

SUPPLEMENTARY INFORMATION

**Design, Synthesis and Anticancer evaluation of Imamine-1,3,5-triazine derivatives**

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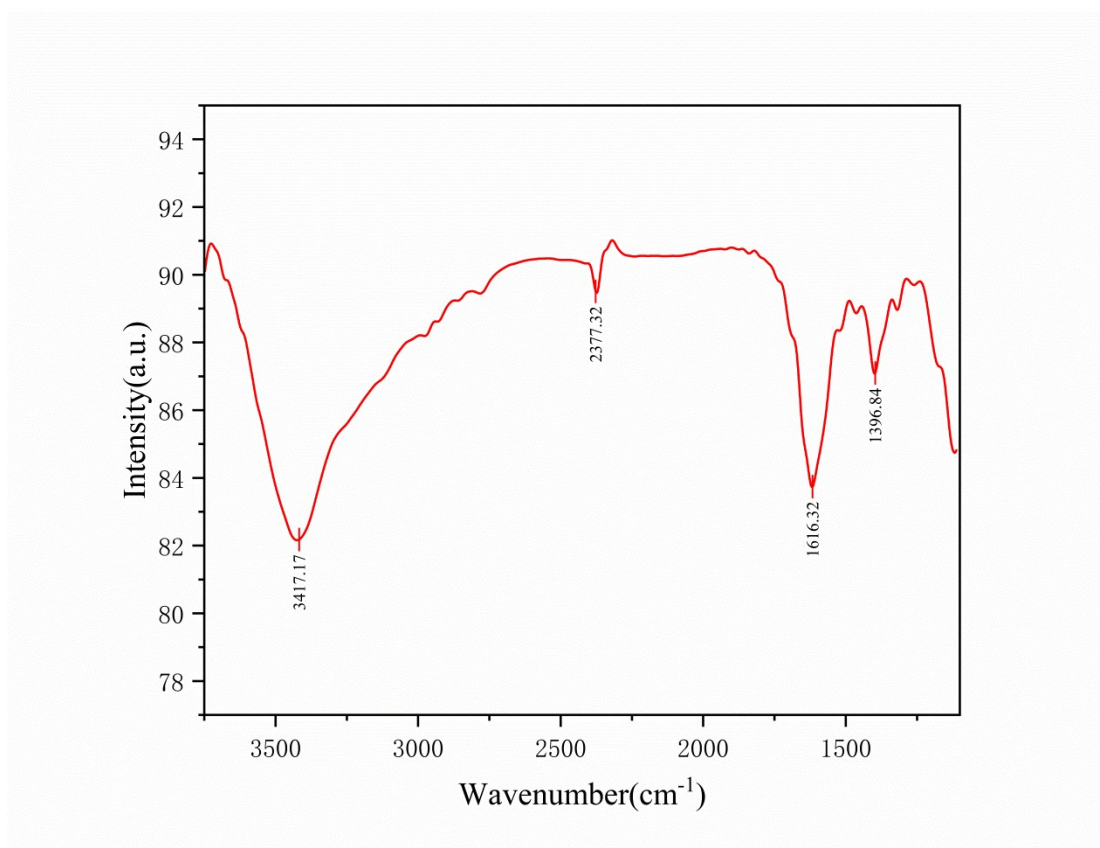


Figure 1 The IR spectrum of compound 4a

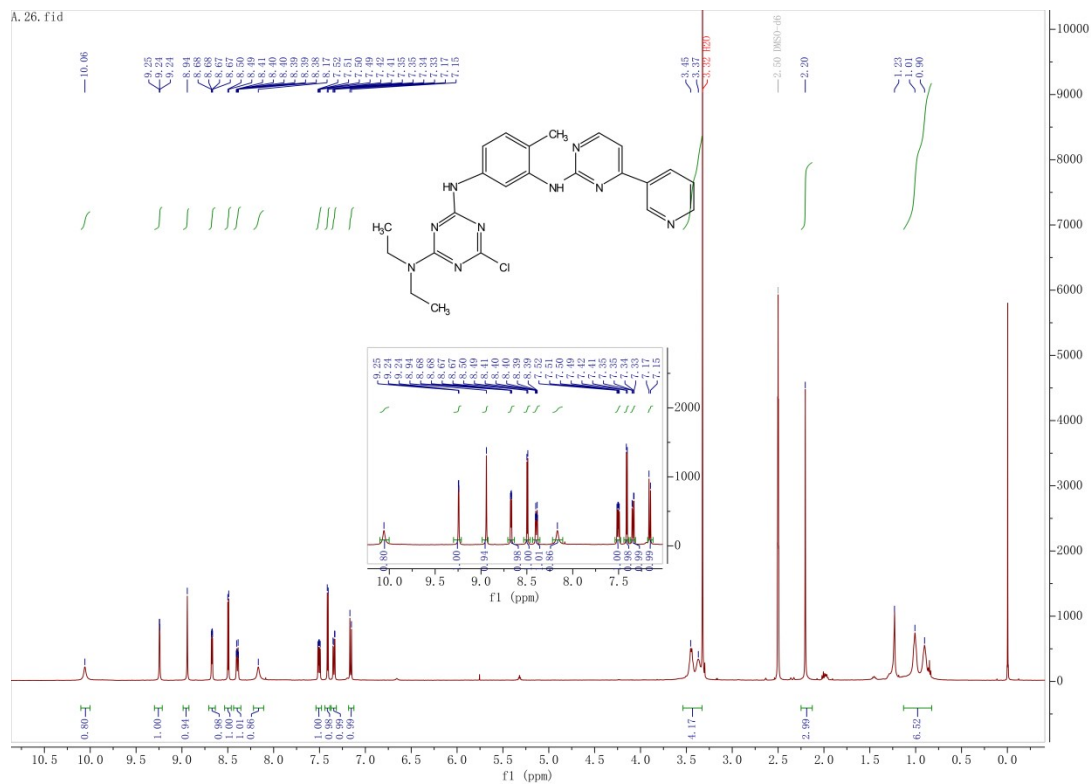


Figure 2 The <sup>1</sup>H NMR spectrum of compound 4a

15 C/11

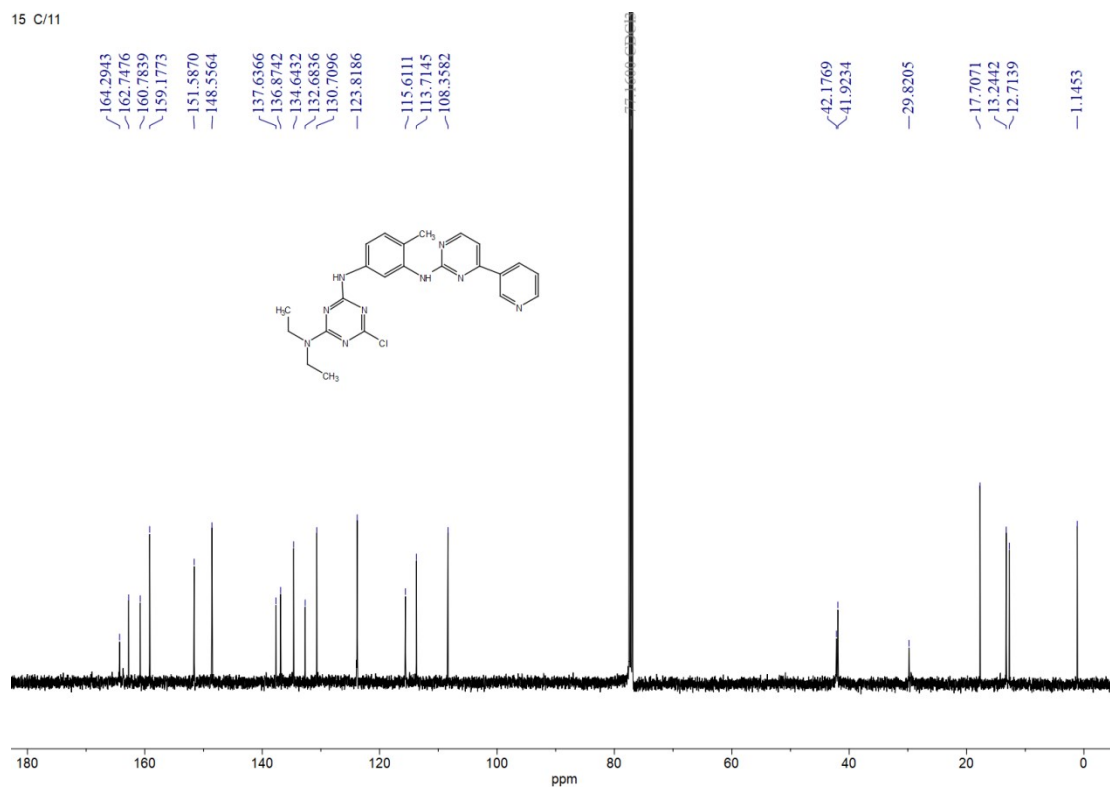


Figure 3 The <sup>13</sup>C NMR spectrum of compound 4a

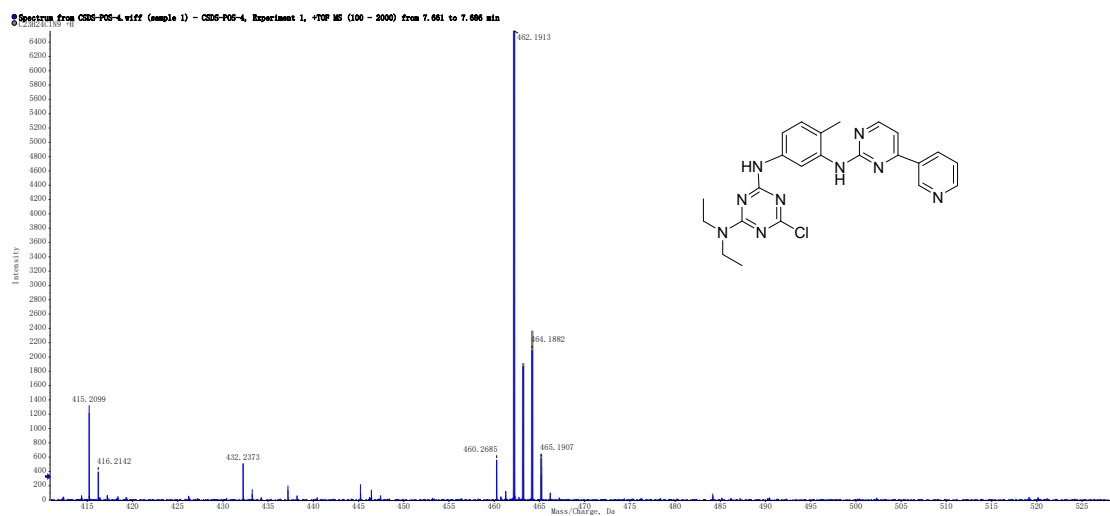
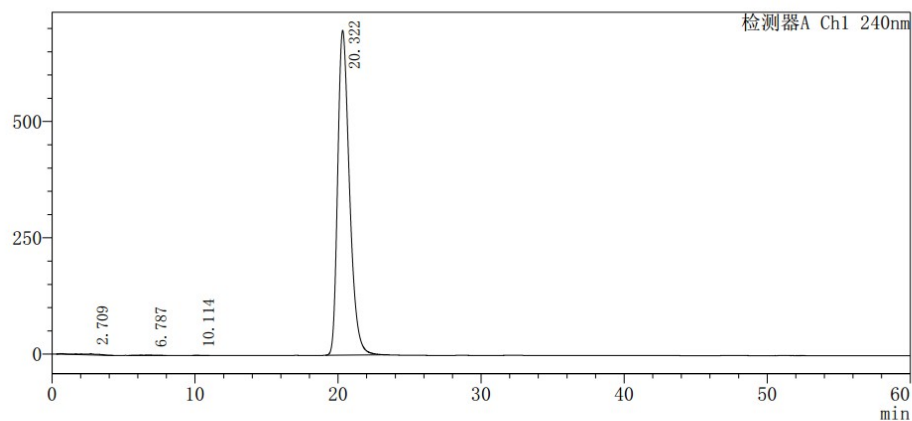


Figure 4 The HRMS spectrum of compound 4a

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mV



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	2.709	264143	2922	0.656		M	
2	6.787	71808	724	0.178		M	
3	10.114	9297	417	0.023		M	
4	20.322	39933254	697798	99.143		M	
总计		40278502	701861				

Figure 5 The HPLC of compound 4a

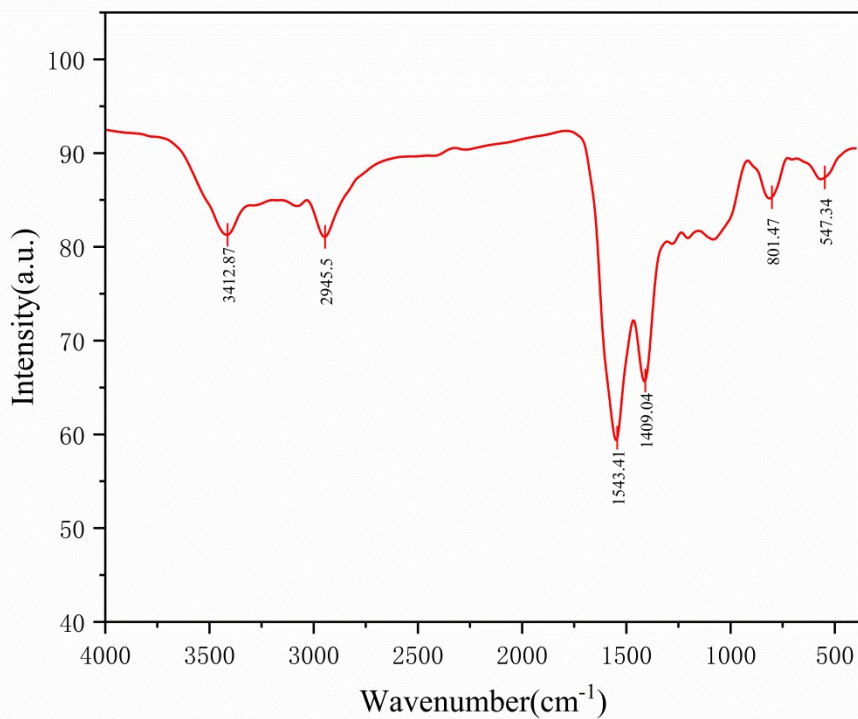


Figure 6 The IR spectrum of compound 4b

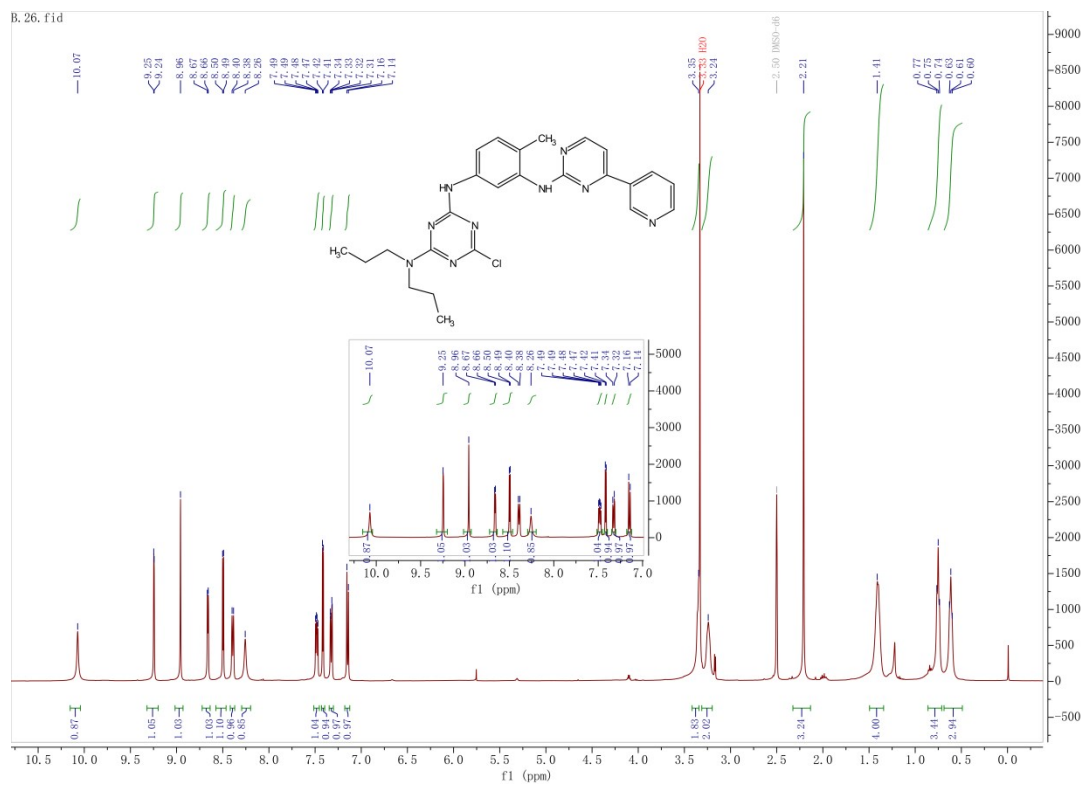


Figure 7 The  $^1\text{H}$  NMR spectrum of compound **4b**

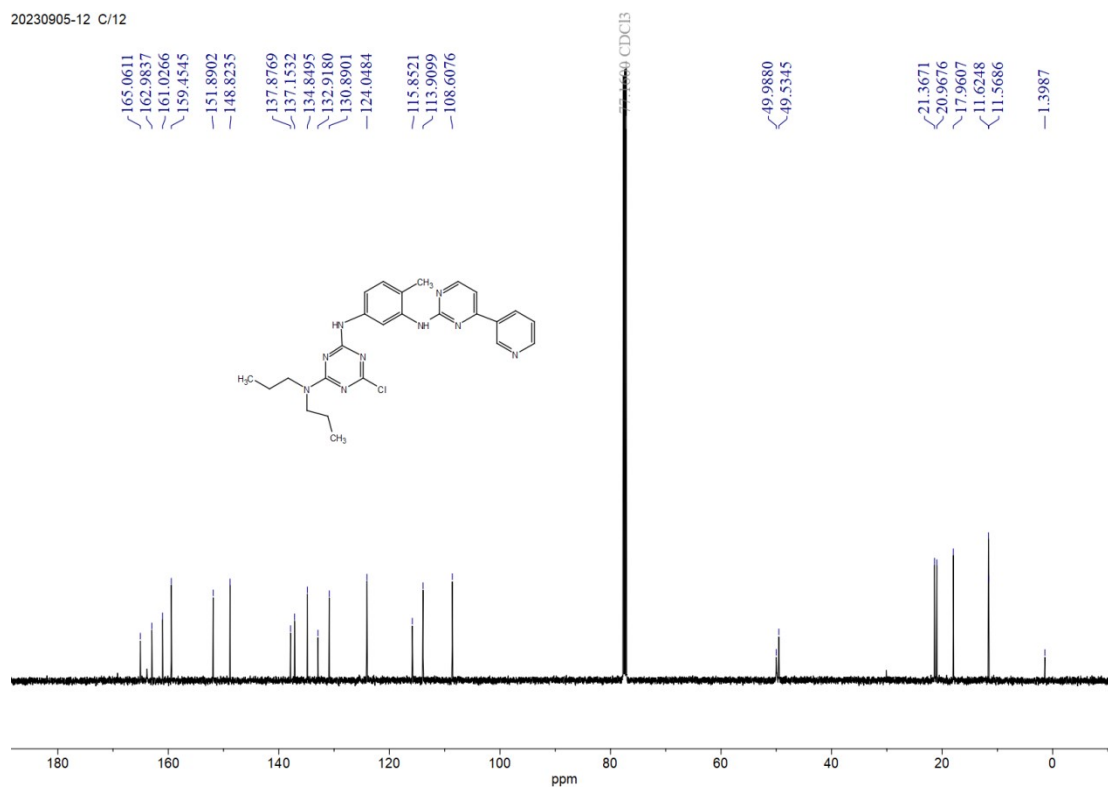


Figure 8 The  $^{13}\text{C}$  NMR spectrum of compound **4b**

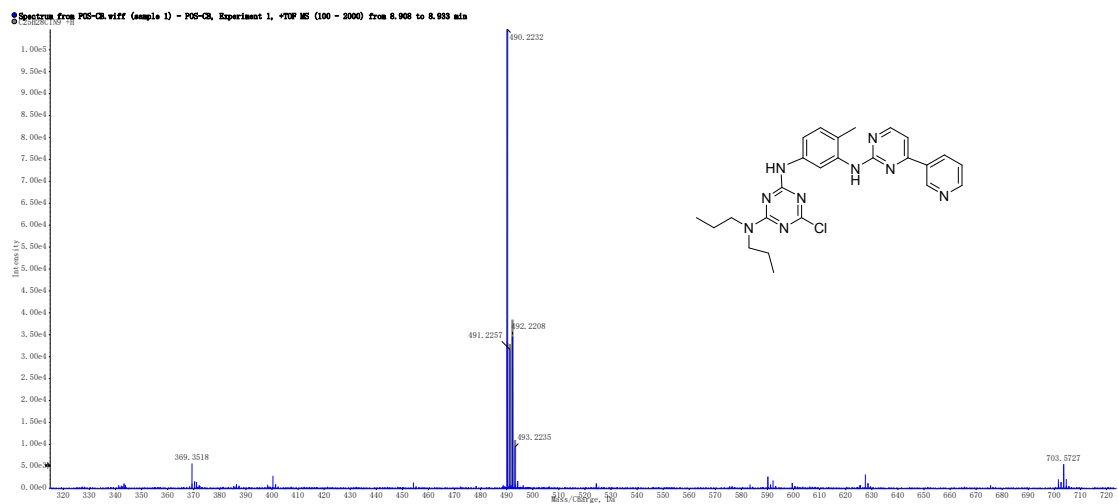
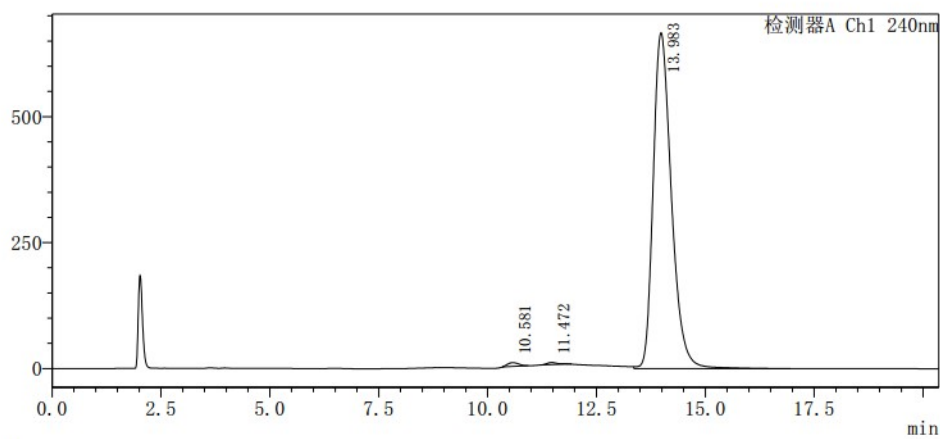


