

# NMR and HRMS Spectra of Selected Synthesized Compounds

## Supporting Information

### SYNTHESIS OF PYRROLO[2,3]PYRIDO[2,4-*d*]PYRIMIDIN-6- ONES AND RELATED NEW HETEROCYCLES

**Tamás Zelenyák<sup>a</sup>, Imre Fejes<sup>a</sup>, Jérôme-Benoît Starck<sup>b</sup>, Miklós Nyerges<sup>a,\*</sup>**

<sup>a</sup>Servier Research Institute of Medicinal Chemistry, 7 Záhony utca., 1031, Budapest, Hungary

<sup>b</sup>Institut de Recherches Servier, 3 rue de la République, 92150 Suresnes, France

# NMR and HRMS Spectra of Selected Synthesized Compounds

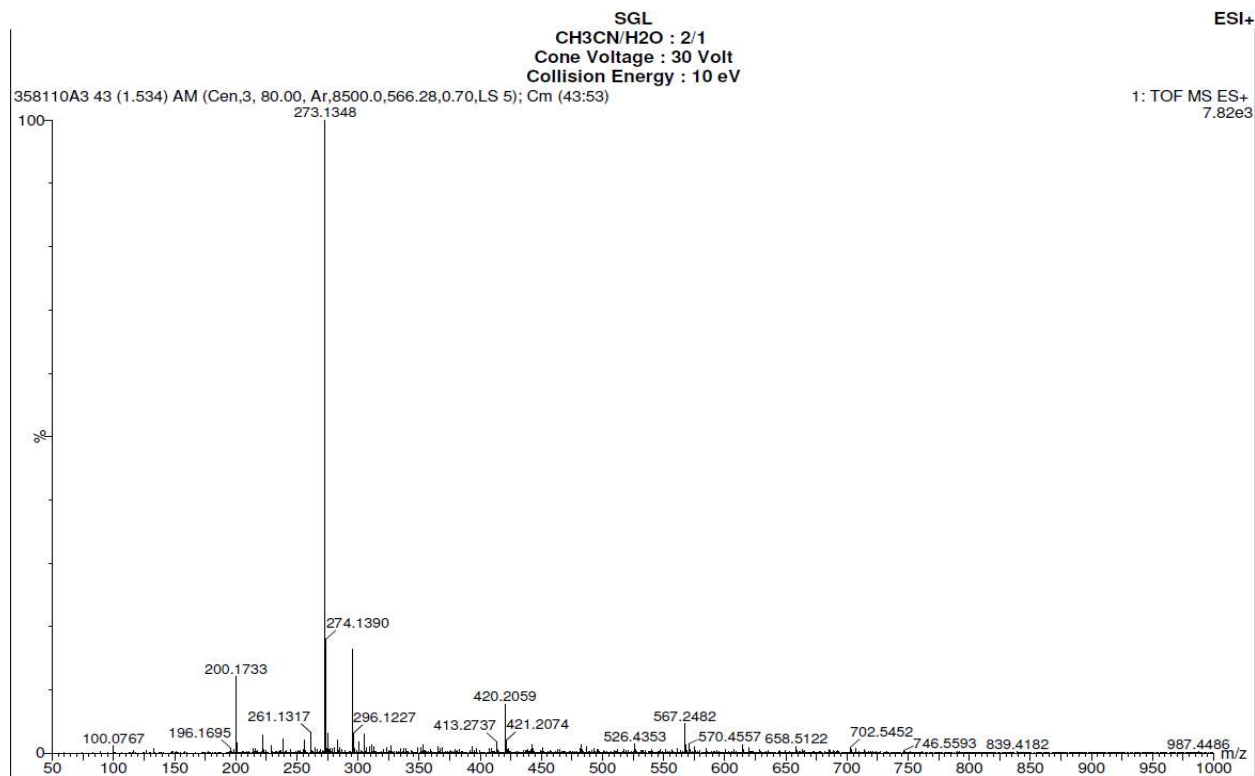


Figure S1. HRMS spectrum of **6**

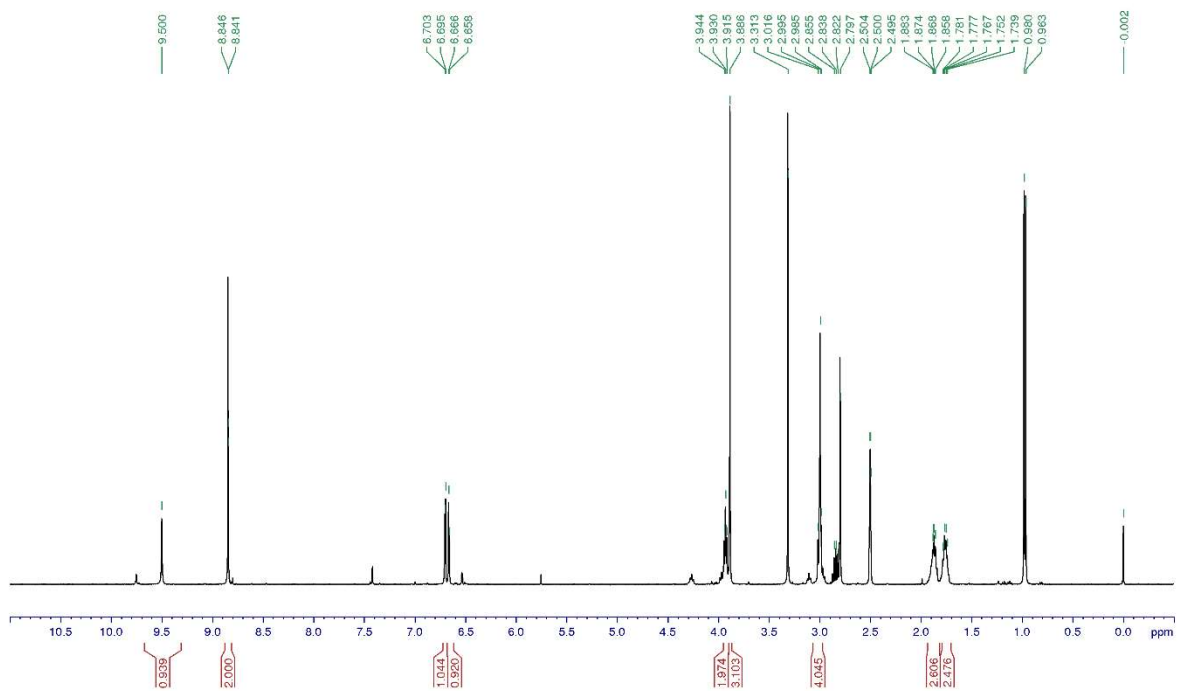


Figure S2.  $^1\text{H-NMR}$  spectrum of **6** measured at 400 MHz in  $\text{DMSO-d}_6$

# NMR and HRMS Spectra of Selected Synthesized Compounds

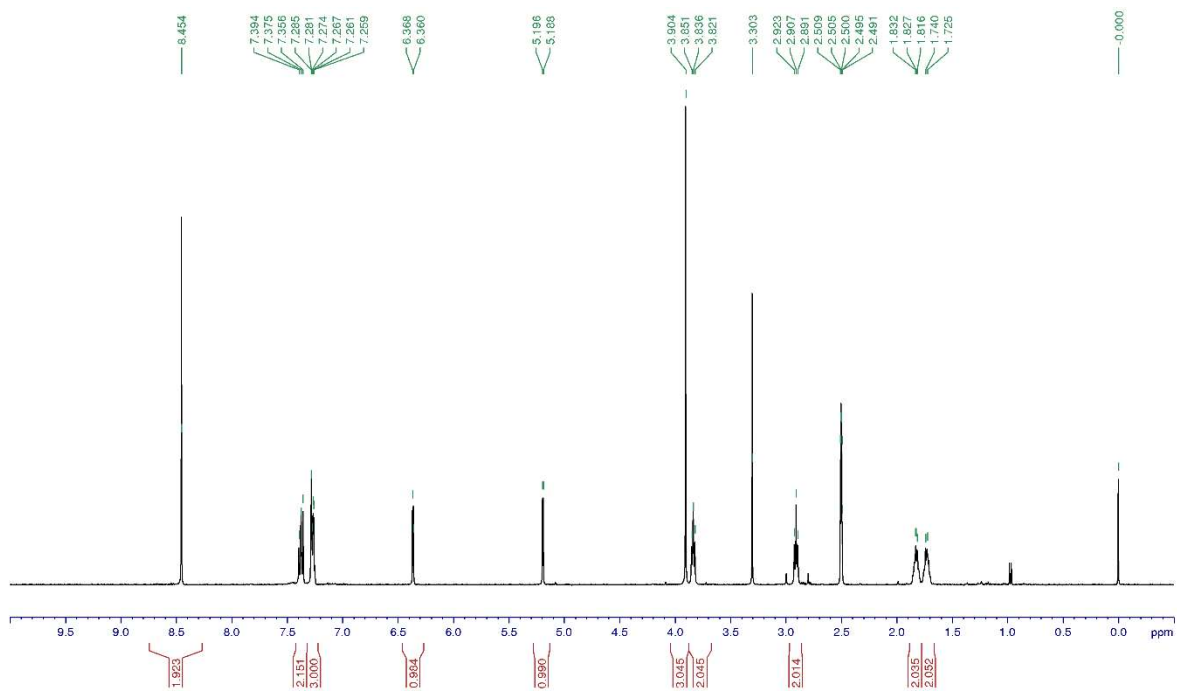


Figure S3. <sup>1</sup>H-NMR spectrum of 7 measured at 400 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

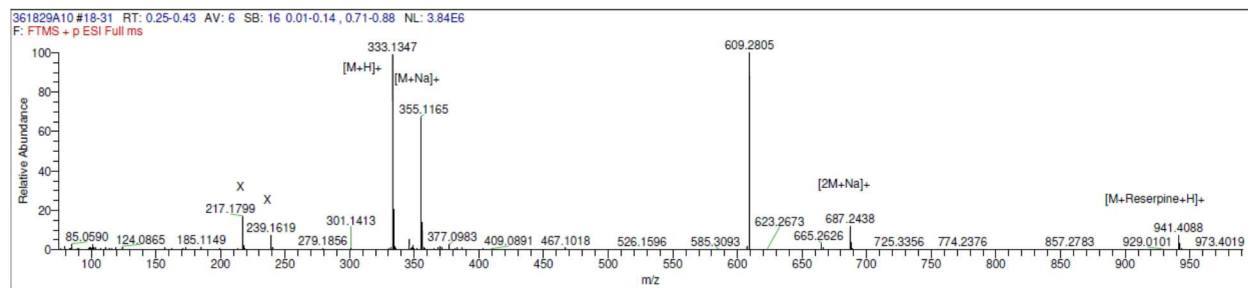


Figure S4. HRMS spectrum of **8**

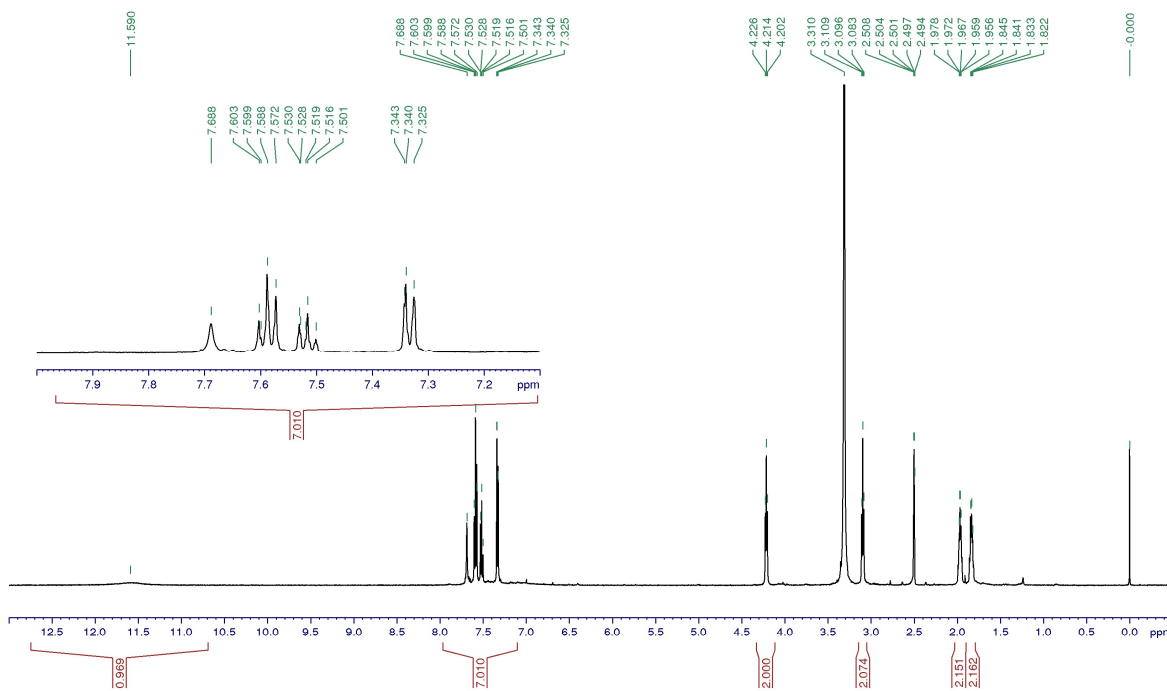


Figure S5.  $^1\text{H-NMR}$  spectrum of **8** measured at 400 MHz in  $\text{DMSO-d}_6$

# NMR and HRMS Spectra of Selected Synthesized Compounds

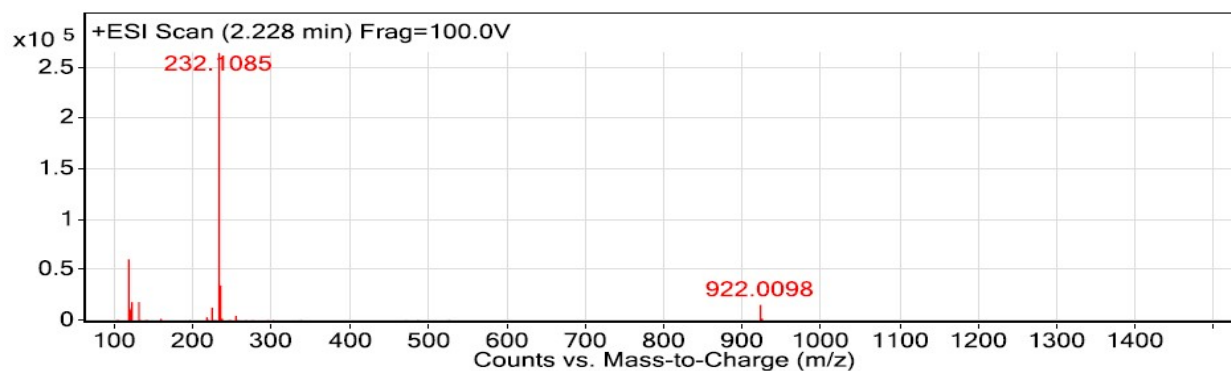


Figure S6. HRMS spectrum of **11a**

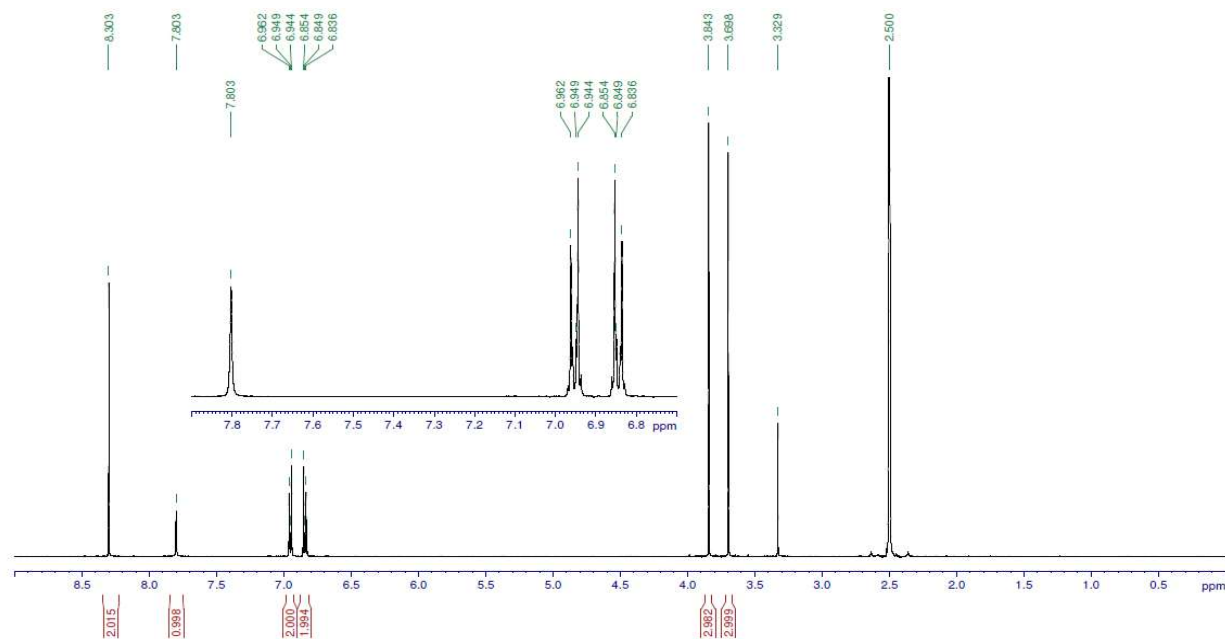


Figure S7. <sup>1</sup>H-NMR spectrum of **11a** measured at 500 MHz in DMSO-d<sub>6</sub>

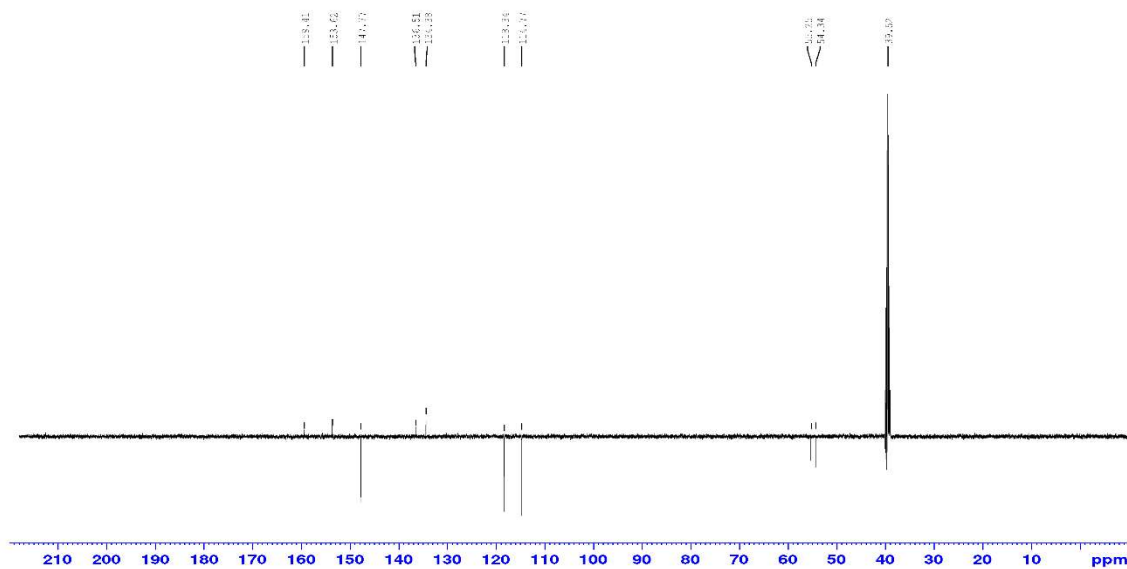


Figure S8. DEPT spectrum of **11a** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

