Supporting Information

Visible Light-Promoted Intermolecular Cyclization/Aromatization of Chalcones and 2-Mercaptobenzimidazoles via EDA Complex and Mechanism Study

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1. General information

^{1}H NMR or ^{19}F NMR and ^{13}C NMR data analyses were performed with Varian Mercuryplus-400 instrument and plus-600 instrument respectively. NMR employed $CDCl_3$ as solvent and tetramethylsilane (TMS) as internal standard. Chemical shifts were reported in units (ppm) by specifying TMS resonance in the ^{1}H NMR spectrum as 0.00 ppm. The data of ^{1}H NMR was reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet and br = broad), coupling constant (J values) in Hz and integration. Chemical shift for ^{13}C NMR spectra were recorded in ppm from TMS using the central peak of $CDCl_3$ (77.0ppm) as the internal standard. Flash chromatography was performed using 200-300 mesh silica gel with the indicated solvent system according to standard techniques. Analytical thin-layer chromatography (TLC) was performed on pre-coated, glass-backed silica gel plates. Melting points were measured with an XT-4 apparatus. High-resolution mass spectra (HRMS) (ESI) were obtained with a Bruker Daltonics APEX II 47e and Orbitrap Elite mass spectrometer. Column chromatography was generally performed on silica gel (200–300 mesh) and TLC analyses were conducted on silica gel GF254 plates. All the chemical reagents were purchased from commercial sources and used as received unless otherwise indicated. Chalcones were prepared according to the existing literature, and other reagents were purchased from domestic analytical reagents.

2. Experimental sections

2.1 Experimental setup

The reaction device includes ordinary magnetic stirring and LUYOR-3416 LED parallel light reactor of Shanghai Luyang Instrument company. The reaction was carried out in an open 10 mL borosilicate glass tube (Figure S1). During the reaction, the room temperature was 25-30℃ for all the reactions.

Figure S1. Reaction setup for this reaction.

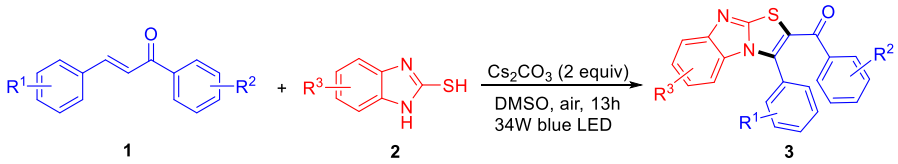
2.2 Optimization of reaction conditions

Table S1. Optimization of reaction conditions [a]

Entry	Solvent	Base	2a	Yield (%) [b]
1	EtOH	Cs_2CO_3	4	NR
2	CH_3CN	Cs_2CO_3	4	Trace
3	$PhCH_3$	Cs_2CO_3	4	NR
4	THF	Cs_2CO_3	4	NR
5	NMP	Cs_2CO_3	4	NR
6	Dioxane	Cs_2CO_3	4	NR
7	DMSO	$NaCO_3$	4	25
8	DMSO	K_3PO_4	4	Trace
9	DMSO	CH_3COONa	4	Trace
10	DMSO	Cs_2CO_3	2	--
11	DMSO	Cs_2CO_3	3	--
12	DMSO	Cs_2CO_3	3.5	33
13	**DMSO**	**Cs_2CO_3**	**4**	**65**

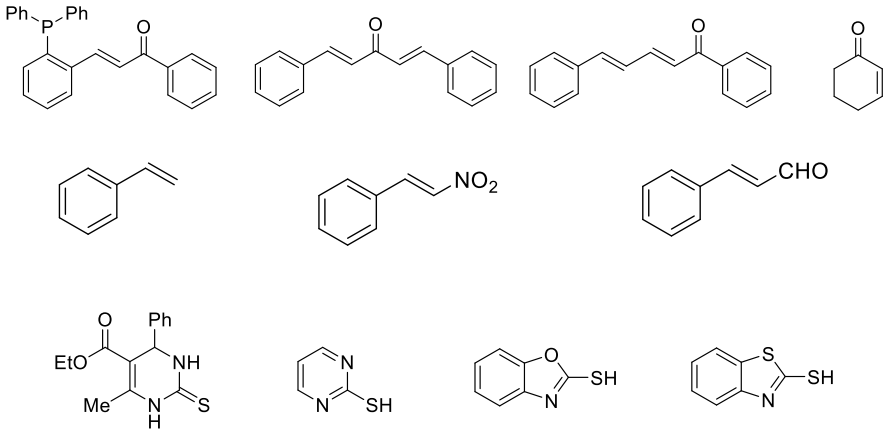
[a] Reaction conditions: 1a (0.1 mmol), 34W blue LED, solvent (2 mL), base (2 equiv.), 13h, rt, air.
[b] Isolated yield.

2.3 General Procedure for synthesis of products

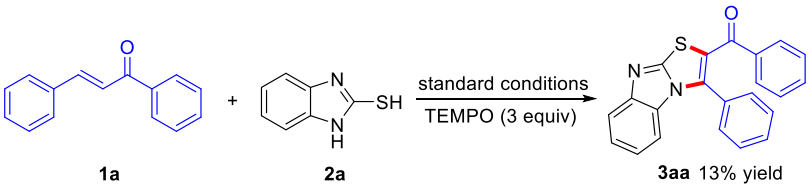


An oven-dried 10 mL borosilicate glass tube was charged with the mixture of chalcone **1** (0.1 mmol), 2-mercaptobenzimidazole **2** (4 equiv.), Cs_2CO_3 (2 equiv., 65.2 mg). Then the reaction mixture was stirred in 2 mL DMSO with a 34W blue LED light irradiation for 13 h in air. After the completion of the reaction detected by TLC. The reaction was quenched with saturated brine (10 mL) and extracted with ethyl acetate (3×10 mL). The organic layers were combined and dried over anhydrous $MgSO_4$, and concentrated under reduced pressure to obtain crude product. The crude product was isolated by silica gel column chromatography with petroleum ether/ethyl acetate (5:1), to obtain the purified product **3**.

2.4 Substrate limitations



2.5 Free radical capture



An oven-dried 10 mL borosilicate glass was charged with the mixture of chalcone **1a** (0.1 mmol, 20.8 mg), 2-mercaptobenzimidazole **2a** (4 equiv., 60.1 mg), Cs_2CO_3 (2 equiv., 65.2 mg) and TEMPO (3.0 equiv., 46.9mg). Then the reaction mixture was stirred in 2 mL DMSO with a 34W blue LED light irradiation for 13 h in air. After the reaction finished, the reaction mixture was detected by HRMS, and the TEMPO-trapped product was found (Figure S2).

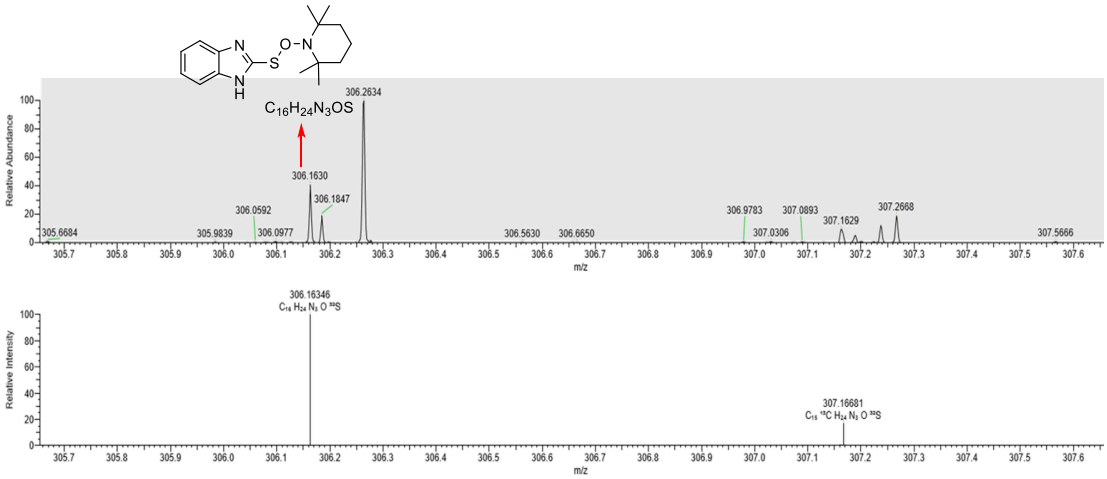


Figure S2. HRMS spectrum of the TEMPO trapping experiment

2.6 UV−vis spectroscopic measurements

The UV-vis absorption spectra of chalcone **1a** (0.005 M), 2-mercaptobenzoimidazole **2a** (0.02 M) and Cs_2CO_3 (0.01 M) in DMSO were recorded in 1 cm path quartz cuvettes respectively (Figure S3). As shown in Figure S3, when **1a**, **2a**, and Cs_2CO_3 were mixed in DMSO, the obvious color changes of the solution and an red-shift in the visible region was observed, demonstrating the formation of EDA complex.

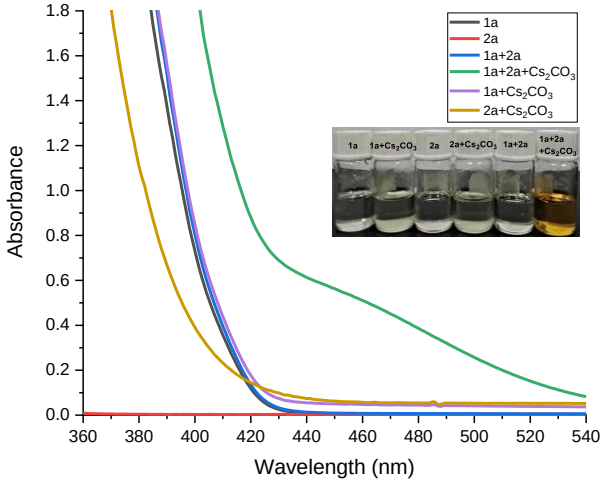


Figure S3. UV−vis spectroscopic measurements on various combinations of 1a, 2a, and Cs_2CO_3 in DMSO.

3. Computational details

All the calculations were performed using the Gaussian 09 programs[1]. All of the structures were fully optimized with the B3LYP[2-3] method and Ahlrichs' split-valence def2-SVP basis set[4] in DiMethyl Sulfoxide employing the Polarizable Continuum Model (PCM)[5]. Grimmes's DFT-D3 dispersion correction was used to describe the van der waals interaction.[6] Vibrational frequency calculations were performed to ensure that a transition state has only one imaginary frequency and a local minimum has no imaginary frequency. Transition states connecting relevant minima were further examined by running intrinsic reaction coordinate (IRC) calculations.

Cartesian Coordinates

1a

C	-1.29893	0.05147	-0.22515
C	-2.75091	-0.05485	-0.39647
C	-3.67439	0.89900	-0.13864
C	-5.12368	0.79600	-0.41422
C	-5.79777	-0.54234	-0.53499
O	-5.77951	1.82364	-0.56346
C	-5.44022	-1.65102	0.25273
C	-6.14477	-2.85354	0.13983
C	-7.20484	-2.96397	-0.76584
C	-7.57354	-1.86132	-1.54783
C	-6.88325	-0.65582	-1.42255
C	-0.66469	1.20554	0.28448
C	0.72039	1.24887	0.43167
C	1.50542	0.14335	0.07425
C	0.89306	-1.00764	-0.43180
C	-0.49488	-1.05191	-0.57947
H	-3.09413	-1.01360	-0.79685
H	-3.37745	1.89574	0.20059
H	-4.62704	-1.56815	0.97588
H	-5.86650	-3.70548	0.76497
H	-7.74911	-3.90720	-0.85870
H	-8.40470	-1.94342	-2.25263
H	-7.17092	0.21628	-2.01335
H	-1.25926	2.07590	0.56911
H	1.19472	2.15006	0.82790
H	2.59126	0.18185	0.19126
H	1.49785	-1.87347	-0.71212
H	-0.96984	-1.95415	-0.97440

2a

C	2.09208	0.71498	-0.00218
C	2.07859	-0.69653	-0.00158
C	0.88053	-1.41295	-0.00081
C	-0.32241	-0.68926	-0.00064
C	-0.28850	0.73120	-0.00125
C	0.90669	1.45528	-0.00202
N	-1.63614	-1.13434	0.00009
C	-2.36338	-0.04169	-0.00012
N	-1.61838	1.11326	-0.00087
S	-4.12589	0.03444	0.00057
H	3.05006	1.24084	-0.00277
H	3.02850	-1.23724	-0.00172
H	0.86757	-2.50511	-0.00034
H	0.91410	2.54718	-0.00247
H	-1.97328	2.06320	-0.00108
H	-4.26893	-1.30935	0.00131

A1

C	3.73730	0.89567	0.63922
C	3.93238	-0.42242	0.17112
C	2.86801	-1.19232	-0.29868
C	1.58642	-0.62056	-0.29010
C	1.40645	0.70141	0.19777
C	2.46839	1.48040	0.66453
N	0.37478	-1.13322	-0.72913
C	-0.49360	-0.16756	-0.53320
N	0.05607	0.95125	0.04384
S	-2.21101	-0.20494	-0.93793
H	4.59793	1.47129	0.98852
H	4.94164	-0.84083	0.16498
H	3.01946	-2.20408	-0.68037
H	2.31597	2.50165	1.01874
H	-0.40375	1.84745	0.15541
H	-2.06007	-1.12339	-1.91929
C	4.34702	-0.44544	-4.18336
C	2.95555	0.01163	-4.12515
C	2.40360	0.79891	-3.17555
C	1.01636	1.30756	-3.17546
C	-0.08800	0.56769	-3.87593
O	0.76354	2.35220	-2.57916
C	-0.11689	-0.83374	-3.98318
C	-1.22222	-1.47441	-4.55128
C	-2.30278	-0.72349	-5.02766

C	-2.28284	0.67293	-4.92144
C	-1.18865	1.31087	-4.33768
C	5.29165	-0.15758	-3.17394
C	6.59982	-0.62821	-3.27013
C	6.99789	-1.39489	-4.37458
C	6.07446	-1.68871	-5.38310
C	4.76260	-1.21925	-5.28667
H	2.32631	-0.32153	-4.95619
H	3.00421	1.20443	-2.35700
H	0.69610	-1.42830	-3.56781
H	-1.24302	-2.56516	-4.61322
H	-3.16438	-1.22671	-5.47358
H	-3.12794	1.26204	-5.28597
H	-1.17107	2.39645	-4.22325
H	4.99658	0.42722	-2.30169
H	7.31633	-0.39856	-2.47749
H	8.02479	-1.76196	-4.44574
H	6.37621	-2.28635	-6.24677
H	4.04309	-1.45404	-6.07586

A2

C	1.31654	2.05860	0.52406
C	2.40110	1.17168	0.70090
C	2.23924	-0.21066	0.58836
C	0.95739	-0.69943	0.29254
C	-0.11644	0.20856	0.09631
C	0.03642	1.59188	0.21556
N	0.52130	-2.00157	0.09280
C	-0.74617	-1.88846	-0.22774
N	-1.19633	-0.59064	-0.23496
S	-1.83645	-3.21439	-0.62882
H	1.48389	3.13430	0.62058
H	3.39021	1.57978	0.92425
H	3.08396	-0.89532	0.68395
H	-0.79911	2.27575	0.05484
H	-2.11769	-0.27324	-0.51354
H	-0.86760	-4.15131	-0.53199
C	0.62992	-0.98893	-3.20226
C	1.70295	-1.92777	-2.86939
C	2.92703	-1.62023	-2.38557
C	3.88561	-2.60119	-1.84076
C	3.90696	-4.01971	-2.33483
O	4.65409	-2.25634	-0.94412

C	3.61385	-4.36711	-3.66548
C	3.70078	-5.69879	-4.08254
C	4.07200	-6.69593	-3.17451
C	4.37367	-6.35711	-1.84865
C	4.30345	-5.02669	-1.43609
C	0.75907	0.40796	-3.05469
C	-0.31009	1.25457	-3.33944
C	-1.53408	0.72732	-3.77205
C	-1.67823	-0.65596	-3.92636
C	-0.60556	-1.50361	-3.64673
H	1.43618	-2.98321	-2.97552
H	3.20931	-0.58384	-2.18607
H	3.34018	-3.59191	-4.38320
H	3.48130	-5.95734	-5.12132
H	4.13197	-7.73751	-3.50026
H	4.66730	-7.13414	-1.13849
H	4.55013	-4.74486	-0.41043
H	1.69382	0.83460	-2.68753
H	-0.19565	2.33270	-3.20516
H	-2.37340	1.39417	-3.98481
H	-2.63119	-1.07545	-4.25781
H	-0.72733	-2.58444	-3.74932

EDA complex A

C	1.35705	1.43063	0.83348
C	2.15008	0.27103	0.95162
C	1.61690	-1.00327	0.72884
C	0.26131	-1.10673	0.38125
C	-0.51910	0.07623	0.24993
C	0.00464	1.34992	0.47841
N	-0.50584	-2.21431	0.08088
C	-1.72097	-1.75784	-0.24084
N	-1.76032	-0.37539	-0.14185
S	-3.11213	-2.67157	-0.71283
H	1.80644	2.41069	1.01418
H	3.20673	0.37101	1.21456
H	2.24533	-1.89417	0.78863
H	-0.60915	2.24627	0.36482
H	-2.56281	0.18836	-0.39189
H	-2.11923	-3.84959	-2.35378
C	0.03834	-0.98690	-3.12775
C	0.96576	-2.07917	-2.82112
C	2.23976	-1.94066	-2.38495

C	3.13560	-3.01880	-1.93247
C	2.94583	-4.44463	-2.37617
O	4.04901	-2.75150	-1.15153
C	2.42284	-4.80165	-3.63174
C	2.30726	-6.14749	-3.99290
C	2.70397	-7.15179	-3.10418
C	3.24269	-6.80723	-1.85705
C	3.37536	-5.46362	-1.50341
C	0.32213	0.36433	-2.83788
C	-0.59861	1.36503	-3.14107
C	-1.82468	1.04094	-3.73743
C	-2.12200	-0.29457	-4.02958
C	-1.20132	-1.29812	-3.72461
H	0.53924	-3.07883	-2.93712
H	2.65795	-0.94849	-2.19764
H	2.12757	-4.02692	-4.34044
H	1.90354	-6.41176	-4.97306
H	2.60225	-8.20306	-3.38498
H	3.56266	-7.58814	-1.16263
H	3.80654	-5.17969	-0.54109
H	1.25380	0.63197	-2.33770
H	-0.36814	2.40398	-2.89288
H	-2.54746	1.82812	-3.96719
H	-3.07984	-0.55709	-4.48560
H	-1.43917	-2.34194	-3.93489
C	-2.09657	-5.69401	-3.00252
O	-1.46637	-4.48009	-2.75269
O	-3.33510	-5.67649	-3.17163
O	-1.32569	-6.68382	-3.00666
Cs	-3.60233	-8.67965	-3.65566
Cs	-0.14428	-5.36901	-0.09293

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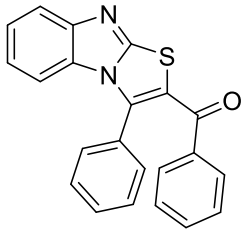
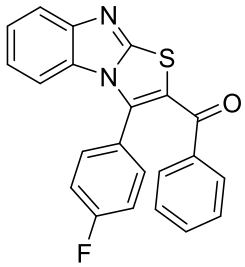
4. Analytical data for all compounds[1]

Phenyl(3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)methanone (3aa)



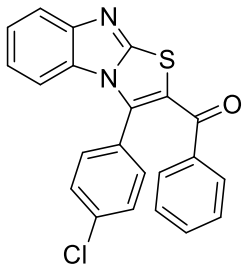
Light yellow crystal, (23.2 mg, 65%), m.p. = 208-210 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.4 Hz, 1H), 7.49 (d, *J* = 7.6 Hz, 2H), 7.41 (d, *J* = 7.2 Hz, 3H), 7.38 – 7.29 (m, 4H), 7.15 (t, *J* = 7.6 Hz, 2H), 7.01 (t, *J* = 7.8 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.9, 155.3, 149.0, 138.7, 137.0, 132.0, 130.6, 130.1, 130.1, 128.6, 128.6, 127.8, 127.7, 124.6, 121.1, 119.4, 112.0. **HRMS** (ESI) m/z: Calcd for $C_{22}H_{15}N_2OS$ $[M+H]^+$ 355.0900, Found 355.0898.

