Supporting Information

Copper-catalyzed three-component *N*-alkylation of quinazolinones and azoles

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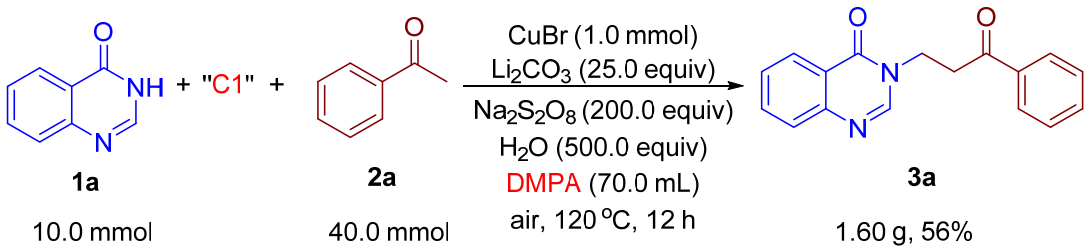
1. General information

The reaction via general procedure was carried out under an atmosphere of air unless otherwise noted. Column chromatography was performed using silica gel (200-300 mesh) or thin layer chromatography was performed using silica gel (GF254). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument using $CDCl_3$ and DMSO-d_6 as solvents. Mass spectra were measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra (ESI) were obtained with the Thermo Scientific LTQ Orbitrap XL mass spectrometer. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and HRMS data with those in literature. Melting points were measured with a YUHUA X-5 melting point instrument and were uncorrected. All reagents were directly used without purification as received from commercial supplier.

2. General procedure for synthetic reaction

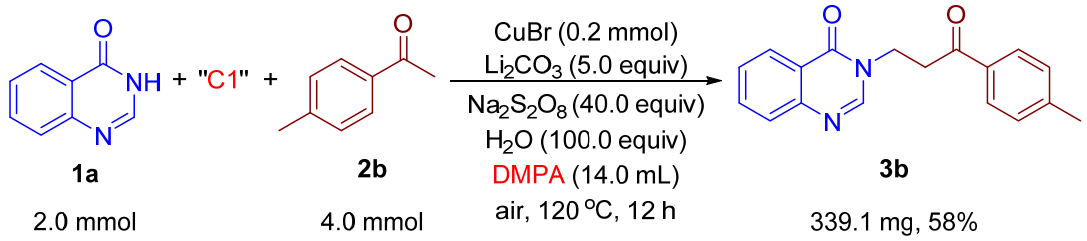
Standard reaction conditions: 4-hydroxyquinazoline (**1a**, 29.2 mg, 0.2 mmol), acetophenone (**2a**, 37 μL, 0.4 mmol, 2.0 equiv), CuBr (2.9 mg, 0.02 mmol), Li_2CO_3 (7.4 mg, 0.5 equiv), $Na_2S_2O_8$ (190.5 mg, 4.0 equiv), H_2O (36 μL, 10 equiv) and DMPA (1.4 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred under air at 120 ℃ for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to yield the desired product **3a.**

Gram scale reaction for the synthesis of 3a: 4-hydroxyquinazoline (**1a**, 1.46 g, 10.0 mmol), acetophenone (**2a**, 2.4 mL, 20.0 mmol, 2.0 equiv), CuBr (145.0 mg, 1.0 mmol), Li_2CO_3 (370.0 mg, 25.0 equiv), $Na_2S_2O_8$ (9.5 g, 200.0 equiv), H_2O (1.8 mL, 500.0 equiv) and DMPA (70.0 mL) were added successfully to a 250 mL ovendried reaction flask. The sealed reaction flask was stirred under air at 120 °C for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (100 mL) and water (100 mL). The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (100 mL) for three times. The combined organic layer was brine and dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (PE/EA: 5/1) to yield the desired product **3a** as a white solid.



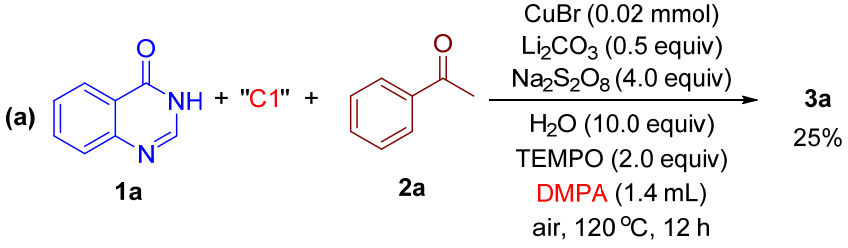
2 mmol Scale experiment for the synthesis of 3b: 4-hydroxyquinazoline (**1a**, 292.0 mg, 2.0 mmol), 4-methylacetophenone (**2b**, 533 μL, 4.0 mmol, 20.0 equiv), CuBr (29.0 mg, 0.2 mmol), Li_2CO_3 (74.0 mg, 5.0 equiv), $Na_2S_2O_8$ (1.9 g, 40.0 equiv), H_2O (360 μL, 100.0 equiv) and DMPA (14.0 mL) were added successfully to a 25 mL ovendried reaction flask. The sealed reaction flask

was stirred under air at 120 °C for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (50 mL) and water (50 mL). The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (50 mL) for three times. The combined organic layer was brine and dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (PE/EA: 5/1) to yield the desired product **3b** (339.1 mg, 58%) as a white solid.

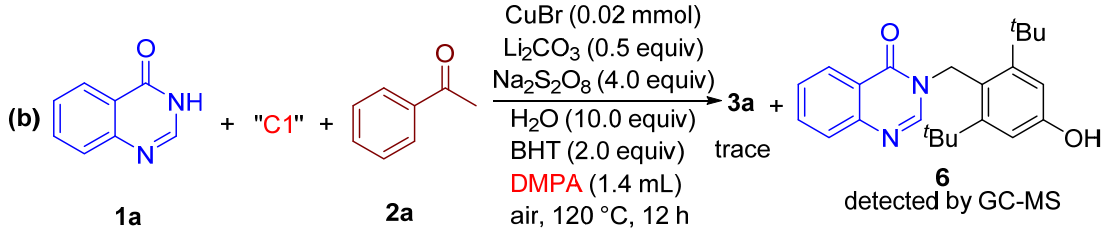


3. General procedures for the control experiments:

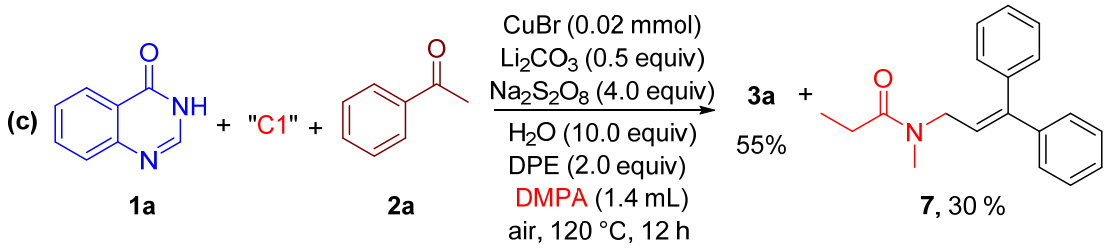
(a): 4-hydroxyquinazoline (**1a**, 29.2 mg, 0.2 mmol), acetophenone (**2a**, 37 μL, 0.4 mmol, 2.0 equiv), CuBr (2.9 mg, 0.02 mmol), Li_2CO_3 (7.4 mg, 0.5 equiv), $Na_2S_2O_8$ (190.5 mg, 4.0 equiv), H_2O (36 μL, 10.0 equiv), 2,2,6,6-Tetramethylpiperidine oxide (TEMPO, 62.3 mg, 2.0 equiv) and DMPA (1.4 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred under air at 120 ℃ for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to receive the desired product **3a** (13.9 mg, 25%).



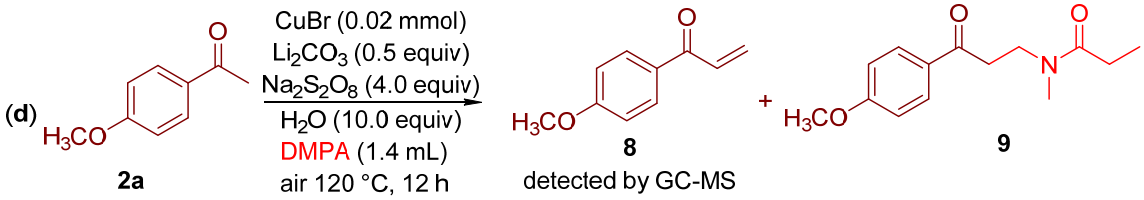
(b): 4-hydroxyquinazoline (**1a**, 29.2 mg, 0.2 mmol), acetophenone (**2a**, 37 μL, 0.4 mmol, 2.0 equiv), CuBr (2.9 mg, 0.02 mmol), Li_2CO_3 (7.4 mg, 0.5 equiv), $Na_2S_2O_8$ (190.5 mg, 4.0 equiv), H_2O (36 μL, 10.0 equiv), 2,6-di-tert-butyl-4-methylphenol (BHT, 88.1 mg, 2.0 equiv) and DMPA (1.4 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred under air at 120 ℃ for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. Only a small amount of **3a** and the BHT-coupled compound **6** was detected by GC-MS.



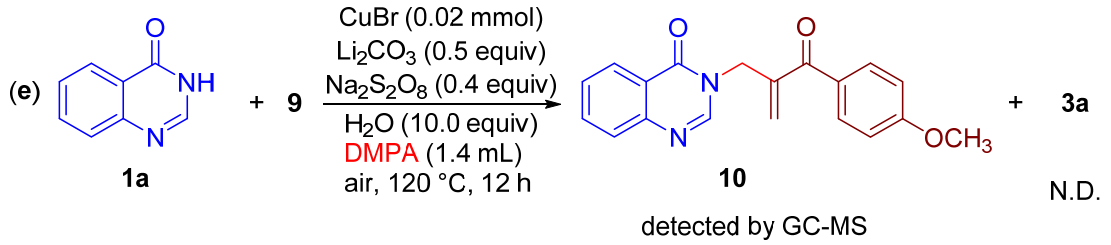
(c): 4-hydroxyquinazoline (**1a**, 29.2 mg, 0.2 mmol), acetophenone (**2a**, 37 μL, 0.4 mmol, 2.0 equiv), CuBr (2.9 mg, 0.02 mmol), Li_2CO_3 (7.4 mg, 0.5 equiv), $Na_2S_2O_8$ (190.5 mg, 4.0 equiv), H_2O (36 μL, 10.0 equiv), 1,1′-diphenylethylene (DPE, 71 μL, 2.0 equiv) and DMPA (1.4 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred under air at 120 ℃ for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to receive the desired product **3a** (30.6 mg, 55%)**,** also can obtain compound **7** (16.7 mg, 30%) as a white oil.



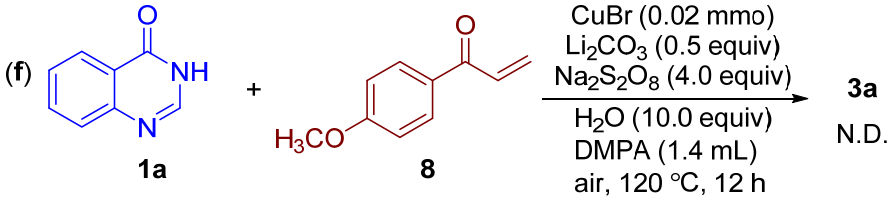
(d): 4-methyacetophenone (**2a**, 51 μL, 0.4 mmol, 2.0 equiv), CuBr (2.9 mg, 0.02 mmol), Li_2CO_3 (7.4 mg, 0.5 equiv), $Na_2S_2O_8$ (190.5 mg, 4.0 equiv), H_2O (36 μL, 10.0 equiv) and DMPA (1.4 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred under air at 120 ℃ for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. The enone **8** and β-amino ketone **9** with low yields were detected by GC-MS.



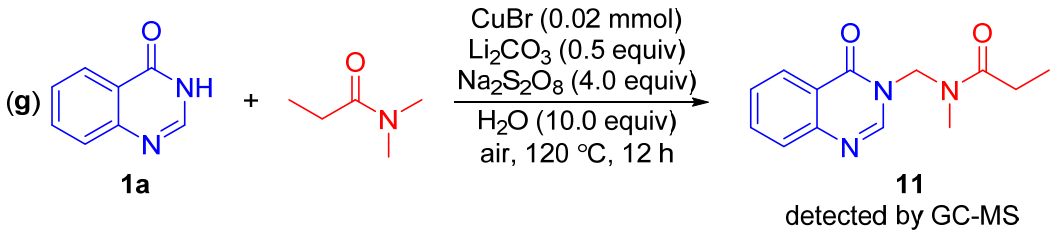
(e): 4-hydroxyquinazoline (**1a**, 29.2 mg, 0.2 mmol), **9** (99.6 μL, 0.4 mmol, 2.0 equiv), CuBr (2.9 mg, 0.02 mmol), Li_2CO_3 (7.4 mg, 0.5 equiv), $Na_2S_2O_8$ (190.5 mg, 4.0 equiv), H_2O (36 μL, 10.0 equiv) and DMPA (1.4 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred under air at 120 ℃ for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. The expected product **3a** was not detected. However, compound **10** was detected with low yield.



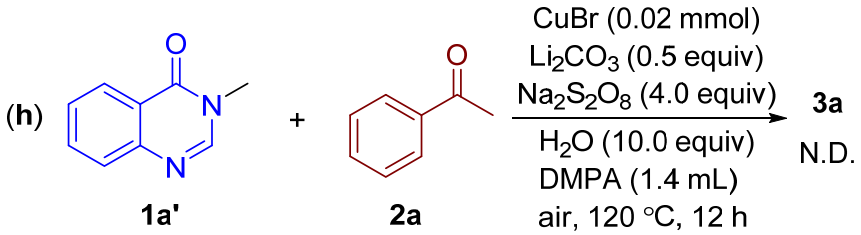
(f): 4-hydroxyquinazoline (**1a**, 29.2 mg, 0.2 mmol), **8** (53 μL, 0.4 mmol, 2.0 equiv), CuBr (2.9 mg, 0.02 mmol), Li_2CO_3 (7.4 mg, 0.5 equiv), $Na_2S_2O_8$ (190.5 mg, 4.0 equiv), H_2O (36 μL, 10.0 equiv), and DMPA (1.4 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred under air at 120 ℃ for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. However, the target compound **3a** was not detected.



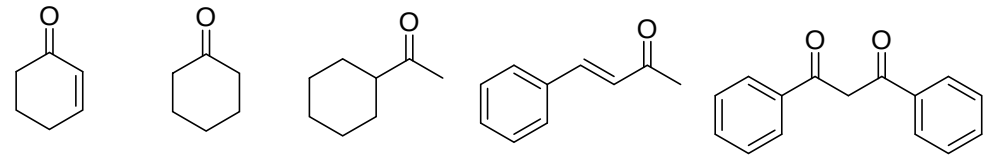
(g): 4-hydroxyquinazoline (**1a**, 29.2 mg, 0.2 mmol), CuBr (2.9 mg, 0.02 mmol), Li_2CO_3 (7.4 mg, 0.5 equiv), $Na_2S_2O_8$ (190.5 mg, 4.0 equiv), H_2O (36 μL, 10.0 equiv) and DMPA (1.4 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred under air at 120 ℃ for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. Then, the C-N coupling product **11** was detected by GC-MS.

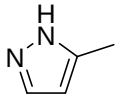


(h): 3-methylquinazolin-4(3*H*)-one (**1a′**, 29.2 mg, 0.2 mmol), acetophenone (**2a**, 37 μL, 0.4 mmol, 2.0 equiv), CuBr (2.9 mg, 0.02 mmol), Li_2CO_3 (7.4 mg, 0.5 equiv), $Na_2S_2O_8$ (190.5 mg, 4.0 equiv), H_2O (36 μL, 10.0 equiv) and DMPA (1.4 mL) were added successfully to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred under air at 120 ℃ for 12 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. However, the desired product **3a** was not detected.



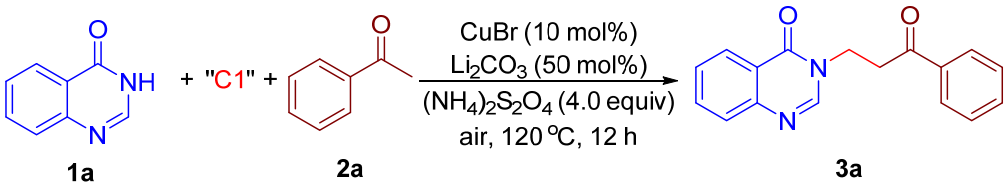
Substrates with no or very low reactivity:





4. Optimization of Reaction Conditions

Table S1. Screening of carbon source[a]

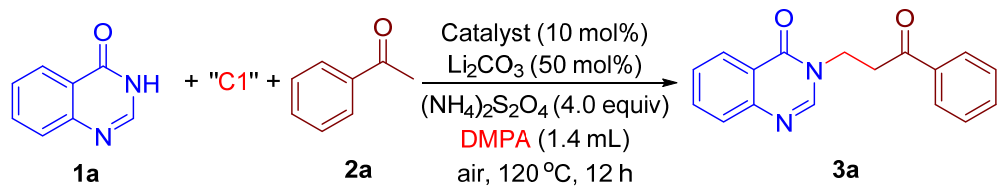


1a 2a 3a

Entry	Catalyst	Base	Oxidant	"C1"	Yield(%)[b]
1	CuBr	Li_2CO_3	$(NH_4)_2S_2O_4$	DMSO	13
2	CuBr	Li_2CO_3	$(NH_4)_2S_2O_4$	DMA	7
3	CuBr	Li_2CO_3	$(NH_4)_2S_2O_4$	DMF	trace
4	CuBr	Li_2CO_3	$(NH_4)_2S_2O_4$	TMEDA	trace
5	CuBr	Li_2CO_3	$(NH_4)_2S_2O_4$	DEF	N.D.
6	CuBr	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	40
7[c]	CuBr	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	56

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), CuBr (10 mol%), Li_2CO_3 (50 mol%), $(NH_4)_2S_2O_4$ (4.0 equiv), "C1" (2.0 mL) at 120 ºC under air atmosphere for 12 h. [b] Isolated yield. [c] DMPA (1.4 mL).

Table S2. Screening of Catalyst[a]

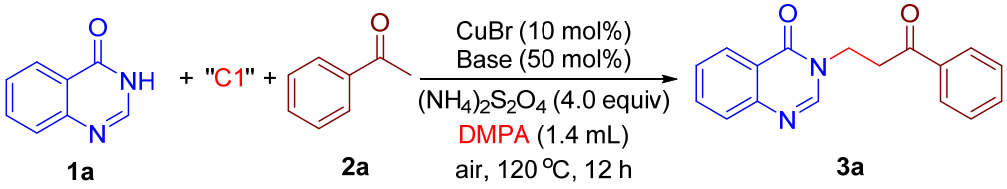


1a 2a 3a

Entry	Catalyst	Base	Oxidant	"C1"	Yield(%)[b]
1	$FeCl_3$	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	trace
2	$ZnCl_2$	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	trace
3	$AlCl_3$	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	trace
4	CuI	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	46
5	CuCl	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	53
6	$CuBr_2$	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	50
7	$Cu(OAc)_2$	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	46
8	$Cu(OTf)_2$	Li_2CO_3	$(NH_4)_2S_2O_4$	DMPA	30

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), Catalyst (10 mol%), Li_2CO_3 (50 mol%), $(NH_4)_2S_2O_4$ (4.0 equiv), DMPA (1.4 mL) at 120 ºC under air atmosphere for 12 h. [b] Isolated yield.

Table S3. Screening of Base[a]

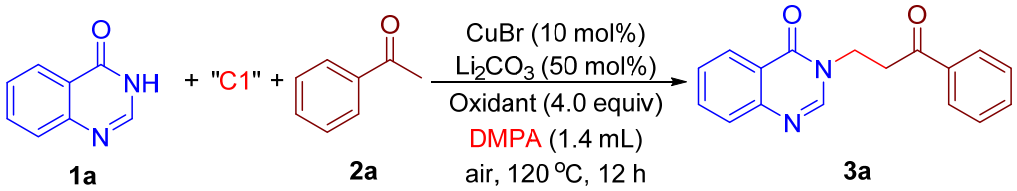


1a 2a 3a

Entry	Catalyst	Base	Oxidant	"C1"	Yield(%)[b]
1	CuBr	Na_2CO_3	$(NH_4)_2S_2O_4$	DMPA	48
2	CuBr	K_2CO_3	$(NH_4)_2S_2O_4$	DMPA	45
3	CuBr	Cs_2CO_3	$(NH_4)_2S_2O_4$	DMPA	30
4	CuBr	$KHCO_3$	$(NH_4)_2S_2O_4$	DMPA	51
5	CuBr	Et_3N	$(NH_4)_2S_2O_4$	DMPA	48
6	CuBr	DBU	$(NH_4)_2S_2O_4$	DMPA	30
7	CuBr	DABCO	$(NH_4)_2S_2O_4$	DMPA	46

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), CuBr (10 mol%), Base (50 mol%), $(NH_4)_2S_2O_4$ (4.0 equiv), DMPA (1.4 mL) at 120 ºC under air atmosphere for 12 h. [b] Isolated yield.

Table S4. Screening of Oxidant[a]

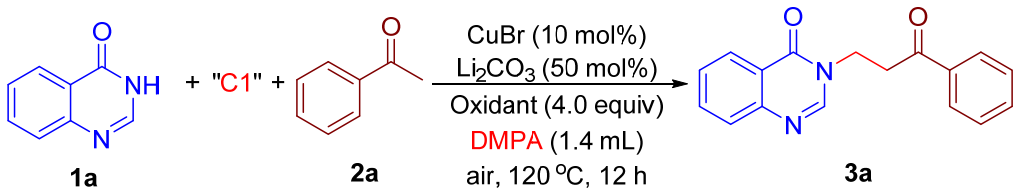


1a 2a 3a

Entry	Catalyst	Base	Oxidant	"C1"	Yield(%)[b]
1	CuBr	Li_2CO_3	$K_2S_2O_8$	DMPA	56
2	CuBr	Li_2CO_3	$Na_2S_2O_8$	DMPA	59
3	CuBr	Li_2CO_3	Oxone	DMPA	trace
4	CuBr	Li_2CO_3	TBHP	DMPA	N.D.
5	CuBr	Li_2CO_3	DTBP	DMPA	N.D.
6	CuBr	Li_2CO_3	O_2	DMPA	Trace

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), CuBr (10 mol%), Li_2CO_3 (50 mol%), Oxidant (4.0 equiv), DMPA (1.4 mL) at 120 ºC under air atmosphere for 12 h. [b] Isolated yield.

Table S5. Screening of H_2O[a]

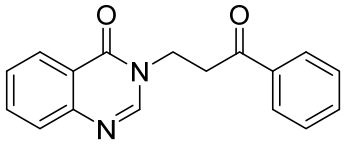


Entry	Catalyst	Base	Oxidant	"C1"	H_2O	Yield(%)[b]
1	CuBr	Li_2CO_3	$Na_2S_2O_8$	DMPA	3.0 equiv	50
2	CuBr	Li_2CO_3	$Na_2S_2O_8$	DMPA	5.0 equiv	49
3	CuBr	Li_2CO_3	$Na_2S_2O_8$	DMPA	10.0 equiv	63
4	CuBr	Li_2CO_3	$Na_2S_2O_8$	DMPA	20.0 equiv	54
5[c]	CuBr	Li_2CO_3	$Na_2S_2O_8$	DMPA	10.0 equiv	59
6[d]	CuBr	Li_2CO_3	$Na_2S_2O_8$	DMPA	10.0 equiv	60

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), CuBr (10 mol%), Li_2CO_3 (50 mol%), $Na_2S_2O_8$ (4.0 equiv), H_2O and DMPA (1.4 mL) at 120 ºC under air atmosphere for 12 h. [b] Isolated yield, [c] Li_2CO_3 (1.0 equiv), [d] Li_2CO_3 (1.5 equiv).

5. Characterization data of products

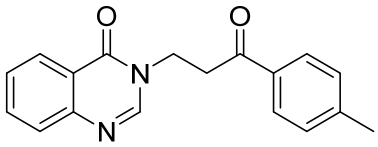
3-(3-oxo-3-phenylpropyl) quinazolin-4(3*H*)-one (3a)[1]



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and acetophenone (37 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3a** (35.1 mg, 63%) as a white solid. mp:188-189 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (s, 1H), 8.28 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.94 – 7.92(m, 2H), 7.76 – 7.69(m, 2H), 7.58 – 7.54(m, 1H), 7.50 – 7.42 (m, 3H), 4.43 (t, *J* = 5.9 Hz, 2H), 3.60 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.5 (C), 161.5 (C), 148.2 (CH), 147.7 (C), 136.1 (C), 134.3 (CH), 133.7 (C), 128.8 (CH), 128.1 (CH), 127.5 (CH), 127.2 (CH), 126.4 (CH), 122.0 (CH), 42.8 (CH_2), 36.9 (CH_2).

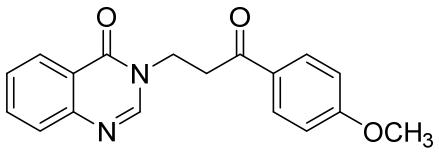
3-(3-oxo-3-(p-tolyl) propyl) quinazolin-4(3*H*)-one (3b)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3b** (42.6 mg, 73%) as a white solid. mp:190-191 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (s, 1H), 8.25 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.82 – 7.79 (m, 2.2 Hz, 2H), 7.73 – 7.66 (m, 2H), 7.47 – 7.43 (m, 1H), 7.21-7.19 (m, 2H), 4.39 (t, *J* = 5.9 Hz, 2H), 3.53 (t, *J* = 5.9 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.1 (C), 161.4 (C), 148.2 (CH), 147.8 (C), 144.6 (C), 134.2 (CH), 133.7 (C), 129.4 (CH), 128.2 (CH), 127.5 (CH), 127.1 (CH), 126.4 (CH), 122.0 (C), 42.9 (CH_2), 36.7 (CH_2), 21.7 (CH_3). HRMS (ESI) m/z calcd for $C_{18}H_{17}N_2O_2^+$ $(M+H)^+$ 293.1285, found 293.1286.

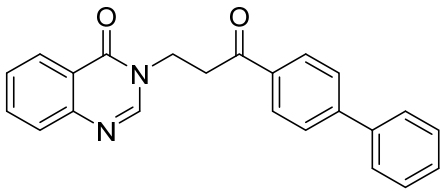
3-(3-(4-methoxyphenyl)-3-oxopropyl) quinazolin-4(3*H*)-one (3c)[1]



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 4-methoxyacetophenone (58 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3c** (43.2 mg, 70%) as a white solid. mp:193-194 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 (s, 1H), 8.26 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.91 – 7.87 (m, 2H), 7.73 – 7.66 (m, 3H), 7.47 – 7.43 (m, 1H), 6.89 – 6.85 (m, 2H), 4.39 (t, *J* = 5.9 Hz, 2H), 3.82 (s, 3H), 3.51 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9 (C), 163.9 (C), 161.4 (C), 148.2 (CH), 147.8 (C), 134.2 (CH), 130.4 (C), 129.3 (CH), 127.5 (CH), 127.1 (CH), 126.4 (CH), 122.0 (C), 113.8 (C), 55.5 (CH_3), 42.9 (CH_2), 36.5 (CH_2).

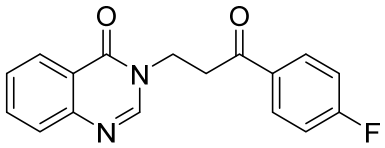
3-(3-([1,1'-biphenyl]-4-yl)-3-oxopropyl) quinazolin-4(3*H*)-one (3d)[1]



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 4-phenyl-acetophenon (78.5 mg, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3d** (43.2 mg, 70%) as a white solid. mp:201-202 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 (s, 1H), 8.29 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.76 – 7.69 (m, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.60 – 7.58 (m, 2H), 7.50 – 7.43 (m, 3H), 7.40 – 7.37 (m, 1H), 4.45 (t, *J* = 5.2 Hz, 2H), 3.62 (t, *J* = 5.7 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.1 (C), 161.5 (C), 148.2 (CH), 147.7 (C), 146.3 (C), 139.6 (C), 134.8 (C), 134.3 (CH), 129.0 (CH), 128.7 (CH), 128.4 (CH), 127.6 (CH), 127.3 (CH), 127.3 (CH), 127.2 (CH), 126.4 (CH), 122.0 (CH), 42.9 (CH_2), 36.9 (CH_2).

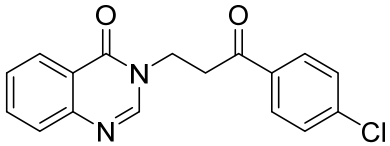
3-(3-(4-fluorophenyl)-3-oxopropyl) quinazolin-4(3*H*)-one (3e)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 4-fluoroacetophenone (48 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3e** (28.4 mg, 48%) as a white solid. mp:197-198 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (s, 1H), 8.26 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.97 – 7.93 (m, 2H), 7.74 – 7.67 (m, 2H), 7.49 –7.45 (m, 1H), 7.12 – 7.07 (m, 2H), 4.40 (t, *J* = 5.9 Hz, 2H), 3.55 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.9 (C), 166.0 (d, *J* = 254 Hz), 161.5 (C), 148.2 (CH), 147.7 (C), 134.3 (CH), 132.6 (C) (d, *J* = 3 Hz), 130.8 (C) (d, *J* = 10 Hz), 127.6 (CH), 127.2 (CH), 126.4 (CH), 122.0, 115.9 (d, *J* = 22 Hz), 42.8 (CH_2), 36.7 (CH_2); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -103.9. HRMS (ESI) m/z calcd for $C_{17}H_{14}FN_2O_2^+$ $(M+H)^+$ 297.1034, found 297.1037.

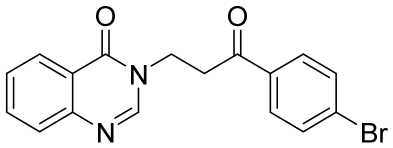
3-(3-(4-chlorophenyl)-3-oxopropyl) quinazolin-4(3*H*)-one (3f)[1]



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 4-chloroacetophenone (53 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3f** (31.3 mg, 50%) as a white solid. mp:197-198 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 (s, 1H), 8.28 (dd, *J* = 8.0 Hz, 1.5 Hz, 1H), 7.89 – 7.87 (m, 2H), 7.77 – 7.69 (m, 2H), 7.51 – 7.49 (m, 1H), 7.43 – 7.41 (m, 2H), 4.42 (t, *J* = 5.9 Hz, 2H), 3.57 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.3 (C), 161.5 (C), 148.2 (CH), 147.6 (C), 140.2 (C), 134.4 (CH), 134.4 (CH), 129.5 (CH), 129.1 (CH), 127.6 (CH), 127.3 (CH), 126.4 (CH), 122.0 (C), 42.8 (CH_2), 36.8 (CH_2).

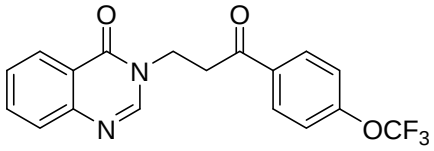
3-(3-(4-bromophenyl)-3-oxopropyl) quinazolin-4(3*H*)-one (3g)



The reaction was conducted with quinazolin-4(3*H*)-one (29.2 mg, 0.2 mmol) and 4-bromoacetophenone (79.7 mg, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3g** (34.3mg, 48%) as a white solid. mp:185-186 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 (s, 1H), 8.26 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.80 – 7.75 (m, 2H), 7.74 – 7.68 (m, 2H), 7.59 – 7.55 (m, 2H), 7.50 – 7.46 (m, 1H), 4.40 (t, *J* = 5.9 Hz, 2H), 3.55 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.6 (C), 161.5 (C), 148.1 (CH), 147.6 (C), 134.8 (C), 134.4 (CH), 132.1 (CH), 129.6 (CH), 129.0 (C), 127.6 (CH), 127.3 (CH), 126.4 (CH), 122.0 (C), 42.8 (CH_2), 36.8 (CH_2). HRMS (ESI) m/z calcd for $C_{17}H_{14}BrN_2O_2^+$ $(M+H)^+$ 357.0233, found 357.0247.

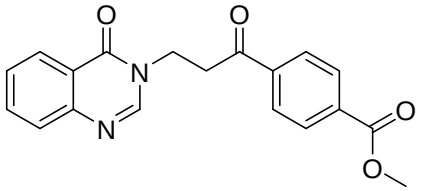
3-(3-oxo-3-(4-(trifluoromethoxy) phenyl) propyl) quinazolin-4(3*H*)-one (3h)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 4-trifluoromethoxyacetophenone (62.8 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3h** (25.3 mg, 35%) as a white solid. mp:185-186 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (s, 1H), 8.28 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.02 – 7.99 (m, 2H), 7.77 – 7.70 (m, 2H), 7.52 – 7.47 (m, 1H), 7.28 (d, *J* = 1.5 Hz, 2H), 4.43 (t, *J* = 5.9 Hz, 2H), 3.59 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.0 (C), 161.4 (C), 153.0 (C), 148.1 (CH), 147.6 (C), 134.4 (CH), 134.3 (C), 130.2 (CH), 127.6 (CH), 127.2 (CH), 126.4 (CH), 121.9 (C), 121.5 (C) (q, *J* = 258 Hz), 120.5 (CH), 42.8 (CH_2), 36.8 ((CH_2); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.6. HRMS (ESI) m/z calcd for $C_{18}H_{14}F_3N_2O_3^+$ $(M+H)^+$ 363.0951, found 363.0955.

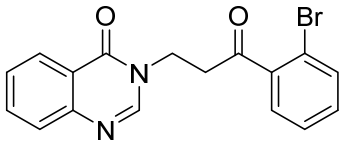
methyl 4-(3-(4-oxoquinazolin-3(4*H*)-yl) propanoyl) benzoate (3i)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and methyl 4-acetylbenzoate (64 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3i** (33.6 mg, 50%) as a white solid. mp:168-169 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 (s, 1H), 8.28 – 8.25 (m, 1H), 8.08 (d, *J* = 8.5 Hz, 2H), 7.97 (d, *J* = 8.5 Hz, 2H), 7.76 – 7.68 (m, 2H), 7.50 – 7.46 (m, 1H), 4.42 (t, *J* = 5.9 Hz, 2H), 3.92 (s, 3H), 3.62 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.1 (C), 166.0 (C), 161.5 (C), 148.2 (CH), 147.6 (C), 139.2 (C), 134.4 (CH), 129.9 (C), 128.0 (CH), 127.6 (CH), 127.3 (CH), 126.4 (CH), 122.0 (C), 52.5 (CH_3), 42.7 (CH_2), 37.2 (CH_2). HRMS (ESI) m/z calcd for $C_{19}H_{17}N_2O_4^+$ $(M+H)^+$ 337.1183, found 337.1177.

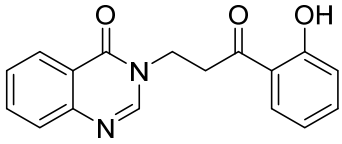
3-(3-(2-bromophenyl)-3-oxopropyl) quinazolin-4(3*H*)-one (3j)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 2-bromoacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3j** (14.3 mg, 20%) as a yellow liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 7.77 – 7.70 (m, 2H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.40 – 7.28 (m, 3H), 4.41 (t, *J* = 5.9 Hz, 2H), 3.54 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 201.3 (C), 161.4 (C), 148.2 (CH), 147.4 (C), 140.2 (C), 134.4 (CH), 134.0 (CH), 132.2 (CH), 128.8 (CH), 127.6 (CH), 127.6 (CH), 126.4 (CH), 122.0 (C), 118.9 (C), 42.7 (CH_2), 40.8 (CH_2). HRMS (ESI) m/z calcd for $C_{17}H_{14}BrN_2O_2^+$ $(M+H)^+$ 357.0233, found 357.0229.

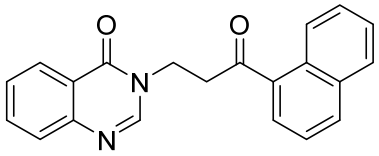
3-(3-(2-hydroxyphenyl)-3-oxopropyl) quinazolin-4(3*H*)-one (3k)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 2-hydroxyacetophenone (50 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 2/1) to yield **3k** (11.8 mg, 20%) as a purple solid. mp:184-185 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.95 (s, 1H), 8.36 (s, 1H), 8.28 (d, *J* = 8.6 Hz, 1H), 7.78 – 7.70 (m, 3H), 7.52 – 7.44 (m, 2H), 6.97 – 6.95 (m, 1H), 6.90 – 6.86 (m, 1H), 4.42 (t, *J* = 5.9 Hz, 2H), 3.65 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 203.4 (C), 162.4 (C), 161.5 (C), 148.1 (CH), 147.6 (C), 137.0 (CH), 134.4 (CH), 129.8 (CH), 127.6 (CH), 127.3 (CH), 126.4 (CH), 122.0 (C), 119.2 (C), 119.0 (CH), 118.6 (CH), 42.5 (CH_2), 36.4 (CH_2). HRMS (ESI) m/z calcd for $C_{17}H_{15}N_2O_3^+$ $(M+H)^+$ 295.1077, found 295.1078.

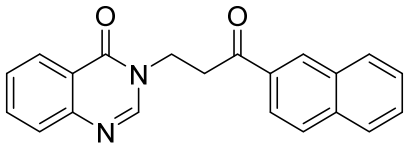
3-(3-(naphthalen-1-yl)-3-oxopropyl) quinazolin-4(3*H*)-one (3l)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 1-acetonaphthone (68 mg, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3l** (39.4 mg, 60%) as a white solid. 151-152 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.72 (d, *J* = 8.6 Hz, 1H), 8.40 (s, 1H), 8.29 (d, *J* = 7.9 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.91 (d, *J* = 7.2 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.75 –7.69 (m, 2H), 7.59 – 7.55 (m, 1H), 7.52 – 7.42 (m, 3H), 4.47 (t, *J* = 5.9 Hz, 2H), 3.68 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 200.9 (C), 161.4 (C), 148.2 (CH), 147.6 (C), 134.3 (C), 134.1 (CH), 134.0 (C), 133.7 (C), 130.2 (CH), 128.8 (CH), 128.5 (CH), 128.4 (CH), 127.6 (CH), 127.2 (CH), 126.6 (CH), 126.4 (CH), 125.7 (CH), 124.3 (CH), 122.1 (C), 43.2 (CH_2), 39.7 (CH_2). HRMS (ESI) m/z calcd for $C_{21}H_{17}N_2O_2^+$ $(M+H)^+$ 329.1285, found 329.1293.

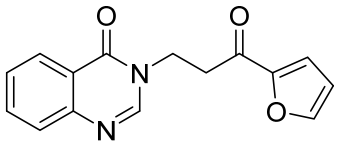
3-(3-(naphthalen-2-yl)-3-oxopropyl) quinazolin-4(3*H*)-one (3m)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 2-acetonaphthone (68 mg, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3m** (41.4 mg, 63%) as a white solid. mp:201-202 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 (s, 1H), 8.40 (s, 1H), 8.29 (d, *J* = 8.0 Hz, 1H), 7.98 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.86 – 7.82 (m, 2H), 7.74 – 7.68 (m, 2H), 7.60 –7.45 (m, 3H), 4.47 (t, *J* = 5.8 Hz, 2H), 3.72 (t, *J* = 5.8 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.4 (C), 161.5 (C), 148.2 (CH), 147.7 (C), 135.8 (CH), 134.3 (C), 133.5 (C), 132.4 (C), 130.1 (C), 129.6 (CH), 128.8 (CH), 128.6 (CH), 127.8 (CH), 127.6 (CH), 127.2 (CH), 127.0 (CH), 126.4 (CH), 123.5 (CH), 122.0 (C), 42.9 (CH_2), 36.9 (CH_2). HRMS (ESI) m/z calcd for $C_{21}H_{17}N_2O_2^+$ $(M+H)^+$ 329.1285, found 329.1280.

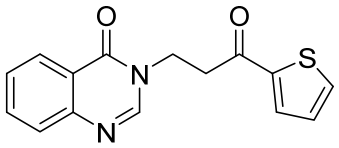
3-(3-(furan-2-yl)-3-oxopropyl) quinazolin-4(3*H*)-one (3n)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 1-(furan-2-yl)ethan-1-one (43 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3n** (10.7 mg, 20%) as a white solid. mp:188-189 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 (s, 1H), 8.28 (d, *J* = 8.1 Hz, 1H), 7.76 – 7.69 (m, 2H), 7.56 (d, *J* = 1.6 Hz, 1H), 7.51 – 7.47 (m, 1H), 7.21 (d, *J* = 3.6 Hz, 1H), 6.51 (dd, *J* = 3.6, 1.6 Hz, 1H), 4.40 (t, *J* = 6.0 Hz, 2H), 3.45 (t, *J* = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 186.4 (C), 161.4 (C), 152.1 (C), 148.2 (CH), 147.5 (C), 146.9 (CH), 134.3 (CH), 127.6 (CH), 127.2 (CH), 126.4 (CH), 122.0 (C), 117.9 (CH), 112.5 (CH), 42.3 (CH_2), 36.7 (CH_2). HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2O_3^+$ $(M+H)^+$ 269.0921, found 269.0917.

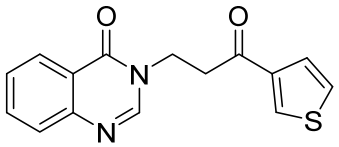
3-(3-oxo-3-(thiophen-2-yl) propyl) quinazolin-4(3*H*)-one (3o)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 1-(thiophen-2-yl)ethan-1-one (46.6 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3o** (35.3 mg, 62%) as a white solid. mp:203-204 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 8.28 – 8.26 (m, 1H), 7.76 – 7.68 (m, 3H), 7.63 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.11 – 7.07 (m, 1H), 4.40 (t, *J* = 5.9 Hz, 2H), 3.52 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 190.4 (C), 161.4 (C), 148.2 (CH), 147.6 (C), 143.3 (C), 134.4 (CH), 134.3 (CH), 132.6 (CH), 128.3 (CH), 127.6 (CH), 127.2 (CH), 126.4 (CH), 122.0 (C), 42.7 (CH_2), 37.4 (CH_2). HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2O_2S^+$ $(M+H)^+$ 285.0692, found 285.0701.

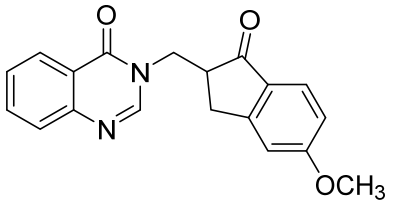
3-(3-oxo-3-(thiophen-3-yl) propyl) quinazolin-4(3*H*)-one (3p)



The reaction was conducted with quinazolin-4(*3H*)-one (29.2 mg, 0.2 mmol) and 3-acetylthiophene (50.5 mg, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3p** (28.5 mg, 50%) as a white solid. mp:206-207 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.34 (s, 1H), 8.28 – 8.26 (m, 1H), 8.07 (dd, *J* = 2.9, 1.3 Hz, 1H), 7.75 – 7.68 (m, 2H), 7.51 – 7.45 (m, 2H), 7.29 (dd, *J* = 5.1, 2.9 Hz, 1H), 4.39 (t, *J* = 5.9 Hz, 2H), 3.49 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 191.7 (C), 161.4 (C), 148.2 (CH), 147.6 (C), 141.5 (C), 134.3 (CH), 132.8 (CH), 127.6 (CH), 127.2 (CH), 126.7 (CH), 126.7 (CH), 126.4 (C), 122.0 (CH), 42.7 (CH_2), 38.0 (CH_2). HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2O_2S^+$ $(M+H)^+$ 285.0692, found 285.0701.

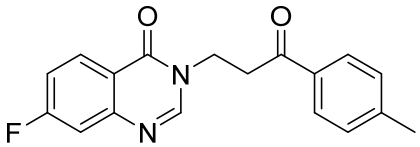
3-((5-methoxy-1-oxo-2,3-dihydro-1*H*-inden-2-yl) methyl) quinazolin-4(3*H*)-one (3q)



The reaction was conducted with quinazolin-4(3*H*)-one (13.6 mg, 0.2 mmol) and 5-methoxy-2,3-dihydro-1*H*-inden-1-one (65 mg, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3q** (16.1 mg, 25%) as a white solid. mp; 189-190 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.13 (s, 1H), 7.78 – 7.70 (m, 2H), 7.53 – 7.48 (m, 1H), 7.35 – 7.33 (m, 2H), 7.05 – 7.02 (m, 1H), 4.45 – 4.32 (m, 2H), 3.86 (s, 3H), 3.33 – 3.22 (m, 2H), 2.95 – 2.86 (m, 1H); ^{13}C NMR (100MHz, Chloroform-*d*) δ 205.7 (C), 161.5 (C), 156.9 (C), 148.0 (C), 146.9 (CH), 142.1 (C), 137.5 (CH), 134.4 (C), 129.4 (CH), 127.6 (CH), 127.3 (CH), 126.8 (CH), 122.0 (C), 115.6 (CH), 115.4 (CH), 55.5 (CH_3), 46.9 (CH_2), 46.8 (CH), 27.5 (CH_2). HRMS (ESI) m/z calcd for $C_{19}H_{17}N_2O_3^+$ (M+H)+ 321.1234, found 321.1232.

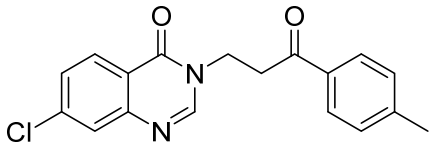
6-fluoro-3-(3-oxo-3-(p-tolyl) propyl) quinazolin-4(3*H*)-one (3r)



The reaction was conducted with 7-fluoroquinazolin-4(3*H*)-one (38.2 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3r** (31.0 mg, 50%) as a white solid. mp:191-192 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (s, 1H), 8.27 – 8.23 (m, 1H), 7.82 – 7.78 (m, 2H), 7.32 – 7.28 (m, 1H), 7.21 – 7.12 (m, 3H), 4.40 – 4.36 (m, 2H), 3.55 – 3.53 (m, 2H), 2.36 (d, *J* = 2.3 Hz, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.1 (C), 167.6 (C) (d, *J* = 253 Hz), 160.7 (C), 150.4 (C) (d, *J* = 129 Hz), 149.06 (CH), 144.66 (C), 133.62 (C), 129.40 (CH), 129.2 (C) (d, *J* = 105 Hz), 128.18 (CH), 118.7 (C) (d, *J* = 19 Hz), 116.0 (C) (d, *J* = 23 Hz), 112.9 (C) (d, *J* = 22 Hz), 42.8 (CH_2), 36.6 (CH_2), 21.7 (CH_3); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -103.2. HRMS (ESI) m/z calcd for $C_{18}H_{16}FN_2O_2^+$ $(M+H)^+$ 311.1190, found 311.1196.

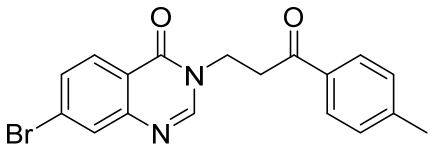
7-chloro-3-(3-oxo-3-(p-tolyl) propyl) quinazolin-4(3*H*)-one (3s)



The reaction was conducted with 7-chloroquinazolin-4(3*H*)-one (35.9 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3s** (19.6 mg, 30%) as a white solid. mp:194-195 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (s, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 2H), 7.63 (s, 1H), 7.38 – 7.35 (m, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 4.37 (t, *J* = 5.8 Hz, 2H), 3.52 (t, *J* = 5.8 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.1 (C), 160.8 (C), 149.1 (CH), 149.0 (C), 144.7 (C), 140.4 (C), 133.6 (C), 129.4 (CH), 128.2 (CH), 127.9 (CH), 127.7 (CH), 127.0 (CH), 120.5 (C), 42.9 (CH_2), 36.6 (CH_2), 21.7 (CH_3). HRMS (ESI) m/z calcd for $C_{18}H_{16}ClN_2O_2^+$ $(M+H)^+$ 327.0895, found, 327.0894.

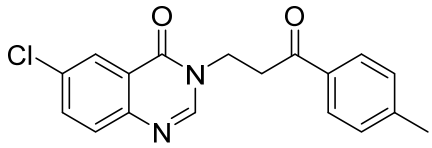
6-bromo-3-(3-oxo-3-(p-tolyl) propyl) quinazolin-4(3*H*)-one (3t)



The reaction was conducted with 7-bromoquinazolin-4(3*H*)-one (44.8 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3t** (25.9 mg, 35%) as a white solid. mp:195-196 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (s, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.86 (d, *J* = 1.8 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 2H), 7.56 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.22 (d, *J* = 8.1 Hz, 2H), 4.39 (t, *J* = 5.8 Hz, 2H), 3.54 (t, *J* = 5.8 Hz, 2H), 2.38 (s, 4H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.1 (C), 161.0 (C), 149.2 (CH), 149.0 (C), 144.7 (C), 133.6 (C), 130.5 (CH), 130.3 (CH), 129.4 (CH), 129.0 (CH), 128.2 (CH), 127.9 (C), 120.8 (C), 43.0 (CH_2), 36.7 (CH_2), 21.7 (CH_3). HRMS (ESI) m/z calcd for $C_{18}H_{16}BrN_2O_2^+$ $(M+H)^+$ 371.0390, found 371.0378.

