Supporting Information

tert-Butyl peroxide (TBHP)/KI-mediated dual C(sp^2)-H bond amination of arylamines with α-diazo carbonyls toward 1,2,4-benzotriazines

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Context

General Information

^{1}H NMR (^{13}C NMR) spectra were measured on a Bruker DPX 400 MHz spectrometer in $CDCl_3$ (DMSO-*d6*) with chemical shift (δ) given in ppm relative to TMS as internal standard [(s = singlet, d = doublet, t = triplet, brs = broad singlet, m = multiplet), coupling constant (Hz)]. HRMS (APCI) was determined by using microTOF-QII HRMS/MS instrument (BRUKER). X-Ray crystallographic analysis was performed with a Siemens SMART CCD and a Siemens P4 diffractometer.

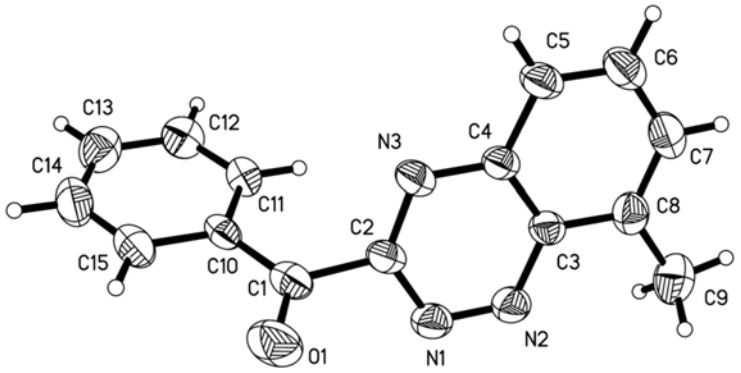
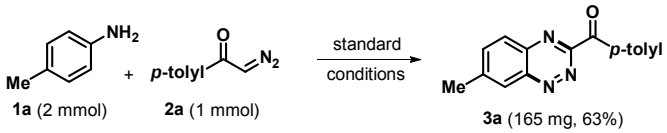


Figure S1. X-Ray Structure of Product **3j** (CCDC 1868192)

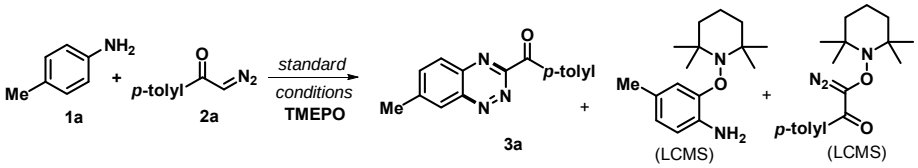
Gram-Scale Experiment of 3a:



under the air conditions, sodium benzenesulfinate (1.0 mmol, 1.0 equiv, 165 mg), KI (30 mol %, 50 mg) ,4 Å MS (500 mg) and ethanol (5.0 mL) were added into a 25-mL reaction tube. Then, *α*-diazo ketone **2a** (1.0 mmol, 1.0 equiv, 160 g) and *p*-toluidine **1a** (2.0 mmol, 2.0 equiv, 215 mg) was added into the reaction system. Subsequently, TBHP (0.4 mL, 2.0 equiv, 5.5 M in nonane) in ethanol solution (5.0 mL) was added into the suspension over 1.0 hour *via* a syringe pump at room temperature. After completion of the addition, the reaction mixture was stirred at room temperature for an additional 19.0 h until complete consumption of **2a** as monitored by TLC analysis. After completion of the reaction, the mixture was poured into the water and was extracted with ethyl acetate (3×10 mL). The organic layers were combined and dried over sodium sulfate and was then concentrated in vacuum. The resulting residue was purified by column chromatography on silica gel (eluent, petroleum ether/ethyl acetate = 15:1) to afford the desired product **3a** (165 mg, 63%) as a yellow solid.

Radical-Trapping Experiment:

TEMPO as the radical trapping reagent —— General procedure



Under the air conditions, sodium benzenesulfinate (0.2 mmol, 1.0 equiv, 33 mg), KI (30 mol%, 10 mg), 4 Å MS (100 mg), and 1.0 mL of ethanol were added into a reaction tube. Then, α-diazo ketone **2a** (0.2 mmol, 1.0 equiv, 32 mg),

p-toluidine **1a** (0.4 mmol, 2.0 equiv, 43 mg) and TEMPO (0.4 mmol, 2.0 equiv, 62 mg) was added into the reaction system. Subsequently, TBHP (0.08 mL, 2.0 equiv, 5.5 M in nonane) in ethanol solution (1.0 mL) was added into the suspension over 1.0 h via a syringe pump at room temperature. Next, the reaction mixture was stirred at room temperature for an additional 19.0 h. After, the mixture was poured into the water and was extracted with ethyl acetate (3×5 mL). The organic layers were combined and dried over sodium sulfate, which is further detected by LC-MS analysis.

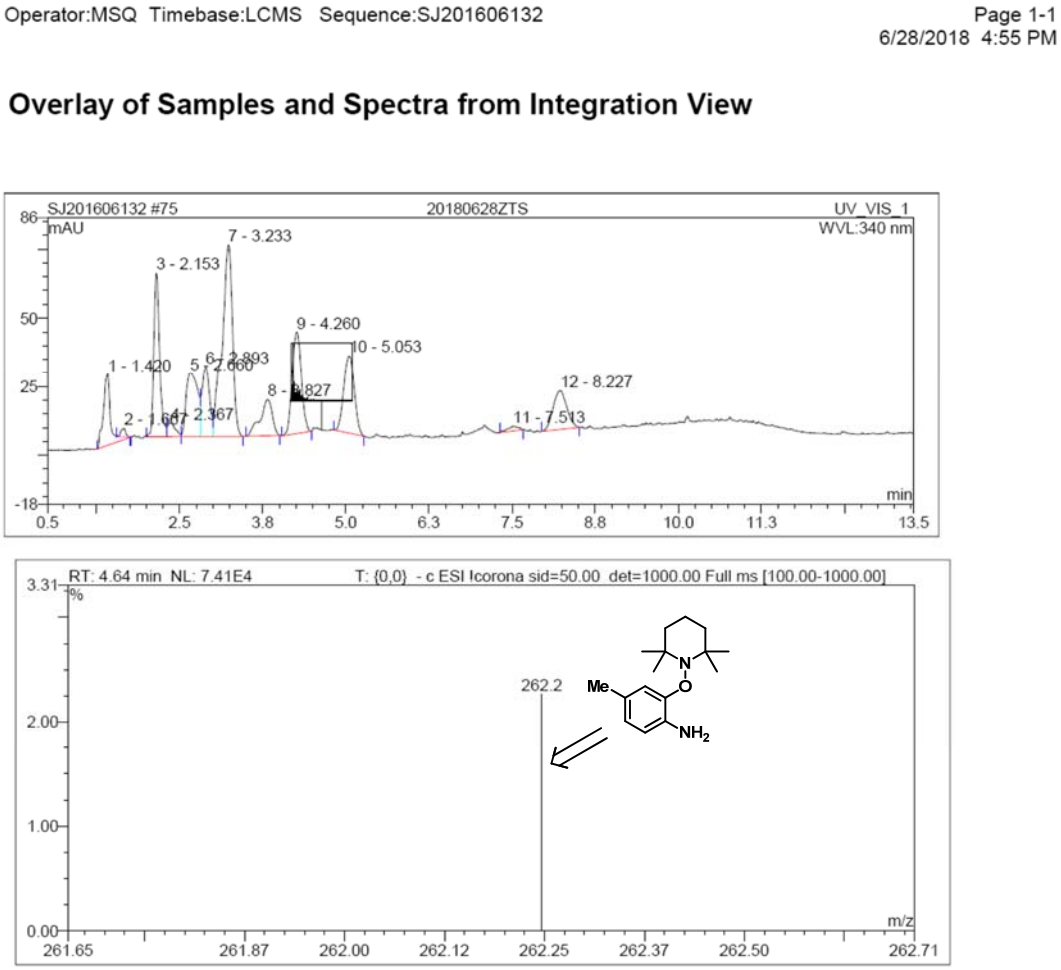


Figure S2 Copy of LC-MS Spectrum for *p*-Toluidine-TEMPO Adduct

Overlay of Samples and Spectra from Integration View

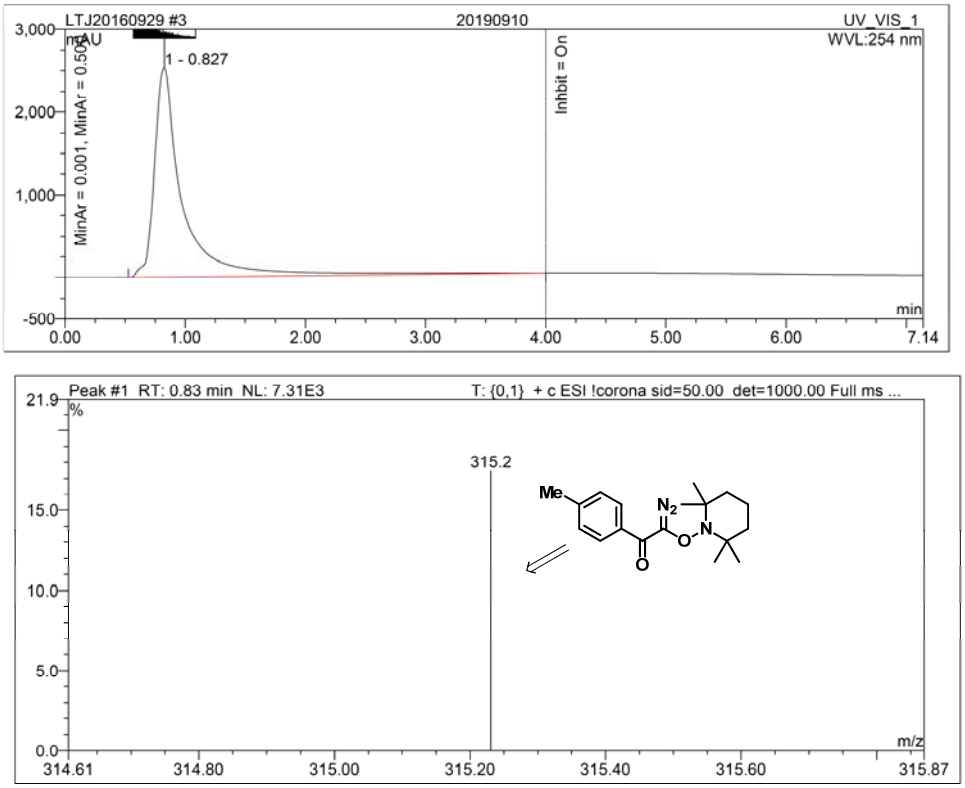


Figure S3 Copy of LC-MS Spectrum for TEMPO-α-Diazoketone Adduct

Computational Section

Computational details

All calculations were carried out by using Gaussian 09 program[1]. The geometries of all species were optimized using DFT with the B3LYP functional[2,3] and 6-311+g(d) basis sets. To illuminate the influence of the solvent (ethanol) on the reaction, the SMD model[4] single-point energy calculations were carried out based on the gas-phase geometries by using SMD-M06[5] functional and 6-311+ G (d, p) basis set. The free energy of each species in solution was deemed as the sum of the gas-phase free energy and the free energy of solvation.

References

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; et al. *Gaussian 09*, Revision A.02; Gaussian, Inc.: Wallingford, CT, 2009.
2. Becke, A. D. *J. Chem. Phys.* 1993, 98, 5648-5652.
3. Lee, C.; Yang, W. T.; Parr, R. G. *Phys. Rev. B.* 1988, 37, 785-789.
4. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B.* 2009, 113, 6378-6396.
5. Zhao, Y.; Truhlar, D. G. *Theor. Chem. Account.* 2008, 120, 215-241.

Computational Results

Toward molecular-level understanding of mechanism of this reaction, we performed a density functional theory (DFT) study on various possible processes. As shown in **Figure S1-S7**, the substrate **2** is easier to be activated by ^{t}BuO radical to give radical **B** (an energy barrier 16.3 kcal/mol for **Sub→A→TS-A/B→B**) than by $PhSO_2$ radical (an energy barrier 34.7 kcal/mol). The radical **B** can spontaneously bind to the aniline (exothermic 2.0 kcal/mol), but its subsequent cyclization step is very difficult to overcome in either presence or absence of $PhSO_2^-$ (**C'→F'** or **D'→E'**, **Figure S3** and **Figure S4**). Reversely, the radical **B** can also spontaneously bind to the aniline radical to give the intermediate **C** (exothermic by 49.8 kcal/mol), because the aniline radical is very easy to form in the presence of ^{t}BuO radical (an energy barrier of 0.1 kcal/mol, **Figure S7**).

When intermediate **C** forms, its N-H bond is easy to be activated by ^{t}BuO radical to afford an intermediate **D** (an energy barrier of 12.1 kcal/mol for **C→TS-C/D→D**), **D** then undergoes a cyclization process (an energy barrier of 12.7 kcal/mol for **D→TS-D/E→E**) to give an intermediate **E**, in which $PhSO_2^-$ play an absorbing benzene proton role. The intermediate **E** finally releases the desired product with an energy barrier of 0.9 kcal/mol. Reversely, **C** is relatively difficult to undergo a direct cyclization process to give an intermediate **F** (an energy barrier of 20.3 kcal/mol for **C→TS-C/F→F**); and its C-H bond is also very difficult to be activated by ^{t}BuO radical to afford an intermediate **G** (an energy barrier of 29.8 kcal/mol for **C→TS-C/G→G**) which then involves in a cyclization process to give H (**G→TS-G/H→H**) in the absence of $PhSO_2^-$. In addition, the N-H bond of aniline is very easy to be activated by ^{t}BuO radical to give the aniline radical, but its subsequent process is very difficult to occur (**Figure S6** and **S7**).

To sum up, **Sub→A→B→C→D→E→Product** is the most possible mechanism in the whole catalytic process.

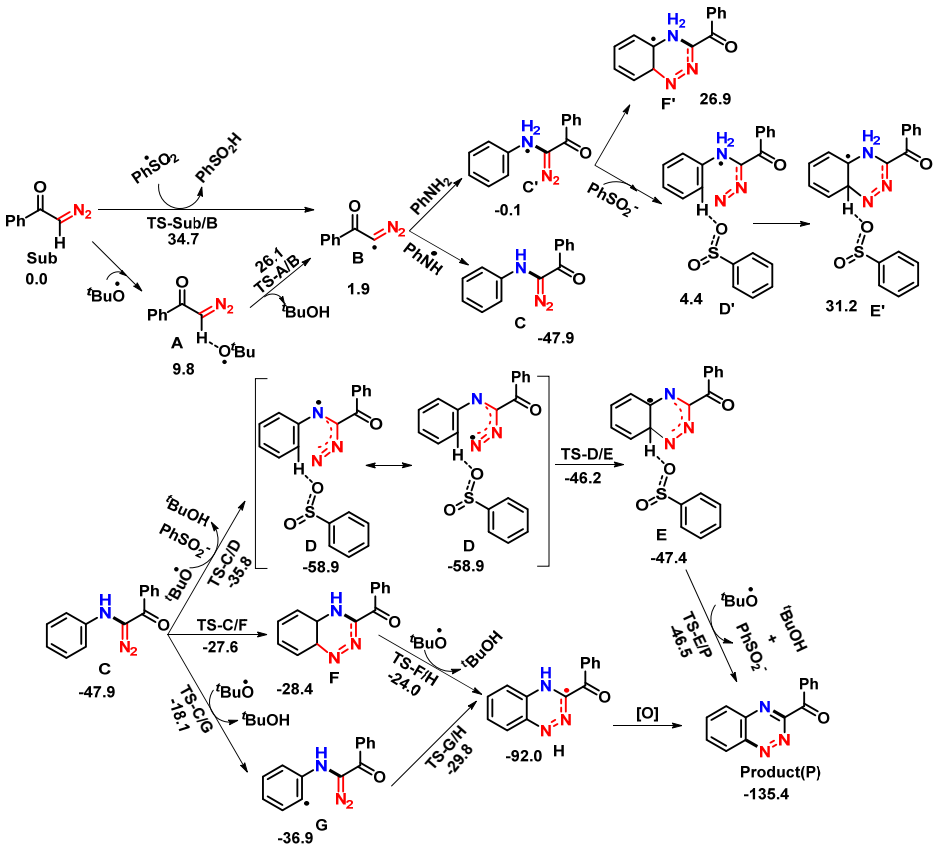


Figure S1. Possible pathways of the reaction (kcal/mol)

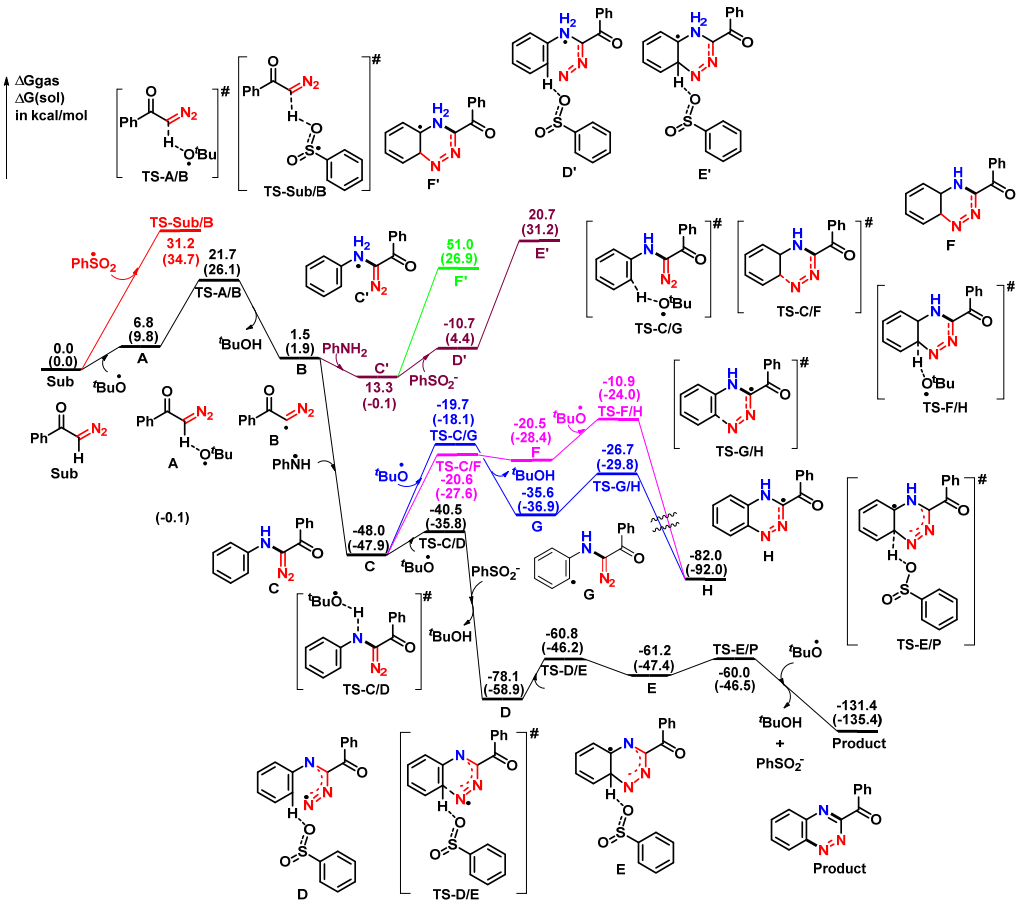


Figure S2. Gibbs free energy profiles from the beginning of Sub

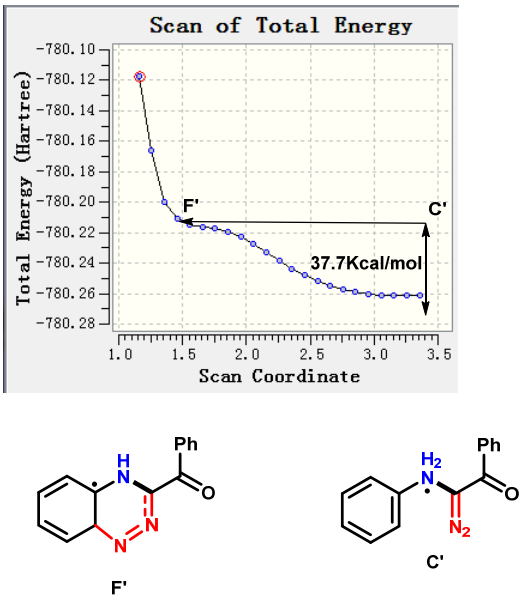


Figure S3. The relaxed potential energy surface scans from C' to F'.

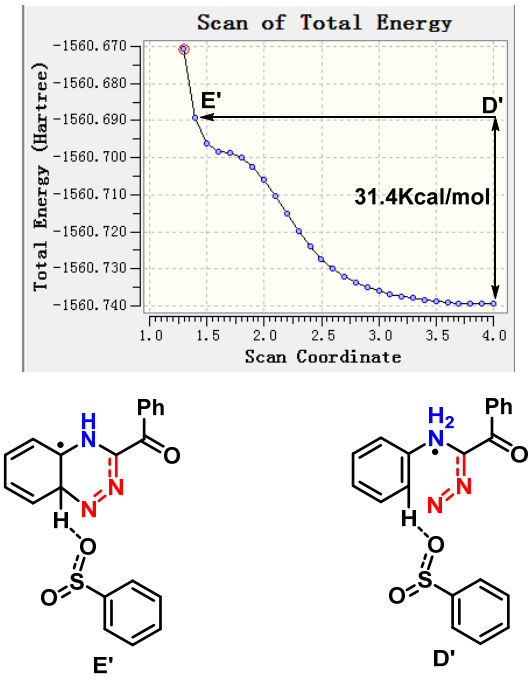


Figure S4. The relaxed potential energy surface scans from D' to E'

Many attempts are made to locate their transition states from C' to F' (and from D' to E'), but the transition state is still elusive. Herein, the relaxed potential energy surface scans of these two processes are performed. As shown in Figure S2(from C' to F') and Figure S3 (from D' to E'), the energies are always increased, showing that it is impossible for the radical B bound to aniline to occur.

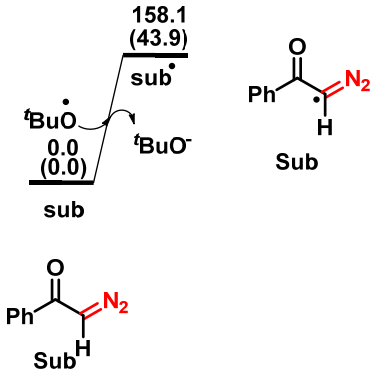


Figure S5. Gibbs free energy profile from the beginning of the Sub electronics withdrawn by ᵗBuO radicals. This energy barrier is impossible to overcome.

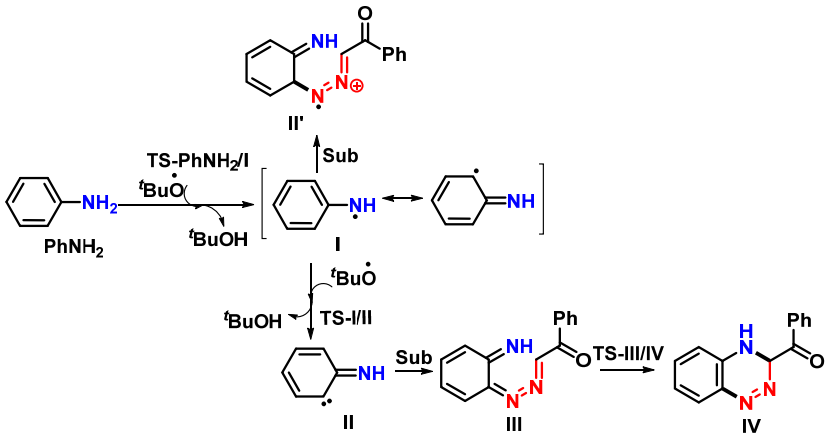


Figure S6. Possible pathways from the beginning of aniline N-H activation

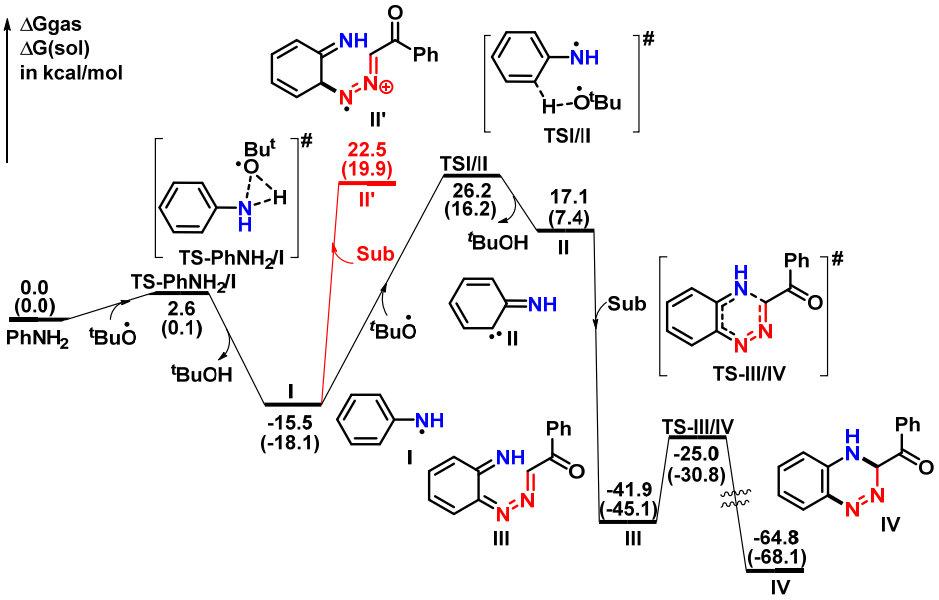
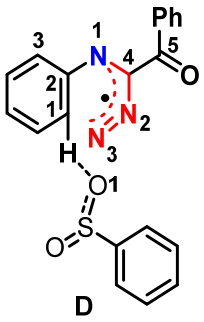


Figure S7. Gibbs free energy profiles from the beginning of aniline N-H activation

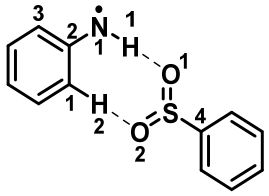
Table S1 The NBO charge of the key atoms from **D** to **E**



D

atom / species	S	O1	H	C1	C2	C3	C4	C5	N1	N2	N3
D-noPhS$^-$			0.213	0.154	-0.629	0.597	0.031	-0.812	0.225	0.462	-0.216
D	0.188	-0.528	0.456	0.24	-0.516	-0.044	-0.091	-0.836	0.31	0.016	0.064
TSDE	0.344	-0.526	0.526	0.255	-0.008	-0.681	0.327	-1.124	0.333	-0.064	0.224
E	0.428	-0.503	0.552	0.105	0.172	-1.53	0.268	-0.531	0.328	-0.105	0.269

Table S2 The NBO charge of the key atoms of $PhNH_2$-$PhSO_2H$



atom / species	S	O1	O2	C1	C2	C3	C4	N	H1	H2
PhNH				0.386	-0.75	0.18		-0.338	0.268	0.21
PhS$^-$	0.291	-0.515	-0.514				-0.138			
PhNH-PhS-	0.217	-0.582	-0.511	0.763	-0.746	0.196	-0.073	-0.492	0.488	0.408

Table S3. Electronic energies (E_{elec}), Zero-point energies(ZPE), Gibbs free energies (G_{gas}), high accurate single-point energies (E_{sp}) and solvent free energies ($\triangle G_{sol}$) of all stationary points. The E_{elec}, ZPE, G_{gas}, E_{sp} energies are in a. u. and G_{sol} are in kcal/mol.

Species	E_{elec}	**ZPE**	E_{sp}	G_{gas}	$\triangle G_{sol}$
Sub	-493.2600801	0.124066	-492.9394529	-493.171511	-7.56
^{t}BuO·	-233.0668091	0.122149	-232.9096636	-232.974195	-5.11
A	-726.3324445	0.247179	-725.8506686	-726.134923	-9.64

^{t}BuOH	-233.7337242	0.135257	-233.5890228	-233.627507	-7.37
$PhSO_2^-$	-780.4200396	0.096459	-780.239319	-780.357302	-64.05
$PhSO_2$·	-780.3210966	0.098145	-780.0501699	-780.256686	-8.62
TS-A/B	-726.3055018	0.242627	-725.8277564	-726.111064	-8.31
TS-Sub/B	-1273.543125	0.216733	-1272.956247	-1273.378479	-12.72
B	-492.590613	0.111271	-492.266629	-492.515824	-4.87
$PhNH_2$	-287.6638215	0.116421	-287.4580699	-287.576272	-7.09
C'	-780.2614755	0.23359	-779.759002	-780.073222	-25.84
PhNH·	-287.0214993	0.103389	-286.8150849	-286.947661	-7.48
C	-779.7182748	0.22115	-779.1978994	-779.542358	-12.69
TS-C/G	-1012.754142	0.338333	-1012.087378	-1012.471525	-16.22
G	-779.031556	0.208018	-778.5137294	-778.869272	-11.8
TS-G/H	-779.019639	0.207711	-778.5018132	-778.855133	-13.61
H	-779.1113318	0.21074	-778.5987009	-778.943223	-20.54
D'	-1560.739394	0.331191	-1560.013955	-1560.468798	-61.35
E'					-65.91
F'					-32.6
TS-C/F	-779.678251	0.221383	-779.1661148	-779.49862	-19.79
F	-779.6783039	0.221971	-779.1675507	-779.498565	-20.65
TS-F/H	-1012.746631	0.343899	-1012.085327	-1012.457396	-25.91
TS-C/D	-1012.790274	0.341022	-1012.110857	-1012.504536	-13.24
D	-1559.535736	0.304534	-1558.797522	-1559.294358	-55.33

TS-D/E	-1559.513126	0.305346	-1558.784155	-1559.266662	-59.97
E	-1559.514789	0.30577	-1558.789165	-1559.267303	-60.84
TS-E/P	-1559.510221	0.302654	-1558.783604	-1559.265541	-61.07
Product	-778.5268762	0.200402	-778.0042411	-778.368603	-14.98
$^{t}BuO^{-}$	-233.1316184	0.120055	-233.0804291	-233.040249	-69.5
Sub·	-492.9379599	0.121622	-492.6930695	-492.853431	-57.44
TS-$PhNH_2$/I	-520.7387537	0.235302	-520.546264	-520.3829505	-14.72
I	-287.021497	0.1034	-286.947646	-286.8150895	-7.48
TS-I/II	-520.036298	0.221698	-519.855428	-519.6858941	-19.92
II	-286.303611	0.090326	-286.242402	-286.0912344	-12.23
III	-779.6855306	0.221111	-779.508	-779.1603366	-13.24
TS-III/IV	-779.6592798	0.220639	-779.481037	-779.1382641	-15.92
IV	-779.726051	0.223476	-779.544376	-779.2035039	-13.46
II'	-780.2425078	0.230235	-780.058652	-779.7189004	-14.97

Table S4. Calculated Cartesian coordinates of all stationary points

Sub

C	-2.71213300	-0.72882300	-0.45149200
C	-1.32599200	-0.63207900	-0.54796300
C	-0.70581200	0.62152600	-0.62106600
C	-1.49899900	1.77614400	-0.59016900

C	-2.88299200	1.67857900	-0.50410400
C	-3.49326200	0.42537400	-0.43504400
H	-3.18119100	-1.70501700	-0.38474700
H	-0.73640800	-1.54223400	-0.53618300
H	-1.00808600	2.74114800	-0.63364000
H	-3.48780000	2.57939700	-0.48834100
H	-4.57353300	0.34882100	-0.36433000
C	0.78060500	0.80603700	-0.70910200
O	1.30487200	1.88568500	-0.46640200
C	1.57078900	-0.35401900	-1.11798800
H	1.19646700	-1.31213200	-1.44165000
N	2.87229000	-0.20446300	-1.17241400
N	3.98335500	-0.01795300	-1.19726200

^{t}BuO·

C	-1.27621800	-0.79140700	-0.31526700
H	-2.16503400	-0.22653900	-0.02681800
H	-1.30972900	-0.97266900	-1.39339400
H	-1.30968800	-1.75923800	0.19147500
C	0.00000100	-0.02758700	0.08258400
C	-0.00009500	1.38808200	-0.57739000
H	-0.88830000	1.95027200	-0.28656400
H	0.88818100	1.95028800	-0.28681100
H	-0.00025600	1.25840800	-1.66282400
C	1.27631900	-0.79123900	-0.31528300
H	2.16505400	-0.22641000	-0.02651200

H	1.30976400	-1.75921400	0.19118700
H	1.31001400	-0.97218000	-1.39345700
O	-0.00000600	0.26127400	1.43073100

A

C	-2.43351300	1.47271000	-0.88768800
C	-1.36611000	1.08136700	-0.08200900
C	-1.05610600	1.80234800	1.07898200
C	-1.83525400	2.91822900	1.41476000
C	-2.89900700	3.30697700	0.60908300
C	-3.20130200	2.58443200	-0.54602500
H	-2.66391300	0.90670700	-1.78459700
H	-0.79039200	0.21135000	-0.37508100
H	-1.58661000	3.46666900	2.31550400
H	-3.49358700	4.17346700	0.88031900
H	-4.03153200	2.88690500	-1.17656800
C	0.07441500	1.45222000	2.00413000
O	0.28533400	2.10285900	3.02199900
C	0.91110200	0.31092500	1.64249900
H	0.82304900	-0.32888700	0.77729600
N	1.89470500	0.01716800	2.45681500
N	2.72748500	-0.19773200	3.18620000
C	0.44101100	-2.95203000	-3.05955400
H	0.63399500	-3.89069400	-3.58599500
H	-0.63499000	-2.76670800	-3.05943900
H	0.92610500	-2.14665100	-3.61672600
C	0.98132700	-3.00333100	-1.61991200
C	2.49514500	-3.27552700	-1.57637500
H	2.84985300	-3.31748700	-0.54456700
H	2.73772200	-4.22200800	-2.06704100
H	3.03777000	-2.47931900	-2.09207400

C	0.21893300	-4.09993000	-0.80308900
H	0.57462500	-4.13304200	0.22705500
H	-0.85439900	-3.90842200	-0.80644000
H	0.41166700	-5.06471600	-1.27884900
O	0.66863600	-1.84628900	-0.93727700

^{t}BuOH

H	0.71758700	1.44311100	-0.80983100
C	-0.25037100	-0.95905200	-0.51488000
H	-1.03531400	-0.87099400	-1.26979700
H	-0.20100800	-2.00252300	-0.18979100
H	-0.54663000	-0.35932800	0.35316200
C	1.09300900	-0.48290900	-1.08128000
C	1.47964000	-1.28652300	-2.32095800
H	0.70792100	-1.19655500	-3.08898800
H	2.41764800	-0.91408400	-2.73925400
H	1.60476000	-2.34510900	-2.07881400
C	2.19253400	-0.55498600	-0.01455200
H	3.13712400	-0.17842700	-0.41415800
H	1.93138900	0.04851400	0.86211700
H	2.34936300	-1.58139000	0.33016800
O	0.96424100	0.87543400	-1.55104400

$PhSO_2^-$

C	-3.96814600	1.16075600	0.44813900
C	-2.62520600	1.32663600	0.79172000
C	-1.95988400	2.50769100	0.46792000
C	-2.64017100	3.52515500	-0.19875300
C	-3.98321600	3.36284200	-0.54338800
C	-4.65278400	2.18157200	-0.21538700
H	-4.48159500	0.23232900	0.69020200

H	-2.06566600	0.53538900	1.28249600
H	-2.09268800	4.42337300	-0.46985800
H	-4.50845500	4.15348400	-1.07557000
H	-5.69861700	2.05355000	-0.48402000
S	-0.18359600	2.77442800	1.03397400
O	0.35038700	3.68066900	-0.07432300
O	0.35522000	1.34476700	1.00721700

$PhSO_2$·

C	-3.96318200	1.15888300	0.45340100
C	-2.61825400	1.30599200	0.78510100
C	-1.97319400	2.48655400	0.42463000
C	-2.63047900	3.52888300	-0.22409400
C	-3.97545300	3.36368400	-0.54748800
C	-4.63906600	2.18437500	-0.20836400
H	-4.48085000	0.24103800	0.71044100
H	-2.07422400	0.51674200	1.28976500
H	-2.09569700	4.43316300	-0.48841500
H	-4.50250400	4.15651500	-1.06725100
H	-5.68727800	2.06400900	-0.46081400
S	-0.23520900	2.71678200	0.91242500
O	0.35337300	3.73618400	0.00793400
O	0.36759800	1.36983900	1.07310000

TS-A/B

C	-2.87550300	-0.14009000	-1.48527900
C	-1.51923200	-0.41050700	-1.31627600
C	-0.70084200	0.51271200	-0.65249100
C	-1.25905600	1.70528200	-0.16464400
C	-2.61183900	1.96732900	-0.33356300
C	-3.42396300	1.04325400	-0.99506200

H	-3.50352900	-0.85829300	-2.00194000
H	-1.11381400	-1.33405900	-1.71045800
H	-0.61453900	2.41206800	0.34442700
H	-3.03598200	2.89017800	0.04826000
H	-4.48172700	1.24760000	-1.12786200
C	0.75567200	0.30656300	-0.44097300
O	1.46274600	1.15078600	0.09804600
C	1.38986200	-0.98197300	-0.80958400
H	0.84002400	-2.06629100	-1.32358600
N	2.69004100	-0.97990100	-0.88314900
N	3.81839000	-1.05881800	-0.94416100
C	2.05596300	-3.38972600	-3.71996200
H	2.62756900	-4.20775100	-4.16760800
H	1.45876000	-2.91566500	-4.50176100
H	2.77197100	-2.65231600	-3.34721800
C	1.14508500	-3.90358900	-2.59253800
C	1.95719700	-4.55740300	-1.46493200
H	1.29676700	-4.89120200	-0.66105900
H	2.51375500	-5.42368800	-1.83328900
H	2.68478300	-3.86134200	-1.03798100
C	0.12947900	-4.91572800	-3.16750000
H	-0.54105800	-5.27272400	-2.38356000
H	-0.47019100	-4.45063500	-3.95203500
H	0.65913900	-5.77301500	-3.59302600

TS-Sub/B

C	-3.34088300	-0.16801900	-0.68637400
C	-2.00583500	-0.56361300	-0.68855100
C	-0.98920200	0.40096400	-0.73084000
C	-1.33001200	1.76284600	-0.77375100
C	-2.66237100	2.15078800	-0.77485900

C	-3.67116900	1.18477200	-0.73004500
H	-4.12194000	-0.91969500	-0.65200300
H	-1.77013900	-1.61927900	-0.65206100
H	-0.53544900	2.49888300	-0.80409600
H	-2.91911100	3.20432500	-0.80966200
H	-4.71299100	1.48914000	-0.72960500
C	0.45355000	0.05335700	-0.72804200
O	1.33553800	0.90170300	-0.67575300
C	0.83850100	-1.38698300	-0.70867100
H	0.11619000	-2.59576100	-0.56885200
N	2.09593600	-1.62333500	-0.99711300
N	3.16316100	-1.91891900	-1.20716100
C	-3.96424800	-3.88748400	-3.31274100
C	-2.86944500	-4.24315900	-2.52851200
C	-1.58743700	-3.91411900	-2.96644400
C	-1.37698600	-3.26525700	-4.17803100
C	-2.48049800	-2.90974700	-4.95432800
C	-3.76937800	-3.22043900	-4.52376100
H	-4.96792700	-4.13454100	-2.98206500
H	-3.01277300	-4.76002400	-1.58470000
H	-0.36440000	-3.04327100	-4.49564700
H	-2.33099200	-2.39483500	-5.89777300
H	-4.62432200	-2.94863200	-5.13433100
S	-0.14811600	-4.44211600	-1.96204900
O	-0.41590700	-3.64562200	-0.59816300
O	1.04298300	-3.83208500	-2.65625400

B

C	-2.53018500	-0.63390400	-0.55129200
C	-1.15267900	-0.44230600	-0.49746200
C	-0.62428600	0.85437600	-0.48151700

C	-1.48708700	1.95871800	-0.51645700
C	-2.86125400	1.76362500	-0.57099400
C	-3.38395400	0.46801900	-0.58894900
H	-2.93735000	-1.63931800	-0.55756800
H	-0.48441800	-1.29626100	-0.44859500
H	-1.06308200	2.95623200	-0.50213400
H	-3.52865400	2.61845900	-0.59996100
H	-4.45813700	0.31876300	-0.62966400
C	0.83854000	1.09237300	-0.44847900
O	1.35154000	2.18606200	-0.27698000
C	1.72485100	-0.08644500	-0.54556700
N	2.66323500	-0.21816000	-1.37714900
N	3.54155900	-0.46175700	-2.08706000

$PhNH_2$

C	-2.80832200	2.27223100	-0.05276100
C	-1.41451500	2.26284400	-0.05219900
C	-0.69412600	3.46298300	-0.05269800
C	-1.39436100	4.67047200	-0.05377000
C	-2.78893000	4.68206600	-0.05435200
C	-3.49969900	3.48338400	-0.05384500
H	-3.35398300	1.33373200	-0.05235600
H	-0.87735000	1.31823100	-0.05136400
H	-0.82673100	5.59440700	-0.05413600
H	-3.31964800	5.62899200	-0.05519300
H	-4.58494200	3.49146500	-0.05428600
N	0.74909900	3.51320400	-0.05213700
H	1.13349200	3.04884400	0.76488200
H	1.13415000	3.04842000	-0.8686060

C'

C	-4.68902700	2.13058800	-0.38349500
C	-4.05229700	0.98674500	0.10267600
C	-2.97181500	0.42342100	-0.58829700
C	-2.52461100	1.03596600	-1.76295500
C	-3.16715100	2.16887200	-2.25577200
C	-4.25407900	2.71608100	-1.57108700
H	-5.51000000	2.57149300	0.17325000
H	-4.36060100	0.56441700	1.05729700
H	-1.66556700	0.62126000	-2.27927600
H	-2.81505000	2.63292200	-3.17167200
H	-4.74709800	3.60454100	-1.95215800
C	-2.23258600	-0.78661500	-0.04548800
O	-1.03256000	-0.68853700	0.20672600
C	-2.99889200	-1.97119200	0.16095600
N	-2.57079800	-3.07944900	0.82271600
N	-3.16515800	-4.10101000	1.02599700
C	-4.18598000	-3.82942400	-2.15942200
C	-4.54509800	-2.53388100	-1.79980400
C	-5.02575400	-1.61928600	-2.72879900
C	-5.15401800	-2.01635800	-4.05905400
C	-4.80366500	-3.30943100	-4.44066400
C	-4.32136300	-4.21111500	-3.49185600
H	-3.80673400	-4.52065800	-1.41546300
H	-5.28364800	-0.60822000	-2.43130000
H	-5.52626100	-1.31041600	-4.79328700
H	-4.90399200	-3.61473100	-5.47658800
H	-4.04666100	-5.21794000	-3.78648900
N	-4.40039600	-2.11100500	-0.38647500
H	-4.90824400	-1.23359700	-0.25570900
H	-4.83688200	-2.82486900	0.21773600

PhNH·

C	-5.22832300	0.84017500	0.27873600
C	-4.05426900	0.25093400	-0.21545600
C	-3.14021400	1.00447500	-0.92397200
C	-3.36685300	2.39737500	-1.17047800
C	-4.57539600	2.97063100	-0.65273700
C	-5.47948200	2.20242800	0.05417700
H	-5.94293100	0.24280500	0.83490500
H	-3.86598900	-0.80309400	-0.03818100
H	-4.76819000	4.02567200	-0.82740300
H	-6.38910100	2.65276200	0.43880300
N	-2.44276200	3.07044300	-1.86419000
H	-2.73192700	4.04787700	-1.96565100
H	-2.22677700	0.57086200	-1.31528700

C

C	-4.31637100	2.30073700	-1.20645300
C	-4.09007500	1.03078600	-0.68011500
C	-2.78557500	0.53113100	-0.57243100
C	-1.71539000	1.33105100	-1.00045300
C	-1.94471200	2.59035500	-1.54142200
C	-3.24760400	3.07964100	-1.64487200
H	-5.33054300	2.68073400	-1.27546400
H	-4.93089000	0.43762300	-0.34846600
H	-0.70766700	0.94746400	-0.89383800
H	-1.10798100	3.19404400	-1.87772900
H	-3.42799000	4.06519100	-2.06233300
C	-2.43142000	-0.79527100	0.03099700
O	-1.31347500	-0.98384800	0.50586600
C	-3.40188000	-1.89325300	0.03866800
N	-2.94124100	-3.00515300	0.62640200

