Electronic Supplementary Material (ESI) for RSC Advances.

Iodine(III)-Mediated Construction of Dibenzoxazepinone Skeleton from 2-(Aryloxy)benzamides through Oxidative C-N Formation

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Supporting Information

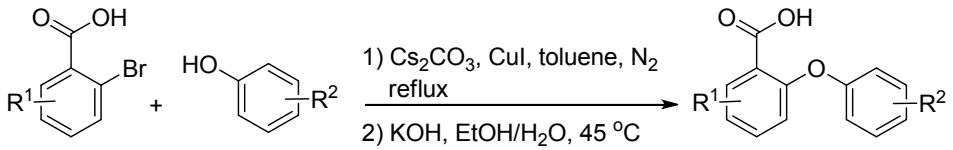
I. General Information

All reactions were carried out at room temperature under air unless otherwise noted. ^{1}H and ^{13}C NMR spectra were recorded on 600 MHz or 400 MHz spectrometer at 25 ^{o}C. Chemical shifts values are given in ppm and referred as the internal standard to TMS: 0.00 ppm. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; qui, quintet; m, multiplet and dd, doublet of doublets, brs, broad singlet. The coupling constants *J*, are reported in Hertz (Hz). High resolution mass spectrometry (HRMS) was obtained on a Q-TOF micro spectroMeter. Melting points were determined with a MicroMelting point apparatus without corrections. Organic solutions were concentrated by rotary evaporation below 40 °C in vacuum. TLC plates were visualized by exposure to ultraviolet light.

Reagents and solvents were purchased as reagent grade and were used without further purification. All reactions were performed in standard glassware, heated at 70 ^{o}C for 3 h before use. Flash column chromatography was performed over silica gel 200-300 m and the eluent was a mixture of ethyl acetate (EA) and petroleum ether (PE).

II. Procedures for the Synthesis of Amides 1.[1-3]

1. General Procedure for the Synthesis of Acids 3a-p and 3r.

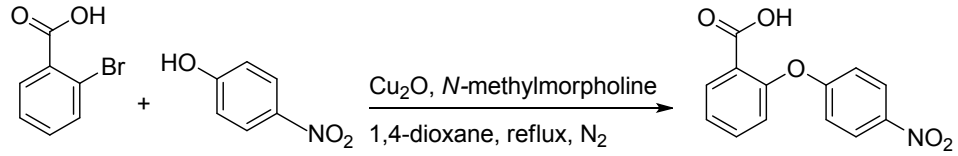


5 **4** **3**

To a mixture of substituted 2-bromobenzoic ester (10 mmol) and substitutedphenol (12 mmol) in toluene (20 mL) was added Cs_2CO_3 (3.78 g, 15 mmol) and CuI (1.90 g 10 mmol) and the flask was purged with N_2. After stirring for 5 minutes at room temperature, the mixture was stirred at 125 ^{o}C for 15 hours. After the completion of the reaction (monitored by TLC), the reaction mixture was cooled down to room temperature, filtered over celite, washed with ethyl acetate, and evaporated. To the crude material was added MeOH (40 mL), KOH (2.8 g) and the mixture was stirred for 3 hours at 45 ^{o}C. After completion of the hydrolysis, aq. HCl solution (3 M, 45

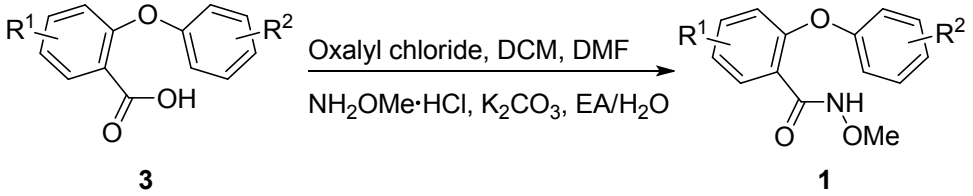
mL) was used to adjust pH to 3-4. Then extracted with ethyl acetate (3 × 100 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude product can be used for the next step without any purification.

2. Procedure for the Synthesis of Acid 3q.



2-Bromobenzoic acid (2.0 g, 10 mmol), 4-nitrophenol (1.4 g, 10 mmol), *N*-methylmorpholine (1.7 mL, 15 mmol) and Cu(I) oxide (0.72 g, 5 mmol) were heated to reflux in dioxane (30 mL) under nitrogen for 16 h. The resulting reaction mixture was allowed to cool slowly to room temperature before HCl (4 M, 20 mL) was added. The precipitate was filtrated, washed with water (10 mL × 2), and then concentrated under reduced pressure.[4]

3. General Procedure for Converting Acids 3a-r into Amides 1a-r.

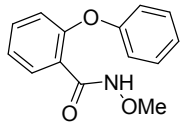


3 **1**

To a solution of the substituted 2-bromobenzoic acid in DCM (0.3 M) was added a catalytic amount of DMF (2 drops). At ambient temperature, oxalyl chloride (1.2 equiv) was added dropwise over a period of 0.5 h. The resulting solution was kept at room temperature until TLC indicated the total consumption of the acid. Then, the solvent was removed under reduced pressure. The residue was dissolved in dry DCM (5 mL) and slowly added dropwise to a solution of the $NH_2OMe{\cdot}HCl$ (1.2 equiv) and K_2CO_3 (3 equiv) in EA/H_2O = 2:1 (40 mL). The reaction mixture was maintained at ambient temperature and monitored by TLC. Upon completion, the mixture was

extracted with EA (3 × 50 mL) and the combined organic phase was washed with NH_4Cl (80 mL) and brine (80 mL). Dried over Na_2SO_4 and evaporation of the solvent under reduced pressure and purification of the crude residue by flash column chromatography on silica gel (EA/PE) afforded the desired amides.

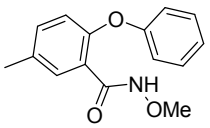
<u>*N*-Methoxy-2-phenoxybenzamide (1a)</u>



1a

Following the general procedure, **1a** was obtained as a white solid (1.34 g), yield: 55% (over three steps), mp. 66 – 68 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.10 (s, 1H), 8.25 (d, *J* = 7.2 Hz, 1H), 7.44 – 7.40 (m, 2H), 7.40 – 7.36 (m, 1H), 7.26 – 7.18 (m, 2H), 7.10 – 7.05 (m, 2H), 6.81 – 6.76 (d, *J* = 8.3 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.6, 155.5, 154.9, 133.2, 132.2, 130.3, 125.2, 123.6, 121.6, 120.1, 117.6, 64.5; HRMS (ESI) calcd for $C_{14}H_{13}NNaO_3^+$ [M + Na^+] 266.0788, found 266.0790.

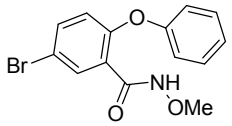
<u>*N*-Methoxy-5-methyl-2-phenoxybenzamide (1b)</u>



1b

Following the general procedure, **1b** was obtained as a light yellow oil (1.16 g), yield: 45% (over three steps). ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.08 (s, 1H), 8.03 (s, 1H), 7.39 (dd, *J* = 8.3, 7.7 Hz, 2H), 7.24 – 7.15 (m, 2H), 7.04 (d, *J* = 7.8 Hz, 2H), 6.71 (d, *J* = 8.4 Hz, 1H), 3.83 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.7, 155.5, 153.0, 133.8, 133.6, 132.2, 130.2, 124.8, 121.5, 119.6, 118.2, 64.5, 20.5; HRMS (ESI) calcd for $C_{15}H_{15}NNaO_3^+$ [M + Na^+] 280.0944, found 280.0947.

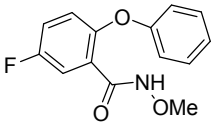
<u>5-Bromo-*N*-methoxy-2-phenoxybenzamide (1c)</u>



1c

Following the general procedure, **1c** was obtained as light yellow oil (1.67 g), yield: 52% (over three steps).^{1}H NMR (600 MHz, $CDCl_3$) δ 10.10 (s, 1H), 8.35 (s, 1H), 7.50 – 7.38 (m, 3H), 7.30 – 7.25 (m, 1H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.67 (d, *J* = 8.8 Hz, 1H), 3.85 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.4, 154.9, 154.3, 133.3, 132.3, 124.1, 122.0, 121.6, 117.8, 64.6; HRMS (ESI) calcd for $C_{14}H_{12}{}^{79}BrNNaO_3^+$ [M + Na^+] 343.9893, found 343.9895.

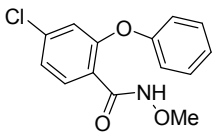
5-Fluoro-*N*-methoxy-2-phenoxybenzamide (1d)



1d

Following the general procedure, **1d** was obtained as a light yellow oil (1.17 g), yield: 45% (over three steps). ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.11 (s, 1H), 7.94 (dd, *J* = 9.0, 3.0 Hz, 1H), 7.47 – 7.35 (m, 2H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.09 (ddd, *J* = 9.1, 7.1, 3.3 Hz, 1H), 7.06 – 7.03 (m, 2H), 6.79 (dd, *J* = 9.0, 4.3 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2 , 158.6 (d, $J_{C\text{-}F}$ = 243.9 Hz), 155.3 , 151.3 , 130.4 , 125.2 , 123.5 (d, $J_{C\text{-}F}$ = 7.4 Hz), 120.0 (d, $J_{C\text{-}F}$ = 23.9 Hz), 119.7 (d, $J_{C\text{-}F}$ = 7.6 Hz), 119.6 , 118.3 (d, $J_{C\text{-}F}$ = 25.4 Hz), 64.6; ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -118.48 (s, 1F); HRMS (ESI) calcd for $C_{14}H_{12}{}^{19}FNNaO_3^+$ [M + Na^+] 284.0693, found 284.0692.

4-Chloro-*N*-methoxy-2-phenoxybenzamide (1e)

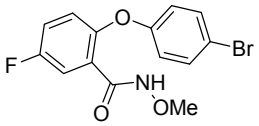


1e

Following the general procedure, **1e** was obtained as a light yellow oil (1.39 g), yield: 50% (over three steps). ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.22 – 7.15 (m, 1H), 7.10 (d, *J* = 8.3 Hz, 2H), 6.74 (s, 1H), 3.87 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ

162.7, 156.2, 154.1, 138.9, 133.4, 130.4, 125.9, 123.8, 120.4, 119.8, 117.3, 64.6; HRMS (ESI) calcd for $C_{14}H_{12}{}^{35}ClNNaO_3^+$ [M + Na^+] 300.0398, found 300.0398.

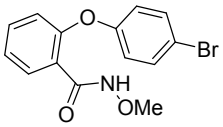
2-(4-Bromophenoxy)-5-fluoro-N-methoxybenzamide (1f)



1f

Following the general procedure, **1f** was obtained as a white solid (1.64 g), yield: 48% (over three steps), mp. 106 – 108 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.96 (s, 1H), 7.91 (d, *J* = 8.9 Hz, 1H), 7.52 (dd, *J* = 8.1, 3.4 Hz, 2H), 7.17 – 7.05 (m, 1H), 6.93 (d, *J* = 8.7 Hz, 2H), 6.80 (dd, *J* = 8.9, 4.0 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.0, 158.8 (d, J_{C-F} = 244.7 Hz), 154.6, 150.6, 133.36, 123.9 (d, J_{C-F} = 7.1 Hz), 121.1, 120.1 (d, J_{C-F} = 23.8 Hz), 119.9 (d, J_{C-F} = 7.7 Hz), 118.4 (d, J_{C-F} = 25.2 Hz), 117.9, 64.6; ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -117.46 (s, 1F); HRMS (ESI) calcd for $C_{14}H_{11}{}^{79}Br^{19}FNNaO_3^+$ [M + Na^+] 361.9799, found 361.9802.

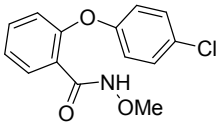
2-(4-Bromophenoxy)-*N*-methoxybenzamide (1g)



1g

Following the general procedure, **1g** was obtained as a beige solid (1.51 g), yield: 47% (over three steps), mp. 88 – 90 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.96 (s, 1H), 8.23 (d, *J* = 7.7 Hz, 1H), 7.53 (d, *J* = 8.7 Hz, 2H), 7.46 – 7.36 (m, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.79 (d, *J* = 8.3 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.4, 154.9, 154.3, 133.3, 132.3, 124.1, 122.0, 121.6, 117.8, 64.6 (one carbon peak was missing due to overlapping); HRMS (ESI) calcd for $C_{14}H_{11}{}^{79}Br^{19}FNNaO_3^+$ [M + Na^+] 361.9799, found 361.9801.

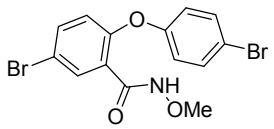
2-(4-Chlorophenoxy)-*N*-methoxybenzamide (1h)



1h

Following the general procedure, **1h** was obtained as a white solid (1.33 g), yield: 48% (over three steps), mp. 86 – 88 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.92 (s, 1H), 8.22 (d, *J* = 7.5 Hz, 1H), 7.42 – 7.39 (m, 1H), 7.38 – 7.35 (m, 2H), 7.25 – 7.21 (m, 1H), 7.09 – 6.92 (m, 2H), 6.79 (d, *J* = 8.2 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.4, 154.9, 153.80, 133.2, 132.1, 130.2, 130.2, 124.0, 122.2, 121.1, 117.9, 64.4; HRMS (ESI) calcd for $C_{14}H_{12}{}^{35}ClNNaO_3^+$ [M + Na^+] 300.0398, found 300.0396

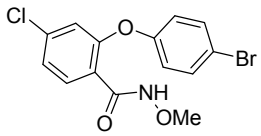
5-Bromo-2-(4-bromophenoxy)-*N*-methoxybenzamide (1i)



1i

Following the general procedure, **1i** was obtained as a white solid (1.56 g), yield: 39% (over three steps), mp. 77 – 79 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 2.5 Hz, 1H), 7.58 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.47 – 7.38 (m, 2H), 6.87 (d, *J* = 8.7 Hz, 1H), 6.84 – 6.79 (m, 2H), 3.82 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.0, 154.1, 153.8, 136.0, 134.9, 133.5, 123.4, 121.7, 119.4, 118.4, 116.9, 64.6; HRMS (ESI) calcd for $C_{14}H_{11}{}^{79}Br_2NNaO_3^+$ [M + Na^+] 421.8998, found 421.9001.

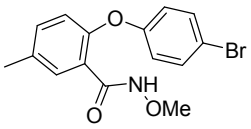
2-(4-Bromophenoxy)-4-chloro-*N*-methoxybenzamide (1j)



1j

Following the general procedure, **1j** was obtained as a white solid (1.28 g), yield: 36% (over three steps), mp. 116 – 118 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.90 (s, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.8 Hz, 2H), 7.20 (dd, *J* = 8.5, 1.9 Hz, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.74 (d, *J* = 1.7 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.5, 155.6, 153.3, 139.0, 133.6, 133.5, 124.3, 122.1, 120.1, 118.8, 117.4, 64.6; HRMS (ESI) calcd for $C_{14}H_{11}{}^{79}Br^{35}ClNNaO_3^+$ [M + Na^+] 377.9503, found 377.9504.

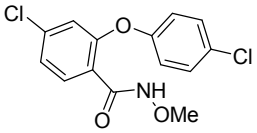
2-(4-Bromophenoxy)-*N*-methoxy-5-methylbenzamide (1k)



1k

Following the general procedure, **1k** was obtained as a tan solid (1.71 g), yield: 51% (over three steps), mp. 62 – 64 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.91 (s, 1H), 8.01 (s, 1H), 7.49 (d, *J* = 8.8 Hz, 2H), 7.24 – 7.16 (m, 1H), 6.92 (d, *J* = 8.8 Hz, 2H), 6.71 (d, *J* = 8.4 Hz, 1H), 3.83 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.5, 154.9, 152.4, 134.2, 133.9, 133.1, 132.3, 121.9, 121.0, 118.4, 117.3, 64.5, 20.5; HRMS (ESI) calcd for $C_{15}H_{14}{}^{79}BrNNaO_3^+$ [M + Na^+] 358.0049, found 358.0047.

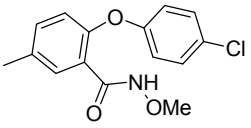
4-Chloro-2-(4-chlorophenoxy)-*N*-methoxybenzamide (1l)



1l

Following the general procedure, **1l** was obtained as a white solid (1.25 g), yield: 40% (over three steps), mp. 63 – 65 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.74 (s, 1H), 3.84 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.5, 155.7, 152.9, 138.9, 133.3, 131.1, 130.5, 124.2, 121.6, 120.3, 117.5, 64.5; HRMS (ESI) calcd for $C_{14}H_{11}{}^{35}Cl_2NNaO_3^+$ [M + Na^+] 334.0008, found 334.0010.

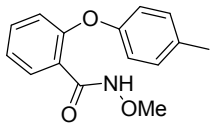
2-(4-Chlorophenoxy)-*N*-methoxy-5-methylbenzamide (1m)



1m

Following the general procedure, **1m** was obtained as a white solid (1.49 g), yield: 51%, mp. 62 – 64 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.98 (s, 1H), 7.41 – 7.31 (m, 2H), 7.21 (d, *J* = 8.4 Hz, 1H), 7.05 – 6.91 (m, 2H), 6.71 (d, *J* = 8.3 Hz, 1H), 3.83 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.5, 154.3, 152.5, 134.1, 133.9, 132.2, 130.1, 129.8, 121.8, 120.7, 118.3, 64.5, 20.5; HRMS (ESI) calcd for $C_{15}H_{14}{}^{35}ClNNaO_3^+$ [M + Na^+] 314.0554, found 314.0557.

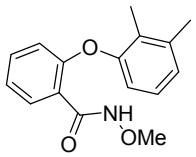
***N*-Methoxy-2-(*p*-tolyloxy)benzamide (1n)**



1n

Following the general procedure, **1n** was obtained as a beige solid (1.39 g), yield: 54%, mp. 96 – 98 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.18 (s, 1H), 8.24 (d, *J* = 7.7 Hz, 1H), 7.40 – 7.32 (m, 1H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.18 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 2H), 6.76 (d, *J* = 8.3 Hz, 1H), 3.87 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.7, 156.0, 152.5, 135.0, 133.1, 132.2, 130.8, 123.3, 121.2, 120.2, 117.1, 64.5, 20.8; HRMS (ESI) calcd for $C_{15}H_{15}NNaO_3^+$ [M + Na^+] 280.0944, found 280.0943.

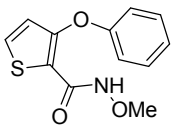
2-(2,3-Dimethylphenoxy)-*N*-methoxybenzamide (1o)



1o

Following the general procedure, **1o** was obtained as a brown solid (1.02 g), yield: 37%, mp. 104 – 106 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.32 (s, 1H), 8.27 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.32 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1H), 7.20 – 7.06 (m, 3H), 6.86 (d, *J* = 7.8 Hz, 1H), 6.56 (dd, *J* = 8.3, 0.6 Hz, 1H), 3.90 (s, 3H), 2.35 (s, 3H), 2.12 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 156.2, 152.0, 139.6, 133.2, 132.3, 129.2, 127.4, 126.9, 122.7, 120.1, 118.9, 115.3, 64.6, 20.1, 12.4; HRMS (ESI) calcd for $C_{16}H_{17}NNaO_3^+$ [M + Na^+] 294.1101, found 294.1103.

***N*-Methoxy-3-phenoxythiophene-2-carboxamide (1p)**

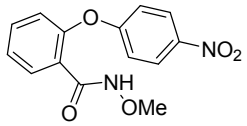


1p

Following the general procedure, **1p** was obtained as a light yellow oil (1.27 g), yield: 37%, mp. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.64 (s, 1H), 7.41 (t, *J* = 7.7 Hz, 3H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 2H), 6.53 (d, *J* = 5.5 Hz, 1H), 3.85 (s,

3H).^{13}C NMR (150 MHz, $CDCl_3$) δ 160.3, 155.9, 153.5, 130.2, 130.0, 125.3, 119.2, 118.1, 64.9 (one carbon peak was missing due to overlapping); HRMS (ESI) calcd for $C_{12}H_{11}NNaO_3S^+$ [M + Na^+] 272.0352, found 272.0355.

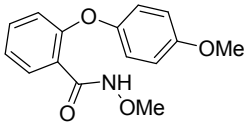
<u>*N*-Methoxy-2-(4-nitrophenoxy)benzamide (1q)</u>



1q

Following the general procedure, **1q** was obtained as a beige solid (1.12 g), yield: 41%, mp. 108 – 110 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.51 (s, 1H), 8.27 (d, *J* = 9.1 Hz, 2H), 8.16 (d, *J* = 6.3 Hz, 1H), 7.58 – 7.46 (m, 1H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.11 (d, *J* = 9.1 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 1H), 3.79 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.0, 161.3, 152.6, 143.9, 133.5, 132.2, 126.2, 125.9, 123.9, 120.2, 118.3, 64.6; HRMS (ESI) calcd for $C_{14}H_{12}N_2NaO_5^+$ [M + Na^+] 311.0638, found 311.0637.

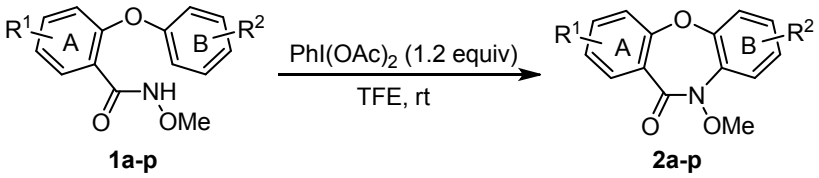
<u>*N*-Methoxy-2-(4-methoxyphenoxy)benzamide (1r)</u>



1r

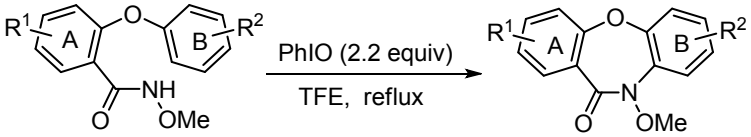
Following the general procedure, **1r** was obtained as a beige solid (1.47 g), yield: 54%, mp. 88 – 90 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.24 (s, 1H), 8.24 (s, 1H), 7.35 (dd, *J* = 3.0, 1.8 Hz, 1H), 7.23 – 7.10 (m, 1H), 7.03 (dd, *J* = 8.7, 4.5 Hz, 2H), 6.98 – 6.90 (m, 2H), 6.76 – 6.66 (m, 1H), 3.89 (s, 3H), 3.83 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.7, 157.1, 156.6, 147.8, 133.1, 132.2, 123.0, 121.7, 120.7, 116.4, 115.3, 64.6, 55.7; HRMS (ESI) calcd for $C_{15}H_{15}NNaO_4^+$ [M + Na^+] 296.0893, found 296.0896.