Figure 9 The HRMS spectrum of compound 4b

<色谱图>

mV



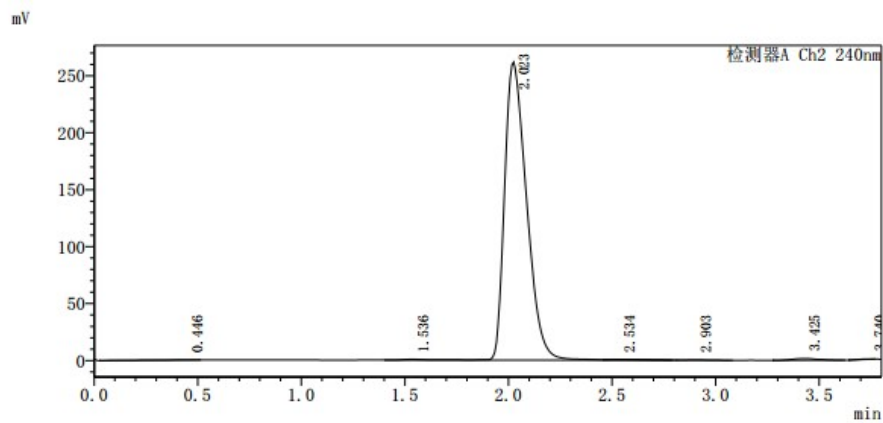
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检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	10.581	133831	7501	0.682		M	
2	11.472	74567	4306	0.380		M	
3	13.983	19407139	666412	98.938		S	
总计		19615537	678219				

Figure 10 The HPLC of compound 4b





峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	0.446	1483	68	0.000			
2	1.536	8648	733	0.000		V	
3	2.023	1929635	261661	0.000		SV	
4	2.534	3237	329	0.000		T	
5	2.903	1623	183	0.000			
6	3.425	13292	1516	0.000			
7	3.740	1725	272	0.000			
总计		1959644	264762				

Figure 11 The HPLC of DMSO

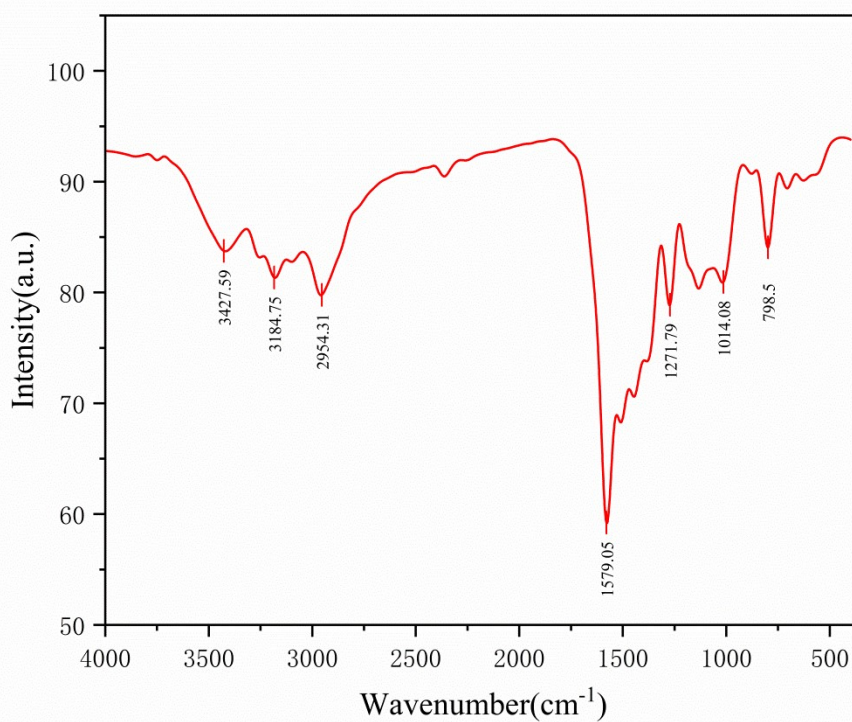


Figure 12 The IR spectrum of compound 4c

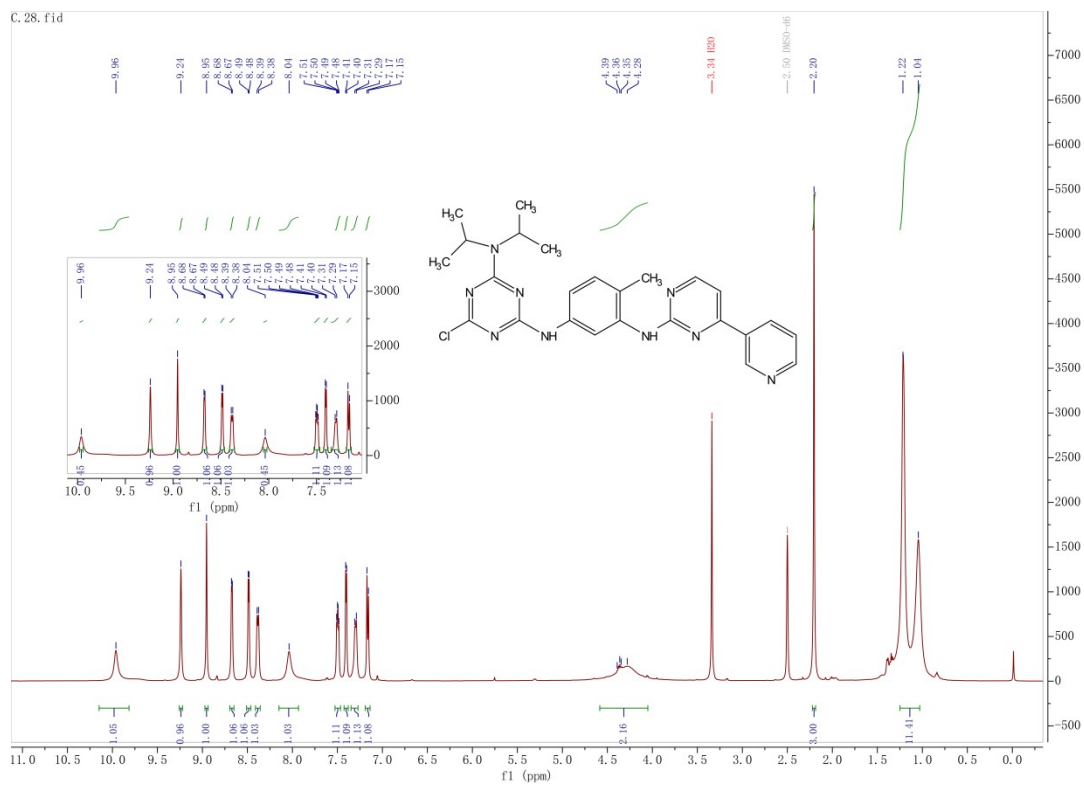


Figure 13 The  $^1\text{H}$  NMR spectrum of compound **4c**

22 C/100

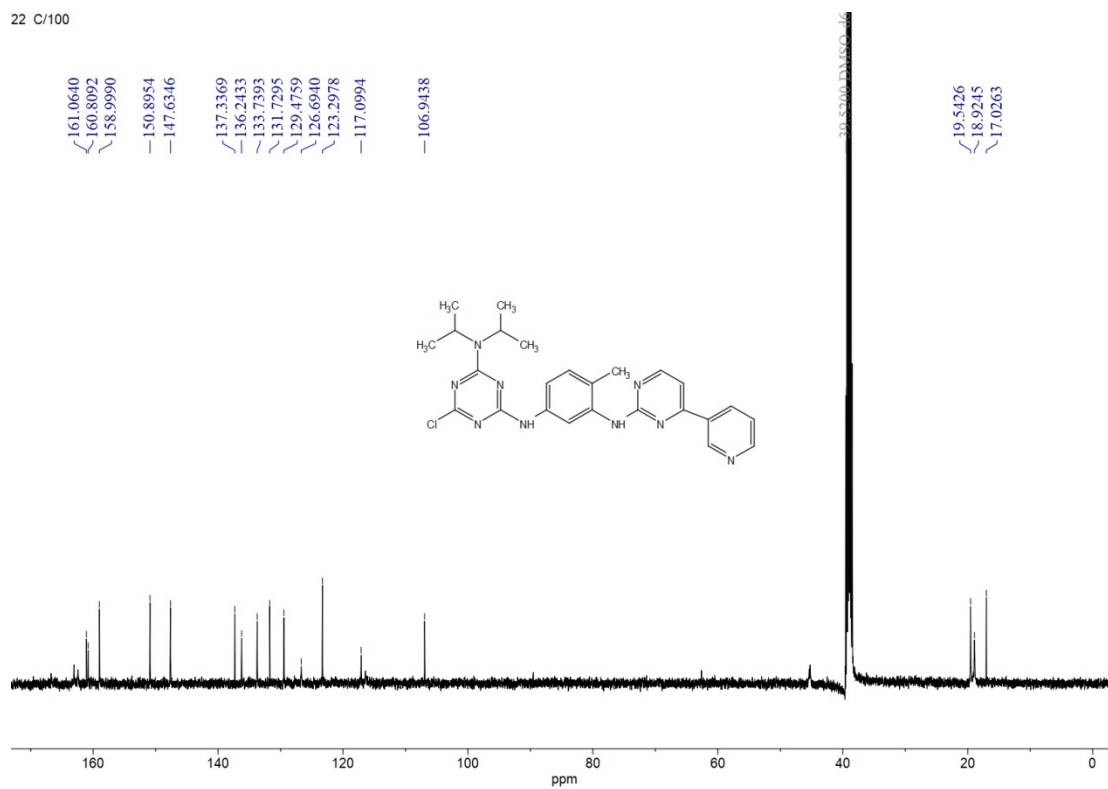


Figure 14 The  $^{13}\text{C}$  NMR spectrum of compound **4c**

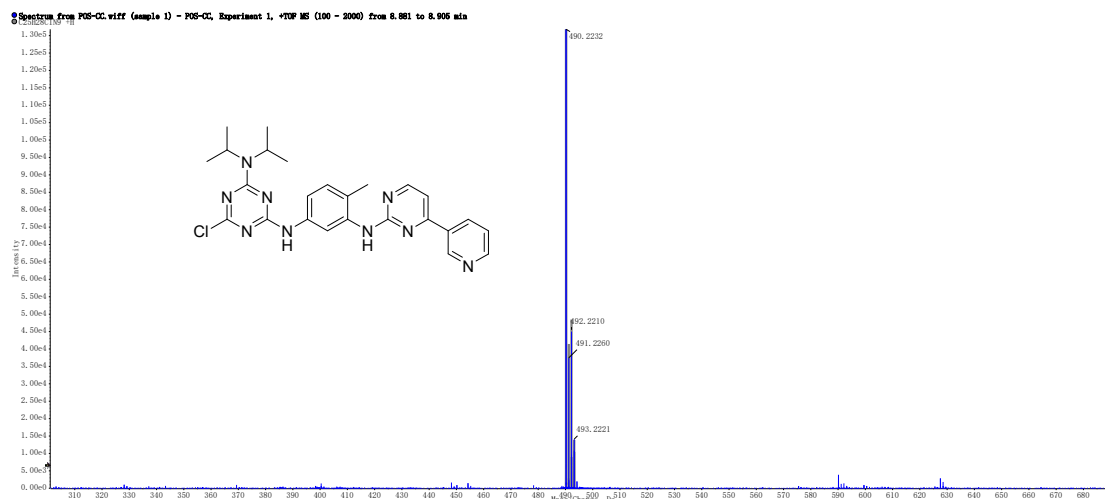
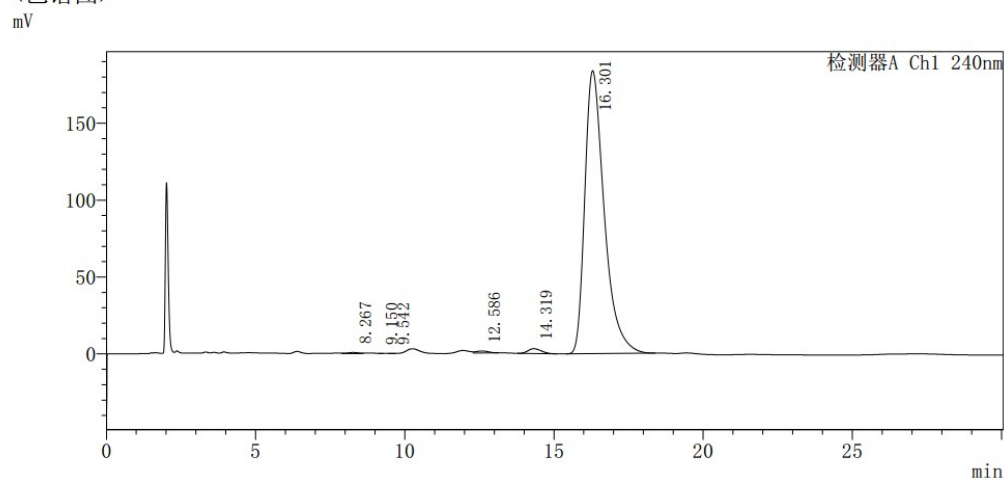


Figure 15 The HRMS spectrum of compound 4c

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<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.267	19920	720	0.235			
2	9.150	1852	189	0.022			
3	9.542	2357	169	0.028			
4	12.586	40175	1366	0.474			
5	14.319	96656	3150	1.140			
6	16.301	8315557	183994	98.101			
总计		8476515	189589				

Figure 16 The HPLC of compound 4c

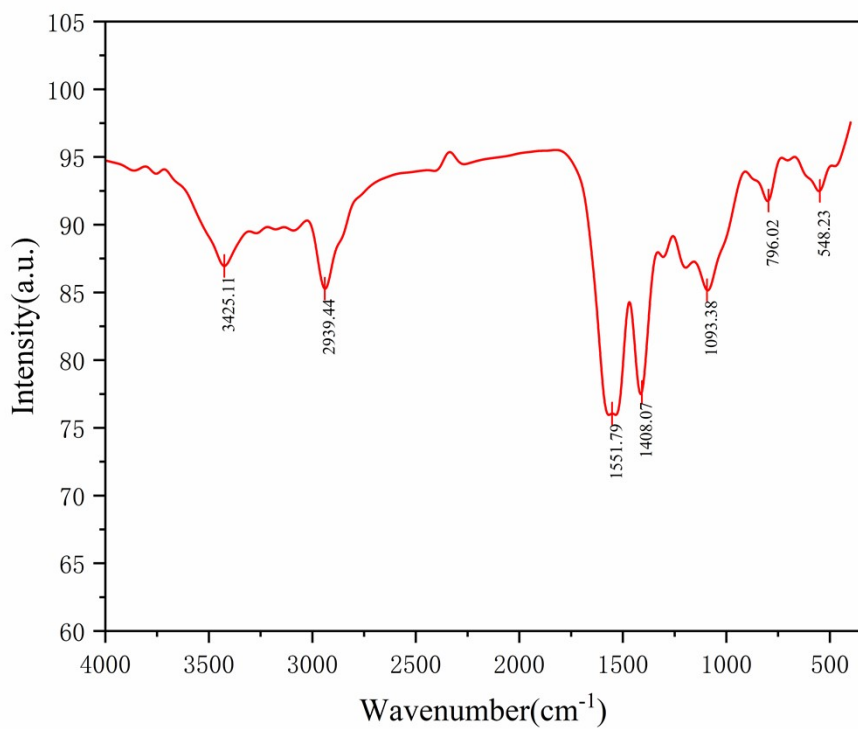


Figure 17 The IR spectrum of compound 4d

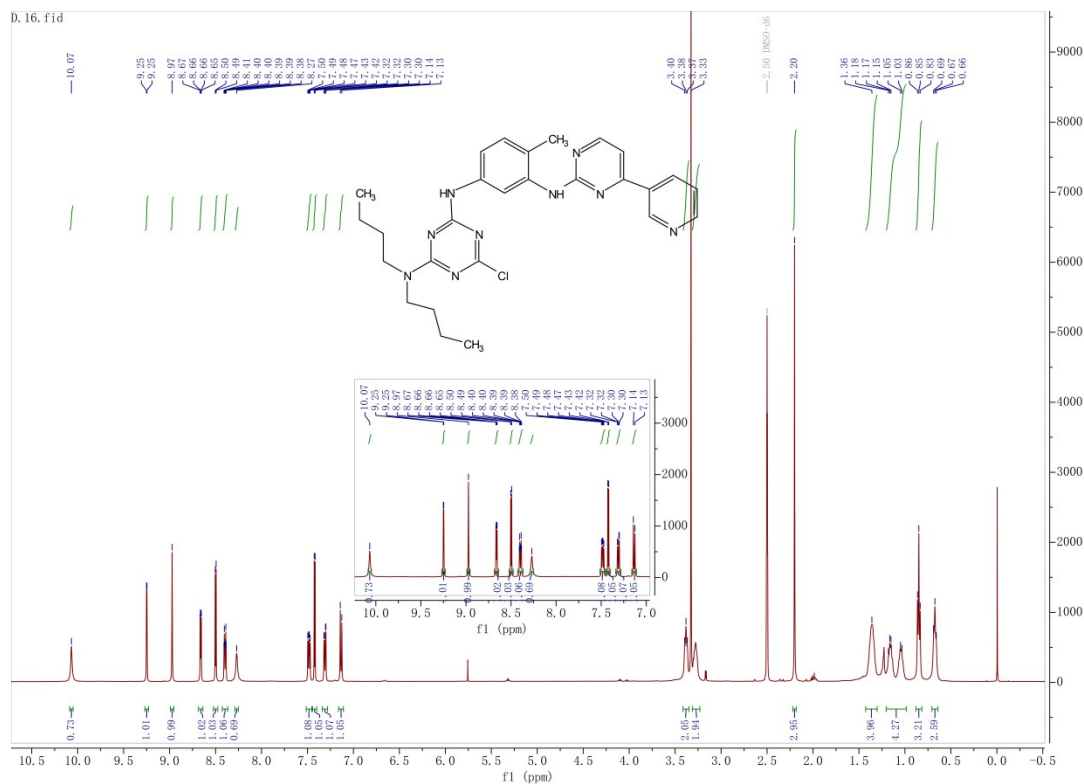


Figure 18 The <sup>1</sup>H NMR spectrum of compound 4d

05 C/11

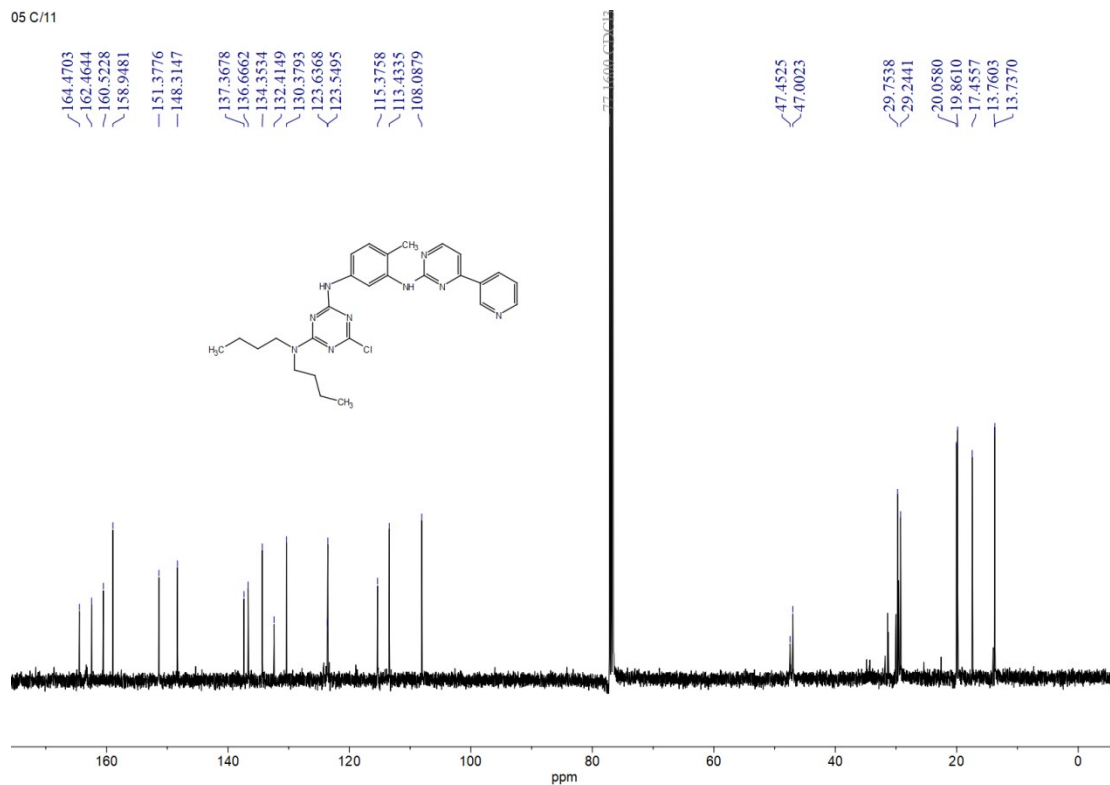


Figure 19 The <sup>13</sup>C NMR spectrum of compound 4d

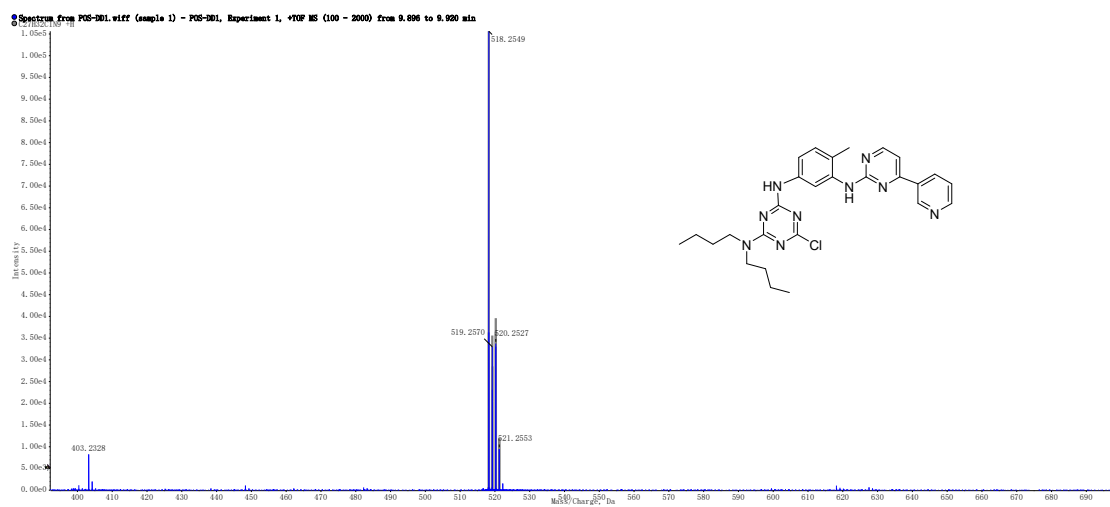
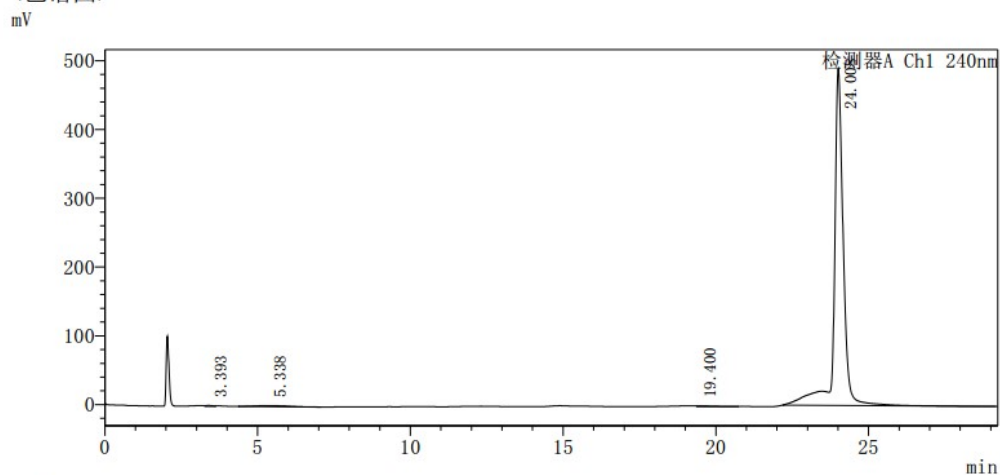