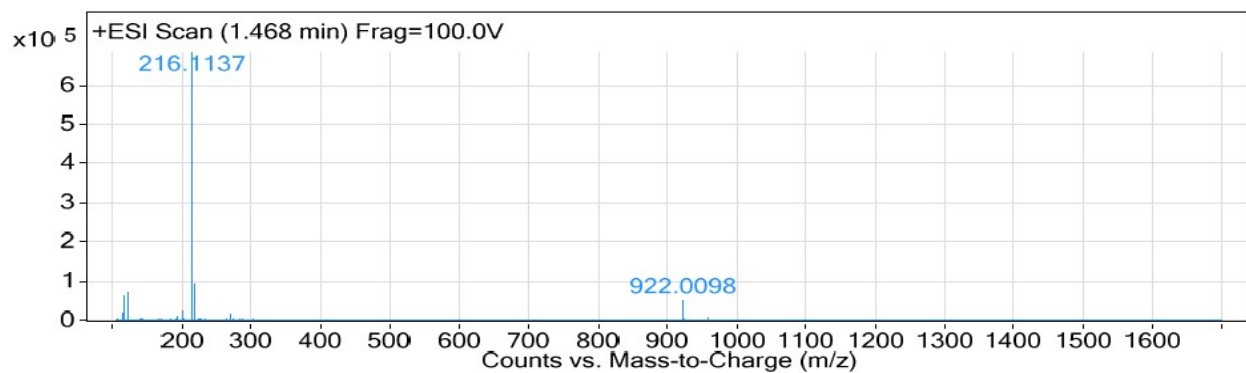


Figure S9. HRMS spectrum of **11b**

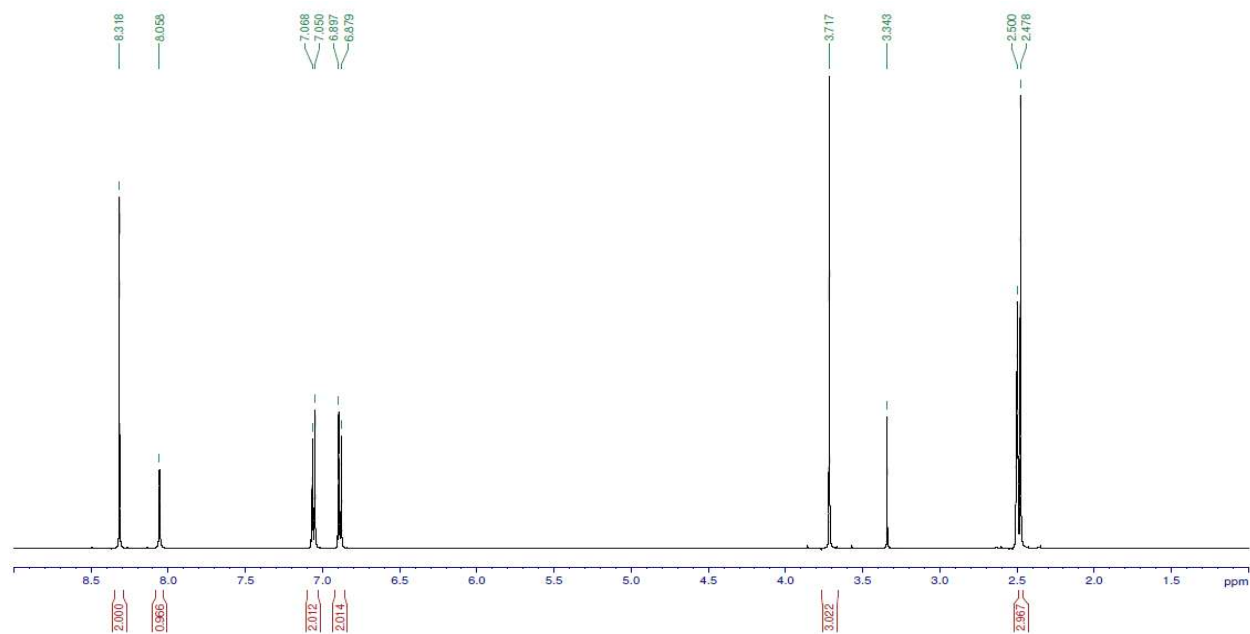


Figure S10. <sup>1</sup>H-NMR spectrum of **11b** measured at 500 MHz in DMSO-d<sub>6</sub>

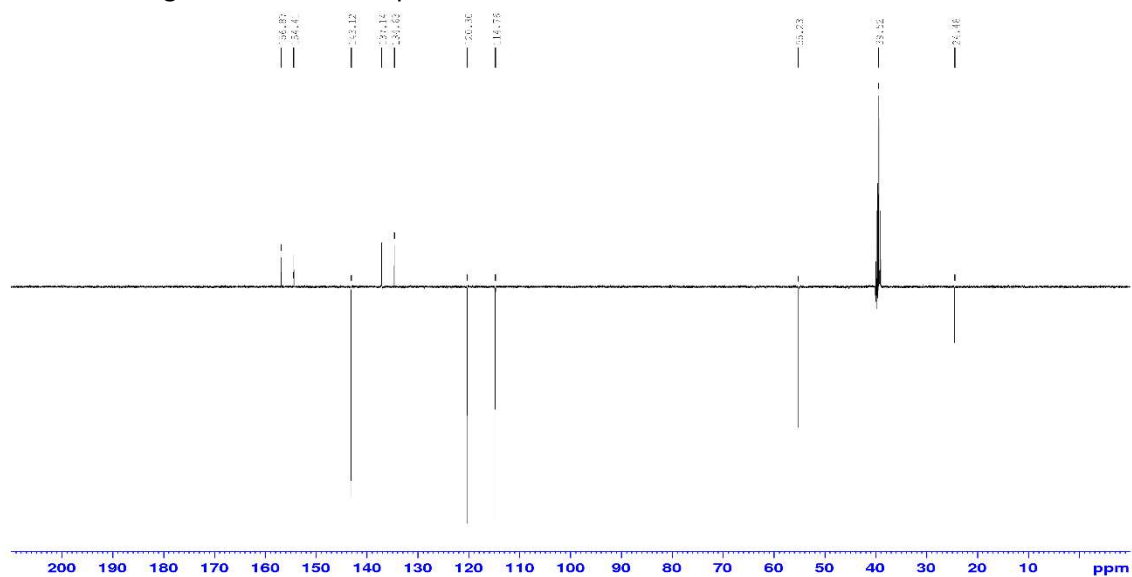


Figure S11. DEPT spectrum of **11b** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

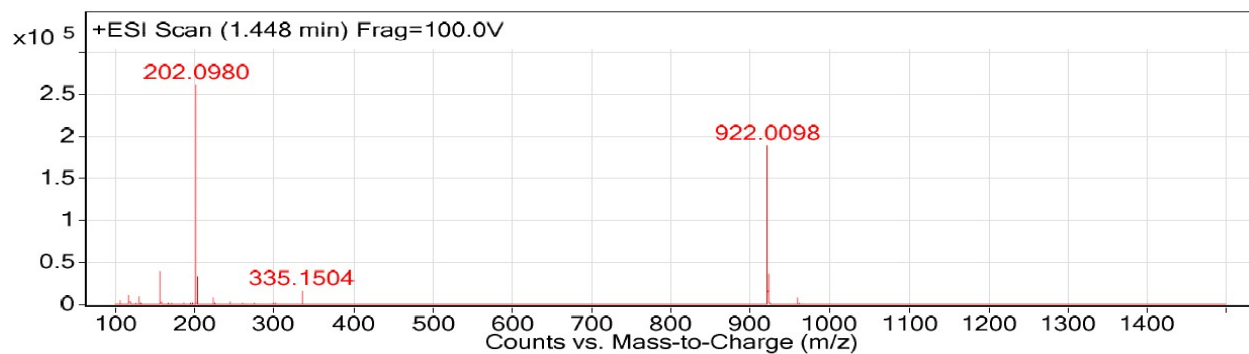


Figure S12. HRMS spectrum of **11c**

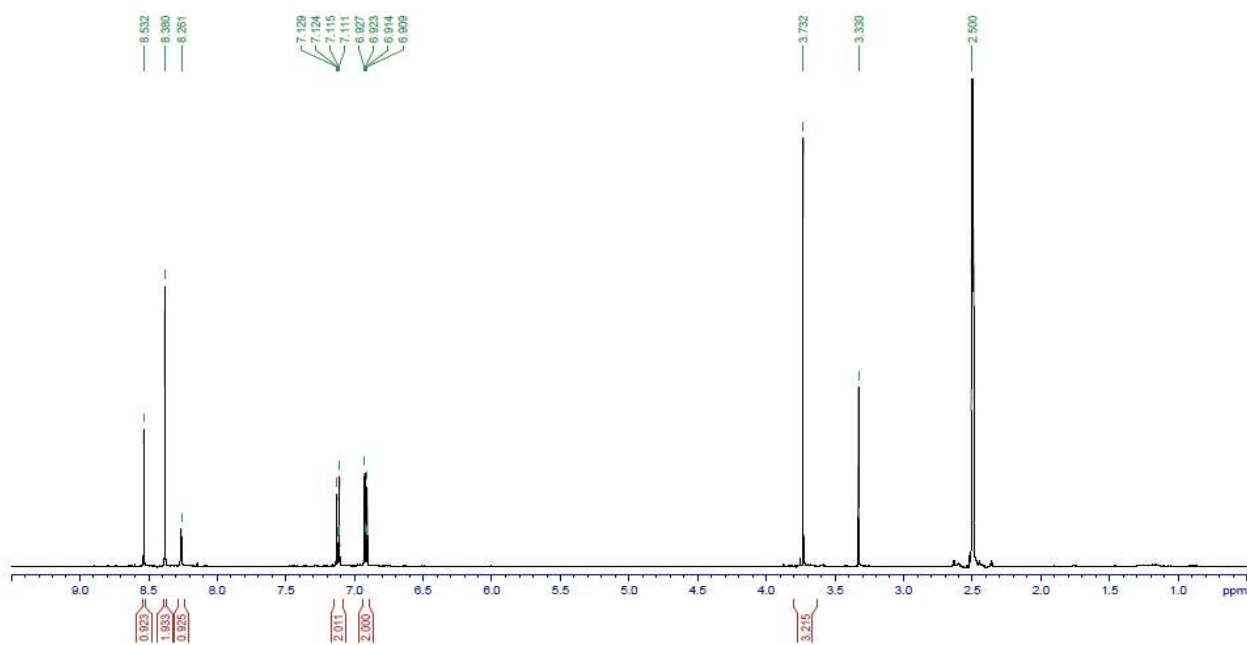


Figure S13.  $^1\text{H-NMR}$  spectrum of **11c** measured at 500 MHz in  $\text{DMSO-d}_6$

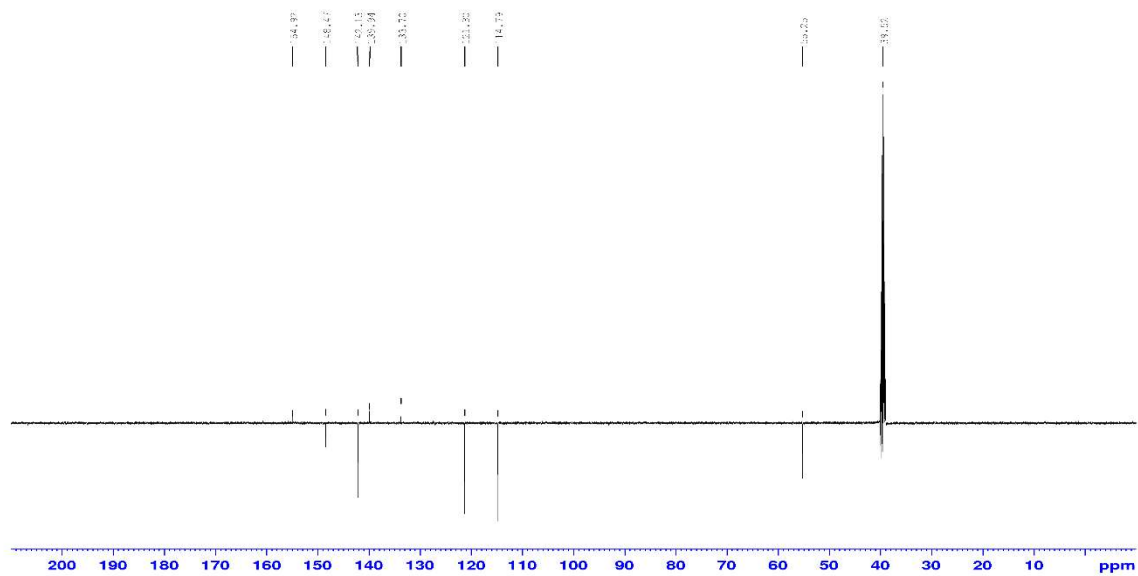


Figure S14. DEPT spectrum of **11c** measured at 125 MHz in  $\text{DMSO-d}_6$

# NMR and HRMS Spectra of Selected Synthesized Compounds

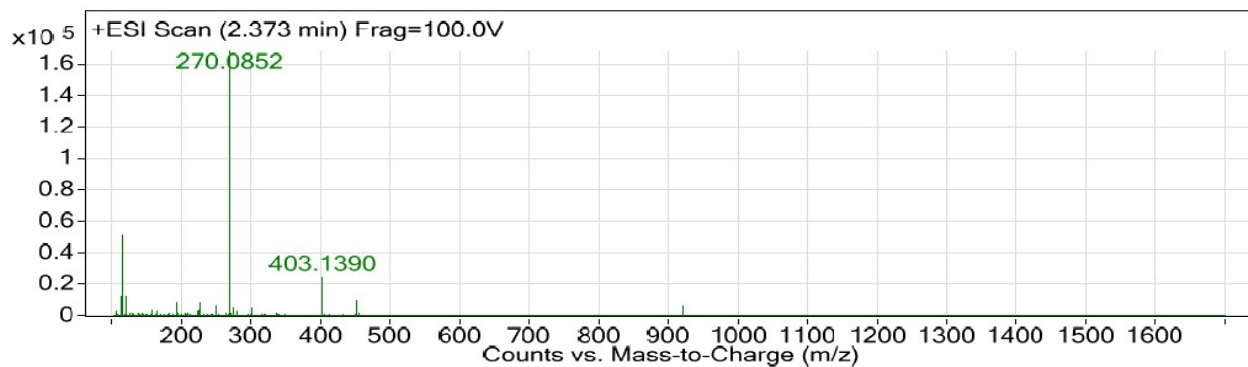


Figure S15. HRMS spectrum of **11d**

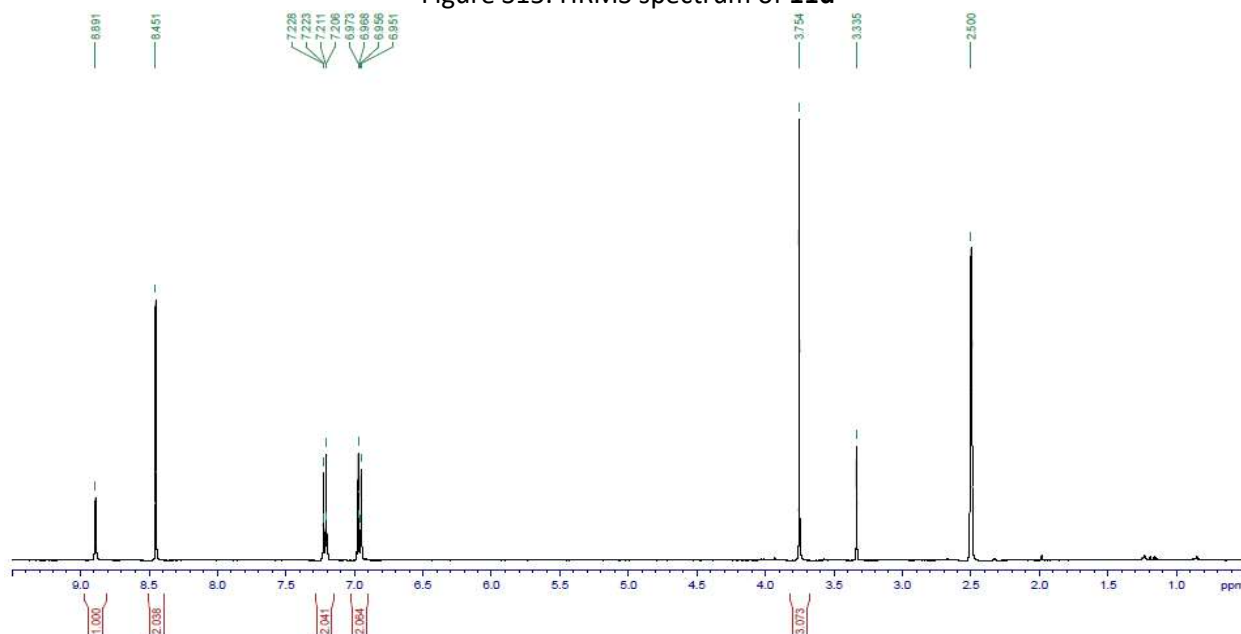


Figure S16.  $^1\text{H-NMR}$  spectrum of **11d** measured at 500 MHz in DMSO-d<sub>6</sub>

