

Supporting Information

One-Pot Two-Step Catalytic Synthesis of Rationally Designed 6-amino-2-pyridone-3,5-dicarbonitriles Enabling Anti-Cancer Bioactivity

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1. Copies of 1D and 2D NMR spectra of **5(a-p)**

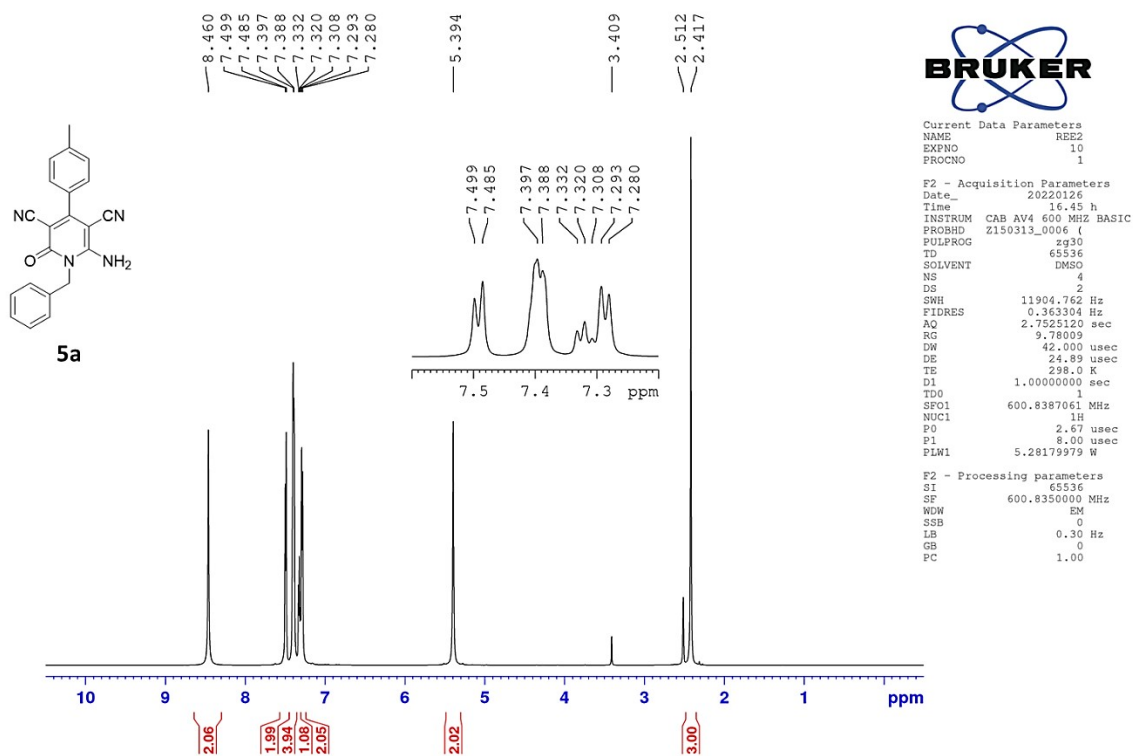


Figure S1. ^1H NMR spectrum of compound **5a** at 600 MHz in DMSO-d_6

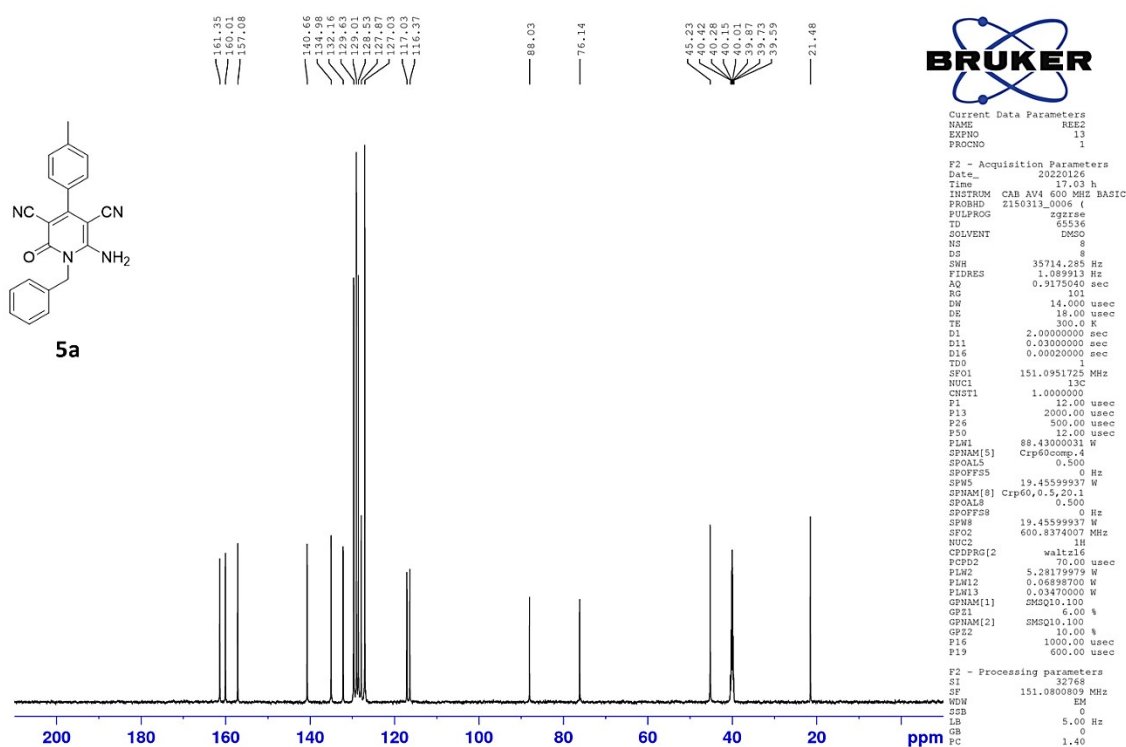
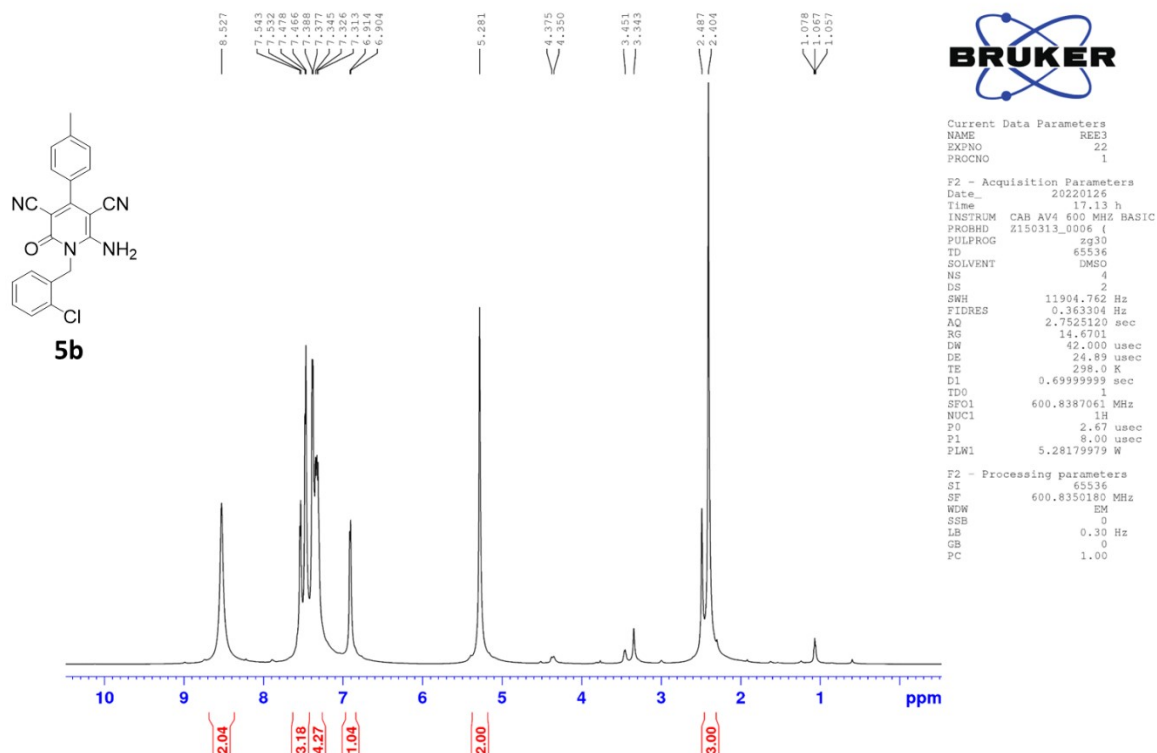
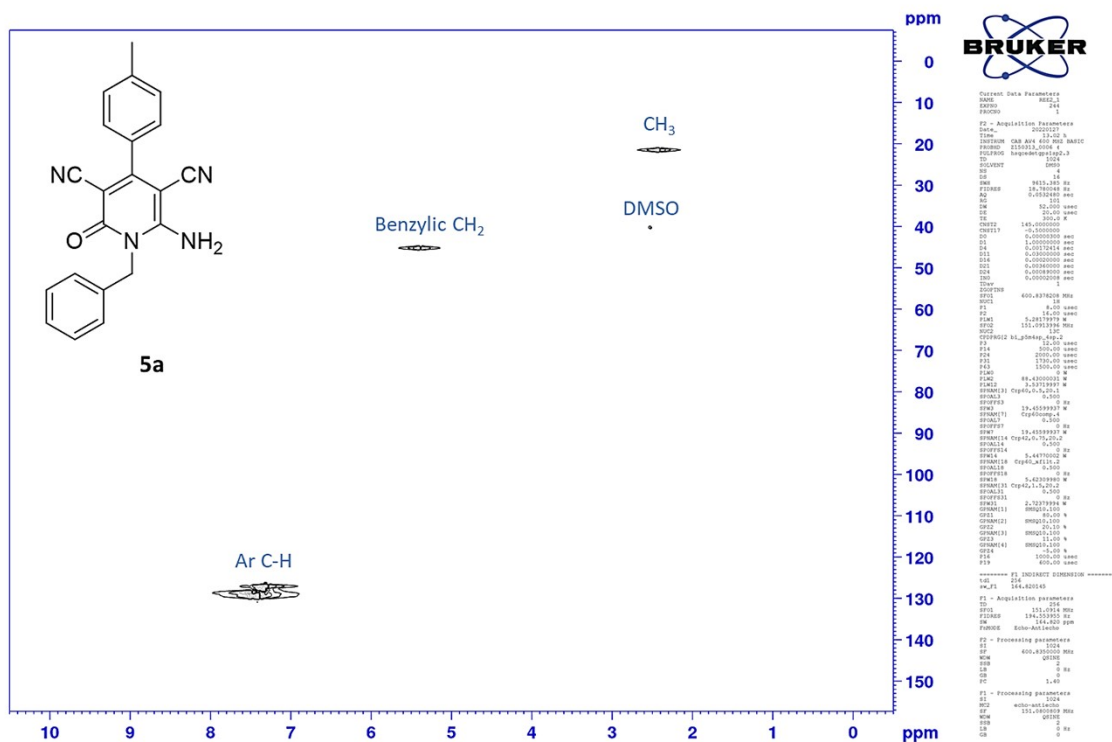


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5a** at 151 MHz in DMSO-d_6



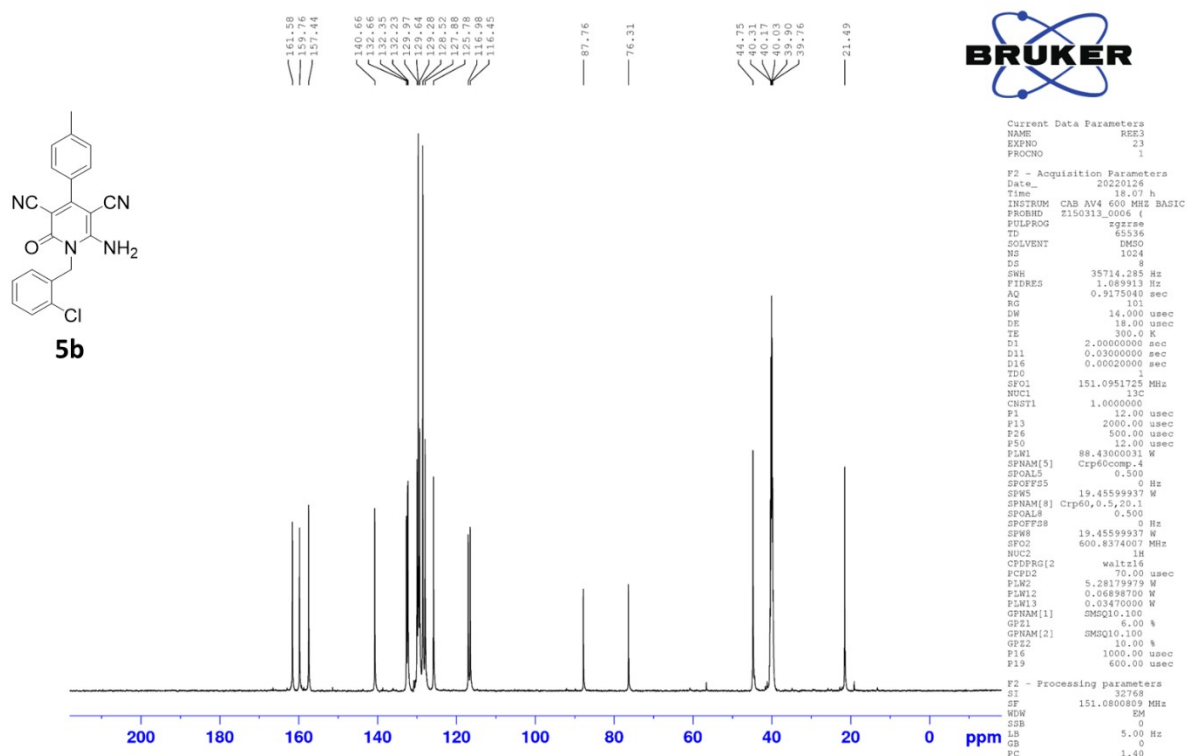


Figure S5. ¹³C{¹H} NMR spectrum of compound **5b** at 151 MHz in DMSO-d₆

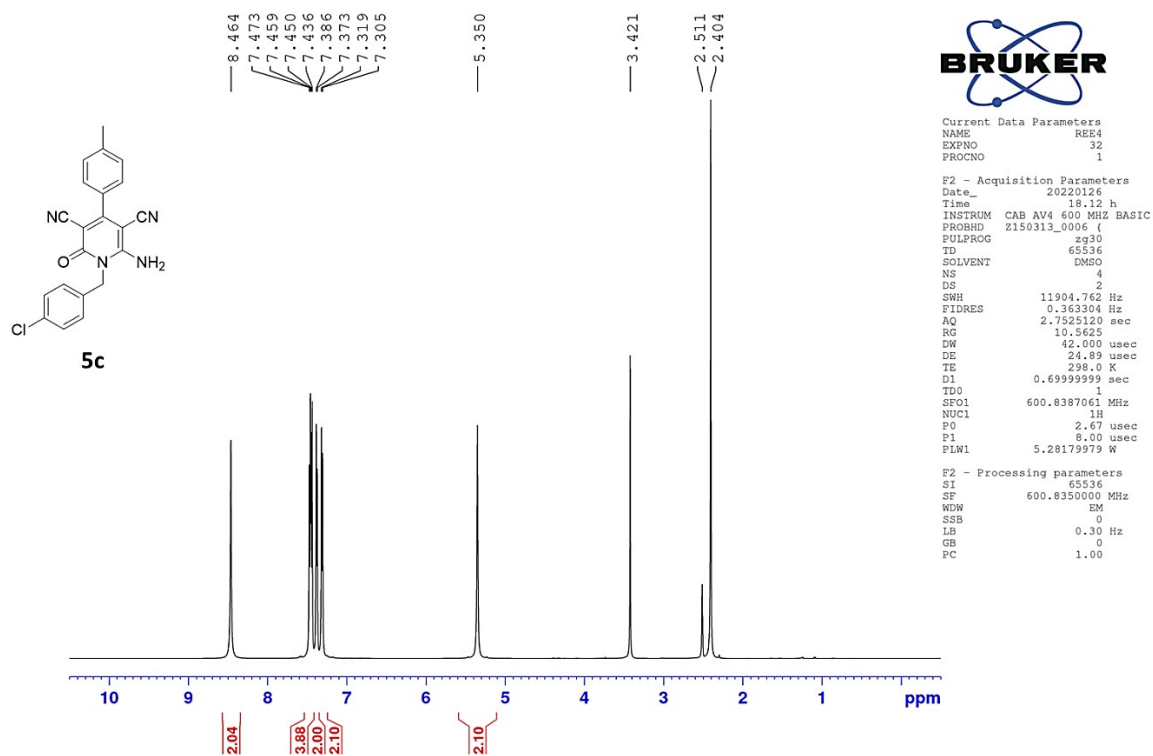


Figure S6. ¹H NMR spectrum of compound **5c** at 600 MHz in DMSO-d₆

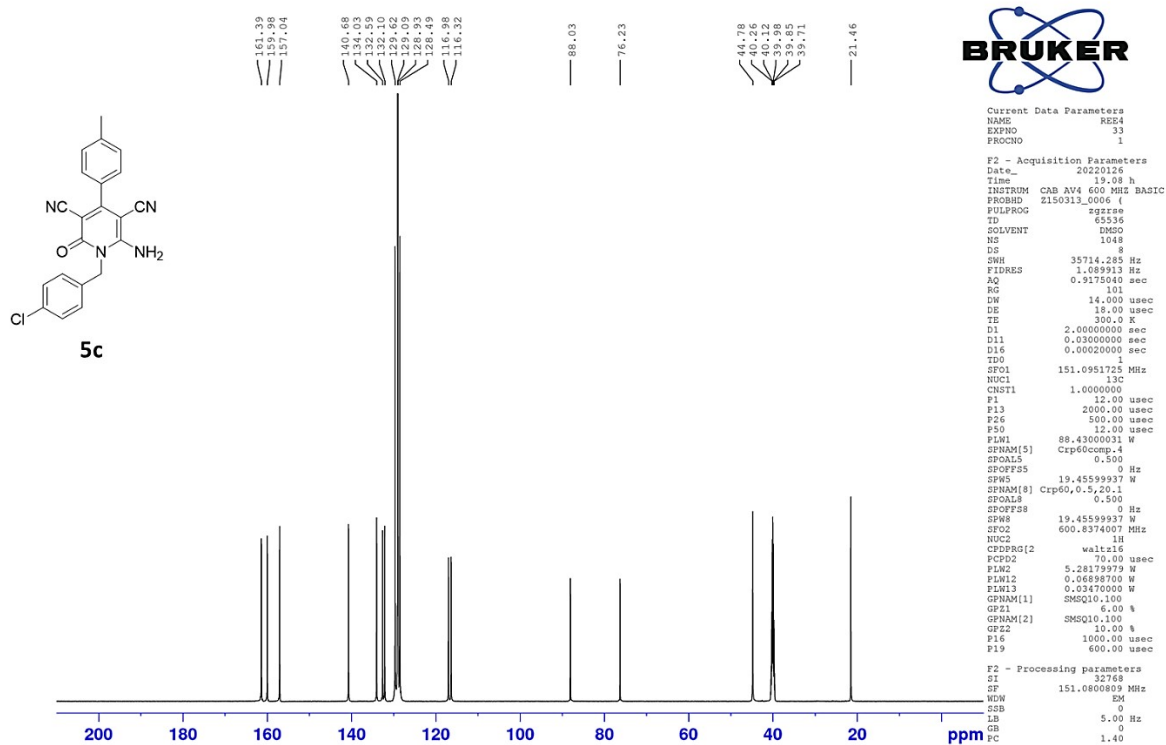


Figure S7. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5c** at 151 MHz in DMSO-d_6

