Supporting Information

Electrochemical Intramolecular C-H/N-H Functionalization for the Synthesis of Isoxazolidine-Fused Isoquinolin-1(2*H*)-ones

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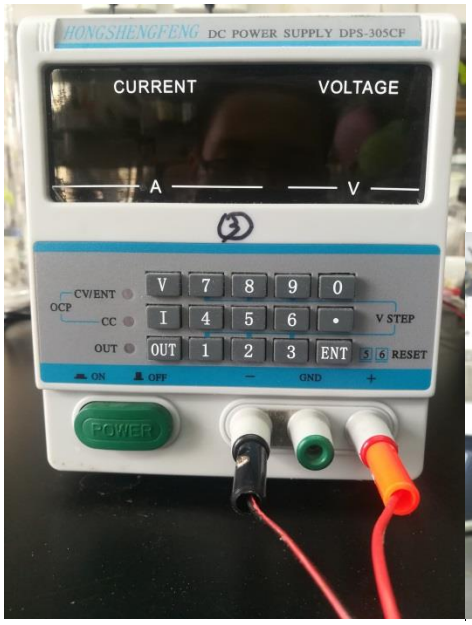
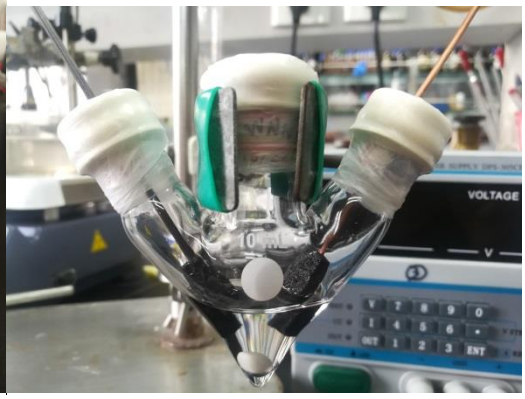
General methods

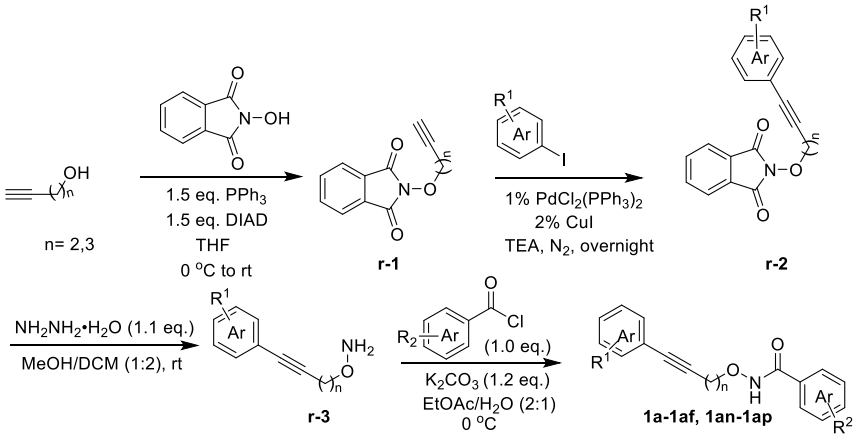
Unless noted, all commercial reagents and solvents were used without further purification. Melting points were recorded on a RY-1 microscopic melting apparatus and uncorrected. NMR spectra were recorded in $CDCl_3$ on 400 MHz or 500 MHz spectrometers. ^1H NMR chemical shifts (δ) are reported in parts per million relative to tetramethylsilane (0 ppm) or residual $CHCl_3$ (7.26 ppm). ^{13}C NMR chemical shifts are reported relative to the center line signal of the $CDCl_3$ triplet at 77.0 ppm. The following abbreviations are used for multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, and m = multiplet. Mass spectra were obtained on an Ultima Global spectrometer with an ESI source. Silica gel (200–300 mesh) for column chromatography and silica GF254 for TLC were produced by Qingdao Marine Chemical Company (China). DC power supply DPS-305CF was used for all experiments. Cyclic voltammograms were obtained on a CHI 660E potentiostat.





Preparation of starting materials

General procedure A for the synthesis of substrate 1a-1af, 1an-1ap. [1]



1) To a 50 mL Schlenk tube, under N_2, was added *N*-Hydroxyphthalimide (6.5 mmol, 1.3 equiv.), triphenylphosphine (PPh_3, 7.5 mmol, 1.5 equiv.), 30 mL of anhydrous THF, and then alcohol (5 mmol, 1.0 equiv.) was added. The tube is immersed in an ice bath, and diisopropyl azodicarboxylate (DIAD, 7.5 mmol, 1.5 equiv.) in 5 mL of anhydrous THF was added dropwise, upon completion of the addition, the flask is removed from the ice bath and the solution is allowed to stir at room temperature overnight. The solvent was removed and the residue purified by flash column chromatography on silica gel (using 30% EtOAc/petroleum ether as eluent) to give compound **r-1**.

2) To a 50 mL Schlenk tube, under N_2, was added $PdCl_2$ $(PPh_3)_2$ (0.05 mmol, 0.01 equiv.), CuI (0.1

mmol, 0.02 equiv.), iodobenzene (6 mmol, 1.2 equiv.), compound **r-1** (5 mmol, 1.0 equiv.) and anhydrous TEA (10 mL), then the tube was placed in a pre-heated oil bath (60 ºC). The reaction was stirred overnight and then cooled to room temperature and checked by TLC. The reaction is filtered over celite, washing with dichloromethane. The solvent was removed and the residue purified by flash column chromatography on silica gel (using 30% EtOAc/petroleum ether as eluent) to give compound **r-2**.

3) In a 50 mL round-bottom flask was charged alkoxyphthalimide starting material (5.0 mmol), solvent 20 mL [MeOH/DCM (ratio 1:2)], and then slowly added hydrazine monohydrate (5.5 mmol, 1.1 equiv.), then stirred at room temperature for 1 h. Upon completion (indicated by TLC), the solvent was then removed under reduce pressure. The residue was washed with DCM and filtered, collect the DCM part and removed the solvent to give the crude *O*-alkoxylamine **r-3**, which was used in next step without further purification.

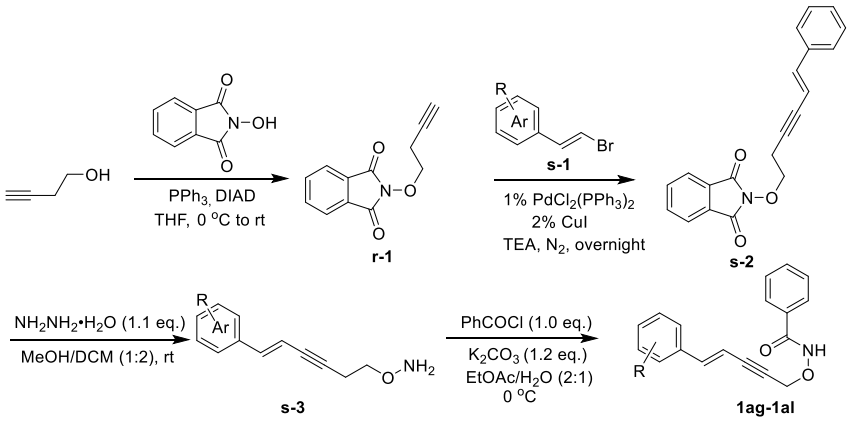
4) The crude *O*-alkoxylamine which was obtained in the previous step was added to a biphasic mixture of K_2CO_3 (10 mmol, 2.0 equiv.) in a 2:1 mixture of EtOAc: H_2O (0.2 M). The resulting solution was cooled to 0 ºC followed by dropwise addition of the acid chloride dissolved in a minimum amount of EtOAc. The flask containing the acid chloride was then rinsed with additionnal EtOAc. The reaction was allowed to stir at same temperature for 1 h. Upon completion (indicated by TLC), the phases were separated and the aqueous phase was extracted twice with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered, and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (using 30% EtOAc/petroleum ether as eluent) to give product **1a-1af**, **1an-1ap**.

5) Acid chloride was prepared according to the literature [2].

To a suspension of the carboxylic acid (5 mmol, 1.0 equiv.) in dry CH_2Cl_2 (5 mL) at room temperature under a nitrogen atmosphere was added a catalytic amount of dry DMF (2 drops). Oxalyl chloride (7.5 mmol, 1.5 equiv., 2 M in DCM) was added dropwise over about 10 minutes with care as effervescence occurs. The reaction was allowed to stir at room temperature until completion which was judged to be when no further effervescence could be seen and in some cases,

the solution became homogeneous. The solvent was then removed under reduced pressure to afford the corresponding crude acid chloride.

General procedure B for the synthesis of substrate 1ag-1al. [1],[3]



1) To a 50 mL Schlenk tube, under N_2, was added *N*-hydroxyphthalimide (1.054g, 6.5 mmol), triphenylphosphine (PPh_3, 1.967 g, 7.5 mmol), 30 mL of anhydrous THF, and then alcohol (0.47 mL, 5 mmol) was added. The tube is immersed in an ice bath, and diisopropyl azodicarboxylate (DIAD, 1.48 mL, 7.5 mmol) in 5 mL of anhydrous THF was added dropwise, upon completion of the addition, the flask is removed from the ice bath and the solution is allowed to stir at room temperature overnight. The solvent was removed and the residue purified by flash column chromatography on silica gel (using 30% EtOAc/petroleum ether as eluent) to give compound **r-1**.

2) To a 50 mL Schlenk tube, under N_2, was added $PdCl_2(PPh_3)_2$ (0.05 mmol, 0.01 equiv.), CuI (0.1 mmol, 0.02 equiv.), **s-1** (6 mmol, 1.2 equiv.) and anhydrous TEA (10 mL), then the tube was placed in a pre-heated oil bath (60 °C). The reaction was stirred overnight and then cooled to room temperature and checked by TLC. The reaction is filtered over celite, washing with dichloromethane. The solvent was removed and the residue was purified by flash column chromatography on silica gel (using 30% EtOAc/petroleum ether as eluent) to give compound **s-2**.

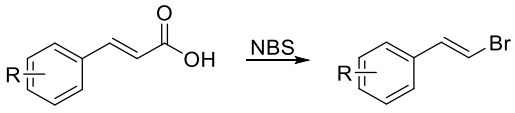
3) In a 50 mL round-bottom flask was charged compound **s-2** (5.0 mmol), solvent 20 mL [MeOH/DCM (ratio 1:2)], and then slowly added hydrazine monohydrate (5.5 mmol, 1.1 equiv.), then stirred at room temperature for 1 h. Upon completion (indicated by TLC), the solvent was then removed under reduce pressure. The residue was washed with DCM and filtered, collect the DCM part and removed the solvent to give the crude *O*-alkoxylamine **s-3**, which was used in next step without further purification.

4) The crude *O*-alkoxylamine which was obtained in the previous step was added to a biphasic mixture of K_2CO_3 (10 mmol, 2.0 equiv.) in a 2:1 mixture of EtOAc: H_2O (0.2 M). The resulting solution was cooled to 0 °C followed by dropwise addition of the acid chloride dissolved in a minimum amount of EtOAc. The flask containing the acid chloride was then rinsed with additional

EtOAc. The reaction was allowed to stir at same temperature for 1 h. Upon completion (indicated by TLC), the phases were separated and the aqueous phase was extracted twice with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (using 30% EtOAc/petroleum ether as eluent) to give product **1ag-1al**.

General procedure C for the synthesis of *β*-bromostyrene compounds. [4]

1ag, 1ah, 1aj, 1ak was prepared according to general procedure B, **s-1** was prepared according to procedure C**.**

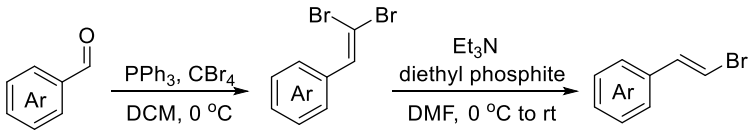


s-1

To a solution of cinnamic acid (5.0 mmol, 1.0 equiv.) in methylene chloride (5 mL) was added Et_3N (0.25 mmol, 0.05 equiv.) at room temperature and stirred for 5 minutes. *N*-bromosuccinimide (6 mmol, 1.2 equiv.) was added in one portion and stirred for 30 minutes. The solvent was removed under reduced pressure. The crude was purified by flash column chromatography (silica gel hexanes) to afford product **s-1**.

General procedure D for the synthesis of *β*-bromostyrene compounds.[5]

1ai was prepared according to general procedure B, **s-1** was prepared according to procedure D**.**



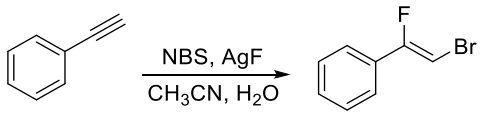
s-1

1) A flame-dried round-bottom flask equipped with a stir bar under argon was charged with the corresponding aldehyde (10 mmol, 1.0 equiv.), CBr_4 (15 mmol, 1.5 equiv.) and DCM (80 mL). The reaction mixture was cooled at 0 °C, then a solution of PPh_3 (30 mmol, 3.0 equiv.) in DCM (80 mL) was added dropwise over 20 min. After another 1 h at 0 °C, the mixture was concentrated under reduce pressure to half of the volume. Next, pentane was added and triphenylphosphine oxide precipitated out. The mixture was filtered and concentrated under reduced pressure. Pentane was added again to further precipitate the triphenylphosphine oxide. After filtration and evaporation of the solvent, the crude dibromide was used directly in the next step without any further purification.

2) To a mixture of the above dibromide and diethyl phosphite (30 mmol, 3.0 equiv.) in DMF (10 mL) was added Et_3N (30 mmol, 3.0 equiv.) at 0 °C. The reaction was then warmed to room temperature and stirred overnight. The mixture was quenched with water. The aqueous layer was extracted with DCM. The combined organics were washed with brine, dried over Na_2SO_4, and concentrated in vacuo. The product **s-1** was purified by chromatography.

General procedure E for the reaction of bromofluorination of terminal alkynes.[6]

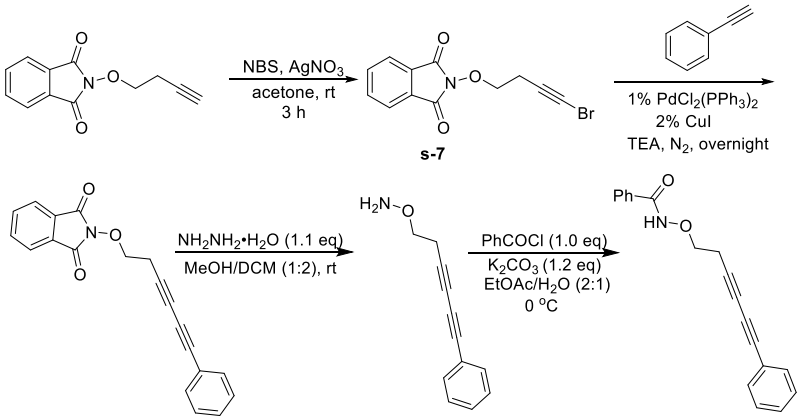
1al was prepared according to general procedure B, **s-1** was replaced by **s-4.**



s-4

A mixture of NBS (5.5 mmol, 1.1 equiv.), AgF (12.5 mmol, 2.5 equiv.), CH_3CN (wet, 10 mL), phenylacetylene (5.0 mmol, 1.0 equiv.) was added successively in Schlenk tube. After stirring for 10 h at 80 °C, the solution was filtered through a small amount of silica gel. The residue was purified by silica gel preparative TLC (*n*-hexane), which furnished product **s-4**.

General procedure F for the synthesis of 1am. [1],[3]



s-8 **s-7** **s-9** **1aq**

1) To a solution of terminal alkyne (10 mmol) in acetone (60 mL) was added NBS (12 mmol) and $AgNO_3$ (5 mmol %) at room temperature with magnetic stirring. After 2-4 hours, the solution was filtered through a small amount of silica gel. Then the solvent was removed under reduced pressure. The crude was purified by flash column chromatography on silica gel (using 30% EtOAc/ petroleum ether as eluent) to afford product **s-7**.

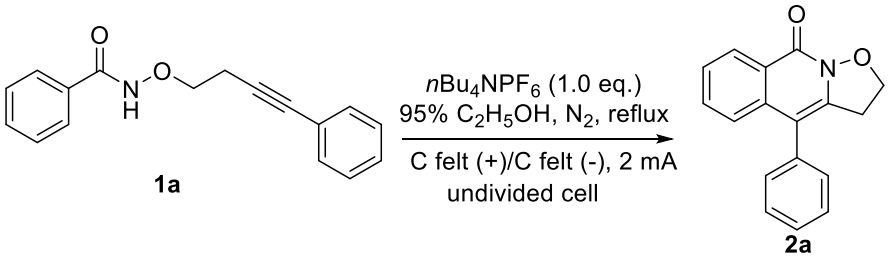
2) To a 50 mL Schlenk tube, under N_2, was added $PdCl_2(PPh_3)_2$ (0.05 mmol, 0.01 equiv.), CuI (0.1 mmol, 0.02 equiv.), compound **s-7** (5 mmol, 1.2 equiv.) and 4-chlorophenylacetylene (6 mmol, 1.2 equiv.) and anhydrous TEA (10 mL), then the tube was placed in a pre-heated oil bath (60 °C). The reaction was stirred overnight and then cooled to room temperature and checked by TLC. The reaction is filtered over celite, washing with dichloromethane. The solvent was removed and the residue was purified by flash column chromatography on silica gel (using 30% EtOAc/ petroleum ether as eluent) to give compound **s-8**.

2) In a 50 mL round-bottom flask was charged compound **s-8** (5.0 mmol), solvent 20 mL [MeOH/DCM (ratio 1:2)], and then slowly added hydrazine monohydrate (5.5 mmol, 1.1 equiv.), then stirred at room temperature for 1 h. Upon completion (indicated by TLC), the solvent was then removed under reduce pressure. The residue was washed with DCM and filtered, collect the DCM part and removed the solvent to give the crude *O*-alkoxylamine **s-9**, which was used in next step without further purification.

4) The crude *O*-alkoxylamine **s-9** which was obtained in the previous step was added to a biphasic

mixture of K_2CO_3 (10 mmol, 2.0 equiv.) in a 2:1 mixture of EtOAc: H_2O (0.2 M). The resulting solution was cooled to 0 ºC followed by dropwise addition of the acid chloride dissolved in a minimum amount of EtOAc. The flask containing the acid chloride was then rinsed with additionnal EtOAc. The reaction was allowed to stir at same temperature for 1 h. Upon completion (indicated by TLC), the phases were separated and the aqueous phase was extracted twice with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered, and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (using 30% EtOAc/ petroleum ether as eluent) to give product **1am**.

Optimization of the Reaction Conditions[a]

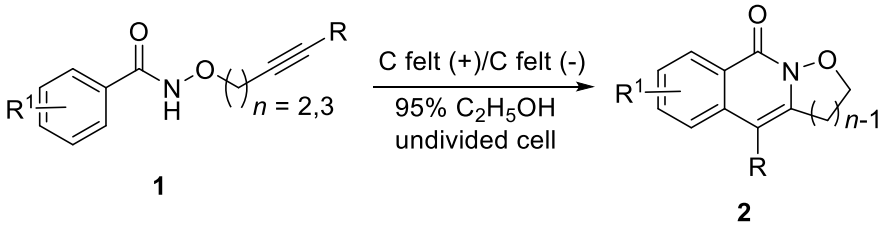


Entry	Variation from standard conditions	Yield (%)[b]
1	none	93
2	5 mA	62
3	3 mA	75
4	Pt(+)|Pt(-)	40
5	C(+)|C(-)	63
6	C(+)|Pt(-)	65
7	MeCN as the solvent	81
8	MeOH as the solvent	85
9	EtOH as the solvent	90
10	without *n*-Bu_4NBF_4	trace
11	under air	n.r
12	no electric current	n.r
13	Reaction at RT	16
14	Reaction at 50 ºC	62
15	Reaction at 70 ºC	90

[a]Reaction conditions: **1a** (0.1 mmol), *n*-Bu_4NBF_4 (0.1 mmol), 95% EtOH (5.0 mL) in undivided cell with carbon felt anode and cathode (2.0 cm × 1.0 cm × 0.5 cm), constant current = 2.0 mA, nitrogen, reflux, 4 h. [b]Isolated yield of **2a**. n.r = no reaction.

Synthesis of compounds 2

A 10-mL three-necked flask was charged with the substrate **1** (0.1 mmol, 1.0 equiv) and nBu$_4$NPF$_6$ (0.1 mmol, 1.0 equiv). The flask was equipped with a rubber stopper, a carbonc felt anode (2 cm x 1 cm x 0.5 cm) and a carbonc felt cathode (2 cm x 1 cm x 0.5 cm) and then flushed with nitrogen. EtOH (5.0 mL) were added. The constant current electrolysis was carried out at 80 °C (oil bath temperature) until complete consumption of the substrate (monitored by TLC). The reaction mixture was cooled to RT and concentrated under reduced pressure. The residue was chromatographed through silica gel eluting with petroleum ether /EtOAc to give the product.



1 **2**

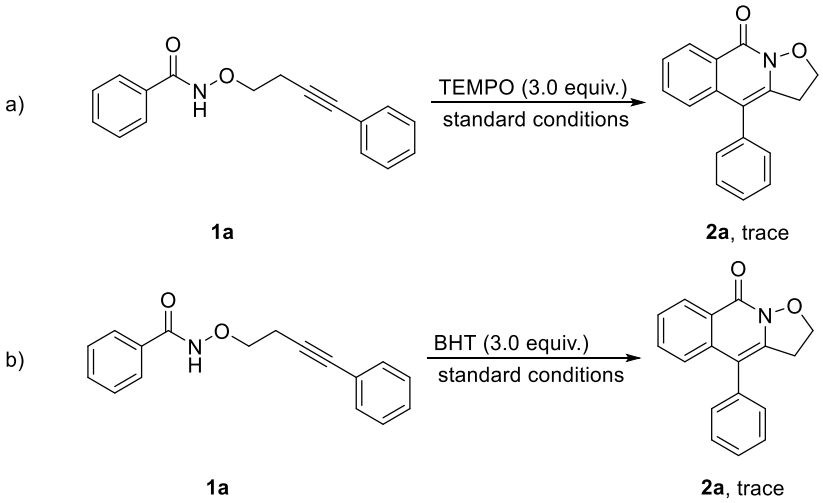
Gram-scale reaction

A 250-mL three-necked flask was charged with the substrate 1 (5 mmol, 1.0 equiv) and nBu$_4$NPF$_6$ (5 mmol, 1.0 equiv). The flask was equipped with a rubber stopper, a carbonc felt anode (4 cm x 2 cm x 0.5 cm) and a carbonc felt cathode (4 cm x 2 cm x 0.5 cm) and then flushed with argon. EtOH (150 mL) were added. The constant current (2 mA) electrolysis was carried out at 80 °C (oil bath temperature) until complete consumption of the substrate (monitored by TLC). The reaction mixture was cooled to RT and concentrated under reduced pressure. The residue was chromatographed through silica gel eluting with petroleum ether /EtOAc to give the product.

Control experiments

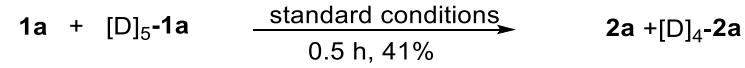
TEMPO/BHT inhibiting experiment:

A 10-mL three-necked flask was charged with the substrate **1** (0.1 mmol, 1.0 equiv) ,TEMPO (0.3mmol, 3.0 equiv) or BHT (0.3 mmol, 3.0 equiv) and nBu$_4$NPF$_6$ (0.1 mmol, 1.0 equiv). The flask was equipped with a rubber stopper, a carbonc felt anode (2 cm x 1 cm x 0.5 cm) and a carbonc felt cathode (2 cm x 1 cm x 0.5 cm) and then flushed with nitrogen. EtOH (5.0 mL) were added. The constant current (2 mA) electrolysis was carried out at 80 °C (oil bath temperature) for 4 h. (monitored by TLC).

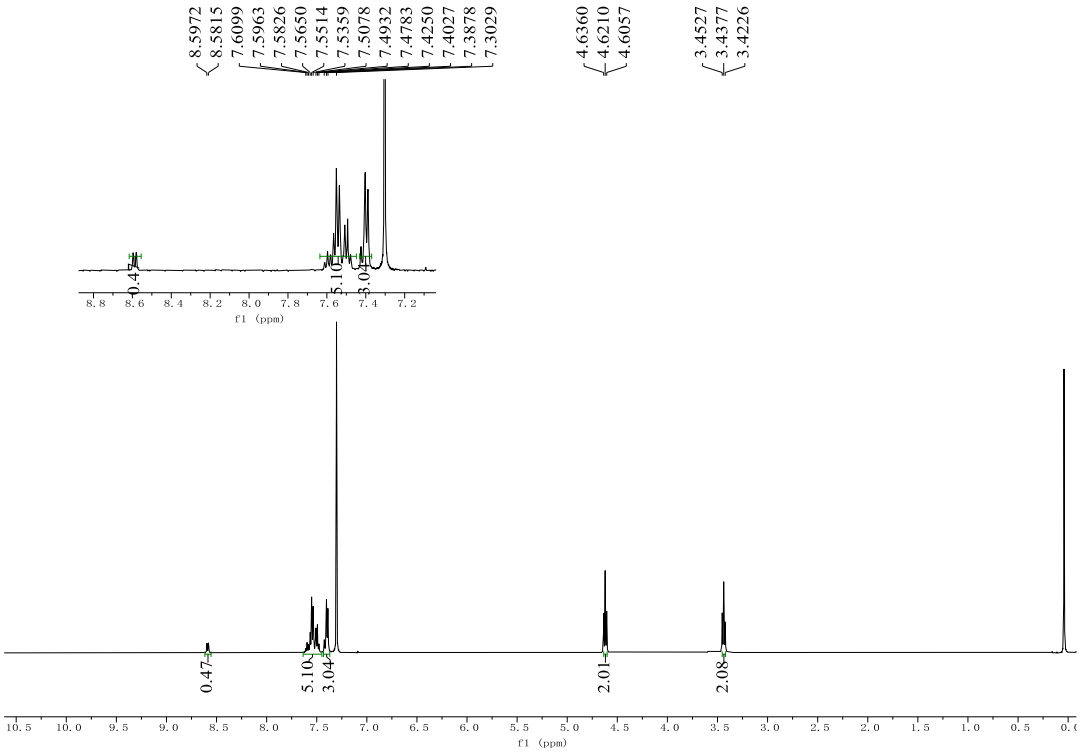


Kinetic Isotope Effect (KIE) Study

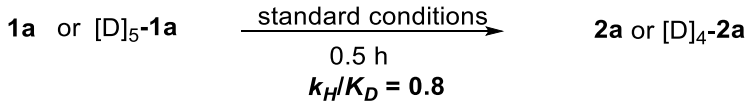
Intermolecular Kinetic Isotopic Effect



A 10-mL three-necked flask was charged with the substrate **1a** (0.1 mmol, 1.0 equiv) , $[D]_5$-**1a** (0.1 mmol, 1.0 equiv) and nBu$_4$NPF$_6$ (0.1 mmol, 1.0 equiv). The flask was equipped with a rubber stopper, a carbonc felt anode (2 cm x 1 cm x 0.5 cm) and a carbonc felt cathode (2 cm x 1 cm x 0.5 cm) and then flushed with nitrogen. EtOH (5.0 mL) were added. The constant current (2 mA) electrolysis was carried out at 80 °C (oil bath temperature). The reaction was stopped after 0.5 h, then the products was isolated by using column chromatography on silica gel. A mixture of the products was analyzed by ^{1}H NMR spectroscopy. A Kinetic isotopic effect of this reaction was determined to be kH/kD = 0.8 (0.44/0.56).



Two parallel reactions for KIE value measurement

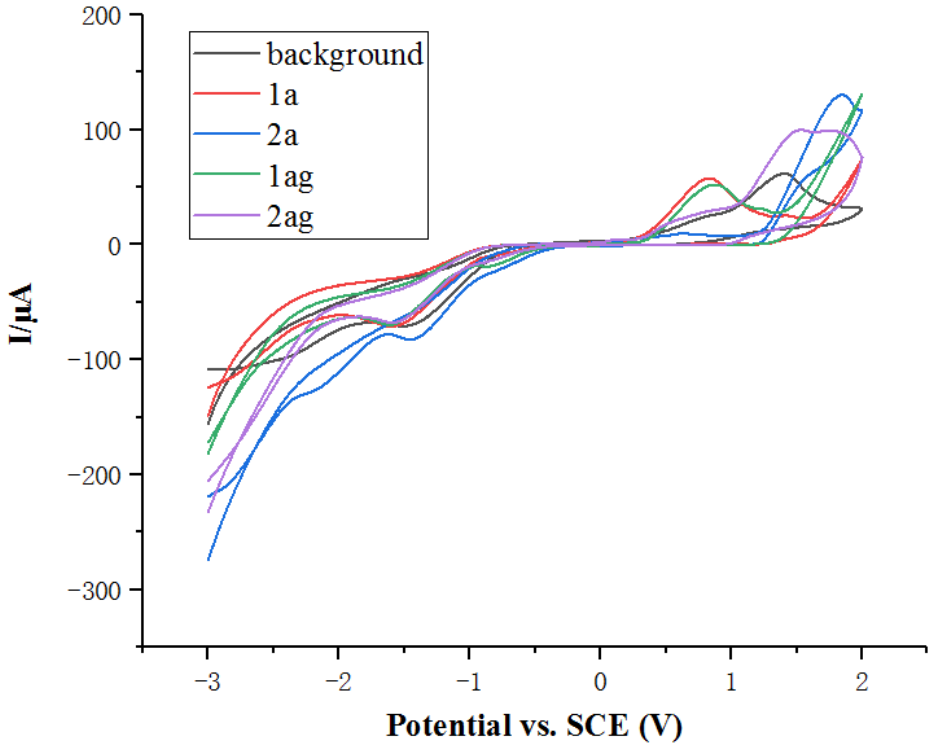


A 10-mL three-necked flask was charged with the substrate **1a** (0.1 mmol, 1.0 equiv) and nBu$_4$NPF$_6$ (0.1 mmol, 1.0 equiv). The flask was equipped with a rubber stopper, a carbonc felt anode (2 cm x 1 cm x 0.5 cm) and a carbonc felt cathode (2 cm x 1 cm x 0.5 cm) and then flushed with nitrogen. EtOH (5.0 mL) were added. The constant current (2 mA) electrolysis was carried out at 80 °C (oil bath temperature). The reaction was stopped after 0.5 h, then the product **2a** (38%, 10 mg) was isolated by using column chromatography on silica gel.

A 10-mL three-necked flask was charged with the substrate [D]$_5$-**1a** (0.1 mmol, 1.0 equiv) and nBu$_4$NPF$_6$ (0.1 mmol, 1.0 equiv). The flask was equipped with a rubber stopper, a carbonc felt anode (2 cm x 1 cm x 0.5 cm) and a carbonc felt cathode (2 cm x 1 cm x 0.5 cm) and then flushed with nitrogen. EtOH (5.0 mL) were added. The constant current (2 mA) electrolysis was carried out at 80 °C (oil bath temperature). The reaction was stopped after 0.5 h, then the product [D]$_4$-**2a** (48.6%, 13 mg) was isolated by using column chromatography on silica gel.

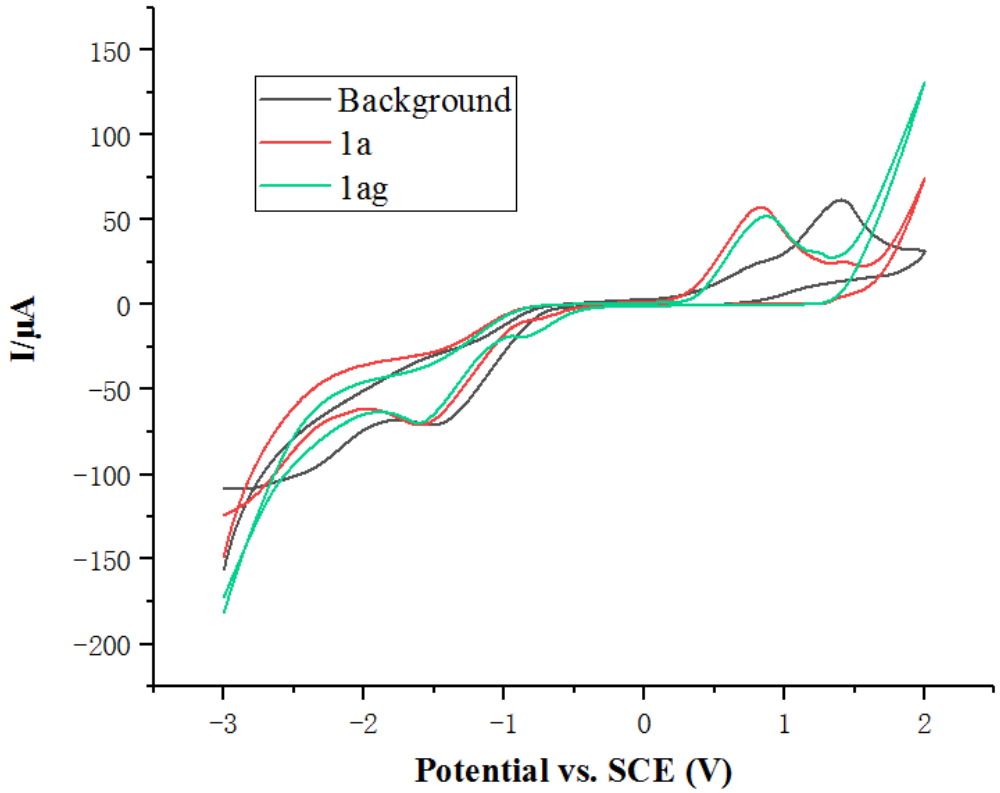
Cyclic Voltammetry Studies

The cyclic voltammograms were recorded in an electrolyte of nBu$_4$NPF$_6$ (0.02 M) in EtOH using glassy carbon electrode working electrode, Pt wire, and SCE as counter and reference electrodes at 100 mV/s scan rate.



background): nBu$_4$NPF$_6$ (0.02M). 1a): **1a** (0.02 M), nBu$_4$NPF$_6$ (0.02M). 2a): **2a** (0.02M),

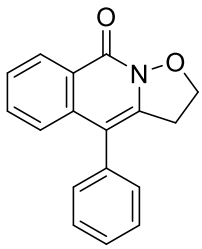
nBu$_4$NPF$_6$ (0.02M). 1ag): **1ag** (0.02 M), nBu$_4$NPF$_6$ (0.02M). 2ag): **2ag** (0.02M), nBu$_4$NPF$_6$ (0.02M).



background): nBu$_4$NPF$_6$ (0.02M). 1a): **1a** (0.02 M), nBu$_4$NPF$_6$ (0.02M). 1ag): **1ag** (0.02M), nBu$_4$NPF$_6$ (0.02M).

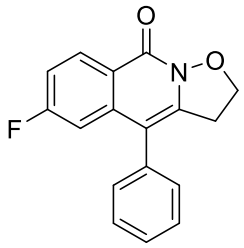
Characterization of compounds 2

4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2a).[7]



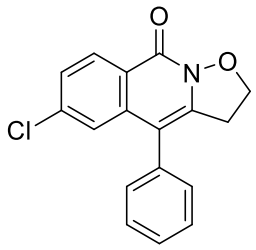
White solid, 49 mg, 93 % yield, M.p. = 206-208°C;
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.54 (d, J = 7.1 Hz, 1H), 7.59-7.43 (m, 5H), 7.38-7.32 (m, 3H), 4.58 (t, J = 7.6 Hz, 2H), 3.39 (t, J = 7.6 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 153.95, 136.20, 135.02, 132.52, 131.63, 130.31, 128.93, 128.10, 127.47, 126.32, 126.30, 124.71, 113.03, 69.55, 32.46.

6-fluoro-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2b).



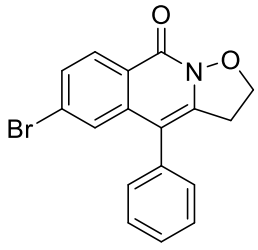
White solid, 48 mg, 85% yield, M.p. =230-232 °C;
^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.15 (d, J = 9.3, 2.5 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.48 – 7.42 (m, 1H), 7.38 – 7.31 (m, 3H), 7.28 – 7.24 (m, 1H), 4.58 (t, J = 7.6 Hz, 2H), 3.38 (t, J = 7.6 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 161.10 (d, $^1J_{C,F}$ = 248.2 Hz), 152.94, 134.69, 132.76, 131.90, 130.15, 128.98, 128.24, 127.87 (d, $^3J_{C,F}$ = 7.6 Hz), 127.14 (d, $^3J_{C,F}$ = 7.4 Hz), 120.31 (d, $^2J_{C,F}$ = 23.5 Hz), 112.66, 112.46 (d, $^2J_{C,F}$ = 23.2 Hz), 69.74, 32.25; **HRMS** (ESI) m/z calcd for $C_{17}H_{12}FNNaO_2^+$ $[M+Na]^+$ 304.0750, found 304.0754.

6-chloro-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2c). [7]



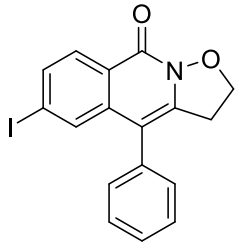
Pale yellow solid, 54 mg, 91% yield, M.p. = 236-238 °C;
^{1}H NMR (500 MHz $CDCl_3$): δ 8.47 (d, J = 3.6 Hz, 1H), 7.53-7.49 (m, 2H), 7.48 – 7.42 (m, 2H), 7.34-7.28 (m, 3H), 4.58 (t, J = 7.6 Hz, 2H), 3.39 (t, J = 7.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 152.76, 134.51, 134.43, 132.89, 132.53, 132.02, 130.14, 129.01, 128.29, 127.29, 126.71, 126.34, 112.60, 69.69, 32.36.

6-bromo-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2d).



White solid, 58 mg, 85% yield, M.p. = 204-206 °C;
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.65 (d, J = 2.1 Hz, 1H), 7.64 – 7.57 (m, 1H), 7.55 – 7.43 (m, 3H), 7.36 – 7.30 (m, 2H), 7.23 (d, J = 8.7 Hz, 1H), 4.59 (t, J = 7.6 Hz, 2H), 3.39 (t, J = 7.6 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 152.72,134.90, 134.81, 134.43, 133.12, 130.20, 129.91, 129.08, 128.36, 127.60, 126.52, 120.50, 112.73, 69.74, 32.47; **HRMS** (ESI) m/z calcd for $C_{17}H_{12}BrNNaO_2^+$ $[M+Na]^+$ 363.9949, found 363.9949.

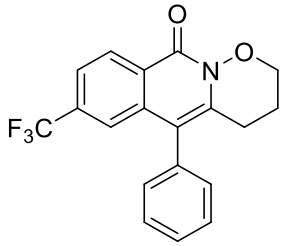
6-iodo-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2e).



White solid, 54 mg, 70% yield, M.p. = 218-220 °C

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.87 (d, J = 1.7 Hz, 1H), 7.85 – 7.74 (m, 1H), 7.51 (t, J = 7.4 Hz, 2H), 7.46 (t, J = 7.3 Hz, 1H), 7.32 (d, J = 7.1 Hz, 2H), 7.09 (d, J = 8.6 Hz, 1H), 4.59 (t, J = 7.6 Hz, 2H), 3.38 (t, J = 7.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 150.61, 138.42, 134.21, 133.40, 132.46, 131.39, 128.27, 127.15, 126.43, 125.79, 124.54, 110.85, 89.54, 67.78, 30.59; **HRMS** (ESI) m/z calcd for $C_{17}H_{12}INNaO_2^+$ $[M+Na]^+$ 411.9810, found 411.9808.

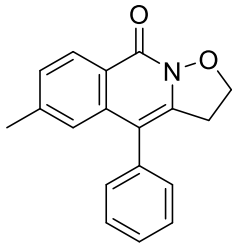
5-phenyl-7-(trifluoromethyl)-3,4-dihydro-[1,2]oxazino[2,3-*b*]isoquinolin-10(2*H*)-one(2f).[7]



Pale yellow solid, 24 mg, 35% yield, M.p. = 219-221 °C;

^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.66 (d, J = 8.6 Hz, 1H), 7.75 – 7.61 (m, 2H), 7.57-7.45 (m, 3H), 7.36-7.32 (m, 2H), 7.28 (d, J = 9.8 Hz, 1H), 4.62 (t, J = 7.6 Hz, 2H), 3.43 (t, J = 7.6 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 125 MHz): **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 153.13, 136.20, 134.28, 133.97, 133.46 (q, $^2J_{C,F}$ = 34.9 Hz), 130.15, 129.29, 129.19 (q, $^1J_{C,F}$ = 275.1 Hz) , 128.65, 128.40, 122.38 (q, $^3J_{C,F}$ = 3.5 Hz), 122.03 (q, $^3J_{C,F}$ = 4.3 Hz), 112.98, 69.76, 32.56.

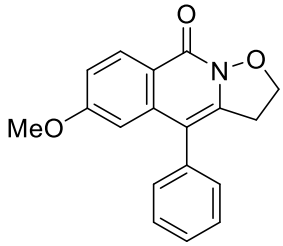
6-methyl-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2g). [7]



Pale yellow solid, 48mg, 86% yield, M.p. = 219-221 °C;

^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.34 (s, 1H), 7.50 (t, J = 7.5 Hz, 2H), 7.44 (t, J = 6.9 Hz, 1H), 7.36 (d, J = 8.5 Hz, 1H), 7.34 (d, J = 7.8 Hz, 2H), 7.27 (d, J = 8.2 Hz, 1H), 4.57 (t, J = 7.5 Hz, 2H), 3.38 (t, J = 7.6 Hz, 2H), 2.48 (s, 3H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 153.90, 136.50, 135.16, 133.90, 133.17, 131.51, 130.27, 128.86, 128.00, 127.00, 126.23, 124.65, 113.02, 109.98, 69.58, 32.32, 21.20.

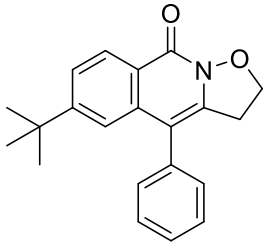
6-methoxy-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2h). [7]



Pale yellow solid, 47 mg, 80% yield, M.p. = 160-162 °C;

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (d, J = 2.7 Hz, 1H), 7.47 (t, J = 7.3 Hz, 2H), 7.42 (t, J = 7.4 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.30 – 7.25 (m, 1H), 7.13 (dd, J = 9.0, 2.7 Hz, 1H), 4.56 (t, J = 7.5 Hz, 2H), 3.91 (s, 3H), 3.36 (t, J = 7.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 158.33, 153.43, 135.12, 130.19,130.07, 128.81, 127.97, 127.53, 126.28, 122.21, 113.01, 107.13, 69.71, 55.71, 32.13.

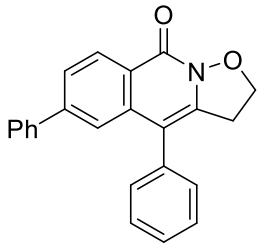
6-(tert-butyl)-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2i).



White solid, 58 mg, 91% yield, M.p. = 206-208 °C;

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.52 (d, J = 2.0 Hz, 1H), 7.61 (dd, J = 8.6, 2.1 Hz, 1H), 7.49 (t, J = 7.3 Hz, 2H), 7.44 (t, J = 7.3 Hz, 1H), 7.38 – 7.29 (m, 3H), 4.56 (t, J = 7.5 Hz, 2H), 3.38 (t, J = 7.5 Hz, 2H), 1.38 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 154.10, 149.69, 135.13, 133.83, 131.63, 130.22, 129.64, 128.80, 127.94, 125.99, 124.49, 123.29, 112.58, 69.52, 34.94, 32.27, 31.24. **HRMS** (ESI) m/z calcd for $C_{21}H_{21}NNaO_2^+$ $[M+Na]^+$ 342.1470, found 342.1470.

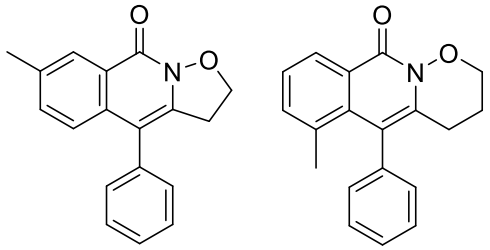
4,6-diphenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2j).



White solid, 58 mg, 85% yield, M.p. = 160-162 °C;

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (d, J = 2.0 Hz, 1H), 7.77 (dd, J = 8.6, 2.1 Hz, 1H), 7.69 (d, J = 7.4 Hz, 2H), 7.53 – 7.40 (m, 6H), 7.40 – 7.33 (m, 3H), 4.58 (t, J = 7.6 Hz, 2H), 3.40 (t, J = 7.6 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 154.01, 139.68, 139.05, 135.13, 134.96, 132.55, 130.51, 130.32, 128.98, 128.92, 128.15, 127.76, 127.23, 126.64, 125.38, 125.34, 112.90, 69.67, 32.45.. **HRMS** (ESI) m/z calcd for $C_{23}H_{17}NNaO_2^+$ $[M+Na]^+$ 362.1157, found 362.1159.

7-methyl-4-phenyl-2,3-dihydro-9H-isoxazolo[2,3-b]isoquinolin-9-one (2k). [7]
6-methyl-5-phenyl-3,4-dihydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one (2k'). [7]

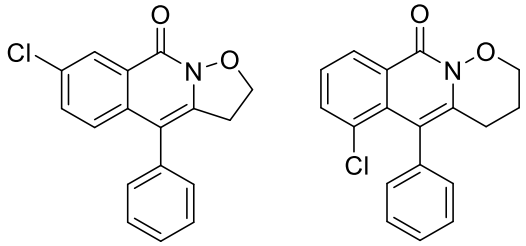


2k 1:0.7 **2k'**

White solid; 53mg, 95% yield;

^{1}H NMR (500 MHz $CDCl_3$): δ 8.49 (d, J = 7.0 Hz, 0.68H), 8.33 (s, 1H), 7.54 – 7.22 (m, 12H), 4.56 (t, J = 7.3 Hz, 2H), 4.50 (t, J = 7.6 Hz, 1.46H), 3.38 (t, J = 7.3 Hz, 2H), 3.20 (t, J = 7.4 Hz, 1.41H), 2.47 (s, 3H), 1.85 (s, 2.19H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 154.07, 153.83, 139.16, 136.44, 135.52, 135.10, 134.67, 134.24, 133.83, 133.40, 133.12, 131.46, 130.21, 128.81, 128.53, 127.95, 127.78, 127.44, 126.94, 126.10, 126.03, 124.60, 112.96, 69.55, 69.37, 33.03, 32.28, 23.83, 21.17.

7-chloro-4-phenyl-2,3-dihydro-9H-isoxazolo[2,3-b]isoquinolin-9-one (2l). [7]
6-chloro-5-phenyl-3,4-dihydro-[1,2]oxazino[2,3-b]isoquinolin-10(2H)-one (2l'). [7]

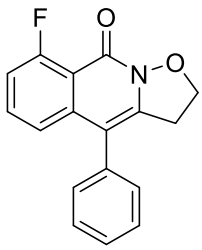


2l 1:0.65 **2l'**

White solid; 58mg, 97% yield;

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.55-8.52 (m, 0.58H) ,8.51 (d, J = 2.3 Hz, 1H), 7.60 – 7.58 (m, 0.59H),7.53 – 7.26 (m, 3.84H), 7.42 – 7.37 (m, 11H), 7.35 – 7.31 (m, 2.54H), 4.59 (t, J = 7.6 Hz, 2H), 4.55 (t , 1.24H), 3.39 (t, J = 7.6 Hz, 2H), 3.25 (t, 1.29H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.17, 152.81, 137.67, 135.22, 135.06, 134.52, 134.47, 132.86, 132.61, 132.52, 132.06, 130.55, 130.18, 130.14, 129.01, 128.82, 128.28, 128.26, 127.69, 127.36, 126.98, 126.78, 126.49, 126.32, 112.60, 111.49, 69.66, 69.49, 33.20, 32.37.

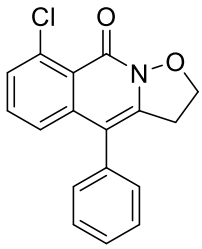
8-fluoro-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2m).



White solid, 39mg, 69% yield, M.p. =180-182 °C;

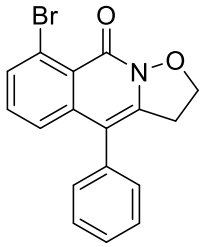
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 8.1 Hz, 1H), 7.46 – 7.37 (m, 4H), 7.32 (d, J = 5.9 Hz, 2H), 7.26 – 7.18 (m, 1H), 4.56 (t, J = 7.6 Hz, 2H), 3.30 (t, J = 7.7 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 158.34 (d, $^1J_{C,F}$ = 254.8 Hz), 152.91, 137.14, 134.57, 129.37, 129.34, 128.49, 128.27, 127.73, 126.91 (d, $^3J_{C,F}$ = 8.4 Hz), 125.11 (d, $^3J_{C,F}$ = 10.5 Hz), 123.60, 118.40 (d, $^2J_{C,F}$ = 21.8 Hz), 109.25, 69.64, 32.68; **HRMS** (ESI) m/z calcd for $C_{17}H_{12}FNNaO_2^+$ $[M+Na]^+$ 304.0750, found 304.0754.

8-chloro-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2n). [7]



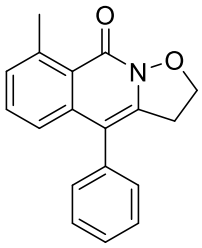
White solid, 55 mg, 92% yield, M.p. = 207-209 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.51 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 7.6 Hz, 1H), 7.40-7.32 (m, 4H), 7.27 (d, J = 6.7 Hz, 2H), 4.54 (t, J = 7.6 Hz, 2H), 3.24 (t, J = 7.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 153.12, 137.66, 135.25, 135.03, 132.48, 130.51, 130.18, 128.78, 128.24, 127.67, 126.94, 126.47, 111.44, 69.50, 33.19.

8-bromo-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2o).



White solid, 58 mg, 85% yield, M.p. = 196-198°C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.57 (d, J = 8.0 Hz, 1H), 7.81 (d, J = 7.6 Hz, 1H), 7.40-7.38 (m, 3H), 7.29-7.26 (m, 3H), 4.53 (t, J = 7.7 Hz, 2H), 3.23 (t, J = 7.7 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.15, 139.20, 137.14, 135.40, 133.55, 130.80, 128.96, 128.34, 127.88, 127.65, 126.78, 118.83, 112.30, 69.52, 33.37; **HRMS** (ESI) m/z calcd for $C_{17}H_{12}BrNNaO_2^+$ $[M+Na]^+$ 363.9949, found 363.9947.

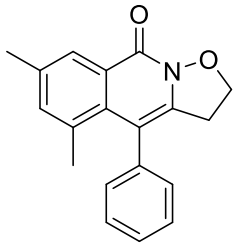
8-methyl-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2p).



White solid, 29 mg, 53% yield, M.p. =180-182 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 (d, J = 8.7 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.38 – 7.32 (m, 2H), 7.33 – 7.28 (m, 2H), 4.53 (t, J = 7.6 Hz, 2H), 3.22 (t, J = 7.6 Hz, 2H), 1.87 (s, 3H); **^{13}C NMR** (125

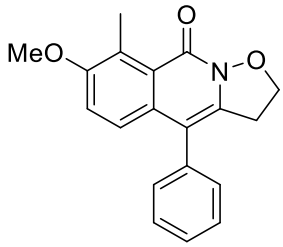
MHz, $CDCl_3$): δ 154.15, 139.23, 135.59, 134.72, 134.30, 133.43, 130.22, 128.59, 127.84, 127.51, 126.18, 126.11, 113.06, 69.41, 33.09, 23.87; **HRMS** (ESI) m/z calcd for $C_{18}H_{15}NNaO_2^+$ $[M+Na]^+$ 300.1000, found 300.1002.

5,7-dimethyl-4-phenyl-2,3-dihydro-9H-isoxazolo[2,3-b]isoquinolin-9-one (2q).



