

Design, Synthesis and Biological Evaluation of *N*-phenylindole Derivatives as Pks13 Inhibitors against *Mycobacterium tuberculosis*

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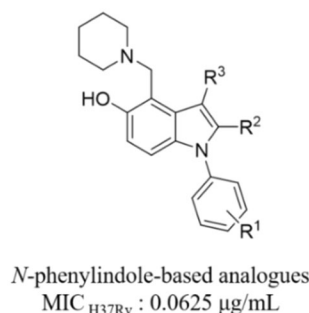
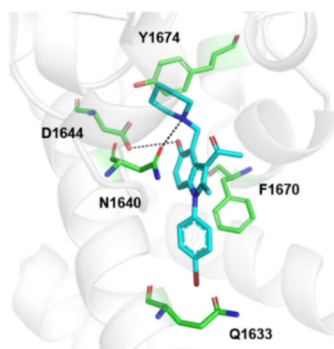
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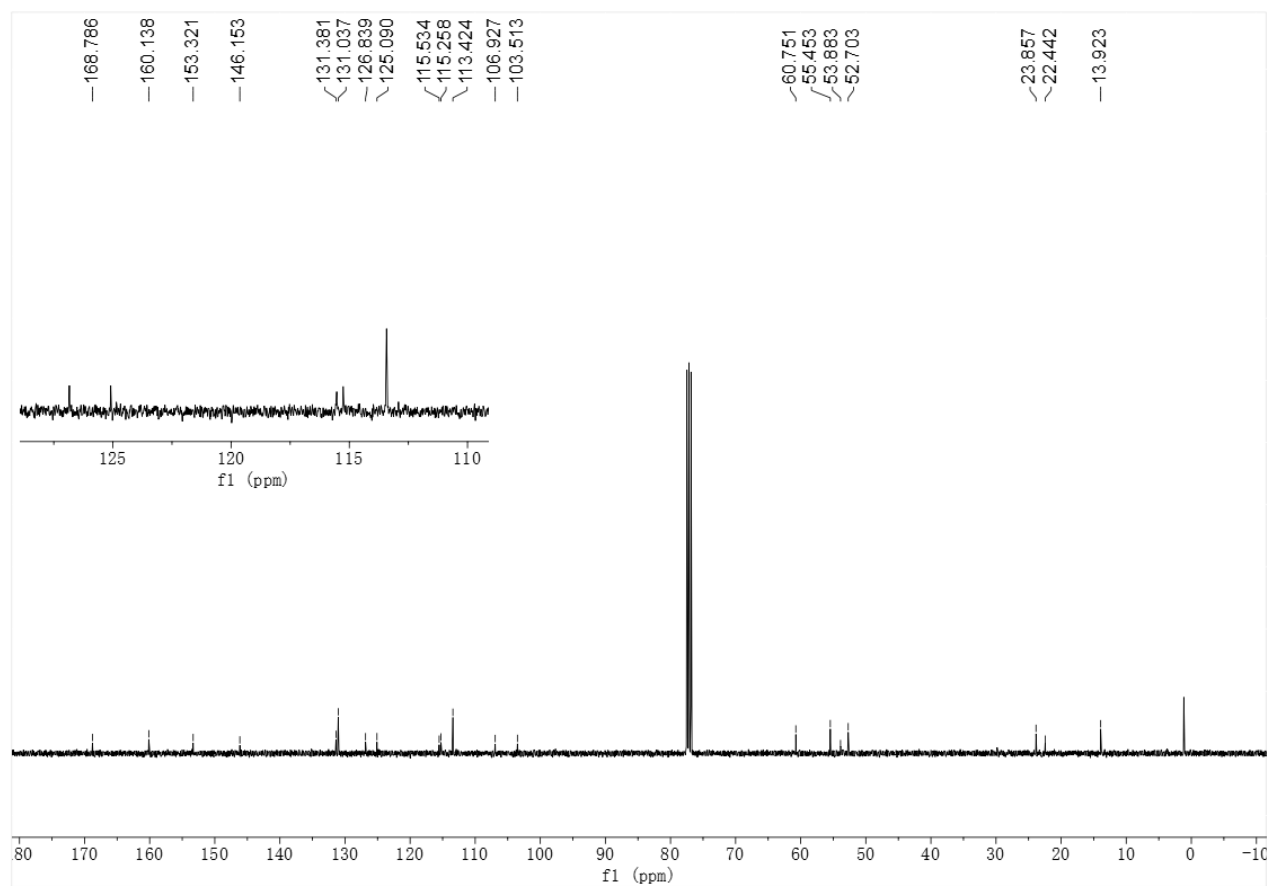
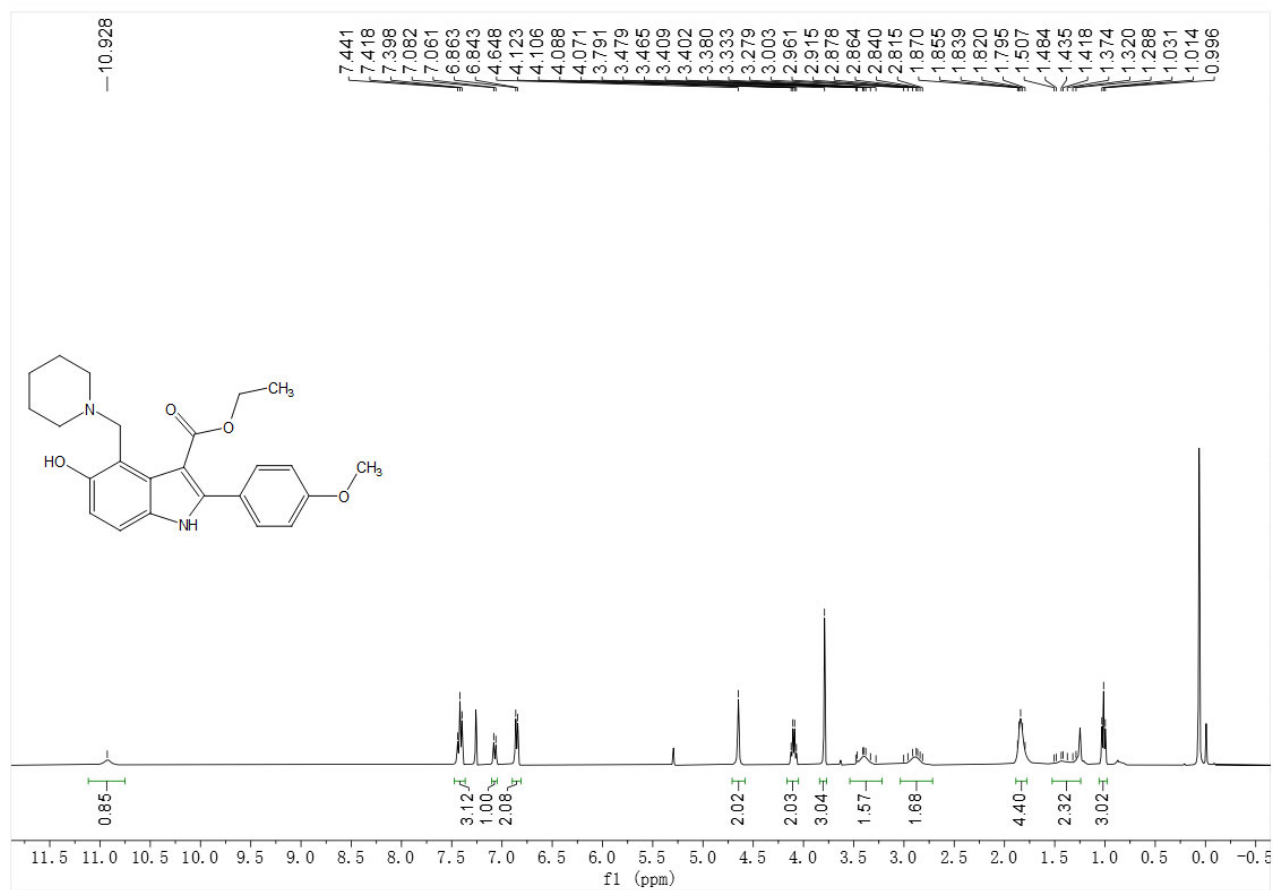
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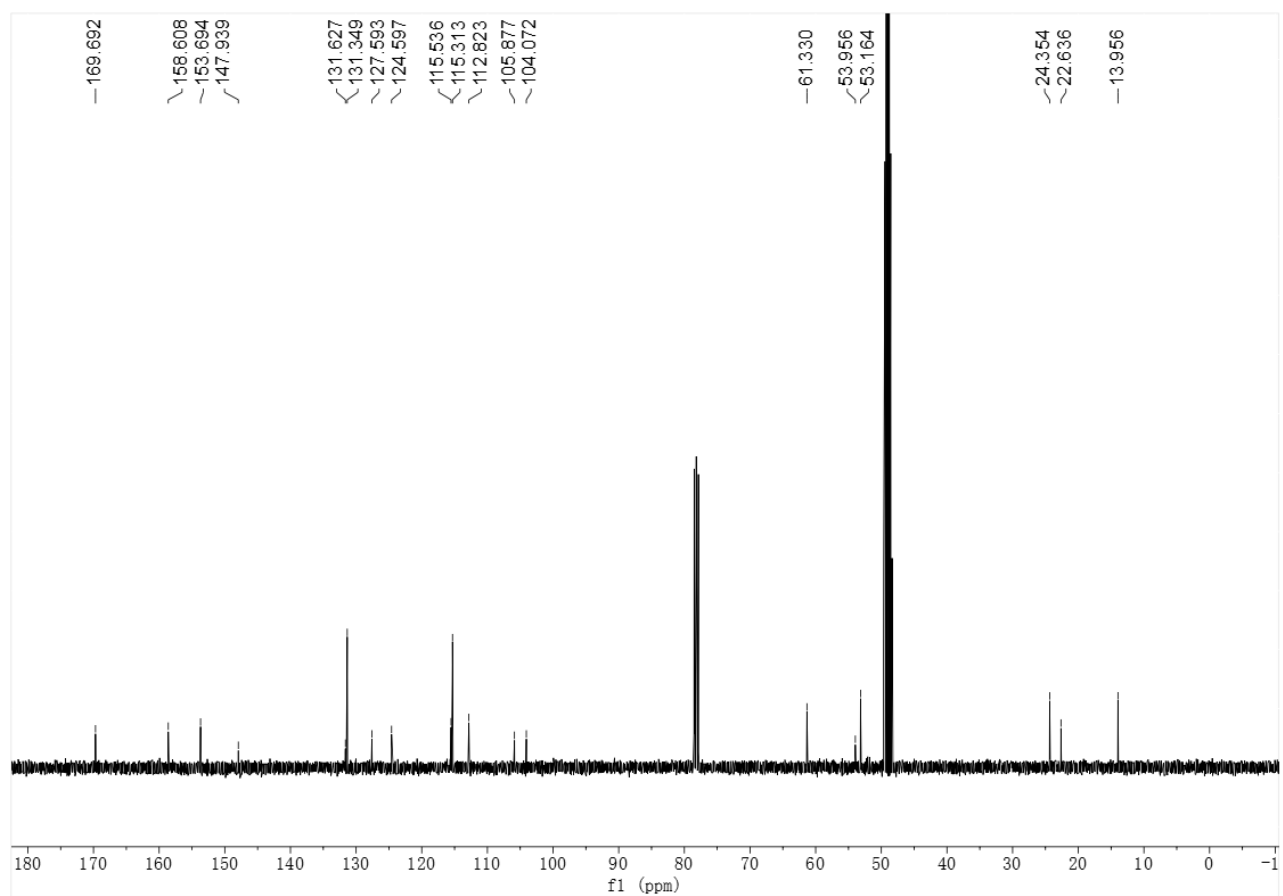
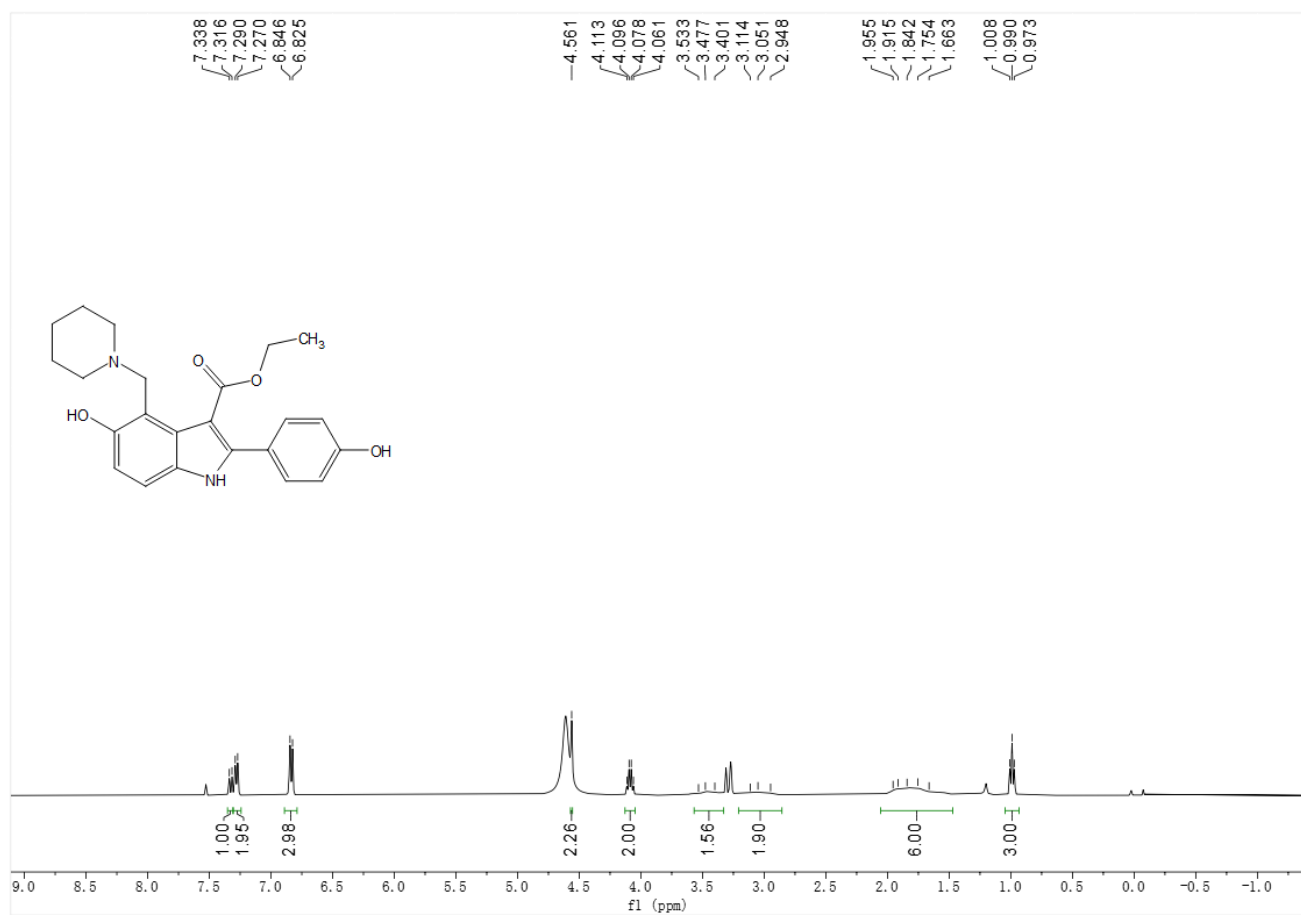
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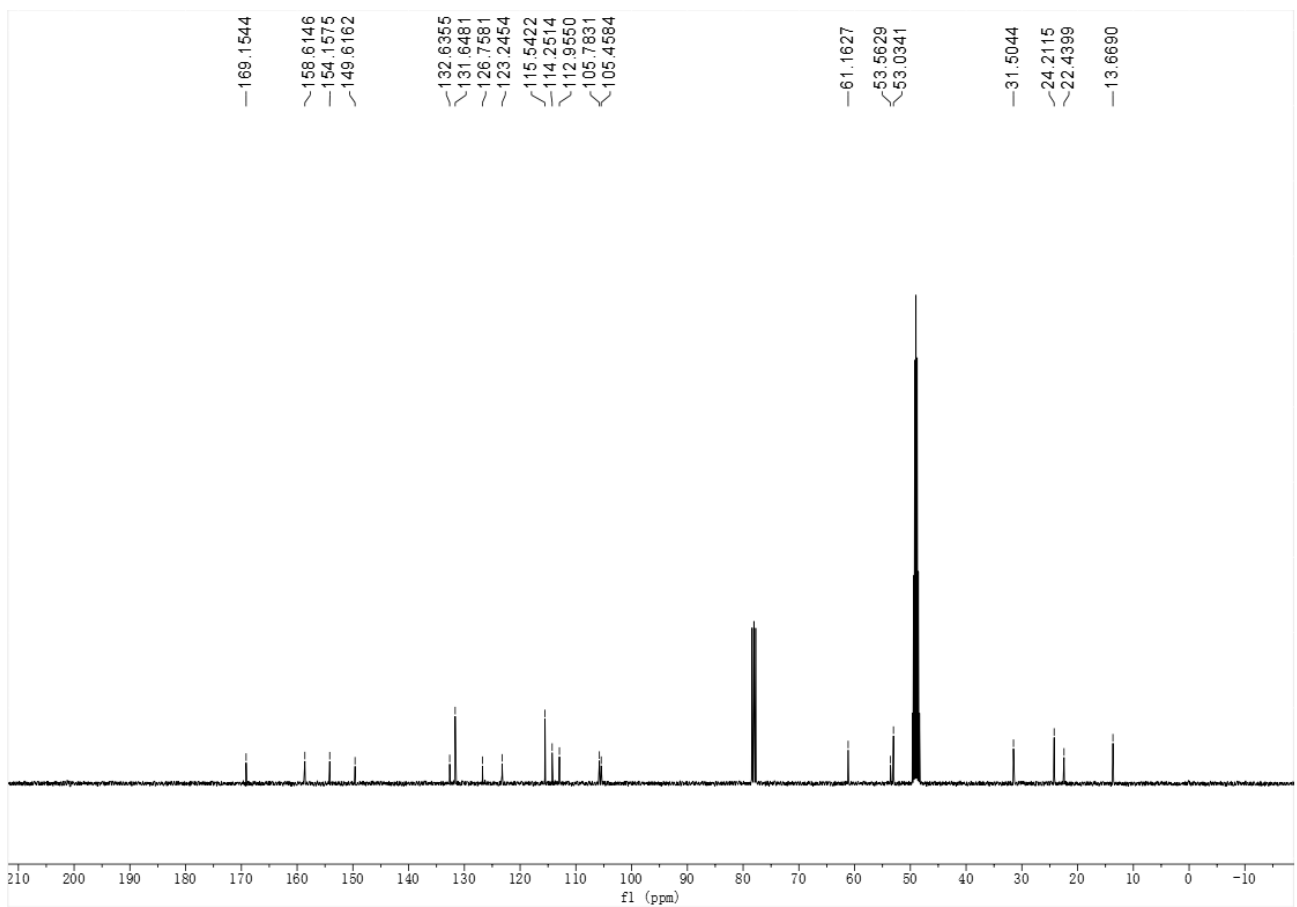
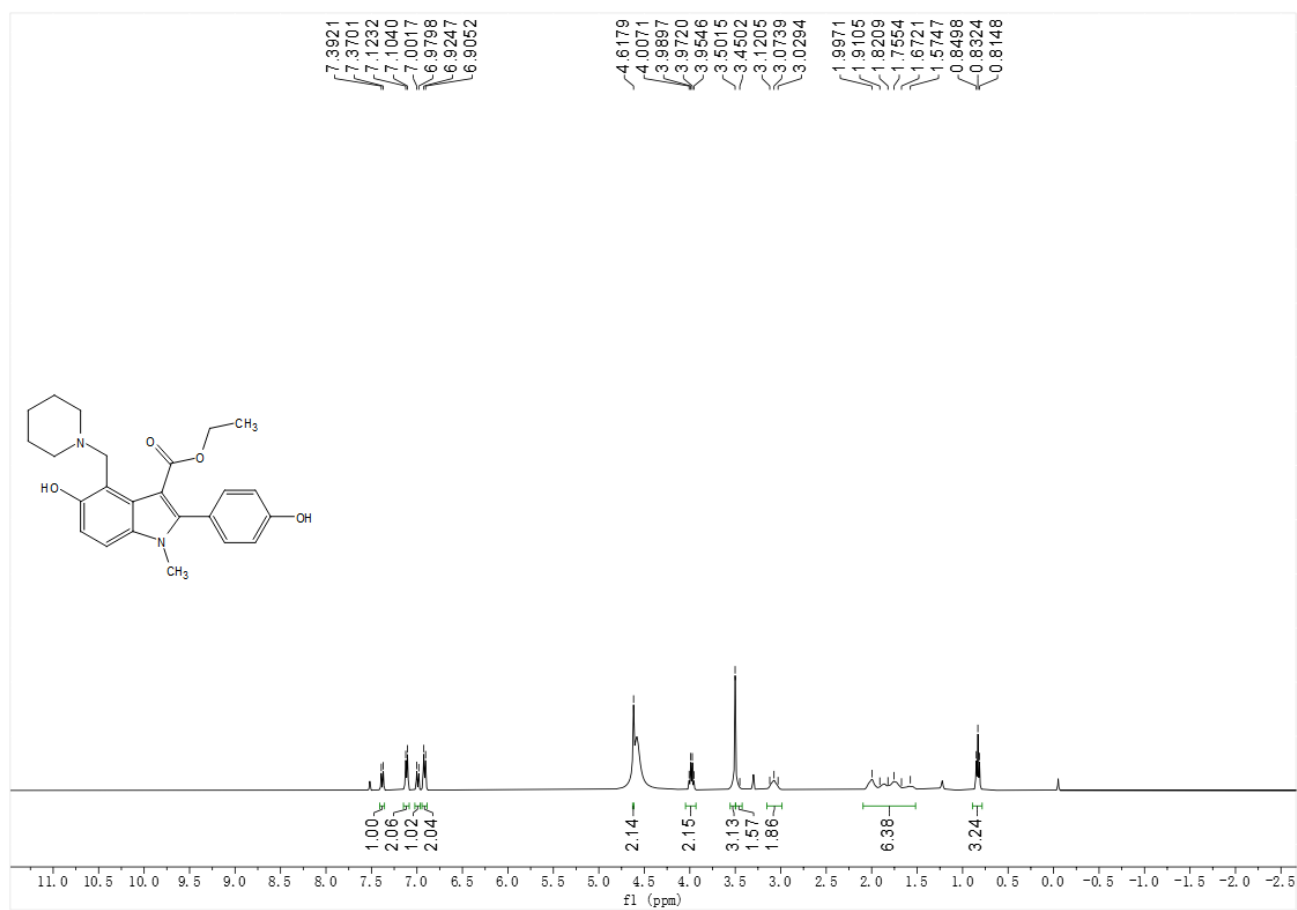
† These authors contributed equally to this work.

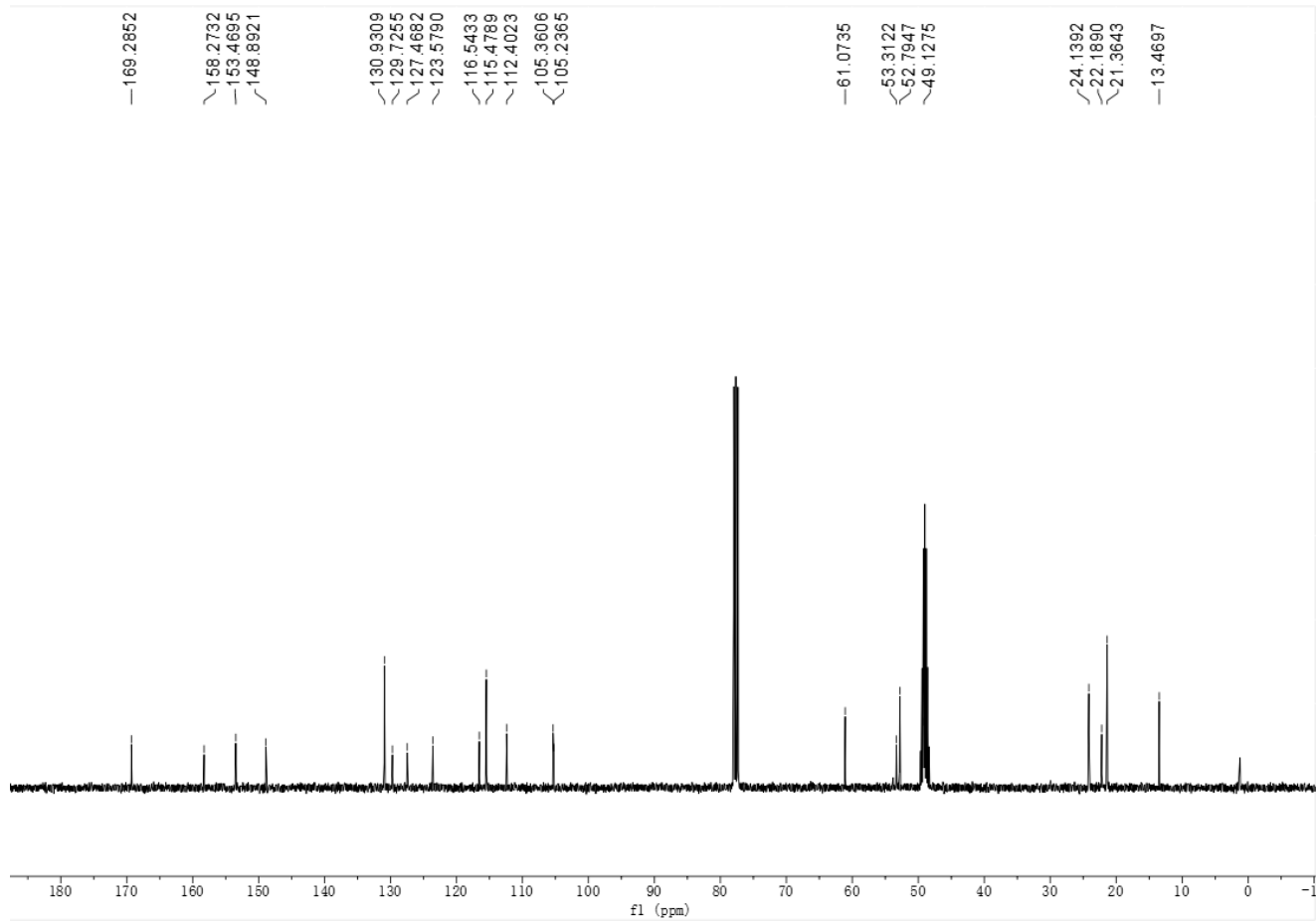
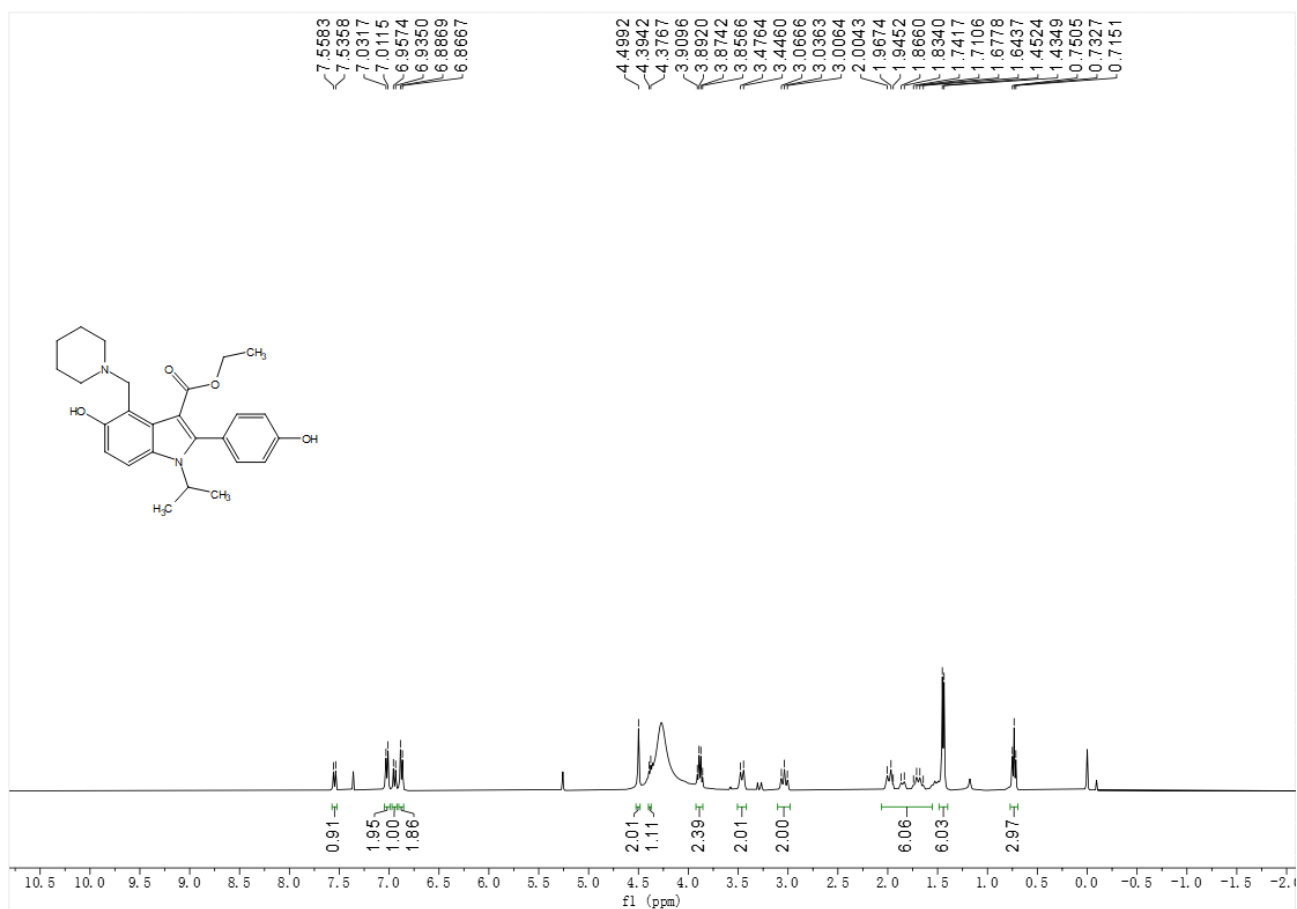
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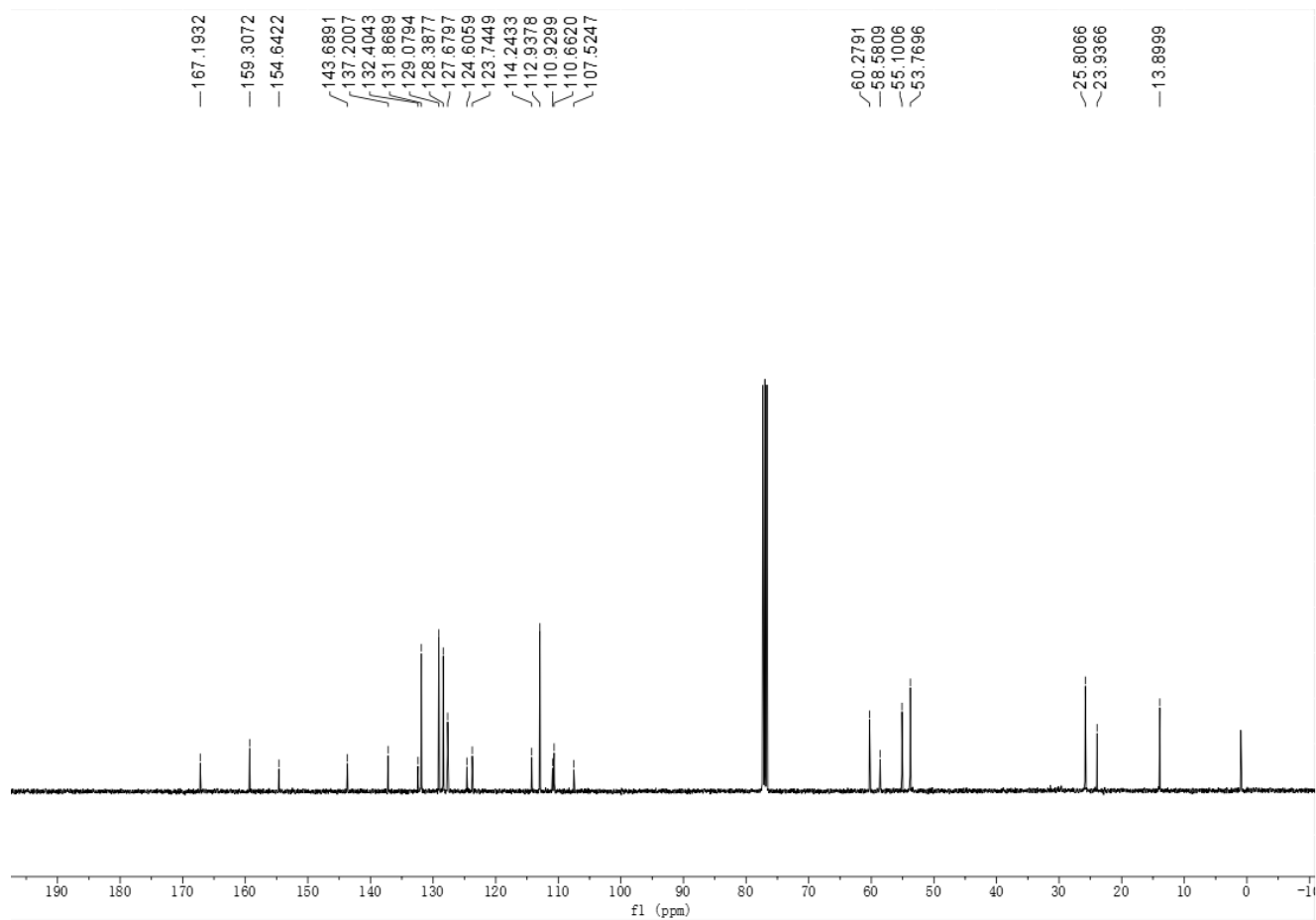
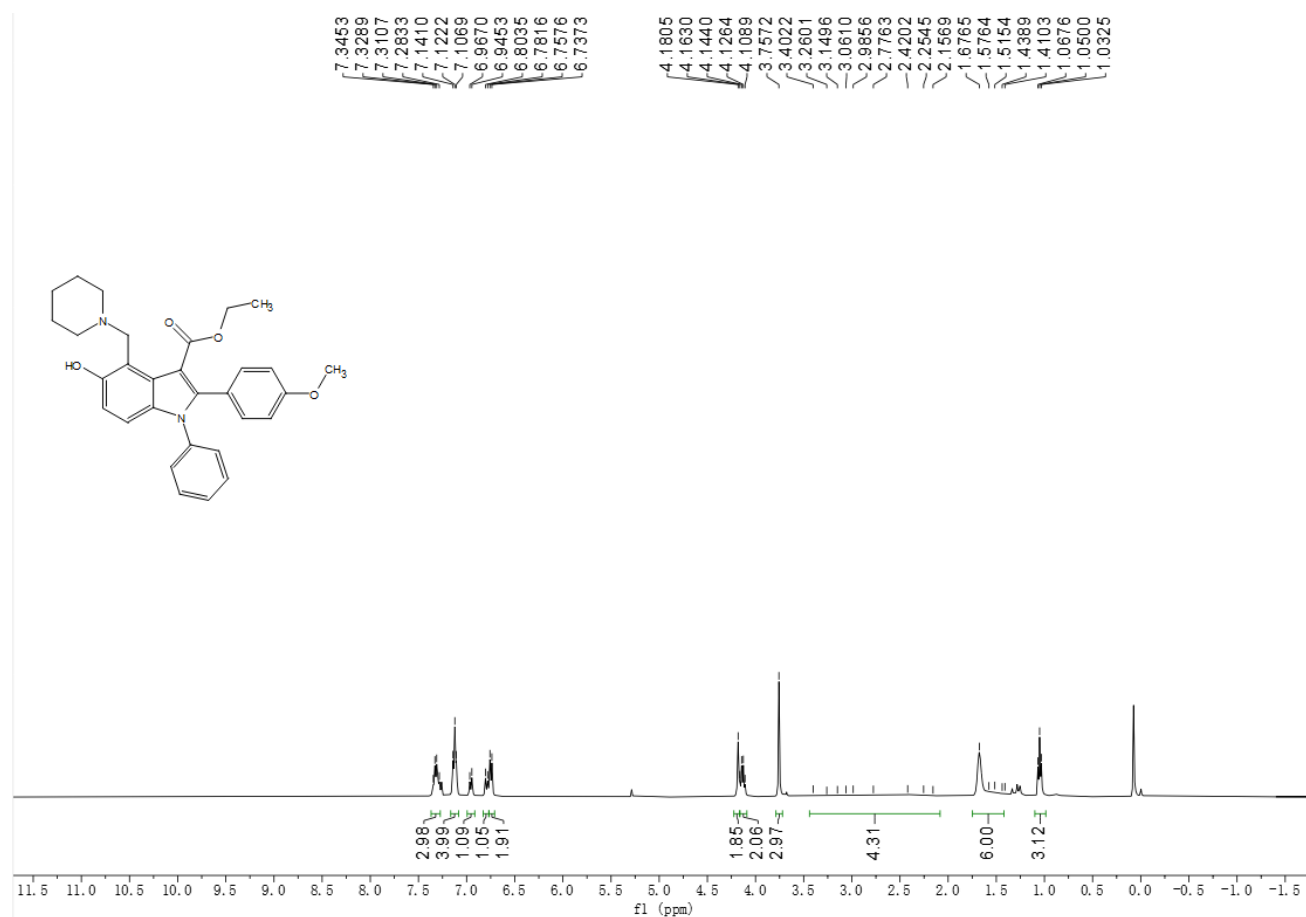