III. General Procedure for the Synthesis of 2a-m and 2q.



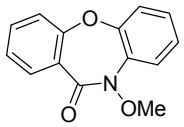
To a stirred solution of **1** (0.5 mmol) in TFE (10 mL) was added PIDA (1.2 mmol) slowly at room temperature. The resulting mixture was kept at the same temperature until the TLC indicated that the total consumption of **1**. The reaction was quenched by sat. $NaHCO_3$ (25 mL) and extracted with ethyl acetate (3 × 20 mL). The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4 and then evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford the desired product **2**.

IV. Procedures for the synthesis of 2n-p and 2r



To a stirred solution of **1** (0.5 mmol) in TFE (10 mL) was added PhIO (2.2 mmol) slowly at rt. The resulting mixture was heat at reflux for 15 hours. The reaction was quenched by sat. $NaHCO_3$ (25 mL) and extracted with ethyl acetate (3 × 20 mL). The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4

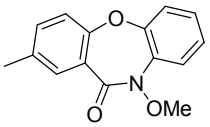
10-Methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2a)



2a

Following the general procedure, **2a** was obtained as a light yellow oil (108 mg), yield: 89%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.45 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.40 (td, *J* = 8.0, 1.7 Hz, 1H), 7.20 – 7.17 (m, 1H), 7.16 (dd, *J* = 8.2, 2.1 Hz, 2H), 7.14 – 7.13 (m, 1H), 7.10 (td, *J* = 7.7, 1.6 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.6, 159.8, 151.4, 134.2, 132.7, 132.2, 127.0, 126.0, 125.4, 124.5, 121.2, 120.5, 120.4, 62.7; HRMS (ESI) calcd for $C_{14}H_{11}NNaO_3^+$ [M + Na^+] 264.0631, found 264.0633.

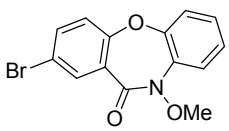
10-Methoxy-2-methyldibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2b)



2b

Following the general procedure, **2b** was obtained as a light yellow oil (120 mg), yield: 93%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.52 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.27 (s, 1H), 7.26 – 7.24 (m, 1H), 7.22 (td, *J* = 7.8, 1.4 Hz, 1H), 7.17 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 3.92 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.8, 157.748, 151.7, 135.2, 134.8, 132.7, 132.1, 127.0, 125.9, 124.0, 121.1, 120.6, 120.1, 62.6, 20.6; HRMS (ESI) calcd for $C_{15}H_{13}NNaO_3^+$ [M + Na^+] 278.0788, found 278.0786.

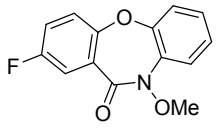
2-Bromo-10-methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2c)



2c

Following the general procedure, **2c** was obtained as a light yellow oil (152 mg), yield: 95%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, J = 2.4 Hz, 1H), 7.58 (dd, J = 8.6, 2.4 Hz, 1H), 7.54 (d, J = 8.2 Hz, 1H), 7.27 – 7.24 (m, 2H), 7.21 (dd, J = 10.9, 4.3 Hz, 1H), 7.11 (d, J = 8.6 Hz, 1H), 3.92 (s, 3H).^{13}C NMR (150 MHz, $CDCl_3$) δ 161.3, 158.8, 151.2, 136.9, 134.7, 132.3, 127.3, 126.3, 126.2, 122.3, 121.1, 120.7, 118.3, 62.8; HRMS (ESI) calcd for $C_{14}H_{10}{}^{79}BrNNaO_3^+$ [M + Na^+] 341.9736, found 341.9739.

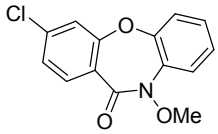
2-Fluoro-10-methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2d)



2d

Following the general procedure, **2d** was obtained as a white solid (117 mg), yield: 89%, mp. 127 – 129 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (dd, J = 8.5, 2.3 Hz, 1H), 7.54 (d, J = 8.6 Hz, 1H), 7.28 – 7.24 (m, 2H), 7.19 (ddd, J = 6.2, 4.2, 3.7 Hz, 3H), 3.93 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.5 , 159.5 (d, $J_{C\text{-}F}$ = 245.0 Hz), 155.7 (d, $J_{C\text{-}F}$ = 2.6 Hz), 151.5 , 132.4 , 127.3 , 126.2 , 126.0 (d, $J_{C\text{-}F}$ = 7.9 Hz), 122.0 (d, $J_{C\text{-}F}$ = 8.1 Hz), 121.1 , 120.9 (d, $J_{C\text{-}F}$ = 23.7 Hz), 120.7 , 118.2 (d, $J_{C\text{-}F}$ = 25.5 Hz), 62.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.54 (s, 1F); HRMS (ESI) calcd for $C_{14}H_{10}{}^{19}FNNaO_3^+$ [M + Na^+] 282.0537, found 282.0540.

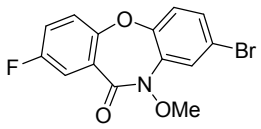
3-Chloro-10-methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2e)



2e

Following the general procedure, **2e** was obtained as a beige solid (133 mg), yield: 96%, mp. 107 – 109 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, J = 8.4 Hz, 1H), 7.54 (dd, J = 8.4, 1.5 Hz, 1H), 7.27 (ddd, J = 8.3, 3.6, 1.7 Hz, 3H), 7.22 (ddd, J = 9.2, 8.0, 2.1 Hz, 2H), 3.92 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.8, 159.9, 150.9, 139.7, 133.2, 132.5, 127.2, 126.4, 125.9, 123.0, 121.2, 120.9, 120.6, 62.7; HRMS (ESI) calcd for $C_{14}H_{10}{}^{35}ClNNaO_3^+$ [M + Na^+] 298.0241, found 298.0243.

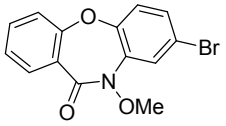
8-Bromo-2-fluoro-10-methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2f)



2f

Following the general procedure, **2f** was obtained as a colorless oil (135 mg), yield: 80%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 – 7.58 (m, 2H), 7.30 (d, J = 8.3 Hz, 1H), 7.20 (d, J = 5.0 Hz, 2H), 7.14 (d, J = 8.6 Hz, 1H), 3.95 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.3 , 159.6 (d, $J_{C\text{-}F}$ = 245.6 Hz), 155.3 (d, $J_{C\text{-}F}$ = 2.4 Hz), 150.1 , 133.8 , 130.0 , 125.5 (d, $J_{C\text{-}F}$ = 7.9 Hz), 123.4 , 122.6 , 122.0 (d, $J_{C\text{-}F}$ = 8.1 Hz), 121.3 (d, $J_{C\text{-}F}$ = 23.7 Hz), 118.9 , 118.3 (d, $J_{C\text{-}F}$ = 25.5 Hz), 63.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.94 (s, 1F); HRMS (ESI) calcd for $C_{14}H_9{}^{79}Br^{19}FNNaO_3^+$ [M + Na^+] 359.9642, found 359.9645.

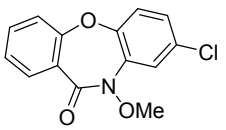
8-Bromo-10-methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2g)



2g

Following the general procedure, **2g** was obtained as a light yellow solid (146 mg), yield: 91%, mp. 66 – 68 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (dd, J = 7.8, 1.6 Hz, 1H), 7.68 (d, J = 2.3 Hz, 1H), 7.59 – 7.46 (m, 1H), 7.31 – 7.26 (m, 2H), 7.21 (d, J = 8.1 Hz, 1H), 7.15 (d, J = 8.6 Hz, 1H), 3.95 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.4, 159.3, 150.2, 134.5, 134.2, 132.3, 129.7, 125.7, 124.1, 123.3, 122.7, 120.3, 118.7, 63.1; HRMS (ESI) calcd for $C_{14}H_{10}{}^{79}BrNNaO_3^+$ [M + Na^+] 341.9736, found 341.9734.

8-Chloro-10-methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2h)

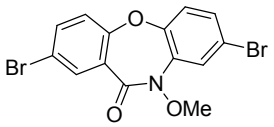


2h

Following the general procedure, **2h** was obtained as a reddish-brown oil (126 mg), yield: 91%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 (dd, J = 7.8, 1.5 Hz, 1H), 7.54 (t, J =

2.8 Hz, 1H), 7.52 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.29 (dd, *J* = 5.6, 2.3 Hz, 1H), 7.25 – 7.19 (m, 2H), 7.15 (dd, *J* = 8.6, 2.4 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.4, 159.4, 149.6, 134.4, 133.9, 132.3, 131.4, 126.7, 125.6, 124.1, 122.3, 120.3, 120.3, 63.0; HRMS (ESI) calcd for $C_{14}H_{10}{}^{35}ClNNaO_3^+$ [M + Na^+] 298.0241, found 298.0238.

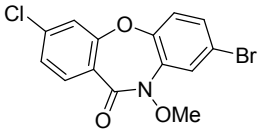
2,8-Dibromo-10-methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2i)



2i

Following the general procedure, **2i** was obtained as a beige solid (147 mg), yield: 74%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.68 (d, *J* = 2.3 Hz, 1H), 7.60 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.31 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.11 (dd, *J* = 8.5, 8.6 Hz, 2H), 3.94 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.1, 158.3, 149.9, 137.2, 134.8, 133.8, 130.0, 125.8, 123.4, 122.6, 122.2, 119.1, 118.6, 63.1; HRMS (ESI) calcd for $C_{14}H_9{}^{79}Br_2NNaO_3^+$ [M + Na^+] 419.8841, found 419.8844.

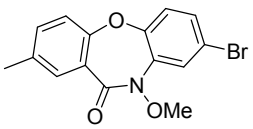
8-Bromo-3-chloro-10-methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2j)



2j

Following the general procedure, **2j** was obtained as a white solid (133 mg), yield: 75%, mp. 121 – 123 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 – 7.88 (m, 1H), 7.73 – 7.64 (m, 1H), 7.34 – 7.28 (m, 1H), 7.26 – 7.21 (m, 2H), 7.13 (dd, *J* = 8.6, 1.4 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.6, 159.5, 149.6, 140.1, 134.0, 133.3, 129.9, 126.1, 123.3, 122.6, 122.6, 120.9, 119.1, 63.1; HRMS (ESI) calcd for $C_{14}H_9{}^{79}Br^{35}ClNNaO_3^+$ [M + Na^+] 375.9347, found 375.9349.

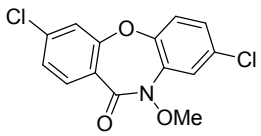
8-Bromo-10-methoxy-2-methyldibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2k)



2k

Following the general procedure, **2k** was obtained as a tan solid (159 mg), yield: 95%, mp. 119 – 121 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, *J* = 1.4 Hz, 1H), 7.66 (d, *J* = 2.3 Hz, 1H), 7.28 (td, *J* = 8.7, 2.0 Hz, 2H), 7.11 (dd, *J* = 8.4, 8.4 Hz, 2H), 3.94 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.6, 157.3, 150.4, 135.5, 135.1, 134.2, 132.2, 129.7, 123.5, 123.3, 122.6, 120.1, 118.6, 63.0, 20.6; HRMS (ESI) calcd for $C_{16}H_{14}{}^{79}BrNNaO_2^+$ [M + Na^+] 354.0100, found 354.0101.

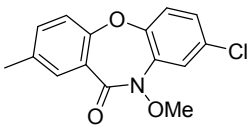
3,8-Dichloro-10-methoxydibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2l)



2l

Following the general procedure, **2l** was obtained as a white solid (112 mg), yield: 72%, mp. 132 – 134 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.1 Hz, 1H), 7.53 (s, 1H), 7.27 – 7.23 (m, 2H), 7.19 (d, *J* = 8.5 Hz, 1H), 7.15 (d, *J* = 8.6 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.6, 159.5, 149.0, 140.0, 133.7, 133.3, 131.8, 126.9, 126.1, 122.6, 122.3, 120.8, 120.4, 63.1; HRMS (ESI) calcd for $C_{14}H_9{}^{35}Cl_2NNaO_3^+$ [M + Na^+] 331.9852, found 331.9850.

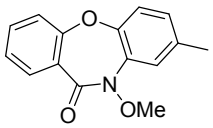
8-Chloro-10-methoxy-2-methyldibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2m)



2m

Following the general procedure, **2m** was obtained as a tan solid (124 mg), yield: 85%, mp. 117 – 119 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, *J* = 1.3 Hz, 1H), 7.52 (d, *J* = 2.4 Hz, 1H), 7.29 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.18 (d, *J* = 8.6 Hz, 1H), 7.13 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.09 (d, *J* = 8.2 Hz, 1H), 3.94 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.6, 157.4, 149.9, 135.5, 135.1, 134.0, 132.2, 131.2, 126.7, 123.5, 122.2, 120.4, 120.1, 63.0, 20.6; HRMS (ESI) calcd for $C_{15}H_{12}{}^{35}ClNNaO_3^+$ [M + Na^+] 312.0398, found 312.0401.

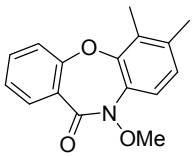
10-Methoxy-8-methyldibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2n)



2n

Following the general procedure, **2n** was obtained as a light yellow oil (76 mg), yield: 59%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.48 (ddd, *J* = 9.2, 7.8, 1.7 Hz, 1H), 7.33 (d, *J* = 1.4 Hz, 1H), 7.22 (ddd, *J* = 8.0, 7.5, 3.2 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 1H), 6.98 (dd, *J* = 8.2, 1.5 Hz, 1H), 3.93 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7, 159.9, 149.4, 136.0, 134.1, 132.1, 127.6, 125.3, 124.6, 120.8, 120.3, 62.7, 21.0 (two carbon peak was missing due to overlapping); HRMS (ESI) calcd for $C_{15}H_{13}NNaO_3^+$ [M + Na^+] 278.0788, found 278.0791.

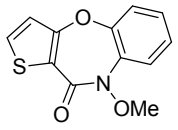
10-Methoxy-6,7-dimethyldibenzo[*b*,*f*][1,4]oxazepin-11(10*H*)-one (2o)



2o

Following the general procedure, **2o** was obtained as a white solid (59 mg), yield: 43%, mp. 117 – 119 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.48 (td, *J* = 8.2, 1.7 Hz, 1H), 7.31 – 7.18 (m, 3H), 7.01 (d, *J* = 8.3 Hz, 1H), 3.90 (s, 3H), 2.43 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6, 159.8, 149.9, 136.2, 133.8, 132.2, 130.4, 129.1, 126.6, 125.3, 125.1, 120.6, 117.5, 62.8, 19.8, 12.6; HRMS (ESI) calcd for $C_{16}H_{15}NNaO_3^+$ [M + Na^+] 292.0944, found 292.0941.

9-Methoxybenzo[*b*]thieno[2,3-*f*][1,4]oxazepin-10(9*H*)-one (2p)

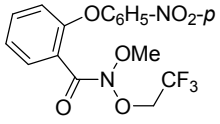


2p

Following the general procedure, **2p** was obtained as a tan solid (41 mg), yield: 33%, mp. 123 – 125 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 1H), 7.51 (d, *J* = 5.3 Hz, 1H), 7.32 – 7.22 (m, 1H), 7.18 (d, *J* = 3.9 Hz, 2H), 6.85 (d, *J* = 5.3 Hz, 1H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 150.1, 133.2, 132.3, 126.9, 126.2,

121.1, 120.8, 120.3, 118.8, 62.9 (one carbon peak was missing due to overlapping); HRMS (ESI) calcd for $C_{12}H_9NNaO_3S^+$ [M + Na^+] 270.0195, found 270.0197.

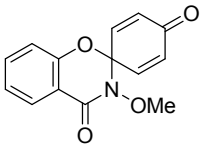
<u>*N*-Methoxy-2-(4-nitrophenoxy)-*N*-(2,2,2-trifluoroethoxy)benzamide (2q)</u>



2q

Following the general procedure, **2q** was obtained as a colorless oil (110 mg), yield: 57%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 (d, *J* = 2.1 Hz, 1H), 8.20 (d, *J* = 2.1 Hz, 1H), 7.58 (m, 2H), 7.35 (td, *J* = 7.6, 0.8 Hz, 1H), 7.11 (d, *J* = 8.1 Hz, 1H), 7.03 – 6.98 (m, 2H), 4.30 (q, *J* = 8.4 Hz, 2H), 3.77 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.8 , 161.7 , 151.1 , 142.1 , 132.1 , 128.9 , 125.7 , 125.0 , 124.4 , 121.7 (q, *J* = 272.6 Hz) 120.4 , 116.2 , 69.3 (q, *J* = 34.8 Hz), 60.2; HRMS (ESI) calcd for $C_{16}H_{13}{}^{19}F_3N_2NaO_6^+$ [M + Na^+] 409.0618, found 409.0621.

<u>3-Methylspiro[benzo[*e*][1,3]oxazine-2,1'-cyclohexa[2,5]diene]-4,4'(3*H*)-dione (2r)</u>



2r

Following the general procedure, **2r** was obtained as a yellow solid (85 mg), yield: 66%, mp. 103 – 105 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 6.9 Hz, 1H), 7.53 (t, *J* = 6.9 Hz, 1H), 7.19 (t, *J* = 6.5 Hz, 1H), 7.01 (d, *J* = 9.8 Hz, 2H), 6.97 (d, *J* = 7.8 Hz, 1H), 6.39 (d, *J* = 9.7 Hz, 2H), 3.88 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 183.9, 162.6, 154.0, 140.2, 135.6, 131.7, 128.2, 123.4, 117.1, 116.3, 86.9, 65.5; HRMS (ESI) calcd for $C_{14}H_{11}NNaO_4^+$ [M + Na^+] 280.0580, found 280.0577.

V. References:

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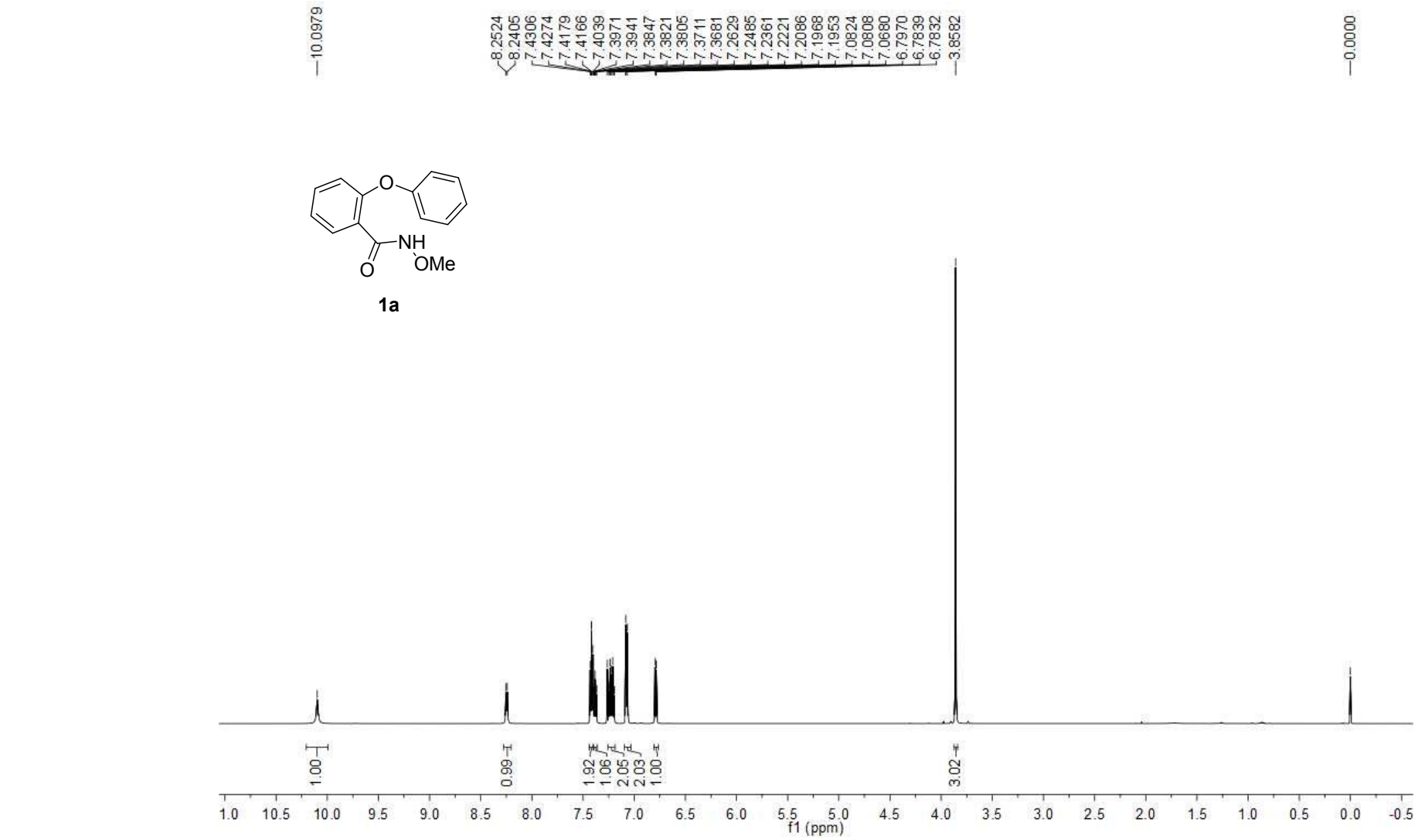
P. R. Likhar, M. L. Kantam, P. Saravanan, T. Magdaleno and S. H. Kwonc, *Adv. Synth. Catal.,* 2011, **353**, 1591.