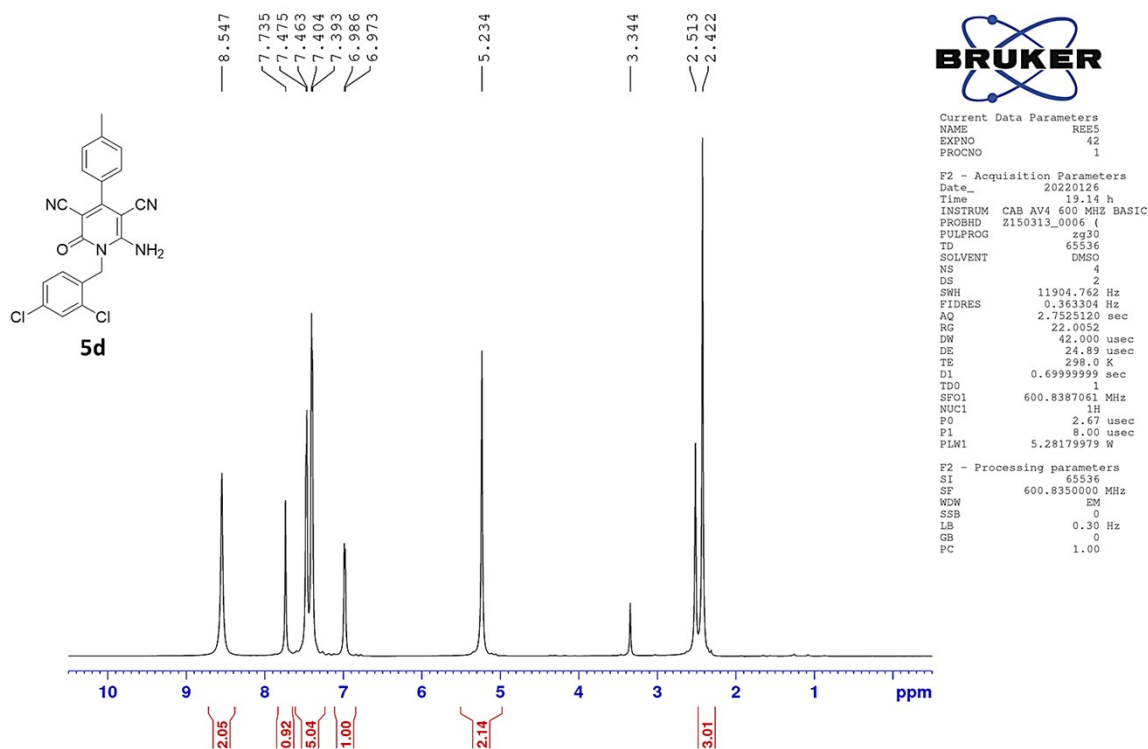


Figure S8. ^1H NMR spectrum of compound **5d** at 600 MHz in DMSO-d_6

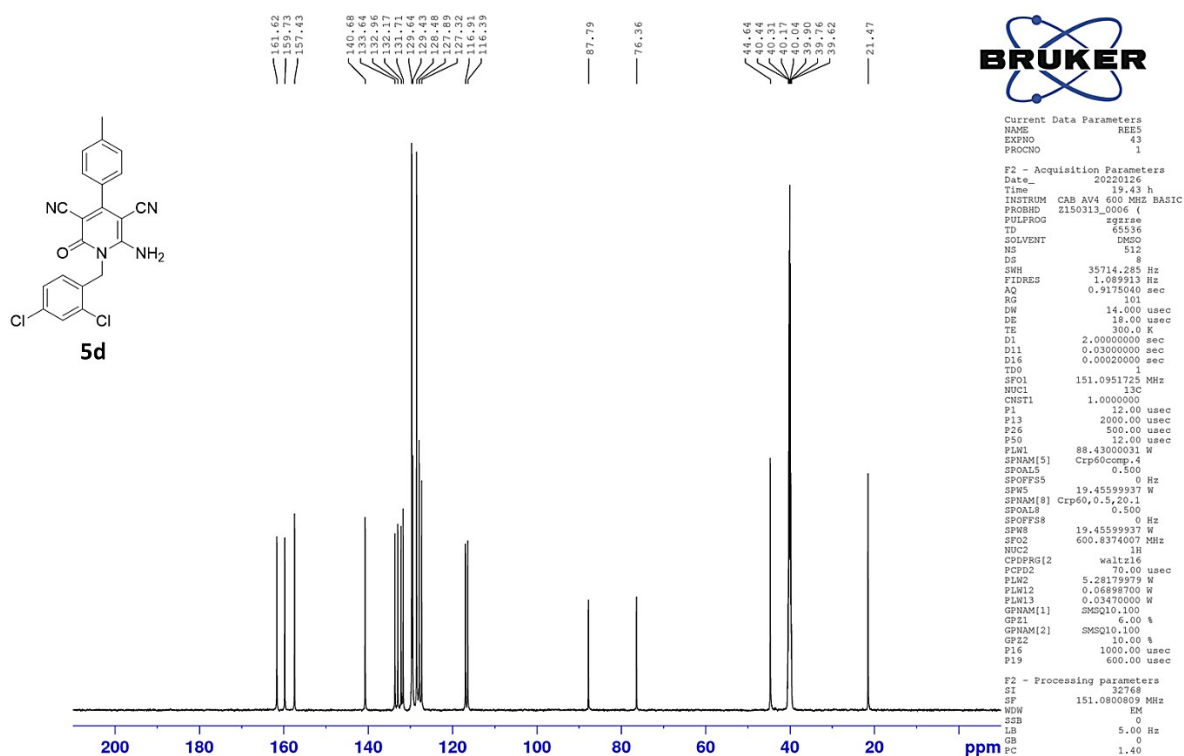


Figure S9. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5d** at 151 MHz in DMSO-d_6

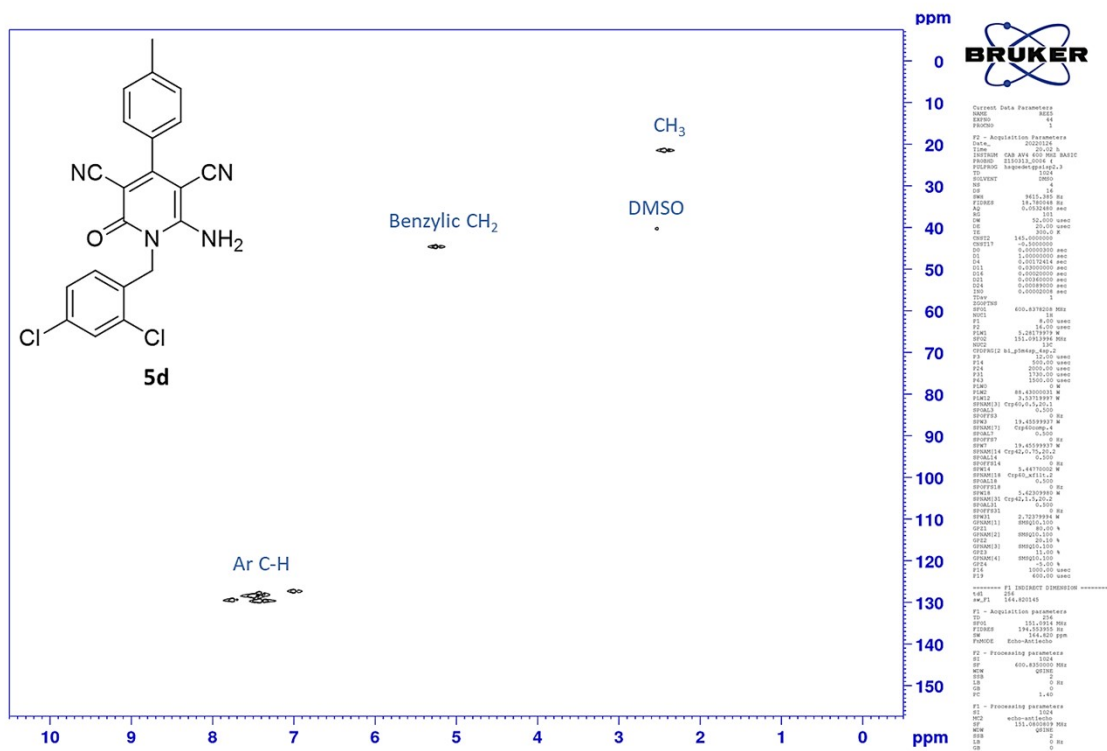


Figure S10. HSQC spectrum of compound **5d** in DMSO-d_6

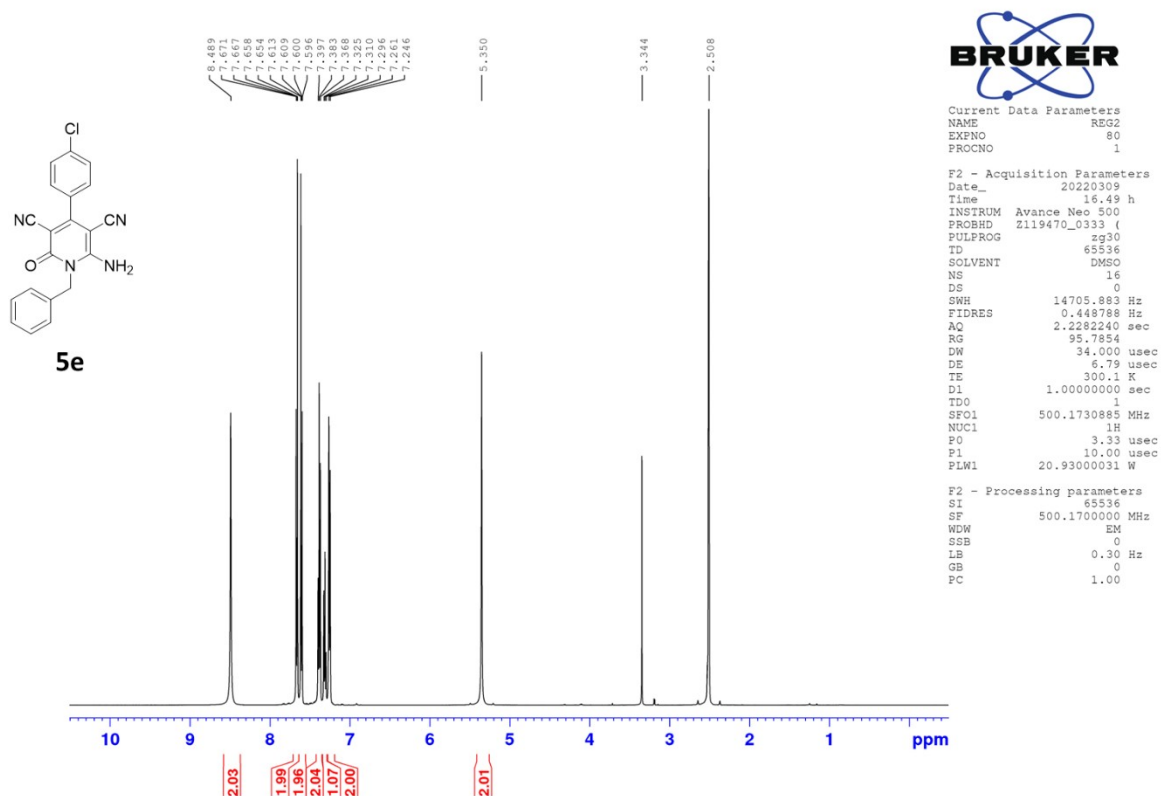


Figure S11. ^1H NMR spectrum of compound **5e** at 500 MHz in DMSO-d_6

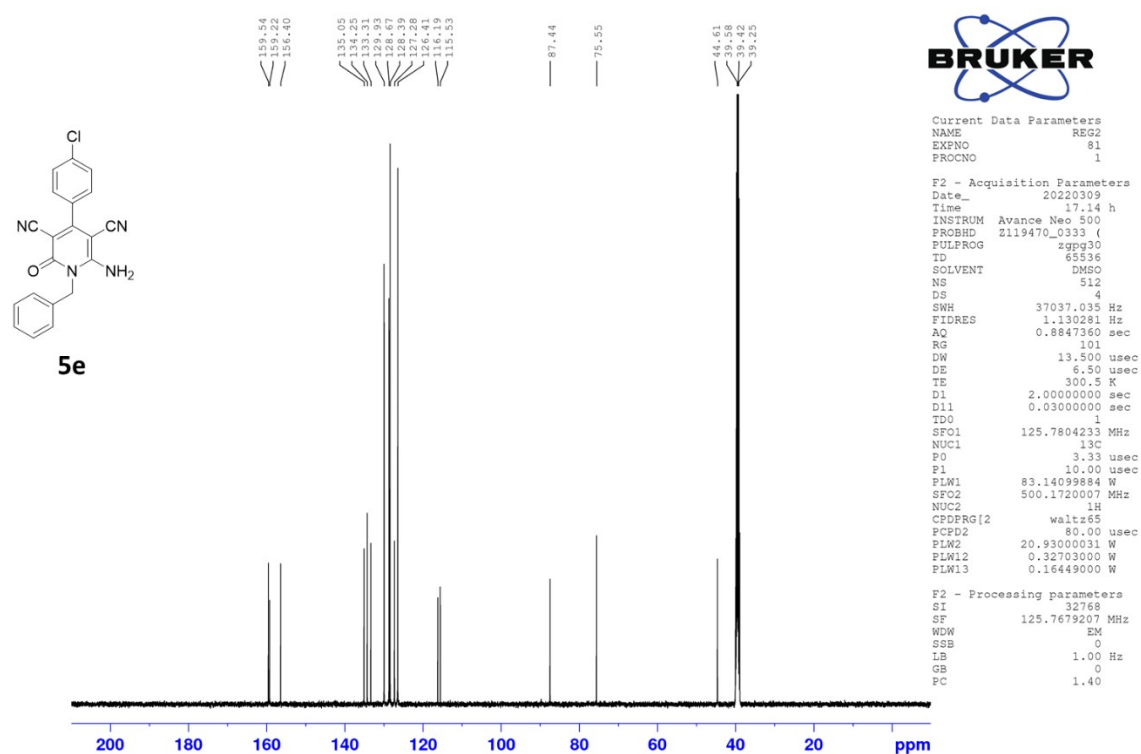


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5e** at 125 MHz in DMSO-d_6

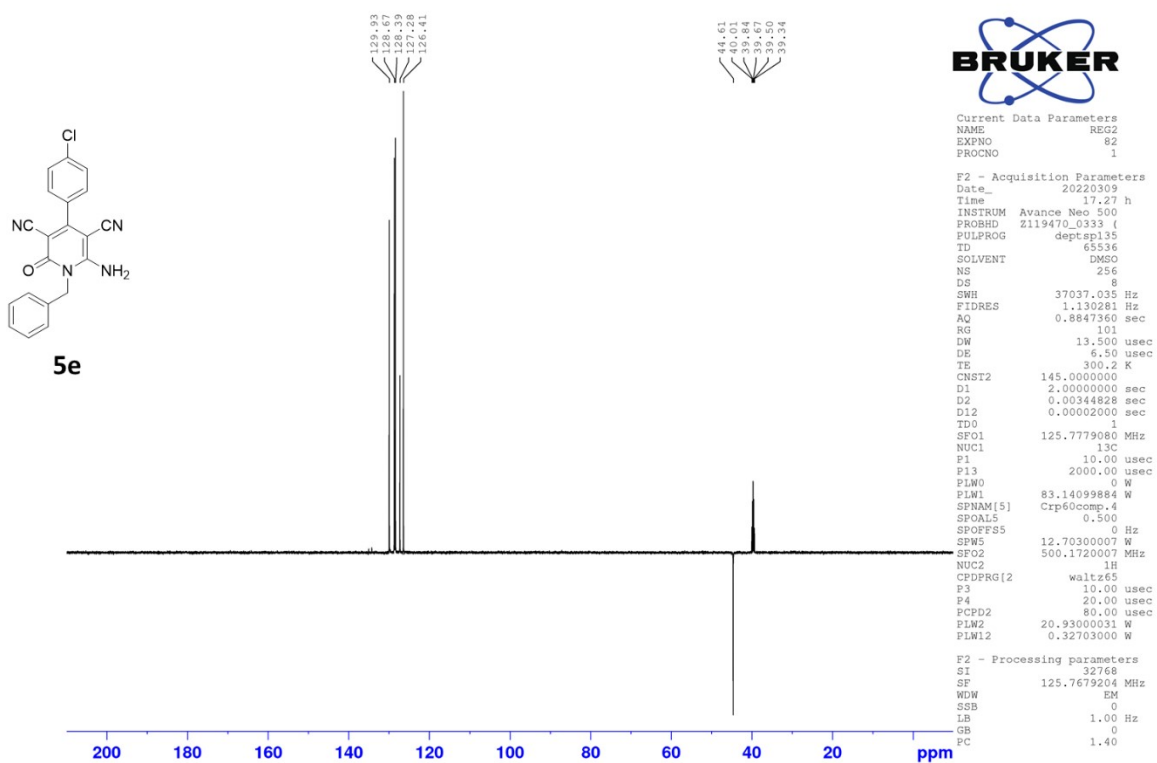


Figure S13. DEPT-135 spectrum of compound **5e** at 125 MHz in DMSO-d₆

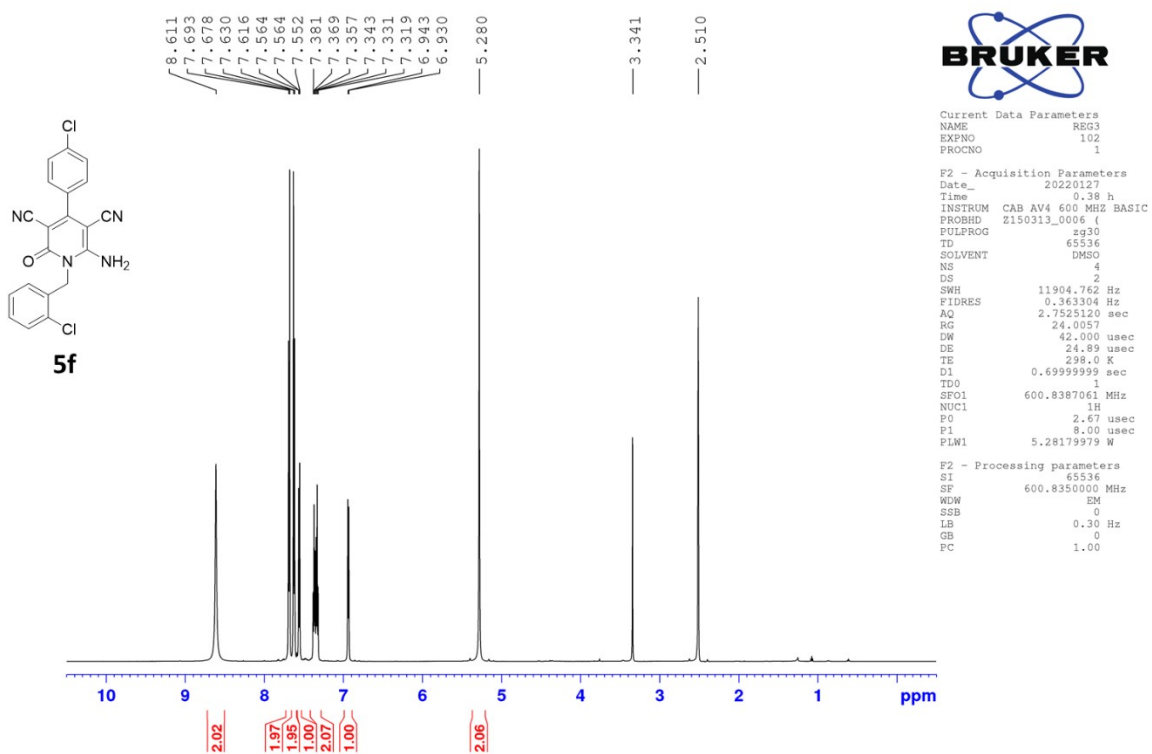


Figure S14. ¹H NMR spectrum of compound **5f** at 600 MHz in DMSO-d₆

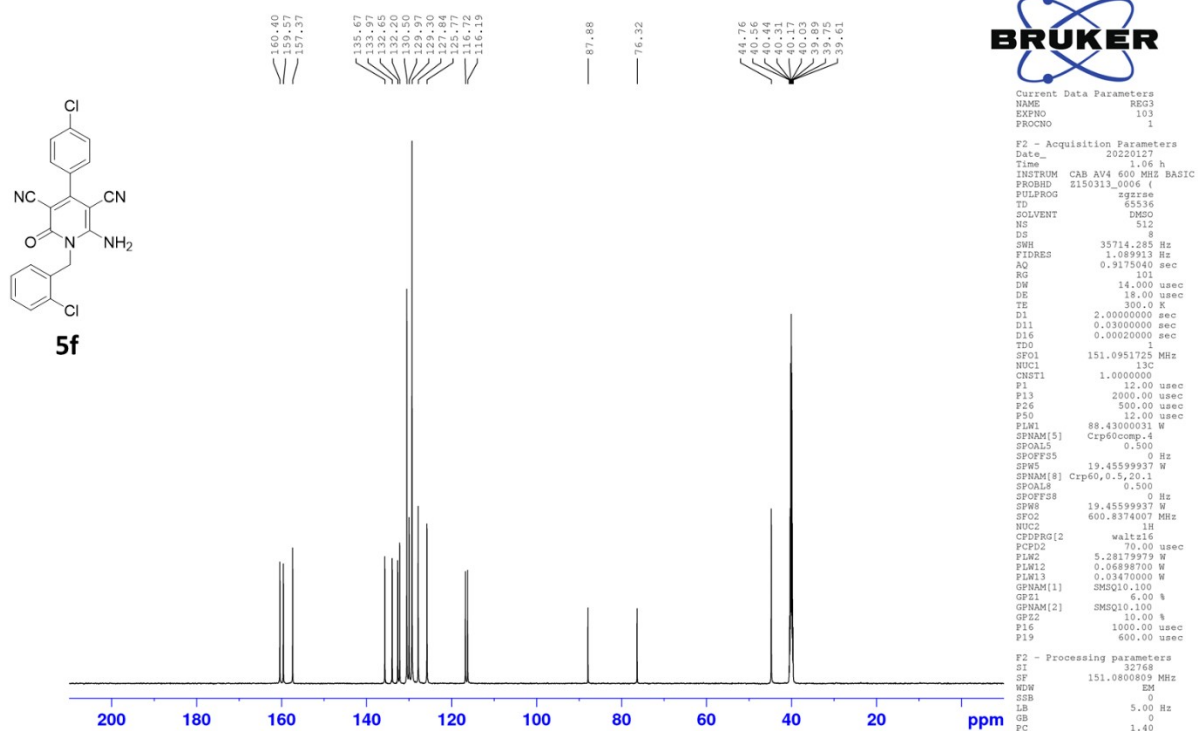


Figure S15. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5f** at 151 MHz in DMSO-d_6

