

Synthesis of novel dibenzo[*b,f*]imidazo[1,2-*d*][1,4]oxazepine-6,7-dicarbonitriles

Supporting information

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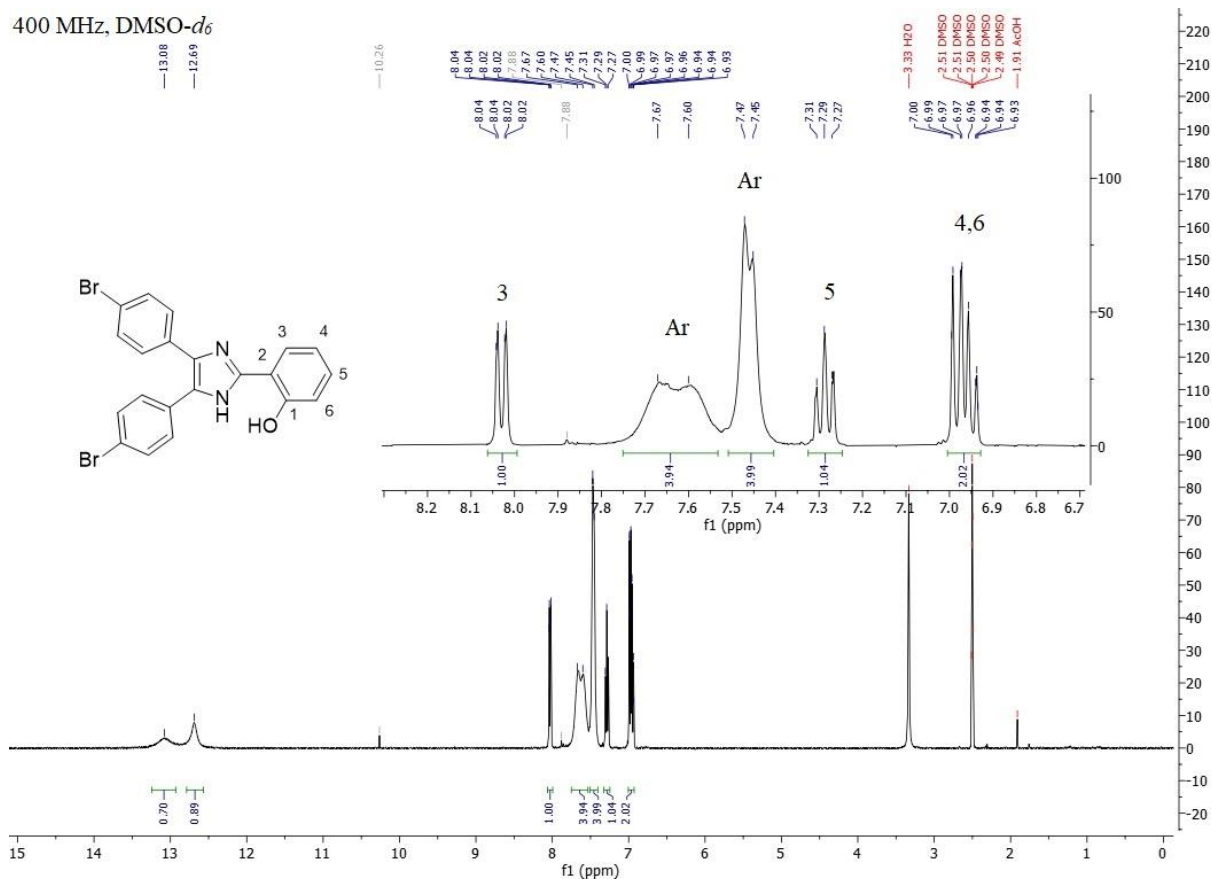


Figure SI-1. ¹H NMR spectrum of compound **1e**.

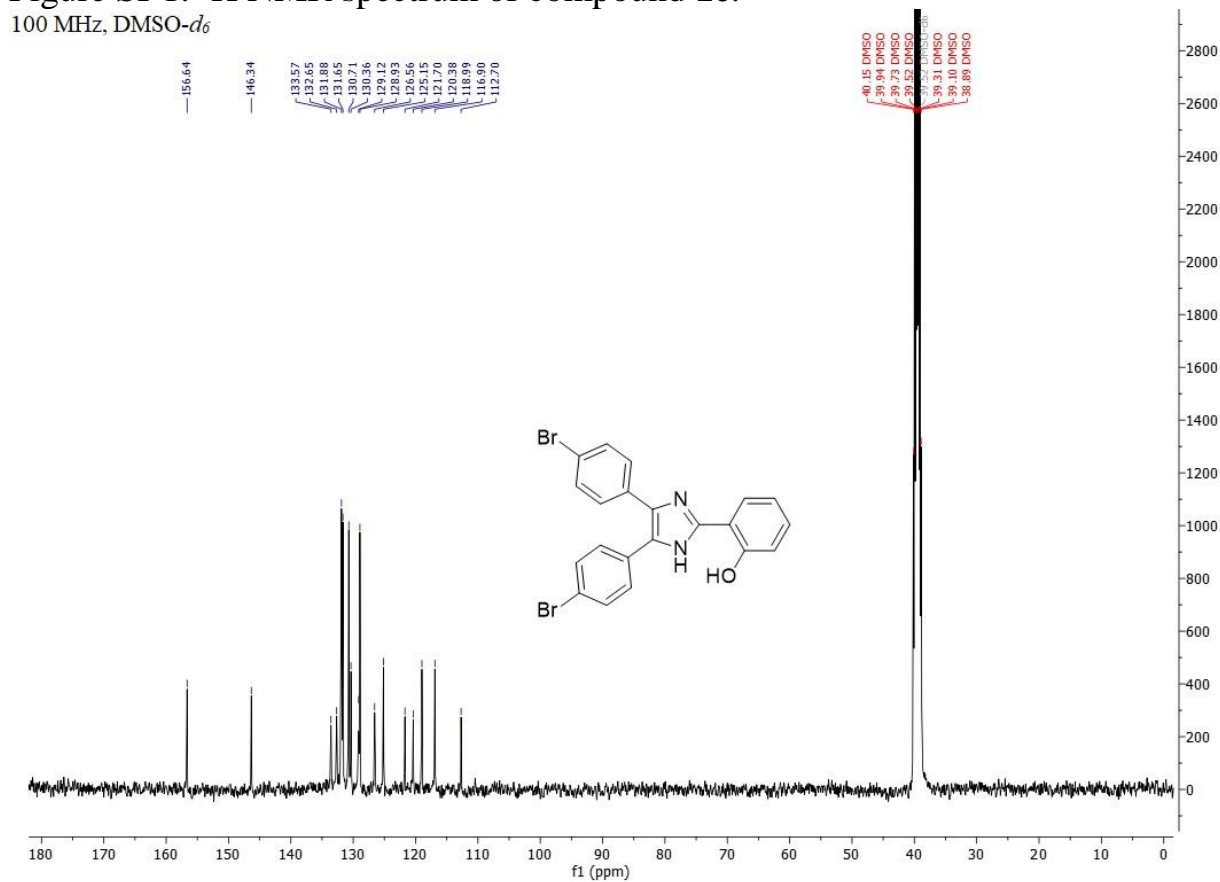


Figure SI-2. ¹³C NMR spectrum of compound **1e**.

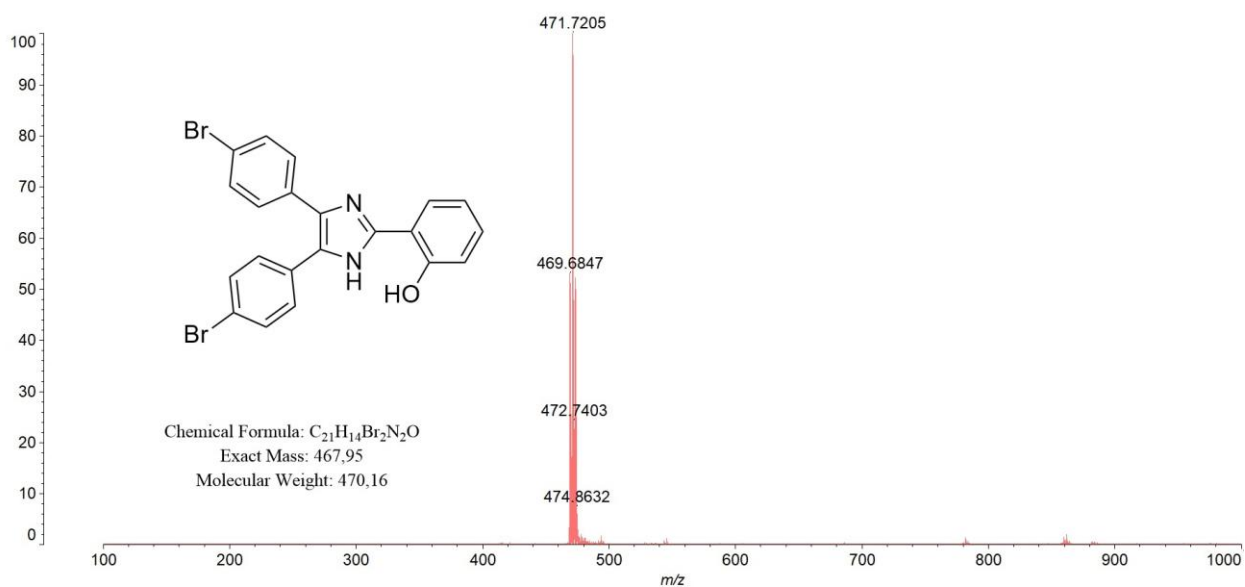


Figure SI-4. High-resolution mass spectrum (MALDI MS) of compound **1e**.

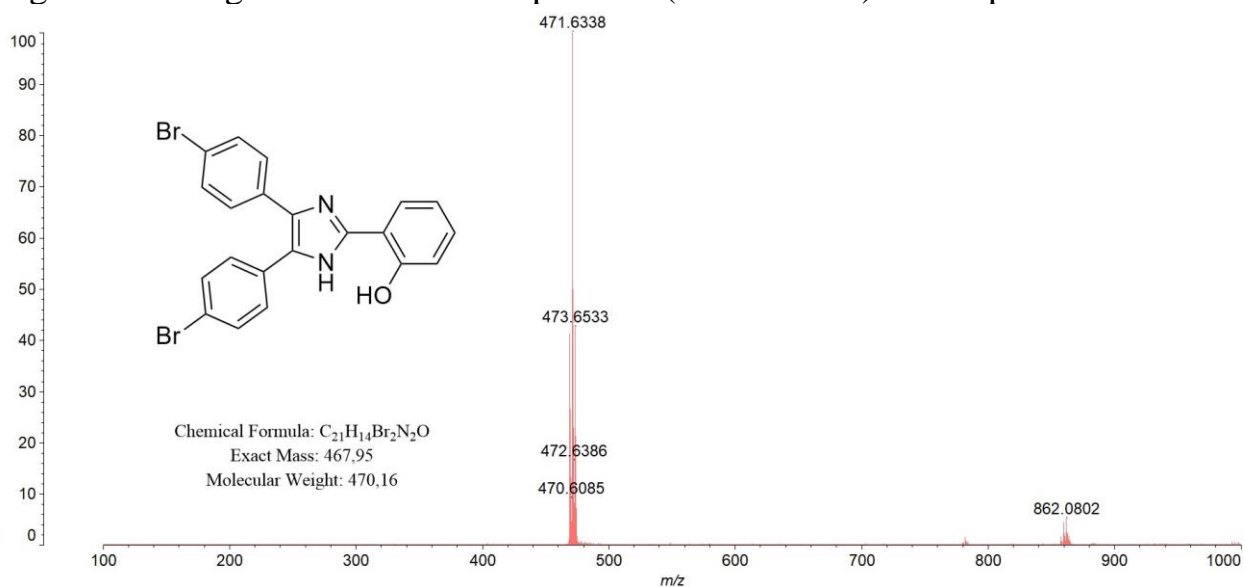


Figure SI-3. High-resolution mass spectrum (LDI MS) of compound **1e**.

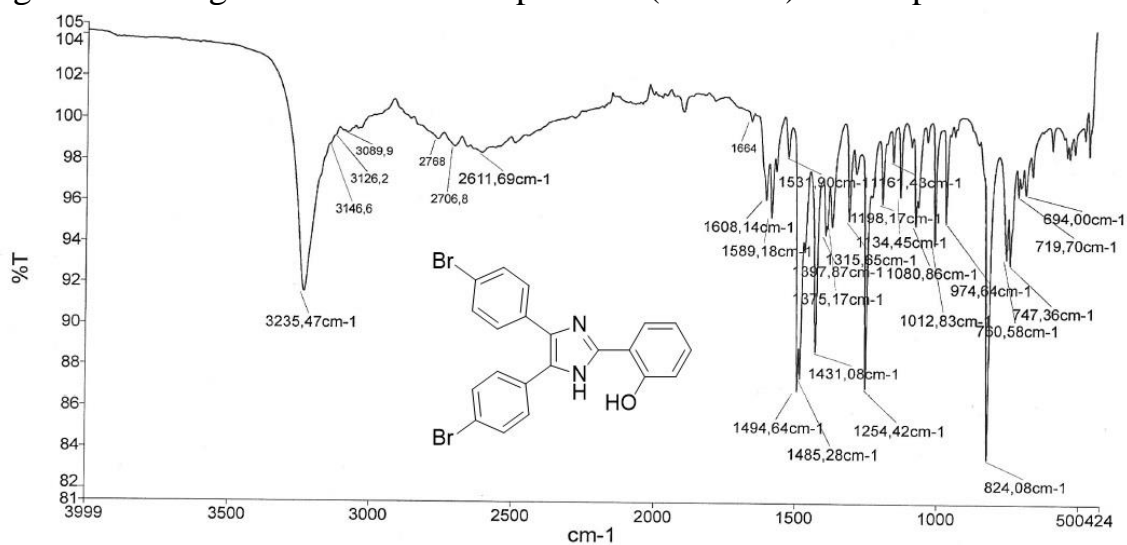


Figure SI-5. IR spectrum of compound **1e**.

400 MHz, DMSO-*d*₆

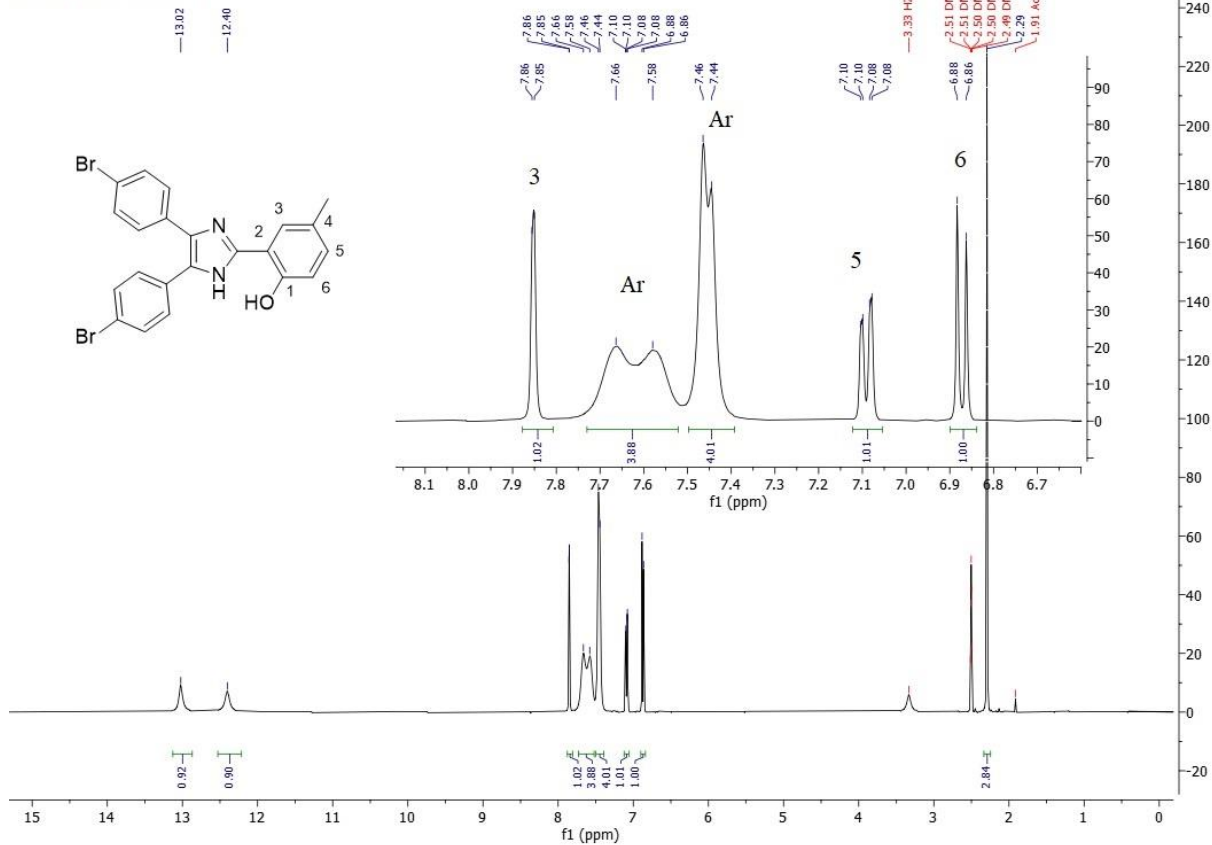


Figure SI-6. ¹H NMR spectrum of compound **1f**.

100 MHz, DMSO-*d*₆

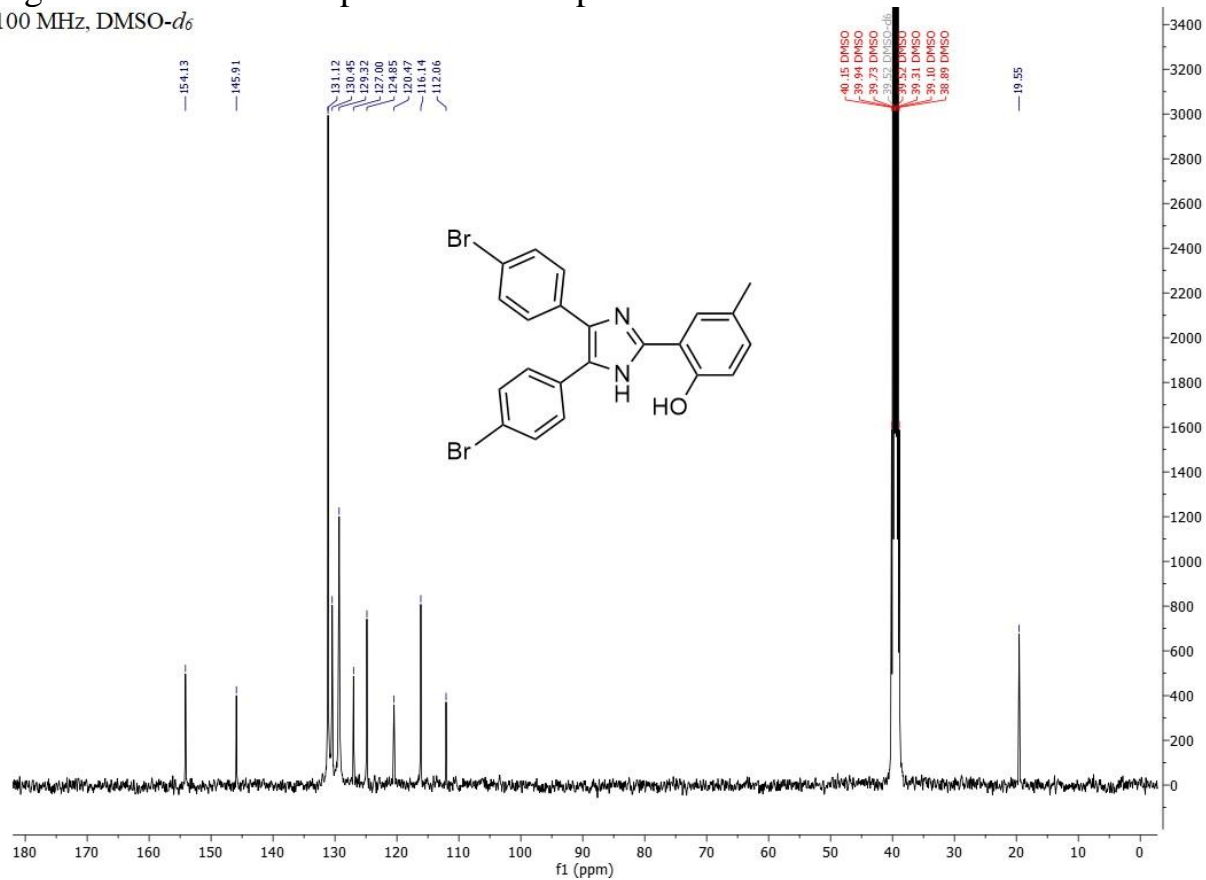


Figure SI-7. ¹³C NMR spectrum of compound **1f**.

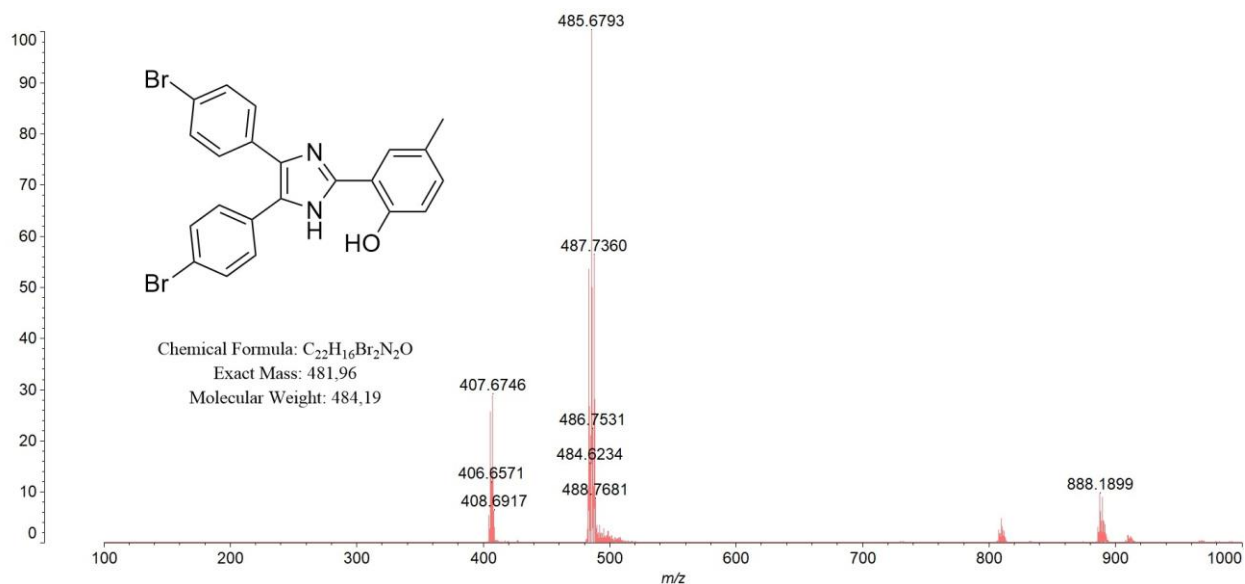


Figure SI-8. High-resolution mass spectrum (MALDI MS) of compound **1f**.