(3-(4-fluorophenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ab)[1]



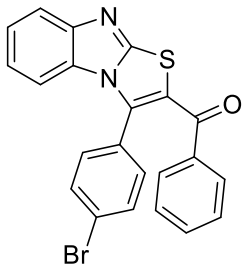
Light yellow crystal, (22.0 mg, 59%), m.p. = 186-188 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.49 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.46 – 7.32 (m, 4H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.11 – 7.01 (m, 3H), 6.85 (d, *J* = 8.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.7, 163.8 (d, *J* = 250.5 Hz), 155.1, 149.0, 137.5, 137.0, 132.3, 130.0, 128.6, 128.0, 124.7 (d, *J* = 7.5 Hz), 123.8, (d, *J* = 4.5 Hz), 121.2, 119.5, 116.0 (d, *J* = 22.5 Hz), 111.8. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -108.38 – -108.46 (m).

(3-(4-chlorophenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ac)[1]



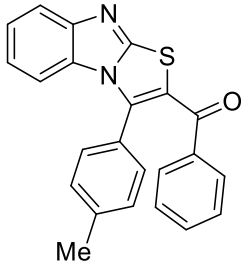
Light yellow crystal, (25.2 mg, 65%), m.p. = 191-193 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.0 Hz, 1H), 7.50 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.43 – 7.32 (m, 6H), 7.22 (t, *J* = 7.8 Hz, 2H), 7.05 (t, *J* = 7.8 Hz, 1H), 6.87 (d, *J* = 8.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.5, 155.1, 148.9, 137.3, 137.0, 132.2, 131.4, 129.9, 129.0, 128.7, 128.0, 126.2, 124.7, 124.6, 121.3, 119.5, 111.9.

(3-(4-bromophenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ad)[1]



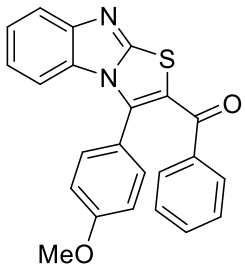
Light yellow crystal, (27.5 mg, 64%), m.p. = 205-206 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 4H), 7.46 – 7.28 (m, 4H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.05 (t, *J* = 7.8 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.5, 155.1, 148.9, 137.3, 137.0, 132.2, 131.9, 131.6, 129.9, 128.7, 128.0, 126.6, 125.3, 124.7, 124.6, 121.3, 119.5, 111.9.

Phenyl(3-(p-tolyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)methanone (3ae)[1]



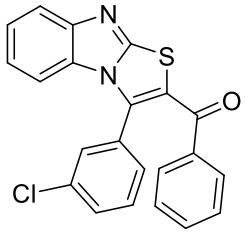
White crystal, (18.6 mg, 51%), m.p. = 176-177 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.57 – 7.45 (m, 2H), 7.39 – 7.26 (m, 4H), 7.24 – 7.09 (m, 4H), 7.02 (t, *J* = 7.8 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 2.37 (s, 3H). **^{13}C NMR** (150 MHz, CDCl3): δ 189.06, 155.4, 149.0, 141.0, 139.1, 137.1, 131.8, 130.1, 130.0, 129.3, 128.7, 127.8, 124.7, 124.5, 124.2, 121.1, 119.3, 112.2, 21.4.

(3-(4-methoxyphenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3af)[1]



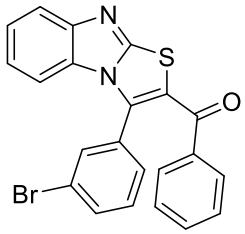
Light yellow crystal, (18.5 mg, 48%), m.p. = 192-194 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.48 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.37 – 7.30 (m, 4H), 7.17 (d, *J* = 7.6 Hz, 2H), 7.06 – 6.95 (m, 2H), 6.87 – 6.78 (m, 2H), 3.82 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 189.1, 161.2, 155.3, 149.0, 138.9, 137.1, 131.8, 131.6, 130.2, 128.7, 127.8, 124.5, 124.2, 121.1, 119.5, 119.3, 114.1, 112.1, 55.4.

(3-(3-chlorophenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ag)



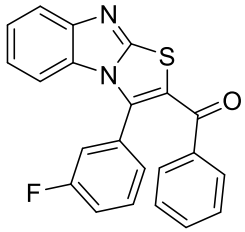
New compound. White crystal, (26.0 mg, 67%), m.p. = 194-196 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (td, *J* = 8.4, 0.8 Hz, 1H), 7.51 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.43 – 7.29 (m, 6H), 7.22 (t, *J* = 7.6 Hz, 2H), 7.05 (t, *J* = 8.4 Hz, 1H), 6.85 (d, *J* = 8.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.6, 155.1, 149.0, 137.0, 136.9, 134.8, 132.3, 130.7, 130.3, 129.9, 129.9, 129.4, 128.5, 128.1, 128.0, 125.0, 124.7, 121.4, 119.6, 111.8. **HRMS** (ESI) m/z: Calcd for $C_{22}H_{14}ClN_2OS$ $[M+H]^+$ 389.0510, Found 389.0505.

(3-(3-bromophenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ah)



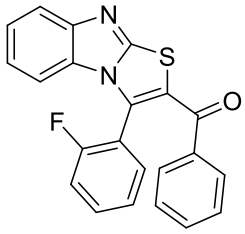
New compound. White crystal, (25.9 mg, 60%), m.p. = 207-209 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.63 – 7.44 (m, 4H), 7.43 – 7.34 (m, 3H), 7.29 – 7.19 (m, 3H), 7.06 (t, *J* = 7.8 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.6, 155.1, 149.0, 137.0, 136.8, 133.7, 133.2, 132.3, 130.1, 129.9, 129.6, 128.5, 128.5, 128.0, 125.1, 124.8, 122.7, 121.4, 119.6, 111.8. **HRMS** (ESI) m/z: Calcd for $C_{22}H_{14}BrN_2OS$ $[M+H]^+$ 433.0005, Found 433.0005.

(3-(3-fluorophenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ai)[1]



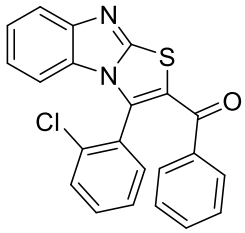
Light yellow crystal, (22.7 mg, 61%), m.p. = 208-210 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.4 Hz, 1H), 7.52 (dd, *J* = 8.2, 1.0 Hz, 2H), 7.41 – 7.32 (m, 3H), 7.29 – 7.19 (m, 3H), 7.18 – 7.10 (m, 2H), 7.04 (t, *J* = 7.8 Hz, 1H), 6.84 (d, *J* = 8.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.5, 162.3 (d, *J* = 247.5 Hz), 155.1, 148.9, 137.0, 136.8, 132.3, 130.6 (d, *J* = 9.0 Hz), 129.9, 129.7 (d, *J* = 7.5 Hz), 128.6, 128.0, 126.0 (d, *J* = 4.5 Hz), 124.8, 124.7, 121.3, 119.5, 117.8 (d, *J* = 21 Hz), 117.4 (d, *J* = 24 Hz), 111.8. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -111.16 – -111.22(m).

(3-(2-fluorophenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3aj)



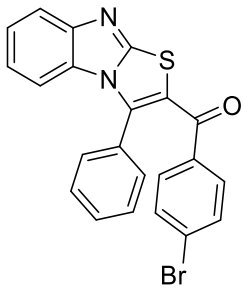
New compound. White crystal, (15.3 mg, 41%), m.p. = 198-200 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 7.2 Hz, 2H), 7.48 – 7.41 (m, 1H), 7.39 – 7.28 (m, 3H), 7.20 (t, *J* = 7.6 Hz, 2H), 7.15 – 7.02 (m, 3H), 6.83 (d, *J* = 8.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.5, 160.0 (d, *J* = 249.0 Hz), 155.1, 148.8, 137.0, 133.2 (d, *J* = 7.5 Hz), 132.4, 132.2, 132.0, 132.0, 130.0, 128.4, 127.9, 125.9, 124.7, 124.6 (d, *J* = 4.5 Hz), 121.4, 119.4, 116.4 (d, *J* = 15 Hz), 116.1 (d, *J* = 19.5 Hz), 111.4. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -110.88 – -110.94 (m). **HRMS** (ESI) m/z: Calcd for $C_{22}H_{14}FN_2OS$ $[M+H]^+$ 373.0805, Found 373.0806.

(3-(2-chlorophenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ak)[1]



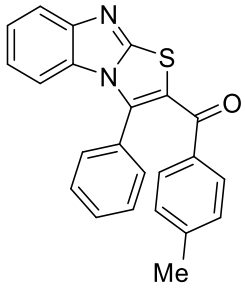
Yellow crystal, (14.7 mg, 38%), m.p. = 190-192 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.4 Hz, 1H), 7.65 – 7.55 (m, 2H), 7.47 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.41 – 7.31 (m, 3H), 7.29 – 7.24 (m, 1H), 7.23 – 7.17 (m, 3H), 7.03 (t, *J* = 8.2 Hz, 1H), 6.63 (d, *J* = 8.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.6, 154.9, 148.7, 137.3, 135.4, 134.5, 132.4, 132.1, 132.1, 129.9, 129.9, 128.2, 127.9, 127.6, 127.1, 125.9, 124.7, 121.5, 119.4, 111.4.

(4-bromophenyl)(3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)methanone (3al)[1]



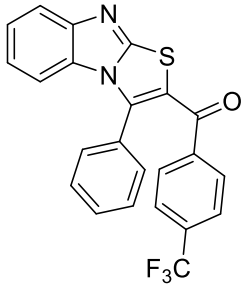
Light yellow crystal, (25.0 mg, 58%), m.p. = 200-202 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.4 Hz, 1H), 7.54 – 7.45 (m, 1H), 7.43 – 7.27 (m, 9H), 7.02 (t, *J* = 7.8 Hz, 1H), 6.85 (d, *J* = 8.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 187.9, 155.2, 149.0, 139.0, 135.8, 131.1, 130.8, 130.1, 130.1, 128.8, 127.6, 126.9, 124.7, 124.4, 121.3, 119.5, 112.1.

(3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)(p-tolyl)methanone (3am)[1]



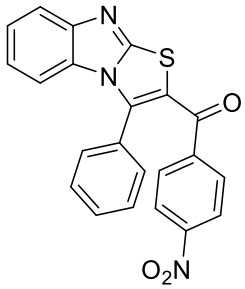
Light yellow crystal, (23.7 mg, 64%), m.p. = 191-192 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.48 – 7.40 (m, 5H), 7.40 – 7.31 (m, 3H), 7.04 – 6.94 (m, 3H), 6.86 (d, *J* = 8.0 Hz, 1H), 2.29 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.4, 155.3, 148.9, 143.0, 138.2, 134.3, 130.4, 130.1, 130.1, 129.0, 128.6, 128.5, 127.9, 124.5, 124.2, 121.0, 119.3, 112.0, 109.9.

(3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)(4-(trifluoromethyl)phenyl)meth anone (3an)[1]



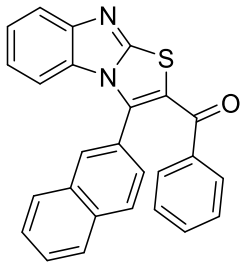
Light yellow crystal, (16.9 mg, 40%), m.p. = 270-271 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.4 Hz, 1H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.45 – 7.39 (m, 1H), 7.38 – 7.29 (m, 7H), 7.01 (d, *J* = 7.8 Hz, 1H), 6.81 (d, *J* = 8.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.1, 155.1, 149.1, 140.3, 139.7, 132.9 (d, *J* = 31.5 Hz), 130.9, 130.1, 128.8, 128.6, 127.3, 124.9, 124.9, 124.7 (q, *J* = 12.0 Hz), 123.3 (d, *J* = 270.0 Hz), 121.4, 119.5, 112.0. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -63.79 (s).

(4-nitrophenyl)(3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)methanone (3ao)[1]



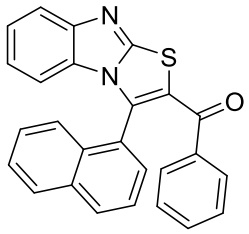
Orange crystal, (17.9 mg, 45%), m.p. = 179-181 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 8.8 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 2H), 7.47 – 7.30 (m, 6H), 7.03 (t, *J* = 7.8 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 187.4, 155.1, 149.1, 148.9, 142.5, 140.0, 131.2, 130.1, 130.0, 129.2, 128.9, 127.2, 125.1, 124.8, 122.9, 121.5, 119.7, 112.0.

(3-(naphthalen-2-yl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ap)[1]



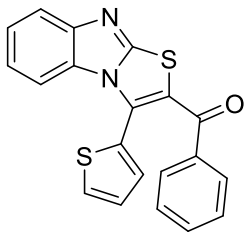
Yellow crystal, (18.2 mg, 45%), m.p. = 192-194 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.92 – 7.76 (m, 4H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.63 – 7.42 (m, 5H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.04 (t, *J* = 7.4 Hz, 1H), 7.00 – 6.91 (m, 3H), 6.86 (d, *J* = 8.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 189.1, 155.4, 149.0, 138.8, 137.1, 133.6, 132.3, 131.7, 131.0, 130.1, 128.5, 128.4, 128.2, 127.8, 127.7, 127.7, 127.0, 125.9, 124.8, 124.6, 121.2, 119.4, 112.2.

(3-(naphthalen-1-yl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3aq)



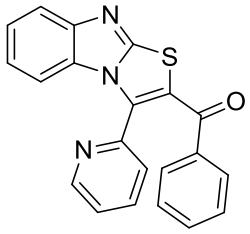
New compound. Light yellow crystal, (20.4 mg, 50%), m.p. =244-245 °C. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.87 (t, *J* = 9.6 Hz, 2H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.48 – 7.44 (m, 1H), 7.39 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.33 – 7.27 (m, 3H), 7.26 – 7.22 (m, 1H), 7.09 – 7.05 (m, 1H), 6.81 – 6.73 (m, 3H), 6.07 (d, *J* = 8.4 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 189.2, 155.2, 148.9, 137.6, 137.2, 133.1, 131.6, 131.5, 131.2, 129.9, 129.8, 128.7, 128.0, 127.7, 127.2, 126.8, 126.4, 125.3, 124.9, 124.5, 124.5, 121.2, 119.2, 112.1. **HRMS** (ESI) m/z: Calcd for $C_{26}H_{17}N_2OS$ $[M+H]^+$ 405.1056, Found 405.1056.

phenyl(3-(thiophen-2-yl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)methanone (3ar)



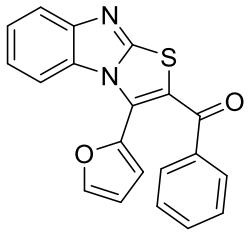
New compound. Light yellow crystal, (17.3 mg, 48%), m.p. = 196-197 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.4 Hz, 1H), 7.60 (dd, *J* = 8.2, 1.0 Hz, 2H), 7.48 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.44 – 7.33 (m, 2H), 7.29 – 7.21 (m, 3H), 7.11 – 6.98 (m, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.6, 154.6, 148.8, 137.1, 132.3, 131.0, 130.2, 130.0, 128.5, 128.0, 127.4, 126.7, 126.7, 124.6, 121.3, 119.4, 112.0. **HRMS** (ESI) m/z: Calcd for $C_{20}H_{13}N_2OS_2$ $[M+H]^+$ 361.0464, Found 361.0464.

phenyl(3-(pyridin-2-yl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)methanone(3as)



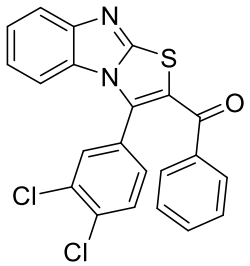
New compound. Light yellow crystal, (19.2 mg, 54%), m.p. = 192-194 °C. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.77 (d, *J* = 4.8 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.55 – 7.45 (m, 3H), 7.35 – 7.28 (m, 3H), 7.24 (t, *J* = 7.8 Hz, 1H), 7.14 (t, *J* = 7.8 Hz, 2H), 7.04 (t, *J* = 7.8 Hz, 1H), 6.88 (d, *J* = 7.8 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.5, 155.1, 149.8, 148.9, 147.2, 137.1, 137.0, 136.4, 132.2, 130.0, 128.9, 127.9, 127.1, 125.9, 125.0, 124.6, 121.2, 119.3, 112.6. **HRMS** (ESI) m/z: Calcd for $C_{21}H_{14}N_3OS$ $[M+H]^+$ 356.0852, Found 356.0852.

(3-(furan-2-yl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3at)



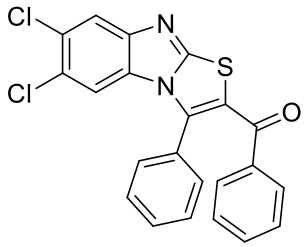
New compound. Orange solid, (18.2 mg, 53%), m.p. = 163-164 °C. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.79 (d, *J* = 7.8 Hz, 1H), 7.60 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.57 – 7.55 (m, 1H), 7.43 – 7.36 (m, 2H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.17 – 7.12 (m, 2H), 6.50 (d, *J* = 3.0 Hz, 1H), 6.32 (dd, *J* = 3.6, 1.8 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.3, 154.5, 148.6, 144.4, 139.1, 137.1, 132.4, 129.8, 128.6, 128.1, 127.5, 127.1, 124.7, 121.6, 119.4, 117.2, 112.1, 112.0. **HRMS** (ESI) m/z: Calcd for $C_{20}H_{13}N_2O_2S$ $[M+H]^+$ 345.0692, Found 345.0685.