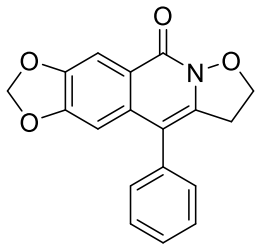
White solid, 41 mg, 70% yield, M.p. = 179-181 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.29 (s, 1H), 7.45-7.35 (m, 3H), 7.30 – 7.26 (m, 2H), 7.17 (s, 1H), 4.51 (td, J = 7.6, 1.2 Hz, 2H), 3.19 (t, J = 7.6 Hz, 2H), 2.42 (s, 3H), 1.82 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 154.03, 139.27, 137.10, 136.04, 134.51, 132.36, 131.98, 130.14, 128.49, 127.70, 127.48, 125.67, 112.98, 69.38, 32.88, 23.65, 20.85; **HRMS** (ESI) m/z calcd for $C_{19}H_{17}NNaO_2^+$ $[M+Na]^+$ 314.1157, found 314.1158.

7-methoxy-8-methyl-4-phenyl-2,3-dihydro-9H-isoxazolo[2,3-b]isoquinolin-9-one (2r).



Yellow solid, 33mg, 53% yield, M.p. = 179-181 °C;
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 – 7.40 (m, 3H), 7.31 (d, J = 6.7 Hz, 2H), 7.18 – 7.09 (m, 2H), 4.51 (t, J = 7.5 Hz, 2H), 3.86 (s, 3H), 3.30 (t, J = 7.5 Hz, 2H), 2.93 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 155.97, 155.23, 135.91, 131.59, 130.41, 130.09, 129.70, 129.23, 128.85, 127.88, 125.68, 123.42, 115.53, 112.37, 69.20, 56.38, 32.35, 13.26.; **HRMS** (ESI) m/z calcd for $C_{19}H_{17}NNaO_3^+$ $[M+Na]^+$ 330.1106, found 330.1107.

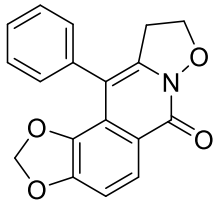
10-phenyl-8,9-dihydro-5*H*-[1,3]dioxolo[4,5-*g*]isoxazolo[2,3-*b*]isoquinolin-5-one (2s).



White solid, 36 mg, 58% yield, M.p. = 236-238 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.83 (s, 1H), 7.48 (t, J = 7.3 Hz, 2H), 7.42 (t, J = 7.4 Hz, 1H), 7.32 –

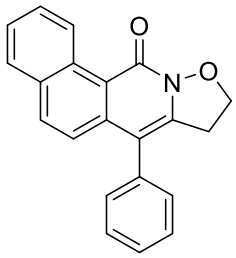
7.29 (m, 2H), 6.66 (s, 1H), 6.01 (s, 2H), 4.54 (t, *J* = 7.6 Hz, 2H), 3.33 (t, *J* = 7.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): *δ* 153.13, 151.56, 147.38, 135.18, 133.47, 131.19, 130.16, 128.91, 128.05, 121.83, 112.66, 105.11, 102.76, 101.82, 69.61, 32.39; **HRMS** (ESI) m/z calcd for $C_{18}H_{13}NNaO_4^+$ $[M+Na]^+$ 330.0742, found 330.0743.

11-phenyl-9,10-dihydro-6H-[1,3]dioxolo[4,5-f]isoxazolo[2,3-b]isoquinolin-6-one (2s').



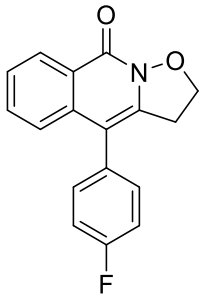
White solid, 25 mg, 41% yield, M.p. = 223-221 °C;
^{1}H NMR (400 MHz, $CDCl_3$): *δ* 8.17 (d, *J* = 8.5 Hz, 1H), 7.45 – 7.37 (m, 3H), 7.35-7.28 (m, 2H), 7.04 (d, *J* = 8.5 Hz, 1H), 5.82 (s, 2H), 4.52 (t, *J* = 7.5 Hz, 2H), 3.30 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): *δ* 153.56, 150.18, 141.94, 136.06, 133.53, 129.99, 127.95, 127.71, 123.13, 121.60, 120.68, 108.94, 108.69, 101.62, 69.51, 32.55.; **HRMS** (ESI) m/z calcd for $C_{18}H_{13}NNaO_4^+$ $[M+Na]^+$ 330.0742, found 330.0742.

7-phenyl-8,9-dihydro-12*H*-benzo[*h*]isoxazolo[2,3-*b*]isoquinolin-12-one (2t).



White solid, 60mg, 95% yield, M.p. = 232-234 °C;
^{1}H NMR (500 MHz, $CDCl_3$): *δ* 10.33 (d, *J* = 8.7 Hz, 1H), 7.86 (d, *J* = 8.8 Hz, 2H), 7.75 (t, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.45 (m, 3H), 7.41 – 7.30 (m, 3H), 4.63 (t, *J* = 7.8 Hz, 2H), 3.46 (t, *J* = 7.7 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): *δ* 154.74, 137.27, 135.58, 133.58, 132.83, 132.19, 131.76, 130.56, 129.00, 128.28, 128.13, 127.90, 127.57, 126.50, 122.64, 119.64, 112.87, 100.00, 69.36, 32.96; **HRMS** (ESI) m/z calcd for $C_{21}H_{15}NNaO_2^+$ $[M+Na]^+$ 336.1000, found 336.1002.

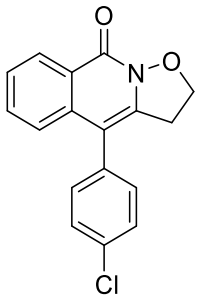
4-(4-fluorophenyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2u).



White solid, 55 mg, 97% yield, M.p. = 218-220 °C;
^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.53 (d, *J* = 8.0 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.49 (t, *J* = 7.5 Hz, 1H),

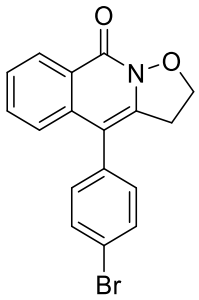
7.37 – 7.28 (m, 3H), 7.21 (m, 2H), 4.58 (t, J = 7.6 Hz, 2H), 3.38 (t, J = 7.6 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 162.51 (d, $^1J_{C,F}$ = 247.9 Hz), 153.93, 136.17, 132.77, 132.05 (d, $^3J_{C,F}$ = 8.1 Hz), 131.75, 130.88 (d, $^4J_{C,F}$ =3.5 Hz), 127.54, 126.42, 126.27, 124.47, 116.04 (d, $^2J_{C,F}$ = 21.5 Hz), 111.94, 69.53, 32.44; **HRMS** (ESI) m/z calcd for $C_{17}H_{12}FNNaO_2^+$ $[M+Na]^+$ 304.0750, found 304.0753.

4-(4-chlorophenyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2v). [7]



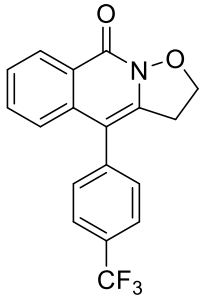
Pale yellow solid, 50 mg, 84% yield, M.p. = 233-235 °C;
^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.51 (d, J = 8.0 Hz, 1H), 7.58-7.52 (m, 1H), 7.50-7.44 (m, 3H), 7.35-7.26 (m, 3H), 4.58 (t, J = 7.6 Hz, 2H), 3.38 (t, J = 7.6 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 153.87, 135.88, 134.18, 133.43, 132.75, 131.77, 131.69, 129.22, 127.52, 126.44, 126.24, 124.39, 111.72, 69.53, 32.43.

4-(4-bromophenyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2w). [7]



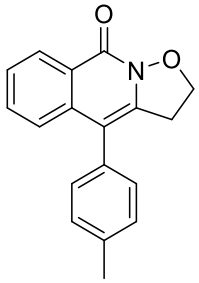
White solid, 57 mg, 83% yield, M.p. =224-226°C;
^{1}H NMR ($CDCl_3$, 400MHz): δ 8.63 – 8.43 (m, 1H), 7.71 – 7.60 (m, 2H), 7.59 – 7.44 (m, 2H), 7.35 – 7.28 (m, 1H), 7.26-7.23 (m, 2H), 4.67 – 4.46 (m, 2H), 3.38 (t, J = 7.5 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 153.89, 135.80, 133.93, 132.70, 132.21, 132.01, 131.81, 127.55, 126.47, 126.25, 124.39, 122.34, 111.75, 69.54, 32.45.

4-(4-(trifluoromethyl)phenyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2x).



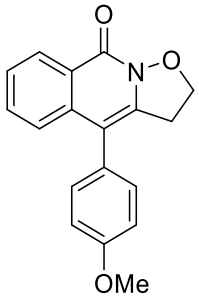
White solid, 53 mg, 80% yield, M.p. = 199-201 °C;
^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.54 (d, J = 8.0 Hz, 1H), 7.78 (d, J = 7.9 Hz, 2H), 7.57 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 7.2 Hz, 3H), 7.30 (d, J = 8.1 Hz, 1H), 4.59 (t, J = 7.5 Hz, 2H), 3.39 (t, J = 7.5 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 153.86, 138.87, 135.54, 132.88, 131.87, 130.77, 130.33 (q, $^1J_{C,F}$ = 32.5 Hz), 127.62, 126.56, 126.26, 125.90, 124.20, 123.94 (q, $^1J_{C,F}$ = 271.3 Hz), 111.49, 69.47, 32.42; **HRMS** (ESI) m/z calcd for $C_{18}H_{12}F_3NNaO_2^+$ $[M+Na]^+$ 354.0718, found 354.0718.

4-(p-tolyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2y). [7]



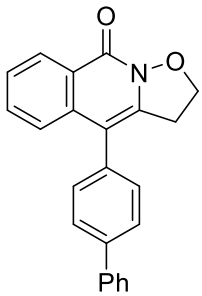
Pale yellow solid, 46 mg, 83% yield, M.p. = 195-197 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.52 (d, J = 8.0 Hz, 1H), 7.55-7.51 (m, 1H), 7.46 (t, J = 7.2 Hz, 1H), 7.38 (d, J = 8.1 Hz, 1H), 7.30 (d, J = 7.9 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 4.56 (t, J = 7.6 Hz, 2H), 3.39 (t, J = 7.6 Hz, 2H), 2.44 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.91, 137.87, 136.34, 132.44, 131.93, 131.53, 130.13, 129.59, 127.40, 126.29, 126.20, 124.76, 112.99, 69.54, 32.44,21.27;

4-(4-methoxyphenyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2z). [7]



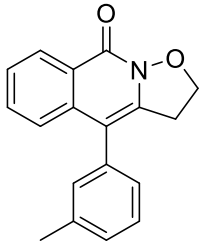
Pale yellow solid, 42 mg, 72% yield, M.p. =238-240°C;
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.54 (d, J = 8.0 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.52 – 7.45 (m, 1H), 7.39 (d, J = 7.9 Hz, 1H), 7.29-7.24 (m, 3H), 7.06 – 6.99 (m, 2H), 4.57 (t, J = 7.6 Hz, 2H), 3.89 (s, 3H), 3.39 (t, J = 7.6 Hz, 2H); **^{13}C NMR** ($CDCl_3$, 125 MHz): δ 159.37, 153.96, 136.54, 132.53, 131.58, 131.42, 127.47, 127.08, 126.29, 124.75, 114.34, 112.72, 69.55, 55.38, 32.46.

4-([1,1'-biphenyl]-4-yl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2aa).



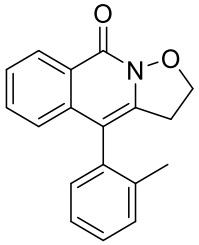
White solid, 57 mg, 84% yield, M.p. = 146-148 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.54 (d, J = 8.1 Hz, 1H), 7.72 (d, J = 8.2 Hz, 2H), 7.67 (d, J = 8.5 Hz, 2H), 7.60 – 7.53 (m, 1H), 7.51 – 7.46 (m, 4H), 7.44-7.37 (m, 3H), 4.58 (t, J = 7.6 Hz, 2H), 3.44 (t, J = 7.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.95, 140.91, 140.38, 136.16, 133.92, 132.65, 131.69, 130.75, 128.95, 127.68, 127.58, 127.48, 127.08, 126.35, 126.31, 124.75, 112.68, 69.63, 32.55; **HRMS** (ESI) m/z calcd for $C_{23}H_{17}NNaO_2^+$ $[M+Na]^+$ 362.1157, found 362.1156.

4-(*m*-tolyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2ab).



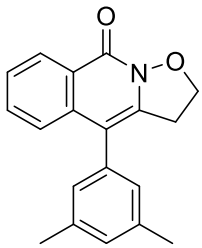
Pale yellow solid, 39 mg, 70% yield, M.p. = 189-191 °C;
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.53 (d, J = 8.1 Hz, 1H), 7.59 – 7.51 (m, 1H), 7.52 – 7.43 (m, 1H), 7.39 (t, J = 7.7 Hz, 2H), 7.27 (s, 1H), 7.14 (d, J = 11.7 Hz, 2H), 4.57 (t, J = 7.6 Hz, 2H), 3.39 (t, J = 7.6 Hz, 2H), 2.43 (s, 3H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 153.95, 138.63, 136.27, 134.91, 132.40, 131.59, 130.90, 128.84, 128.80, 127.42, 127.33, 126.26, 124.81, 113.20, 69.58, 32.46, 21.47; **HRMS** (ESI) m/z calcd for $C_{18}H_{15}NNaO_2^+$ $[M+Na]^+$ 300.1000, found 300.1003.

4-(*o*-tolyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2ac). [7]



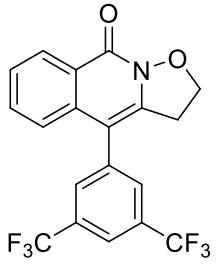
Pale yellow solid, 52 mg, 93% yield, M.p. = 140-142 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.52 (dd, J = 8.0, 1.4 Hz, 1H), 7.54 – 7.42 (m, 2H), 7.39-7.34 (m ,2H), 7.31-7.28 (m, 1H), 7.19 (d, J = 7.3 Hz, 1H), 7.05 (d, J = 7.8 Hz, 1H), 4.57 (t, J = 7.7 Hz, 2H), 3.37 –3.12 (m, 2H), 2.06 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 154.00, 137.59, 136.08, 134.05, 132.35, 131.69, 130.58, 130.46, 128.60, 127.40, 126.41, 126.24, 126.16, 124.50, 112.21, 69.45, 32.12, 19.63.

4-(3,5-dimethylphenyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2ad). [7]



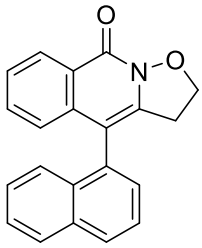
Pale yellow solid, 43 mg, 74% yield, M.p. =249-251 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.53 (d, J = 7.9 Hz, 1H), 7.54 (t, J = 7.1 Hz, 1H), 7.47 (t, J = 7.3 Hz, 1H), 7.38 (d, J = 8.1 Hz, 1H), 7.08 (s, 1H), 6.95 (s, 2H), 4.57 (t, J = 7.6 Hz, 2H), 3.40 (t, J = 7.6 Hz, 2H), 2.38 (s, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.94, 138.47, 136.35, 134.82, 132.28, 131.54, 129.69, 127.97, 127.37, 126.24, 126.20, 124.89, 113.34, 69.58, 32.46, 21.35.

4-(3,5-bis(trifluoromethyl)phenyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2ae).



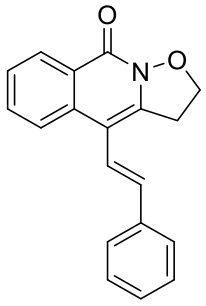
White solid, 41 mg, 51% yield, M.p. = 238-240 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.54 (d, J = 8.8 Hz, 1H), 7.99 (s, 1H), 7.87 (s, 2H), 7.62-7.58 (m, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.19 (d, J = 8.1 Hz, 1H), 4.62 (t, J = 7.6 Hz, 2H), 3.41 (t, J = 7.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.82, 137.43, 135.09, 133.63, 132.53 (q, $^2J_{C,F}$ = 32.5 Hz) ,132.27, 130.58, 127.87,126.88, 126.25, 123.58, 123.02 (d, $^1J_{C,F}$ = 272.3 Hz), 109.95, 109.78, 69.41, 32.44; **HRMS** (ESI) m/z calcd for $C_{19}H_{11}F_6NNaO_2^+$ $[M+Na]^+$ 422.0592, found 422.0588.

4-(naphthalen-1-yl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2af). [7]



Pale yellow solid; 47 mg, 75% yield, M.p. = 222-224 °C;
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.58 (dd, J = 7.9, 1.3 Hz, 1H), 7.97 (t, J = 7.8 Hz, 2H), 7.62-7.58 (m, 1H), 7.56 – 7.34 (m, 6H), 7.07 – 6.95 (m, 1H), 4.62-4.50 (m, 2H), 3.34-3.26 (m, 1H), 3.14-3.06 (m, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 154.17, 136.86, 133.96, 133.50, 132.41, 132.28, 131.74, 129.00, 128.70, 128.66, 127.41, 126.80, 126.37, 126.32, 126.19, 125.73, 125.26, 125.10, 110.85, 69.55, 32.26..

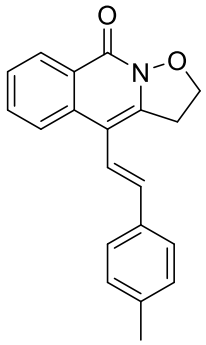
(*E*)-4-styryl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2ag).



White solid, 45 mg, 78% yield, M.p. = 206-208°C;

^{1}H NMR (500 MHz $CDCl_3$): δ 8.52 (d, J = 7.3 Hz, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.54-7.47 (m, 3H), 7.41 (t, J = 7.6 Hz, 2H), 7.33 (t, J = 7.4 Hz, 1H), 7.22 (d, J = 16.3 Hz, 1H), 6.76 (d, J = 16.3 Hz, 1H), 4.60 (t, J = 7.5 Hz, 2H), 3.69 (t, J = 7.5 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.89, 136.81, 135.39, 134.10, 132.37, 131.83, 128.88, 128.21, 127.71, 126.56, 126.39, 126.20, 123.52, 121.45, 109.31, 69.97, 32.20; **HRMS** (ESI) m/z calcd for $C_{19}H_{15}NNaO_2^+$ $[M+Na]^+$ 312.1000, found 312.1004.

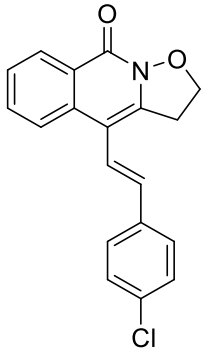
(*E*)-4-(4-methylstyryl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2ah).



White solid, 42 mg, 69% yield, M.p. = 210-212°C;

^{1}H NMR (500 MHz $CDCl_3$): δ 8.51 (d, J = 8.1 Hz, 2H), 7.82 (d, J = 8.2 Hz, 1H), 7.66 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 7.6 Hz, 1H), 7.42 (d, J = 7.7 Hz, 2H), 7.21 (d, J = 7.8 Hz, 2H), 7.17 (d, J = 16.2 Hz, 1H), 6.73 (d, J = 16.2 Hz, 1H), 4.59 (t, J = 7.4 Hz, 2H), 3.68 (t, J = 7.5 Hz, 2H), 2.39 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.87, 138.23, 135.45, 134.07, 132.19, 131.78, 129.56, 127.68, 126.51, 126.30, 126.20, 123.55, 120.39, 109.51, 69.45, 33.02, 21.28; **HRMS** (ESI) m/z calcd for $C_{20}H_{17}NNaO_2^+$ $[M+Na]^+$ 326.1157, found 326.1164.

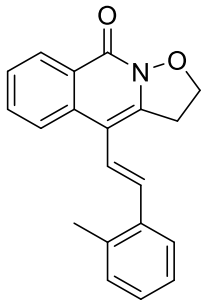
(*E*)-4-(4-chlorostyryl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2ai).



White solid, 38 mg, 59% yield, M.p. = 202-204°C;

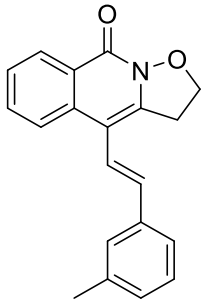
^{1}H NMR (500 MHz $CDCl_3$): δ 8.49 (d, J = 8.0 Hz, 1H), 7.78 (d, J = 8.2 Hz, 1H), 7.65 (t, J = 7.6 Hz, 1H), 7.50 (t, J = 7.5 Hz, 1H), 7.44 (d, J = 8.1 Hz, 2H), 7.36 (d, J = 8.2 Hz, 2H), 7.18 (d, J = 16.2 Hz, 1H), 6.70 (d, J = 16.2 Hz, 1H), 4.59 (t, J = 7.3 Hz, 2H), 3.67 (t, J = 7.5 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.79, 135.27, 135.18, 133.78, 132.62, 132.49, 131.82, 128.97, 127.67, 127.49, 126.55, 126.13, 123.36, 122.02, 108.92, 69.37, 33.02; **HRMS** (ESI) m/z calcd for $C_{19}H_{14}ClNNaO_2^+$ $[M+Na]^+$ 346.0611, found 346.0612.

(*E*)-4-(2-methylstyryl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2aj).



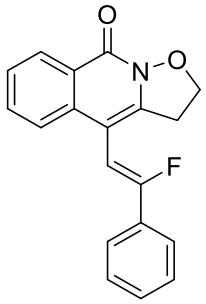
White solid, 38 mg, 62% yield, M.p. = 222-224°C;
^{1}H NMR (500 MHz $CDCl_3$): δ 8.51 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.69 – 7.61 (m, 2H), 7.50 (t, J = 7.5 Hz, 1H), 7.30-7.20 (m, 3H), 7.09 (d, J = 16.1 Hz, 1H), 6.99 (d, J = 16.1 Hz, 1H), 4.60 (t, J = 7.4 Hz, 2H), 3.69 (t, J = 7.5 Hz, 2H), 2.41 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.86, 136.05, 135.64, 135.41, 132.34, 132.18, 131.81, 130.57, 127.67, 126.52, 126.41, 126.19, 125.44, 123.50, 122.75; **HRMS** (ESI) m/z calcd for $C_{20}H_{17}NNaO_2^+$ $[M+Na]^+$ 326.1157, found 326.1163.

(*E*)-4-(3-methylstyryl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2ak).



White solid, 39 mg, 65% yield, M.p. = 228-230°C;
^{1}H NMR (500 MHz $CDCl_3$): δ 8.50 (d, J = 8.1 Hz, 1H), 7.80 (d, J = 8.2 Hz, 1H), 7.68 – 7.61 (m, 1H), 7.53 – 7.46 (m, 1H), 7.36 – 7.27 (m, 3H), 7.22 – 7.12 (m, 2H), 6.72 (d, J = 16.3 Hz, 1H), 4.58 (t, J = 7.5 Hz, 2H), 3.66 (t, J = 7.5 Hz, 2H), 2.40 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.86, 136.05, 135.64, 135.41, 132.34, 132.18, 131.82, 130.57, 128.12, 127.67, 126.52, 126.41, 126.19, 125.44, 123.50, 122.75, 109.65, 69.43, 33.08, 19.99; **HRMS** (ESI) m/z calcd for $C_{20}H_{17}NNaO_2^+$ $[M+Na]^+$ 326.1157, found 326.1160.

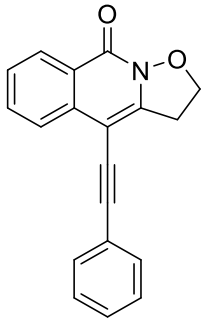
(*Z*)-4-(2-fluoro-2-phenylvinyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2al).



White solid, 36 mg, 58% yield, M.p. = 200-202°C;
^{1}H NMR (500 MHz $CDCl_3$): δ 8.51 (d, J = 8.1 Hz, 1H), 7.76 – 7.60 (m, 4H), 7.55 – 7.39 (m, 4H), 6.48

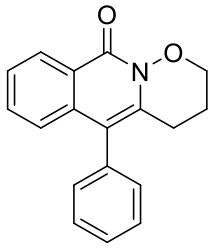
(d, J = 37.1 Hz, 1H), 4.61 (t, J = 7.6 Hz, 2H), 3.55 (t, J = 7.6 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 157.88 (d, $^1J_{C,F}$ = 255.5 Hz) , 153.99, 135.47, 134.02, 131.75, 131.51, 129.73, 128.76, 127.62, 126.43, 125.99, 124.54 (d, $^3J_{C,F}$ = 7.2 Hz), 123.57, 103.50, 98.27 (d,$^2J_{C,F}$ = 15.6 Hz), 69.57, 33.10; **HRMS** (ESI) m/z calcd for $C_{19}H_{14}FNNaO_2$ $[M+Na]^+$ 330.0906, found 330.0914.

4-(phenylethynyl)-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2am).



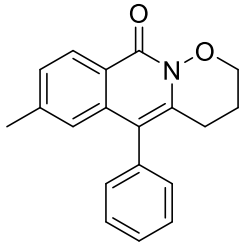
White solid, 41 mg, 72% yield, M.p. = 158-160°C;
^{1}H NMR (500 MHz $CDCl_3$): δ 8.48 (d, J = 9.6 Hz, 1H), 8.03 (d, J = 8.1 Hz, 1H), 7.73 (t, J = 7.6 Hz, 1H), 7.63 – 7.57 (m, 2H), 7.54 (t, J = 7.6 Hz, 1H), 7.47 – 7.37 (m, 3H), 4.68 (t, J = 7.8 Hz, 2H), 3.78 (t, J = 7.8 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.78, 138.68, 135.38, 132.24, 131.42, 128.63, 128.54, 127.42, 126.90, 125.55, 124.76, 122.84, 96.07, 95.19, 82.13, 69.46, 33.21; **HRMS** (ESI) m/z calcd for $C_{19}H_{13}NNaO_2^+$ $[M+Na]^+$ 310.0844, found 310.0850.

5-phenyl-3,4-dihydro-[1,2]oxazino[2,3-*b*]isoquinolin-10(2*H*)-one (2an). [7]



White solid, 47 mg, 85% yield, M.p. = 190-192°C;
^{1}H NMR (500 MHz $CDCl_3$): δ 8.52 (d, J = 9.5 Hz, 1H), 7.54-7.45 (m, 3H), 7.46 – 7.40 (m, 2H), 7.27 (t, J = 6.4 Hz, 2H), 7.16 (d, J = 8.1 Hz, 1H), 4.43 (t, J = 6.9 Hz , 2H), 2.70 (t, J = 6.9 Hz, 2H), 2.10-2.02 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 138.38, 136.11, 135.05, 131.06, 128.80, 127.90, 127.75, 125.91, 125.51, 125.00, 70.82, 21.77, 21.36.

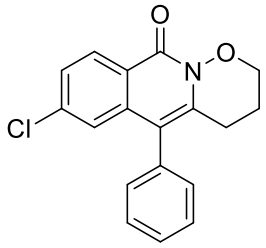
7-methyl-5-phenyl-3,4-dihydro-[1,2]oxazino[2,3-*b*]isoquinolin-10(2*H*)-one (2ao). [7]



White solid, 51mg, 87% yield, M.p. = 198-200°C;

^{1}H NMR (500 MHz $CDCl_3$): δ 8.41 (d, J = 8.2 Hz, 1H), 7.50 (t, J = 7.2 Hz, 2H), 7.45 (t, J = 7.3 Hz, 1H), 7.27 (t, J = 7.3 Hz, 3H), 6.91 (s, 1H), 4.46 – 4.37 (m, 2H), 2.67 (t, J = 6.9 Hz, 2H), 2.33 (s, 3H), 2.08-2.01 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 156.53, 138.38, 136.11, 135.05, 131.87, 131.06, 128.80, 127.90, 127.75, 125.91, 125.51, 125.00, 115.22, 70.82, 21.77, 21.36.

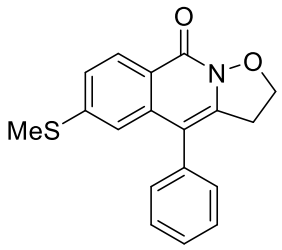
7-chloro-5-phenyl-3,4-dihydro-[1,2]oxazino[2,3-*b*]isoquinolin-10(2*H*)-one (2ap). [7]



Pale yellow solid; 51 mg, 82% yield, M.p. = 168-170°C;

^{1}H NMR (500 MHz $CDCl_3$): δ 8.45 (d, J = 8.6 Hz, 1H), 7.56 – 7.44 (m, 3H), 7.38 (dd, J = 8.7, 2.0 Hz, 1H), 7.29-7.24 (m, 2H), 7.12 (d, J = 2.1 Hz, 1H), 4.44 (t, J = 6.9 Hz, 2H), 2.70 (t, J = 6.9 Hz, 2H), 2.11-2.04 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 157.78, 139.90, 138.63, 137.42, 134.32, 130.94, 129.57, 129.03, 128.22, 126.48, 124.32, 123.81, 114.52, 70.85, 21.62, 21.49.

6-(methylthio)-4-phenyl-2,3-dihydro-9*H*-isoxazolo[2,3-*b*]isoquinolin-9-one (2aq).



White solid, 54 mg, 87% yield, M.p. = 199-201°C;

^{1}H NMR (500 MHz $CDCl_3$): δ 8.41 (d, J = 8.1 Hz, 1H), 7.53-7.49 (m, 2H), 7.47-7.43 (m, 1H), 7.36-7.29 (m, 3H), 7.11 (s, 1H), 4.56 (t, J = 7.8 Hz, 2H), 3.37 (t, J = 7.6 Hz, 2H), 2.39 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 153.79, 144.08, 136.57, 134.76, 133.38, 130.26, 128.98, 128.20, 127.71, 123.93, 123.12, 120.13, 112.26, 69.53, 32.54, 14.85. **HRMS** (ESI) m/z calcd for $C_{18}H_{15}NNaO_2S^+$ $[M+Na]^+$ 332.0721, found 332.0721.

References

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Computational Details

The B3LYP functional was used for all calculations, which were carried out with the Gaussian 09

program[1]. Basis set 6-31G(d) was used for geometry optimizations and frequency calculations.[2,3,4] Geometric structures of all species in this work were optimized in solvation with the SMD solvent model at T = 298.15 K and 1 atm pressure. The harmonic vibrational frequencies and the number of imaginary frequencies determine the nature of all intermediates (no imaginary frequency) and transition state structures (only one imaginary frequency). The latter were also confirmed to connect appropriate intermediates, reactants, or products by intrinsic reaction coordinate (IRC) calculations.[5,6] The energy were refined with bigger basis set 6-311++G(d,p). The same methodology has been widely used in previous works.[7]

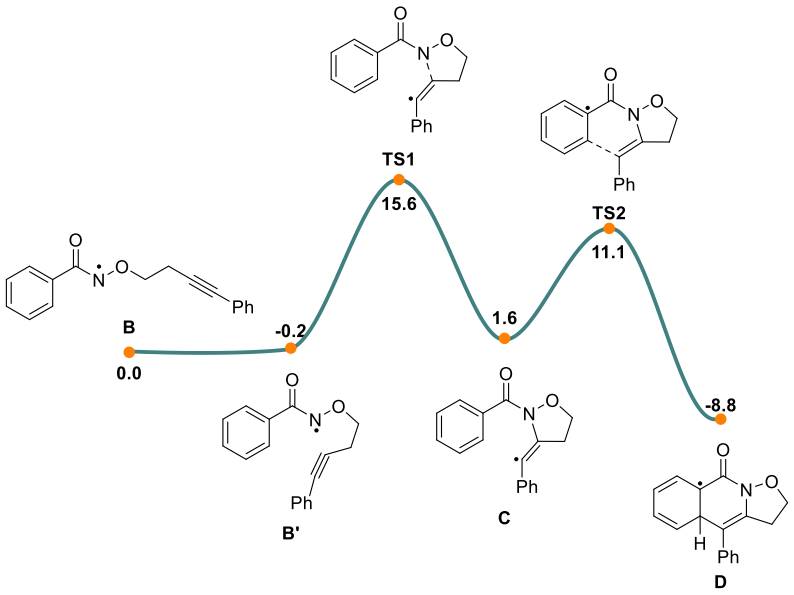

Figure S1. Computed free energy profile (in kcal mol^{-1}) of this react

Cartesian Coordinates of all the intermediate and transition states

B

C	-4.37912500	-0.54076300	-0.99468800
C	-3.12036900	-0.65746700	-0.40638800
C	-2.61982700	0.38445600	0.39525400
C	-3.39734200	1.53812700	0.59519400
C	-4.65342300	1.64913500	0.00641400
C	-5.14682100	0.60914700	-0.78995300
H	-4.76092000	-1.34795800	-1.61363500
H	-2.52731500	-1.55045600	-0.56767100
H	-3.00389700	2.33782500	1.21469000
H	-5.24931800	2.54349900	0.16614800
H	-6.12757800	0.69606300	-1.25006900
C	-1.28646700	0.32052000	1.04722100
O	-0.82161200	1.23296400	1.73168900
N	-0.60697100	-0.89380900	0.80449500
O	0.57751400	-0.85228600	1.42284100
C	1.32078800	-2.08346600	1.21902900
C	2.68481500	-1.87285800	1.87725800
H	1.40693900	-2.26040500	0.14401900
H	0.76289500	-2.90021000	1.68459900
H	3.17646500	-1.00697600	1.41532500
H	2.53958200	-1.63429200	2.93874800
C	3.52284500	-3.06290800	1.73815800
C	4.20464400	-4.05918900	1.61328400
C	5.01117900	-5.23276700	1.46853100
C	5.09491400	-6.17640100	2.51235000
C	5.73134800	-5.46277800	0.27881200
C	5.87813100	-7.31990200	2.36465700
H	4.54242300	-6.00477400	3.43159800
C	6.51228700	-6.60894000	0.14058100
H	5.67170000	-4.73868700	-0.52859900
C	6.58804700	-7.54040300	1.18051000
H	5.93368300	-8.04109300	3.17583800
H	7.06287600	-6.77556000	-0.78153600
H	7.19706900	-8.43342900	1.06843100

B'

C	-4.15906700	0.65813900	-1.31089200
C	-3.00924600	0.21495600	-0.65856200

C	-2.96912100	0.17405000	0.74689700
C	-4.09522500	0.58174100	1.48242300
C	-5.24030200	1.02425200	0.82642300
C	-5.27421700	1.06351800	-0.57225100
H	-4.18458200	0.68661000	-2.39674700
H	-2.14672900	-0.10023500	-1.23446900
H	-4.05793400	0.54677900	2.56659400
H	-6.10698300	1.33811700	1.40172100
H	-6.16854000	1.40890600	-1.08416900
C	-1.77308800	-0.29107900	1.49761500
O	-1.72468600	-0.34921700	2.72799800
N	-0.70067300	-0.65207500	0.65631400
O	0.32556200	-1.06289300	1.41413200
C	1.43496300	-1.52828100	0.60976800
C	1.35958500	-3.04801000	0.40915700
H	2.32316900	-1.27585300	1.19267800
H	1.43385600	-0.98545100	-0.33710500
H	2.30520500	-3.34889200	-0.06254400
H	1.33063300	-3.53371800	1.39289000
C	0.23013000	-3.49100300	-0.40590700
C	-0.70635700	-3.86531900	-1.08257500
C	-1.80747900	-4.31089400	-1.88007000
C	-2.91684800	-4.94009500	-1.27917500
C	-1.79904300	-4.12792100	-3.27796300
C	-3.98659000	-5.37424000	-2.05993900
H	-2.92943300	-5.08381000	-0.20270100
C	-2.87392300	-4.56468200	-4.05023500
H	-0.94762600	-3.64334800	-3.74695000
C	-3.96947800	-5.18851400	-3.44567500
H	-4.83596700	-5.85834400	-1.58526500
H	-2.85638800	-4.41731800	-5.12688300
H	-4.80570300	-5.52776100	-4.05123400

TS1

C	-3.65675500	0.19634000	-1.76181200
C	-2.53911900	-0.02993700	-0.95764900
C	-2.70107100	-0.35575700	0.39902100
C	-3.99558500	-0.44501200	0.93641700
C	-5.10934800	-0.22494100	0.12930500
C	-4.94191600	0.09724300	-1.22177900
H	-3.52360800	0.45606400	-2.80853600
H	-1.54154600	0.06280200	-1.37291100

H	-4.11515100	-0.69046500	1.98723100
H	-6.10762700	-0.30238700	0.55158300
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C	-1.54322700	-0.57453200	1.31190200
O	-1.64780400	-0.49225400	2.54035900
N	-0.33346300	-0.79891500	0.64896600
O	0.69067600	-0.89955400	1.58966600
C	1.78284100	-1.48553500	0.88439100
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C	-2.19014700	-3.59301800	-1.50761000
C	-3.18448200	-4.37086300	-0.85792900
C	-2.32571500	-3.32810500	-2.89612800
C	-4.27012000	-4.85775100	-1.57547100
H	-3.08553800	-4.57761900	0.20333000
C	-3.41505100	-3.82633800	-3.59960000
H	-1.56735400	-2.73545100	-3.39854300
C	-4.39034600	-4.59051800	-2.94543000
H	-5.02750400	-5.44967800	-1.06900600
H	-3.50907300	-3.61947100	-4.66211600
H	-5.24056500	-4.97632800	-3.50101600

C

C	-3.74142700	0.39170900	-1.67105400
C	-2.58200000	0.14612900	-0.93488900
C	-2.66656100	-0.09770300	0.44461600
C	-3.91674400	-0.07829100	1.07976300
C	-5.07472000	0.14672900	0.33604200
C	-4.98842100	0.38339100	-1.03921800
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H	-6.04241300	0.14526400	0.83018700
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C	-1.44715800	-0.25284100	1.29435900
O	-1.31270600	0.35473200	2.35893800
N	-0.44712400	-1.06024800	0.80195000

O	0.71357300	-1.08745900	1.62231500
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C	0.86759900	-2.93118200	0.19376800
H	2.45138200	-2.13923500	1.52356000
H	2.11063200	-1.13627100	0.07421200
H	1.27752700	-3.27259700	-0.75931800
H	0.78426500	-3.78823300	0.87056000
C	-0.50250500	-2.27512300	0.02458400
C	-1.52294400	-2.71937800	-0.65956400
C	-2.27948900	-3.53393800	-1.49278900
C	-3.08957100	-4.58336500	-0.95739300
C	-2.31316100	-3.31866100	-2.90578400
C	-3.86538100	-5.37362500	-1.79305000
H	-3.08353600	-4.75516800	0.11502300
C	-3.09606400	-4.12060700	-3.72381000
H	-1.71073300	-2.52067100	-3.32971600
C	-3.87609800	-5.15154600	-3.17847400
H	-4.46923000	-6.17117800	-1.36760800
H	-3.10297800	-3.94594200	-4.79674400
H	-4.48770800	-5.77372300	-3.82589800

TS2

C	-4.40141800	-0.99802100	-0.45742100
C	-3.27300500	-1.02424700	0.40809800
C	-2.46107600	0.14926500	0.49006400
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C	-4.64390000	0.10155500	-1.26687500
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H	-4.01782500	2.09841100	-1.82835600
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C	-4.15715000	-0.95209500	-0.89520300
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C	-2.88521700	1.42387100	-0.01430700
C	-4.00797600	1.47544600	-0.85088300
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H	-3.50096900	-1.45868400	1.02440400
H	-2.39390000	2.34246800	0.29458800
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C	0.39423200	-2.99157000	0.54661300
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H	1.83356700	-1.35928300	0.31227500
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H	-2.88328000	-3.82245400	-4.50841700
H	-2.79693400	-6.19472500	-3.75623500

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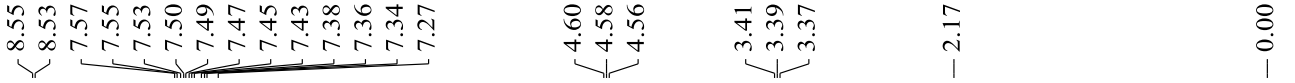
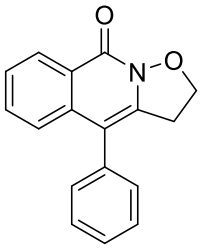
^{1}H NMR and ^{13}C NMR spectra of 2.





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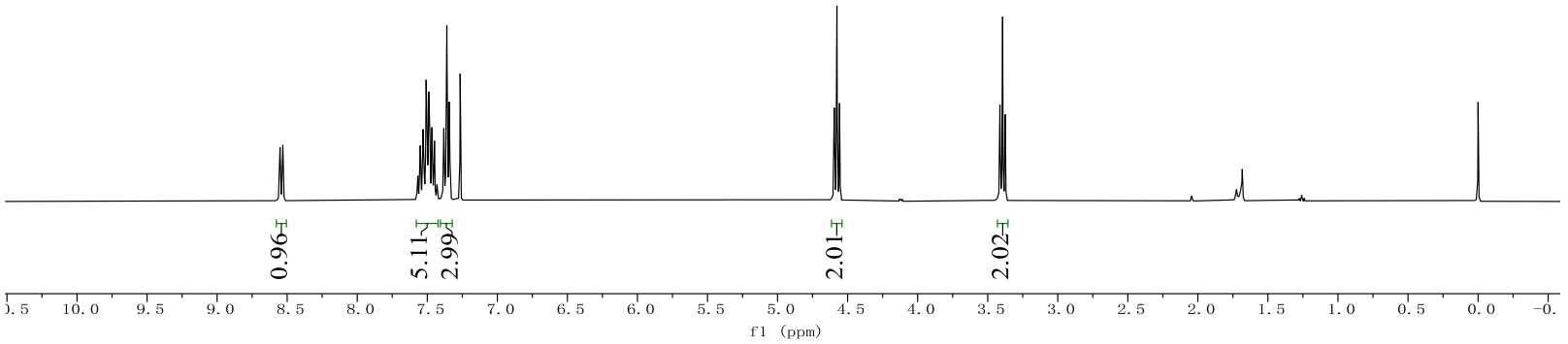