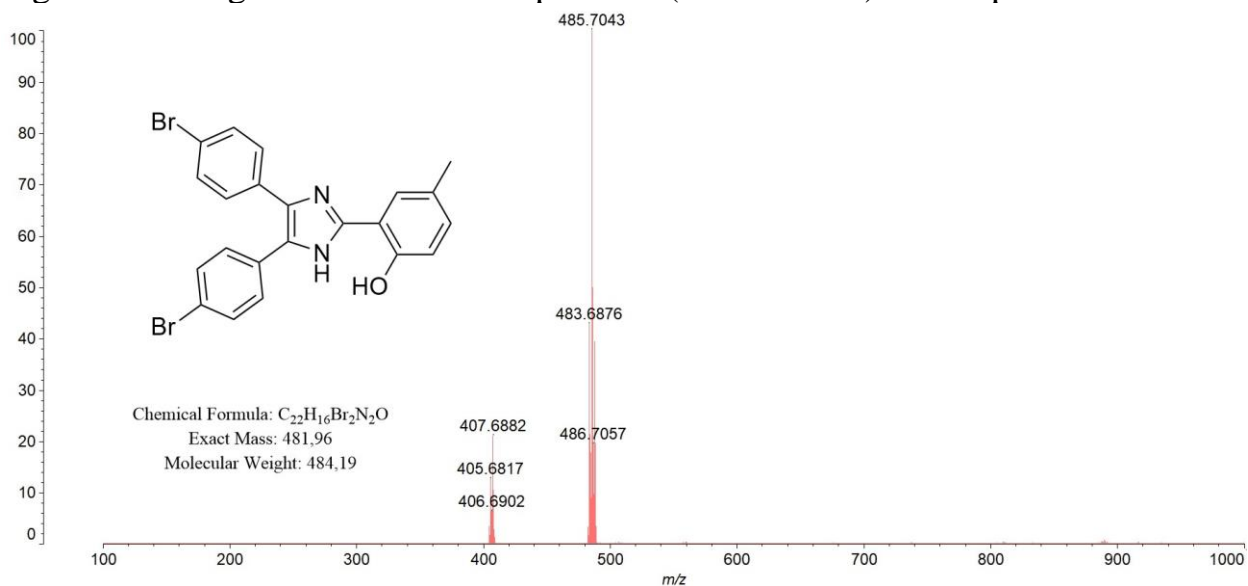


Figure SI-9. High-resolution mass spectrum (LDI MS) of compound **1f**.

400 MHz, DMSO-*d*₆

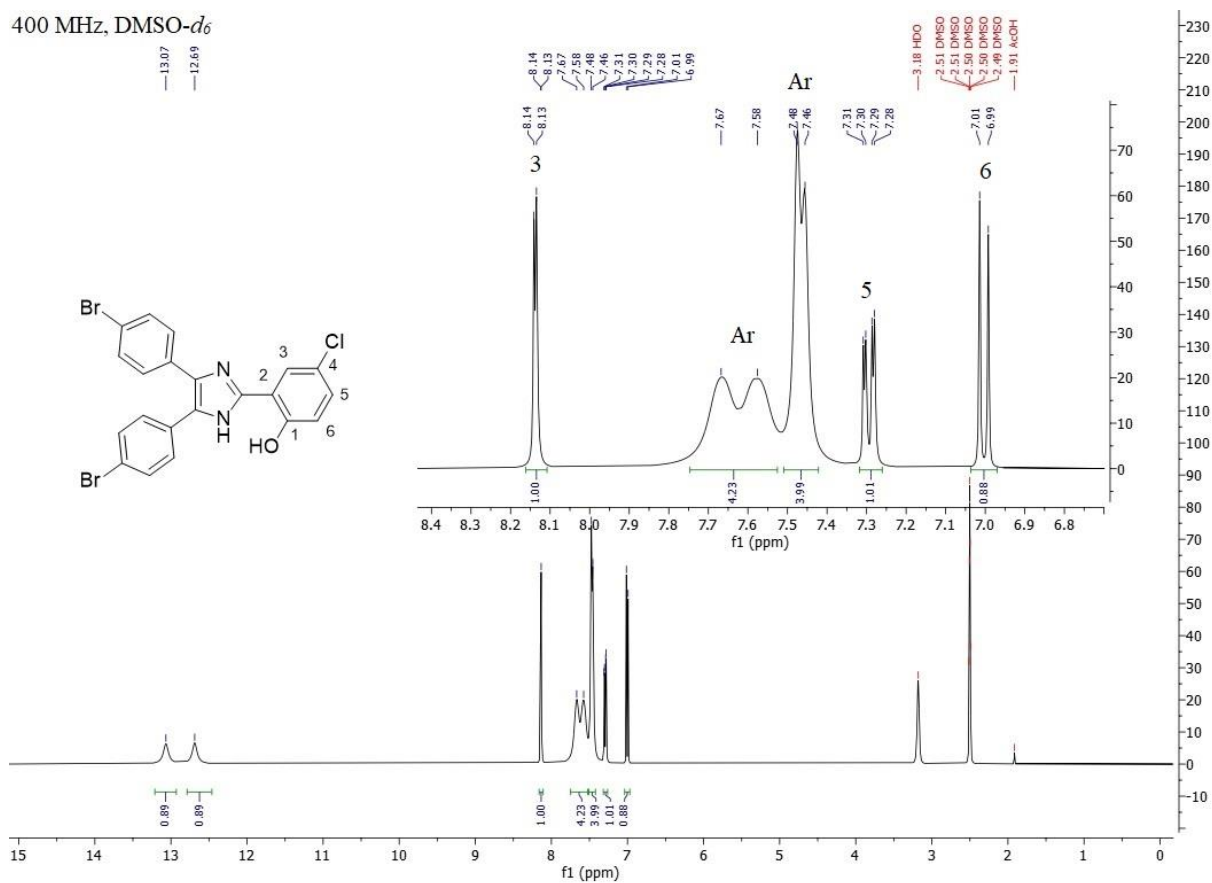


Figure SI-10. ¹H NMR spectrum of compound **1g**.

100 MHz, DMSO-*d*₆

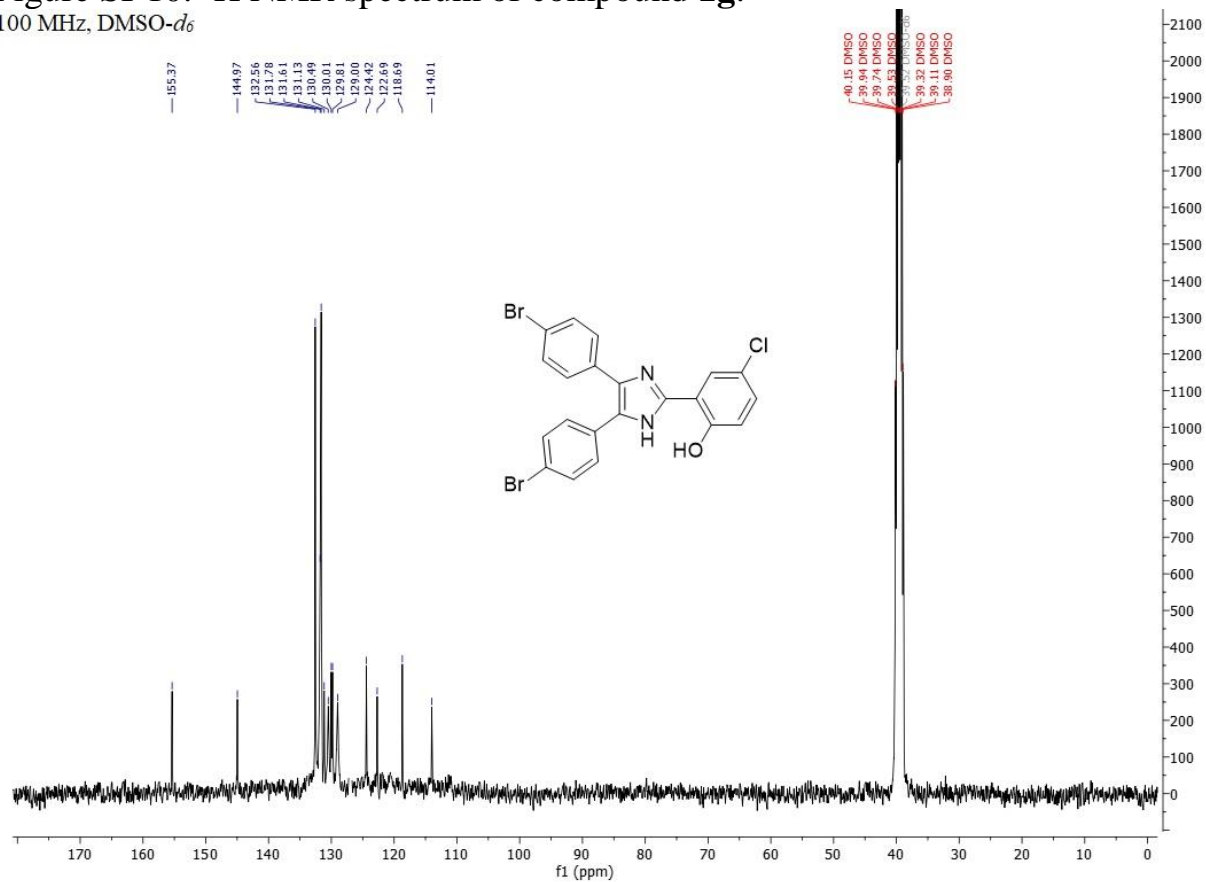


Figure SI-11. ¹³C NMR spectrum of compound **1g**.

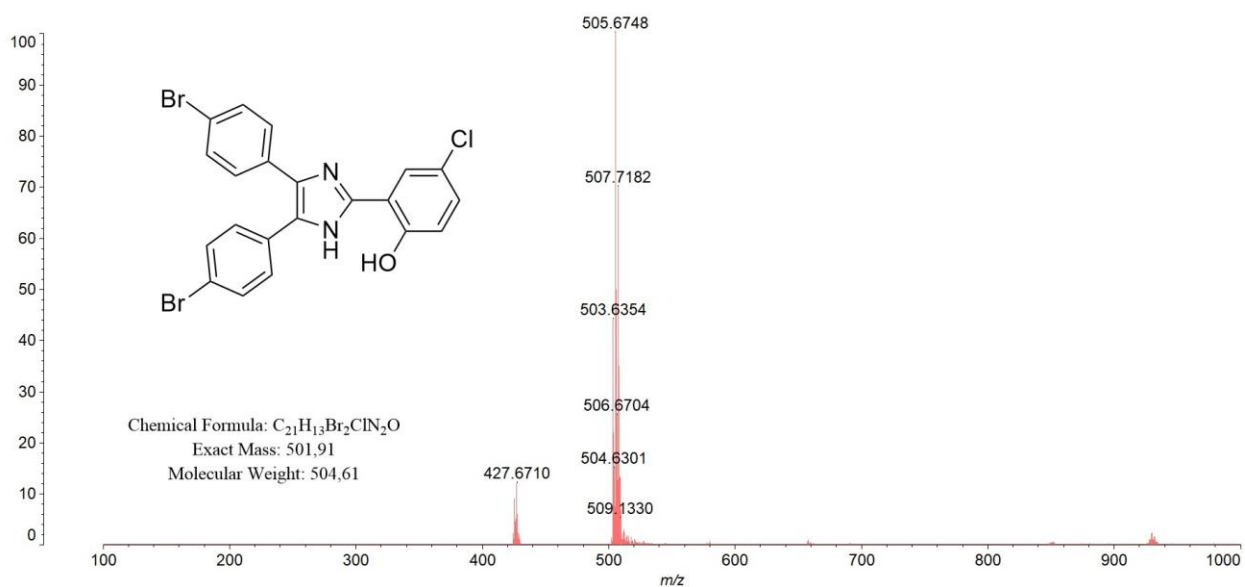


Figure SI-12. High-resolution mass spectrum (MALDI MS) of compound **1g**.

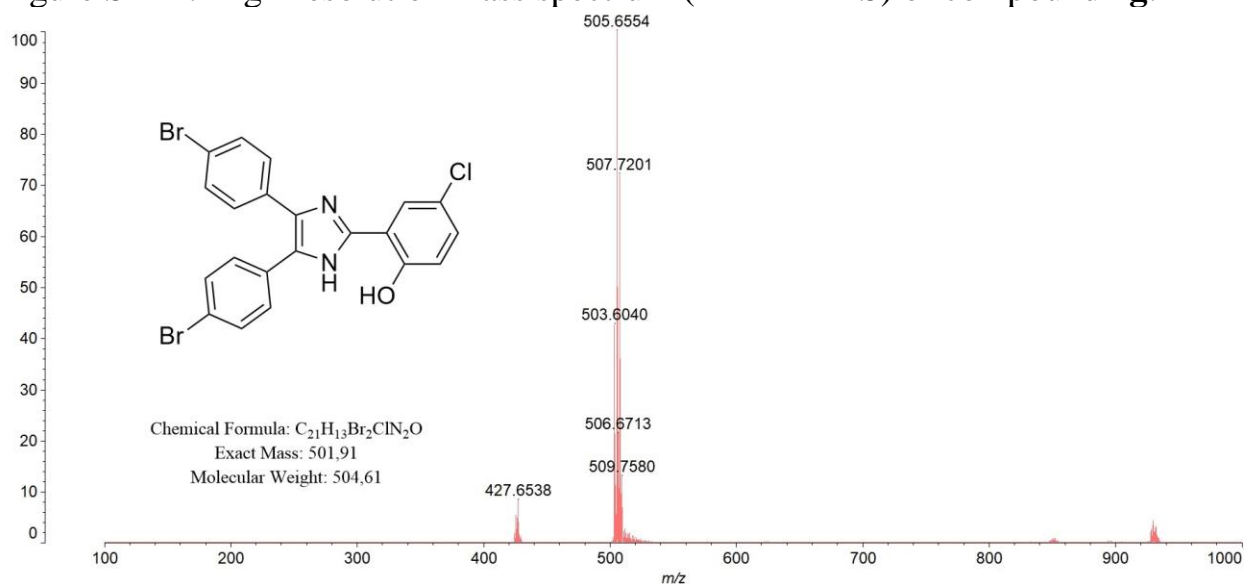


Figure SI-13. High-resolution mass spectrum (LDI MS) of compound **1g**.

400 MHz, DMSO-*d*₆

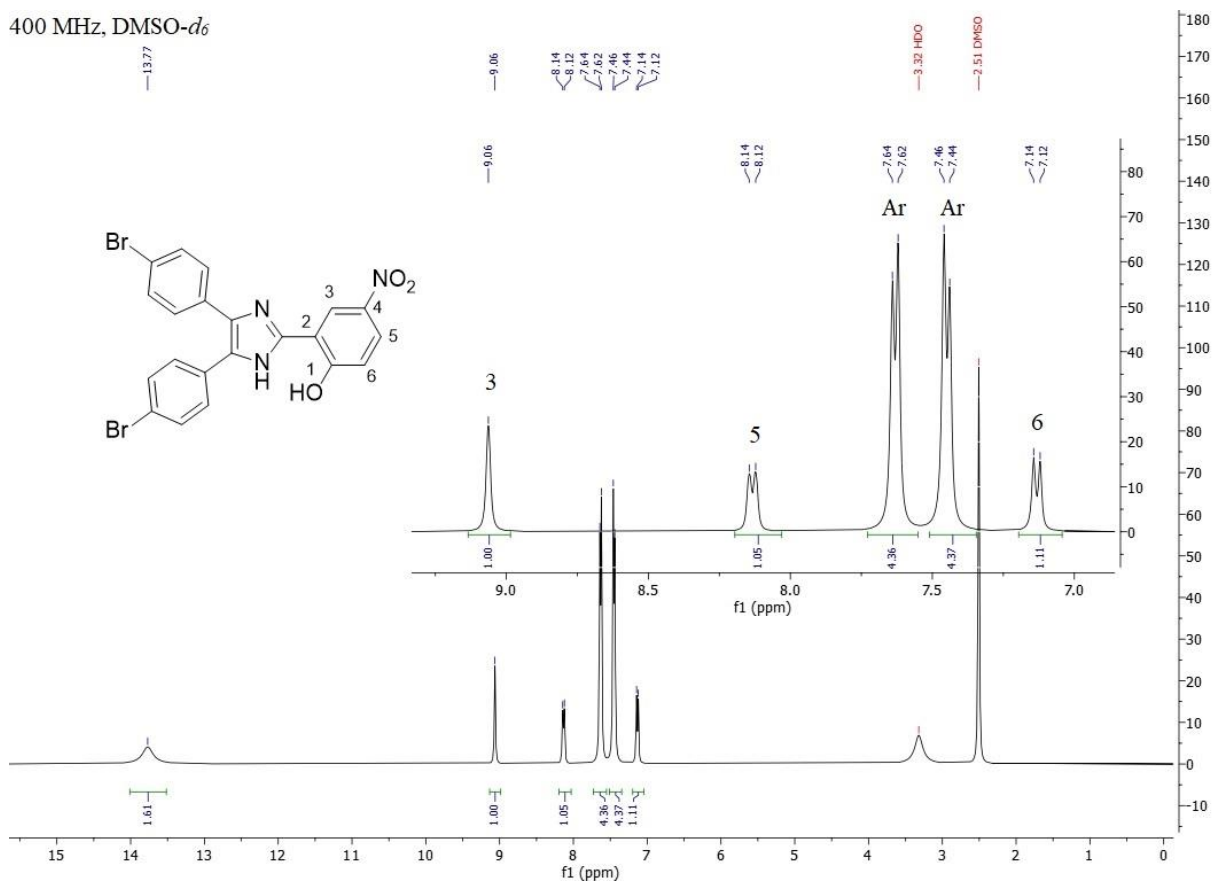


Figure SI-14. ¹H NMR spectrum of compound **1h**.
100 MHz, DMSO-*d*₆

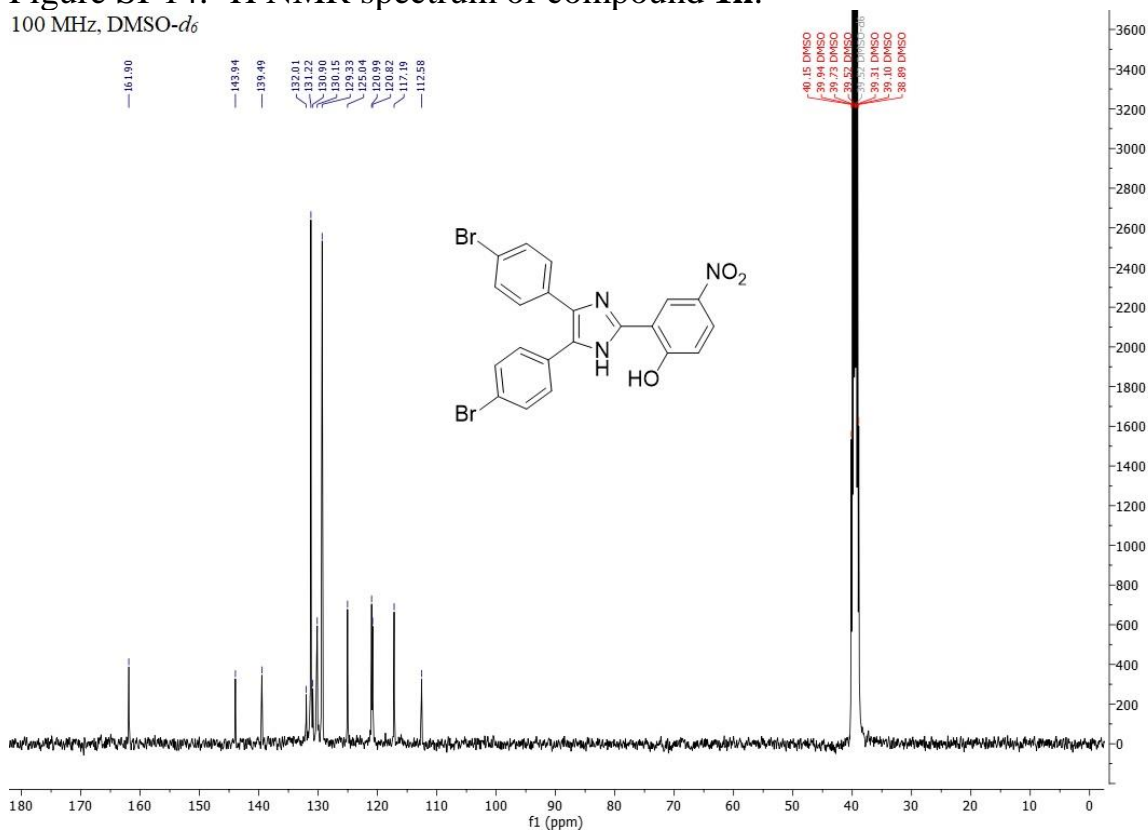


Figure SI-15. ¹³C NMR spectrum of compound **1h**.

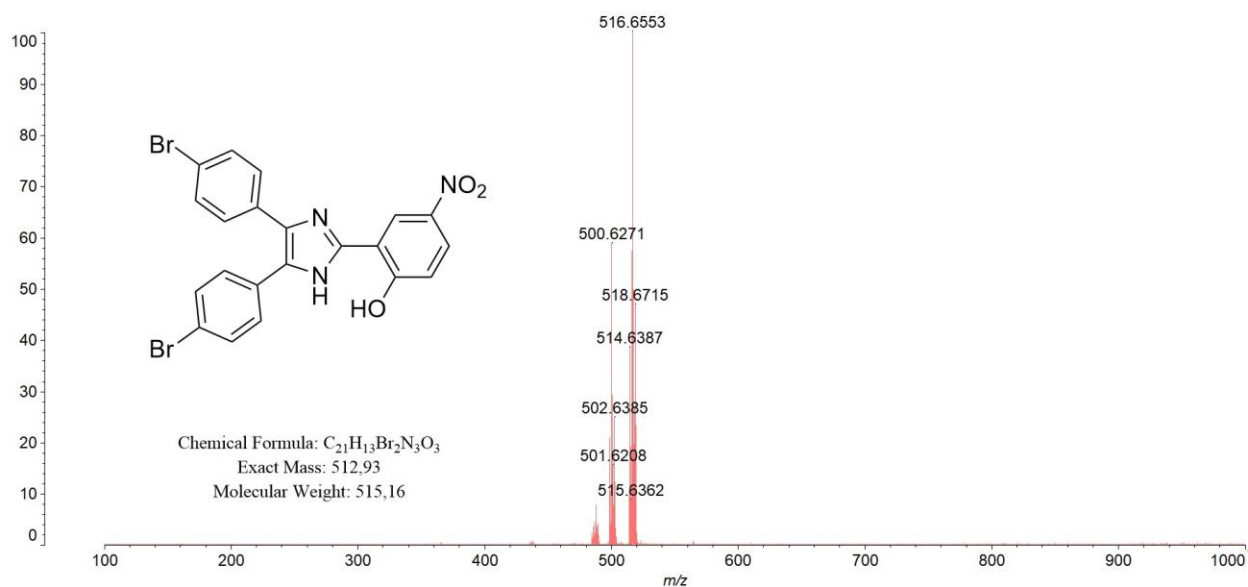


Figure SI-16. High-resolution mass spectrum (MALDI MS) of compound **1h**.