Figure 20 The HRMS spectrum of compound 4d

<色谱图>



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	3.393	22573	1330	0.218			
2	5.338	115605	1486	1.117			
3	19.400	41508	1058	0.401			
4	24.008	10171510	489794	98.264		S M	
总计		10351195	493668				

Figure 21 The HPLC of compound 4d

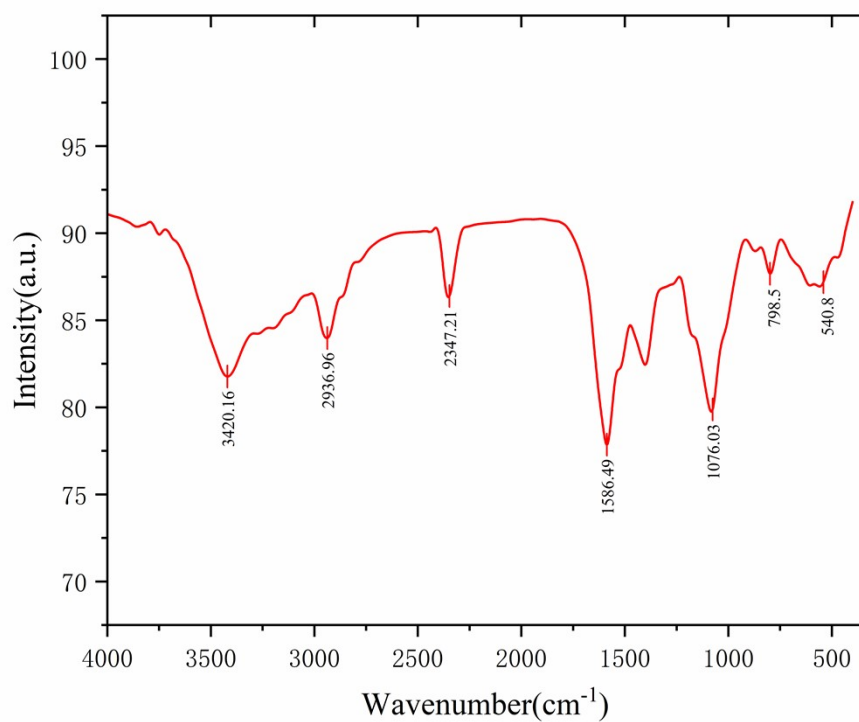


Figure 22 The IR spectrum of compound 4e

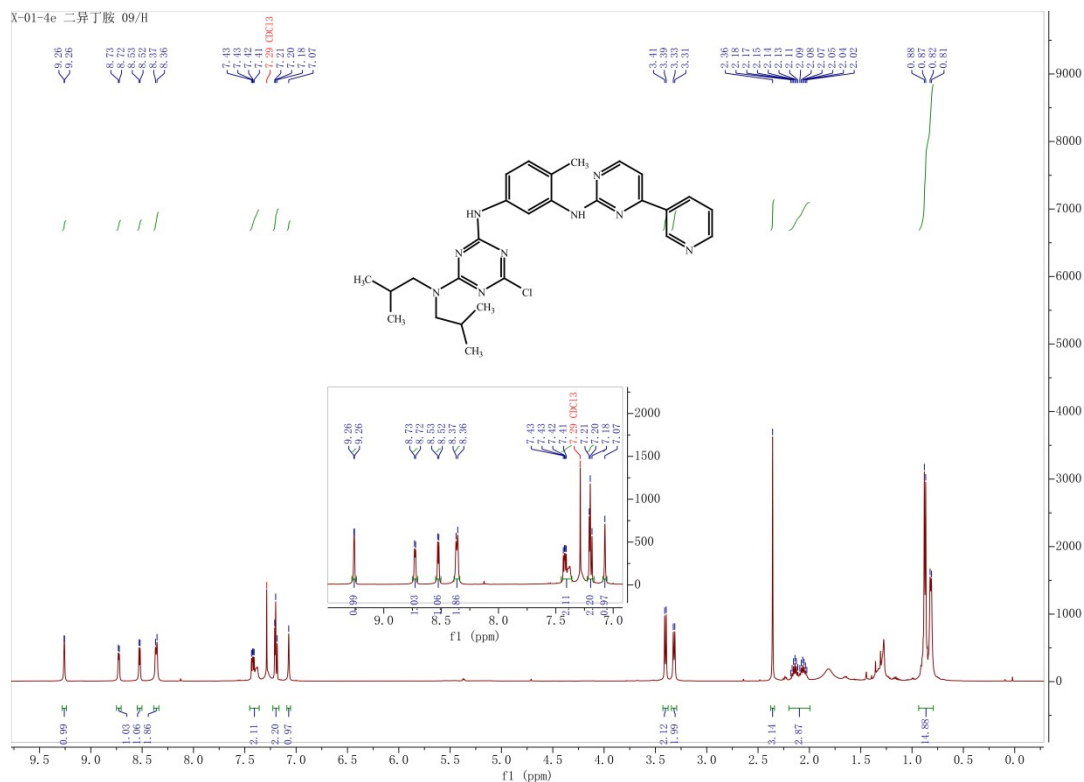


Figure 23 The  $^1\text{H}$  NMR spectrum of compound 4e

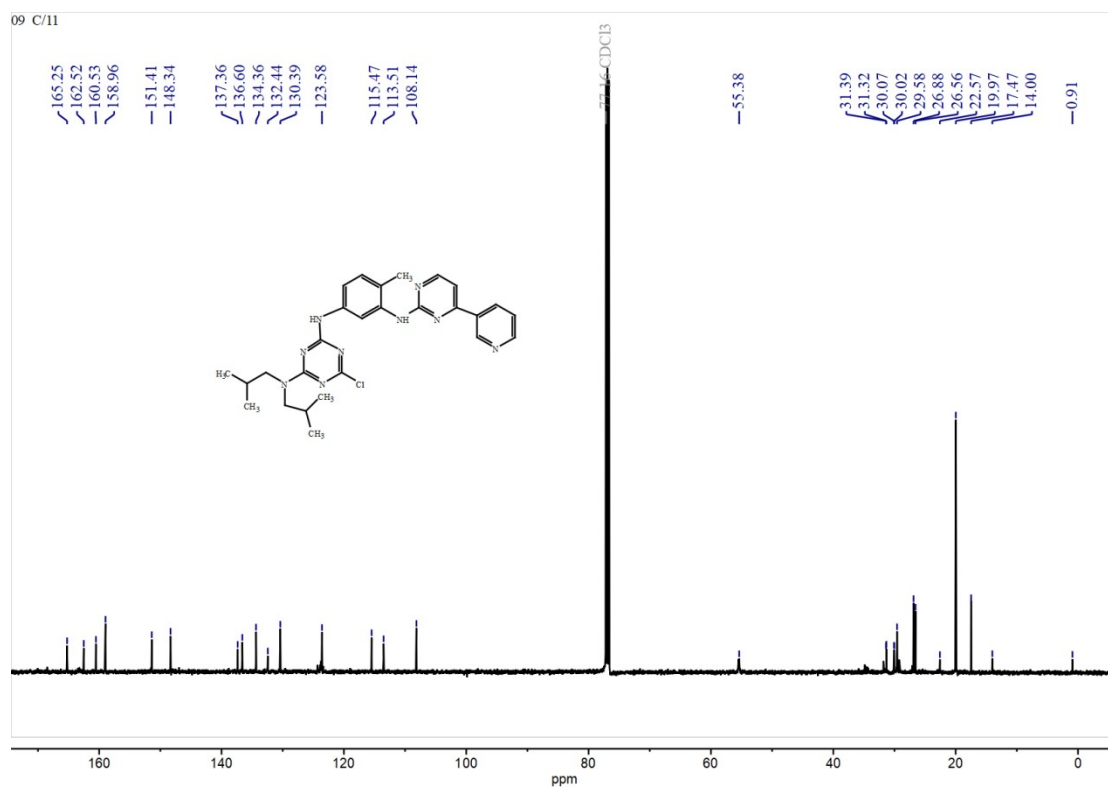


Figure 24 The  $^{13}\text{C}$  NMR spectrum of compound 4e

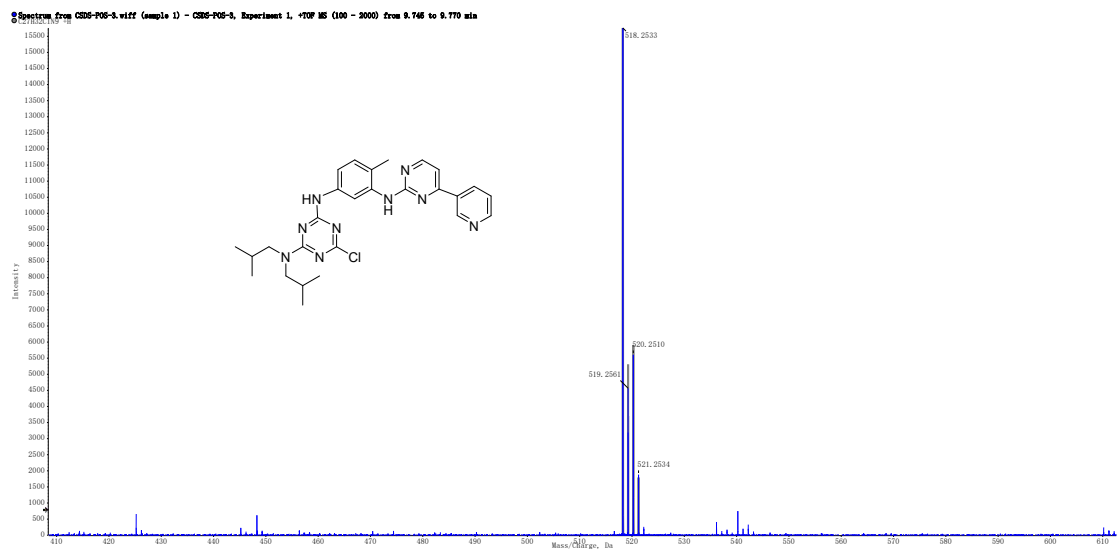
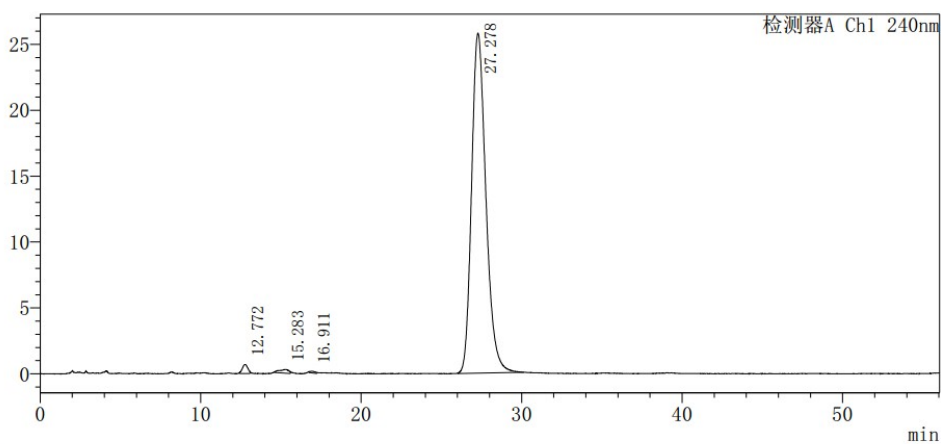


Figure 25 The HRMS spectrum of compound 4e

<色谱图>

mV



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.772	15728	681	0.966		M	
2	15.283	11090	279	0.681		M	
3	16.911	2824	120	0.173		M	
4	27.278	1598611	25793	98.180		SV	
总计		1628253	26873				

