

# Novel *N*-Substituted Amino Acid Hydrazone-Isatin Derivatives: Synthesis, Antioxidant Activity, and Anticancer Activity in 2D and 3D Models *In Vitro*

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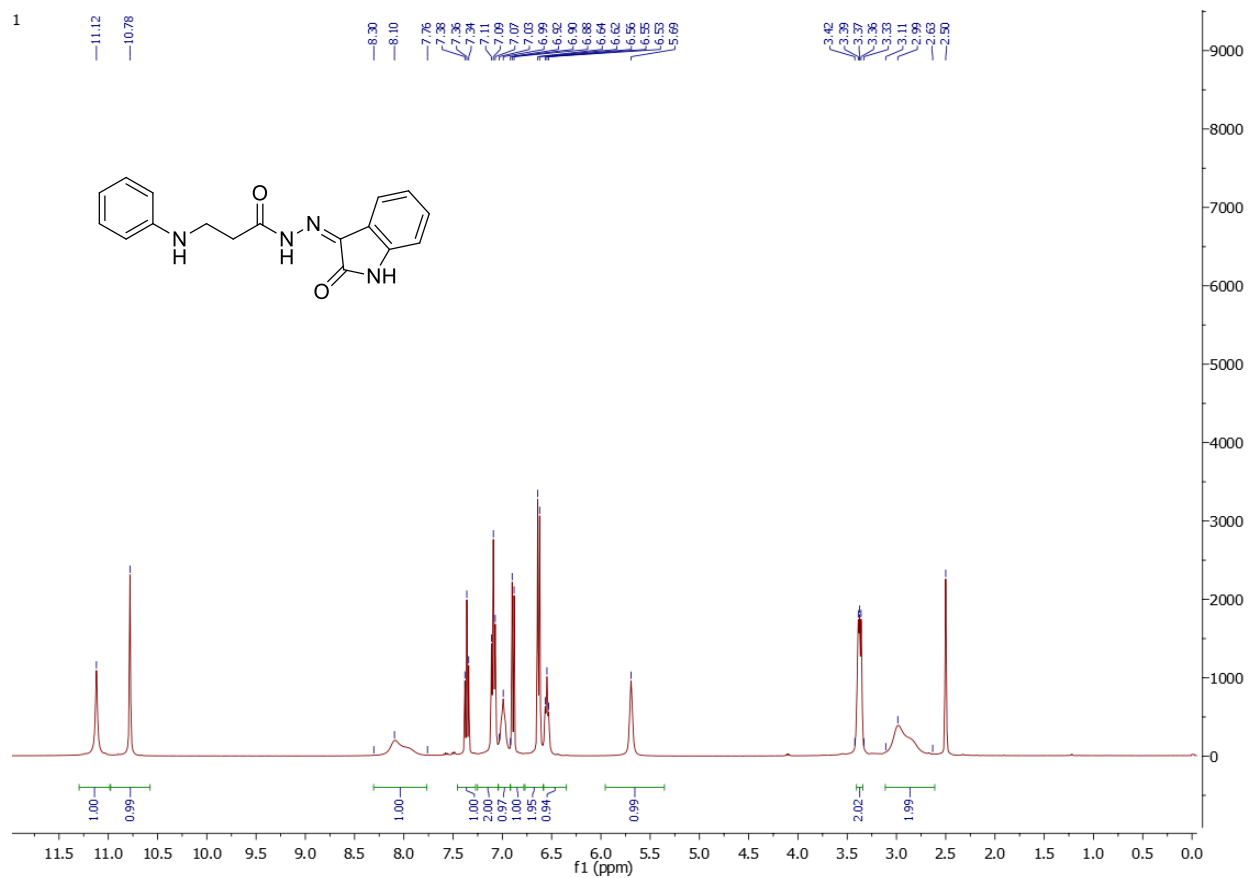


Figure S1. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of 12

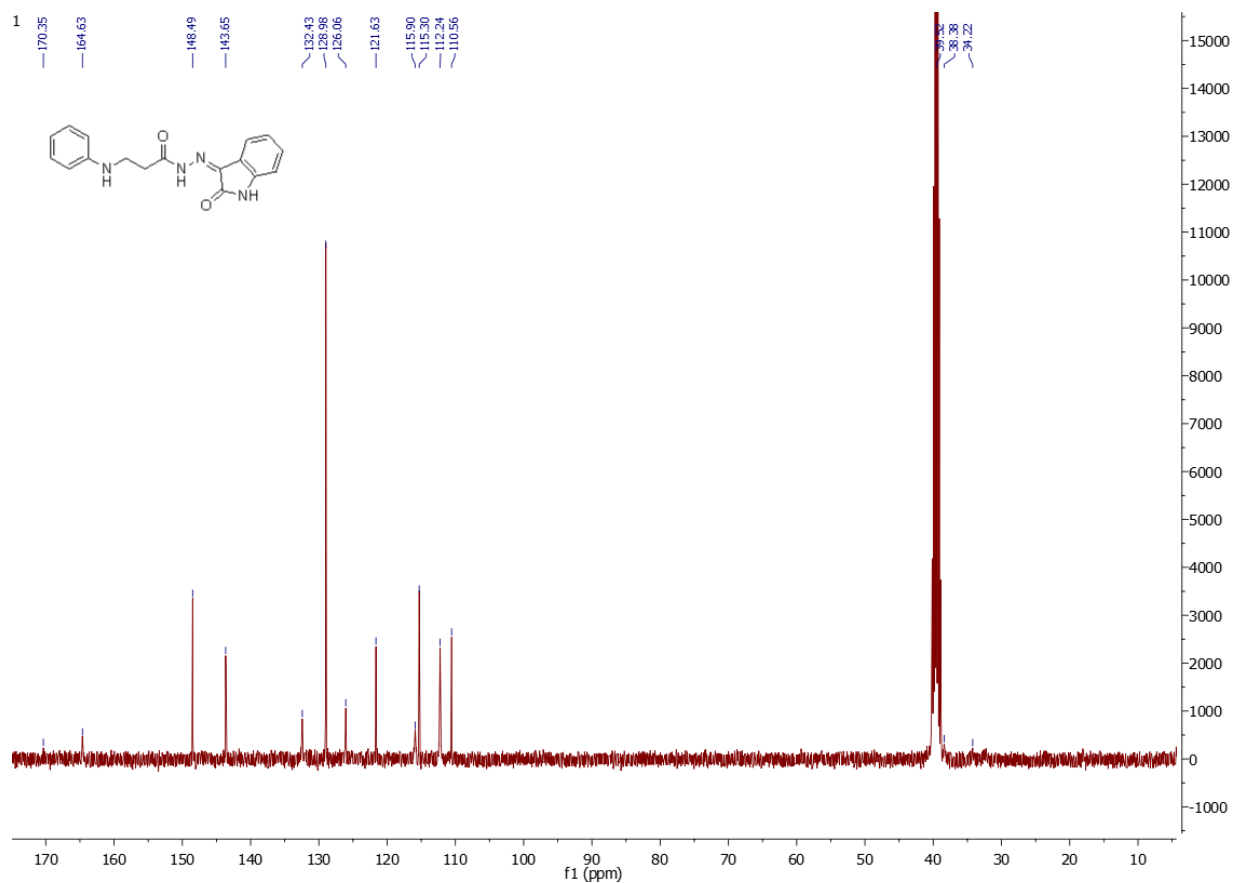


Figure S2.  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ ) spectrum of 12

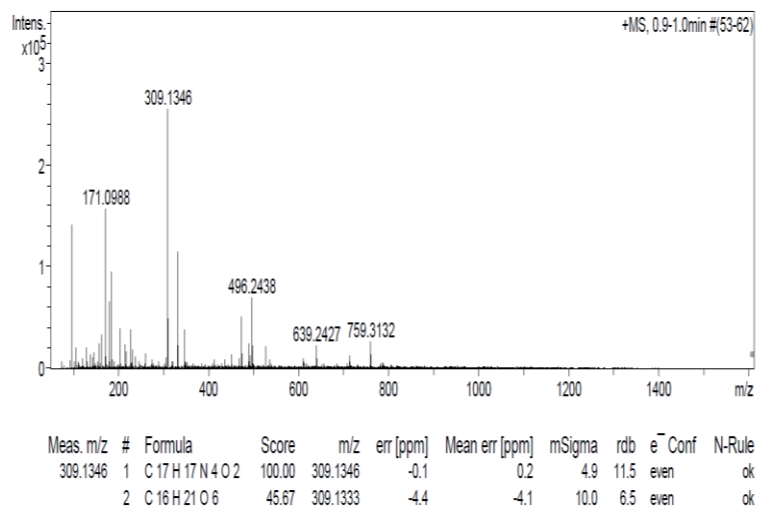
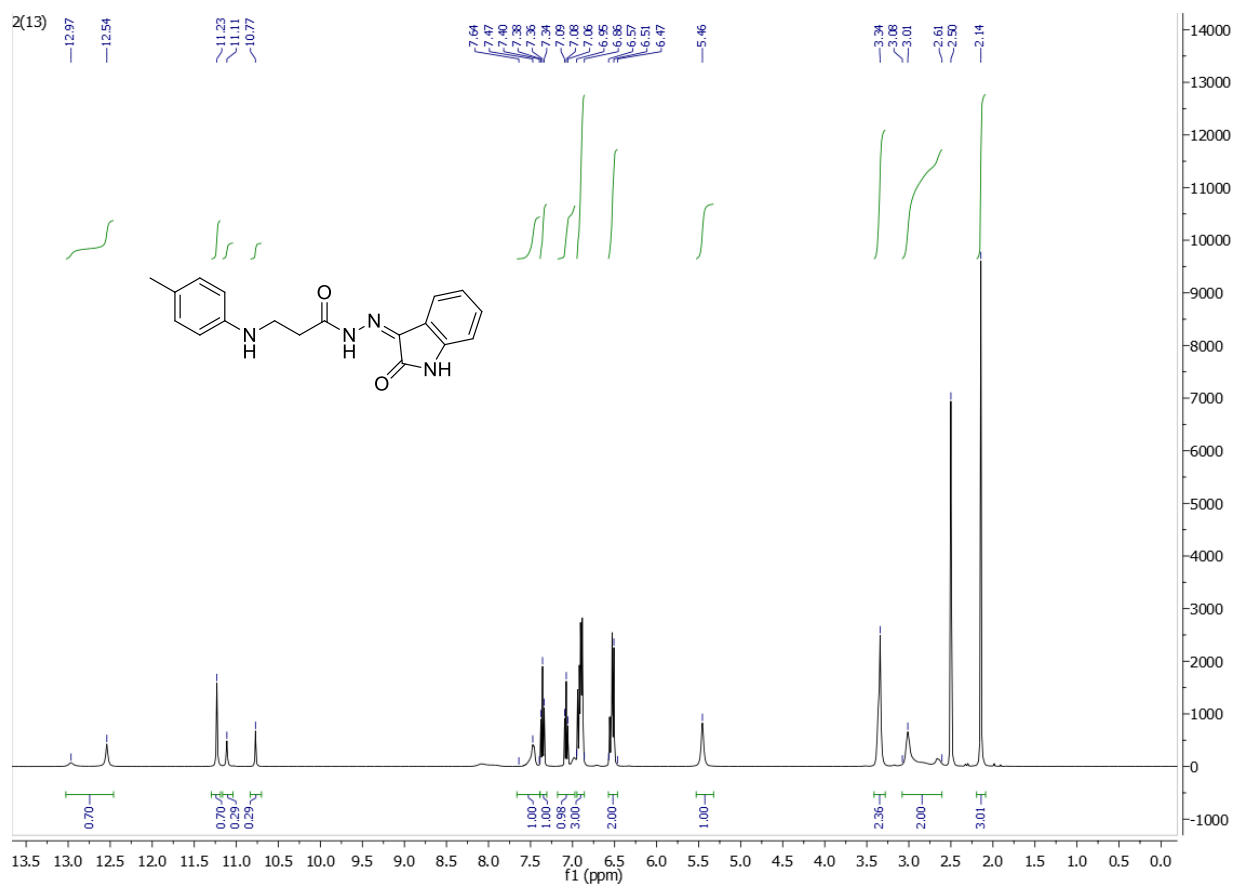
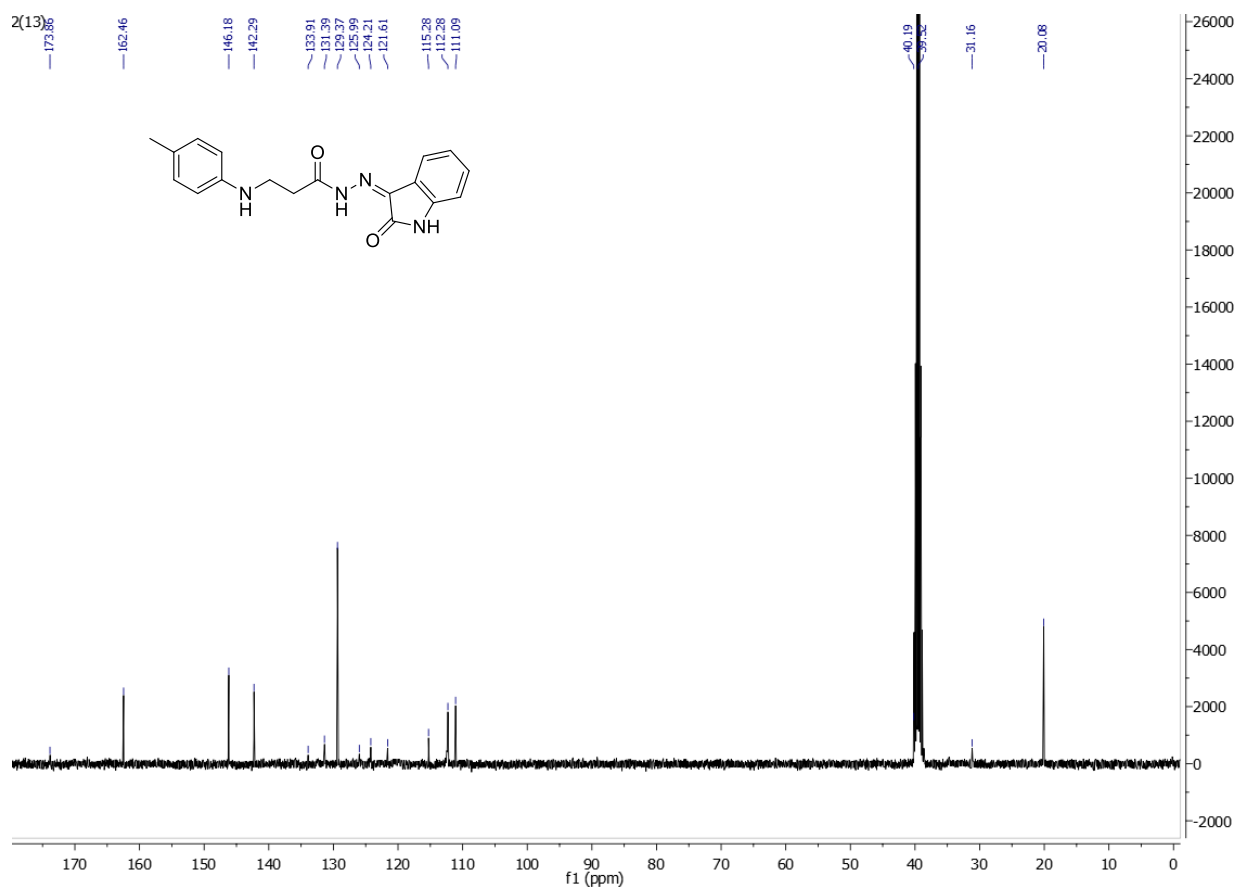


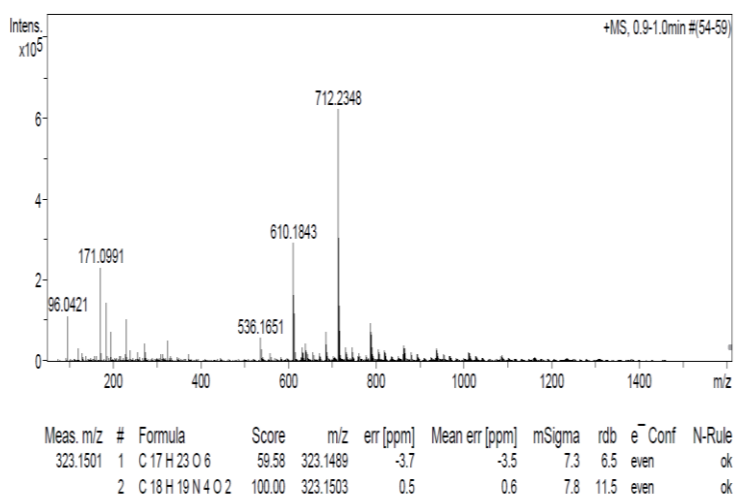
Figure S3. HRMS spectrum of 12



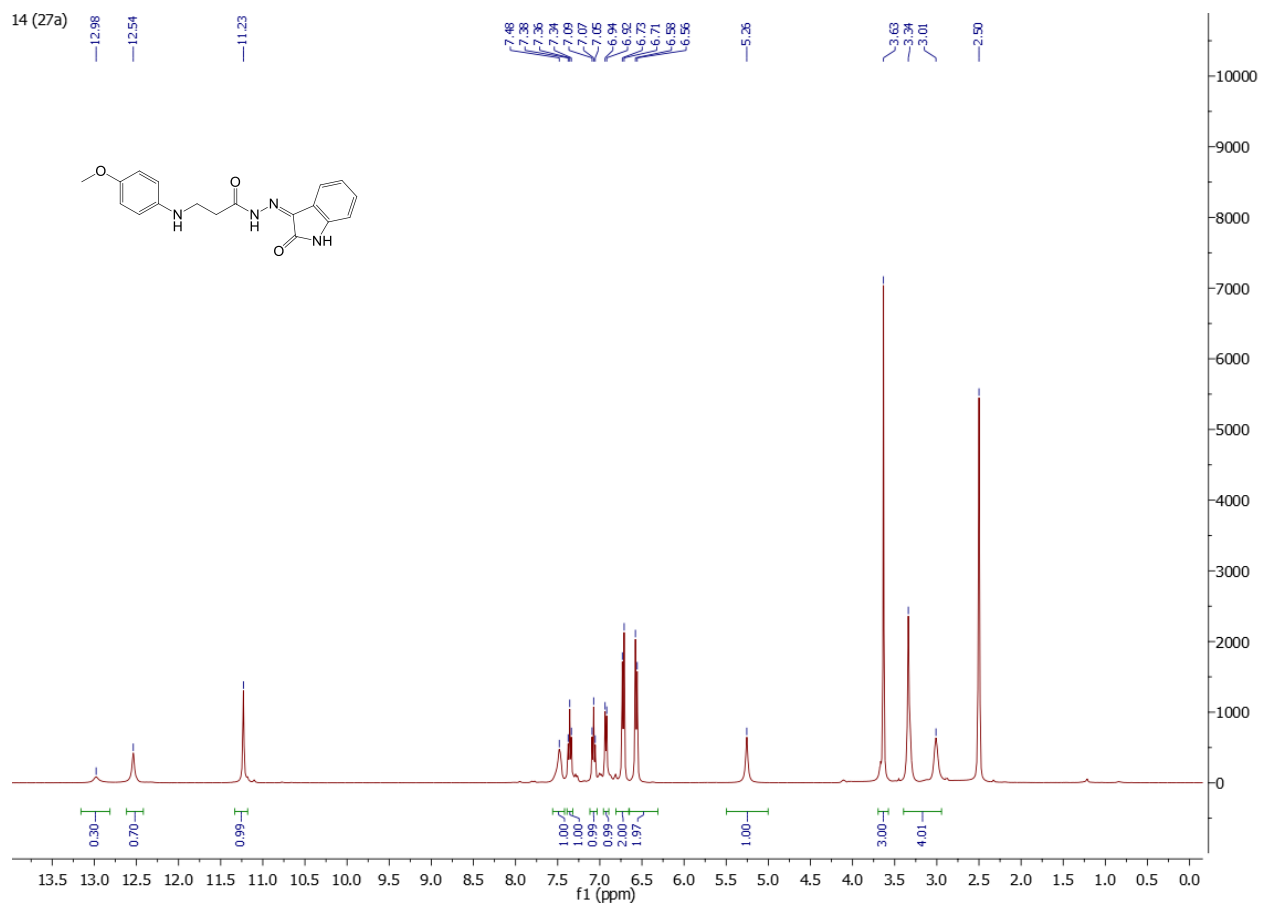
**Figure S4.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **13**