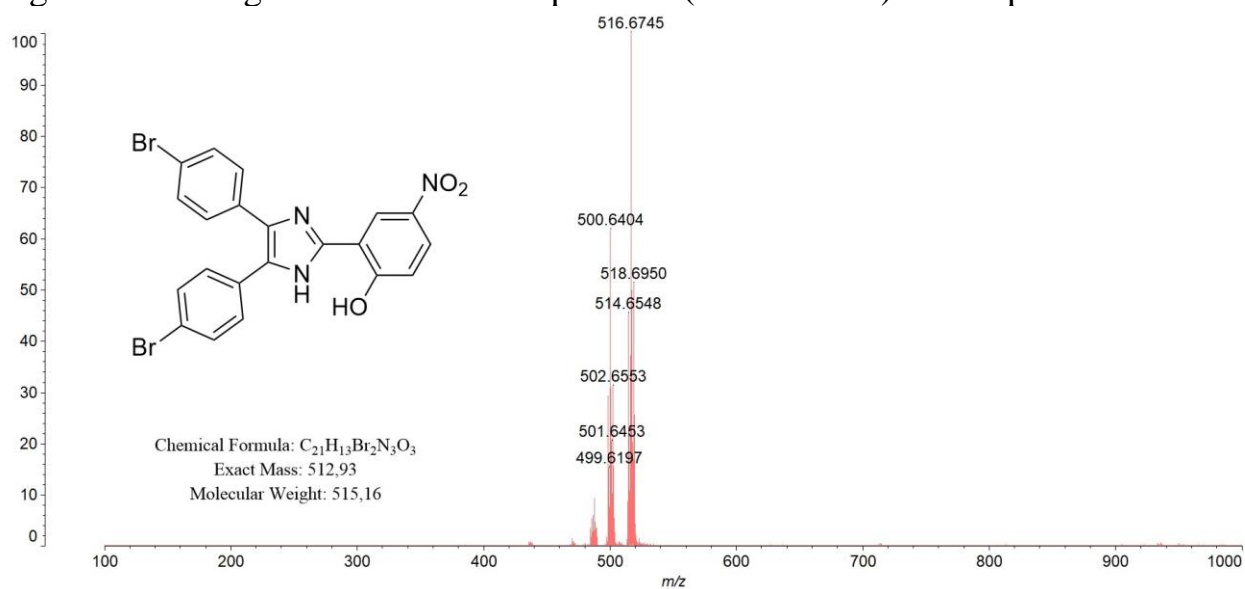


Figure SI-17. High-resolution mass spectrum (LDI MS) of compound **1h**.

400 MHz, DMSO-*d*₆

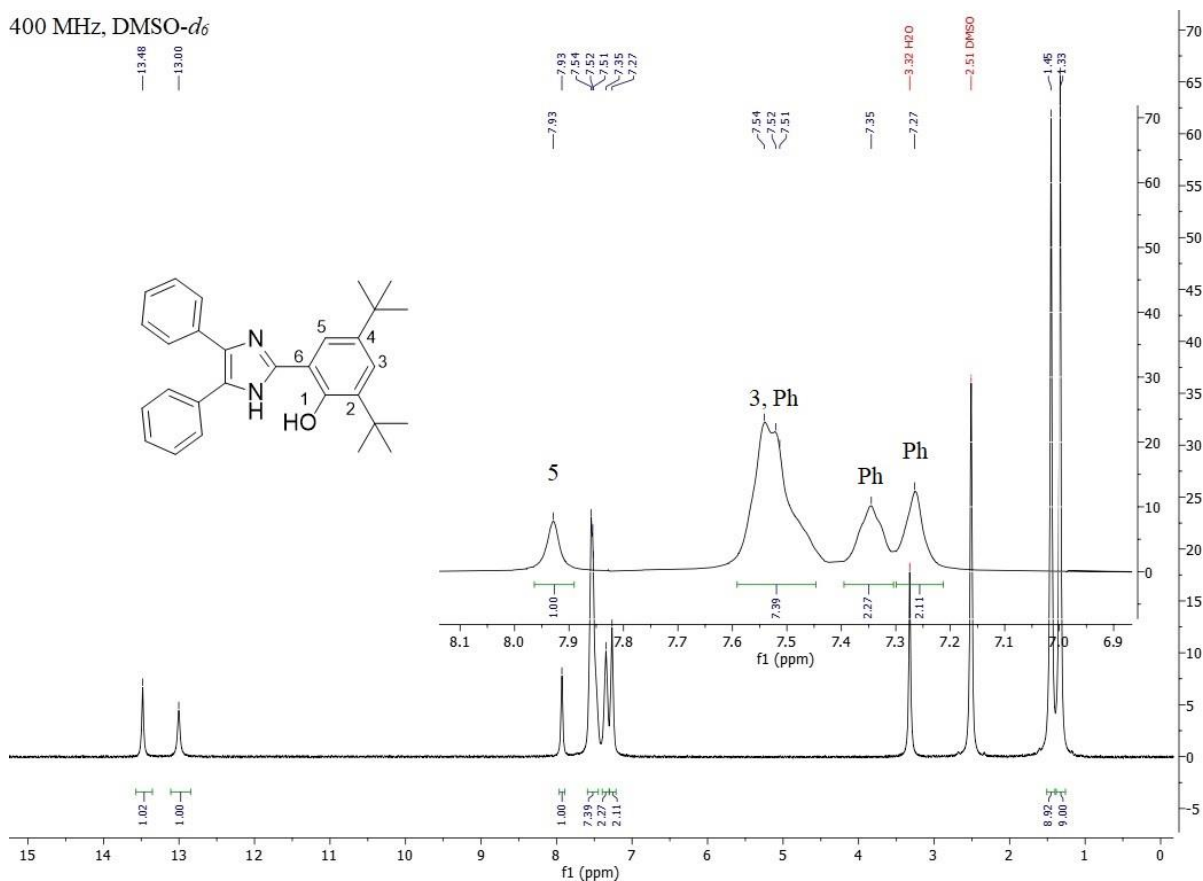


Figure SI-18. ¹H NMR spectrum of compound **1j**.
100 MHz, DMSO-*d*₆

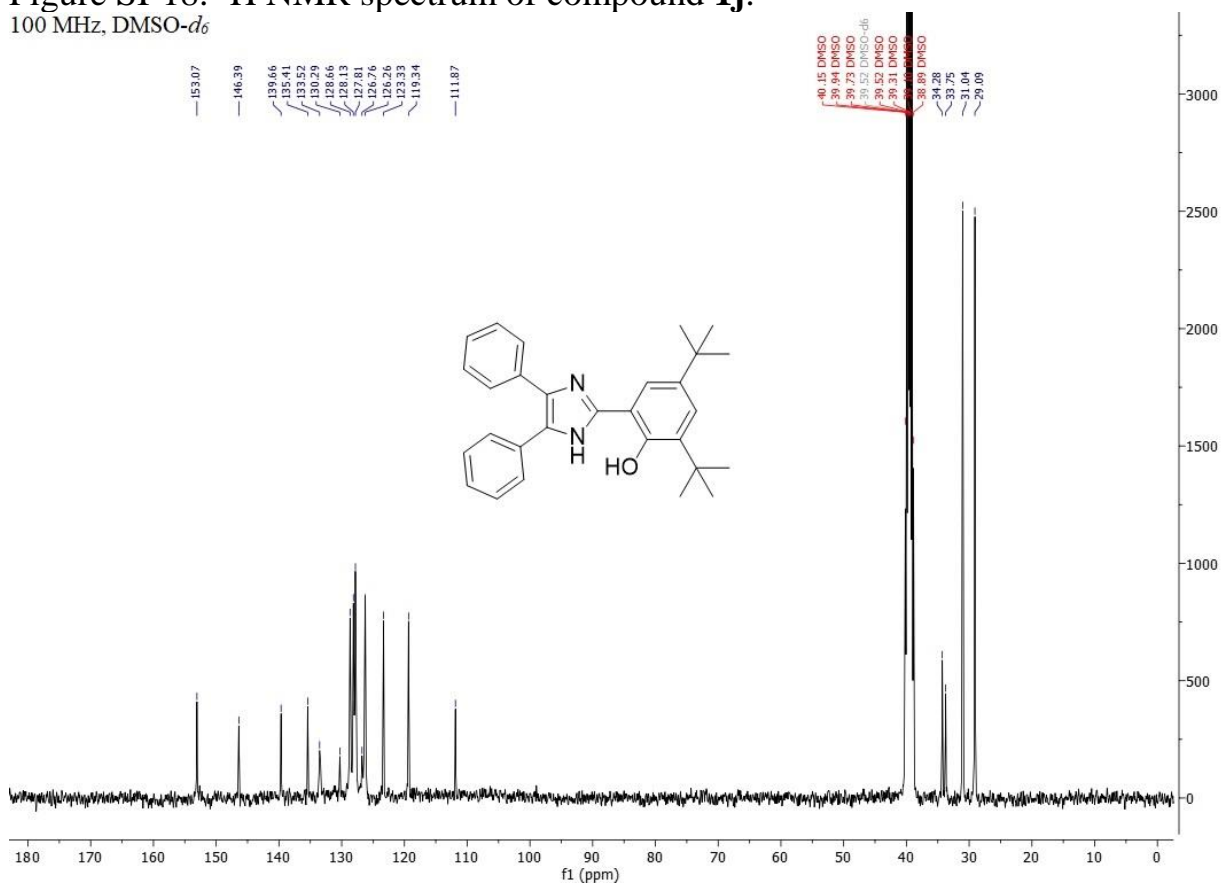


Figure SI-19. ¹³C NMR spectrum of compound **1j**.

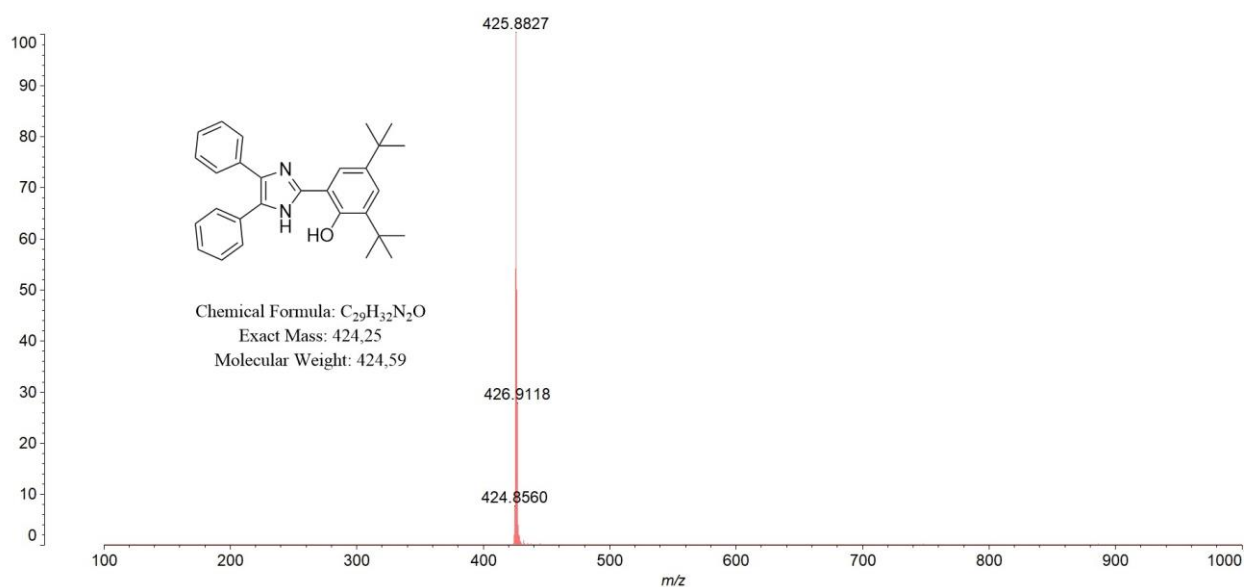


Figure SI-20. High-resolution mass spectrum (MALDI MS) of compound **1j**.

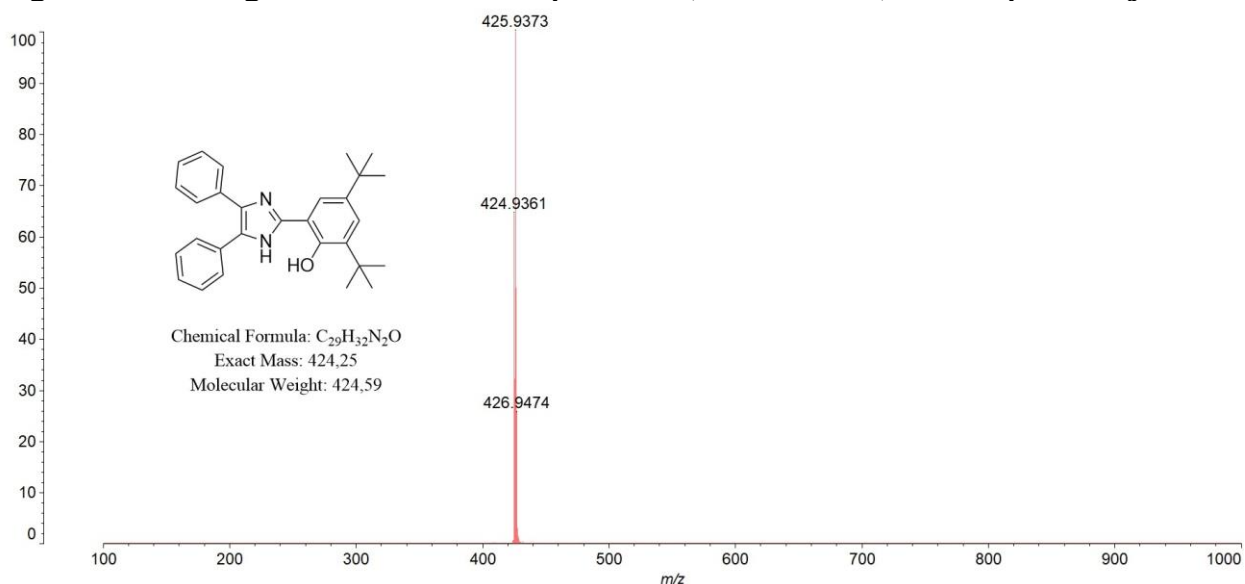


Figure SI-21. High-resolution mass spectrum (LDI MS) of compound **1j**.

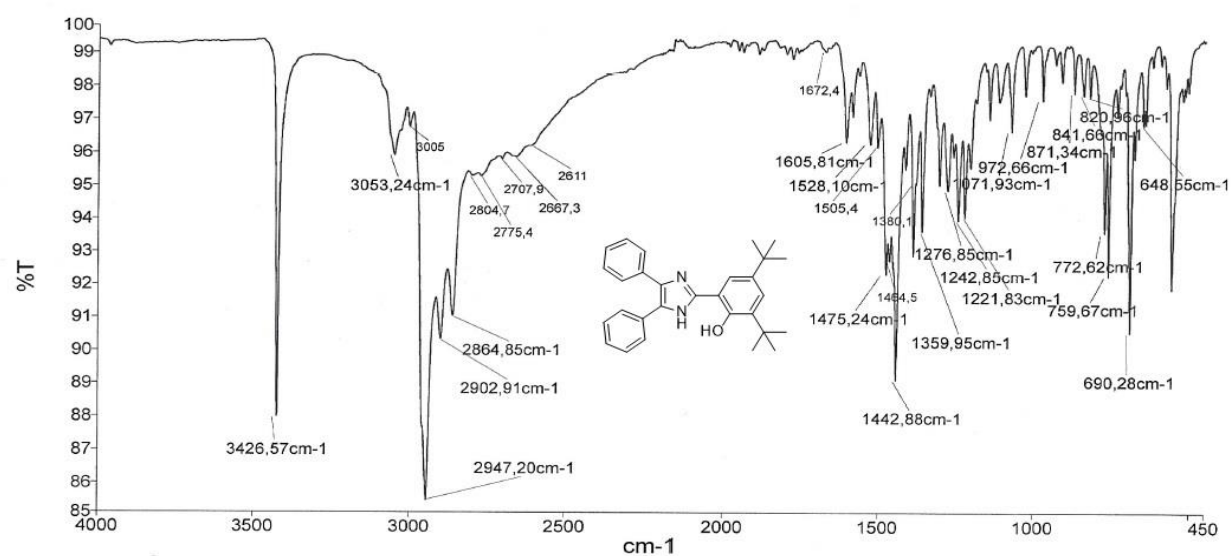


Figure SI-22. IR spectrum of compound **1j**.

400 MHz, DMSO-*d*₆

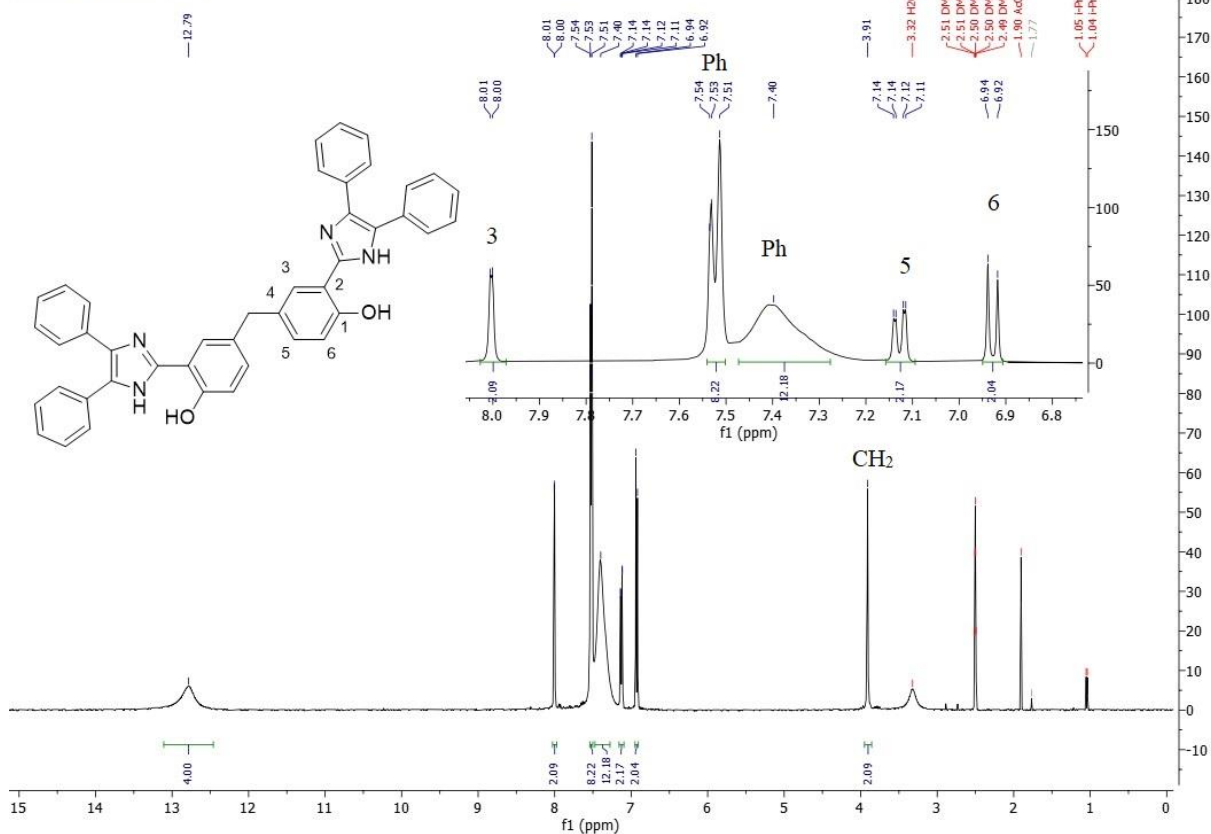


Figure SI-23. ¹H NMR spectrum of compound 4.

100 MHz, DMSO-*d*₆

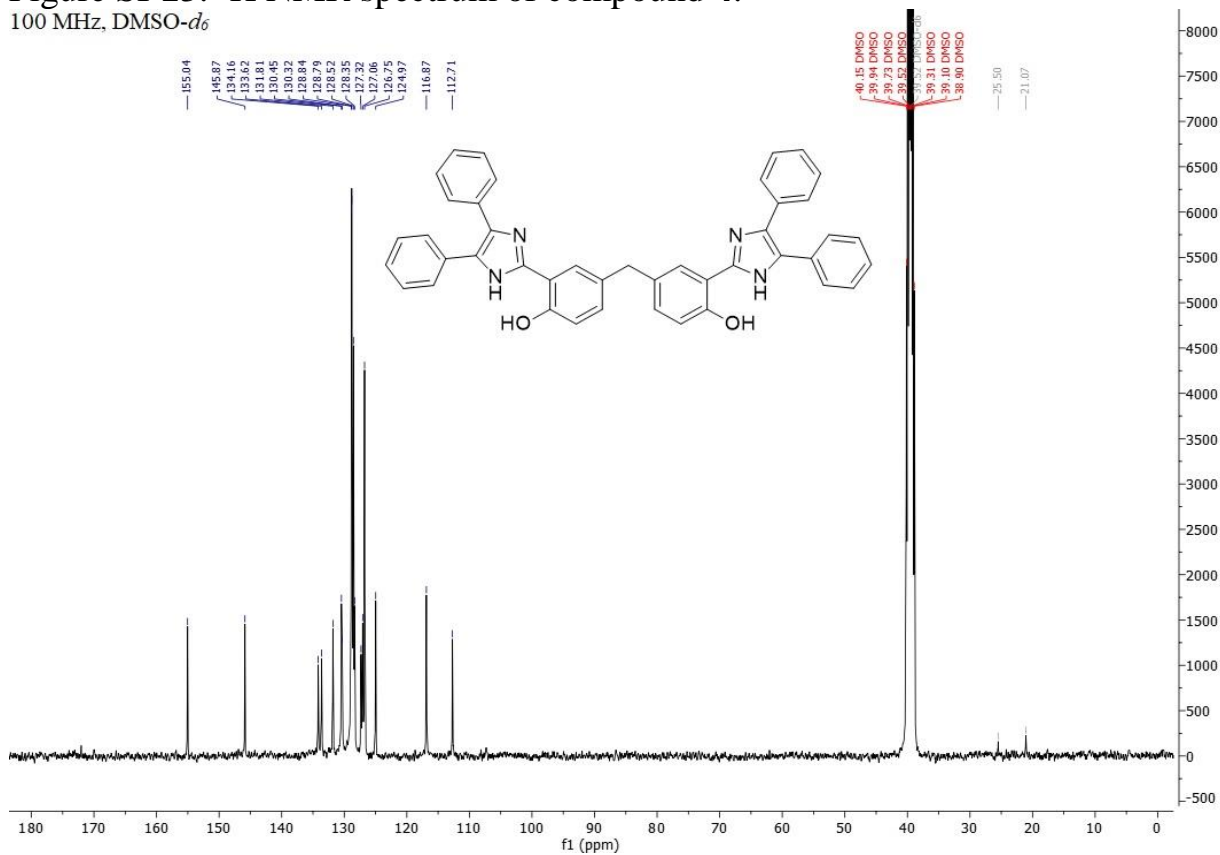


Figure SI-24. ¹³C NMR spectrum of compound 4.