N	-2.60924500	-3.95775500	1.12416800
C	-3.84542900	-2.81405500	-2.72307200
C	-4.89285500	-2.55808600	-1.83117700
C	-6.20890100	-2.83730200	-2.22487700
C	-6.46919100	-3.35685700	-3.48816900
C	-5.42655100	-3.61153500	-4.37891200
C	-4.11868800	-3.33636500	-3.98516200
H	-2.82214300	-2.60328400	-2.43325900
H	-7.02961700	-2.64441100	-1.53853300
H	-7.49469400	-3.56681700	-3.77514800
H	-5.63107400	-4.01932100	-5.36273500
H	-3.29497200	-3.52858900	-4.66521100
N	-4.66429300	-2.00126600	-0.55694100
H	-5.46863600	-1.98214600	0.05517700

TS-C/G

C	-2.32910500	0.08738400	-2.76834500
C	-2.98483400	-0.80442900	-1.92217800
C	-2.43310000	-1.12793400	-0.67637300
C	-1.21482700	-0.54820800	-0.29686800
C	-0.57296000	0.35770800	-1.13440600
C	-1.12938200	0.67749100	-2.37342200
H	-2.75574800	0.31945200	-3.73896400
H	-3.90694300	-1.26700200	-2.24891400
H	-0.78180900	-0.82515500	0.65748100
H	0.36464700	0.80881900	-0.82567400
H	-0.62591300	1.37870700	-3.03157600
C	-3.04029200	-2.12227200	0.26863000
O	-2.33130400	-2.81129900	0.99472900
C	-4.49848900	-2.22036200	0.35747900
N	-4.93523900	-3.18631800	1.16371900

N	-5.32518700	-4.02871500	1.79943900
C	-6.40002100	-2.83859000	-1.92536700
C	-6.43162600	-1.69135300	-1.12875200
C	-7.50881900	-0.80696500	-1.34160300
C	-8.48182900	-1.07255300	-2.29569400
C	-8.42722100	-2.23367200	-3.06530700
C	-7.37081000	-3.12672000	-2.86662900
H	-5.32436100	-3.73160200	-1.80510200
H	-7.57512000	0.09455800	-0.73700100
H	-9.29600600	-0.36804700	-2.43141000
H	-9.18739500	-2.44609800	-3.80917600
H	-7.31358800	-4.03343900	-3.45869000
N	-5.47078600	-1.36025500	-0.17021900
H	-5.64128200	-0.49704600	0.32733300
C	-4.30011000	-5.27091600	-3.88921900
H	-3.43913900	-4.62525000	-4.07658400
H	-4.18710000	-6.17753500	-4.49079100
H	-5.19403100	-4.74907700	-4.24109700
C	-4.39844100	-5.60677300	-2.39486700
C	-3.10221600	-6.29058900	-1.92043900
H	-2.23939500	-5.64780700	-2.10343000
H	-3.14878800	-6.50331400	-0.85096400
H	-2.95837400	-7.23202300	-2.45869900
C	-5.60728700	-6.50221800	-2.09053600
H	-5.65782300	-6.72122300	-1.02162000
H	-6.54489400	-6.01910500	-2.37833300
H	-5.54166800	-7.44988000	-2.63313500
O	-4.43515000	-4.41659200	-1.60750200

G

C	-2.41048400	0.19785200	-2.72395300

C	-3.06930900	-0.70542100	-1.89237500
C	-2.46752500	-1.13451300	-0.70244900
C	-1.19726000	-0.64750700	-0.36389900
C	-0.55200600	0.27046100	-1.18499400
C	-1.15783000	0.69509600	-2.36819200
H	-2.87682200	0.51105700	-3.65246200
H	-4.03515900	-1.09280700	-2.18985900
H	-0.72767700	-1.00500200	0.54521400
H	0.42658400	0.64897700	-0.90785500
H	-0.65156300	1.40539300	-3.01422700
C	-3.07373500	-2.15190600	0.21649700
O	-2.36407000	-2.91468300	0.86562200
C	-4.53021400	-2.20150400	0.37174900
N	-4.95737400	-3.17912300	1.17700200
N	-5.34926000	-4.01499900	1.81941600
C	-6.39627700	-2.79871300	-1.79440300
C	-6.44982700	-1.62588000	-1.05973900
C	-7.51096900	-0.75602200	-1.37512900
C	-8.42483200	-1.08965900	-2.37211900
C	-8.32174100	-2.28789200	-3.07945700
C	-7.27485300	-3.17243600	-2.77737700
H	-7.61411600	0.18083000	-0.83226900
H	-9.23285100	-0.40073600	-2.59553400
H	-9.03974400	-2.53893300	-3.85296300
H	-7.16849100	-4.11385400	-3.30775300
N	-5.50534000	-1.30491100	-0.08166300
H	-5.67224200	-0.46548000	0.45541400

TS-G/H

C	-3.10012800	2.05719800	-0.13292500
C	-3.45290800	0.71387800	-0.24673900

C	-2.76292200	-0.26228100	0.48544100
C	-1.71186600	0.13155700	1.32530900
C	-1.37550200	1.47459300	1.45247700
C	-2.06907400	2.44124400	0.72276100
H	-3.62825700	2.80338400	-0.71782700
H	-4.24780700	0.42661800	-0.92407300
H	-1.16477000	-0.63255200	1.86529900
H	-0.56715600	1.76867300	2.11412300
H	-1.80112700	3.48896500	0.81510900
C	-3.03768300	-1.73376400	0.37181600
O	-2.13780100	-2.55366500	0.53862000
C	-4.38689400	-2.18159900	0.07507500
N	-4.56167500	-3.49761200	-0.17915600
N	-5.20636200	-4.30303600	-0.68511100
C	-6.69716300	-2.70597700	-1.64272000
C	-6.70124200	-1.76517900	-0.61958900
C	-7.93126200	-1.11686700	-0.36611600
C	-9.04307800	-1.39847000	-1.14467800
C	-8.98145700	-2.33477600	-2.18571500
C	-7.78017900	-2.99892700	-2.44204100
H	-7.98928200	-0.37266500	0.42522400
H	-9.97465500	-0.88080300	-0.94160000
H	-9.86346200	-2.55628800	-2.77761600
H	-7.71129900	-3.74520700	-3.22738700
N	-5.57410700	-1.45790700	0.14644100
H	-5.76305000	-0.96338400	1.01019200

H

C	1.97066500	3.26068500	-0.02664200
C	1.61716500	1.92367200	-0.19735700
C	2.04542300	0.95583900	0.72268200

C	2.83514700	1.34911100	1.81198800
C	3.16825000	2.68676400	1.99181100
C	2.73700900	3.64490300	1.07261200
H	1.65462200	3.99968300	-0.75553500
H	1.04089500	1.63055500	-1.06887400
H	3.18487000	0.59071000	2.50318300
H	3.77127500	2.98375500	2.84354400
H	3.00582700	4.68745100	1.20846800
C	1.76320000	-0.50866300	0.54397600
O	2.55822900	-1.34929000	0.91467300
C	0.45816500	-0.91635600	-0.07206900
N	0.40702600	-2.04635700	-0.74824900
N	-0.72195700	-2.47596700	-1.30271300
C	-1.86625700	-1.71068200	-1.14448500
C	-1.87380400	-0.49605000	-0.41707200
C	-3.04201000	0.24728400	-0.26694400
C	-4.22168400	-0.21663200	-0.84606000
C	-4.23347300	-1.41366800	-1.57176700
C	-3.06819100	-2.15325900	-1.72038700
H	-3.02959300	1.17532500	0.29767300
H	-5.13451800	0.35740700	-0.73015200
H	-5.15761000	-1.76449800	-2.01799700
H	-3.04920000	-3.08433900	-2.27545600
N	-0.65272500	-0.11758200	0.12079500
H	-0.58198800	0.71936900	0.68249500

D'

C	-0.24852200	0.15024300	-3.02713300
C	-0.30105400	0.88814000	-1.84163600
C	-1.45559200	1.60720600	-1.50068500
C	-2.54550200	1.58838300	-2.38137900

C	-2.49686400	0.84502000	-3.55603600
C	-1.34673300	0.12123400	-3.88247200
H	0.65585200	-0.39725700	-3.27371100
H	0.57104400	0.91158100	-1.19325800
H	-3.42129000	2.17954300	-2.13542700
H	-3.35460100	0.83104700	-4.22301700
H	-1.30814100	-0.45726100	-4.80108500
C	-1.53610500	2.49543700	-0.26636400
O	-1.93800300	3.65901500	-0.43186600
C	-1.14567100	1.94836600	0.98406500
N	-1.01928400	2.72786800	2.10361400
N	-0.71096500	2.40681200	3.21745200
C	-1.22136400	-1.50040800	2.53621300
C	-1.70959000	-0.28485600	2.06502100
C	-2.97990200	0.16971500	2.39429300
C	-3.78421000	-0.61200000	3.22126200
C	-3.31711500	-1.83288700	3.70600300
C	-2.03942500	-2.27182000	3.36081100
H	-0.22714600	-1.84791900	2.26064900
H	-3.32120900	1.12874400	2.02236400
H	-4.77394000	-0.25802100	3.49277300
H	-3.94545700	-2.43745000	4.35355900
H	-1.66639100	-3.22057400	3.73347600
N	-0.84941100	0.49961100	1.14210500
H	-0.94562100	0.08435200	0.21249100
C	3.63402700	-3.16119700	-2.20503900
C	3.14671700	-2.87469500	-0.92833700
C	3.20483300	-1.57159300	-0.44347600
C	3.75805700	-0.55356000	-1.21938400
C	4.24720100	-0.84168100	-2.49325700
C	4.18734900	-2.14695900	-2.98721100

H	3.57892100	-4.17566800	-2.59145800
H	2.69476200	-3.63943200	-0.30460000
H	3.77976000	0.46116000	-0.83413900
H	4.66808400	-0.04793000	-3.10455600
H	4.56692600	-2.37023900	-3.98043400
S	2.61407900	-1.20584500	1.28174000
O	1.73495200	-2.41795600	1.58223600
O	1.76166900	0.06500700	1.01505000
H	0.18394900	0.33303700	1.34546000

E'

C	-0.66941900	2.17426100	-3.39225100
C	-0.70783200	2.23204400	-1.99659700
C	-1.89790300	2.56205200	-1.33517900
C	-3.03967700	2.84151900	-2.10060500
C	-3.00412300	2.76517000	-3.48901100
C	-1.81441200	2.43213100	-4.14176800
H	0.26516500	1.92901400	-3.88811000
H	0.20081100	2.03213600	-1.43714800
H	-3.94779900	3.13562200	-1.58532700
H	-3.90119500	2.97403300	-4.06560100
H	-1.78183900	2.38113100	-5.22655600
C	-2.00217500	2.74027400	0.17375900
O	-2.55679000	3.77106500	0.57598100
C	-1.49371800	1.70895300	1.02796600
N	-1.57345600	1.78185100	2.36179000
N	-1.26766100	0.86512800	3.18942600
C	-0.78265300	-0.35544300	2.70796100
C	-1.24377000	-0.68655700	1.32514800
C	-1.88222400	-1.82896300	0.95487100
C	-2.11194000	-2.84571500	1.91124600

C	-1.71332900	-2.63421600	3.25740100
C	-1.10786000	-1.47957800	3.65557100
H	0.32861800	-0.27175900	2.66043000
H	-2.21197200	-1.96629500	-0.07342400
H	-2.60380000	-3.76638900	1.61838500
H	-1.91517900	-3.41122600	3.99090600
H	-0.84449500	-1.31273600	4.69482800
N	-0.99382000	0.41069000	0.41133000
H	-1.45914300	0.24716900	-0.48218200
C	3.53016800	-4.00105700	-0.09459300
C	3.27969900	-2.75404600	0.48082400
C	3.01482500	-1.65806700	-0.33480000
C	3.01015300	-1.79590400	-1.72215900
C	3.26418200	-3.04133100	-2.29554400
C	3.52669900	-4.14572400	-1.48196600
H	3.72329700	-4.86149500	0.54056800
H	3.25951100	-2.61758500	1.55725600
H	2.78295700	-0.93583000	-2.34435700
H	3.25002600	-3.15380600	-3.37646500
H	3.72240400	-5.11630600	-1.92927900
S	2.76407600	0.01431100	0.43774400
O	2.40408300	-0.34083000	1.87165900
O	1.51552500	0.50498500	-0.36422900
H	0.06505600	0.45163000	0.17678000

F'

C	-4.81344600	2.29856300	0.31136300
C	-4.20445900	1.04488800	0.37386800
C	-2.99550900	0.80535500	-0.29180100
C	-2.40157200	1.84621600	-1.01502200
C	-3.01932700	3.09251100	-1.09389300

C	-4.22646100	3.32117000	-0.43213300
H	-5.73593600	2.47994500	0.85390000
H	-4.64449800	0.26365500	0.98975600
H	-1.44605100	1.67395500	-1.49944400
H	-2.55248900	3.89074400	-1.66207100
H	-4.69982900	4.29622700	-0.48415100
C	-2.27542100	-0.52915200	-0.17836400
O	-1.15083100	-0.55520600	0.30672700
C	-2.98476300	-1.69170500	-0.65540400
N	-2.51860800	-2.93186400	-0.62658200
N	-3.06110700	-3.97047100	-1.12598800
C	-4.26912500	-3.85776700	-1.73156500
C	-4.50812600	-2.53511700	-2.40648000
C	-4.78658200	-2.34972500	-3.72493300
C	-4.97869400	-3.47344200	-4.55928100
C	-4.83132600	-4.77750200	-4.01861700
C	-4.49783800	-4.98350000	-2.71438500
H	-5.05242800	-3.96542600	-0.93699100
H	-4.86507100	-1.34768500	-4.14214800
H	-5.21437600	-3.33405500	-5.60714100
H	-4.96267600	-5.63239300	-4.67494000
H	-4.33205500	-5.98227500	-2.32616800
N	-4.26293400	-1.41654100	-1.50028800
H	-4.15029700	-0.54022700	-2.01553000
H	-5.06415400	-1.27060600	-0.88005000

TS-C/F

C	-3.43682300	2.68081700	-4.65927200
C	-3.12059000	1.64934200	-3.77527600
C	-2.37294100	0.54787400	-4.20842800
C	-1.93711900	0.49809500	-5.53585100

C	-2.27006400	1.51824100	-6.42290700
C	-3.02162300	2.61032500	-5.98765400
H	-3.99565500	3.54224200	-4.30760100
H	-3.40887900	1.73308600	-2.72985900
H	-1.33102200	-0.33977500	-5.86325900
H	-1.93505500	1.46678300	-7.45388500
H	-3.27156500	3.40898400	-6.67845300
C	-1.95774600	-0.53952800	-3.24641400
O	-0.77343000	-0.79660600	-3.08400200
C	-3.01268300	-1.27015700	-2.55788800
N	-2.73674800	-2.02107500	-1.45783100
N	-3.44378800	-2.88026900	-0.95292800
C	-4.69030000	-3.29449100	-2.04421000
C	-5.26242200	-1.98880900	-2.34820100
C	-6.61740100	-1.68075400	-2.05999500
C	-7.41964400	-2.63787800	-1.50549900
C	-6.90383900	-3.93943100	-1.19067400
C	-5.61572700	-4.26444200	-1.46345000
H	-4.04164300	-3.67286800	-2.84258700
H	-6.99916000	-0.68731500	-2.27770600
H	-8.45595900	-2.40897900	-1.28193900
H	-7.56605400	-4.67093000	-0.73961500
H	-5.23376700	-5.25498500	-1.24036200
N	-4.37731200	-1.07885000	-2.79932200
H	-4.70183300	-0.14361200	-3.01695400

F

C	-3.26363900	2.64637500	-4.60992900
C	-2.94373400	1.54484000	-3.81614700
C	-2.37658600	0.39931000	-4.38814900
C	-2.12521100	0.37570900	-5.76329100

C	-2.46320500	1.46786500	-6.55789900
C	-3.03423800	2.60426200	-5.98384900
H	-3.67941300	3.53914000	-4.15375600
H	-3.08421900	1.60152600	-2.73915200
H	-1.65686600	-0.49934800	-6.20088300
H	-2.27244500	1.43711600	-7.62580100
H	-3.28755800	3.45824000	-6.60359900
C	-1.95574900	-0.77280300	-3.53333600
O	-0.79620700	-1.15794500	-3.54801300
C	-2.98220400	-1.42728100	-2.72951300
N	-2.64803100	-2.22438300	-1.67920700
N	-3.40841200	-3.01401300	-1.10926900
C	-4.74928200	-3.26609500	-1.99947800
C	-5.24784600	-1.90916900	-2.25368600
C	-6.54062200	-1.48762200	-1.84716500
C	-7.36321000	-2.37308900	-1.21289700
C	-6.92560800	-3.71355200	-0.92535600
C	-5.70069900	-4.14646300	-1.30178600
H	-4.29581800	-3.70478600	-2.90091700
H	-6.85767300	-0.46681500	-2.04084500
H	-8.35250300	-2.05968600	-0.89790700
H	-7.60045700	-4.38125000	-0.40003100
H	-5.37687100	-5.15900400	-1.08541700
N	-4.33571000	-1.09185900	-2.80299400
H	-4.58675700	-0.13418900	-3.02176200

TS-F/H

O	-4.58733600	-4.42002100	-4.31901800
C	-2.38081600	2.93988800	-3.79364200
C	-2.28195700	1.65851600	-3.25100900
C	-1.95916200	0.56631300	-4.06685300

C	-1.72701100	0.77701700	-5.43011200
C	-1.84539700	2.05275400	-5.97373600
C	-2.17390200	3.13615100	-5.15763600
H	-2.60538000	3.78379400	-3.14926700
H	-2.39705700	1.52115000	-2.17850000
H	-1.44639600	-0.06474800	-6.05357300
H	-1.67165000	2.20533300	-7.03397600
H	-2.25514400	4.13169700	-5.58158600
C	-1.76549600	-0.81594000	-3.49294700
O	-0.73490800	-1.43267100	-3.70958600
C	-2.85588000	-1.39491300	-2.70458900
N	-2.61880900	-2.42107400	-1.84352400
N	-3.51837800	-3.11201000	-1.32009200
C	-4.91288900	-2.91947800	-1.96624200
C	-5.14036800	-1.47228600	-2.08830400
C	-6.33021900	-0.85121300	-1.63911600
C	-7.28745100	-1.61313700	-1.02721000
C	-7.08517400	-3.01710700	-0.79421000
C	-5.95723100	-3.63601600	-1.21320600
H	-4.76844700	-3.39976800	-2.99488700
H	-6.46486400	0.21855600	-1.77207300
H	-8.19998700	-1.14463000	-0.67456200
H	-7.84792900	-3.57323800	-0.25961800
H	-5.78792900	-4.69088600	-1.02803600
N	-4.10684300	-0.79922400	-2.61834100
H	-4.18146800	0.19935300	-2.78075900
C	-5.03190700	-4.03966400	-5.57948100
C	-4.87154900	-5.32920500	-6.43415500
H	-5.19870600	-5.12999900	-7.45895100
H	-3.82789700	-5.64694600	-6.45168200
H	-5.47609900	-6.13835900	-6.02103000

C	-4.15374000	-2.92036200	-6.16830500
H	-4.44663500	-2.67745900	-7.19451500
H	-4.24432100	-2.01014500	-5.56859000
H	-3.10460200	-3.22313000	-6.16556300
C	-6.51574600	-3.62566900	-5.54223500
H	-6.89136900	-3.38868500	-6.54237800
H	-7.12450500	-4.43083000	-5.12446700
H	-6.65124300	-2.73919400	-4.91534200

TS-C/D

C	-2.25247300	1.94248900	-1.25409300
C	-3.11325000	0.86965900	-1.02906400
C	-2.91134900	0.03399300	0.07799500
C	-1.84476500	0.29513300	0.95264300
C	-0.97908200	1.35419500	0.71089400
C	-1.18187400	2.18130500	-0.39516400
H	-2.42378300	2.59309700	-2.10531500
H	-3.94927400	0.72151400	-1.70004600
H	-1.71077400	-0.34310600	1.81810000
H	-0.14998100	1.53934000	1.38600800
H	-0.50963600	3.01267000	-0.58258100
C	-3.79910500	-1.11018600	0.43866700
O	-3.95530600	-1.45408500	1.60523200
C	-4.45299900	-1.91707000	-0.61680300
N	-5.20015800	-2.91326800	-0.11804500
N	-5.79947900	-3.79161400	0.24948700
C	-3.53358900	-4.05143200	-2.39920600
C	-4.16000600	-2.87203200	-2.84290800
C	-4.50164000	-2.74586800	-4.20335600
C	-4.22016600	-3.77629800	-5.08810200
C	-3.59956300	-4.94766200	-4.64607000

C	-3.25564200	-5.07284800	-3.30057500
H	-3.22282100	-4.15048700	-1.36535700
H	-4.99187900	-1.83826400	-4.53568800
H	-4.49066600	-3.66712400	-6.13330800
H	-3.38393400	-5.75036400	-5.34280100
H	-2.75777300	-5.96989900	-2.94725100
N	-4.39411000	-1.78820400	-1.98963400
H	-4.95996100	-0.95277100	-2.43239700
C	-7.40865000	0.48812200	-1.31265900
H	-6.81541300	1.33890800	-0.96822900
H	-8.46284600	0.70509700	-1.11538700
H	-7.13337600	-0.38223900	-0.70946400
C	-7.15363000	0.22302400	-2.80781200
C	-7.54385200	1.47589400	-3.63147500
H	-6.95952000	2.33994600	-3.30839100
H	-7.35155500	1.30719200	-4.69290100
H	-8.60618400	1.70222600	-3.49759700
C	-7.98173200	-0.98355900	-3.29331600
H	-7.80956100	-1.16303800	-4.35731200
H	-7.70042900	-1.88930800	-2.74783300
H	-9.05276800	-0.81920300	-3.14087600
O	-5.79383700	0.01961400	-3.06583400

D

C	-0.39122700	1.17923200	-3.09444400
C	-0.96359400	1.30276100	-1.82701700
C	-2.29442000	1.73239400	-1.69440800
C	-3.04459300	2.03204900	-2.84820900
C	-2.47654600	1.89480800	-4.10485900
C	-1.14765000	1.47000600	-4.22663300
H	0.64503800	0.85348000	-3.16363500

H	-0.34122600	1.05723000	-0.97429100
H	-4.06803900	2.36980600	-2.73175600
H	-3.06263500	2.11959300	-4.99165200
H	-0.70134300	1.36756600	-5.21201600
C	-2.96703800	1.94080400	-0.39007400
O	-4.03182800	2.52834000	-0.27151900
C	-2.31941500	1.42251600	0.87466900
N	-2.70867400	2.28593400	2.07627200
N	-2.05550100	3.03460800	2.67966900
C	0.08183700	-0.72834600	2.15559100
C	-1.24969800	-0.28826500	2.15621600
C	-2.08093700	-0.54316800	3.25670600
C	-1.57635600	-1.22638200	4.35971200
C	-0.24537500	-1.64264100	4.37993900
C	0.57444400	-1.38477500	3.27949100
H	0.71276700	-0.52799300	1.29071200
H	-3.11621100	-0.21959400	3.23836700
H	-2.22599600	-1.42893100	5.20625800
H	0.14794600	-2.16936200	5.24434000
H	1.61050300	-1.70920600	3.28612700
N	-1.74062500	0.31873100	0.98826100
C	4.24429200	-3.49201600	0.19311600
C	3.79763300	-2.17318900	0.11465600
C	3.56024000	-1.58750100	-1.12792800
C	3.77781300	-2.31584100	-2.29355800
C	4.21981400	-3.63824900	-2.21734900
C	4.45717600	-4.22786100	-0.97506000
H	4.42004700	-3.95044900	1.16330600
H	3.61643400	-1.59920900	1.01932700
H	3.57606900	-1.83120400	-3.24410700
H	4.37884000	-4.21101300	-3.12805000

H	4.80314400	-5.25640400	-0.91565700
S	3.03481300	0.20836900	-1.23046100
O	1.80130400	0.22591600	-0.31262800
O	2.66761900	0.32425900	-2.71205400

TS-D/E

C	-7.46712700	0.28176900	-8.49804500
C	-7.51127000	0.17457000	-7.10776400
C	-8.38076300	0.99527600	-6.37775900
C	-9.19612000	1.91563800	-7.05287900
C	-9.16755000	1.99675700	-8.44002600
C	-8.29856400	1.17753000	-9.16655800
H	-6.76790100	-0.34163600	-9.04546100
H	-6.83051400	-0.51933800	-6.62544200
H	-9.84556300	2.56156400	-6.47184600
H	-9.81397200	2.70128300	-8.95607600
H	-8.26608100	1.24728300	-10.25065400
C	-8.42368400	0.98888400	-4.88222700
O	-8.68381700	2.00601000	-4.25146800
C	-8.15746500	-0.29031900	-4.17969400
N	-7.87755700	-0.18395500	-2.78692800
N	-7.38911200	-1.08157100	-2.13658600
C	-6.98822300	-2.49369000	-3.08914300
C	-8.10584400	-2.57297800	-4.01397900
C	-8.89058100	-3.75145800	-4.10891700
C	-8.62462700	-4.81785000	-3.28892300
C	-7.55461800	-4.76077200	-2.34013300
C	-6.76141500	-3.65845600	-2.25066800
H	-6.05876800	-2.04789900	-3.50563200
H	-9.70711900	-3.76830200	-4.82329500
H	-9.23352400	-5.71488700	-3.35079600

H	-7.35976700	-5.62578000	-1.71246000
H	-5.91473600	-3.63743900	-1.57170100
N	-8.45004800	-1.46466700	-4.68892100
C	-2.47092400	-5.42034800	-4.41769600
C	-2.84490700	-4.07639000	-4.42673000
C	-3.45097500	-3.53038200	-5.55709300
C	-3.68043900	-4.32235500	-6.67936900
C	-3.31026500	-5.66823700	-6.66895200
C	-2.70076400	-6.21845300	-5.54041600
H	-2.00776800	-5.84934800	-3.53246200
H	-2.69480600	-3.44966400	-3.55293500
H	-4.17554700	-3.87614500	-7.53618500
H	-3.50224700	-6.29062600	-7.53960600
H	-2.41159800	-7.26601000	-5.53257800
S	-3.85595900	-1.70781100	-5.60796400
O	-4.39840900	-1.47666300	-4.18611400
O	-4.94233100	-1.66371500	-6.68128700

E

C	-1.05804200	2.08845300	-3.32688300
C	-1.12616000	2.00651900	-1.93593500
C	-1.99656500	2.84866200	-1.23210000
C	-2.79052200	3.76474900	-1.93724300
C	-2.73876000	3.82264600	-3.32518800
C	-1.86761000	2.98258300	-4.02424600
H	-0.35967500	1.44570100	-3.85283300
H	-0.46855800	1.30753200	-1.43088600
H	-3.44167000	4.42774800	-1.37778400
H	-3.36920400	4.52544600	-3.86306500
H	-1.81691700	3.03343600	-5.10872800
C	-2.05846900	2.87588100	0.26589600

O	-2.32452600	3.91290700	0.86001800
C	-1.80033200	1.61205900	1.00691000
N	-1.48213100	1.74328500	2.36947700
N	-1.00562800	0.77252500	2.99754400
C	-0.72476900	-0.49739400	2.19263400
C	-1.75765000	-0.65098200	1.14849300
C	-2.36257900	-1.91201700	0.90403300
C	-2.05762300	-2.98251500	1.70058500
C	-1.14892000	-2.84920000	2.81067600
C	-0.53646400	-1.67169300	3.07034600
H	0.27748800	-0.24814500	1.70113600
H	-3.07434800	-1.98763000	0.08832700
H	-2.52649100	-3.94468400	1.51729400
H	-0.96401000	-3.71359600	3.44203600
H	0.14885100	-1.56194600	3.90506200
N	-2.12467600	0.43732100	0.47515500
C	3.18019600	-4.08707400	0.81604100
C	3.04365100	-2.69924500	0.79884200
C	2.47646500	-2.07124500	-0.30905500
C	2.04996900	-2.82284200	-1.40030200
C	2.18186200	-4.21246100	-1.38015000
C	2.75110700	-4.84606900	-0.27499400
H	3.61308100	-4.57908200	1.68333900
H	3.35308100	-2.10039100	1.65000200
H	1.59647800	-2.30468300	-2.23929800
H	1.83709300	-4.80217600	-2.22586300
H	2.85571600	-5.92758200	-0.26052500
S	2.39228700	-0.20980000	-0.37897900
O	1.85637300	0.12743500	1.02988900
O	1.36934100	0.01859100	-1.48447000

TS-E/P

C	-3.91317500	2.17049900	-5.04274700
C	-3.60566400	0.89430900	-4.57253300
C	-2.27540300	0.55222100	-4.29889600
C	-1.26740500	1.50255800	-4.50788100
C	-1.58085100	2.78378900	-4.95059400
C	-2.90872400	3.12062000	-5.22098700
H	-4.94603000	2.41332400	-5.27227200
H	-4.40616800	0.17176700	-4.46150700
H	-0.23760600	1.21773300	-4.32049600
H	-0.79148600	3.51688300	-5.09307900
H	-3.15661000	4.11709000	-5.57693900
C	-1.86004800	-0.83004300	-3.87173600
O	-0.80562900	-1.30238200	-4.28457200
C	-2.74221300	-1.57463700	-2.94445300
N	-2.47912100	-2.93541800	-2.80111700
N	-3.29348300	-3.67800300	-2.18076500
C	-4.54174000	-3.05953100	-1.69004400
C	-4.39090700	-1.62980500	-1.38519000
C	-5.13560900	-1.05780500	-0.31194300
C	-5.89378900	-1.85689200	0.49696500
C	-5.93547800	-3.28439700	0.31722200
C	-5.24894200	-3.86871800	-0.69558400
H	-5.29890500	-3.10960600	-2.68422700
H	-5.05991100	0.01317400	-0.15324500
H	-6.45217400	-1.41589500	1.31802100
H	-6.50962300	-3.88754400	1.01439800
H	-5.24487400	-4.94528000	-0.83655400
N	-3.56560300	-0.89838800	-2.12154800
C	-8.30464700	-5.46589800	-6.83331400
C	-7.36383700	-4.81121700	-6.04037800

C	-7.25853900	-3.42265100	-6.10140500
C	-8.07779600	-2.68581500	-6.95005800
C	-9.02251000	-3.34418700	-7.73924400
C	-9.13503700	-4.73332600	-7.68482200
H	-8.39593600	-6.54754800	-6.78302100
H	-6.72830700	-5.36831200	-5.35988600
H	-7.97258500	-1.60579200	-6.96196100
H	-9.67163500	-2.77198800	-8.39681000
H	-9.86828200	-5.24513600	-8.30195100
S	-5.96348900	-2.54308600	-5.12109400
O	-6.29988200	-3.17582100	-3.71204900
O	-6.38265500	-1.09013400	-5.21477500

Product

C	-3.85474100	2.20046700	-5.11062600
C	-3.53020900	1.04475900	-4.40495700
C	-2.18866100	0.70660100	-4.18421500
C	-1.17792800	1.54407800	-4.67985200
C	-1.50414500	2.70036400	-5.37574900
C	-2.84421900	3.02991400	-5.59338300
H	-4.89562100	2.45406000	-5.28204500
H	-4.32277800	0.40984600	-4.02814300
H	-0.14399800	1.26717200	-4.50962900
H	-0.71769900	3.34566800	-5.75309300
H	-3.09875300	3.93218300	-6.14037200
C	-1.78387500	-0.53744500	-3.47542300
O	-0.63186600	-0.91476800	-3.41205800
C	-2.83637300	-1.38282700	-2.77370500
N	-2.89393400	-2.68799900	-3.18688300
N	-3.69377800	-3.50031500	-2.56968700
C	-4.41876800	-3.04148700	-1.50940500

C	-4.34326000	-1.67694400	-1.11776900
C	-5.11880100	-1.22082700	-0.02431200
C	-5.92820900	-2.10985400	0.64118800
C	-6.00218700	-3.47336900	0.24938700
C	-5.26348300	-3.93822400	-0.80997500
H	-5.04839200	-0.17768000	0.26275200
H	-6.52367500	-1.76996200	1.48216900
H	-6.65195200	-4.14761100	0.79687500
H	-5.29882600	-4.97234500	-1.13392200
N	-3.53213500	-0.83422600	-1.80524600

^{t}BuO^{-}

C	-0.24835500	-0.96183900	-0.51684000
H	-1.04059400	-0.87675400	-1.26936600
H	-0.18320700	-2.01456200	-0.19438200
H	-0.54435300	-0.35173400	0.34415200
C	1.08332200	-0.38351900	-1.11425600
C	1.48261000	-1.30325500	-2.32195000
H	0.71375700	-1.22190400	-3.09872900
H	2.42325300	-0.93794000	-2.74958200
H	1.60598900	-2.36786500	-2.06171300
C	2.19252100	-0.55876500	-0.01706000
H	3.14313400	-0.18115600	-0.41060700
H	1.92984600	0.05293400	0.85356900
H	2.34038700	-1.59917700	0.31768400
O	0.94750800	0.89765700	-1.48659100

Sub.

C	-2.71913000	-0.73773600	-0.52991700
C	-1.34240300	-0.63450500	-0.67143000
C	-0.71411700	0.64319000	-0.68572500

C	-1.49501400	1.80265900	-0.55614100
C	-2.86766700	1.69328100	-0.41552400
C	-3.48452900	0.41881500	-0.40218700
H	-3.19273300	-1.71197000	-0.51958400
H	-0.76916600	-1.54819400	-0.76901400
H	-1.00771100	2.76973500	-0.56796900
H	-3.47640000	2.58447500	-0.31483400
H	-4.56093900	0.34757000	-0.29181200
C	0.74789600	0.83544900	-0.83079200
O	1.30509800	1.91154900	-0.84129600
C	1.56870000	-0.40912800	-0.97338100
H	1.26307900	-1.44571000	-0.99213900
N	2.88361100	-0.21042900	-1.10056300
N	3.96359500	0.05694100	-1.19958900

TS-PhNH$_2$/I

C	3.34865900	-1.76714000	-1.14602900
H	3.81056200	-2.27641400	-0.29728700
H	3.61453400	-2.30270500	-2.06297900
H	3.75704000	-0.75578000	-1.20086100
C	1.81457400	-1.71147400	-0.96553400
C	1.25251900	-3.14150100	-0.85948900
H	1.67079100	-3.65025100	0.01291100
H	0.16250800	-3.12586700	-0.75041400
H	1.48342600	-3.73661700	-1.74854600
C	1.18509700	-0.97249000	-2.16393800
H	0.09856300	-0.90974400	-2.04666300
H	1.57514600	0.04621800	-2.22416100
H	1.39448600	-1.48261400	-3.10979400
O	1.59406500	-0.98845200	0.21278700
C	-2.69839000	2.14399500	1.84018300

C	-2.33950700	0.86561500	1.44712700
C	-0.99406900	0.43043200	1.55798700
C	-0.02328200	1.34101300	2.05198500
C	-0.39547800	2.62058500	2.42133500
C	-1.73166100	3.03119500	2.32621200
H	-3.73340500	2.46023600	1.76158600
H	-3.08835900	0.18037200	1.05983300
H	1.00830400	1.01373000	2.11233700
H	0.35568500	3.31096100	2.79077000
H	-2.01554500	4.03462600	2.62439500
N	-0.61597300	-0.84003300	1.25217400
H	-1.34420900	-1.39071500	0.80616200
H	0.46008400	-1.03438700	0.83947300

I

C	-2.84173400	2.22865600	1.27076400
C	-2.55039000	0.92414100	0.92450500
C	-1.21075100	0.41890800	1.01374700
C	-0.19647500	1.31994300	1.47349000
C	-0.50481900	2.62127100	1.81552200
C	-1.82516700	3.08659800	1.71817900
H	-3.86113800	2.59405500	1.19726900
H	-3.33614300	0.25835800	0.57780300
H	0.81629300	0.93882200	1.54143300
H	0.27670100	3.28992800	2.16188300
H	-2.06112300	4.11031000	1.98871900
N	-0.84651800	-0.82848500	0.69843300
H	-1.66617400	-1.35814900	0.38706200

TS-I/II

C	-2.36193500	2.75199900	0.37672800

C	-2.09930500	1.46909900	0.74655900
C	-0.76906900	0.89126600	0.54406500
C	0.24198300	1.74409200	-0.06166500
C	-0.06754600	3.04946000	-0.42523900
C	-1.34301000	3.55599900	-0.21518400
H	-3.34956300	3.17500700	0.52905800
H	-2.86754500	0.84686100	1.19825200
H	1.51059700	1.36826800	-0.31277200
H	0.69878400	3.67275700	-0.87655500
H	-1.57630500	4.57694400	-0.50238500
N	-0.45580100	-0.33048100	0.87539000
H	-1.26260400	-0.80844500	1.28785500
C	2.60055300	-1.05688300	-1.17892000
H	2.58652700	-0.81353700	-2.24462000
H	3.12112500	-2.01132000	-1.04972600
H	1.57019400	-1.18558300	-0.83768800
C	3.28994800	0.06791300	-0.38622700
C	4.74080000	0.24965700	-0.88180900
H	4.75020100	0.49800500	-1.94540400
H	5.22942700	1.05987500	-0.33610900
H	5.31453900	-0.67040400	-0.73145400
C	3.28534800	-0.24921000	1.11990000
H	3.74815300	0.56866900	1.67846500
H	2.26096200	-0.37929900	1.47825200
H	3.83783100	-1.16970800	1.33452200
O	2.66320800	1.30722800	-0.63507700

II

C	-3.27856900	1.69138800	0.39757100
C	-3.02141100	0.40960600	0.76832900
C	-1.68898400	-0.18290300	0.57030800

C	-0.70633900	0.69219900	-0.03476500
C	-0.98828700	2.00004900	-0.40701200
C	-2.26184300	2.50433200	-0.19654200
H	-4.26649300	2.11428700	0.55015700
H	-3.79370000	-0.20882800	1.22000500
H	-0.22546300	2.62849900	-0.85911800
H	-2.49788100	3.52542700	-0.48274000
N	-1.37706000	-1.40197100	0.90192400
H	-2.19011500	-1.87089500	1.31325500

III

C	-3.02469200	2.73837800	-0.60171700
C	-2.71894000	1.51672000	-0.11229400
C	-1.33785200	1.04296700	-0.02810900
C	-0.28375200	2.01388000	-0.45508500
C	-0.69089700	3.30921200	-0.96695800
C	-1.99490800	3.65485800	-1.04186300
H	-4.06266000	3.04944900	-0.66869100
H	-3.49897300	0.83406800	0.21307400
H	0.10044000	3.98159200	-1.27756400
H	-2.28392200	4.62794100	-1.42339800
N	-0.98730700	-0.13055900	0.37698300
H	-1.80773400	-0.66290300	0.67792700
C	1.69202800	-1.64315600	3.71628200
C	1.76560000	-1.27495500	2.37400300
C	2.97119300	-1.42674700	1.67463600
C	4.09106800	-1.95376500	2.33585200
C	4.01616600	-2.30086400	3.67868100
C	2.81363400	-2.14674100	4.37199400
H	0.75408900	-1.53460400	4.25168700
H	0.89049900	-0.89013400	1.86744500

H	5.01225700	-2.08336000	1.77953700
H	4.89064300	-2.69549200	4.18595400
H	2.75232200	-2.42302300	5.42010600
C	3.11540900	-1.10814000	0.22409800
O	3.96327400	-1.65494000	-0.46754300
C	2.26662400	-0.08776500	-0.45366100
H	2.34962100	-0.07270600	-1.54173700
N	1.54853300	0.76108000	0.17895500
N	0.99966400	1.80297500	-0.39270000

TS-III/IV

C	-4.10016600	0.18884900	-0.87710900
C	-2.84513800	0.70304800	-0.77897300
C	-2.45713900	1.51155200	0.34530600
C	-3.49394500	1.90702300	1.31565200
C	-4.72580000	1.15048500	1.27579300
C	-5.03484000	0.38648900	0.19185300
H	-4.38198300	-0.42364200	-1.72619900
H	-2.07567600	0.47875600	-1.50939500
H	-5.44617000	1.30512800	2.07407000
H	-6.00809500	-0.09140400	0.13575300
N	-3.29824500	2.90623800	2.14602200
H	-3.95622000	2.89895600	2.93015700
N	-1.14029900	1.56186700	0.59278300
N	-0.70252600	2.13103200	1.68313000
C	-1.18536600	3.28065900	2.08086900
H	-1.46428200	4.00457300	1.32201000
C	-0.82354400	3.77533000	3.46621800
C	-1.21385100	5.17163200	3.83272900
C	-2.14643500	5.92358200	3.10317600
C	-0.61967700	5.73830200	4.97064500

C	-2.47318900	7.21693300	3.50499000
H	-2.64735800	5.49373900	2.24415900
C	-0.93879100	7.03212300	5.36190700
H	0.09348300	5.14581500	5.53185700
C	-1.86706200	7.77481800	4.62899900
H	-3.20280600	7.78818200	2.94040500
H	-0.46643700	7.46459600	6.23783300
H	-2.11828700	8.78515500	4.93578800
O	-0.22907800	3.05301500	4.23871900

IV

C	-1.80206400	-3.20095300	-3.32532100
C	-0.99847800	-2.07590400	-3.27922500
C	-0.69569600	-1.48267200	-2.04454400
C	-1.21321000	-2.02009900	-0.84565600
C	-1.95429600	-3.21255800	-0.89483800
C	-2.25082100	-3.77912000	-2.12445700
H	-2.05589700	-3.65667100	-4.27569300
H	-0.56398000	-1.64875600	-4.17692000
H	-2.31720500	-3.65890000	0.02580000
H	-2.84743900	-4.68527400	-2.15792900
N	-0.92971900	-1.33554400	0.30846600
H	-0.70556100	-1.80653300	1.17644000
N	0.35116800	-0.54063500	-1.98365300
N	0.58098900	0.12538500	-0.95448400
C	-0.44487000	0.00334900	0.15888000
H	-1.26689000	0.67815200	-0.13080900
C	0.16891100	0.47795700	1.48400800
C	0.56478100	1.90190400	1.64046300
C	0.49860800	2.83177500	0.59265300
C	1.01796400	2.32149900	2.90132700

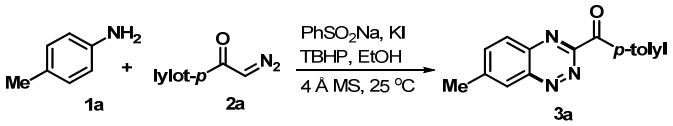
C	0.87410200	4.15515800	0.80674500
H	0.18449200	2.52510200	-0.39650400
C	1.38874500	3.64270600	3.11191800
H	1.06945100	1.59441200	3.70308800
C	1.31657400	4.56286900	2.06387300
H	0.82707700	4.86655500	-0.01093100
H	1.73522800	3.95852900	4.09040600
H	1.60823600	5.59547700	2.22727000
O	0.29364100	-0.32942400	2.38806700

II'

C	-0.79238300	-3.19140300	-3.55323200
C	-1.00205600	-1.88548400	-3.76723700
C	-1.92355500	-1.08033600	-2.87533600
C	-2.81593700	-1.92386200	-1.96577100
C	-2.40799900	-3.30747100	-1.71340000
C	-1.47017400	-3.90342100	-2.47520700
H	-0.10424300	-3.74418900	-4.18511500
H	-0.47695400	-1.34385100	-4.54604600
H	-2.91835800	-3.85136100	-0.92315400
H	-1.20952900	-4.94310300	-2.30193000
N	-3.87035500	-1.36457600	-1.50284500
H	-4.37969100	-2.00654500	-0.88890800
N	-1.02481200	-0.12675600	-2.18257400
N	-0.95658800	-0.30974800	-0.90251500
C	-0.16568300	0.57437900	-0.29231700
H	0.34837900	1.34168500	-0.87203600
C	0.15671500	0.51525500	1.14734100
C	-0.67163500	-0.24338500	2.13001100
C	-2.02512700	-0.54458300	1.92159800
C	-0.06754500	-0.60354100	3.34428200

C	-2.75595900	-1.19233800	2.91514900
H	-2.50946700	-0.27218800	0.99332300
C	-0.79495100	-1.26812400	4.32334600
H	0.97441700	-0.35093800	3.50257400
C	-2.14364800	-1.56134200	4.11139800
H	-3.80759100	-1.40676700	2.75424800
H	-0.31574400	-1.55234600	5.25451300
H	-2.71569800	-2.07204800	4.87970500
O	1.16926000	1.11728900	1.49619600
H	-2.57113500	-0.44611300	-3.49151600

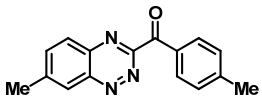
General Procedure for the Synthesis of Products 3



Example for the synthesis of **3a**:

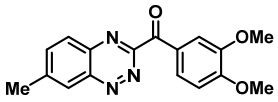
Under the air conditions, sodium benzenesulfinate (0.2 mmol, 1.0 equiv, 33 mg), KI (30 mol%, 10 mg) and 4 Å MS (100 mg) and ethanol (1.0 mL) were added into a reaction tube. Then, *α*-diazo ketone **2a** (0.2 mmol, 1.0 equiv, 32 mg) and *p*-toluidine **1a** (0.4 mmol, 2.0 equiv, 43 mg) was added into the reaction system. Subsequently, TBHP (0.08 mL, 2.0 equiv, 5.5 M in nonane) in ethanol solution (1.0 mL) was added into the suspension over 1.0 h via a syringe pump at room temperature. After completion of the addition, the reaction mixture was stirred at room temperature for an additional 19.0 h until complete consumption of **2a** as monitored by TLC analysis. After completion of the reaction, the mixture was poured into the water and was extracted with ethyl acetate (3 × 5 mL). The organic layers were combined and dried over sodium sulfate and was then concentrated in vacuum. The resulting residue was purified by column chromatography on silica gel (eluent, petroleum ether/ethyl acetate =15:1) to afford the desired product **3a** as a yellow solid.