**Figure S5.** <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of 13



**Figure S6.** HRMS spectrum of 13



**Figure S7.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **14**



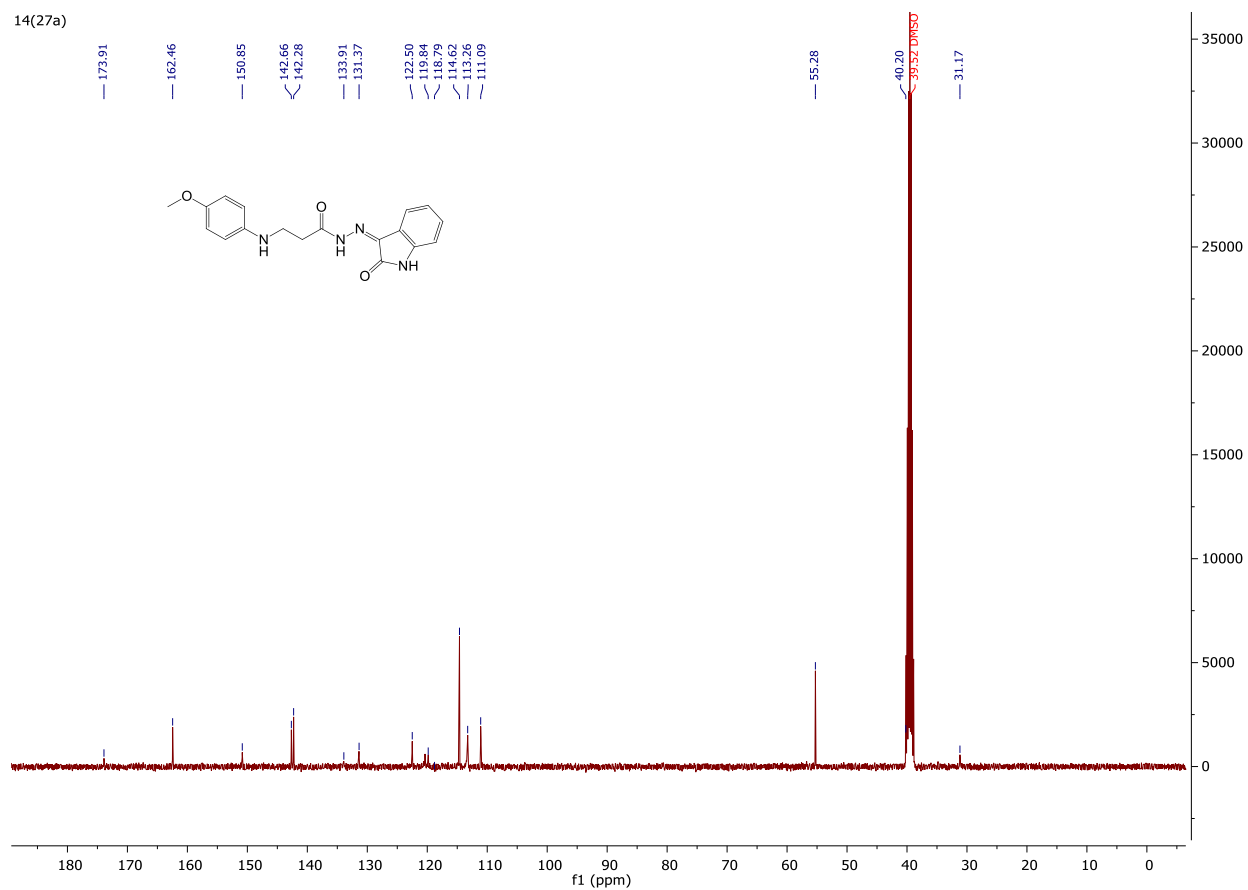


Figure S8.  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ ) spectrum of **14**

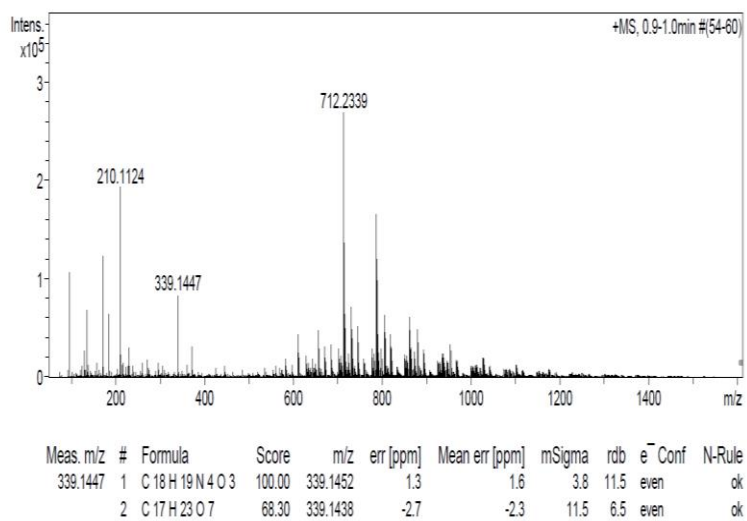
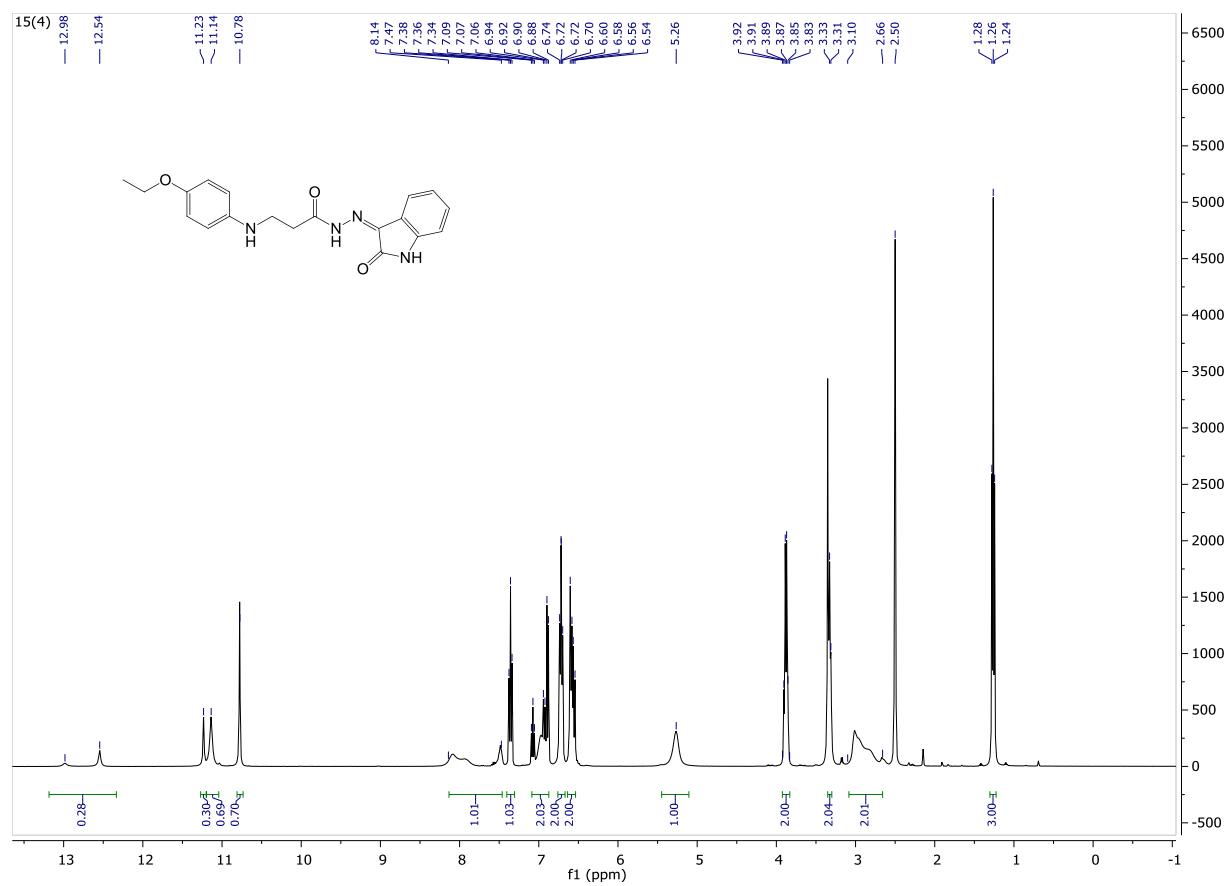
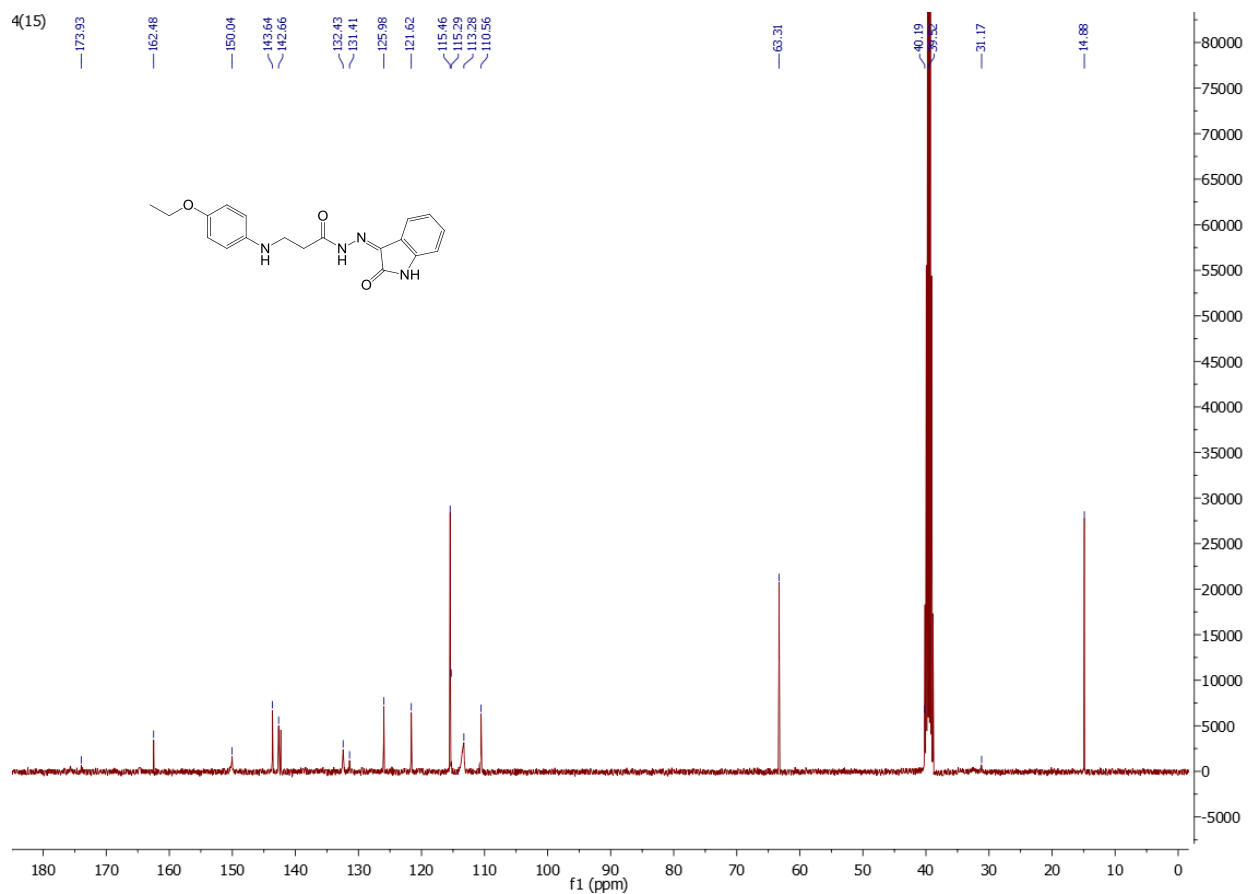


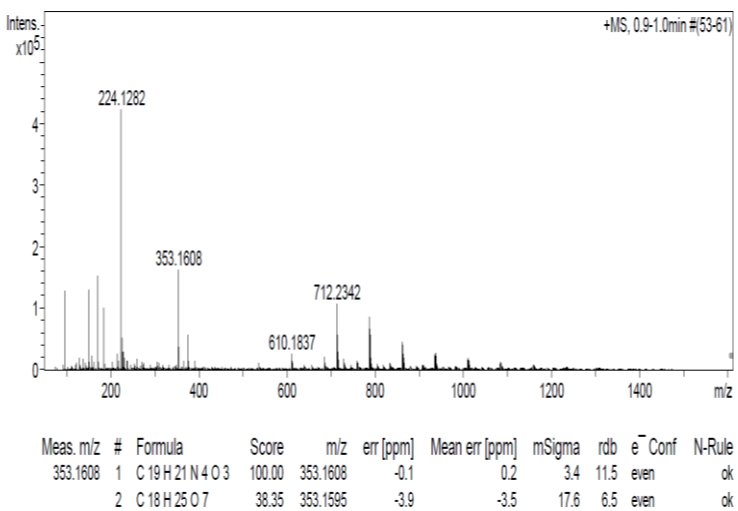
Figure S9. HRMS spectrum of **14**



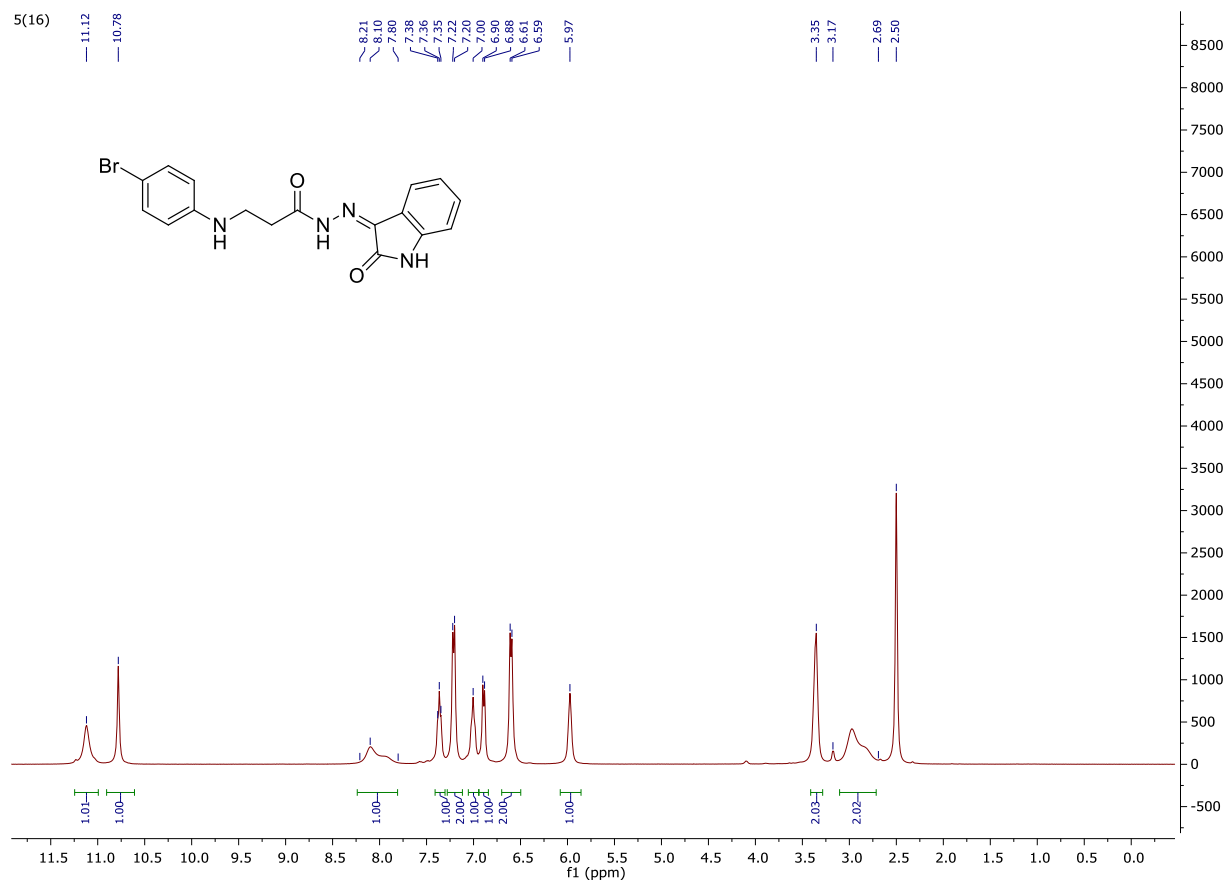
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**Figure S11.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ ) spectrum of **15**



**Figure S12.** HRMS spectrum of **15**



**Figure S13.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **16**

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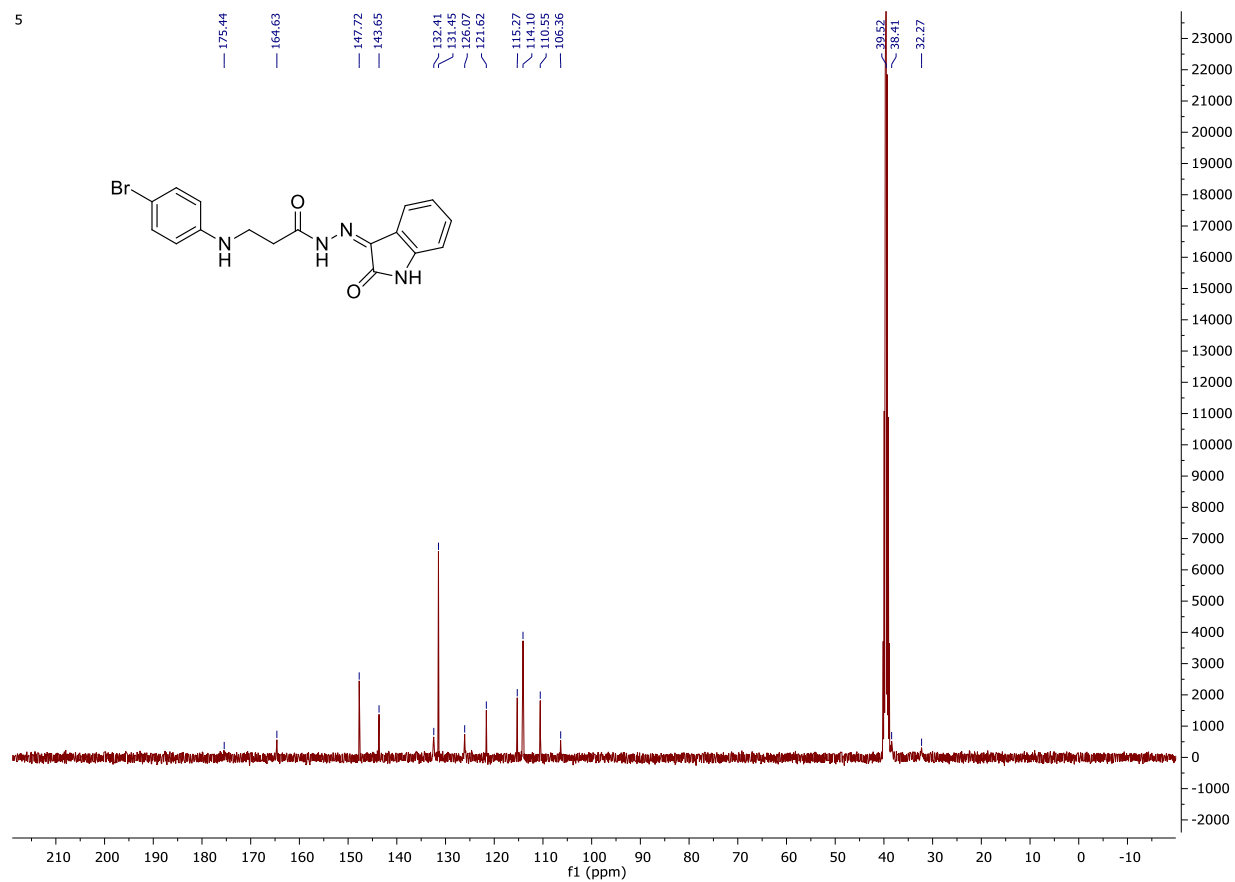


Figure S14. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of 16

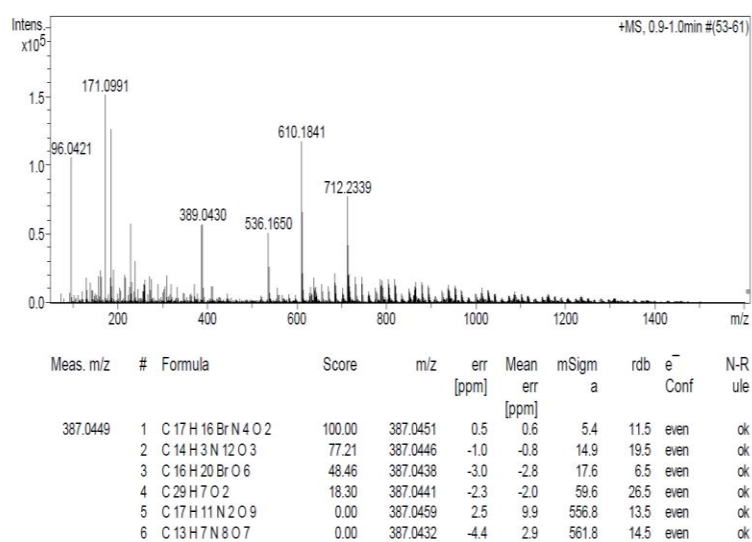
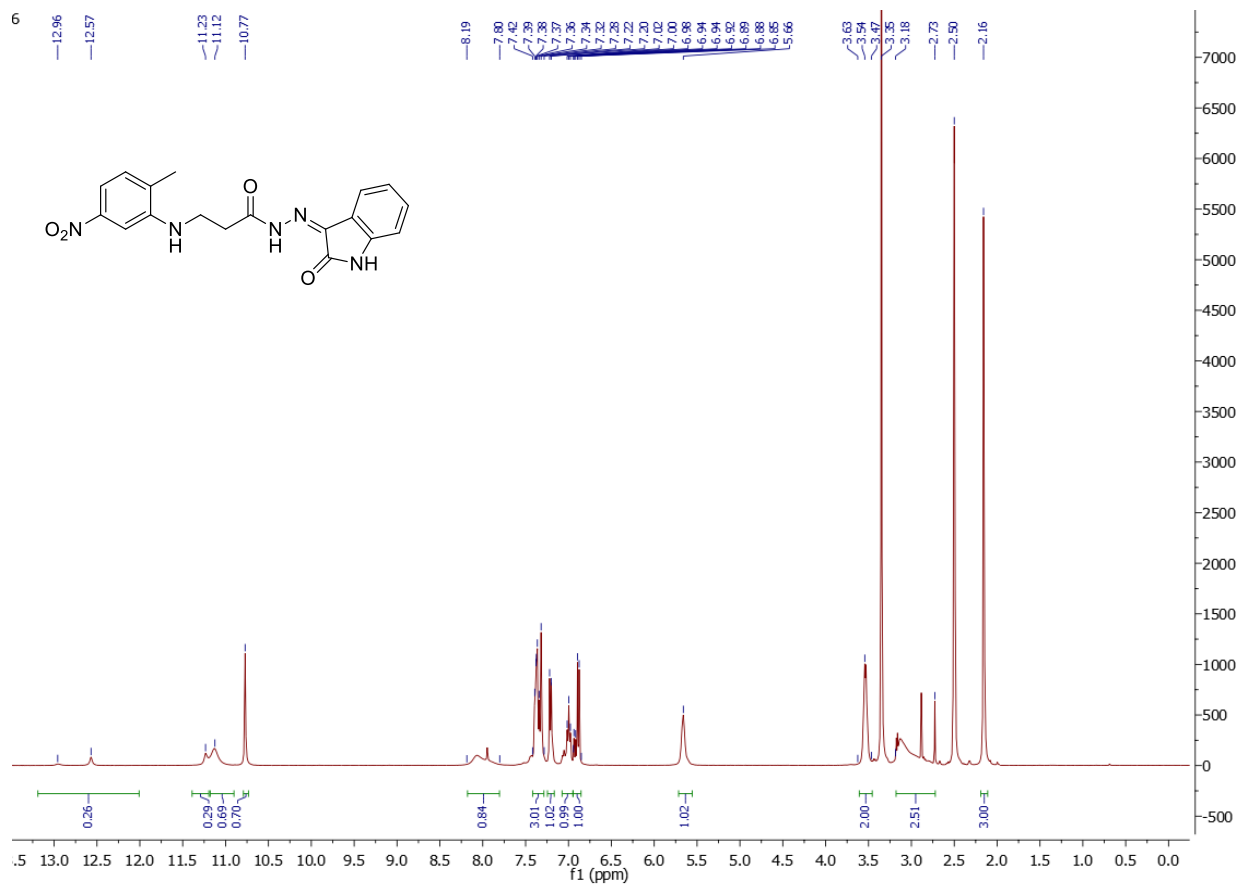