Figure 26 The HPLC of compound 4e



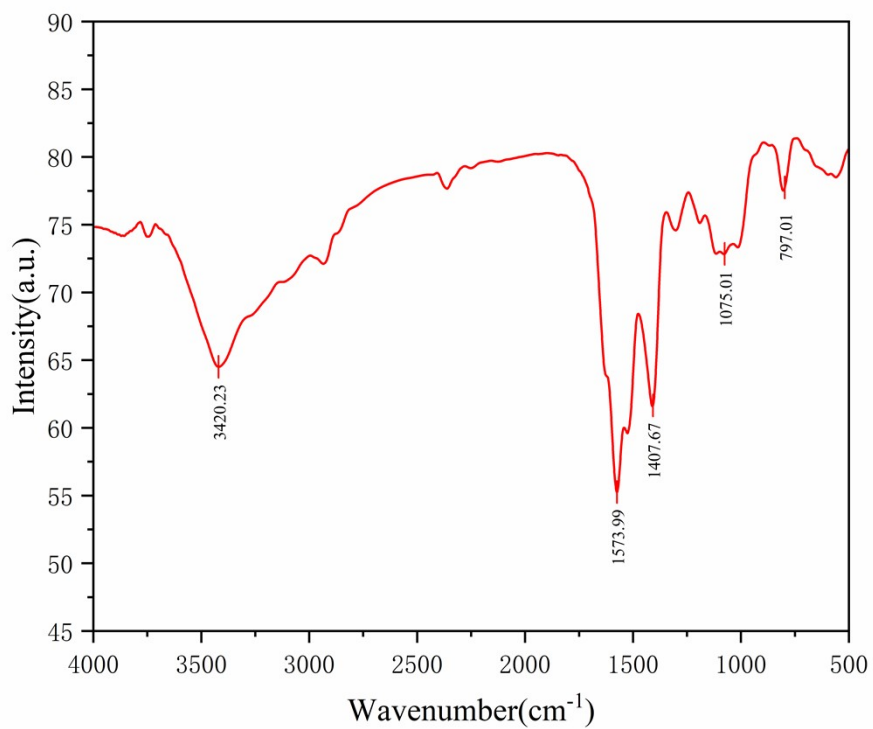


Figure 27 The IR spectrum of compound 4f

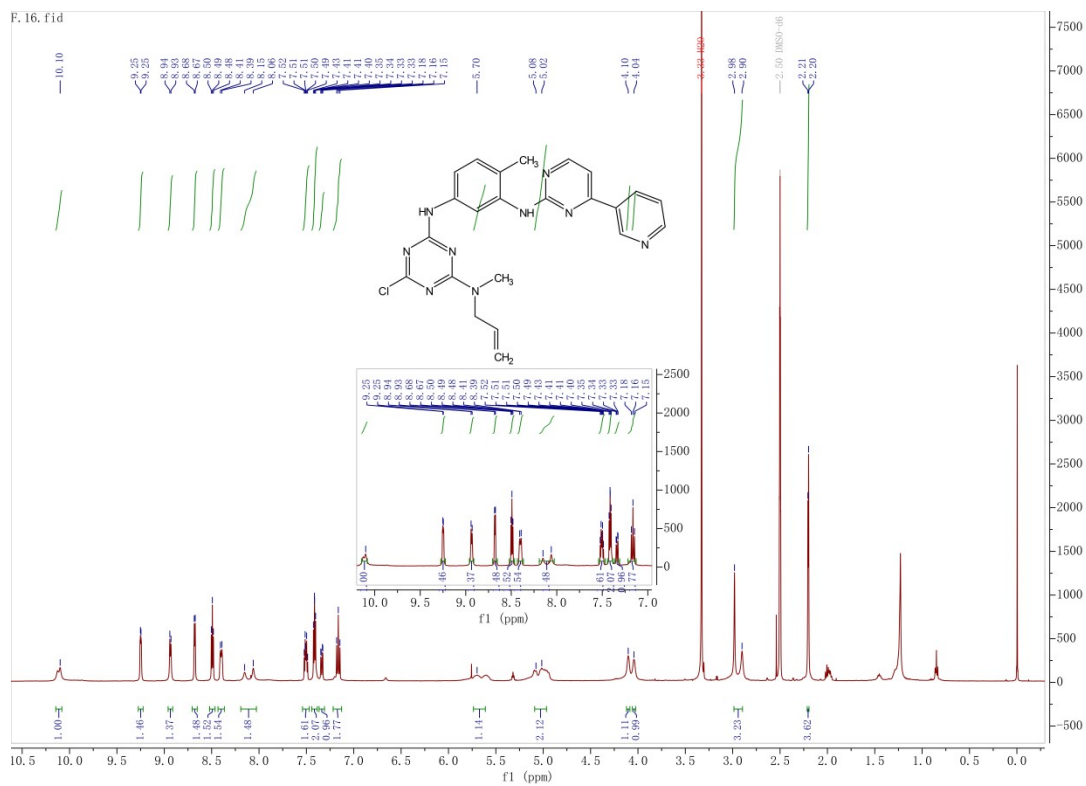


Figure 28 The <sup>1</sup>H NMR spectrum of compound 4f

X-01-4fN-甲基烯丙基胺 24/108

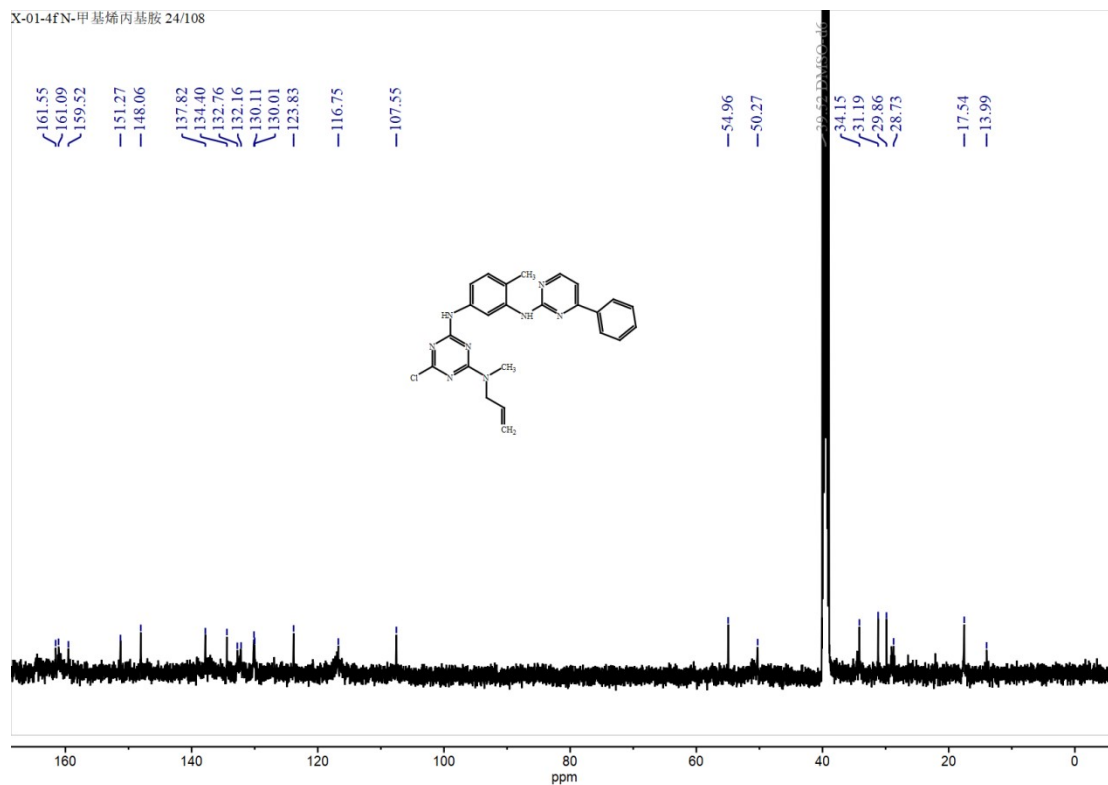


Figure 29 The  $^{13}\text{C}$  NMR spectrum of compound 4f

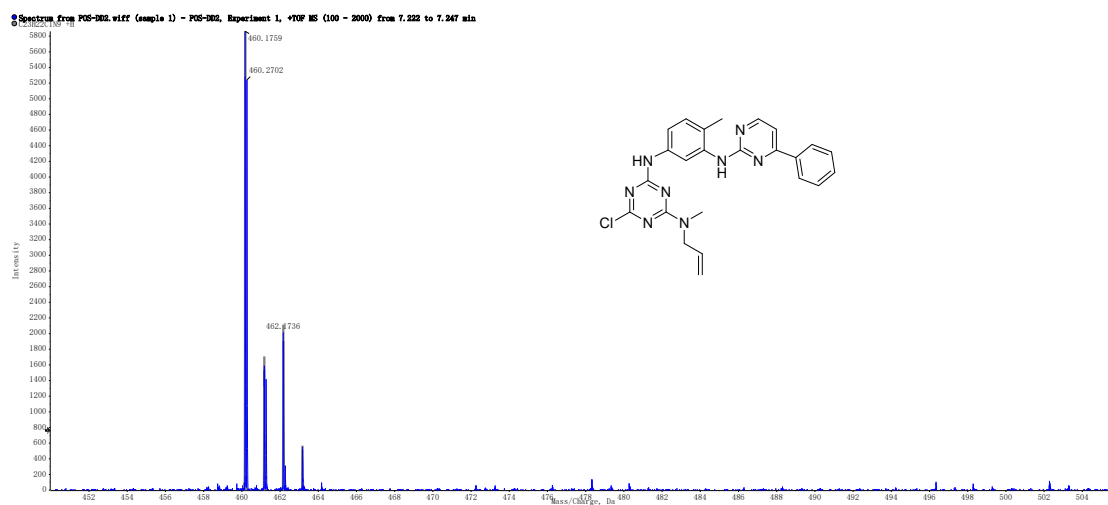
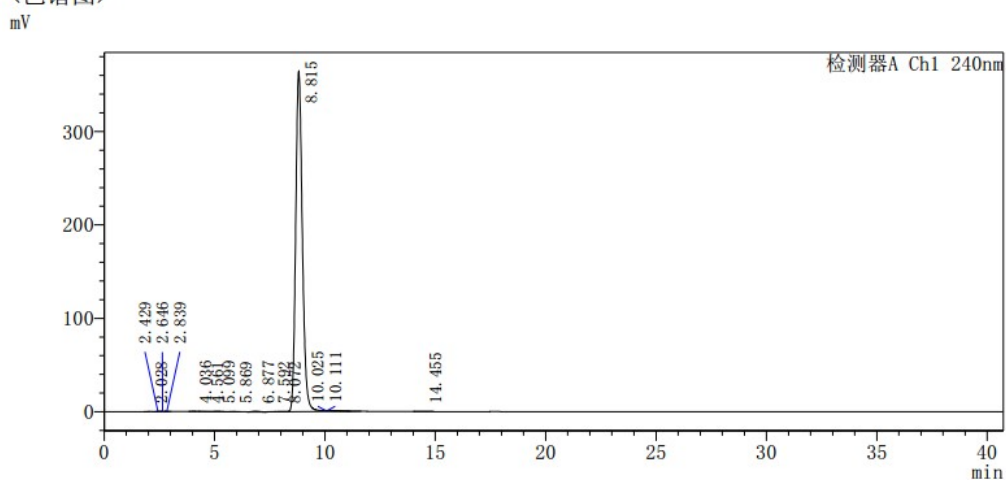


Figure 30 The HRMS spectrum of compound 4f

<色谱图>



<峰表>

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	2.028	1792	190	0.000			
2	2.429	2299	272	0.000		V	
3	2.646	1221	116	0.000		V	
4	2.839	1177	159	0.000		V	
5	4.036	2750	281	0.000			
6	4.561	5413	257	0.000			
7	5.099	11777	519	0.000		V	
8	5.869	3048	262	0.000			
9	6.877	15631	714	0.000			
10	7.592	2238	135	0.000			
11	8.072	8062	370	0.000		V	
12	8.815	7682331	364233	0.000		SV	
13	10.025	1258	168	0.000		T	
14	10.111	7706	231	0.000		TV	
15	14.455	3484	121	0.000			
总计		7750187	368027				

Figure 31 The HPLC of compound 4f

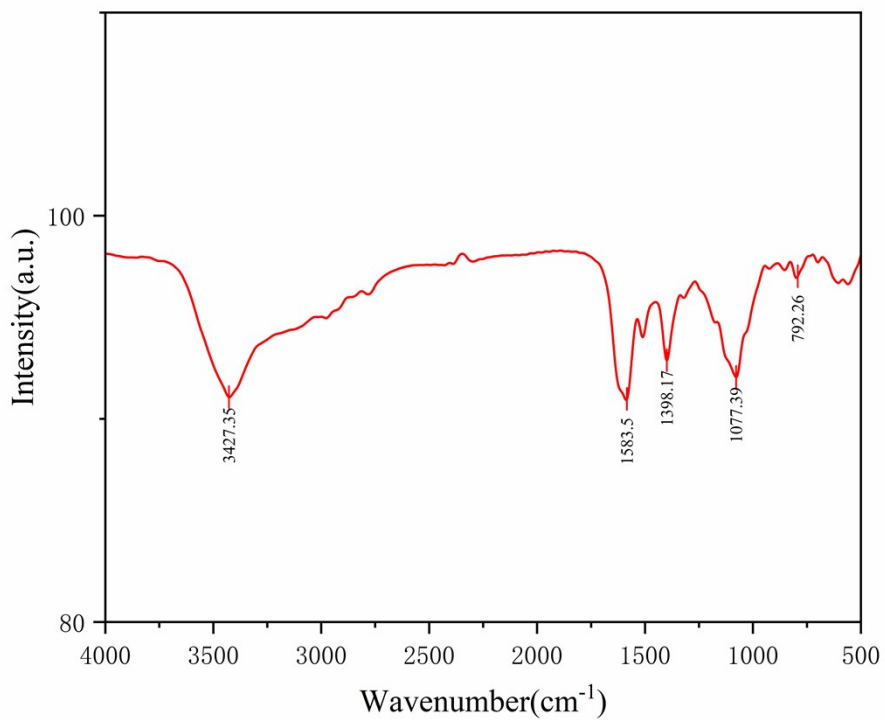


Figure 32 The IR spectrum of compound 4g

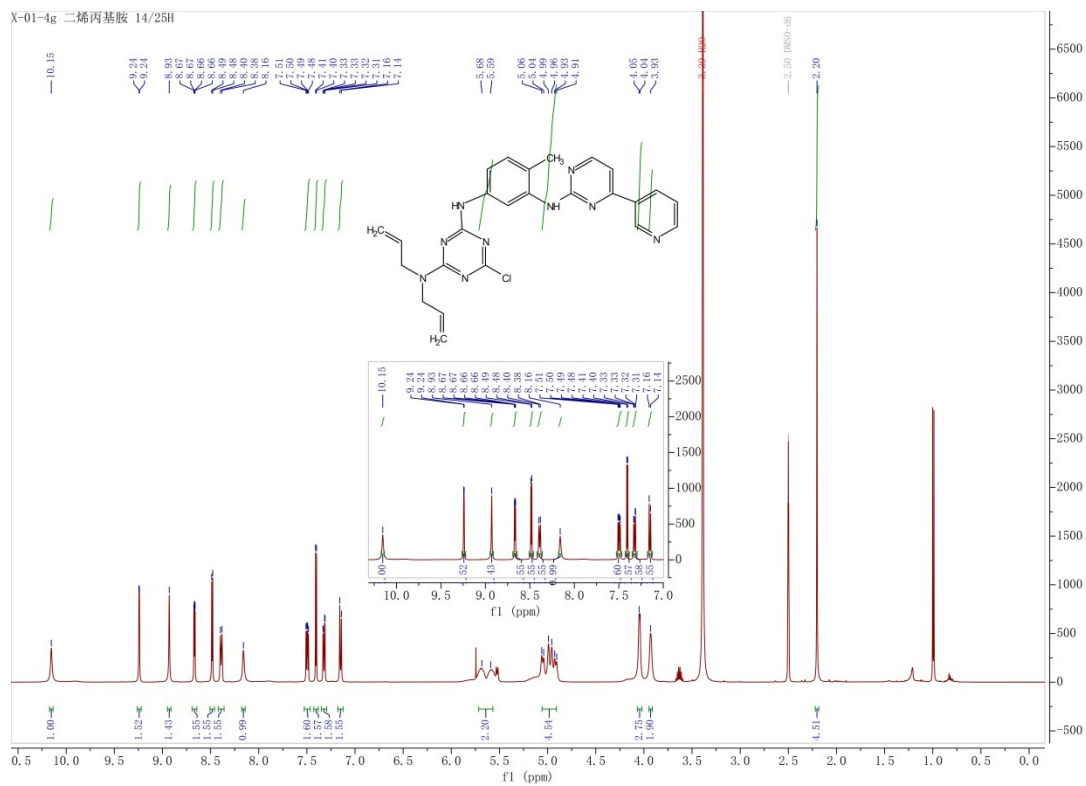


Figure 33 The <sup>1</sup>H NMR spectrum of compound 4g

X-01-4g 二烯丙基胺 14/C

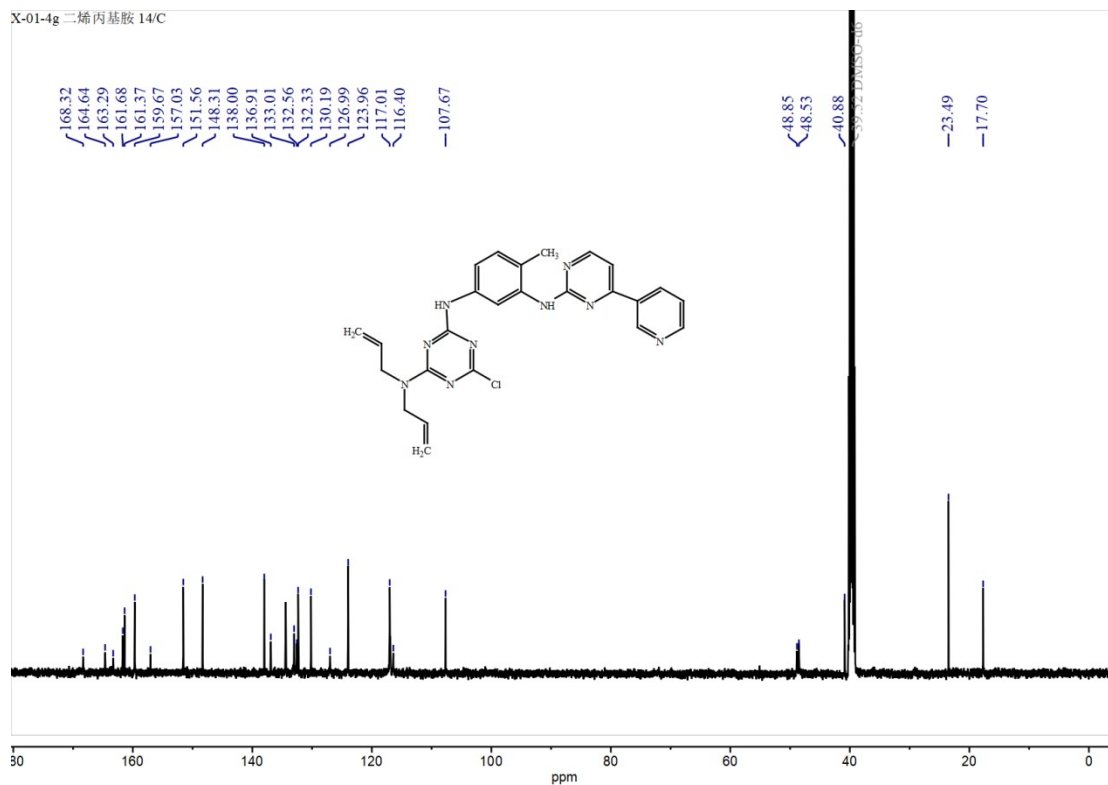


Figure 34 The <sup>1</sup>H NMR spectrum of compound 4g

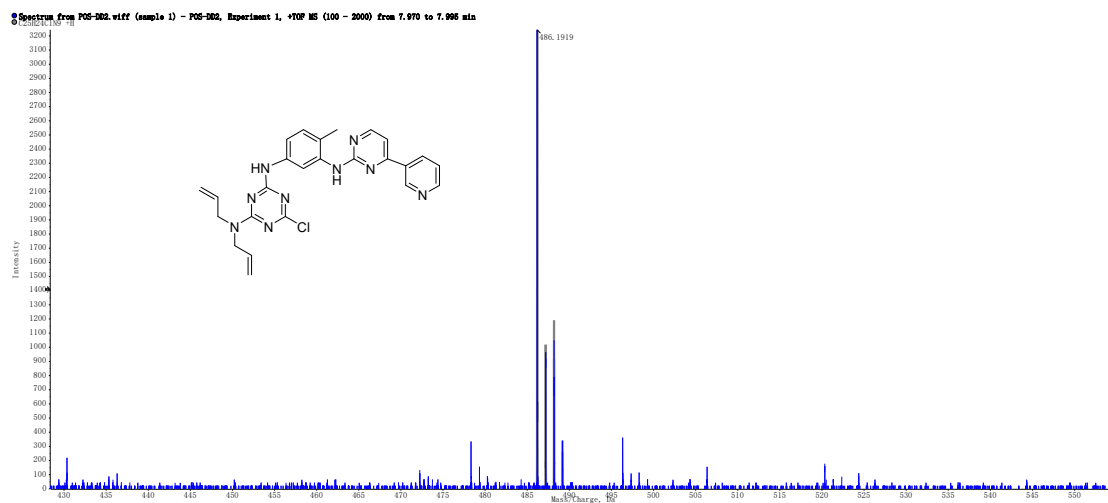
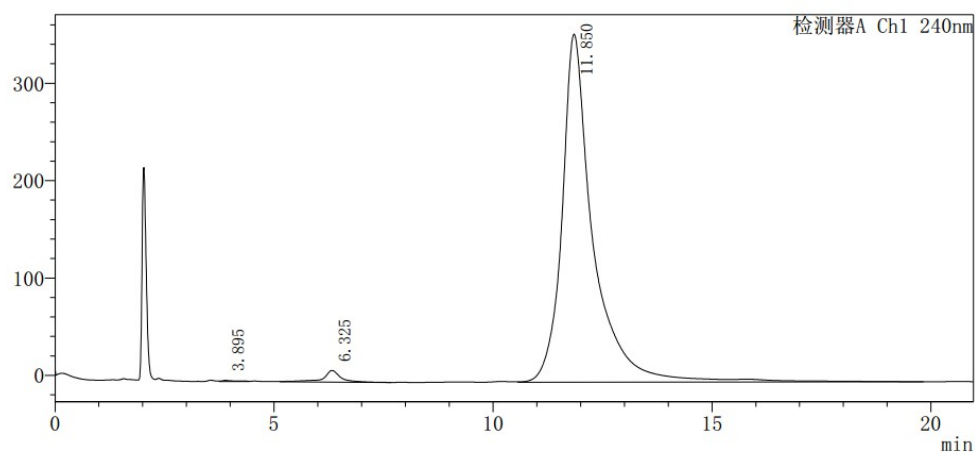


Figure 35 The HRMS spectrum of compound 4g

<色谱图>

mV



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	3.895	28350	1221	0.157			
2	6.325	326513	11851	1.808		V	
3	11.850	17708448	357481	98.035		S	
总计		18063311	370553				