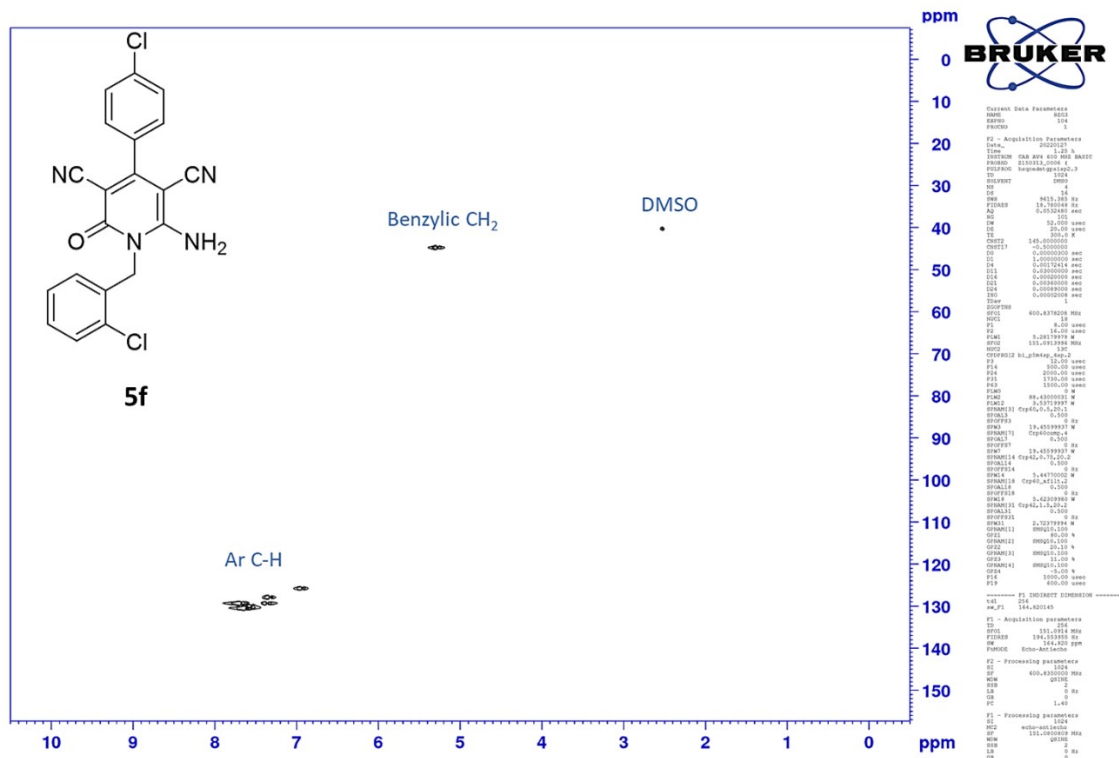
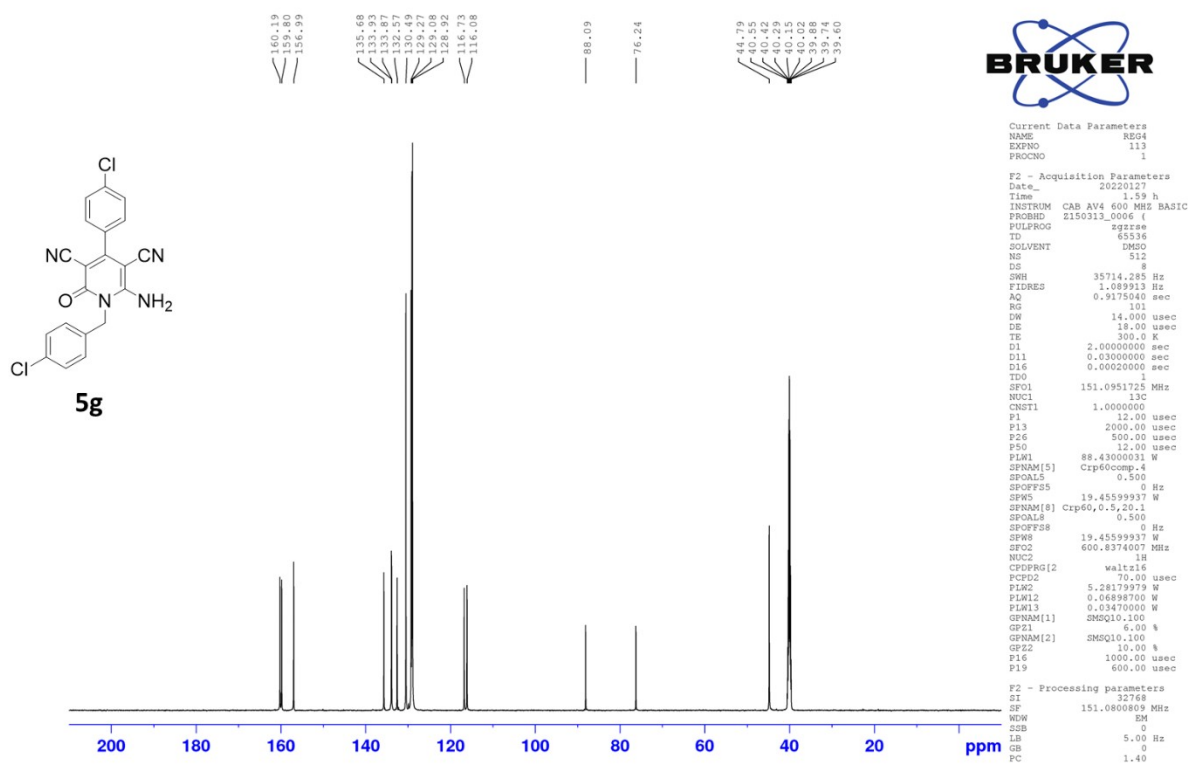
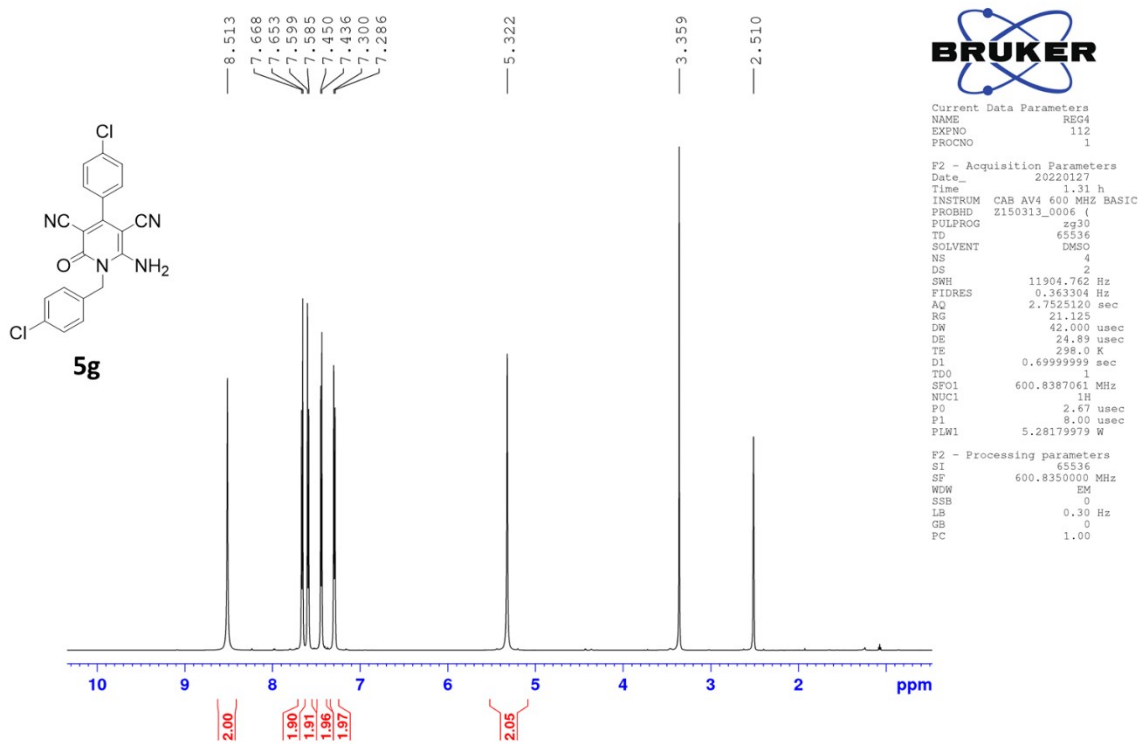


Figure S16. HSQC spectrum of compound **5f** in DMSO-d_6



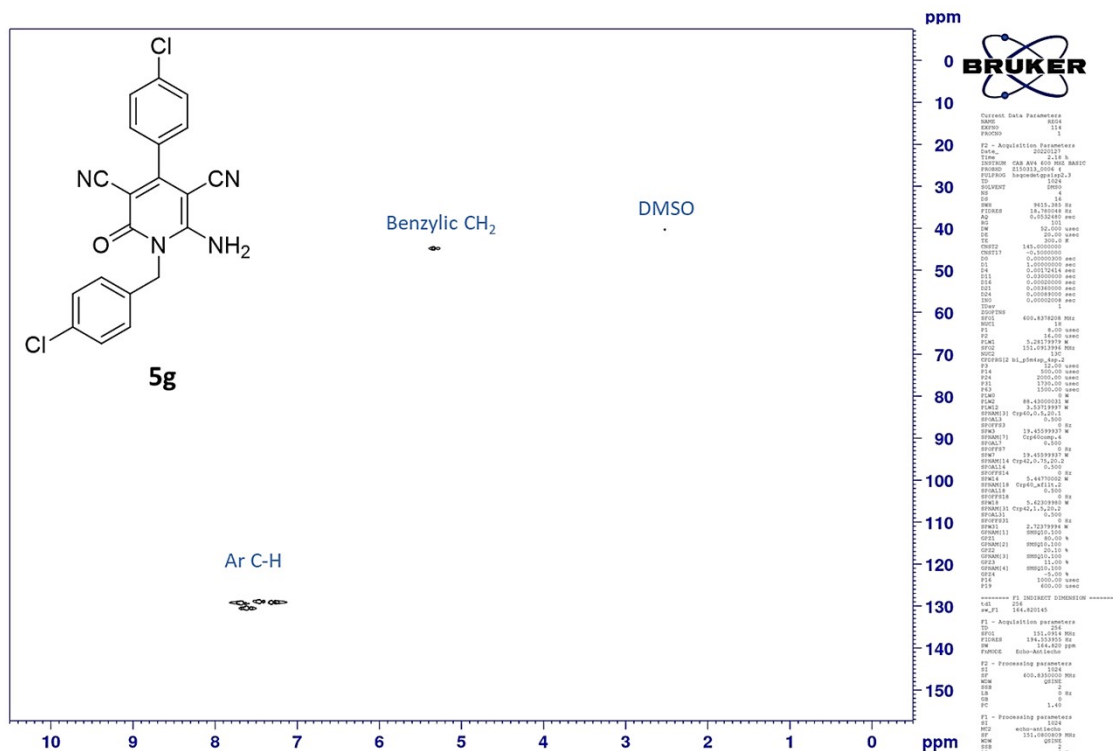


Figure S19. DEPT-135 spectrum of compound **5g** at 125 MHz in DMSO-d₆

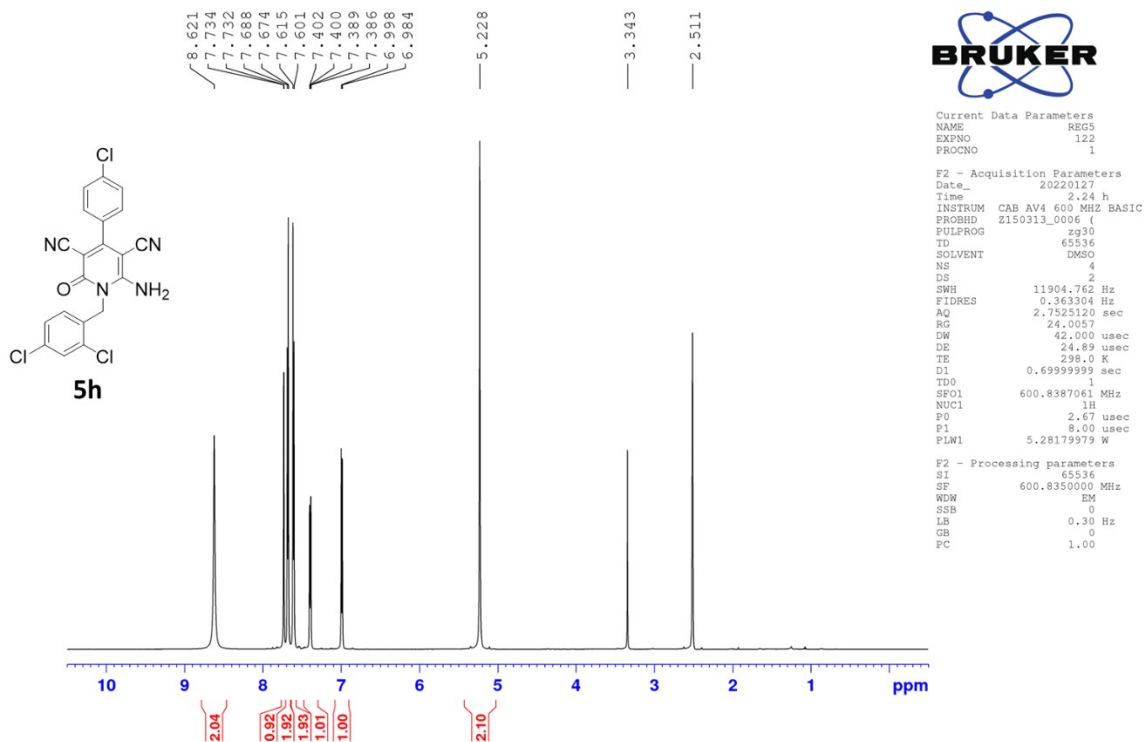


Figure S20. ¹H NMR spectrum of compound **5h** at 600 MHz in DMSO-d₆

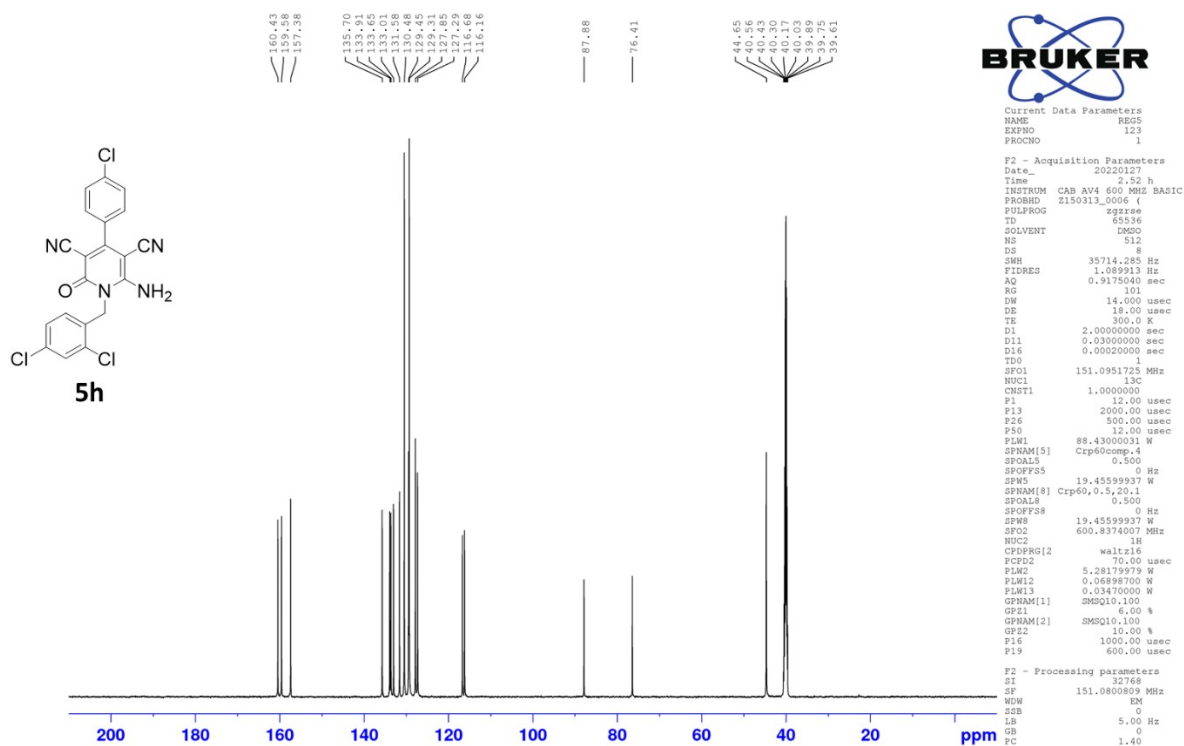


Figure S21. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5h** at 151 MHz in DMSO-d_6