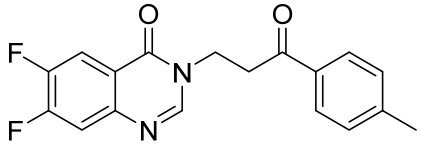
6-chloro-3-(3-oxo-3-(p-tolyl) propyl) quinazolin-4(3*H*)-one (3u)



The reaction was conducted with 6-chloroquinazolin-4(3*H*)-one (35.9 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3u** (39.2 mg, 60%) as a white solid. mp:184-185 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (s, 1H), 8.23 (d, *J* = 2.1 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 2H), 7.68 – 7.63 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 4.41 (t, *J* = 5.8 Hz, 2H), 3.56 (t, *J* = 5.8 Hz, 2H), 2.39 (s, 3H); 13C NMR (100 MHz, Chloroform-d) δ 197.1 (C), 160.4 (C), 148.0 (CH), 146.7 (C), 144.7 (C), 134.7 (C), 133.6 (CH), 133.0 (CH), 129.4 (CH), 129.2 (CH), 128.2 (CH), 125.8 (CH), 123.0 (C), 43.0 (CH_2), 36.5 (CH_2), 21.7 (CH_3). HRMS (ESI) m/z calcd for $C_{18}H_{16}ClN_2O_2^+$ $(M+H)^+$ 327.0895, found, 327.0898.

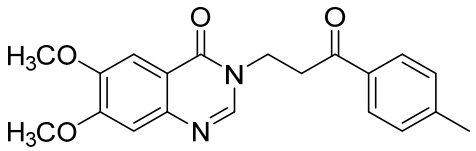
6,7-difluoro-3-(3-oxo-3-(p-tolyl) propyl) quinazolin-4(3*H*)-one (3v)



The reaction was conducted with 6,7-difluoroquinazolin-4(3*H*)-one (36.4 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3v** (16.4 mg, 25%) as a white solid. mp:184-185 ^{o}C

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 (s, 1H), 7.81 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.14 (m, 1H), 6.90 – 6.84 (m, 1H), 4.37 (t, *J* = 5.7 Hz, 2H), 3.55 (t, *J* = 5.7 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.1 (C), 166.9 (C) (d, *J* = 253.7 Hz), 164.4 (C) (d, *J* = 253.8 Hz), 163.7 (C) (d, *J* = 14.7 Hz, 161.0 (C) (d, *J* = 14.6 Hz), 157.9 (C) (d, *J* = 4.1 Hz), 151.6 (C) (d, *J* = 14.5 Hz), 149.8 (CH), 144.7 (C), 133.6 (C), 129.4 (CH), 128.2 (CH), 109.5 (C) (d, *J* = 4.5 Hz), 109.2 (C) (d, *J* = 4.7 Hz), 103.6 (C) (q, *J* = 25.5 Hz), 42.9 (CH_2), 36.3 (CH_2), 21.7 (CH_3); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -99.8, -105.3. HRMS (ESI) m/z calcd for $C_{18}H_{15}F_2N_2O_2^+$ $(M+H)^+$ 329.1096, found 329.1095.

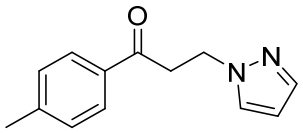
6,7-dimethoxy-3-(3-oxo-3-(p-tolyl) propyl) quinazolin-4(3*H*)-one (3w)



The reaction was conducted with 6,7-dimethoxyquinazolin-4(3*H*)-one (41.2 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **3w** (35.3 mg, 50%) as a white solid. mp:219-220 ^{o}C

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.34 (s, 1H), 7.86 (d, J = 8.1 Hz, 2H), 7.43 (s, 1H), 7.30 (d, J = 8.1 Hz, 2H), 7.11 (s, 1H), 4.27 (t, J = 6.7 Hz, 2H), 3.88 (s, 3H), 3.85 (s, 3H), 3.52 (t, J = 6.7 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 198.1 (C), 160.1 (C), 154.9 (C), 149.1 (CH), 147.6 (C), 144.5 (C), 144.4 (C), 134.2 (C), 129.8 (CH), 128.5 (CH), 115.1 (C), 108.2 (CH), 105.3 (CH), 56.4 (CH_3), 56.2 (CH_3), 42.7 (CH_2), 37.4 (CH_2), 21.6 (CH_3). HRMS (ESI) m/z calcd for $C_{20}H_{21}N_2O_4^+$ $(M+H)^+$ 353.1496, found 353.1499.

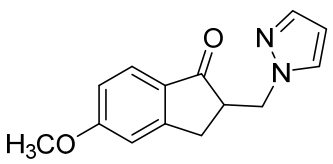
3-(1*H*-pyrazol-1-yl)-1-(p-tolyl) propan-1-one (5a)[2]



The reaction was conducted with pyrazole (13.6 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 10/1) to yield **5a** (29.1 mg, 68%) as a white oil.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.82 (d, J = 8.2 Hz, 2H), 7.49 (d, J = 2.2 Hz, 2H), 7.23 (d, J = 8.5 Hz, 2H), 6.19 (t, J = 2.1 Hz, 1H), 4.58 (t, J = 6.6 Hz, 2H), 3.55 (t, J = 6.6 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 197.1 (C), 144.4 (C), 139.6 (CH), 133.9 (C), 130.1 (CH), 129.4 (CH), 128.2 (CH), 105.3 (CH), 46.7 (CH_2), 38.7 (CH_2), 21.7 (CH_3).

2-((1*H*-pyrazol-1-yl) methyl)-5-methoxy-2,3-dihydro-1*H*-inden-1-one (5b)

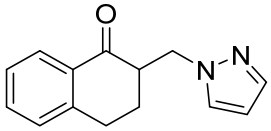


The reaction was conducted with pyrazole (13.6 mg, 0.2 mmol) and 5-methoxy-2,3-dihydro-1*H*-inden-1-one (65 mg, 0.4 mmol). Purification by thin layer

chromatography was performed (petroleum ether/ethyl acetate = 10/1) to yield **5b** (22.8 mg, 47%) as a white solid. mp: 85-86 ^{o}C

^{1}H NMR (400 MHz, Chloroform-d) δ 7.46 (d, *J* = 1.8 Hz, 1H), 7.40 (d, *J* = 2.3 Hz, 1H), 7.35 – 7.27 (m, 2H), 7.03 – 6.99 (m, 1H), 6.20 (t, *J* = 1.9 Hz, 1H), 4.66 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.41 (dd, *J* = 8.1 Hz, 7.0 Hz, 1H), 3.85 (s, 3H), 3.23 – 3.15 (m, 2H), 2.95 – 2.87 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-d) δ 205.7 (C), 157.0 (C), 142.6 (C), 139.5 (CH), 137.7 (C), 129.7 (CH), 129.1 (CH), 115.5 (CH), 115.3 (CH), 105.7 (CH), 55.5 (CH_3), 52.0 (CH_2), 48.5 (CH), 27.3 (CH_2). HRMS (ESI) m/z calcd for $C_{14}H_{15}N_2O_2^+$ $(M+H)^+$ 243.1128, found 243.1130.

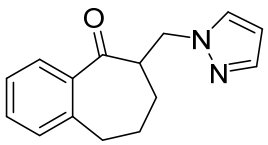
2-((1*H*-pyrazol-1-yl) methyl)-3,4-dihydronaphthalen-1(2*H*)-one (5c)



The reaction was conducted with pyrazole (13.6 mg, 0.2 mmol) and 3,4-dihydronaphthalen-1(2*H*)-one (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 10/1) to yield **5c** (20.4 mg, 45%) as a yellow liquid.

^{1}H NMR (400 MHz, Chloroform-d) δ 8.03 (d, J = 7.8 Hz, 1H), 7.50 – 7.45 (m, 3H), 7.31 (t, J = 7.5 Hz, 1H), 7.22 (d, J = 7.7 Hz, 1H), 6.24 (s, 1H), 4.80 – 4.75 (m, 1H), 4.42 – 4.37 (m, 1H), 3.11 – 2.90 (m, 3H), 2.12 – 2.08 (m, 1H), 1.84 – 1.74 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.8 (C), 144.1 (C), 139.4 (CH), 133.7 (C), 132.2 (CH), 130.4 (CH), 128.9 (CH), 127.4 (CH), 126.8 (CH), 105.5 (CH), 51.6 (CH_2), 48.8 (CH), 28.8 (CH_2), 27.0 (CH_2). HRMS (ESI) m/z calcd for $C_{14}H_{14}N_2ONa^+$ $(M+Na)^+$ 249.0998, found 249.0998.

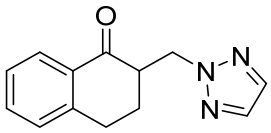
6-((1*H*-pyrazol-1-yl) methyl)-6,7,8,9-tetrahydro-5*H*-benzo [7] annulen-5-one (5d)



The reaction was conducted with pyrazole (13.6 mg, 0.2 mmol) and 6,7,8,9-tetrahydro-5*H*-benzo[7]annulen-5-one (59.8 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 10/1) to yield **5d** (12.1 mg, 25%) as a yellow liquid.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.64 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.46 (dd, *J* = 4.7, 2.0 Hz, 2H), 7.40 – 7.36 (m, 1H), 7.27 (d, *J* = 3.9 Hz, 1H), 7.21 (d, *J* = 7.6 Hz, 1H), 6.19 (s, 1H), 4.75 – 4.70 (m, 1H), 4.30 – 4.25 (m, 1H), 3.63 – 3.55 (m, 1H), 3.09 – 2.93 (m, 2H), 2.17 – 2.10 (m, 1H), 1.94 – 1.90 (m, 1H), 1.73 – 1.55 (m, 2H); ^{13}C NMR (100 MHz, Chloroform-d) δ 204.2 (C), 142.8 (C), 139.5 (C), 138.9 (CH), 131.8 (CH), 130.5 (CH), 130.1 (CH), 128.6 (CH), 126.5 (CH), 105.1 (CH), 52.3 (CH_2), 50.5 (CH), 33.5 (CH_2), 28.0 (CH_2), 25.4 (CH_2). HRMS (ESI) m/z calcd for $C_{15}H_{17}N_2O^+$ $(M+H)^+$ 241.1335, found 241.1330.

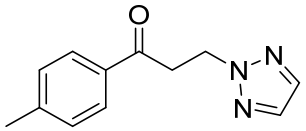
2-((2*H*-1,2,3-triazol-2-yl) methyl)-3,4,8,8a-tetrahydronaphthalen-1(2*H*)-one (5e)



The reaction was conducted with 1,2,3-triazole (13.8 mg, 0.2 mmol) and 3,4-dihydronaphthalen-1(2*H*)-one (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **5e** (15.1 mg, 63%) as a white solid. mp: 117-118 ^{o}C

^{1}H NMR (400 MHz, Chloroform-d) δ 8.04 (d, J = 7.8 Hz, 1H), 7.70 (d, J = 14.7 Hz, 1H), 7.50 (t, J = 7.5 Hz, 1H), 7.32 (t, J = 7.6 Hz, 1H), 7.24 (d, J = 7.7 Hz, 1H), 4.95 – 4.92 (m, 1H), 4.81 – 4.76 (m, 1H), 3.13 – 2.93 (m, 3H), 2.26 – 2.20 (m, 1H), 1.83 – 1.72 (m, 2H); ^{13}C NMR (100 MHz, Chloroform-d) δ 197.2 (C), 144.0 (C), 134.0 (C), 133.9 (CH), 131.9 (CH), 128.9 (CH), 127.5 (CH), 126.9 (CH), 124.9(CH), 49.6 (CH_2), 48.6 (CH), 28.8 (CH_2), 27.0 (CH_2). HRMS (ESI) m/z calcd for $C_{13}H_{14}N_3O^+$ $(M+H)^+$ 228.1131, found 228.1139.

1-(p-tolyl)-3-(2*H*-1,2,3-triazol-2-yl) propan-1-one (5f)

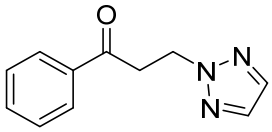


The reaction was conducted with 1,2,3-triazole (13.8 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **5f** (23.7 mg, 55%) as a white solid. mp:125-126 ^{o}C

^{1}H NMR (400 MHz, Chloroform-d) δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.72 (s, 1H), 7.65 (s, 1H), 7.24 (d, *J* = 7.7 Hz, 1H), 4.84 (t, *J* = 6.9 Hz, 2H), 3.63 (t, *J* = 6.9 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (100

MHz, Chloroform-d) δ 196.2 (C), 144.8 (C), 133.6 (C), 133.5 (CH), 129.5 (CH), 128.2 (CH), 124.8 (CH), 44.7 (CH_2), 38.6 (CH_2), 21.7 (CH_3). HRMS (ESI) m/z calcd for $C_{12}H_{14}N_3O^+$ $(M+H)^+$ 216.1131, found 216.1141.

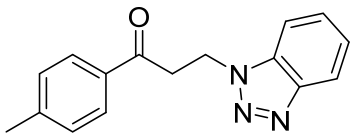
1-phenyl-3-(2*H*-1,2,3-triazol-2-yl) propan-1-one (5g)



The reaction was conducted with 1,2,3-triazole (13.8 mg, 0.2 mmol) and acetophenone (37 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **5g** (15.1 mg, 63%) as a white solid. mp: 123-124 ^oC

^1H NMR (400 MHz, Chloroform-d) δ 7.94 – 7.92 (m, 2H), 7.73 (s, 1H), 7.66 (s, 1H), 7.61 – 7.57 (m, 1H), 7.49 –7.45 (m, 2H), 4.86 (t, *J* = 6.2 Hz, 2H), 3.67 (t, *J* = 6.2 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-d) δ 196.6 (C), 135.9 (C), 133.9 (CH), 133.7 (CH), 128.8 (CH), 128.1 (CH), 124.8 (CH), 44.6 (CH_2), 38.7 (CH_2). HRMS (ESI) m/z calcd for $C_{11}H_{11}N_3ONa^+$ $(M+Na)^+$ 224.0794, found 224.0792.

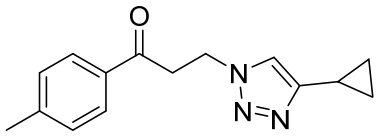
3-(1*H*-benzo[d][1,2,3] triazol-1-yl)-1-(p-tolyl) propan-1-one (5h)



The reaction was conducted with benzotriazole (23.2 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **5h** (28.1 mg, 53%) as a white solid. mp:133-134 ^oC

^1H NMR (400 MHz, Chloroform-d) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 2H), 7.70 (d, *J* = 8.3 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 5.04 (t, *J* = 6.8 Hz, 2H), 3.77 (t, *J* = 6.8 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 196.3 (C), 145.8 (C), 144.7 (C), 133.6 (C), 133.2 (C), 129.5 (CH), 128.2 (CH), 127.4 (CH), 124.0 (CH), 119.9 (CH), 109.8 (CH), 42.7 (CH_2), 38.2 (CH_2), 21.7 (CH_3). HRMS (ESI) m/z calcd for $C_{16}H_{16}N_3O^+$ $(M+H)^+$ 266.1288, found 266.1295.

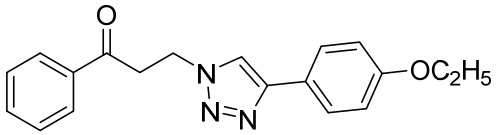
3-(4-cyclopropyl-1*H*-1,2,3-triazol-1-yl)-1-(p-tolyl) propan-1-one (5i)



The reaction was conducted with 4-cyclopropyl-1*H*-1,2,3-triazole (21.8 mg, 0.2 mmol) and 4-methyacetophenone (54 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 10/1) to yield **5i** (12.8 mg, 25%) as a white solid. mp:124-125 ^{o}C

^{1}H NMR (400 MHz, Chloroform-d) δ 7.86 (d, *J* = 8.1 Hz, 2H), 7.25 (s, 1H), 4.78 (t, *J* = 7.3 Hz, 2H), 3.63 (t, *J* = 7.3 Hz, 2H), 2.41 (s, 3H), 1.94 – 1.88 (m, 1H), 0.97 – 0.92 (m, 2H), 0.76 – 0.72 (m, 2H); ^{13}C NMR (100 MHz, Chloroform-d) δ 196.4 (C), 150.8 (C), 144.4 (C), 133.9 (C), 131.0 (CH), 129.4 (CH), 128.2 (CH), 49.7 (CH_2), 37.9 (CH_2), 21.7 (CH_3), 8.0 (CH), 6.7 (CH_2). HRMS (ESI) m/z calcd for $C_{14}H_{14}N_3ONa^+$ $(M+Na)^+$ 278.1264, found 278.1262.

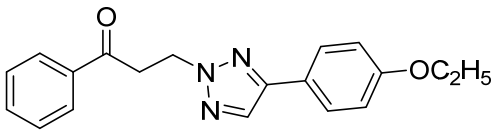
3-(4-(4-ethoxyphenyl)-1*H*-1,2,3-triazol-1-yl)-1-phenylpropan-1-one (5j)



The reaction was conducted with 4-(4-ethoxyphenyl)-1*H*-1,2,3-triazole (37.8 mg, 0.2 mmol) and acetophenone (37 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **5j** (15.4 mg, 25%) as a white solid. mp:122-123 ^{o}C

^{1}H NMR (400 MHz, Chloroform-d) δ 7.95 (d, *J* = 7.9 Hz, 2H), 7.86 (s, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 6.94 (d, *J* = 8.5 Hz, 2H), 4.87 (t, *J* = 6.1 Hz, 2H), 4.06 (q, *J* = 7.0 Hz, 2H), 3.70 (t, *J* = 6.1 Hz, 2H), 1.43 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 196.7 (C), 158.9 (C), 147.6 (C), 135.9 (C), 133.9 (CH), 128.8 (CH), 128.1 (CH), 127.0 (CH), 123.1 (C), 120.3 (CH), 114.7 (CH), 63.5 (CH_2), 44.7 (CH_2), 38.8 (CH_2), 14.9 (CH_3). HRMS (ESI) m/z calcd for $C_{19}H_{20}N_3O_2^+$ $(M+H)^+$ 322.1550, found 322.1560.

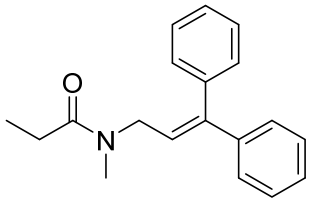
3-(4-(4-ethoxyphenyl)-2*H*-1,2,3-triazol-2-yl)-1-phenylpropan-1-one (5k)



The reaction was conducted with 4-(4-ethoxyphenyl)-1*H*-1,2,3-triazole (37.8 mg, 0.2 mmol) and acetophenone (37 μL, 0.4 mmol). Purification by thin layer chromatography was performed (petroleum ether/ethyl acetate = 5/1) to yield **5k** (12.8 mg, 20%) as a white solid. mp:122-123 ^{o}C

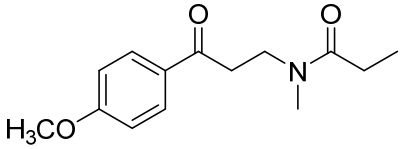
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 – 7.98 (m, 2H), 7.75 (s, 1H), 7.68 (d, *J* = 8.7 Hz, 2H), 7.61 – 7.57 (m, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 6.95 – 6.93 (m, 2H), 4.91 (t, *J* = 7.2 Hz, 2H), 4.07 (q, *J* = 7.0 Hz, 2H), 3.75 (t, *J* = 7.2 Hz, 2H), 1.44 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.7 (C), 158.9 (C), 147.6 (C), 135.9 (C), 133.9 (CH), 128.8 (CH), 128.1 (CH), 127.0 (CH), 123.1 (C), 120.3 (CH), 114.7 (CH), 63.5 (CH_2), 44.7 (CH_2), 38.8 (CH_2), 14.9 (CH_3). HRMS (ESI) m/z calcd for $C_{19}H_{20}N_3O_2^+$ $(M+H)^+$ 322.1550, found 322.1560.

***N*-(3,3-diphenylallyl)-*N*-methylpropionamide (7)[3]**



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.34 (m, 3H), 7.30 – 7.16 (m, 7H), 6.06 – 5.99 (m, 1H), 4.10 (d, *J* = 6.9 Hz, 1H), 3.96 (d, *J* = 6.5 Hz, 1H), 2.92 (s, 1H), 2.87 (s, 1H), 2.33 (q, *J* = 7.4 Hz, 1H), 2.23 (q, *J* = 7.4 Hz, 1H), 1.16 (t, *J* = 7.4 Hz, 1H), 1.09 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.7 (C), 172.6 (C), 144.1 (C), 143.6 (C), 140.5 (C), 140.1 (C), 138.0 (C), 137.6 (C), 128.7 (CH), 128.6 (CH), 127.5 (CH), 127.3 (CH), 127.3 (CH), 127.1 (CH), 126.8 (CH), 126.4 (CH), 126.4 (CH), 126.3 (CH), 126.2 (CH), 123.5 (CH), 122.5 (CH), 47.8 (CH_2), 45.3 (CH_2), 33.6 (CH_3), 32.4 (CH_3), 25.7 (CH_2), 25.3 (CH_2), 8.5 (CH_3), 8.3 (CH_3).

***N*-(3-(4-methoxyphenyl)-3-oxopropyl)-*N*-methylpropionamide (9)[3]**



According to previous literature reports, compound **7** was obtained. The specific operation is as follows:

To a test tube equipped with a magnetic stir bar was added *N,N*'-dimethylpropionamide. (1.5 mL), $CuF_2{\cdot}2H_2O$ (0.05 mmol, 6.9 mg), 4-methoxystyrene (0.5 mmol, 67 μL), and tert-butylhydroperoxide (TBHP, 2 mmol, 0.267 mL) in air. The resulting reaction mixture was kept stirring at 100 °C for 48 h. At the end of the reaction, the reaction mixture was cooled to

room temperature. After removal of the solvent, the residue was subjected to column chromatography on silica gel using ethyl acetate and petroleum ether mixtures (1:1) to afford the desired product **7** (54.8 mg, 50 %) as a white oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 – 7.90 (m, 2H), 6.93 – 6.91 (m, 2H), 3.86 (d, *J* = 6.5 Hz, 3H), 3.76 – 3.70 (m, 2H), 3.21 – 3.16 (m, 2H), 3.05 (s, 2H), 2.95 (s, 1H), 2.43 – 2.27 (m, 2H), 1.12 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.8 (C), 174.0 (C), 163.6 (C), 130.5 (CH), 130.4 (C), 130.3 (C), 129.8 (C), 113.9 (C), 113.8 (C), 113.6 (CH), 55.5 (CH_3), 45.1 (CH_2), 45.0 (CH_2), 36.7 (CH_3), 36.7 (CH_3), 26.9 (CH_2), 26.2 (CH_2), 9.7 (CH_3), 9.2 (CH_3).

6. references

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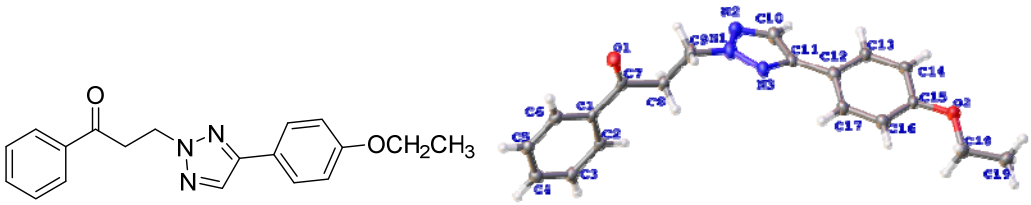
2 K. Sun, Z. Zhu, J. Sun, L. Liu and X. Wang, *J. Org. Chem*., 2016, **81**, 1476-83.

3 H. Yan, L. Lu, G. Rong, D. Liu, Y. Zheng, J. Chen and J. Mao, *J. Org. Chem*., 2014, **79**, 7103-7111.

7. Crystal data and structure refinement for 5k



5k

CCDC: 2131274

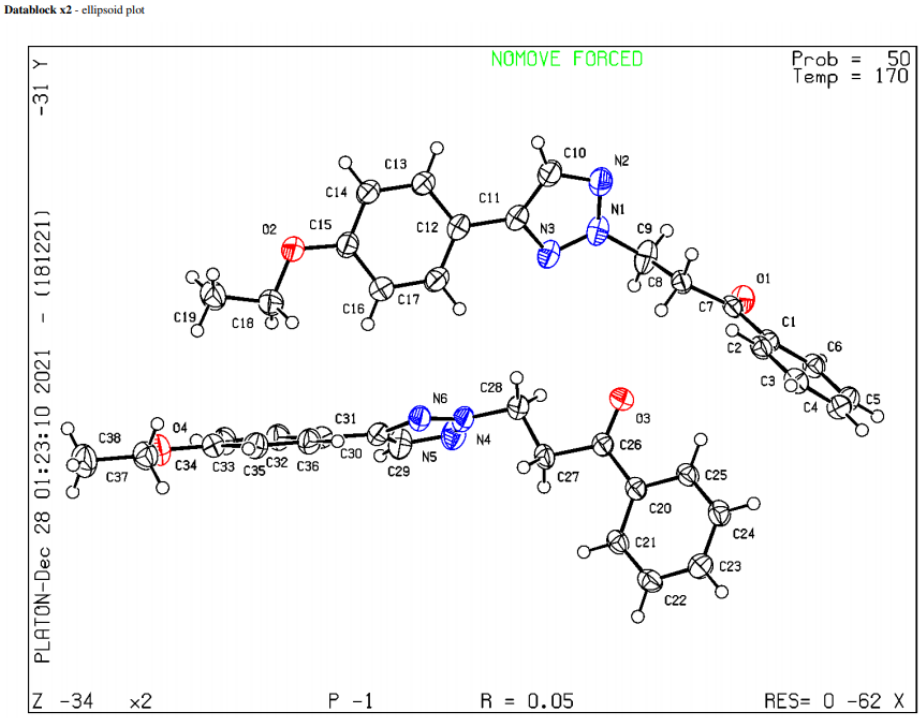


Table 1 Crystal data and structure refinement for **5k**

Empirical formula	$C_{19}H_{19}N_3O_2$
Formula weight	321.37
Temperature/K	169.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.5358(4)
b/Å	9.3335(3)
c/Å	20.6119(9)
α/°	95.328(3)
β/°	91.723(4)
γ/°	90.573(3)
Volume/Å^3	1634.16(12)
Z	4
ρ_{calc}g/cm^3	1.306
μ/mm^{-1}	0.697

F(000)	680.0
Crystal size/mm^3	0.15 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.622 to 147.93
Index ranges	-10 ≤ h ≤ 8, -11 ≤ k ≤ 11, -21 ≤ l ≤ 25
Reflections collected	11022
Independent reflections	6398 [R_{int} = 0.0319, R_{sigma} = 0.0441]
Data/restraints/parameters	6398/0/435
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0461, wR_2 = 0.1117
Final R indexes [all data]	R_1 = 0.0629, wR_2 = 0.1219
Largest diff. peak/hole / e Å^{-3}	0.16/-0.26

Crystal structure determination of [5k]

Crystal Data for $C_{19}H_{19}N_3O_2$ (*M* =321.37 g/mol): triclinic, space group P-1 (no. 2), *a* = 8.5358(4) Å, *b* = 9.3335(3) Å, *c* = 20.6119(9) Å, *α* = 95.328(3)°, *β* = 91.723(4)°, *γ* = 90.573(3)°, *V* = 1634.16(12) Å^3, *Z* = 4, *T* = 169.99(10) K, μ(Cu Kα) = 0.697 mm^{-1}, *Dcalc* = 1.306 g/cm^3, 11022 reflections measured (8.622° ≤ 2Θ ≤ 147.93°), 6398 unique (R_{int} = 0.0319, R_{sigma} = 0.0441) which were used in all calculations. The final R_1 was 0.0461 (I > 2σ(I)) and wR_2 was 0.1219 (all data).

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×1^3) f0or X2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	14563.9(14)	7715.6(13)	4207.6(6)	39.5(3)
O2	4066.2(14)	8917.4(16)	700.3(6)	45.9(3)
N1	11688.4(18)	9218.8(17)	2774.7(8)	41.3(4)
N2	12072(2)	10476.2(19)	2566.2(8)	46.5(4)
N3	10324.0(18)	8650.6(17)	2540.6(7)	40.2(3)
C1	13400.9(17)	8926.3(16)	5121.9(8)	28.3(3)
C2	12333.5(18)	9928.1(17)	5377.3(9)	32.0(3)
C3	12202.3(19)	10186.7(18)	6048.0(9)	35.9(4)
C4	13121(2)	9443.8(19)	6464.5(9)	38.5(4)
C5	14210(2)	8462.6(19)	6213.7(9)	37.0(4)
C6	14350.0(18)	8214.3(17)	5550.5(9)	32.3(3)
C7	13574.4(17)	8561.4(16)	4408.2(8)	29.9(3)
C8	12473.1(18)	9224.1(18)	3932.2(8)	31.6(3)
C9	12676(2)	8546(2)	3248.9(10)	47.4(5)
C10	10862(2)	10738(2)	2169.5(9)	44.2(4)
C11	9777(2)	9609.3(19)	2145.7(8)	35.8(4)
C12	8289(2)	9387.3(19)	1771.7(8)	35.9(4)

C13	7989(2)	10107(2)	1216.4(9)	38.9(4)
C14	6583(2)	9914(2)	866.7(9)	41.1(4)
C15	5430(2)	9008(2)	1069.9(9)	38.4(4)
C16	5704(2)	8268(2)	1614.3(9)	41.1(4)
C17	7130(2)	8467(2)	1957.0(9)	40.0(4)
C18	2781(2)	8139(2)	931.9(10)	46.1(5)
C19	1383(2)	8382(3)	496.0(11)	54.3(5)
O3	9839.4(14)	6849.2(13)	4196.9(6)	38.8(3)
O4	-751.8(14)	4186.8(16)	778.5(7)	46.3(3)
N4	7028.1(18)	4651.8(17)	2751.1(7)	39.4(3)
N5	7355(2)	3311.8(18)	2533.3(9)	47.8(4)
N6	5655.6(17)	5140.0(16)	2543.0(7)	38.6(3)
C20	8481.7(17)	6184.0(16)	5106.6(8)	28.8(3)
C21	7306.5(18)	5377.5(17)	5359.0(9)	32.2(3)
C22	7100.1(19)	5457.4(19)	6024.8(9)	36.5(4)
C23	8054(2)	6356.5(19)	6444.0(9)	37.4(4)
C24	9247(2)	7144.3(18)	6197.4(9)	37.0(4)
C25	9467.2(18)	7054.2(17)	5535.5(9)	32.3(3)
C26	8738.7(18)	6184.4(16)	4392.9(8)	30.3(3)
C27	7589.6(18)	5382.0(18)	3912.8(8)	33.3(4)
C28	8069(2)	5490(2)	3217.4(9)	41.8(4)
C29	6106(2)	2906(2)	2153.5(10)	45.8(4)
C30	5045(2)	4026.6(19)	2152.1(8)	35.9(4)
C31	3535(2)	4106.3(19)	1797.0(8)	34.5(4)
C32	3155(2)	3141(2)	1256.6(9)	38.8(4)
C33	1728(2)	3205(2)	925.2(9)	40.5(4)
C34	628(2)	4230(2)	1132.1(9)	37.2(4)
C35	985(2)	5201(2)	1667.9(9)	39.1(4)
C36	2433(2)	5131.8(19)	1991.5(9)	38.3(4)
C37	-1930(2)	5202(2)	976.4(10)	46.5(5)
C38	-3325(2)	4894(3)	518.0(12)	57.3(6)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **5k**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
O1	37.9(6)	36.8(6)	43.1(7)	1.2(5)	-3.7(5)	9.8(5)
O2	36.5(7)	65.2(9)	37.3(7)	14.2(6)	-4.9(5)	-6.9(6)
N1	45.2(8)	41.9(8)	35.3(8)	-0.8(6)	-10.5(6)	6.3(7)
N2	49.0(9)	49.0(9)	40.8(9)	4.2(7)	-10.0(7)	-3.8(7)
N3	44.9(8)	40.2(8)	35.0(8)	2.9(6)	-9.0(6)	5.4(7)

C1	22.5(7)	24.7(7)	37.5(9)	4.3(6)	-4.3(6)	-5.0(6)
C2	25.1(7)	28.3(8)	42.7(9)	6.6(7)	-4.5(6)	-1.2(6)
C3	31.0(8)	30.9(8)	45.3(10)	1.2(7)	1.1(7)	1.2(7)
C4	41.2(9)	38.5(9)	35.9(9)	5.4(7)	0.2(7)	-1.9(7)
C5	34.4(8)	37.2(9)	40.0(10)	9.5(7)	-5.8(7)	1.8(7)
C6	26.8(8)	29.0(8)	41.3(9)	4.9(7)	-2.2(6)	2.2(6)
C7	23.8(7)	24.9(7)	40.7(9)	4.0(6)	-4.1(6)	-4.7(6)
C8	26.7(8)	31.5(8)	36.4(9)	3.7(7)	-4.6(6)	-1.9(6)
C9	52.2(11)	47.0(11)	41.1(10)	-3.4(8)	-14.8(9)	15.9(9)
C10	50.3(11)	45.5(10)	37.1(10)	8.0(8)	-8.1(8)	-1.3(8)
C11	39.8(9)	39.7(9)	27.9(8)	2.8(7)	-1.1(7)	5.3(7)
C12	39.8(9)	39.2(9)	28.5(8)	1.7(7)	-1.6(7)	5.6(7)
C13	36.7(9)	48.4(10)	32.7(9)	9.9(8)	-0.1(7)	-0.3(8)
C14	38.2(9)	53.4(11)	33.2(9)	13.2(8)	-1.6(7)	1.0(8)
C15	36.1(9)	48.6(10)	30.3(9)	3.6(7)	-2.7(7)	0.9(8)
C16	43.8(10)	43.8(10)	36.2(10)	8.0(8)	-1.1(8)	-4.9(8)
C17	47.8(10)	40.9(9)	32.1(9)	8.9(7)	-2.6(7)	1.9(8)
C18	39.0(10)	61.3(12)	38.0(10)	4.6(9)	2.6(8)	-6.6(9)
C19	35.5(10)	76.9(15)	50.3(12)	6.2(11)	-0.3(8)	-6.9(10)
O3	37.3(6)	37.7(6)	42.3(7)	9.8(5)	-2.7(5)	-8.0(5)
O4	34.0(6)	57.7(8)	45.1(8)	-4.3(6)	-6.7(5)	1.0(6)
N4	41.8(8)	40.5(8)	36.3(8)	9.5(6)	-10.3(6)	-0.9(6)
N5	51.6(9)	43.9(9)	47.4(10)	5.0(7)	-12.1(7)	7.2(7)
N6	39.0(8)	39.6(8)	37.3(8)	6.9(6)	-8.2(6)	-2.2(6)
C20	23.9(7)	23.6(7)	39.1(9)	5.5(6)	-3.7(6)	4.4(6)
C21	24.8(7)	28.5(8)	43.1(9)	3.3(7)	-3.0(6)	1.3(6)
C22	27.8(8)	34.1(9)	48.4(10)	9.2(7)	1.6(7)	-0.8(7)
C23	38.5(9)	35.6(9)	38.3(9)	5.3(7)	0.4(7)	4.6(7)
C24	36.6(9)	31.9(8)	41.7(10)	1.7(7)	-6.4(7)	-1.3(7)
C25	28.4(8)	27.3(8)	41.5(9)	6.1(7)	-2.9(7)	-1.7(6)
C26	27.8(8)	24.3(7)	39.1(9)	7.0(6)	-5.2(6)	3.9(6)
C27	25.3(7)	33.7(8)	40.7(9)	4.2(7)	-6.9(6)	0.4(6)
C28	42.5(10)	43.4(10)	40.0(10)	12.0(8)	-12.2(8)	-8.1(8)
C29	50.8(11)	40.4(10)	44.8(11)	0.8(8)	-12.5(8)	3.4(8)
C30	41.4(9)	37.0(9)	29.3(8)	5.8(7)	-3.5(7)	-3.9(7)
C31	36.2(9)	36.4(9)	31.2(8)	6.9(7)	-1.8(7)	-5.3(7)
C32	36.8(9)	42.1(10)	36.7(9)	-0.1(8)	-0.5(7)	-0.4(7)
C33	40.0(9)	44.0(10)	35.6(9)	-4.6(8)	-2.5(7)	-3.8(8)
C34	33.4(8)	42.7(9)	35.6(9)	6.6(7)	-2.0(7)	-5.1(7)
C35	40.0(9)	39.9(9)	36.8(9)	1.2(7)	0.5(7)	2.2(7)

C36	43.0(10)	37.9(9)	33.2(9)	0.8(7)	-4.2(7)	-3.1(7)
C37	35.5(9)	56.4(12)	47.4(11)	5.4(9)	-1.7(8)	0.8(8)
C38	36.7(10)	73.7(15)	60.4(14)	4.2(11)	-7.3(9)	4.1(10)

Table 4 Bond Lengths for **5k**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C7	1.217(2)	O3	C26	1.220(2)
O2	C15	1.369(2)	O4	C34	1.364(2)
O2	C18	1.428(2)	O4	C37	1.431(2)
N1	N2	1.328(2)	N4	N5	1.324(2)
N1	N3	1.333(2)	N4	N6	1.335(2)
N1	C9	1.461(2)	N4	C28	1.456(2)
N2	C10	1.336(2)	N5	C29	1.334(2)
N3	C11	1.342(2)	N6	C30	1.345(2)
C1	C2	1.391(2)	C20	C21	1.390(2)
C1	C6	1.398(2)	C20	C25	1.399(2)
C1	C7	1.491(2)	C20	C26	1.494(2)
C2	C3	1.389(3)	C21	C22	1.384(3)
C3	C4	1.383(2)	C22	C23	1.387(3)
C4	C5	1.388(3)	C23	C24	1.386(2)
C5	C6	1.374(3)	C24	C25	1.378(3)
C7	C8	1.516(2)	C26	C27	1.514(2)
C8	C9	1.505(3)	C27	C28	1.514(3)
C10	C11	1.392(3)	C29	C30	1.390(3)
C11	C12	1.469(2)	C30	C31	1.469(2)
C12	C13	1.398(2)	C31	C32	1.394(2)
C12	C17	1.389(3)	C31	C36	1.390(3)
C13	C14	1.383(3)	C32	C33	1.383(2)
C14	C15	1.391(3)	C33	C34	1.395(3)
C15	C16	1.386(3)	C34	C35	1.386(3)
C16	C17	1.391(3)	C35	C36	1.392(3)
C18	C19	1.504(3)	C37	C38	1.506(3)

Table 5 Bond Angles for **5k**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C15	O2	C18	117.71(14)	C34	O4	C37	118.02(15)
N2	N1	N3	115.41(15)	N5	N4	N6	115.59(15)
N2	N1	C9	121.69(16)	N5	N4	C28	121.42(15)
N3	N1	C9	122.85(16)	N6	N4	C28	122.89(16)
N1	N2	C10	103.19(15)	N4	N5	C29	103.10(15)

N1	N3	C11	104.06(15)	N4	N6	C30	103.88(15)
C2	C1	C6	118.92(16)	C21	C20	C25	119.06(16)
C2	C1	C7	123.02(14)	C21	C20	C26	123.12(15)
C6	C1	C7	118.06(14)	C25	C20	C26	117.82(14)
C3	C2	C1	120.00(15)	C22	C21	C20	120.29(16)
C4	C3	C2	120.28(16)	C21	C22	C23	120.14(16)
C3	C4	C5	120.05(17)	C24	C23	C22	119.93(17)
C6	C5	C4	119.72(16)	C25	C24	C23	120.03(16)
C5	C6	C1	121.00(16)	C24	C25	C20	120.50(15)
O1	C7	C1	120.63(15)	O3	C26	C20	120.61(15)
O1	C7	C8	120.07(16)	O3	C26	C27	120.18(16)
C1	C7	C8	119.28(14)	C20	C26	C27	119.19(14)
C9	C8	C7	110.77(14)	C26	C27	C28	111.09(14)
N1	C9	C8	111.91(15)	N4	C28	C27	111.76(15)
N2	C10	C11	109.74(17)	N5	C29	C30	109.98(17)
N3	C11	C10	107.60(16)	N6	C30	C29	107.44(16)
N3	C11	C12	122.26(17)	N6	C30	C31	122.56(16)
C10	C11	C12	130.14(16)	C29	C30	C31	129.98(17)
C13	C12	C11	120.82(16)	C32	C31	C30	120.86(17)
C17	C12	C11	121.46(16)	C36	C31	C30	121.29(16)
C17	C12	C13	117.72(16)	C36	C31	C32	117.85(16)
C14	C13	C12	121.06(17)	C33	C32	C31	120.98(17)
C13	C14	C15	120.09(17)	C32	C33	C34	120.41(17)
O2	C15	C14	115.62(16)	O4	C34	C33	115.80(16)
O2	C15	C16	124.38(17)	O4	C34	C35	124.76(17)
C16	C15	C14	120.00(17)	C35	C34	C33	119.44(16)
C15	C16	C17	119.08(17)	C34	C35	C36	119.40(17)
C12	C17	C16	122.03(17)	C31	C36	C35	121.90(17)
O2	C18	C19	106.96(16)	O4	C37	C38	106.94(17)

Table 6 Torsion Angles for**5k**.

A	**B**	**C**	**D**	**Angle/˚**	**A**	**B**	**C**	**D**	**Angle/˚**
O1	C7	C8	C9	7.2(2)	O3	C26	C27	C28	2.6(2)
O2	C15	C16	C17	-178.96(18)	O4	C34	C35	C36	179.64(17)
N1	N2	C10	C11	-0.5(2)	N4	N5	C29	C30	0.0(2)
N1	N3	C11	C10	-0.6(2)	N4	N6	C30	C29	0.53(19)
N1	N3	C11	C12	178.75(16)	N4	N6	C30	C31	-178.14(15)
N2	N1	N3	C11	0.3(2)	N5	N4	N6	C30	-0.6(2)
N2	N1	C9	C8	78.0(2)	N5	N4	C28	C27	-93.7(2)
N2	C10	C11	N3	0.7(2)	N5	C29	C30	N6	-0.4(2)

N2	C10	C11	C12	-178.55(18)	N5	C29	C30	C31	178.18(18)
N3	N1	N2	C10	0.1(2)	N6	N4	N5	C29	0.4(2)
N3	N1	C9	C8	-99.4(2)	N6	N4	C28	C27	82.5(2)
N3	C11	C12	C13	-158.43(18)	N6	C30	C31	C32	160.22(17)
N3	C11	C12	C17	21.9(3)	N6	C30	C31	C36	-20.5(3)
C1	C2	C3	C4	-0.5(2)	C20	C21	C22	C23	0.8(2)
C1	C7	C8	C9	-171.12(15)	C20	C26	C27	C28	-179.03(14)
C2	C1	C6	C5	1.8(2)	C21	C20	C25	C24	-1.9(2)
C2	C1	C7	O1	177.34(15)	C21	C20	C26	O3	-175.98(15)
C2	C1	C7	C8	-4.3(2)	C21	C20	C26	C27	5.7(2)
C2	C3	C4	C5	1.7(3)	C21	C22	C23	C24	-1.9(3)
C3	C4	C5	C6	-1.2(3)	C22	C23	C24	C25	1.2(3)
C4	C5	C6	C1	-0.6(3)	C23	C24	C25	C20	0.8(3)
C6	C1	C2	C3	-1.2(2)	C25	C20	C21	C22	1.2(2)
C6	C1	C7	O1	-3.2(2)	C25	C20	C26	O3	4.8(2)
C6	C1	C7	C8	175.08(14)	C25	C20	C26	C27	-173.54(14)
C7	C1	C2	C3	178.18(14)	C26	C20	C21	C22	-178.06(14)
C7	C1	C6	C5	-177.67(15)	C26	C20	C25	C24	177.35(15)
C7	C8	C9	N1	-176.89(15)	C26	C27	C28	N4	176.53(14)
C9	N1	N2	C10	-177.48(17)	C28	N4	N5	C29	176.83(17)
C9	N1	N3	C11	177.89(16)	C28	N4	N6	C30	-176.99(16)
C10	C11	C12	C13	20.8(3)	C29	C30	C31	C32	-18.1(3)
C10	C11	C12	C17	-158.9(2)	C29	C30	C31	C36	161.18(19)
C11	C12	C13	C14	-179.27(17)	C30	C31	C32	C33	179.37(16)
C11	C12	C17	C16	178.74(17)	C30	C31	C36	C35	-178.65(16)
C12	C13	C14	C15	0.9(3)	C31	C32	C33	C34	-0.9(3)
C13	C12	C17	C16	-0.9(3)	C32	C31	C36	C35	0.7(3)
C13	C14	C15	O2	178.44(17)	C32	C33	C34	O4	-178.95(17)
C13	C14	C15	C16	-1.6(3)	C32	C33	C34	C35	0.9(3)
C14	C15	C16	C17	1.1(3)	C33	C34	C35	C36	-0.2(3)
C15	O2	C18	C19	172.02(17)	C34	O4	C37	C38	-178.65(17)
C15	C16	C17	C12	0.2(3)	C34	C35	C36	C31	-0.6(3)
C17	C12	C13	C14	0.4(3)	C36	C31	C32	C33	0.0(3)
C18	O2	C15	C14	-172.69(17)	C37	O4	C34	C33	179.11(17)
C18	O2	C15	C16	7.4(3)	C37	O4	C34	C35	-0.8(3)

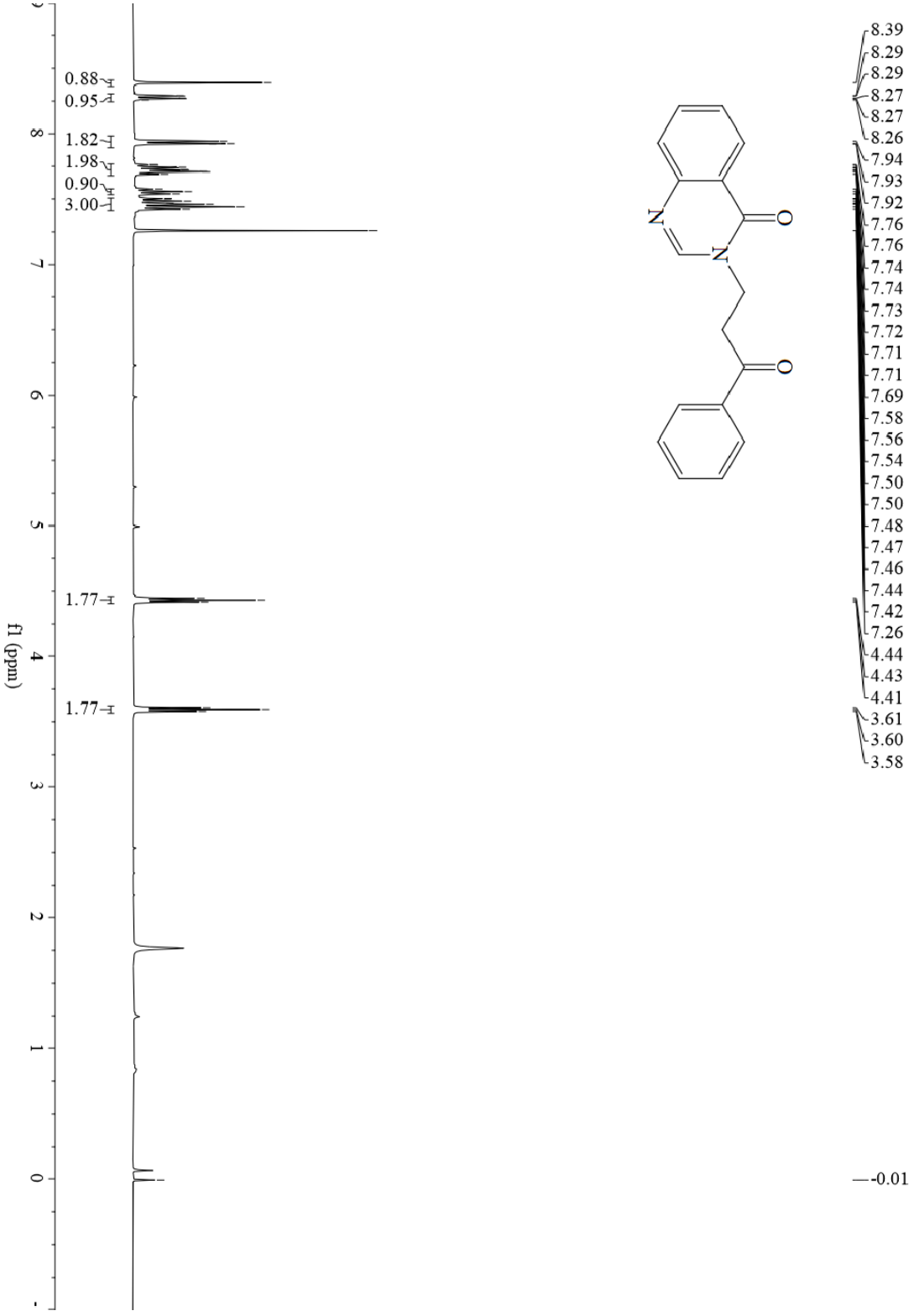
Table 7 Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **5k**.

