

Supporting Information

**Synthesis and biological evaluation of hybrids from farnesylthiosalicylic acid and hydroxycinnamic acid with dual inhibitory activities of Ras-related signaling and phosphorylated NF- $\kappa$ B**

Yong Ling,<sup>a,b</sup> Zhiqiang Wang,<sup>a,b</sup> Xuemin Wang,<sup>a</sup> Ying Zhao,<sup>a</sup> Wei Zhang,<sup>a</sup> Xinyang Wang,<sup>a</sup> Li Chen,<sup>b,c</sup> Zhangjian Huang<sup>b,c,\*</sup> and Yihua Zhang<sup>b,c,\*</sup>

<sup>a</sup> School of Pharmacy, Nantong University, Nantong, 226001, PR China.

<sup>b</sup> State Key Laboratory of Natural Medicines, China Pharmaceutical University, Nanjing, 210009, PR China.

<sup>c</sup> Center of Drug Discovery, China Pharmaceutical University, Nanjing, 210009, PR China.

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Table 1. The number of experiments and the related SD values for Figure 1 legend in the manuscript.

Compound	<i>In vitro</i> inhibitory activity (%)		
	Mcf-7	SMMC-7721	SGC-7901
FTS	55.16 ± 3.23	45.79 ± 4.95	57.04 ± 4.66
Sorafenib	90.35 ± 4.53	92.78 ± 5.28	93.03 ± 6.83
<b>5a</b>	91.32 ± 6.06	93.01 ± 5.21	94.64 ± 4.97
<b>5b</b>	35.70 ± 3.28	43.08 ± 2.68	32.69 ± 3.55
<b>5c</b>	93.52 ± 4.93	87.98 ± 6.56	94.96 ± 4.67
<b>5d</b>	38.39 ± 4.16	39.02 ± 3.16	36.49 ± 4.04
<b>5e</b>	92.46 ± 5.47	89.11 ± 6.10	87.56 ± 5.09
<b>5f</b>	91.54 ± 6.85	97.43 ± 4.18	96.21 ± 6.87
<b>5g</b>	88.65 ± 5.92	87.72 ± 6.18	91.58 ± 5.65
<b>5h</b>	12.56 ± 2.61	11.53 ± 2.12	8.56 ± 1.35
<b>5i</b>	62.76 ± 4.86	64.46 ± 4.62	60.96 ± 4.16
<b>5j</b>	28.09 ± 2.42	36.55 ± 2.78	21.66 ± 3.54
<b>5k</b>	72.03 ± 5.23	78.07 ± 5.64	79.58 ± 5.74
<b>5l</b>	11.43 ± 1.86	7.42 ± 1.41	8.81 ± 1.73
<b>5m</b>	70.21 ± 4.68	75.37 ± 3.85	63.04 ± 4.98
<b>5n</b>	86.83 ± 4.29	87.68 ± 5.92	84.98 ± 5.15
<b>5o</b>	61.99 ± 4.52	62.95 ± 3.66	51.59 ± 3.51
<b>5p</b>	14.86 ± 2.67	23.40 ± 1.35	13.66 ± 1.69
<b>5q</b>	61.98 ± 4.32	67.21 ± 4.06	55.09 ± 3.93
<b>5r</b>	49.64 ± 2.65	44.48 ± 3.02	42.98 ± 2.06

#### HPLC assessment of compound **5f** purity.

Compounds (**5f**) with a purity of 99.1% (HPLC analysis) were used for subsequent experiments. We provided the spectra of HPLC assays as below: Column: Shimadzu C18 (150mm×4.6mm×5μm); Mobile phase: Methanol: aqueous solution of triethylamine (28.5 mmol/L) = 65: 35; Wavelength: 254 nm; Rate: 1 mL/min; Temperature: 30 °C; Pressure: 85-142 kgf.