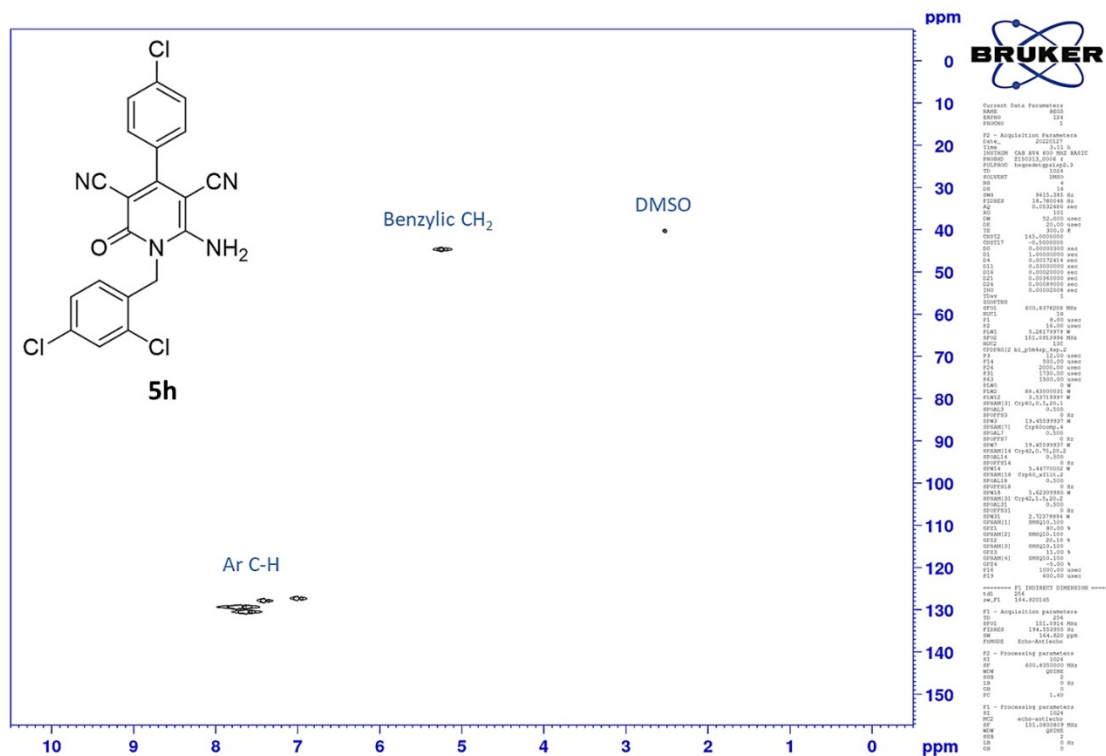


Figure S22. HSQC spectrum of compound **5h** in DMSO-d_6

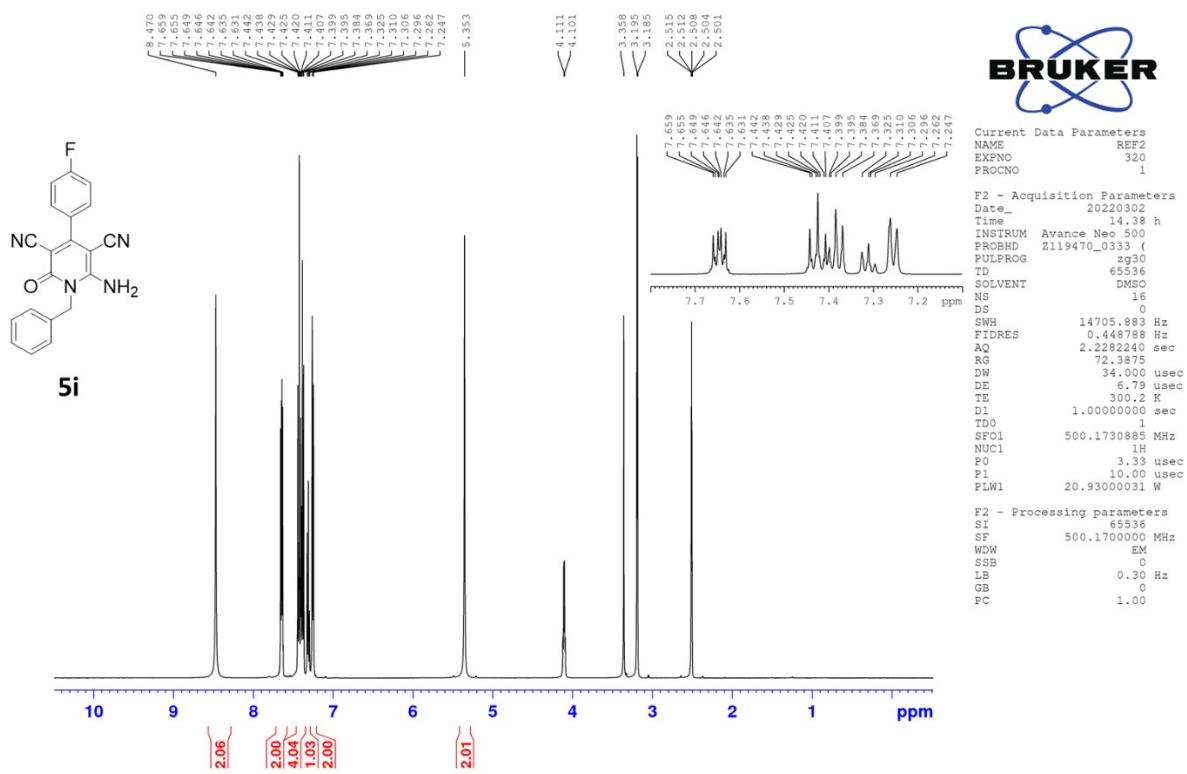


Figure S23. ^1H NMR spectrum of compound **5i** at 500 MHz in DMSO-d_6

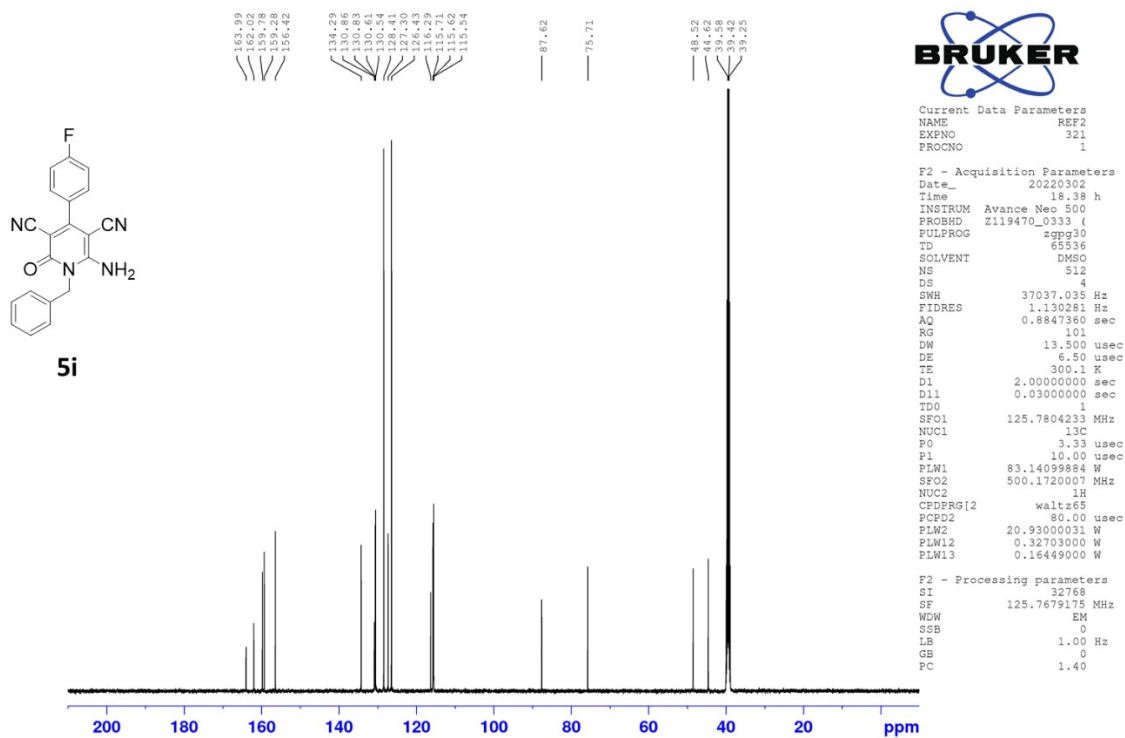


Figure S24. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5i** at 125 MHz in DMSO-d_6

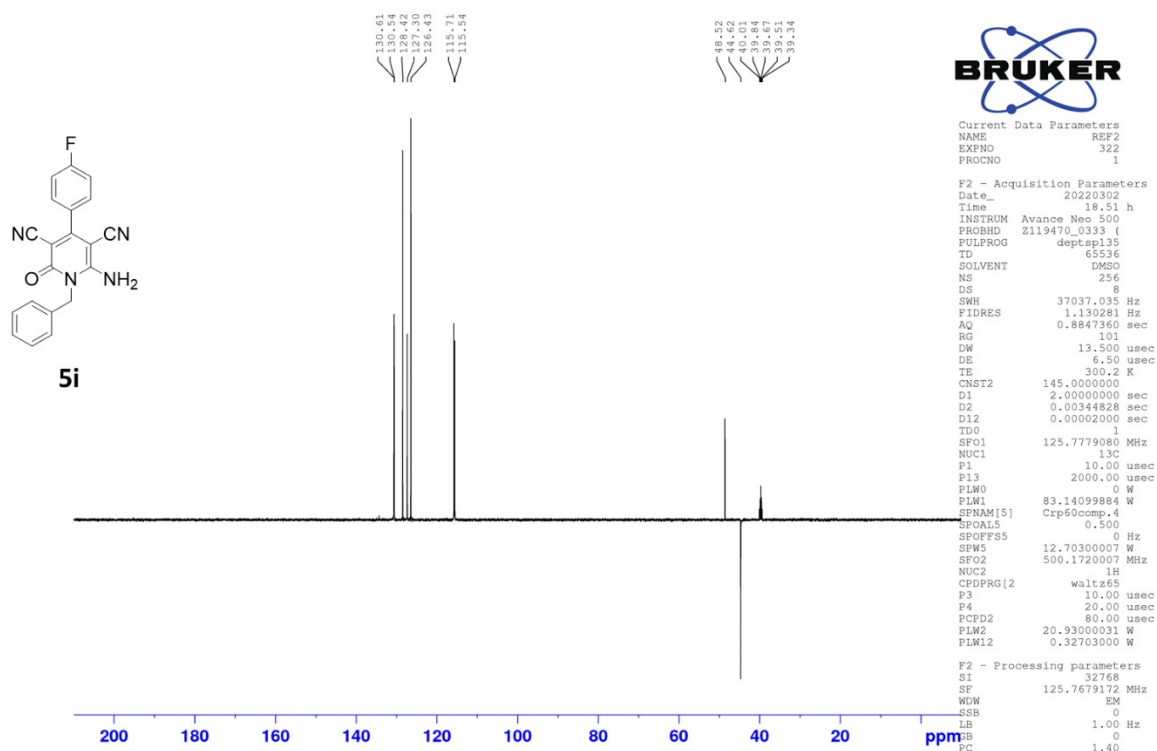


Figure S25. DEPT-135 spectrum of compound **5i** at 125 MHz in DMSO- d_6

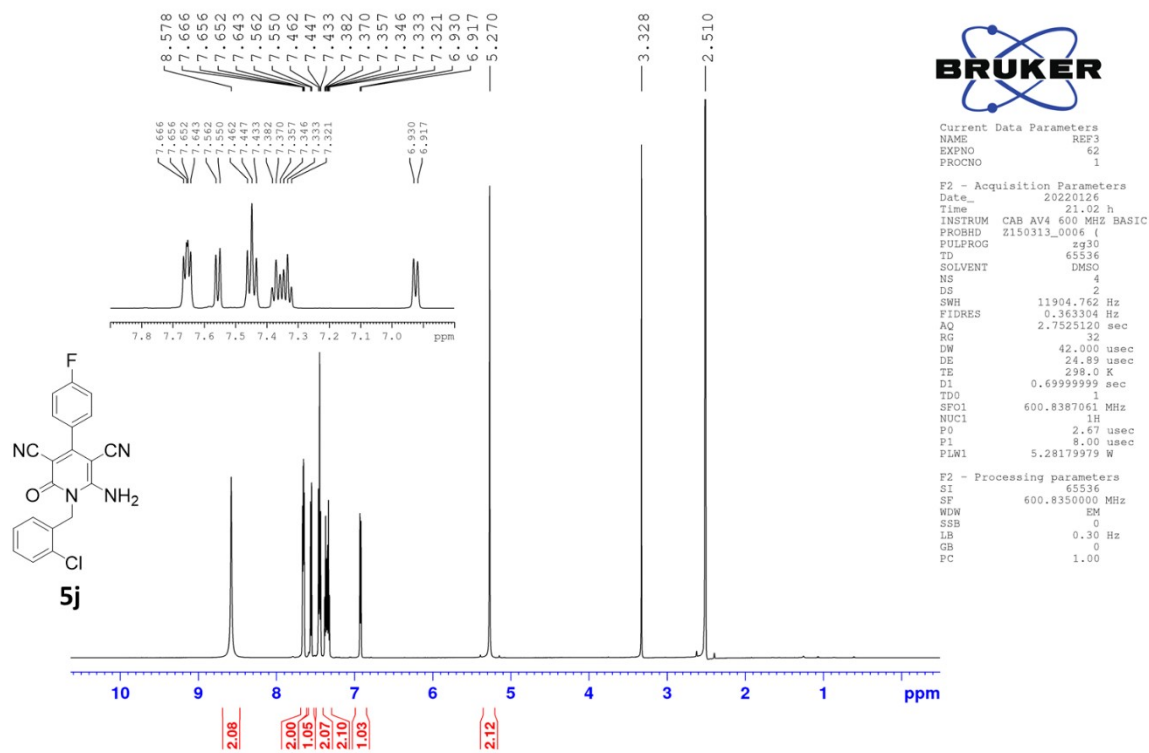


Figure S26. ^1H NMR spectrum of compound **5j** at 600 MHz in DMSO- d_6

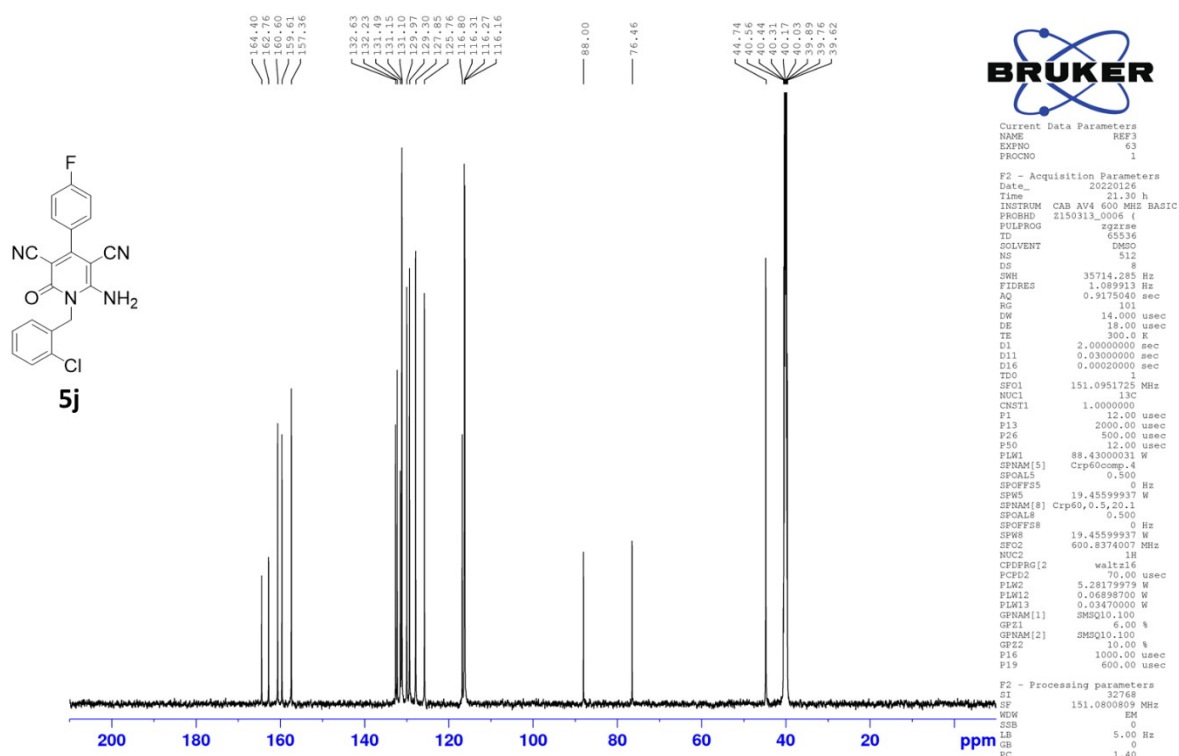


Figure S27. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5j** at 151 MHz in DMSO- d_6