(3-(3,4-dichlorophenyl)benzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3au)[1]



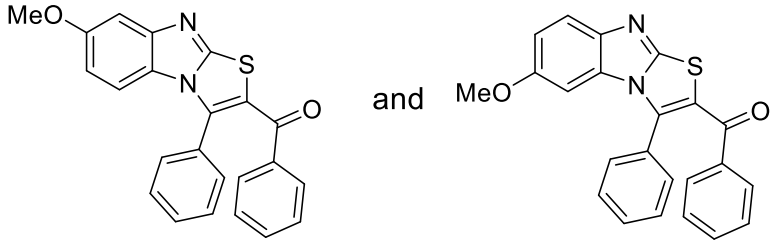
Yellow solid, (19.0 mg, 45%), m.p. = 200-201 °C. **^{1}H NMR** (400 MHz, CDCl3): δ 7.78 (d, J = 8.0 Hz, 1H), 7.62 – 7.39 (m, 5H), 7.39 – 7.30 (m, 2H), 7.25 (d, J = 7.8 Hz, 2H), 7.07 (t, J = 7.7 Hz, 1H), 6.89 (d, J = 8.0 Hz, 1H). **^{13}C NMR** (150 MHz, CDCl3): δ 188.2, 154.9, 148.9, 137.0, 135.8, 135.2, 133.2, 132.3, 132.1, 130.7, 129.7, 129.0, 128.5, 128.1, 127.4, 125.0, 124.8, 121.5, 119.6, 111.7.

(6,7-dichloro-3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3av)[1]



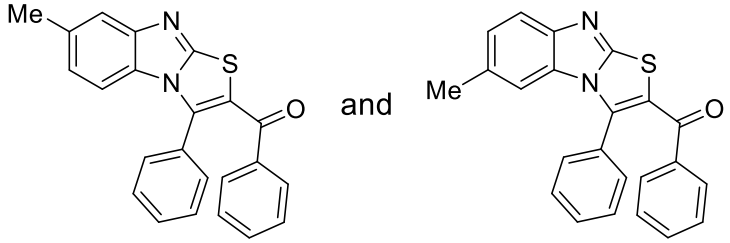
White crystal, (14.9 mg, 35%), m.p. = 218-220 °C. **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.84 (s, 1H), 7.48 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.46 – 7.42 (m, 1H), 7.39 – 7.30 (m, 5H), 7.15 (d, *J* = 7.8 Hz, 2H), 6.91 (s, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.6, 157.0, 148.0, 138.0, 136.6, 132.3, 131.1, 129.9, 128.9, 128.9, 128.8, 128.7, 127.9, 127.0, 125.5, 125.0, 120.3, 113.2.

(7-methoxy-3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3aw) and (6-methoxy-3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3aw')[1]



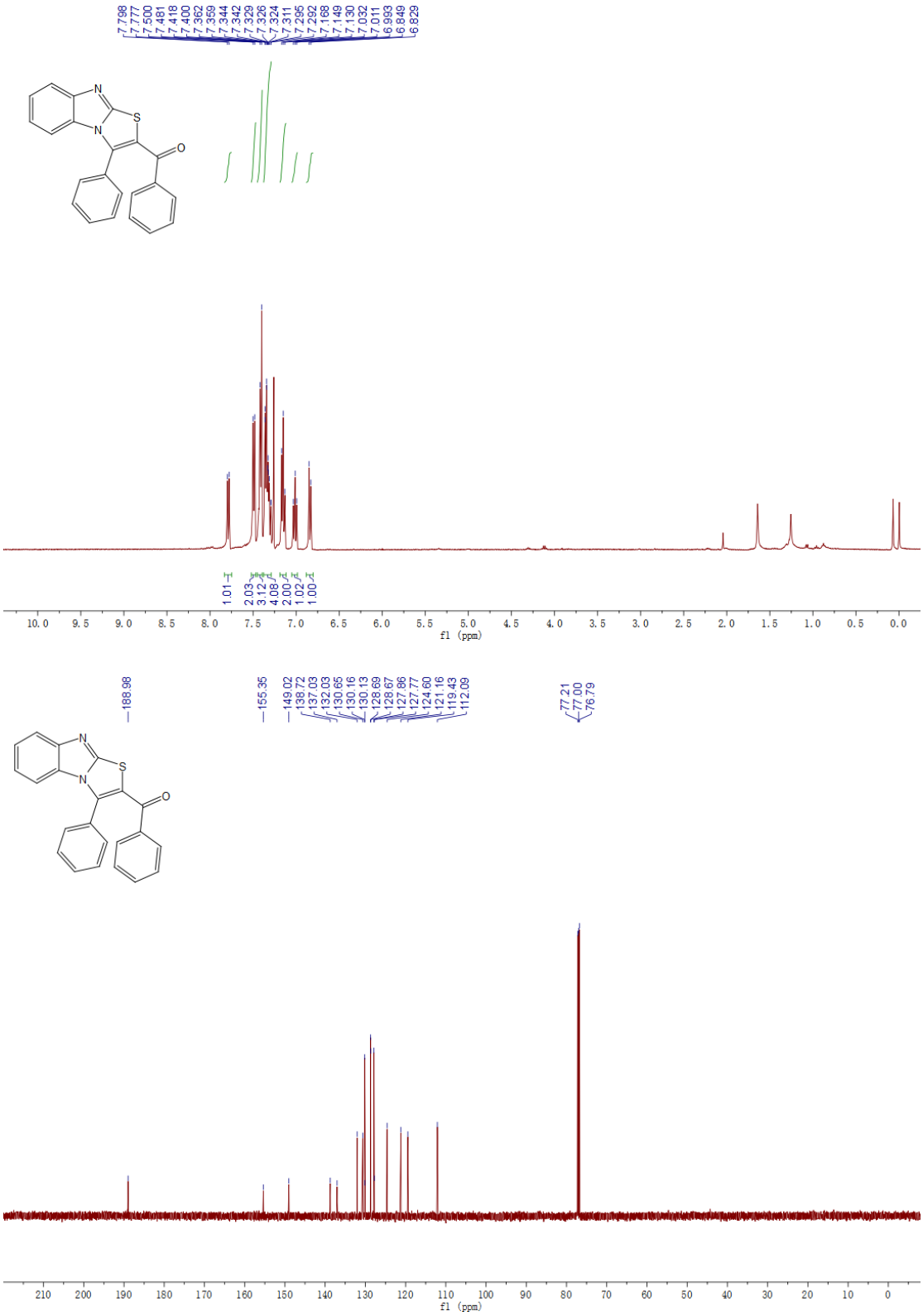
Yellow crystal, (26.1 mg, 68%). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.64 (d, *J* = 8.4 Hz, 1H), 7.51 – 7.44 (m, 4H), 7.44 – 7.36 (m, 6H), 7.36 – 7.27 (m, 6H), 7.23 (d, *J* = 2.4 Hz, 1H), 7.13 (q, *J* = 7.8 Hz, 4H), 6.95 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.71 (d, *J* = 9.0 Hz, 1H), 6.62 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.28 (d, *J* = 2.4 Hz, 1H), 3.83 (s, 3H), 3.57 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 188.9, 188.9, 157.5, 155.5, 154.7, 153.8, 150.1, 143.3, 138.5, 138.4, 137.0, 131.9, 131.8, 130.5, 130.5, 130.3, 130.2, 130.0, 128.6, 128.6, 128.5, 127.8, 127.7, 127.7, 127.7, 124.4, 124.0, 119.6, 113.0, 112.3, 110.5, 101.8, 96.6, 55.6, 55.4.

(7-methyl-3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ax) and (6-methyl-3-phenylbenzo[4,5]imidazo[2,1-b]thiazol-2-yl)(phenyl)methanone (3ax')[1]

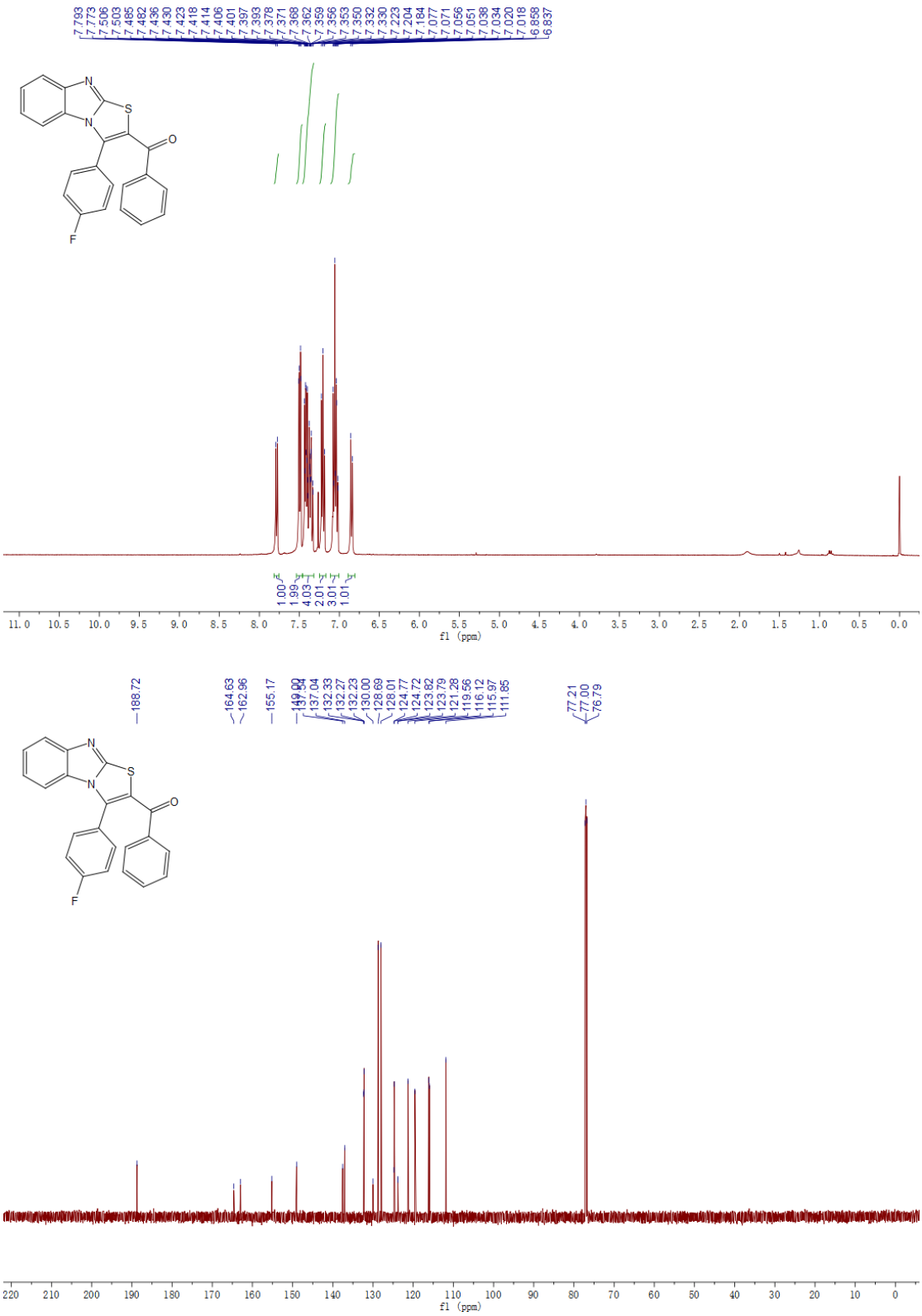


Yellow crystal, (21.0 mg, 57%). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.64 (d, *J* = 8.4 Hz, 1H), 7.55 (s, 1H), 7.49 – 7.45 (m, 4H), 7.43 – 7.36 (m, 6H), 7.35 – 7.27 (m, 6H), 7.16 – 7.10 (m, 5H), 6.81 (d, *J* = 9.0 Hz, 1H), 6.70 (d, *J* = 8.4 Hz, 1H), 6.59 (s, 1H), 2.44 (s, 3H), 2.27 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$): δ 189.0, 155.3, 154.7, 149.3, 147.1, 138.7, 137.0, 134.6, 131.9, 131.9, 131.0, 130.6, 130.5, 130.2, 130.1, 130.1, 128.6, 128.6, 128.5, 128.1, 127.8, 127.8, 126.0, 124.4, 124.2, 122.5, 119.2, 118.8, 112.1, 111.5, 21.8, 21.6.

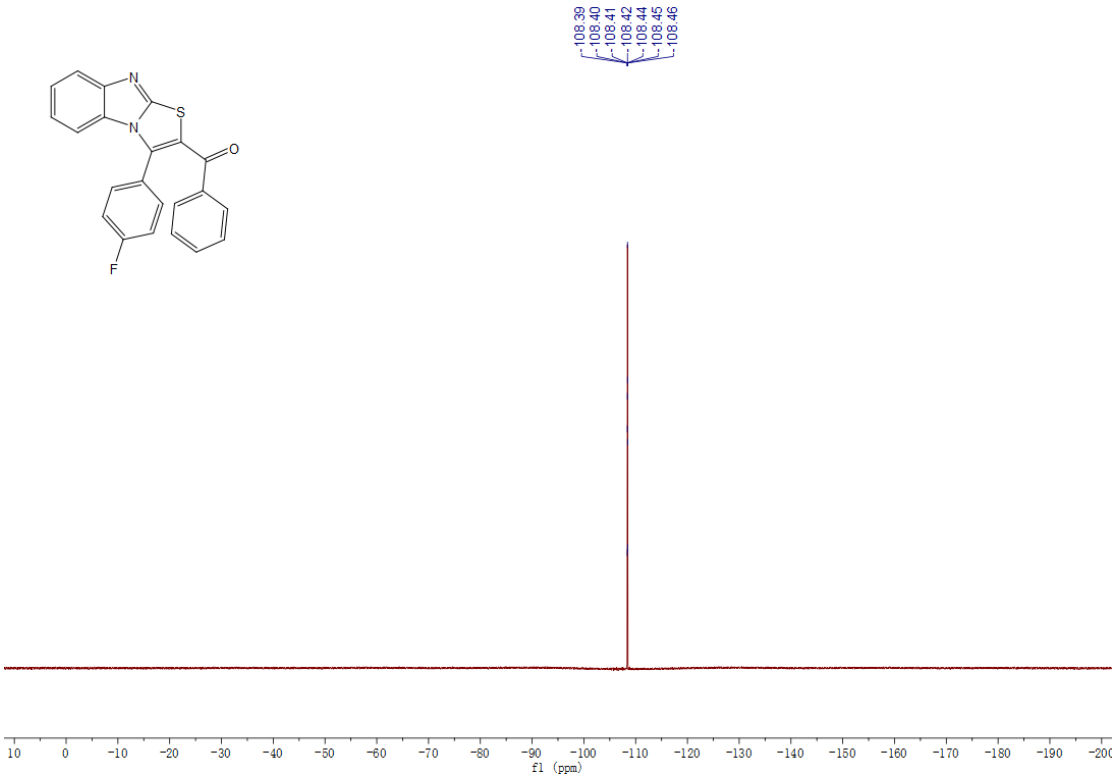
5. NMR Spectra



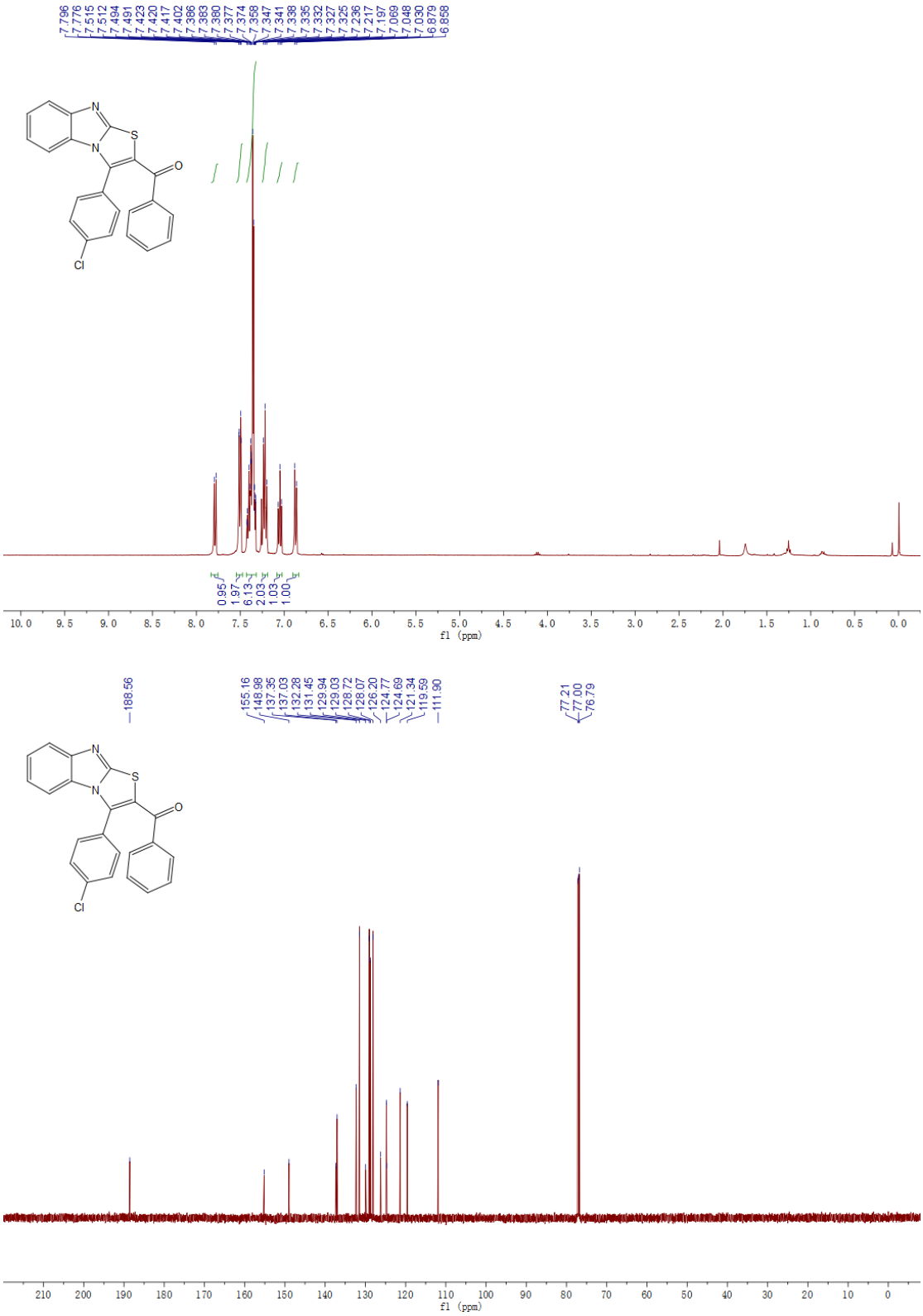
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3aa in $CDCl_3$