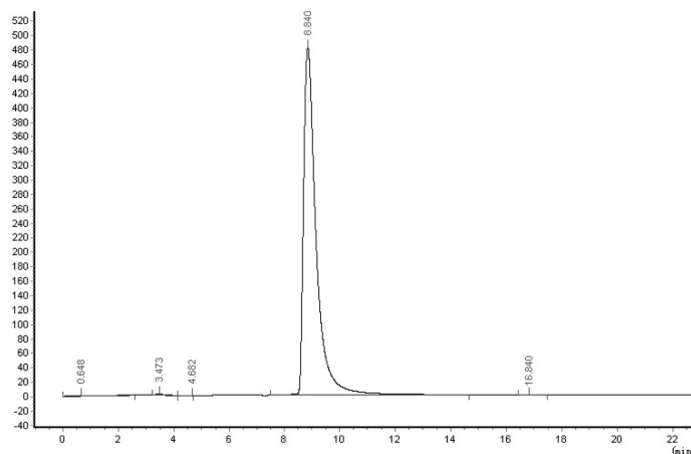


Fig. 1. HPLC spectrum of **5f**

The  $^1\text{H}$  NMR spectra for **5a-5r**

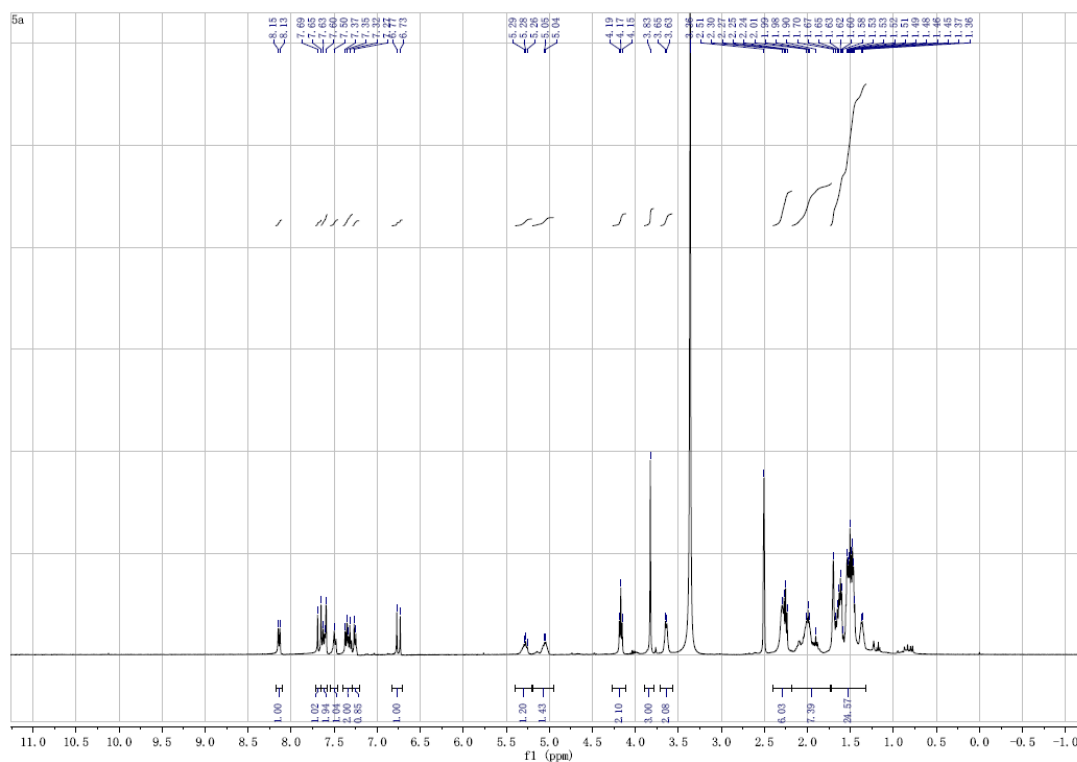


Fig. 2. The  $^1\text{H}$  NMR spectra of **5a**

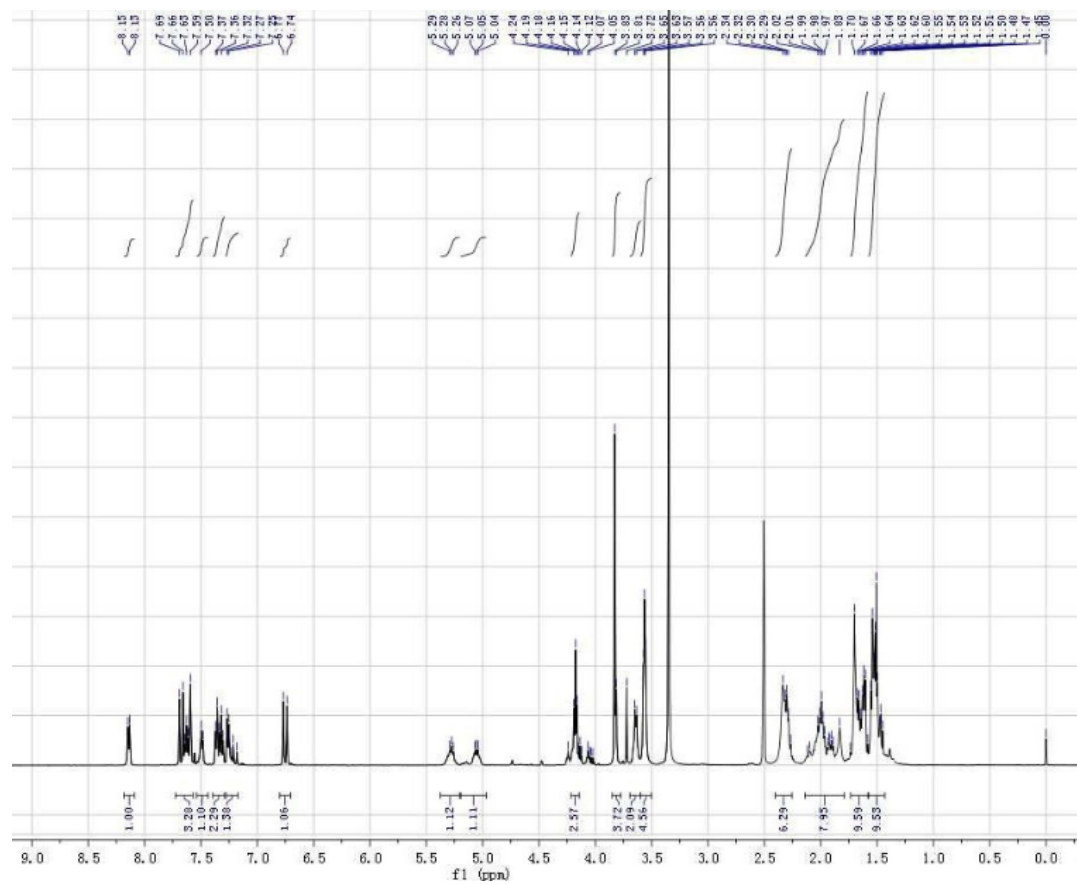


Fig. 3. The  $^1\text{H}$  NMR spectra for **5b**

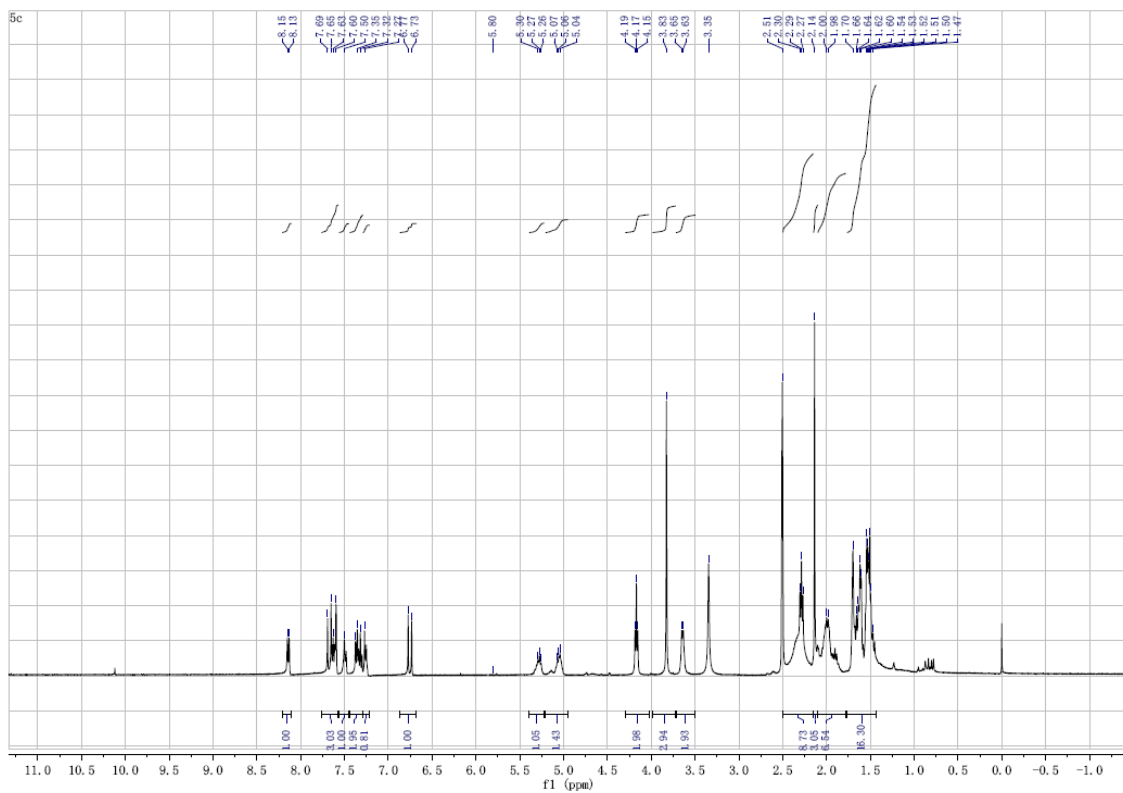


Fig. 4. The  $^1\text{H}$  NMR spectra for **5c**

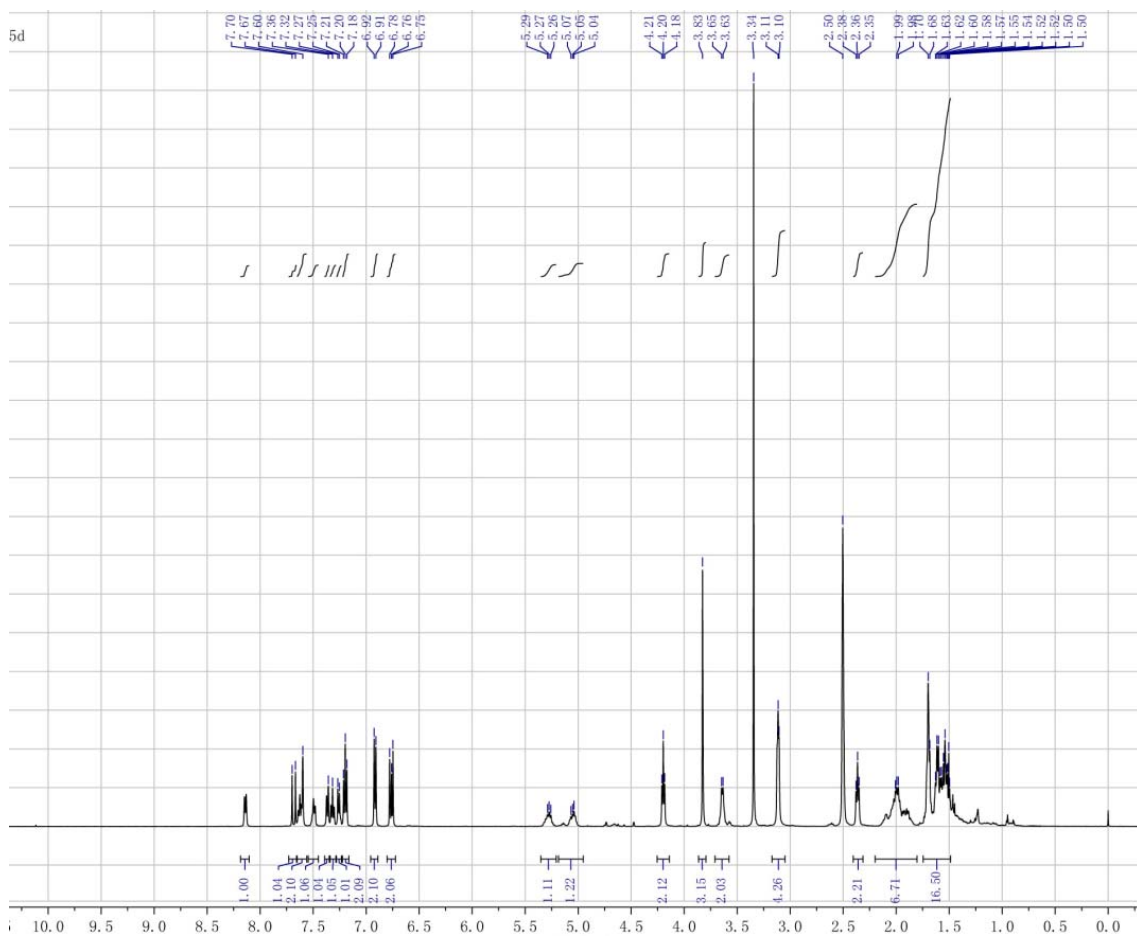


Fig. 5. The  $^1\text{H}$  NMR spectra for **5d**

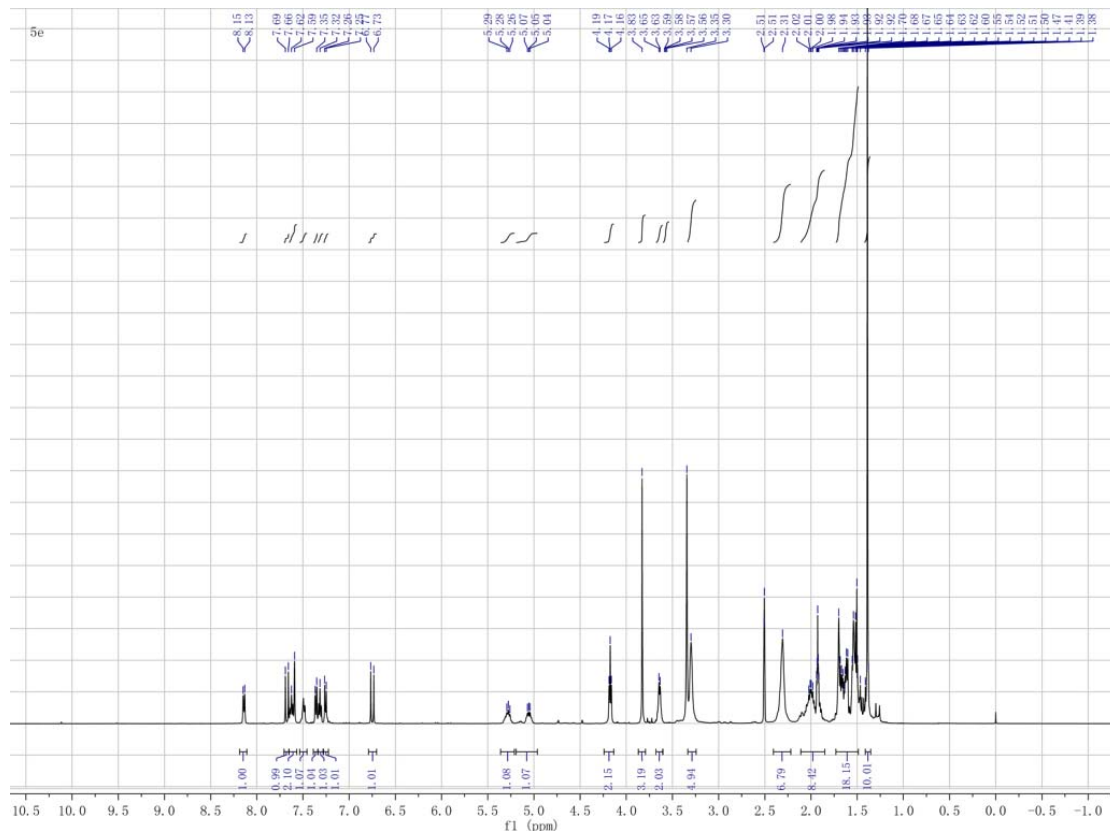


Fig. 6. The  $^1\text{H}$  NMR spectra for **5e**

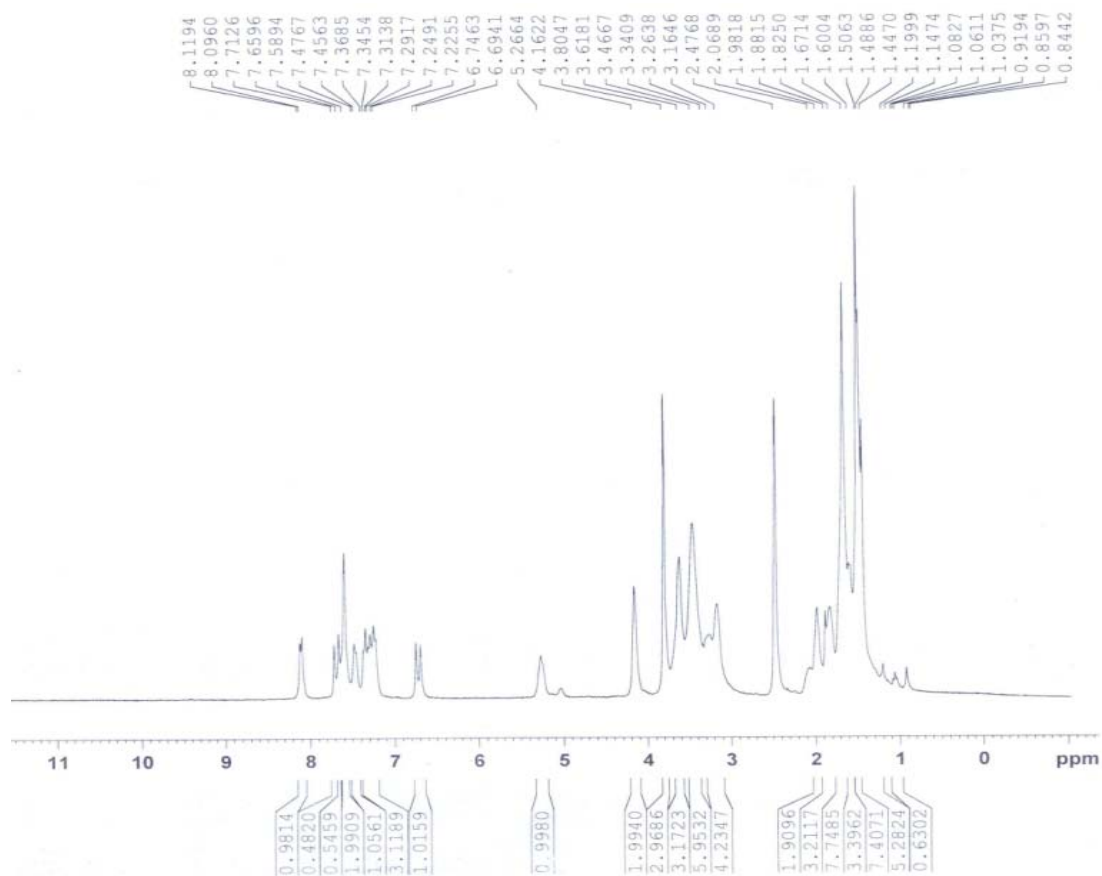


Fig. 7. The  $^1\text{H}$  NMR spectra for **5f**

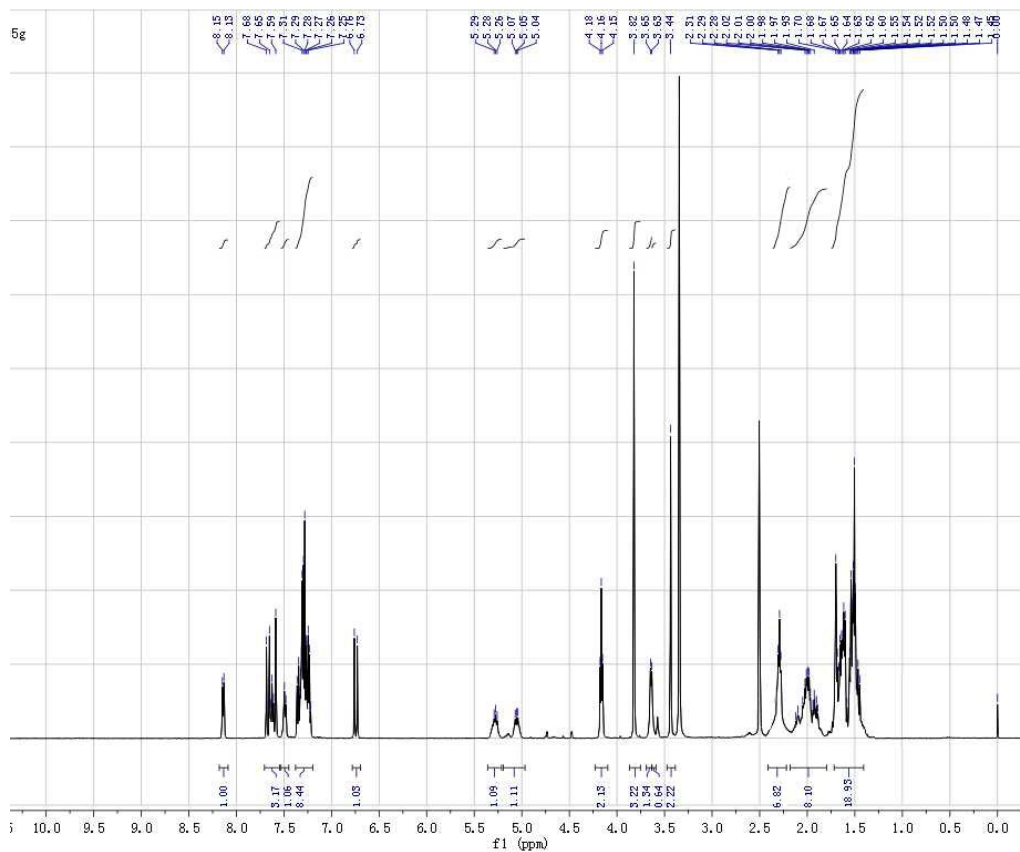


Fig. 8. The  $^1\text{H}$  NMR spectra for **5g**

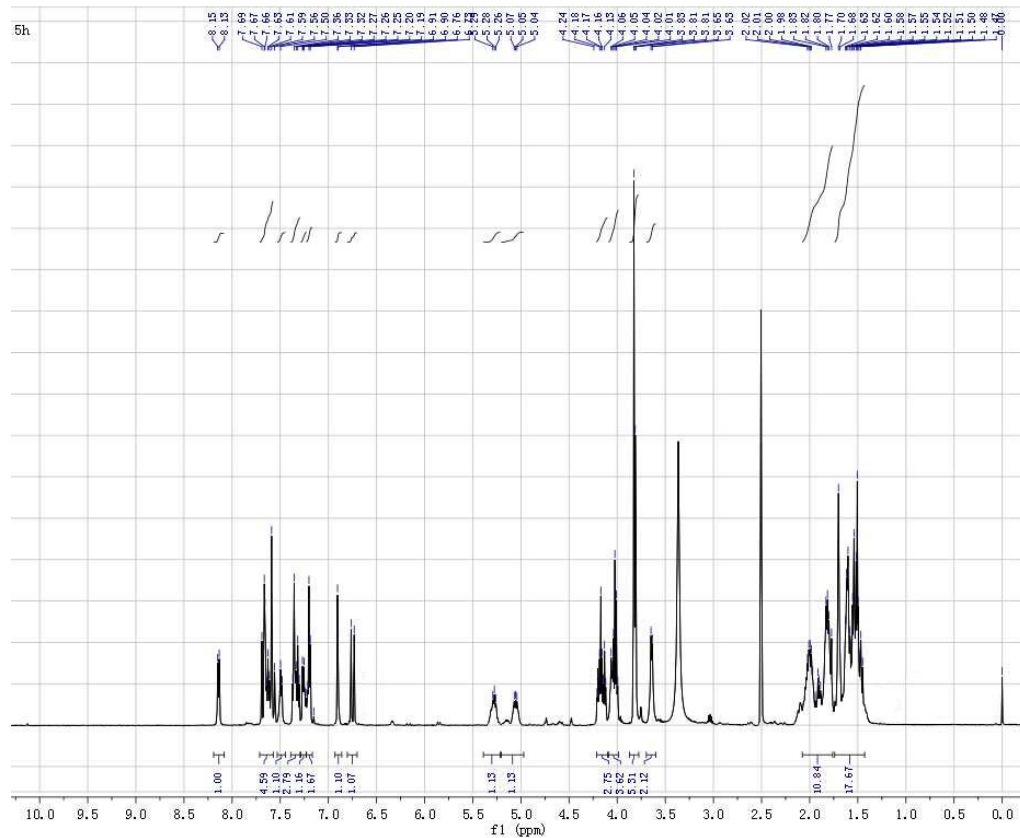


Fig. 9. The  $^1\text{H}$  NMR spectra for **5h**

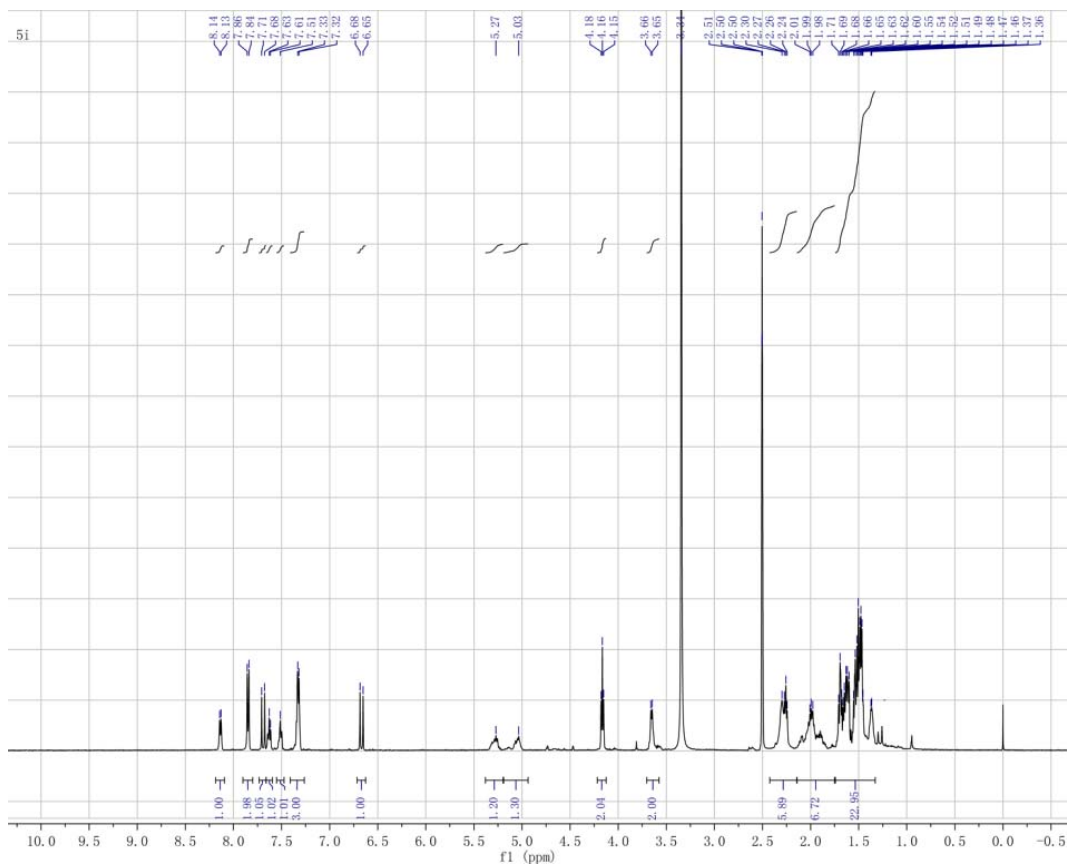