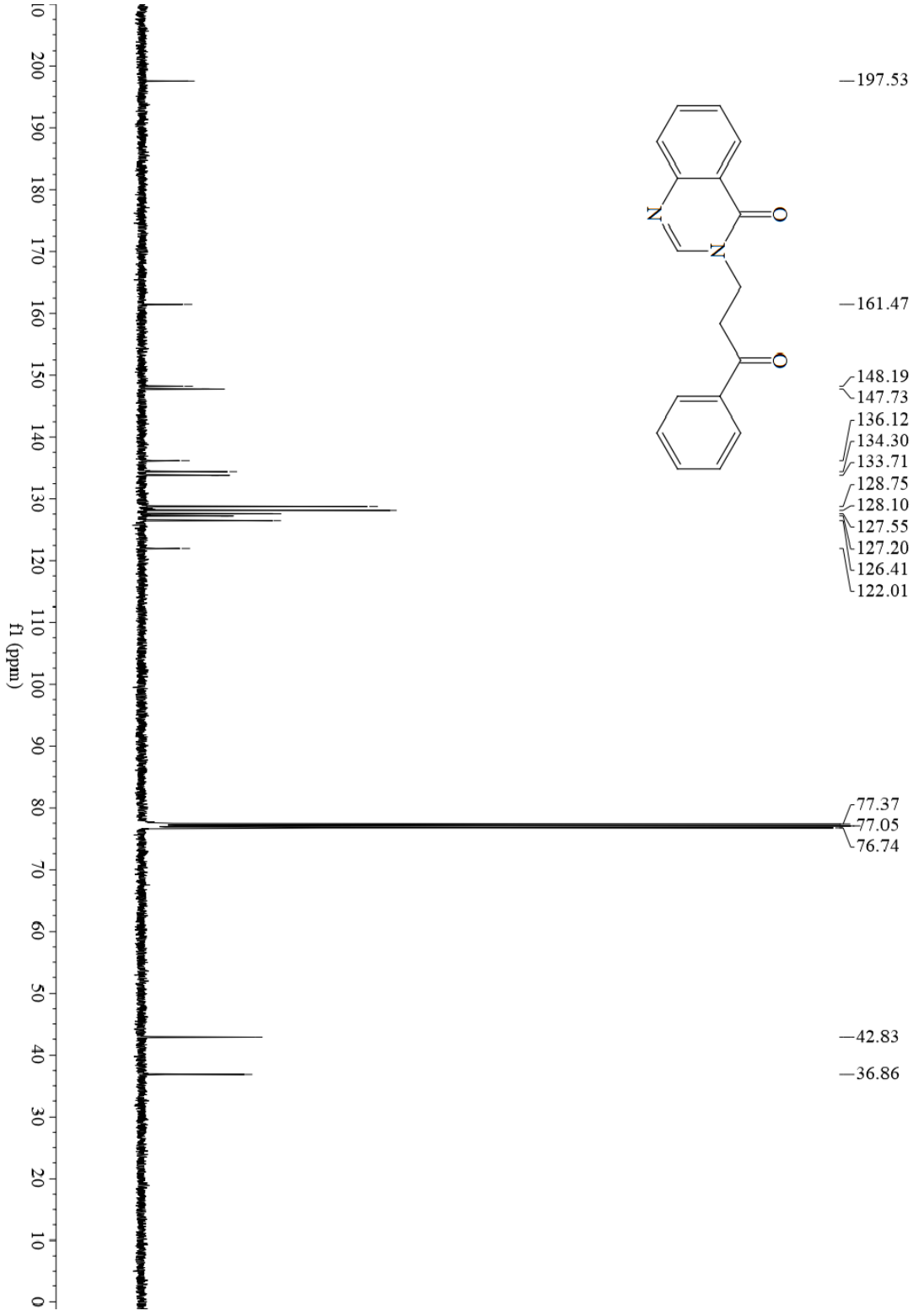
Atom	*x*	*y*	*z*	U(eq)
H2	11707.76	10424.57	5099.01	38
H3	11493.84	10862.03	6217.76	43
H4	13009.57	9601.67	6912.75	46
H5	14842.29	7975.58	6493.35	44
H6	15087.04	7562.85	5384.21	39
H8A	11398.62	9088.43	4056.67	38
H8B	12683.89	10250.12	3948.09	38
H9A	13765.22	8633.75	3135.75	57
H9B	12412.63	7529.14	3230.16	57
H10	10761.19	11550.44	1943.43	53
H13	8748.22	10725.27	1080.16	47
H14	6408.9	10391.63	495.11	49
H16	4944.41	7647.84	1748.5	49
H17	7313.08	7967.79	2321.38	48
H18A	2575.92	8485.01	1379.35	55
H18B	3014.1	7121.78	914.63	55
H19A	1586.83	8003.73	57.9	81
H19B	1188.49	9394.87	505.41	81
H19C	481.77	7902.34	646.24	81
H21	6656.17	4781.62	5079.31	39
H22	6320.01	4907.01	6191.36	44
H23	7893.34	6430.94	6890.03	45
H24	9899.9	7733.88	6478.95	44
H25	10276.85	7575.75	5372.6	39
H27A	6552.41	5779.99	3970.98	40
H27B	7543.27	4377.73	3997.69	40
H28A	8054.39	6491.03	3125.69	50
H28B	9131.72	5148.69	3167.79	50
H29	5965.68	2006.35	1923.49	55
H32	3872.71	2444.2	1116.79	47
H33	1500.73	2560.51	562.12	49
H35	262.88	5891.84	1809.88	47
H36	2669.91	5791.08	2348.29	46
H37A	-1544.99	6176.72	952.32	56
H37B	-2215.9	5097.26	1421.54	56
H38A	-3027.89	5010.61	80.25	86
H38B	-4148.07	5550.89	637.85	86

H38C	-3687.29	3924.8	543.81	86

8. Copies of ^{1}H and ^{13}C NMR spectra of all products

^{1}H and ^{13}C NMR spectra of 3a

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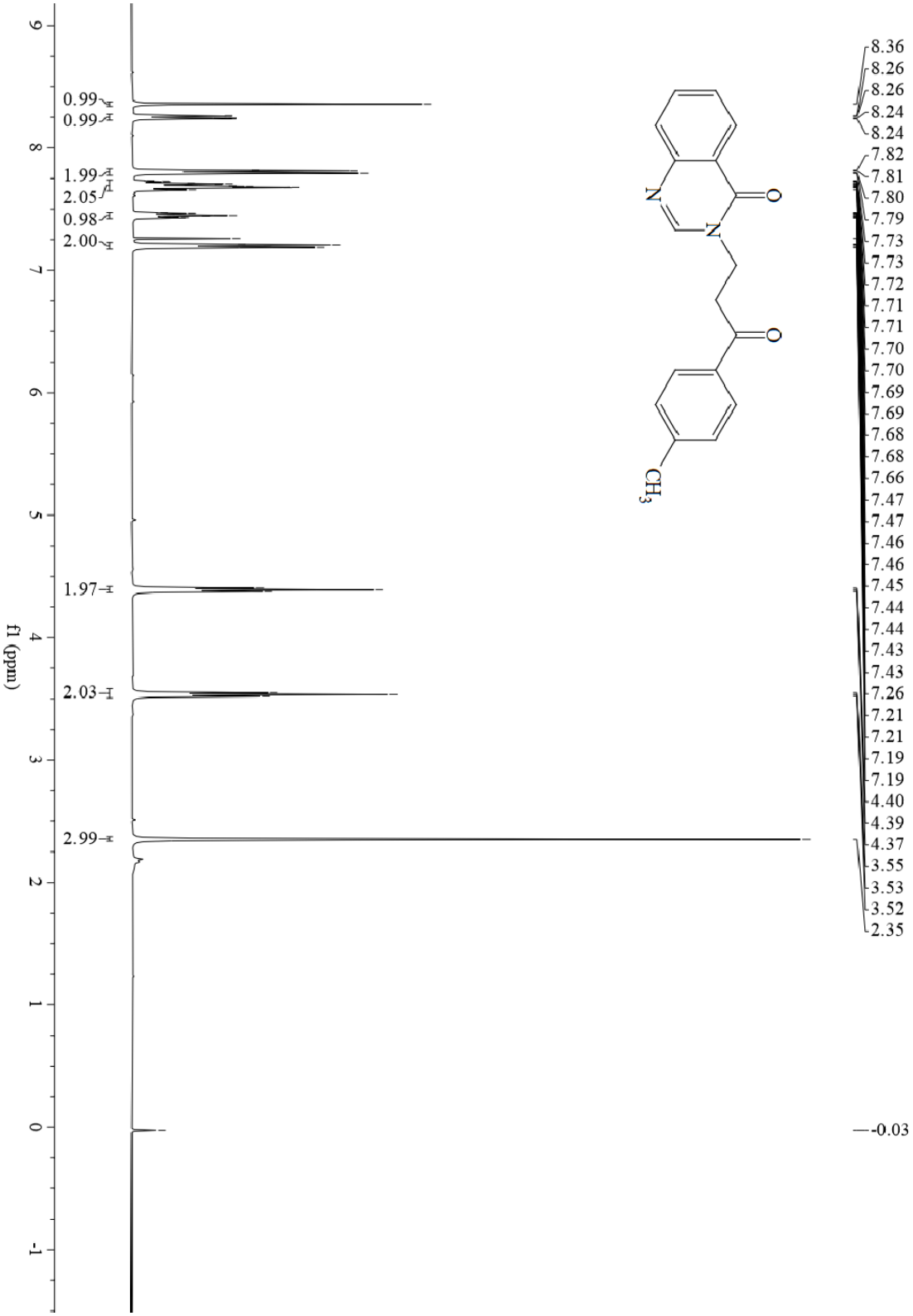
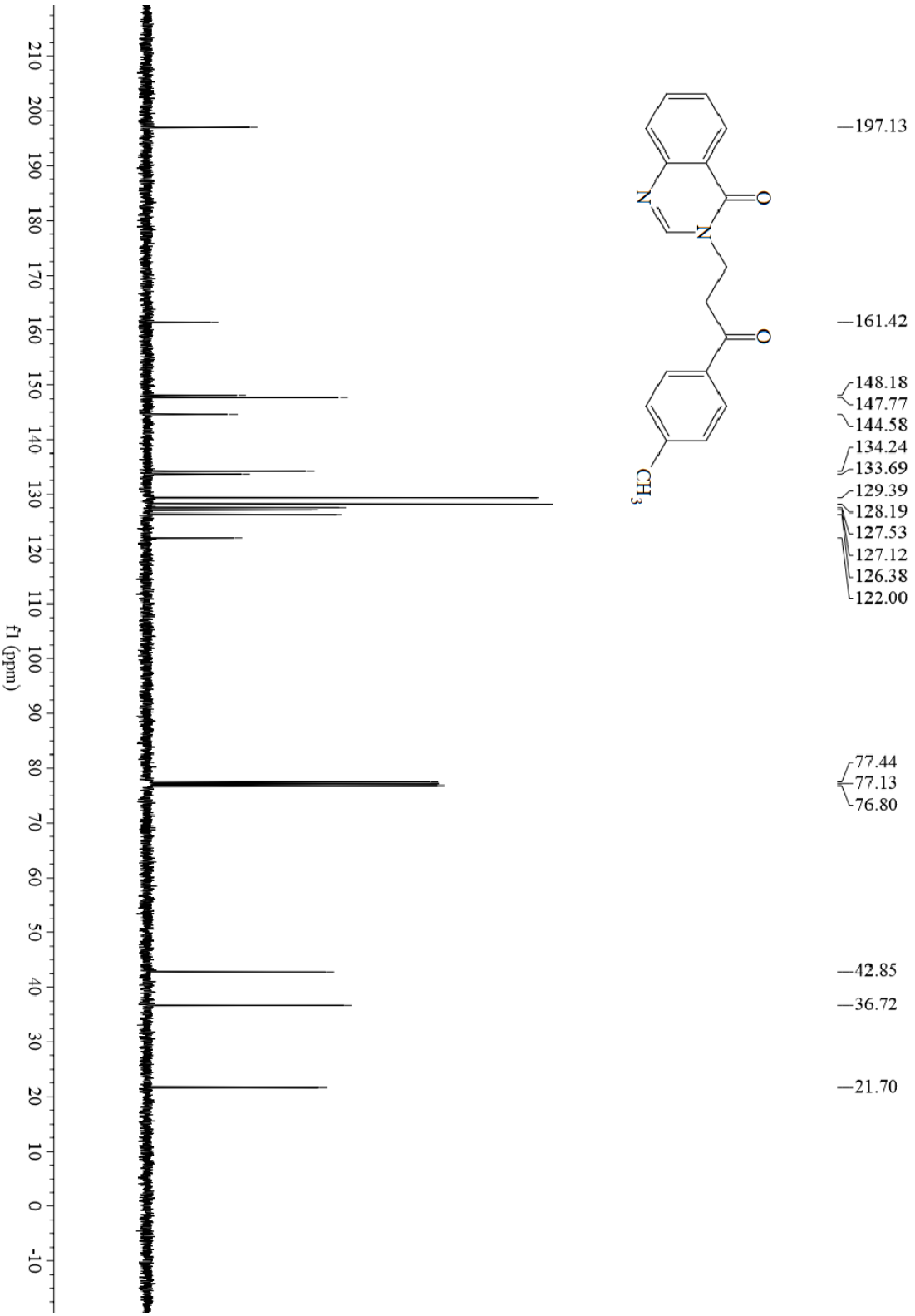
f1 (ppm)

^{1}H and ^{13}C NMR spectra of 3b

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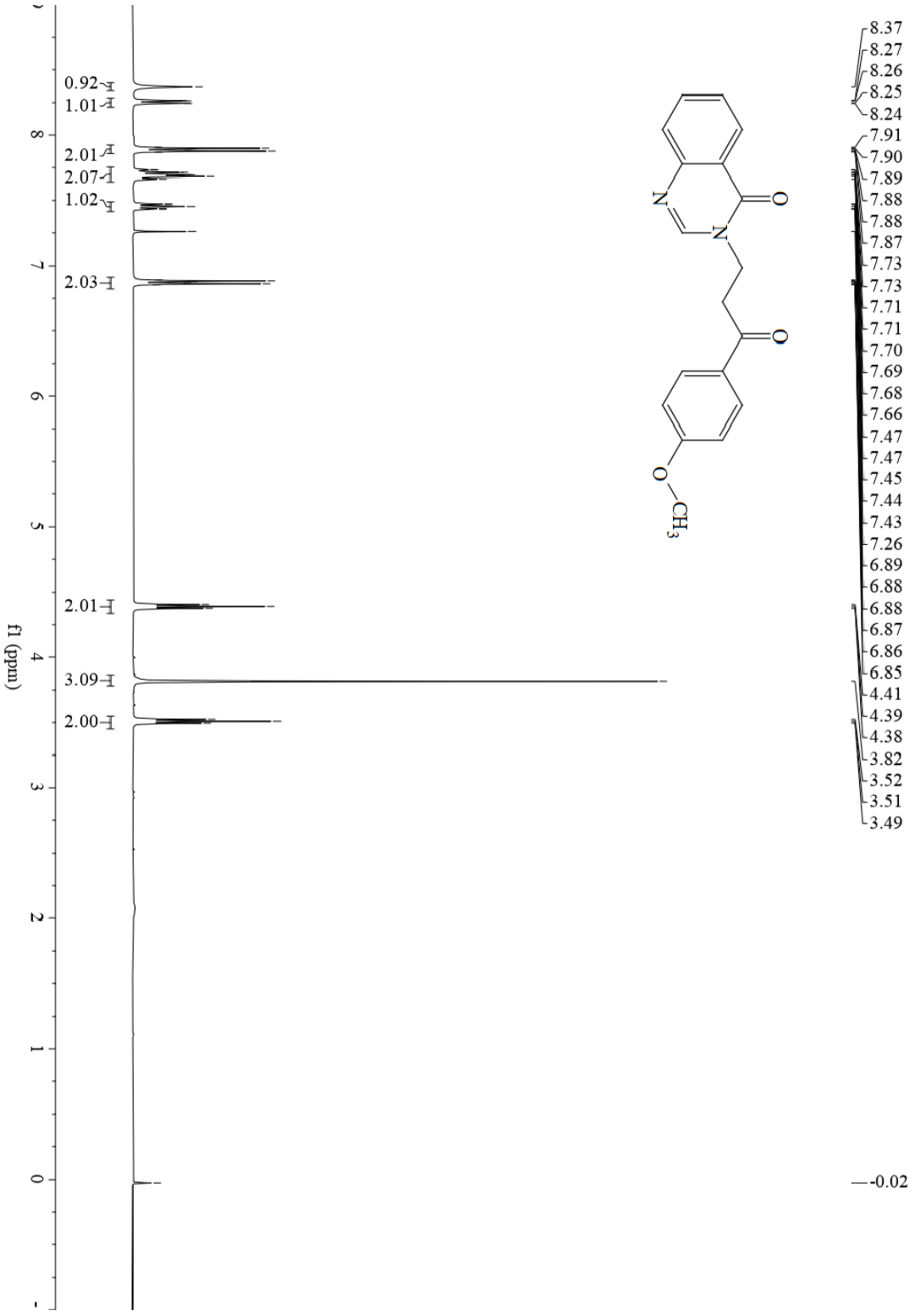
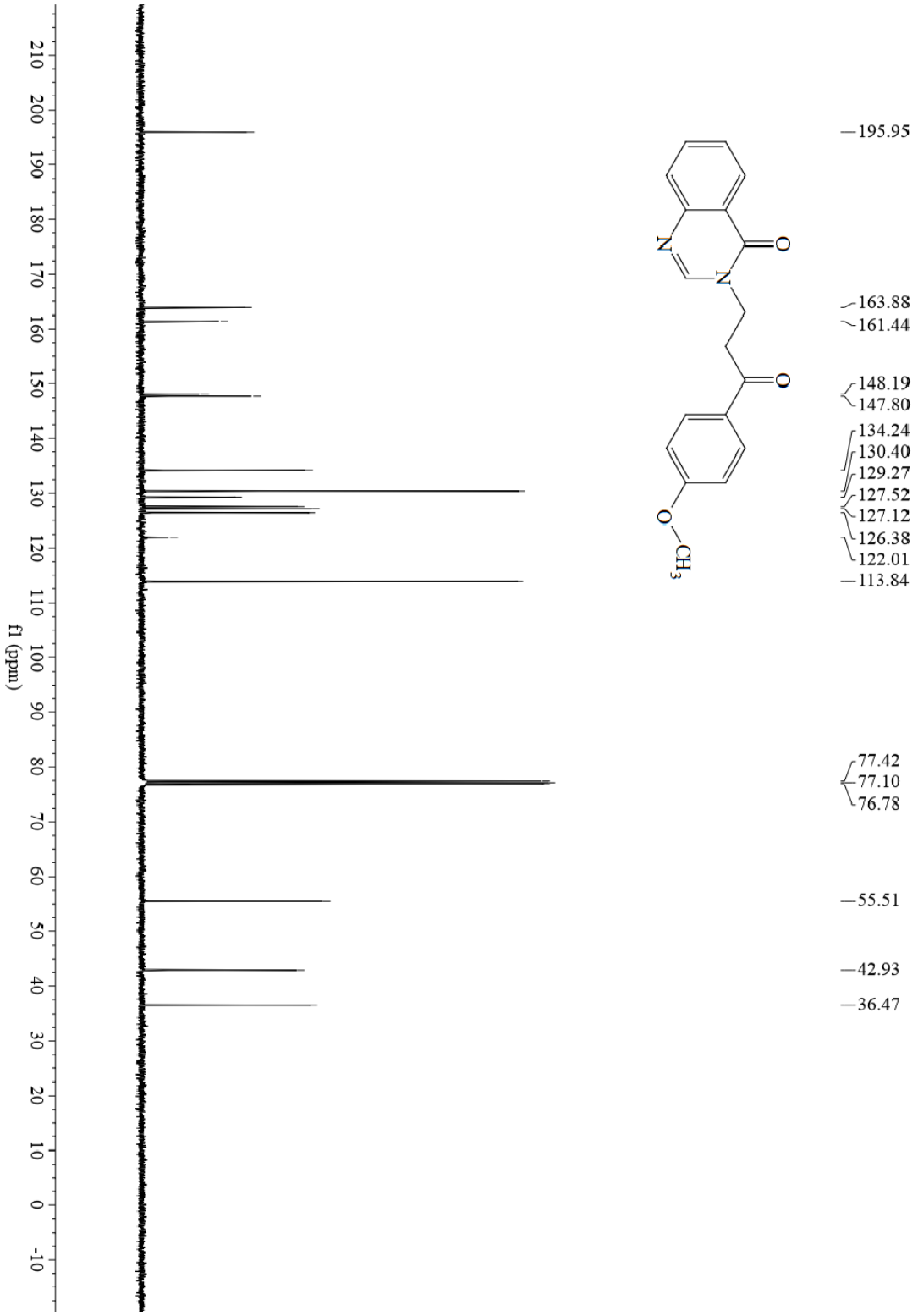
N
N
O
O
CH3

^{1}H and ^{13}C NMR spectra of 3c

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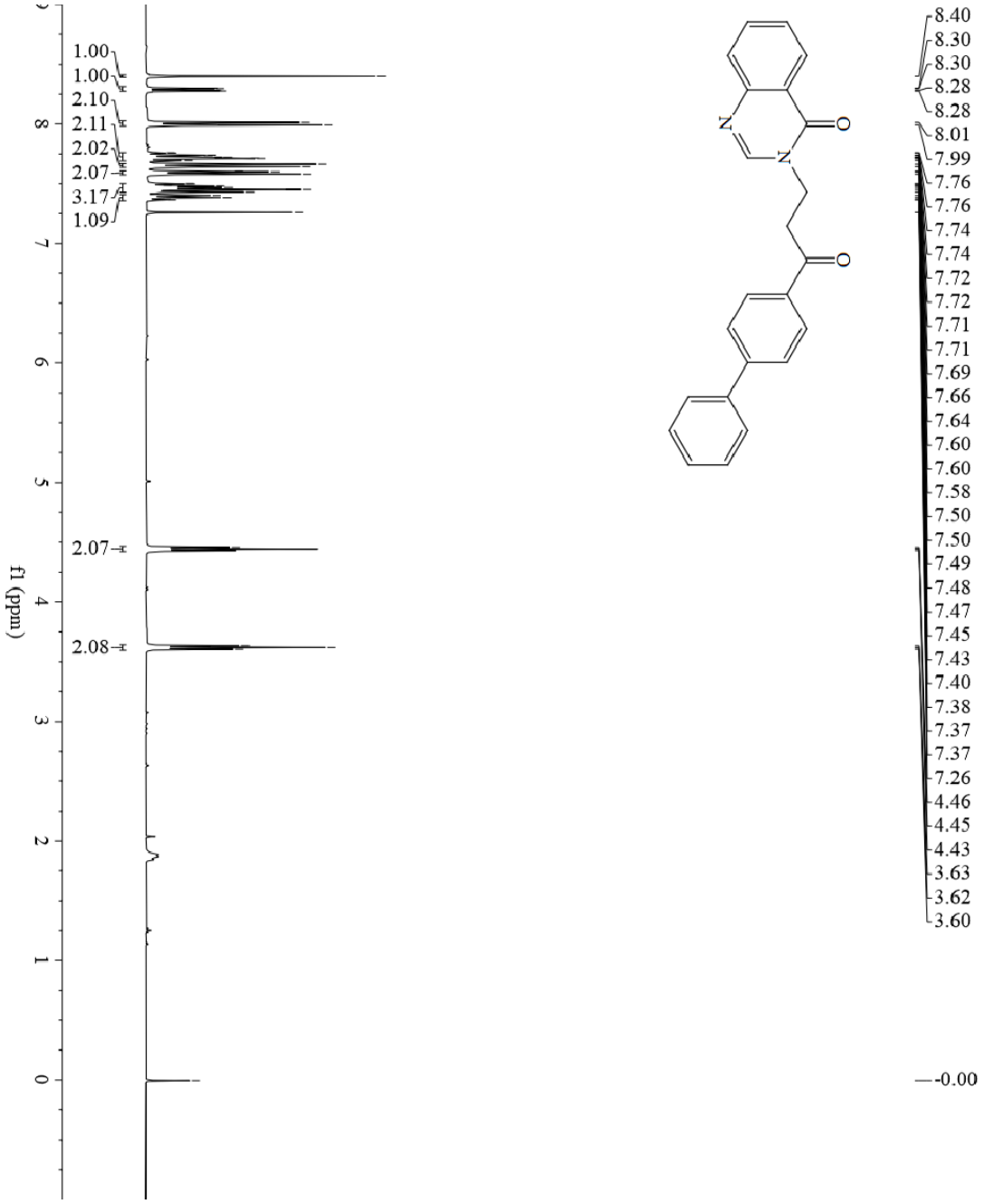
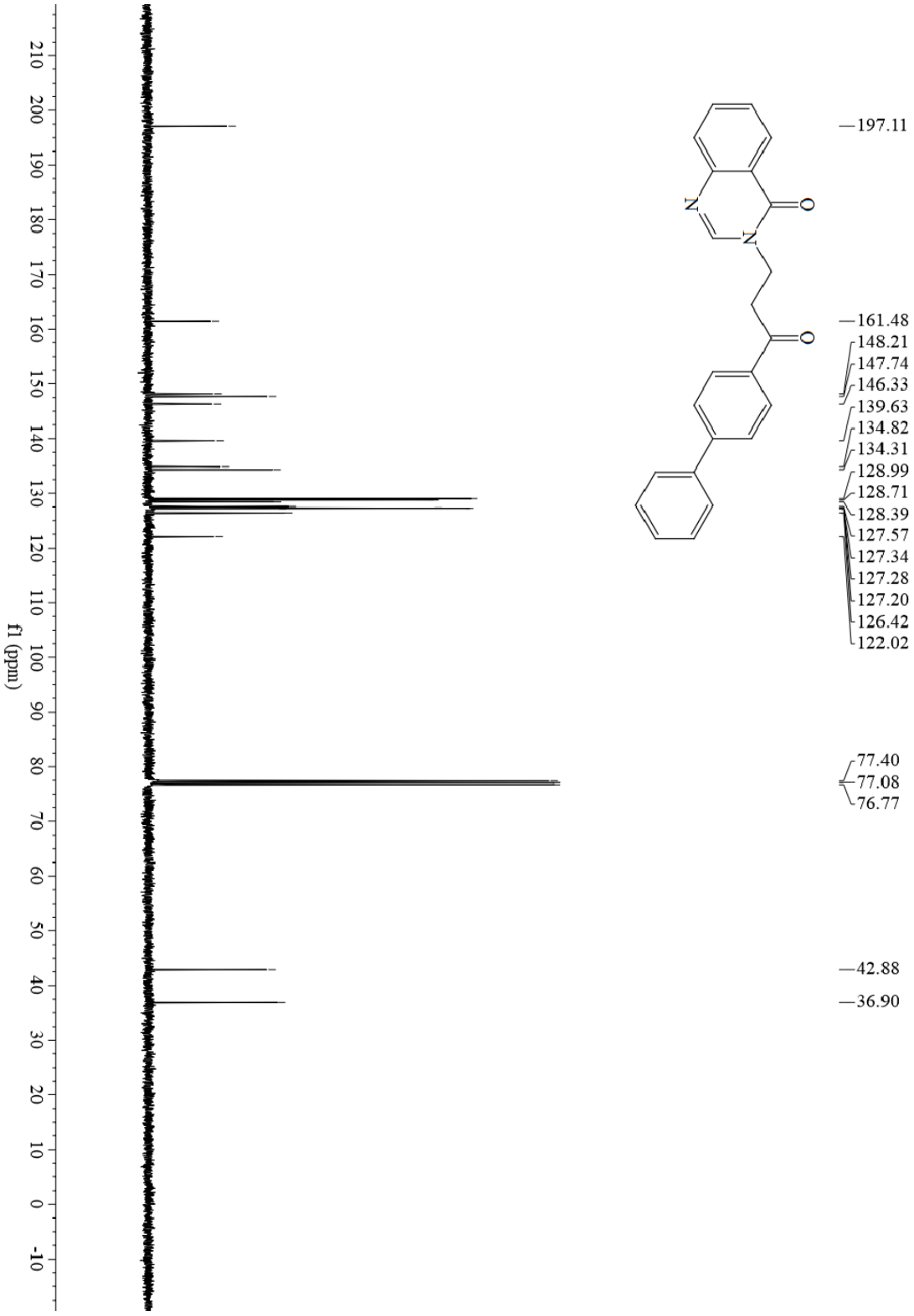
f1 (ppm)

^{1}H and ^{13}C NMR spectra of 3d

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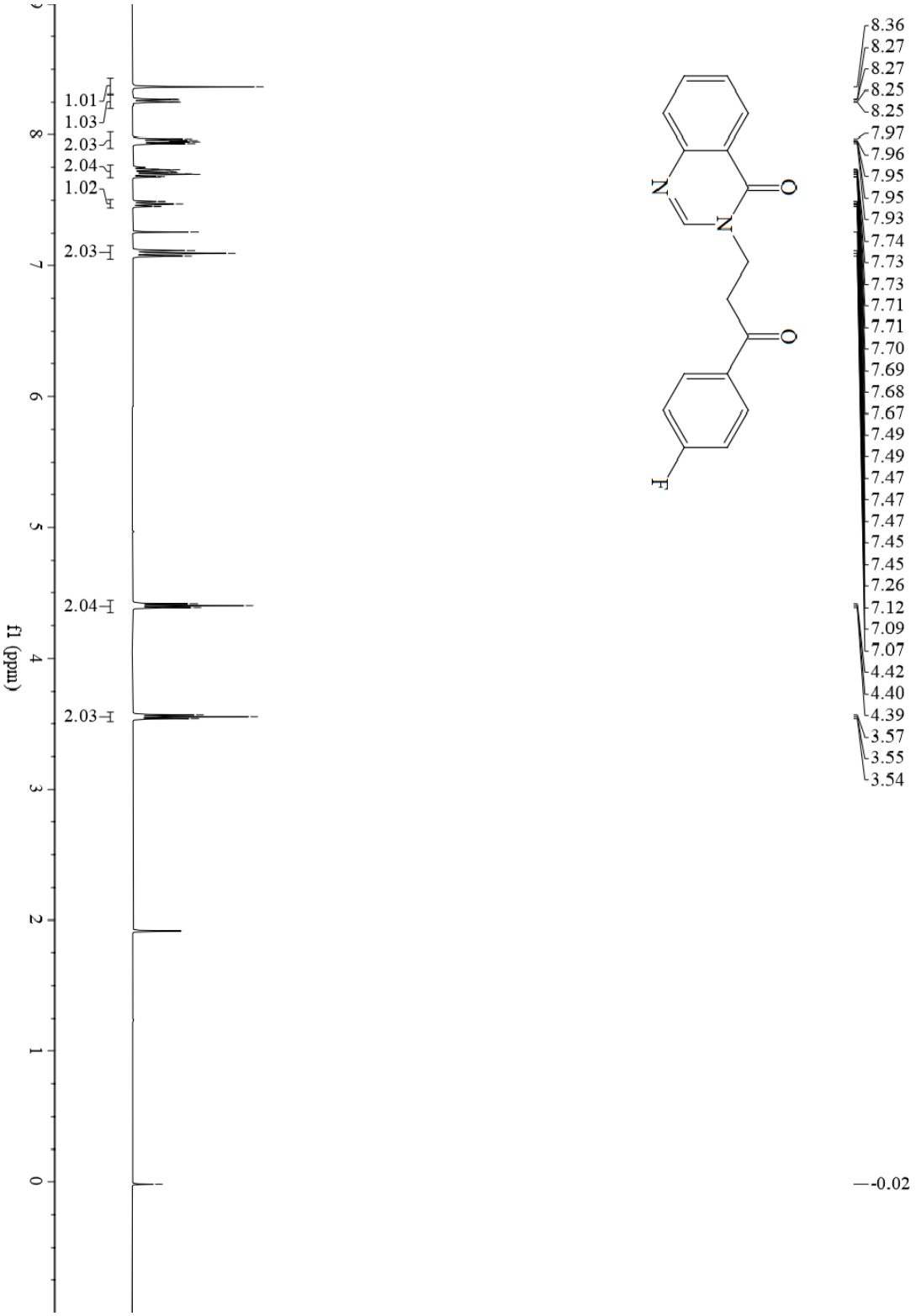
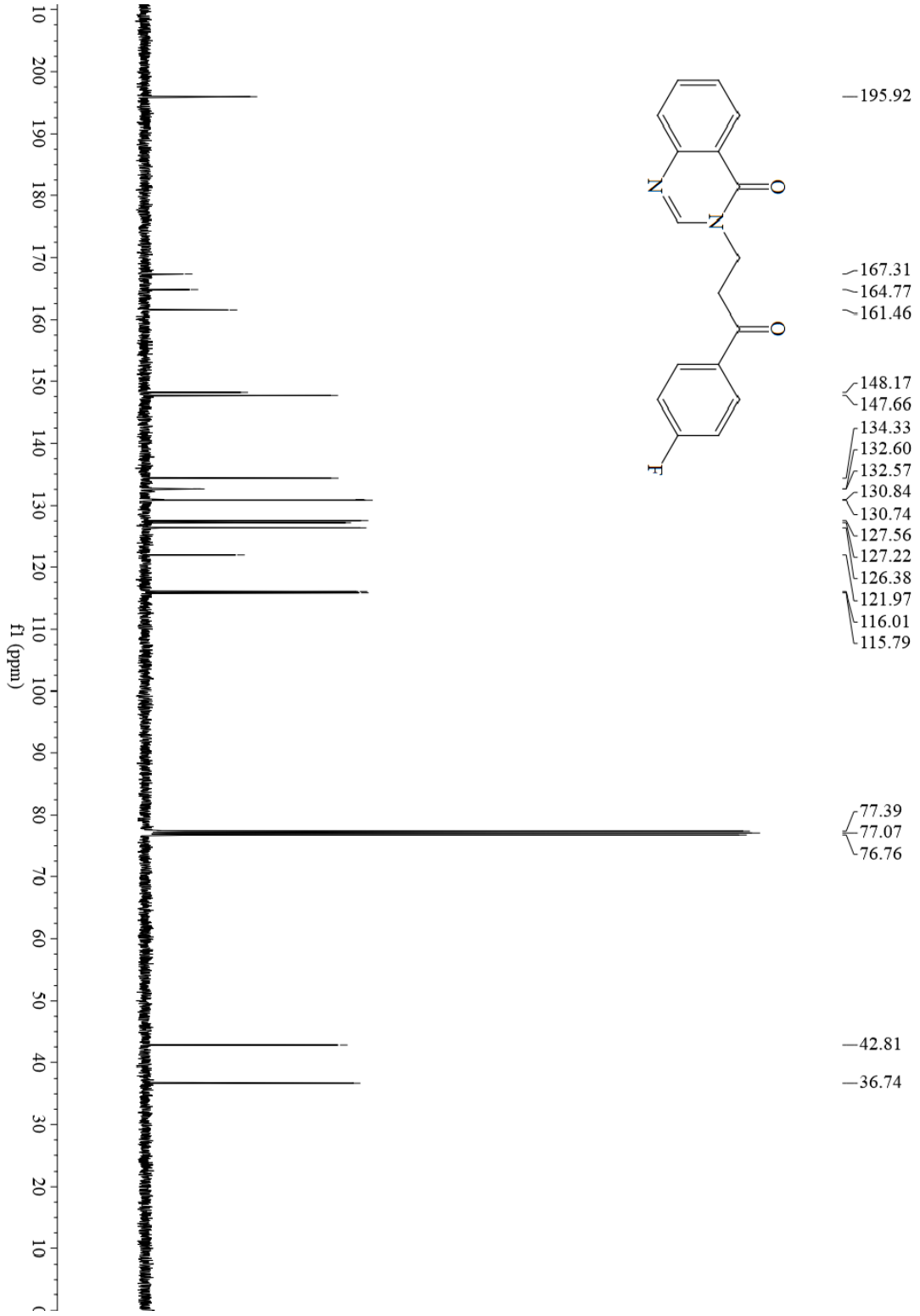
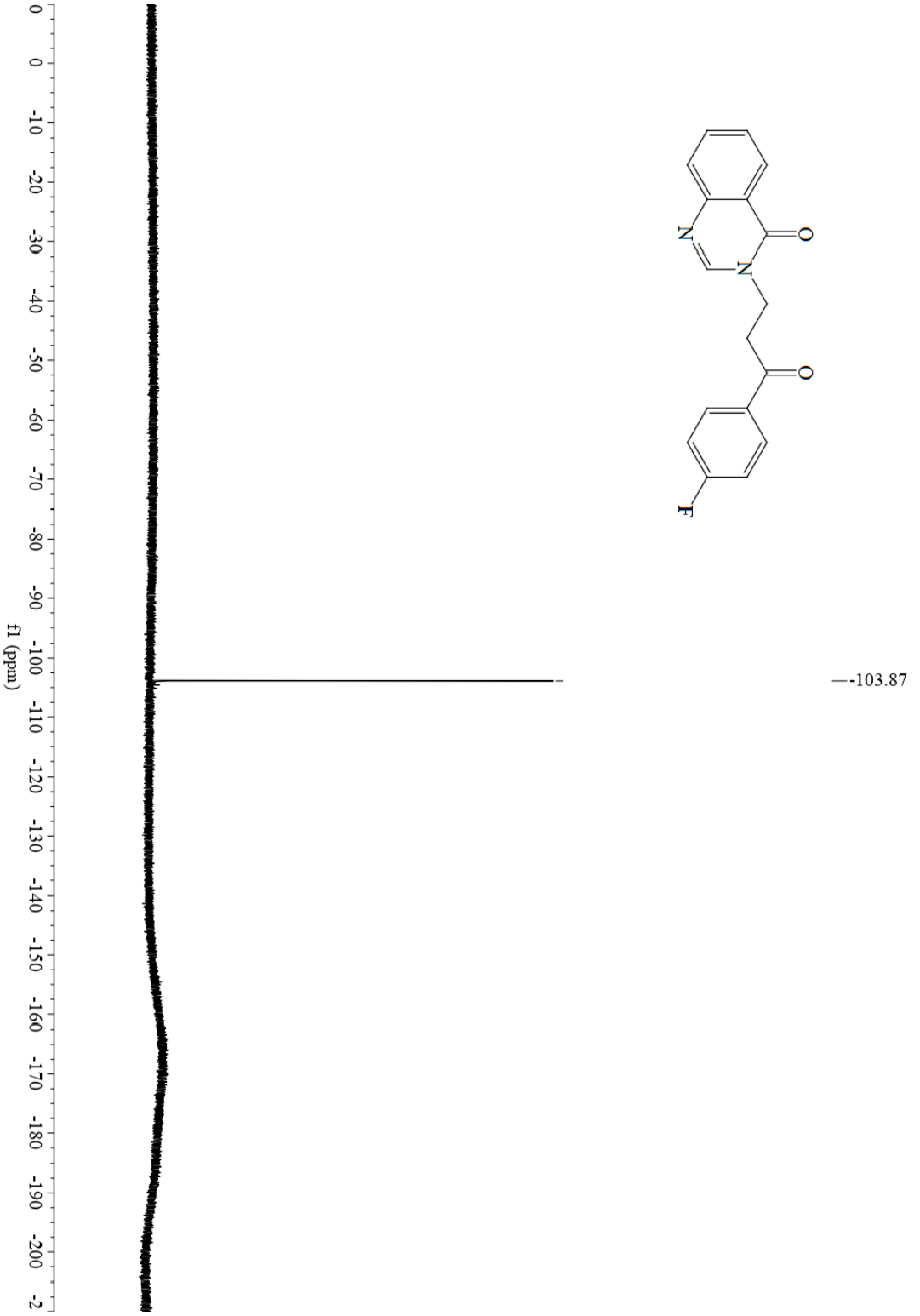
42.88
36.90
f1 (ppm)

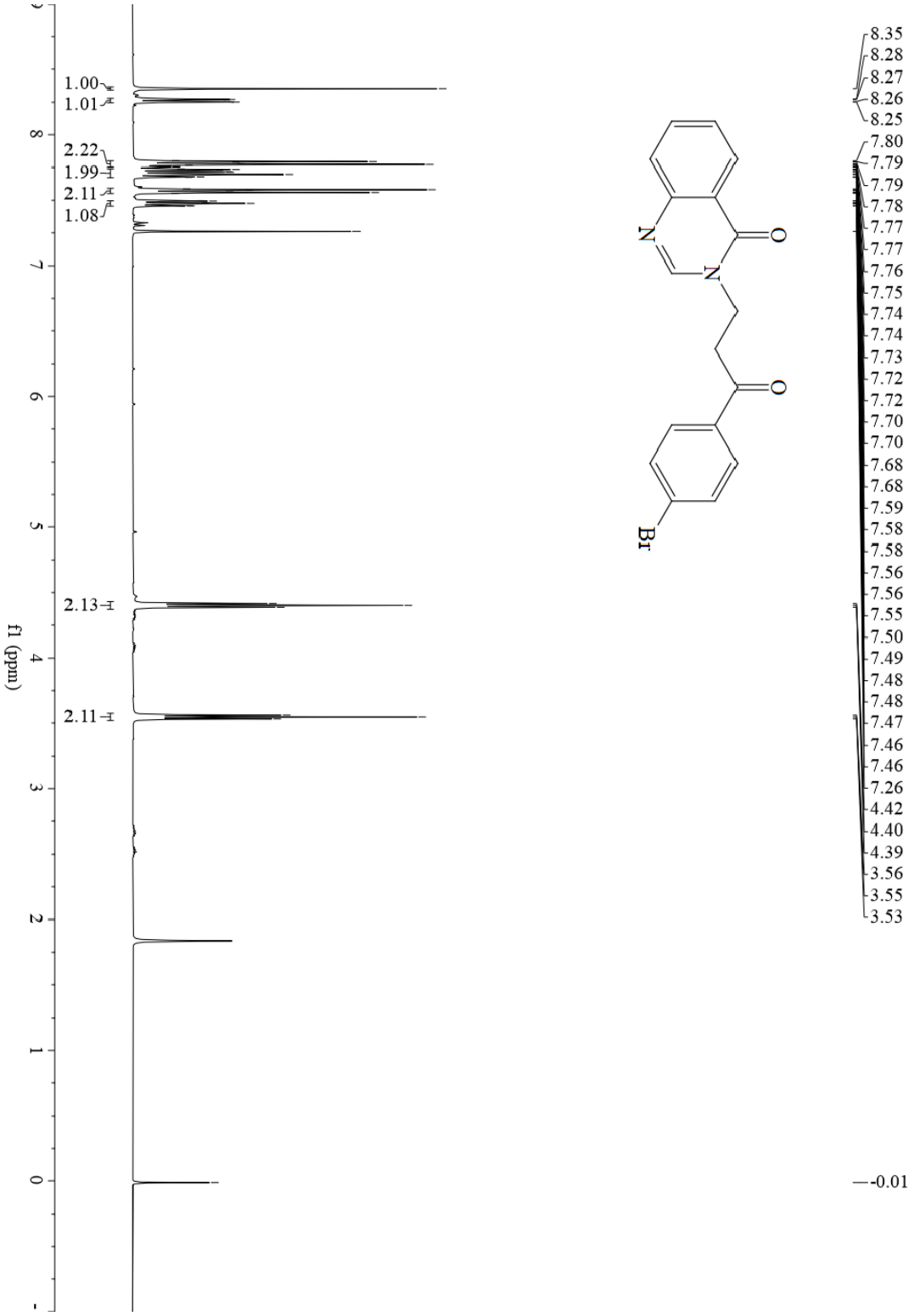
^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of 3e

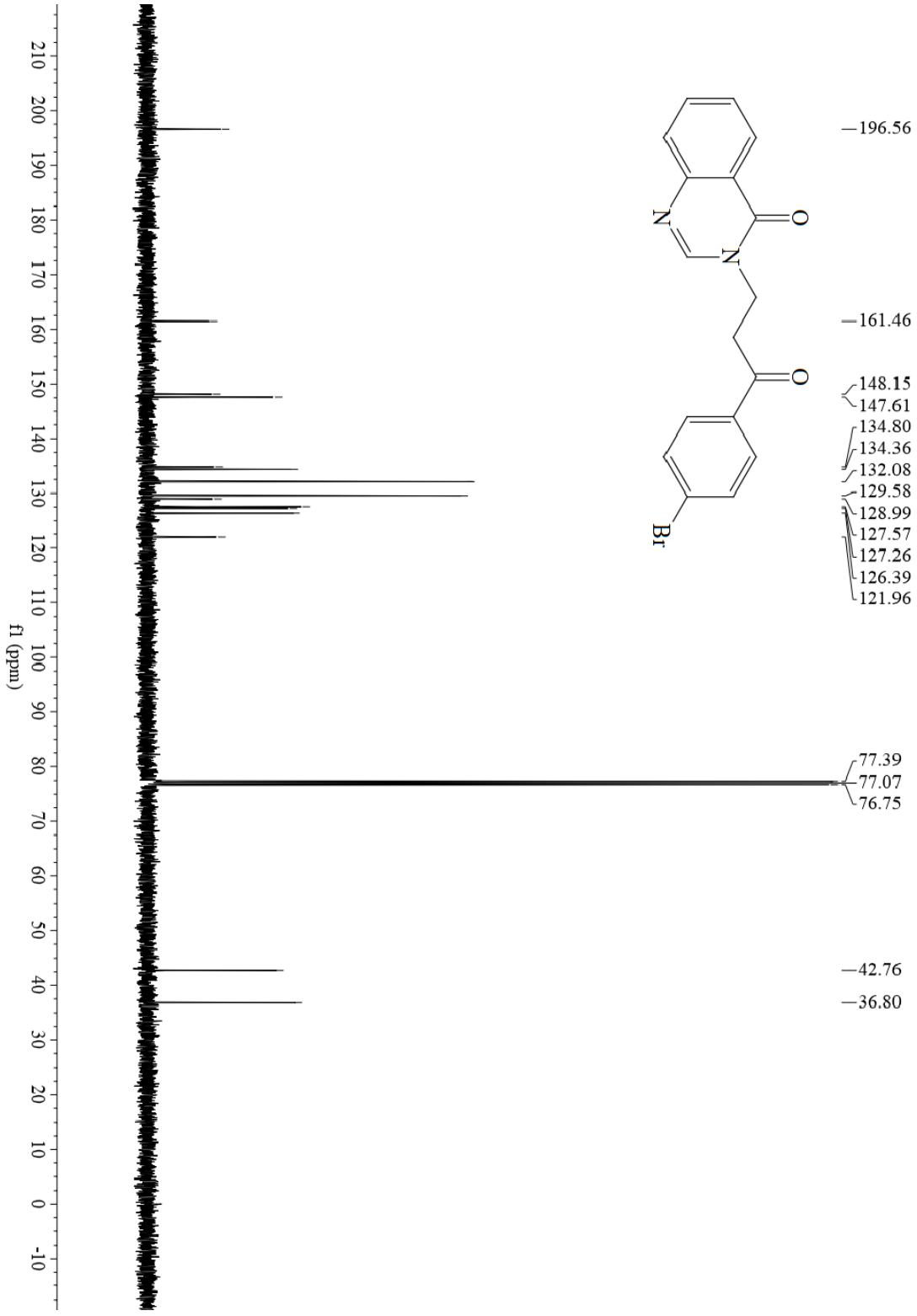



195.92
167.31
164.77
161.46
148.17
147.66
134.33
132.60
132.57
130.84
130.74
127.56
127.22
126.38
121.97
116.01
115.79
77.39
77.07
76.76
42.81
36.74
f1 (ppm)

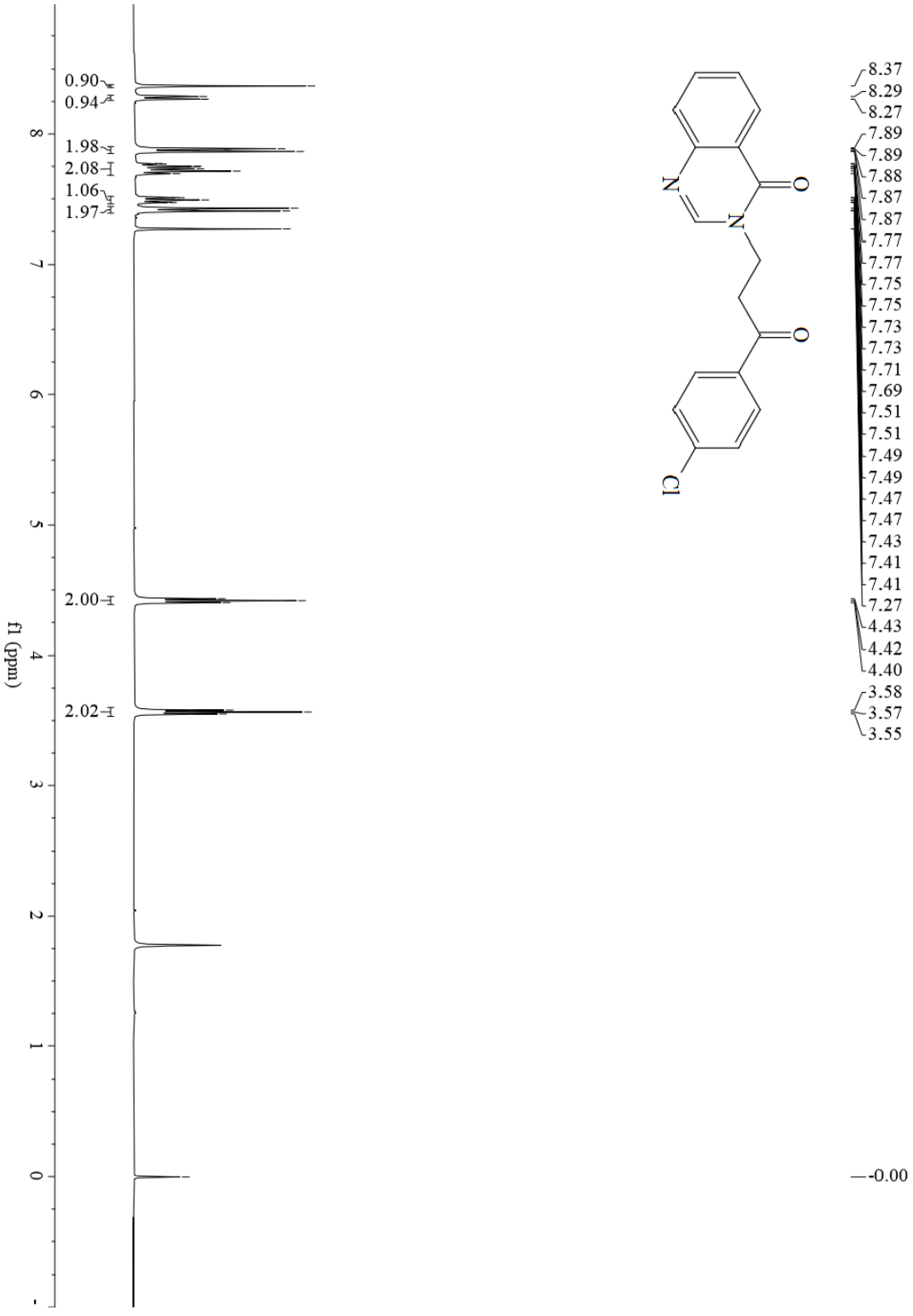

0
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-2
f1 (ppm)
-103.87
N
N
O
O
F