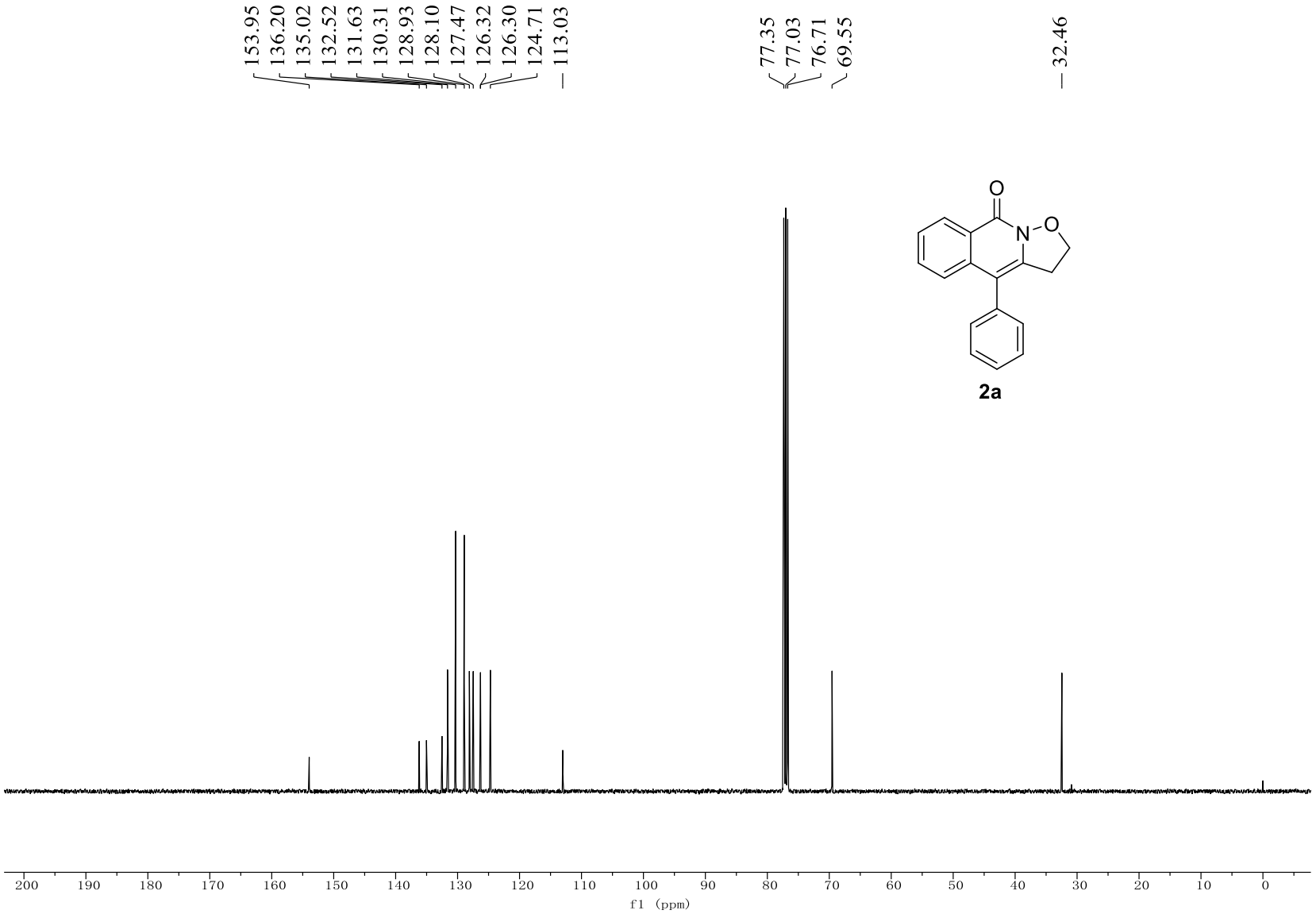
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76.71
69.55
32.46
O
N
O
2a
200
190
180
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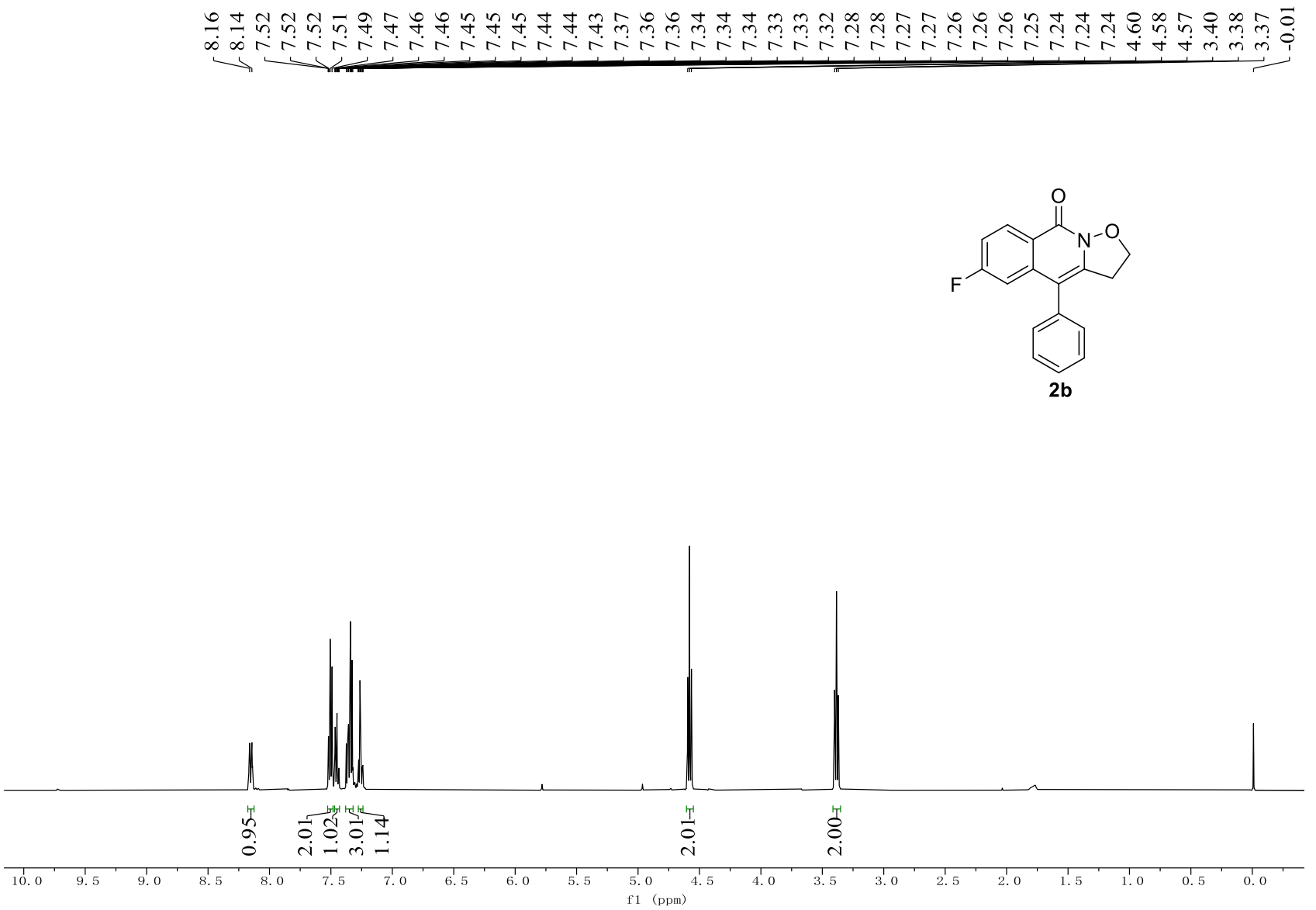
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7.28
7.27
7.27
7.26
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7.24
7.24
7.24
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4.58
4.57
3.40
3.38
3.37
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N
O
F
2b
0.95
2.01
1.02
3.01
1.14
2.01
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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6.0
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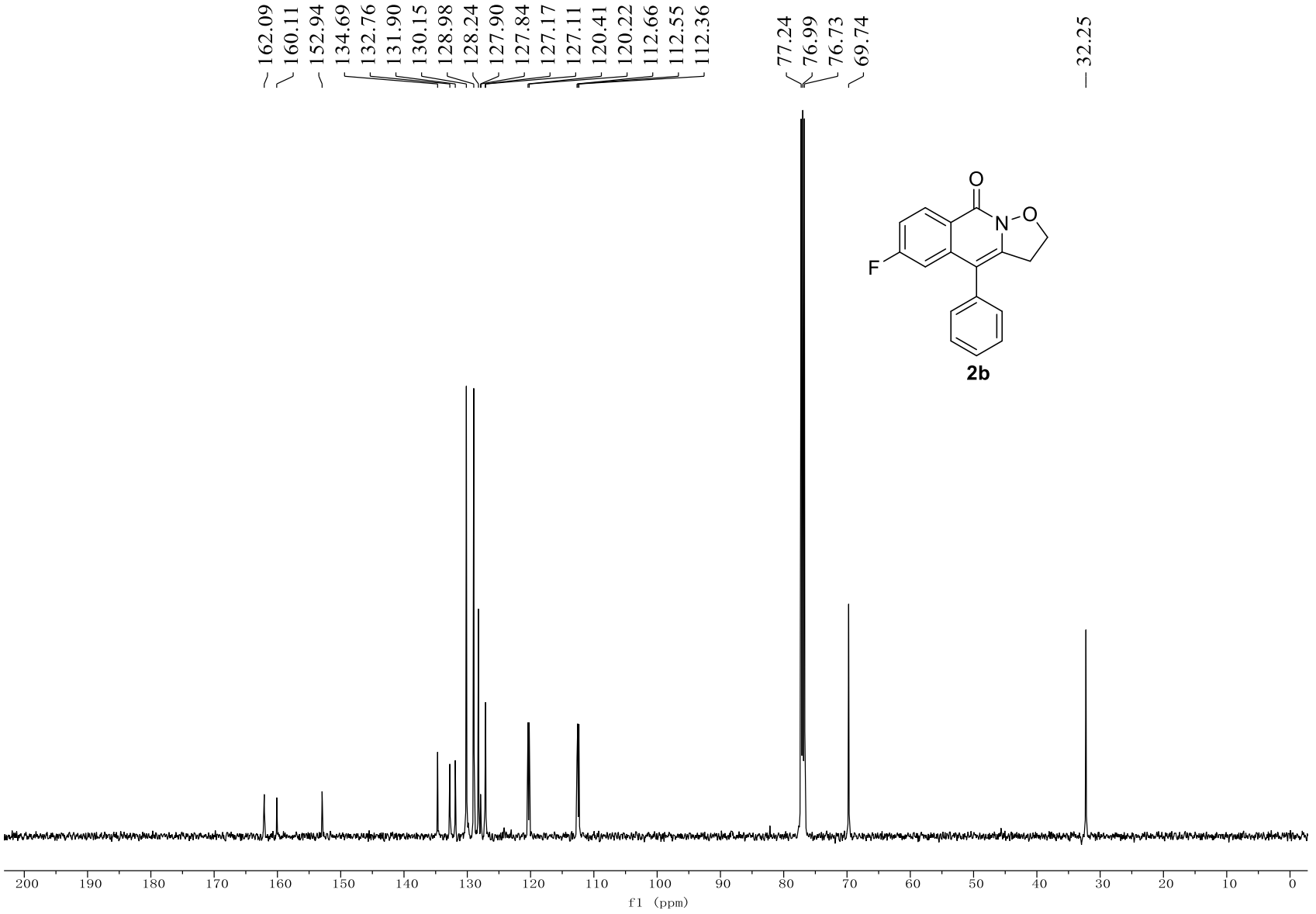
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127.11
120.41
120.22
112.66
112.55
112.36
77.24
76.99
76.73
69.74
32.25
O
N
O
F
2b
200
190
180
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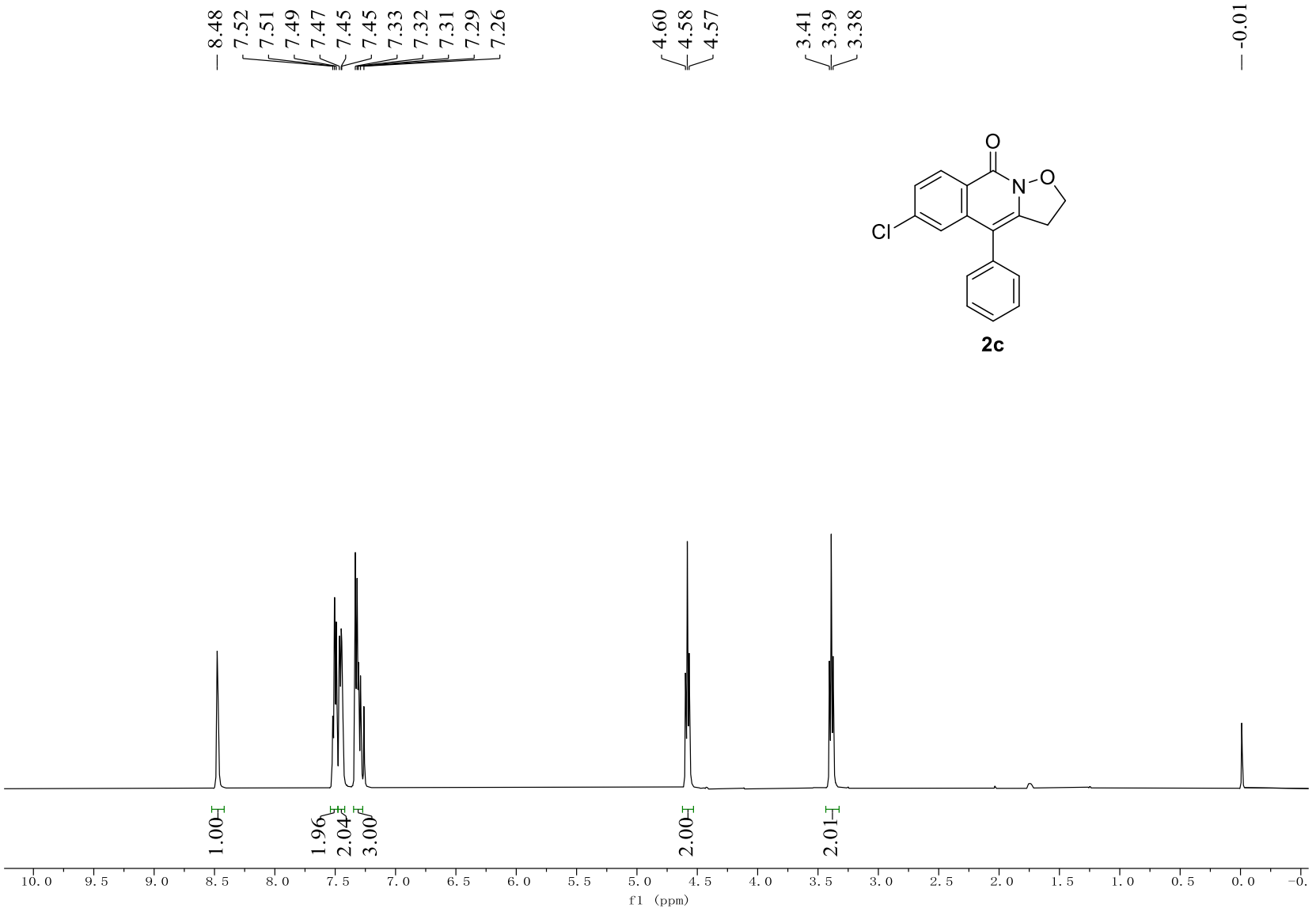
f1 (ppm)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4.58
4.57
3.41
3.39
3.38
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N
O
Cl
2c
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1.96
2.04
3.00
2.00
2.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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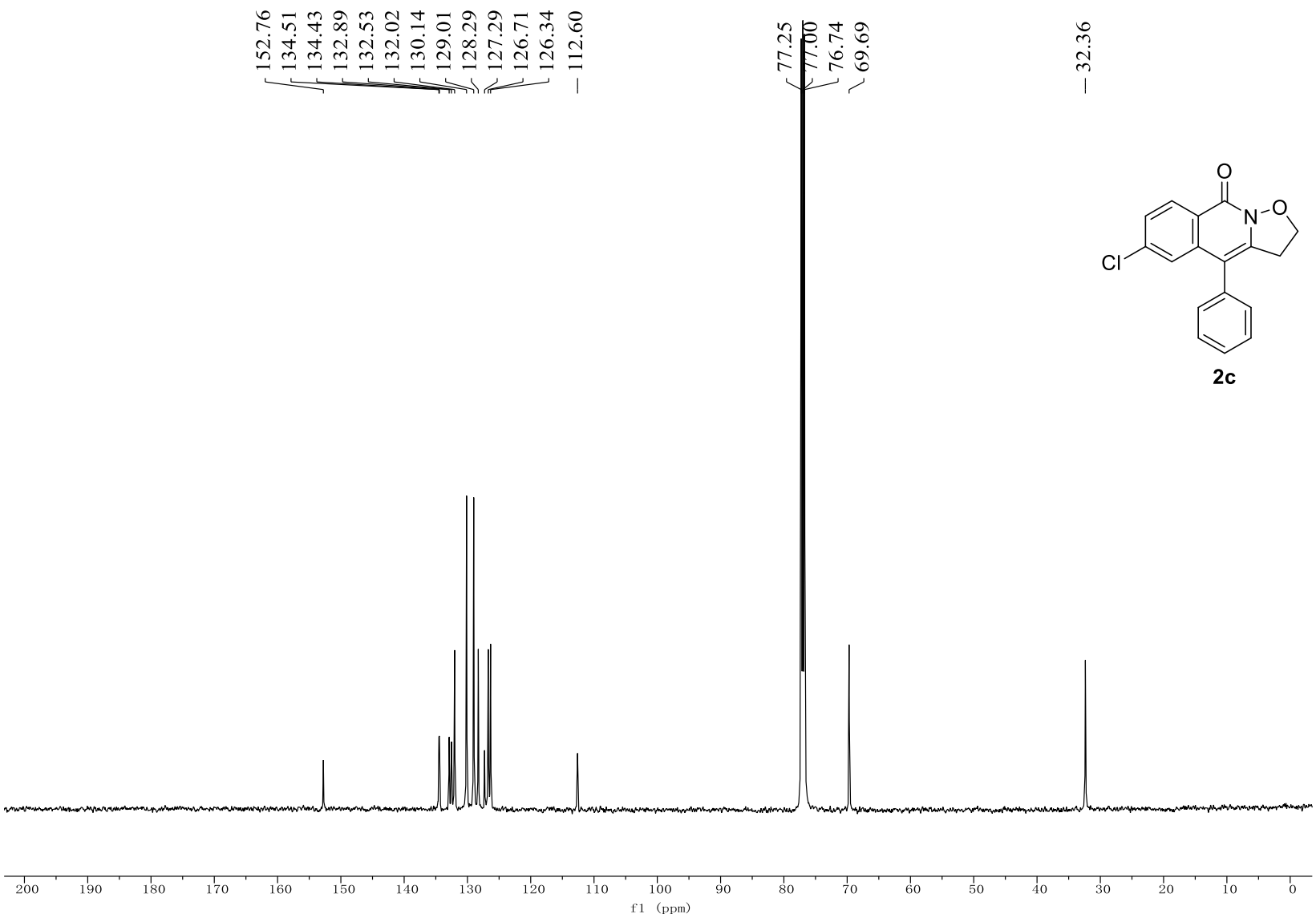
f1 (ppm)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112.60
77.25
77.00
76.74
69.69
32.36
O
N
O
Cl
2c
200
190
180
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150
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130
120
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100
90
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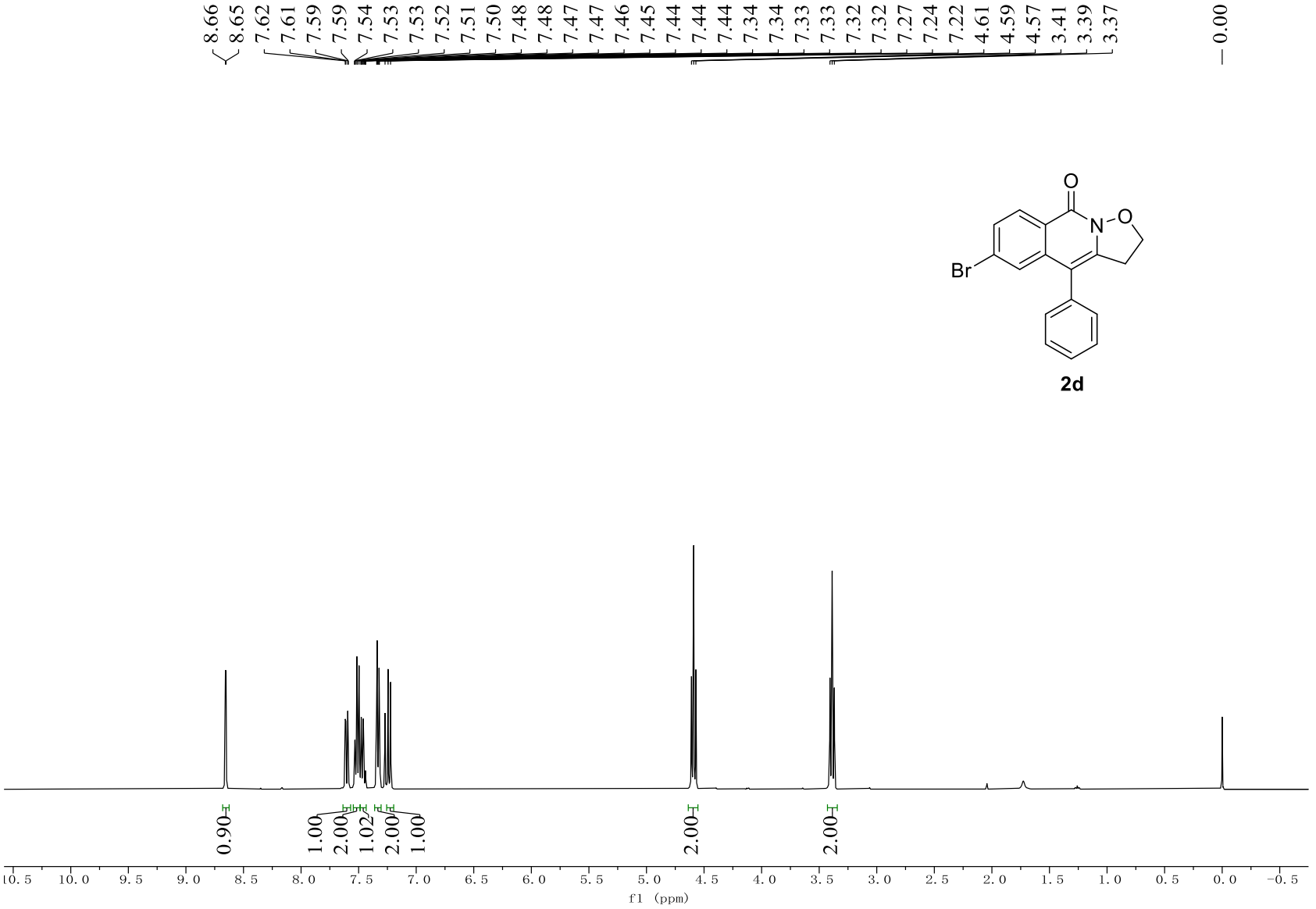
70
60
50
40
30
20
10
0
f1 (ppm)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7.48
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7.47
7.47
7.46
7.45
7.44
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7.34
7.33
7.33
7.32
7.32
7.27
7.24
7.22
4.61
4.59
4.57
3.41
3.39
3.37
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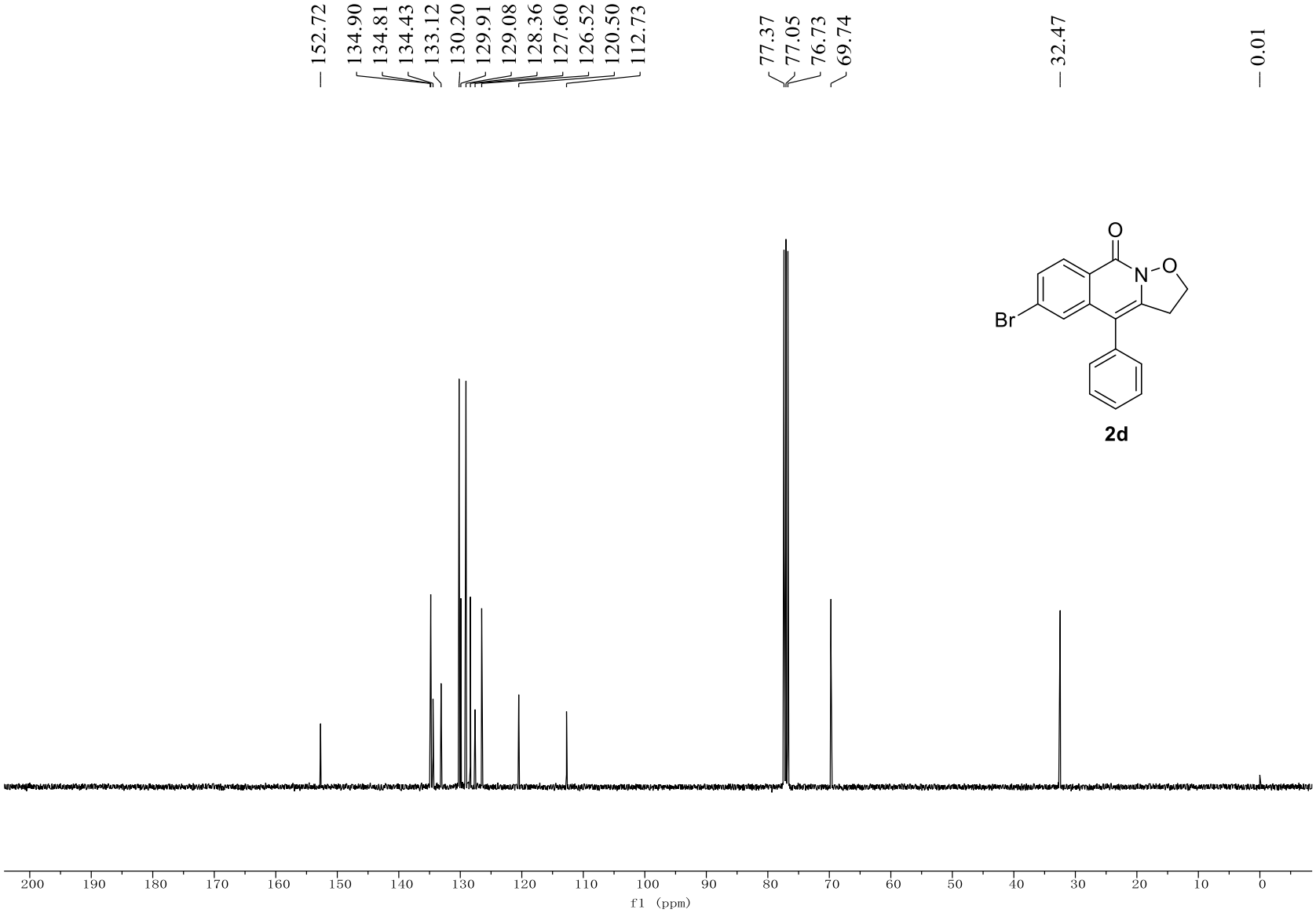
2.00
f1 (ppm)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76.73
69.74
32.47
0.01
O
N
O
Br
2d
200
190
180
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50
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10
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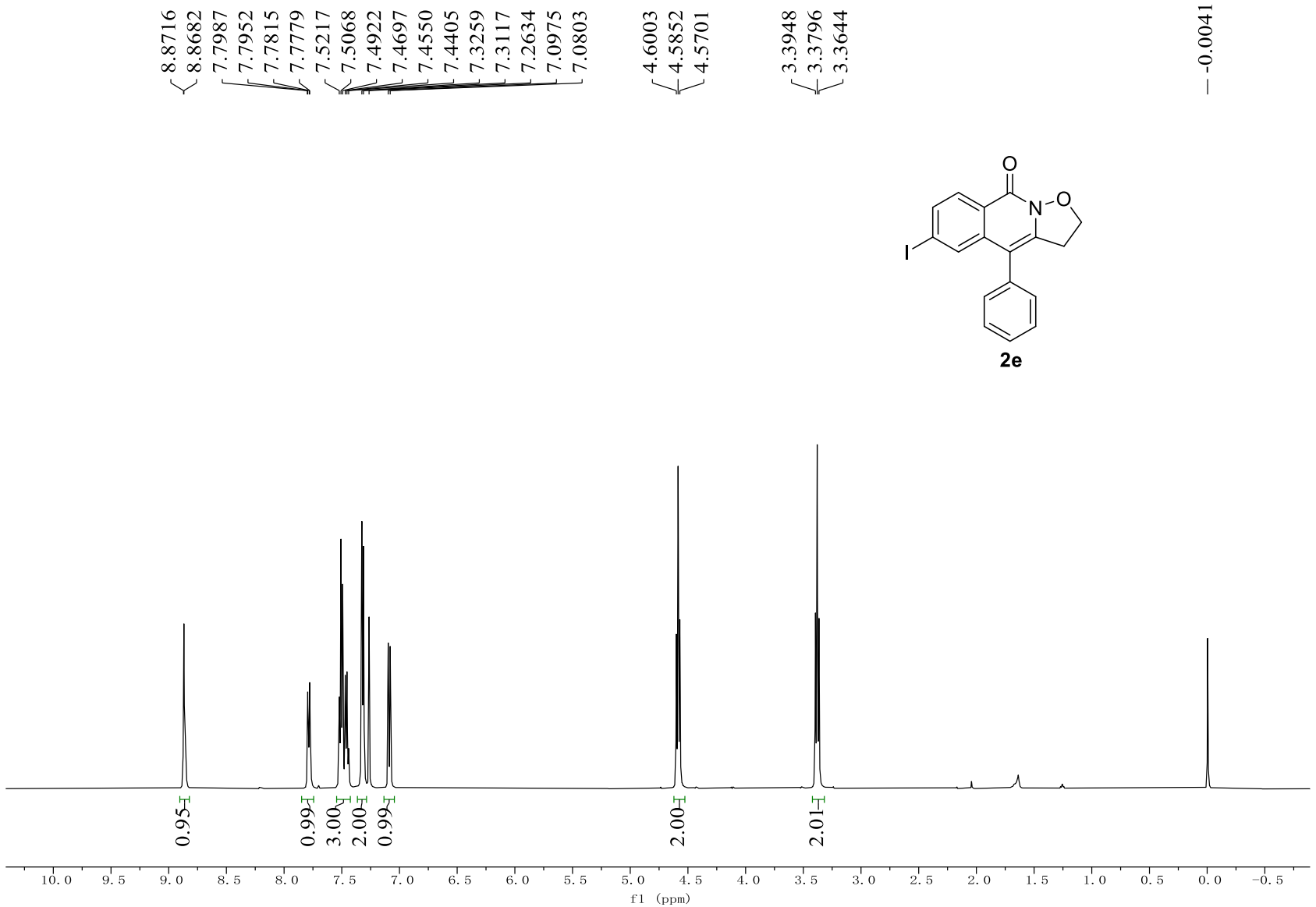
f1 (ppm)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7.3117
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4.5852
4.5701
3.3948
3.3796
3.3644
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O
N
O
I
2e
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0.99
2.00
2.01
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8.0
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6.5
6.0
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5.0
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2.0
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0.0
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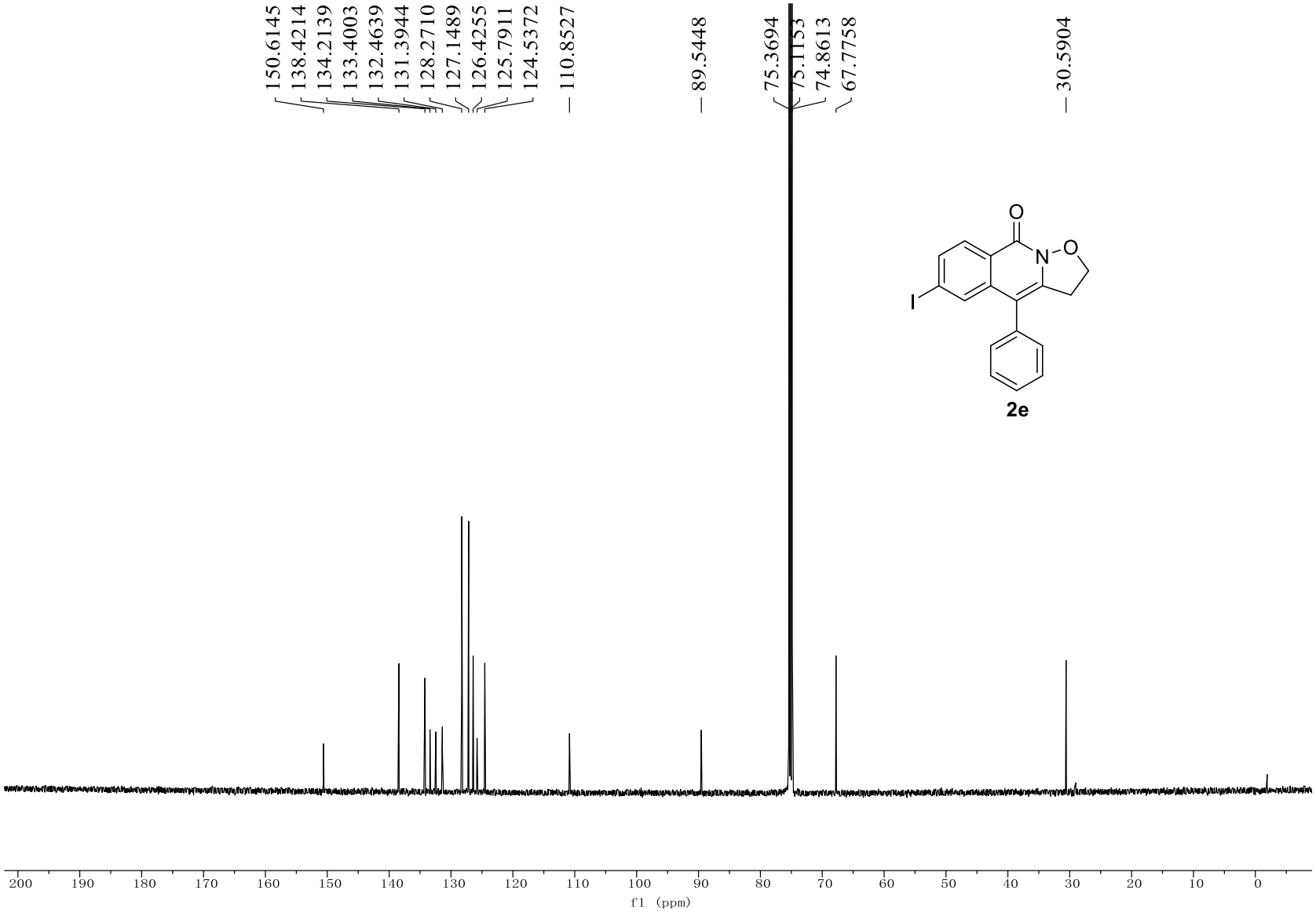
f1 (ppm)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75.3694
75.1153
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67.7758
30.5904
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N
O
I
2e
200
190
180
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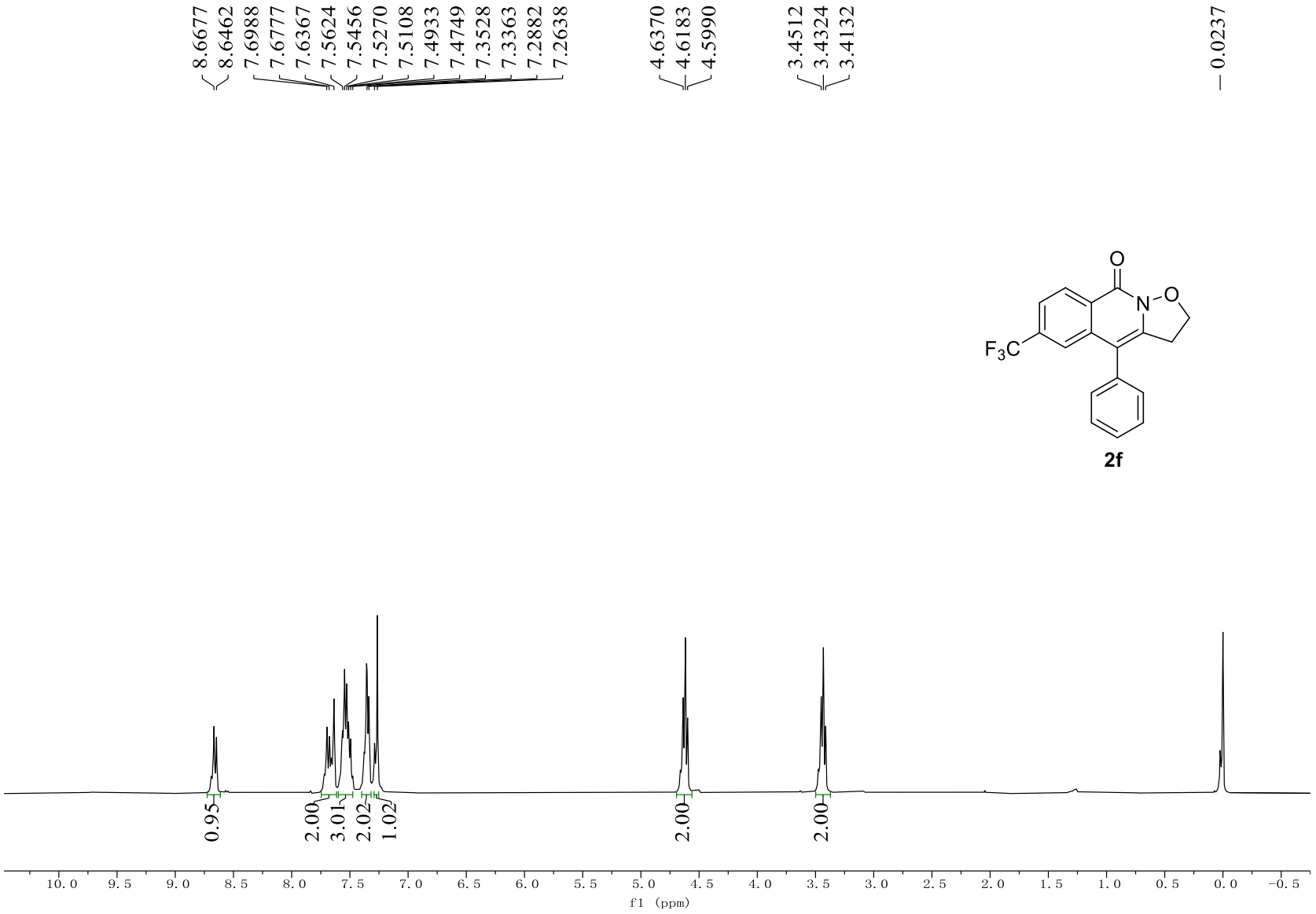
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7.2882
7.2638
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4.5990
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3.4324
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O
F3C
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3.01
2.02
1.02
2.00
2.00
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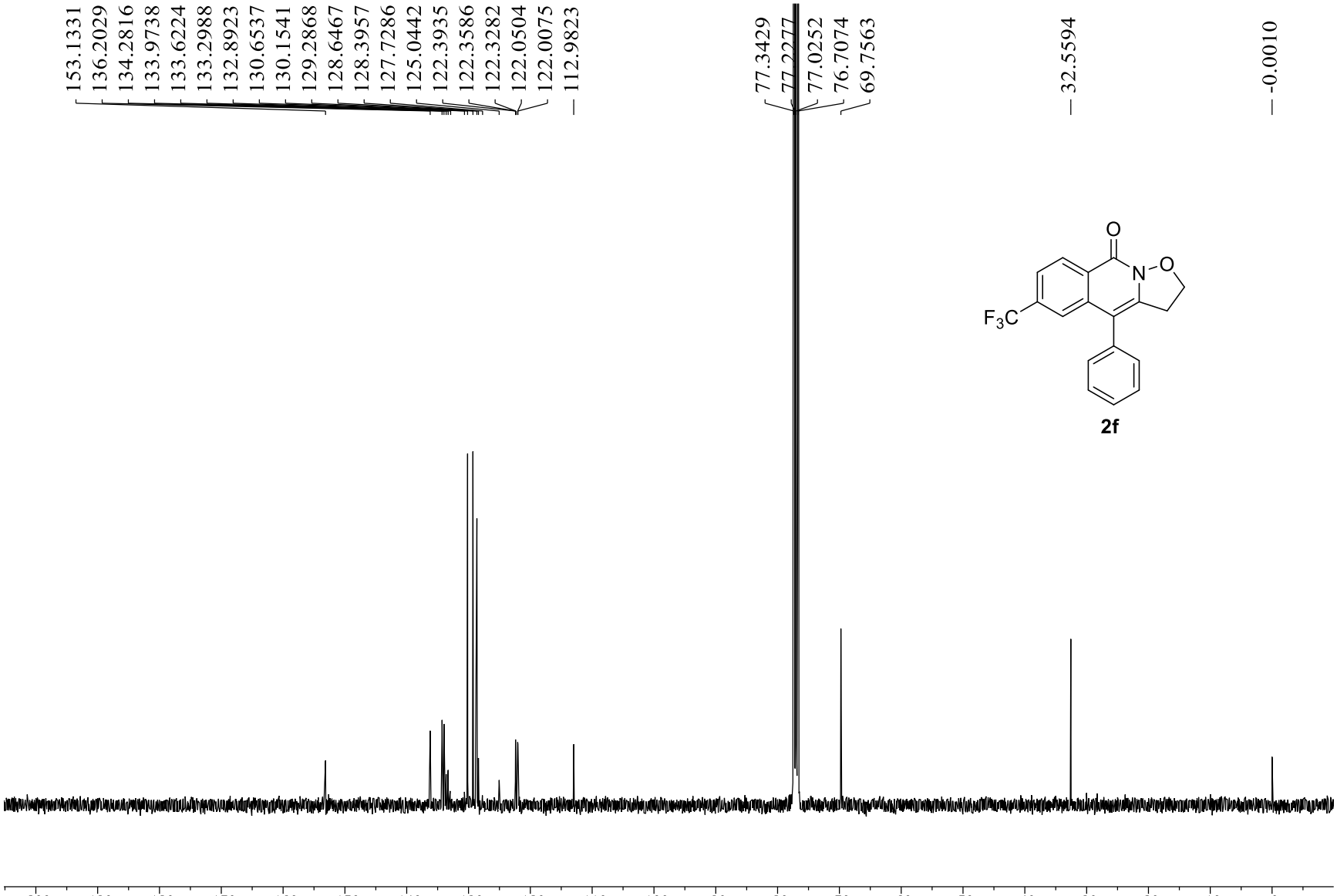
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77.0252
76.7074
69.7563
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O
N
O
F3C
2f
200
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180
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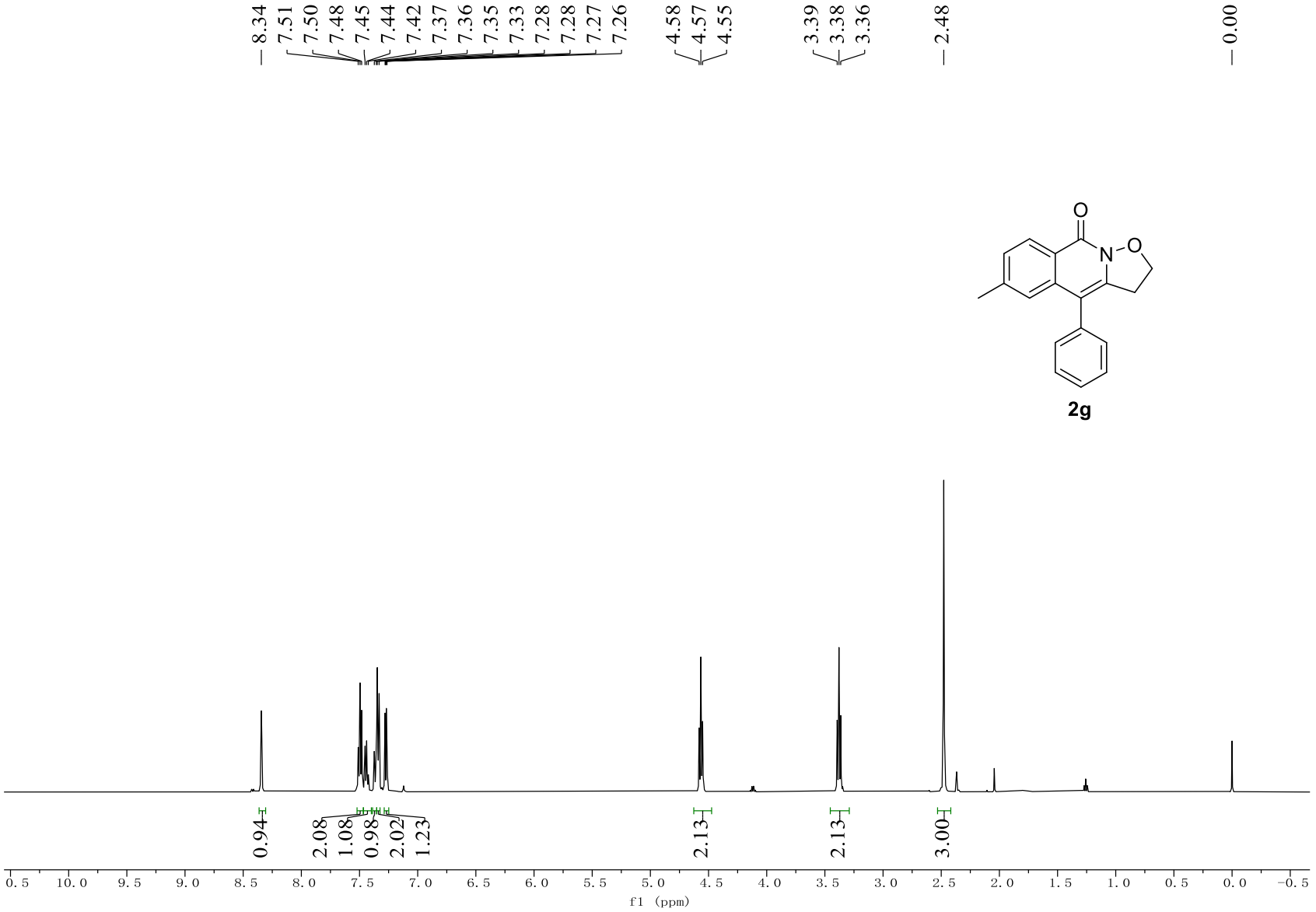
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4.55
3.39
3.38
3.36
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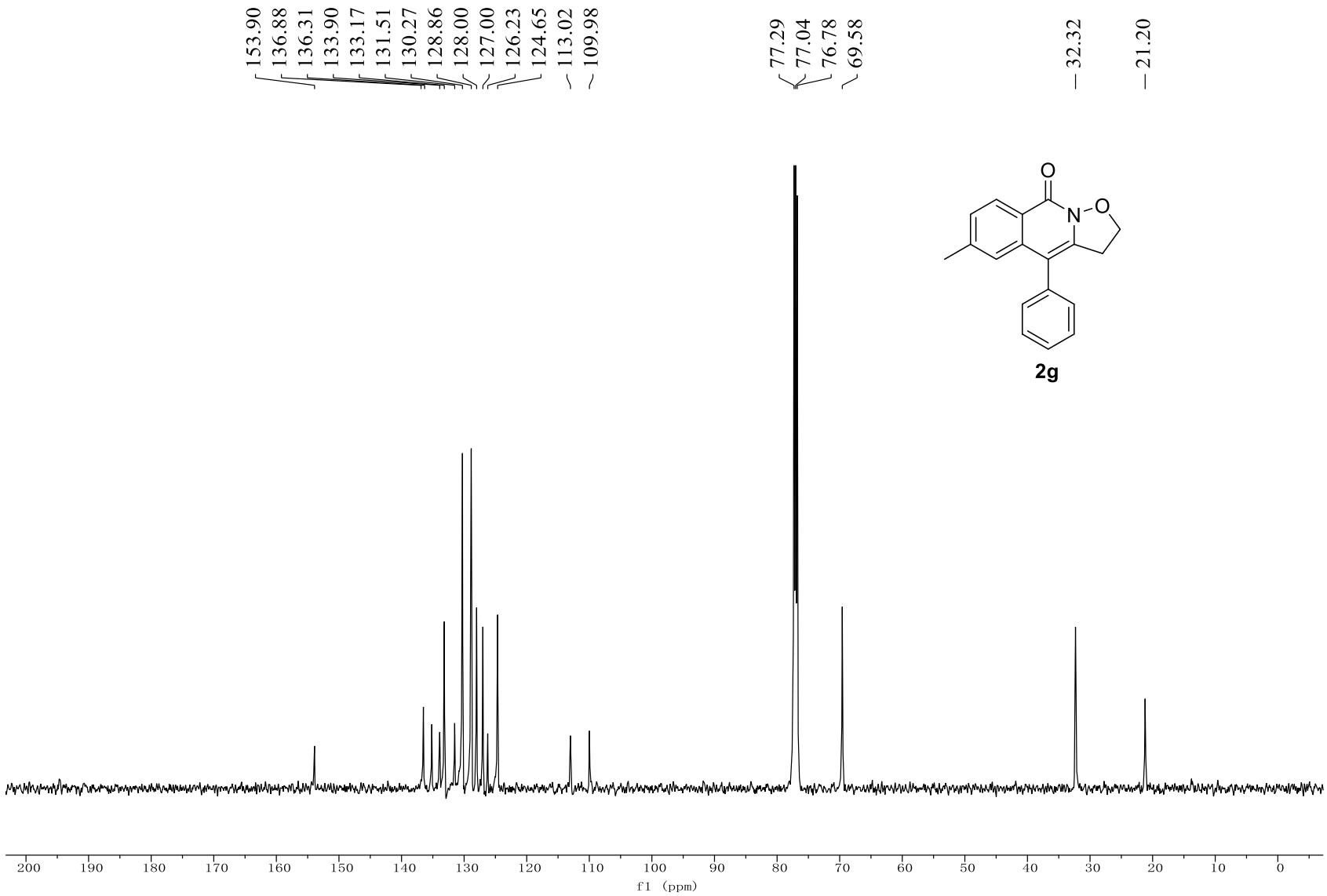
f1 (ppm)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76.78
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32.32
21.20
O
N
O
2g
200
190
180
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120
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90
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50
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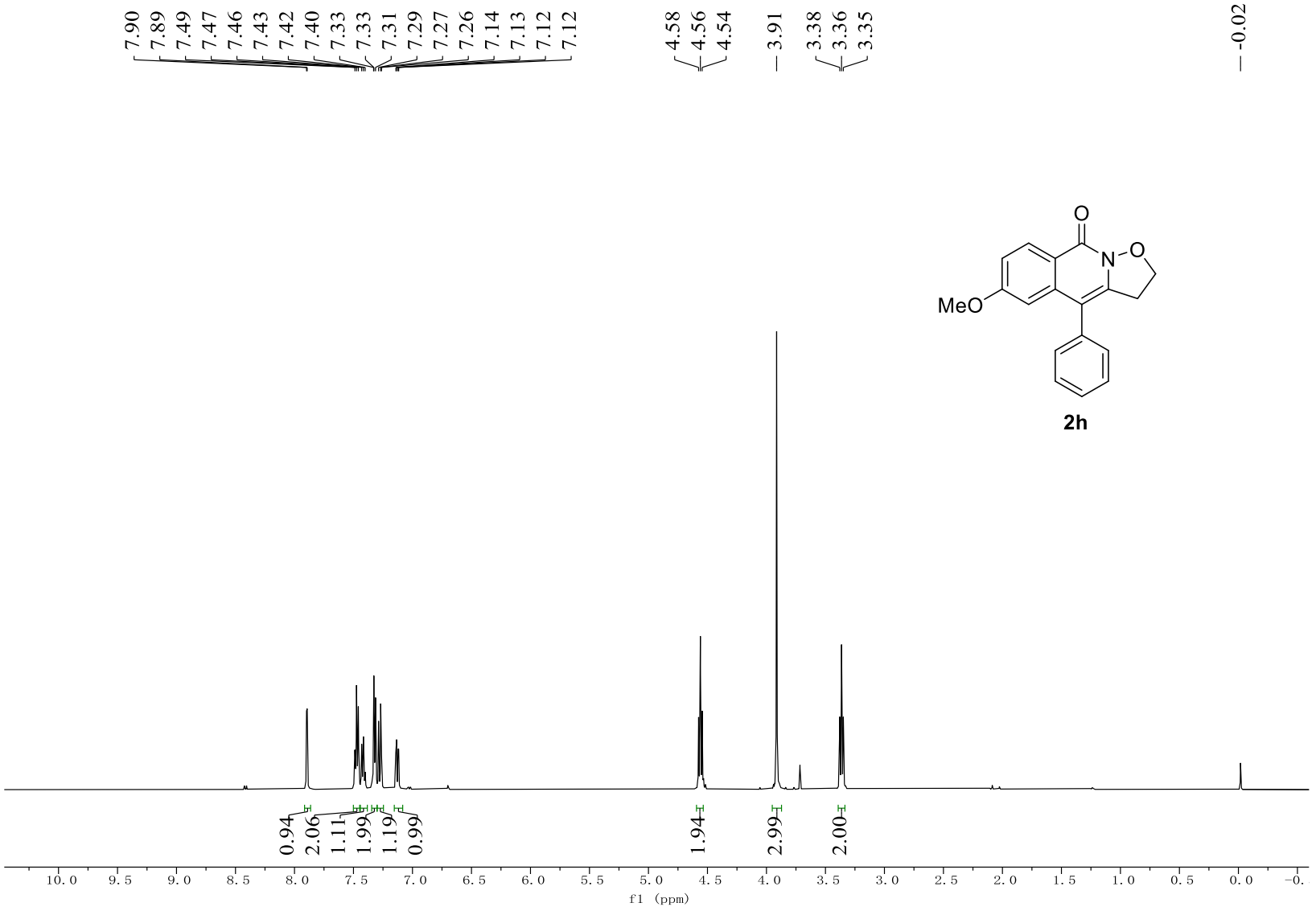
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7.13
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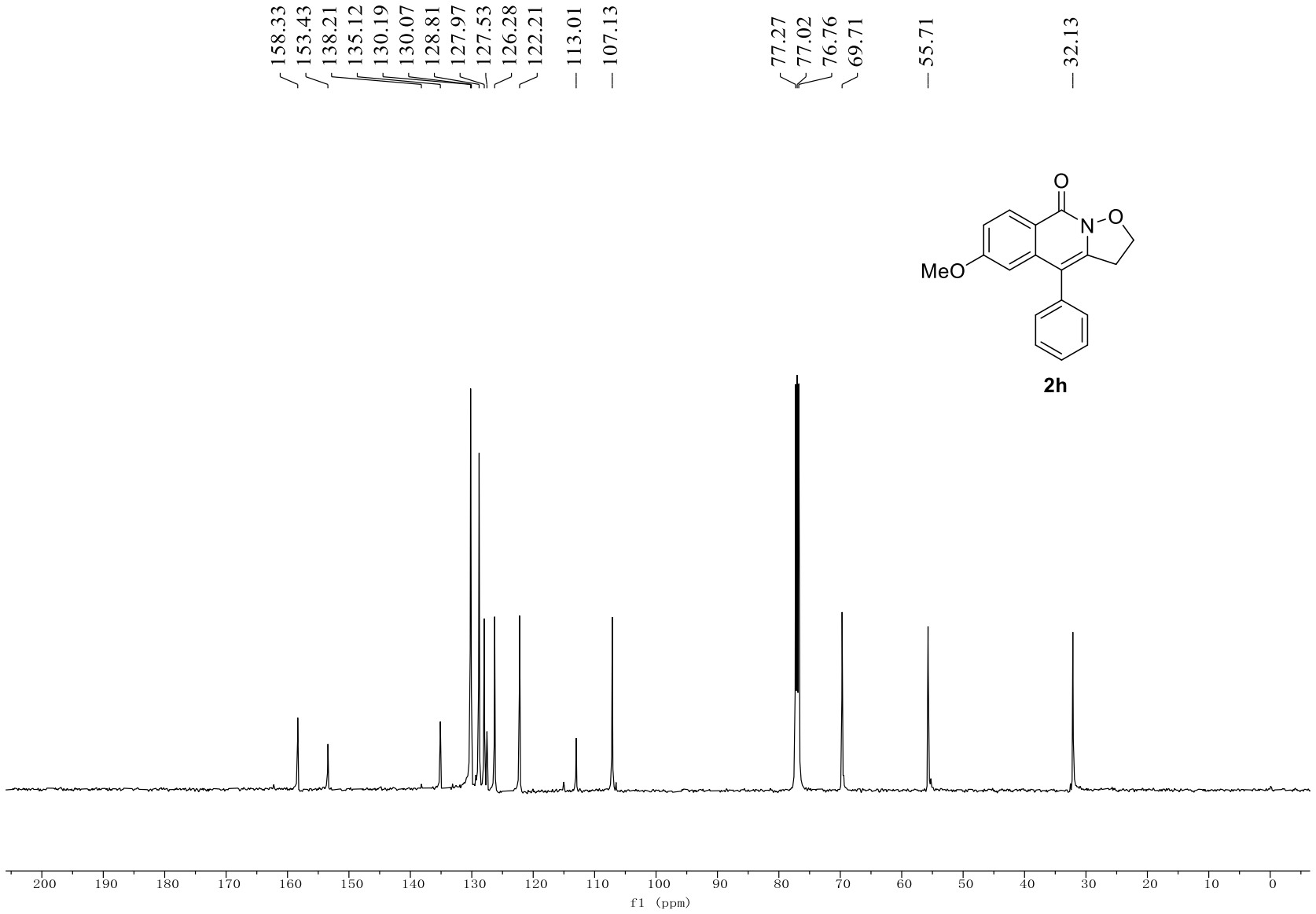
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76.76
69.71
55.71
32.13
O
N
O
MeO
2h
200
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180
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100
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80
70
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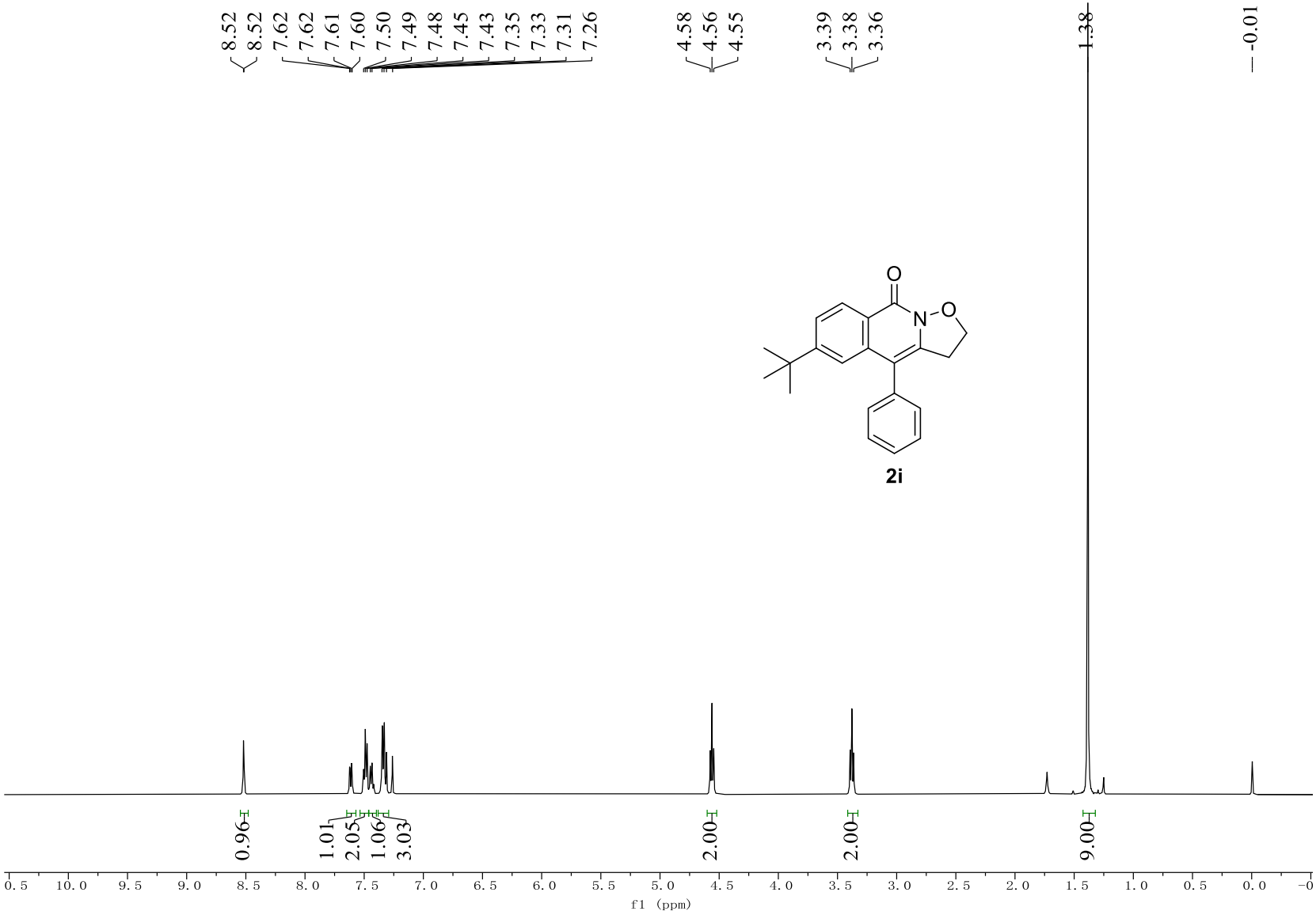
50
40
30
20
10
0
f1 (ppm)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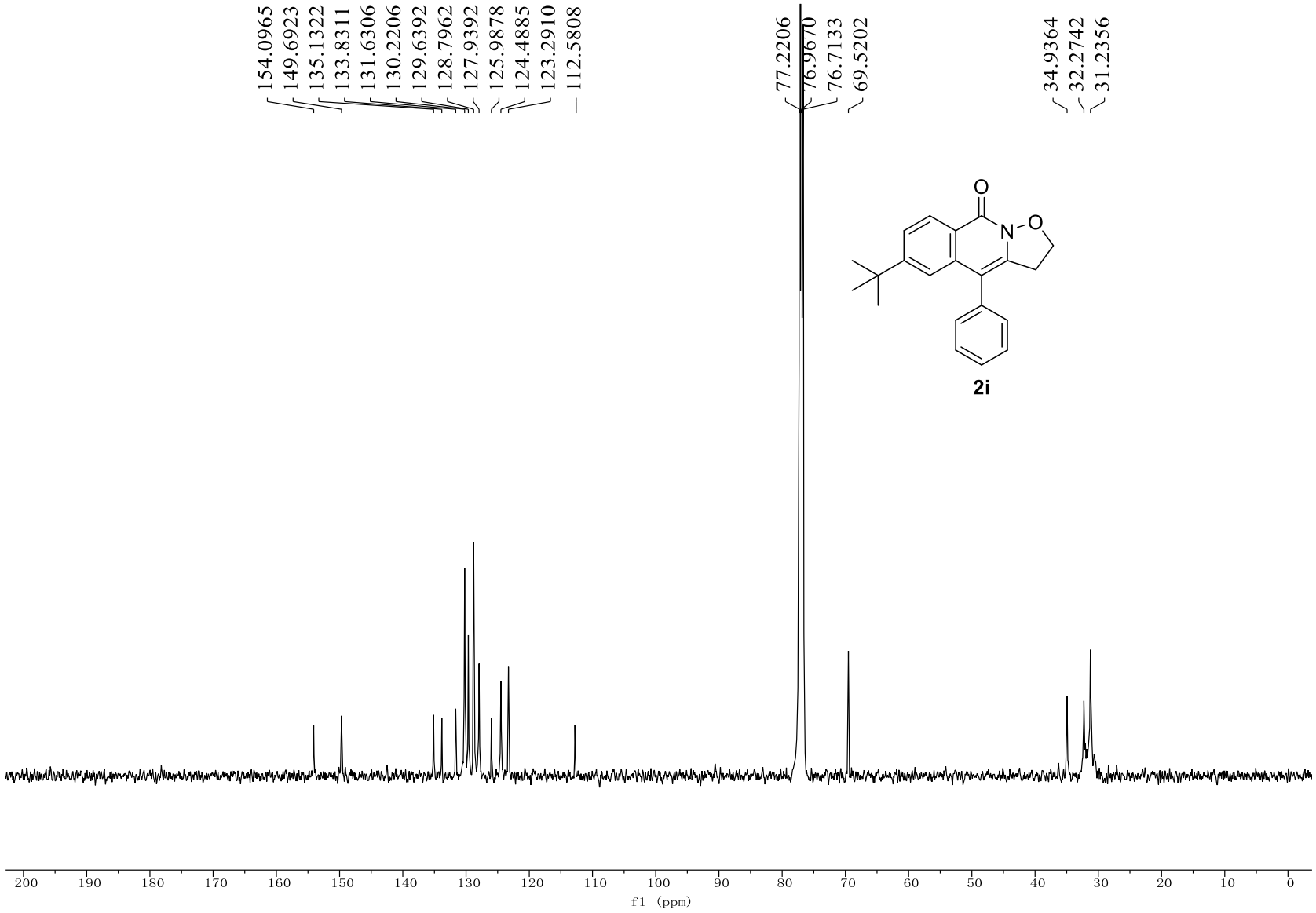
8.52
7.62
7.62
7.61
7.60
7.50
7.49
7.48
7.45
7.43
7.35
7.33
7.31
7.26
4.58
4.56
4.55
3.39
3.38
3.36
1.38
-0.01
O
N
O
2i
0.96
1.01
2.05
1.06
3.03
2.00
2.00
9.00
f1 (ppm)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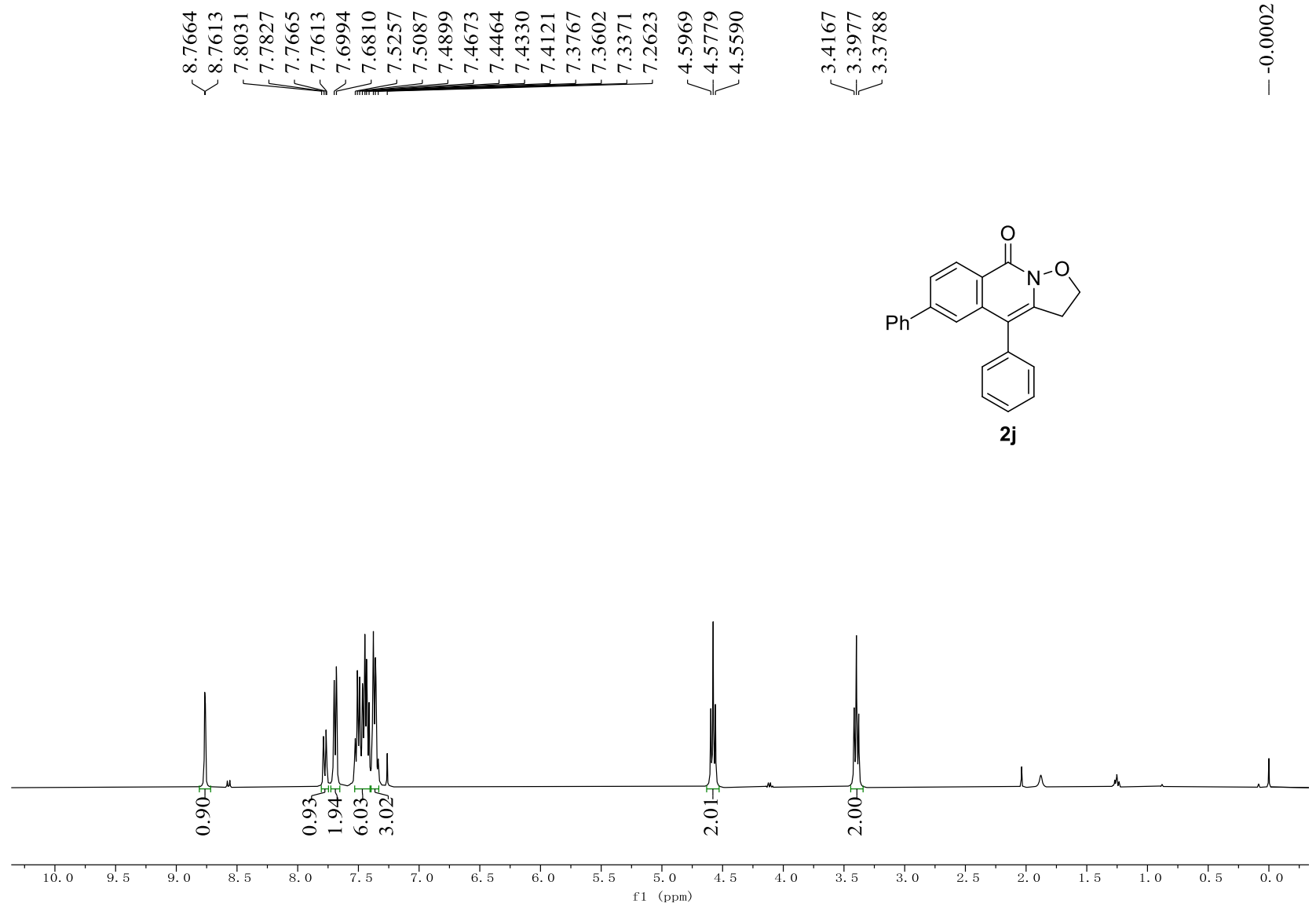
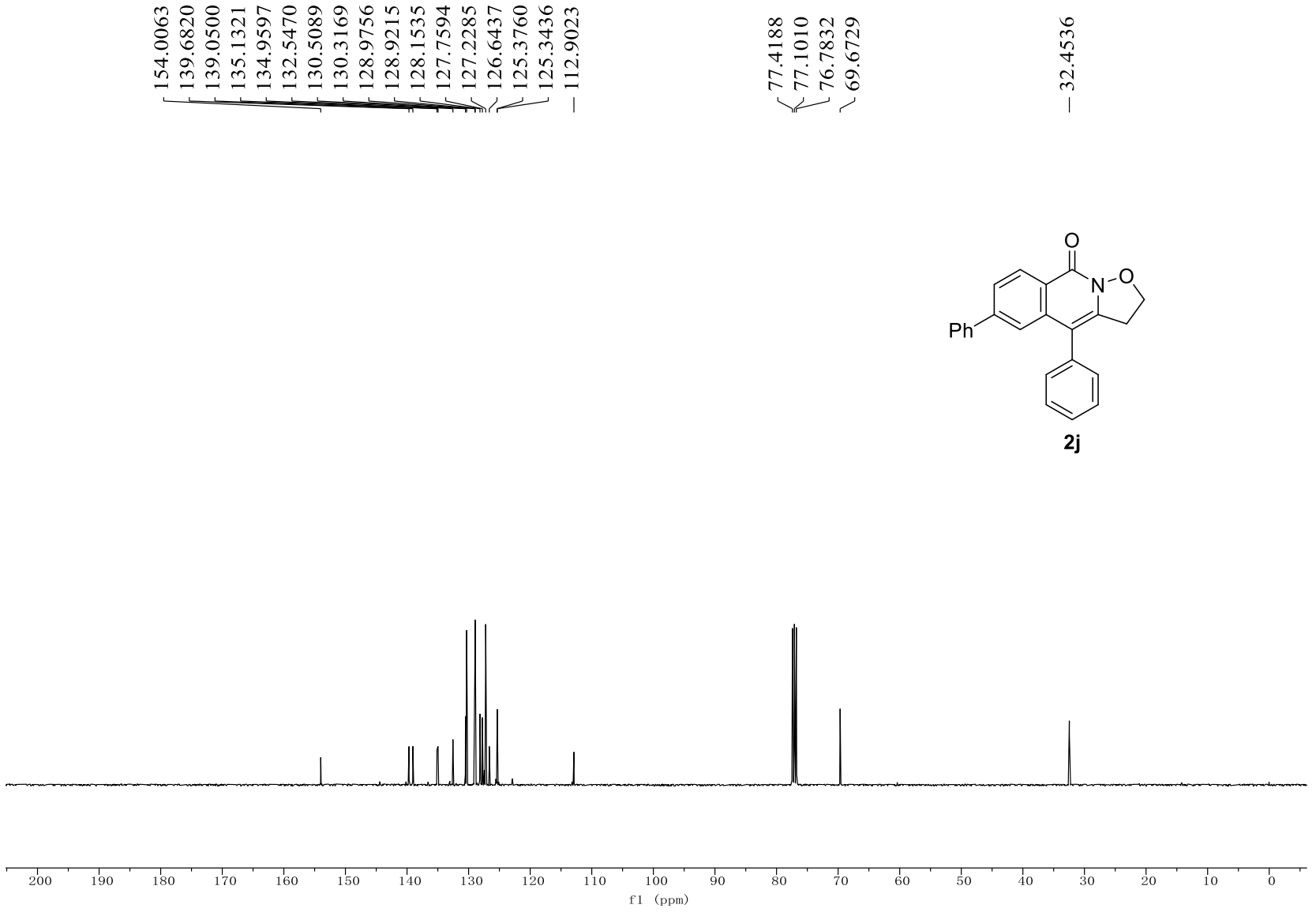
135.1322
133.8311
131.6306
130.2206
129.6392
128.7962
127.9392
125.9878
124.4885
123.2910
112.5808
77.2206
76.9670
76.7133
69.5202
34.9364
32.2742
31.2356
O
N
O
2i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.7664
8.7613
7.8031
7.7827
7.7665
7.7613
7.6994
7.6810
7.5257
7.5087
7.4899
7.4673
7.4464
7.4330
7.4121
7.3767
7.3602
7.3371
7.2623
4.5969
4.5779
4.5590
3.4167
3.3977
3.3788
-0.0002
O
N
O
Ph
2j
0.90
0.93
1.94
6.03
3.02
2.01
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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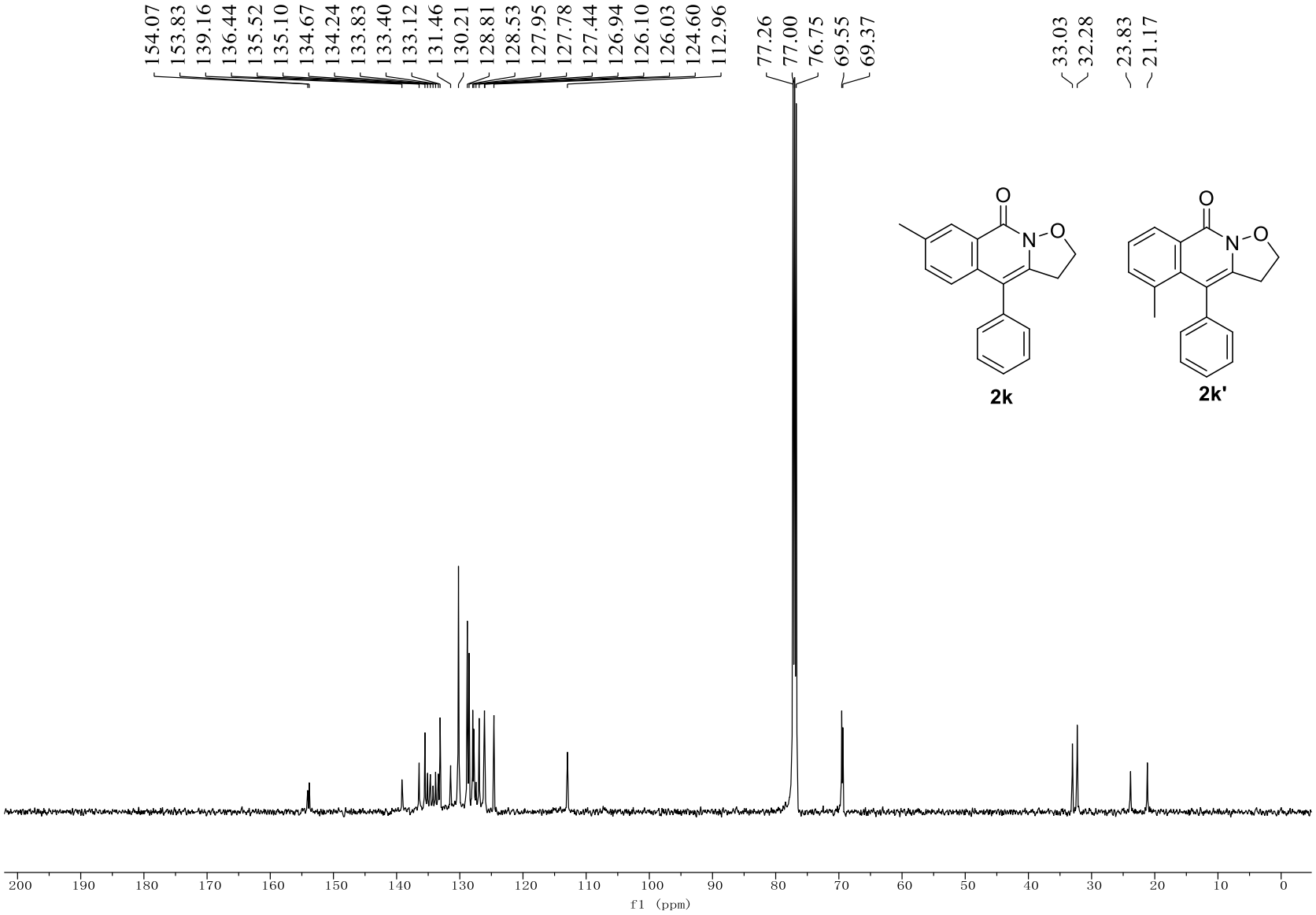
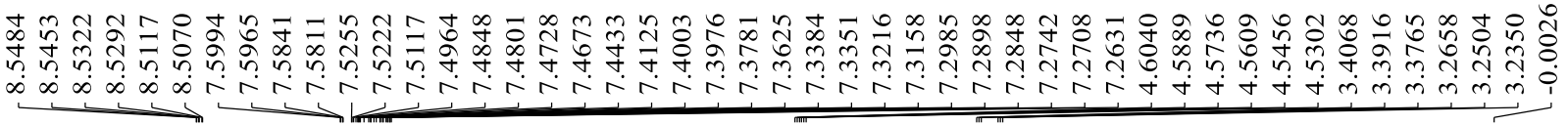
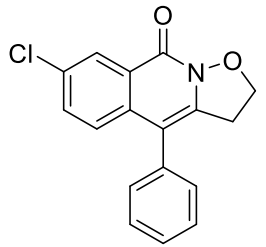
139.6820
139.0500
135.1321
134.9597
132.5470
130.5089
130.3169
128.9756
128.9215
128.1535
127.7594
127.2285
126.6437
125.3760
125.3436
112.9023
77.4188
77.1010
76.7832
69.6729
32.4536
O
N
O
Ph
2j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

