

## Supporting Information

### Design, synthesis, and structure-activity relationship studies of 6,7-dihydro-5H-pyrrolo[1,2-*b*][1,2,4]triazole derivatives as necroptosis inhibitors

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## 1. Preparation of key intermediates

Intermediates **S5b–S5g** and **S9a–S9e** were synthesized *via* similar routes to intermediates **S5a**.

### **5-(3-(2-Amino-5-fluoropyridin-4-yl)-4-methylphenoxy)-2-methylpentan-2-ol (S5b)**

Purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a brown oil. Yield 75%. <sup>1</sup>H NMR (400 MHz, methanol-*d*<sub>4</sub>) δ 7.85 (d, *J* = 3.8 Hz, 1H), 7.20 (d, *J* = 8.5 Hz, 1H), 6.91 (dd, *J* = 8.5, 2.7 Hz, 1H), 6.75 (d, *J* = 2.7 Hz, 1H), 6.48 (d, *J* = 3.8 Hz, 1H), 3.99 (t, *J* = 6.4 Hz, 2H), 2.14 (s, 3H), 1.90 – 1.83 (m, 2H), 1.67 – 1.62 (m, 2H), 1.24 (s, 6H). LC/MS (ESI) *m/z*: 319.2 [M + H]<sup>+</sup>.

### **5-(3-(2-Amino-5-chloropyridin-4-yl)-4-methylphenoxy)-2-methylpentan-2-ol (S5c)**

Purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a pale-yellow oil. Yield 75%. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.96 (s, 1H), 7.17 (d, *J* = 8.5 Hz, 1H), 6.86 (dd, *J* = 8.5, 2.8 Hz, 1H), 6.61 (d, *J* = 2.8 Hz, 1H), 6.29 (s, 1H), 6.18 (s, 2H), 4.16 (s, 1H), 3.91 (t, *J* = 6.6 Hz, 2H), 1.98 (s, 3H), 1.76 – 1.67 (m, 2H), 1.48 – 1.41 (m, 2H), 1.07 (s, 6H). LC/MS (ESI) *m/z*: 335.2 [M + H]<sup>+</sup>.

### **5-(3-(2-Amino-5-methylpyridin-4-yl)-4-methylphenoxy)-2-methylpentan-2-ol (S5d)**

Purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a pale-yellow oil. Yield 89%. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.79 (s, 1H), 7.16 (d, *J* = 8.4 Hz, 1H), 6.82 (dd, *J* = 8.4, 2.7 Hz, 1H), 6.54 (d, *J* = 2.7 Hz, 1H), 6.15 (s, 1H), 5.69 (s, 2H), 4.16 (s, 1H), 3.90 (t, *J* = 6.6 Hz, 2H), 1.91 (s, 3H), 1.89 (s, 2H), 1.76 (s, 3H), 1.74 – 1.67 (m, 2H), 1.47 – 1.42 (m, 2H), 1.07 (s, 6H). LC/MS (ESI) *m/z*: 315.3 [M + H]<sup>+</sup>.

### **5-(3-(6-Aminopyridazin-4-yl)-4-methylphenoxy)-2-methylpentan-2-ol (S5e)**

Purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a gray solid. Yield 50%. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.55 (d, *J* = 2.7 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 1H), 6.96 (dd, *J* = 8.4, 2.7 Hz, 1H), 6.94 (d, *J* = 2.7 Hz, 1H), 6.90 (d, *J* = 2.7 Hz, 1H), 6.73 (s, 2H), 4.19 (s, 1H), 3.97 (t, *J* = 6.6 Hz, 2H),

2.19 (s, 3H), 1.81 – 1.72 (m, 2H), 1.53 – 1.46 (m, 2H), 1.11 (s, 6H). LC/MS (ESI)  $m/z$ : 302.2 [M + H]<sup>+</sup>.

***5-(3-(2-Aminopyridin-4-yl)-4-chlorophenoxy)-2-methylpentan-2-ol (S5f)***

Purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a black solid. Yield 83%. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 7.95 (d,  $J$  = 5.3 Hz, 1H), 7.43 (d,  $J$  = 8.8 Hz, 1H), 6.98 (dd,  $J$  = 8.8, 3.0 Hz, 1H), 6.87 (d,  $J$  = 3.0 Hz, 1H), 6.51 (d,  $J$  = 1.5 Hz, 1H), 6.45 (s, 1H), 6.03 (s, 2H), 4.19 (s, 1H), 3.98 (t,  $J$  = 6.6 Hz, 2H), 1.79 – 1.69 (m, 2H), 1.50 – 1.42 (m, 2H), 1.09 (s, 6H). LC/MS (ESI)  $m/z$ : 321.2 [M + H]<sup>+</sup>.

***5-(3-(2-Aminopyridin-4-yl)phenoxy)-2-methylpentan-2-ol (S5g)***

Purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a black solid. Yield 83%. <sup>1</sup>H NMR (400 MHz, chloroform-*d*) δ 8.07 (s, 1H), 7.35 (d,  $J$  = 8.2 Hz, 1H), 7.15 (d,  $J$  = 5.6 Hz, 1H), 7.10 (s, 1H), 6.94 (d,  $J$  = 8.2 Hz, 1H), 6.87 (d,  $J$  = 5.6 Hz, 1H), 6.72 (s, 1H), 4.78 (s, 2H), 4.04 (t,  $J$  = 6.3 Hz, 2H), 1.96 – 1.86 (m, 2H), 1.72 – 1.64 (m, 2H), 1.27 (s, 6H). LC/MS (ESI)  $m/z$ : 287.2 [M + H]<sup>+</sup>.

***4-(5-Methoxy-2-methylphenyl)pyridin-2-amine (S9a)***

The title compound was purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a black solid and directly used in the next step. Yield 73%. LC/MS (ESI)  $m/z$ : 215.1 [M + H]<sup>+</sup>.

***1-(3-(2-Aminopyridin-4-yl)-4-methylphenoxy)-2-methylpropan-2-ol (S9b)***

Purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a black solid. Yield 52%. <sup>1</sup>H NMR (400 MHz, chloroform-*d*) δ 8.05 (d,  $J$  = 5.2 Hz, 1H), 7.16 (d,  $J$  = 8.4 Hz, 1H), 6.86 (dd,  $J$  = 8.4, 2.3 Hz, 1H), 6.76 (d,  $J$  = 2.3 Hz, 1H), 6.62 (d,  $J$  = 5.2 Hz, 1H), 6.47 (s, 1H), 4.81 (s, 2H), 3.79 (s, 2H), 2.19 (s, 3H), 1.34 (s, 6H). LC/MS (ESI)  $m/z$ : 272.2 [M + H]<sup>+</sup>.

***4-(2-Methyl-5-(2-(tetrahydro-2H-pyran-4-yl)ethoxy)phenyl)pyridin-2-amine (S9c)***

Purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a gray solid. Yield 55%. <sup>1</sup>H NMR (400 MHz, chloroform-*d*) δ 8.08 (d,  $J$  = 5.2 Hz, 1H), 7.15 (d,  $J$  = 8.4 Hz, 1H), 6.82 (dd,  $J$  = 8.4, 2.7 Hz, 1H), 6.73 (d,  $J$  = 2.7

Hz, 1H), 6.62 (dd,  $J = 5.3, 1.5$  Hz, 1H), 6.44 (s, 1H), 4.50 (s, 2H), 4.04 – 3.92 (m, 4H), 3.46 – 3.34 (m, 2H), 2.19 (s, 3H), 1.77 – 1.69 (m, 3H), 1.69 – 1.62 (m, 2H), 1.41 – 1.29 (m, 2H). LC/MS (ESI)  $m/z$ : 313.2  $[M + H]^+$ .

***4-(3-(2-Aminopyridin-4-yl)-4-methylphenoxy)butanenitrile (S9d)***

The title compound was purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a gray solid and directly used in the next step. Yield 58%. LC/MS (ESI)  $m/z$ : 268.2  $[M + H]^+$ .

***4-(2-Methyl-5-(2-morpholinoethoxy)phenyl)pyridin-2-amine (S9e)***

Purified by preparative thin layer chromatography (dichloromethane: methanol = 20: 1, V: V) as a gray solid. Yield 60%.  $^1\text{H}$  NMR (400 MHz, chloroform- $d$ )  $\delta$  8.09 (d,  $J = 5.3$  Hz, 1H), 7.16 (d,  $J = 8.4$  Hz, 1H), 6.84 (dd,  $J = 8.4, 2.8$  Hz, 1H), 6.75 (d,  $J = 2.8$  Hz, 1H), 6.62 (dd,  $J = 5.3, 1.5$  Hz, 1H), 6.44 (t,  $J = 1.5$  Hz, 1H), 4.50 (s, 2H), 4.11 (t,  $J = 5.7$  Hz, 2H), 3.76 – 3.70 (m, 4H), 2.80 (t,  $J = 5.7$  Hz, 2H), 2.62 – 2.54 (m, 4H), 2.19 (s, 3H). LC/MS (ESI)  $m/z$ : 314.2  $[M + H]^+$ .

Intermediates **S7b–S7h** and **S11a–S11b** were synthesized via similar routes to intermediates **S7a**.

***5-(2-Fluorophenyl)-6,7-dihydro-5H-pyrrolo[1,2-b][1,2,4]triazole-2-carboxylic acid (S7b)***

The title compound was obtained through filtration as a white solid and directly used in the next step. Yield 54%. LC/MS (ESI)  $m/z$ : 246.1  $[M - H]^-$ .

***5-(3-Fluorophenyl)-6,7-dihydro-5H-pyrrolo[1,2-b][1,2,4]triazole-2-carboxylic acid (S7c)***

The title compound was obtained through filtration as a white solid and directly used in the next step. Yield 54%.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  13.23 (brs, 1H), 7.46 (dd,  $J = 8.2, 6.0$  Hz, 1H), 7.22 – 7.18 (m, 1H), 7.18 – 7.08 (m, 2H), 5.61 (dd,  $J = 8.2, 6.0$  Hz, 1H), 3.24 – 3.05 (m, 3H), 3.04 – 2.94 (m, 1H), 2.62 – 2.54 (m, 1H). LC/MS (ESI)  $m/z$ : 246.1  $[M - H]^-$ .

***5-(4-Fluorophenyl)-6,7-dihydro-5H-pyrrolo[1,2-b][1,2,4]triazole-2-carboxylic acid (S7d)***

The title compound was obtained through filtration as a white solid and directly

used in the next step. Yield 84%. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 13.20 (brs, 1H), 7.37 – 7.28 (m, 2H), 7.25 – 7.21 (m, 2H), 5.59 (t, *J* = 7.3 Hz, 1H), 3.21 – 3.04 (m, 2H), 3.04 – 2.92 (m, 1H), 2.60 – 2.52 (m, 1H). LC/MS (ESI) *m/z*: 246.1 [M - H]<sup>-</sup>.

***5-Cyclohexyl-6,7-dihydro-5H-pyrrolo[1,2-b][1,2,4]triazole-2-carboxylic acid (S7e)***

The title compound was obtained through filtration as a white solid and directly used in the next step. Yield 99%. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 13.15 (brs, 1H), 4.34 – 4.27 (m, 1H), 2.83 (t, *J* = 7.4 Hz, 2H), 2.76 – 2.65 (m, 1H), 2.47 – 2.39 (m, 1H), 1.94 – 1.84 (m, 1H), 1.83 – 1.66 (m, 3H), 1.63 – 1.58 (m, 1H), 1.29 (s, 1H), 1.28 – 1.06 (m, 4H), 0.94 – 0.83 (m, 1H). LC/MS (ESI) *m/z*: 234.1 [M - H]<sup>-</sup>.

***5-Cyclopentyl-6,7-dihydro-5H-pyrrolo[1,2-b][1,2,4]triazole-2-carboxylic acid (S7f)***

The title compound was obtained through filtration as a white solid and directly used in the next step. Yield 77%. LC/MS (ESI) *m/z*: 220.1 [M - H]<sup>-</sup>.

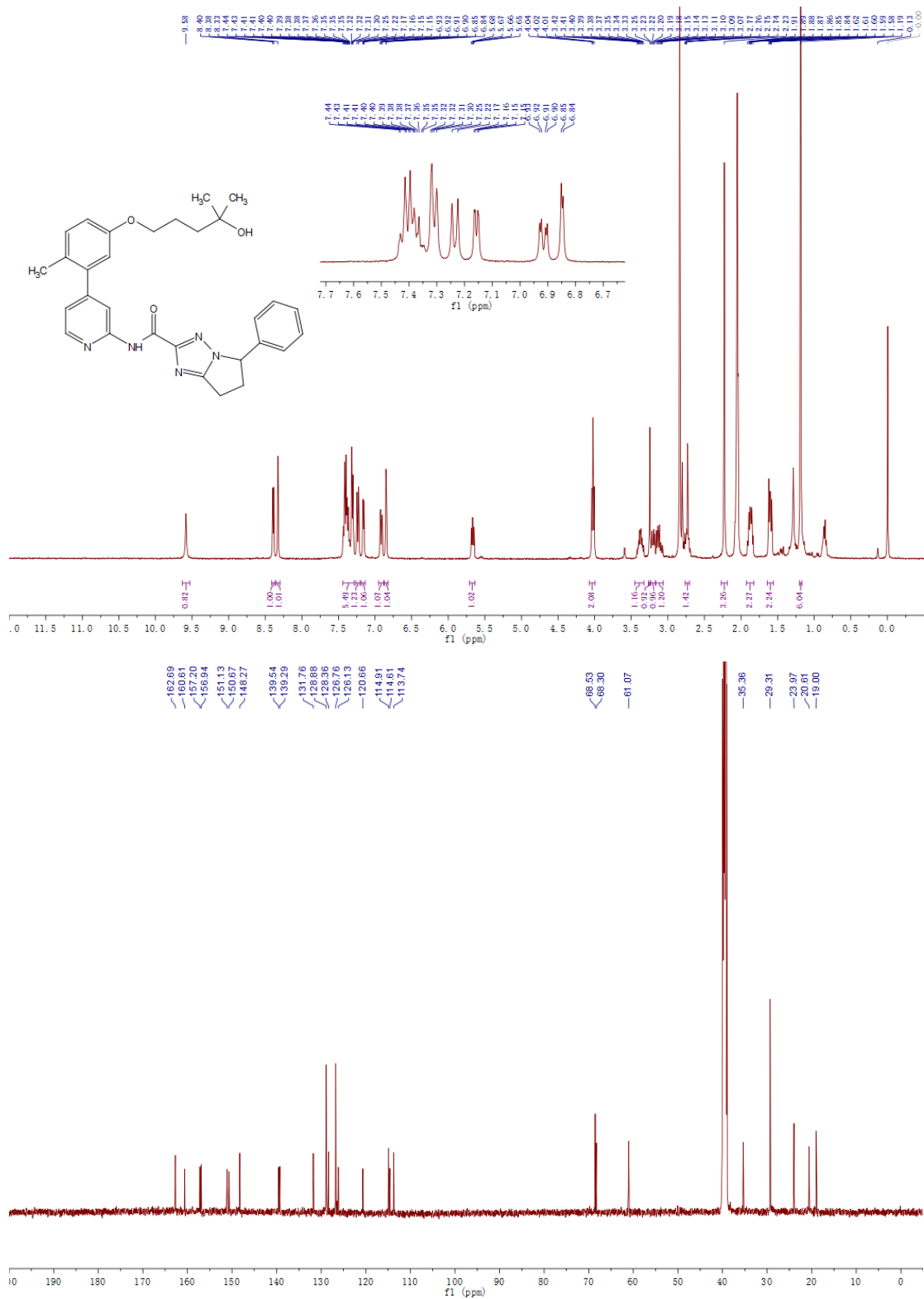
***Trans-7-Fluoro-5-phenyl-6,7-dihydro-5H-pyrrolo[1,2-b][1,2,4]triazole-2-carboxylic acid (S7g)***

The title compound was obtained through filtration as a white solid and directly used in the next step. Yield 99%. LC/MS (ESI) *m/z*: 246.0 [M - H]<sup>-</sup>.

