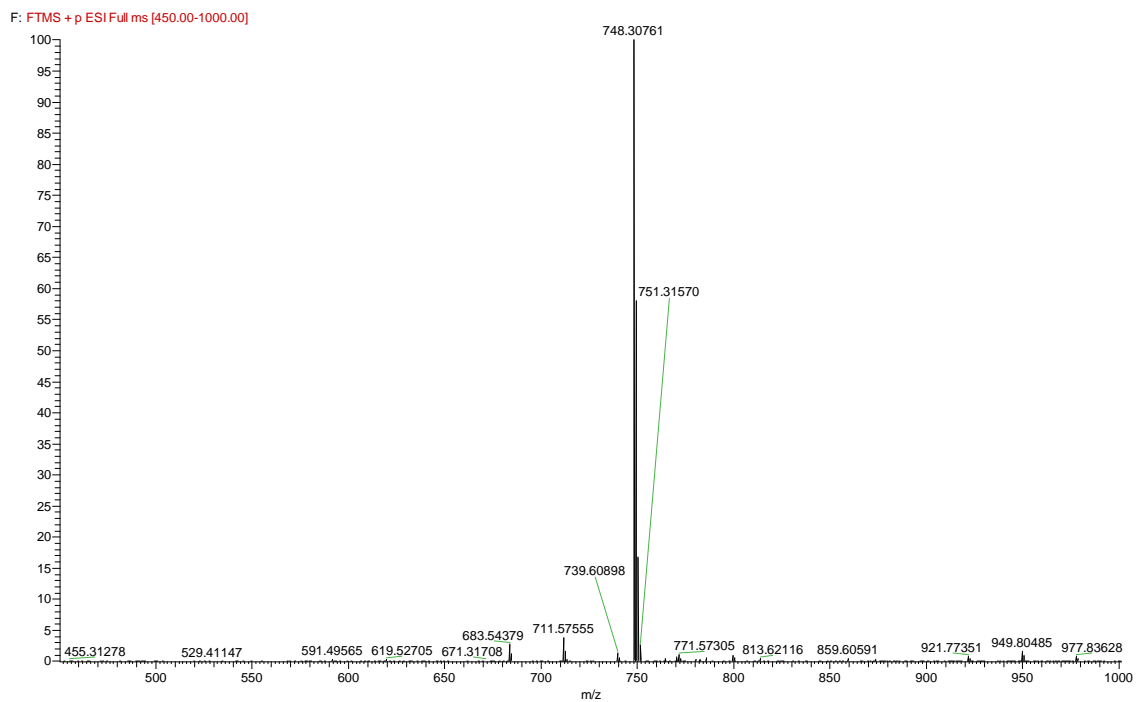


Figure S45. HRMS spectrum of compound **5b** in CDCl_3 .

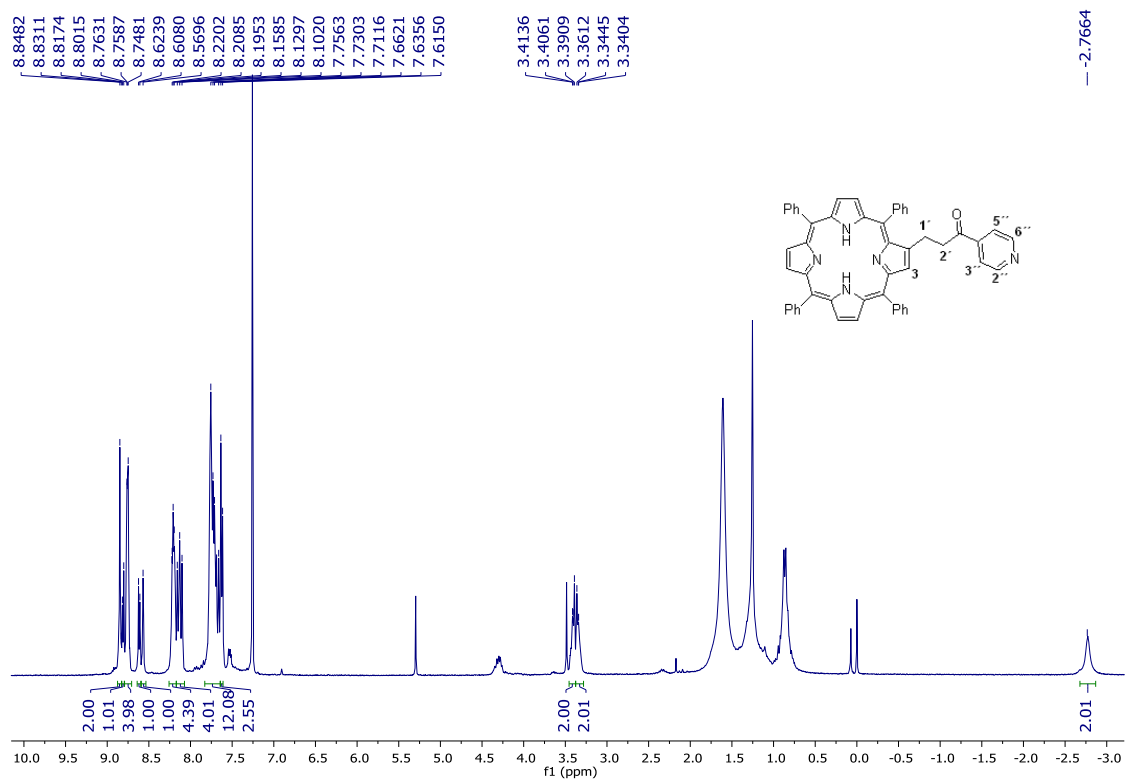


Figure S46. ^1H NMR spectrum of compound **5c** in CDCl_3 .

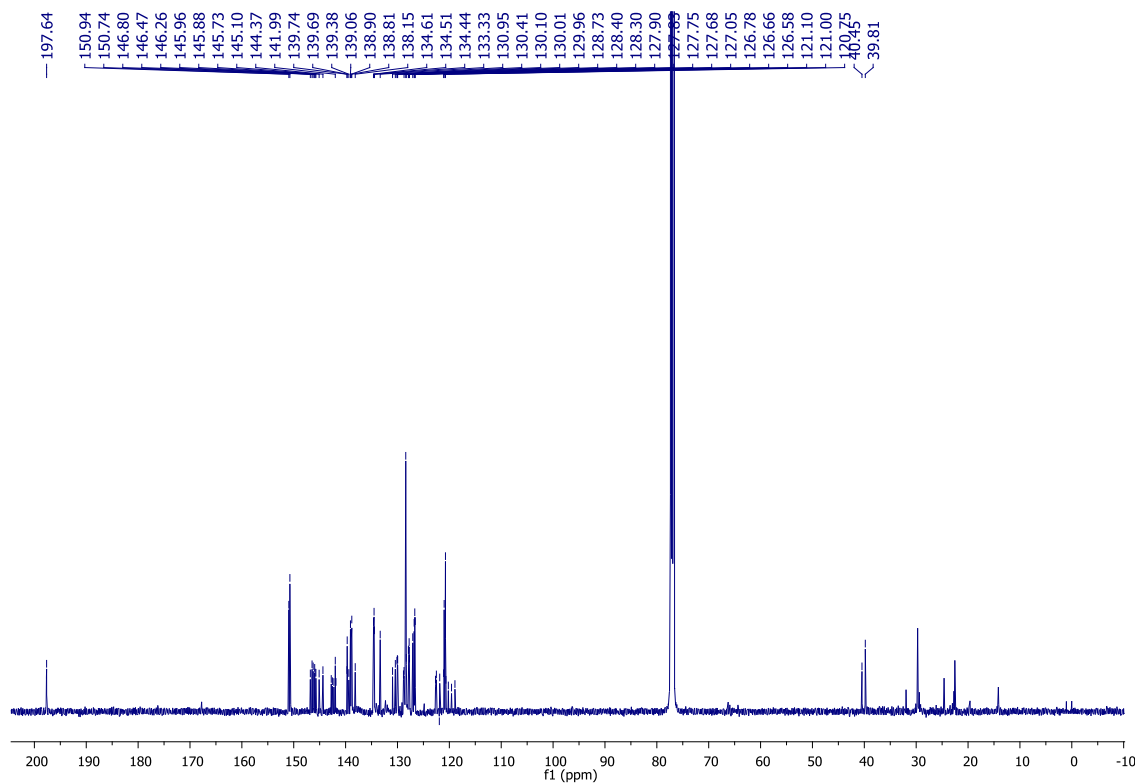


Figure S47. ^{13}C NMR spectrum of compound **5c** in CDCl_3 .