3. Anderson, M. O.; Jamie, M.; John, S.; and Guy, R. K. Synlett 2004, **13**, 2391.

4. D. K. Chalmers, G. H. Scholz, D. J. Topliss, E. Kolliniatis, S. L. A. Munro, D. J. Craik, M. N. Iskander and J. R. Stockigt, *J. Med. Chem.,* 1993, **36**, 1272.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7.3847
7.3821
7.3805
7.3711
7.3681
7.2629
7.2485
7.2361
7.2221
7.2086
7.1968
7.1953
7.0824
7.0808
7.0680
6.7970
6.7839
6.7832
3.8582
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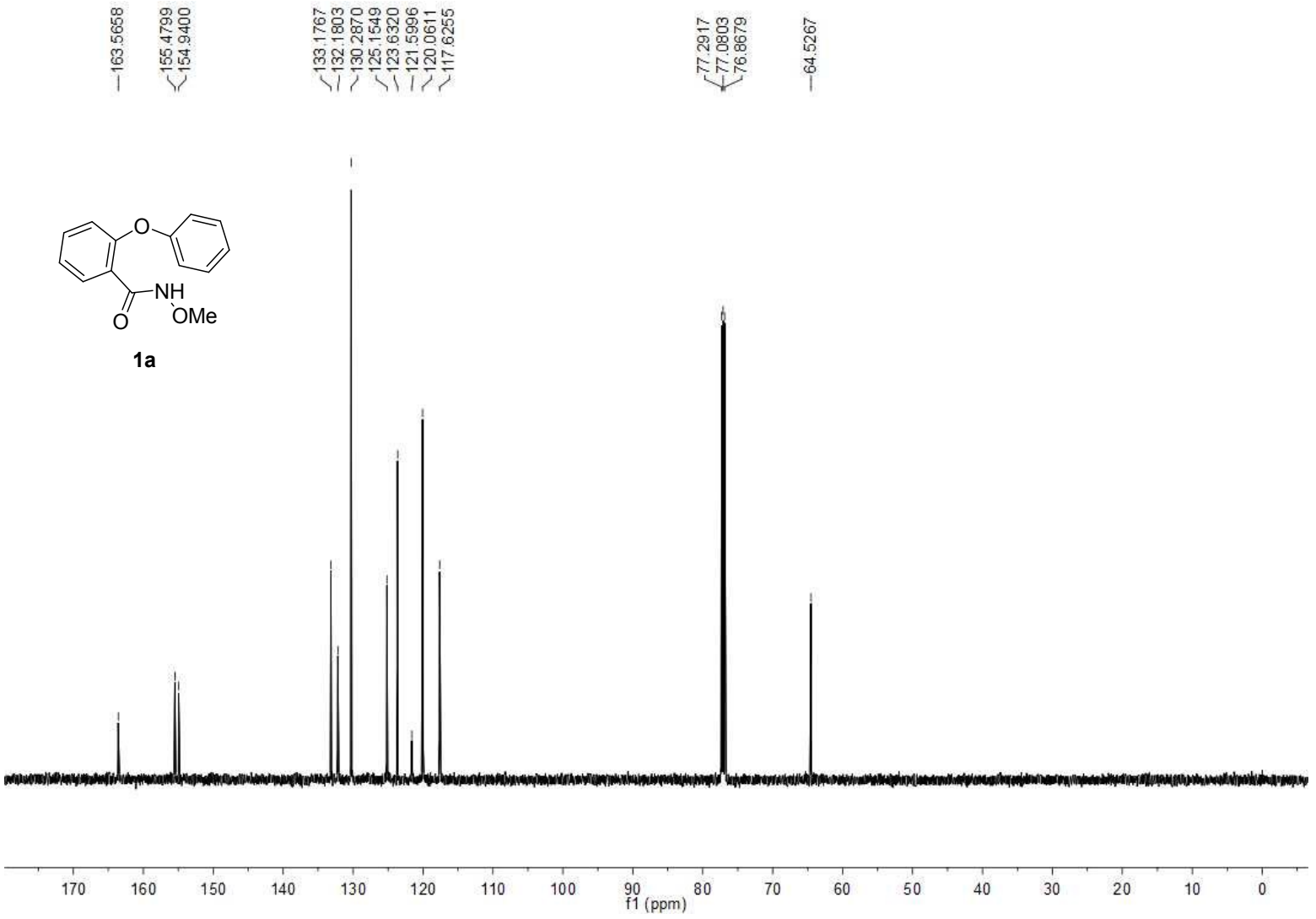
OMe
O
1a
1.00
0.99
1.92
1.06
2.05
2.03
1.00
3.02
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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120.0611
117.6255
77.2917
77.0803
76.8679
64.5267
O
NH
OMe
O
1a
170
160
150
140
130
120
110
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90
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70
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50
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30
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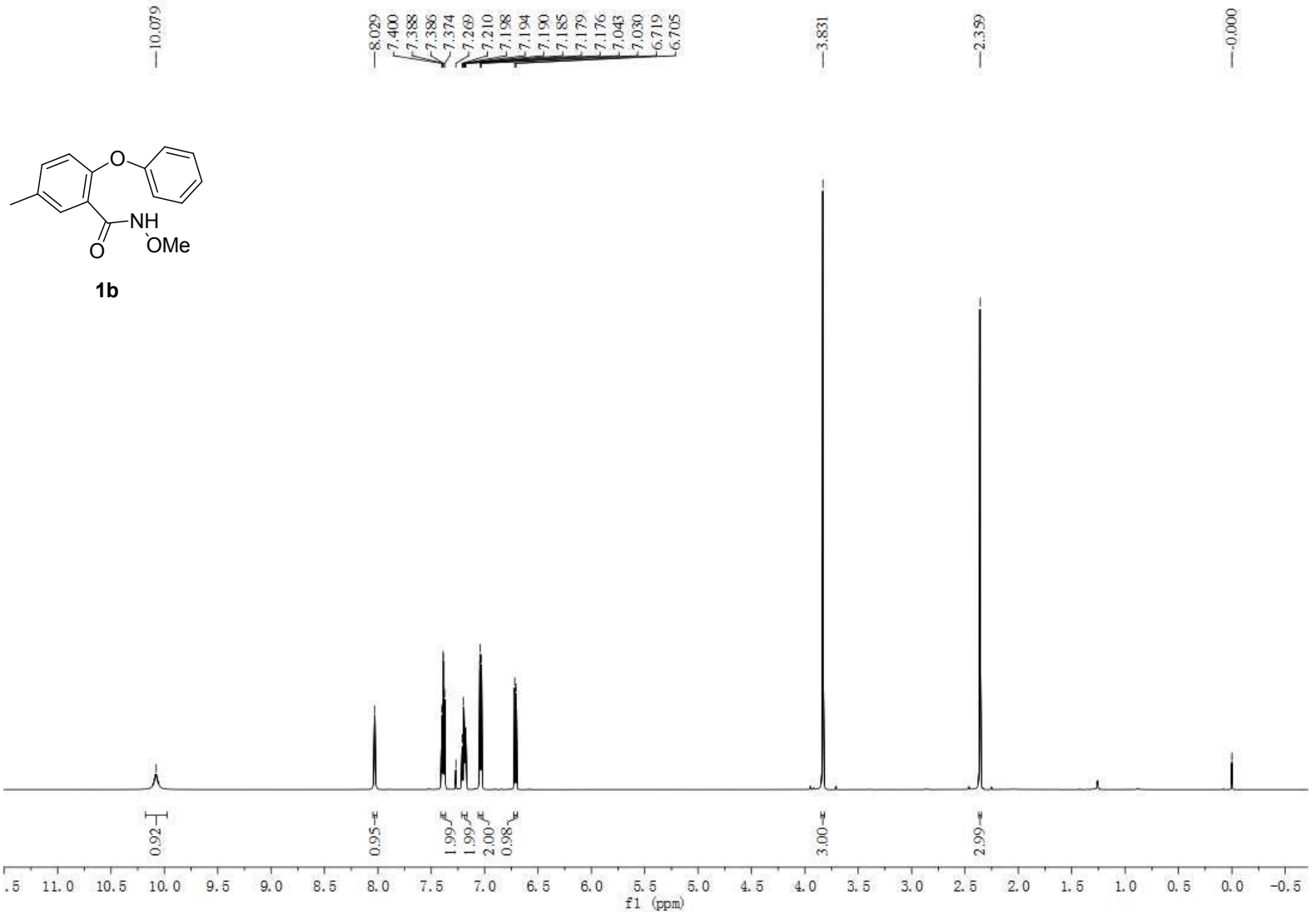
f1 (ppm)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7.194
7.190
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7.179
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7.043
7.030
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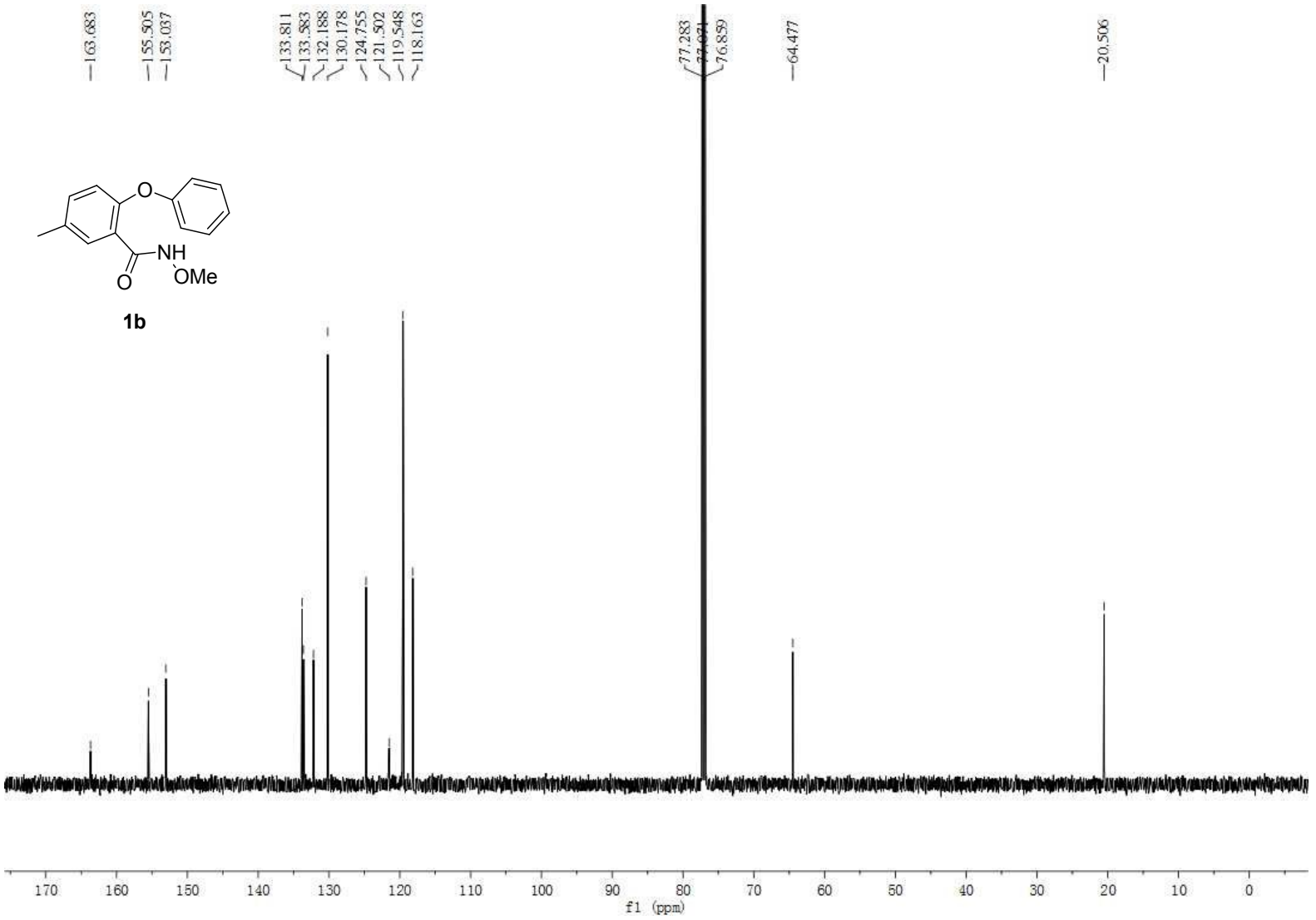
2.99
f1 (ppm)