Fig. 10. The  $^1\text{H}$  NMR spectra for **5i**

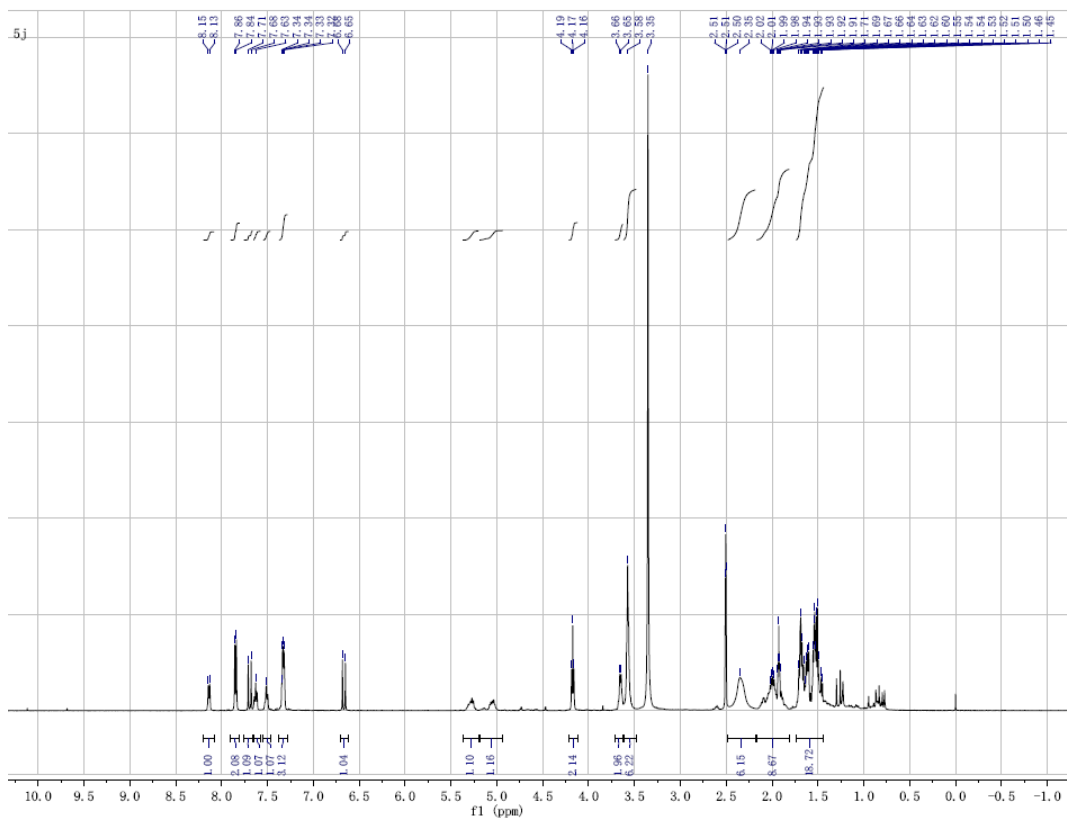


Fig. 11. The  $^1\text{H}$  NMR spectra for **5j**

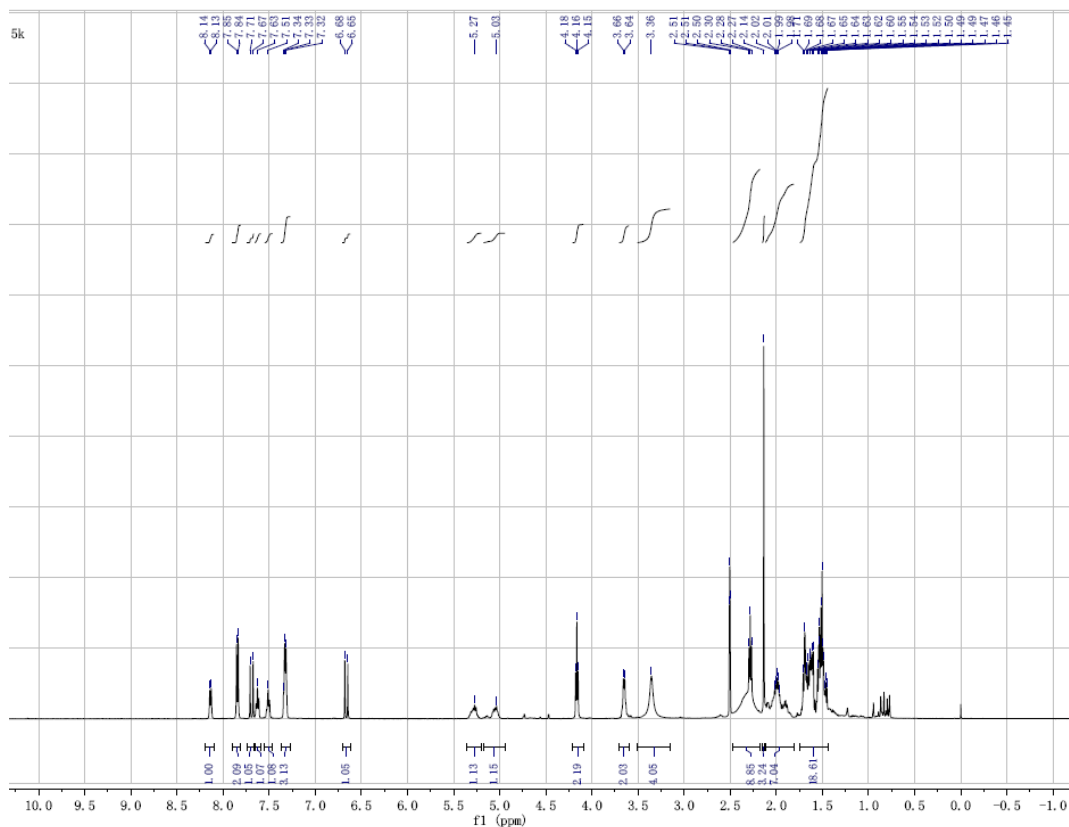


Fig. 12. The  $^1\text{H}$  NMR spectra for **5k**

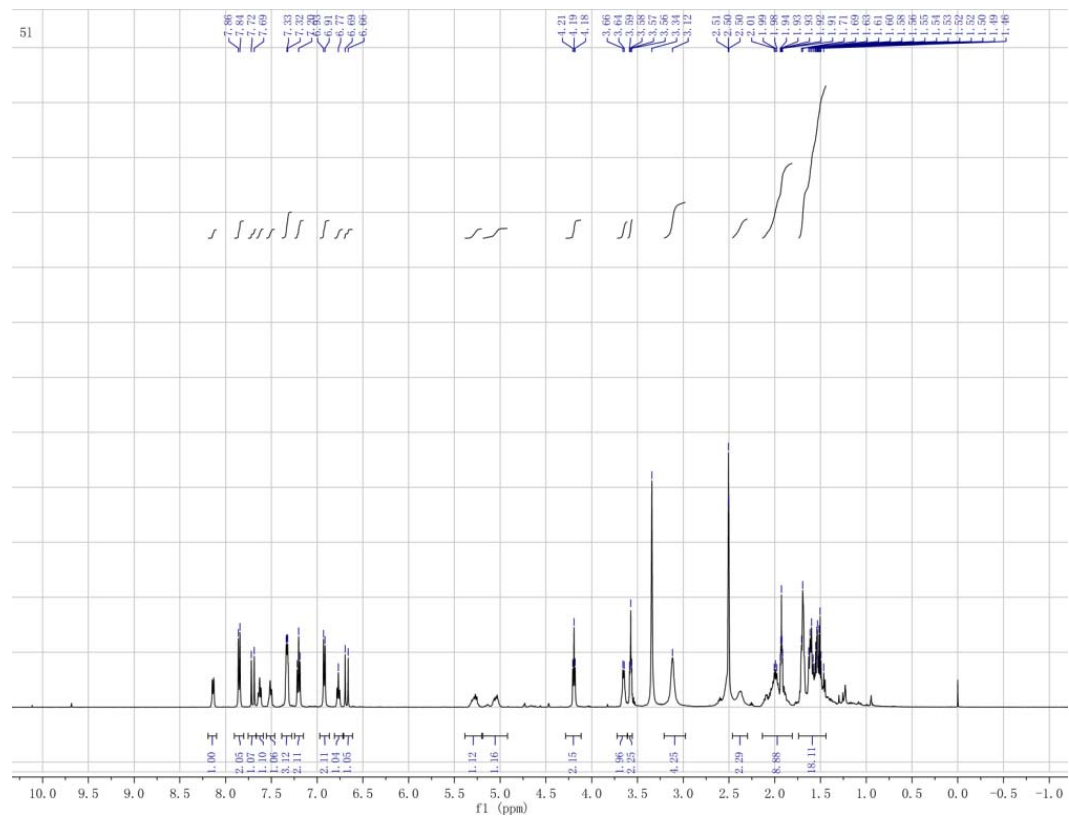


Fig. 13. The  $^1\text{H}$  NMR spectra for **5l**



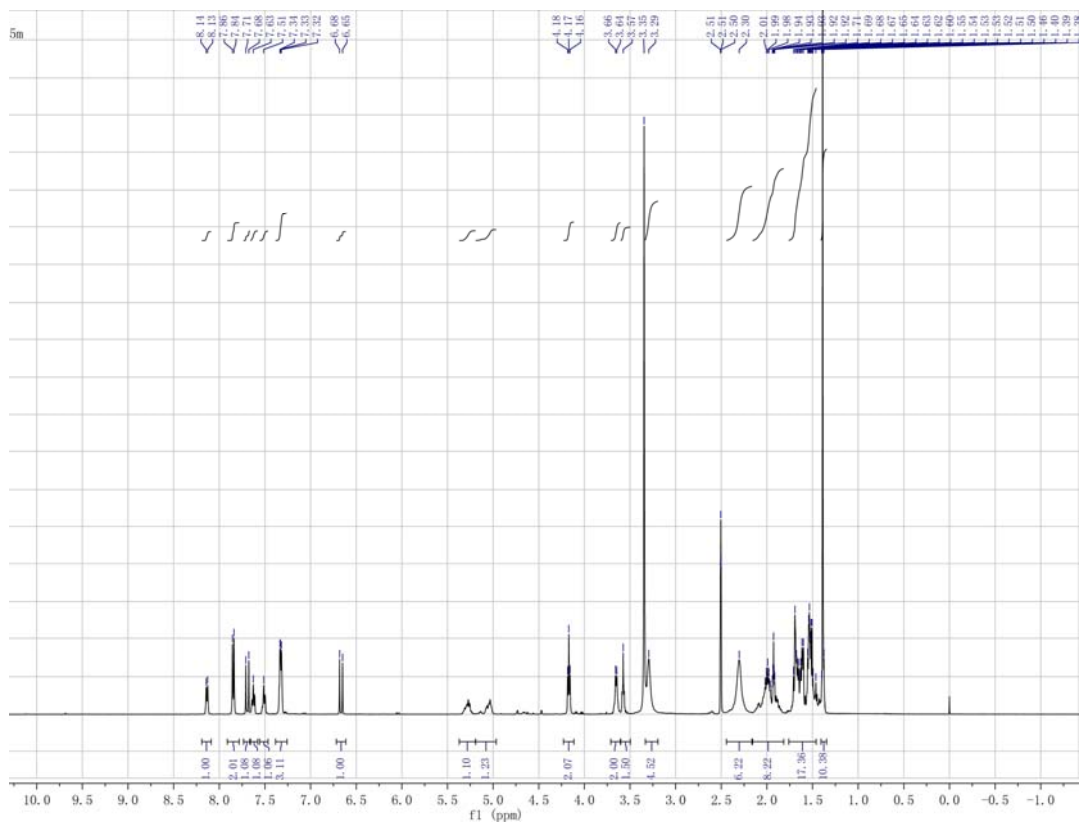


Fig. 14. The  $^1\text{H}$  NMR spectra for **5m**

5n DMSO 1HNMR AV300

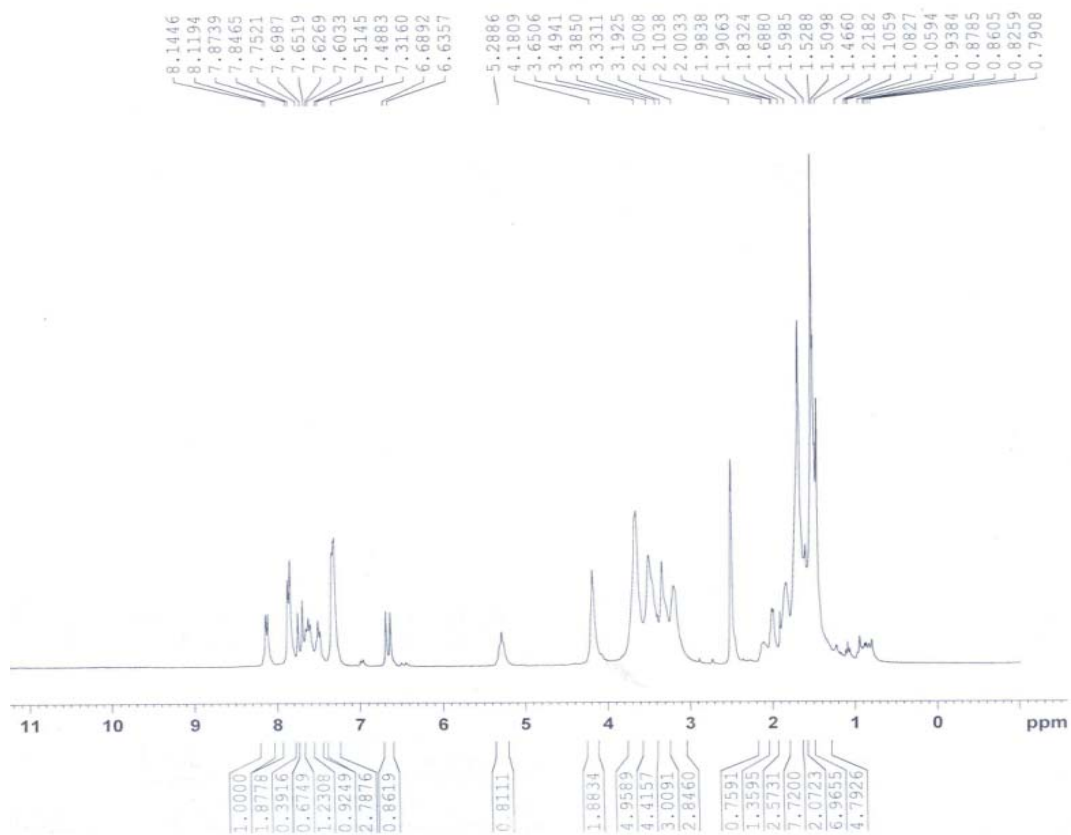


Fig. 15. The  $^1\text{H}$  NMR spectra for **5n**

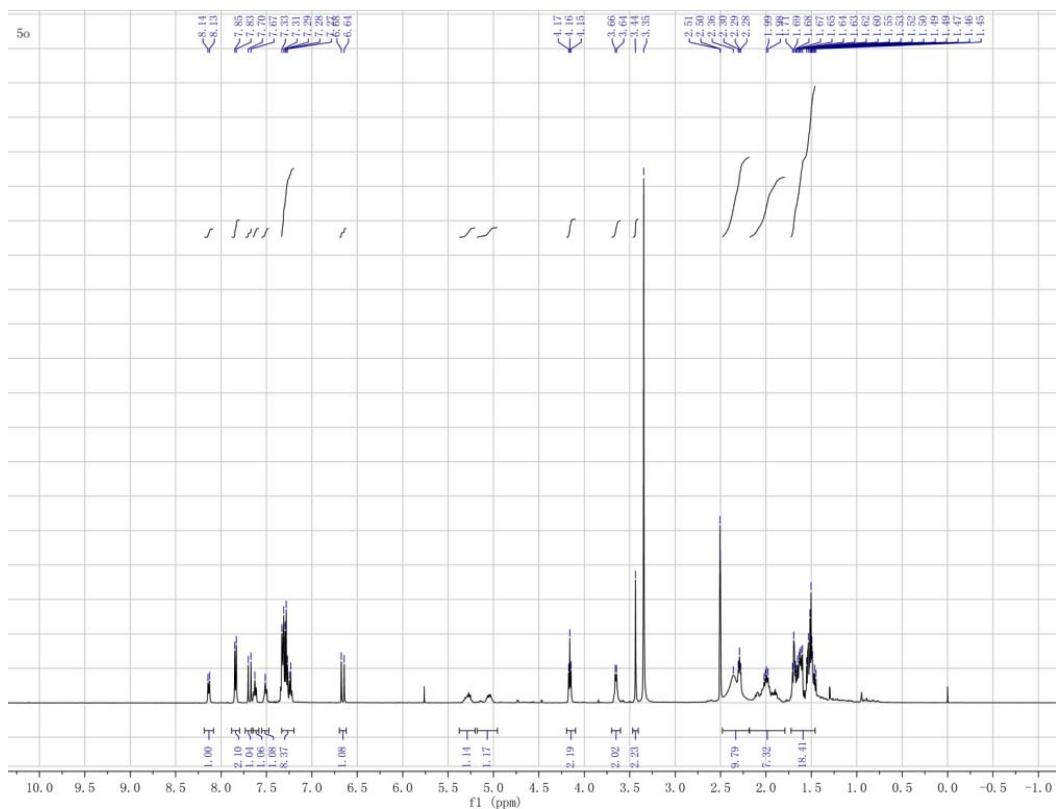


Fig. 16. The  $^1\text{H}$  NMR spectra for **5o**

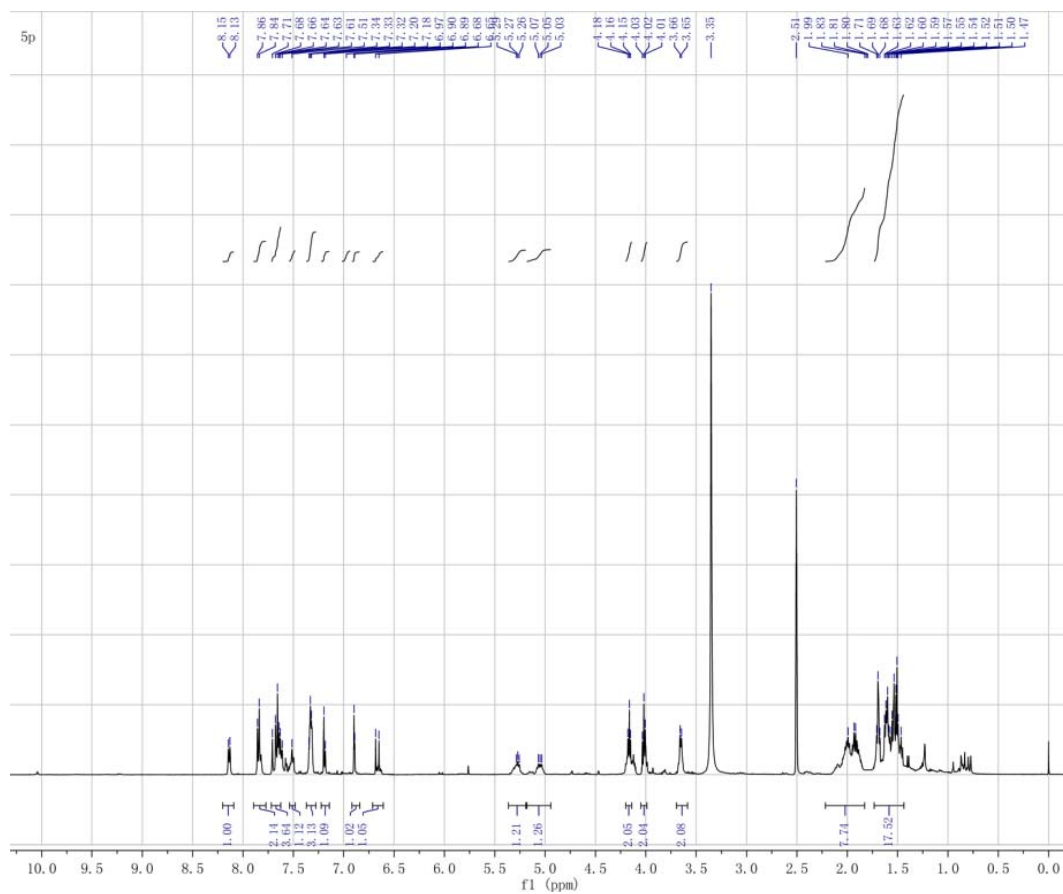


Fig. 17. The  $^1\text{H}$  NMR spectra for **5p**

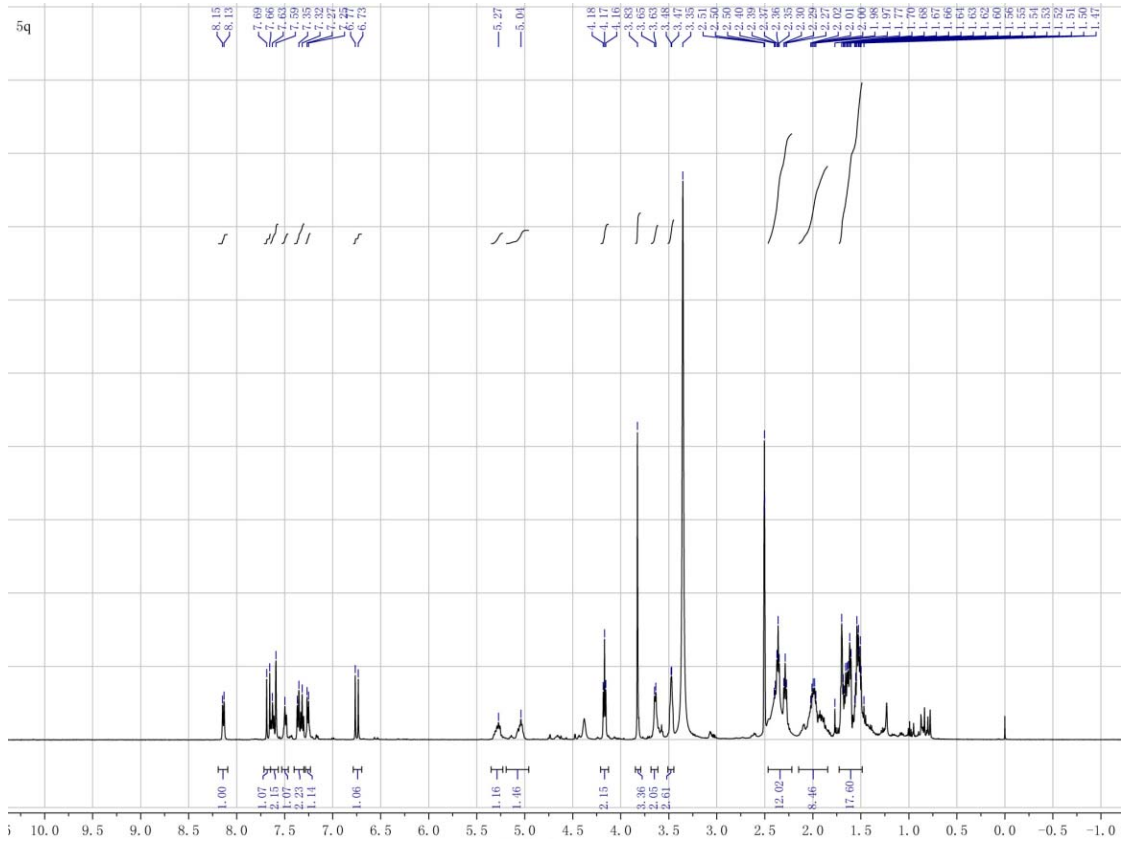


Fig. 19. The  $^1\text{H}$  NMR spectra for **5q**

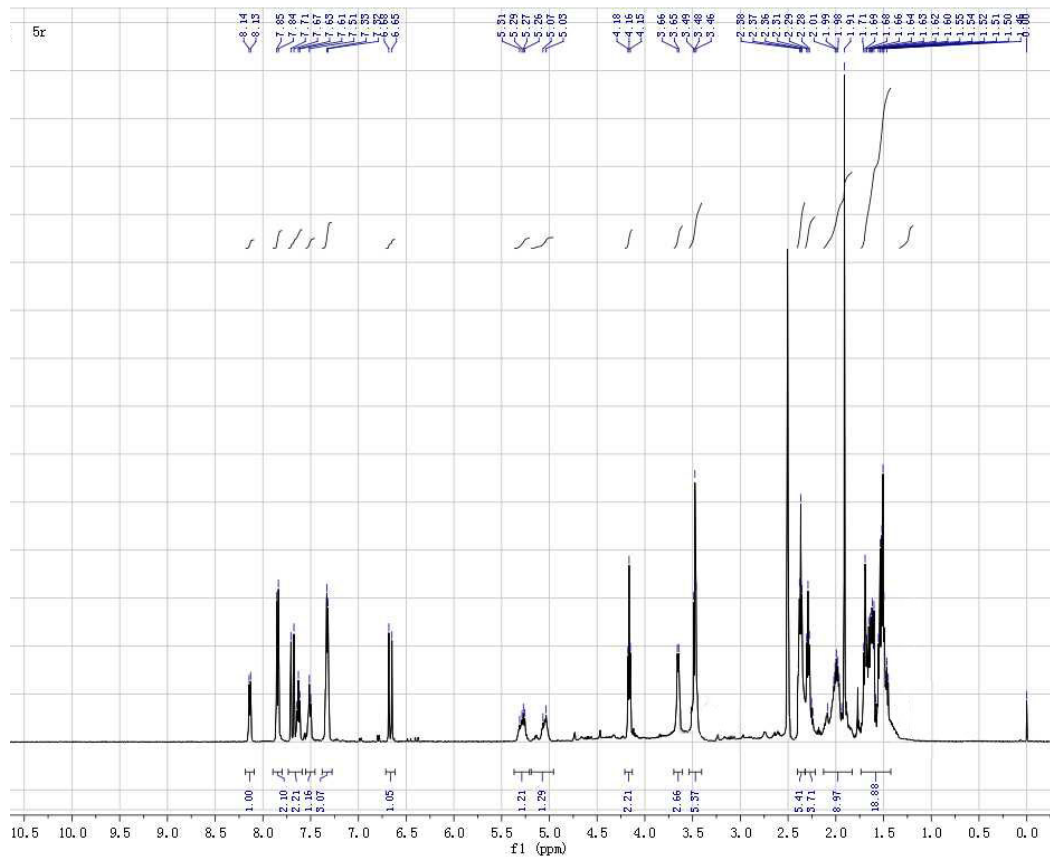
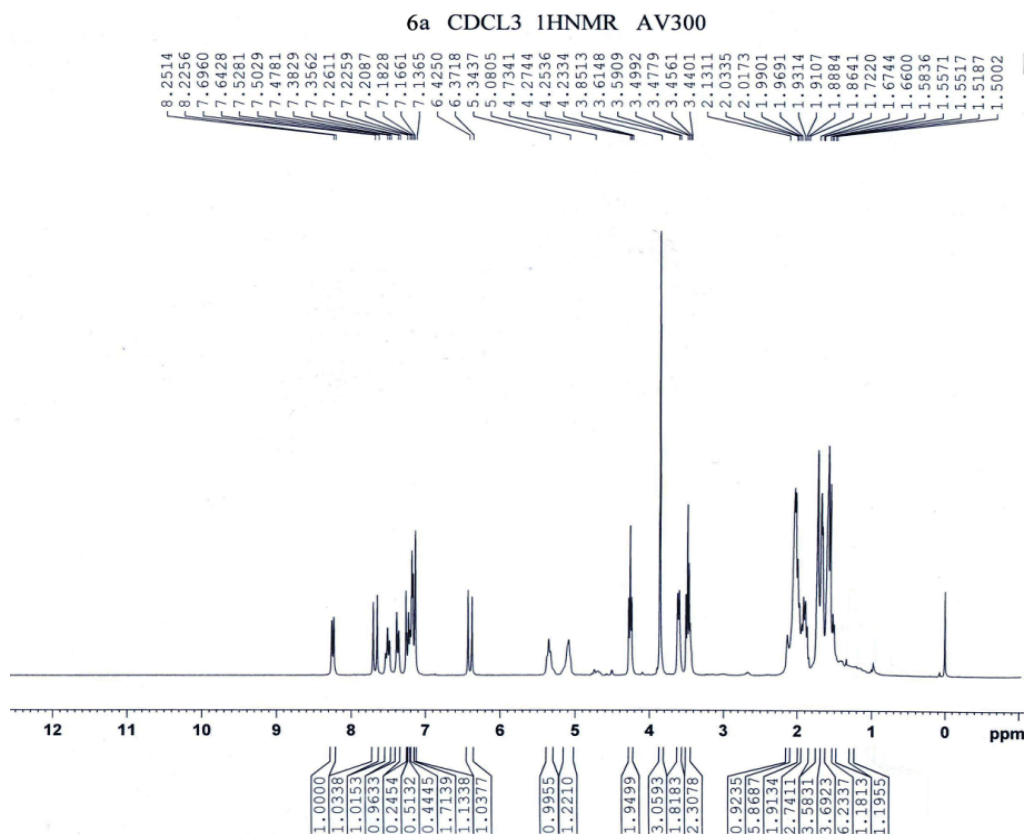
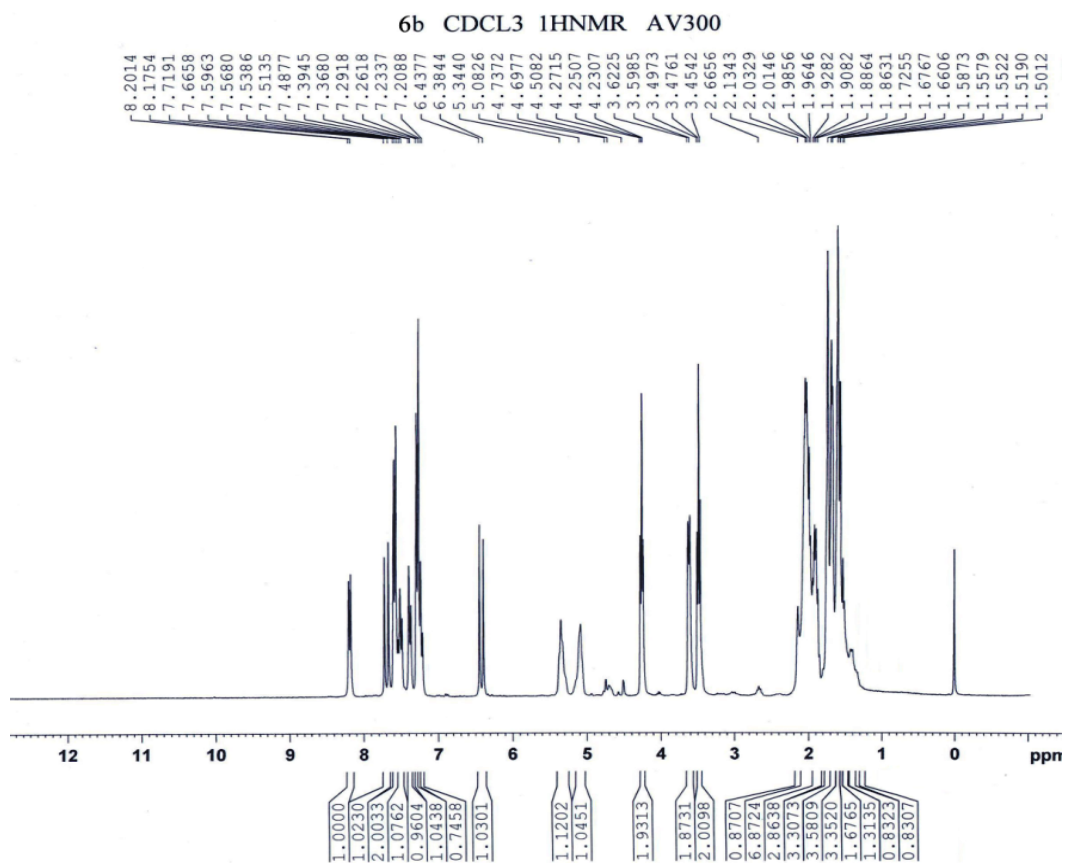