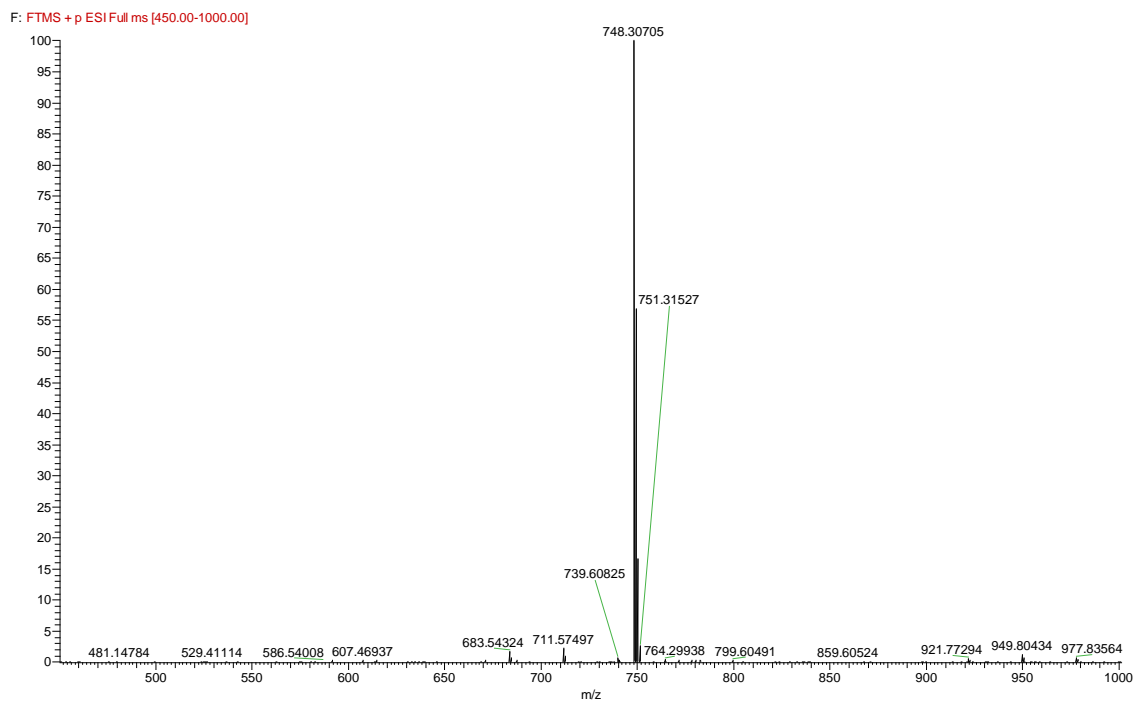


Figure S48. HRMS spectrum of compound **5c** in CDCl_3 .

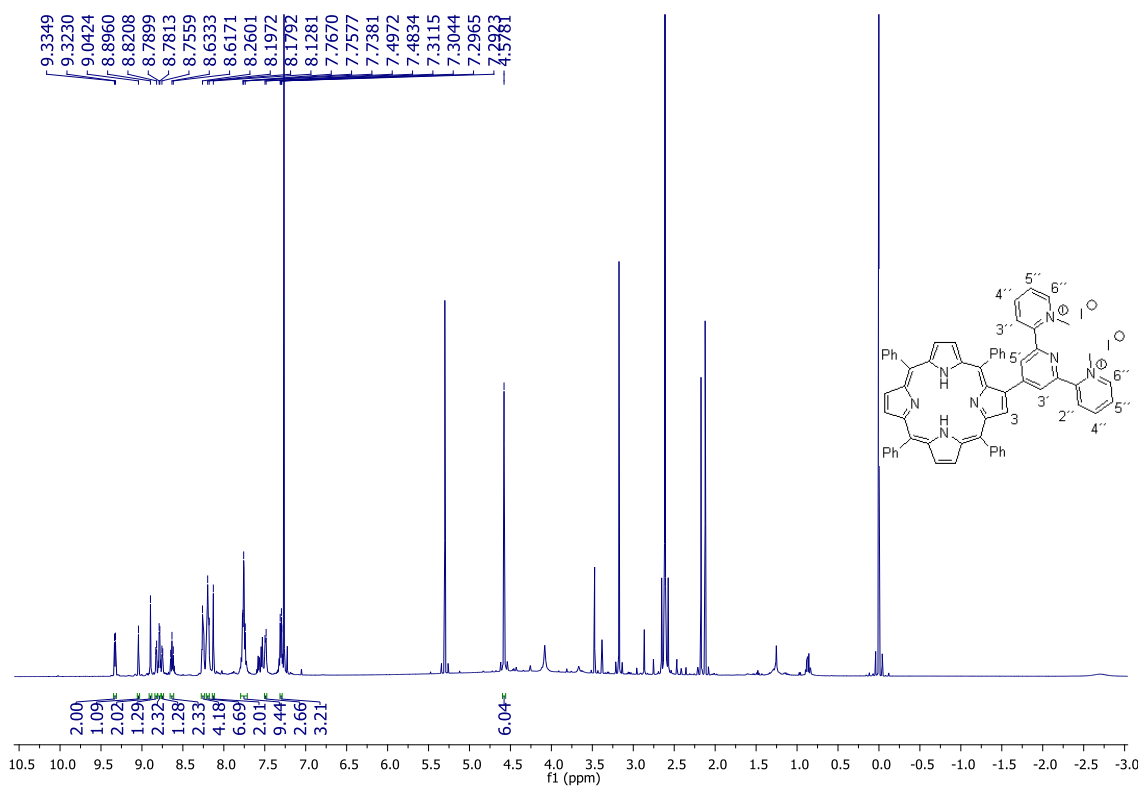


Figure S49. ^1H NMR spectrum of compound **6a** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

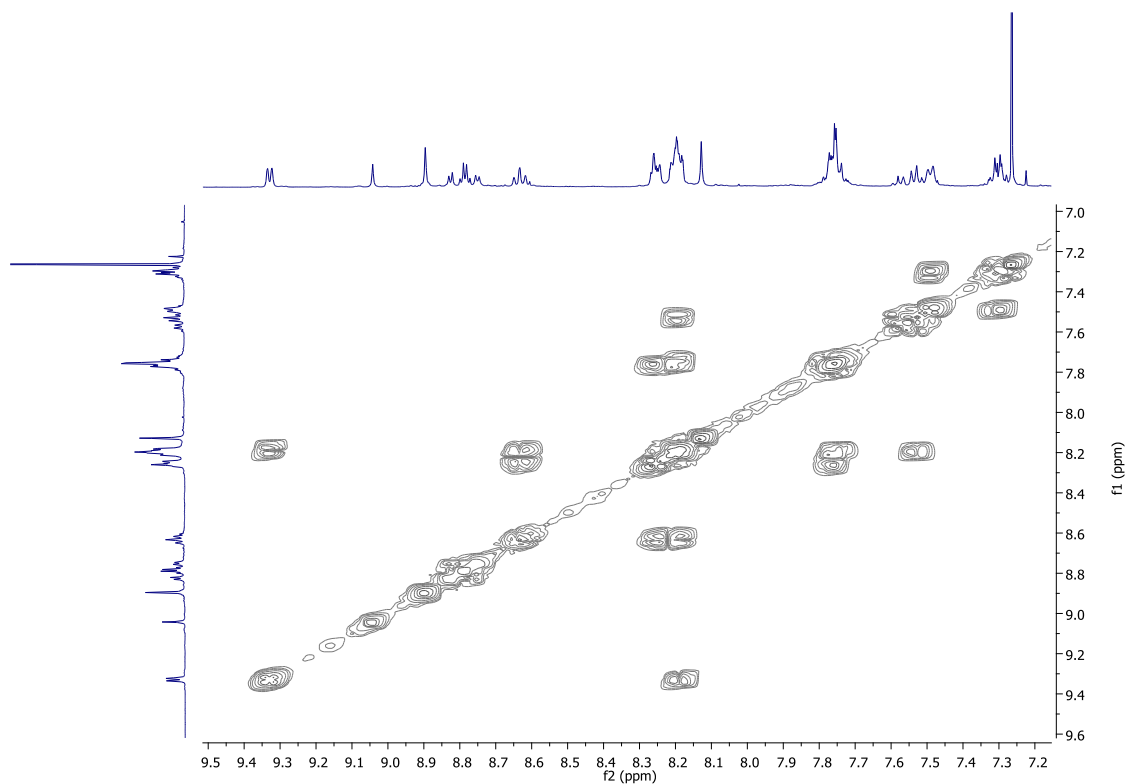


Figure S50. Partial COSY ($^1\text{H}/^1\text{H}$) spectrum of compound **6a** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