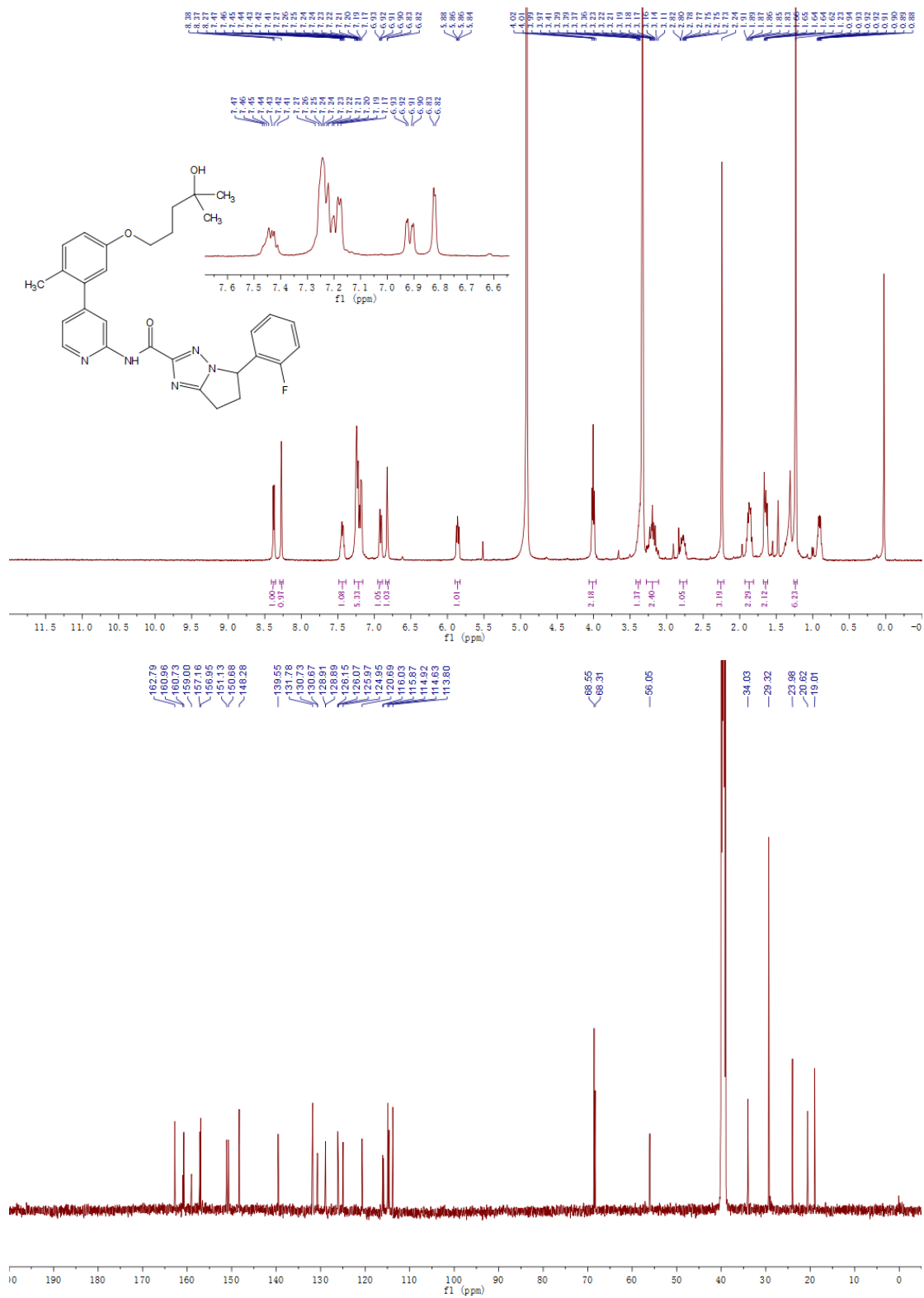
***Cis-7-Fluoro-5-phenyl-6,7-dihydro-5H-pyrrolo[1,2-b][1,2,4]triazole-2-carboxylic acid (S7h), (5R,7R)-7-fluoro-5-phenyl-6,7-dihydro-5H-pyrrolo[1,2-b][1,2,4]triazole-2-carboxylic acid (S11a) and (5S,7S)-7-fluoro-5-phenyl-6,7-dihydro-5H-pyrrolo[1,2-b][1,2,4]triazole-2-carboxylic acid (S11b)***

The title compound was obtained through filtration as a white solid and directly used in the next step. Yield 76%. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 13.51 (brs, 1H), 7.47 – 7.36 (m, 3H), 7.28 – 7.23 (m, 2H), 6.22 (dd, <sup>2</sup>*J*<sub>H-F</sub> = 56.5 Hz, *J* = 6.9 Hz, 1H), 5.73 – 5.67 (m, 1H), 3.82 – 3.65 (m, 1H), 2.70 (dd, <sup>3</sup>*J*<sub>H-F</sub> = 27.8, *J* = 14.8 Hz, 1H). LC/MS (ESI) *m/z*: 246.0 [M - H]<sup>-</sup>.

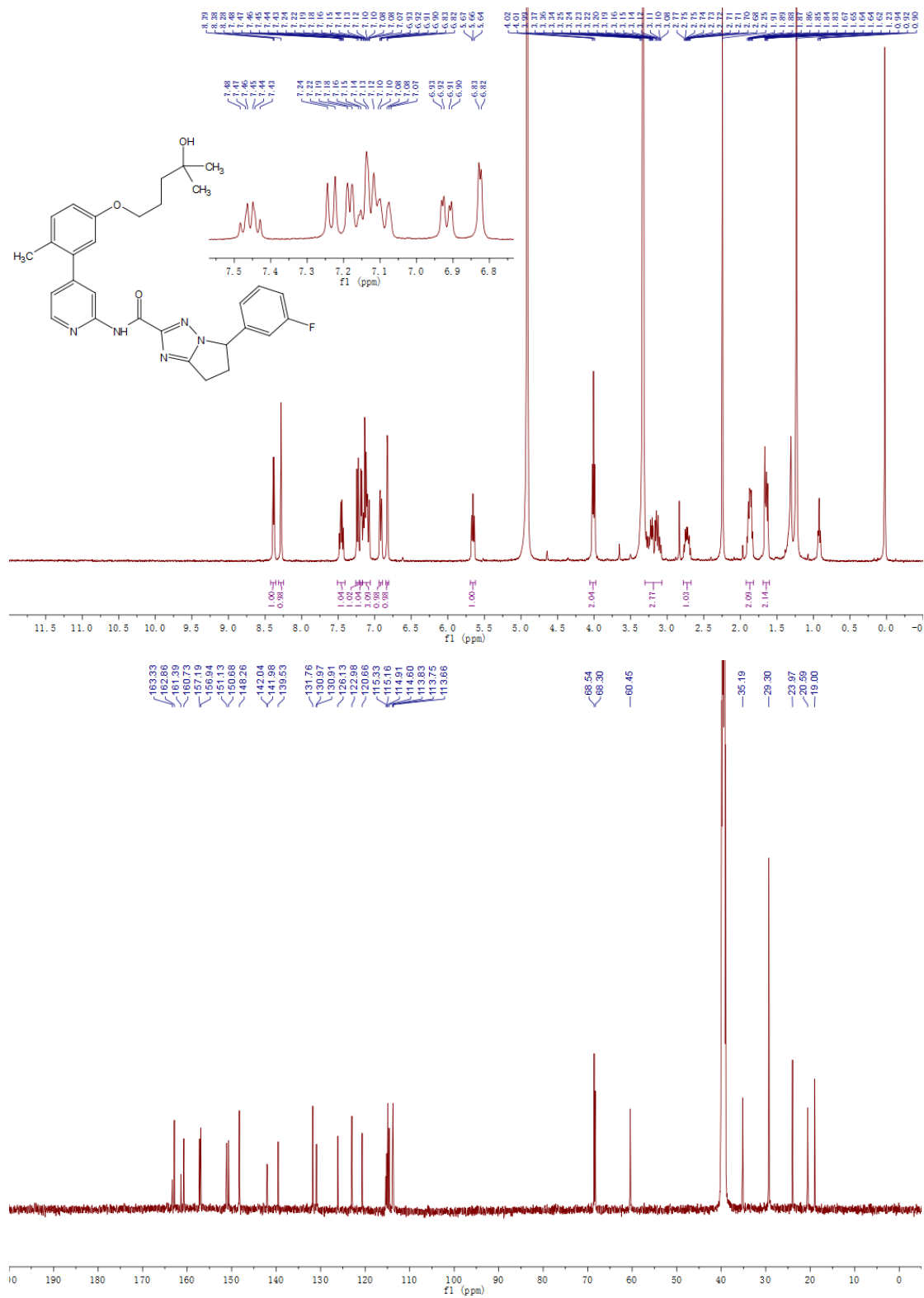
## 2. NMR spectra of target compounds



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 7

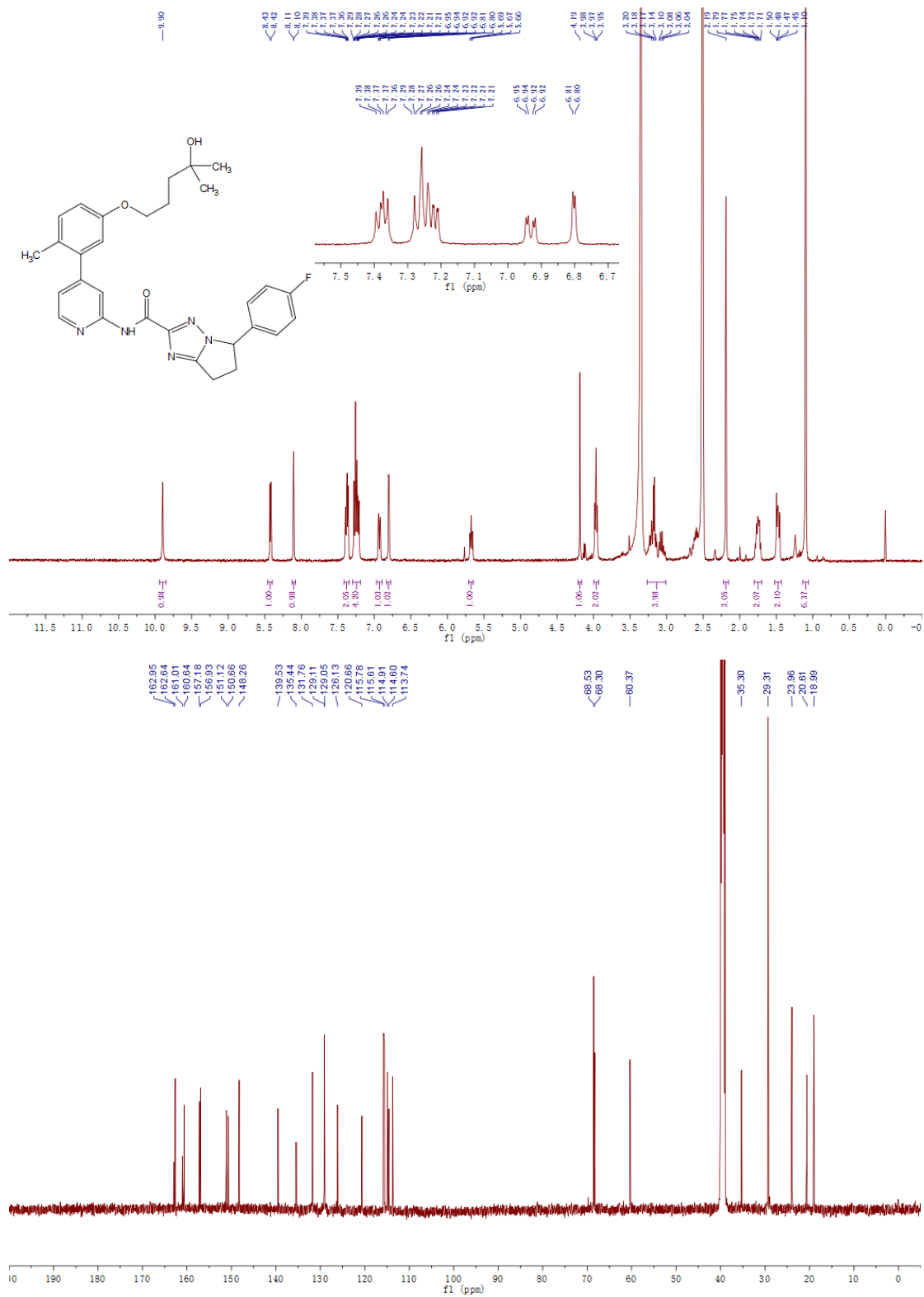


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **8**



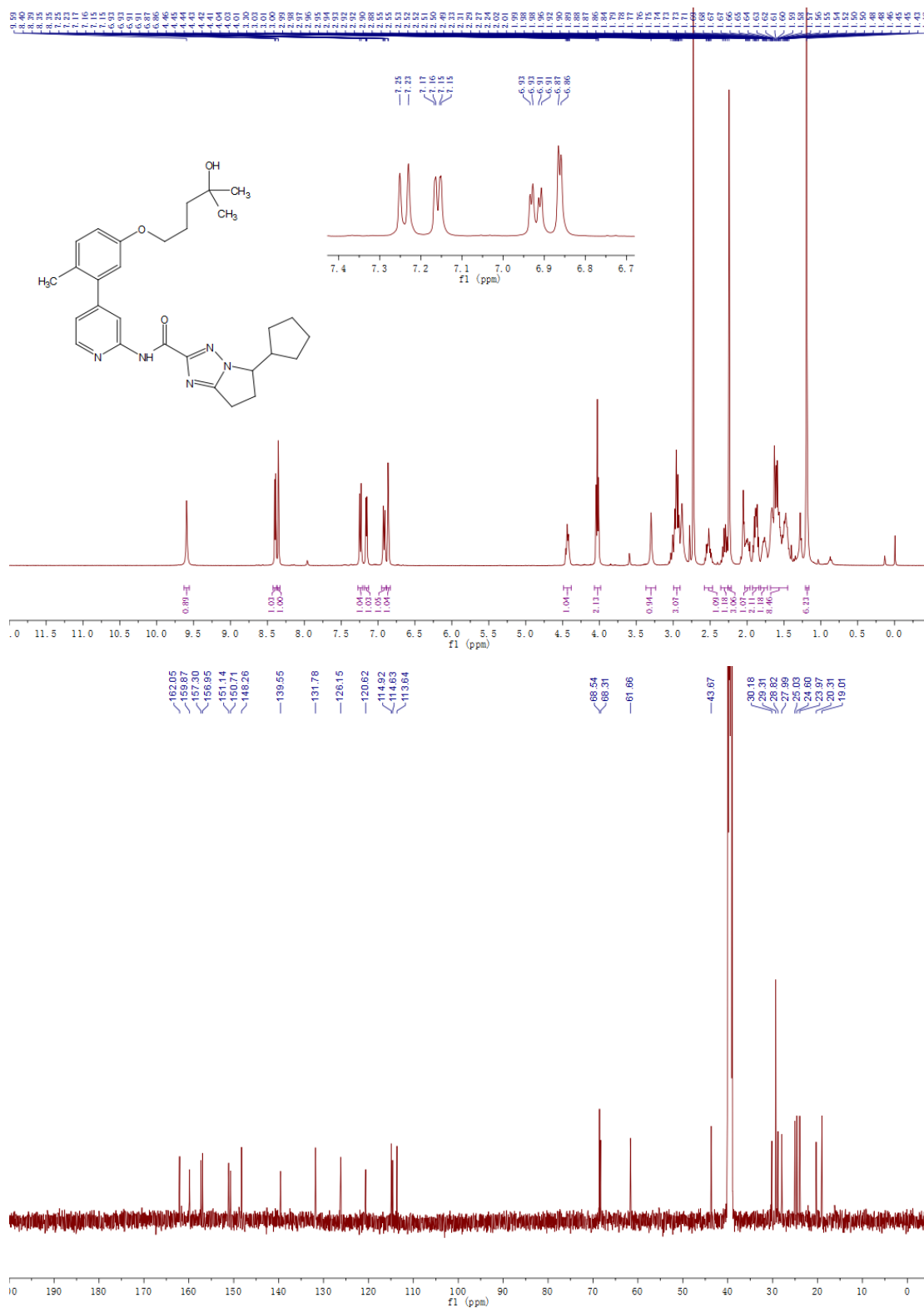
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 9