(7-Methylbenzo[e][1,2,4]triazin-3-yl)(p-tolyl)methanone (3a)



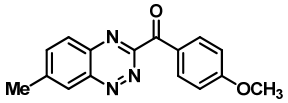
Yellow solid, 43.5 mg, 83% yield; mp 150-152 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.42 (s, 1H), 8.13 (d, J = 8.4 Hz, 1H), 8.04 (d, J = 8.0 Hz, 2H), 7.95-7.92 (m, 1H), 7.33 (d, J = 8.0 Hz, 2H), 2.73 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 190.2, 158.0, 147.5, 145.2, 143.8, 139.1, 132.8, 131.3, 129.8, 129.3, 129.1, 127.9, 22.3, 21.9. IR (KBr, v, cm^{-1}): 1668, 1602, 1557, 1384, 1329, 1272, 1176, 932, 842. HRMS (APCI-TOF, m/z): calcd for $C_{16}H_{14}N_3O$ $[M+H]^+$ 264.1131, found 264.1118.

(3,4-Dimethoxyphenyl)(7-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3b)



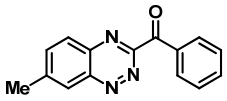
Yellow solid, 43 mg, 70% yield; mp 147-149 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.42 (s, 1H), 8.13 (d, J = 8.8 Hz, 1H), 7.96-7.93 (m, 1H), 7.83 (d, J = 1.6 Hz, 1H), 7.69-7.66 (m, 1H), 6.92 (d, J = 8.4 Hz, 1H), 3.98 (s, 3H), 3.976 (s, 3H), 2.74 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 189.0, 158.3, 154.4, 149.3, 147.5, 143.7, 139.1, 129.0, 128.3, 127.9, 127.5, 112.1, 110.0, 56.2, 56.1, 22.3. IR (KBr, v, cm^{-1}): 1674, 1602, 1546, 1336, 1321, 1227, 1035, 803, 769. HRMS (APCI-TOF, m/z): calcd for $C_{17}H_{16}N_3O_3$ $[M+H]^+$ 310.1192, found 310.1199.

(4-Methoxyphenyl)(7-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3c)



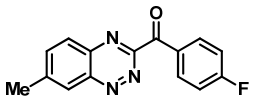
Yellow solid, 49 mg, 87% yield; mp 154-156 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.42 (s, 1H), 8.17-8.12 (m, 3H), 7.95-7.92 (m, 1H), 7.01 (d, J = 8.8 Hz, 2H), 3.91 (s, 3H), 2.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 189.0, 164.4, 143.7, 139.2, 139.0, 134.5, 133.7, 130.9, 129.1, 128.2, 127.9, 113.9, 55.6, 22.3. IR (KBr, v, cm^{-1}): 1672, 1617, 1558, 1489, 1337, 1210, 1064, 843, 690. HRMS (APCI-TOF, m/z): calcd for $C_{16}H_{14}N_3O_2$ $[M+H]^+$ 280.1080, found 280.1077.

(7-Methylbenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3d)



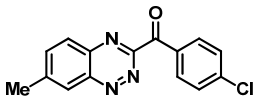
Yellow solid, 44mg, 89% yield; mp 159-161 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.43 (s, 1H), 8.15 (d, J = 8.4 Hz, 3H), 7.96-7.94 (m, 1H), 7.70-7.66 (m, 1H), 7.56-7.52 (m, 2H), 2.66 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 190.6, 157.7, 147.5, 144.1, 139.2, 139.1, 135.3, 134.0, 131.2, 129.1, 128.6, 127. 9, 22.3. IR (KBr, v, cm^{-1}): 1678, 1596, 1552, 1450, 1416, 1327, 1273, 1190, 912, 835, 693. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{12}N_3O$ $[M+H]^+$ 250.0974, found 250.0972.

(4-Chlorophenyl)(7-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3e)



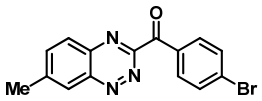
Yellow solid, 48 mg, 90% yield; mp 146-148 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.42 (s, 1H), 8.27-8.19 (m, 2H), 8.14 (d, J = 8.8 Hz, 1H), 7.95 (d, J = 8.8 Hz, 1H), 7.25-7.17 (m, 2H), 2.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 188.9, 166.3 ($^1J_{CF}$ = 255.5 Hz) 157.4, 147.5, 144.2, 139.3, 139.1, 134.0 ($^3J_{CF}$ = 9.6 Hz), 131.7 ($^4J_{CF}$ = 2.8 Hz), 129.1, 127.9, 115.8 ($^2J_{CF}$ = 21.9 Hz), 22.3. IR (KBr, v, cm^{-1}): 1681, 1599, 1506, 1410, 1324, 1238, 1187, 1158, 933, 836. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{11}FN_3O$ $[M+H]^+$ 268.0880, found 268.0872.

(4-chlorophenyl)(7-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3f)



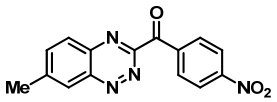
Yellow solid, 46 mg, 81% yield; mp 159-161 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.42 (s, 1H), 8.17-8.09 (m, 3H), 7.98-7.92 (m, 1H), 7.51 (d, J = 8.4 Hz, 2H), 2.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 189.2, 157.2, 147.5, 144.3, 140.6, 139.3, 139.1, 133.7, 132.6, 129.1, 128.9, 127.9, 22.3. IR (KBr, v, cm^{-1}): 1687, 1591, 1494, 1400, 1325, 1270, 1176, 935, 912, 802. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{11}ClN_3O$ $[M+H]^+$ 284.0585, found 284.0596.

(4-Bromophenyl)(7-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3g)



Yellow solid, 54 mg, 83% yield; mp 162-164 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.43 (s, 1H), 8.15 (d, J = 8.4 Hz, 1H), 8.06 (d, J = 8.8 Hz, 2H), 7.98-7.95 (m, 1H), 7.69 (d, J = 8.8 Hz, 2H), 2.74 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 189.4, 157.1, 147.6, 144.4, 139.3, 139.1, 134.1, 132.7, 131.9, 129.5, 129.1, 127.9, 22.3. IR (KBr, v, cm^{-1}): 1686, 1591, 1442, 1405, 1324, 1228, 1189, 948, 802. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{11}BrN_3O$ $[M+H]^+$ 328.0079, found 328.0073.

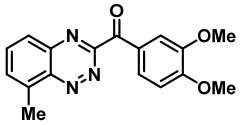
(7-Methylbenzo[e][1,2,4]triazin-3-yl)(4-nitrophenyl)methanone (3h)



Yellow solid, 34 mg, 57% yield; mp 160-162 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.43 (s, 1H), 8.15 (d, J = 8.8 Hz, 1H), 8.10-8.01 (m, 2H), 7.98-7.95 (m, 1H), 7.75-7.64 (m, 2H), 2.74 (d, J = 0.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ,

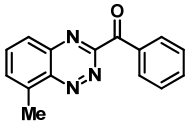
ppm): 189.4, 157.2, 147.6, 144.4, 139.3, 139.1, 134.1, 132.7, 131.9, 129.5, 129.1, 127.9, 22.3. IR (KBr, *v*, cm^{-1}): 1689, 1617, 1557, 1483, 1323, 1221, 1175, 934, 618. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{11}N_4O_3$ $[M+H]^+$ 295.0825, found 295.0827.

(3,4-Dimethoxyphenyl)(6-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3i)



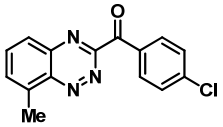
Yellow solid, 37 mg, 60% yield; mp 135-137 °C. ^{1}H NMR (400 MHz, $CDCl_3$; *δ*, ppm): 8.06 (d, *J* = 8.4 Hz, 1H), 8.01-7.98 (m, 1H), 7.84-7.81 (m, 2H), 7.69-7.66 (m, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 3.99 (s, 3H), 3.98 (s, 3H), 3.11 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm): 187.2, 155.8, 145.8, 139.8, 138.3, 137.8, 135.9, 133.9, 132.3, 131.9, 131.8, 129.7, 129.2, 126.4, 15.9. IR (KBr, *v*, cm^{-1}): 1689, 1594, 1515, 1438, 1327, 1269, 1160, 1020, 982, 687. HRMS (APCI-TOF, m/z): calcd for $C_{17}H_{16}N_3O_3$ $[M+H]^+$ 310.1192, found 310.1204.

(6-Methylbenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3j)



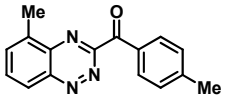
Yellow solid, 37 mg, 74% yield; mp 117-119 °C. ^{1}H NMR (400 MHz, $CDCl_3$; *δ*, ppm): 8.14 (d, *J* = 7.2 Hz, 2H), 8.06 (d, *J* = 8.4 Hz, 3H), 8.02-7.97 (m, 1H), 7.82 (d, *J* = 6.8 Hz, 1H), 7.69-7.63 (m, 1H), 7.58-7.48 (m, 2H), 3.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm): 190.6, 157.9, 146.7, 140.8, 139.2, 136.6, 136.6, 135.2, 134.0, 132.3, 132.2, 131.3, 131.2, 129.3, 128.6, 127.3, 16.9. IR (KBr, *v*, cm^{-1}): 1678, 1605, 1570, 1449, 1384, 1258, 1175, 1095, 965, 906, 787, 692. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{12}N_3O$ $[M+H]^+$ 250.0974, found 250.0972.

(4-chlorophenyl)(7-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3k)



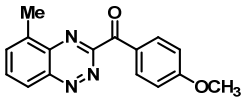
Yellow solid, 31 mg, 54% yield; mp 169-171 °C. ^{1}H NMR (400 MHz, $CDCl_3$; *δ*, ppm): 8.17-8.13 (m, 2H), 8.08 (d, *J* = 8.4 Hz, 1H), 8.04-7.99 (m, 1H), 7.84 (d, *J* = 6.8 Hz, 1H), 7.54-7.49 (m, 2H), 3.11 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm): 189.3, 157.4, 146. 8, 140.8, 140.7, 139.3, 136.8, 133.6, 132.6, 132.5, 128.9, 127.3, 16.9. IR (KBr, *v*, cm^{-1}): 1682, 1586, 1571, 1495, 1380, 1299, 1104, 1090, 907, 719. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{11}ClN_3O$ $[M+H]^+$ 284.0585, found 284.0586.

(5-Methylbenzo[e][1,2,4]triazin-3-yl)(p-tolyl)methanone (3l)



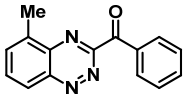
Yellow solid, 29 mg, 56% yield; mp 113-115 °C. ^{1}H NMR (400 MHz, $CDCl_3$; *δ*, ppm): 8.48 (m, 1H), 8.04 (d, *J* = 8.0 Hz, 2H), 7.95-7.87 (m, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 2.81 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm): 190.2, 157.6, 147.7, 145.2, 139.5, 138.7, 135.7, 132.8, 132.1, 131.3, 129.3, 127.3, 21.9, 16.2. IR (KBr, *v*, cm^{-1}): 1672, 1604, 1573, 1455, 1337, 1253, 1178, 894, 776. HRMS (APCI-TOF, m/z): calcd for $C_{16}H_{14}N_3O$ $[M+H]^+$ 264.1136, found 264.1127.

(4-Methoxyphenyl)(5-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3m)



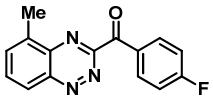
Yellow solid, 31 mg, 56% yield; mp 122-125 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.50-8.43 (m, 1H), 8.13 (d, J = 9.2 Hz, 2H), 7.94-7.85 (m, 2H), 6.99 (d, J = 8.8 Hz, 2H), 3.90 (s, 3H), 2.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 189.0, 164.4, 157.8, 147.7, 139.5, 138.6, 135.7, 133.7, 132.0, 128.2, 127.3, 113. 9, 55.6, 16.2. IR (KBr, ν, cm^{-1}): 1670, 1601, 1573, 1513, 1455, 1340, 1268, 1166, 1023, 951, 830. HRMS (APCI-TOF, m/z): calcd for $C_{16}H_{14}N_3O_2$ $[M+H]^+$ 280.1080, found 280.1094.

(5-Methylbenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3n)



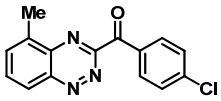
Yellow solid, 25 mg, 50% yield; mp 134-136 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.52-8.49 (m, 1H), 8.14 (d, J = 7.6 Hz, 2H), 7.94-7.92 (m, 2H), 7.70-7.66 (m, 1H), 7.56-7.52 (m, 2H), 2.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 190.6, 157.3, 147.8, 139.5, 138.7, 135.8, 135.2, 134.0, 132.3, 131.2, 128.5, 127.3, 16.3. IR (KBr, ν, cm^{-1}): 1680, 1596, 1572, 1444, 1391, 1334, 1250, 1187, 947, 895, 704. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{12}N_3O$ $[M+H]^+$ 250.0974, found 250.0989.

(4-Fluorophenyl)(5-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3o)



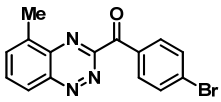
Yellow solid, 49 mg, 92% yield; mp 141-143 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.52-8.50 (m, 1H), 8.25-8.21 (m, 2H), 7.96-7.92 (m, 2H), 7.26-7.20 (m, 2H), 2.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 188.9, 167.4 ($^1J_{CF}$ = 255.4 Hz), 157.0, 147.8, 139.5, 138.7, 135.9, 134.0 ($^3J_{CF}$ = 9.4 Hz), 132.4, 131.7 ($^4J_{CF}$ = 3.0 Hz), 127.4, 115.8 ($^2J_{CF}$ = 21.9 Hz), 16.2. IR (KBr, ν, cm^{-1}): 1682, 1598, 1574, 1506, 1394, 1235, 1184, 895, 782. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{11}FN_3O$ $[M+H]^+$ 268.0880, found 268.0870.

(4-Chlorophenyl)(5-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3p)



Yellow solid, 48 mg, 85% yield; mp 176-178 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.53-8.46 (m, 1H), 8.17-8.10 (m, 2H), 7.97-7.90 (m, 2H), 7.54-7.48 (m, 2H), 2.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 189.2, 156.8, 147.8, 140.7, 139.5, 138.8, 136.0, 133.7, 132.6, 132.5, 128.9, 127.4, 16.2. IR (KBr, ν, cm^{-1}): 1678, 1596, 1552, 1450, 1416, 1327, 1273, 1190, 1177, 912, 835, 693. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{11}ClN_3O$ $[M+H]^+$ 284.0585, found 284.0583.

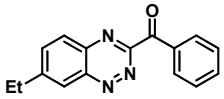
(4-Bromophenyl)(5-methylbenzo[e][1,2,4]triazin-3-yl)methanone (3q)



Yellow solid, 53 mg, 81% yield; mp 180-182 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.53-8.48 (m, 1H), 8.08-8.03 (m, 1H), 7.96-7.92 (m, 1H), 7.71-7.67 (m, 1H), 2.83 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 189.4, 156.7, 147.8,

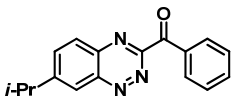
139.5, 138.8, 136.0, 134.1, 132.6, 132.5, 131.9, 129.5, 127.4, 16.2. IR (KBr, *v*, cm^{-1}): 1685, 1584, 1447, 1396, 1250, 1169, 996, 894, 721. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{11}BrN_3O$ $[M+H]^+$ 328.0079, found 328.0080.

(7-Ethylbenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3r)



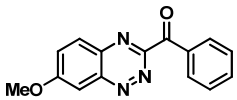
Yellow solid, 50 mg, 95% yield; mp 110-112 °C. ^{1}H NMR (400 MHz, $CDCl_3$; *δ*, ppm): 8.43 (s, 1H), 8.18-8.10 (m, 3H), 8.00-7.94 (m, 1H), 7.70-7.62 (m, 1H), 7.57-7.48 (m, 2H), 3.07-2.97 (m, 2H), 1.49-1.39 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm): 190.6, 157.7, 150.0, 147.7, 139.3, 138.3, 135.3, 134.0, 131.2, 129.2, 128.5, 126.5, 29.3, 14.6. IR (KBr, *v*, cm^{-1}): 1676, 1597, 1450, 1409, 1325, 1176, 1083, 907, 689. HRMS (APCI-TOF, m/z): calcd for $C_{16}H_{14}N_3O$ $[M+H]^+$ 264.1131, found 264.1127.

(7-Isopropylbenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3s)



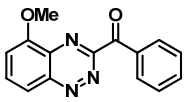
Yellow oli, 53 mg, 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$; *δ*, ppm): 8.45 (s, 1H), 8.17 (d, *J* = 8.8 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 2H), 8.03 (d, *J* = 8.8 Hz, 1H), 7.69-7.63 (m, 1H), 7.55-7.48 (m, 2H), 3.31-3.22 (m, 1H), 1.44 (d, *J* = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm): 189.3, 157.3, 154.8, 147. 8, 140.6, 139.4, 137.3, 133.7, 132.6, 129.3, 128.9, 125.2, 34.6, 23.3. IR (KBr, *v*, cm^{-1}): 1682, 1565, 1480, 1412, 1353, 1150, 1081, 967, 781. HRMS (APCI-TOF, m/z): calcd for $C_{17}H_{17}N_3O$ $[M+H]^+$ 278.1287, found 278.1280.

(7-Methoxybenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3t)



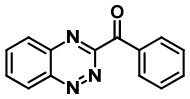
Yellow solid, 38 mg, 72% yield; mp 127-129 °C. ^{1}H NMR (400 MHz, $CDCl_3$; *δ*, ppm): 8.18-8.10 (m, 3H), 7.83 (d, *J* = 2.4 Hz, 1H), 7.76-7.72 (m, 1H), 7.69-7.63 (m, 1H), 7.57-7.50 (m, 2H), 4.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm): 190.6, 162.6, 157.1, 149.0, 137. 6, 135.5, 133.9, 131.3, 131.2, 130.7, 128.5, 105.0, 56.5. IR (KBr, *v*, cm^{-1}): 1681, 1614, 1502, 1472, 1412, 1216, 1178, 1085, 919, 851. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{12}N_3O_2$ $[M+H]^+$ 266.0924, found 266.0920.

(5-Methoxybenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3u)



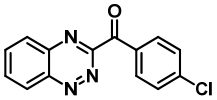
Yellow solid, 22 mg, 42% yield; mp 130-132 °C. ^{1}H NMR (400 MHz, $CDCl_3$; *δ*, ppm): 8.24 (d, *J* = 8.4 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 2H), 7.98-7.92 (m, 1H), 7.69-7.62 (m, 1H), 7.56-7.48 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 1H), 4.12 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; *δ*, ppm): 190.2, 157.5, 155.3, 148.0, 135.2, 134.1, 133.3, 132.8, 131.2, 128. 6, 120.7, 113.0, 56.7. IR (KBr, *v*, cm^{-1}): 1668, 1603, 1567, 1477, 1388, 1297, 1191, 1122, 929, 767. HRMS (APCI-TOF, m/z): calcd for $C_{15}H_{12}N_3O_2$ $[M+H]^+$ 266.0924, found 266.0921.

benzo[e][1,2,4]triazin-3-yl(phenyl)methanone (3v)



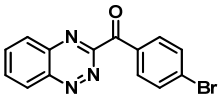
Yellow solid, 42 mg, 88% yield; mp 104-105 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.69 (d, J = 8.4 Hz, 1H), 8.25 (d, J = 8.4 Hz, 1H), 8.22-8.09 (m, 3H), 8.05 (m, 1H), 7.76-7.63 (m, 1H), 7.54 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 190.6, 158.1, 147.6, 140.4, 136.6, 135.2, 134.2, 132.7, 131.3, 129.8, 129.7, 128.7. IR (KBr, v, cm^{-1}): 1675, 1585, 1549, 1441, 1403, 1311, 1286, 1173, 950, 829, 774. HRMS (APCI-TOF, m/z): calcd for $C_{14}H_{10}N_3O$ $[M+H]^+$ 236.0818, found 236.0824.

Benzo[e][1,2,4]triazin-3-yl(4-chlorophenyl)methanone (3w)



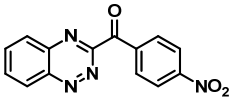
Yellow solid, 46 mg, 85% yield; mp 160-162 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.73-8.65 (m, 1H), 8.28-8.24 (m, 1H), 8.17-8.10 (m, 3H), 8.10-8.04 (m, 1H), 7.55-7.50 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 189.1, 157.6, 147.6, 140.8, 140.3, 136.6, 133.5, 132.8, 132.6, 129.8, 129.7, 129.0. IR (KBr, v, cm^{-1}): 1676, 1607, 1558, 1503, 1478, 1396, 1196, 1087, 928, 771. HRMS (APCI-TOF, m/z): calcd for $C_{14}H_9ClN_3O$ $[M+H]^+$ 270.0426, found 270.0419.

Benzo[e][1,2,4]triazin-3-yl(4-bromophenyl)methanone (3x)



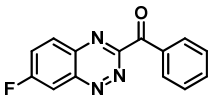
Yellow solid, 50 mg, 80% yield; mp 187-189 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.69 (d, J = 8.4 Hz, 1H), 8.26 (d, J = 8.4 Hz, 1H), 8.17-8.12 (m, 1H), 8.12-7.94 (m, 3H), 7.69 (d, J = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 189.3, 157.5, 147.6, 140.3, 136.7, 133.9, 132.8, 132.6, 132.0, 129.8, 129.7, 129.7. IR (KBr, v, cm^{-1}): 1676, 1582, 1423, 1396, 1307, 1263, 1166, 1026, 926, 772. HRMS (APCI-TOF, m/z): calcd for $C_{14}H_9BrN_3O$ $[M+H]^+$313.9923, found 313.9915.

Benzo[e][1,2,4]triazin-3-yl(4-nitrophenyl)methanone (3y)



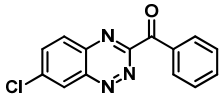
Yellow solid, 41 mg, 73% yield; mp 176-178 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.72 (d, J = 8.0 Hz, 1H), 8.47-8.34 (m, 4H), 8.29 (d, J = 7.6 Hz, 1H), 8.21-8.15 (m, 1H), 8.15-8.08 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 188.8, 156.6, 150.7, 147.7, 140.3, 140.0, 137.0, 133.3, 132.2, 129.8, 129.7, 123.6. IR (KBr, v, cm^{-1}): 1684, 1629, 1527, 1465, 1345, 1169, 938, 691. HRMS (APCI-TOF, m/z): calcd for $C_{14}H_9N_4O_3$ $[M+H]^+$ 281.0669, found 281.0658.

(7-Fluorobenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3z)



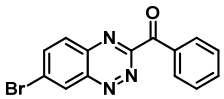
Yellow solid, 31mg, 55% yield; mp 146-148 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.35-8.27 (m, 2H), 8.13 (d, J = 8.0 Hz, 2H), 7.95-7.88 (m, 1H), 7.72-7.66 (m, 1H), 7.58-7.51 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 163.5 ($^1J_{CF}$ = 258.6 Hz), 162.23, 157.90, 148.04, 137.84, 135.02, 134.22, 132.5 ($^4J_{CF}$ = 9.5 Hz), 131.15, 128.63, 127.91 ($^2J_{CF}$ = 27.1 Hz), 112.7 ($^3J_{CF}$ = 22.2 Hz). IR (KBr, v, cm^{-1}): 1682, 1581, 1447, 1402, 1388, 1260, 1196, 1068, 995, 841, 669. HRMS (APCI-TOF, m/z): calcd for $C_{14}H_{10}FN_4O_3$ $[M+H]^+$ 281.0675, found 281.0665.

(7-Chlorobenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3aa)



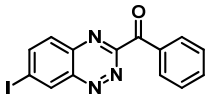
Yellow solid, 38 mg, 71% yield; mp 140-142 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.68 (d, J = 2.0 Hz, 1H), 8.21 (d, J = 8.8 Hz, 1H), 8.12 (d, J = 7.6 Hz, 2H), 8.07-8.02 (m, 1H), 7.73-7.66 (m, 1H), 7.59-7.51 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 190.0, 158.1, 147.4, 139.0, 138.8, 137.8, 134.9, 134.3, 131.1, 128.7, 128.3. IR (KBr, ν, cm^{-1}): 1679, 1598, 1468, 1448, 1399, 1183, 1071, 994, 884, 676. HRMS (APCI-TOF, m/z): calcd for $C_{14}H_{10}ClN_4O_3$ $[M+H]^+$ 270.0428, found 270.0422.

(7-Bromobenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3ab)



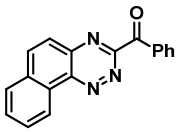
Yellow solid, 32 mg, 51% yield; mp 142-144 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.87 (d, J = 1.2 Hz, 1H), 8.20-8.16 (m, 1H), 8.15-8.08 (m, 3H), 7.72-7.66 (m, 1H), 7.58-7.51 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 190.0, 158.0, 147.6, 140.3, 139.2, 134.9, 134.3, 131.8, 131.1, 131.0, 128.7, 127.1. IR (KBr, ν, cm^{-1}): 1677, 1593, 1544, 1393, 1322, 1261, 1175, 975, 886. HRMS (APCI-TOF, m/z): calcd for $C_{14}H_{10}BrN_4O_3$ $[M+H]^+$ 313.9923, found 313.9929.

(7-Iodobenzo[e][1,2,4]triazin-3-yl)(phenyl)methanone (3ac)



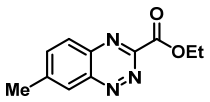
Yellow solid, 33 mg, 45% yield; mp 127-129 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 9.12 (s, 1H), 8.33 (d, J = 8.8 Hz, 1H), 8.11 (d, J = 8.0 Hz, 2H), 7.96 (d, J = 8.8 Hz, 1H), 7.70-7.67 (m, 1H), 7.57-7.52 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 190.1, 158.0, 147.7, 145.4, 139.5, 138.6, 134.9, 134.3, 131.1, 130.7, 128.7, 99.2. IR (KBr, ν, cm^{-1}): 1680, 1586, 1539, 1446, 1393, 1321, 1238, 1174, 936, 879. HRMS (APCI-TOF, m/z): calcd for $C_{14}H_{10}IN_4O_3$ $[M+H]^+$ 361.9784, found 361.9760.

Naphtho[2,3-e][1,2,4]triazin-3-yl(phenyl)methanone (3ad)



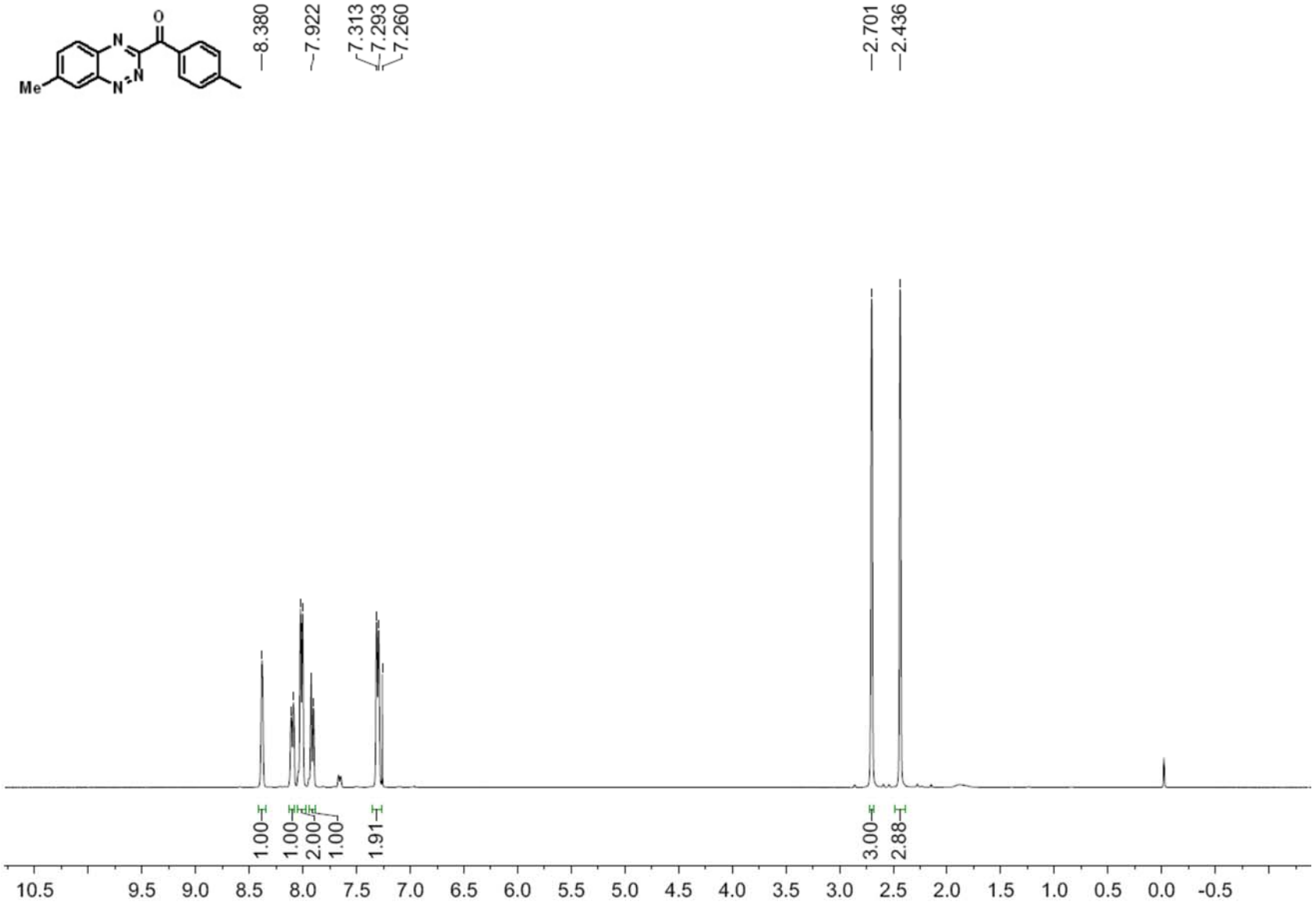
Yellow solid, 34 mg, 60% yield; mp 139-141 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 9.55 (d, J = 7.6 Hz, 1H), 8.31 (d, J = 9.2 Hz, 1H), 8.22-8.14 (m, 2H), 8.04-7.98 (m, 1H), 7.98-7.86 (m, 3H), 7.70-7.63 (m, 1H), 7.57-7.50 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm): 190.6, 159.5, 146.3, 142.9, 139.4, 135.3, 134.0, 133.5, 131.4, 131.2, 129.8, 128.8, 128.8, 128. 6, 125. 5, 124.8. IR (KBr, ν, cm^{-1}): 1676, 1597, 1513, 1431, 1337, 1299, 1180, 981, 904, 761, 688. HRMS (APCI-TOF, m/z): calcd for $C_{18}H_{12}N_3O$ $[M+H]^+$ 286.0974, found 286.0968.

Ethyl 7-methylbenzo[e][1,2,4]triazine-3-carboxylate (3ae)

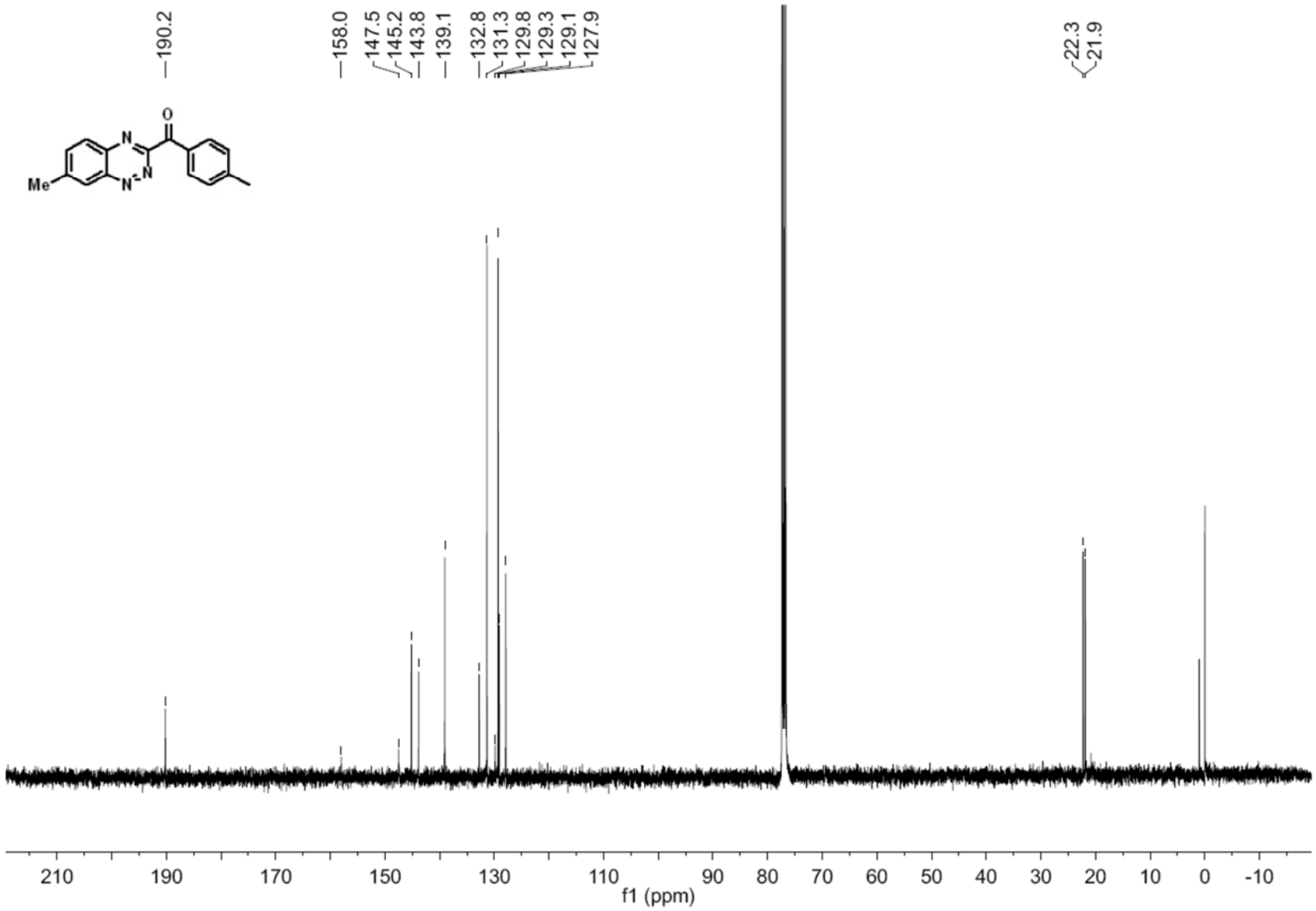


Yellow solid, 37 mg, 86% yield; mp 109-111 °C. ^{1}H NMR (400 MHz, $CDCl_3$; δ, ppm): 8.41 (s, 1H), 8.18 (d, J = 8.8 Hz, 1H), 7.97-7.91 (m, 1H), 4.70-4.62 (m, 2H), 2.71 (s, 3H), 1.53 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$; δ, ppm):

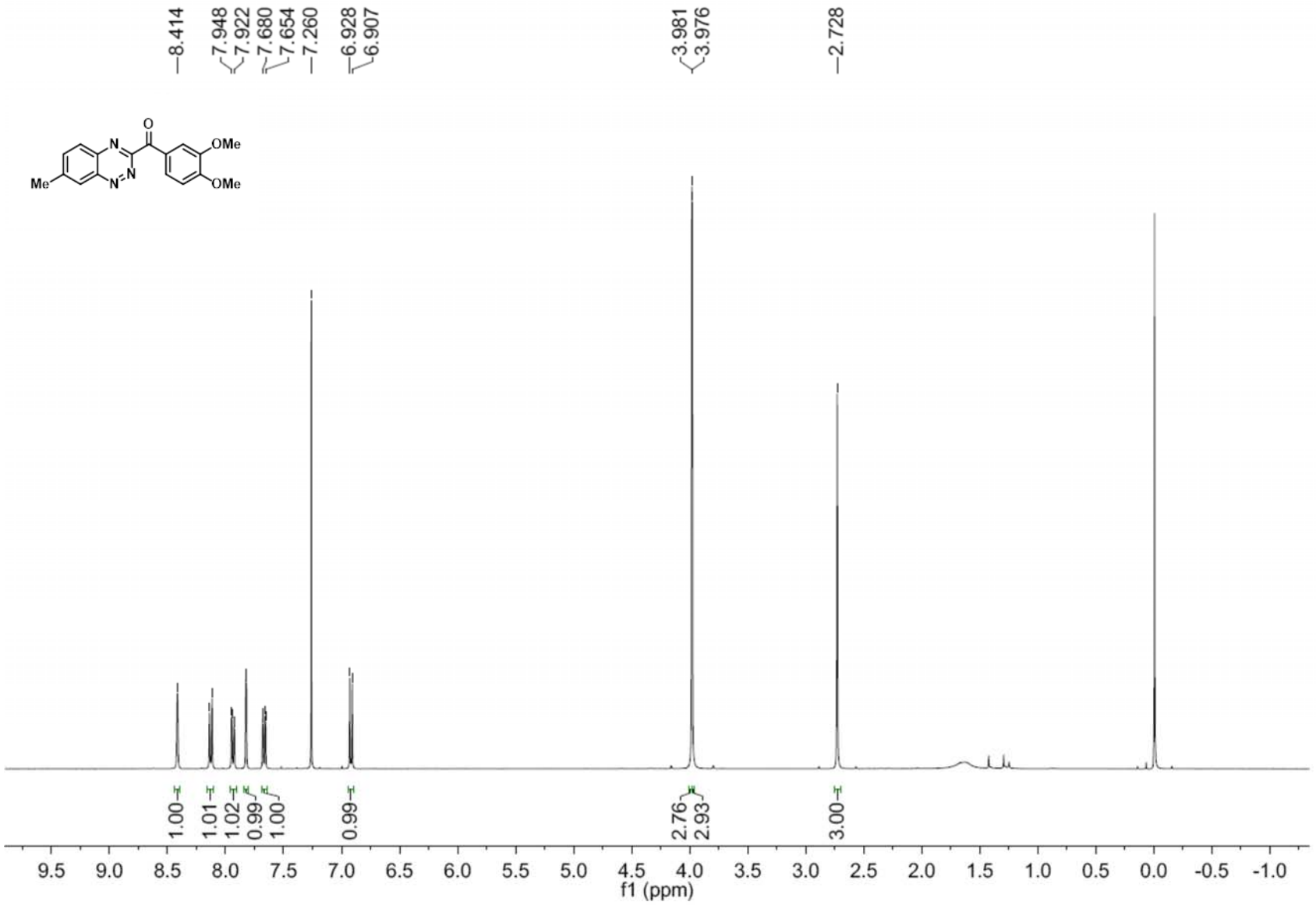
163.1, 152.0, 147.8, 144. 6, 139.3, 139.1, 129.2, 127.9, 63.2, 22.3, 14.3. IR (KBr, *v*, cm^{-1}): 1739, 1557, 1513, 1488, 1319, 1273, 1170, 1077, 1019, 840. HRMS (APCI-TOF, m/z): calcd for $C_{11}H_{11}N_3O_2$ $[M+H]^+$ 218.0924, found 218.0922.