Figure S15. HRMS spectrum of 16



**Figure S16.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **17**

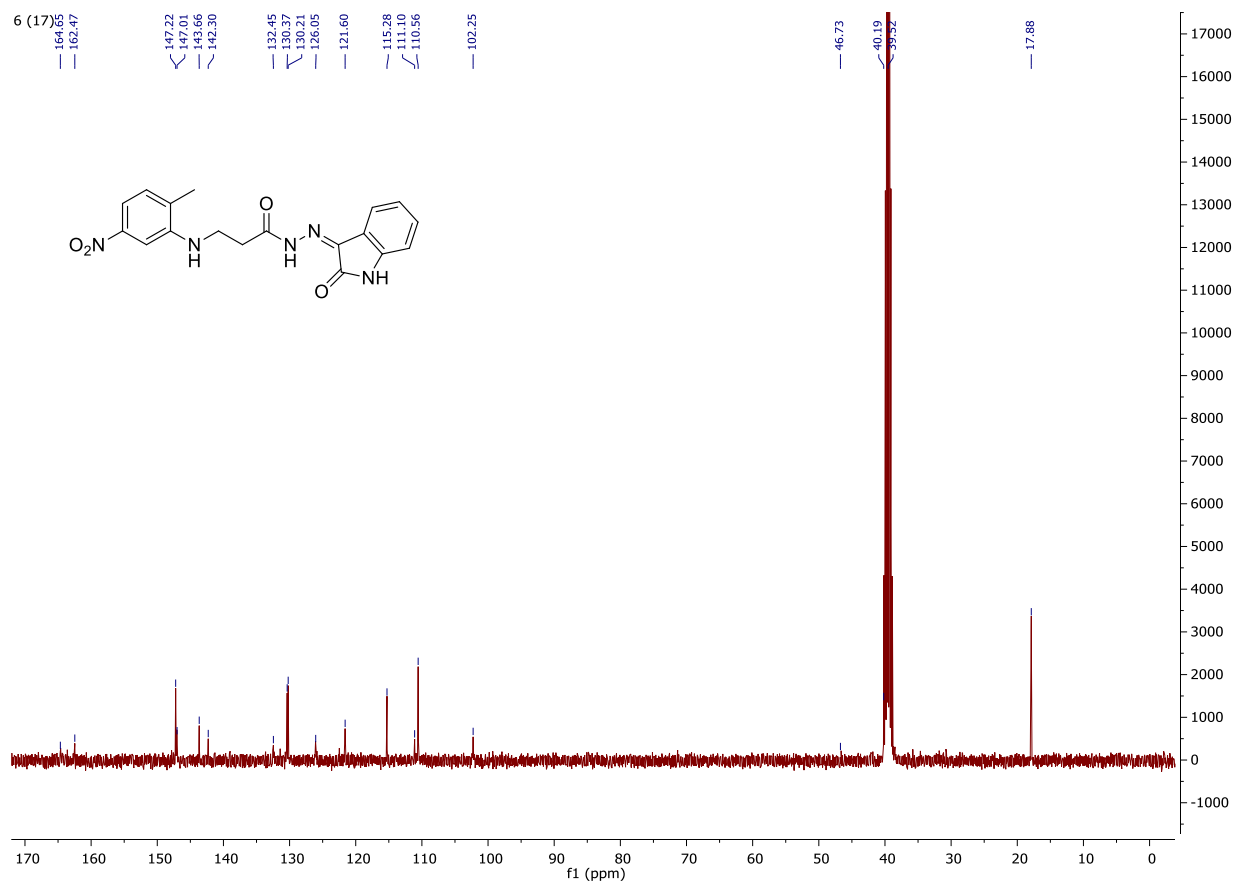


Figure S17.  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ ) spectrum of 17

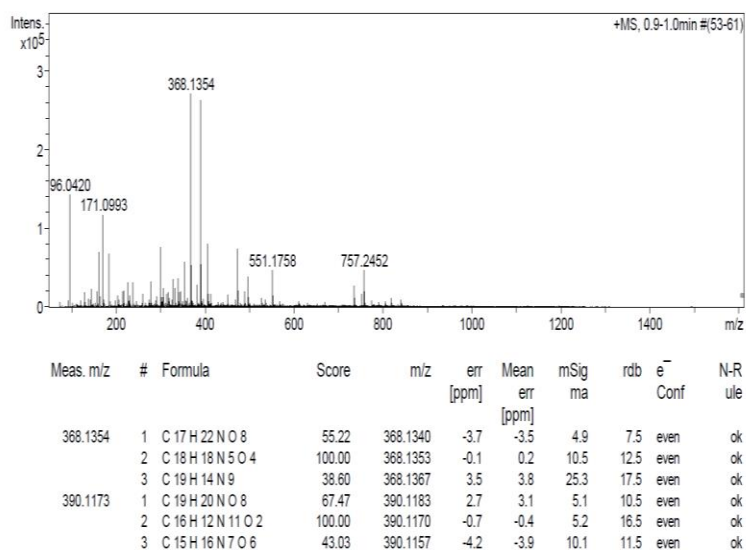


Figure S18. HRMS spectrum of 17

**Figure S19.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) spectrum of **18**



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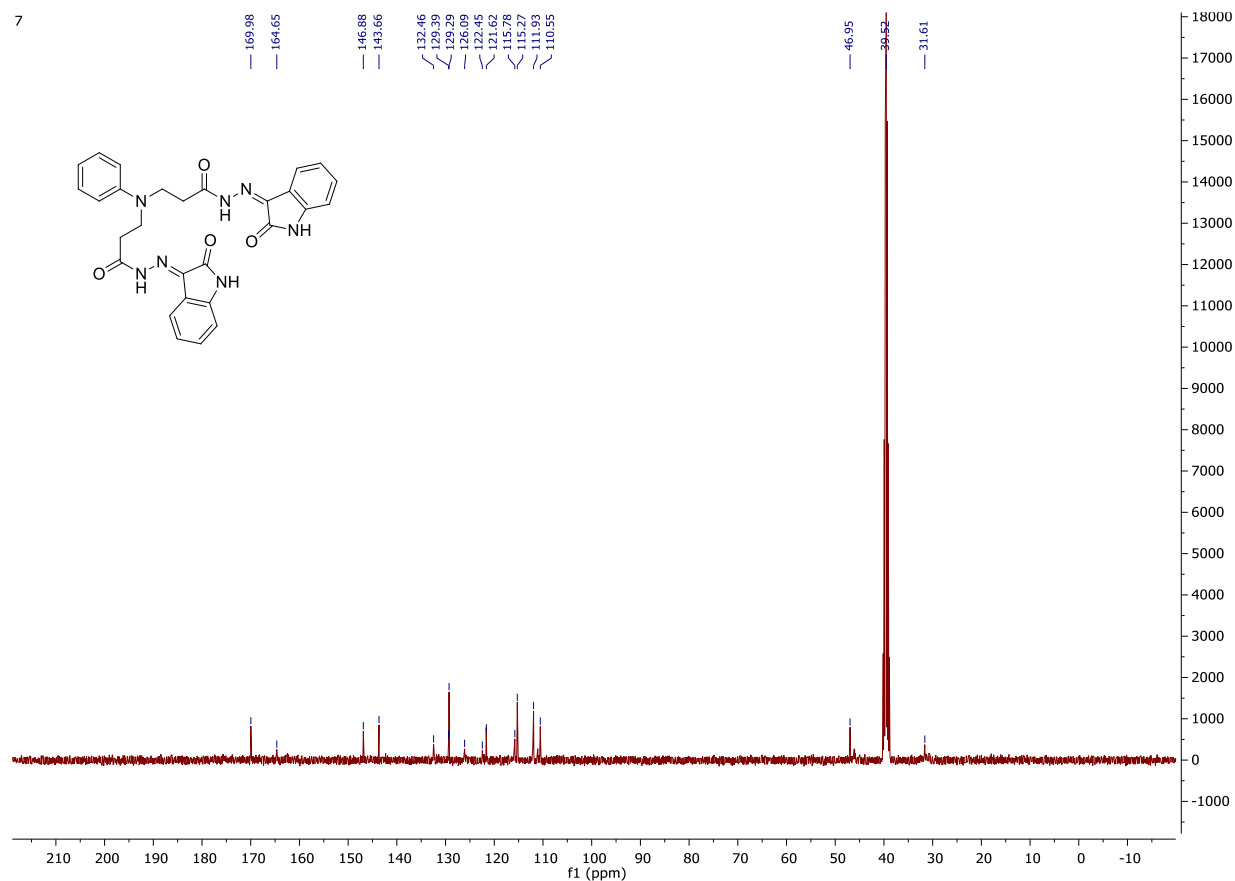


Figure S20. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of 18

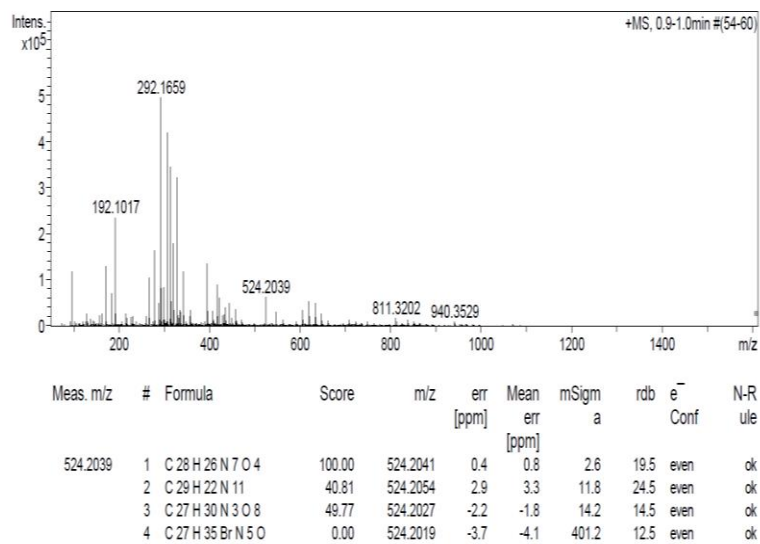
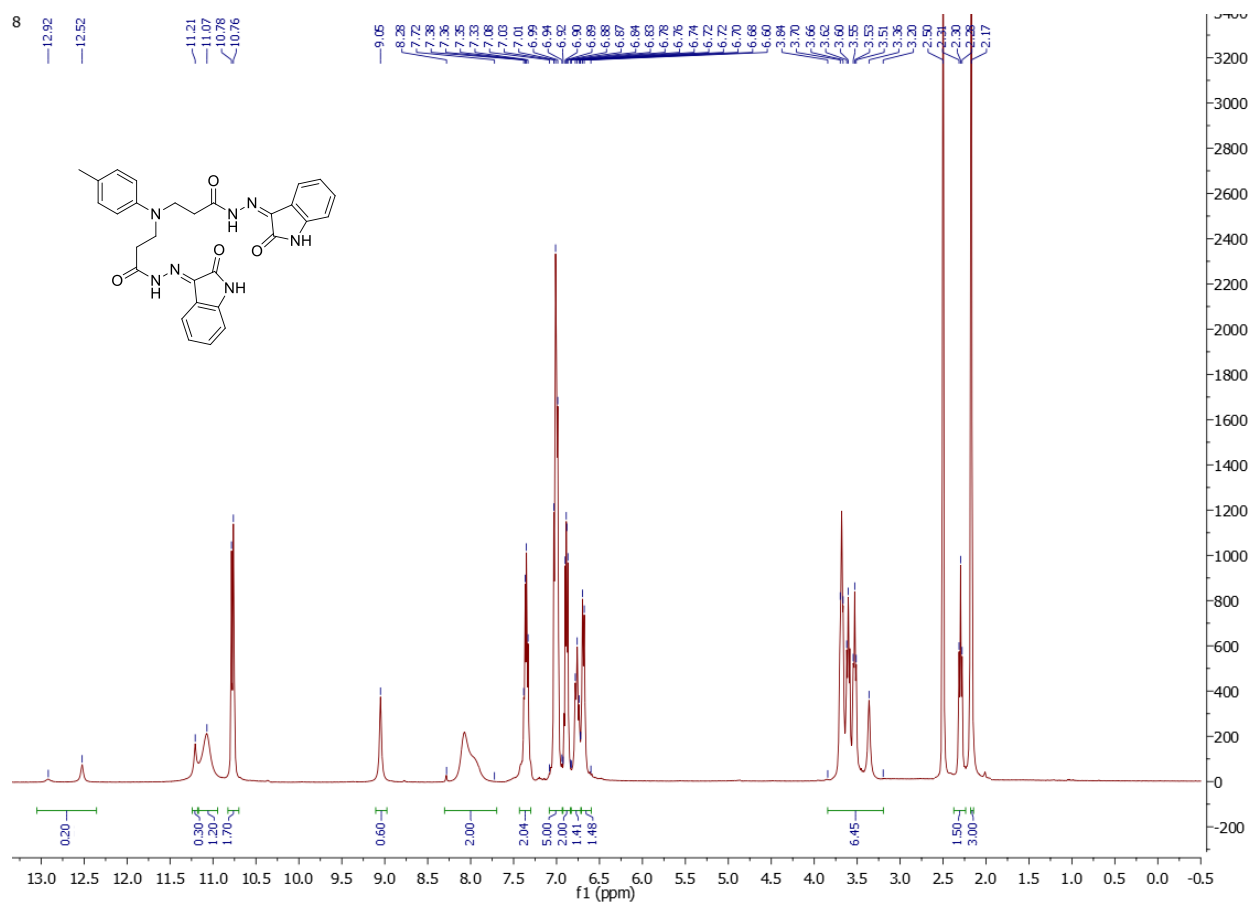
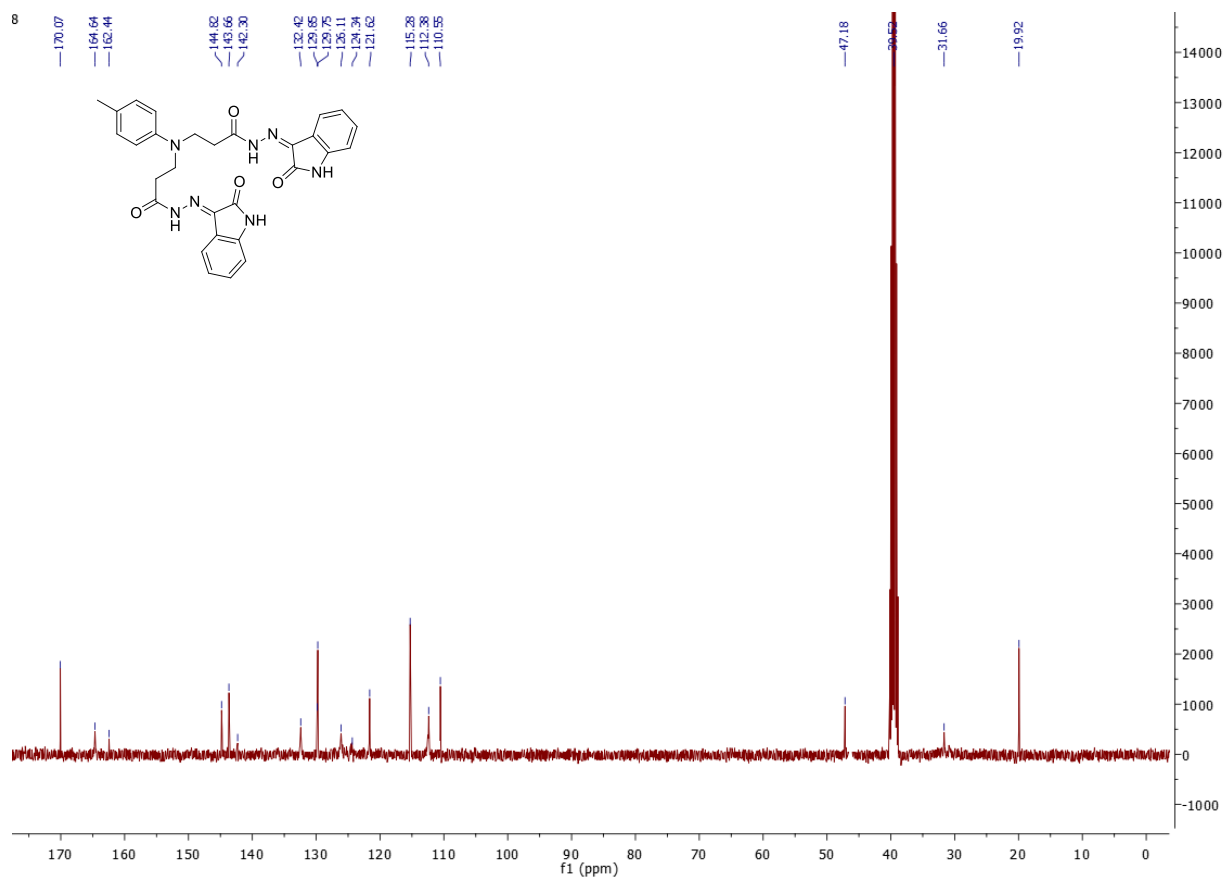


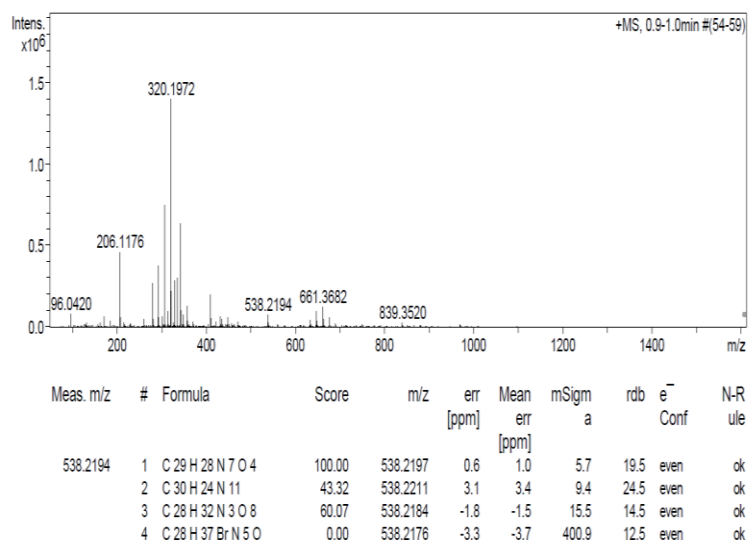
Figure S21. HRMS spectrum of 18



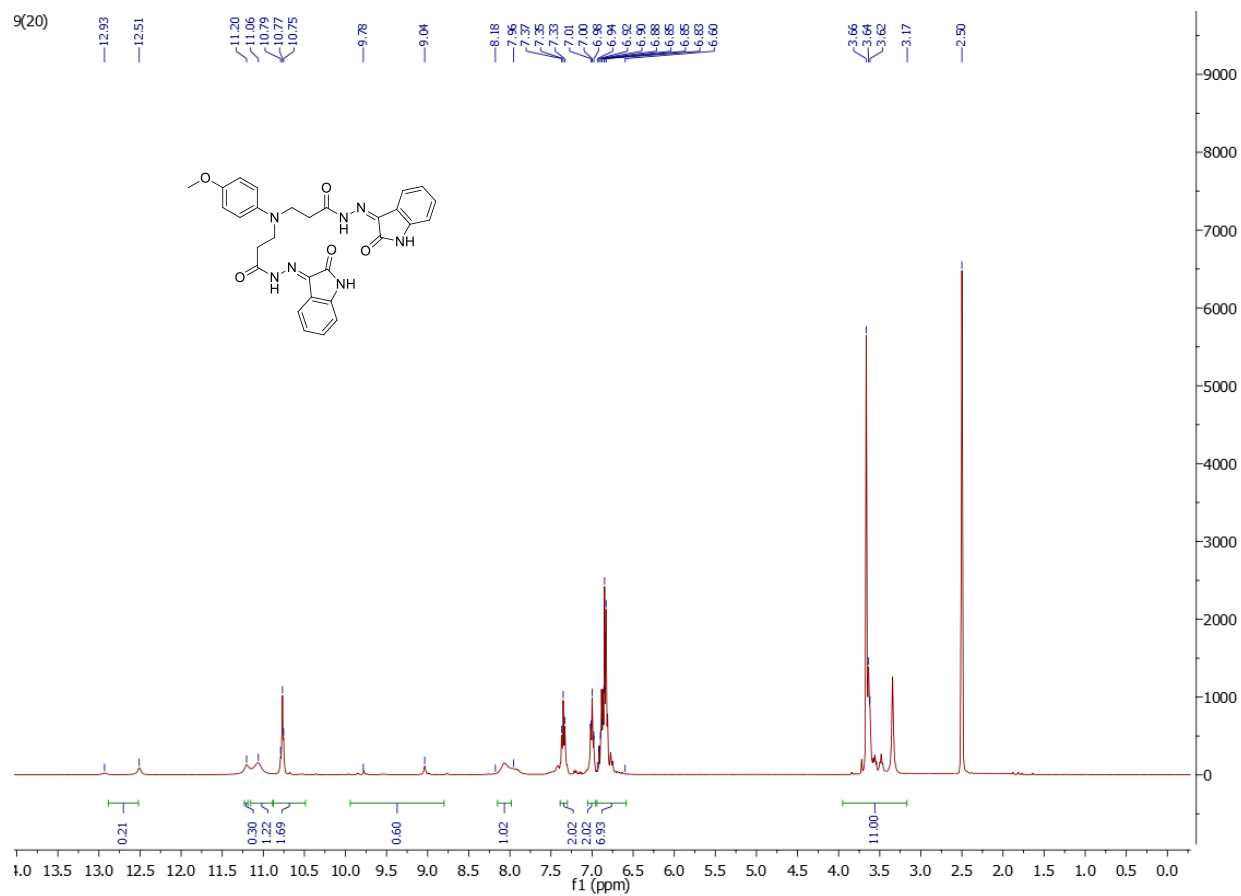
**Figure S22.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **19**