Fig. 19. The  $^1\text{H}$  NMR spectra for **5r**



**Fig. 20.** The <sup>1</sup>H NMR spectra for **6a**



**Fig. 21.** The <sup>1</sup>H NMR spectra for **6b**

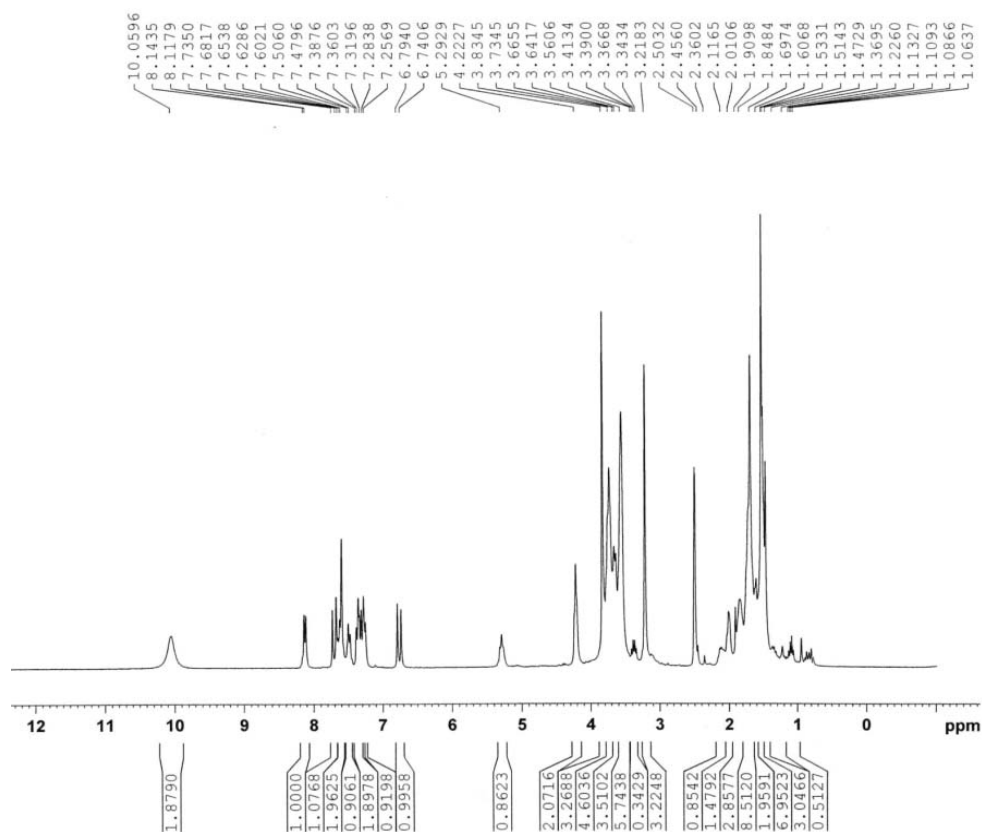


Fig. 22. The  $^1\text{H}$  NMR spectra for **7b**

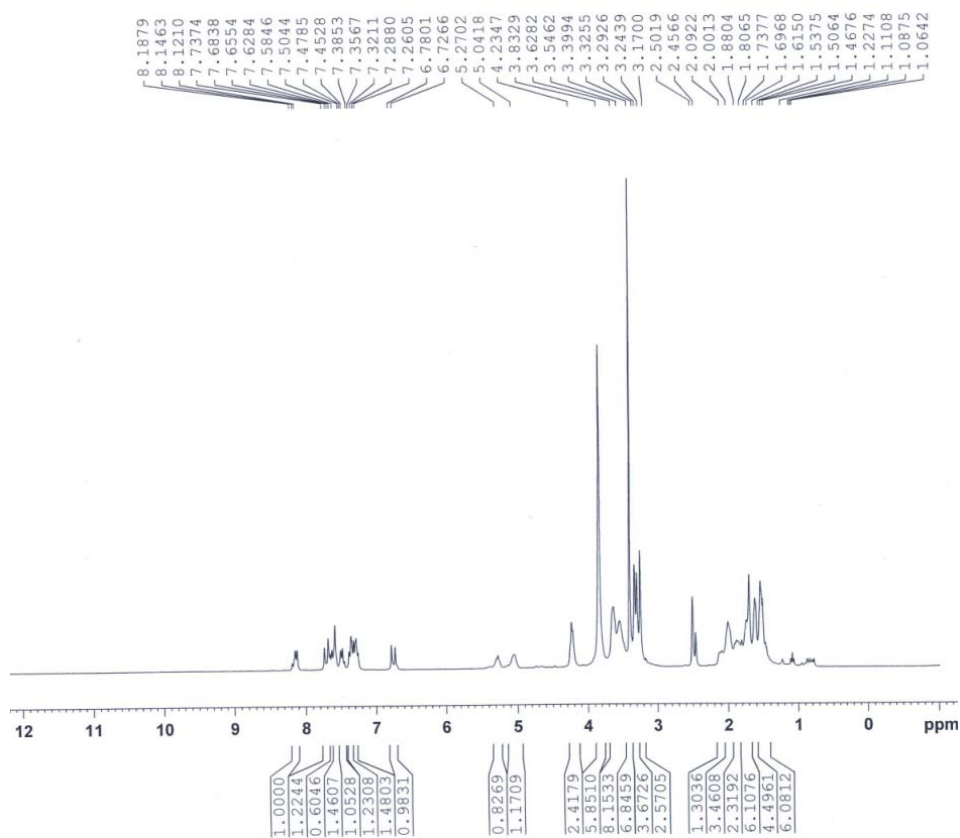


Fig. 23. The  $^1\text{H}$  NMR spectra for **7c**

The  $^{13}\text{C}$  NMR spectra for **5a-5r**

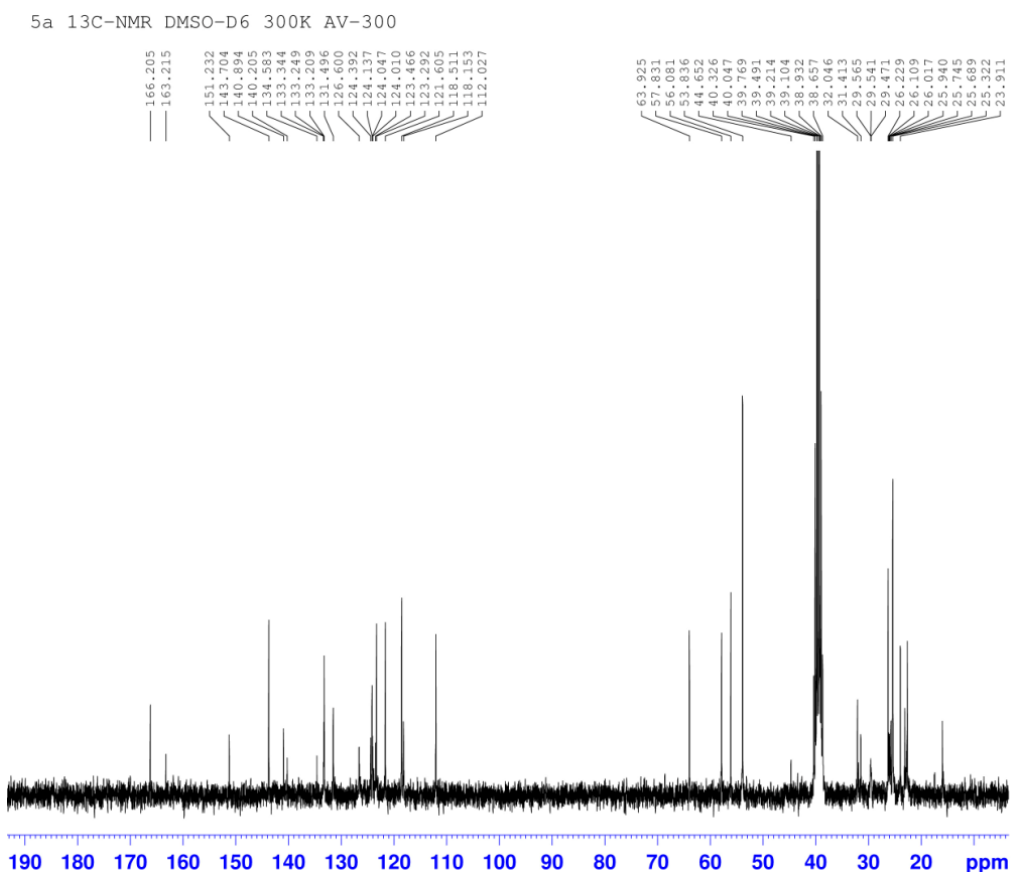


Fig. 24. The  $^{13}\text{C}$  NMR spectra for **5a**

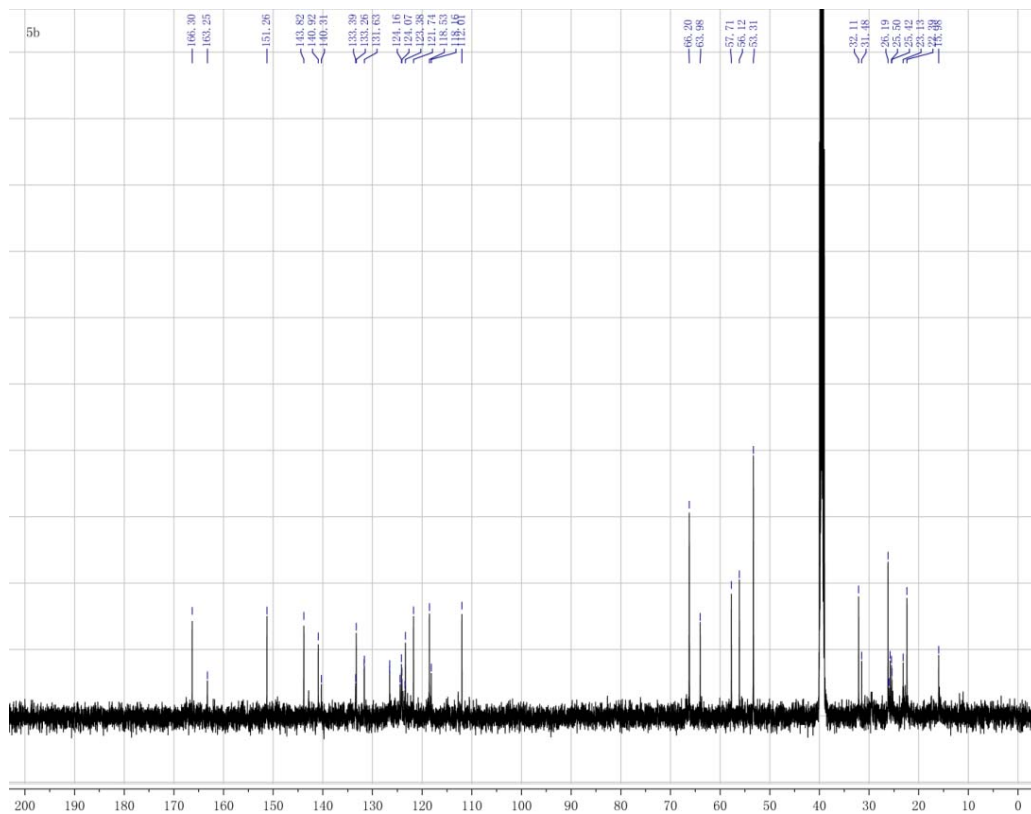


Fig. 25. The  $^{13}\text{C}$  NMR spectra for **5b**

5c <sup>13</sup>C-NMR DMSO-D6 300K AV-300

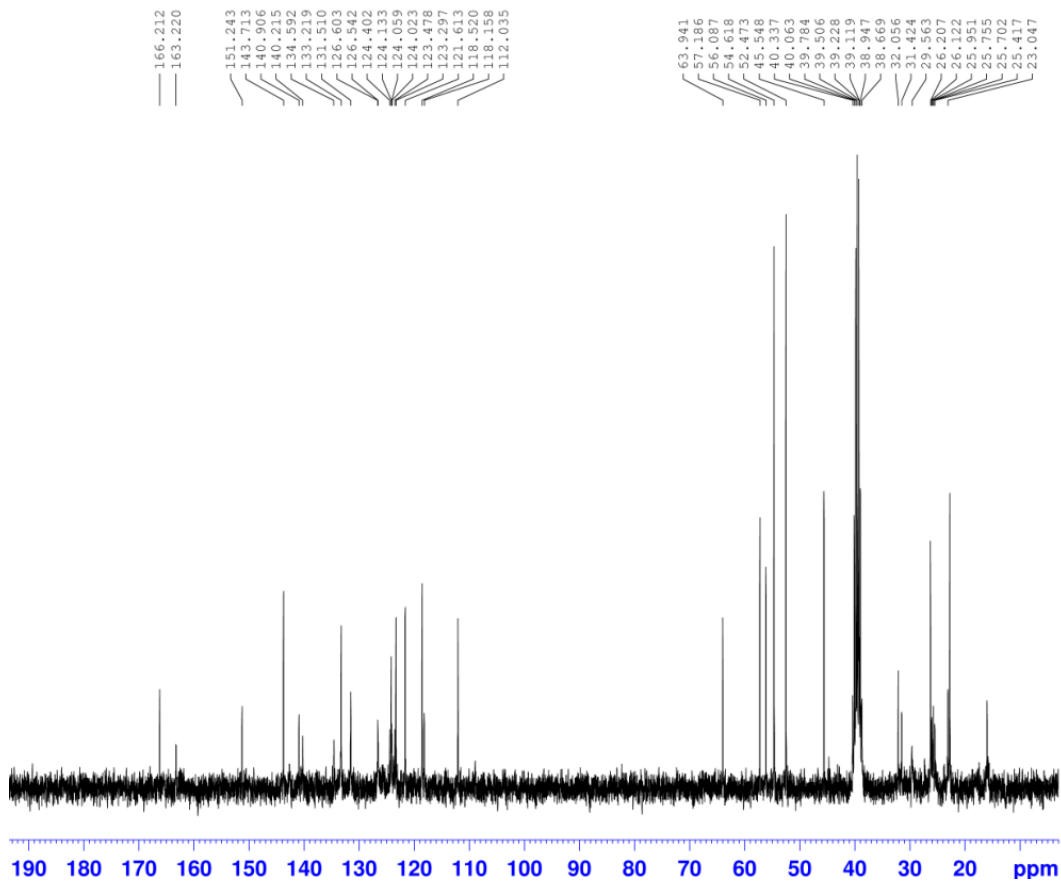


Fig. 26. The <sup>13</sup>C NMR spectra for 5c

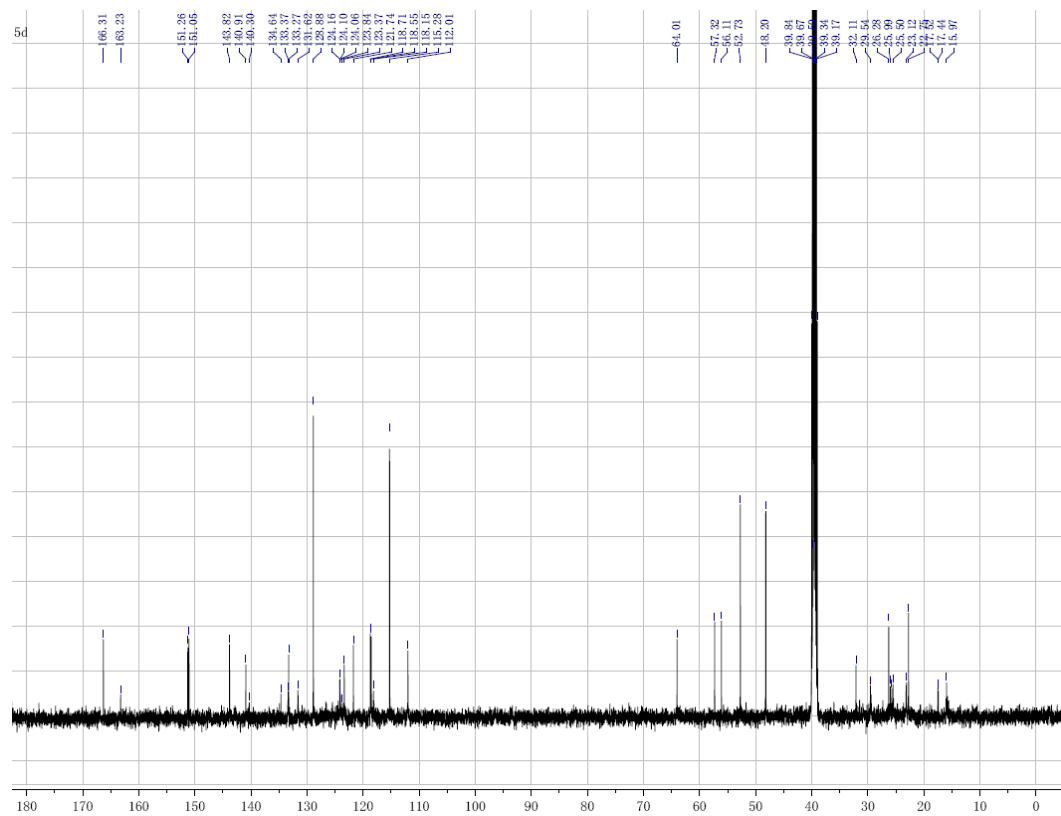


Fig. 27. The <sup>13</sup>C NMR spectra for 5d