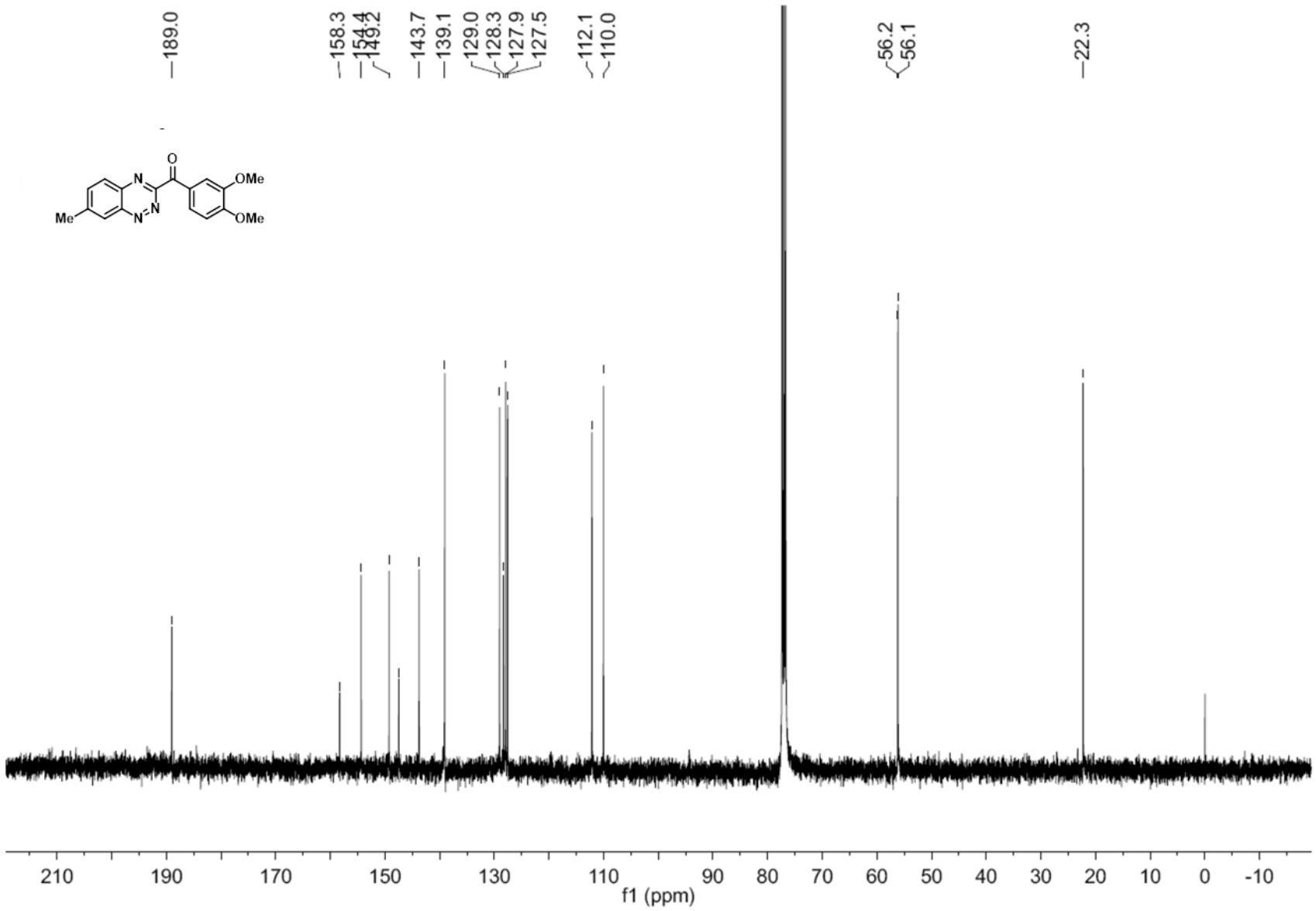
^{1}H NMR Spectrum of Compound **3a**



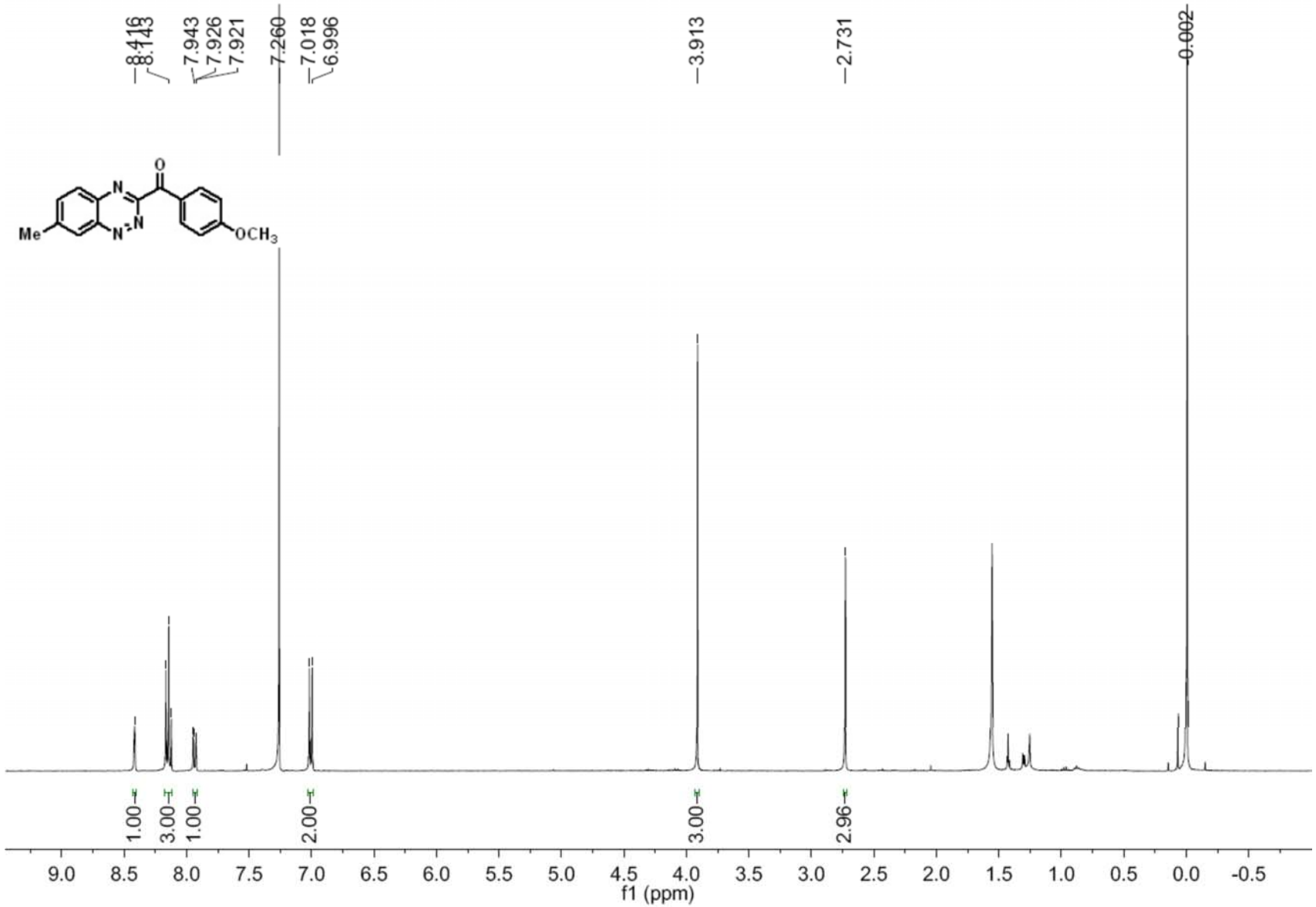
^{13}C NMR Spectrum of Compound **3a**



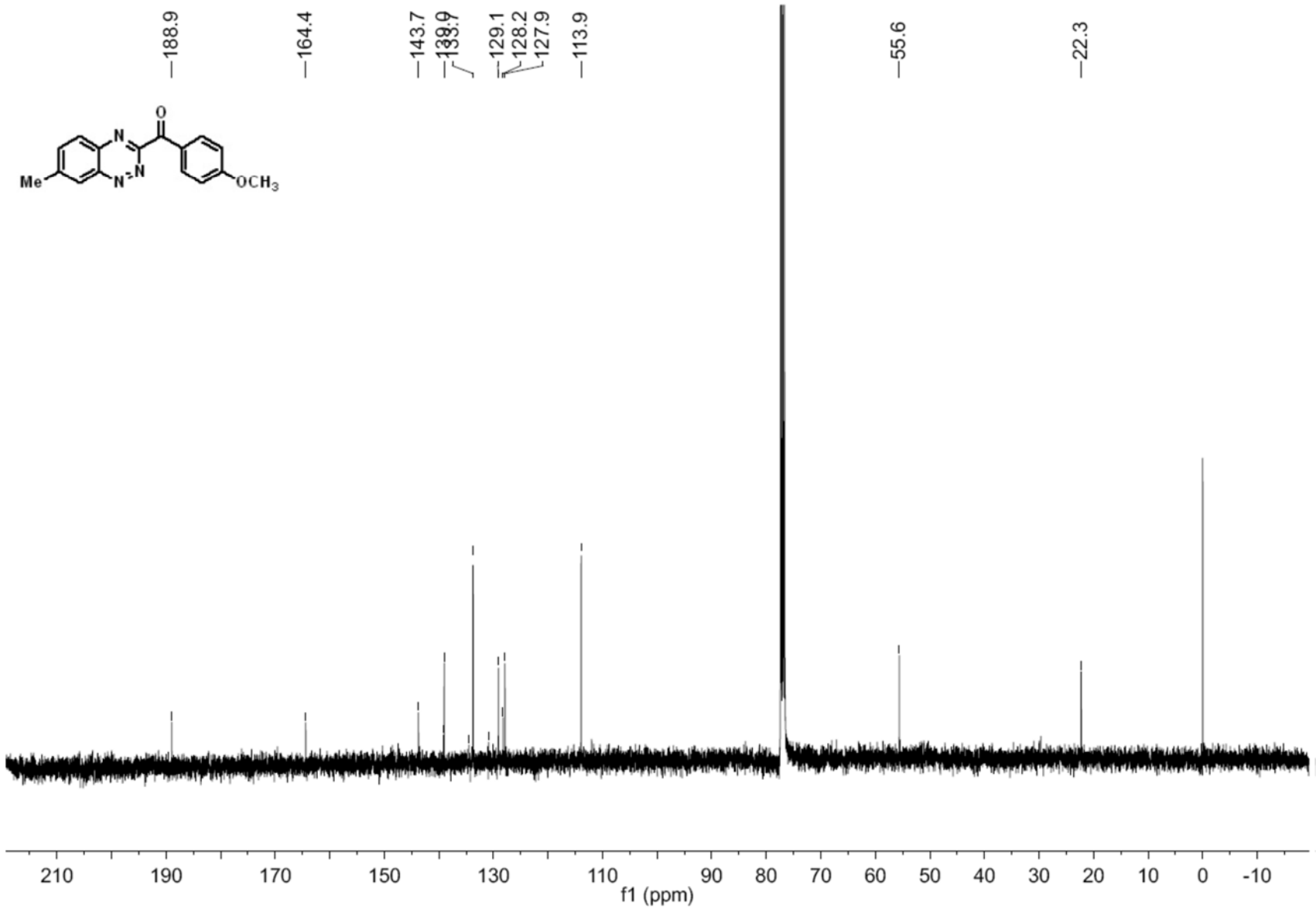
^{1}H NMR Spectrum of Compound **3b**



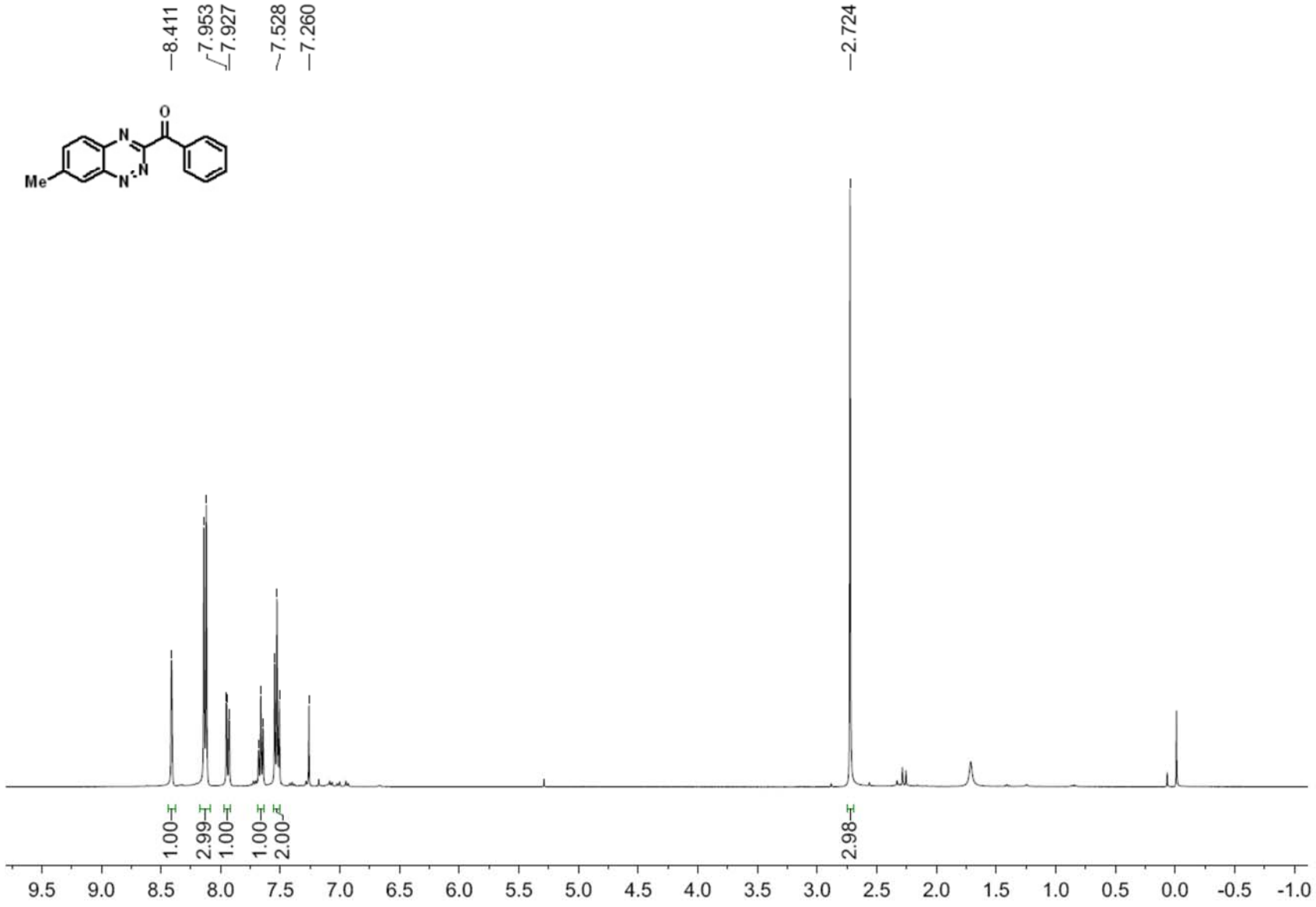
^{13}C NMR Spectrum of Compound **3b**



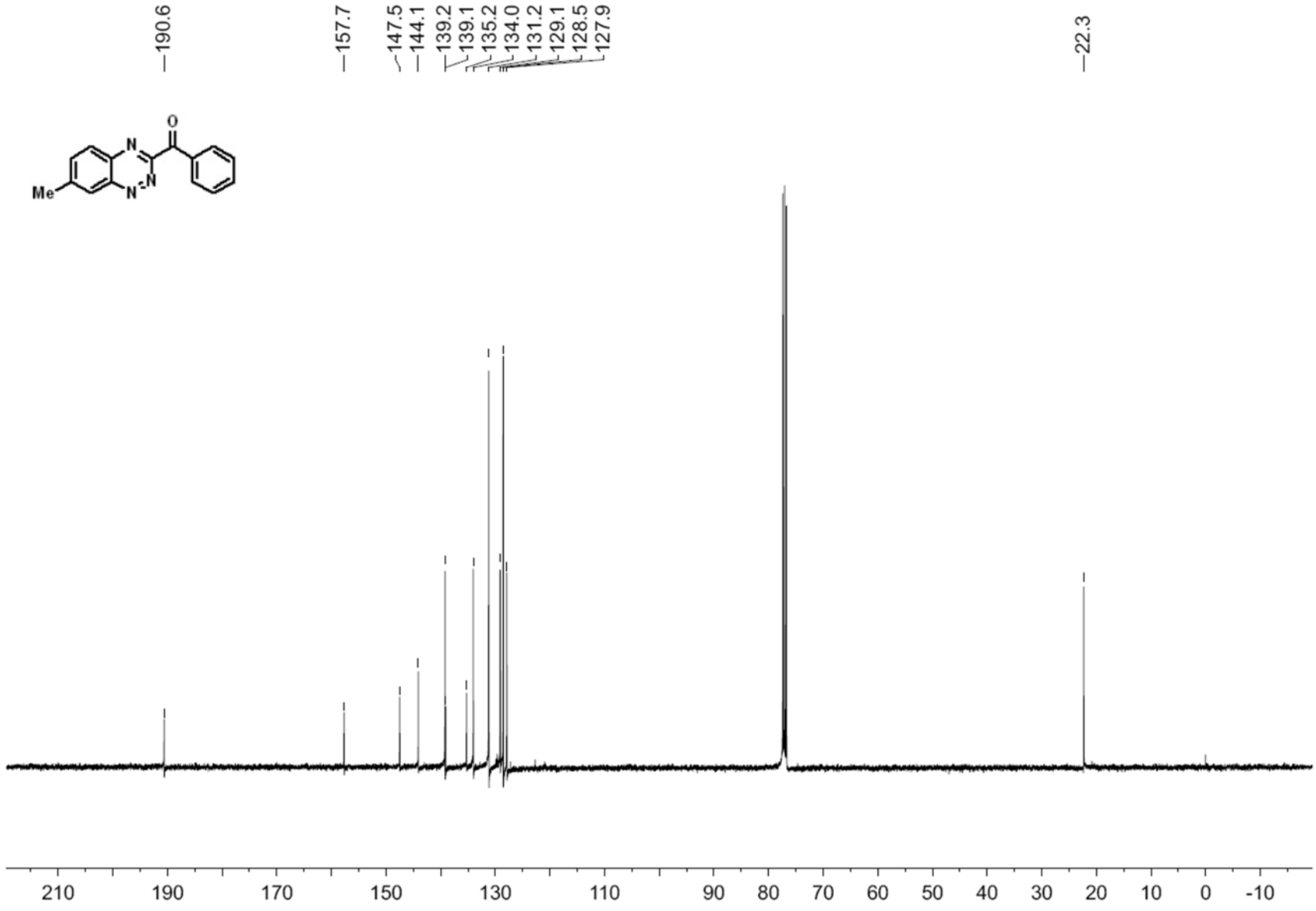
^{1}H NMR Spectrum of Compound **3c**



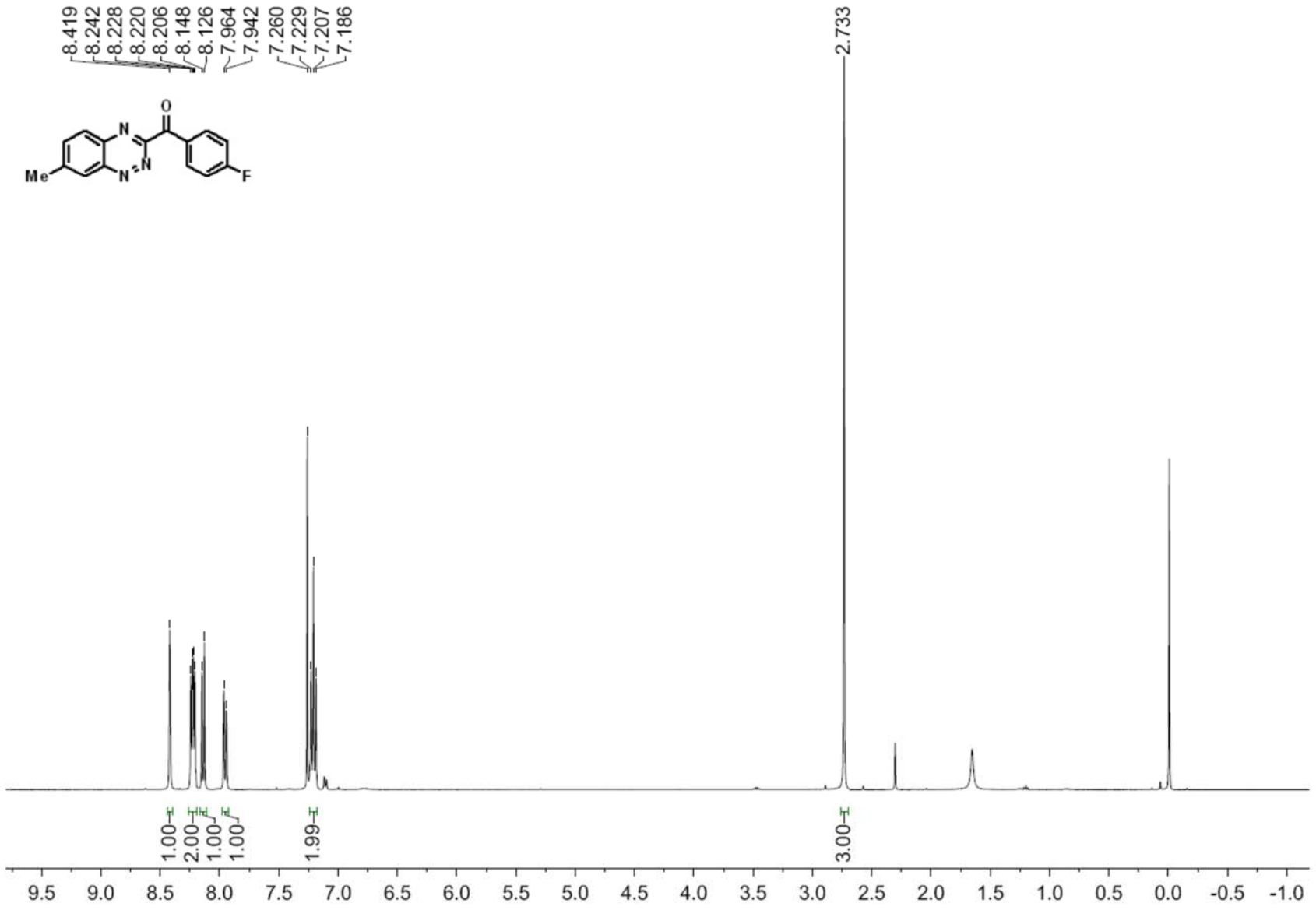
^{13}C NMR Spectrum of Compound **3c**



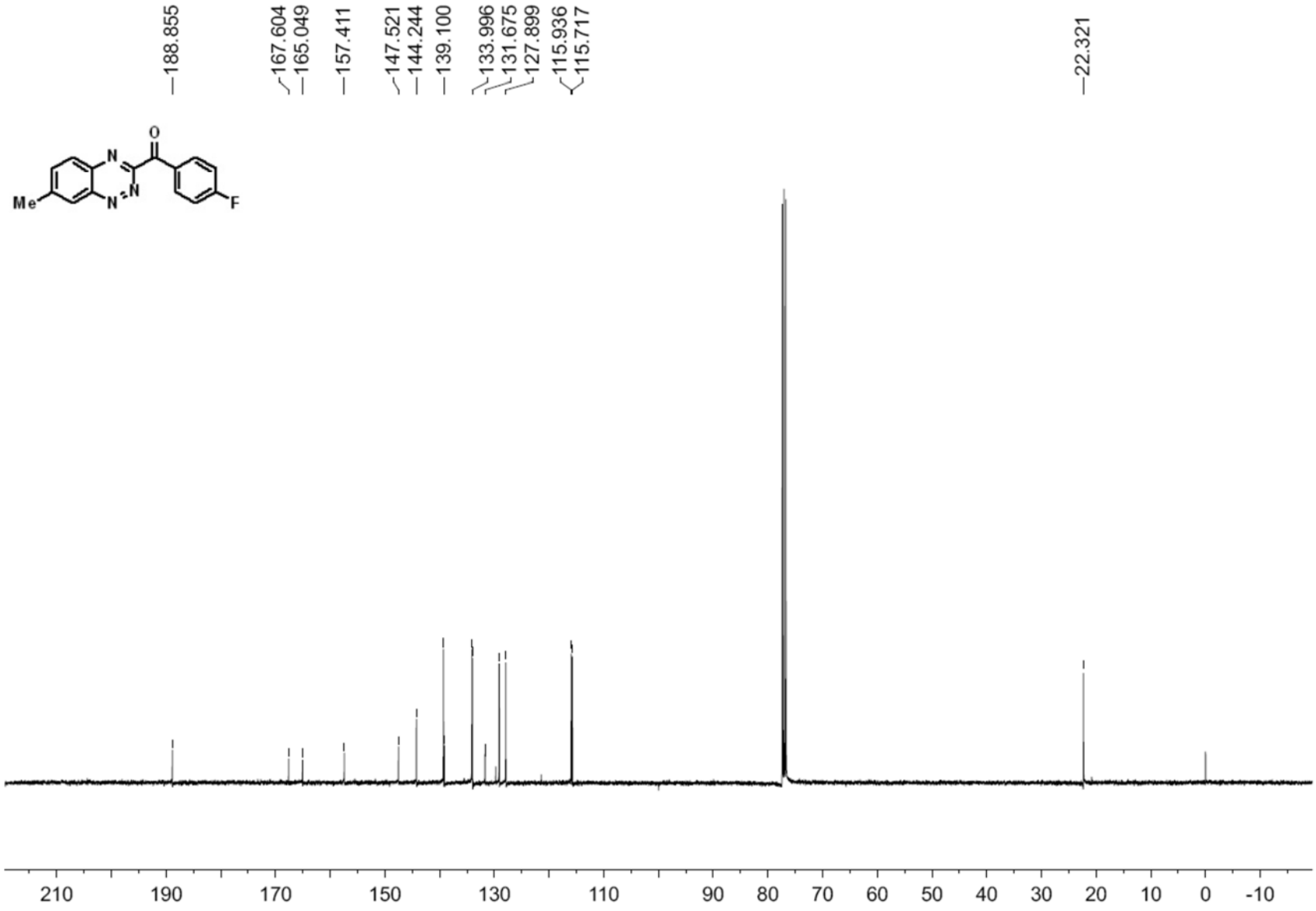
^{1}H NMR Spectrum of Compound **3d**



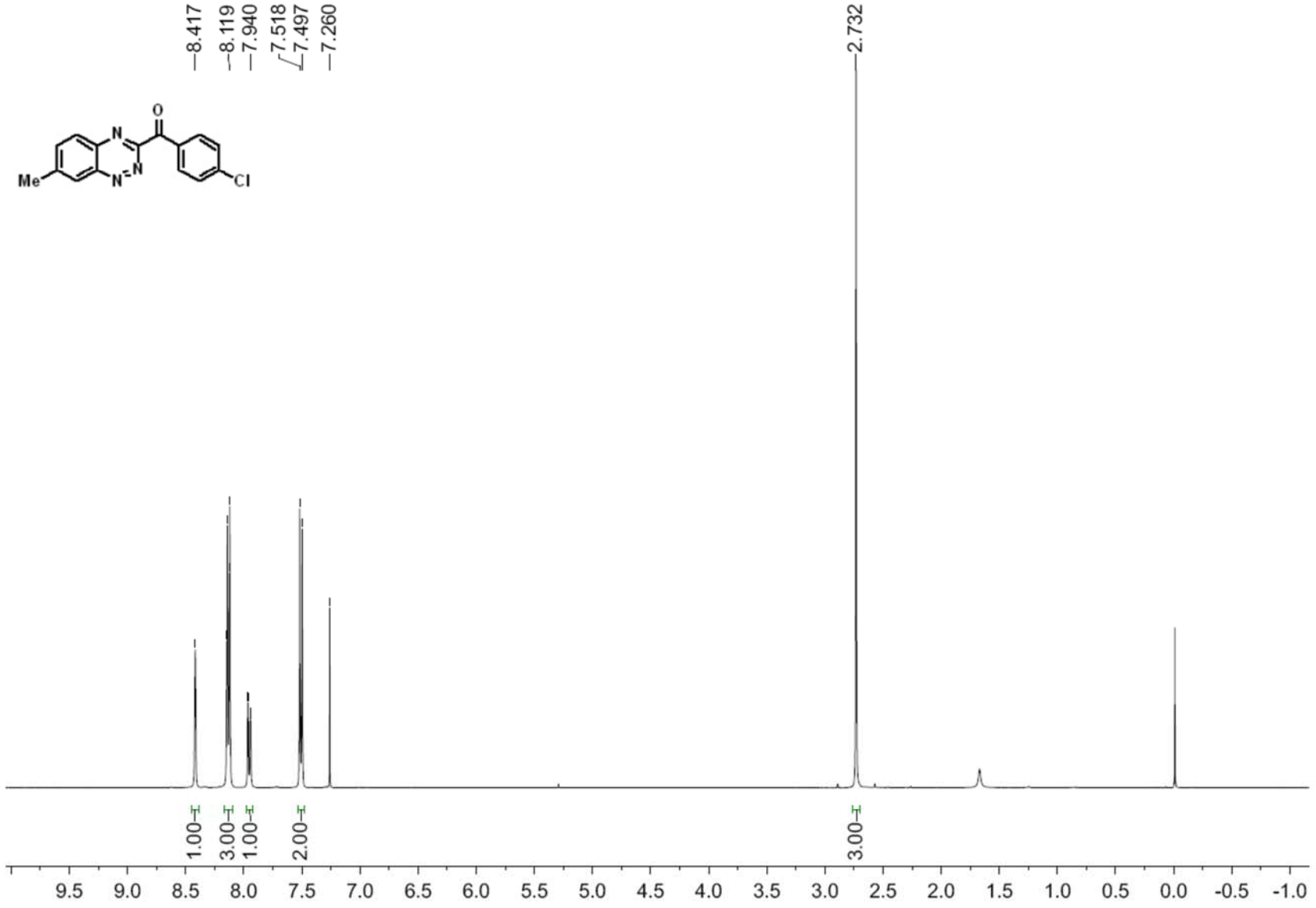
^{13}C NMR Spectrum of Compound **3d**



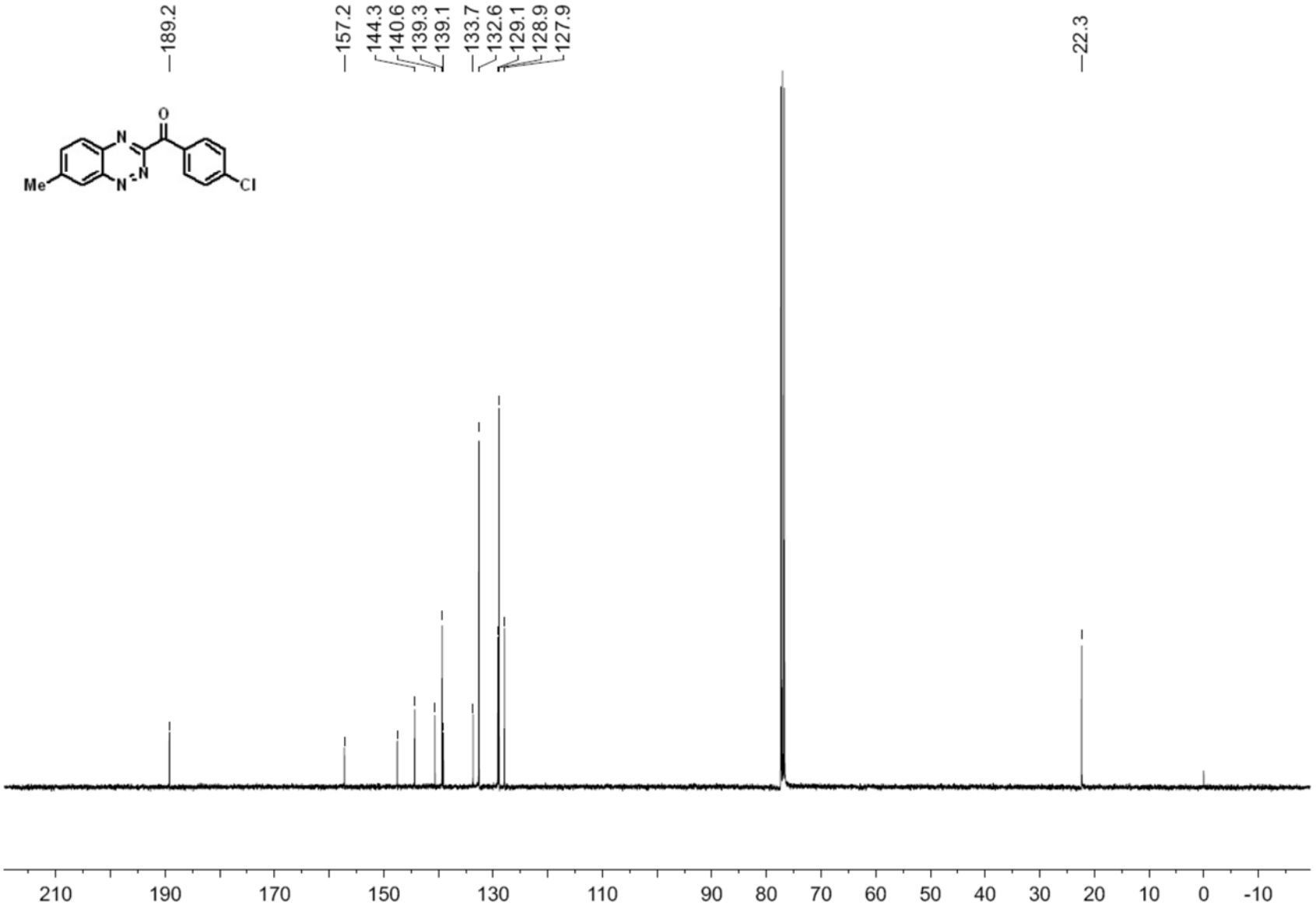
^{1}H NMR Spectrum of Compound **3e**



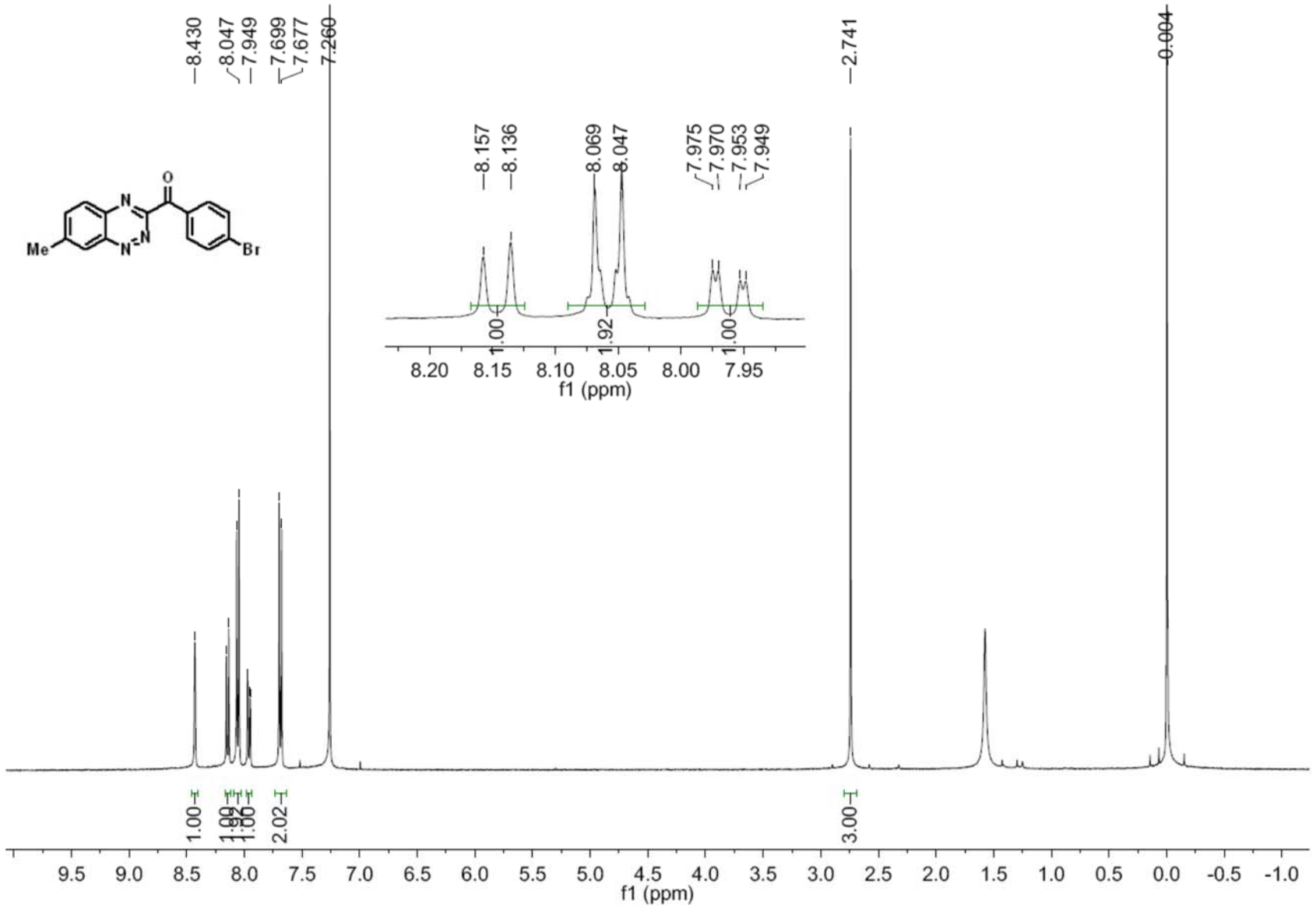
^{13}C NMR Spectrum of Compound **3e**



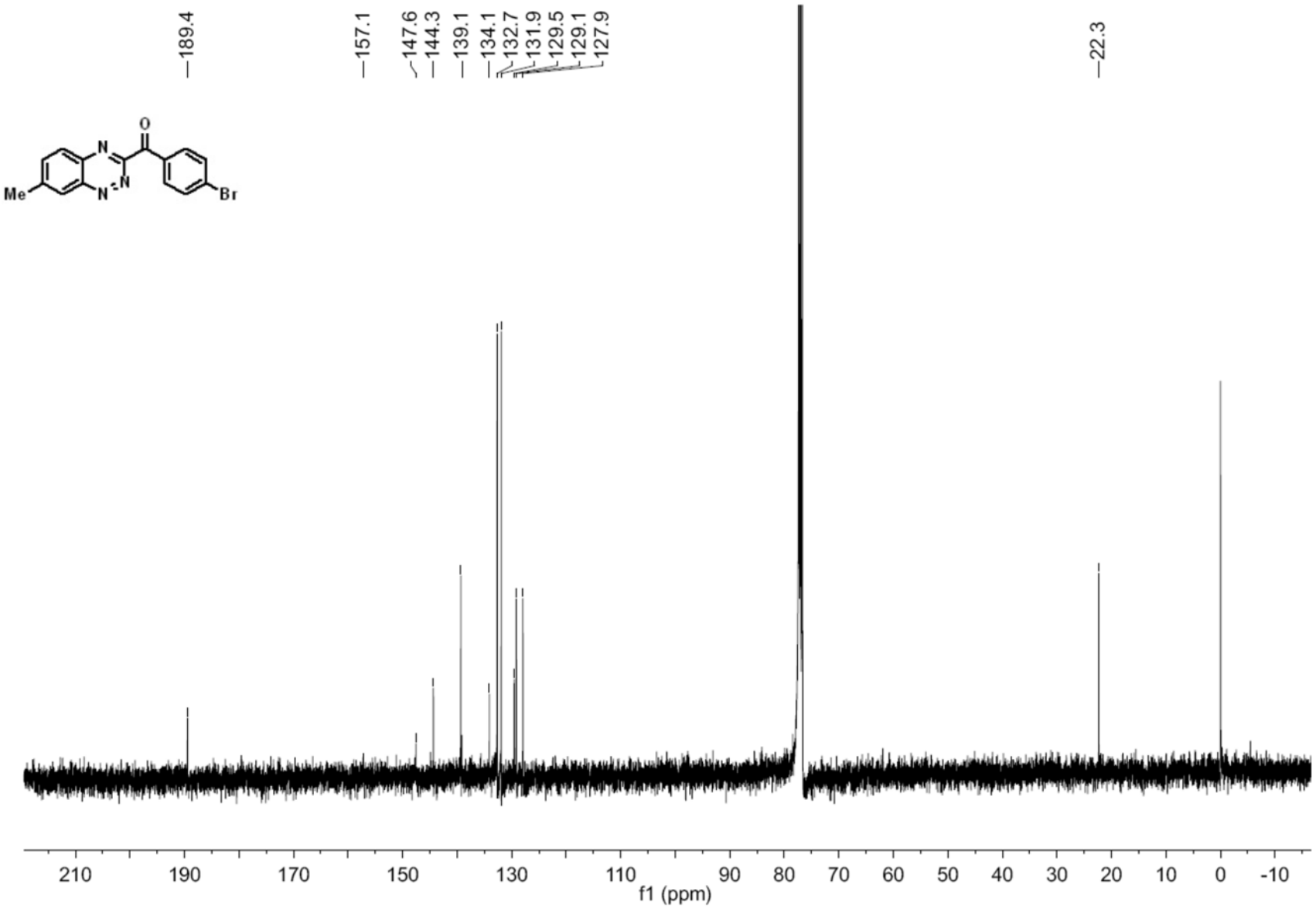
^{1}H NMR Spectrum of Compound **3f**



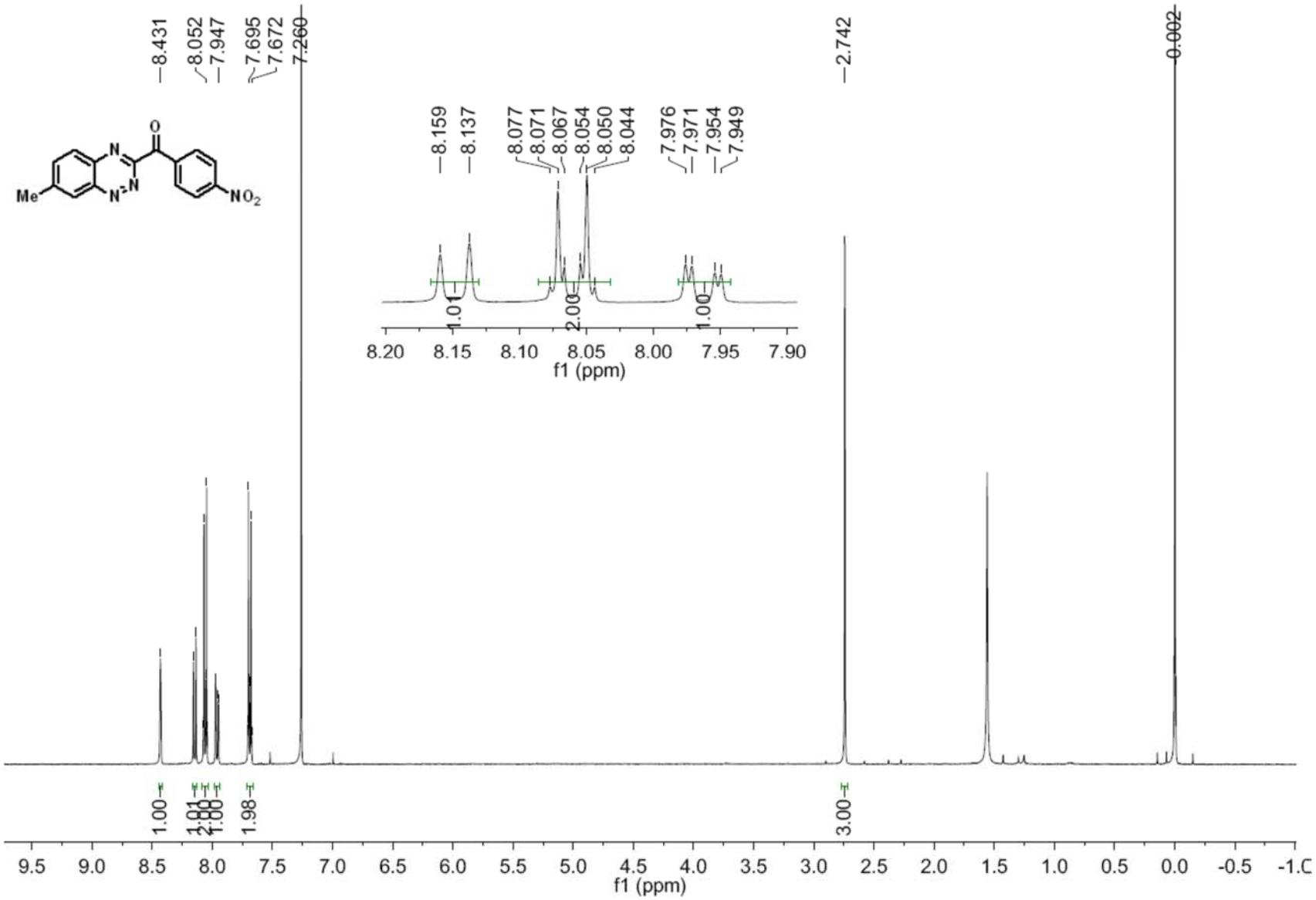
^{13}C NMR Spectrum of Compound **3f**