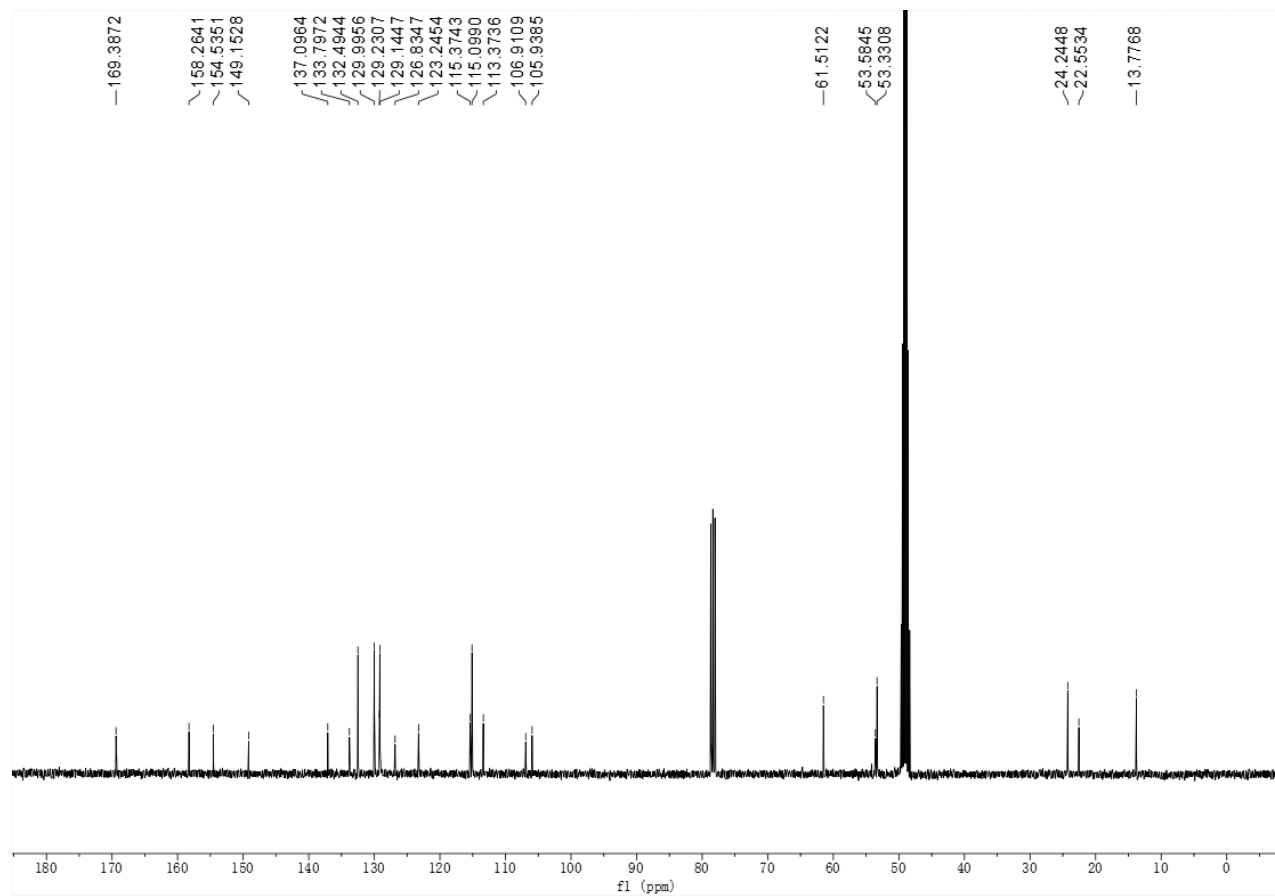
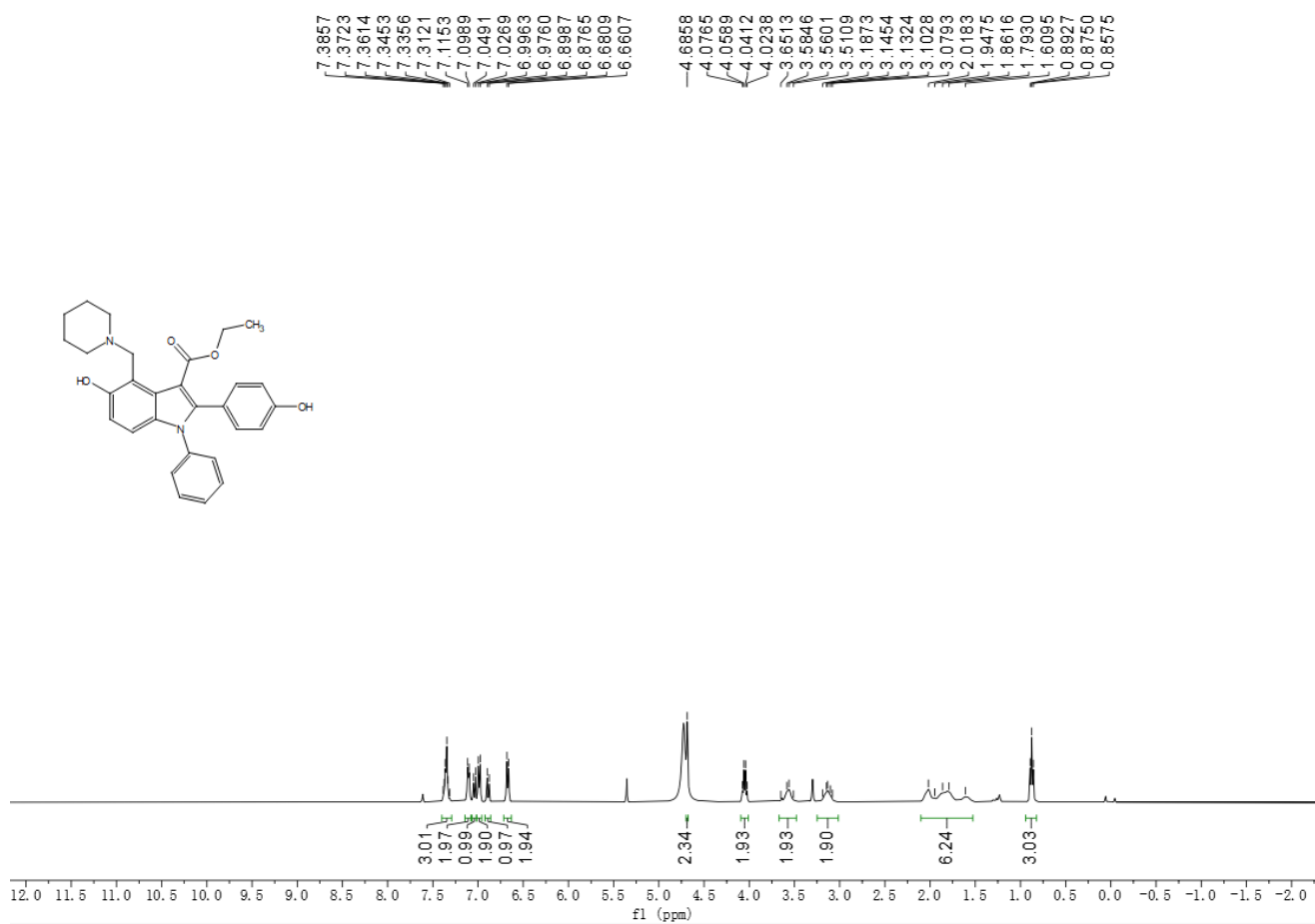


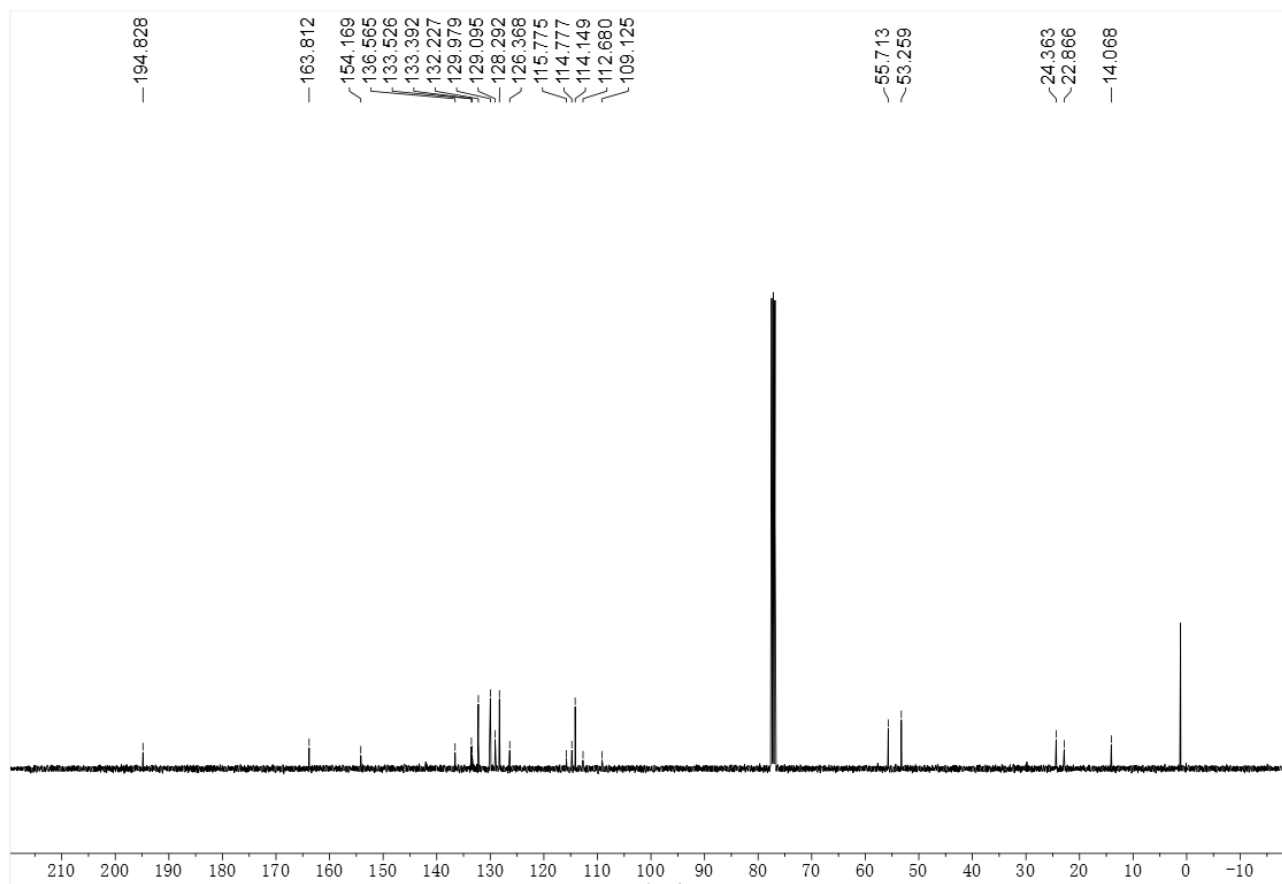
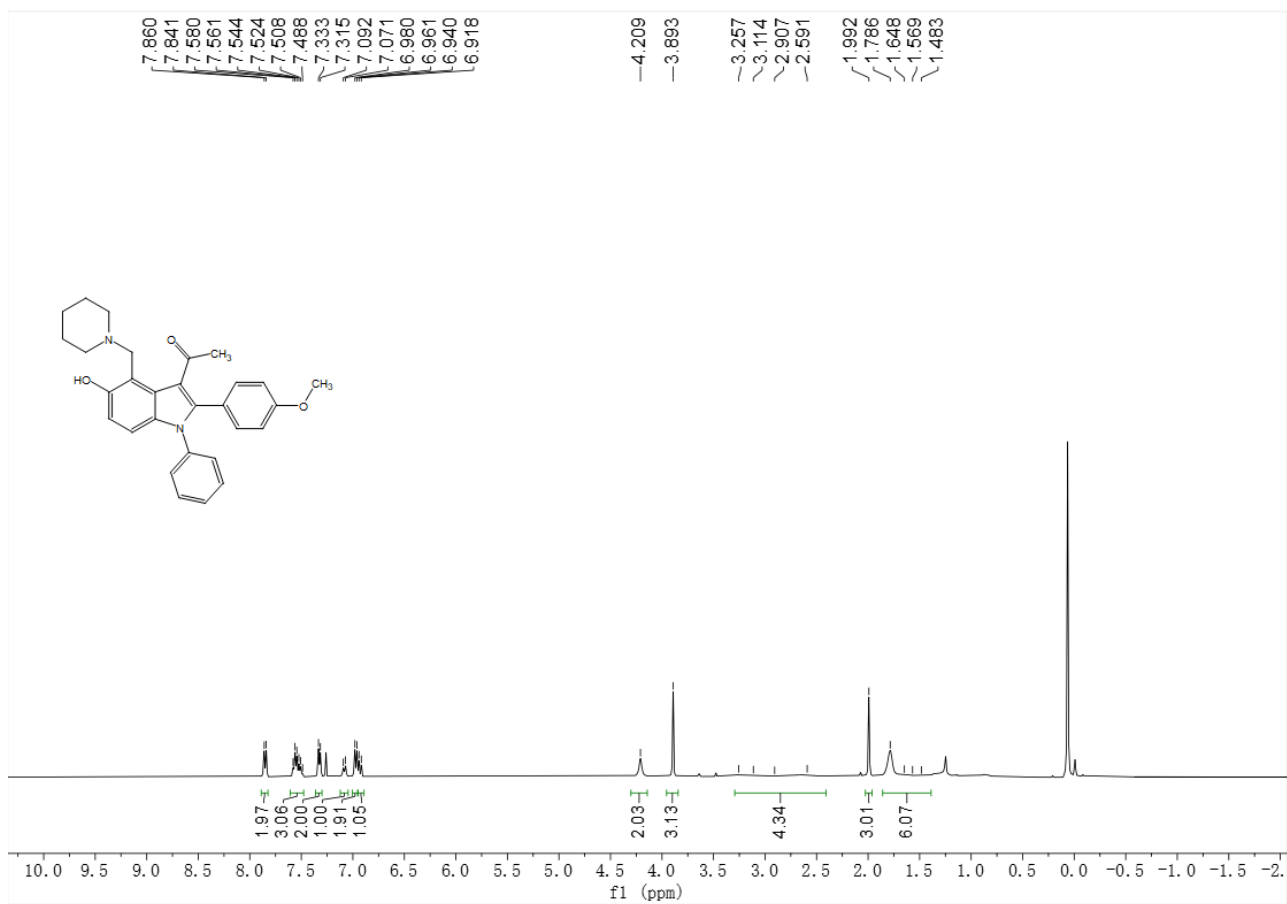


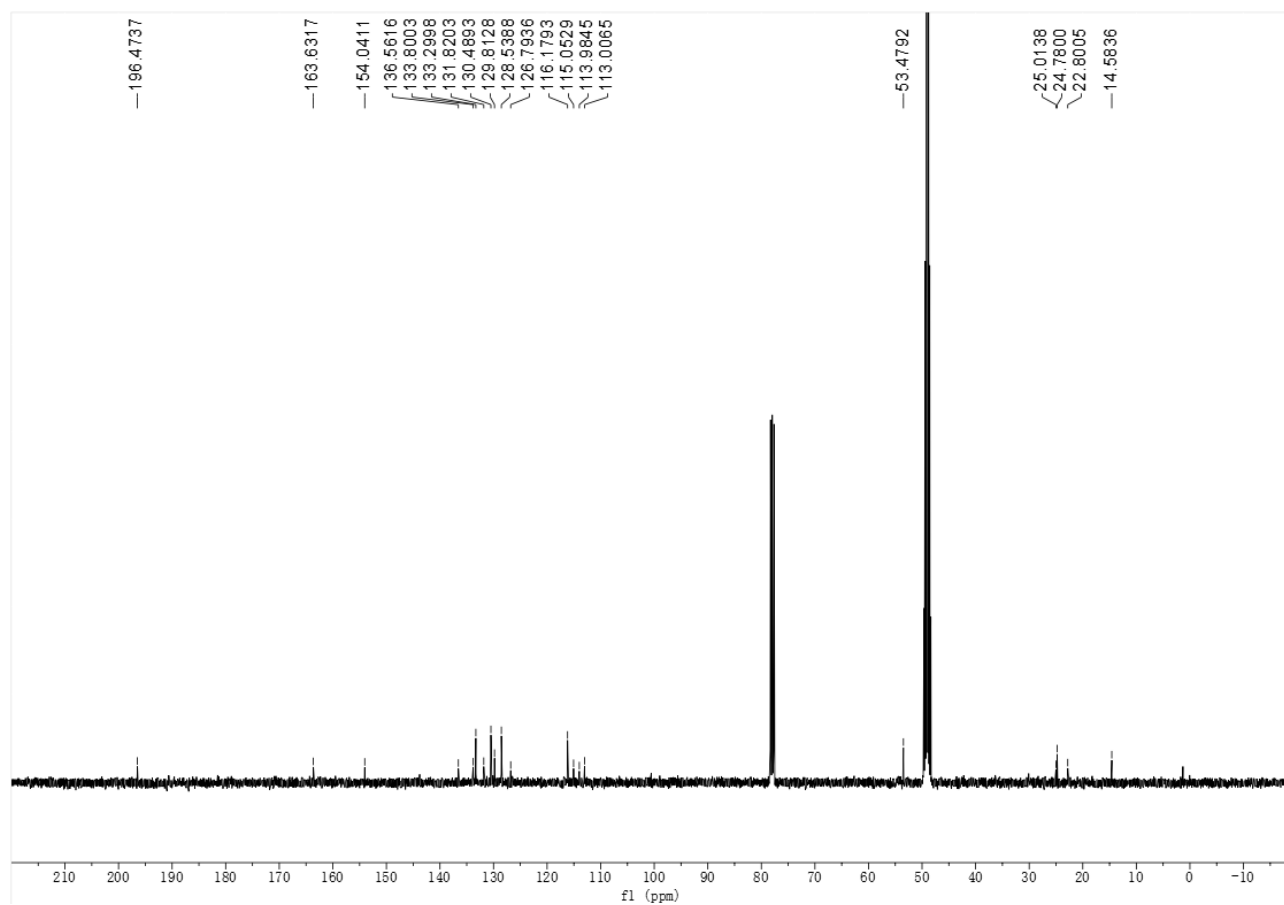
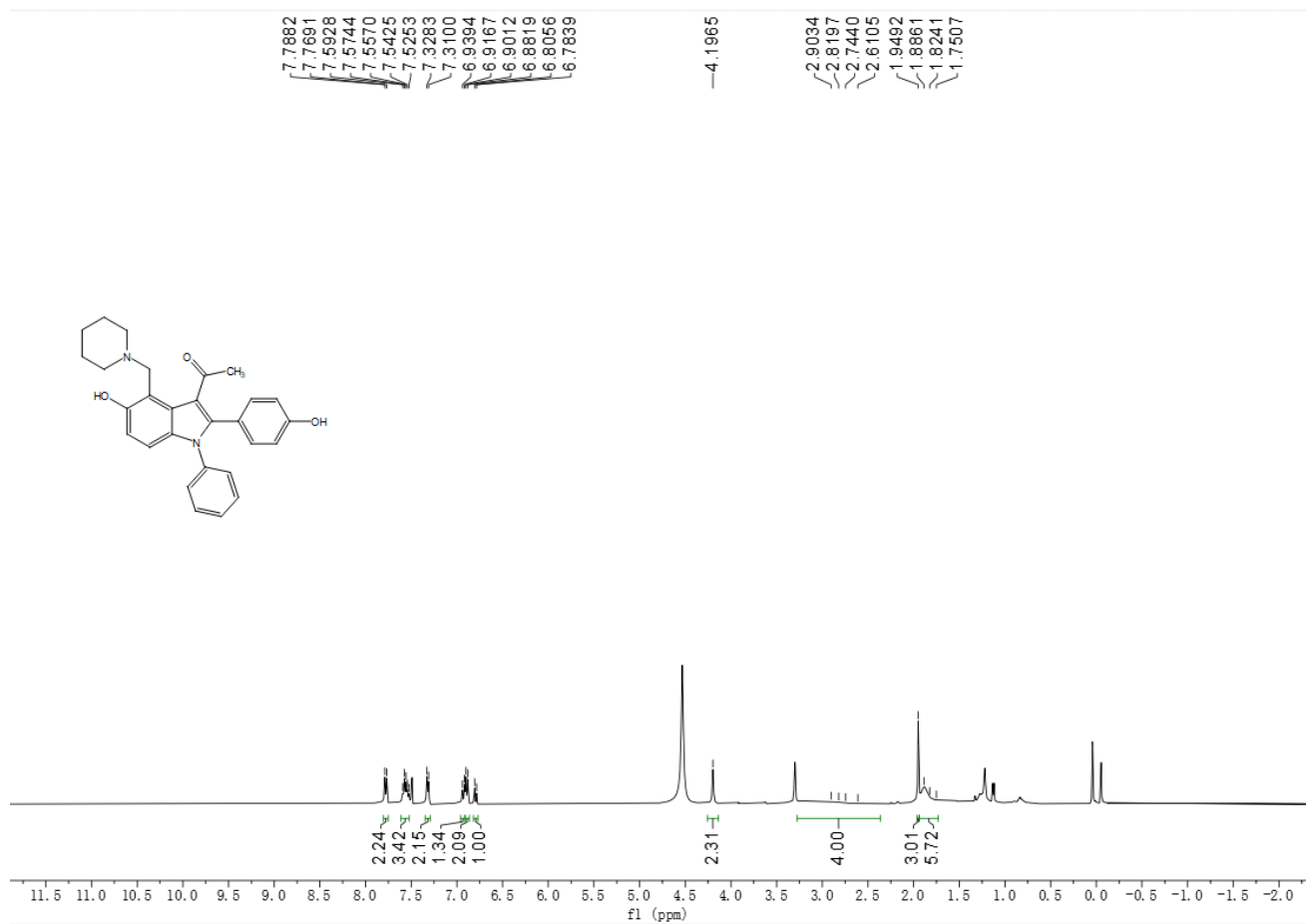