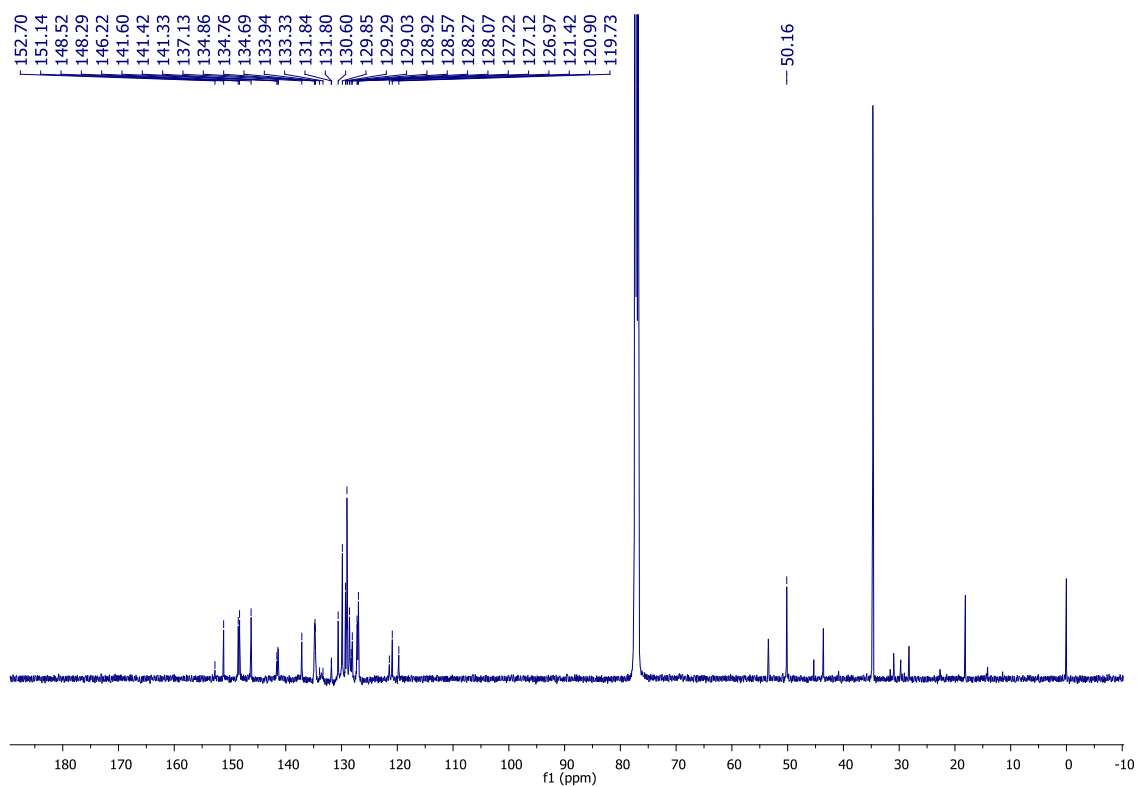


Figure S51. ^{13}C NMR spectrum of compound **6a** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

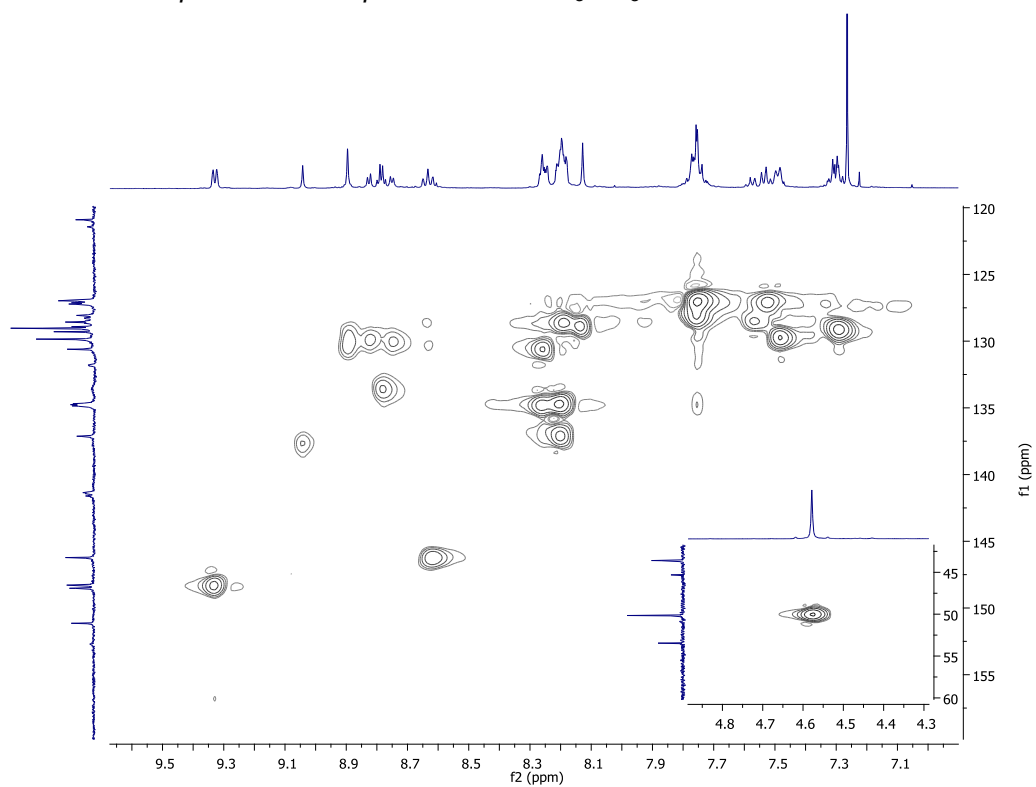


Figure S52. Partial HSQC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **6a** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