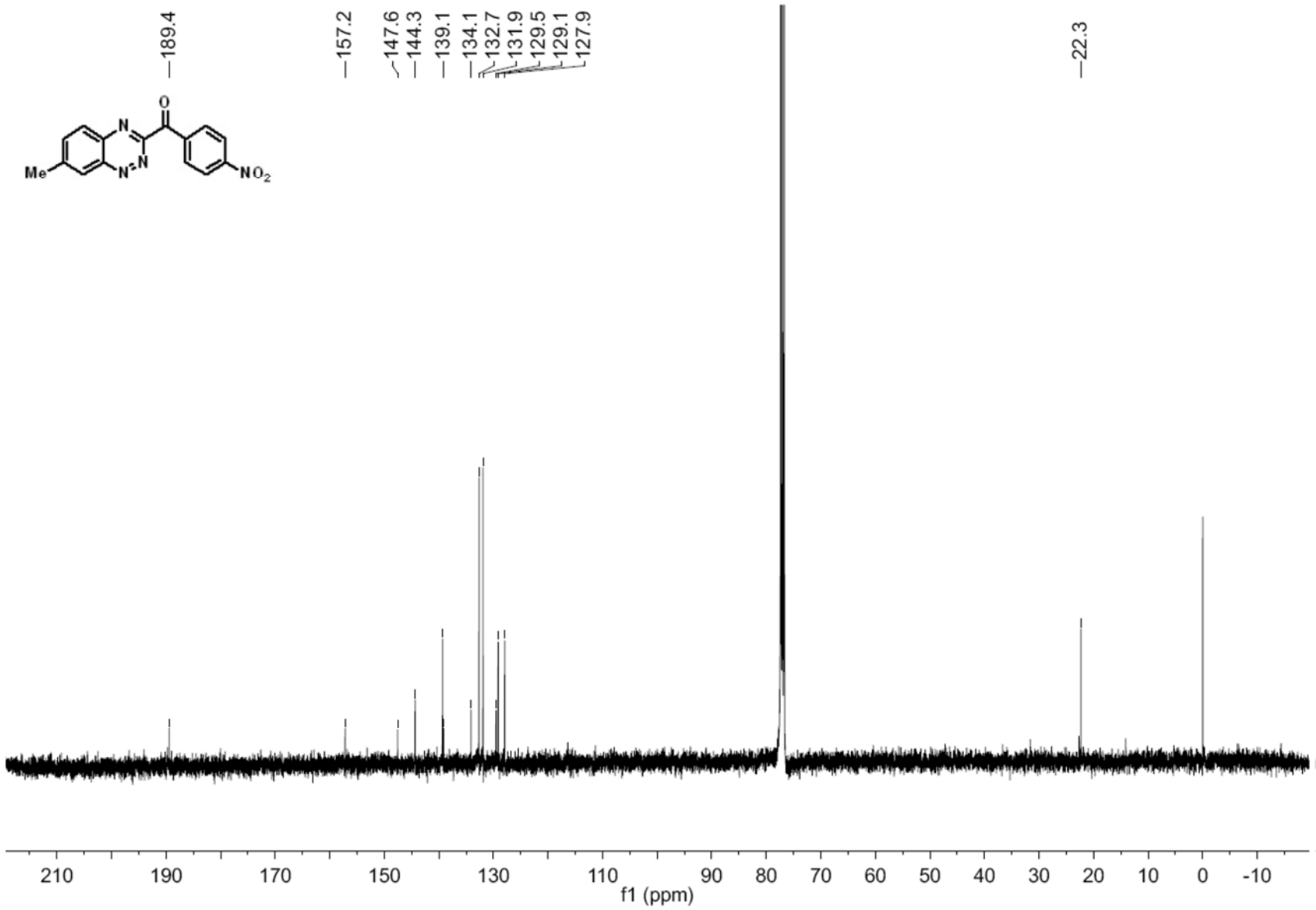
^{1}H NMR Spectrum of Compound **3g**



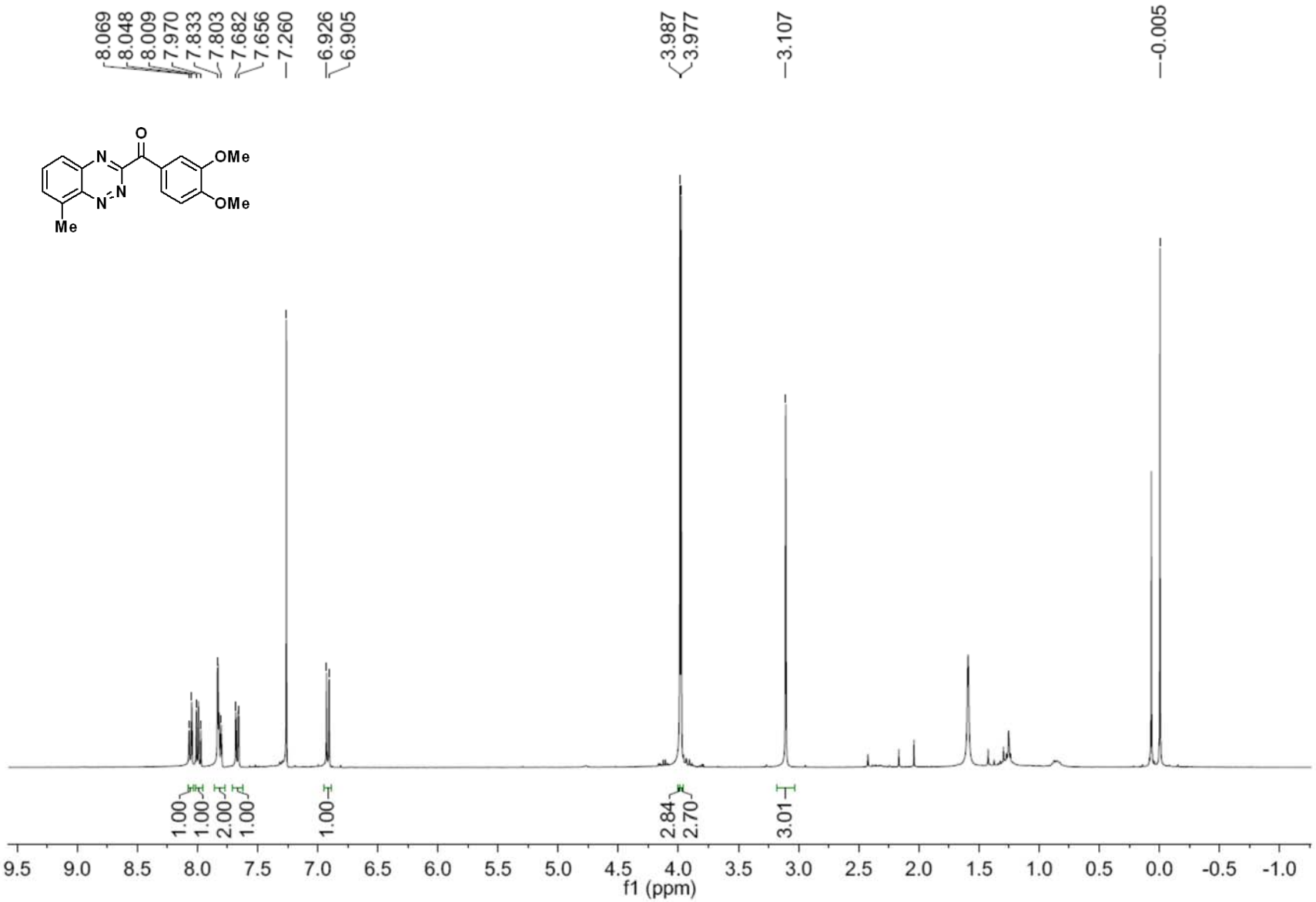
^{13}C NMR Spectrum of Compound **3g**



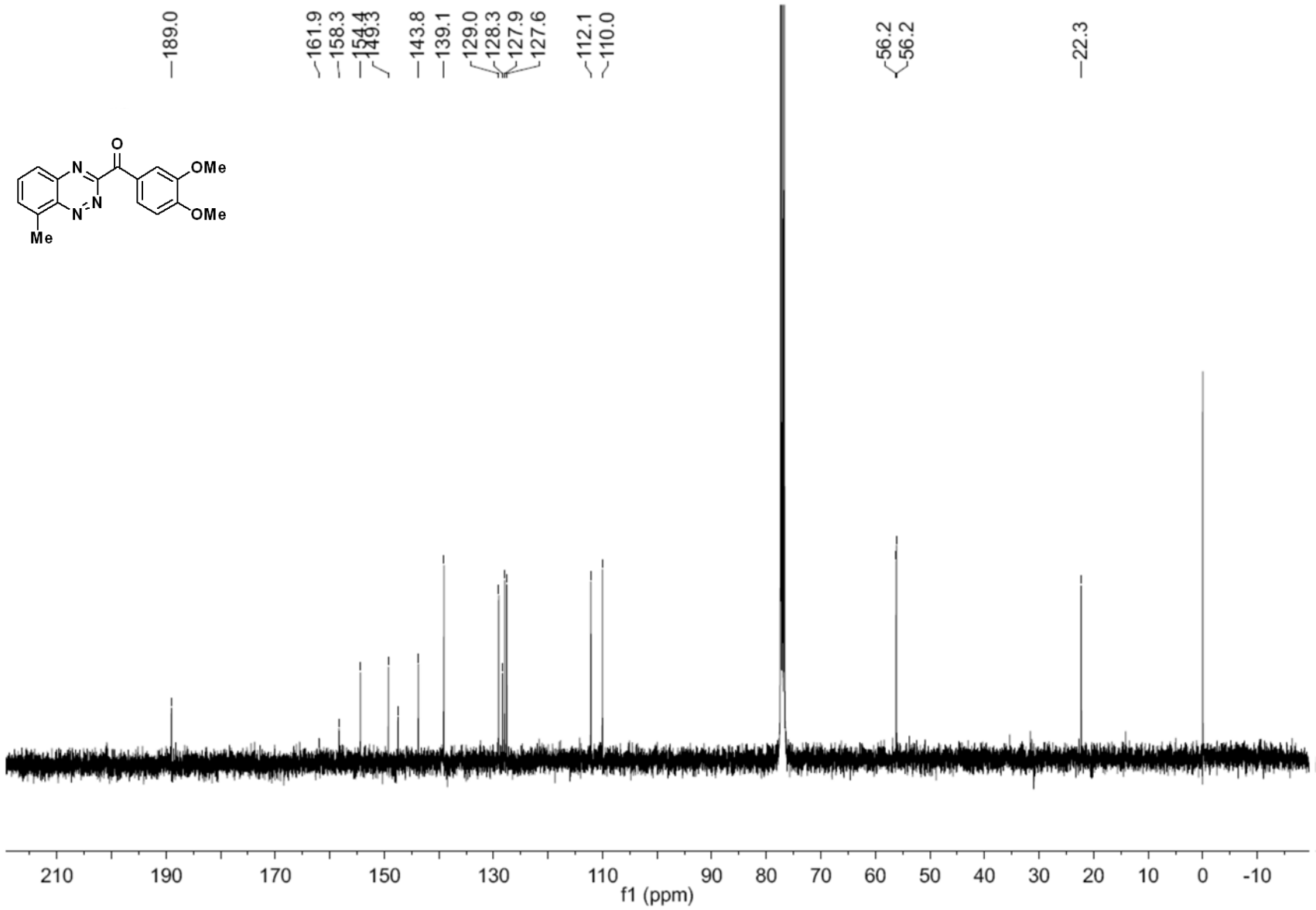
^{1}H NMR Spectrum of Compound **3h**



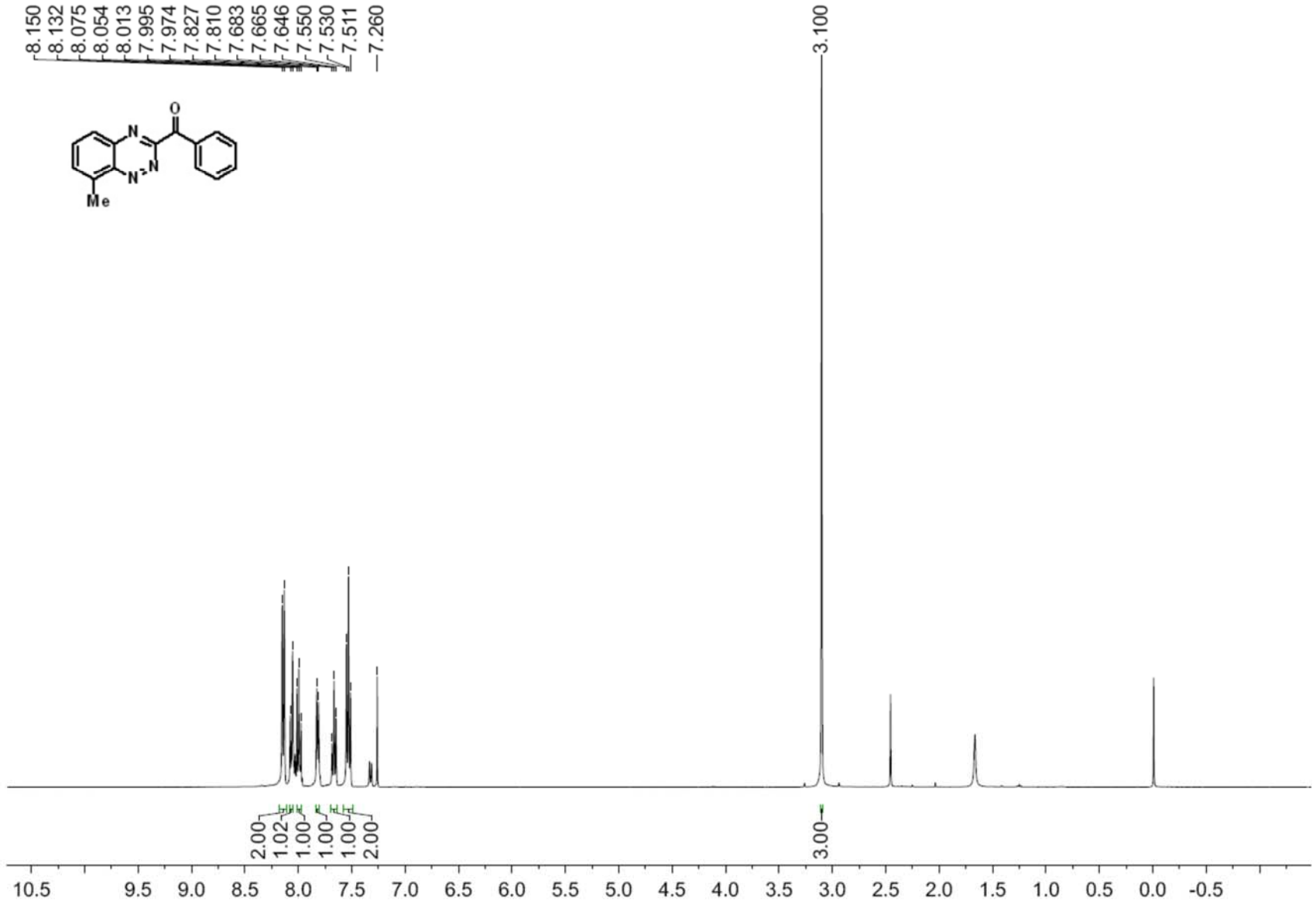
^{13}C NMR Spectrum of Compound **3h**



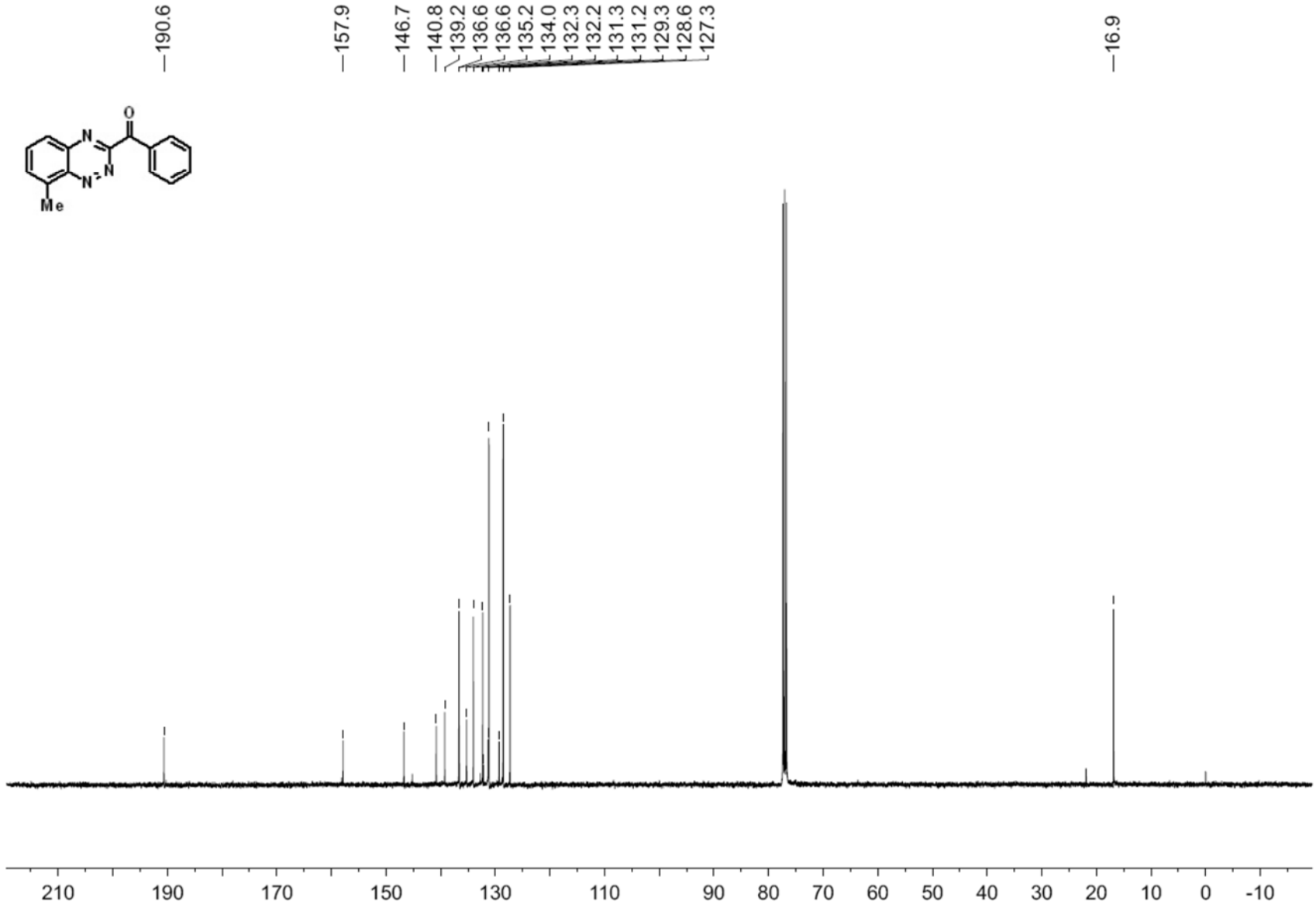
^{1}H NMR Spectrum of Compound **3i**



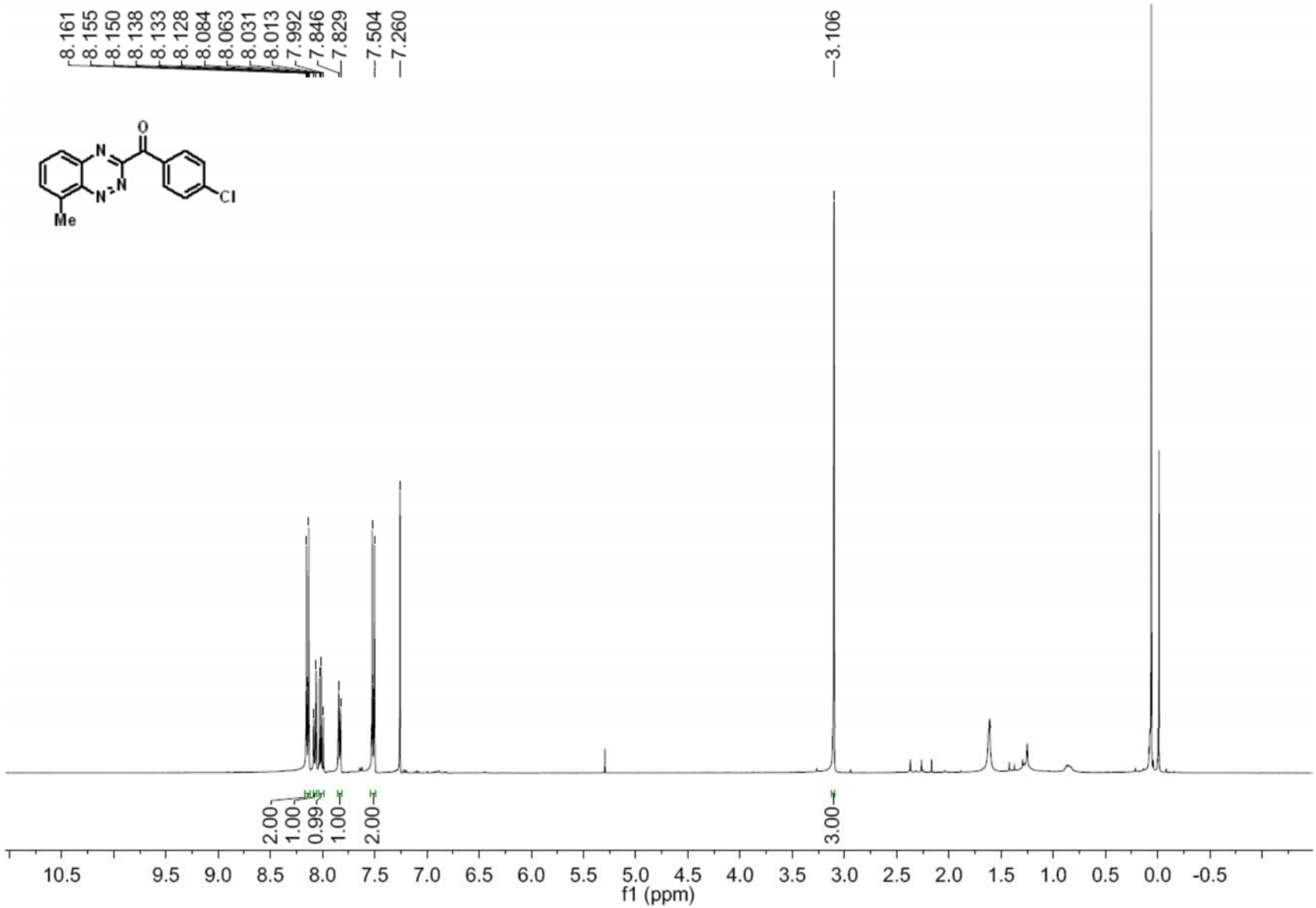
^{13}C NMR Spectrum of Compound **3i**



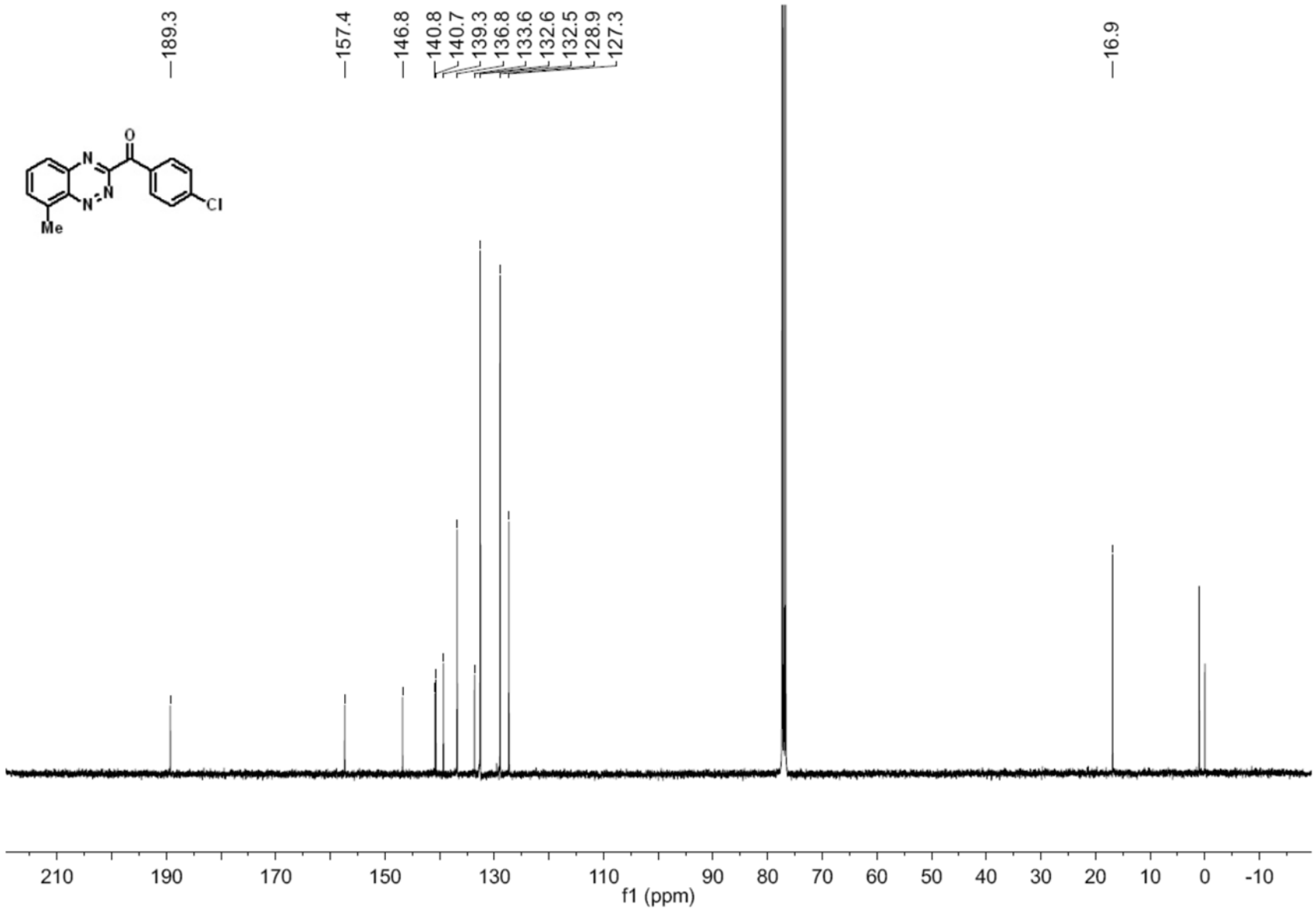
^{1}H NMR Spectrum of Compound **3j**



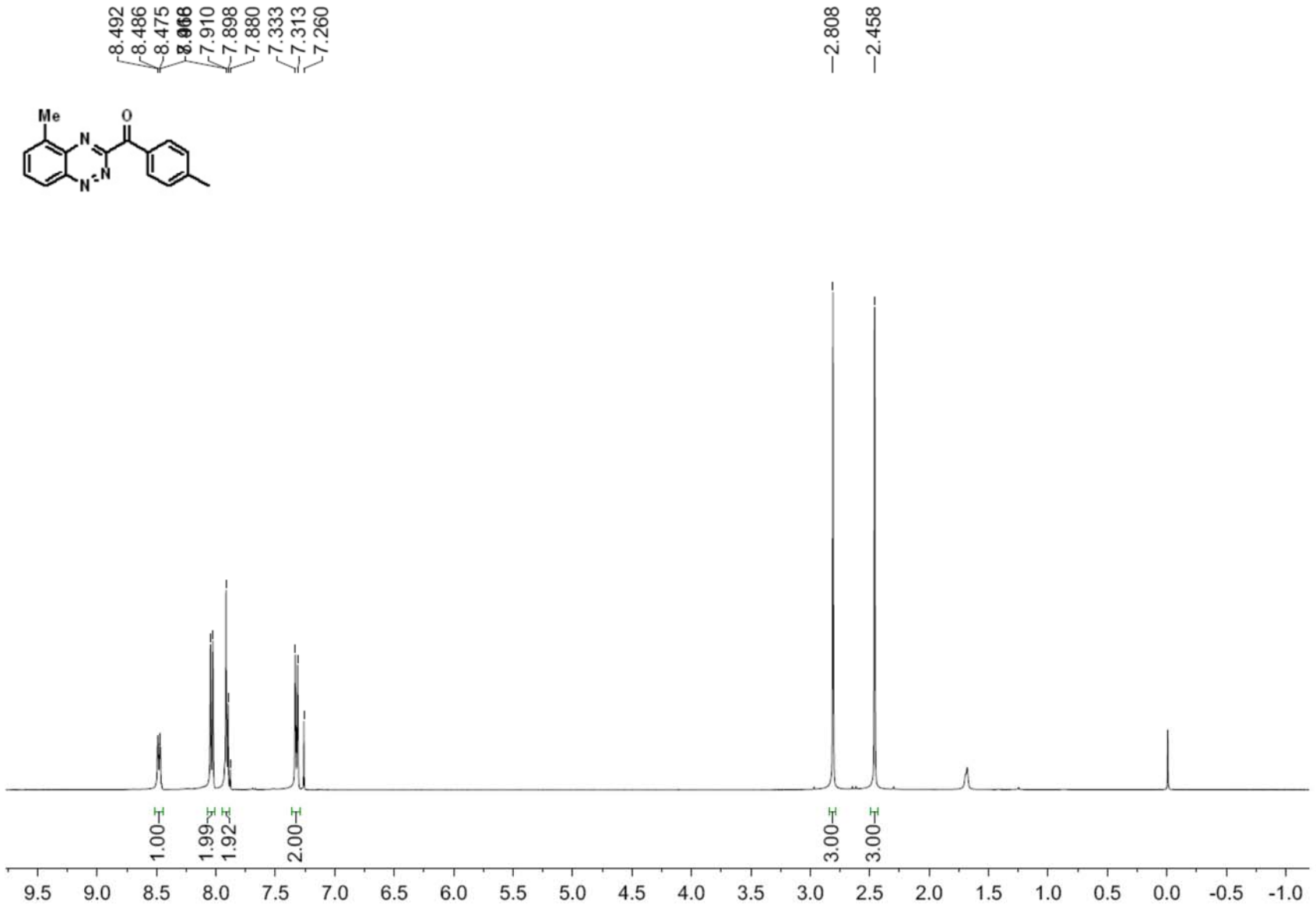
^{13}C NMR Spectrum of Compound **3j**



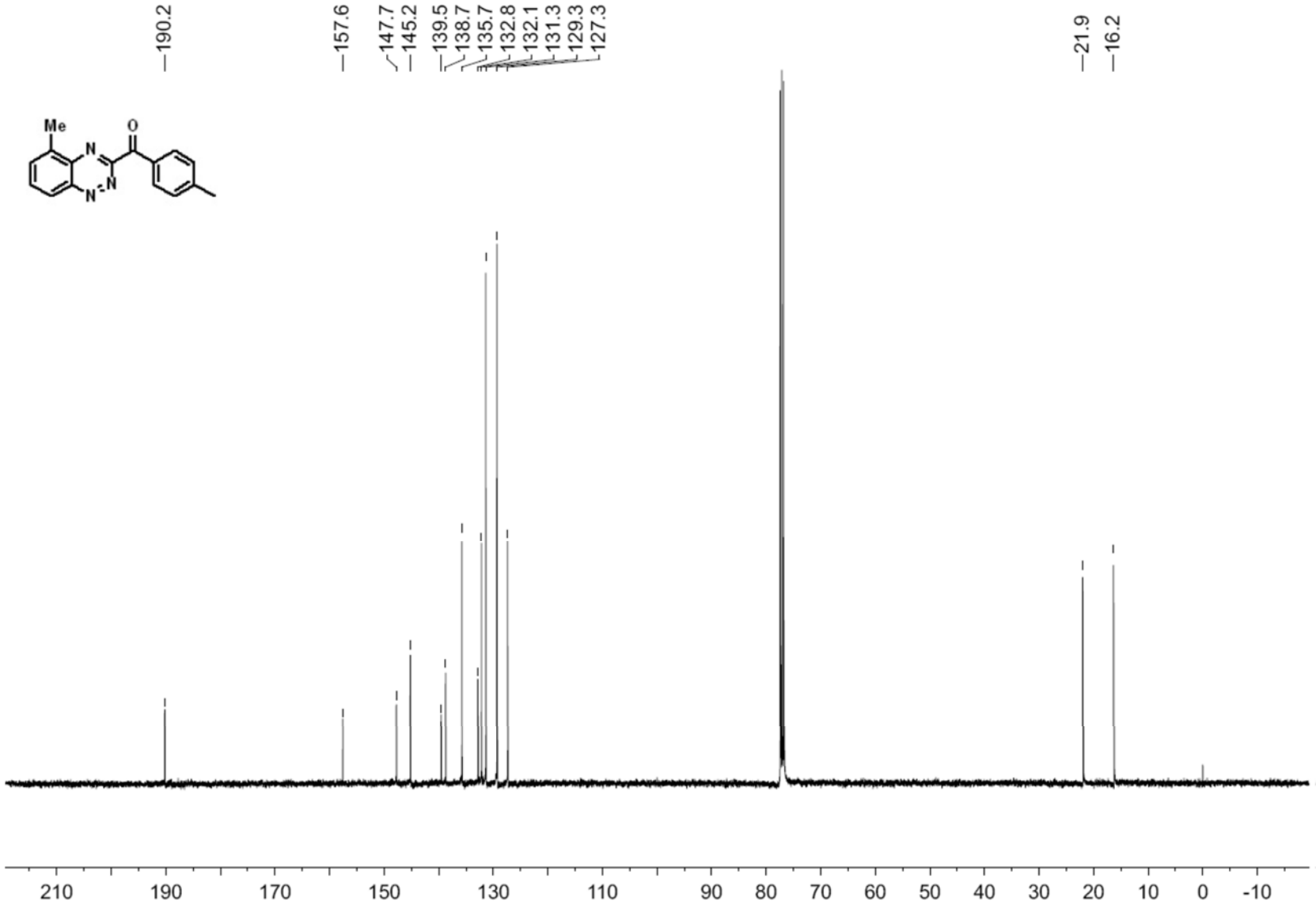
^{1}H NMR Spectrum of Compound **3k**



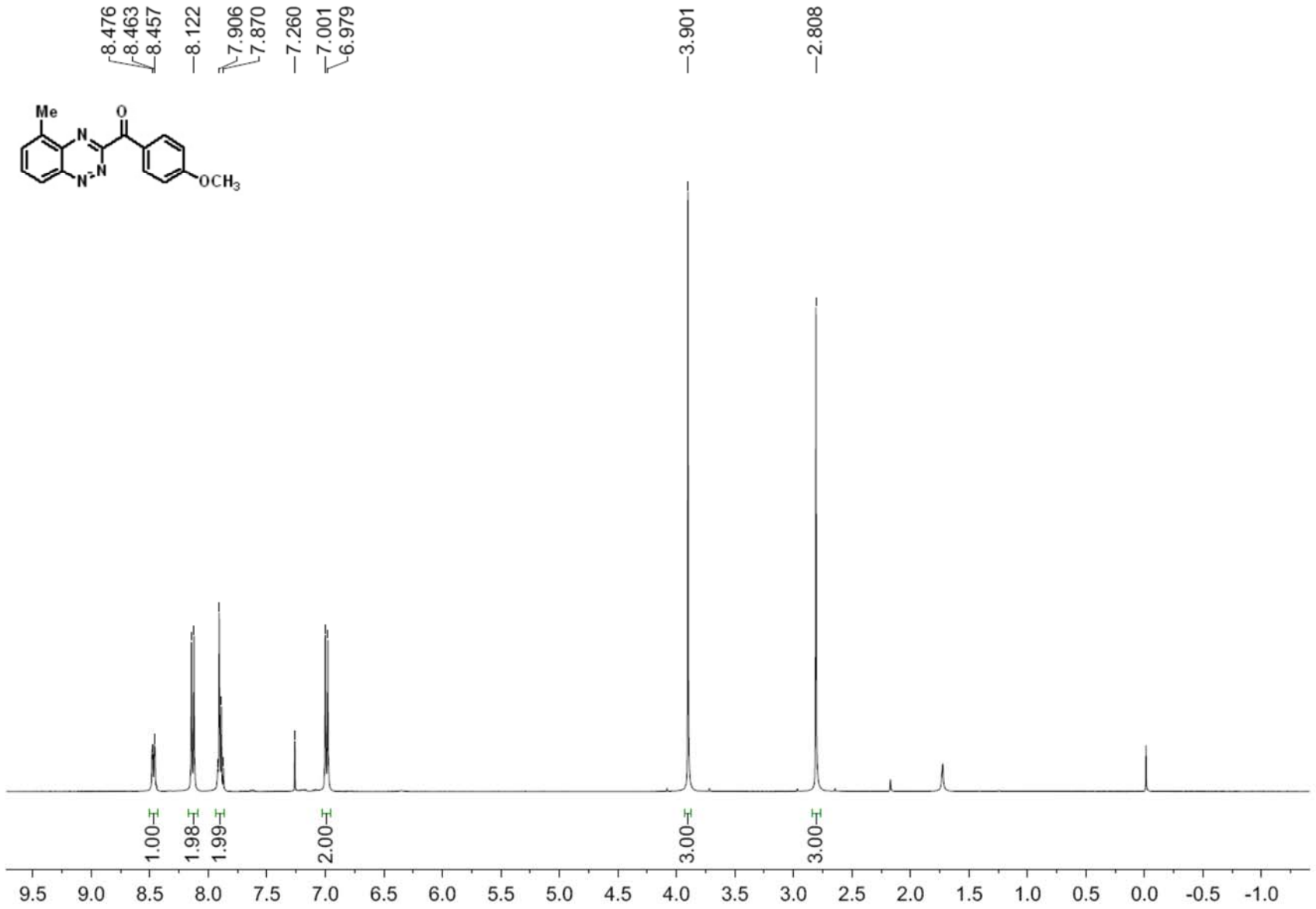
^{13}C NMR Spectrum of Compound **3k**



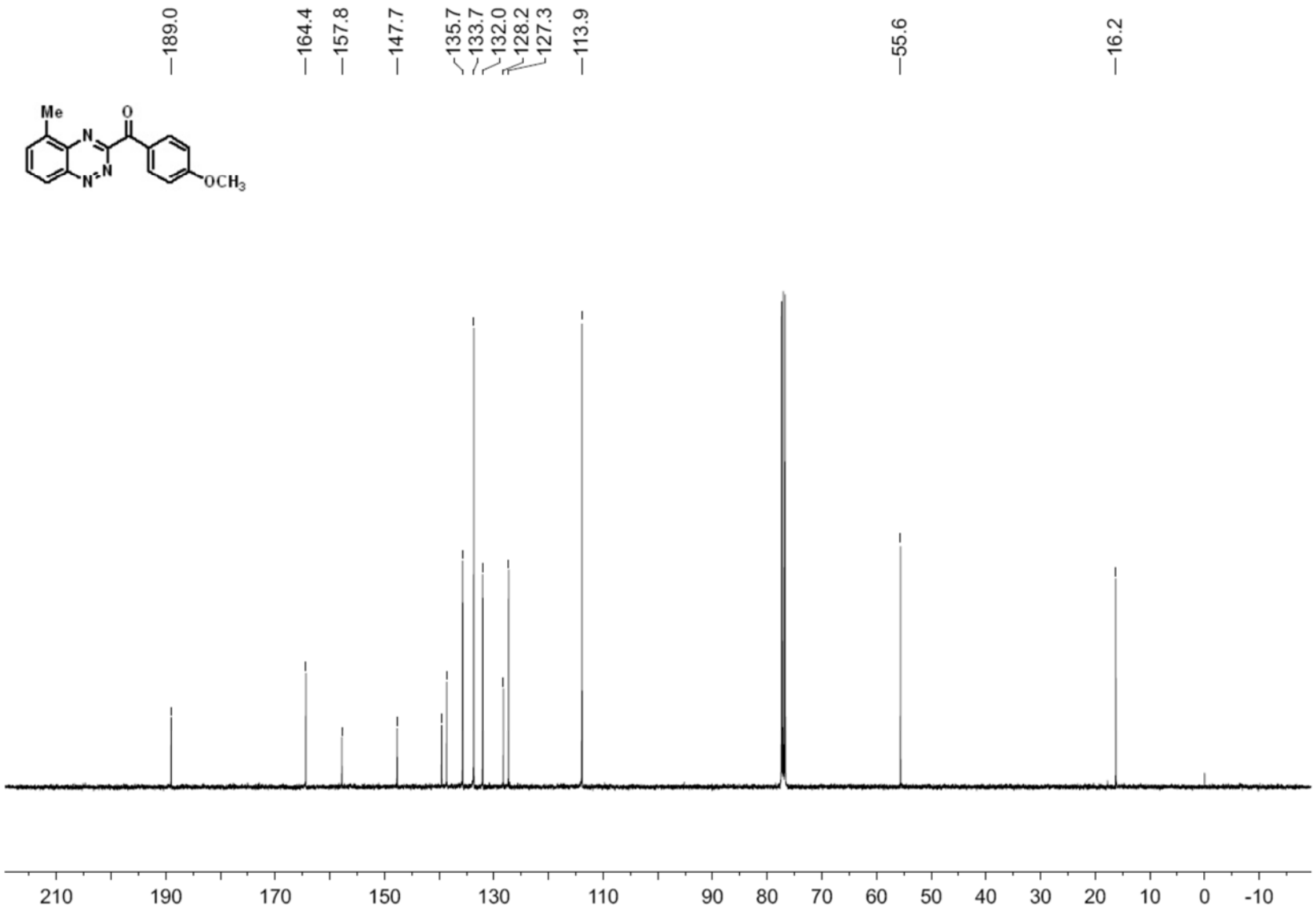
^{1}H NMR Spectrum of Compound **3l**



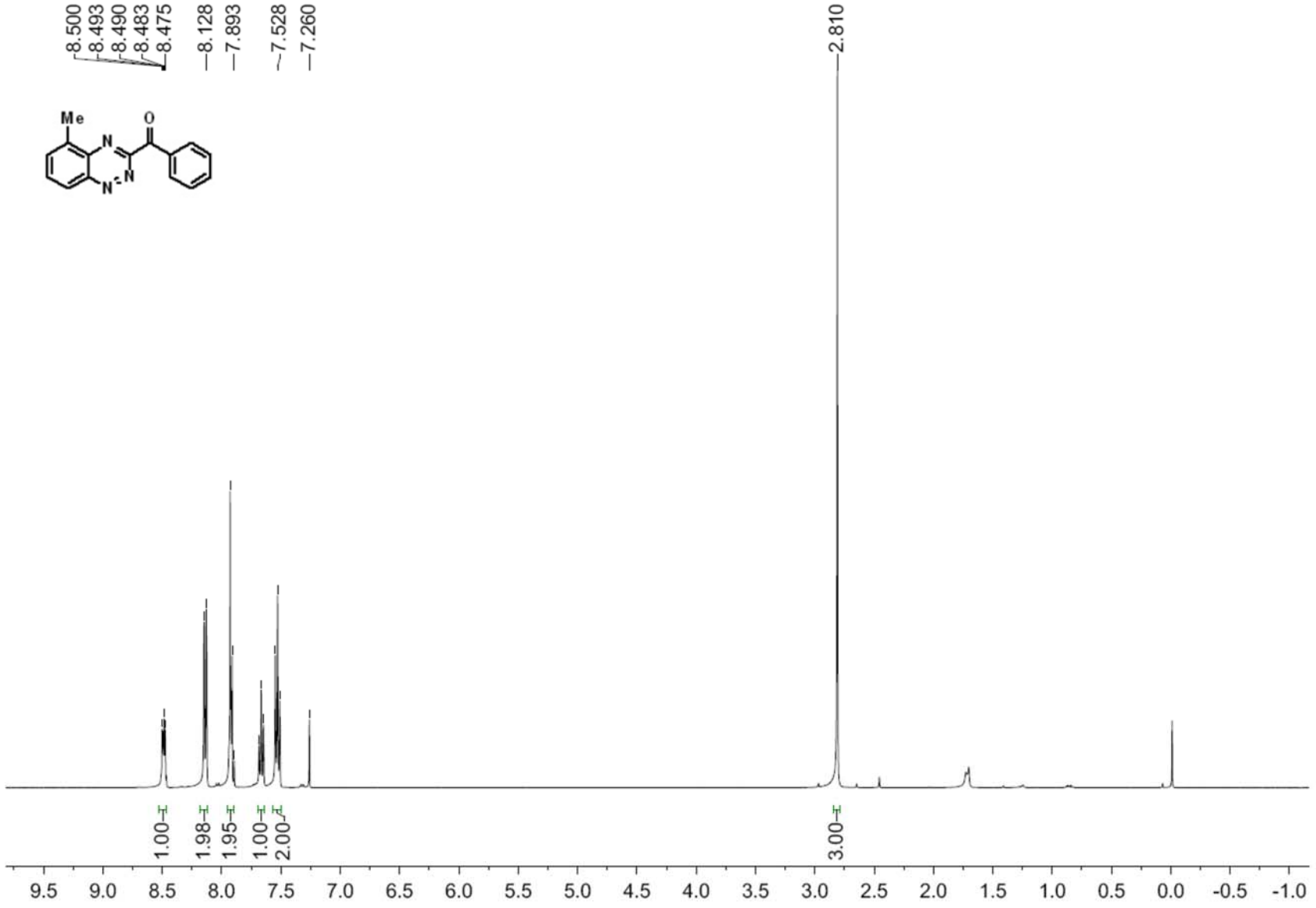
^{13}C NMR Spectrum of Compound **3l**