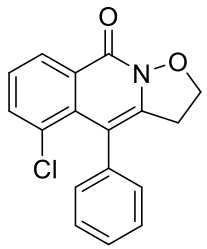
8.5211
8.4655
8.3325
7.5015
7.4864
7.4717
7.4428
7.4232
7.4081
7.3369
7.3235
7.2975
7.2846
7.2719
7.2562
4.5718
4.5565
4.5415
4.5290
4.5131
4.4976
3.3860
3.3706
3.3560
3.2196
3.2044
3.1889
2.4662
1.8516
0.0378
O
N
O
2k
O
N
O
2k'
0.68
0.98
12.16
2.02
1.46
2.00
1.41
3.00
2.19
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


154.07
153.83
139.16
136.44
135.52
135.10
134.67
134.24
133.83
133.40
133.12
131.46
130.21
128.81
128.53
127.95
127.78
127.44
126.94
126.10
126.03
124.60
112.96
77.26
77.00
76.75
69.55
69.37
33.03
32.28
23.83
21.17
2k
2k'
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

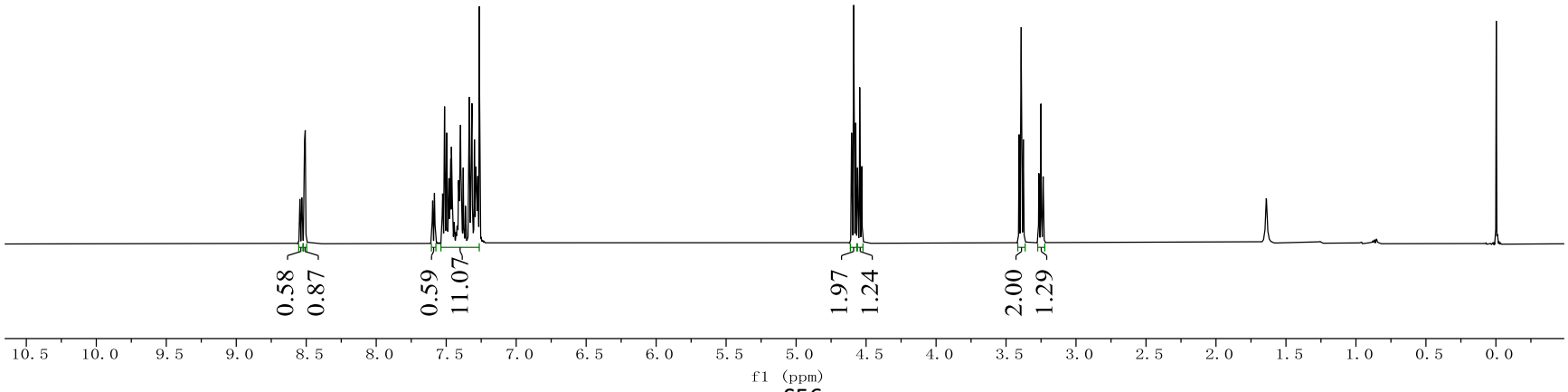

8.5484
8.5453
8.5322
8.5292
8.5117
8.5070
7.5994
7.5965
7.5841
7.5811
7.5255
7.5222
7.5117
7.4964
7.4848
7.4801
7.4728
7.4673
7.4433
7.4125
7.4003
7.3976
7.3781
7.3625
7.3384
7.3351
7.3216
7.3158
7.2985
7.2898
7.2848
7.2742
7.2708
7.2631
4.6040
4.5889
4.5736
4.5609
4.5456
4.5302
3.4068
3.3916
3.3765
3.2658
3.2504
3.2350
-0.0026

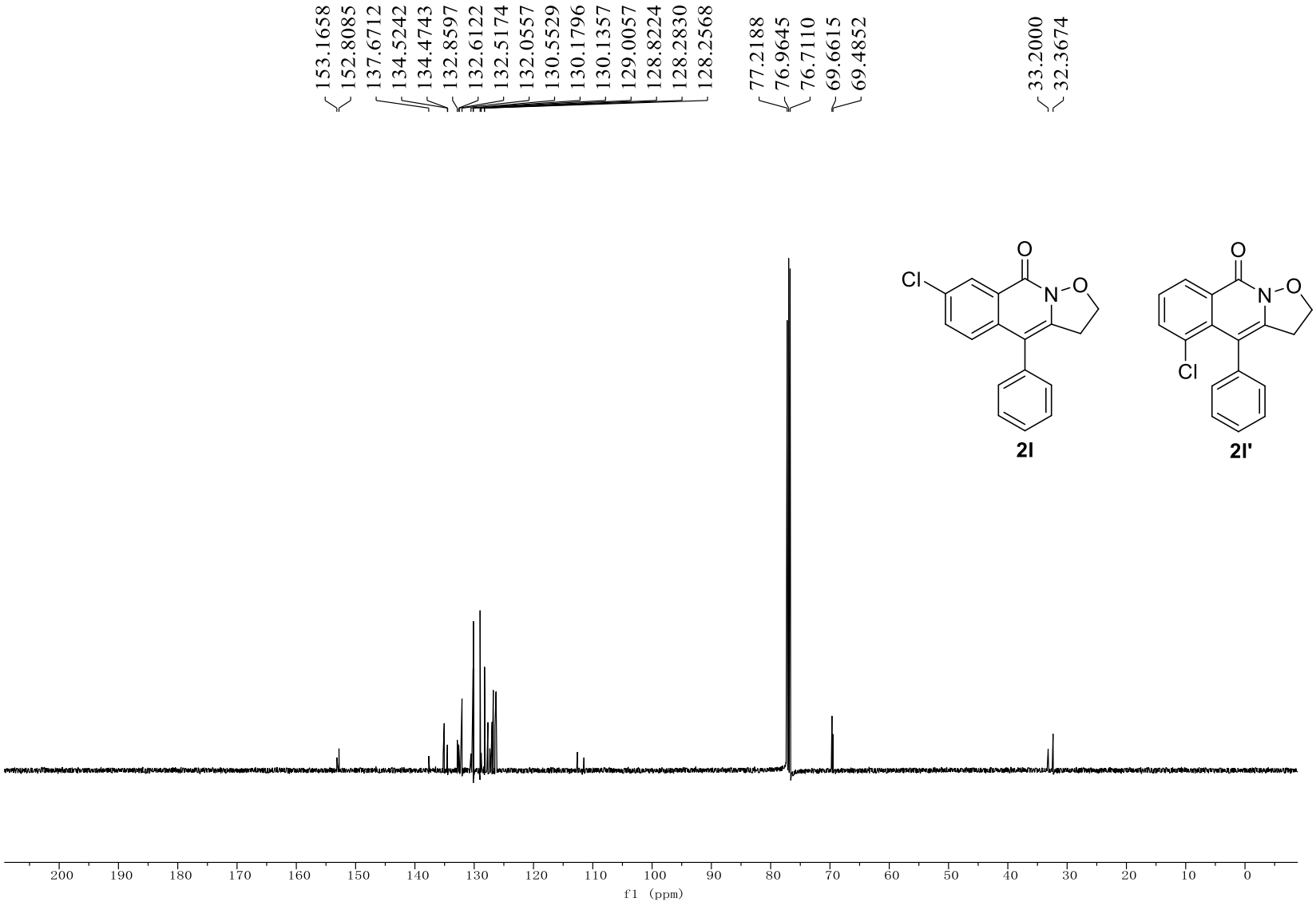

O
Cl
N
O

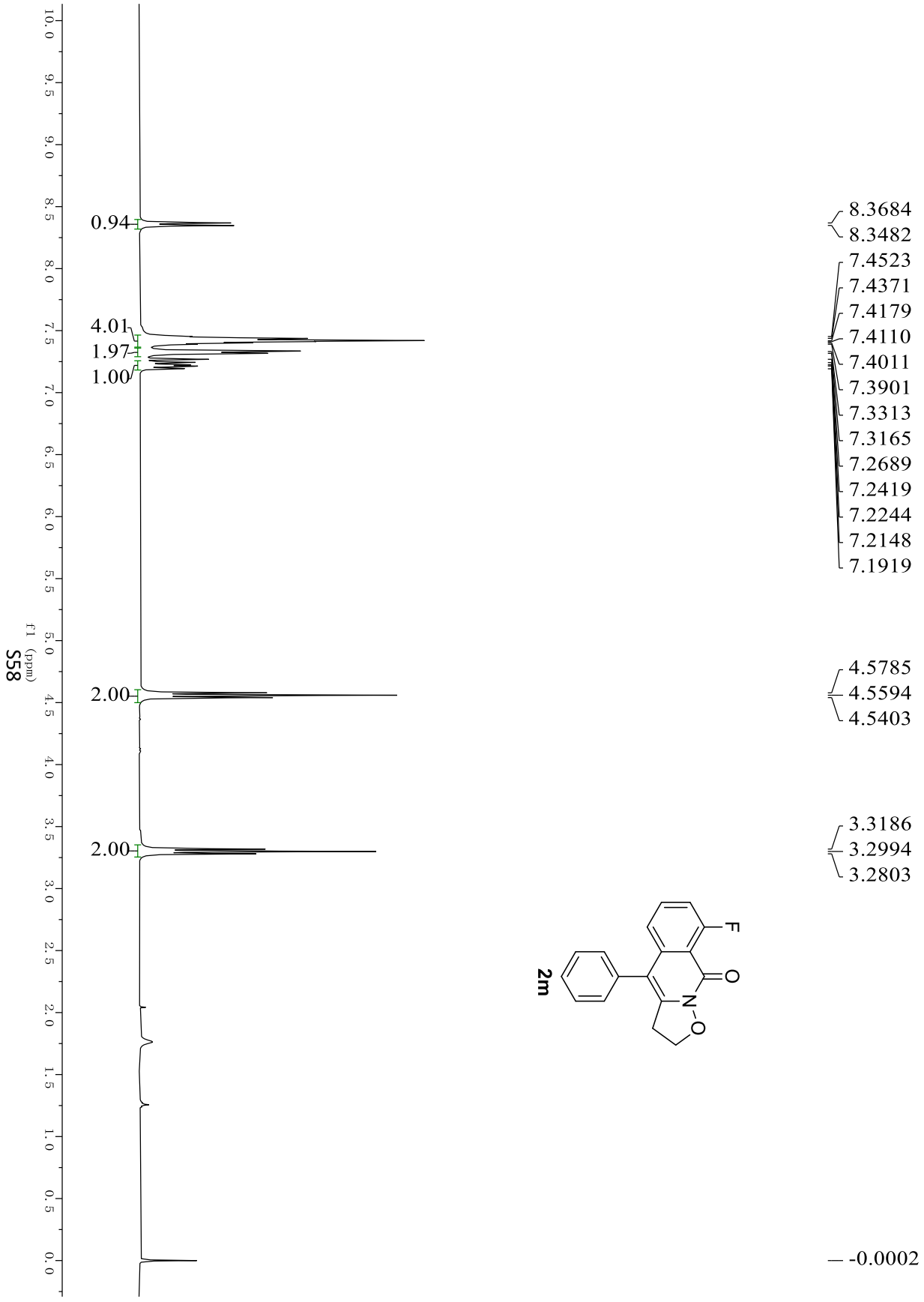
2l

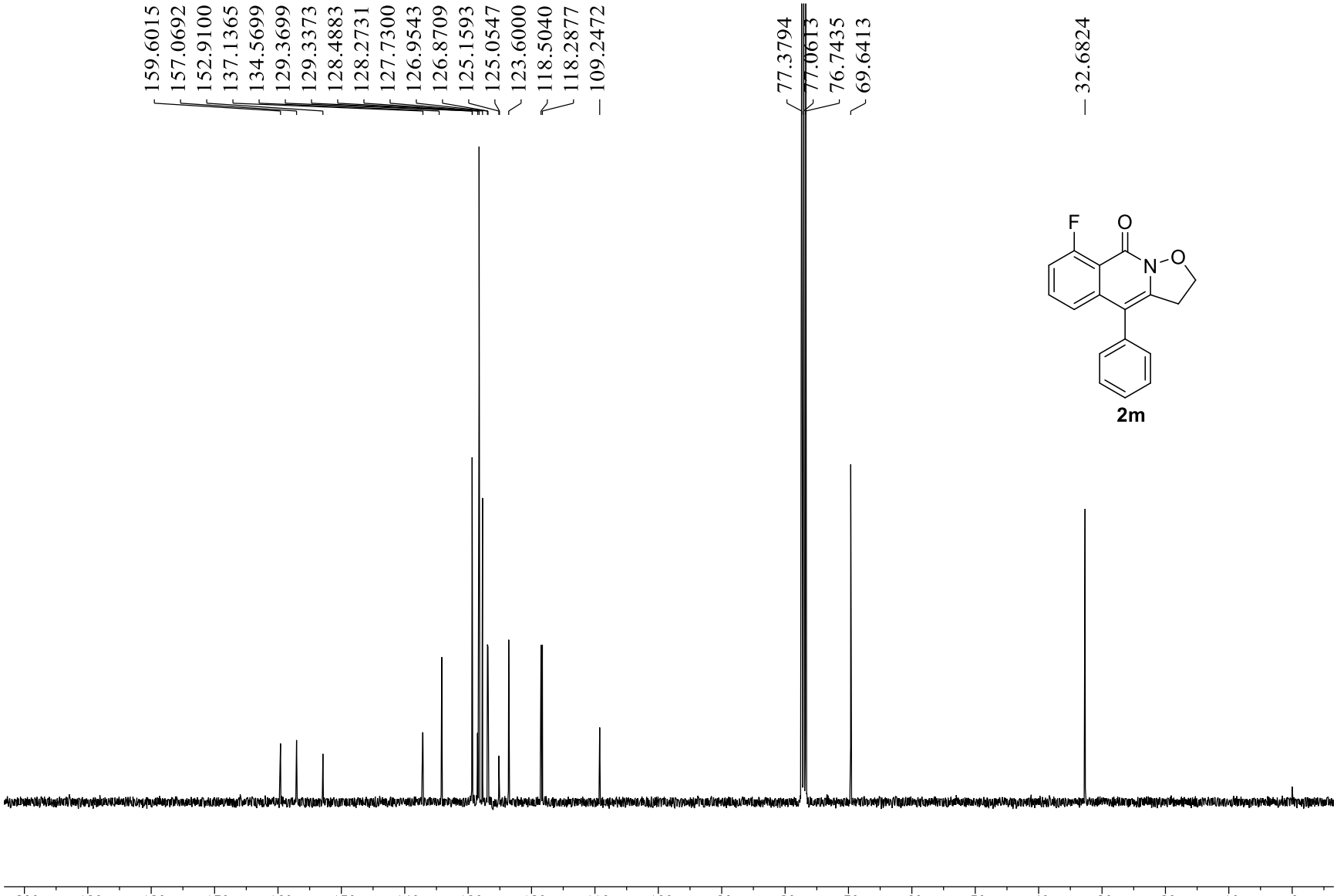

O
Cl
N
O

2l'


0.58
0.87
0.59
11.07
1.97
1.24
2.00
1.29
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.1658
152.8085
137.6712
134.5242
134.4743
132.8597
132.6122
132.5174
132.0557
130.5529
130.1796
130.1357
129.0057
128.8224
128.2830
128.2568
77.2188
76.9645
76.7110
69.6615
69.4852
33.2000
32.3674
Cl
O
N
O
2l
Cl
O
N
O
2l'
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.3684
8.3482
7.4523
7.4371
7.4179
7.4110
7.4011
7.3901
7.3313
7.3165
7.2689
7.2419
7.2244
7.2148
7.1919
4.5785
4.5594
4.5403
3.3186
3.2994
3.2803
-0.0002
0.94
4.01
1.97
1.00
2.00
2.00
f1 (ppm)
F
O
N
O
2m
S58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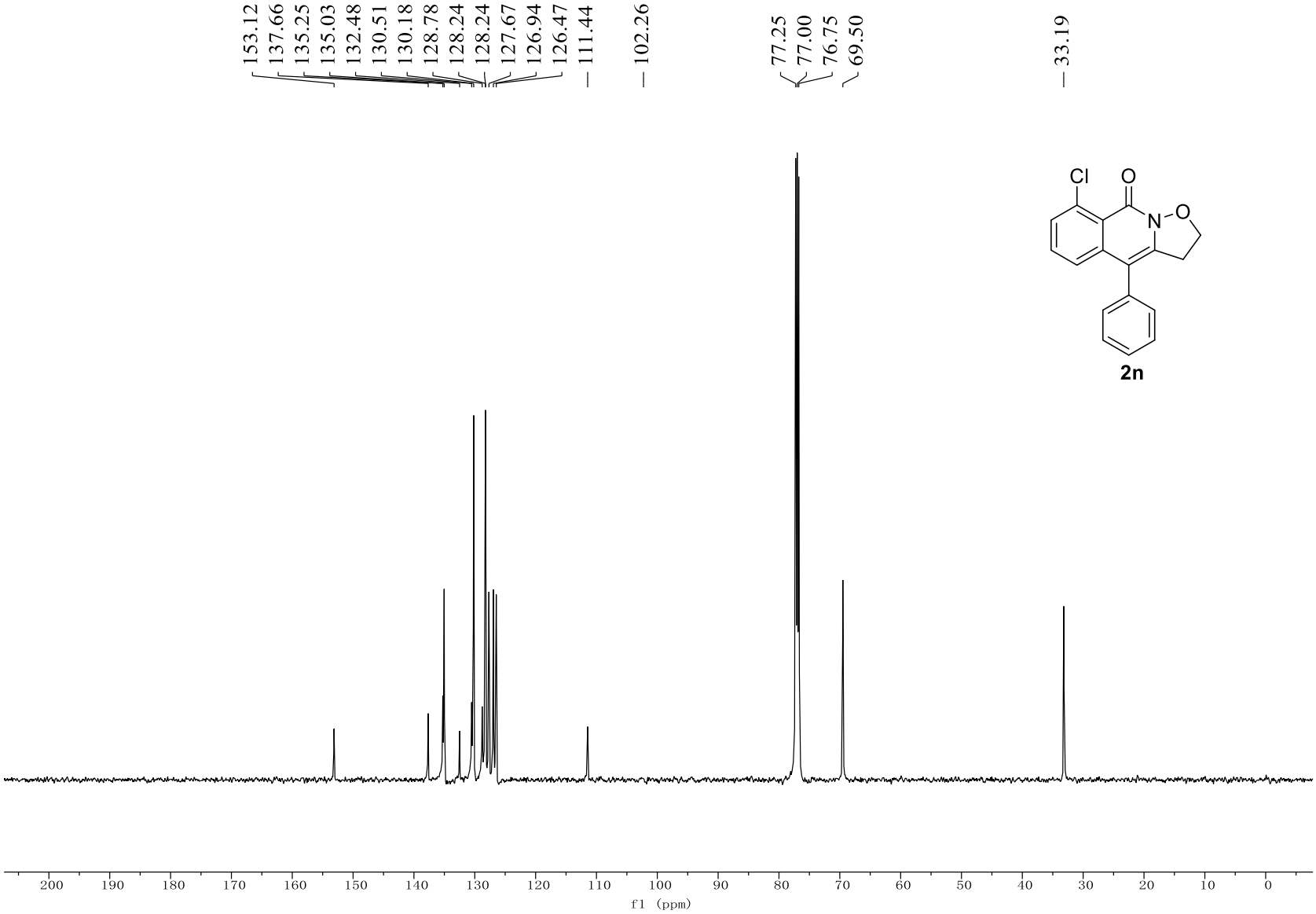
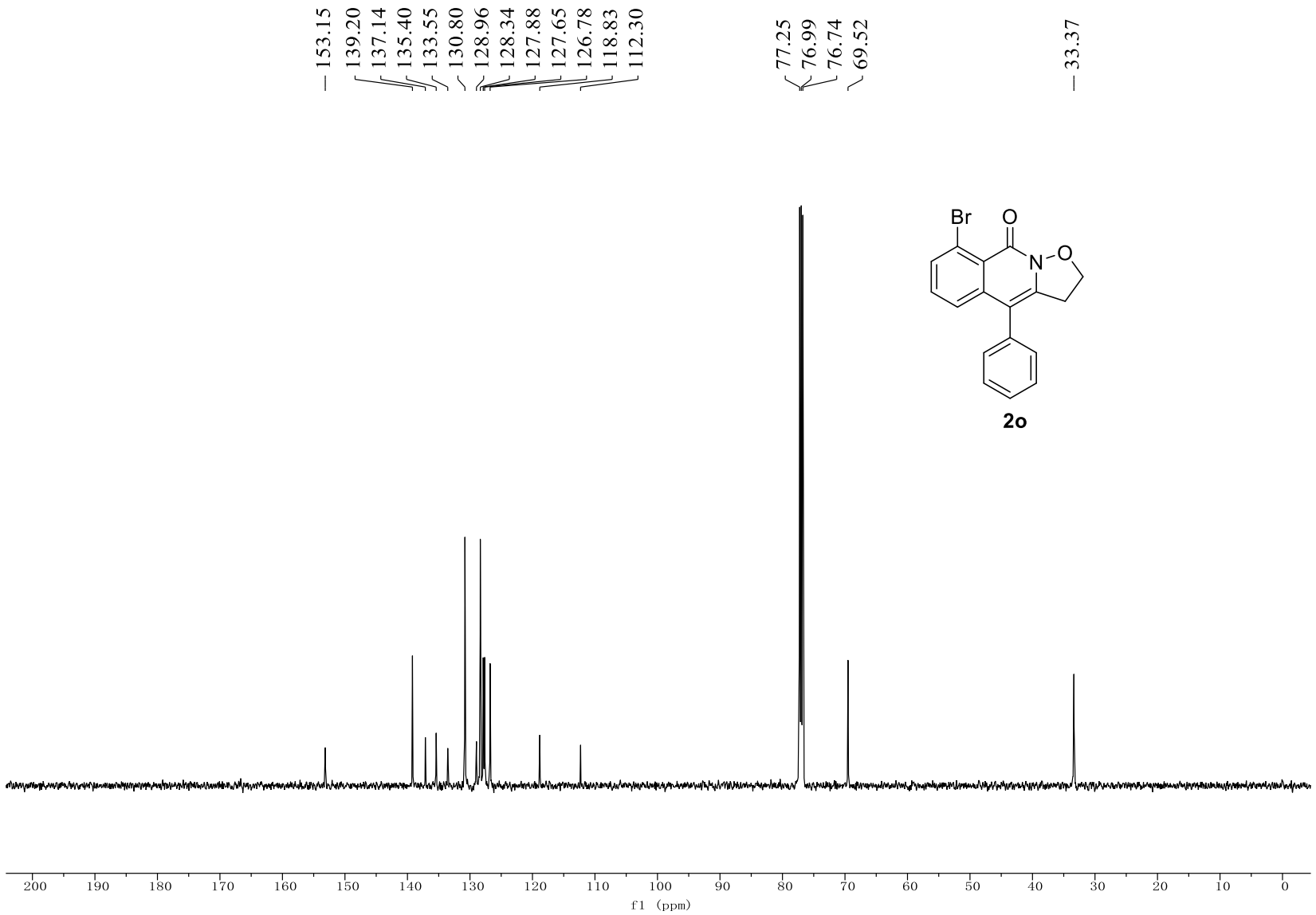
157.0692
152.9100
137.1365
134.5699
129.3699
129.3373
128.4883
128.2731
127.7300
126.9543
126.8709
125.1593
125.0547
123.6000
118.5040
118.2877
109.2472
77.3794
77.0613
76.7435
69.6413
32.6824
F
O
N
O
2m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

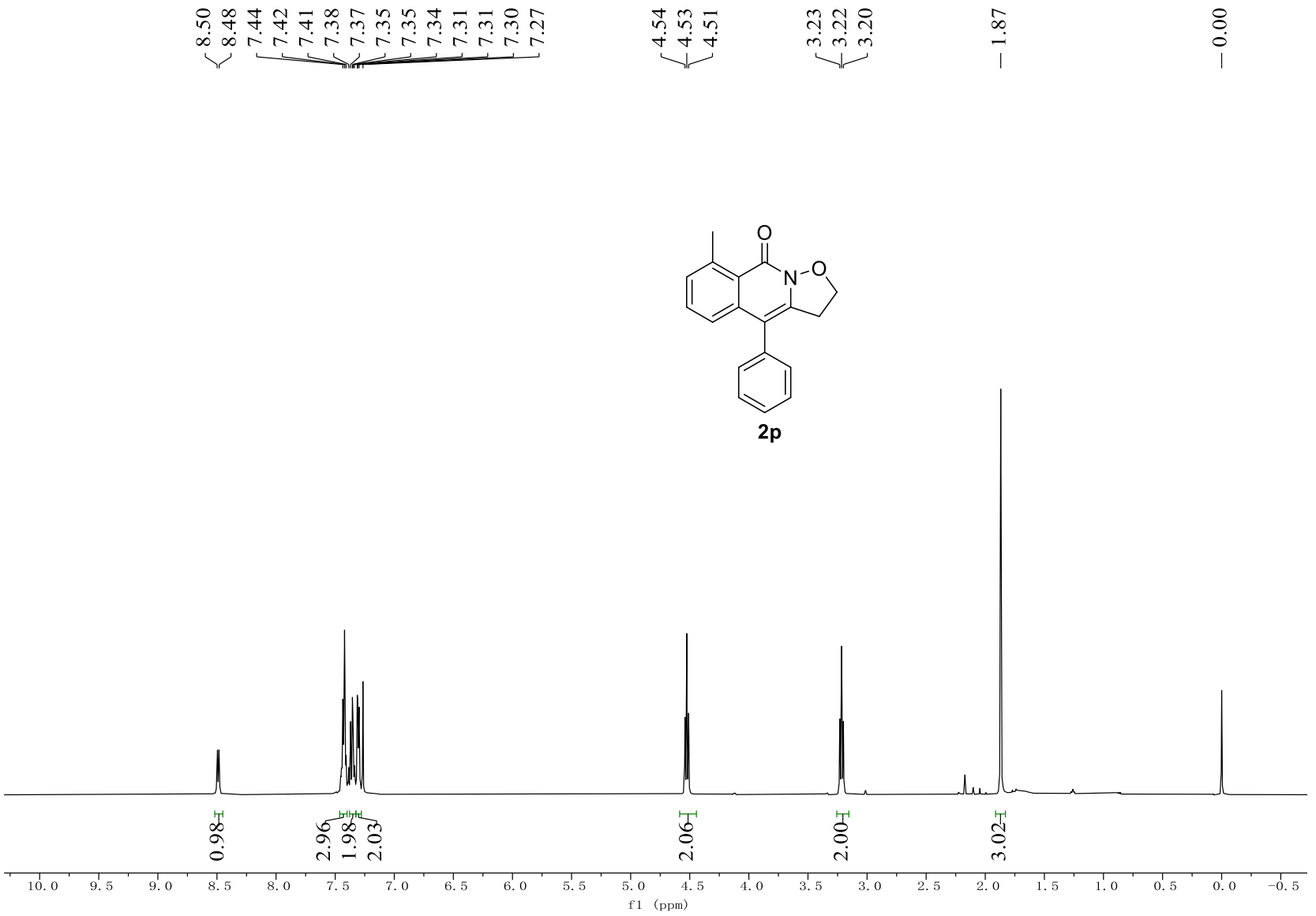

8.52
8.51
7.57
7.56
7.39
7.36
7.34
7.28
7.26
4.55
4.54
4.52
3.26
3.24
3.23
-0.01
Cl
O
N
O
2n
1.00
1.00
4.00
2.13
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


153.12
137.66
135.25
135.03
132.48
130.51
130.18
128.78
128.24
128.24
127.67
126.94
126.47
111.44
102.26
77.25
77.00
76.75
69.50
33.19
Cl
O
N
O
2n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.58
8.56
7.82
7.82
7.81
7.80
7.40
7.39
7.39
7.38
7.28
7.26
7.25
4.54
4.53
4.51
3.25
3.23
3.22
-0.02
Br
O
N
O
1.00
1.00
3.00
3.21
2.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

2o


153.15
139.20
137.14
135.40
133.55
130.80
128.96
128.34
127.88
127.65
126.78
118.83
112.30
77.25
76.99
76.74
69.52
33.37
Br
O
N
O
2o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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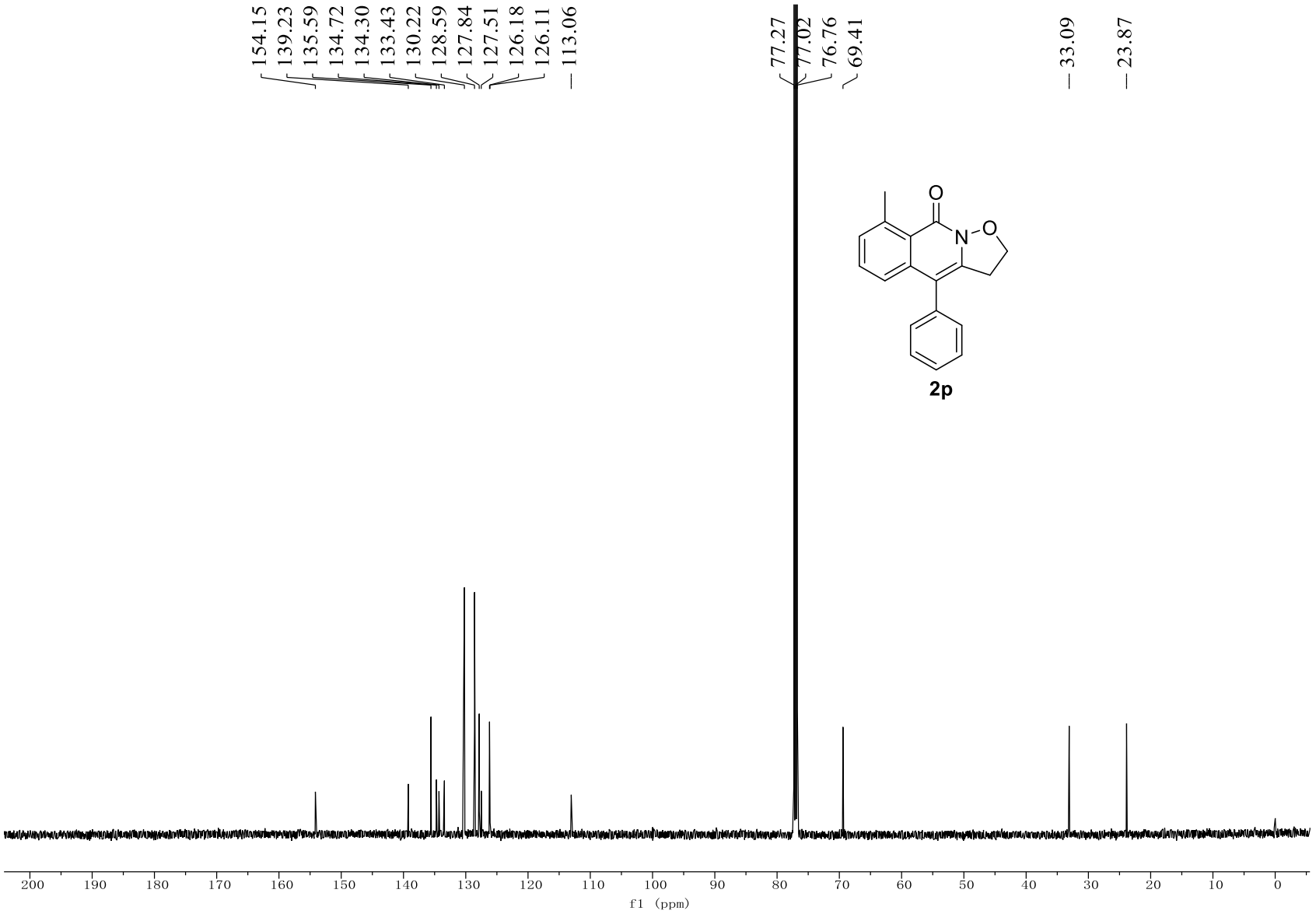
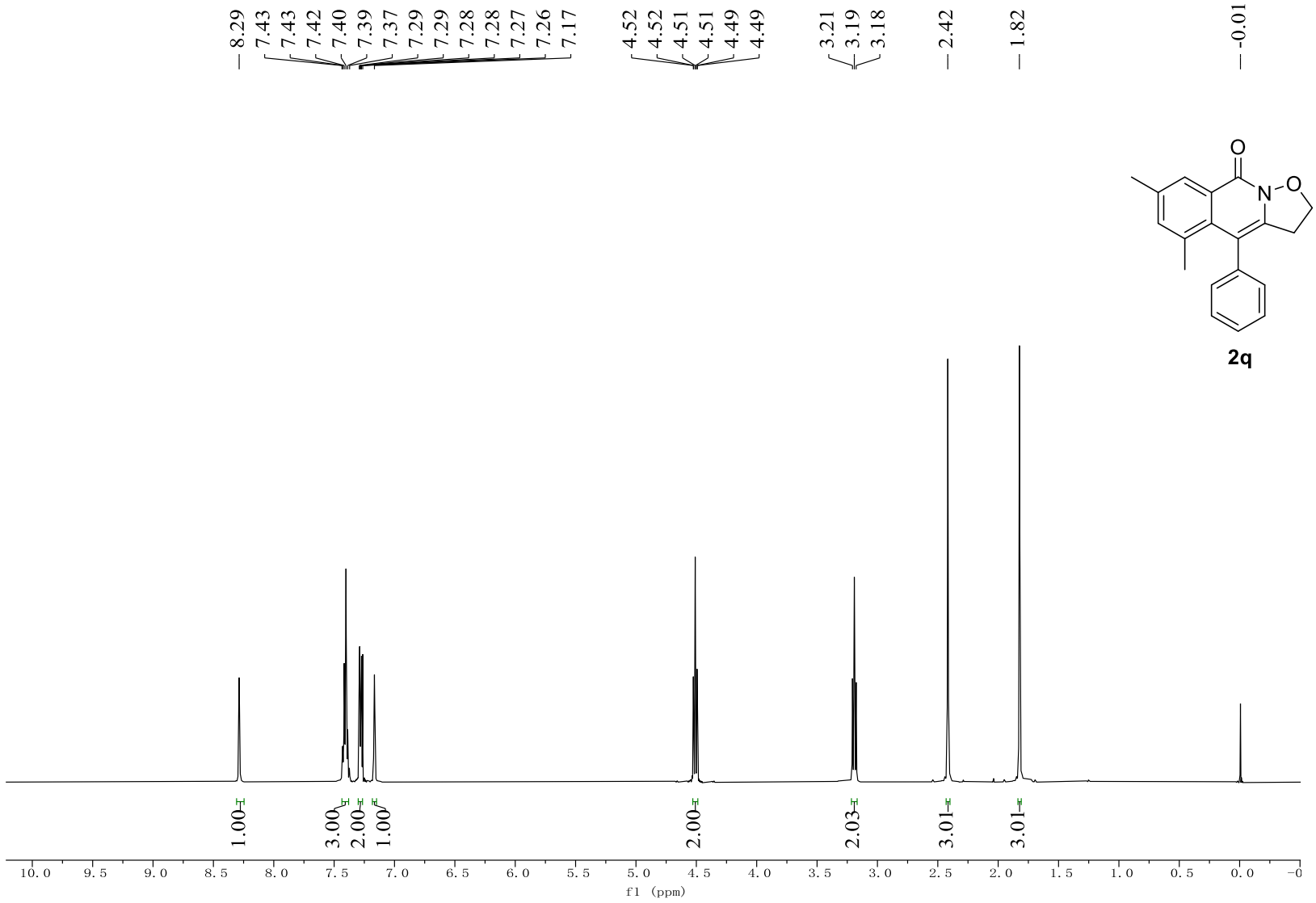
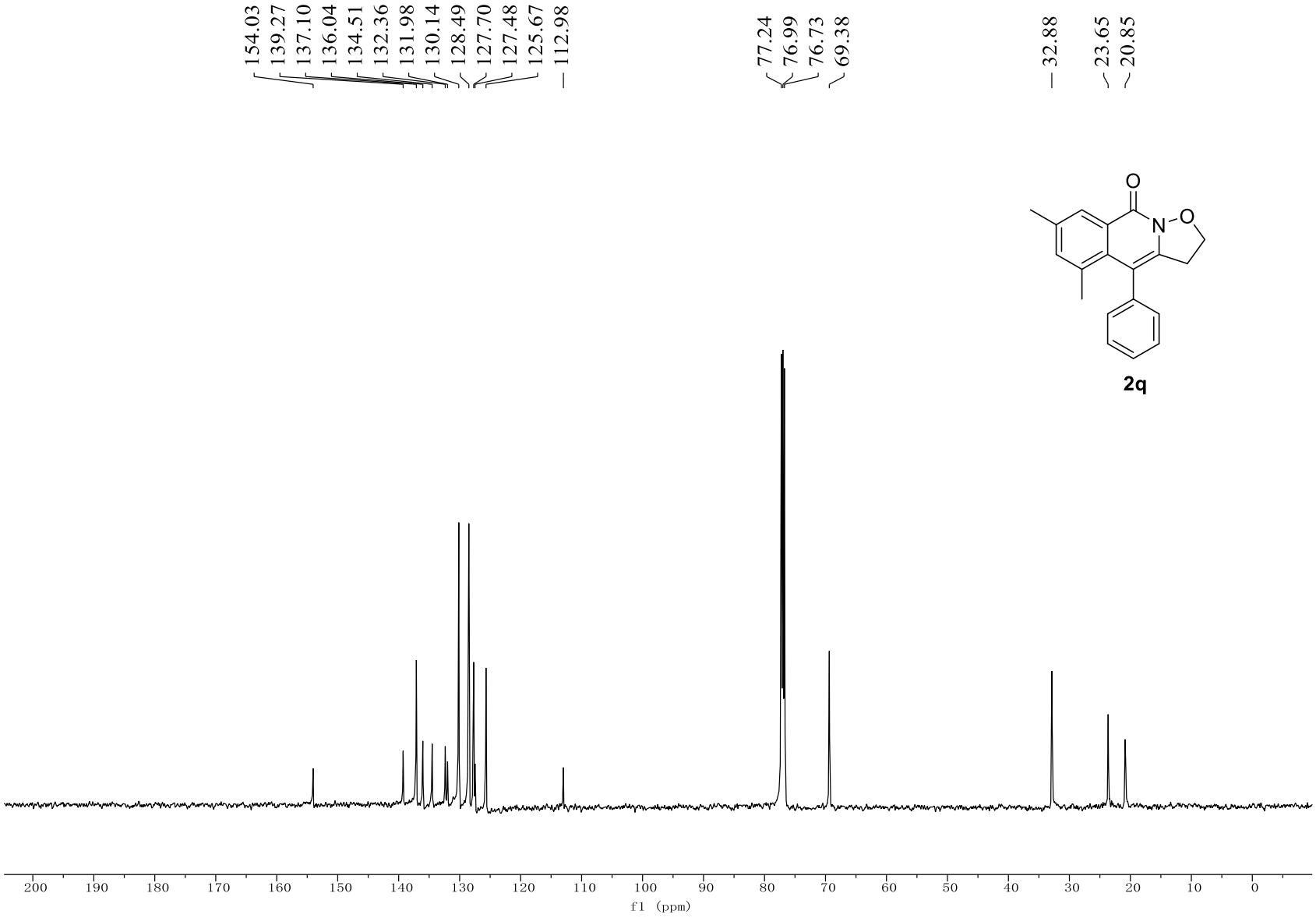
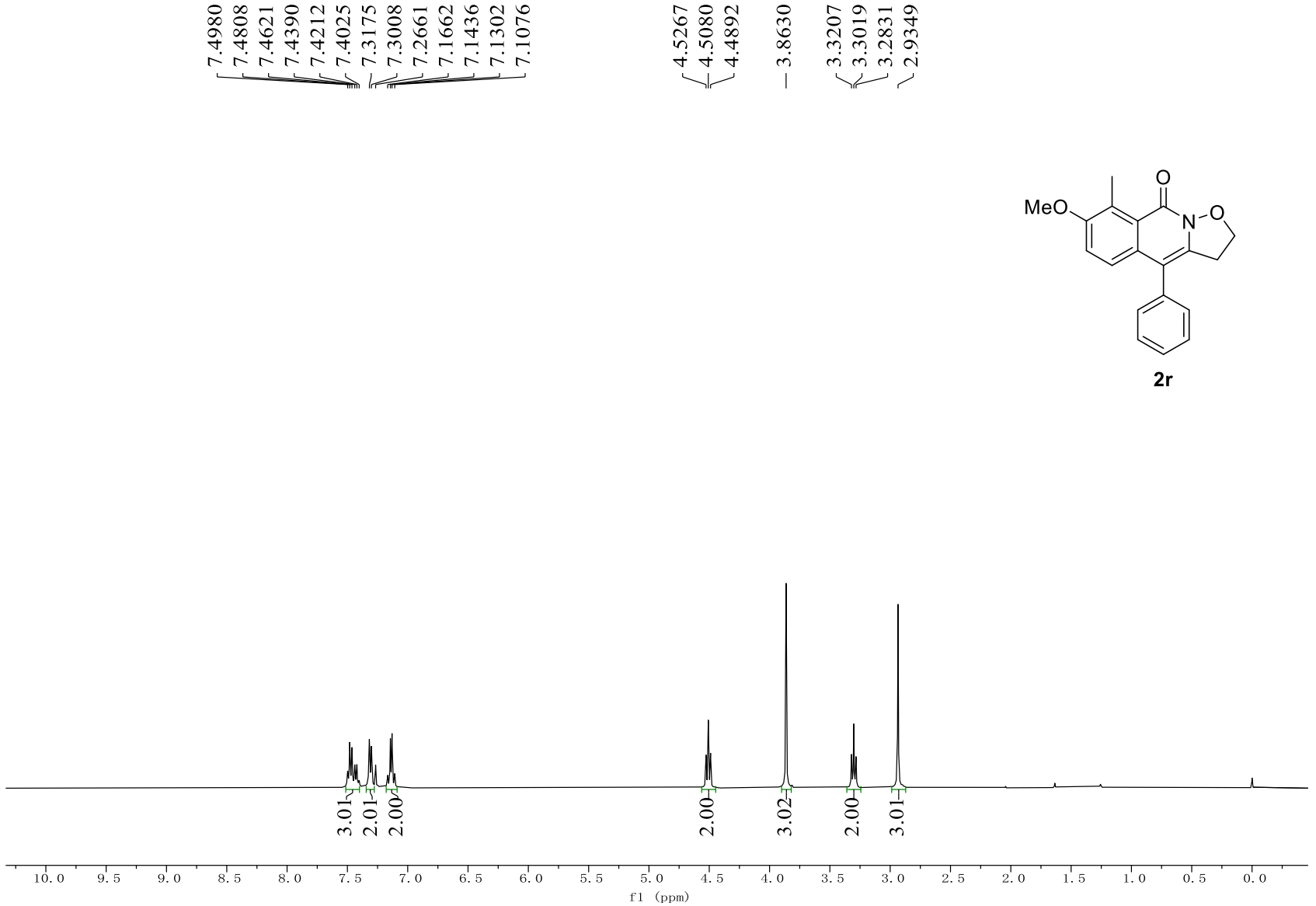
8.48
7.44
7.42
7.41
7.38
7.37
7.35
7.35
7.34
7.31
7.31
7.30
7.27
4.54
4.53
4.51
3.23
3.22
3.20
1.87
0.00
O
N
O
2p
0.98
2.96
1.98
2.03
2.06
2.00
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