**Figure S23.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ ) spectrum of **19**



**Figure S24.** HRMS spectrum of **19**



**Figure S25.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of 20

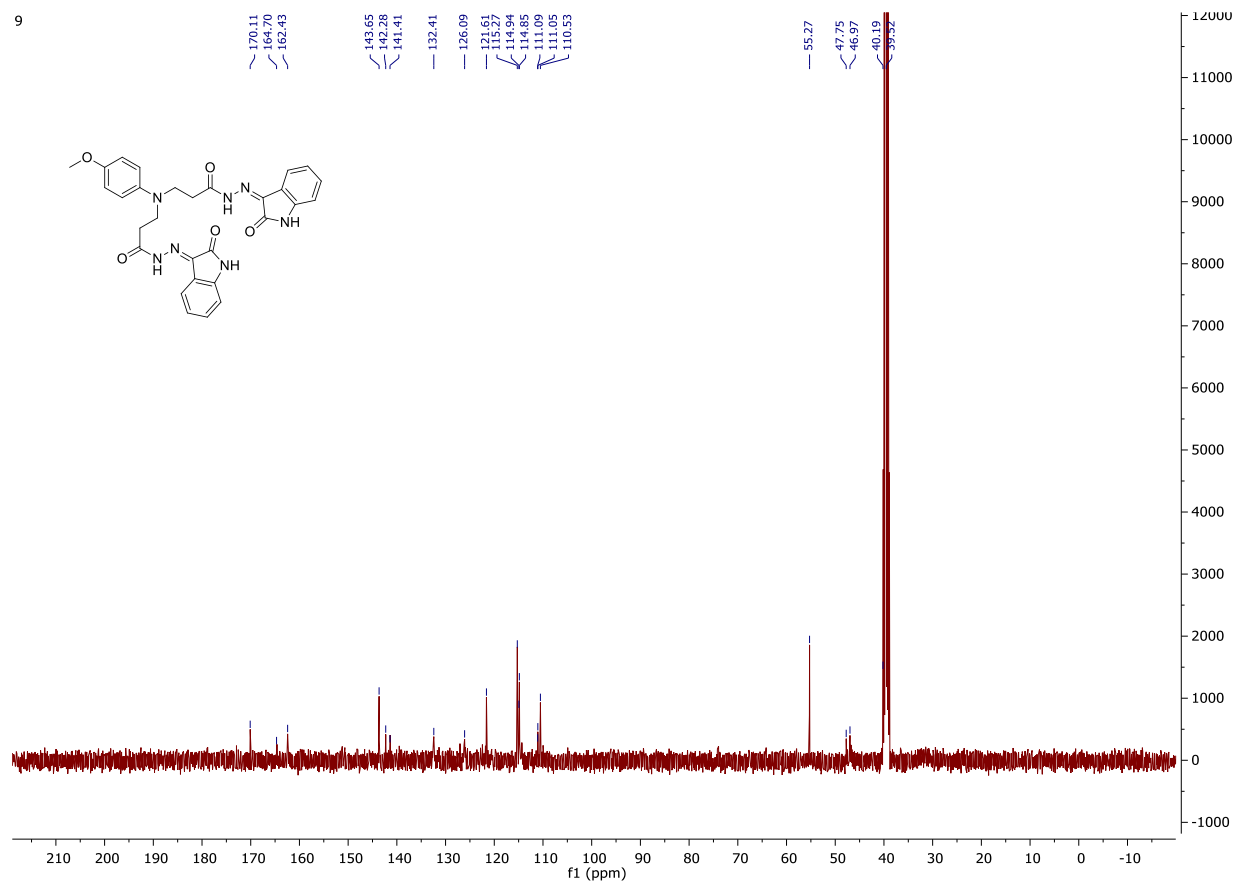


Figure S26. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of 20

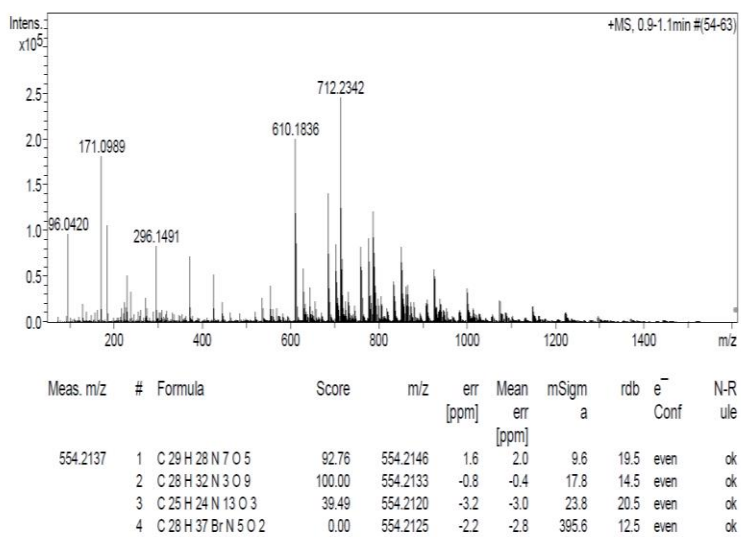
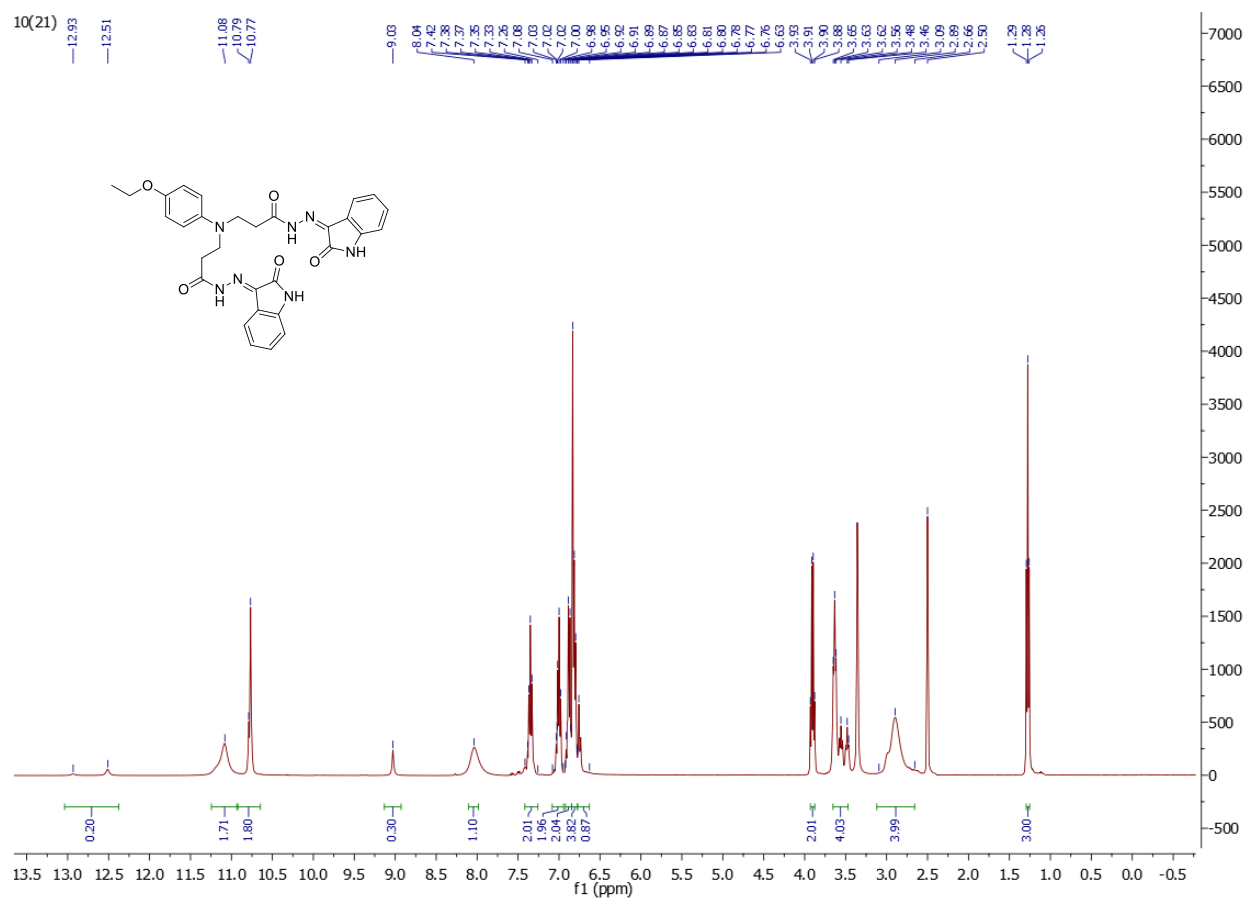


Figure S27. HRMS spectrum of 20



**Figure S28.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21**

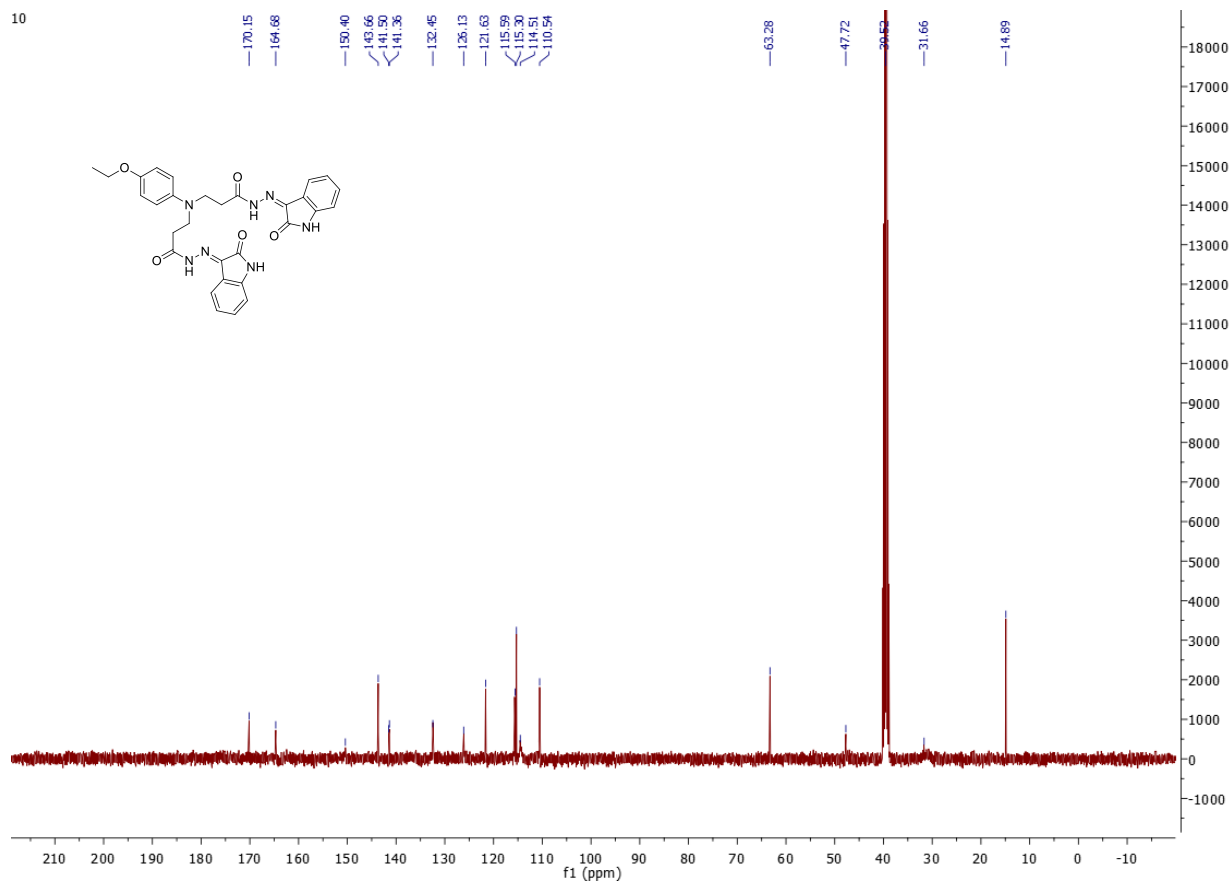


Figure S29. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of 21

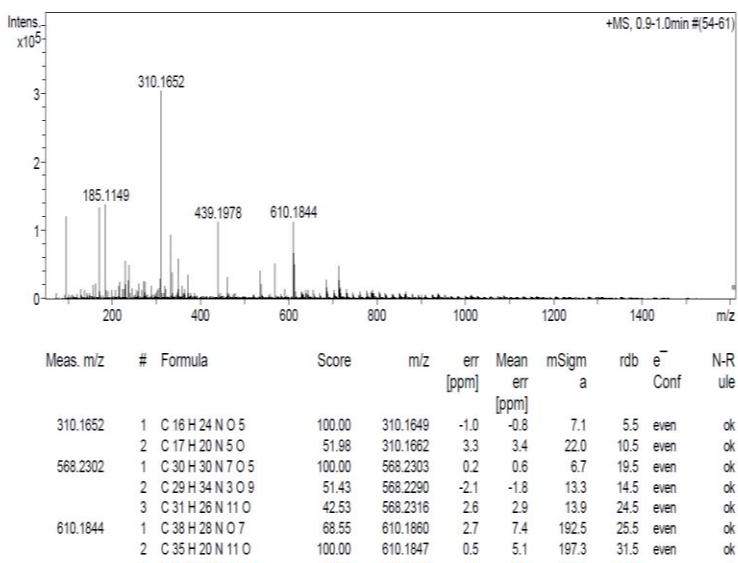
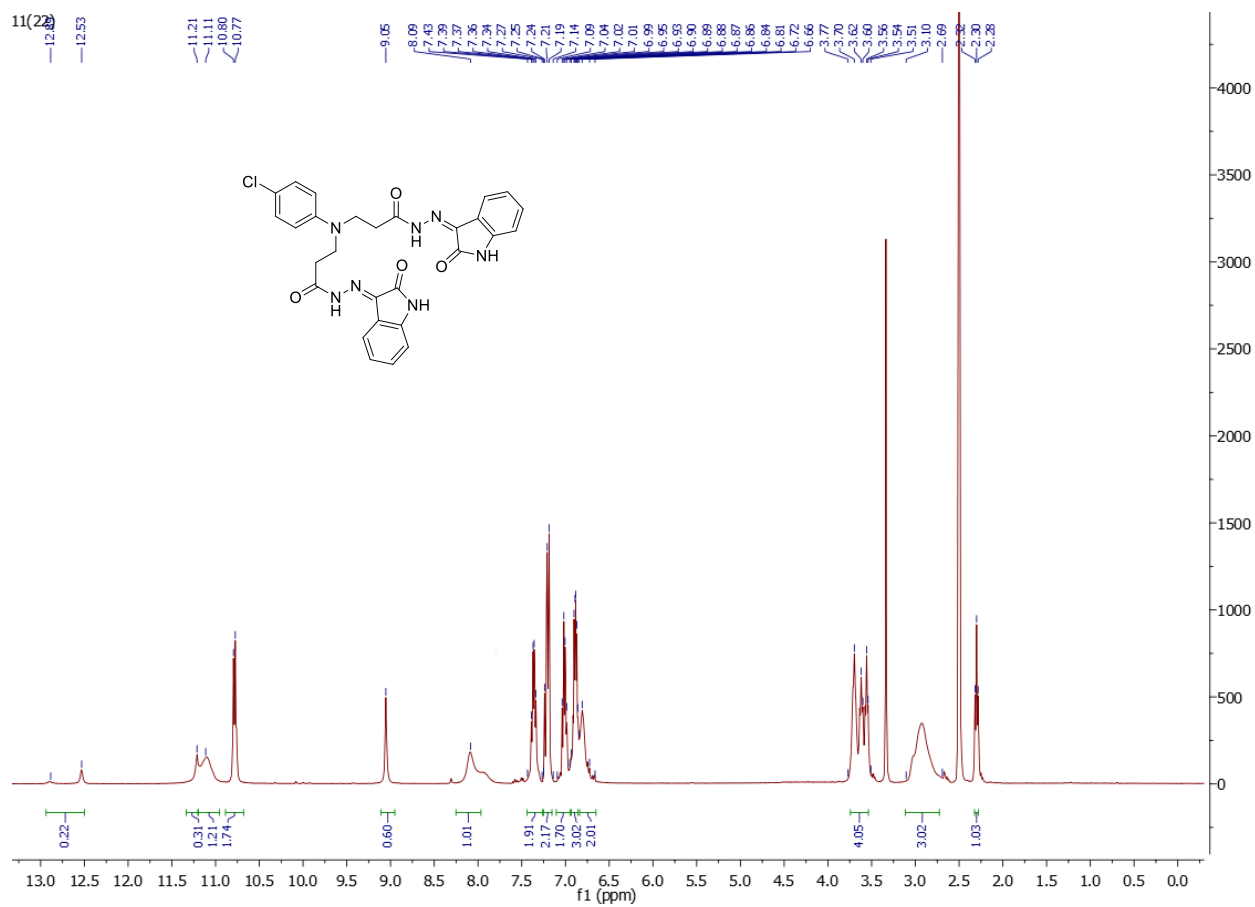


Figure S30. HRMS spectrum of 21



**Figure S31.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **22**



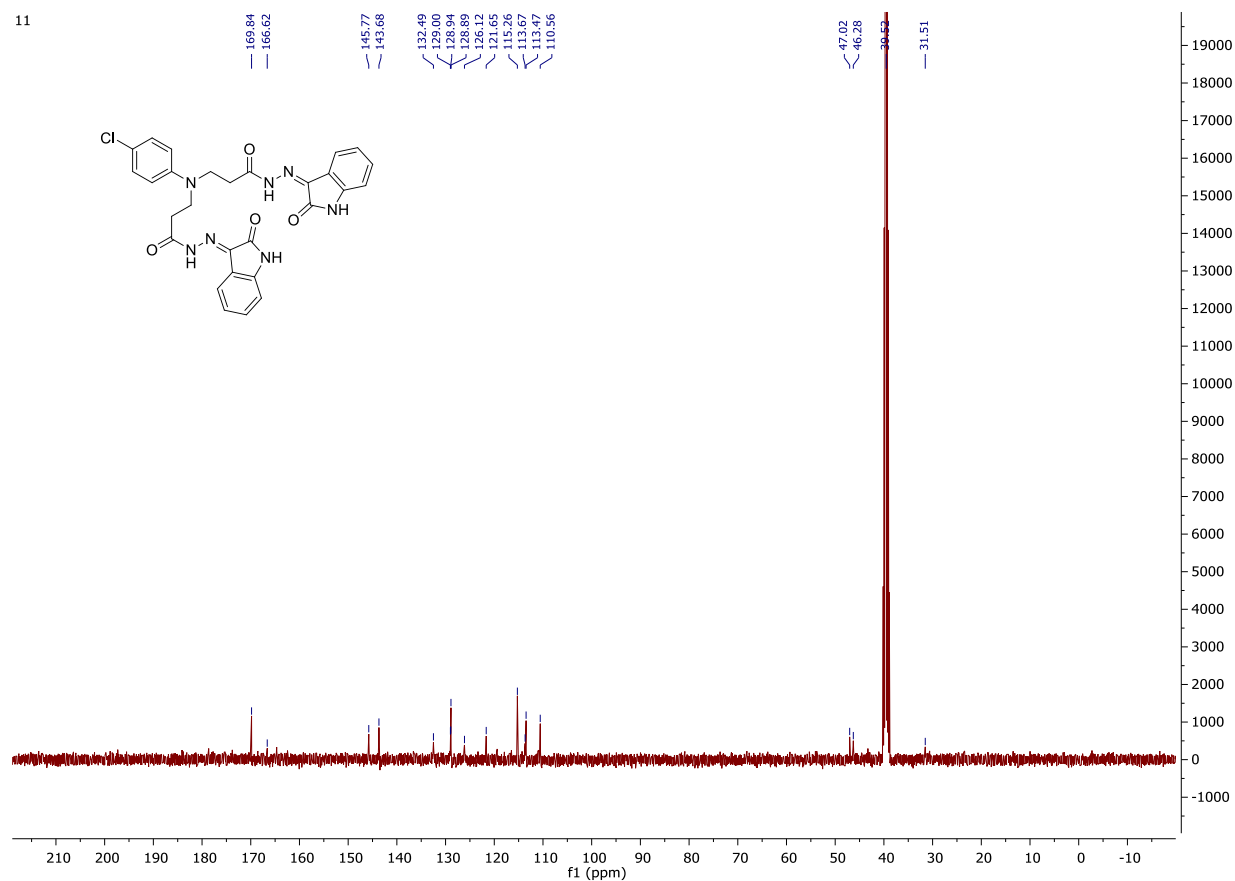


Figure S32.  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ ) spectrum of 22

