

Supporting Information

Visible-Light-Mediated Cascade Cyanoalkylsulfonylation/Cyclization of Alkynoates Leading to Coumarins *via* SO₂ Insertion

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1. General Information

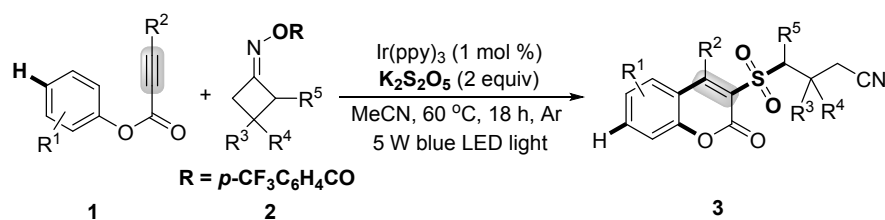
Unless otherwise stated, all commercial reagents were used as received. Acetylenic acid (BK, 99%), aldehydes (Innochem, >98%) and phenol (Innochem, >98%) were used without further treatment. All reagents and solvents were commercially available and used without any further purification unless specified. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (0.25mm, 300-400 mesh). Analytical thin-layer chromatography was performed using glass plates pre-coated with 0.25mm 300-400 mesh silica gel impregnated with a fluorescent indicator (254 nm). All reactions were carried out with magnetic stirring and in dried glassware. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^1H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded in CDCl_3 on a Bruker DRX-400 spectrometer operating at 400 MHz, 376 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. The solvent peak was used as a reference value, for ^1H NMR: TMS = 0.00 ppm, for ^{13}C NMR: CDCl_3 = 77.00 ppm. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, dd = doublet of doublet, t = triplet, td = triplet of doublet, q = quartet, m = multiplet, and br = broad. High-resolution mass spectra (HRMS) were obtained on an Agilent mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

2. Experiment Section

2.1 General Procedure for the Synthesis of Substrates

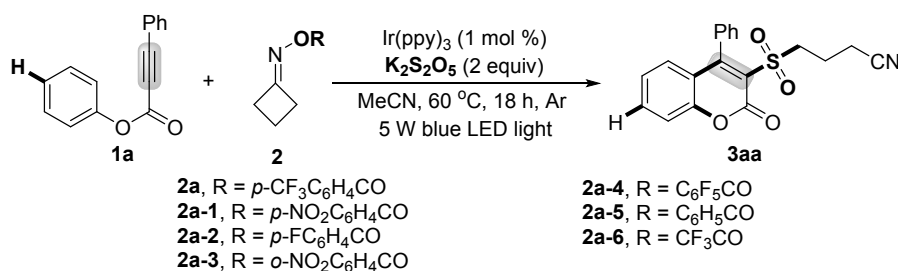
All alkynoates **1**^[1] and cycloketone oxime esters **2**^[2-4] were synthesized according to the known methods.

2.2 Typical Experimental Procedure



To a Schlenk tube were added alkynoates **1** (0.2 mmol, 0.1 M), cyclobutanone oxime compounds **2** (1.5 equiv), Ir(ppy)₃ (1 mol %), K₂S₂O₅ (0.4 mmol, 2 equiv) and MeCN (2 mL) at 60 °C under irradiation of 5 W blue light for 18 h. Until complete consumption of the starting material was observed by TLC and/or GC-MS analysis. After the reaction was finished, the reaction mixture removal of the solvent, the crude product was purified by column chromatography (petroleum ether/ethyl acetate, 3 : 1) to provide the desired products **3**. A scaled-up experiment conducted in the presence of **1a** (1 mmol), **2a** (1.5 mmol, 1.5 equiv), Ir(ppy)₃ (0.01 mmol, 1 mol %), K₂S₂O₅ (2 mmol, 2 equiv) and MeCN (10 mL) at 60 °C under irradiation of 5 W blue light for 72 h gave the target product **3aa** in 68% yield.

2.3 Table S1: Screening of optimal cyclobutanone *O*-acyloximes^a



entry	variation from the standard conditions	yield (%) ^b
1	2a	81
2 ^c	2a-1 instead of 2a	50
3	2a-2 instead of 2a	43
4	2a-3 instead of 2a	40
5	2a-4 instead of 2a	63
6	2a-5 instead of 2a	25
7 ^c	2a-6 instead of 2a	12

^a Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol, 1.5 equiv), Ir(ppy)₃ (1 mol %), K₂S₂O₅ (0.4 mmol, 2 equiv) and MeCN (2 mL) at 60 °C under irradiation of 5 W blue light for 18 h. ^b Isolated yield. ^c Most of starting materials were decomposed.

Several other cyclobutanone *O*-acyloximes **2a-1–2a-6** were examined (Table S1). We found that structural modification of the acyl moiety on the oxime had remarkable effect on the reaction. All of them could afford the sulfonylation products and none of them could afford higher yield than that of cyclobutanone oxime **2a**. This maybe attribute to the leaving ability and basicity of RCOO⁻.

2.4 Figure S1: Profile of 3aa with Light on or off over Time

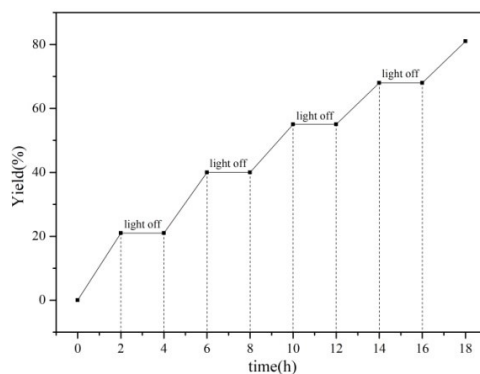
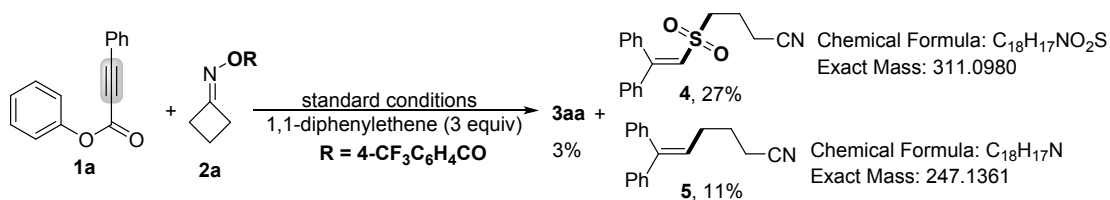


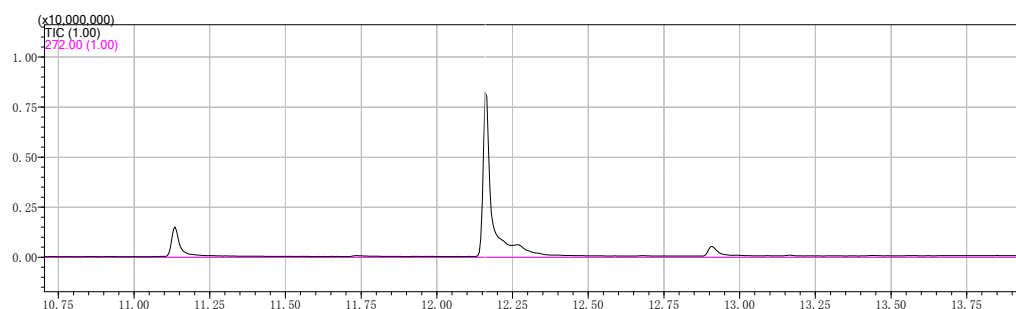
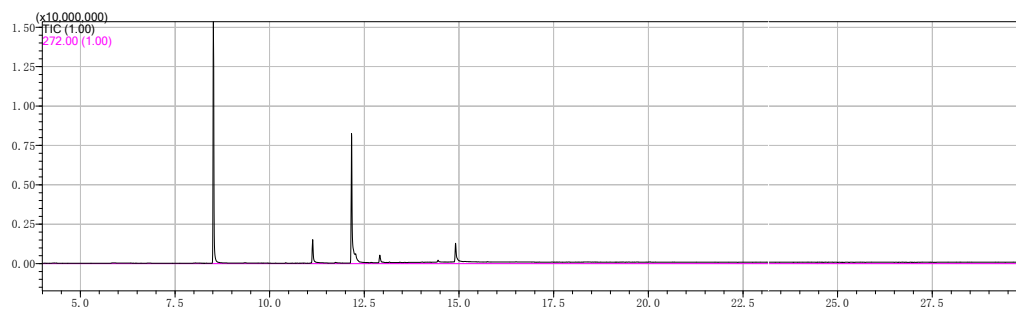
Figure S1. Profile of **3aa** with Light on or off over Time. GC yield using biphenyl as an internal standard.

2.5 GC-MS analysis of Raw Reaction Mixtures in the presence of Radical Inhibitors.

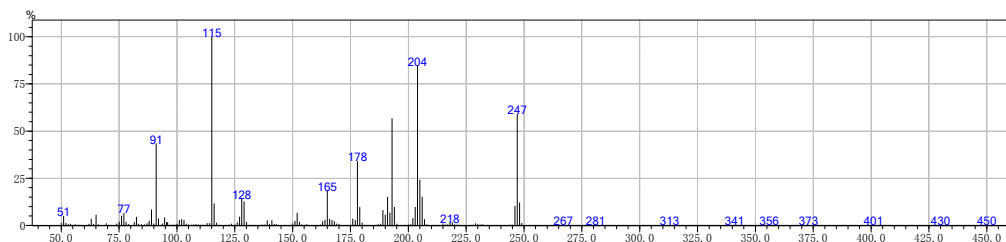
GC-MS Analysis of Raw Reaction Mixture by Using 1,1-diphenylethane as Radical Inhibitor



Spectra of GC-MS



MS Spectra of the peak at 12.16 min



[MS Spectrum]

of Peaks 395

Raw Spectrum 12.160 (scan : 1633)

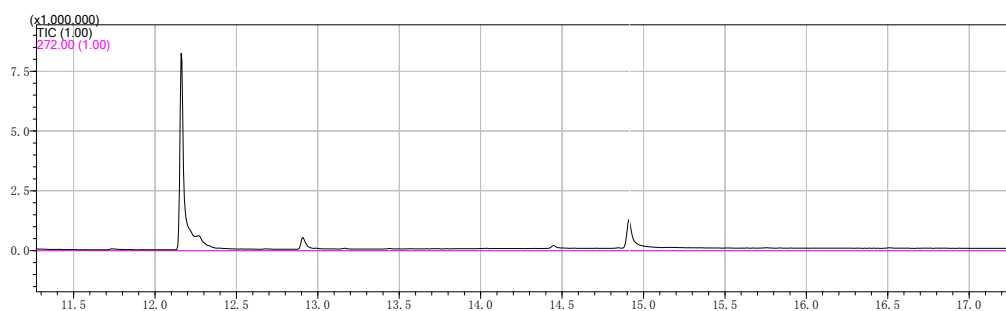
Background No Background Spectrum

Base Peak m/z 115.10 (Inten : 1,148,922)

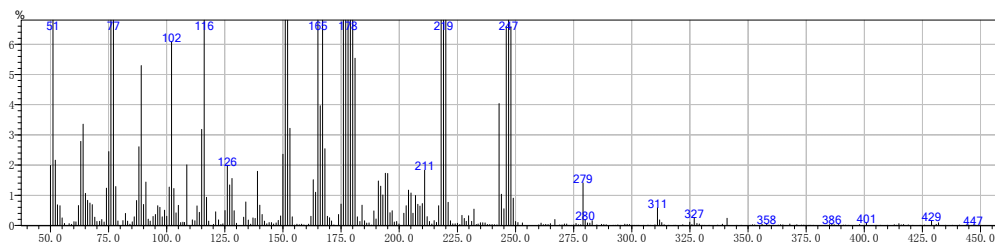
Event# 1

m/z	Absolute Intensity	Relative Intensity
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51.00	55250	4.81
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54.00	80170.70	87.05
55.05	17750.15	88.05
56.05	58950.51	89.05
57.50	17240.15	90.05
58.50	153	0.01
59.50	44	0.00
61.00	636	0.06
62.00	73300.64	94.65
63.00	38052	3.31
64.00	65180.57	96.00
65.05	62840	5.47
66.05	47000.41	98.05
67.05	15280.13	99.05
68.55	11720.10	100.05
69.50	10962	0.95
70.45	23210.20	102.05
71.45	828	0.07
73.00	15320.13	104.05
74.00	87500.76	105.10
75.05	20452	1.78
76.05	56488	4.92
77.05	72828	6.34
78.05	19663	1.71
79.05	60340.53	110.15
80.55	16370.14	111.05
81.55	18569	1.62
82.50	50522	4.40
83.45	81230.71	83.45
84.65	54890.48	84.65
86.05	43950.38	86.05
87.05	10706	0.93
88.05	26411	2.30
89.05	94796	8.25
90.05	94430.82	90.05
91.05	497406	43.29
92.05	40023	3.48
93.65	97180.85	93.65
94.65	47467	4.13
95.55	17887	1.56
96.00	19087	1.66
96.95	21970.19	96.95
98.05	28480.25	98.05
99.05	29970.26	99.05
100.05	72250.63	100.05
101.05	31471	2.74
102.05	36467	3.17
103.05	31333	2.73
104.05	87270.76	104.05
105.10	47340.41	105.10
106.25	25160.22	106.25
107.25	33150.29	107.25
108.20	50260.44	108.20
109.15	43480.38	109.15
110.15	21040.18	110.15
111.05	18380.16	111.05
112.05	740	0.06
113.05	12074	1.05
114.15	11681	1.02
115.10	1148922	100.00
116.10	131602	11.45
117.10	14657	1.28
118.10	18550.16	118.10
119.15	788	0.07
120.65	510	0.04
121.55	10540.09	121.55
122.60	32920.29	122.60
123.60	83020.72	123.60
125.10	22470.20	125.10
126.05	17129	1.49
127.05	51280	4.46
128.05	160662	13.98
129.05	144566	12.58
130.10	20116	1.75
131.05	20680.18	131.05
132.10	258	0.02
133.05	441	0.04
134.00	159	0.01
135.00	209	0.02
136.10	166	0.01
137.10	26170.23	137.10
138.05	32240.28	138.05
139.05	29116	2.53
140.00	68630.60	140.00
141.05	29125	2.53
142.05	60480.53	142.05
143.05	51970.45	143.05

144.00	15320.13		180.00	15257	1.33	216.05	30060.26	
145.00	879	0.08	181.00	22900.20		217.00	48090.42	
146.00	66	0.01	182.10	447	0.04	218.00	17178	1.50
146.95	355	0.03	183.10	52	0.00	219.00	16855	1.47
147.90	202	0.02	184.10	54	0.00	220.00	39000.34	
148.95	10040.09		185.10	94	0.01	221.00	23960.21	
150.00	95800.83		186.00	335	0.03	221.95	34740.30	
151.00	24630	2.14	186.95	56200.49		222.95	644	0.06
152.00	75362	6.56	188.00	71480.62		223.90	159	0.01
153.00	18225	1.59	189.00	91858	8.00	224.90	190	0.02
154.00	48500.42		190.00	63047	5.49	226.00	554	0.05
155.00	18360.16		191.00	171148	14.90	227.00	817	0.07
156.05	59630.52		192.05	76749	6.68	228.00	25380.22	
157.05	660	0.06	193.00	650553	56.62	229.00	11238	0.98
158.10	34	0.00	194.00	110287	9.60	230.00	67460.59	
159.10	6	0.00	195.05	91810.80		231.05	33510.29	
160.00	74	0.01	196.00	734	0.06	232.00	58710.51	
161.00	650	0.06	197.00	116	0.01	233.00	11400.10	
162.00	28490.25		198.00	201	0.02	234.00	121	0.01
163.00	24354	2.12	199.05	468	0.04	235.00	44	0.00
164.00	32593	2.84	200.00	44230.38		236.00	119	0.01
165.00	211087	18.37	201.05	52610.46		237.00	44	0.00
166.00	38518	3.35	201.95	42028	3.66	238.00	175	0.02
167.00	30881	2.69	203.00	110498	9.62	239.00	159	0.01
168.00	23508	2.05	204.00	972580	84.65	240.00	684	0.06
169.00	85140.74		205.00	275674	23.99	240.95	361	0.03
170.05	81020.71		206.00	172255	14.99	241.90	782	0.07
171.05	13870.12		207.00	35921	3.13	243.05	762	0.07
172.00	151	0.01	208.00	39740.35		244.05	32310.28	
173.00	719	0.06	209.05	633	0.06	245.15	26660.23	
173.95	15720.14		210.00	42	0.00	246.05	116683	10.16
175.00	35800.31		211.00	342	0.03	247.05	677335	58.95
176.00	39802	3.46	211.90	162	0.01	248.05	137102	11.93
177.05	30720	2.67	212.95	961	0.08	249.05	13314	1.16
178.00	390034	33.95	214.00	745	0.06	249.95	509	0.04
179.00	110390	9.61	215.00	97690.85		251.00	79	0.01



MS Spectra of the peak at 14.90 min



[MS Spectrum]

of Peaks 309

Raw Spectrum 14.915 (scan : 2184)

Background 14.830 (scan : 2167)

Base Peak m/z 178.00 (Inten : 190,125)

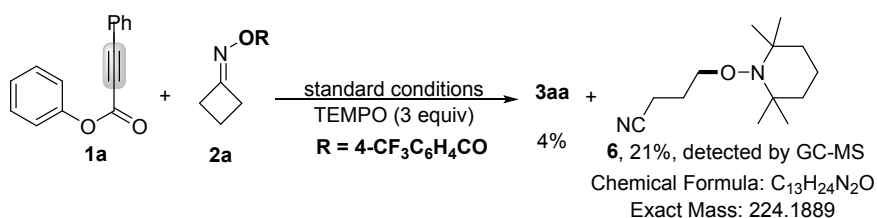
Event# 1

m/z	Absolute Intensity	Relative Intensity
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51.05	20779 10.93	83.15 266 0.14
52.05	41092.16	84.20 80 0.04
53.00	13010.68	85.15 231 0.12
54.05	12440.65	86.05 541 0.28
55.00	471 0.25	87.05 15740.83
56.00	125 0.07	88.05 49552.61
58.00	116 0.06	89.05 10065 5.29
59.05	67 0.04	90.05 13230.70
60.10	235 0.12	91.05 27271.43
60.95	226 0.12	92.05 397 0.21
62.00	12560.66	92.90 272 0.14
63.00	52952.79	94.15 568 0.30
64.00	63763.35	95.10 688 0.36
65.05	20171.06	96.10 12410.65
65.95	15800.83	97.05 11380.60
67.00	14110.74	98.05 544 0.29
68.00	13130.69	99.05 954 0.50
69.05	523 0.28	99.95 581 0.31
69.95	247 0.13	101.05 24101.27
71.10	264 0.14	102.05 11567 6.08
72.05	372 0.20	103.05 23261.22
73.05	217 0.11	104.00 785 0.41
74.05	2351 1.24	105.00 12640.66
75.05	46462.44	106.00 182 0.10
76.00	14009 7.37	106.90 205 0.11
77.05	20546 10.81	107.65 187 0.10
78.10	2449 1.29	108.65 38132.01
79.00	285 0.15	111.00 351 0.18
81.15	302 0.16	112.10 299 0.16
		113.05 12330.65
		114.05 823 0.43
		115.05 60493.18
		116.10 18921 9.95
		117.10 17760.93
		118.05 270 0.14
		120.10 67 0.04
		121.05 856 0.45
		122.30 345 0.18
		123.30 62 0.03
		124.10 96 0.05
		125.05 940 0.49
		126.05 3771 1.98
		127.05 2554 1.34
		128.05 2956 1.55
		129.00 925 0.49
		130.00 140 0.07
		133.05 517 0.27
		134.00 14750.78
		135.10 344 0.18
		136.10 74 0.04
		137.10 475 0.25
		138.05 444 0.23
		139.05 3409 1.79
		140.00 12710.67
		141.00 689 0.36
		142.00 276 0.15
		143.00 103 0.05
		144.00 182 0.10
		145.05 176 0.09

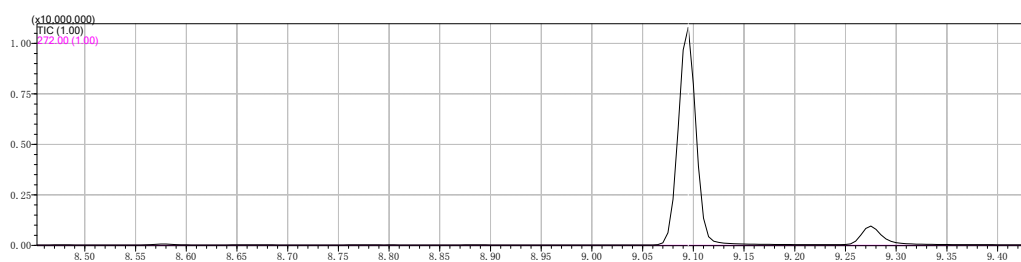
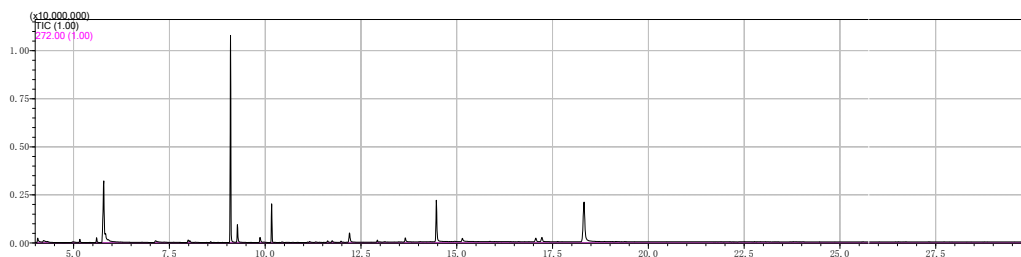
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149.00	596	0.31	194.00	32801.73	238.90	54	0.03	
150.00	44782.36		195.00	32771.72	239.90	52	0.03	
151.00	13308	7.00	196.00	796	0.42	240.90	43	0.02
152.00	34565	18.18	196.95	923	0.49	242.00	38	0.02
153.00	61143.22		197.90	212	0.11	242.95	76714.03	
154.00	545	0.29	198.85	252	0.13	243.95	19651.03	
155.00	26	0.01	199.90	86	0.05	245.00	10520.55	
156.00	78	0.04	202.00	773	0.41	246.05	12532	6.59
157.00	50	0.03	202.95	12400.65	247.05	61299	32.24	
158.00	82	0.04	203.95	22231.17	248.05	12517	6.58	
159.00	31	0.02	205.05	20461.08	249.05	17120.90		
160.00	6	0.00	205.90	773	0.41	250.00	251	0.13
161.00	74	0.04	206.95	18890.99	251.05	175	0.09	
162.00	573	0.30	207.95	13270.70	253.00	159	0.08	
163.00	28751.51		208.90	12230.64	260.00	35	0.02	
164.00	20931.10		209.95	13740.72	261.00	143	0.08	
165.00	35138	18.48	210.95	34791.83	262.00	49	0.03	
166.00	75363.96		212.00	556	0.29	263.00	70	0.04
167.05	30016	15.79	213.00	244	0.13	264.00	52	0.03
168.00	48352.54		214.00	89	0.05	265.00	109	0.06
169.10	580	0.31	215.00	301	0.16	266.95	375	0.20
170.00	487	0.26	216.00	193	0.10	269.00	34	0.02
170.90	287	0.15	216.95	12460.66	270.00	36	0.02	
171.90	31	0.02	218.00	30747	16.17	271.00	85	0.04
173.90	689	0.36	219.00	76861	40.43	272.00	85	0.04
175.00	13440.71		220.00	13847	7.28	273.00	11	0.01
176.00	27156	14.28	221.00	14610.77		274.00	13	0.01
177.00	24266	12.76	222.00	290	0.15	275.00	39	0.02
178.00	190125	100.00	223.00	104	0.05	276.00	128	0.07
179.00	161938	85.17	224.00	98	0.05	277.00	40	0.02
180.00	73503	38.66	225.00	136	0.07	278.00	44	0.02
181.00	10536	5.54	226.00	60	0.03	279.05	26711.40	
182.00	547	0.29	227.00	637	0.34	279.95	373	0.20
183.05	249	0.13	228.00	439	0.23	280.95	157	0.08
184.00	12710.67		228.85	263	0.14	281.95	152	0.08
185.05	296	0.16	229.80	615	0.32	282.95	288	0.15
186.00	144	0.08	231.10	257	0.14	285.00	36	0.02
187.00	156	0.08	232.10	10300.54		287.00	67	0.04
188.10	23	0.01	233.10	60	0.03	288.00	52	0.03
189.10	919	0.48	233.90	88	0.05	289.00	50	0.03
190.05	404	0.21	234.90	166	0.09	292.00	12	0.01