5E <sup>13</sup>C-NMR DMSO-D6 300K AV-300

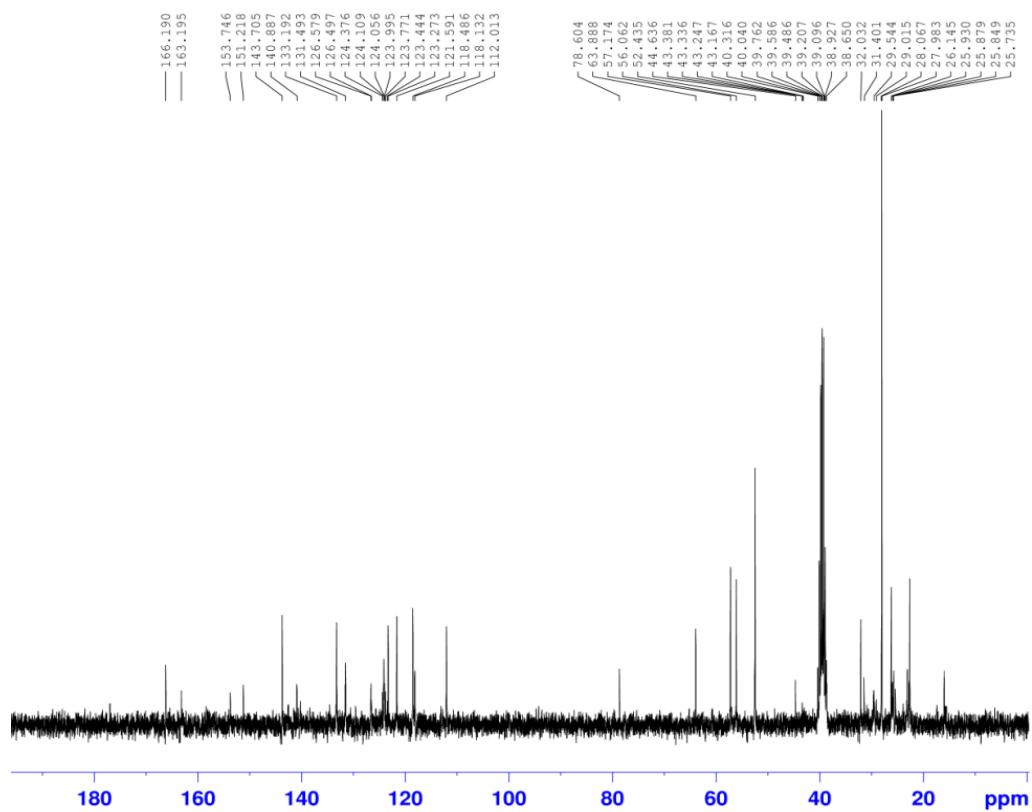


Fig. 28. The <sup>13</sup>C NMR spectra for 5e

5f <sup>13</sup>C-NMR DMSO-D6 300K AV-300

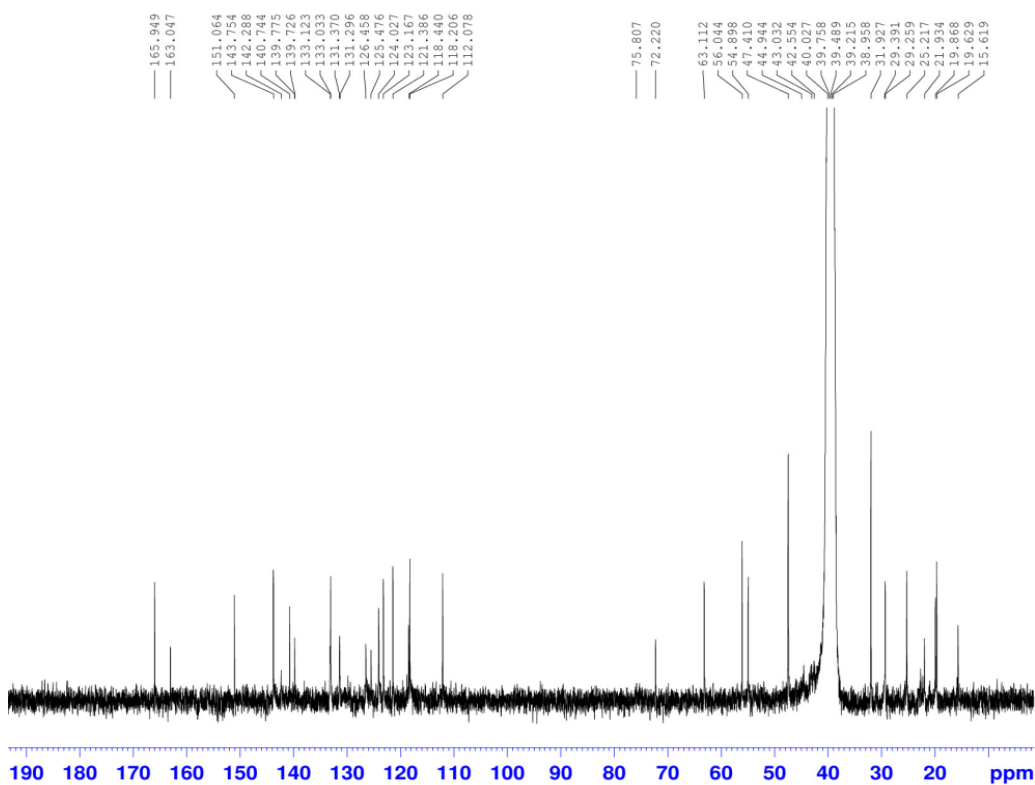


Fig. 29. The <sup>13</sup>C NMR spectra for 5f



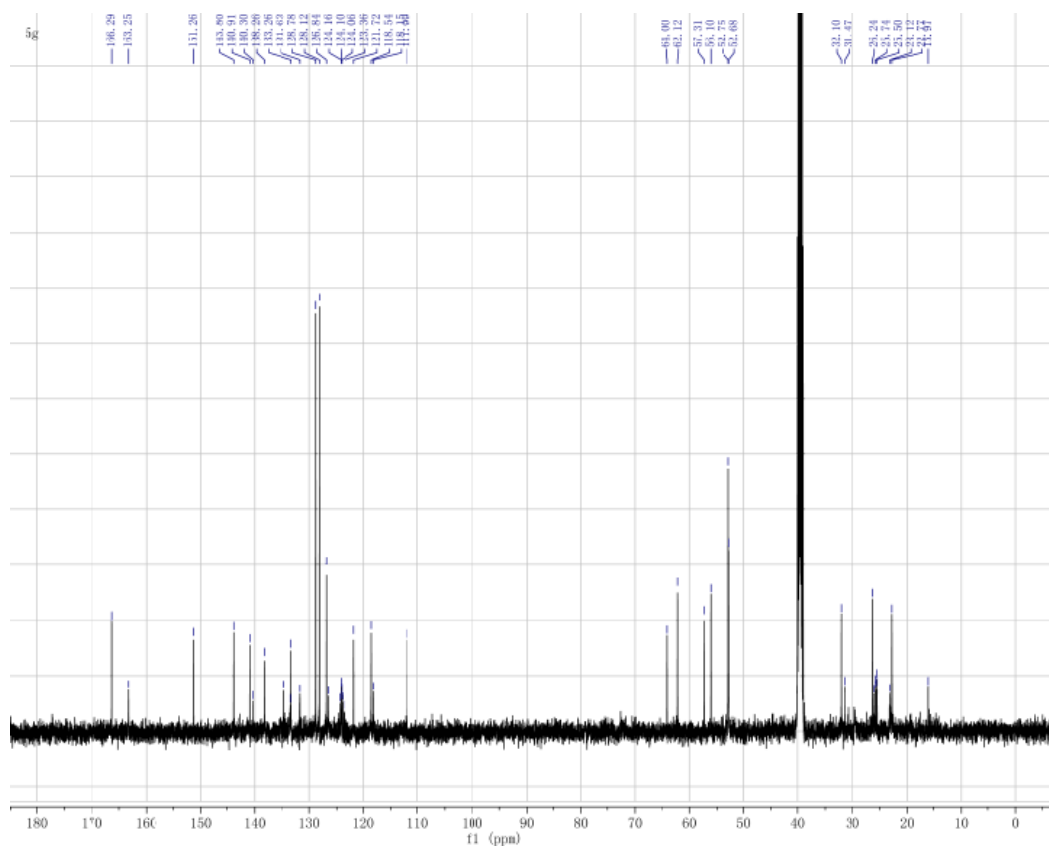


Fig. 30. The  $^{13}\text{C}$  NMR spectra for **5g**

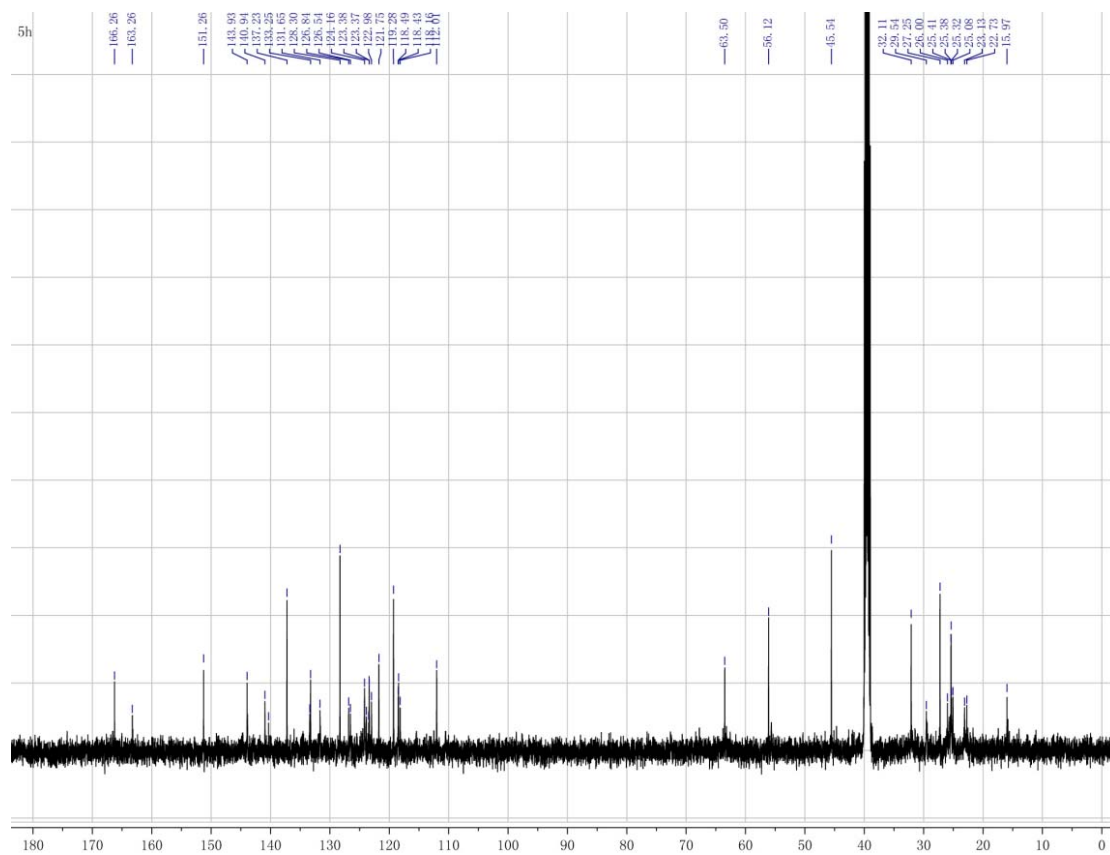


Fig. 31. The  $^{13}\text{C}$  NMR spectra for **5h**

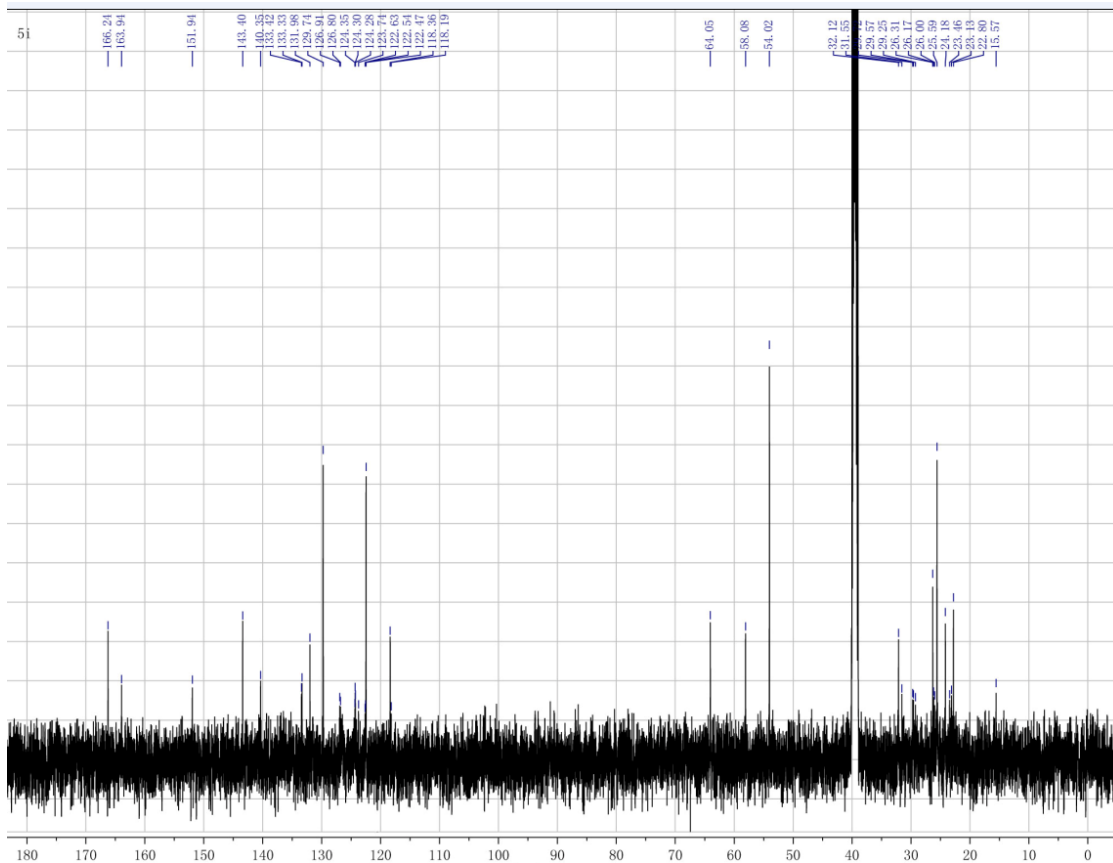


Fig. 32. The  $^{13}\text{C}$  NMR spectra for **5i**

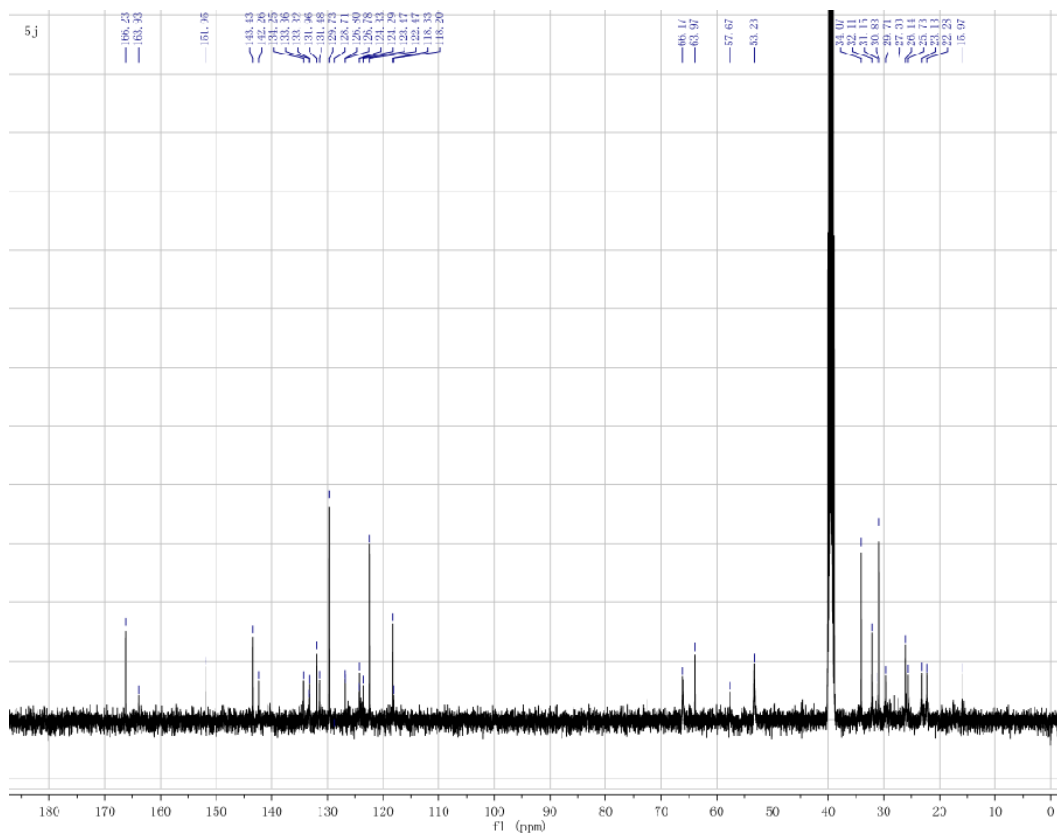


Fig. 33. The  $^{13}\text{C}$  NMR spectra for **5j**

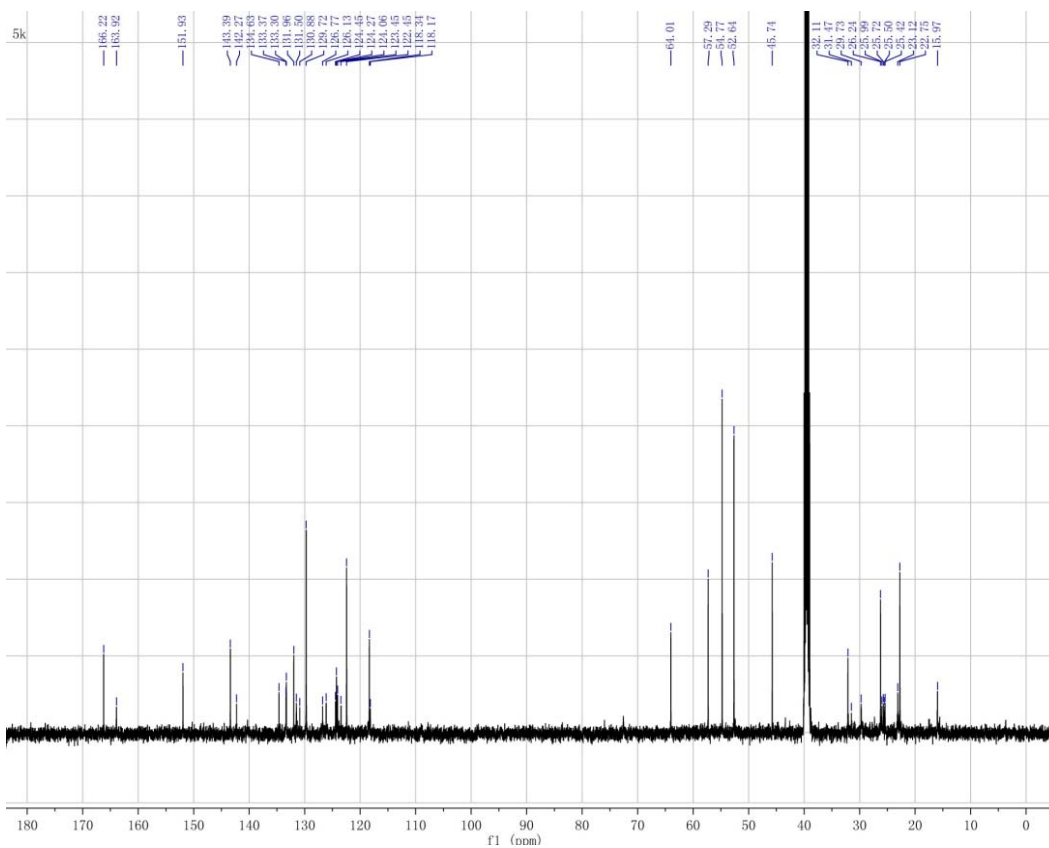


Fig. 34. The  $^{13}\text{C}$  NMR spectra for **5k**

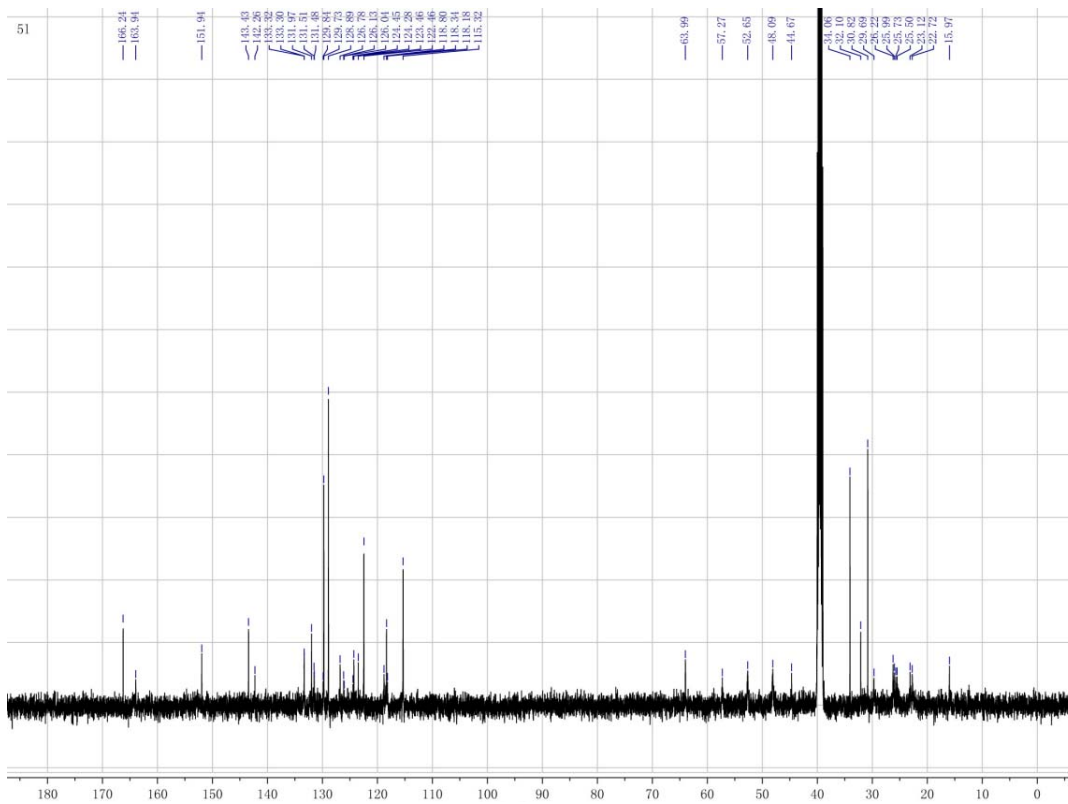


Fig. 35. The  $^{13}\text{C}$  NMR spectra for **5l**