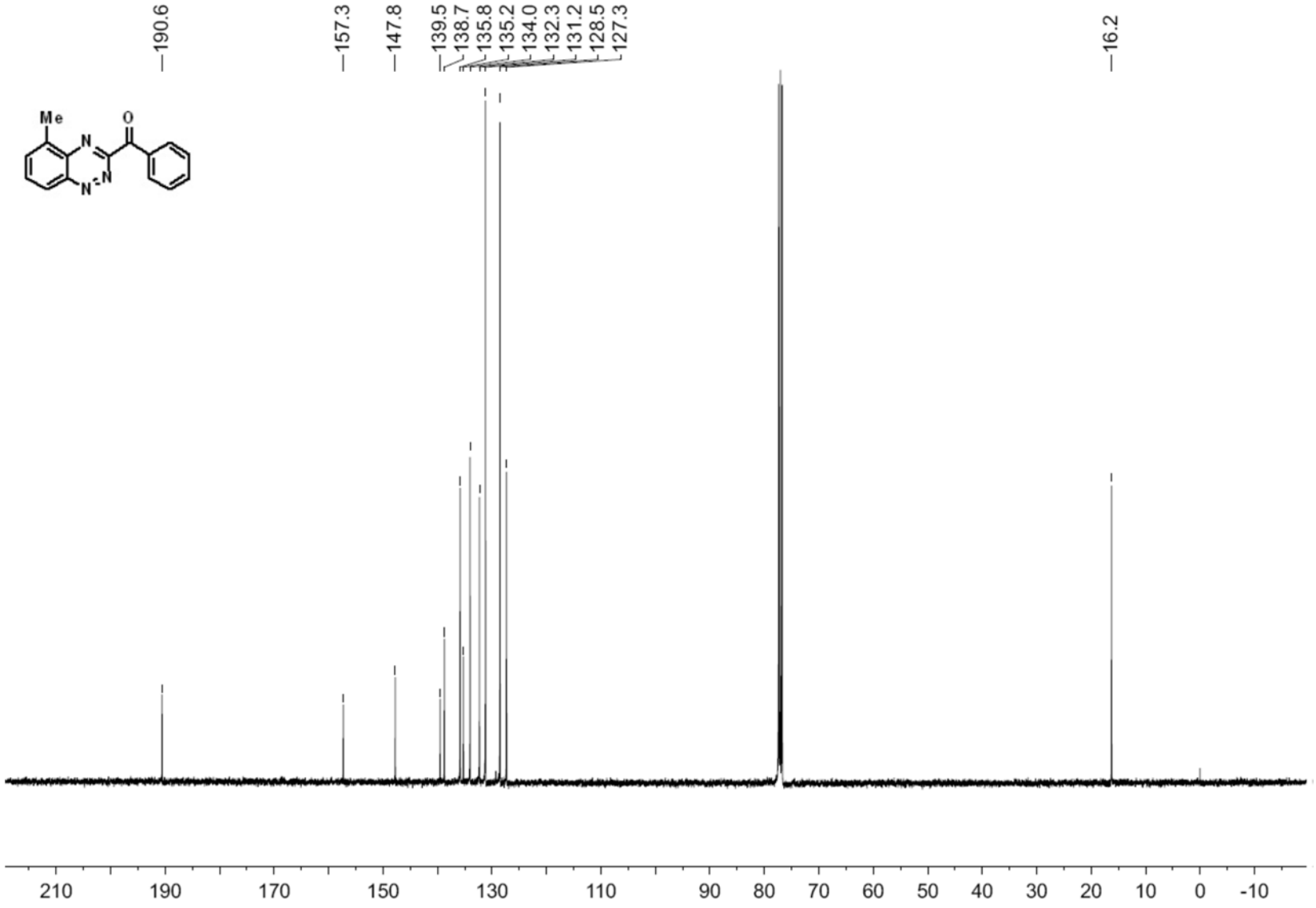
^{1}H NMR Spectrum of Compound **3m**



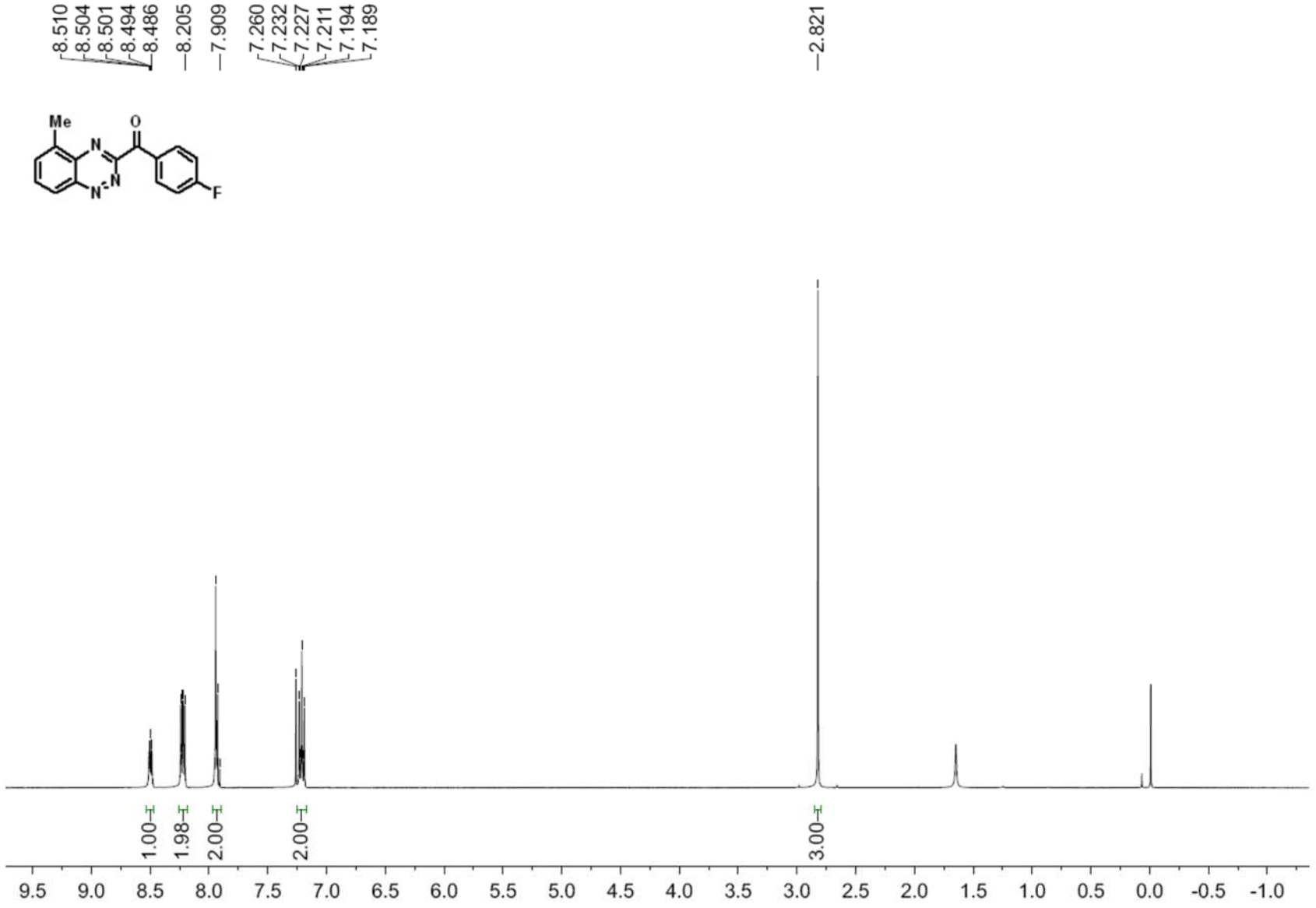
^{13}C NMR Spectrum of Compound **3m**



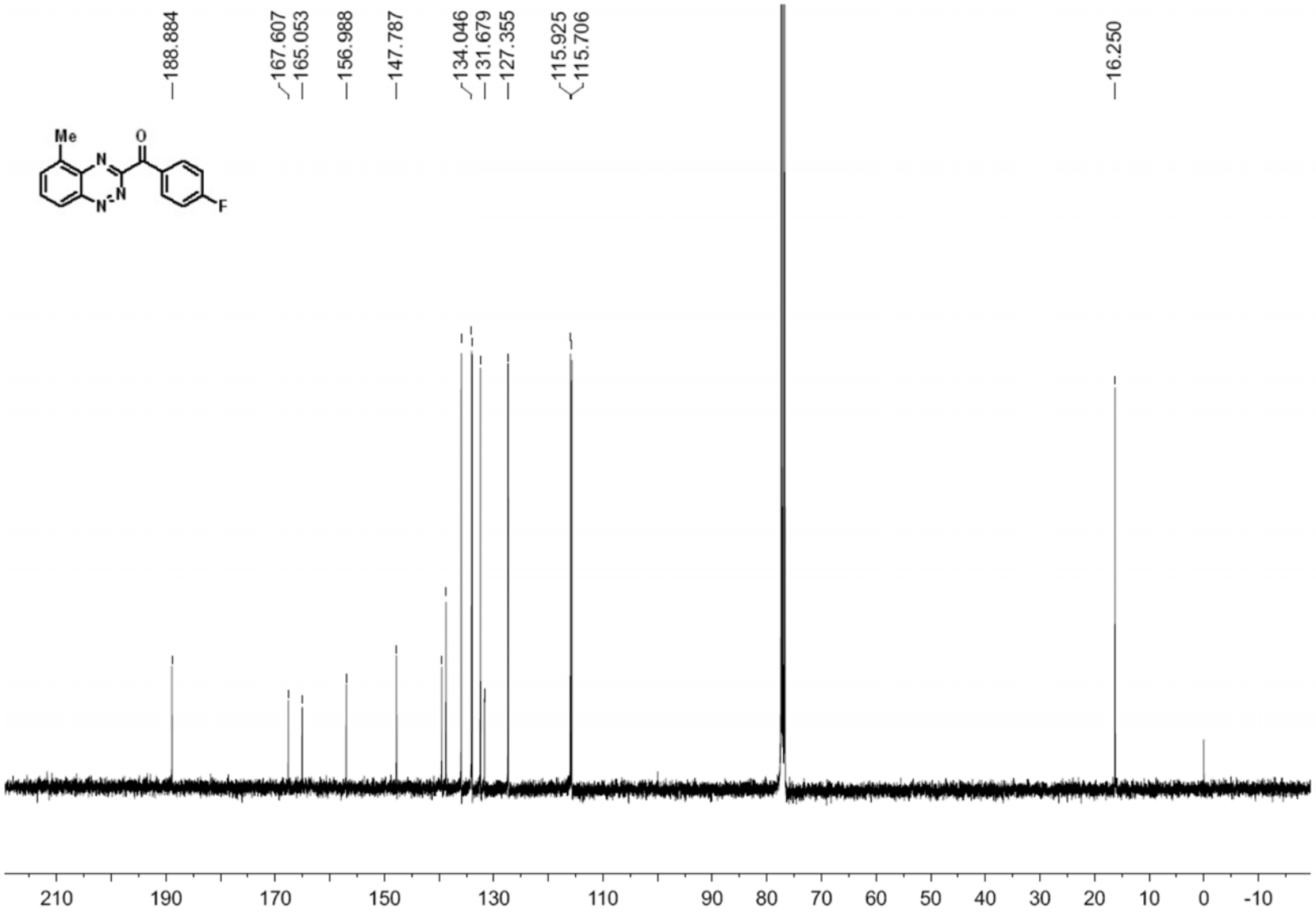
^{1}H NMR Spectrum of Compound **3n**



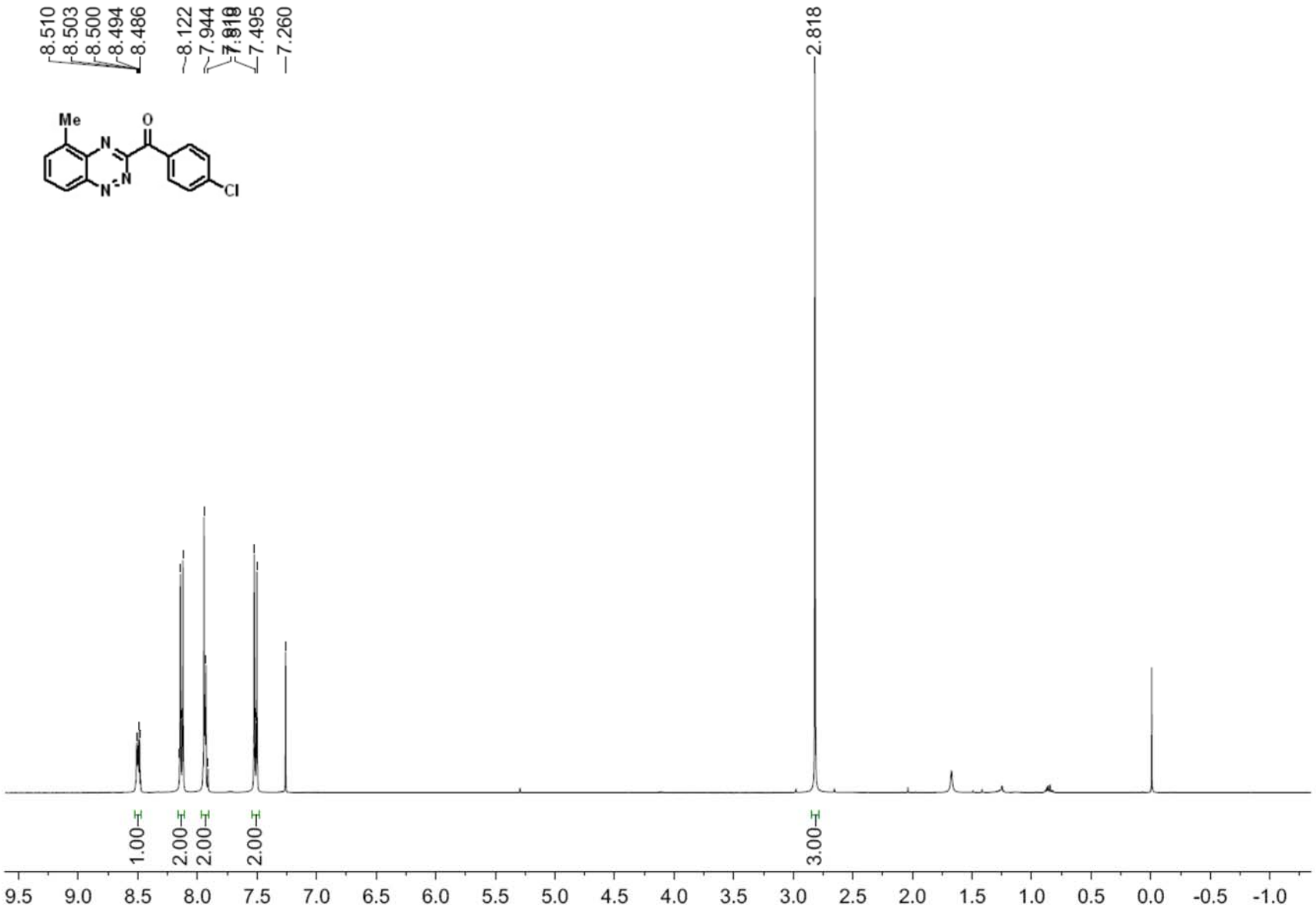
^{13}C NMR Spectrum of Compound **3n**



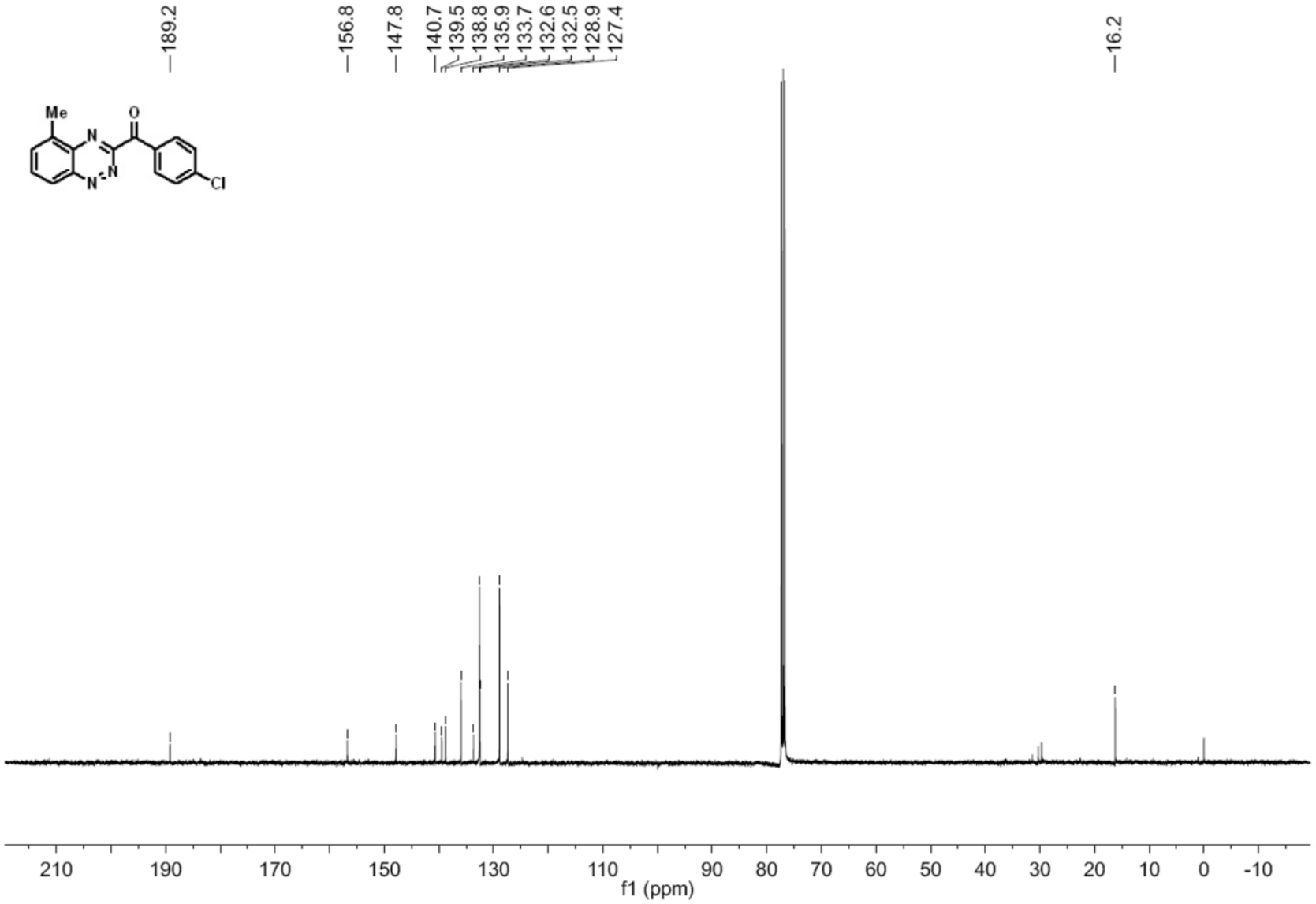
^{1}H NMR Spectrum of Compound **3o**



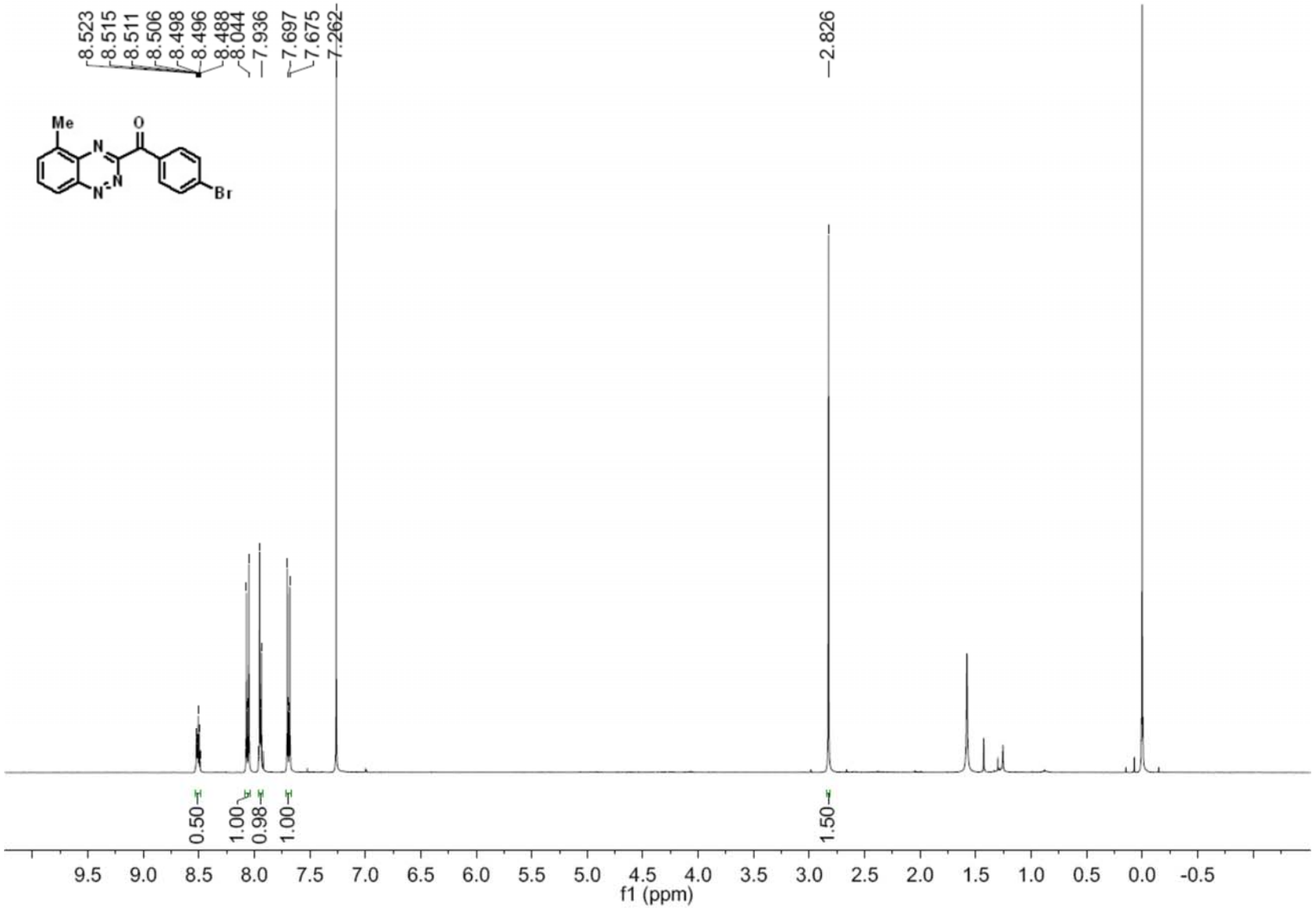
^{13}C NMR Spectrum of Compound **3o**



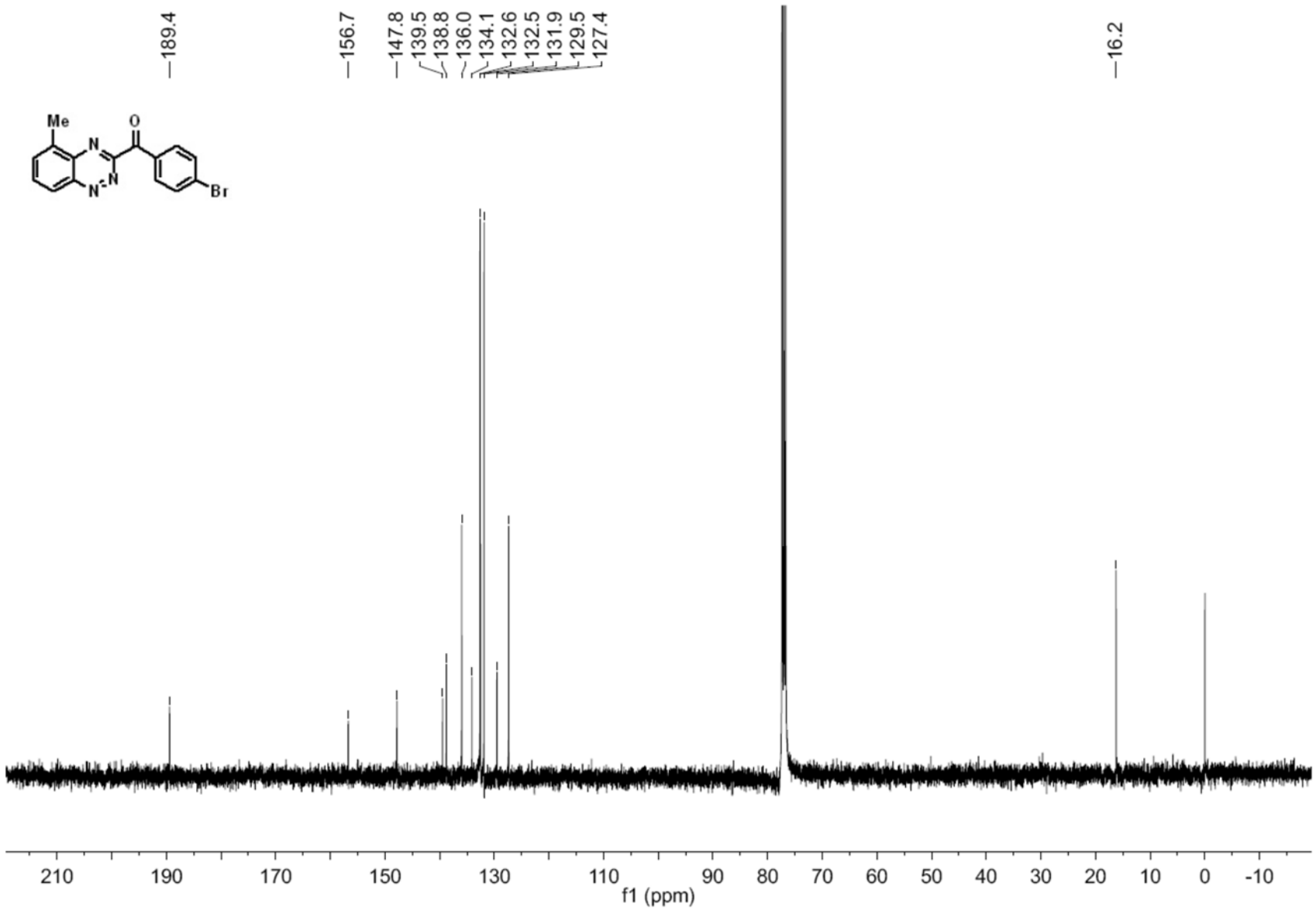
^{1}H NMR Spectrum of Compound **3p**



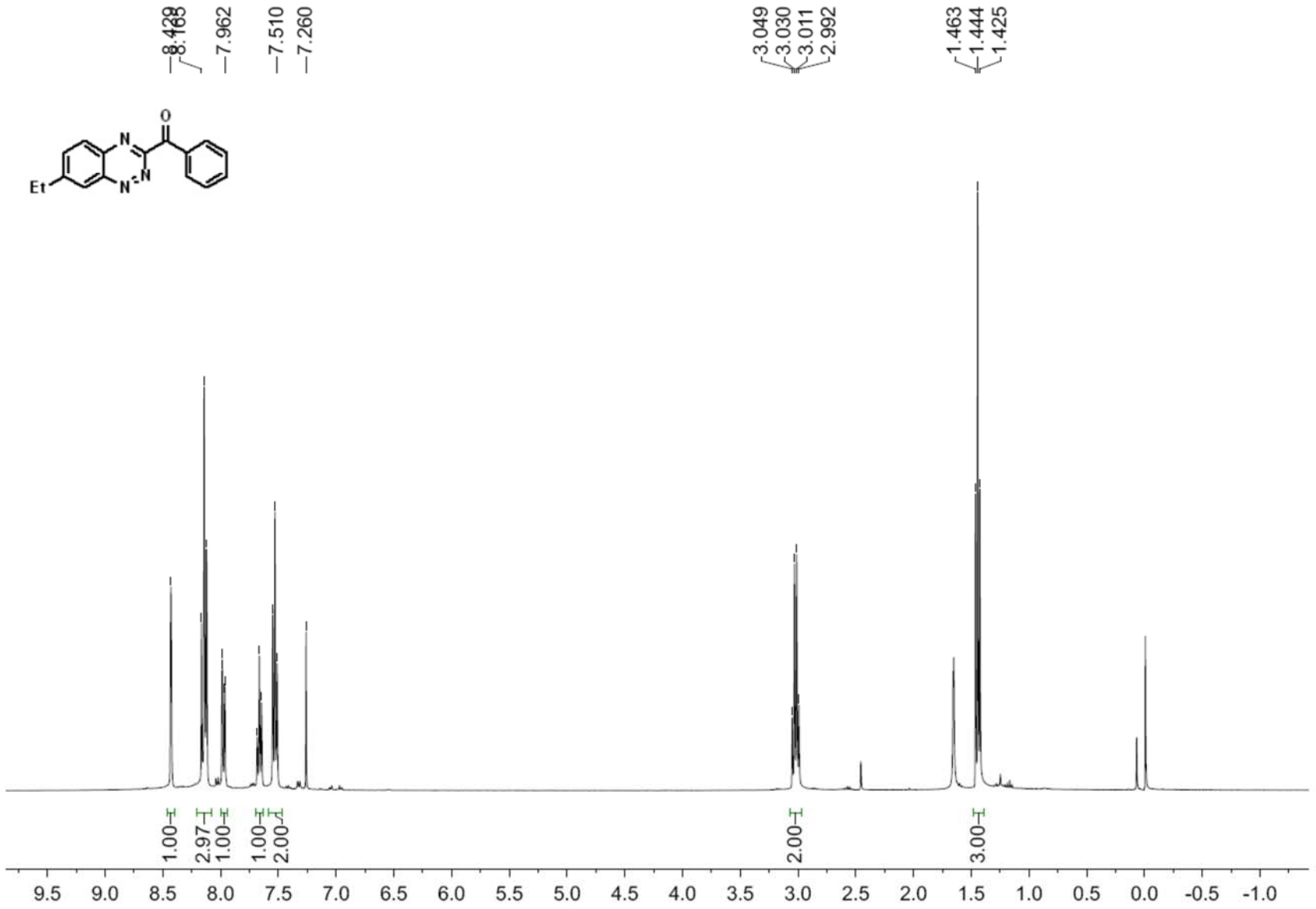
^{13}C NMR Spectrum of Compound **3p**



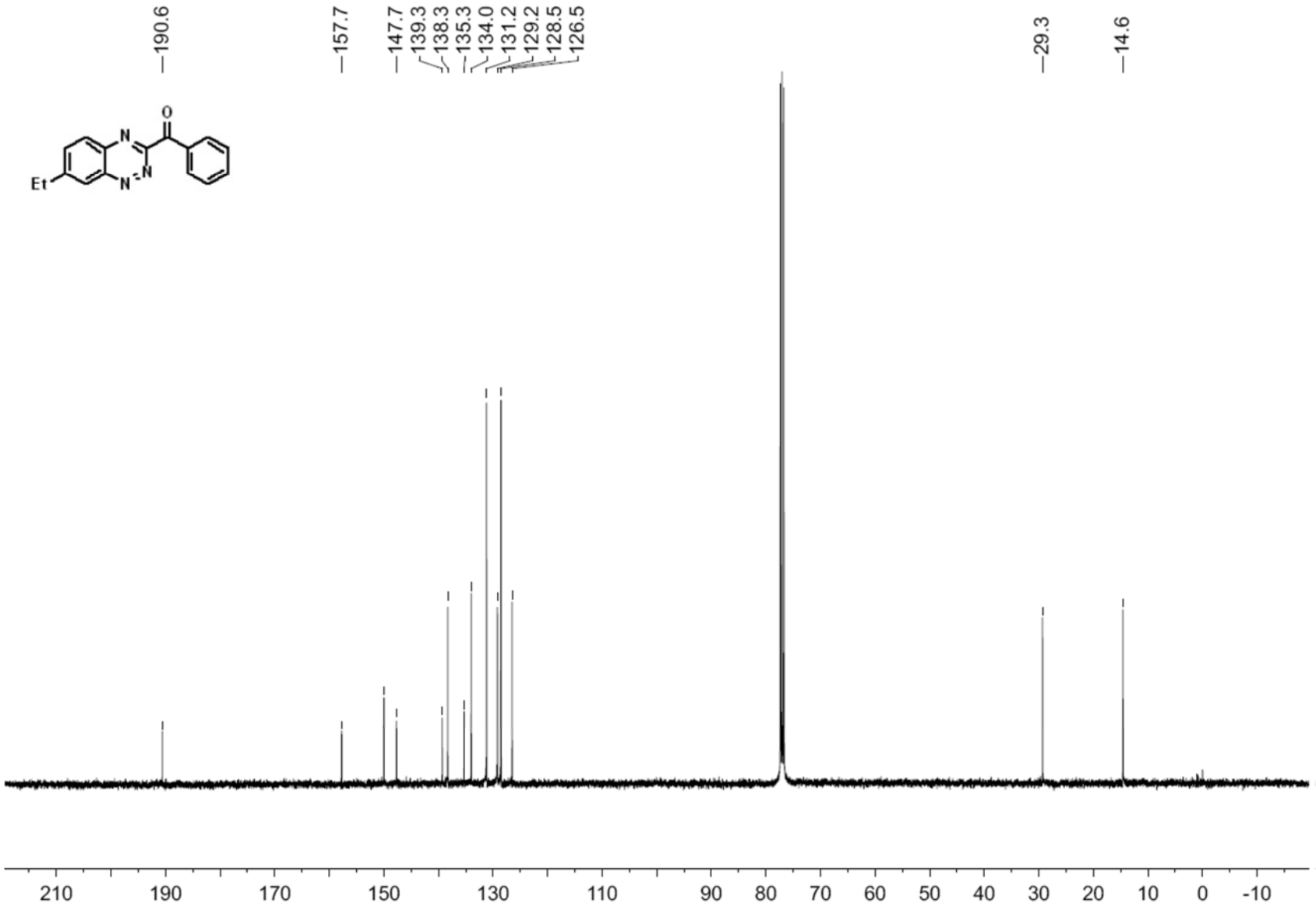
^{1}H NMR Spectrum of Compound **3q**



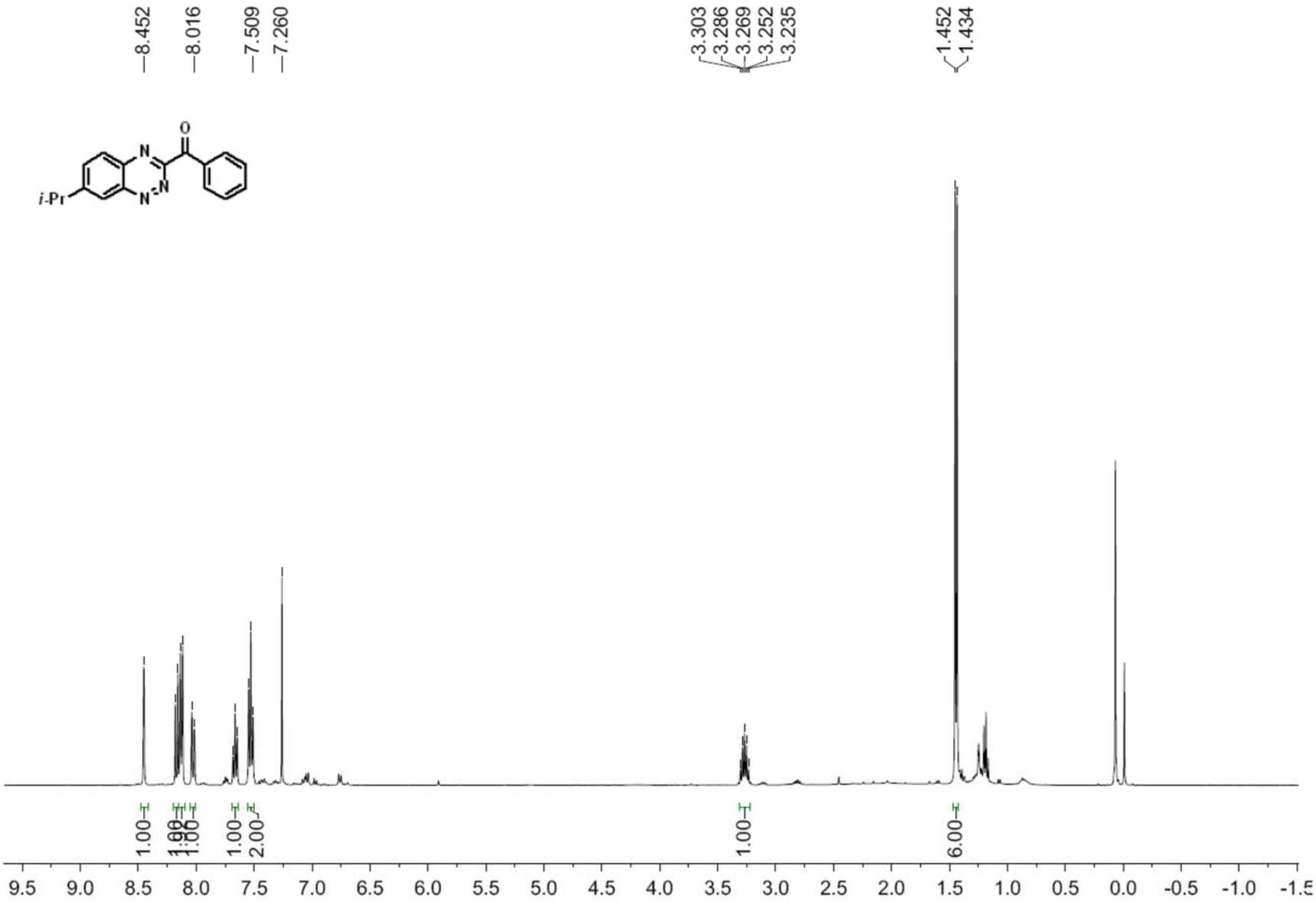
^{13}C NMR Spectrum of Compound **3q**



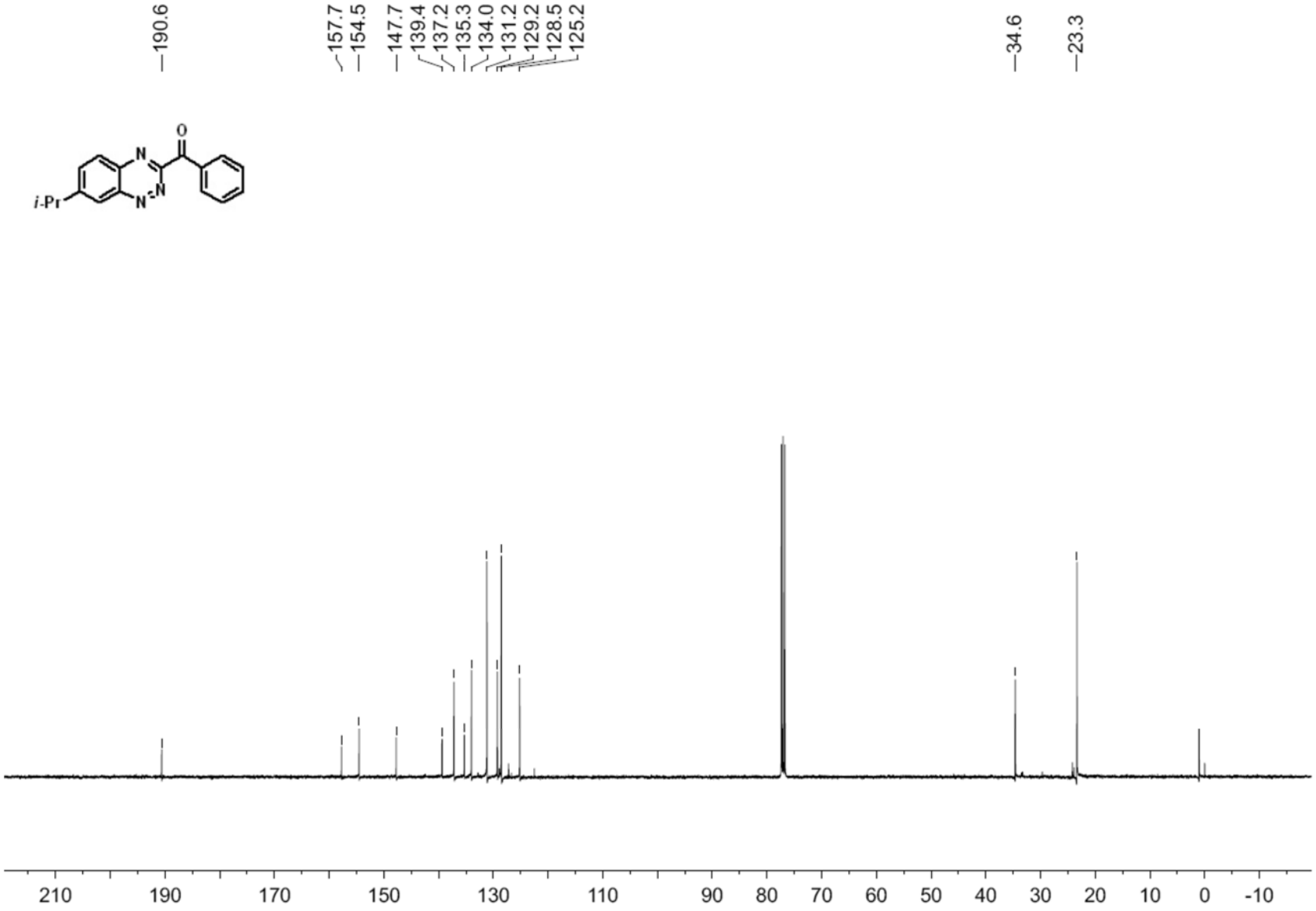
^{1}H NMR Spectrum of Compound **3r**



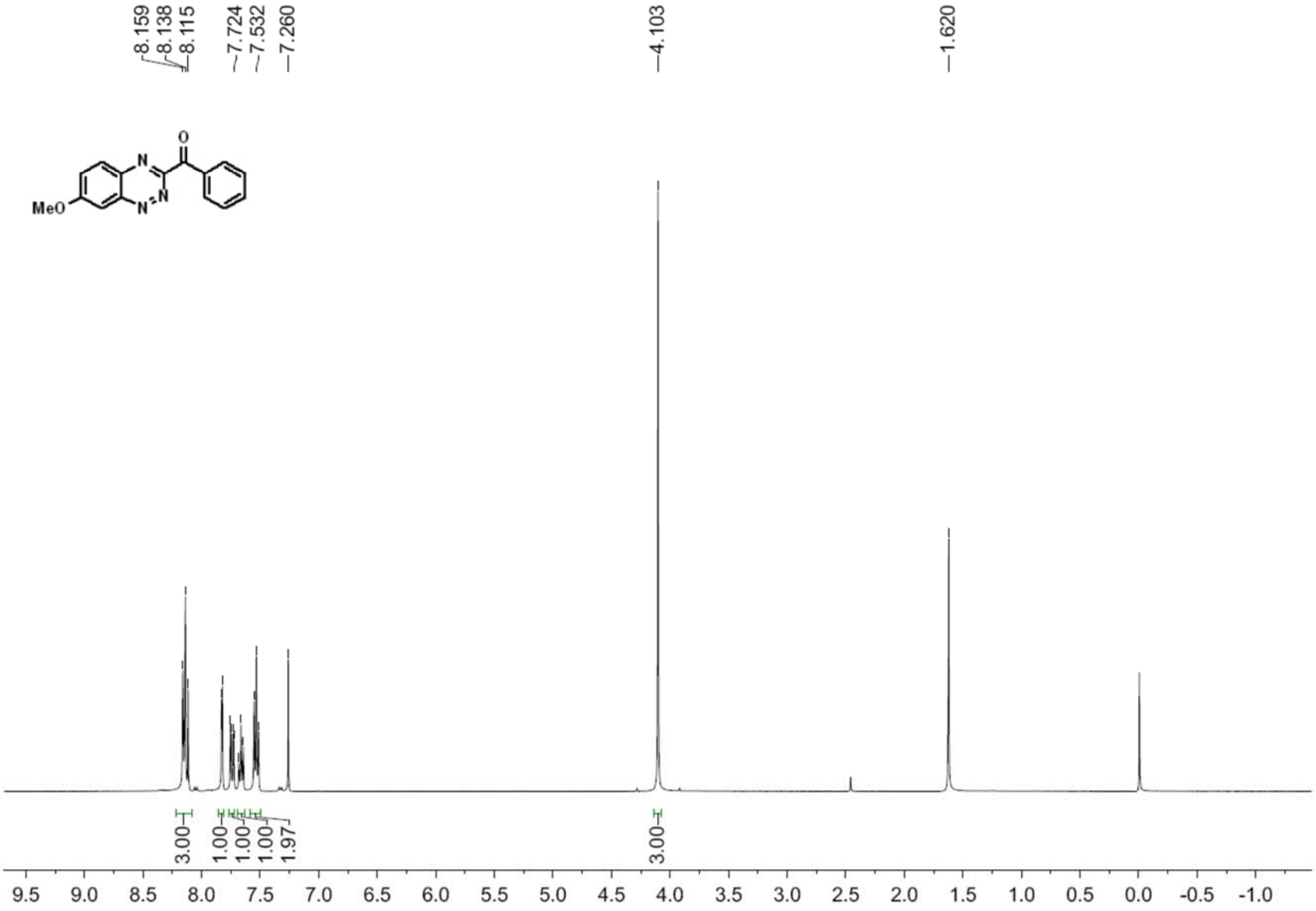
^{13}C NMR Spectrum of Compound **3r**



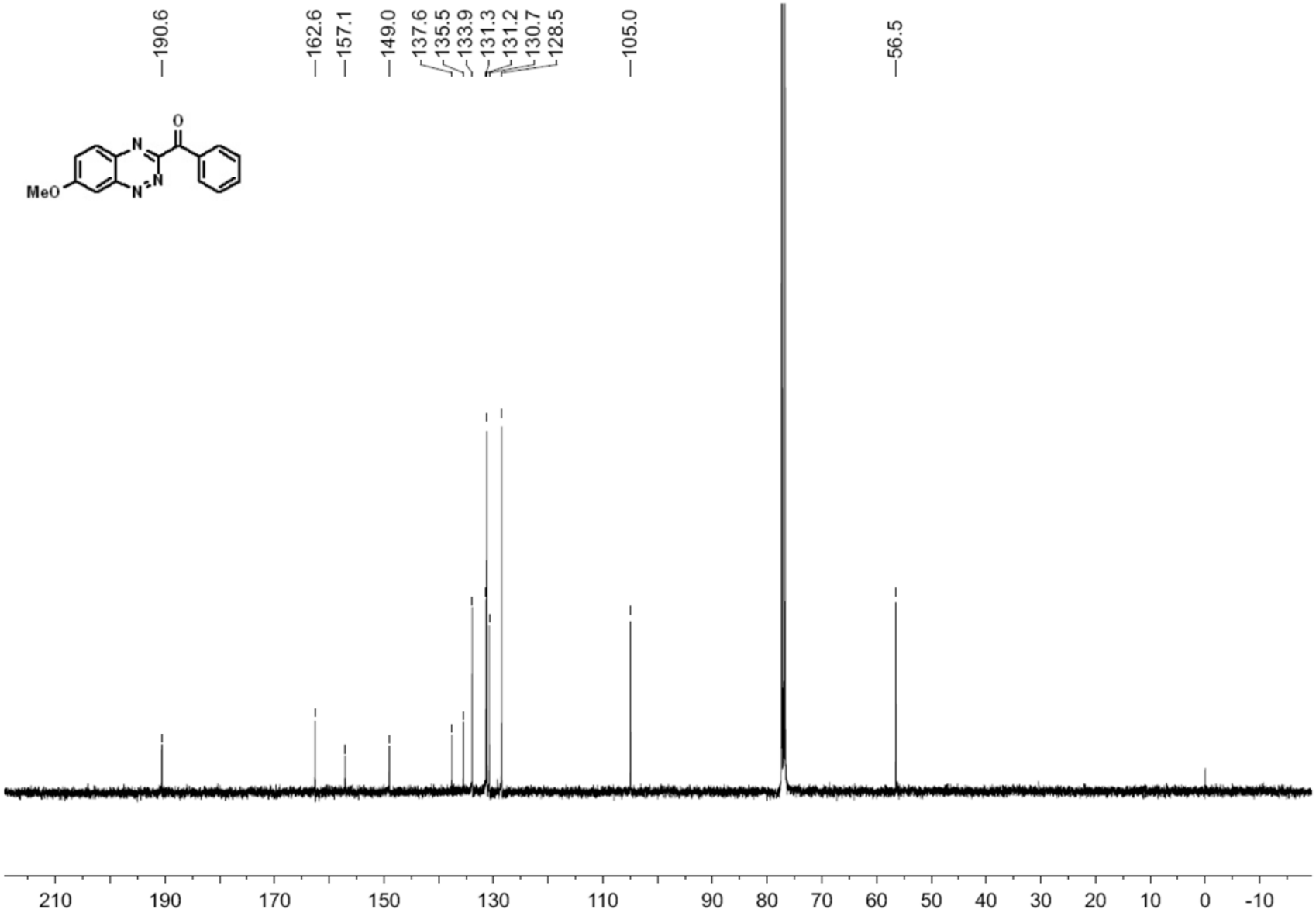