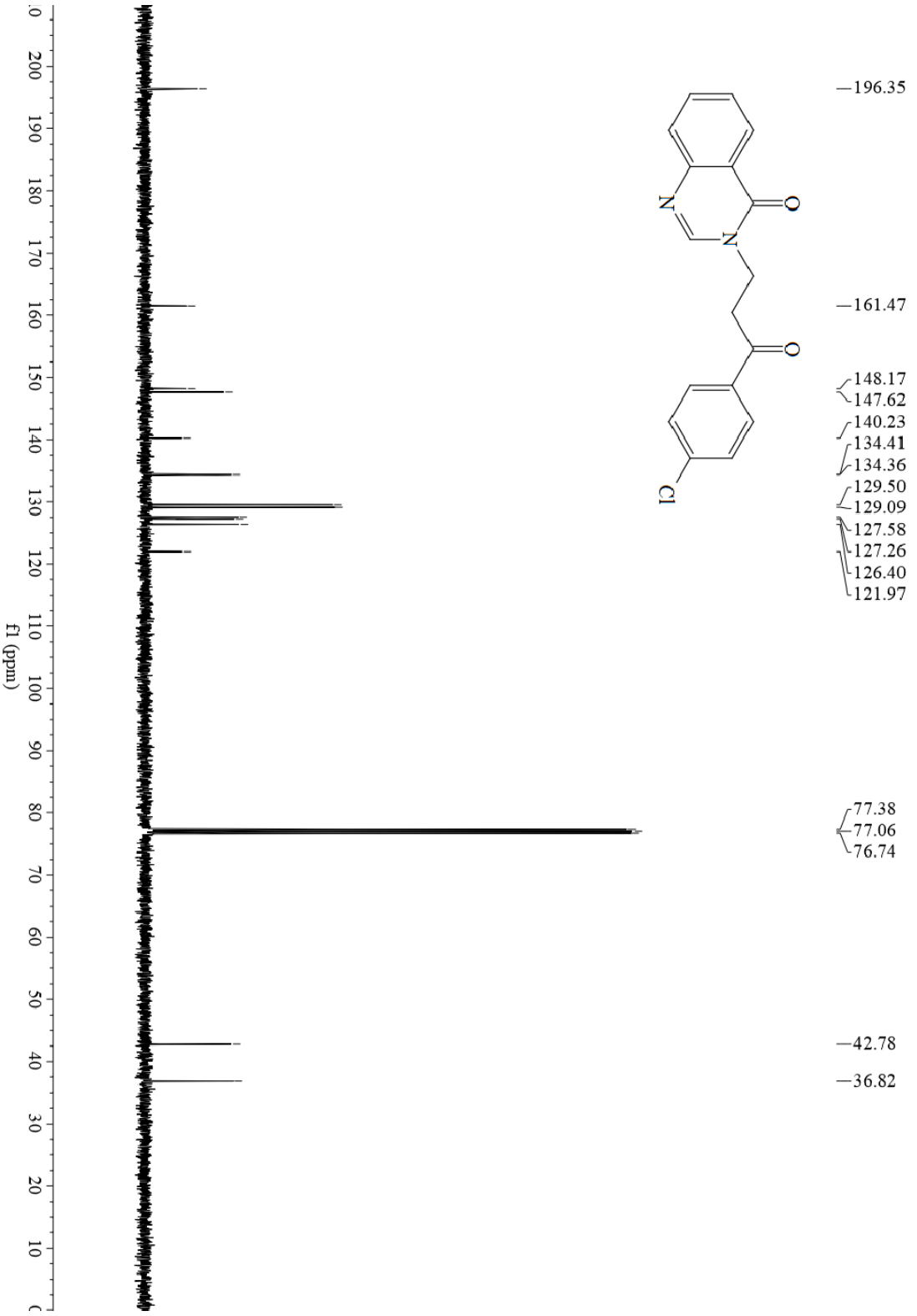
^{1}H and ^{13}C NMR spectra of 3f



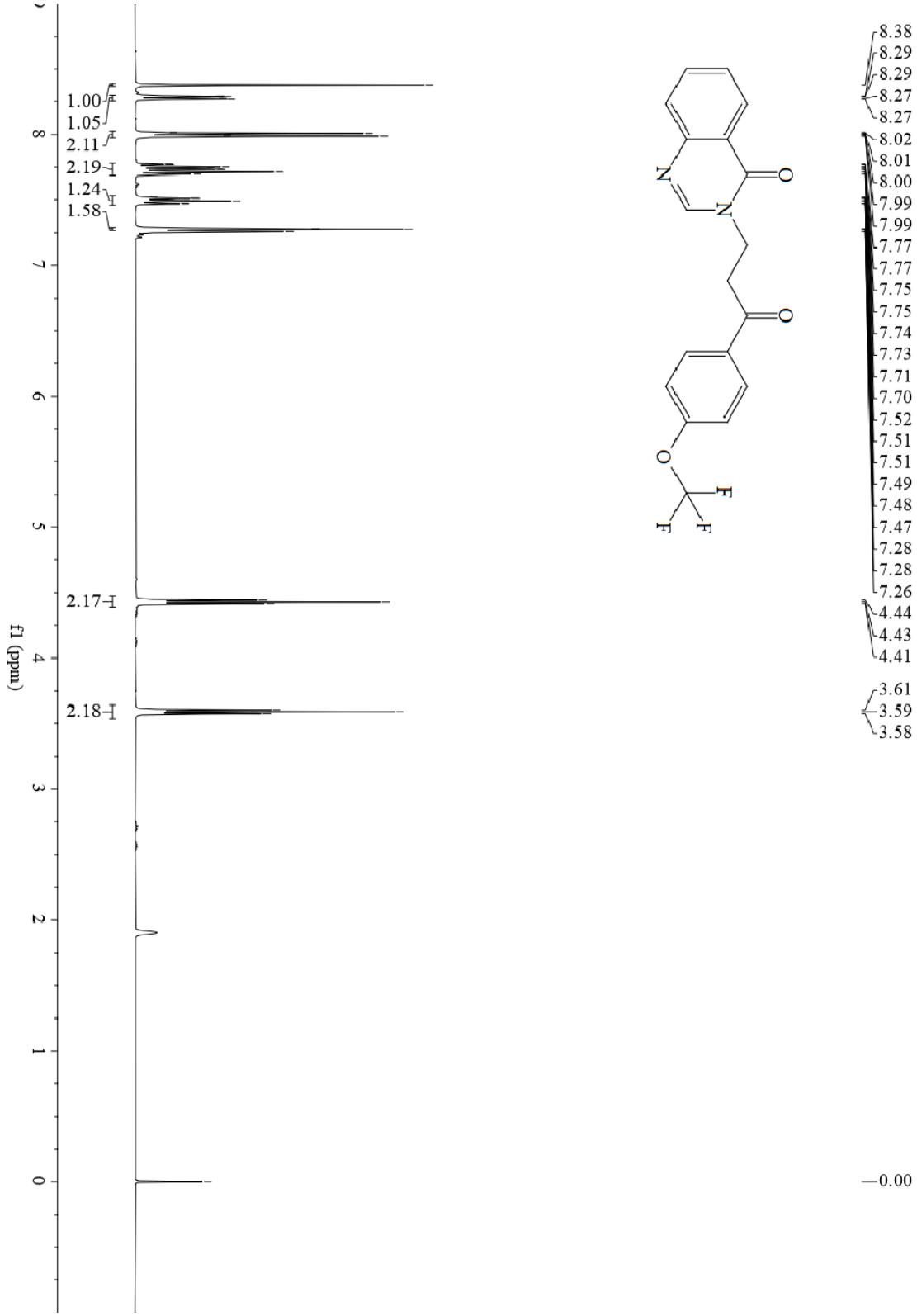

196.56
161.46
148.15
147.61
134.80
134.36
132.08
129.58
128.99
127.57
127.26
126.39
121.96
77.39
77.07
76.75
42.76
36.80
f1 (ppm)

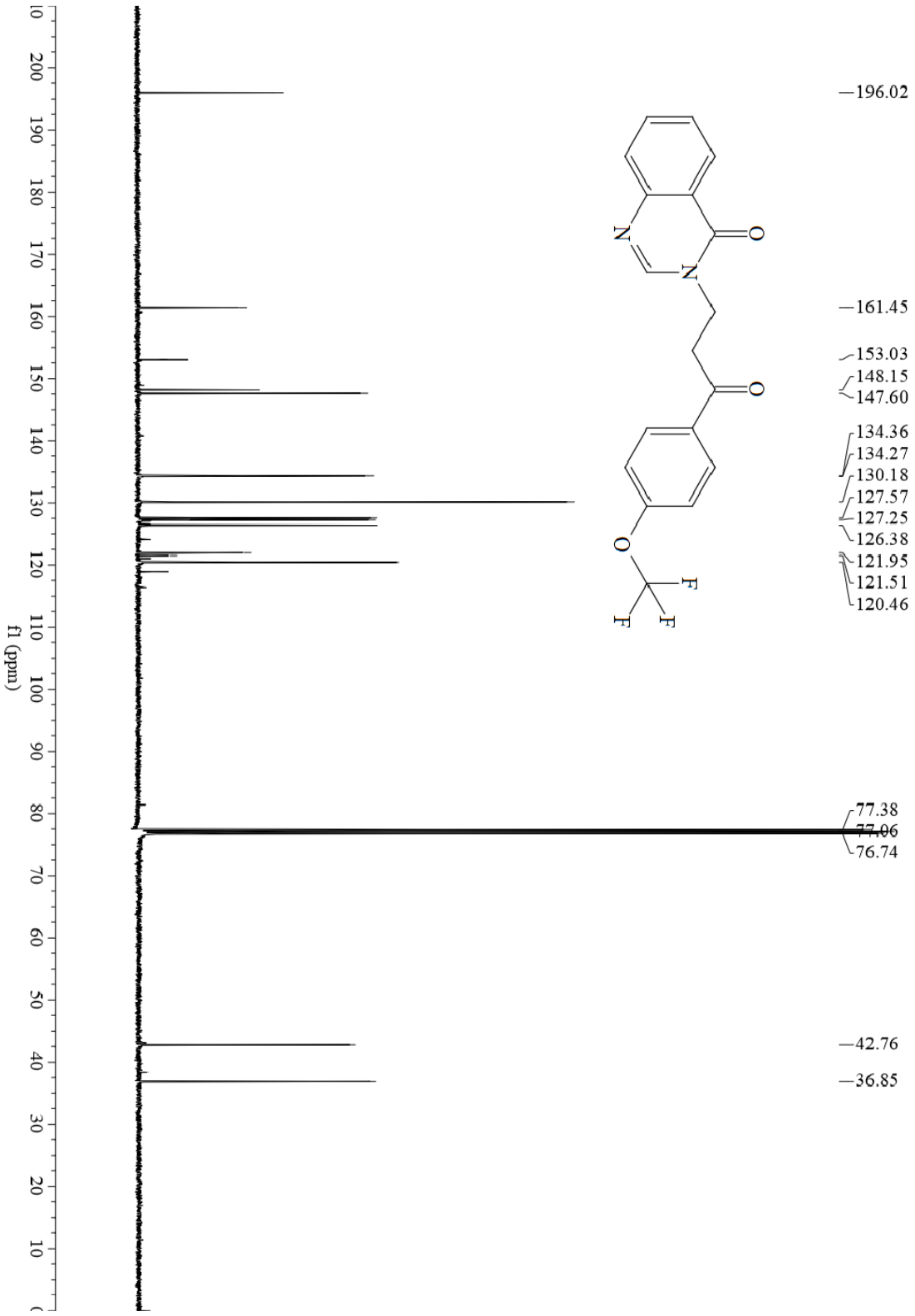
^{1}H and ^{13}C NMR spectra of 3g

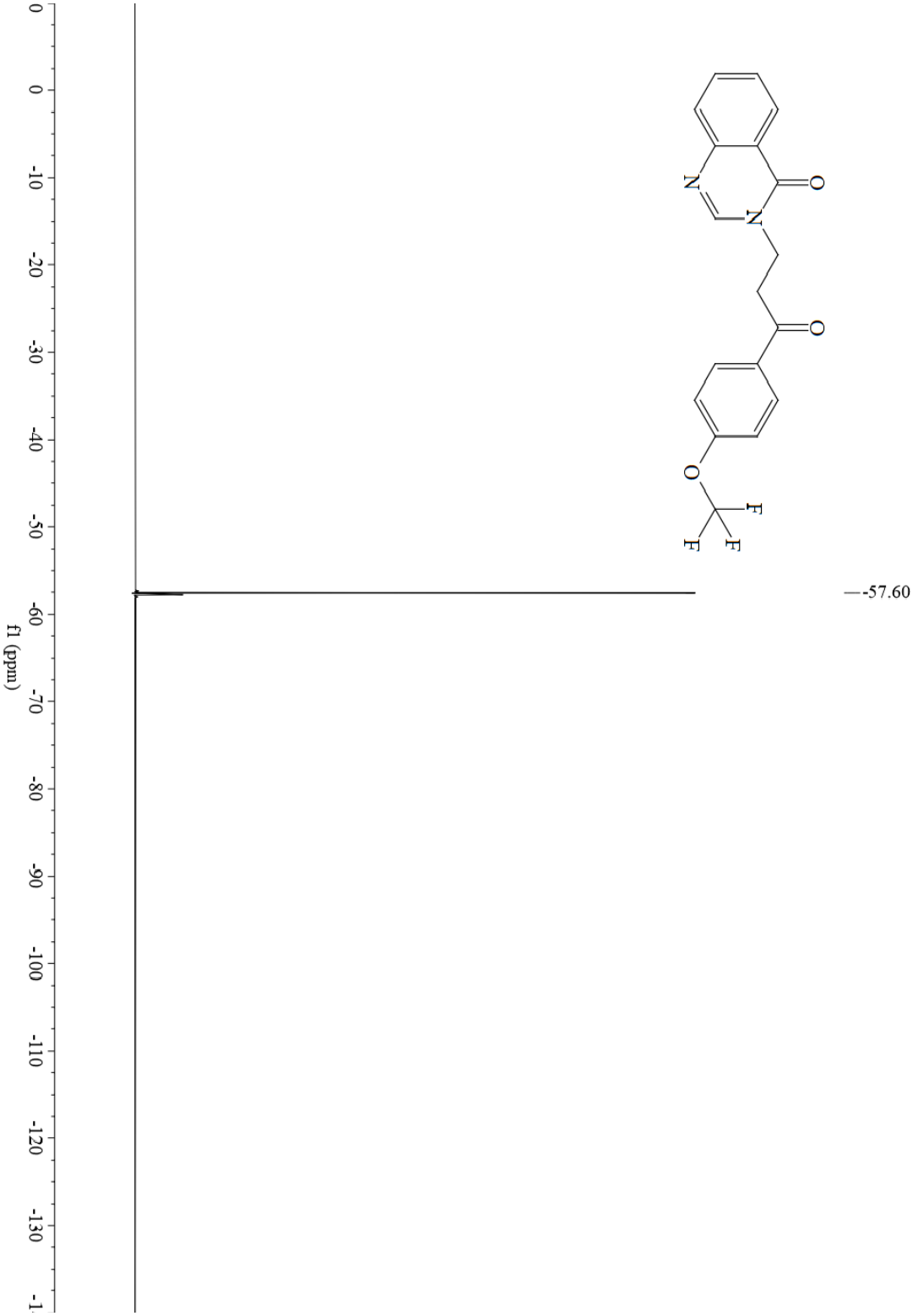



196.35
161.47
148.17
147.62
140.23
134.41
134.36
129.50
129.09
127.58
127.26
126.40
121.97
77.38
77.06
76.74
42.78
36.82
O
N
N
O
Cl
f1 (ppm)

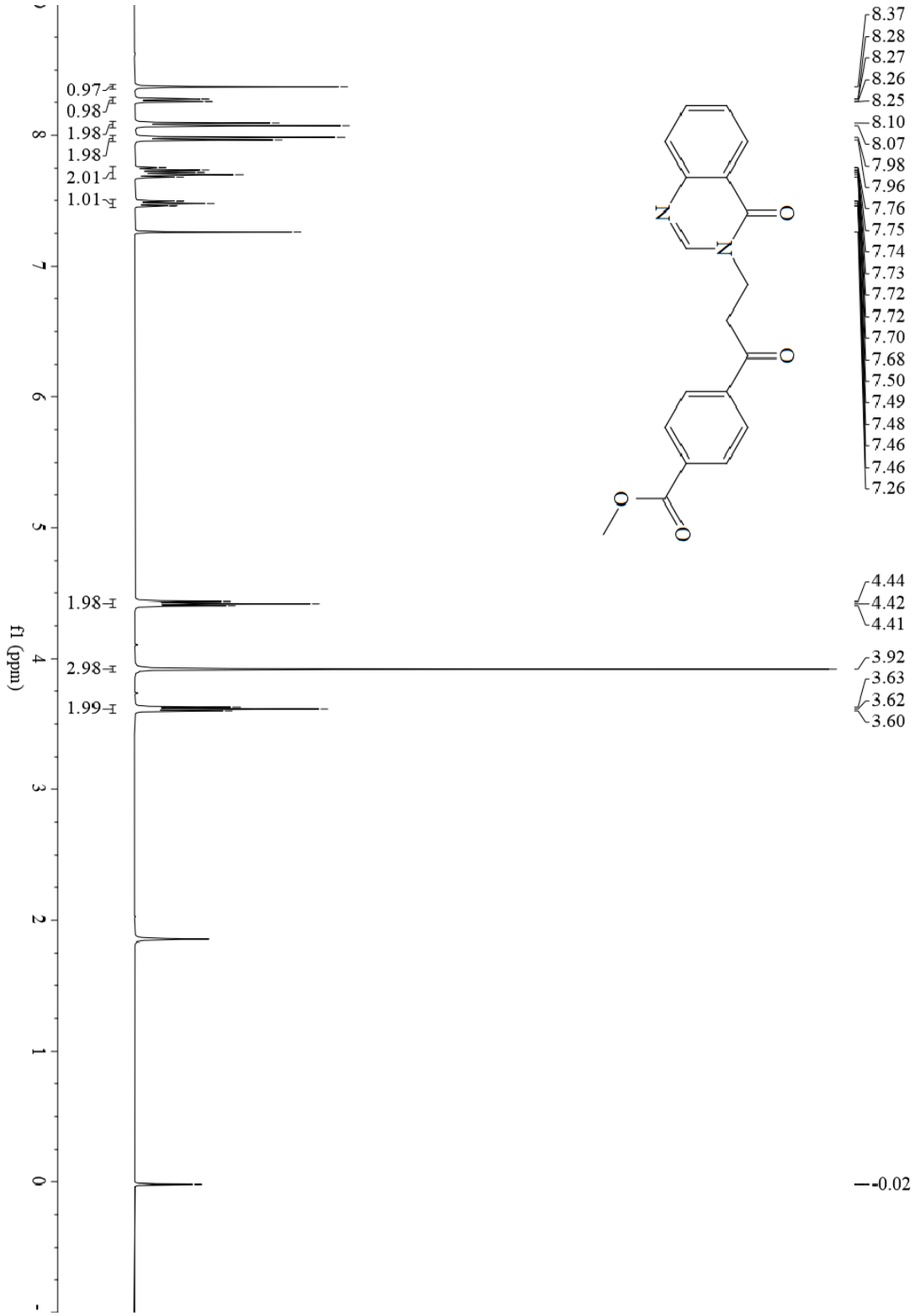
^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of 3h

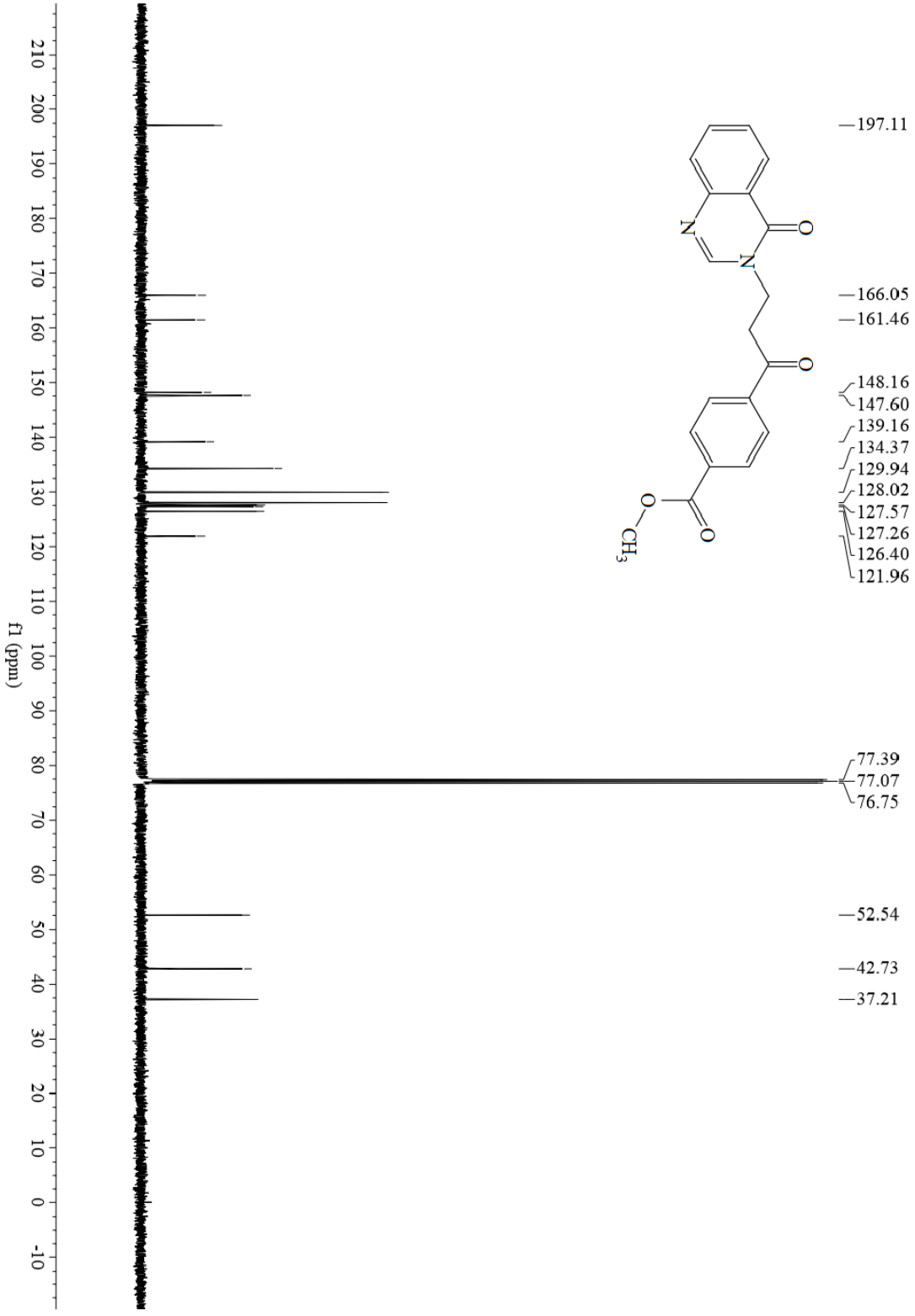



196.02
161.45
153.03
148.15
147.60
134.36
134.27
130.18
127.57
127.25
126.38
121.95
121.51
120.46
77.38
77.06
76.74
42.76
36.85
f1 (ppm)

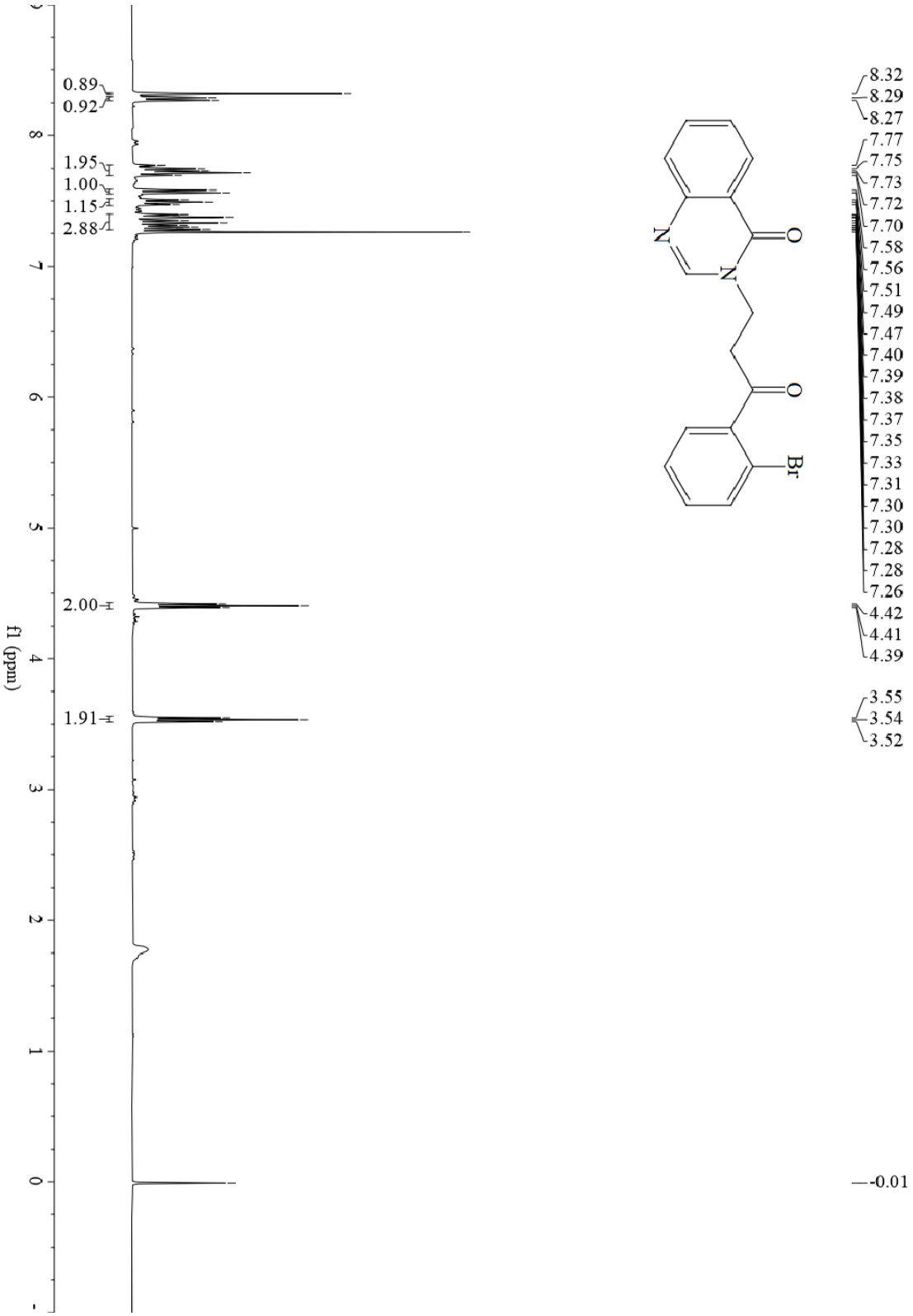

-57.60
f1 (ppm)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130

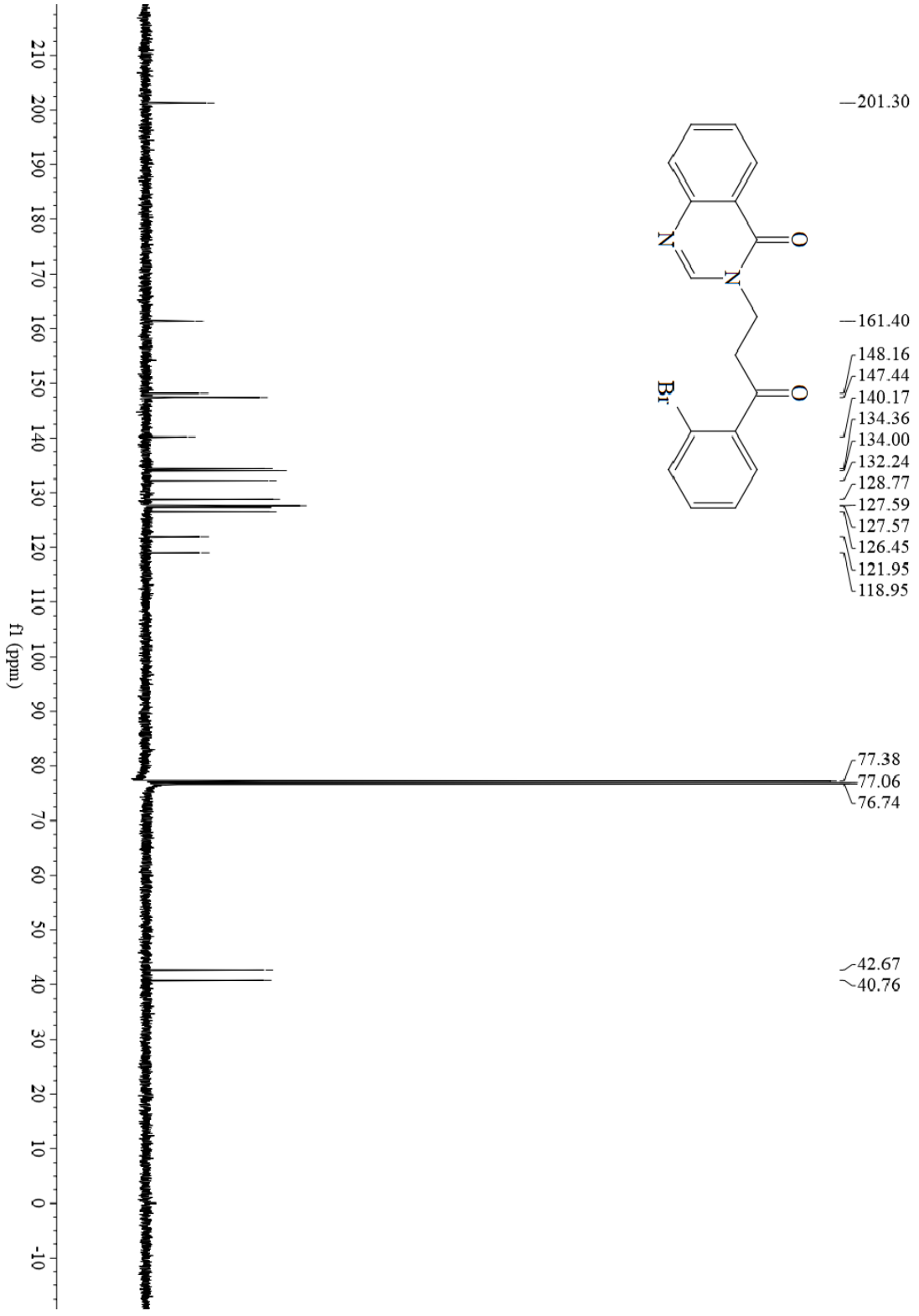
^{1}H NMR, ^{13}C NMR spectra of 3i



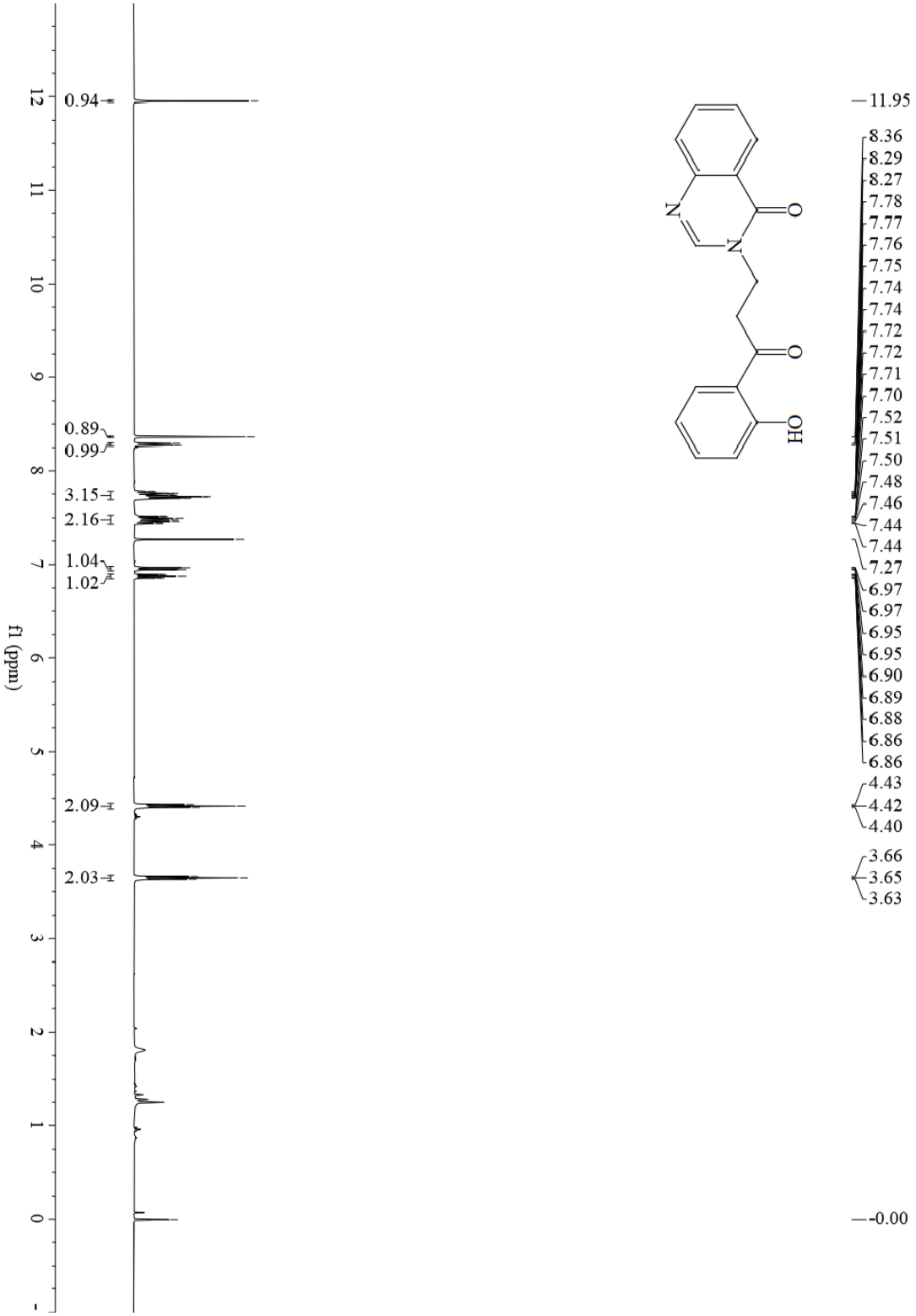

197.11
166.05
161.46
148.16
147.60
139.16
134.37
129.94
128.02
127.57
127.26
126.40
121.96
77.39
77.07
76.75
52.54
42.73
37.21
f1 (ppm)

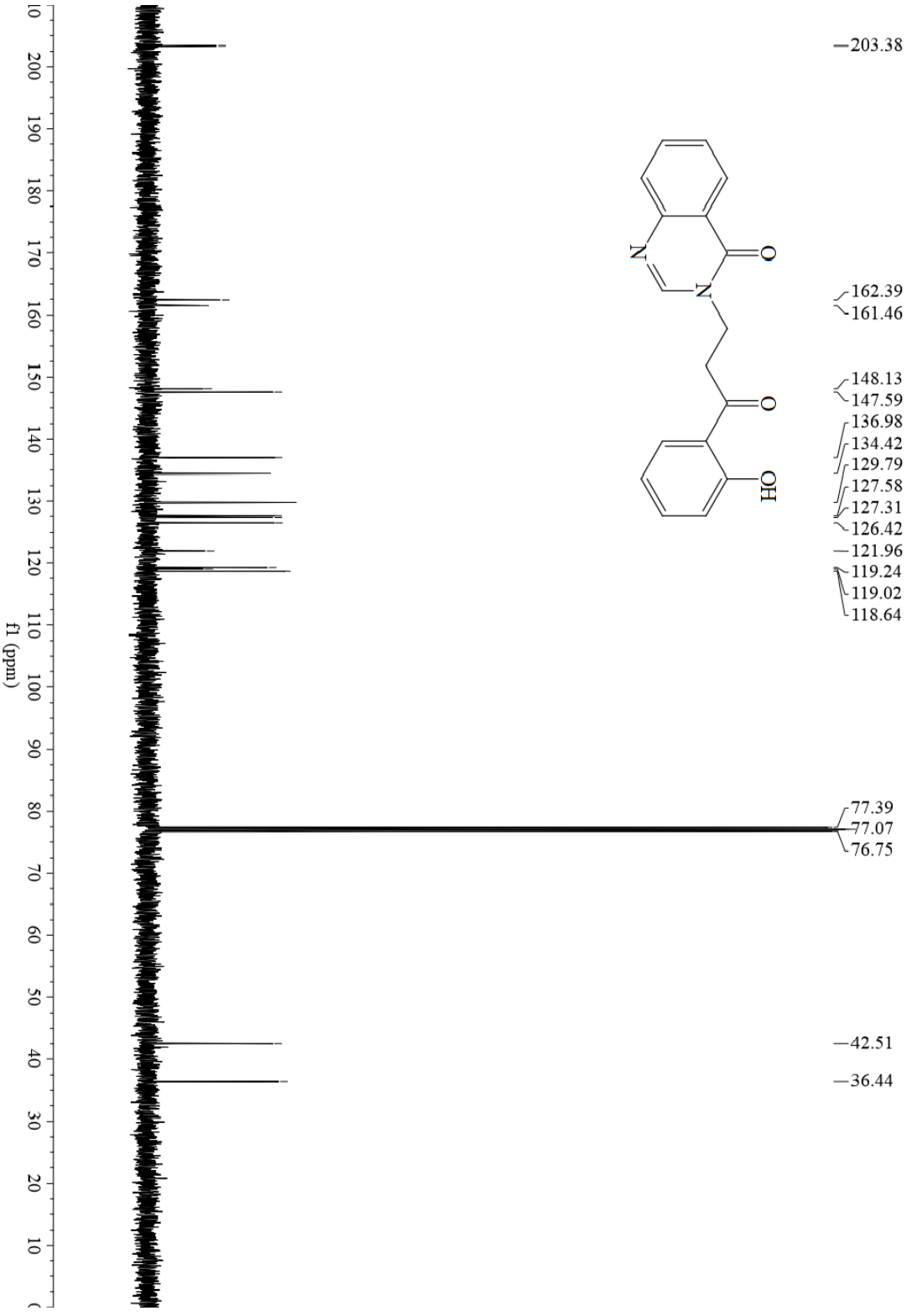
^{1}H and ^{13}C NMR spectra of 3j



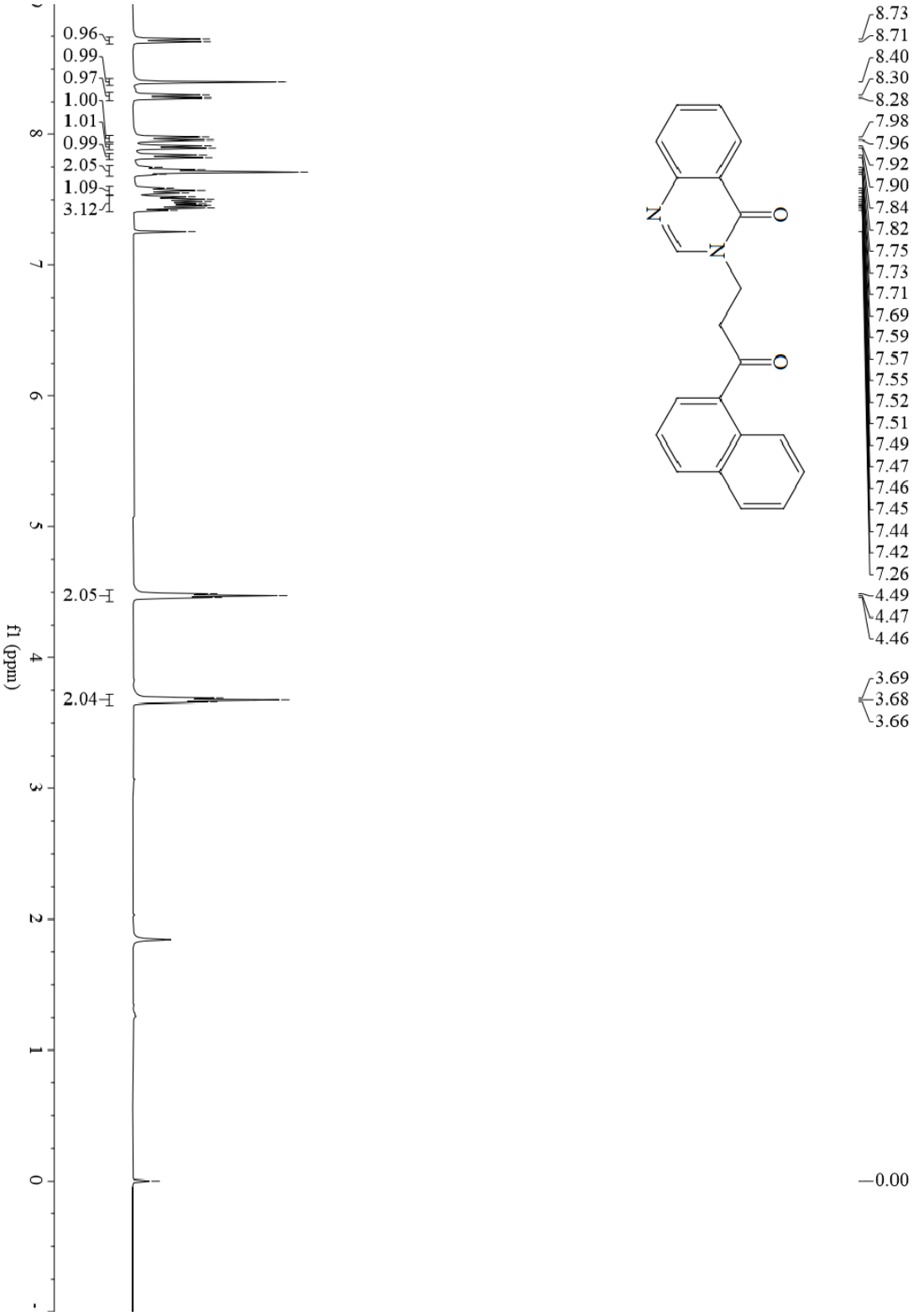

201.30
161.40
148.16
147.44
140.17
134.36
134.00
132.24
128.77
127.59
127.57
126.45
121.95
118.95
77.38
77.06
76.74
42.67
40.76
O
N
N
O
Br
fl (ppm)

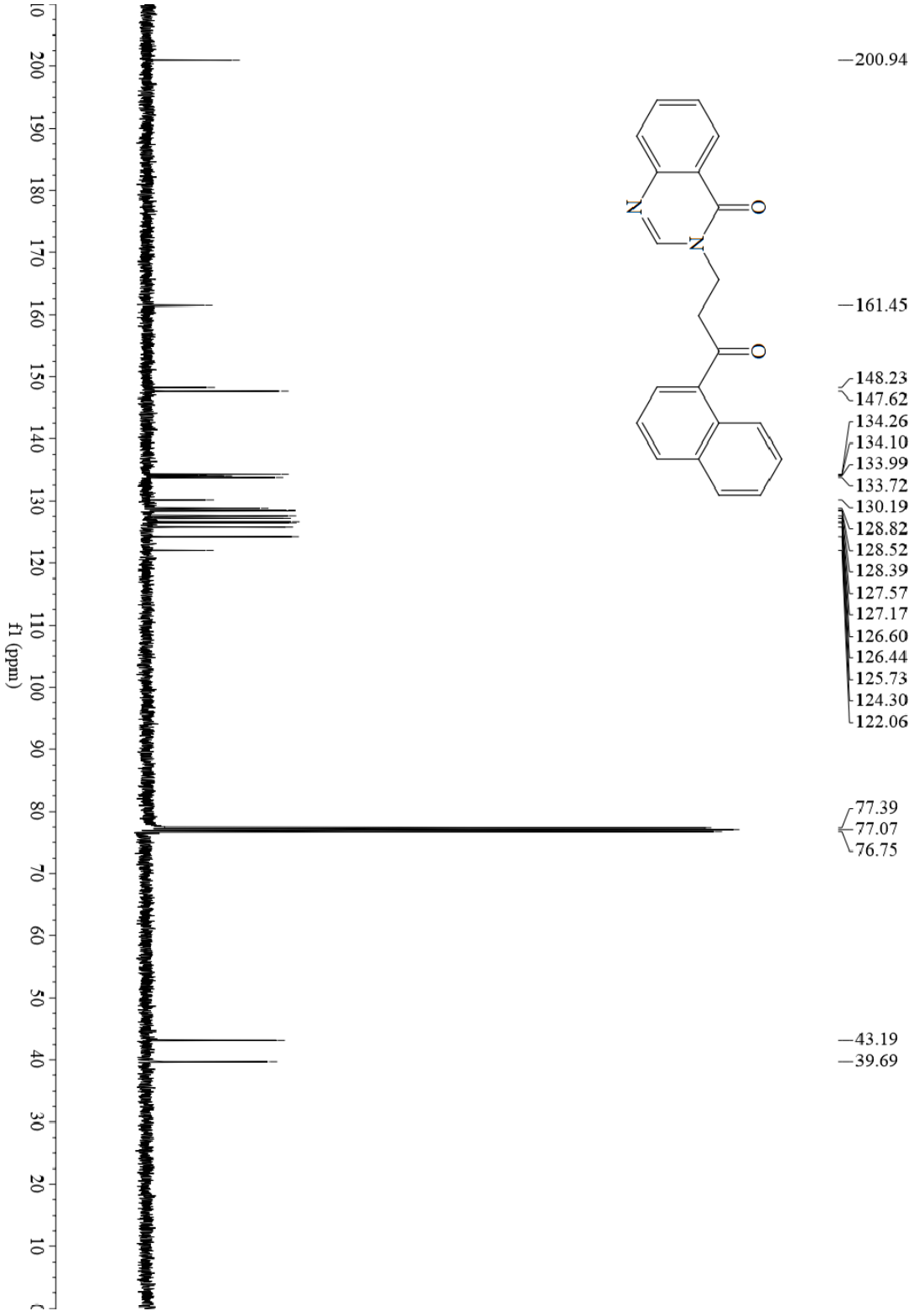
^{1}H and ^{13}C NMR spectra of 3k



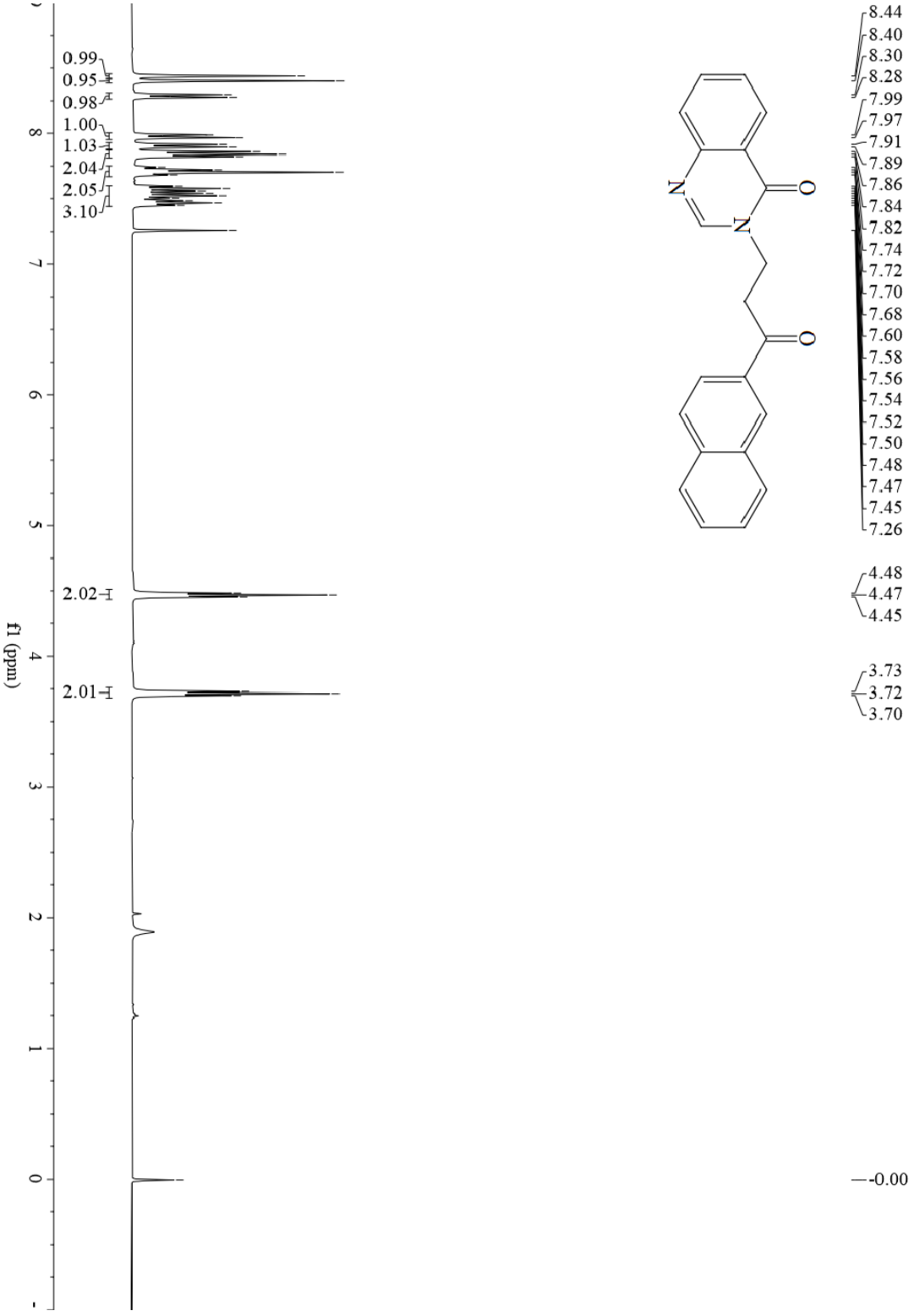

203.38
162.39
161.46
148.13
147.59
136.98
134.42
129.79
127.58
127.31
126.42
121.96
119.24
119.02
118.64
77.39
77.07
76.75
42.51
36.44
f1 (ppm)