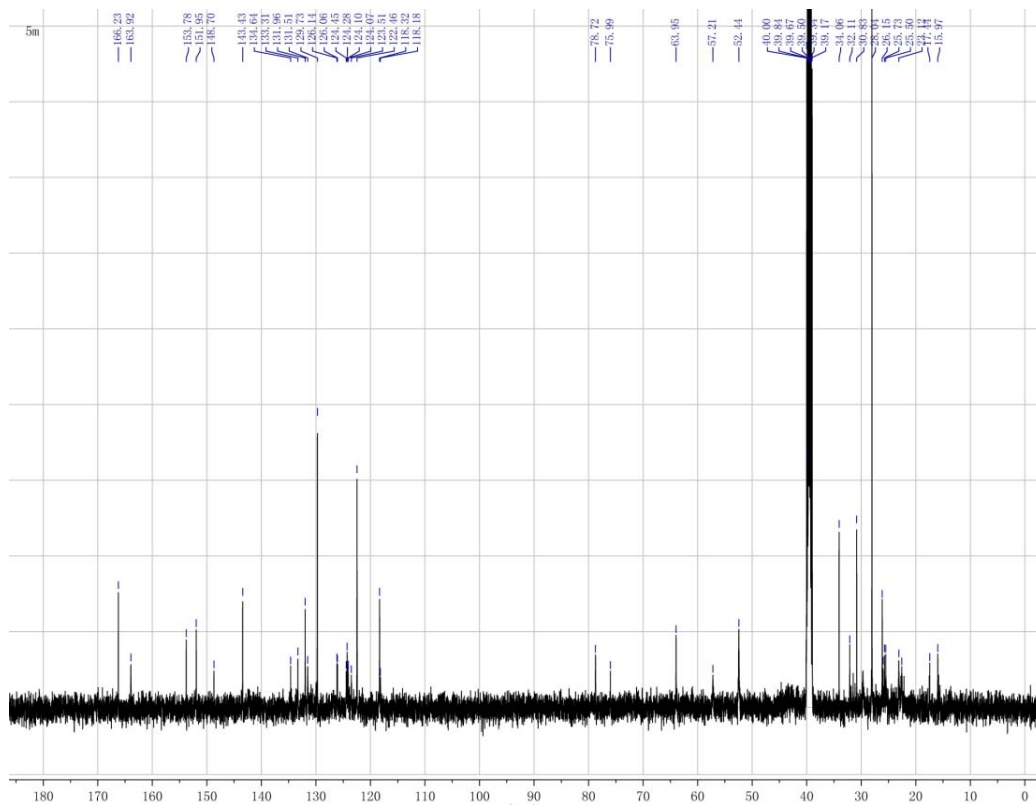


Fig. 36. The  $^{13}\text{C}$  NMR spectra for **5m**

5n  $^{13}\text{C}$ -NMR DMSO-D6 300K AV-300

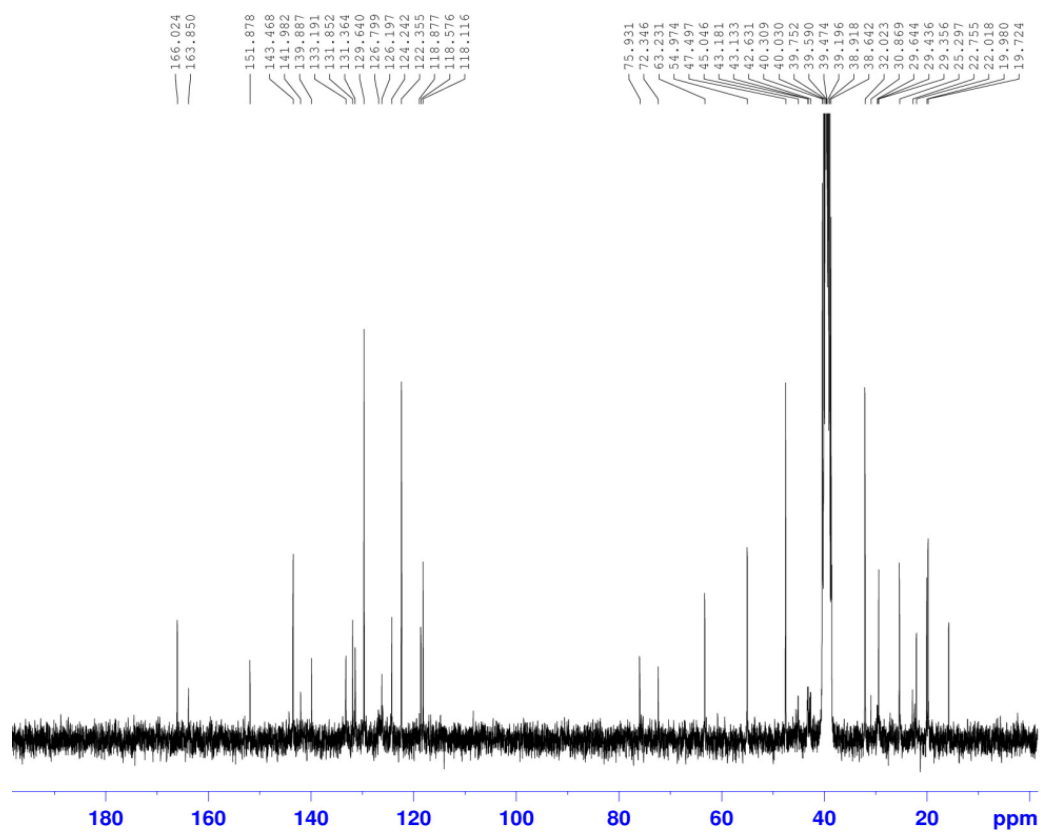


Fig. 37. The  $^{13}\text{C}$  NMR spectra for **5n**

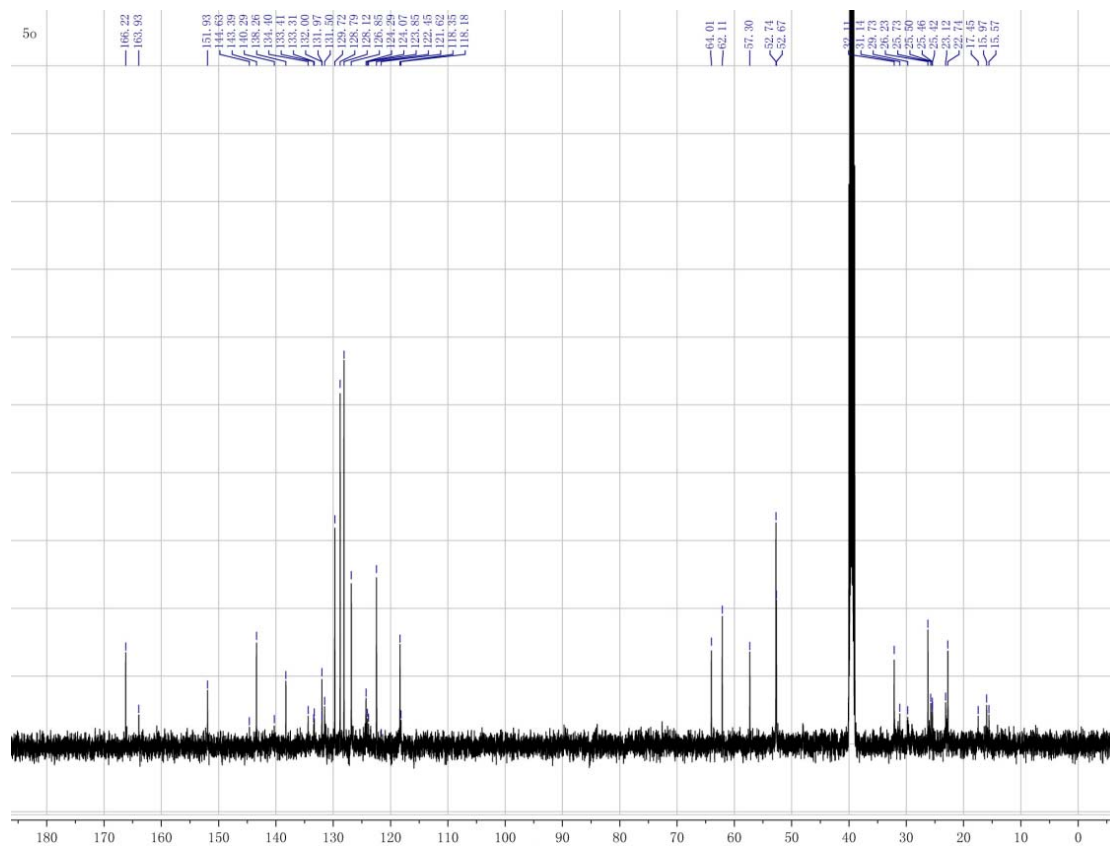


Fig. 38. The  $^{13}\text{C}$  NMR spectra for **5o**

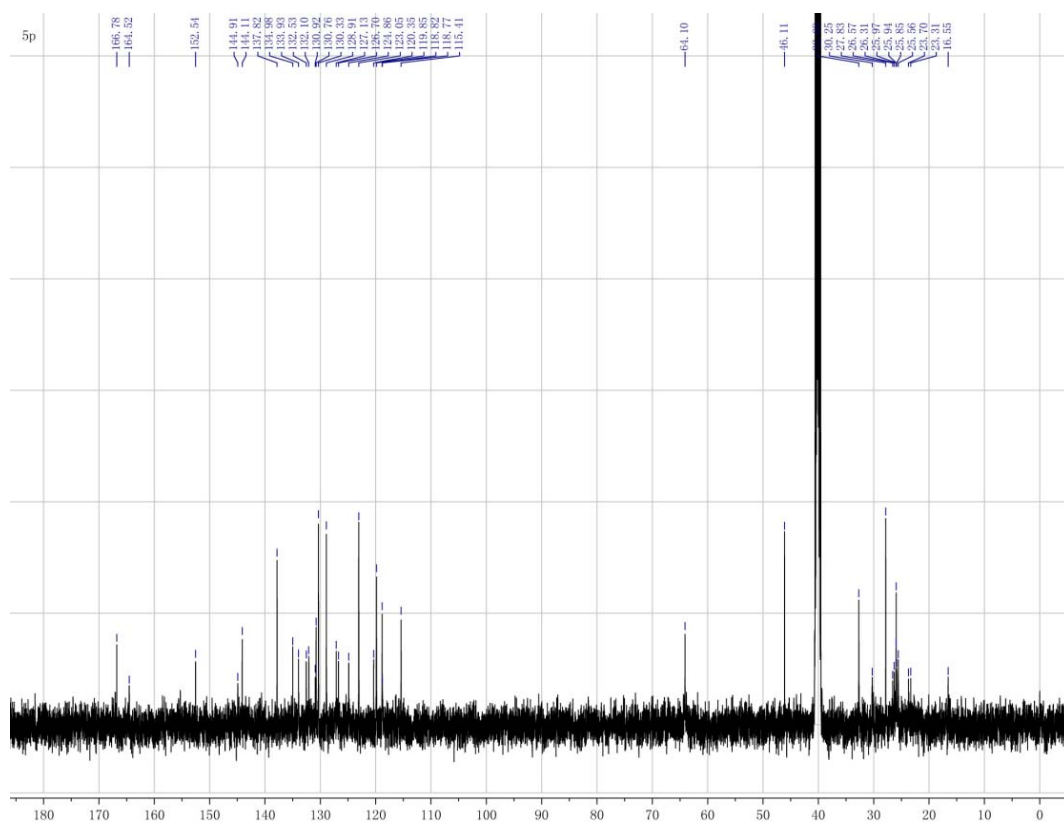


Fig. 39. The  $^{13}\text{C}$  NMR spectra for **5p**

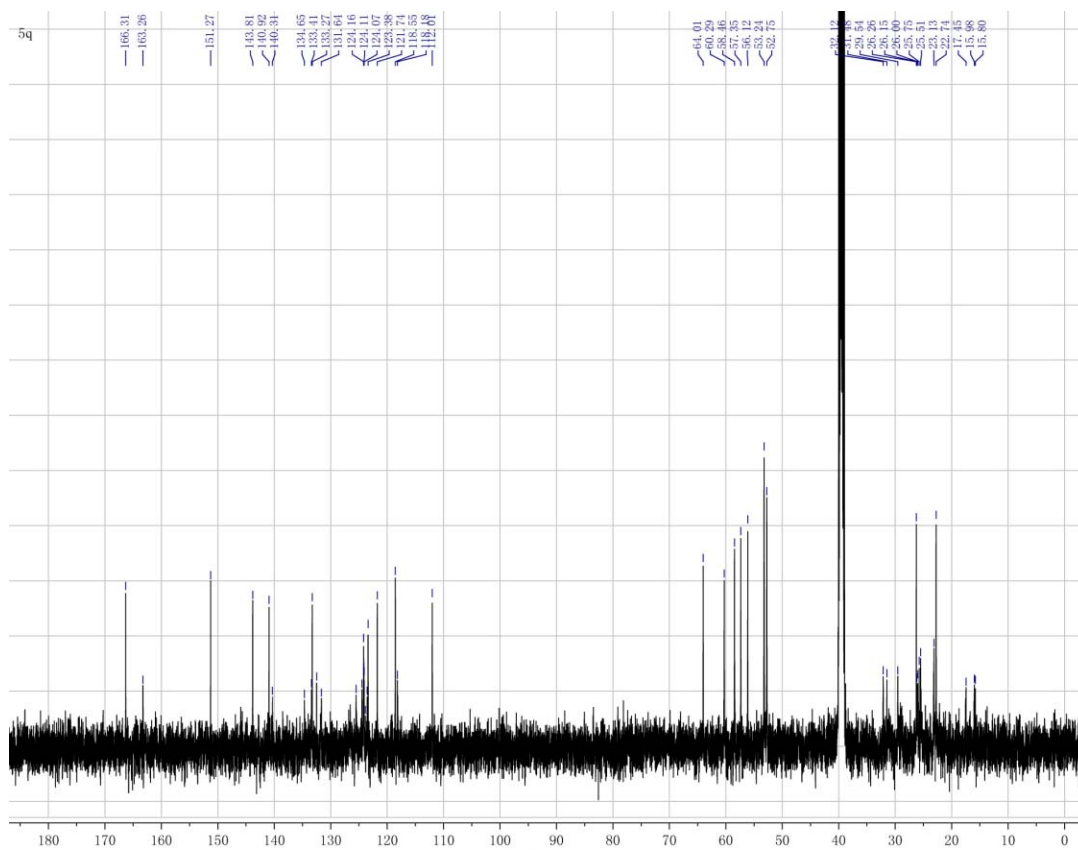


Fig. 40. The  $^{13}\text{C}$  NMR spectra for 5q

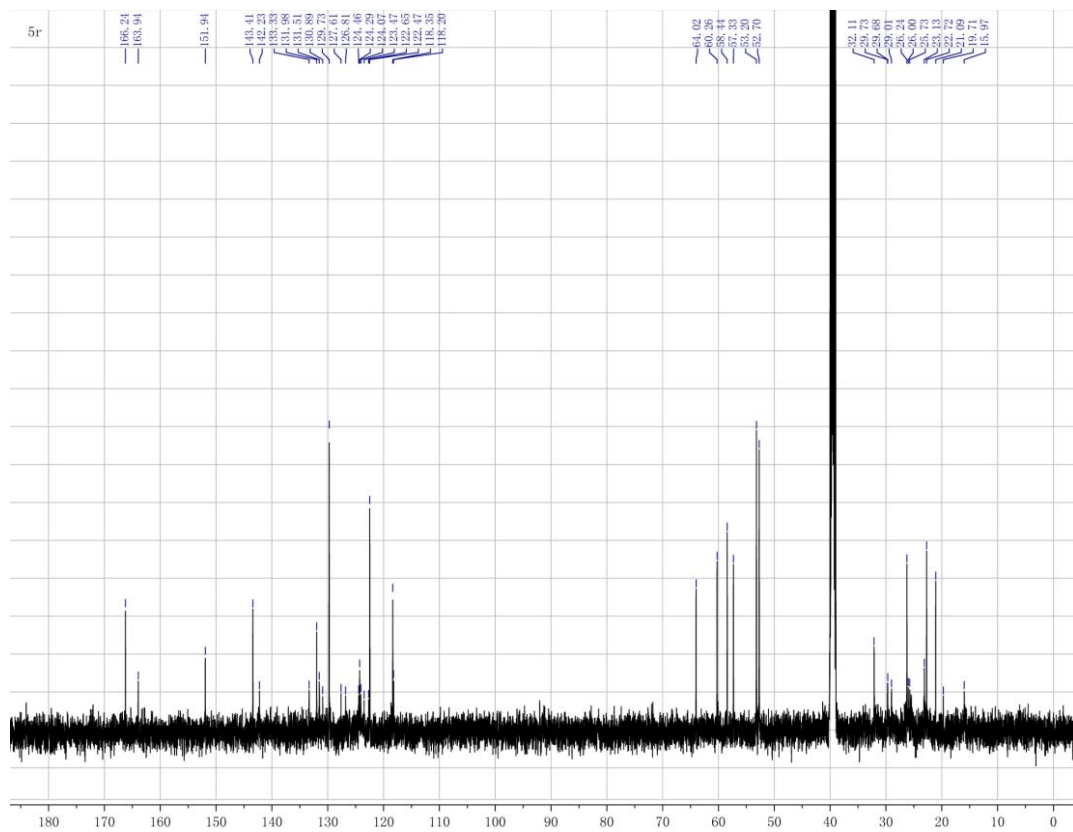


Fig. 41. The  $^{13}\text{C}$  NMR spectra for 5r

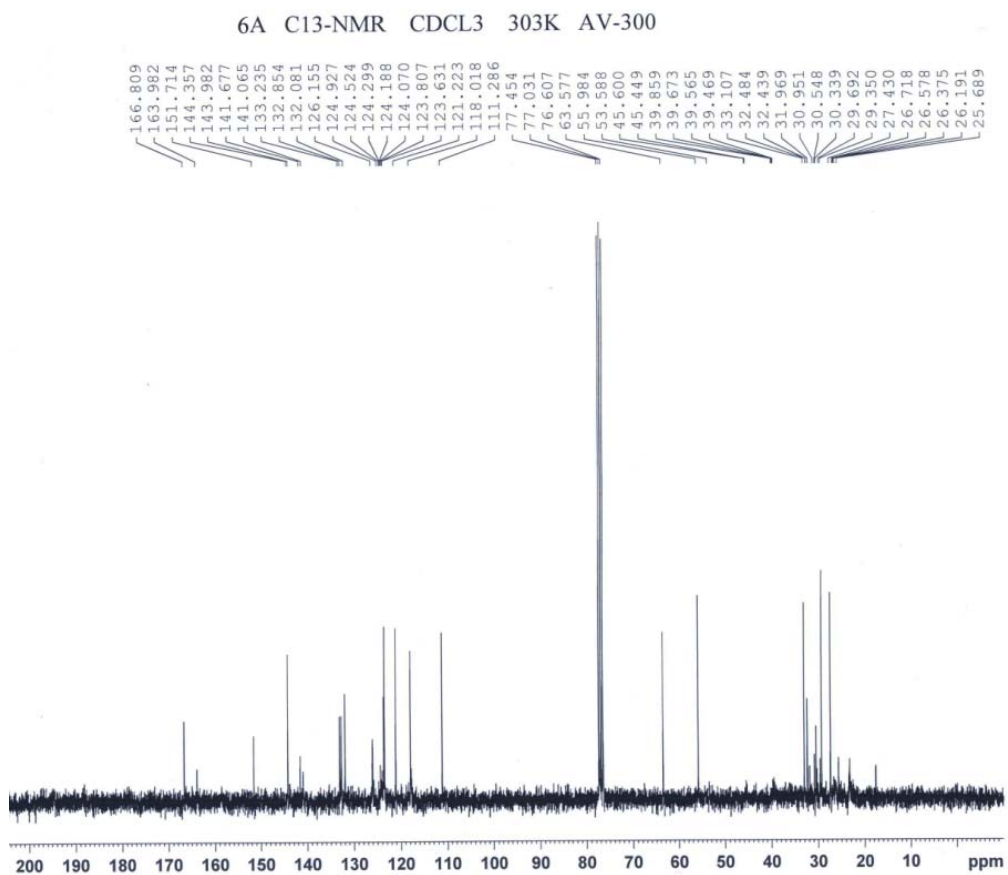


Fig. 42. The  $^{13}\text{C}$  NMR spectra for **6a**

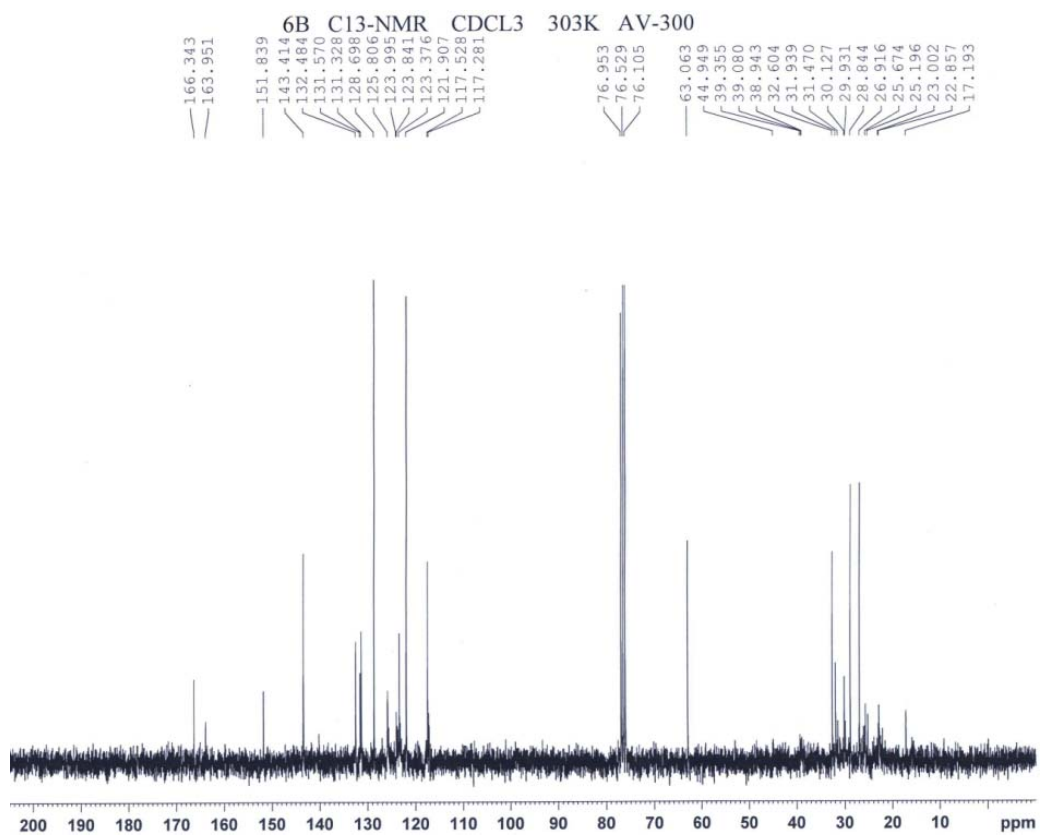


Fig. 43. The  $^{13}\text{C}$  NMR spectra for **6b**

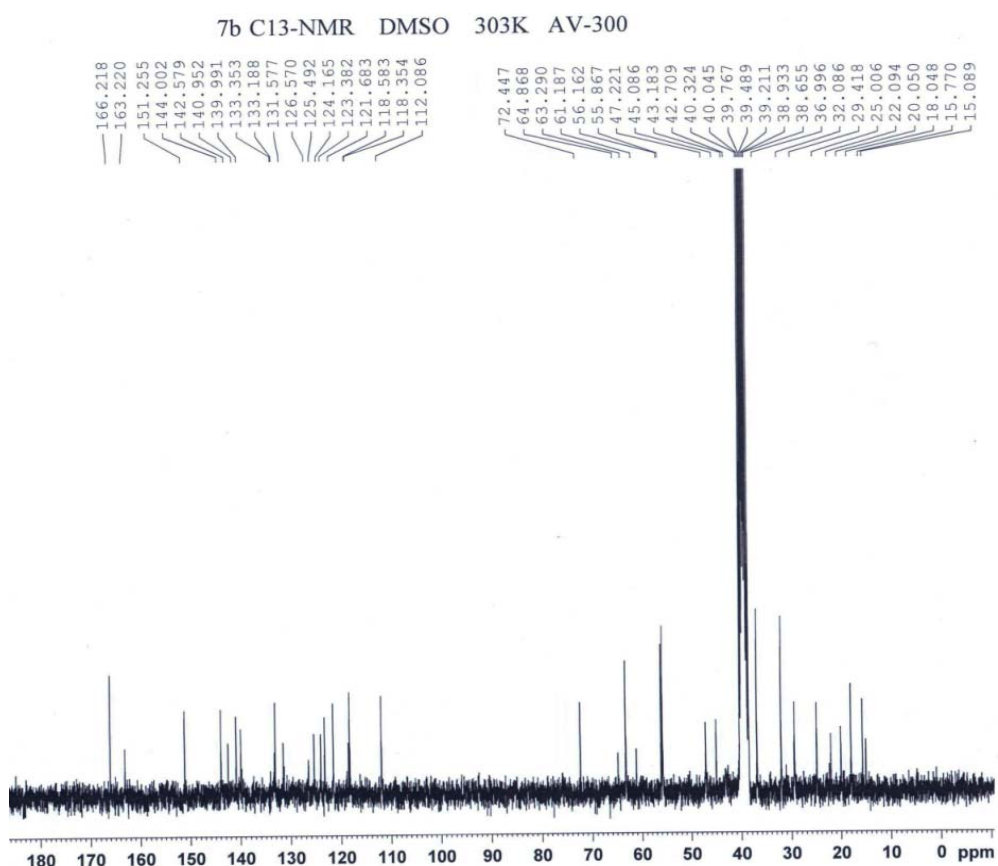