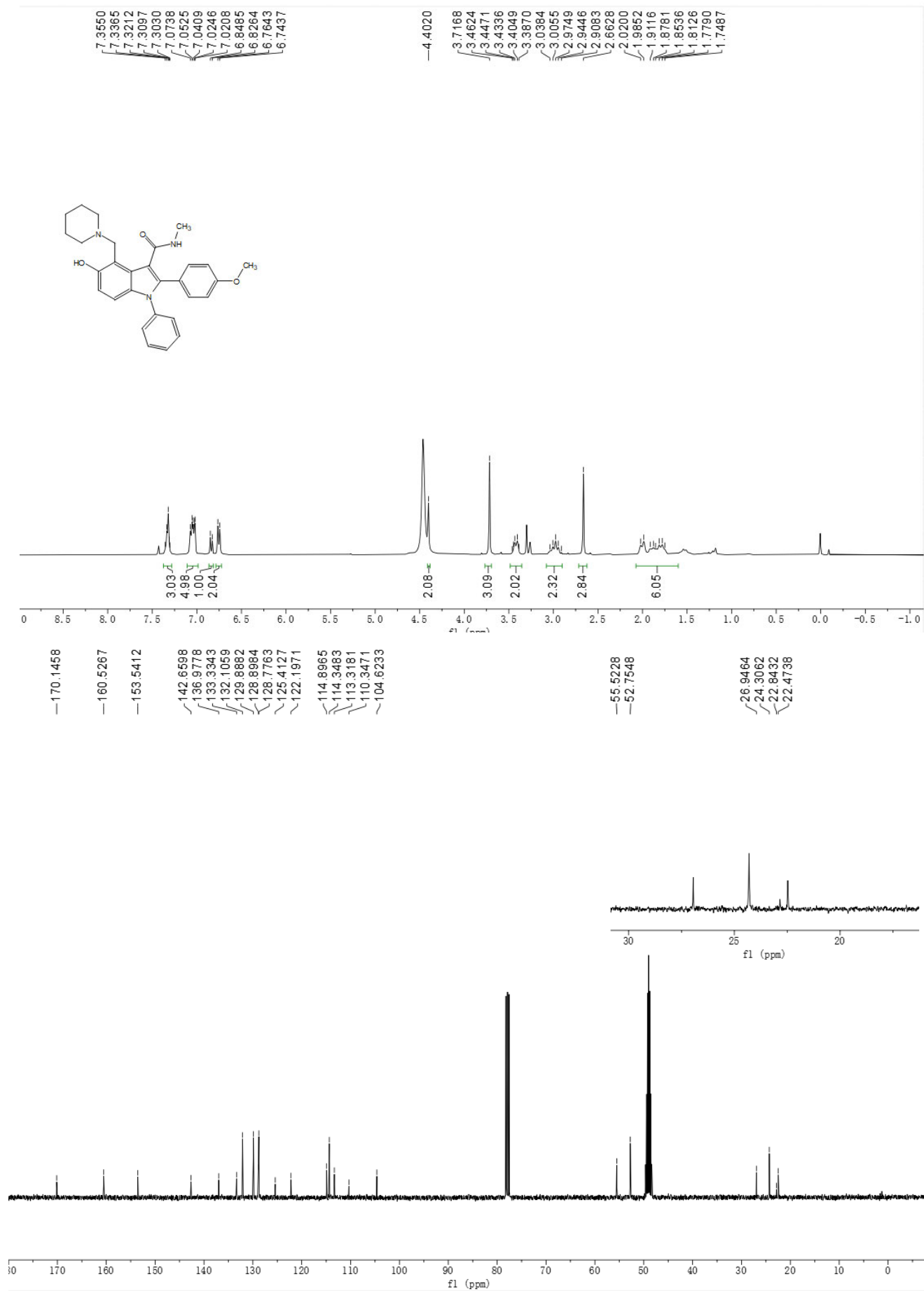


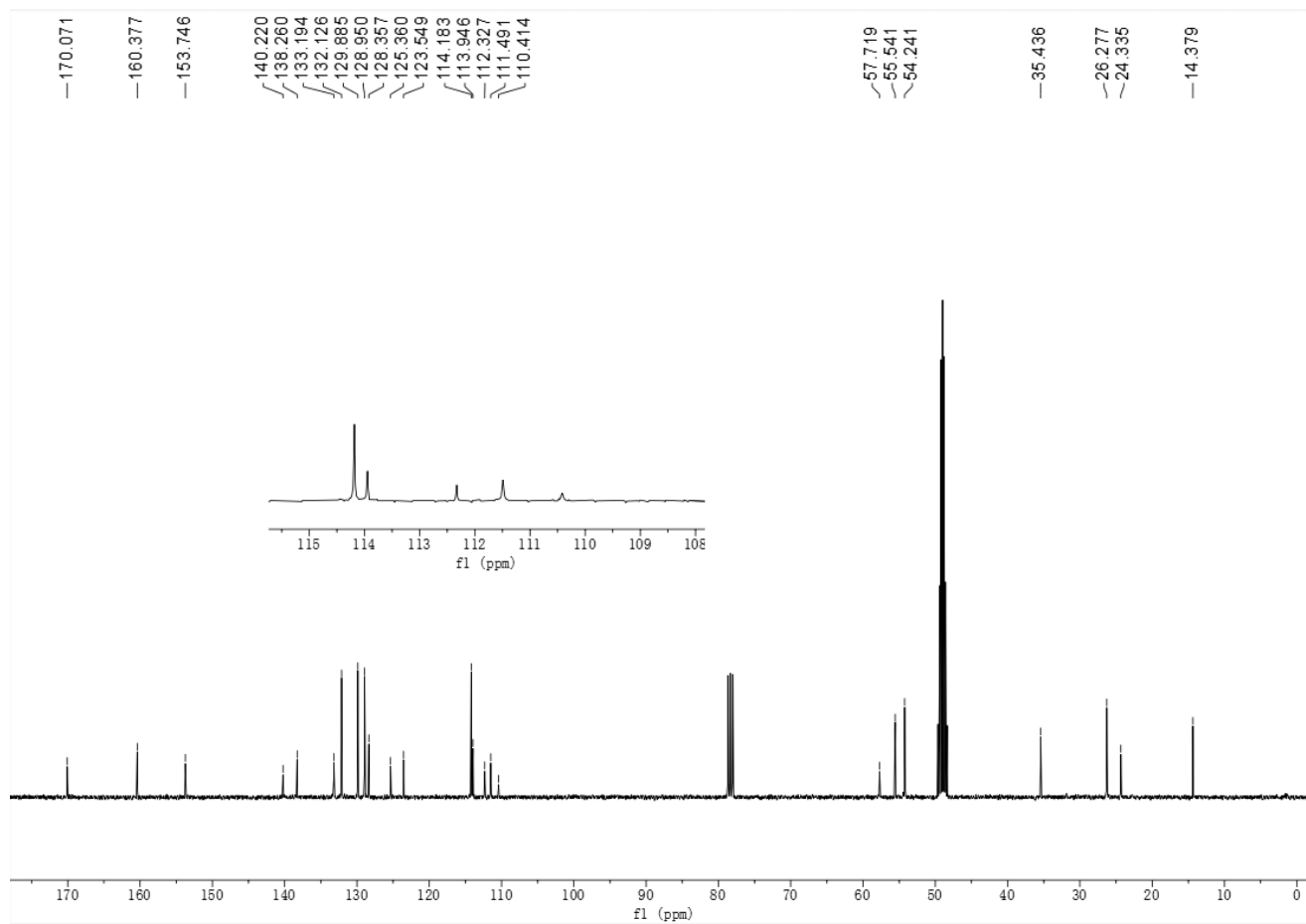
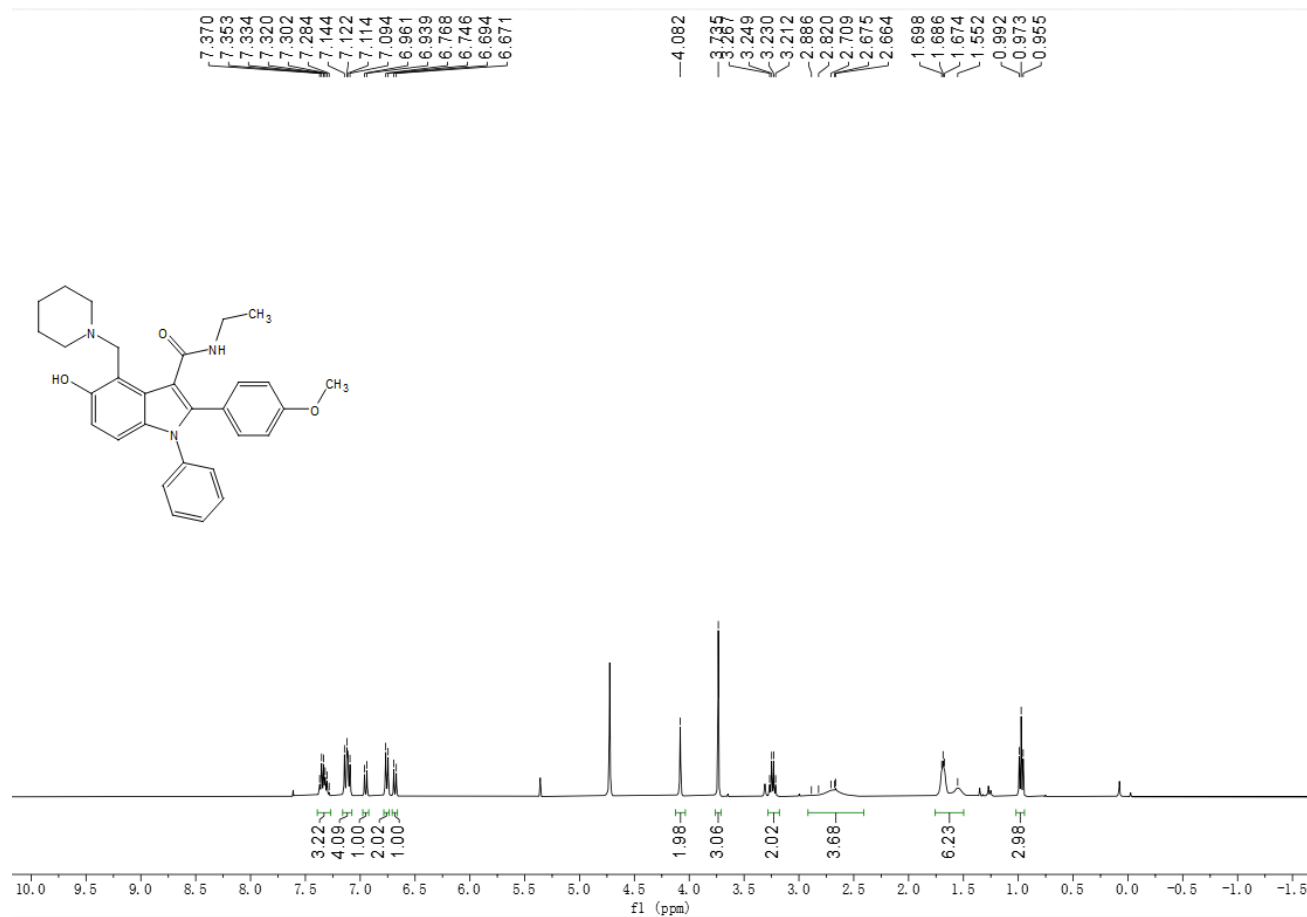


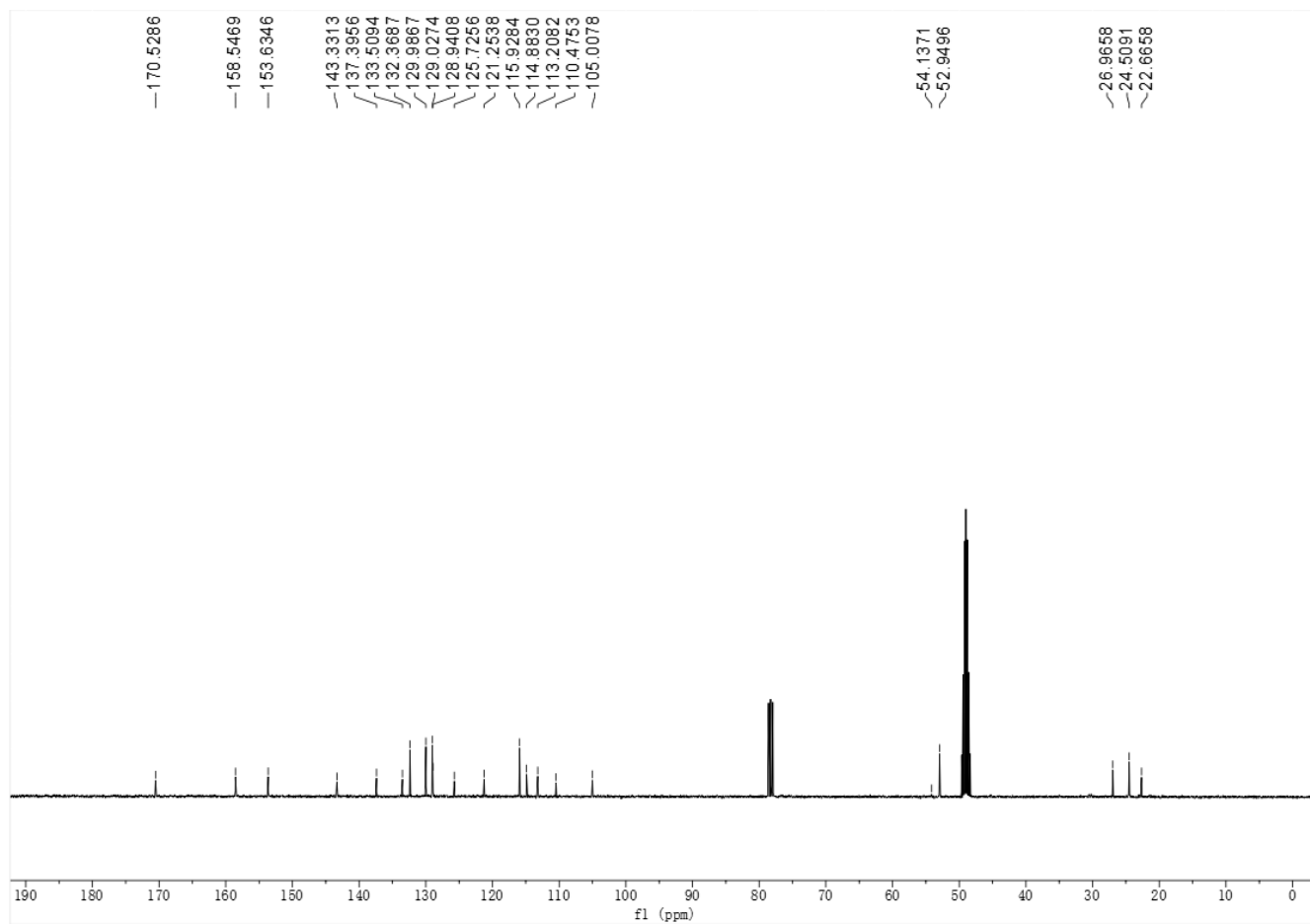
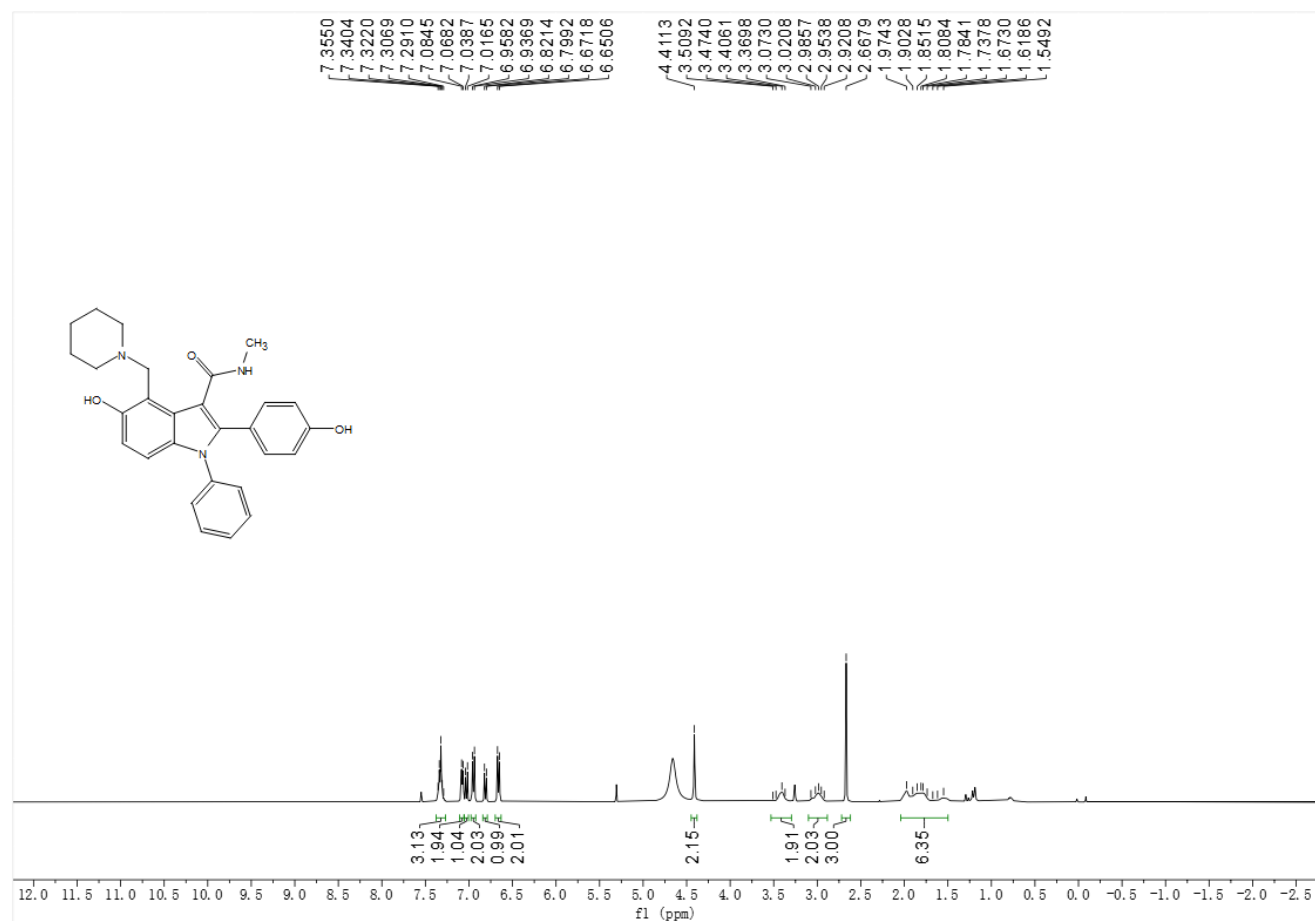


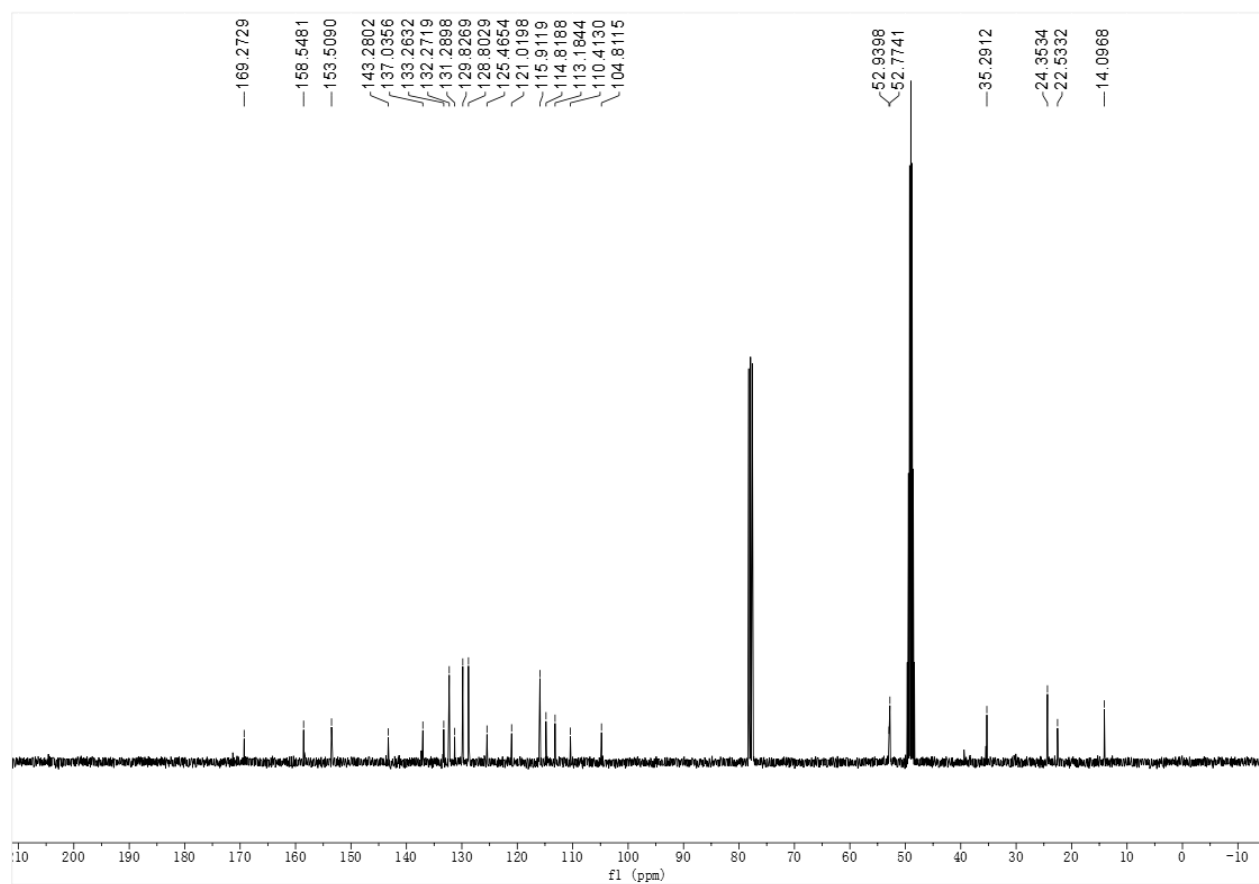
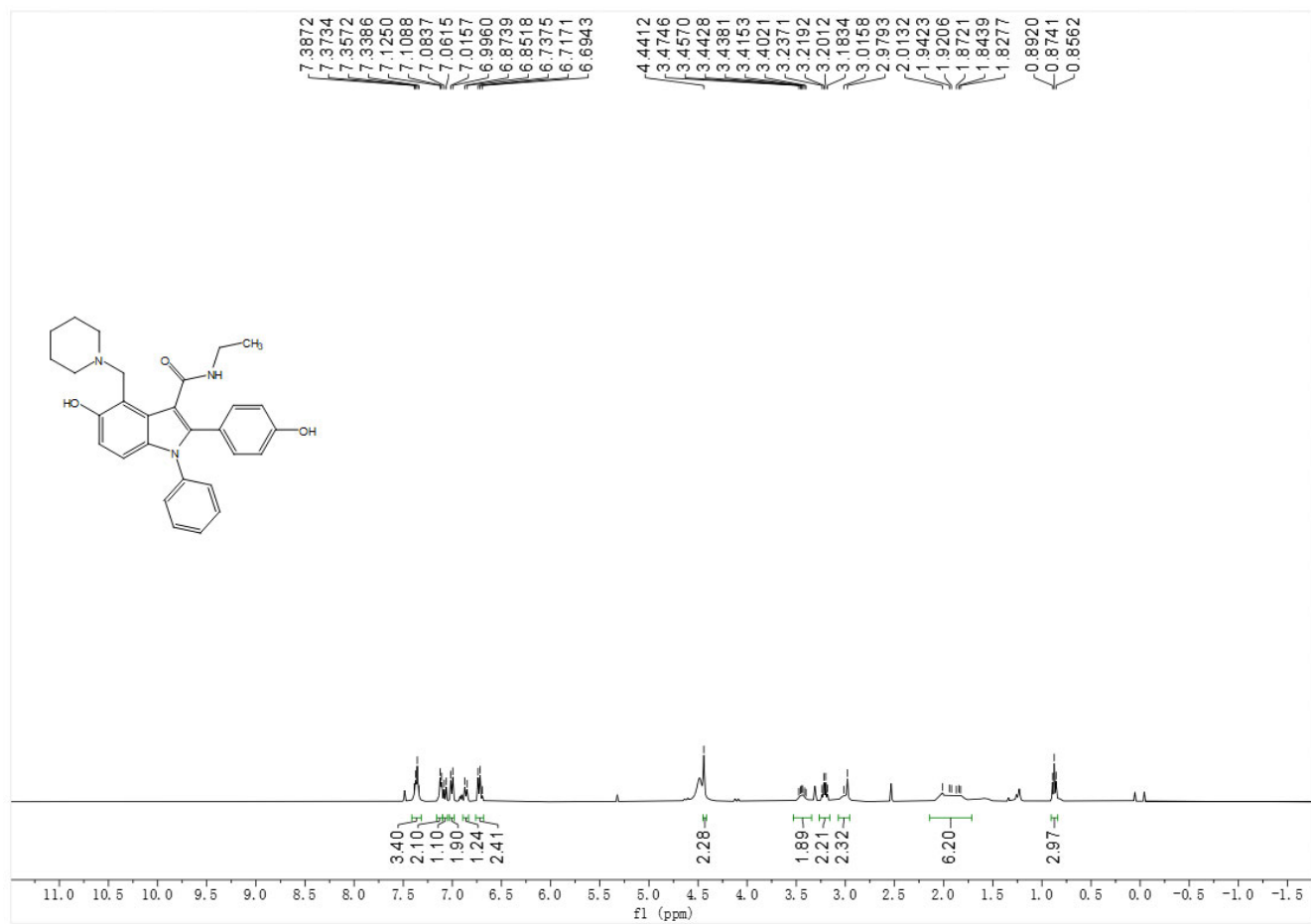


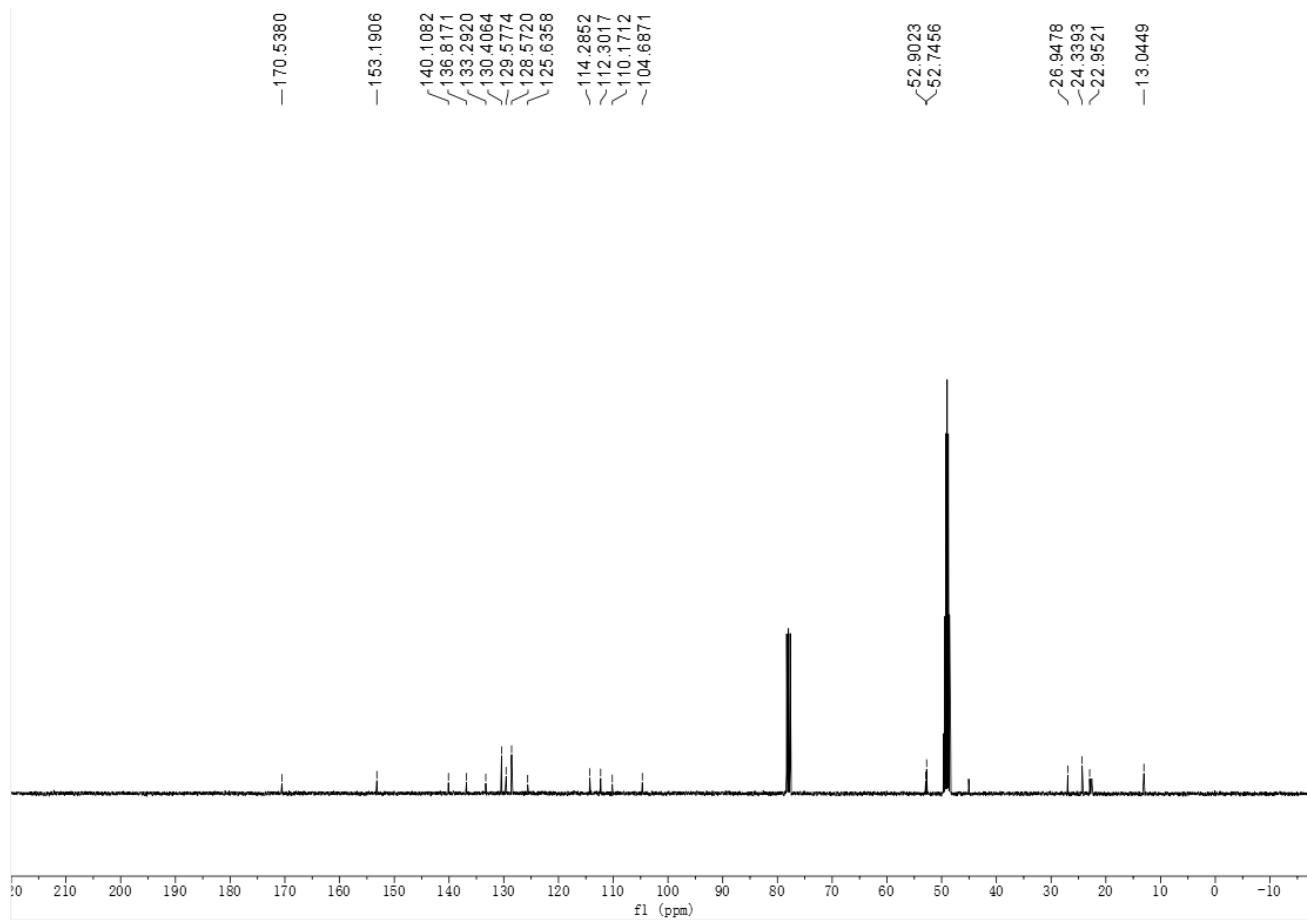
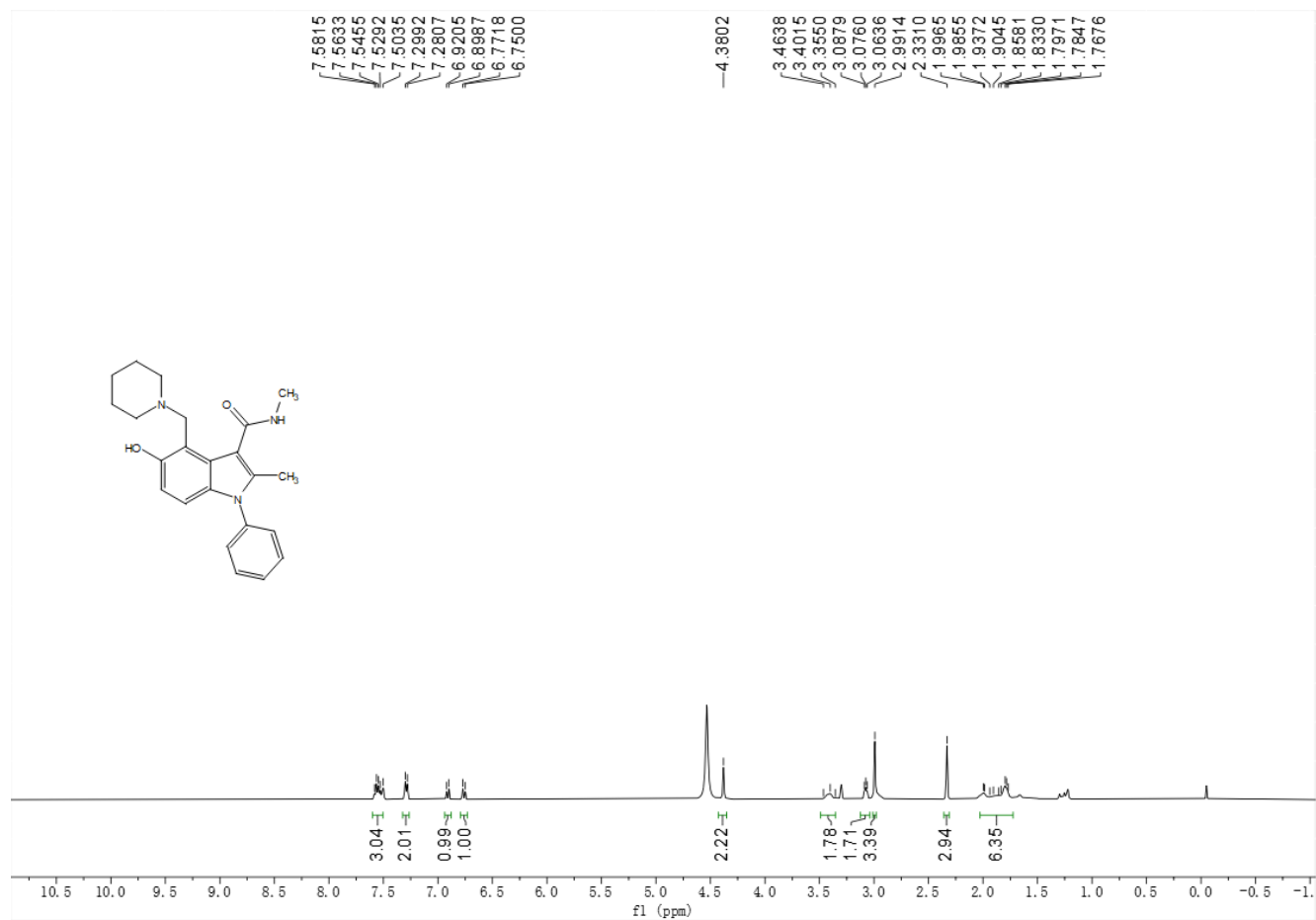