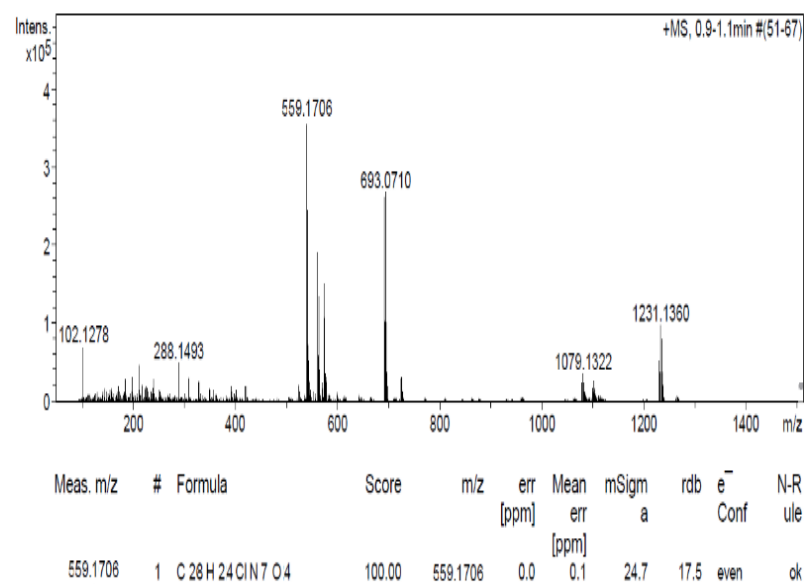
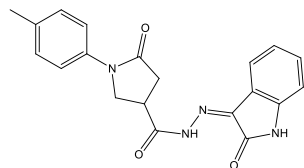


Figure S33. HRMS spectrum of 22



**Figure S34.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) spectrum of **26**

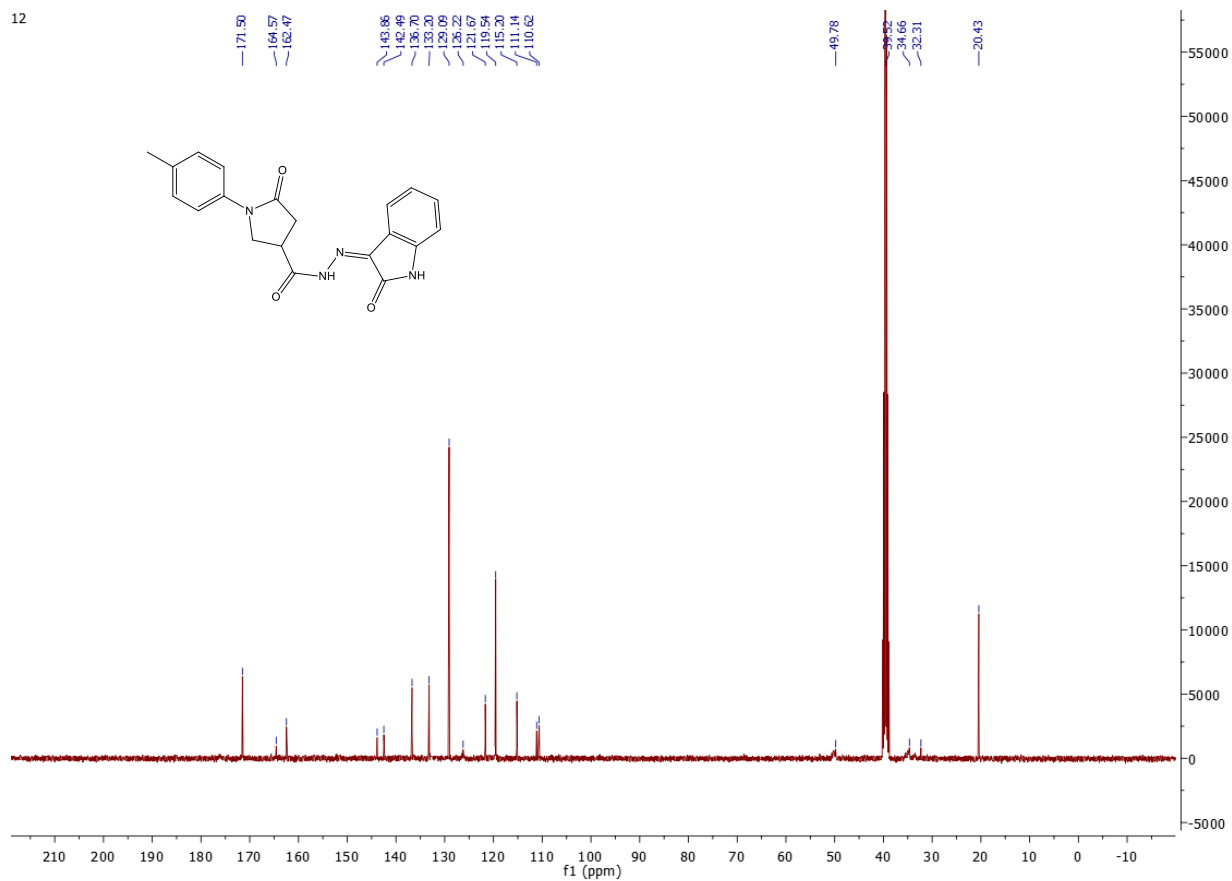


Figure S35. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of 26

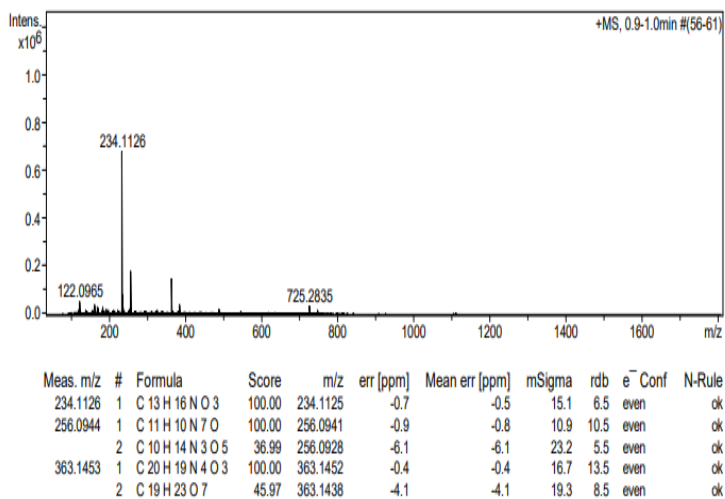


Figure S36. HRMS spectrum of 26

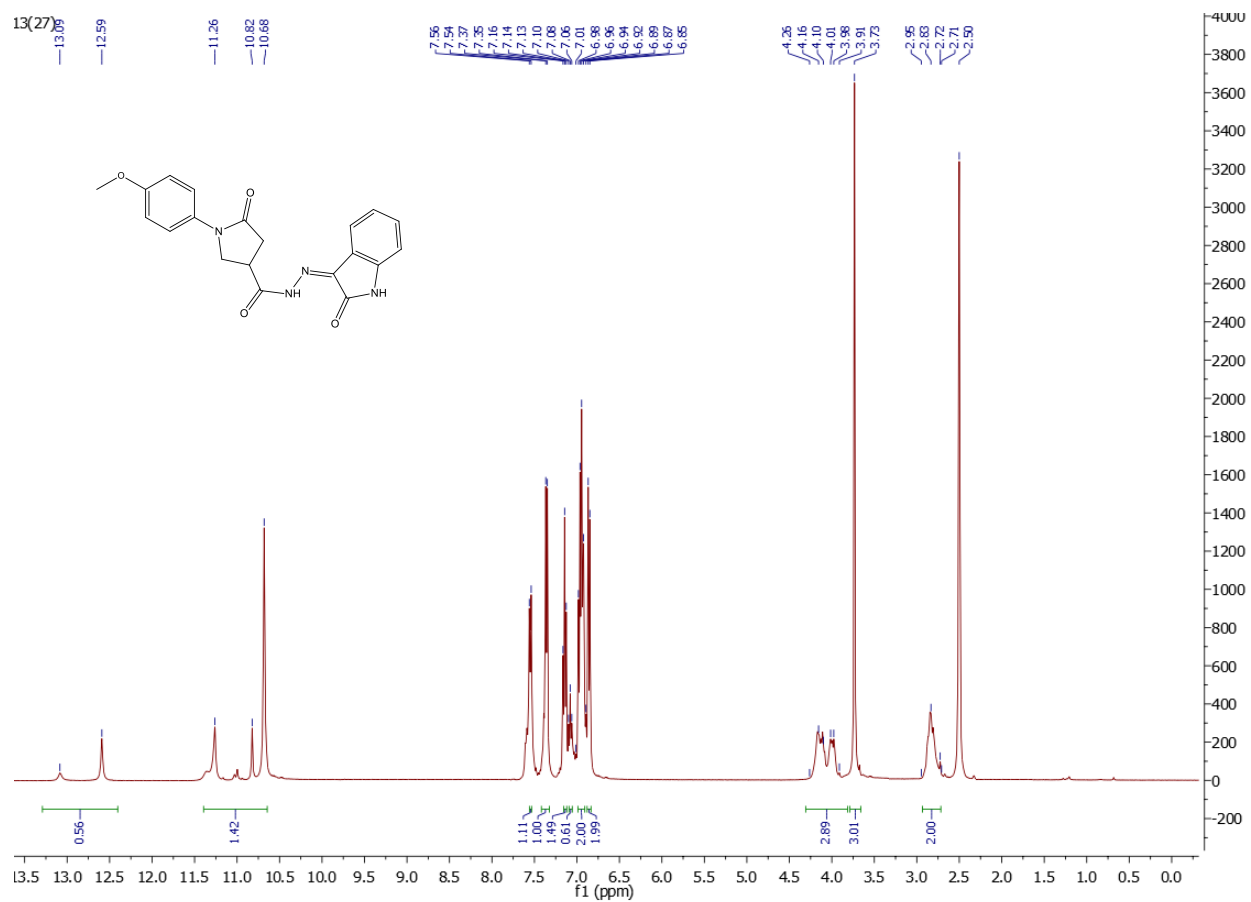


Figure S37. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **27**

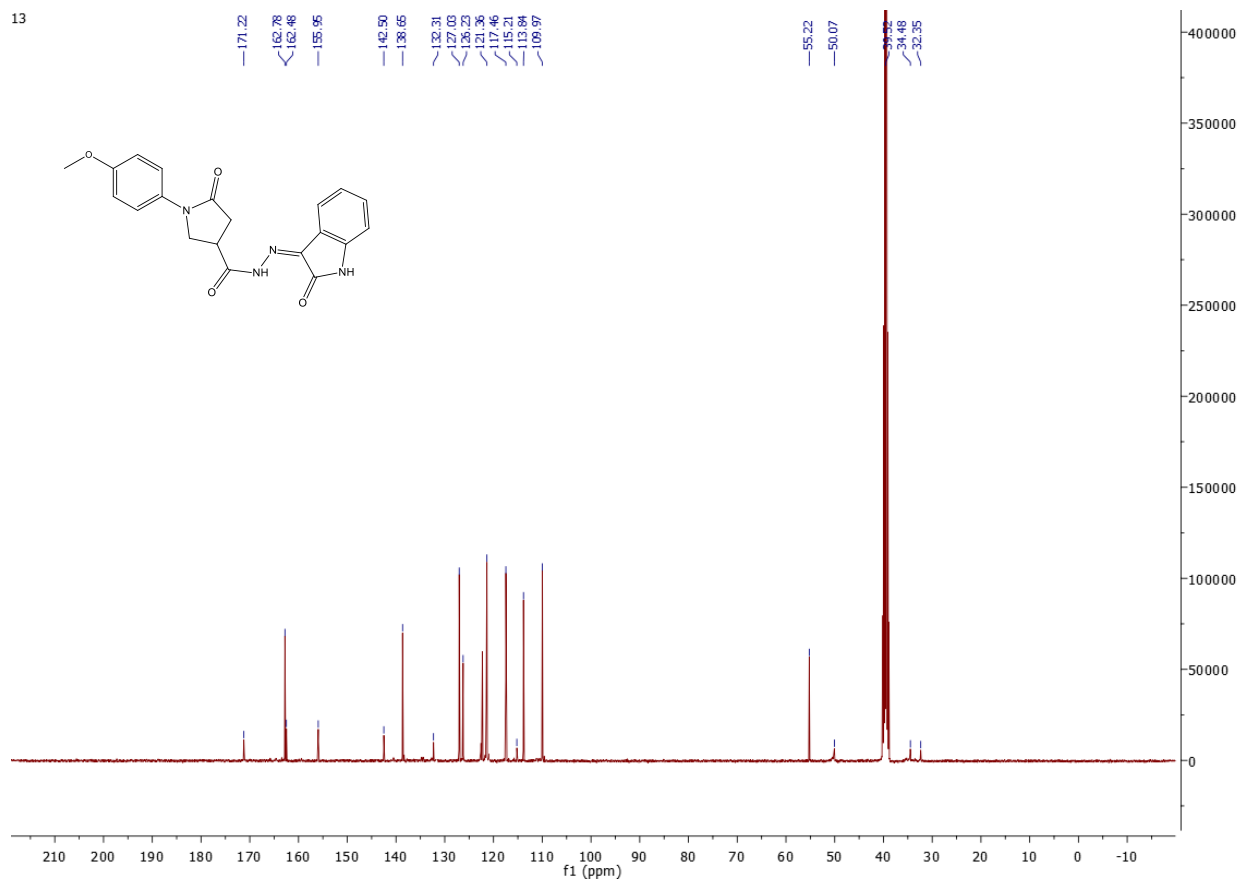


Figure S38. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of 27

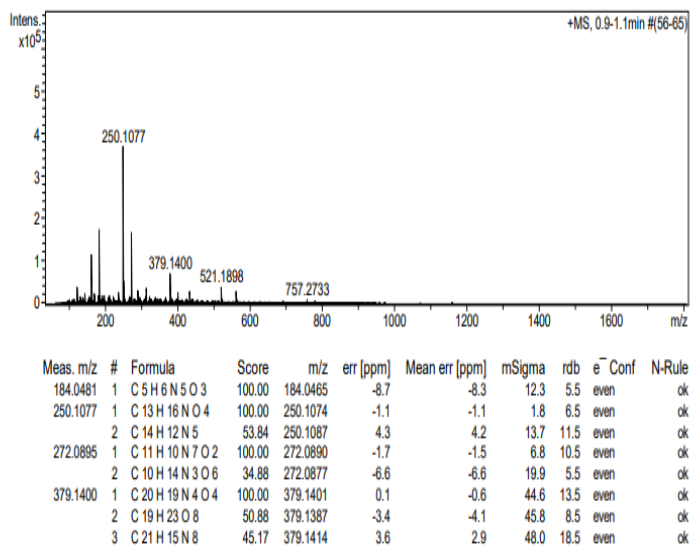
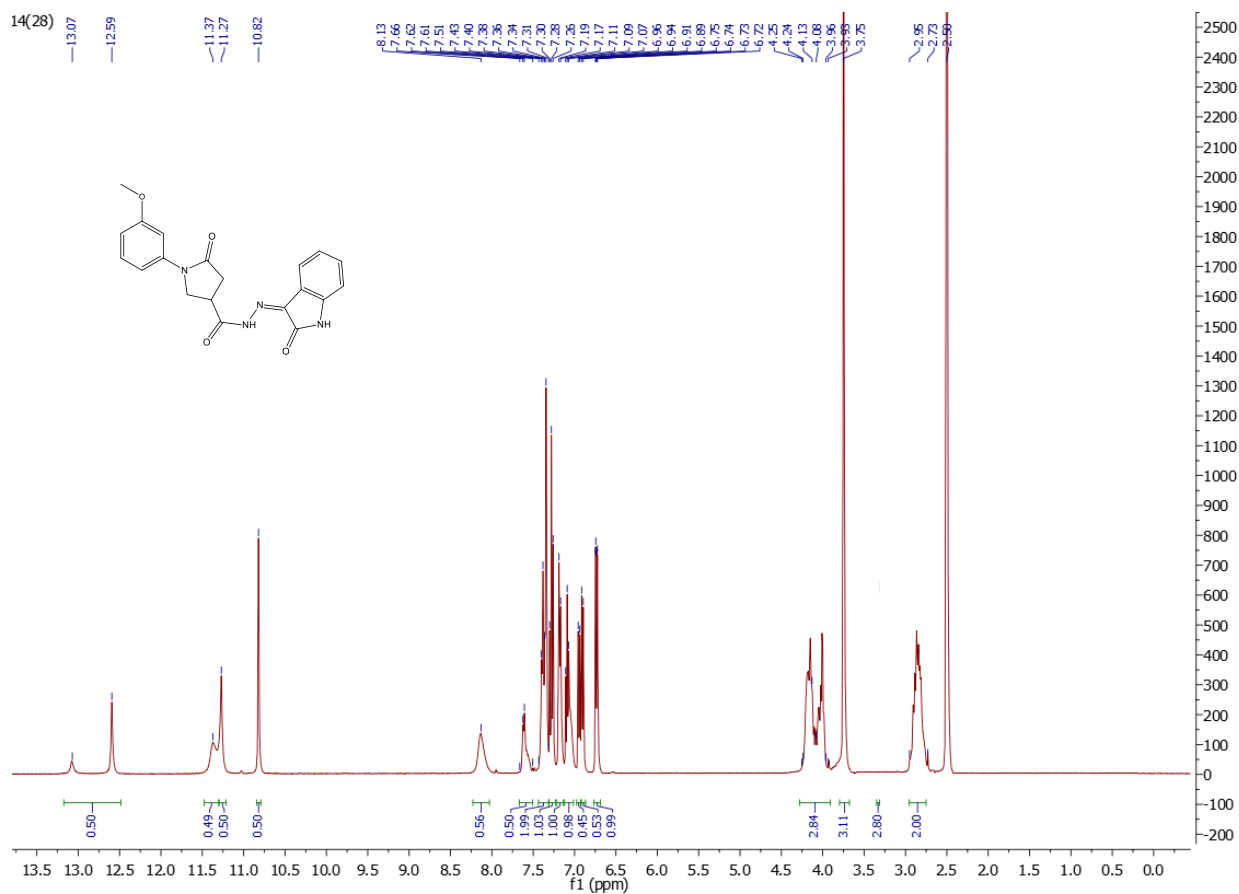