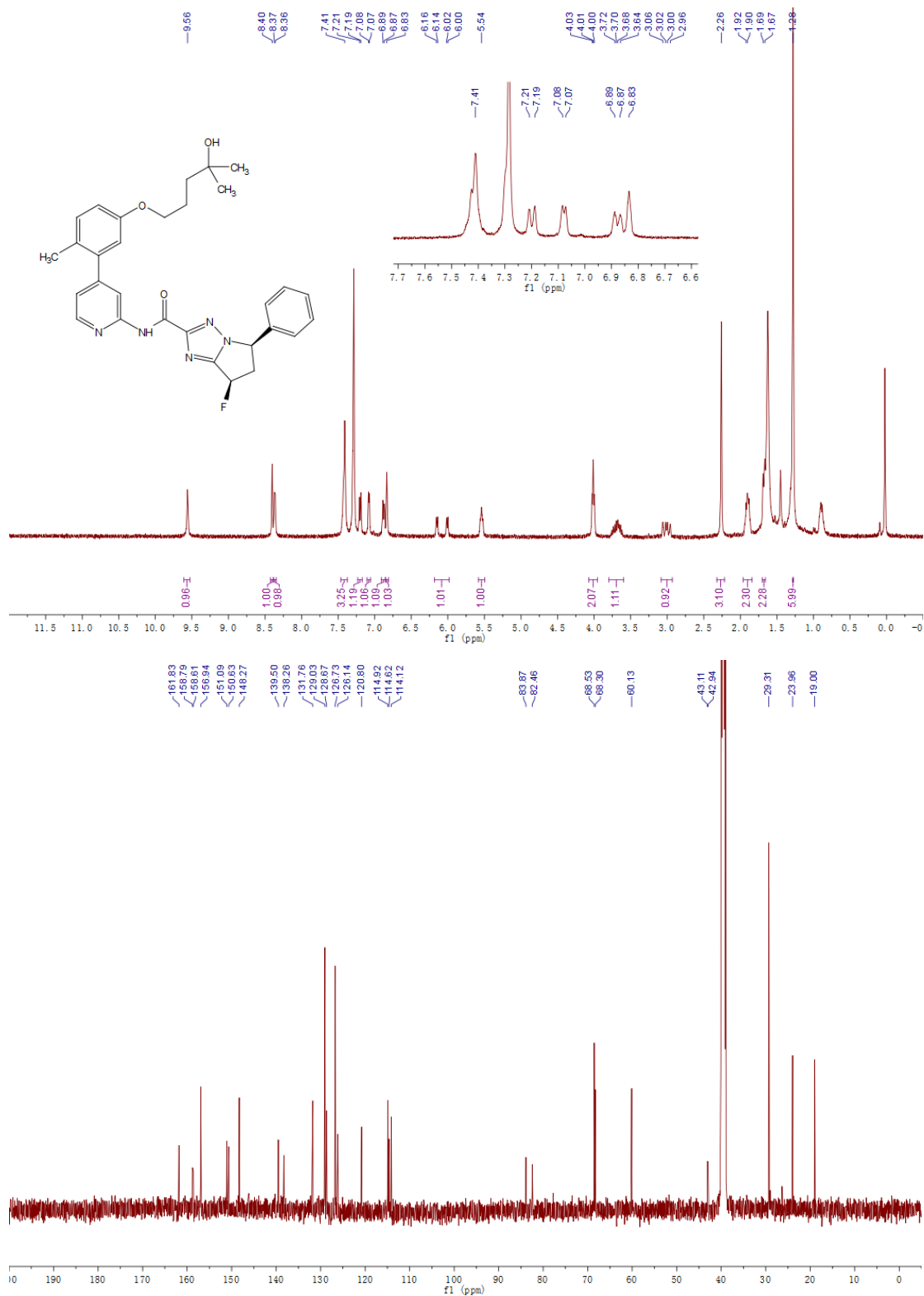
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 10



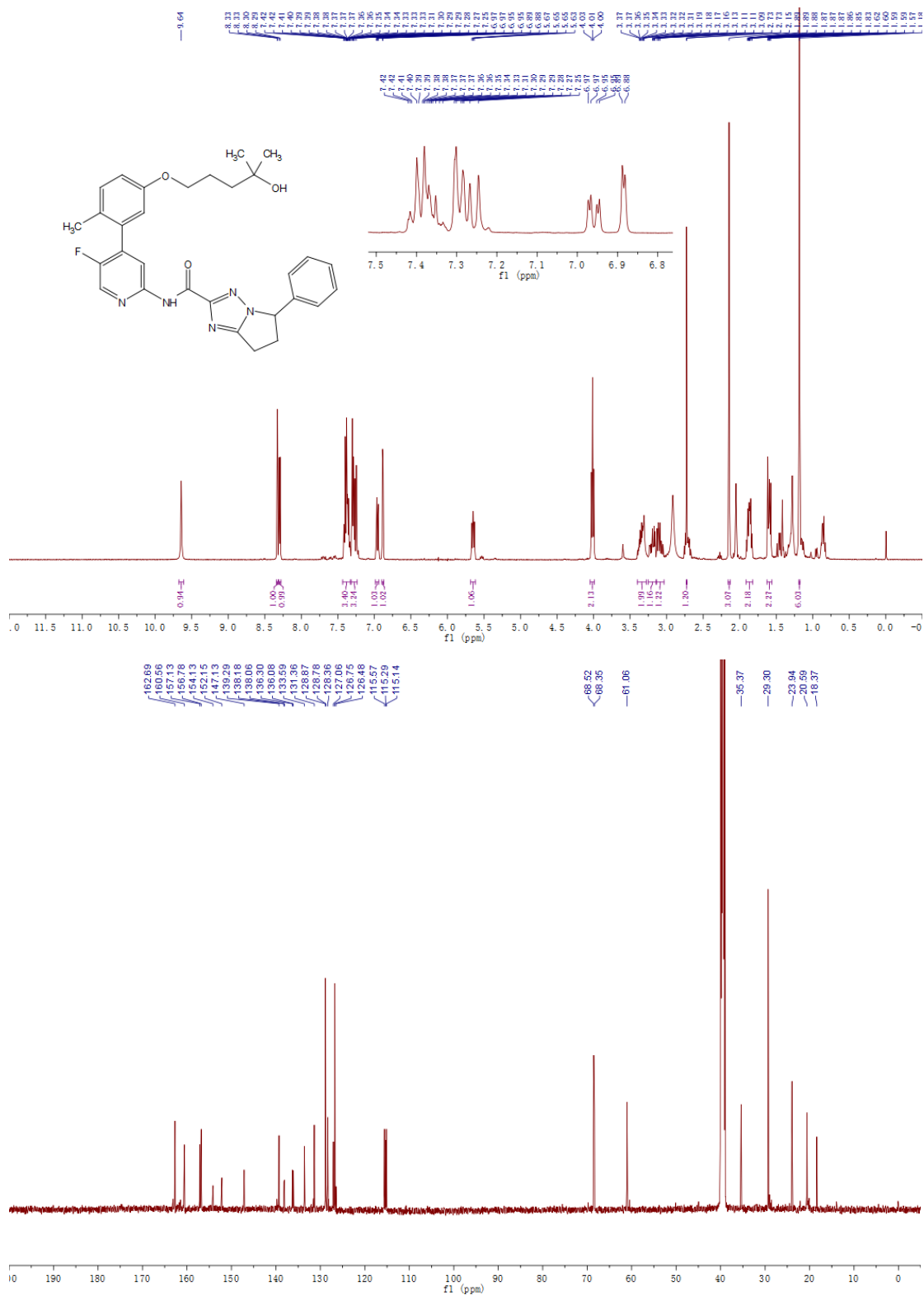


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 12

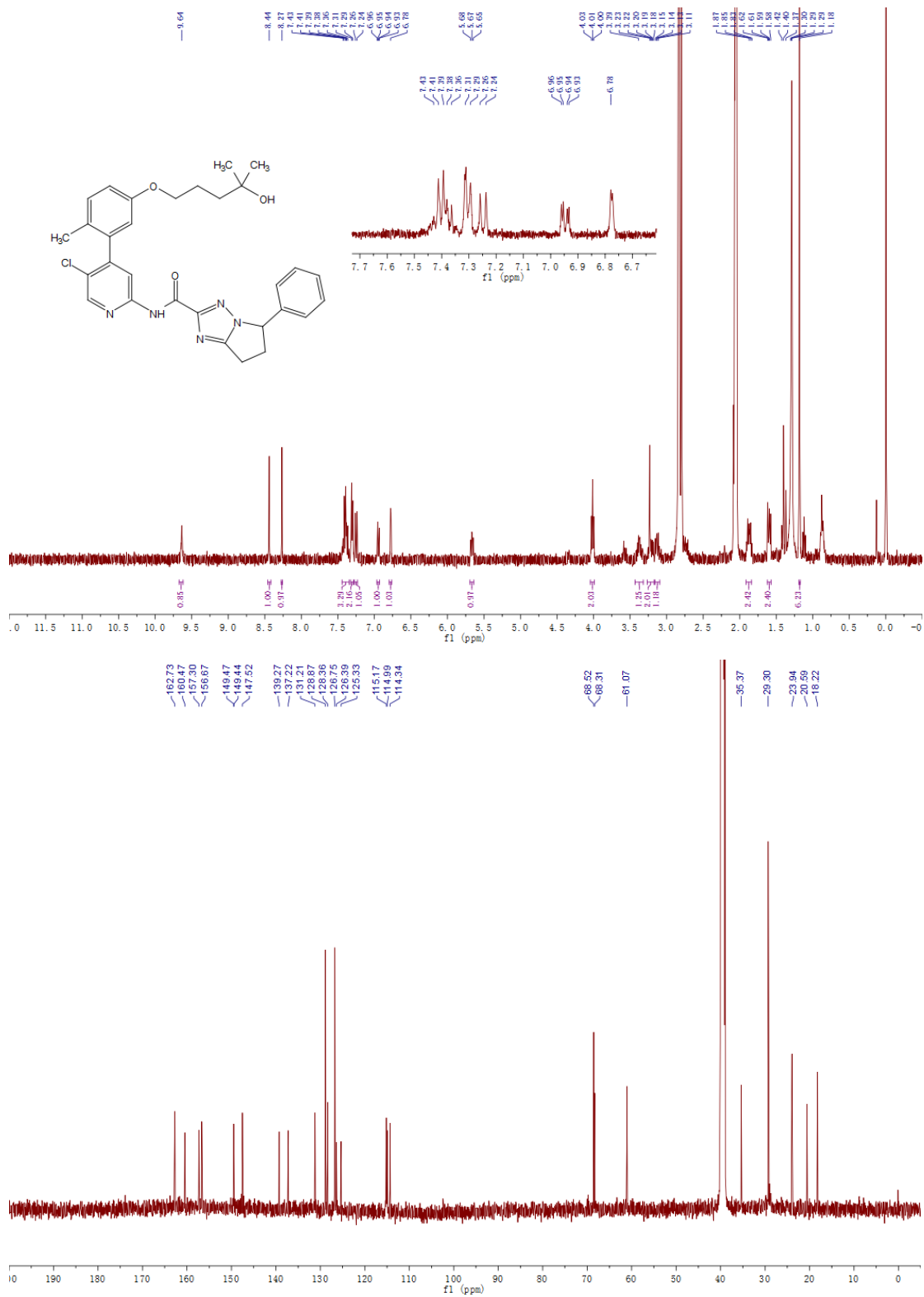




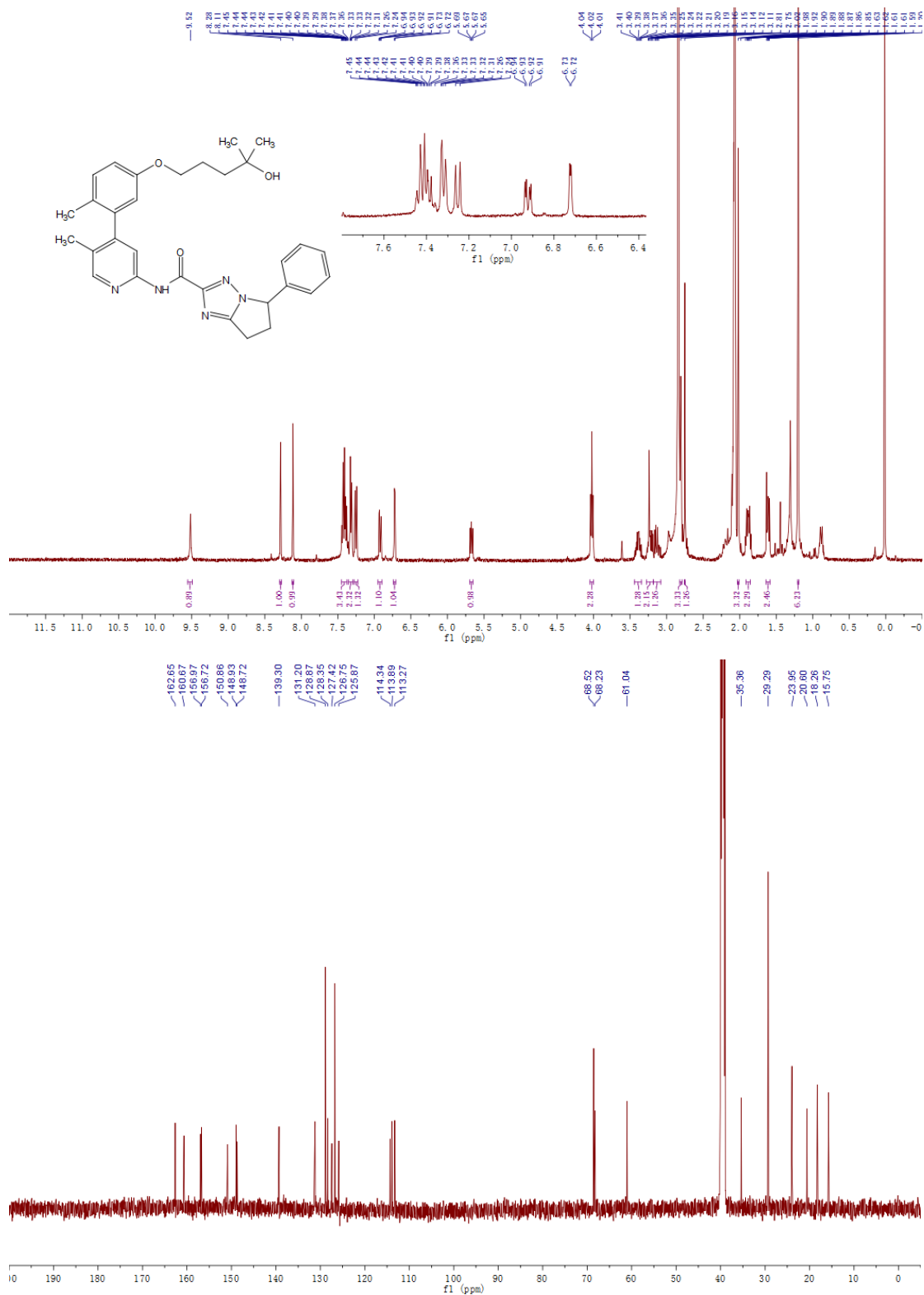
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 14