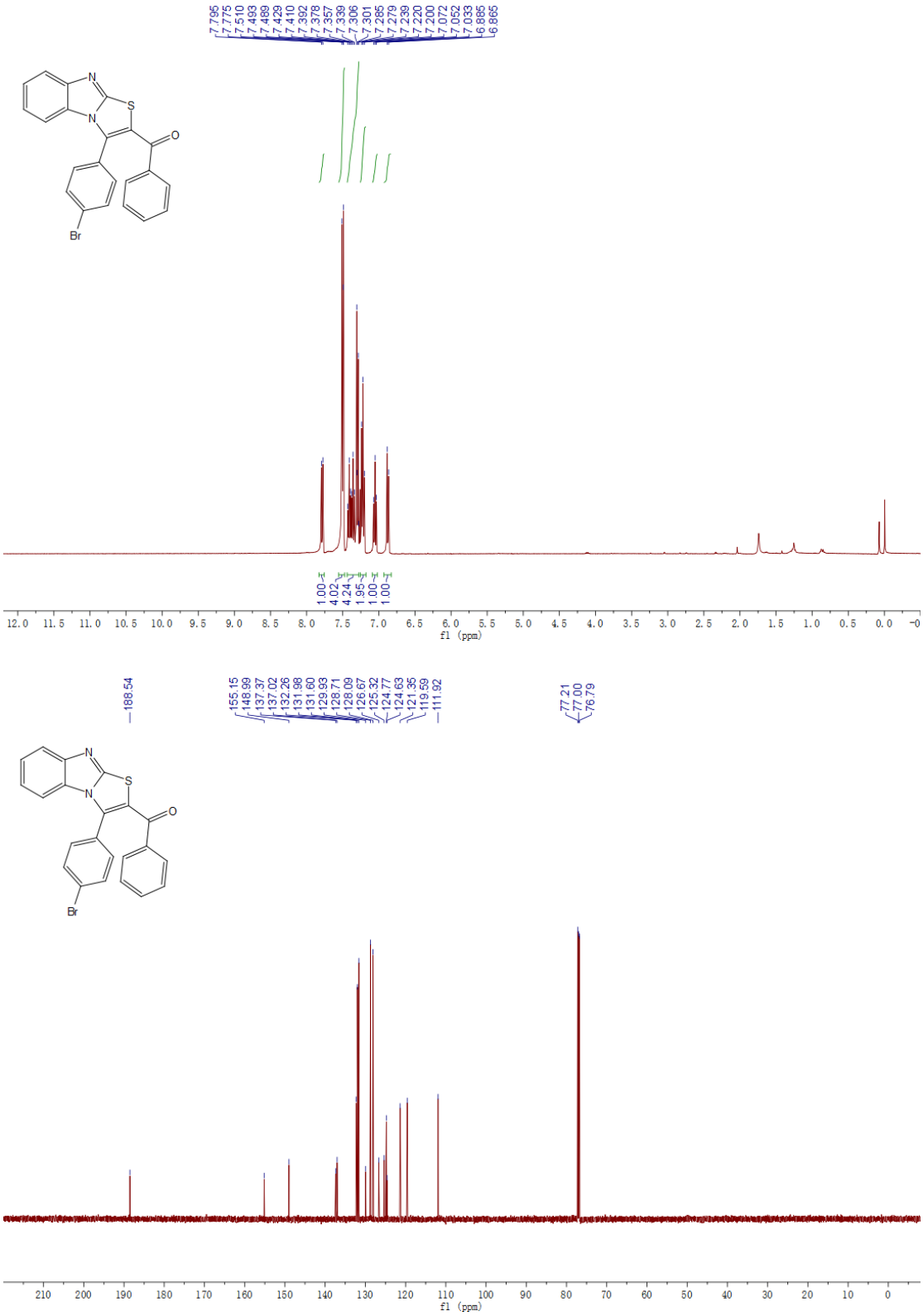
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ab in $CDCl_3$



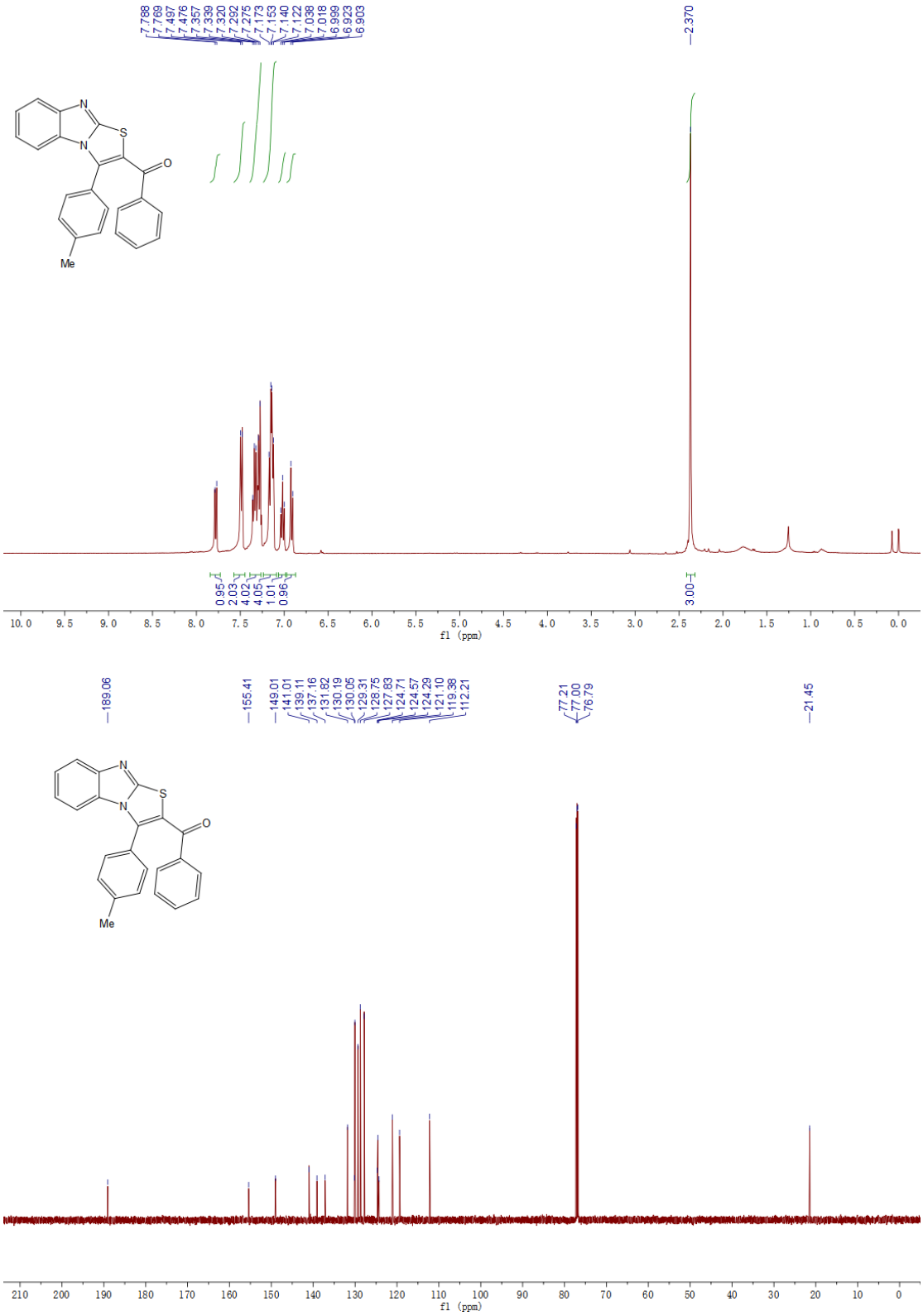
^{19}F NMR of compound 3ab in $CDCl_3$ (376 MHz)



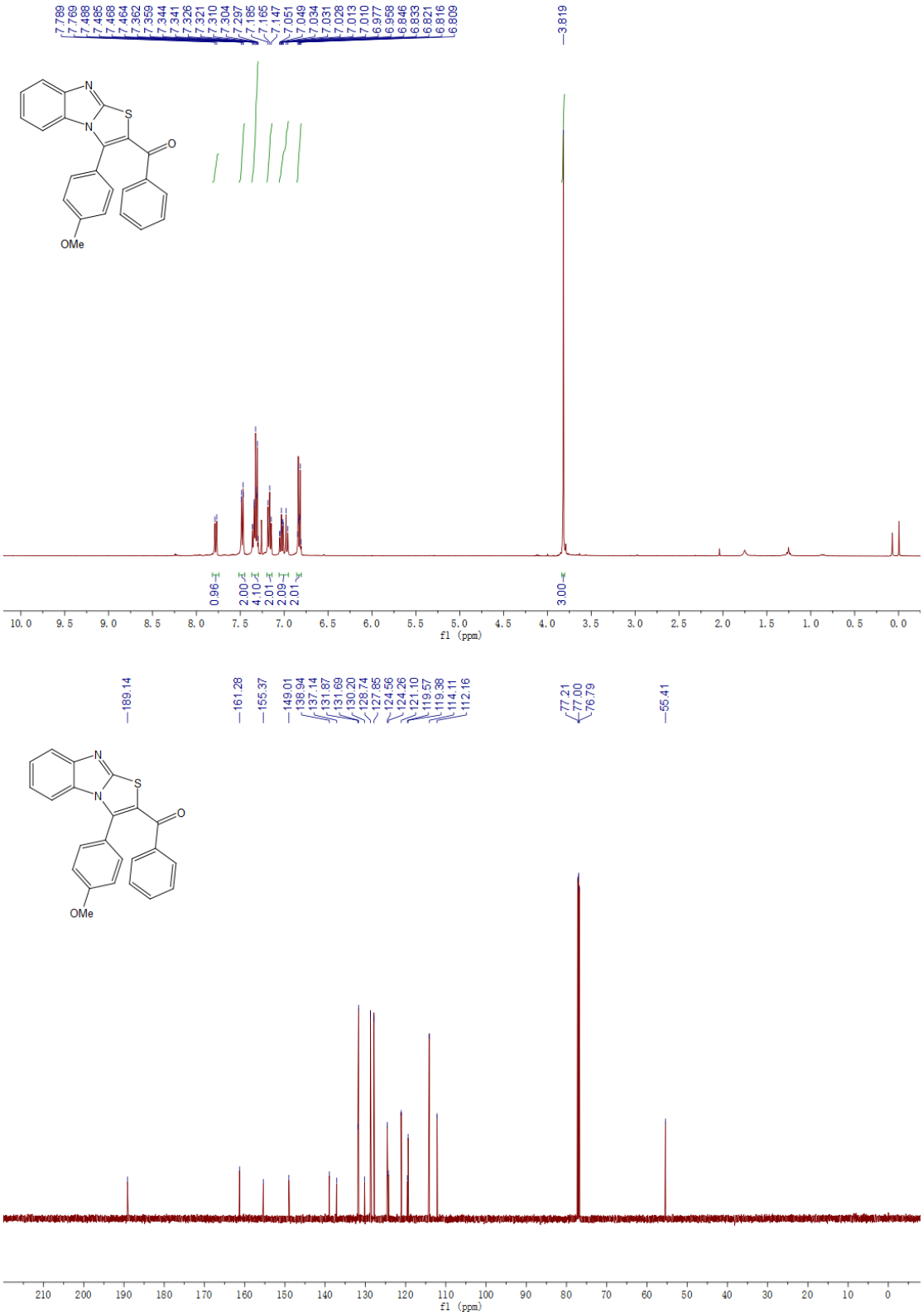
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ac in $CDCl_3$



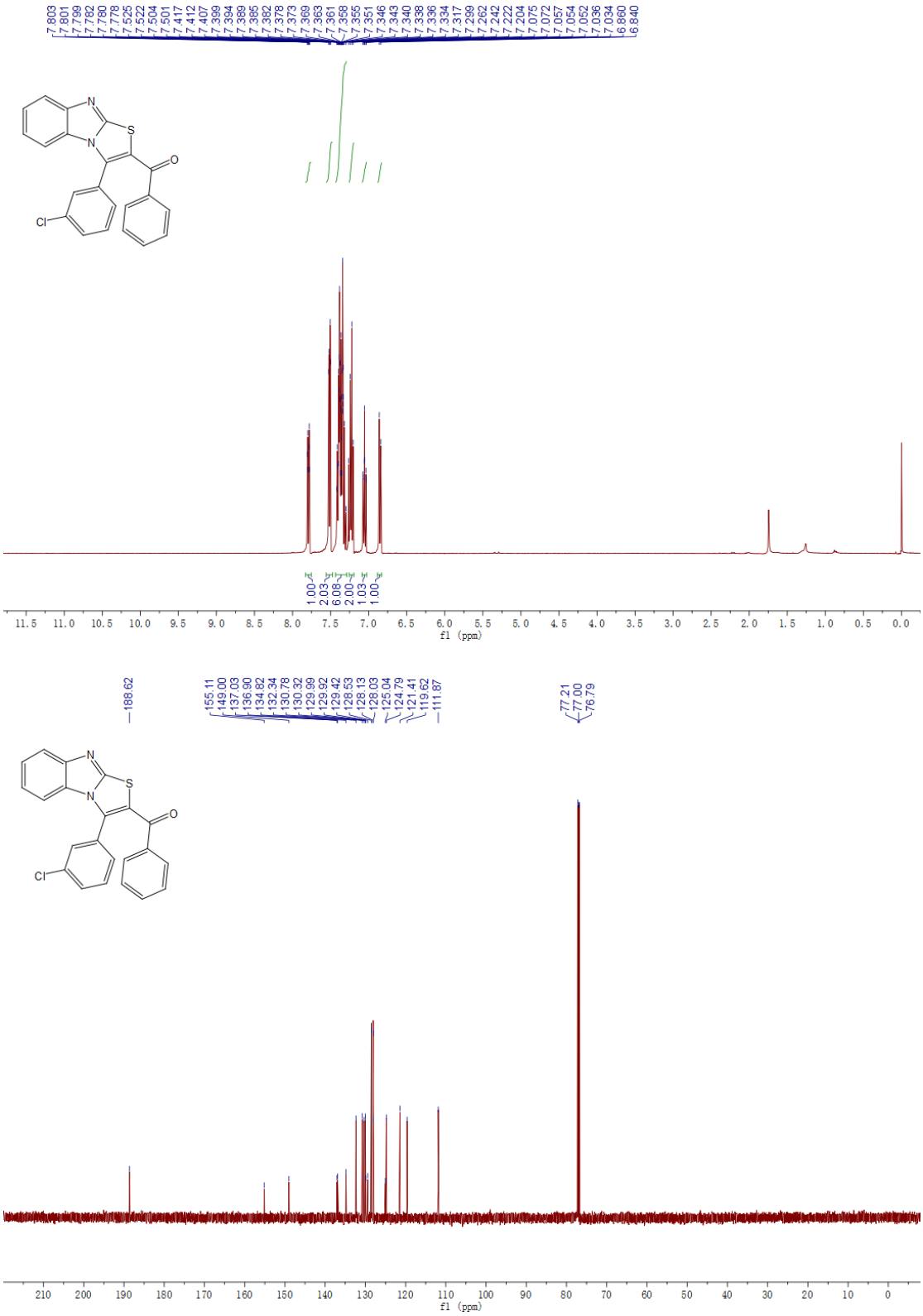
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ad in $CDCl_3$



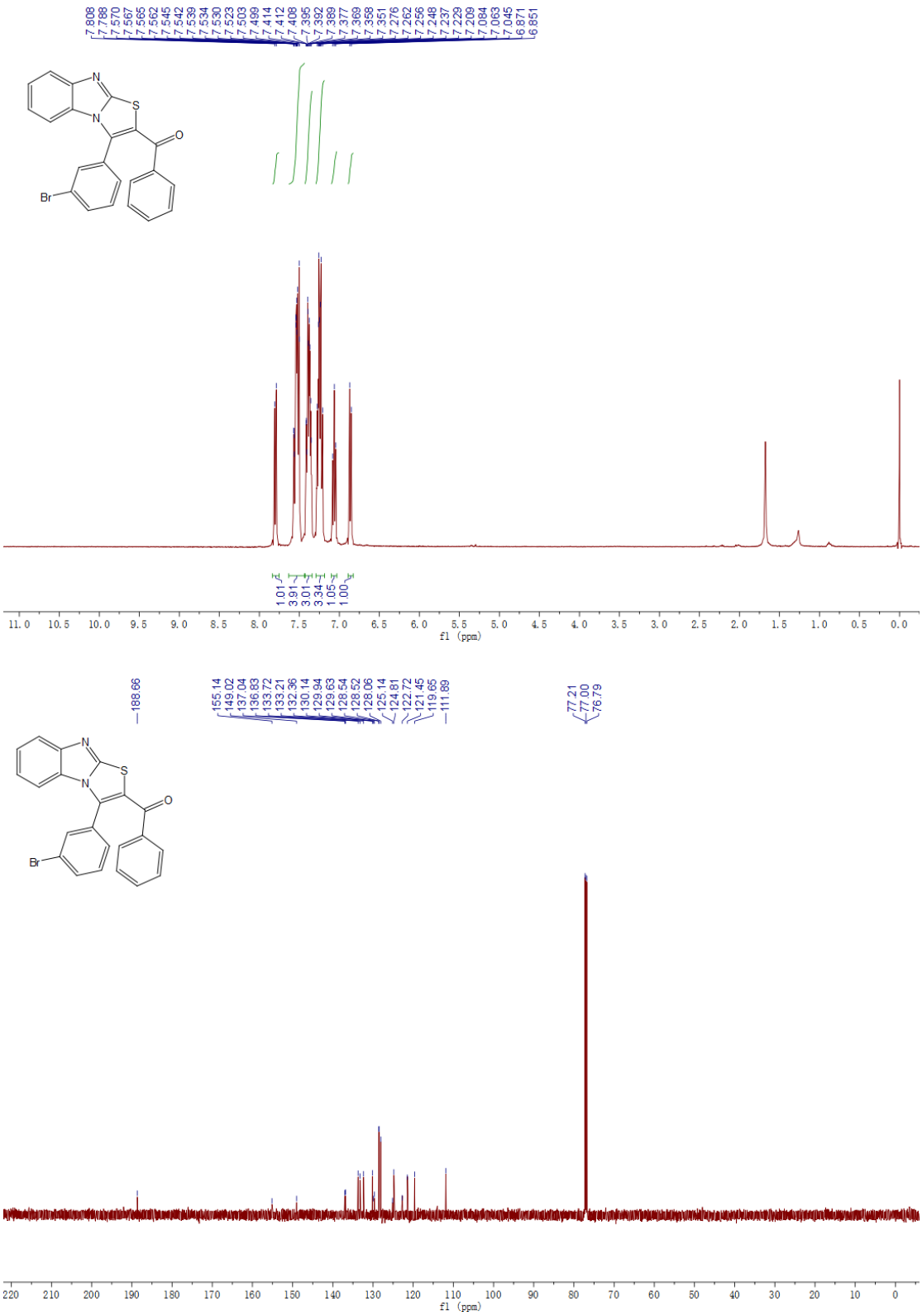
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ae in $CDCl_3$



