

# Supporting Information

## A suitable functionalization of nitroindazoles with triazolyl and pyrazolyl moieties *via* cycloaddition reactions

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# I - NMR and mass spectrum of compounds 2a-d, 3a-d, 4a-d and 5a-d

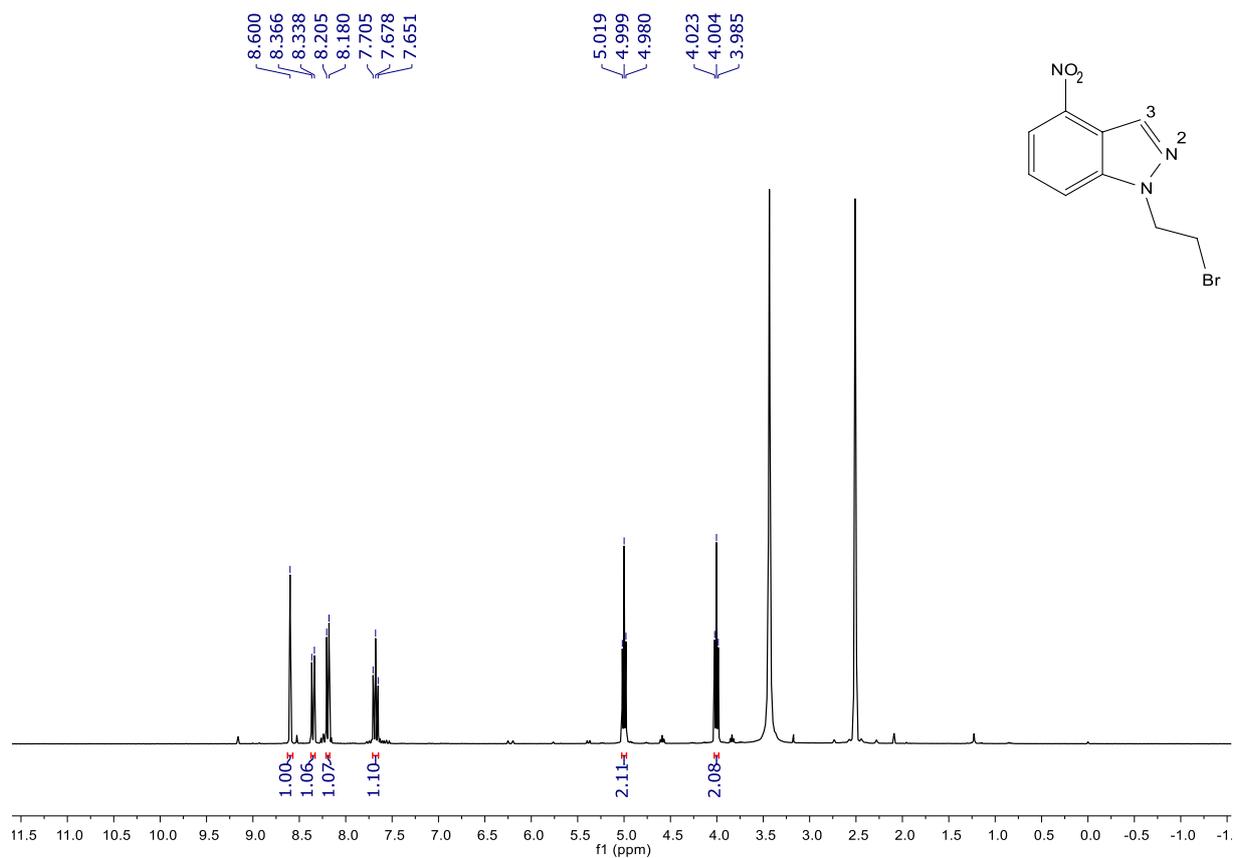


Figure S1. <sup>1</sup>H NMR spectrum of compound 2a in DMSO-d<sub>6</sub>.

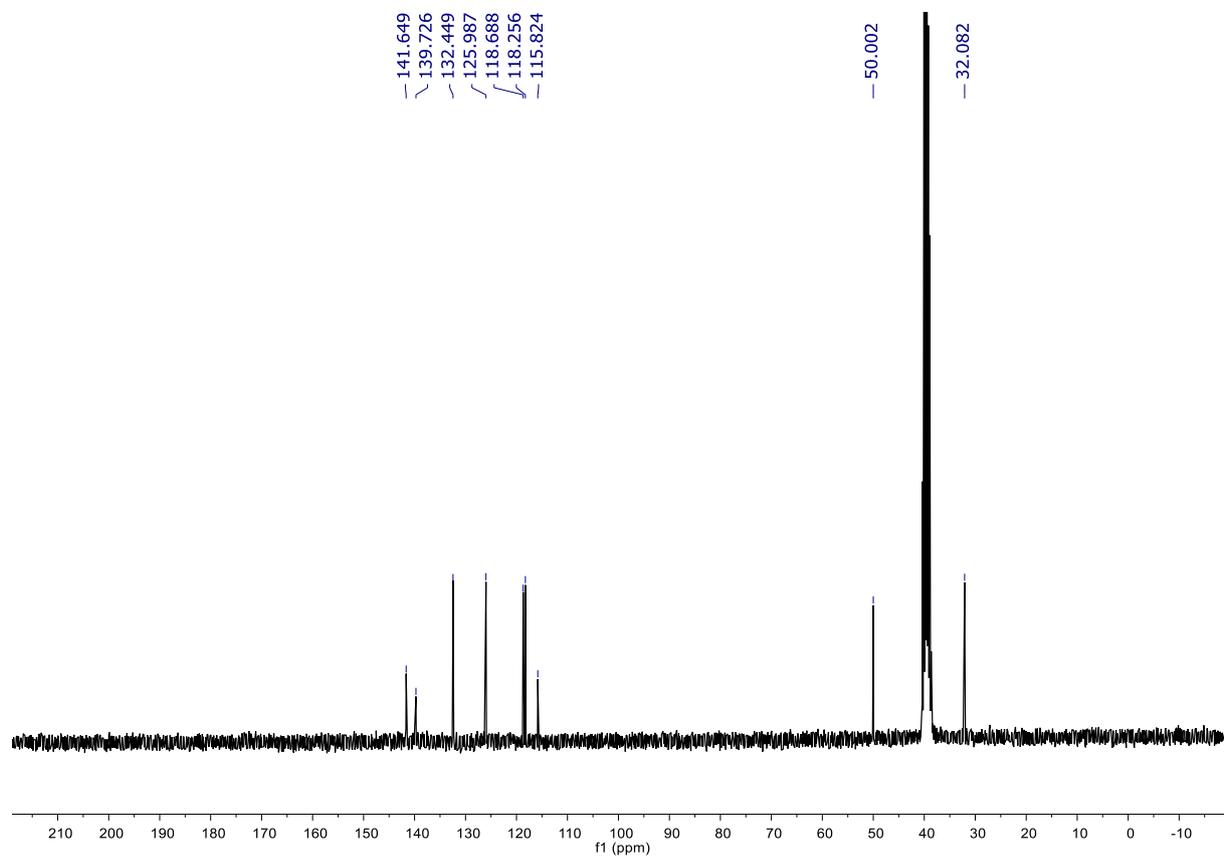


Figure S2. <sup>13</sup>C NMR spectrum of compound 2a in DMSO-d<sub>6</sub>.

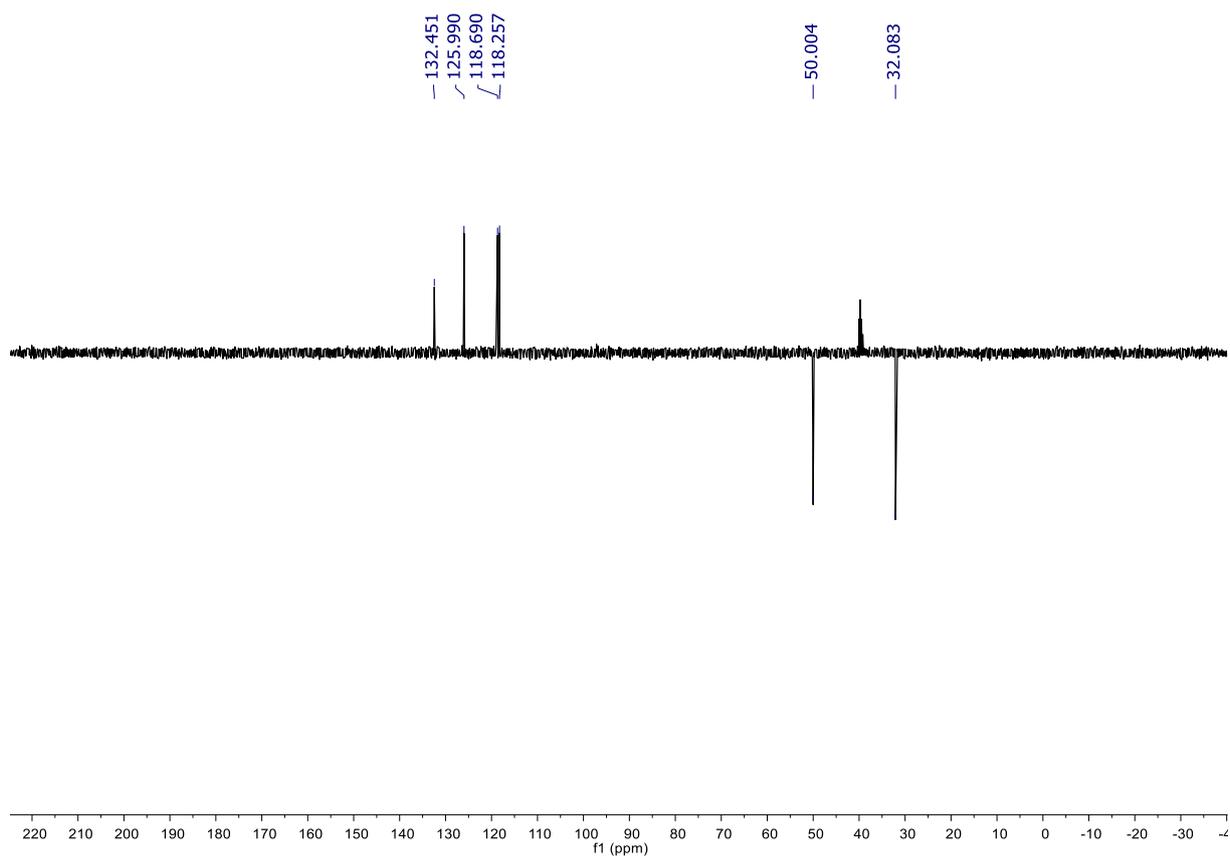


Figure S3. <sup>13</sup>C NMR DEPT 135 spectrum of compound **2a** in DMSO-d<sub>6</sub>.

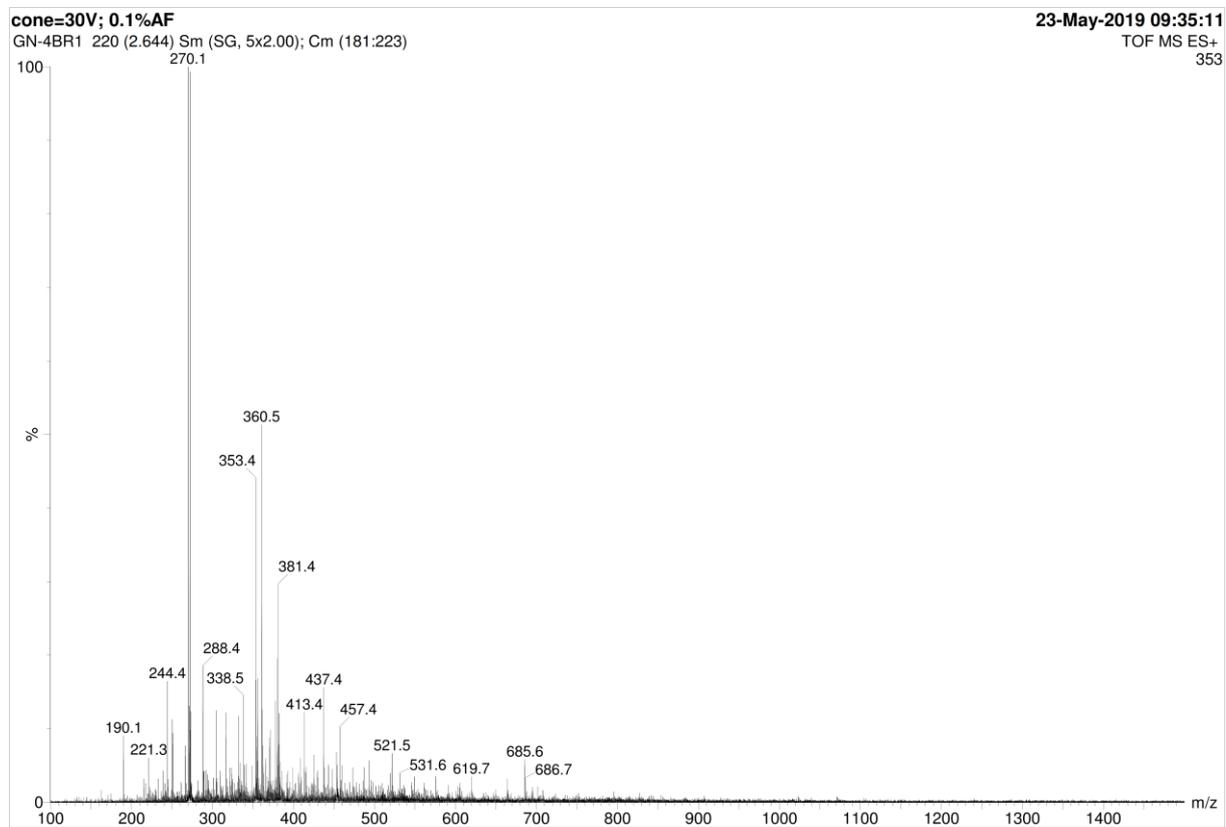
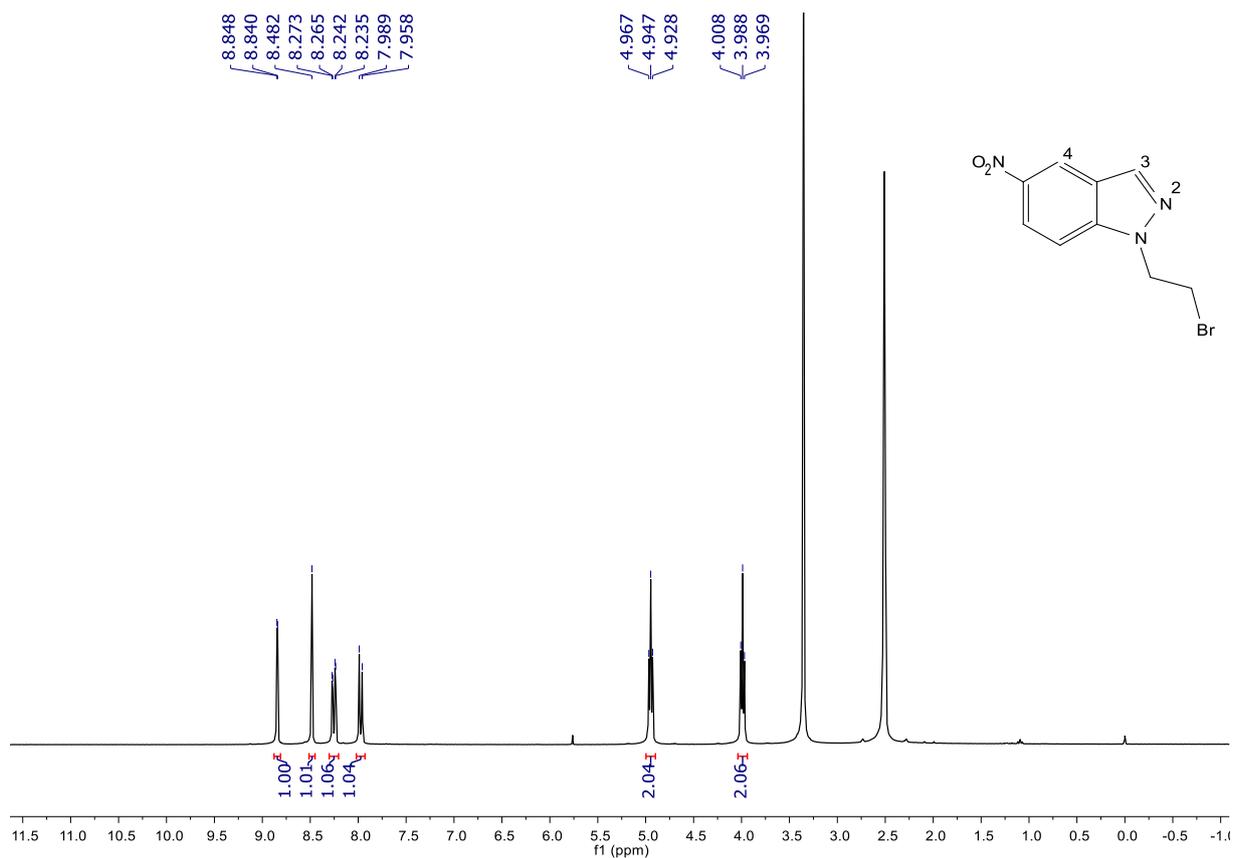
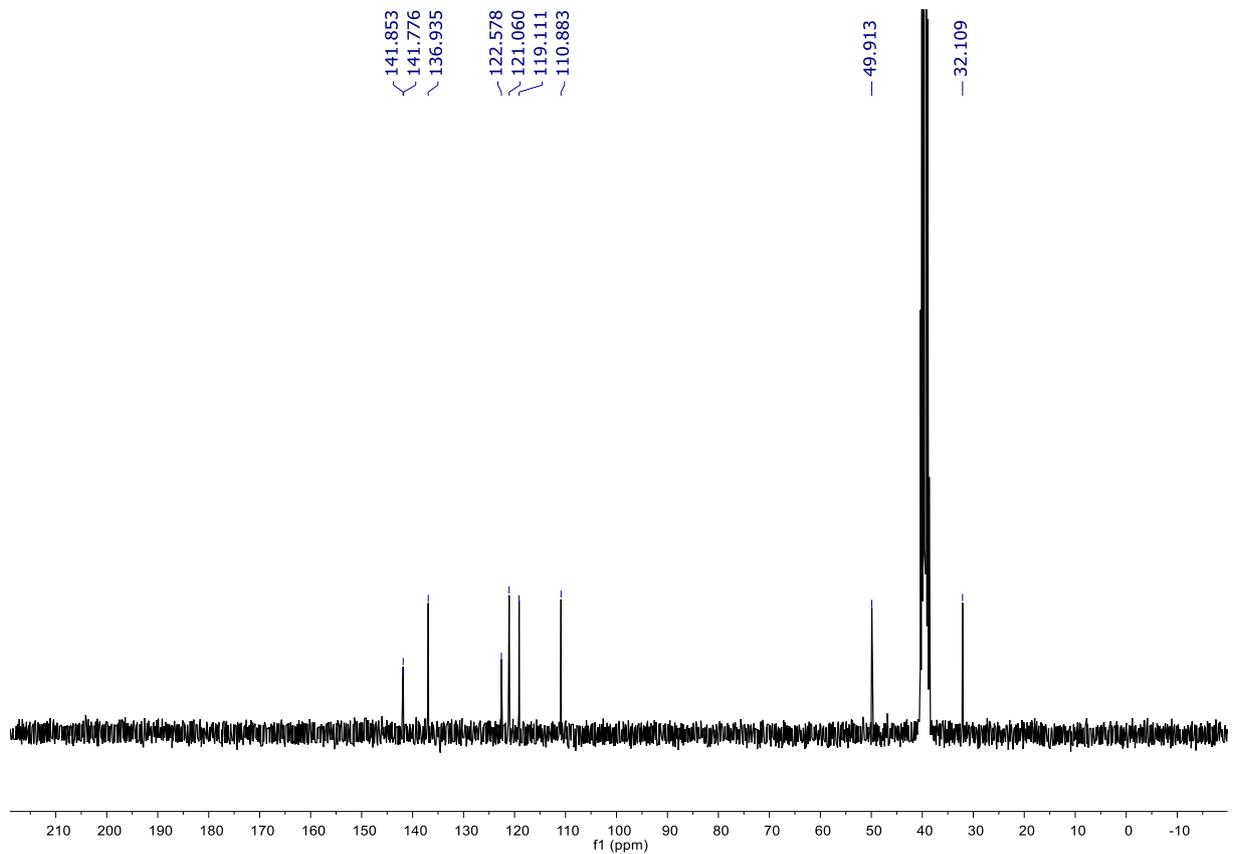


Figure S4. MS-ESI(+) spectrum of compound **2a**.



**Figure S5.** <sup>1</sup>H NMR spectrum of compound **2b** in DMSO-d<sub>6</sub>.



**Figure S6.** <sup>13</sup>C NMR spectrum of compound **2b** in DMSO-d<sub>6</sub>.

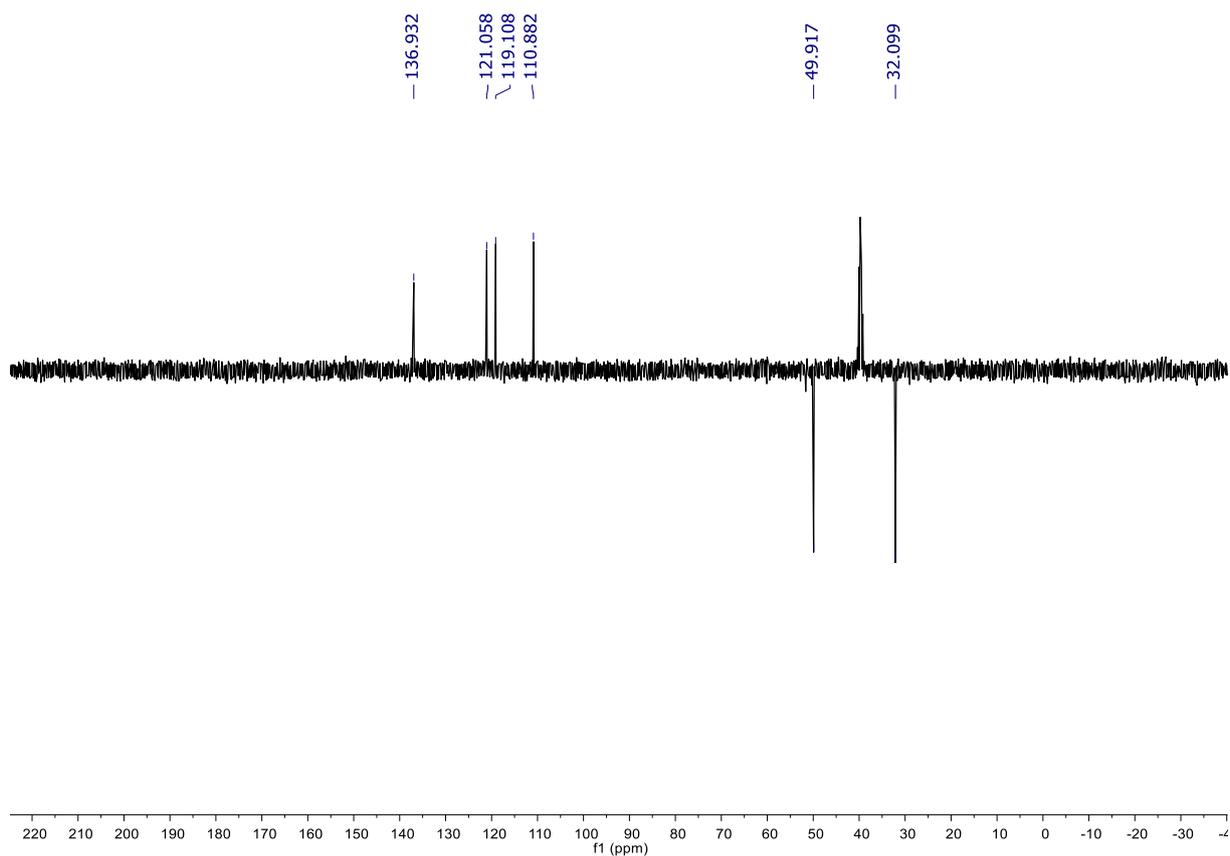


Figure S7.  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **2b** in  $\text{DMSO-d}_6$ .

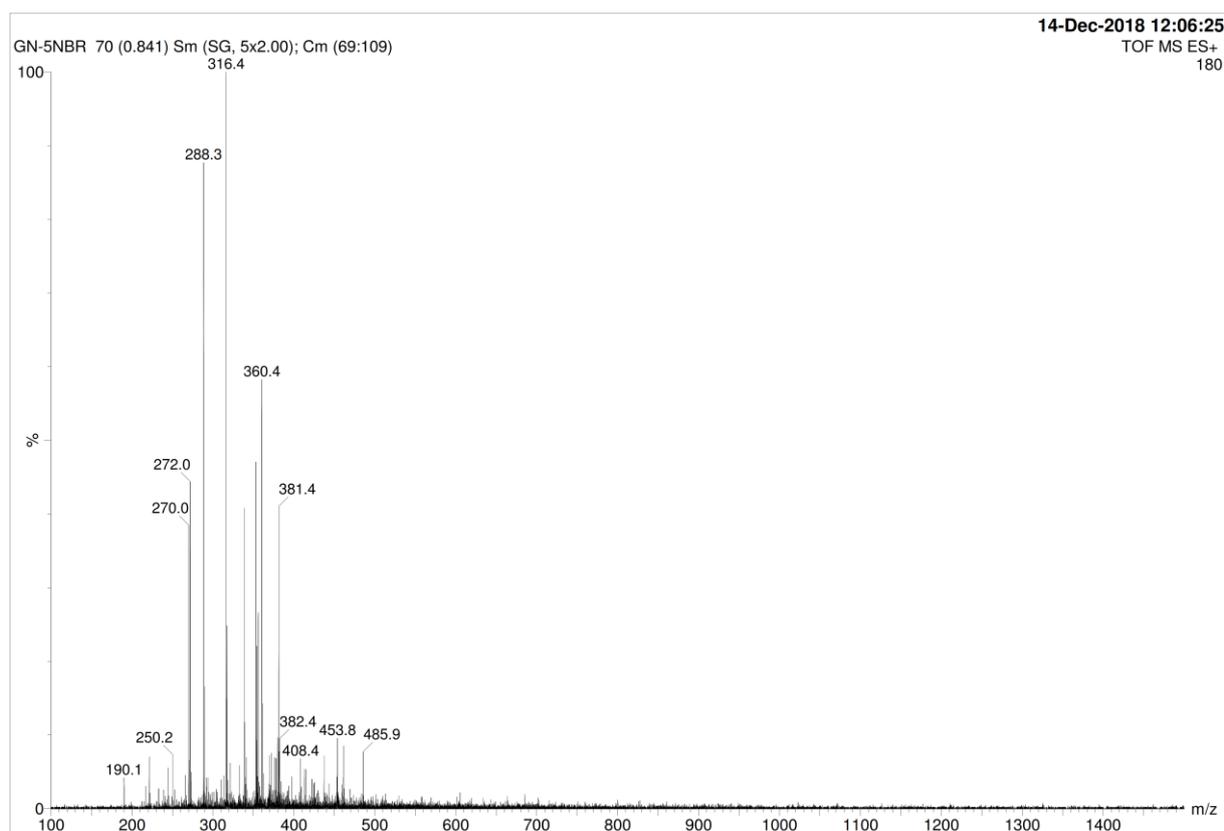


Figure S8. MS-ESI(+) spectrum of compound **2b**.

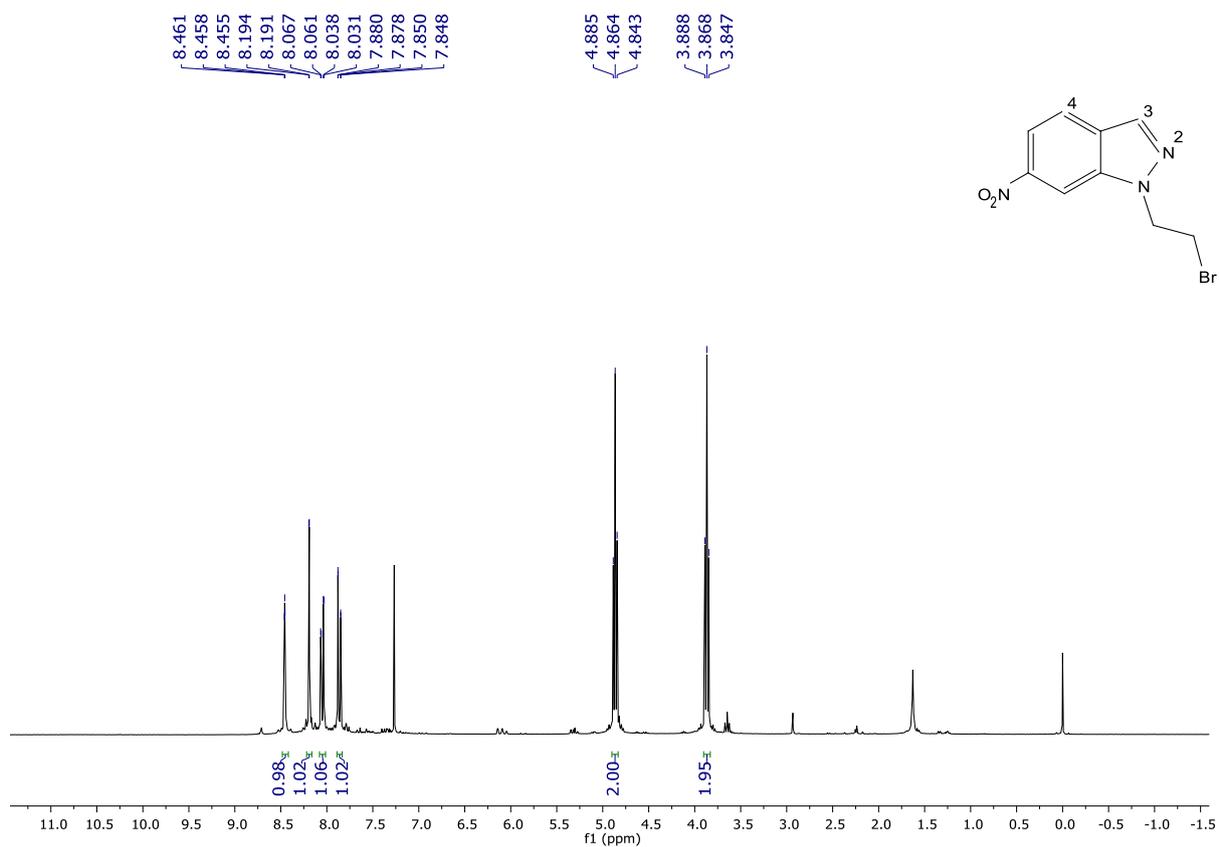


Figure S9. <sup>1</sup>H NMR spectrum of compound **2c** in CDCl<sub>3</sub>.

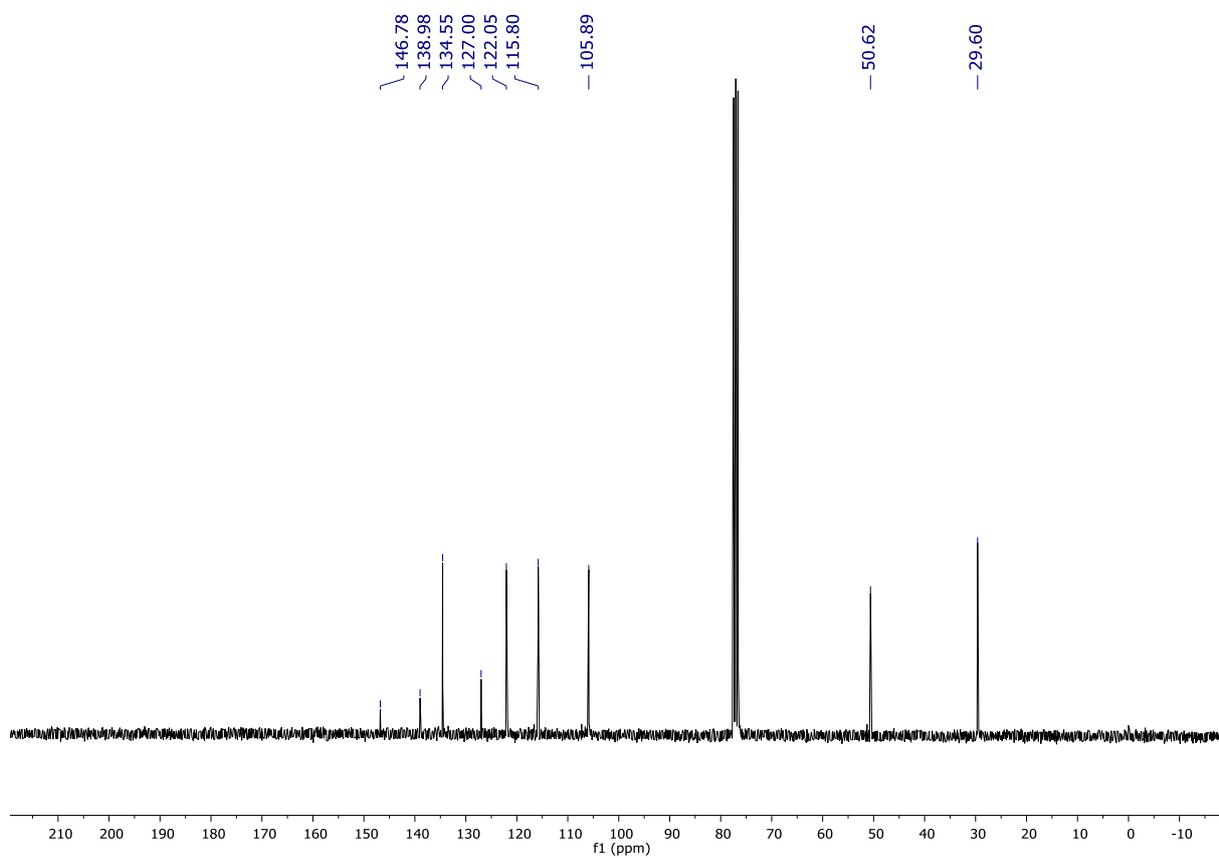
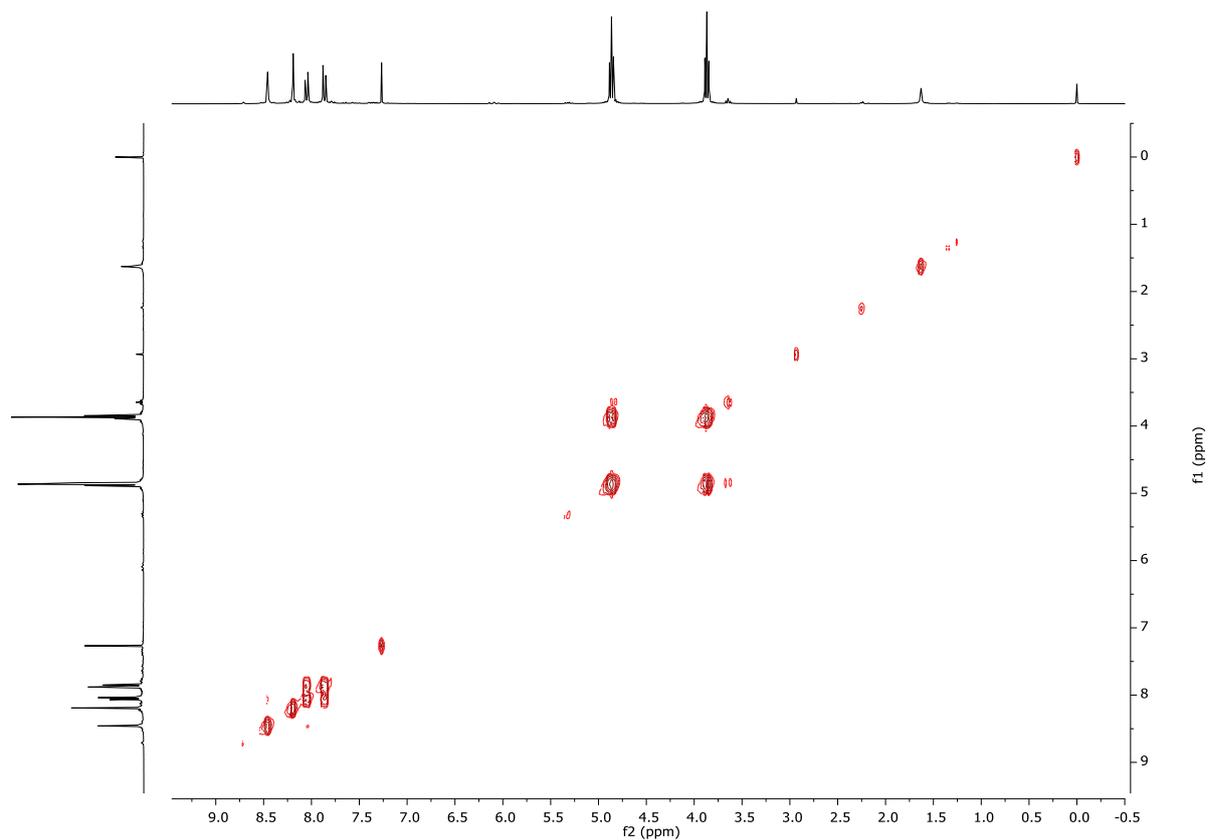
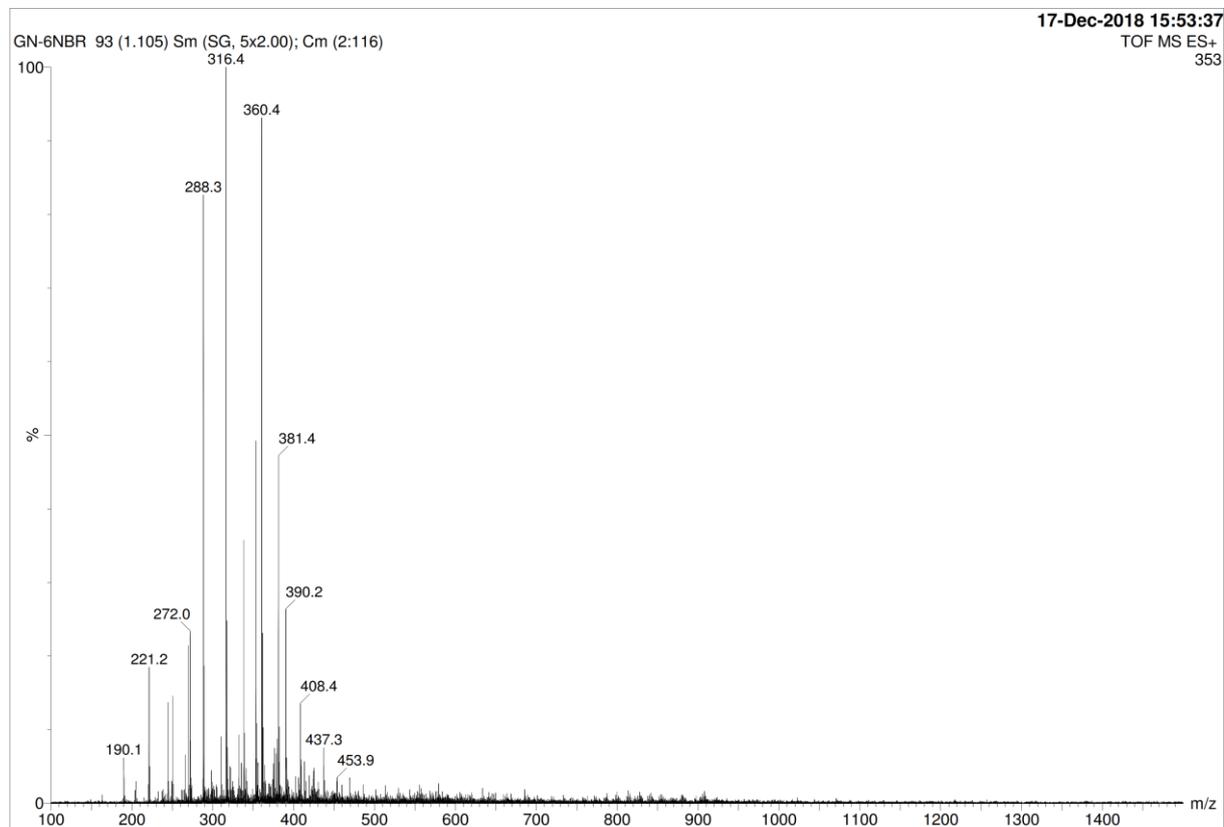


Figure S10. <sup>13</sup>C NMR spectrum of compound **2c** in CDCl<sub>3</sub>.



**Figure S11.** COSY ( $^1\text{H}/^1\text{H}$ ) spectrum of compound **2c** in  $\text{CDCl}_3$ .



**Figure S12.** MS-ESI(+) spectrum of compound **2c**.

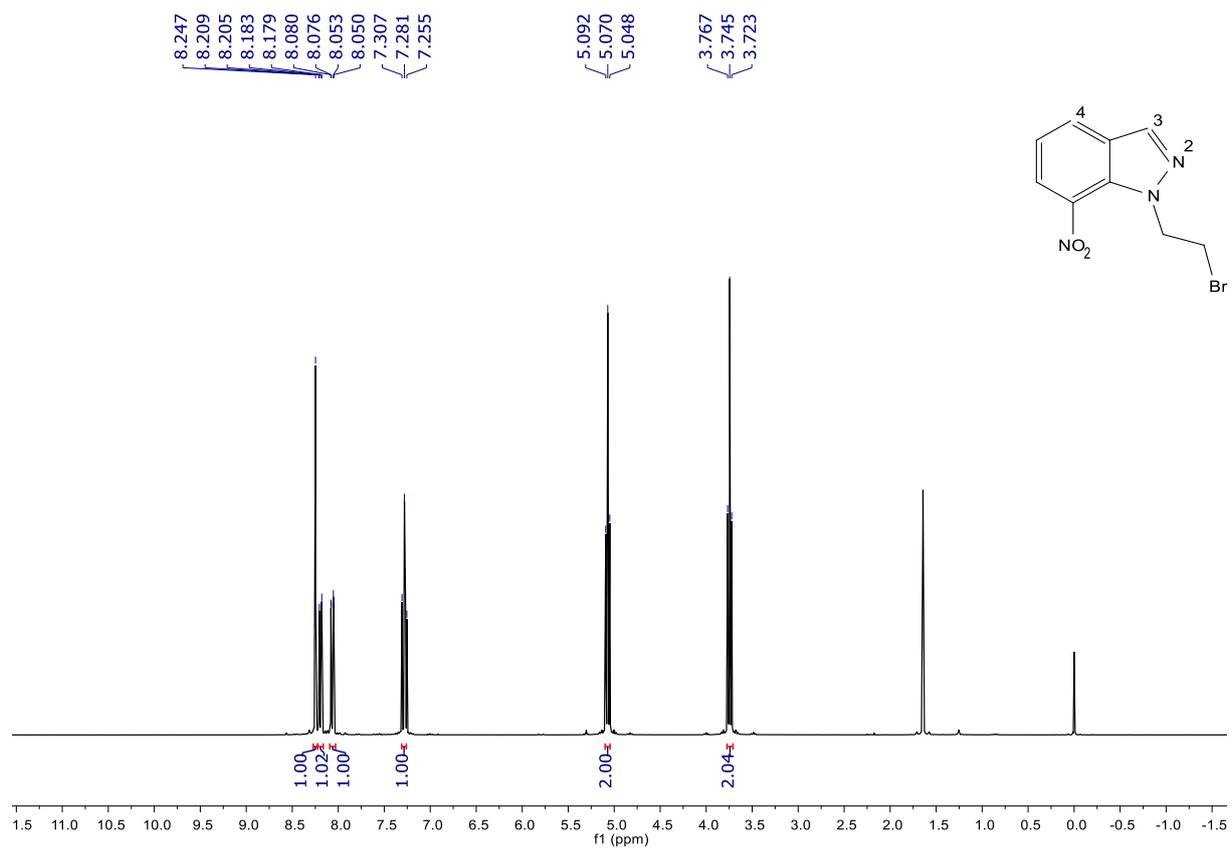


Figure S13. <sup>1</sup>H NMR spectrum of compound **2d** in CDCl<sub>3</sub>.

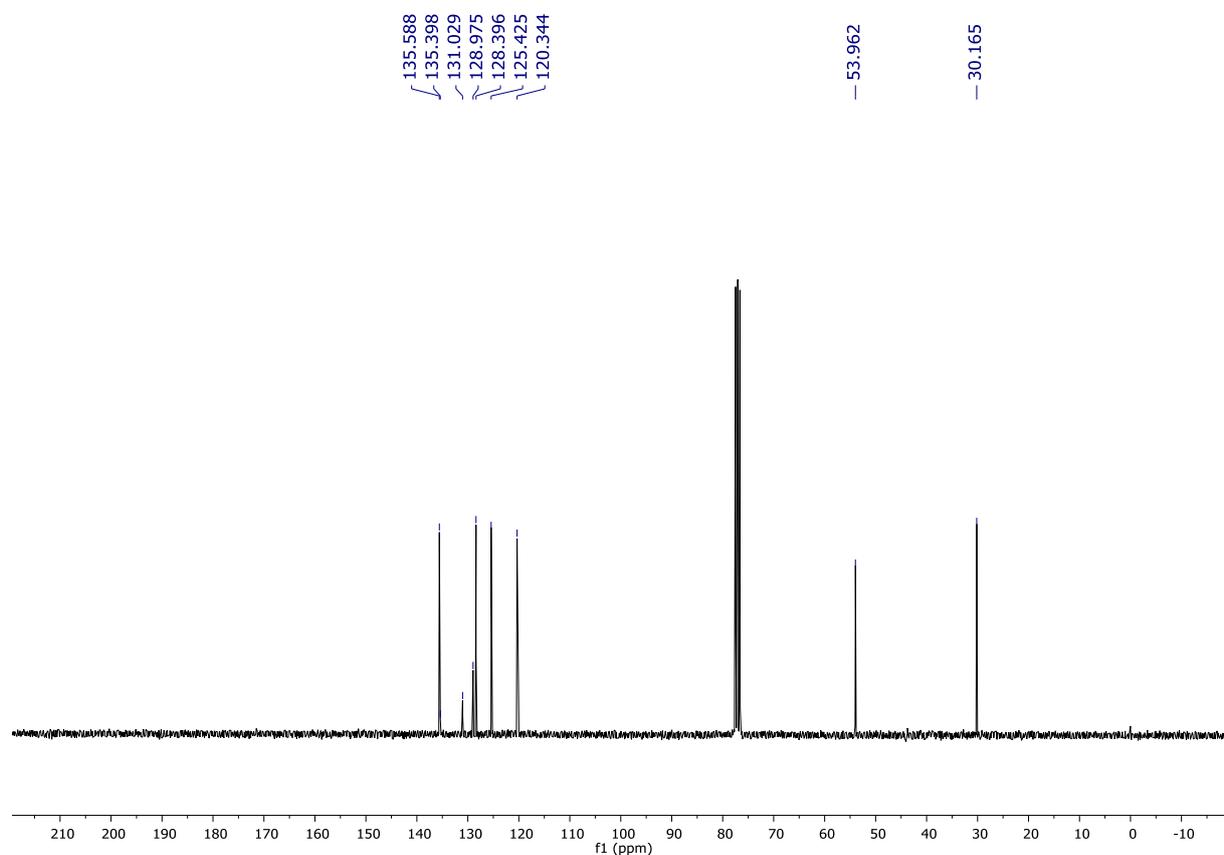
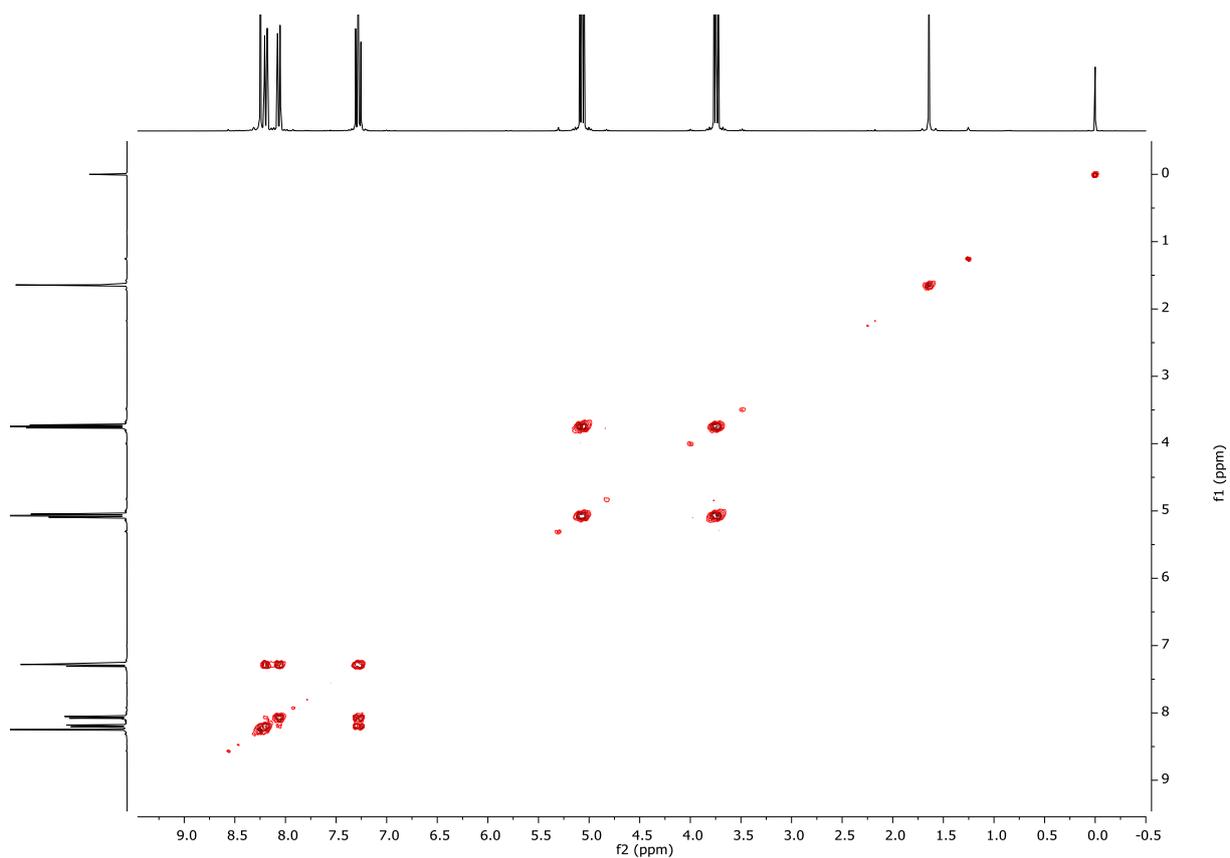
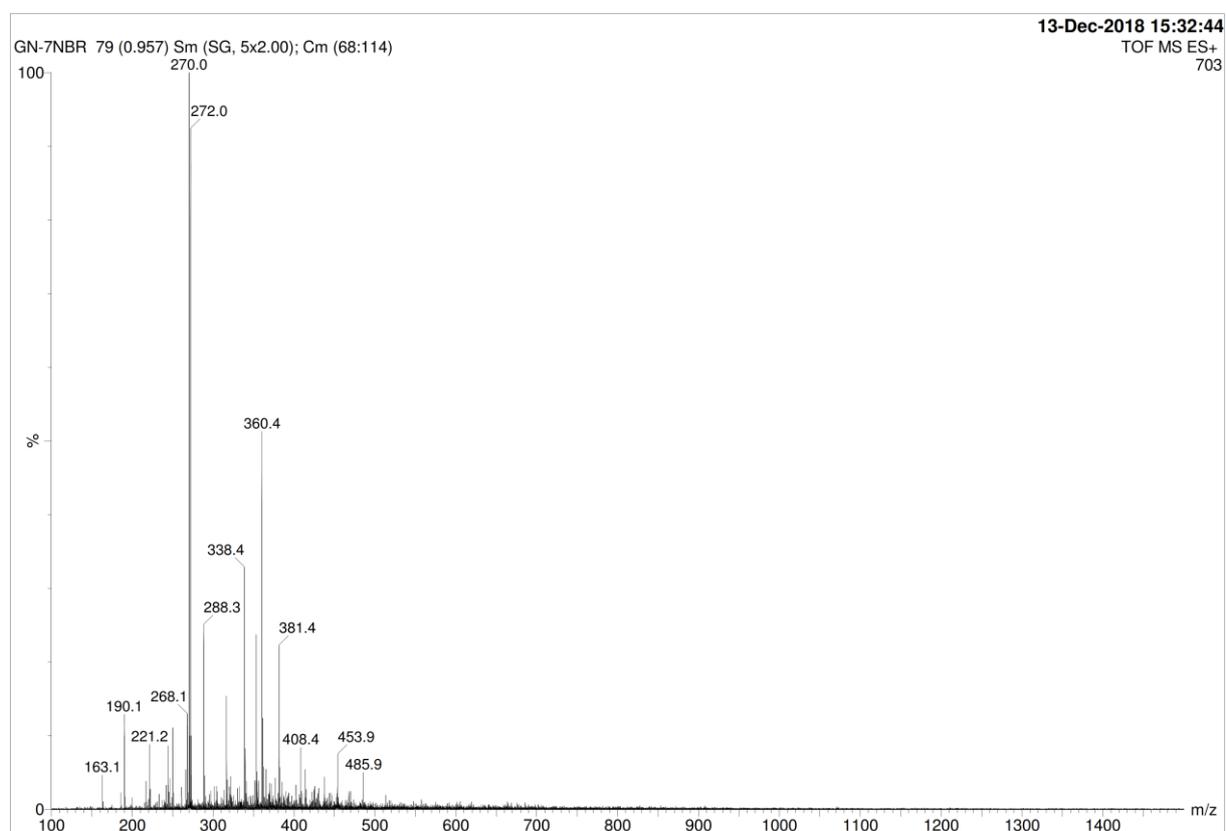