154.15
139.23
135.59
134.72
134.30
133.43
130.22
128.59
127.84
127.51
126.18
126.11
113.06
77.27
77.02
76.76
69.41
33.09
23.87
O
N
O
2p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.29
7.43
7.43
7.42
7.40
7.39
7.37
7.29
7.29
7.28
7.28
7.27
7.26
7.17
4.52
4.52
4.51
4.51
4.49
4.49
3.21
3.19
3.18
2.42
1.82
-0.01
O
N
O
2q
1.00
3.00
2.00
1.00
2.00
2.03
3.01
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


154.03
139.27
137.10
136.04
134.51
132.36
131.98
130.14
128.49
127.70
127.48
125.67
112.98
77.24
76.99
76.73
69.38
32.88
23.65
20.85
O
N
O
2q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4621
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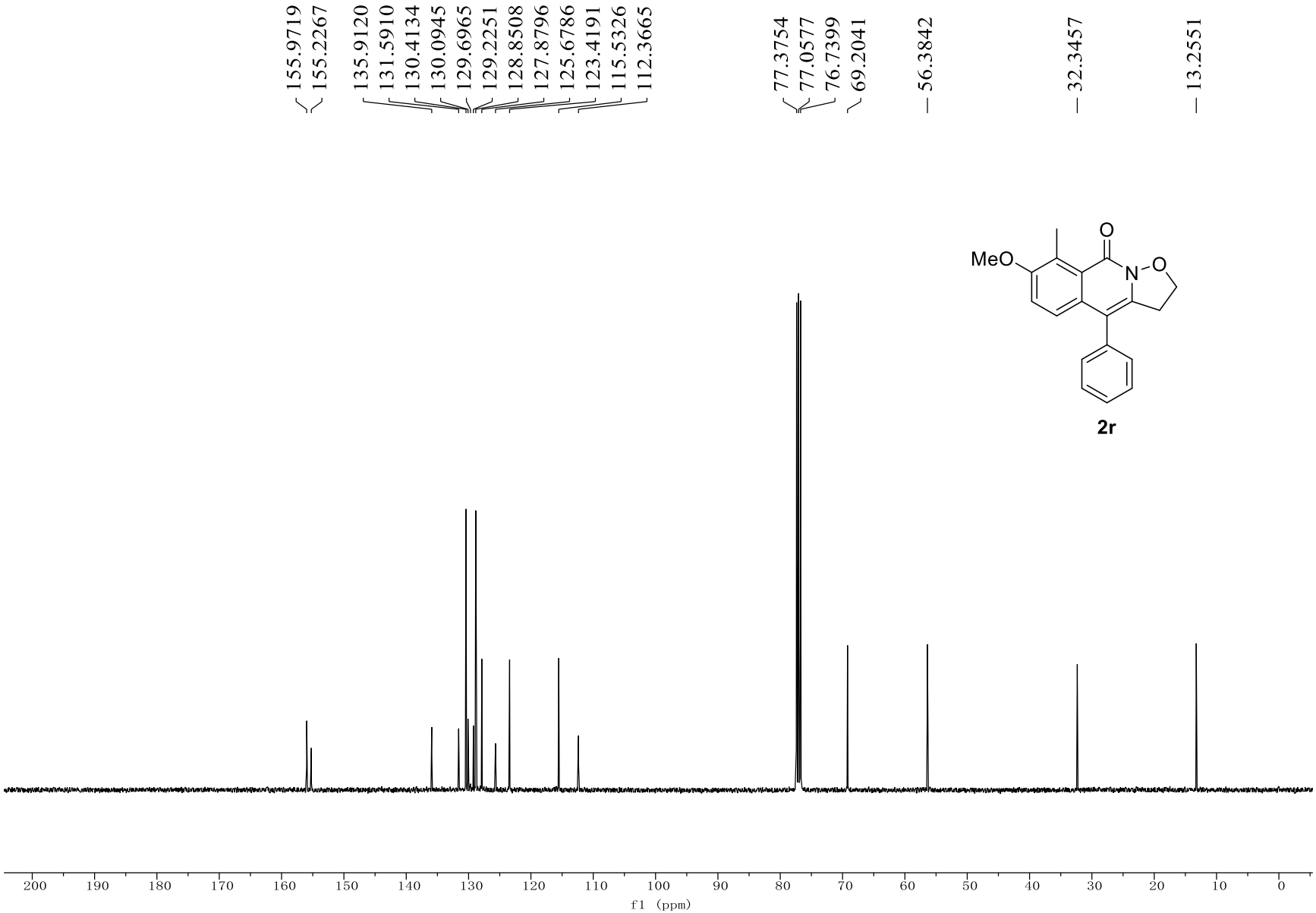
7.4212
7.4025
7.3175
7.3008
7.2661
7.1662
7.1436
7.1302
7.1076
4.5267
4.5080
4.4892
3.8630
3.3207
3.3019
3.2831
2.9349
MeO
O
N
O
2r
3.01
2.01
2.00
2.00
3.02
2.00
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


155.9719
155.2267
135.9120
131.5910
130.4134
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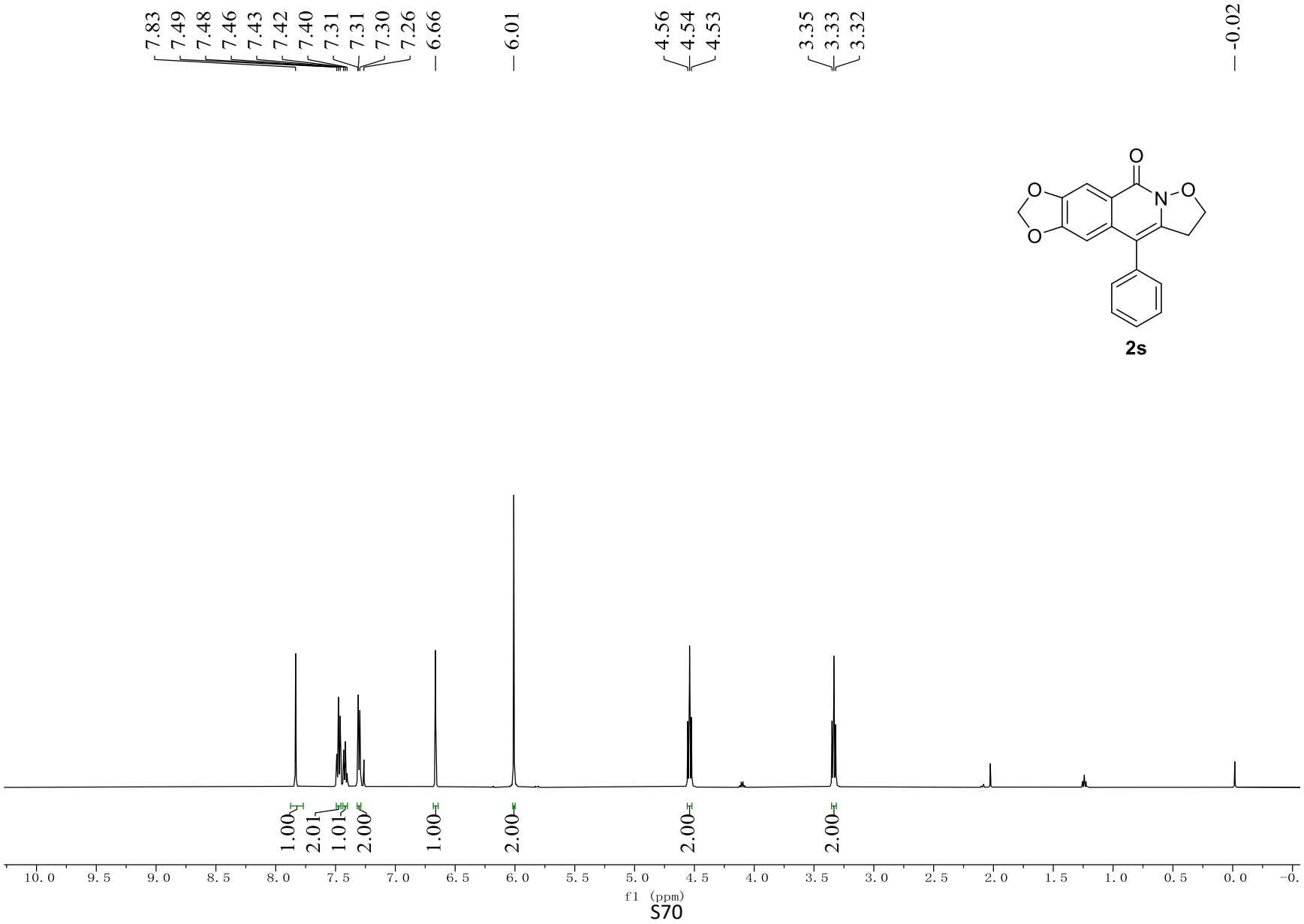
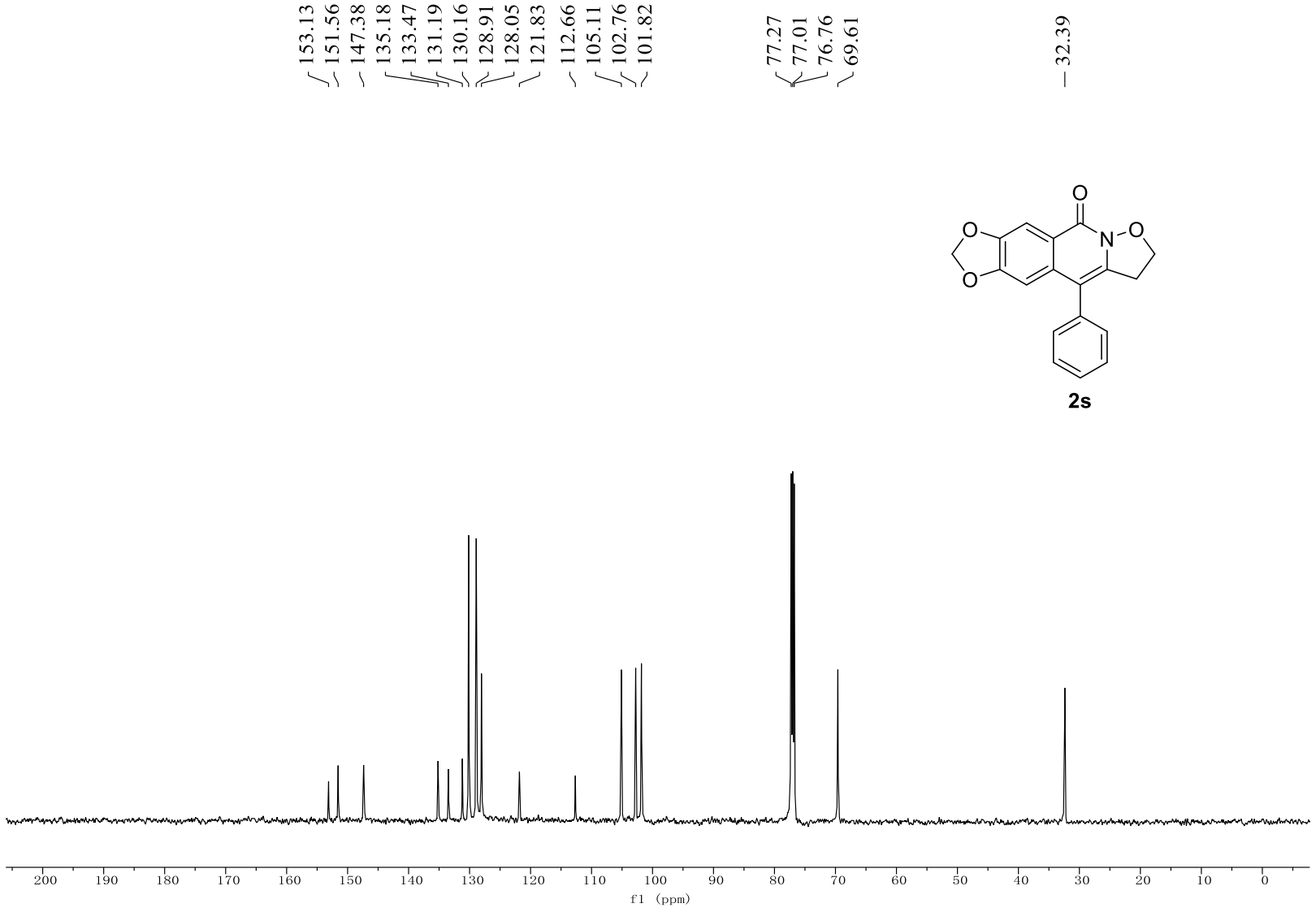
129.6965
129.2251
128.8508
127.8796
125.6786
123.4191
115.5326
112.3665
77.3754
77.0577
76.7399
69.2041
56.3842
32.3457
13.2551
MeO
O
N
O
2r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.83
7.49
7.48
7.46
7.43
7.42
7.40
7.31
7.31
7.30
7.26
6.66
6.01
4.56
4.54
4.53
3.35
3.33
3.32
-0.02
O
O
O
N
O
2s
1.00
2.01
1.01
2.00
1.00
2.00
2.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


153.13
151.56
147.38
135.18
133.47
131.19
130.16
128.91
128.05
121.83
112.66
105.11
102.76
101.82
77.27
77.01
76.76
69.61
32.39
O
O
O
N
O
2s
200
190
180
170
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130
120
110
100
90
80
70
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50
40
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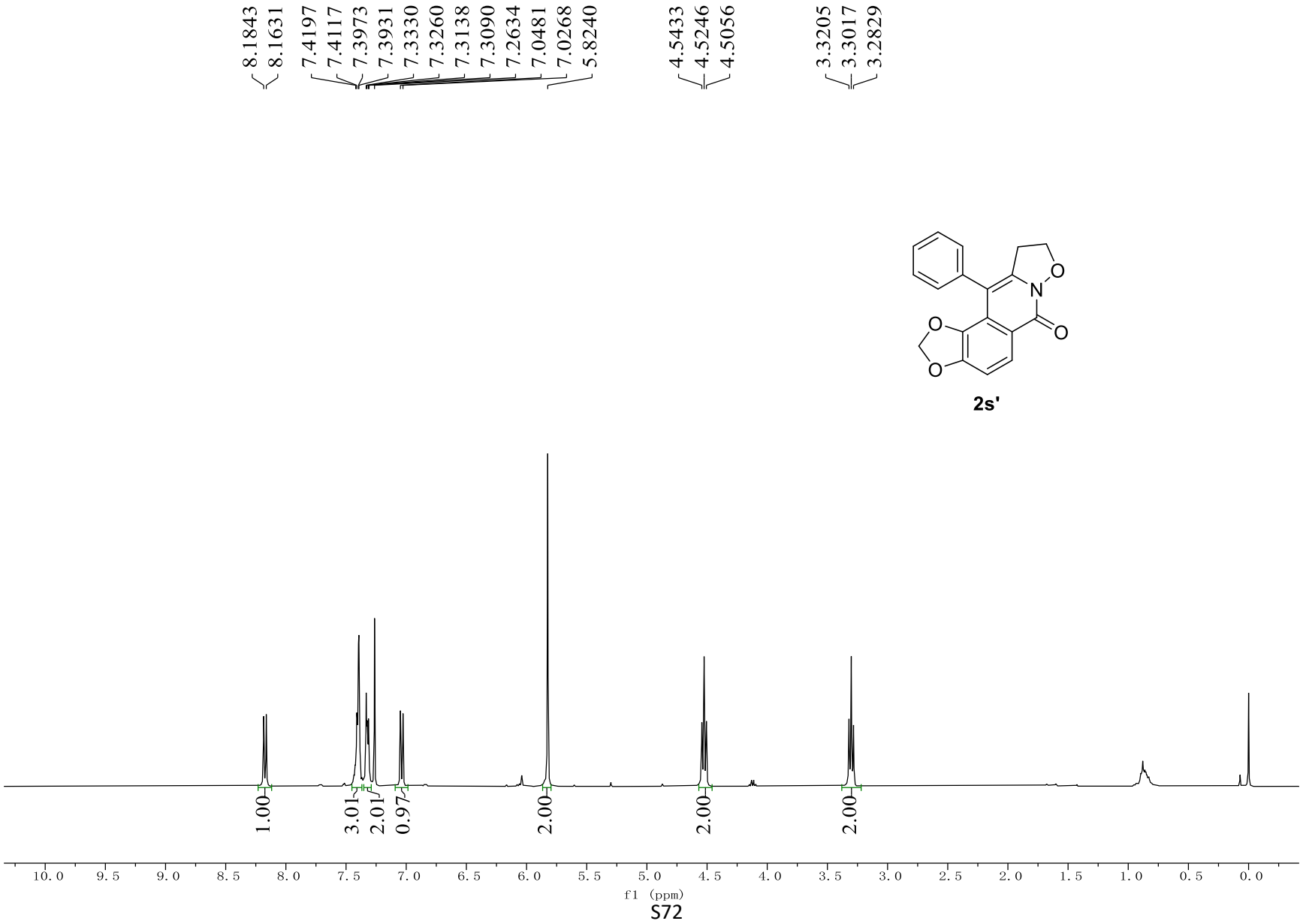
20
10
0
f1 (ppm)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7.3931
7.3330
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7.3138
7.3090
7.2634
7.0481
7.0268
5.8240
4.5433
4.5246
4.5056
3.3205
3.3017
3.2829
O
N
O
O
O
O
2s'
1.00
3.01
2.01
0.97
2.00
2.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
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1.0
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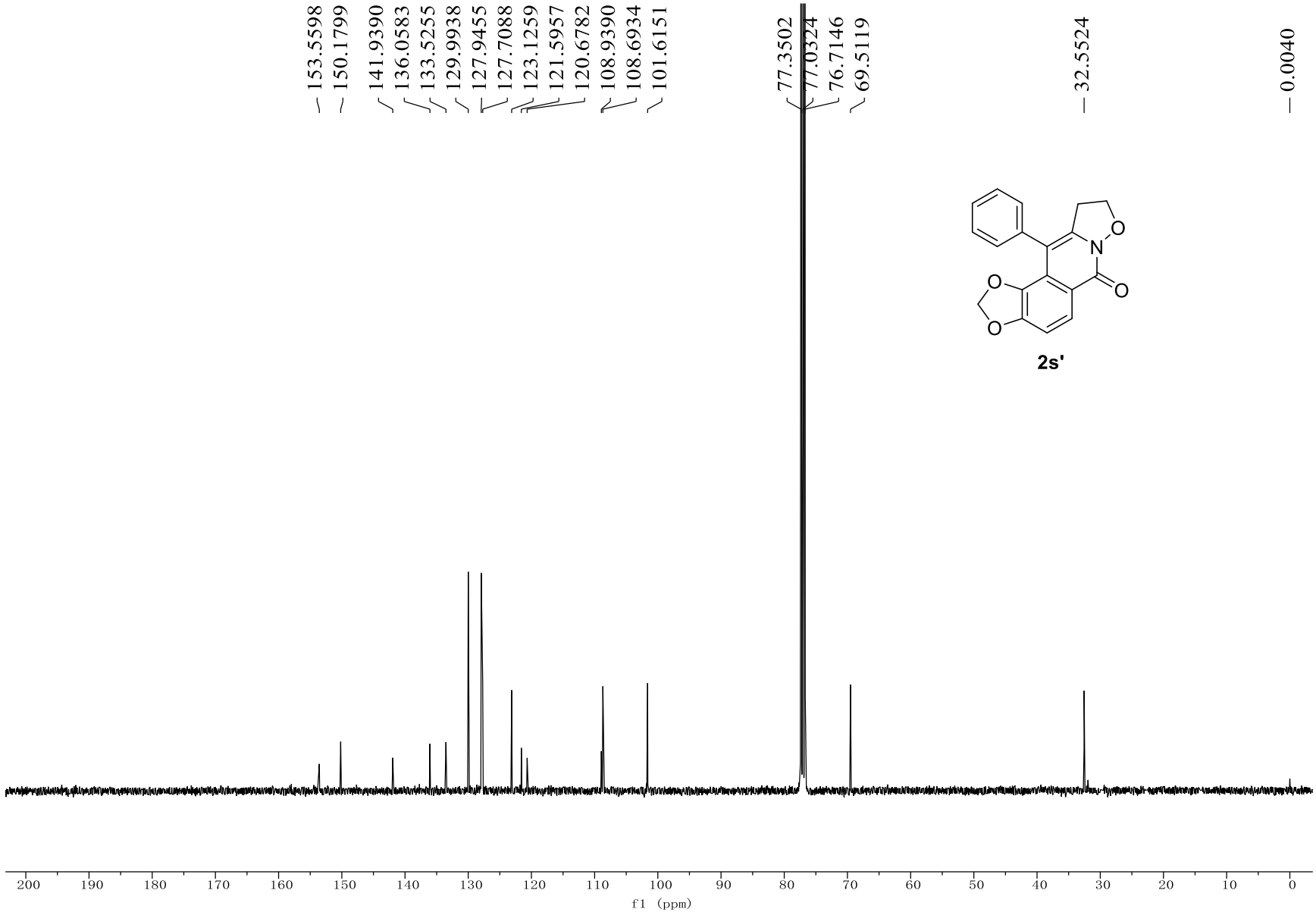
0.0
f1 (ppm)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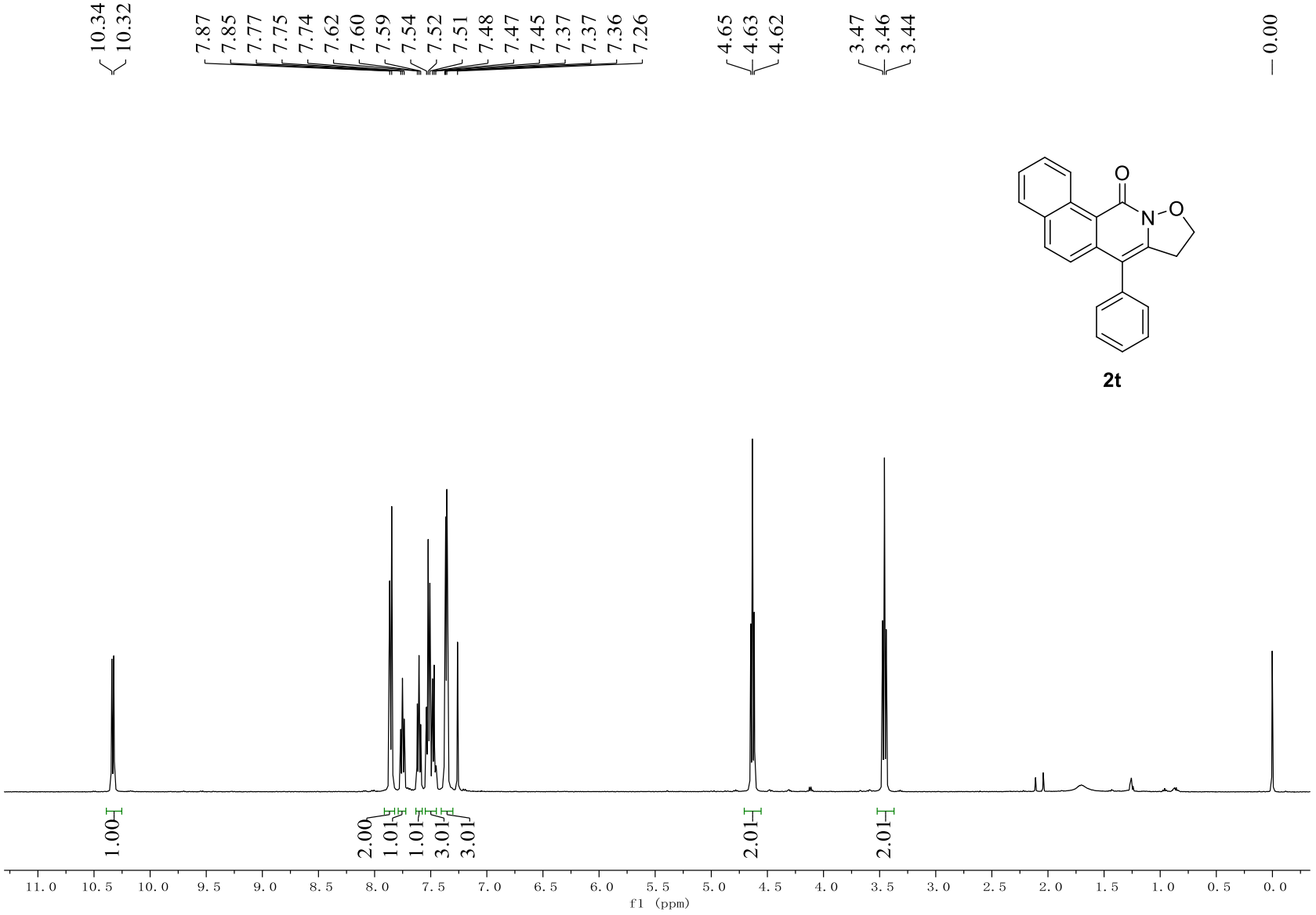
123.1259
121.5957
120.6782
108.9390
108.6934
101.6151
77.3502
77.0324
76.7146
69.5119
32.5524
0.0040
O
N
O
O
O
O
2s'
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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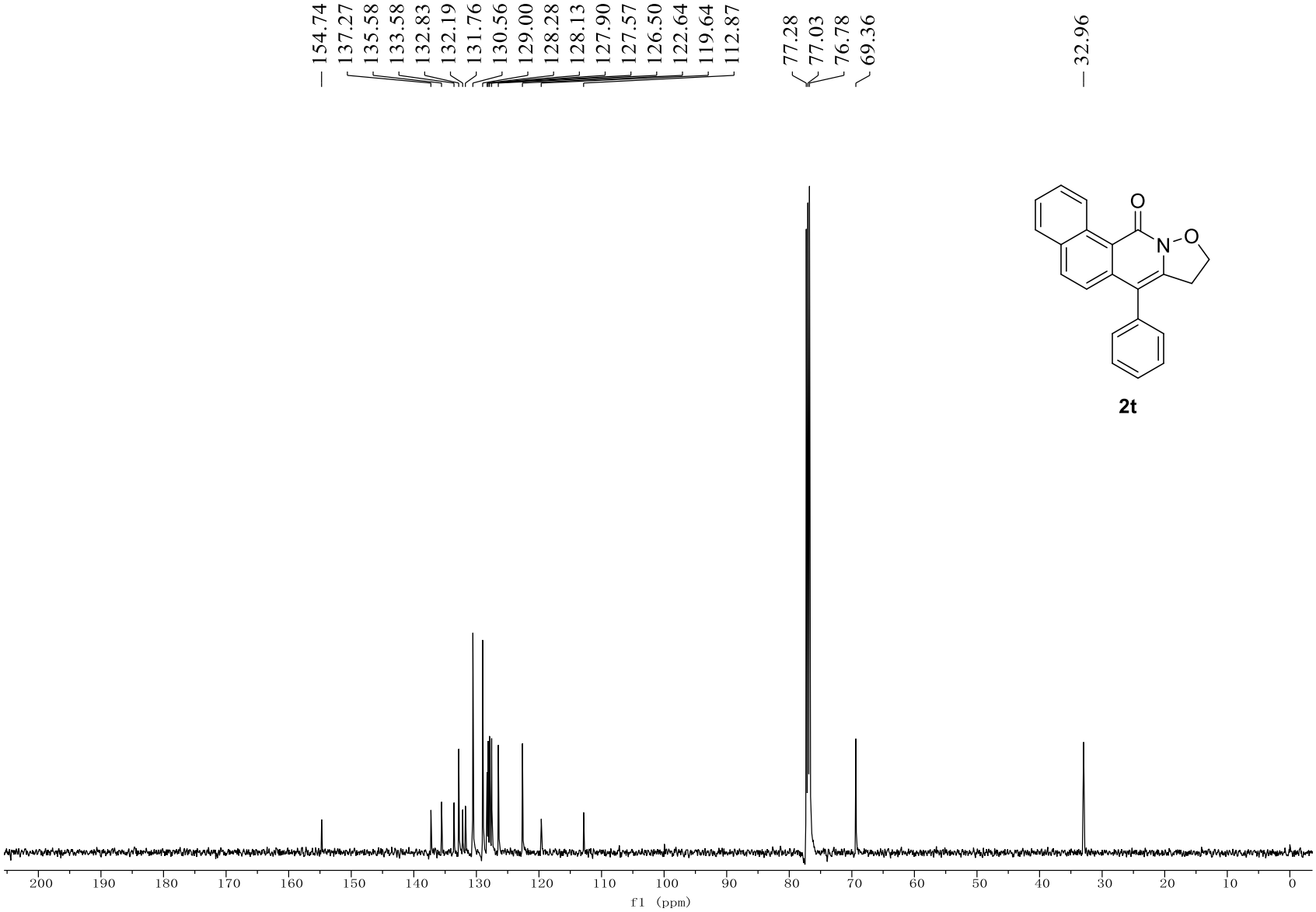
7.59
7.54
7.52
7.51
7.48
7.47
7.45
7.37
7.37
7.36
7.26
4.65
4.63
4.62
3.47
3.46
3.44
0.00
O
N
O
2t
1.00
2.00
1.01
1.01
3.01
3.01
2.01
2.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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137.27
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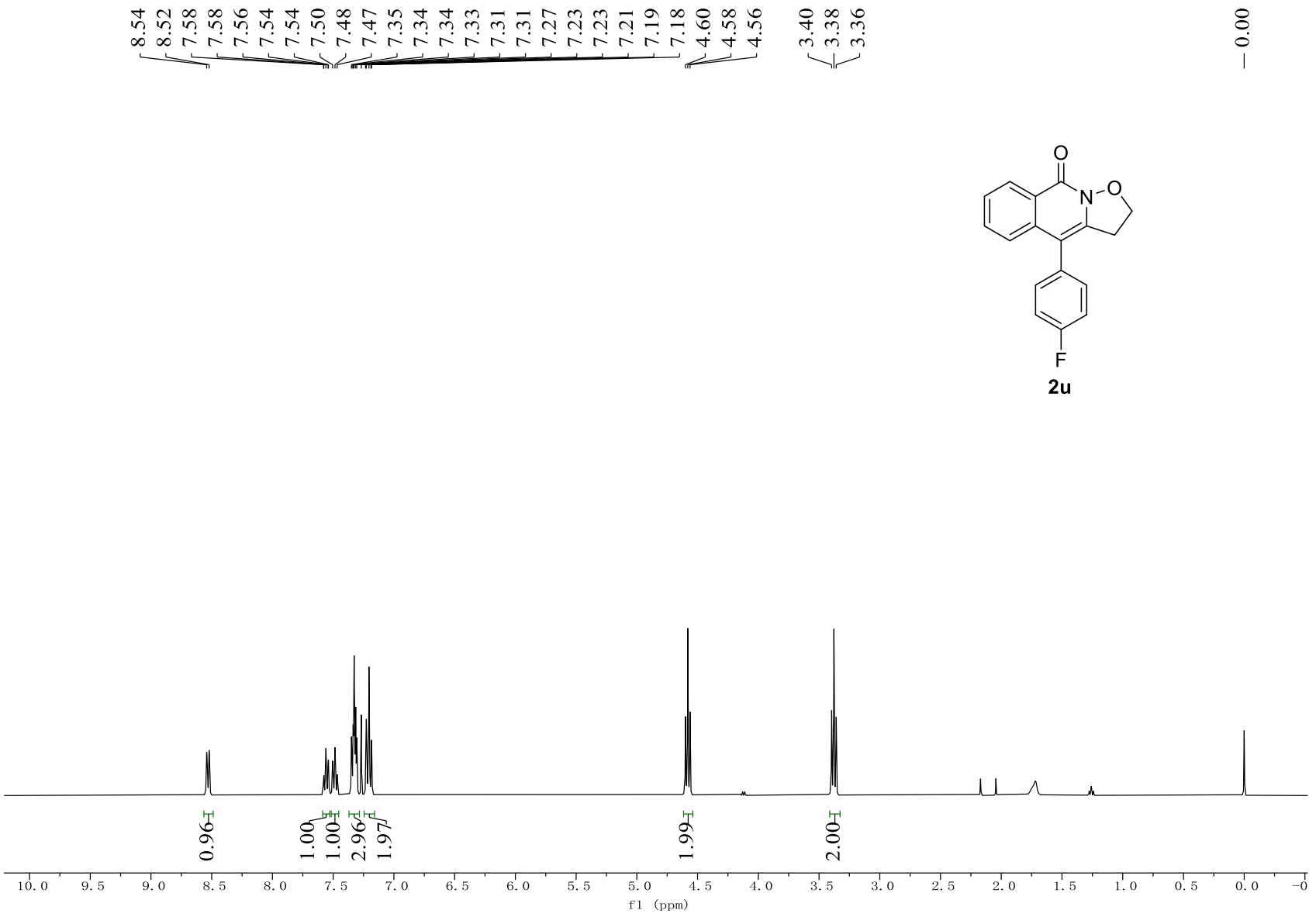
133.58
132.83
132.19
131.76
130.56
129.00
128.28
128.13
127.90
127.57
126.50
122.64
119.64
112.87
77.28
77.03
76.78
69.36
32.96
O
N
O
2t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.35
7.34
7.34
7.33
7.31
7.31
7.27
7.23
7.23
7.21
7.19
7.18
4.60
4.58
4.56
3.40
3.38
3.36
0.00
O
N
O
F
2u
0.96
1.00
1.00
2.96
1.97
1.99
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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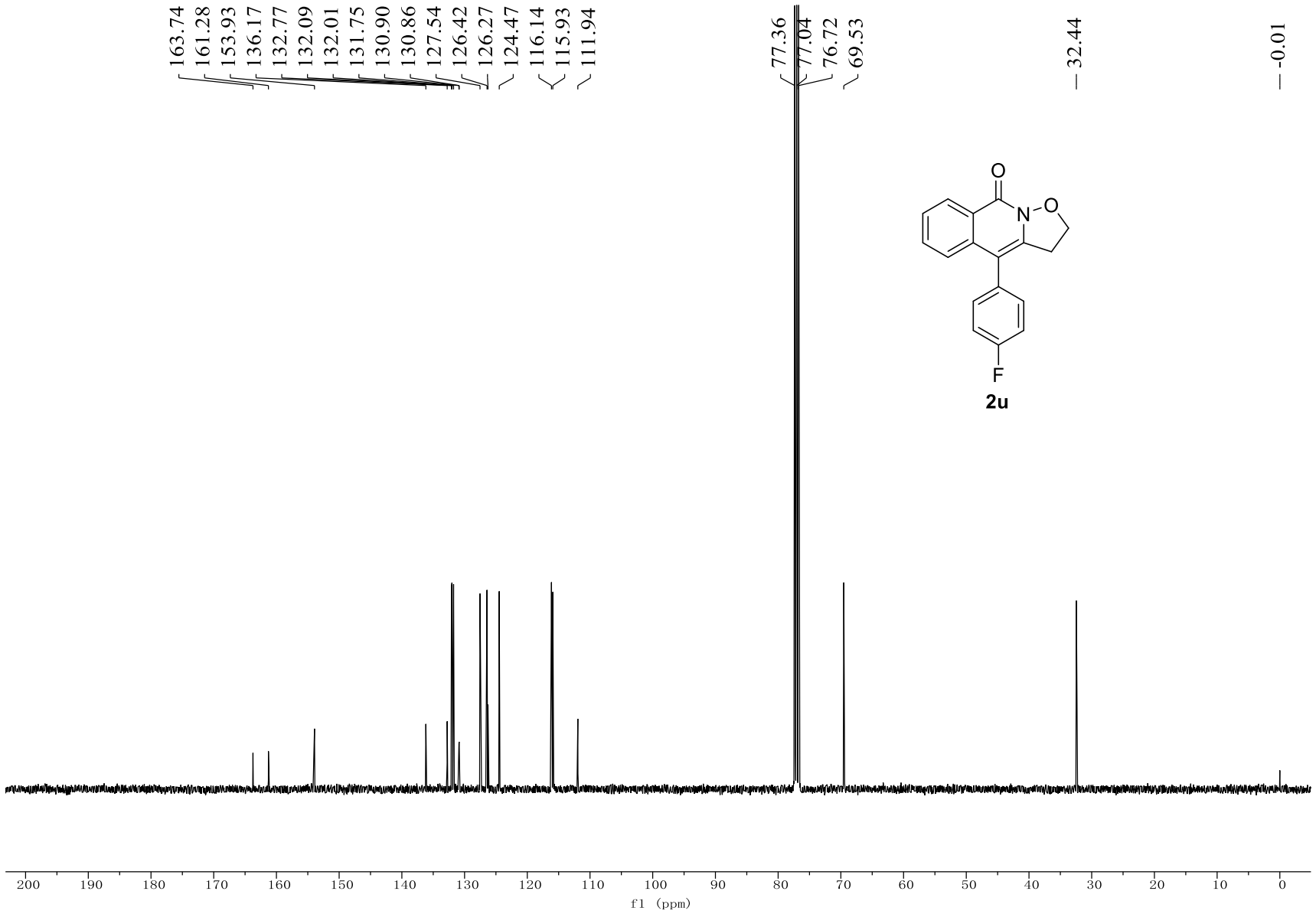
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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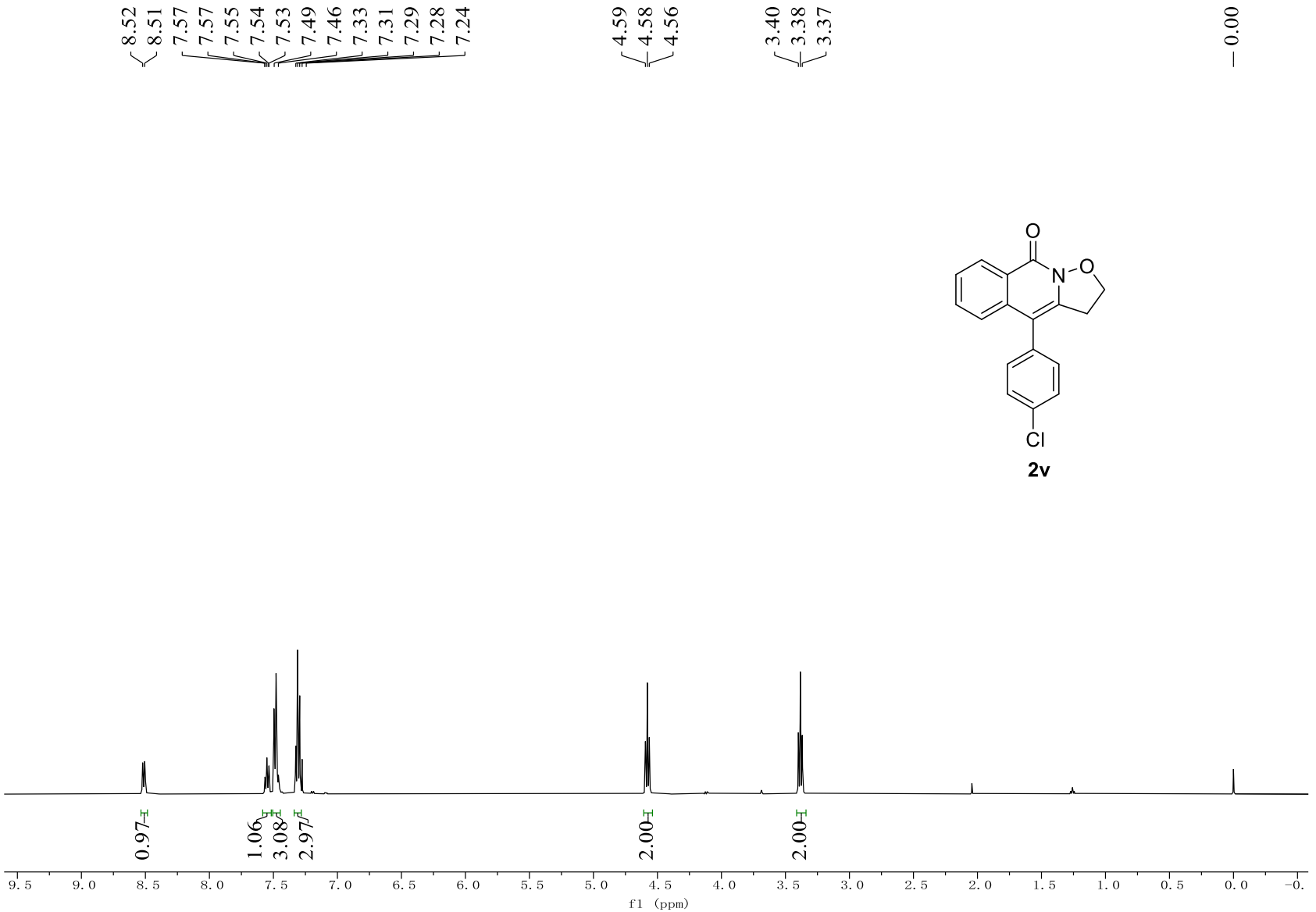
161.28
153.93
136.17
132.77
132.09
132.01
131.75
130.90
130.86
127.54
126.42
126.27
124.47
116.14
115.93
111.94
77.36
77.04
76.72
69.53
32.44
-0.01
O
N
O
F
2u
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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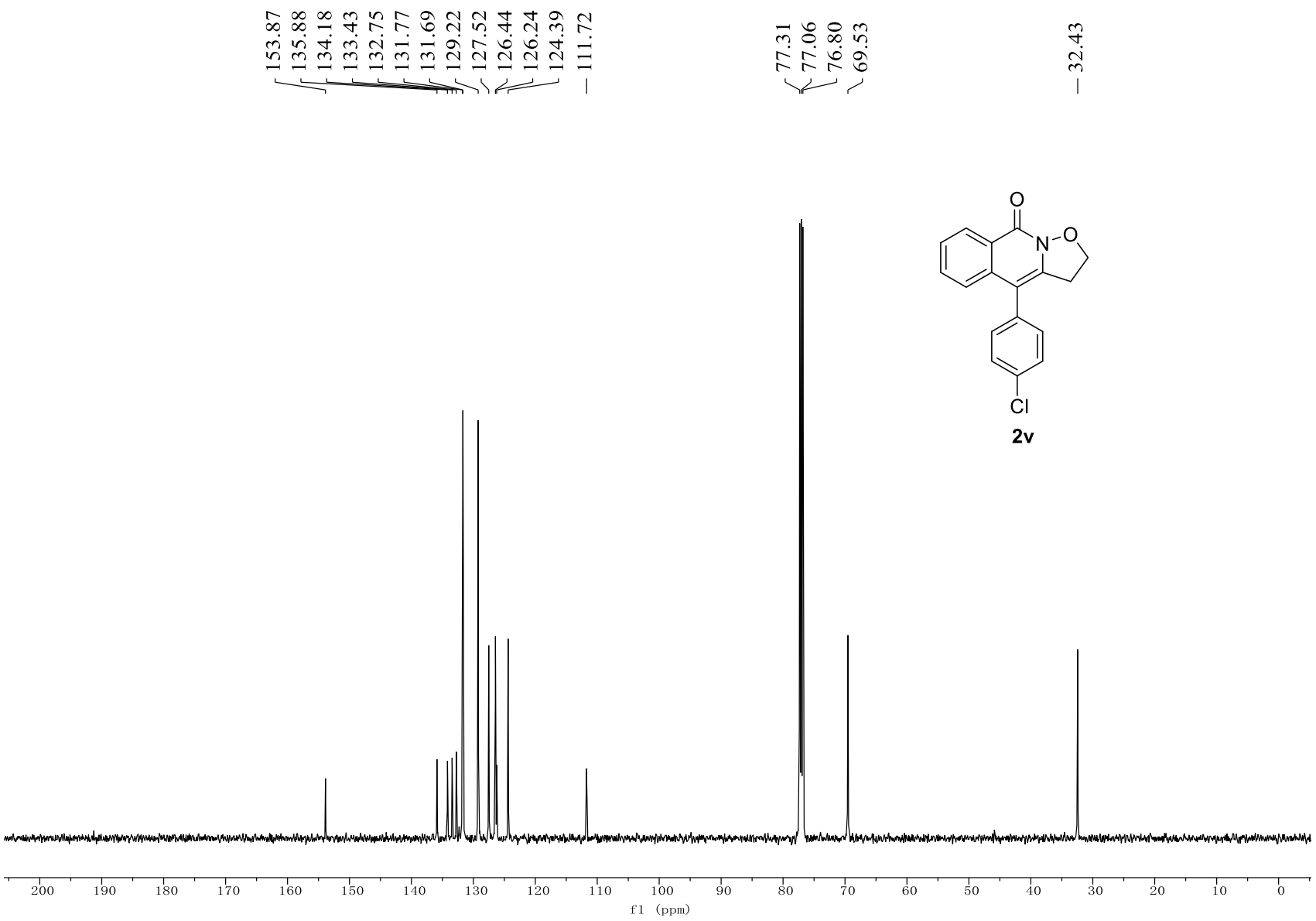
7.57
7.55
7.54
7.53
7.49
7.46
7.33
7.31
7.29
7.28
7.24
4.59
4.58
4.56
3.40
3.38
3.37
0.00
O
N
O
Cl
2v
0.97
1.06
3.08
2.97
2.00
2.00
f1 (ppm)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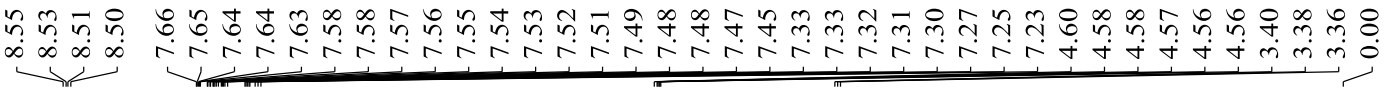
134.18
133.43
132.75
131.77
131.69
129.22
127.52
126.44
126.24
124.39
111.72
77.31
77.06
76.80
69.53
32.43
O
N
O
Cl
2v
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.53
8.51
8.50
7.66
7.65
7.64
7.64
7.63
7.58
7.58
7.57
7.56
7.55
7.54
7.53
7.52
7.51
7.49
7.48
7.48
7.47
7.45
7.33
7.33
7.32
7.31
7.30
7.27
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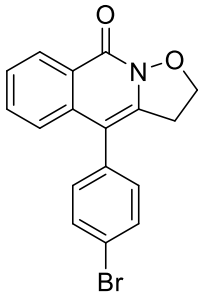
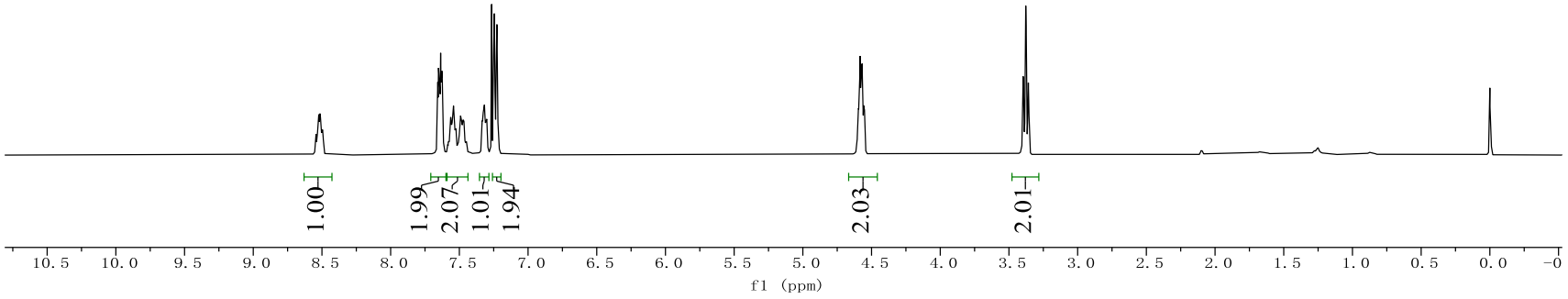
4.56
4.56
3.40
3.38
3.36
0.00