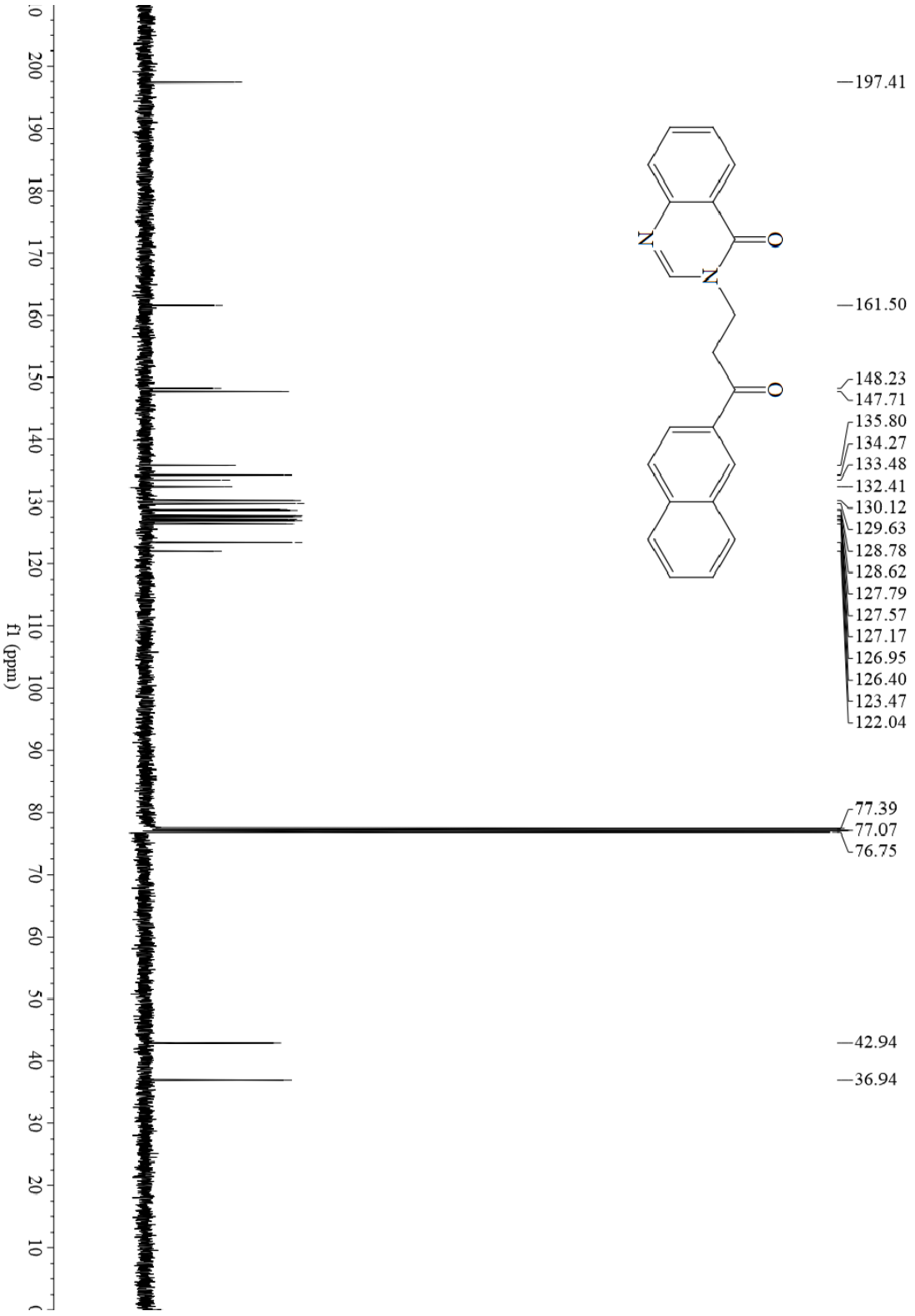
^{1}H and ^{13}C NMR spectra of 3l



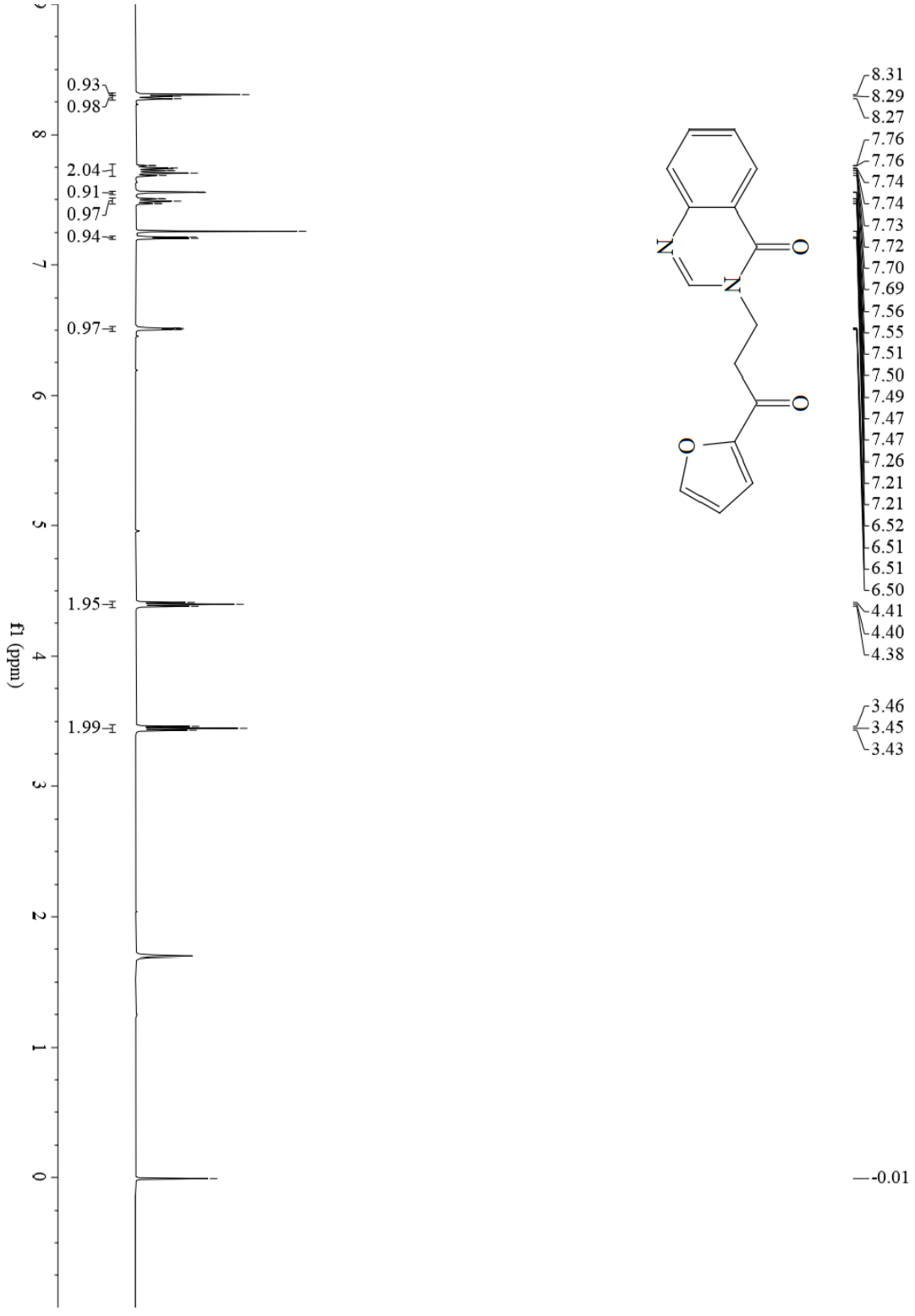

200.94
161.45
148.23
147.62
134.26
134.10
133.99
133.72
130.19
128.82
128.52
128.39
127.57
127.17
126.60
126.44
125.73
124.30
122.06
77.39
77.07
76.75
43.19
39.69
f1 (ppm)

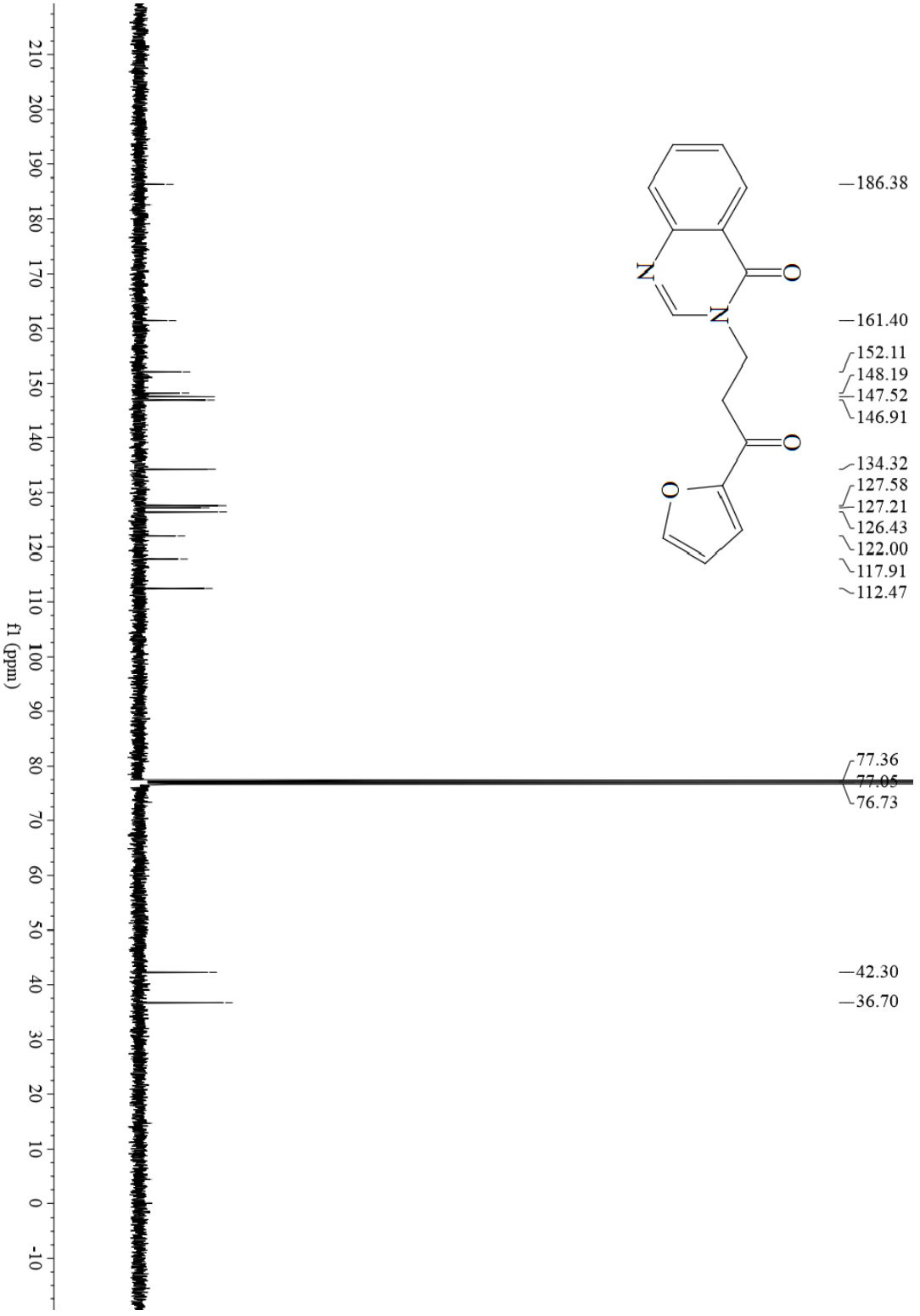
^{1}H and ^{13}C NMR spectra of 3m



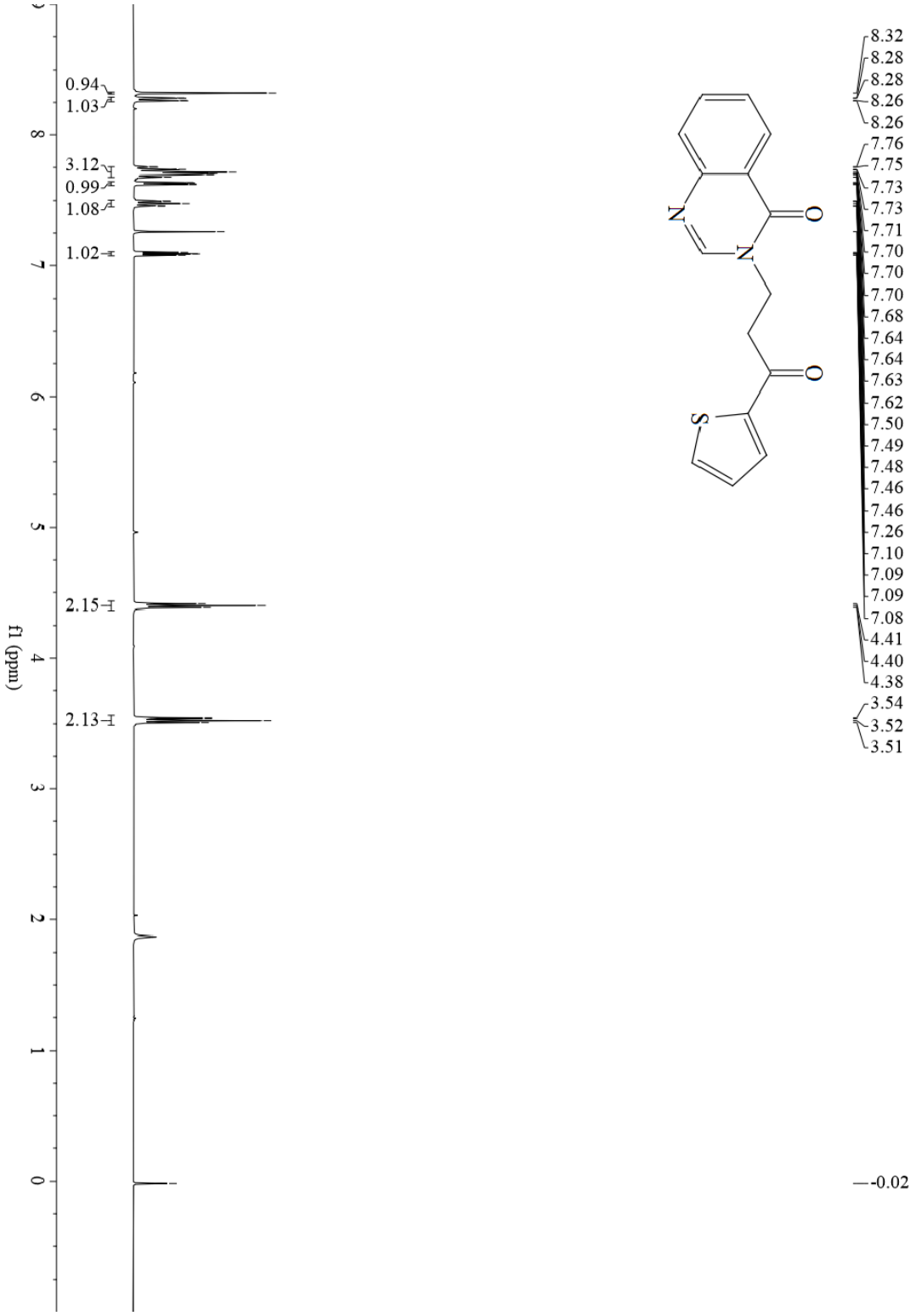

197.41
161.50
148.23
147.71
135.80
134.27
133.48
132.41
130.12
129.63
128.78
128.62
127.79
127.57
127.17
126.95
126.40
123.47
122.04
77.39
77.07
76.75
42.94
36.94
f1 (ppm)

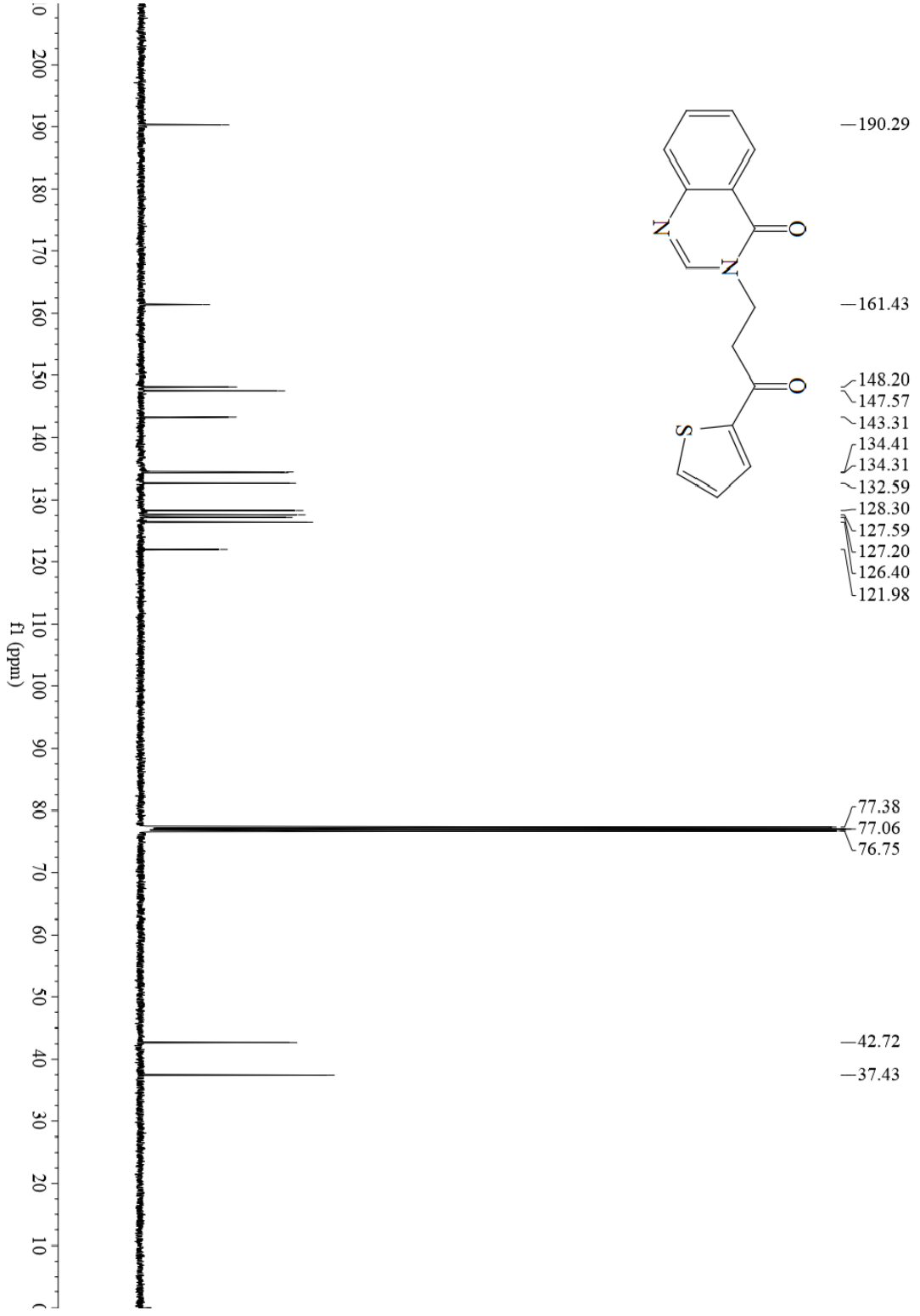
^{1}H and ^{13}C NMR spectra of 3n



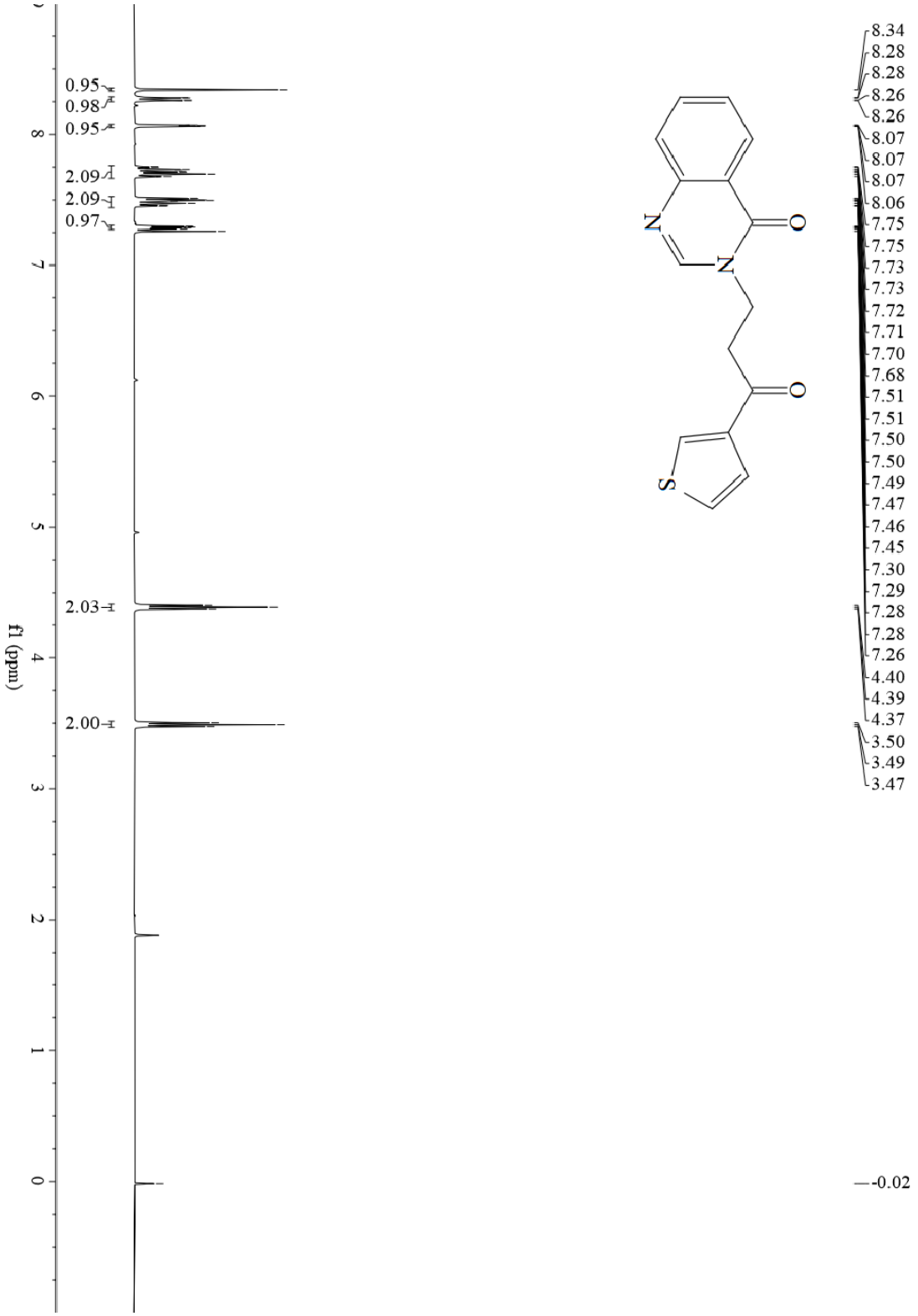

f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
N
N
O
O
O
186.38
161.40
152.11
148.19
147.52
146.91
134.32
127.58
127.21
126.43
122.00
117.91
112.47
77.36
77.05
76.73
42.30
36.70

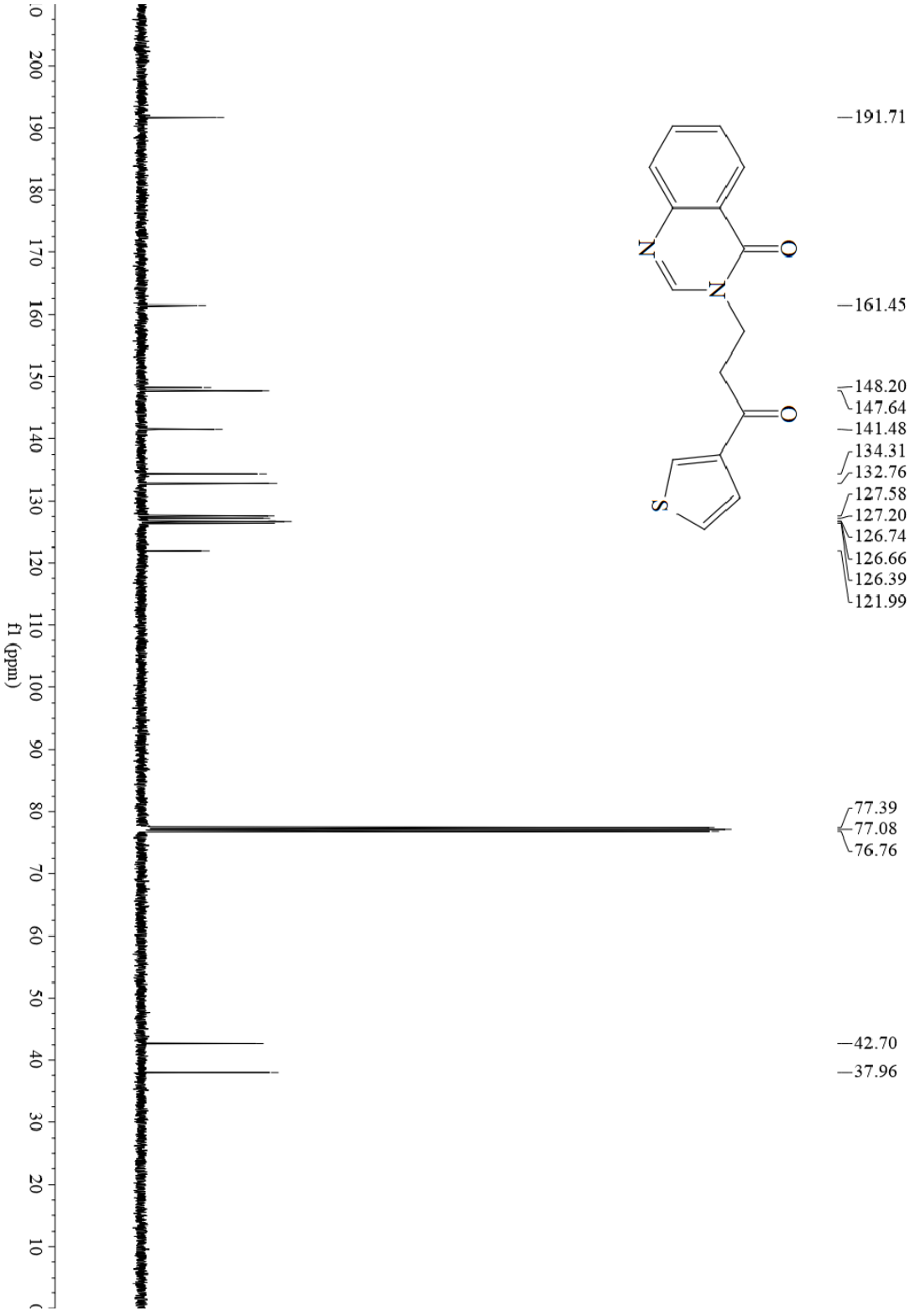
^{1}H and ^{13}C NMR spectra of 3o



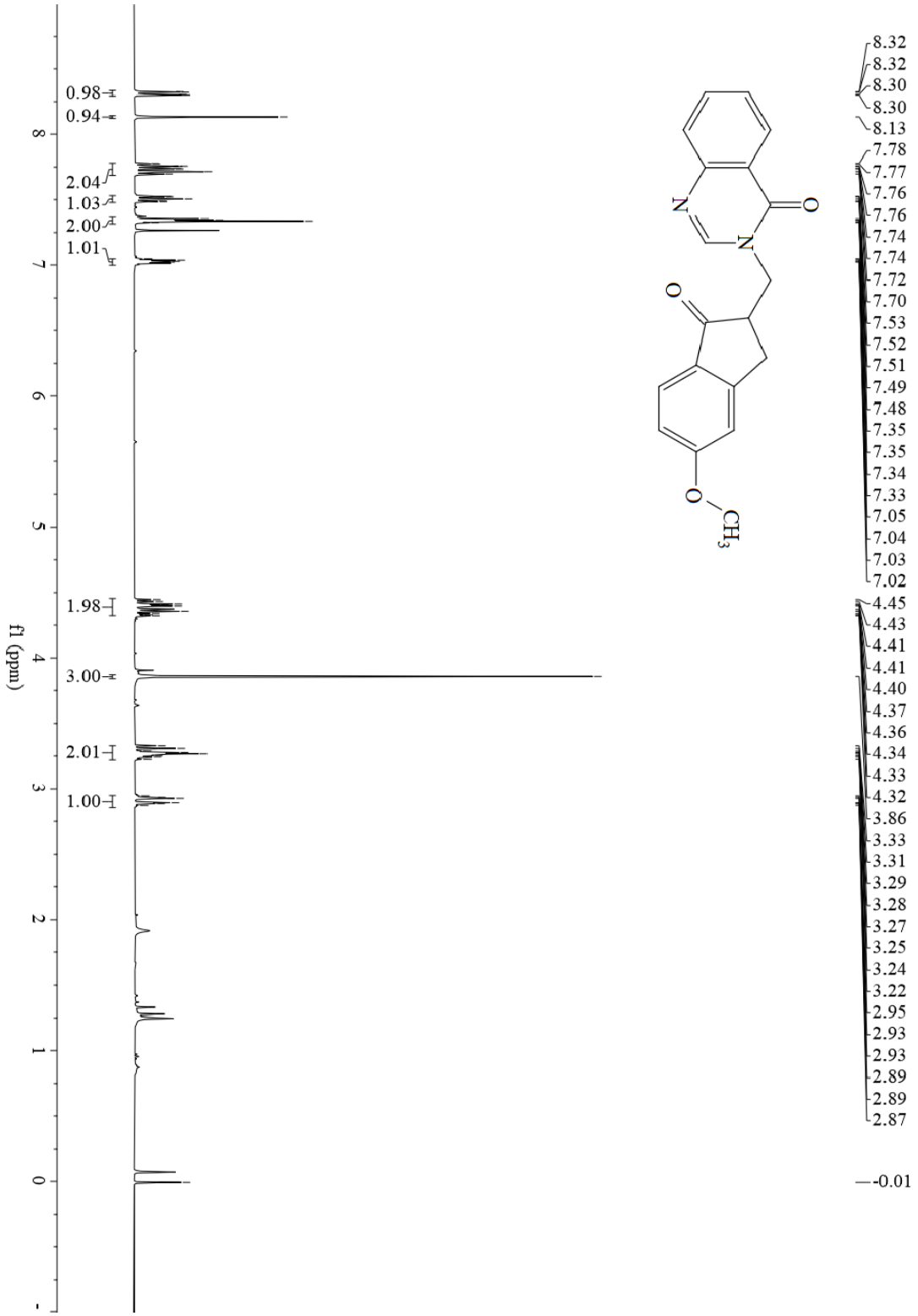

190.29
161.43
148.20
147.57
143.31
134.41
134.31
132.59
128.30
127.59
127.20
126.40
121.98
77.38
77.06
76.75
42.72
37.43
f1 (ppm)

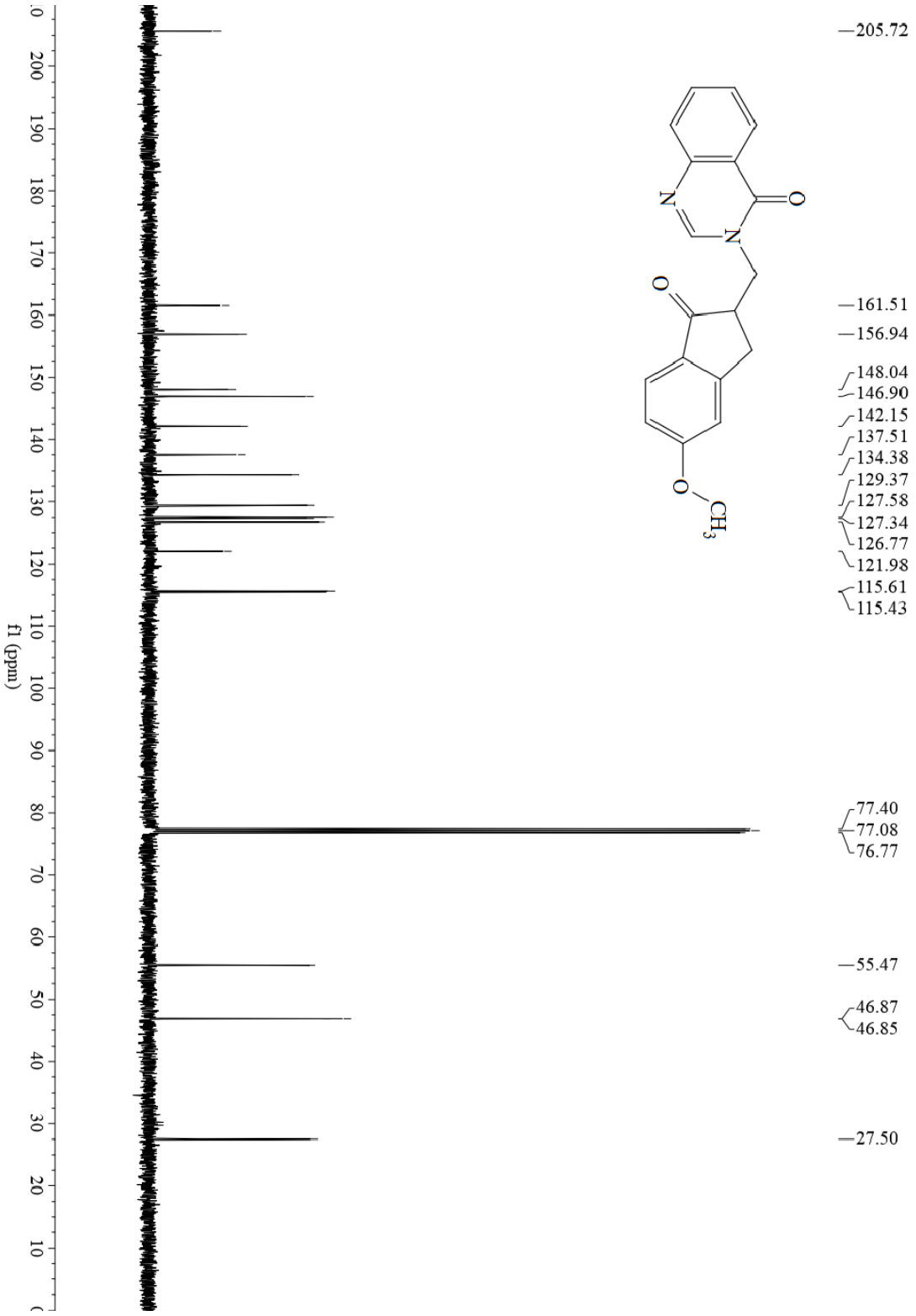
^{1}H and ^{13}C NMR spectra of 3p



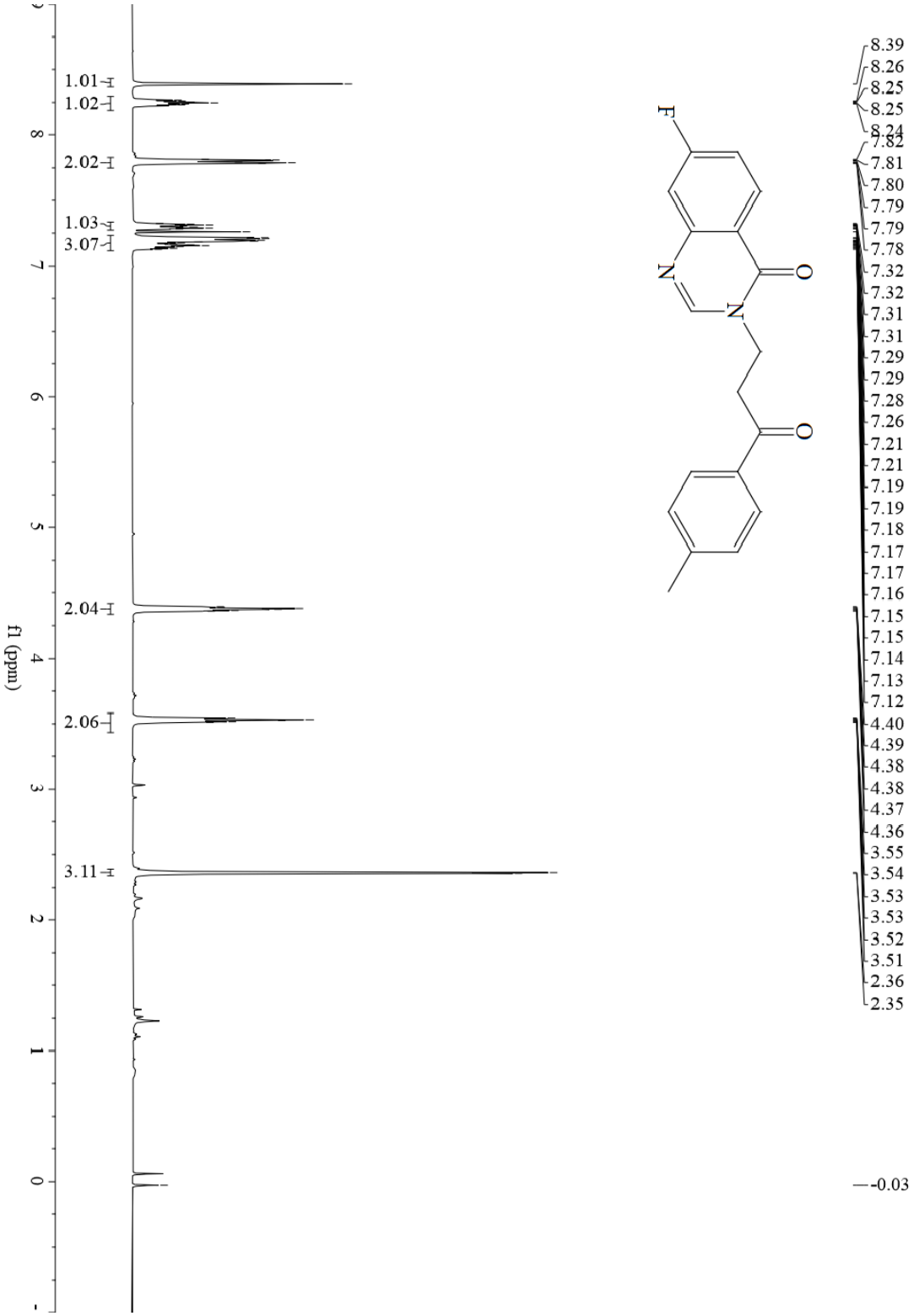

191.71
161.45
148.20
147.64
141.48
134.31
132.76
127.58
127.20
126.74
126.66
126.39
121.99
77.39
77.08
76.76
42.70
37.96
f1 (ppm)

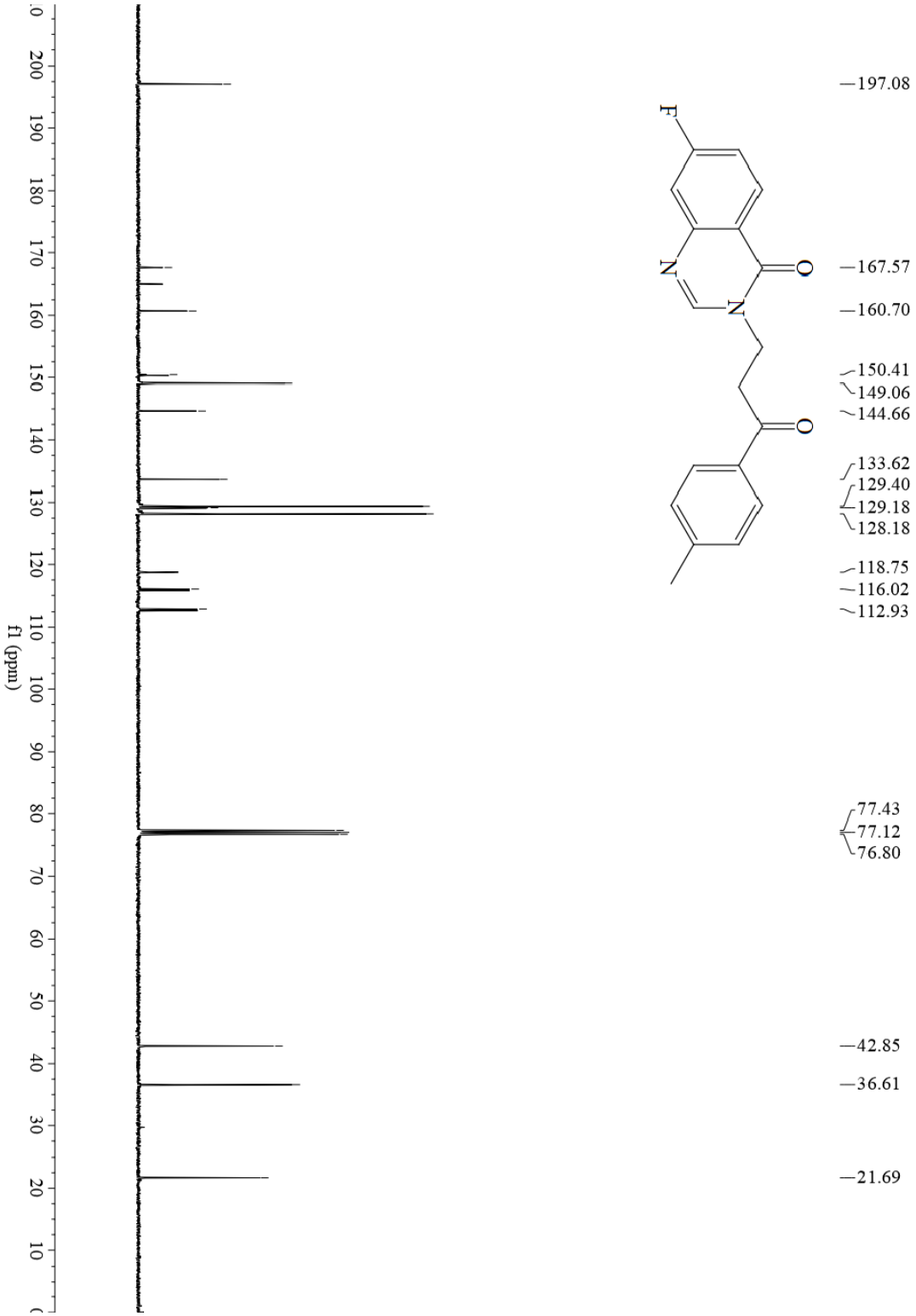
^{1}H and ^{13}C NMR spectra of 3q




205.72
161.51
156.94
148.04
146.90
142.15
137.51
134.38
129.37
127.58
127.34
126.77
121.98
115.61
115.43
77.40
77.08
76.77
55.47
46.87
46.85
27.50
f1 (ppm)

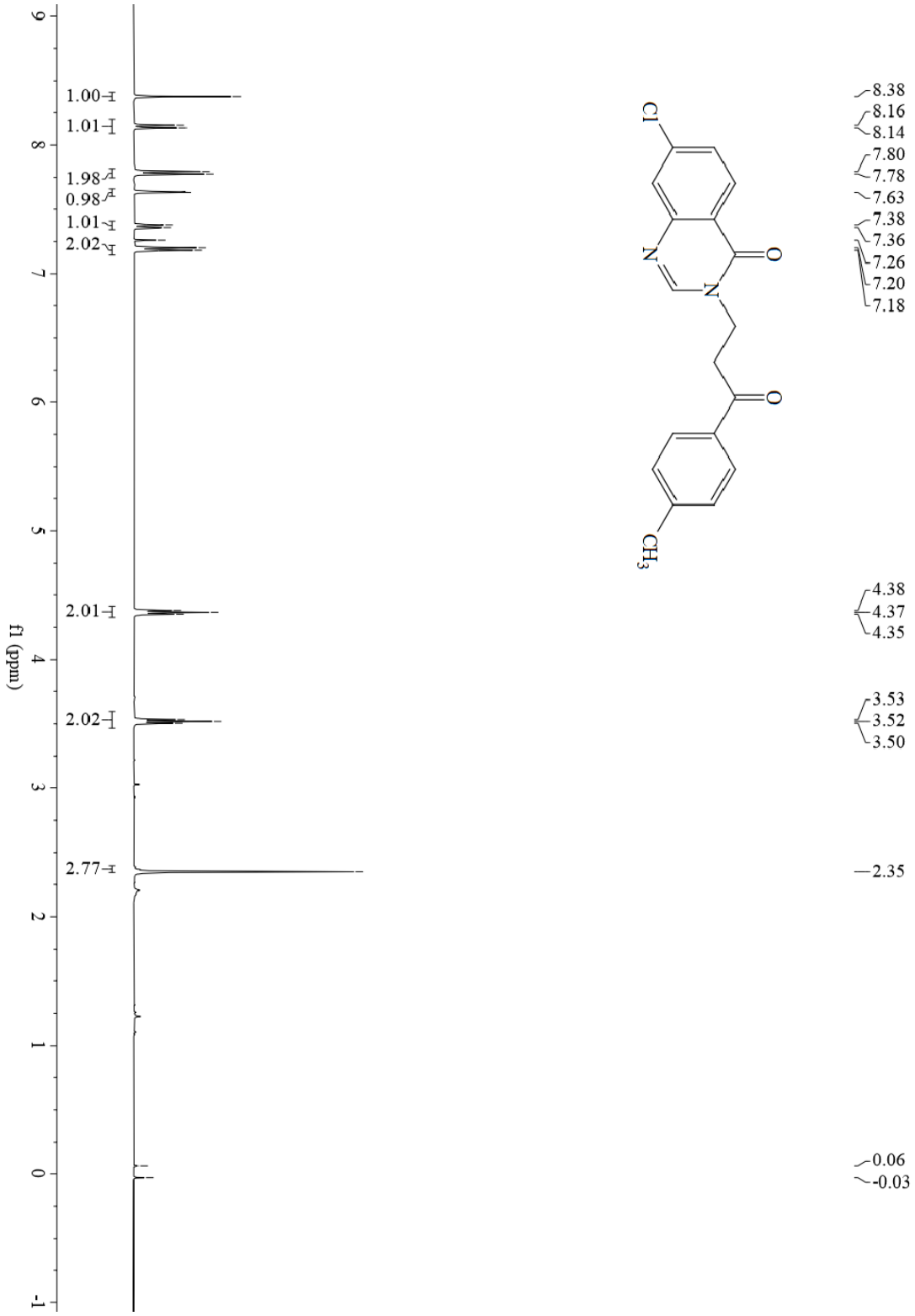
^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of 3r