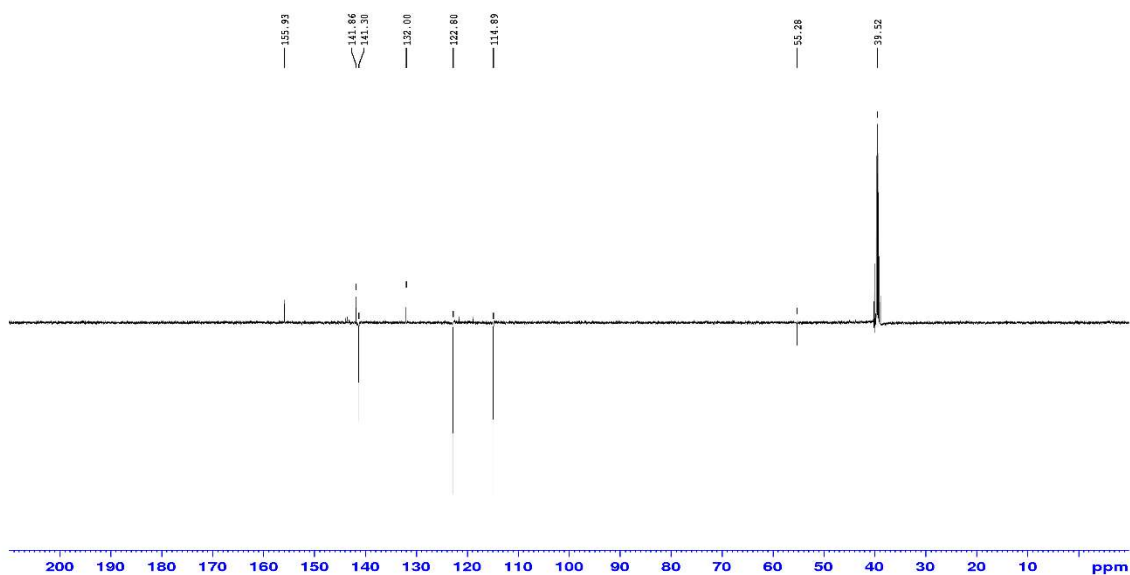


Figure S17. DEPT spectrum of **11d** measured at 100 MHz in DMSO-d<sub>6</sub>



# NMR and HRMS Spectra of Selected Synthesized Compounds

Event#: 1 MS(E+) Ret. Time : 3.462 Scan# : 603

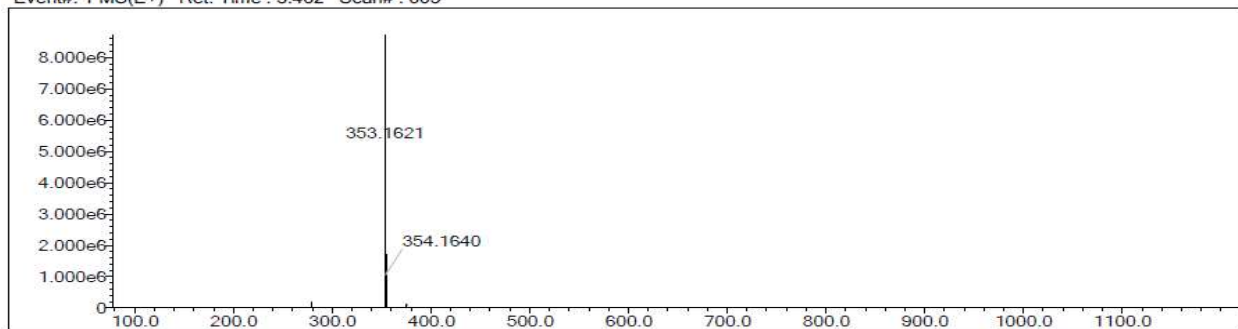


Figure S18. HRMS spectrum of **13a**

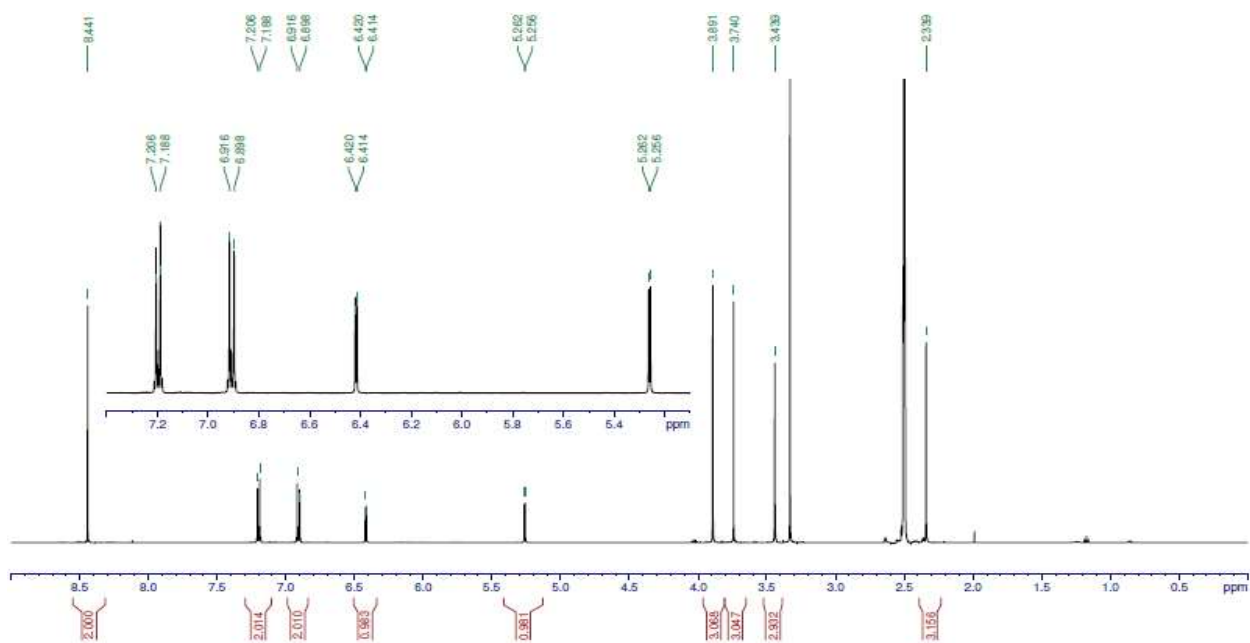


Figure S19.  $^1\text{H-NMR}$  spectrum of **13a** measured at 500 MHz in DMSO- $d_6$

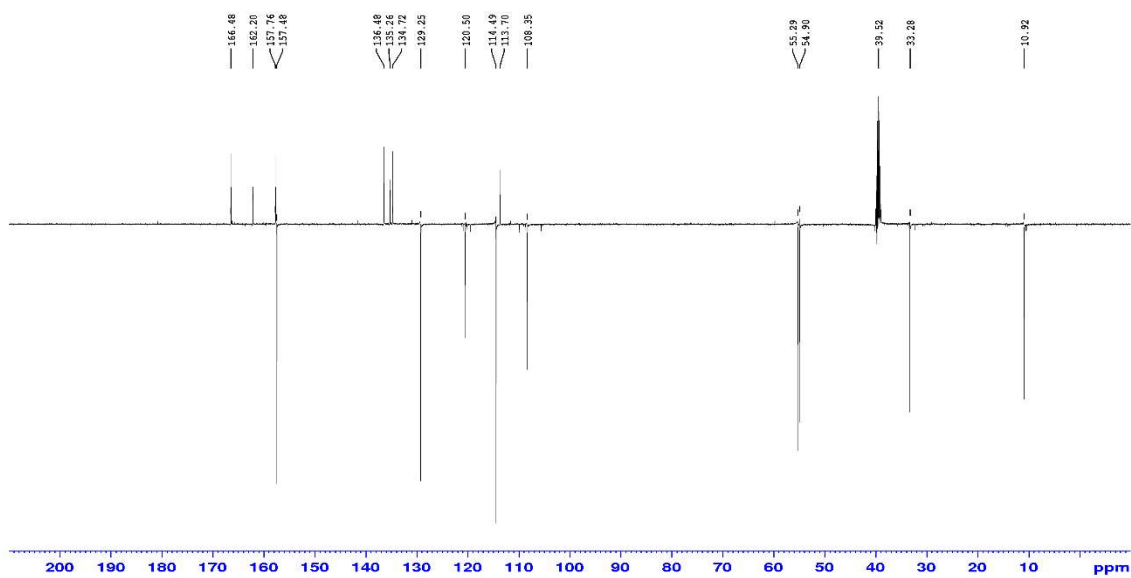


Figure S20. DEPT spectrum of **13a** measured at 125 MHz in DMSO- $d_6$

# NMR and HRMS Spectra of Selected Synthesized Compounds

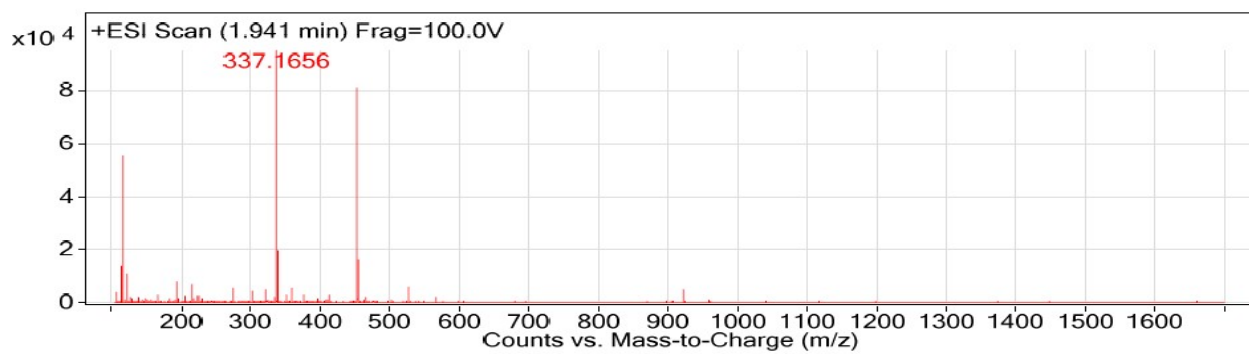


Figure S21. HRMS spectrum of **13b**

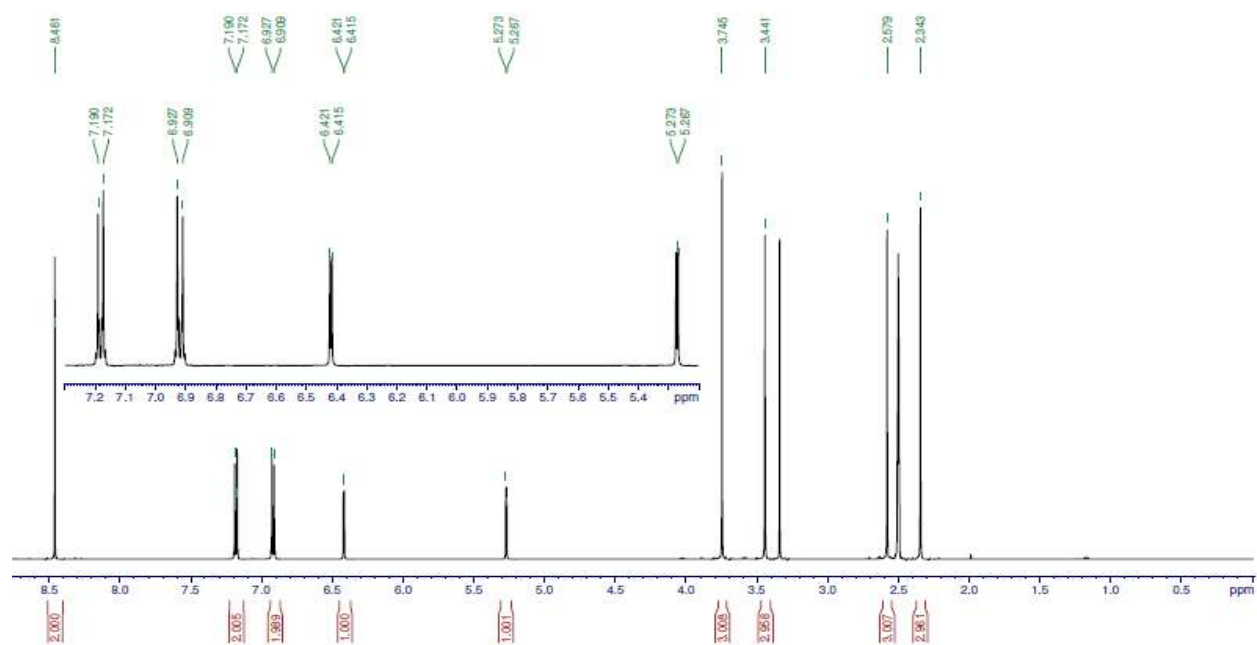


Figure S22.  $^1\text{H-NMR}$  spectrum of **13b** measured at 500 MHz in  $\text{DMSO-d}_6$

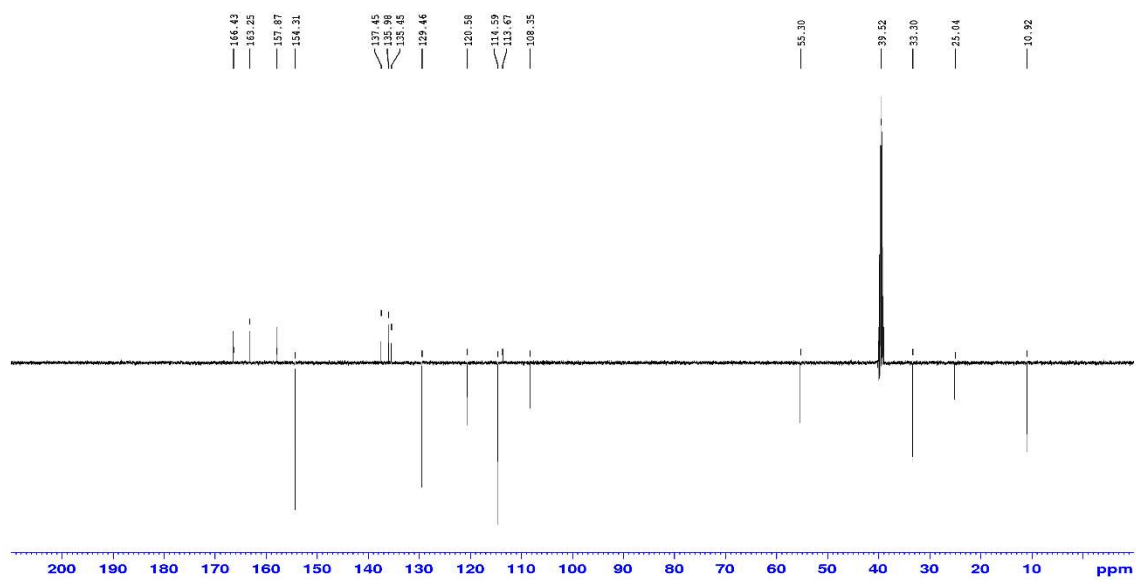


Figure S23. DEPT spectrum of **13b** measured at 125 MHz in  $\text{DMSO-d}_6$

# NMR and HRMS Spectra of Selected Synthesized Compounds

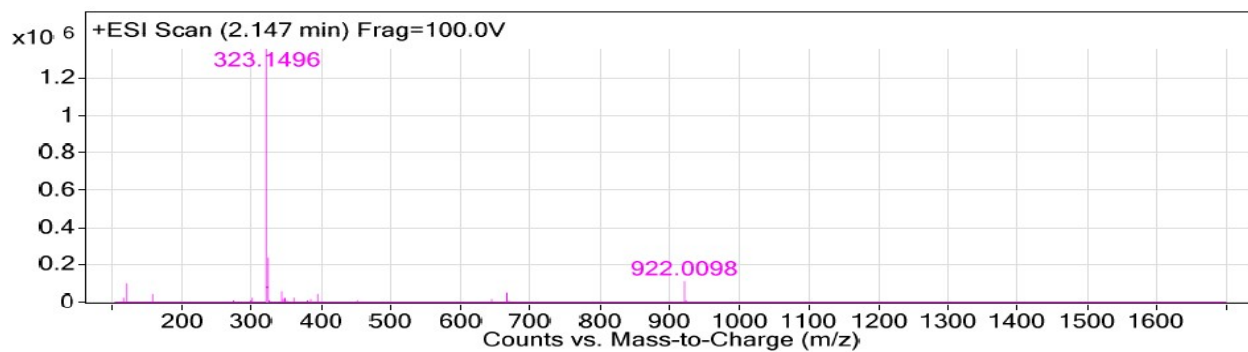


Figure S24. HRMS spectrum of **13c**

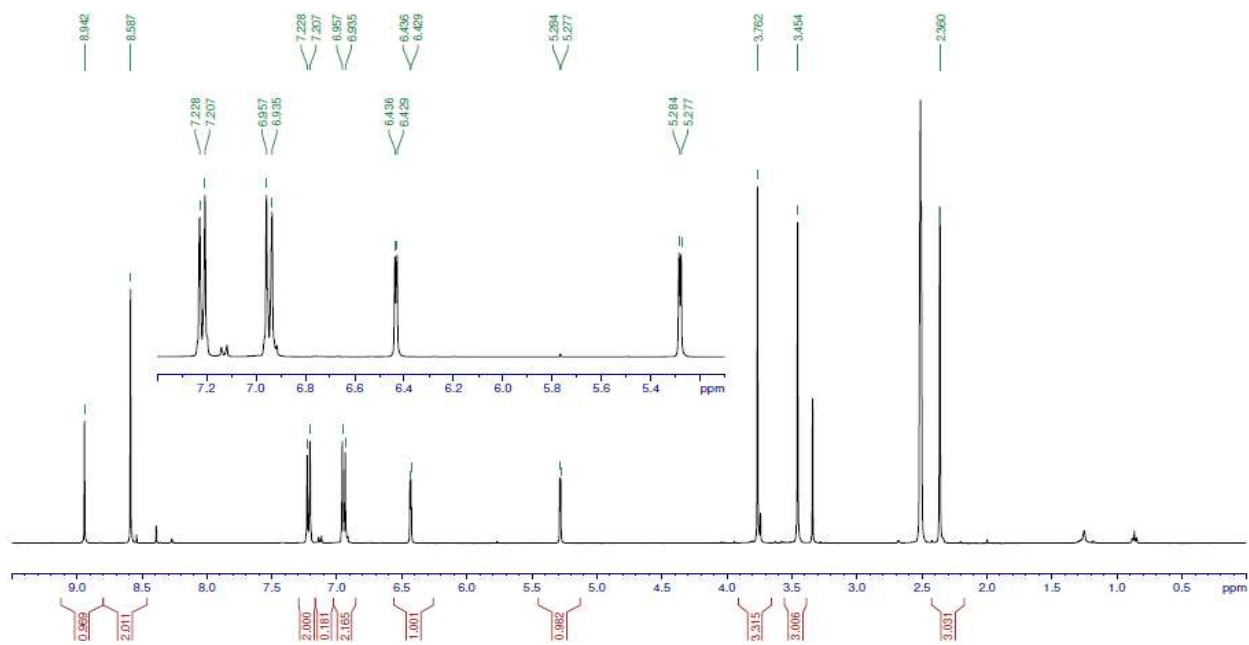


Figure S25.  $^1\text{H-NMR}$  spectrum of **13c** measured at 500 MHz in  $\text{DMSO-d}_6$

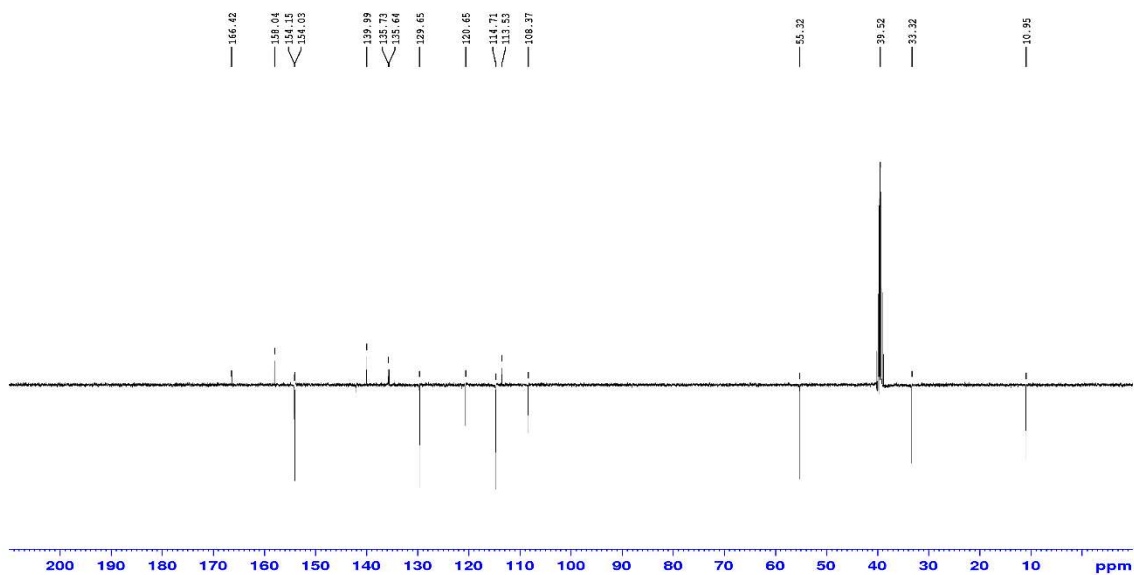


Figure S26. DEPT spectrum of **13c** measured at 100 MHz in  $\text{DMSO-d}_6$

# NMR and HRMS Spectra of Selected Synthesized Compounds

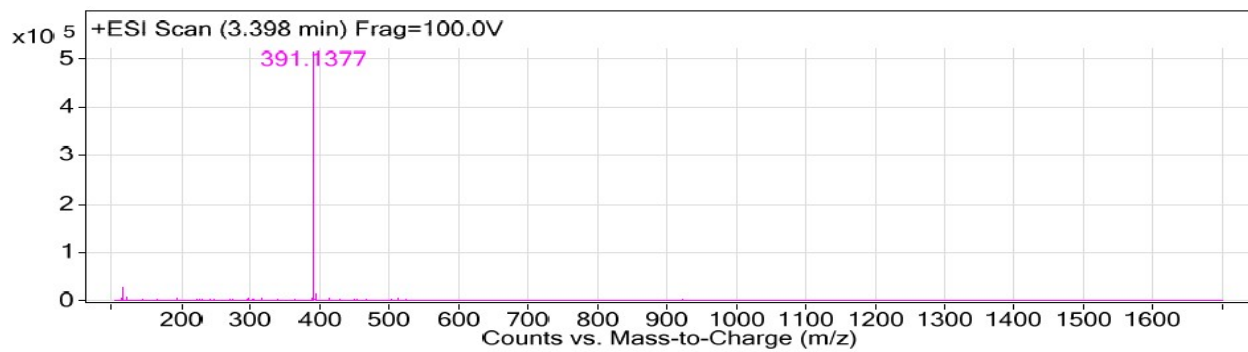


Figure S27. HRMS spectrum of **13d**

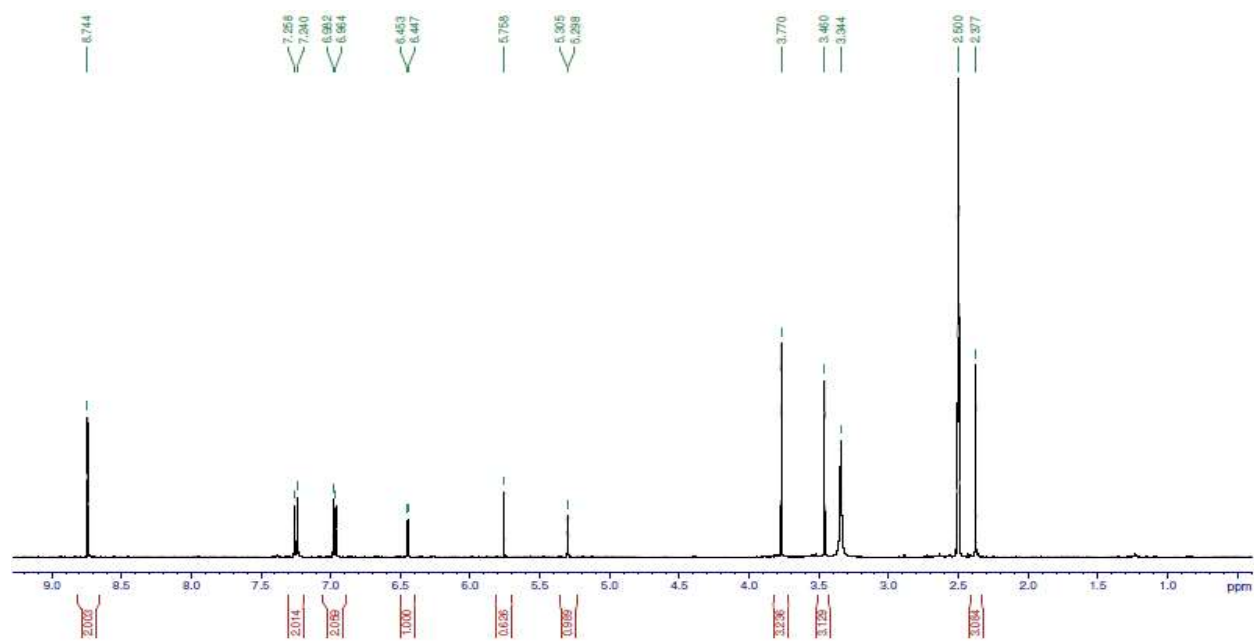


Figure S28. <sup>1</sup>H-NMR spectrum of **13d** measured at 500 MHz in DMSO-d<sub>6</sub>