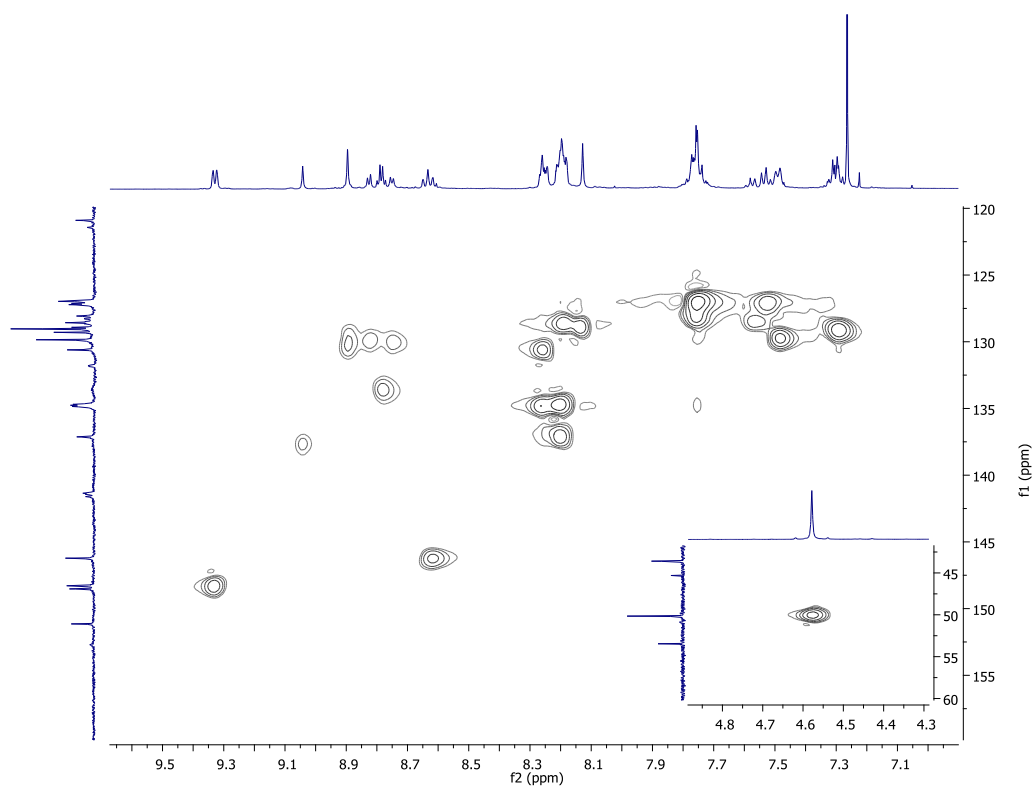


Figure S53. Partial HMBC ($^1\text{H}/^{13}\text{C}$) spectrum of compound **6a** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

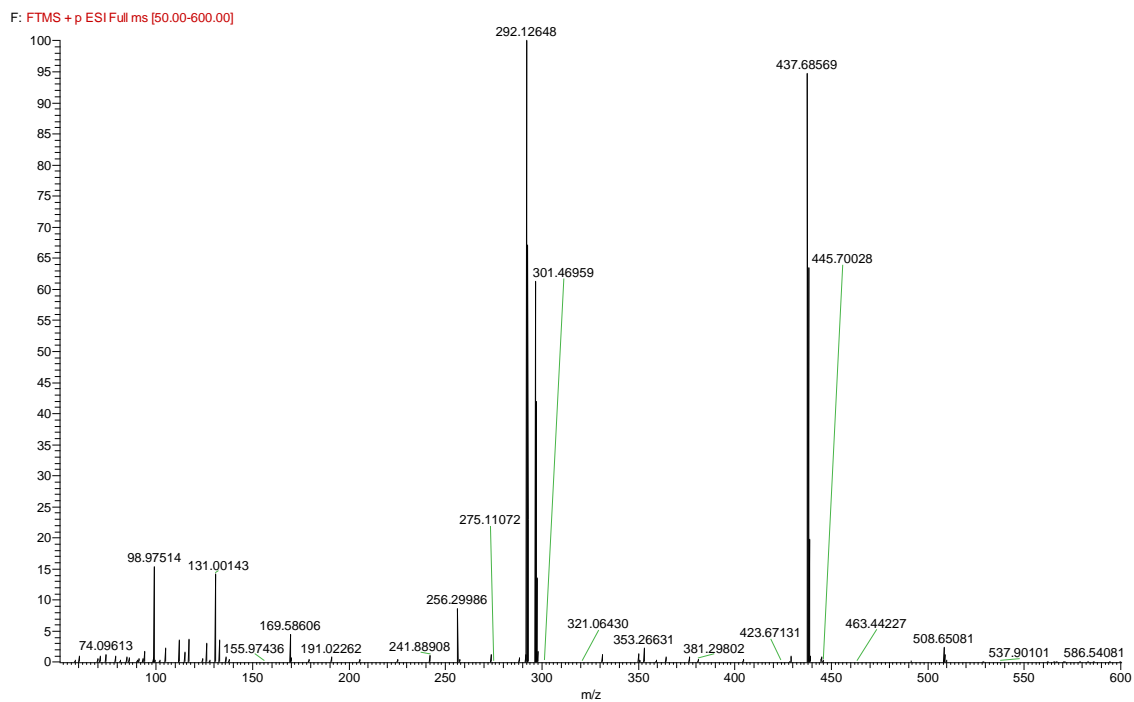


Figure S54. HRMS spectrum of compound **6a**.

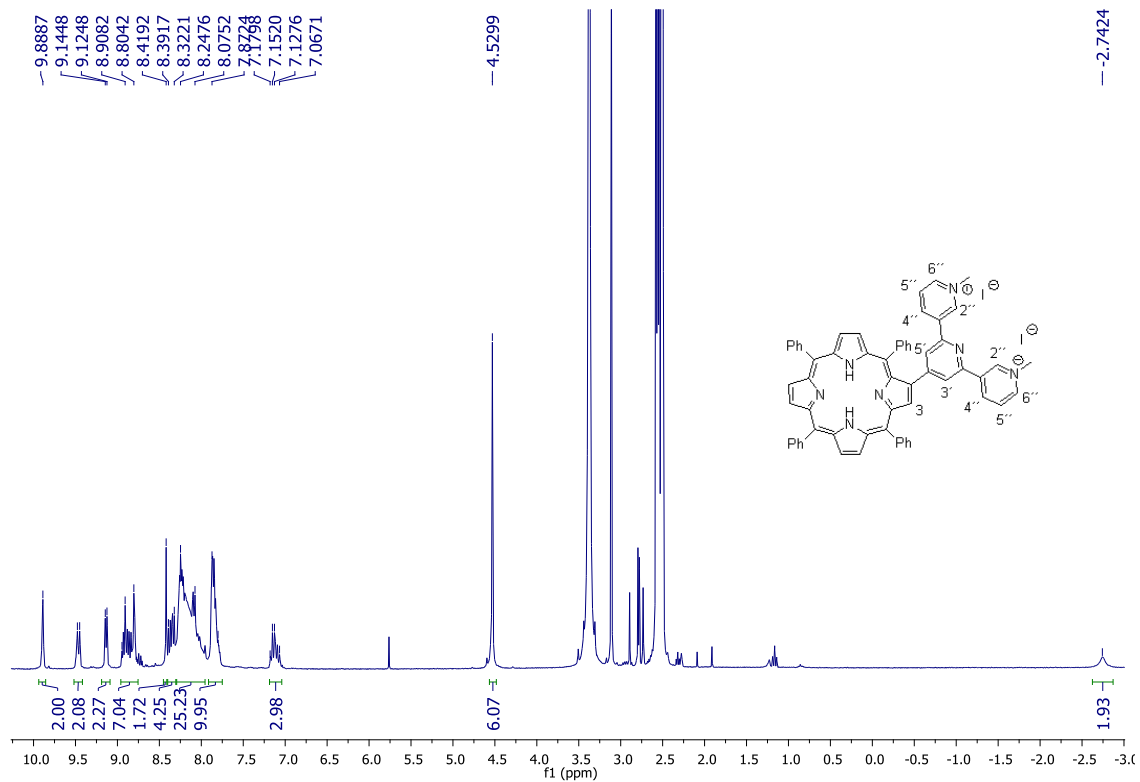


Figure S55. ¹H NMR spectrum of compound **6b** in DMSO-d₆.