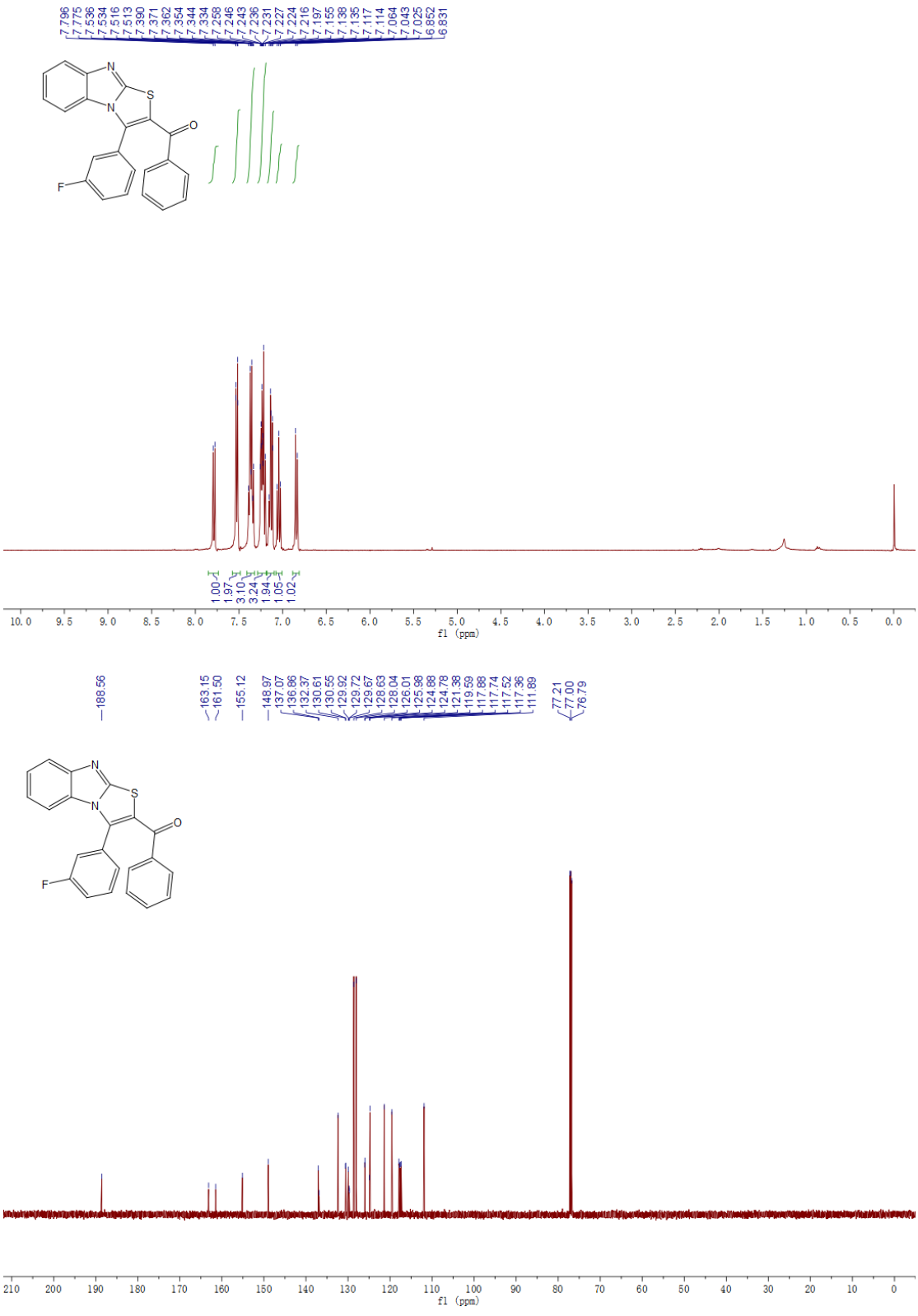
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3af in $CDCl_3$



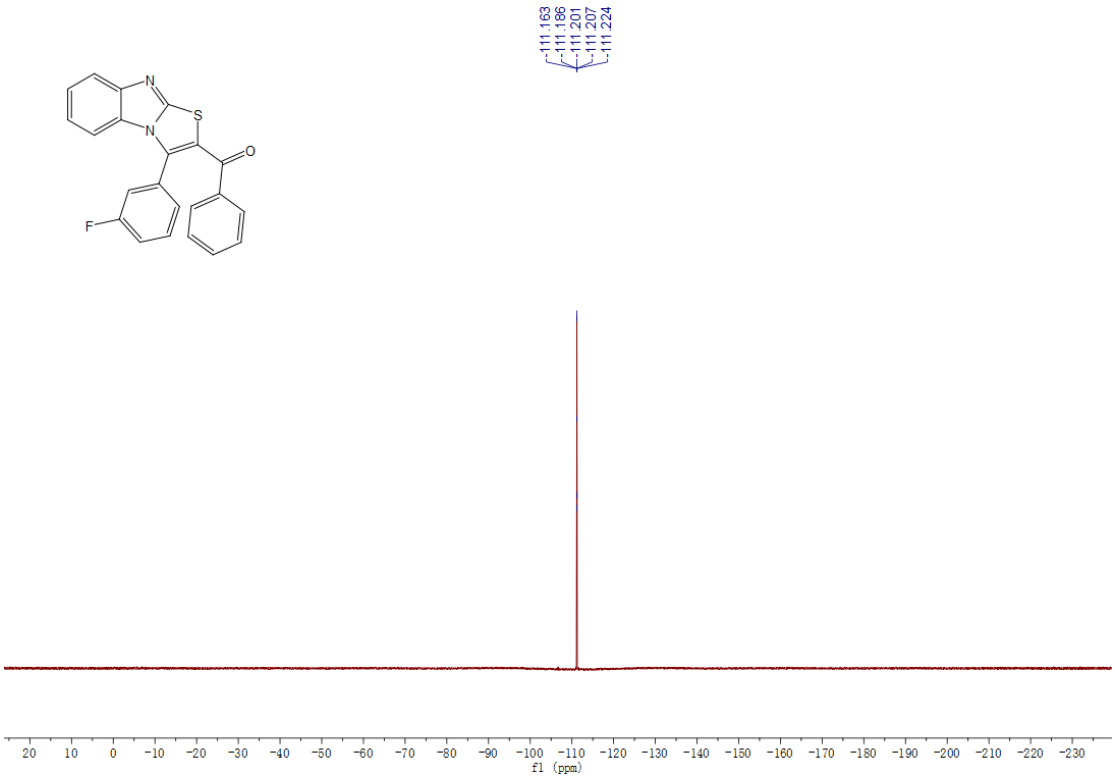
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ag in $CDCl_3$



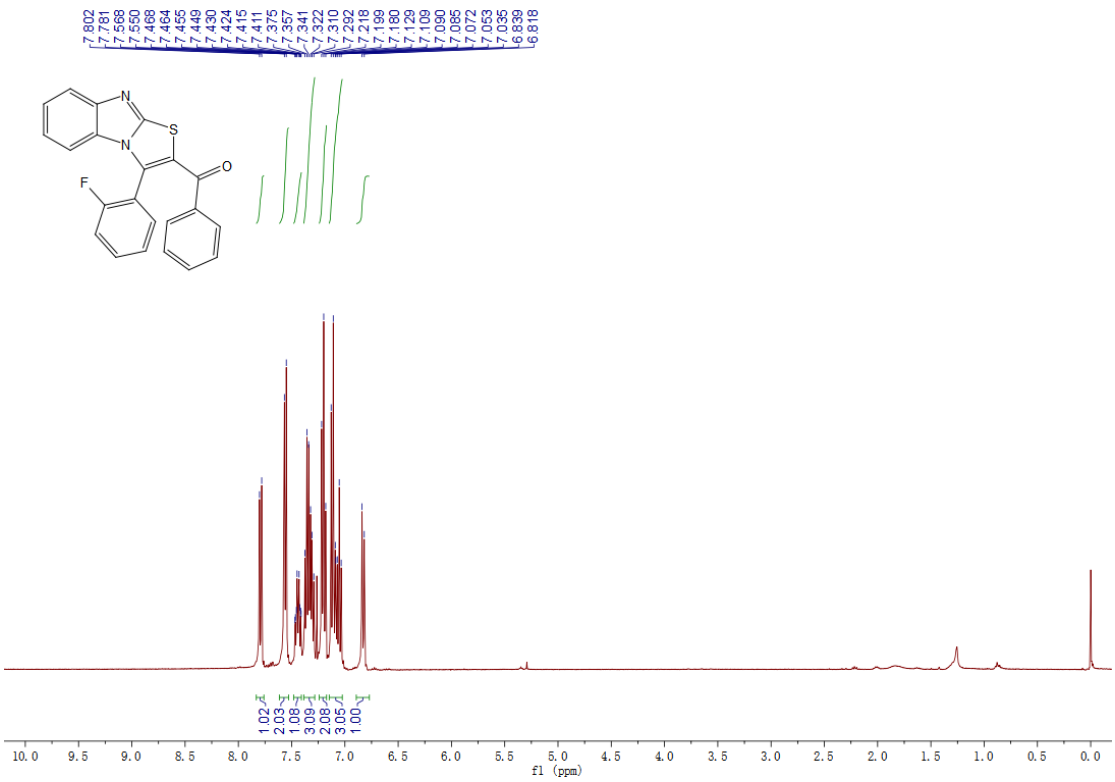
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ah in $CDCl_3$

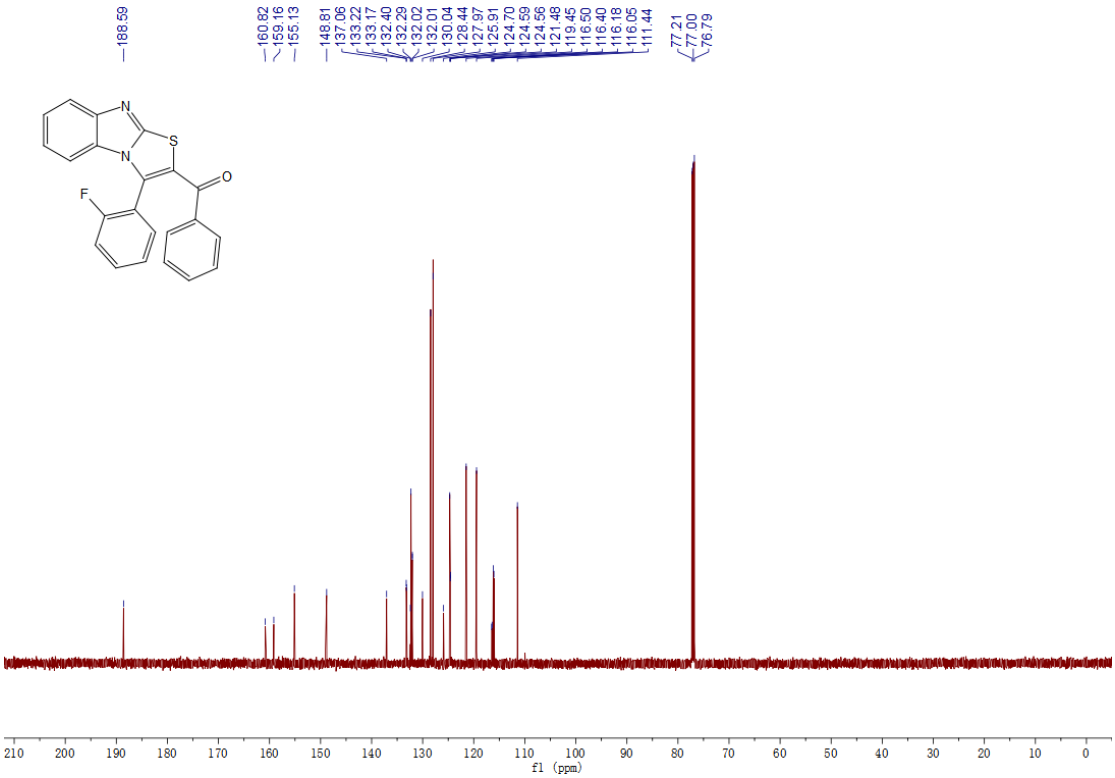


^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ai in $CDCl_3$

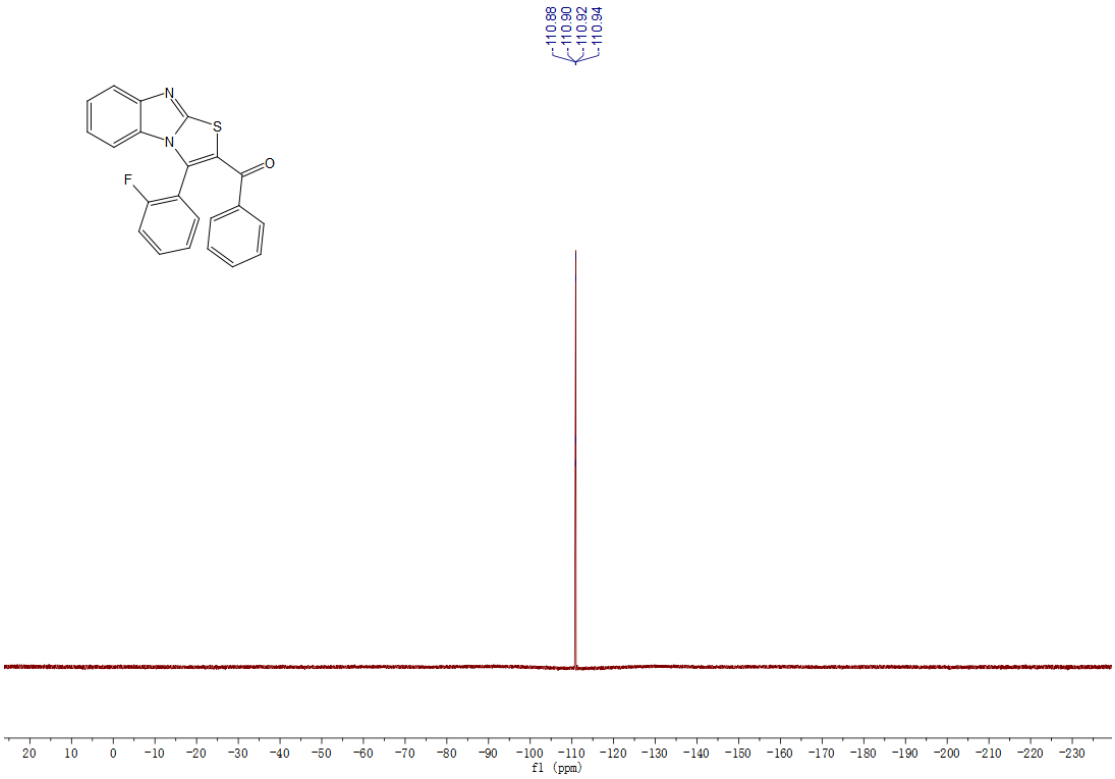


^{19}F NMR of compound 3ai in $CDCl_3$ (376 MHz)