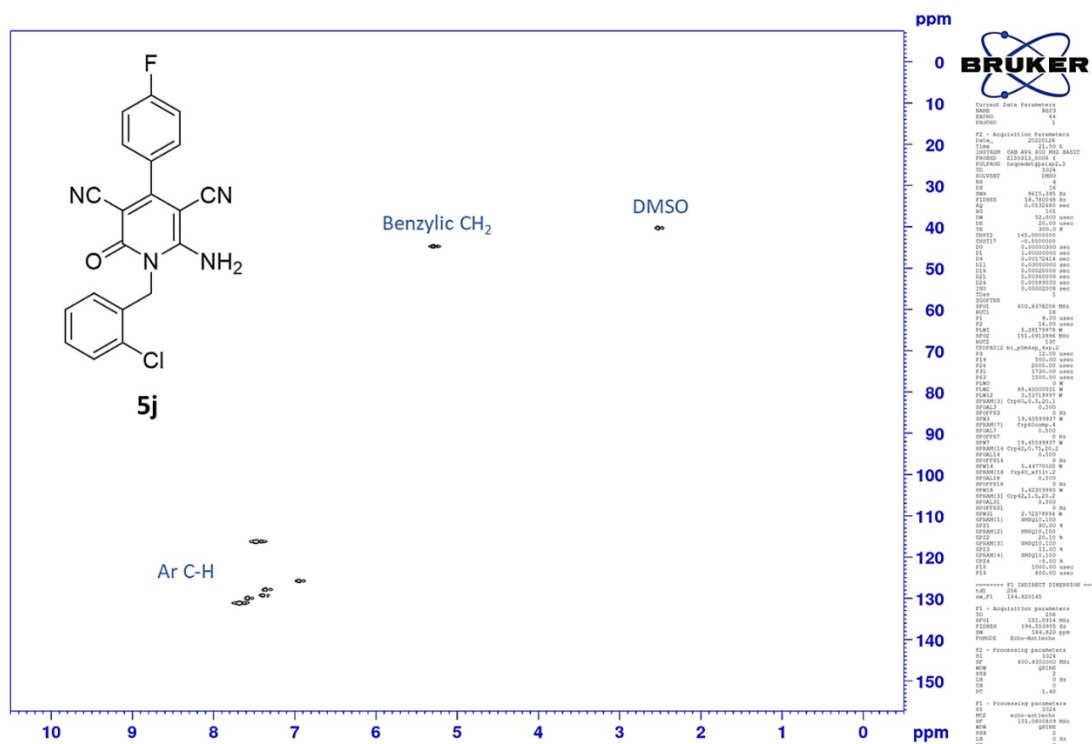


Figure S28. HSQC spectrum of compound **5j** in DMSO- d_6

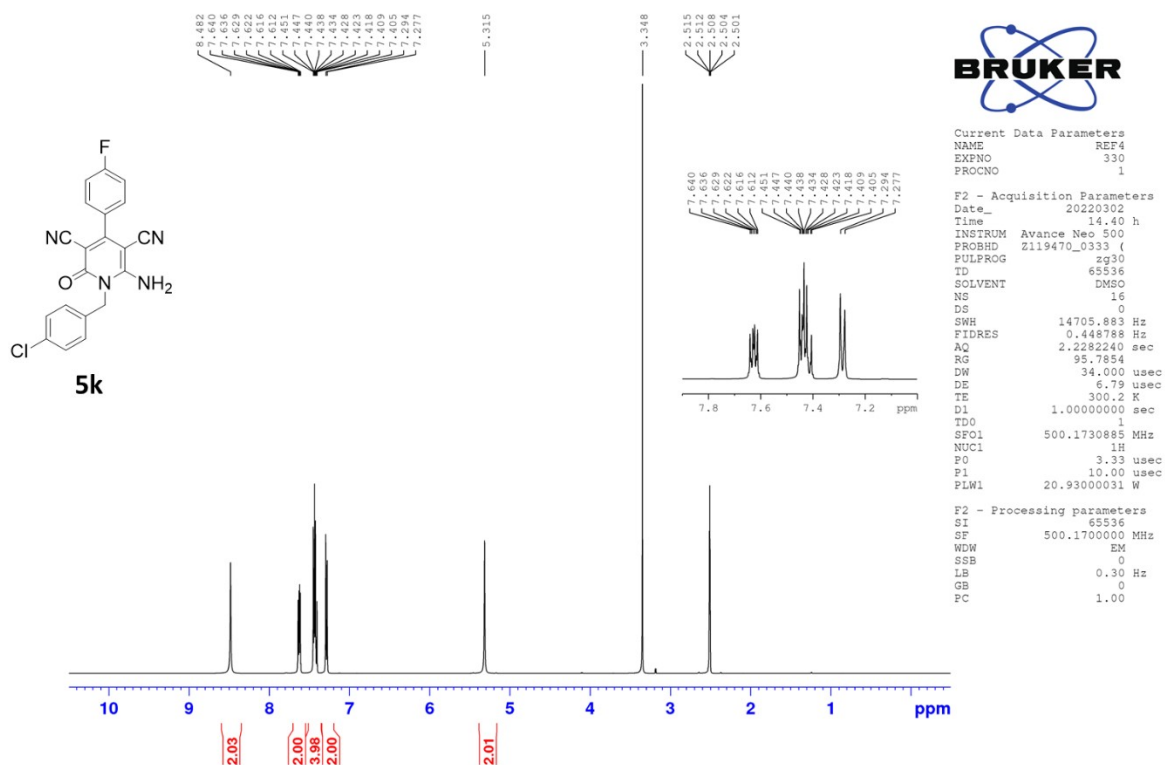


Figure S29. ^1H NMR spectrum of compound **5k** at 600 MHz in DMSO-d_6

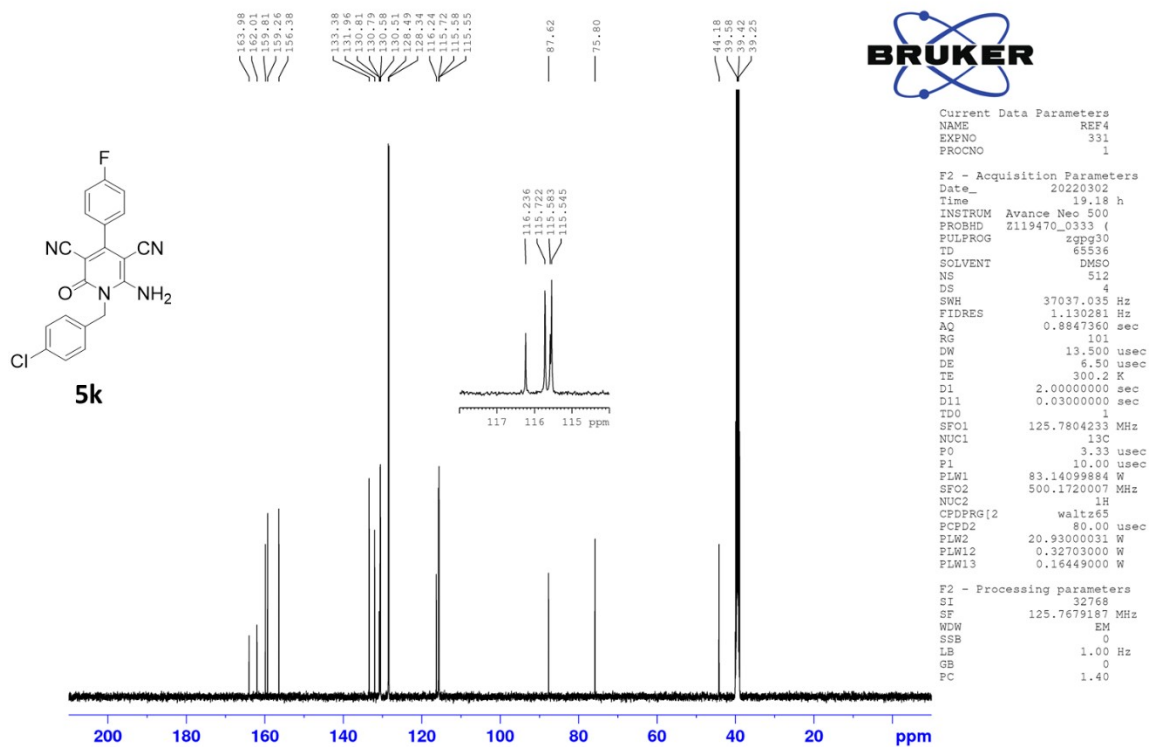


Figure S30. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5k** at 151 MHz in DMSO-d_6

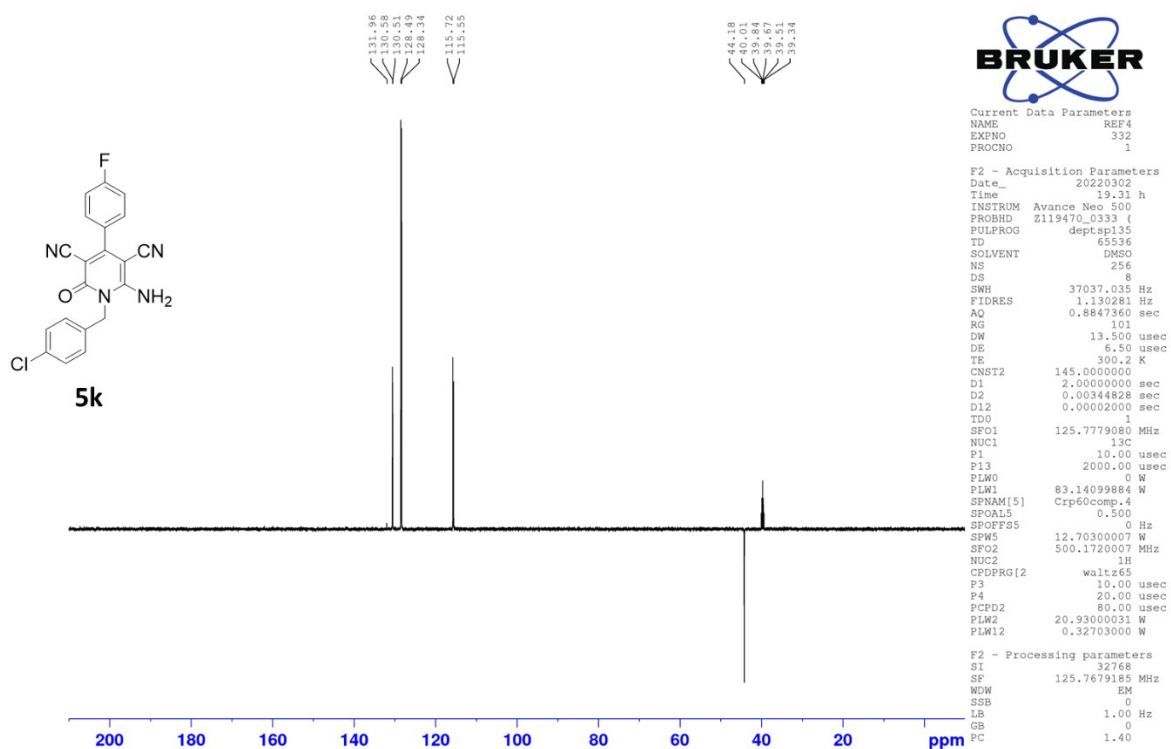


Figure S31. DEPT-135 spectrum of compound **5k** at 125 MHz in DMSO-d₆

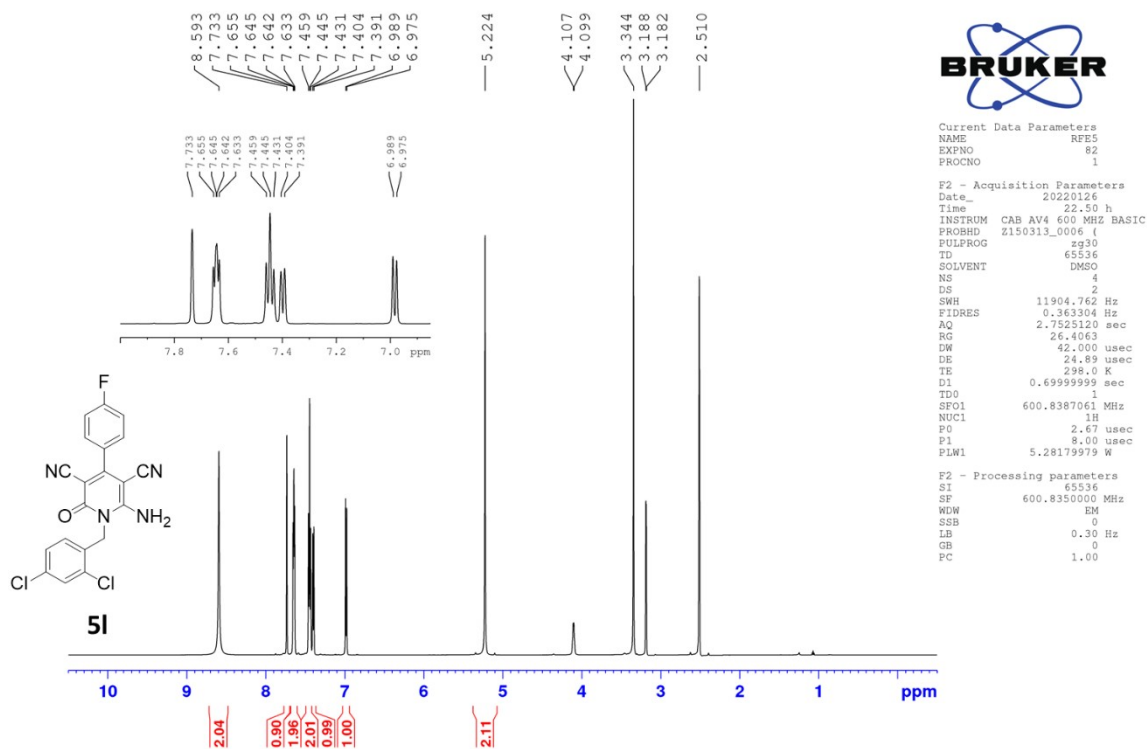


Figure S32. ¹H NMR spectrum of compound **5l** at 600 MHz in DMSO-d₆

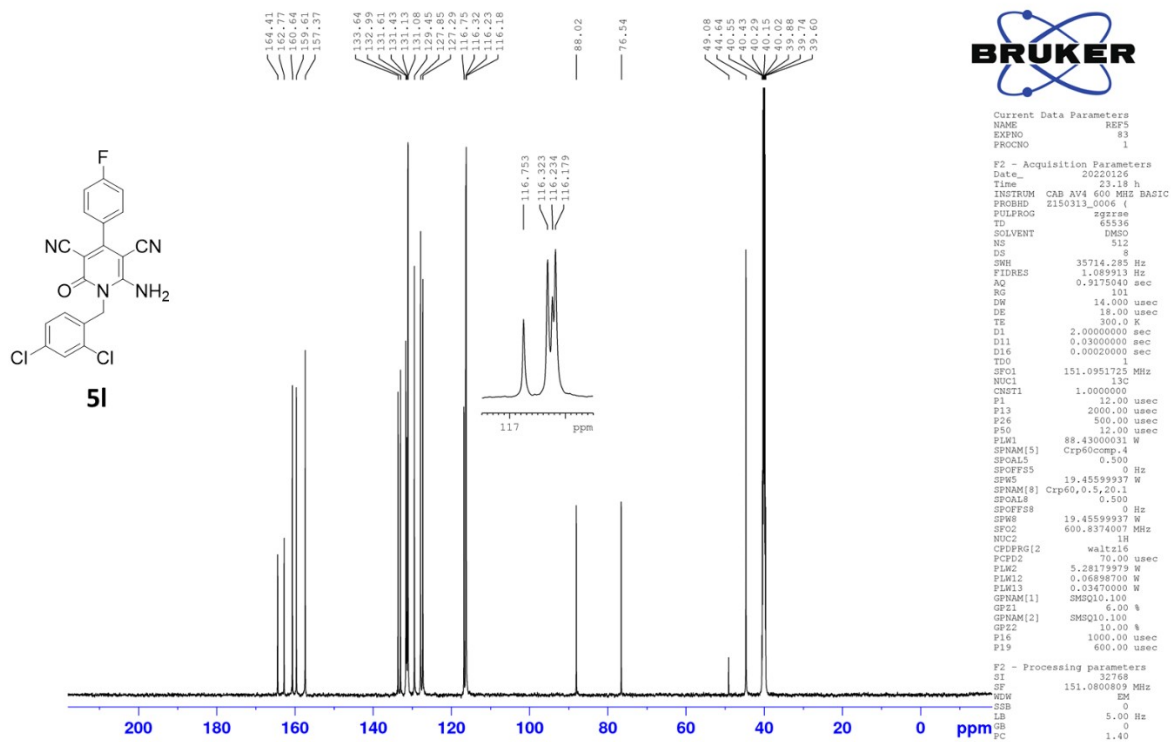


Figure S33. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound 5I at 151 MHz in DMSO- d_6

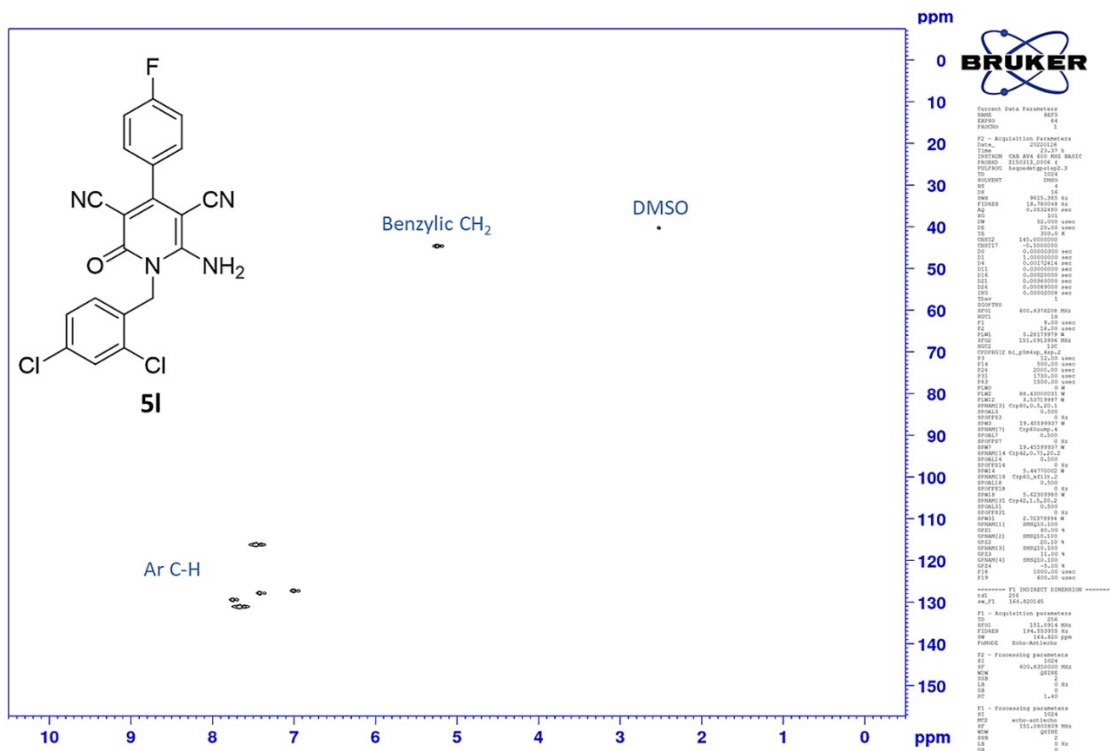


Figure S34. HSQC spectrum of compound 5I in DMSO- d_6

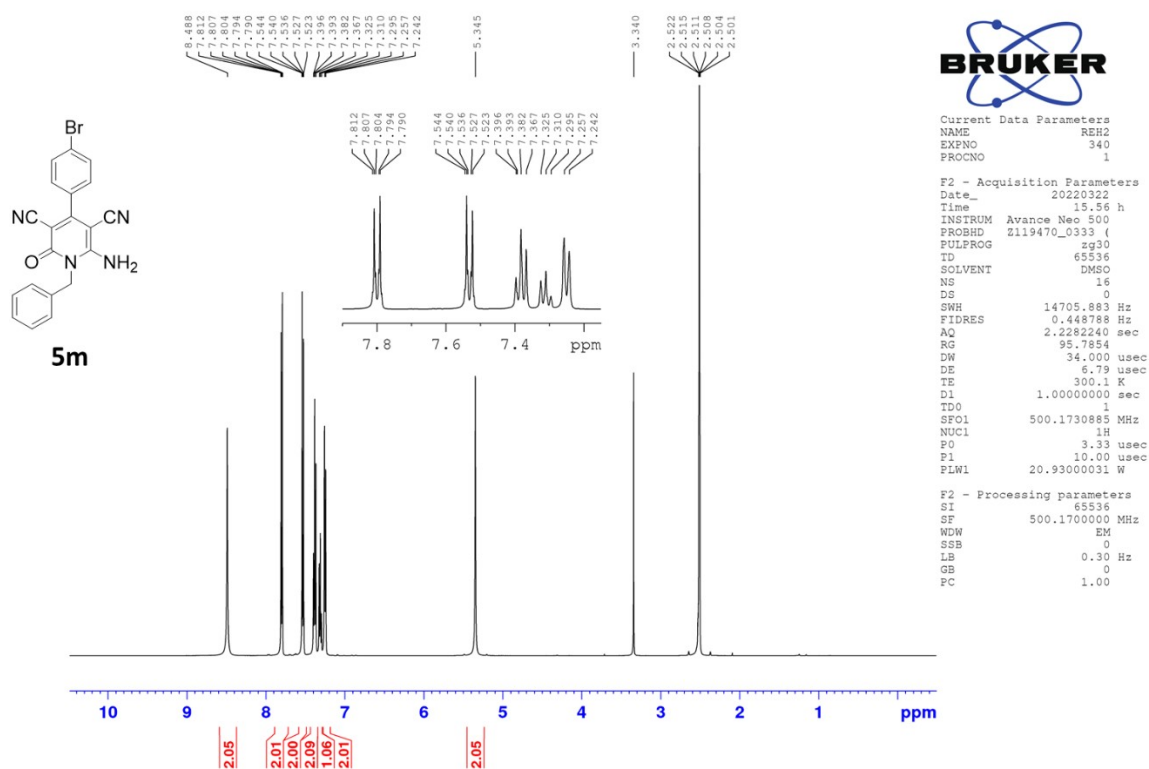


Figure S35. ^1H NMR spectrum of compound **5m** at 500 MHz in DMSO-d_6

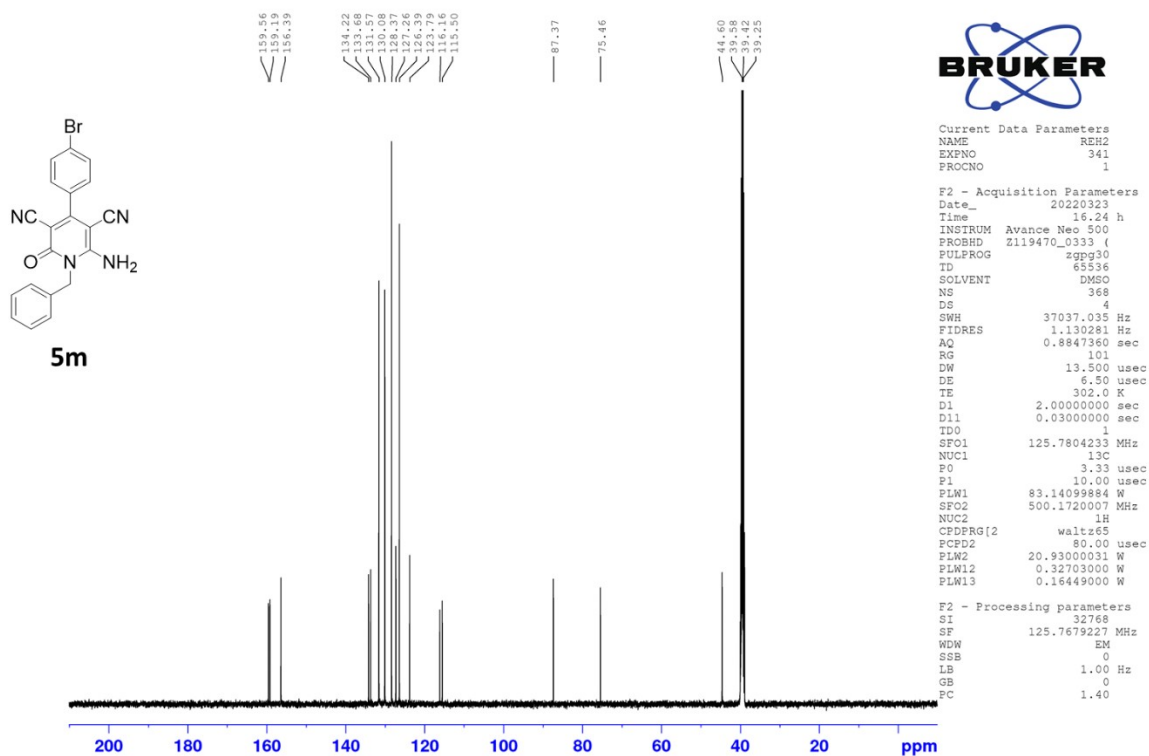


Figure S36. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5m** at 151 MHz in DMSO-d_6