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 15

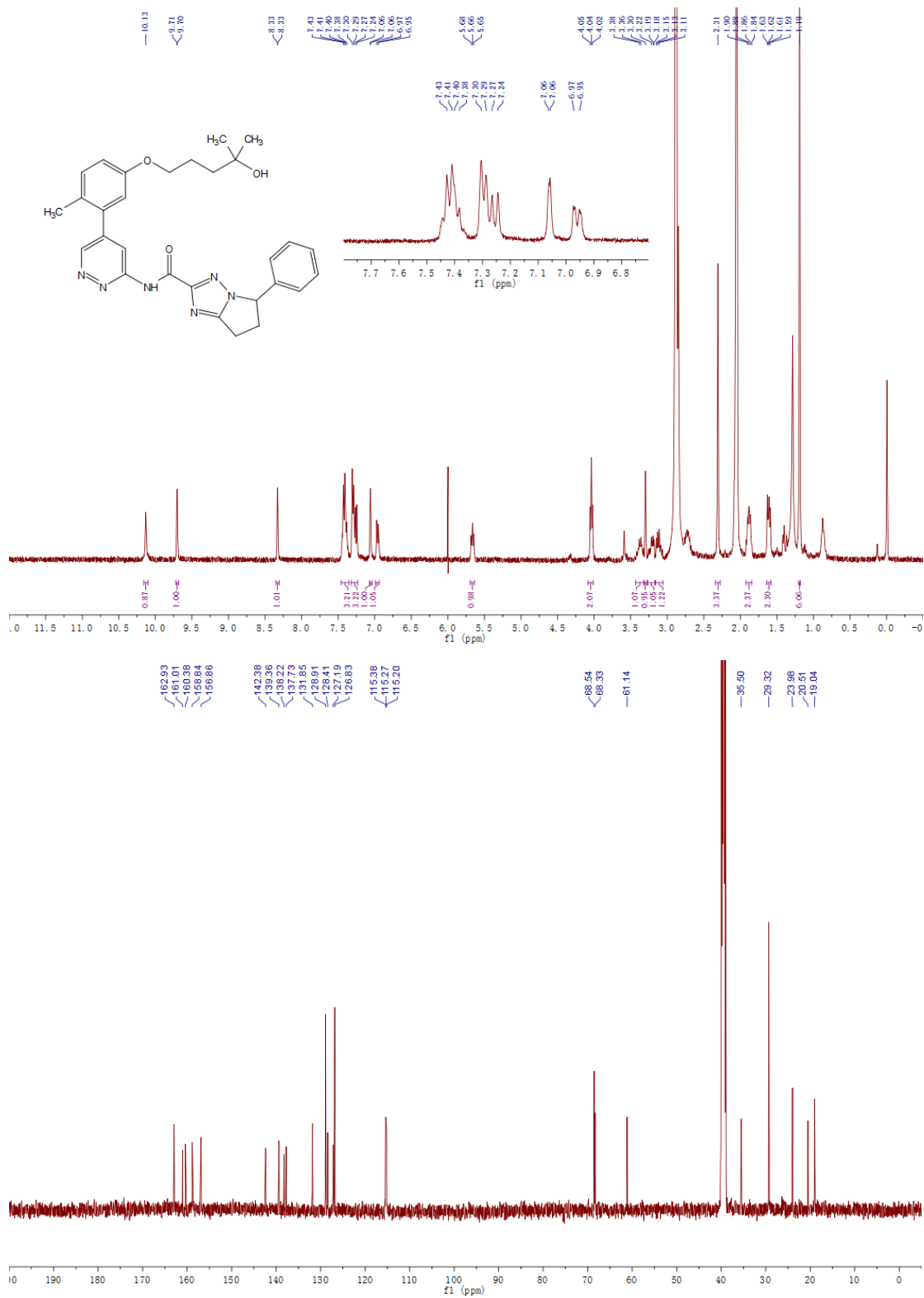


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 16



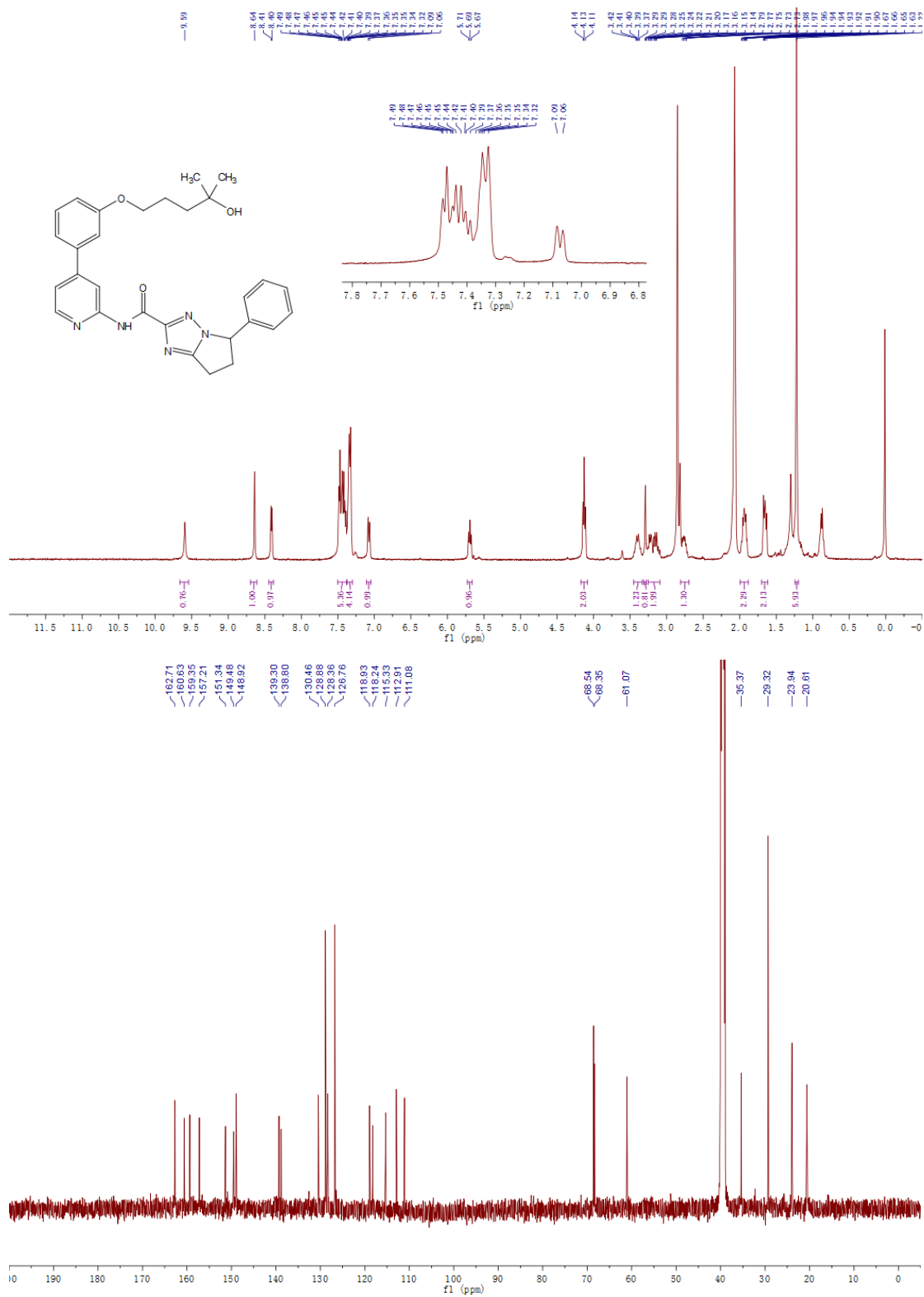
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 17



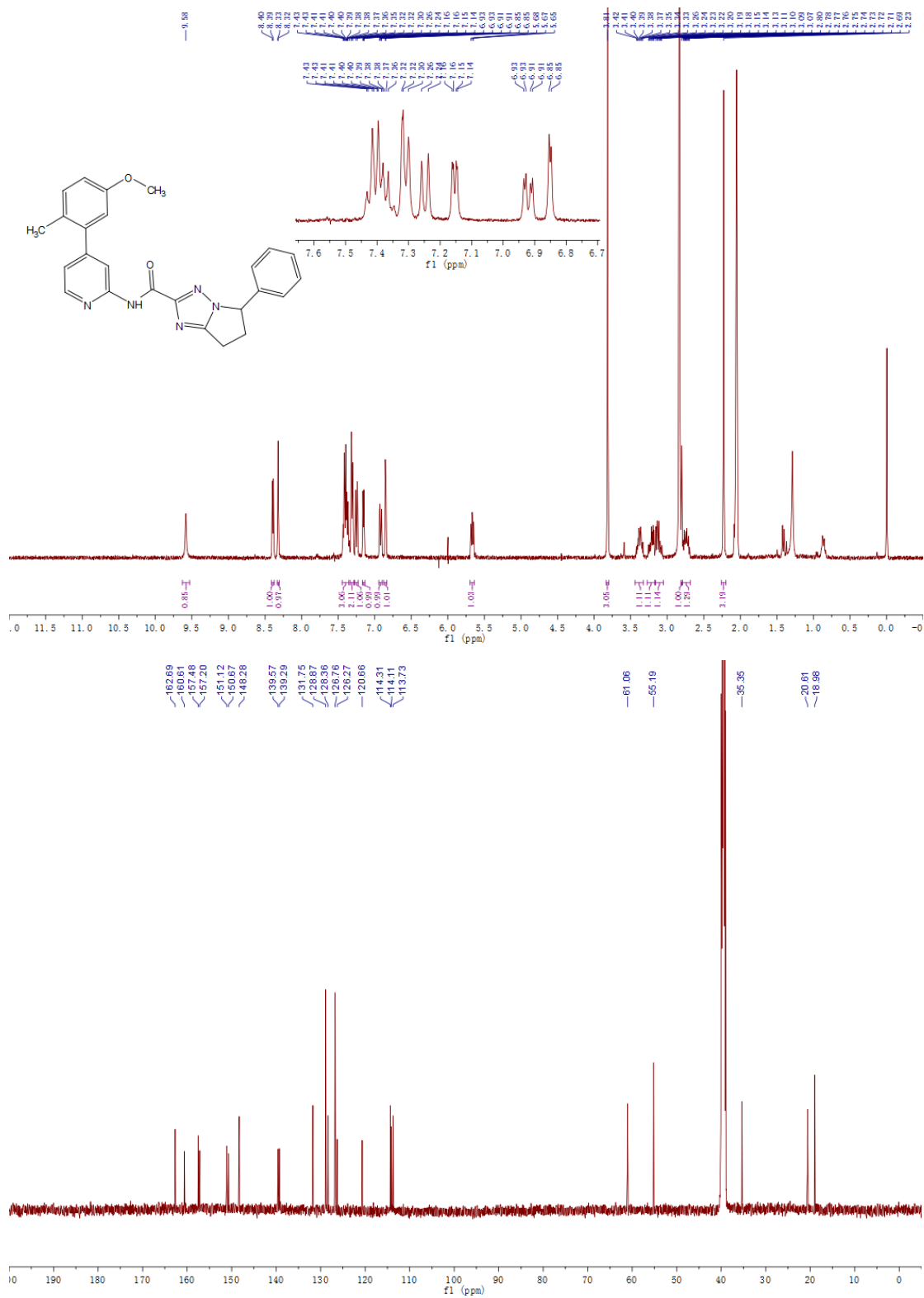


$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound 18

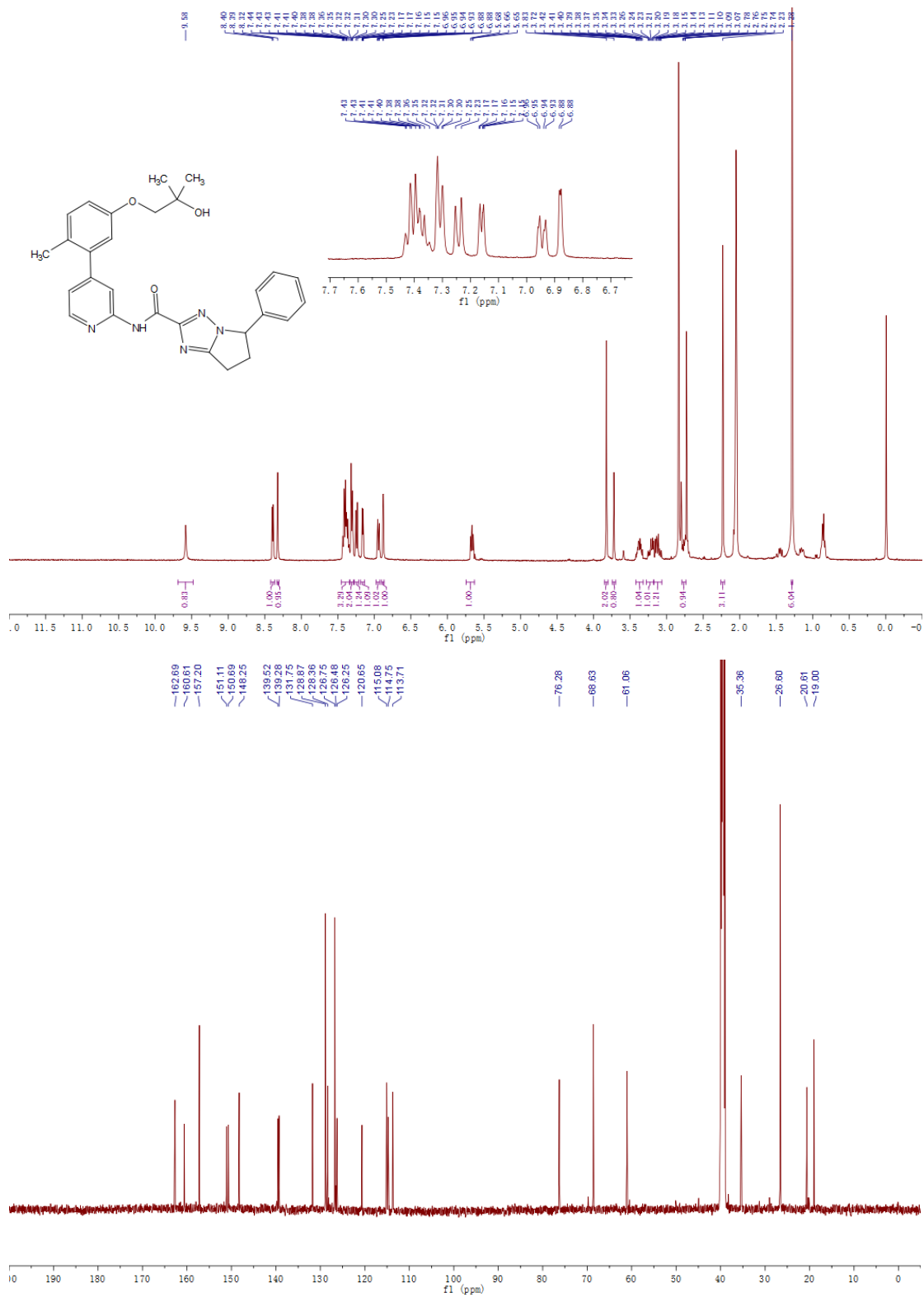




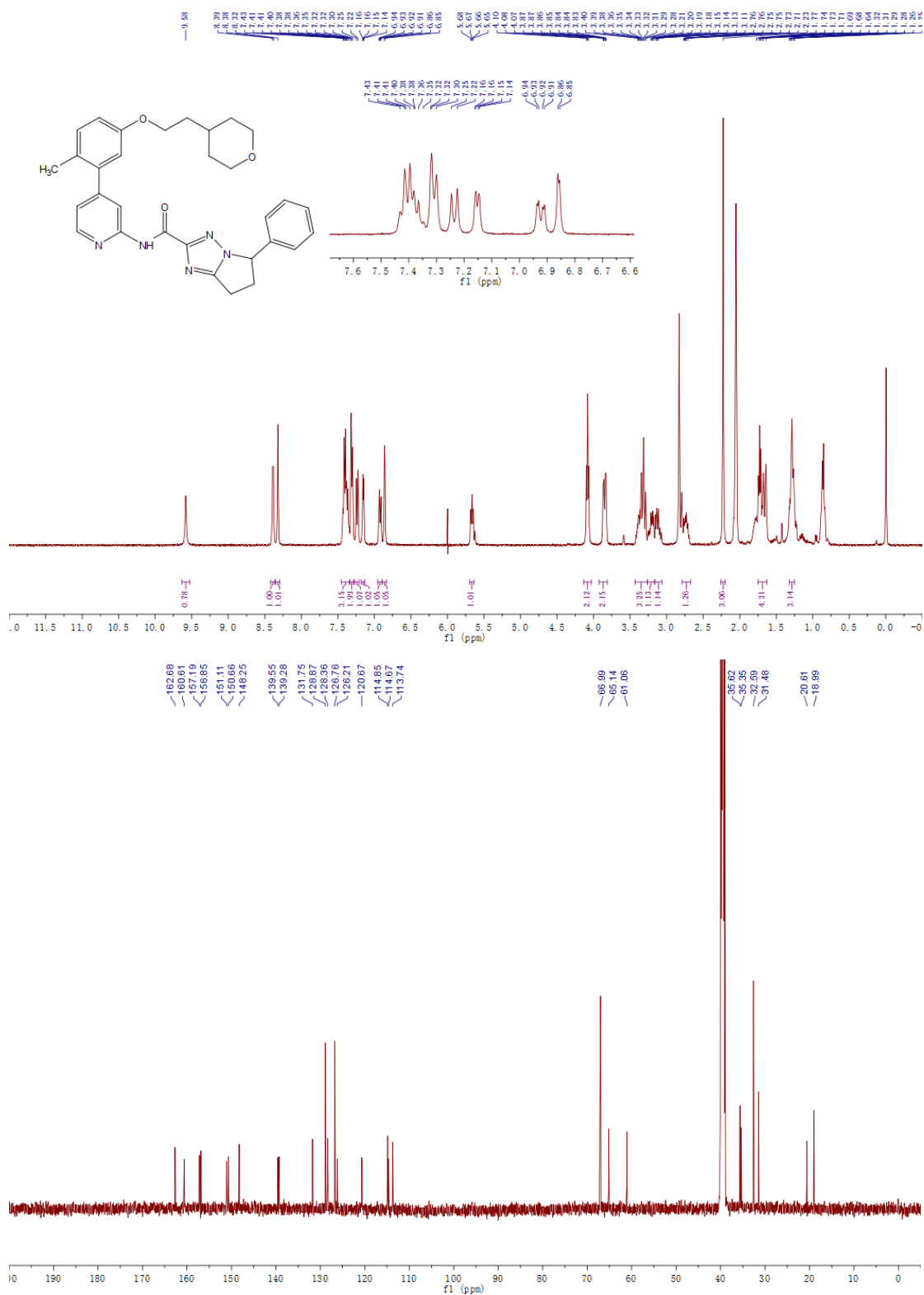
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 20