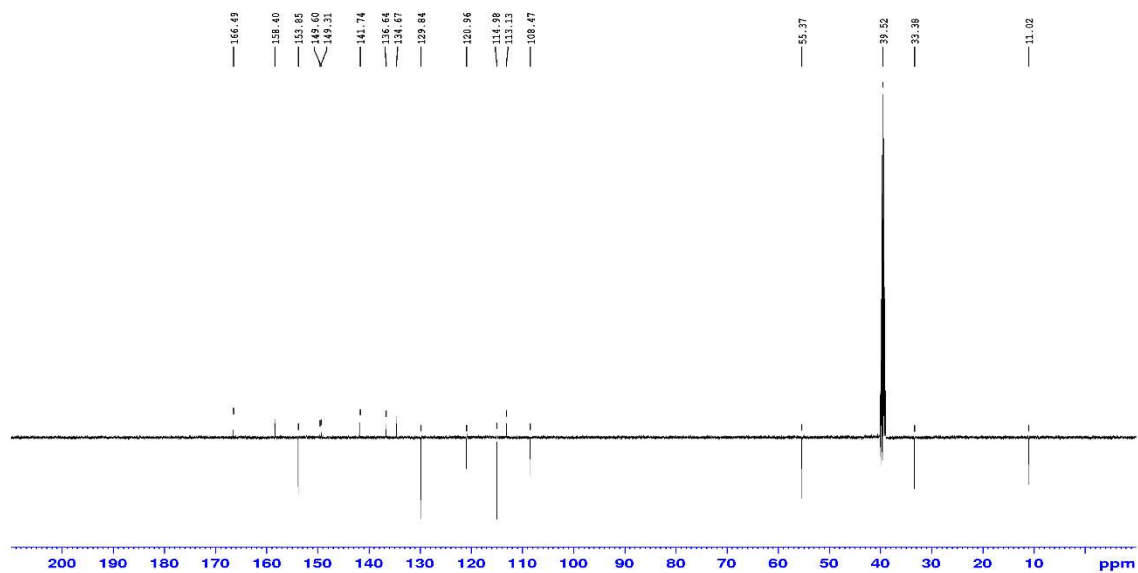


Figure S29. DEPT spectrum of **13d** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

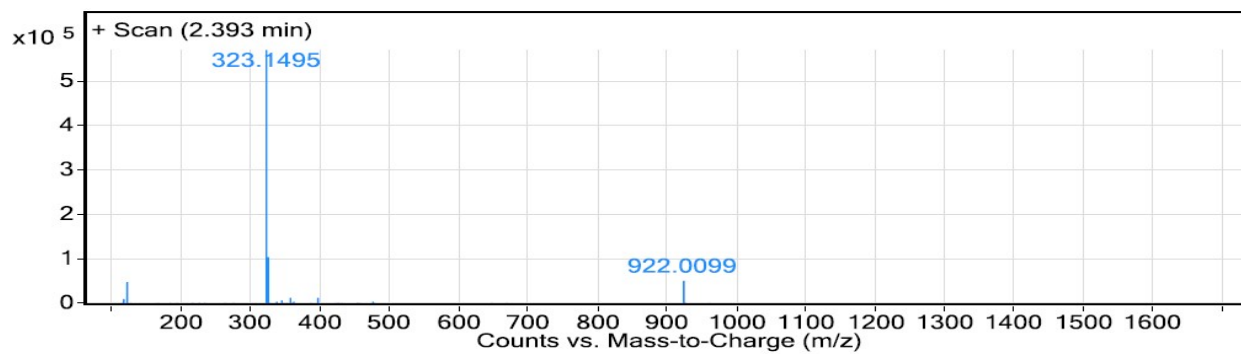


Figure S30. HRMS spectrum of **13e**

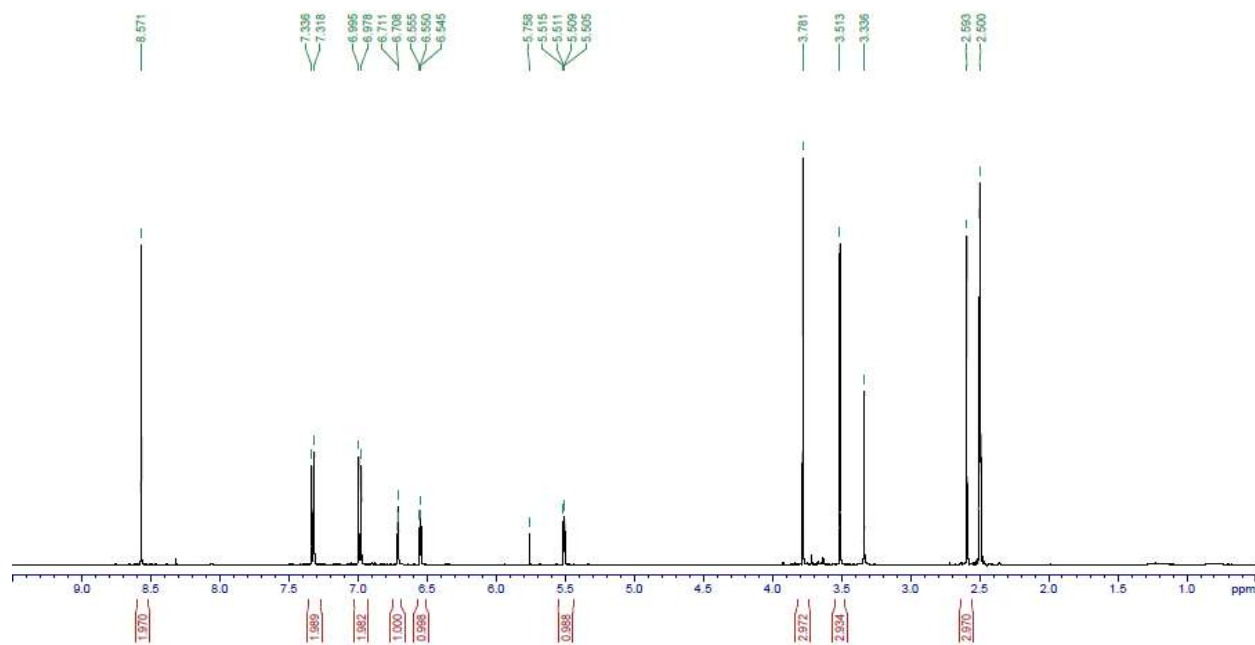


Figure S31.  $^1\text{H}$ -NMR spectrum of **13e** measured at 500 MHz in DMSO- $d_6$

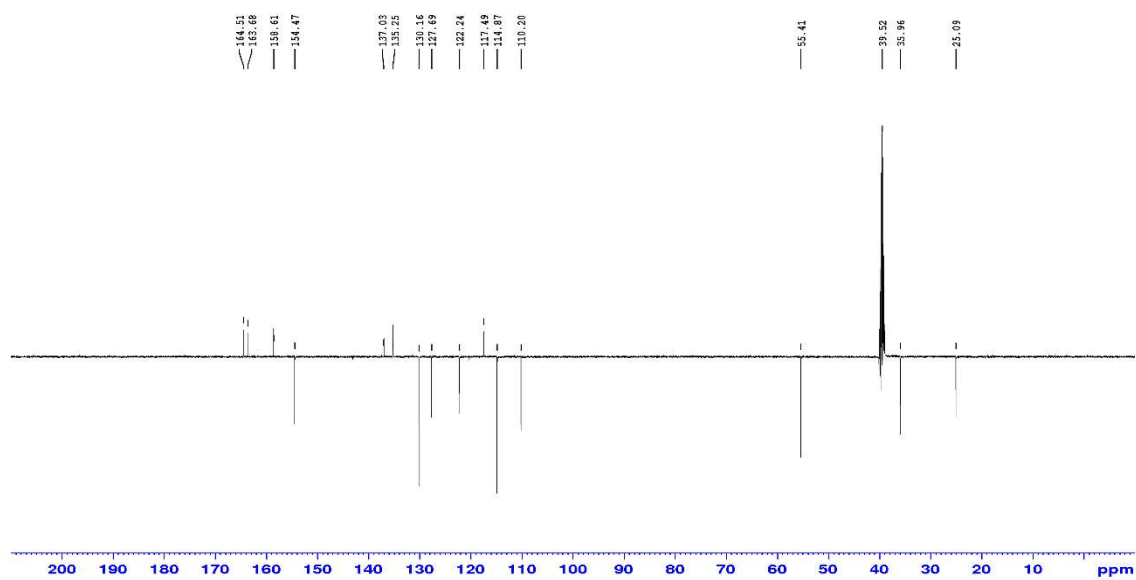


Figure S32. DEPT spectrum of **13e** measured at 125 MHz in DMSO- $d_6$

# NMR and HRMS Spectra of Selected Synthesized Compounds

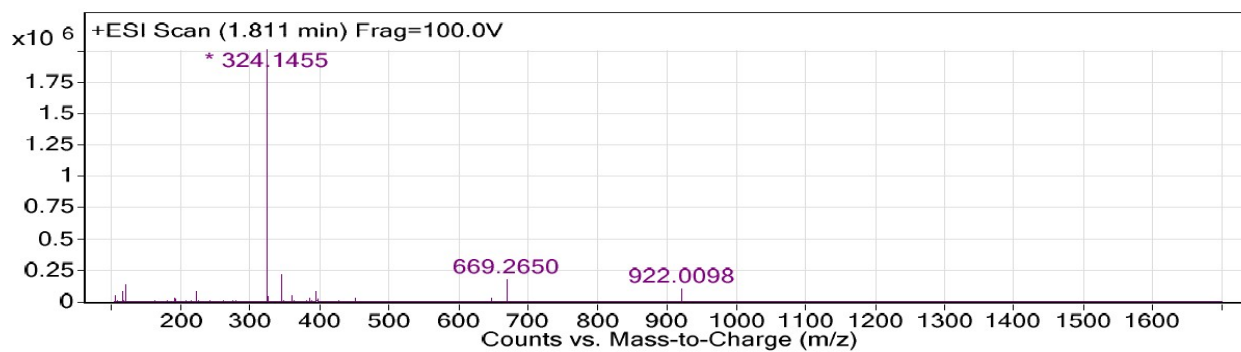


Figure S33. HRMS spectrum of **13f**

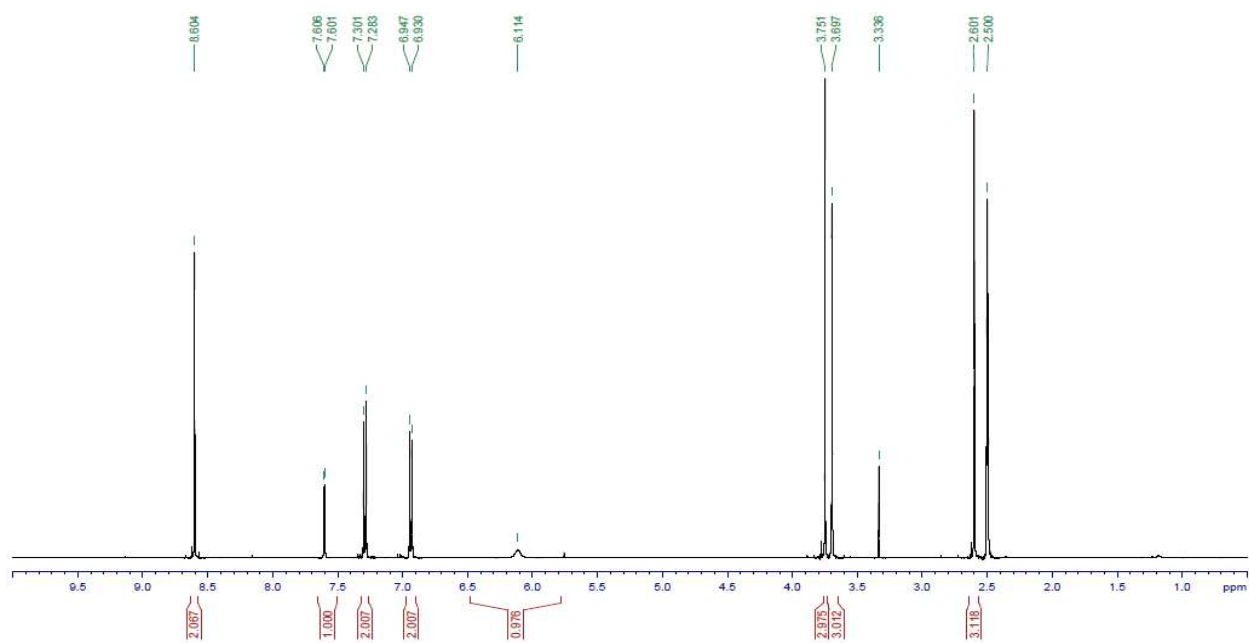


Figure S34.  $^1\text{H-NMR}$  spectrum of **13f** measured at 500 MHz in DMSO-d<sub>6</sub>

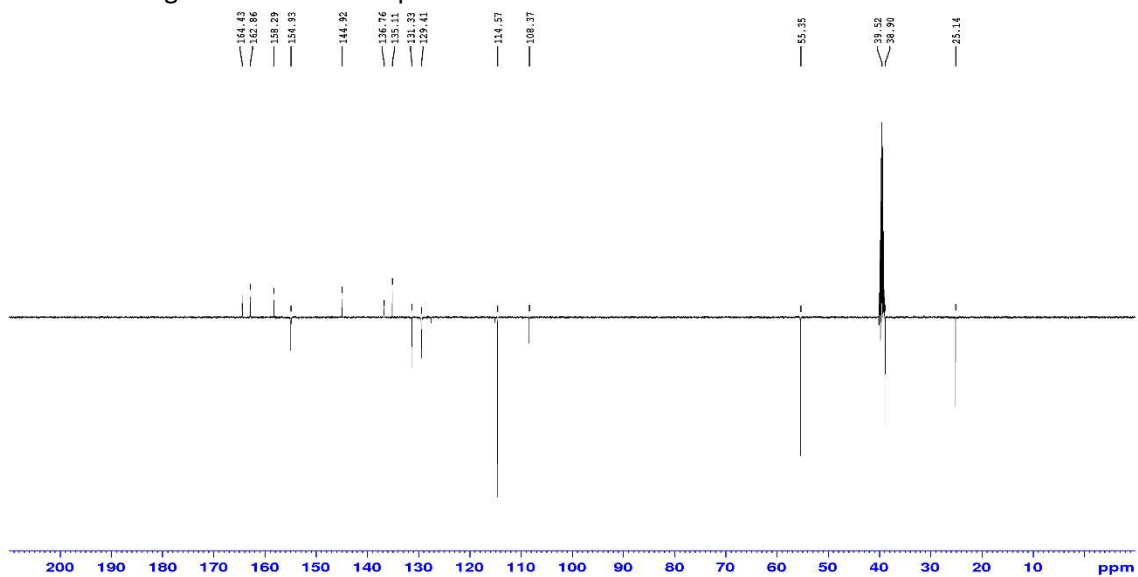


Figure S35. DEPT spectrum of **13f** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