Figure 36 The HPLC of compound 4g

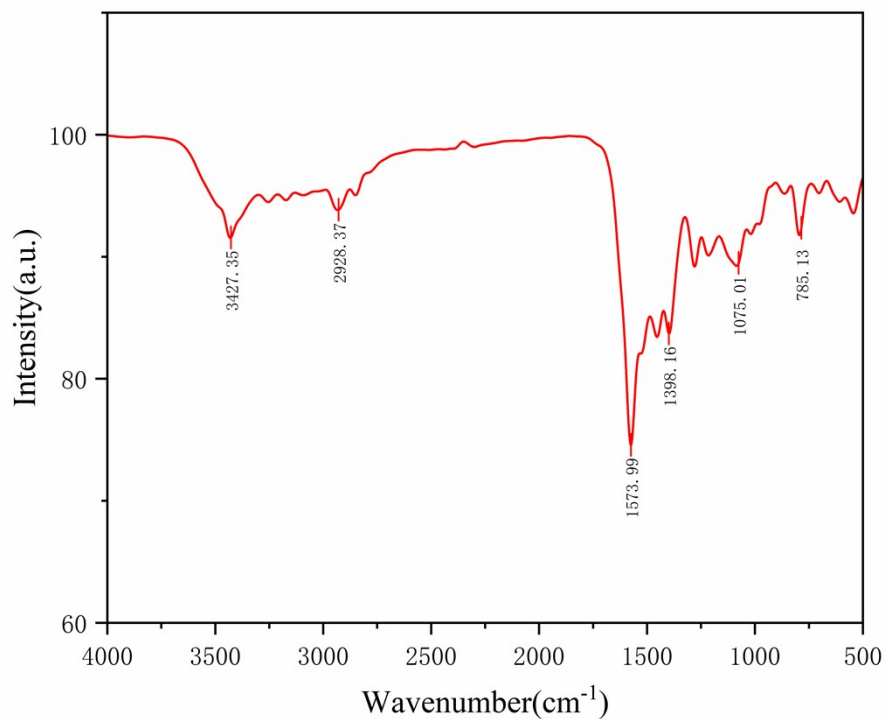


Figure 37 The IR spectrum of compound 4h

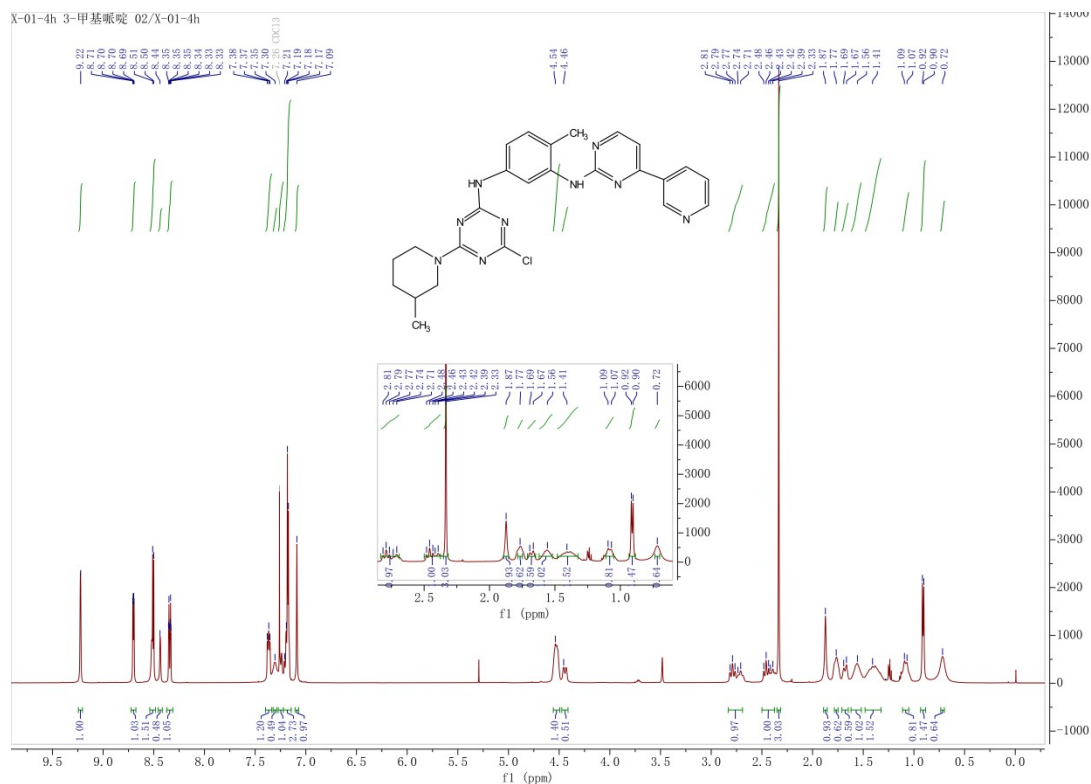


Figure 38 The <sup>1</sup>H NMR spectrum of compound 4h

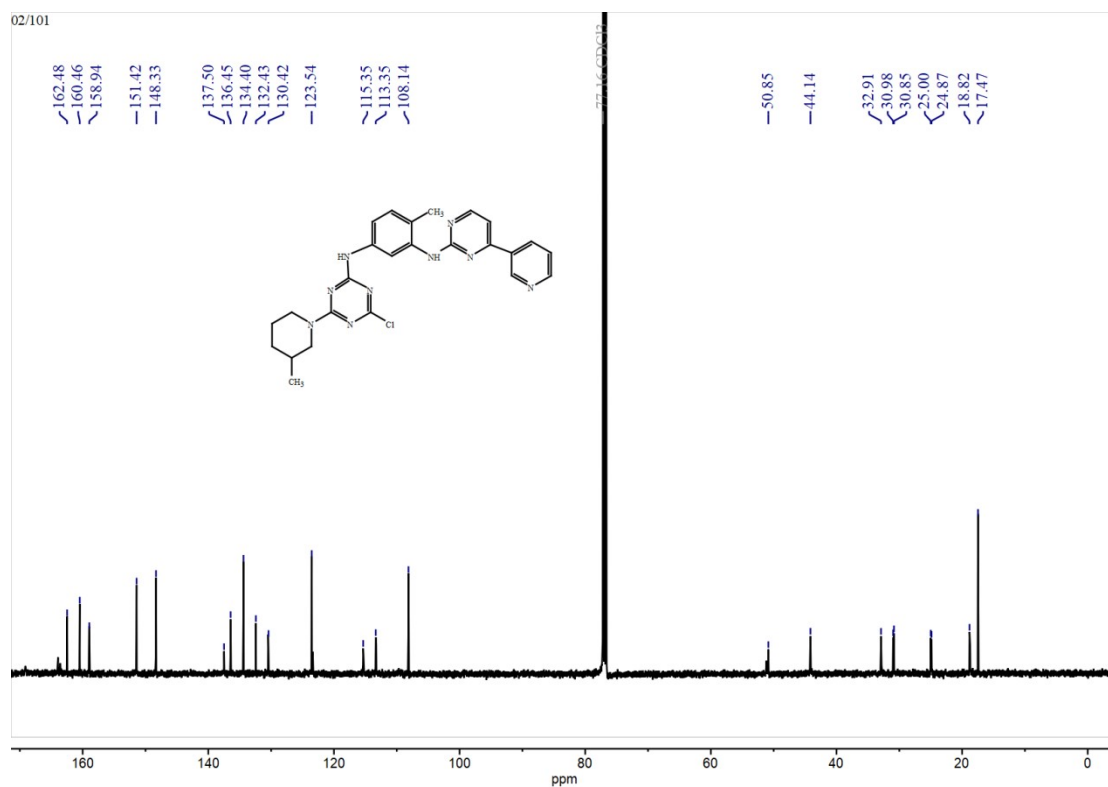


Figure 39 The <sup>13</sup>C NMR spectrum of compound 4h

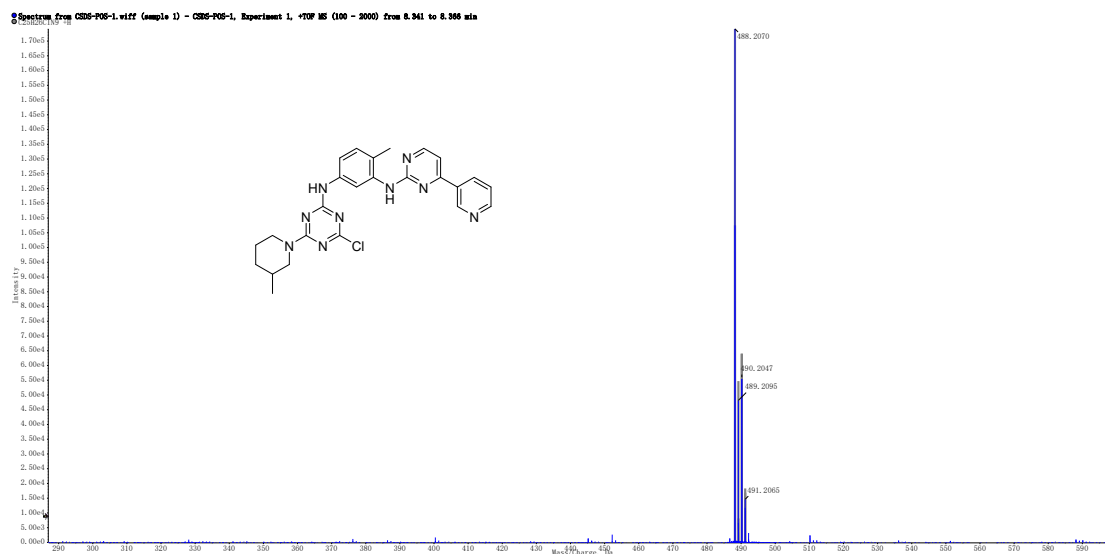
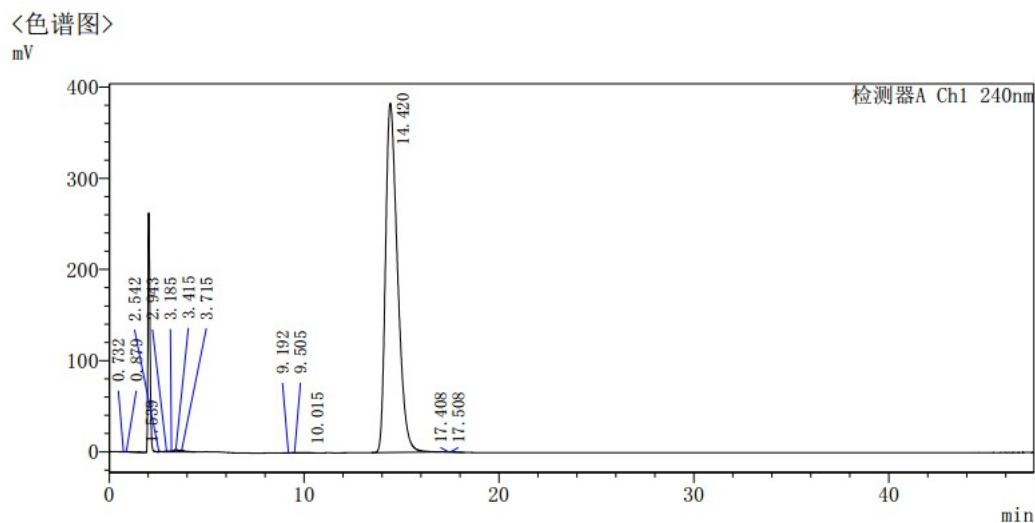


Figure 40 The HRMS spectrum of compound 4h



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	0.732	6985	417	0.042			
2	0.879	8665	458	0.052		V	
3	1.539	3599	586	0.022			
4	2.542	2119	394	0.013			
5	2.943	10715	761	0.065			
6	3.185	13859	1094	0.084		V	
7	3.415	36440	2633	0.221		V	
8	3.715	32185	1901	0.195		V	
9	9.192	2332	126	0.014		V	
10	9.505	4371	230	0.026		V	
11	10.015	10027	324	0.061		V	
12	14.420	16370717	383076	99.166			
13	17.408	2040	169	0.012			
14	17.508	4326	202	0.026		V	
总计		16508381	392369				

Figure 41 The HPLC of compound 4h



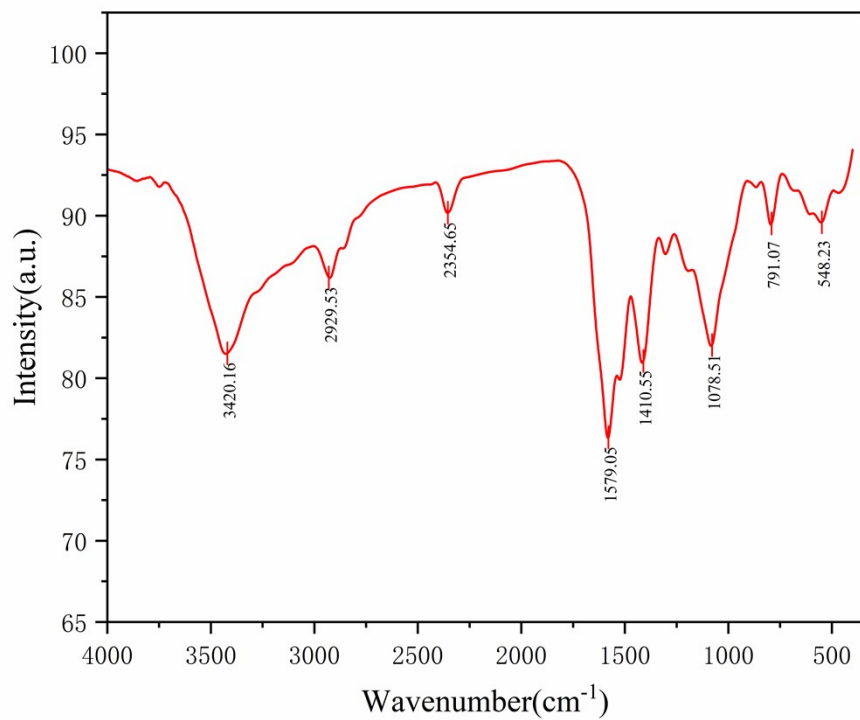


Figure 42 The IR spectrum of compound 4i

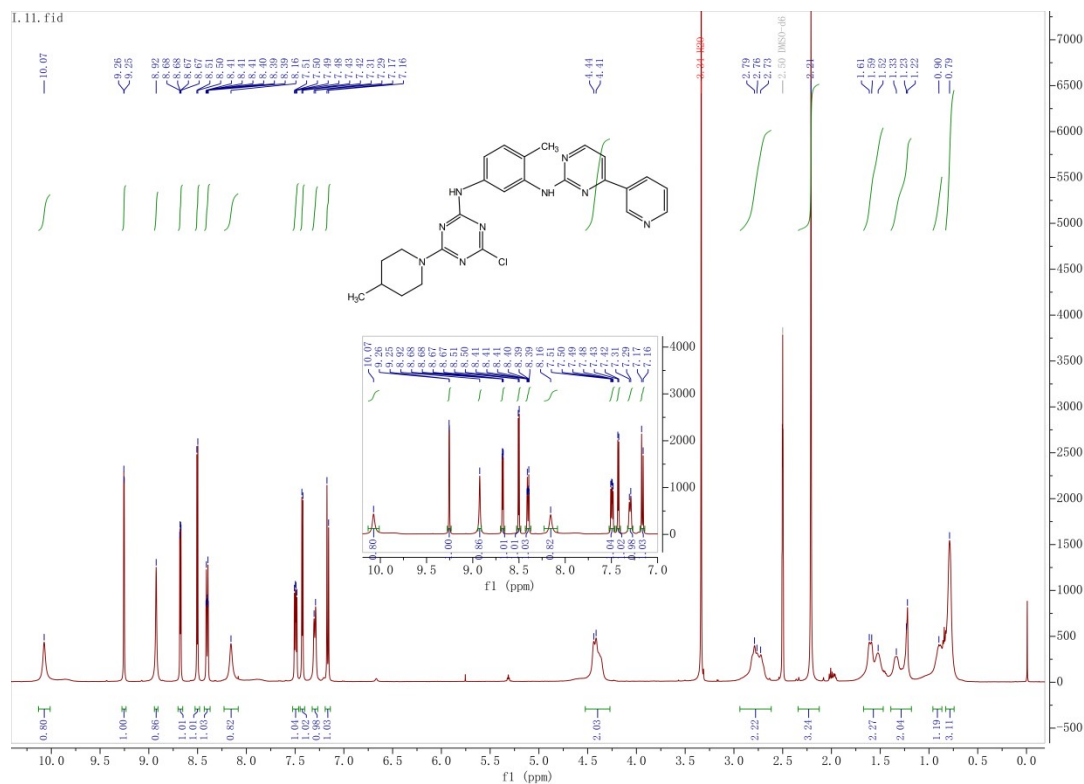


Figure 43 The <sup>1</sup>H NMR spectrum of compound 4i

20230905-13 C/10

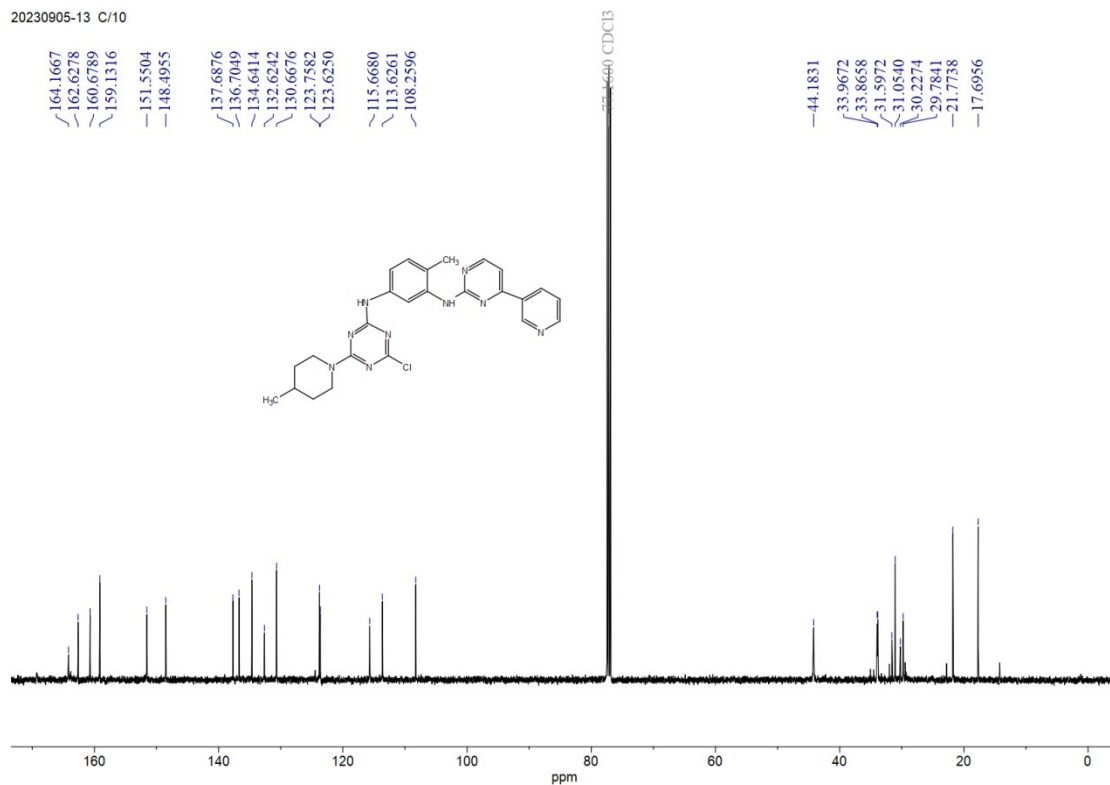


Figure 44 The <sup>13</sup>C NMR spectrum of compound 4i

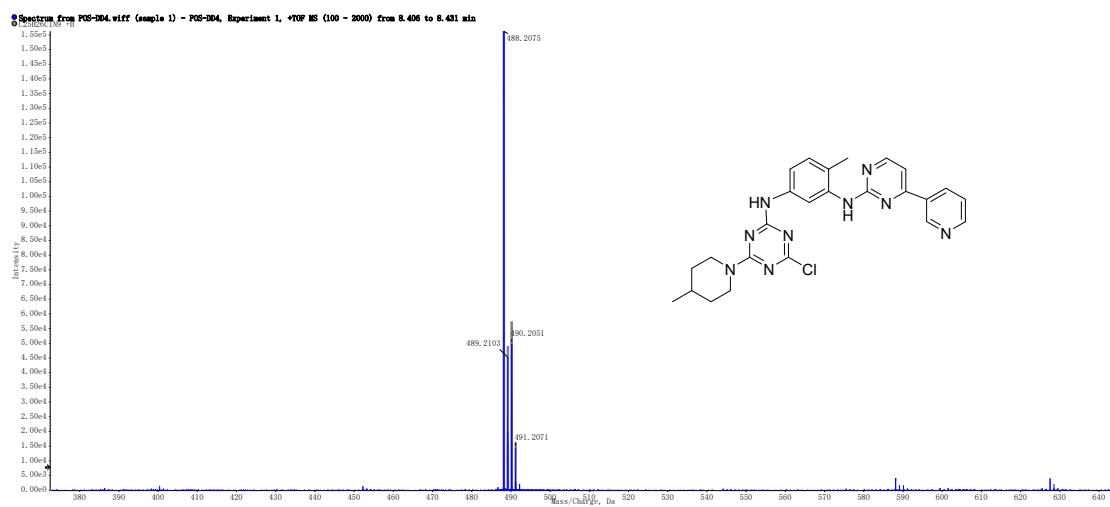
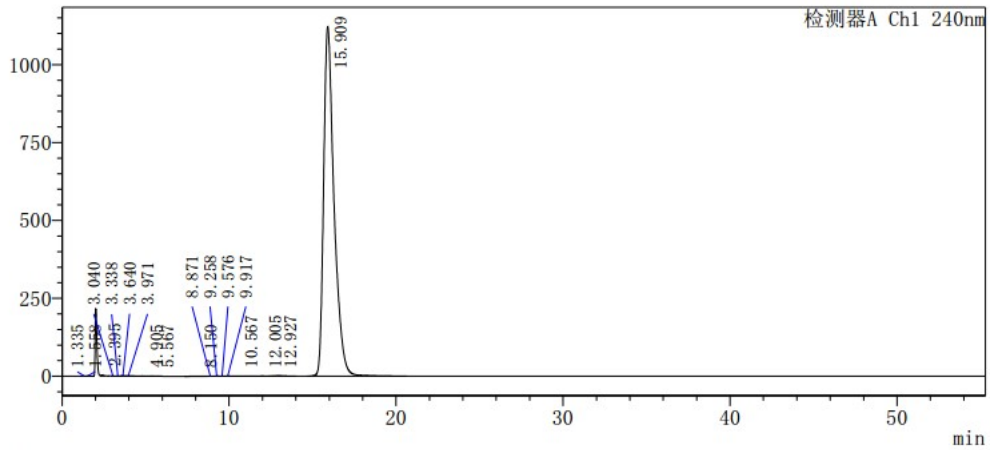


Figure 45 The HRMS spectrum of compound 4i

<色谱图>

mV



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	1.335	2012	149	0.004		V	
2	1.558	14652	1308	0.030		V	
3	2.395	16585	2581	0.034			
4	3.040	1898	191	0.004		V	
5	3.338	1054	128	0.002			
6	3.640	19910	1723	0.041		V	
7	3.971	24990	996	0.051		V	
8	4.905	9865	376	0.020		V	
9	5.567	3354	116	0.007		V	
10	8.150	19687	549	0.040		V	
11	8.871	13525	426	0.028		V	
12	9.258	1088	245	0.002		V	
13	9.576	11898	431	0.024		V	
14	9.917	1107	247	0.002		V	
15	10.567	26285	575	0.054		V	
16	12.005	21041	586	0.043		V	
17	12.927	62339	1518	0.127		V	
18	15.909	48644225	1120991	99.486		SV	
总计		48895516	1133136				