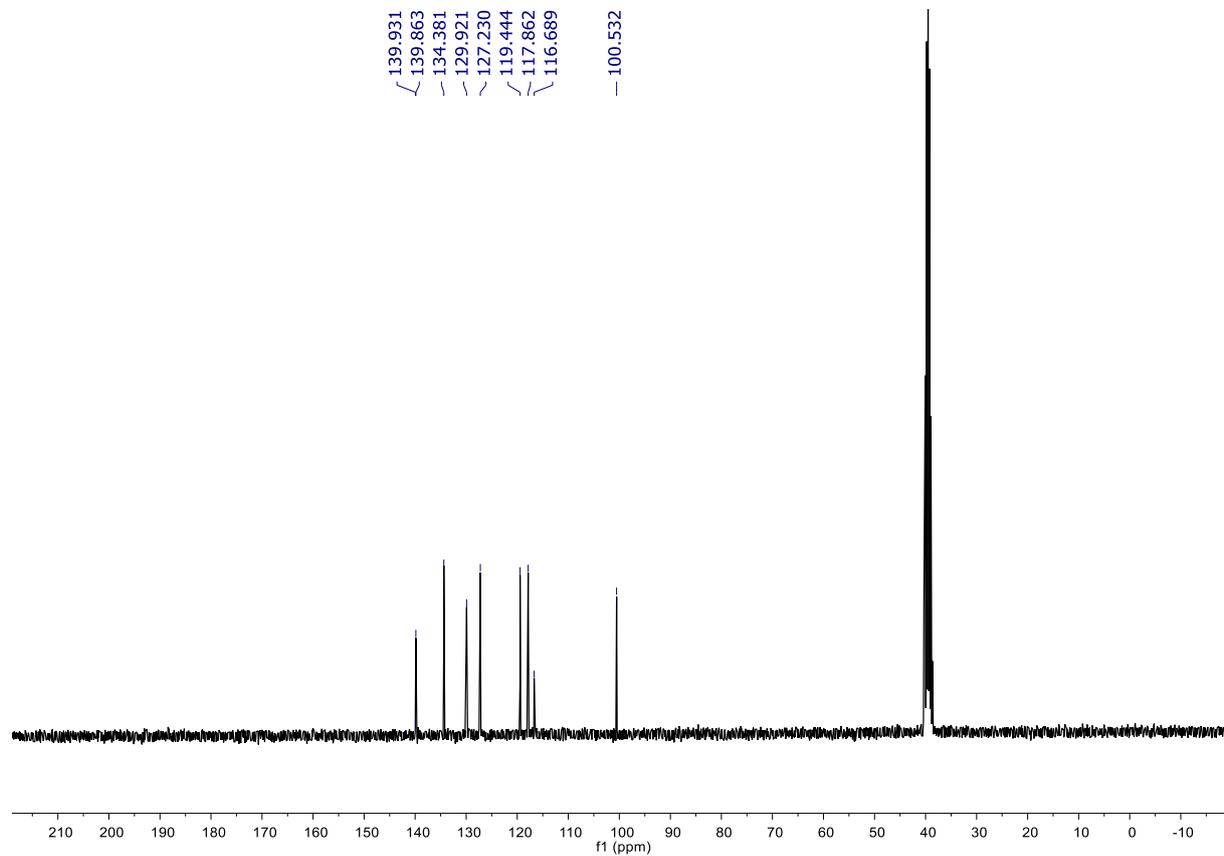
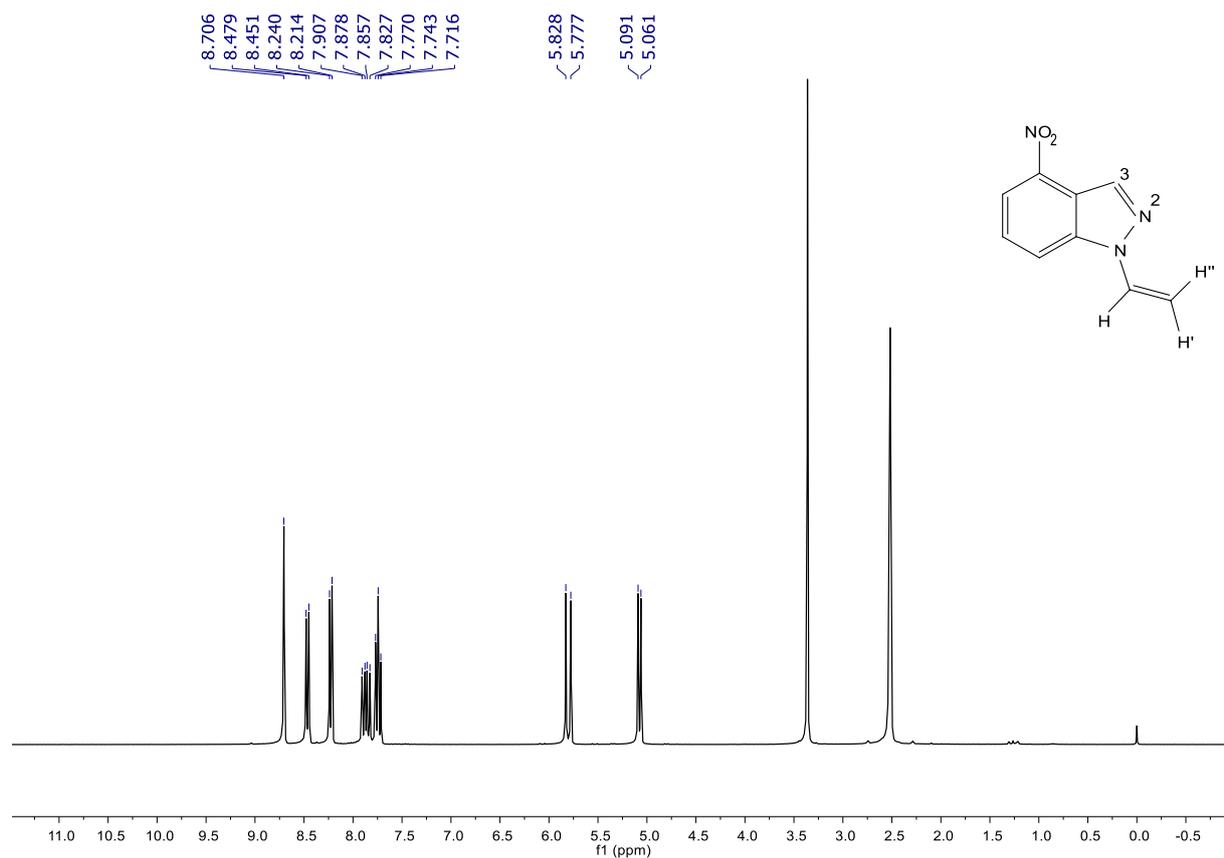
Figure S14. <sup>13</sup>C NMR spectrum of compound **2d** in CDCl<sub>3</sub>.

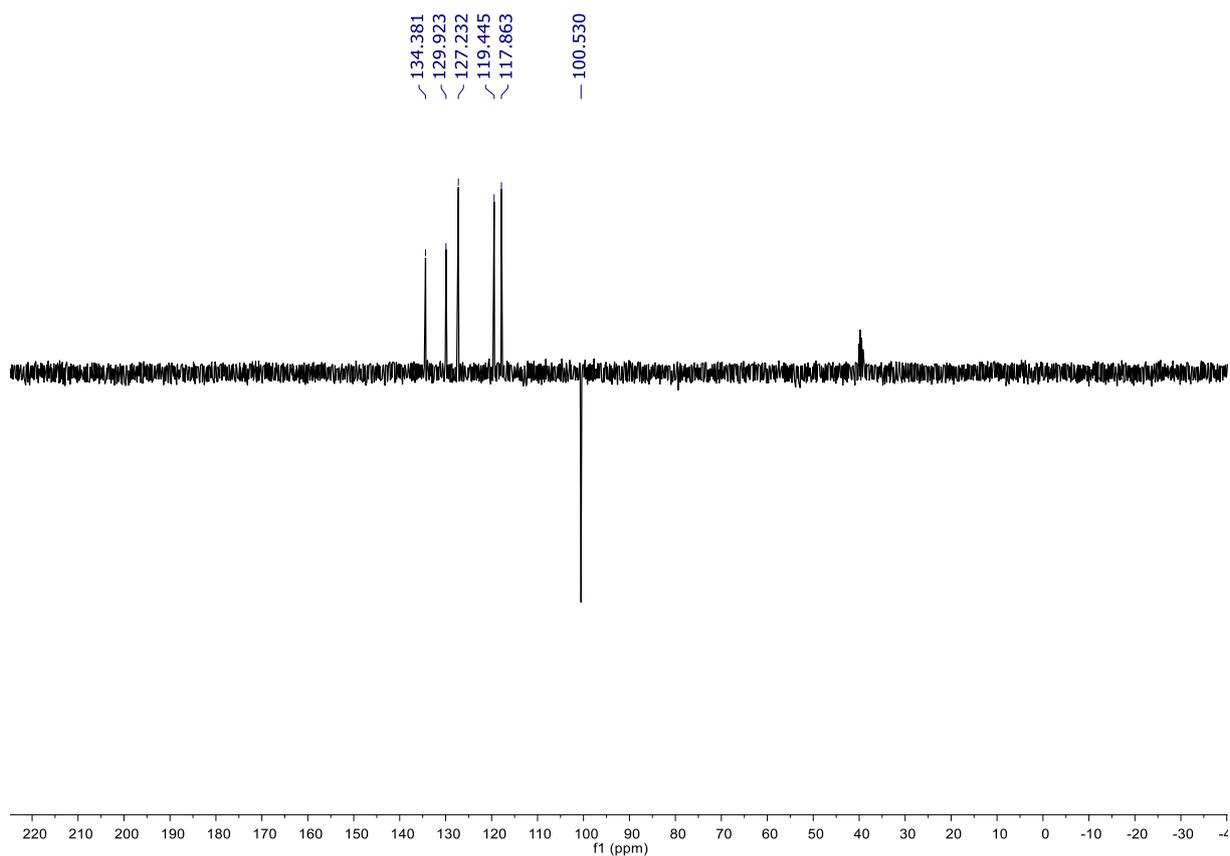


**Figure S15.** COSY (<sup>1</sup>H/<sup>1</sup>H) spectrum of compound **2d** in CDCl<sub>3</sub>.

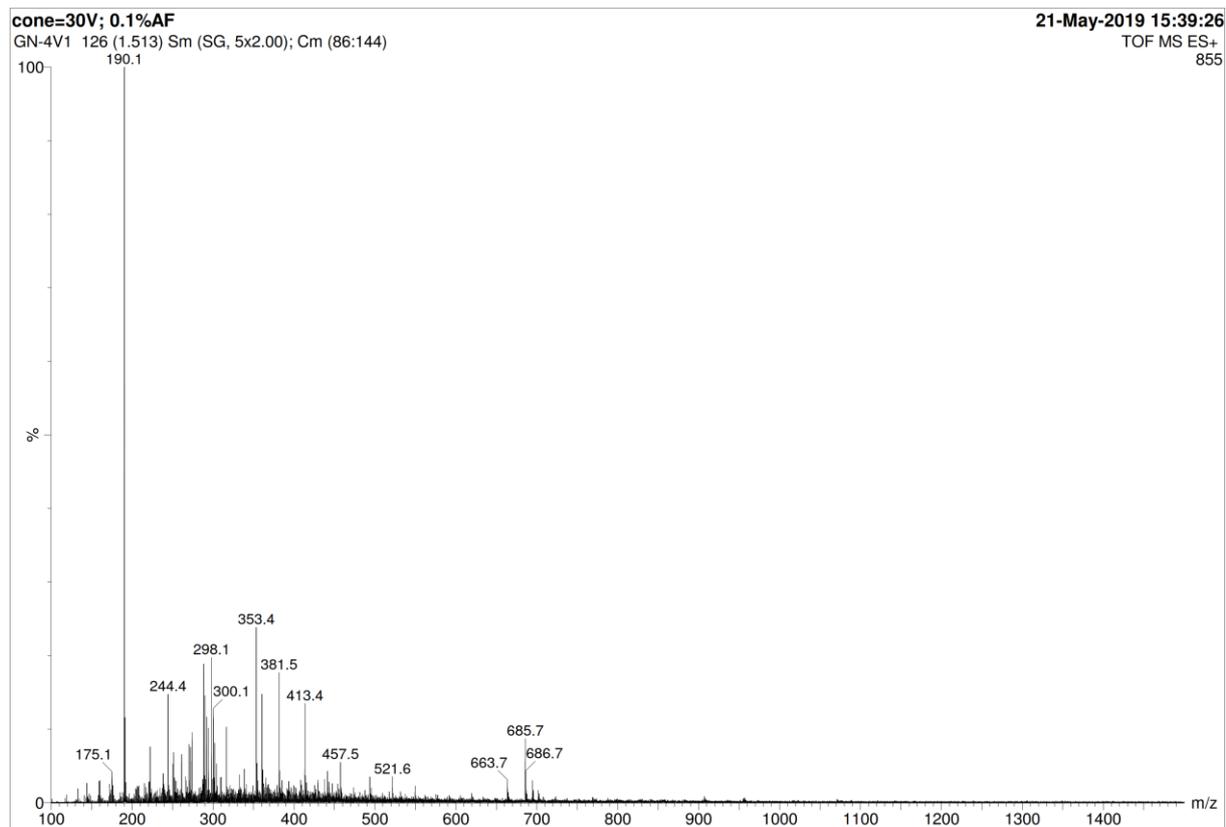


**Figure S16.** MS-ESI(+) spectrum of compound **2d**.

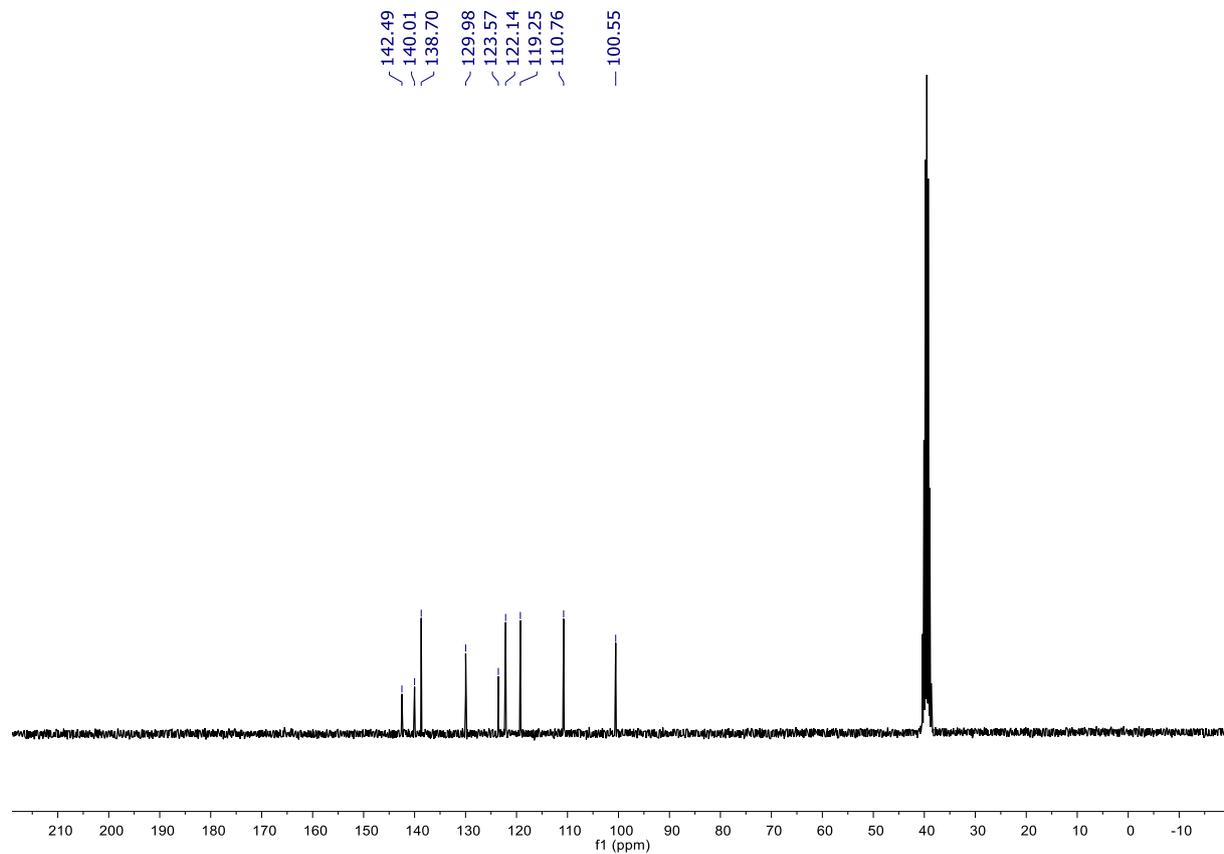
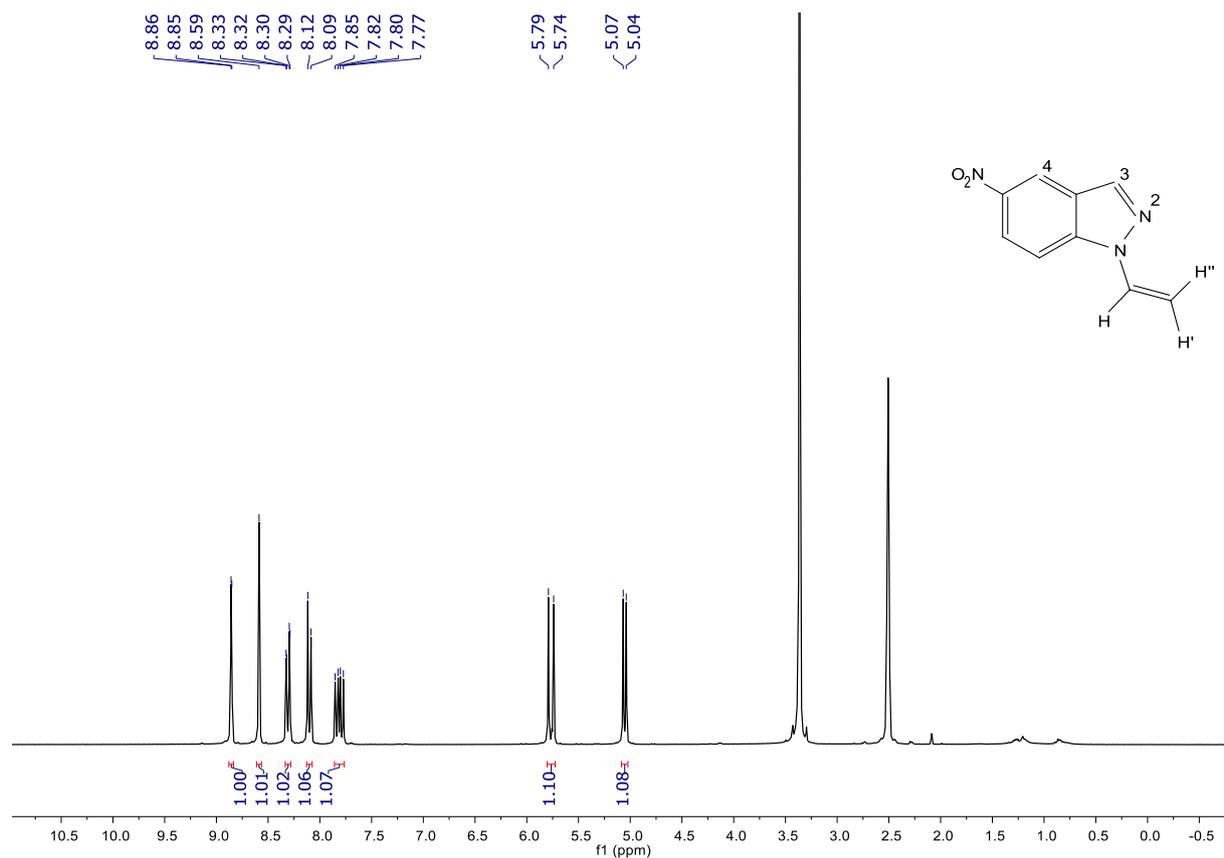


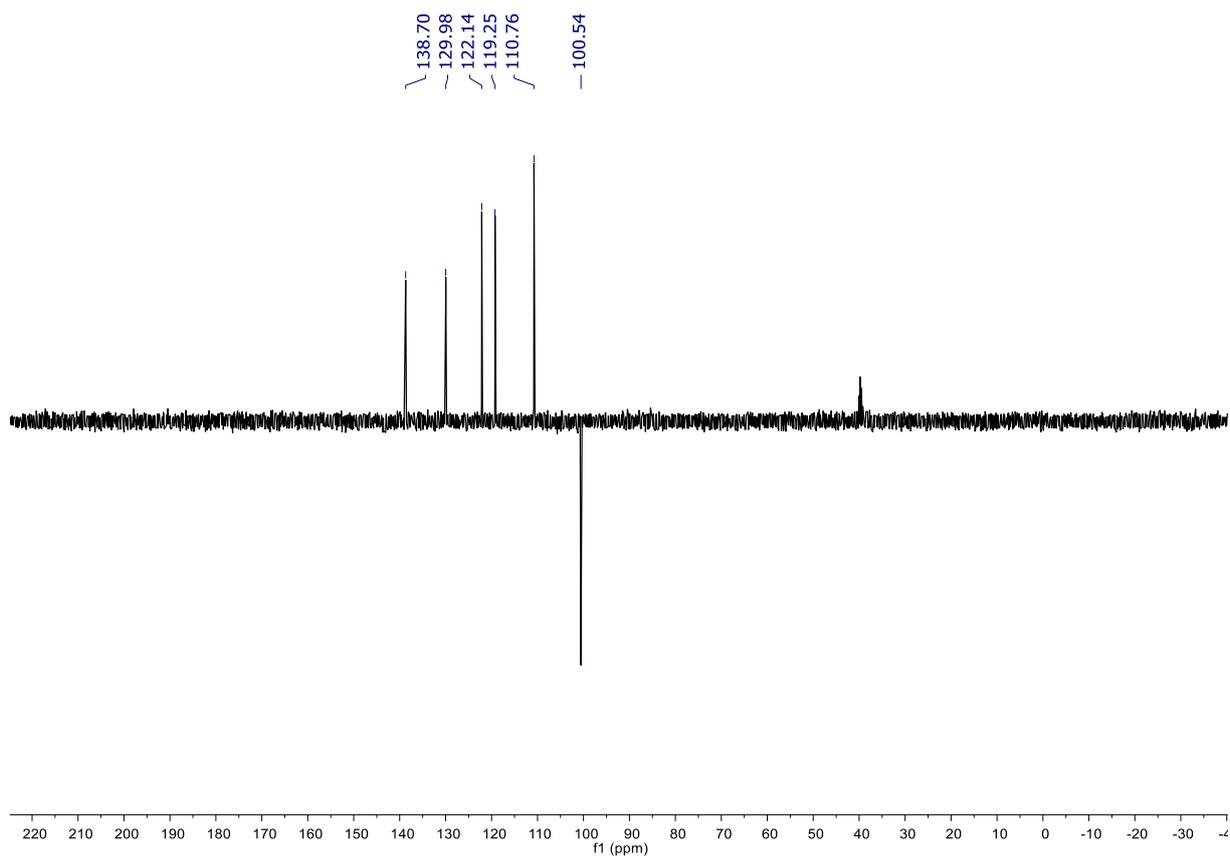


**Figure S19.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **3a** in  $\text{DMSO-d}_6$ .

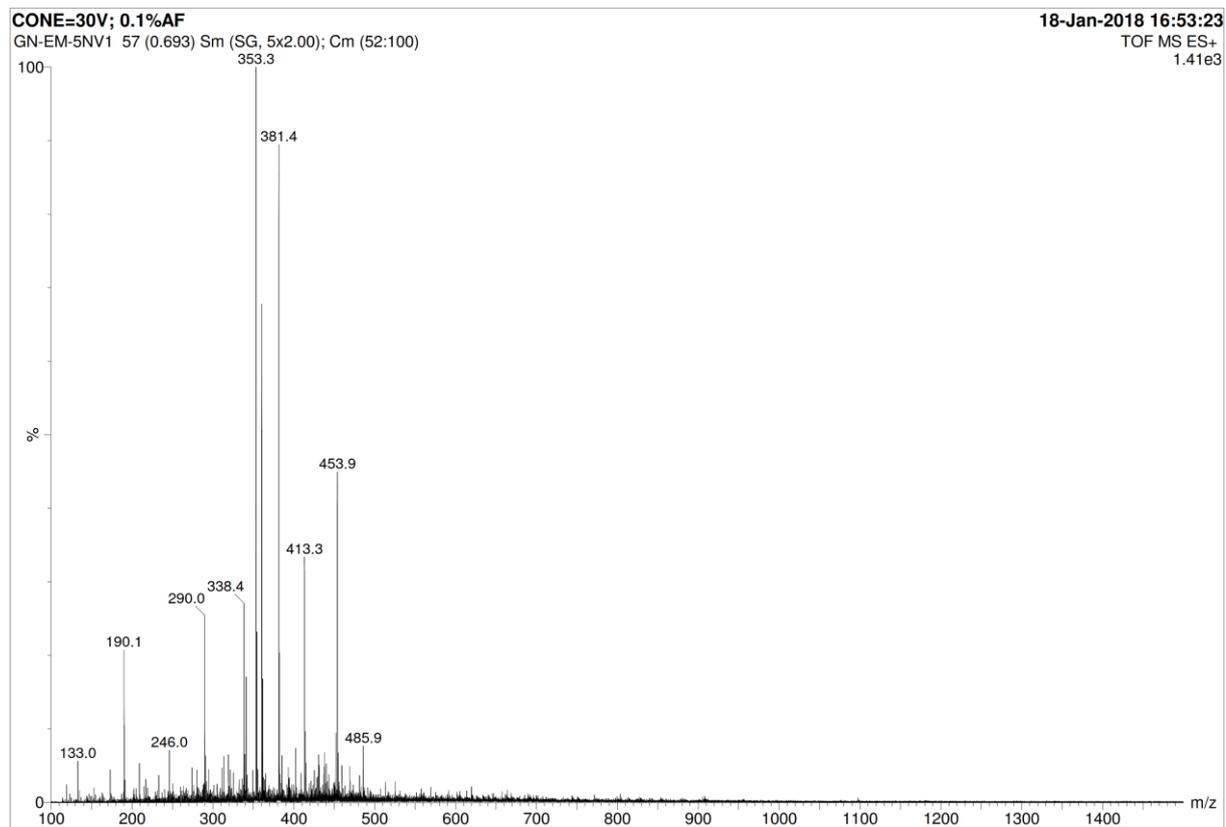


**Figure S20.** MS-ESI(+) spectrum of compound **3a**.

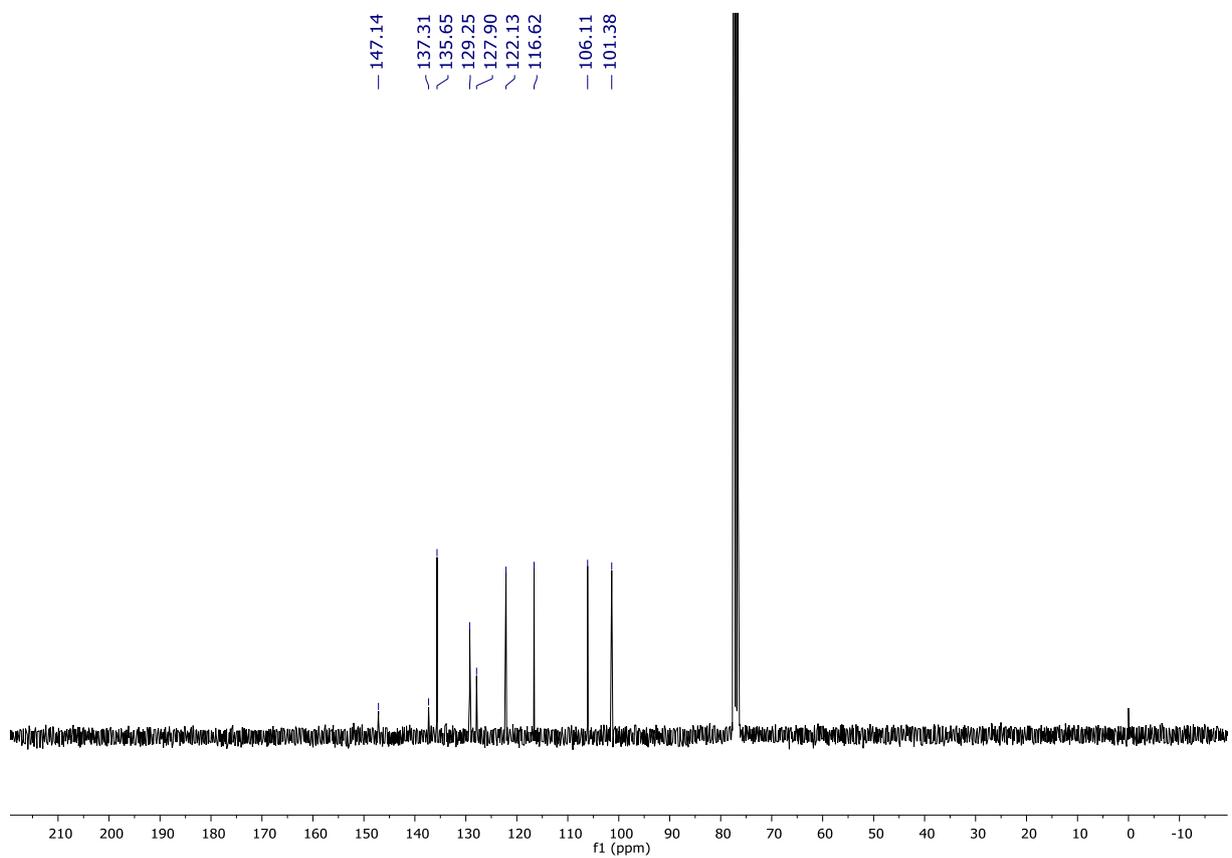
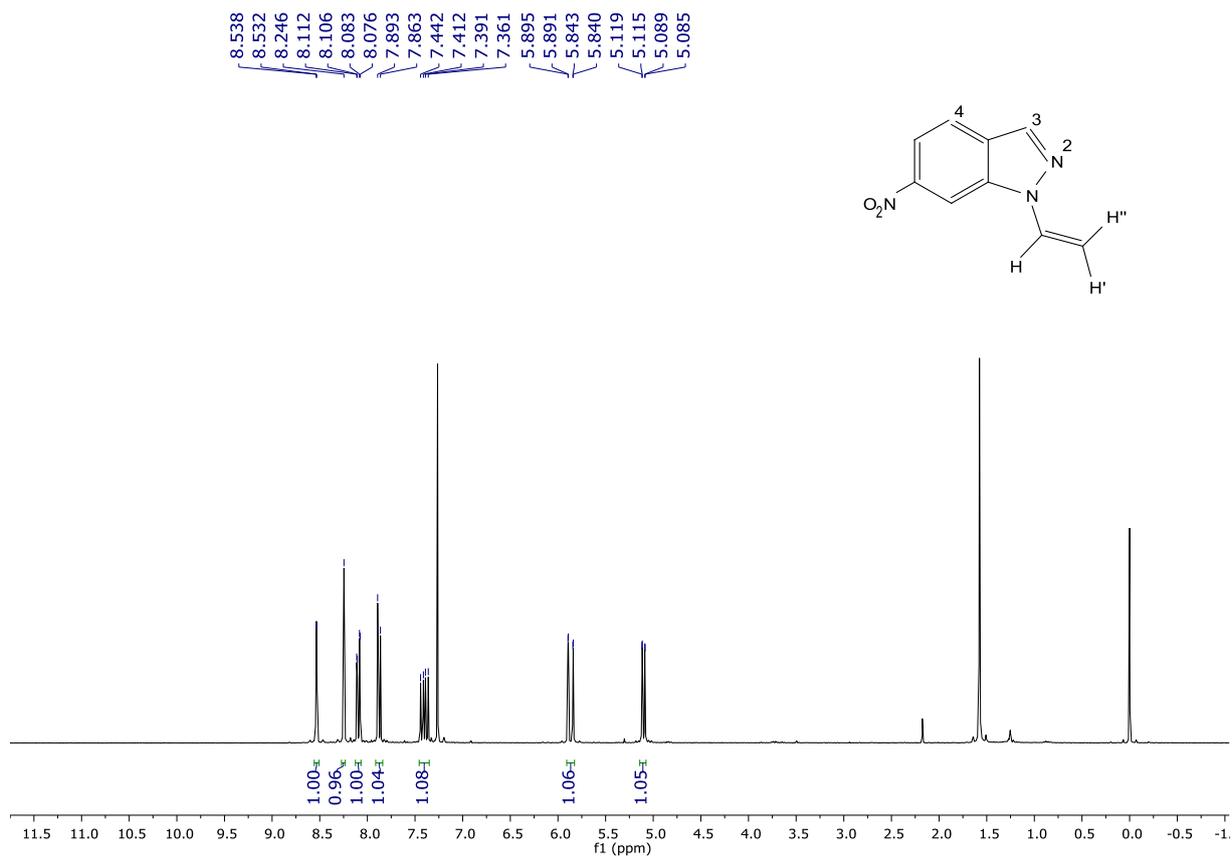




**Figure S23.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **3b** in  $\text{DMSO-d}_6$ .



**Figure S24.** MS-ESI(+) spectrum of compound **3b**.



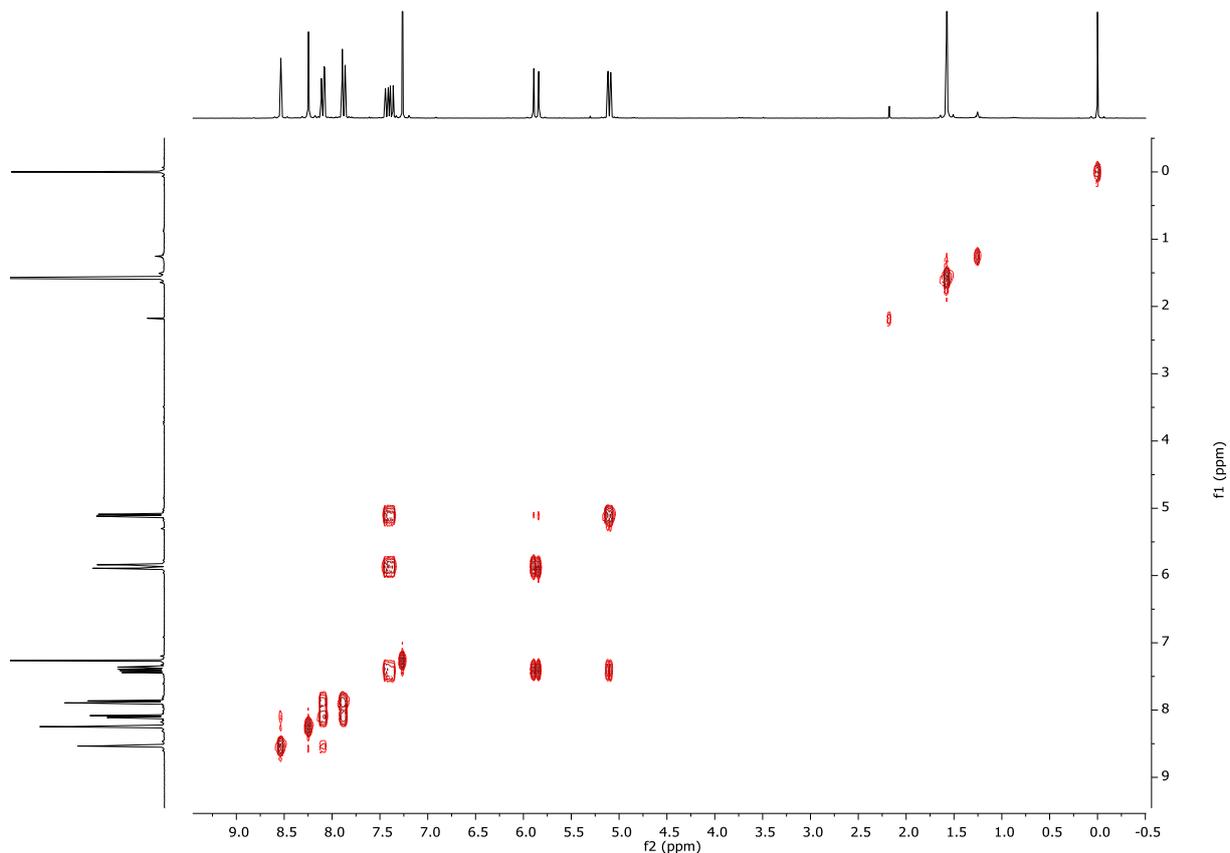


Figure S27. COSY ( $^1\text{H}/^1\text{H}$ ) spectrum of compound **3c** in  $\text{CDCl}_3$ .

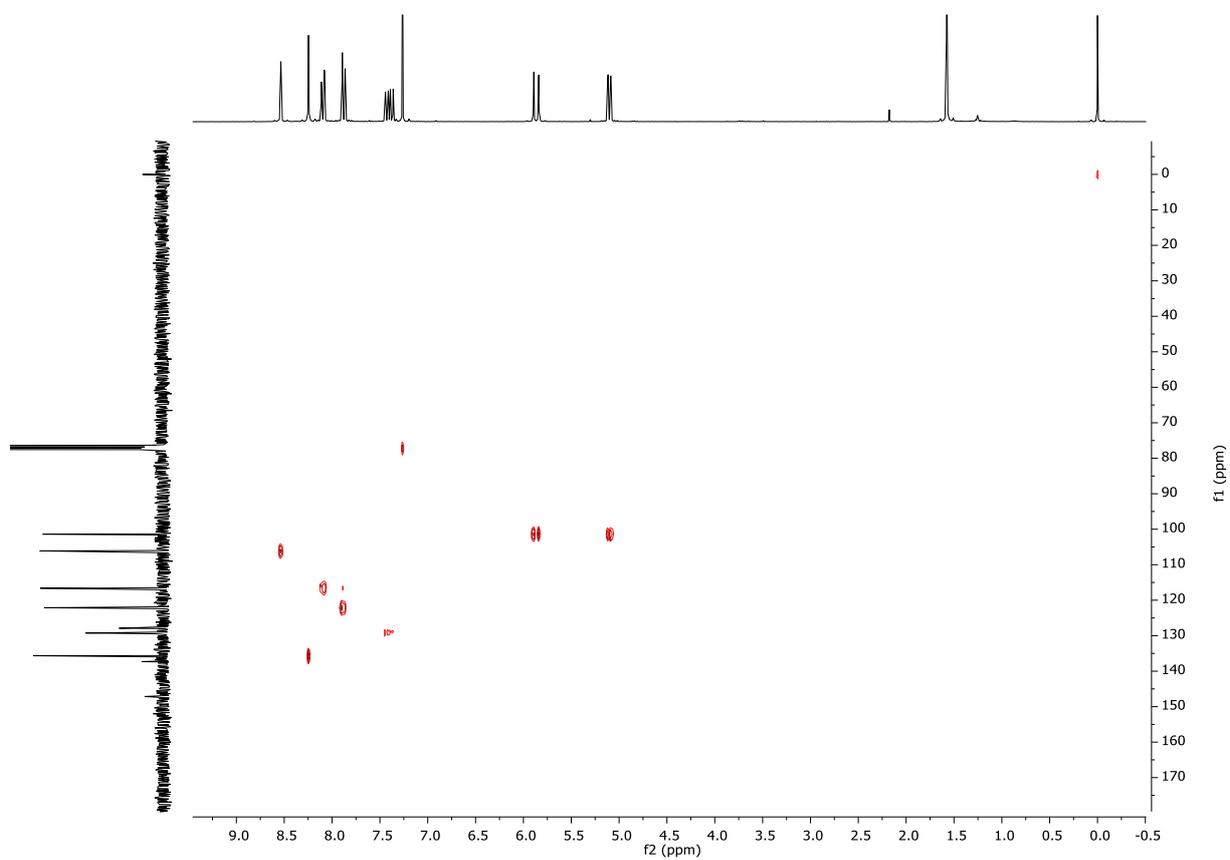


Figure S28. HSQC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **3c** in  $\text{CDCl}_3$ .

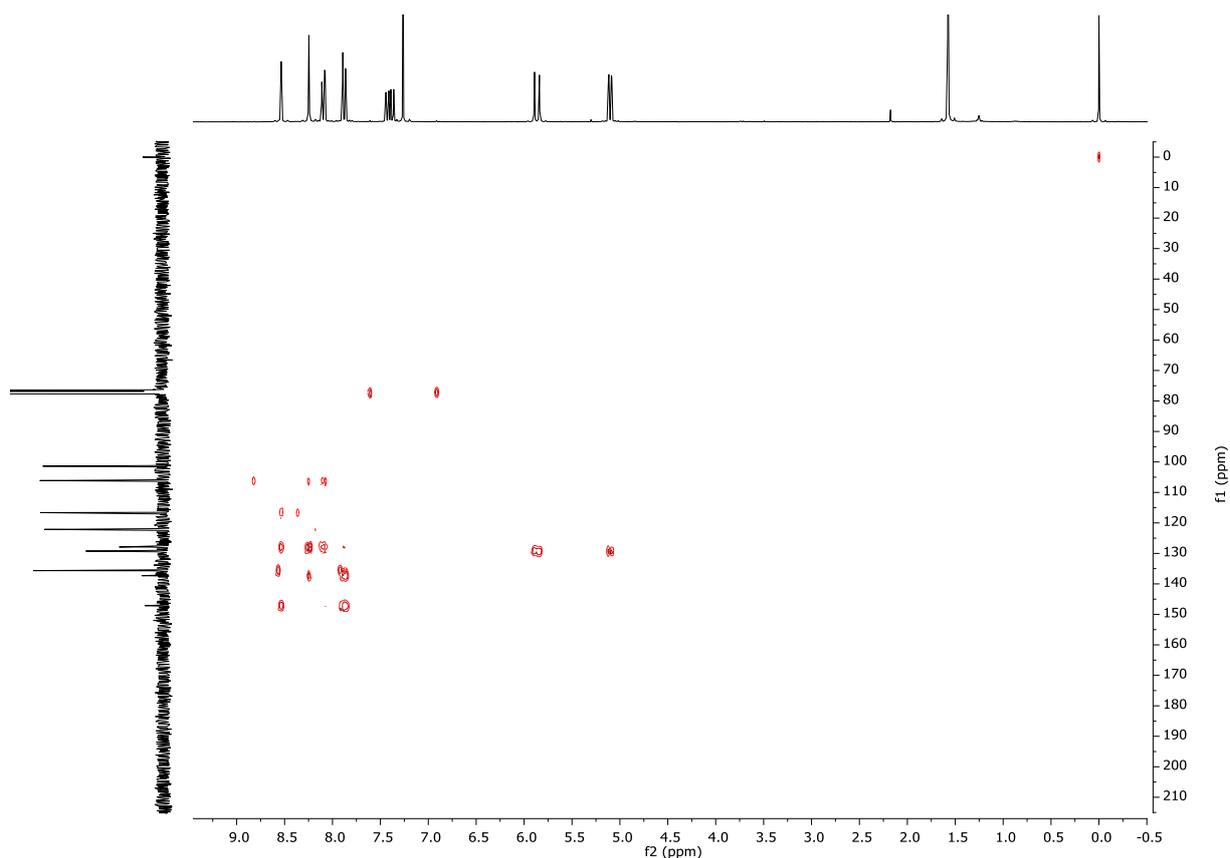


Figure S29. HMBC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **3c** in  $\text{CDCl}_3$ .

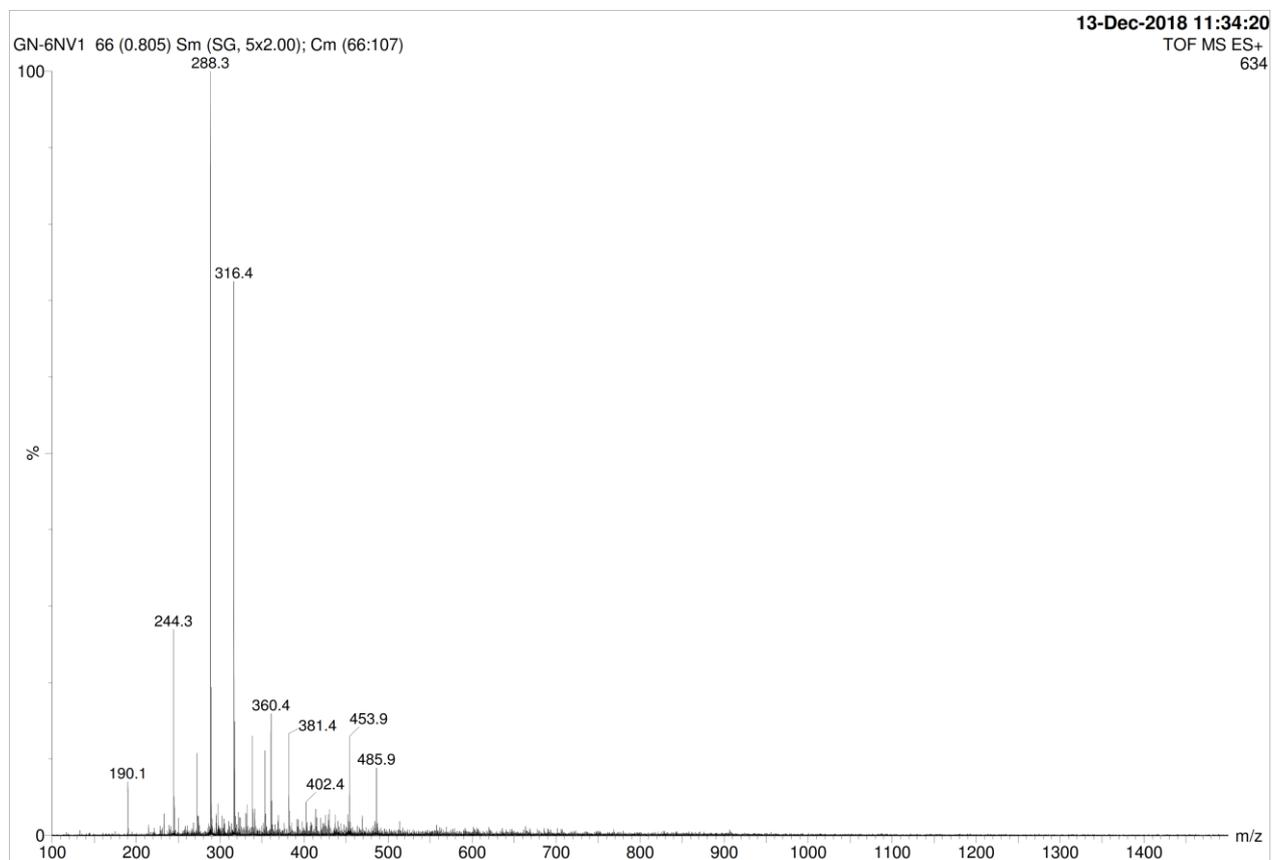


Figure S30. MS-ESI(+) spectrum of compound **3c**.

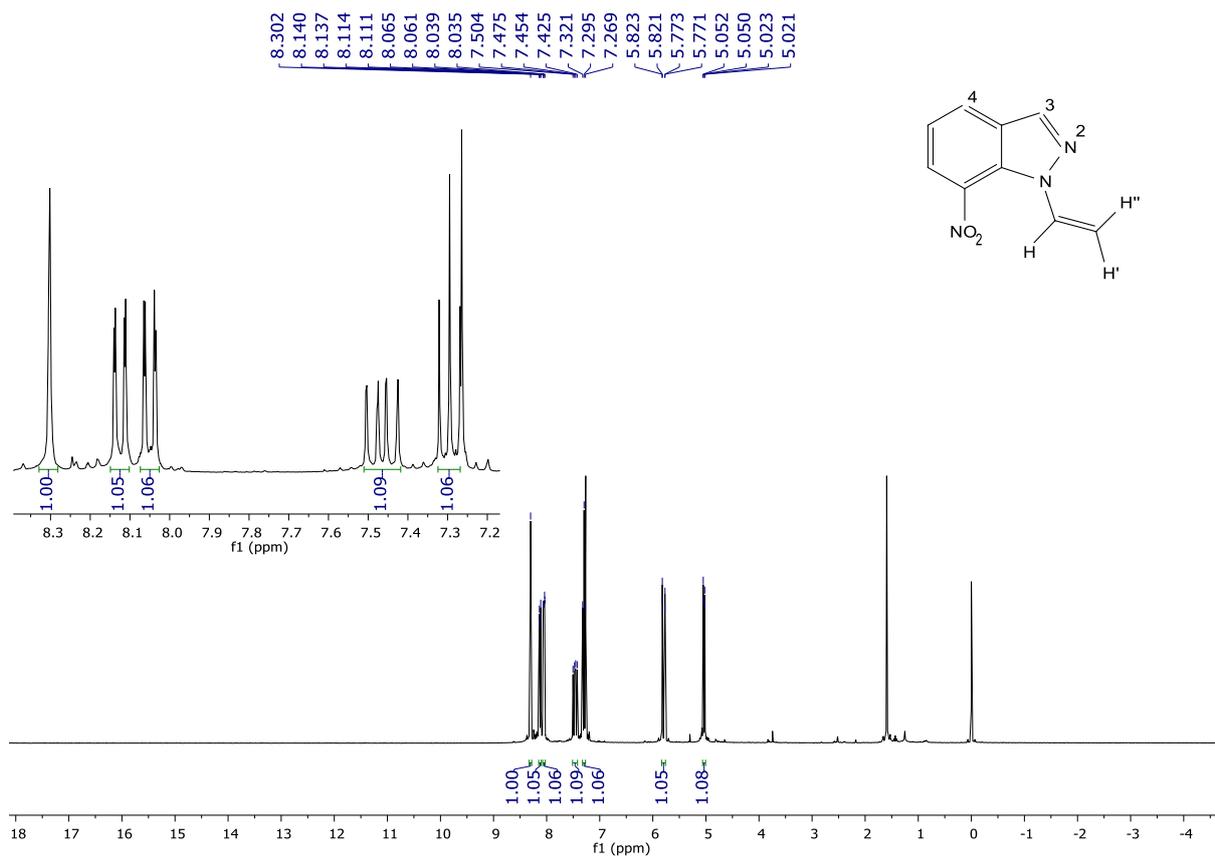


Figure S31. <sup>1</sup>H NMR spectrum of compound **3d** in CDCl<sub>3</sub>.