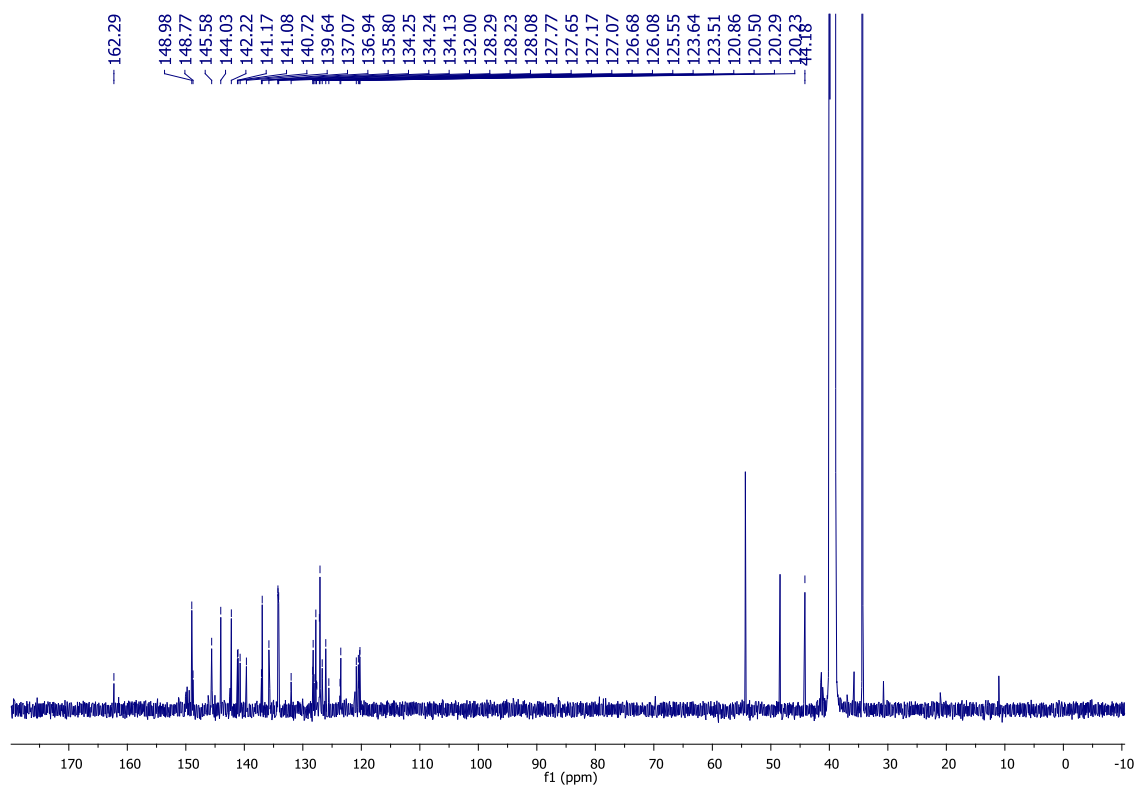


Figure S56. ¹³C NMR spectrum of compound **6b** in DMSO-d₆.

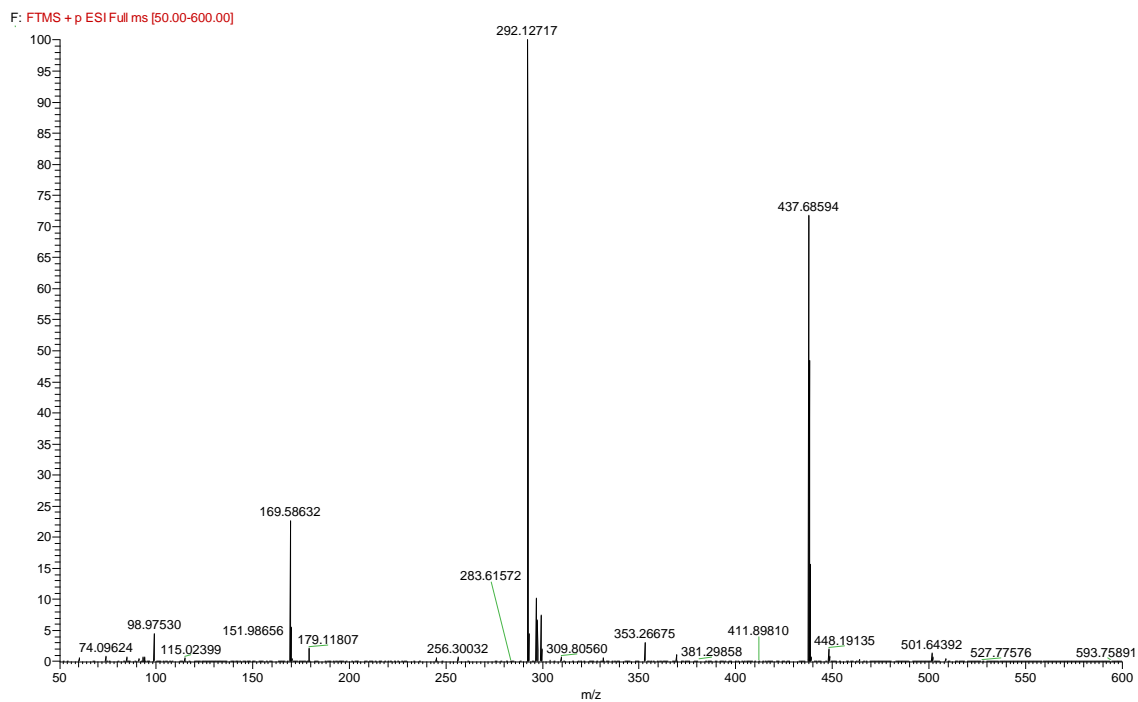


Figure S57. HRMS spectrum of compound **6b**.

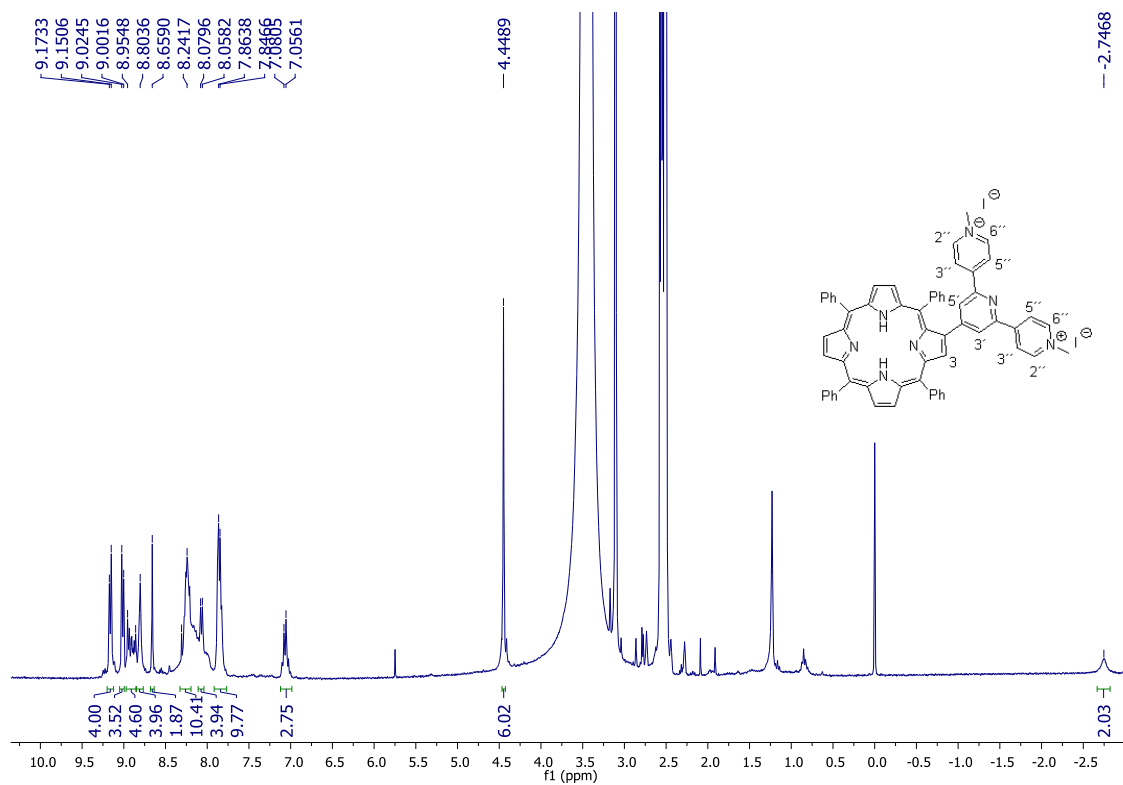


Figure S58. ^1H NMR spectrum of compound **6c** in DMSO-d_6 .