293.00	12	0.01	308.00	9	0.00	326.90	493	0.26
294.00	39	0.02	310.00	39	0.02	328.00	126	0.07
295.00	3	0.00	311.05	11150.59		329.00	87	0.05
297.00	80	0.04	311.95	353	0.19	330.00	4	0.00
298.00	71	0.04	312.90	176	0.09	331.00	1	0.00
299.00	54	0.03	313.90	41	0.02	333.00	3	0.00
300.00	3	0.00	315.90	13	0.01	337.00	26	0.01
301.00	8	0.00	317.90	4	0.00	339.00	78	0.04
302.00	3	0.00	318.90	15	0.01	341.00	446	0.23
303.00	13	0.01	321.90	44	0.02	344.90	3	0.00
305.00	15	0.01	324.90	203	0.11	346.90	3	0.00
307.00	23	0.01	325.90	54	0.03	350.90	8	0.00

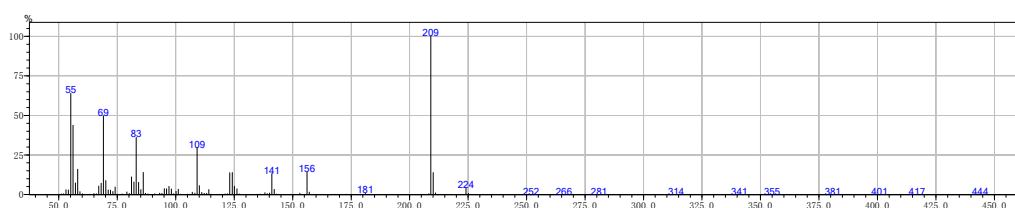
GC-MS Analysis of Raw Reaction Mixture by Using TEMPO as Radical Inhibitor



Spectra of GC-MS



MS Spectra of the peak at 9.100 min



[MS Spectrum]

of Peaks 388

Raw Spectrum 9.095 (scan : 1020)

Background No Background Spectrum

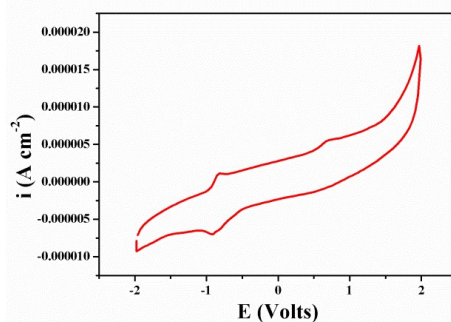
Base Peak m/z 209.05 (Inten : 1,877,707)

Event# 1

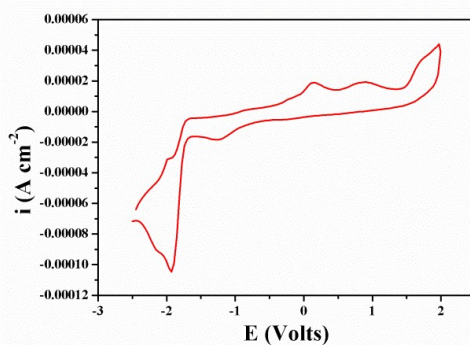
m/z	Absolute Intensity	Relative Intensity						
50.00	13160.07	89.05	570	0.03	128.10	19180.10		
51.05	70210.37	90.00	214	0.01	129.10	188	0.01	
52.05	94720.50	91.05	81930.44		130.10	16	0.00	
53.05	56700	3.02	92.15	16470.09	131.10	148	0.01	
54.10	53818	2.87	93.10	15774	0.84	132.10	60	0.00
55.10	1199618	63.89	94.10	14438	0.77	133.10	438	0.02
56.10	821505	43.75	95.10	69423	3.70	134.15	432	0.02
57.10	136764	7.28	96.10	67230	3.58	135.10	32920.18	
58.10	299102	15.93	97.10	96804	5.16	136.05	52570.28	
59.05	34697	1.85	98.10	65820	3.51	137.15	12840.07	
60.10	81100.43		99.10	87100.46		138.10	22182	1.18
61.10	610	0.03	100.10	38078	2.03	139.10	11015	0.59
62.15	358	0.02	101.10	62583	3.33	140.10	17626	0.94
63.10	27780.15		102.10	36300.19		141.10	246382	13.12
64.10	10360.06		103.10	959	0.05	142.10	61534	3.28
65.05	10805	0.58	104.10	188	0.01	143.10	51140.27	
66.05	85480.46		105.10	49880.27		144.05	283	0.02
67.05	99563	5.30	106.05	23640.13		145.05	17710.09	
68.10	133164	7.09	107.10	26684	1.42	146.00	218	0.01
69.10	934665	49.78	108.15	15288	0.81	147.00	294	0.02
70.10	166722	8.88	109.15	558300	29.73	148.10	538	0.03
71.10	52911	2.82	110.10	105874	5.64	149.10	10060.05	
72.10	51567	2.75	111.15	24885	1.33	150.05	18480.10	
73.10	36458	1.94	112.15	14543	0.77	151.05	24360.13	
74.10	89526	4.77	113.15	13987	0.74	152.05	12210.07	
75.10	38980.21		114.15	59674	3.18	153.05	16340	0.87
76.10	626	0.03	115.10	39610.21		154.00	19320.10	
77.05	71730.38		116.20	559	0.03	155.15	13000.07	
78.10	17510.09		117.20	126	0.01	156.10	265665	14.15
79.10	30446	1.62	118.10	286	0.02	157.10	27943	1.49
80.10	11671	0.62	119.15	780	0.04	158.05	21490.11	
81.10	208857	11.12	120.05	663	0.04	159.00	116	0.01
82.10	148095	7.89	121.10	65930.35		160.00	21	0.00
83.10	677886	36.10	122.10	96740.52		161.00	122	0.01
84.10	144791	7.71	123.10	258479	13.77	162.00	233	0.01
85.10	59068	3.15	124.15	259827	13.84	163.05	359	0.02
86.10	263025	14.01	125.10	97364	5.19	164.00	514	0.03
87.05	13732	0.73	126.15	67248	3.58	165.00	746	0.04
88.10	78200.42		127.15	73100.39		166.10	527	0.03

167.05	810	0.04	188.10	21	0.00	209.05	1877707	100.00
168.05	28390.15		188.90	210	0.01	210.05	261124	13.91
169.15	602	0.03	189.85	700	0.04	211.05	20174	1.07
170.10	156	0.01	190.90	620	0.03	212.15	13120.07	
171.10	284	0.02	191.95	320	0.02	213.20	106	0.01
171.90	63	0.00	192.90	583	0.03	214.20	13	0.00
172.90	29590.16		193.90	164	0.01	215.20	60	0.00
173.90	178	0.01	195.05	398	0.02	216.20	24	0.00
174.90	119	0.01	196.00	62	0.00	217.20	11	0.00
176.05	441	0.02	197.00	63	0.00	218.20	31	0.00
177.00	223	0.01	198.00	68	0.00	219.20	47	0.00
178.10	892	0.05	199.00	41	0.00	220.20	29	0.00
179.10	28630.15		200.00	13	0.00	221.20	90	0.00
180.05	578	0.03	201.00	44	0.00	222.20	137	0.01
181.05	12238	0.65	202.00	26	0.00	223.15	645	0.03
182.00	14040.07		203.00	14	0.00	224.10	80145	4.27
183.00	182	0.01	204.00	29	0.00	225.10	11735	0.62
184.15	721	0.04	205.00	66	0.00	226.00	10180.05	
185.10	95	0.01	206.00	70	0.00	227.00	126	0.01
186.10	31	0.00	207.00	22500.12		228.00	34	0.00
187.10	24	0.00	208.15	92680.49		229.0	14	0.00

2.6 Electrochemical Studies



Blank



1a

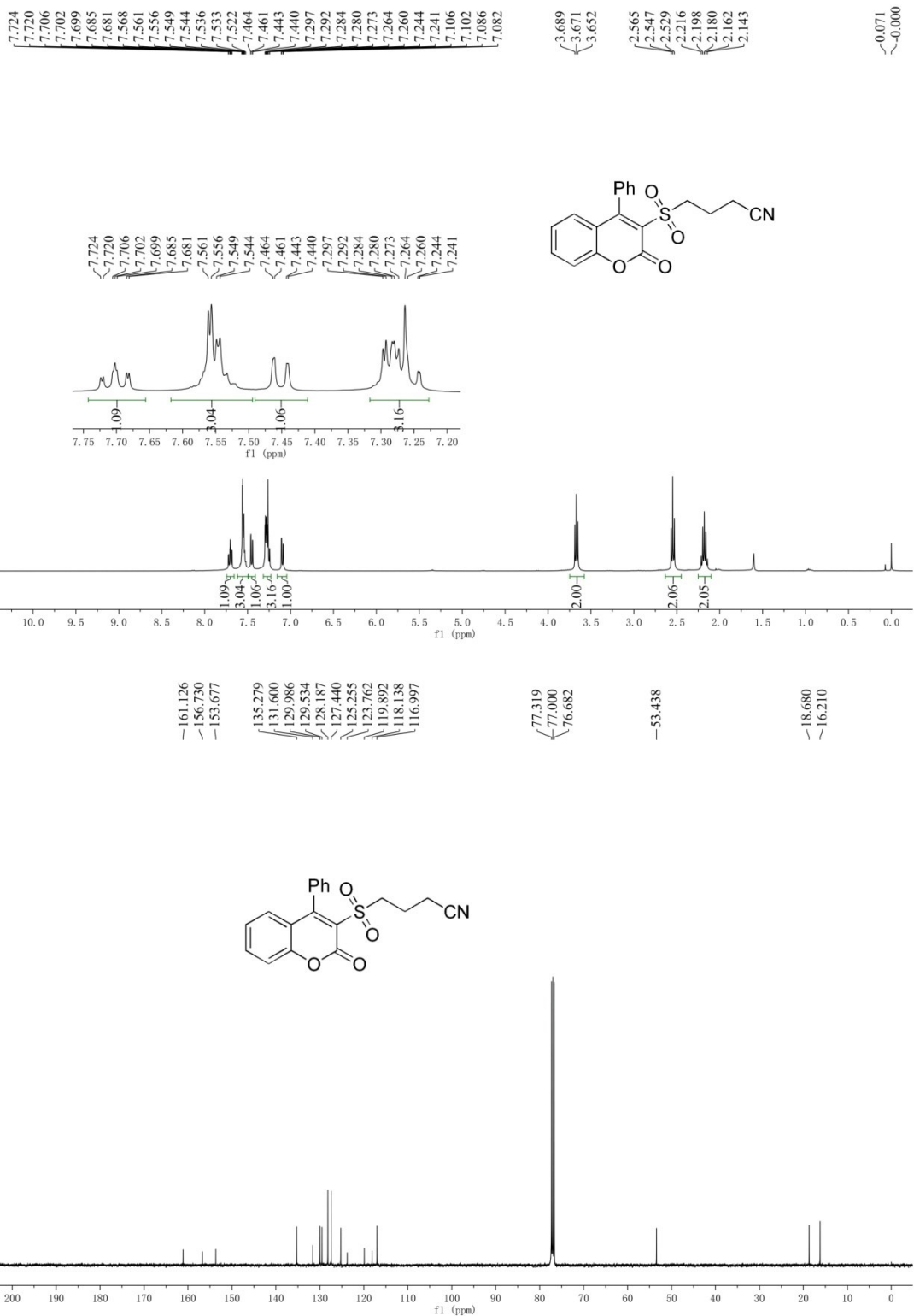
Cyclic voltammetry (CV) was taken using a CHI660D potentiostation. CV measurement of **1a** was carried out in 0.1 M of Bu₄NPF₆/MeCN at a scan rate of 100 mV/s with the protection of Ar. The working electrode is a glassy carbon, the counter electrode is a Pt wire, and the reference electrode is Ag/AgCl. Hence, E_{1a} = -1.88 versus SCE; E_{2a} = -1.64 versus SCE; E_{1/2}(*fac*-Ir(ppy)₃⁺ / *fac*-Ir(ppy)₃^{*}) = -1.73 versus SCE. These results suggested that **2a** was suitable for SET in the excited state of the *Ir^{III} and **1a** was completely unsuitable for SET in the excited state of the *Ir^{III}.

2 References

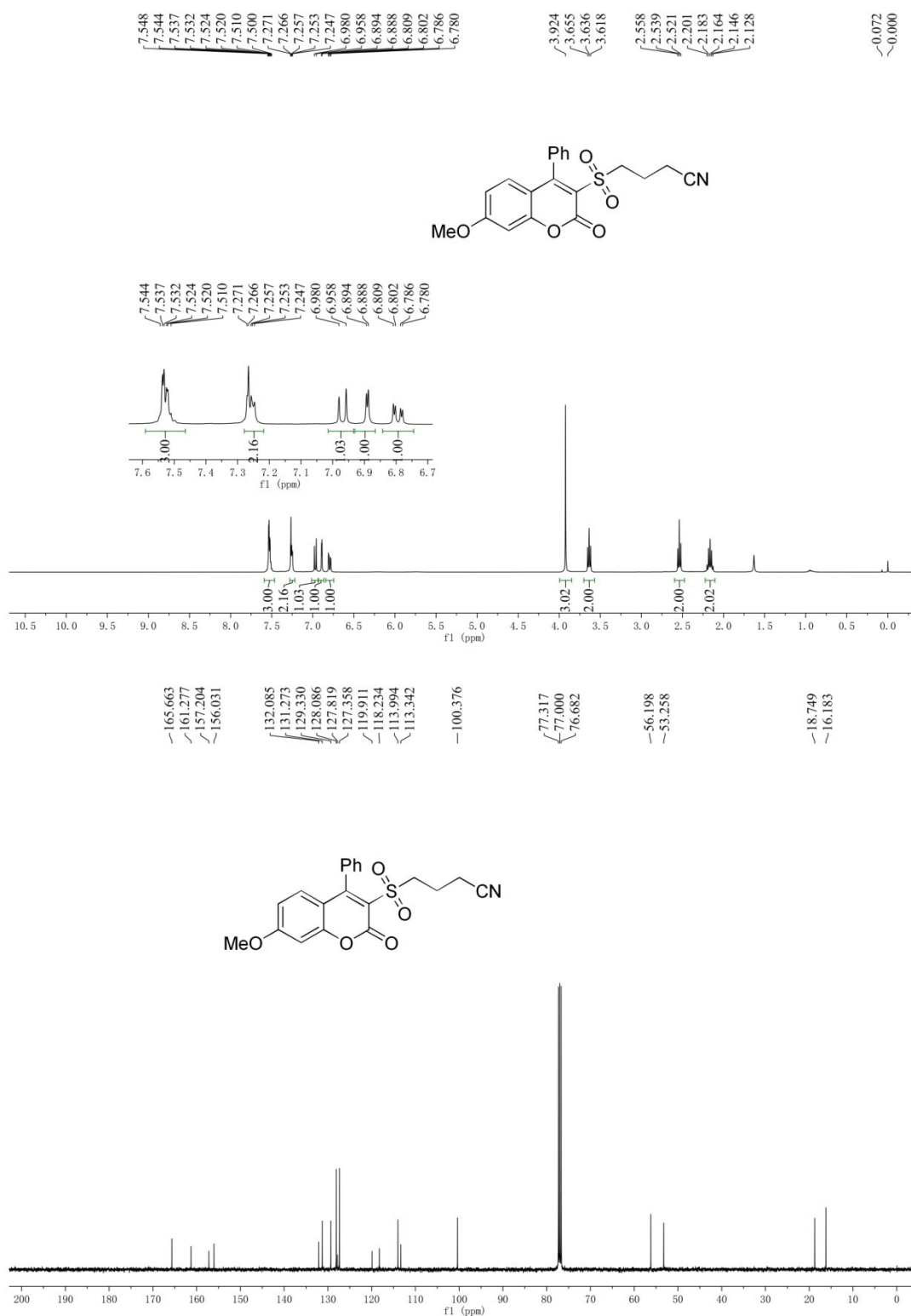
- [1] Y. Liu, Q.-L. Wang, C.-S. Zhou, B.-Q. Xiong, P.-L. Zhang, S.-J. Kang, C.-A. Yang, K.-W. Tang, *Tetrahedron Letter.*, 2018, **59**, 2038.
- [2] J. Chen, B.-Q. He, P.-Z. Wang, X.-Y. Yu, Q.-Q. Zhao, J.-R. Chen and W.-J. Xiao, *Org. Lett.* 2019, **21**, 4359.
- [3] J.-X. Yu, F. Teng, J.-N. Xiang, W. Deng and J.-H. Li, *Org. Lett.* 2019, **21**, 9434.
- [4] J.-J. Zhang, X.-D. Hua, Y. Wu, J.-C. Yang and L.-N. Guo, *Chem. Sci.* 2019, **10**, 161.