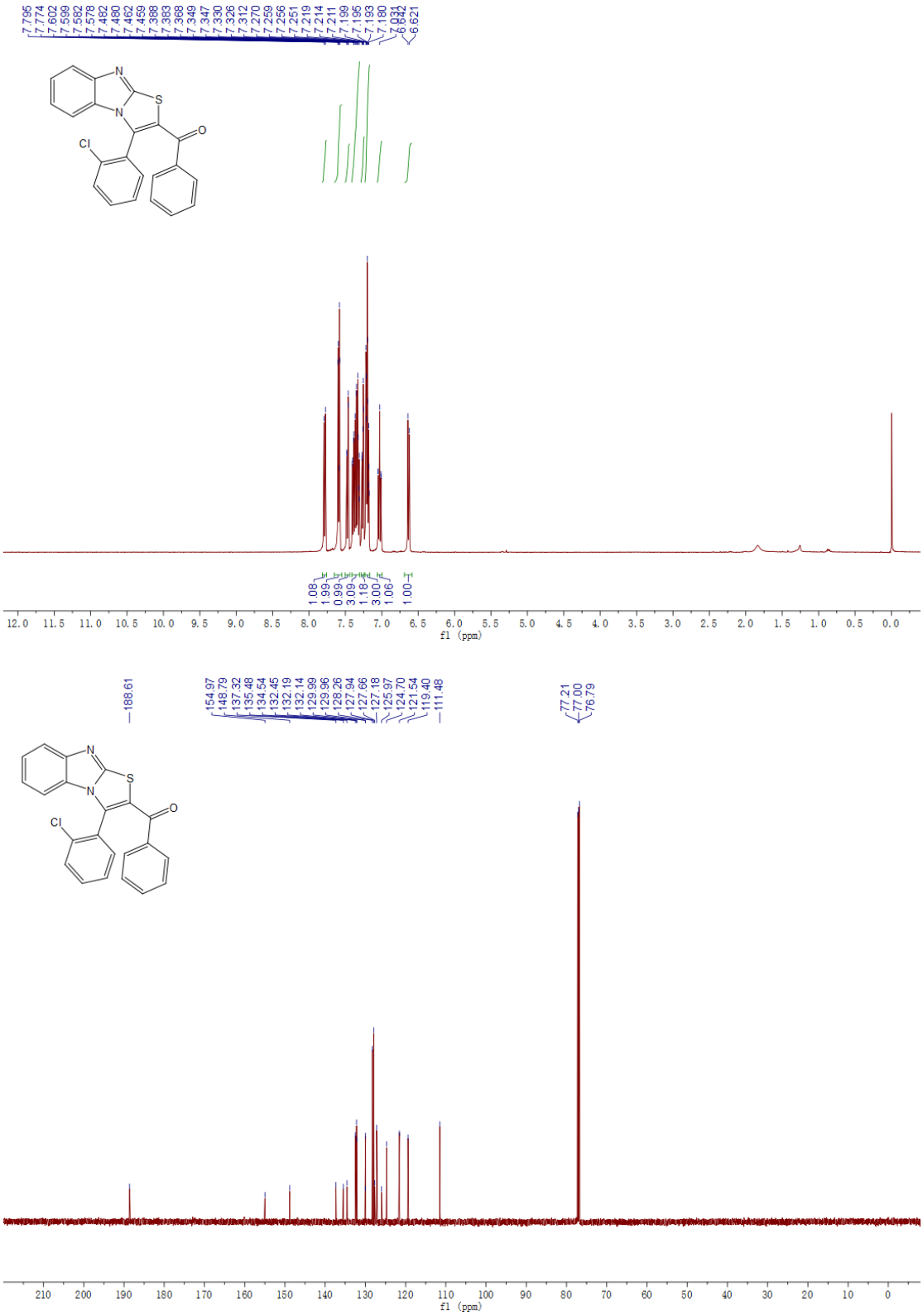




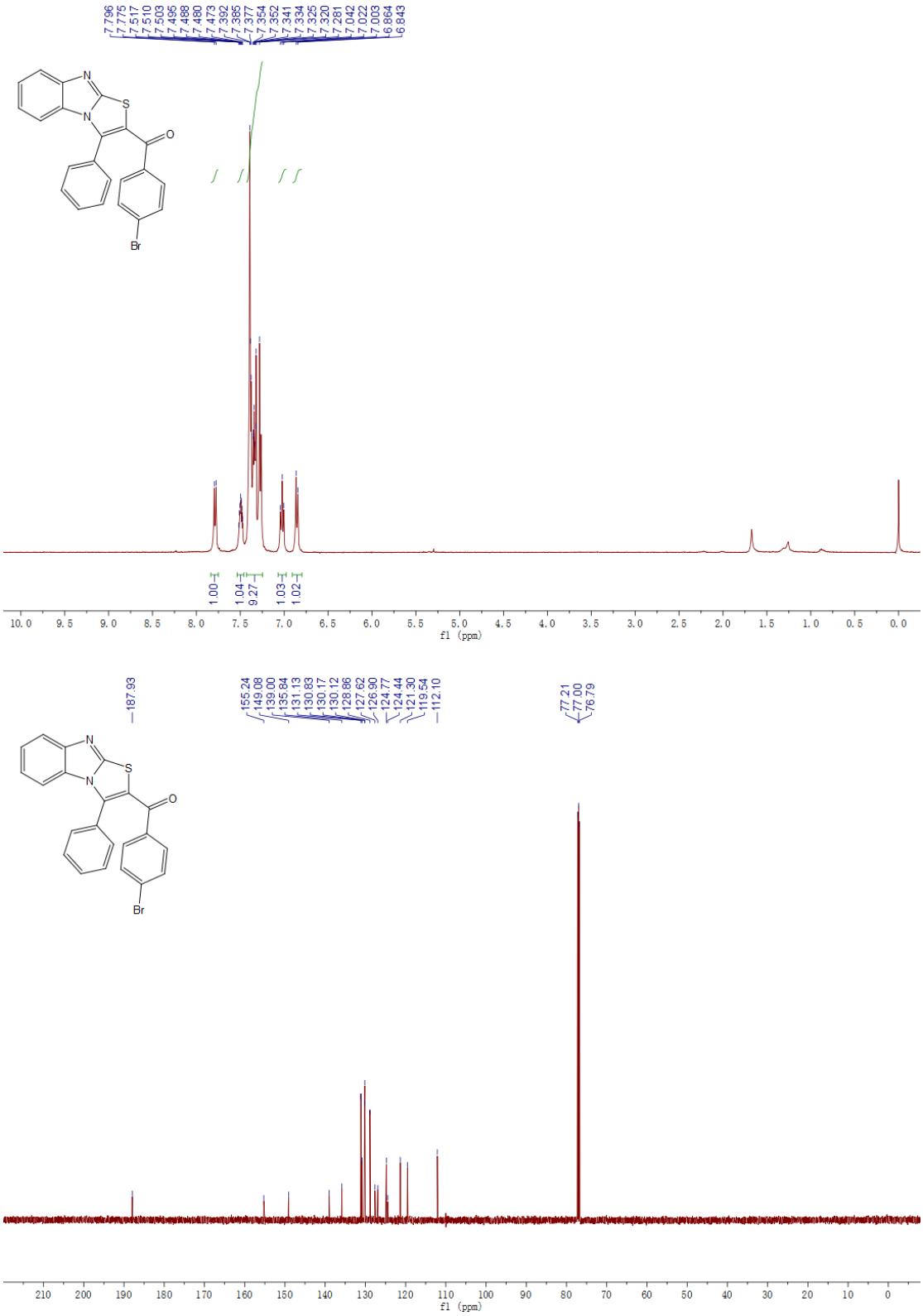
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3aj in $CDCl_3$



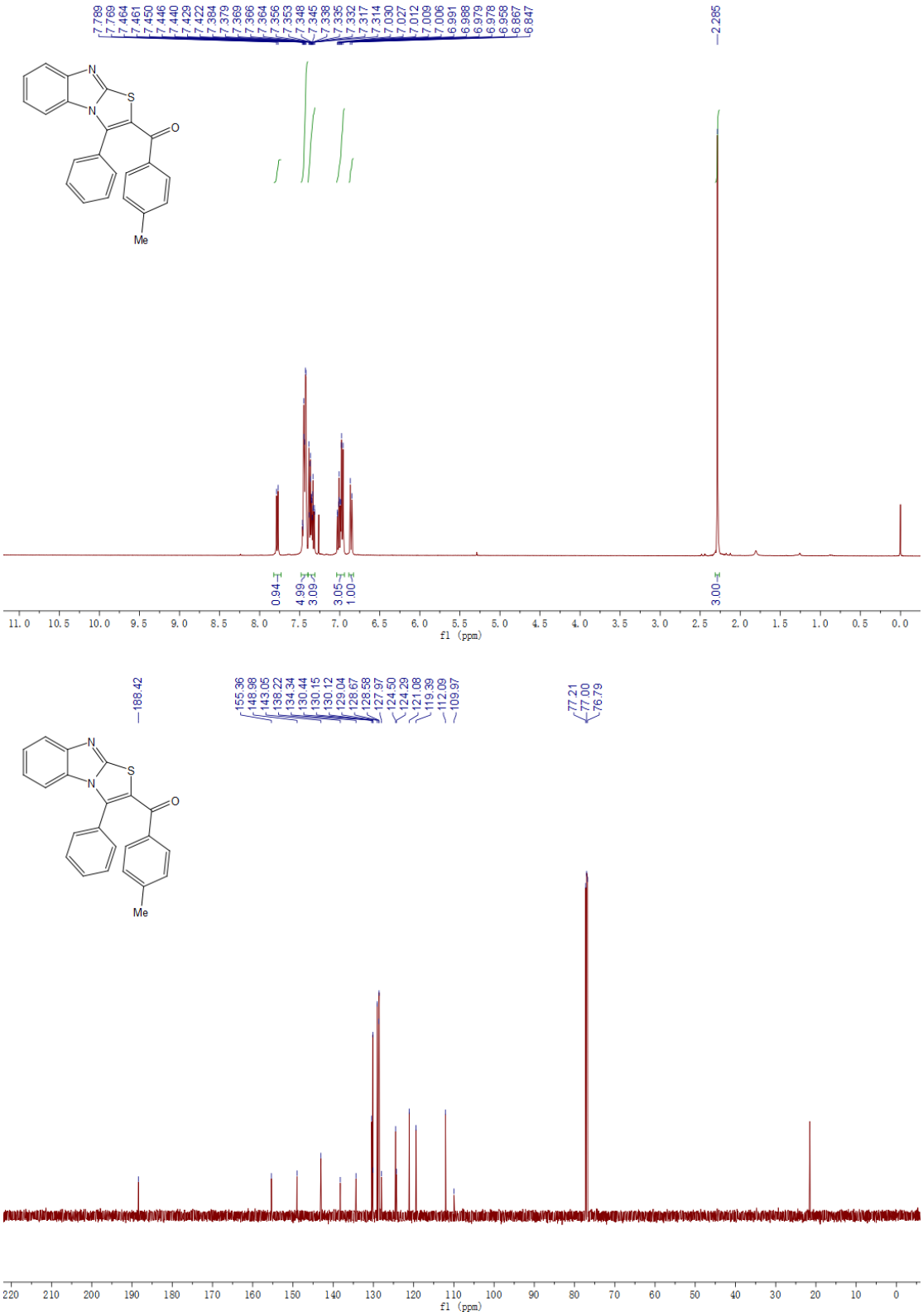
^{19}F NMR of compound 3aj in $CDCl_3$ (376 MHz)



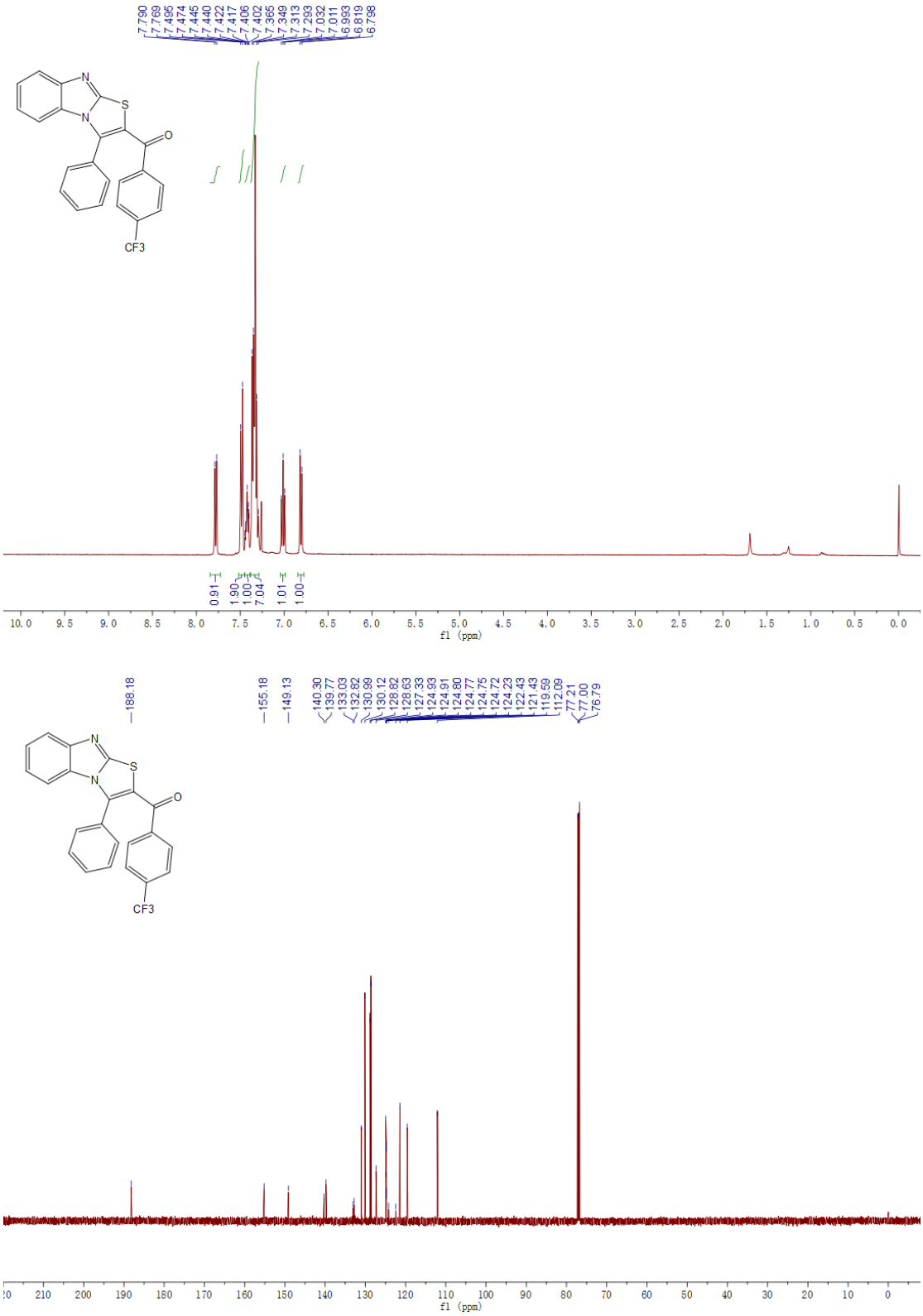
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ak in $CDCl_3$



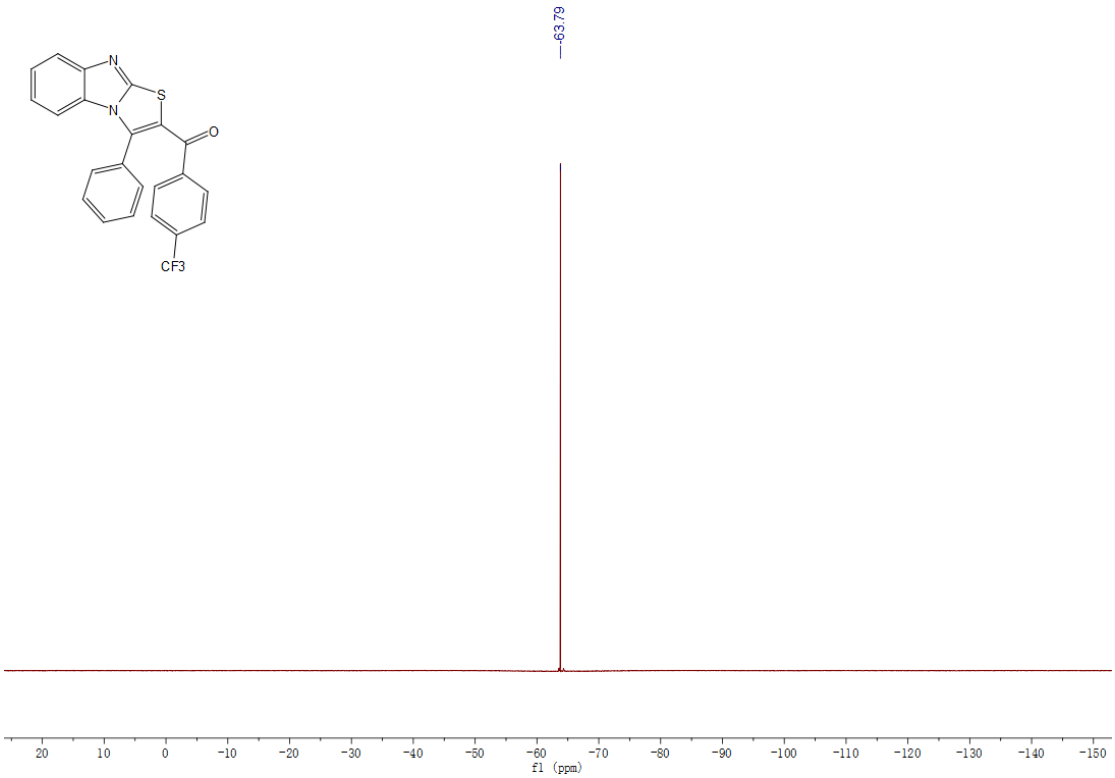
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3al in $CDCl_3$



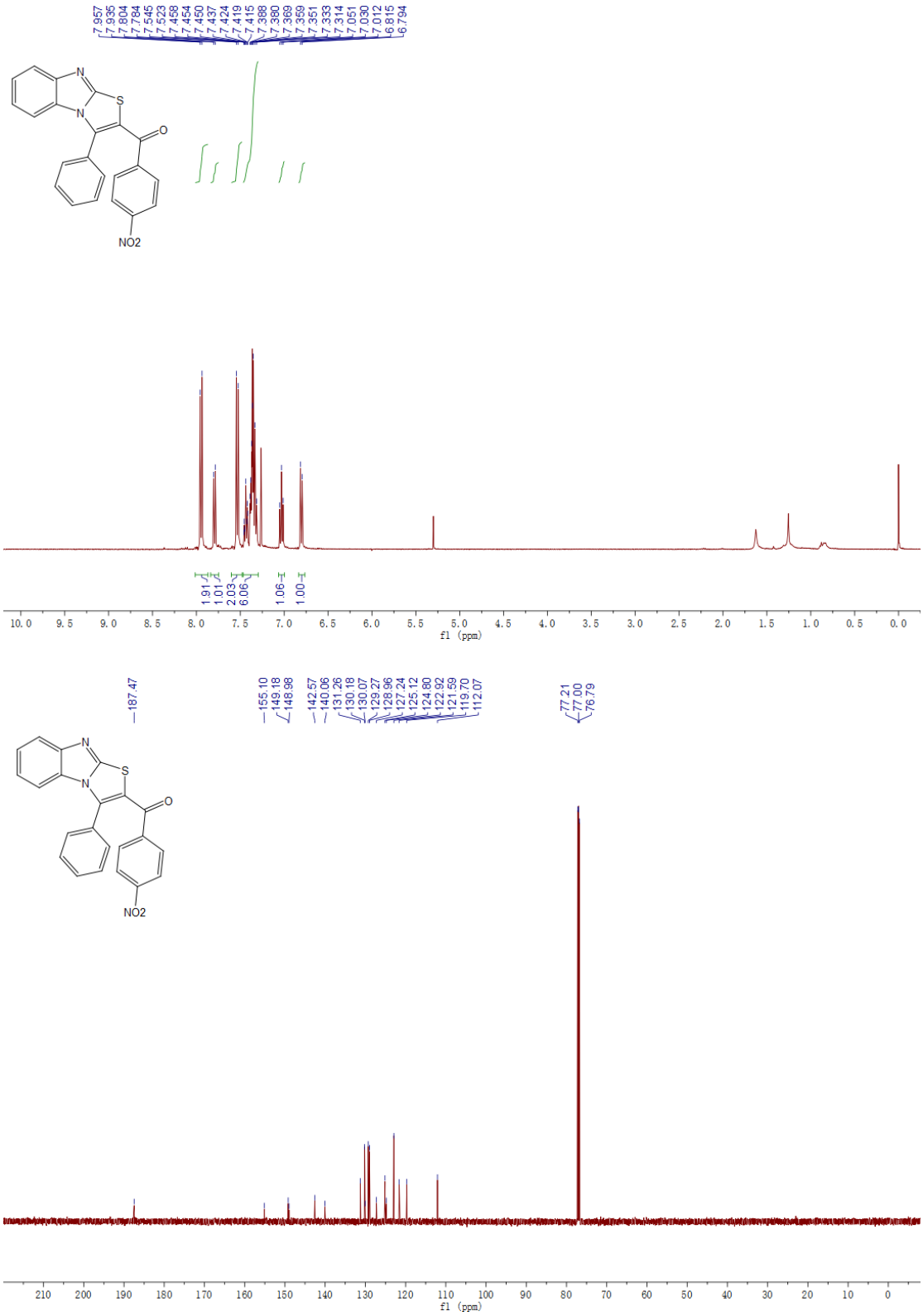
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3am in $CDCl_3$