Figure 46 The HPLC of compound 4i

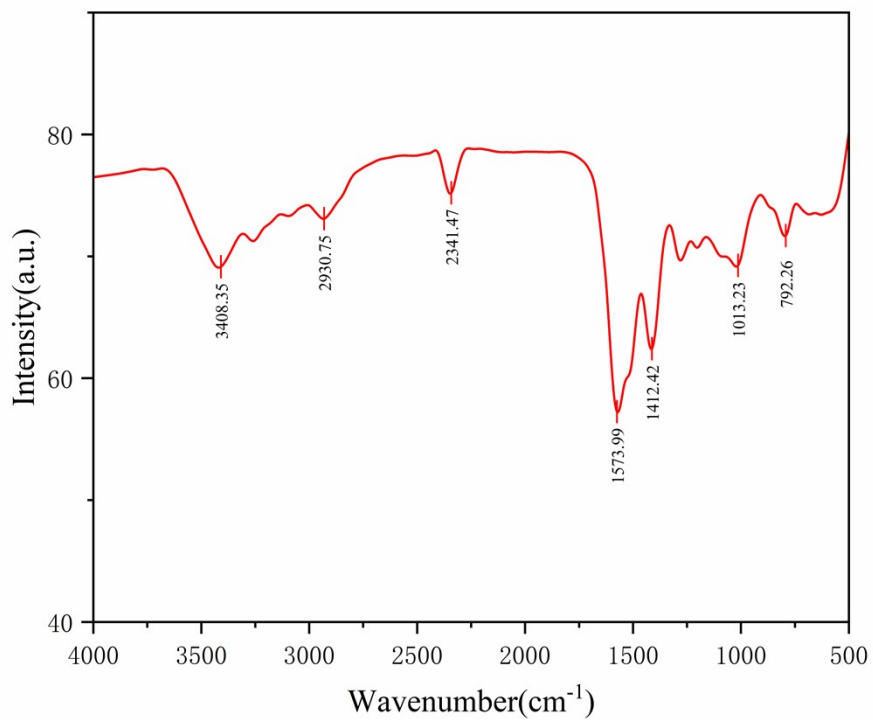


Figure 47 The IR spectrum of compound **4j**

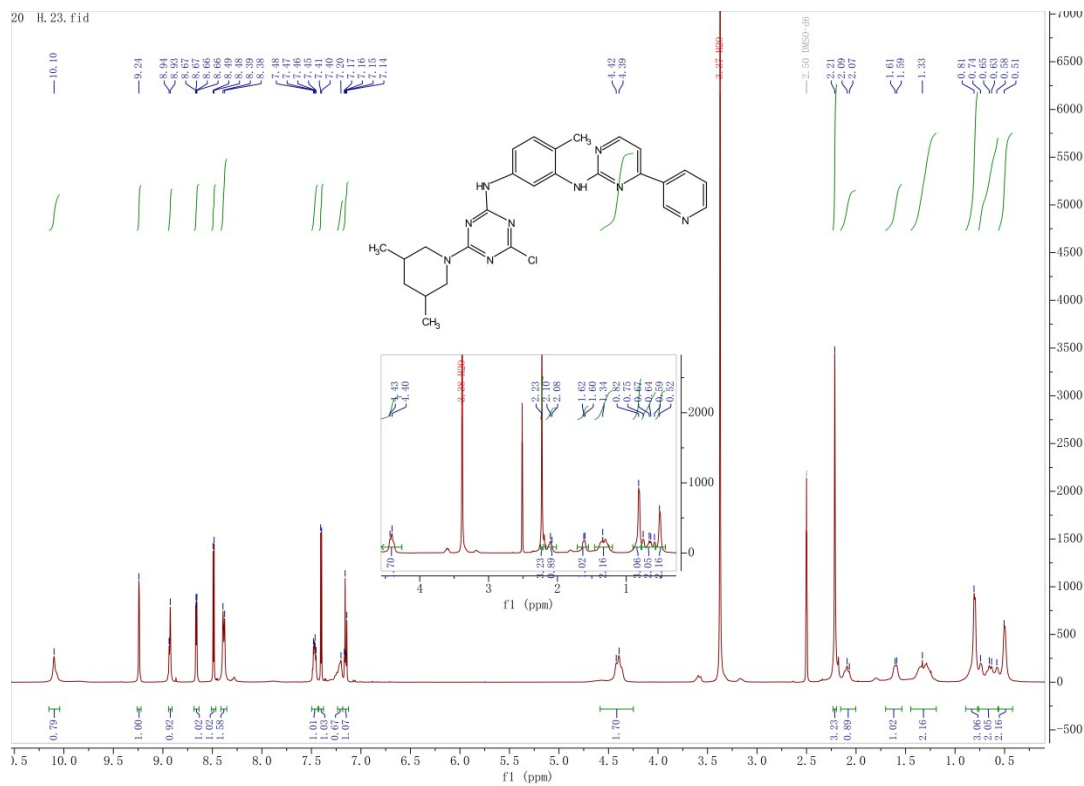


Figure 48 The <sup>1</sup>H NMR spectrum of compound **4j**

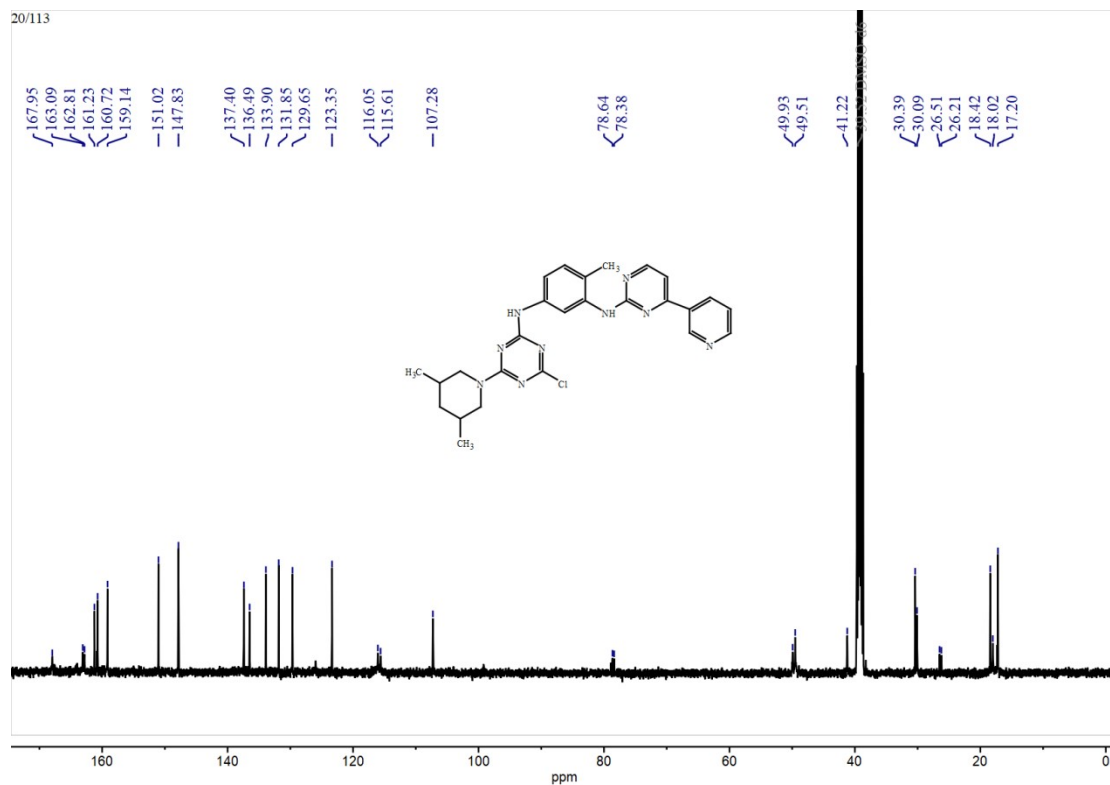


Figure 49 The  $^{13}\text{C}$  NMR spectrum of compound **4j**

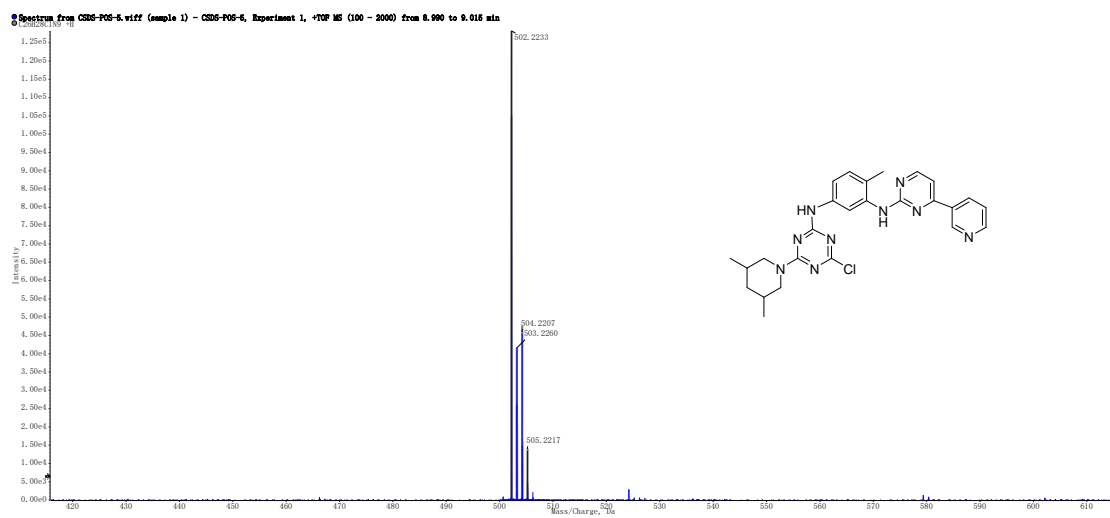
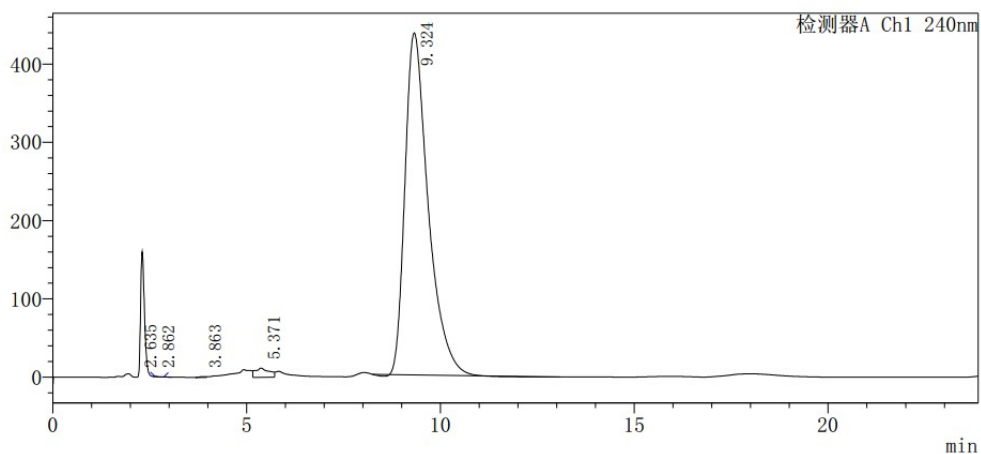


Figure 50 The HRMS spectrum of compound **4j**

<色谱图>

mV



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	2.635	1380	253	0.007			
2	2.862	1786	203	0.010			
3	3.863	10220	1039	0.055			
4	5.371	299356	11805	1.619			
5	9.324	18171909	437106	98.308		S M	
总计		18484651	450405				

Figure 51 The HPLC of compound 4j

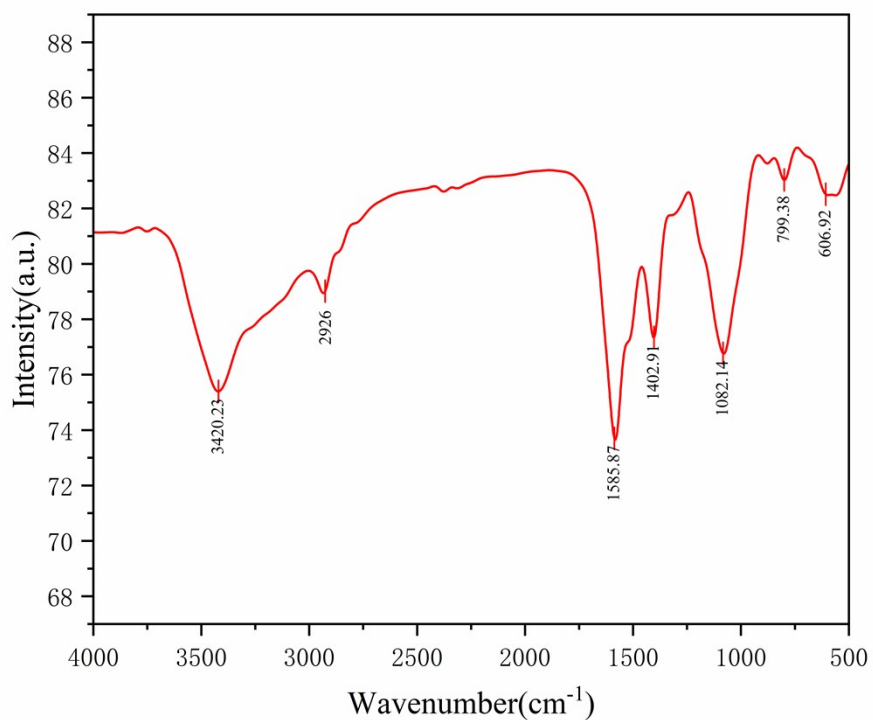
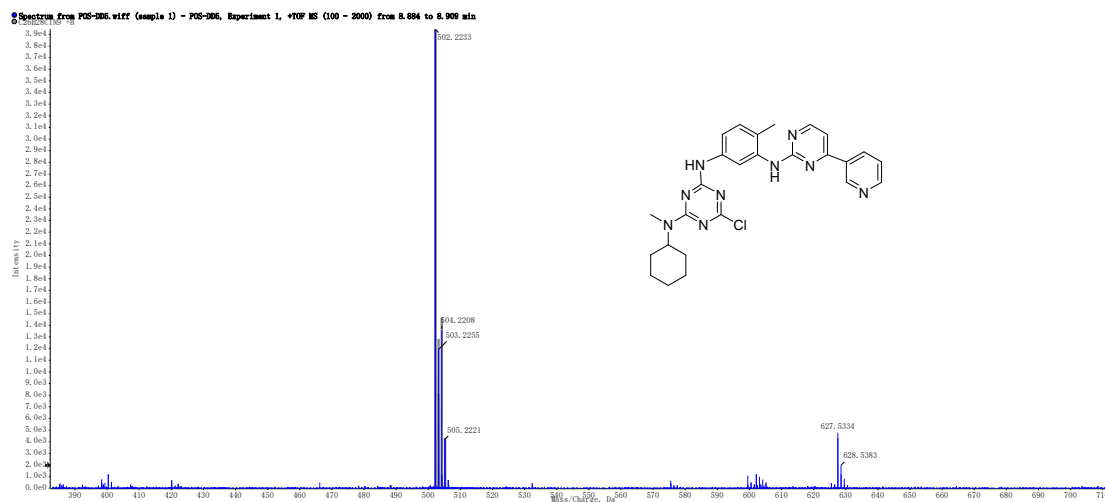
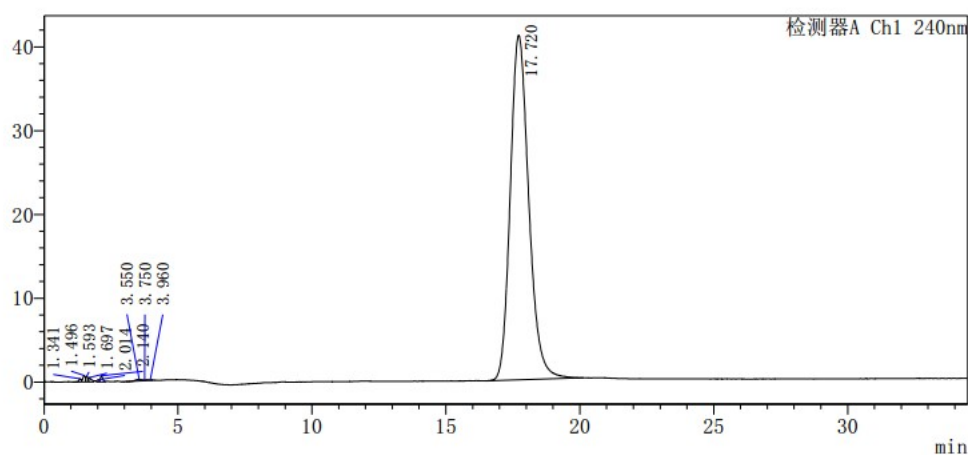


Figure 52 The IR spectrum of compound 4k





<色谱图>  
mV



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	1.341	2325	391	0.116		V	
2	1.496	4874	781	0.244		V	
3	1.593	3694	679	0.185		V	
4	1.697	3720	511	0.186		V	
5	2.014	1436	252	0.072		V	
6	2.140	4587	726	0.229		V	
7	3.550	2897	179	0.145			
8	3.750	1252	111	0.063		V	
9	3.960	1177	93	0.059		V	
10	17.720	1973532	41125	98.701		S	
总计		1999495	44848				

Figure 56 The HPLC of compound 4k



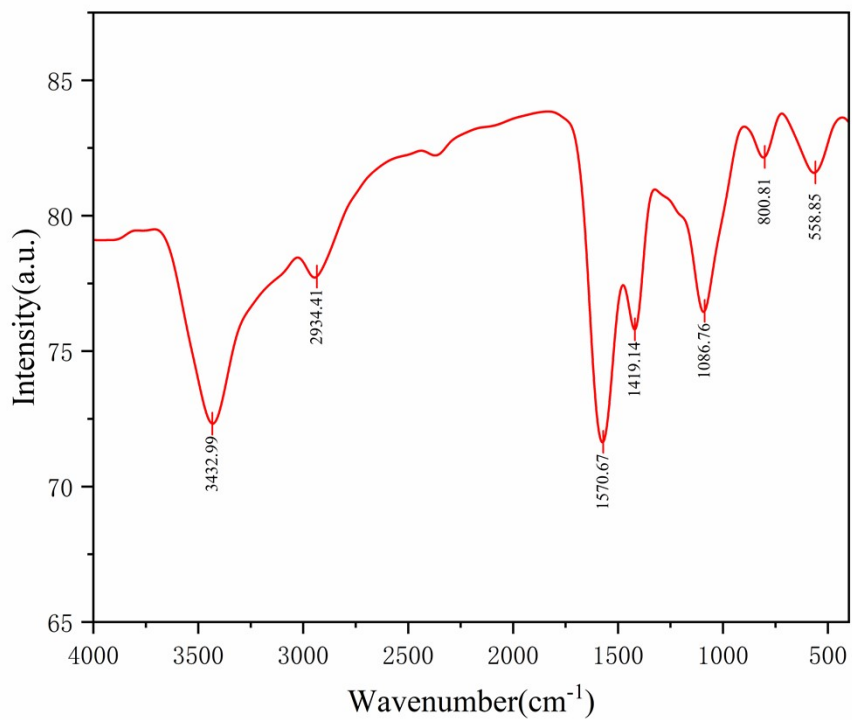


Figure 57 The IR spectrum of compound 41

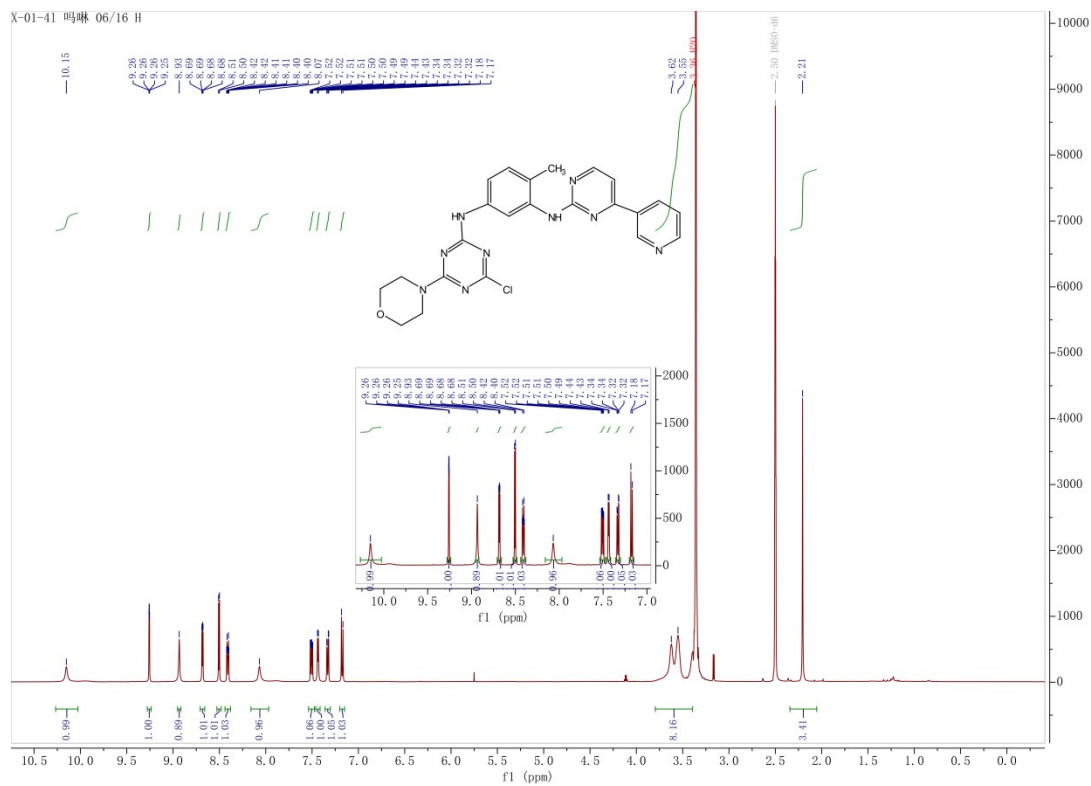


Figure 58 The <sup>1</sup>H NMR spectrum of compound 41

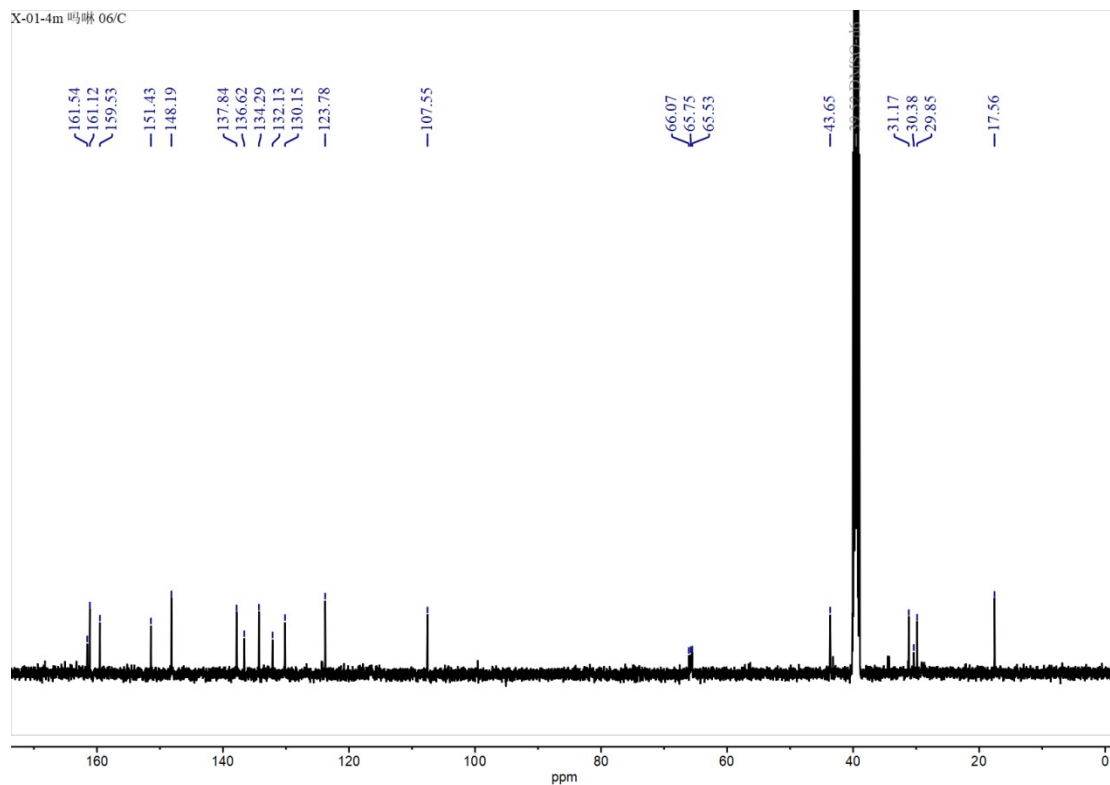


Figure 59 The  $^{13}\text{C}$  NMR spectrum of compound **41**

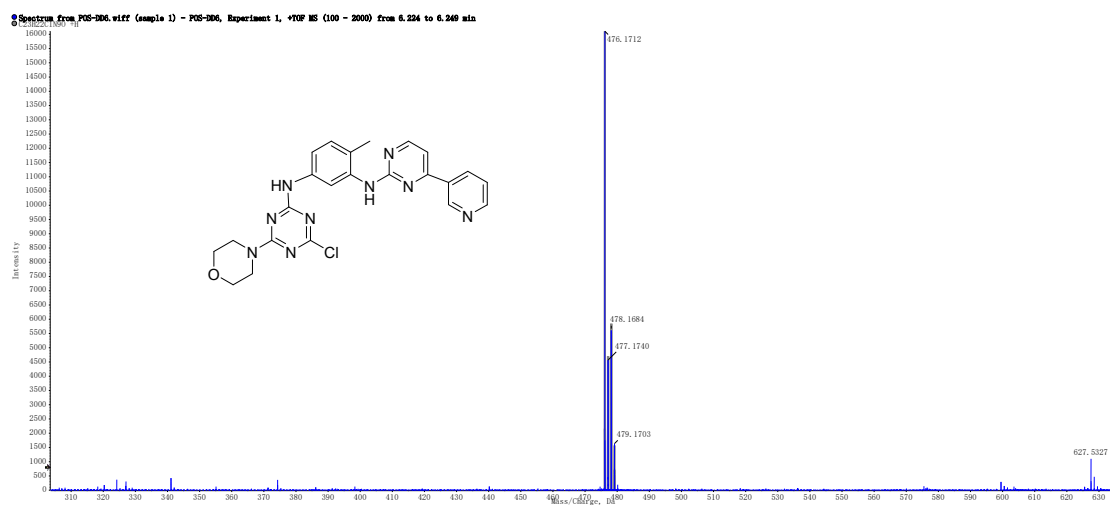
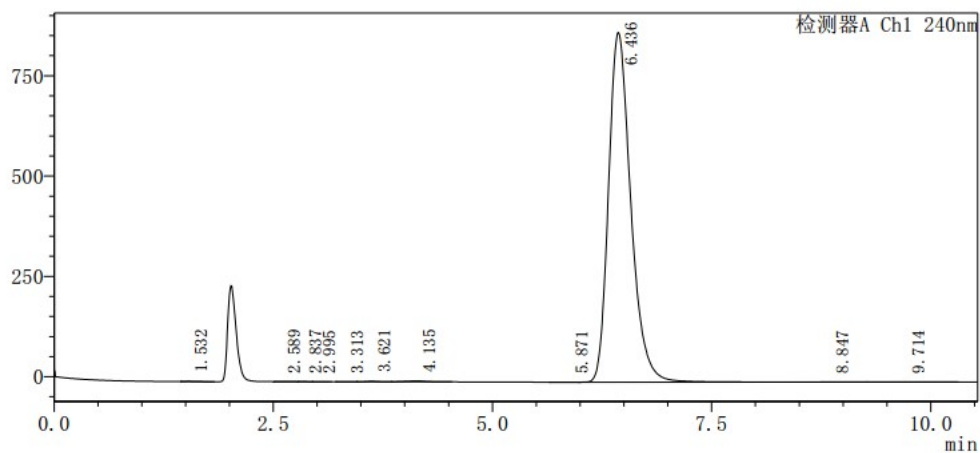