Figure S39. HRMS spectrum of 27



**Figure S40.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **28**

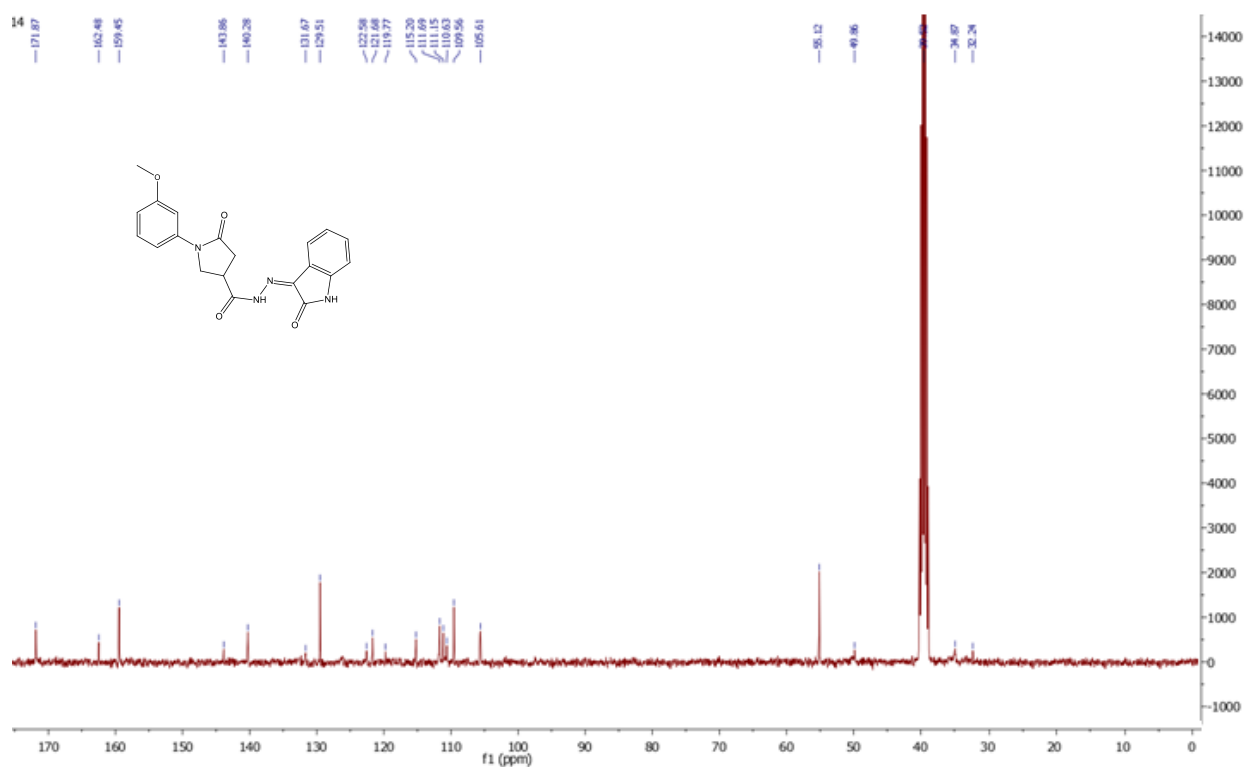


Figure S41. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of 28

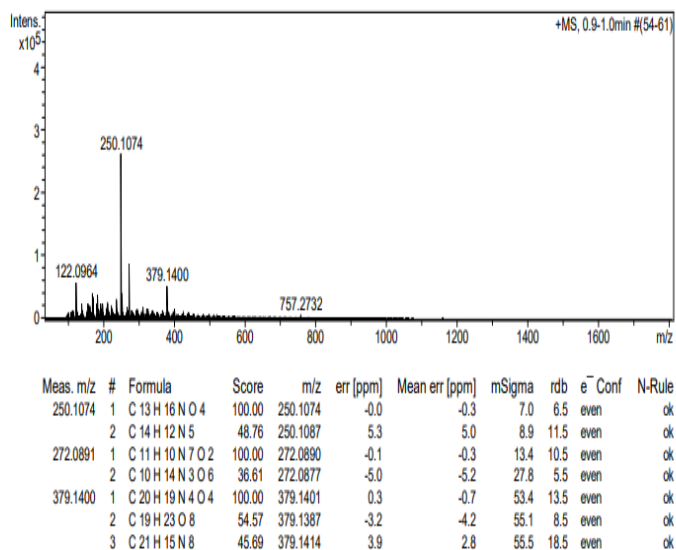


Figure S42. HRMS spectrum of 28

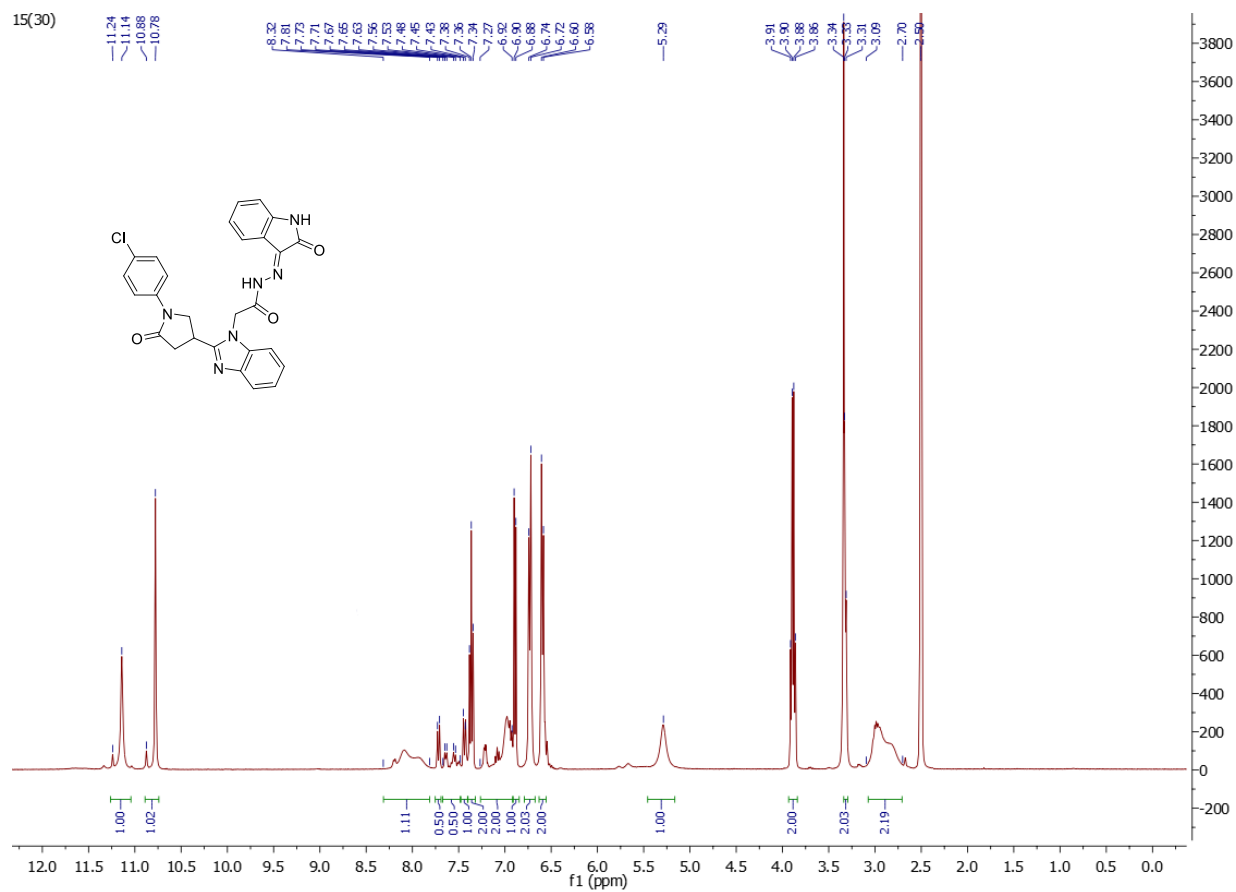


Figure S43. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of 30



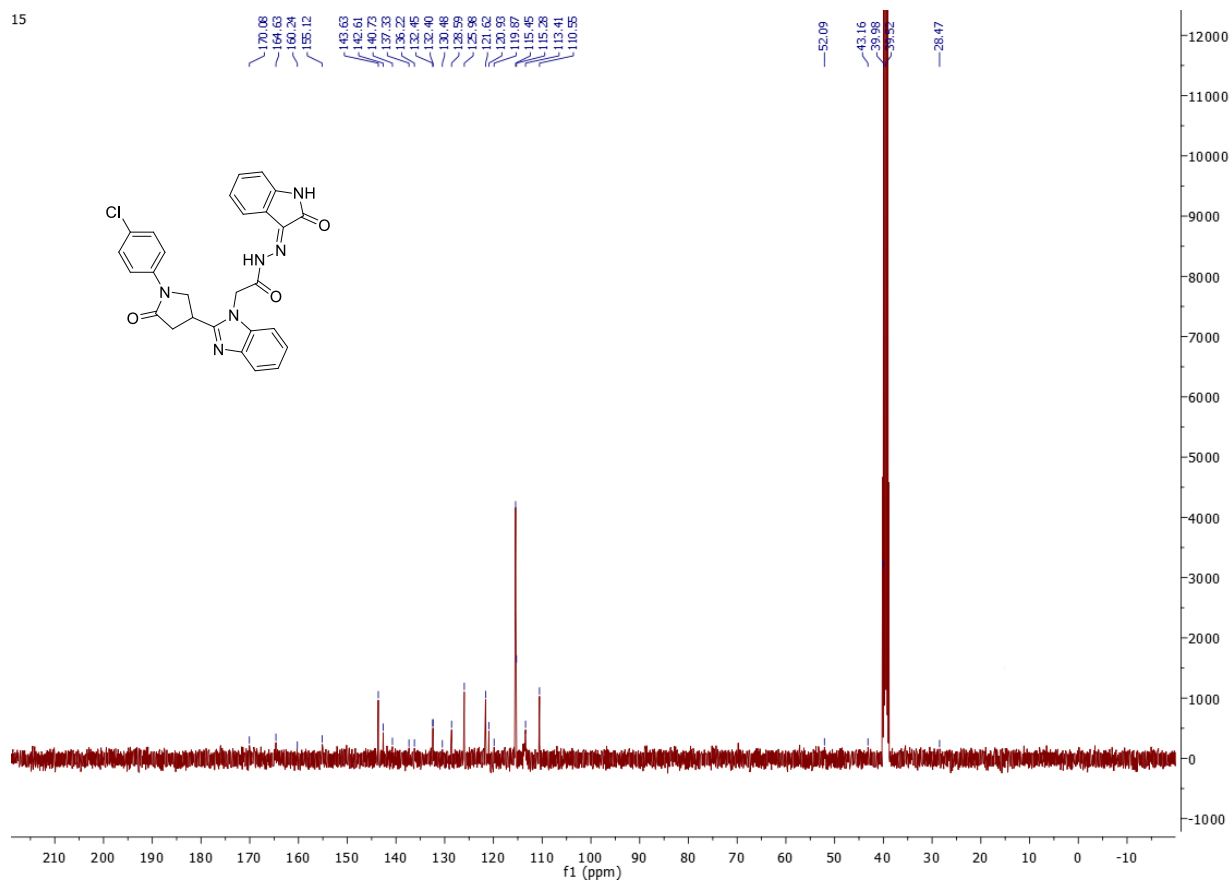


Figure S44. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of 30

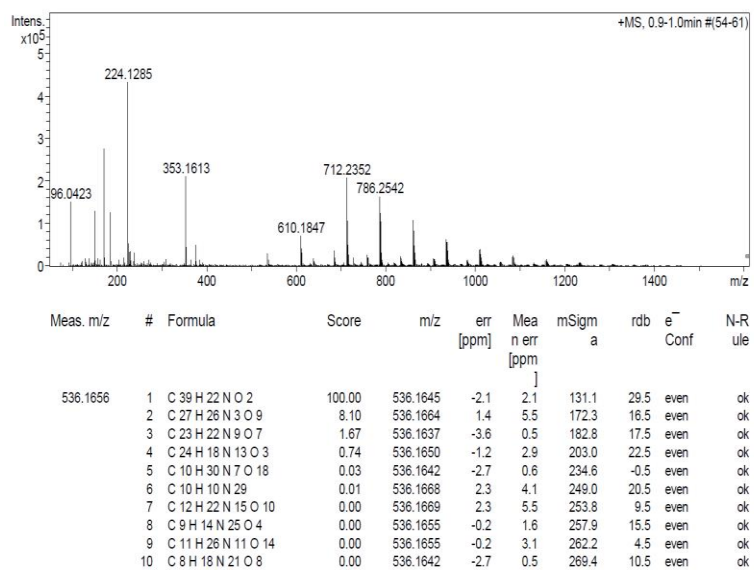
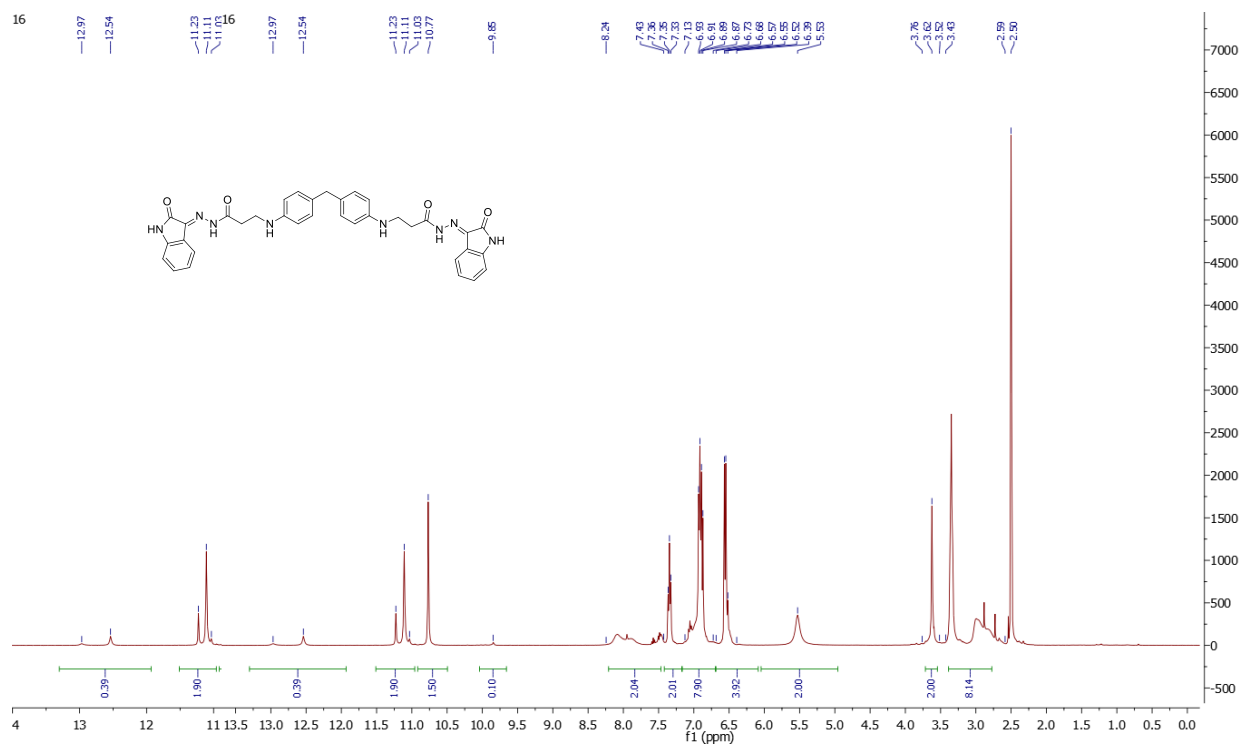


Figure S45. HRMS spectrum of 30



**Figure S46.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **32**

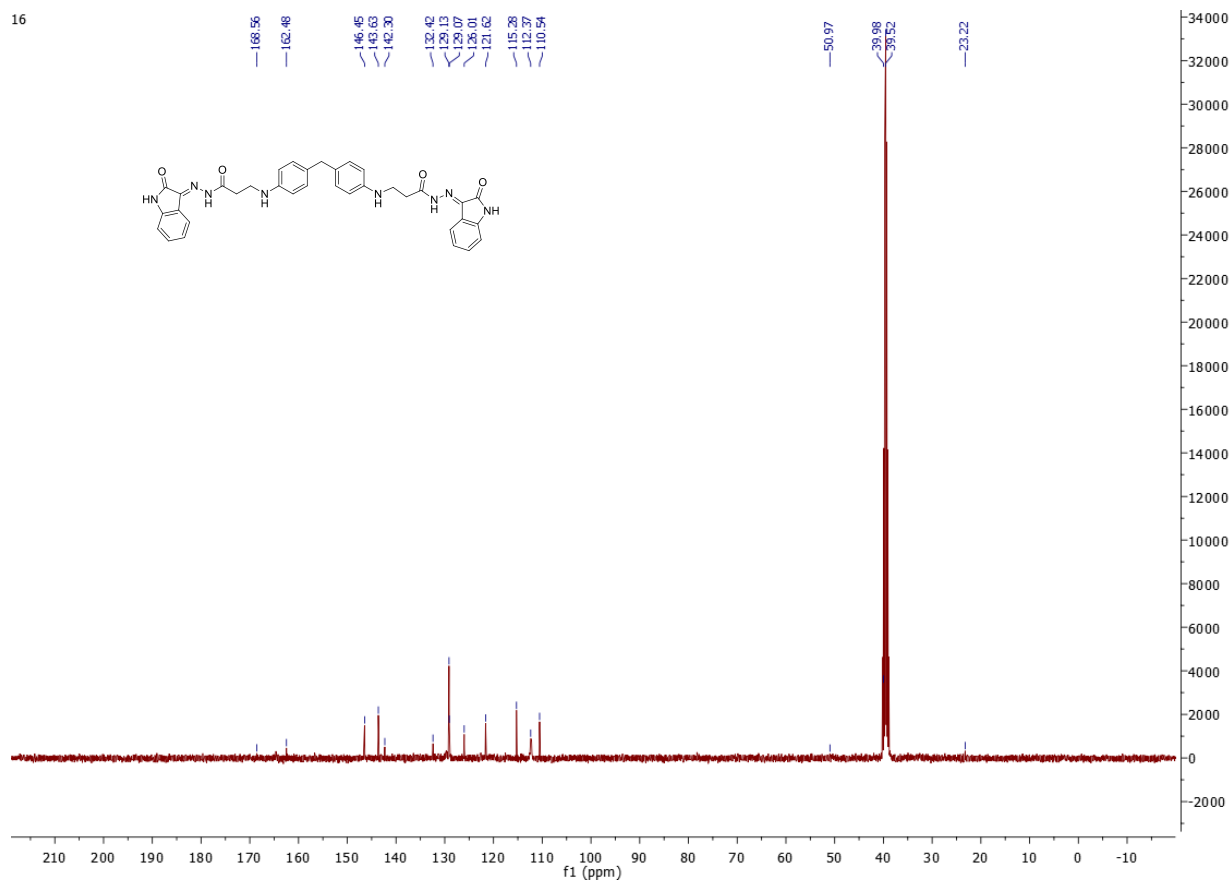


Figure S47. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of **32**

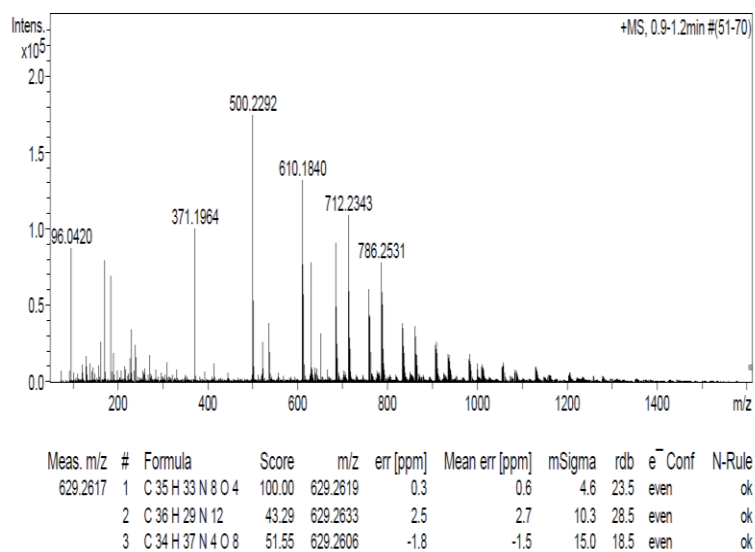
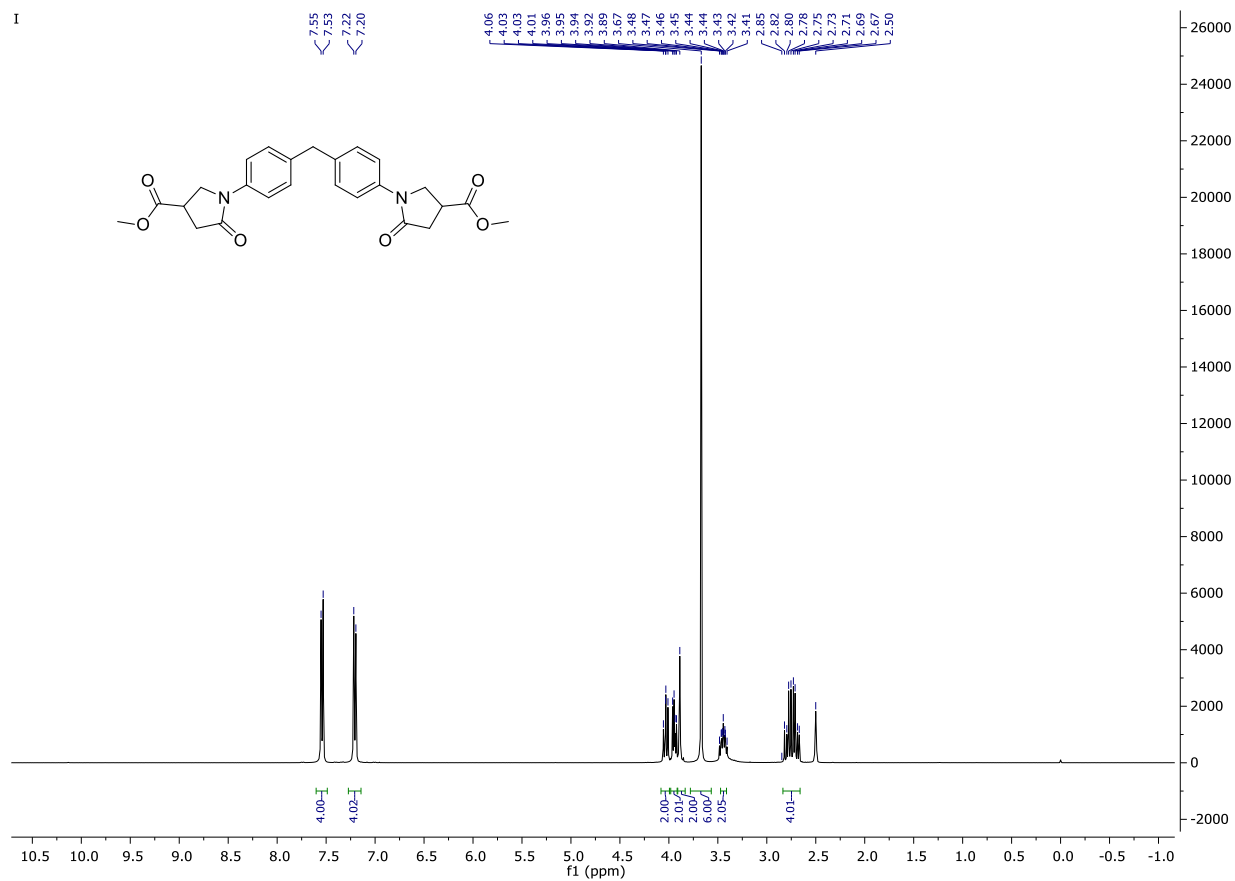