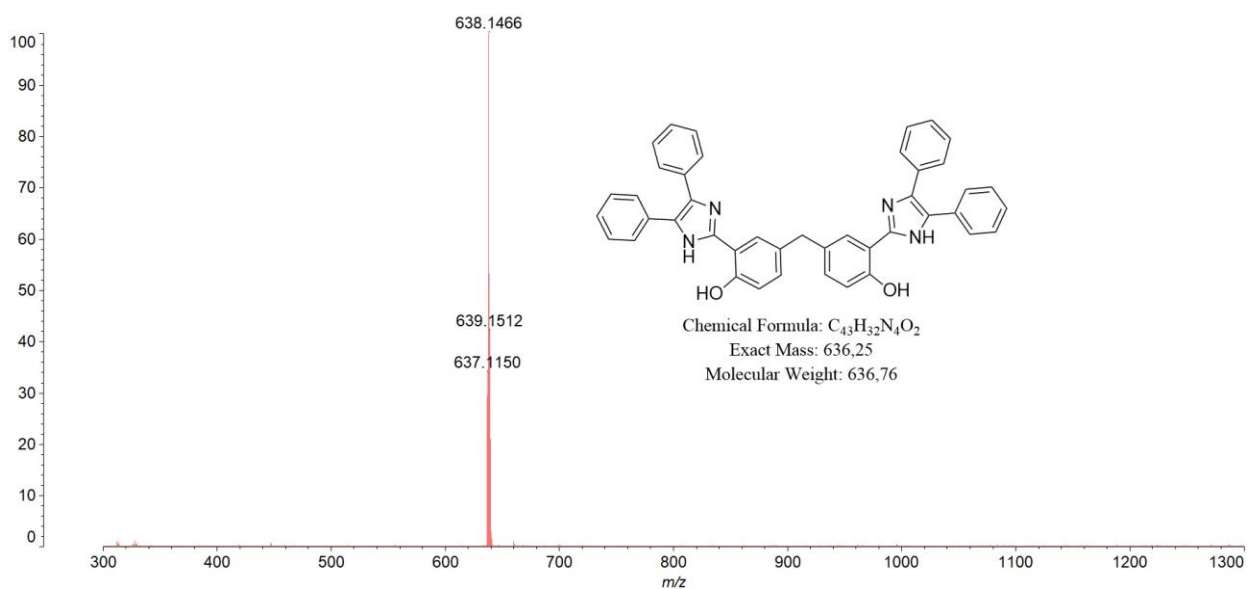


Figure SI-25. High-resolution mass spectrum (MALDI MS) of compound **4**.

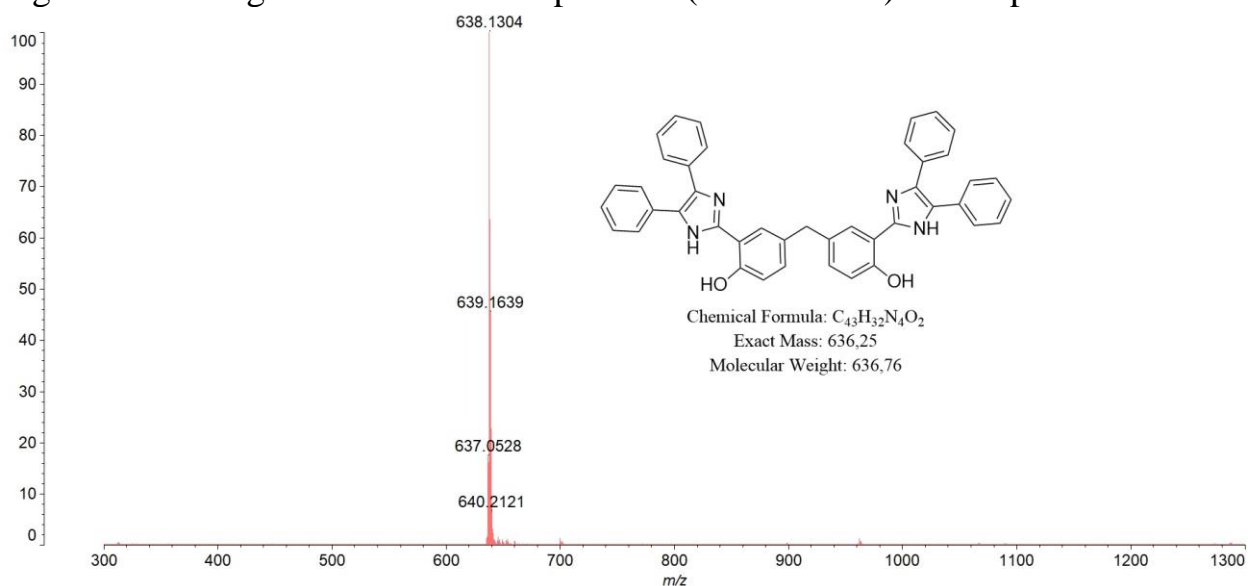


Figure SI-26. High-resolution mass spectrum (LDI MS) of compound **4**.

400 MHz, DMSO-*d*₆

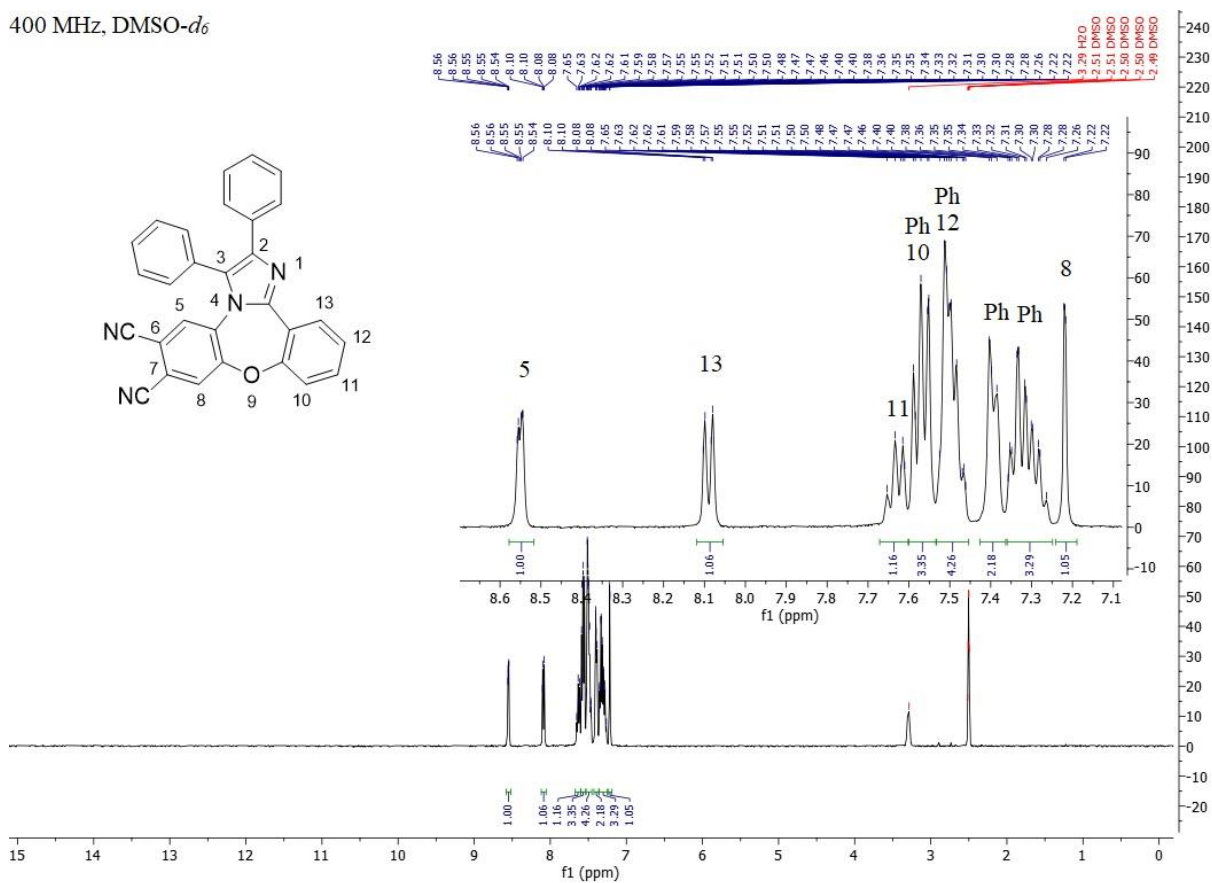


Figure SI-27. ¹H NMR spectrum of compound **3a**.

100 MHz, DMSO-*d*₆

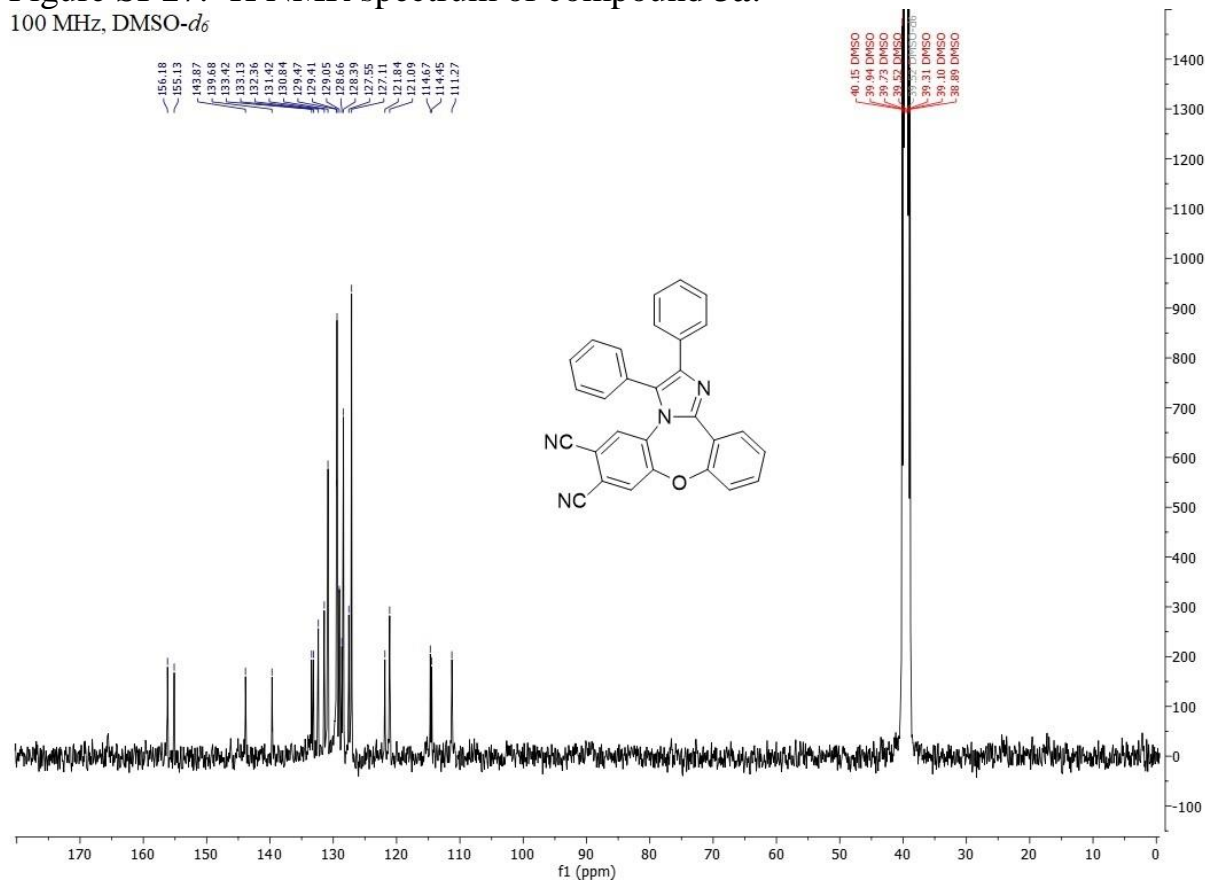


Figure SI-28. ¹³C NMR spectrum of compound **3a**.

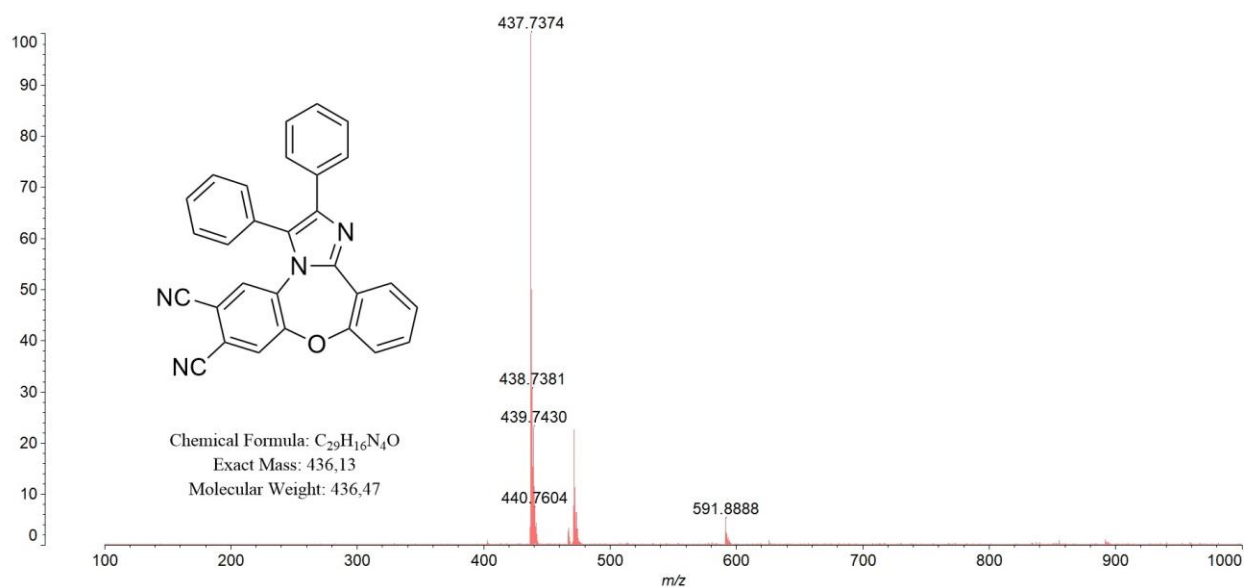


Figure SI-29. High-resolution mass spectrum (MALDI MS) of compound **3a**.

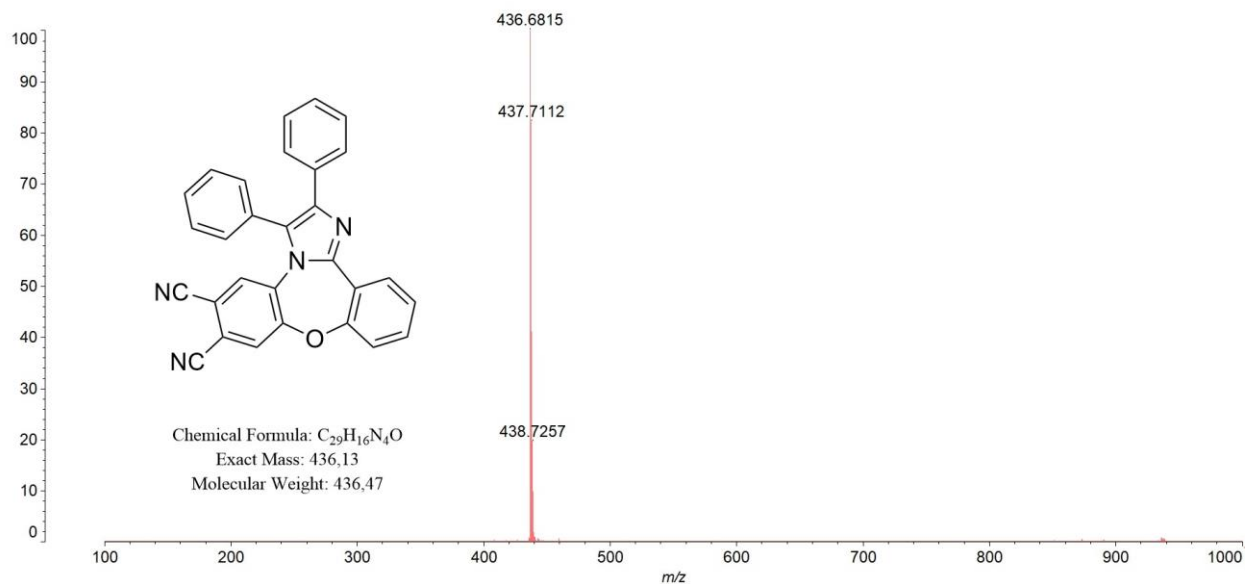


Figure SI-30. High-resolution mass spectrum (LDI MS) of compound **3a**.

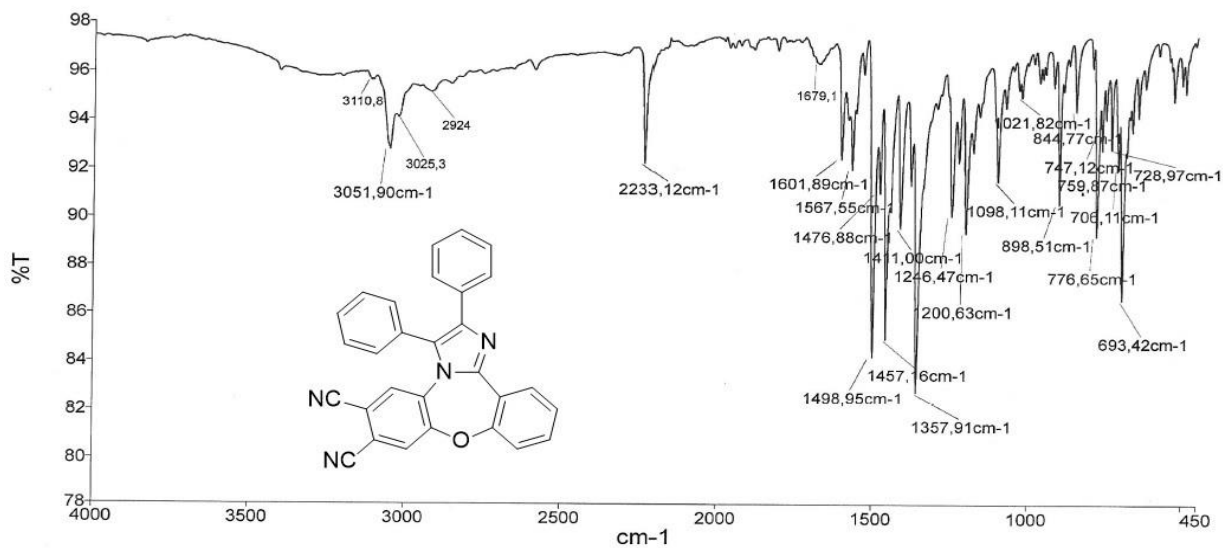


Figure SI-31. IR spectrum of compound **3a**.

400 MHz, DMSO-*d*₆

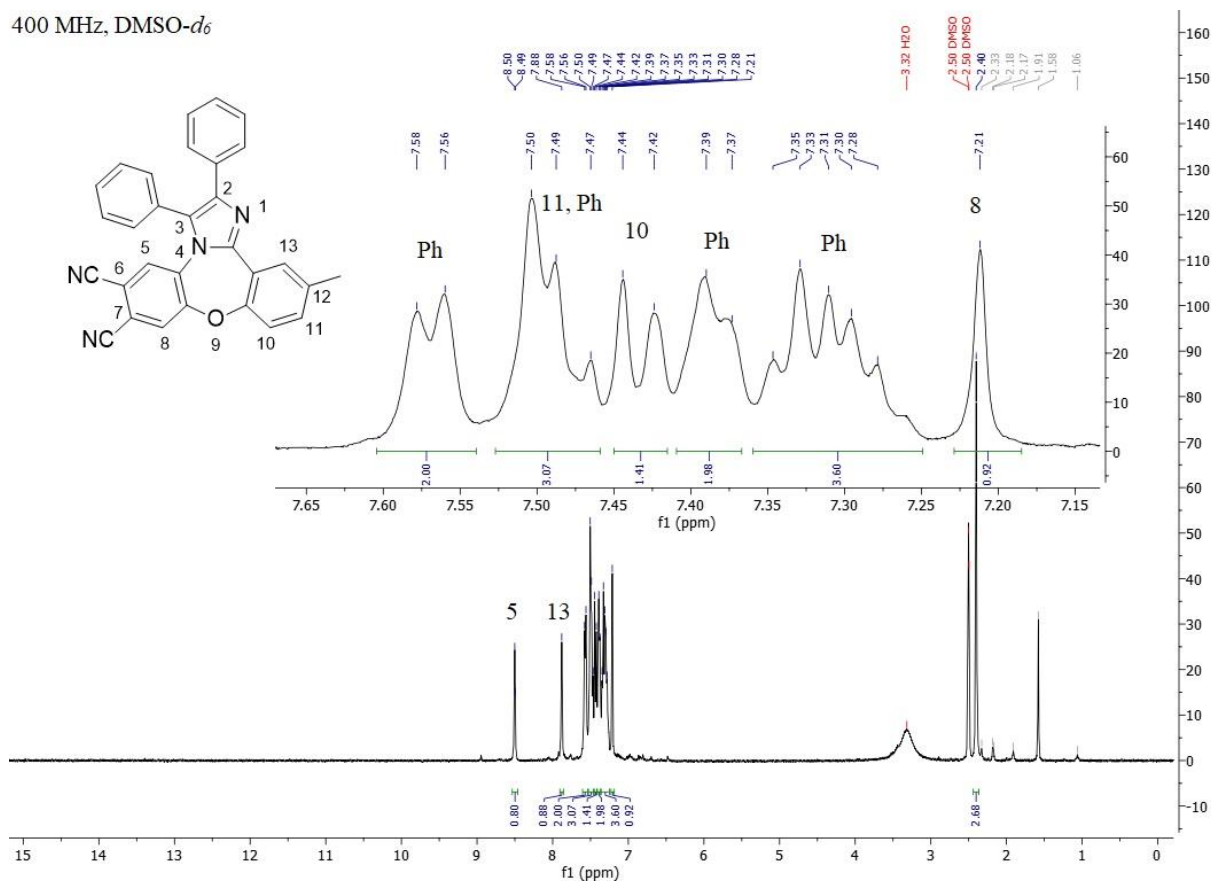


Figure SI-32. ¹H NMR spectrum of compound **3b**.

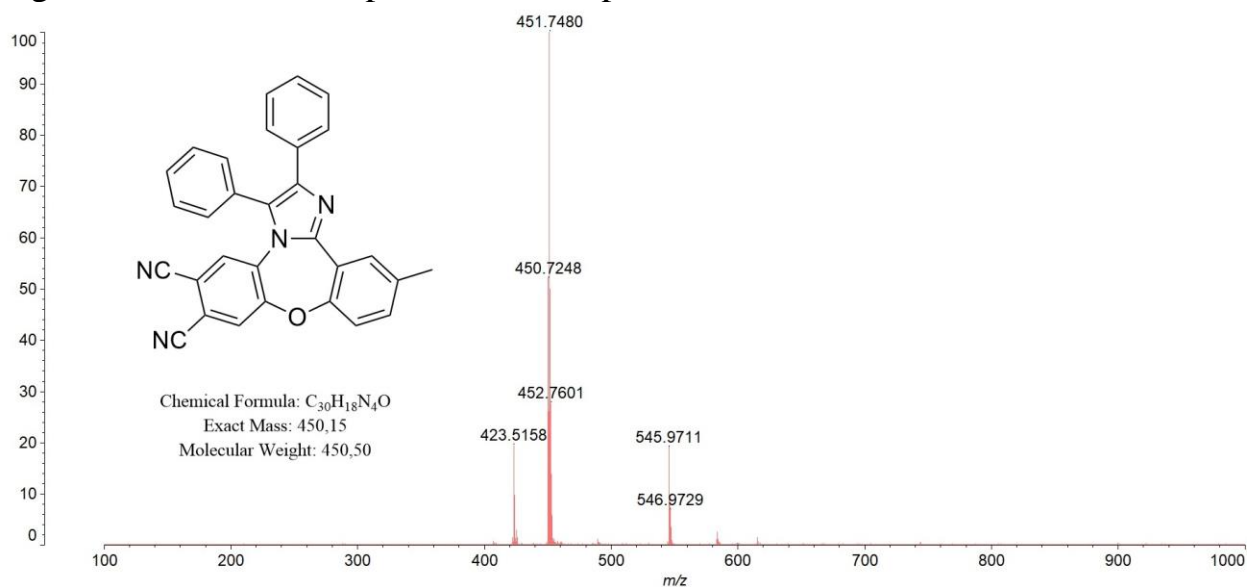


Figure SI-33. High-resolution mass spectrum (MALDI MS) of compound **3b**.