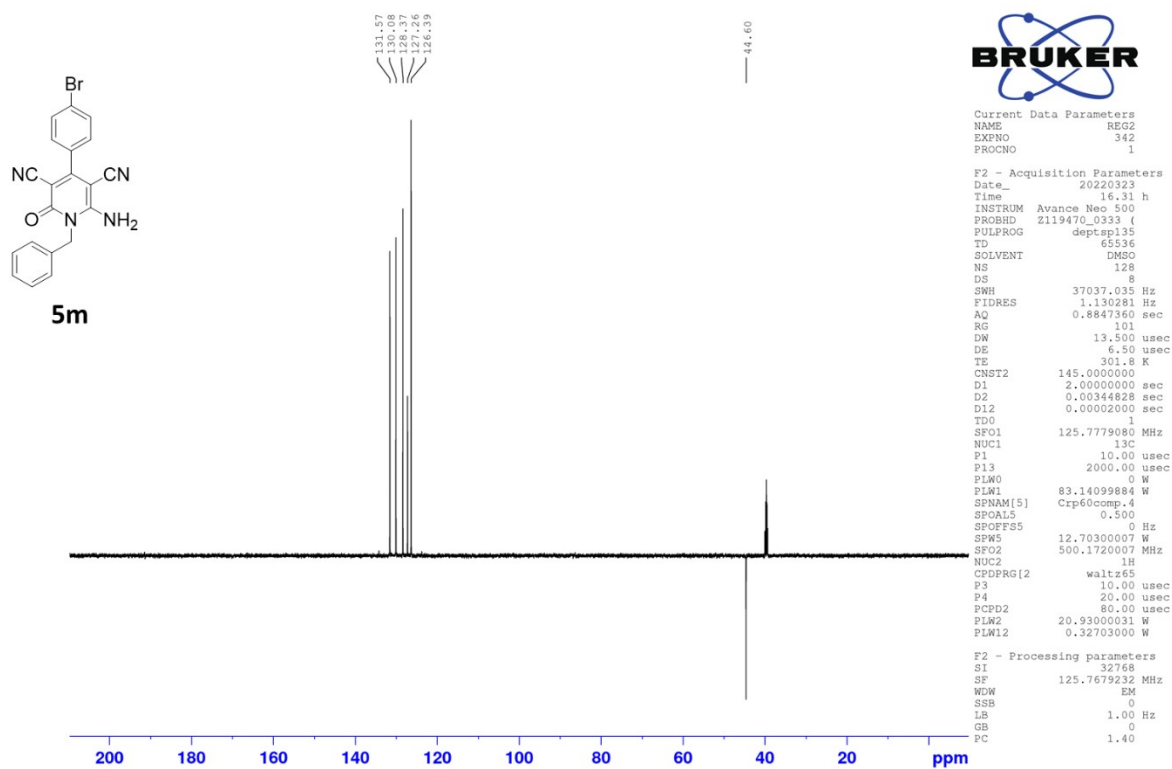


Figure S37. DEPT-135 spectrum of compound **5m** at 125 MHz in DMSO- d_6

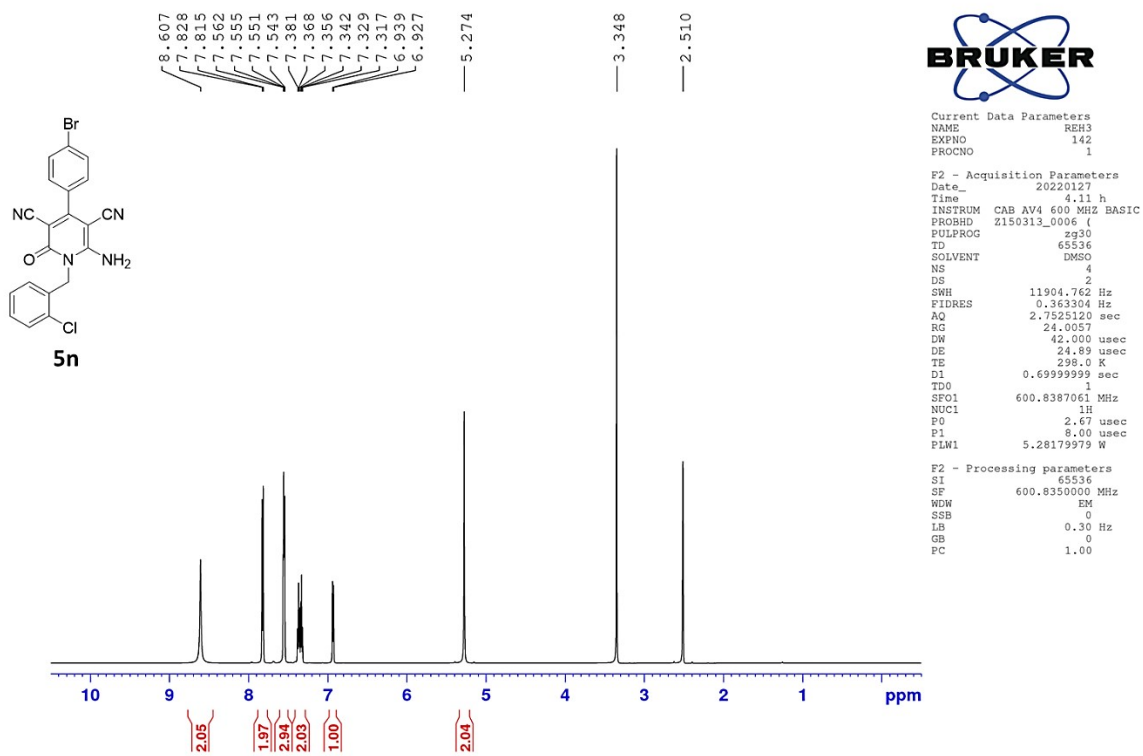


Figure S38. ^1H NMR spectrum of compound **5n** at 600 MHz in DMSO- d_6

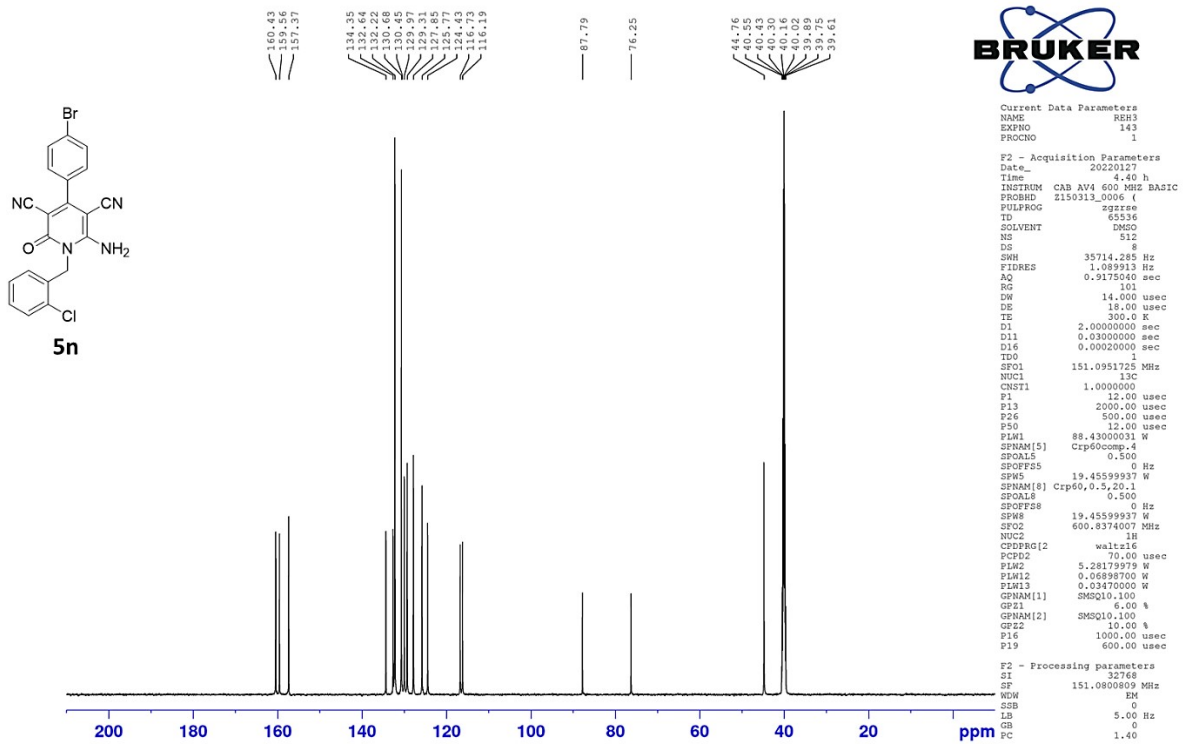


Figure S39. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5n** at 151 MHz in DMSO-d_6

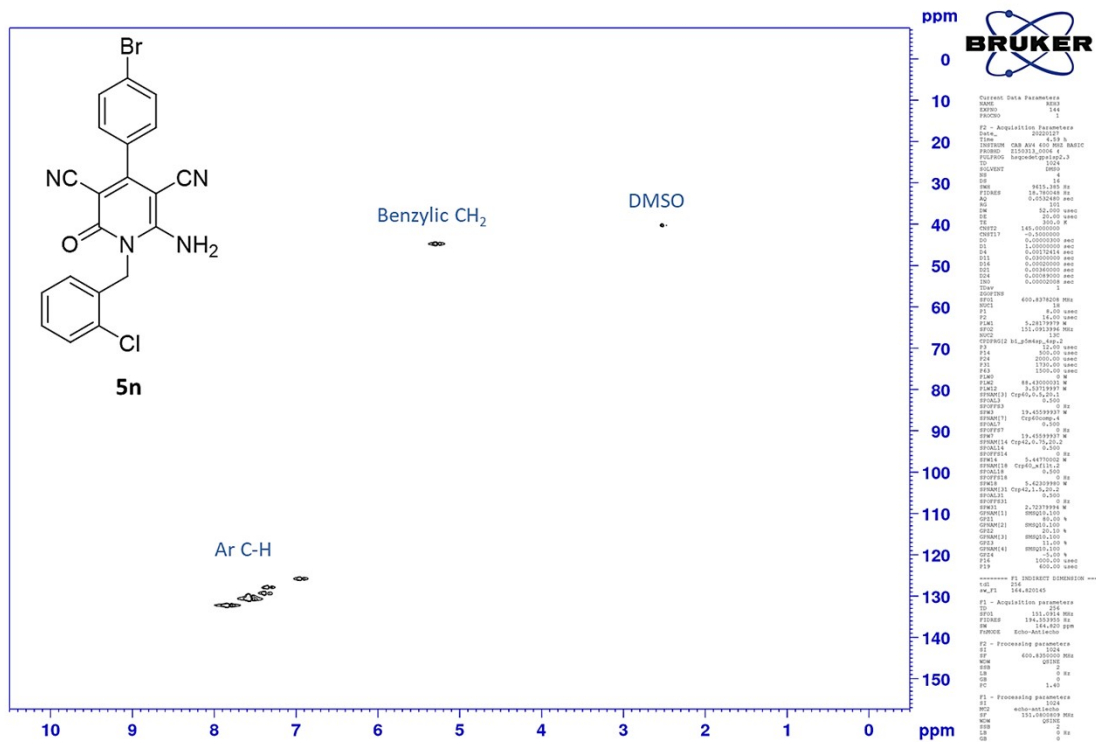


Figure S40. HSQC spectrum of compound **5n** in DMSO-d_6

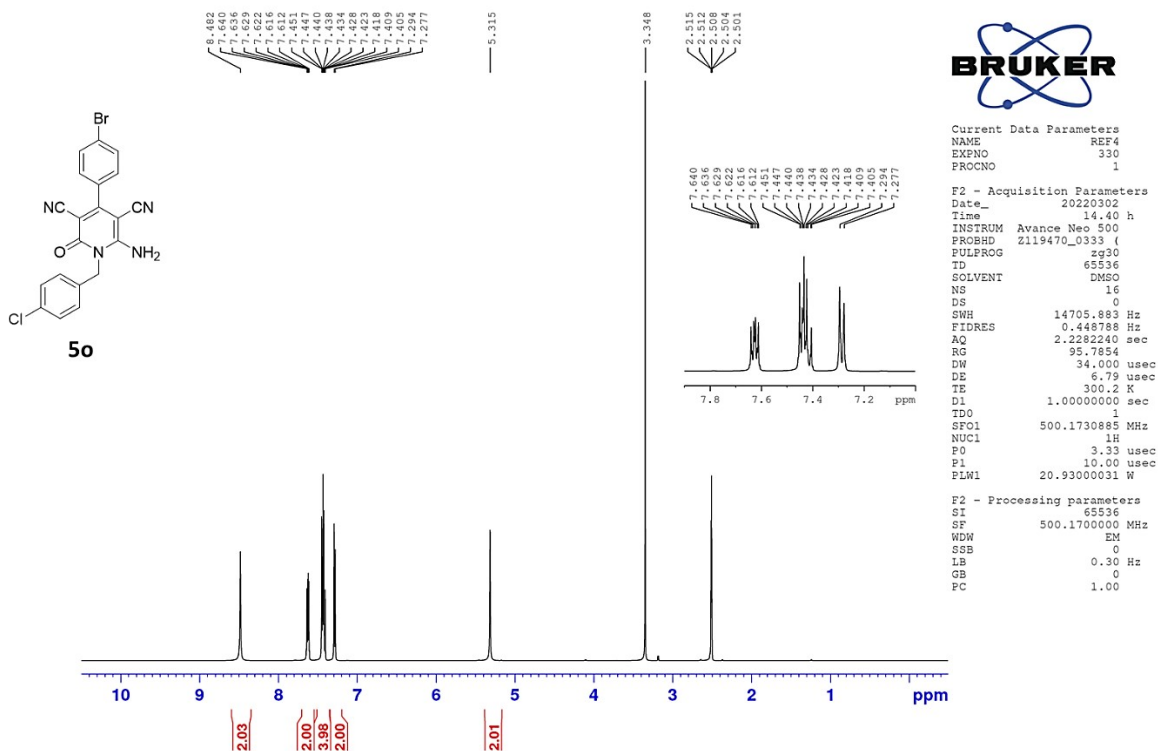


Figure S41. ^1H NMR spectrum of compound **5o** at 600 MHz in DMSO-d_6

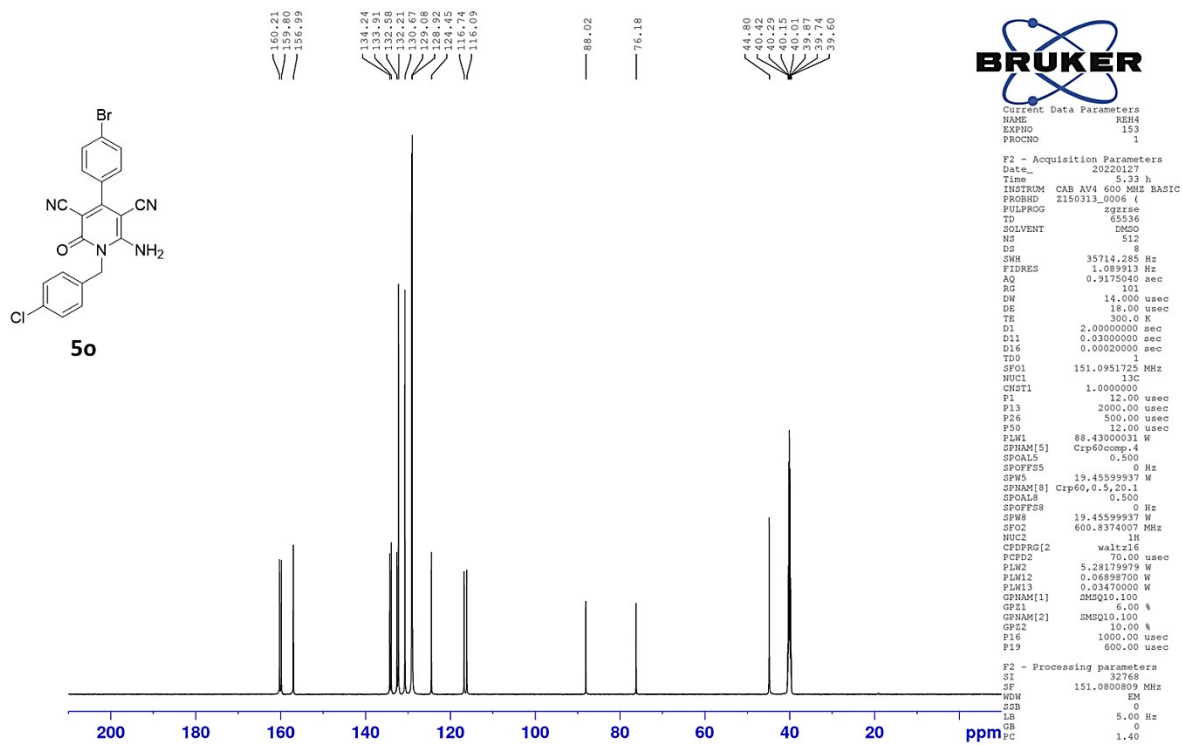


Figure S42. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5o** at 151 MHz in DMSO-d_6