1b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76.859
64.477
20.506
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OMe
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1b
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20
10
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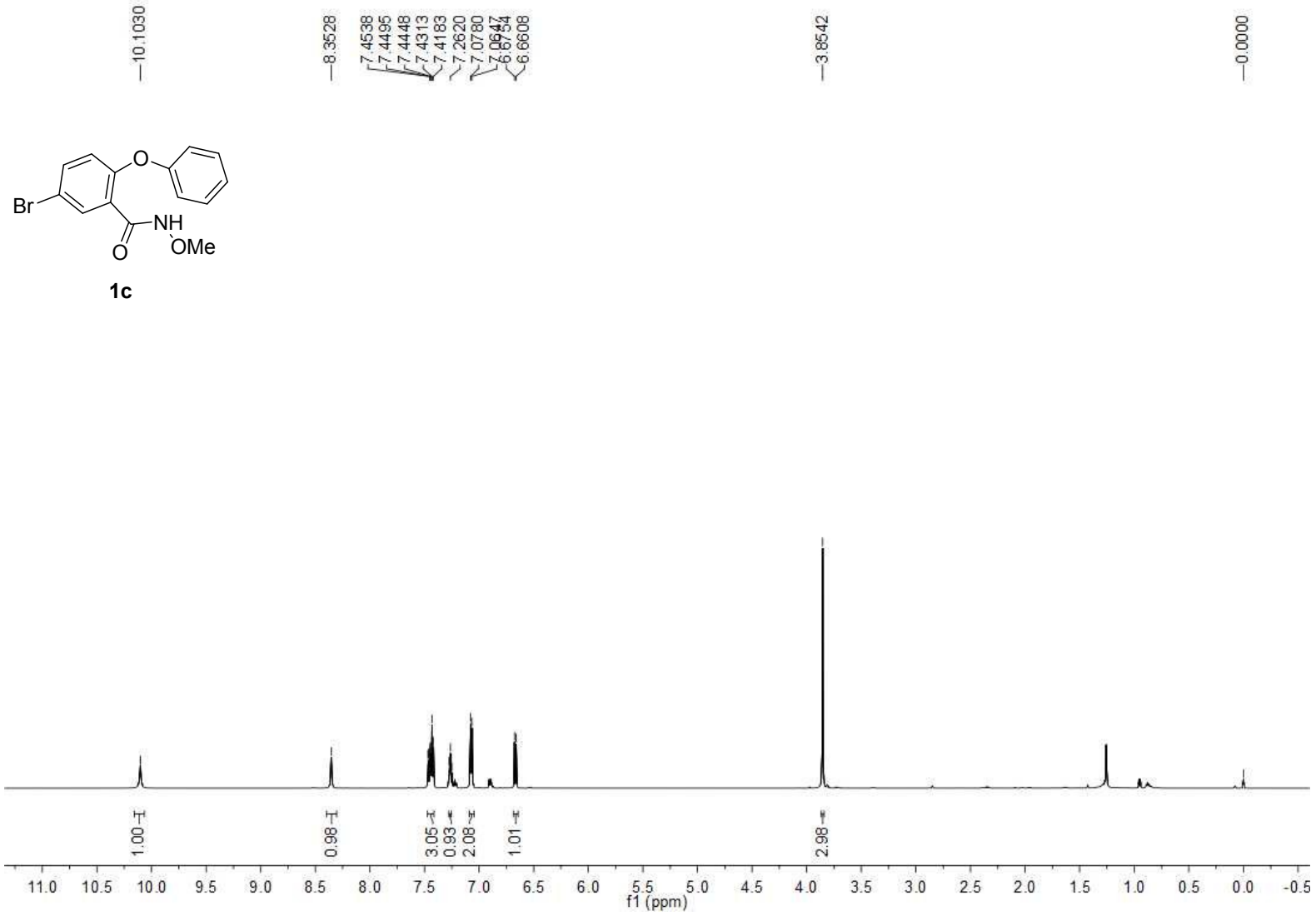
f1 (ppm)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6.6608
3.8542
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OMe
O
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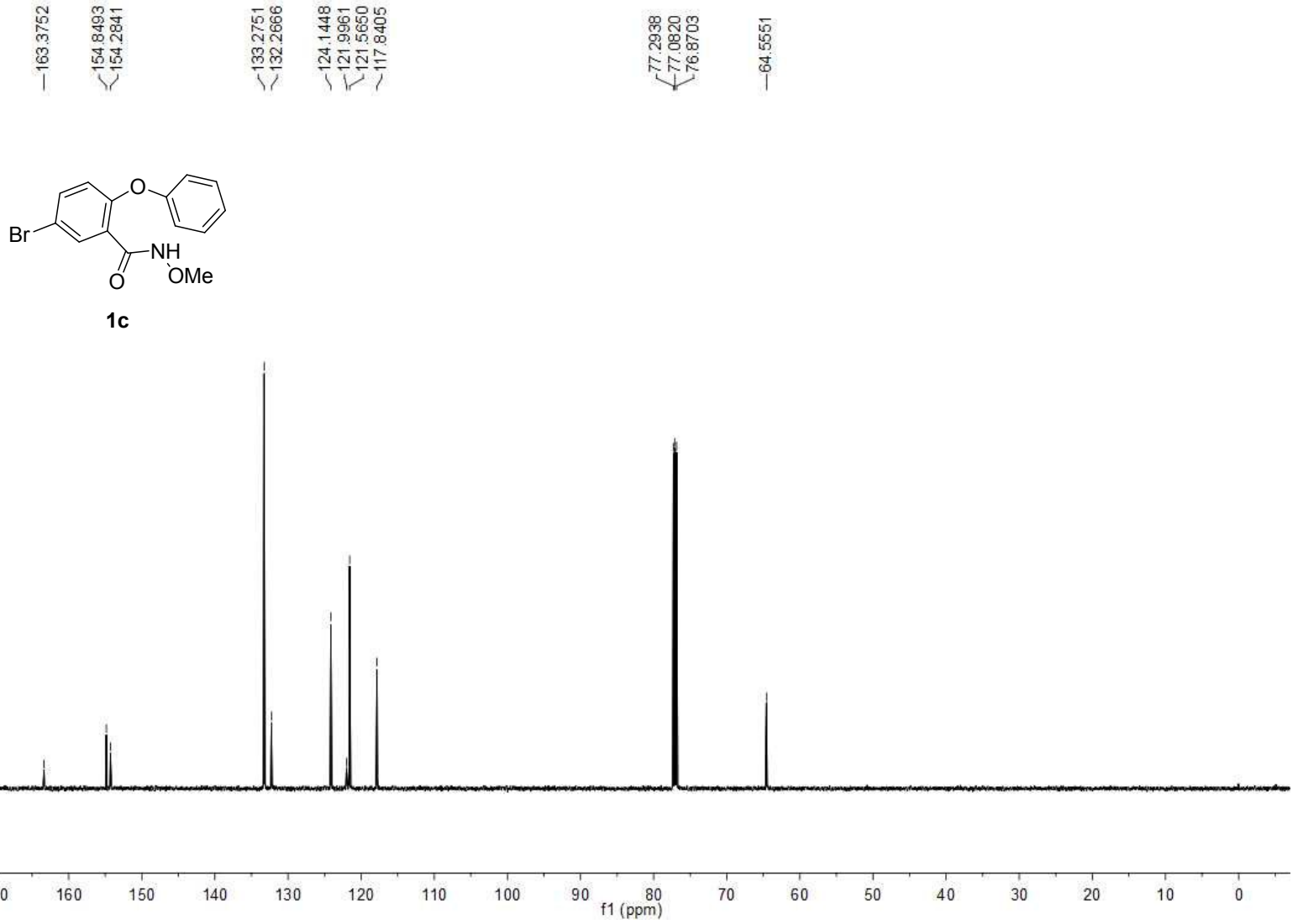
0.98
3.05
0.93
2.08
1.01
2.98
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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76.8703
64.5551
Br
O
NH
OMe
O
1c
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160
150
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130
120
110
100
90
80
70
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50
40
30
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10
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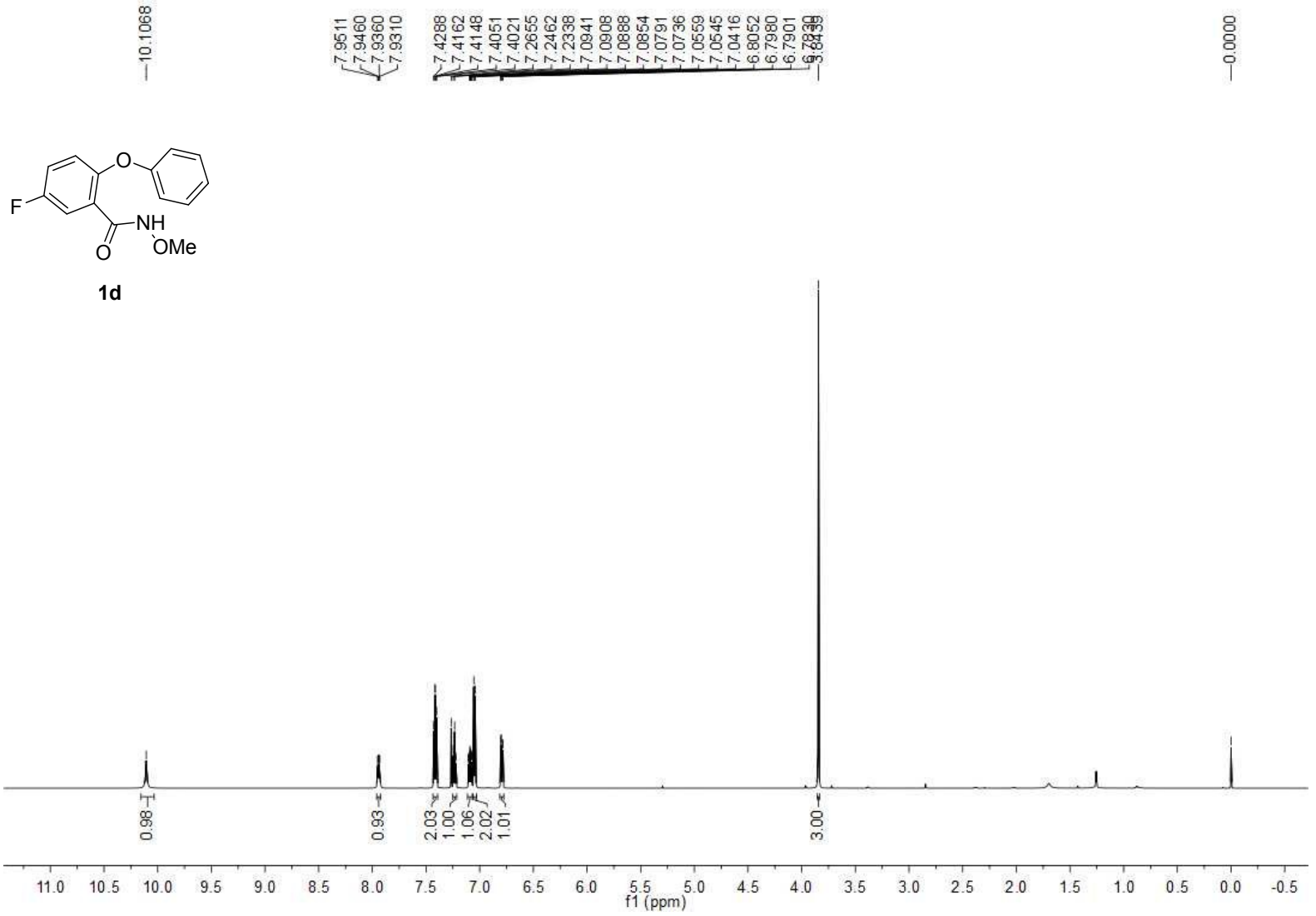
f1 (ppm)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7.2462
7.2338
7.0941
7.0908
7.0888
7.0854
7.0791
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7.0559
7.0545
7.0416
6.8052
6.7980
6.7901
3.8439
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O
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OMe
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1.06
2.02
1.01
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10.0
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9.0
8.5
8.0
7.5
7.0
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6.0
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5.0
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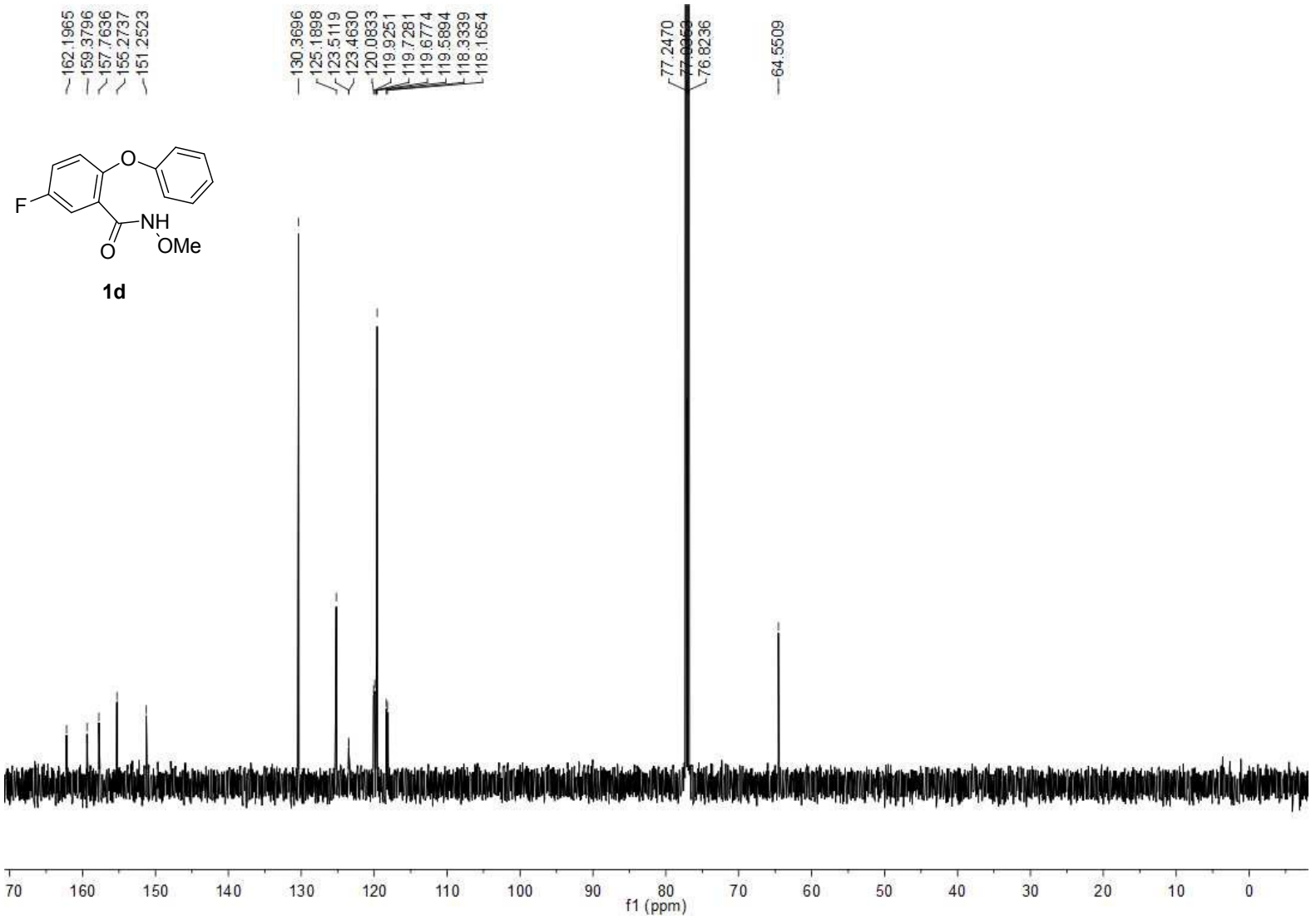
f1 (ppm)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118.1654
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O
OMe
1d
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50
40
30
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10
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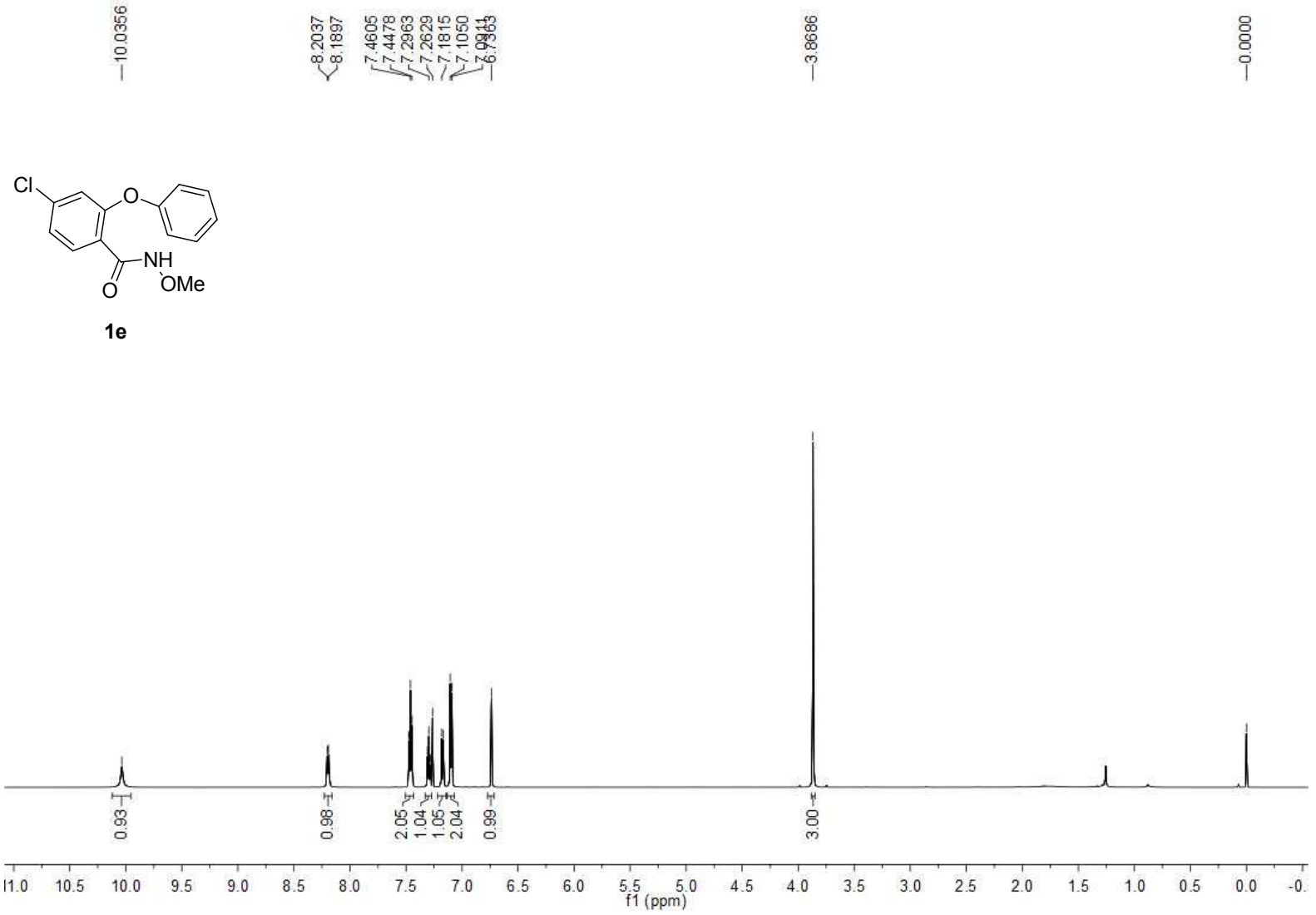
f1 (ppm)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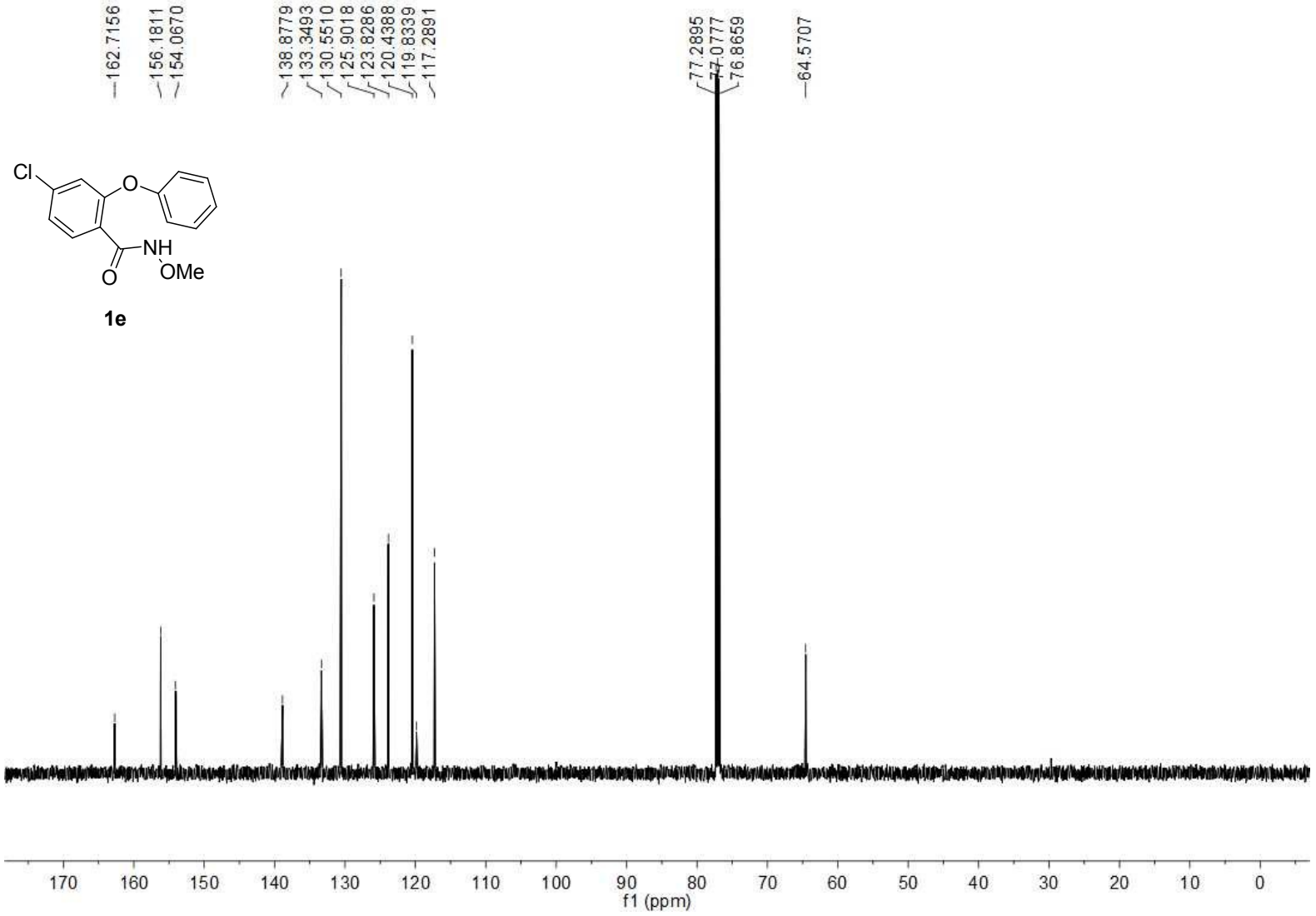
f1 (ppm)

1e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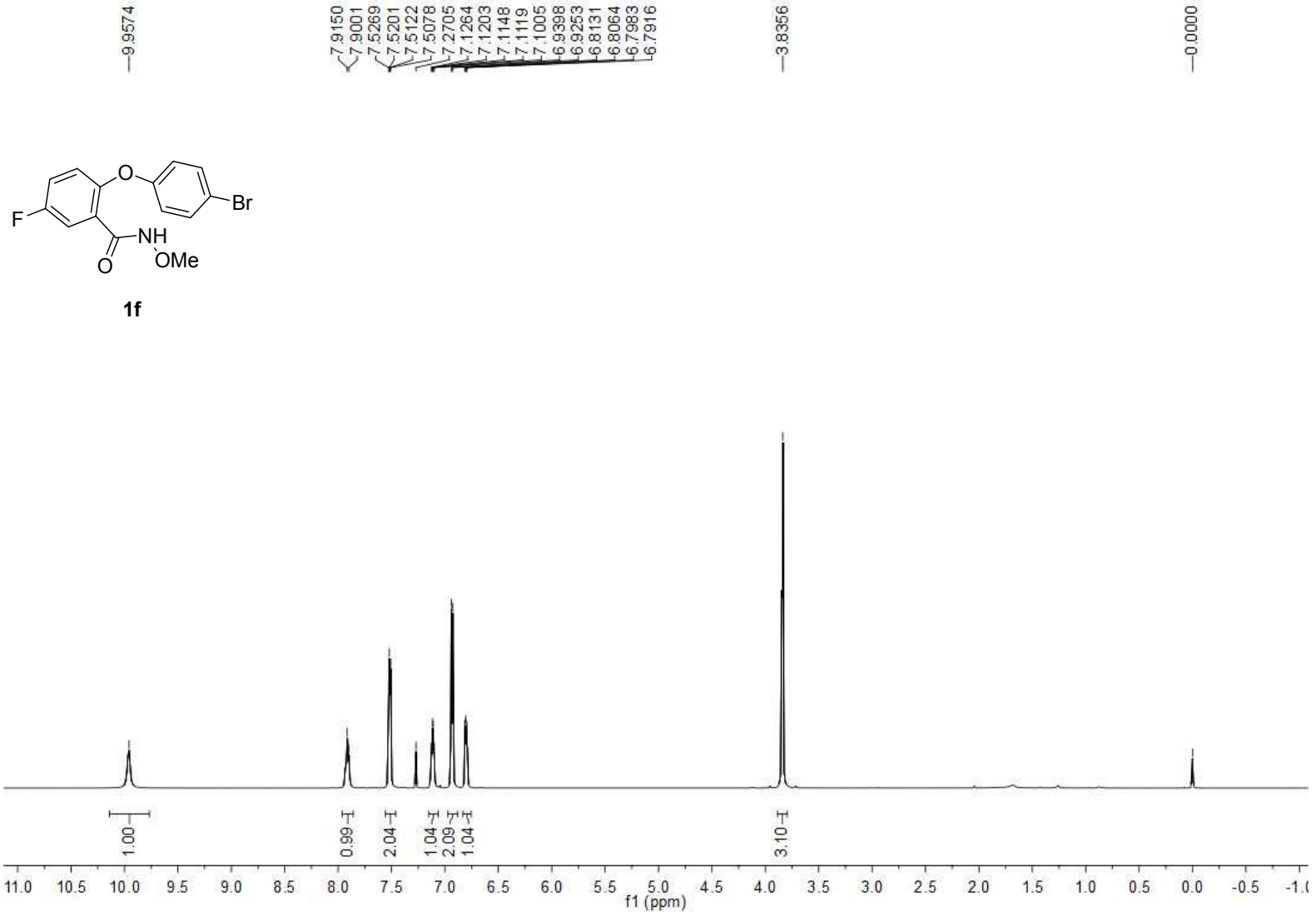
f1 (ppm)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7.1148
7.1119
7.1005
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6.9253
6.8131
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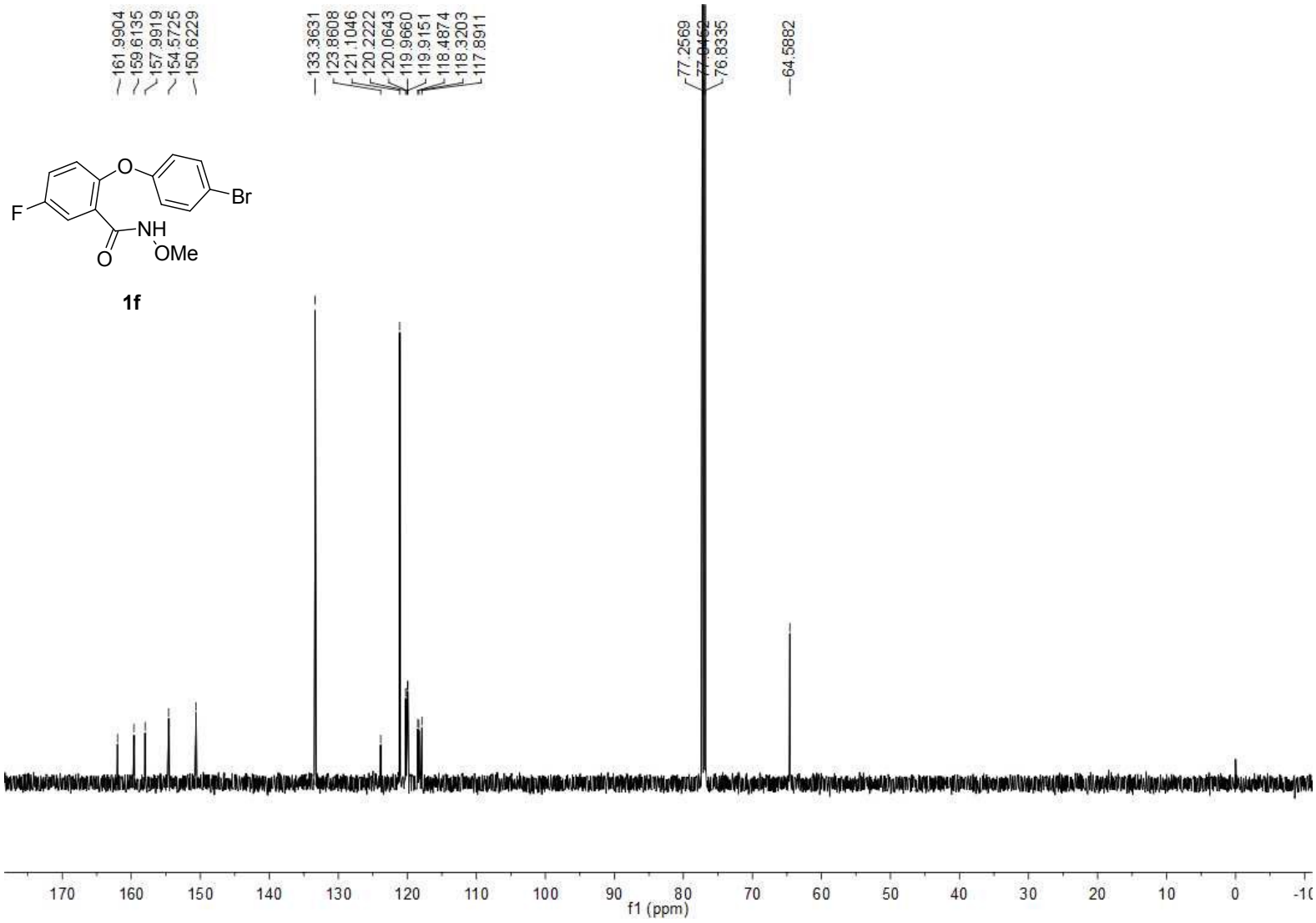
2.09
1.04
3.10
f1 (ppm)