Fig. 44. The  $^{13}\text{C}$  NMR spectra for 7b

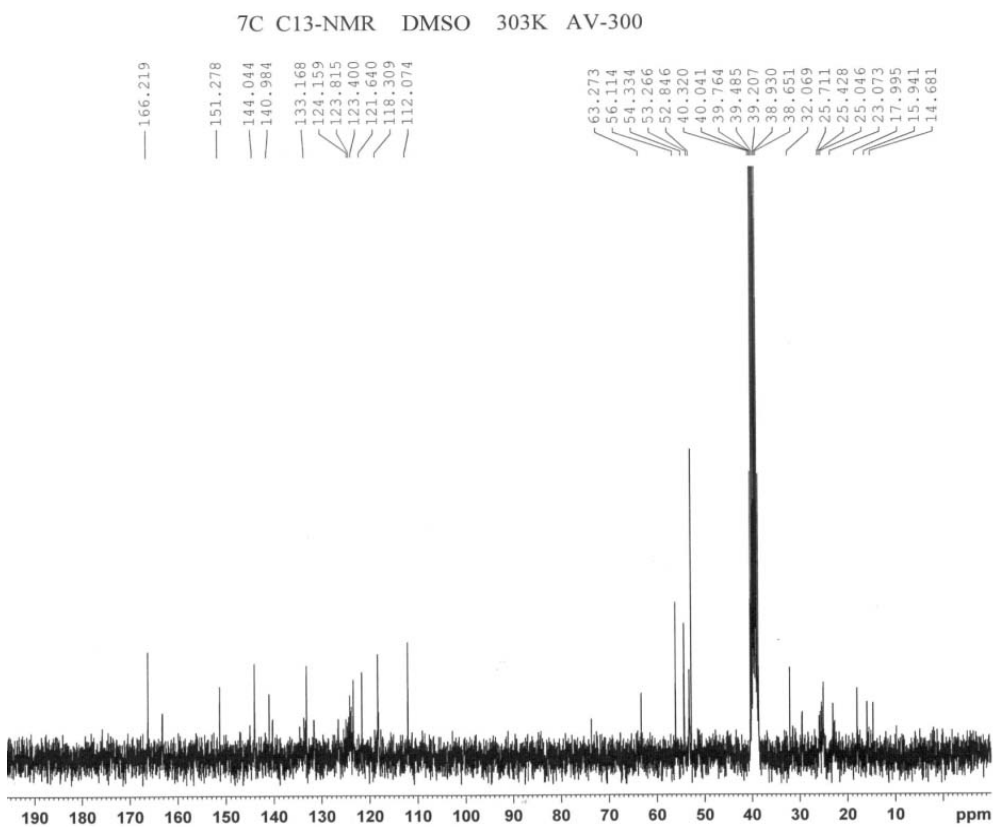


Fig. 45. The  $^{13}\text{C}$  NMR spectra for 7c



The HRMS spectra for **5a-5r**

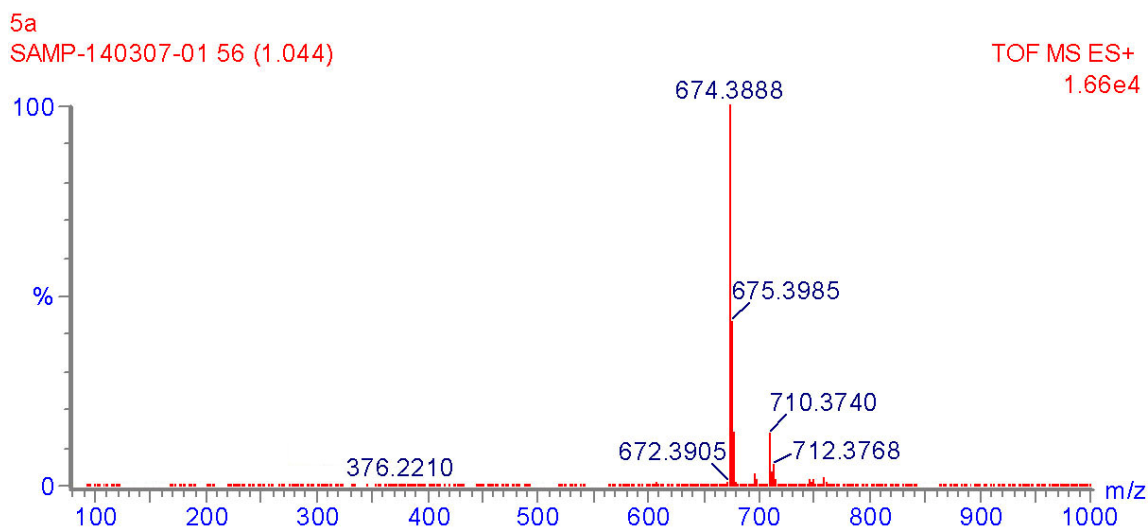


Fig. 46 HRMS spectrum of **5a**

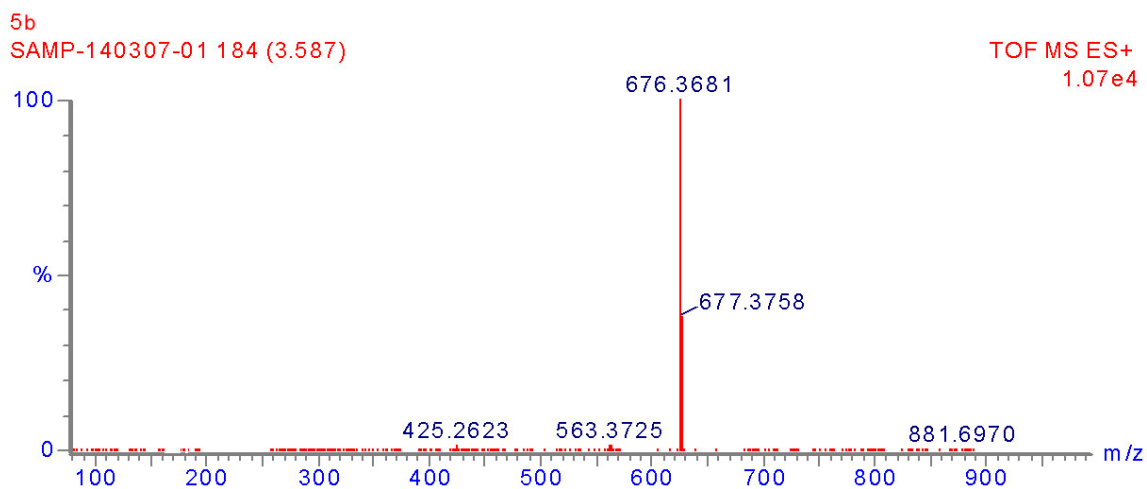


Fig. 47 HRMS spectrum of **5b**

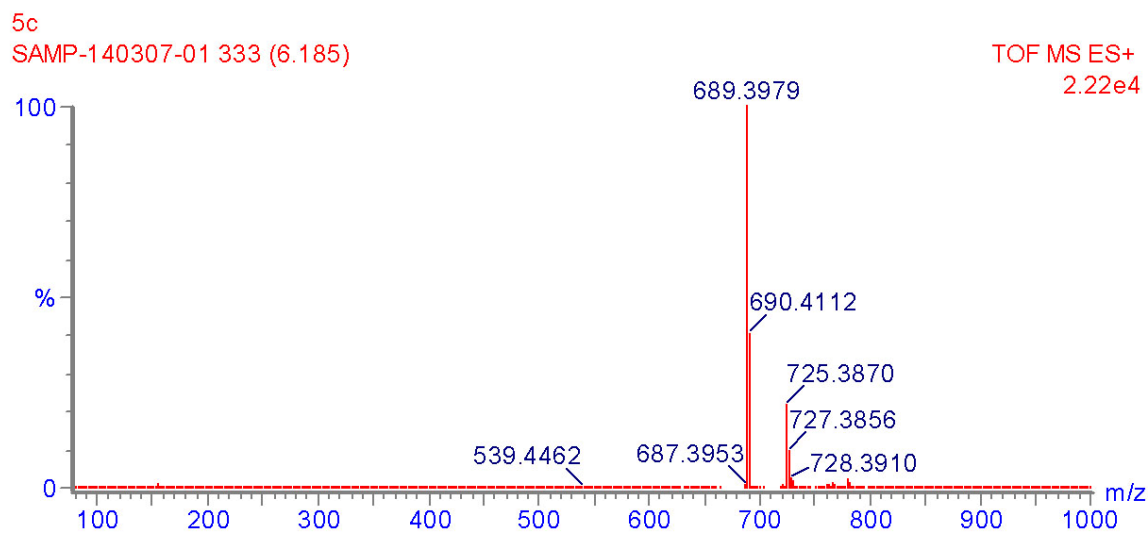


Fig. 48 HRMS spectrum of **5c**

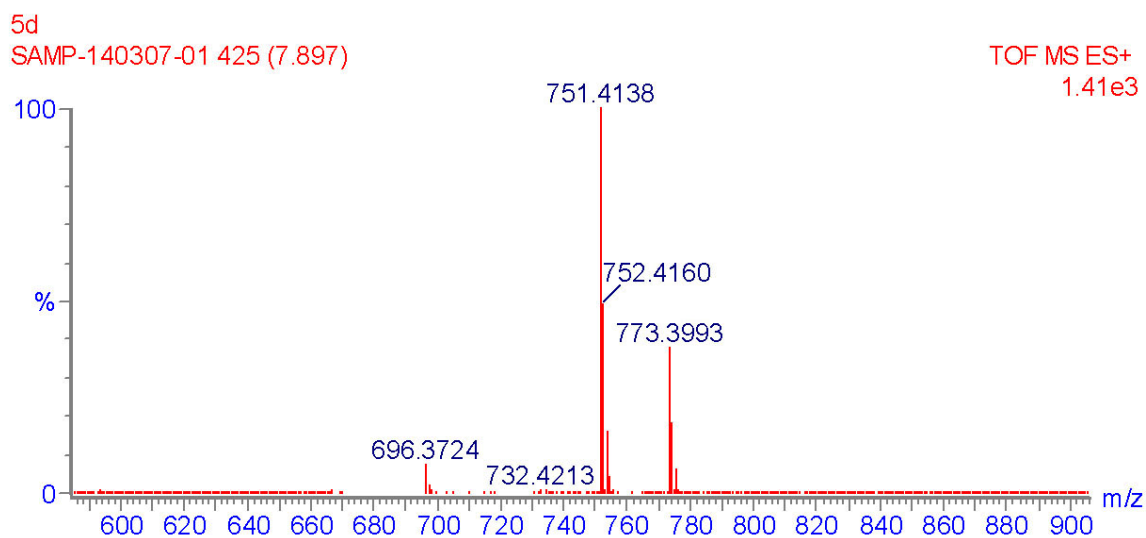


Fig. 49 HRMS spectrum of **5d**

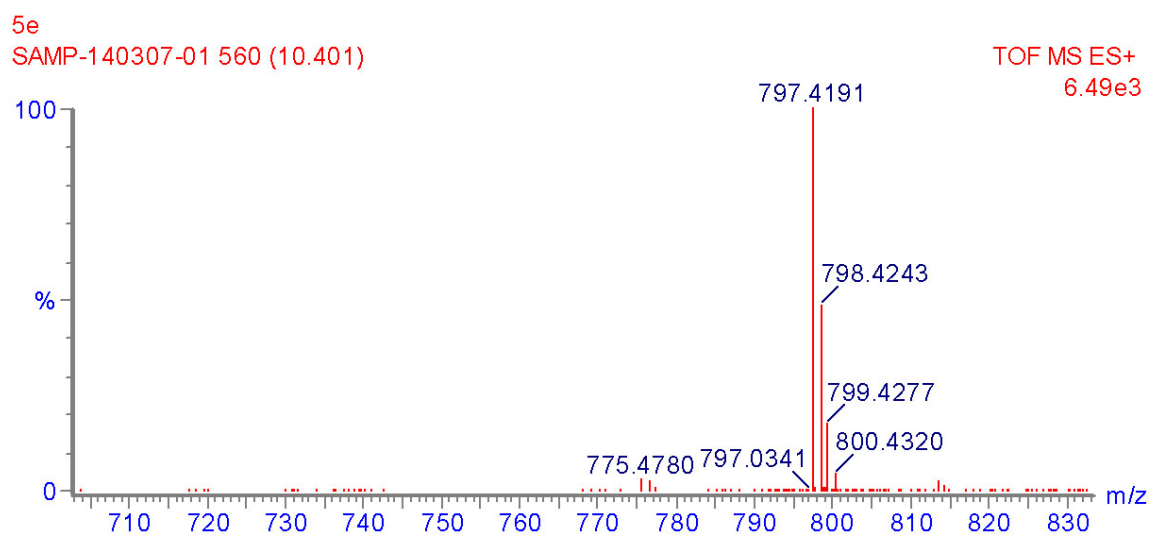


Fig. 50 HRMS spectrum of **5e**

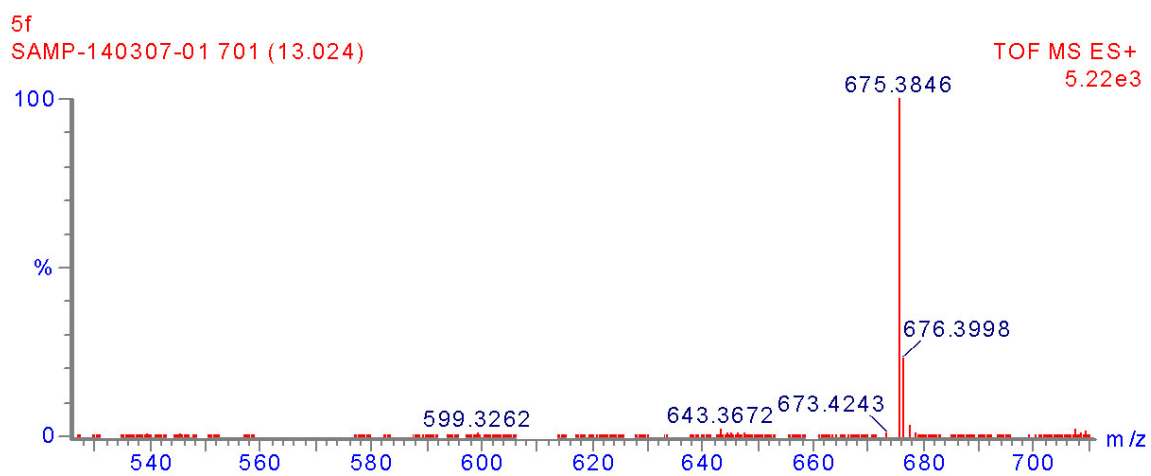


Fig. 51 HRMS spectrum of **5f**

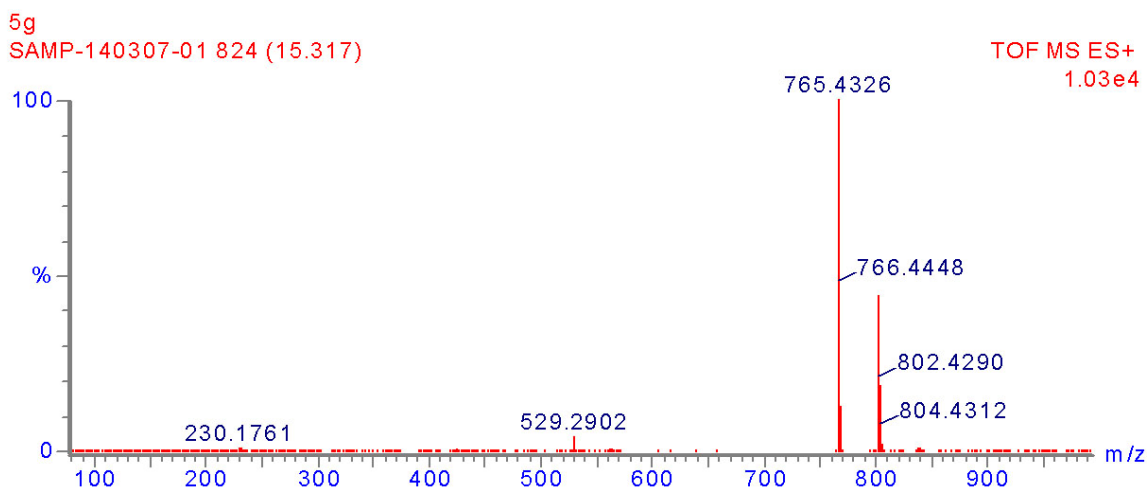


Fig. 52 HRMS spectrum of **5g**

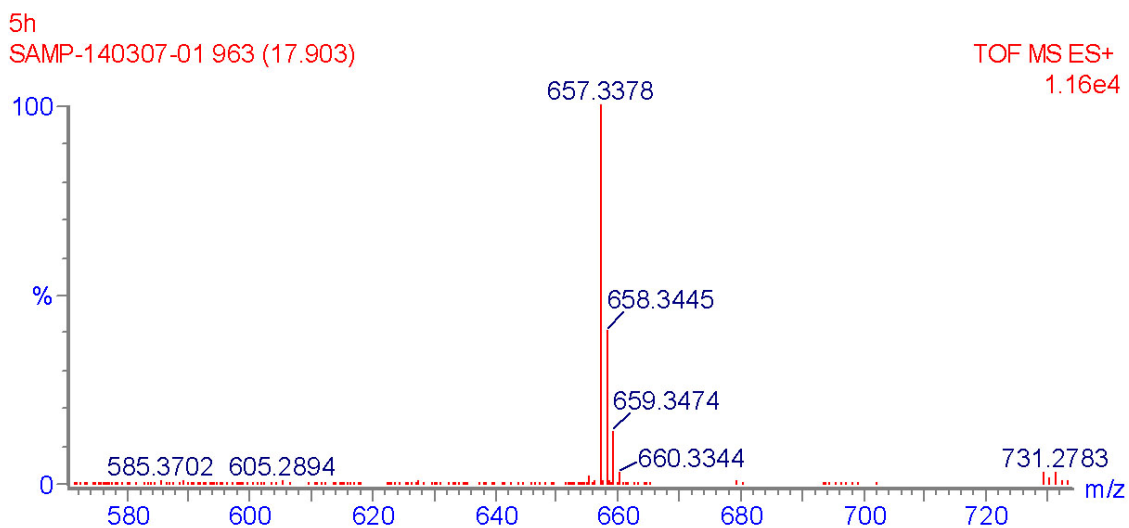


Fig. 53 HRMS spectrum of **5h**

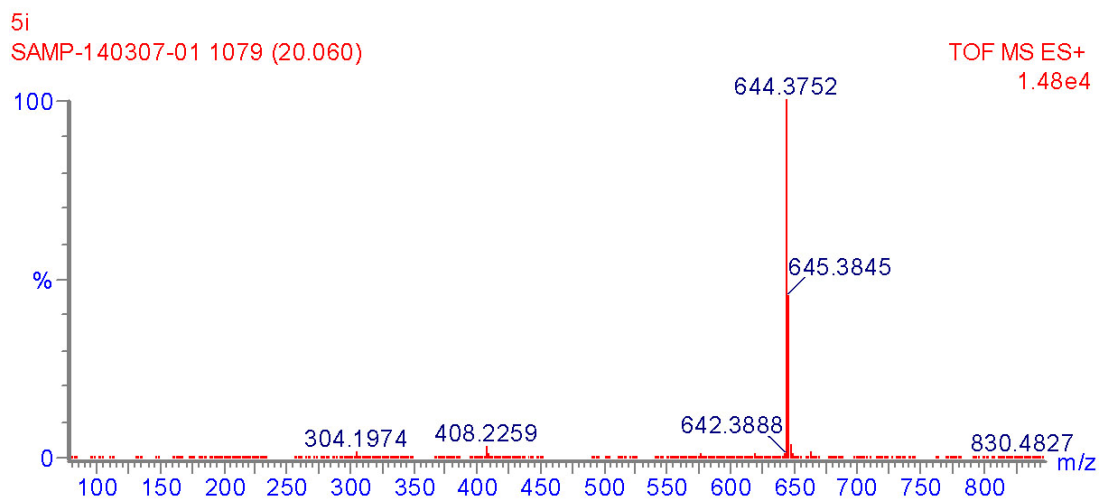