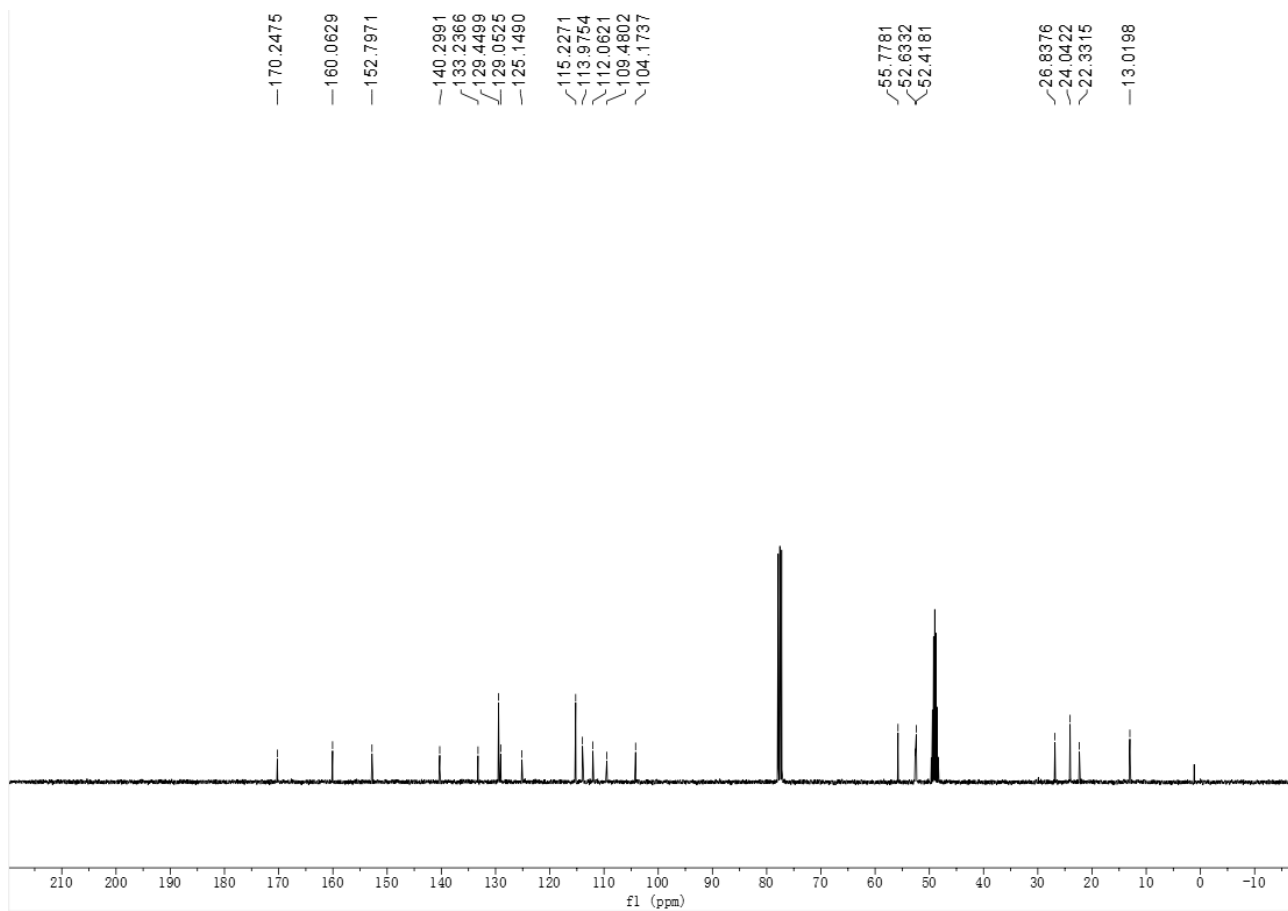
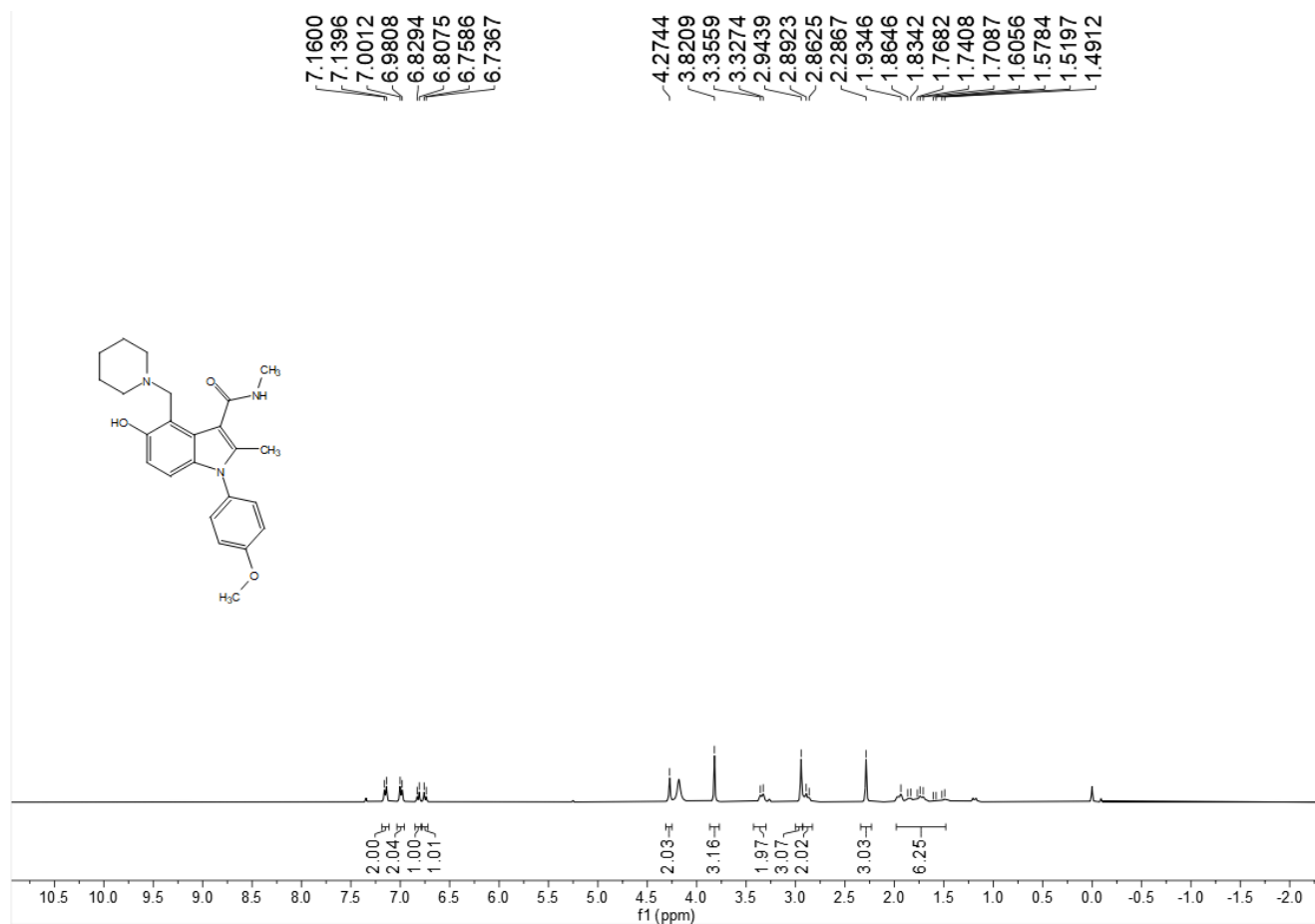


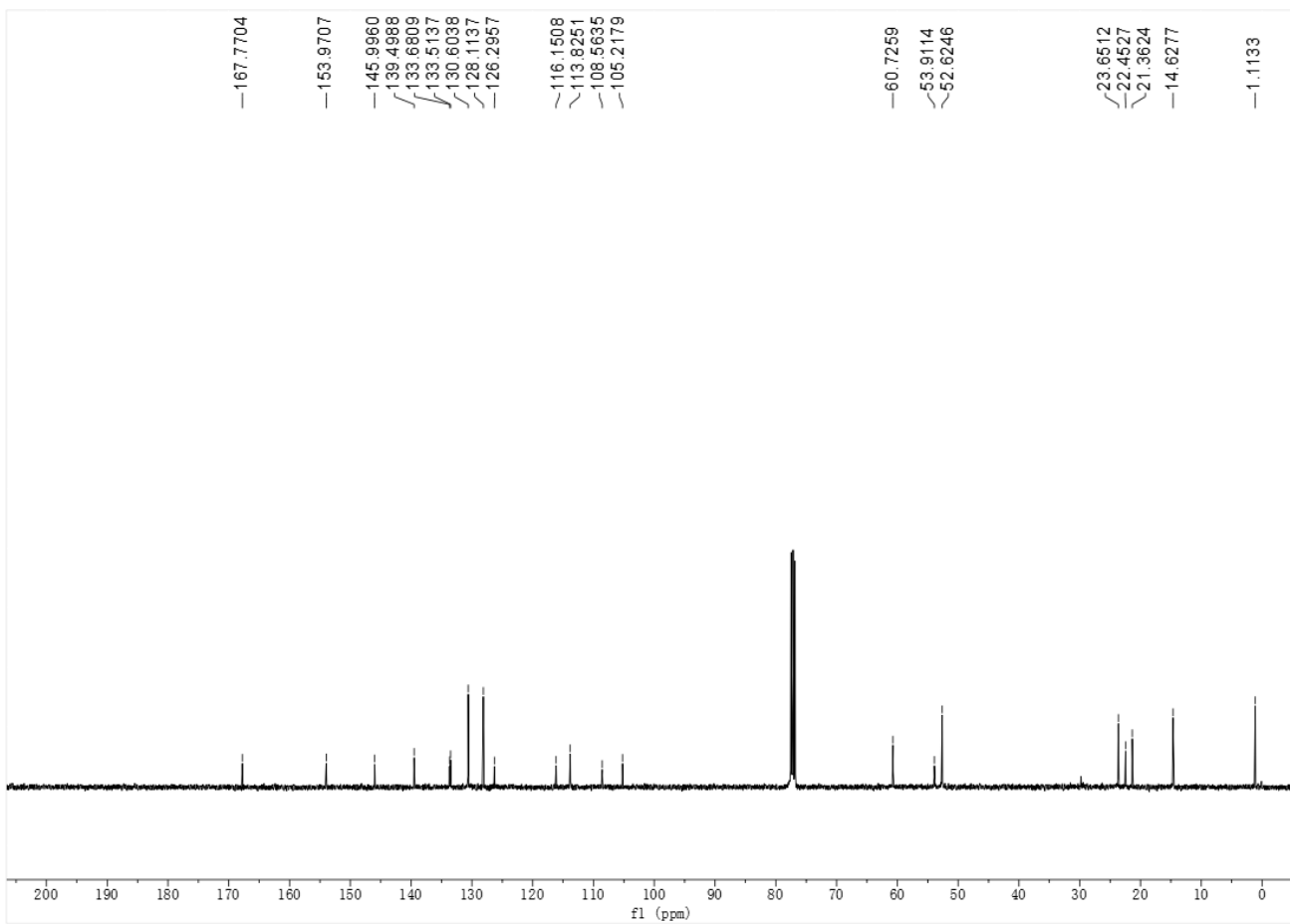
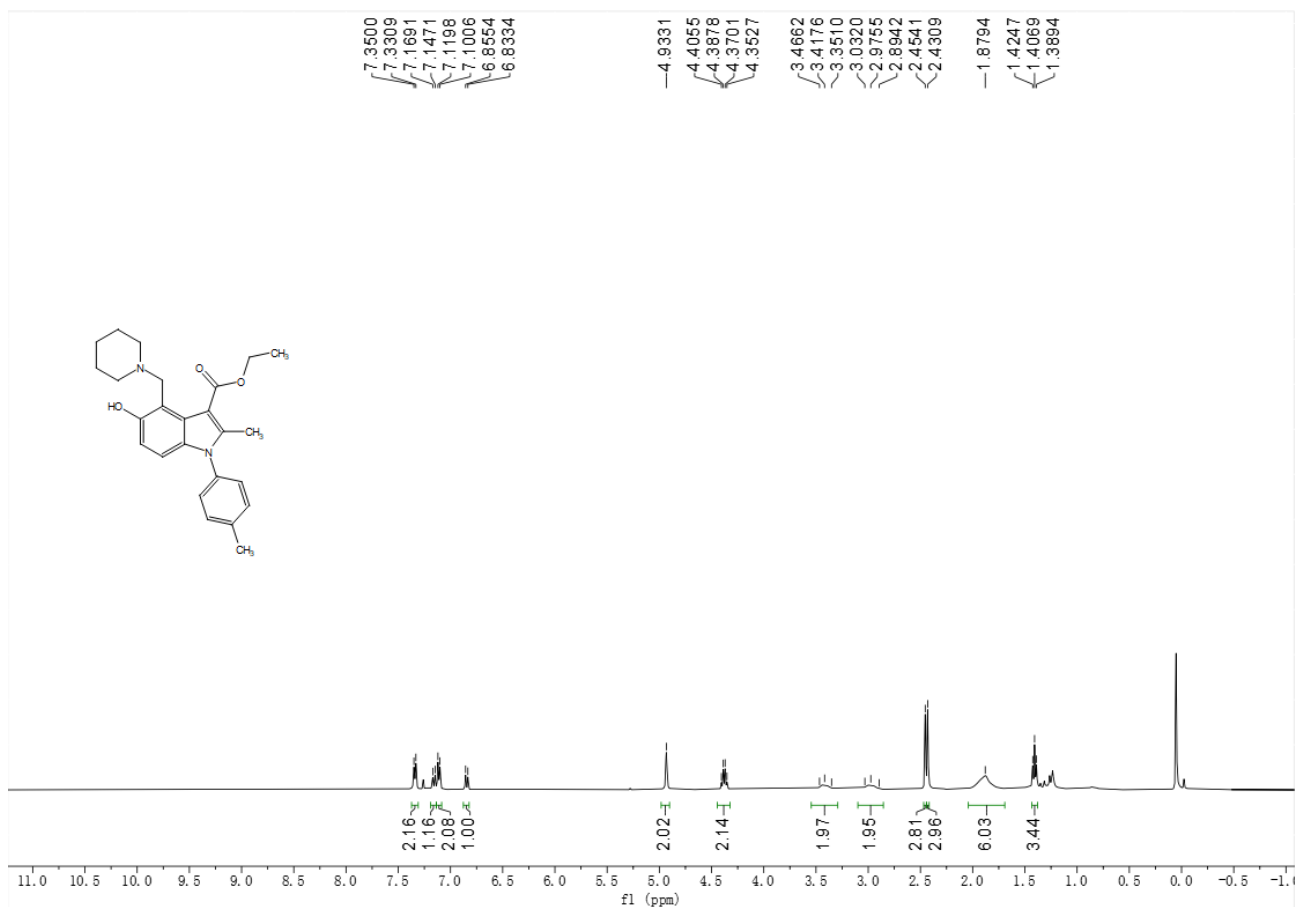


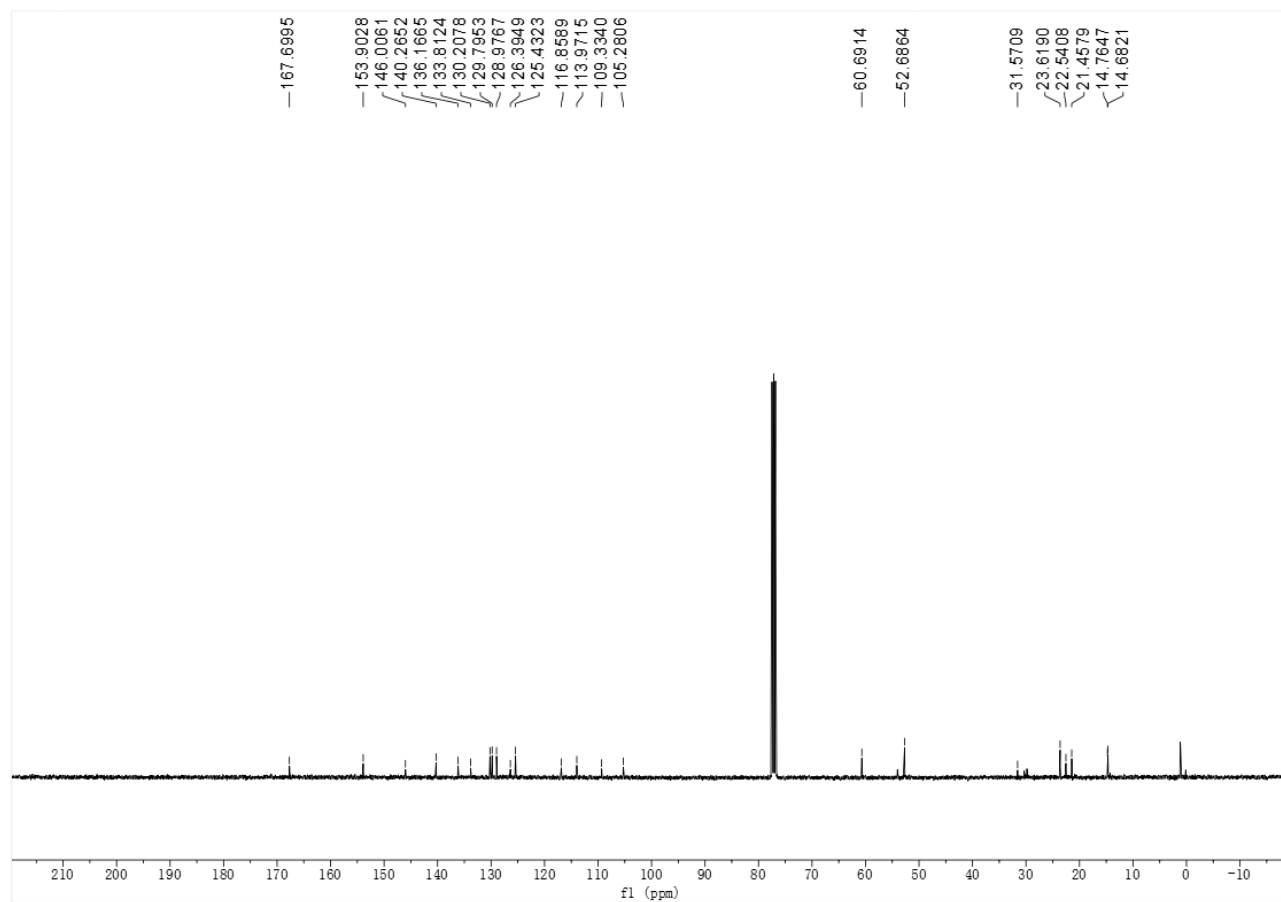
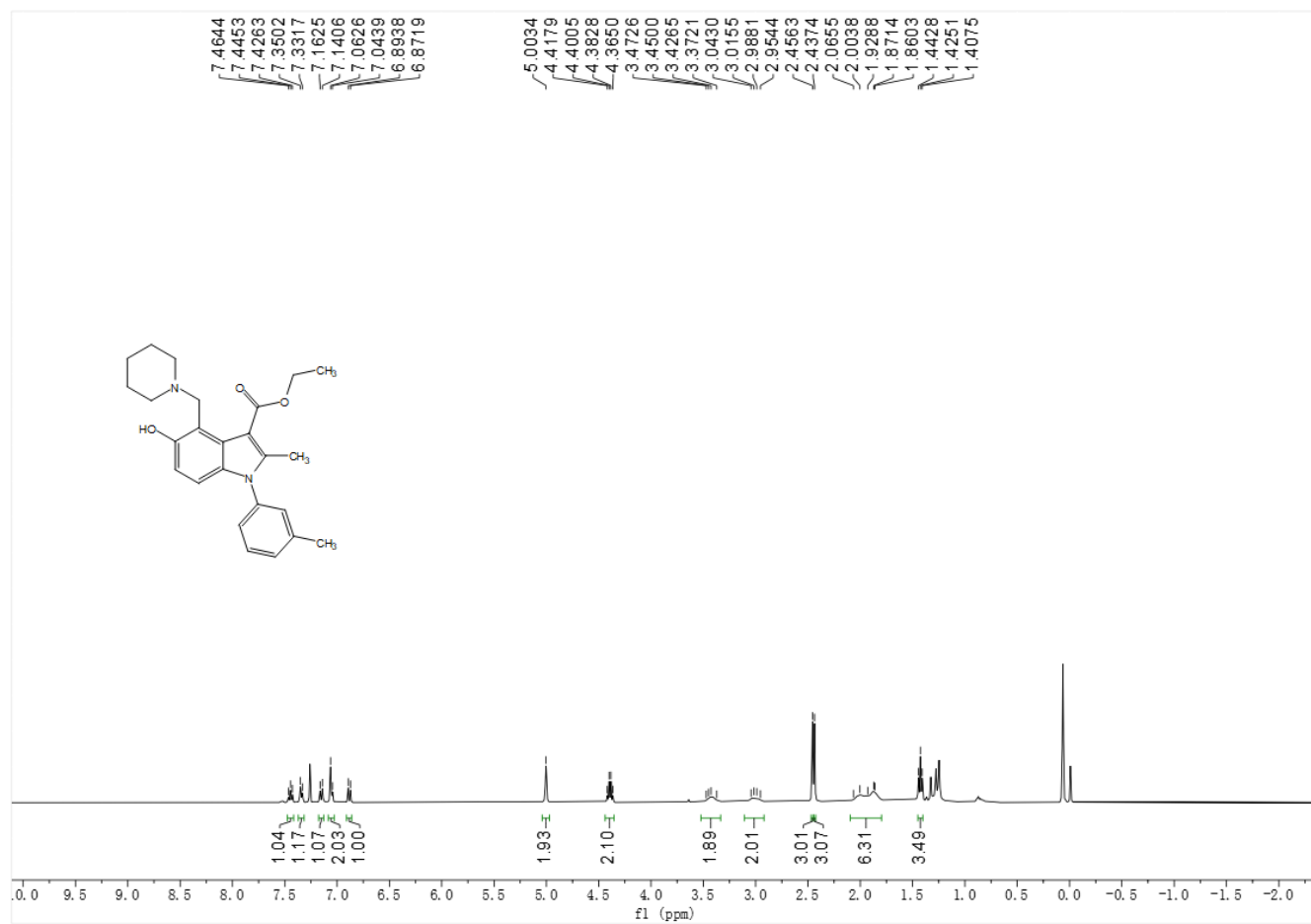


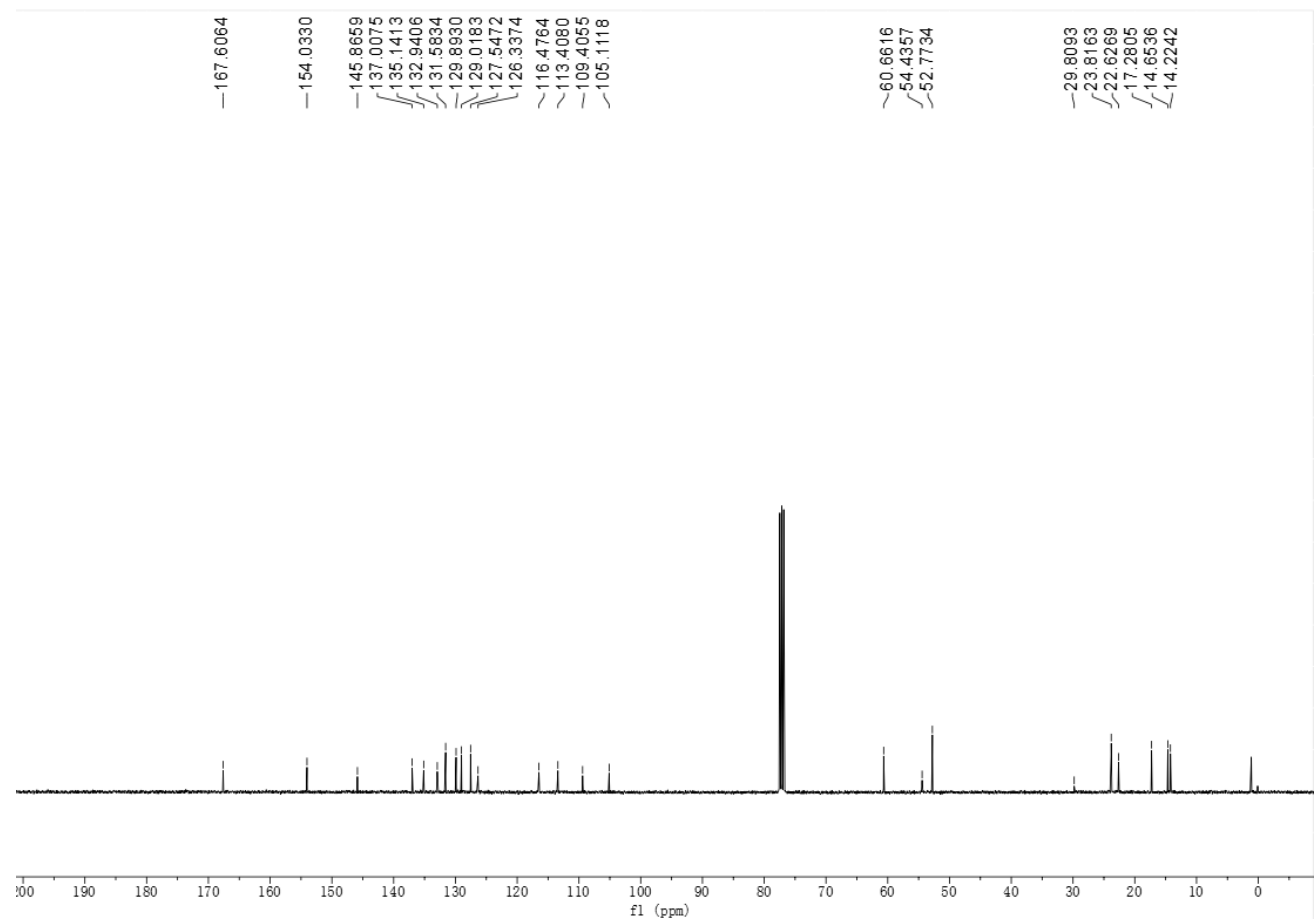
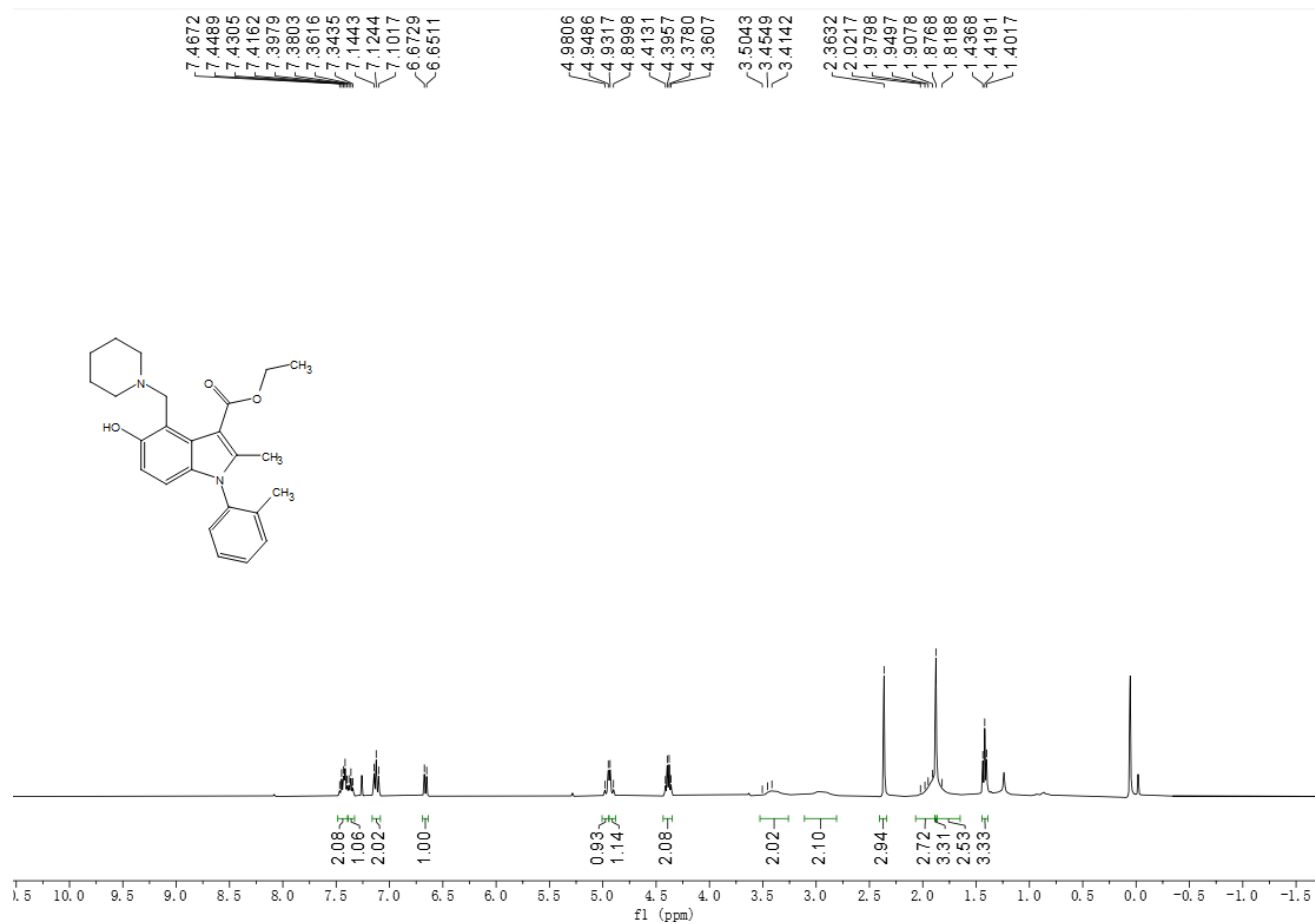