1f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Br
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OMe
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80
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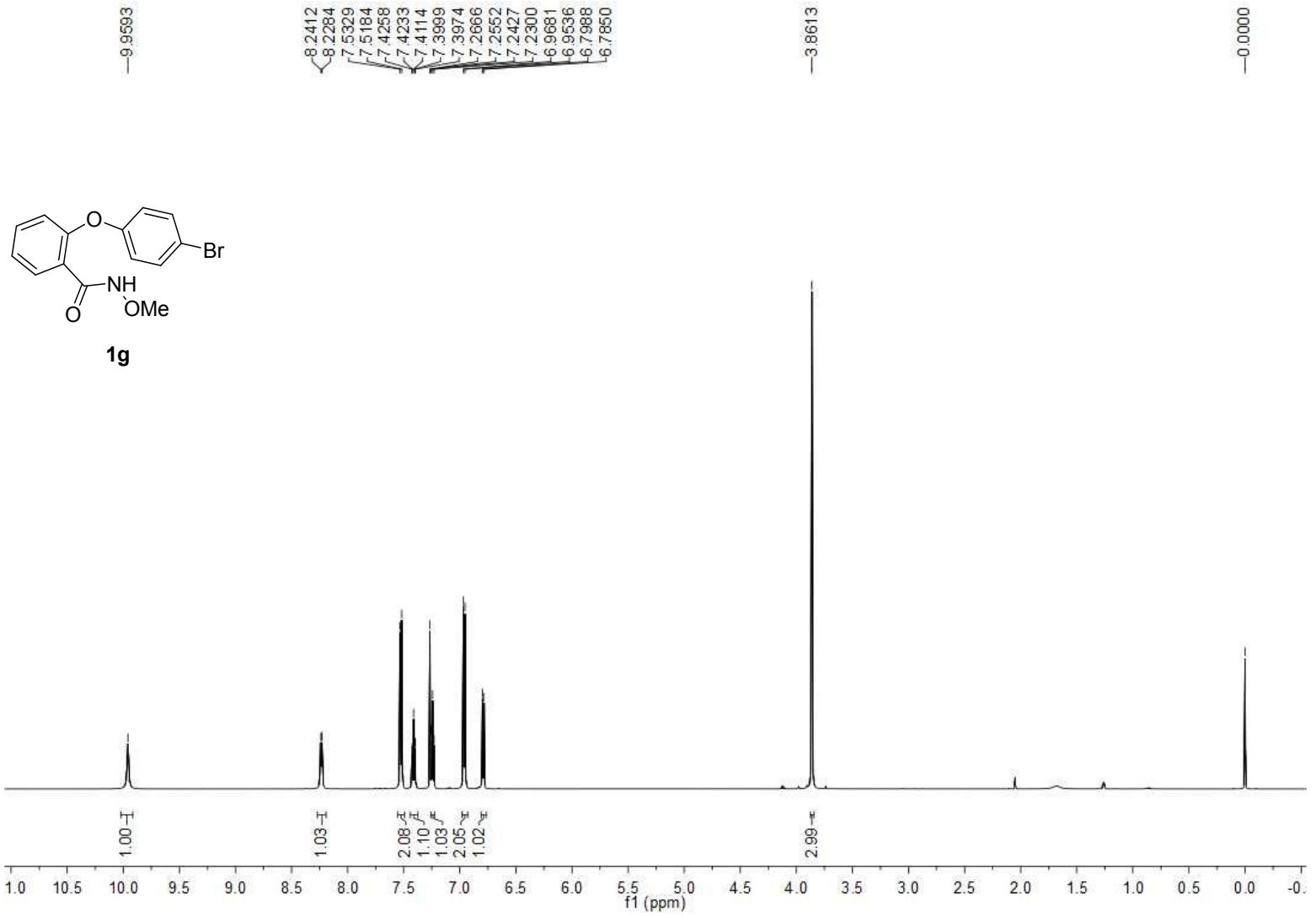
f1 (ppm)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7.3999
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7.2666
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7.2427
7.2300
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6.9536
6.7988
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Br
NH
OMe
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1.03
2.05
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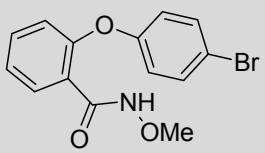
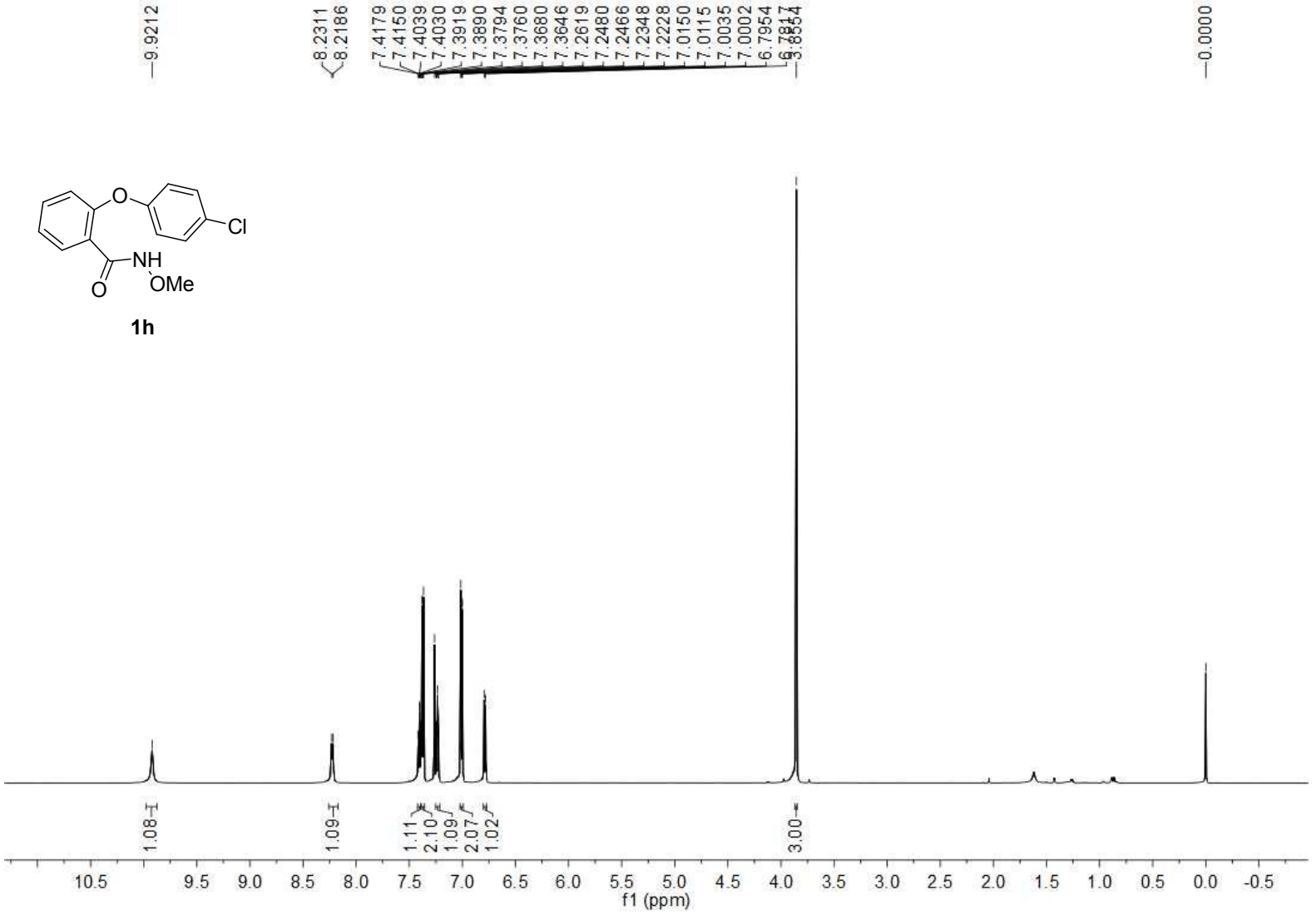
2.99
f1 (ppm)



1g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NH
O
OMe
1h
1.08
1.09
1.11
2.10
1.09
2.07
1.02
3.00
10.5
9.5
9.0
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8.0
7.5
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6.0
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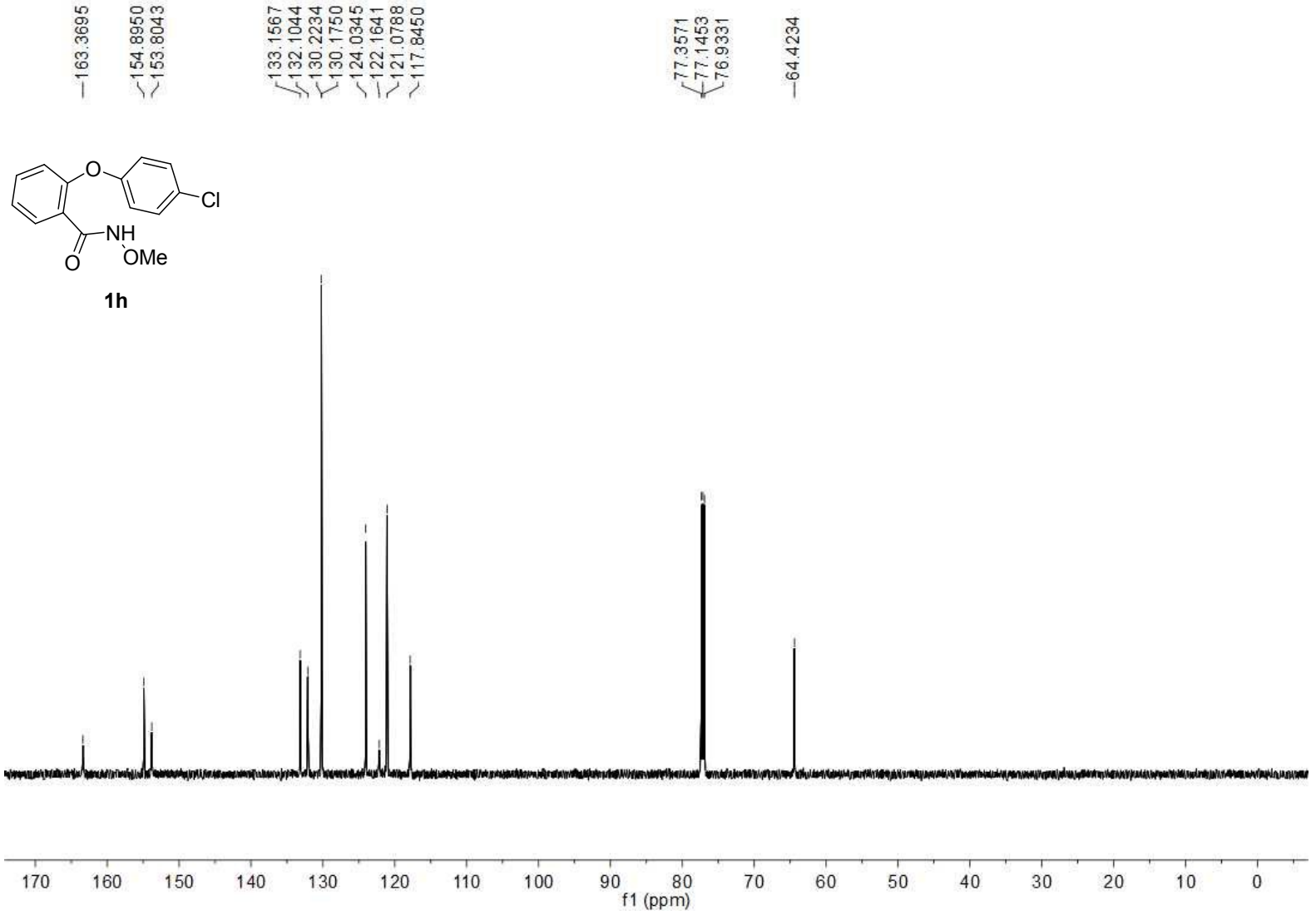
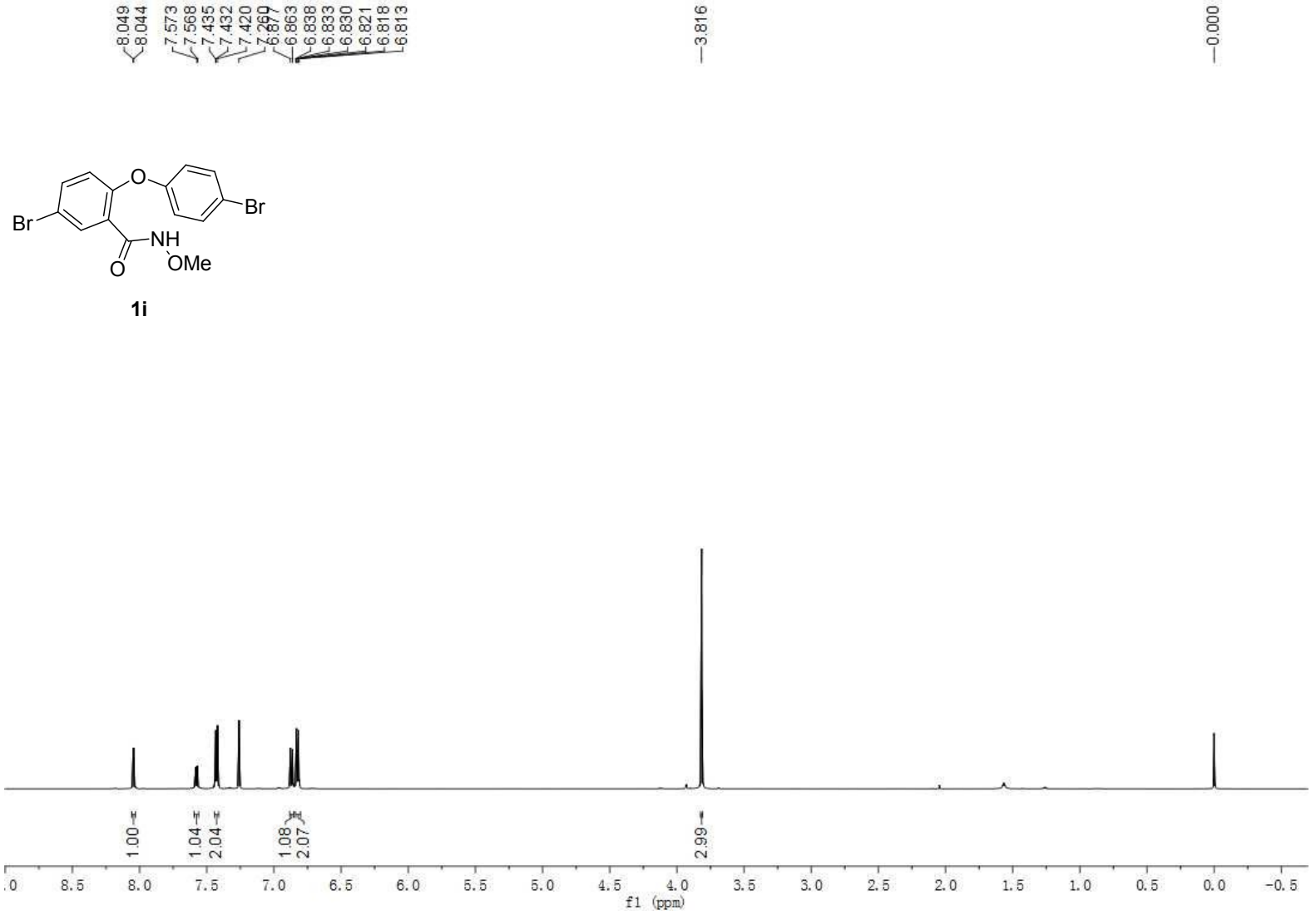
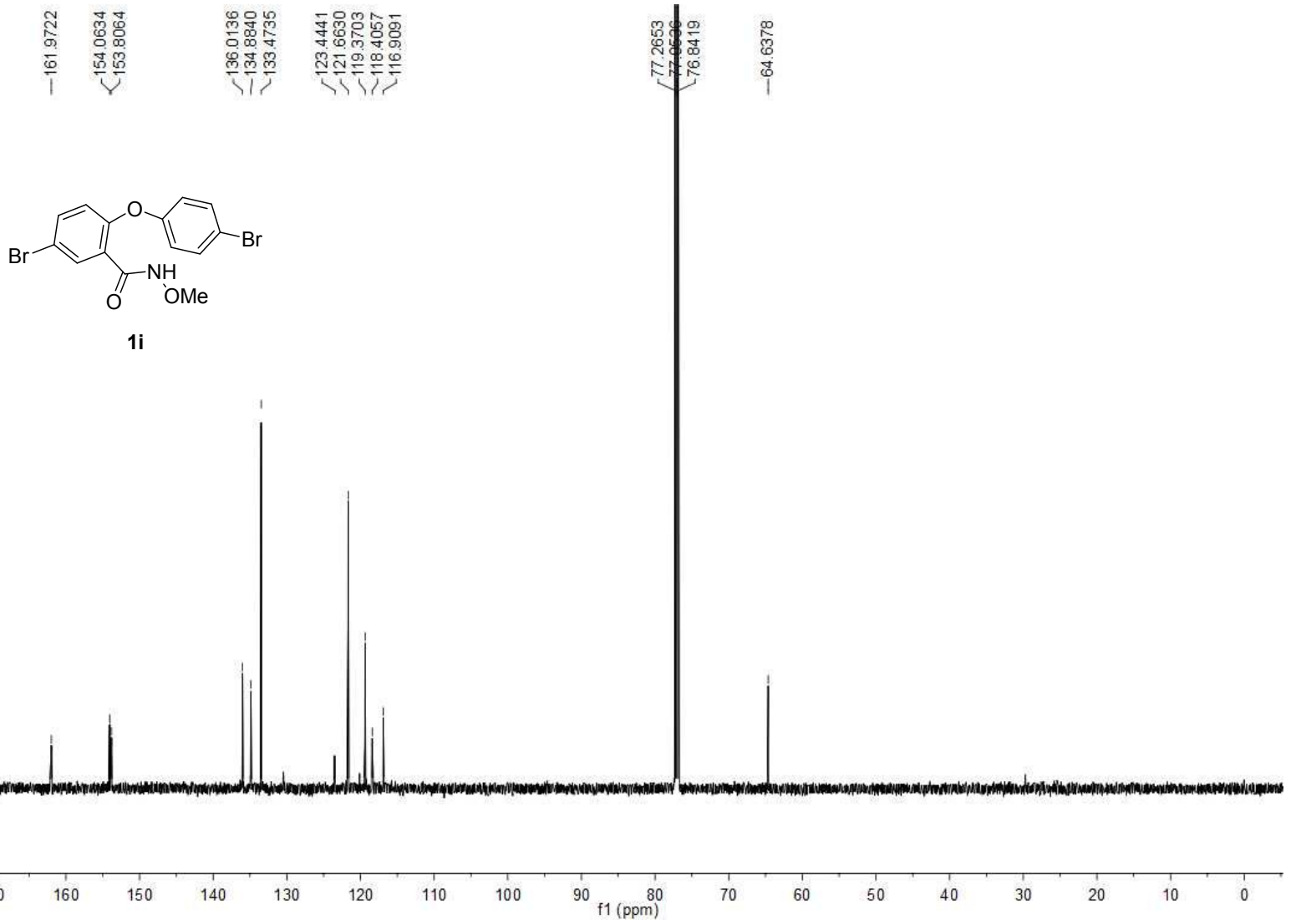
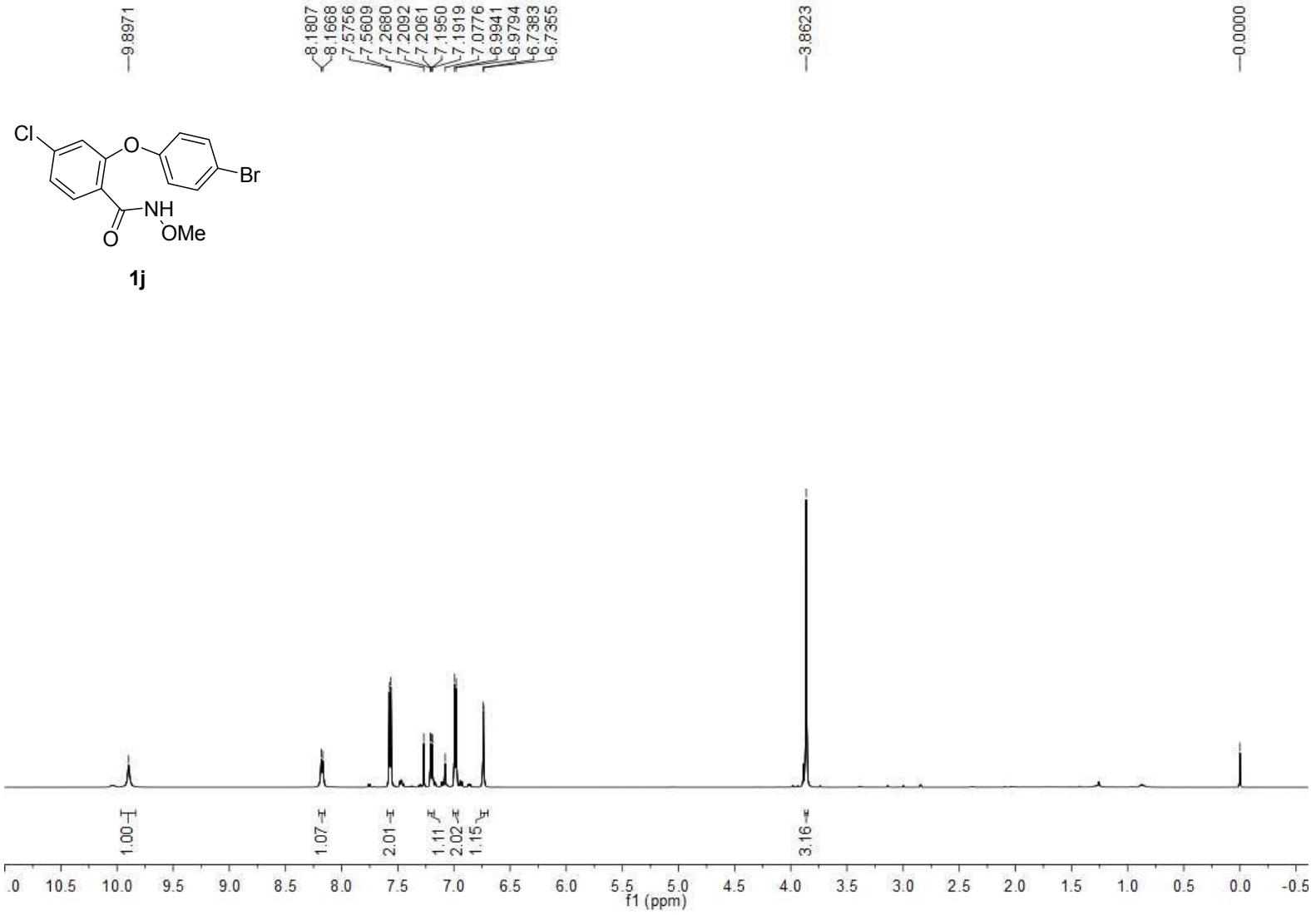
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