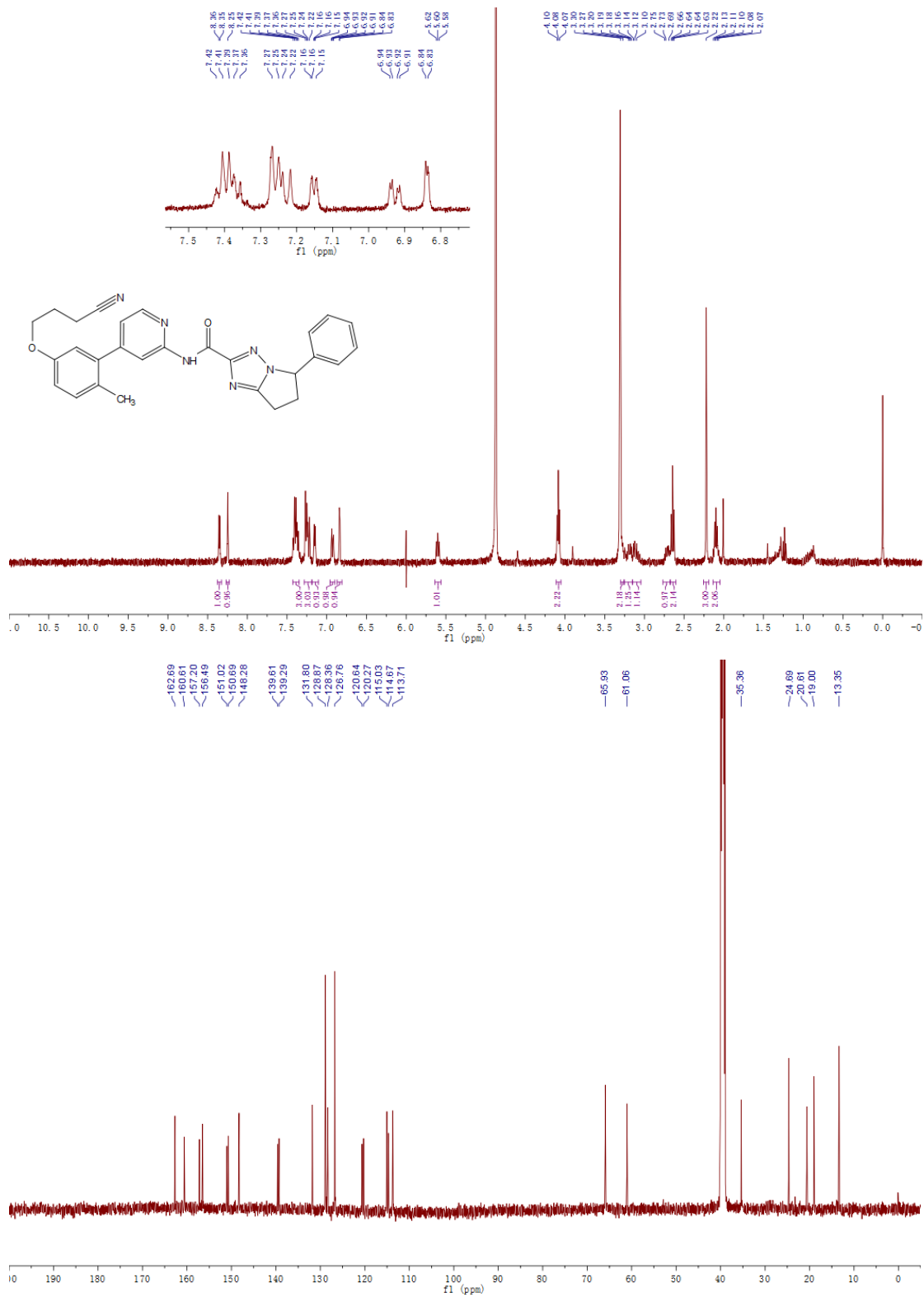
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 21



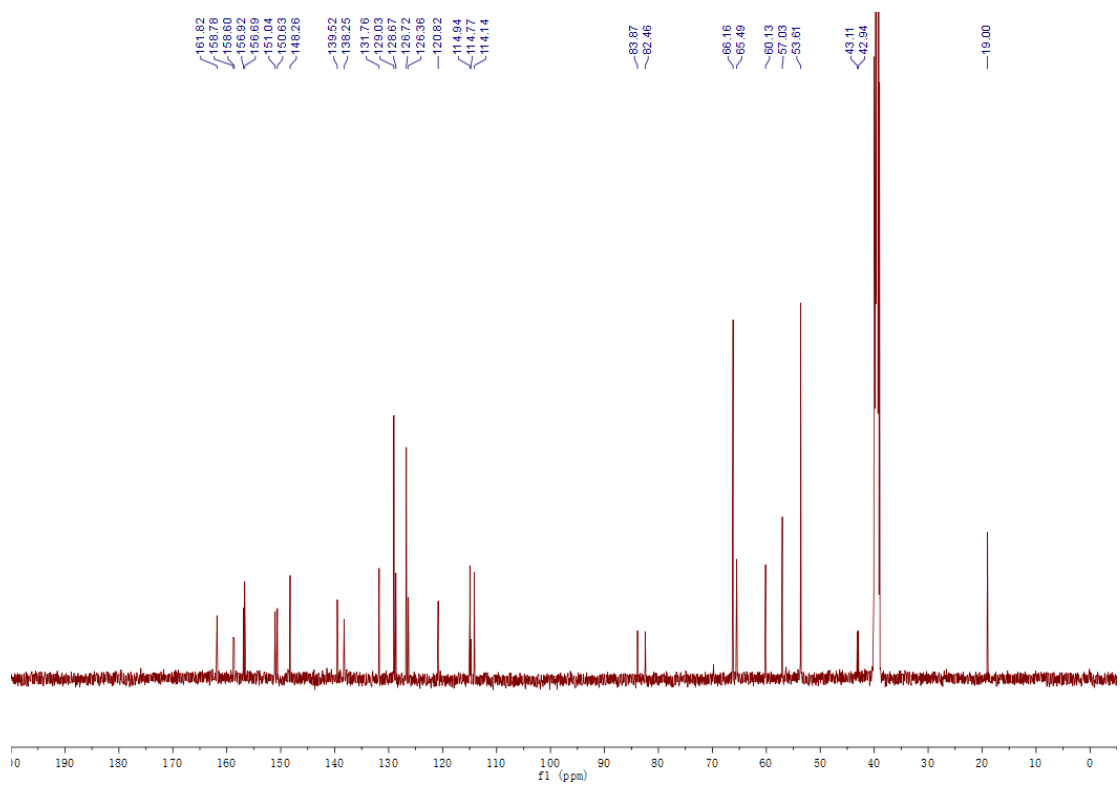
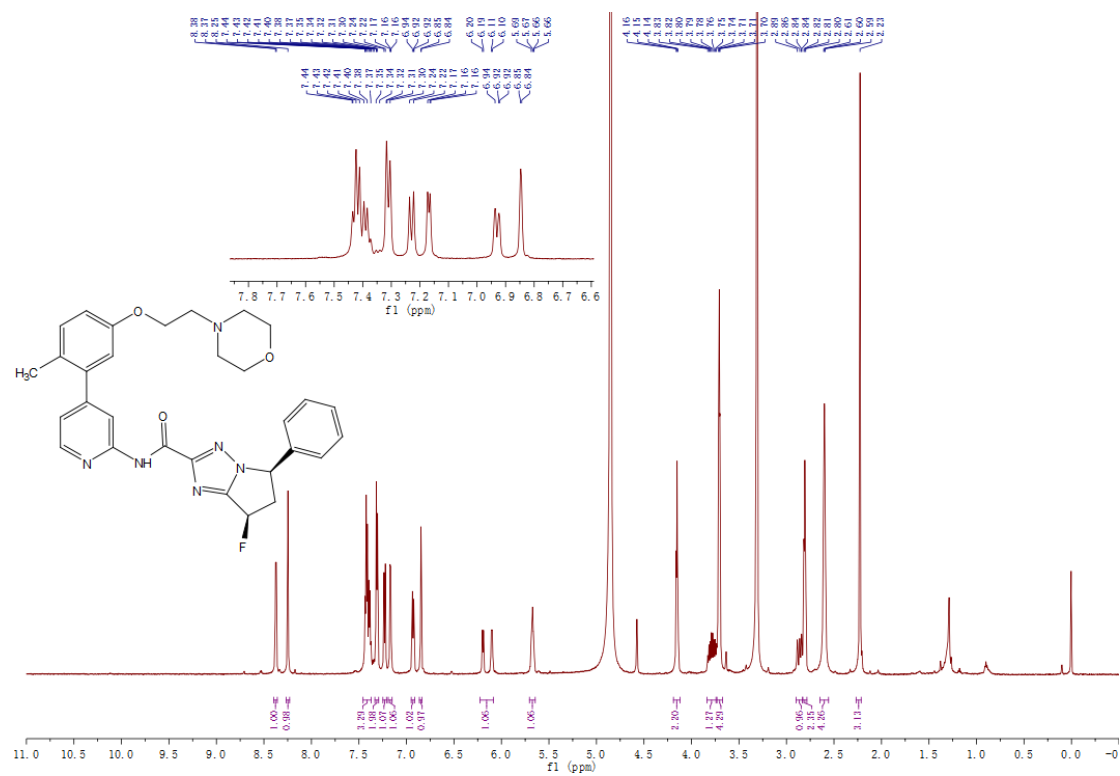
<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 22



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 23

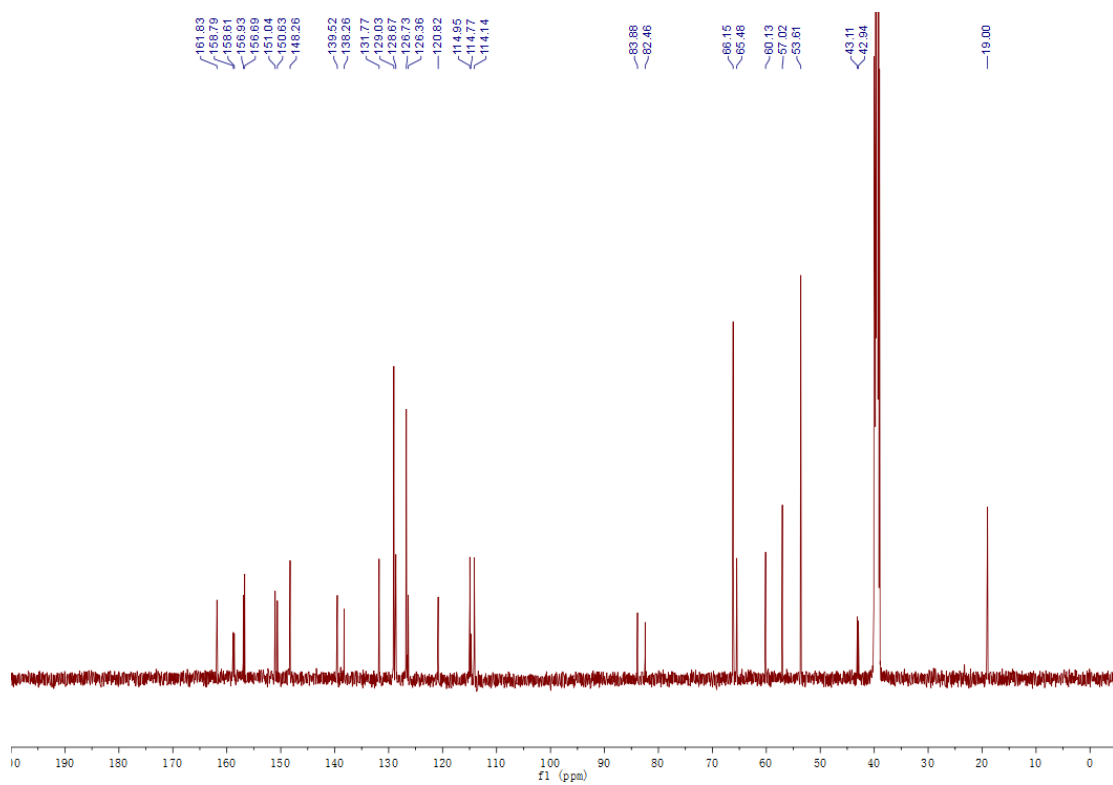
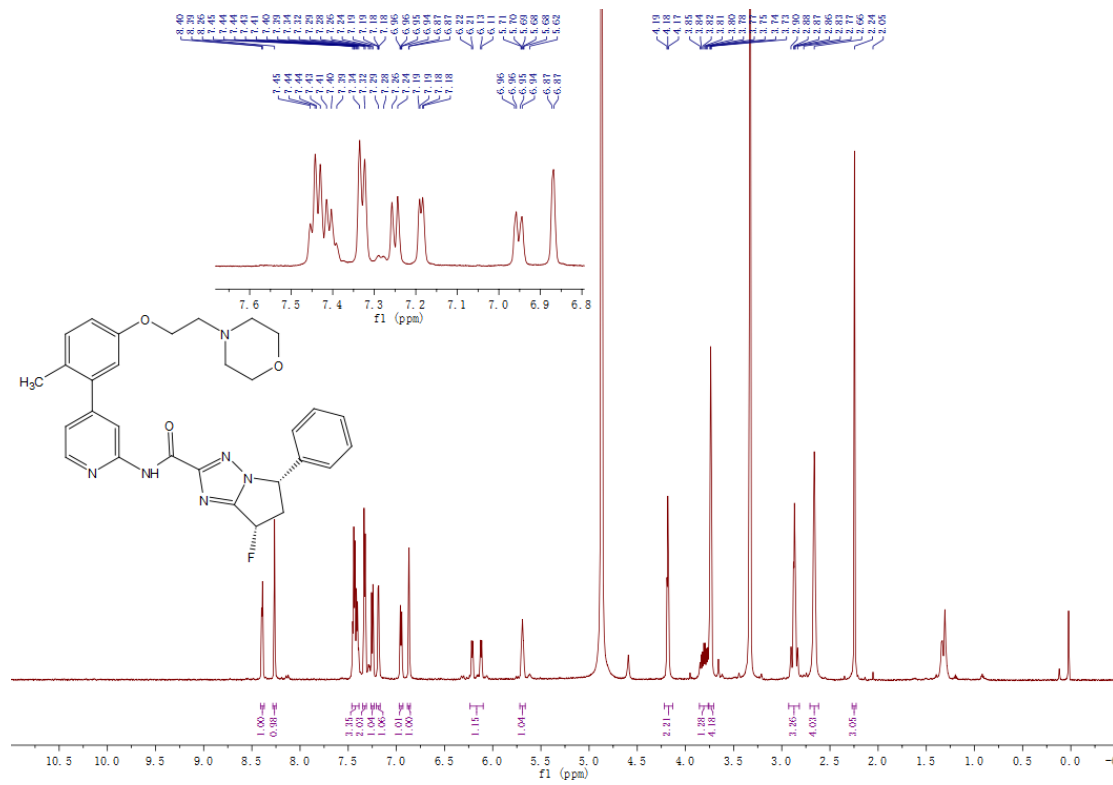