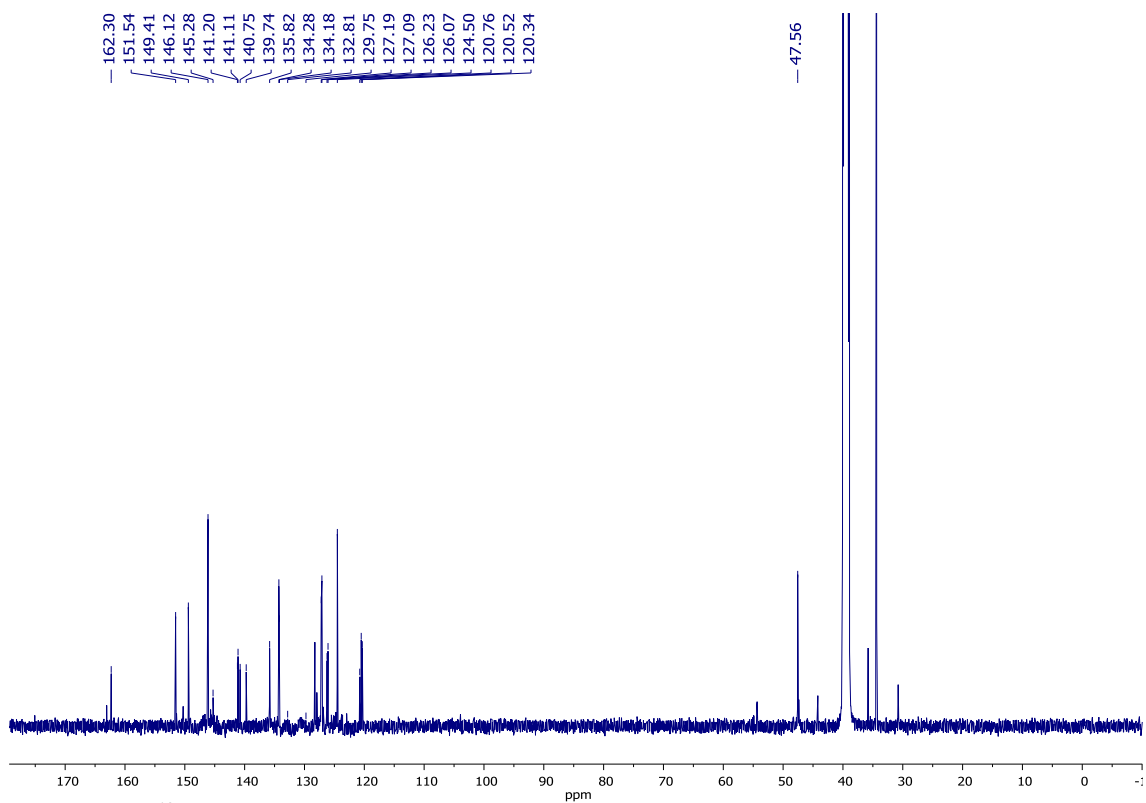


Figure S59. ^{13}C NMR spectrum of compound **6c** in DMSO-d_6 .

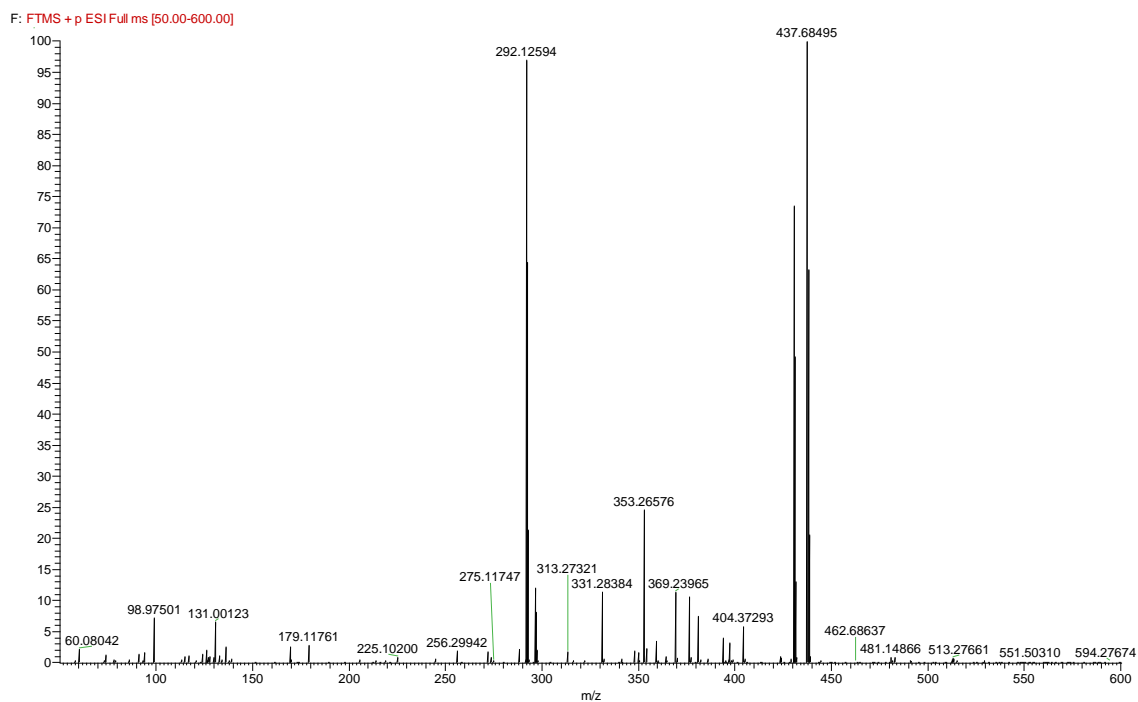
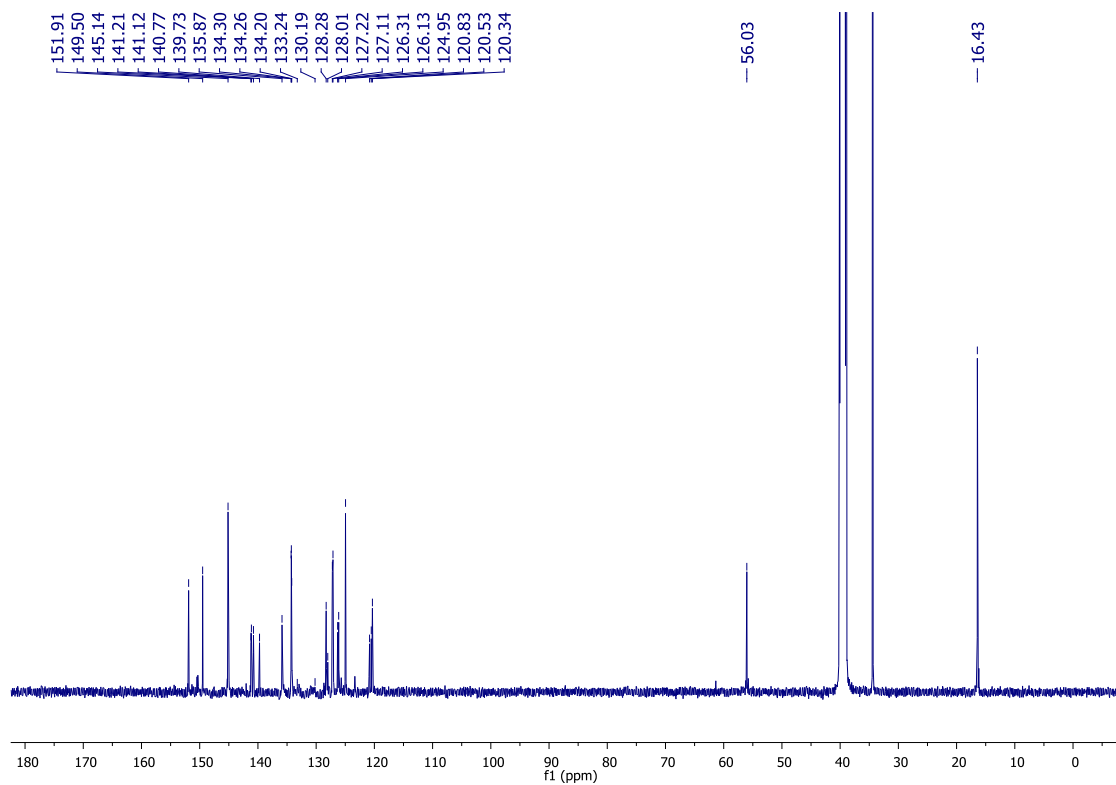
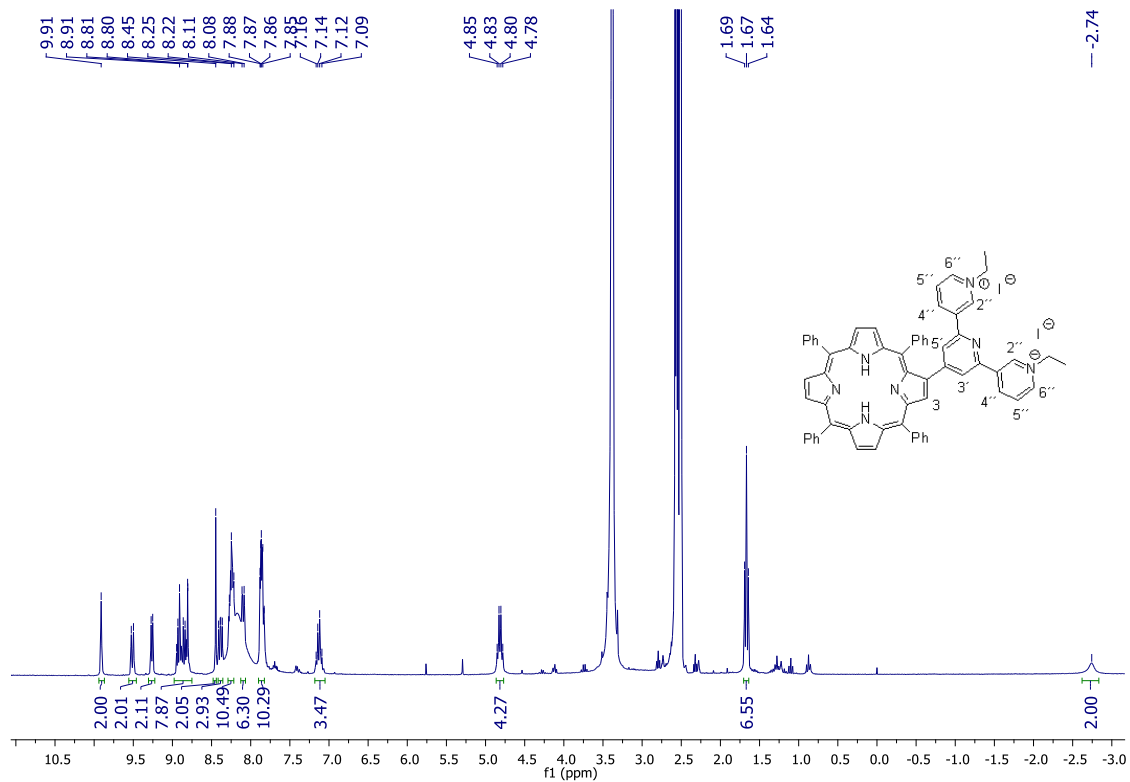