163.3695
154.8950
153.8043
133.1567
132.1044
130.2234
130.1750
124.0345
122.1641
121.0788
117.8450
77.3571
77.1453
76.9331
64.4234
O
Cl
NH
O
OMe
1h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

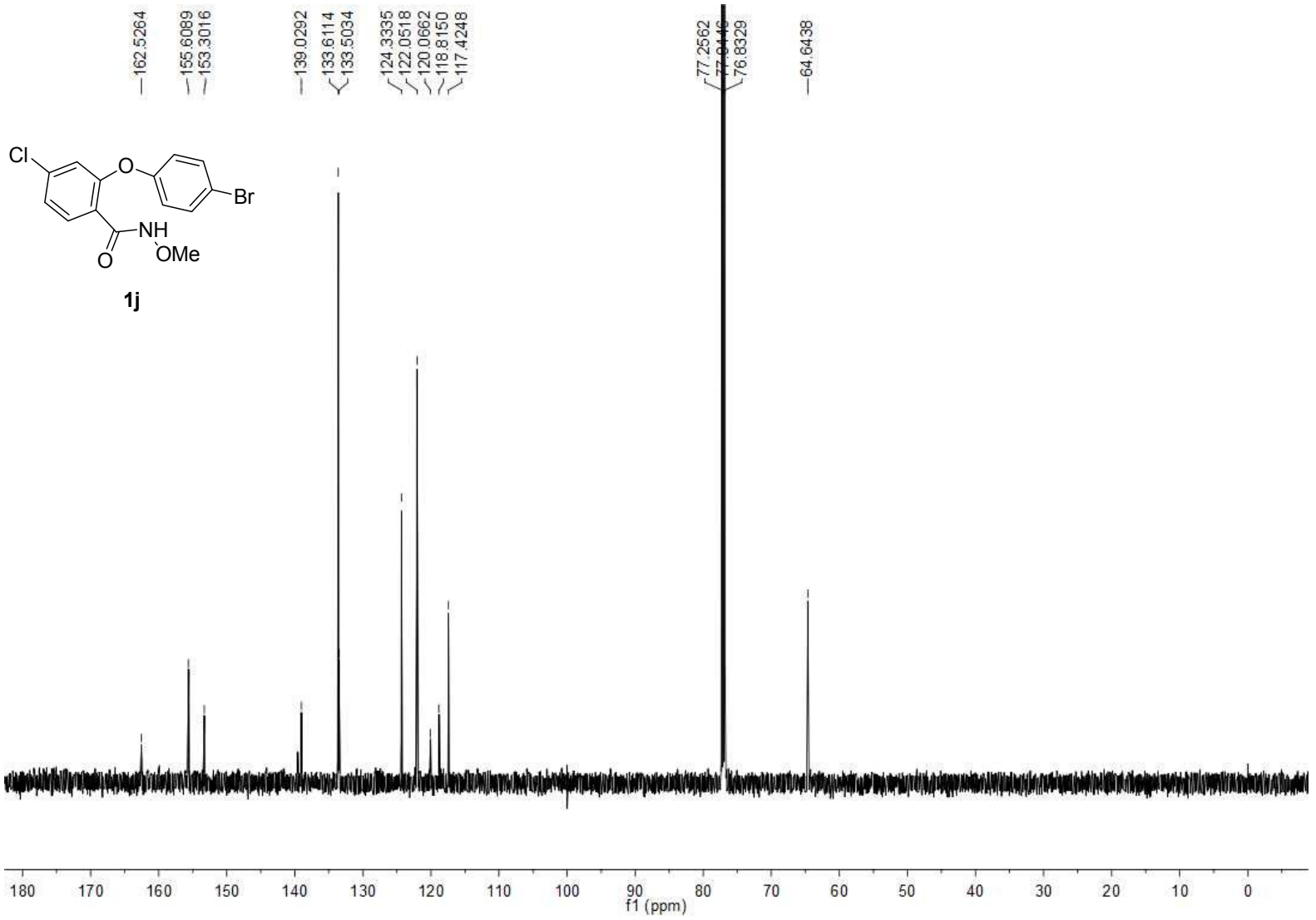

8.049
8.044
7.573
7.568
7.435
7.432
7.420
7.260
6.877
6.863
6.838
6.833
6.830
6.821
6.818
6.813
3.816
0.000
Br
O
Br
NH
O
OMe
1.00
1.04
2.04
1.08
2.07
2.99
f1 (ppm)

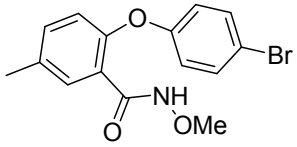
1i


161.9722
154.0634
153.8064
136.0136
134.8840
133.4735
123.4441
121.6630
119.3703
118.4057
116.9091
77.2653
76.8419
64.6378
Br
Br
O
NH
OMe
O
1i
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.8971
8.1807
8.1668
7.5756
7.5609
7.2680
7.2092
7.2061
7.1950
7.1919
7.0776
6.9941
6.9794
6.7383
6.7355
3.8623
0.0000
Cl
O
Br
NH
O
OMe
1.00
1.07
2.01
1.11
2.02
1.15
3.16
f1 (ppm)

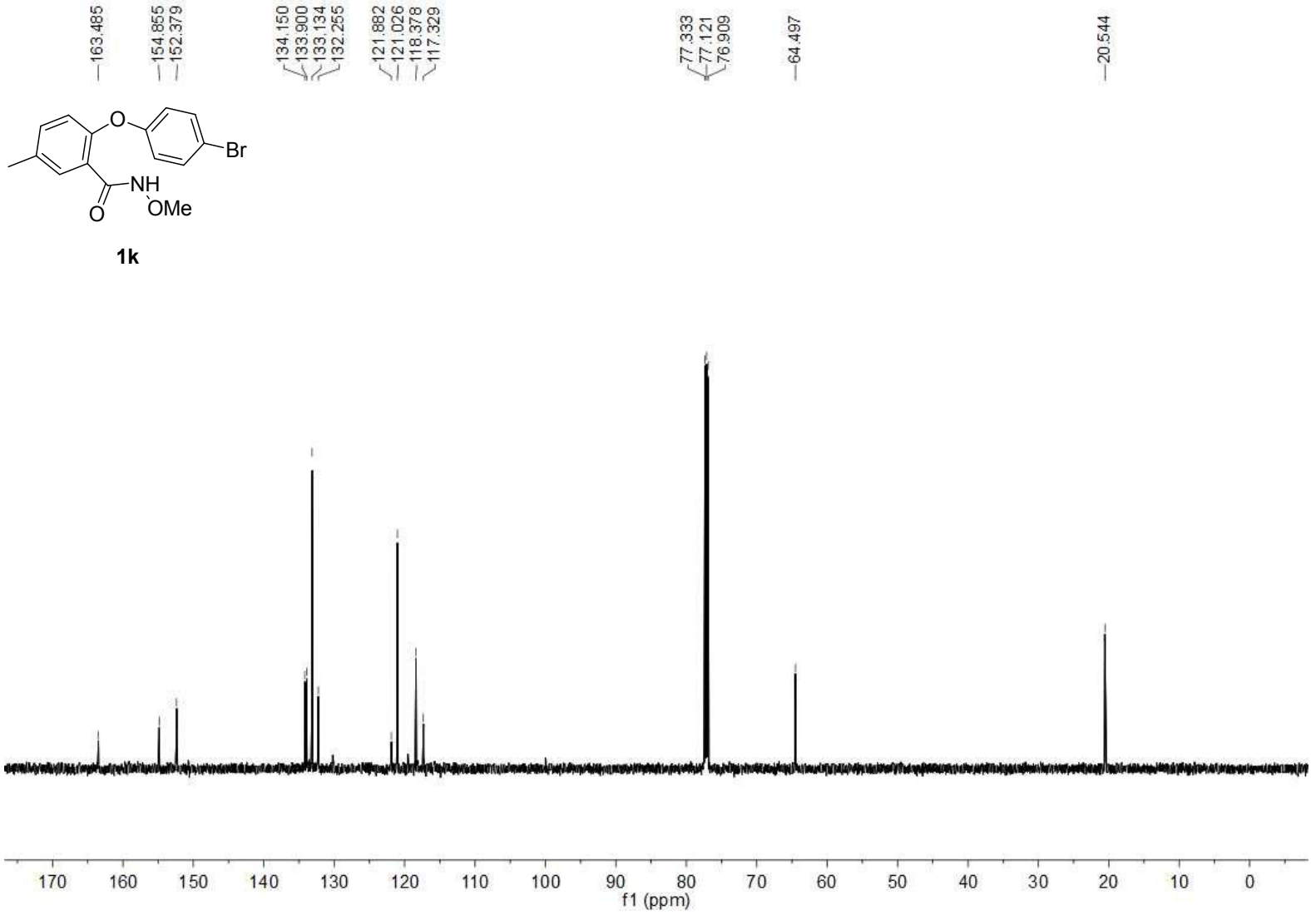
1j


162.5264
155.6089
153.3016
139.0292
133.6114
133.5034
124.3335
122.0518
120.0662
118.8150
117.4248
77.2562
77.0446
76.8329
64.6438
Cl
O
Br
NH
OMe
O
1j
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

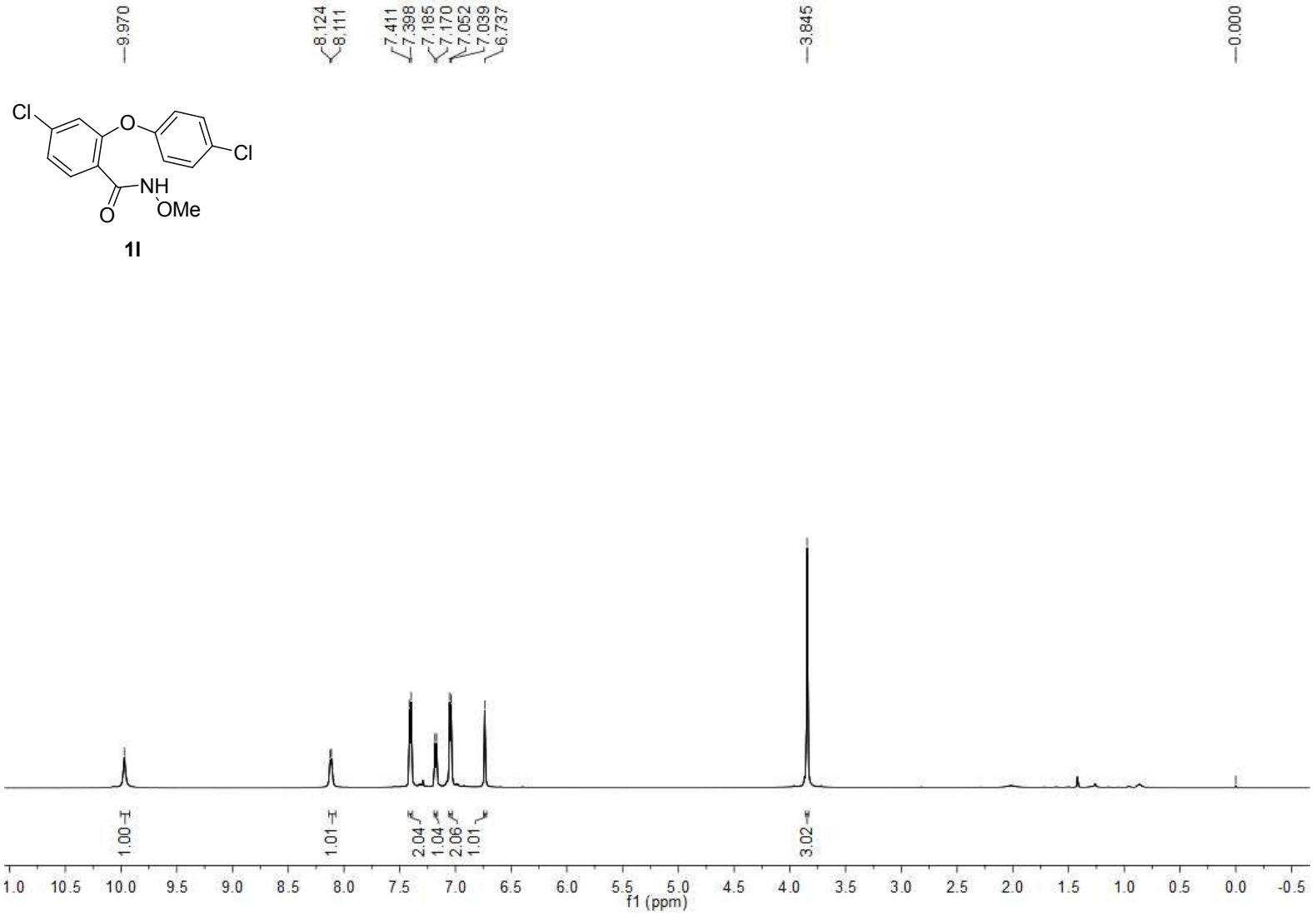

O
Br
NH
O
OMe

1k

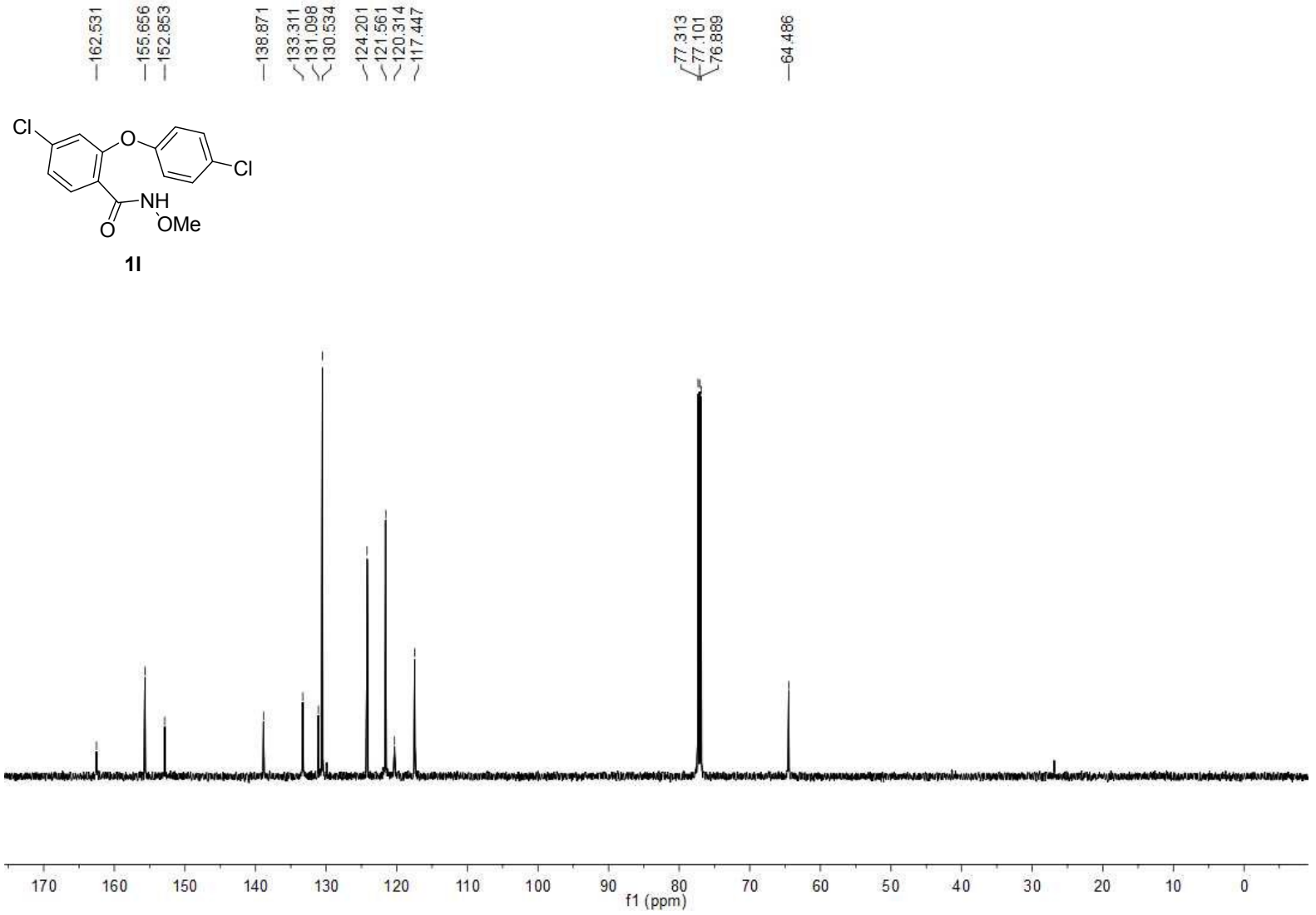
9.908
8.013
7.498
7.483
7.267
7.215
7.204
7.202
6.925
6.911
6.720
6.706
3.833
2.368
0.000
0.96
0.82
1.98
0.97
2.00
0.93
2.94
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

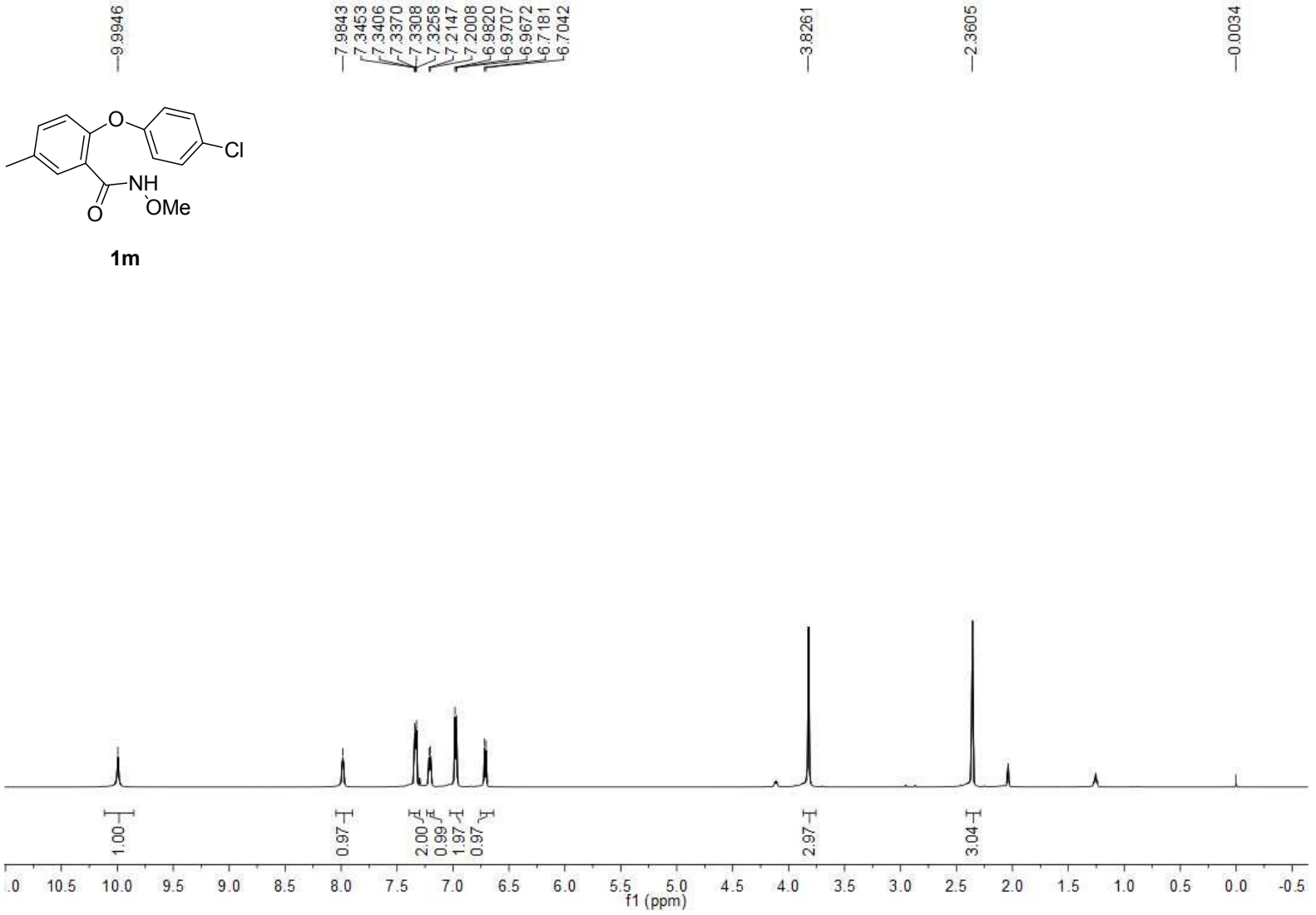

163.485
154.855
152.379
134.150
133.900
133.134
132.255
121.882
121.026
118.378
117.329
77.333
77.121
76.909
64.497
20.544
O
Br
NH
OMe
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