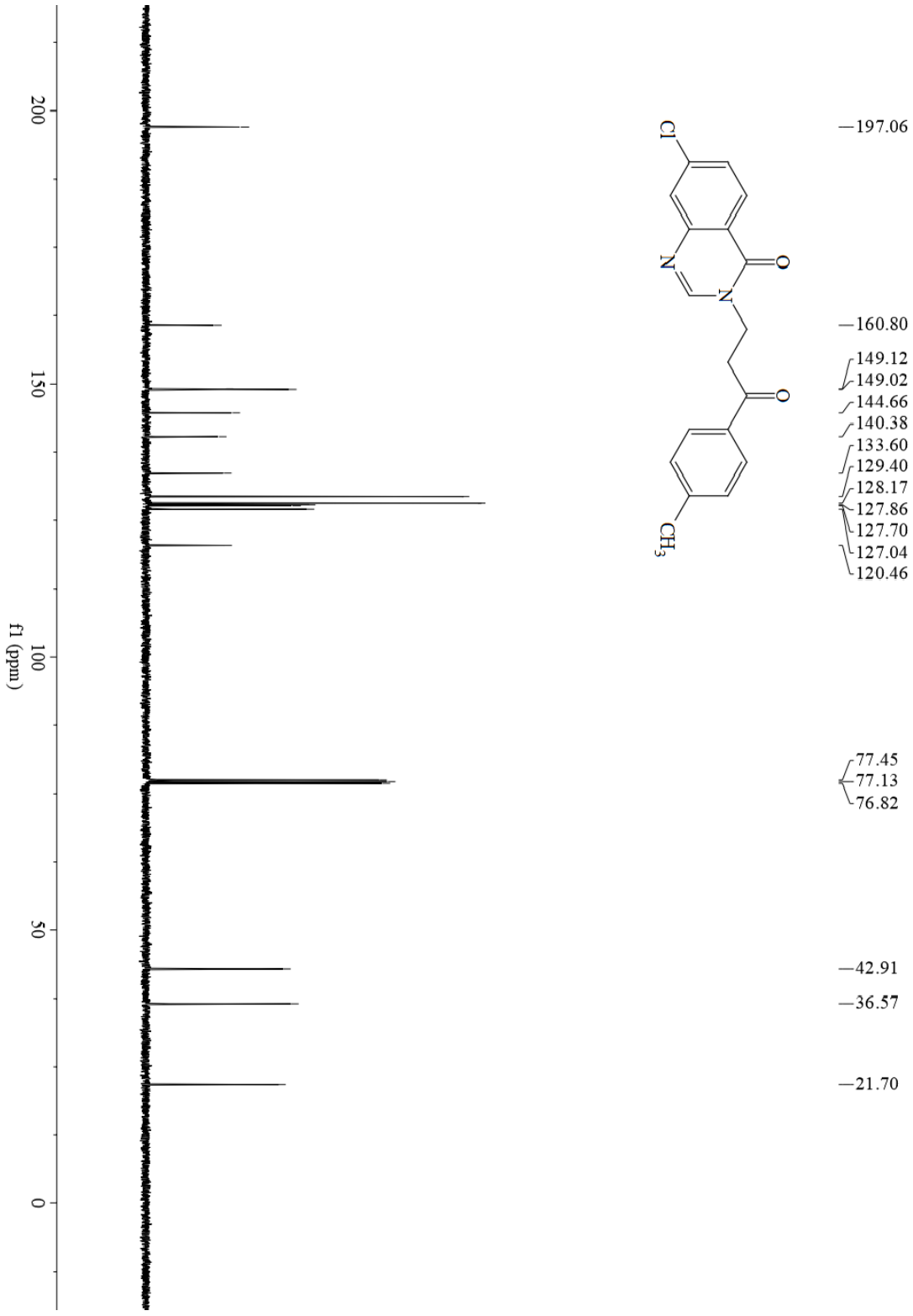



f1 (ppm)
197.08
167.57
160.70
150.41
149.06
144.66
133.62
129.40
129.18
128.18
118.75
116.02
112.93
77.43
77.12
76.80
42.85
36.61
21.69
F
N
N
O
O

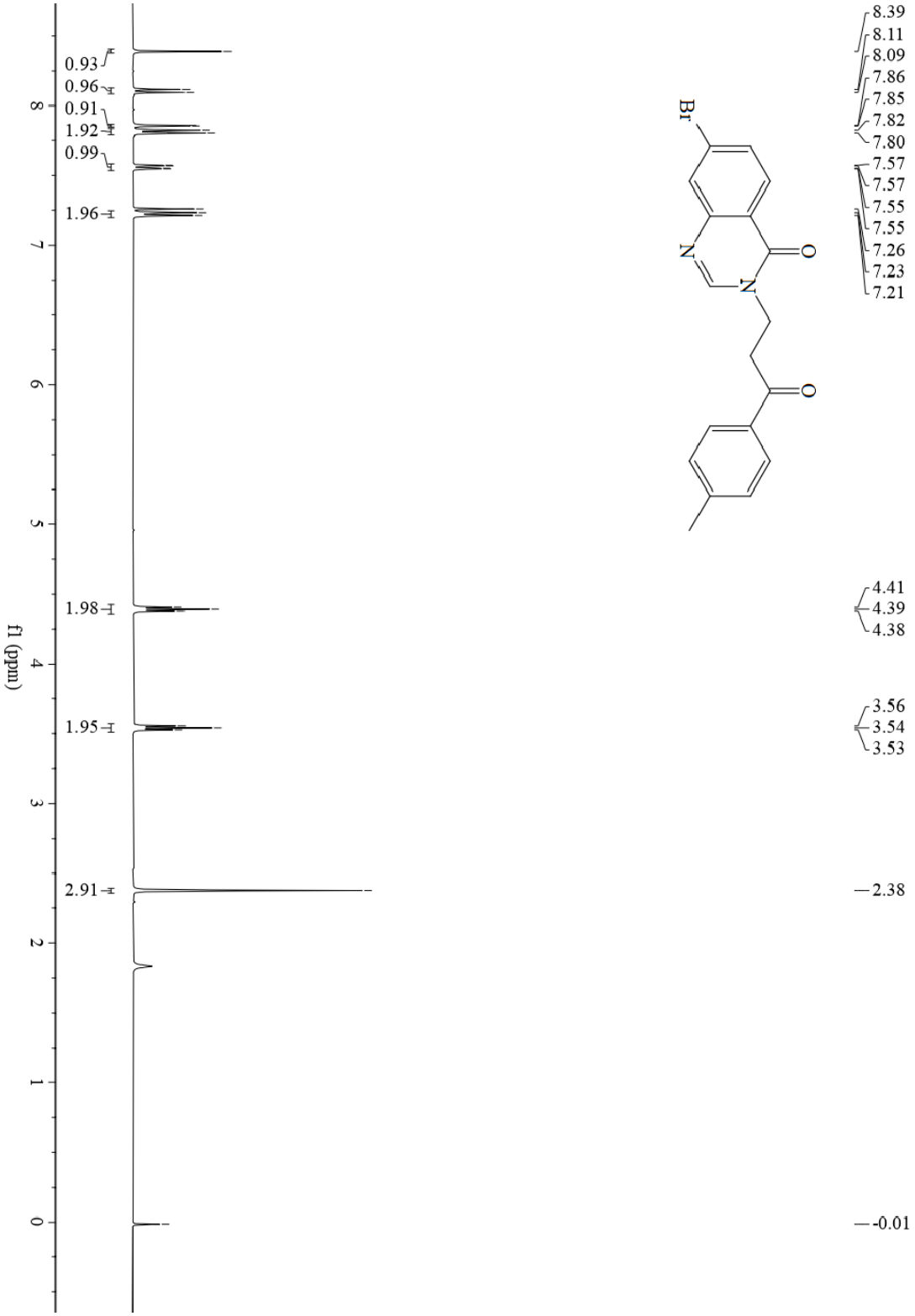

-103.19
O
O
F
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

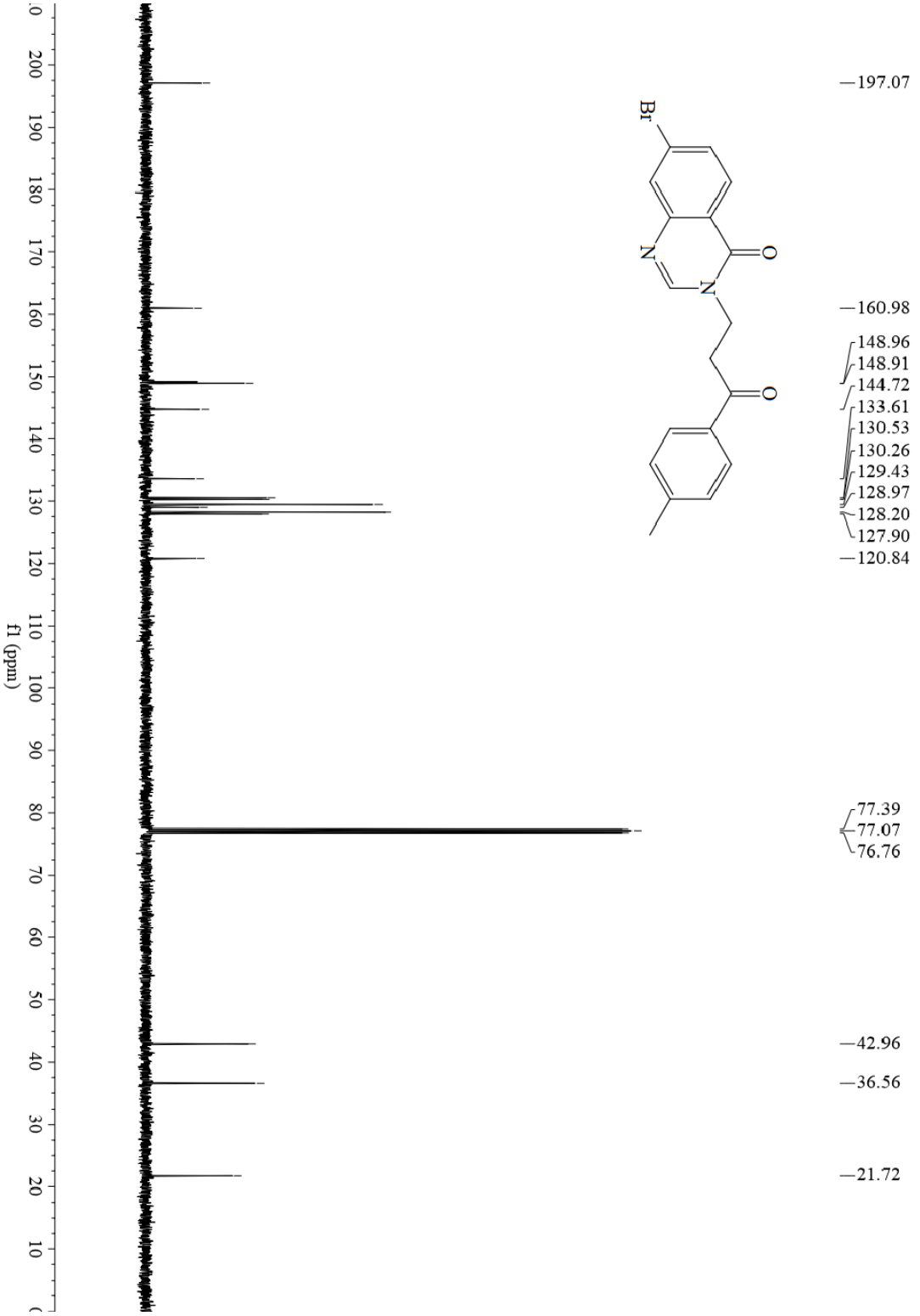
^{1}H and ^{13}C NMR spectra of 3s



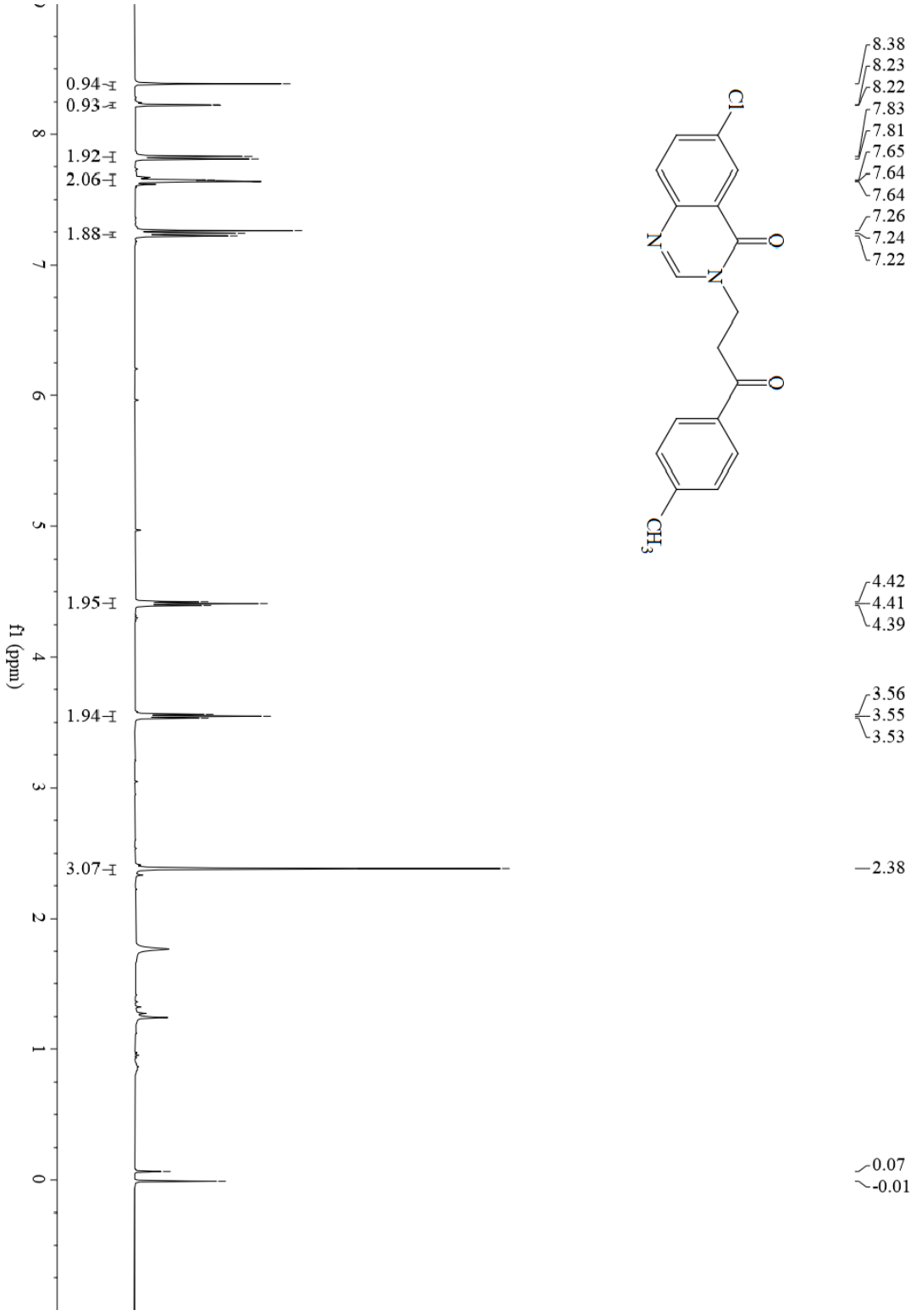

200
150
100
50
0
f1 (ppm)
Cl
N
N
O
O
CH3
197.06
160.80
149.12
149.02
144.66
140.38
133.60
129.40
128.17
127.86
127.70
127.04
120.46
77.45
77.13
76.82
42.91
36.57
21.70

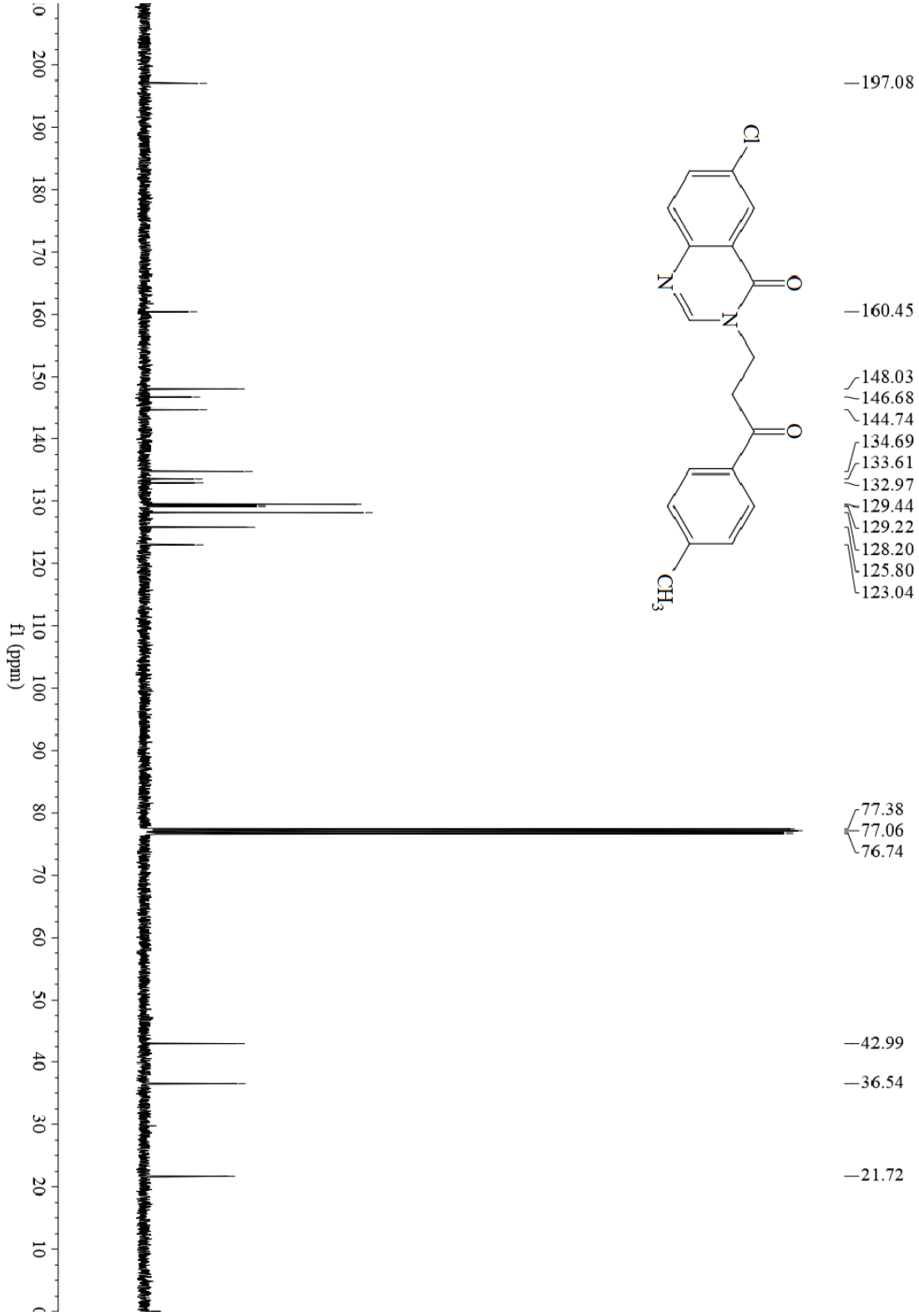
^{1}H and ^{13}C NMR spectra of 3t



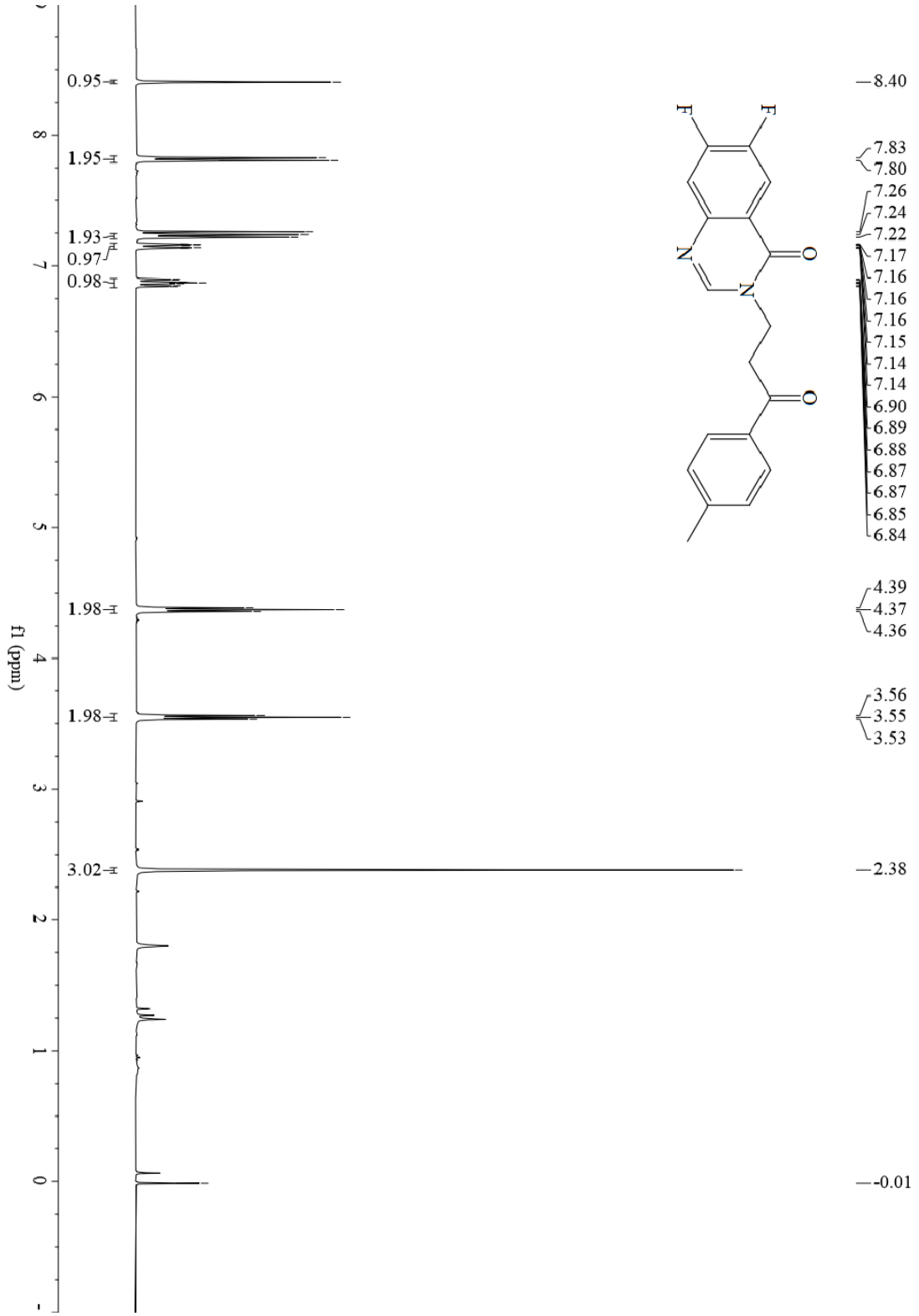

Br
N
N
O
O
f1 (ppm)
—197.07
—160.98
148.96
148.91
144.72
133.61
130.53
130.26
129.43
128.97
128.20
127.90
—120.84
77.39
77.07
76.76
—42.96
—36.56
—21.72

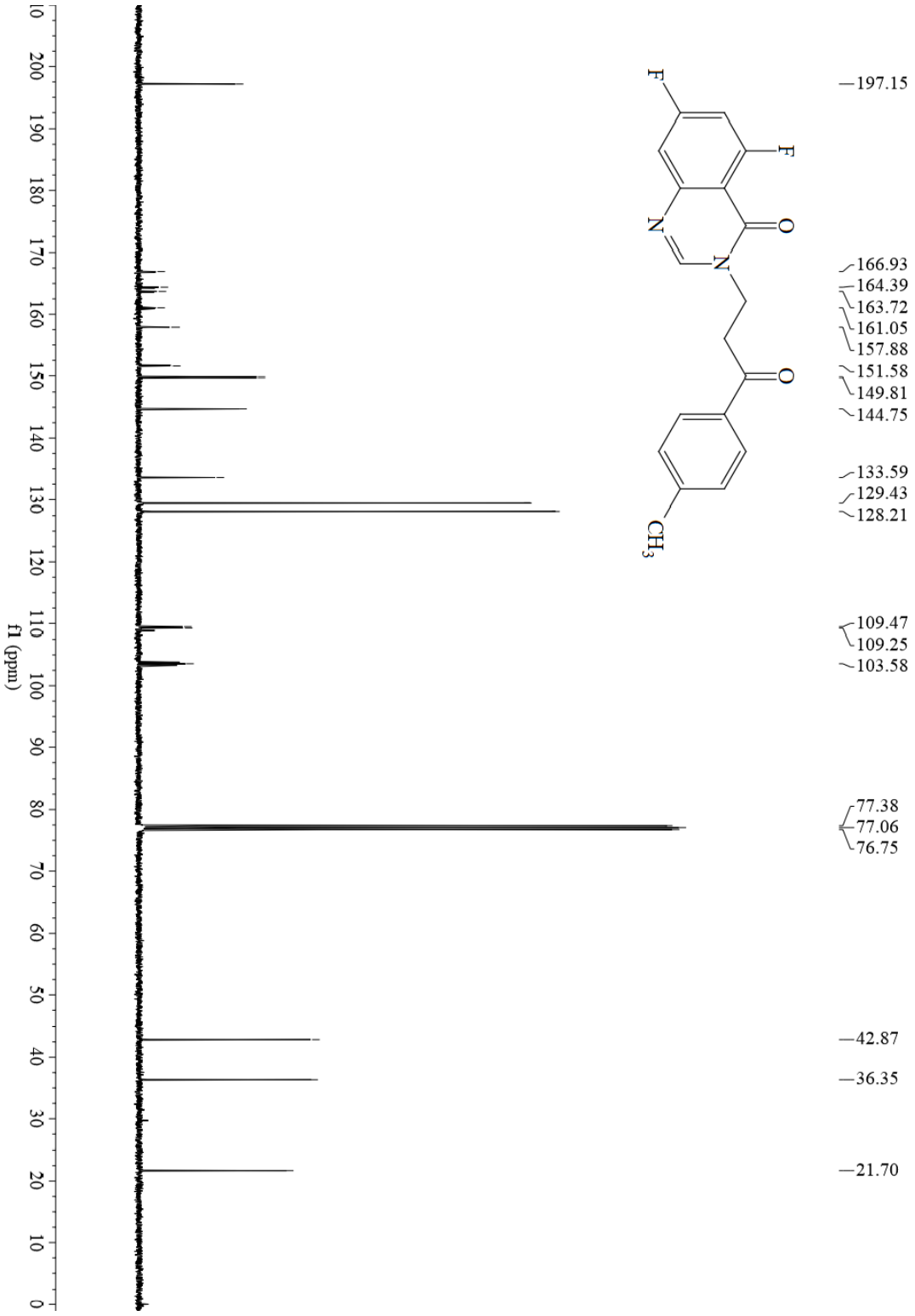
^{1}H and ^{13}C NMR spectra of 3u

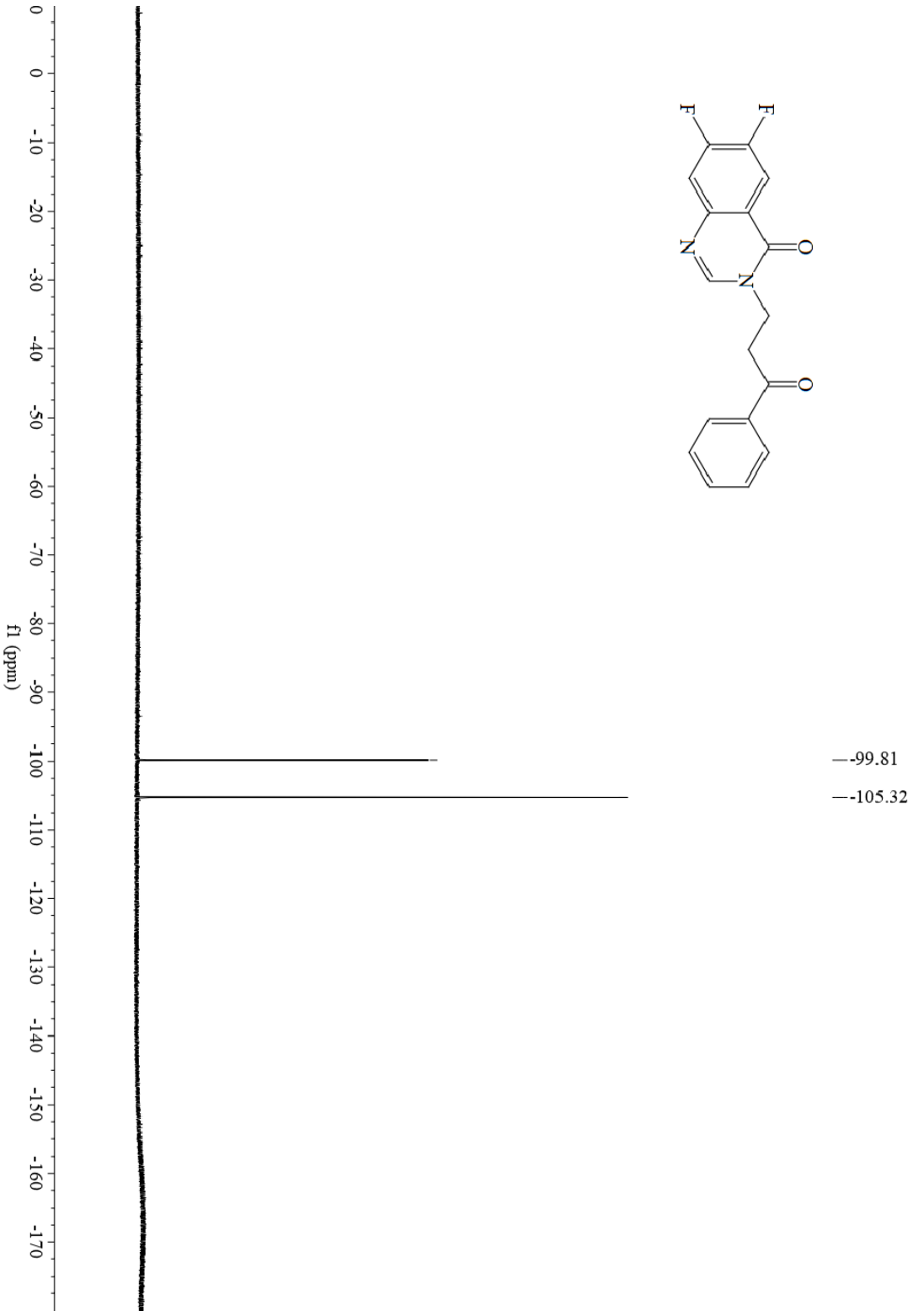



f1 (ppm)
197.08
160.45
148.03
146.68
144.74
134.69
133.61
132.97
129.44
129.22
128.20
125.80
123.04
77.38
77.06
76.74
42.99
36.54
21.72
Cl
N
N
O
O
CH3

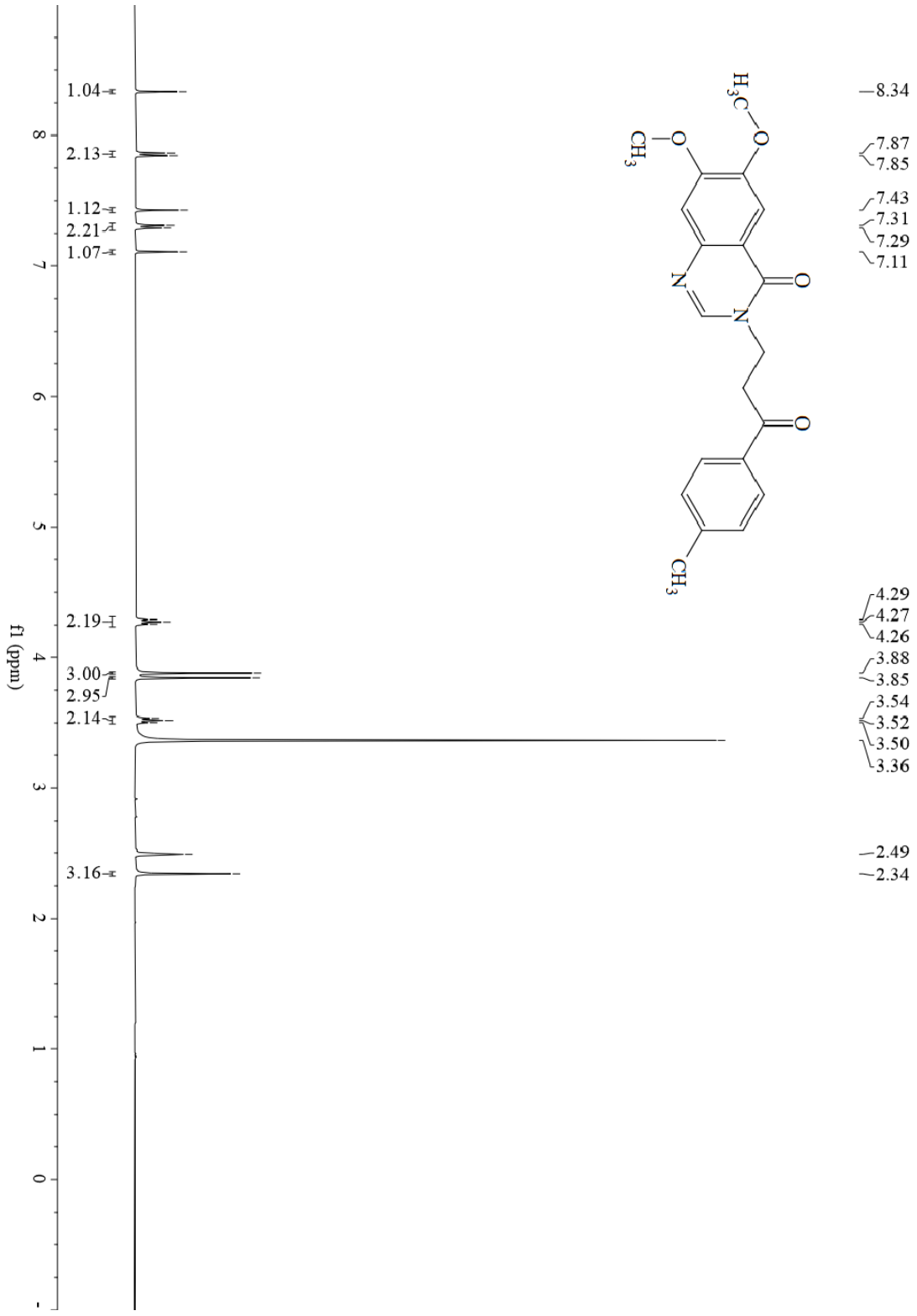
^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of 3v

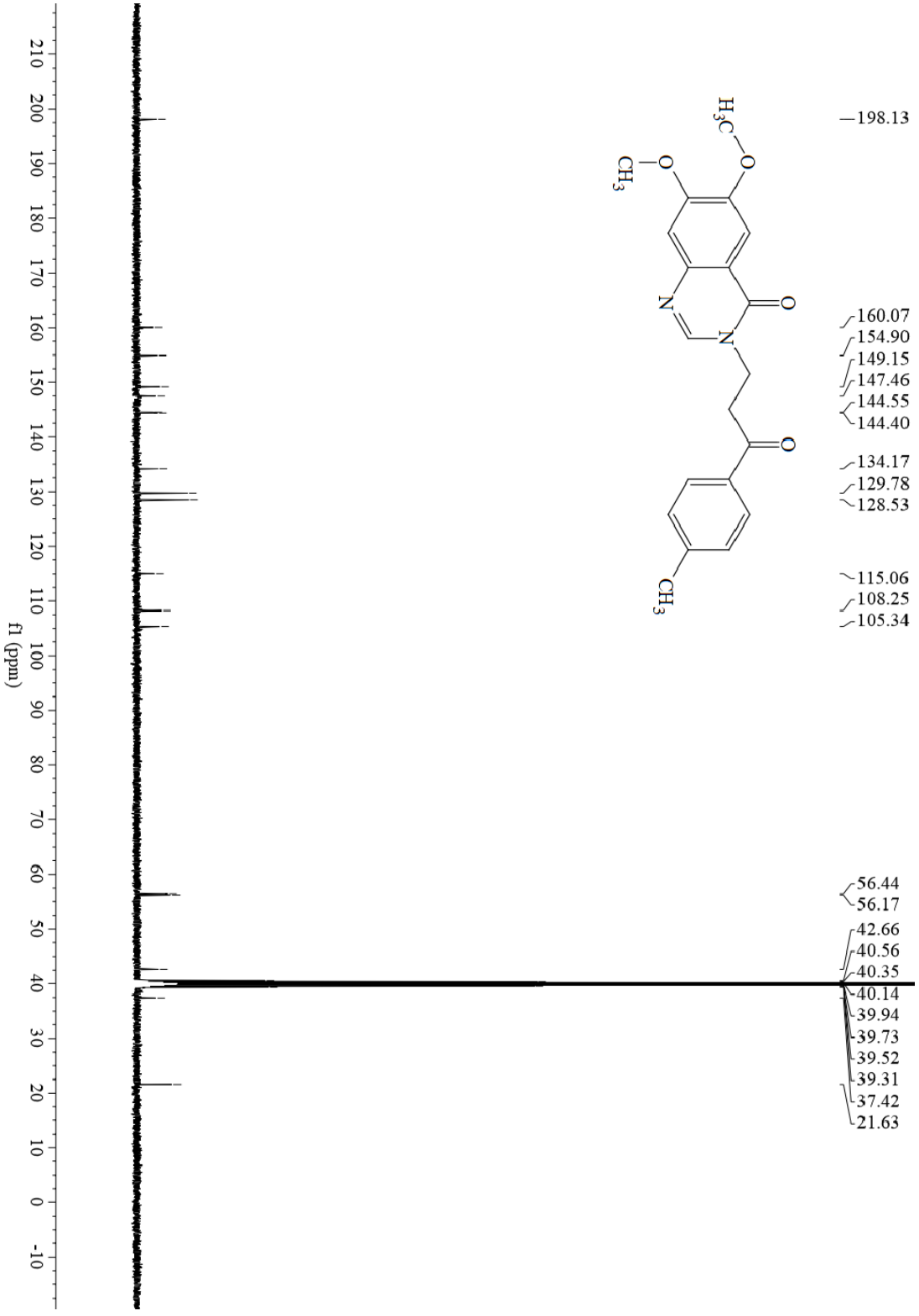



197.15
166.93
164.39
163.72
161.05
157.88
151.58
149.81
144.75
133.59
129.43
128.21
109.47
109.25
103.58
77.38
77.06
76.75
42.87
36.35
21.70
f1 (ppm)
F
F
O
N
N
O
CH3

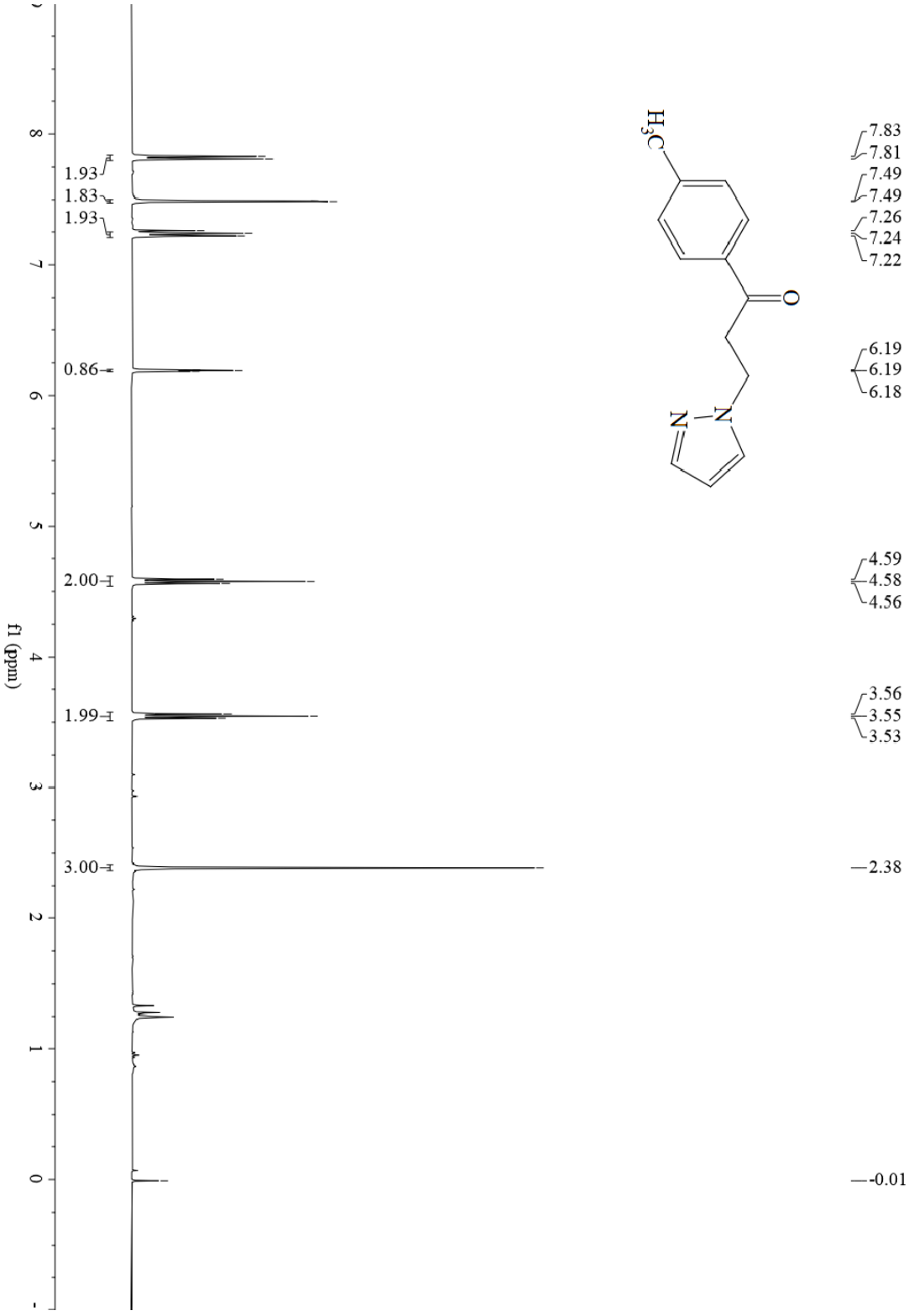

F
F
N
N
O
O
-99.81
-105.32
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
f1 (ppm)

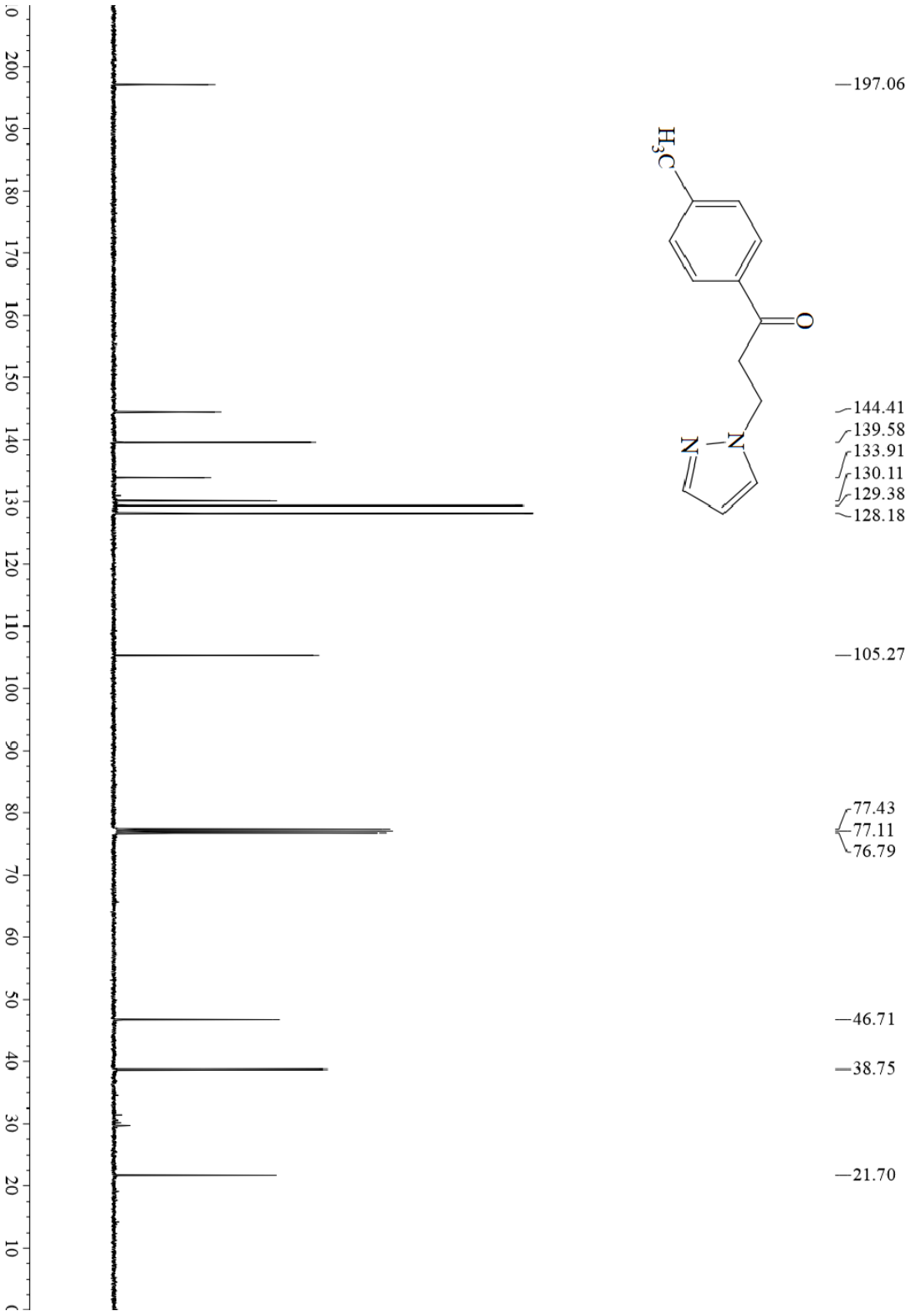
^{1}H and ^{13}C NMR spectra of 3w



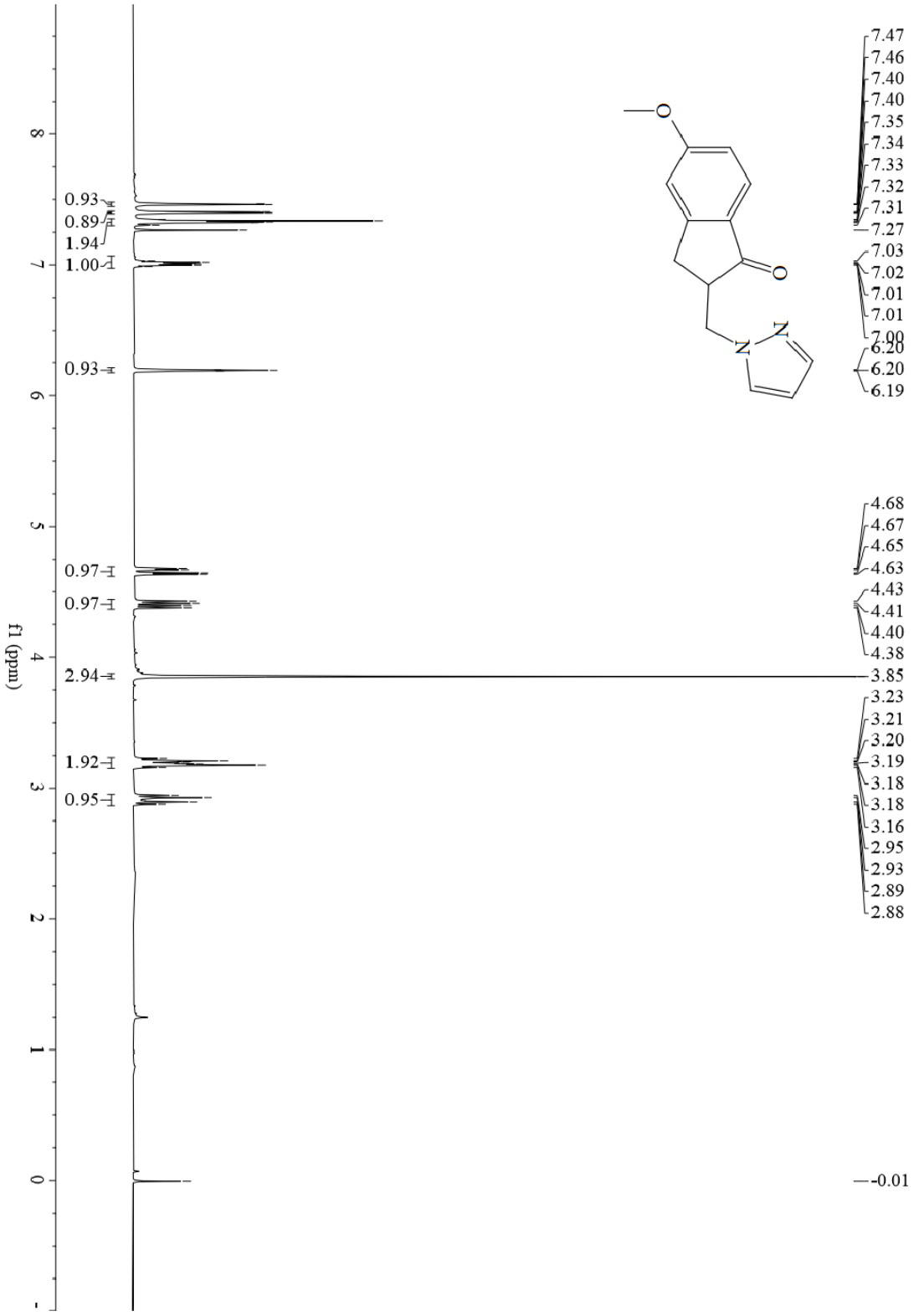

198.13
160.07
154.90
149.15
147.46
144.55
144.40
134.17
129.78
128.53
115.06
108.25
105.34
56.44
56.17
42.66
40.56
40.35
40.14
39.94
39.73
39.52
39.31
37.42
21.63
f1 (ppm)