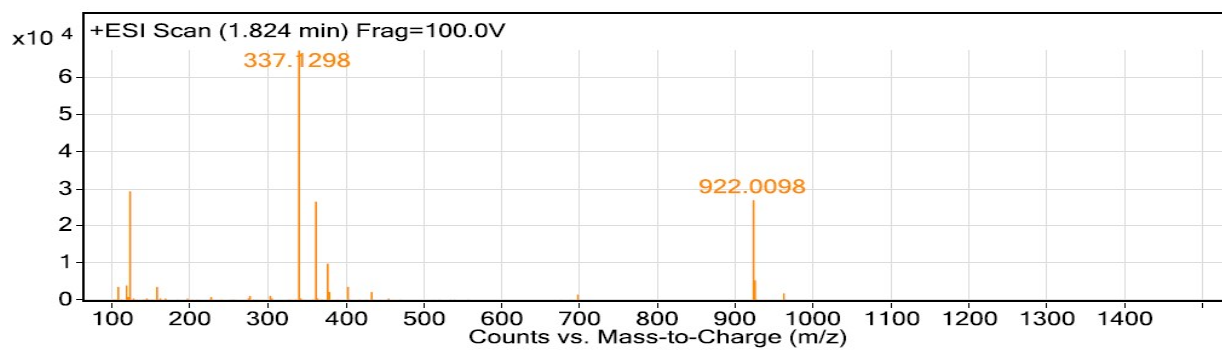


Figure S36. HRMS spectrum of **16**

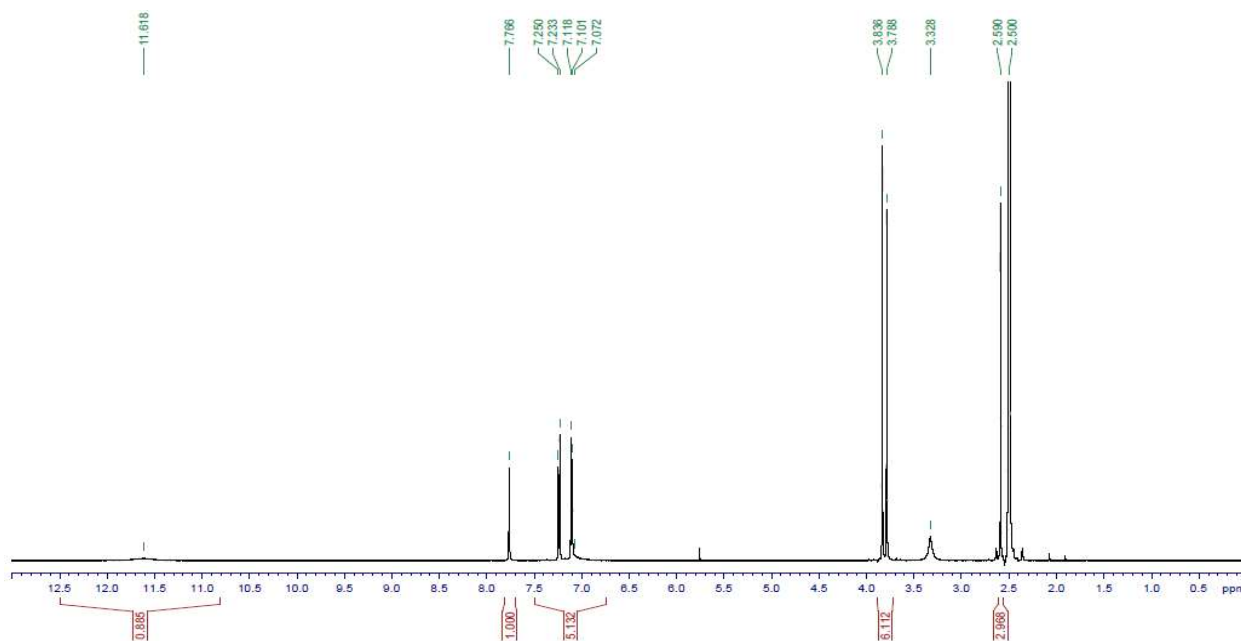


Figure S37. <sup>1</sup>H-NMR spectrum of **16** measured at 500 MHz in DMSO-d<sub>6</sub>

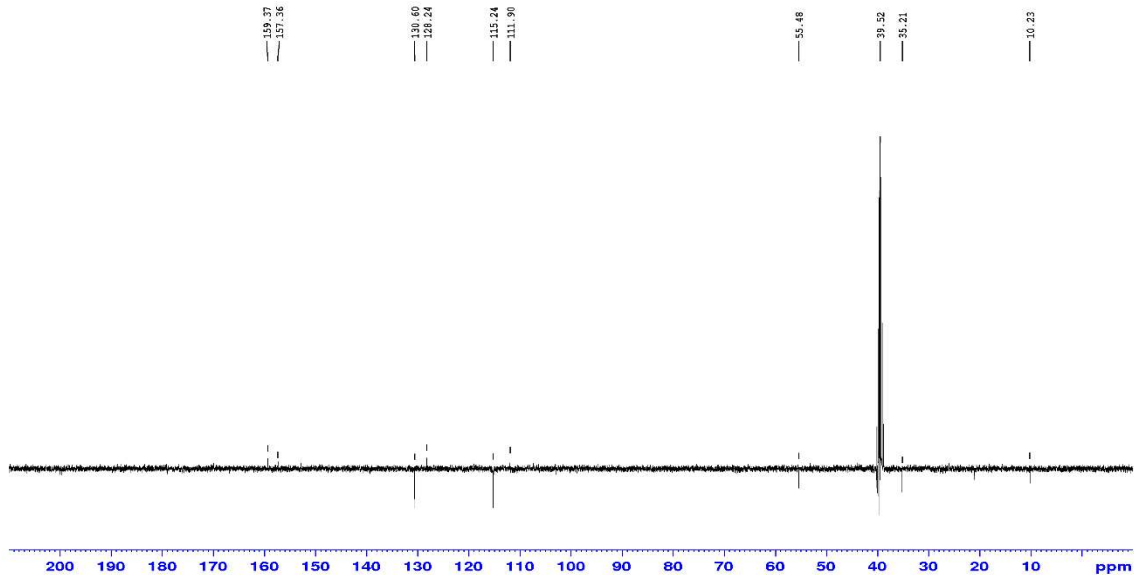


Figure S38. DEPT spectrum of **16** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

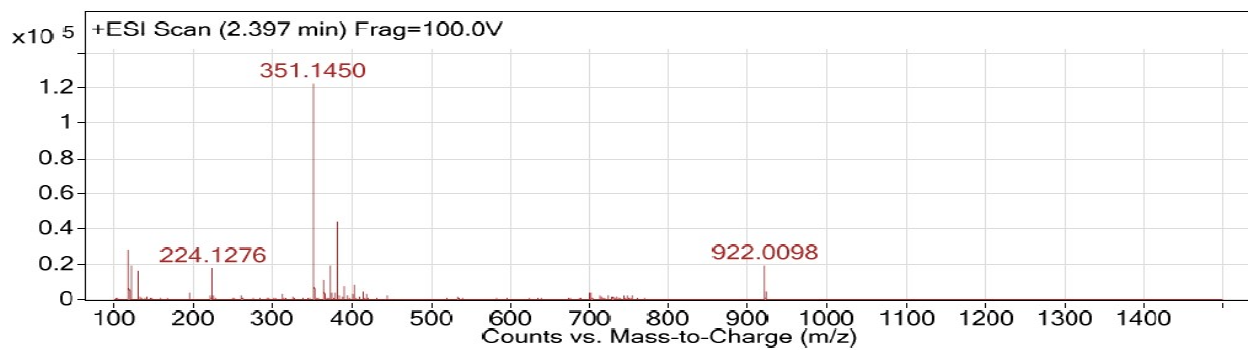


Figure S39. HRMS spectrum of **17a**

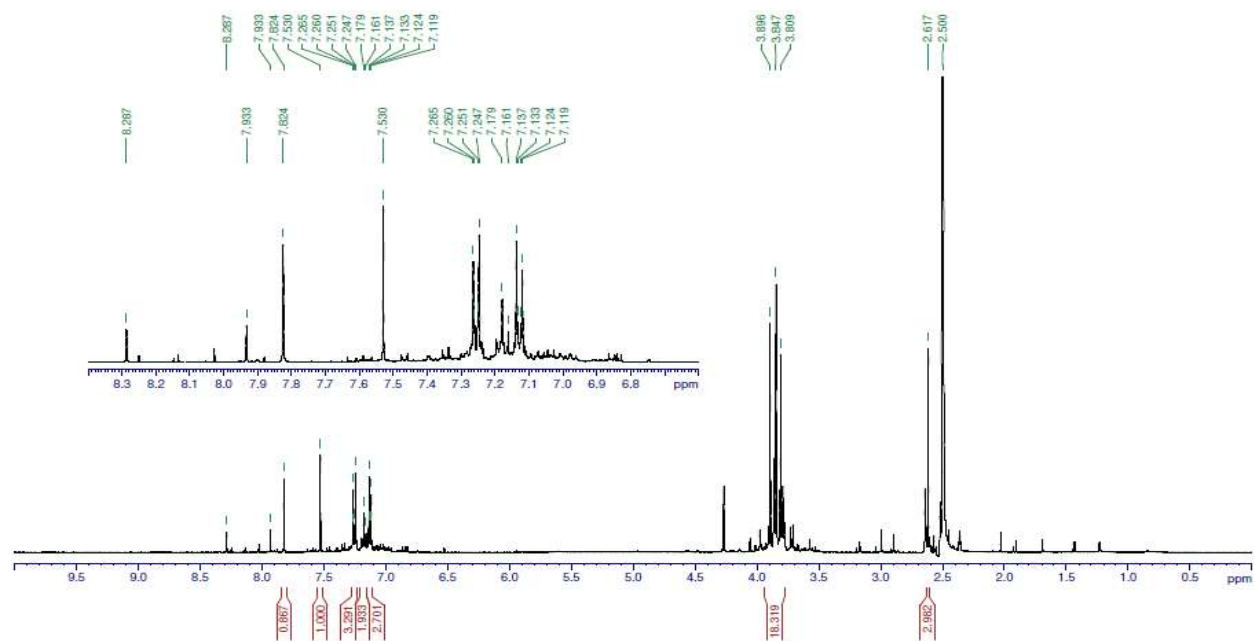


Figure S40. <sup>1</sup>H-NMR spectrum of **17a** measured at 500 MHz in DMSO-d<sub>6</sub>

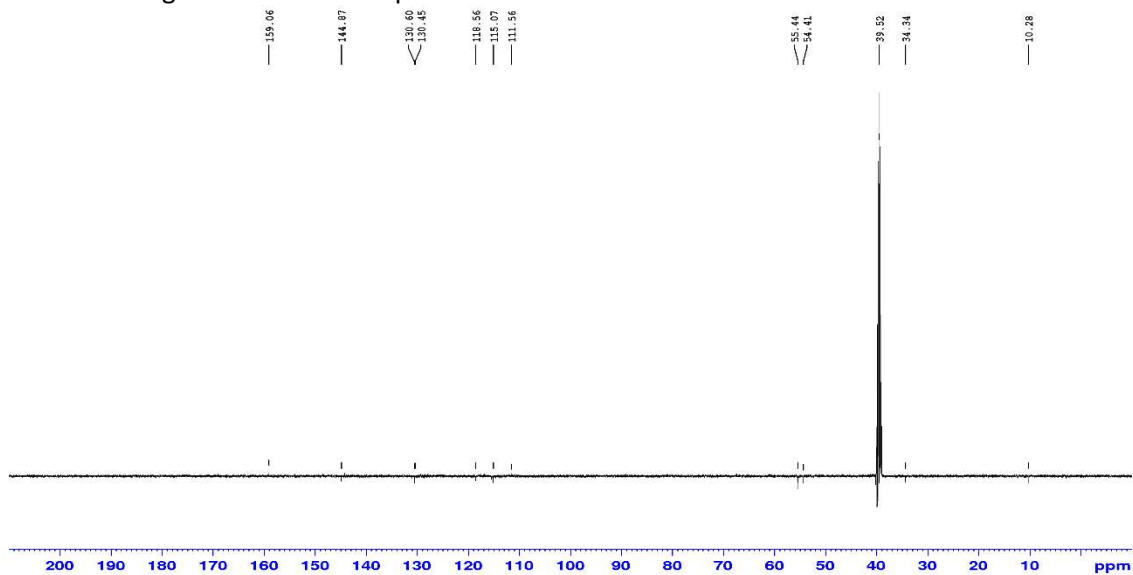


Figure S41. DEPT spectrum of **17a** measured at 125 MHz in DMSO-d<sub>6</sub>



# NMR and HRMS Spectra of Selected Synthesized Compounds

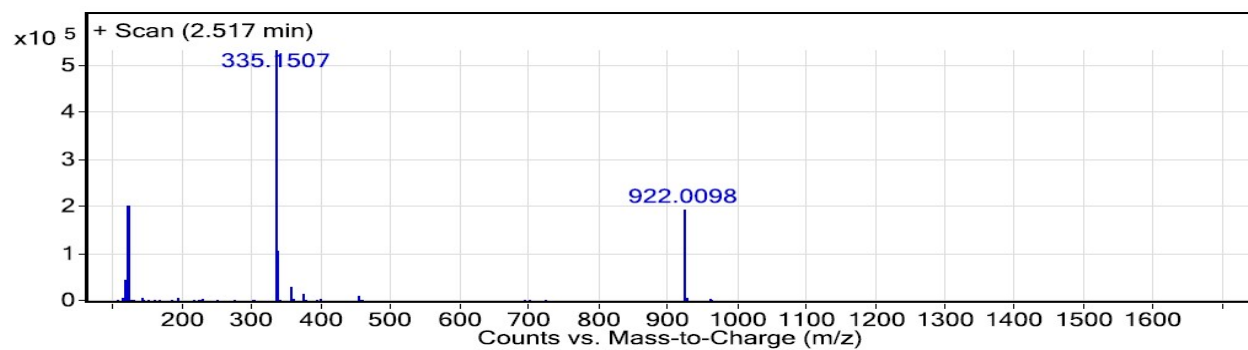


Figure S42. HRMS spectrum of **17b**

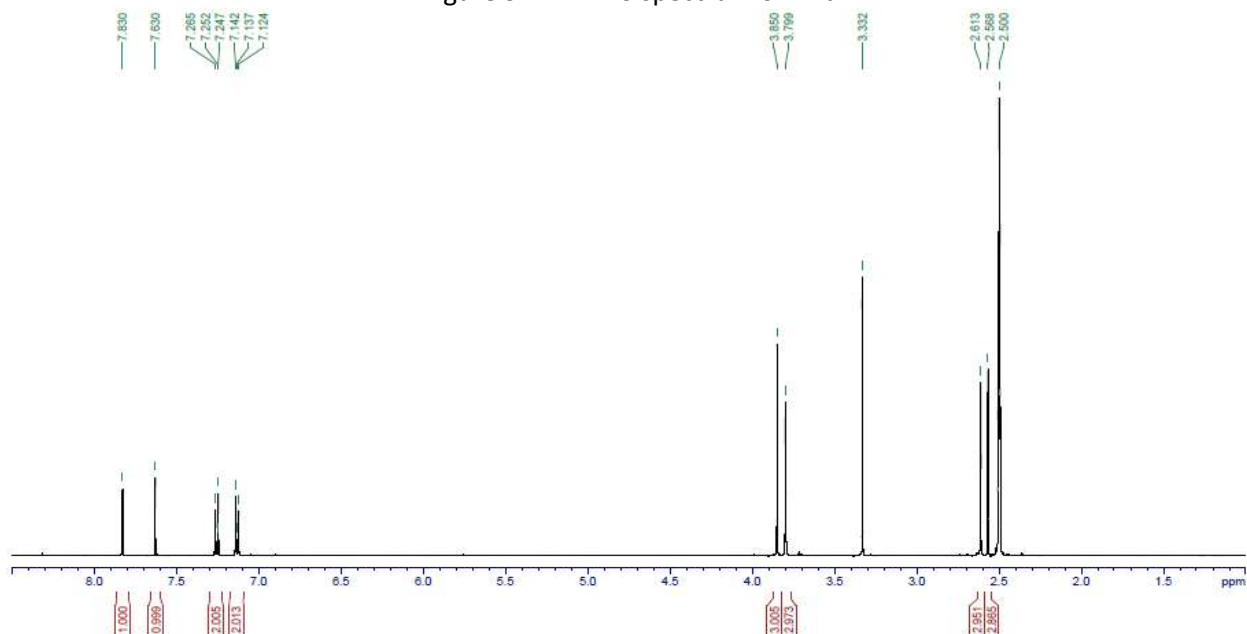


Figure S43. <sup>1</sup>H-NMR spectrum of **17b** measured at 500 MHz in DMSO-d<sub>6</sub>

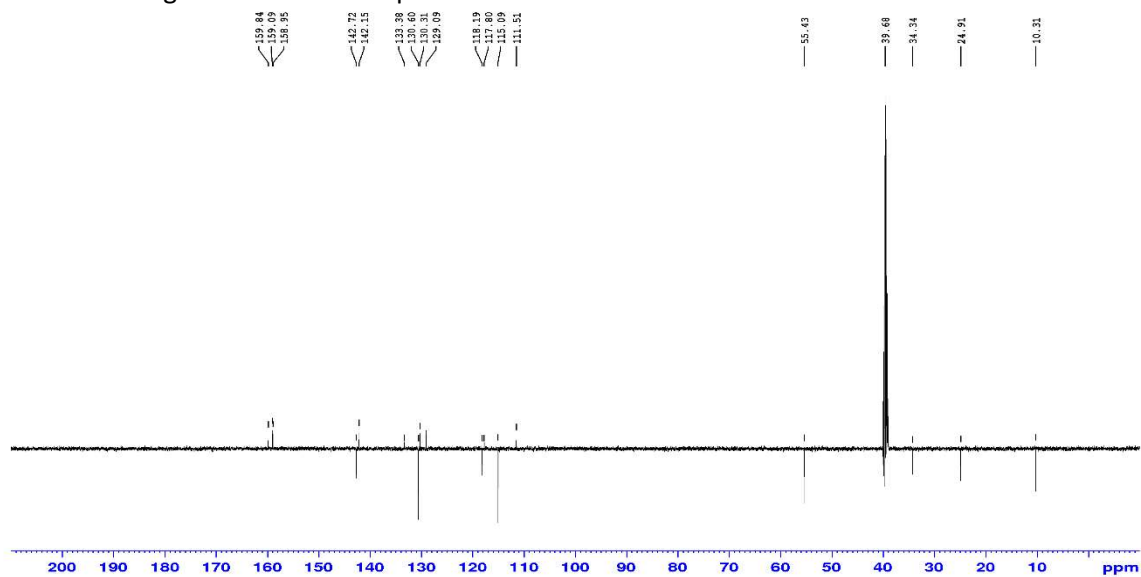


Figure S44. DEPT spectrum of **17b** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

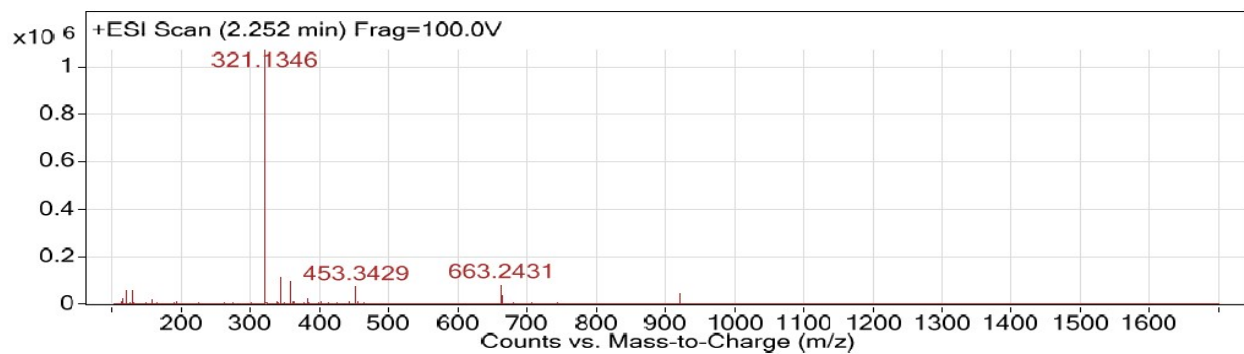


Figure S45. HRMS spectrum of **17c**

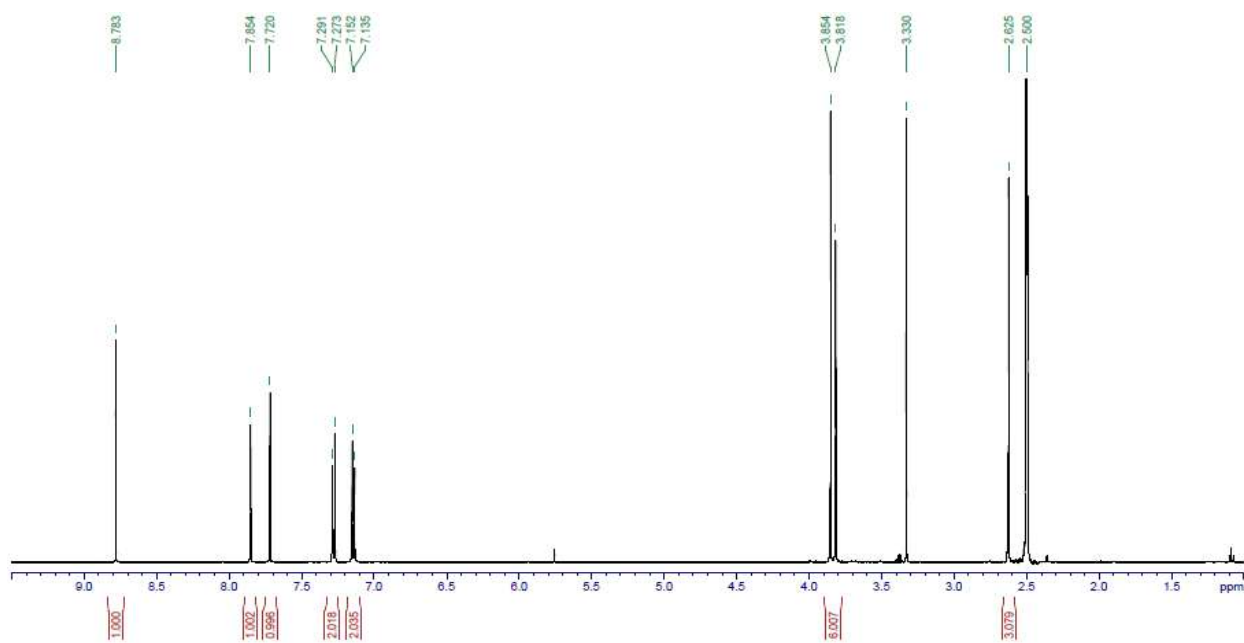


Figure S46. <sup>1</sup>H-NMR spectrum of **17c** measured at 500 MHz in DMSO-d<sub>6</sub>