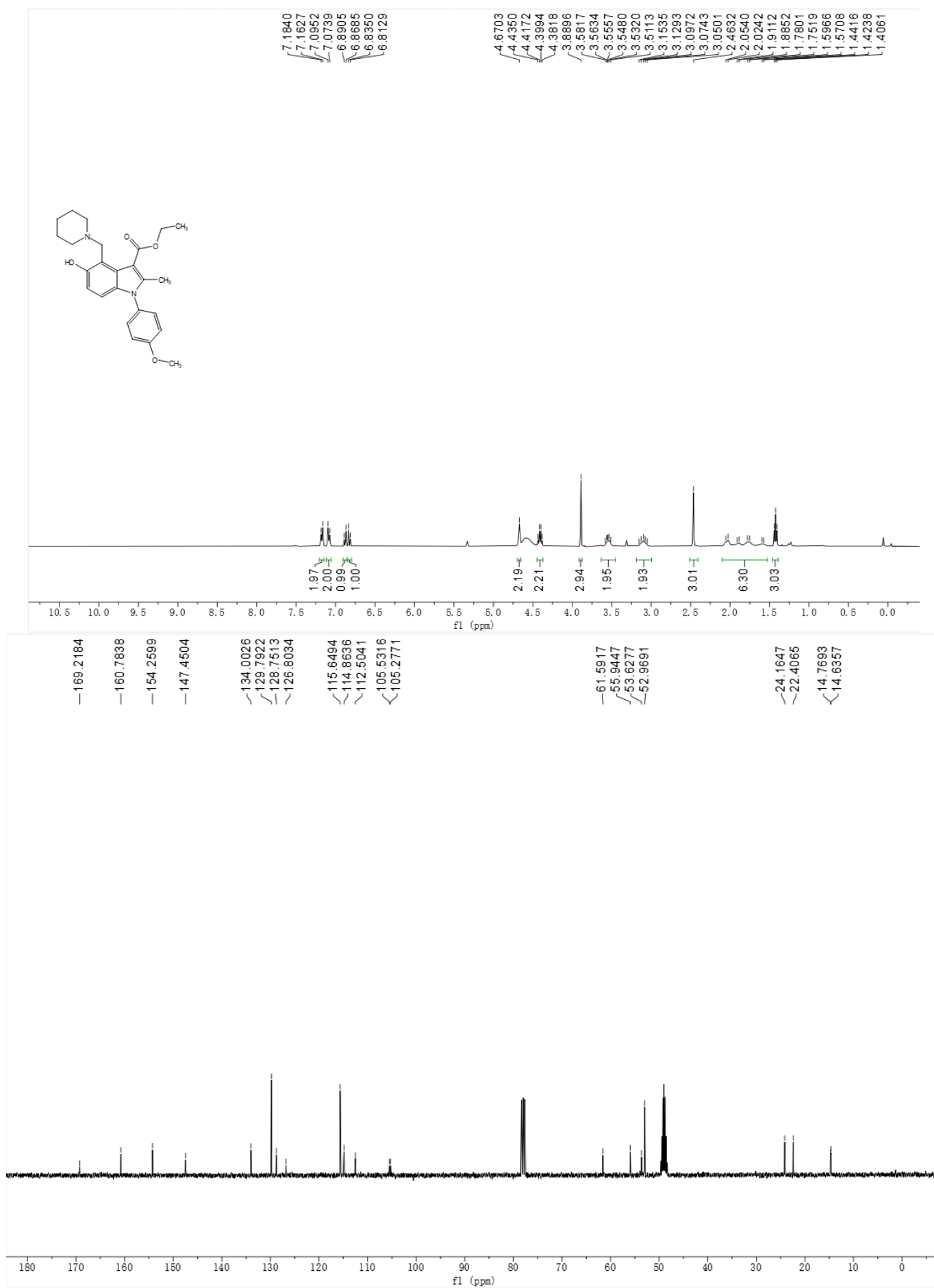


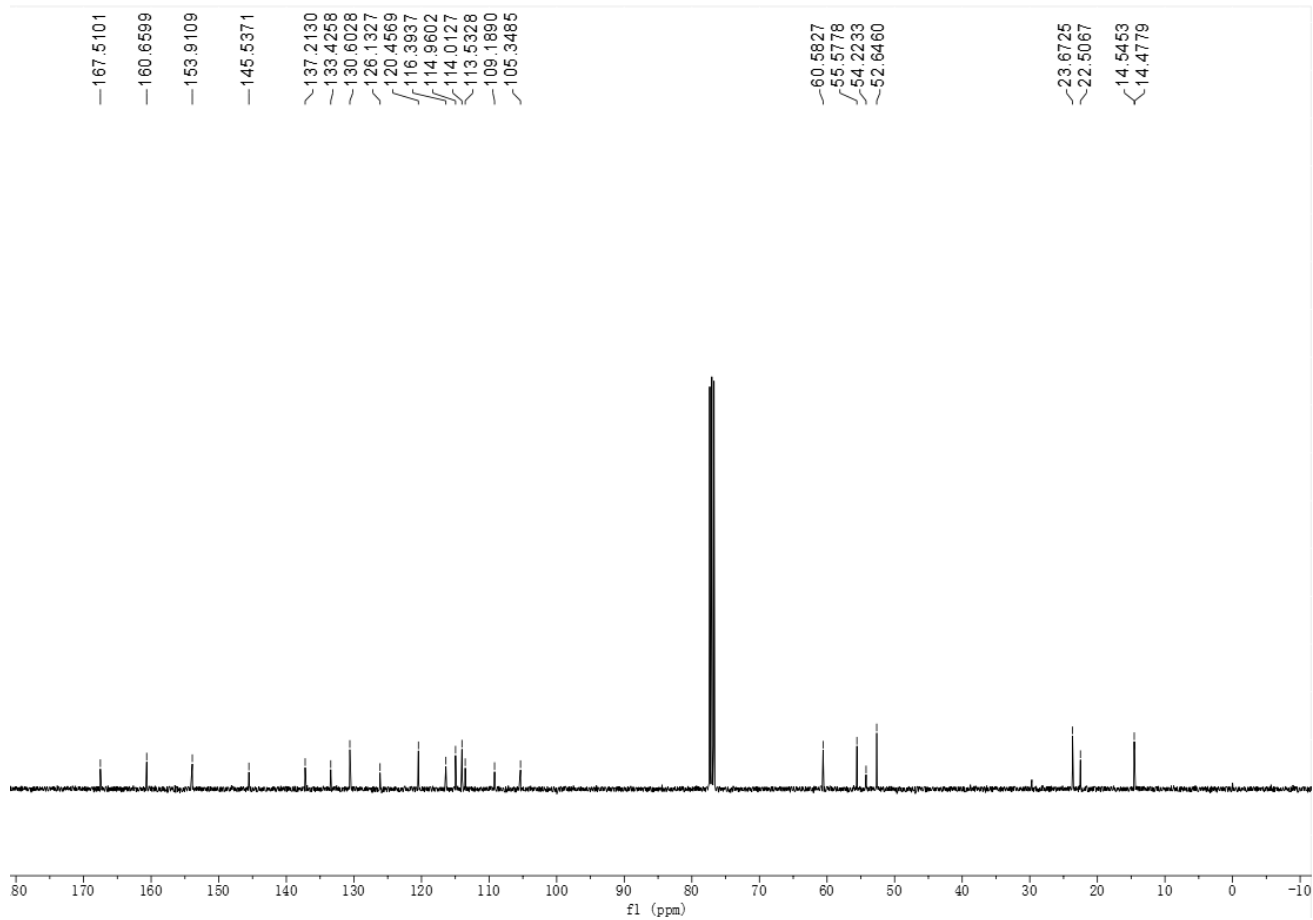
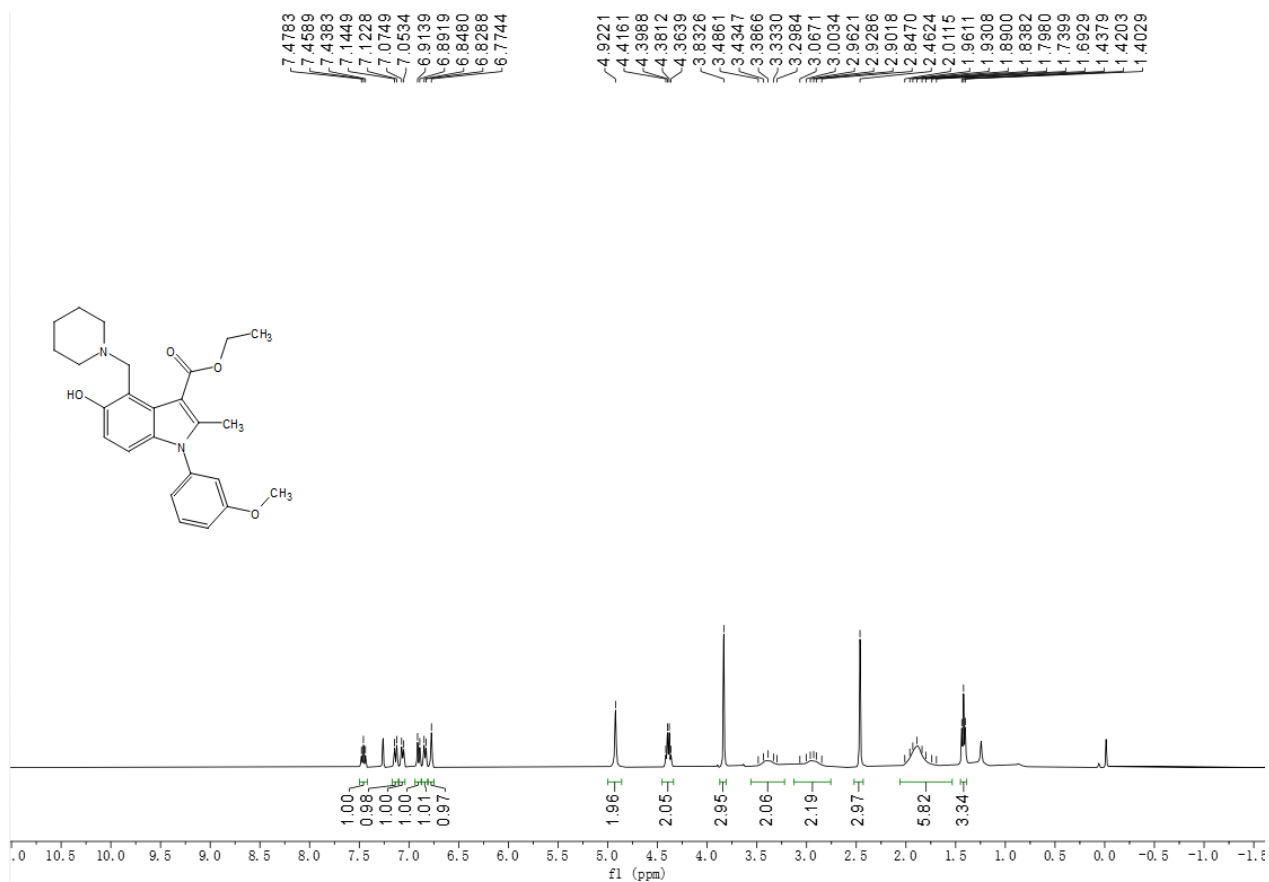


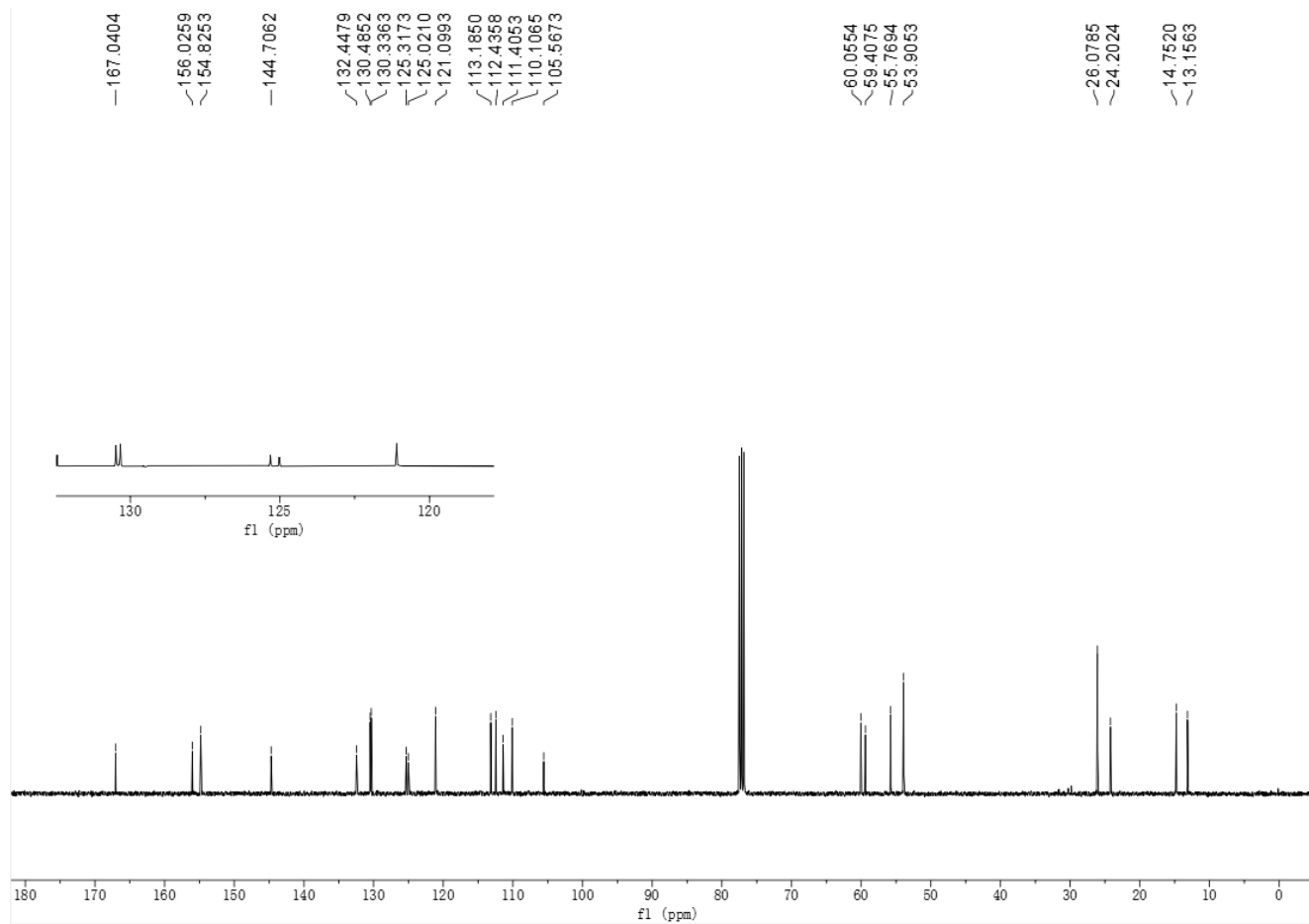
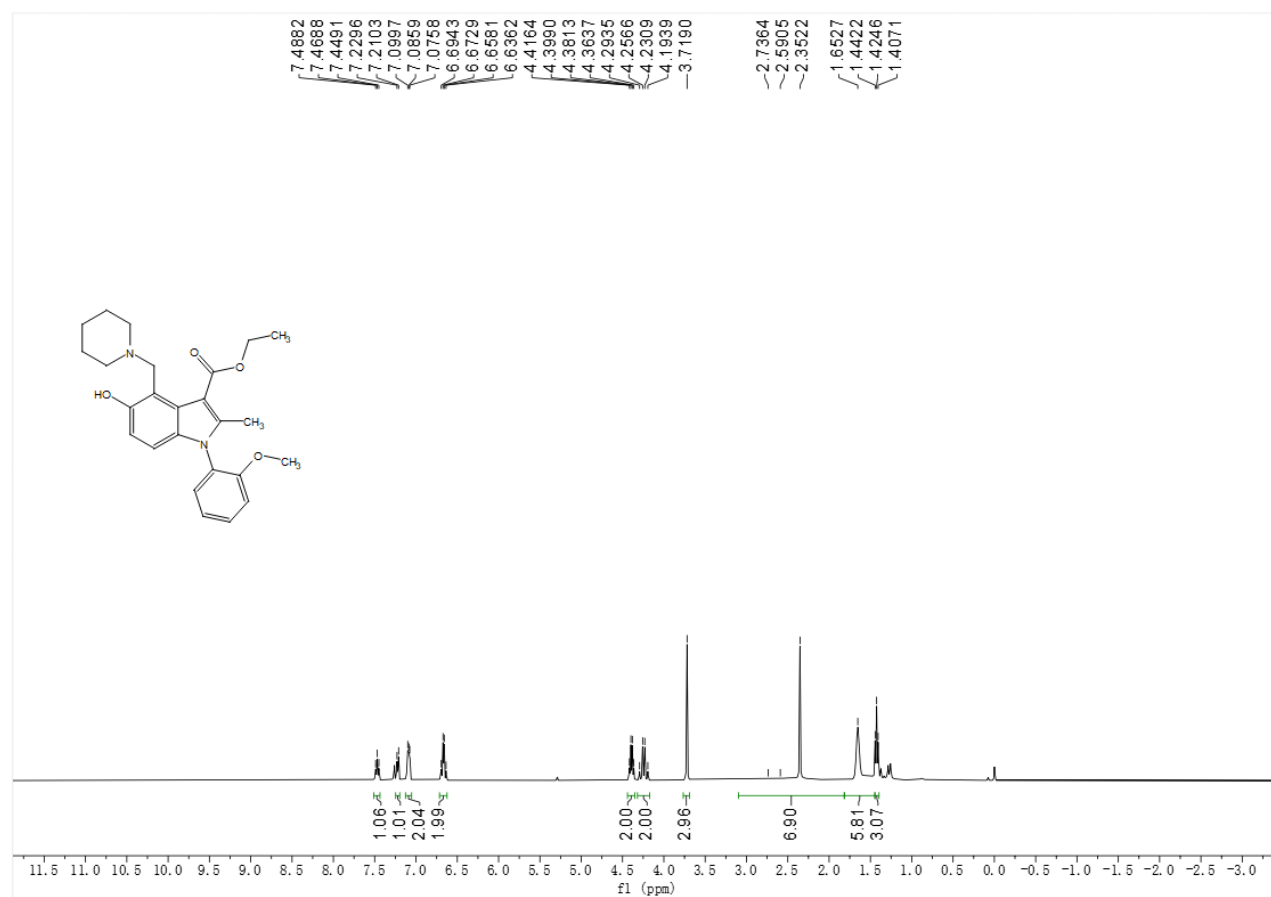


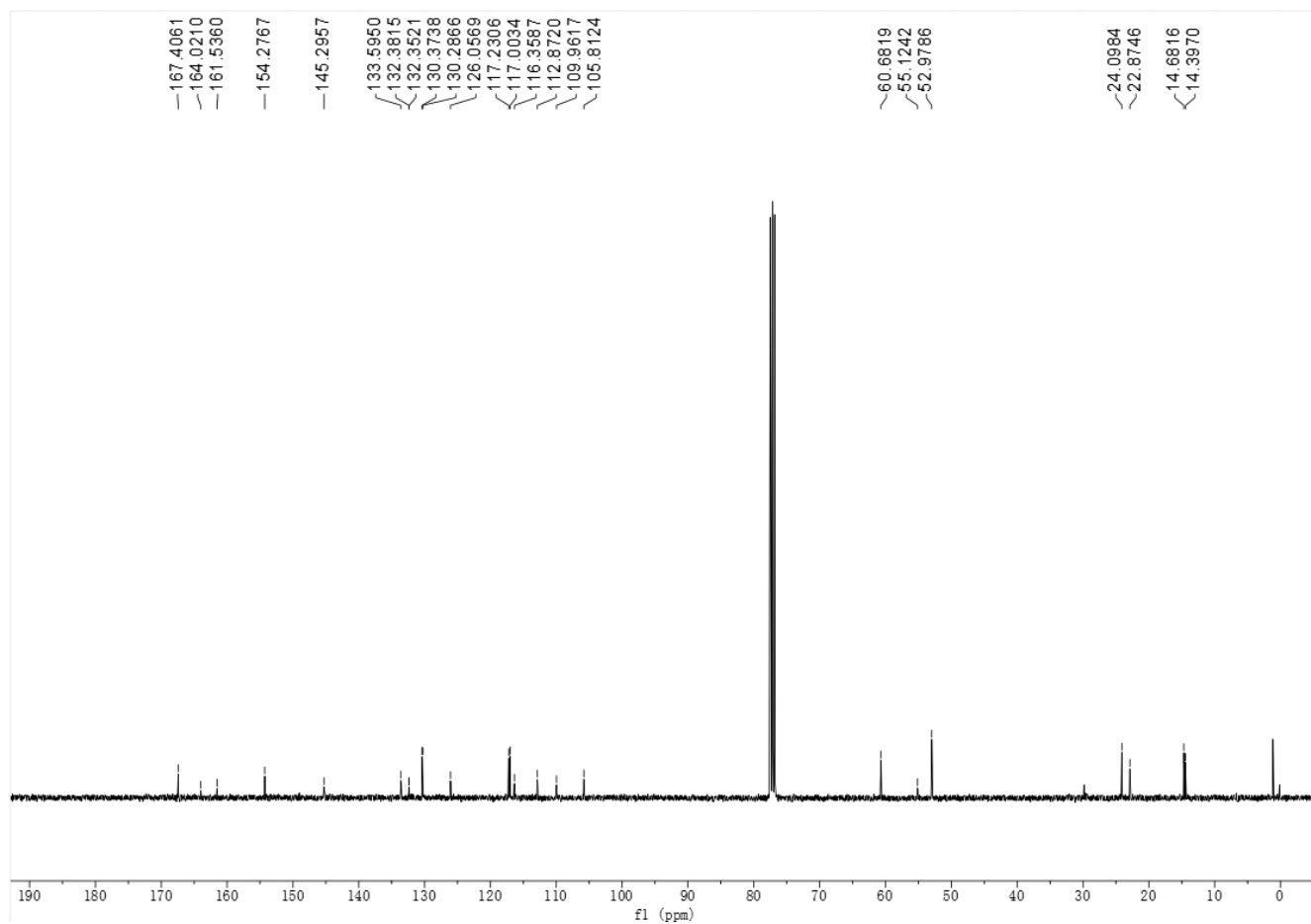
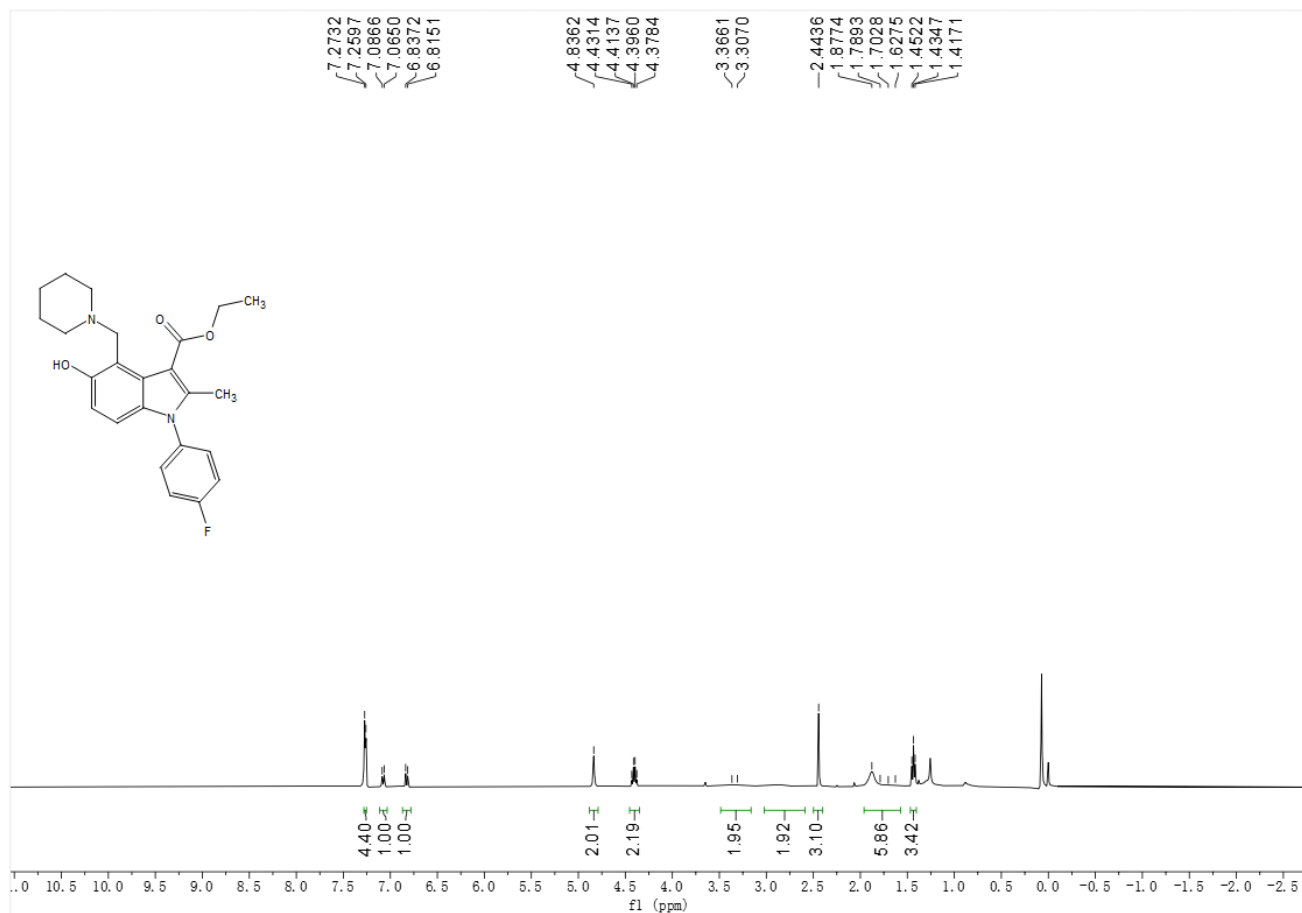


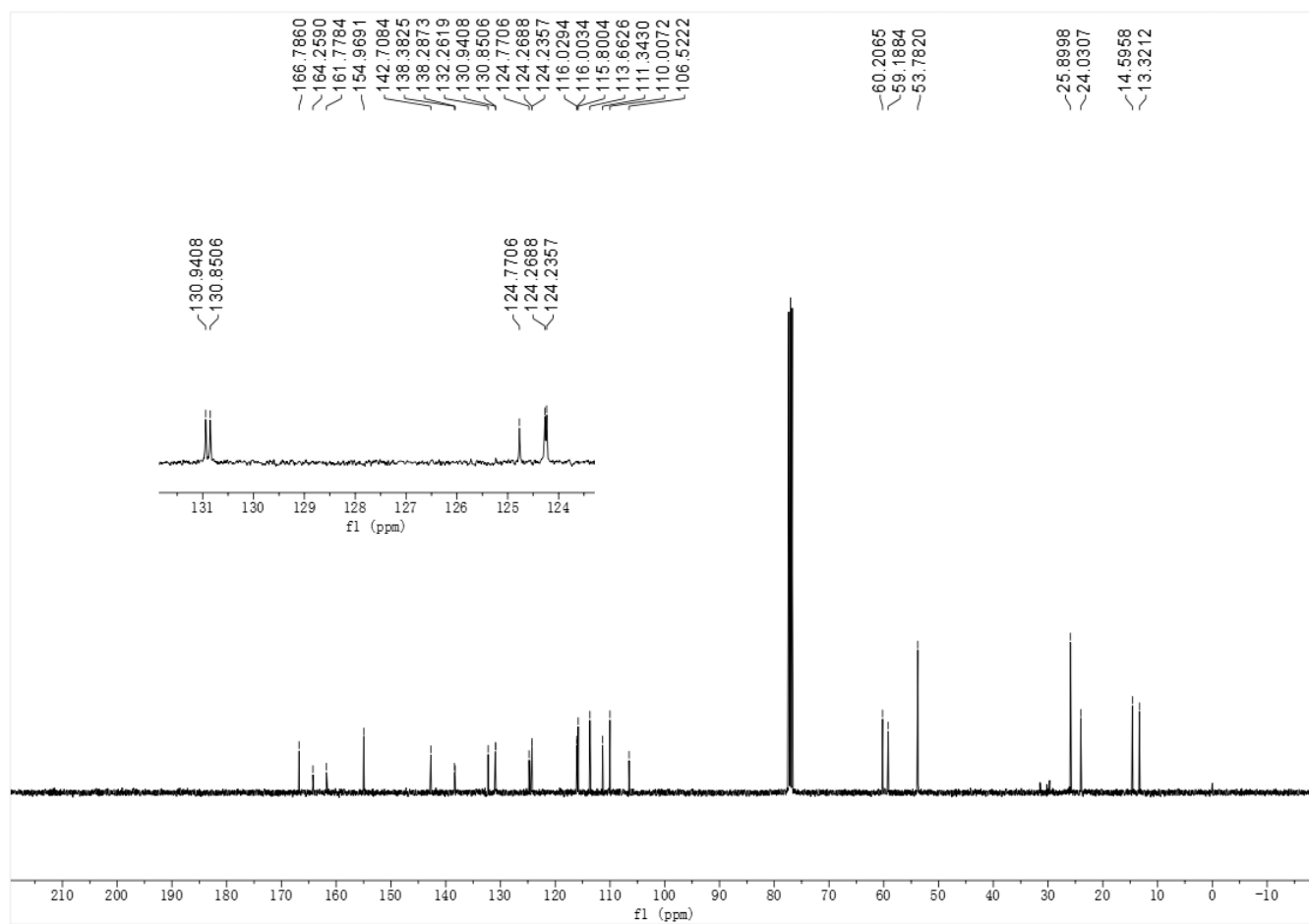
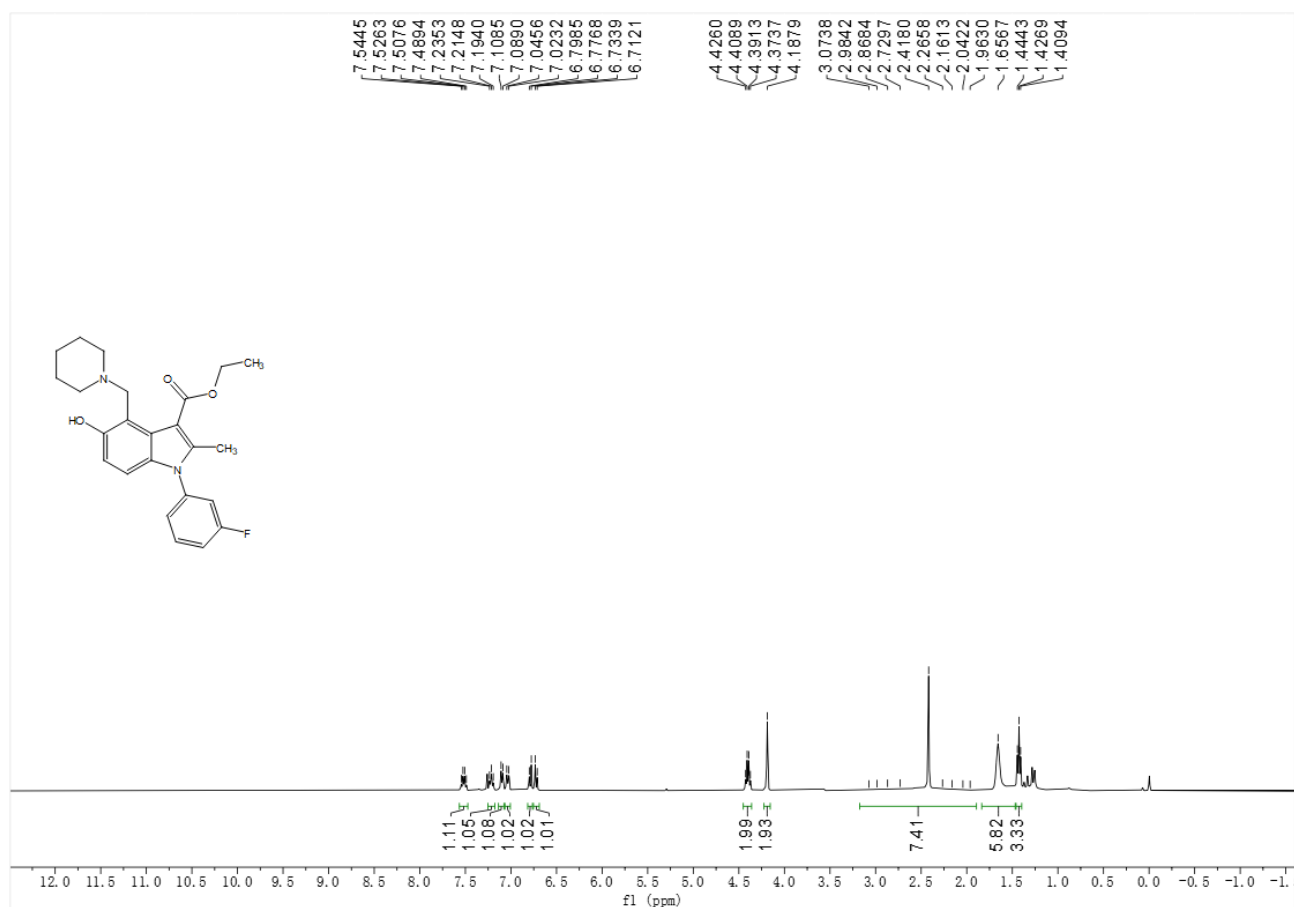