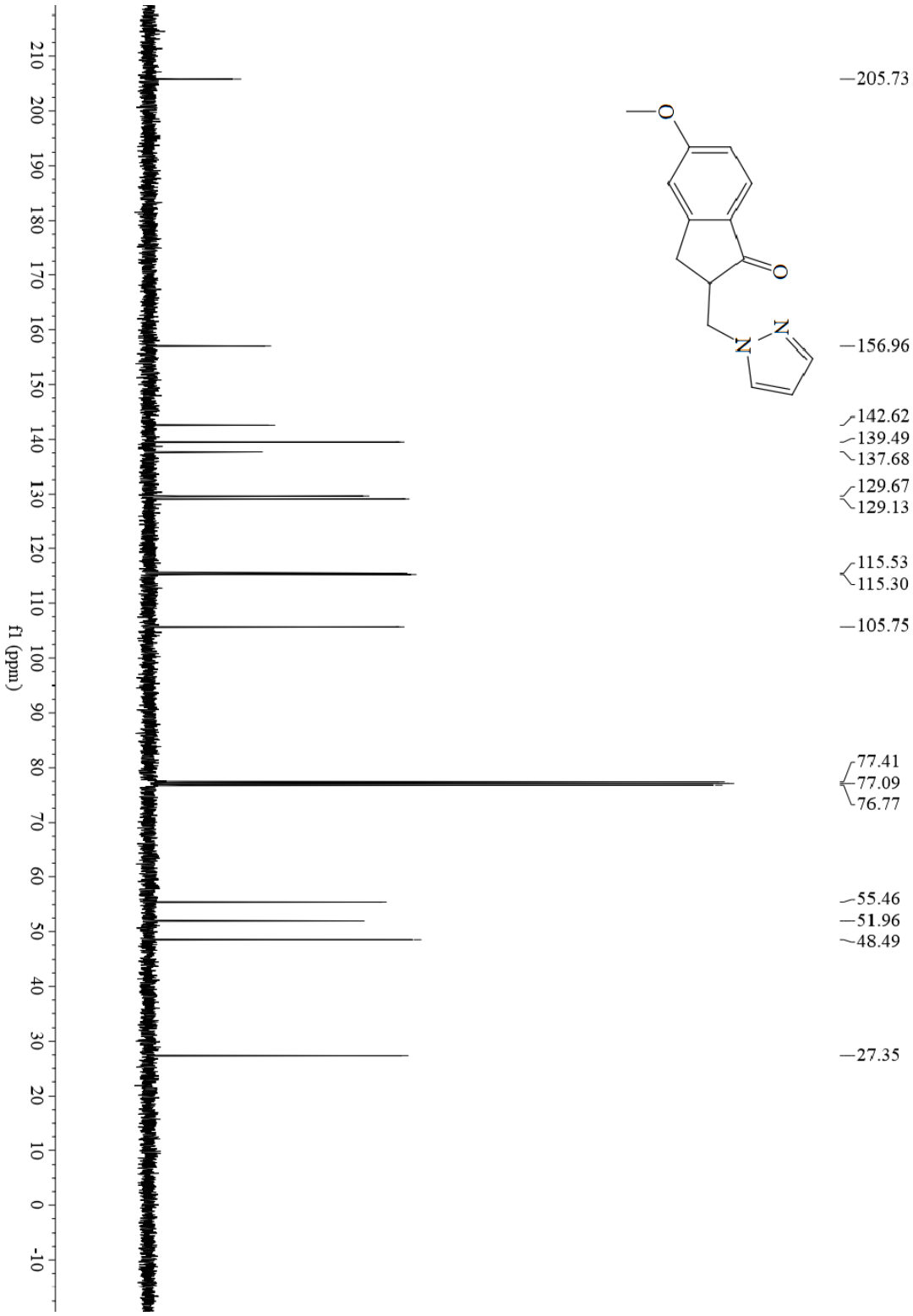
^{1}H and ^{13}C NMR spectra of 5a



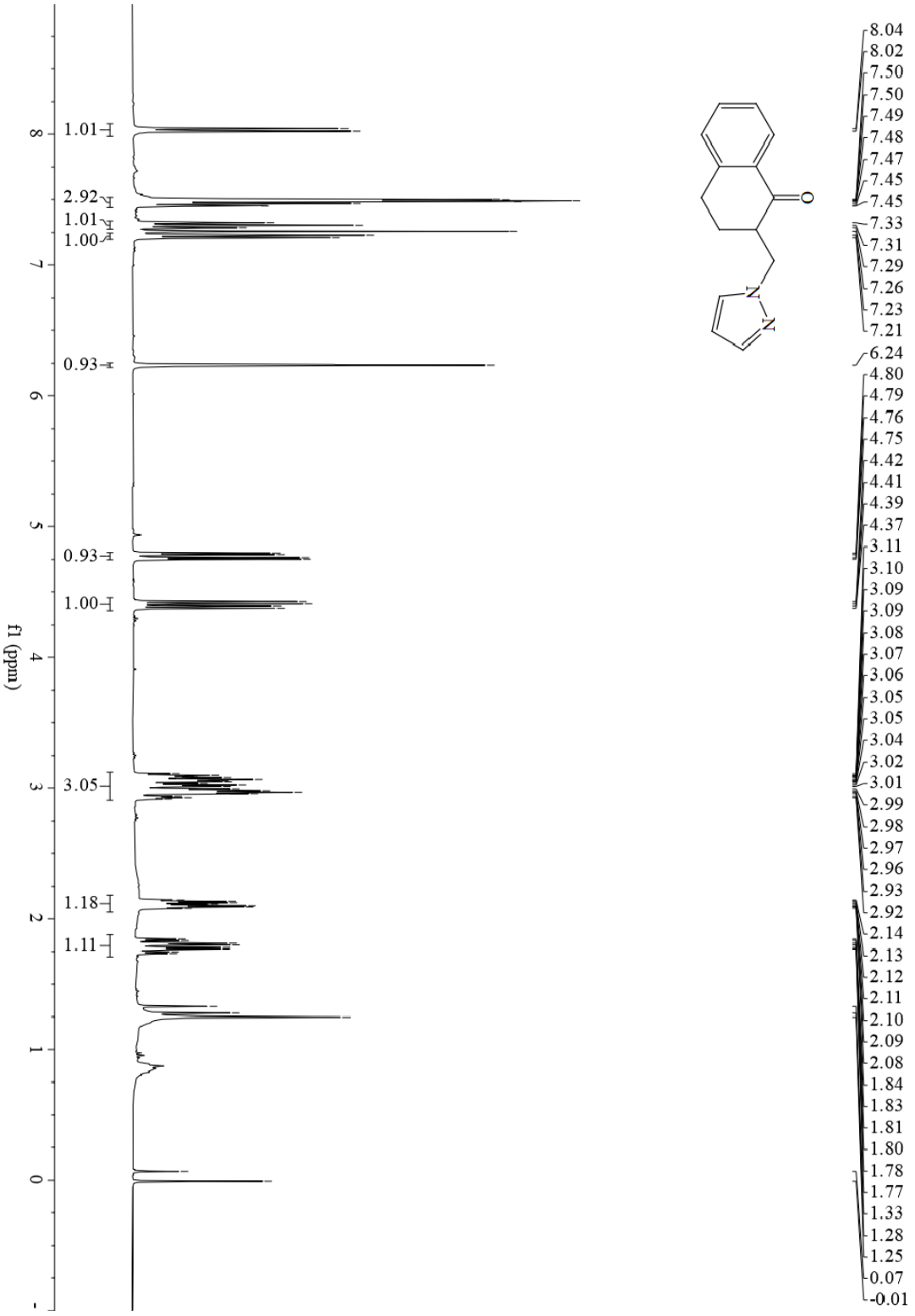

197.06
144.41
139.58
133.91
130.11
129.38
128.18
105.27
77.43
77.11
76.79
46.71
38.75
21.70
H3C
O
N
N

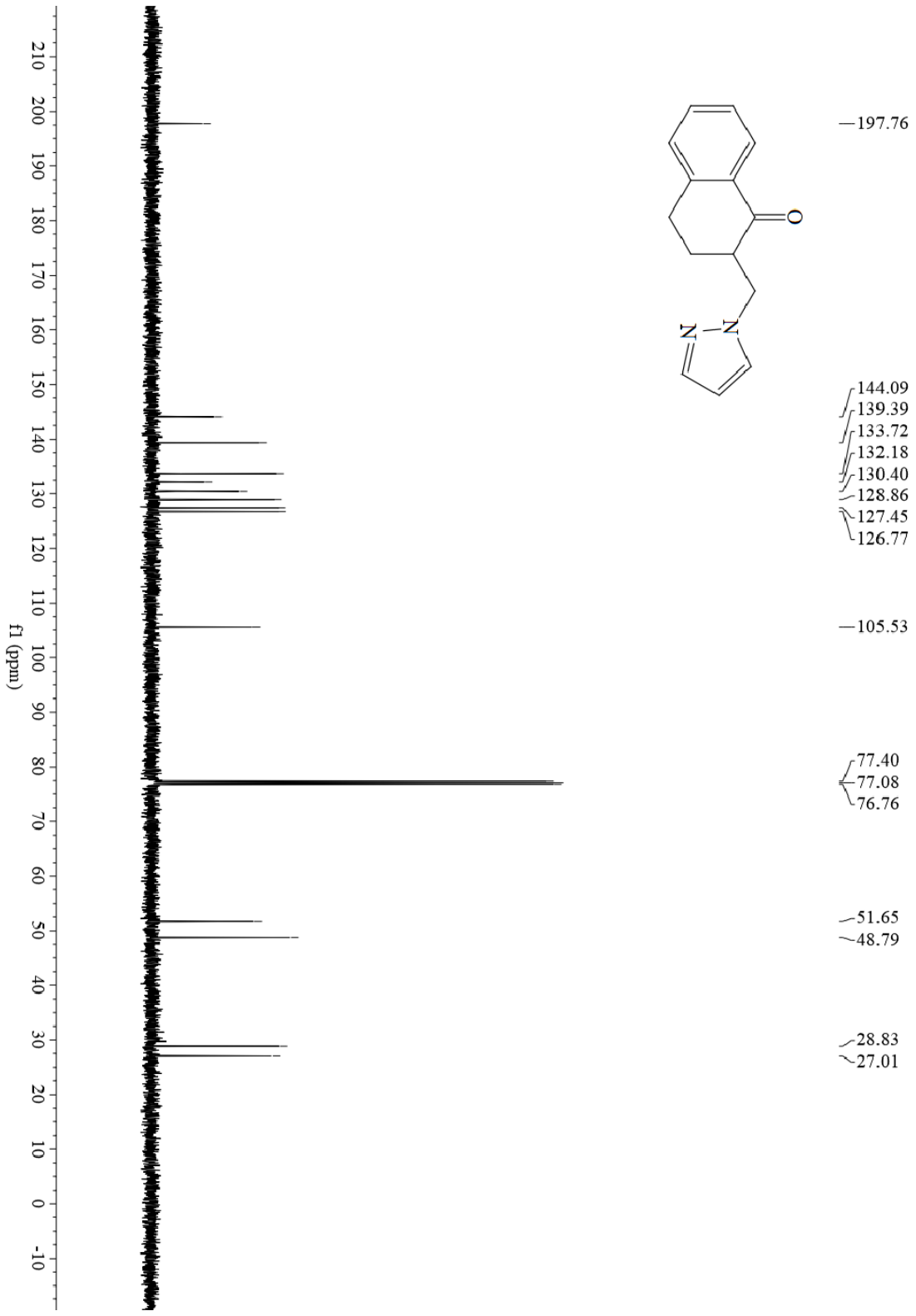
^{1}H and ^{13}C NMR spectra of 5b



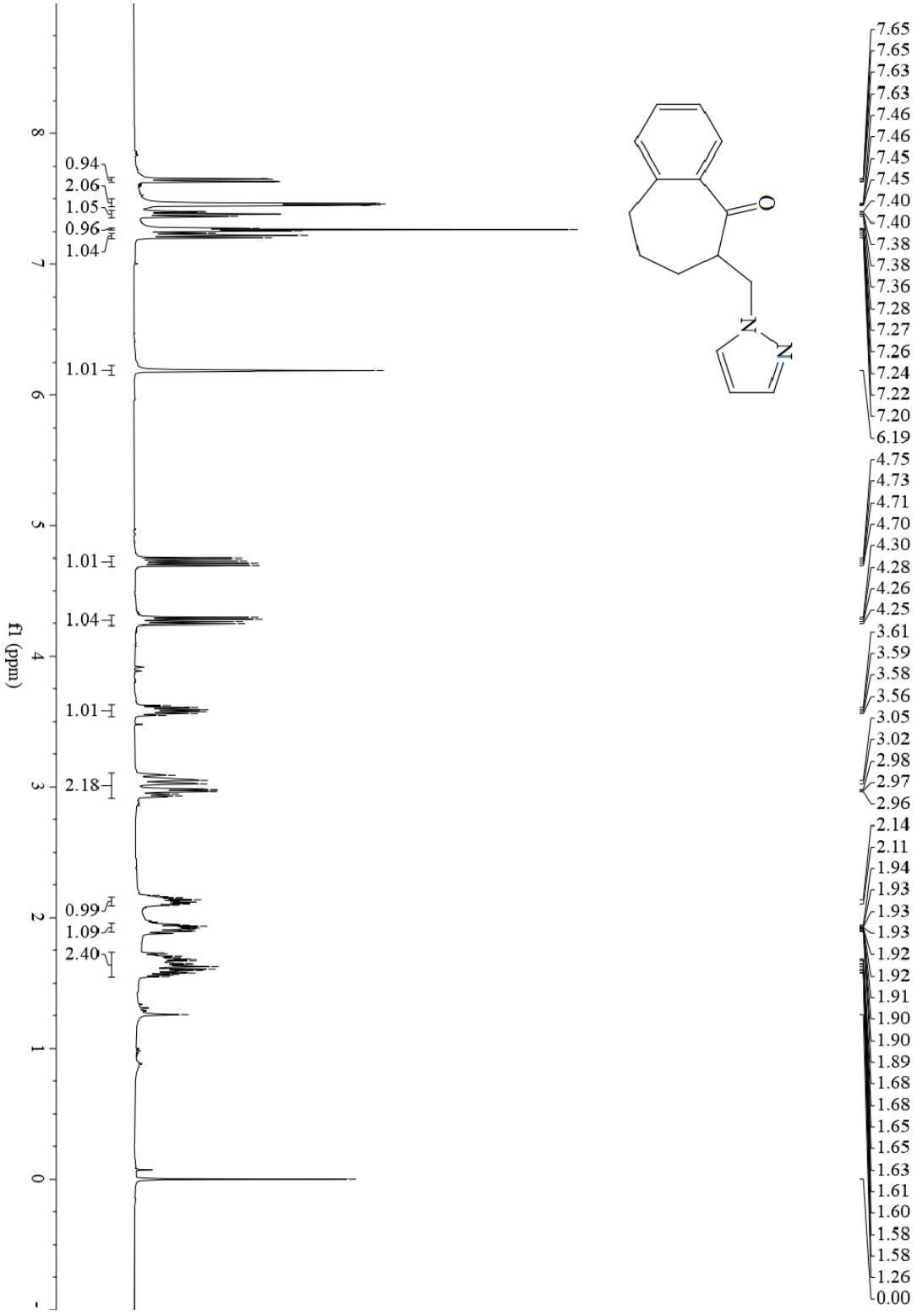

f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
O
O
N
N
205.73
156.96
142.62
139.49
137.68
129.67
129.13
115.53
115.30
105.75
77.41
77.09
76.77
55.46
51.96
48.49
27.35

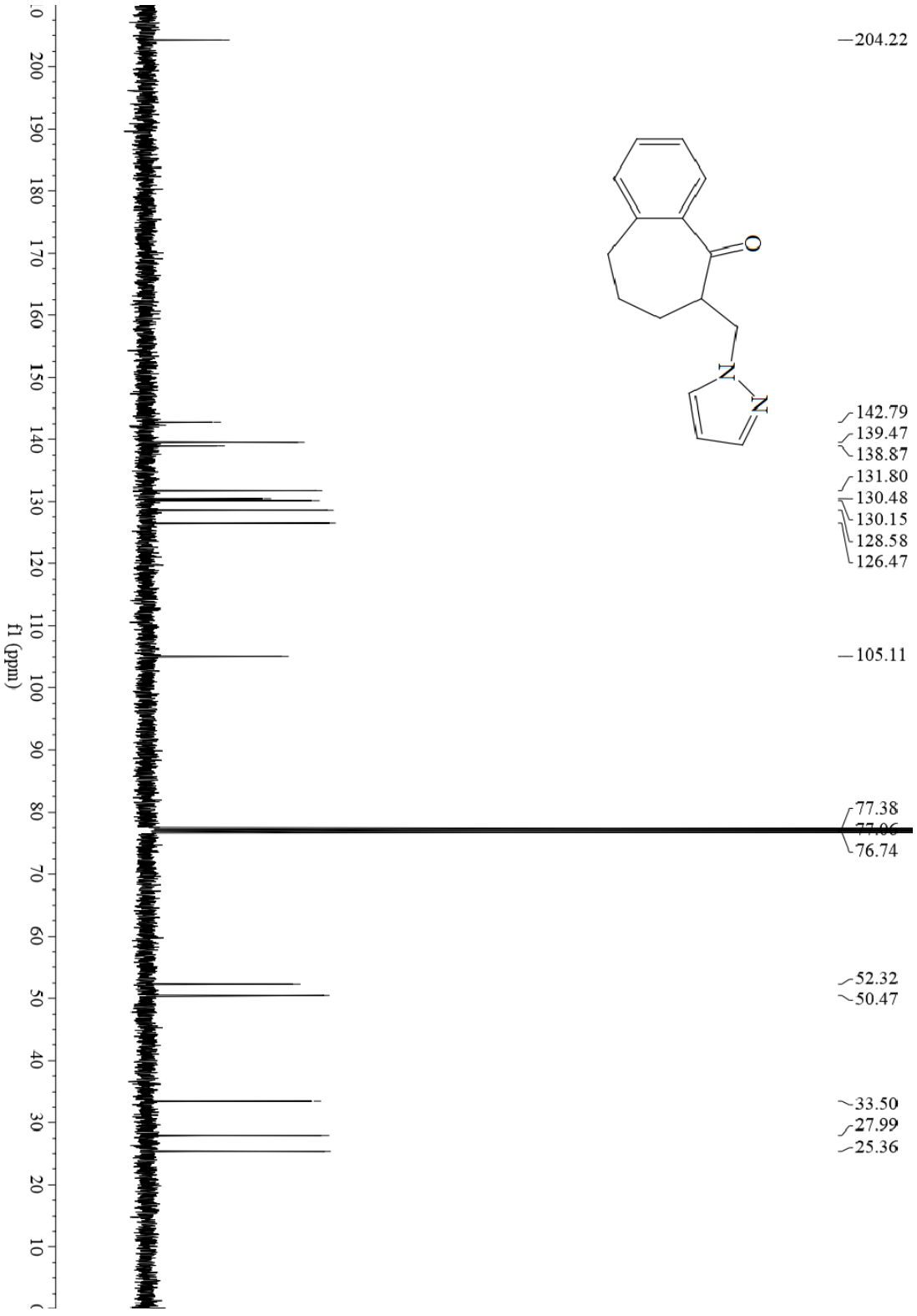
^{1}H and ^{13}C NMR spectra of 5c



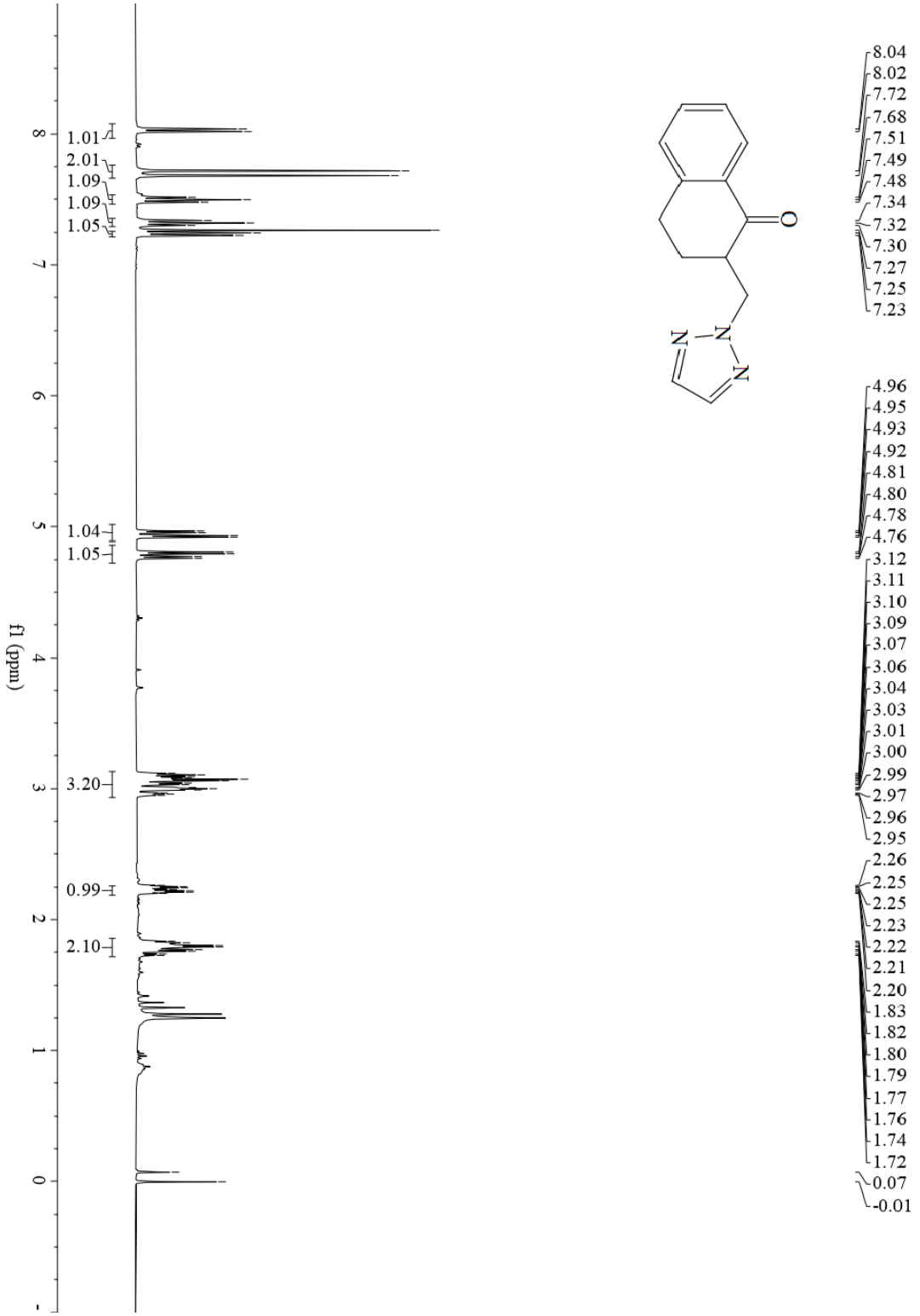

197.76
144.09
139.39
133.72
132.18
130.40
128.86
127.45
126.77
105.53
77.40
77.08
76.76
51.65
48.79
28.83
27.01
O
N
N
f1 (ppm)

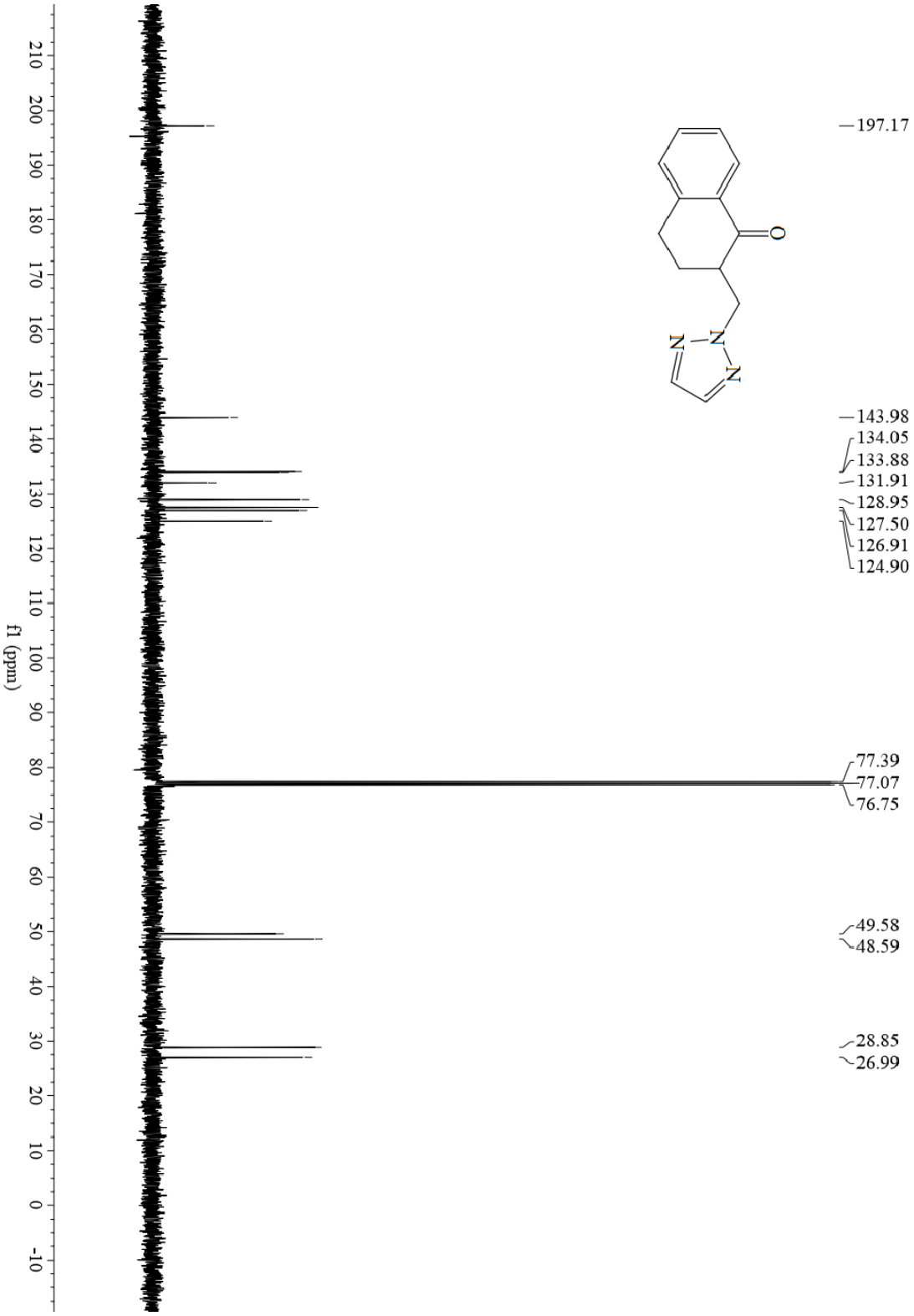
^{1}H and ^{13}C NMR spectra of 5d



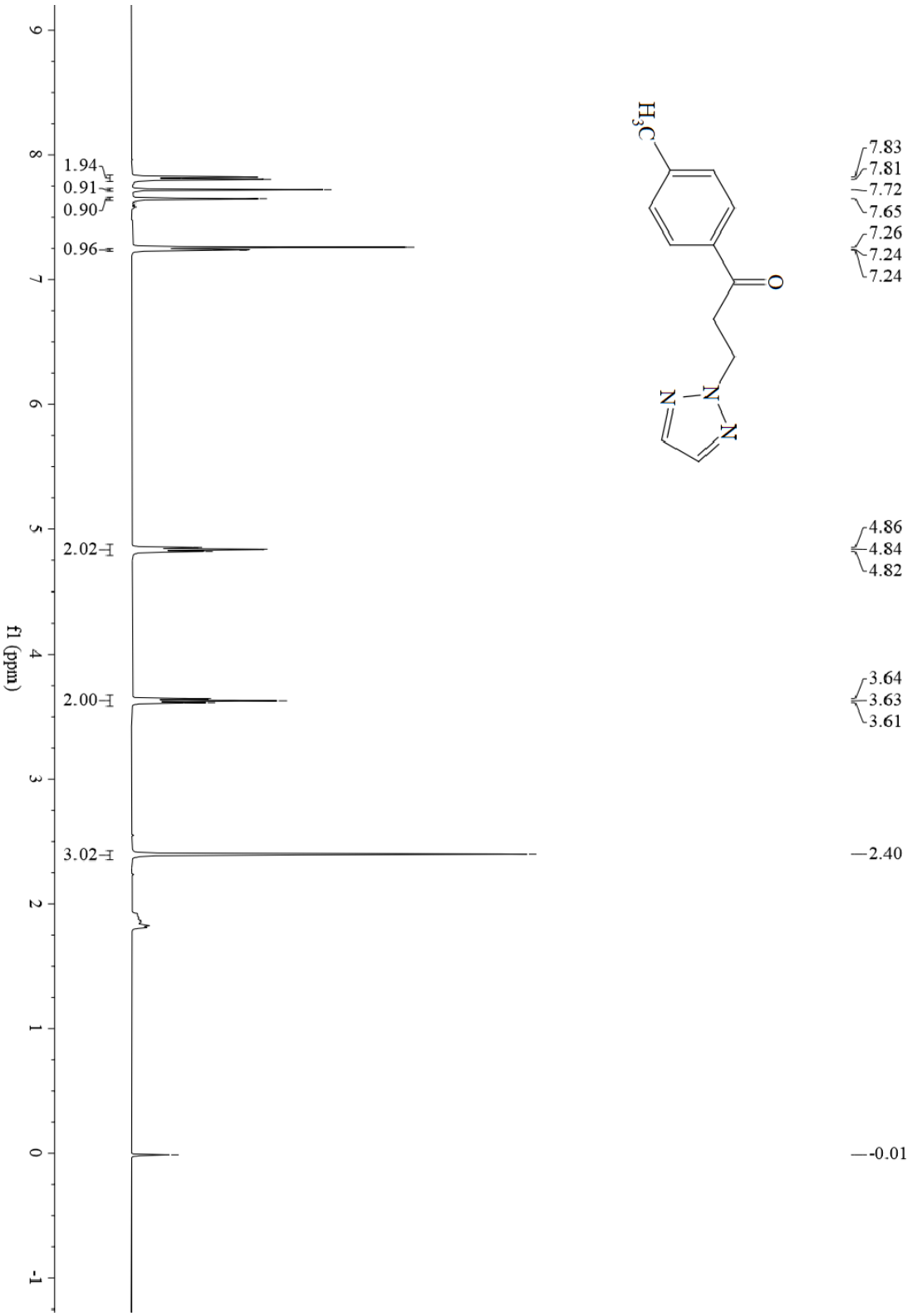

204.22
142.79
139.47
138.87
131.80
130.48
130.15
128.58
126.47
105.11
77.38
77.06
76.74
52.32
50.47
33.50
27.99
25.36
O
N
N
f1 (ppm)

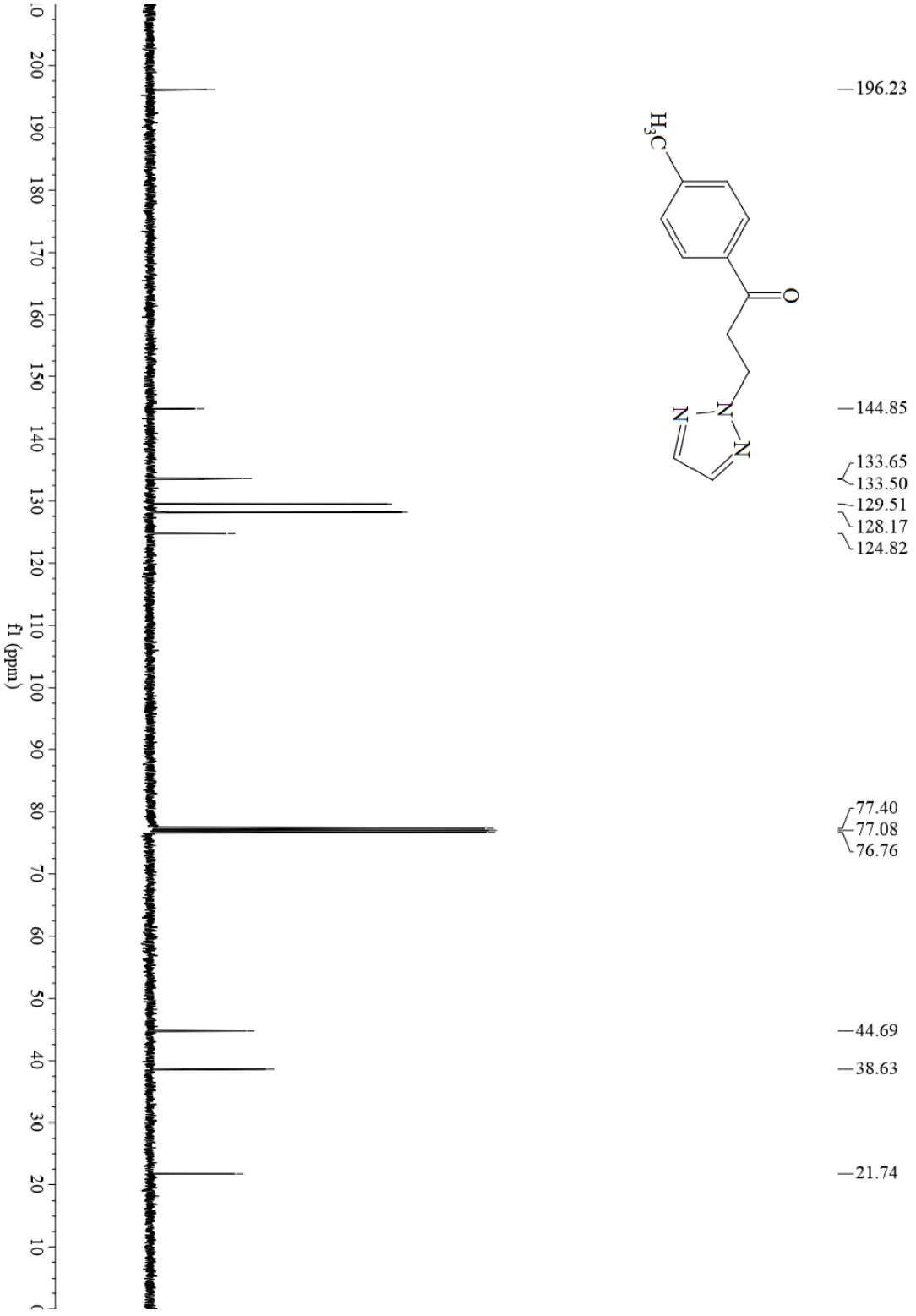
^{1}H and ^{13}C NMR spectra of 5e



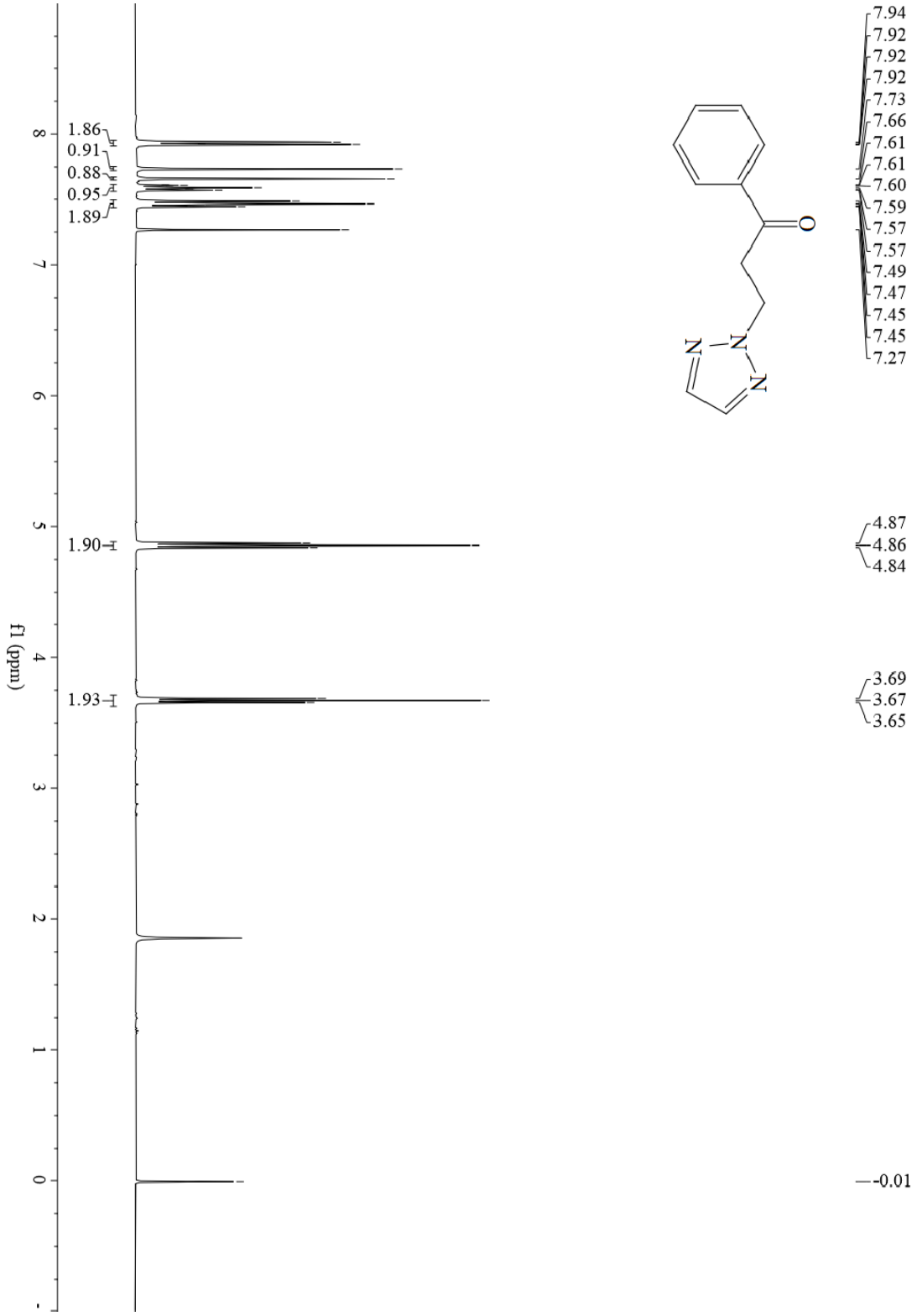

197.17
143.98
134.05
133.88
131.91
128.95
127.50
126.91
124.90
77.39
77.07
76.75
49.58
48.59
28.85
26.99
f1 (ppm)

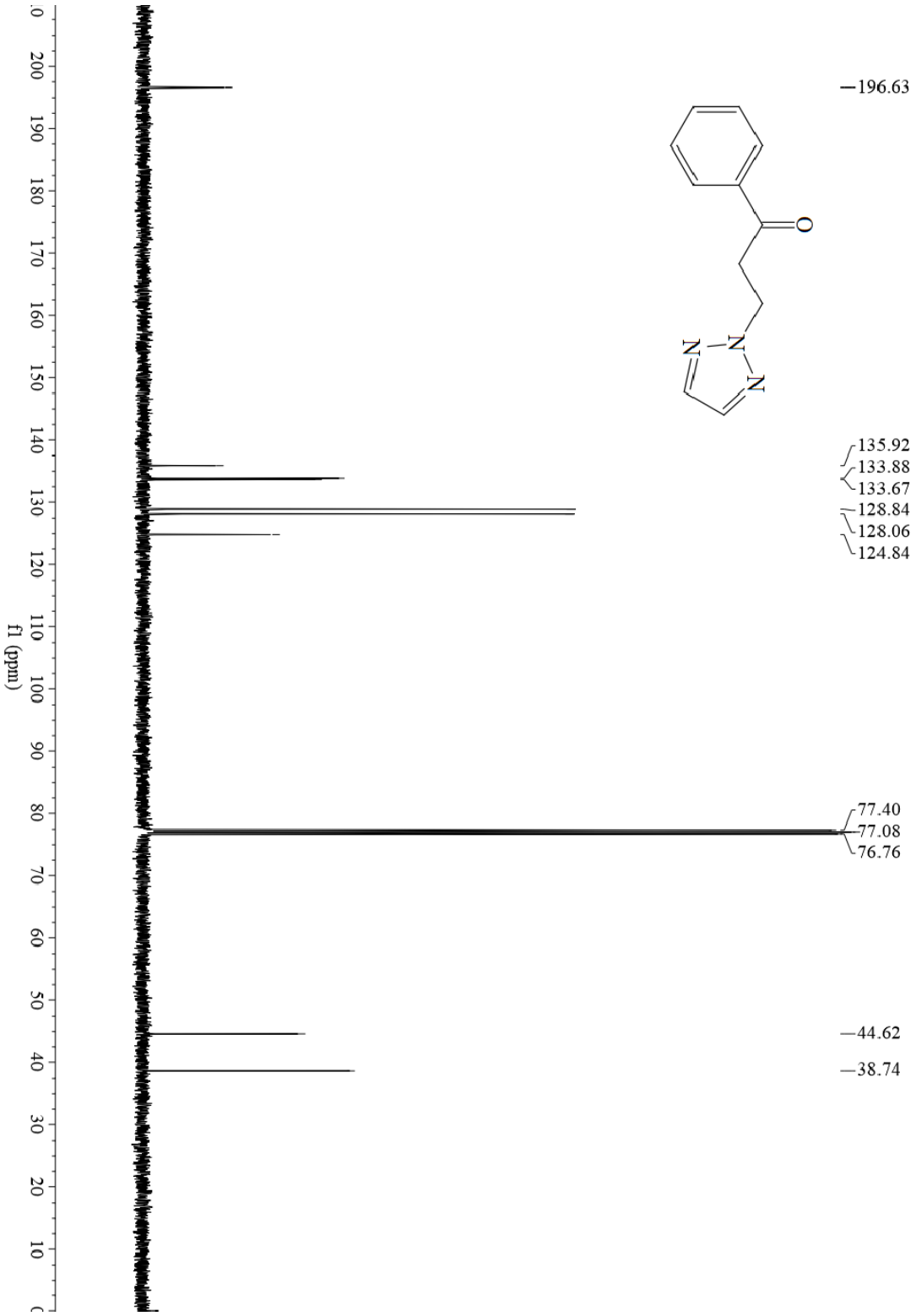
^{1}H and ^{13}C NMR spectra of 5f



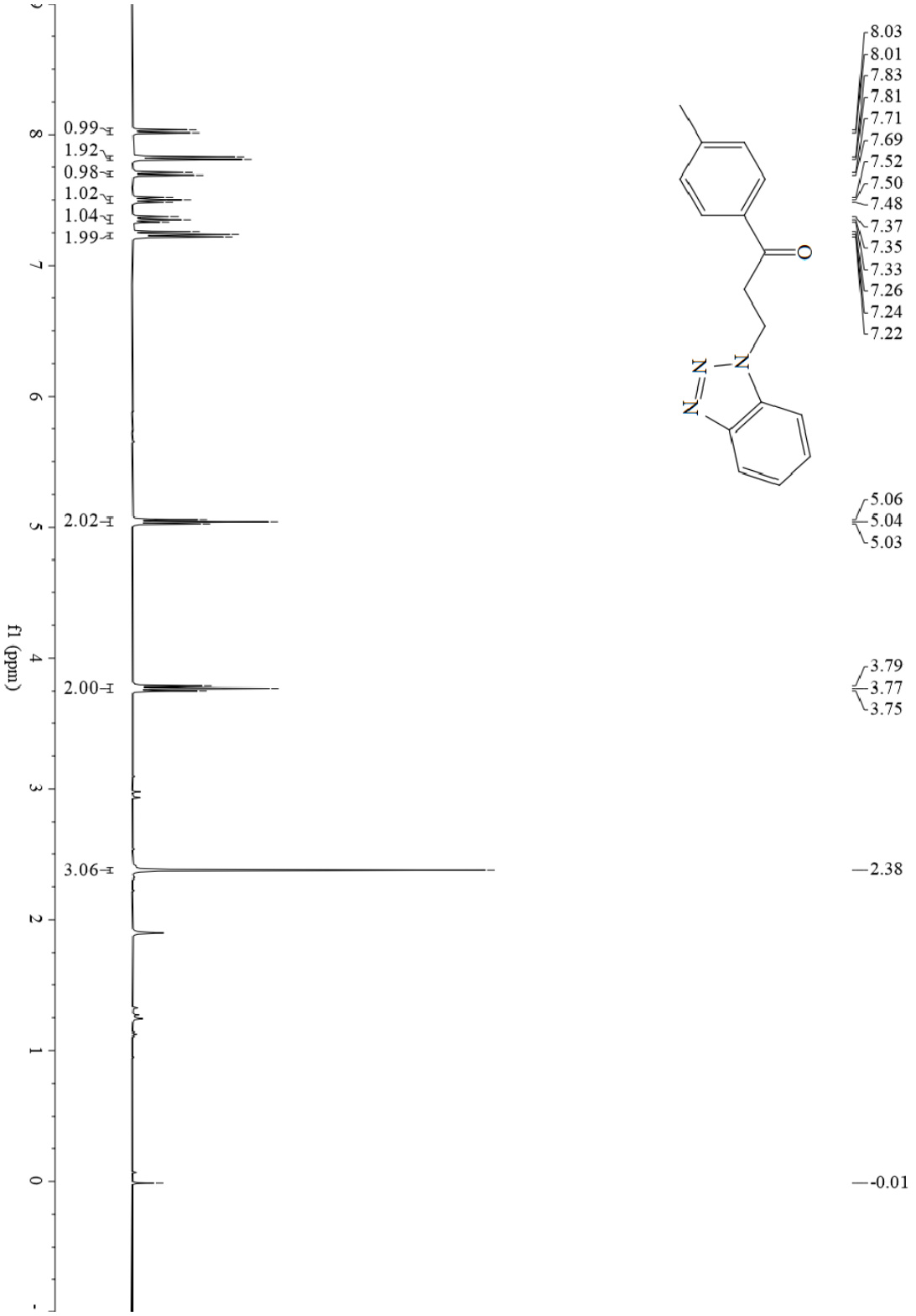

196.23
144.85
133.65
133.50
129.51
128.17
124.82
77.40
77.08
76.76
44.69
38.63
21.74
f1 (ppm)