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 24

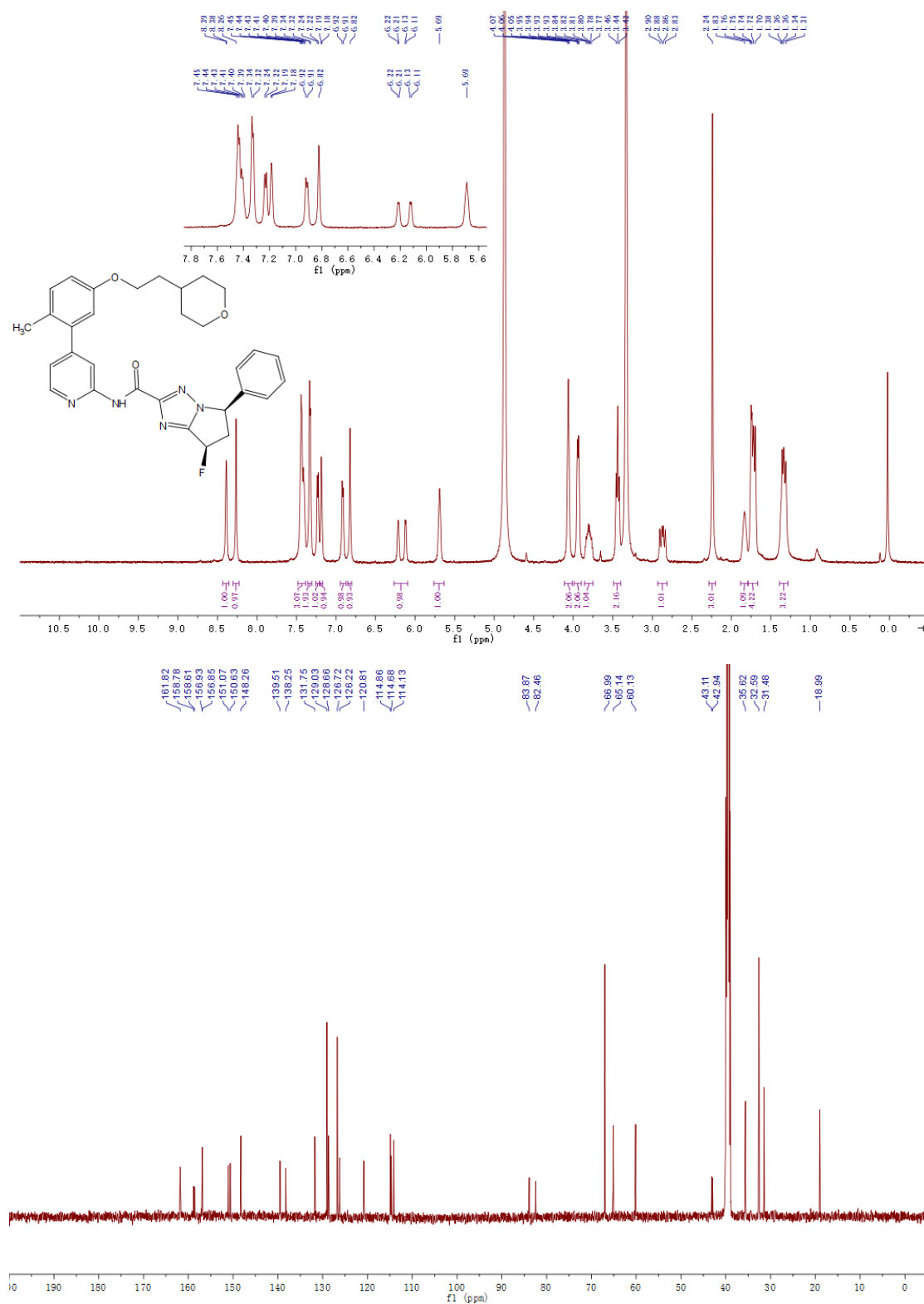


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **25**

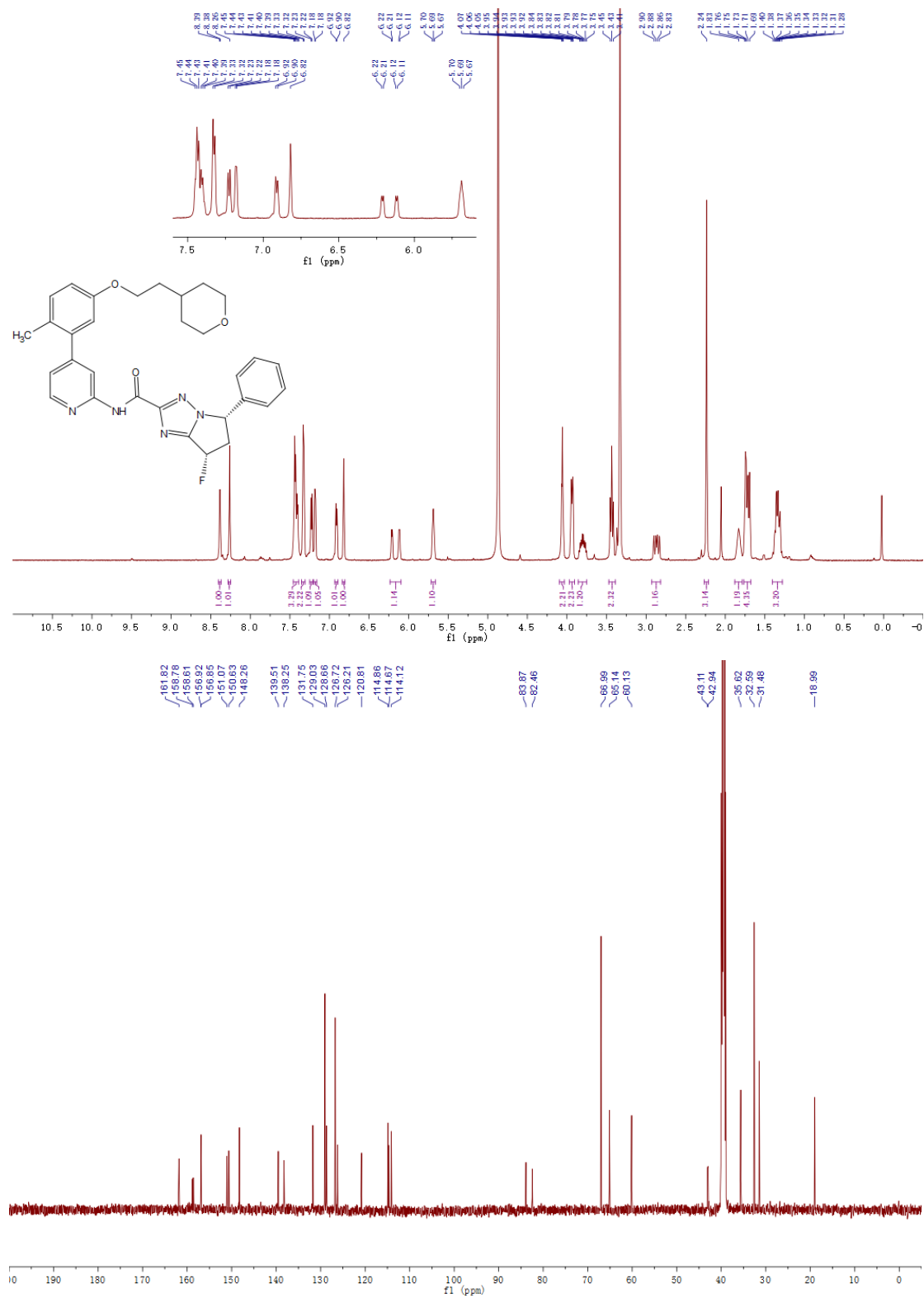




<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **26**

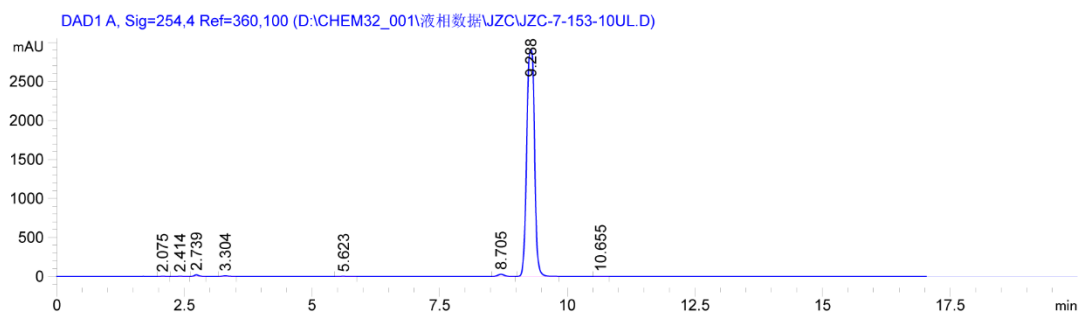


<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 27



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 28

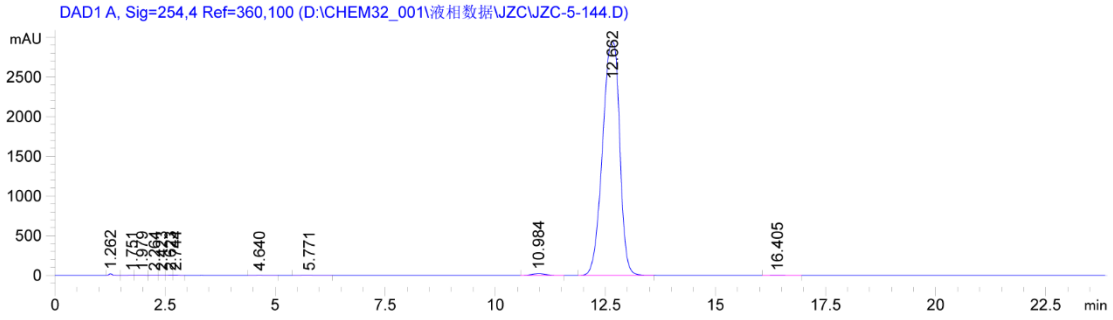
### 3. HPLC traces of target compounds



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 Area Percent Report  
 =====

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.075	BB	0.0971	11.93954	1.80738	0.0381
2	2.414	BB	0.1286	16.61146	1.85195	0.0530
3	2.739	BB	0.0969	121.85189	19.49831	0.3890
4	3.304	BB	0.1098	57.02700	8.13296	0.1821
5	5.623	BB	0.1361	9.47715	1.08323	0.0303
6	8.705	BB	0.1360	244.83781	28.00639	0.7817
7	9.288	BB	0.1677	3.08352e4	2908.52441	98.4470
8	10.655	BV	0.1292	24.68201	2.96116	0.0788
Totals :				3.13216e4	2971.86579	

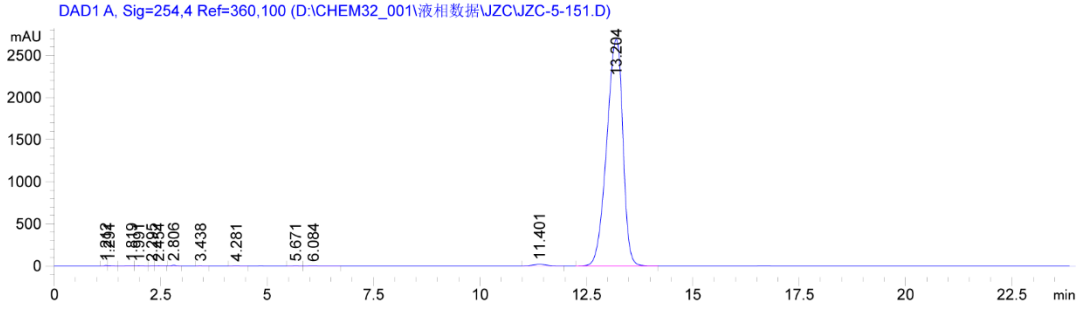
### HPLC traces of compound 7



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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.262	BB	0.0821	103.06296	18.74362	0.1284
2	1.751	BV	0.1492	18.20156	1.54720	0.0227
3	1.979	VV	0.1537	33.94067	3.10127	0.0423
4	2.264	VV	0.1661	21.55850	1.99378	0.0269
5	2.423	VV	0.1110	19.84119	2.60167	0.0247
6	2.623	VV	0.1061	33.90987	4.70468	0.0423
7	2.744	VB	0.1064	36.30606	5.01591	0.0452
8	4.640	VB	0.1389	12.10910	1.45797	0.0151
9	5.771	BB	0.2877	37.17867	1.73694	0.0463
10	10.984	BB	0.3361	442.76932	20.65068	0.5518
11	12.662	BB	0.4231	7.94419e4	2941.80298	99.0105
12	16.405	BB	0.3601	35.09076	1.47201	0.0437
Totals :				8.02359e4	3004.82872	

HPLC traces of compound 8

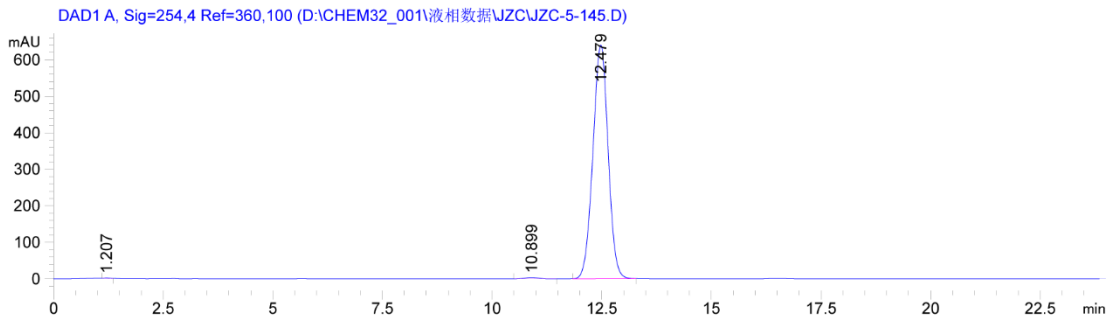


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.212	BV	0.0638	27.69750	6.49320	0.0386
2	1.291	VB	0.0870	32.14153	5.13785	0.0448
3	1.819	BV	0.1607	35.00338	2.82236	0.0488
4	1.991	VV	0.1685	36.06695	3.08347	0.0503
5	2.295	VV	0.1083	11.11665	1.50288	0.0155
6	2.454	VB	0.1330	30.50799	3.20639	0.0425
7	2.806	BB	0.1212	60.91443	7.46528	0.0850
8	3.438	VB	0.1244	10.98609	1.35799	0.0153
9	4.281	BB	0.1642	16.97644	1.59517	0.0237
10	5.671	BV	0.1927	14.08924	1.09062	0.0197
11	6.084	VB	0.2102	22.52876	1.68265	0.0314
12	11.401	BB	0.3374	409.20563	18.84329	0.5707
13	13.204	BB	0.4100	7.09931e4	2689.14307	99.0136

Totals : 7.17004e4 2743.42423

**HPLC traces of compound 9**

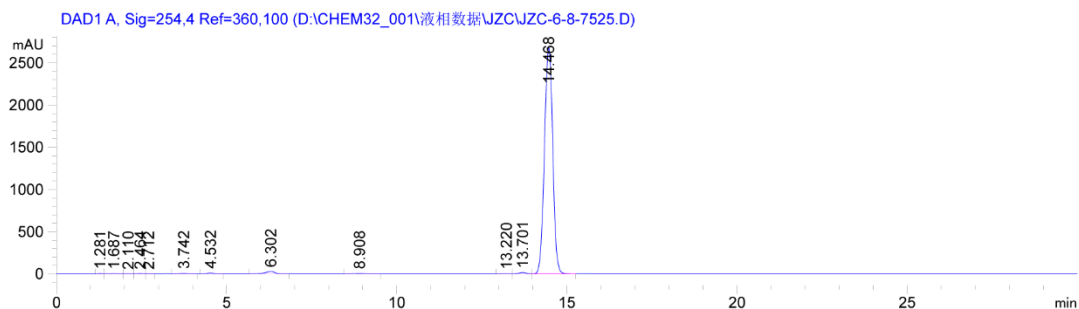


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.207	BB	0.1144	11.22627	1.41681	0.0723
2	10.899	BB	0.3331	77.26126	3.64721	0.4973
3	12.479	BB	0.3756	1.54484e4	640.09253	99.4305