O
N
O
Br

2w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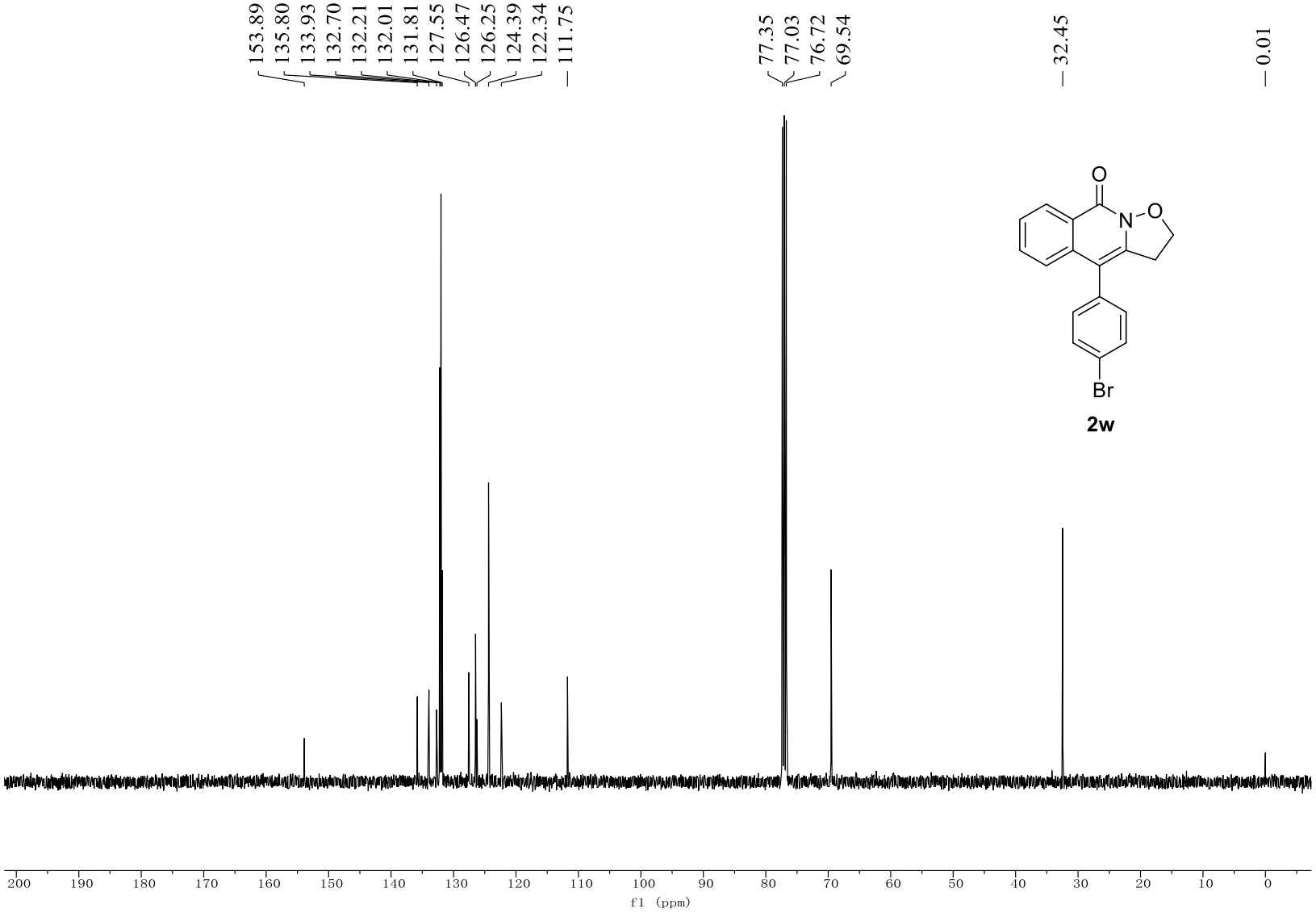
1.01
1.94
2.03
2.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0
f1 (ppm)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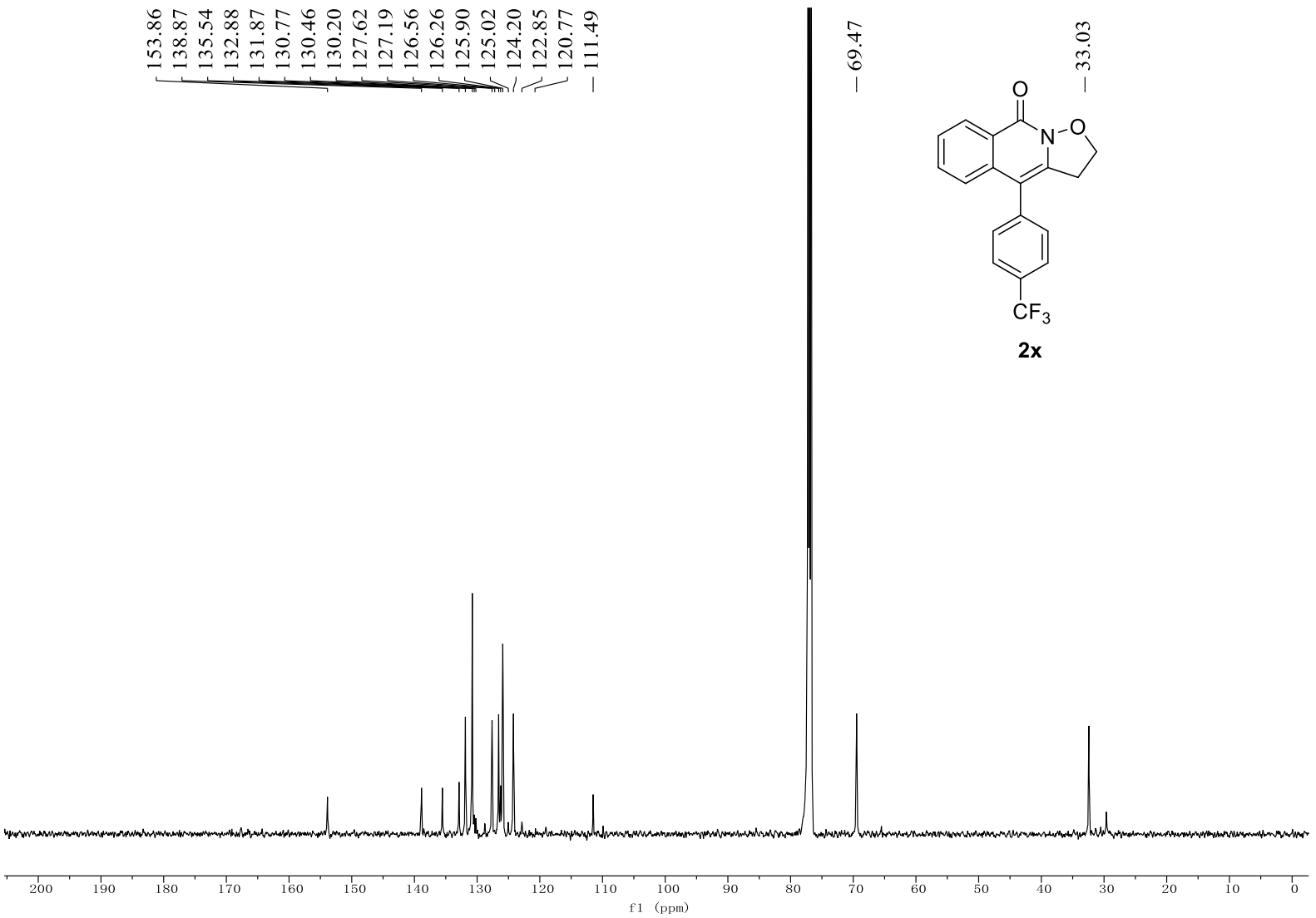
132.21
132.01
131.81
127.55
126.47
126.25
124.39
122.34
111.75
77.35
77.03
76.72
69.54
32.45
0.01
O
N
O
Br
2w
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

8.54
8.53
7.79
7.77
7.58
7.57
7.55
7.51
7.50
7.31
7.29
7.26
4.61
4.59
4.58
3.41
3.39
3.38
-0.01
O
N
O
CF3
1.00
2.01
1.05
3.11
0.98
2.01
1.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

2x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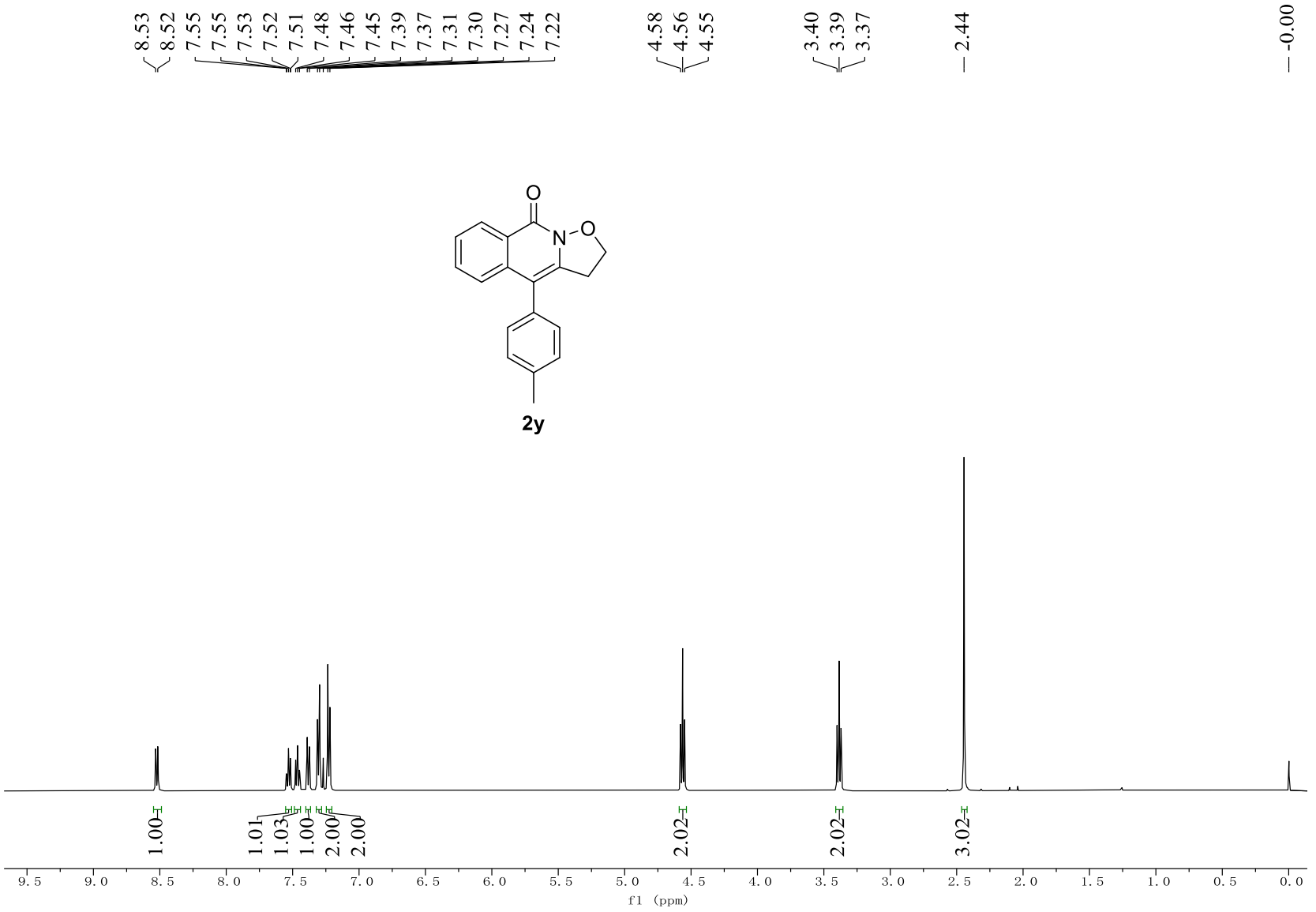
131.87
130.77
130.46
130.20
127.62
127.19
126.56
126.26
125.90
125.02
124.20
122.85
120.77
111.49
69.47
33.03
O
N
O
CF3
2x
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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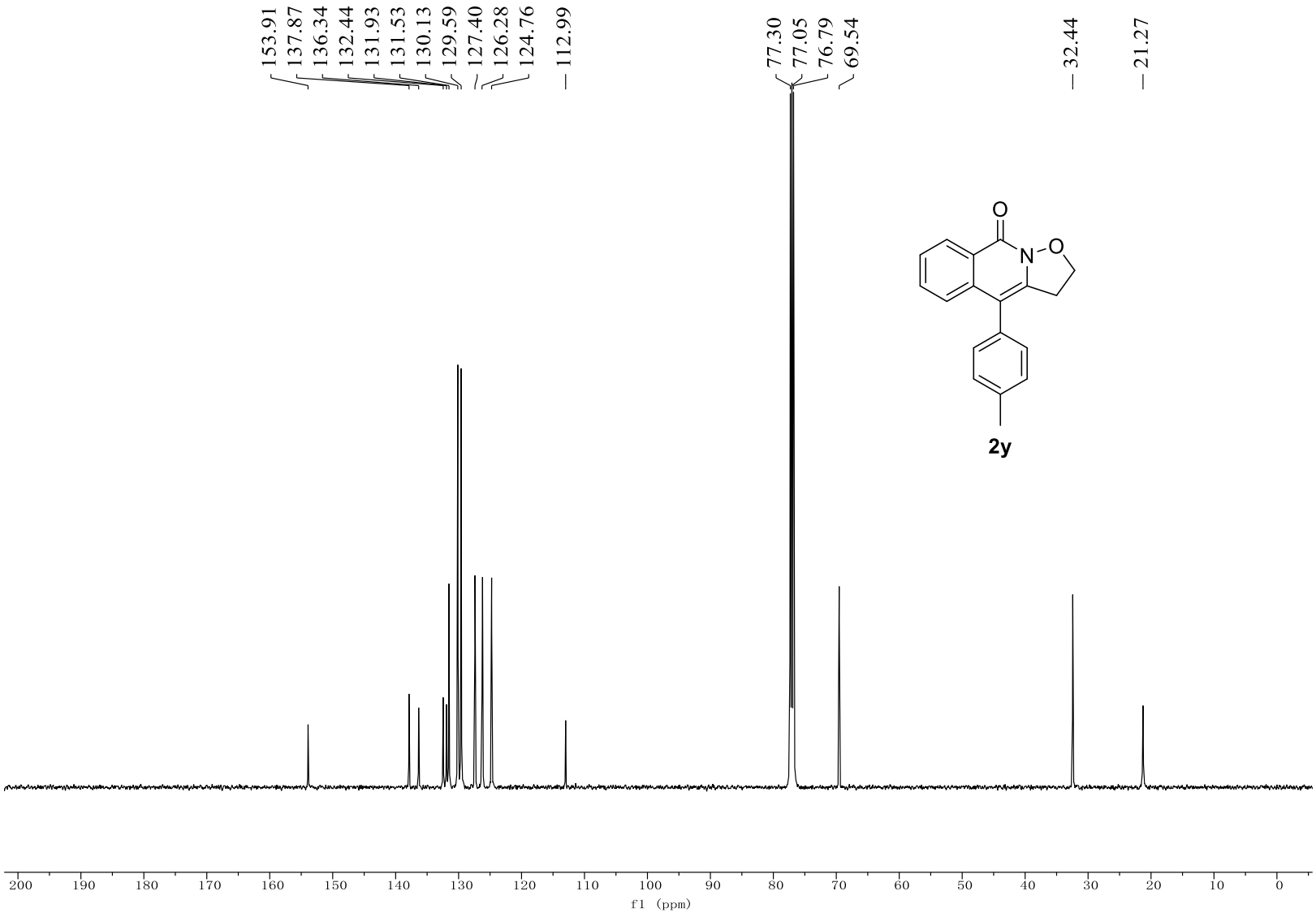
7.53
7.52
7.51
7.48
7.46
7.45
7.39
7.37
7.31
7.30
7.27
7.24
7.22
4.58
4.56
4.55
3.40
3.39
3.37
2.44
-0.00
O
N
O
2y
1.00
1.01
1.03
1.00
2.00
2.00
2.02
2.02
3.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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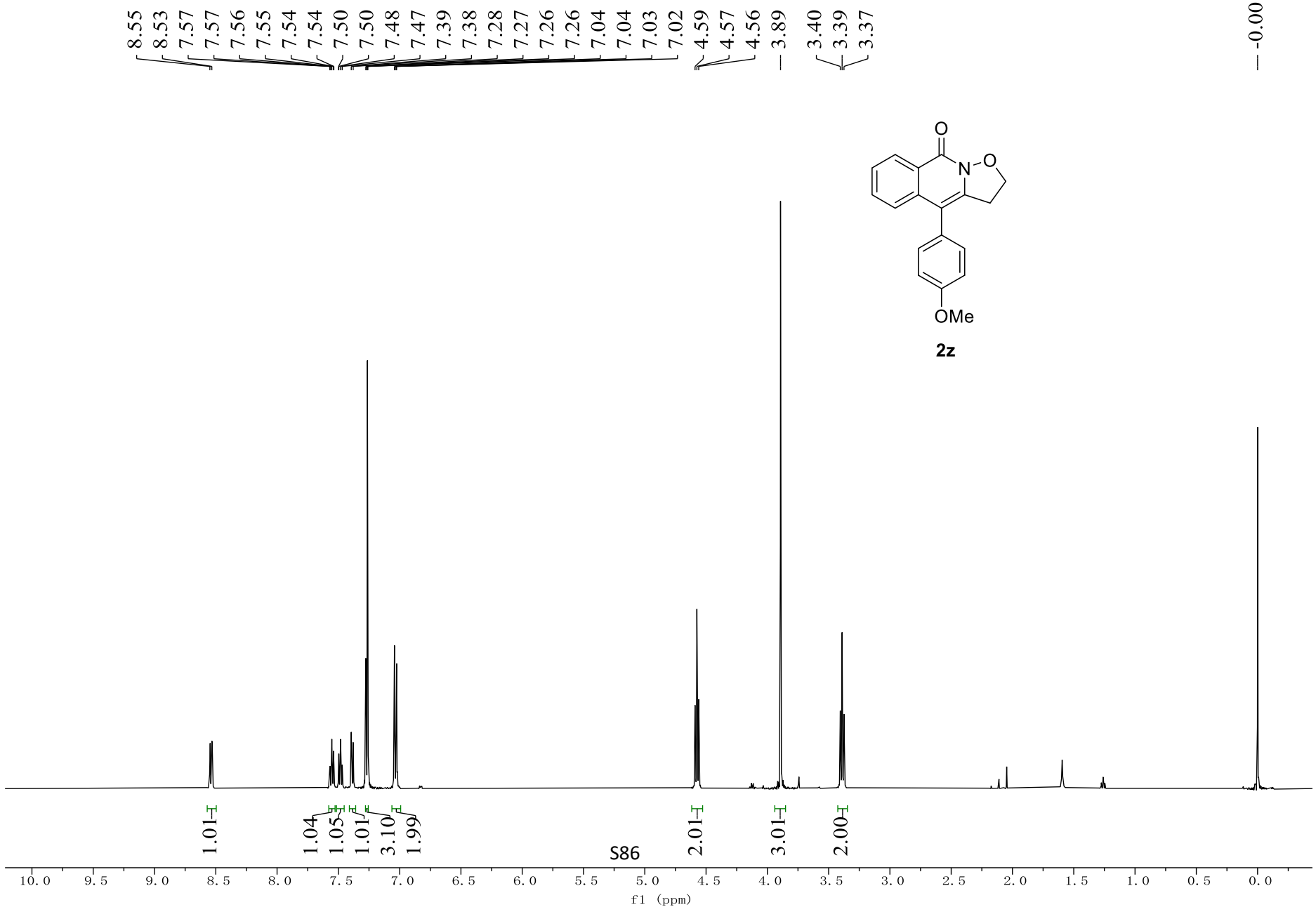
131.93
131.53
130.13
129.59
127.40
126.28
124.76
112.99
77.30
77.05
76.79
69.54
32.44
21.27
O
N
O
2y
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.57
7.56
7.55
7.54
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7.50
7.50
7.48
7.47
7.39
7.38
7.28
7.27
7.26
7.26
7.04
7.04
7.03
7.02
4.59
4.57
4.56
3.89
3.40
3.39
3.37
-0.00
O
N
O
OMe
2z
1.01
1.04
1.05
1.01
3.10
1.99
2.01
3.01
2.00
S86
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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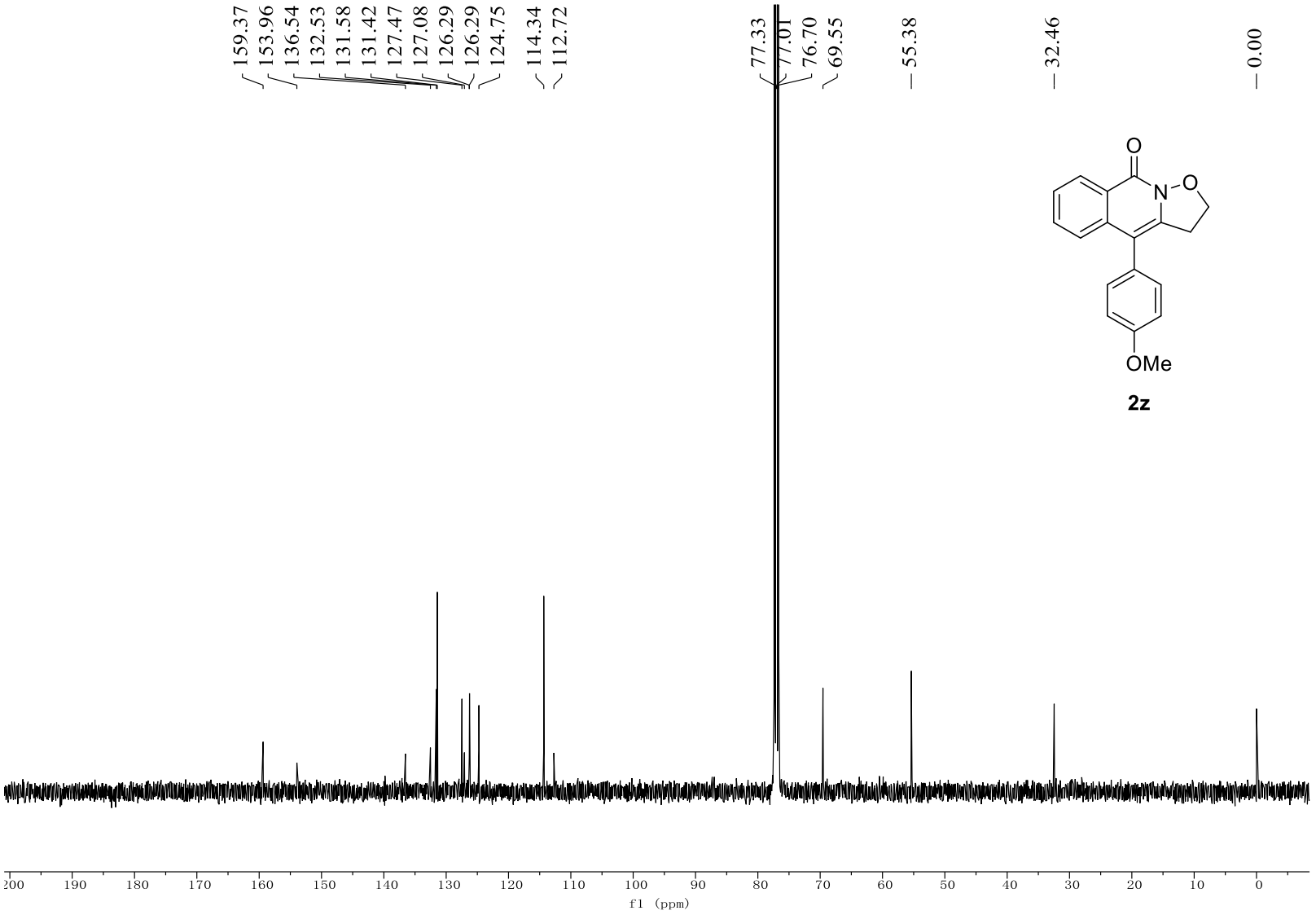
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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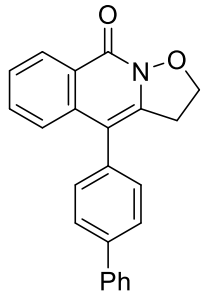
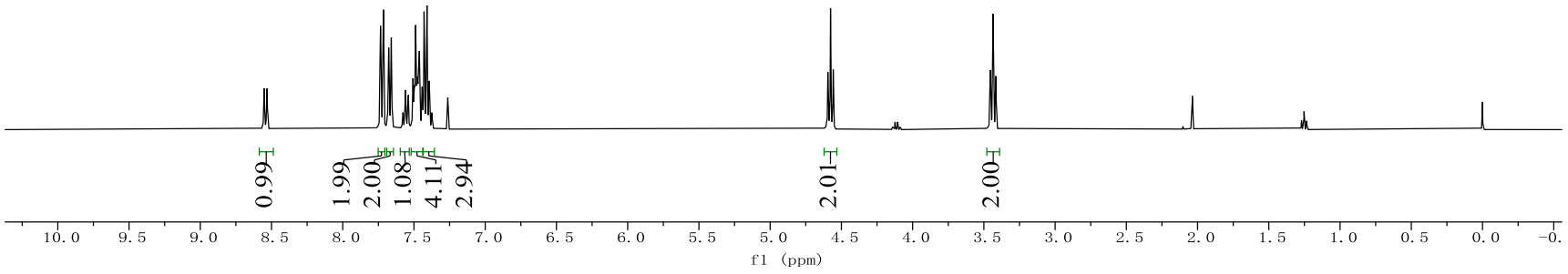
131.42
127.47
127.08
126.29
126.29
124.75
114.34
112.72
77.33
77.01
76.70
69.55
55.38
32.46
0.00
O
N
O
OMe
2z
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.55
8.53
7.73
7.71
7.68
7.66
7.58
7.56
7.54
7.54
7.51
7.50
7.49
7.48
7.47
7.46
7.44
7.43
7.41
7.39
7.37
7.26
4.60
4.58
4.56
3.45
3.44
3.42
0.00


O
N
O
Ph

2aa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2.94
2.01
2.00
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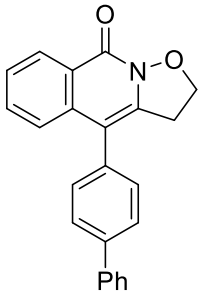
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

153.95
140.91
140.38
136.16
133.92
132.65
131.69
130.75
128.95
127.68
127.58
127.48
127.08
126.35
126.31
124.75
112.68

77.41
77.09
76.78
69.63

32.55



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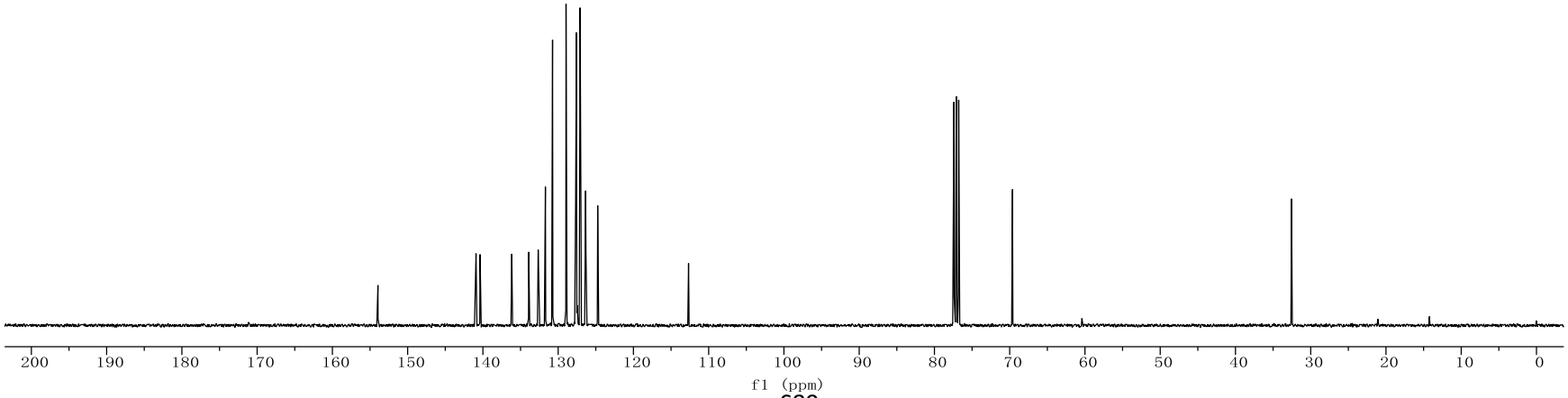

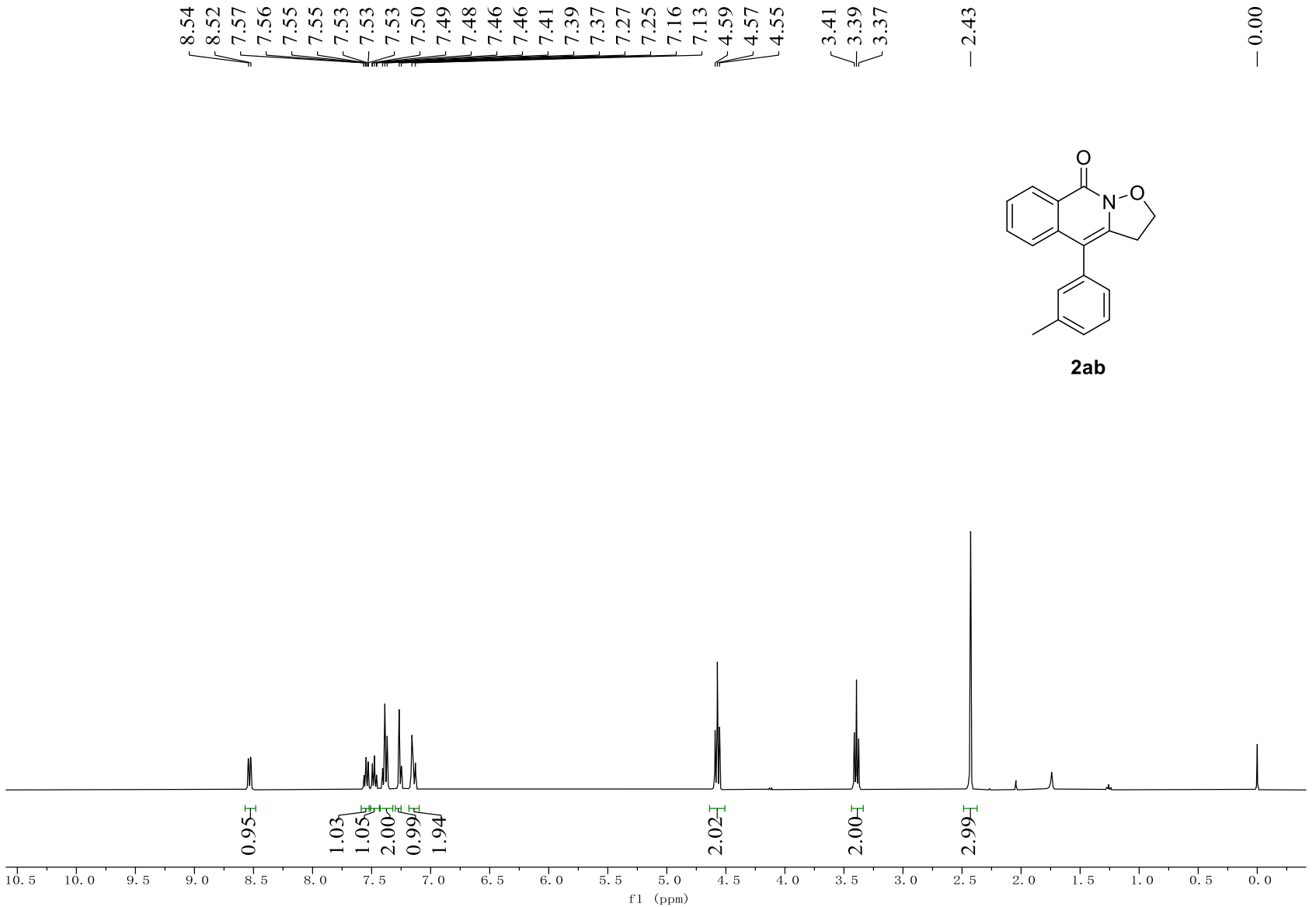
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7.46
7.46
7.41
7.39
7.37
7.27
7.25
7.16
7.13
4.59
4.57
4.55
3.41
3.39
3.37
2.43
0.00
O
N
O
2ab
0.95
1.03
1.05
2.00
0.99
1.94
2.02
2.00
2.99
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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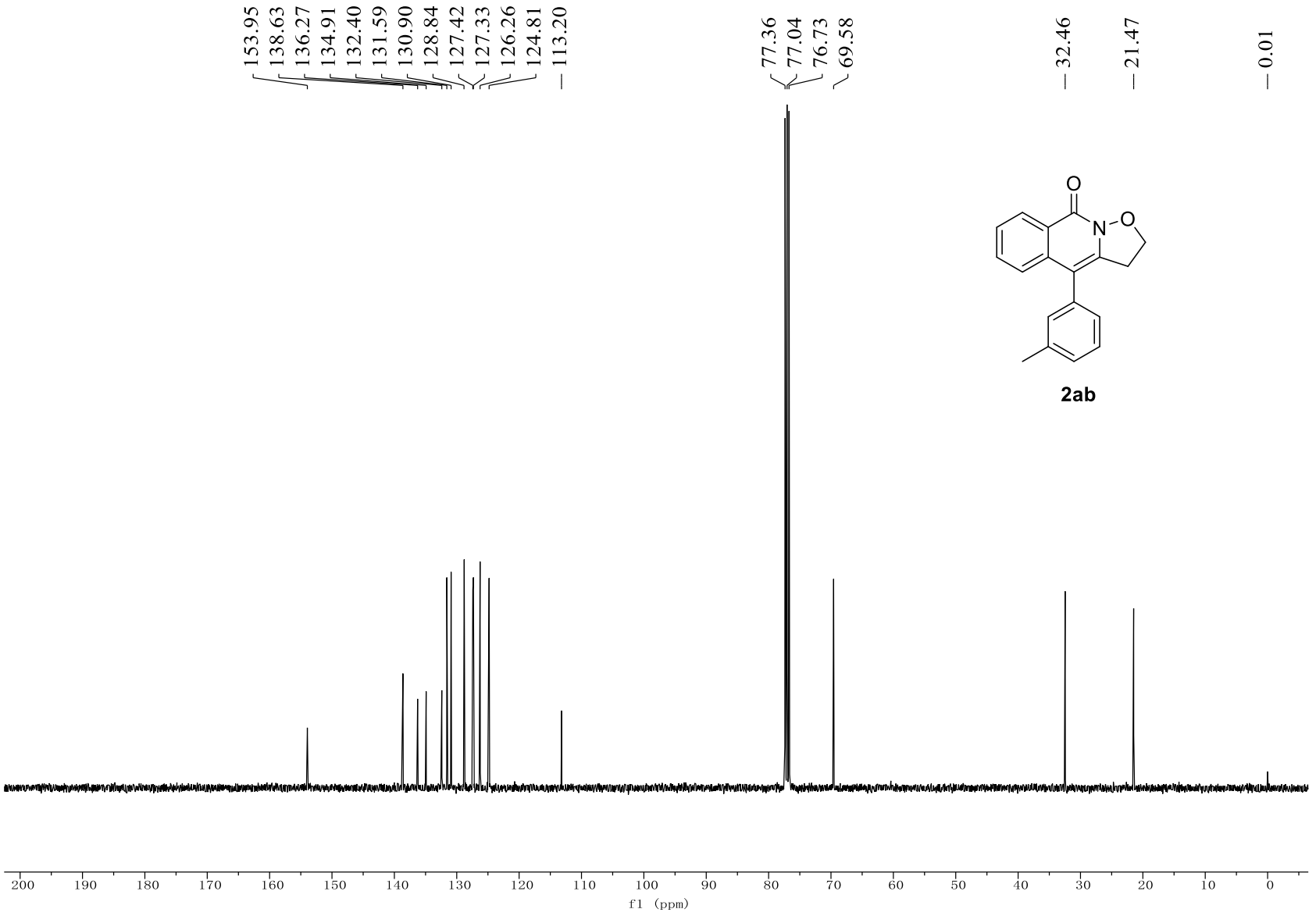
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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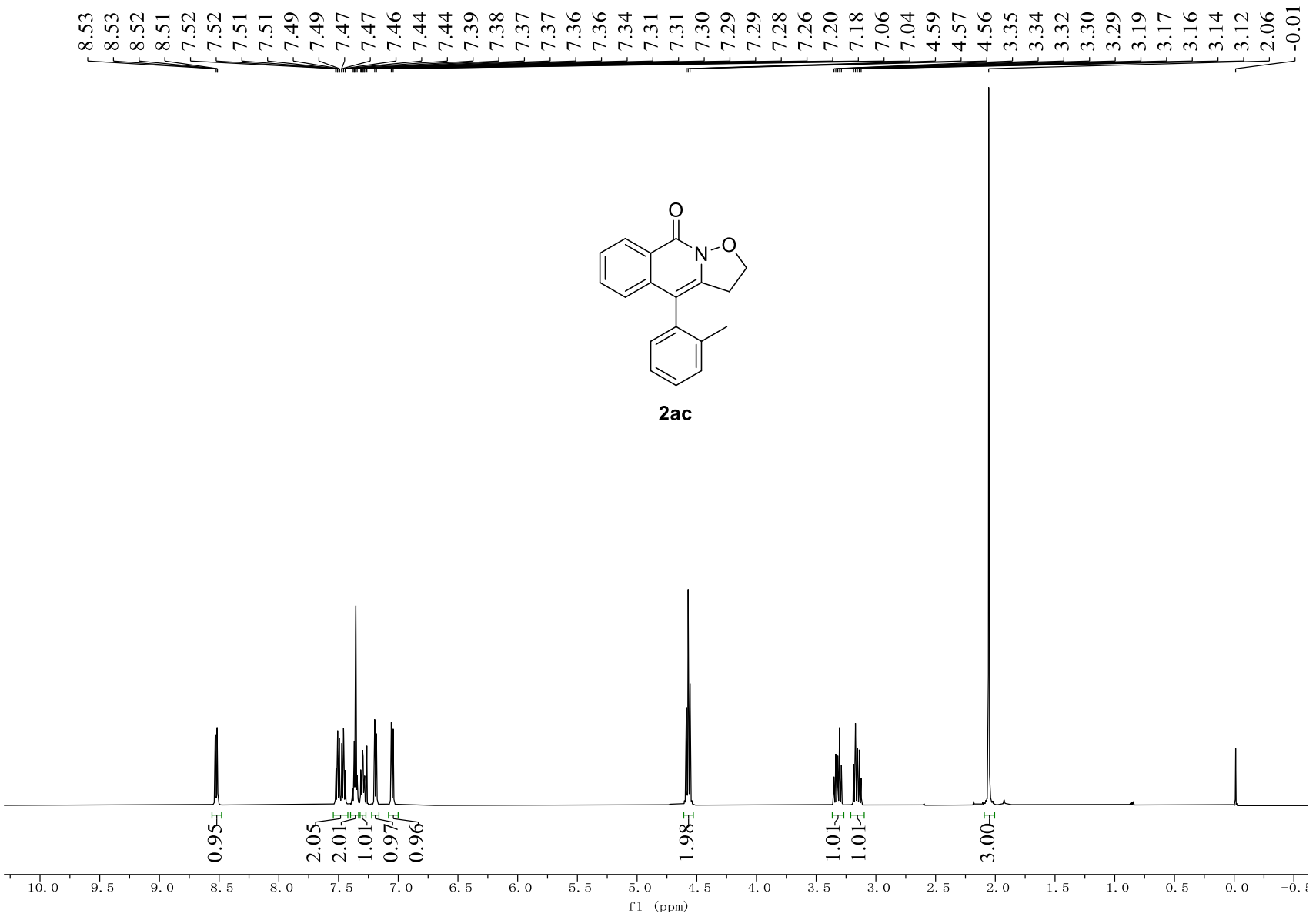
127.42
127.33
126.26
124.81
113.20
77.36
77.04
76.73
69.58
32.46
21.47
0.01
O
N
O
2ab
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.37
7.37
7.36
7.36
7.34
7.31
7.31
7.30
7.29
7.29
7.28
7.26
7.20
7.18
7.06
7.04
4.59
4.57
4.56
3.35
3.34
3.32
3.30
3.29
3.19
3.17
3.16
3.14
3.12
2.06
-0.01
O
N
O
2ac
0.95
2.05
2.01
1.01
0.97
0.96
1.98
1.01
1.01
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
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1.0
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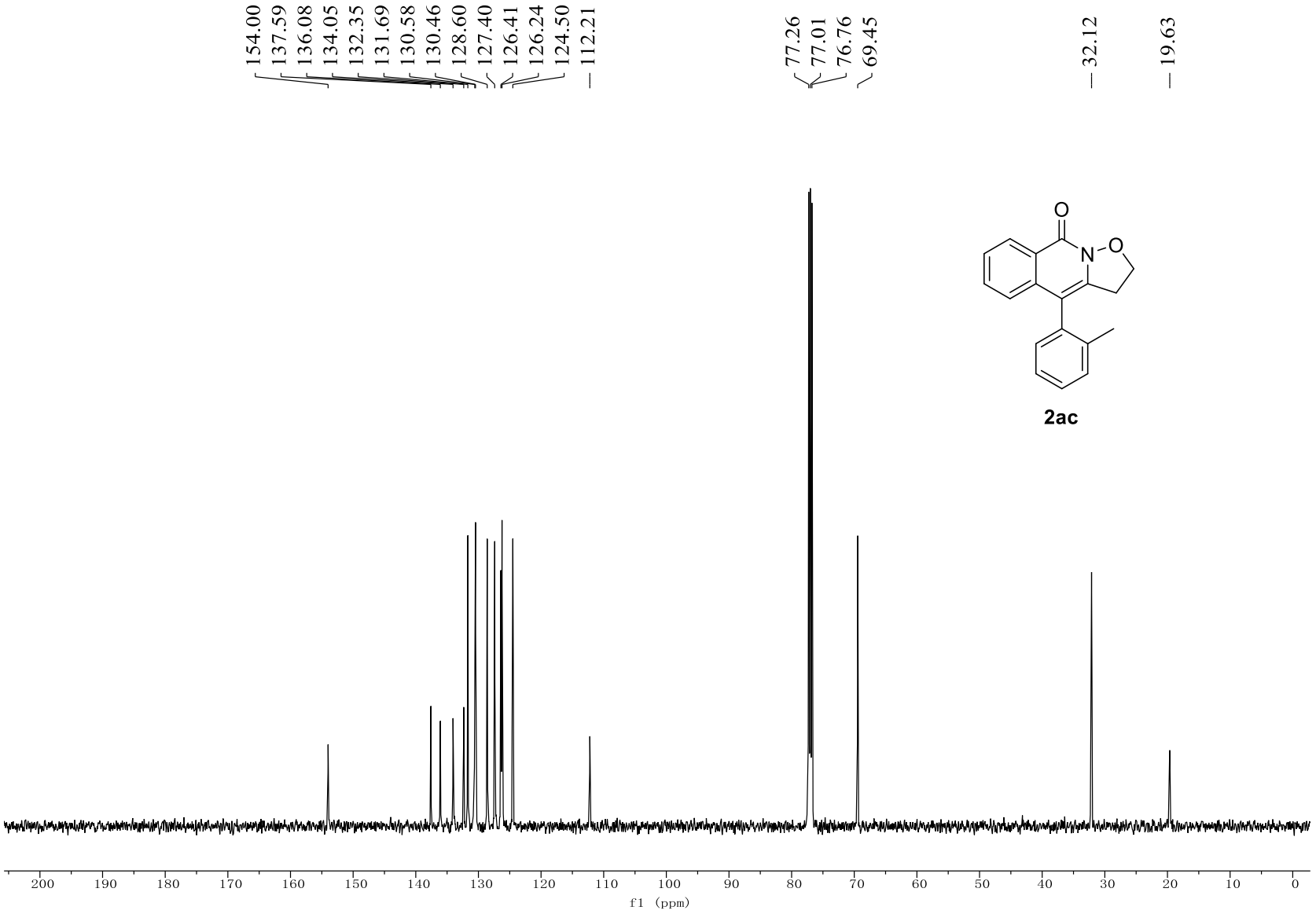
0.0
f1 (ppm)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131.69
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130.46
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127.40
126.41
126.24
124.50
112.21
77.26
77.01
76.76
69.45
32.12
19.63
O
N
O
2ac
200
190
180
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130
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110
100
90
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70
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50
40
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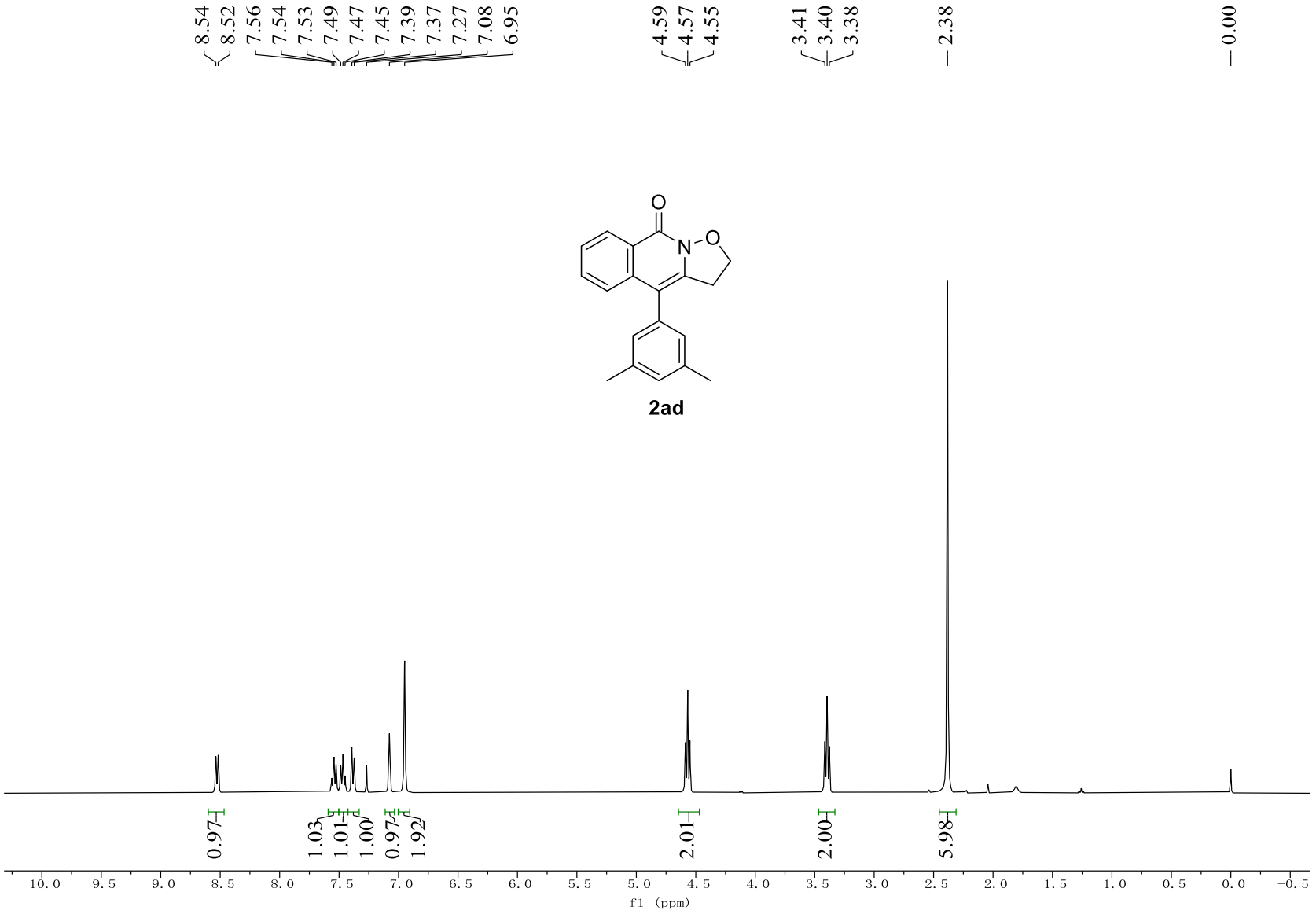
10
0
f1 (ppm)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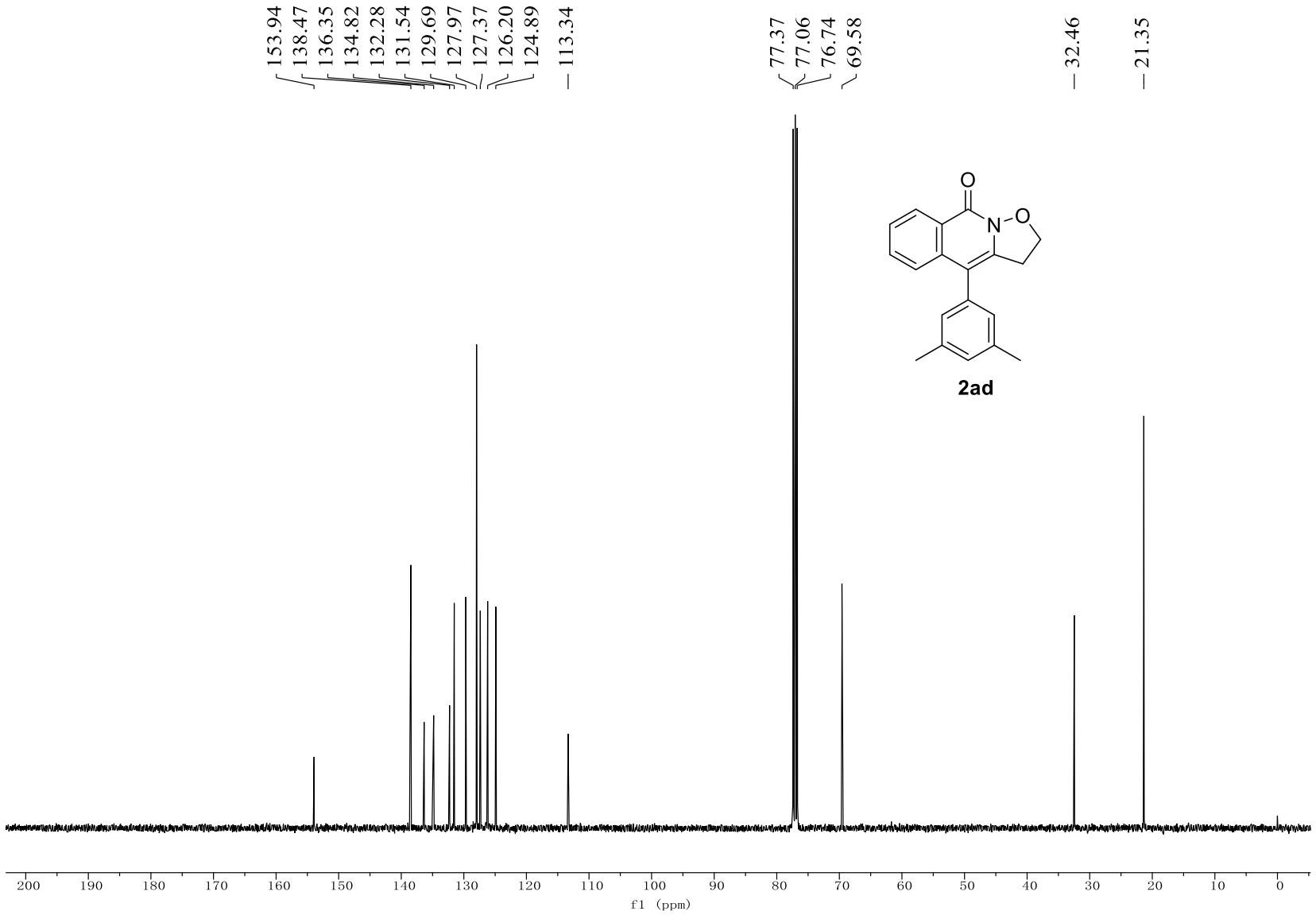
7.47
7.45
7.39
7.37
7.27
7.08
6.95
4.59
4.57
4.55
3.41
3.40
3.38
2.38
0.00
O
N
O
2ad
0.97
1.03
1.01
1.00
0.97
1.92
2.01
2.00
5.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)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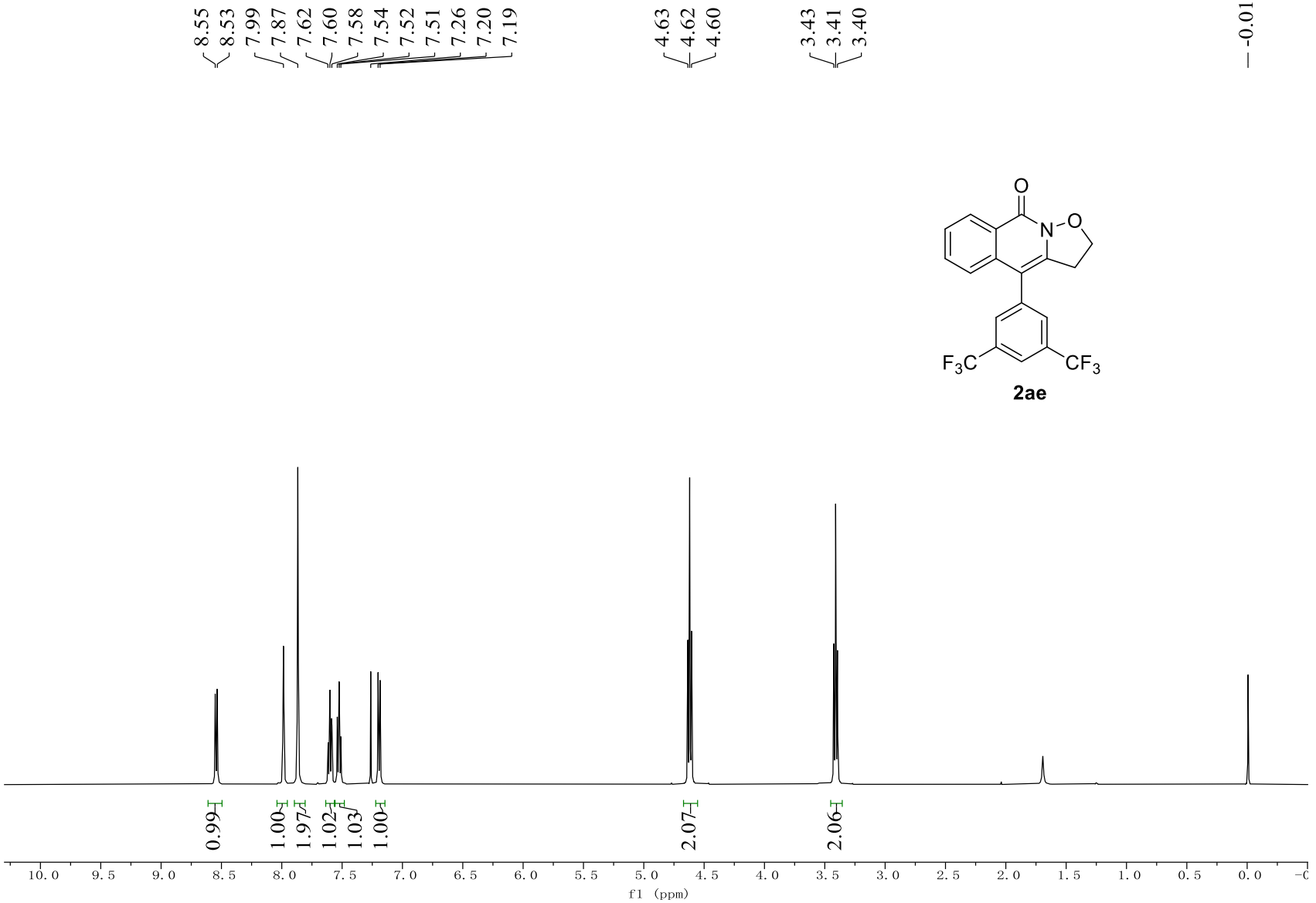
129.69
127.97
127.37
126.20
124.89
113.34
77.37
77.06
76.74
69.58
32.46
21.35
O
N
O
2ad
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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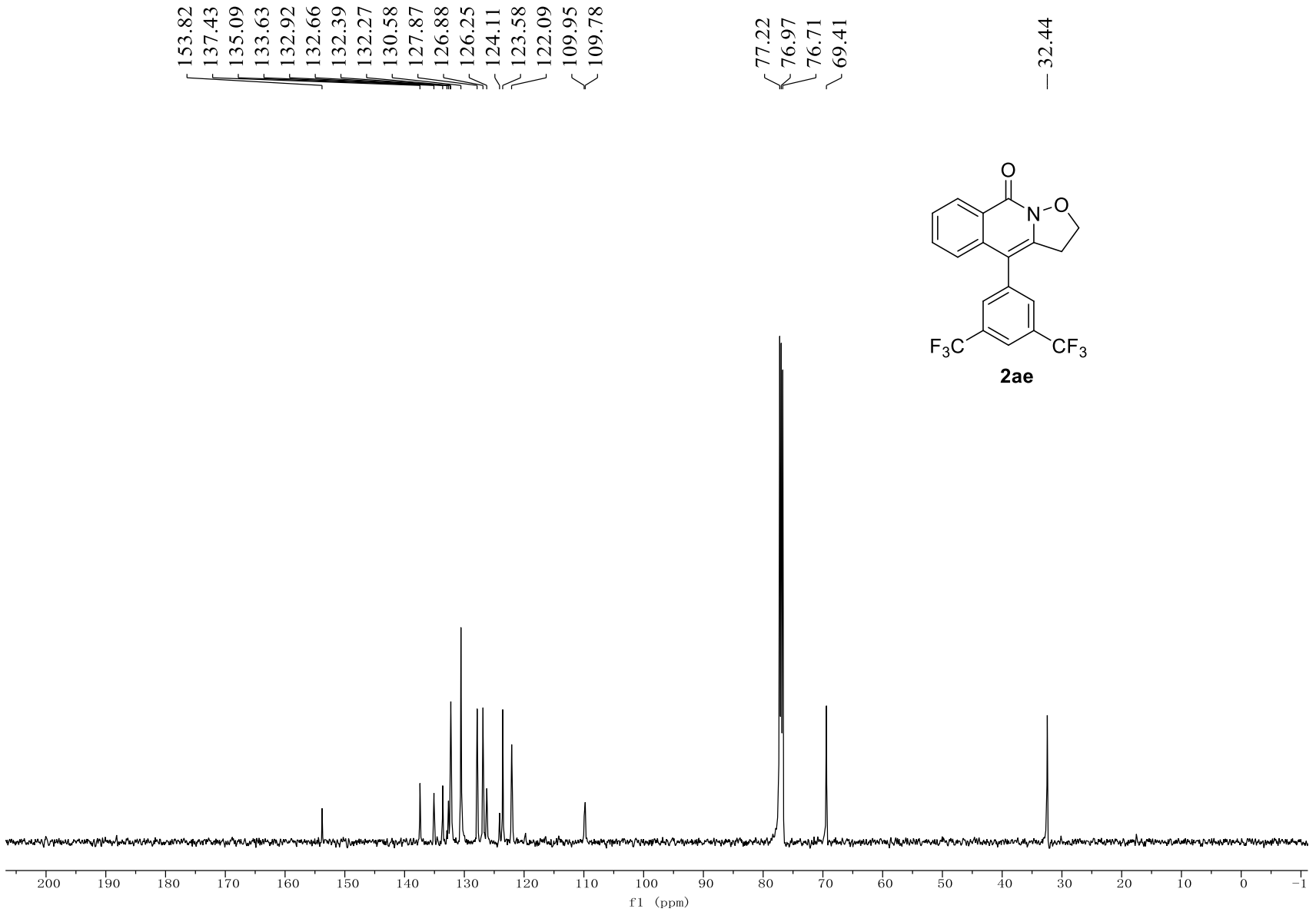
7.60
7.58
7.54
7.52
7.51
7.26
7.20
7.19
4.63
4.62
4.60
3.43
3.41
3.40
-0.01
O
N
O
F3C
CF3
2ae
0.99
1.00
1.97
1.02
1.03
1.00
2.07
2.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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132.27
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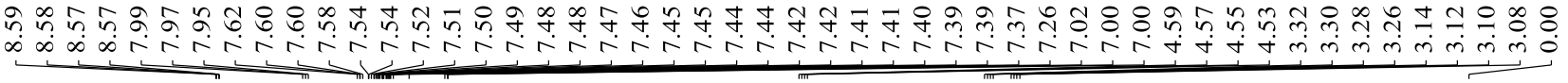
126.88
126.25
124.11
123.58
122.09
109.95
109.78
77.22
76.97
76.71
69.41
32.44
O
N
O
F3C
CF3
2ae
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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7.62
7.60
7.60
7.58
7.54
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7.52
7.51
7.50
7.49
7.48
7.48
7.47
7.46
7.45
7.45
7.44
7.44
7.42
7.42
7.41
7.41
7.40
7.39
7.39
7.37
7.26
7.02
7.00
7.00
4.59
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4.53
3.32
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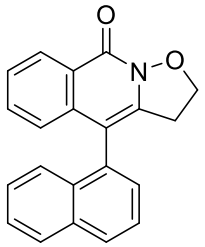
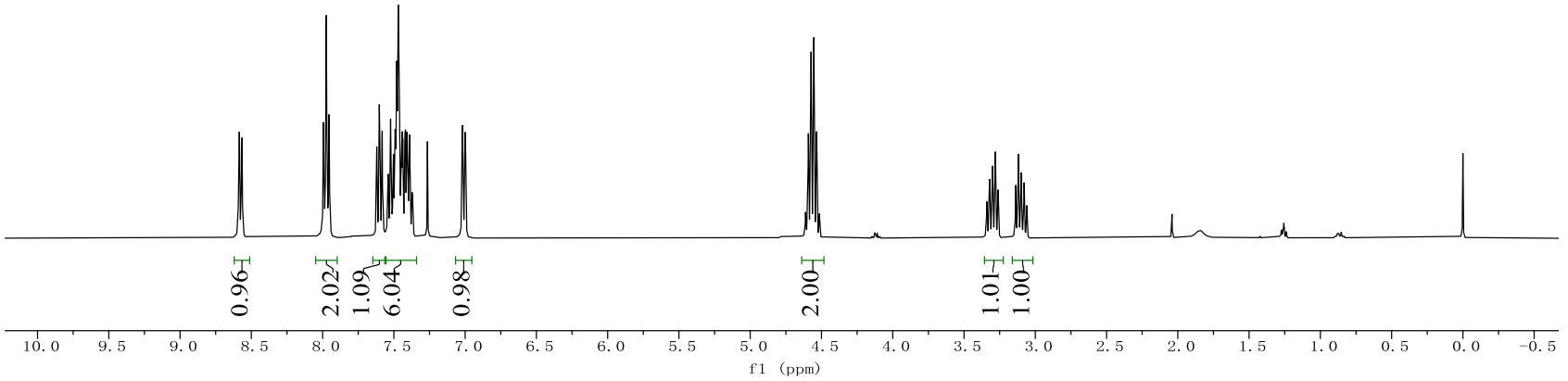
3.28
3.26
3.14
3.12
3.10
3.08
0.00