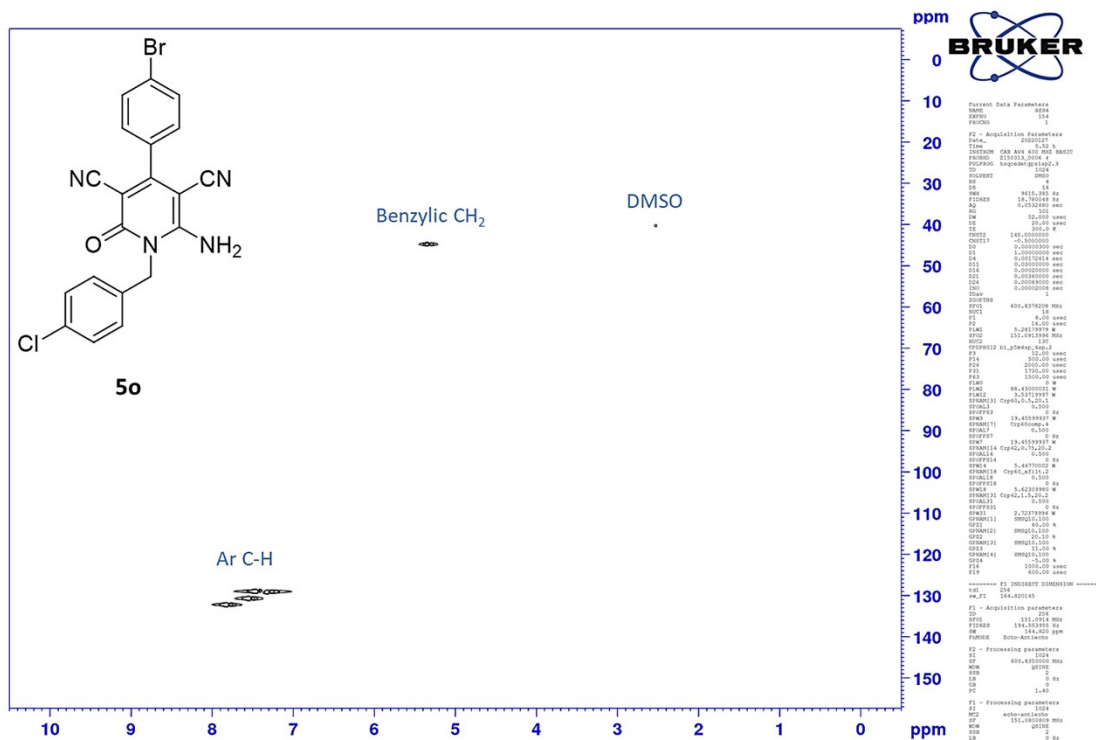


Figure S43. HSQC spectrum of compound **5o** in DMSO-d₆

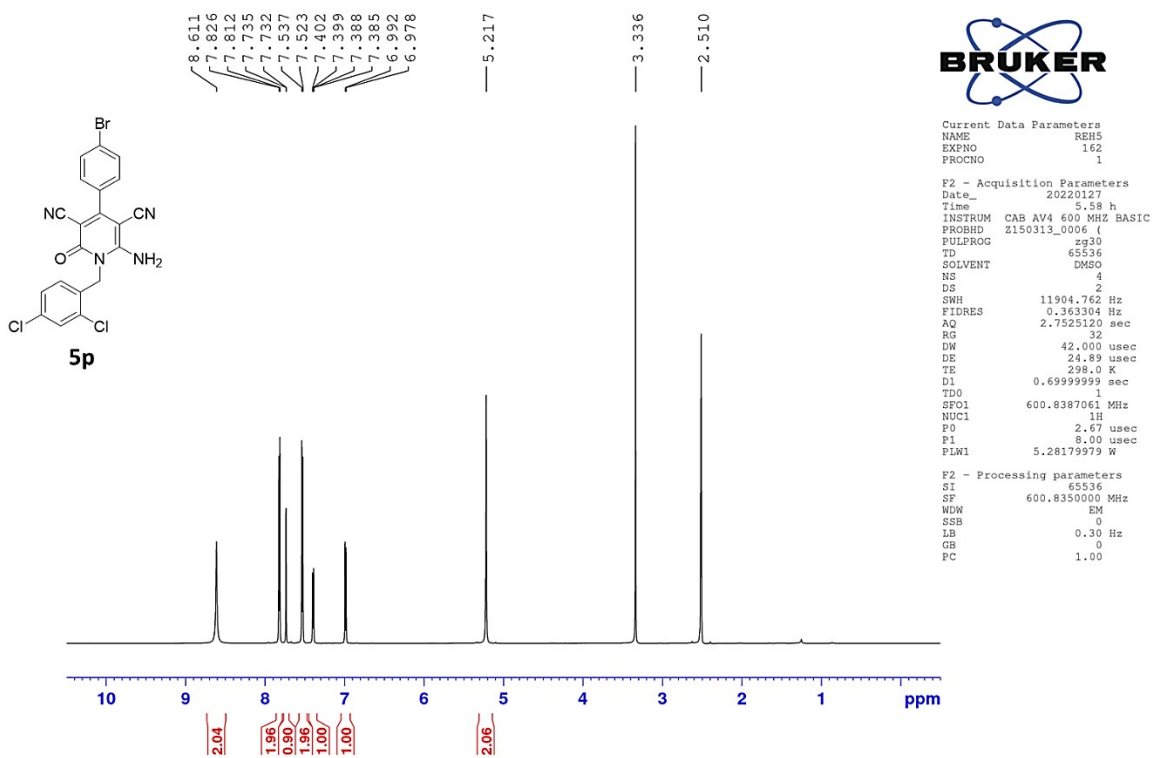


Figure S44. ¹H NMR spectrum of compound **5p** at 600 MHz in DMSO-d₆

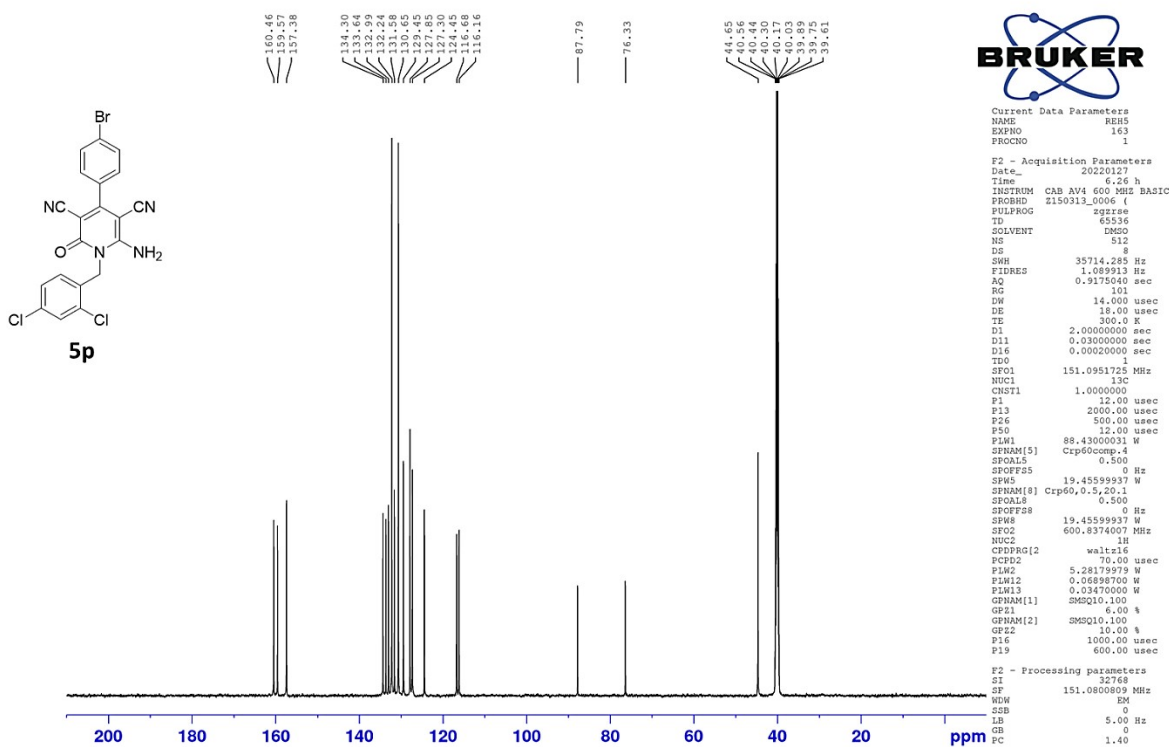


Figure S45. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **5p** at 151 MHz in DMSO-d_6

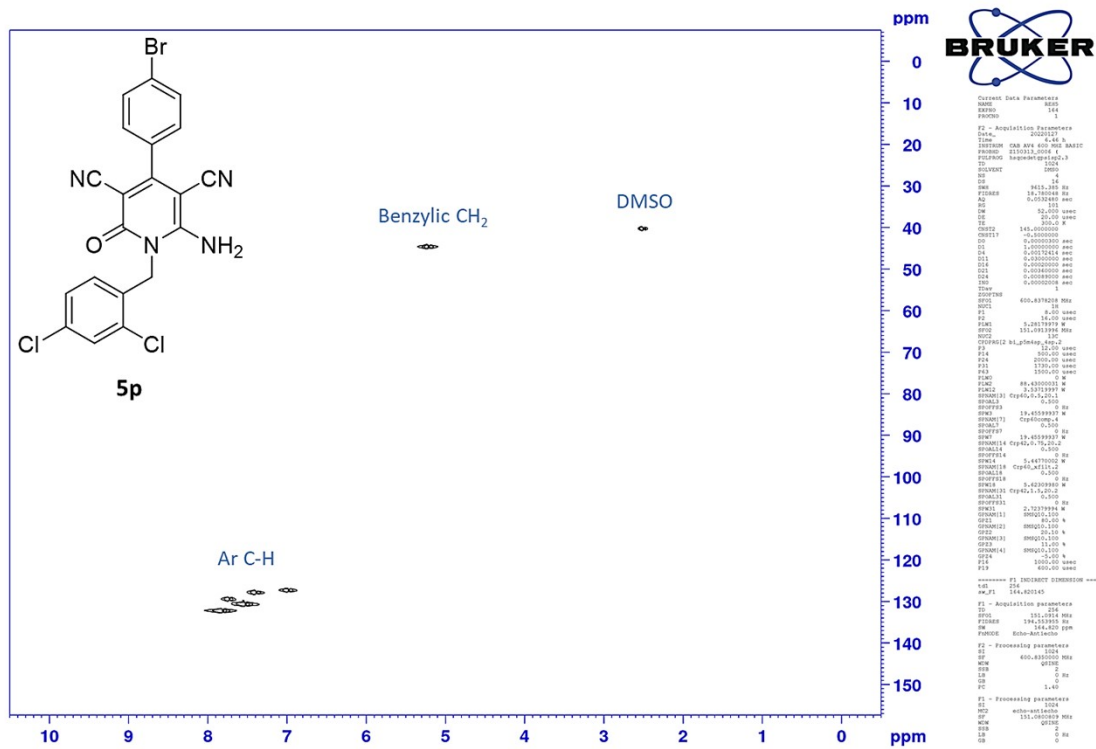


Figure S46. HSQC spectrum of compound **5p** in DMSO-d_6

2. Copies of HRMS of 5(a-p)

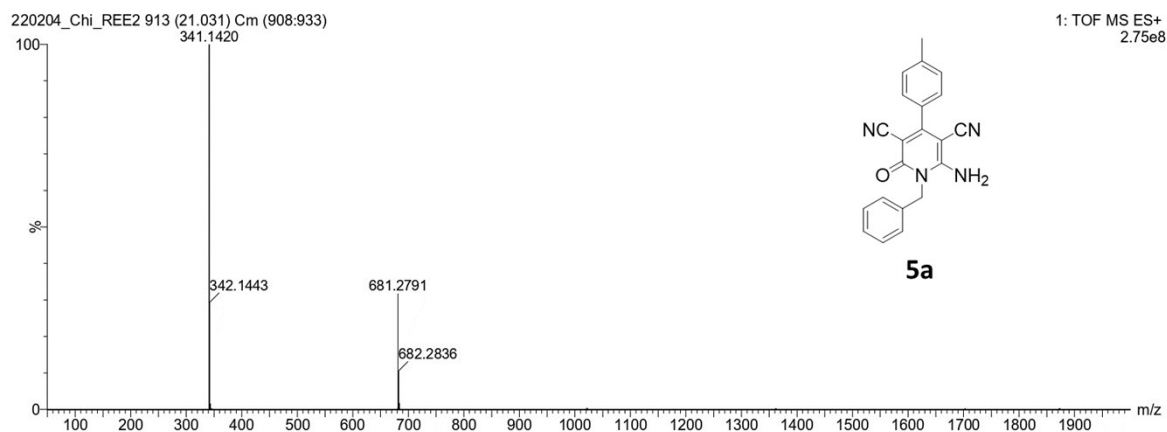


Figure S47. HRMS of compound 5a.

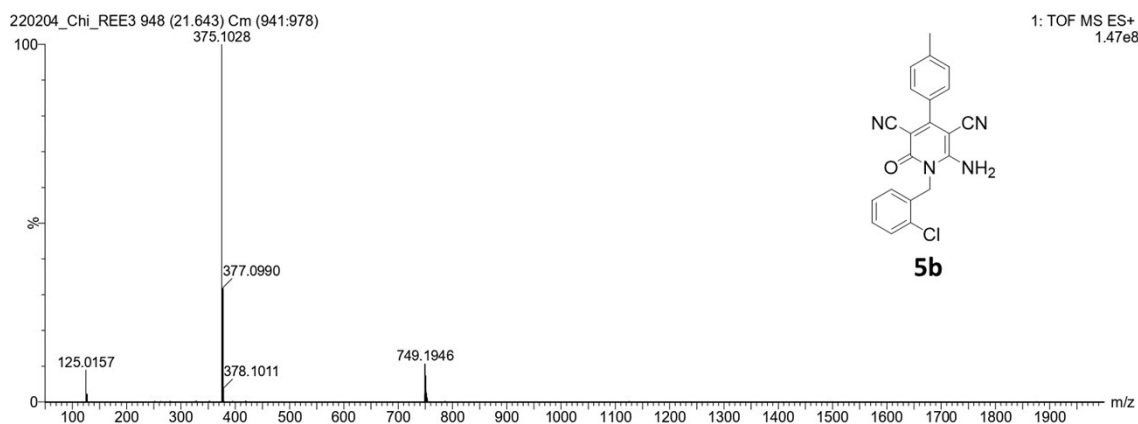


Figure S48. HRMS of compound 5b.

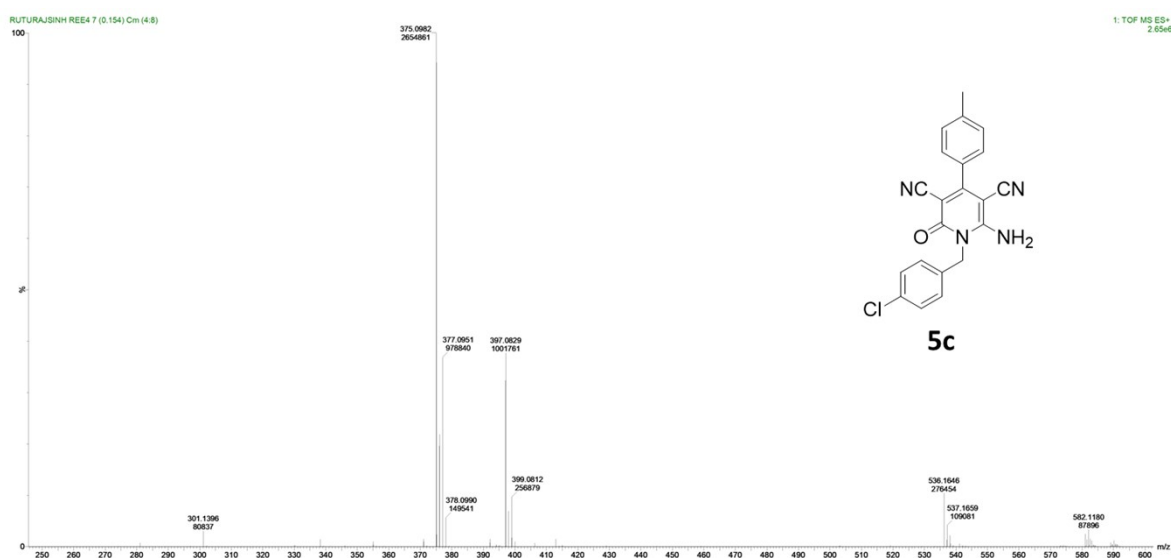


Figure S49. HRMS of compound 5c.

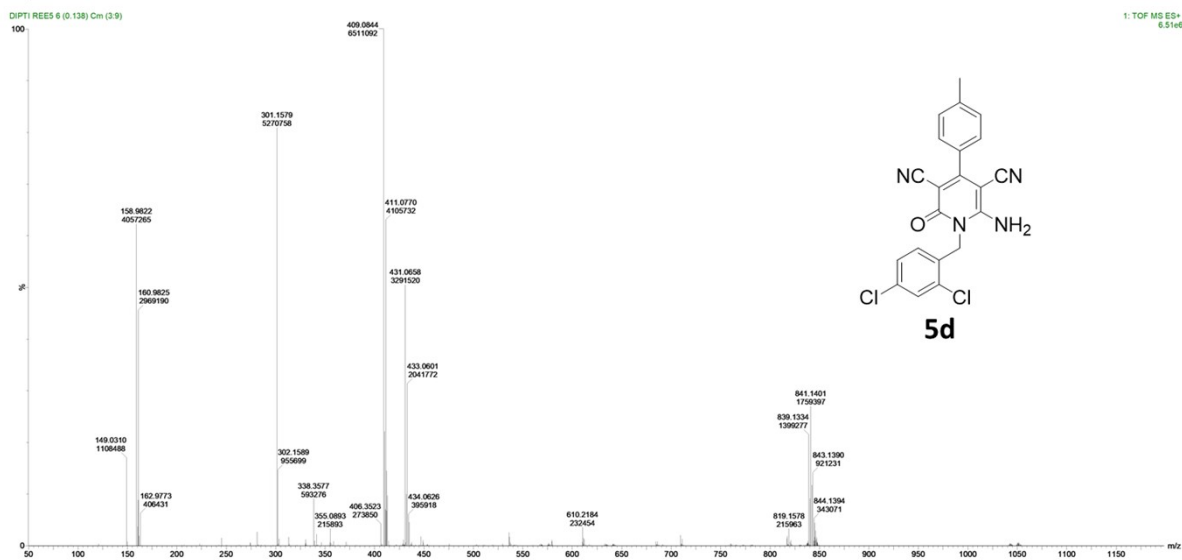


Figure S50. HRMS of compound **5d**.

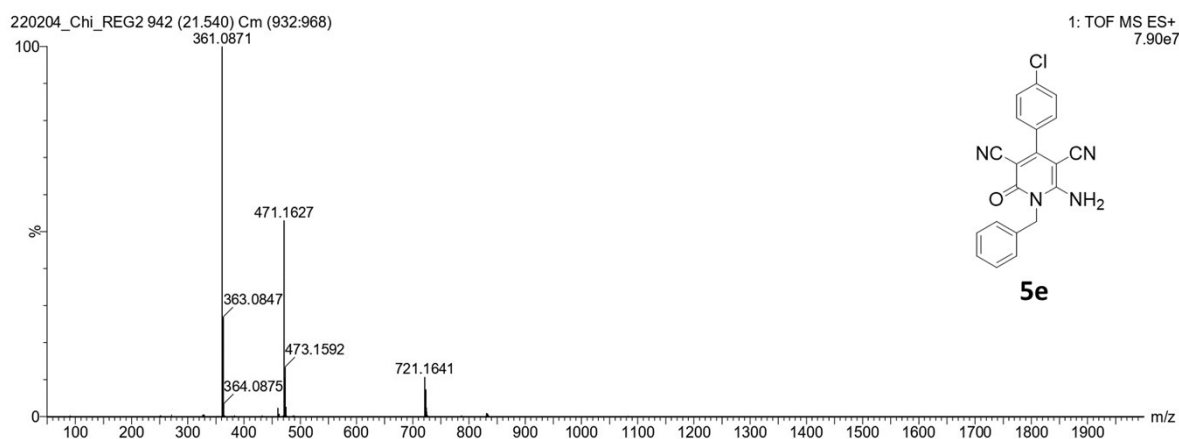


Figure S51. HRMS of compound **5e**.

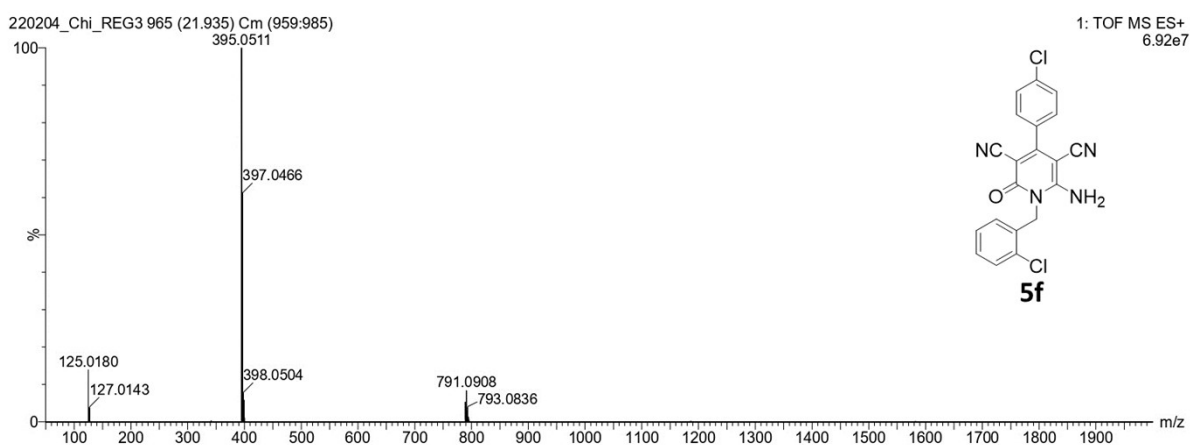


Figure S52. HRMS of compound **5f**.