1k

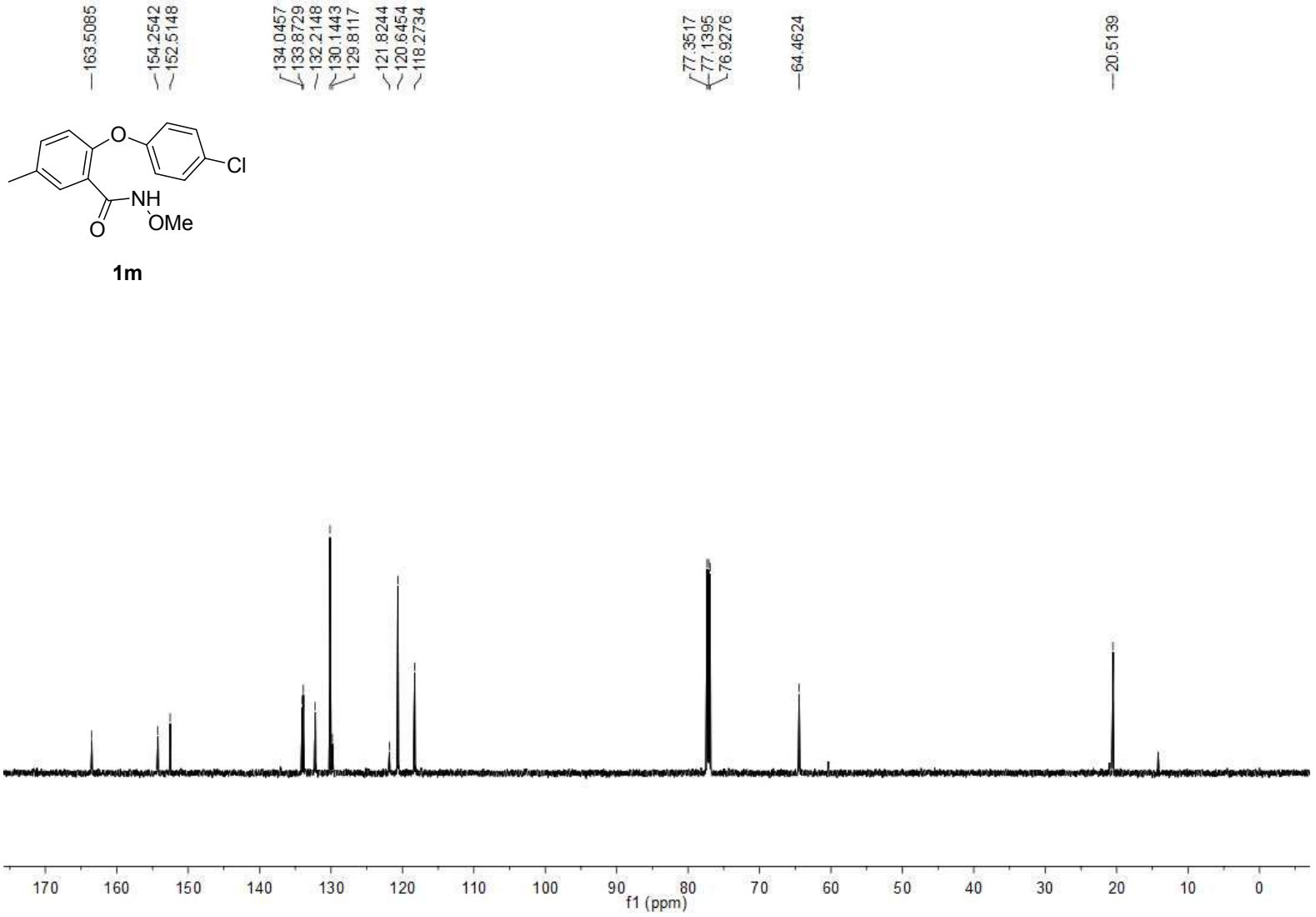

9.970
8.124
8.111
7.411
7.398
7.185
7.170
7.052
7.039
6.737
3.845
0.000
Cl
O
Cl
NH
O
OMe
1.00
1.01
2.04
1.04
2.06
1.01
3.02
f1 (ppm)

1l

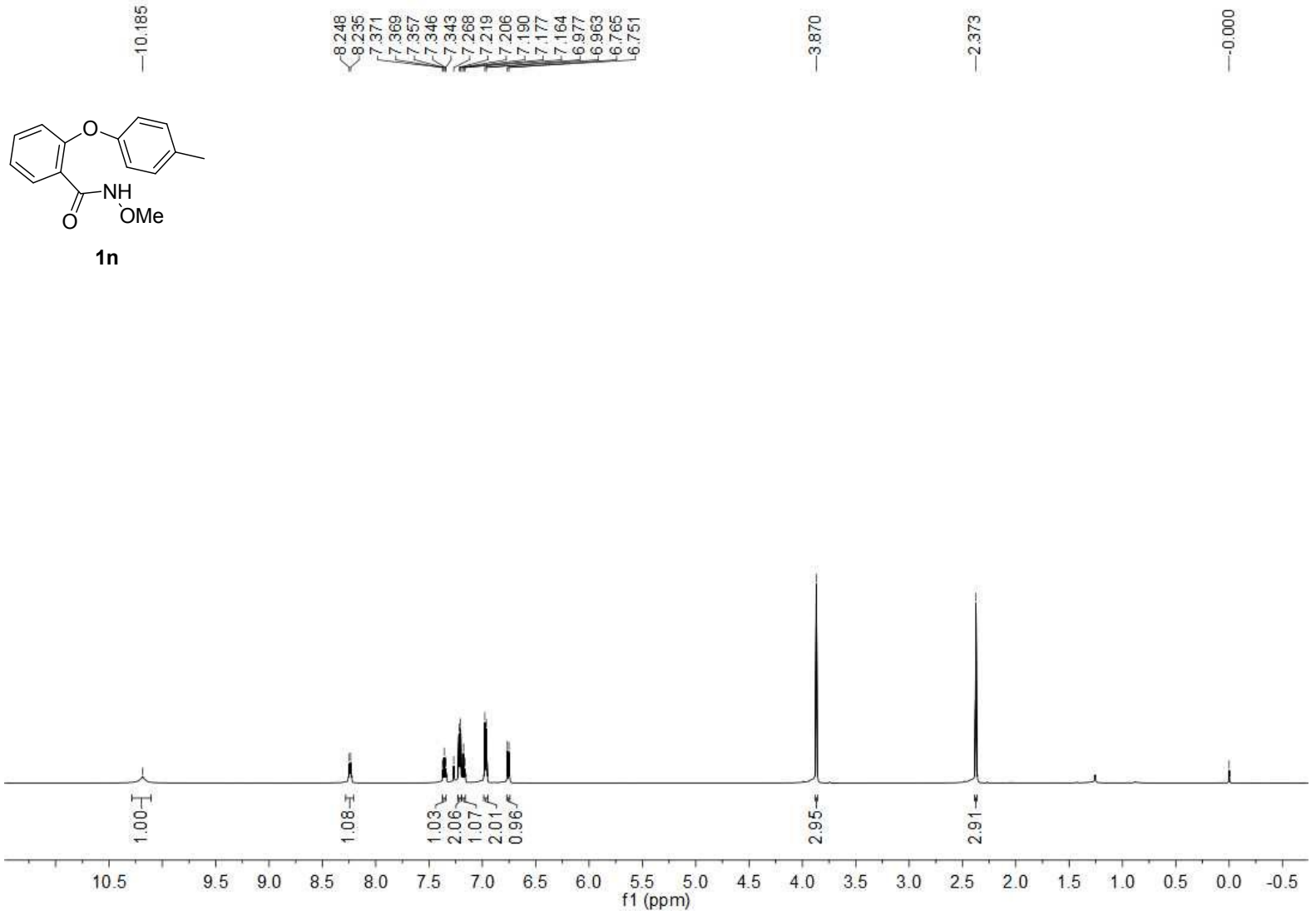

162.531
155.656
152.853
138.871
133.311
131.098
130.534
124.201
121.561
120.314
117.447
77.313
77.101
76.889
64.486
Cl
O
Cl
NH
OMe
O
1l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.9946
7.9843
7.3453
7.3406
7.3370
7.3308
7.3258
7.2147
7.2008
6.9820
6.9707
6.9672
6.7181
6.7042
3.8261
2.3605
0.0034
O
Cl
NH
OMe
O
1.00
0.97
2.00
0.99
1.97
0.97
2.97
3.04
f1 (ppm)

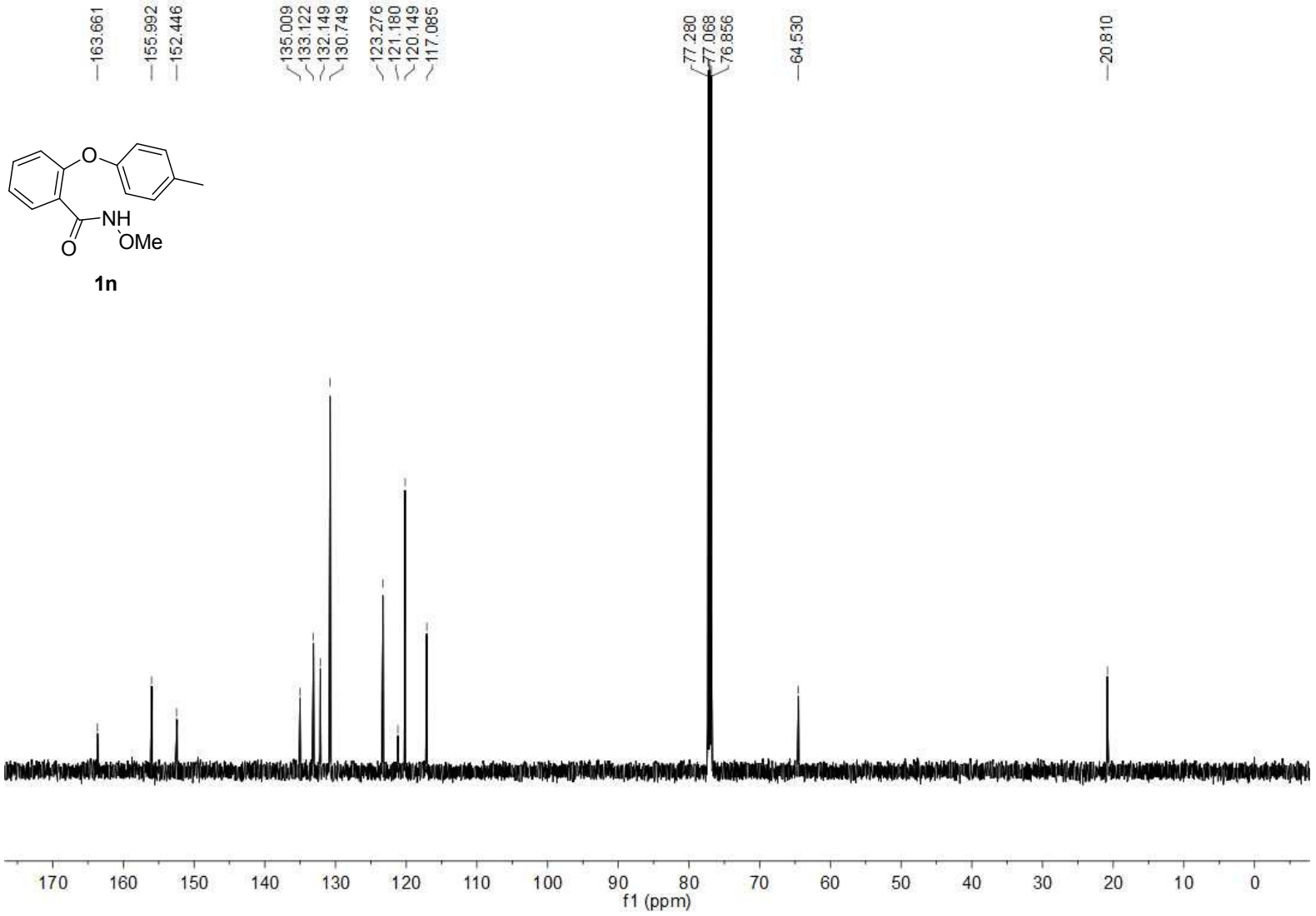
1m

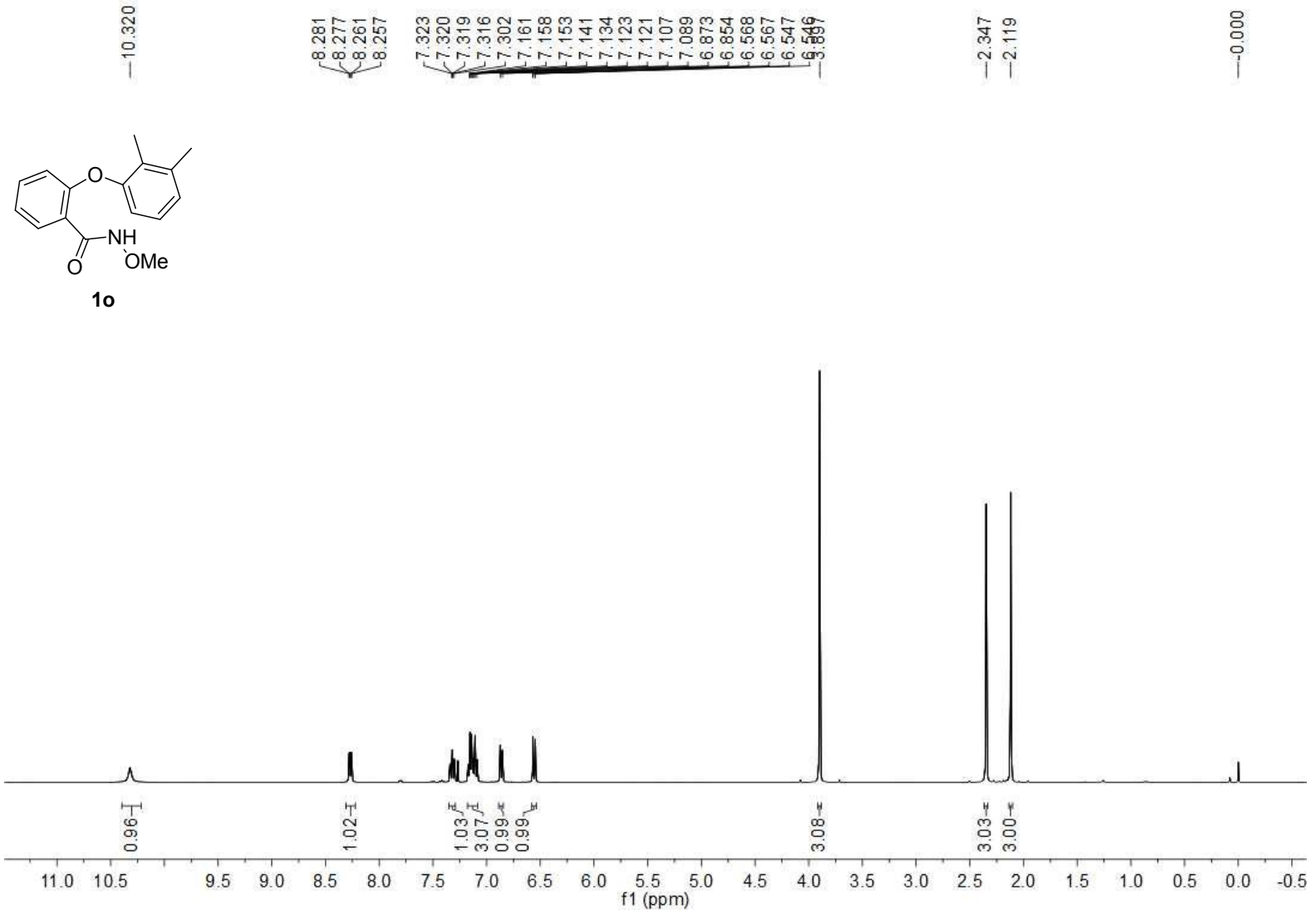

163.5085
154.2542
152.5148
134.0457
133.8729
132.2148
130.1443
129.8117
121.8244
120.6454
118.2734
77.3517
77.1395
76.9276
64.4624
20.5139
O
Cl
NH
O
OMe
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

1m

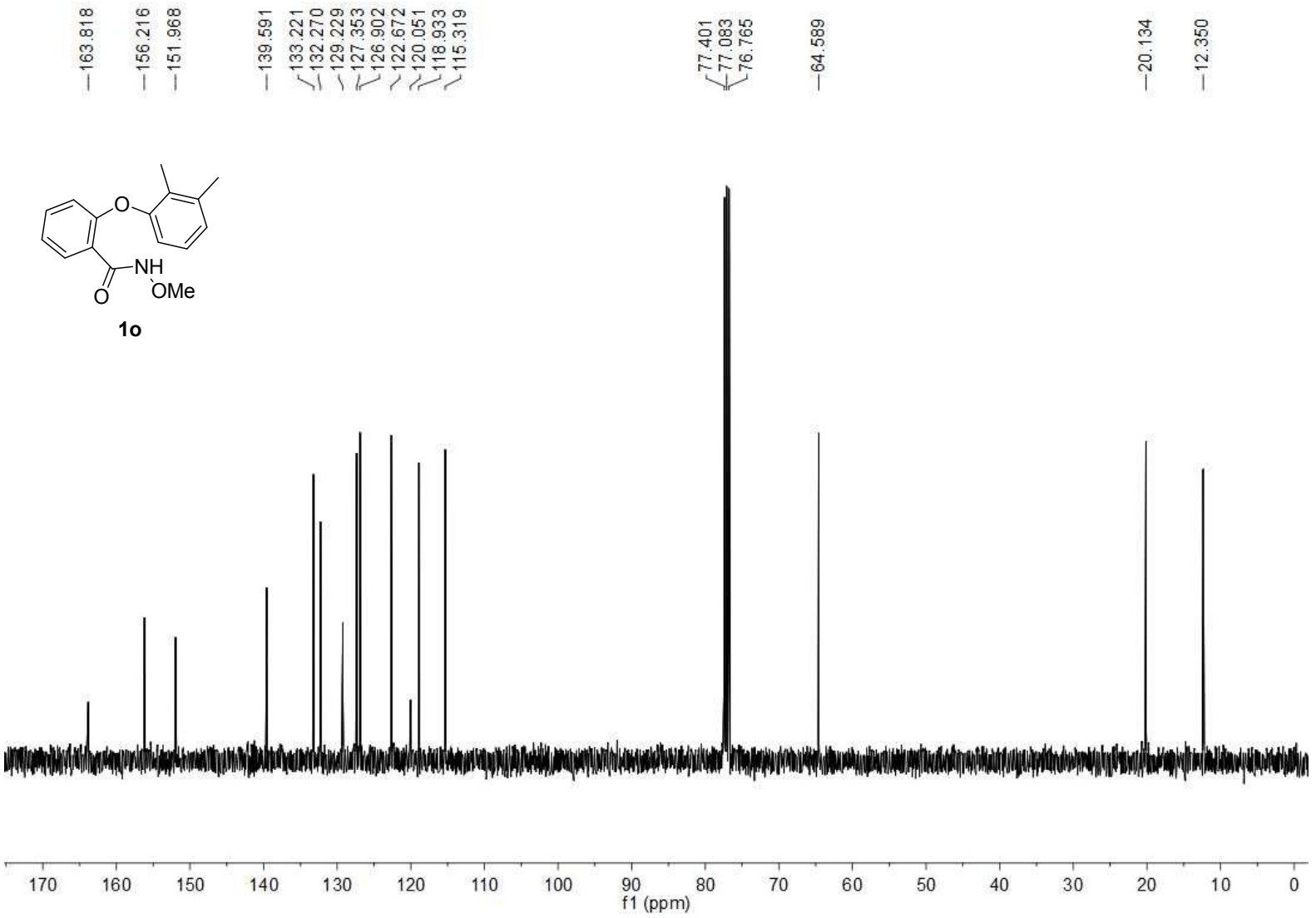

10.185
8.248
8.235
7.371
7.369
7.357
7.346
7.343
7.268
7.219
7.206
7.190
7.177
7.164
6.977
6.963
6.765
6.751
3.870
2.373
0.000
O
NH
OMe
O
1.00
1.08
1.03
2.06
1.07
2.01
0.96
2.95
2.91
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

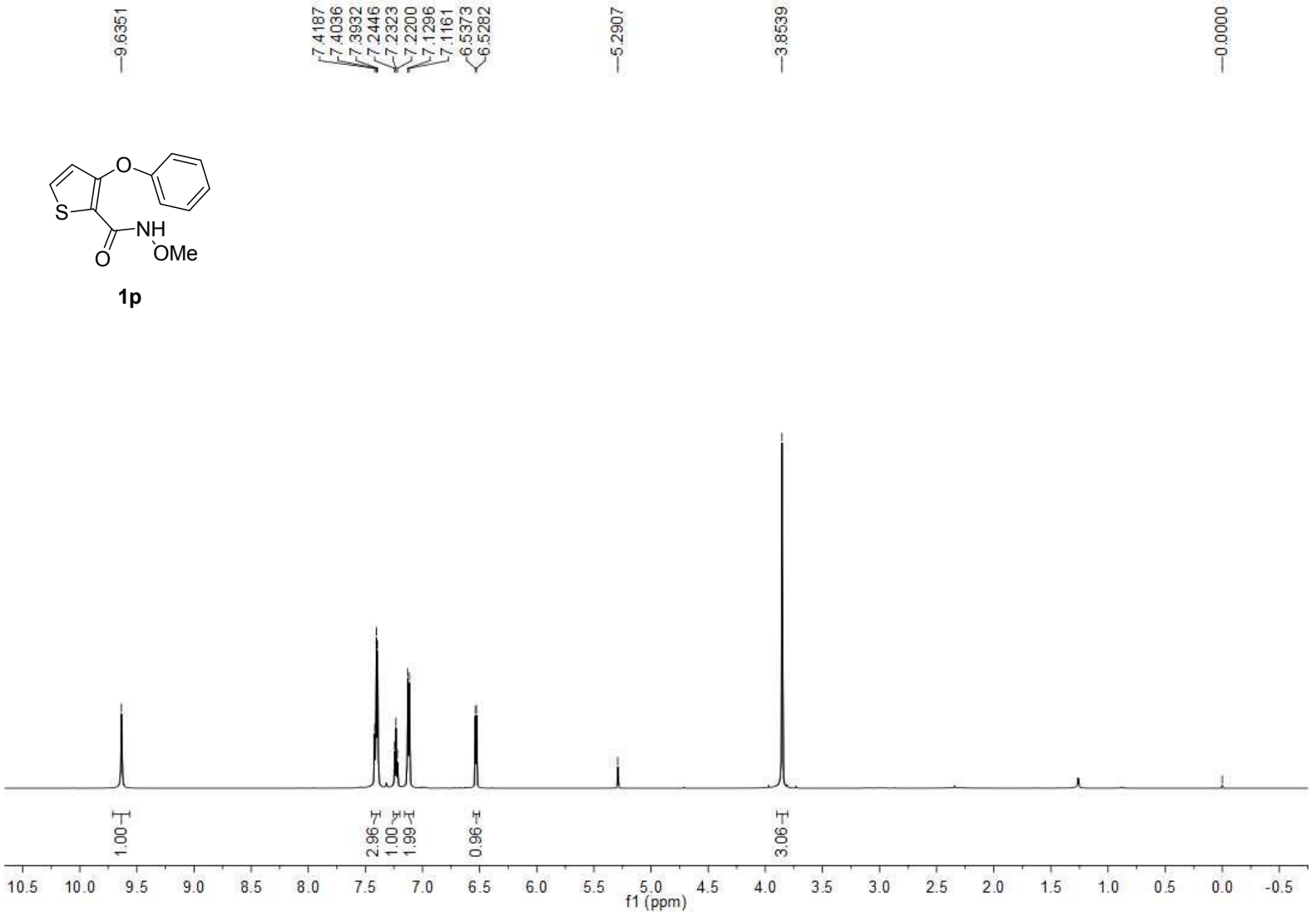
1n


163.661
155.992
152.446
135.009
133.122
132.149
130.749
123.276
121.180
120.149
117.085
77.280
77.068
76.856
64.530
20.810
O
NH
OMe
O
1n
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