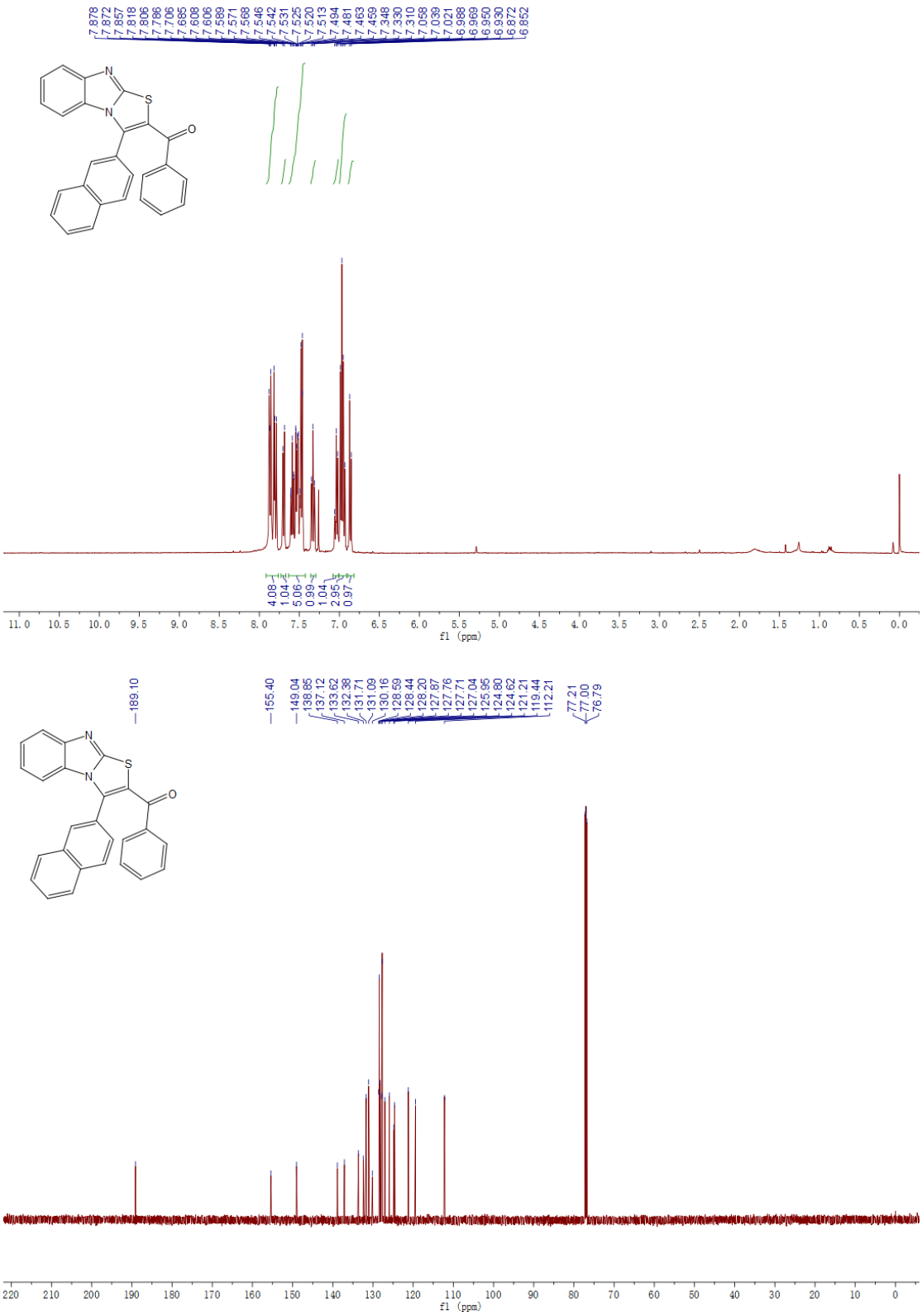
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3an in $CDCl_3$



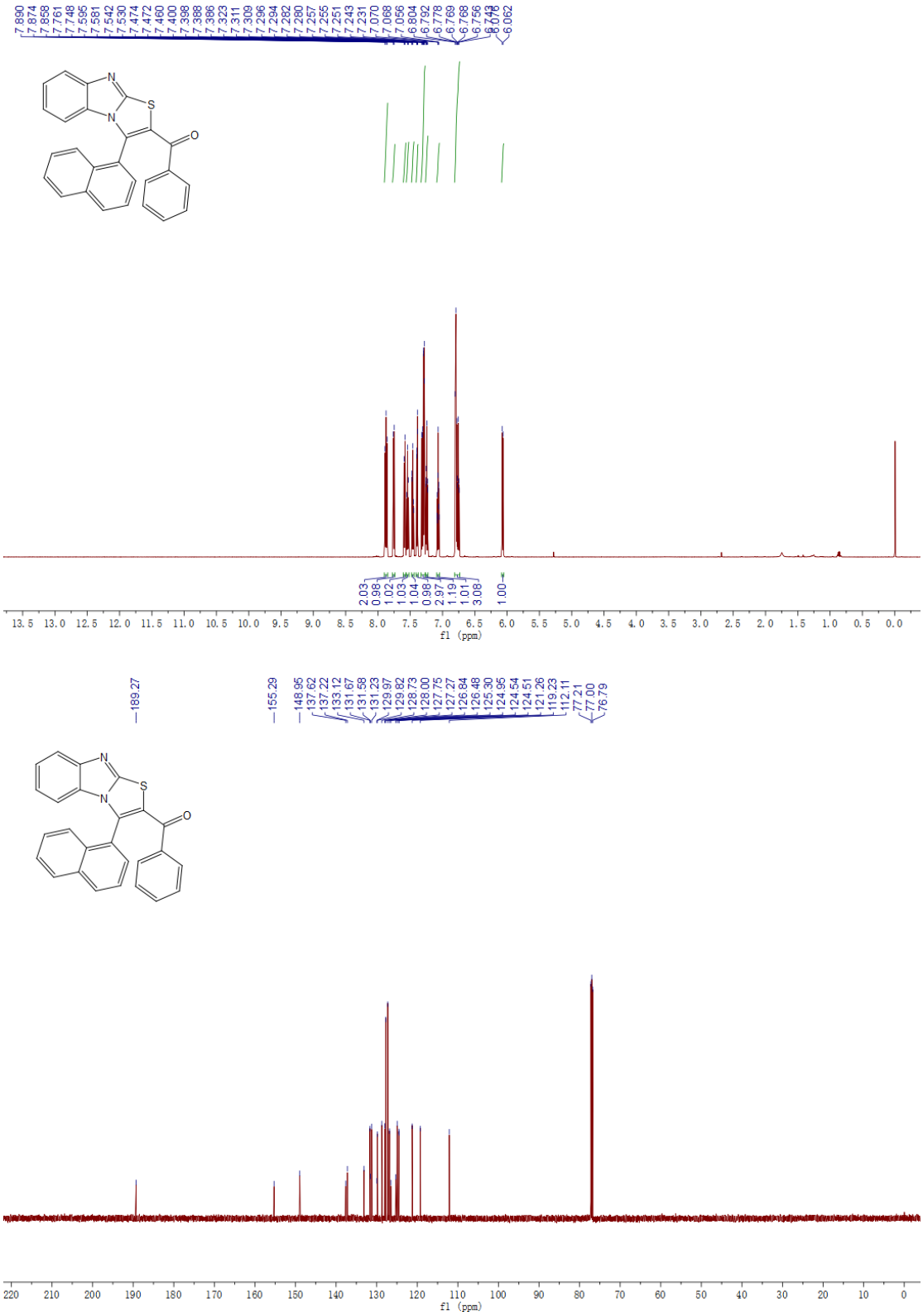
^{19}F NMR of compound 3an in $CDCl_3$ (376 MHz)



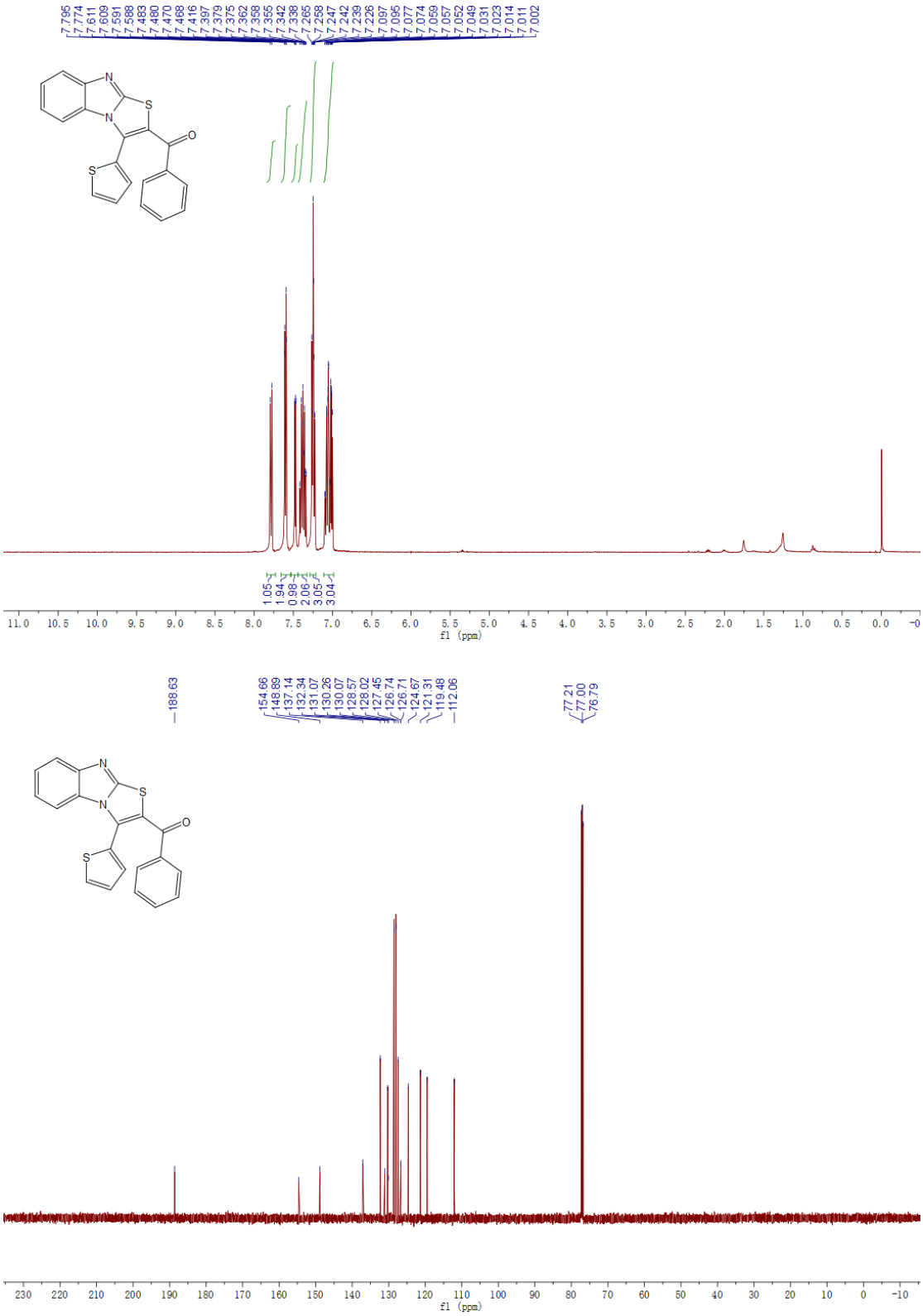
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ao in $CDCl_3$



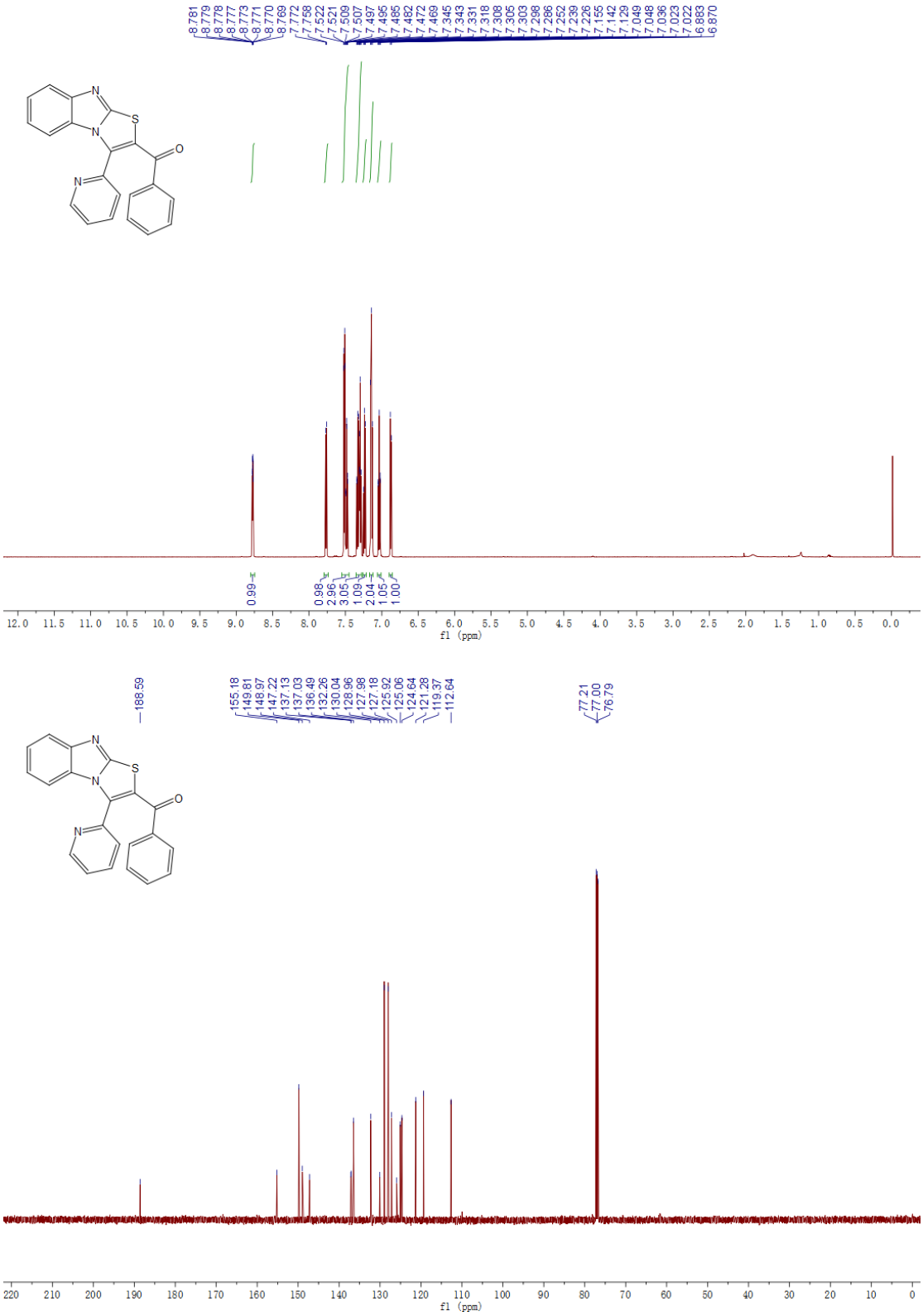
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ap in $CDCl_3$



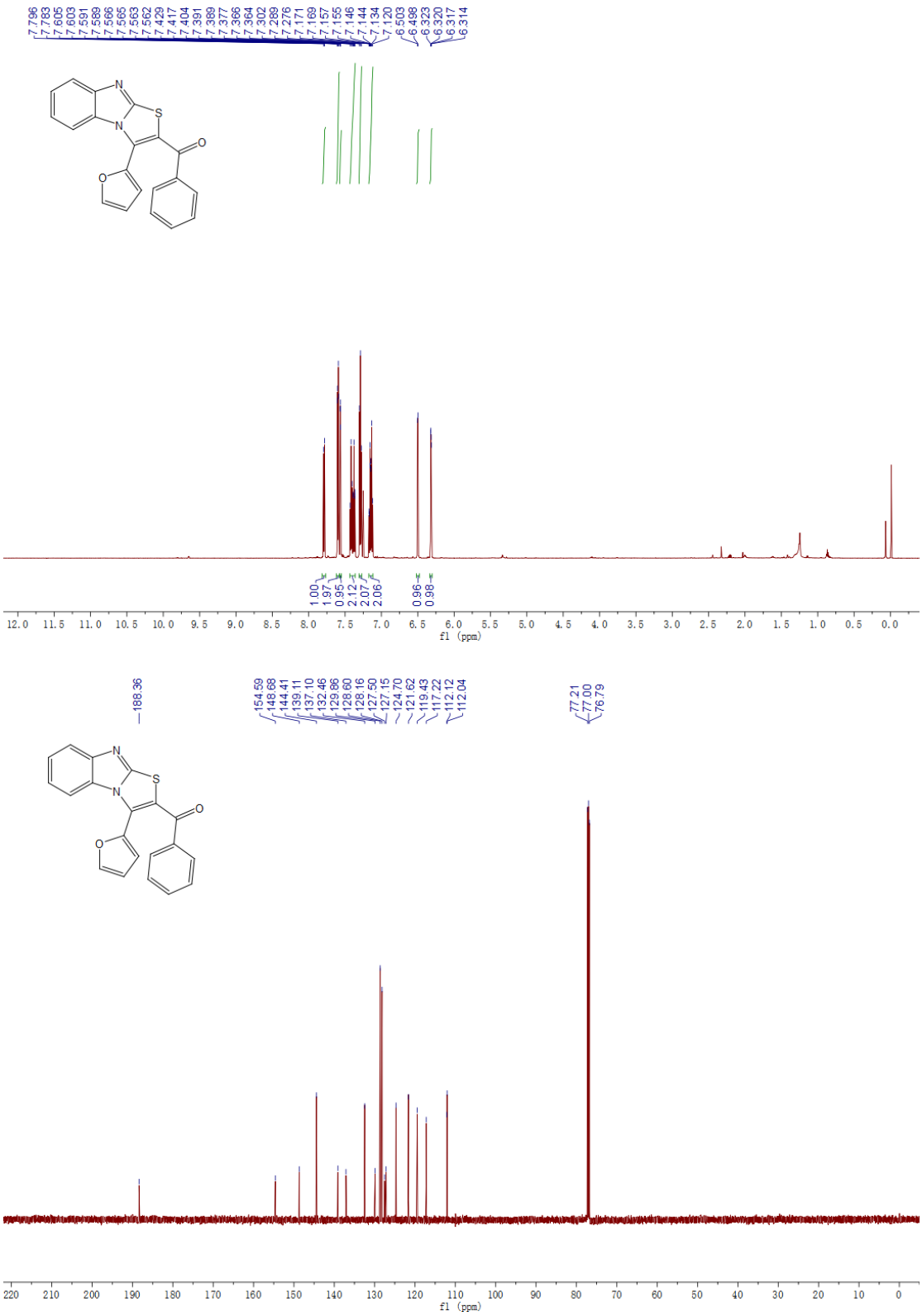
^{1}H NMR(600 MHz)、^{13}C NMR(150 MHz) of compound 3aq in $CDCl_3$