O
N
O

2af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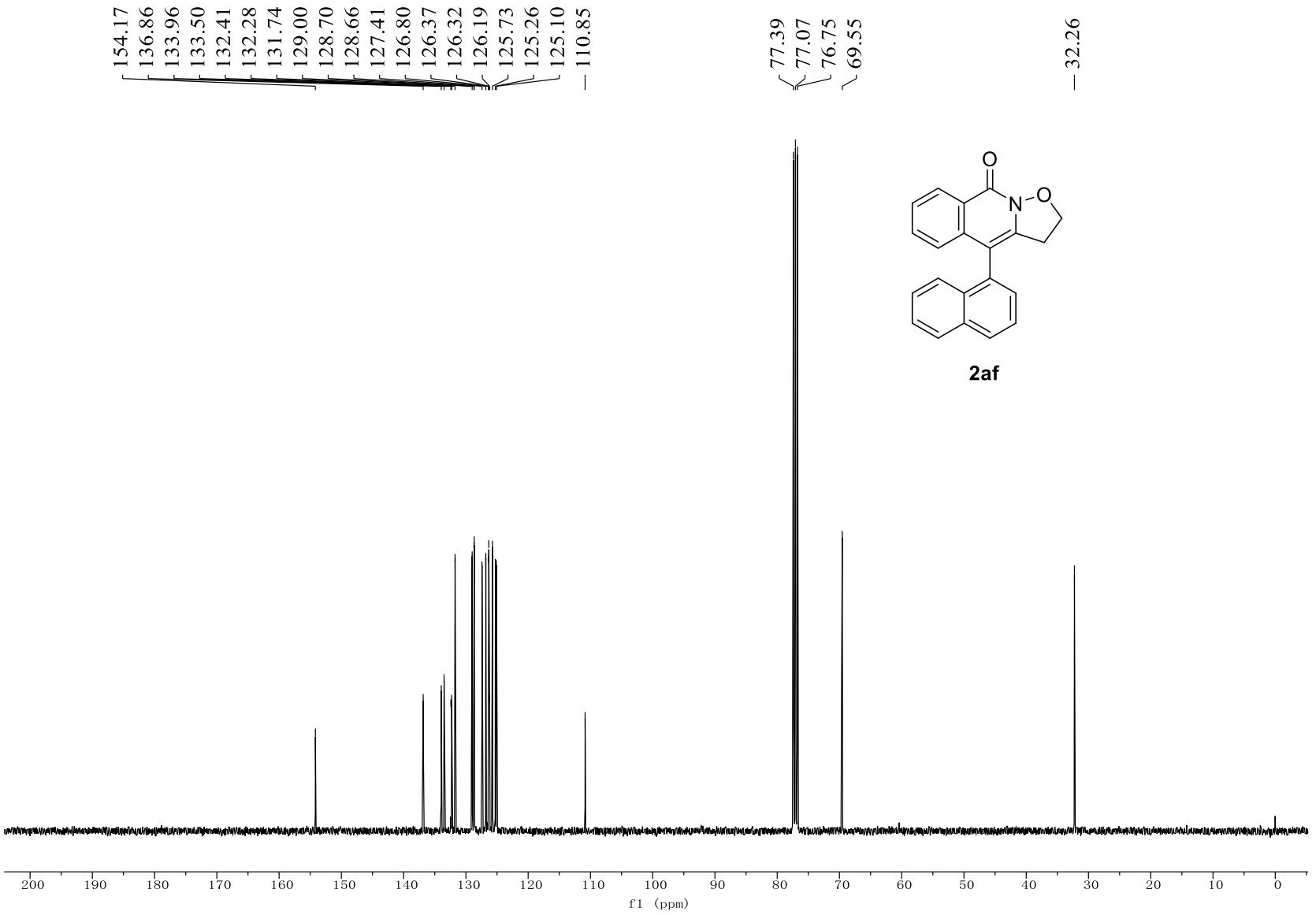
2.02
1.09
6.04
0.98
2.00
1.01
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)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132.28
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129.00
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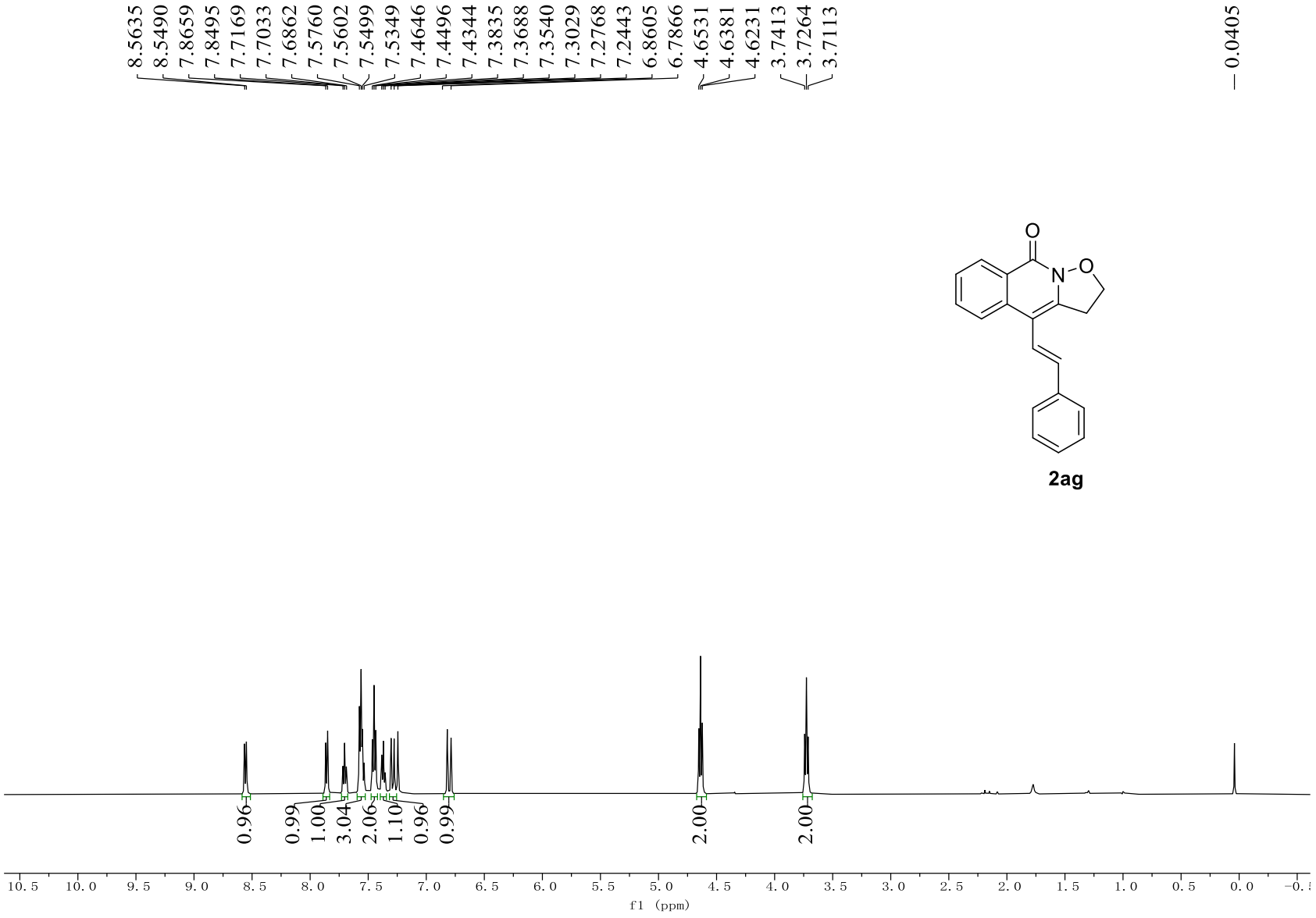
128.66
127.41
126.80
126.37
126.32
126.19
125.73
125.26
125.10
110.85
77.39
77.07
76.75
69.55
32.26
O
N
O
2af
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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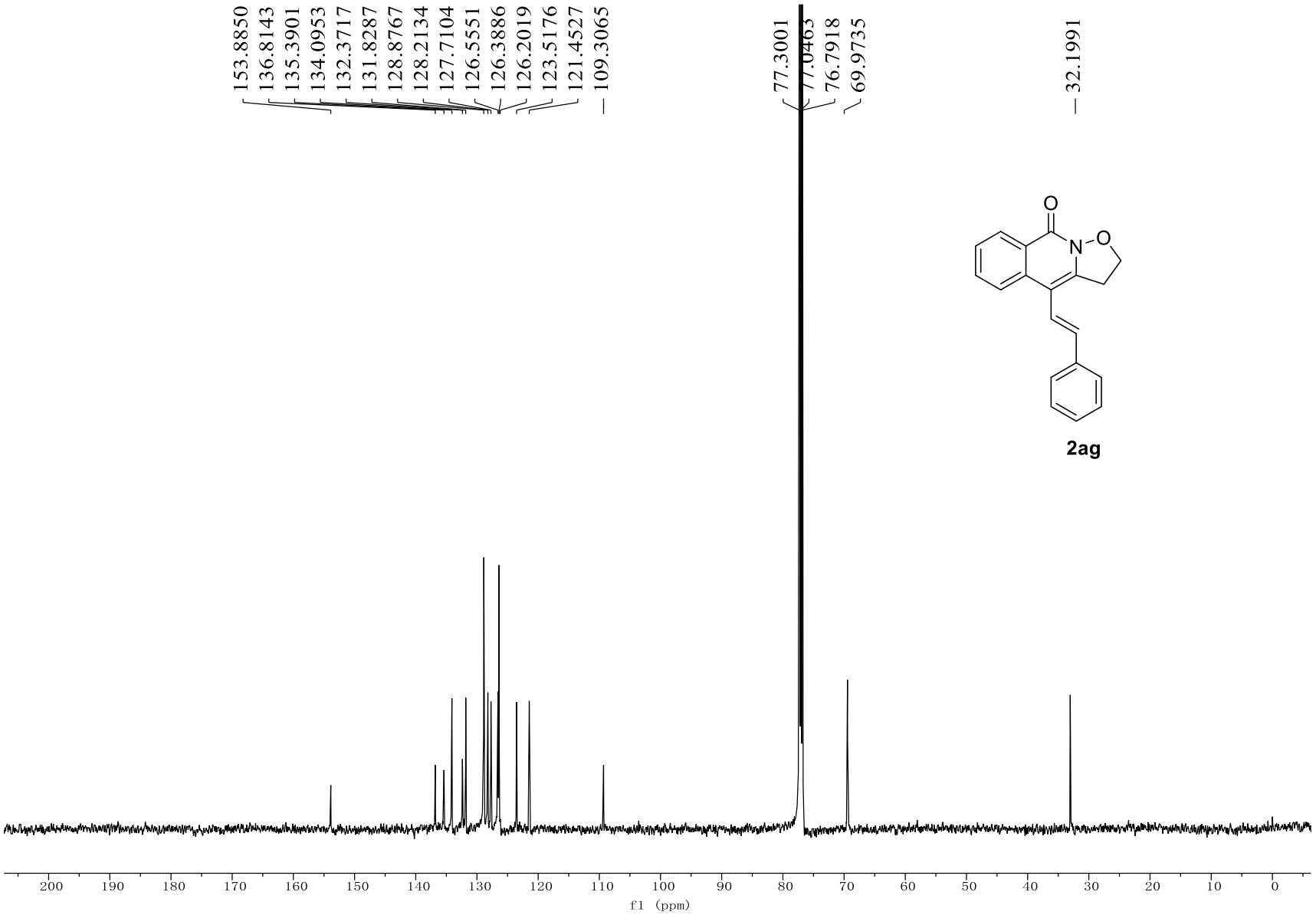
7.7169
7.7033
7.6862
7.5760
7.5602
7.5499
7.5349
7.4646
7.4496
7.4344
7.3835
7.3688
7.3540
7.3029
7.2768
7.2443
6.8605
6.7866
4.6531
4.6381
4.6231
3.7413
3.7264
3.7113
0.0405
O
N
O
2ag
0.96
0.99
1.00
3.04
2.06
1.10
0.96
0.99
2.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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132.3717
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127.7104
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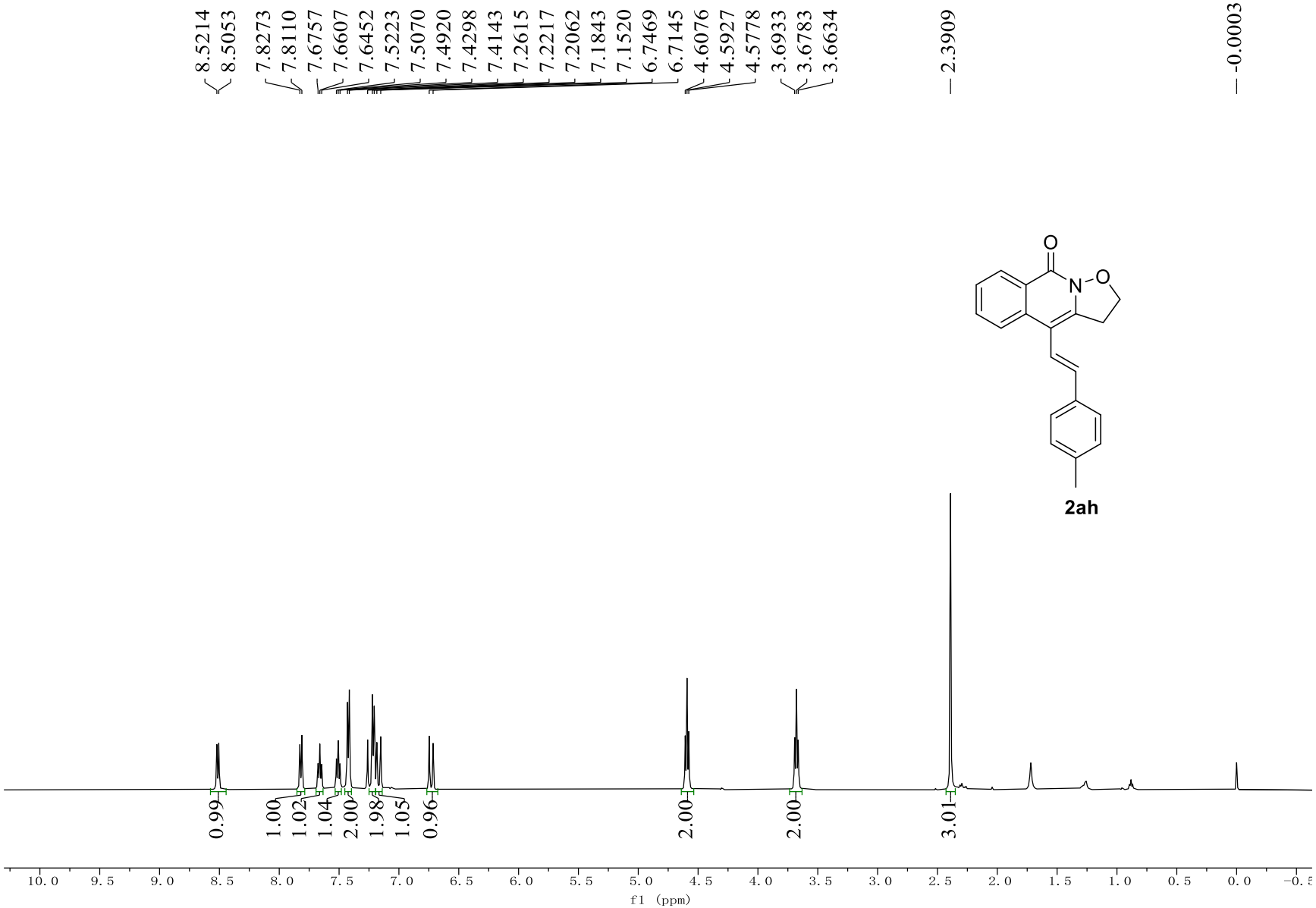
126.3886
126.2019
123.5176
121.4527
109.3065
77.3001
77.0463
76.7918
69.9735
32.1991
O
N
O
2ag
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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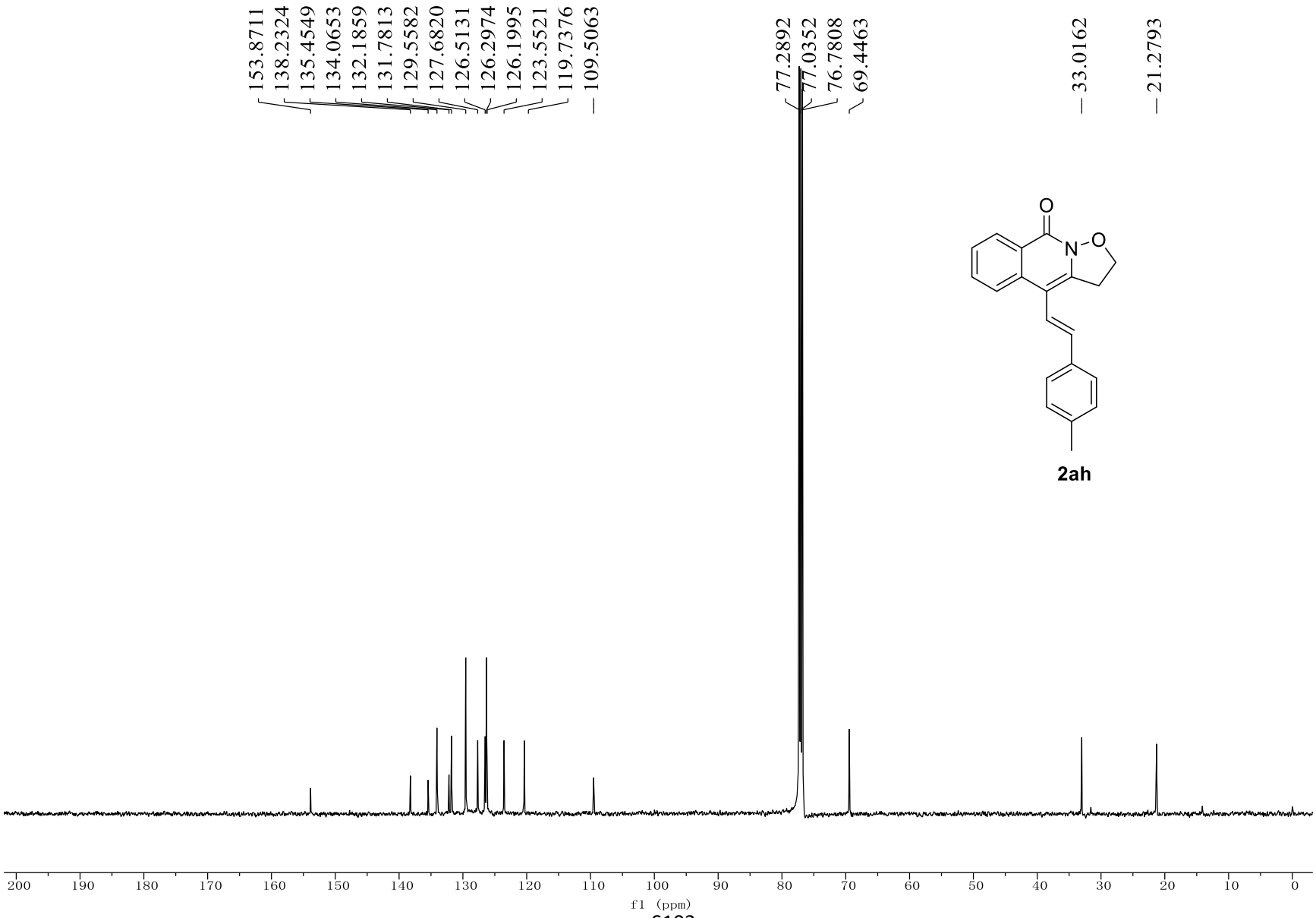
7.8110
7.6757
7.6607
7.6452
7.5223
7.5070
7.4920
7.4298
7.4143
7.2615
7.2217
7.2062
7.1843
7.1520
6.7469
6.7145
4.6076
4.5927
4.5778
3.6933
3.6783
3.6634
2.3909
-0.0003
O
N
O
2ah
0.99
1.00
1.02
1.04
2.00
1.98
1.05
0.96
2.00
2.00
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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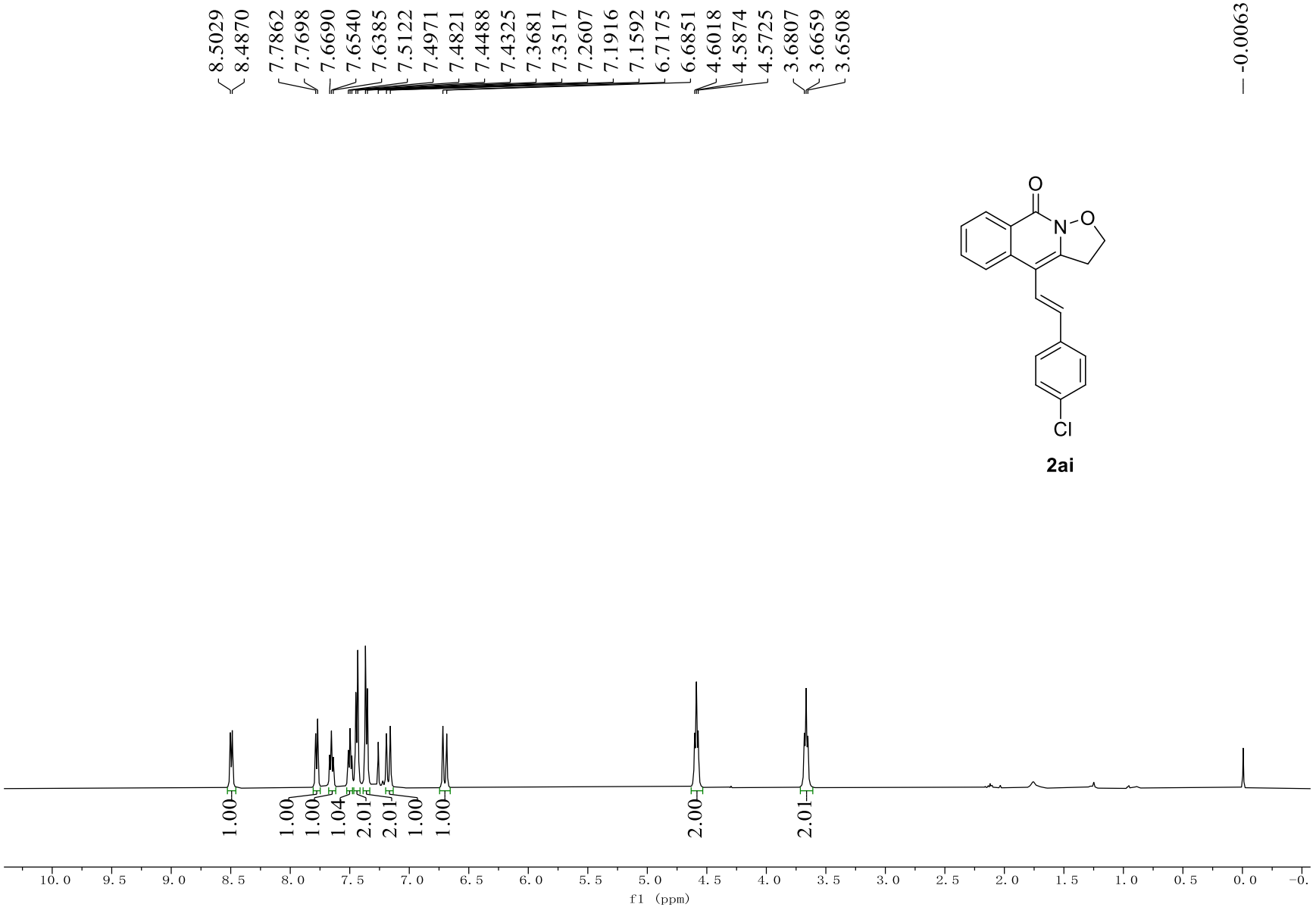
126.1995
123.5521
119.7376
109.5063
77.2892
77.0352
76.7808
69.4463
33.0162
21.2793
O
N
O
2ah
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.6385
7.5122
7.4971
7.4821
7.4488
7.4325
7.3681
7.3517
7.2607
7.1916
7.1592
6.7175
6.6851
4.6018
4.5874
4.5725
3.6807
3.6659
3.6508
-0.0063
O
N
O
Cl
2ai
1.00
1.00
1.00
1.04
2.01
2.01
1.00
1.00
2.00
2.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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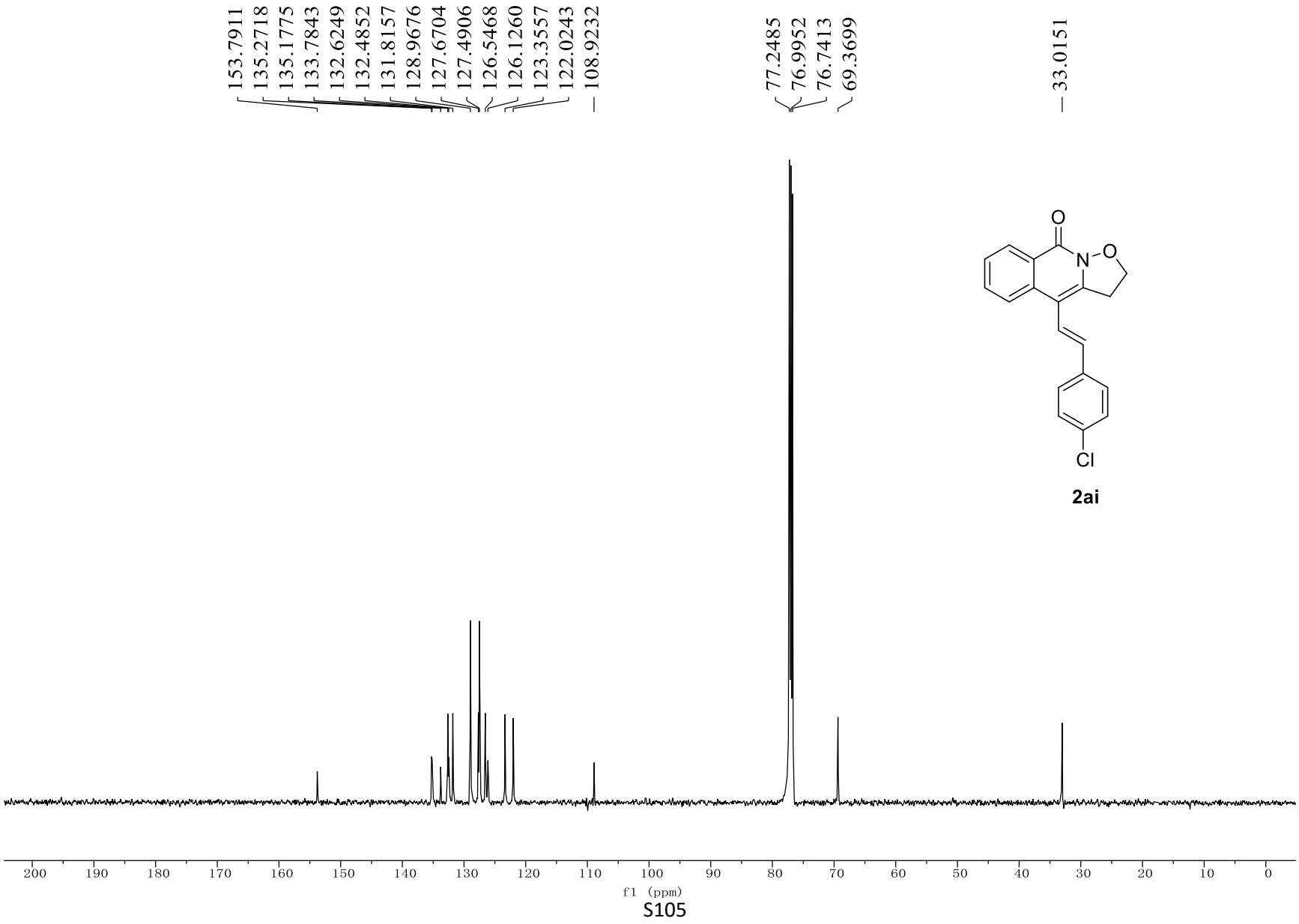
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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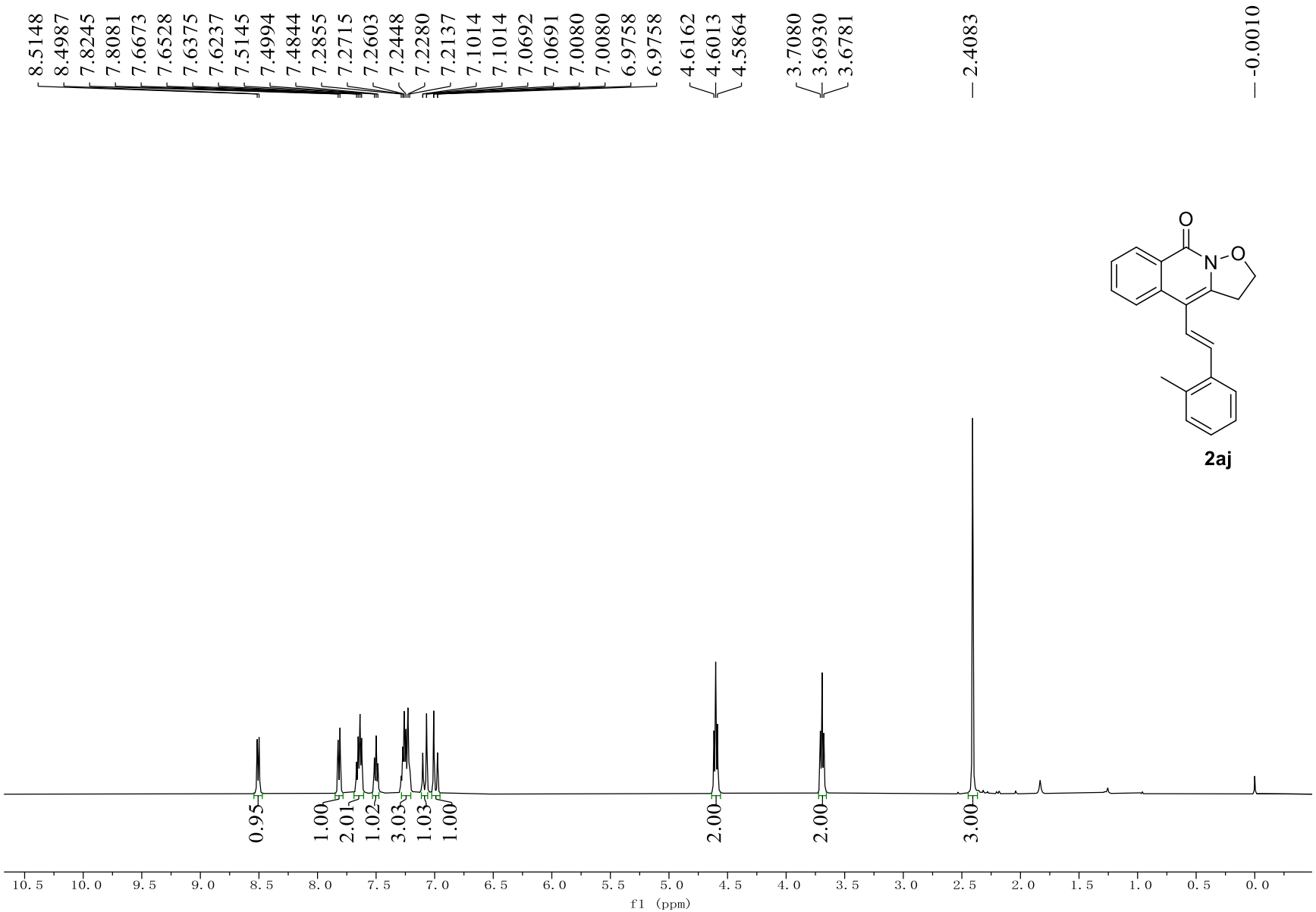
126.5468
126.1260
123.3557
122.0243
108.9232
77.2485
76.9952
76.7413
69.3699
33.0151
O
N
O
Cl
2ai
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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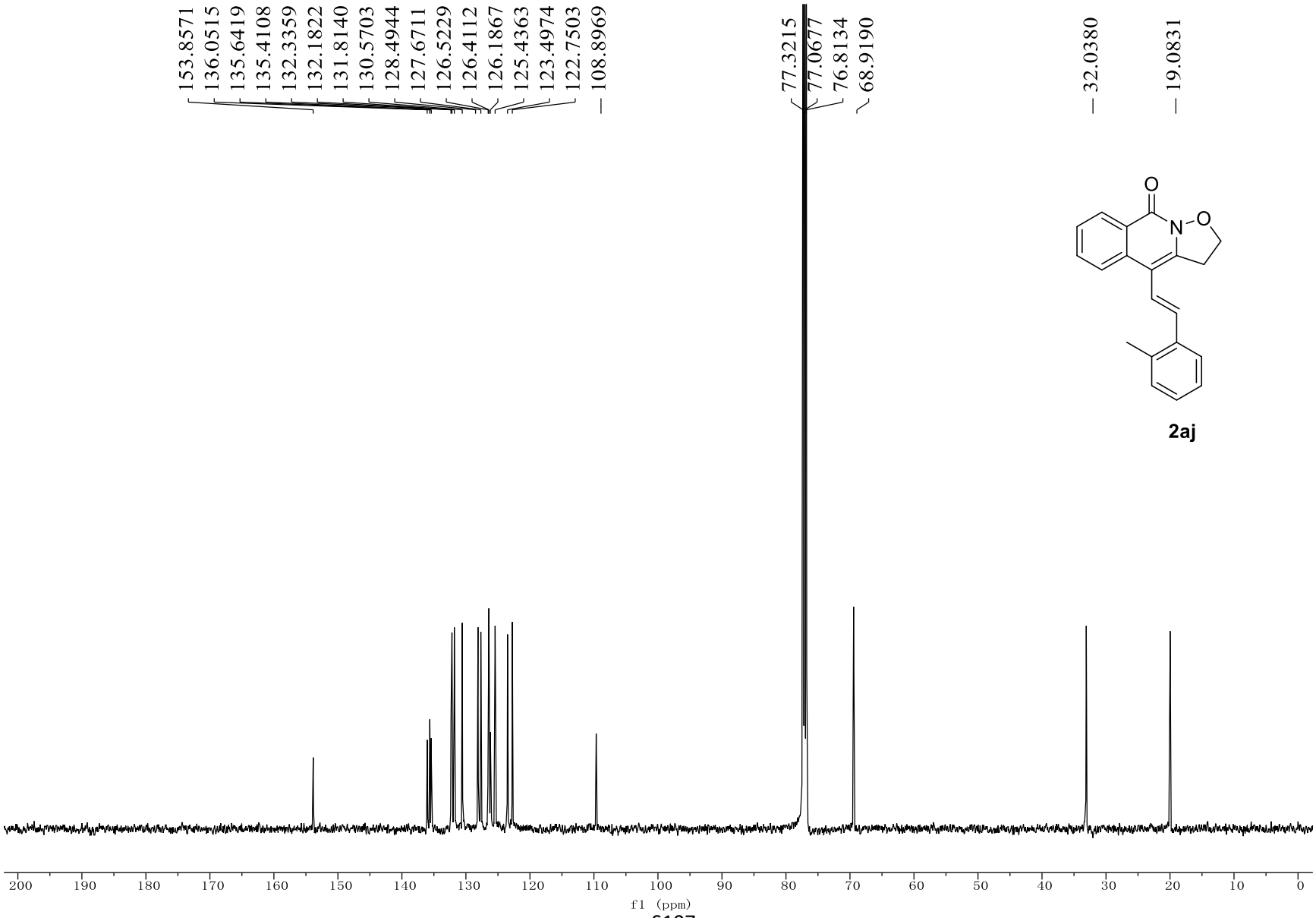
7.5145
7.4994
7.4844
7.2855
7.2715
7.2603
7.2448
7.2280
7.2137
7.1014
7.1014
7.0692
7.0691
7.0080
7.0080
6.9758
6.9758
4.6162
4.6013
4.5864
3.7080
3.6930
3.6781
2.4083
-0.0010
O
N
O
2aj
0.95
1.00
2.01
1.02
3.03
1.03
1.00
2.00
2.00
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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125.4363
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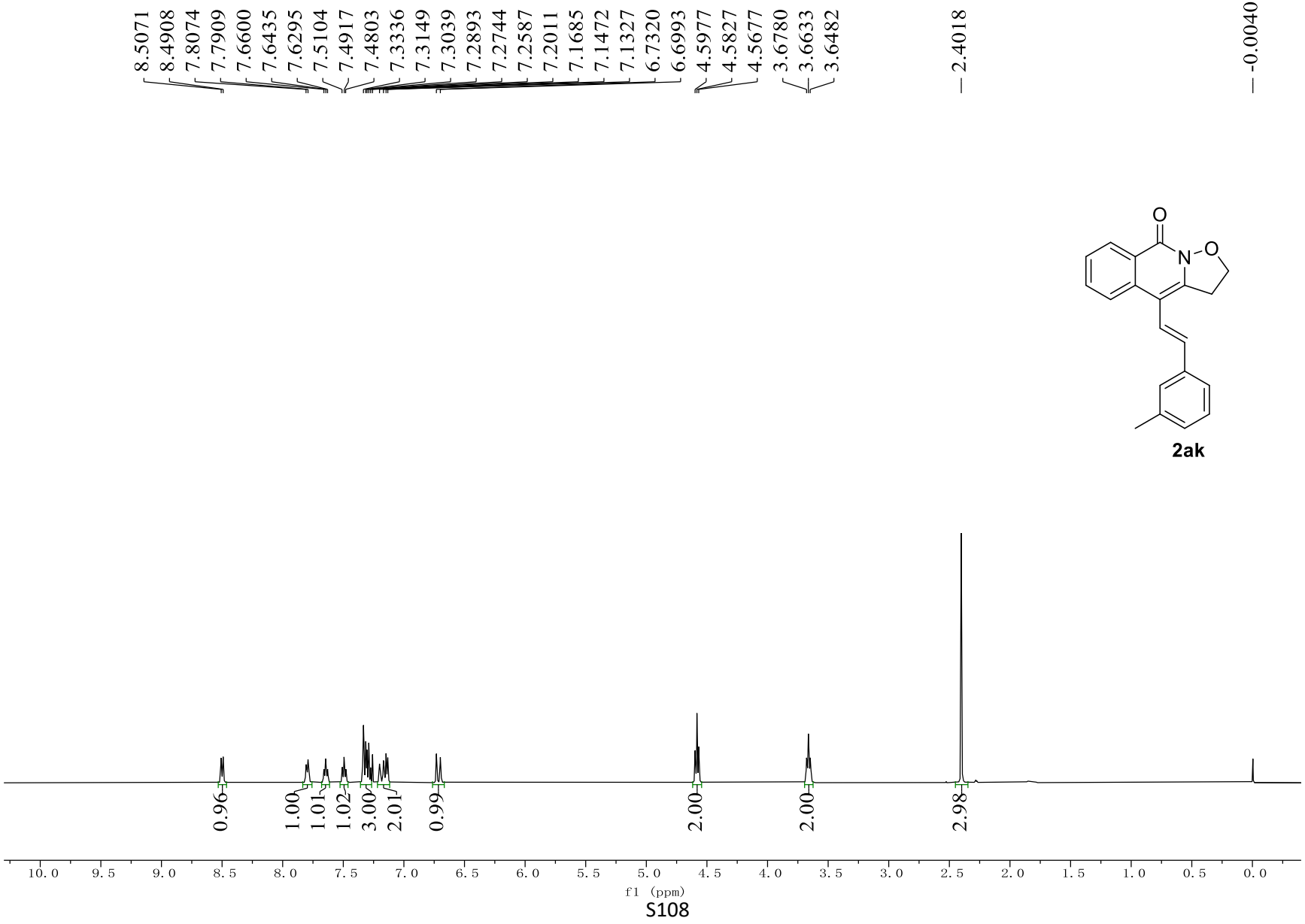
108.8969
77.3215
77.0677
76.8134
68.9190
32.0380
19.0831
O
N
O
2aj
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4917
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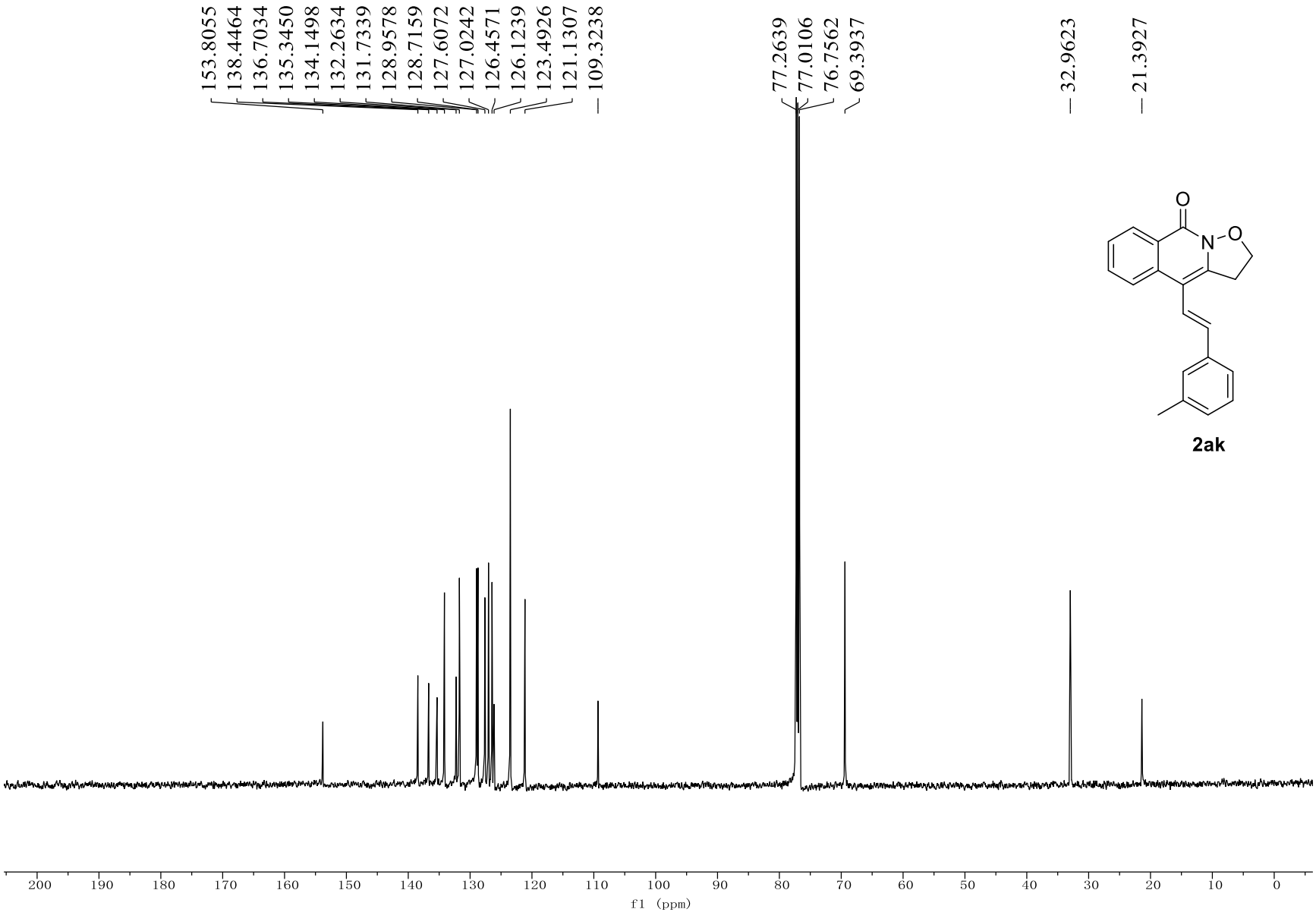
7.3336
7.3149
7.3039
7.2893
7.2744
7.2587
7.2011
7.1685
7.1472
7.1327
6.7320
6.6993
4.5977
4.5827
4.5677
3.6780
3.6633
3.6482
2.4018
-0.0040
O
N
O
2ak
0.96
1.00
1.01
1.02
3.00
2.01
0.99
2.00
2.00
2.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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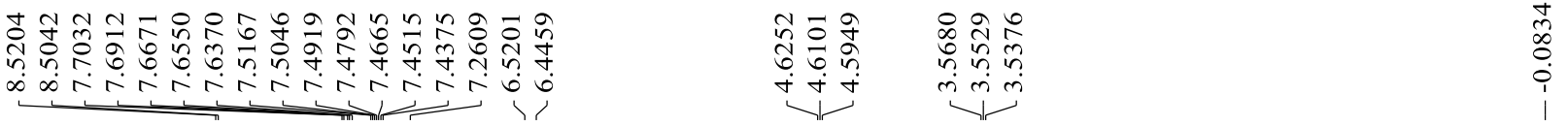
128.7159
127.6072
127.0242
126.4571
126.1239
123.4926
121.1307
109.3238
77.2639
77.0106
76.7562
69.3937
32.9623
21.3927
O
N
O
2ak
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.6370
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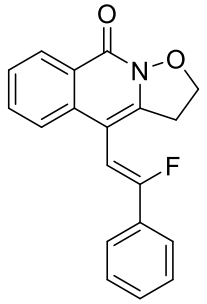
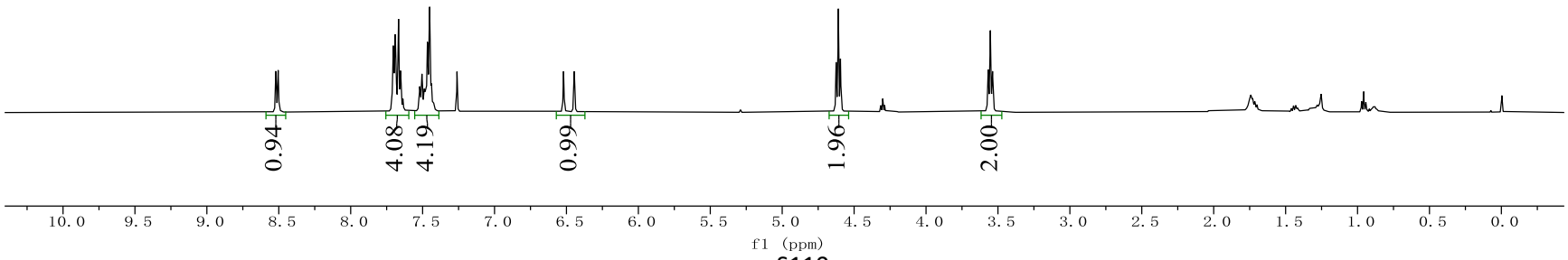
7.5046
7.4919
7.4792
7.4665
7.4515
7.4375
7.2609
6.5201
6.4459
4.6252
4.6101
4.5949
3.5680
3.5529
3.5376
-0.0834