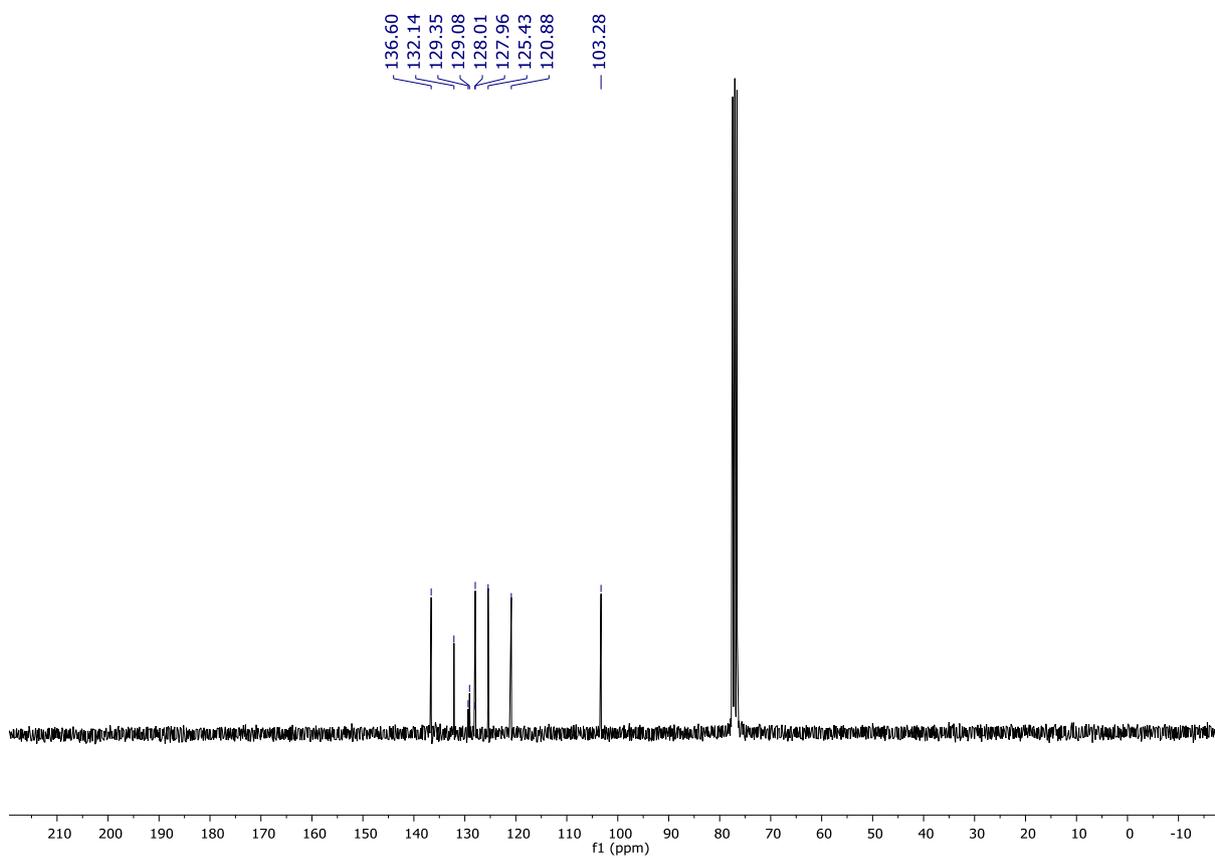
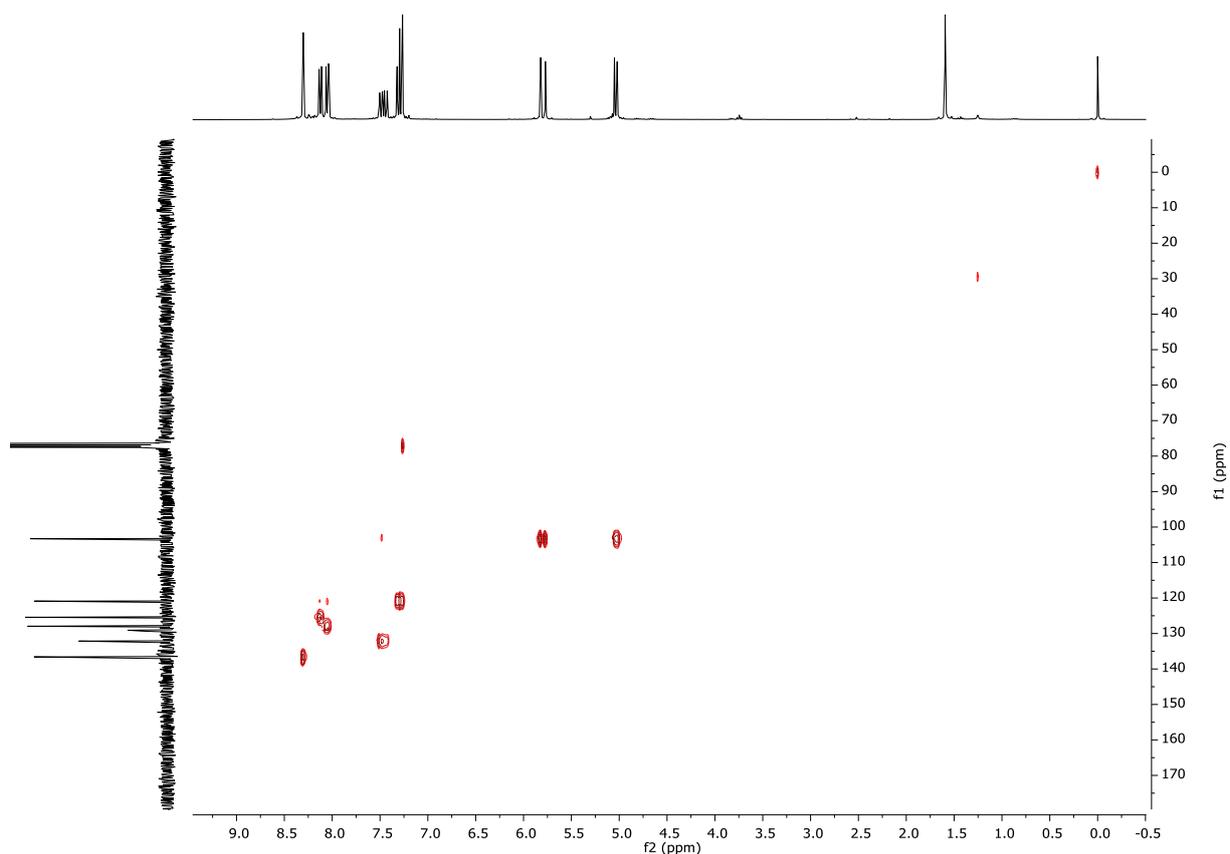
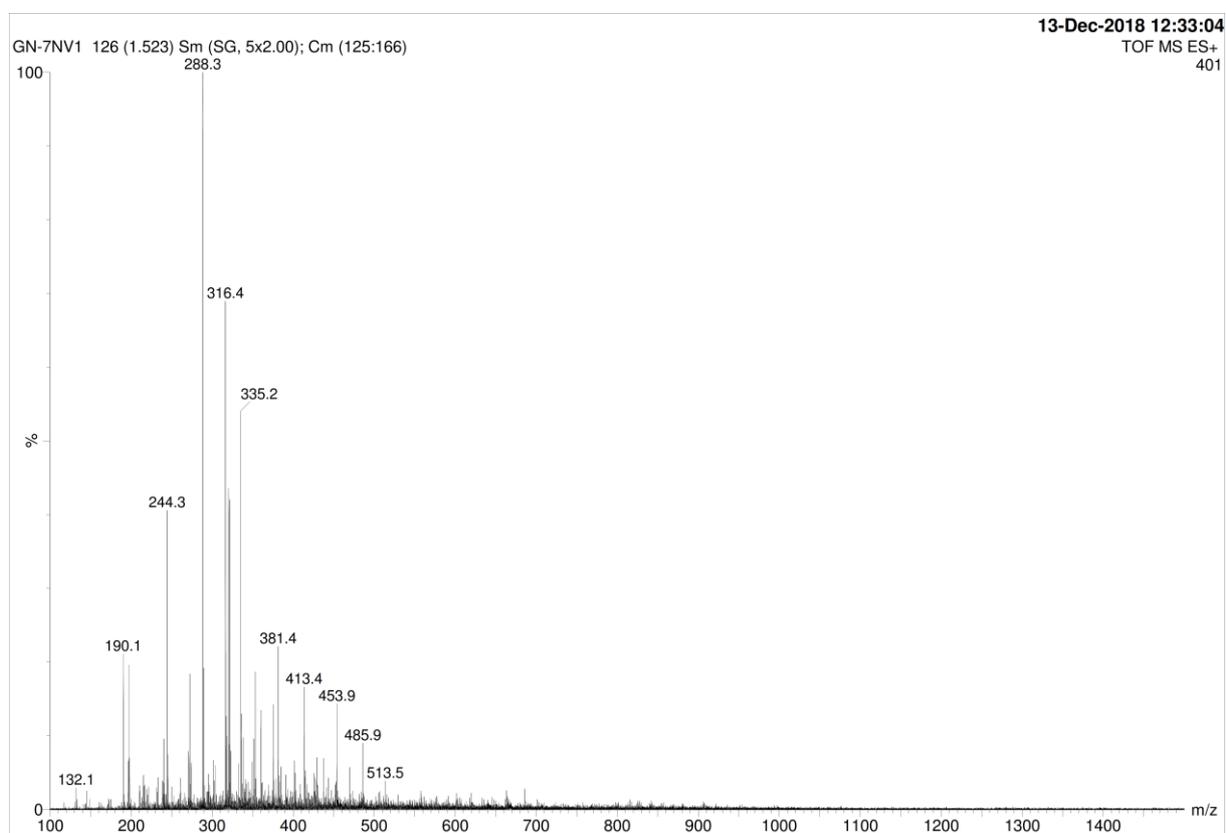


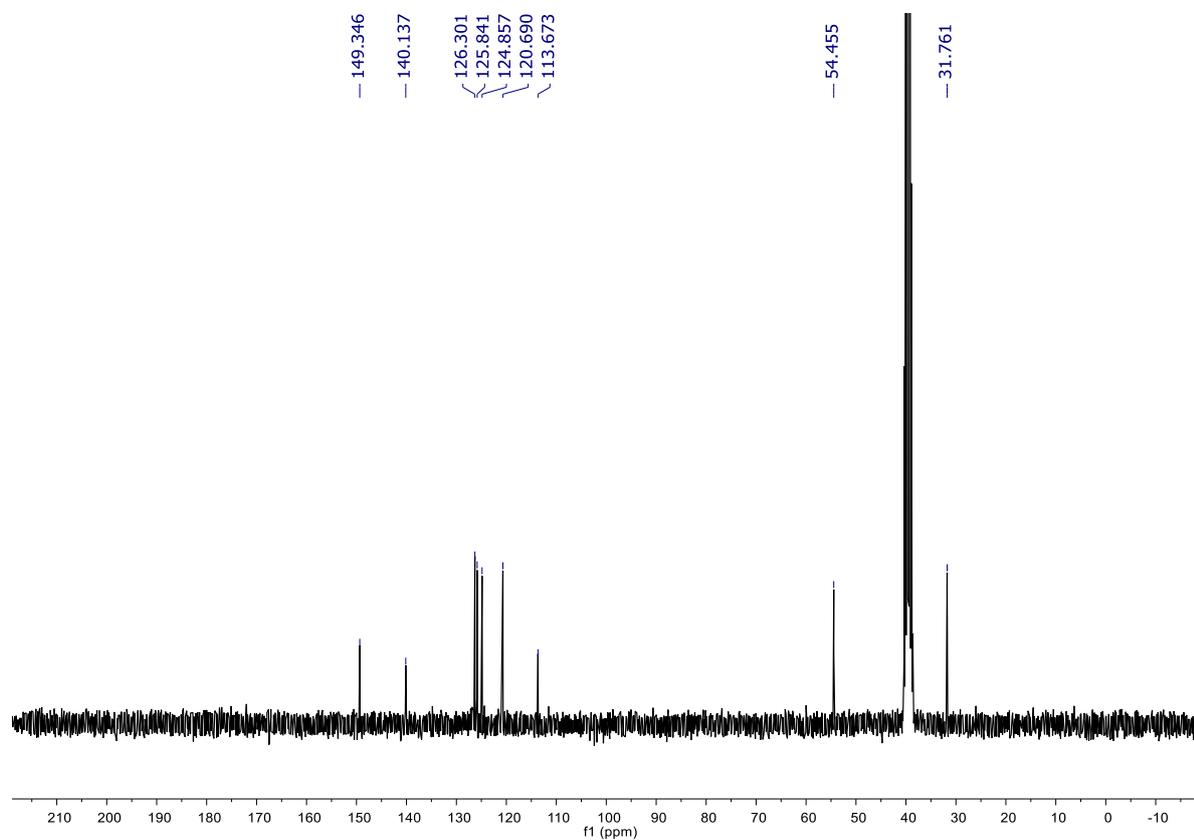
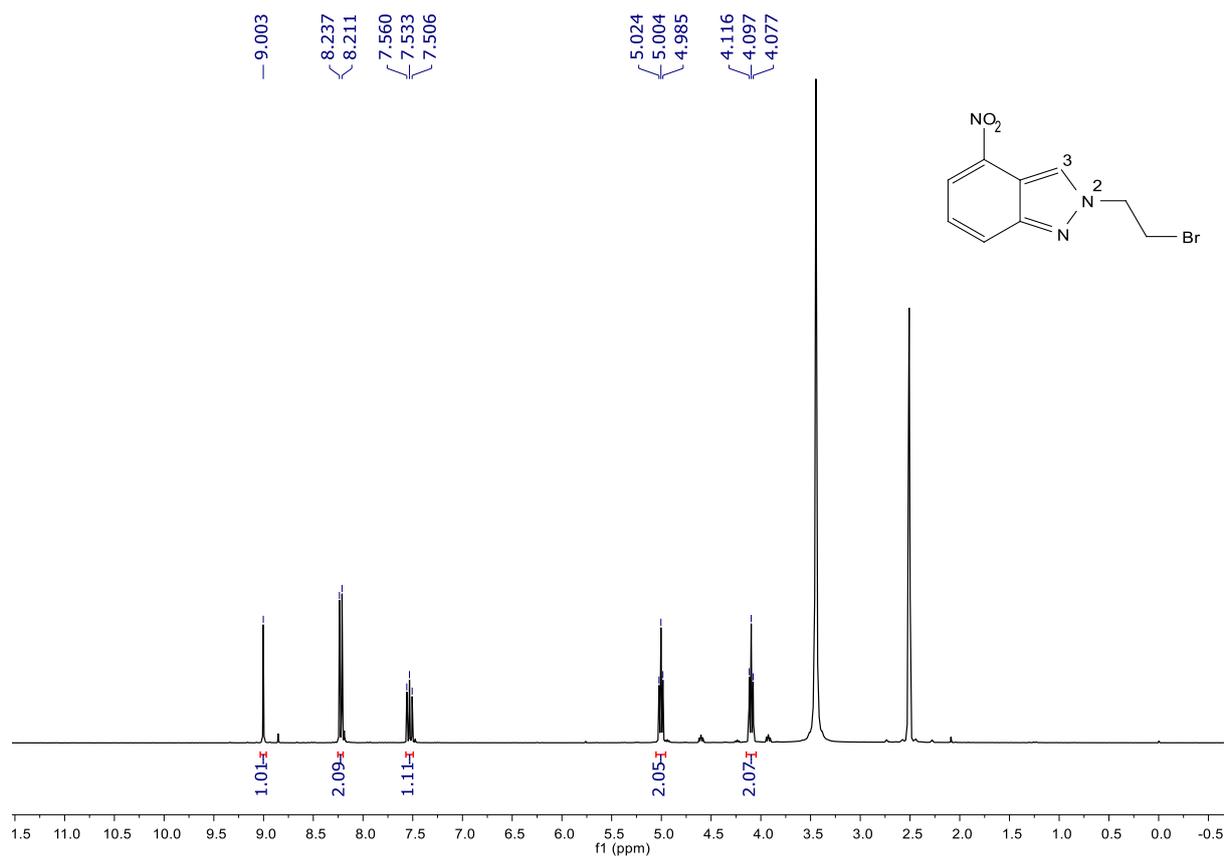
Figure S32. <sup>13</sup>C NMR spectrum of compound **3d** in CDCl<sub>3</sub>.



**Figure S33.** HSQC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **3d** in  $\text{CDCl}_3$ .



**Figure S34.** MS-ESI(+) spectrum of compound **3d**.



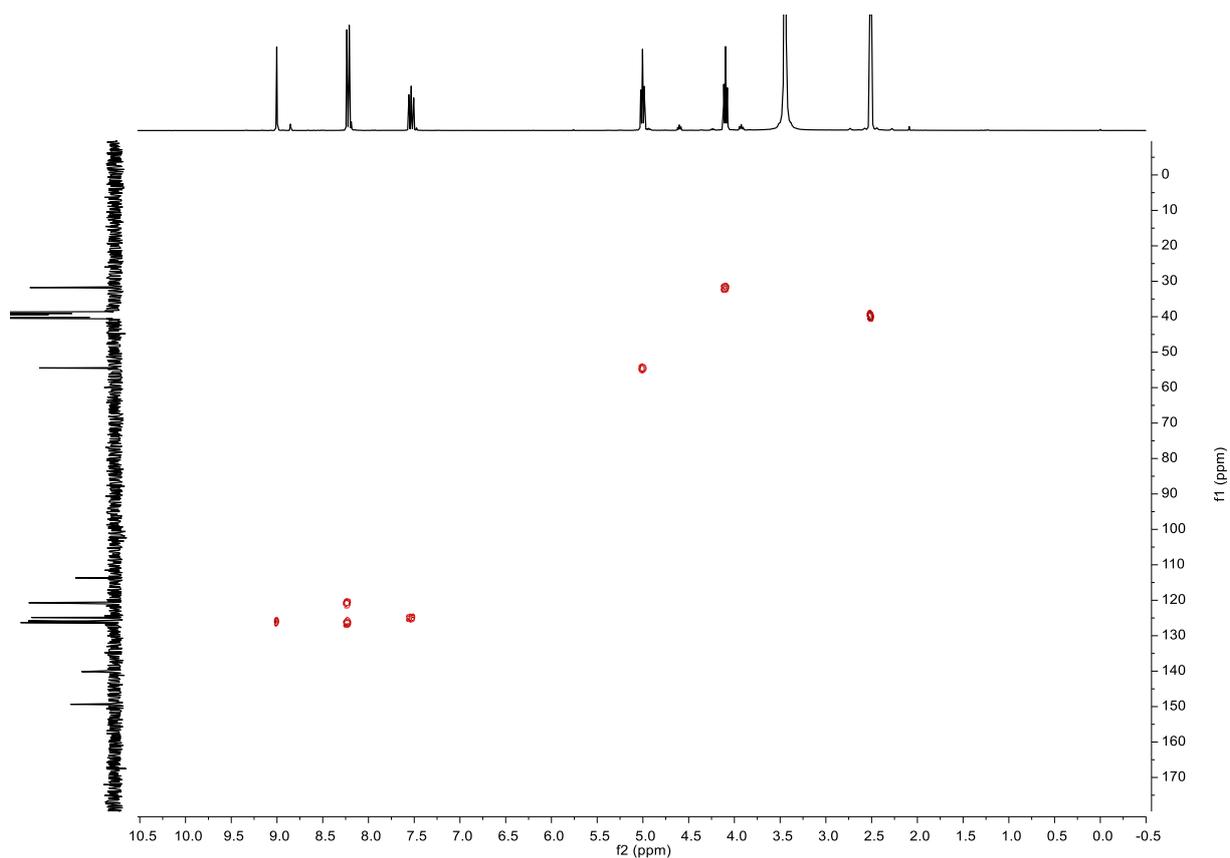


Figure S37. HSQC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **4a** in  $\text{DMSO-d}_6$ .

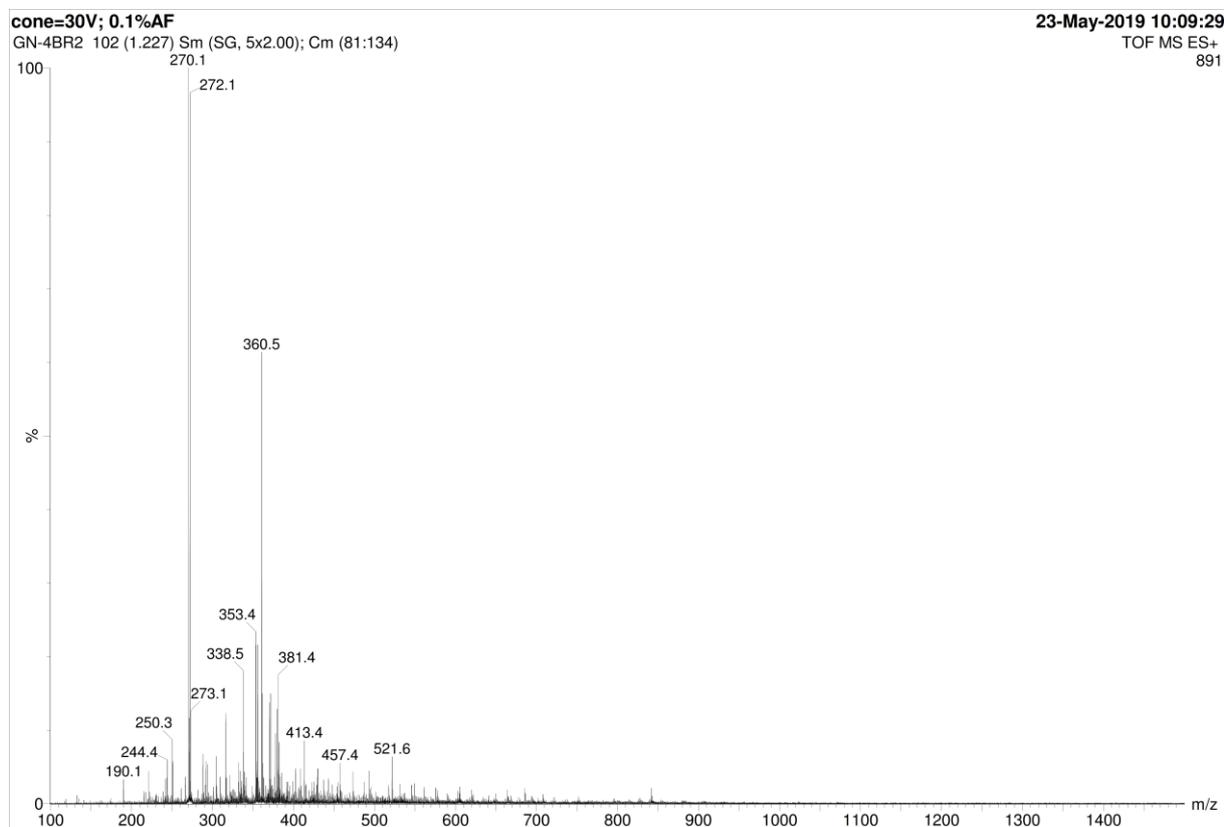


Figure S38. MS-ESI(+) spectrum of compound **4a**.

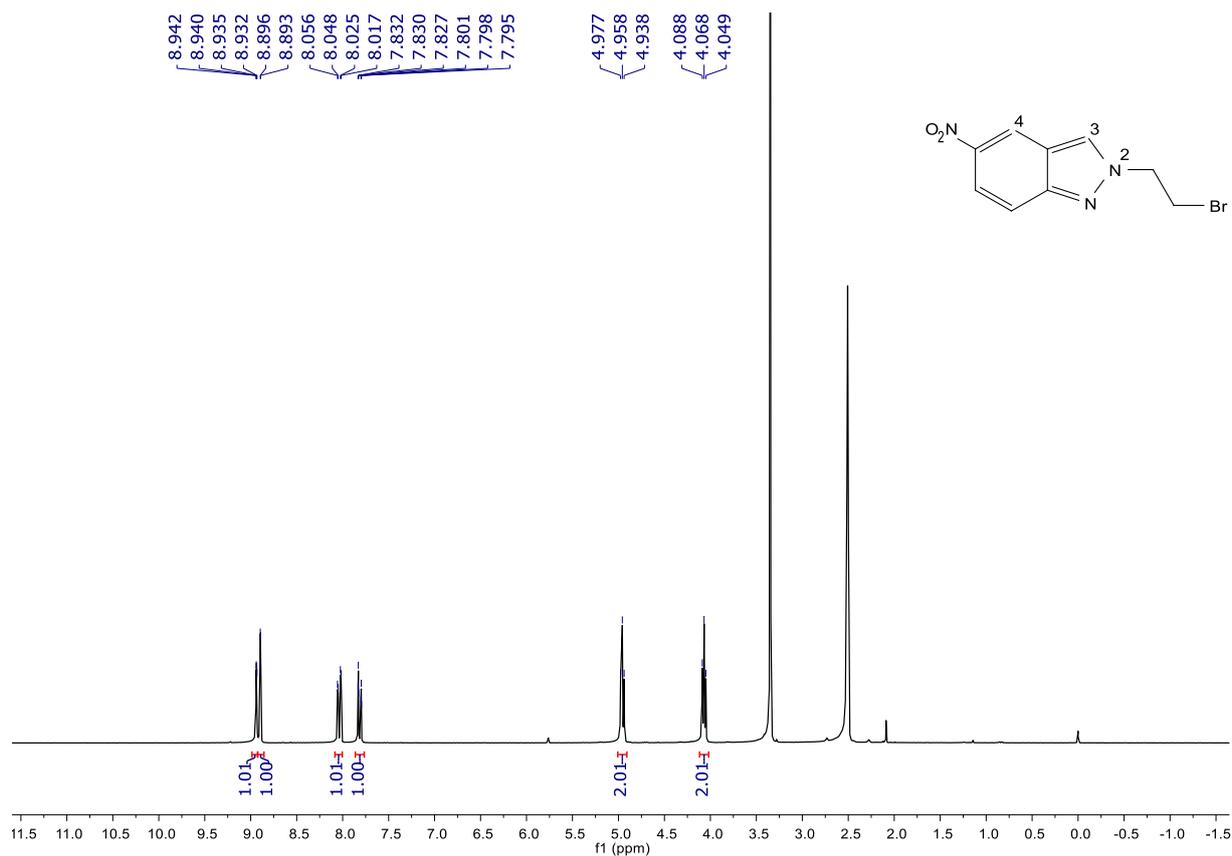


Figure S39. <sup>1</sup>H NMR spectrum of compound **4b** in DMSO-d<sub>6</sub>.

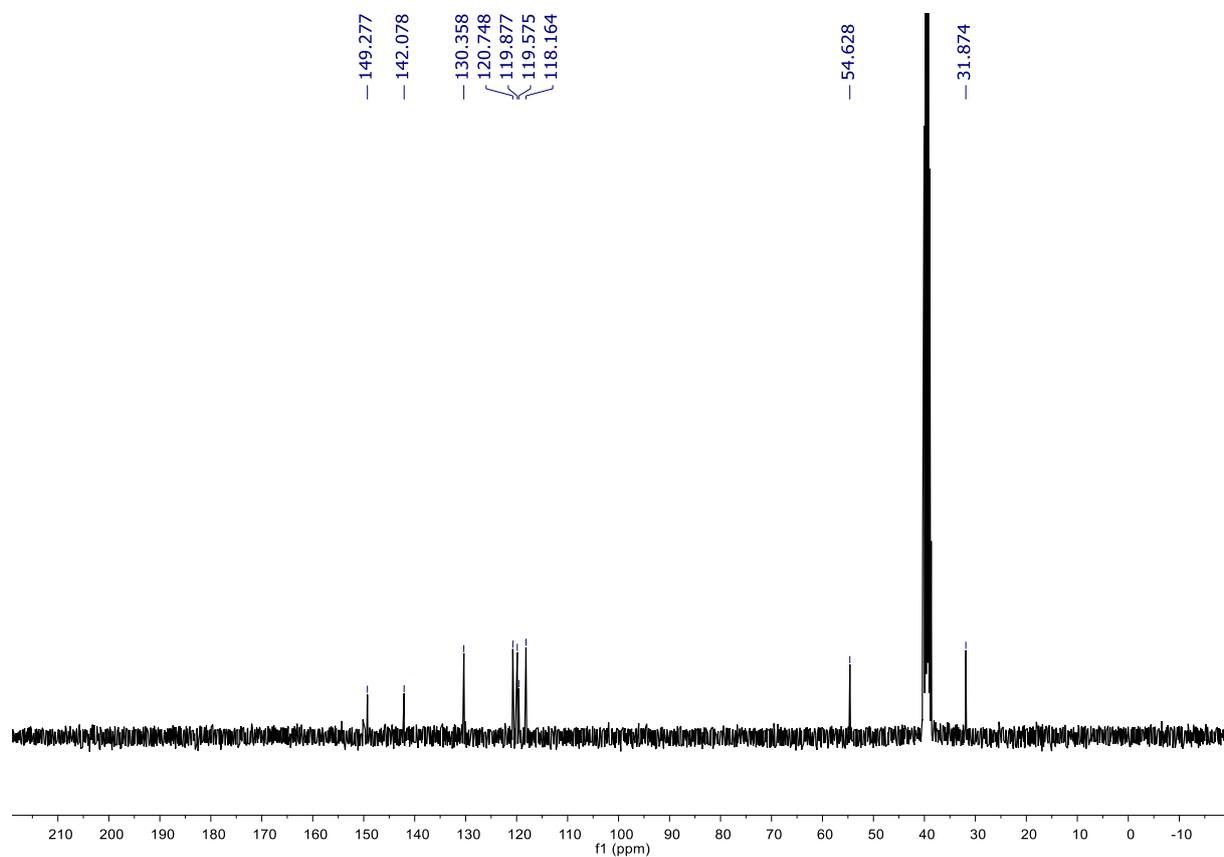
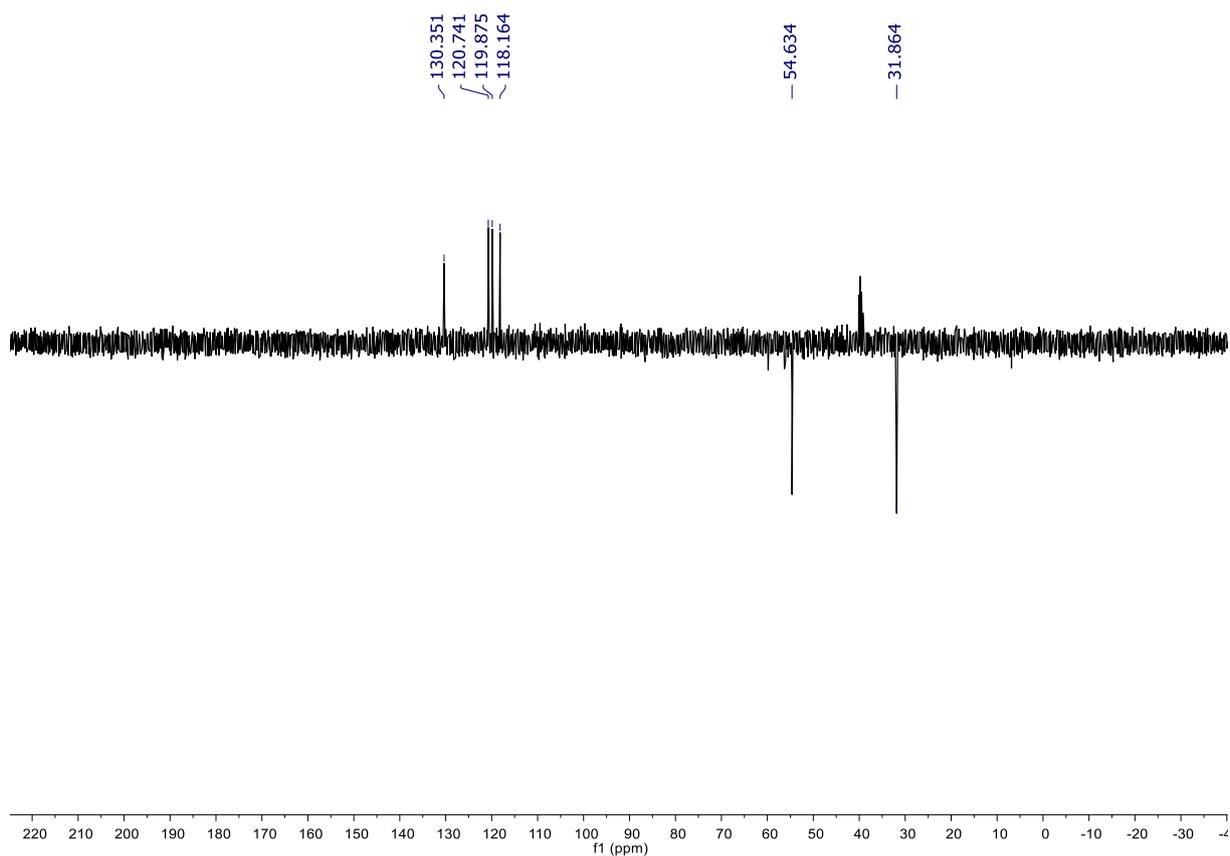
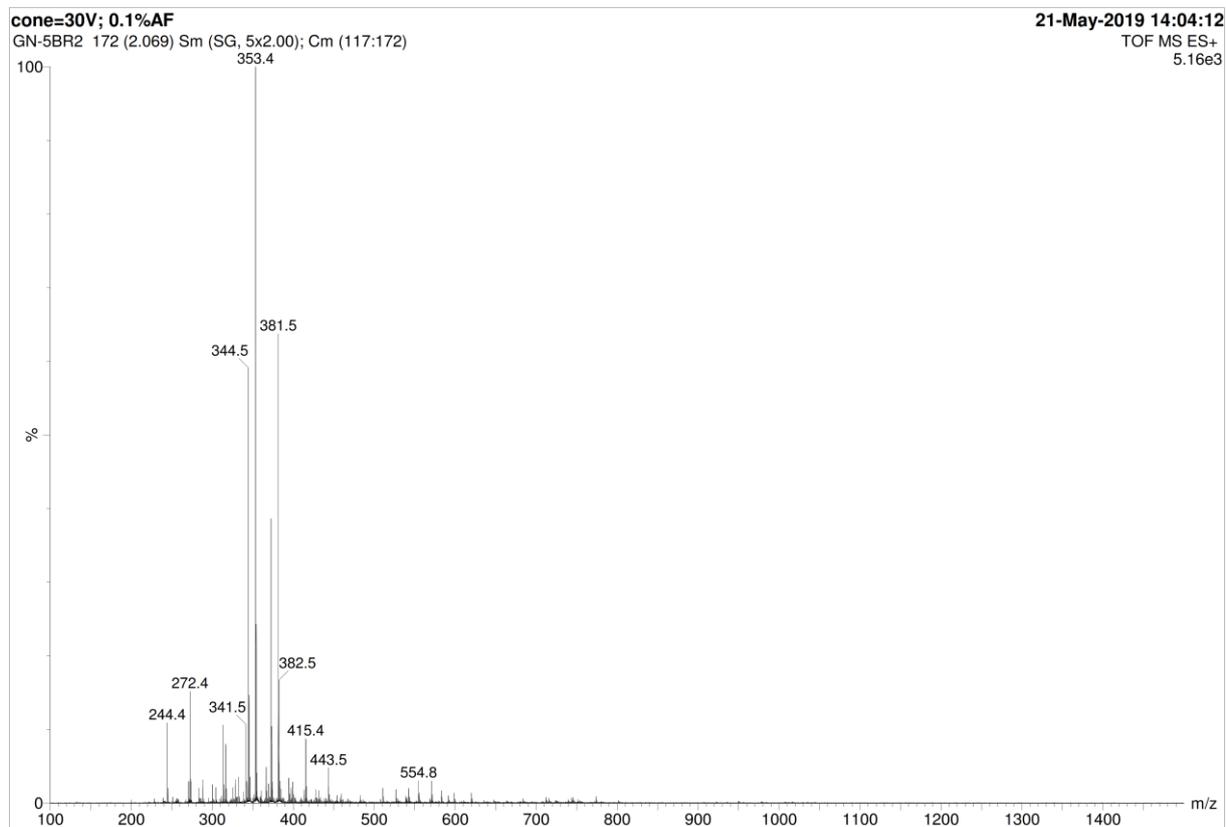


Figure S40. <sup>13</sup>C NMR spectrum of compound **4b** in DMSO-d<sub>6</sub>.



**Figure S41.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **4b** in  $\text{DMSO-d}_6$ .



**Figure S42.** MS-ESI(+) spectrum of compound **4b**.

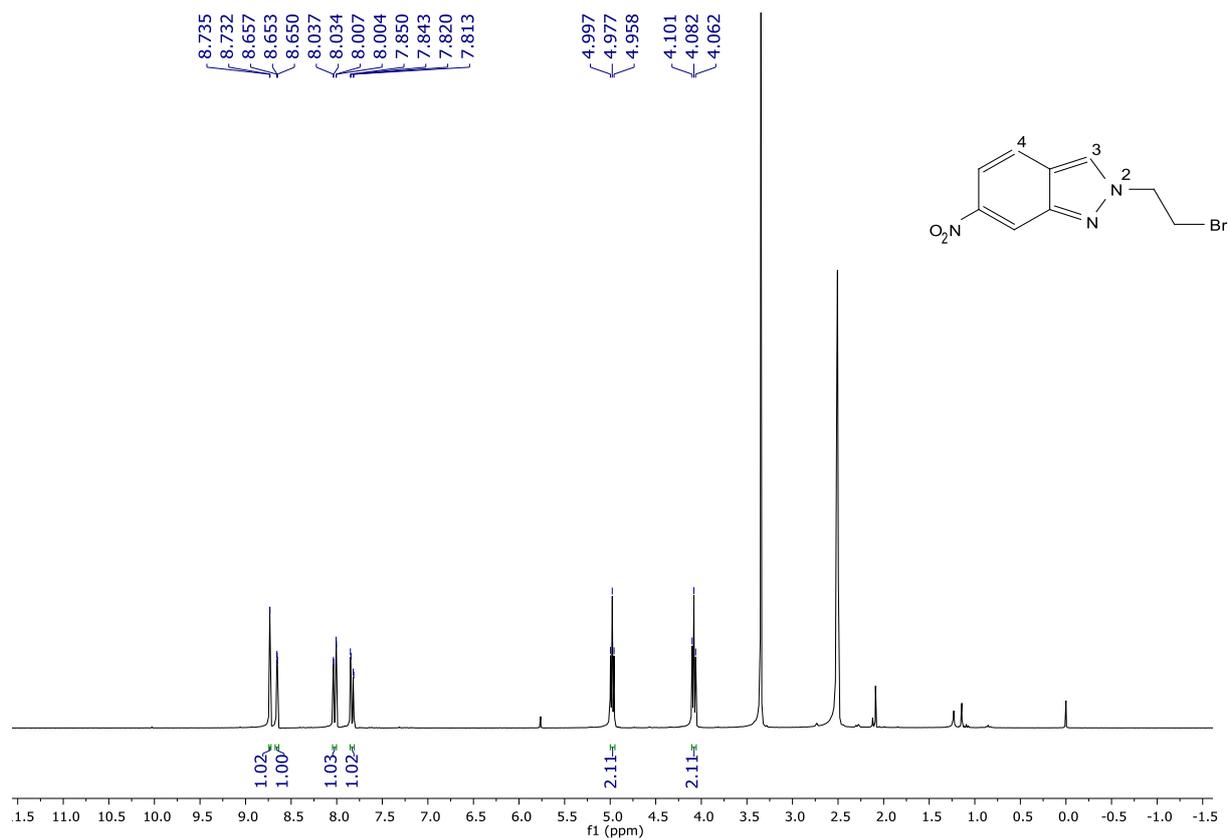


Figure S43. <sup>1</sup>H NMR spectrum of compound **4c** in DMSO-d<sub>6</sub>.

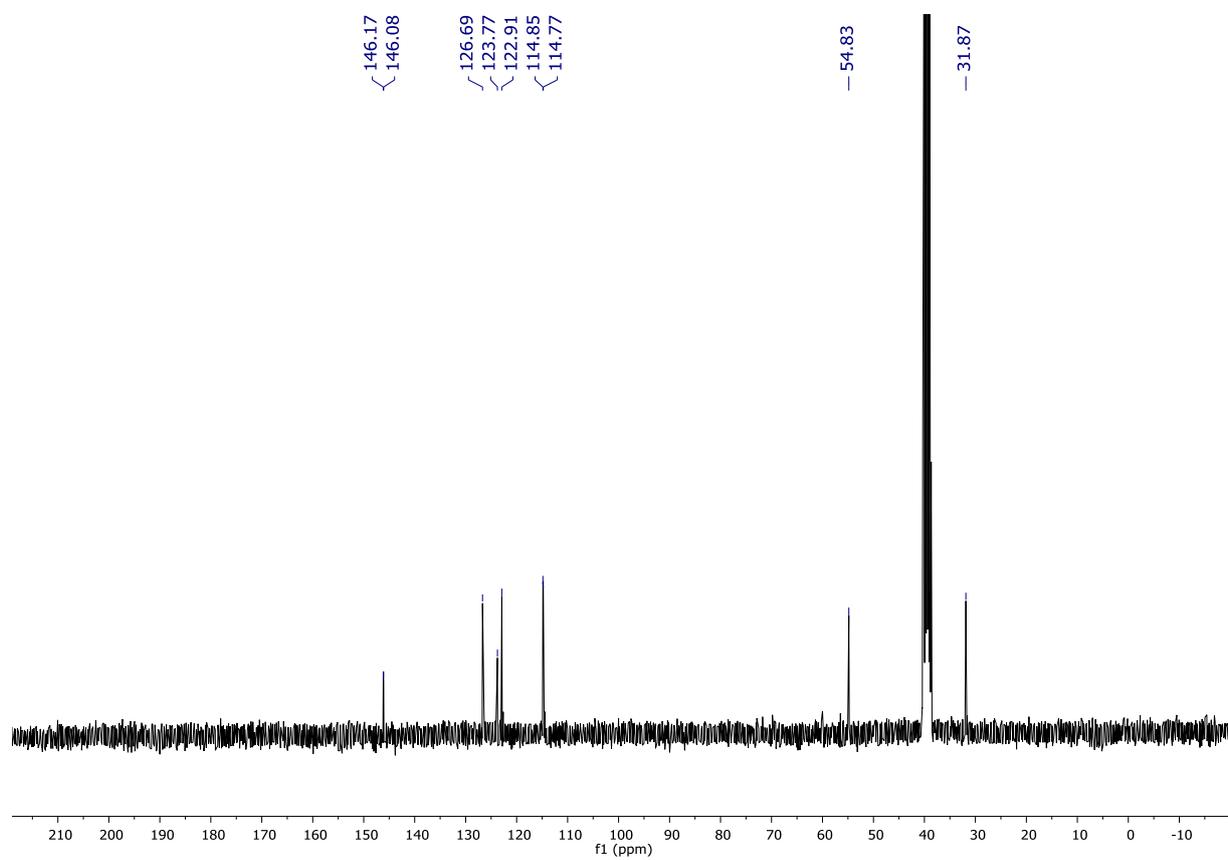
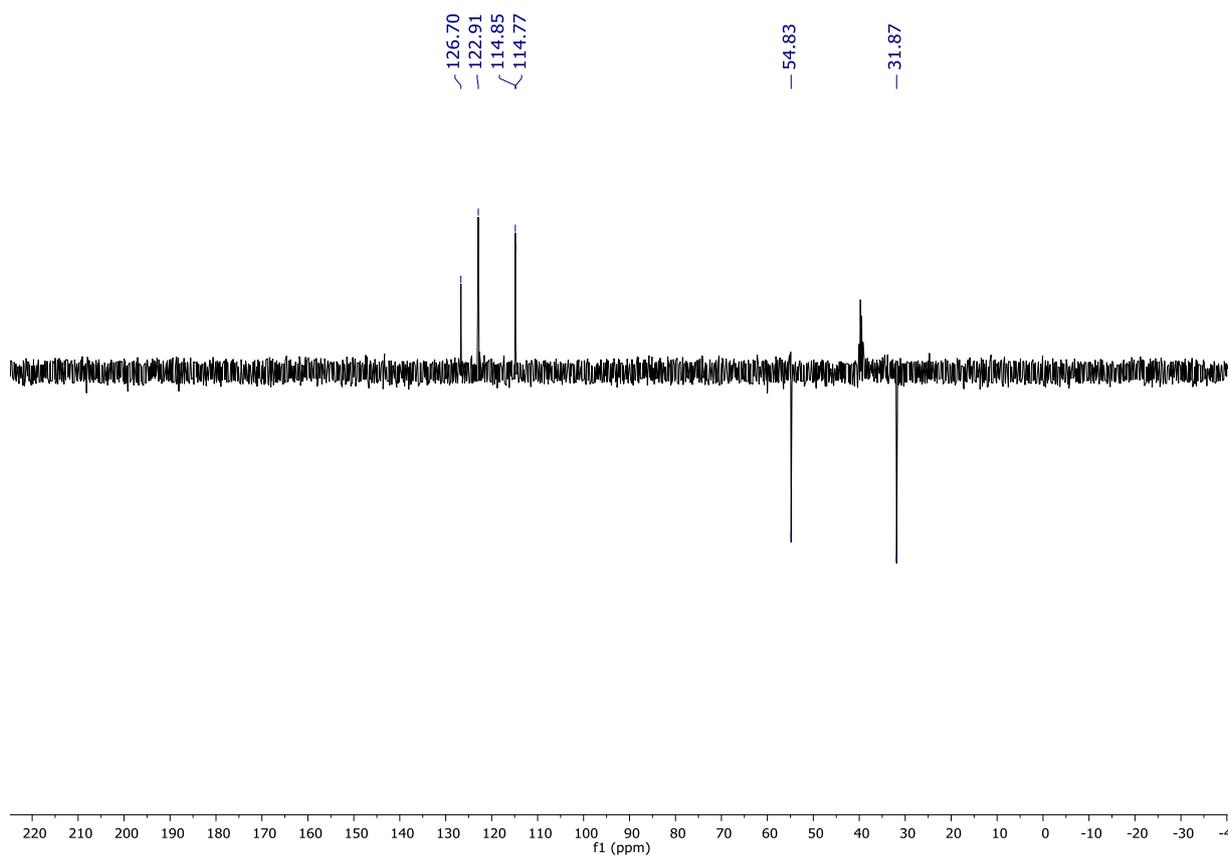
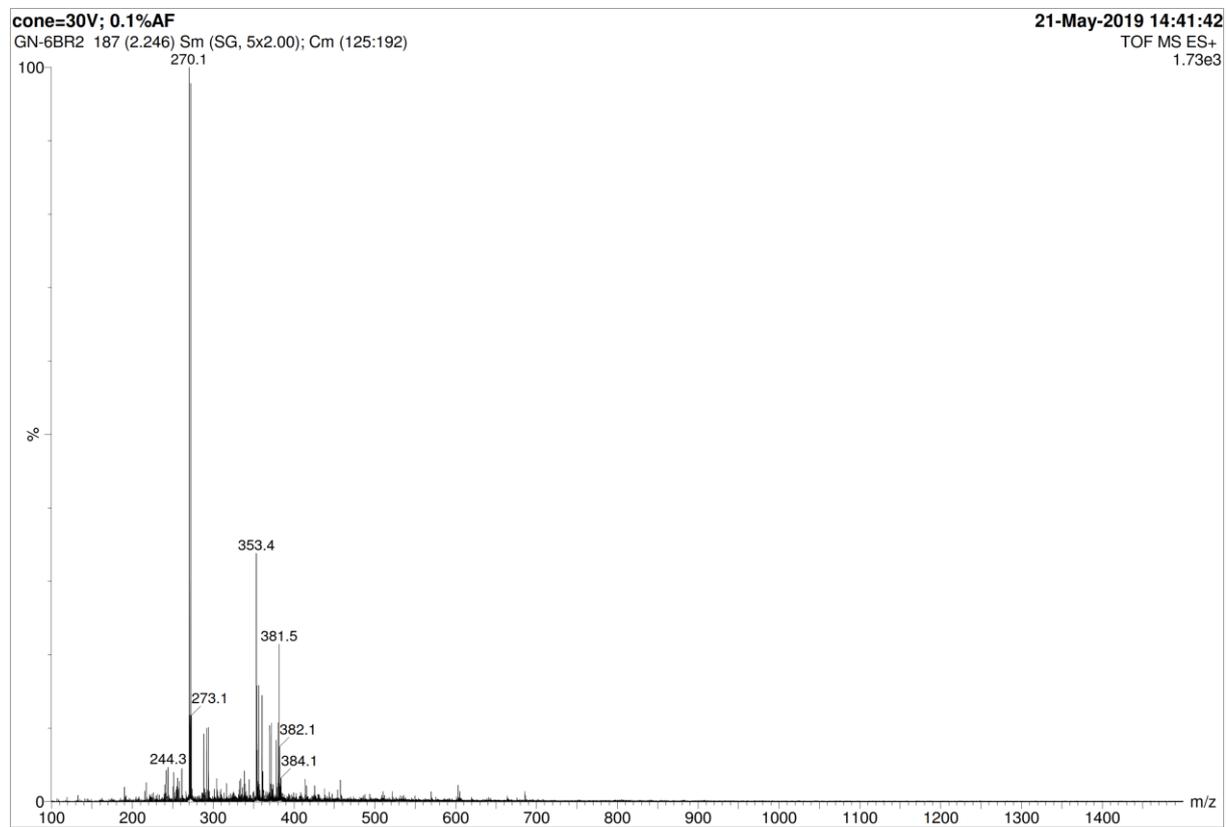


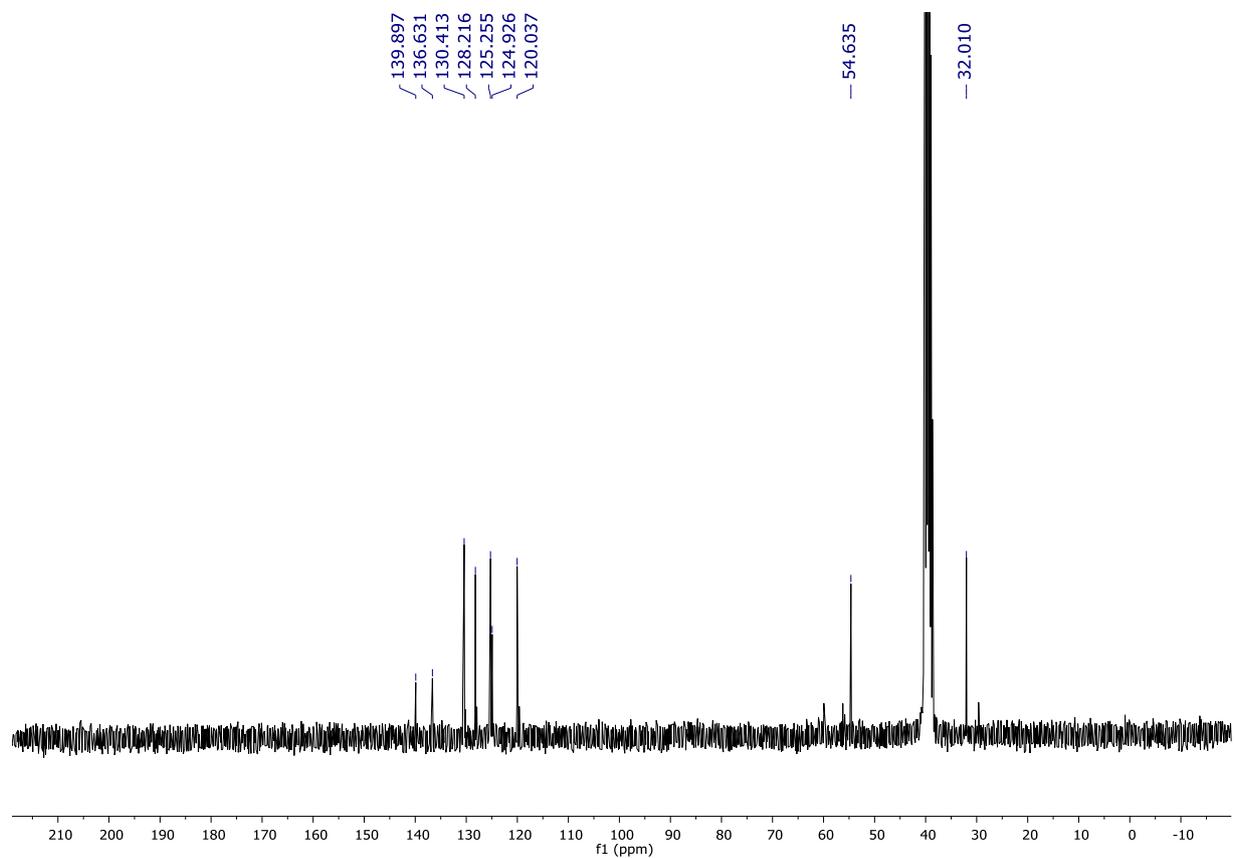
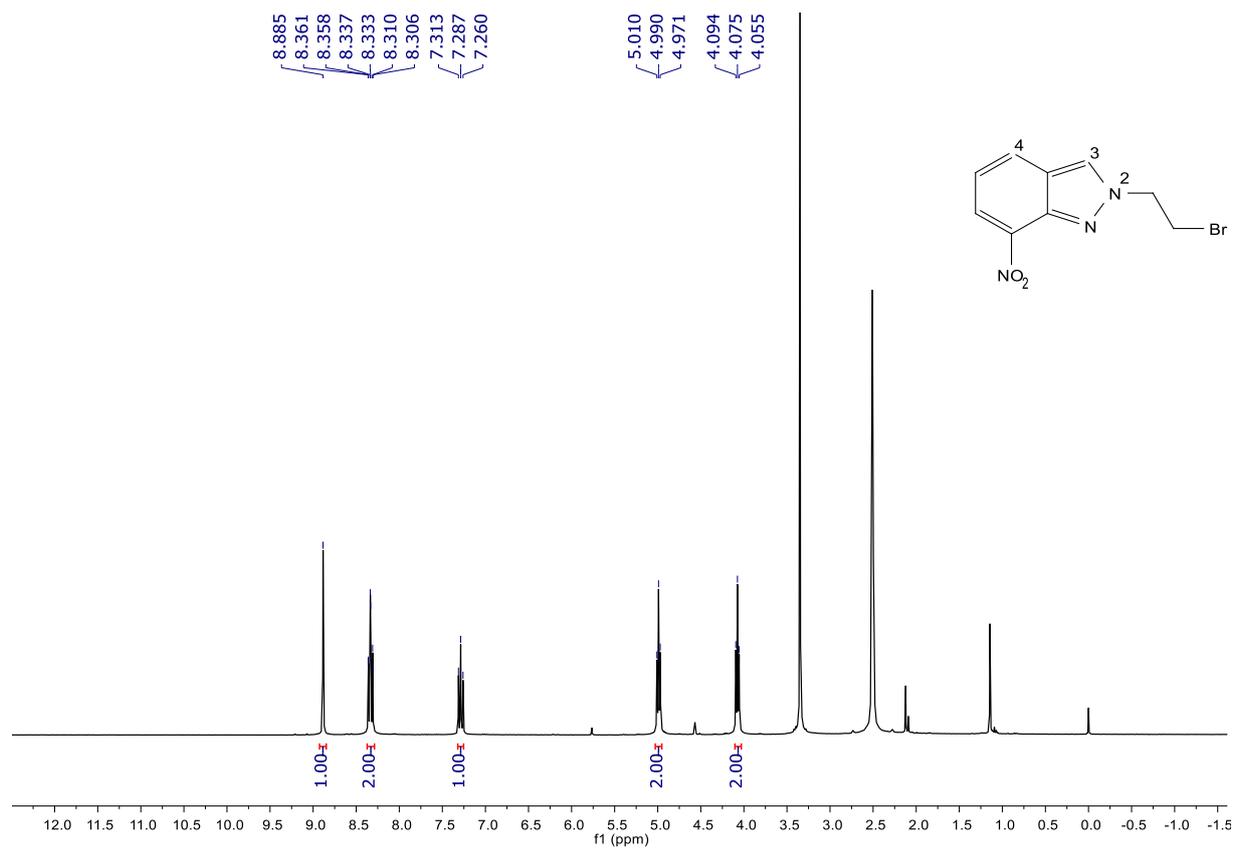
Figure S44. <sup>13</sup>C NMR spectrum of compound **4c** in DMSO-d<sub>6</sub>.