4. Spectra

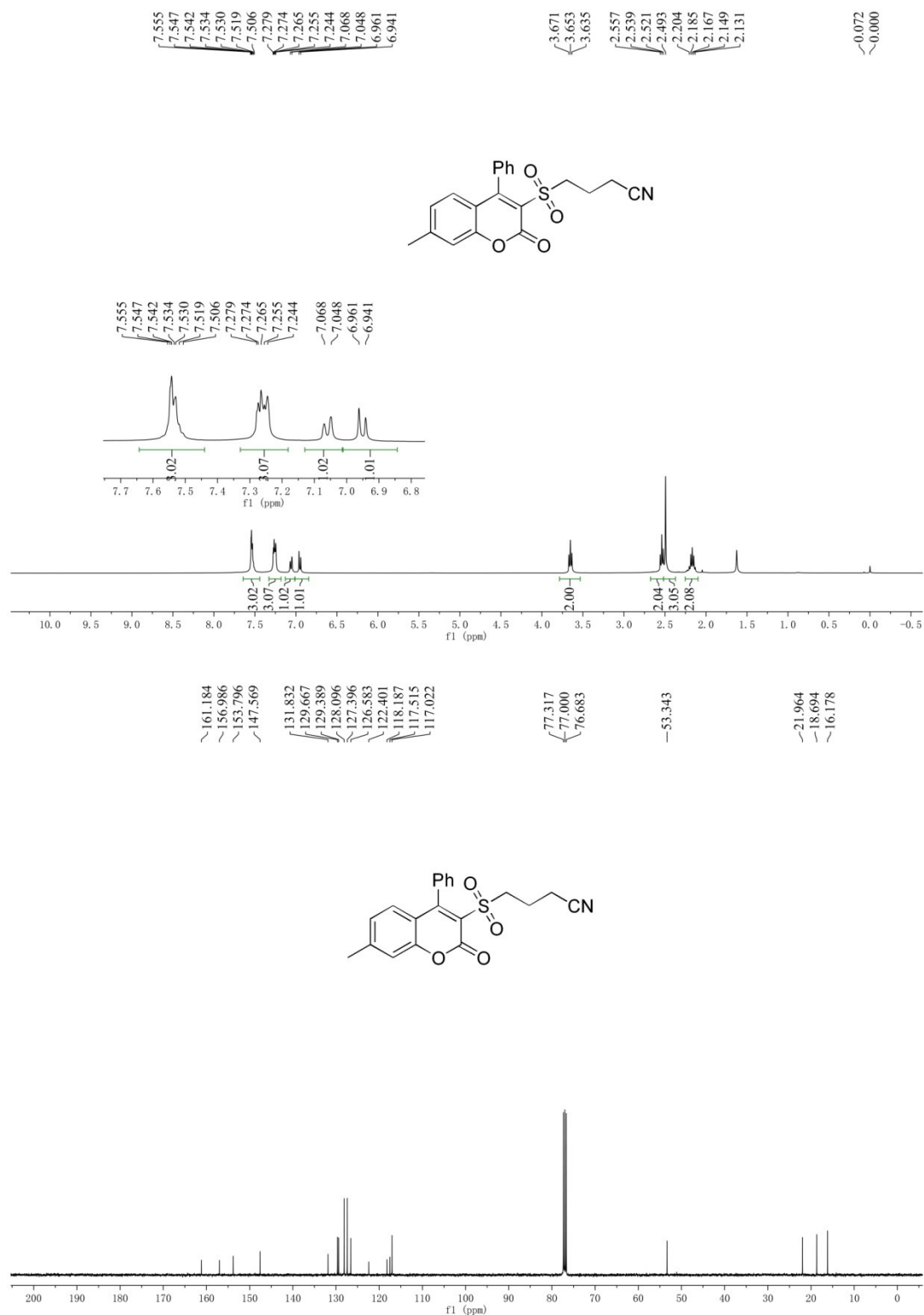
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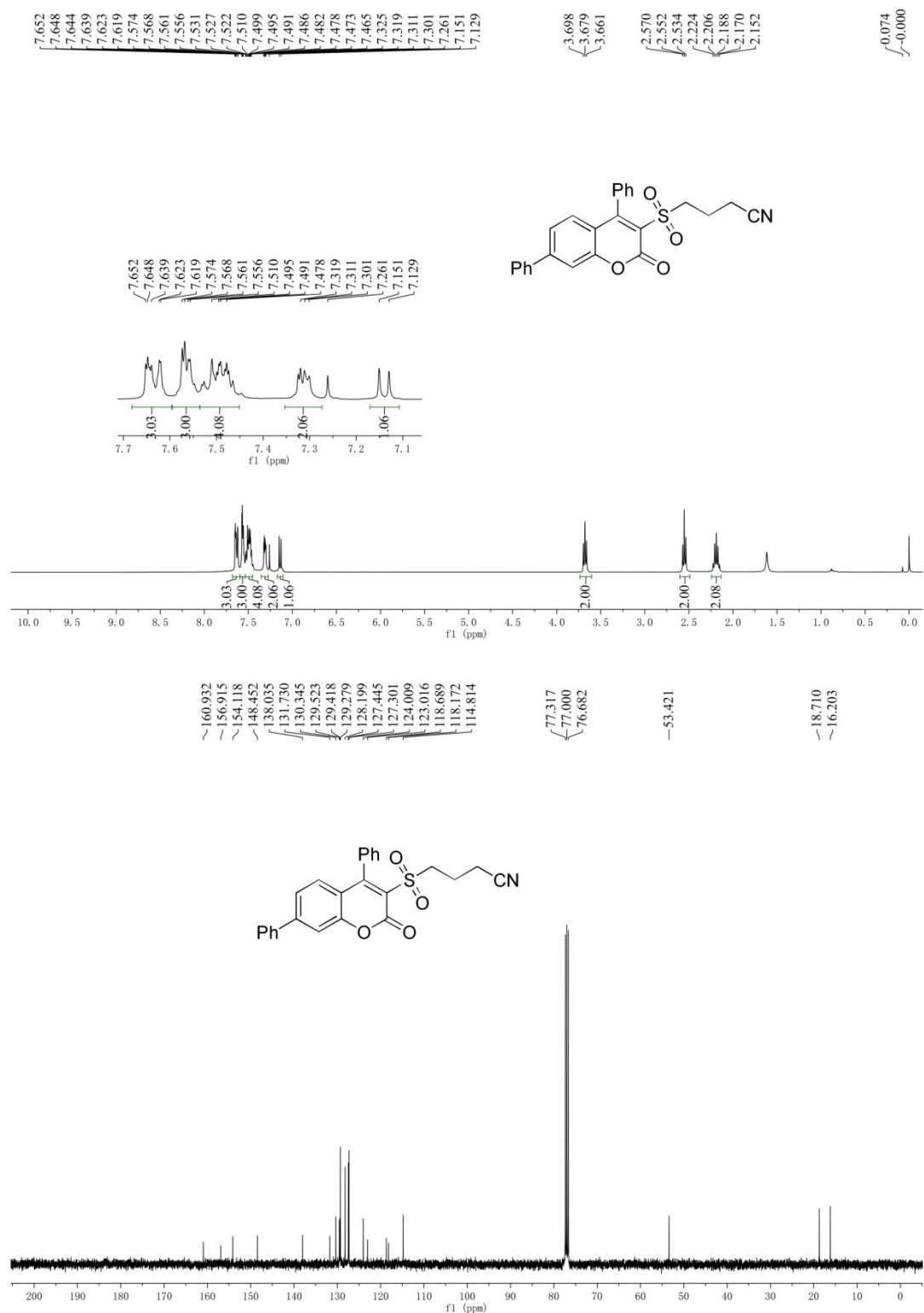
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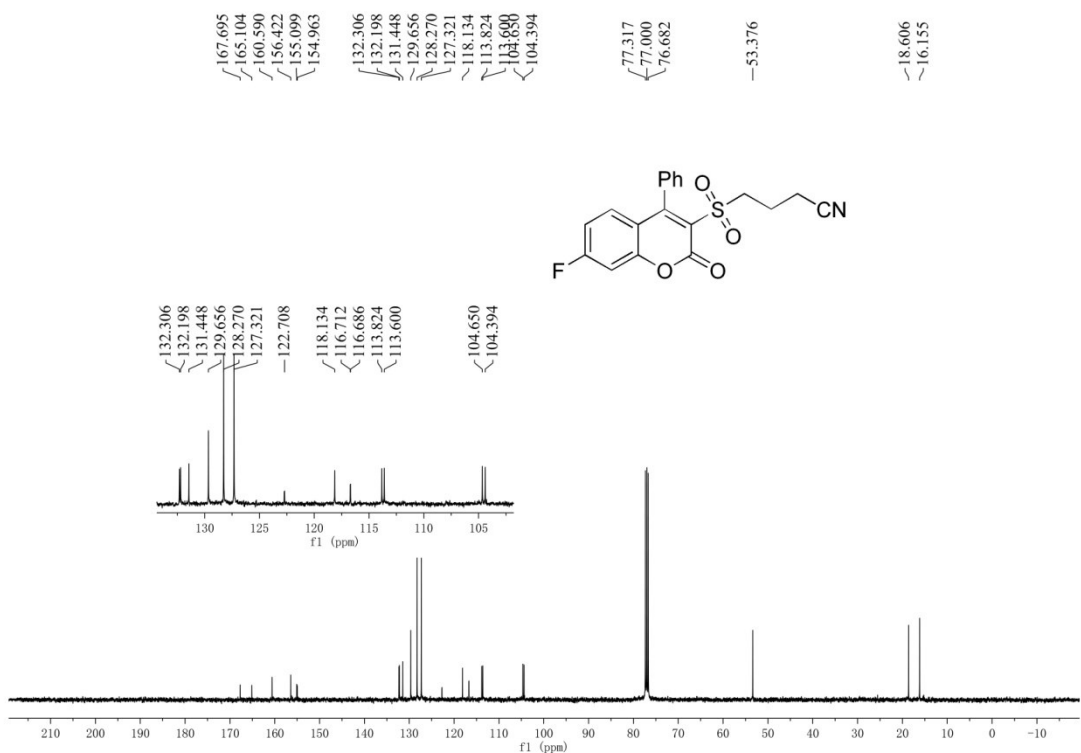
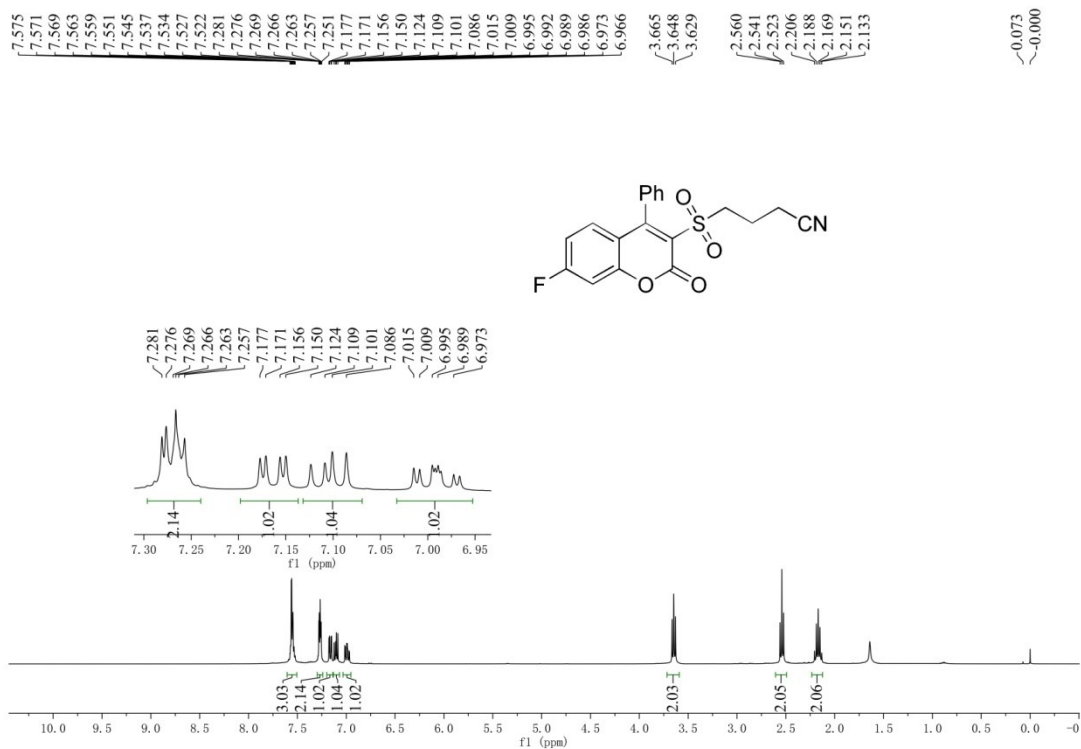
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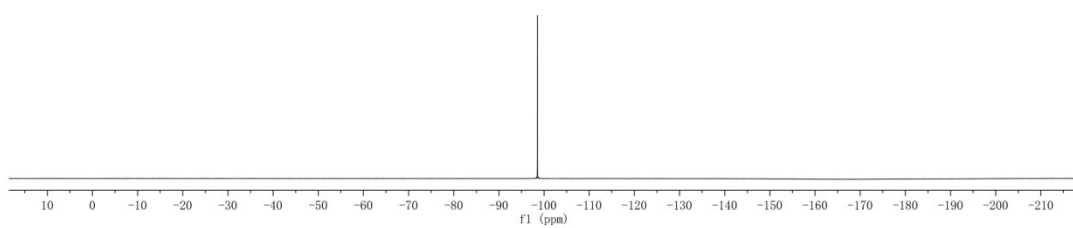
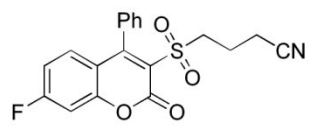
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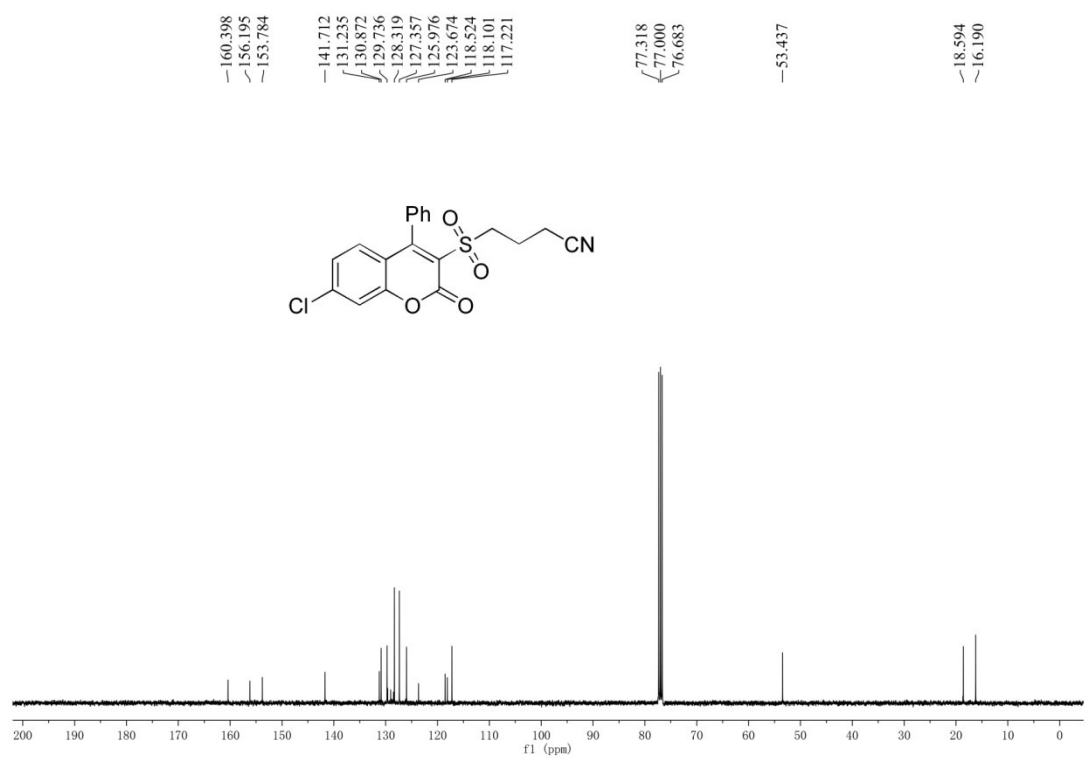
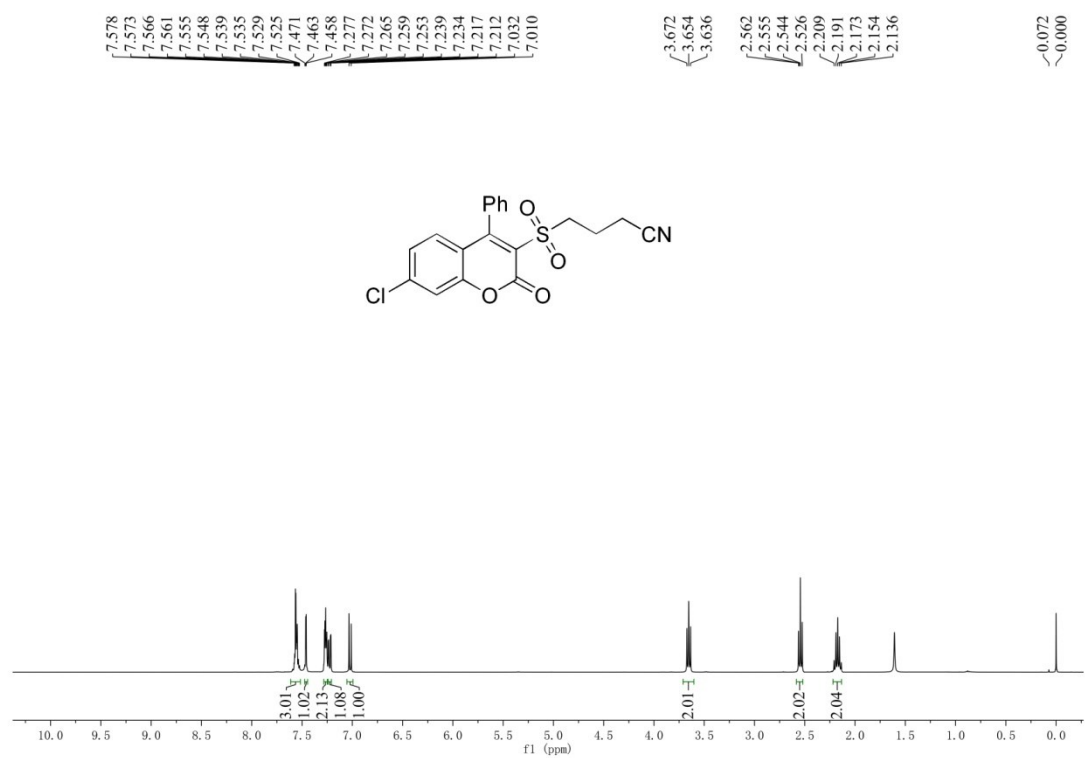
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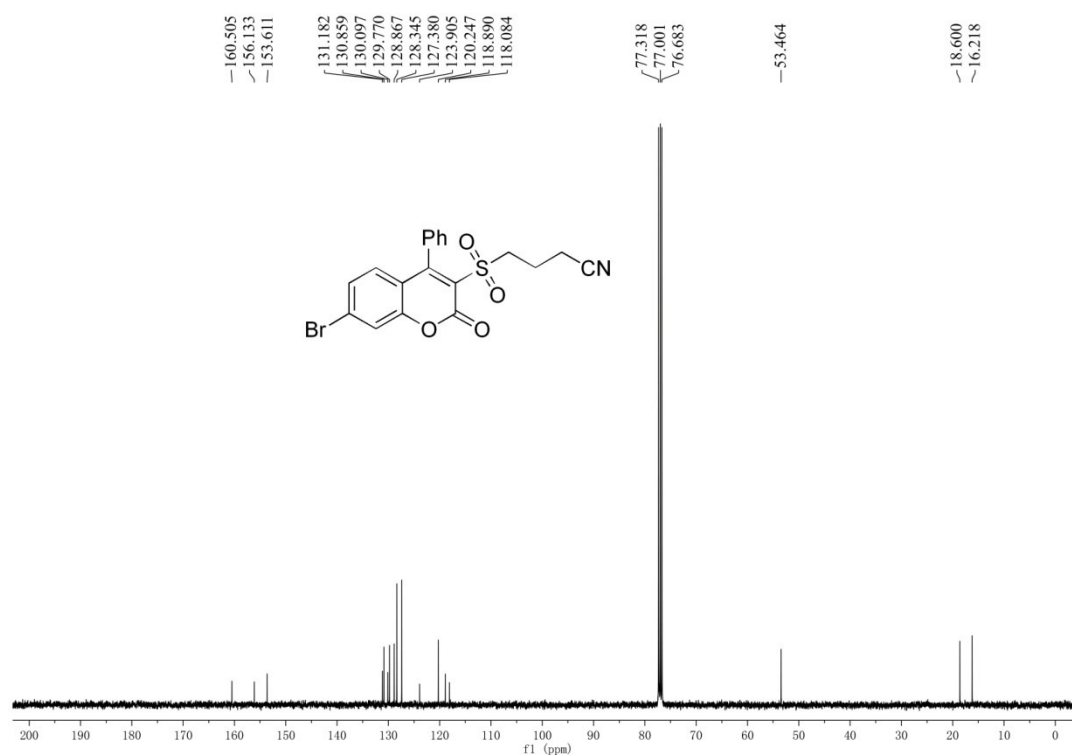
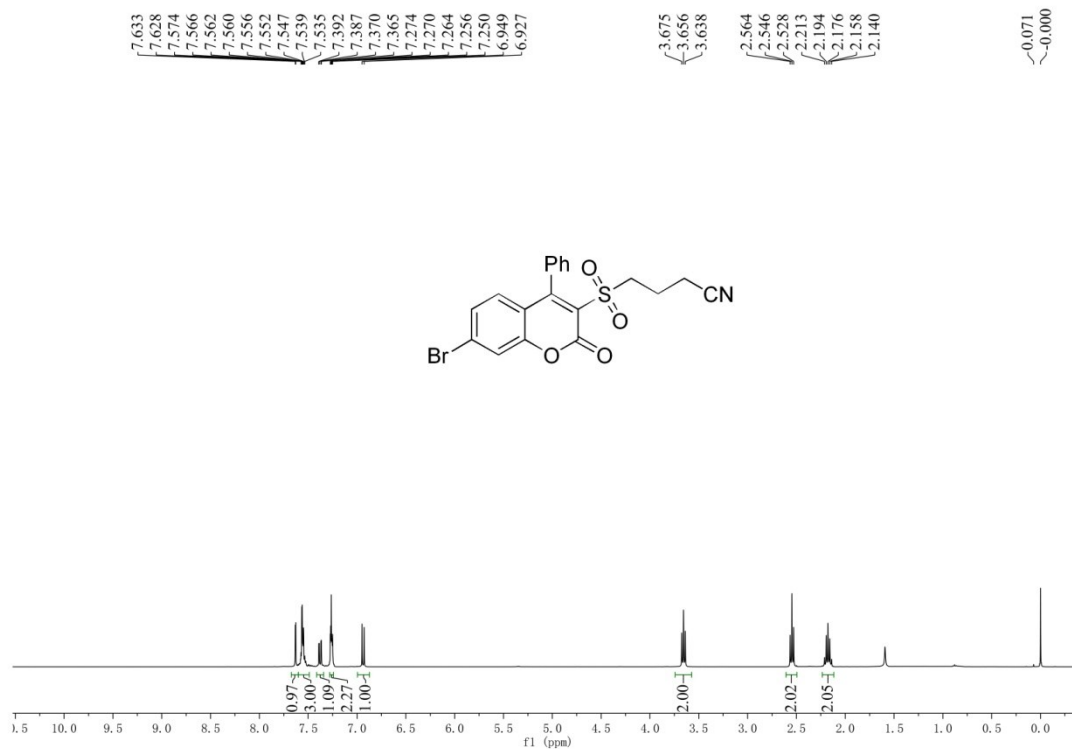
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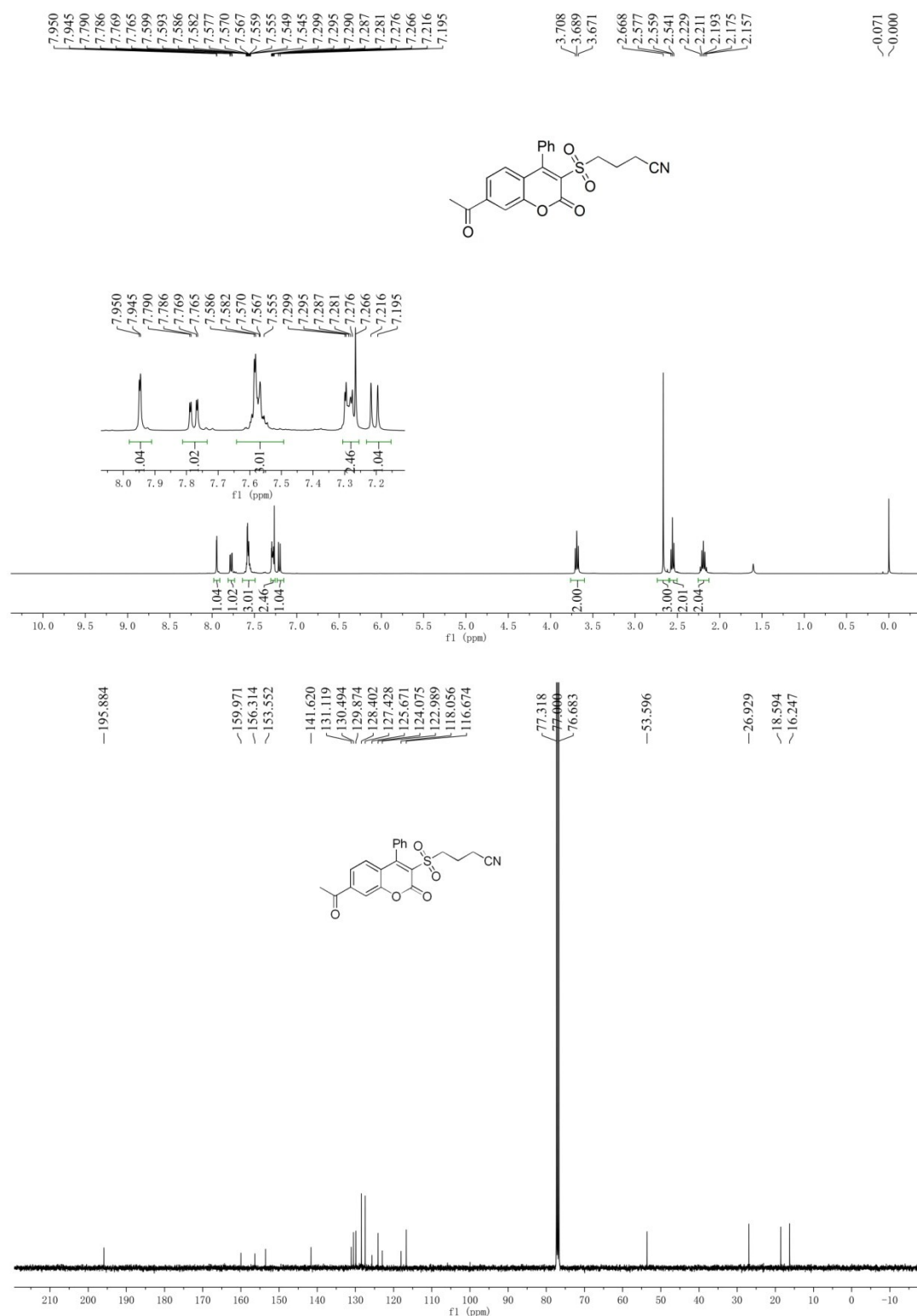
4-((7-Chloro-2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)butanenitrile (3fa)



4-((7-Bromo-2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)butanenitrile (3ga)

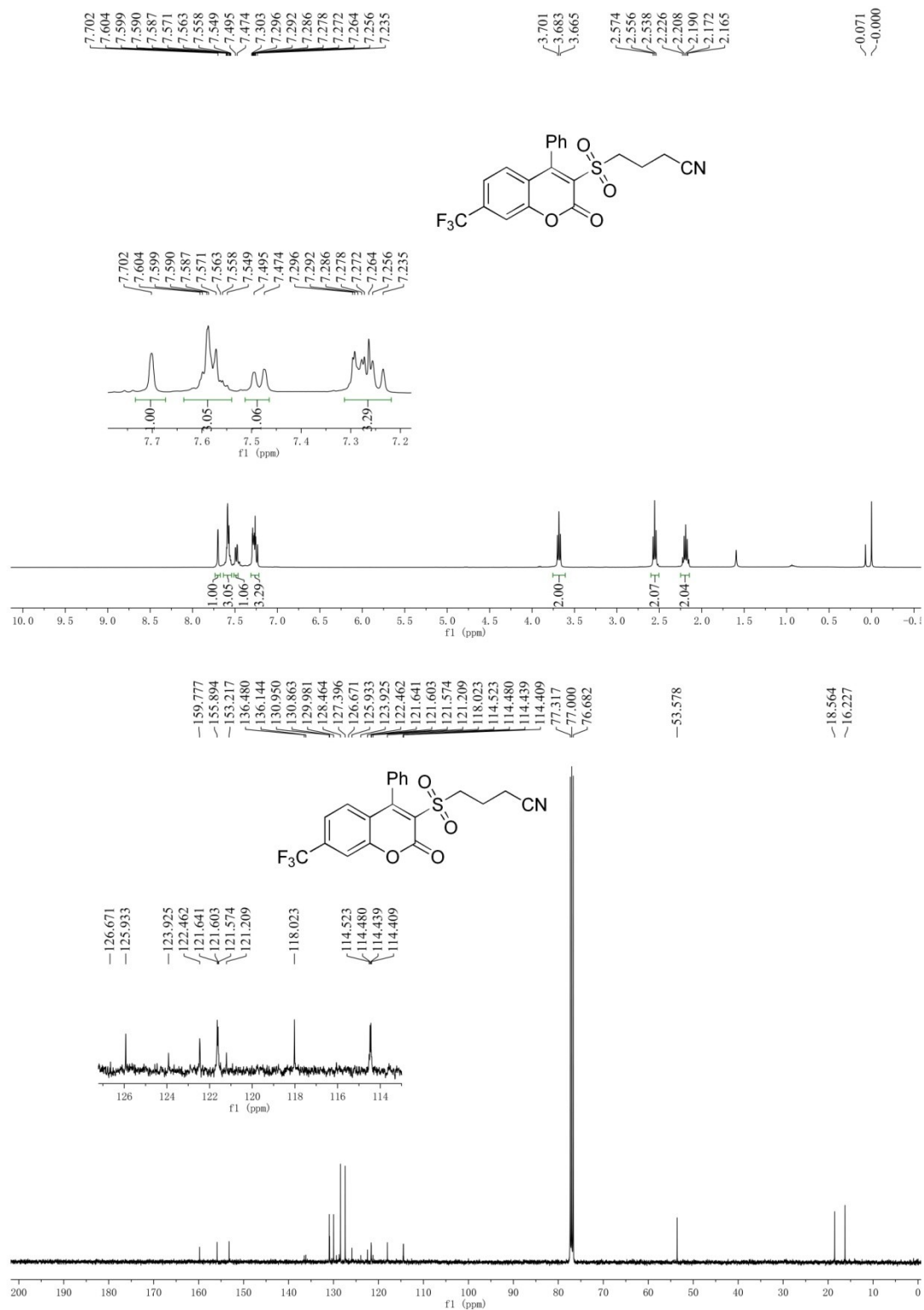


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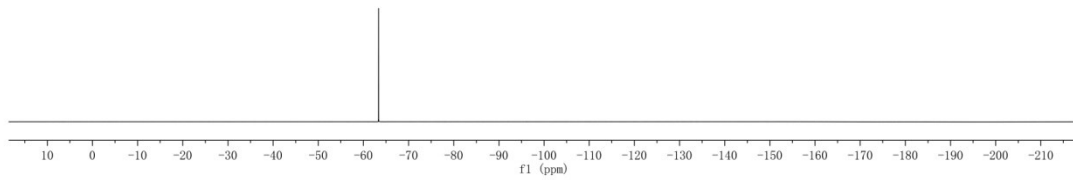
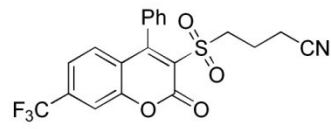