Figure 60 The HRMS spectrum of compound **41**

<色谱图>

mV



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	1.532	4070	612	0.026			
2	2.589	4095	385	0.026			
3	2.837	2050	240	0.013		V	
4	2.995	1958	233	0.013		V	
5	3.313	1433	209	0.009			
6	3.621	12463	1367	0.080			
7	4.135	37697	2296	0.243			
8	5.871	1250	108	0.008			
9	6.436	15411452	871244	99.506		SV	
10	8.847	1139	69	0.007		TV	
11	9.714	10430	421	0.067		T	
总计		15488038	877183				

Figure 61 The HPLC of compound 41

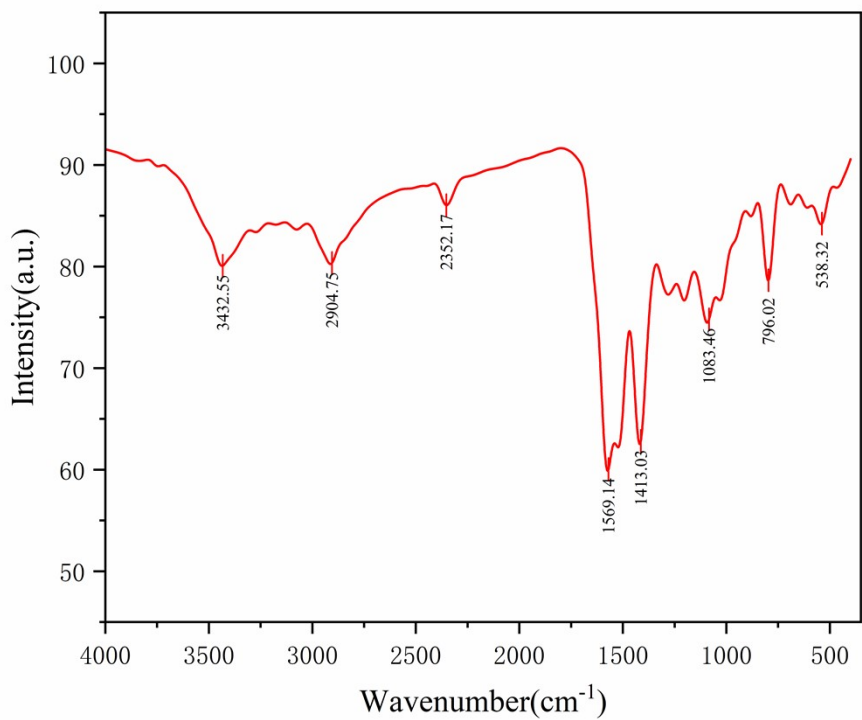


Figure 62 The IR spectrum of compound **4m**

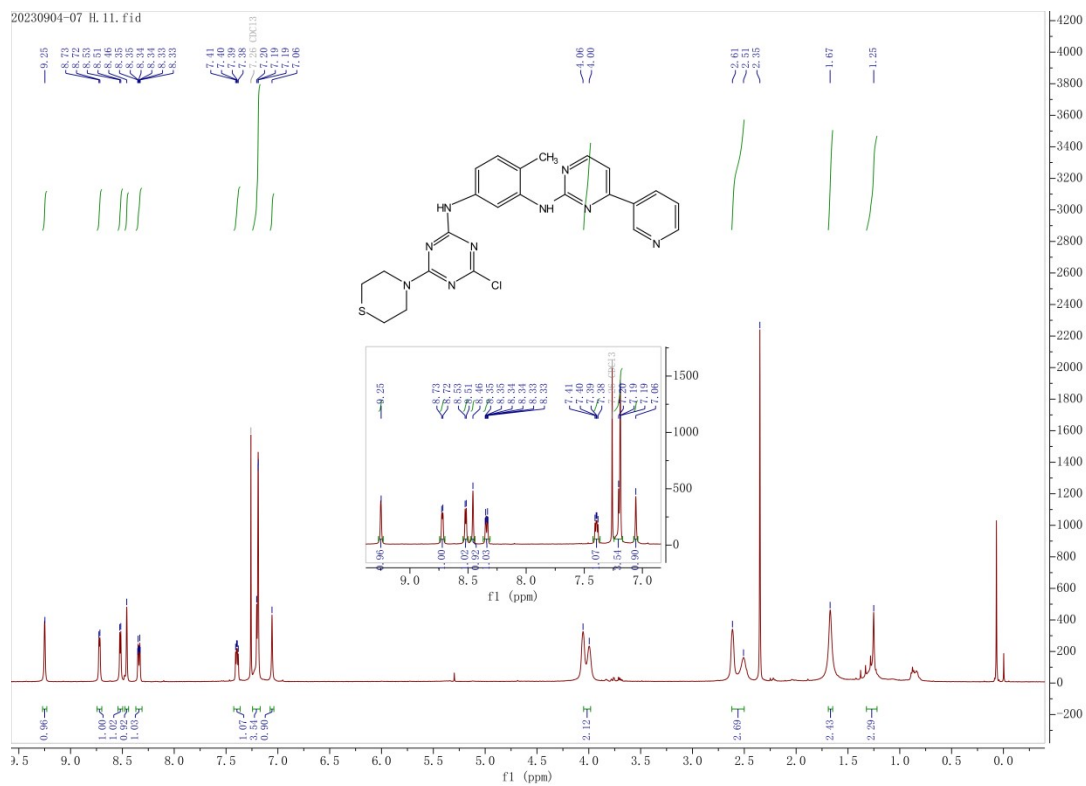


Figure 63 The <sup>1</sup>H NMR spectrum of compound **4m**

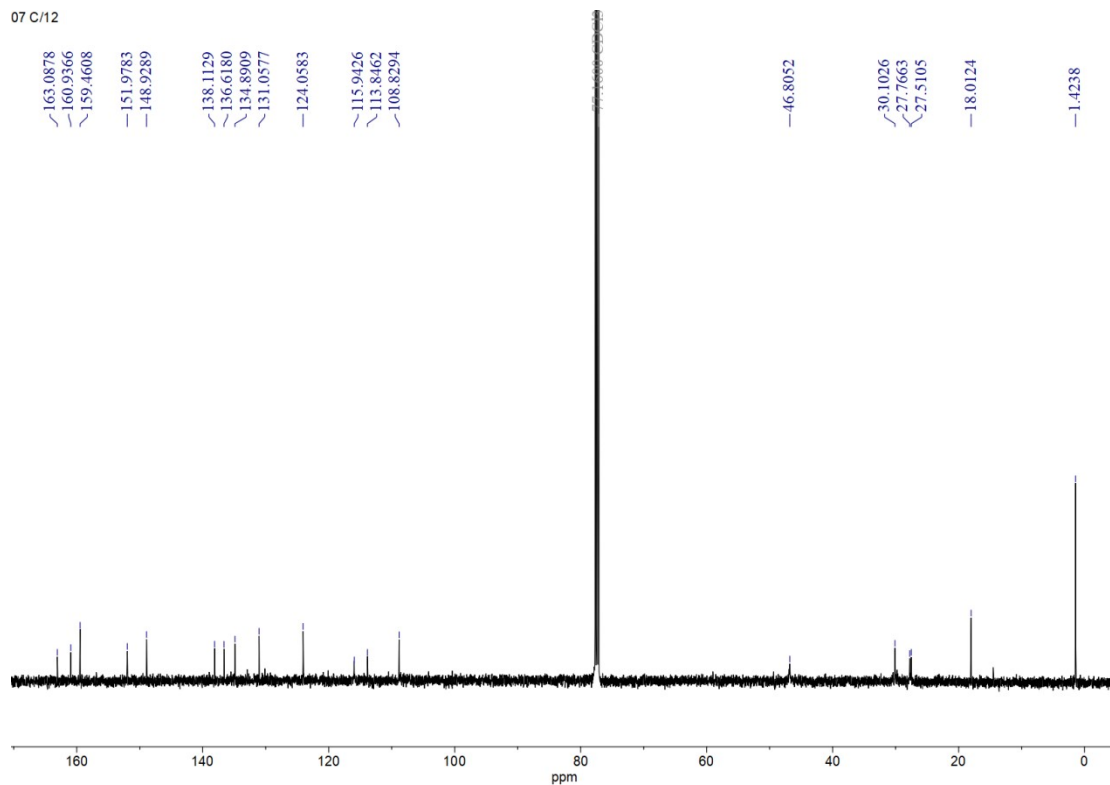


Figure 64 The  $^{13}\text{C}$  NMR spectrum of compound **4m**

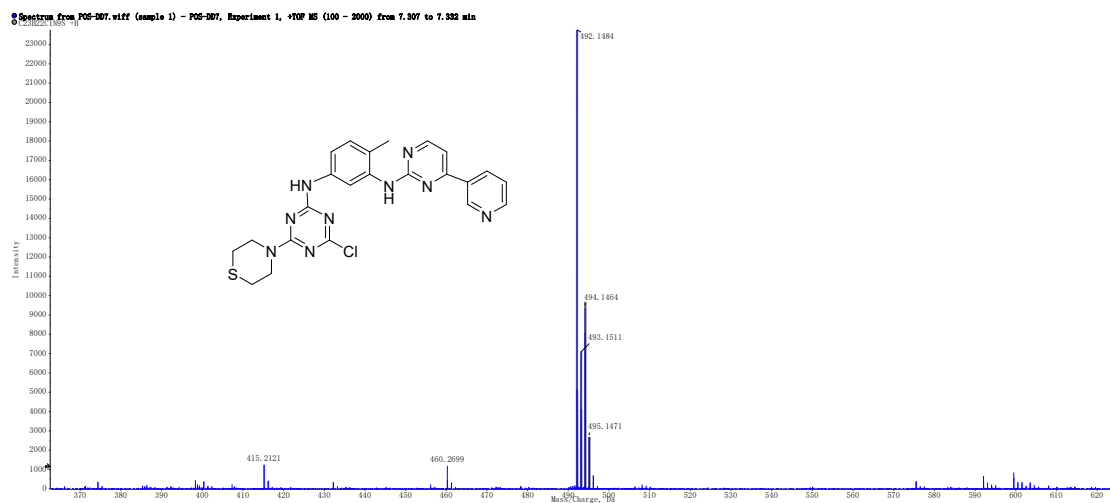
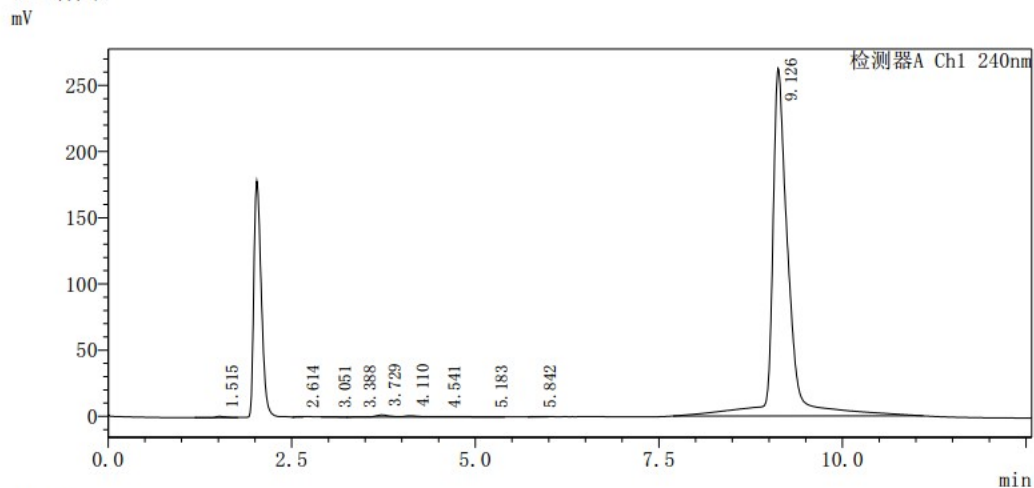


Figure 65 The HRMS spectrum of compound **4m**

<色谱图>



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	1.515	12151	1067	0.297		V	
2	2.614	2362	389	0.058			
3	3.051	2742	249	0.067			
4	3.388	1846	212	0.045			
5	3.729	22139	1646	0.541		V	
6	4.110	14123	1011	0.345		V	
7	4.541	13192	434	0.323		V	
8	5.183	4187	198	0.102		V	
9	5.842	4051	268	0.099			
10	9.126	4012405	262424	98.122		M	
总计		4089199	267898				

Figure 66 The HPLC of compound **4m**

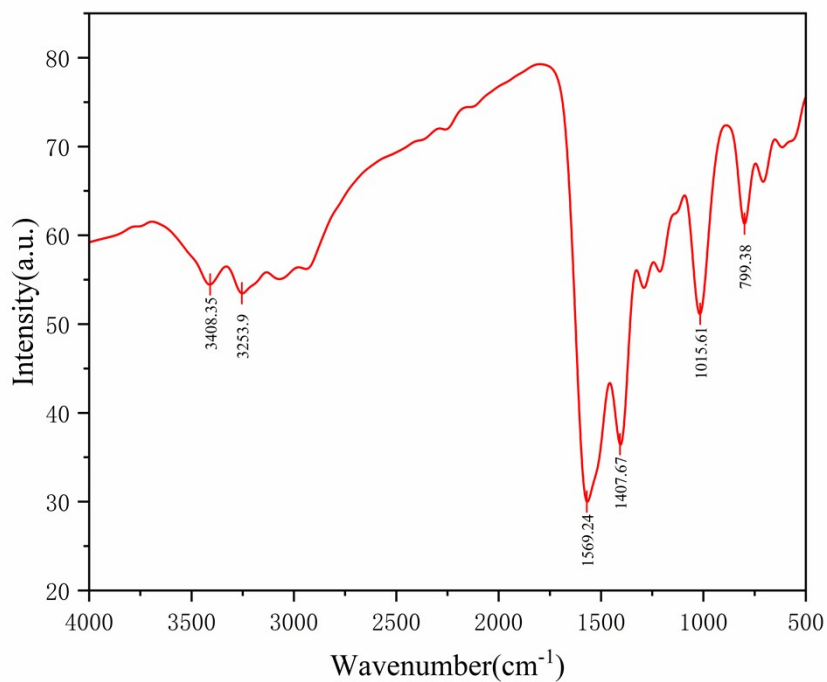


Figure 67 The IR spectrum of compound **4n**



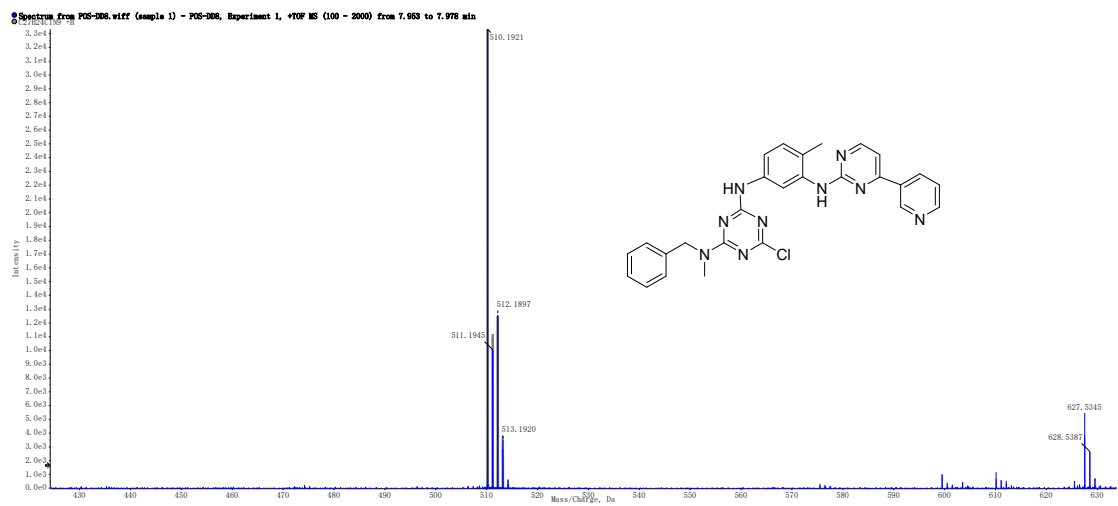
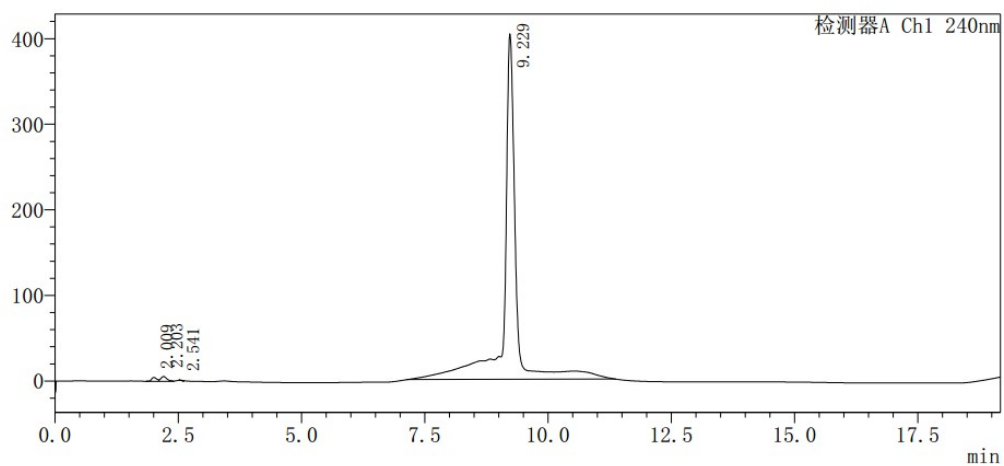


Figure 70 The HRMS spectrum of compound 4n

<色谱图>

mV



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	2.009	32919	4580	0.490			
2	2.203	48854	5752	0.727		V	
3	2.541	1685	-115	0.025		M	
4	9.229	6639792	403310	98.759		M	
总计		6723250	413528				