^{1}H NMR Spectrum of Compound **3s**



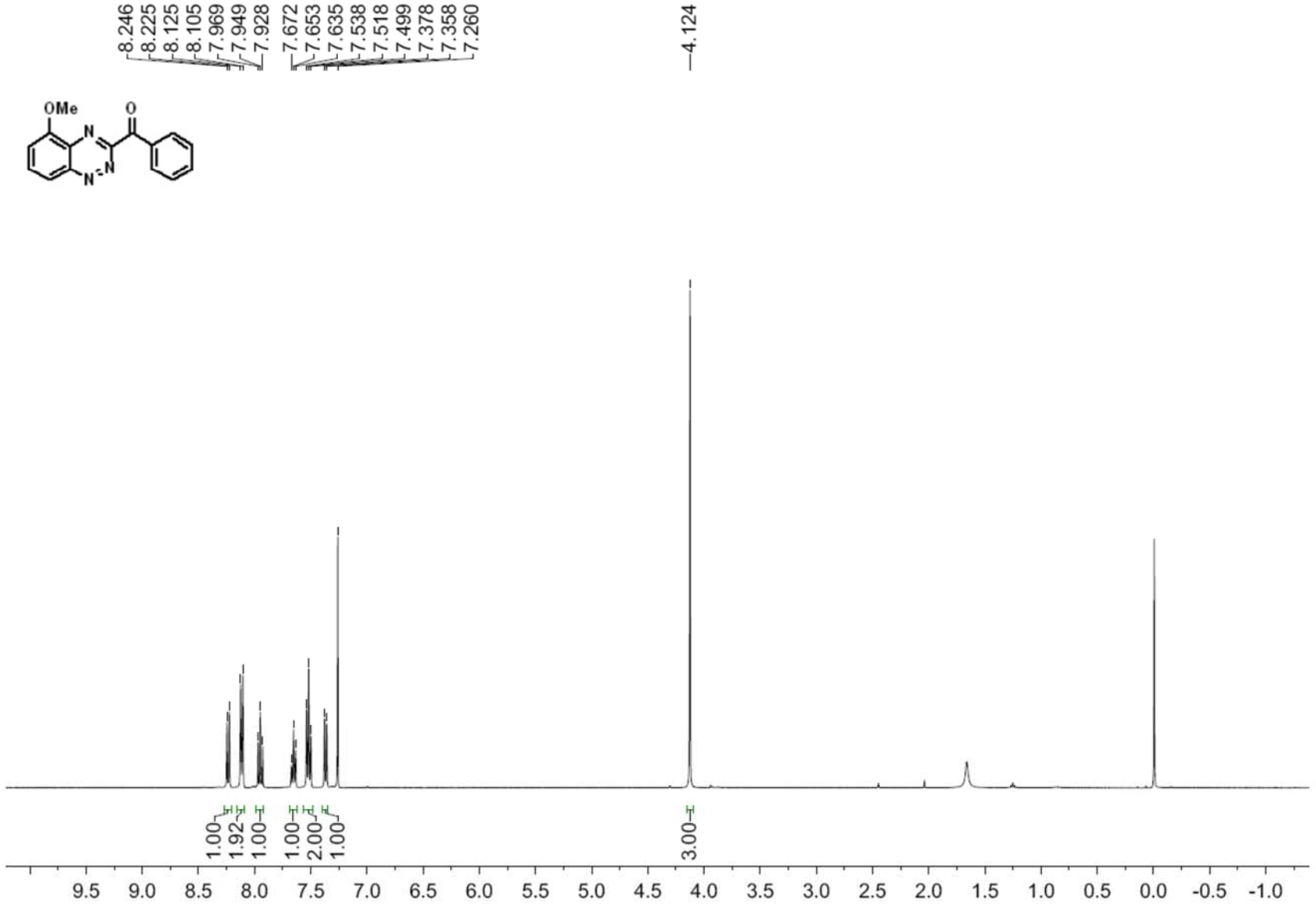
^{13}C NMR Spectrum of Compound **3s**



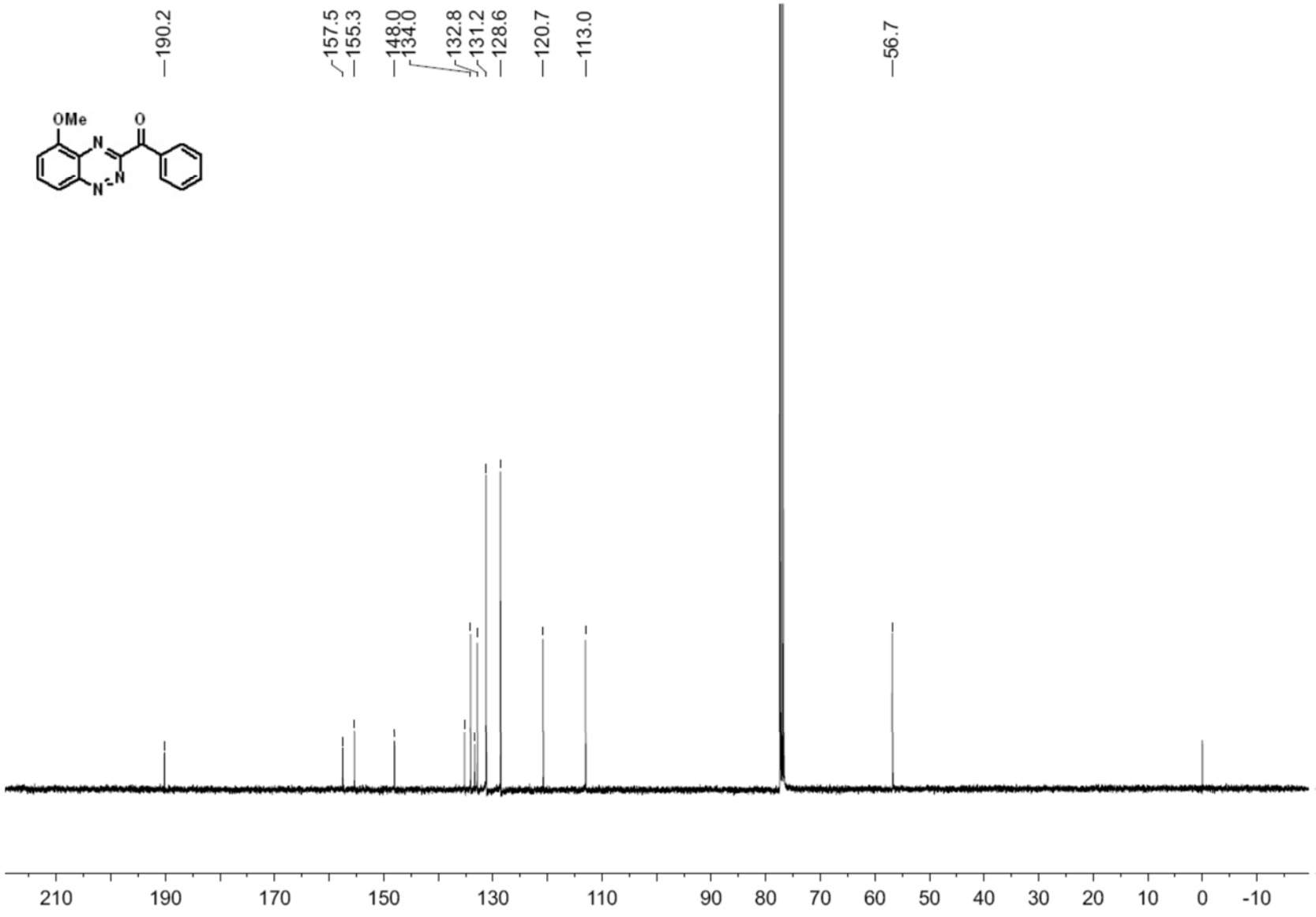
^{1}H NMR Spectrum of Compound **3t**



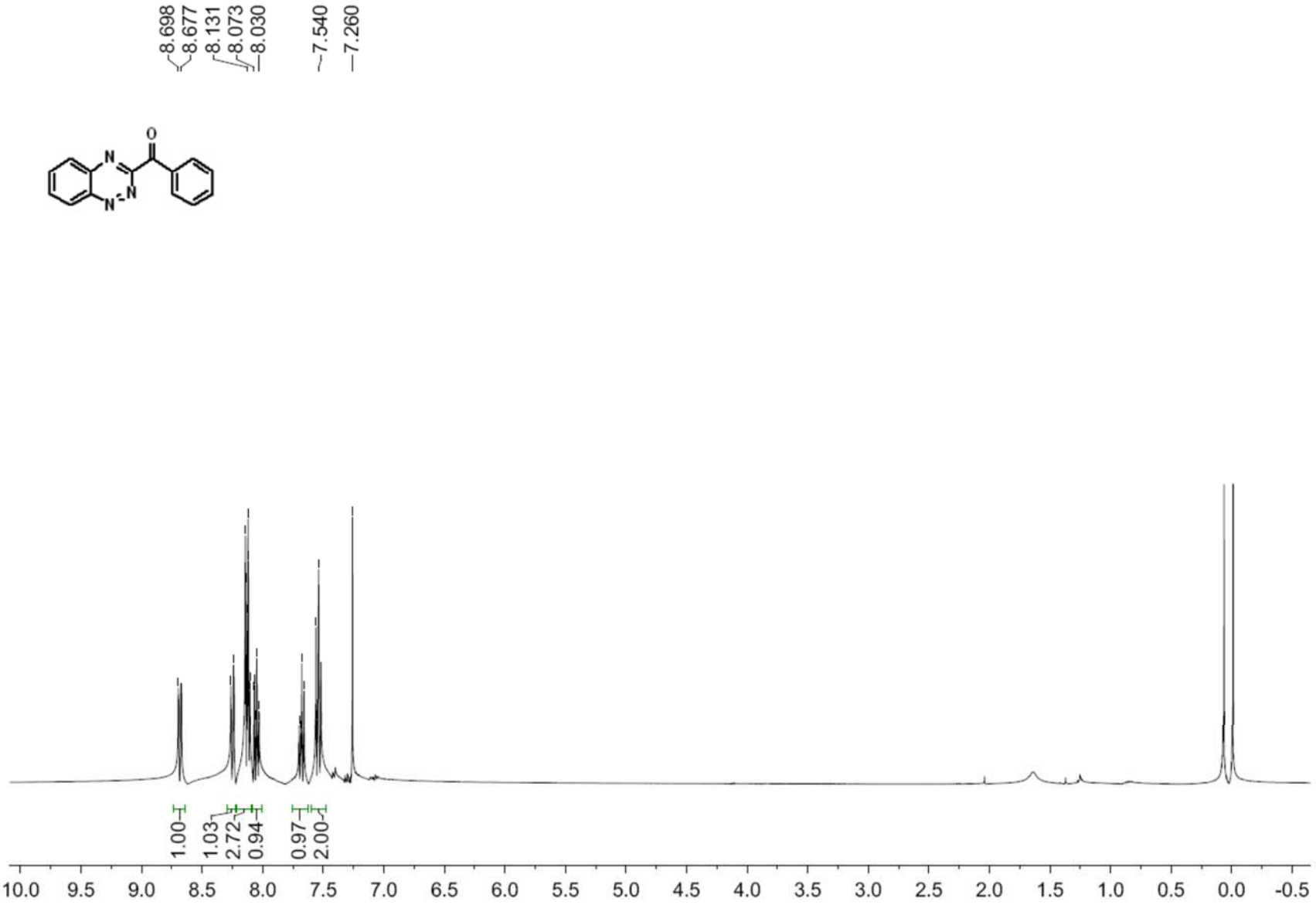
^{13}C NMR Spectrum of Compound **3t**



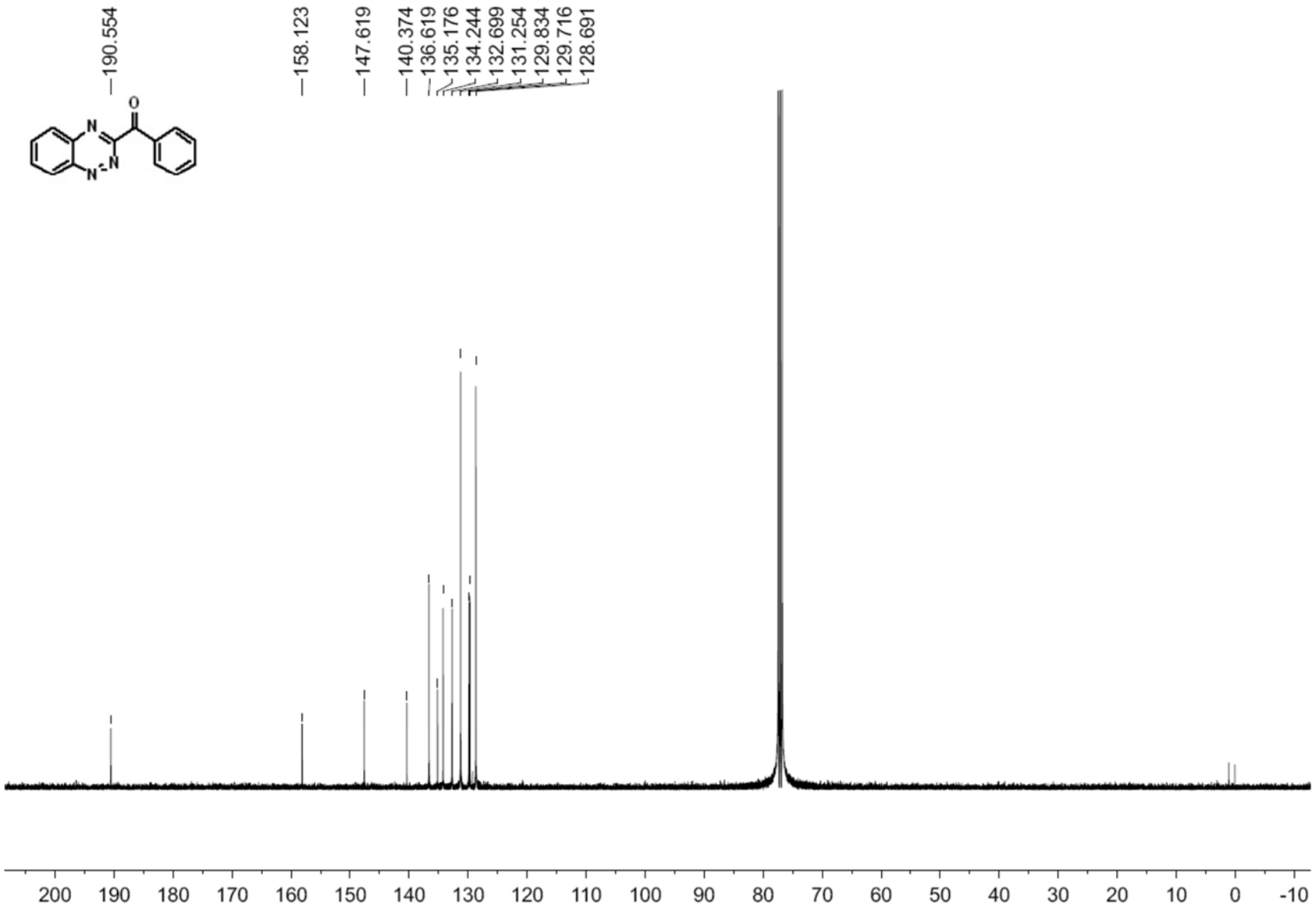
^{1}H NMR Spectrum of Compound **3u**



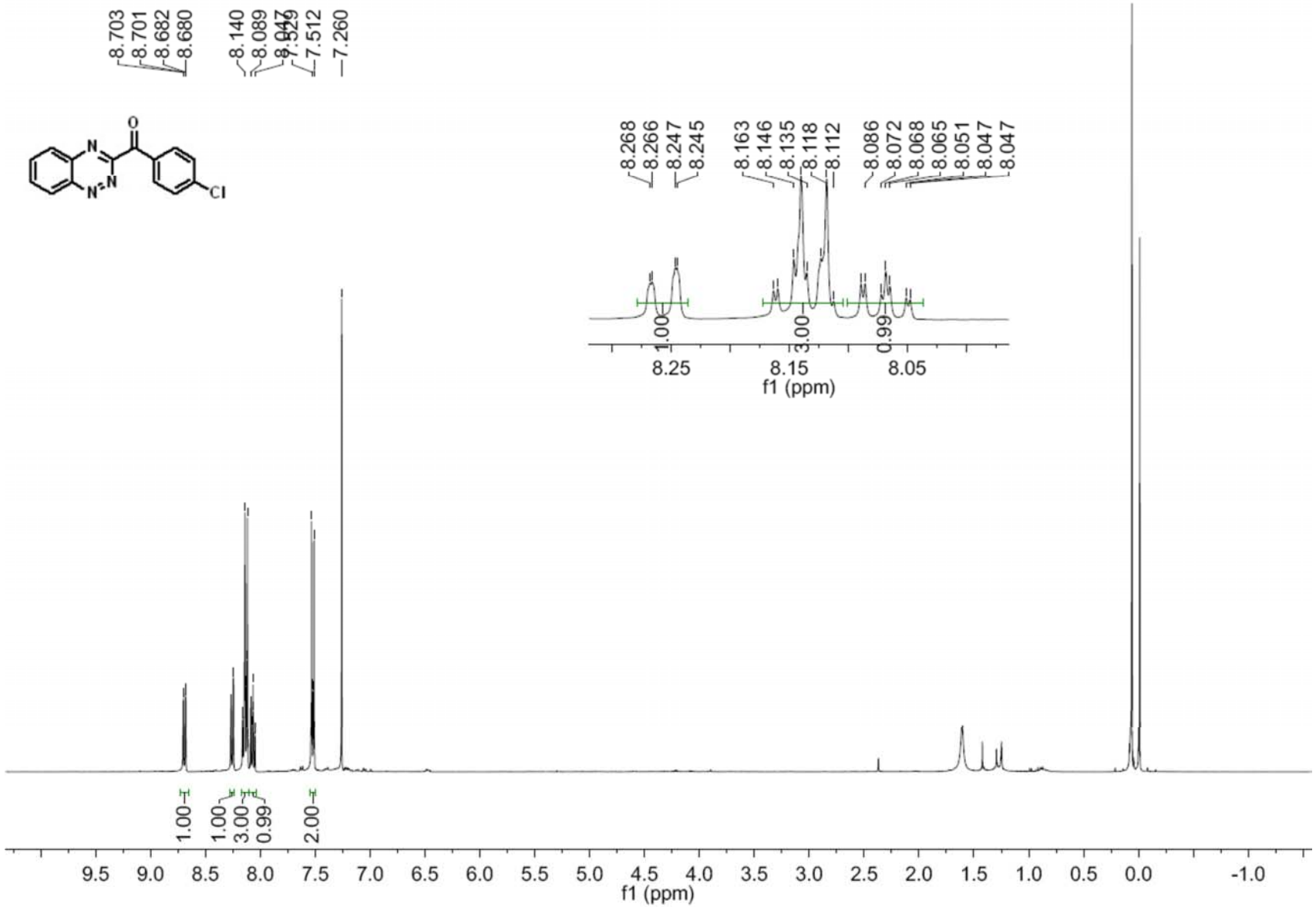
^{13}C NMR Spectrum of Compound **3u**



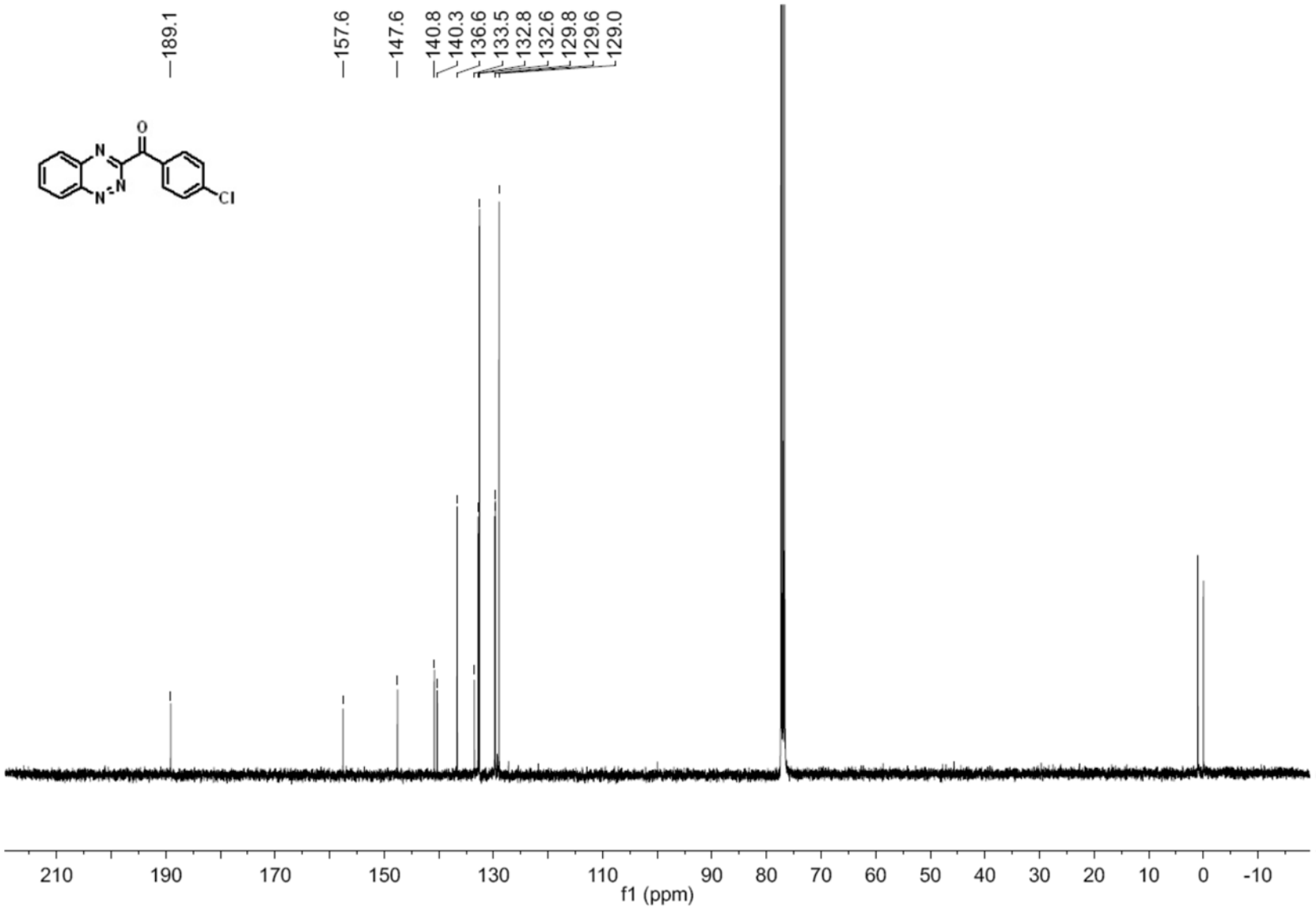
^{1}H NMR Spectrum of Compound **3v**



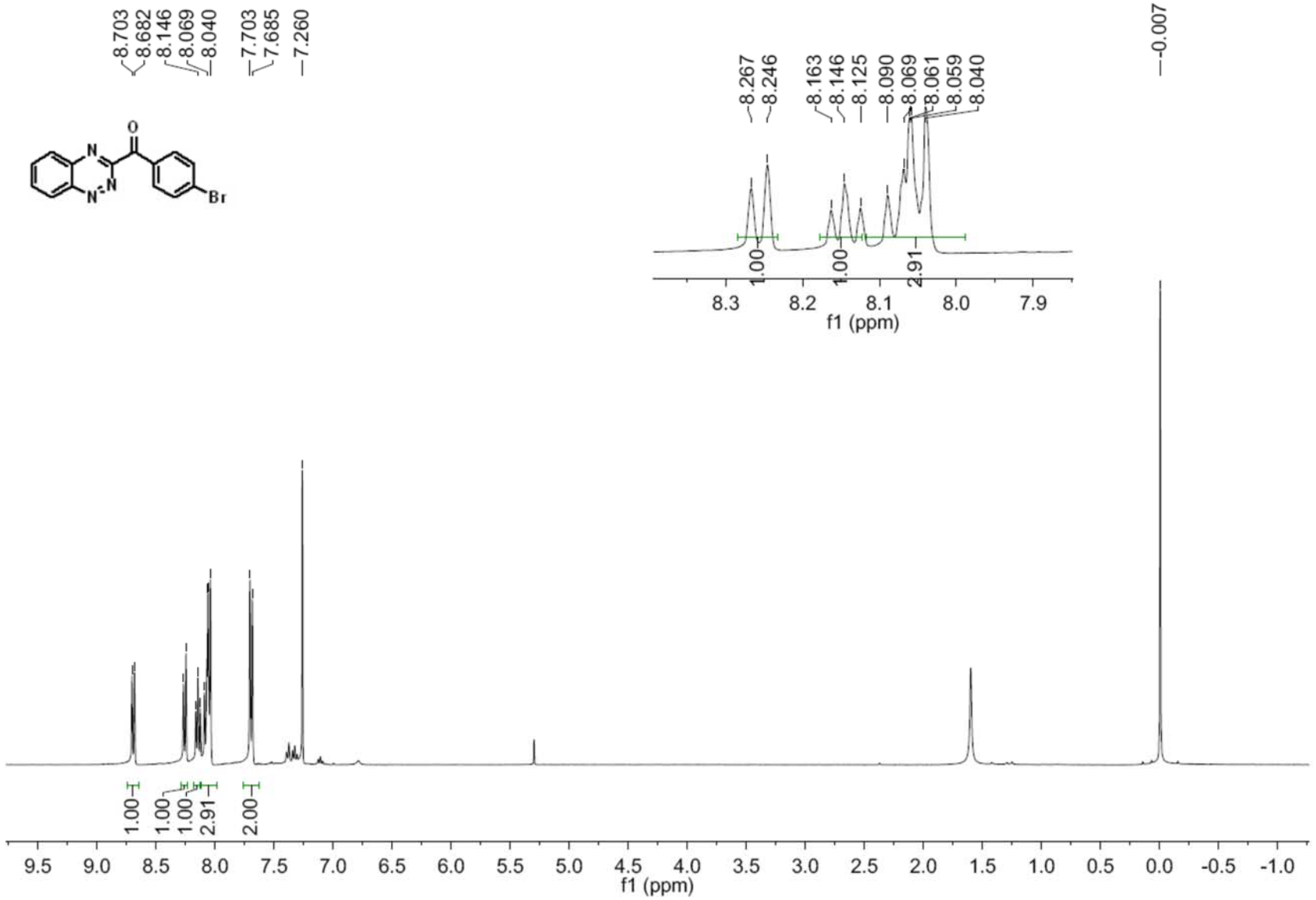
^{13}C NMR Spectrum of Compound **3v**



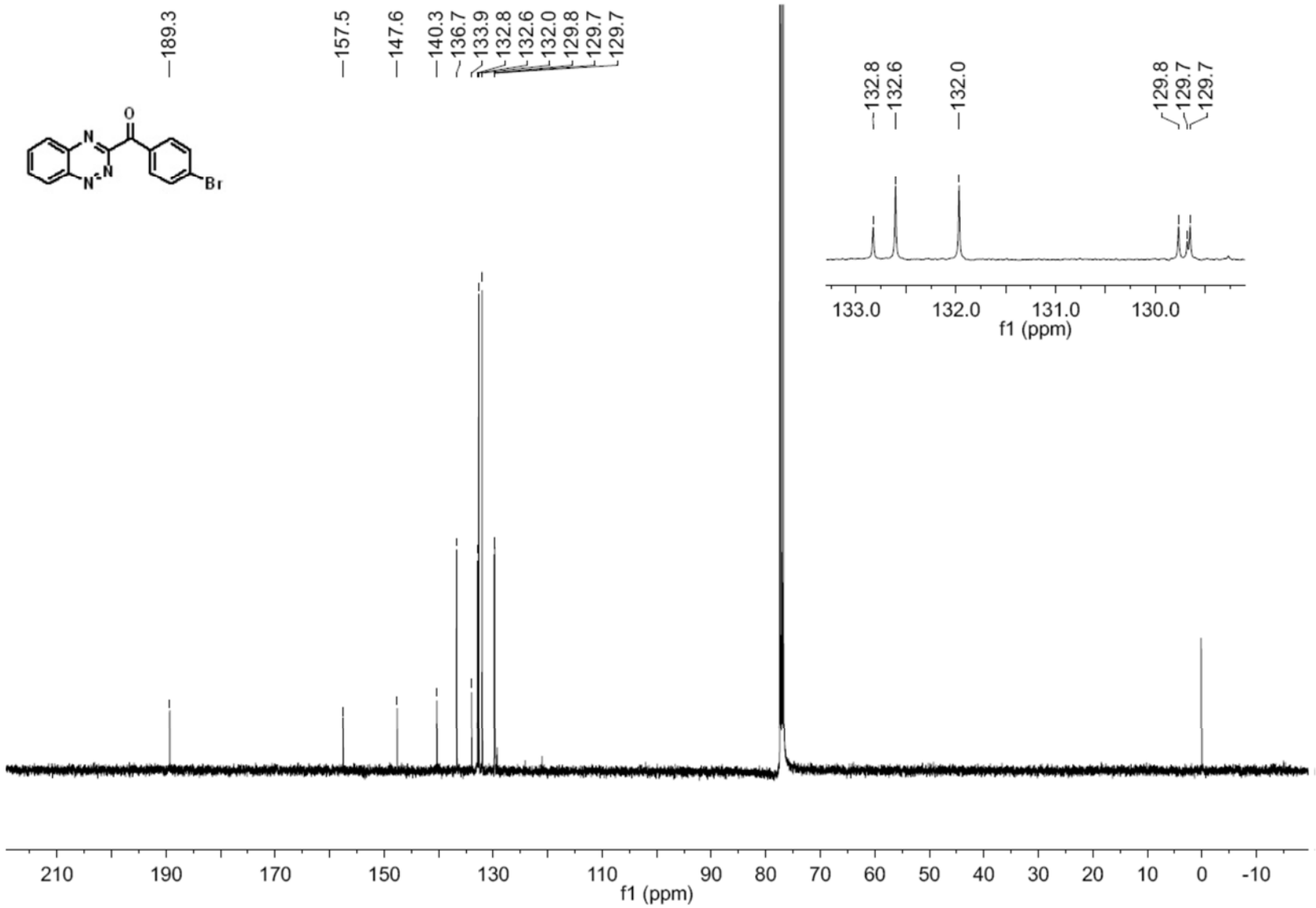
^{1}H NMR Spectrum of Compound **3w**



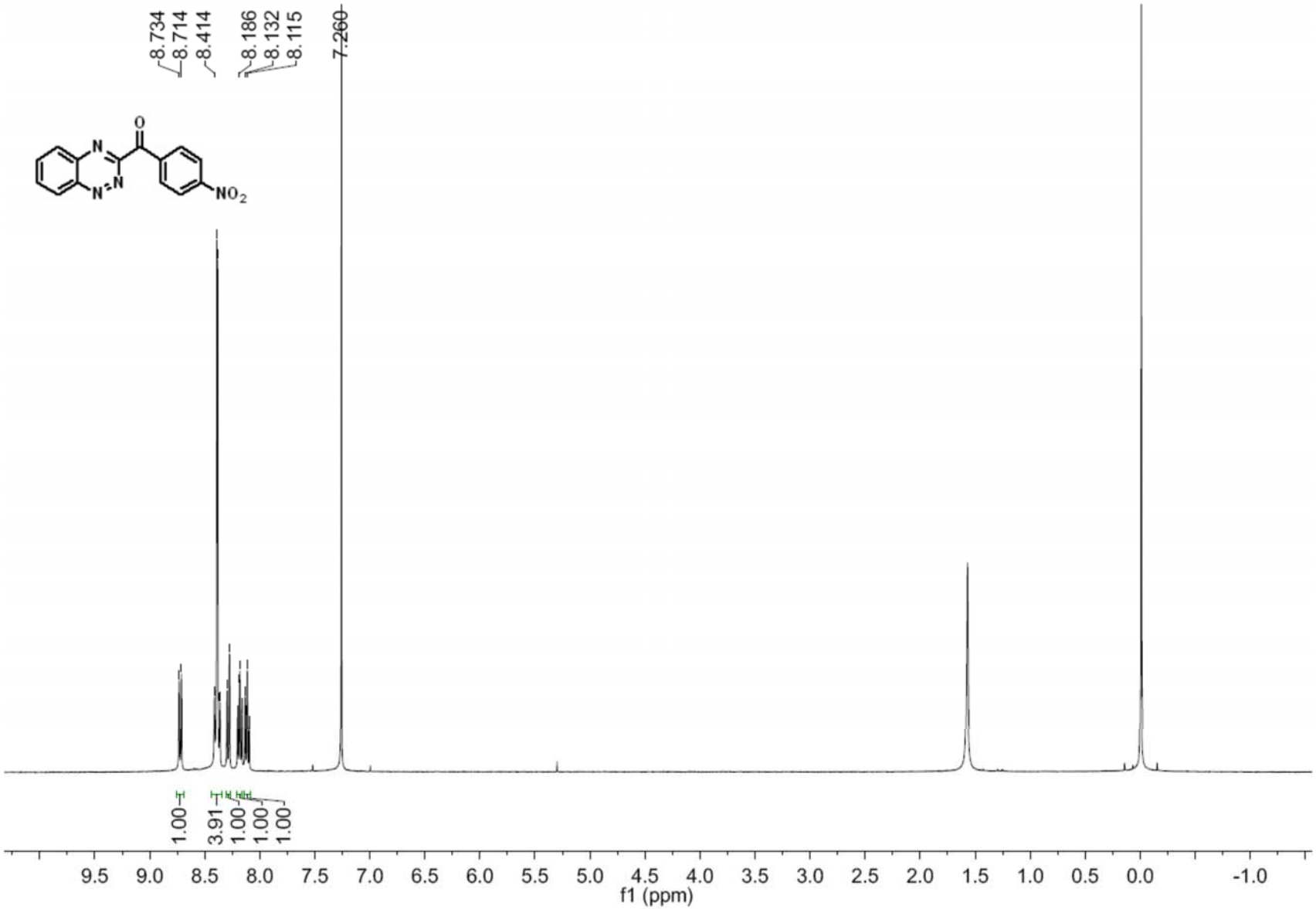
^{13}C NMR Spectrum of Compound **3w**



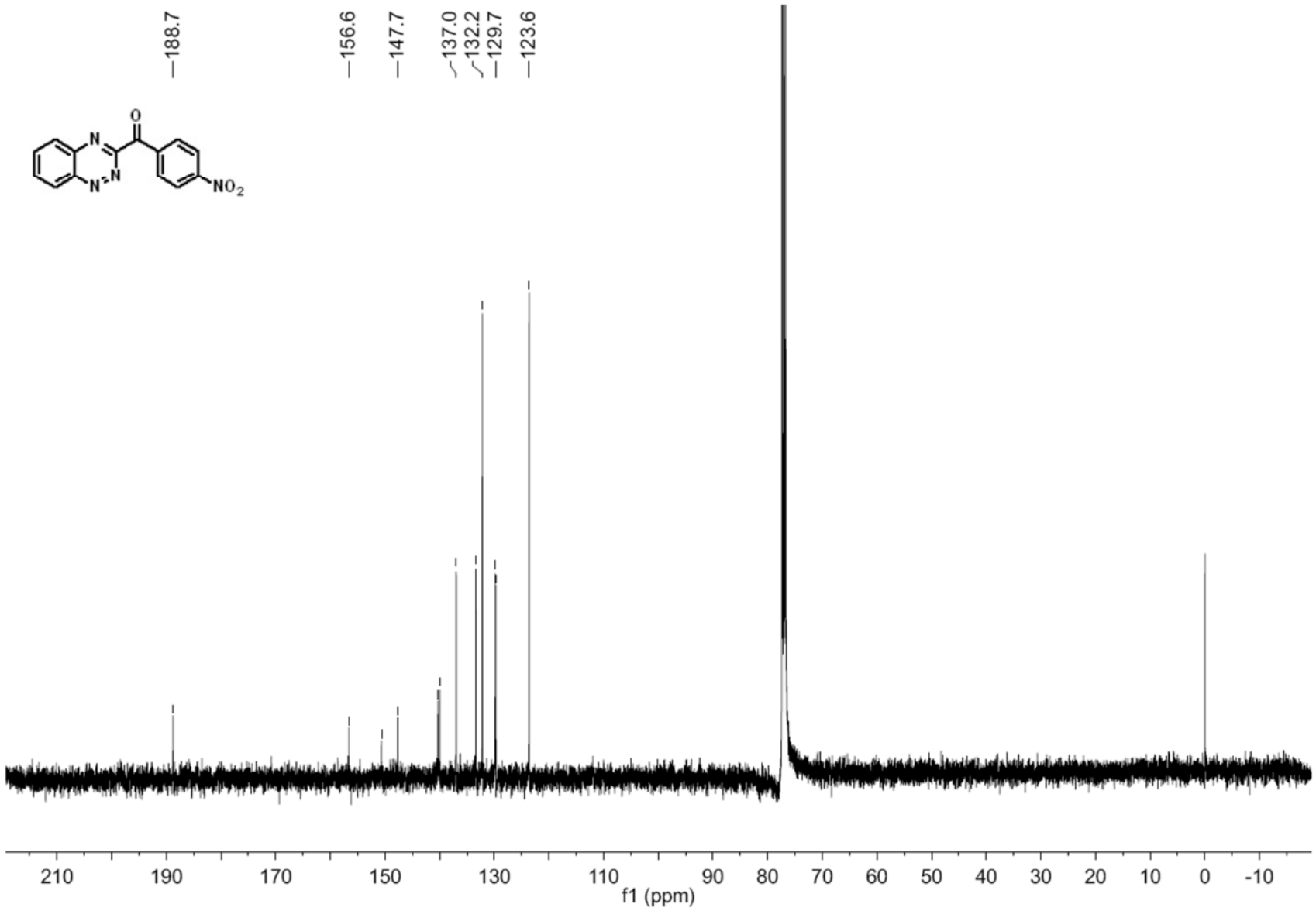
^{1}H NMR Spectrum of Compound **3x**



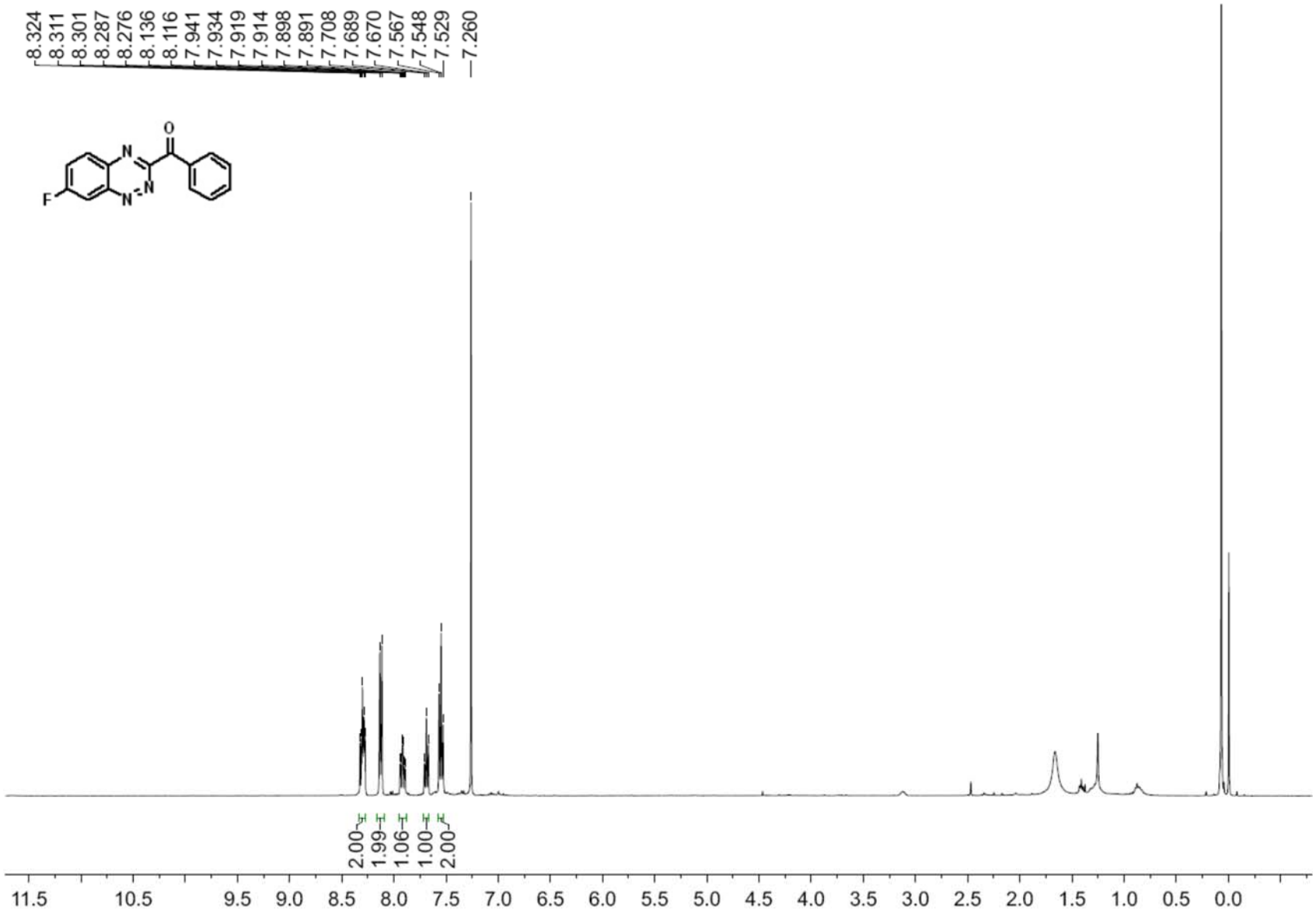
^{13}C NMR Spectrum of Compound **3x**



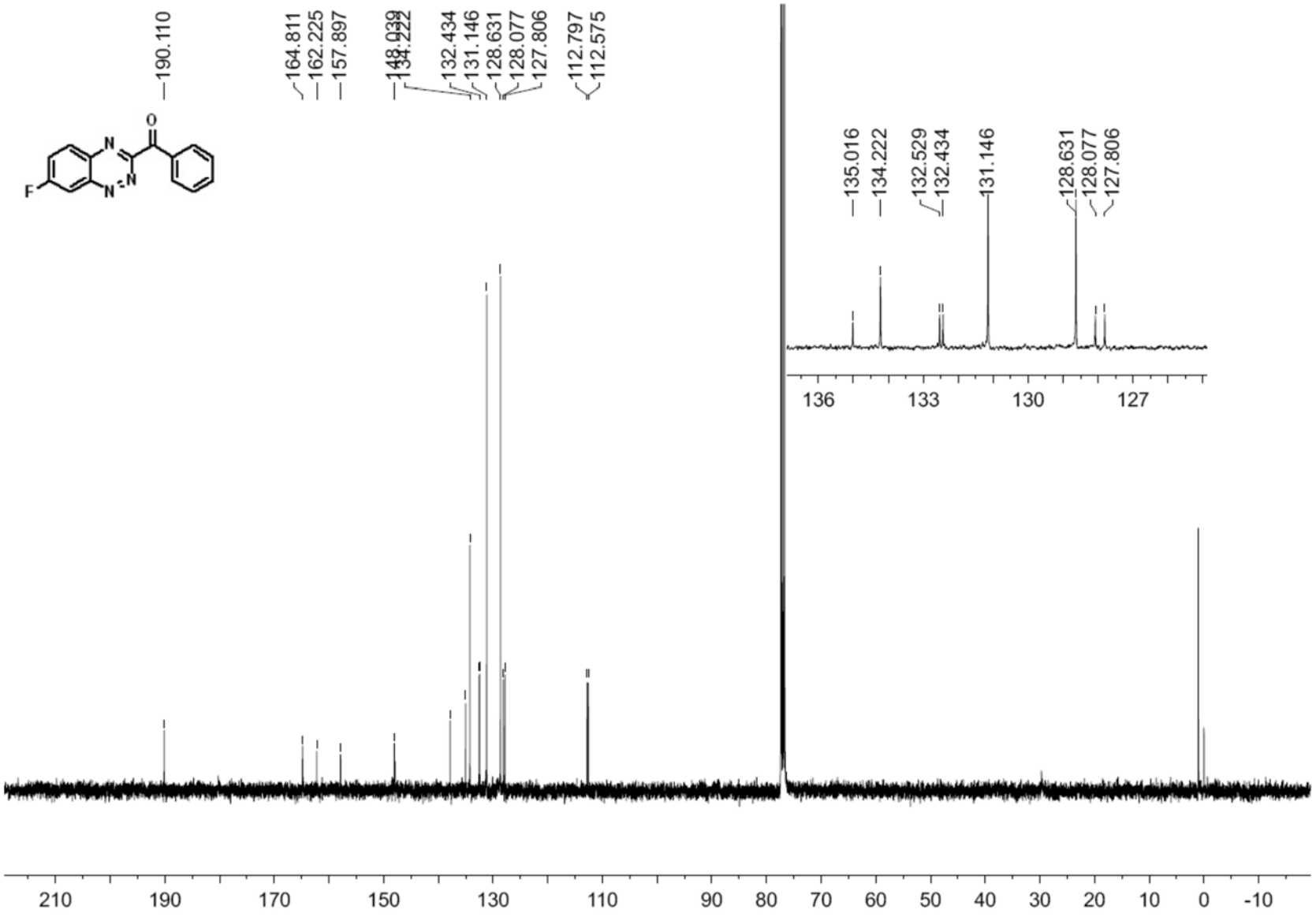