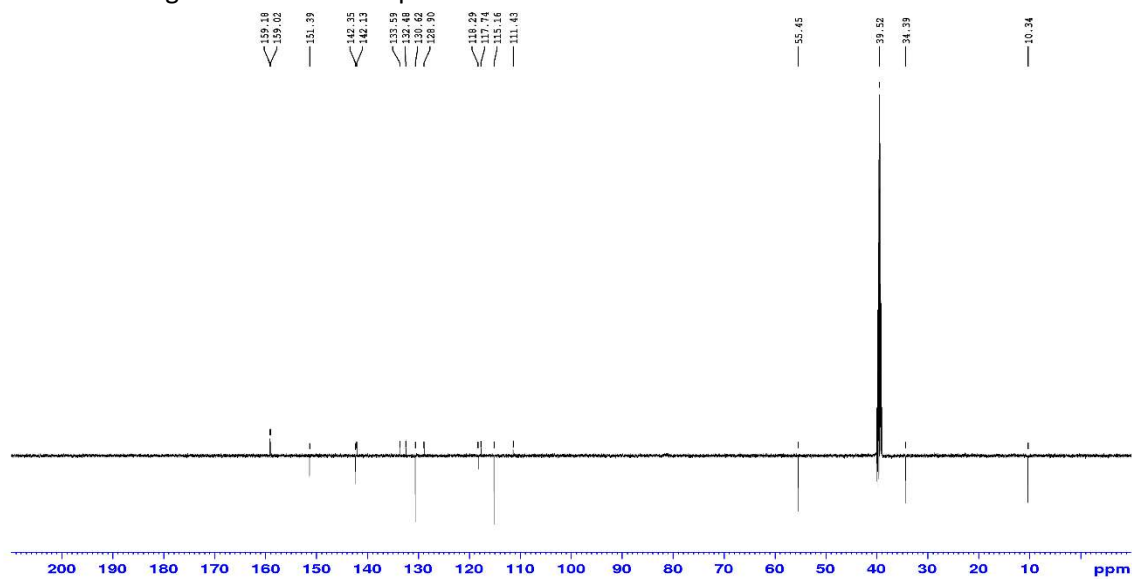


Figure S47. DEPT spectrum of **17c** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

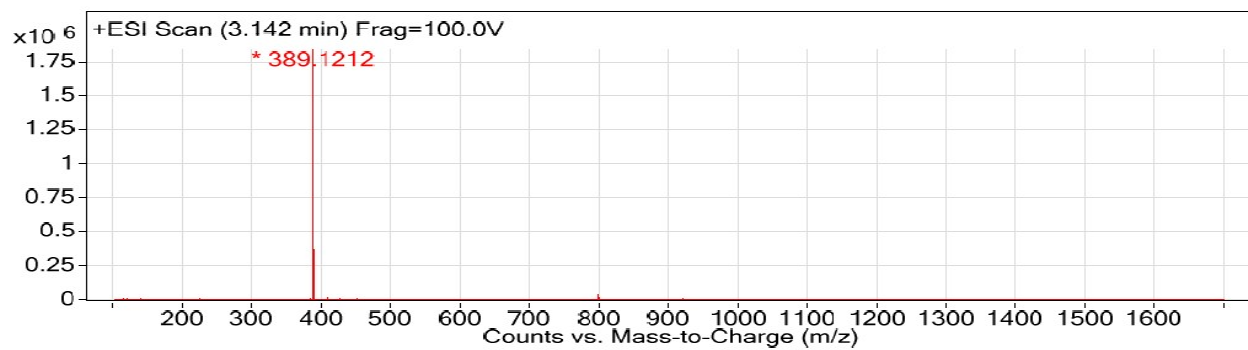


Figure S48. HRMS spectrum of **17d**

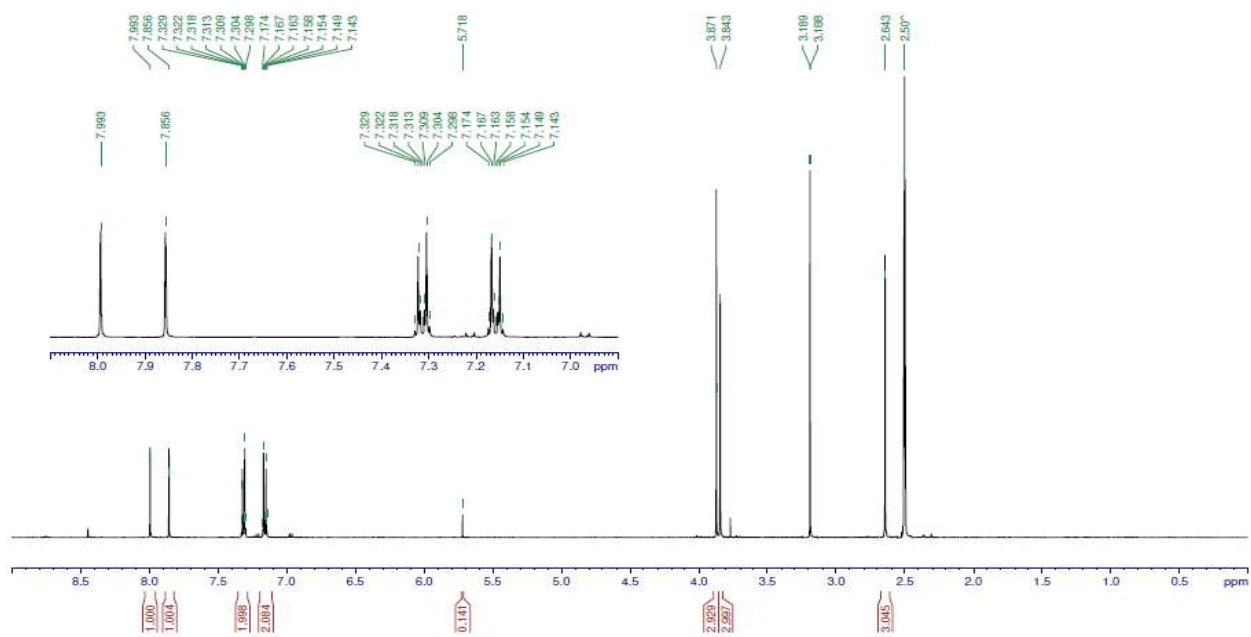


Figure S49. <sup>1</sup>H-NMR spectrum of **17d** measured at 500 MHz in DMSO-d<sub>6</sub>

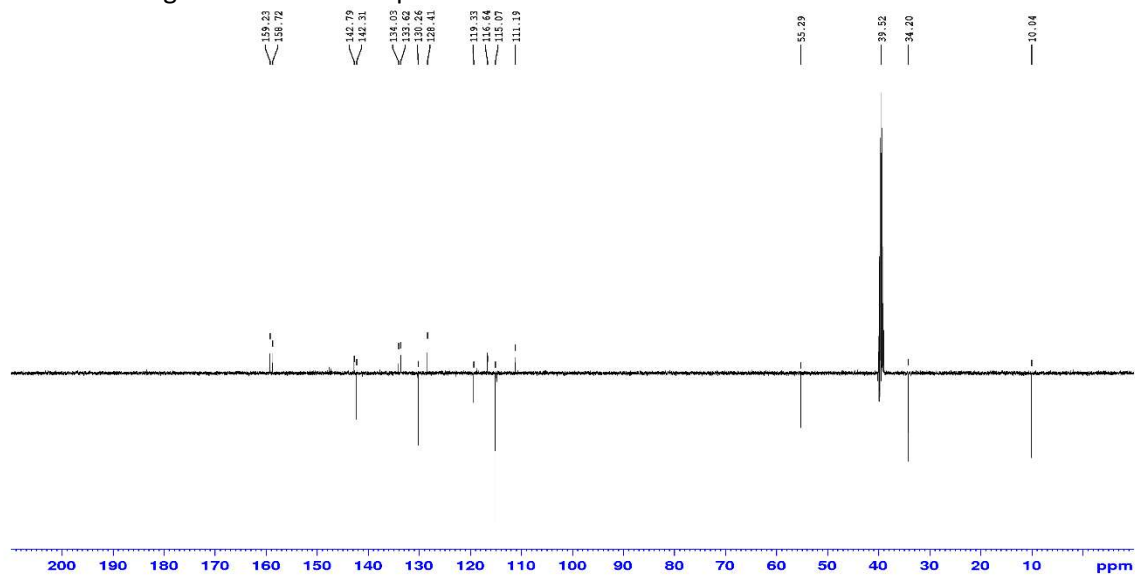


Figure S50. DEPT spectrum of **17d** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

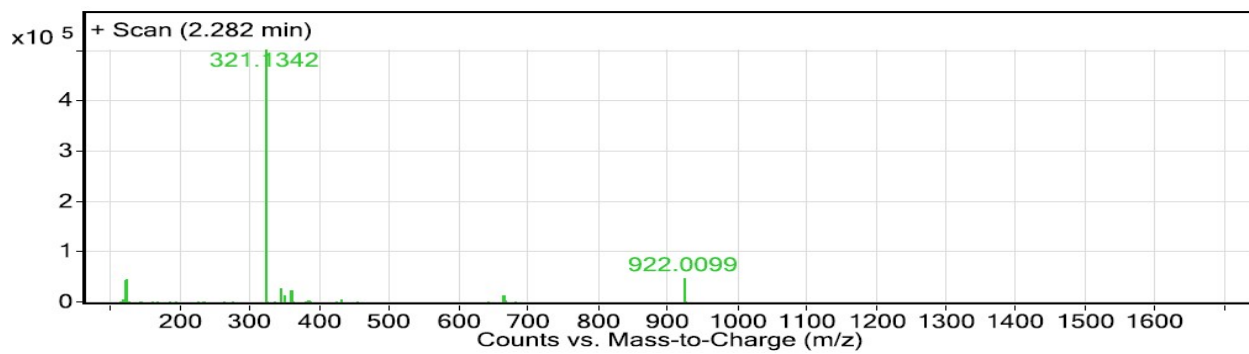


Figure S51. HRMS spectrum of **18**

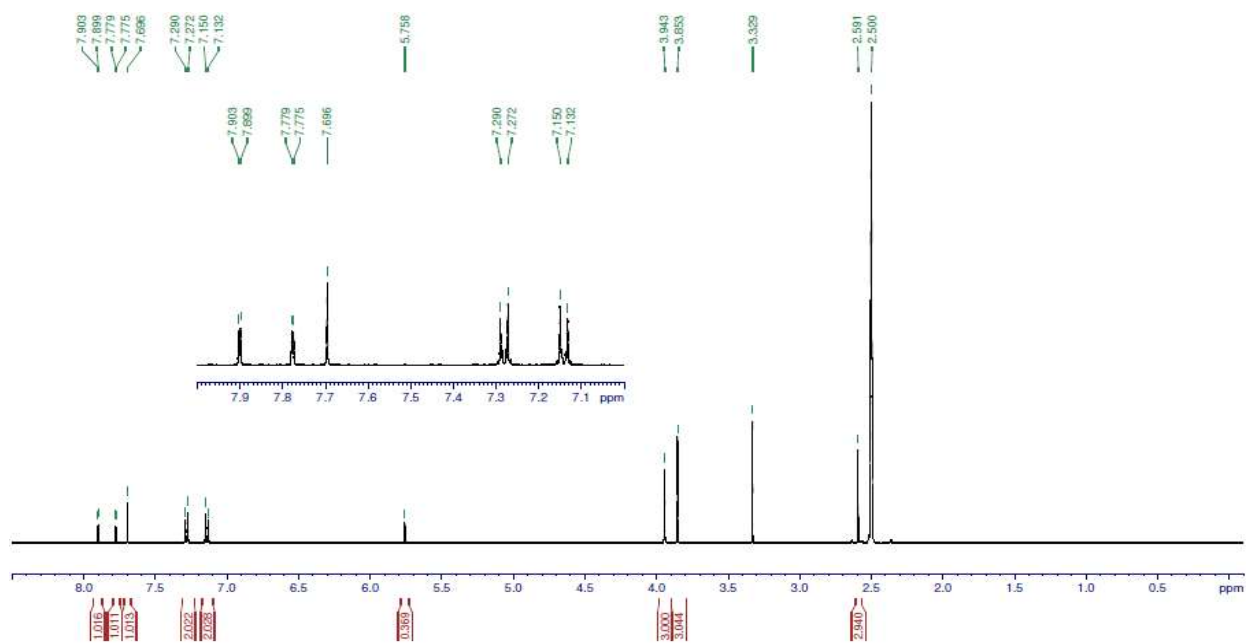


Figure S52. <sup>1</sup>H-NMR spectrum of **18** measured at 500 MHz in DMSO-d<sub>6</sub>

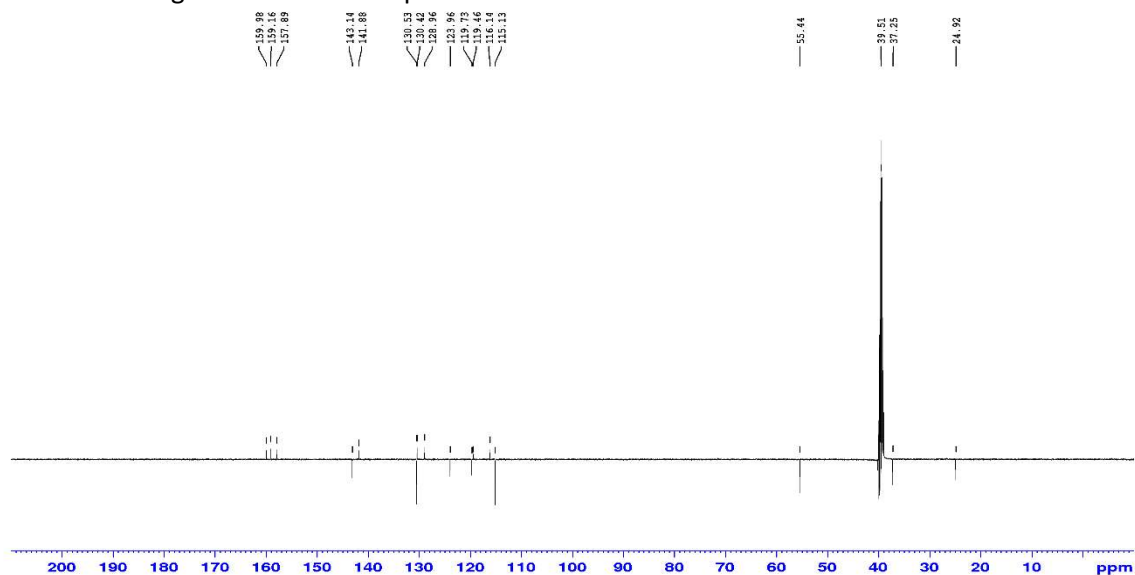


Figure S53. DEPT spectrum of **18** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

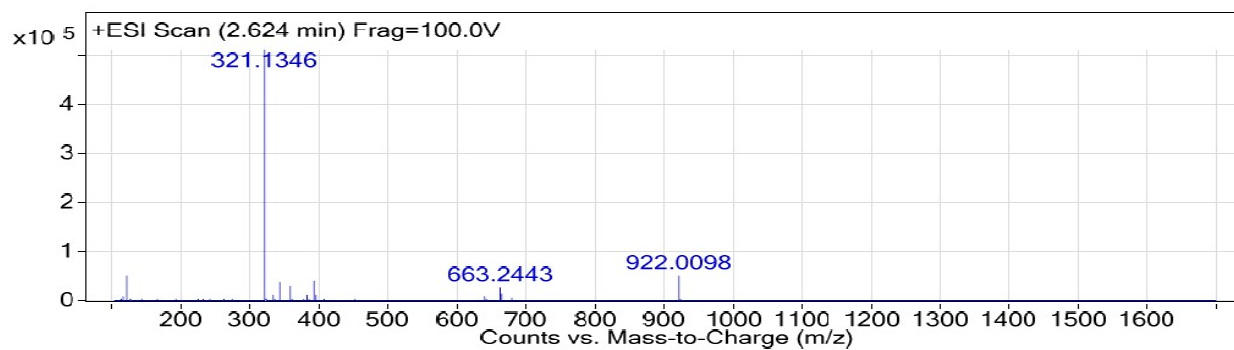


Figure S54. HRMS spectrum of **19**

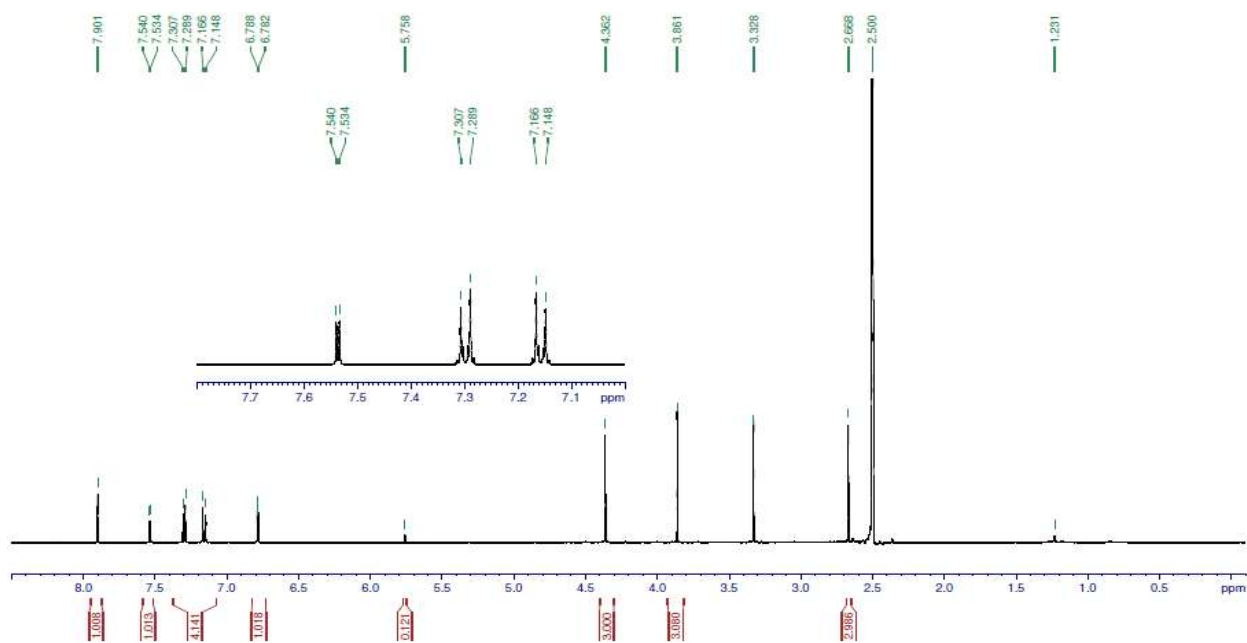


Figure S55. <sup>1</sup>H-NMR spectrum of **19** measured at 500 MHz in DMSO-d<sub>6</sub>