4-((2-Oxo-4-phenyl-7-(trifluoromethyl)-2H-chromen-3-yl)sulfonyl)butanenitrile

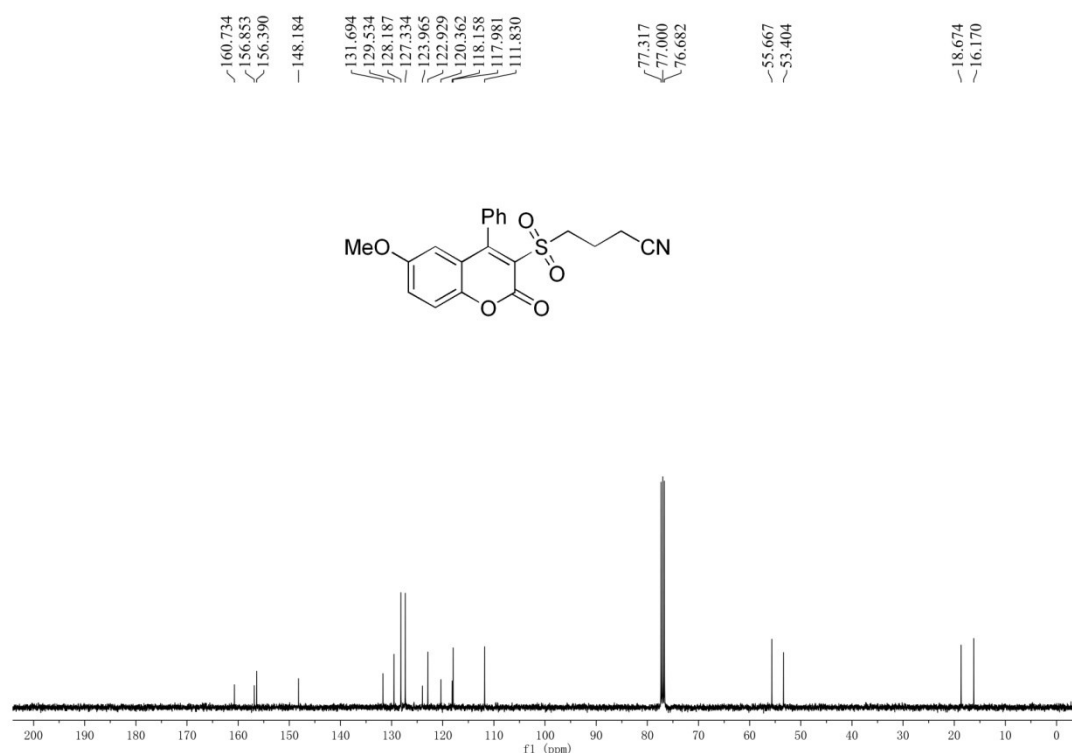
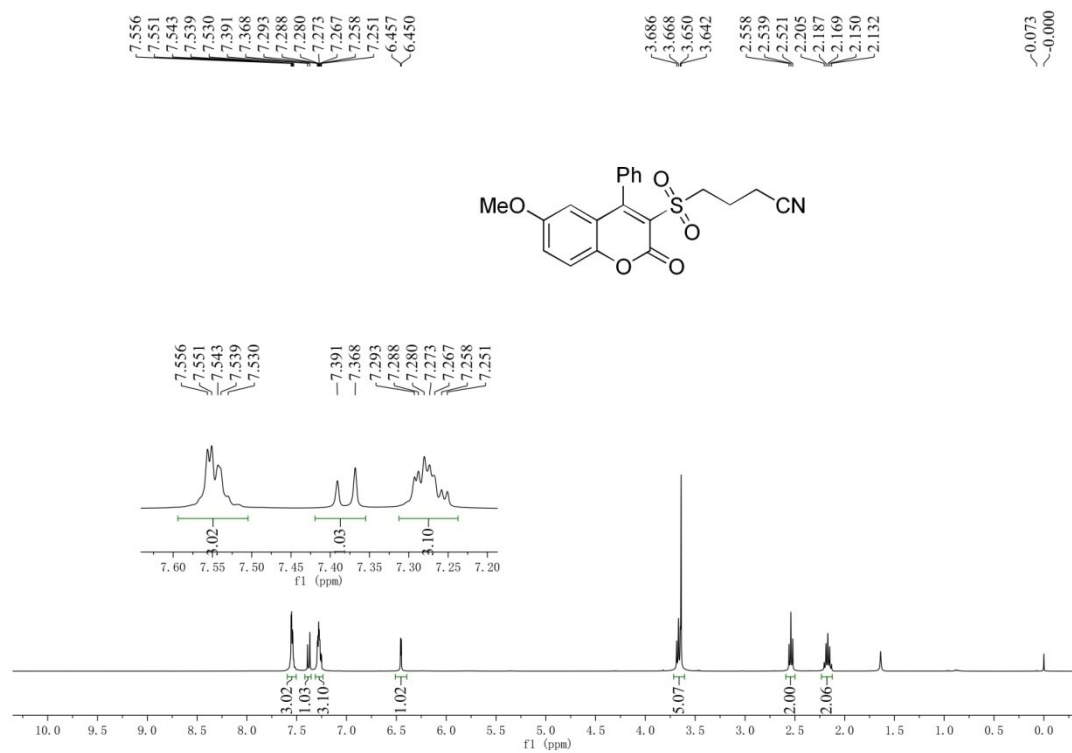
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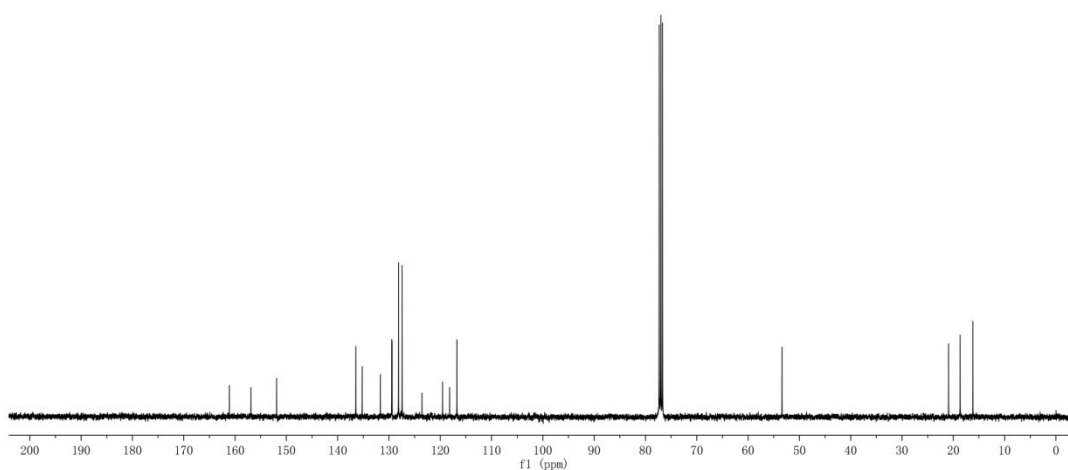
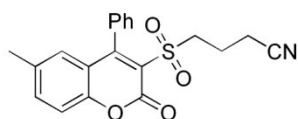
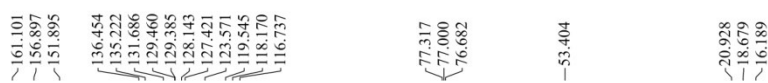
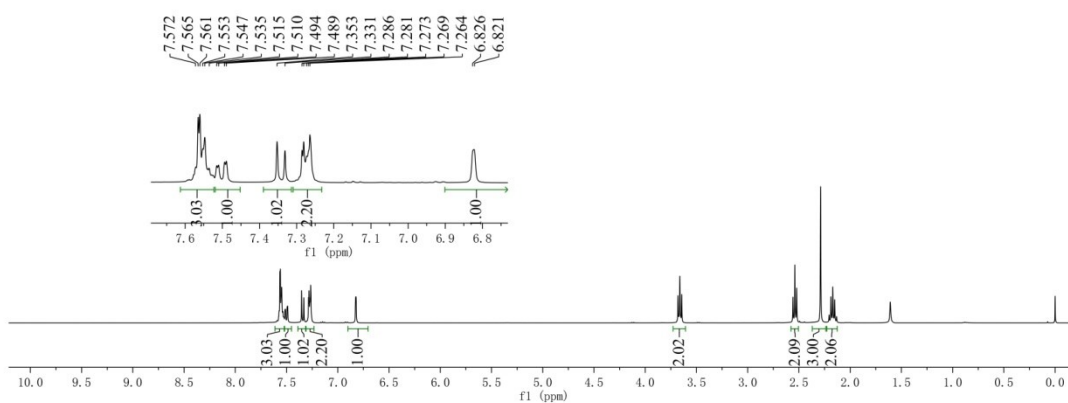
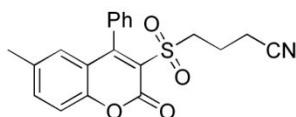
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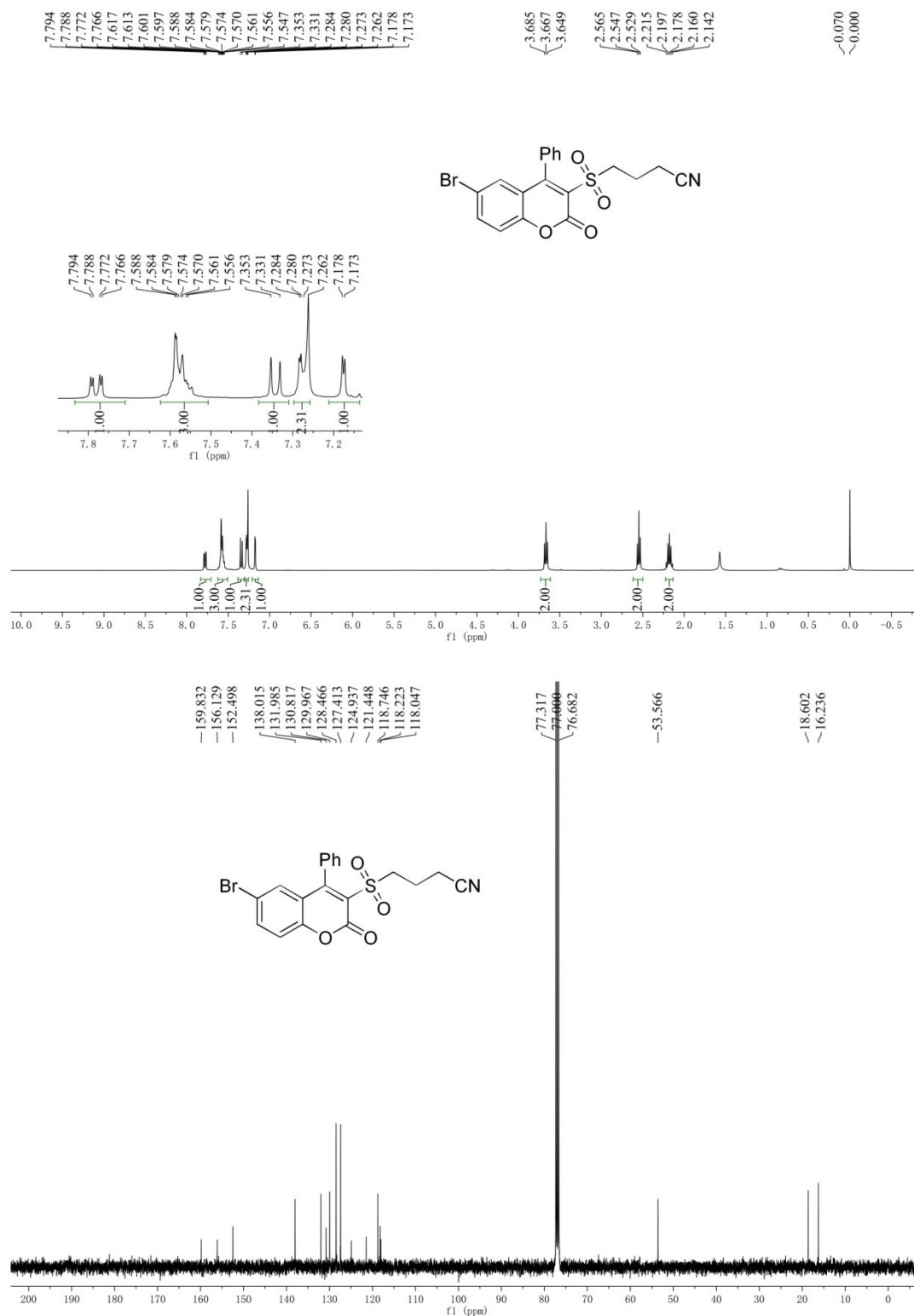
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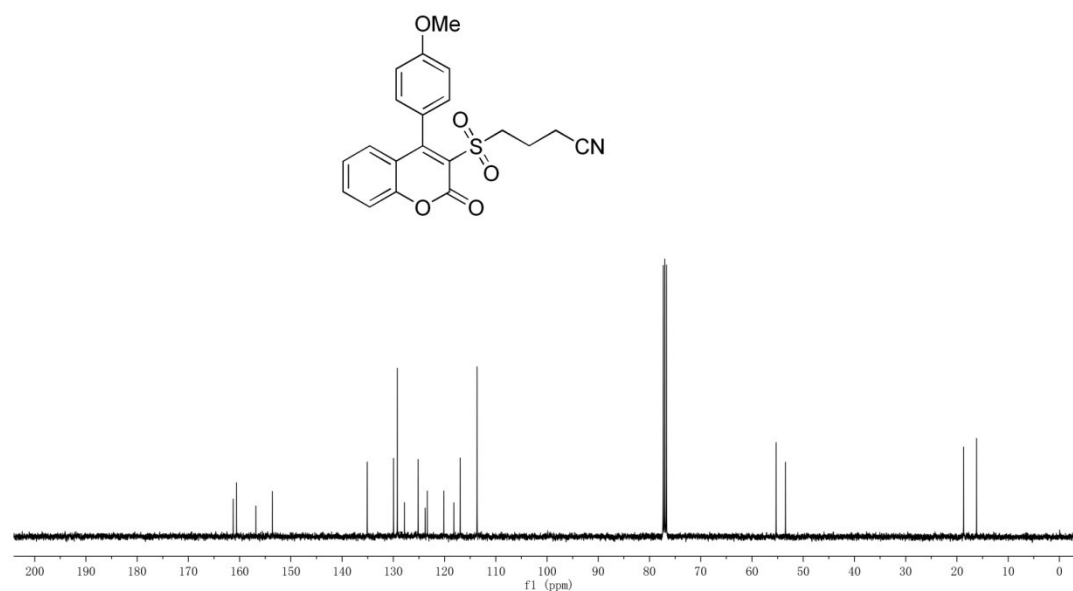
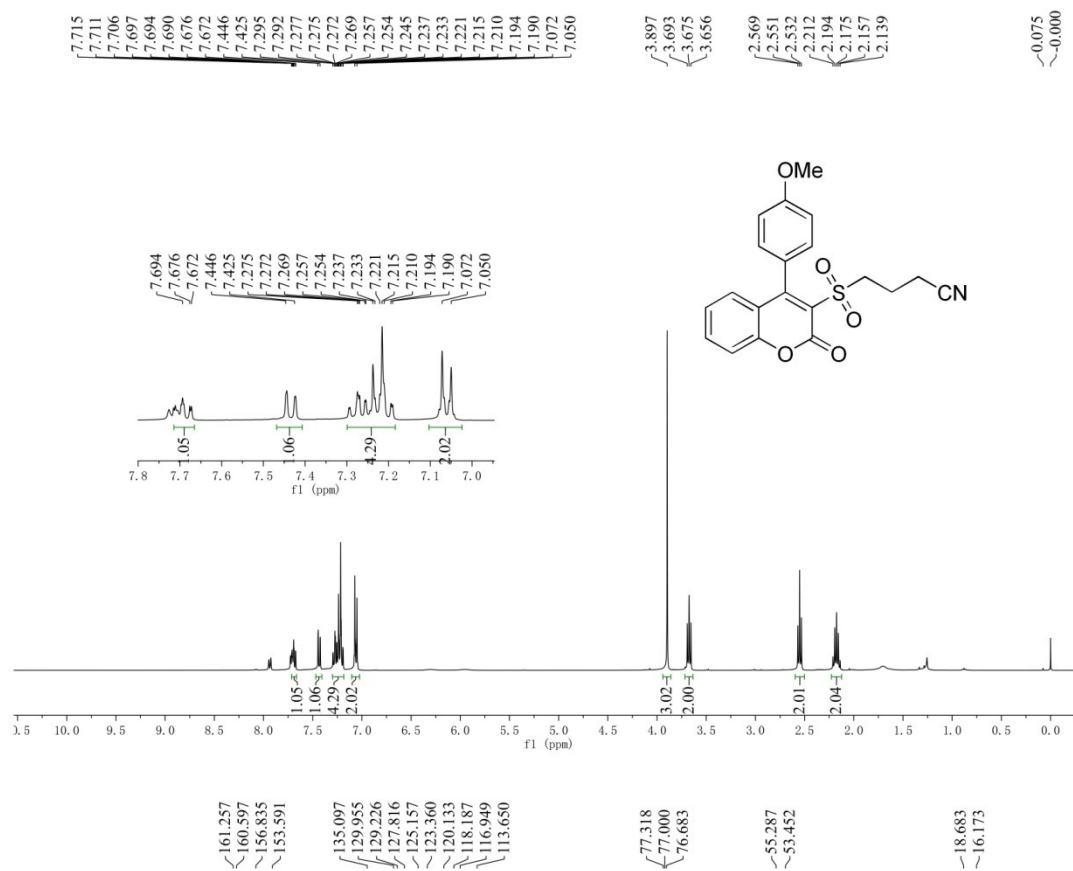
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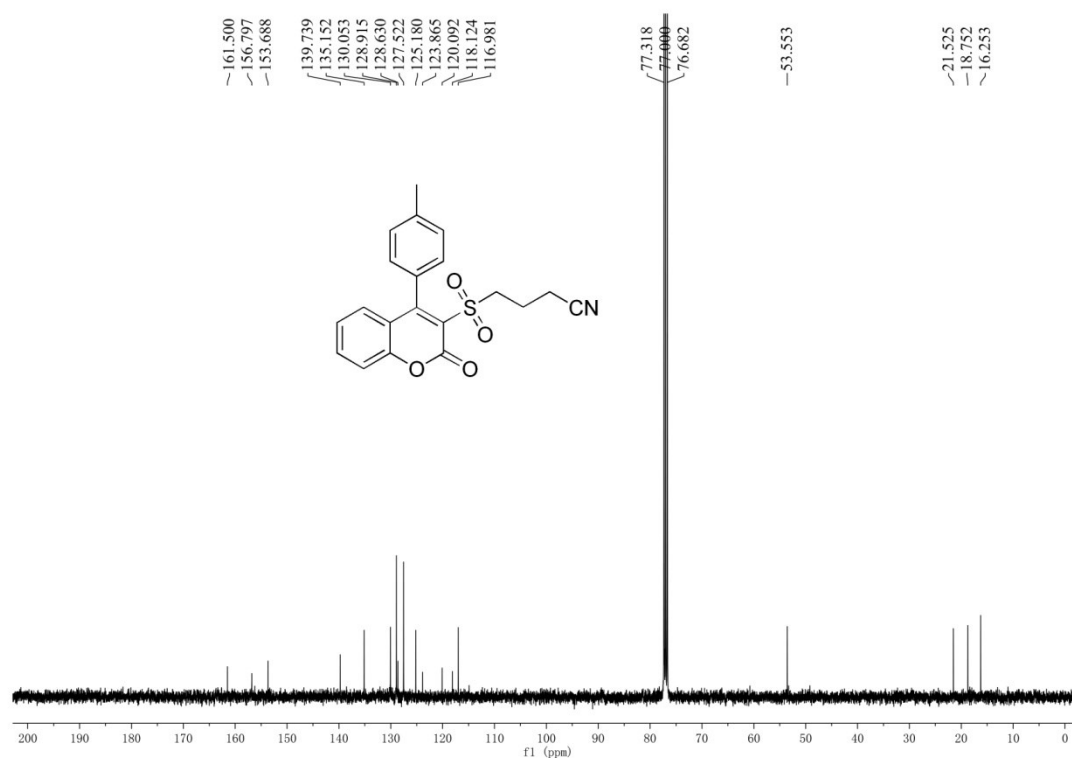
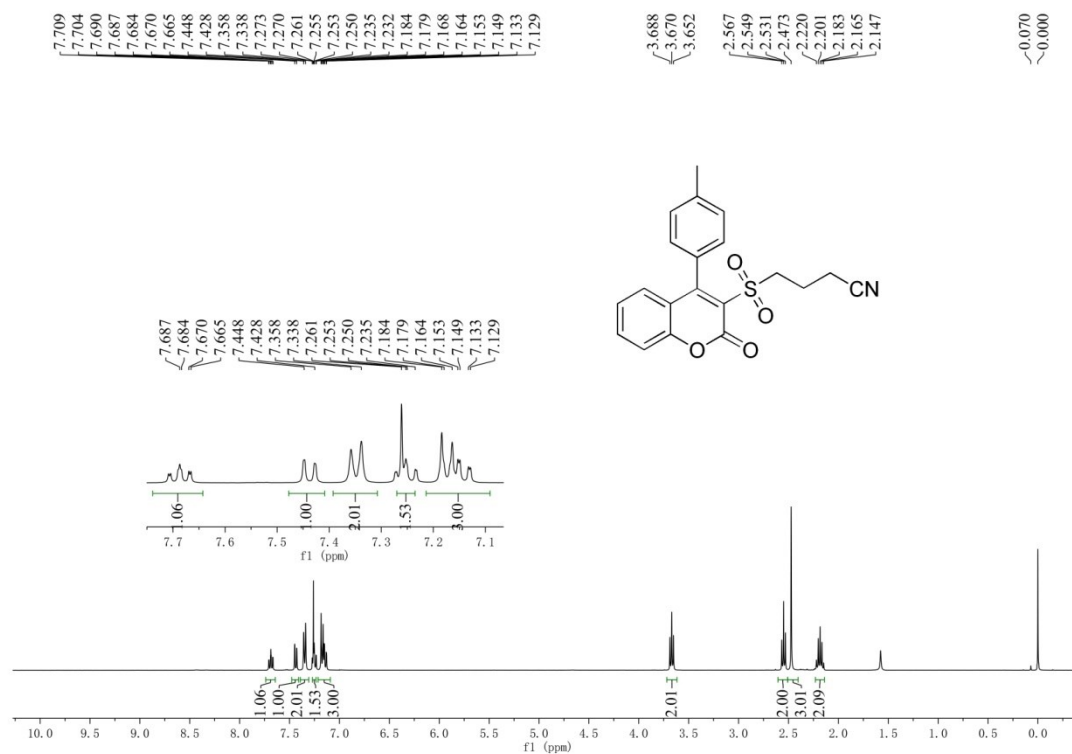
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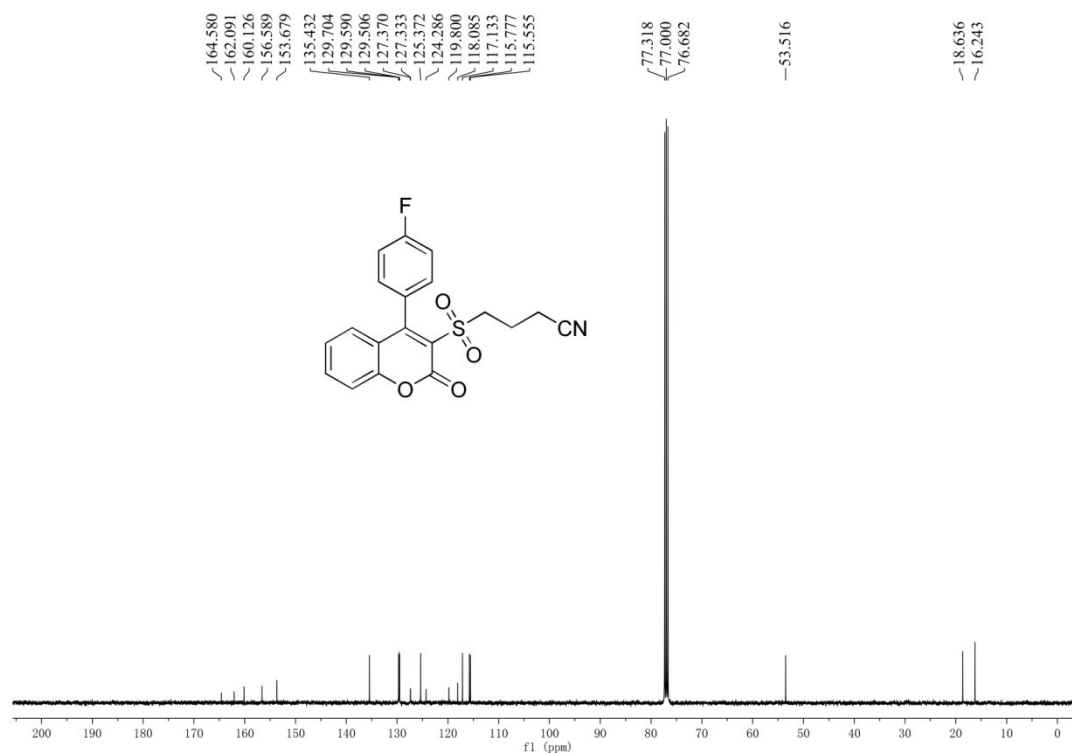
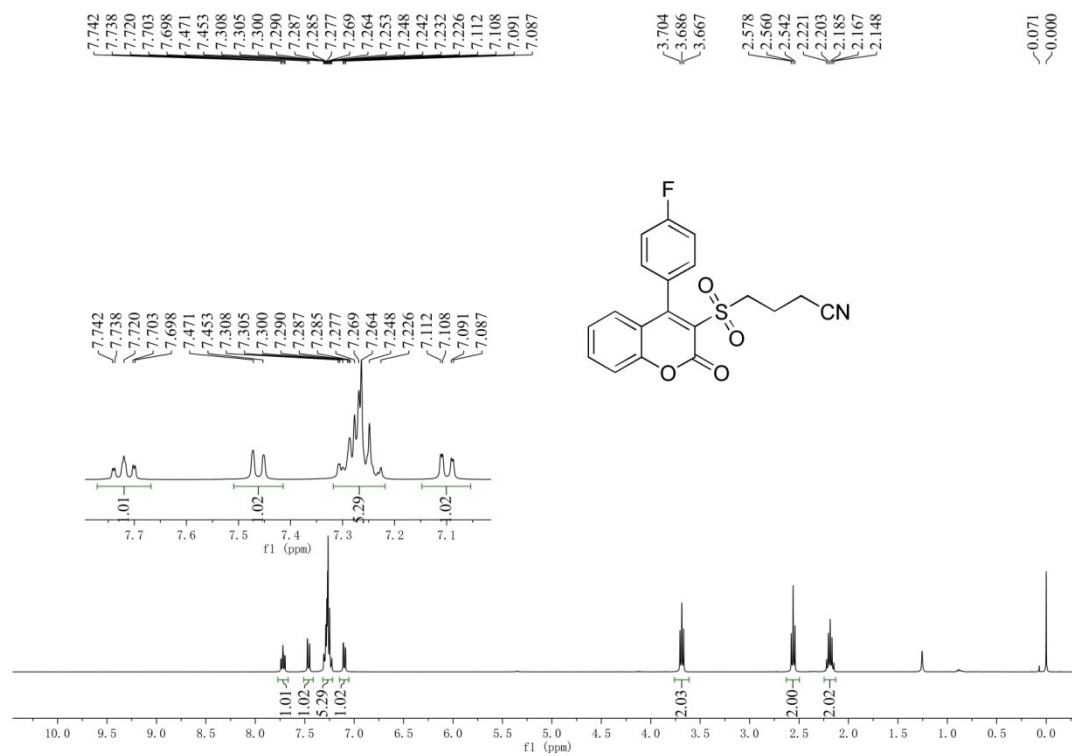
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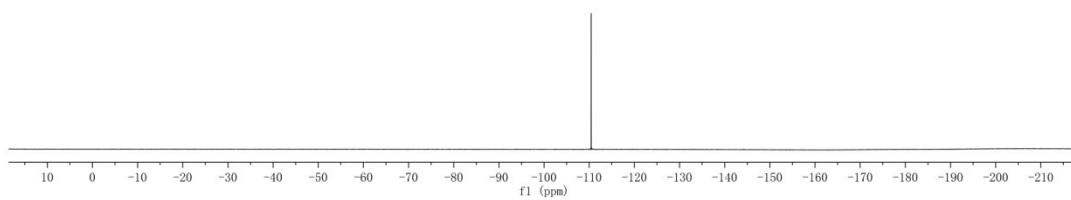
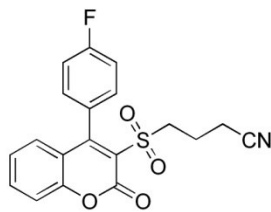
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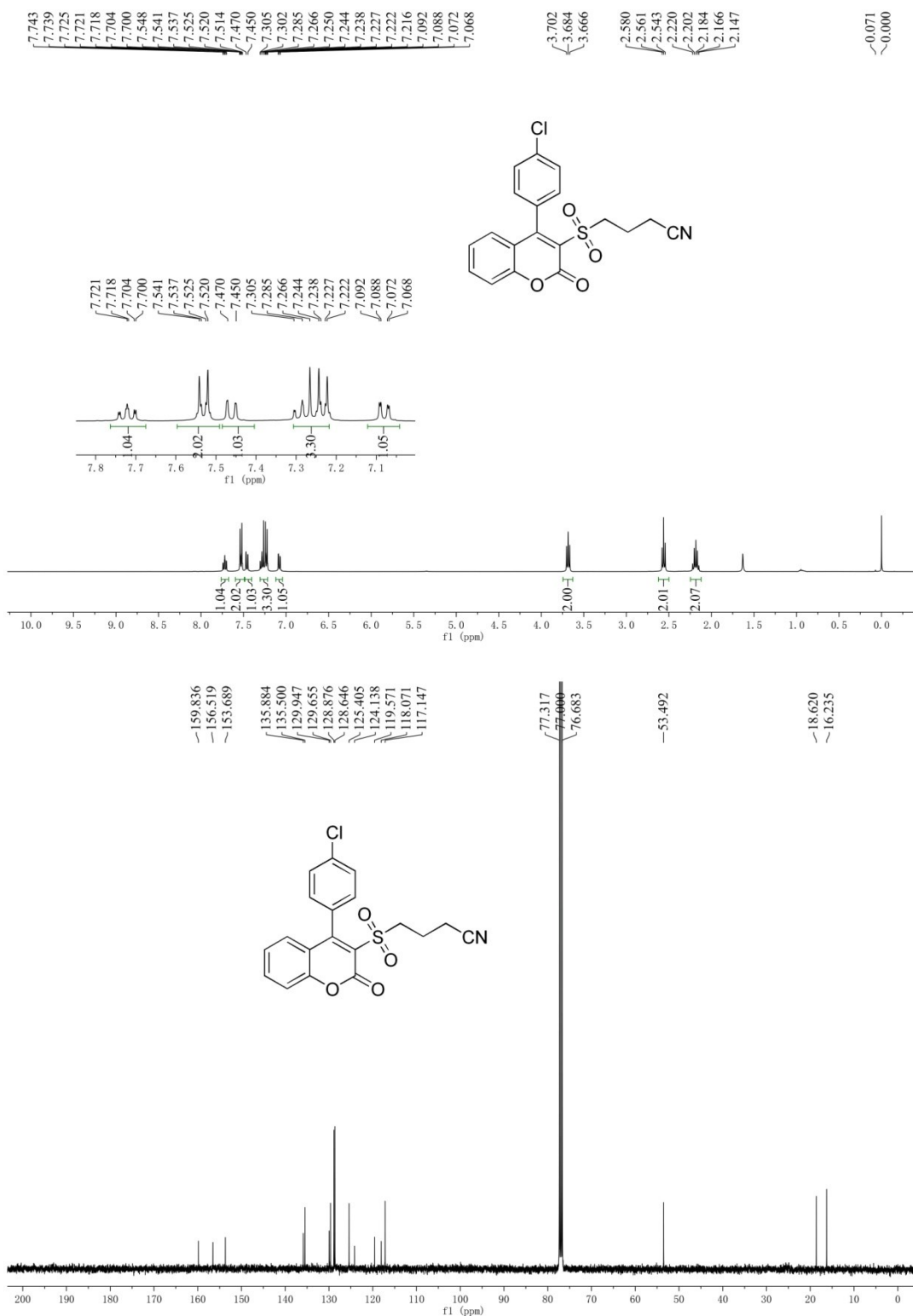
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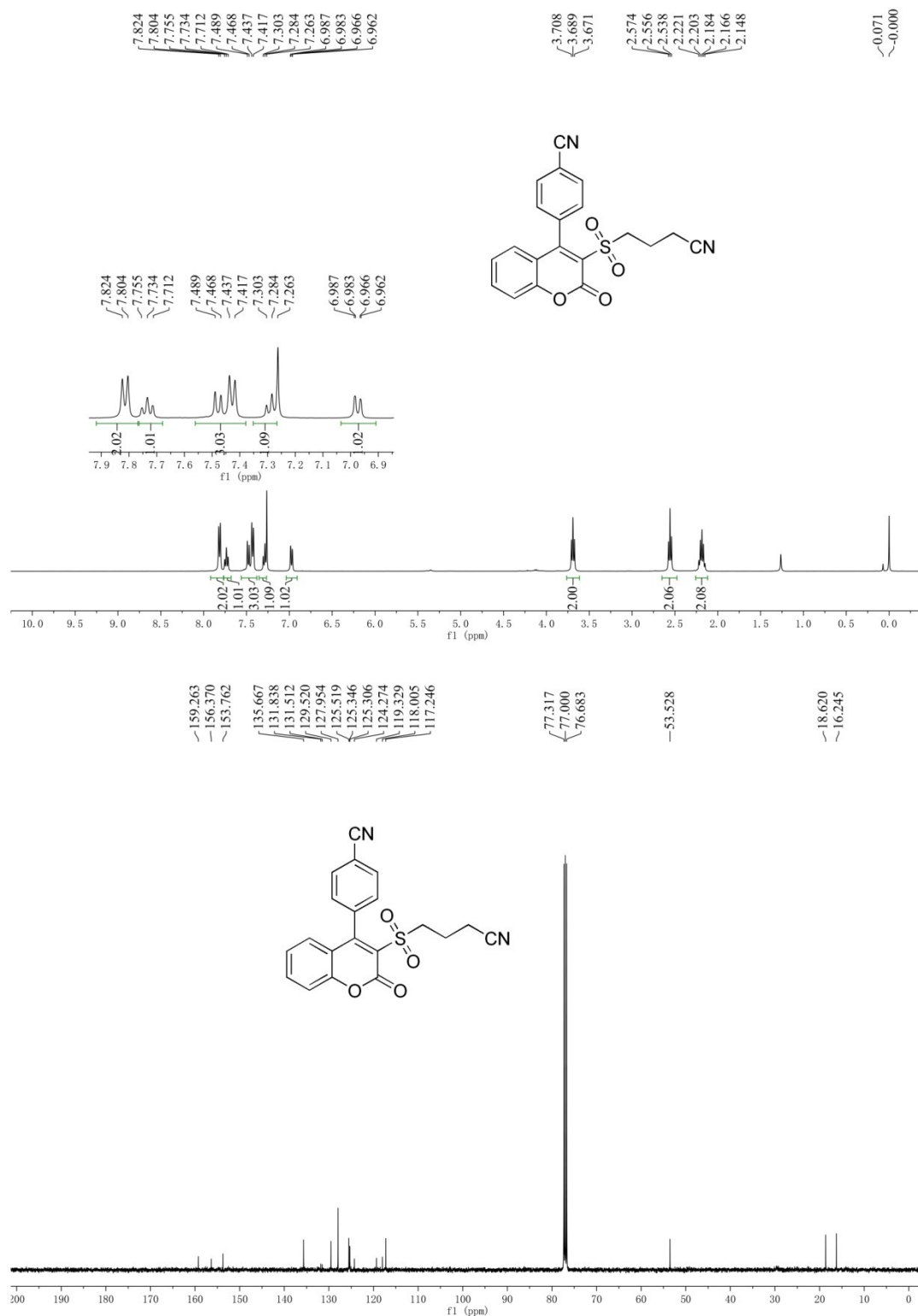
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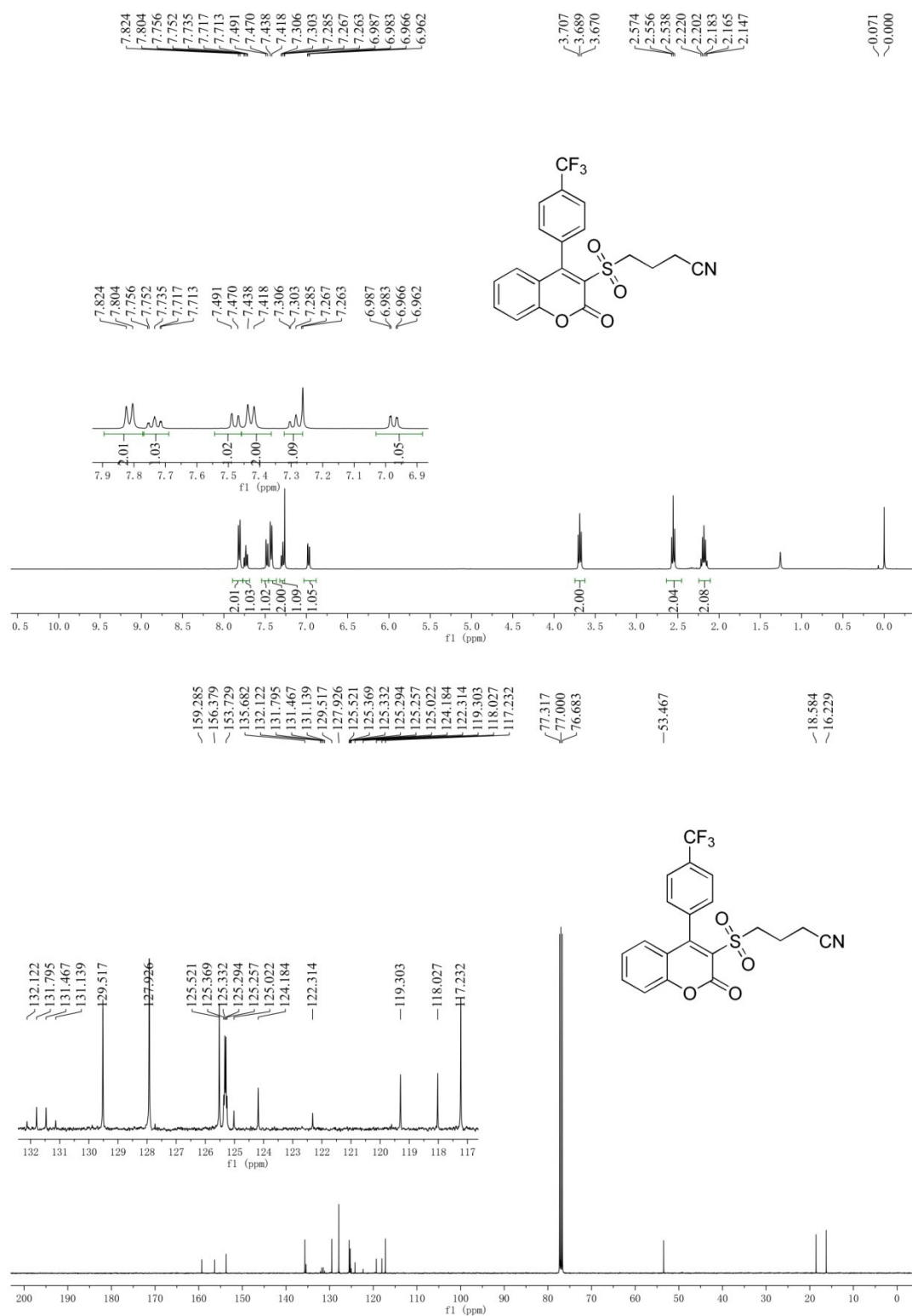