Figure S60. HRMS spectrum of compound **6c**.



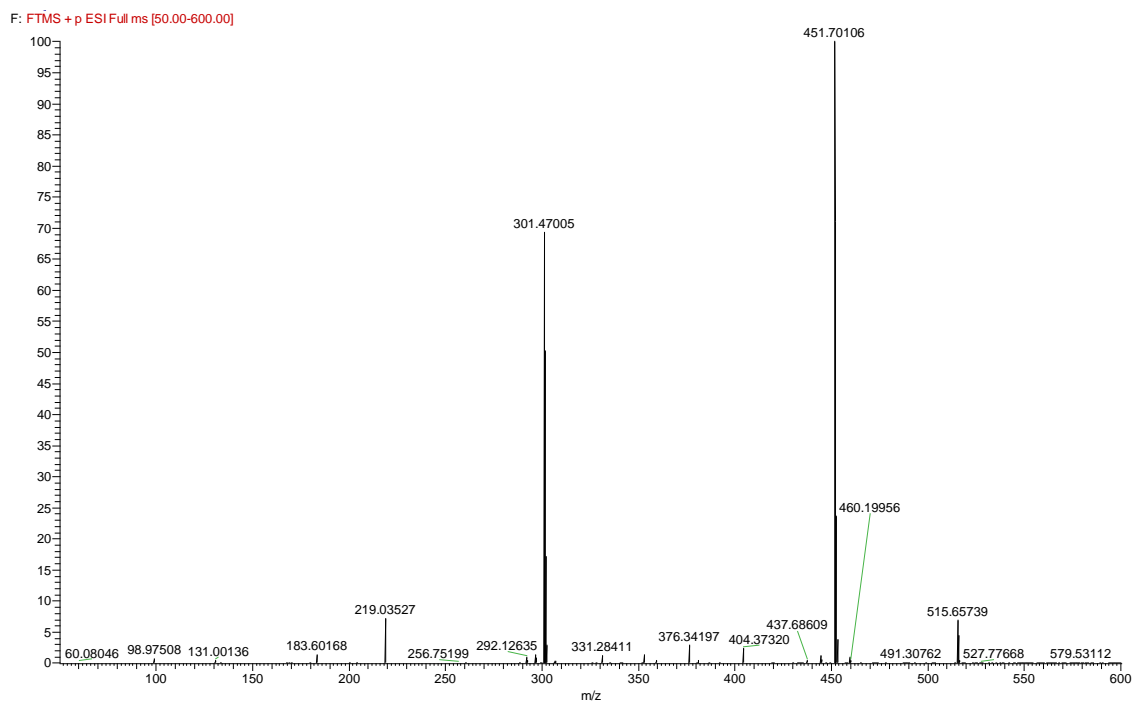


Figure S63. HRMS spectrum of compound **7b**.

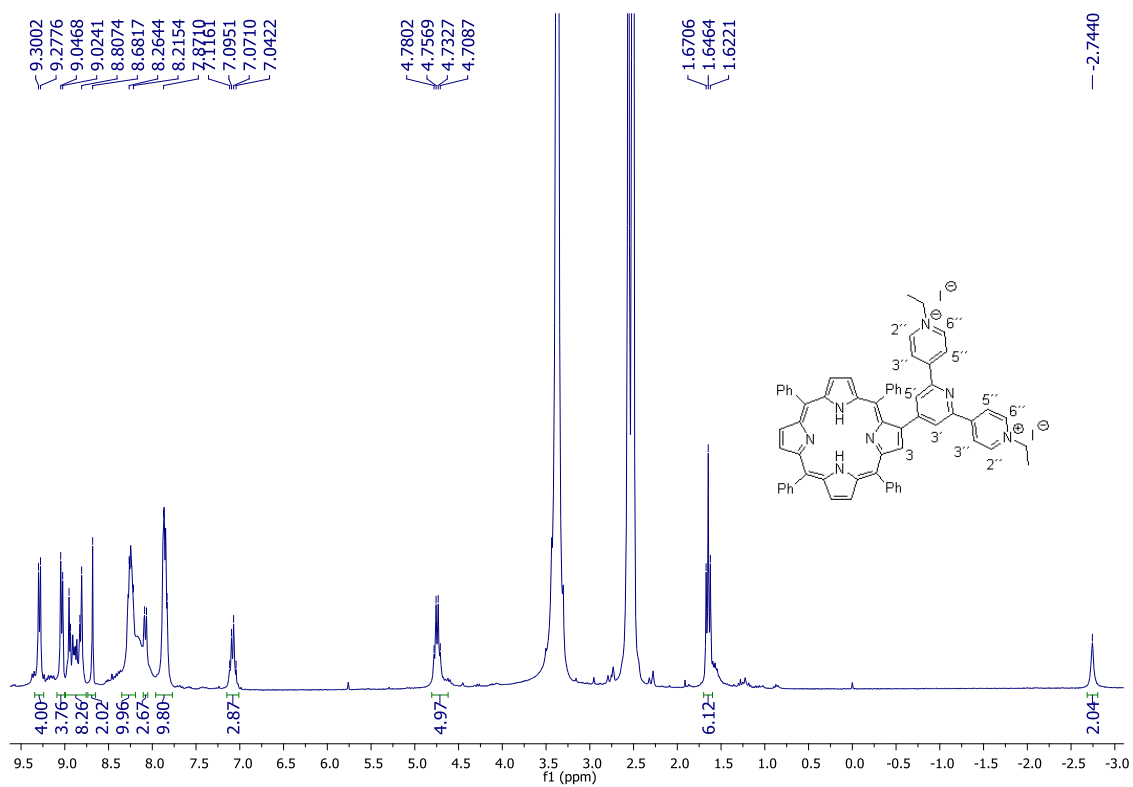


Figure S64. ^1H NMR spectrum of compound **7c** in DMSO-d_6 .