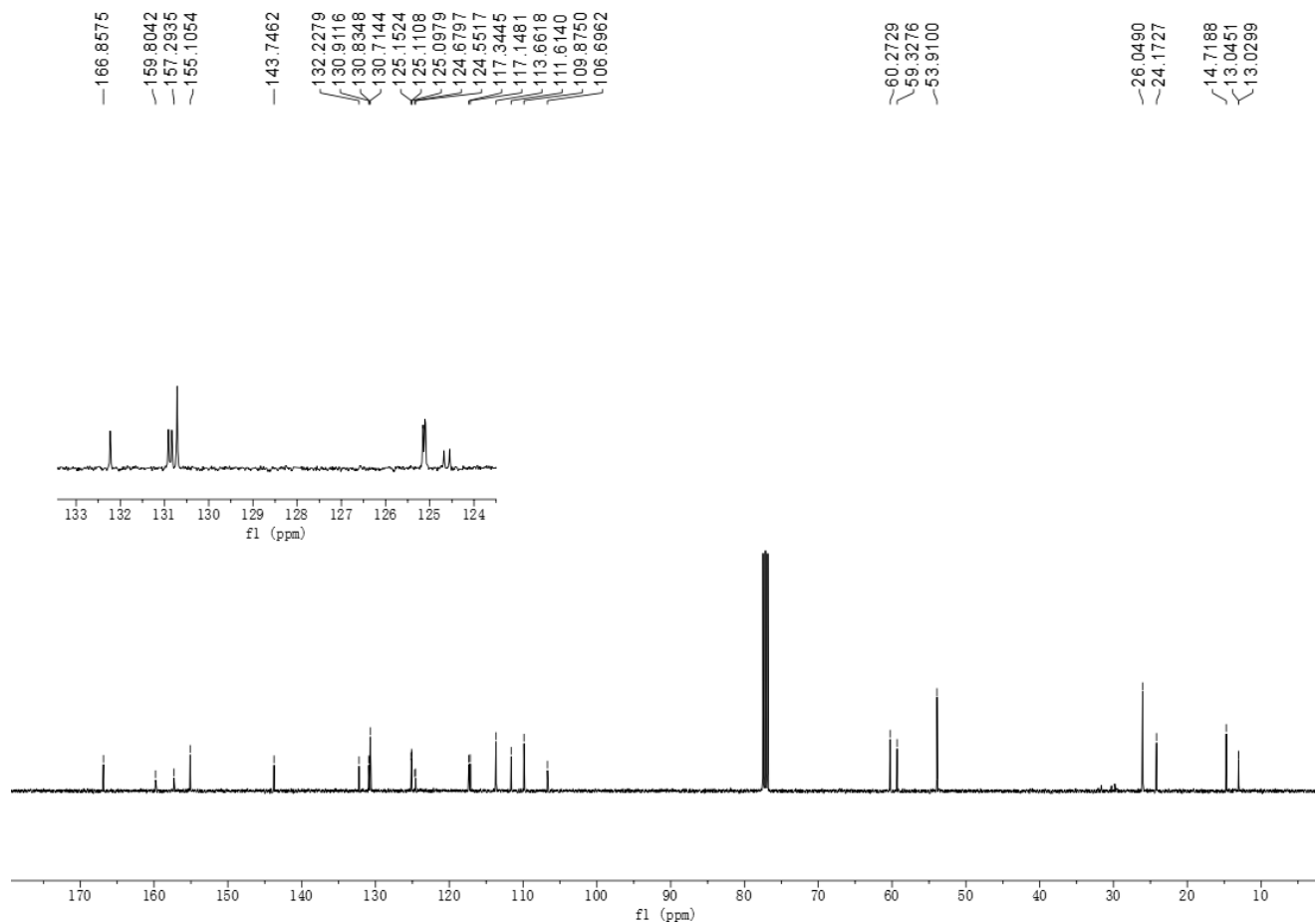
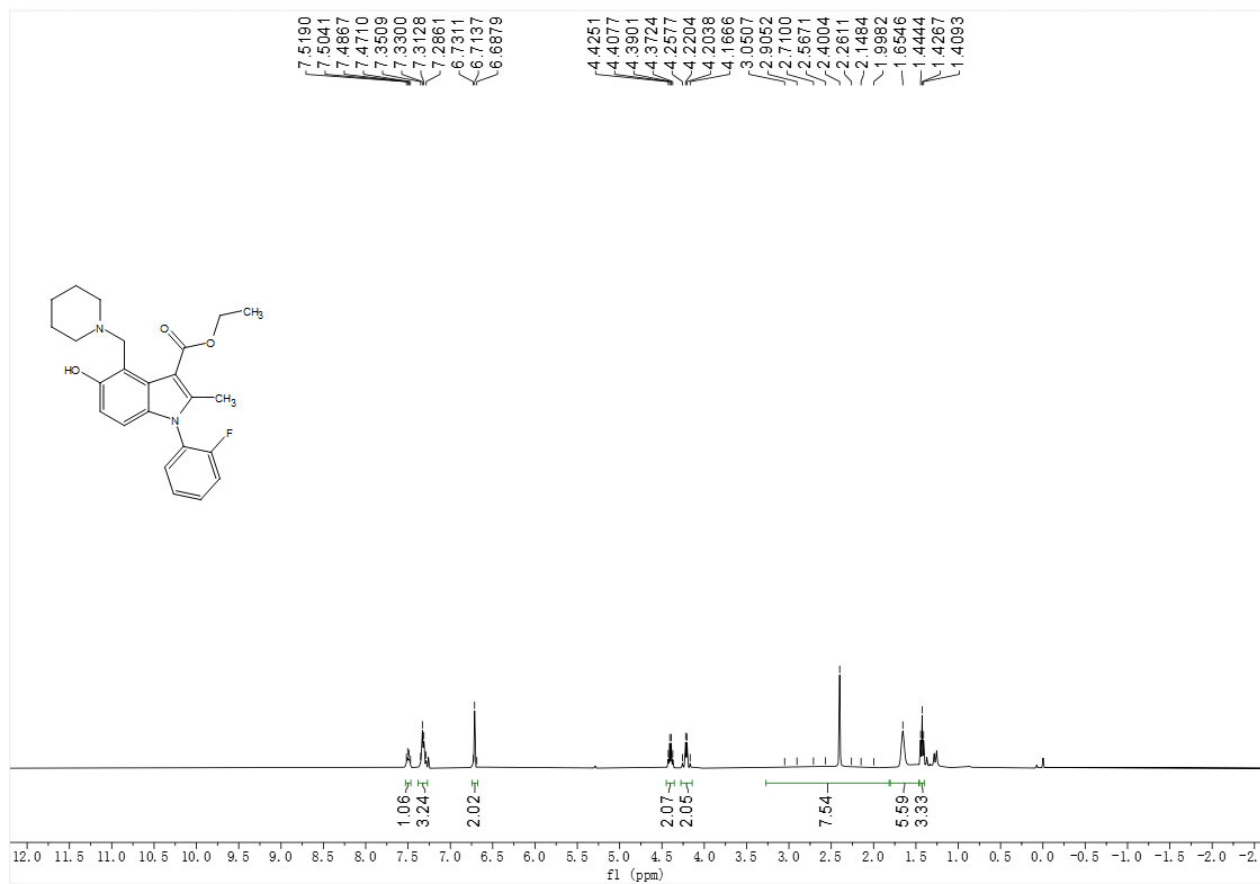


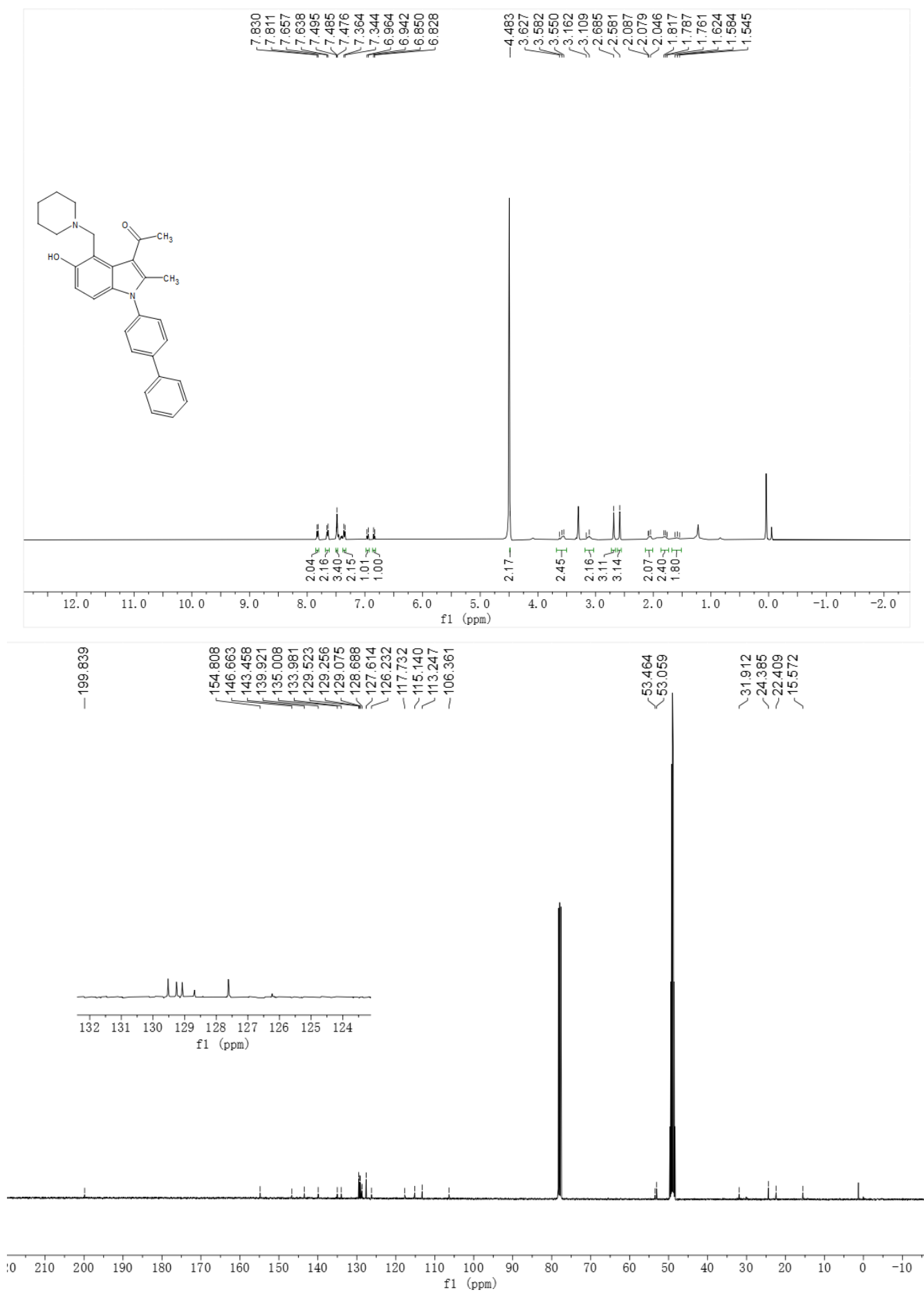


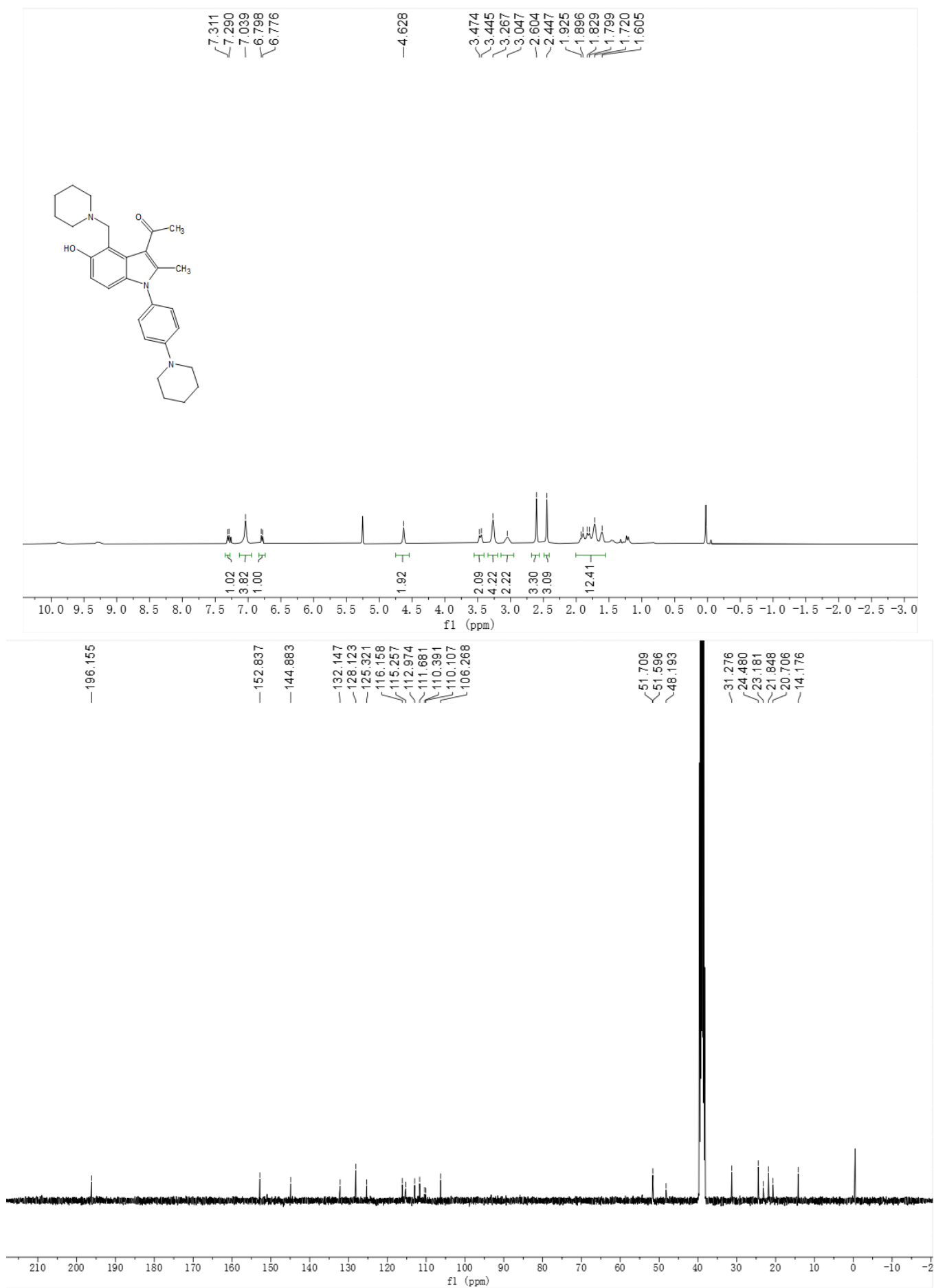


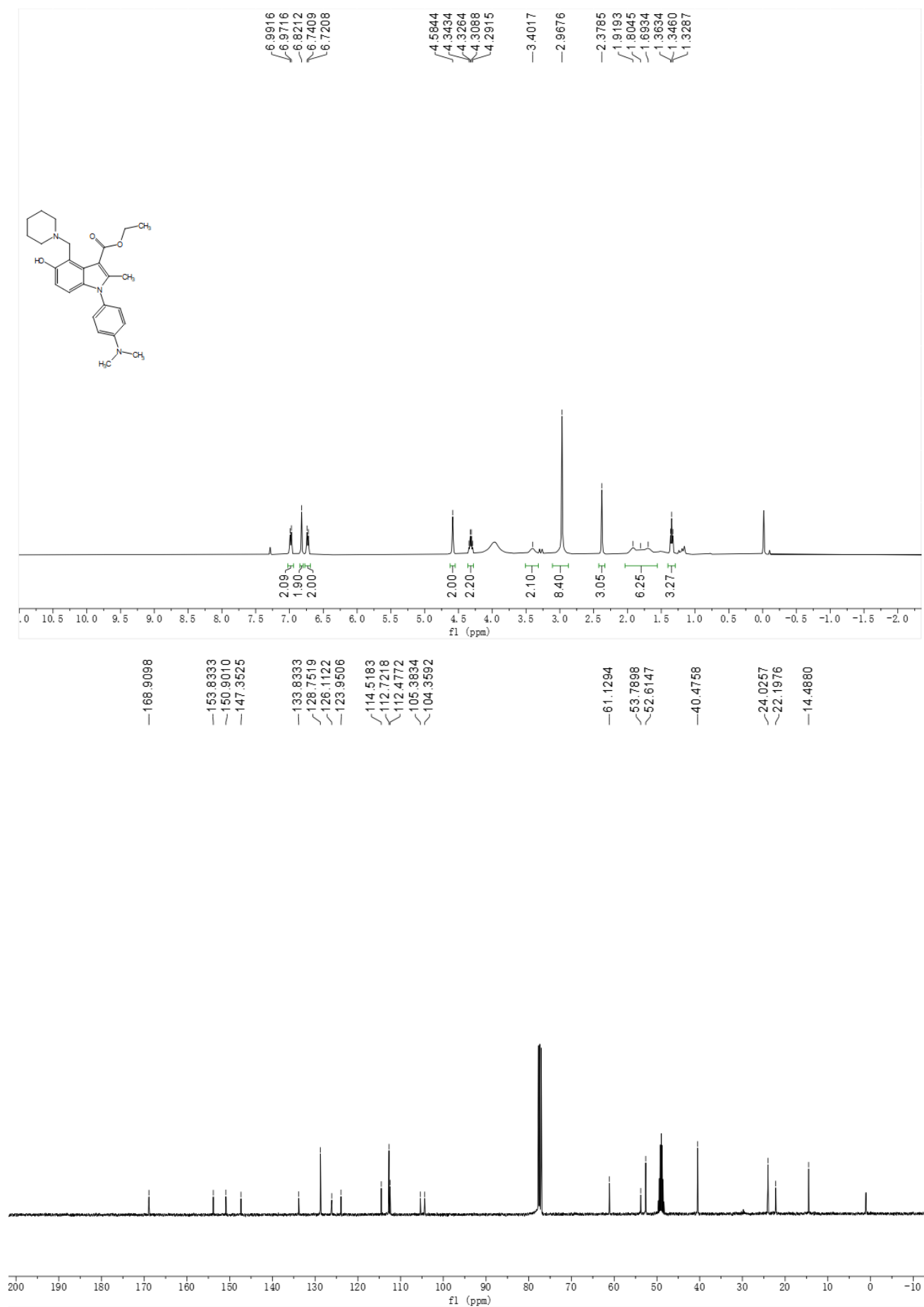


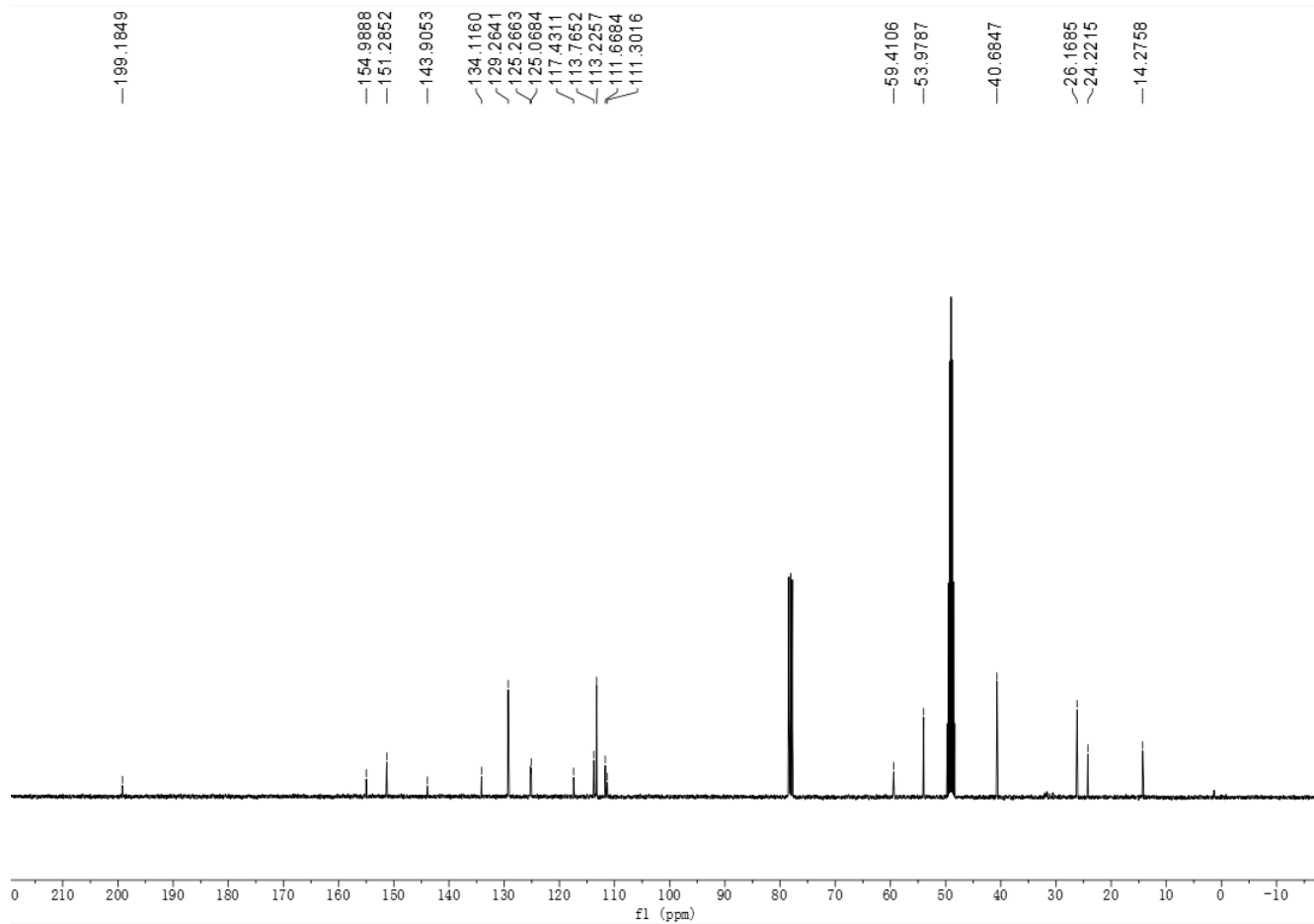
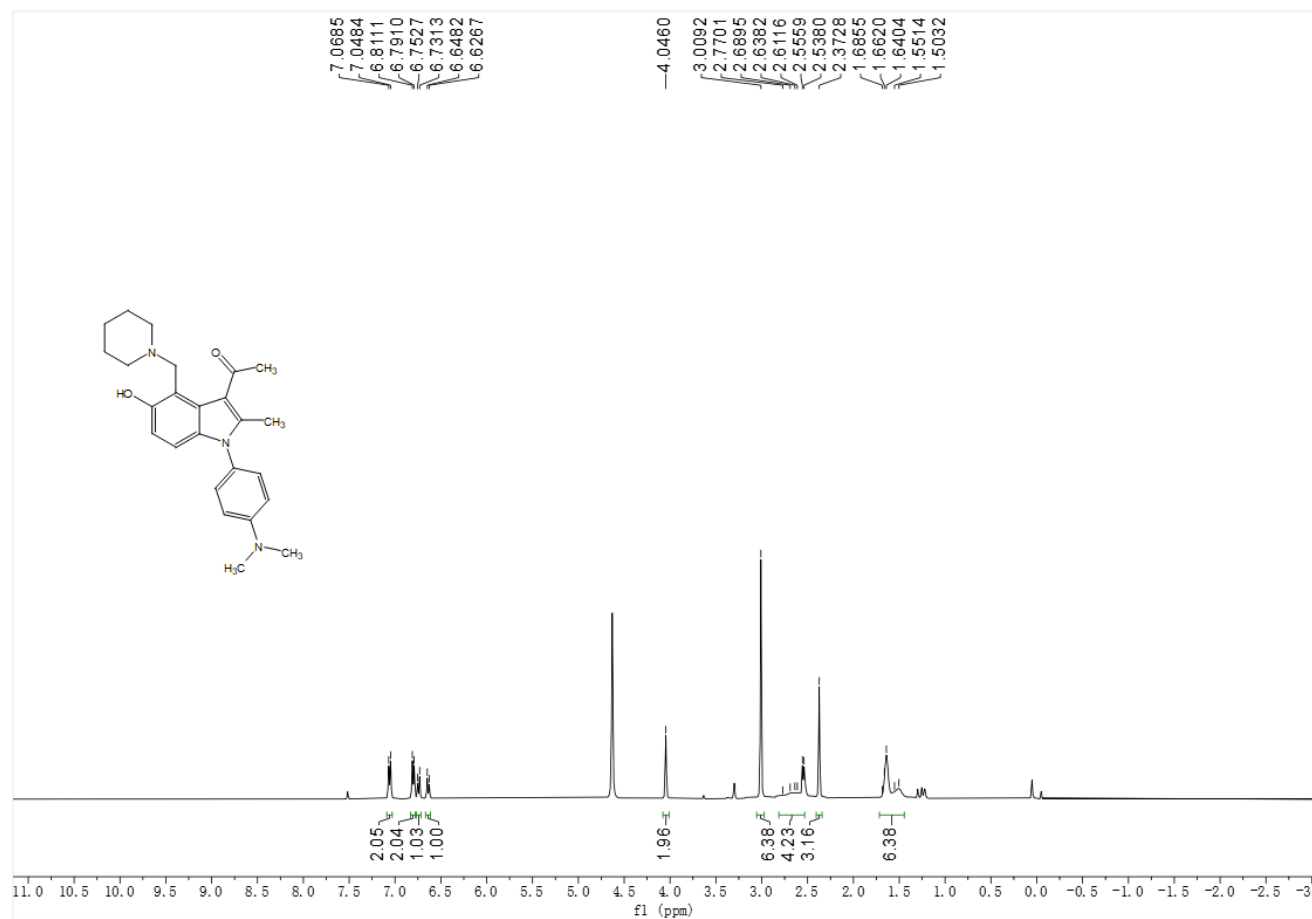




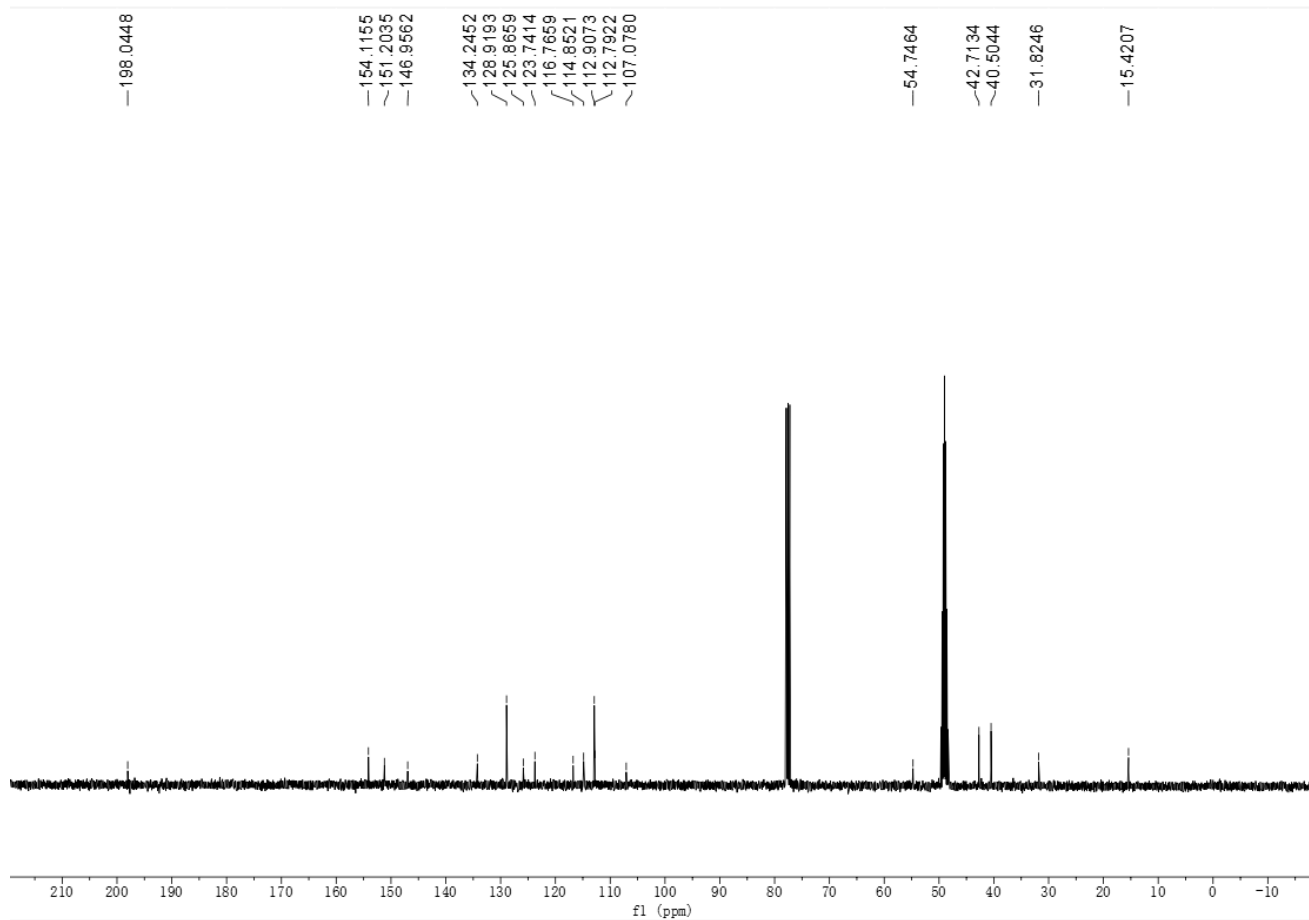
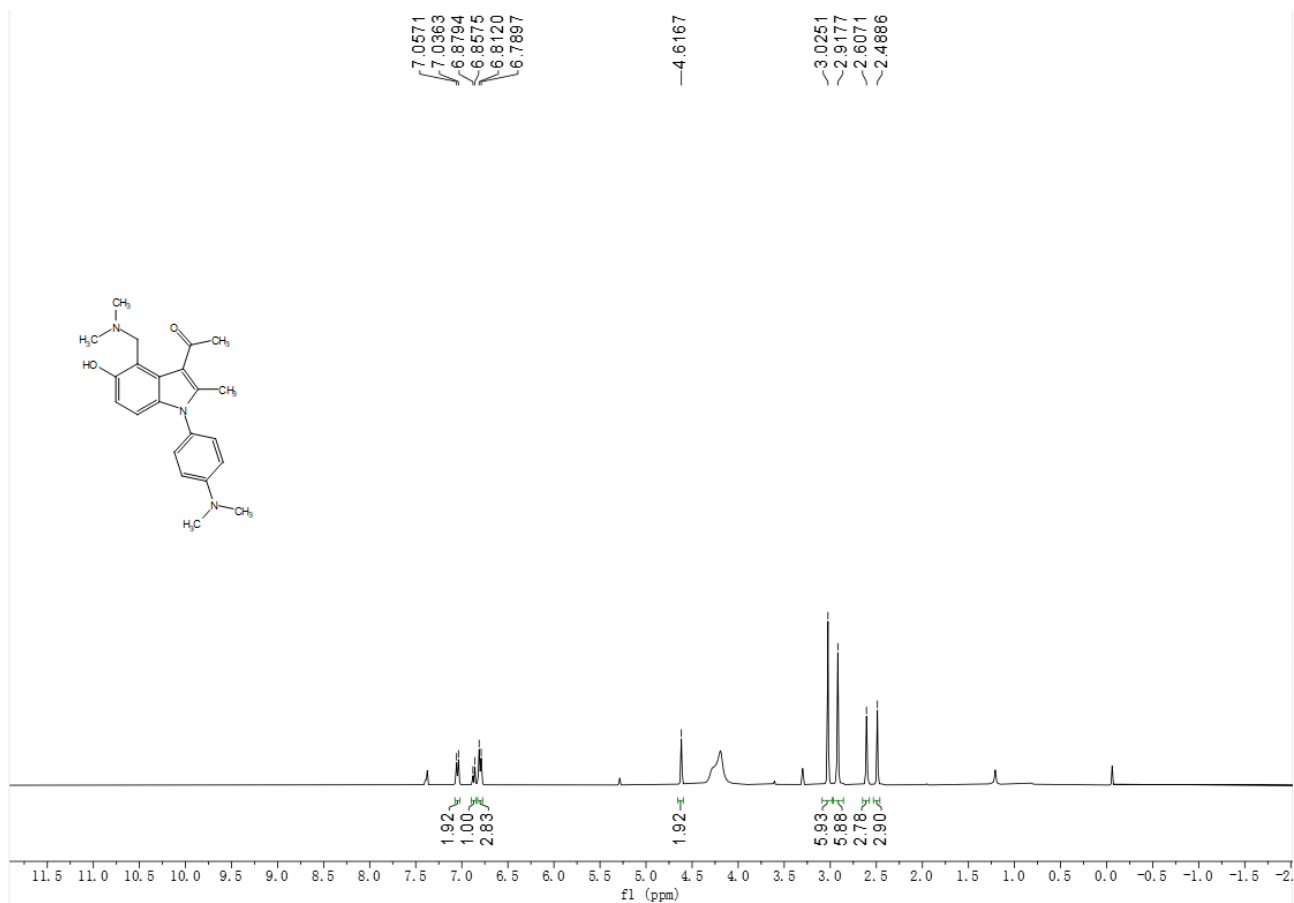