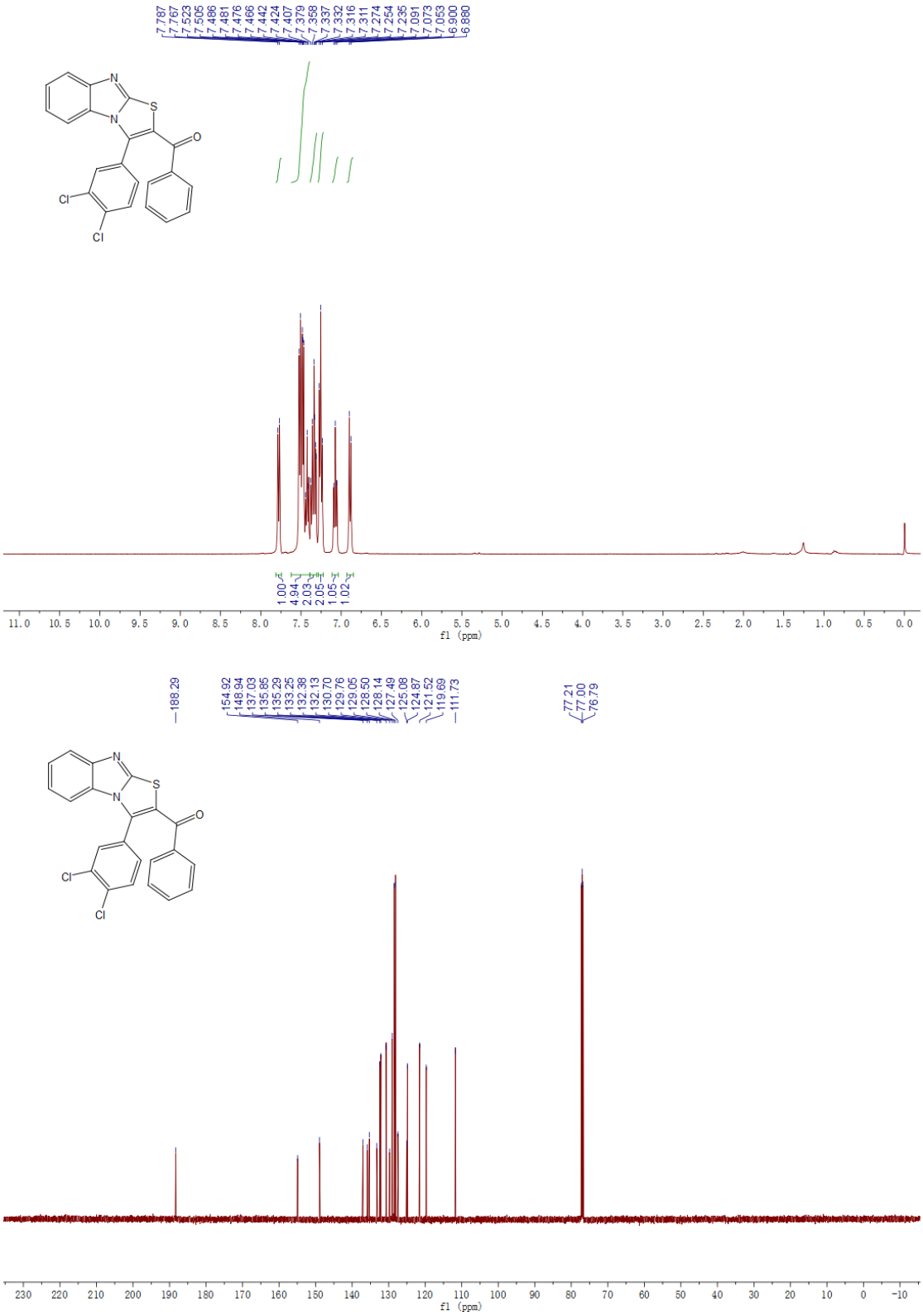
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ar in $CDCl_3$



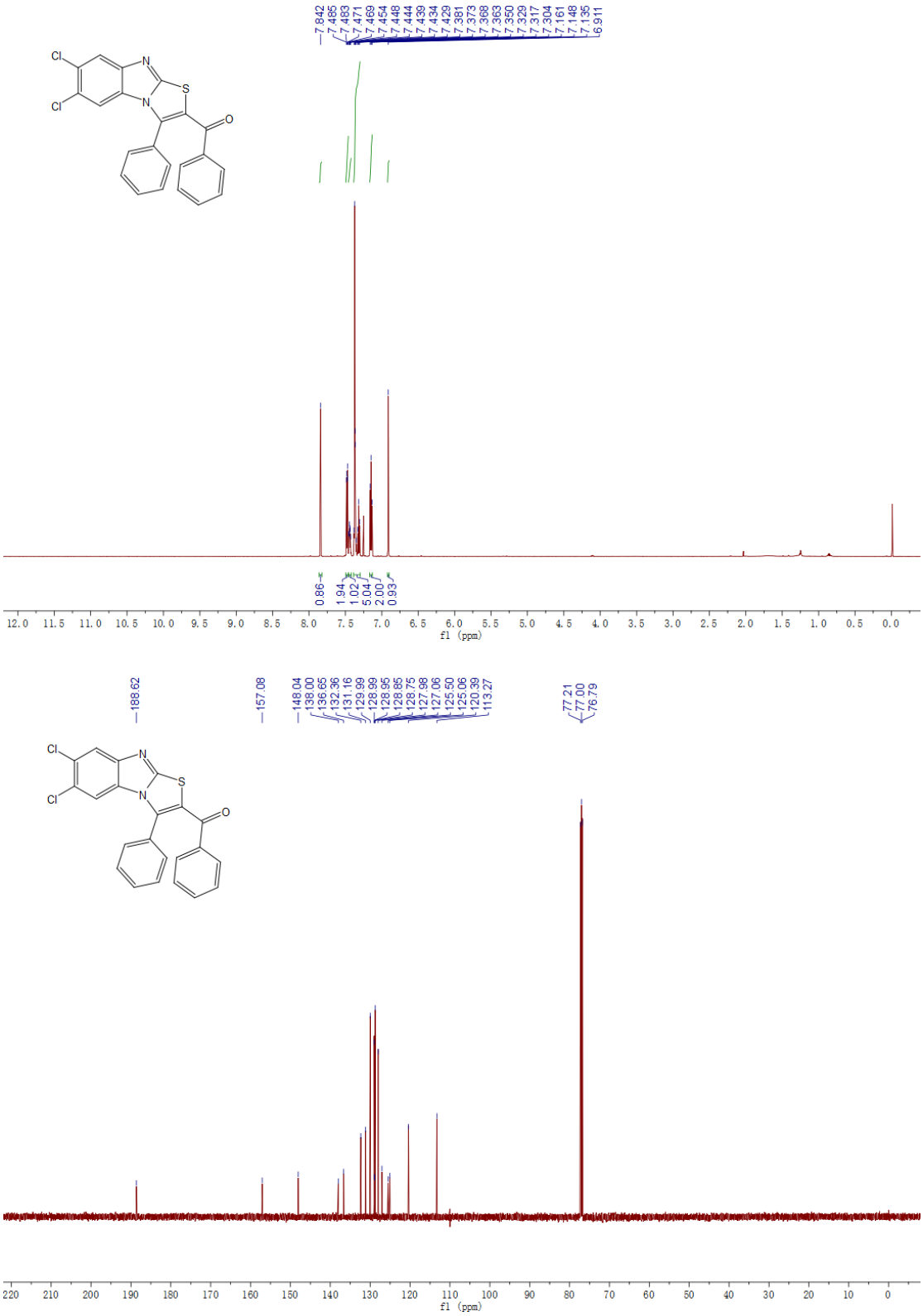
^{1}H NMR(600 MHz)、^{13}C NMR(150 MHz) of compound 3as in $CDCl_3$



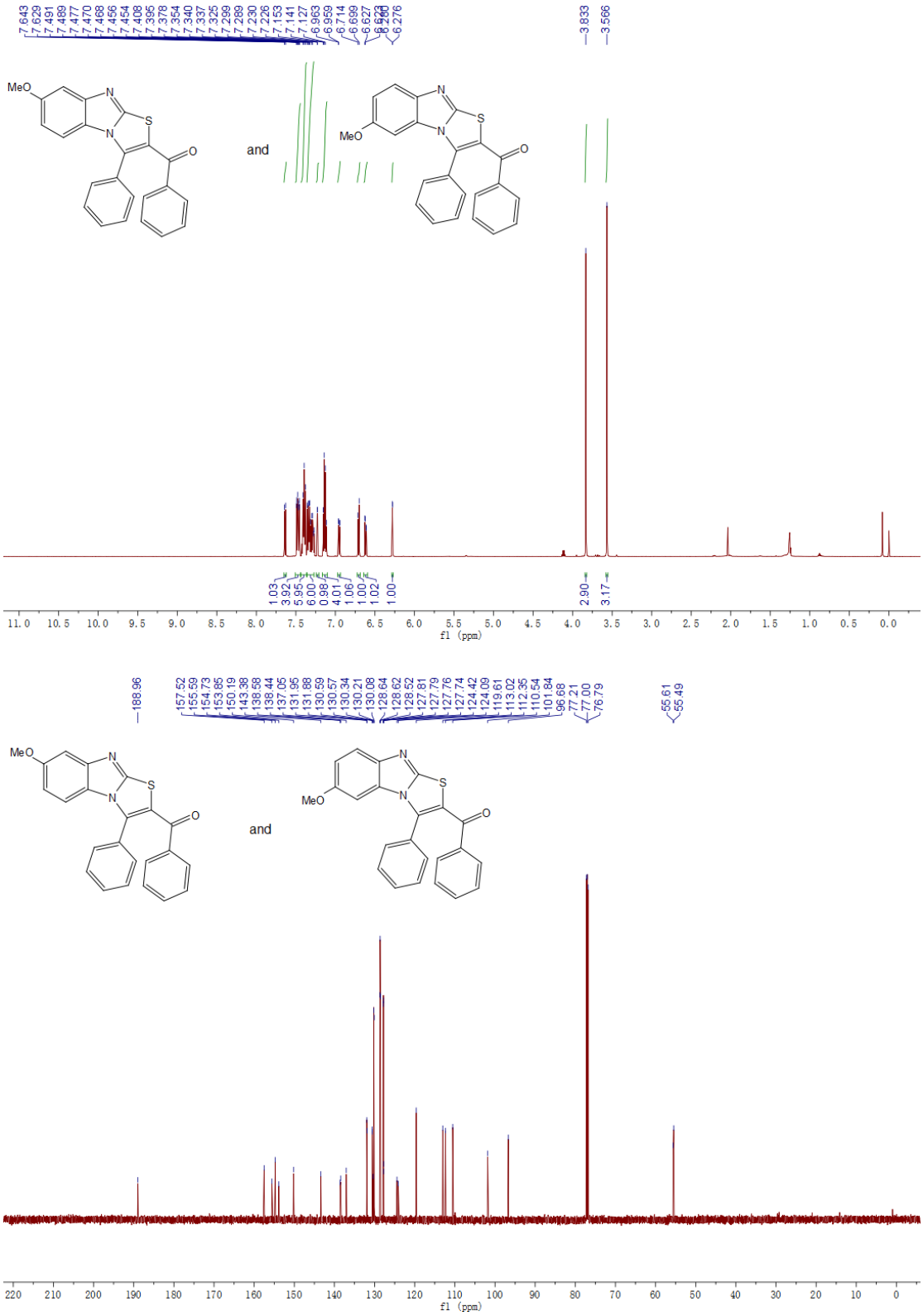
^{1}H NMR(600 MHz)、^{13}C NMR(150 MHz) of compound 3at in $CDCl_3$



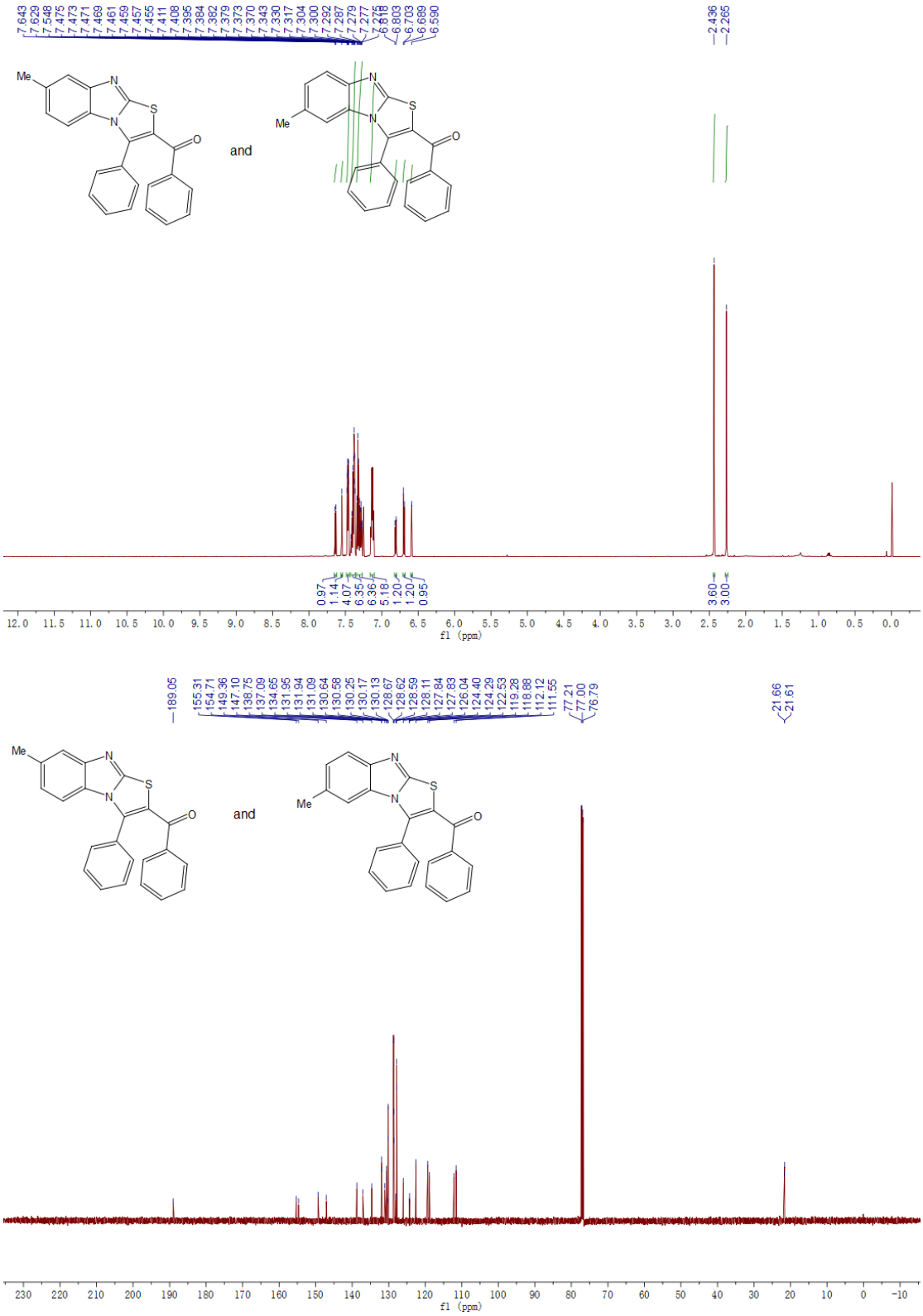
^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3au in $CDCl_3$



^{1}H NMR(600 MHz)、^{13}C NMR(150 MHz) of compound 3av in $CDCl_3$



^{1}H NMR(600 MHz)、^{13}C NMR(150 MHz) of compound 3aw,3aw' in $CDCl_3$



^{1}H NMR(400 MHz)、^{13}C NMR(150 MHz) of compound 3ax,3ax' in $CDCl_3$

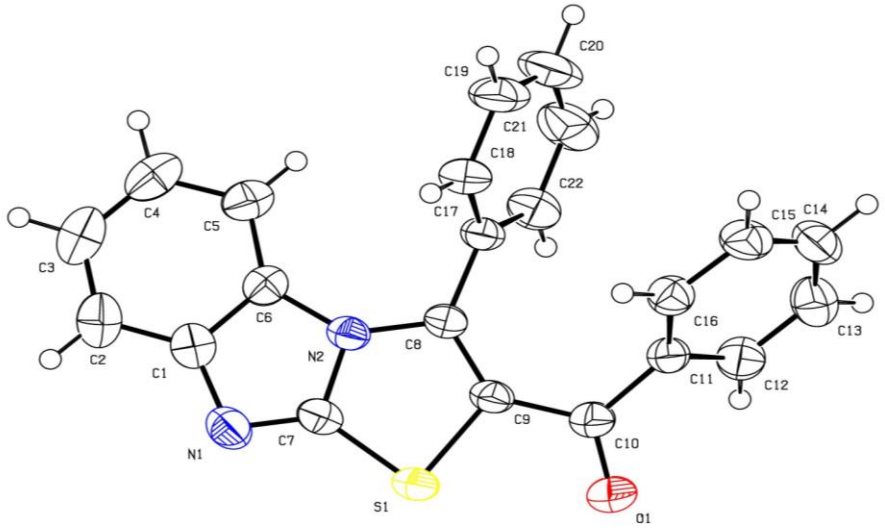


Figure S4. Single crystal data for product 3aa

Bond precision: C-C = 0.0021 A Wavelength=0.71073

Cell: a=11.5640(4) b=8.9788(4) c=17.5497(7)
alpha=90 beta=101.097(4) gamma=90

Temperature: 302 K

	Calculated	Reported
Volume	1788.13(13)	1788.12(13)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H14 N2 O S	C22 H14 N2 O S
Sum formula	C22 H14 N2 O S	C22 H14 N2 O S
Mr	354.41	354.41
Dx,g cm-3	1.316	1.316
Z	4	4
Mu (mm-1)	0.194	0.194
F000	736.0	736.0
F000'	736.76	
h,k,lmax	16,12,25	16,12,22
Nref	5644	4482
Tmin,Tmax	0.961,0.983	0.846,1.000
Tmin'	0.947	

Correction method= # Reported T Limits: Tmin=0.846 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.794 Theta(max)= 30.899

R(reflections)= 0.0382(3383) wR2(reflections)= 0.0990(4482)

S = 1.060 Npar= 236

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.
Click on the hyperlinks for more details of the test.

Alert level G

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1058 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.0 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ 3 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ 3 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 12 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

References:

1. J. Zhang, M. Y. She, L. Liu, X. K. Feng, Y. Li, H. Liu, T. T. Zheng, X. Leng, P. Liu, S. Y. Zhang, J. L. Li, *Org. Lett.* **2021**, *23*, 8396-8401.