Figure S48. HRMS spectrum of **32**



**Figure S49.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of 33

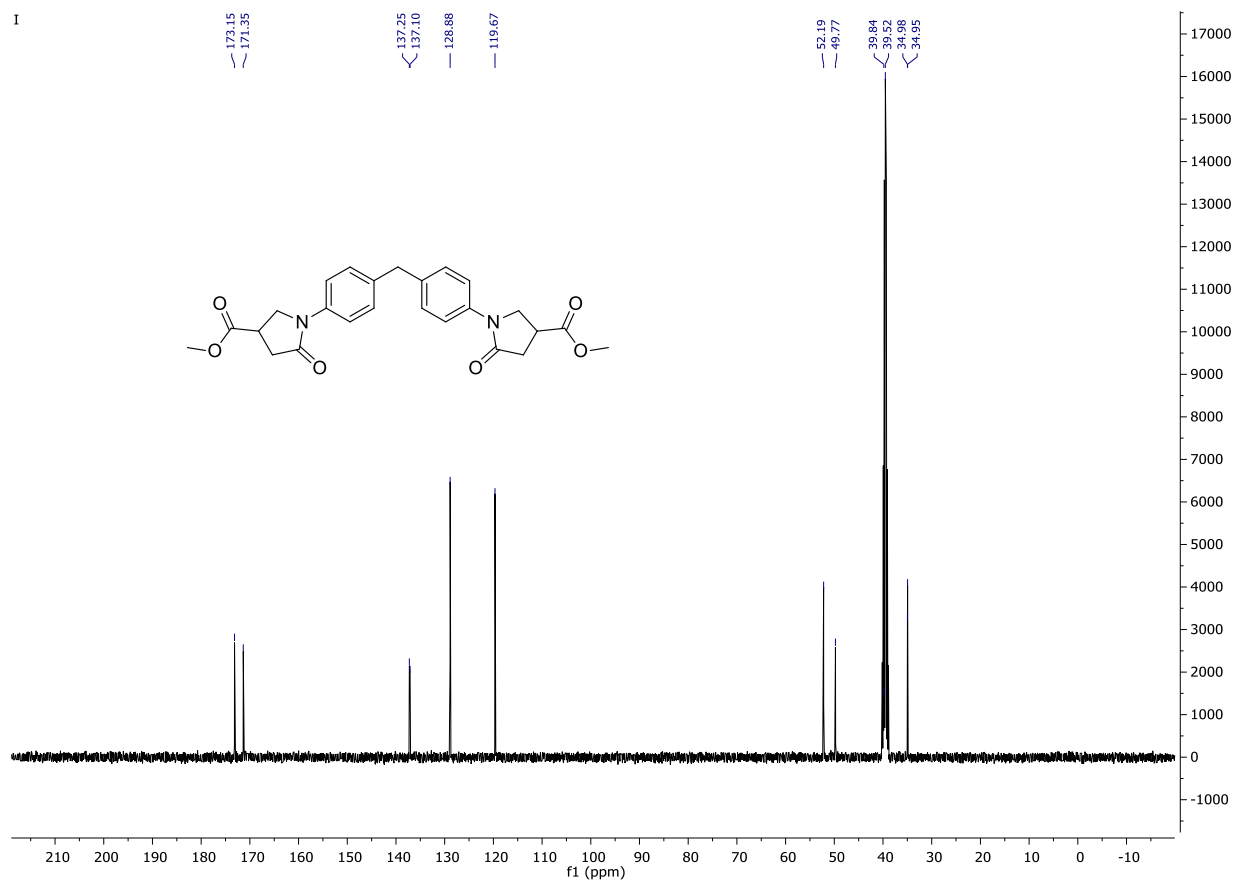


Figure S50. <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of **33**

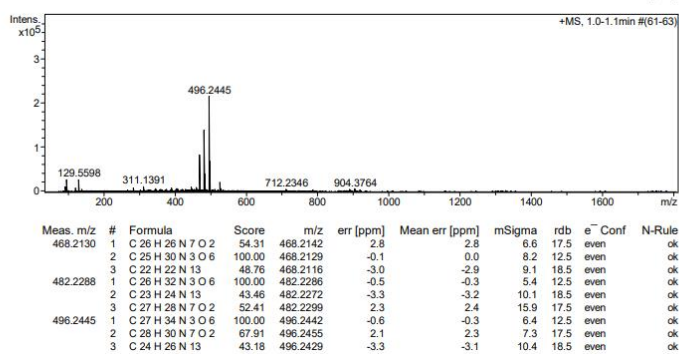
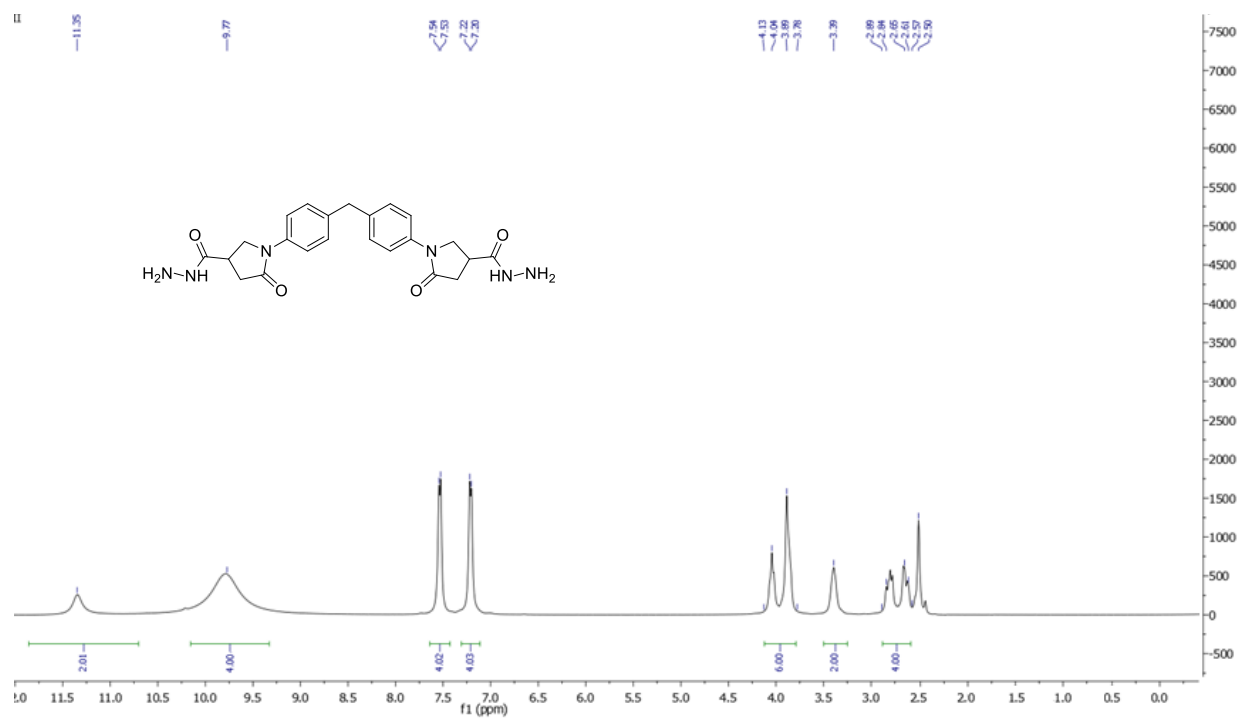


Figure S51. HRMS spectrum of **33**



**Figure S52.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **34**

II

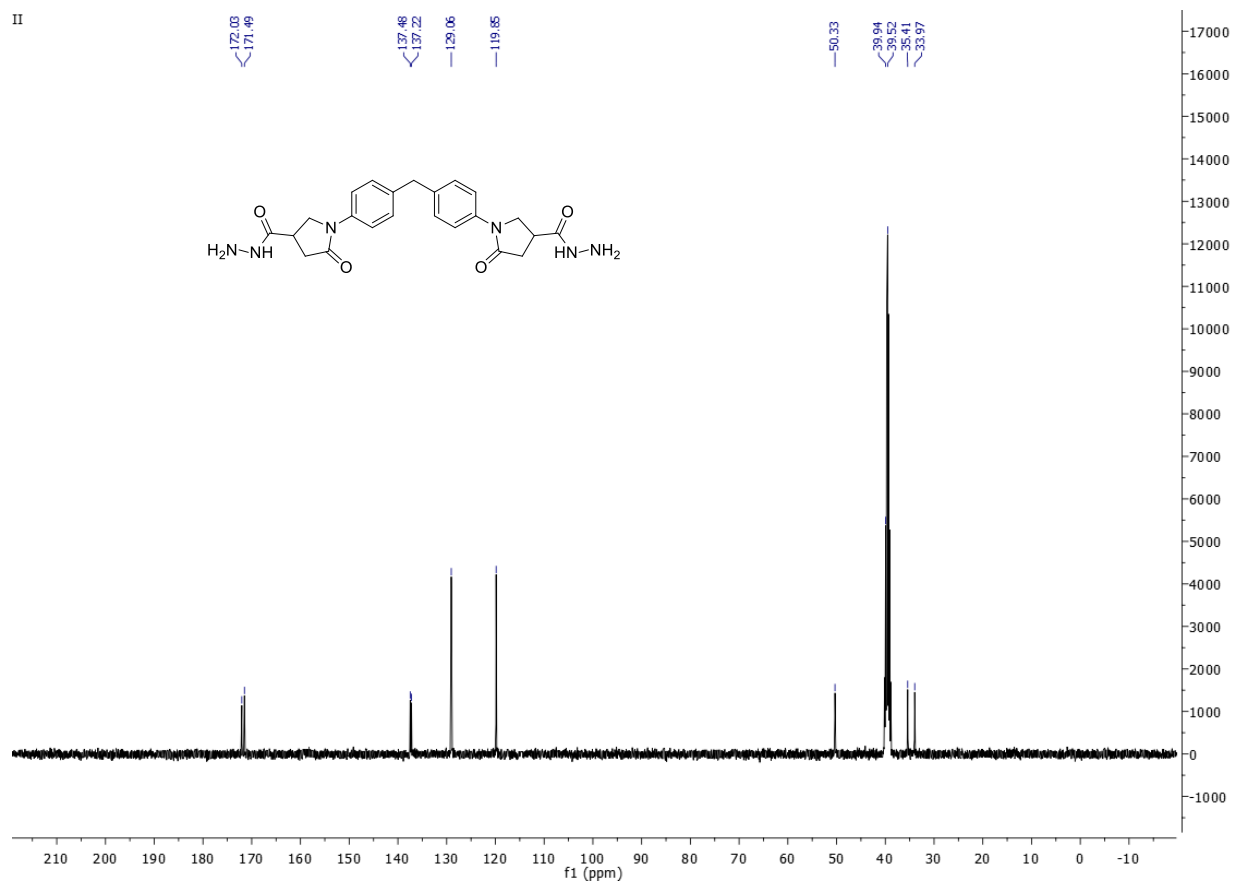


Figure S53.  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-d}_6$ ) spectrum of **34**

**Figure S54** .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) spectrum of **35**



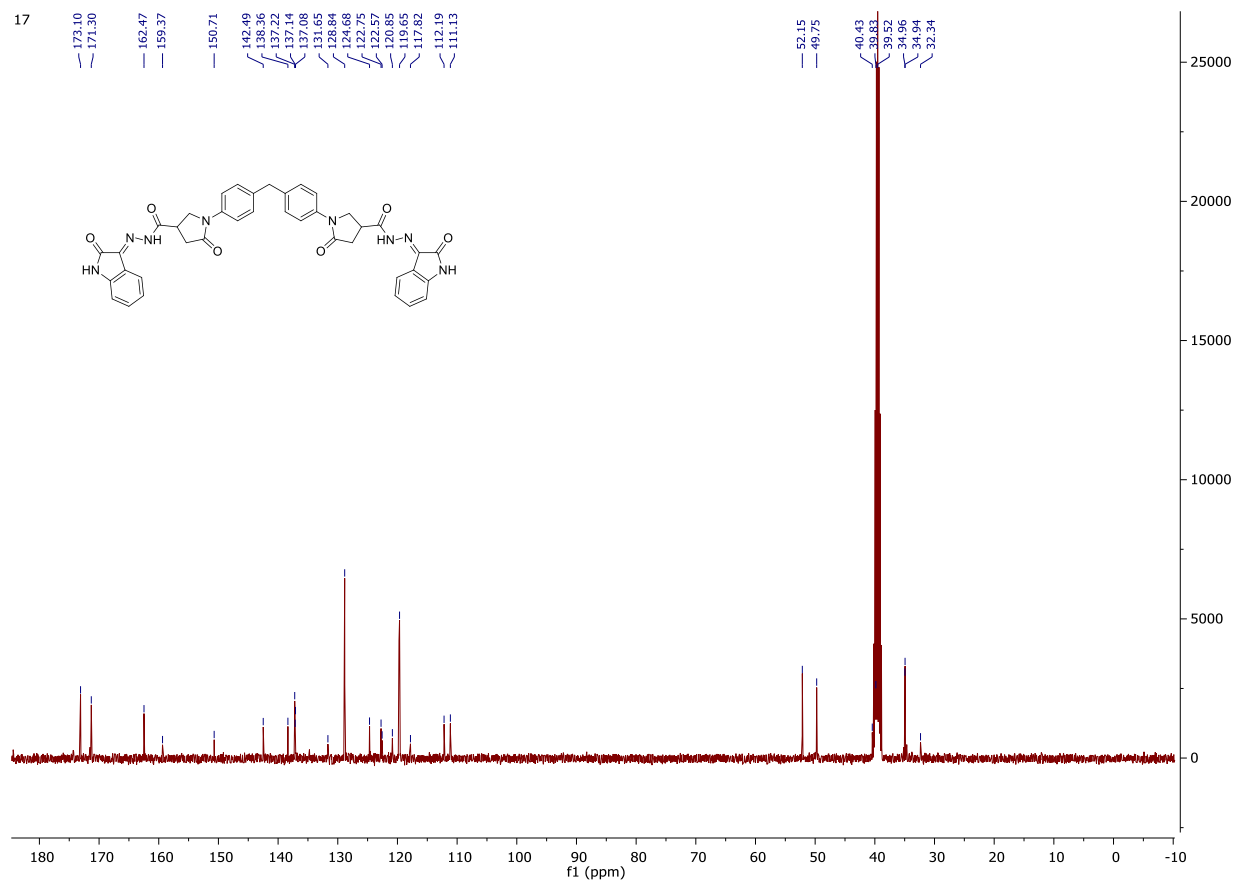


Figure S55.  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ ) spectrum of 35

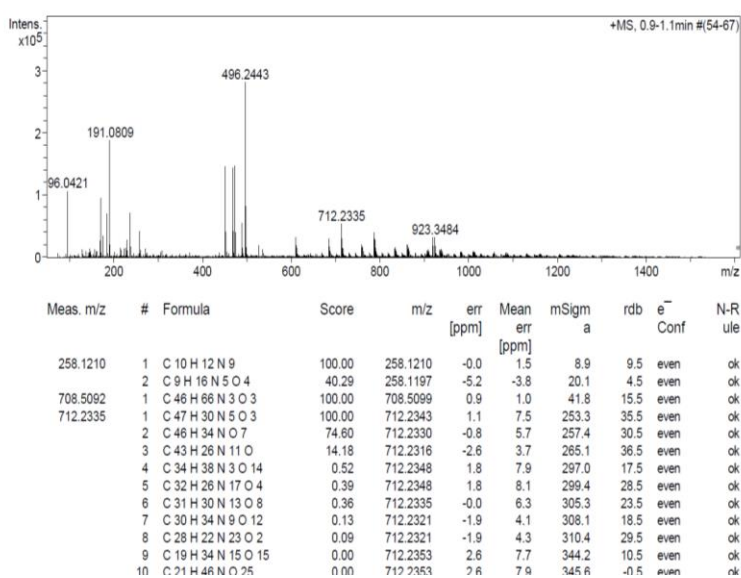


Figure S56. HRMS spectrum of 35

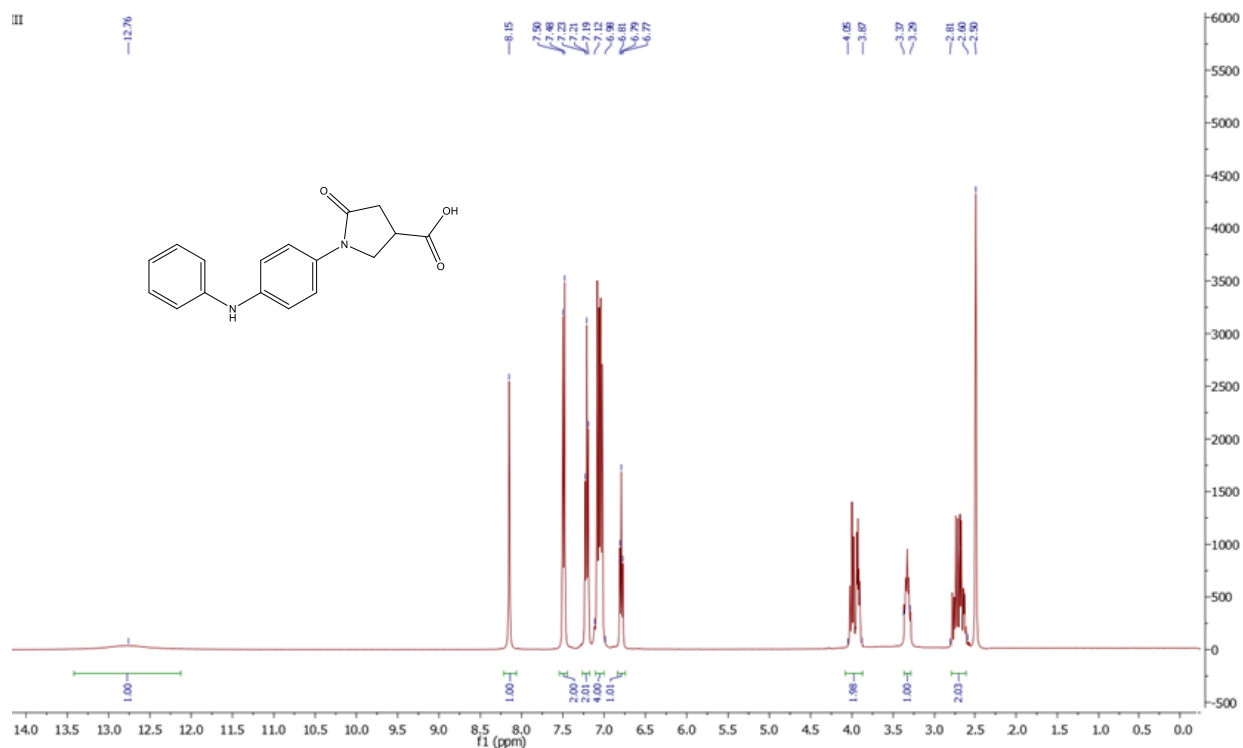
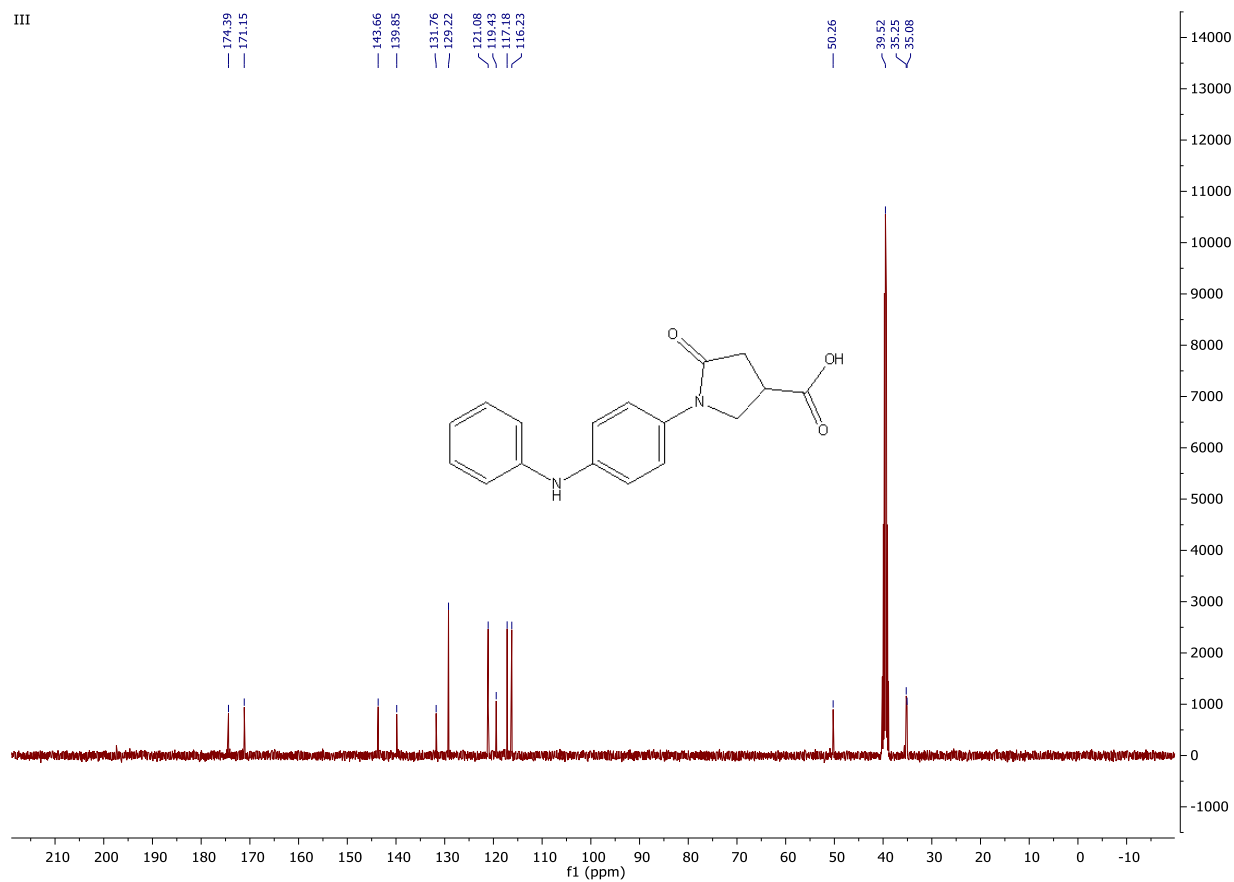
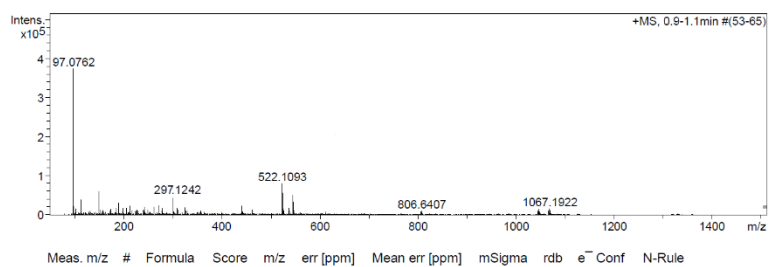