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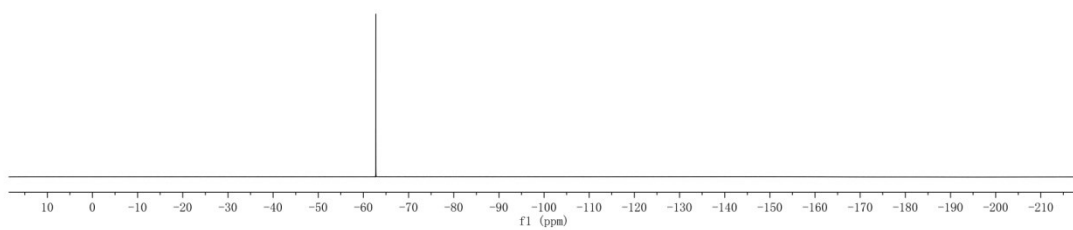
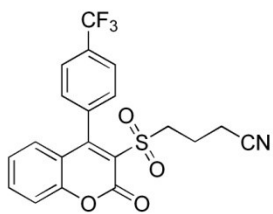


4-((2-Oxo-4-(4-(trifluoromethyl)phenyl)-2H-chromen-3-yl)sulfonyl)butanenitrile

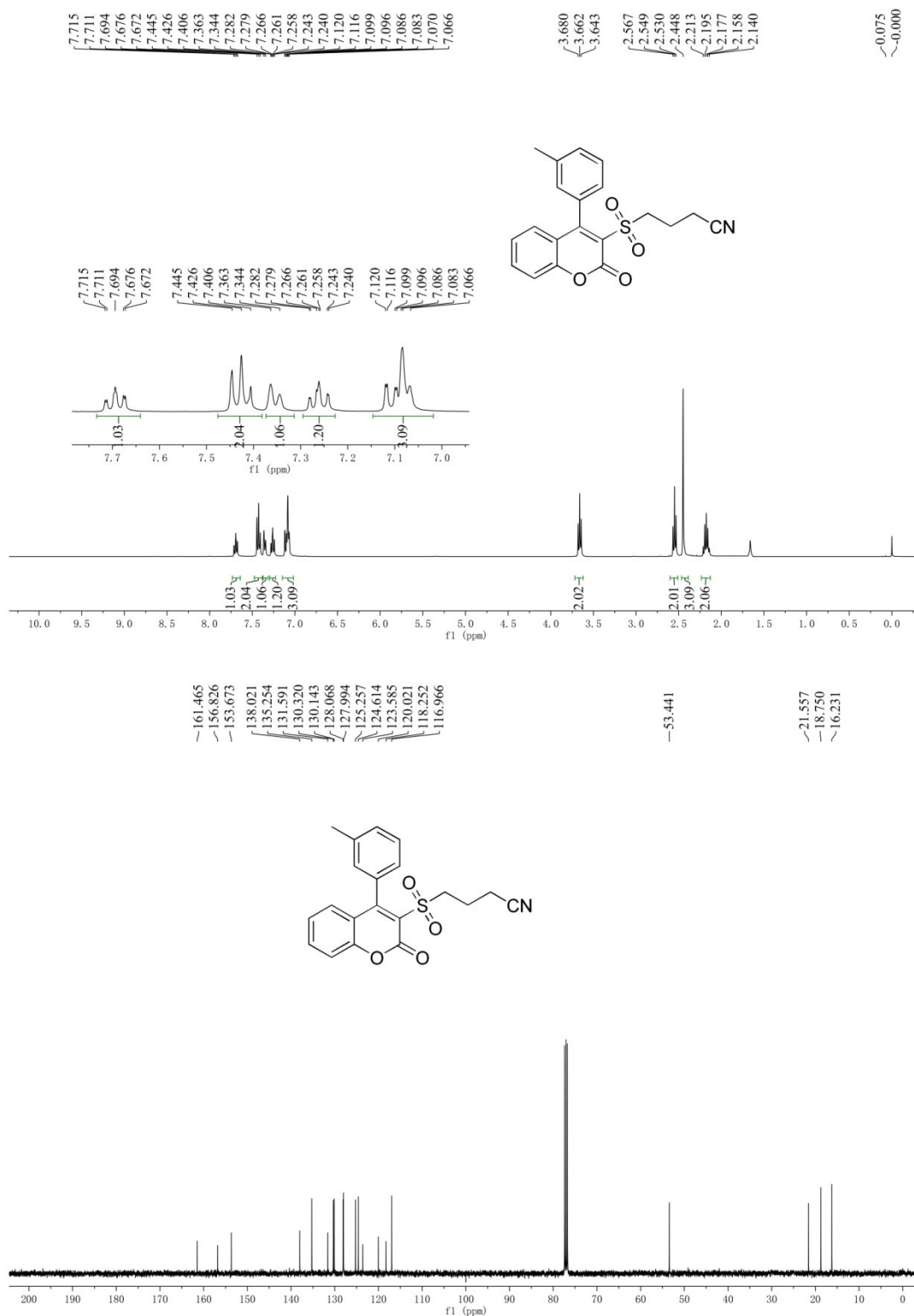
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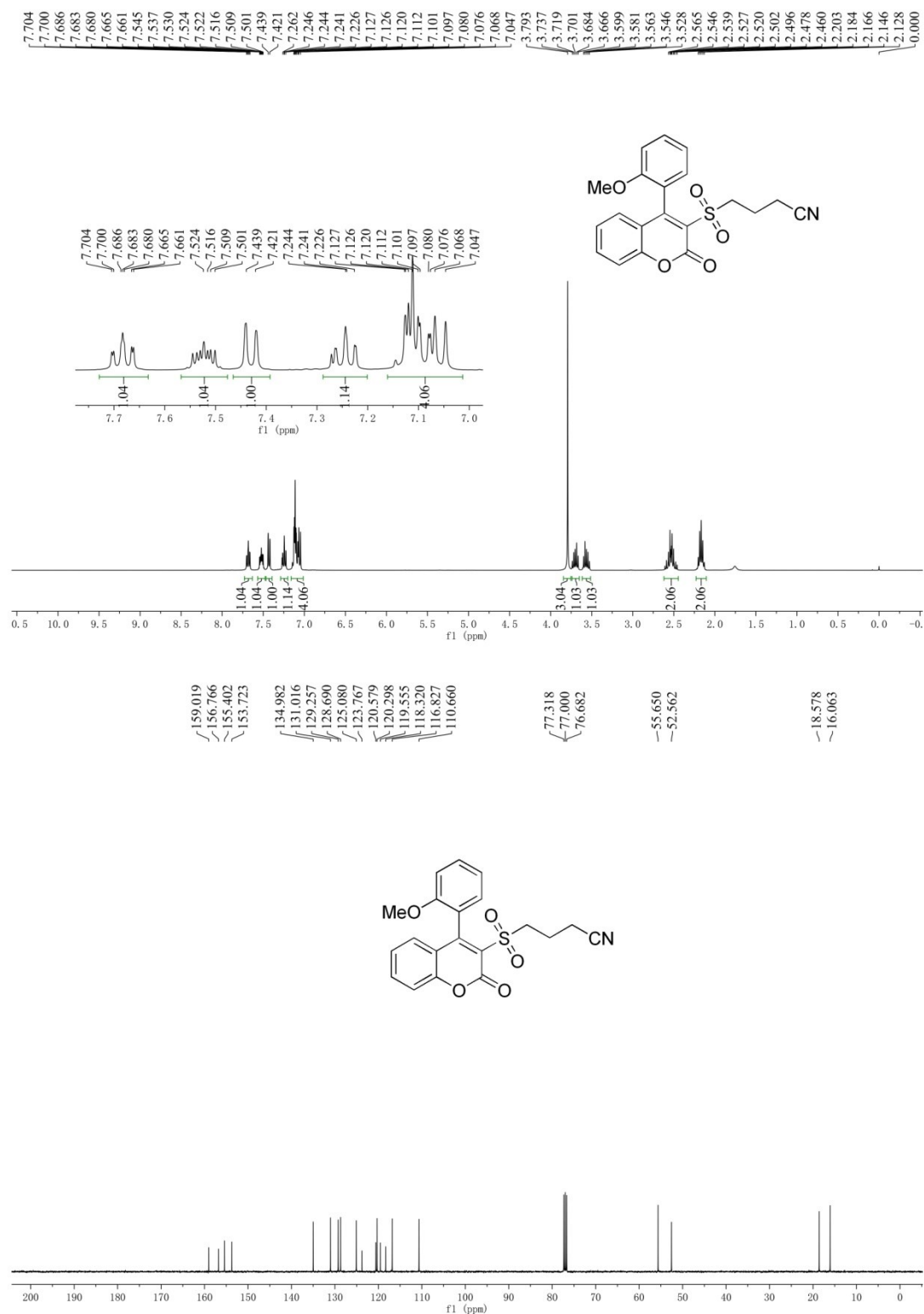
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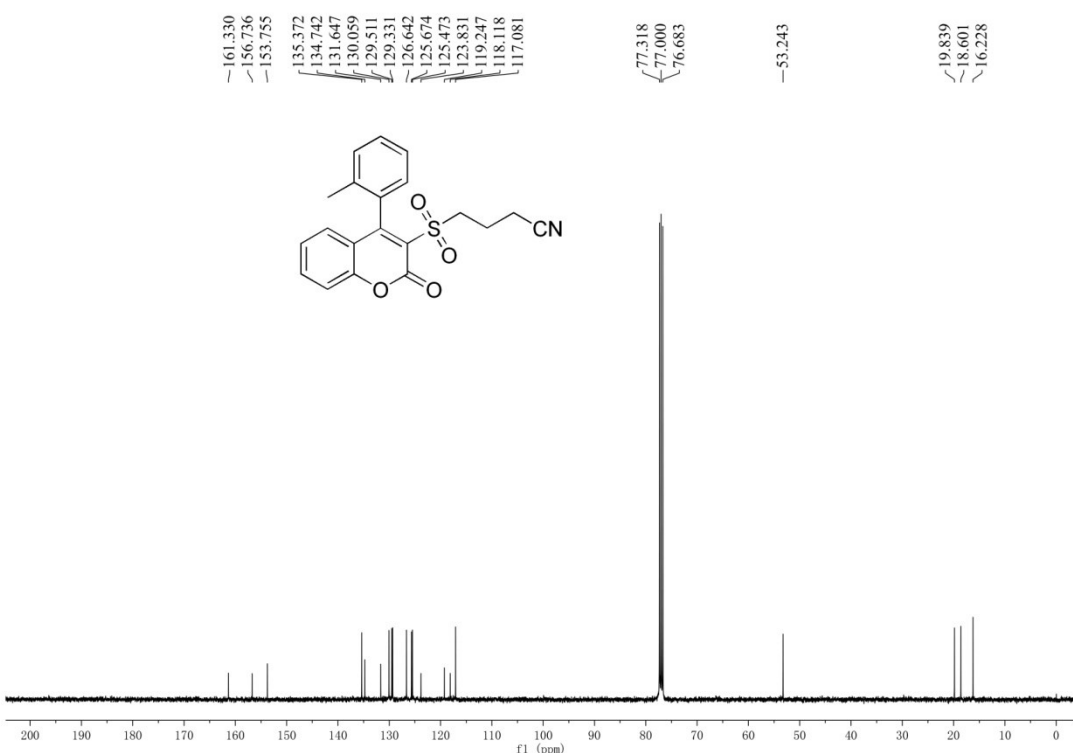
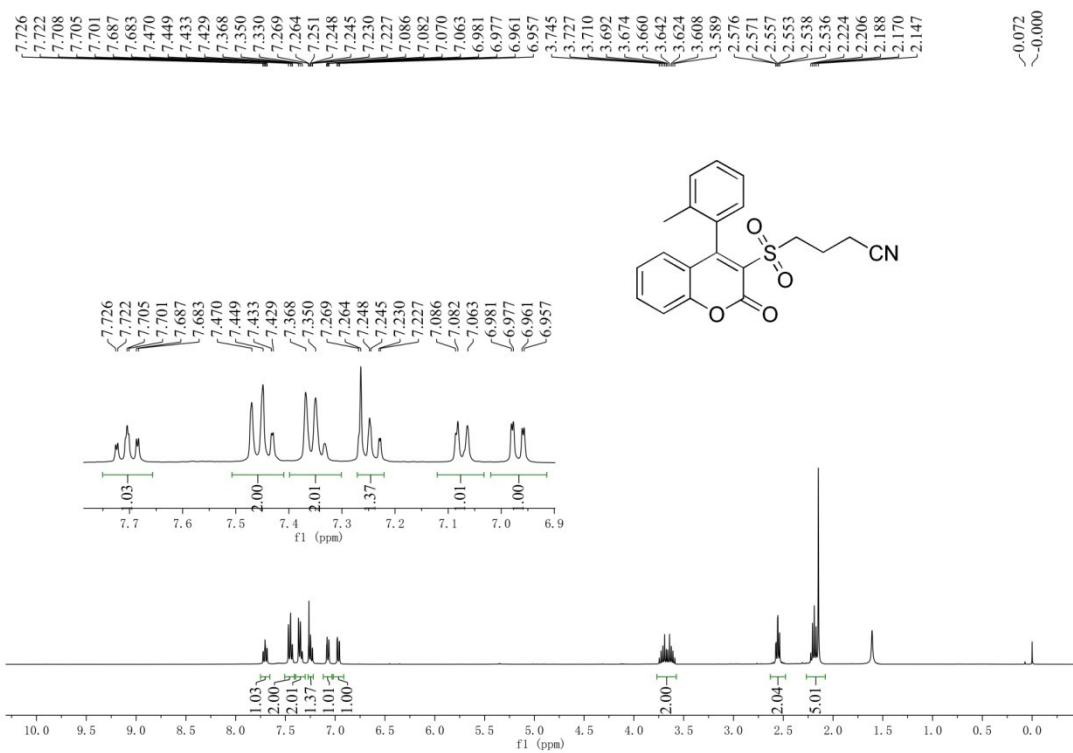
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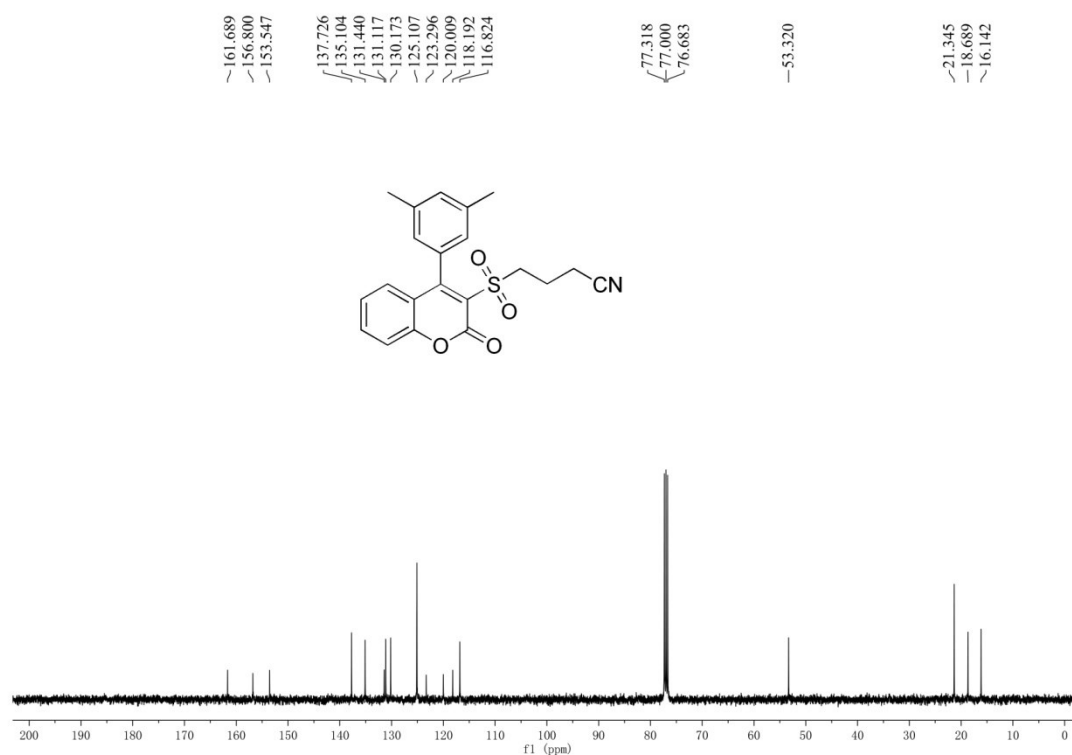
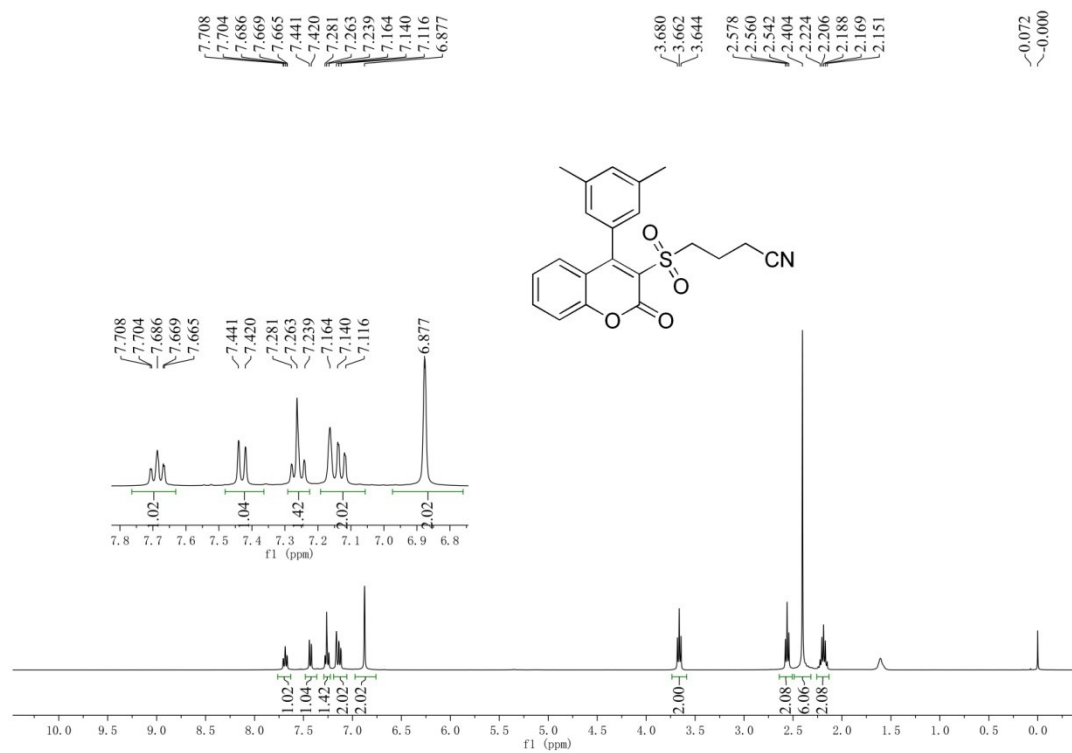
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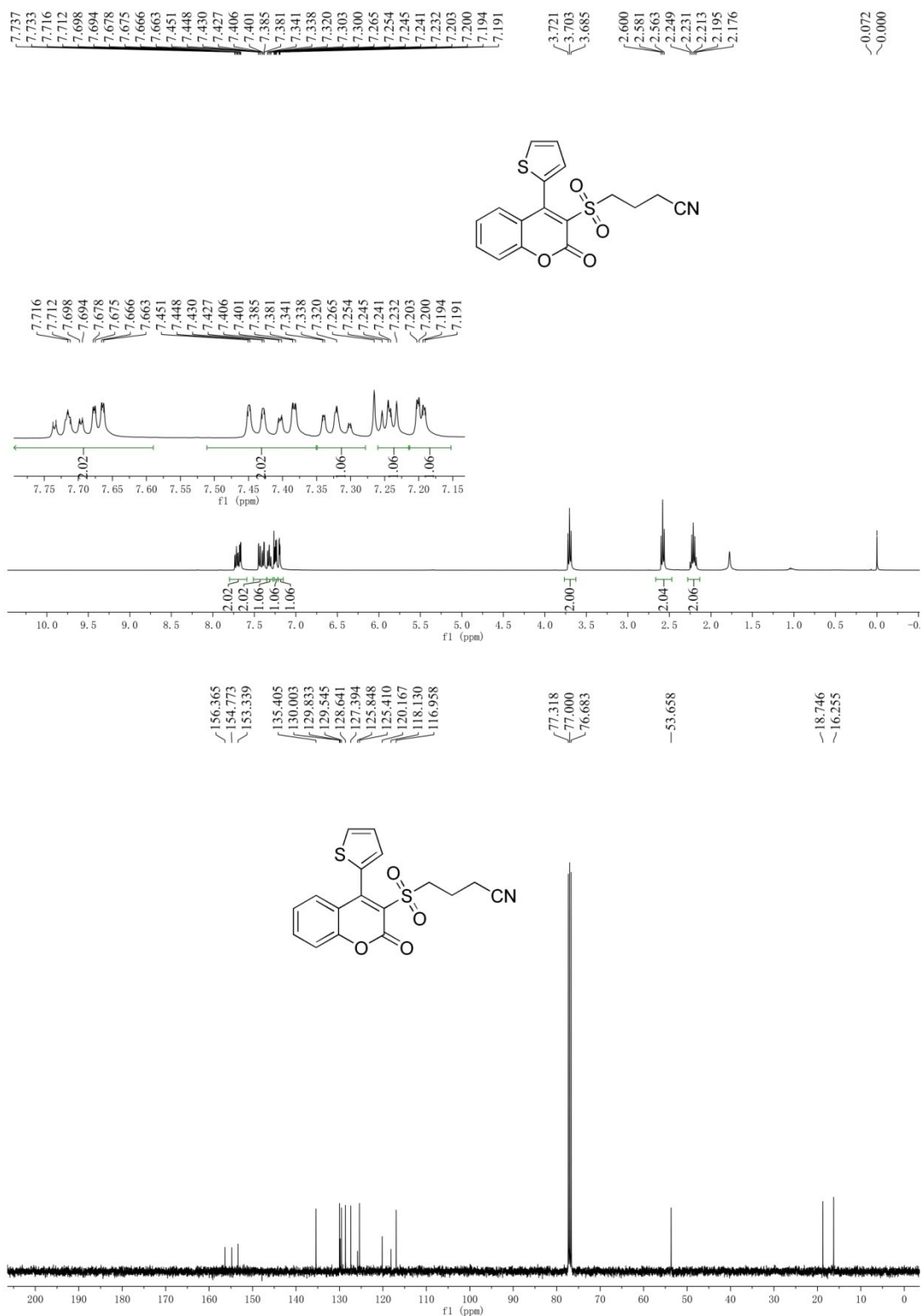
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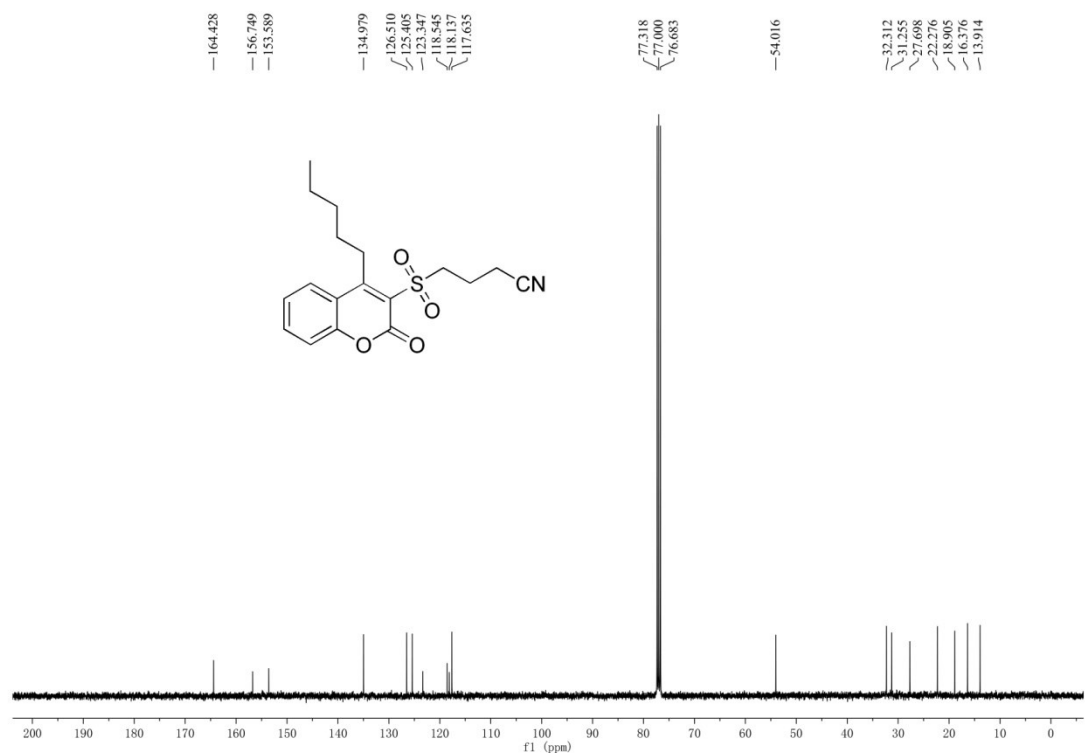