^{1}H NMR Spectrum of Compound **3y**



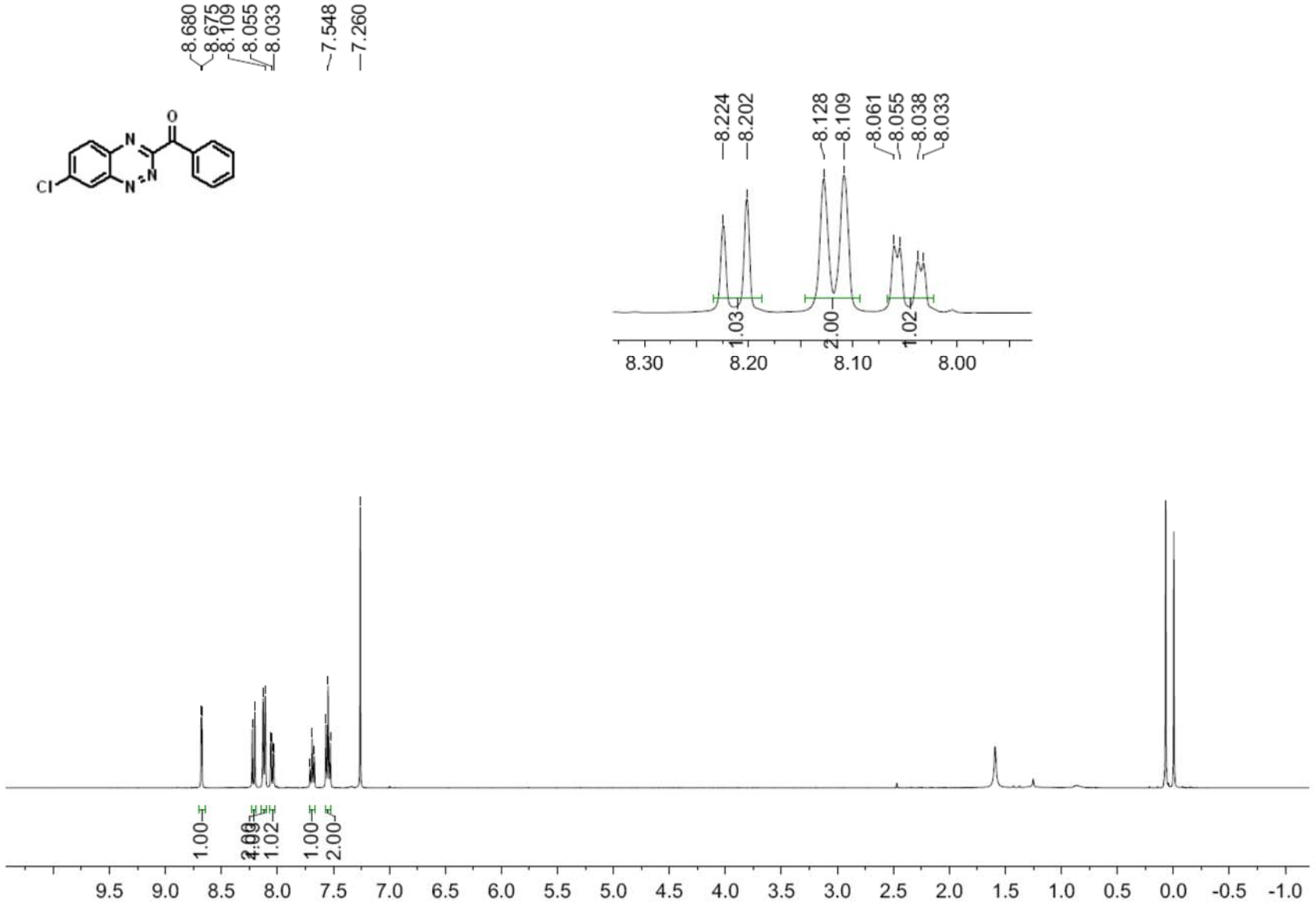
^{13}C NMR Spectrum of Compound **3y**



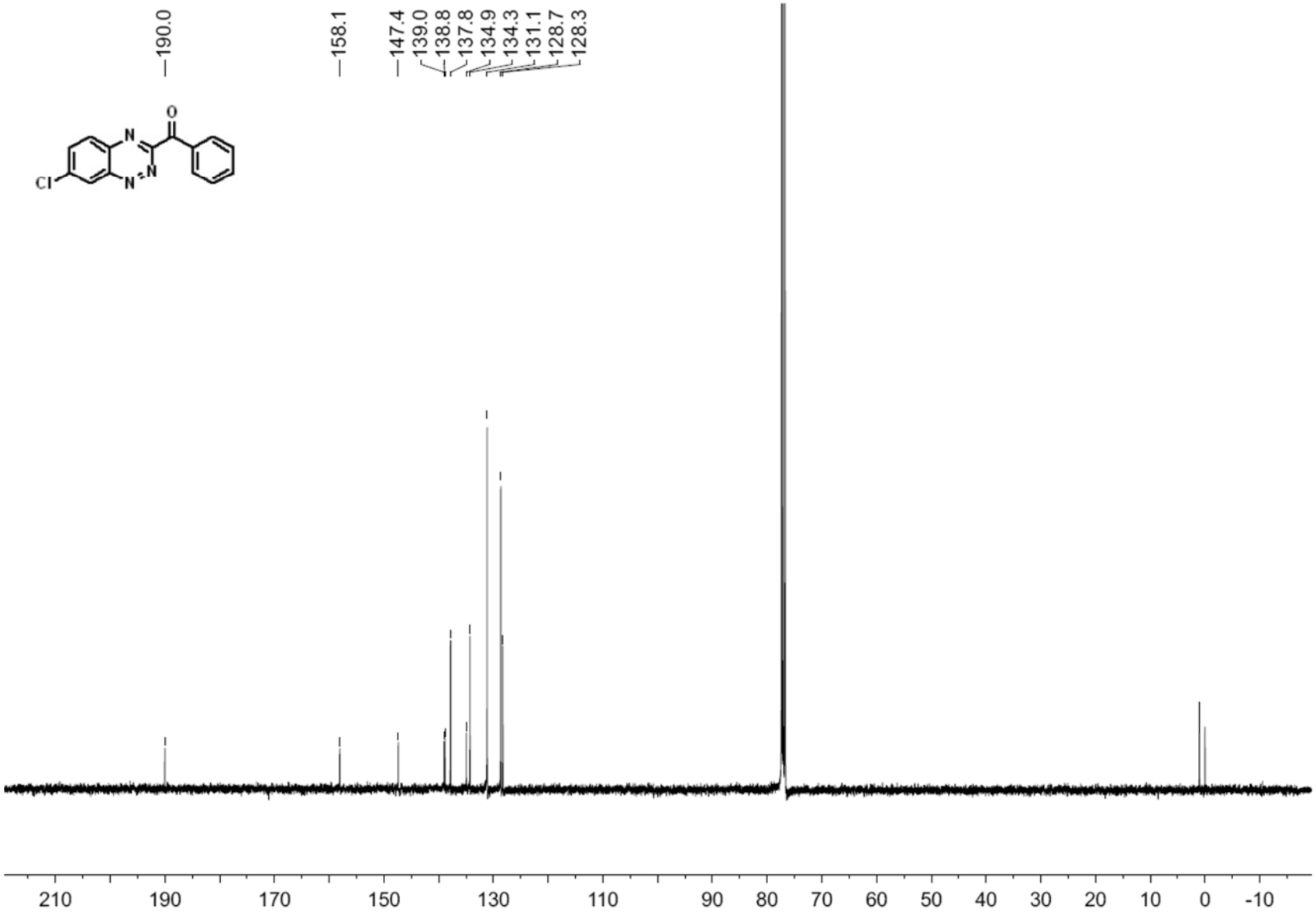
^{1}H NMR Spectrum of Compound **3z**



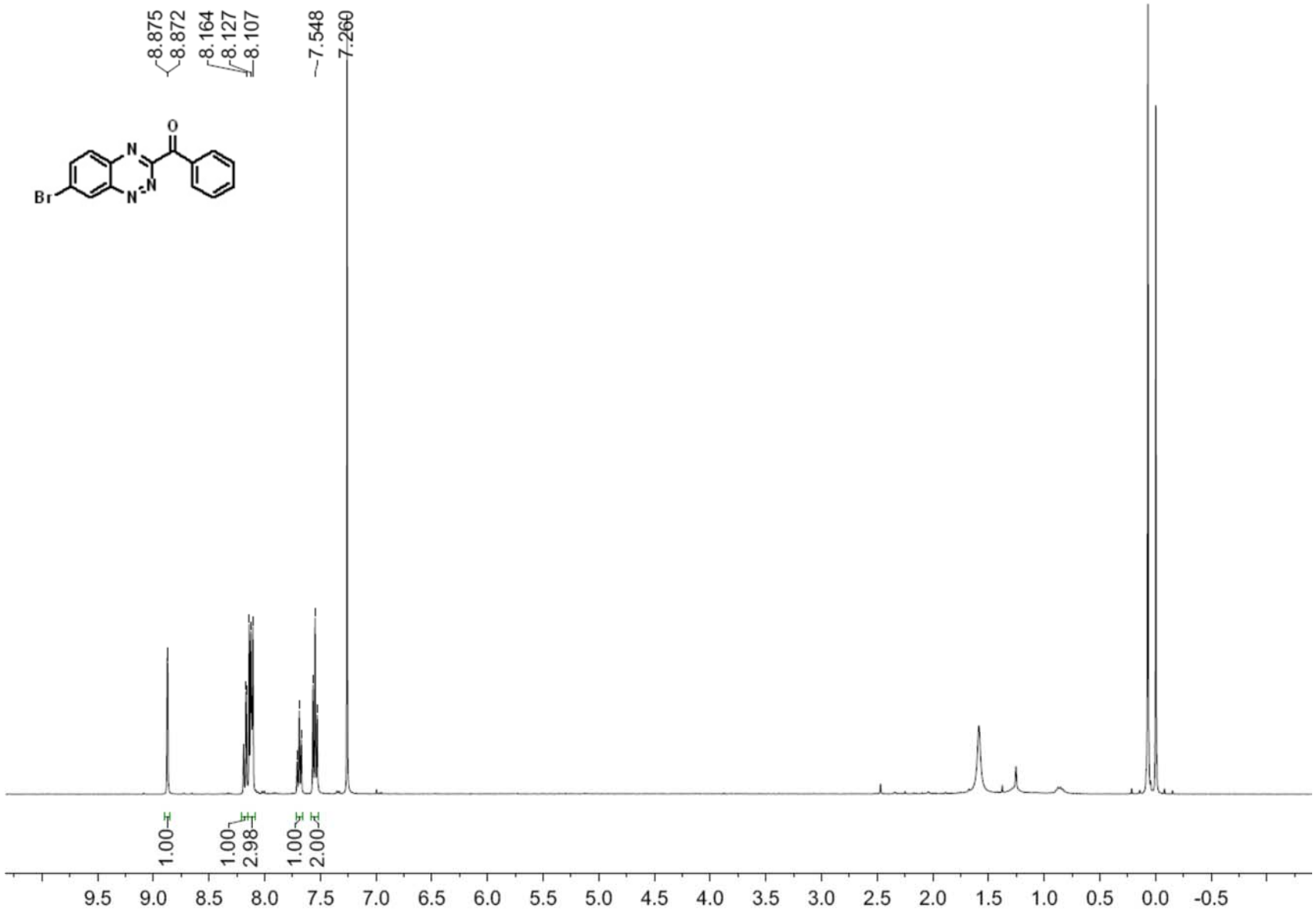
^{13}C NMR Spectrum of Compound **3z**



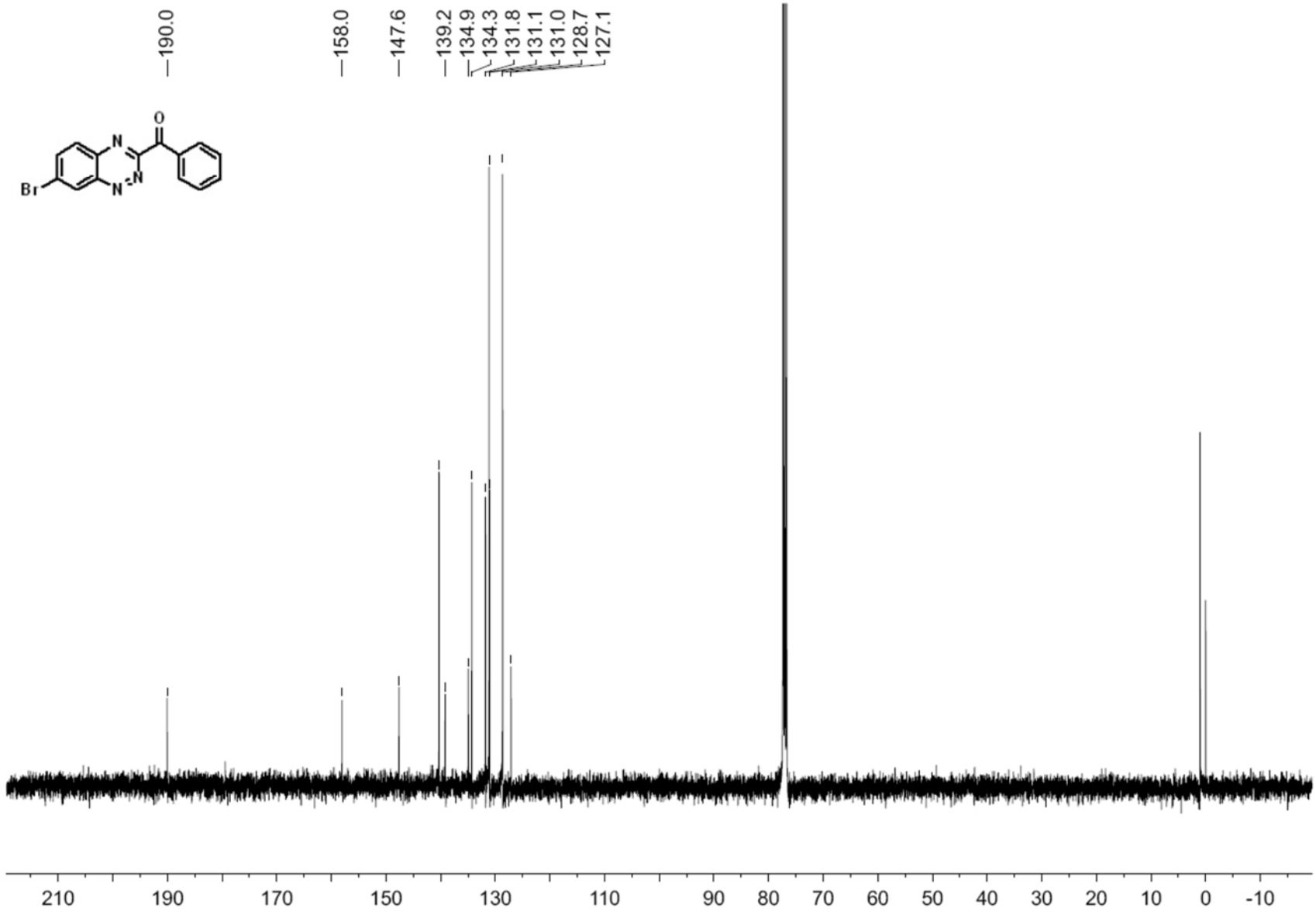
^{1}H NMR Spectrum of Compound **3aa**



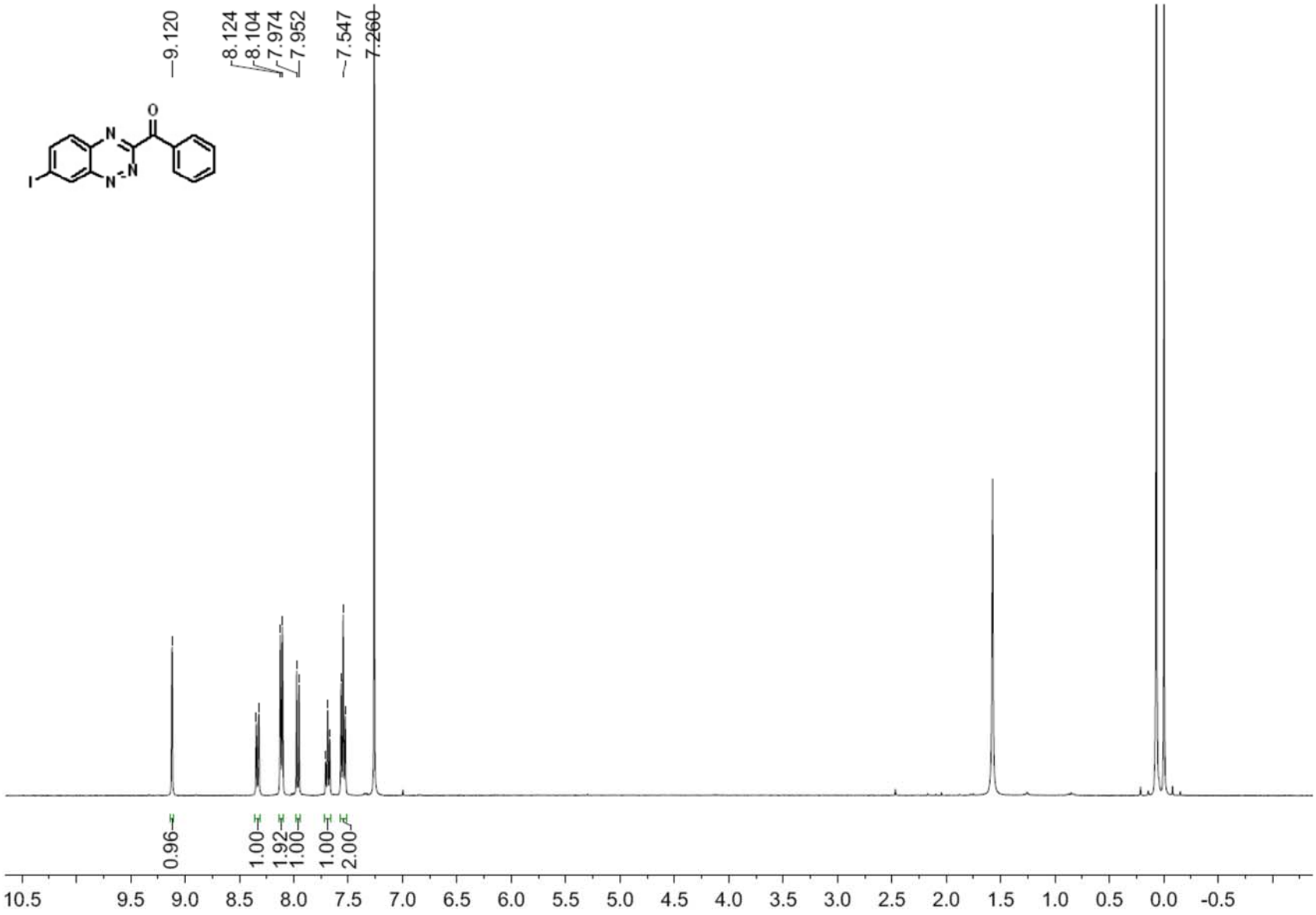
^{13}C NMR Spectrum of Compound **3aa**



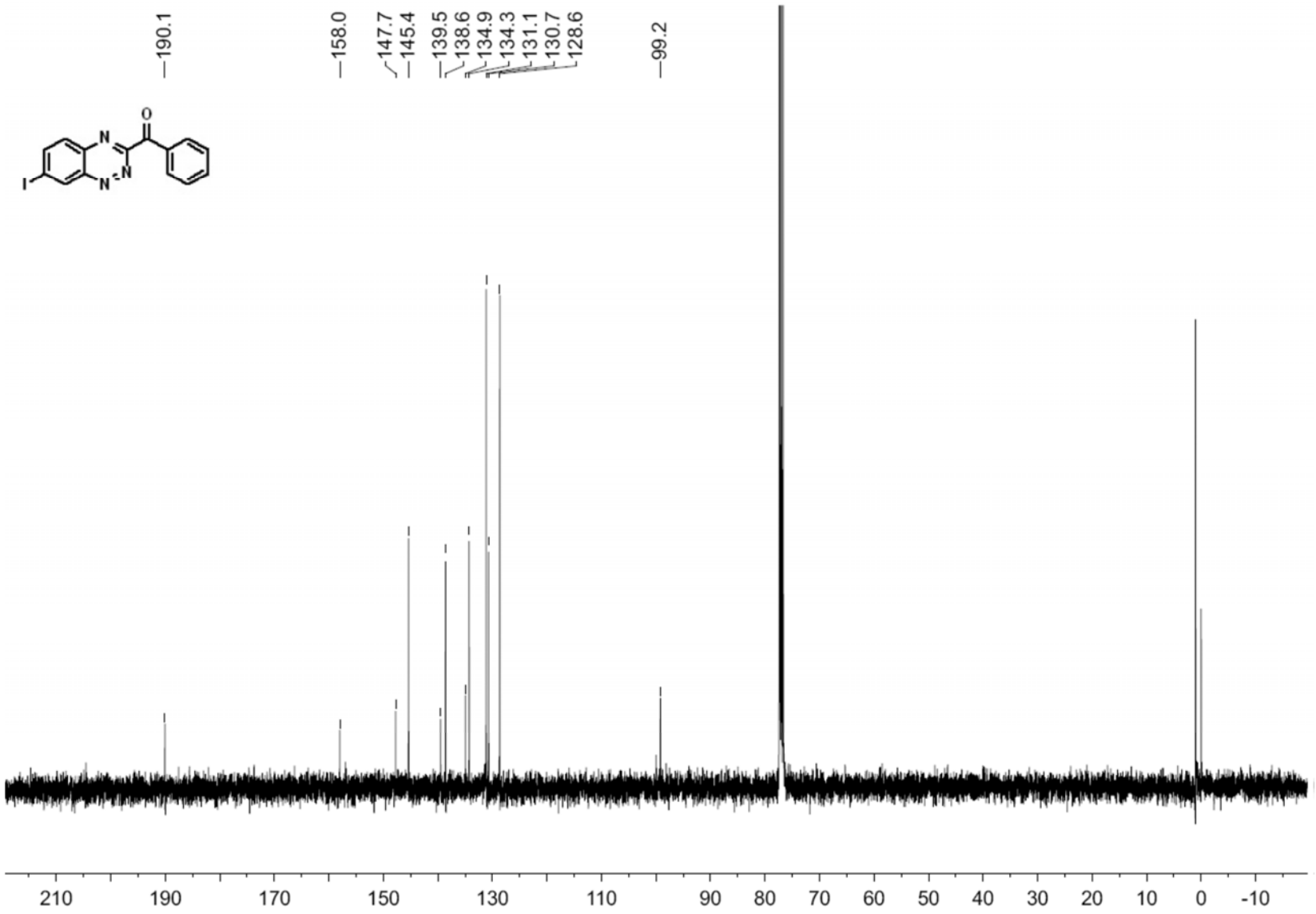
^{1}H NMR Spectrum of Compound **3ab**



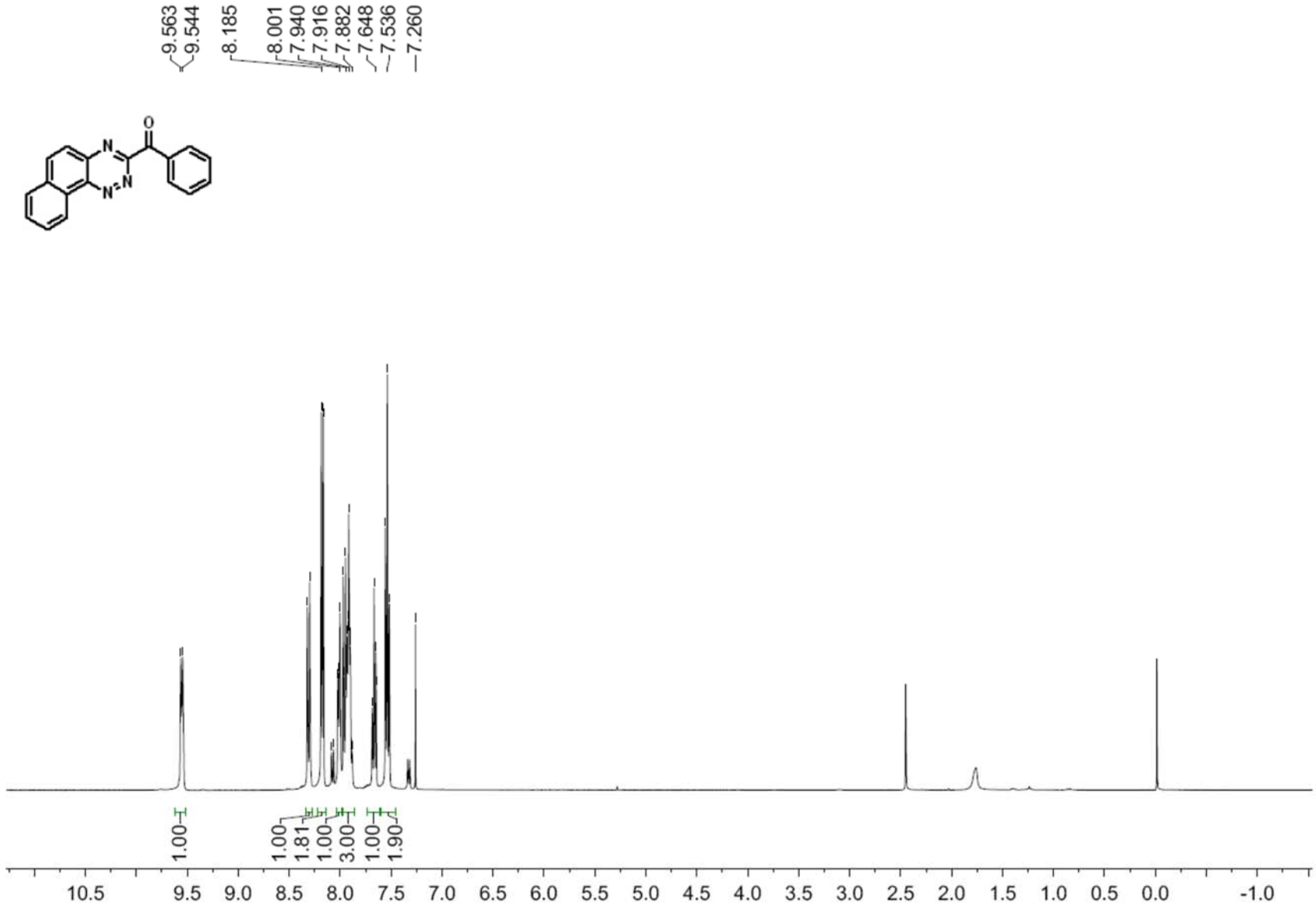
^{13}C NMR Spectrum of Compound **3ab**



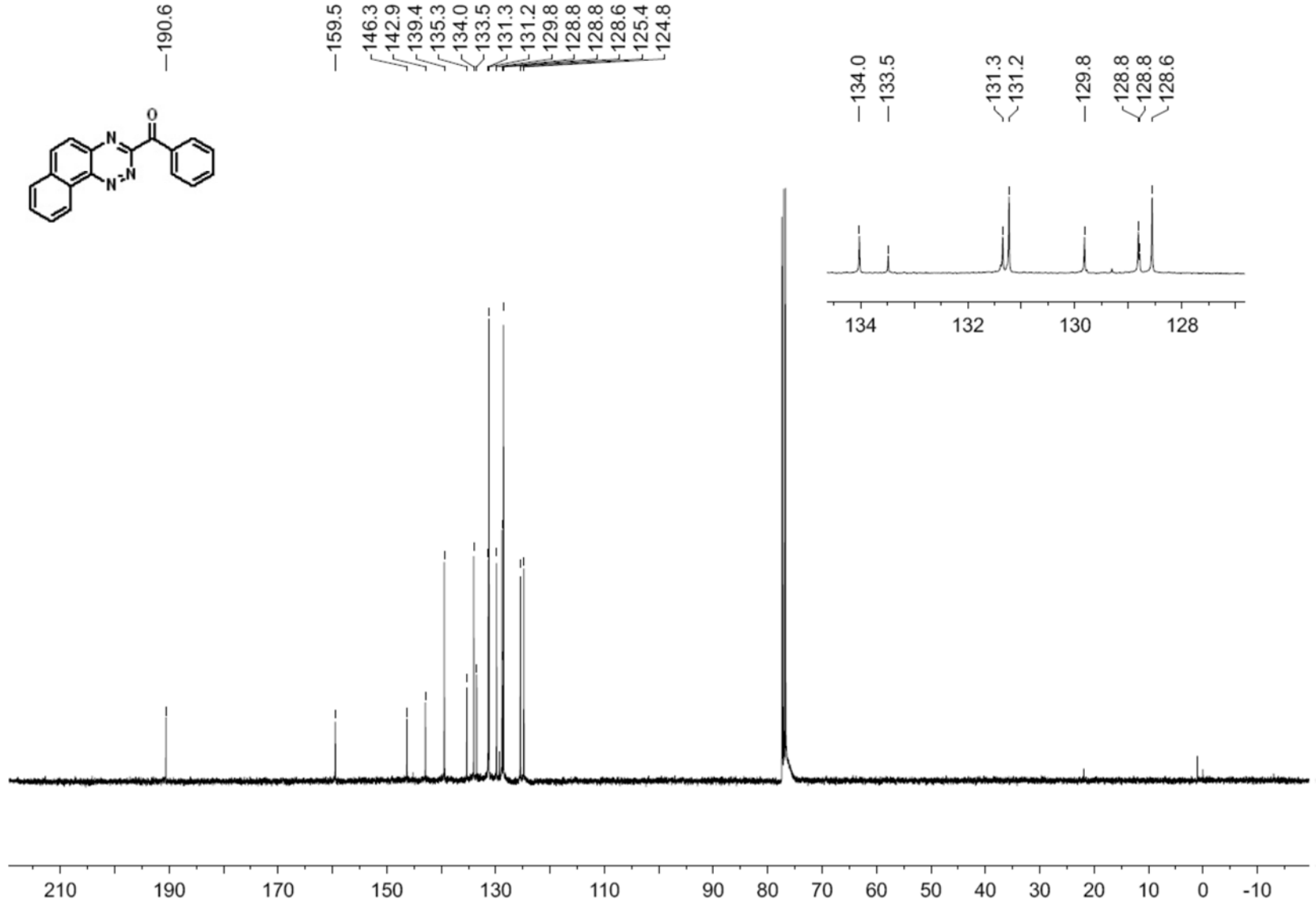
^{1}H NMR Spectrum of Compound **3ac**



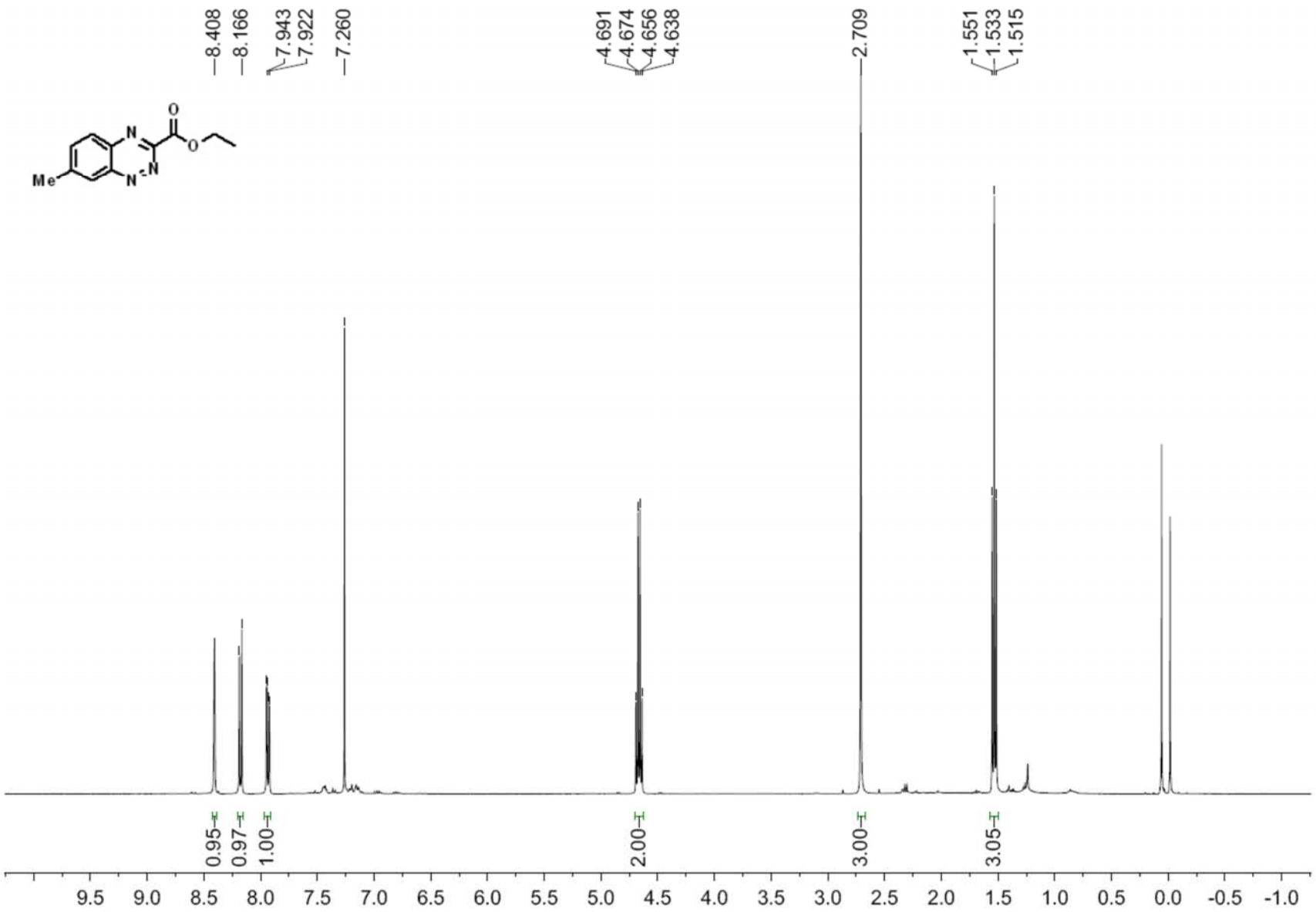
^{13}C NMR Spectrum of Compound **3ac**



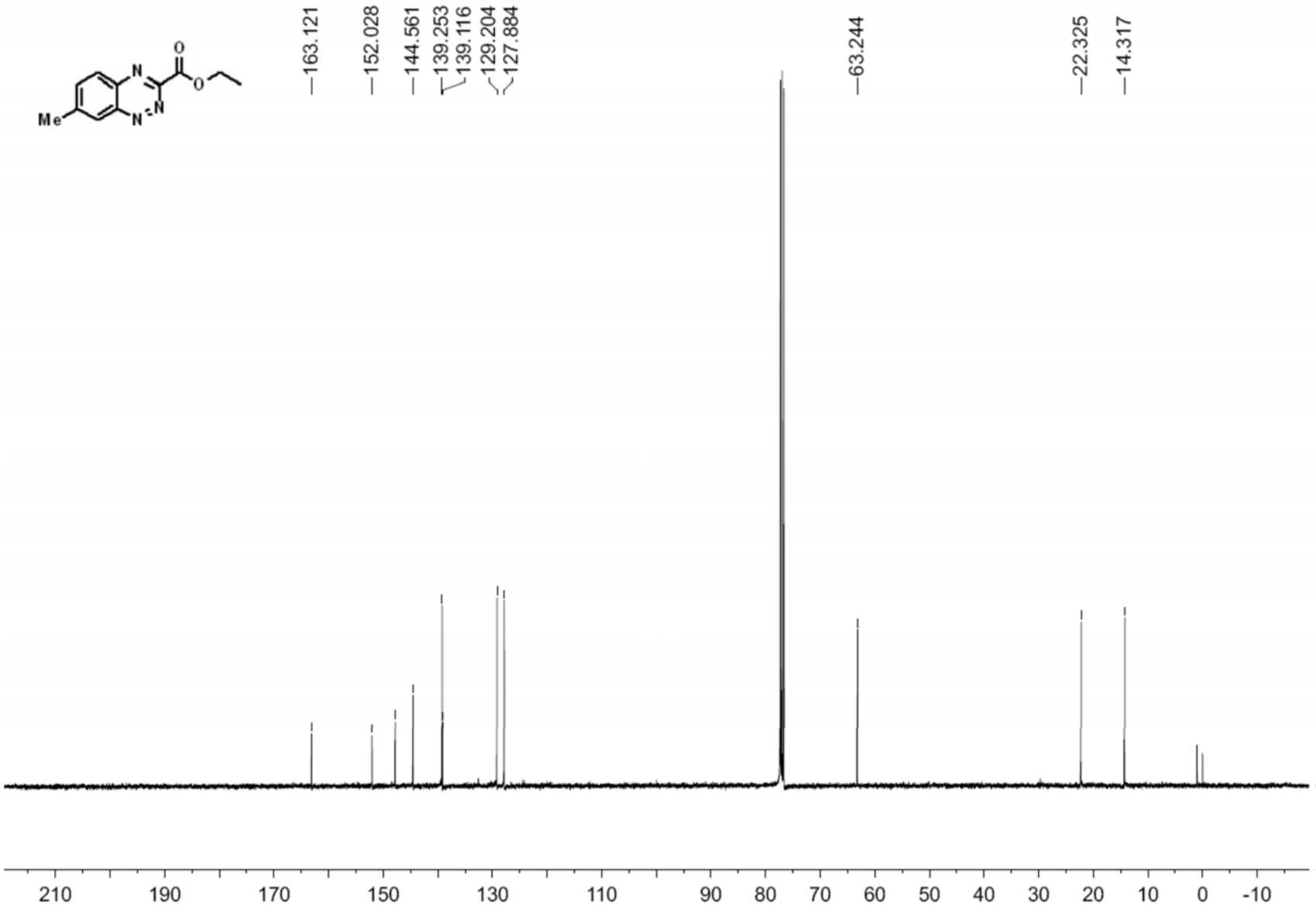
^{1}H NMR Spectrum of Compound **3ad**



^{13}C NMR Spectrum of Compound **3ad**



^{1}H NMR Spectrum of Compound **3ae**



^{13}C NMR Spectrum of Compound **3ae**