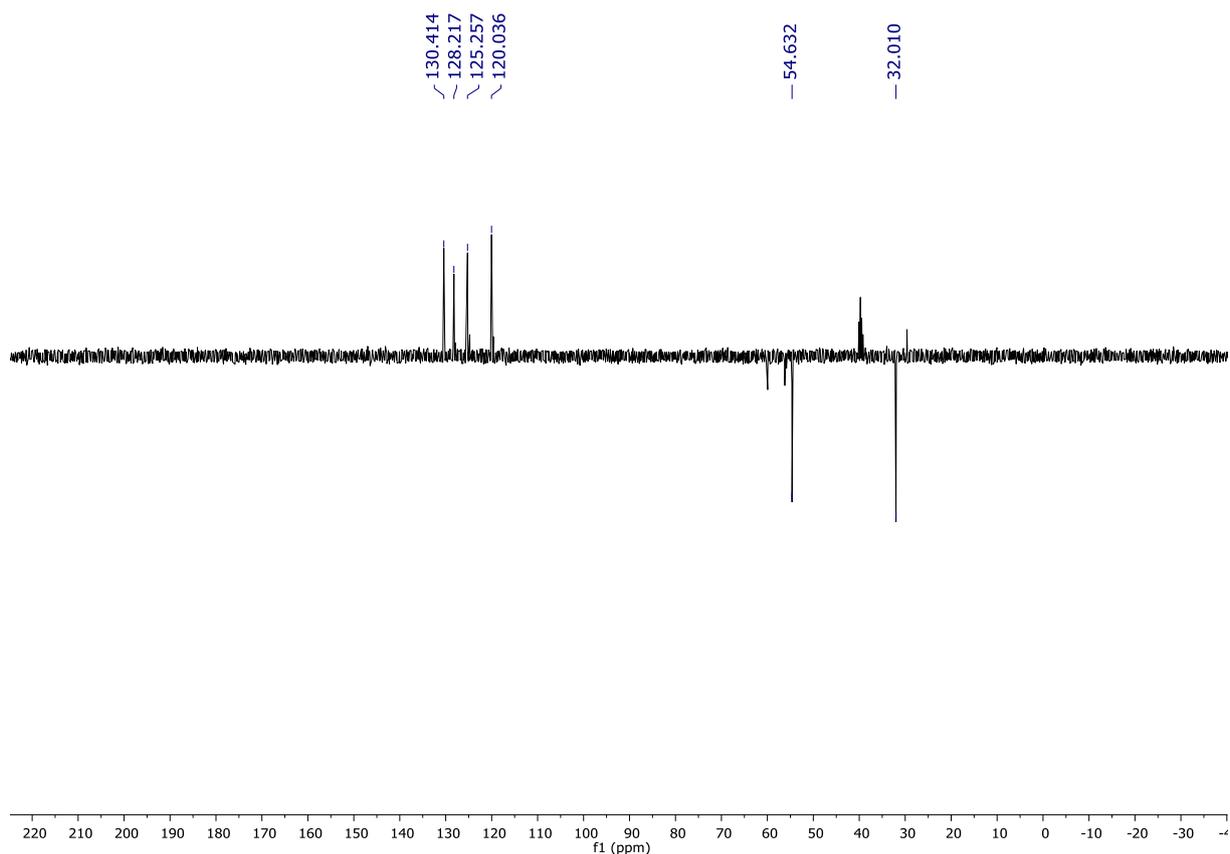


**Figure S45.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **4c** in  $\text{DMSO-d}_6$ .

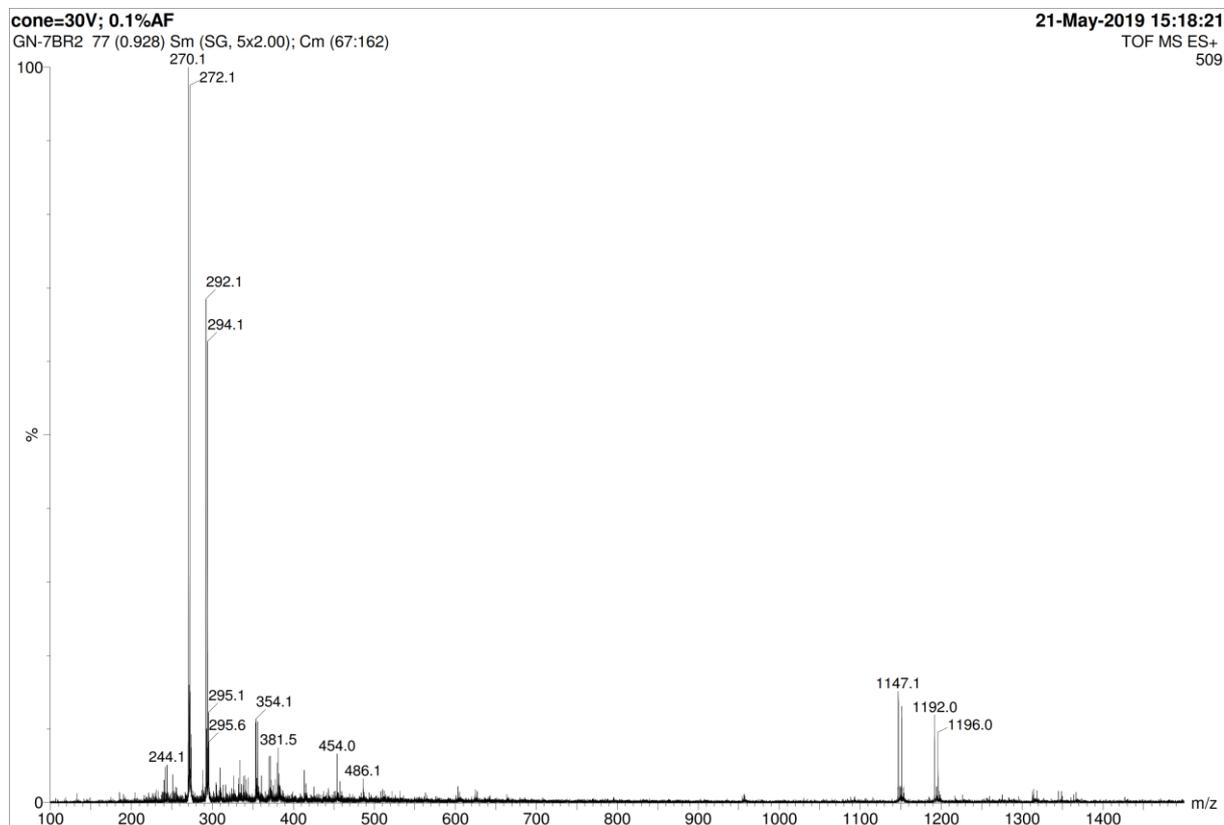


**Figure S46.** MS-ESI(+) spectrum of compound **4c**.





**Figure S49.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **4d** in  $\text{DMSO-d}_6$ .



**Figure S50.** MS-ESI(+) spectrum of compound **4d**.

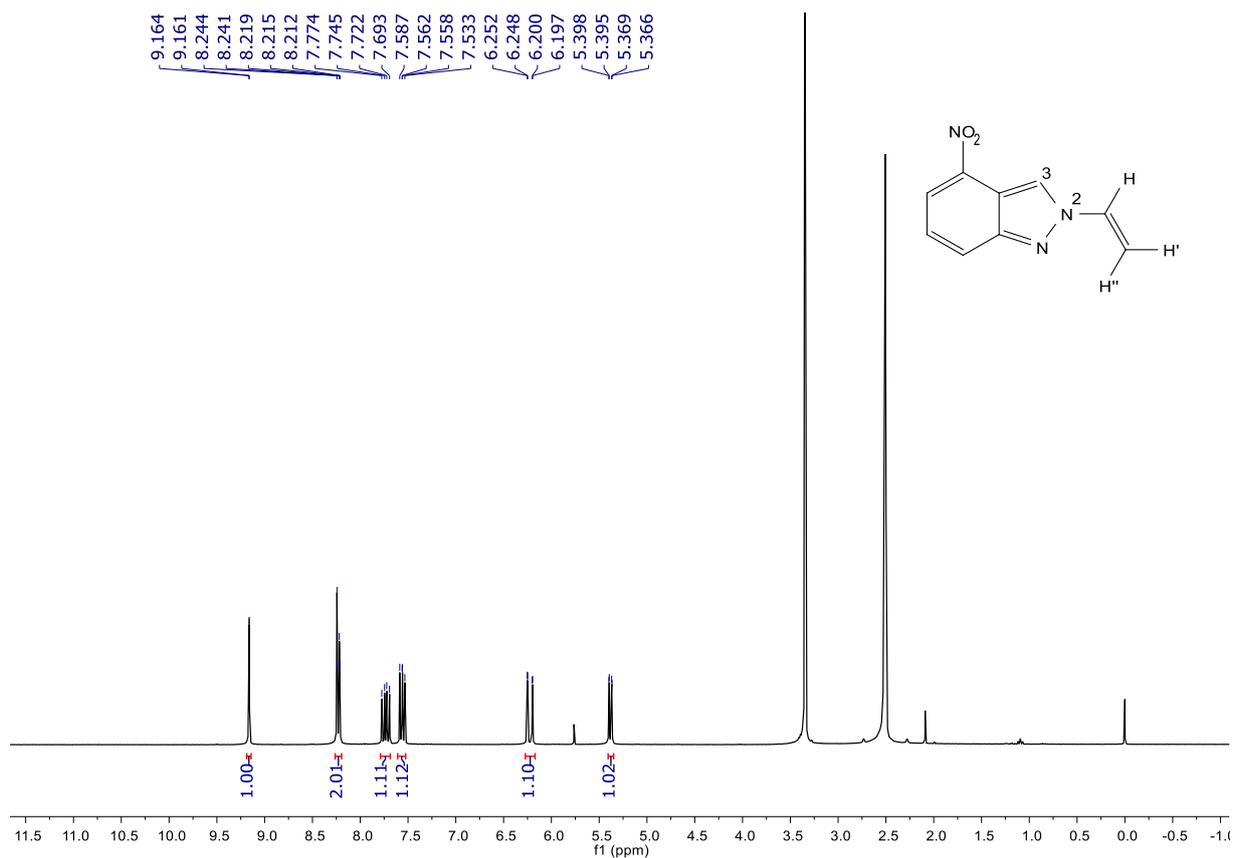


Figure S51.  $^1\text{H}$  NMR spectrum of compound **5a** in  $\text{DMSO-d}_6$ .

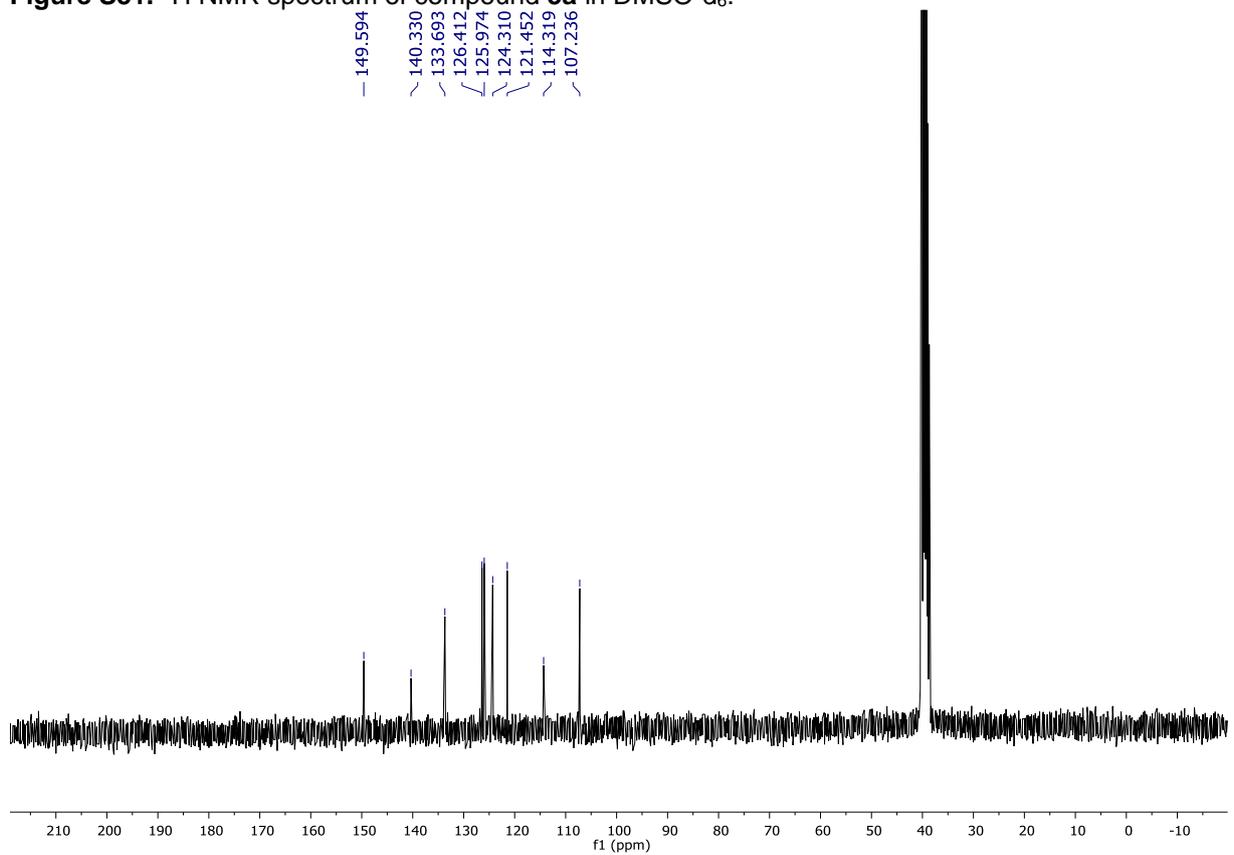


Figure S52.  $^{13}\text{C}$  NMR spectrum of compound **5a** in  $\text{DMSO-d}_6$ .

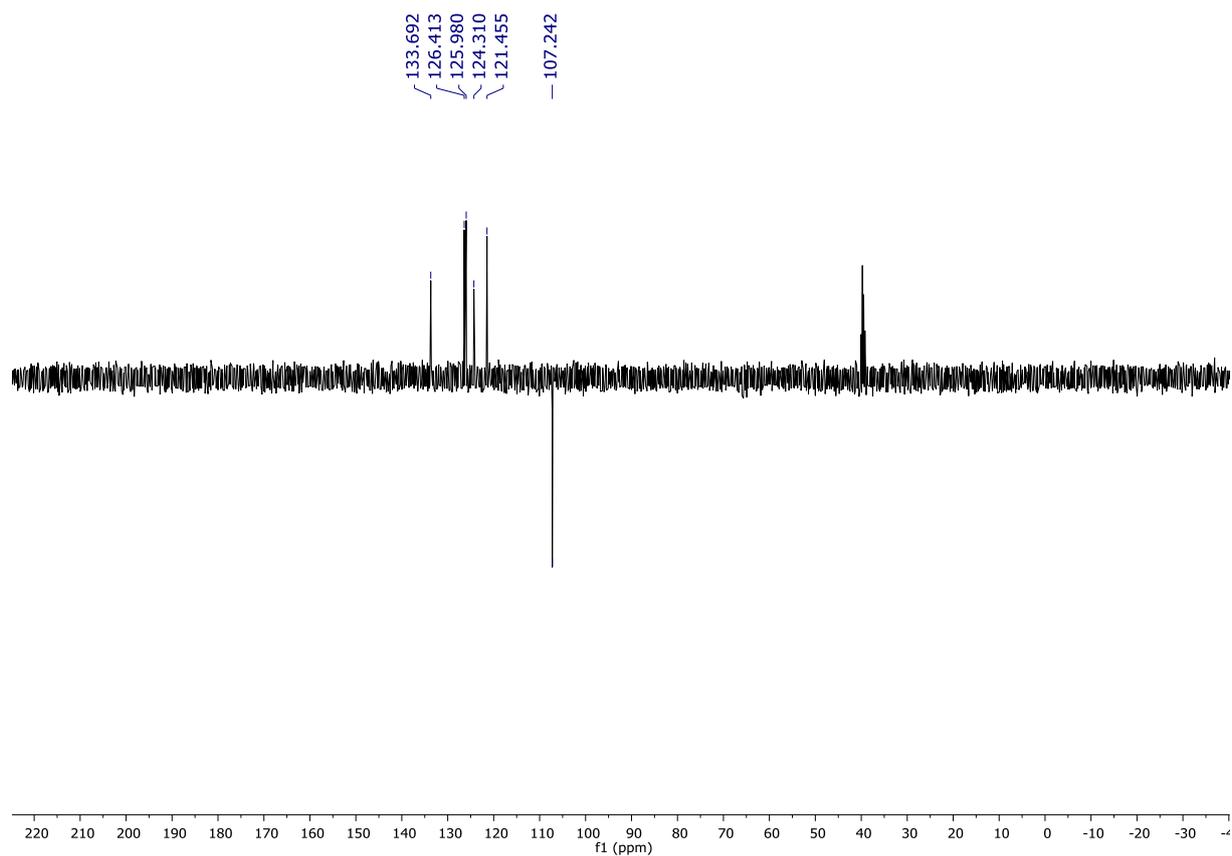


Figure S53.  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **5a** in  $\text{DMSO-d}_6$ .

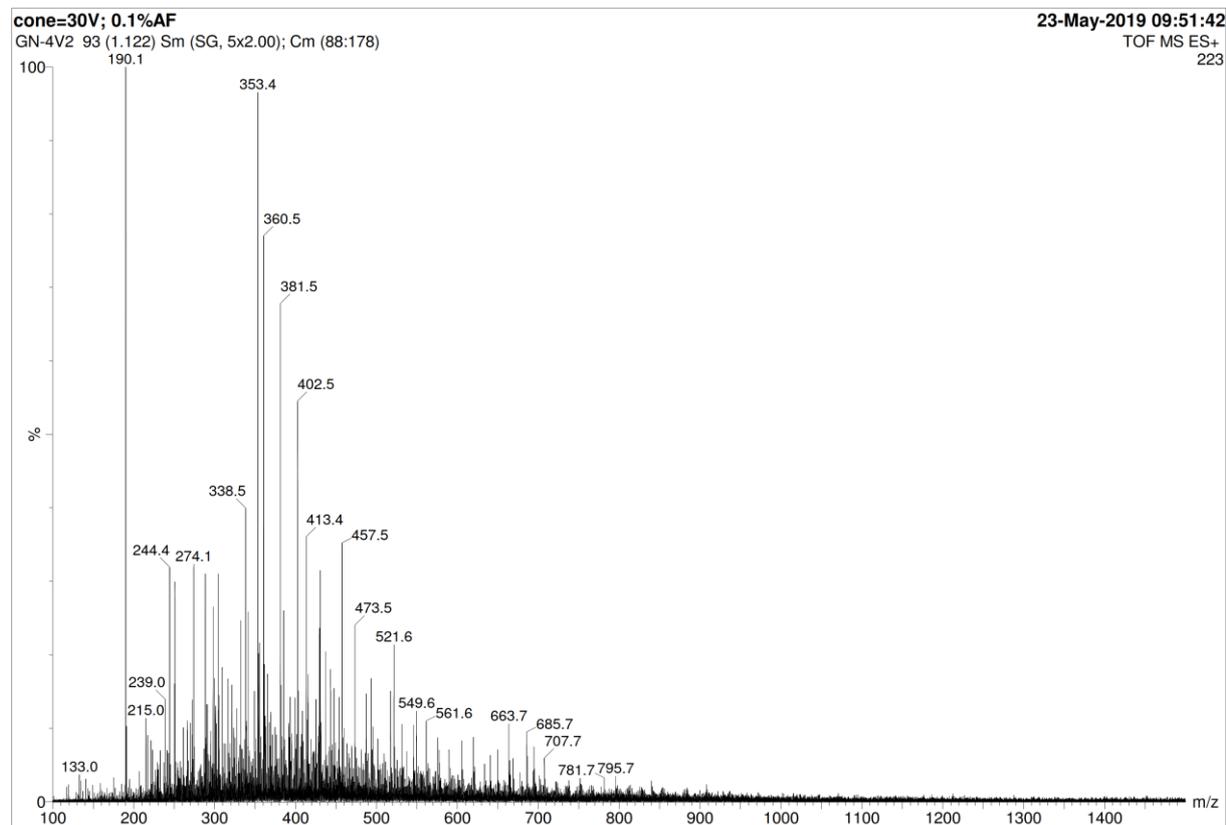


Figure S54. MS-ESI(+) spectrum of compound **5a**.

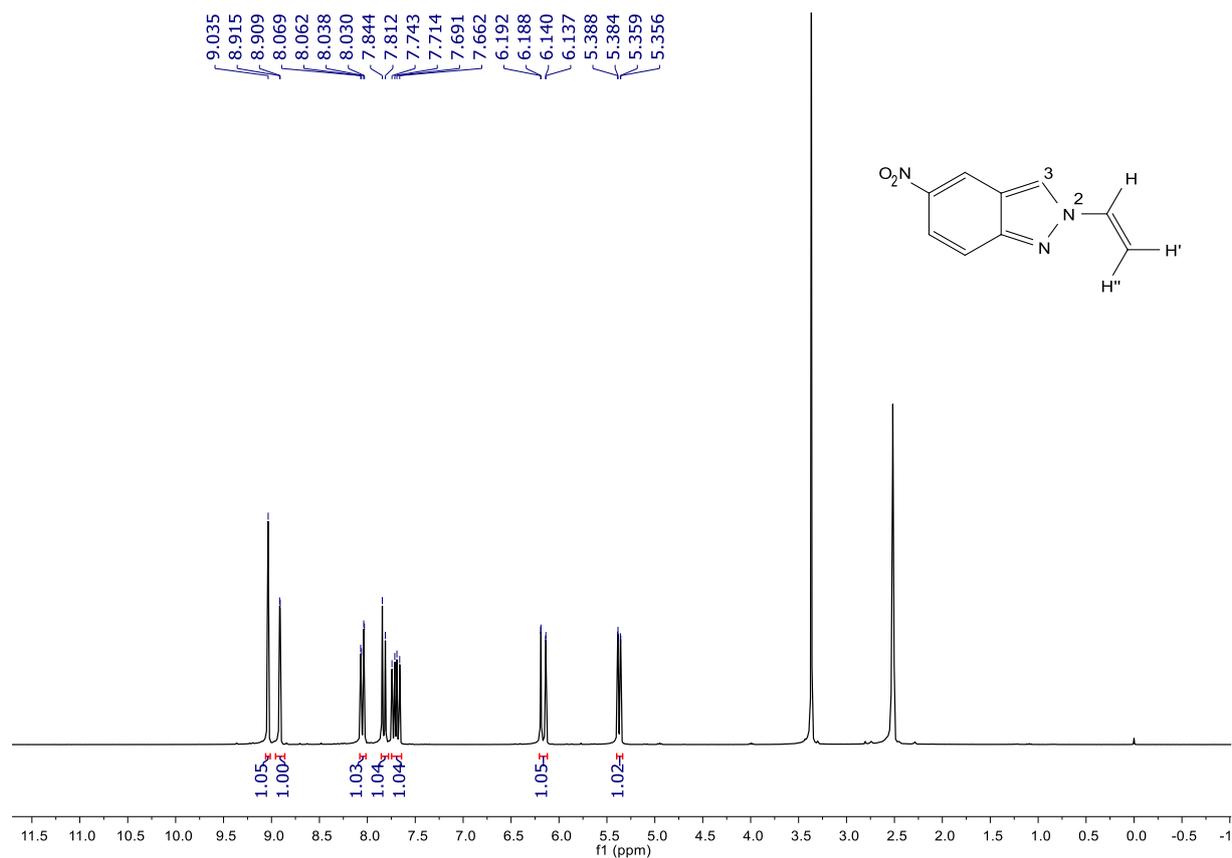


Figure S55. <sup>1</sup>H NMR spectrum of compound **5b** in DMSO-d<sub>6</sub>.

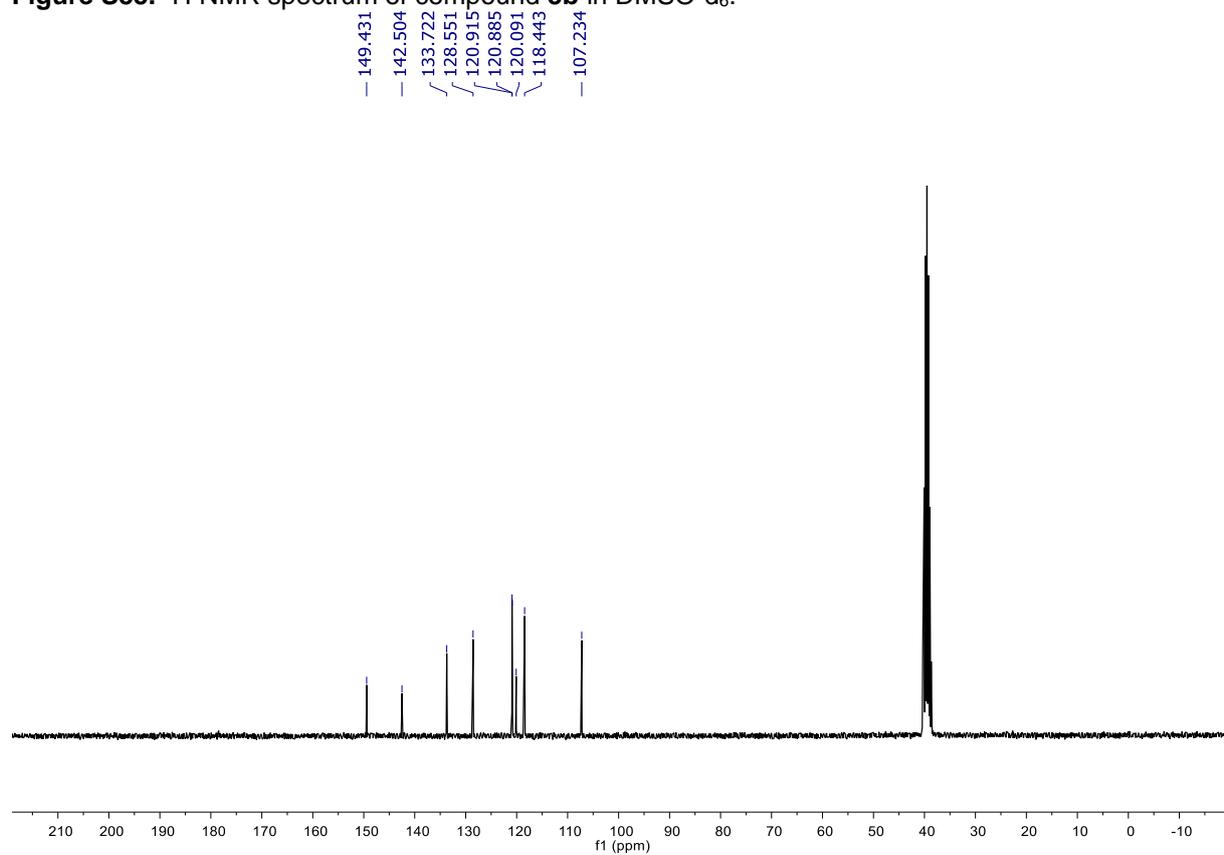
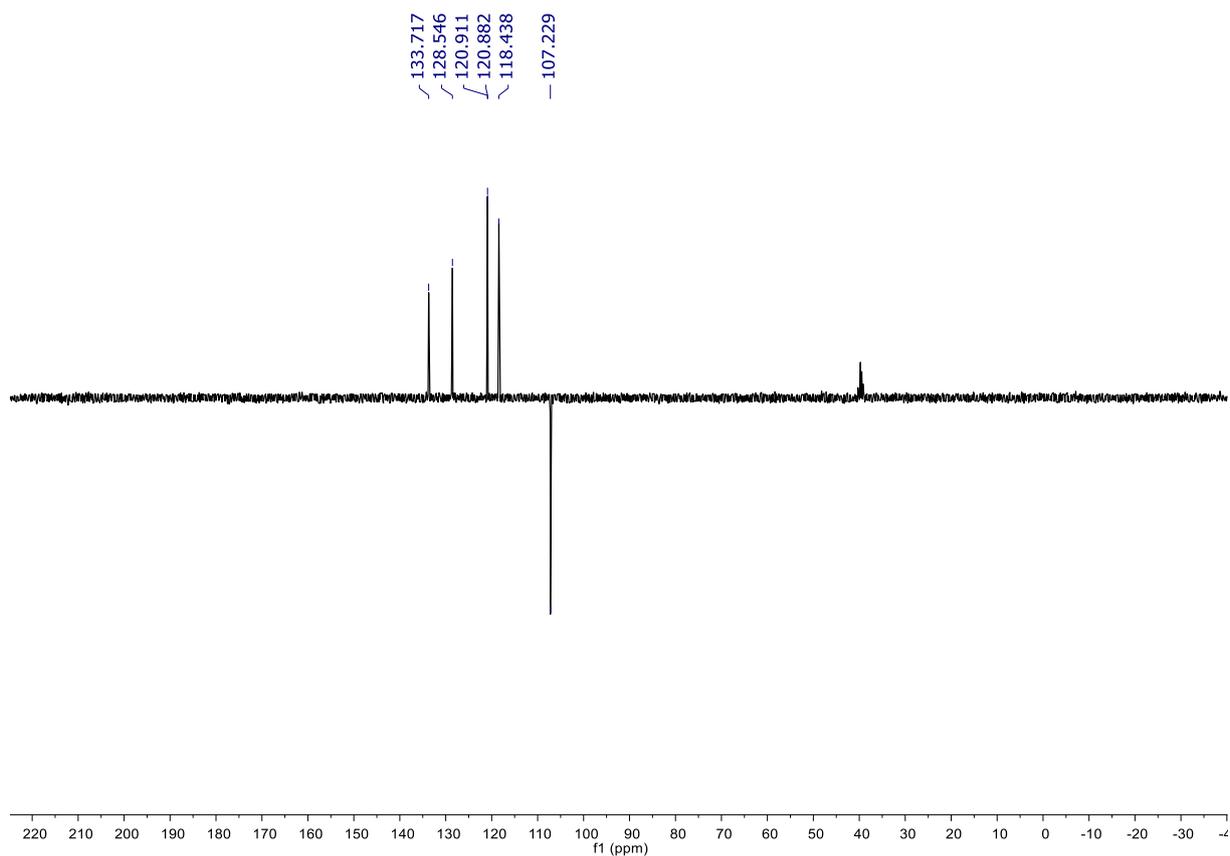
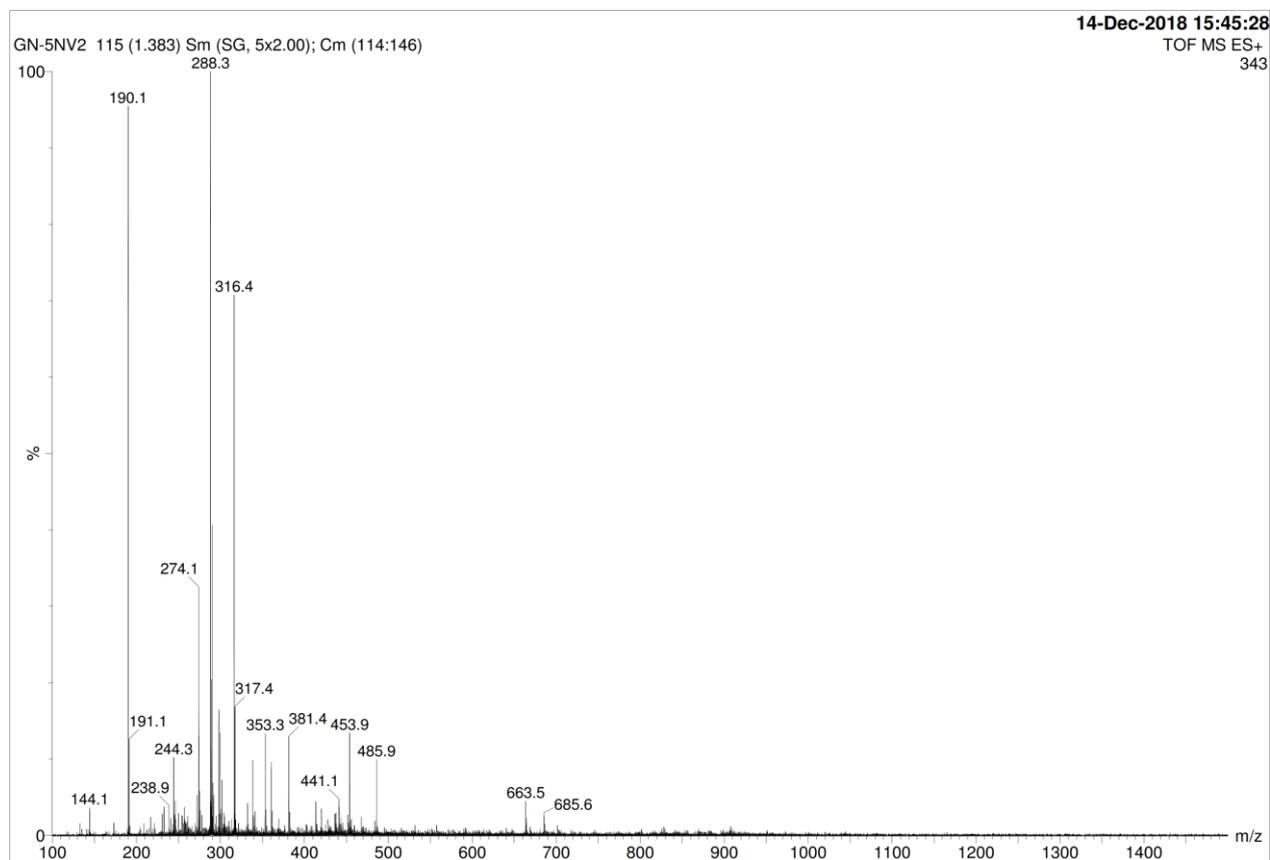


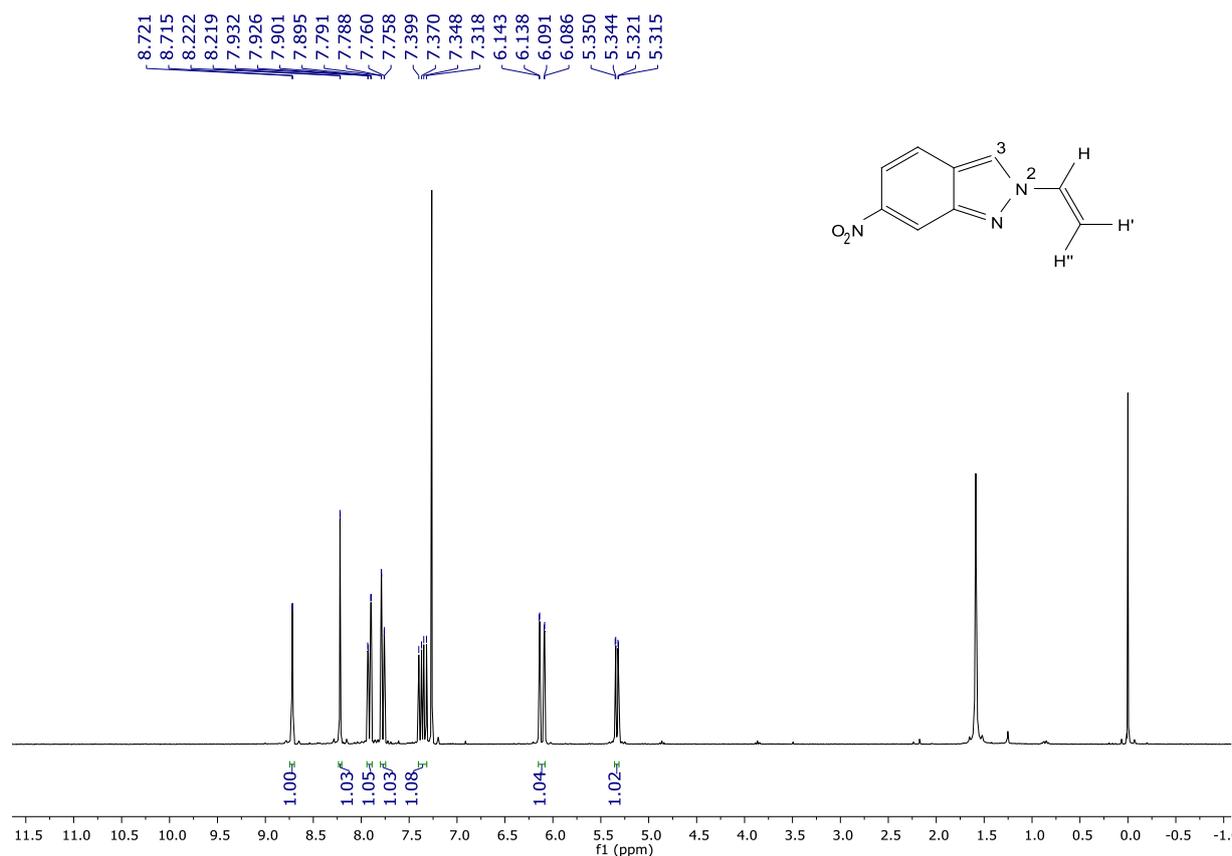
Figure S56. <sup>13</sup>C NMR spectrum of compound **5b** in DMSO-d<sub>6</sub>.



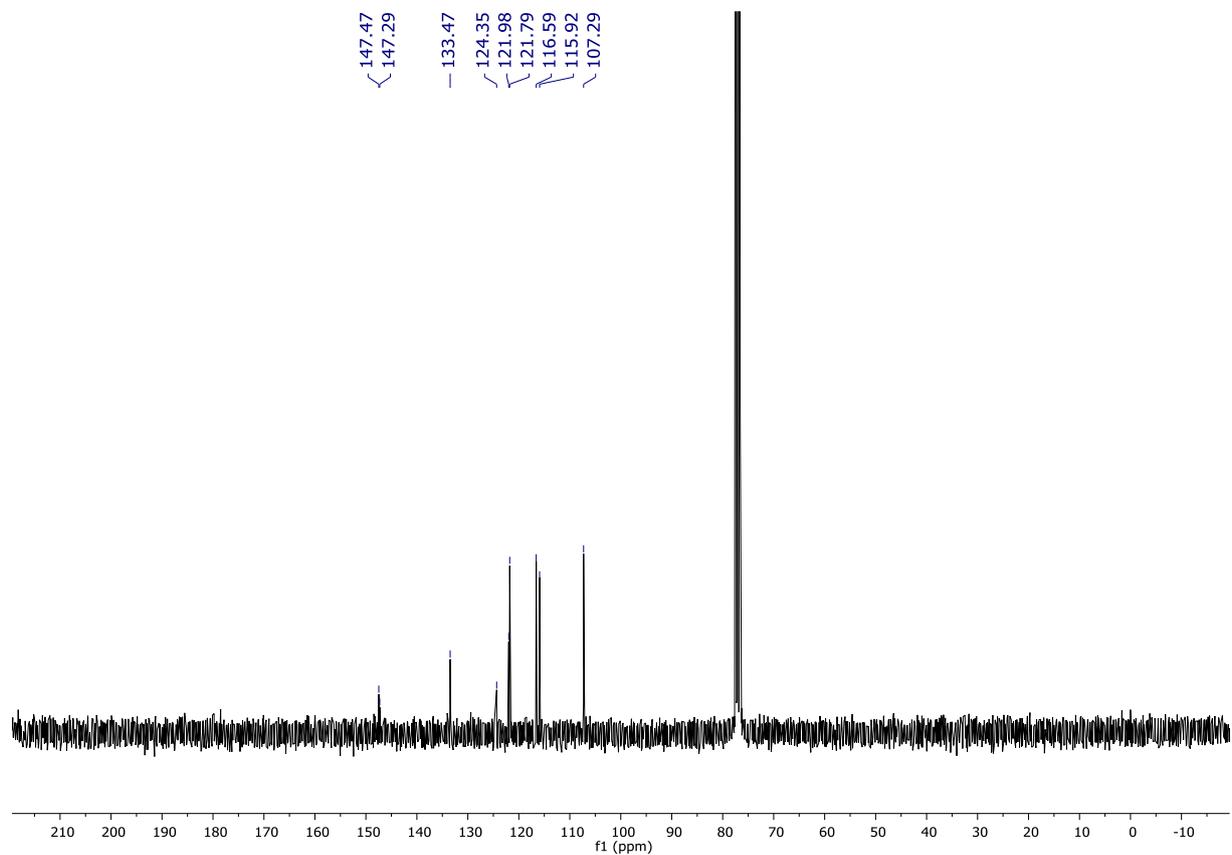
**Figure S57.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **5b** in  $\text{DMSO-d}_6$ .



**Figure S58.** MS-ESI(+) spectrum of compound **5b**



**Figure S59.** <sup>1</sup>H NMR spectrum of compound **5c** in CDCl<sub>3</sub>.



**Figure S60.** <sup>13</sup>C NMR spectrum of compound **5c** in CDCl<sub>3</sub>.

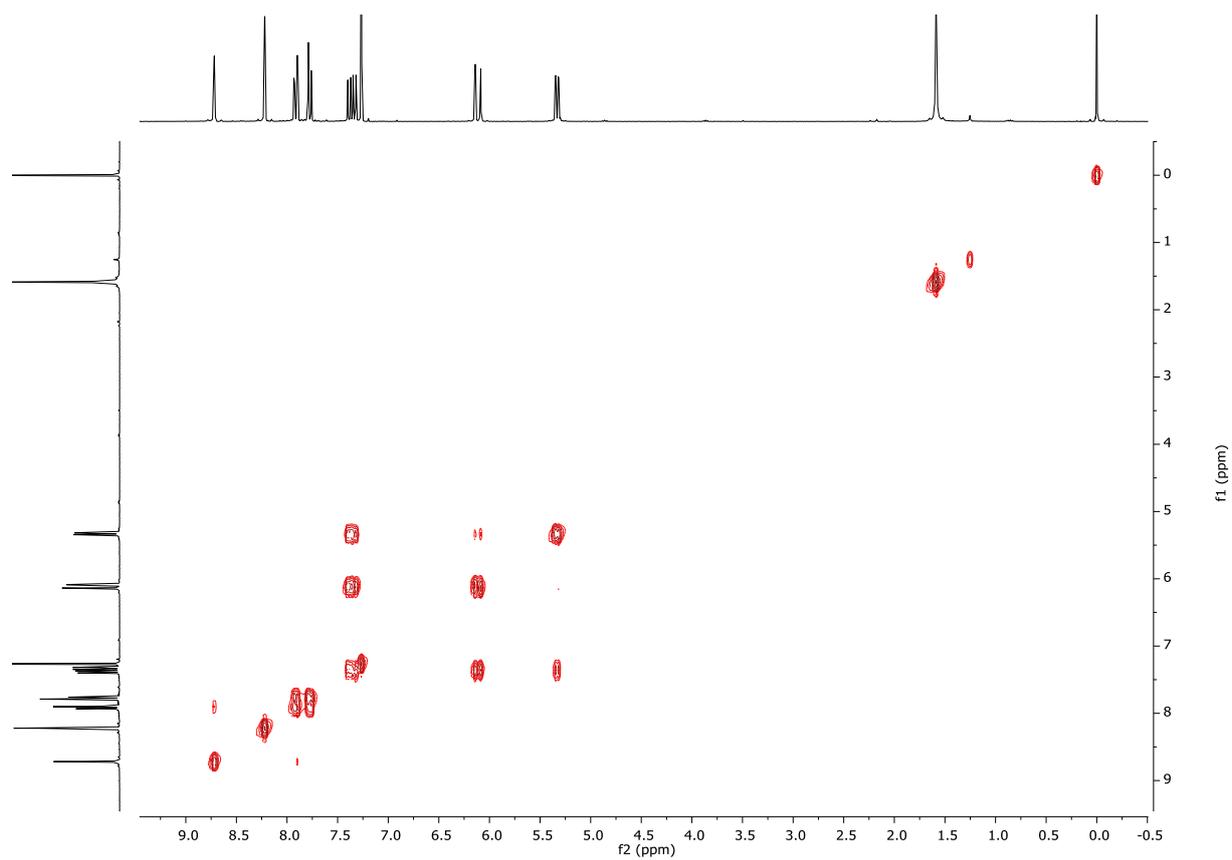


Figure S61. COSY ( $^1\text{H}/^1\text{H}$ ) spectrum of compound **5c** in  $\text{CDCl}_3$ .