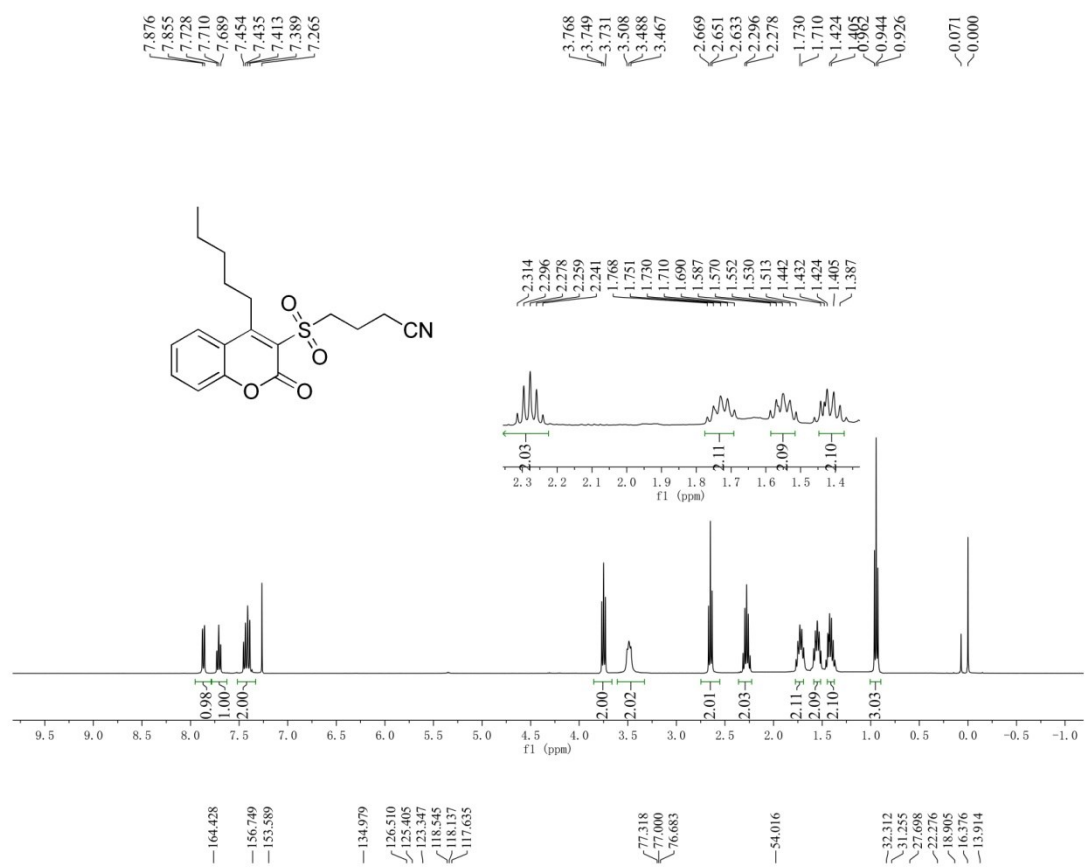
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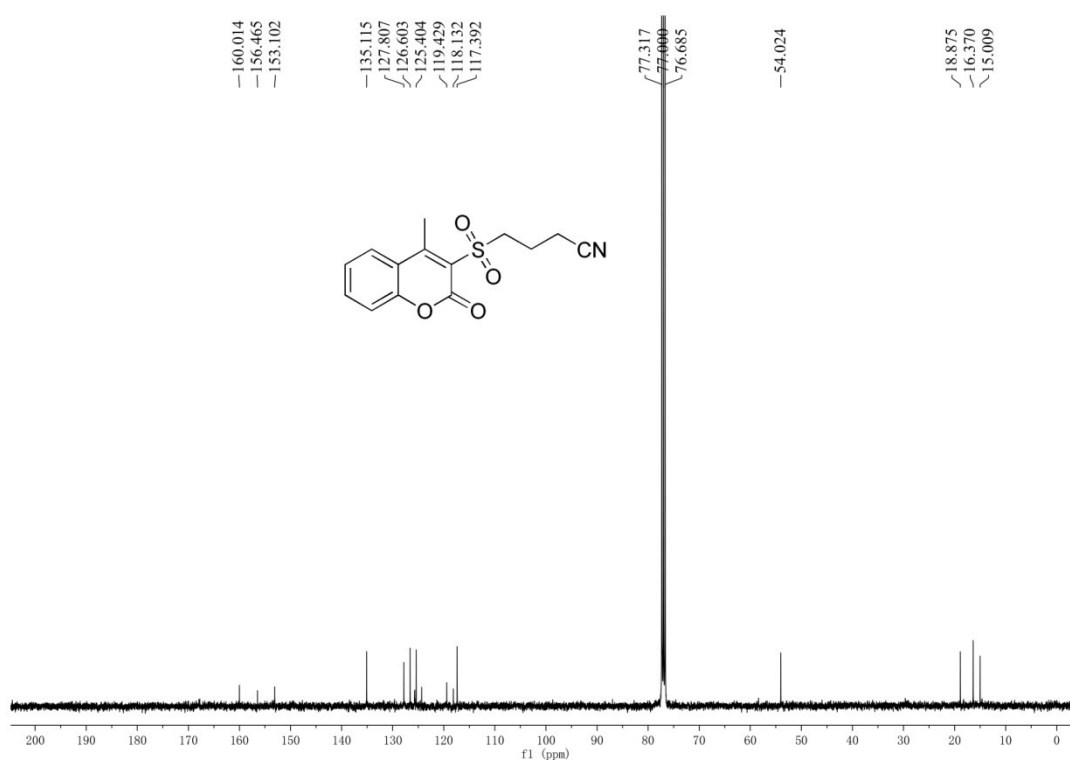
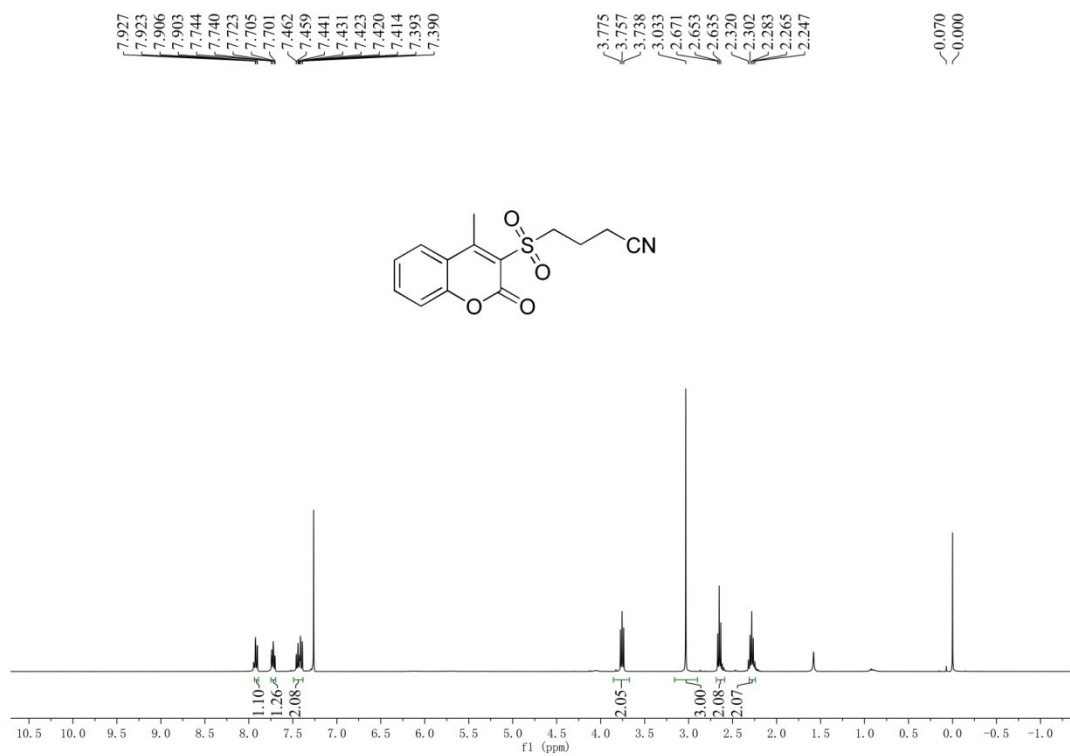
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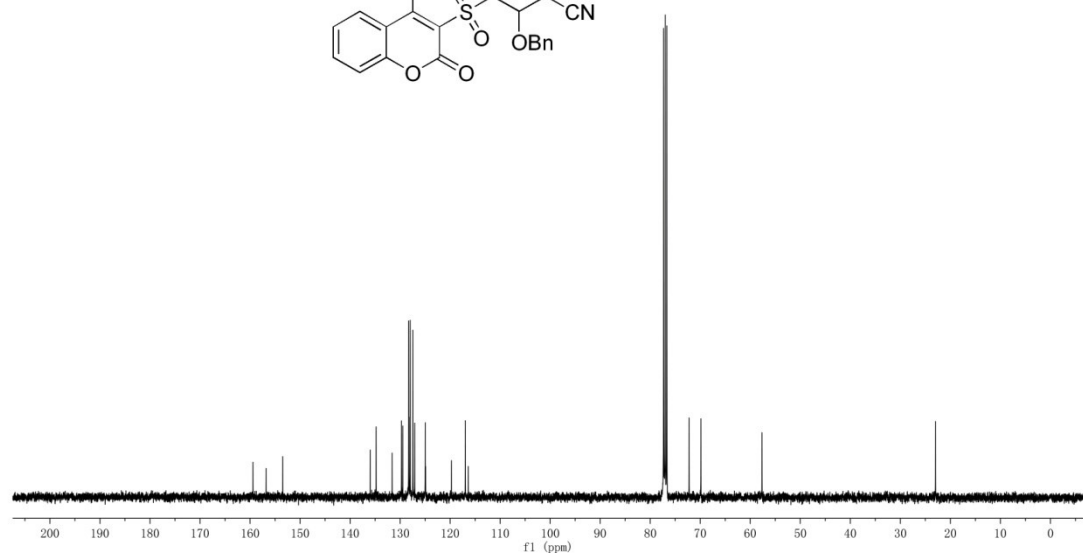
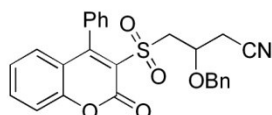
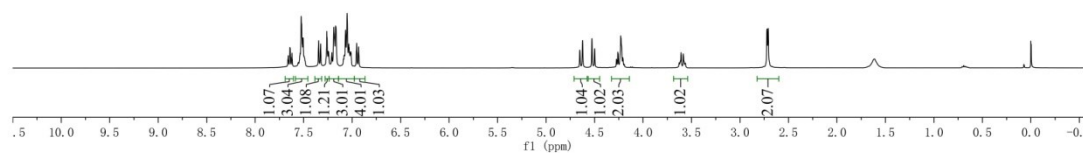
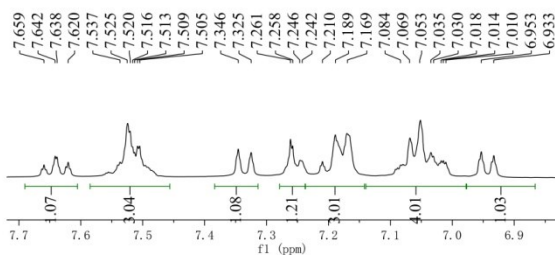
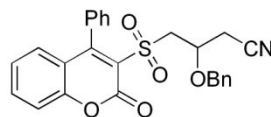
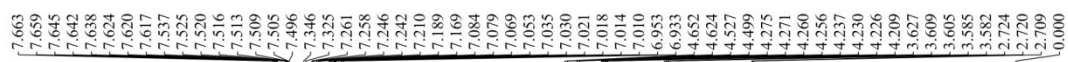
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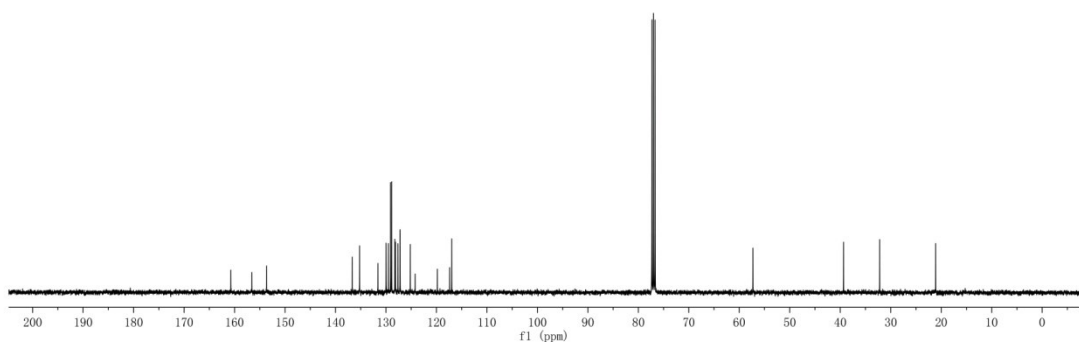
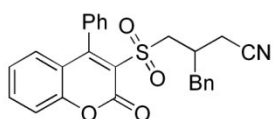
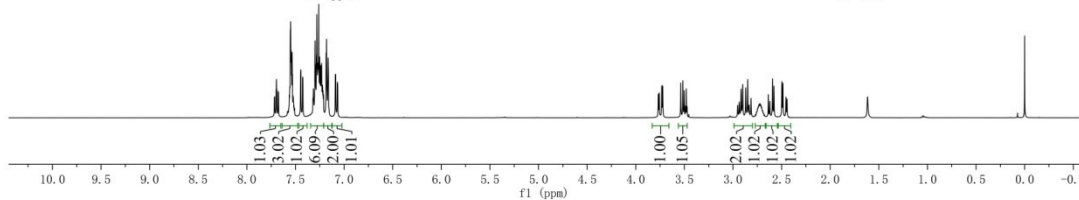
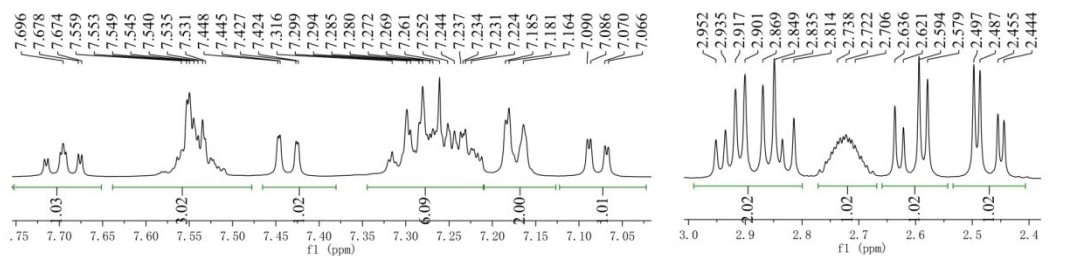
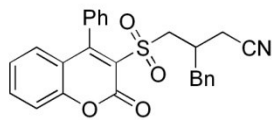
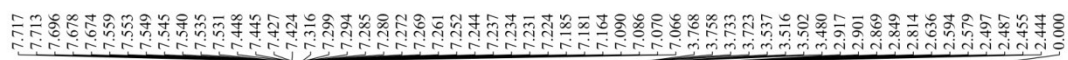
4-((4-Methyl-2-oxo-2H-chromen-3-yl)sulfonyl)butanenitrile (3aaa)