Totals : 1.55369e4 645.15655

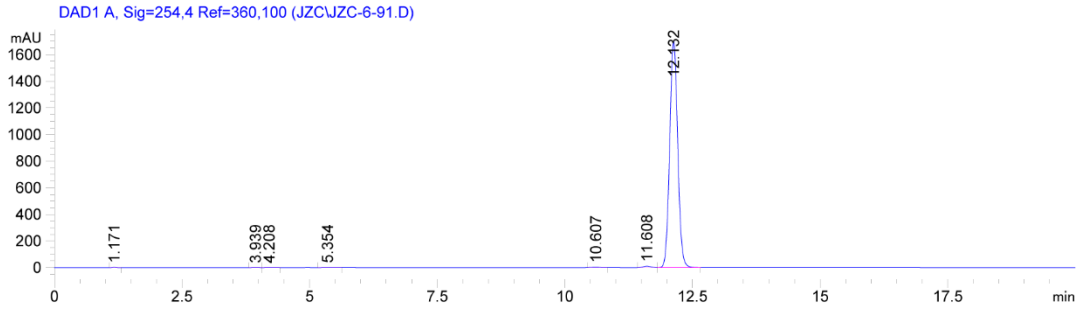
**HPLC traces of compound 10**



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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.281	BV	0.1027	40.22535	5.96332	0.0859
2	1.687	VV	0.2481	60.45518	3.14783	0.1291
3	2.110	VV	0.1676	23.74777	1.90264	0.0507
4	2.464	VV	0.1450	43.38755	4.25412	0.0926
5	2.712	VB	0.1230	8.51706	1.02467	0.0182
6	3.742	VB	0.1889	98.93079	7.54765	0.2113
7	4.532	BB	0.1884	147.13420	11.72375	0.3142
8	6.302	BB	0.2970	586.78662	28.88973	1.2530
9	8.908	BB	0.3535	118.41454	5.24384	0.2529
10	13.220	BV	0.2272	28.65466	1.90778	0.0612
11	13.701	VV	0.2358	249.15660	16.34879	0.5320
12	14.468	VB	0.2658	4.54245e4	2678.79199	96.9989
Totals :				4.68299e4	2766.74611	

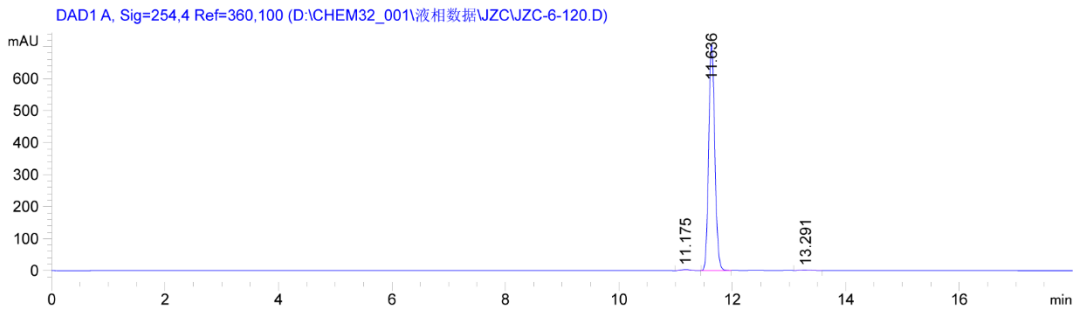
HPLC traces of compound 11



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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.171	BB	0.0725	8.35310	1.72393	0.0446
2	3.939	BV	0.1172	7.64907	1.02310	0.0408
3	4.208	VB	0.1377	10.98770	1.21263	0.0587
4	5.354	BB	0.1571	14.71715	1.44223	0.0786
5	10.607	BB	0.1394	33.54911	3.71434	0.1792
6	11.608	BV	0.1490	106.92207	11.24146	0.5710
7	12.132	VB	0.1711	1.85441e4	1702.25195	99.0272
Totals :				1.87263e4	1722.60965	

**HPLC traces of compound 12**

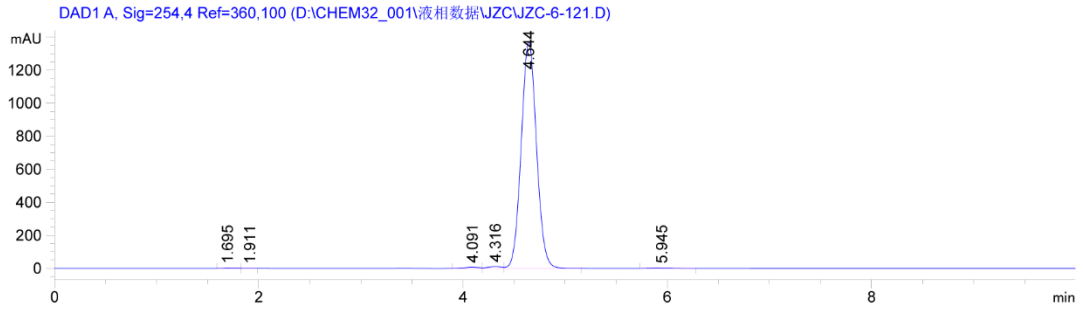


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.175	BB	0.1481	40.07123	4.09747	0.7488
2	11.636	BB	0.1152	5296.68311	708.83722	98.9803
3	13.291	BB	0.1683	14.49667	1.36020	0.2709
Totals :				5351.25101	714.29490	

**HPLC traces of compound 13**

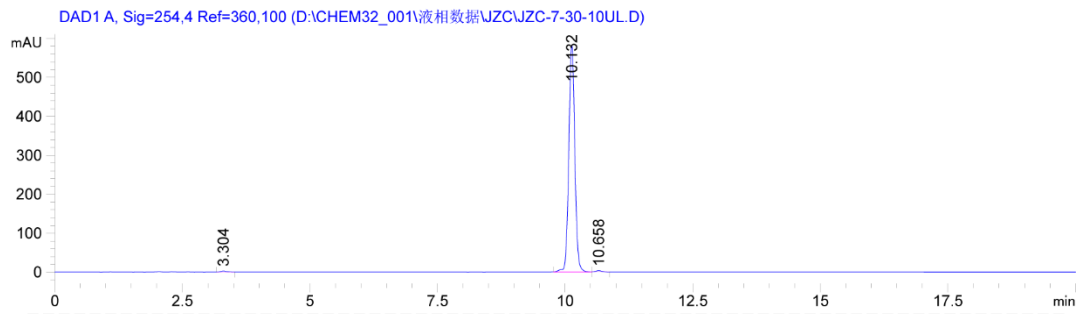




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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.695	VV	0.0933	15.18601	2.35252	0.1050
2	1.911	VV	0.0835	7.58259	1.35032	0.0524
3	4.091	BV	0.1425	62.90701	6.76158	0.4351
4	4.316	VV	0.1355	95.64220	10.78057	0.6615
5	4.644	VB	0.1610	1.42402e4	1373.31177	98.4878
6	5.945	BB	0.1864	37.32717	3.19154	0.2582
Totals :				1.44588e4	1397.74831	

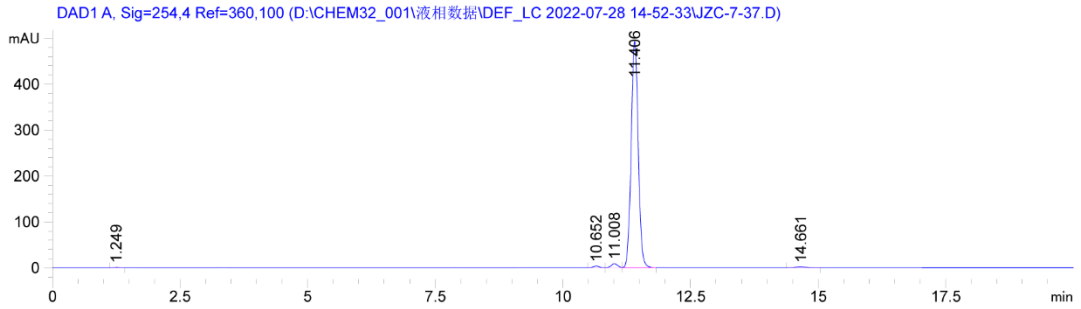
**HPLC traces of compound 14**



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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.304	BB	0.1260	25.30908	3.01205	0.5236
2	10.132	BB	0.1278	4777.45605	581.68475	98.8334
3	10.658	BB	0.1329	31.08210	3.59391	0.6430
Totals :				4833.84724	588.29071	

**HPLC traces of compound 15**

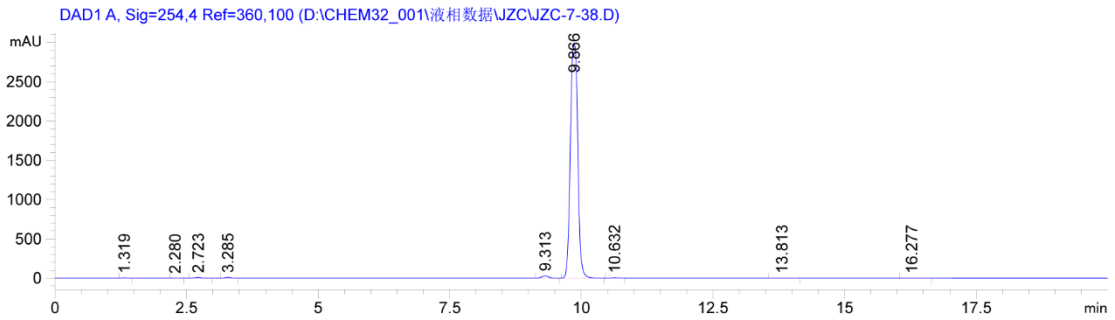


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.249	BB	0.0983	8.02234	1.22601	0.1648
2	10.652	BV	0.1287	27.89470	3.36592	0.5729
3	11.008	VV	0.1349	74.48811	8.60997	1.5297
4	11.406	VB	0.1501	4733.05420	492.53671	97.2014
5	14.661	BB	0.2275	25.86997	1.76008	0.5313

Totals : 4869.32932 507.49870

### HPLC traces of compound 16

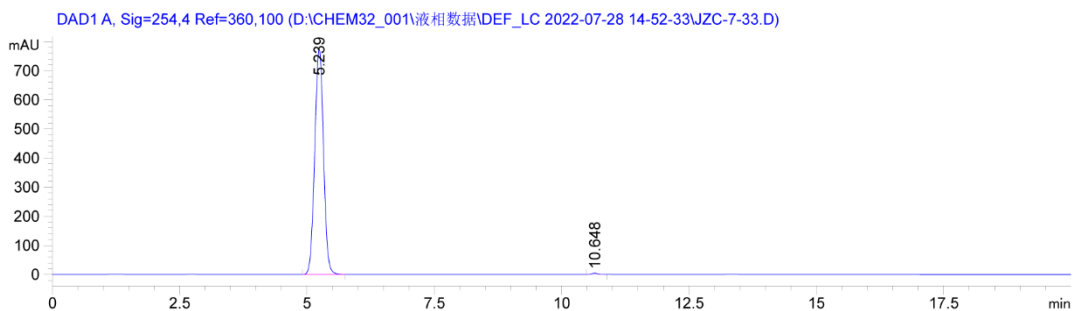


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.319	BB	0.0819	22.57444	4.11992	0.0763
2	2.280	BB	0.0984	7.71739	1.11922	0.0261
3	2.723	BB	0.1109	70.70839	9.28334	0.2390
4	3.285	BB	0.1143	71.52702	9.67087	0.2418
5	9.313	BB	0.1353	263.76694	30.38116	0.8915
6	9.866	BB	0.1540	2.90677e4	2974.27246	98.2505
7	10.632	BV	0.1468	43.22113	4.39314	0.1461
8	13.813	BB	0.2060	20.71740	1.56978	0.0700
9	16.277	BB	0.2256	17.36917	1.19503	0.0587

Totals : 2.95853e4 3036.00492

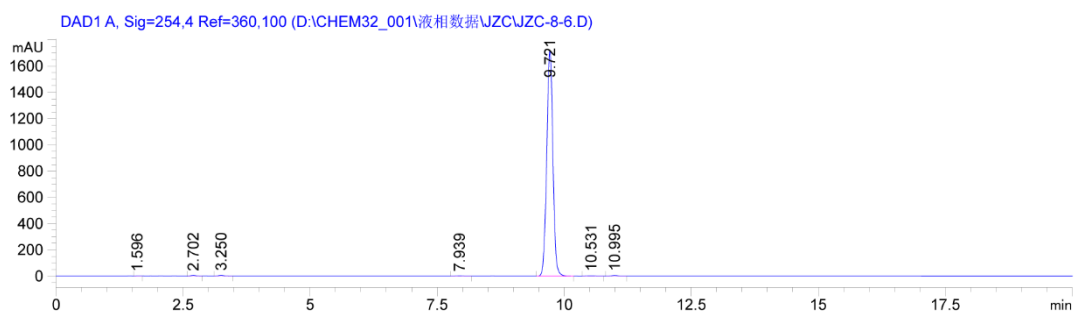
### HPLC traces of compound 17



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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.239	BB	0.1874	9297.32227	777.84552	99.6135
2	10.648	BB	0.1320	36.07273	4.29551	0.3865
Totals :				9333.39499	782.14103	

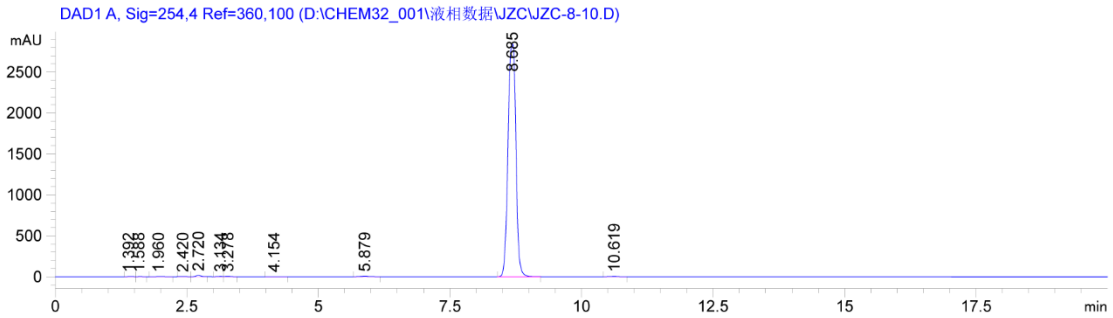
**HPLC traces of compound 18**



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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.596	VB	0.0740	6.96384	1.35303	0.0472
2	2.702	BB	0.0967	42.46932	6.81788	0.2880
3	3.250	BB	0.1102	50.10210	7.10818	0.3398
4	7.939	BB	0.1442	23.80734	2.56635	0.1614
5	9.721	BB	0.1326	1.45377e4	1720.73999	98.5871
6	10.531	BB	0.1354	34.40367	3.87996	0.2333
7	10.995	BB	0.1239	50.59940	6.28404	0.3431
Totals :				1.47461e4	1748.74945	