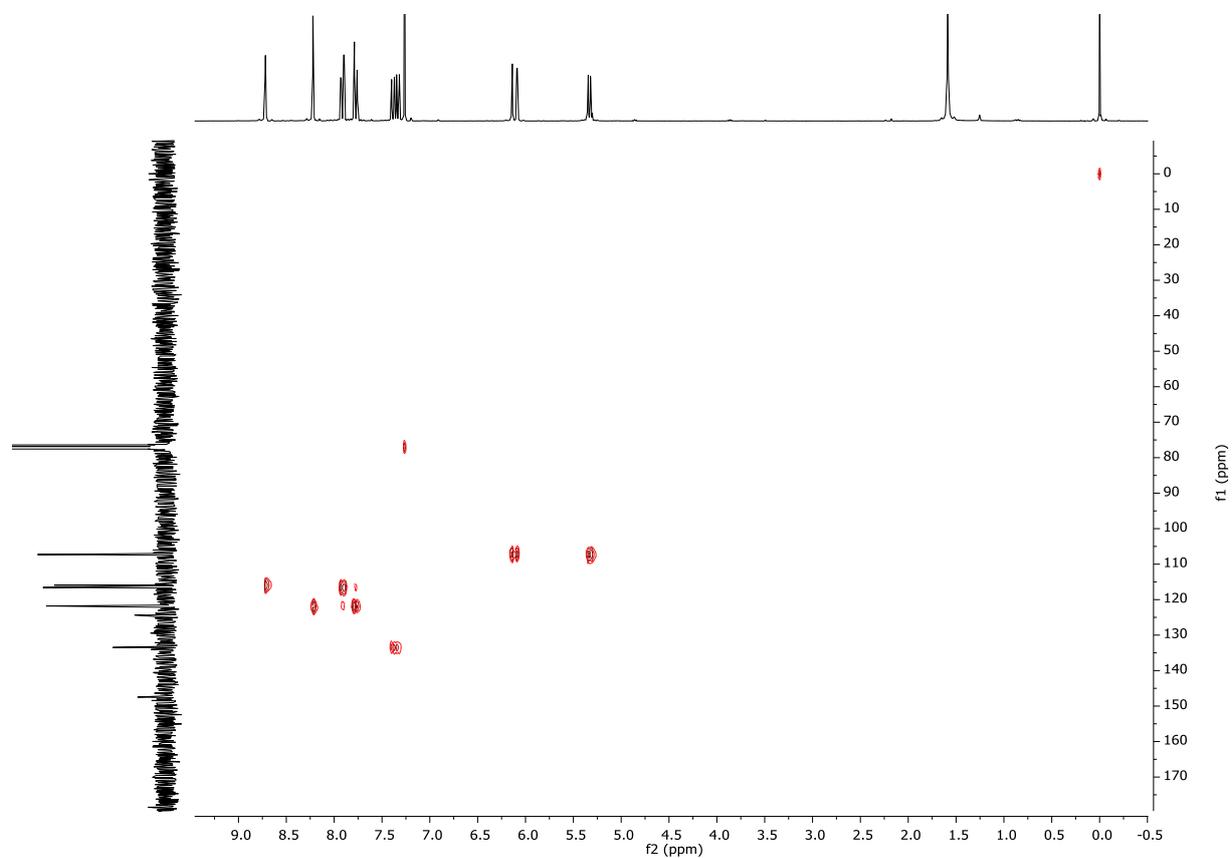
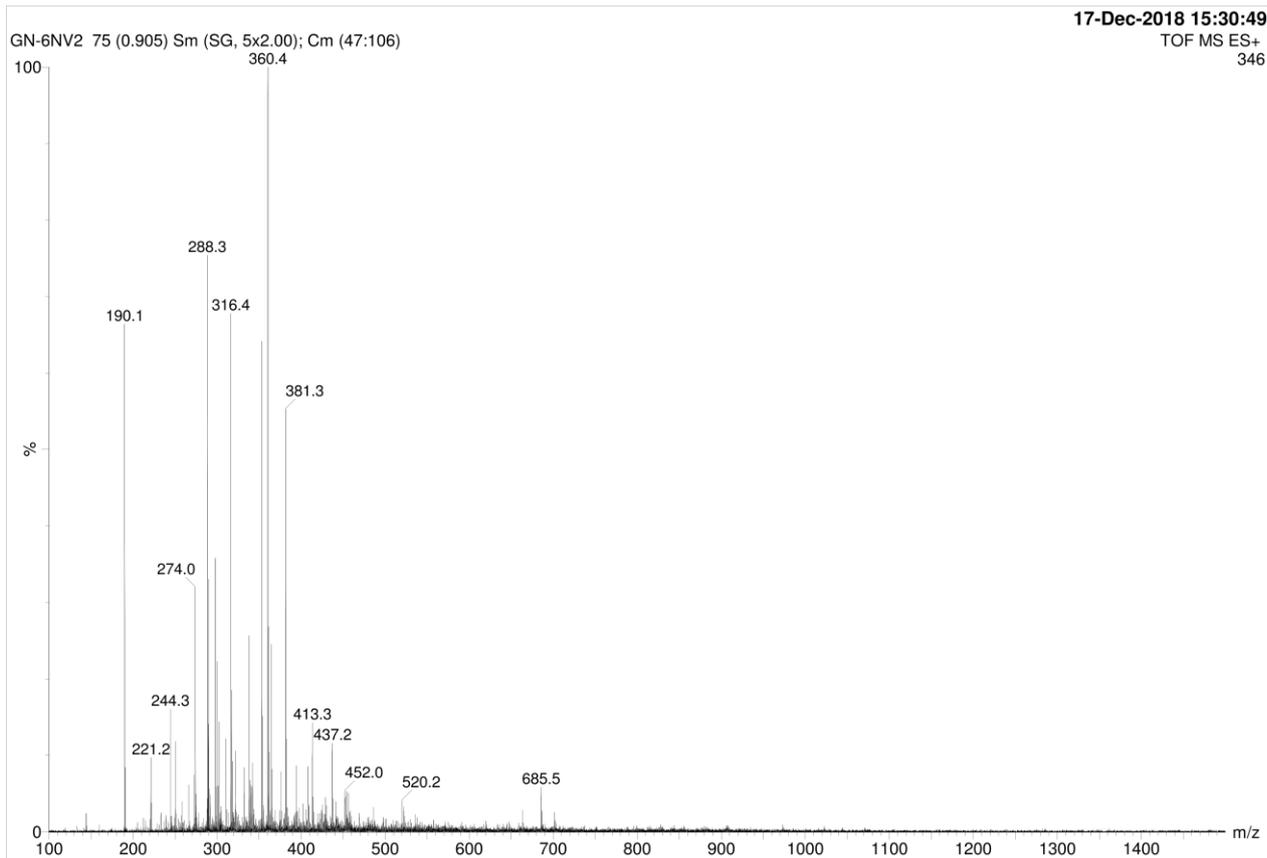
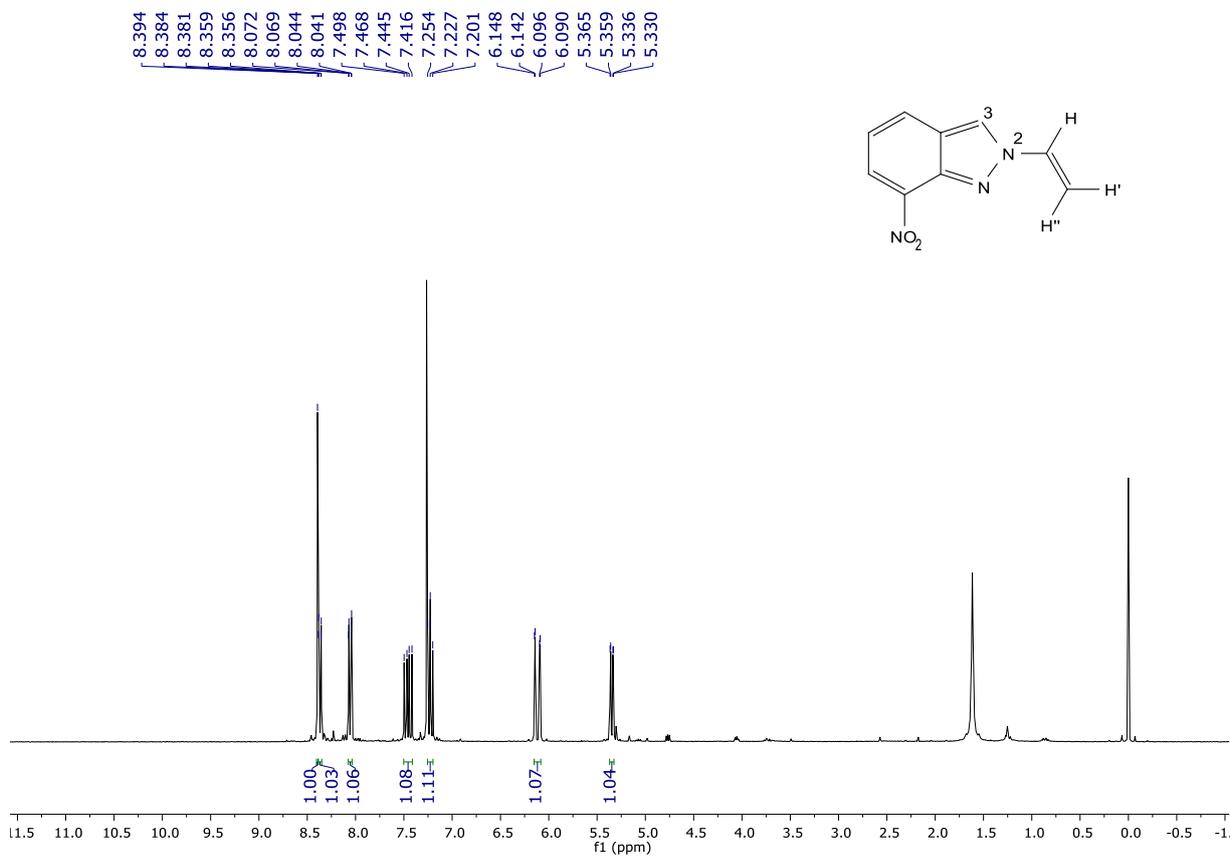


Figure S62. HSQC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **5c** in  $\text{CDCl}_3$ .



**Figure S63.** MS-ESI(+) spectrum of compound **5c**



**Figure S64.** <sup>1</sup>H NMR spectrum of compound **5d** in CDCl<sub>3</sub>.

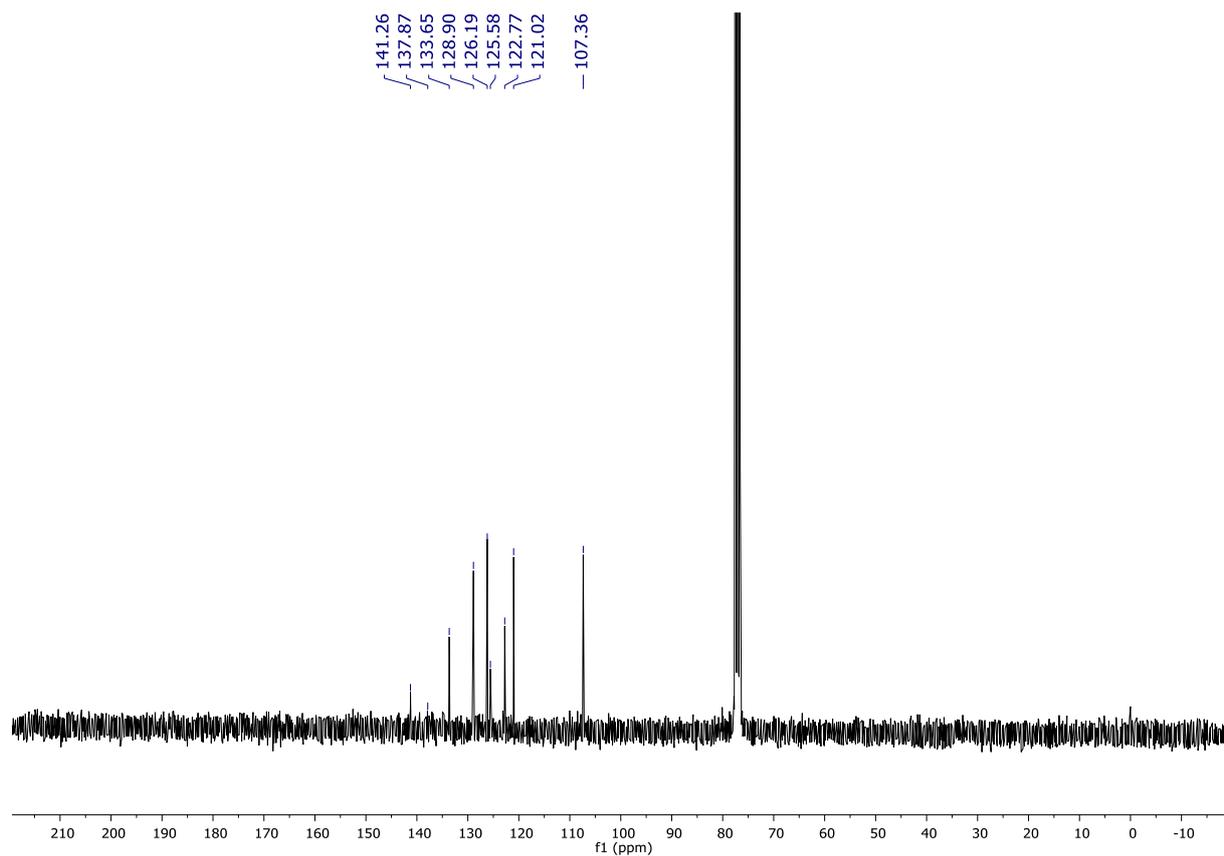


Figure S65.  $^{13}\text{C}$  NMR spectrum of compound **5d** in  $\text{CDCl}_3$ .

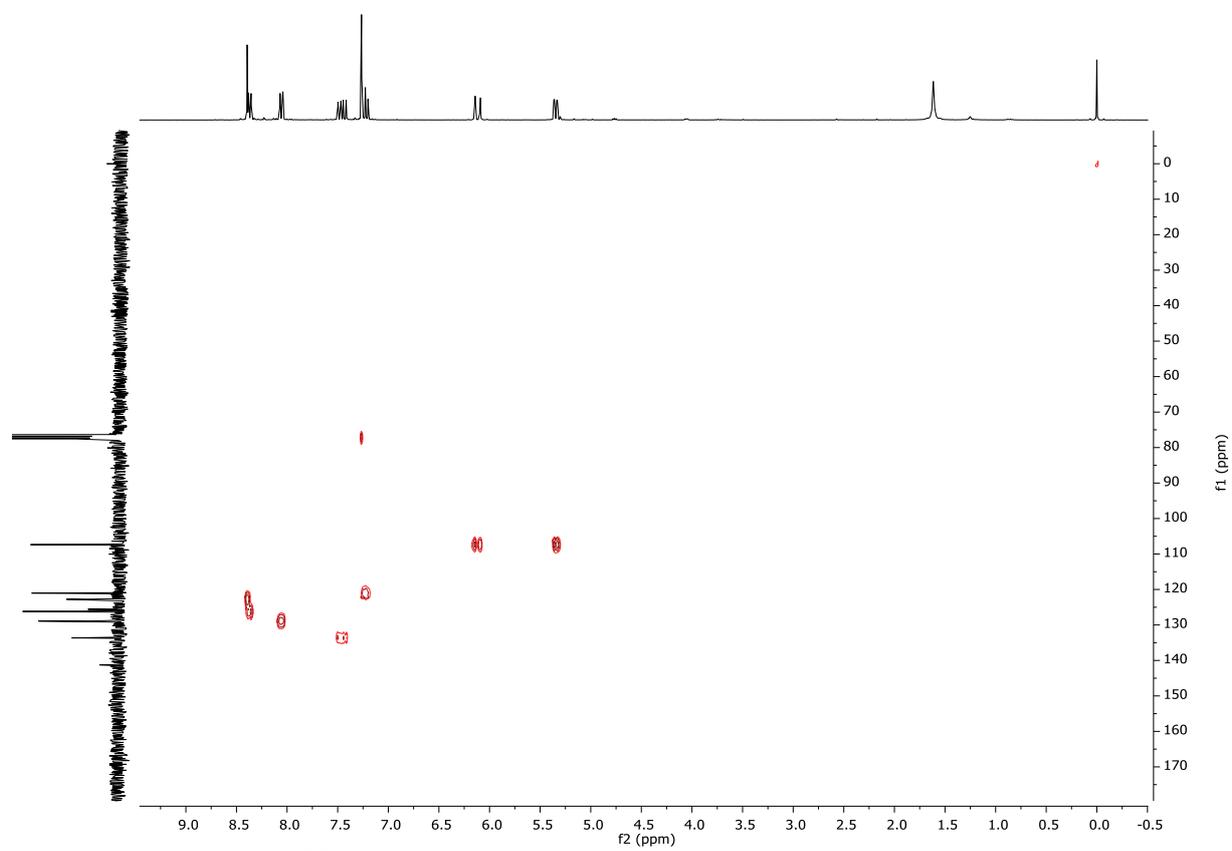
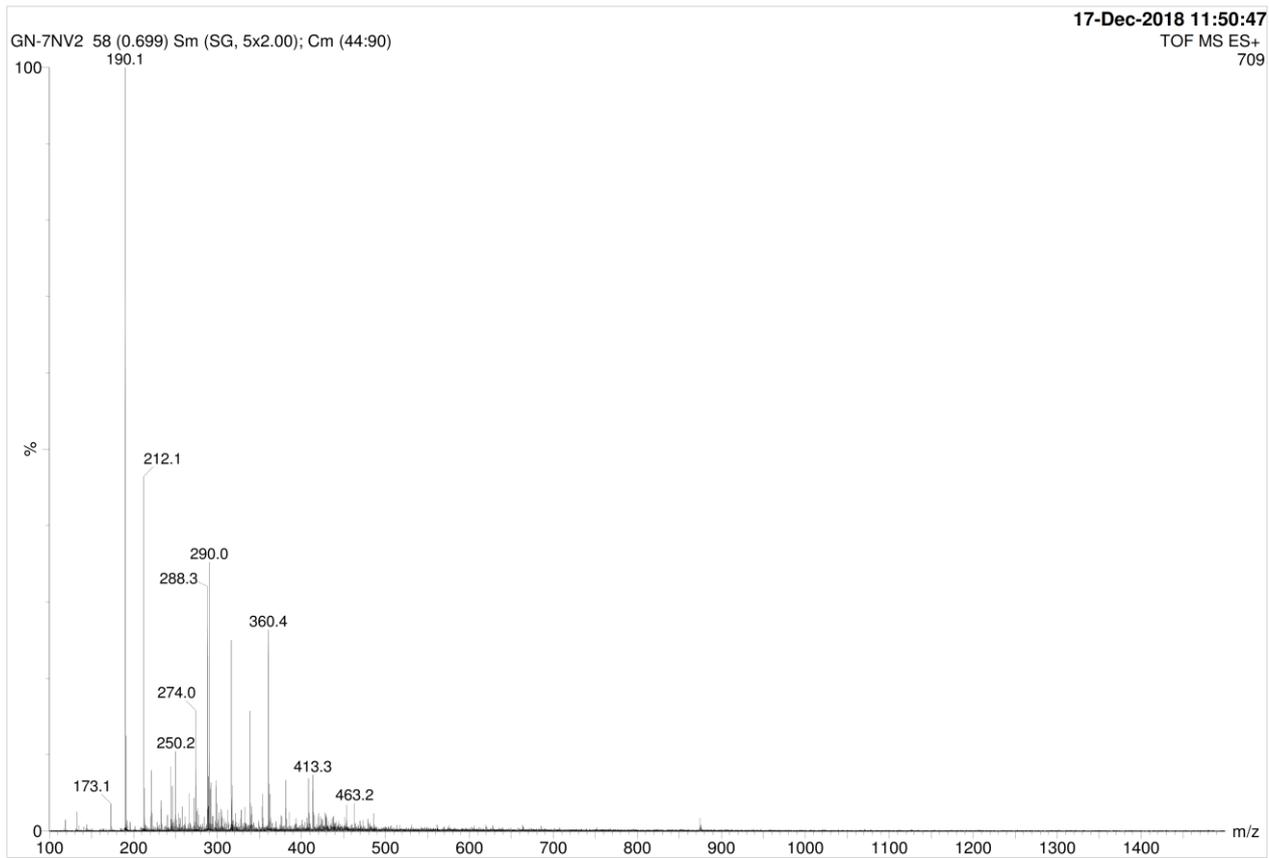


Figure S66. HSQC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **5d** in  $\text{CDCl}_3$ .



**Figure S67.** MS-ESI(+) spectrum of compound **5d**.

## II - NMR and mass spectrum of compounds 6, 7a-d, 8 and 9

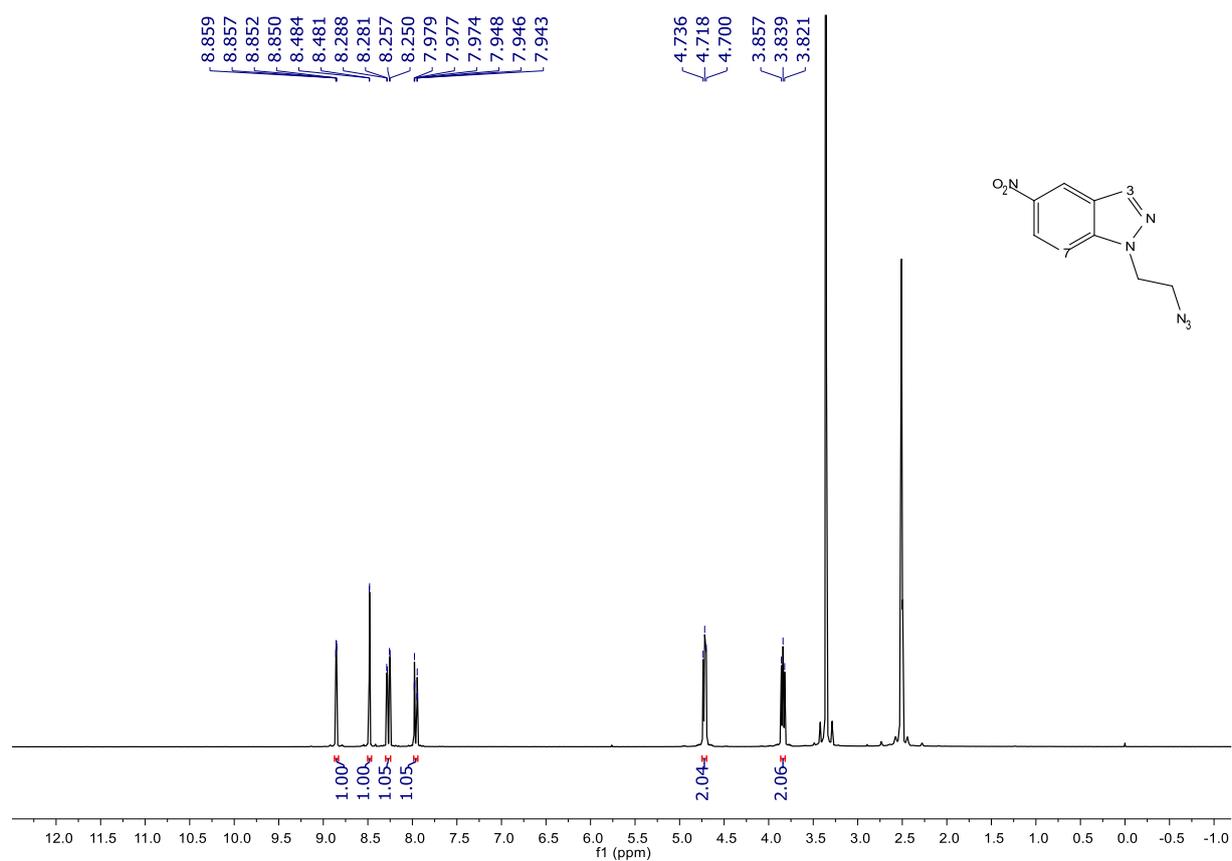


Figure S68. <sup>1</sup>H NMR spectrum of compound 6 in DMSO-d<sub>6</sub>.

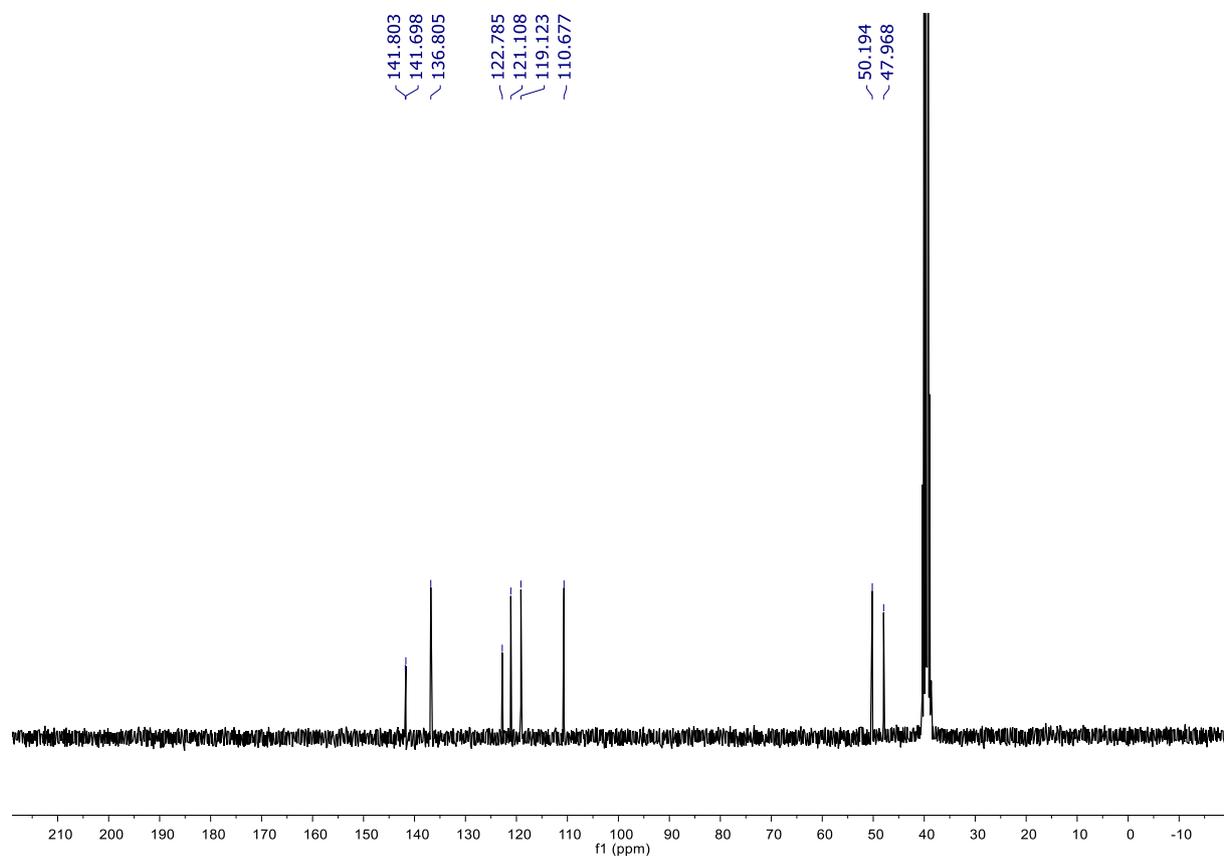


Figure S69. <sup>13</sup>C NMR spectrum of compound 6 in DMSO-d<sub>6</sub>.

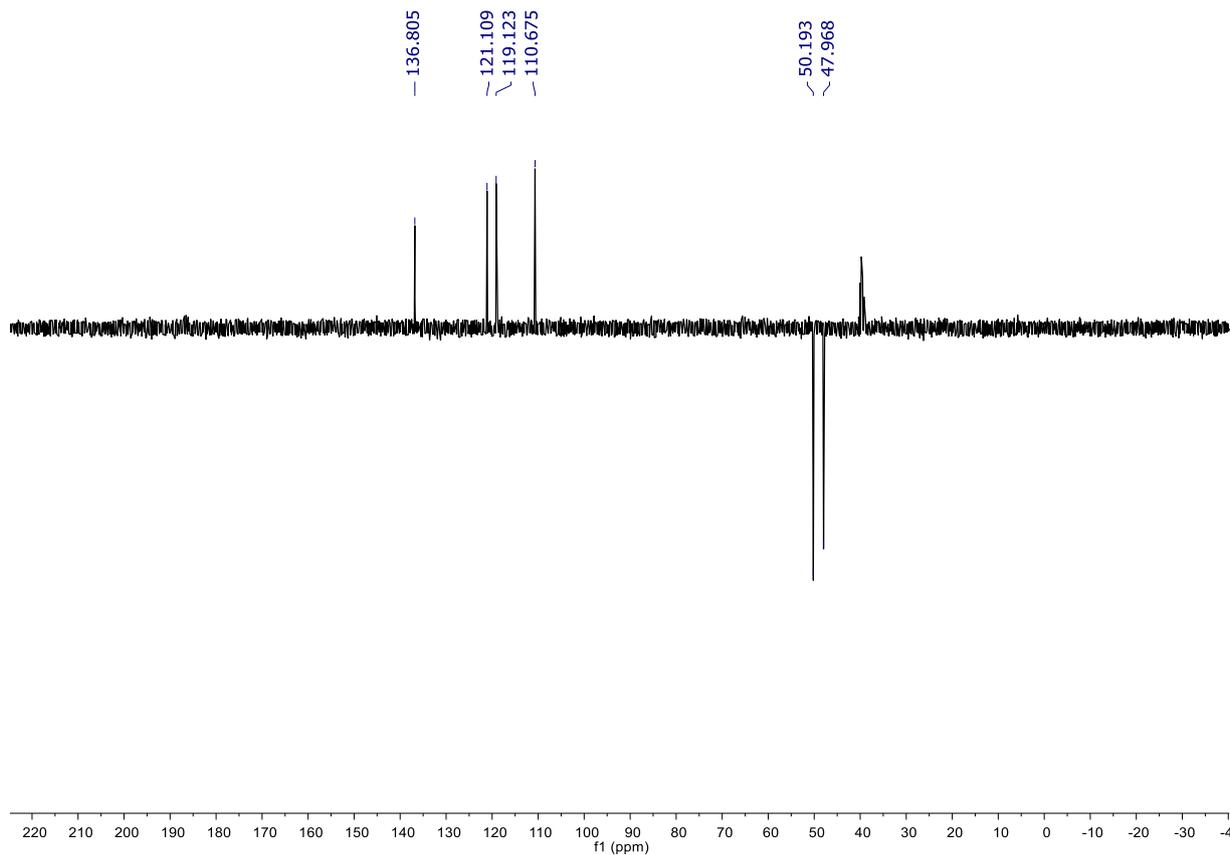


Figure S70.  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **6** in  $\text{DMSO-d}_6$ .

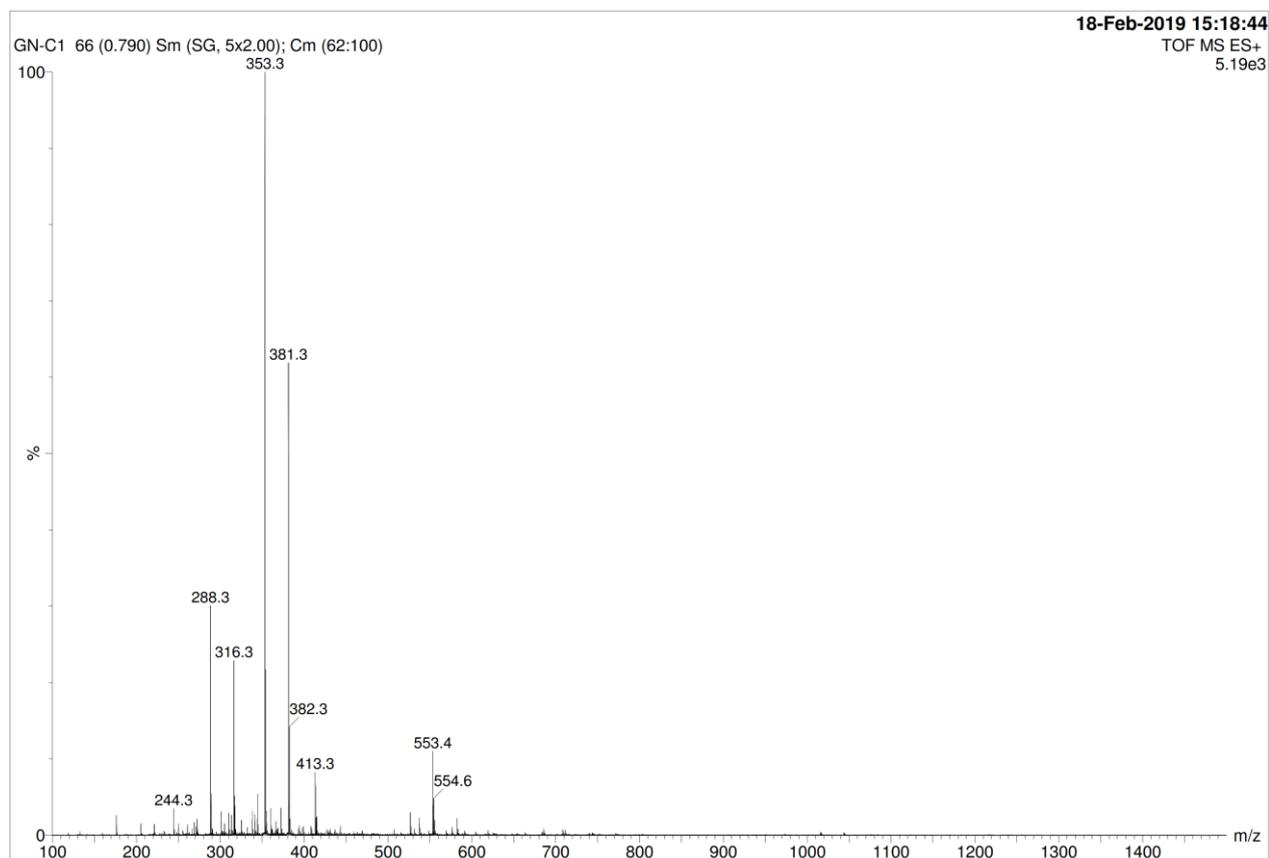


Figure S71. MS-ESI(+) spectrum of compound **6**.

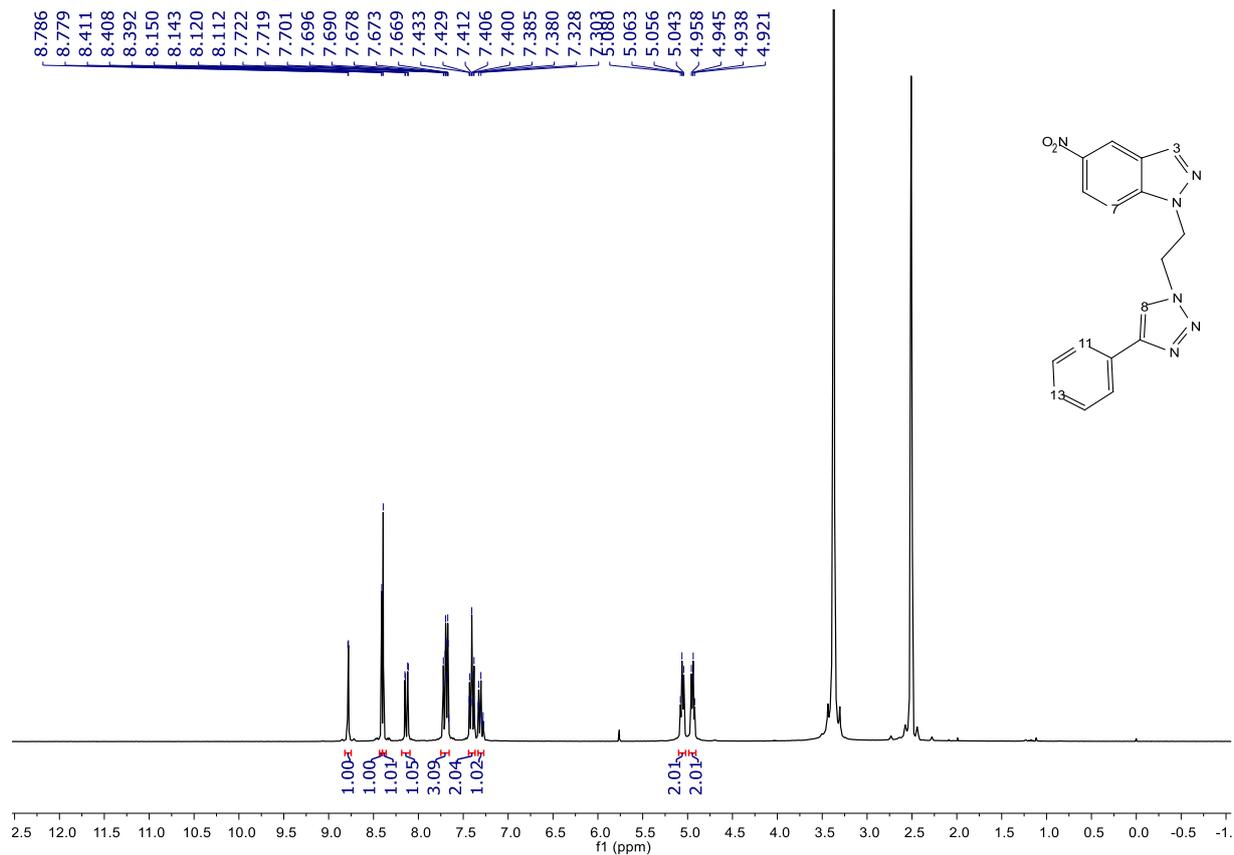


Figure S72. <sup>1</sup>H NMR spectrum of compound 7a in DMSO-d<sub>6</sub>.

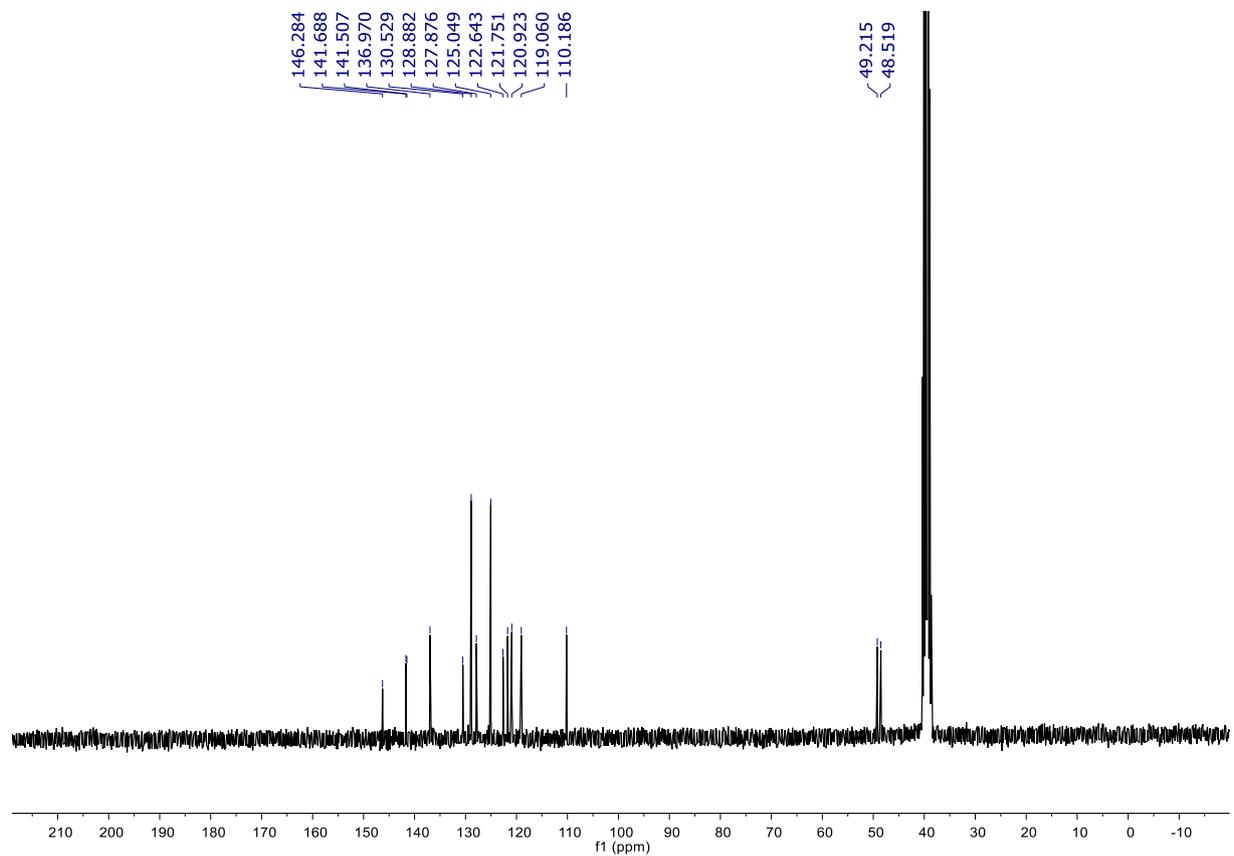


Figure S73. <sup>13</sup>C NMR spectrum of compound 7a in DMSO-d<sub>6</sub>.

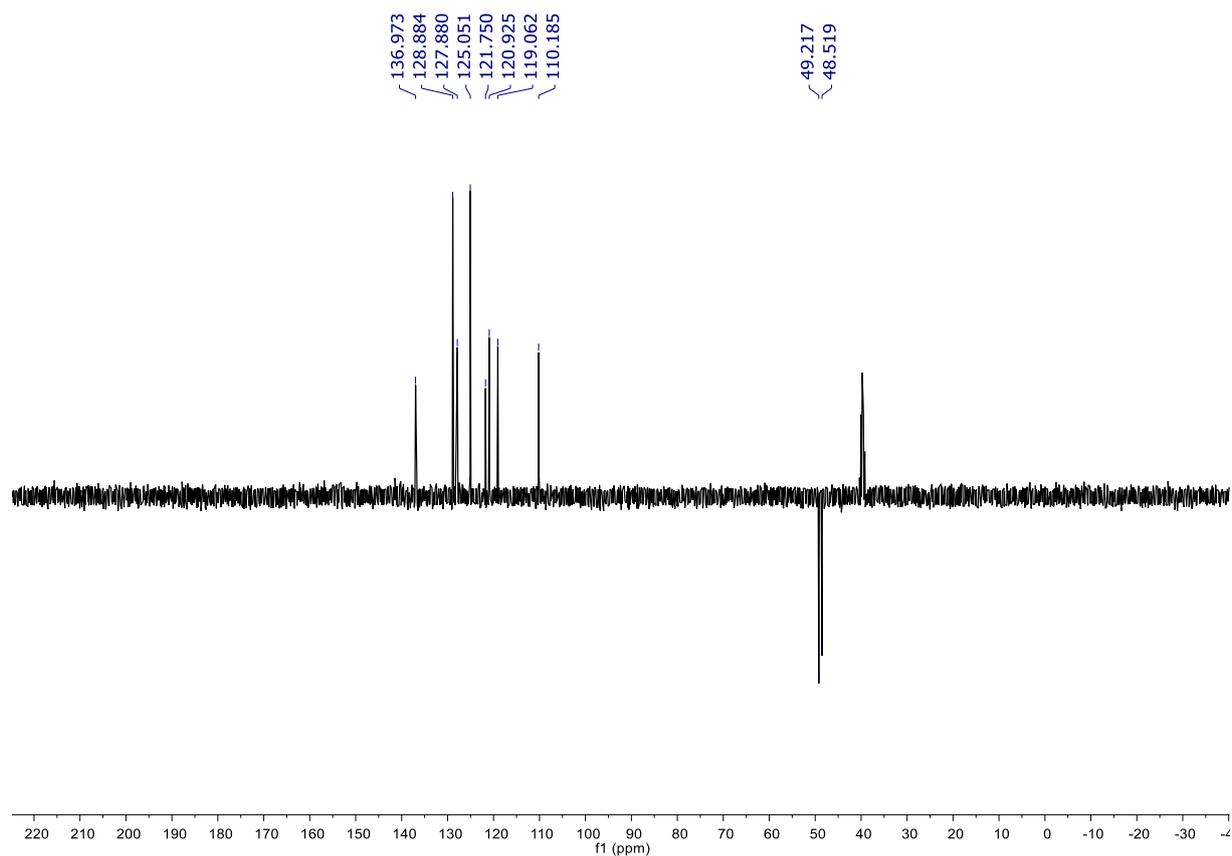


Figure S74.  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **7a** in  $\text{DMSO-d}_6$ .

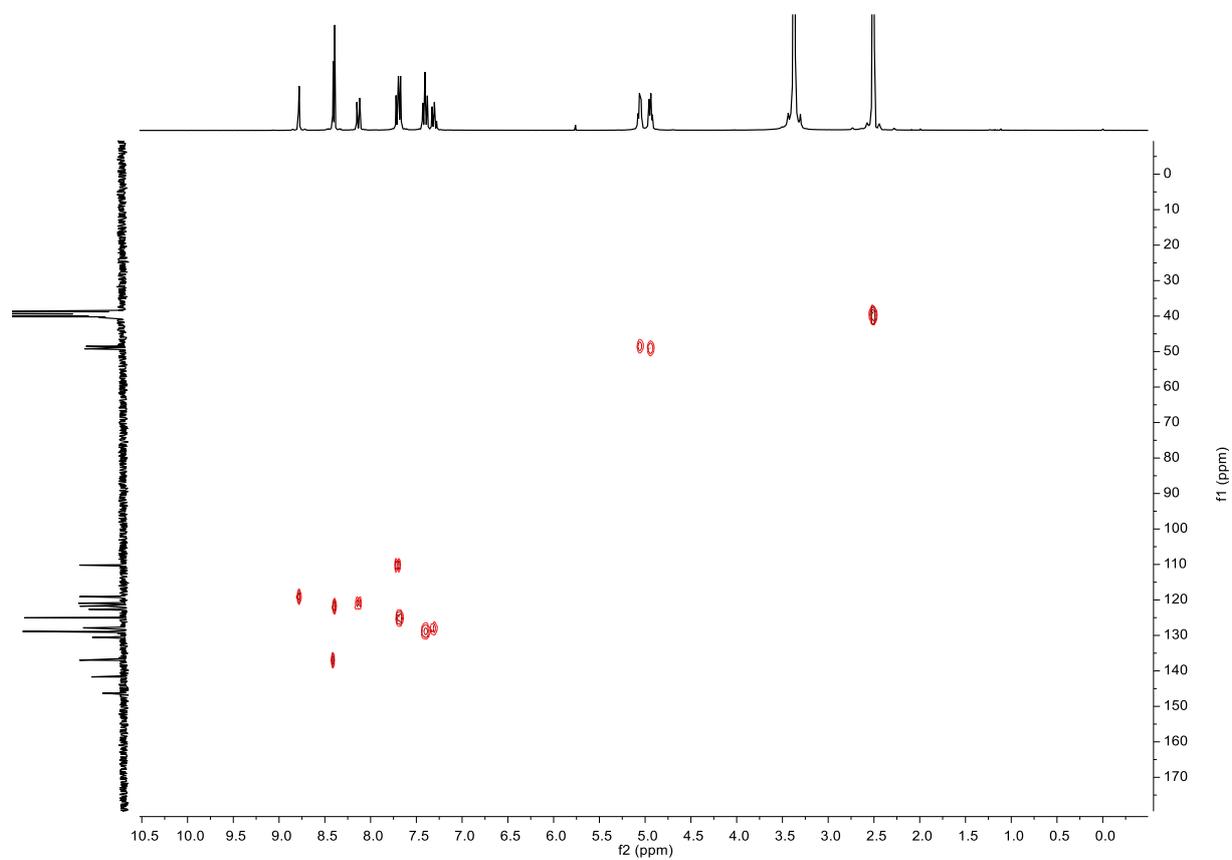


Figure S75. HSQC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **7a** in  $\text{DMSO-d}_6$ .

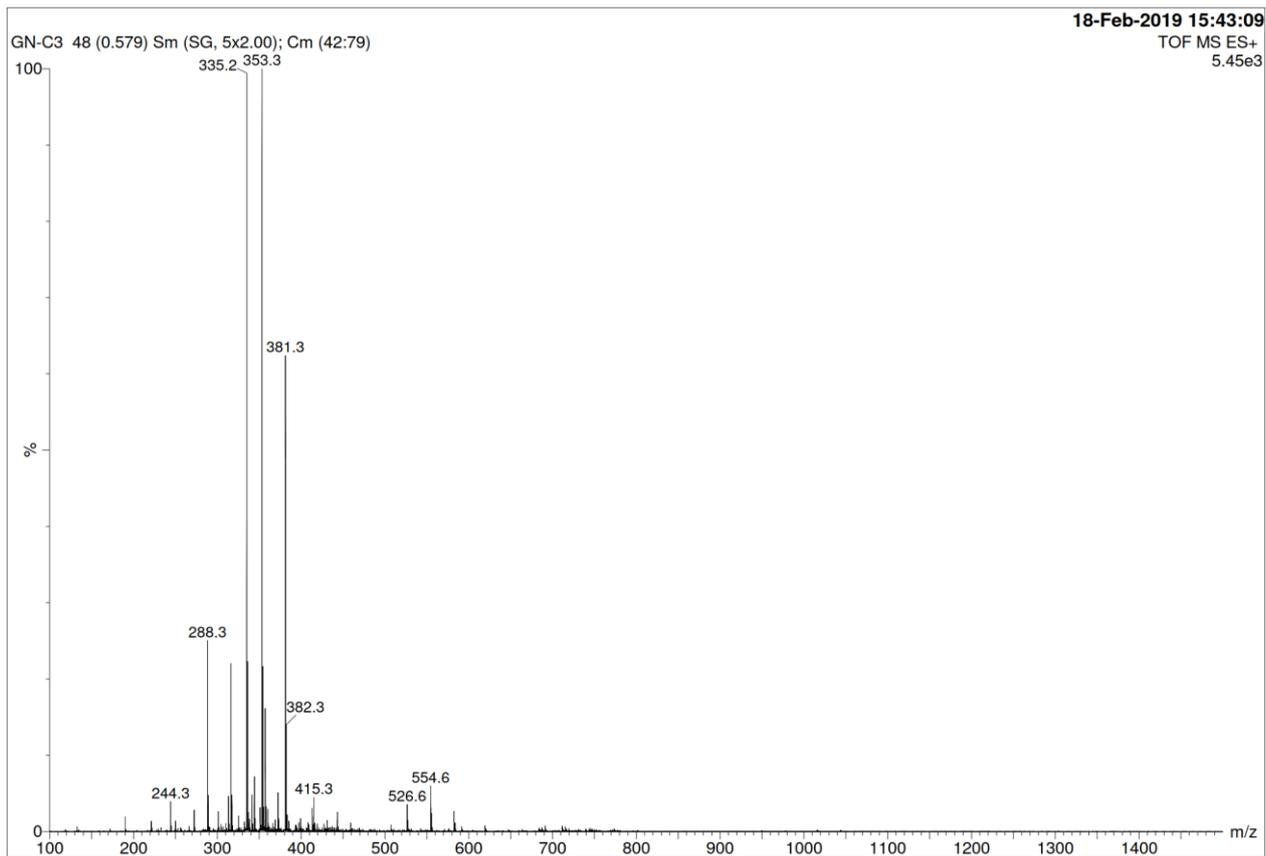


Figure S76. MS-ESI(+) spectrum of compound **7a**.

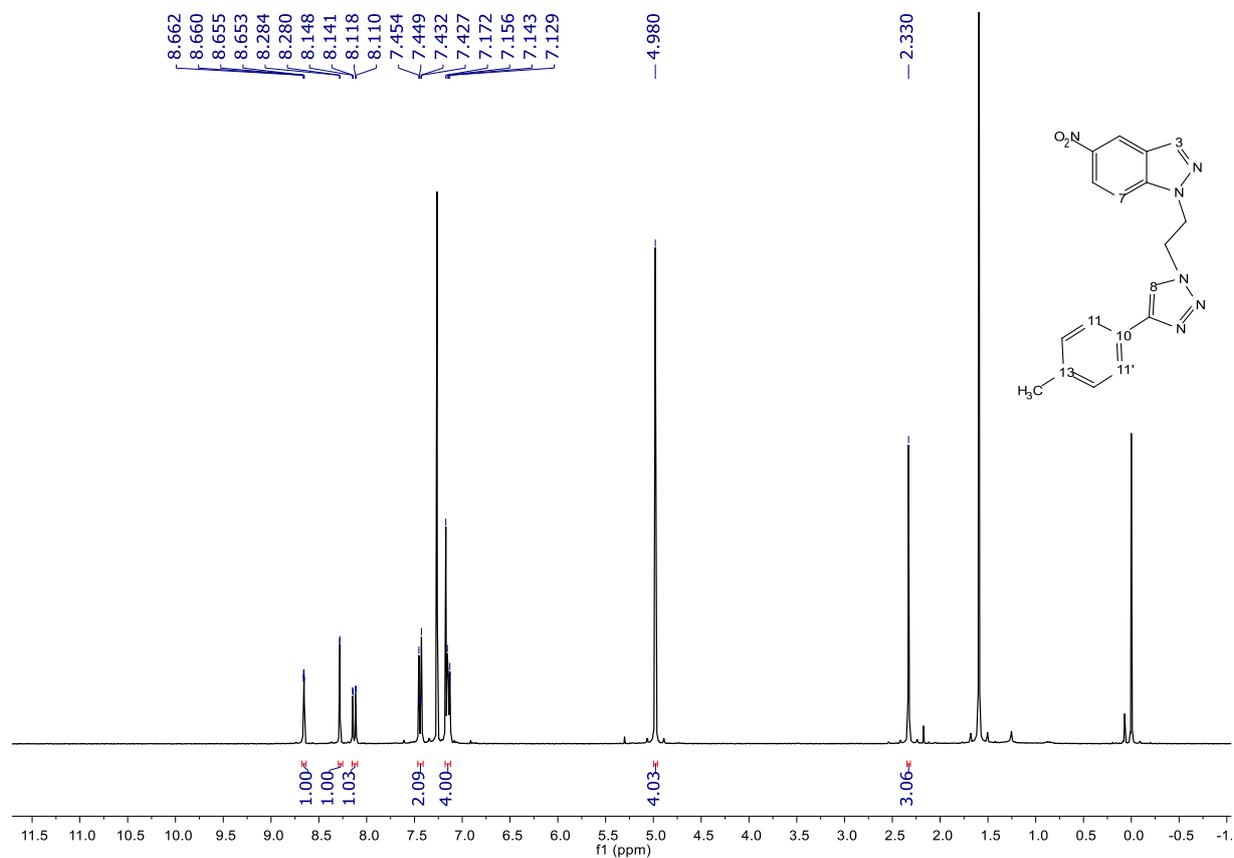


Figure S77. <sup>1</sup>H NMR spectrum of compound **7b** in CDCl<sub>3</sub>.

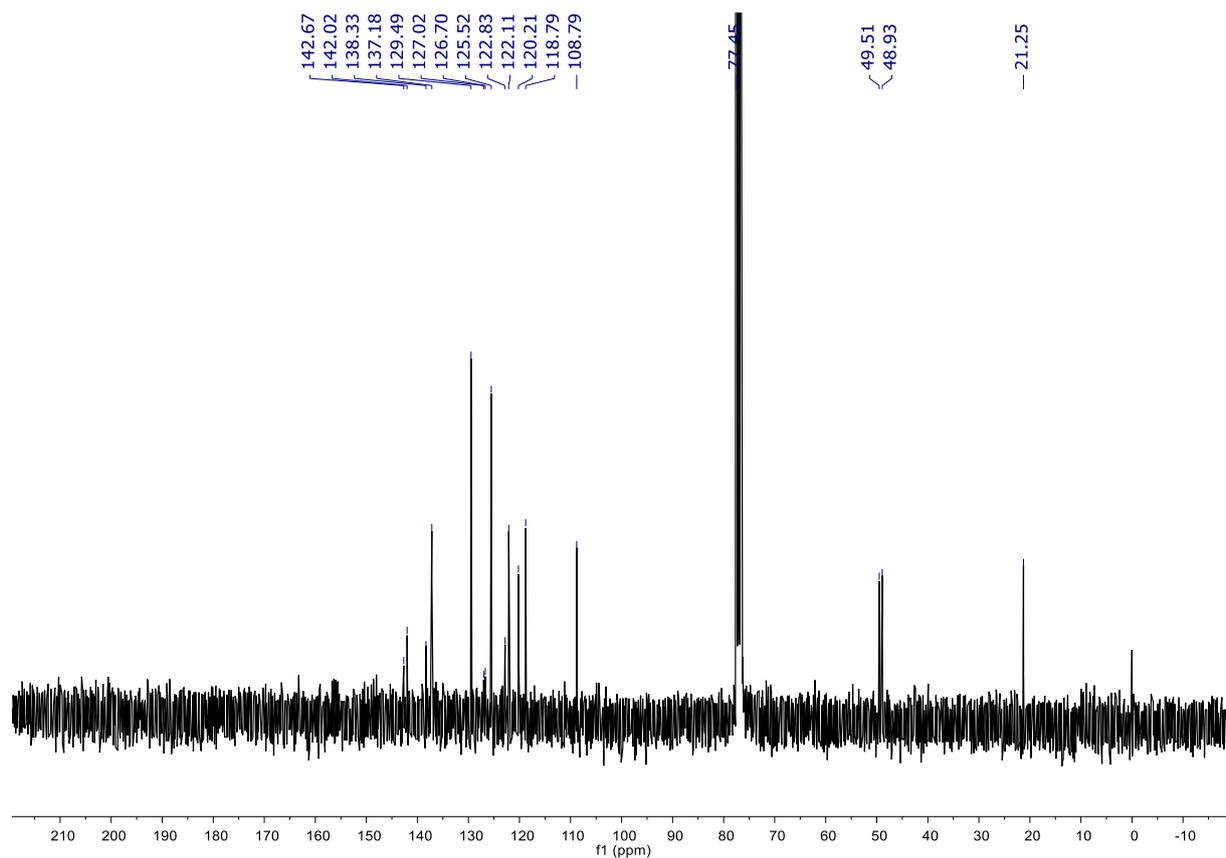


Figure S78.  $^{13}\text{C}$  NMR spectrum of compound **7b** in  $\text{CDCl}_3$ .