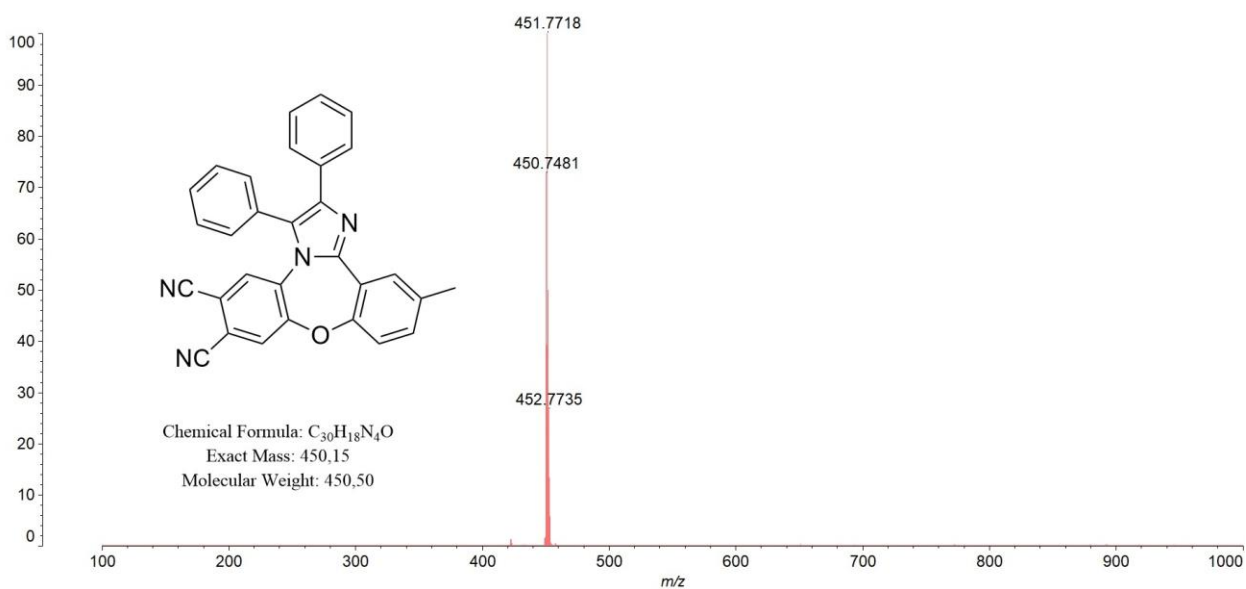


Figure SI-34. High-resolution mass spectrum (LDI MS) of compound **3b**.
 400 MHz, $DMSO-d_6$

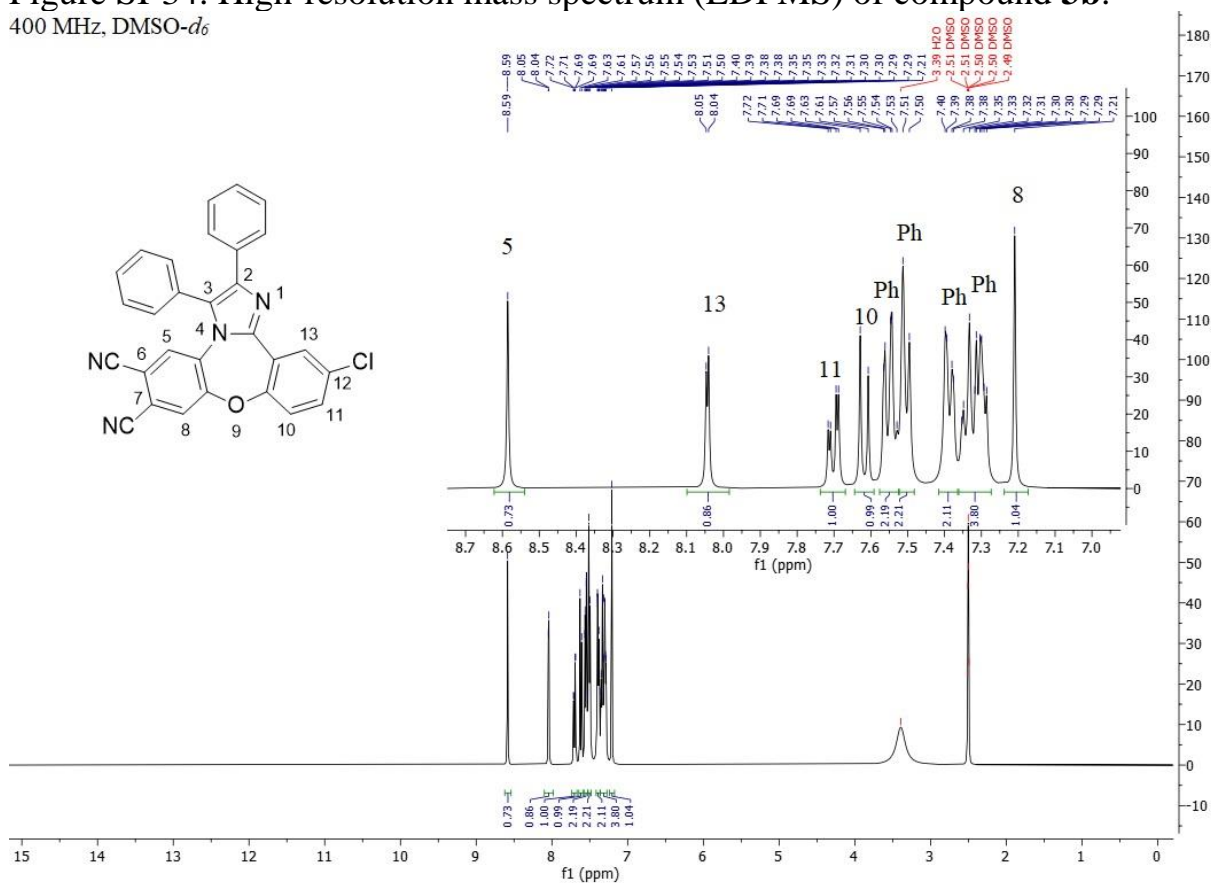


Figure SI-35. 1H NMR spectrum of compound **3c**.

100 MHz, DMSO-*d*₆

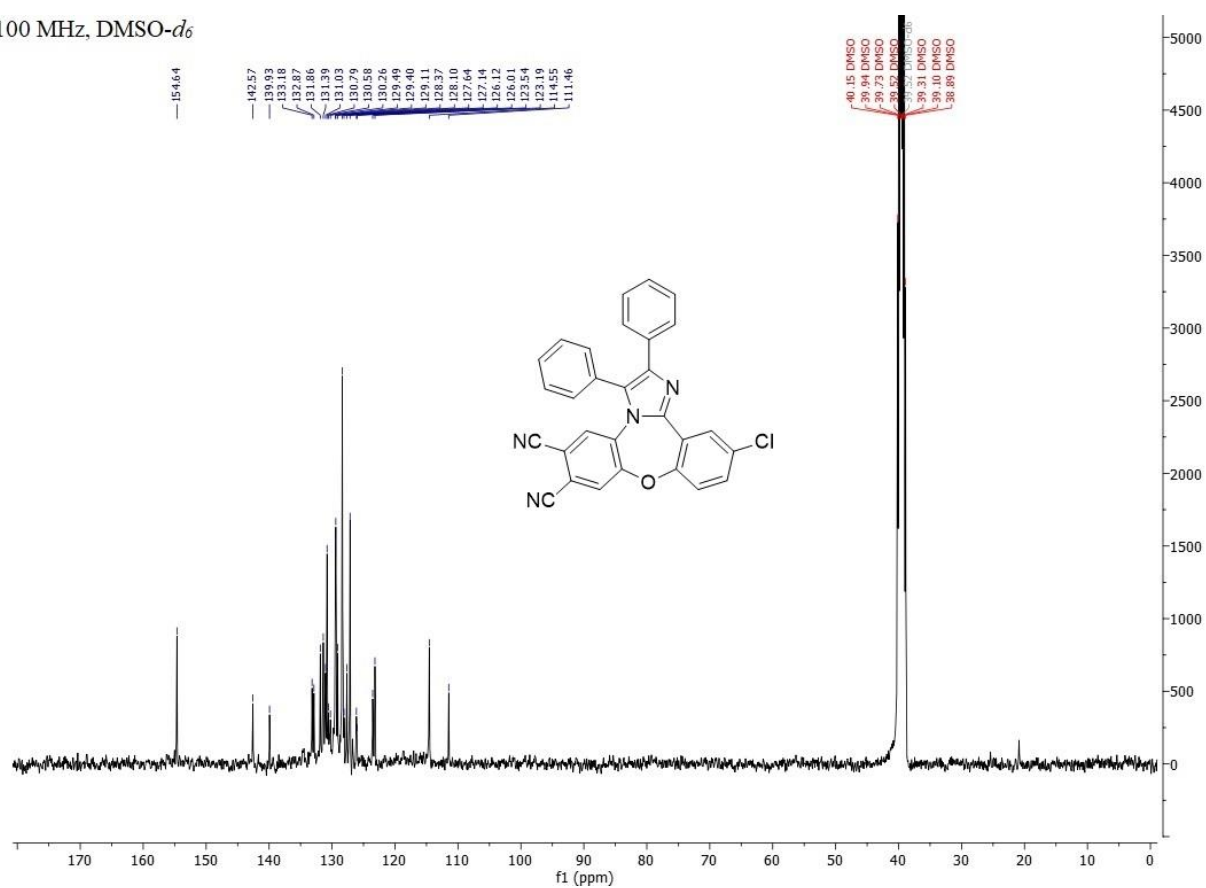


Figure SI-36. ¹³C NMR spectrum of compound **3c**.

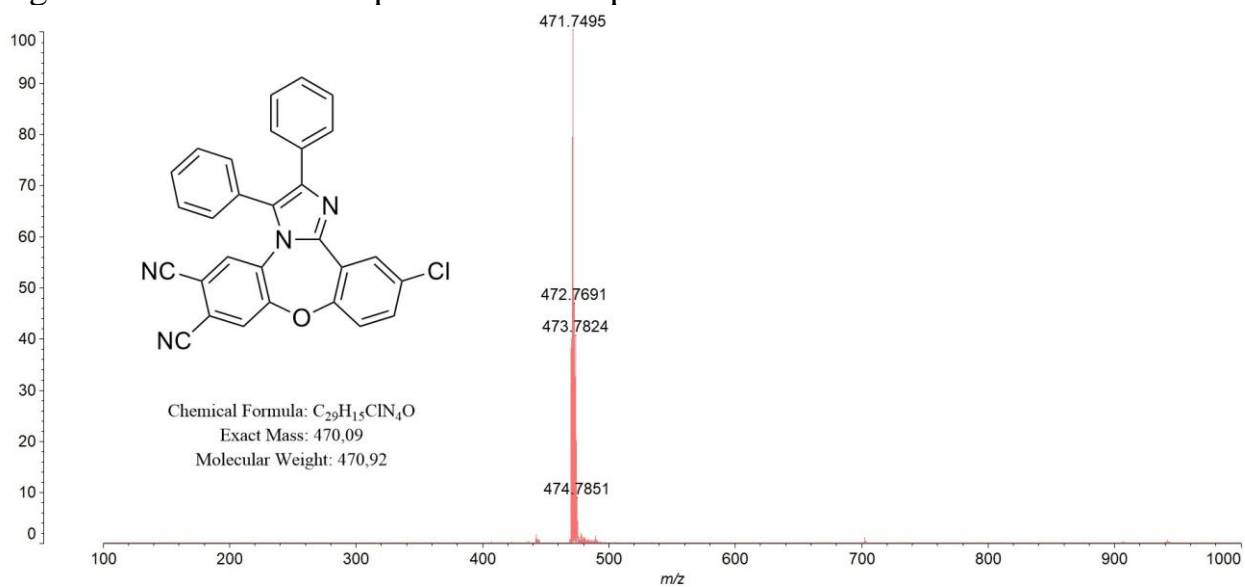


Figure SI-37. High-resolution mass spectrum (MALDI MS) of compound **3c**.

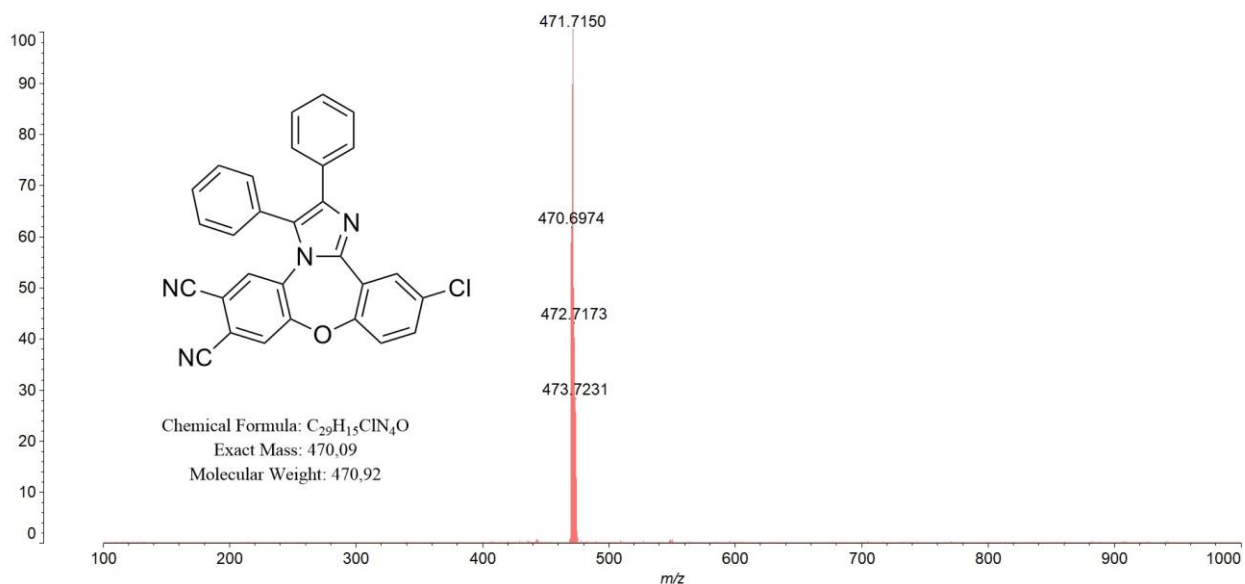


Figure SI-38. High-resolution mass spectrum (LDI MS) of compound **3c**.

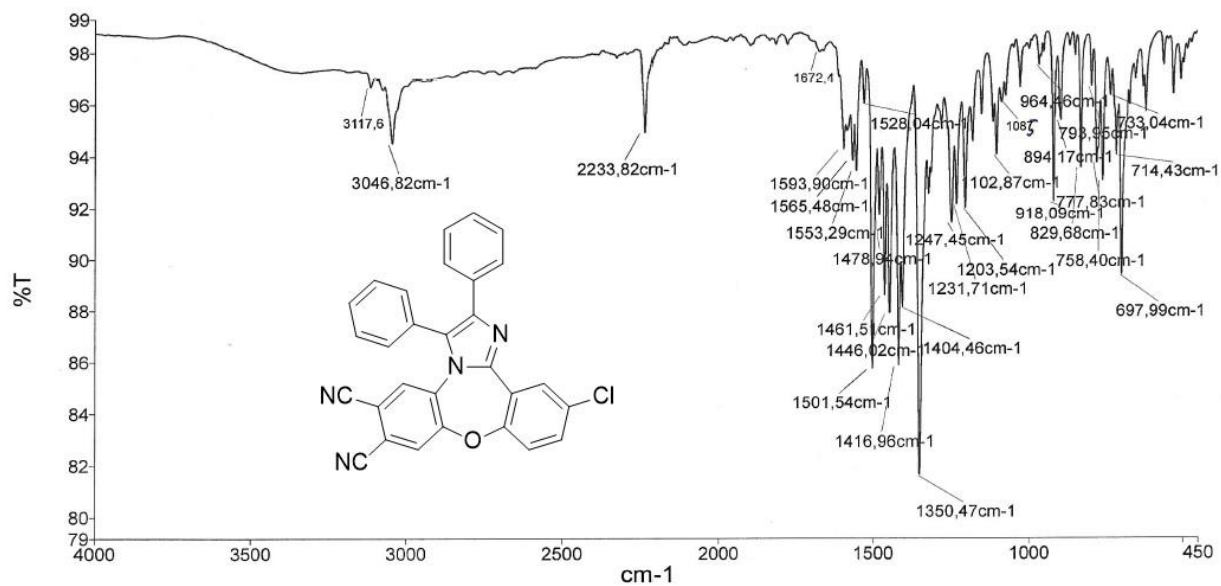


Figure SI-39. IR spectrum of compound **3c**.

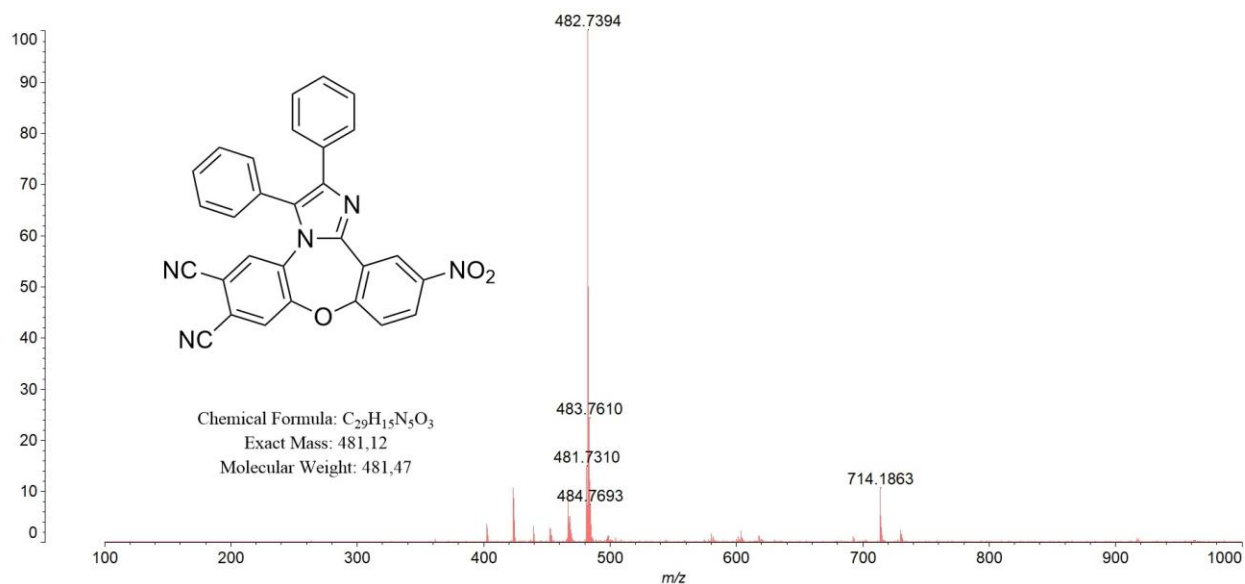


Figure SI-42. High-resolution mass spectrum (MALDI MS) of compound **3d**.

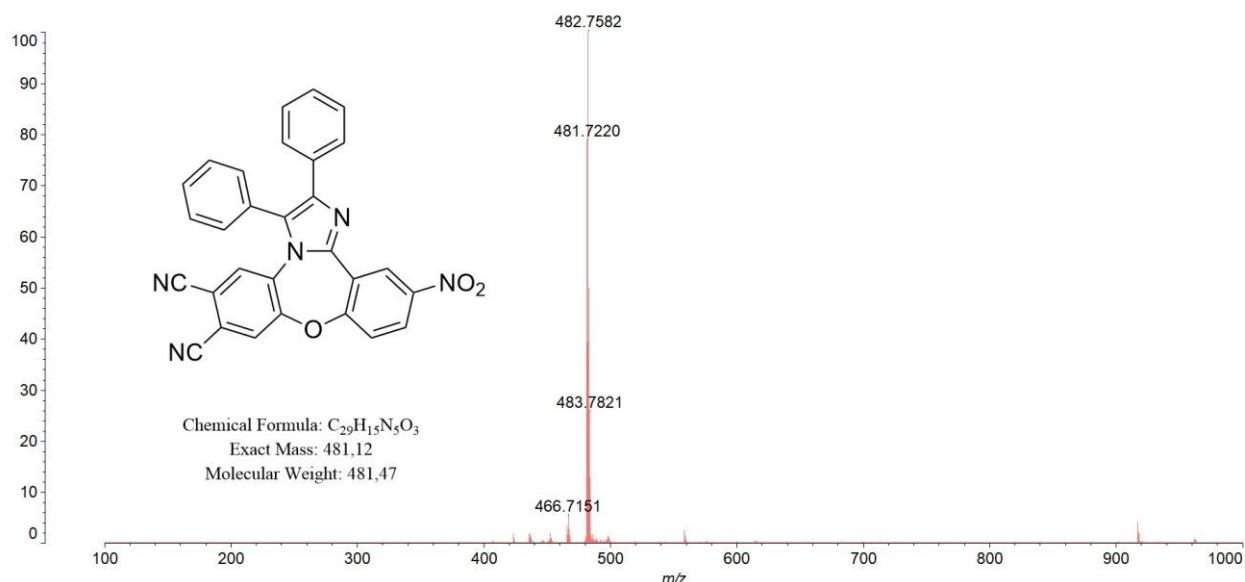


Figure SI-43. High-resolution mass spectrum (LDI MS) of compound **3d**.

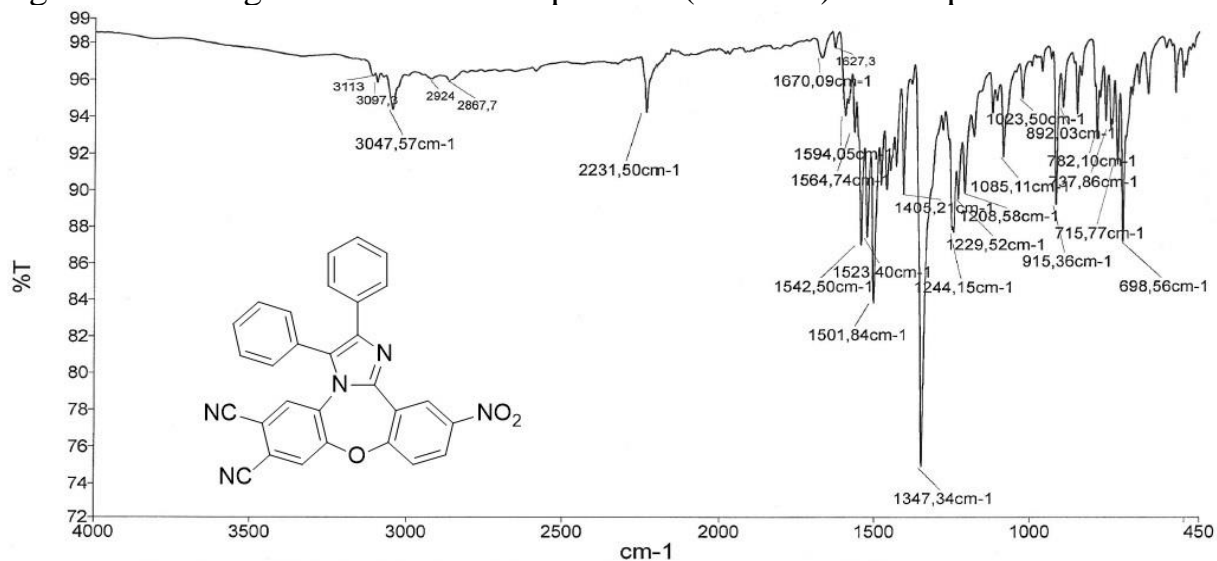


Figure SI-44. IR spectrum of compound **3d**.