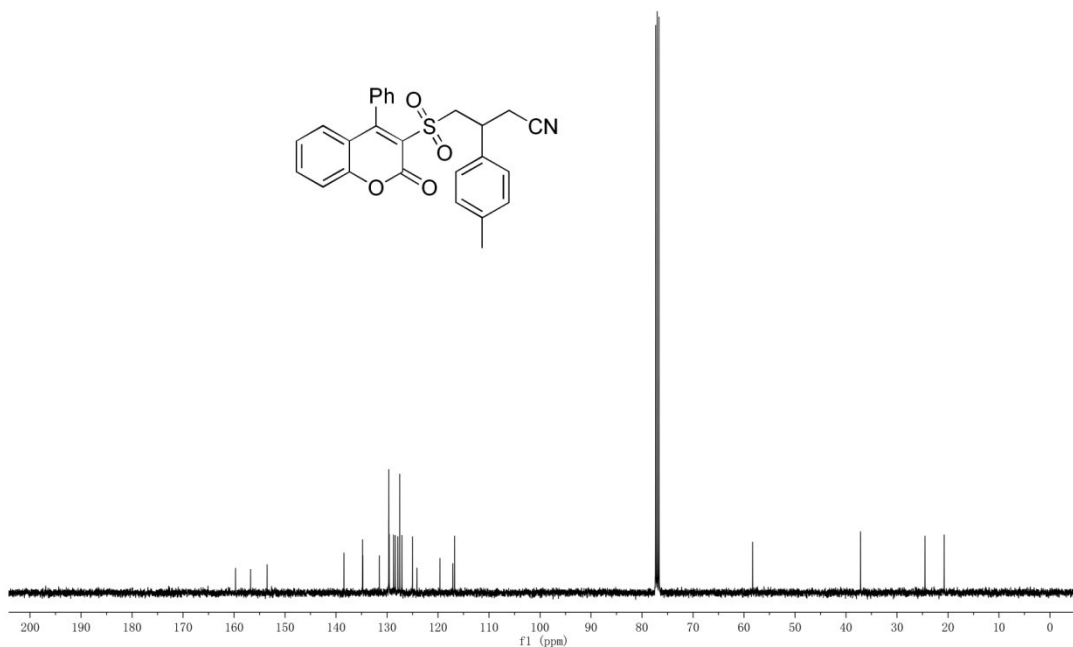
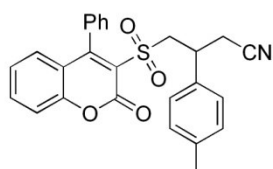
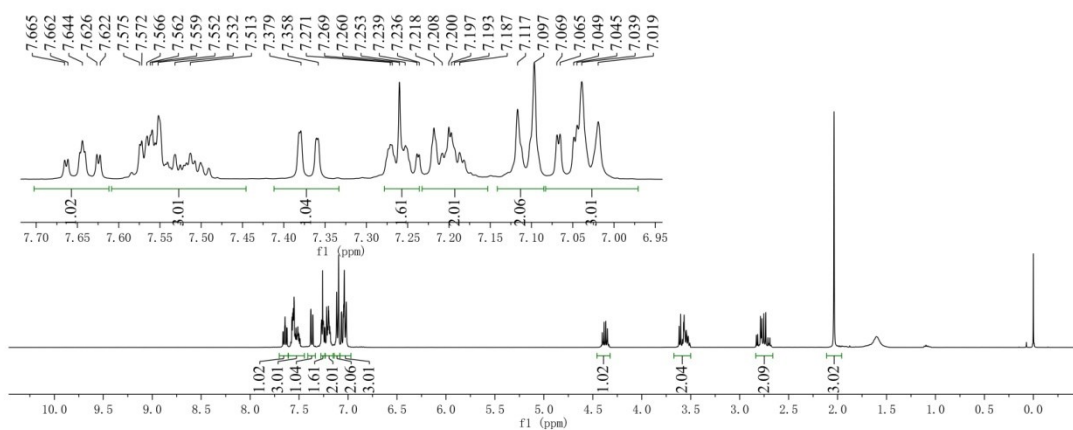
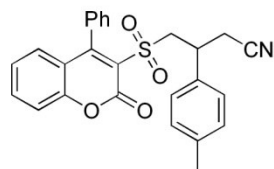
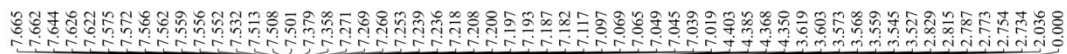
3-(Benzyloxy)-4-((2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)butanenitrile (3ab)



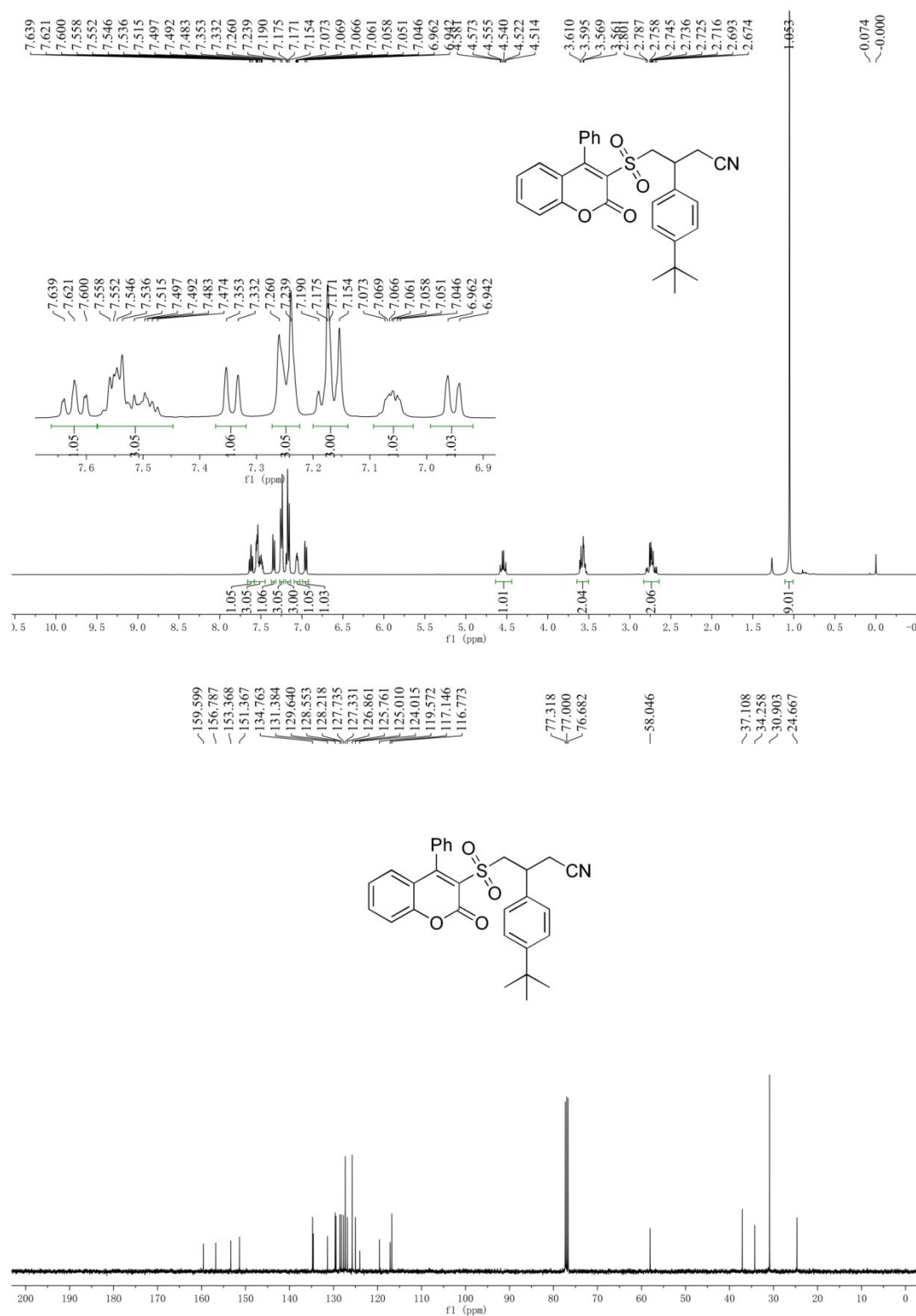
3-Benzyl-4-((2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)butanenitrile (3ac)



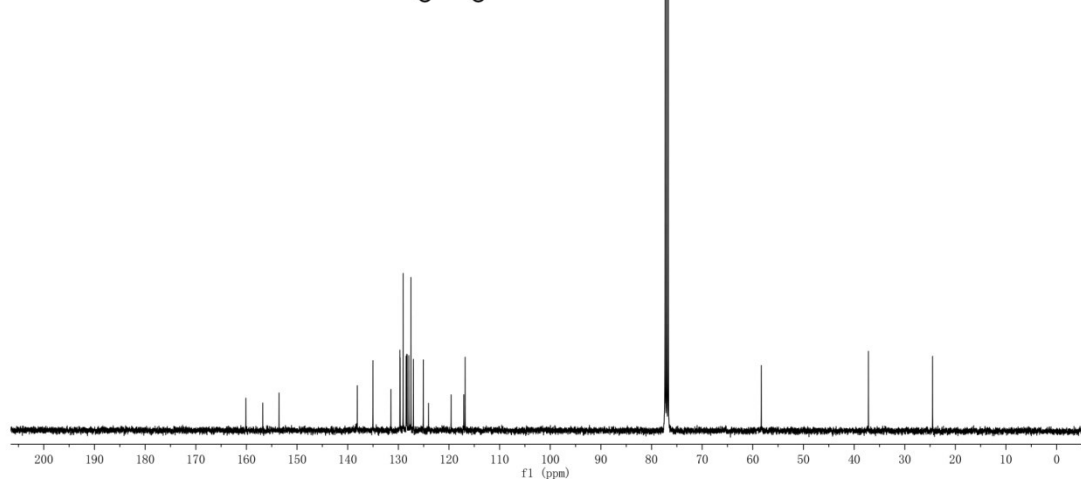
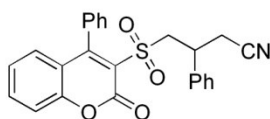
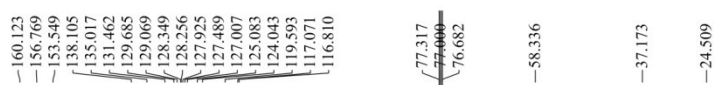
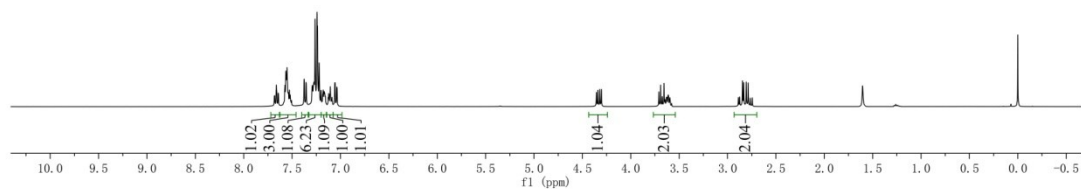
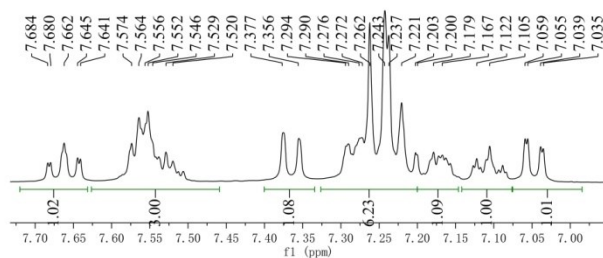
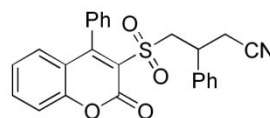
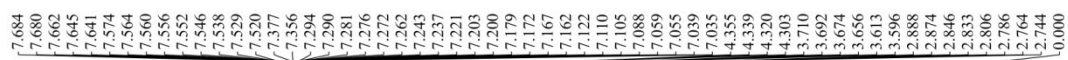
4-((2-Oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)-3-(p-tolyl)butanenitrile (3ad)



3-(4-(Tert-butyl)phenyl)-4-((2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)butanenitrile (3ae)

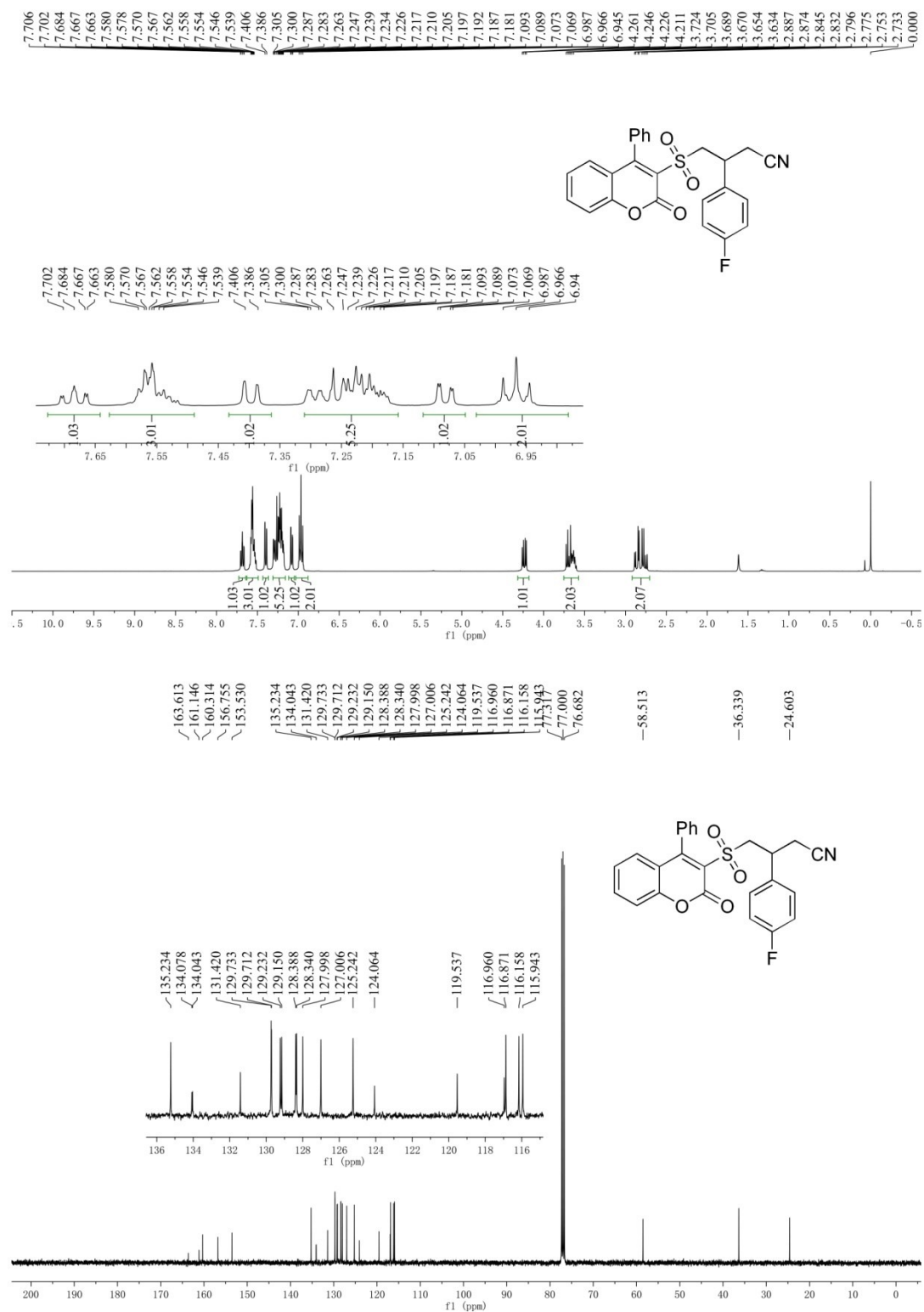


4-((2-Oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)-3-phenylbutanenitrile (3af)

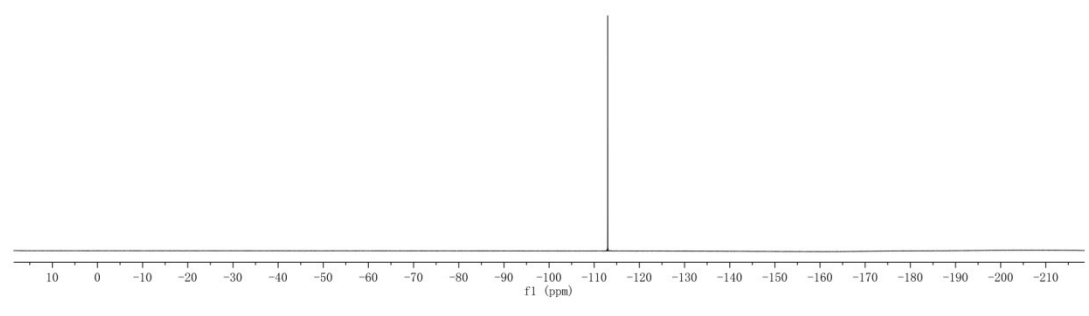
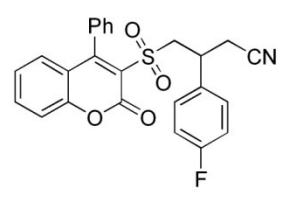


3-(4-Fluorophenyl)-4-((2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)butanenitrile

(3ag)

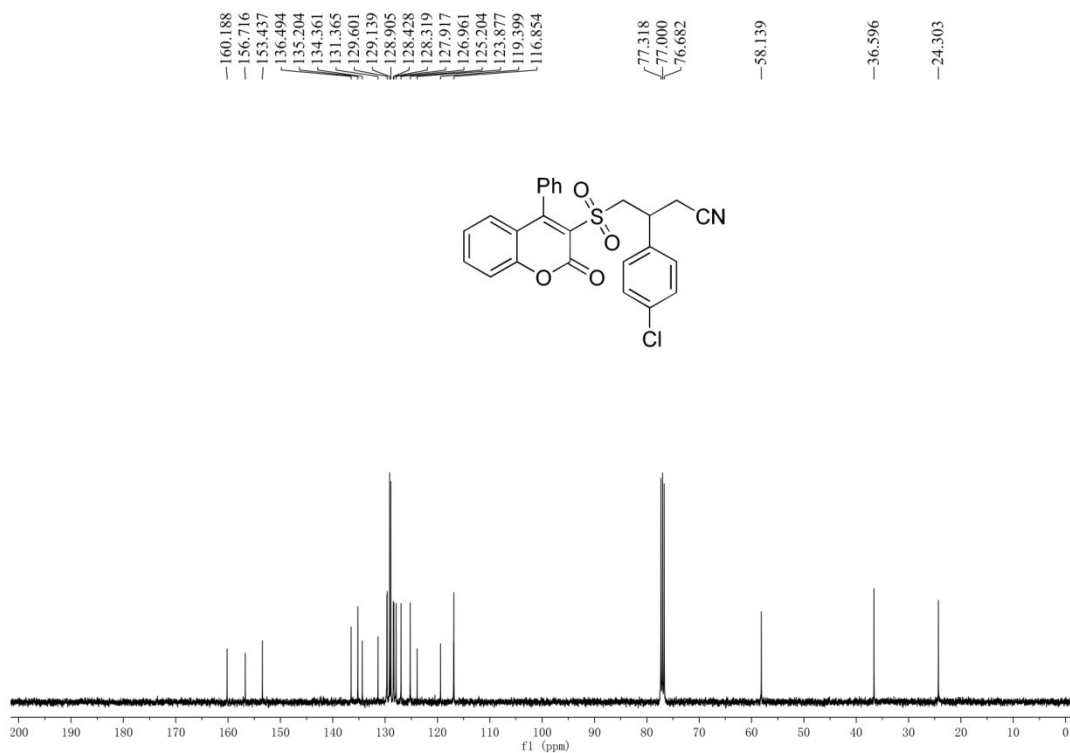
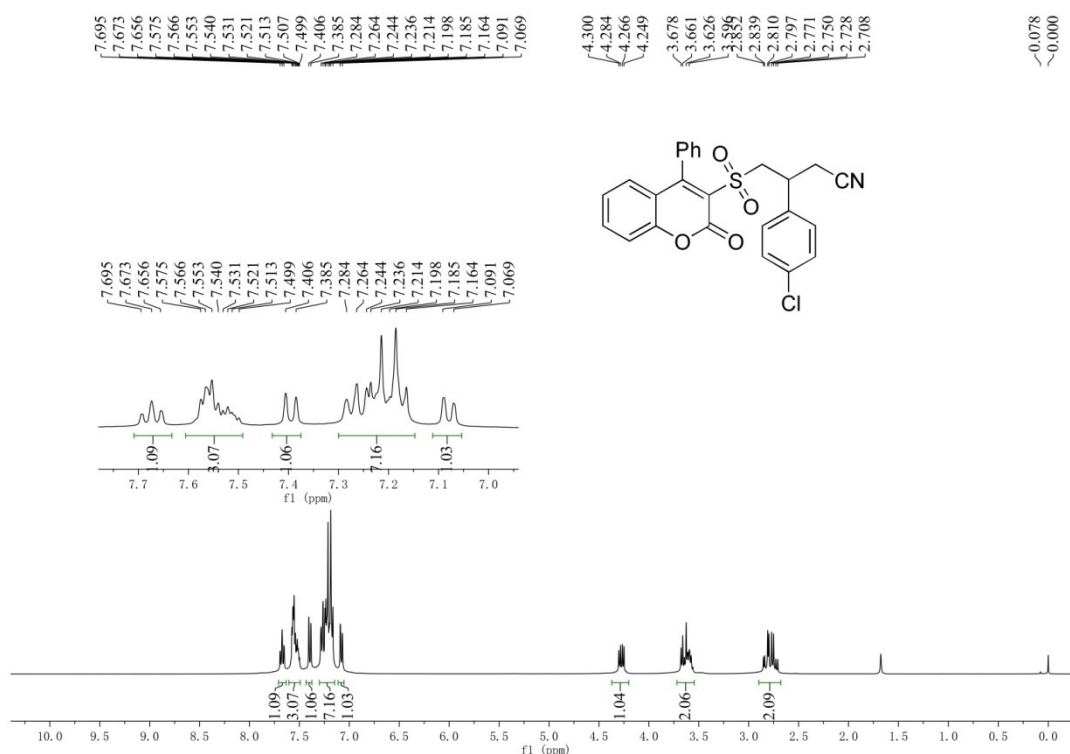