**HPLC traces of compound 19**

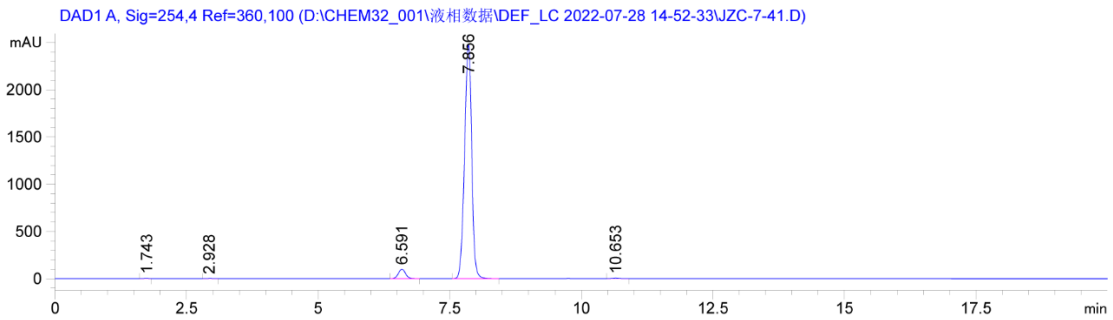


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.392	BV	0.1006	13.15375	1.81341	0.0439
2	1.588	VB	0.0943	12.13883	1.85597	0.0405
3	1.960	BB	0.1749	22.27843	1.65691	0.0744
4	2.420	BV	0.1076	25.46692	3.46900	0.0850
5	2.720	VB	0.1005	104.29250	15.91348	0.3481
6	3.134	BV	0.1098	23.05971	3.13466	0.0770
7	3.278	VB	0.1129	32.49250	4.36212	0.1085
8	4.154	BB	0.1292	22.32992	2.73732	0.0745
9	5.879	BB	0.1746	57.98090	5.17912	0.1935
10	8.685	BB	0.1631	2.96030e4	2851.52466	98.8147
11	10.619	BB	0.1396	41.91390	4.63093	0.1399

Totals : 2.99581e4 2896.27758

HPLC traces of compound 20

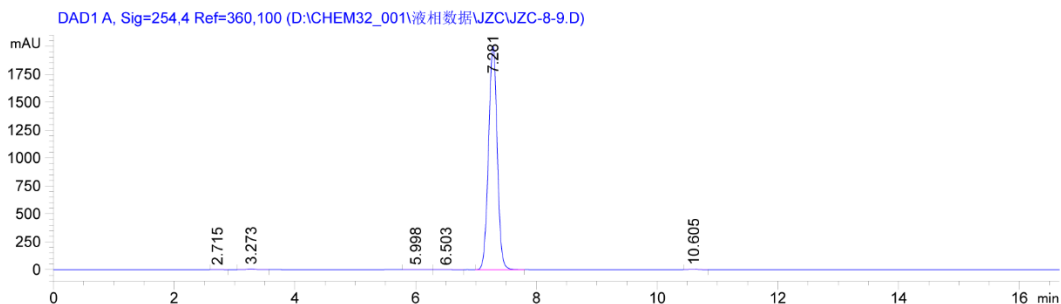


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.743	BV	0.0754	17.39198	3.41546	0.0711
2	2.928	BB	0.1014	11.87218	1.83804	0.0485
3	6.591	BB	0.1470	956.09943	100.50344	3.9088
4	7.856	BB	0.1485	2.34343e4	2473.18701	95.8047
5	10.653	BB	0.1342	40.81966	4.75493	0.1669

Totals : 2.44604e4 2583.69889

HPLC traces of compound 21

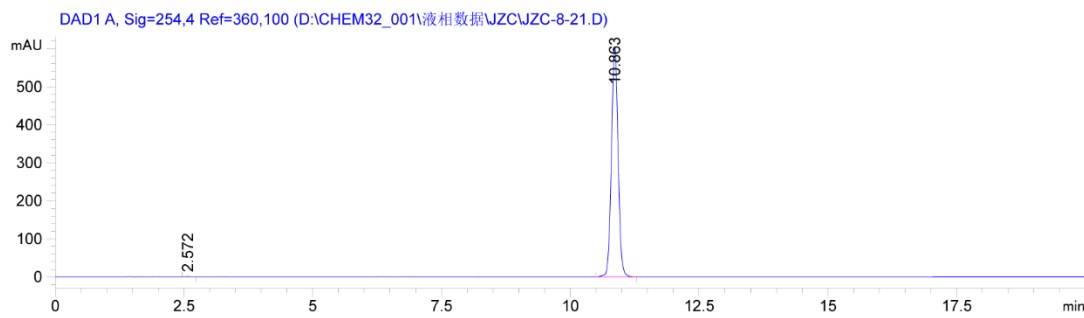


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.715	BB	0.1030	9.60400	1.41908	0.0474
2	3.273	BB	0.1336	64.47256	6.98773	0.3181
3	5.998	BB	0.1664	16.83026	1.57799	0.0830
4	6.503	BB	0.1615	13.98218	1.38864	0.0690
5	7.281	BB	0.1574	2.01275e4	1999.96863	99.2978
6	10.605	BB	0.1338	37.44089	4.37849	0.1847

Totals : 2.02699e4 2015.72056

**HPLC traces of compound 22**

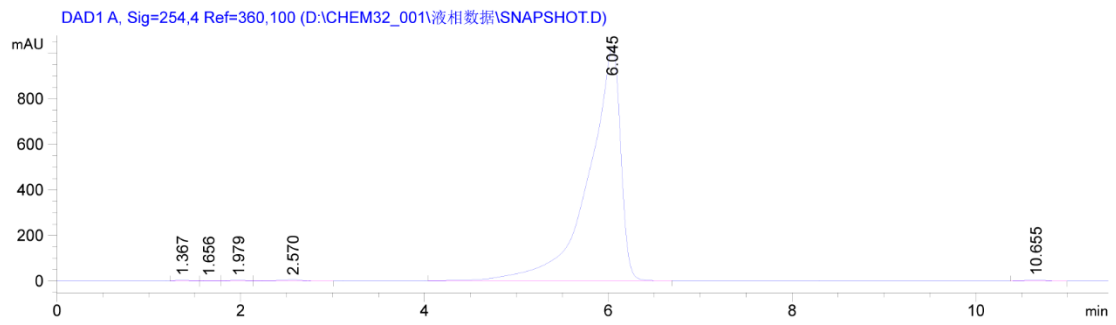


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.572	BB	0.0855	5.75117	1.05718	0.1054
2	10.863	BB	0.1396	5448.19678	602.09296	99.8946

Totals : 5453.94794 603.15014

**HPLC traces of compound 23**

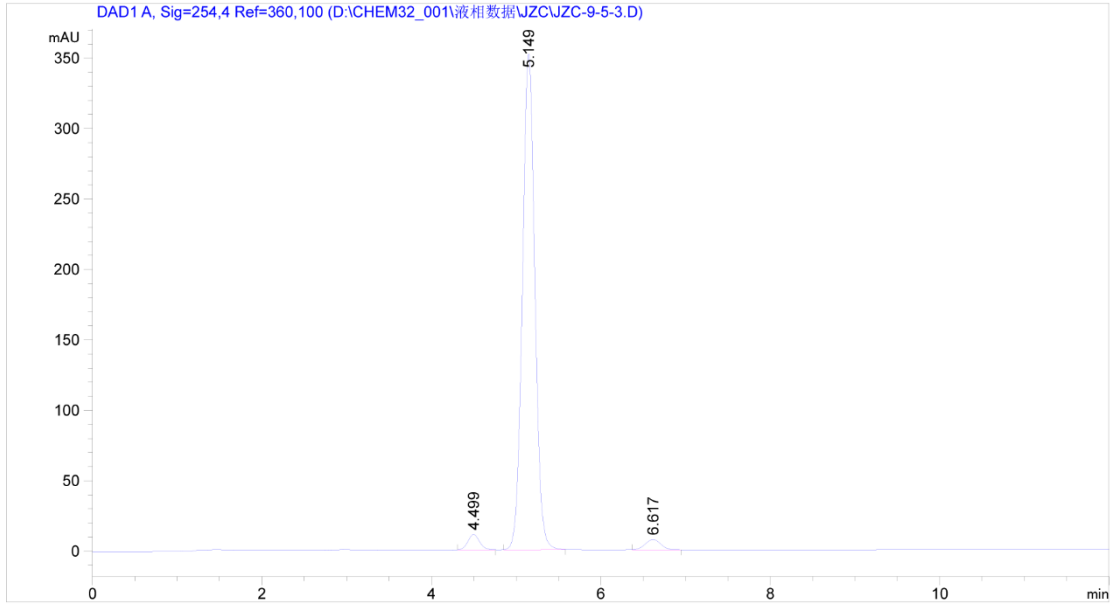


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.367	BV	0.1240	38.35120	4.14352	0.1528
2	1.656	VV	0.1103	15.57590	1.92658	0.0620
3	1.979	VV	0.1600	41.29227	3.64921	0.1645
4	2.570	VB	0.2221	86.95460	5.69633	0.3464
5	6.045	BB	0.3288	2.48560e4	1025.34070	99.0051
6	10.655	BB	0.1982	67.59714	5.25073	0.2692

Totals :                                2.51058e4    1046.00708

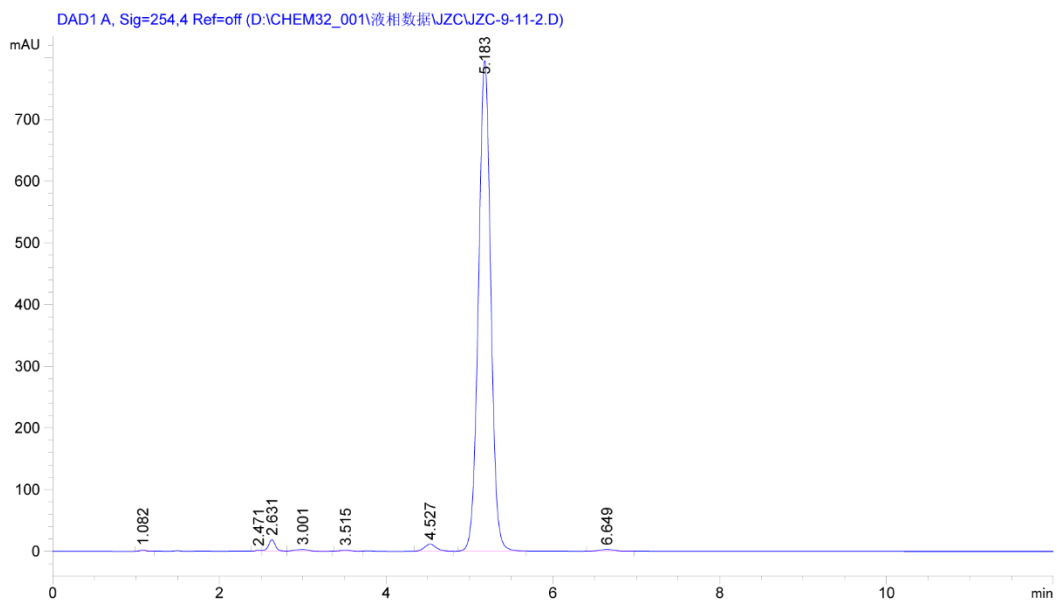
**HPLC traces of compound 24**



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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.499	BB	0.1477	105.05843	10.97565	2.6329
2	5.149	BB	0.1590	3792.07349	352.27576	95.0334
3	6.617	BB	0.1946	93.12179	7.40838	2.3334
Totals :				3990.25371	370.65978	

HPLC traces of compound **25**

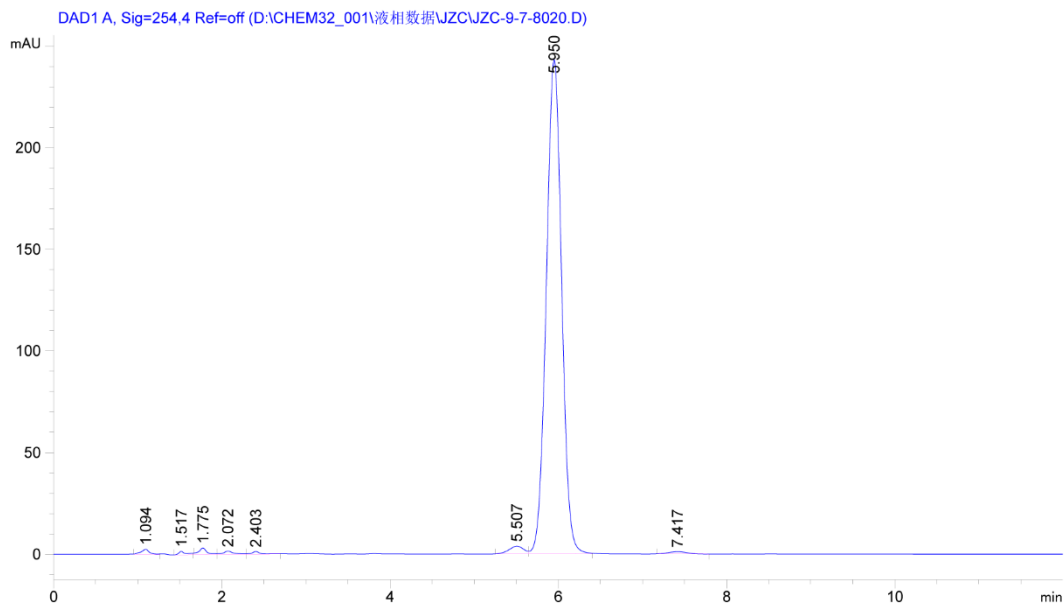


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.082	BB	0.0720	10.67585	2.22602	0.1263
2	2.471	BV	0.0687	6.45290	1.42771	0.0763
3	2.631	VV	0.0863	105.85324	18.62184	1.2521
4	3.001	VB	0.1744	29.05828	2.76954	0.3437
5	3.515	BB	0.1127	11.28000	1.59050	0.1334
6	4.527	BB	0.1522	114.91138	11.53612	1.3592
7	5.183	BB	0.1594	8140.64209	795.58441	96.2892
8	6.649	BB	0.1924	35.49388	2.86717	0.4198
Totals :				8454.36761	836.62331	

HPLC traces of compound 26



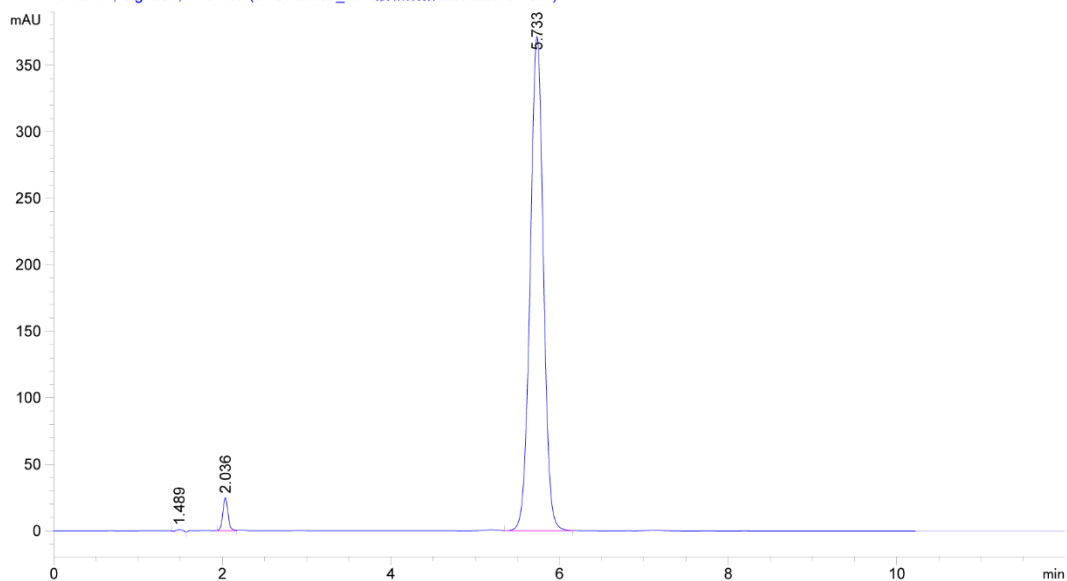


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 Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.094	BB	0.1025	17.32398	2.44844	0.5395
2	1.517	BB	0.0832	10.04524	1.64512	0.3129
3	1.775	BV	0.0948	21.87177	3.23830	0.6812
4	2.072	VV	0.1266	14.32246	1.59787	0.4461
5	2.403	VB	0.1043	9.45238	1.30819	0.2944
6	5.507	BV	0.1870	46.64705	3.80665	1.4528
7	5.950	VB	0.1975	3074.48218	243.20869	95.7524
8	7.417	BB	0.2356	16.72172	1.08649	0.5208
Totals :				3210.86678	258.33974	

HPLC traces of compound 27

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Area Percent Report  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.489	BV	0.0926	8.39113	1.51505	0.2023
2	2.036	BV	0.0660	106.39360	24.83202	2.5644
3	5.733	VB	0.1686	4034.02075	371.62286	97.2333
Totals :				4148.80549	397.96993	

HPLC traces of compound **28**

#### 4. HRMS of compound **26**

##### User Spectra