Figure S57.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **36**



**Figure S58.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ ) spectrum of **36**



**Figure S59.** HRMS spectrum of **36**

IV

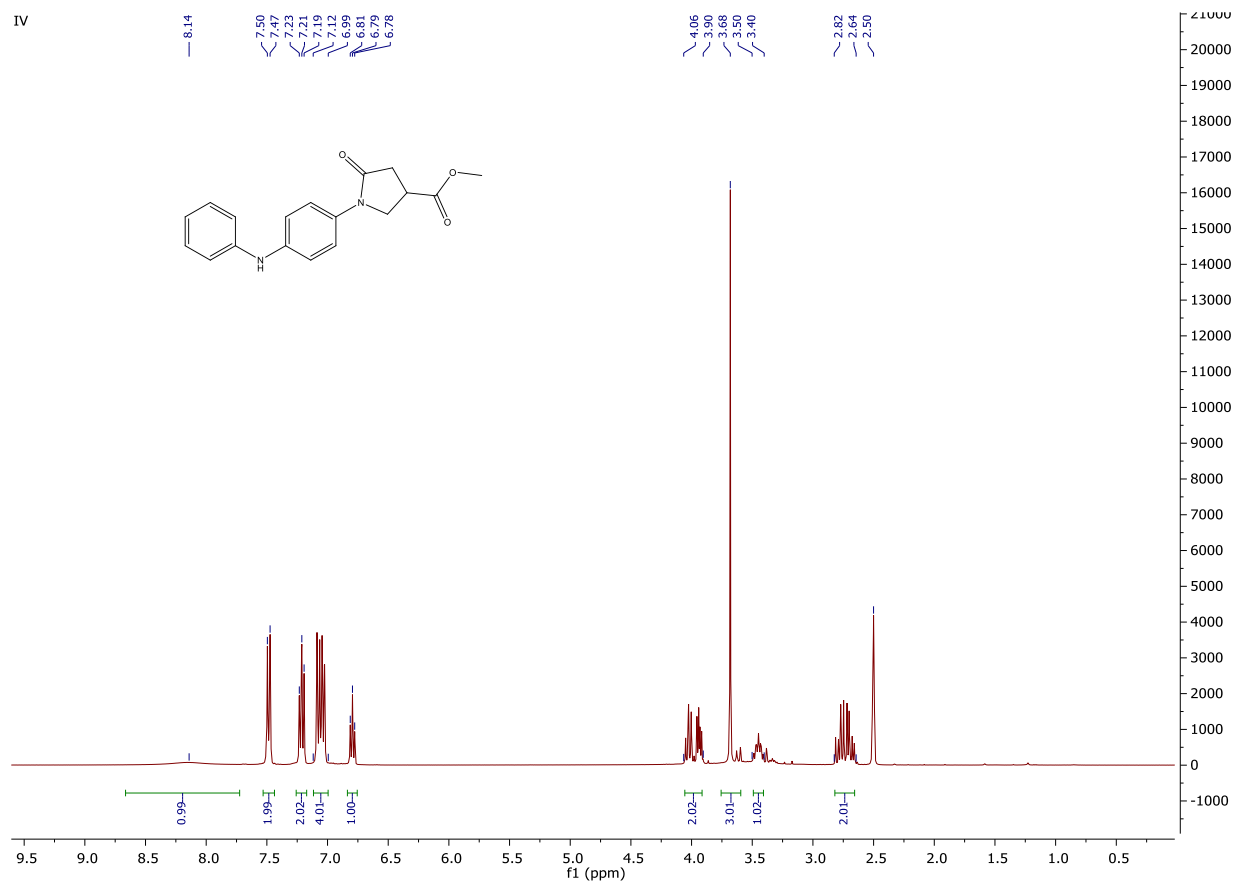
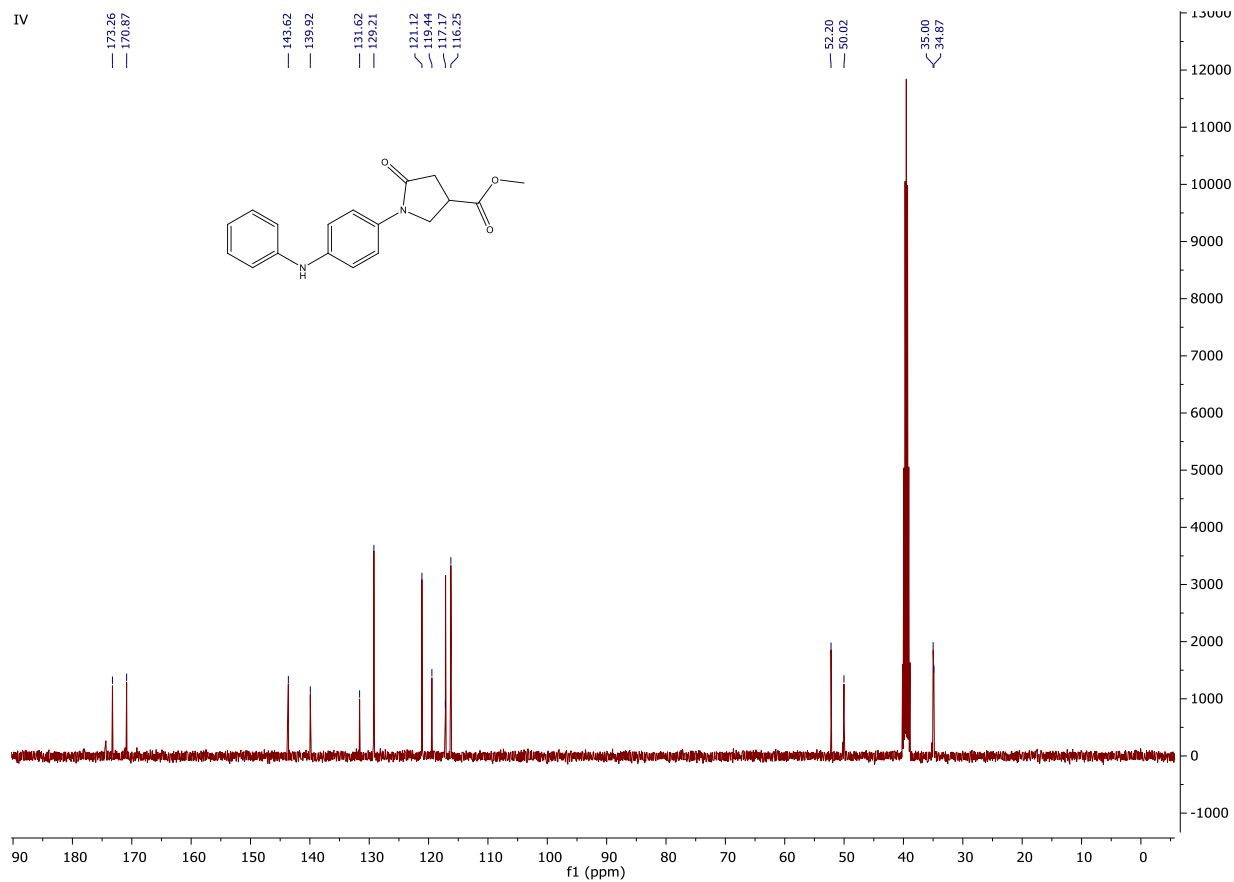
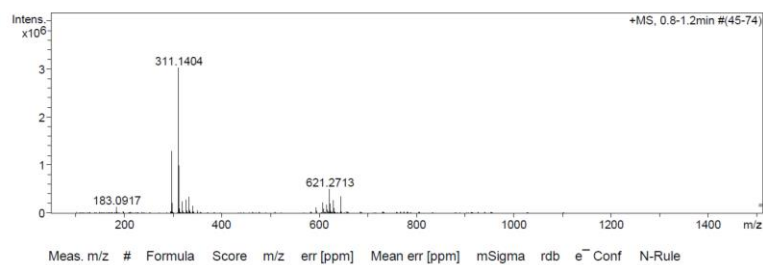


Figure S60. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of 37



**Figure S61.** <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) spectrum of **37**



**Figure S62.** HRMS spectrum of **37**

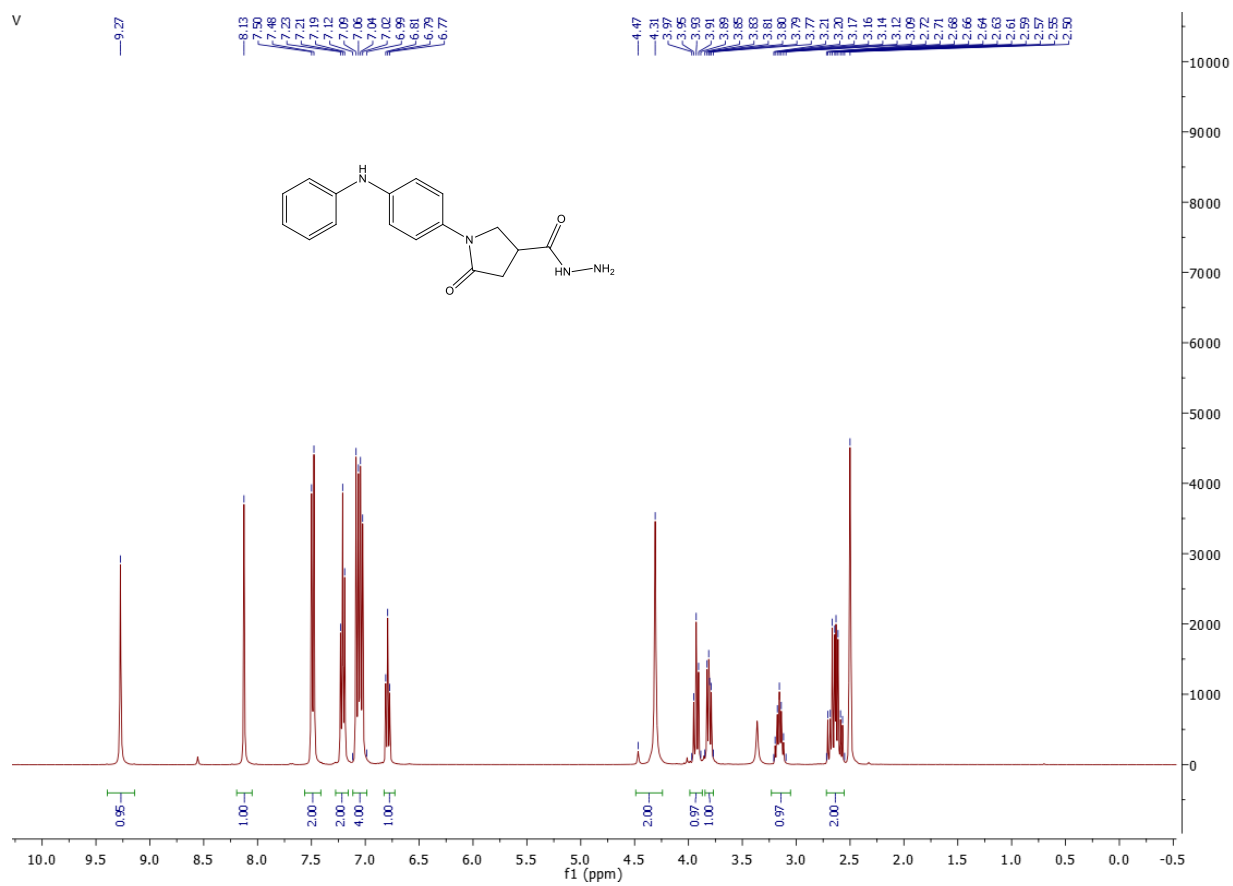


Figure S63. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of 38

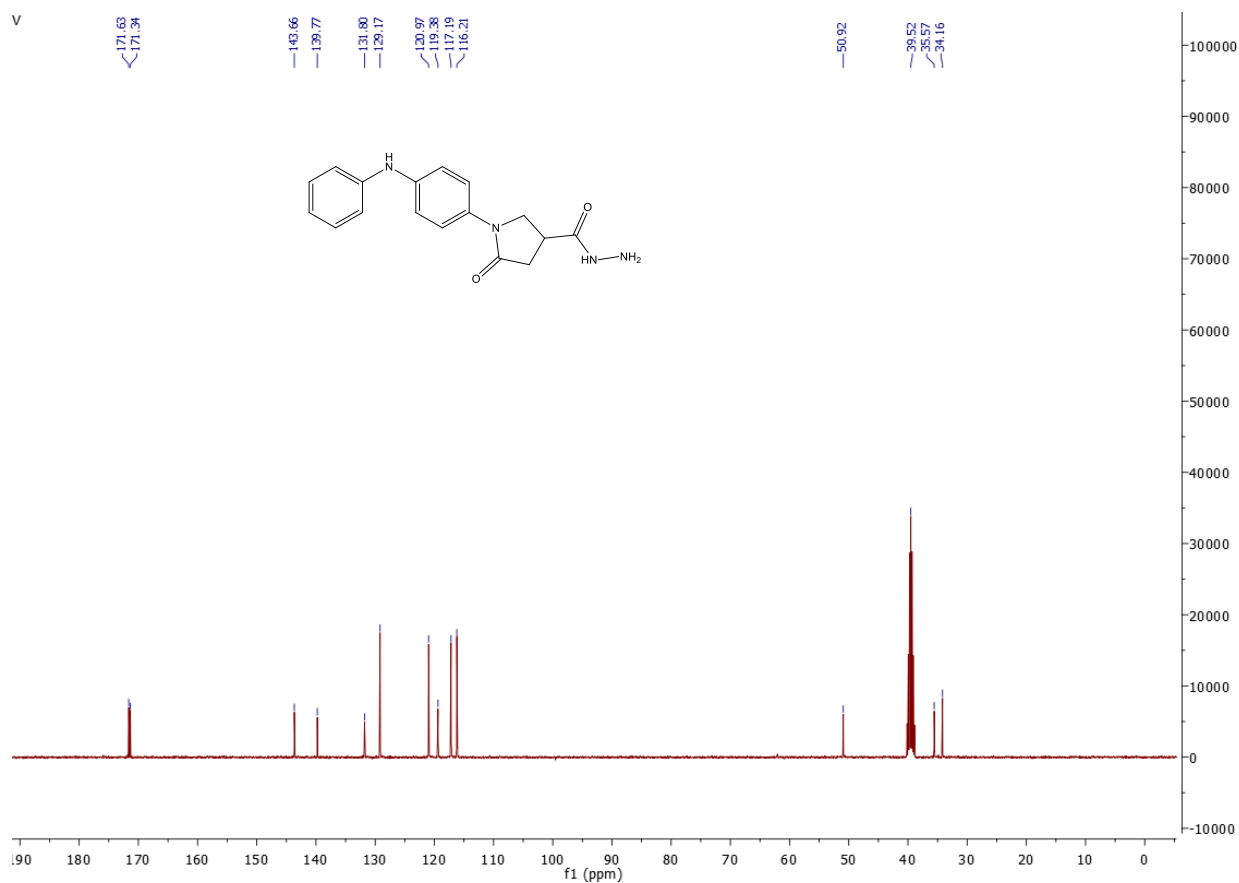


Figure S64.  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO}-d_6$ ) spectrum of 38

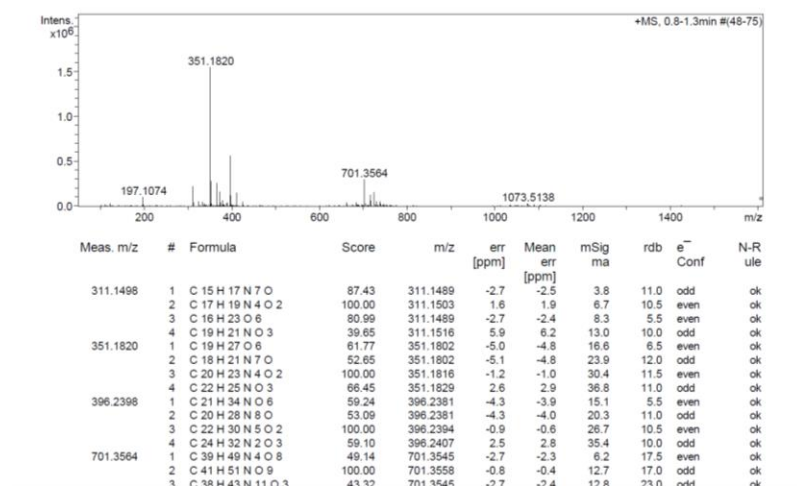
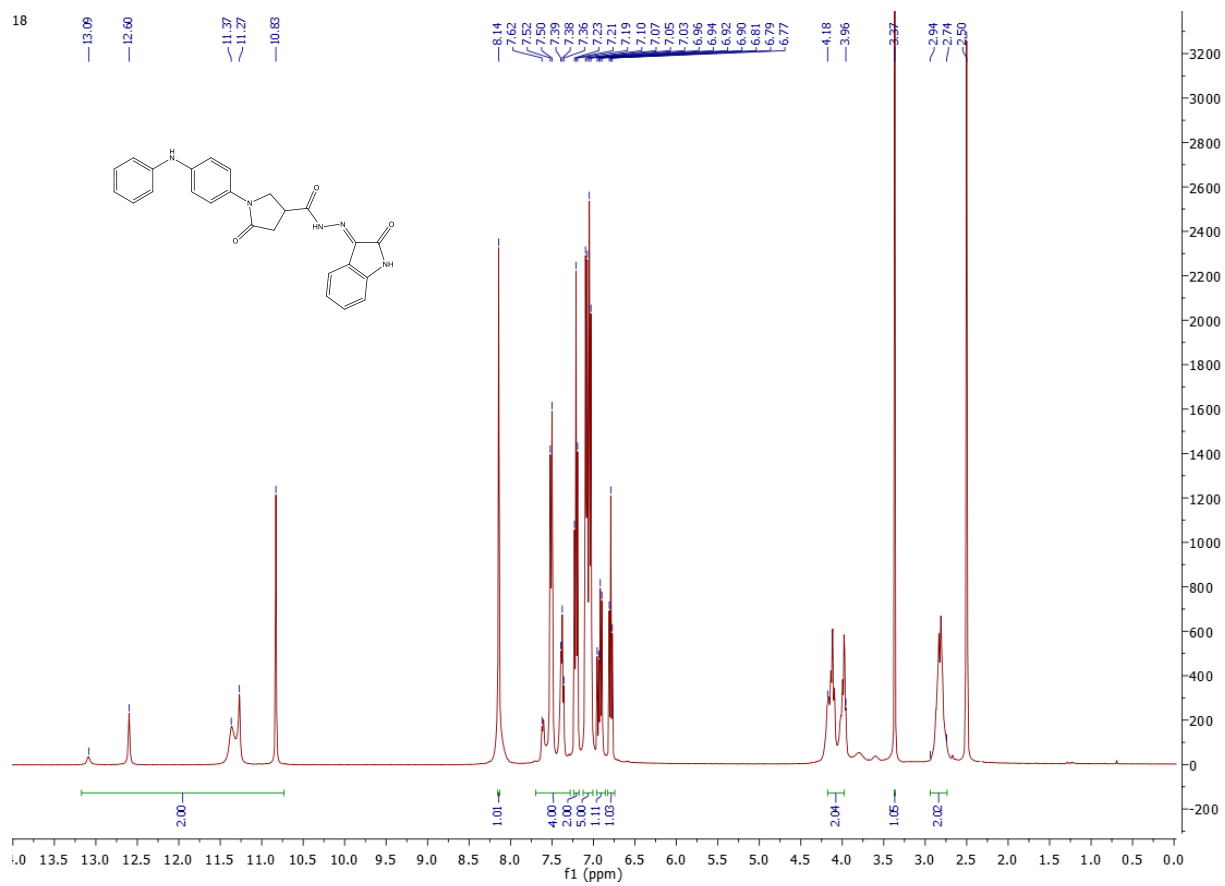


Figure S65. HRMS spectrum of 38





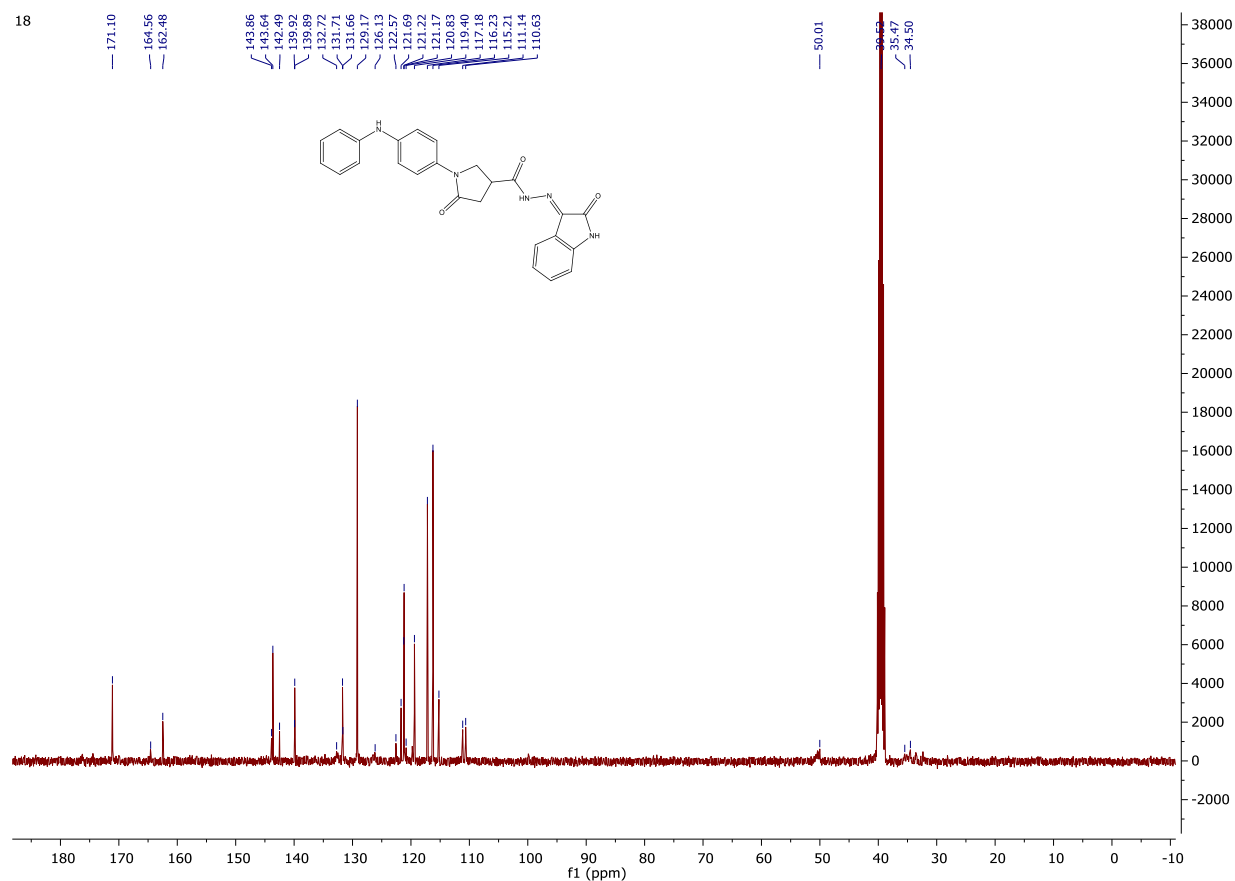
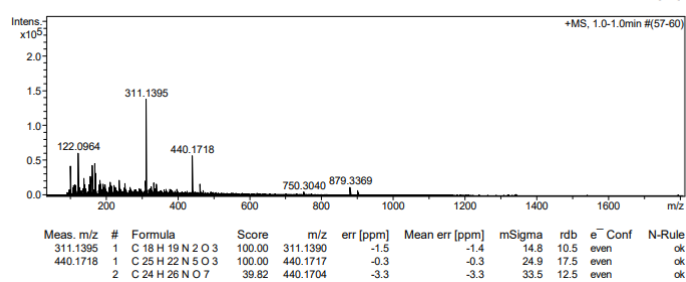
Figure S67. <sup>13</sup>C NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of 39

Figure S68. HRMS spectrum of 39