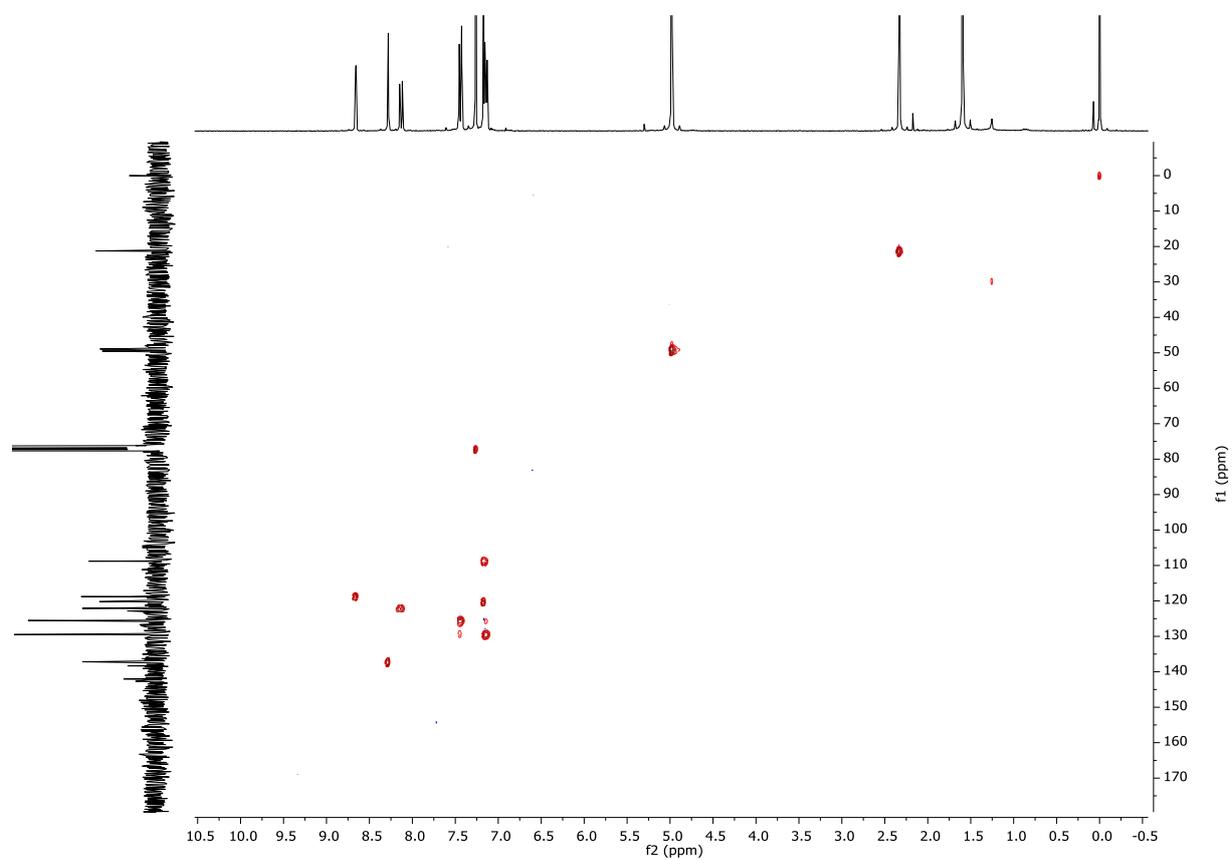
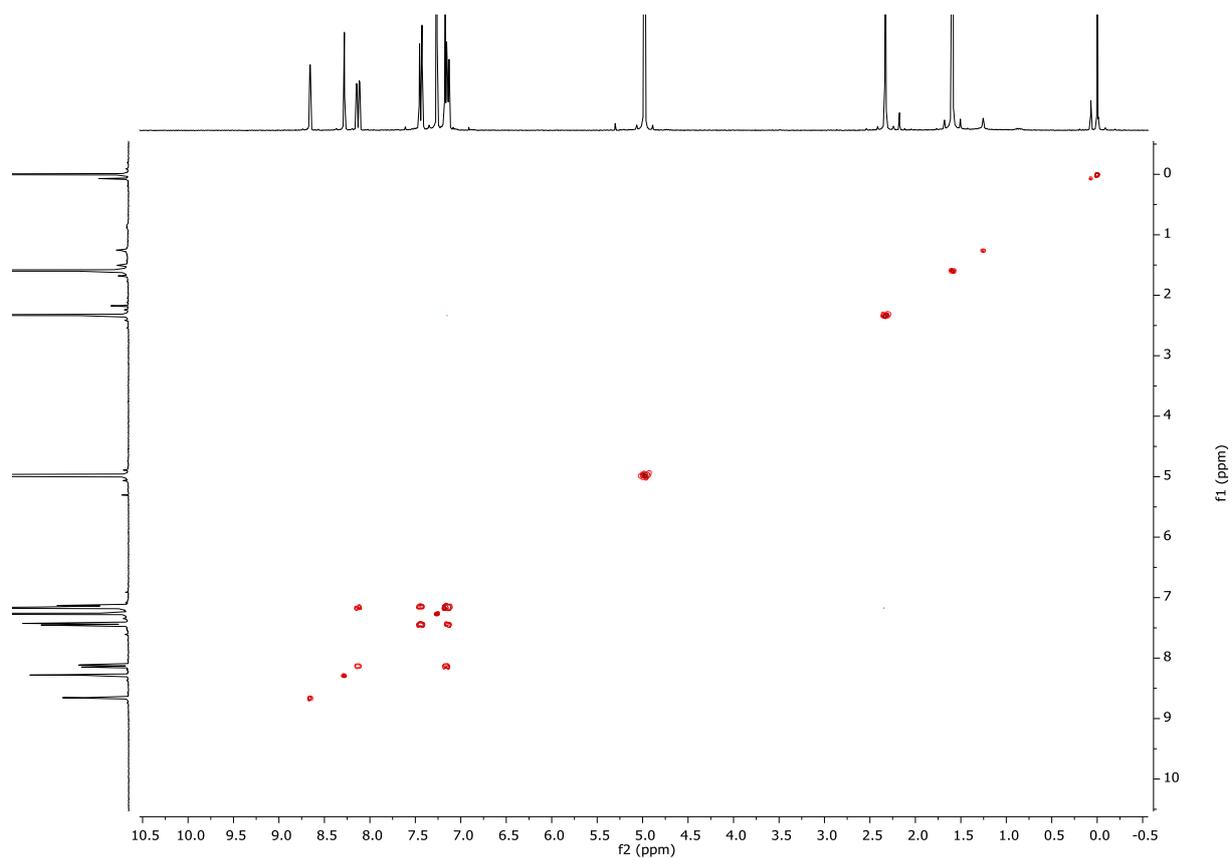
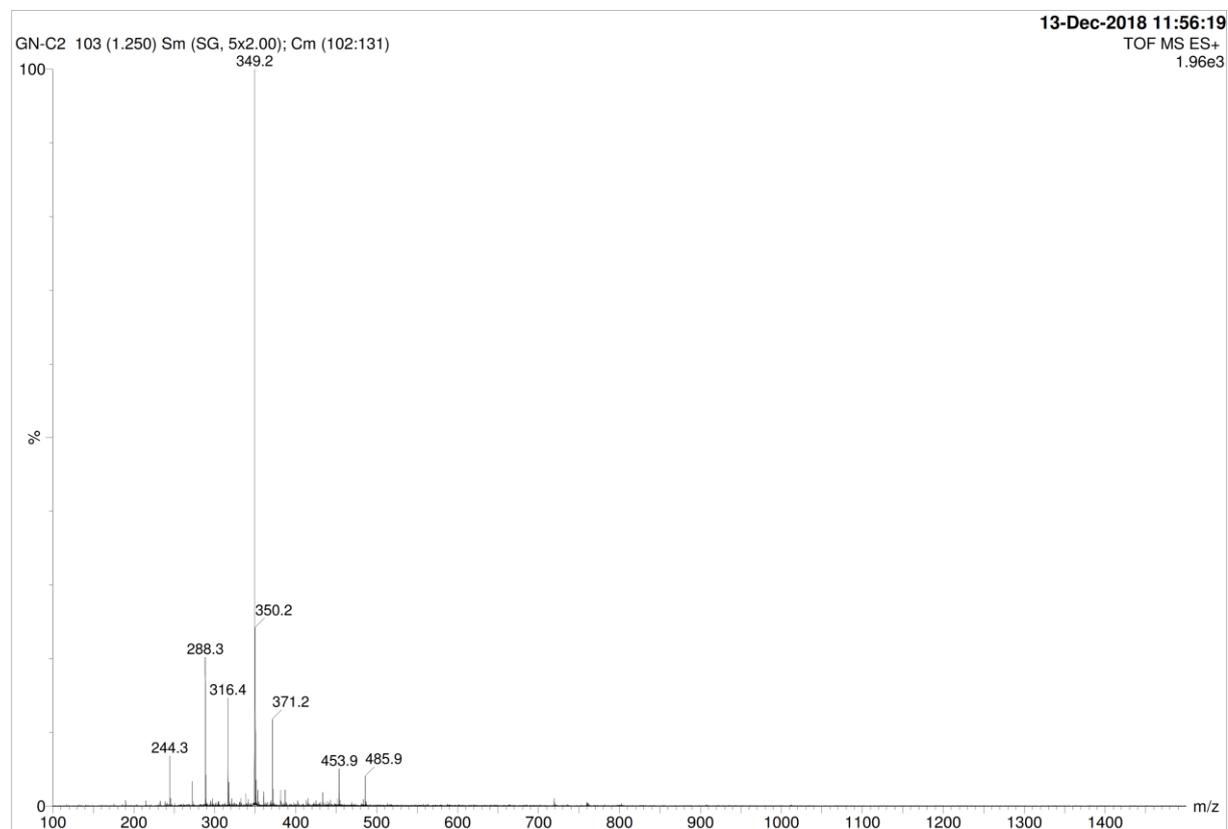


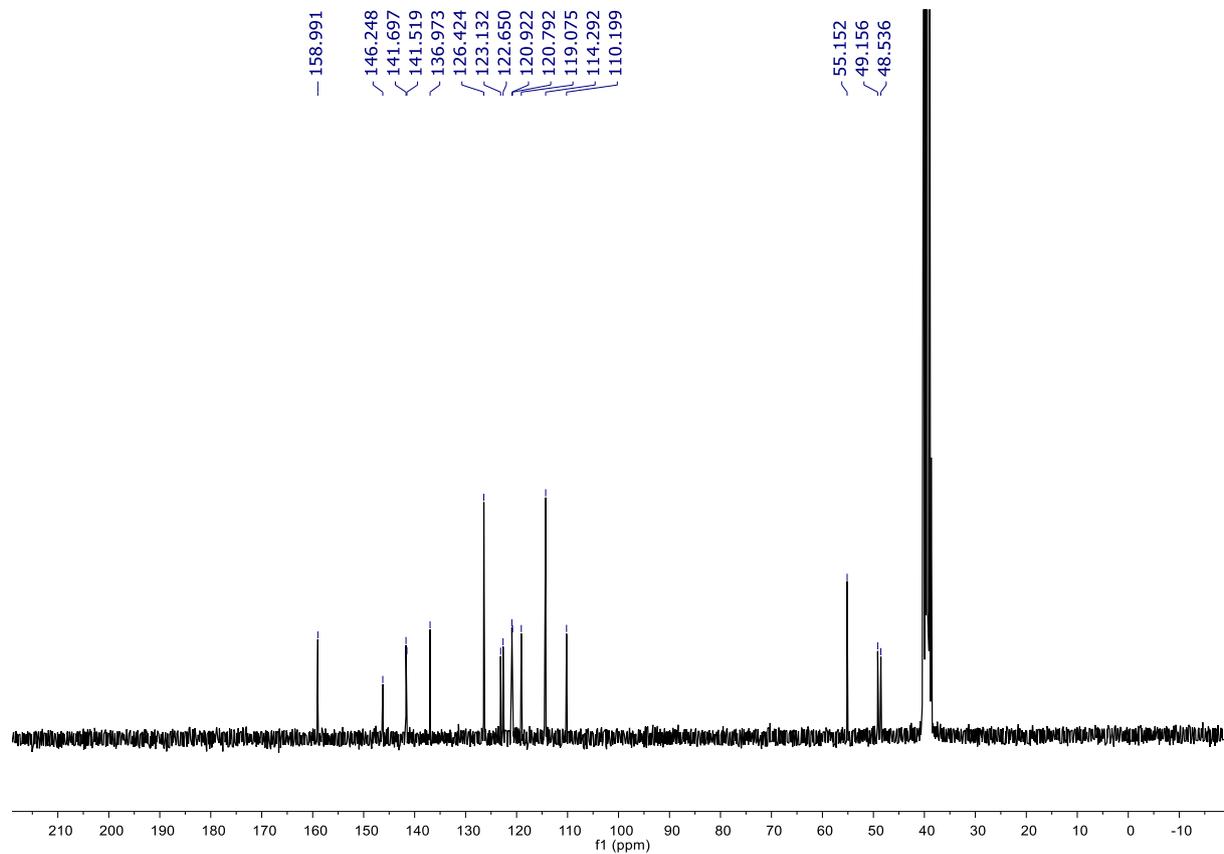
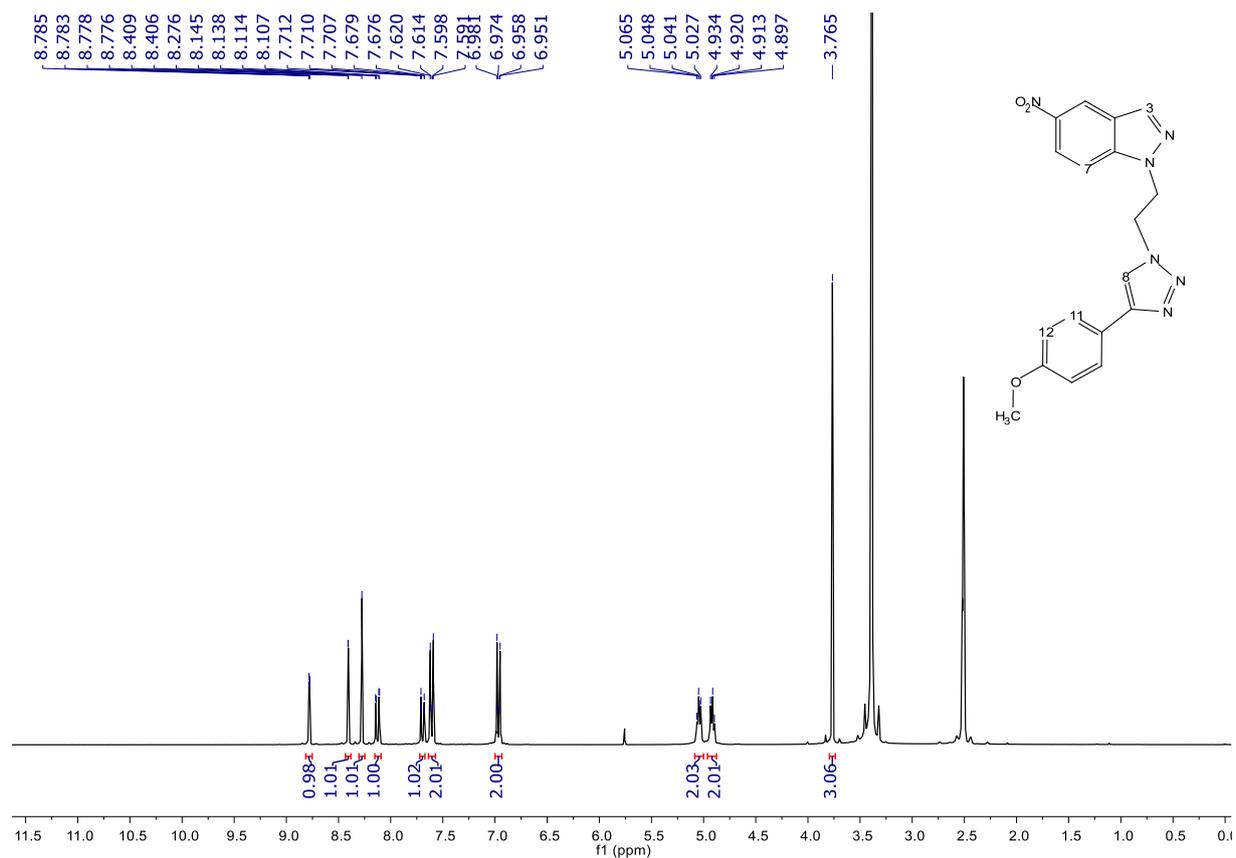
Figure S79. HSQC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **7b** in  $\text{CDCl}_3$ .

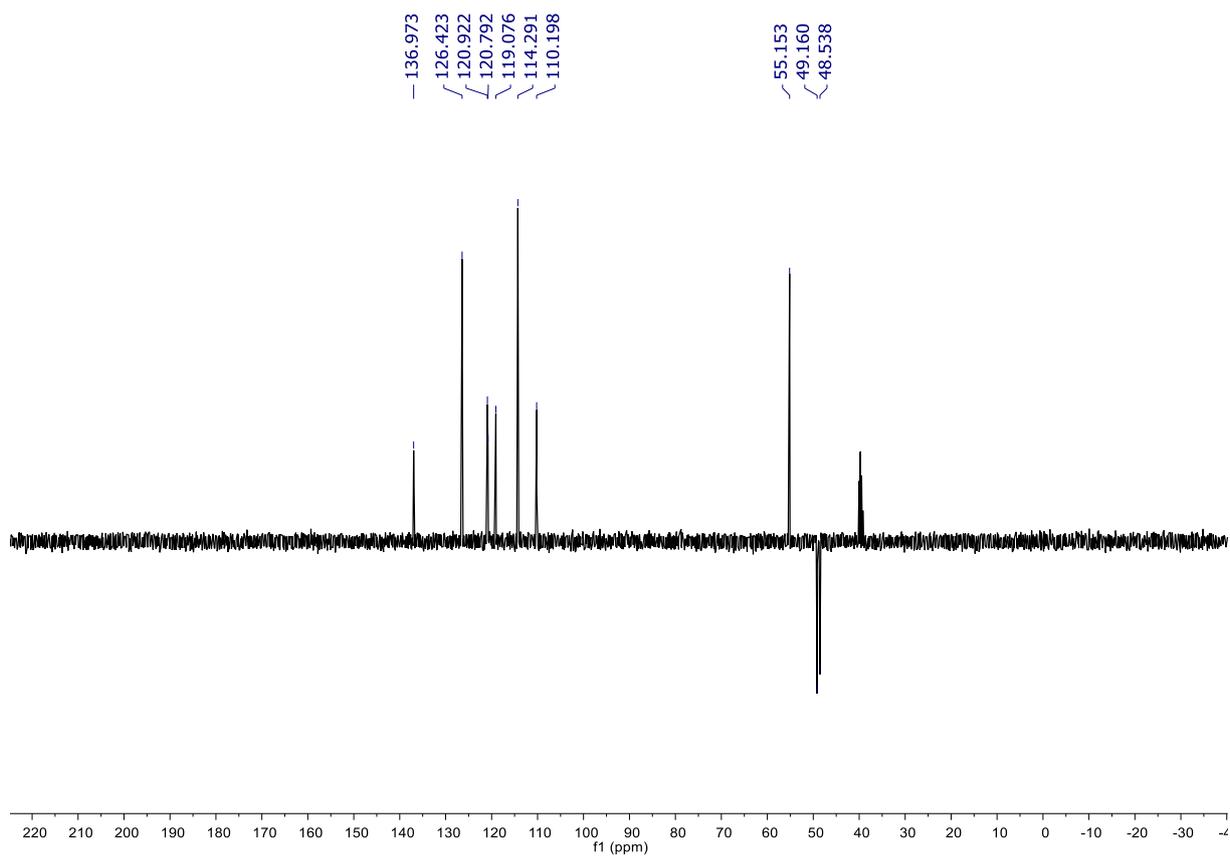


**Figure S80.** COSY (<sup>1</sup>H/<sup>1</sup>H) spectrum of compound **7b** in CDCl<sub>3</sub>.

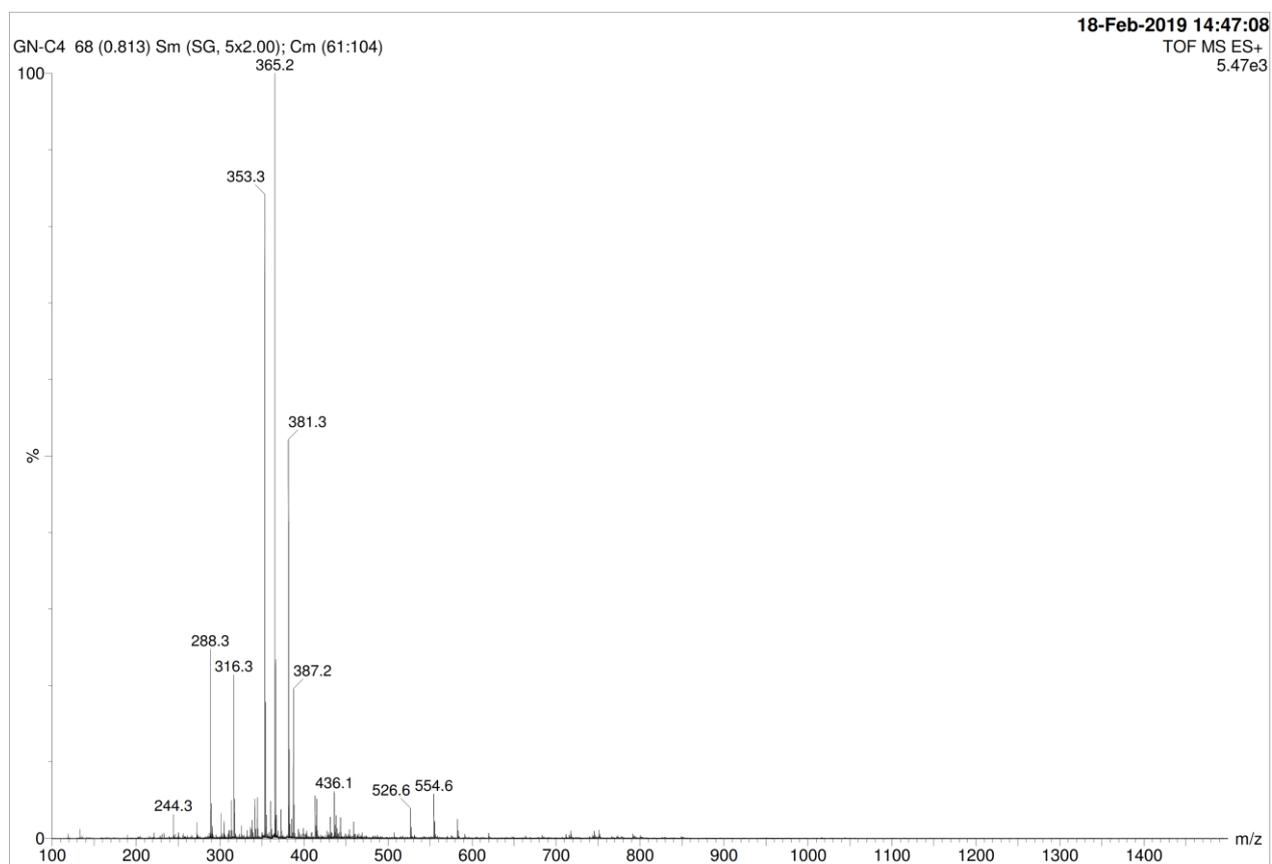


**Figure S81.** MS-ESI(+) spectrum of compound **7b**.

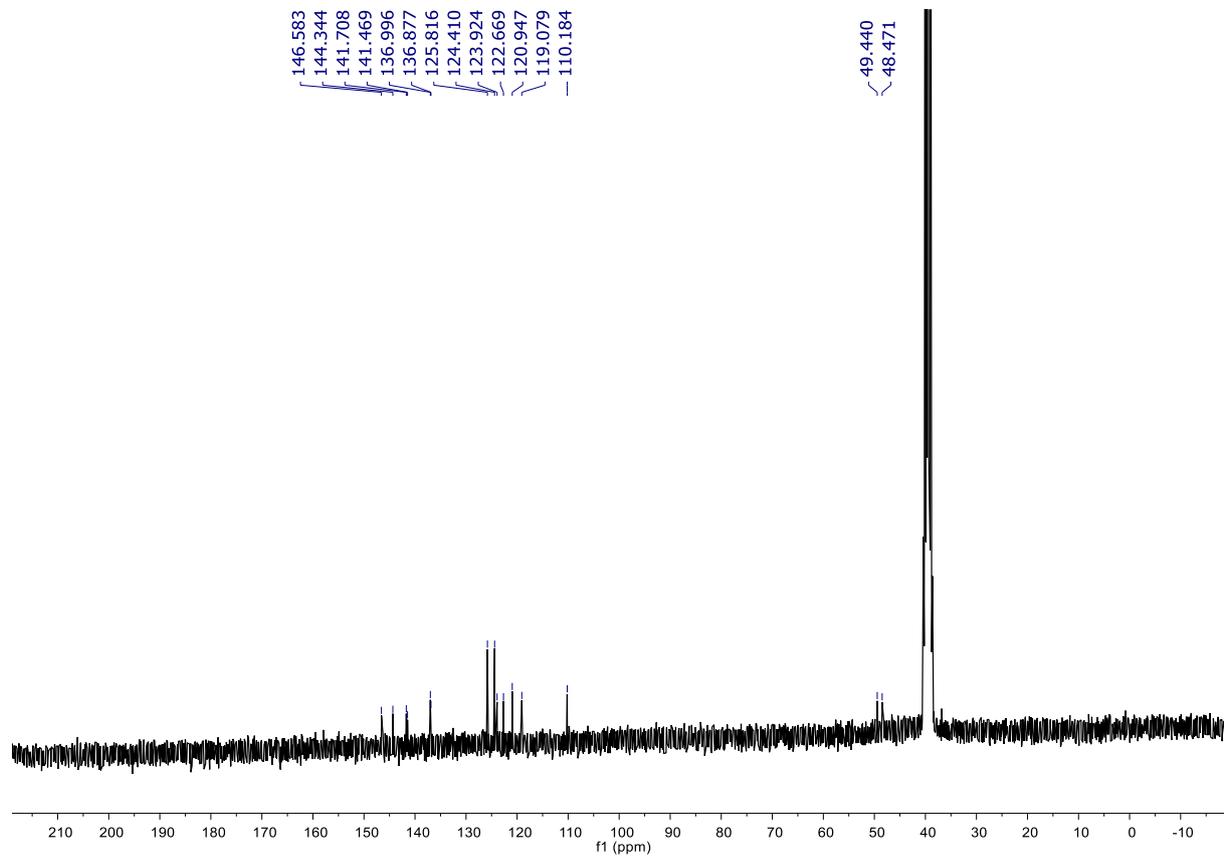
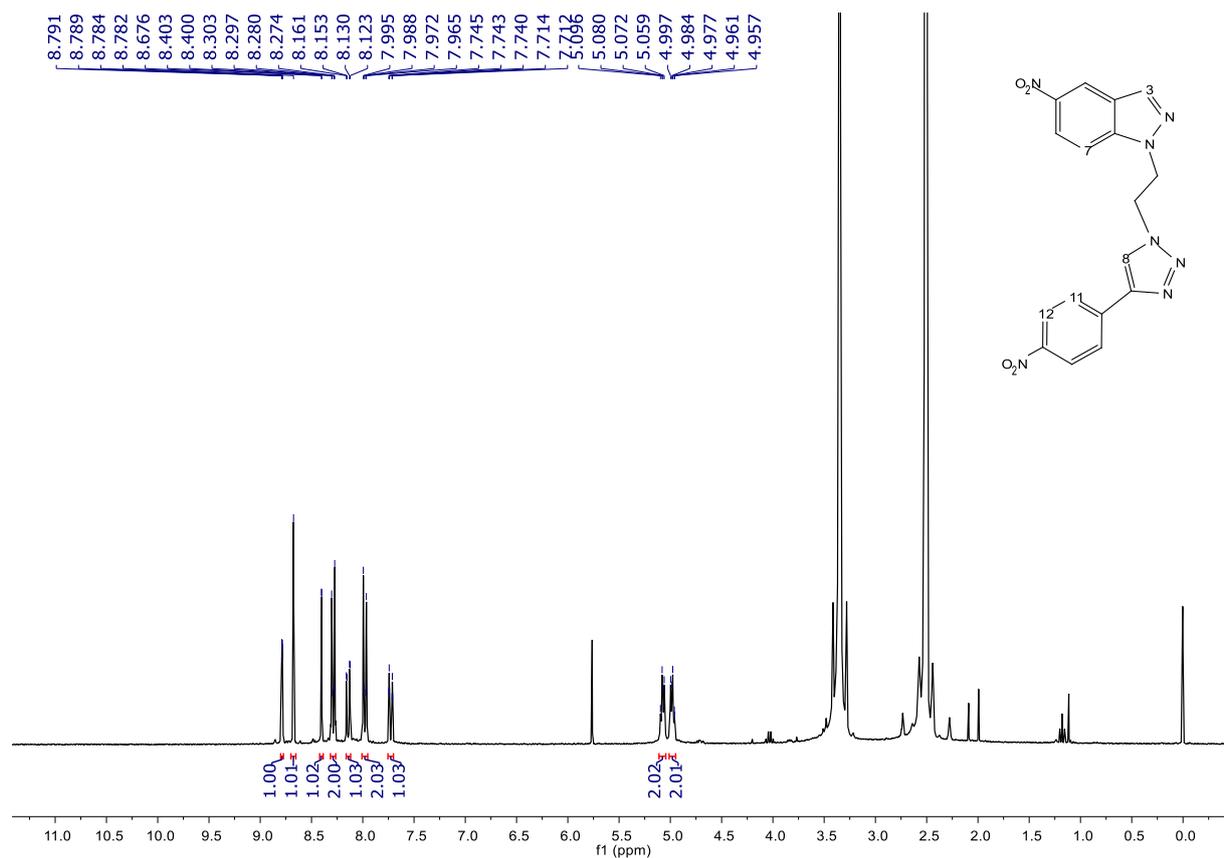


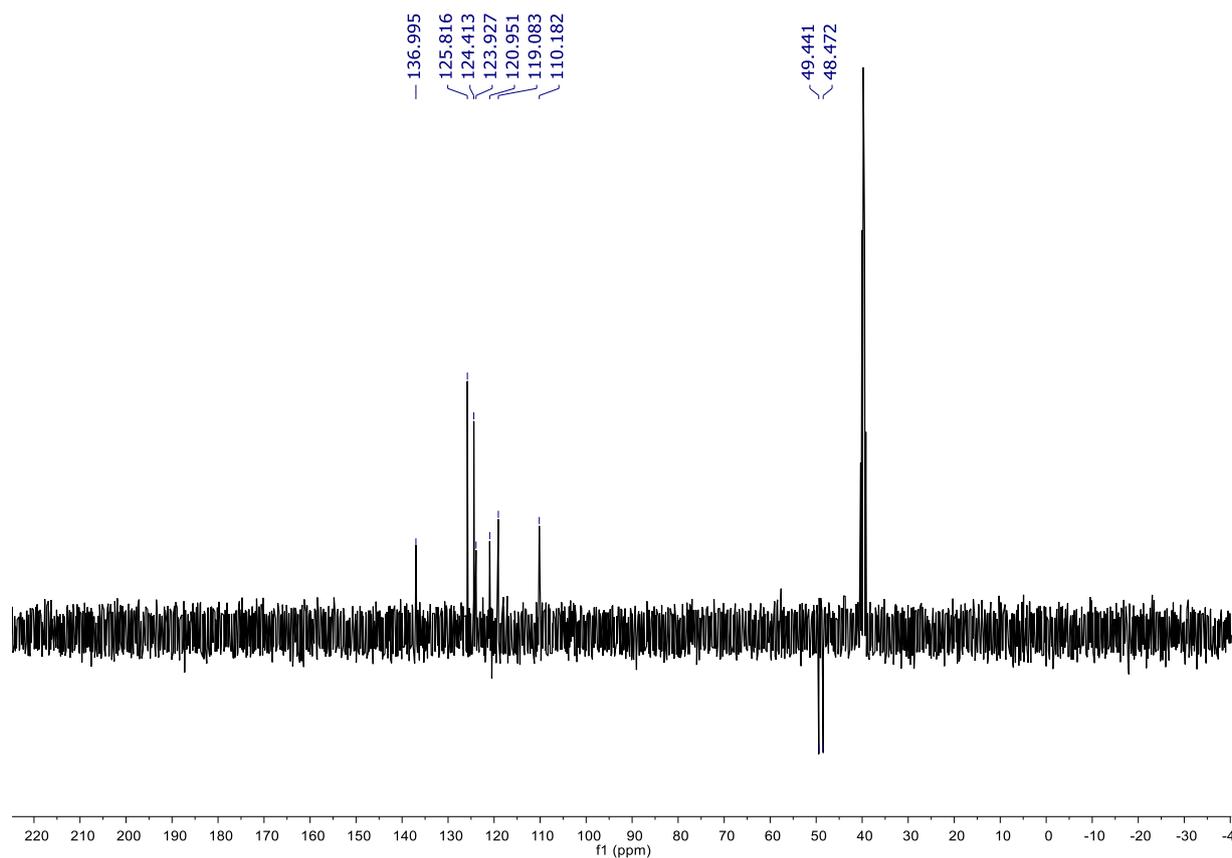


**Figure S84.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **7c** in  $\text{DMSO-d}_6$ .

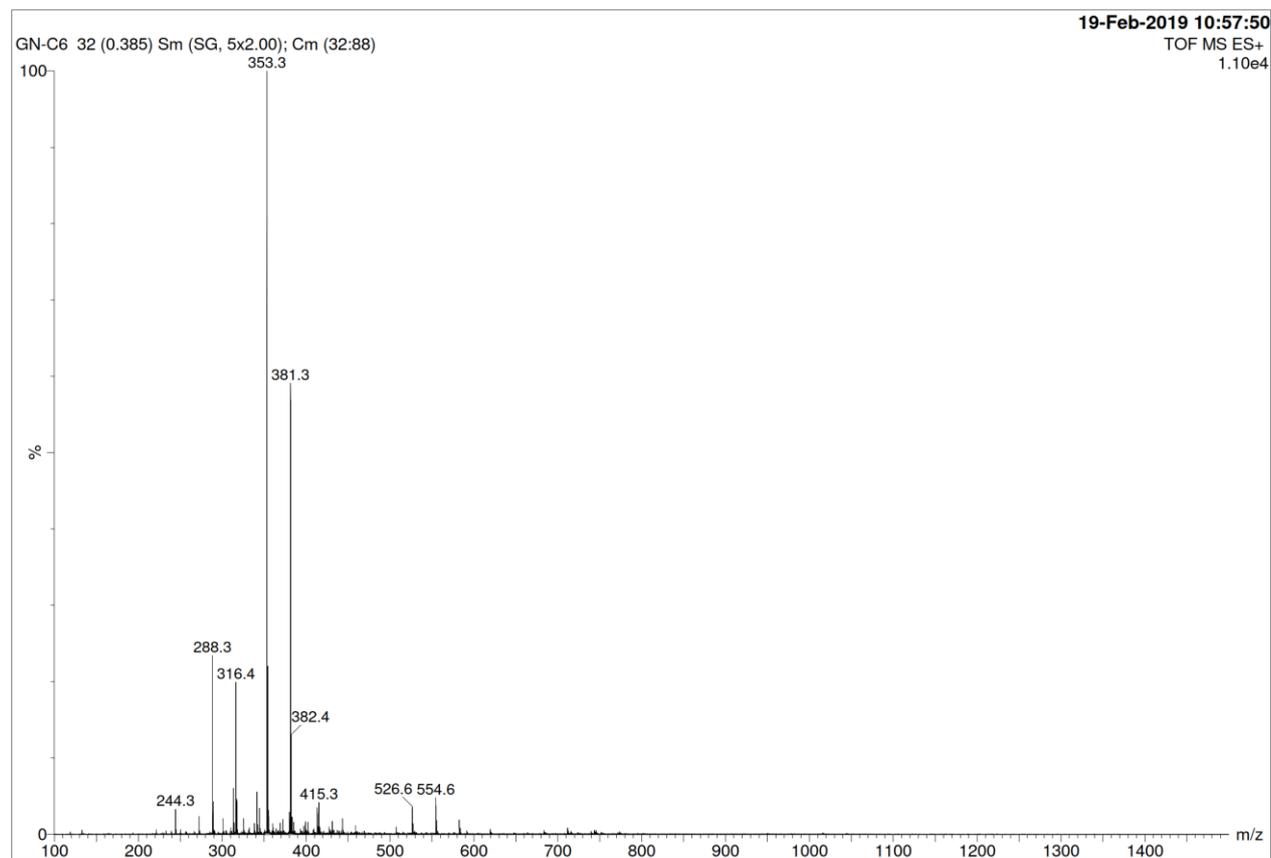


**Figure S85.** MS-ESI(+) spectrum of compound **7c**.

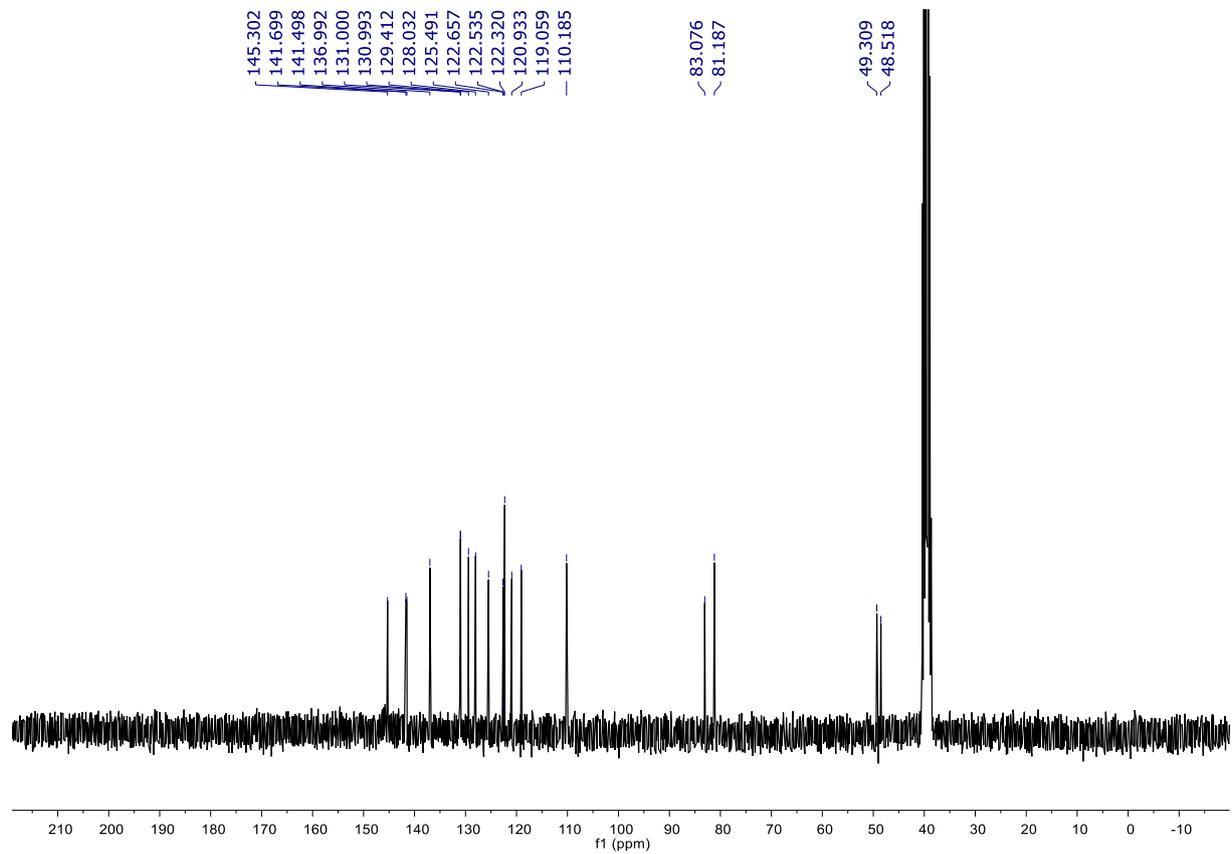
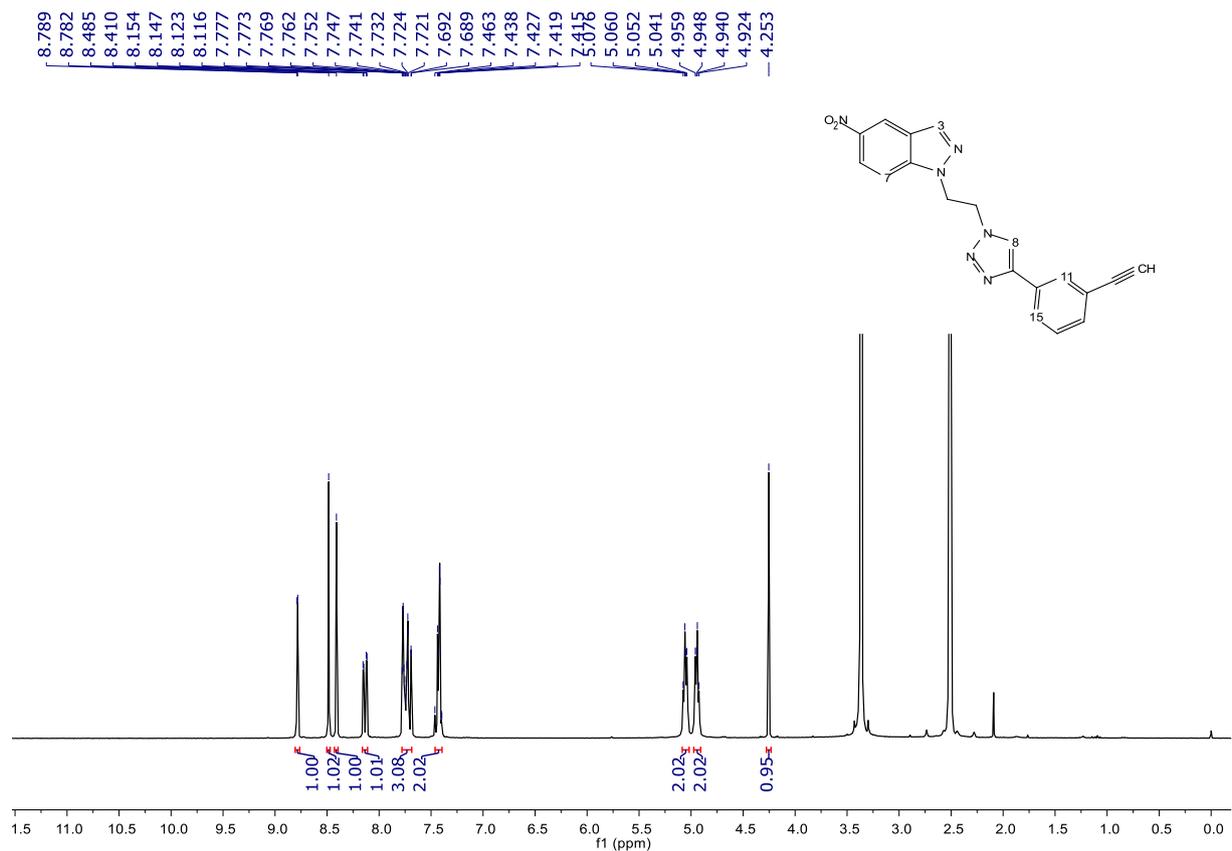




**Figure S88.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **7d** in  $\text{DMSO-d}_6$ .



**Figure S89.** MS-ESI(+) spectrum of compound **7d**.



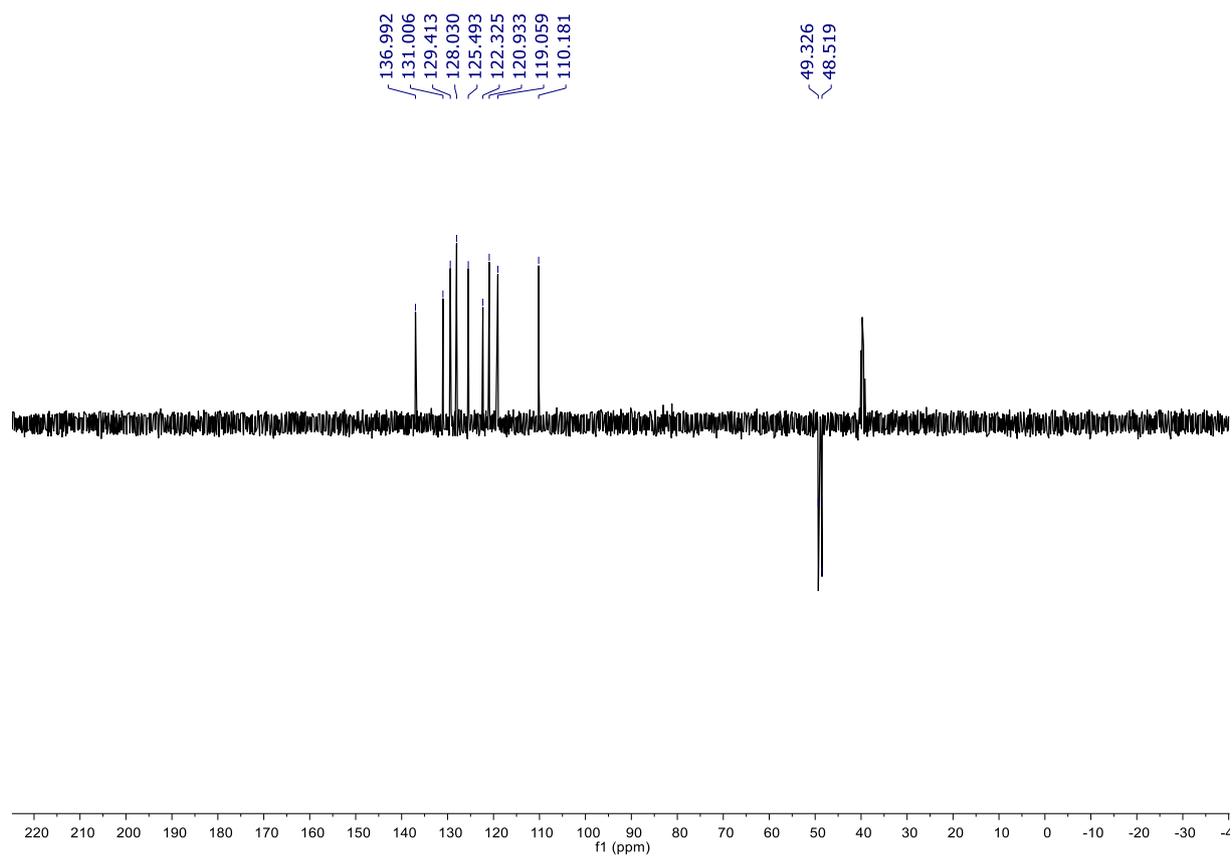


Figure S92.  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **8** in  $\text{DMSO-d}_6$ .

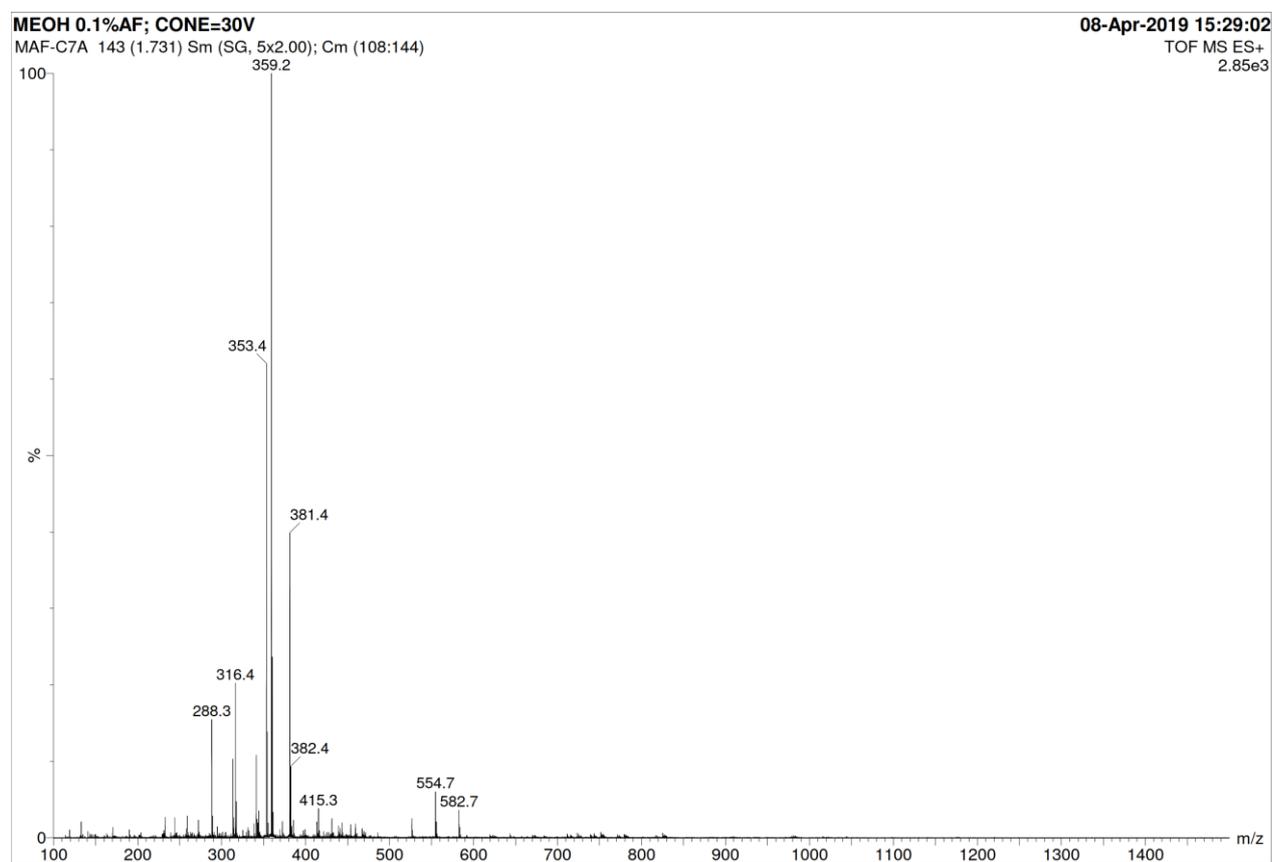


Figure S93. MS-ESI(+) spectrum of compound **8**.