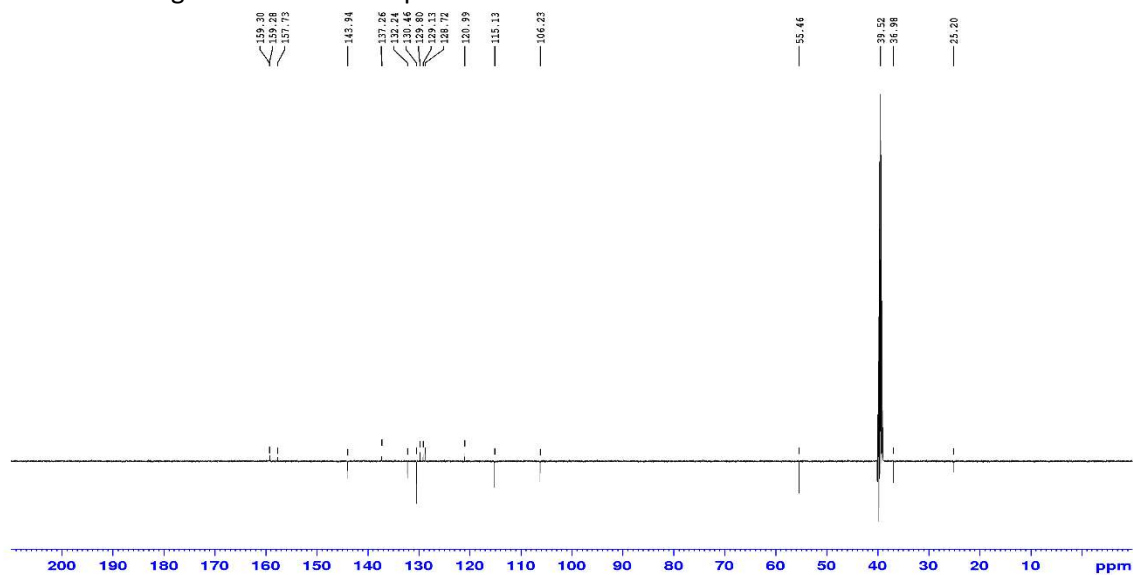


Figure S56. DEPT spectrum of **19** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

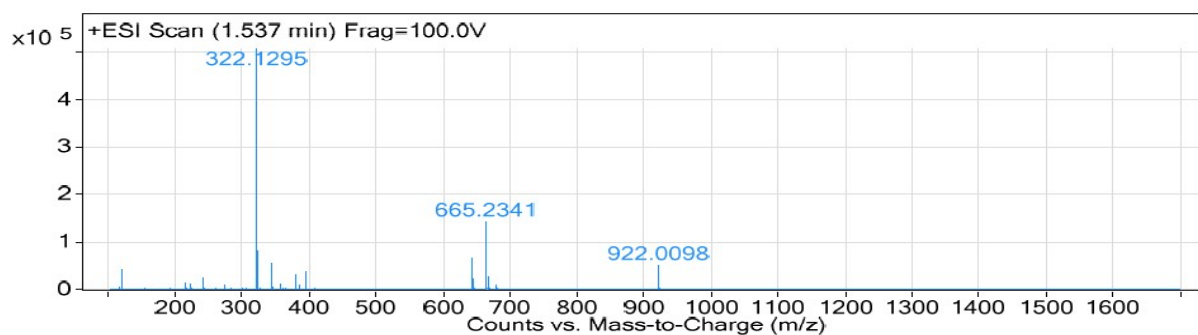


Figure S57. HRMS spectrum of **20**

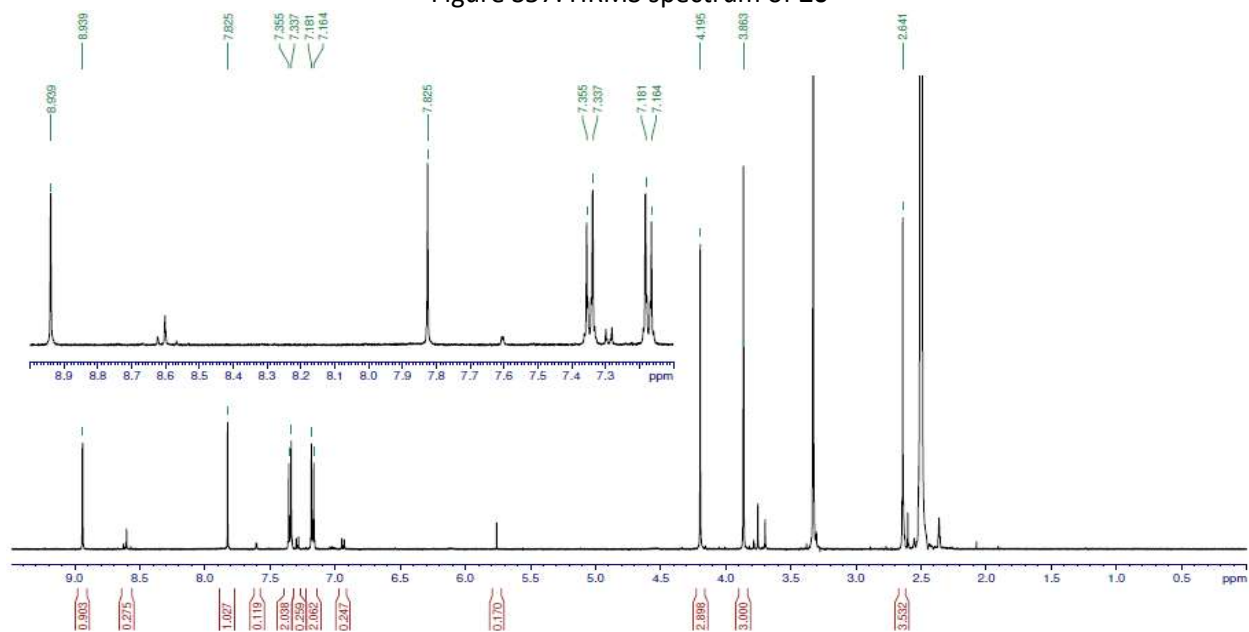


Figure S58. <sup>1</sup>H-NMR spectrum of **20** measured at 500 MHz in DMSO-d<sub>6</sub>

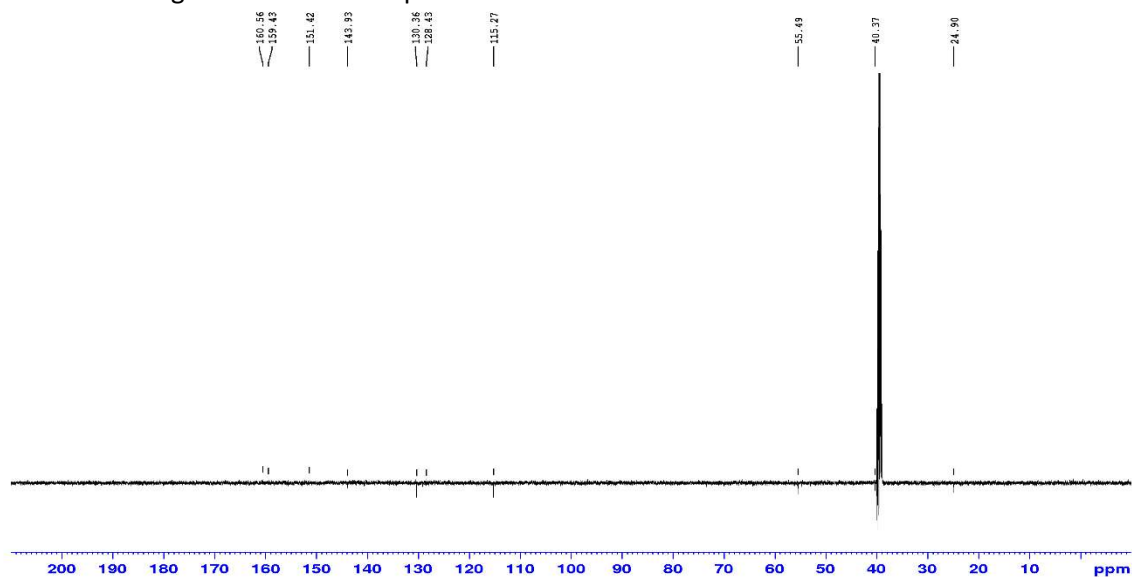


Figure S59. DEPT spectrum of **20** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

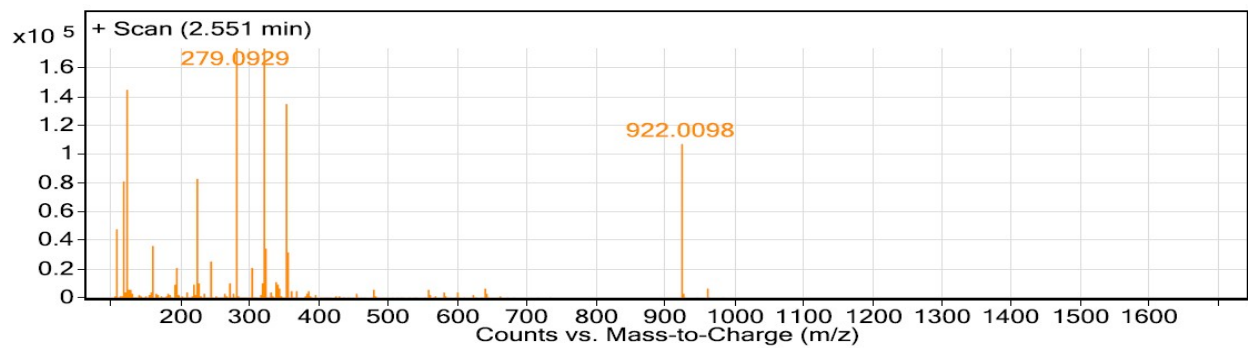


Figure S60. HRMS spectrum of **22a**

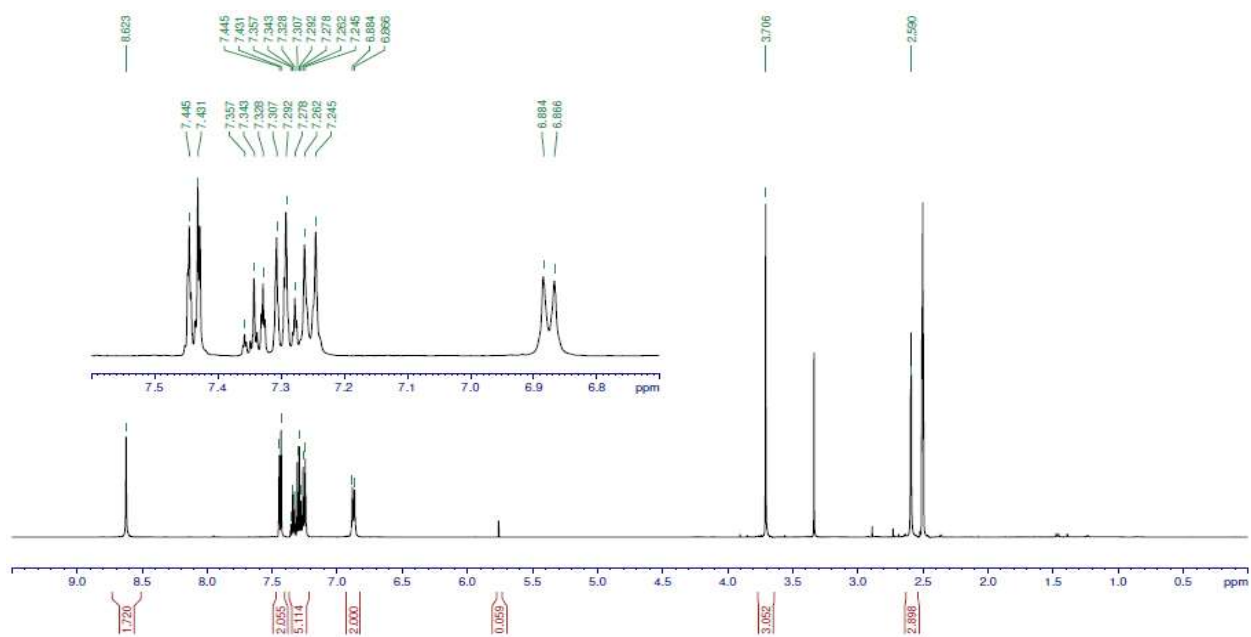


Figure S61.  $^1\text{H-NMR}$  spectrum of **22a** measured at 500 MHz in DMSO-d<sub>6</sub>

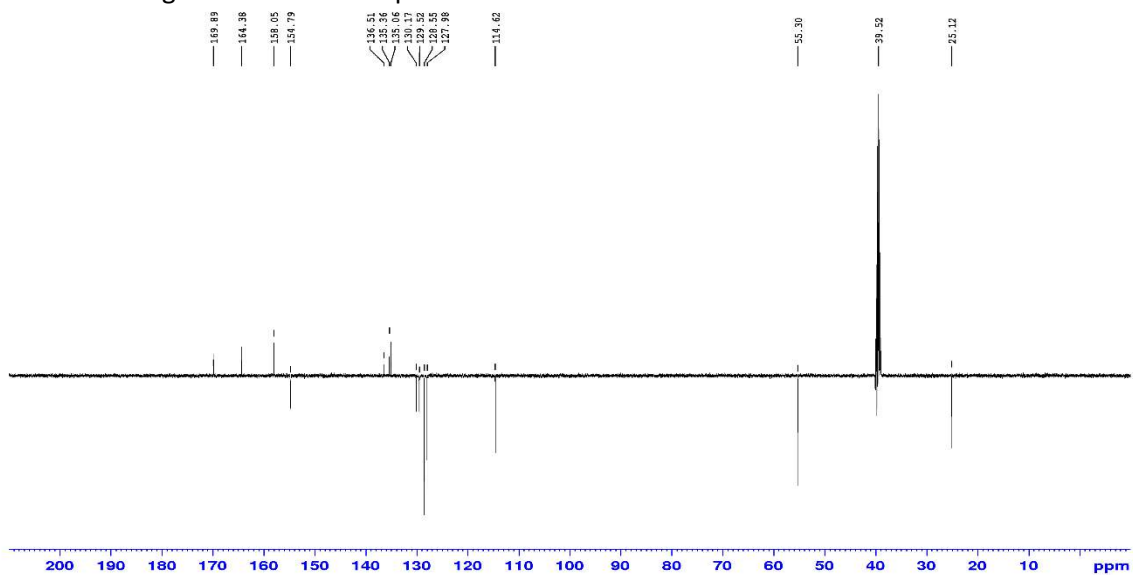


Figure S62. DEPT spectrum of **22a** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

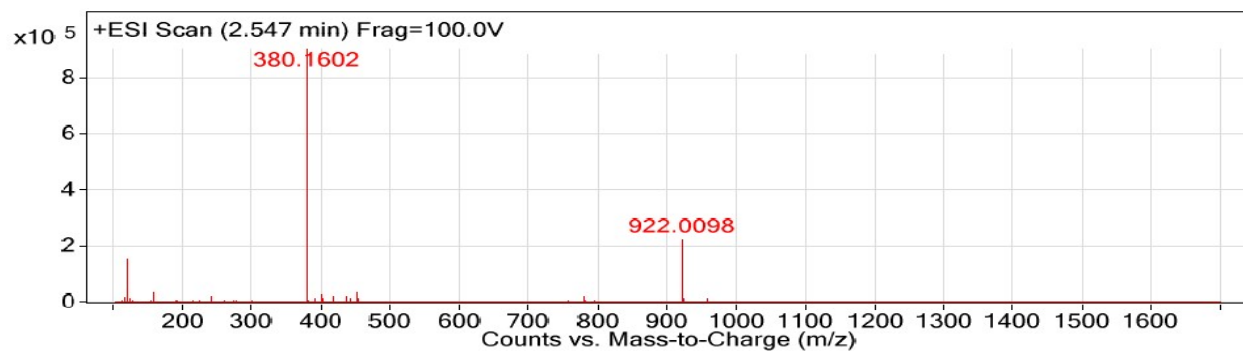


Figure S63. HRMS spectrum of **22b**

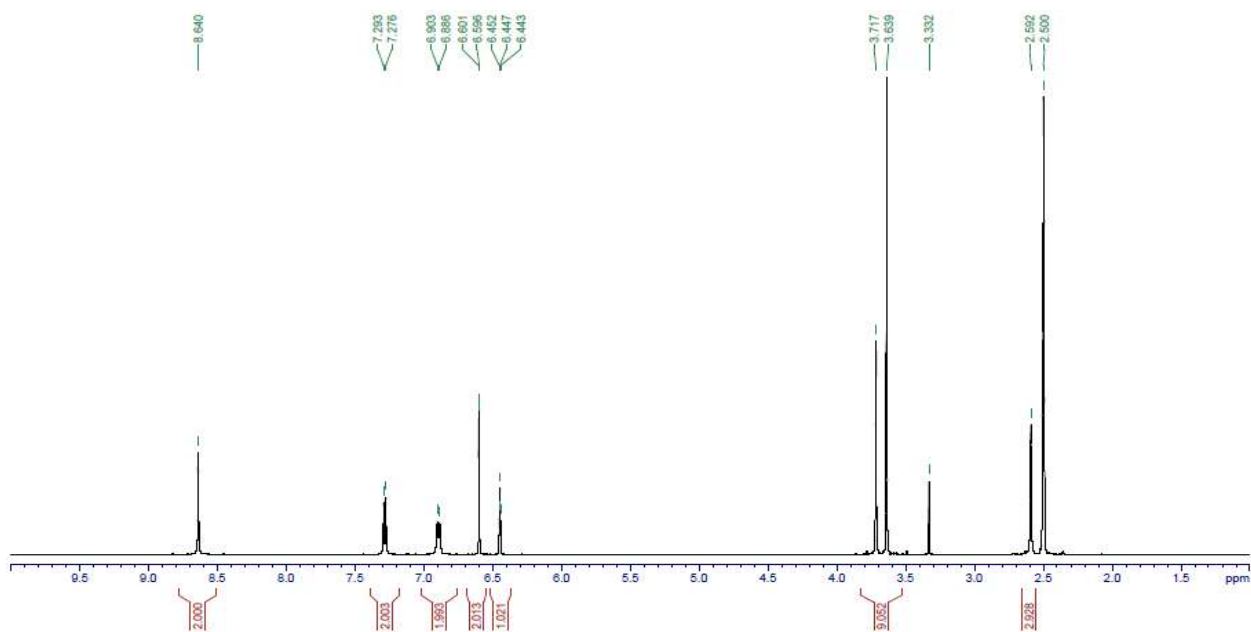


Figure S64. <sup>1</sup>H-NMR spectrum of **22b** measured at 500 MHz in DMSO-d<sub>6</sub>