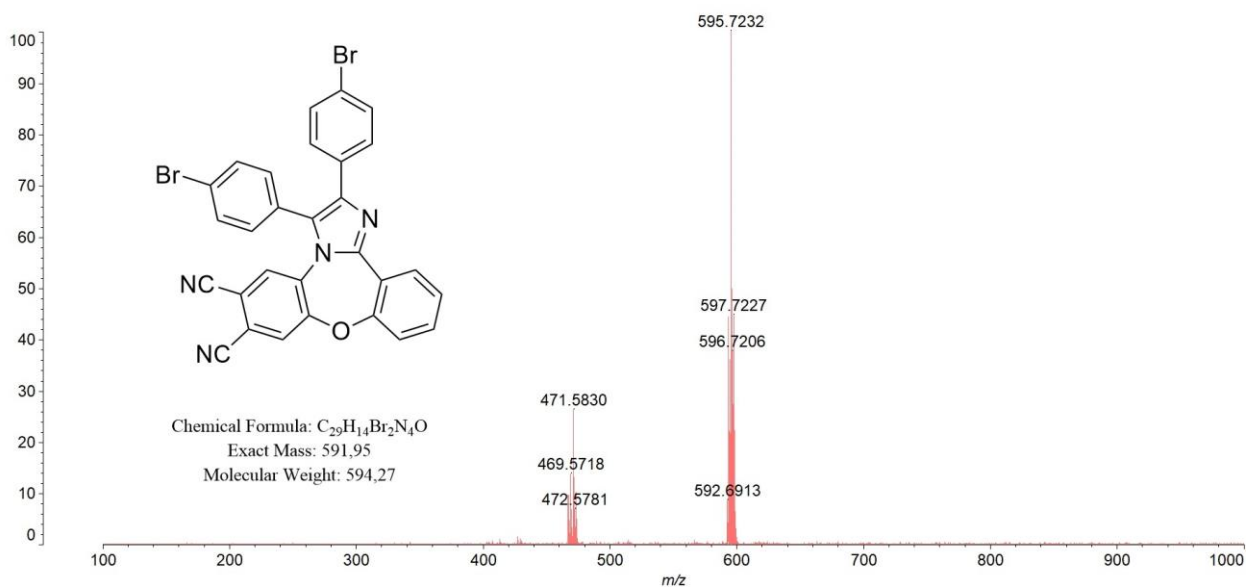


Figure SI-47. High-resolution mass spectrum (MALDI MS) of compound **3e**.

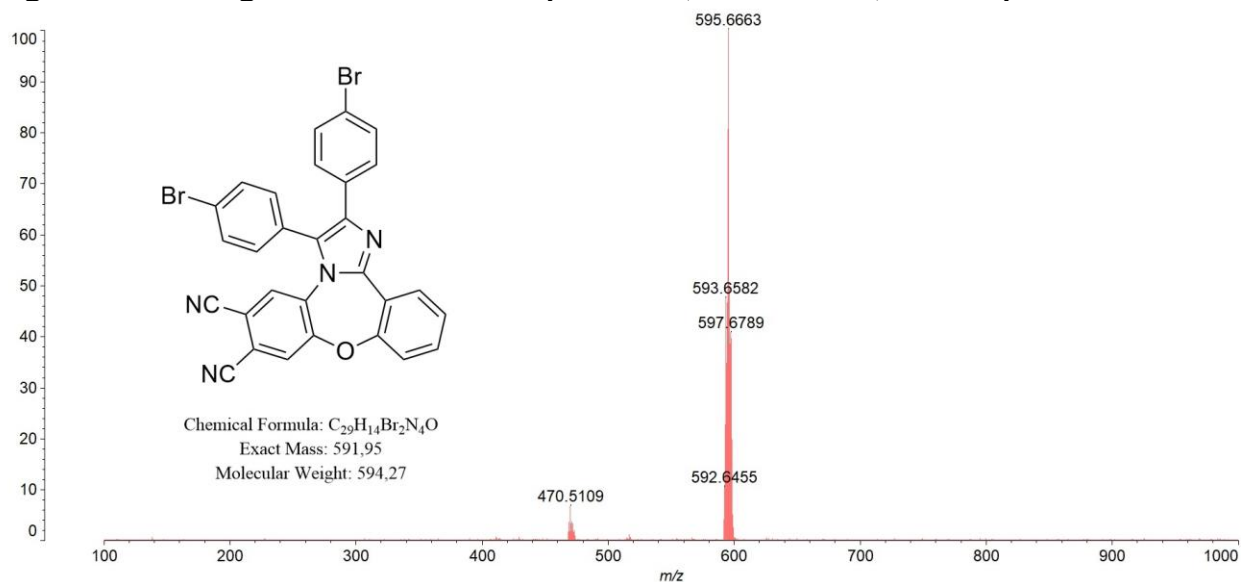


Figure SI-48. High-resolution mass spectrum (LDI MS) of compound **3e**.

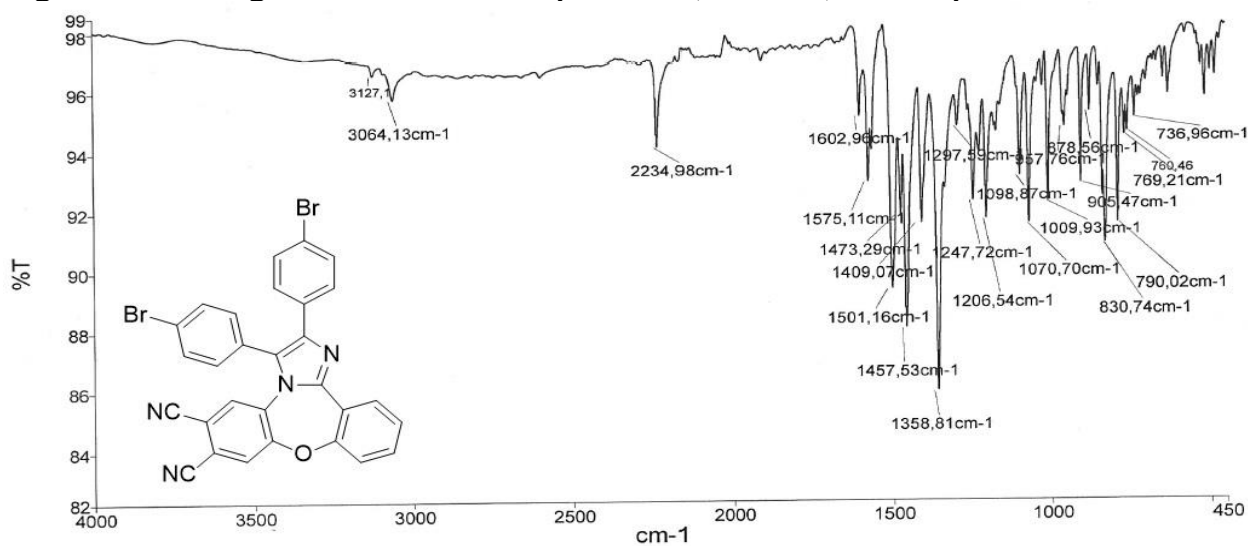


Figure SI-49. IR spectrum of compound **3e**.

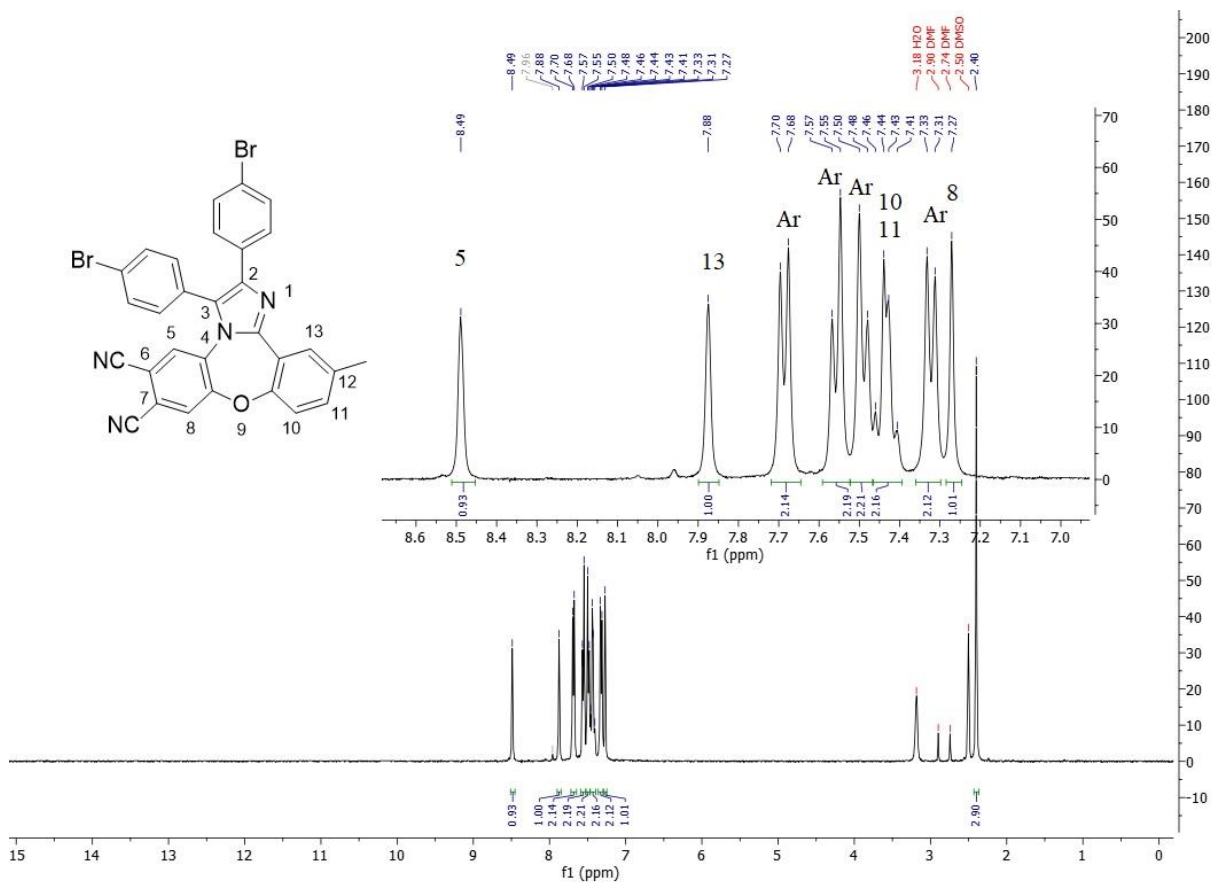


Figure SI-50. ¹H NMR spectrum of compound 3f.
100 MHz, DMSO-*d*₆

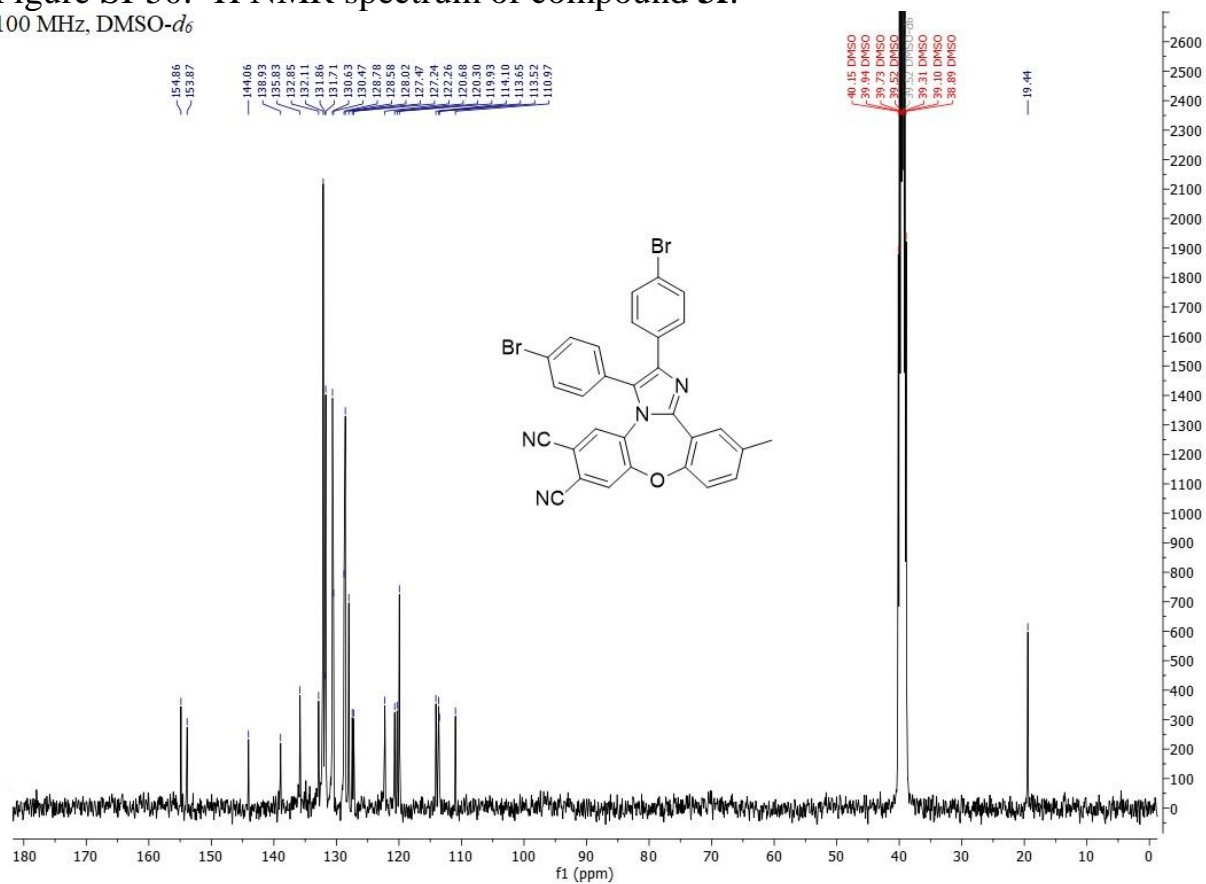


Figure SI-51. ¹³C NMR spectrum of compound 3f.

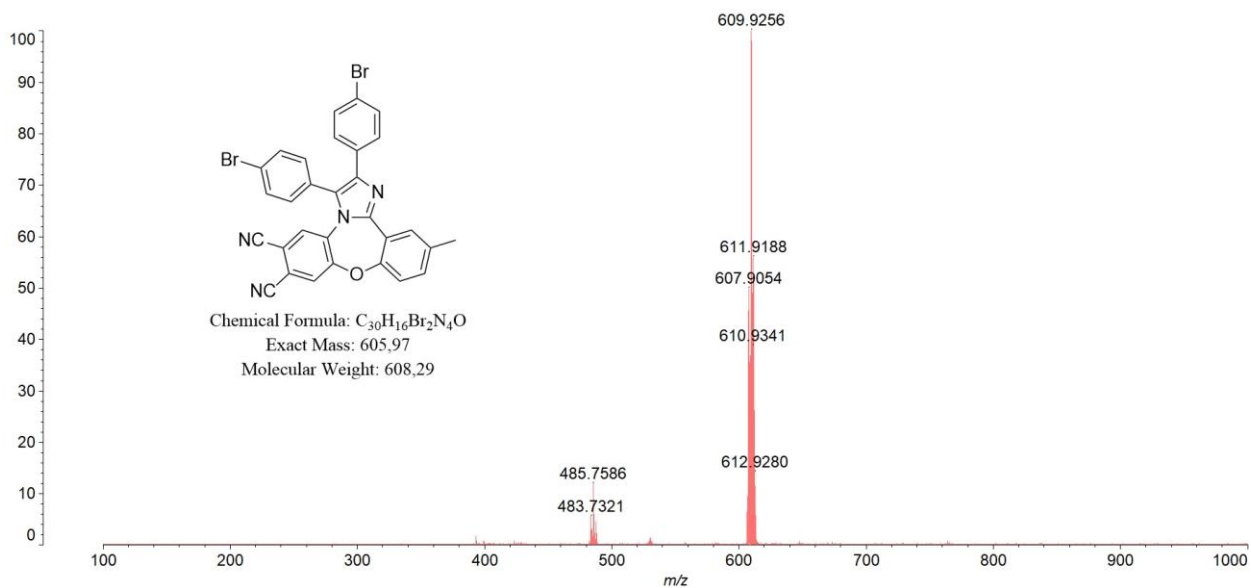


Figure SI-52. High-resolution mass spectrum (MALDI MS) of compound **3f**.

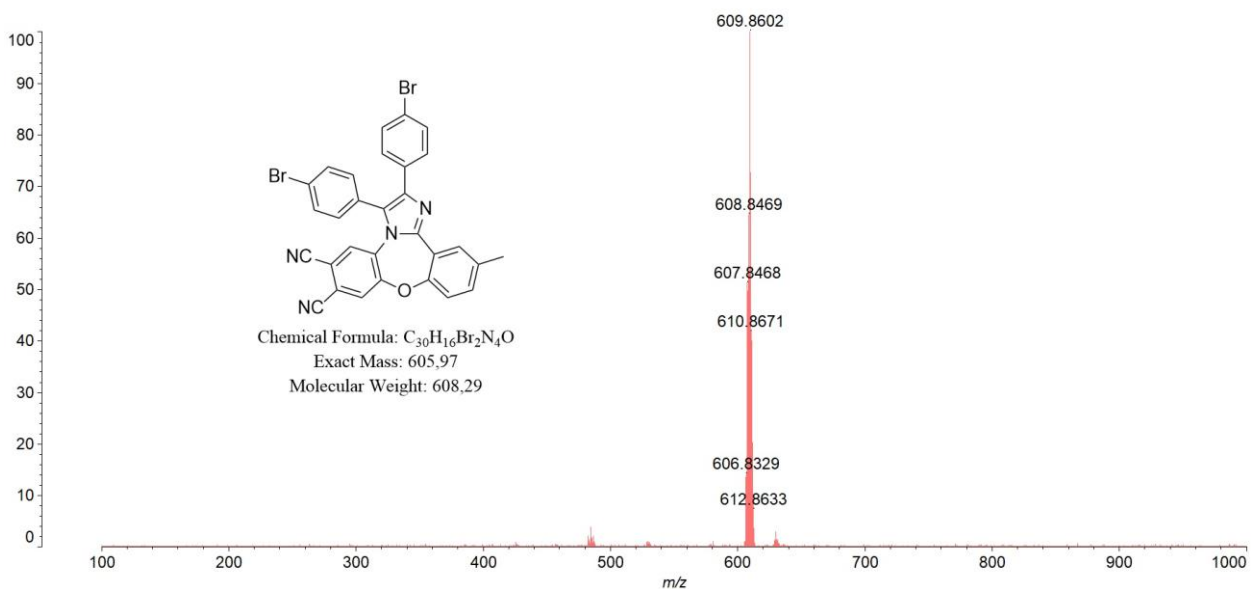


Figure SI-53. High-resolution mass spectrum (LDI MS) of compound **3f**.

400 MHz, DMSO-*d*₆

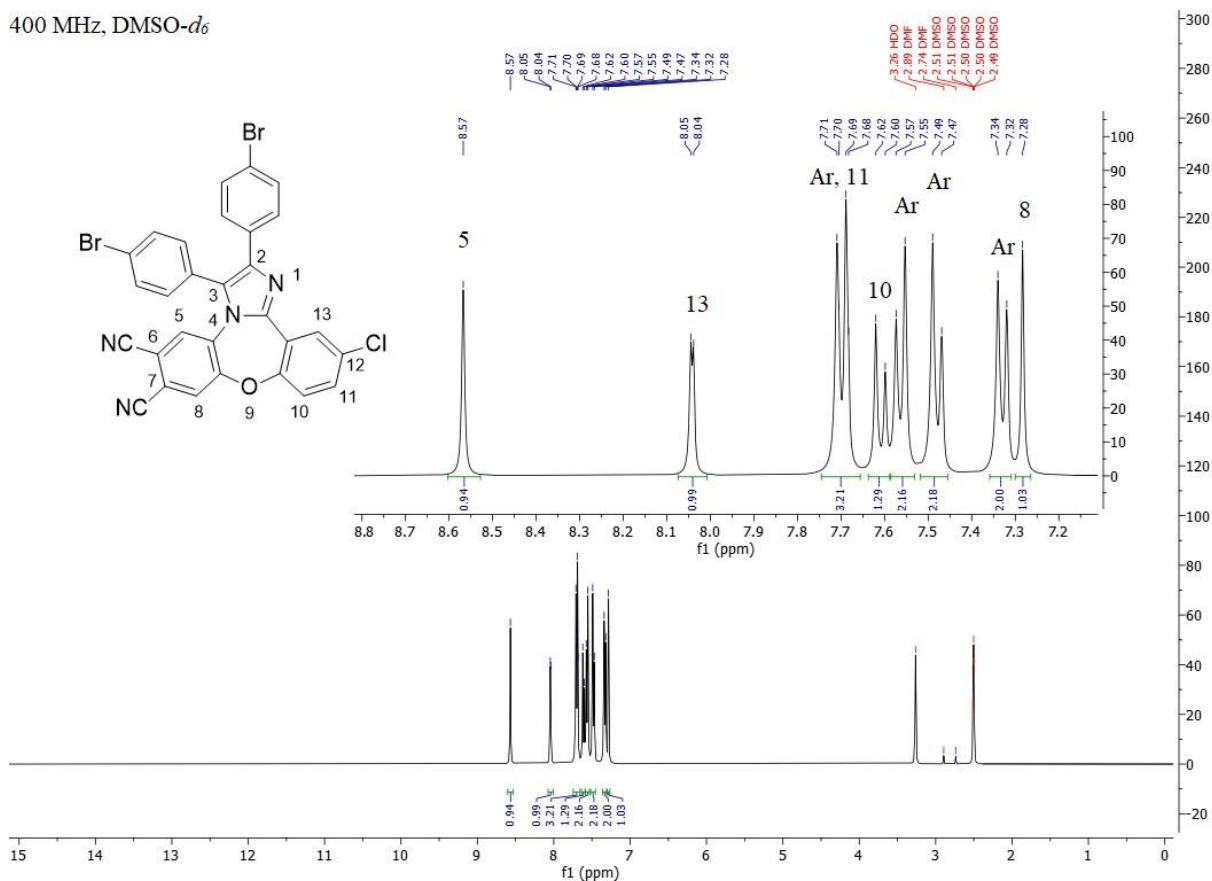


Figure SI-54. ¹H NMR spectrum of compound **3g**.