O
N
O
F

2al


0.94
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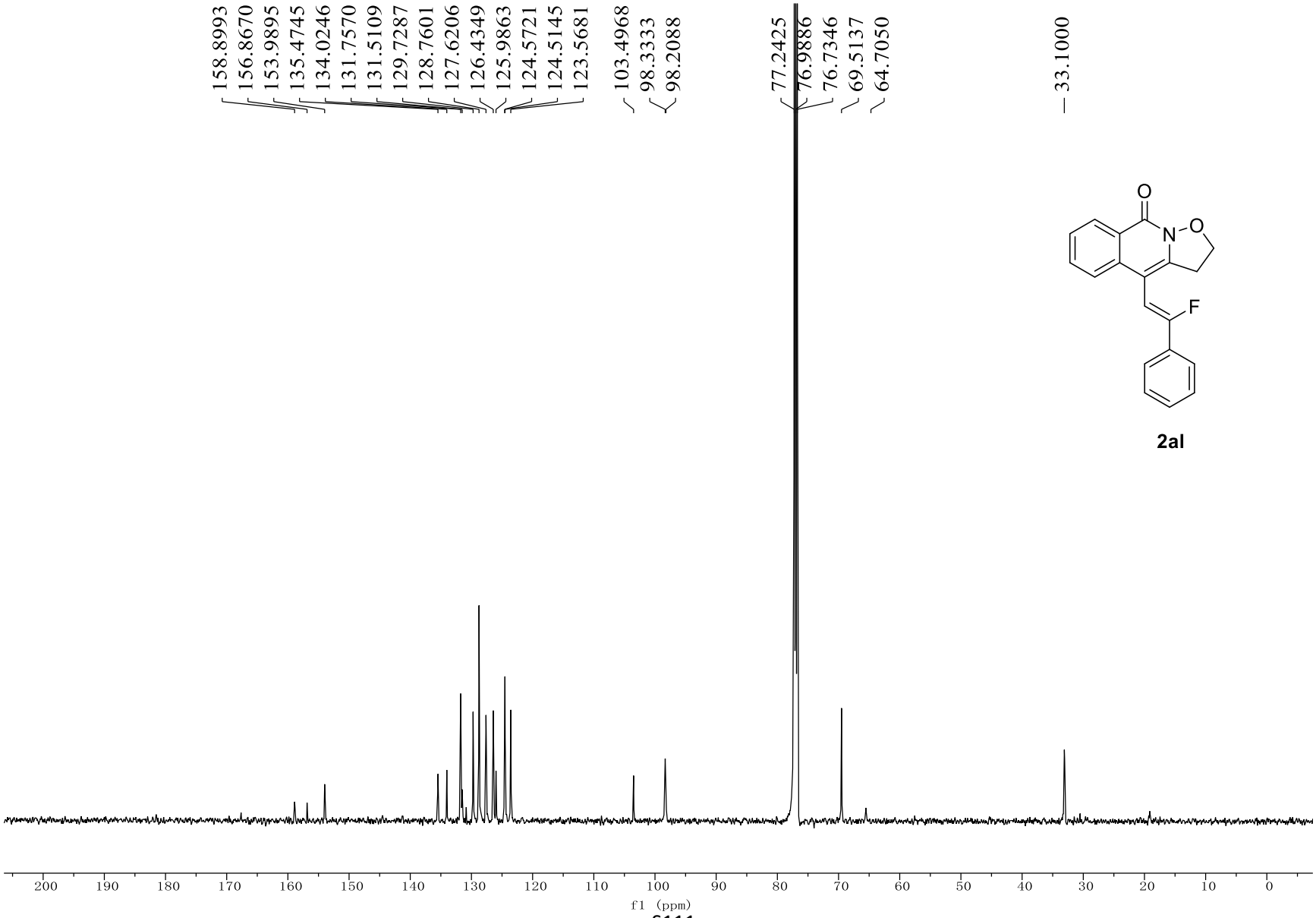
1.96
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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123.5681
103.4968
98.3333
98.2088
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76.9886
76.7346
69.5137
64.7050
33.1000
O
N
O
F
200
190
180
170
160
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140
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120
110
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80
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30
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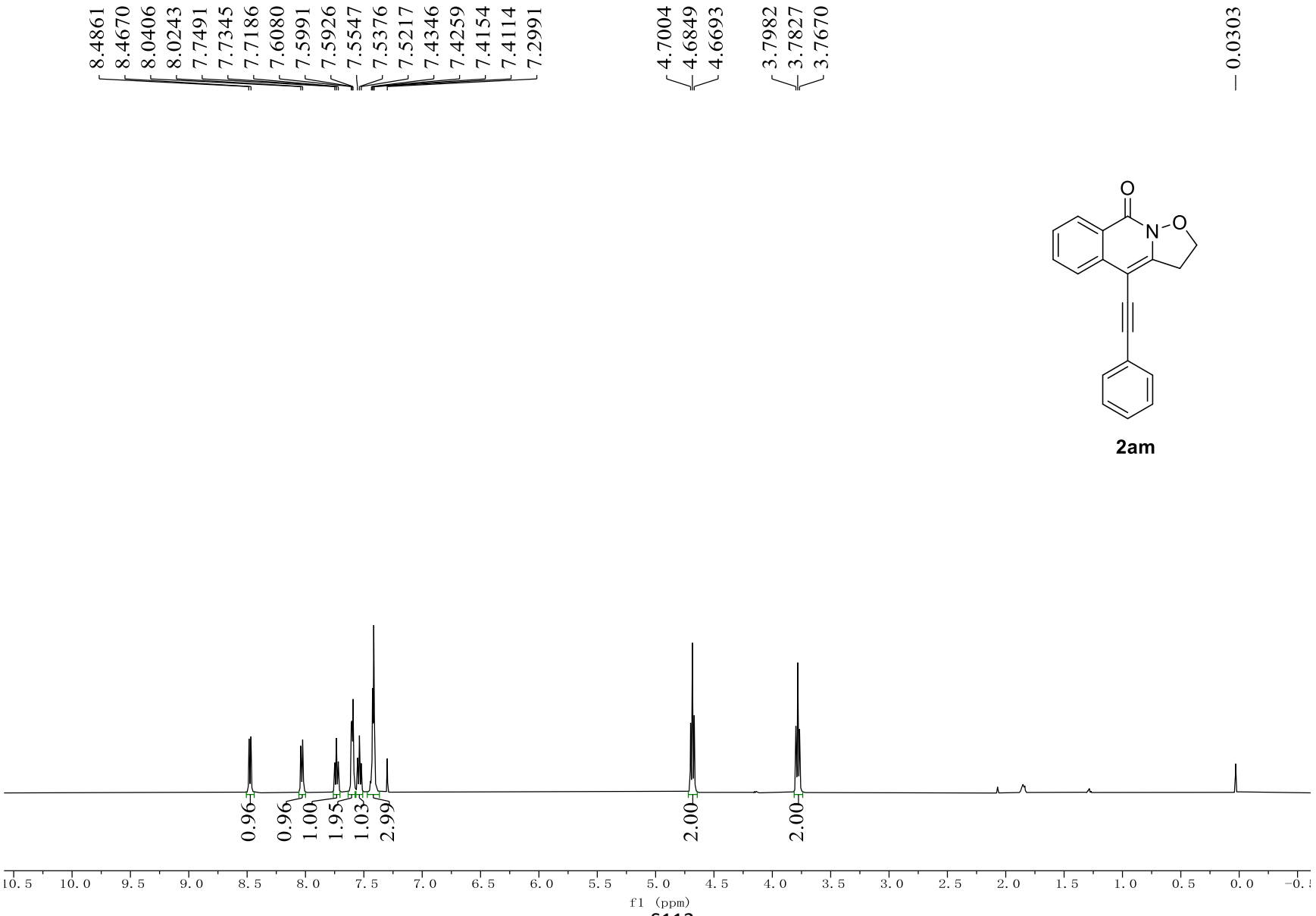
f1 (ppm)

2al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7.5376
7.5217
7.4346
7.4259
7.4154
7.4114
7.2991
4.7004
4.6849
4.6693
3.7982
3.7827
3.7670
0.0303
O
N
O
2am
0.96
0.96
1.00
1.95
1.03
2.99
2.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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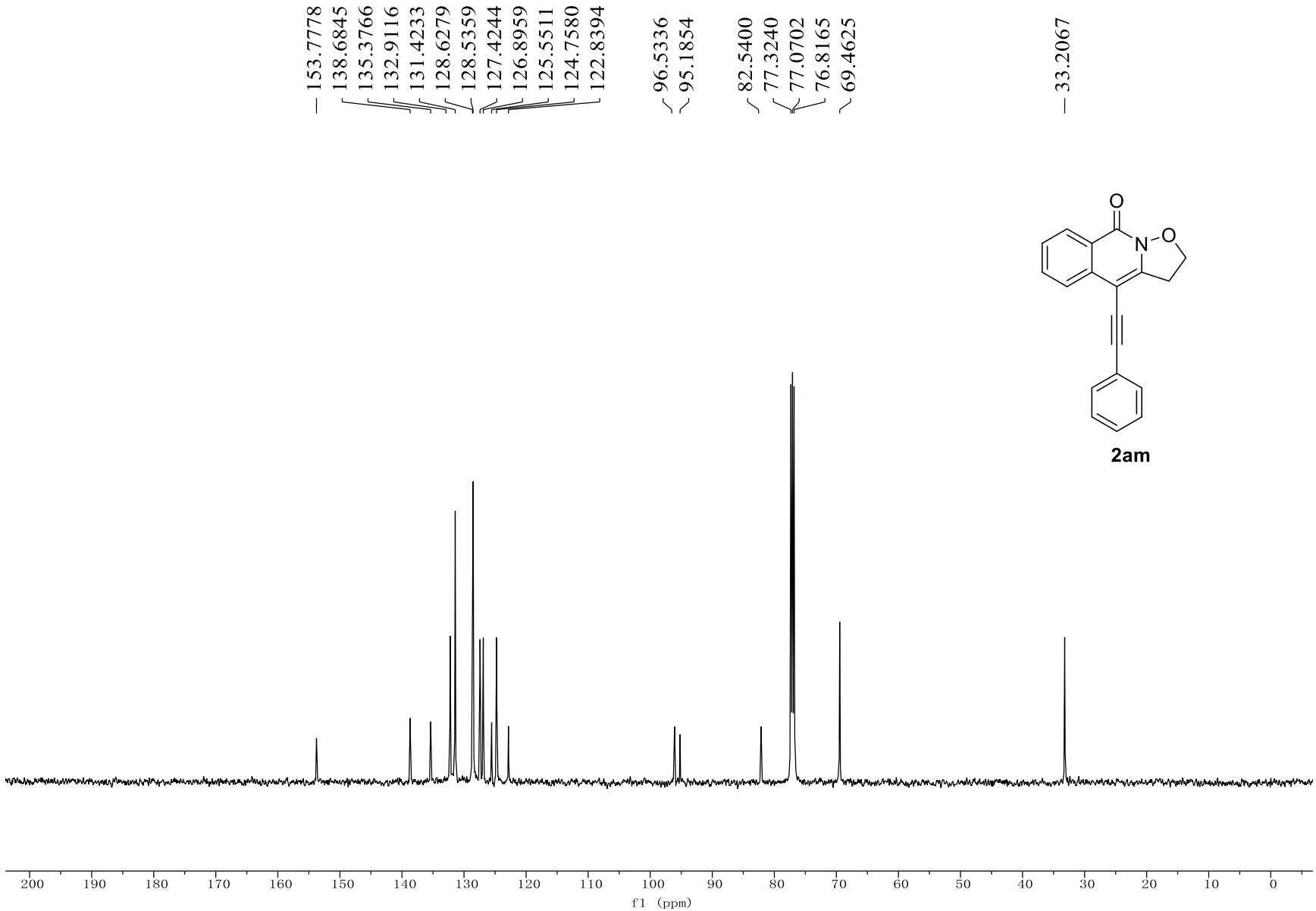
0.0
f1 (ppm)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131.4233
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128.5359
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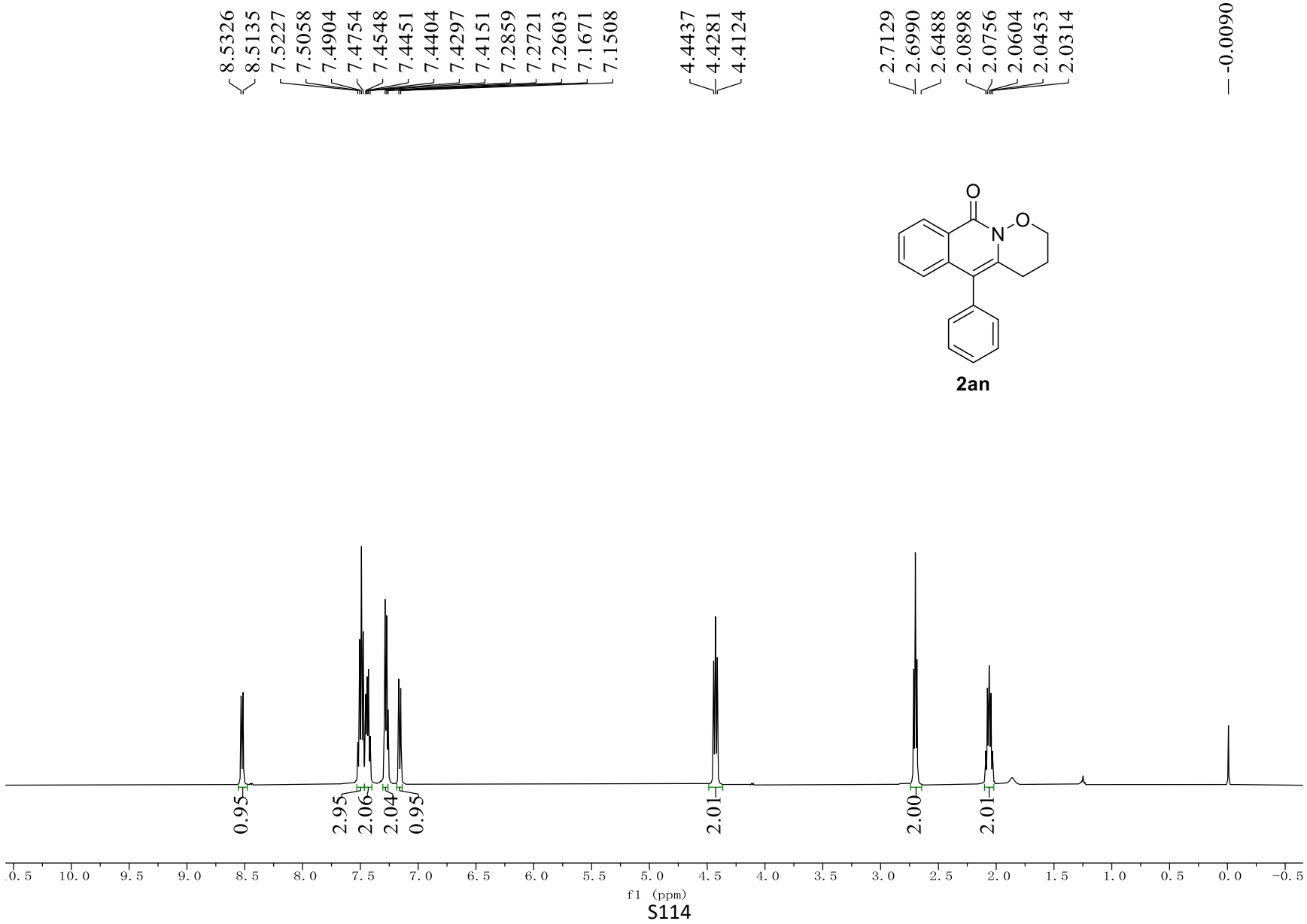
126.8959
125.5511
124.7580
122.8394
96.5336
95.1854
82.5400
77.3240
77.0702
76.8165
69.4625
33.2067
O
N
O
2am
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4904
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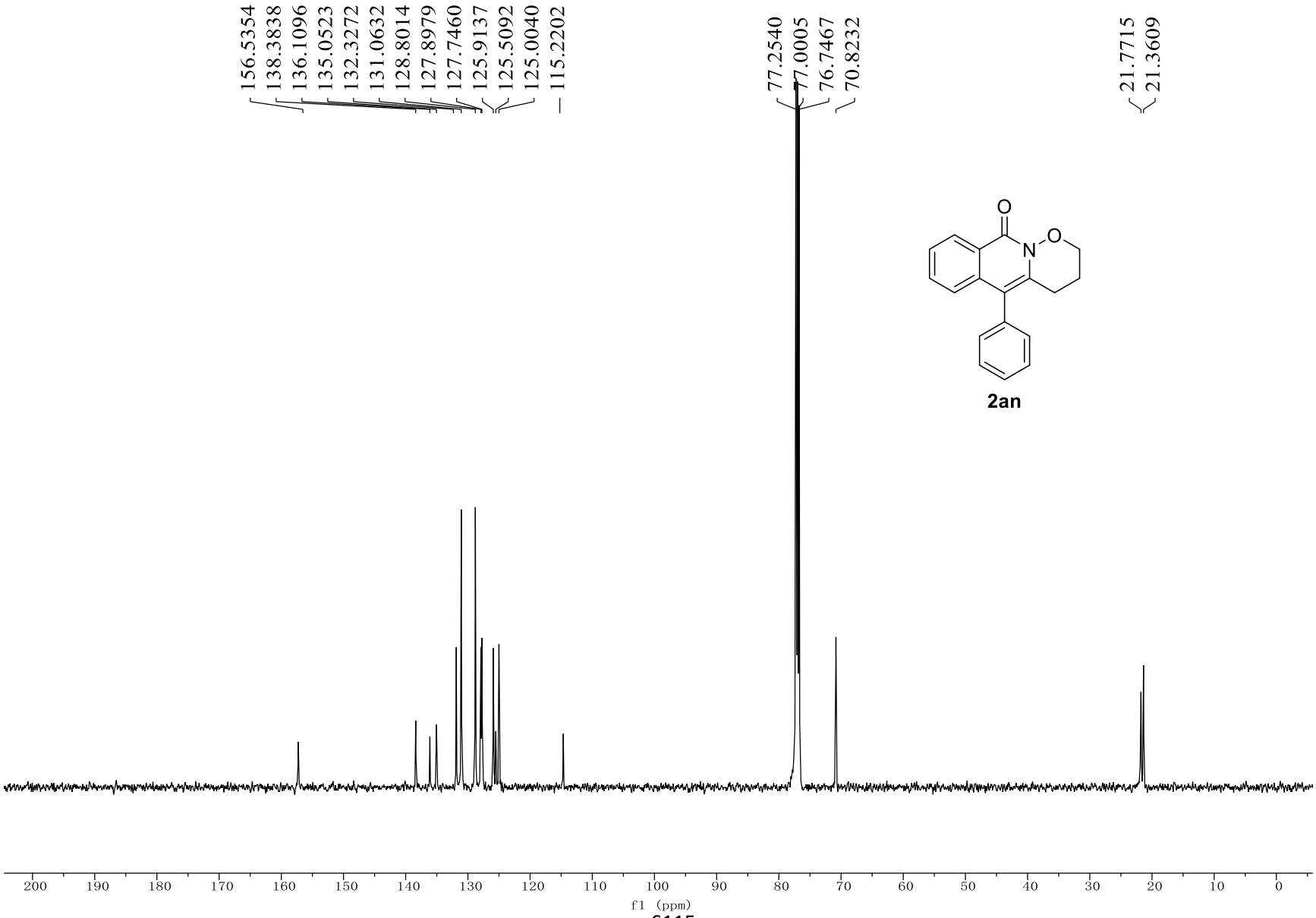
7.4151
7.2859
7.2721
7.2603
7.1671
7.1508
4.4437
4.4281
4.4124
2.7129
2.6990
2.6488
2.0898
2.0756
2.0604
2.0453
2.0314
-0.0090
O
N
O
2an
0.95
2.95
2.06
2.04
0.95
2.01
2.00
2.01
f1 (ppm)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136.1096
135.0523
132.3272
131.0632
128.8014
127.8979
127.7460
125.9137
125.5092
125.0040
115.2202
77.2540
77.0005
76.7467
70.8232
21.7715
21.3609
O
N
O
2an
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
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10
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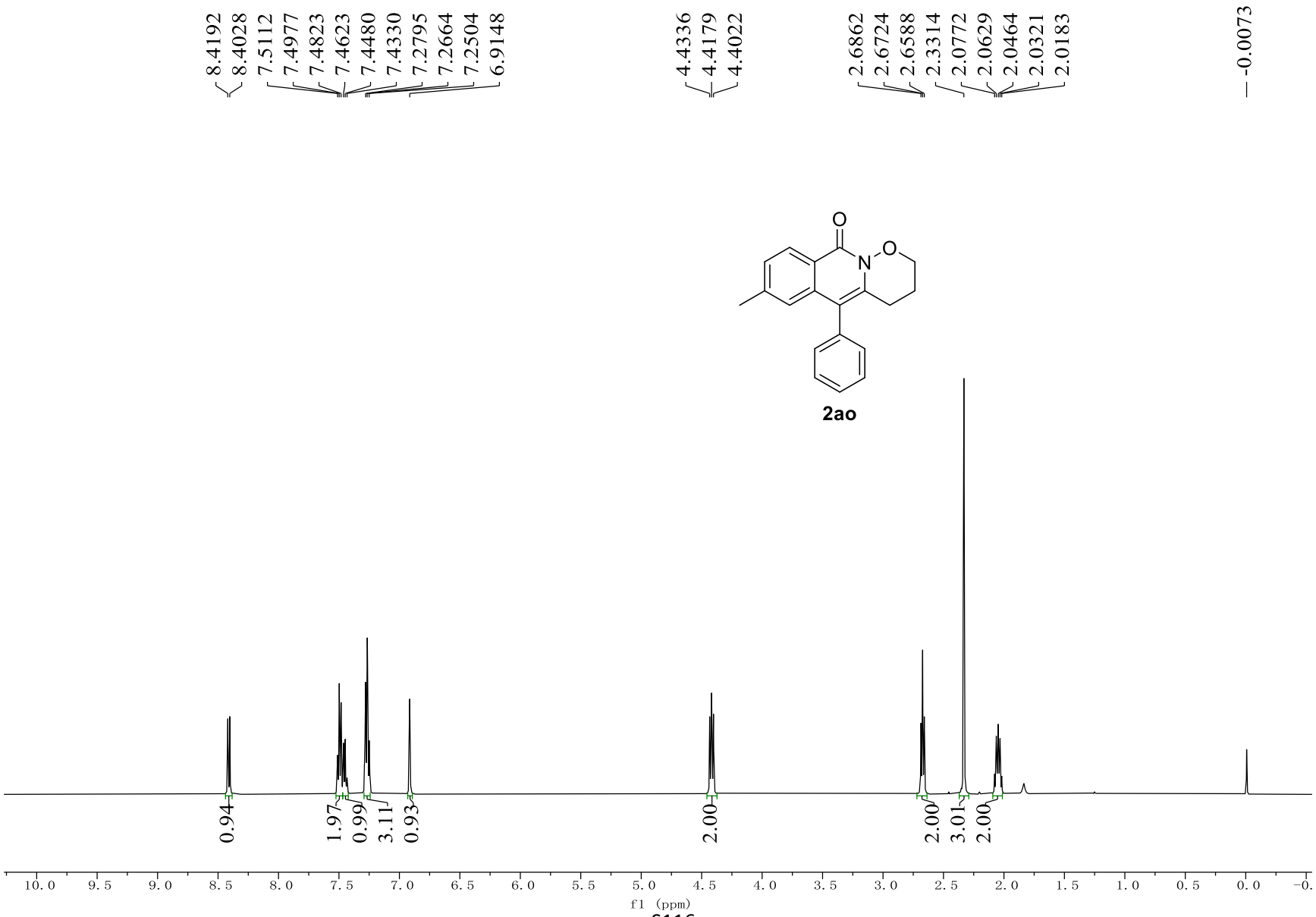
f1 (ppm)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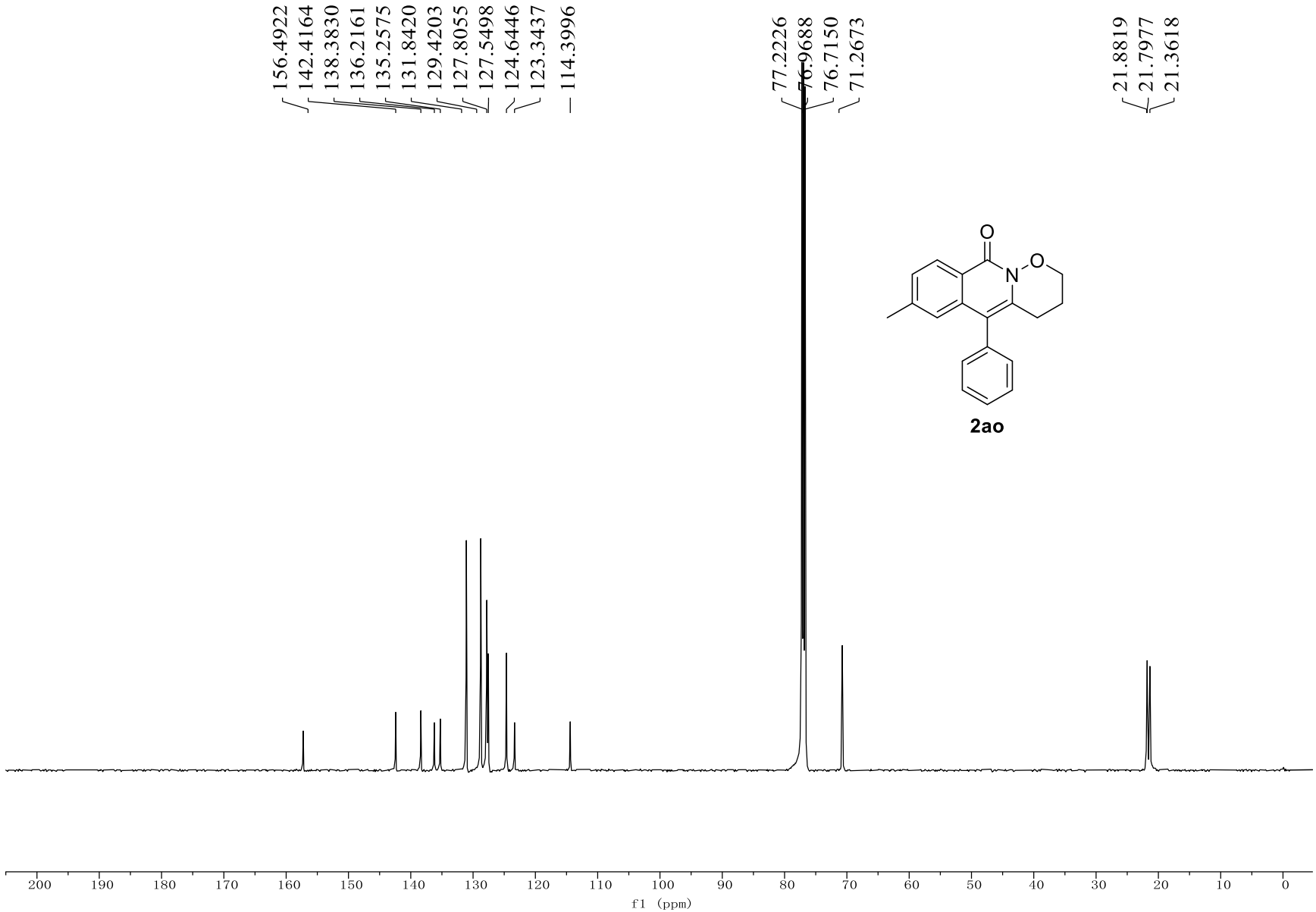
7.4480
7.4330
7.2795
7.2664
7.2504
6.9148
4.4336
4.4179
4.4022
2.6862
2.6724
2.6588
2.3314
2.0772
2.0629
2.0464
2.0321
2.0183
-0.0073
O
N
O
2ao
0.94
1.97
0.99
3.11
0.93
2.00
2.00
3.01
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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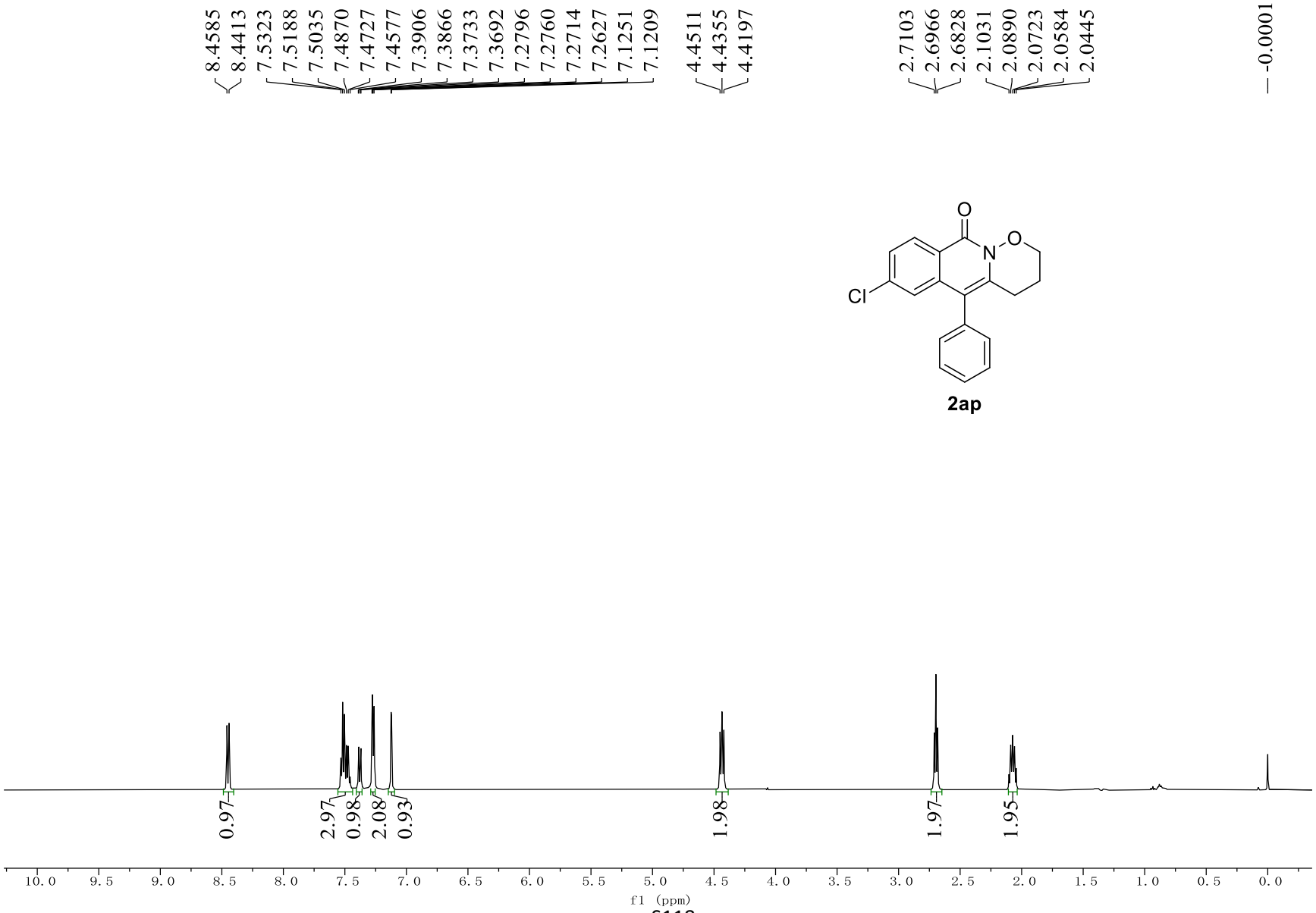
136.2161
135.2575
131.8420
129.4203
127.8055
127.5498
124.6446
123.3437
114.3996
77.2226
76.9688
76.7150
71.2673
21.8819
21.7977
21.3618
O
N
O
2ao
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4577
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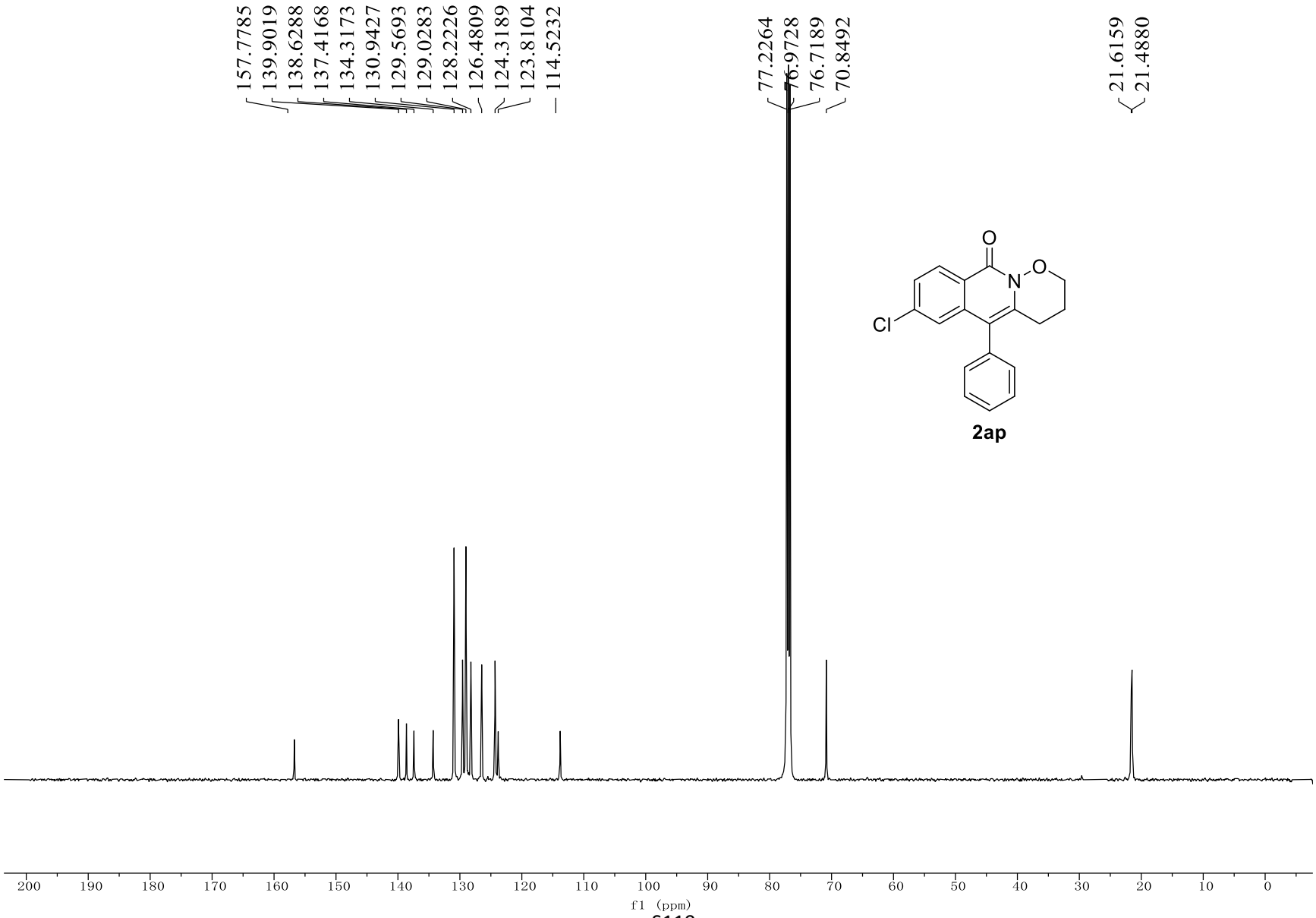
7.3866
7.3733
7.3692
7.2796
7.2760
7.2714
7.2627
7.1251
7.1209
4.4511
4.4355
4.4197
2.7103
2.6966
2.6828
2.1031
2.0890
2.0723
2.0584
2.0445
-0.0001
O
N
O
Cl
2ap
0.97
2.97
0.98
2.08
0.93
1.98
1.97
1.95
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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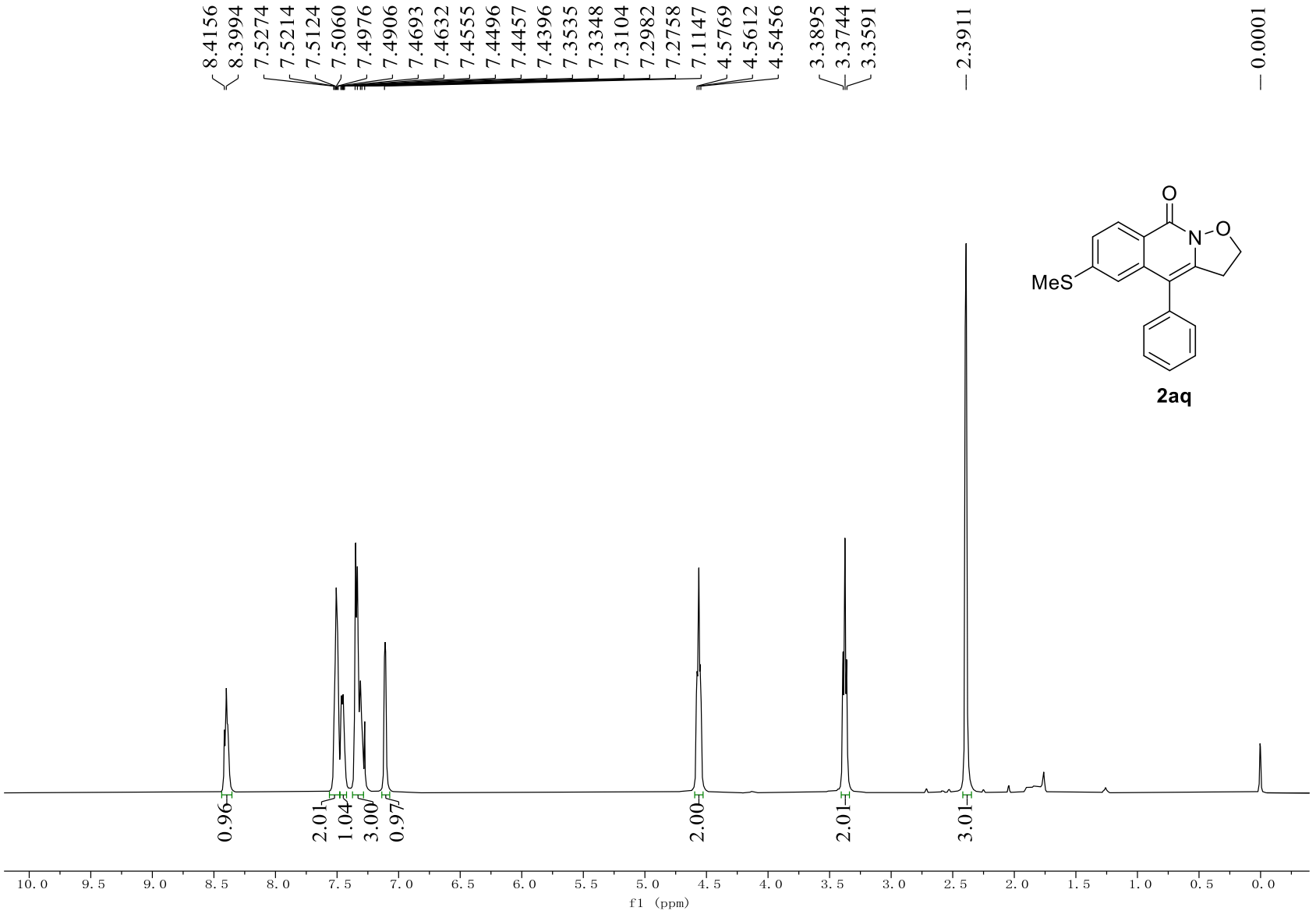
128.2226
126.4809
124.3189
123.8104
114.5232
77.2264
76.9728
76.7189
70.8492
21.6159
21.4880
O
N
O
Cl
2ap
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.5060
7.4976
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7.4693
7.4632
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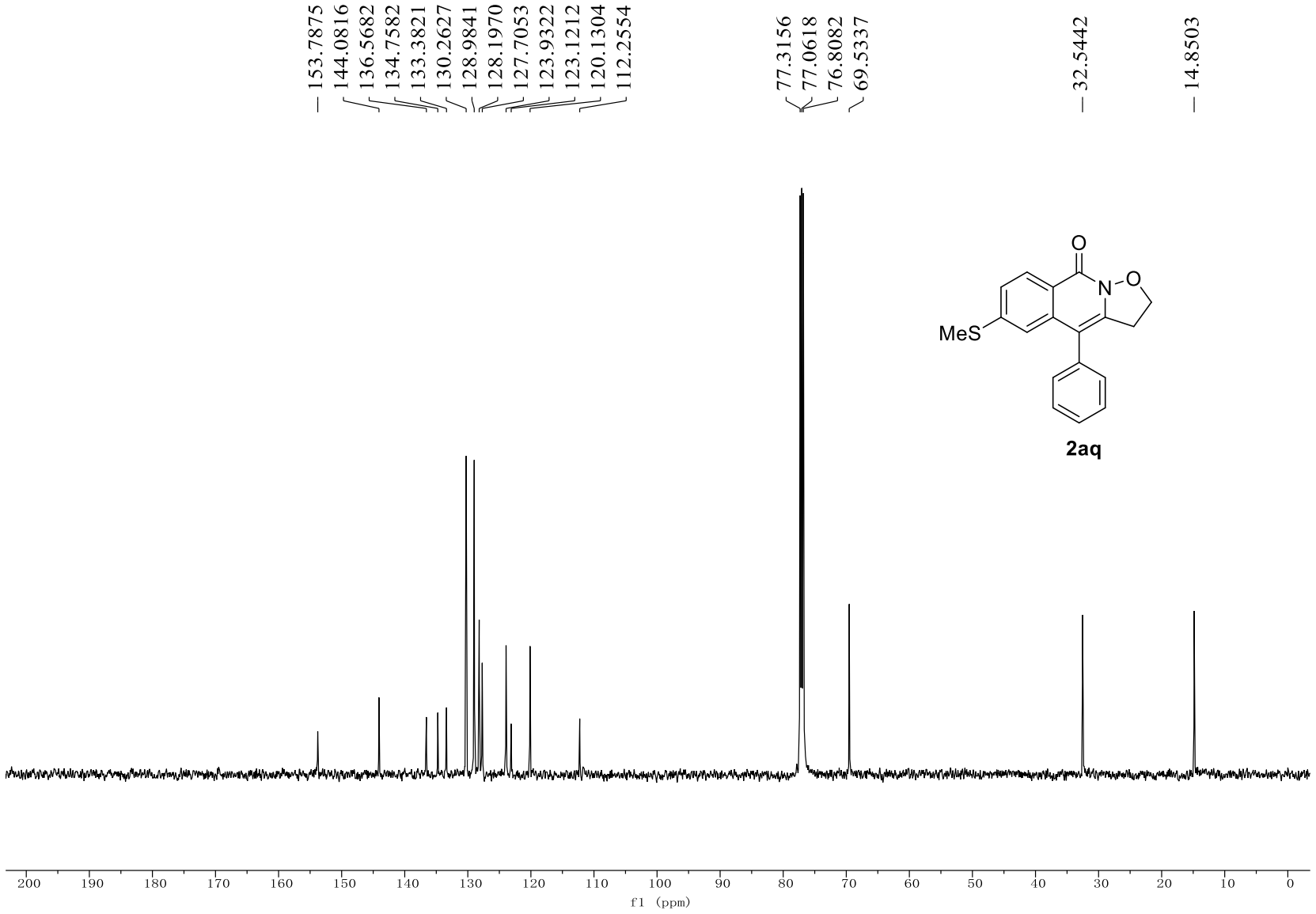
7.4496
7.4457
7.4396
7.3535
7.3348
7.3104
7.2982
7.2758
7.1147
4.5769
4.5612
4.5456
3.3895
3.3744
3.3591
2.3911
0.0001
O
N
O
MeS
2aq
0.96
2.01
1.04
3.00
0.97
2.00
2.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.1970
127.7053
123.9322
123.1212
120.1304
112.2554
77.3156
77.0618
76.8082
69.5337
32.5442
14.8503
O
N
O
MeS
2aq
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)