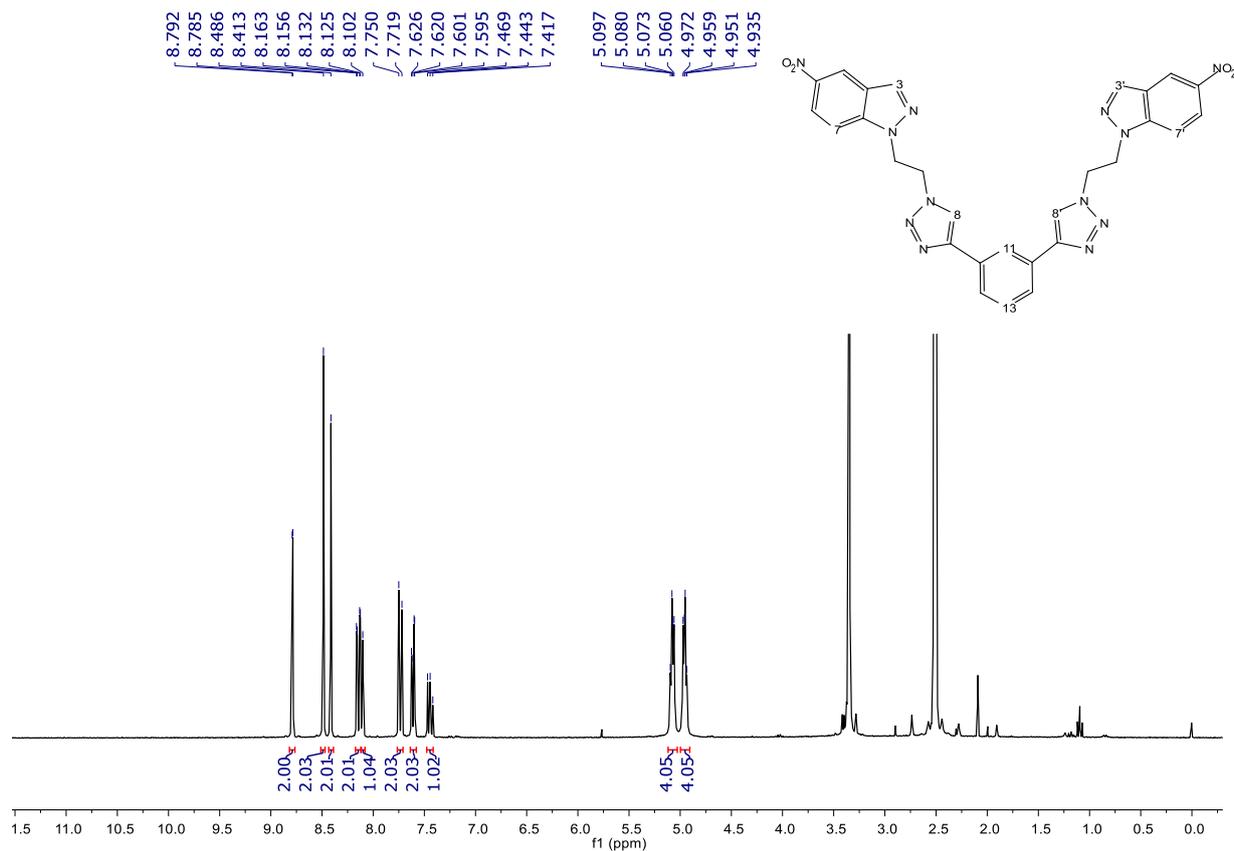


Figure S94. <sup>1</sup>H NMR spectrum of compound **9** in DMSO-d<sub>6</sub>.

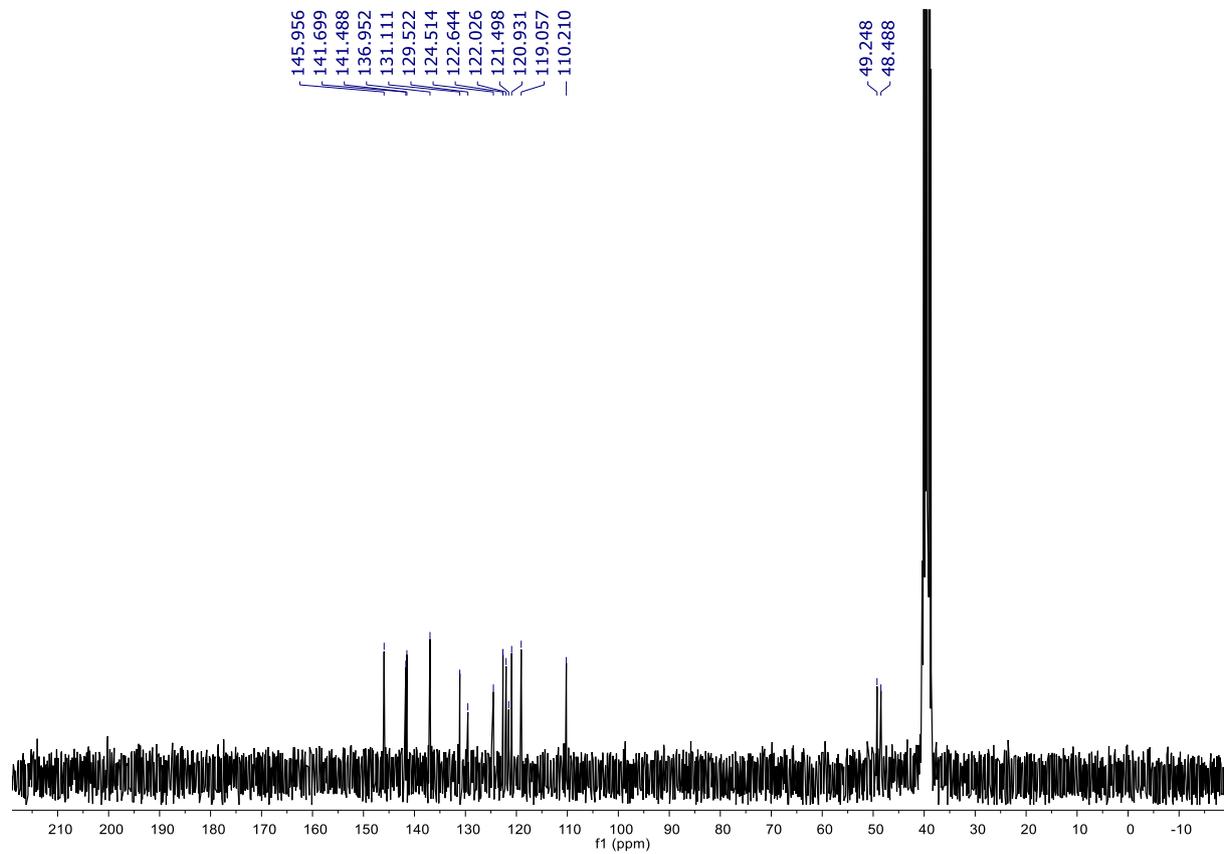
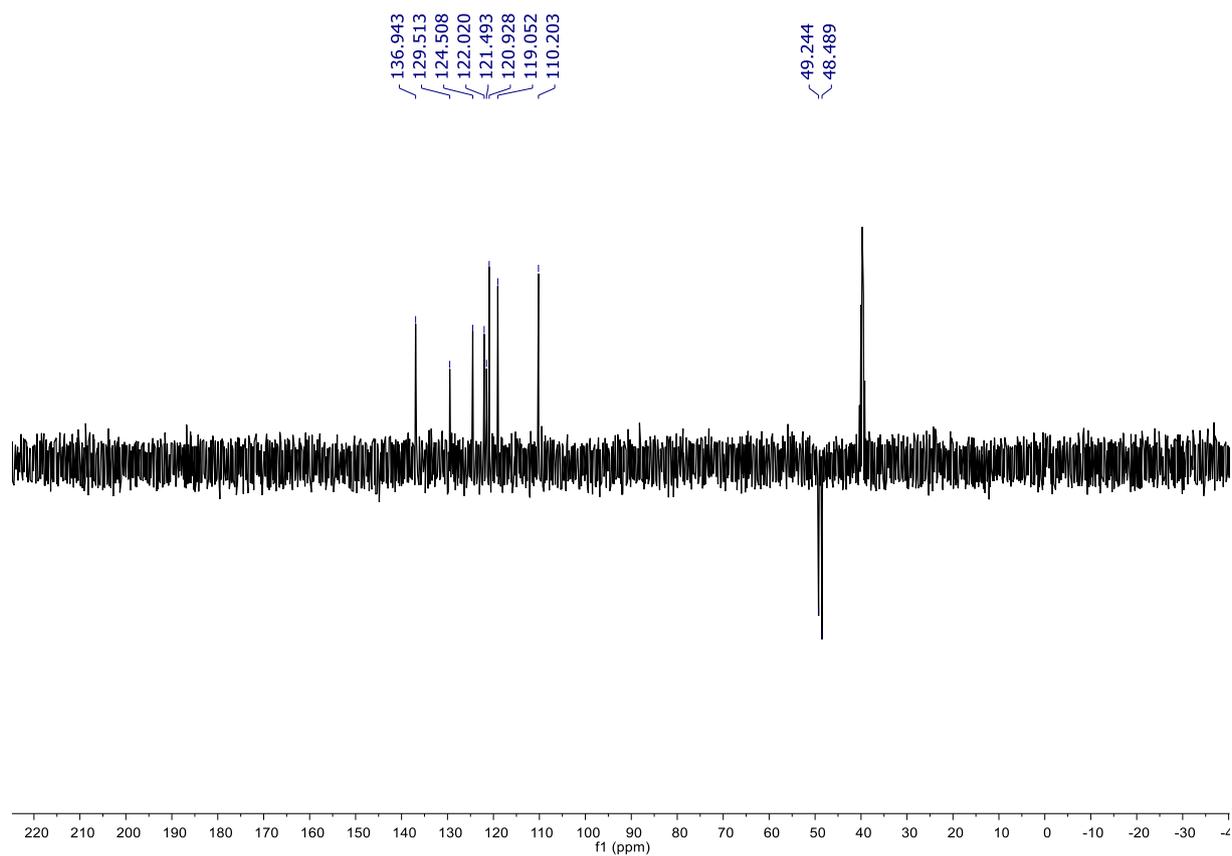
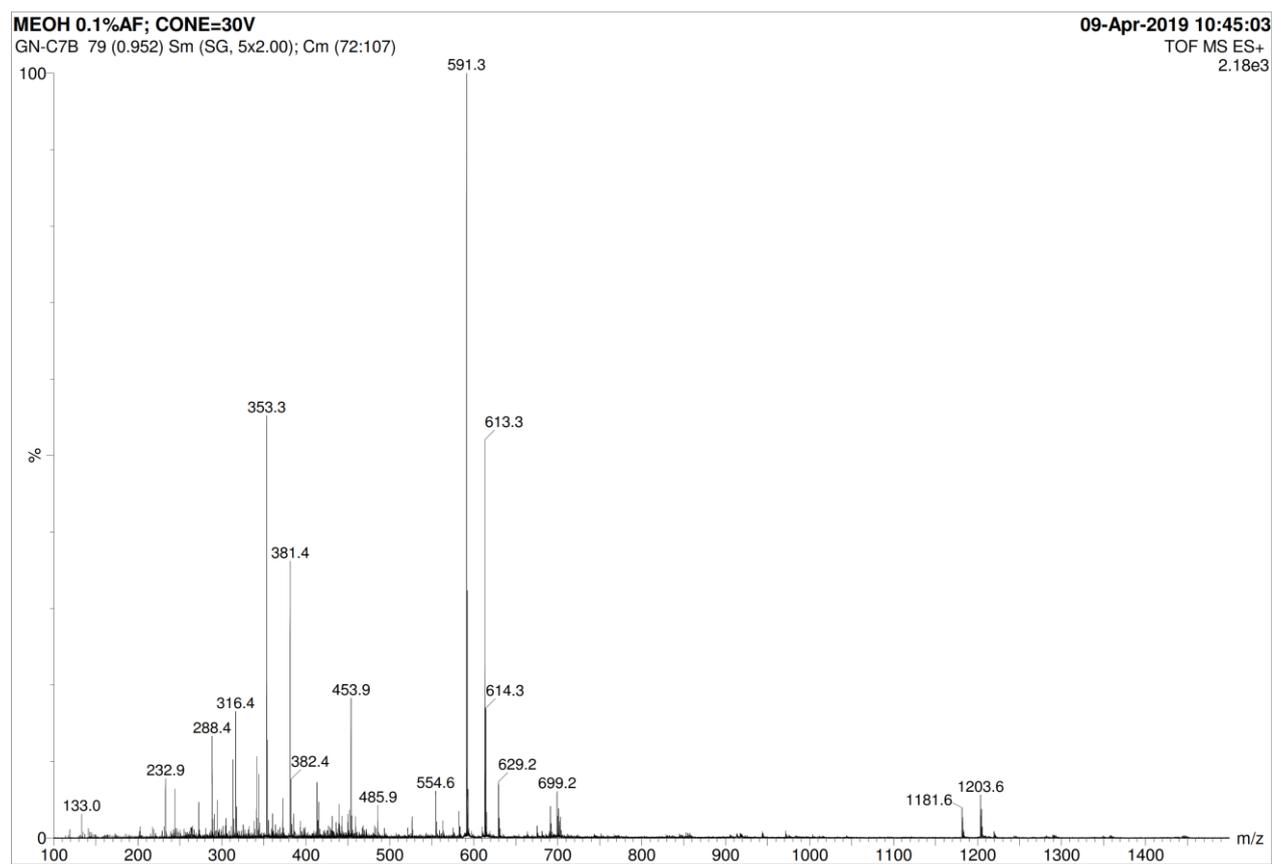


Figure S95. <sup>13</sup>C NMR spectrum of compound **9** in DMSO-d<sub>6</sub>.



**Figure S96.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **9** in  $\text{DMSO-d}_6$ .



**Figure S97.** MS-ESI(+) spectrum of compound **9**.

### III - NMR and mass spectrum of compounds 12a-e

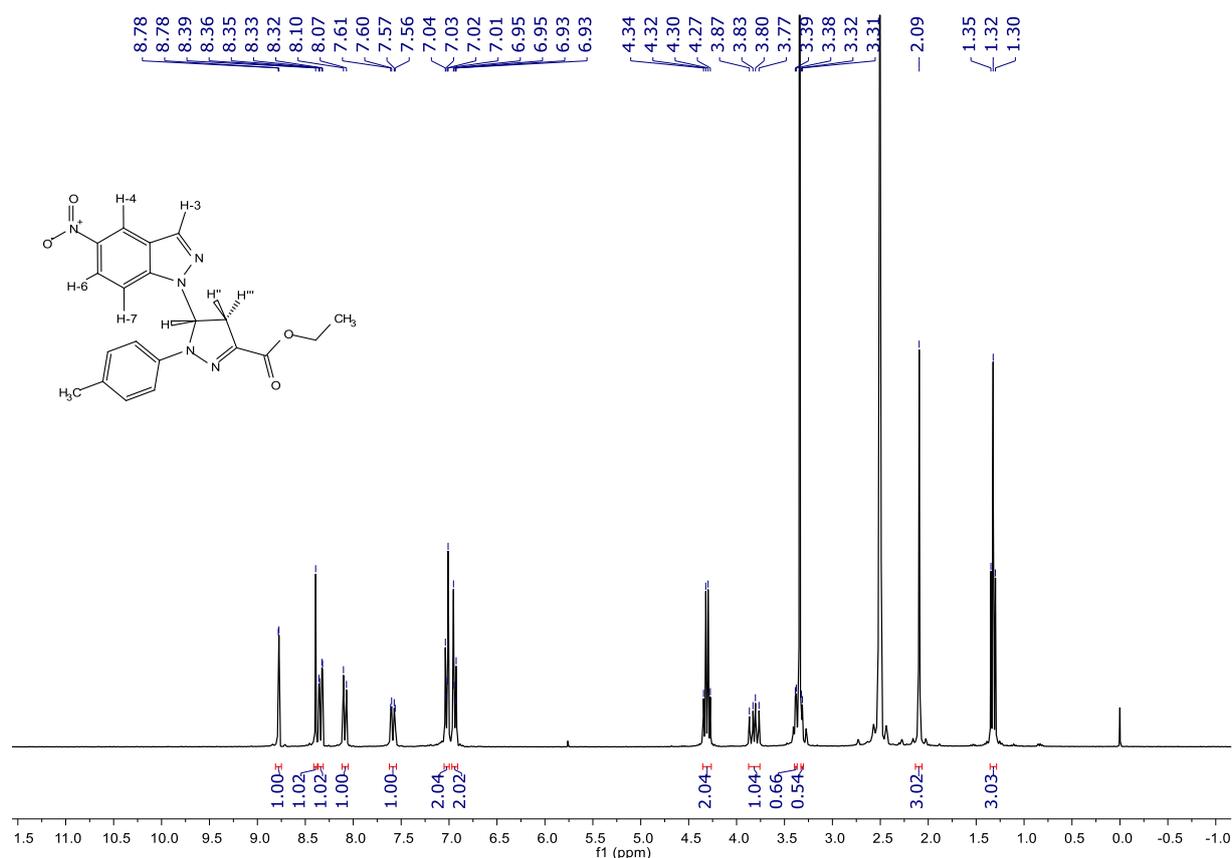


Figure S98. <sup>1</sup>H NMR spectrum of compound 12a in DMSO-d<sub>6</sub>.

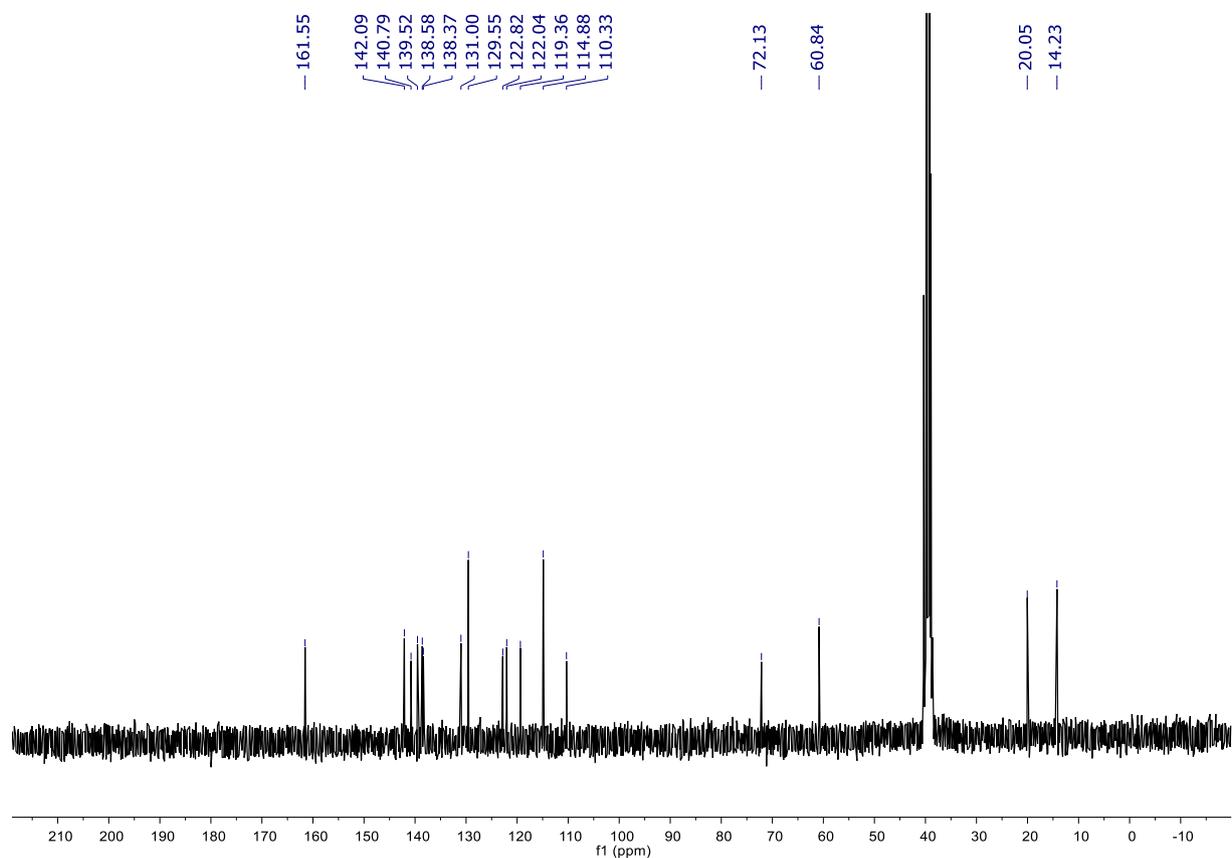
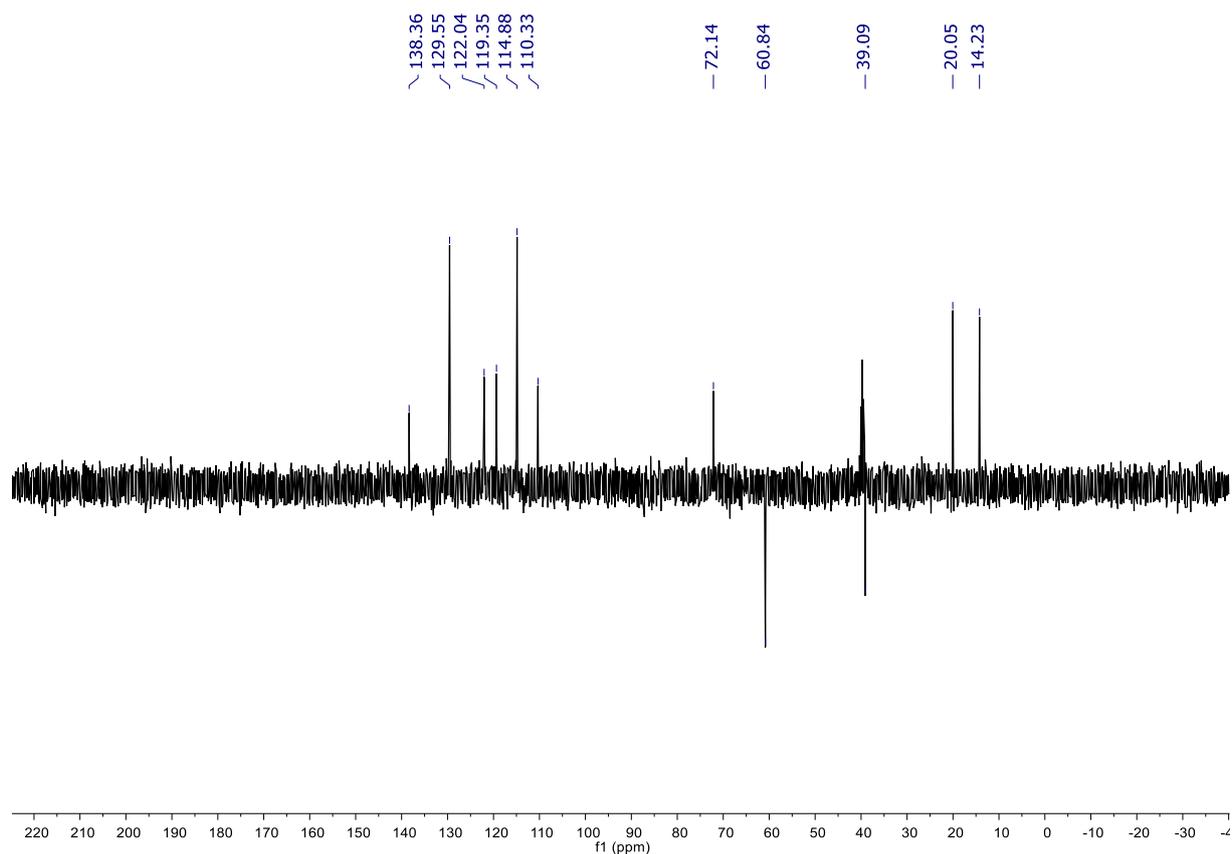
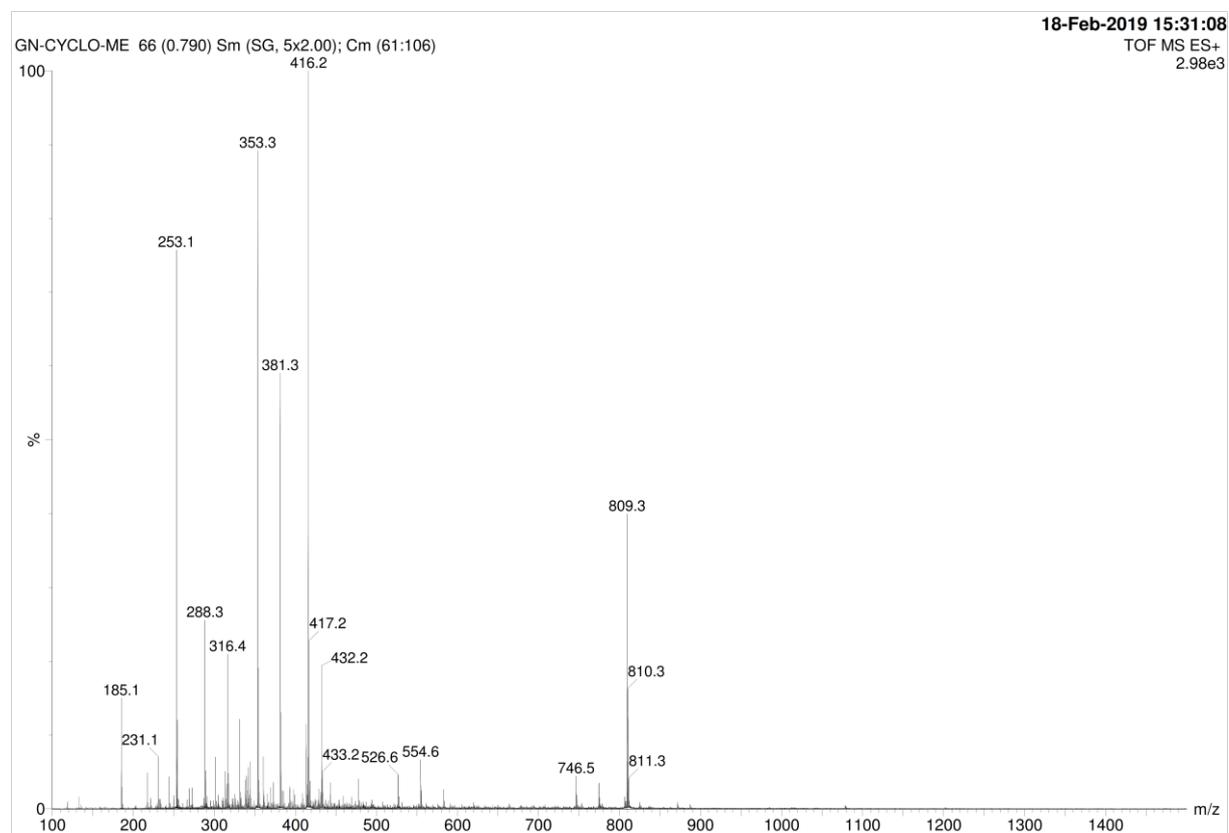


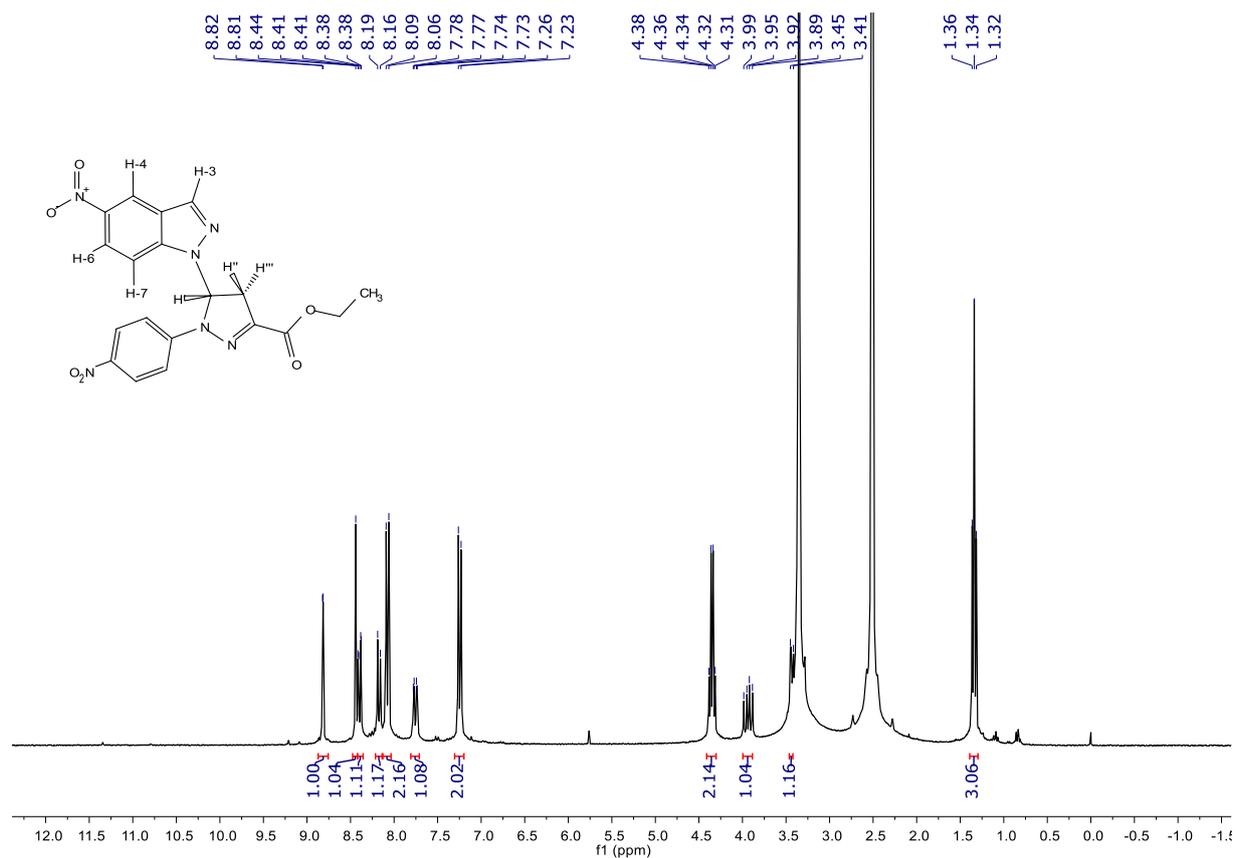
Figure S99. <sup>13</sup>C NMR spectrum of compound 12a in DMSO-d<sub>6</sub>.



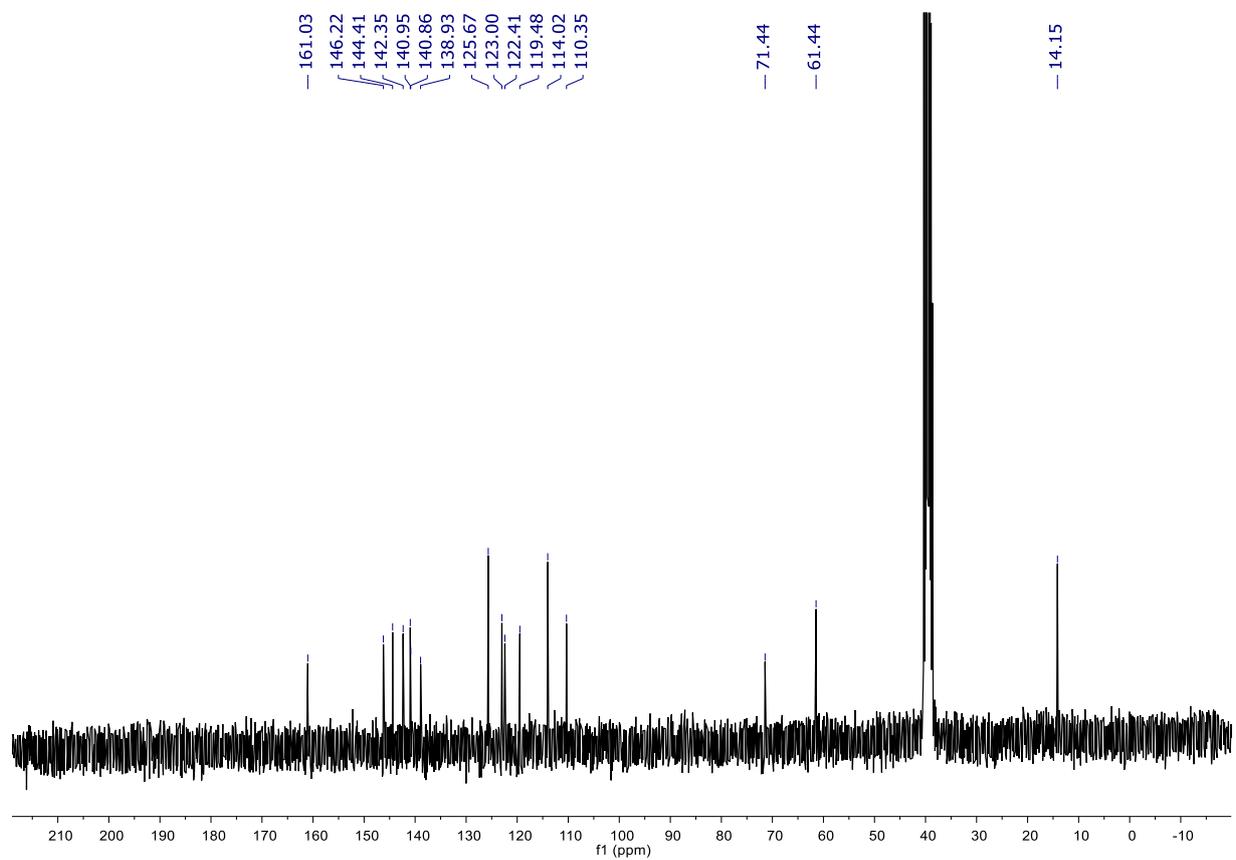
**Figure S100.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **12a** in  $\text{DMSO-d}_6$ .



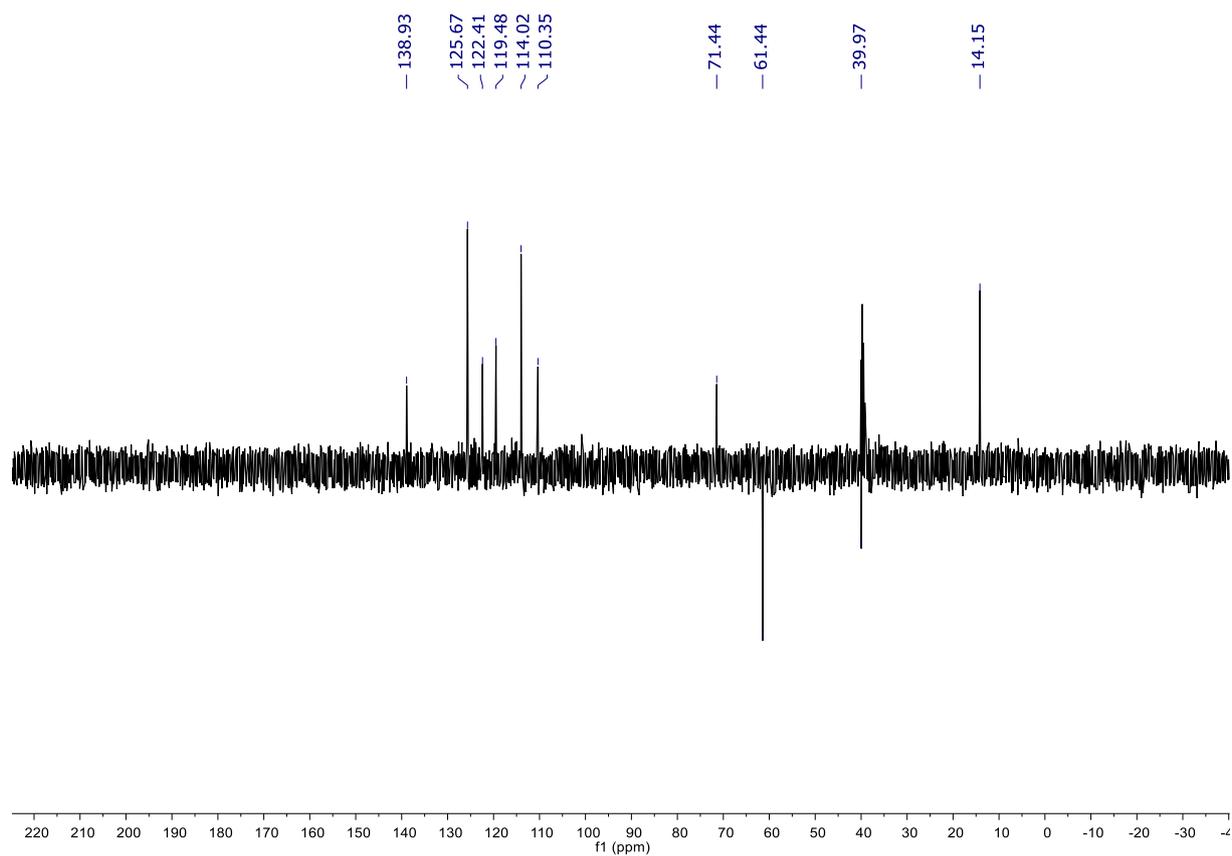
**Figure S101.** MS-ESI(+) spectrum of compound **12a**.



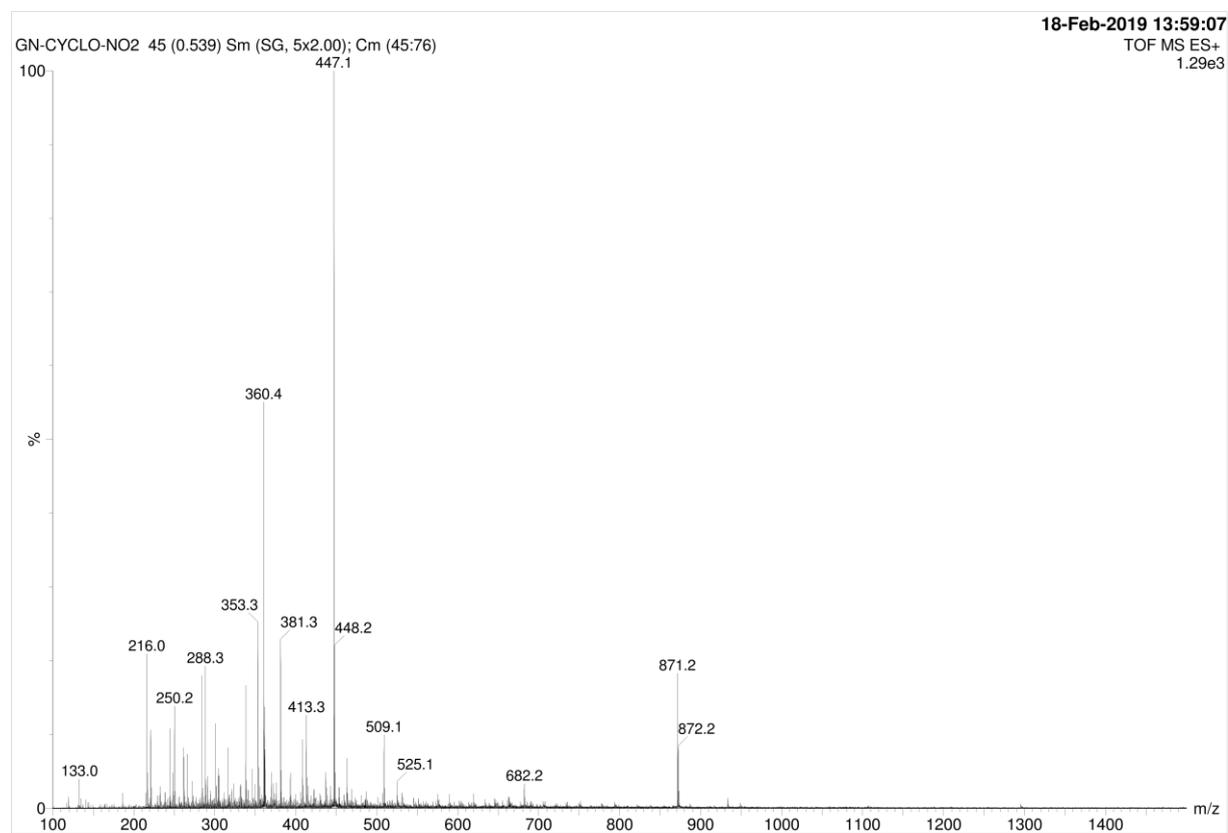
**Figure S102.** <sup>1</sup>H NMR spectrum of compound **12b** in DMSO-d<sub>6</sub>.



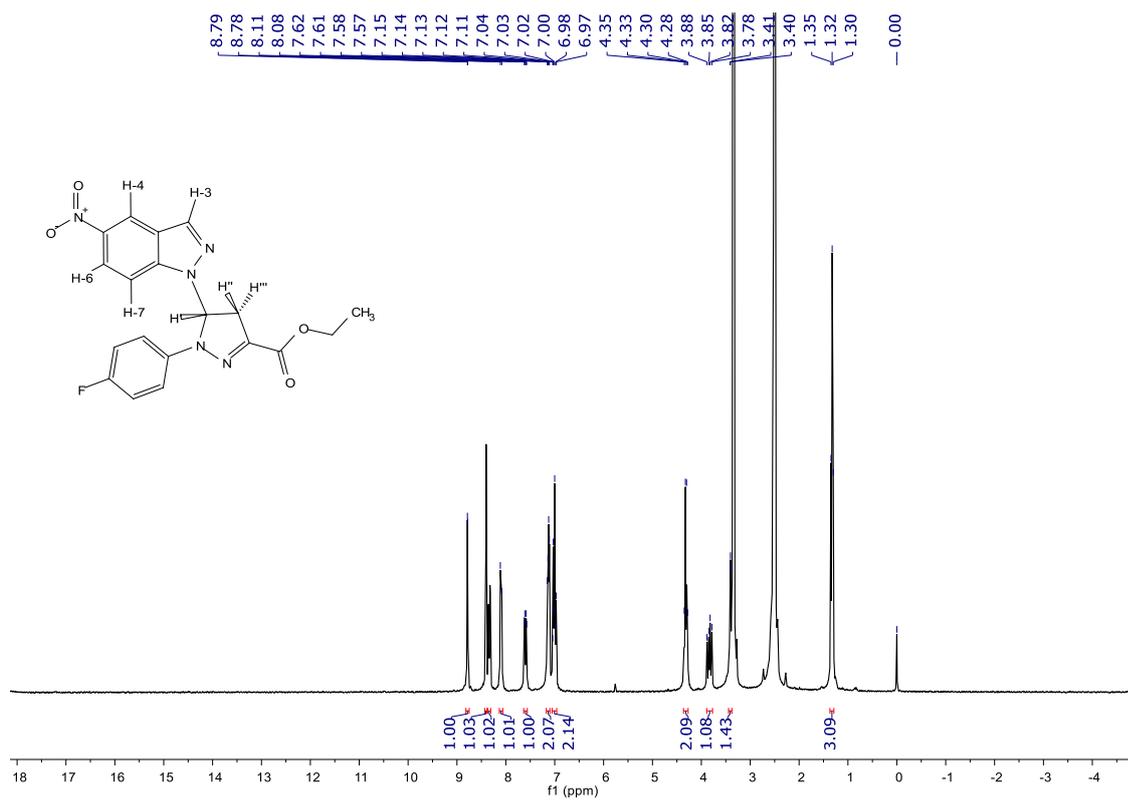
**Figure S103.** <sup>13</sup>C NMR spectrum of compound **12b** in DMSO-d<sub>6</sub>.



**Figure S104.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **12b** in  $\text{DMSO-d}_6$ .

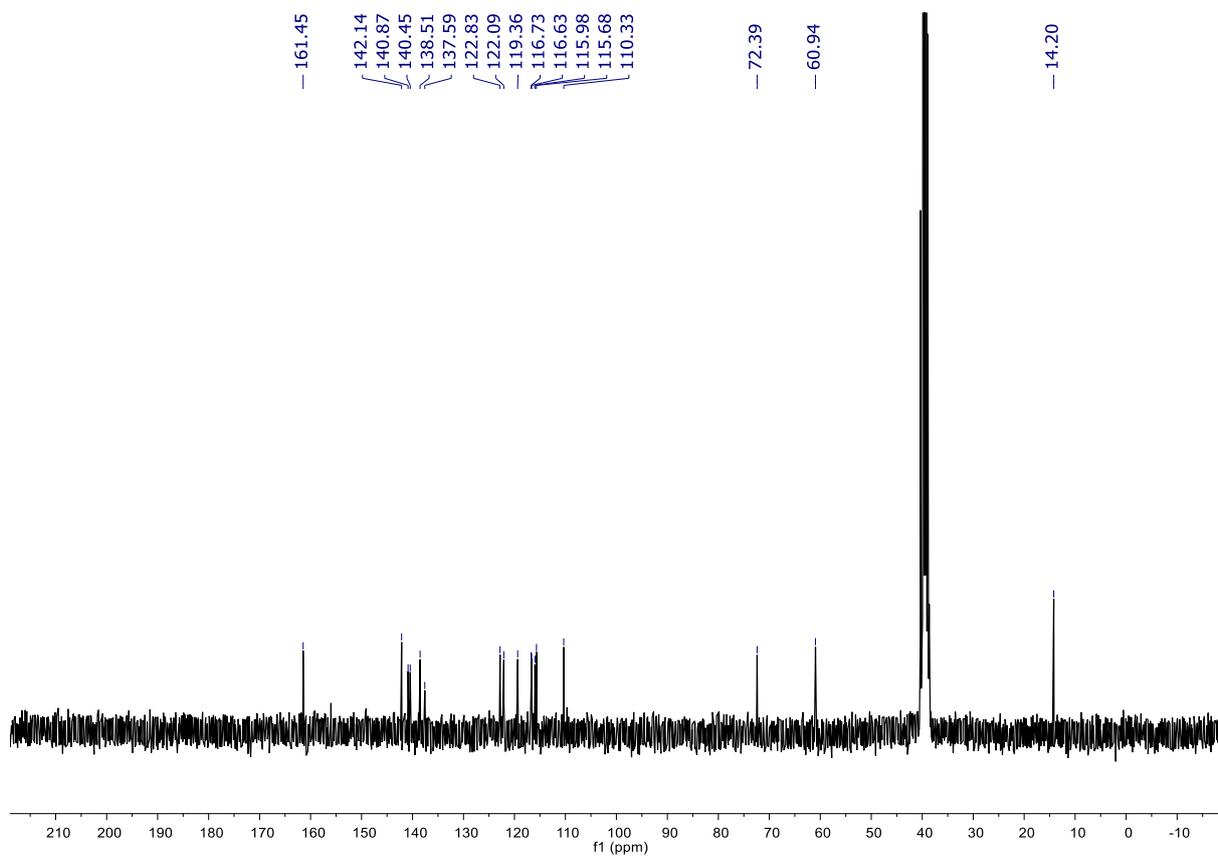


**Figure S105.** MS-ESI(+) spectrum of compound **12b**.

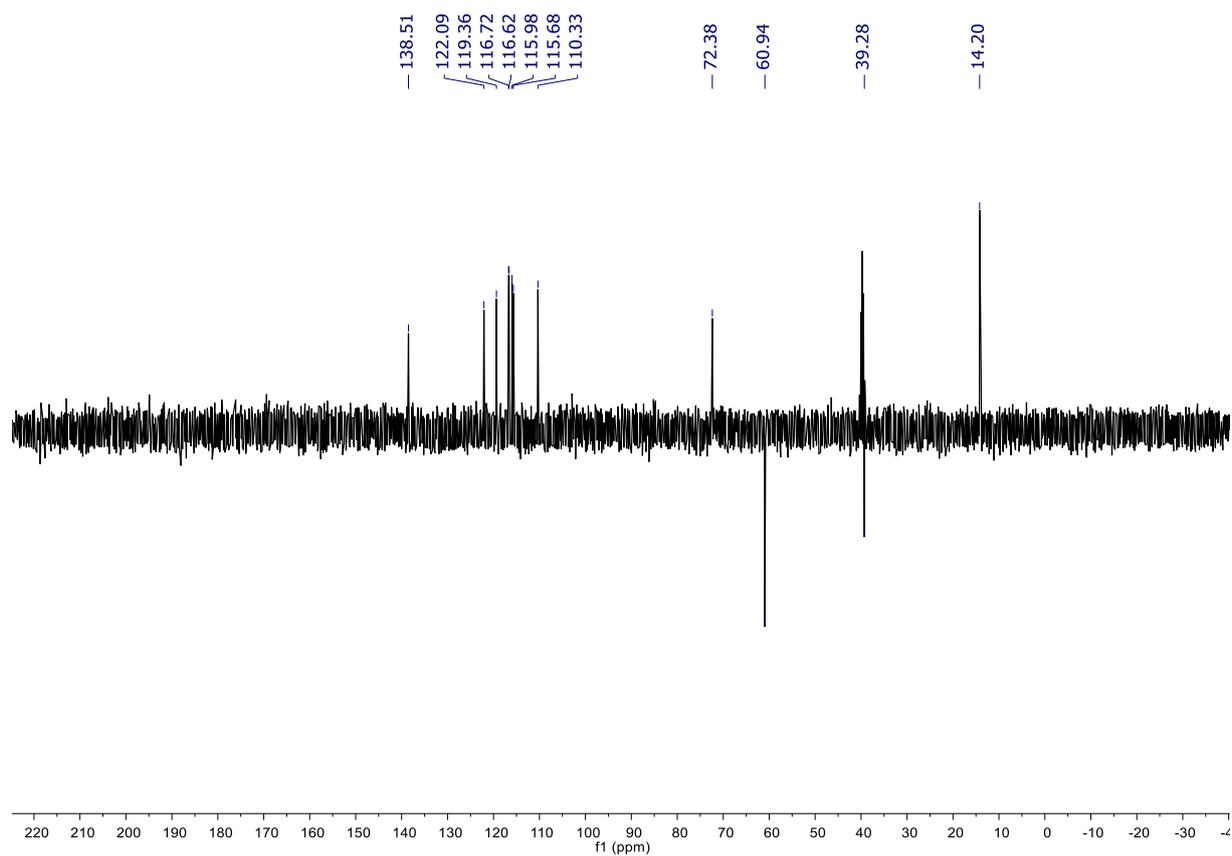


**S106.** <sup>1</sup>H NMR spectrum of compound **12c** in DMSO-d<sub>6</sub>.

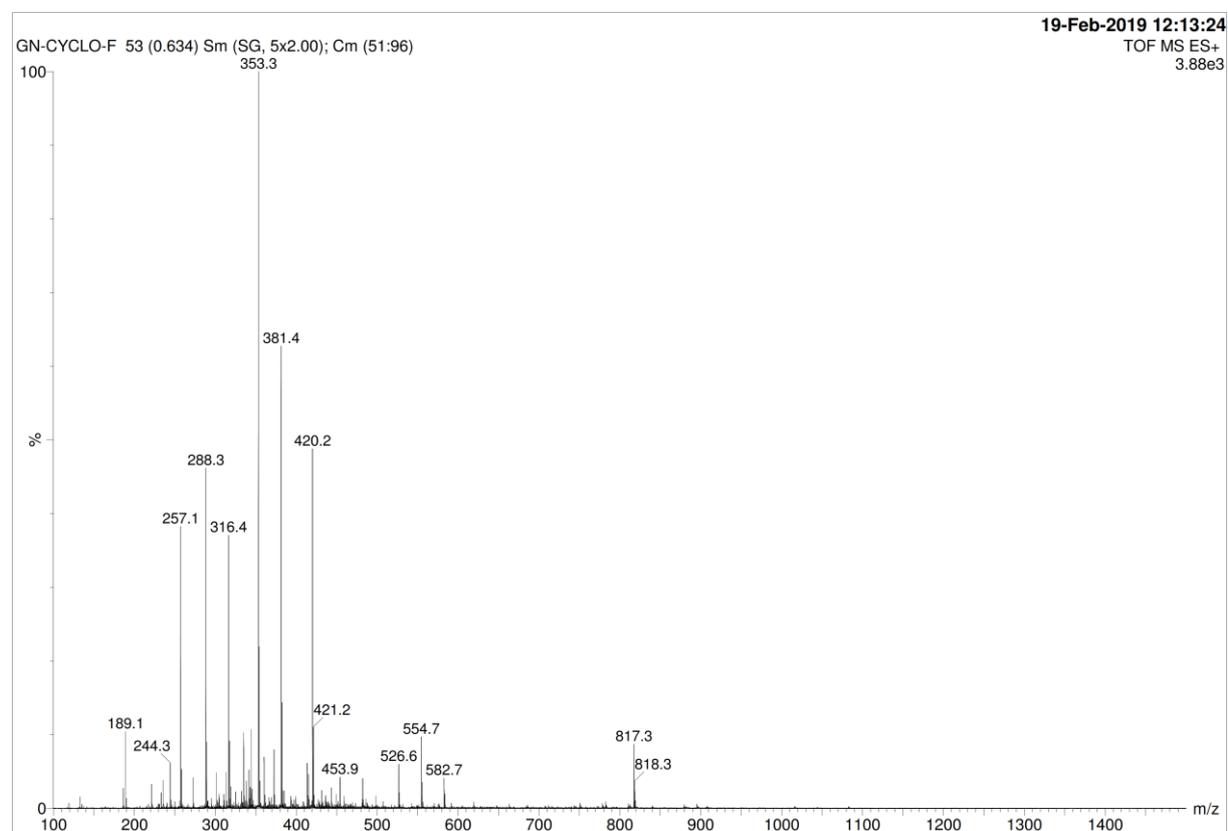
Figure



**Figure S107.** <sup>13</sup>C NMR spectrum of compound **12c** in DMSO-d<sub>6</sub>.



**Figure S108.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **12c** in  $\text{DMSO-d}_6$ .



**Figure S109.** MS-ESI(+) spectrum of compound **12c**.

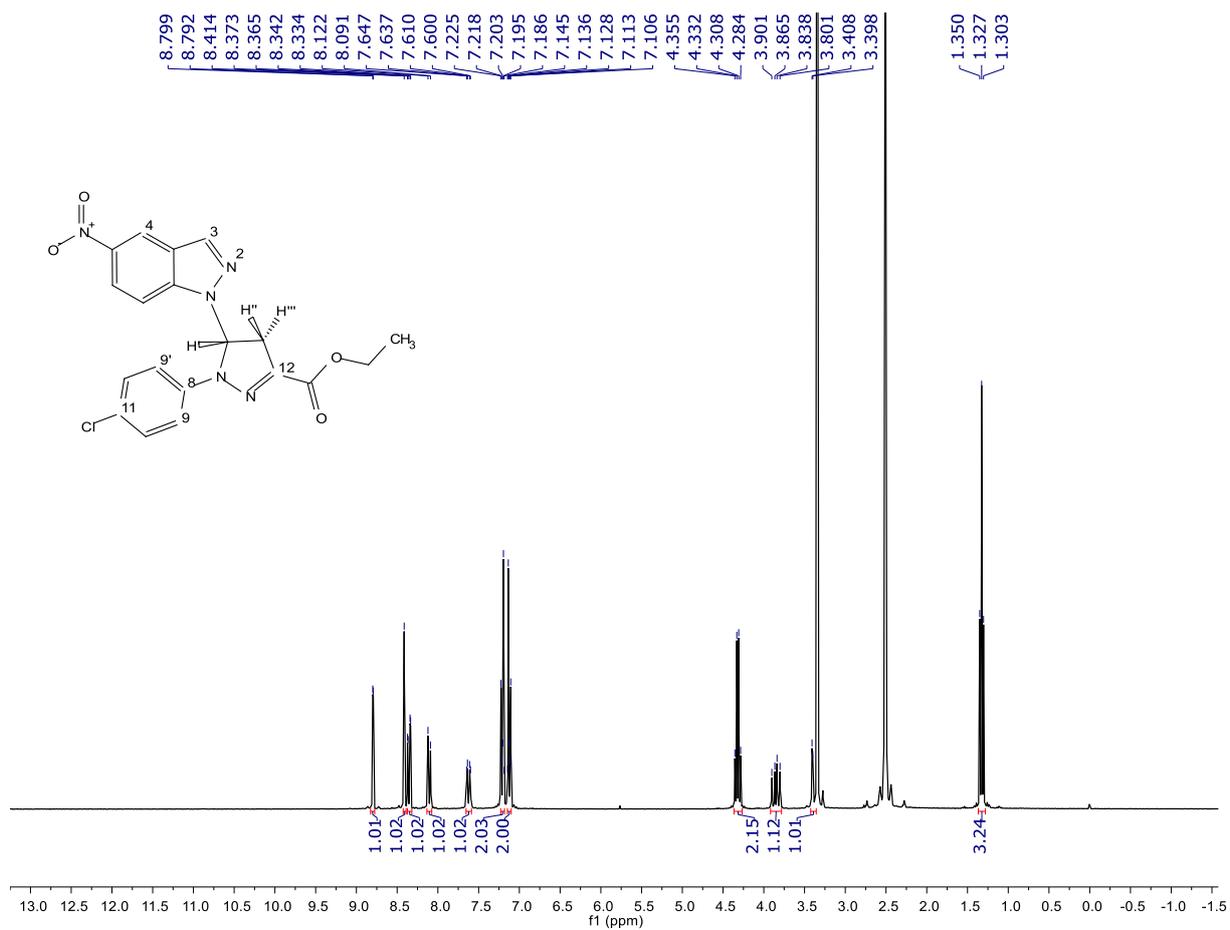


Figure S110. <sup>1</sup>H NMR spectrum of compound 12d in DMSO-d<sub>6</sub>.