100 MHz, DMSO-*d*₆

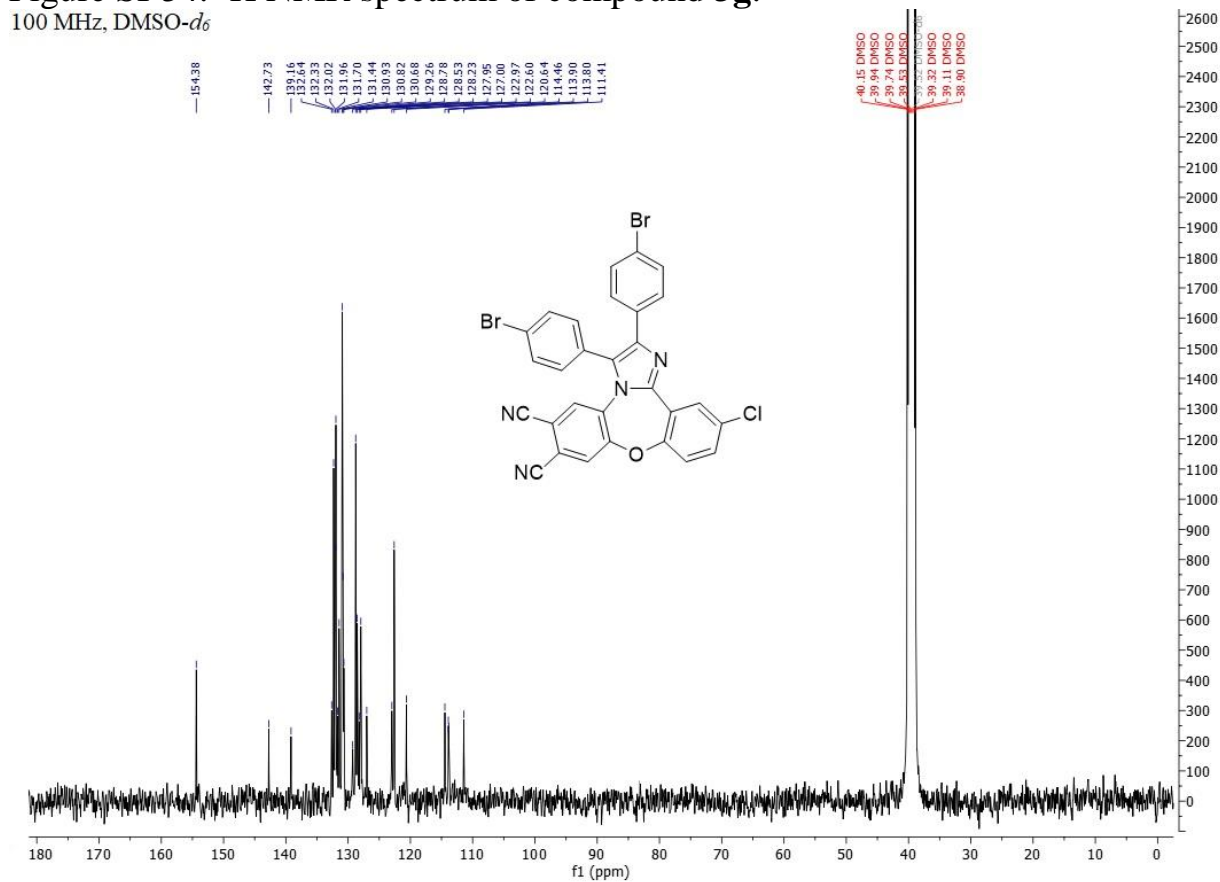


Figure SI-55. ¹³C NMR spectrum of compound **3g**.

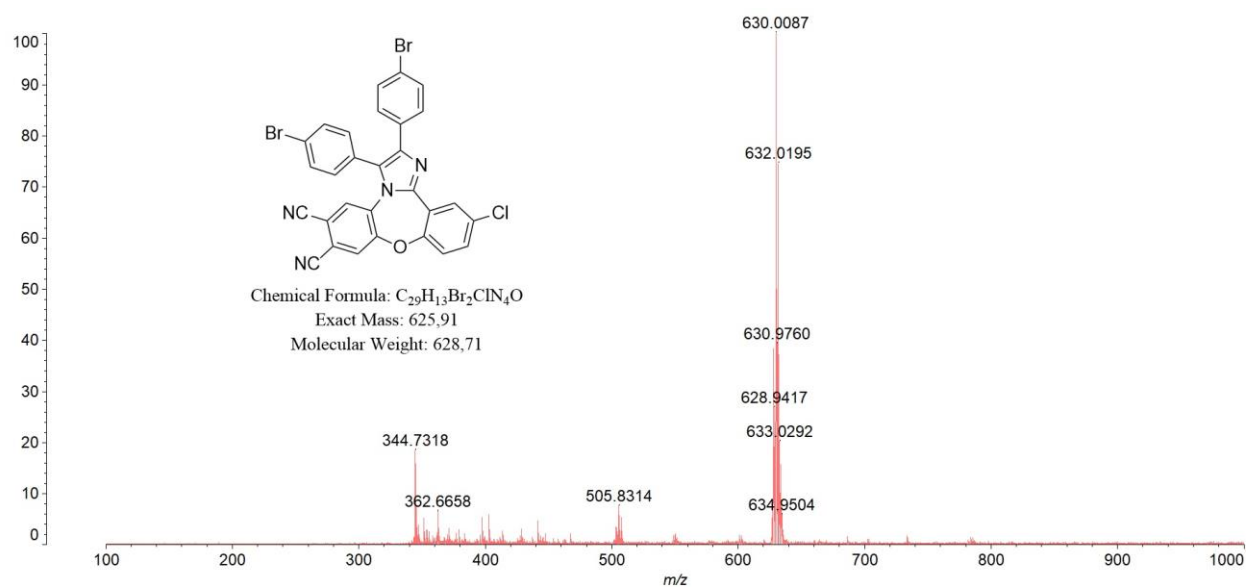


Figure SI-56. High-resolution mass spectrum (MALDI MS) of compound **3g**.

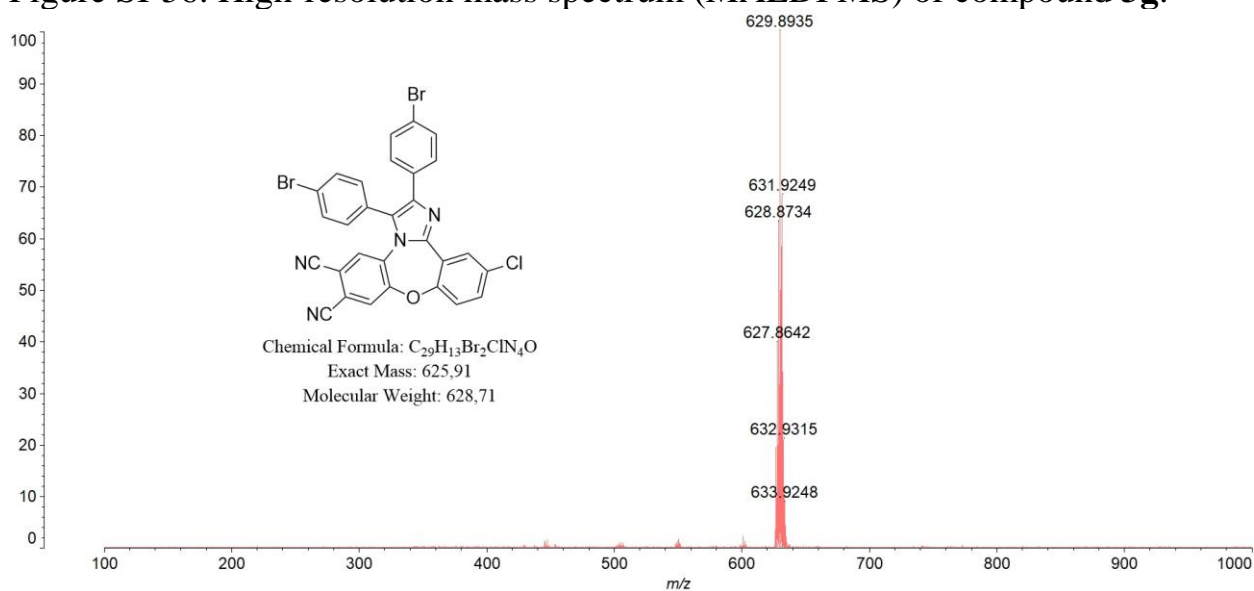


Figure SI-57. High-resolution mass spectrum (LDI MS) of compound **3g**.

400 MHz, DMSO-*d*₆

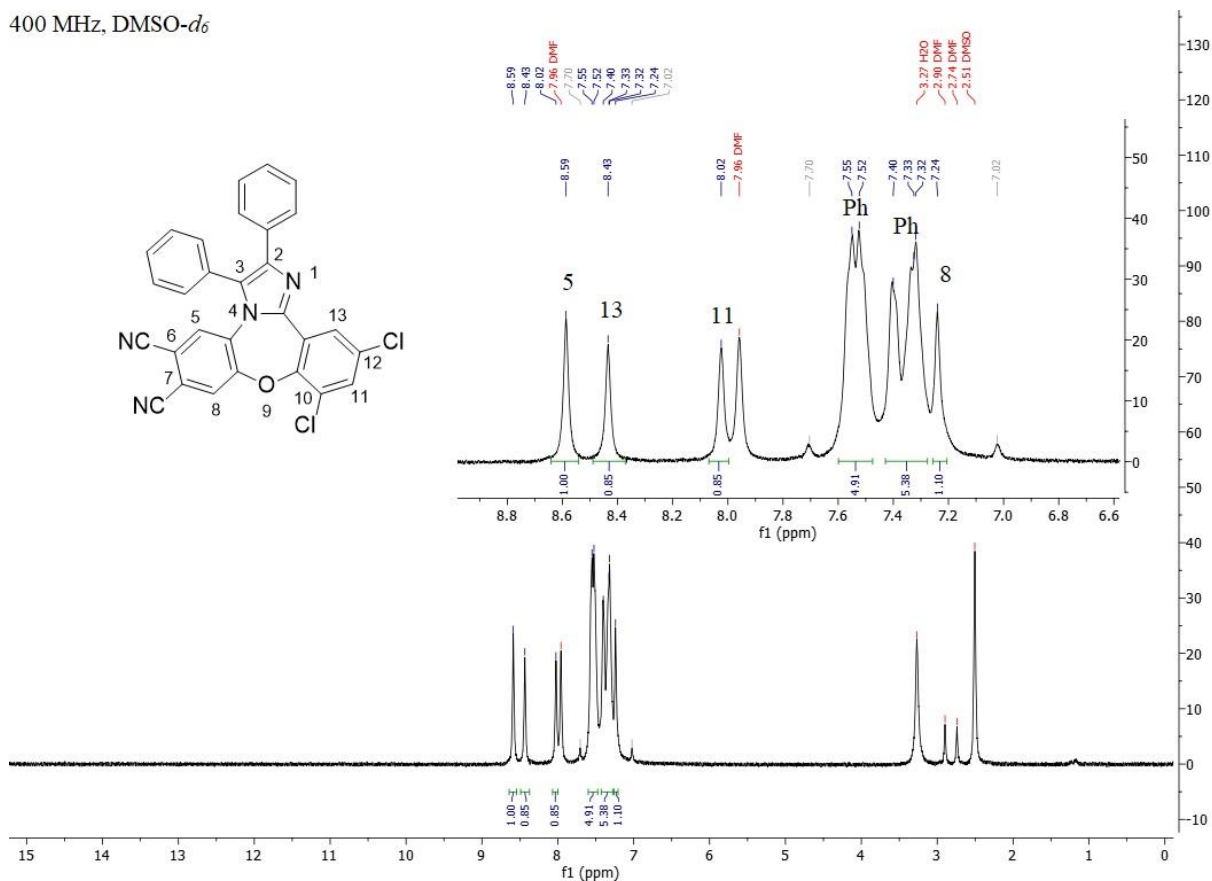


Figure SI-58. ¹H NMR spectrum of compound **3i**.

100 MHz, DMSO-*d*₆

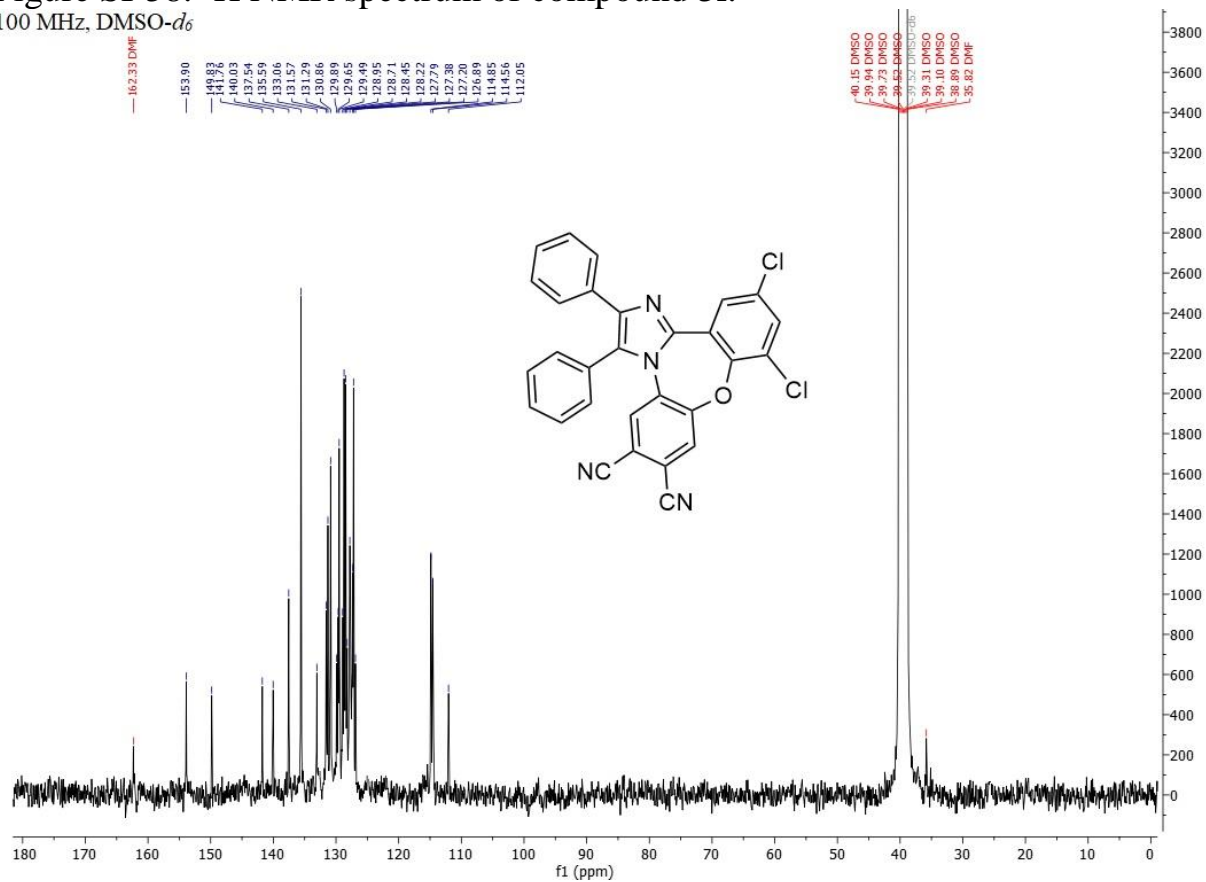


Figure SI-59. ¹³C NMR spectrum of compound **3i**.

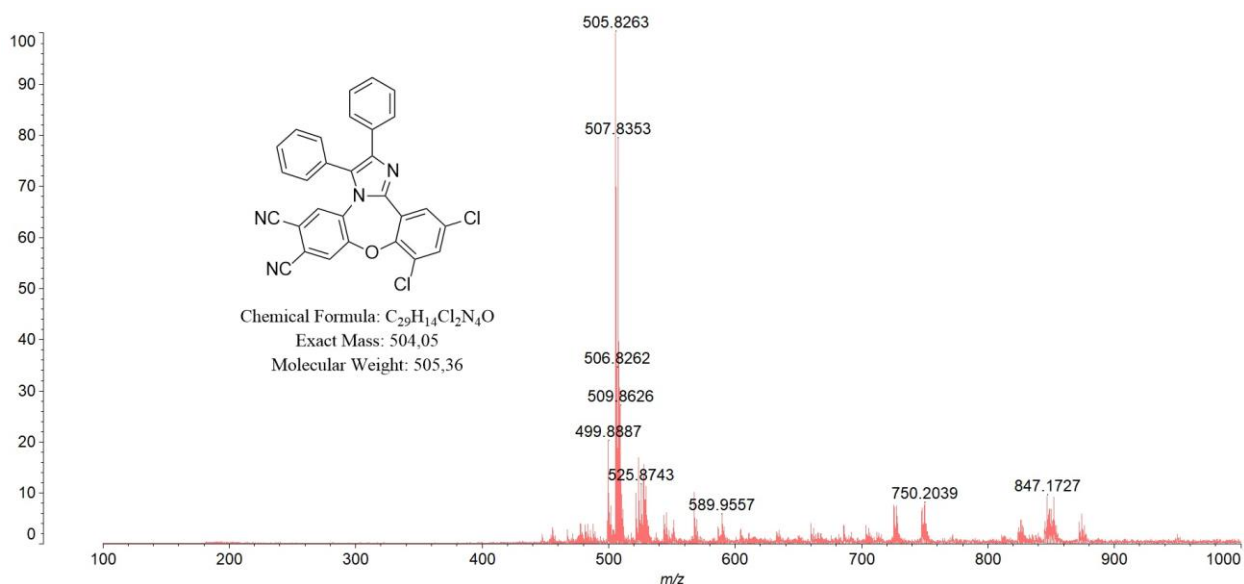


Figure SI-60. High-resolution mass spectrum (MALDI MS) of compound **3i**.

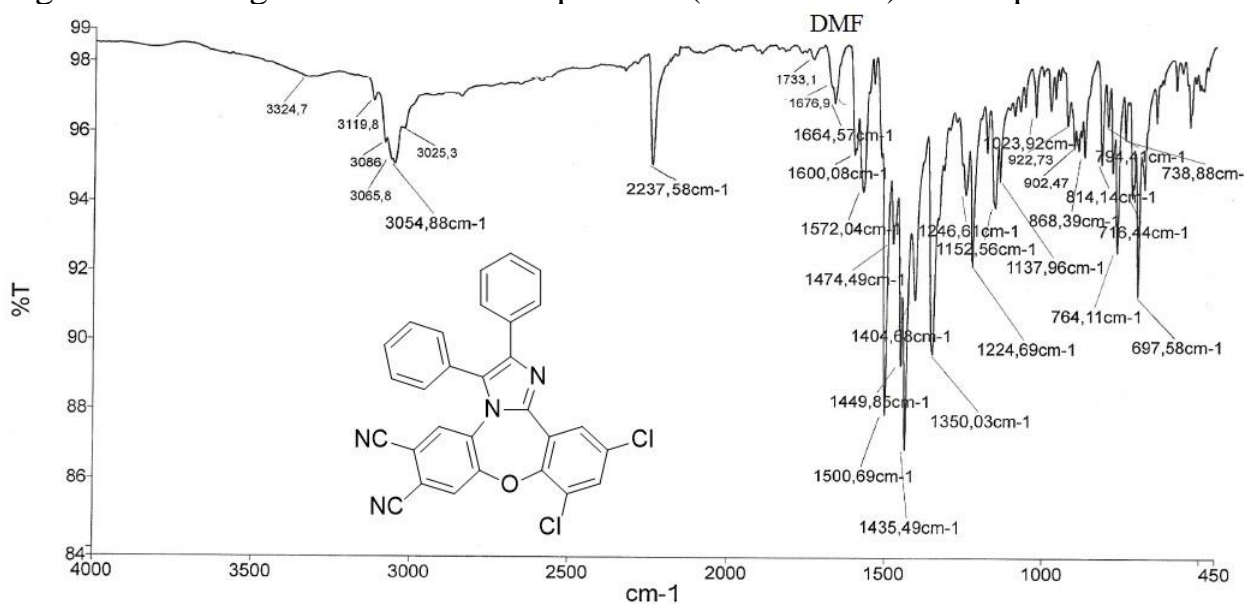


Figure SI-61. IR spectrum of compound **3i**.

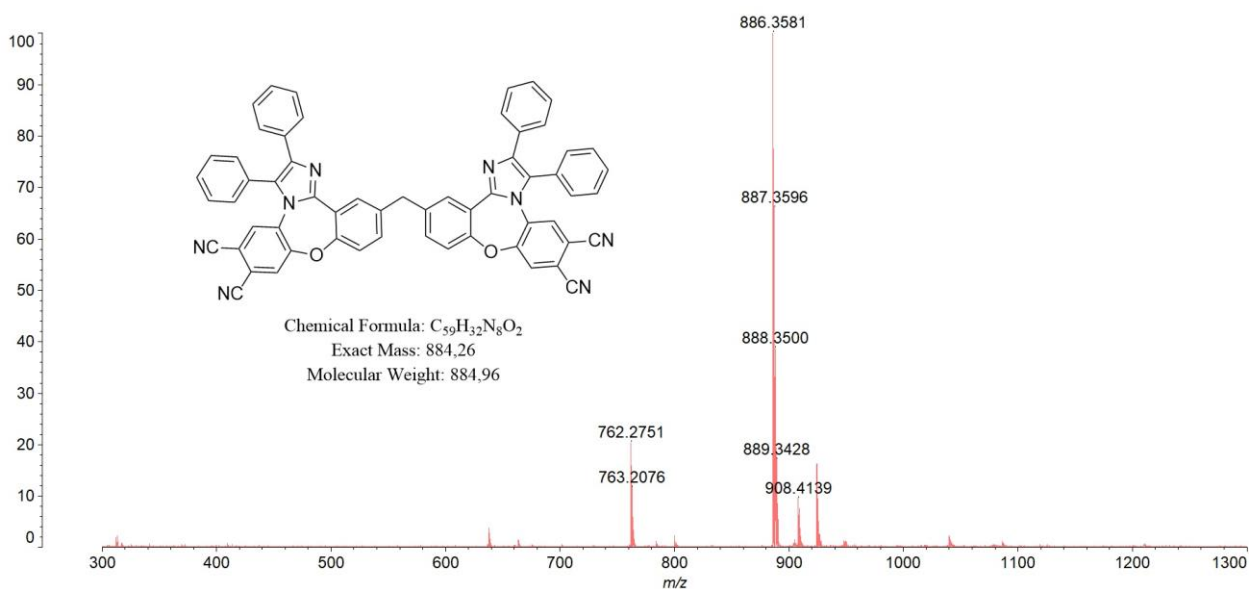


Figure SI-64. High-resolution mass spectrum (MALDI MS) of compound **5**.

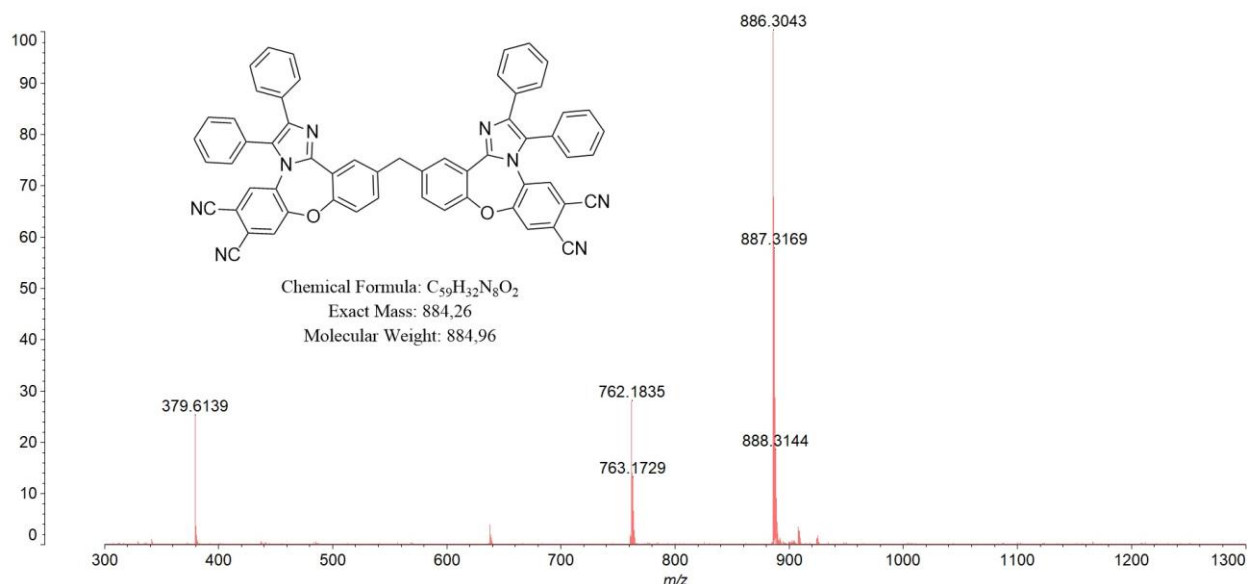


Figure SI-65. High-resolution mass spectrum (LDI MS) of compound **5**.