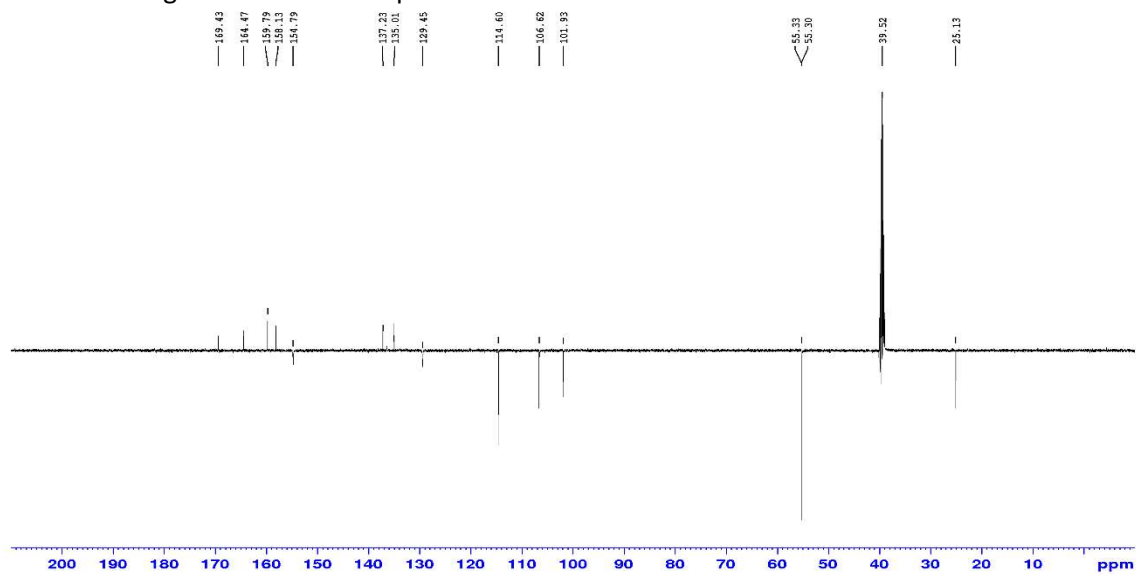


Figure S65. DEPT spectrum of **22b** measured at 125 MHz in DMSO-d<sub>6</sub>



# NMR and HRMS Spectra of Selected Synthesized Compounds

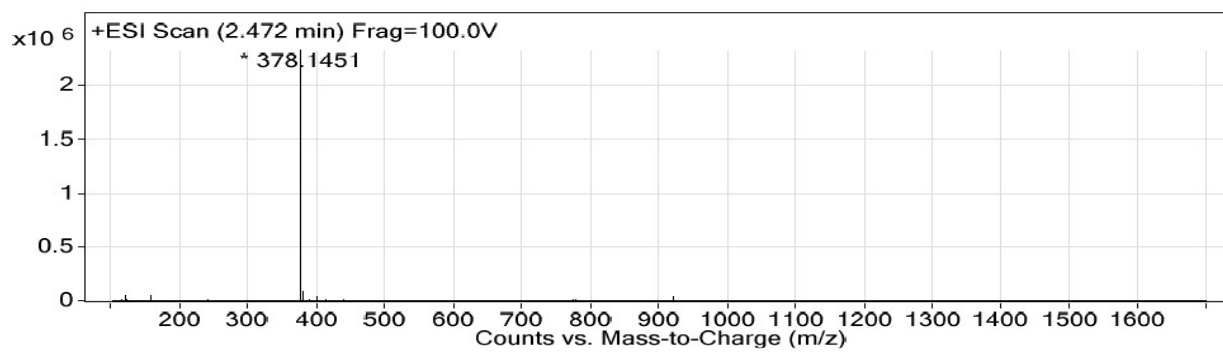


Figure S66. HRMS spectrum of **23**

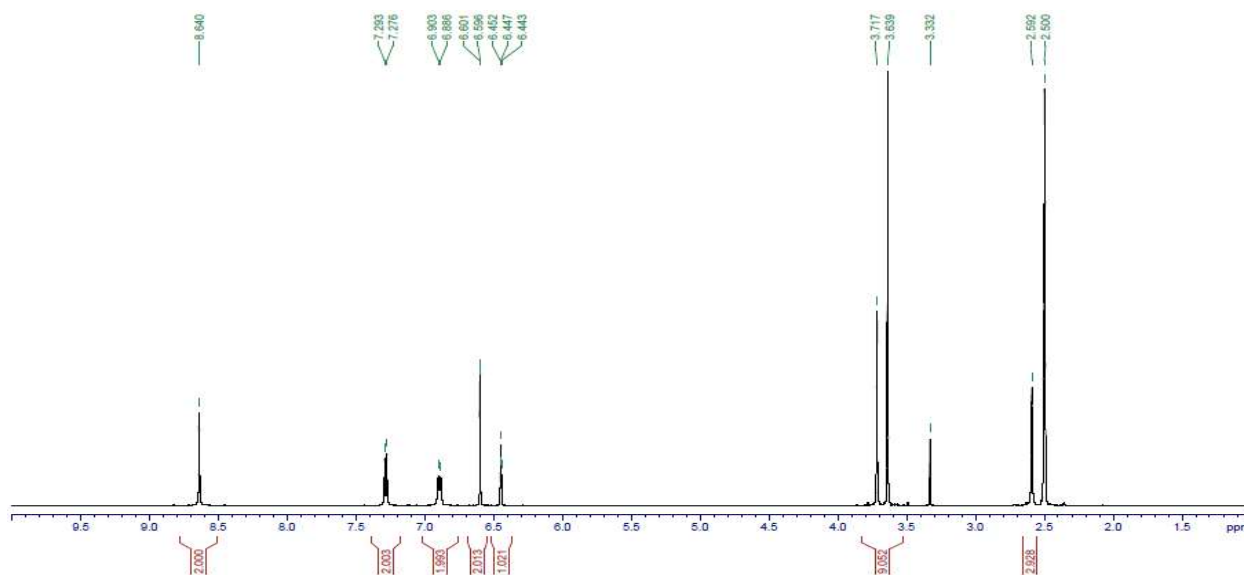


Figure S67. <sup>1</sup>H-NMR spectrum of **23** measured at 500 MHz in DMSO-d<sub>6</sub>

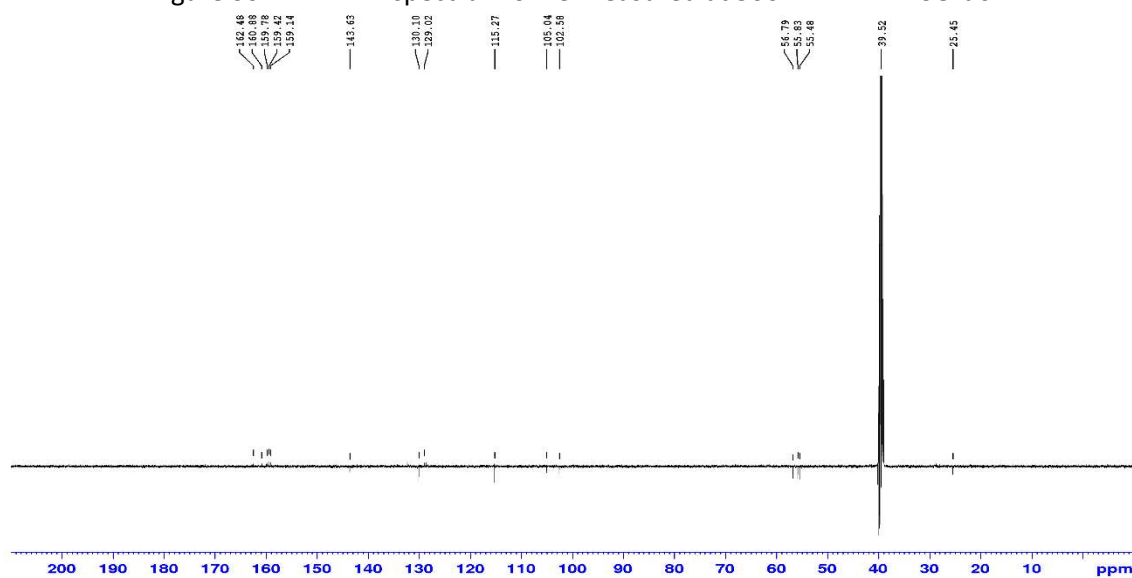


Figure S68. DEPT spectrum of **23** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

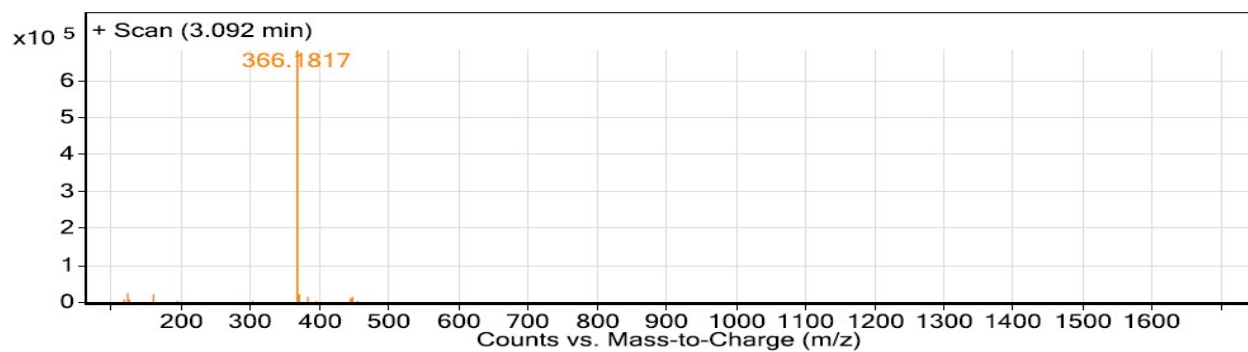


Figure S69. HRMS spectrum of **25**

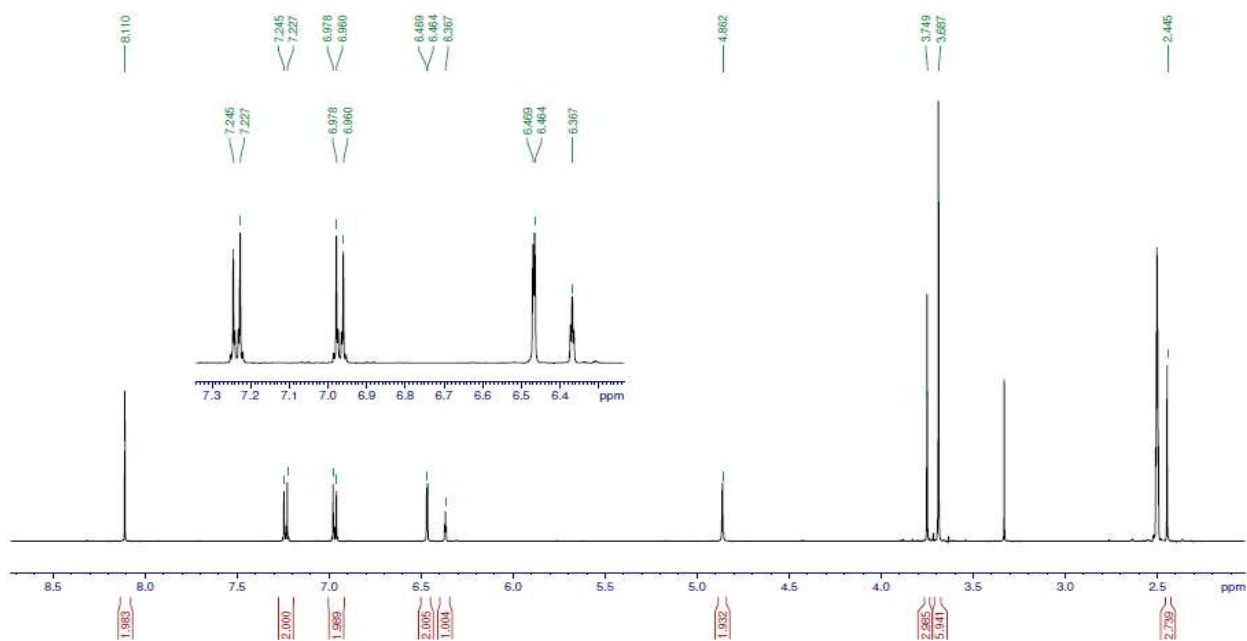


Figure S70. <sup>1</sup>H-NMR spectrum of **25** measured at 500 MHz in DMSO-d<sub>6</sub>

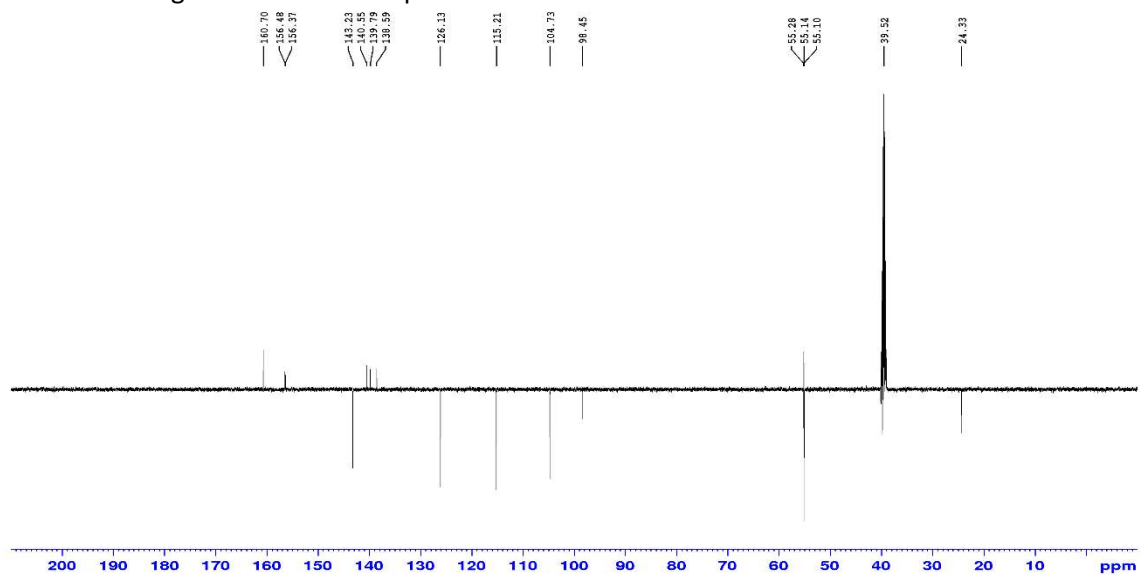


Figure S71. DEPT spectrum of **25** measured at 125 MHz in DMSO-d<sub>6</sub>

# NMR and HRMS Spectra of Selected Synthesized Compounds

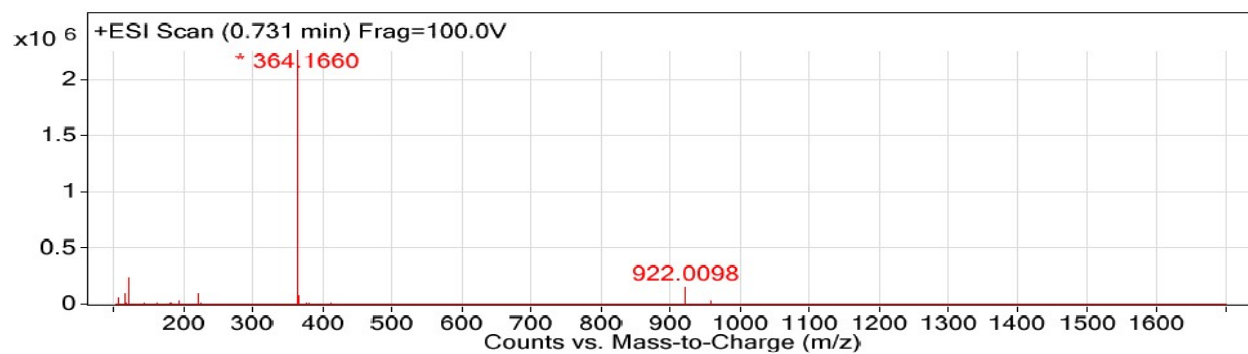


Figure S72. HRMS spectrum of **27**

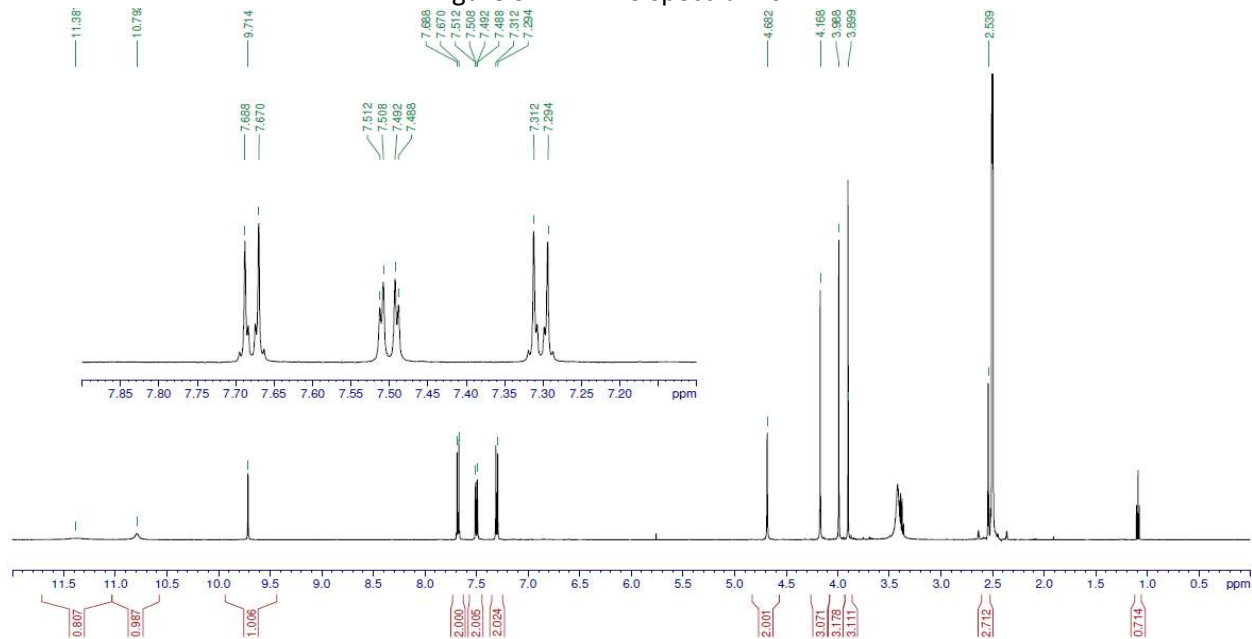


Figure S73. <sup>1</sup>H-NMR spectrum of **27** measured at 500 MHz in DMSO-d<sub>6</sub>

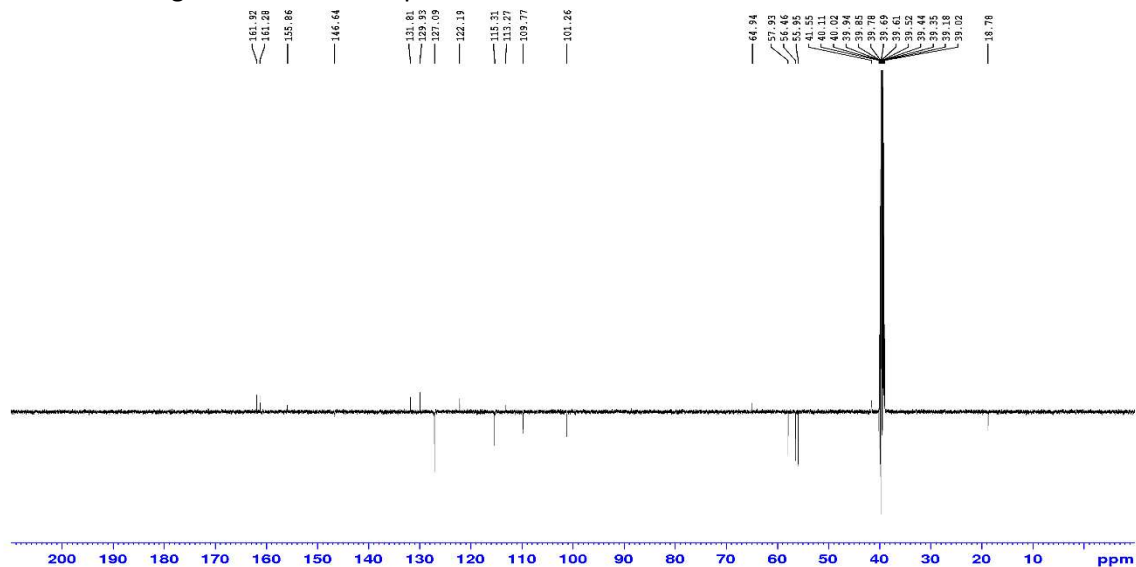


Figure S74. DEPT spectrum of **27** measured at 125 MHz in DMSO-d<sub>6</sub>