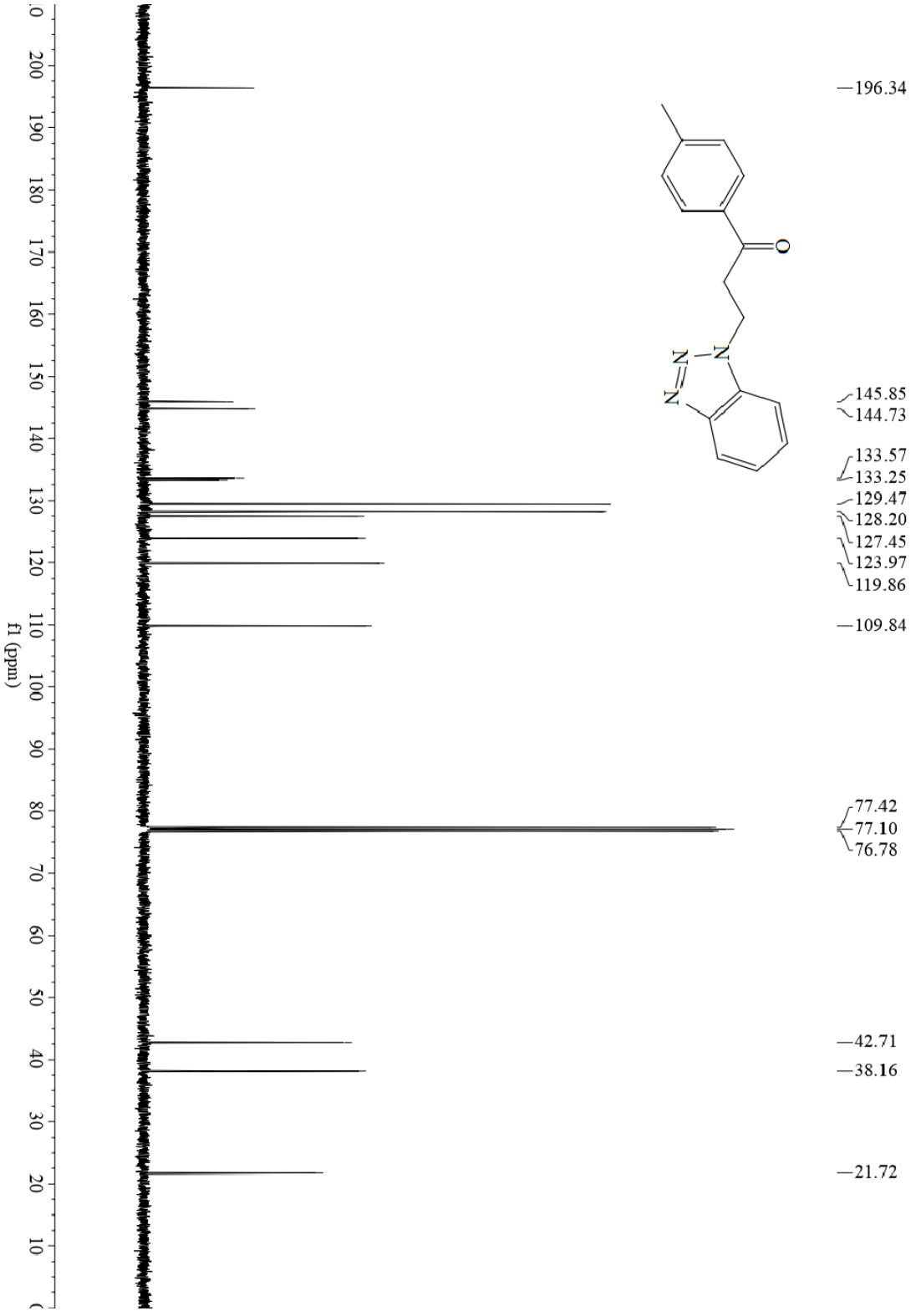
^{1}H and ^{13}C NMR spectra of 5g



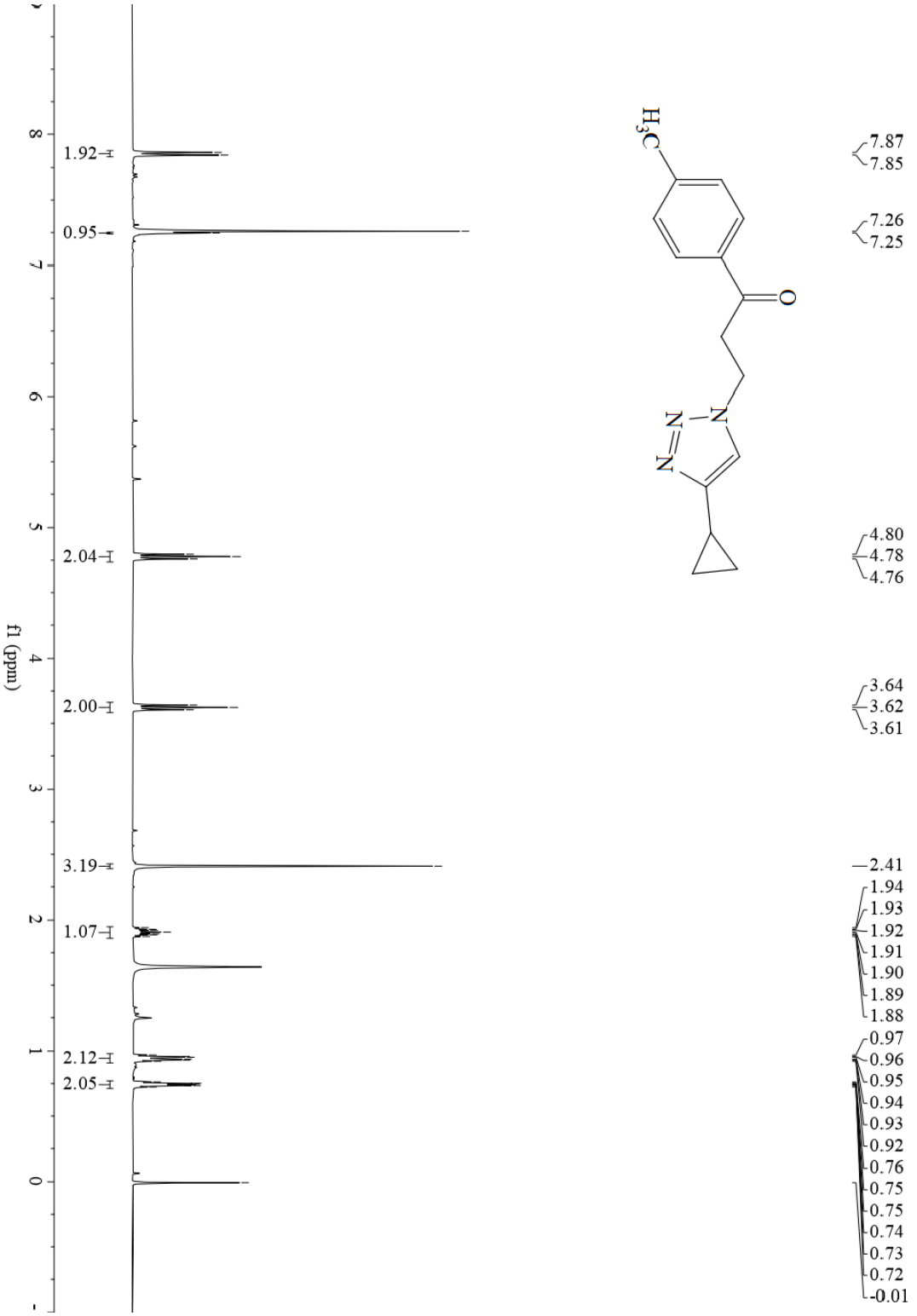

196.63
135.92
133.88
133.67
128.84
128.06
124.84
77.40
77.08
76.76
44.62
38.74
f1 (ppm)

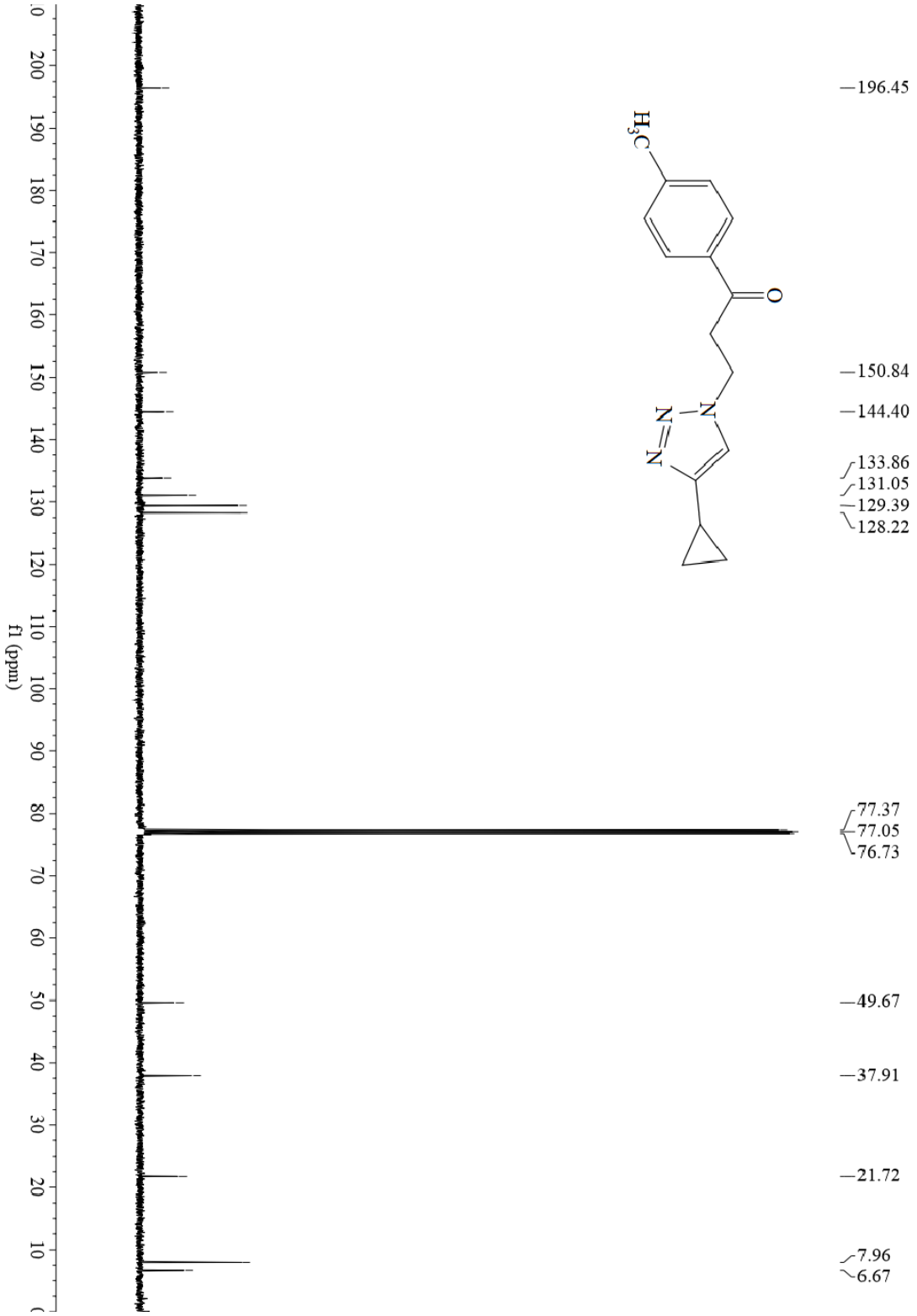
^{1}H and ^{13}C NMR spectra of 5h



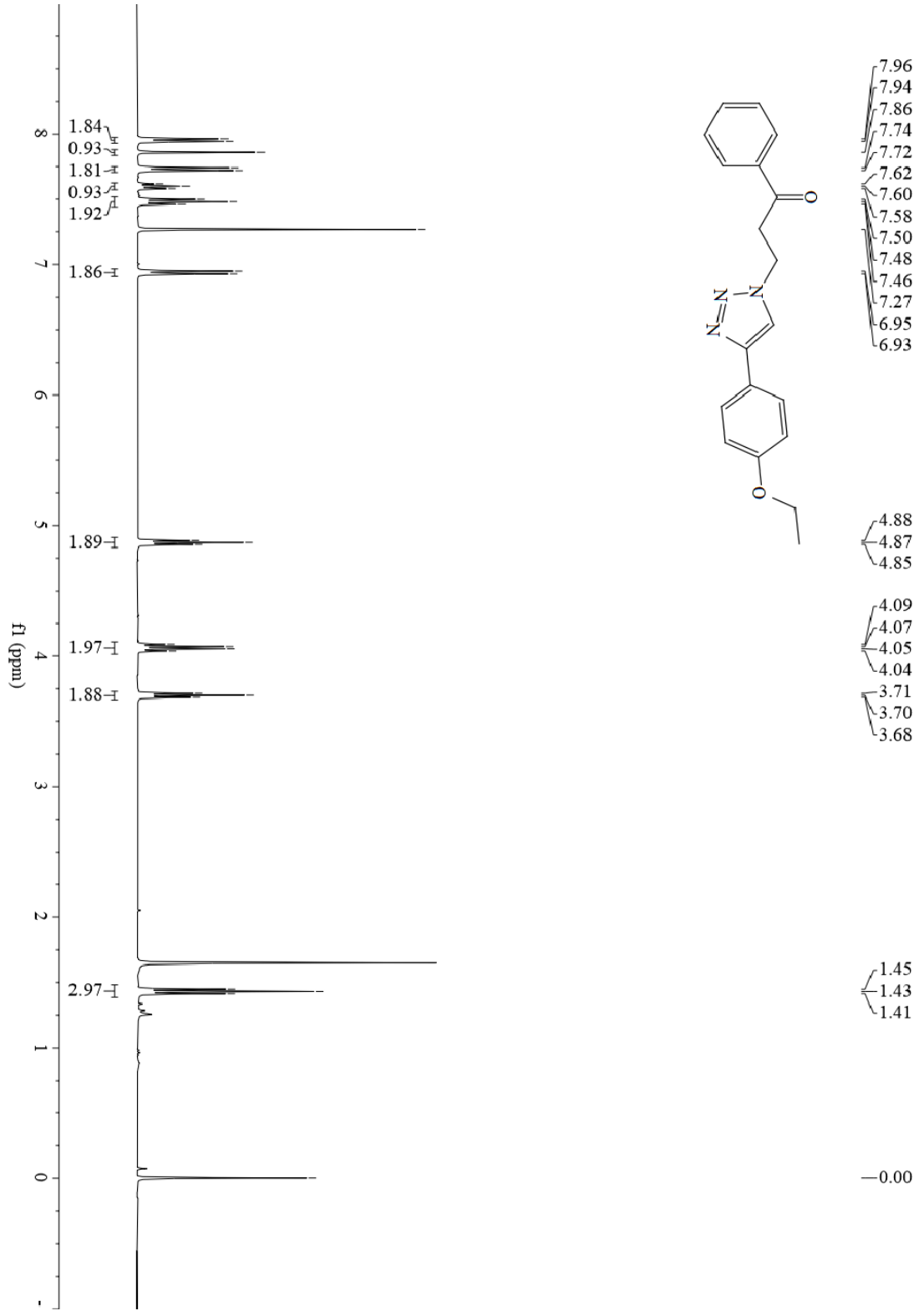

196.34
145.85
144.73
133.57
133.25
129.47
128.20
127.45
123.97
119.86
109.84
77.42
77.10
76.78
42.71
38.16
21.72
f1 (ppm)

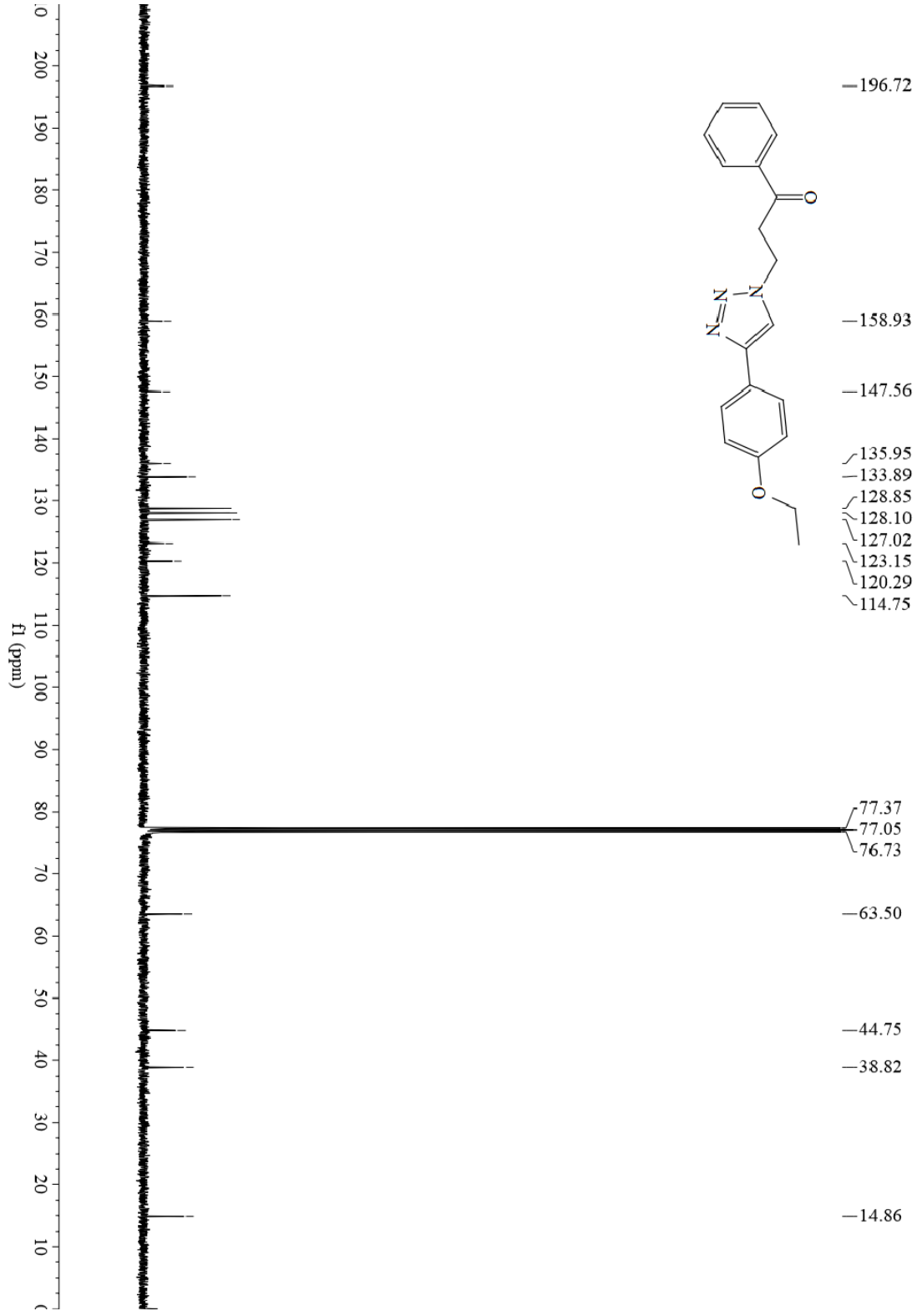
^{1}H and ^{13}C NMR spectra of 5i

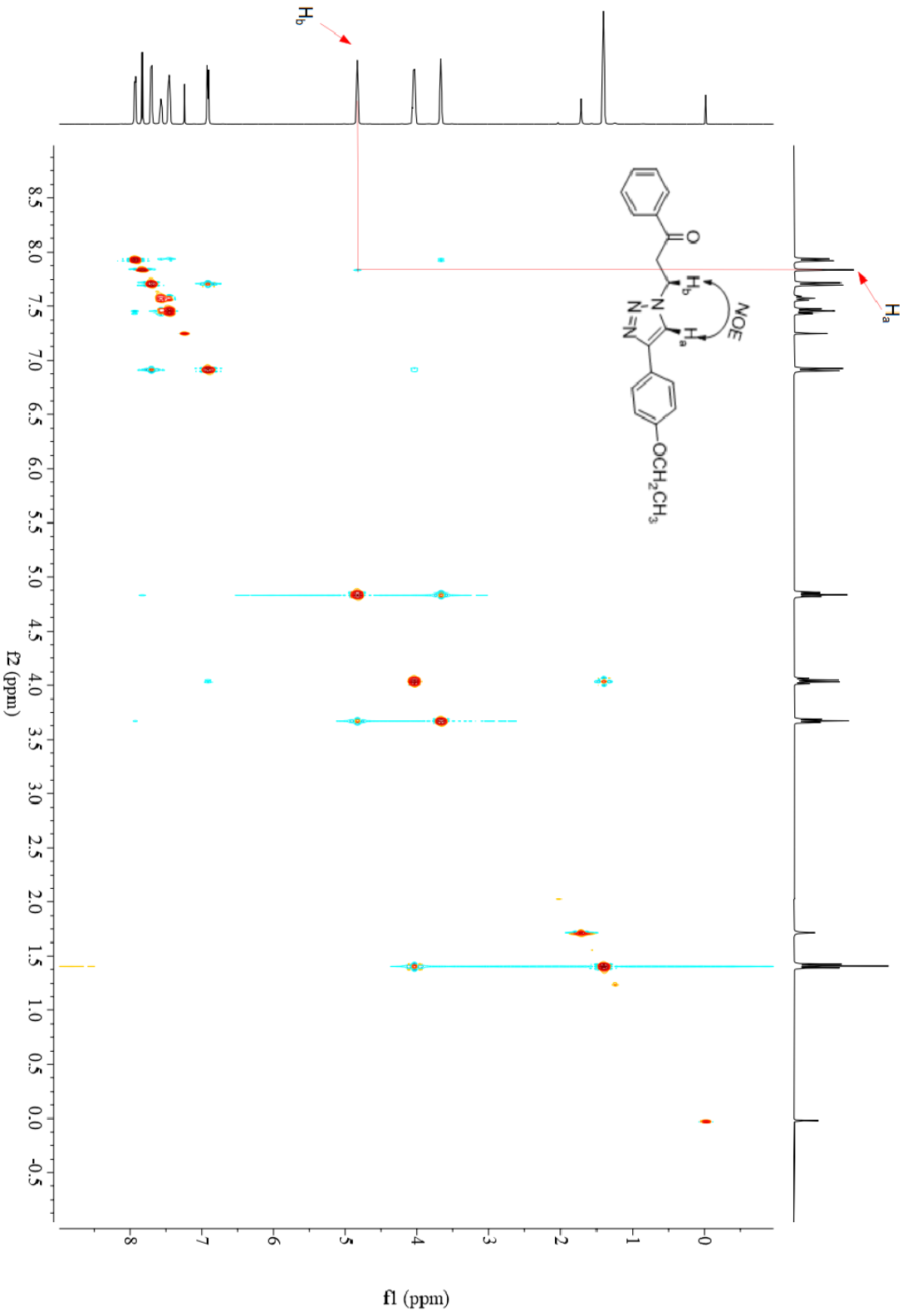



196.45
150.84
144.40
133.86
131.05
129.39
128.22
77.37
77.05
76.73
49.67
37.91
21.72
7.96
6.67
f1 (ppm)

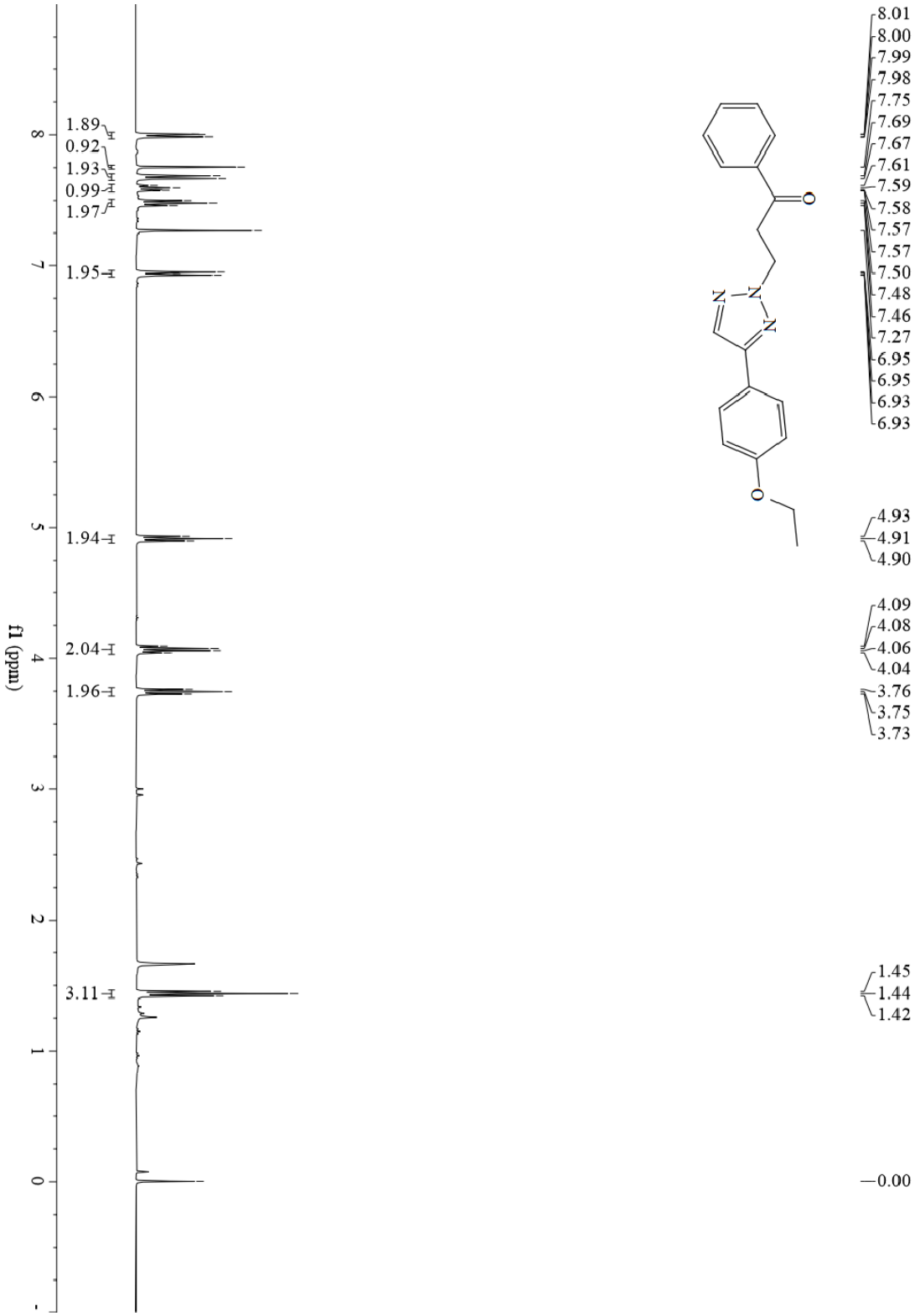
^{1}H NMR, ^{13}C NMR and ^{1}H-^{1}H NOESY spectra of 5j

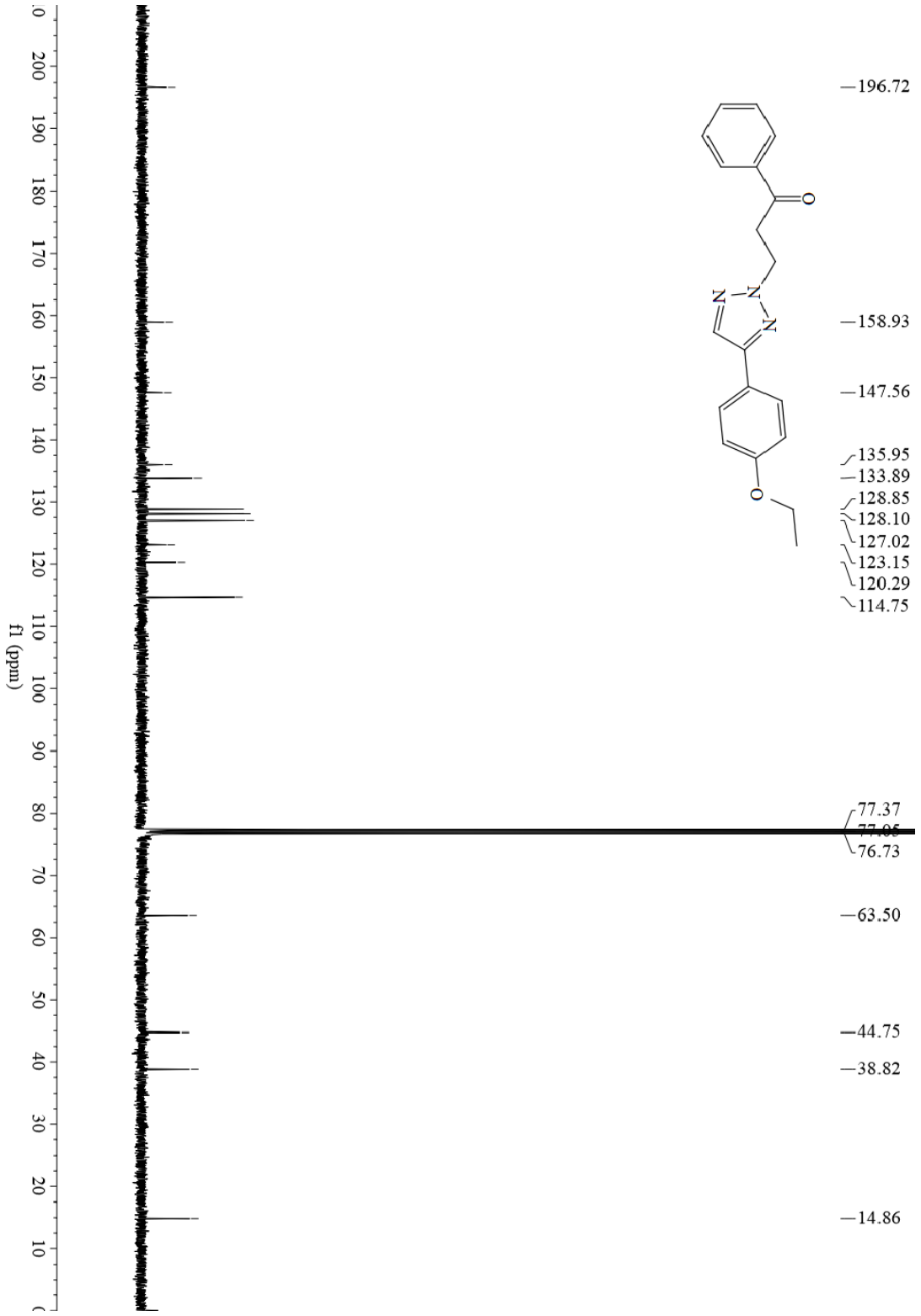


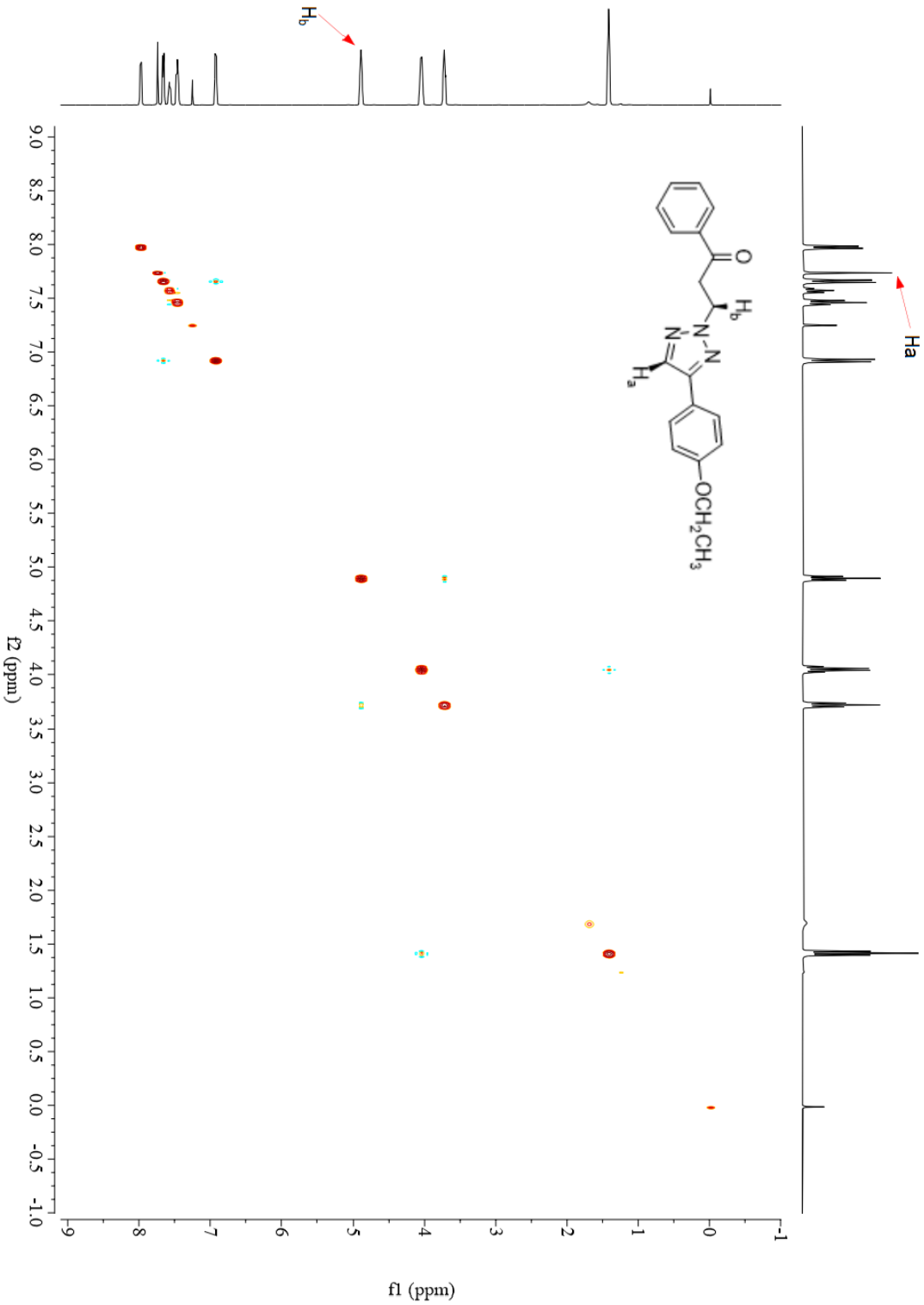

196.72
158.93
147.56
135.95
133.89
128.85
128.10
127.02
123.15
120.29
114.75
77.37
77.05
76.73
63.50
44.75
38.82
14.86
f1 (ppm)


Hb
Ha
NOE
OCH2CH3
f2 (ppm)
f1 (ppm)

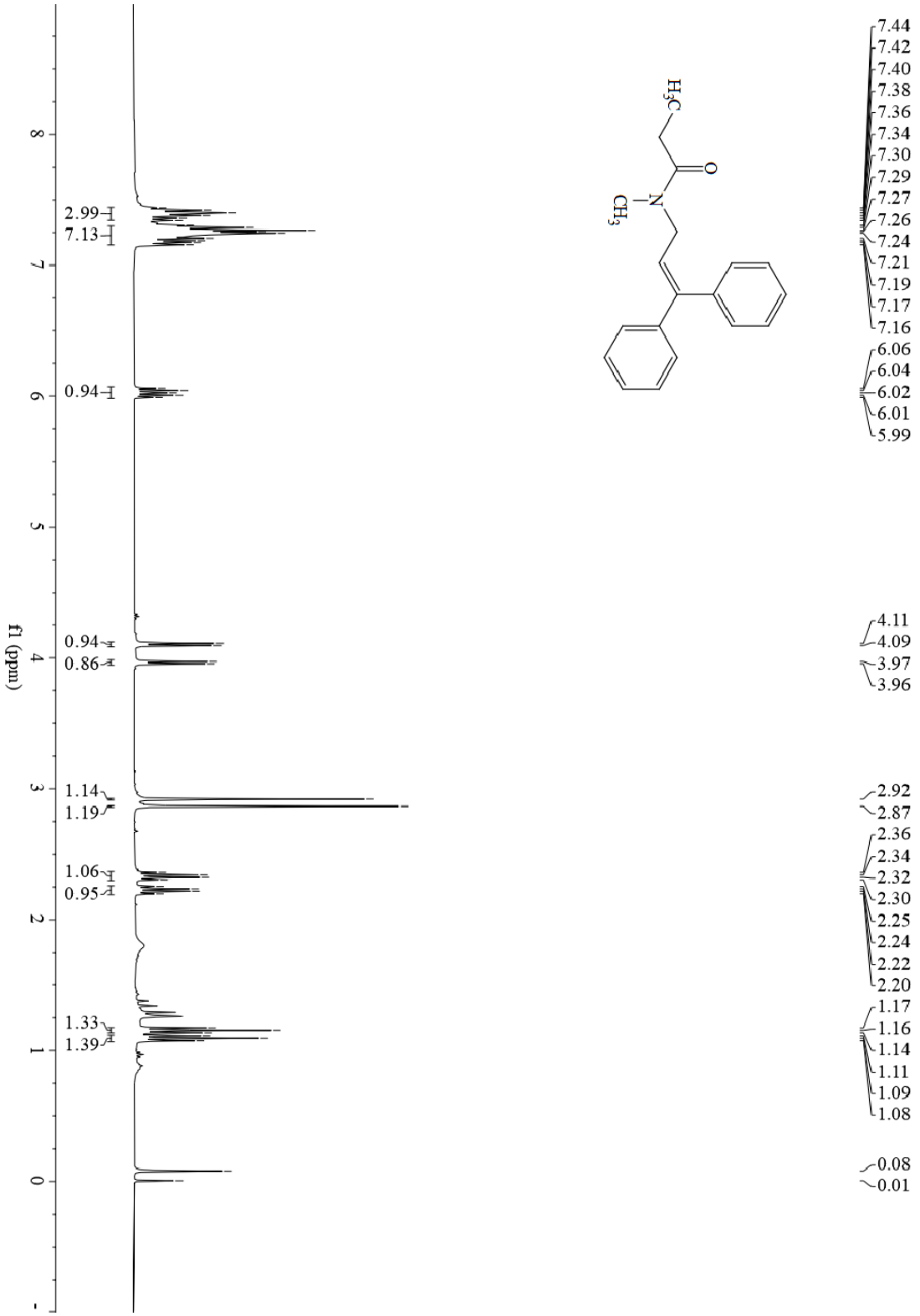
^{1}H NMR, ^{13}C NMR and ^{1}H-^{1}H NOESY spectra of 5k

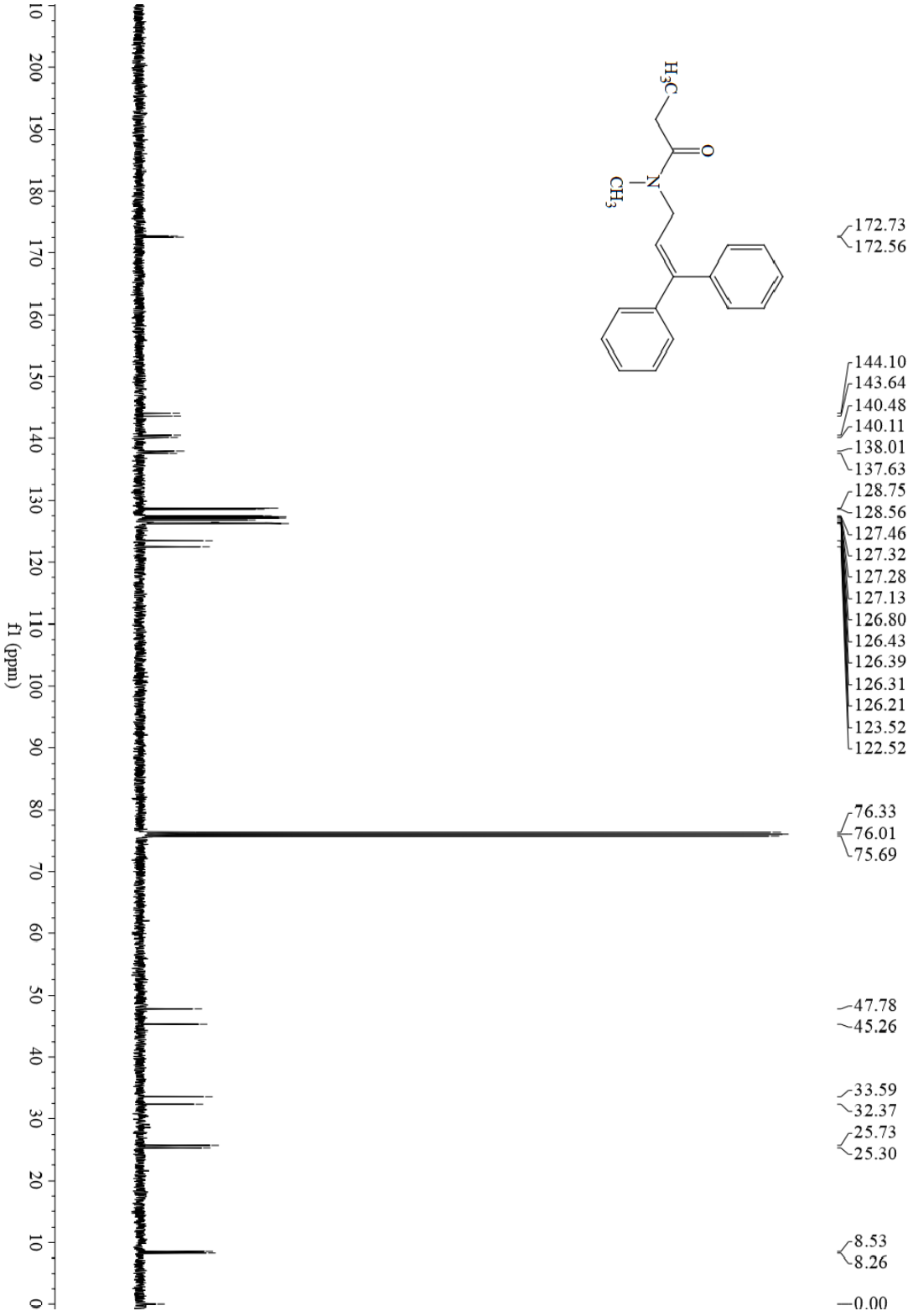



196.72
158.93
147.56
135.95
133.89
128.85
128.10
127.02
123.15
120.29
114.75
77.37
77.05
76.73
63.50
44.75
38.82
14.86
f1 (ppm)

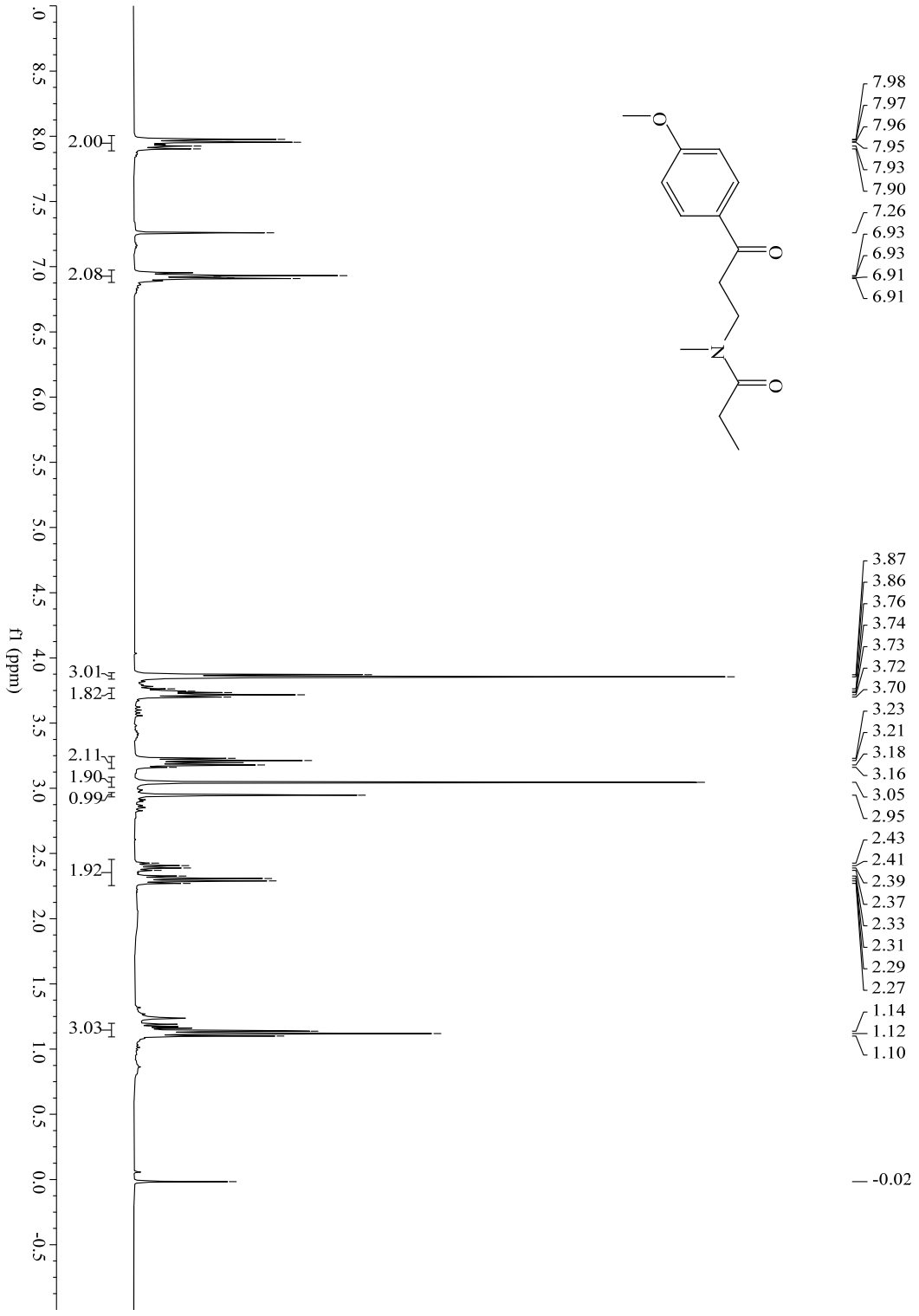

Hb
Ha
Hb
Ha
OCH2CH3
f2 (ppm)
f1 (ppm)

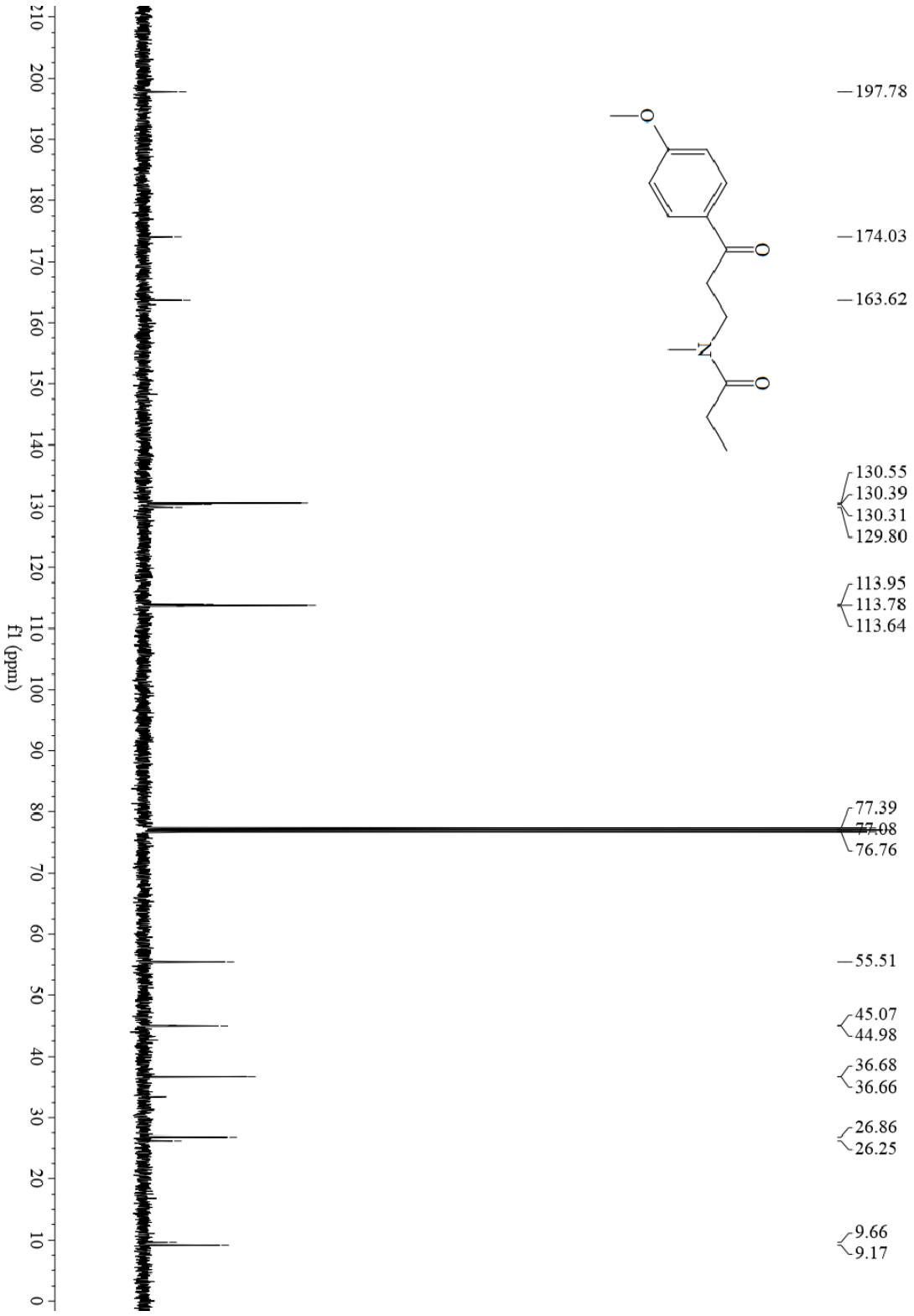
^{1}H and ^{13}C NMR spectra of 7




f1 (ppm)
172.73
172.56
144.10
143.64
140.48
140.11
138.01
137.63
128.75
128.56
127.46
127.32
127.28
127.13
126.80
126.43
126.39
126.31
126.21
123.52
122.52
76.33
76.01
75.69
47.78
45.26
33.59
32.37
25.73
25.30
8.53
8.26
0.00

^{1}H and ^{13}C NMR spectra of 9




197.78
174.03
163.62
130.55
130.39
130.31
129.80
113.95
113.78
113.64
77.39
77.08
76.76
55.51
45.07
44.98
36.68
36.66
26.86
26.25
9.66
9.17
f1 (ppm)