Figure 71 The HPLC of compound 4n



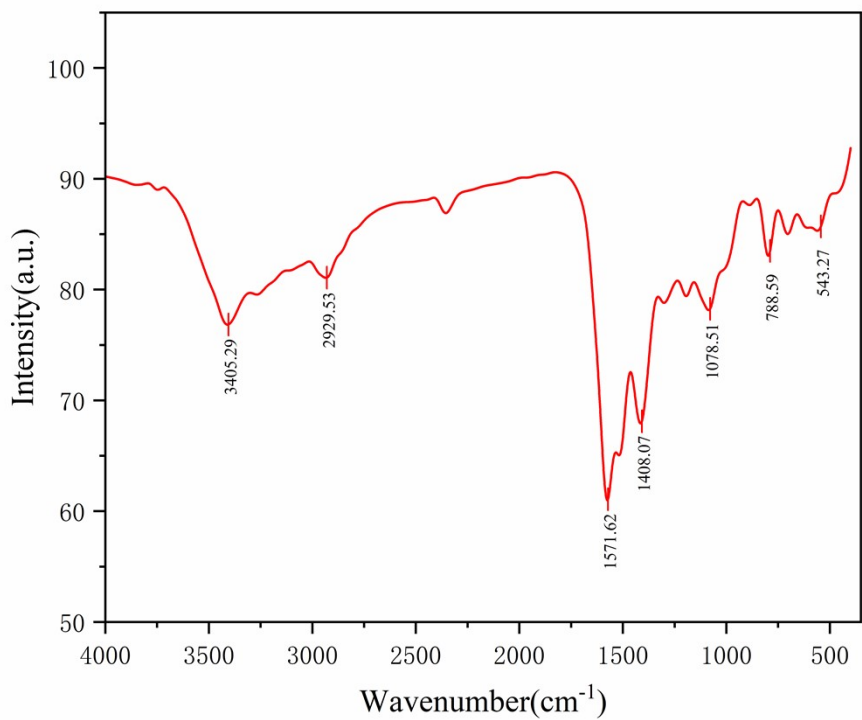


Figure 72 The IR spectrum of compound 4o

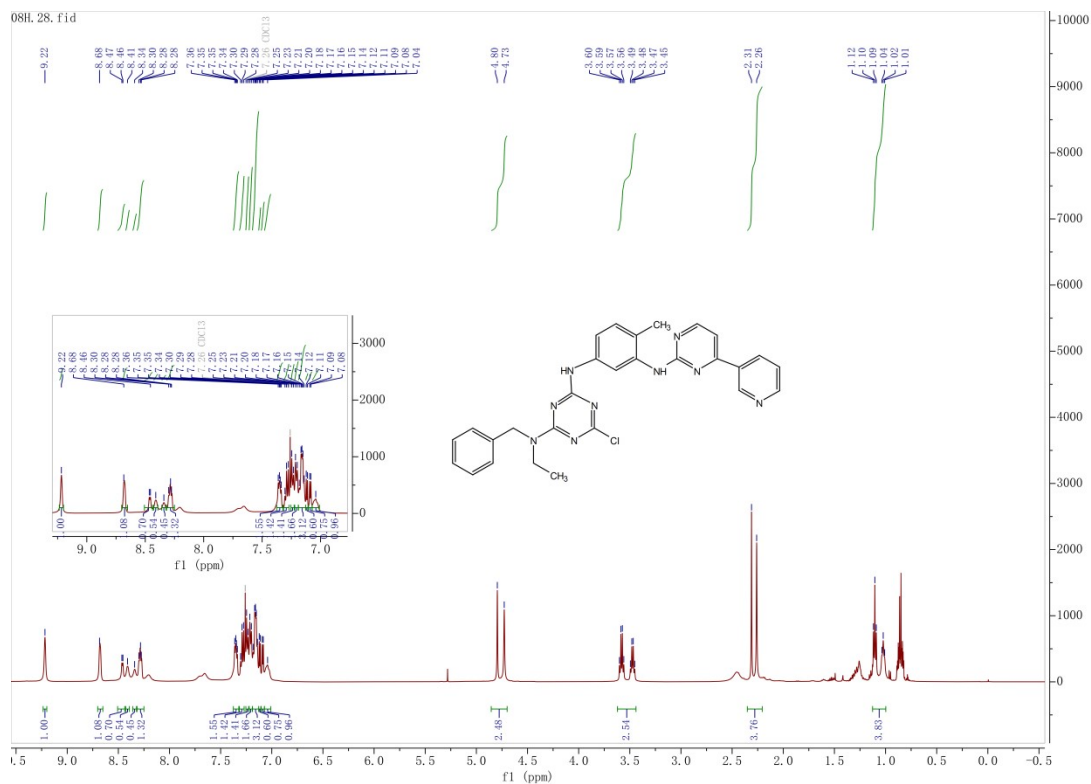


Figure 73 The <sup>1</sup>H NMR spectrum of compound 4o

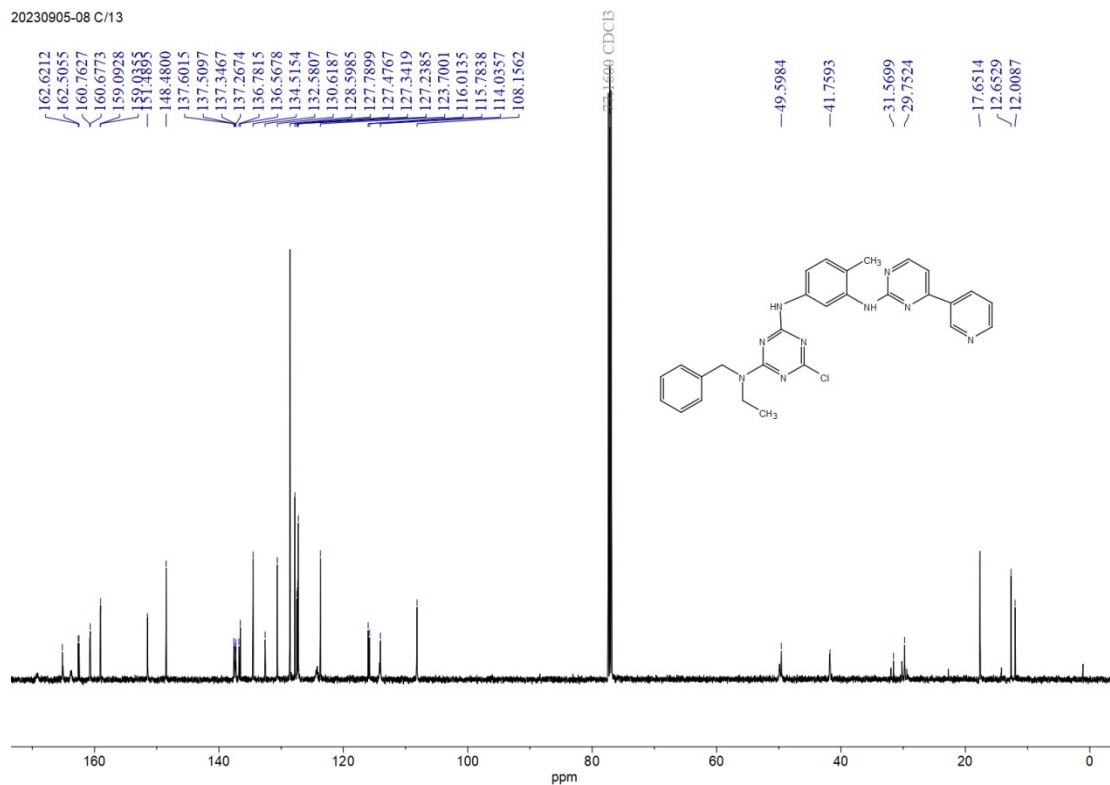


Figure 74 The <sup>13</sup>C NMR spectrum of compound 40

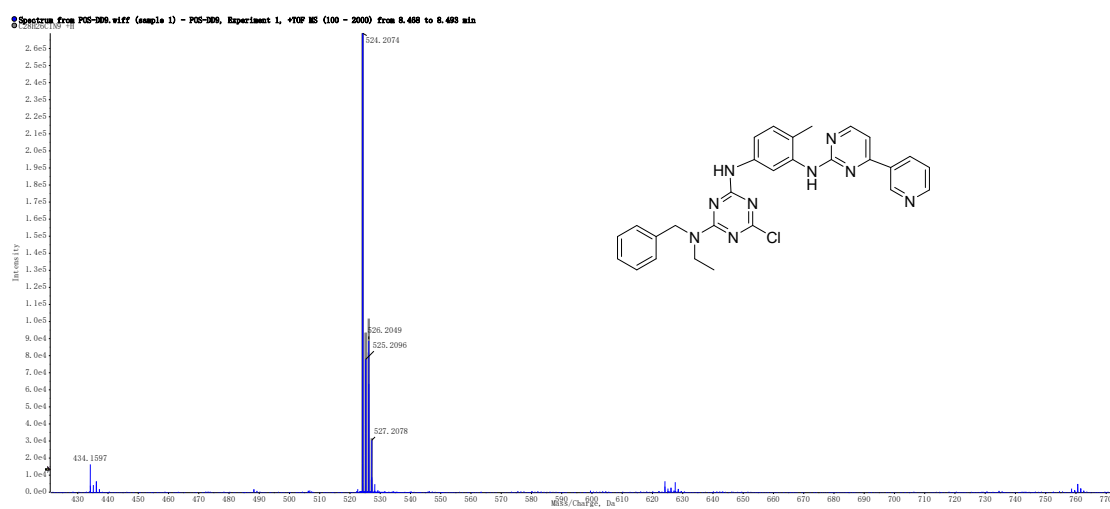
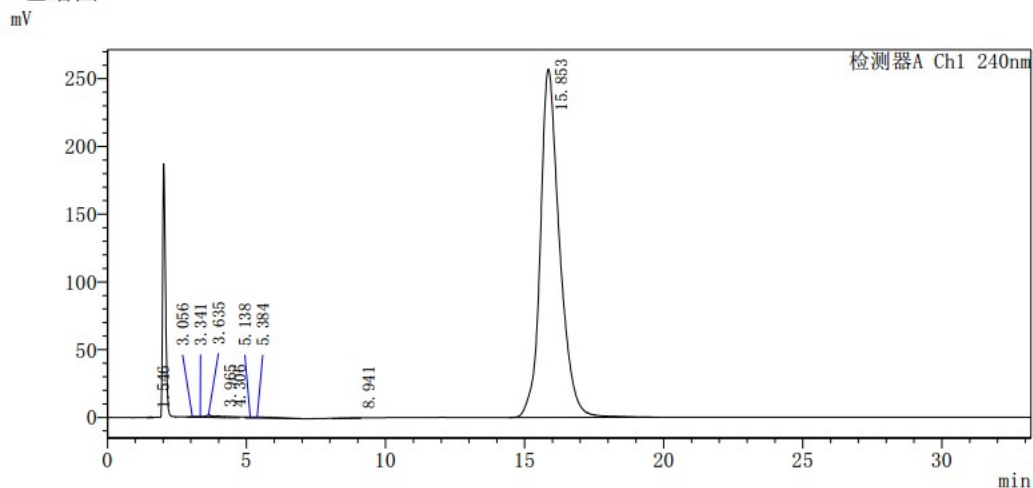


Figure 75 The HRMS spectrum of compound 40

<色谱图>



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	1.546	5517	628	0.044			
2	3.056	7214	527	0.058			
3	3.341	11452	734	0.091		V	
4	3.635	28037	1771	0.224		V	
5	3.965	20888	1274	0.167		V	
6	4.306	25897	860	0.207		V	
7	5.138	12895	756	0.103			
8	5.384	48736	848	0.389		V	
9	8.941	16167	410	0.129			
10	15.853	12340554	257002	98.588		S	
总计		12517357	264811				

Figure 76 The HPLC of compound **4o**

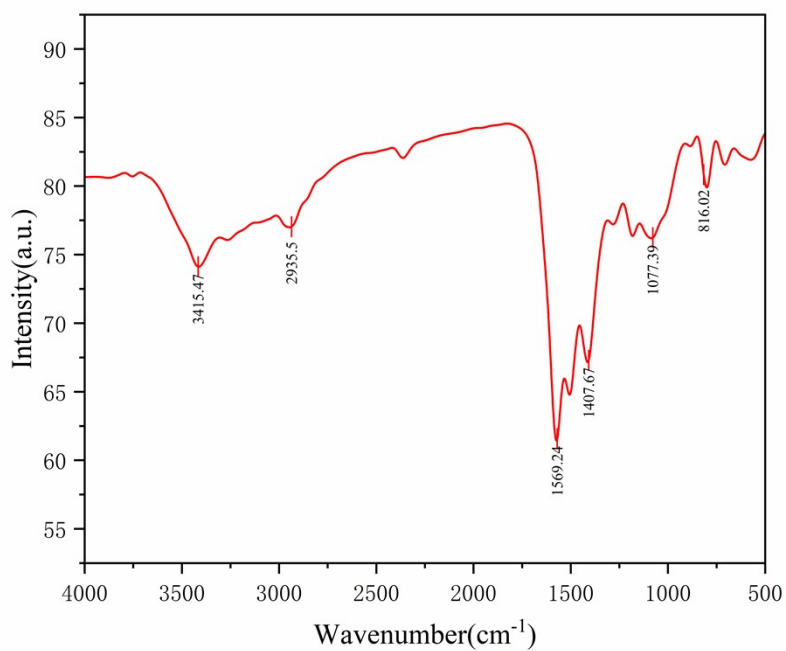


Figure 77 The IR spectrum of compound **4p**

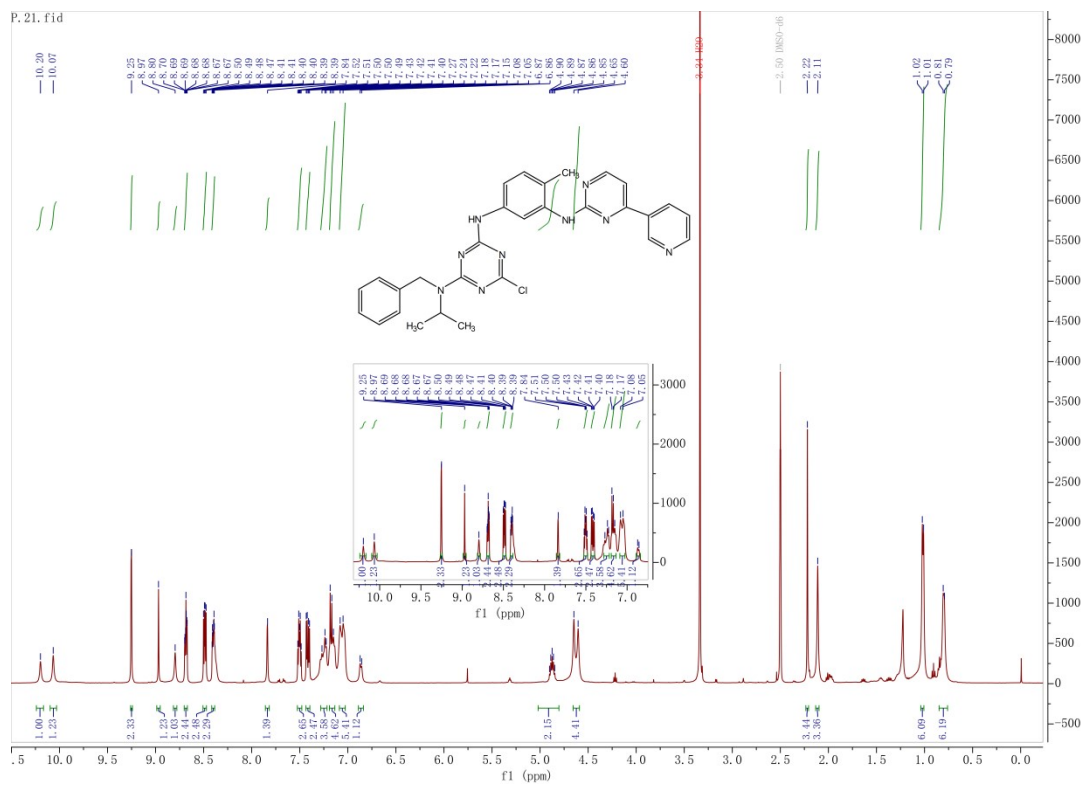


Figure 78 The  $^1\text{H}$  NMR spectrum of compound 4p

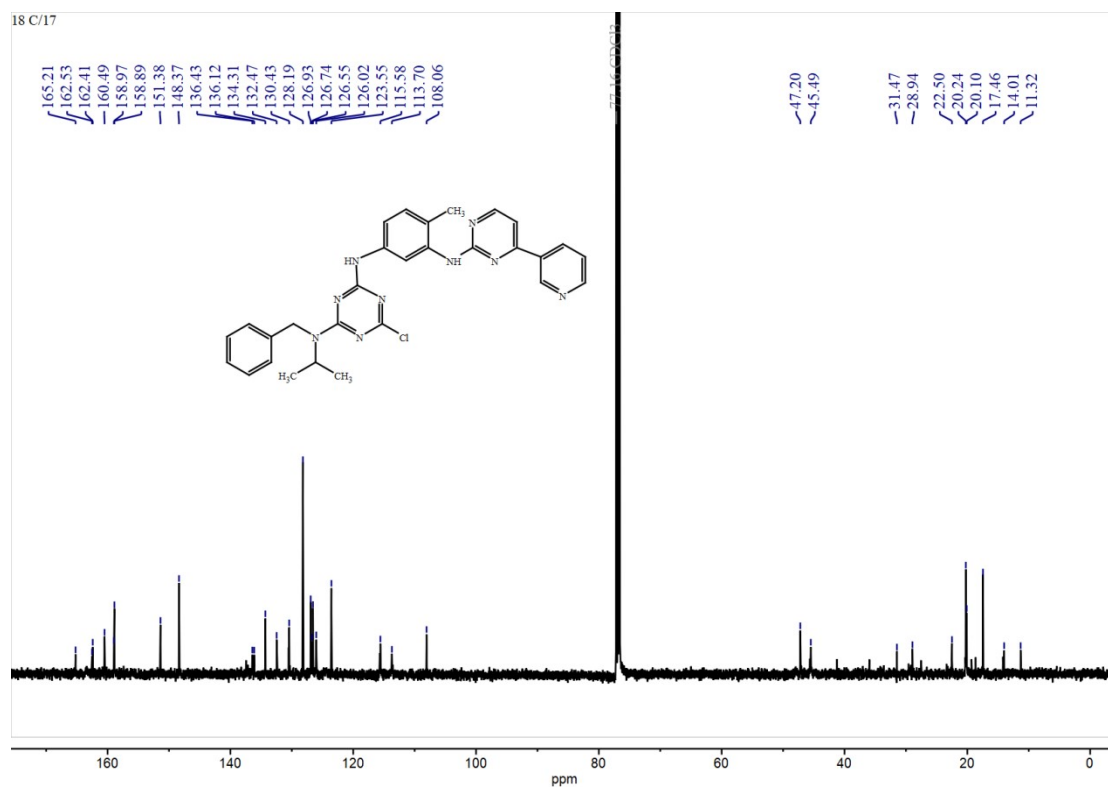


Figure 79 The  $^{13}\text{C}$  NMR spectrum of compound 4p

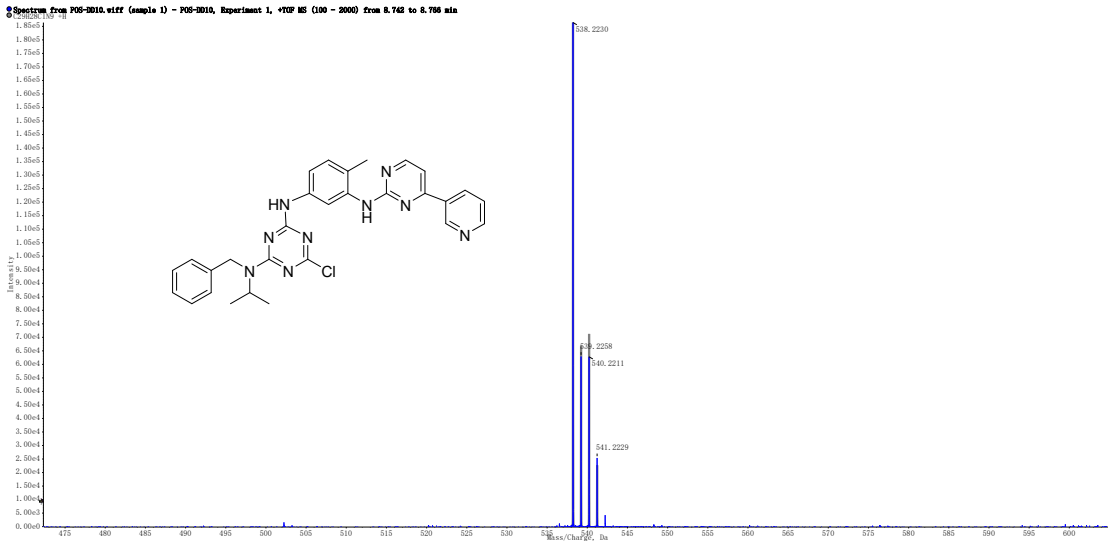
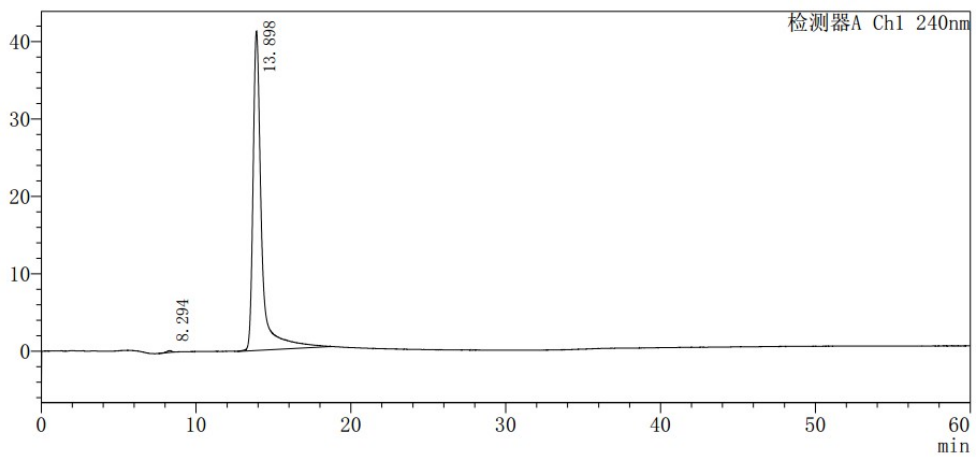


Figure 80 The HRMS spectrum of compound 4p

<色谱图>

mV



<峰表>

检测器A Ch1 240nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.294	5143	234	0.000			
2	13.898	1582608	41247	0.000		S	
总计		1587752	41481				

Figure 81 The HPLC of compound 4p

Table 1 Crystallographic data for compound **4a**

Compound	<b>4a</b>
Formula	C <sub>24</sub> H <sub>25</sub> Cl <sub>4</sub> N <sub>9</sub>
Formula weight	461.96
Crystal shape/color	Plate/yellow
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	9.478(4)
b/Å	12.216(5)
c/Å	13.705(6)
$\alpha$ /°	105.816(5)
$\beta$ /°	107.239(6)
$\gamma$ / °	101.579(6)
Volume /Å <sup>3</sup>	1388.1(10)
Z	2
$\rho_{\text{calc}}$ g/cm <sup>3</sup>	1.391
$\mu$ /mm <sup>-1</sup>	0.458
F (000)	600.0
Crystal size/mm <sup>3</sup>	0.21 × 0.15 × 0.11

Radiation	MoK $\alpha$ ( $\lambda = 0.71073$ )
2 $\Theta$ range for data collection/ $^{\circ}$	3.328 to 55.108
Index ranges	$-8 \leq h \leq 12$ , $-15 \leq k \leq 15$ , $-17 \leq l \leq 17$
Reflections collected	8622
Independent reflections	6174 [Rint = 0.0214, Rsigma = 0.0432]
Data/restraints/parameters	6174/103/337
Goodness-of-fit on F <sup>2</sup>	1.070
Final R indexes [I $\geq$ 2 $\sigma$ (I)]	R1 = 0.0806, wR2 = 0.2349
Final R indexes [all data]	R1 = 0.1091, wR2 = 0.2625
Largest diff. peak/hole / e $\text{\AA}^{-3}$	0.74/-0.71

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