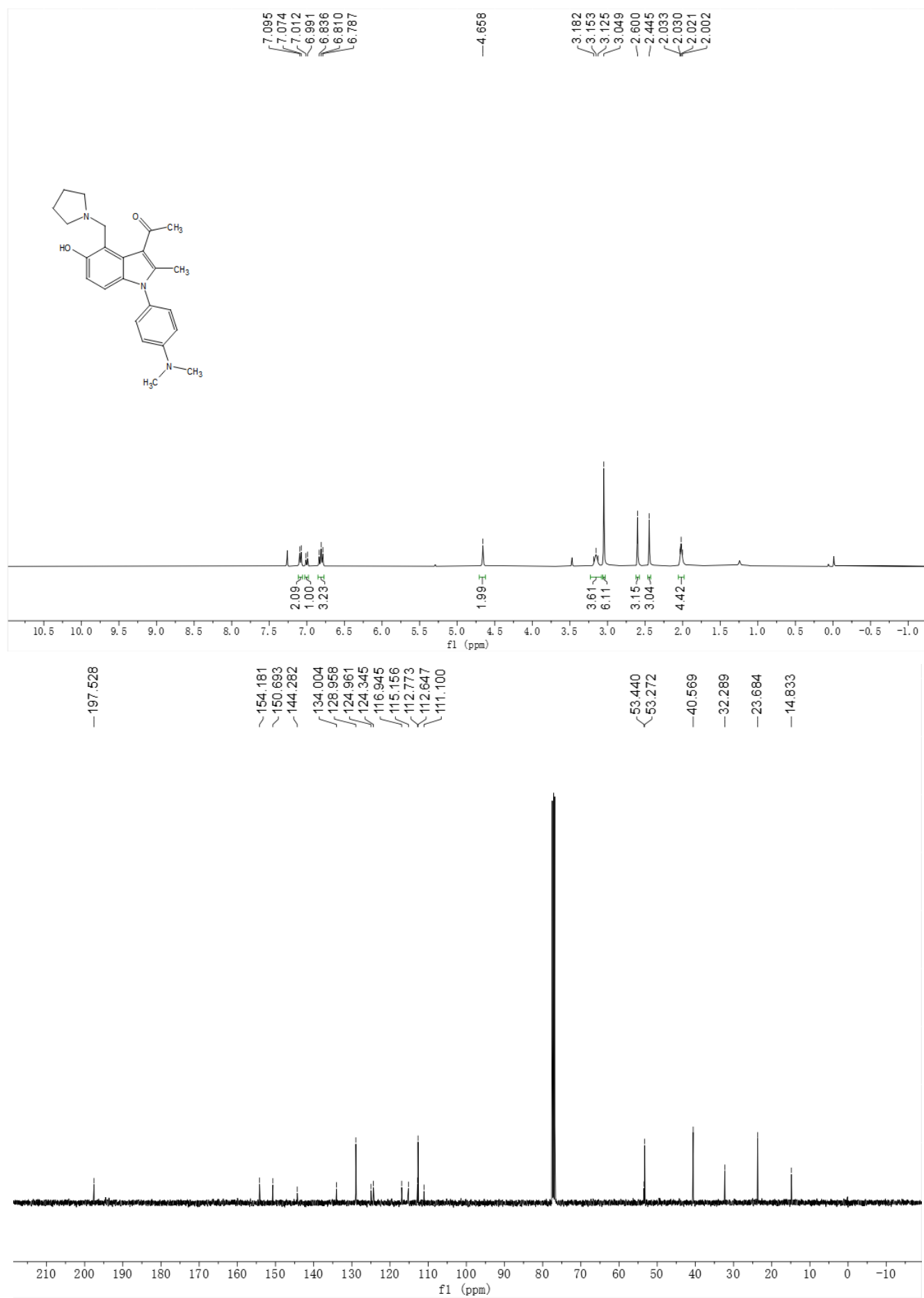


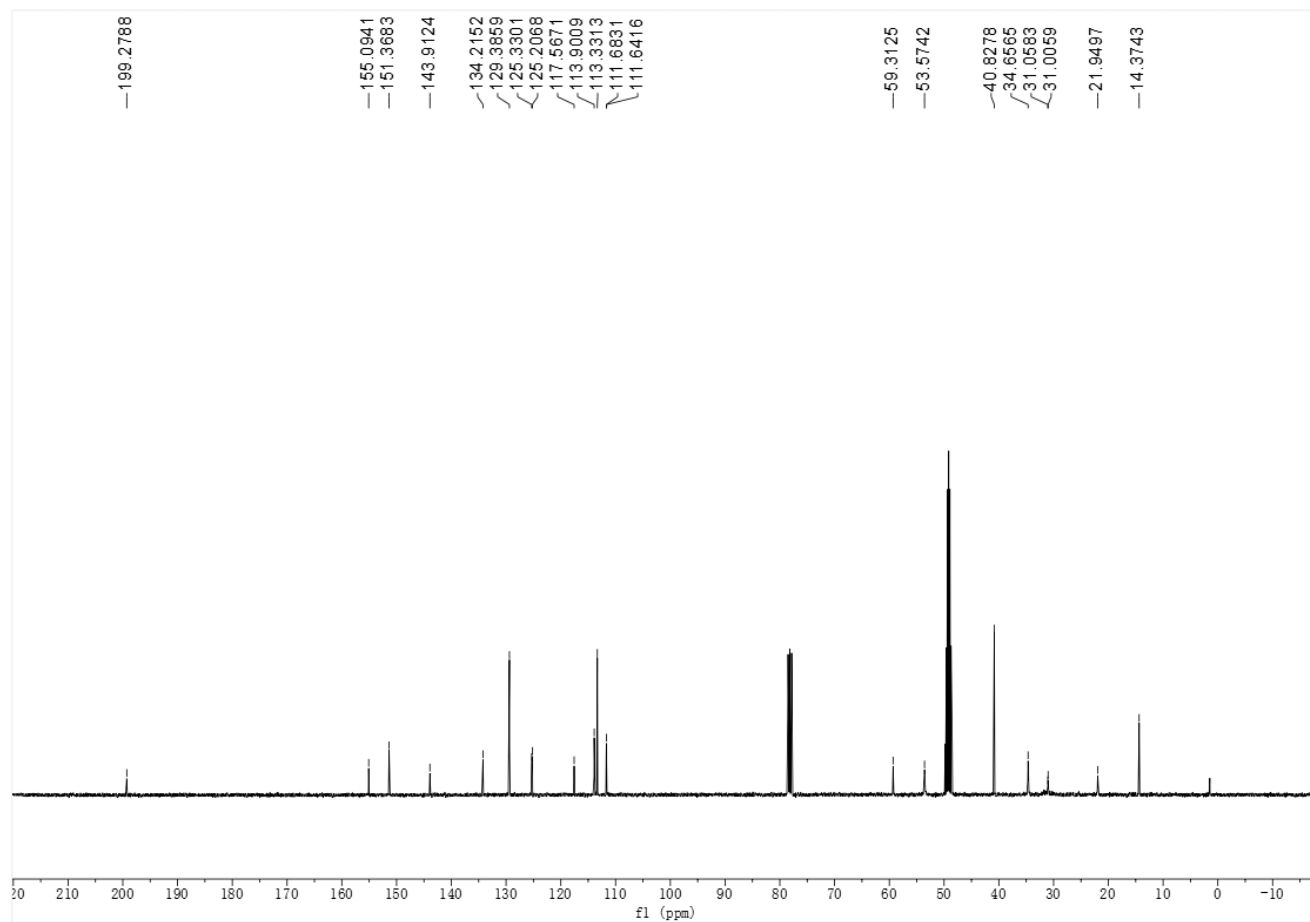
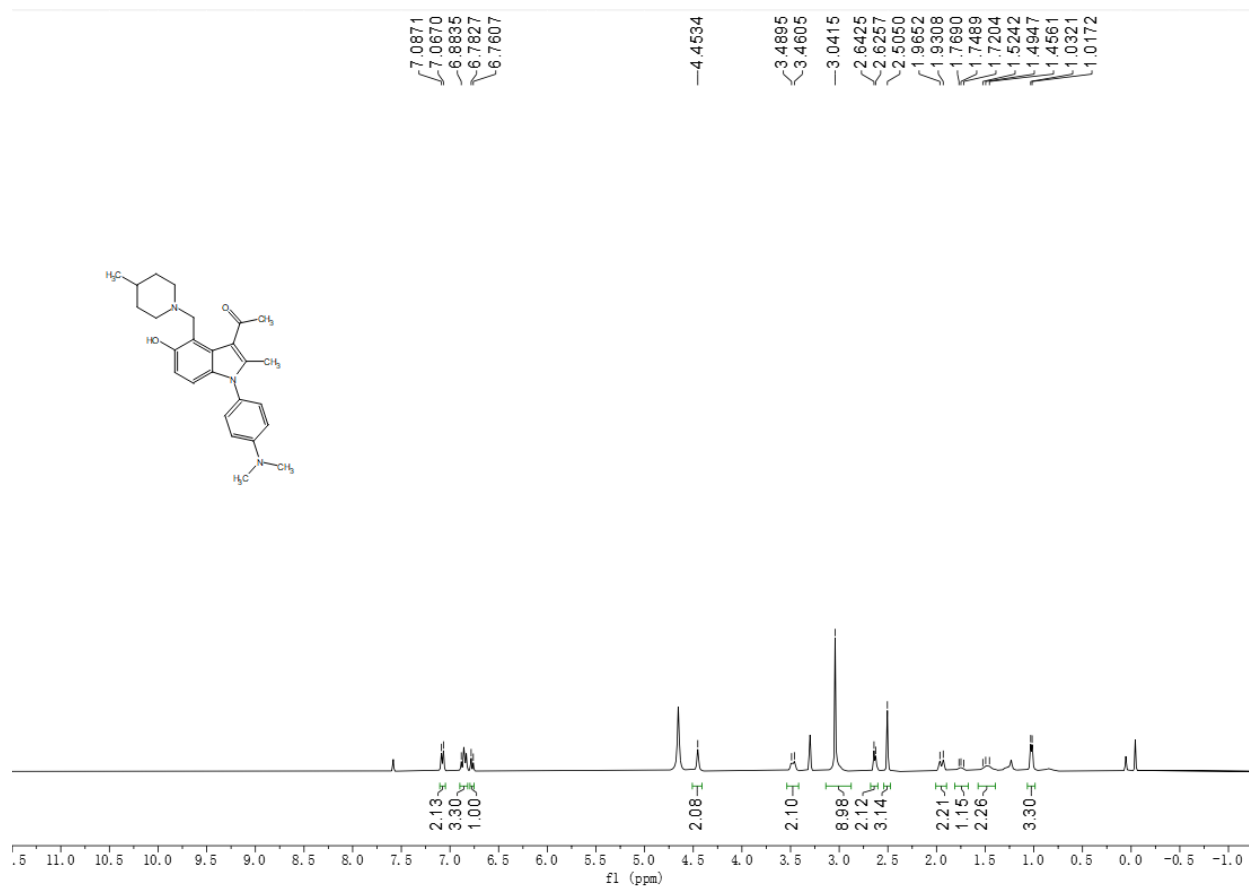


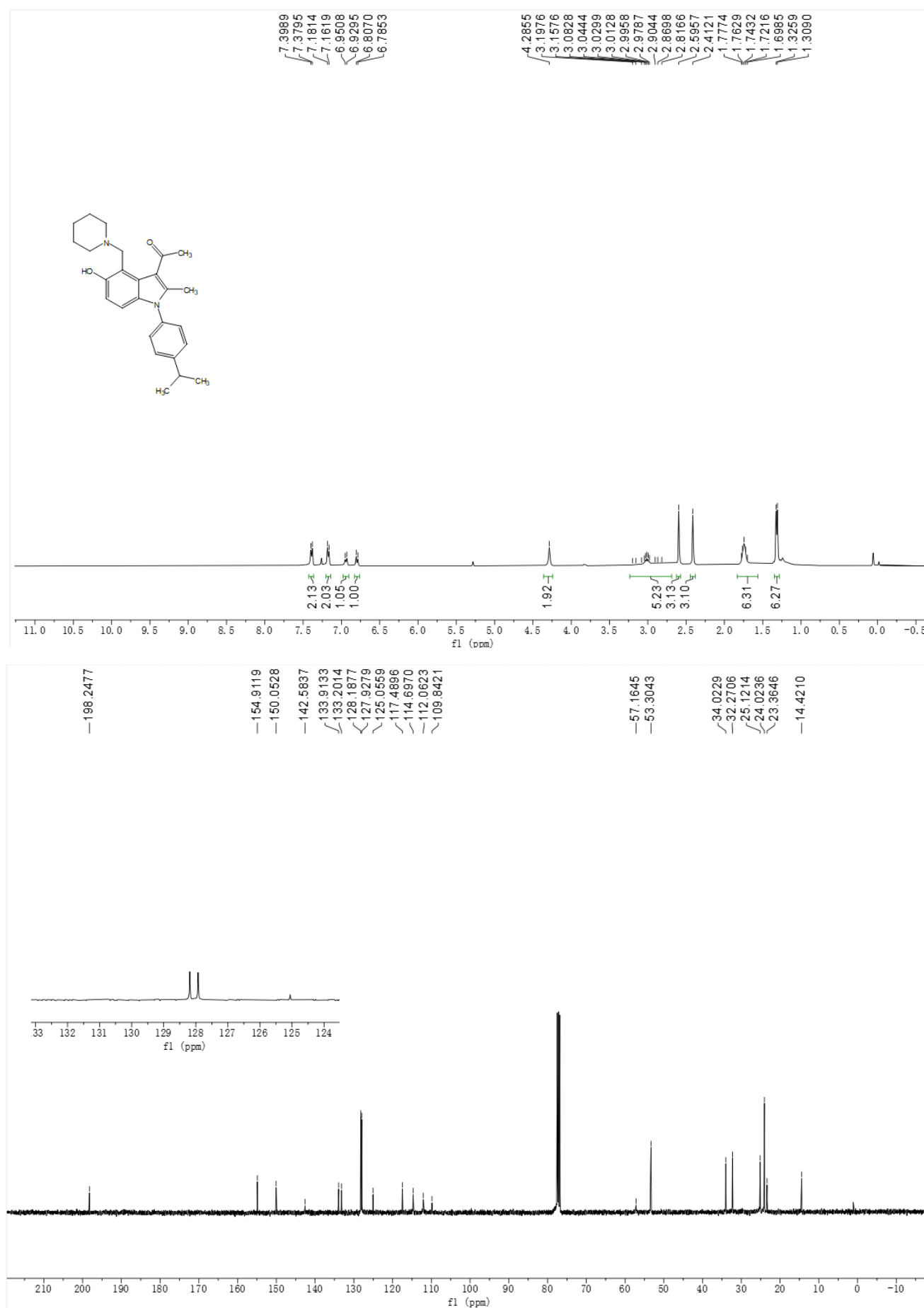


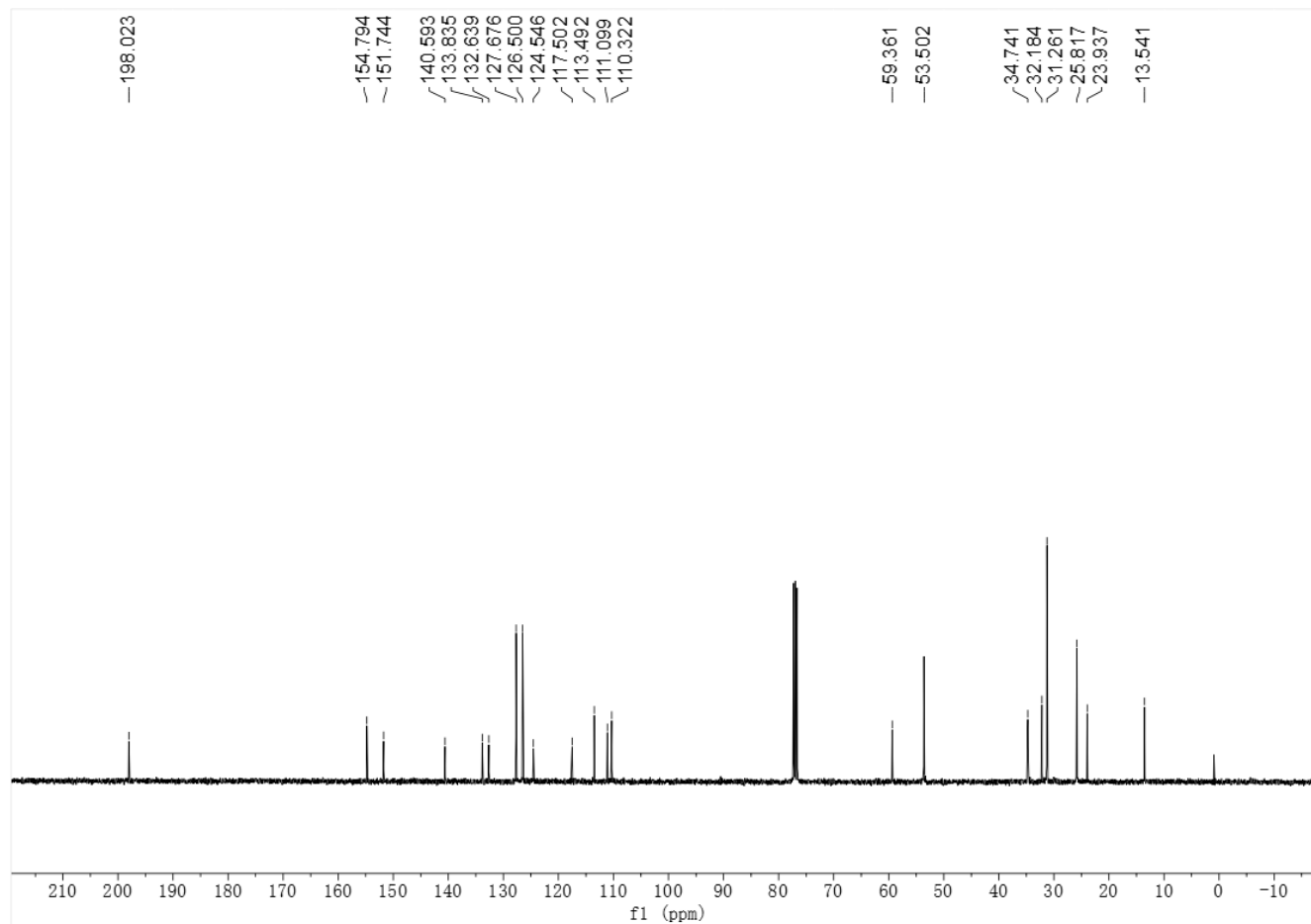
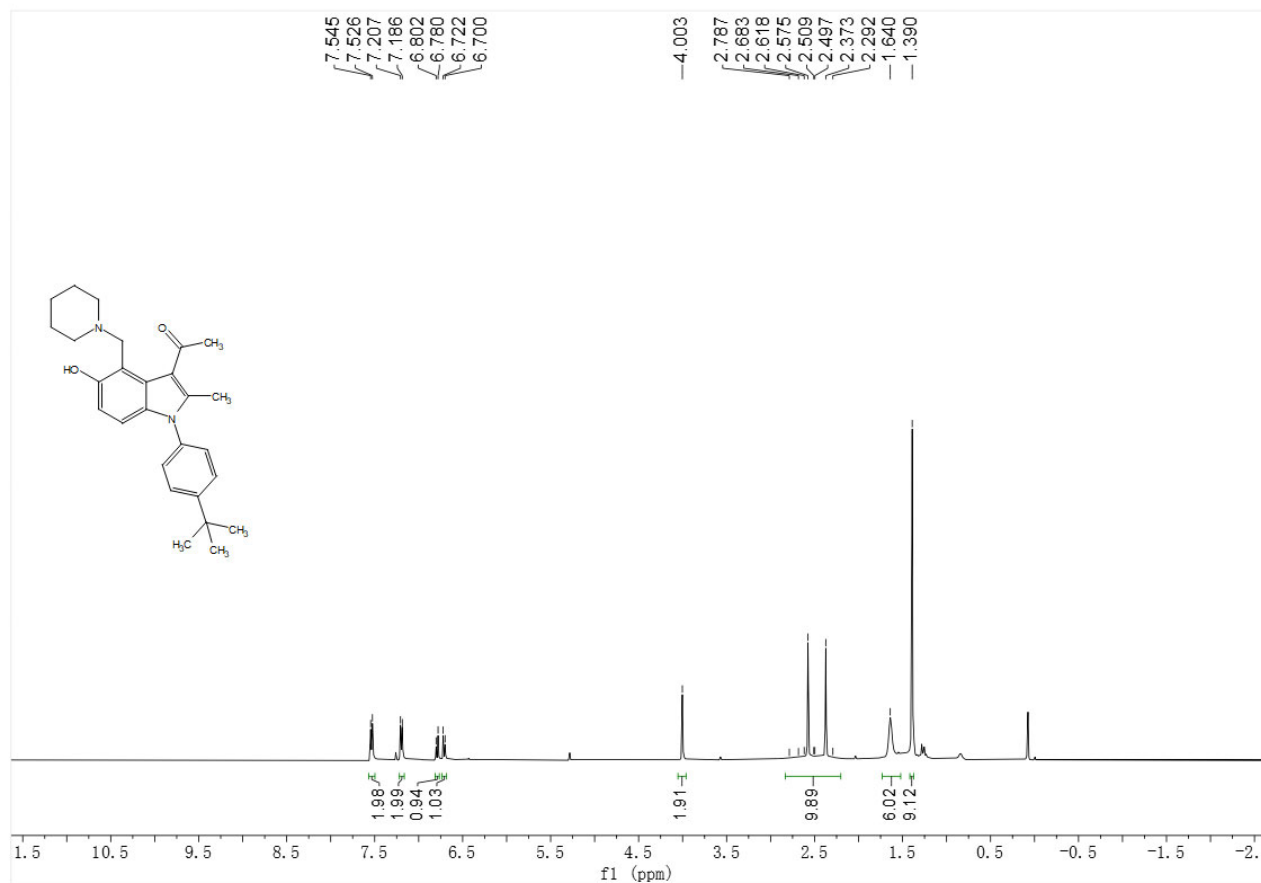
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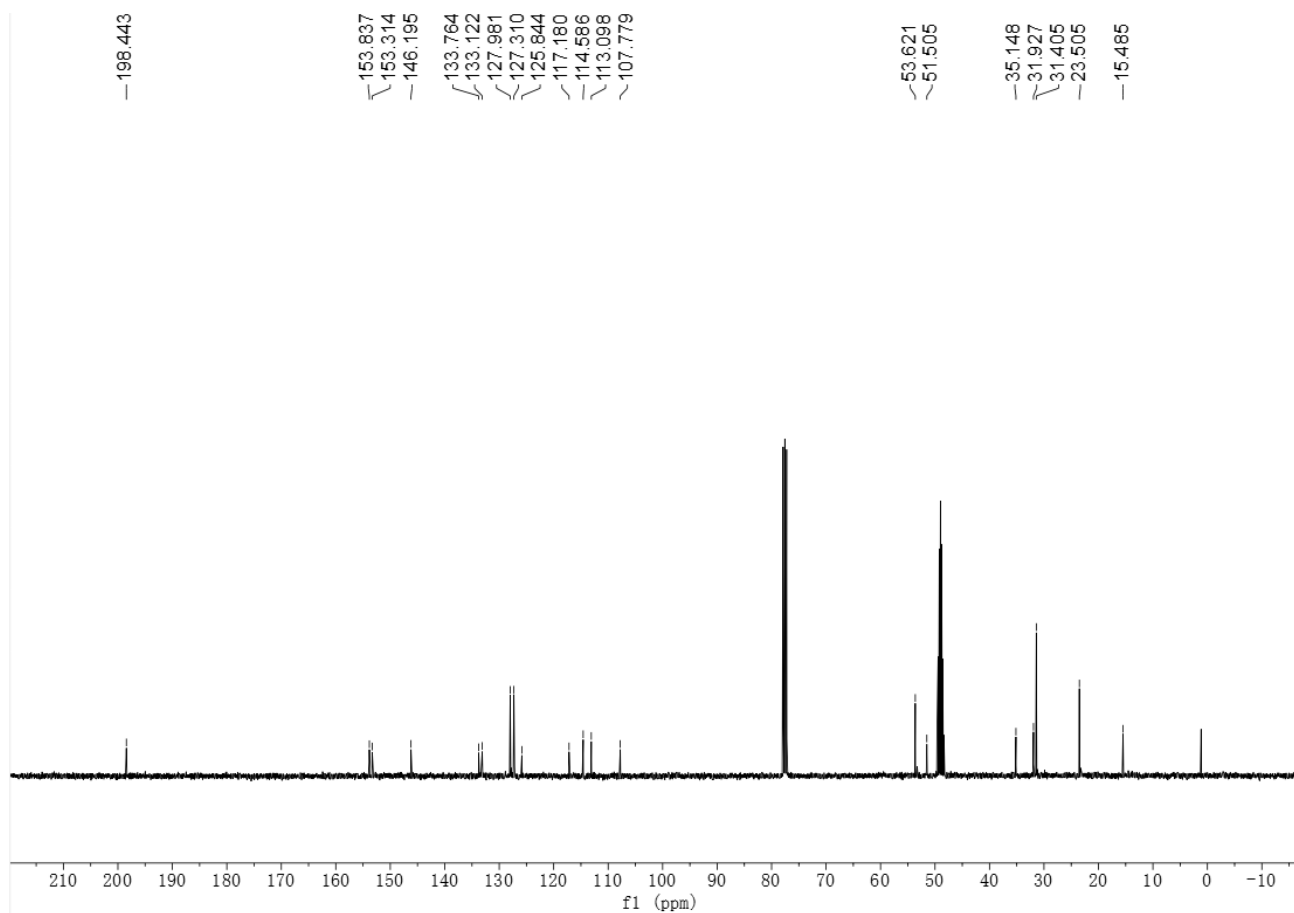
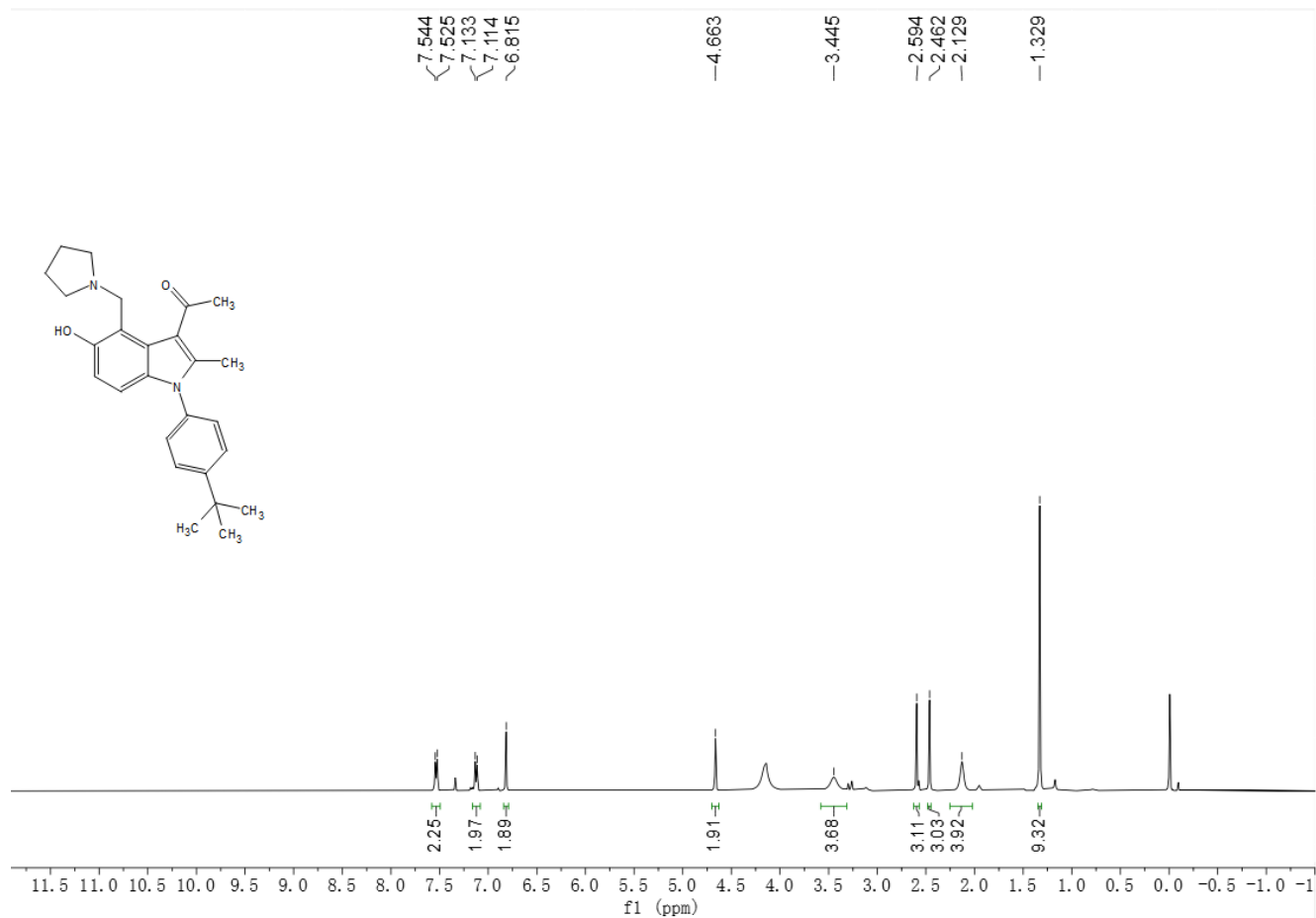