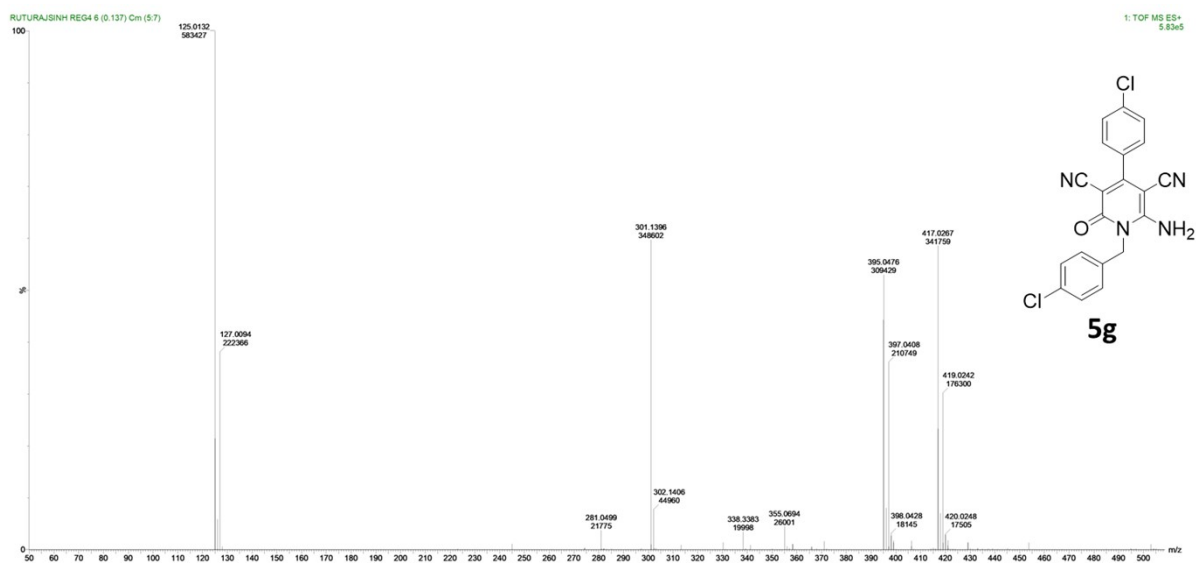


Figure S53. HRMS of compound 5g.

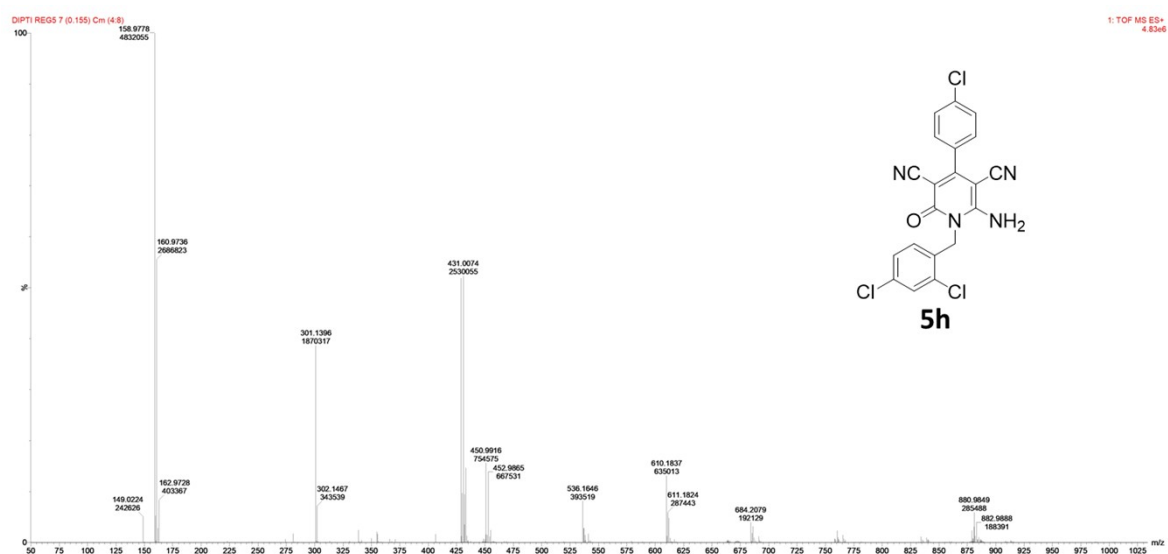


Figure S54. HRMS of compound 5h.

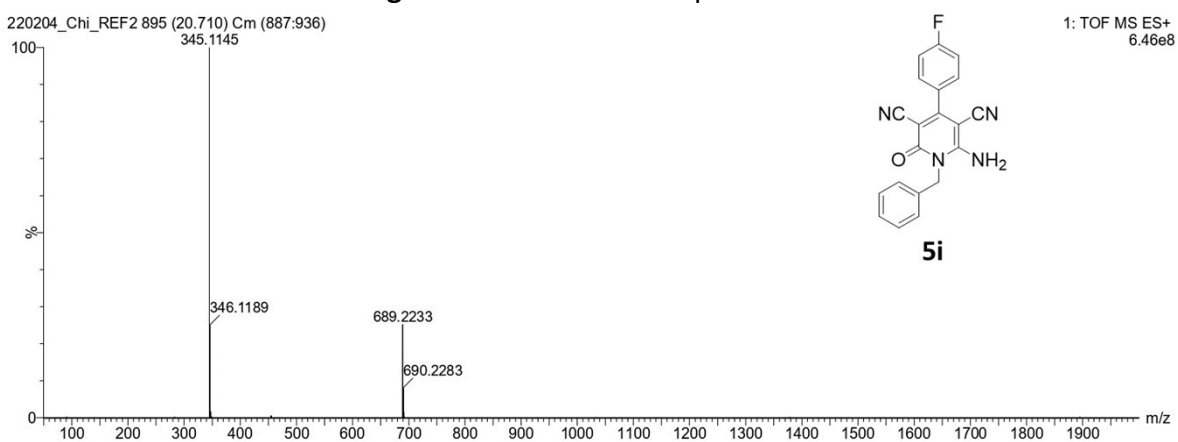


Figure S55. HRMS of compound 5i.

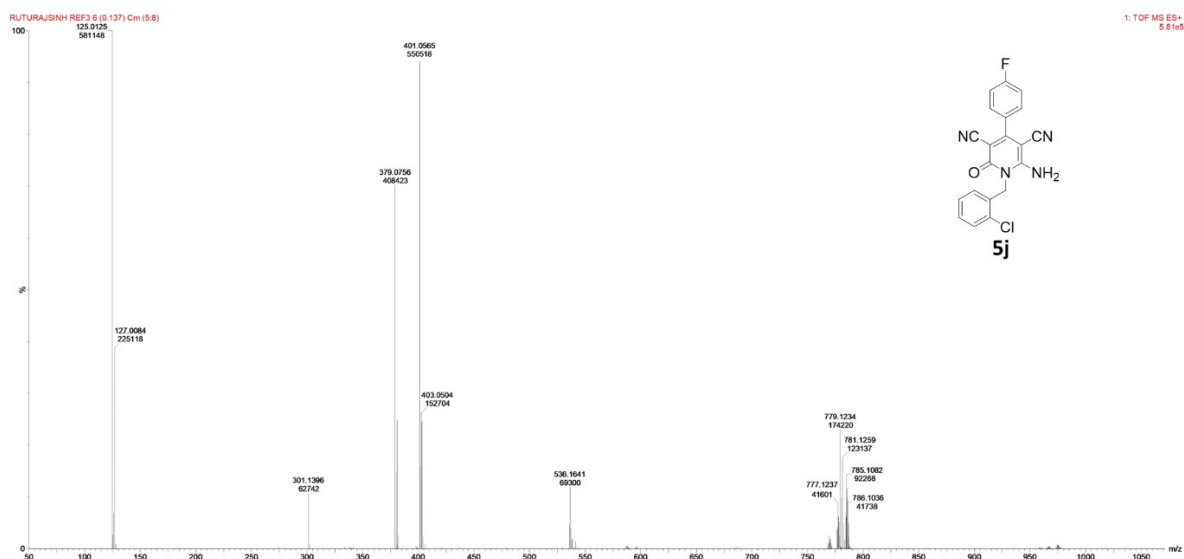


Figure S56. HRMS of compound 5j.

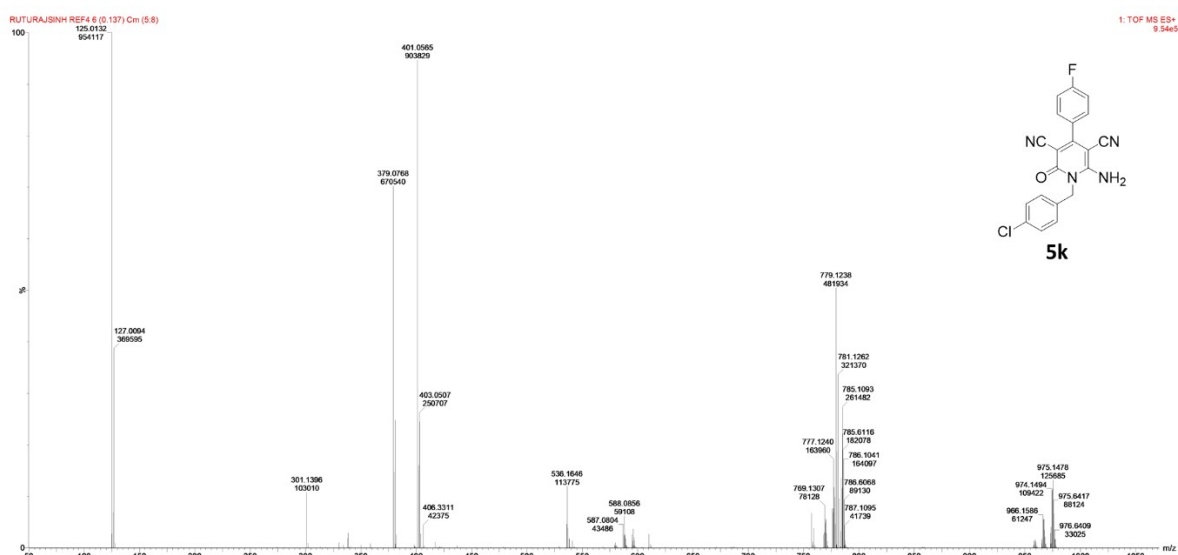


Figure S57. HRMS of compound 5k.

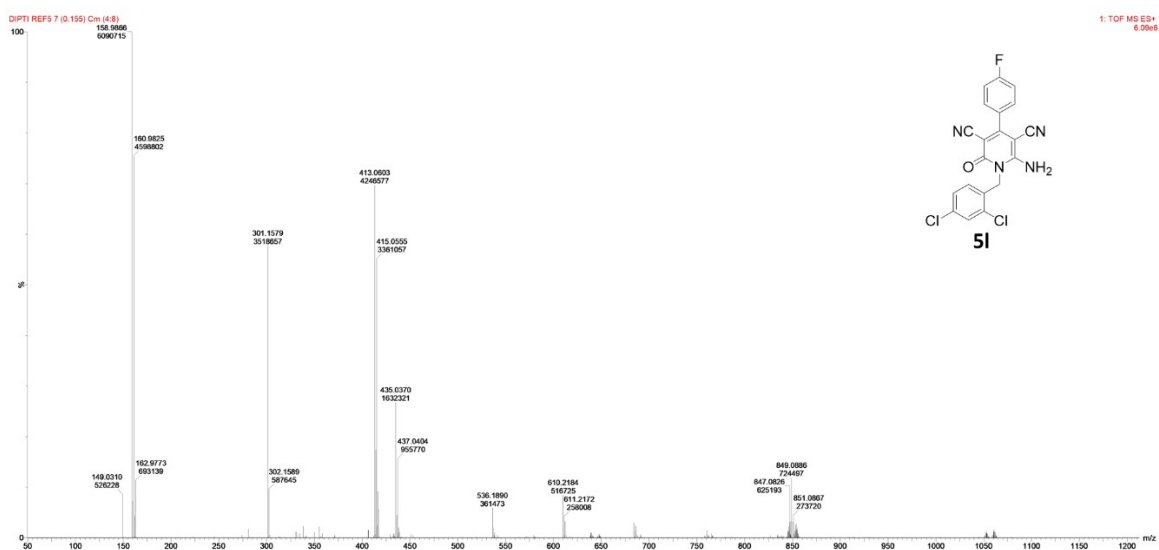


Figure S58. HRMS of compound 5l.

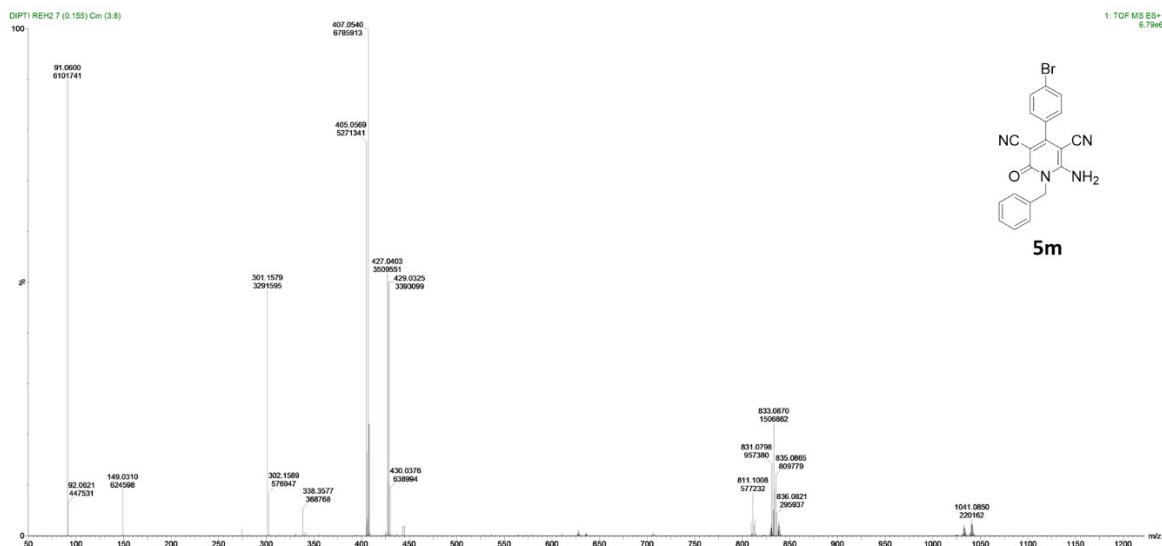


Figure S59. HRMS of compound 5m.

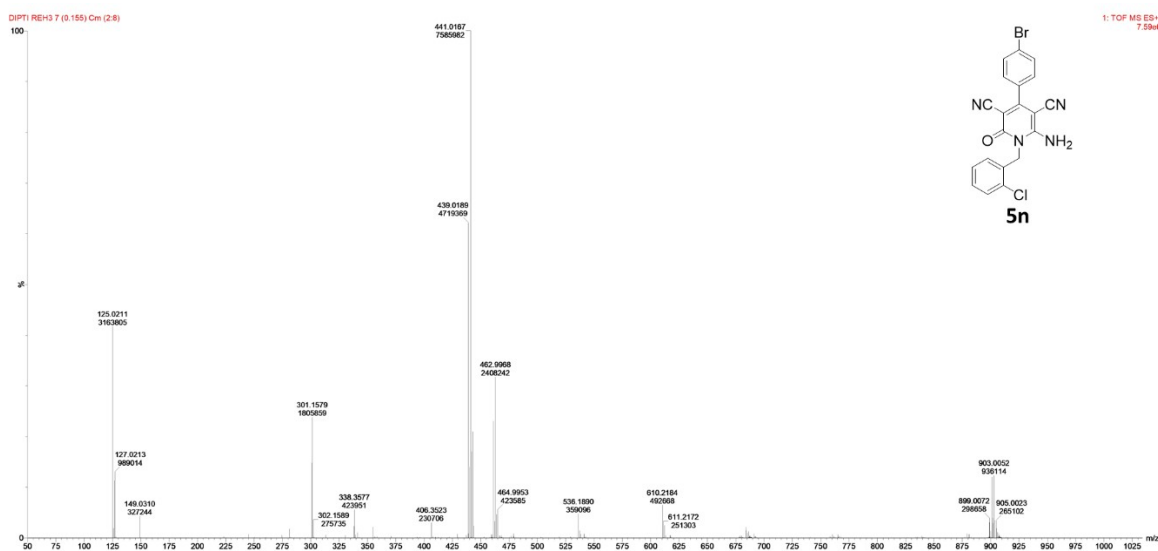


Figure S60. HRMS of compound 5n.

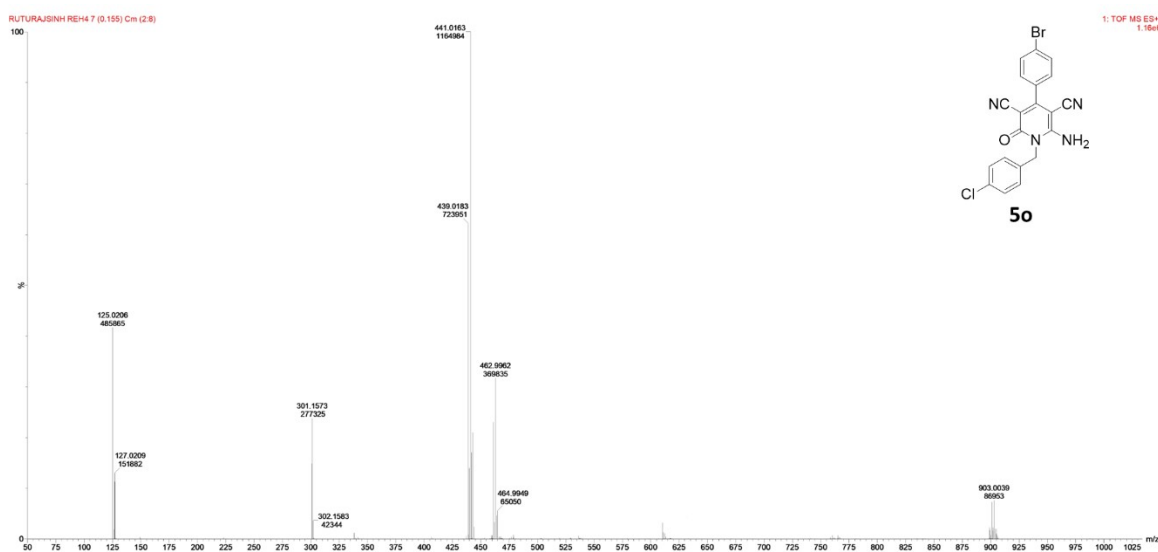


Figure S61. HRMS of compound 5o.

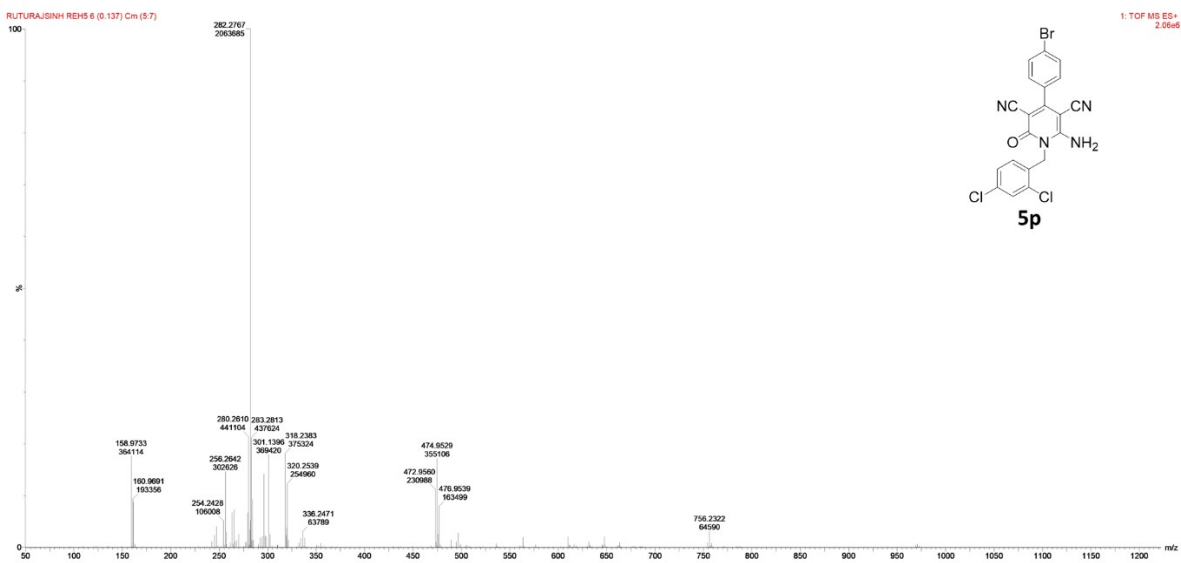


Figure S62. HRMS of compound 5p.