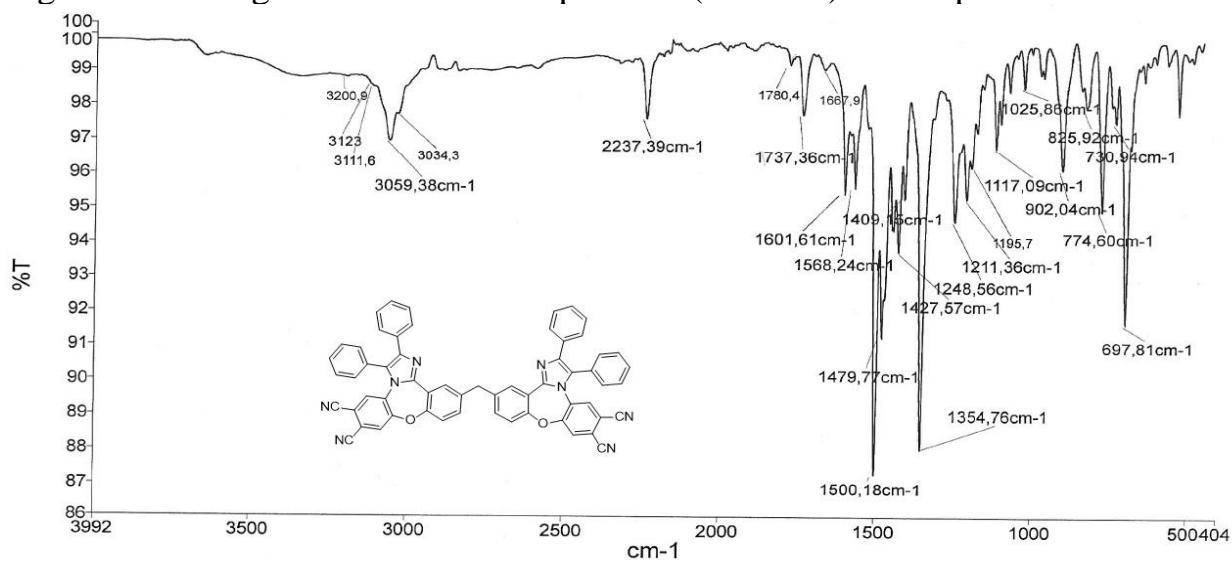


Figure SI-66. IR spectrum of compound **5**.

400 MHz, DMSO-*d*₆

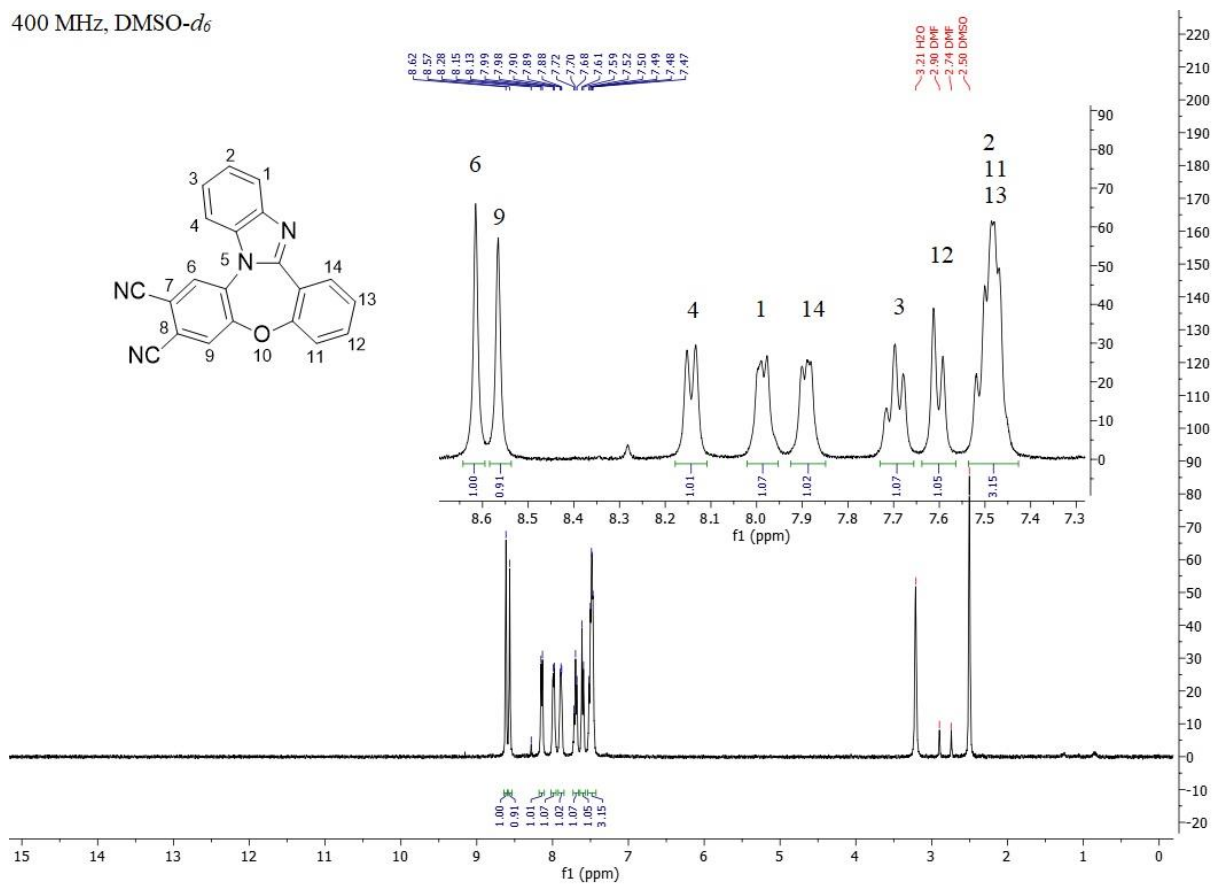


Figure SI-67. ¹H NMR spectrum of compound 7.
100 MHz, DMSO-*d*₆

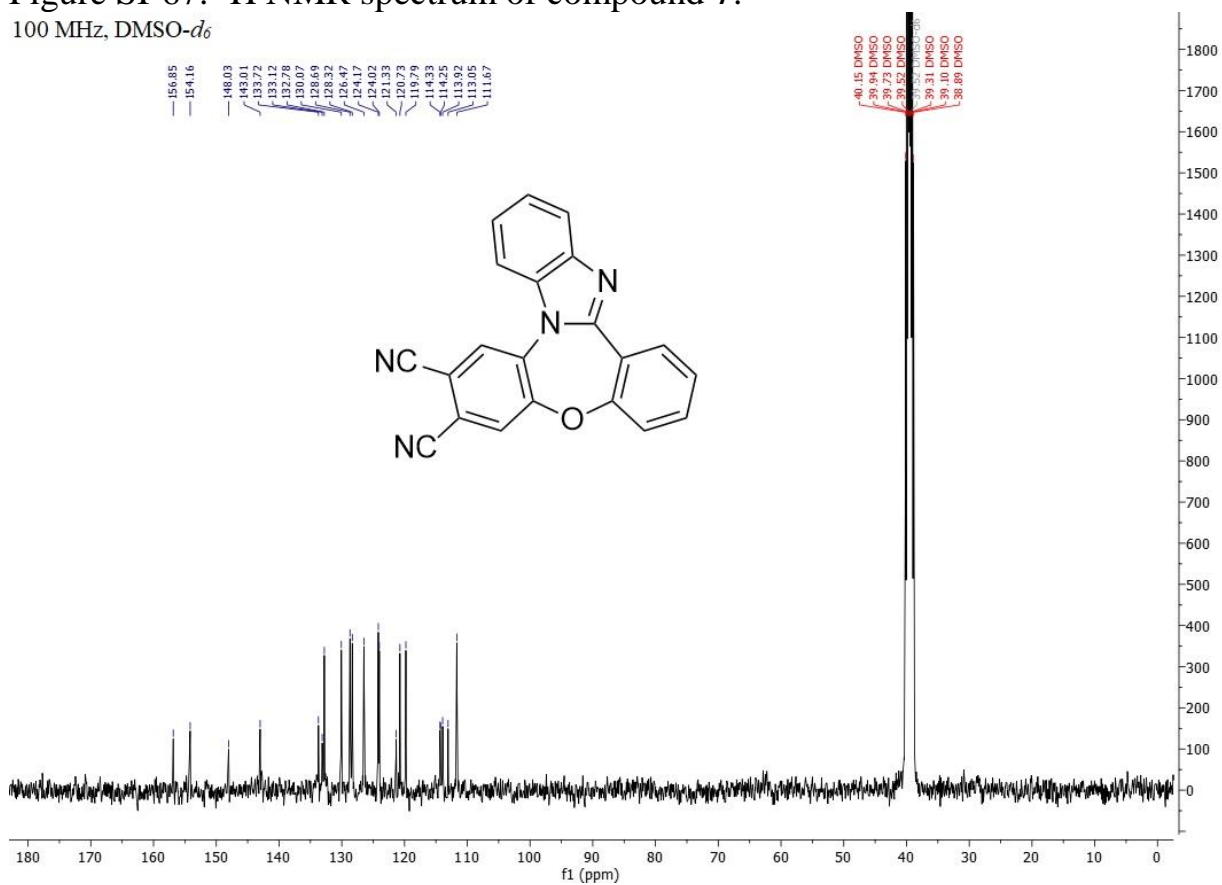


Figure SI-68. ^{13}C NMR spectrum of compound **7**.

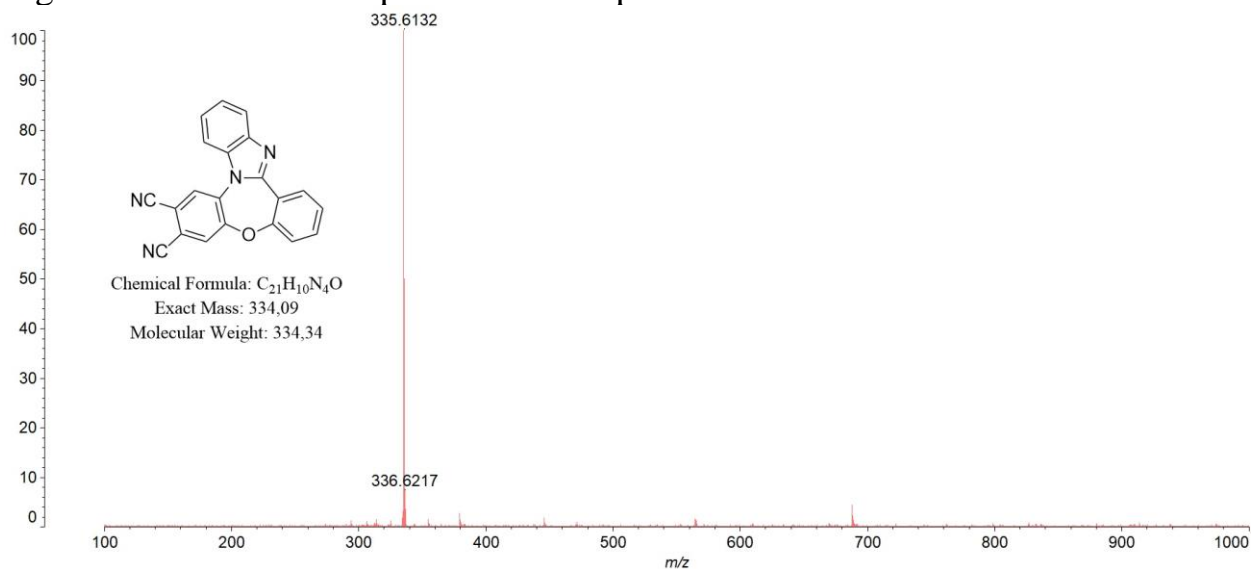


Figure SI-69. High-resolution mass spectrum (MALDI MS) of compound **7**.

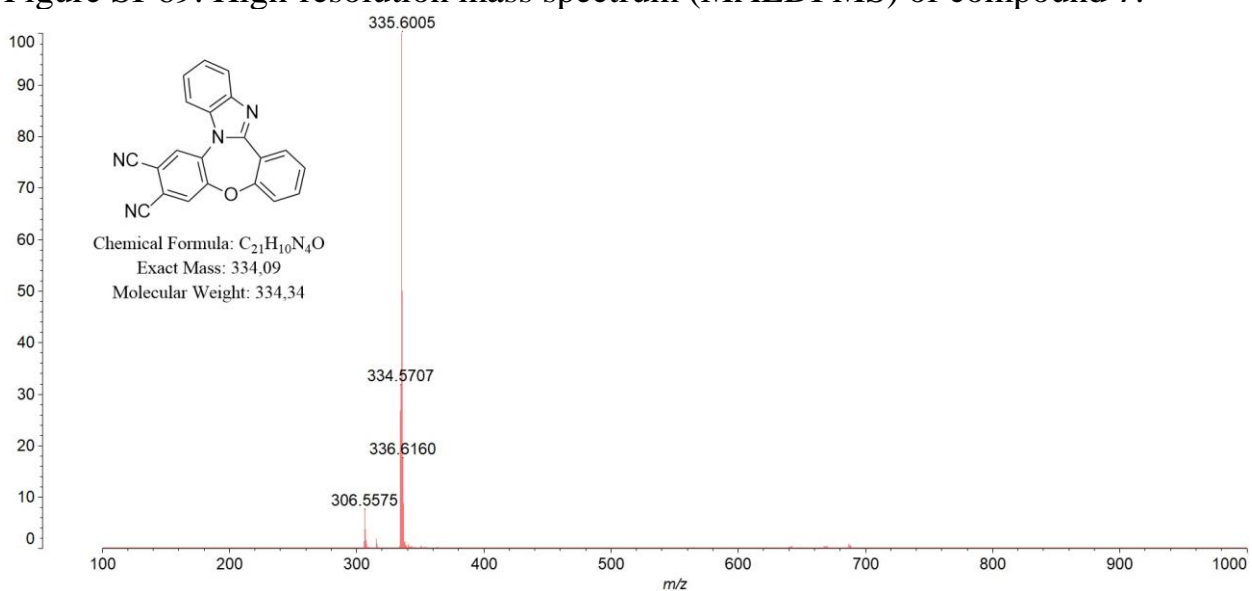


Figure SI-70. High-resolution mass spectrum (LDI MS) of compound **7**.

400 MHz, DMSO-d₆, 100 °C

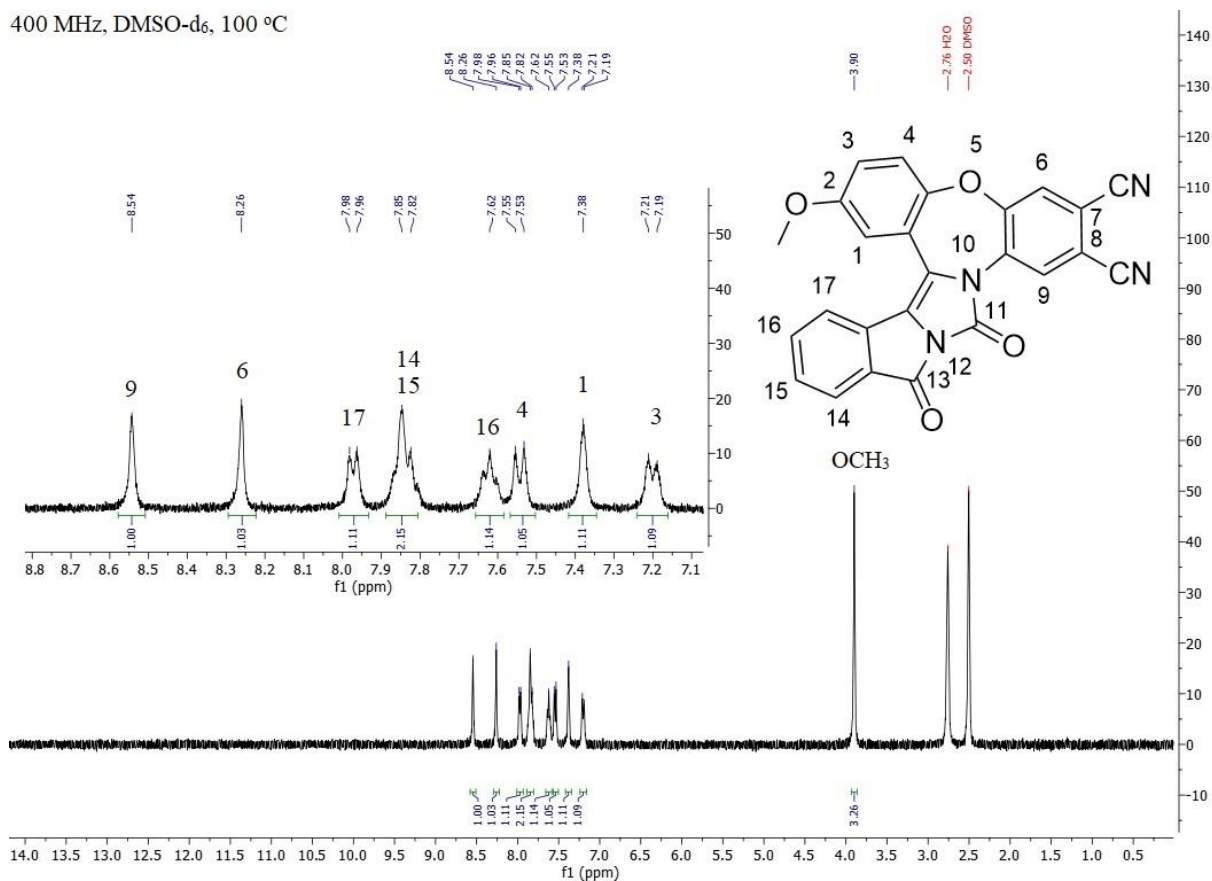


Figure SI-71. ¹H NMR spectrum of compound **9**.

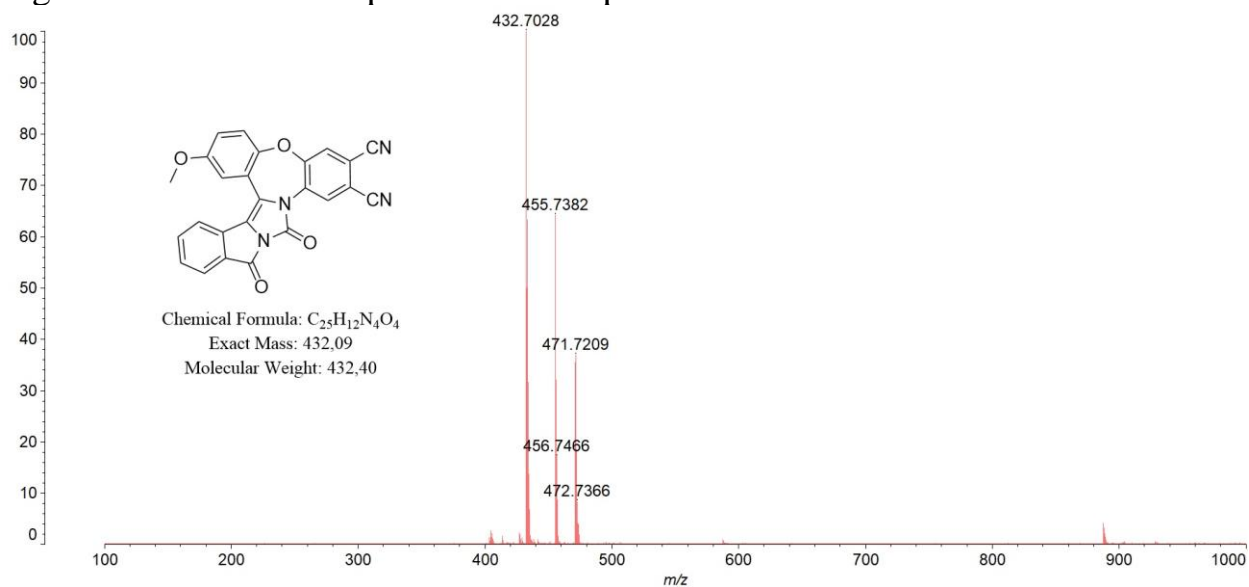


Figure SI-72. High-resolution mass spectrum (MALDI MS) of compound **9**.

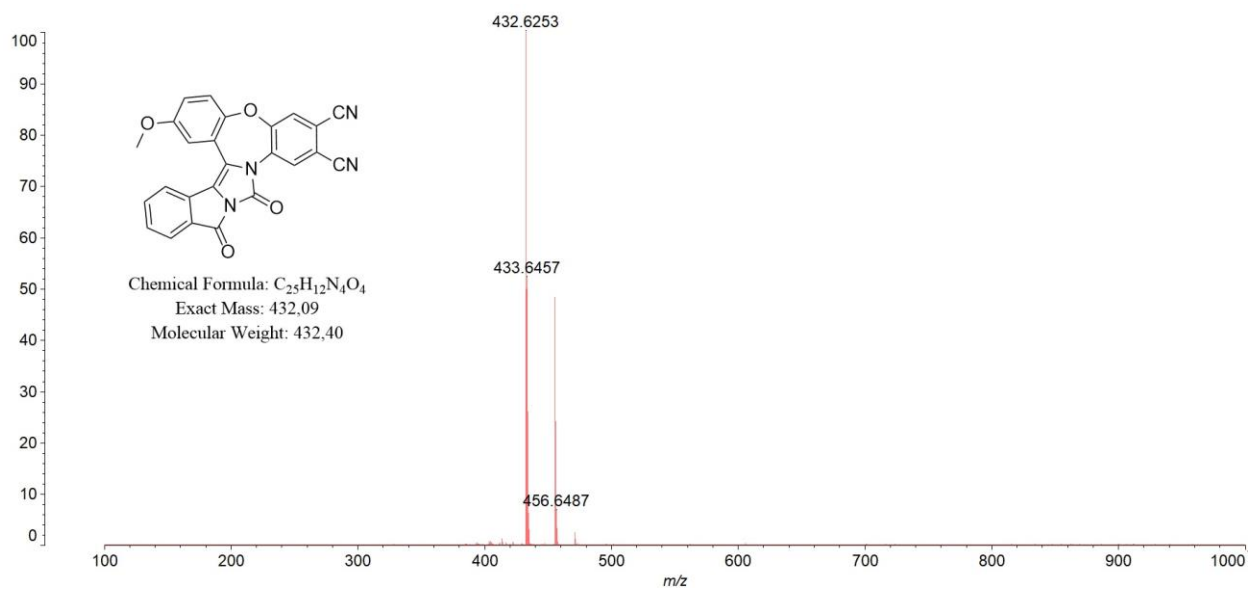


Figure SI-73. High-resolution mass spectrum (LDI MS) of compound **9**.