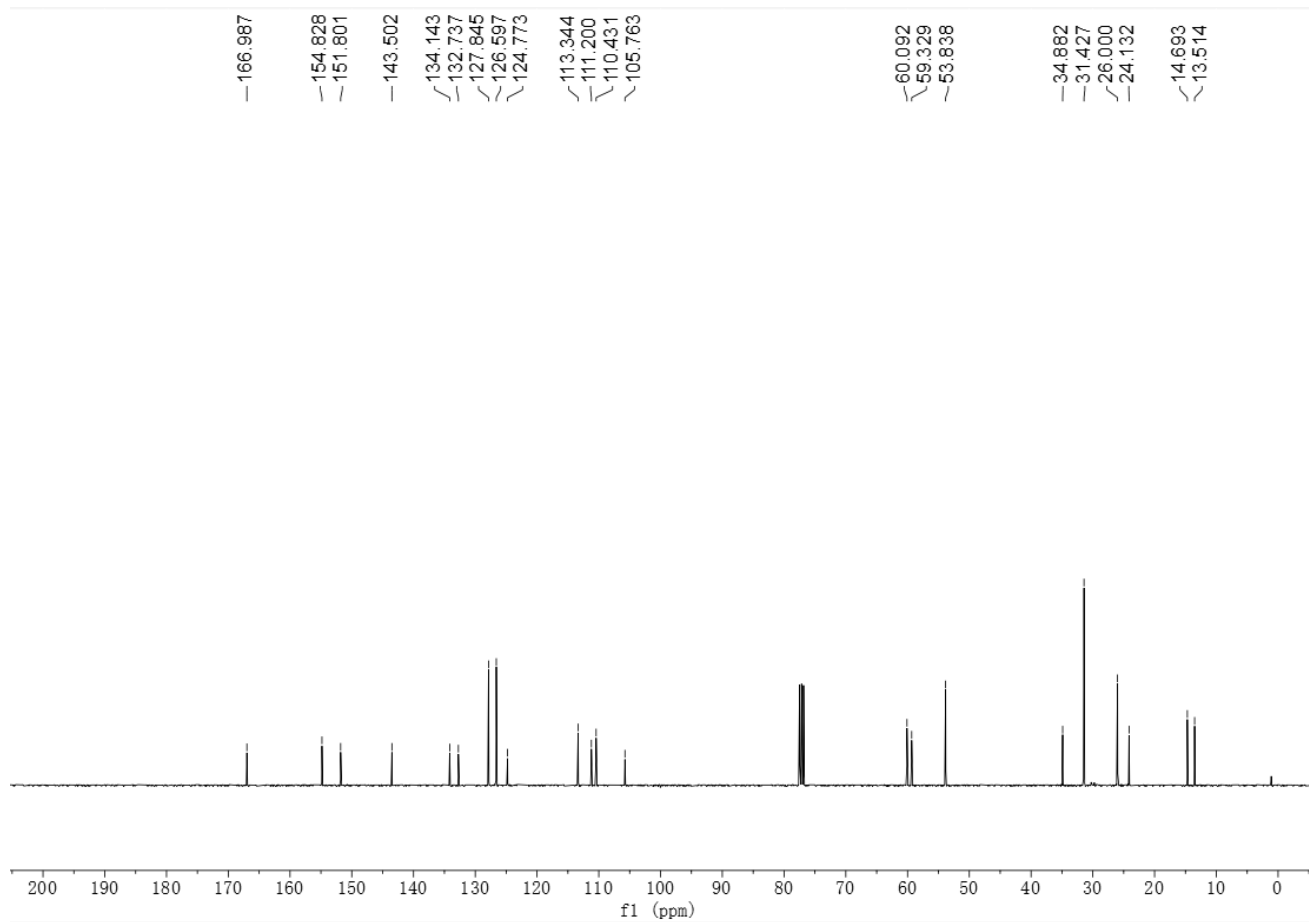
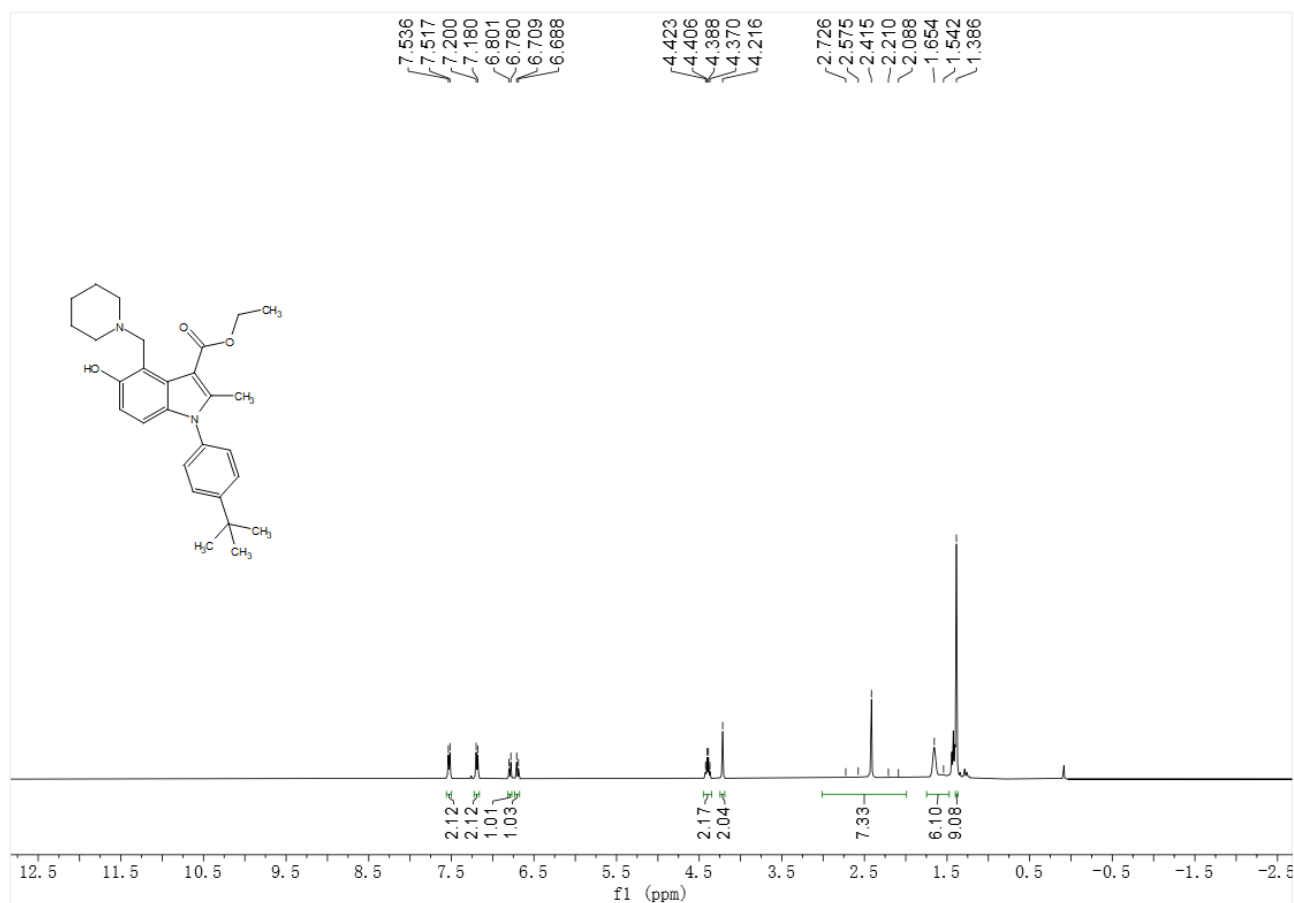












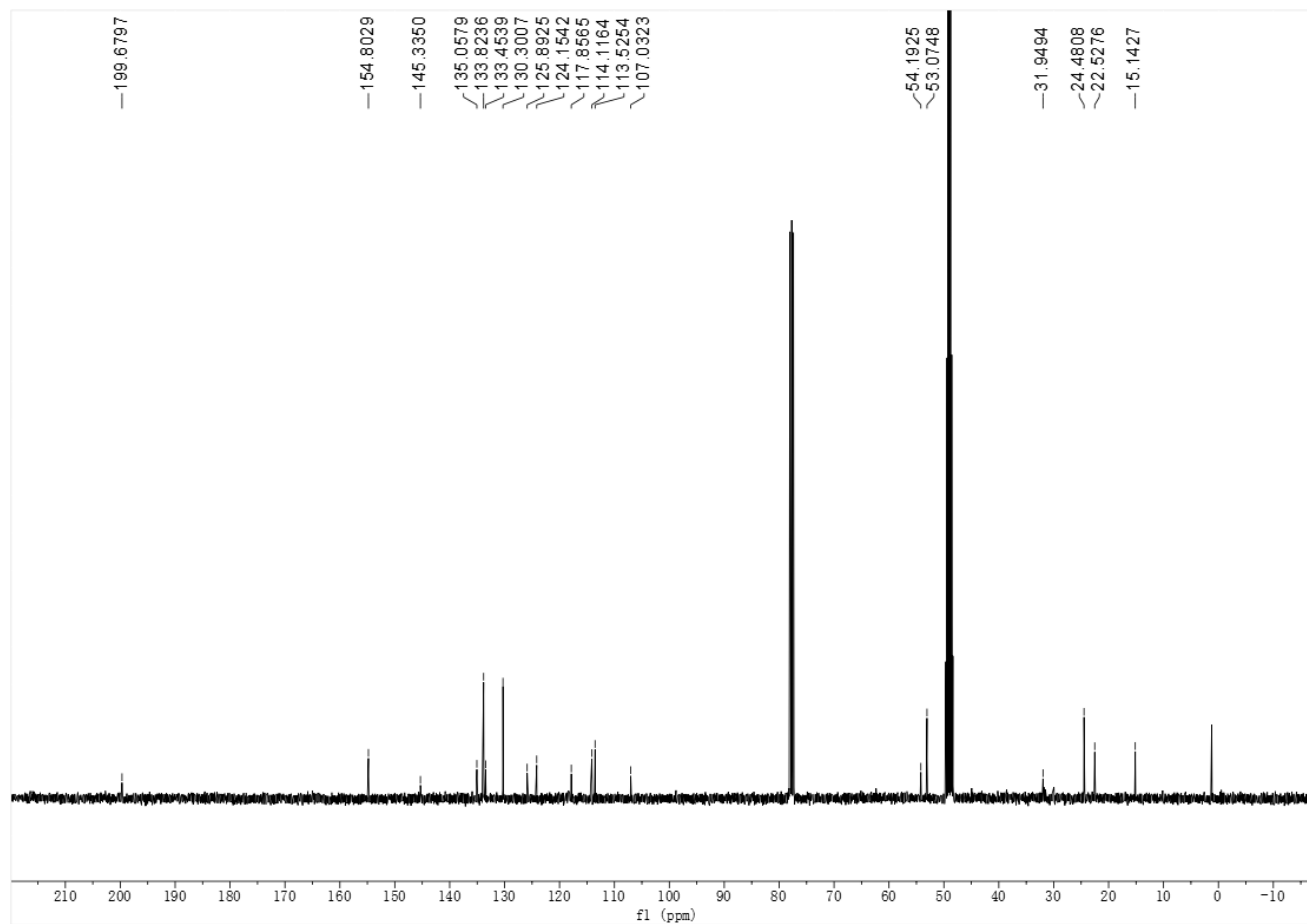
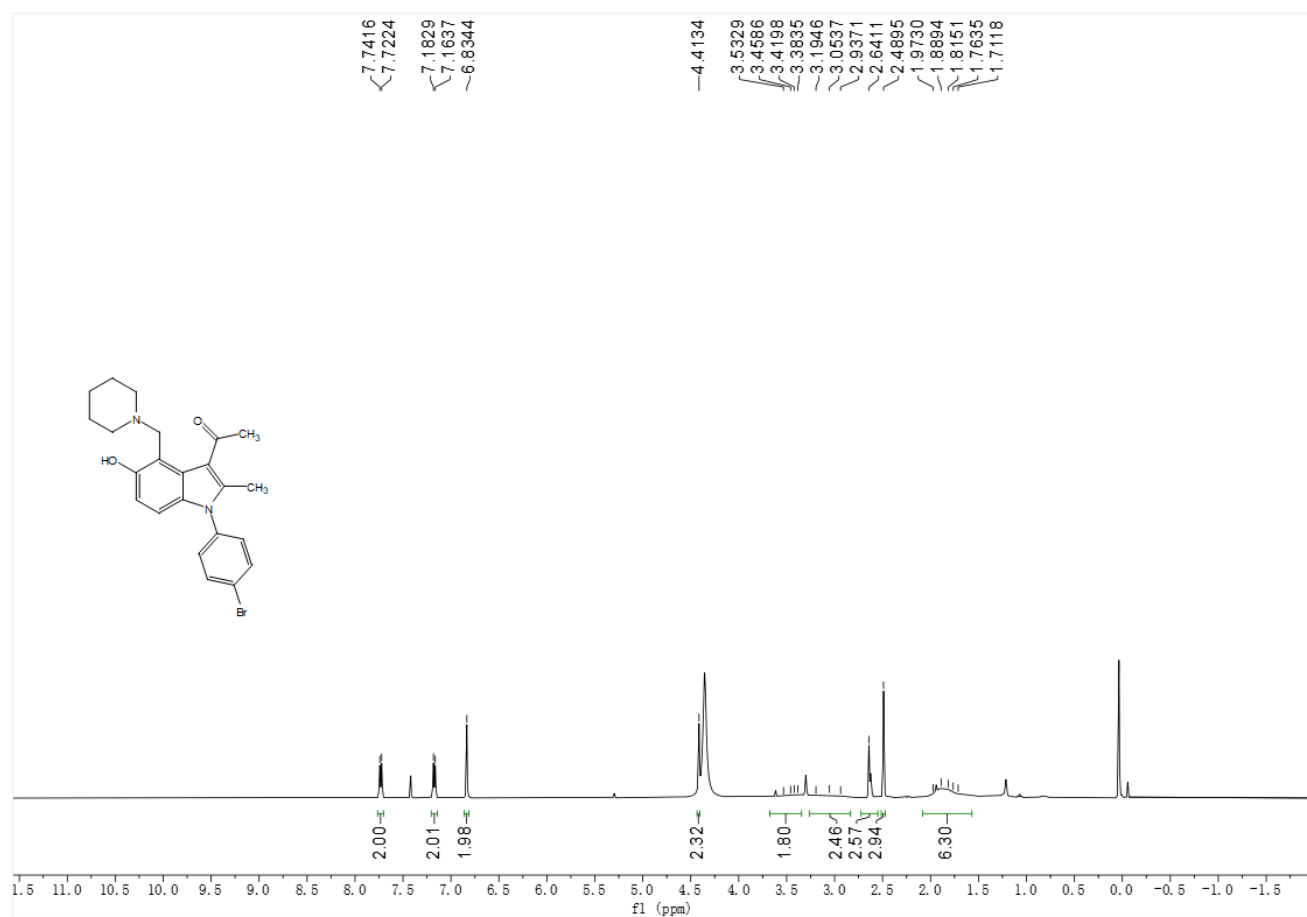


Table S1. Analytical HPLC purities of all final compounds.

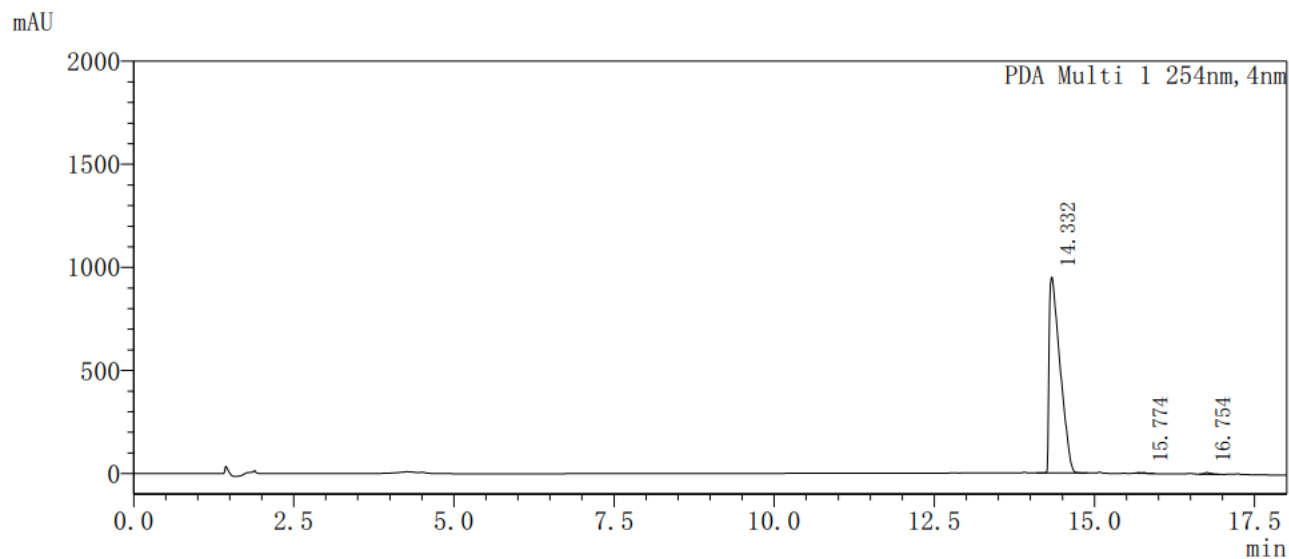
Compd	HPLC			Compd	HPLC		
	t _R (min)	Purity (%)			t _R (min)	Purity (%)	
		254(nm)	280(nm)			254(nm)	280(nm)
13	13.348	96.91	96.67	34	14.132	96.77	95.40
14	12.186	97.67	95.75	35	13.815	96.58	95.75
15	12.770	98.63	97.99	36	14.042	97.28	95.081
16	13.245	99.72	97.20	37	13.955	95.75	95.11
17	13.491	95.95	95.00	38	13.755	97.10	96.13
18	13.569	96.03	95.18	39	13.090	99.29	96.92
19	14.350	97.72	96.62	45	14.322	99.31	98.40
20	13.476	96.91	97.12	48	12.877	97.20	95.81
22	14.535	96.57	95.73	49	14.355	97.01	95.87
23	13.946	96.28	95.36	50	13.253	95.38	95.01
24	12.590	99.30	97.46	51	12.306	97.35	96.93
25	13.035	98.26	95.60	52	13.004	95.01	95.01
28	14.049	98.29	96.17	53	13.829	97.11	96.82
29	12.981	98.71	95.06	54	14.206	95.66	95.86
30	13.090	99.29	96.92	55	14.447	98.82	95.27
31	14.411	97.64	96.59	56	14.721	99.23	97.33
32	14.057	97.91	96.55	57	15.108	99.64	99.64
33	13.989	99.26	98.21	58	13.557	99.50	98.44

HPLC purity determination for the target compounds

Method. Flow rate = 1.0 mL/min; gradient elution over 18 minutes, from 10% ACN-H₂O to 95% ACN-H₂O with 0.5%

HCOOH, 280 nm, 254 nm; InertSustain-C18 column (5 µm 4.6×250 mm).

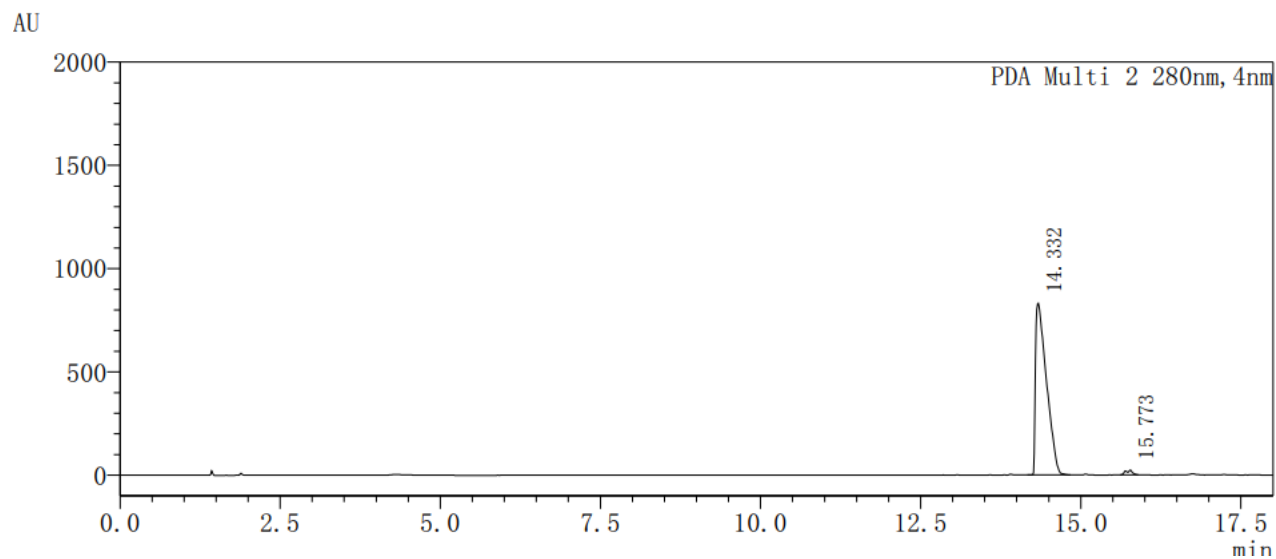
HPLC Traces for **45** (UV=254 nm)



Peak Table

Peak	Ret. time (min)	Area	Area (%)
1	14.332	11279122	99.310
2	15.774	26585	0.234
3	16.754	51781	0.456

HPLC Traces for **45** (UV=280 nm),



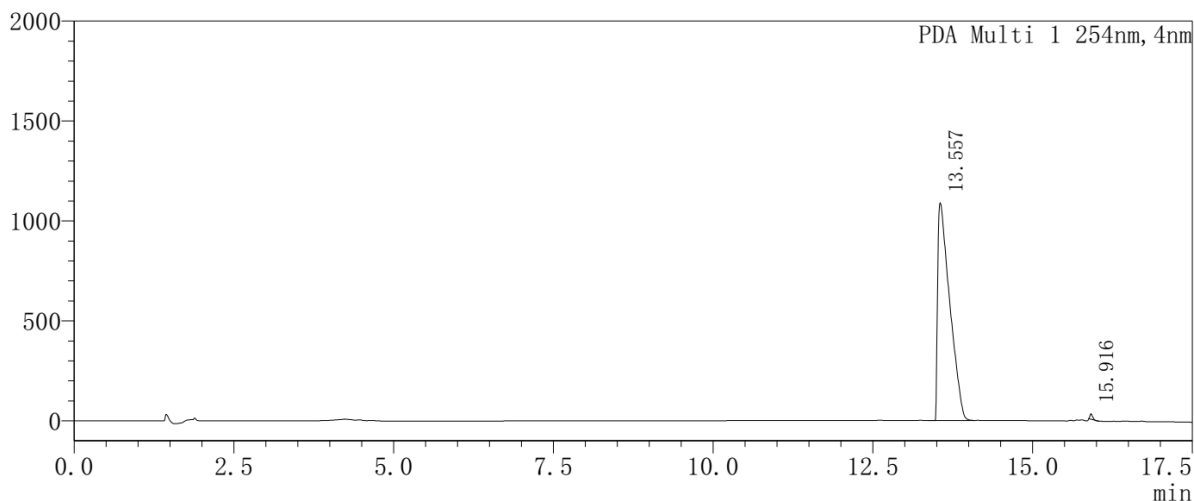
Peak Table

Peak	Ret. time (min)	Area	Area (%)
1	14.332	9946552	98.397
2	15.774	162088	1.603

Method. Flow rate = 1.0 mL/min; gradient elution over 18 minutes, from 10% ACN-H₂O to 95% ACN-H₂O with 0.5% HCOOH, 280 nm, 254 nm;

InertSustain-C18 column (5 μ m 4.6×250 mm).

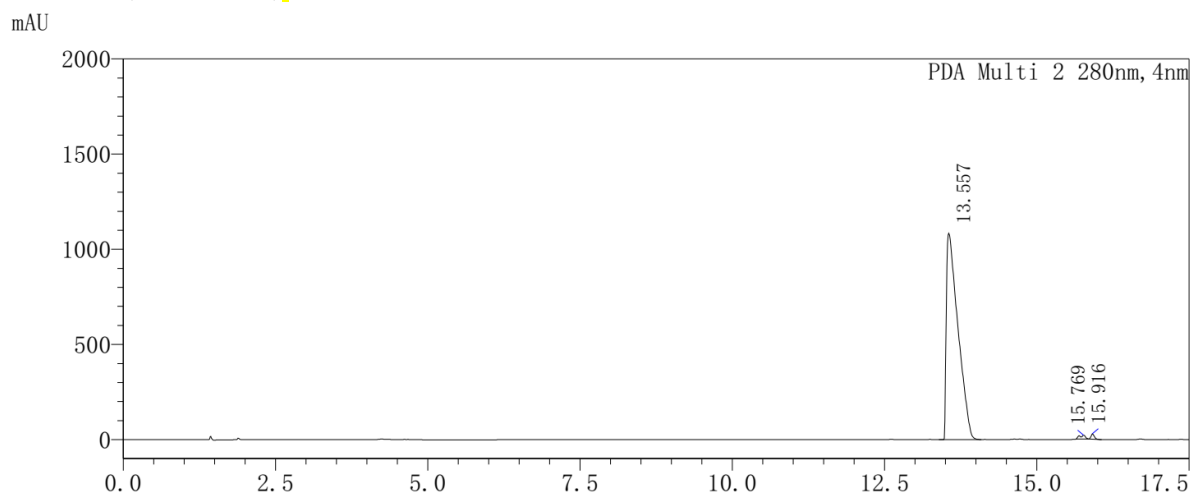
HPLC Traces for **58** (UV=254 nm)



Peak Table

Peak	Ret. time (min)	Area	Area (%)
1	13.557	14408687	99.502
2	15.916	72043	0.498

HPLC Traces for **58** (UV=280 nm),



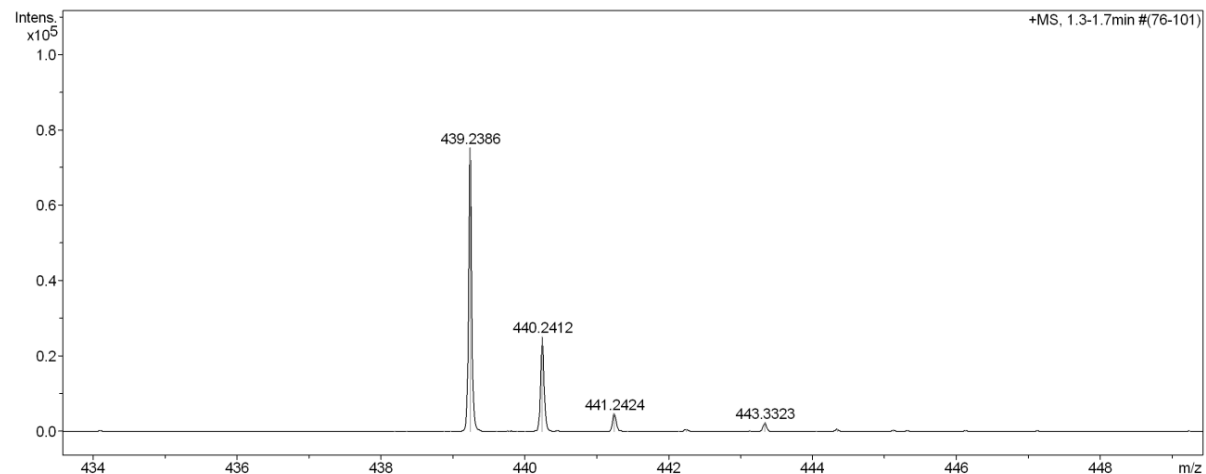
Peak Table

Peak	Ret. time (min)	Area	Area (%)
1	13.557	14464985	98.438
2	15.769	131683	0.896
3	15.916	97870	0.666

Method. Flow rate = 1.0 mL/min; gradient elution over 18 minutes, from 10% ACN-H₂O to 95% ACN-H₂O with 0.5% HCOOH, 280 nm, 254 nm;

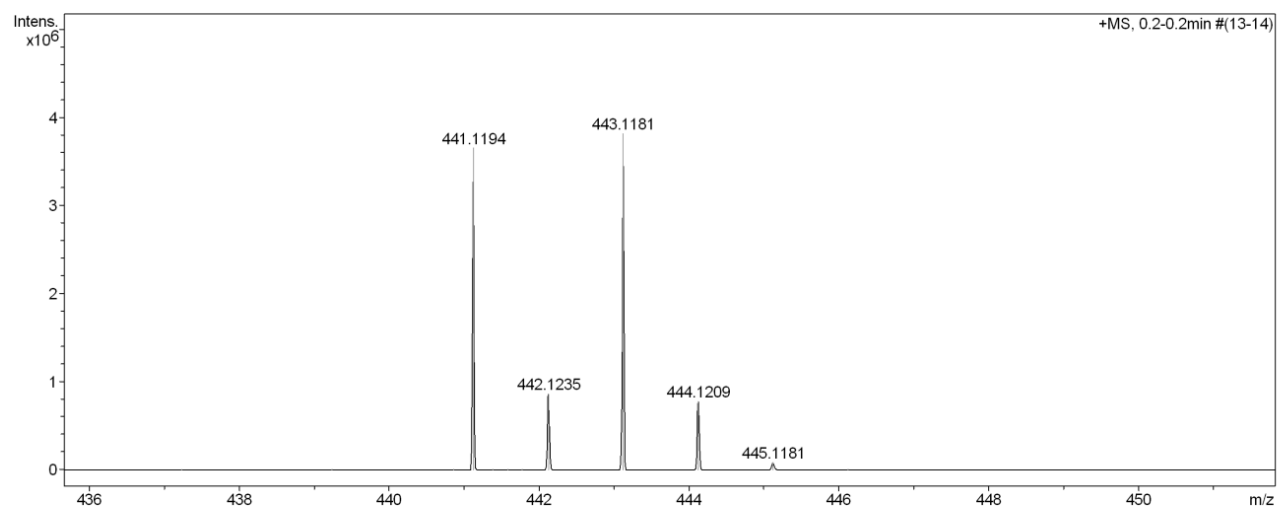
InertSustain-C18 column (5 μ m 4.6×250 mm).

HRMS for **45**.



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
439.2386	1	C ₂₉ H ₃₁ N ₂ O ₂	439.2380	-1.3	-0.5	15.5	ok	even	6.53	0.0121	0.0008	0.0042	0.0017	0.4160

HRMS for 58.



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e ⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
441.1194	1	C ₂₃ H ₂₆ BrN ₂ O ₂	441.1172	-5.0	-5.6	11.5	ok	even	28.99	0.0262	0.0026	0.0095	0.0005	0.7810