--113.002



3-(4-Chlorophenyl)-4-((2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)butanenitrile

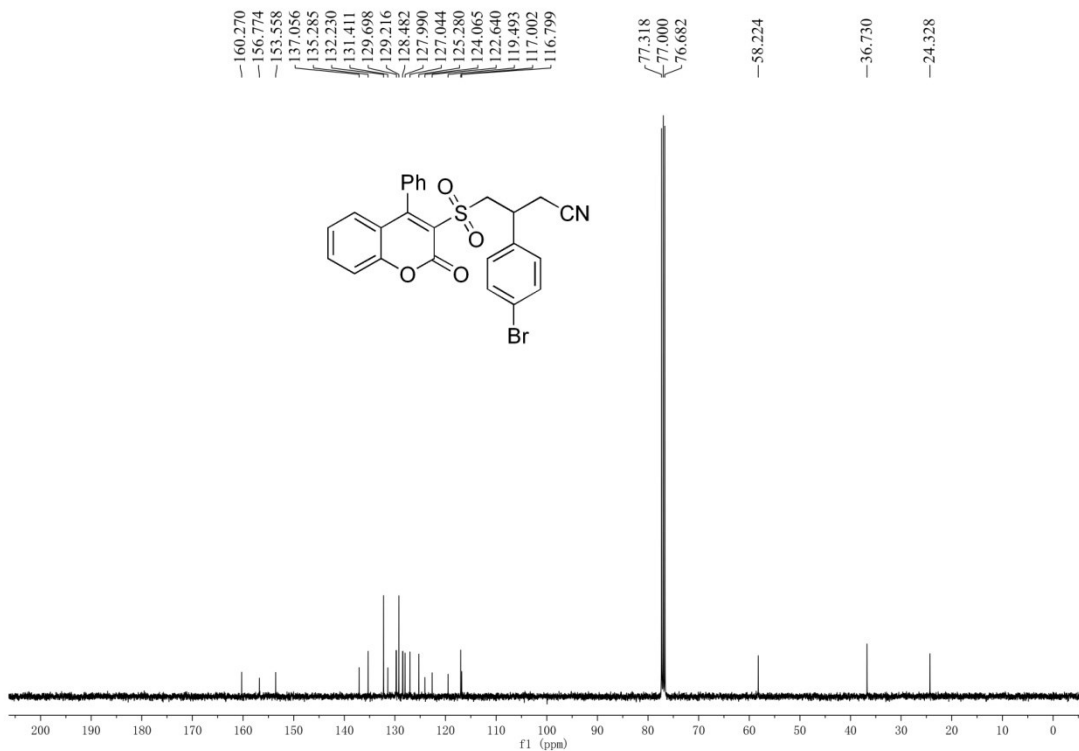
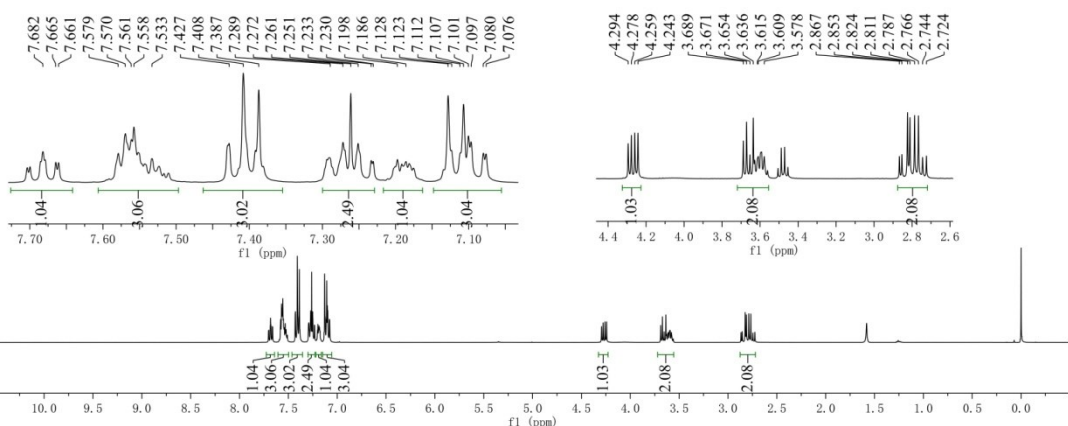
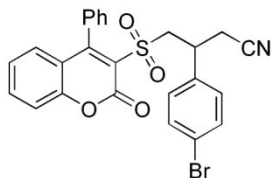
(3ah)



3-(4-Bromophenyl)-4-((2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)butanenitrile

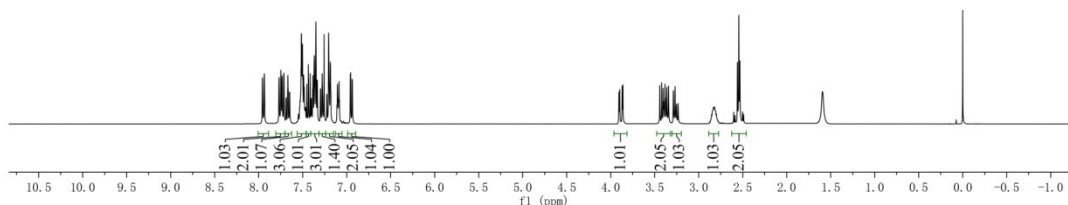
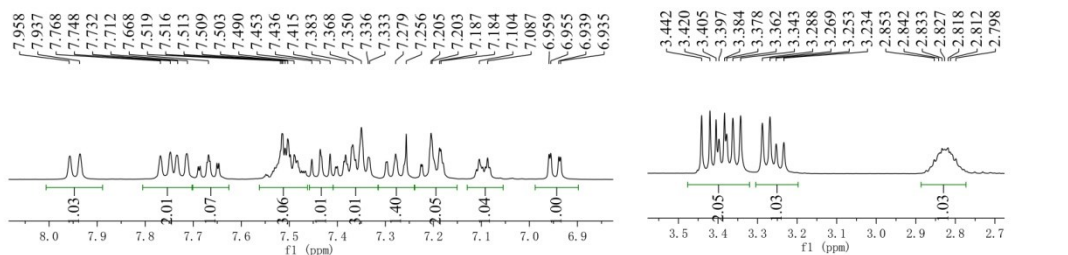
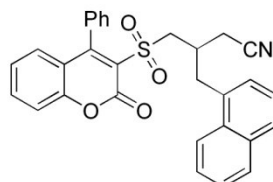
(3ai)

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7.700
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7.682
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7.552
7.543
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7.292
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7.175
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7.107
7.101
7.097
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0.000

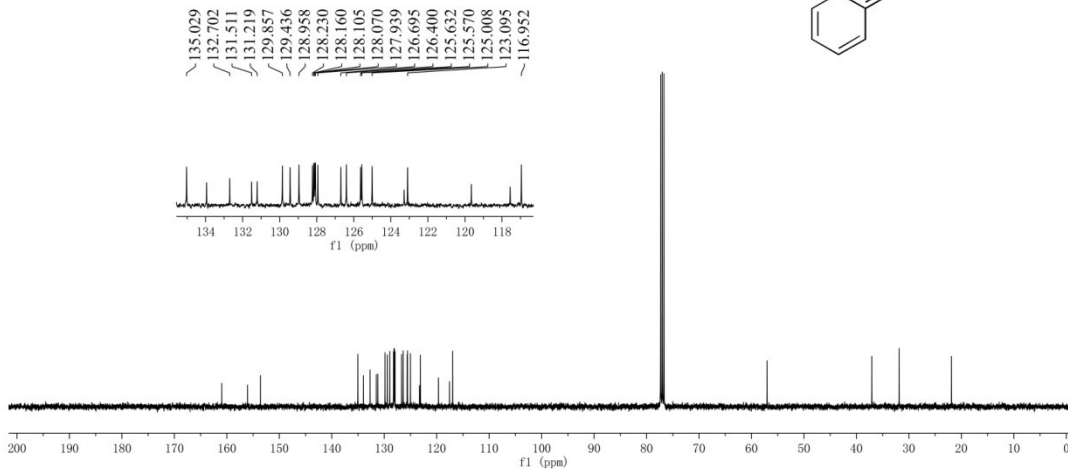
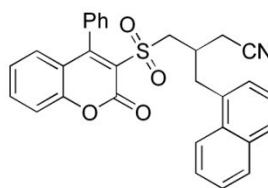


4-(Naphthalen-1-yl)-3-(((2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)methyl)butanenitrile (3aj)

7.958
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7.768
7.748
7.732
7.712
7.668
7.668
7.651
7.647
7.519
7.516
7.513
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7.503
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7.453
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7.279
7.256
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7.223
7.205
7.203
7.187
7.184
7.104
7.087
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6.955
6.939
6.935
6.935
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3.870
3.861
3.442
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3.420
3.384
3.378
3.362
3.343
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3.269
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3.269
2.544
2.532
-0.000

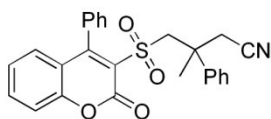
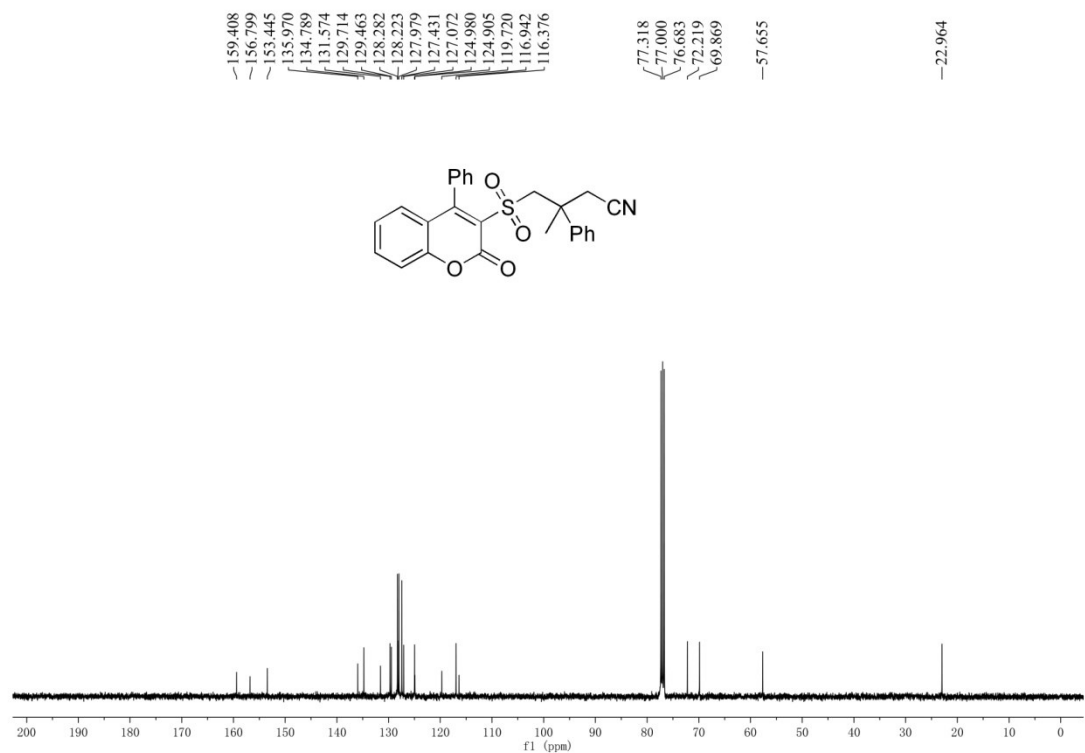
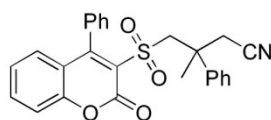
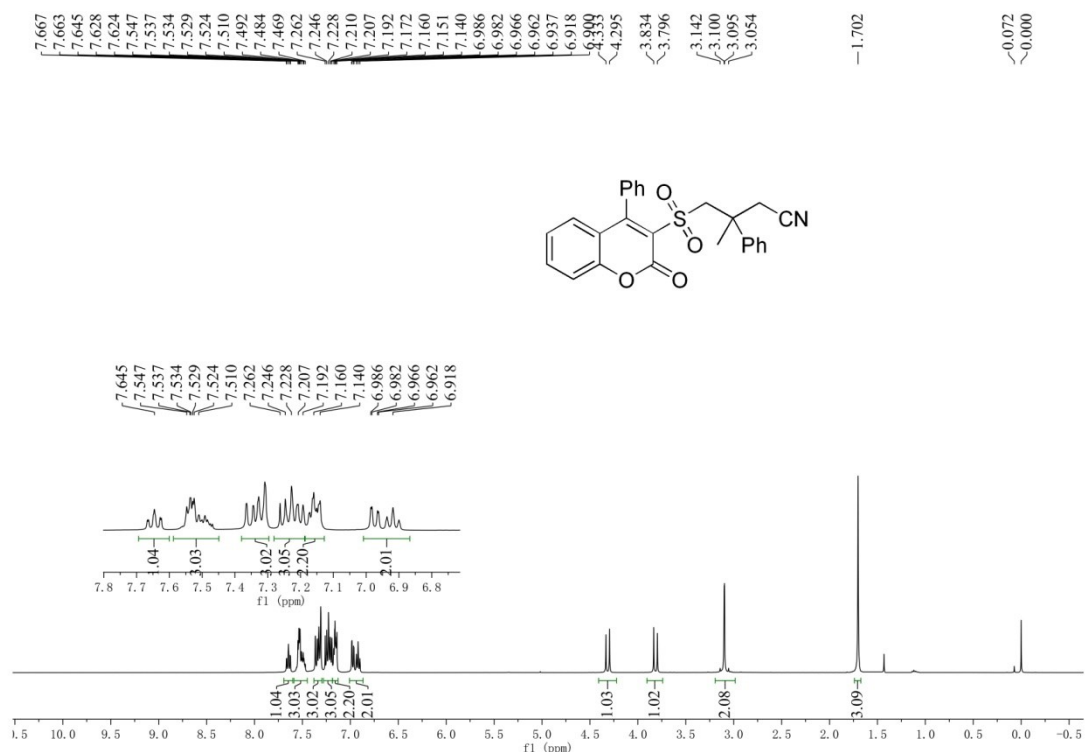


160.964
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135.029
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132.702
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131.219
129.857
129.436
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128.230
128.160
128.105
128.070
127.939
126.695
126.400
125.632
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77.000
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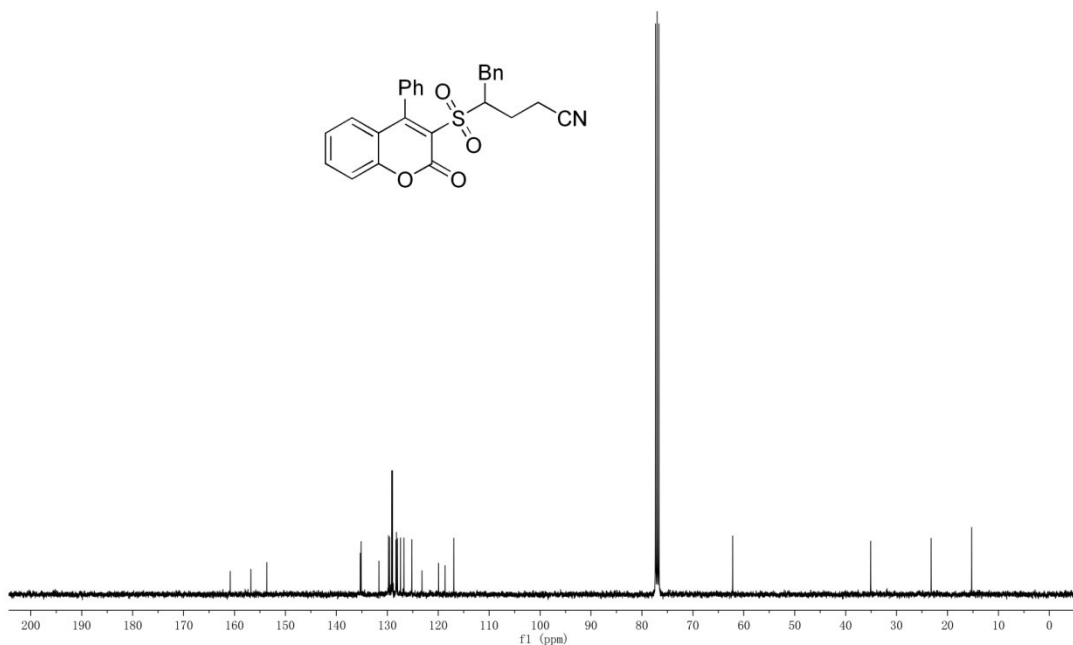
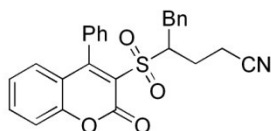
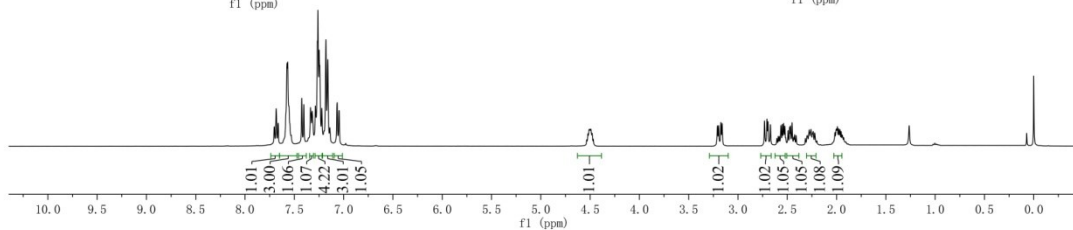
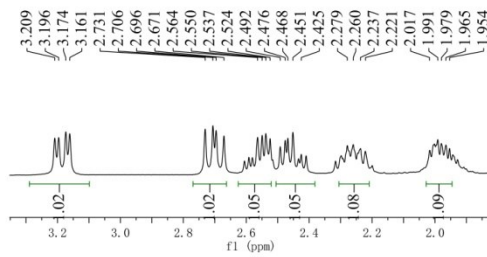
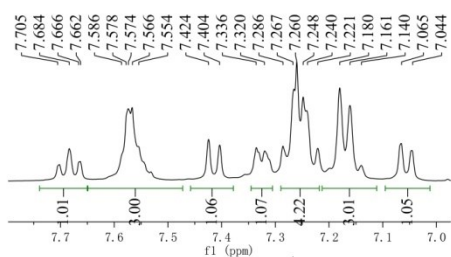
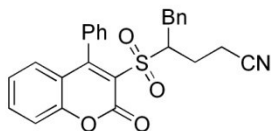
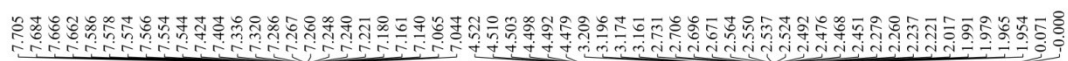


3-Methyl-4-((2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)-3-phenylbutanenitrile

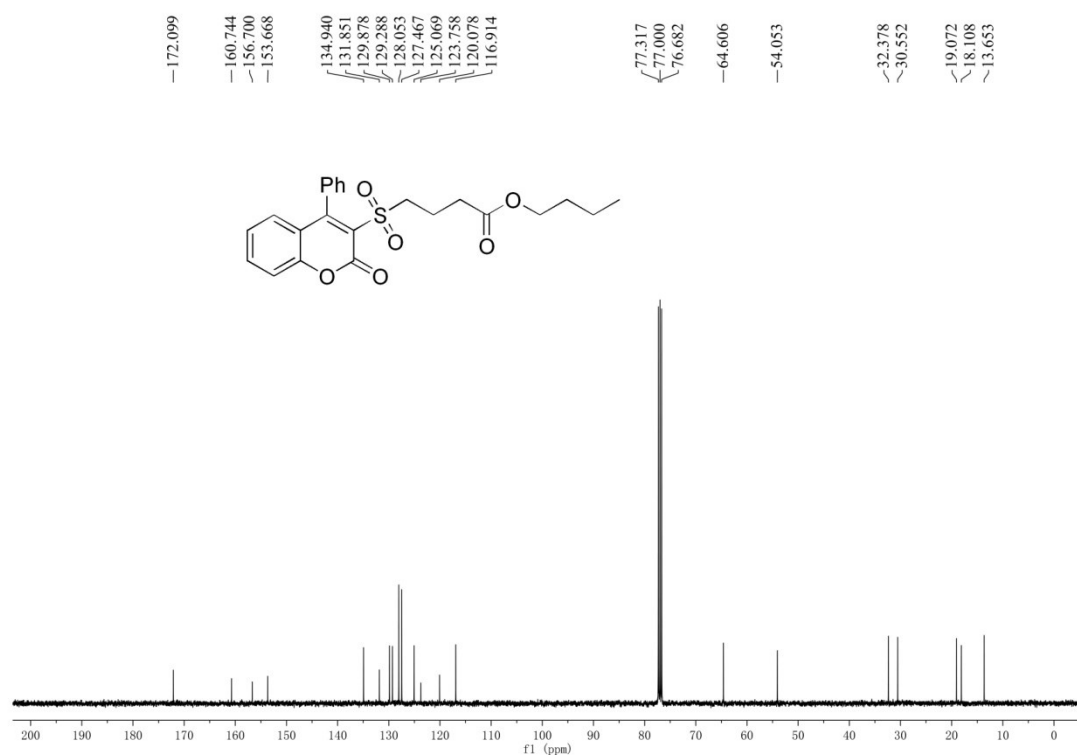
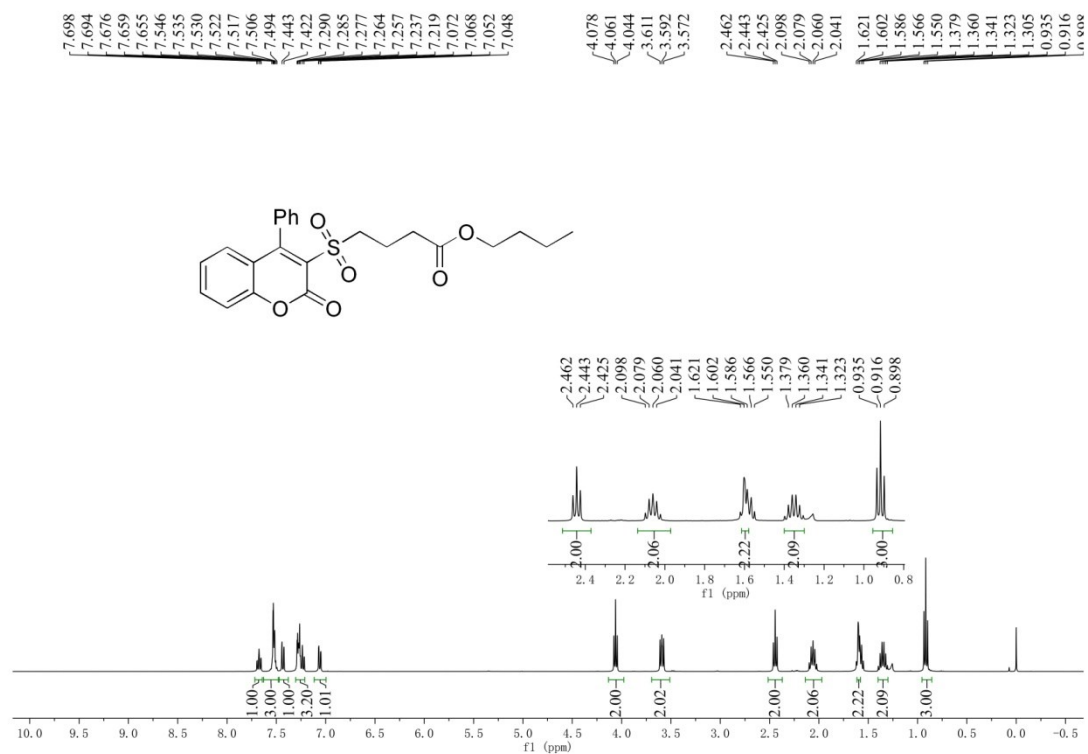
(3ak)



4-((2-Oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)-5-phenylpentanenitrile (3am)



Butyl 4-((2-oxo-4-phenyl-2H-chromen-3-yl)sulfonyl)butanoate (7)



4-((2-Oxo-4-phenylchroman-3-yl)sulfonyl)butanenitrile (8)