Fig. 54 HRMS spectrum of **5i**

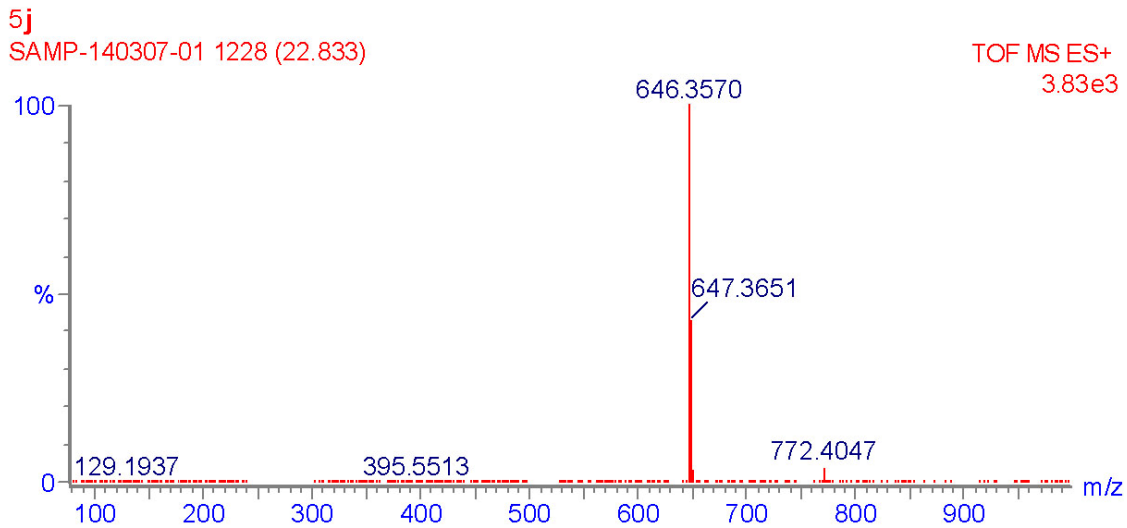


Fig. 55 HRMS spectrum of 5j

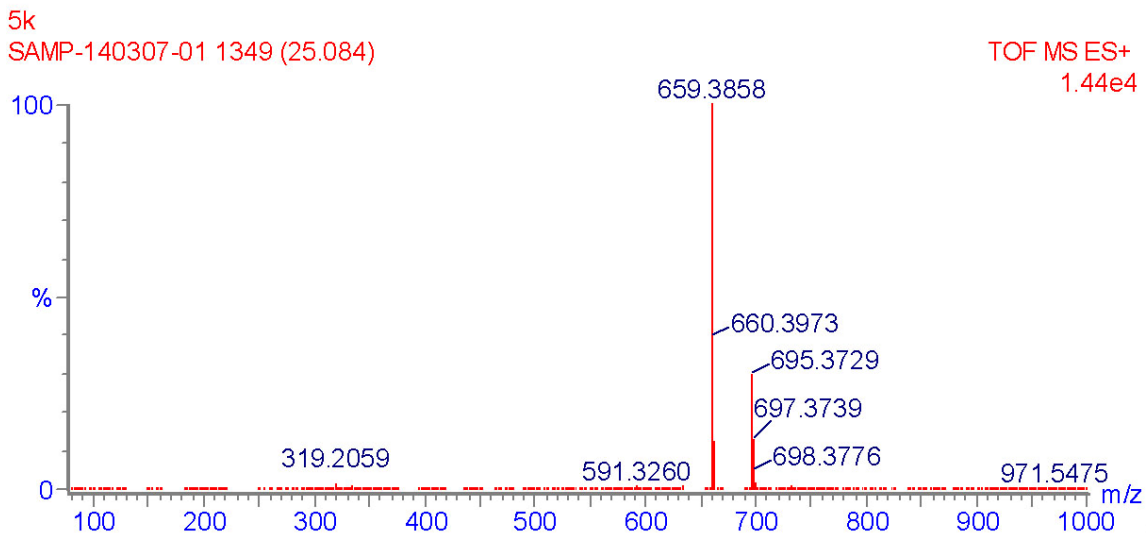


Fig. 56 HRMS spectrum of 5k

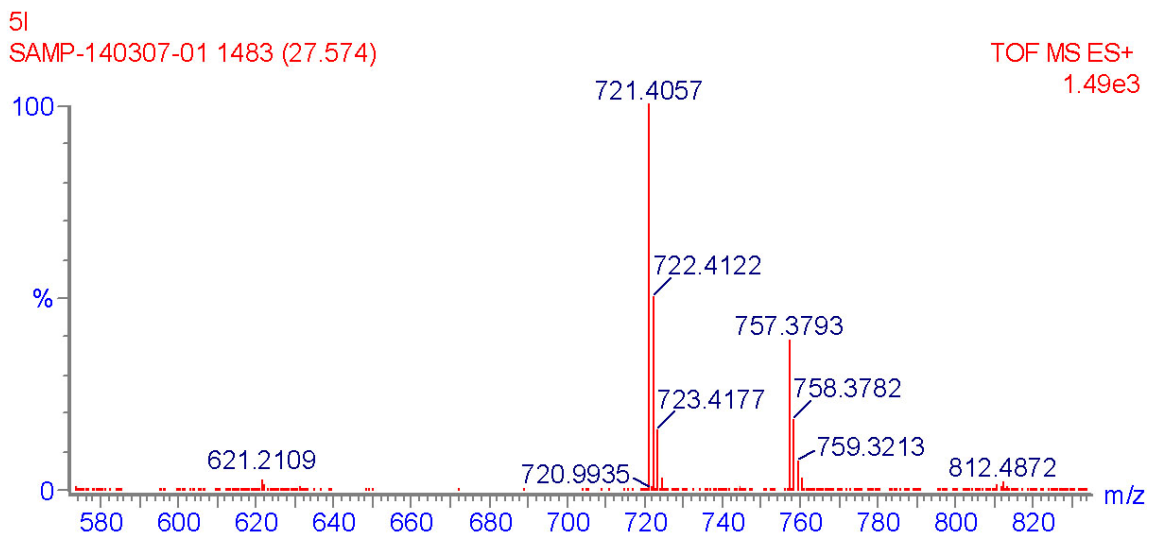


Fig. 57 HRMS spectrum of 5l

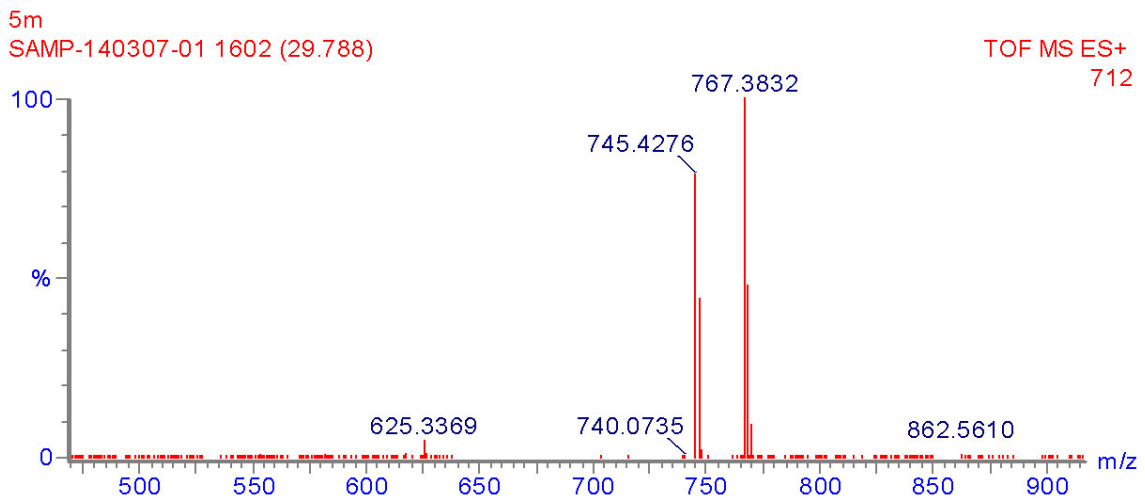


Fig. 58 HRMS spectrum of **5m**

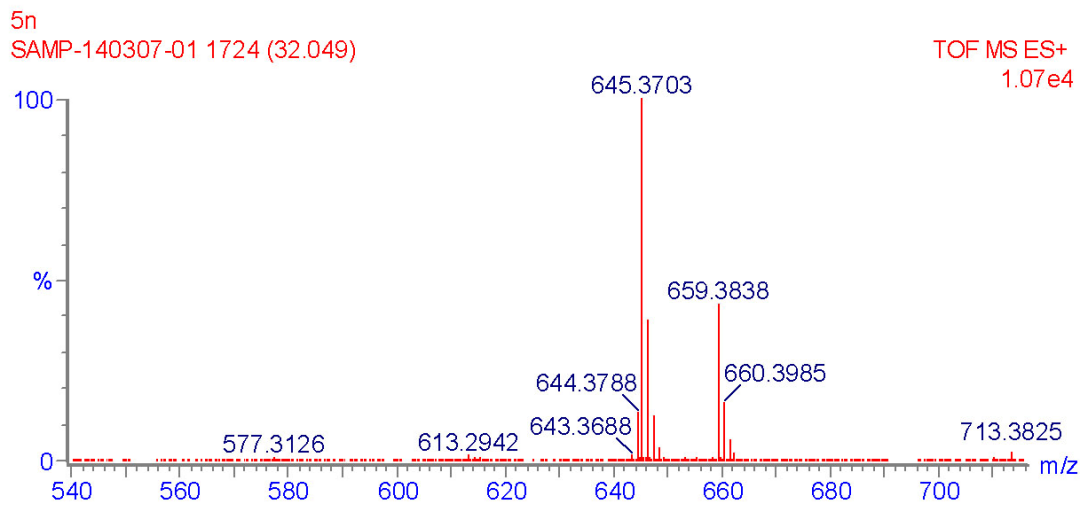


Fig. 59 HRMS spectrum of **5n**

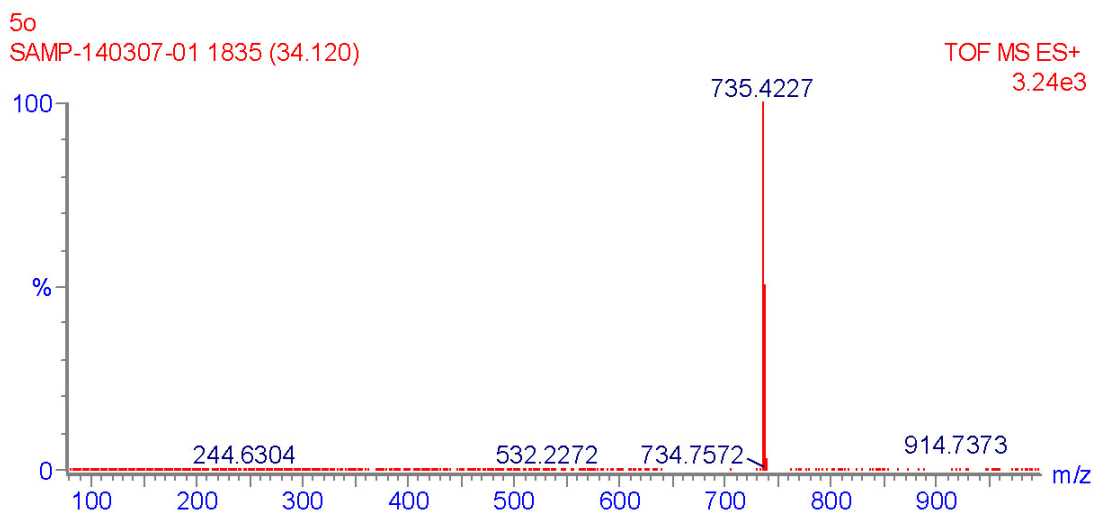


Fig. 60 HRMS spectrum of **5o**

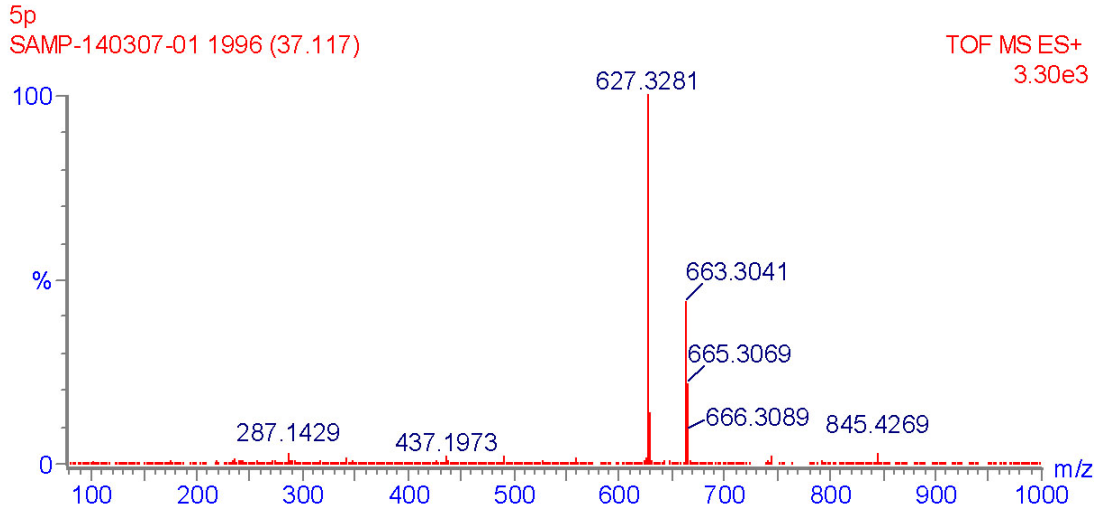


Fig. 61 HRMS spectrum of **5p**

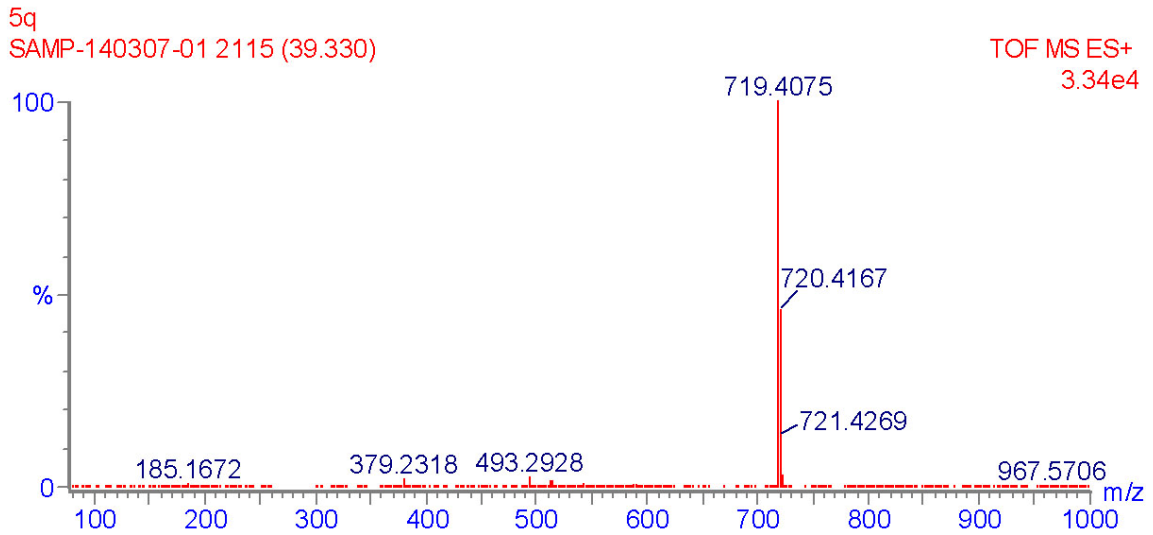


Fig. 62 HRMS spectrum of **5q**

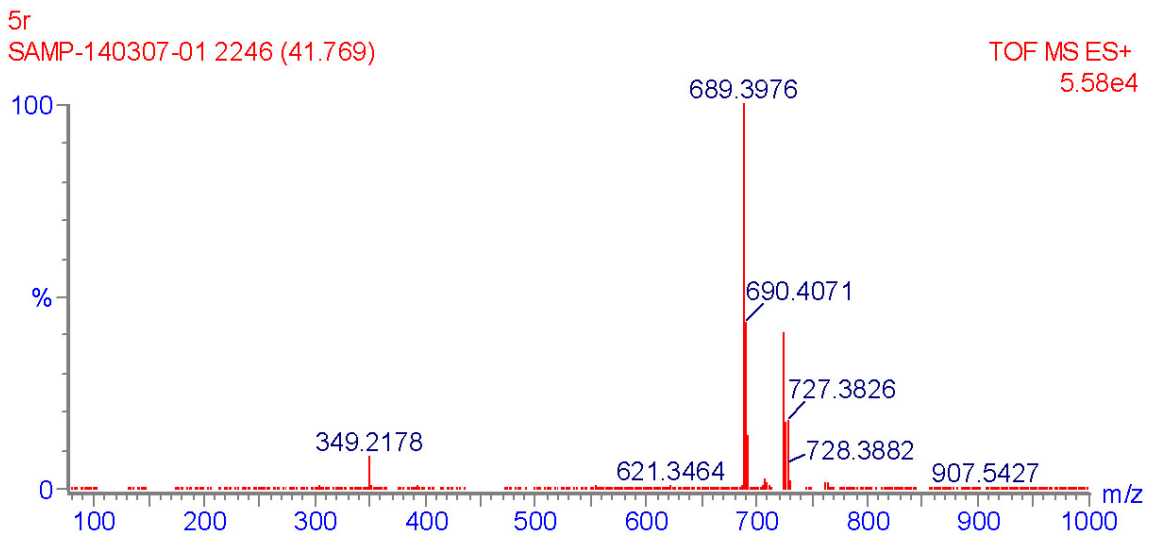


Fig. 63 HRMS spectrum of **5r**

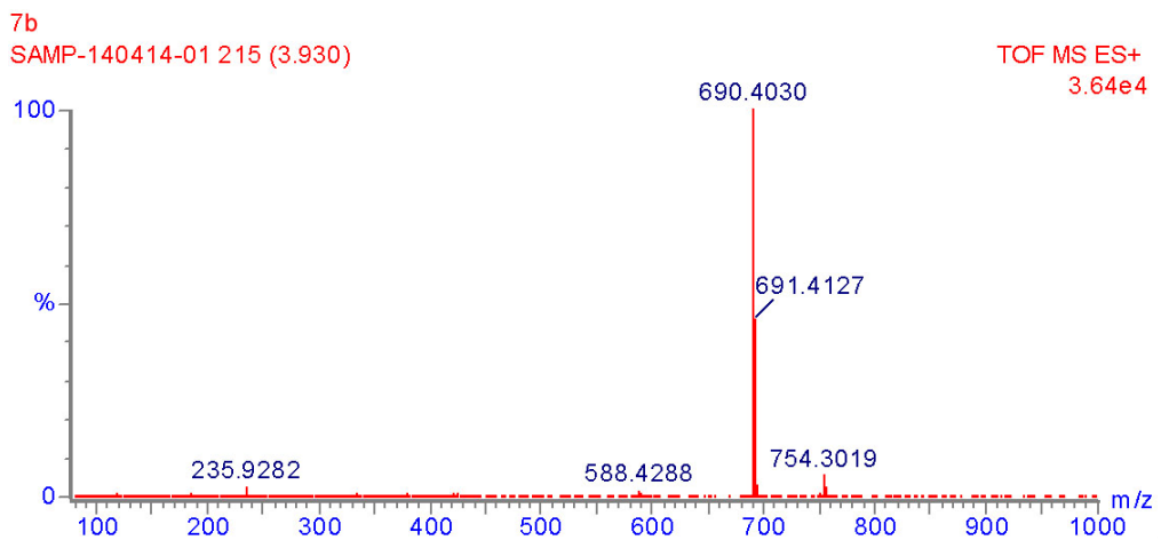


Fig. 64 HRMS spectrum of 7b

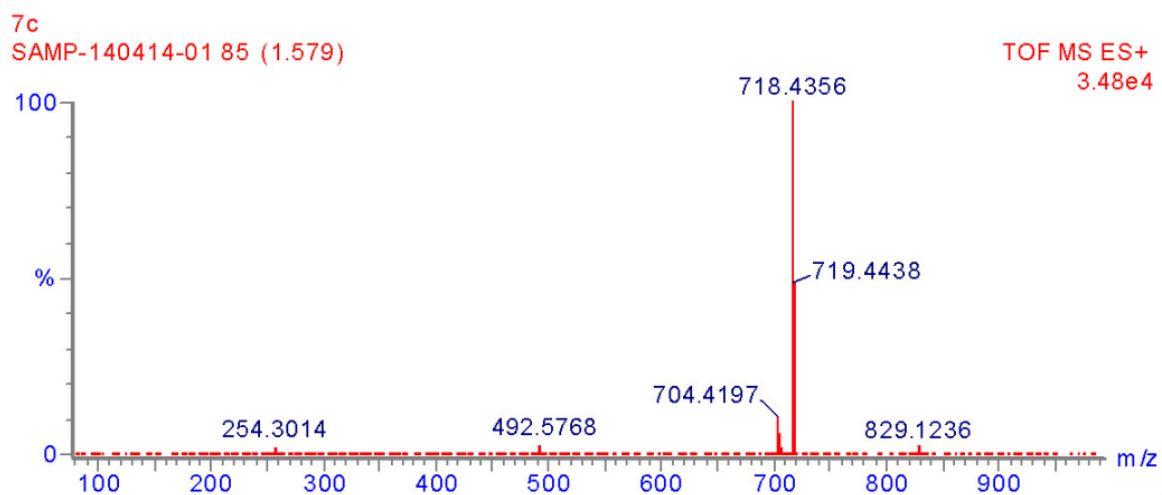


Fig. 65 HRMS spectrum of 7c