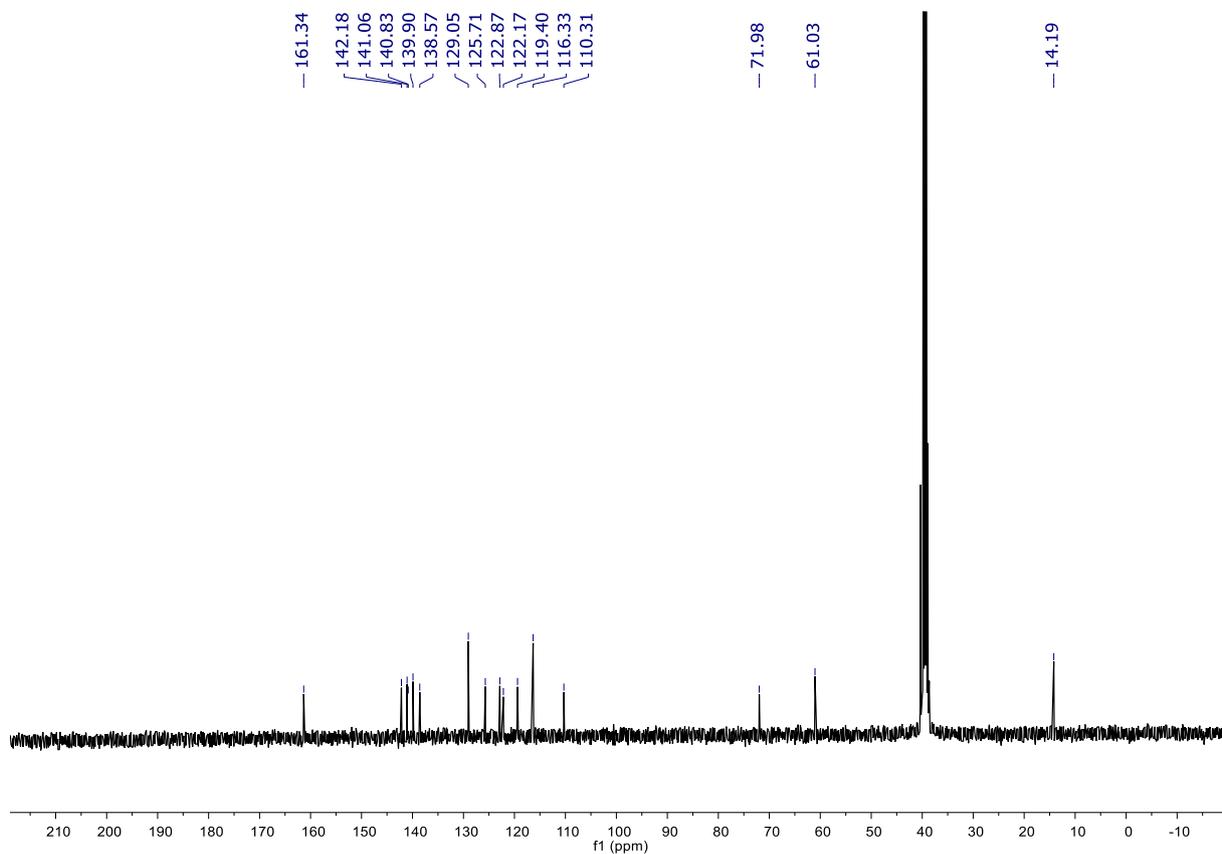
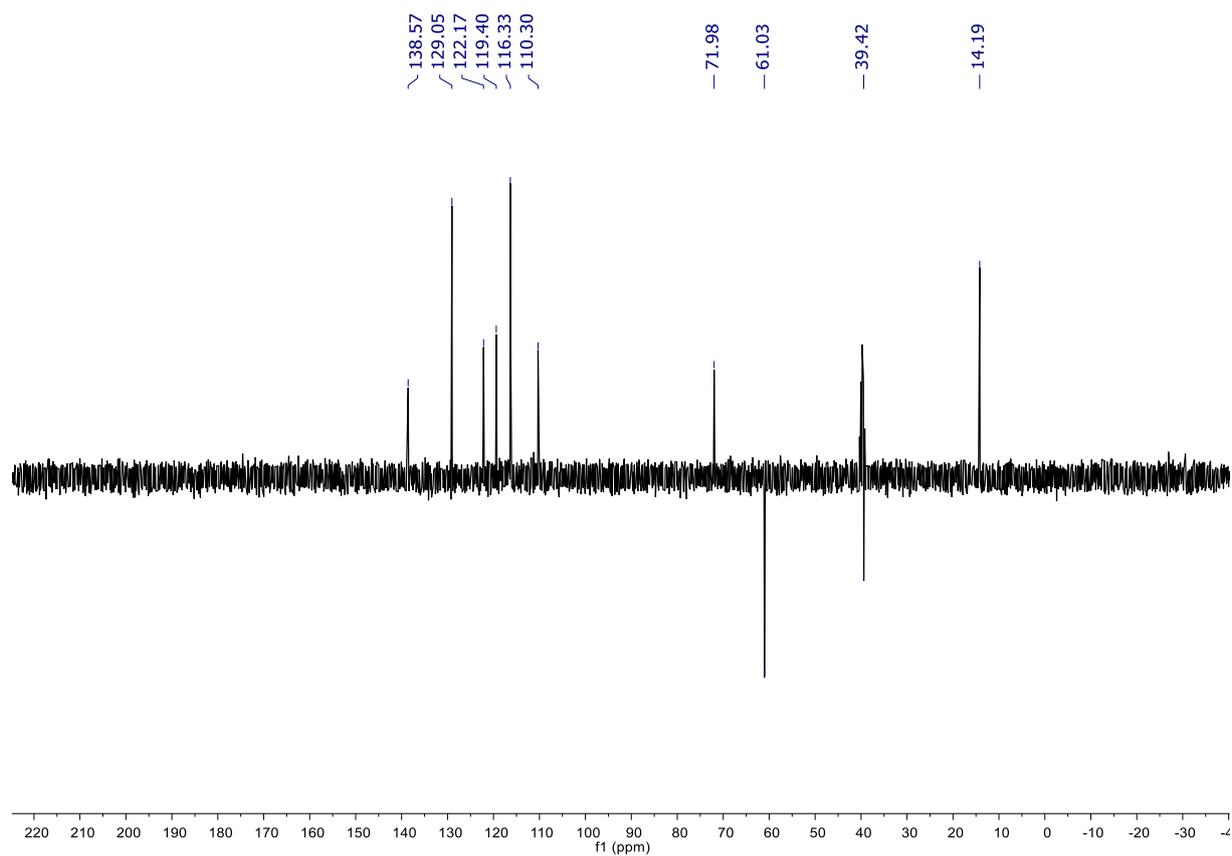
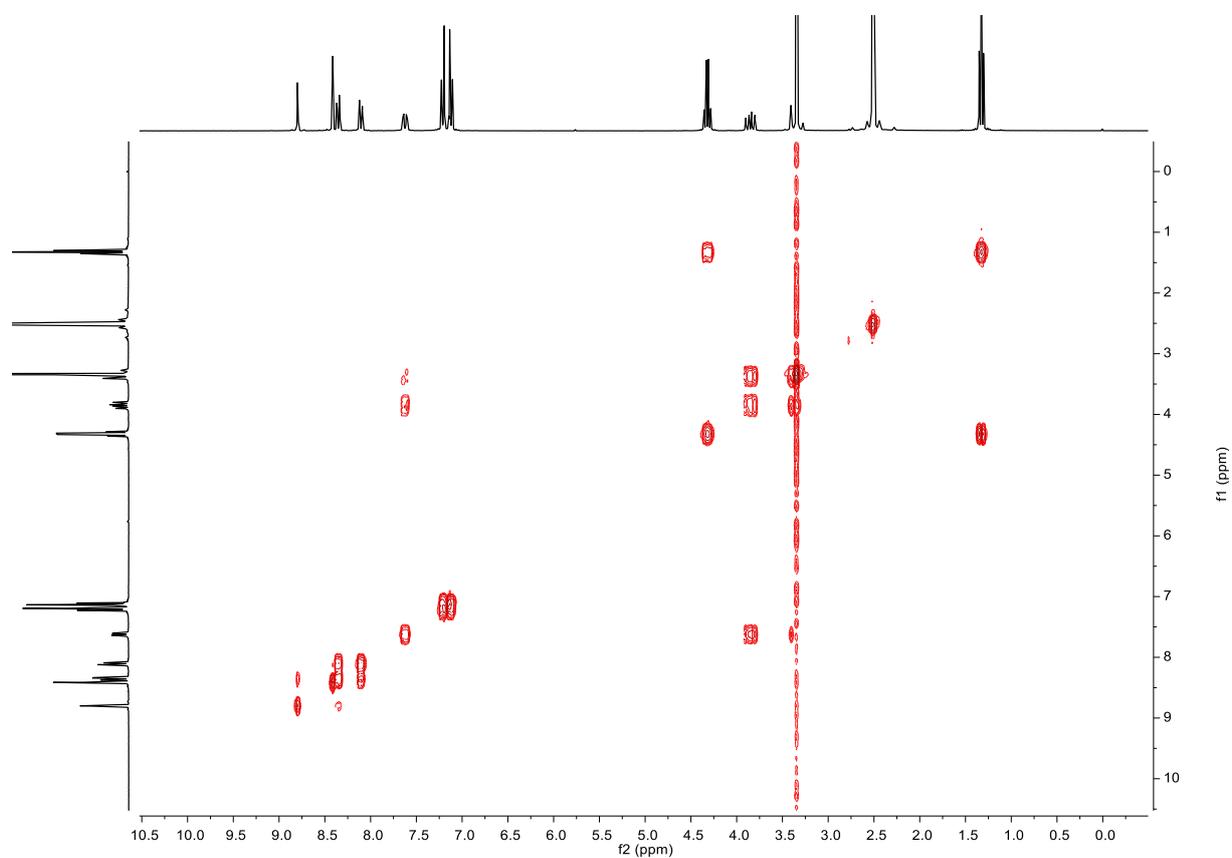


Figure S111. <sup>13</sup>C NMR spectrum of compound 12d in DMSO-d<sub>6</sub>.



**Figure S112.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **12d** in  $\text{DMSO-d}_6$ .



**Figure S113.** COSY ( $^1\text{H}/^1\text{H}$ ) spectrum of compound **12d** in  $\text{DMSO-d}_6$ .

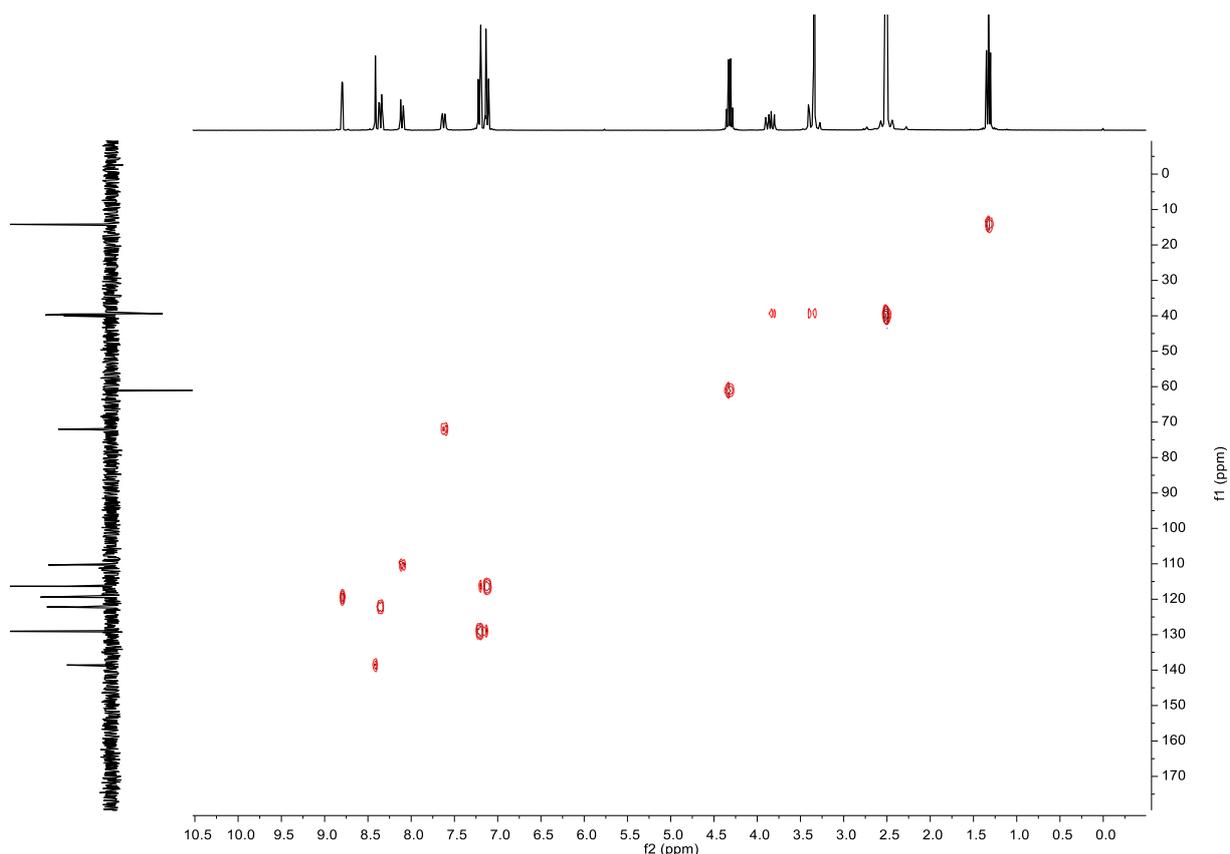


Figure S114. HSQC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **12d** in  $\text{DMSO-d}_6$ .

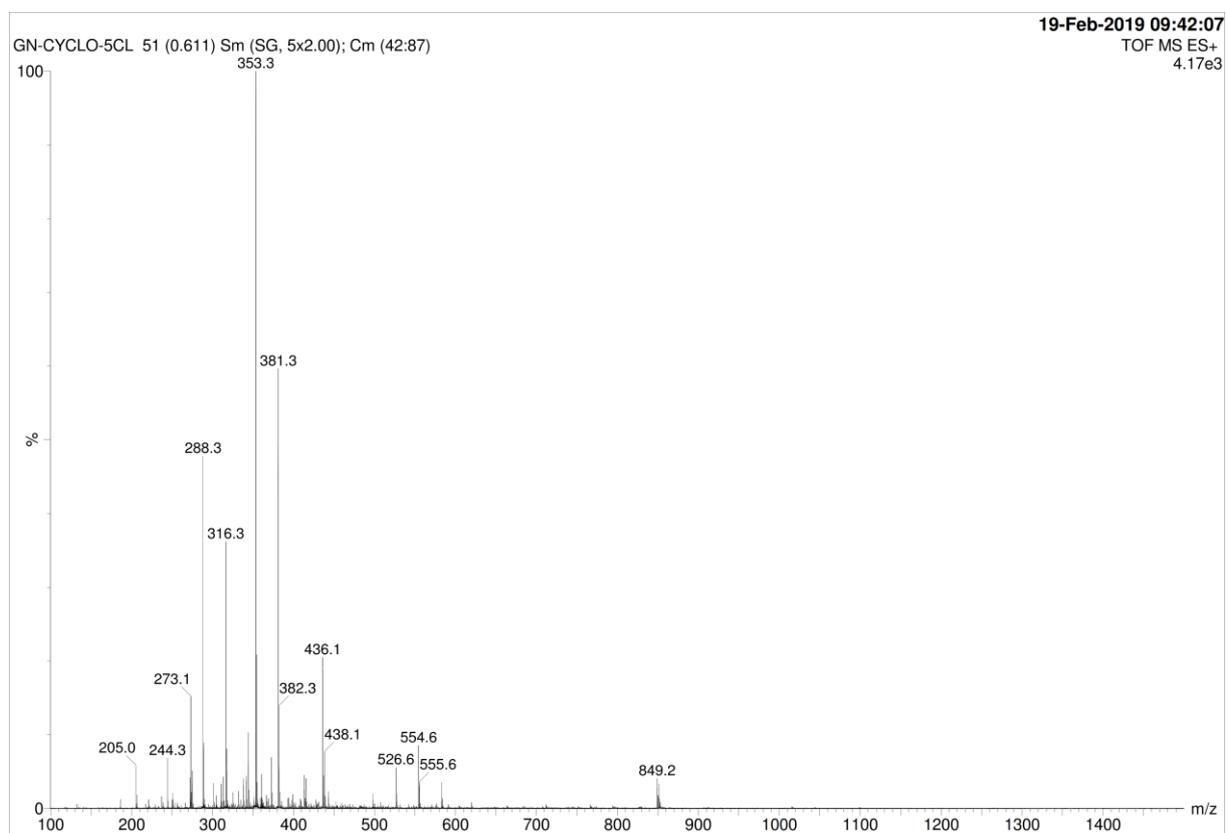
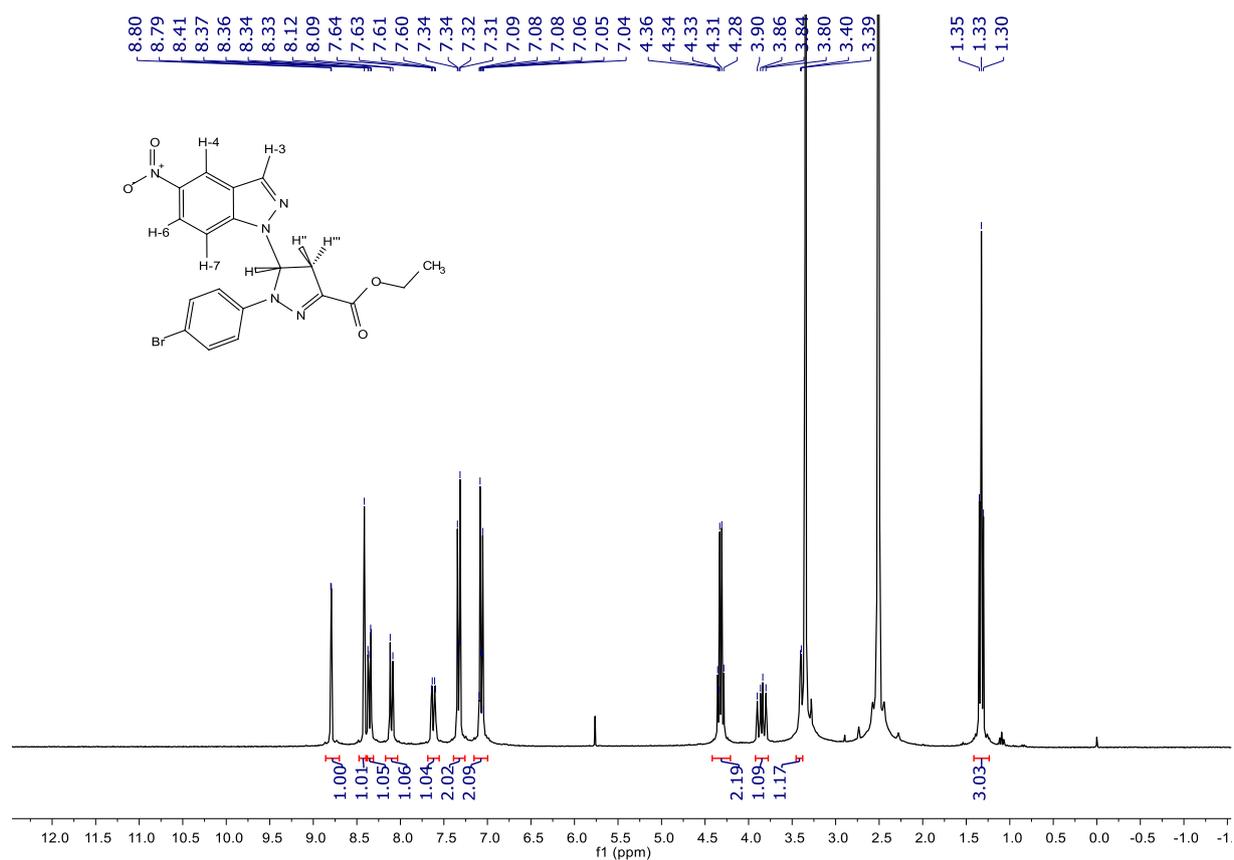
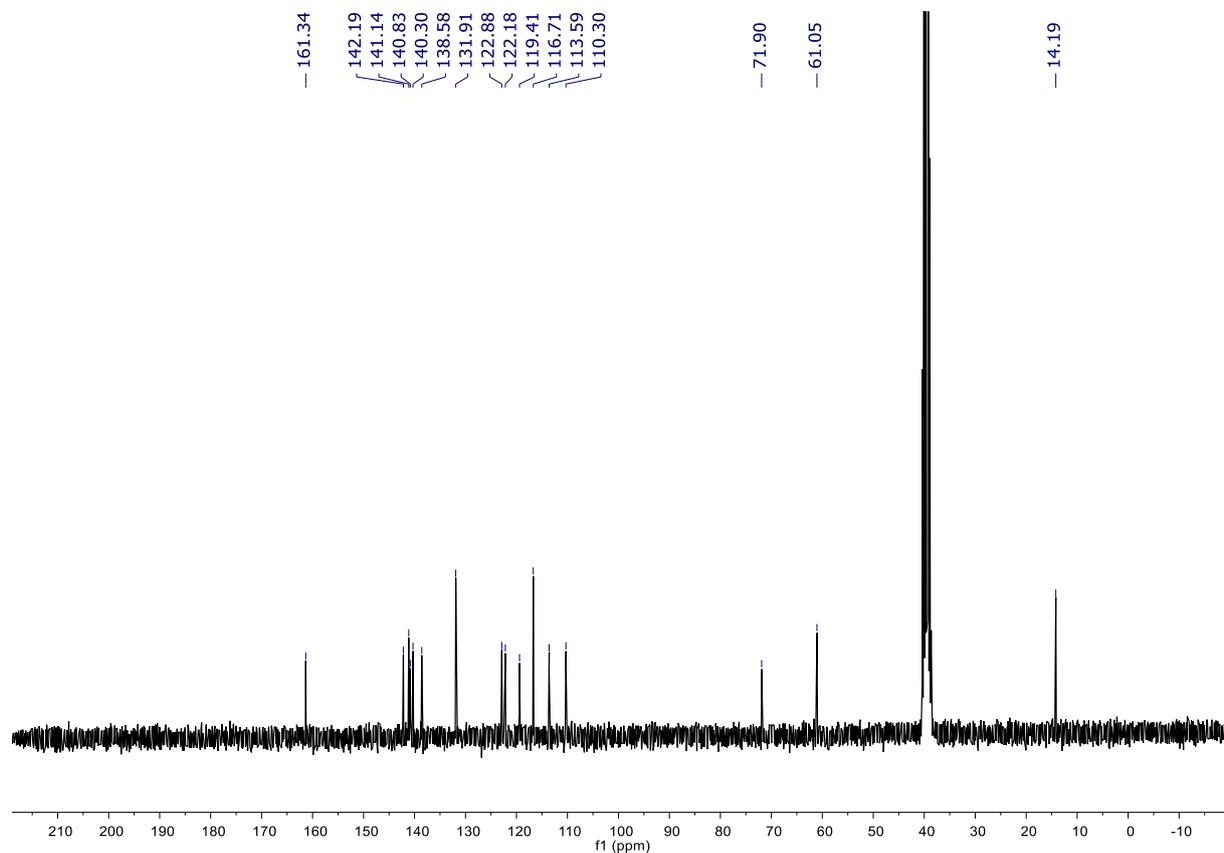


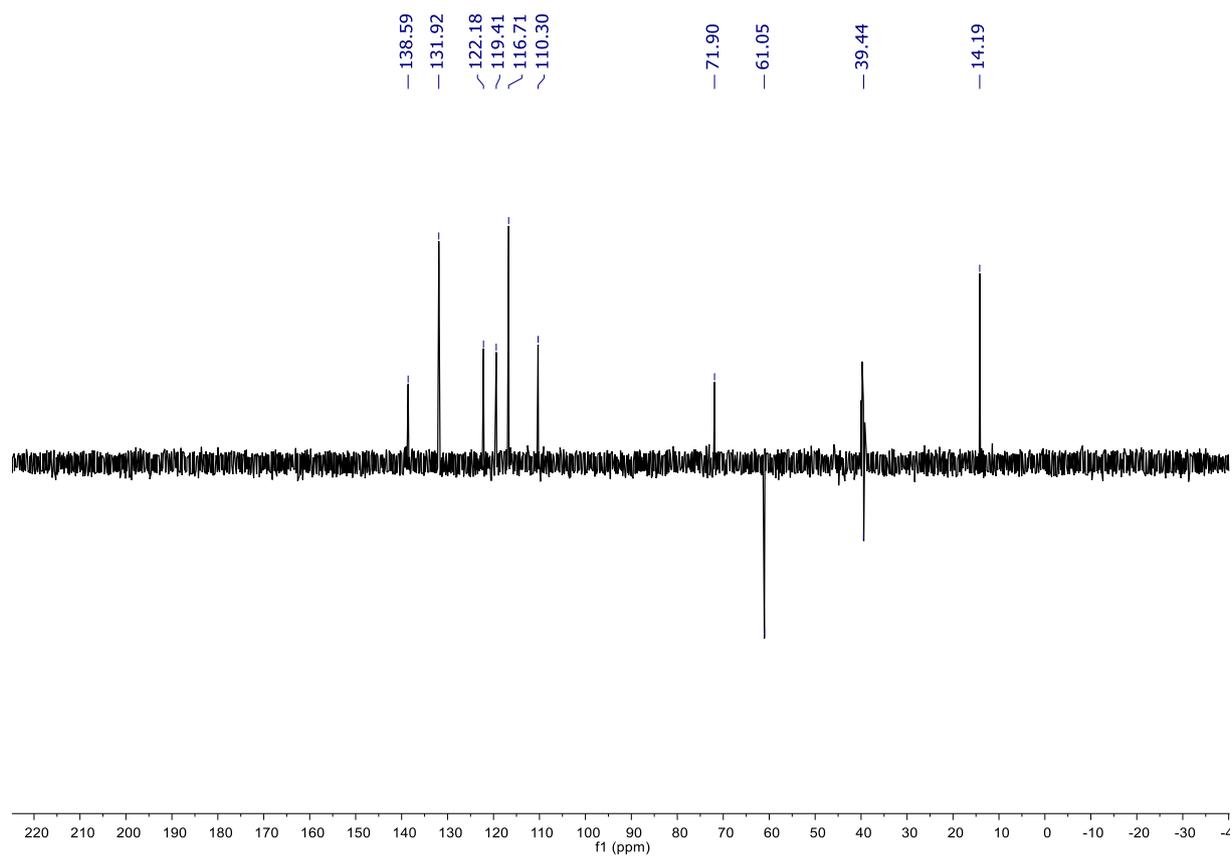
Figure S115. MS-ESI(+) spectrum of compound **12d**.



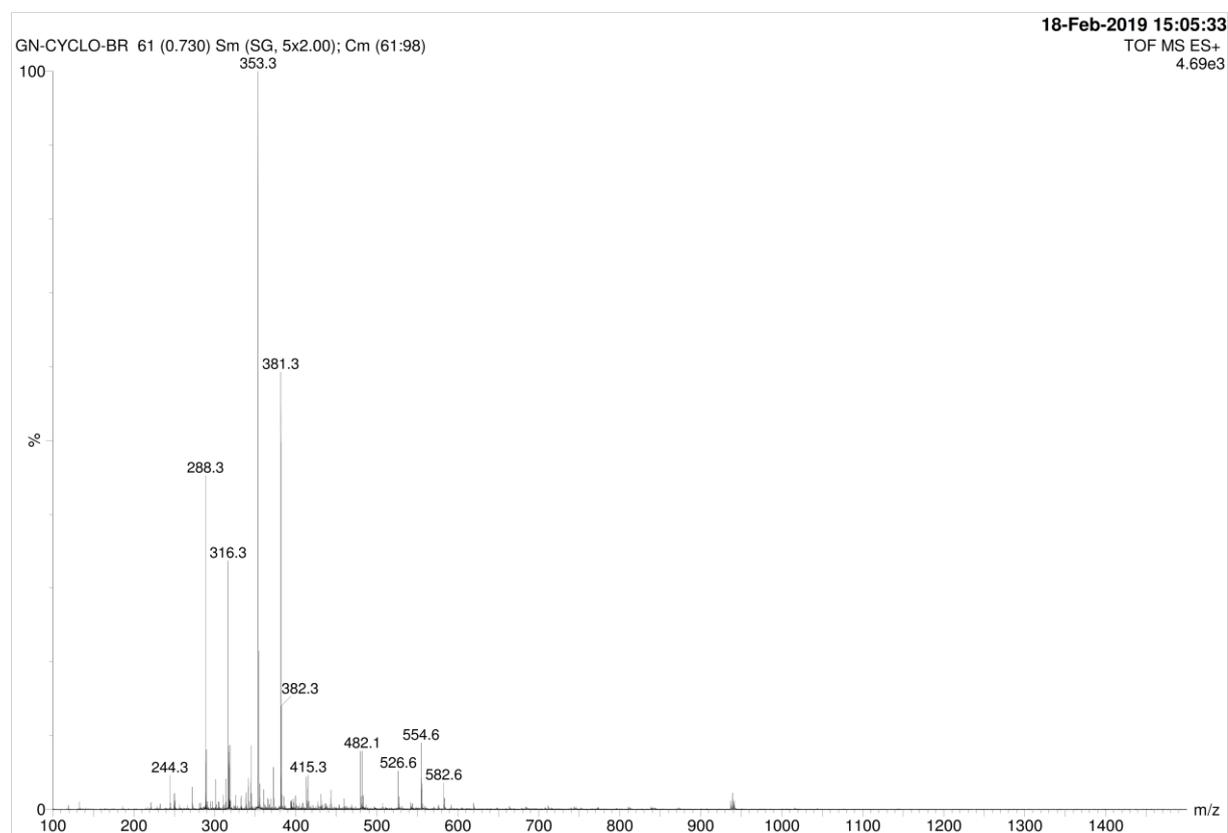
**Figure S116.**  $^1\text{H}$  NMR spectrum of compound **12e** in  $\text{DMSO-d}_6$ .



**Figure S117.**  $^{13}\text{C}$  NMR spectrum of compound **12e** in  $\text{DMSO-d}_6$ .



**Figure S118.**  $^{13}\text{C}$  NMR DEPT 135 spectrum of compound **12e** in  $\text{DMSO-d}_6$ .



**Figure S119.** MS-ESI(+) spectrum of compound **12e**.

#### IV - NMR and mass spectrum of compounds 13

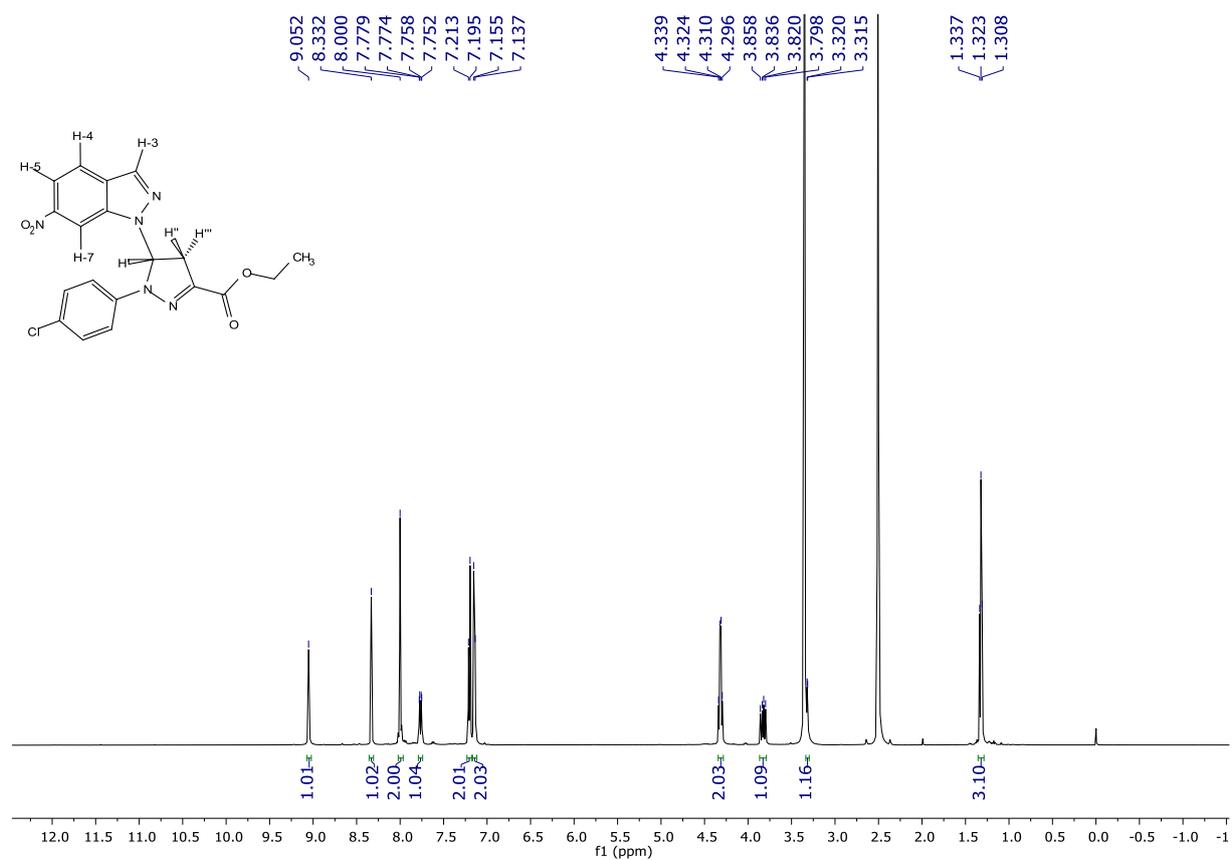


Figure S120. <sup>1</sup>H NMR spectrum of compound 13 in DMSO-d<sub>6</sub>.

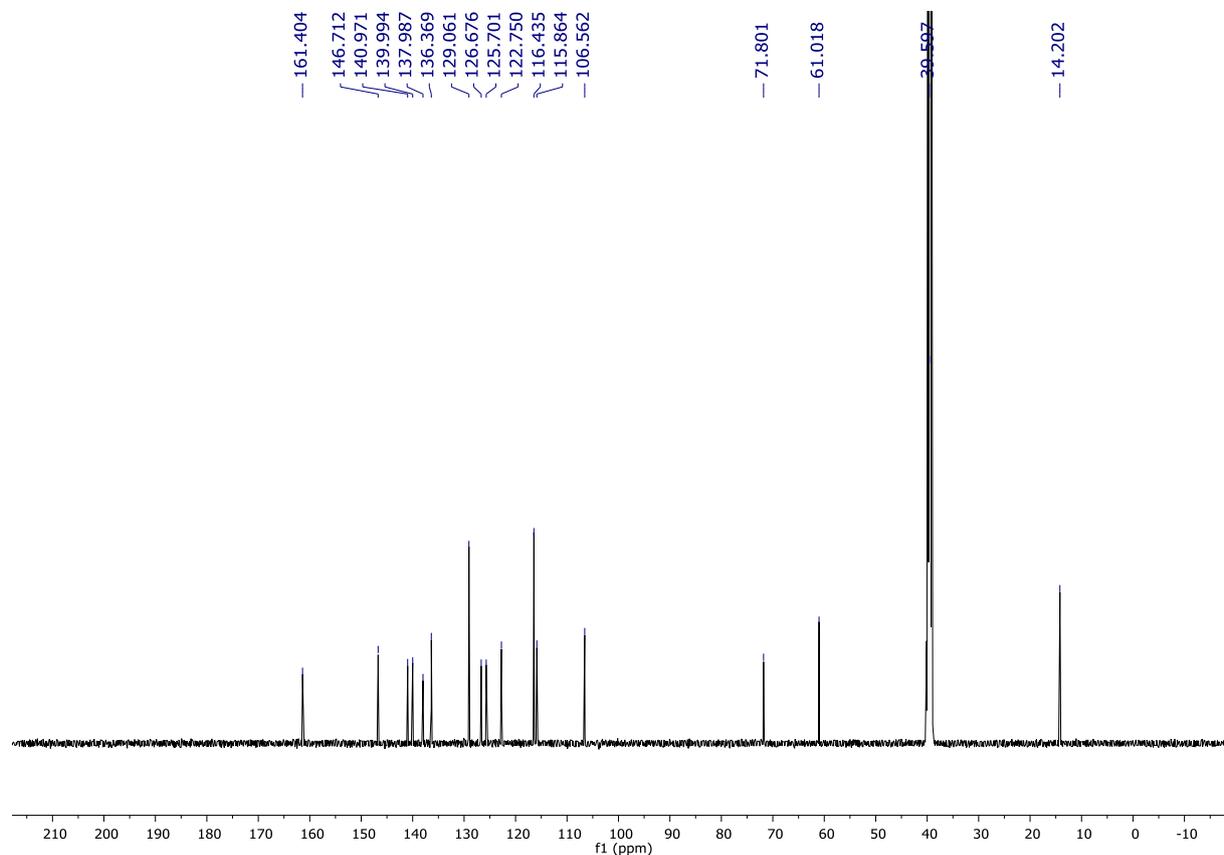
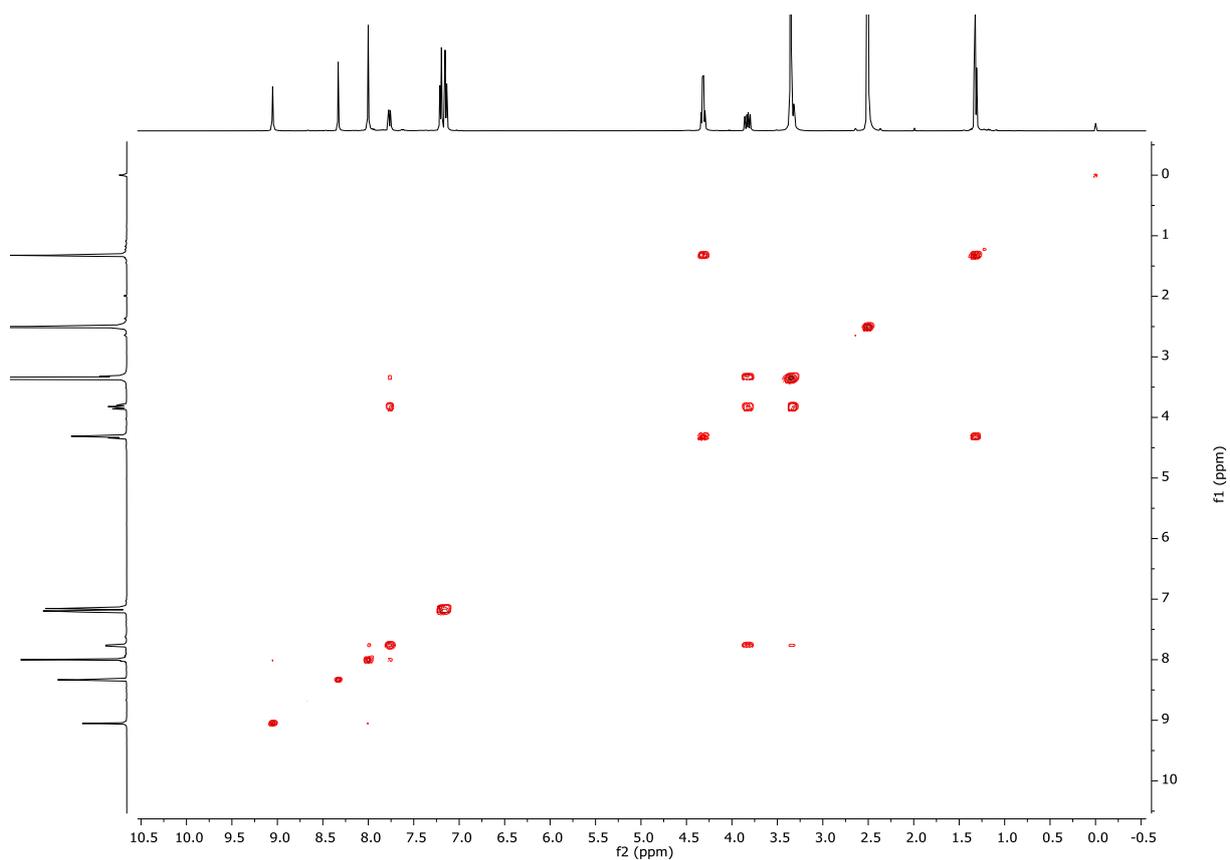
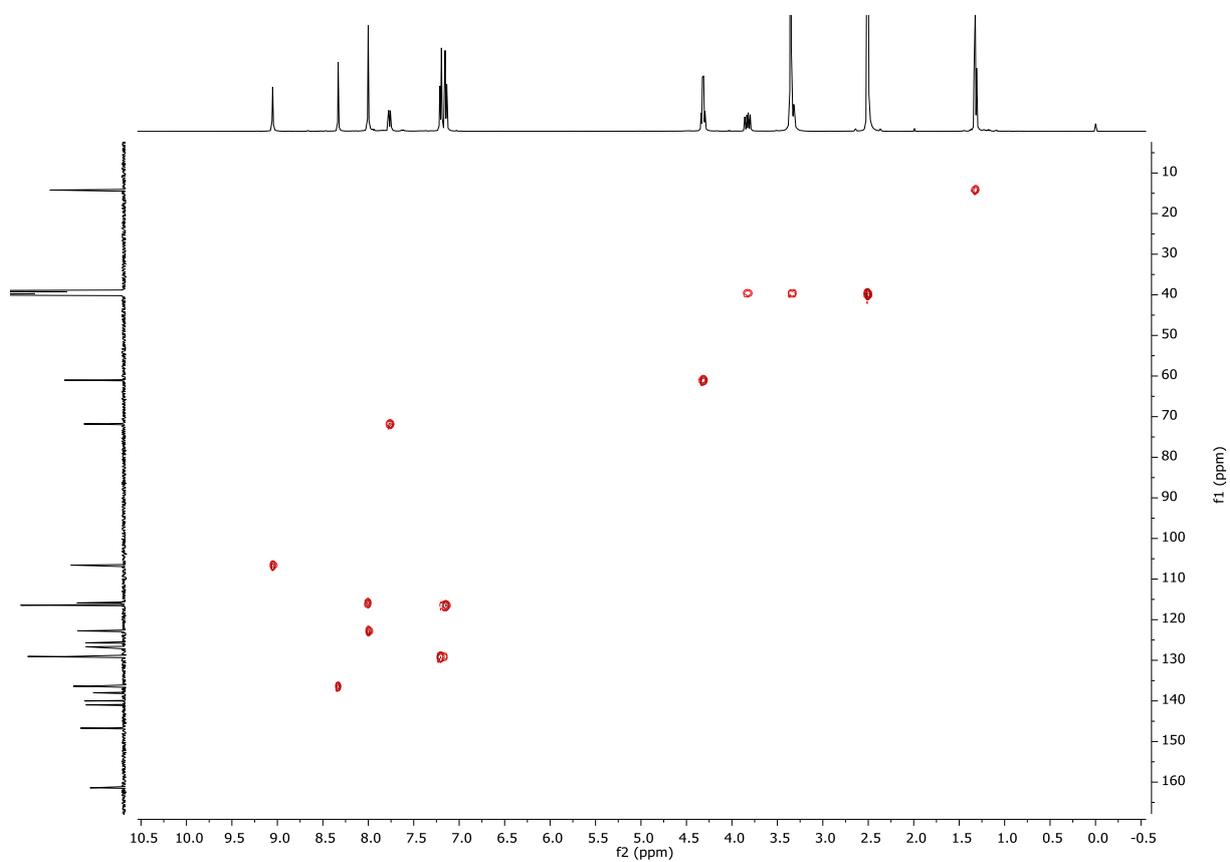


Figure S121. <sup>13</sup>C NMR spectrum of compound 13 in DMSO-d<sub>6</sub>.



**Figure S122.** COSY ( $^1\text{H}/^1\text{H}$ ) spectrum of compound **13** in  $\text{DMSO-d}_6$ .



**Figure S123.** HSQC ( $^1\text{H}/^{13}\text{C}$ ) spectrum of compound **13** in  $\text{DMSO-d}_6$ .

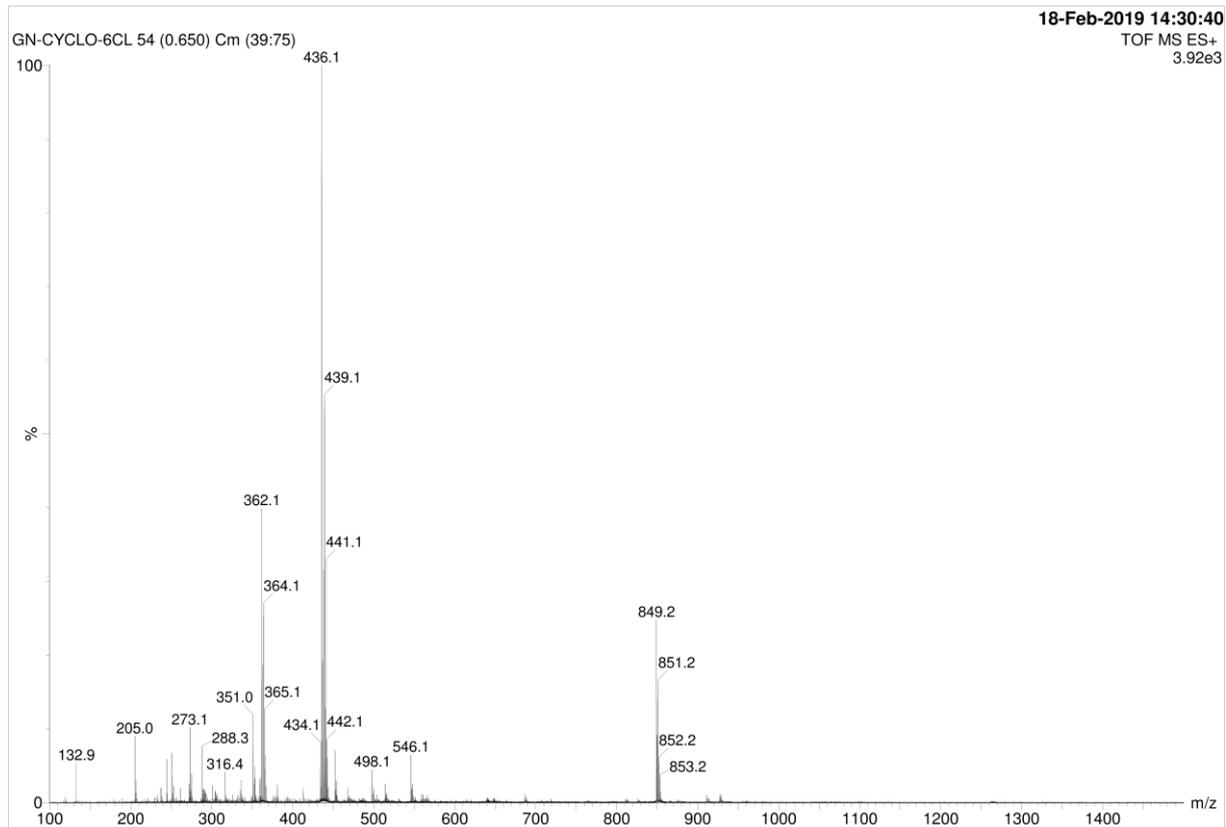


Figure S124. MS-ESI(+) spectrum of compound 13.