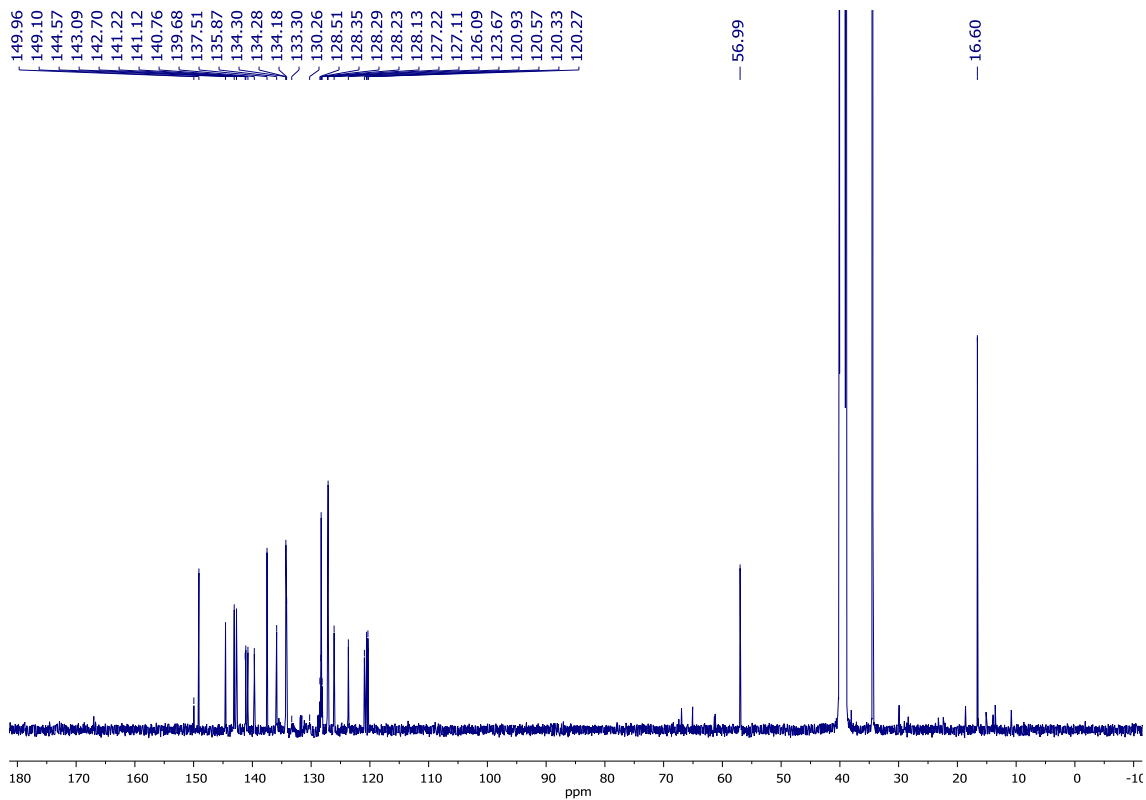


Figure S65. ^{13}C NMR spectrum of compound **7c** in DMSO-d_6 .

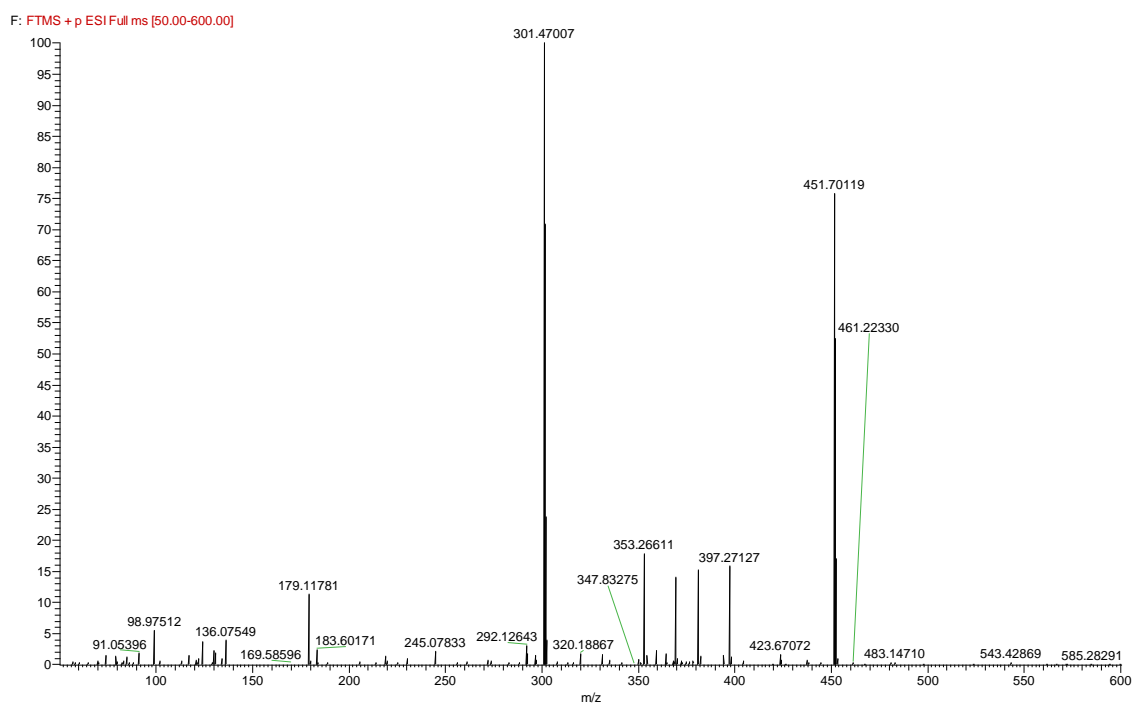


Figure S66. HRMS spectrum of compound **7c**.

III – Biological assays

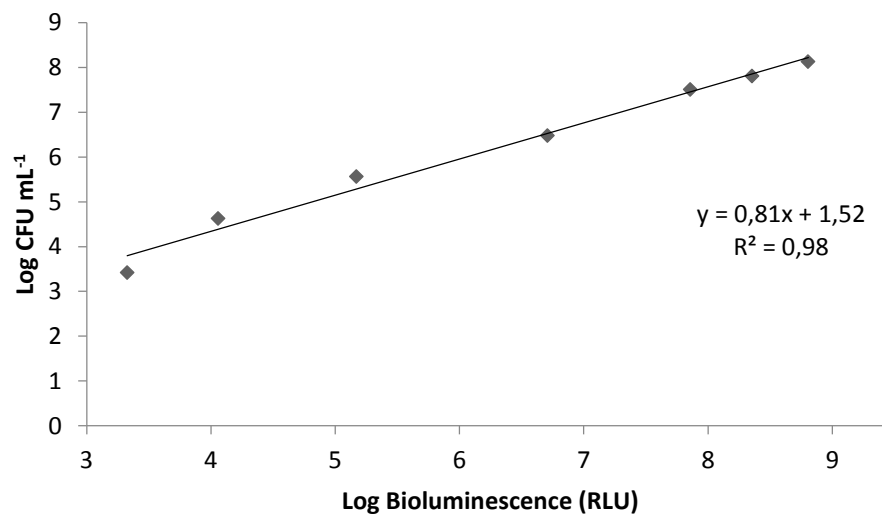


Figure S67. Relationship between bioluminescence and viable counts of overnight cultures of recombinant *E. coli* ($\approx 10^8$ CFU mL⁻¹) serially diluted in PBS. Bioluminescence is expressed in relative light units (RLU) and viable counts in CFU mL⁻¹.