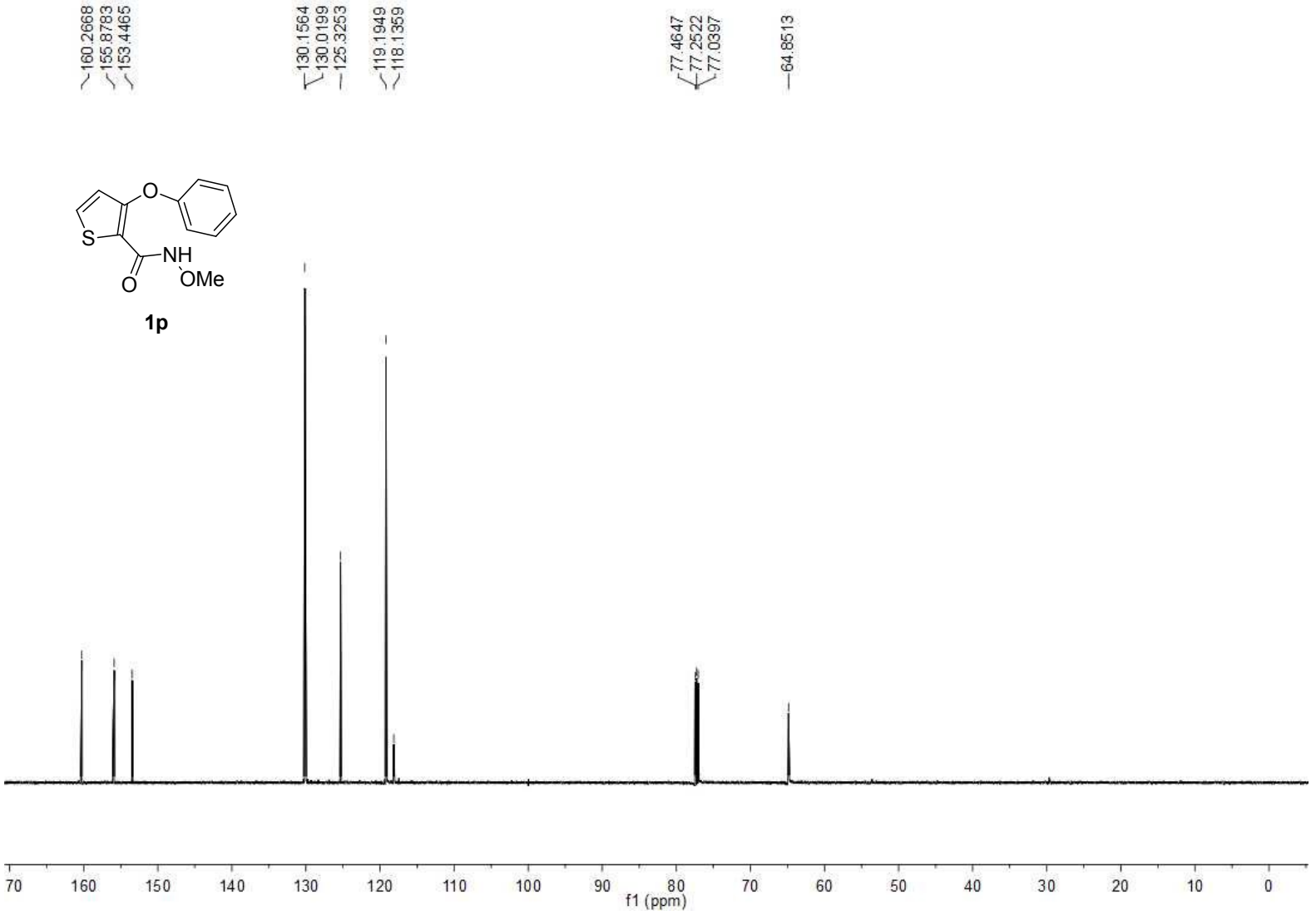

10.320
8.281
8.277
8.261
8.257
7.323
7.320
7.319
7.316
7.302
7.161
7.158
7.153
7.141
7.134
7.123
7.121
7.107
7.089
6.873
6.854
6.568
6.567
6.547
3.897
2.347
2.119
0.000
O
NH
OMe
O
0.96
1.02
1.03
3.07
0.99
0.99
3.08
3.03
3.00
11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

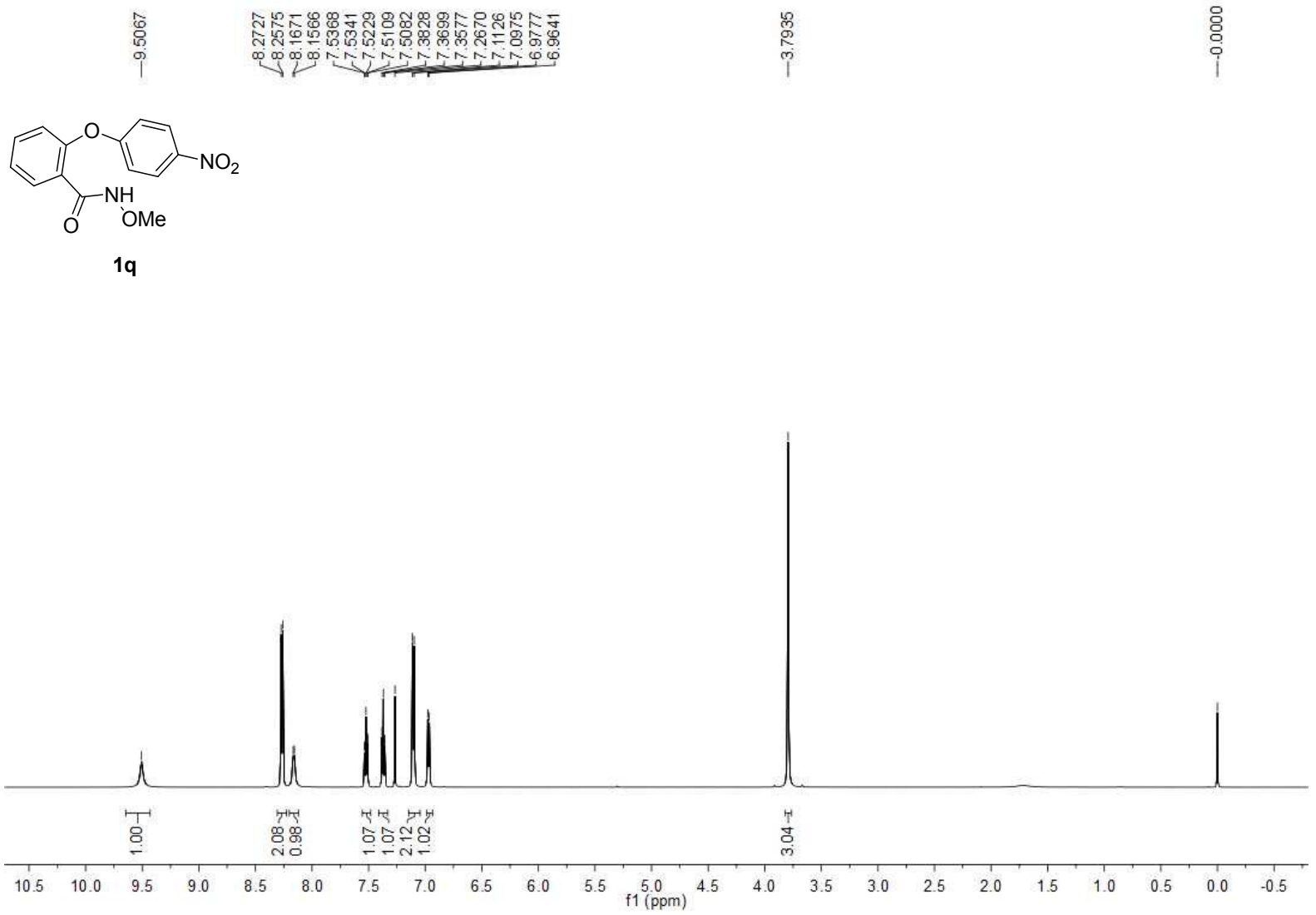
1o


163.818
156.216
151.968
139.591
133.221
132.270
129.229
127.353
126.902
122.672
120.051
118.933
115.319
77.401
77.083
76.765
64.589
20.134
12.350
O
NH
O
OMe
1o
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

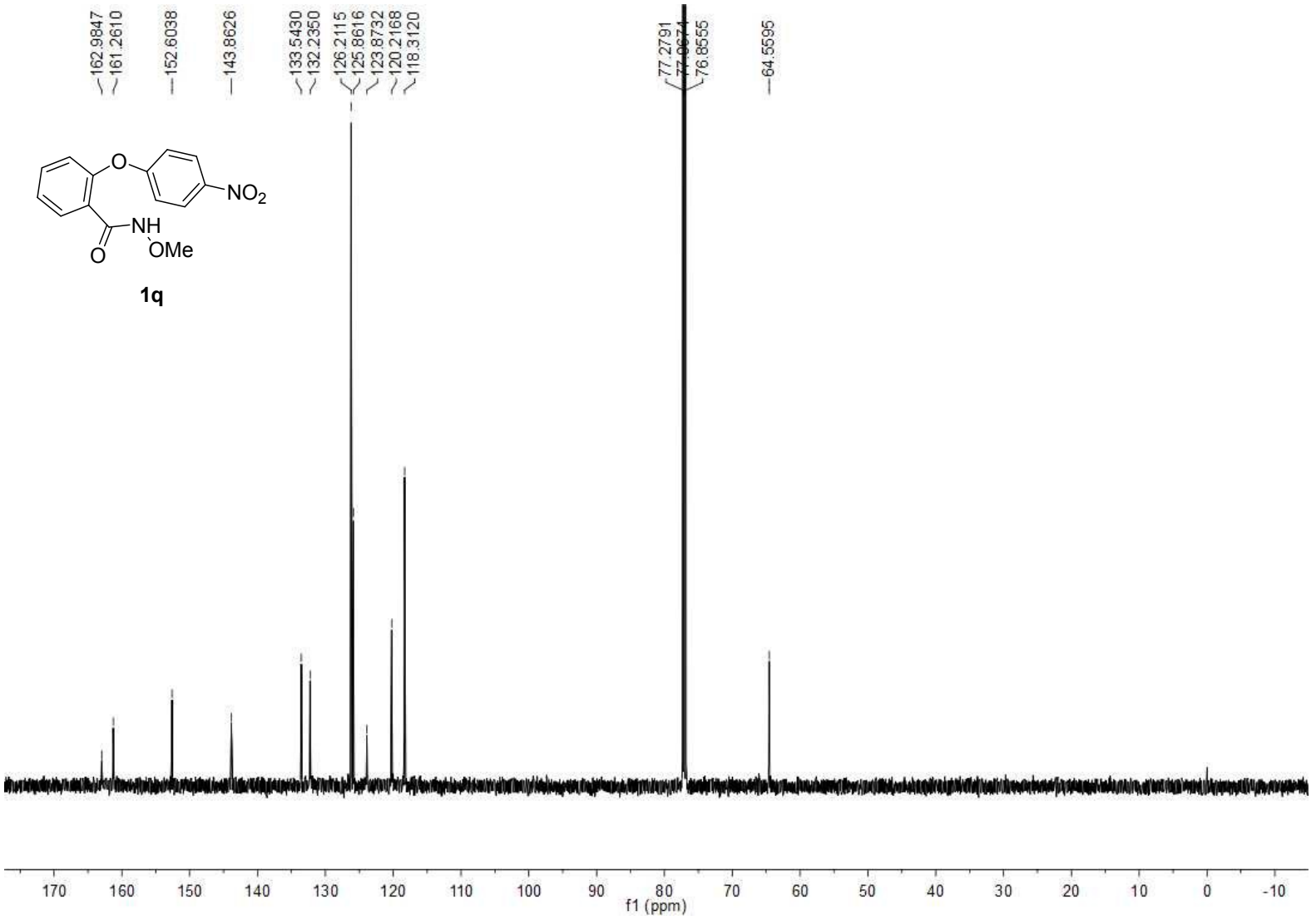

9.6351
7.4187
7.4036
7.3932
7.2446
7.2323
7.2200
7.1296
7.1161
6.5373
6.5282
5.2907
3.8539
0.0000
O
S
NH
OMe
O
1.00
2.96
1.00
1.99
0.96
3.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

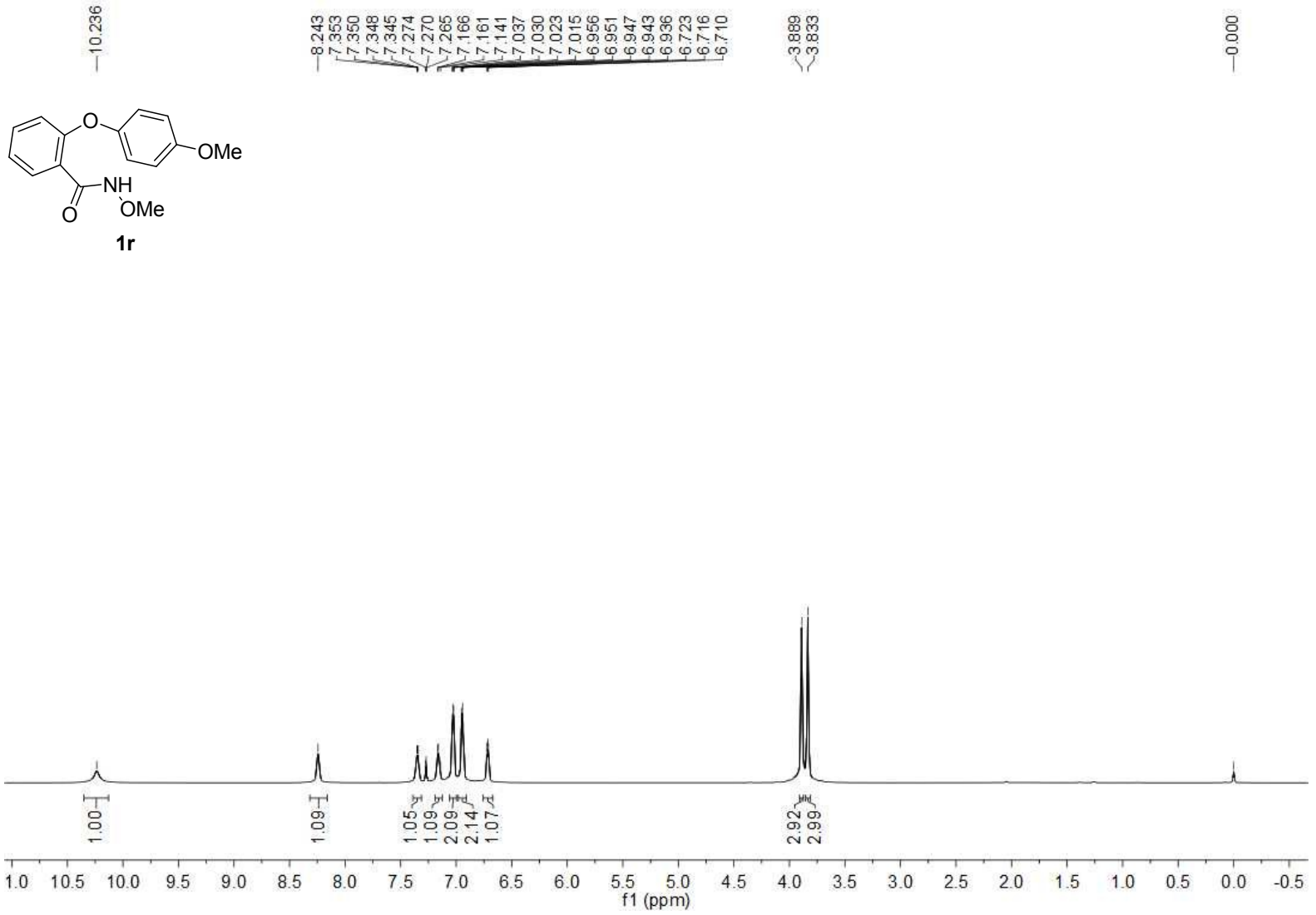
1p

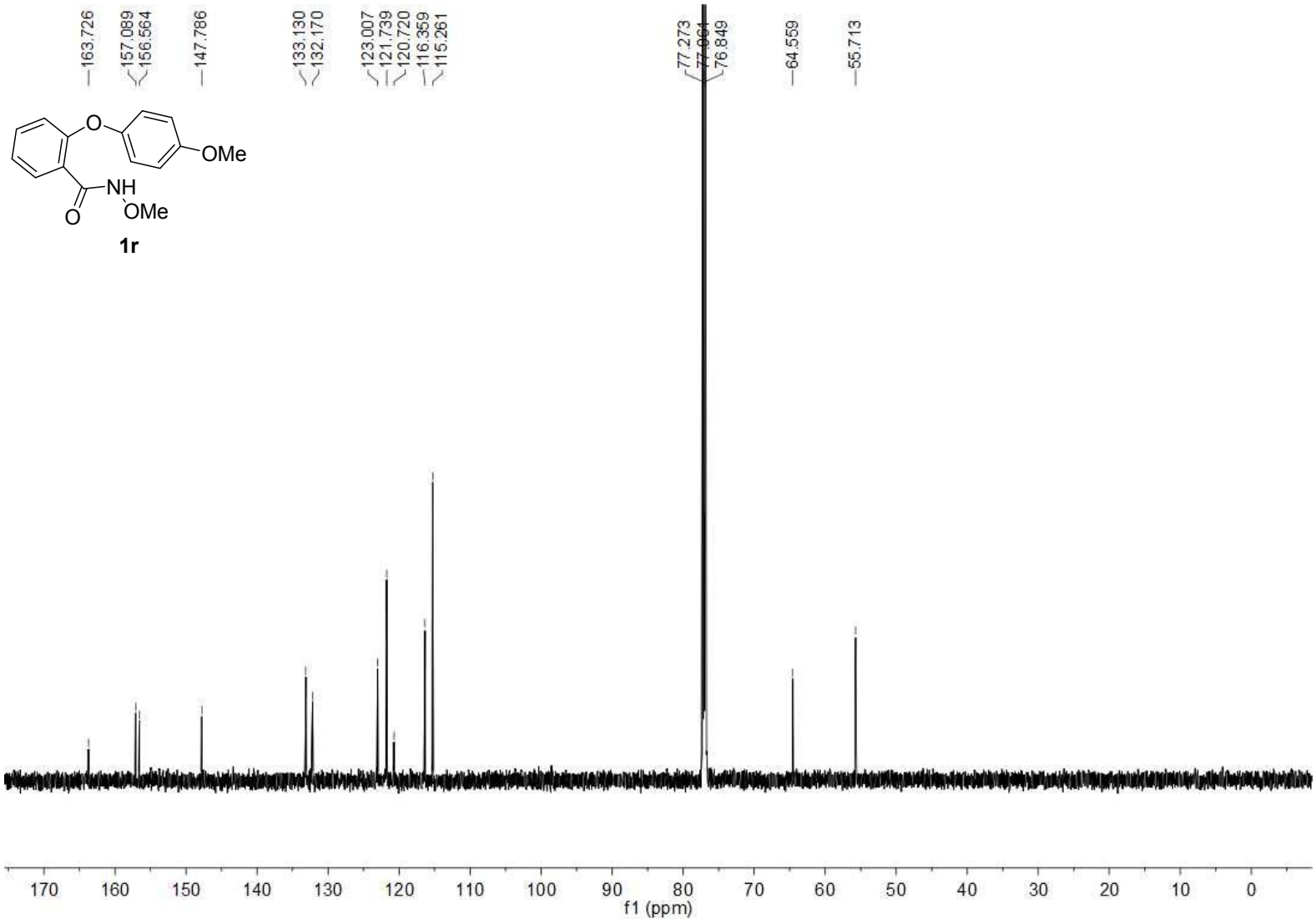

160.2668
155.8783
153.4465
130.1564
130.0199
125.3253
119.1949
118.1359
77.4647
77.2522
77.0397
64.8513
O
S
NH
OMe
O
1p
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

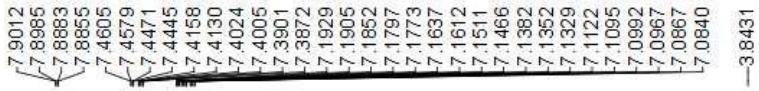

9.5067
8.2727
8.2575
8.1671
8.1566
7.5368
7.5341
7.5229
7.5109
7.5082
7.3828
7.3699
7.3577
7.2670
7.1126
7.0975
6.9777
6.9641
3.7935
0.0000
O
NO2
NH
OMe
O
1.00
2.08
0.98
1.07
1.07
2.12
1.02
3.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

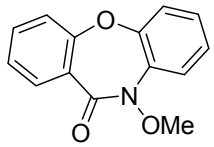
1q


162.9847
161.2610
152.6038
143.8626
133.5430
132.2350
126.2115
125.8616
123.8732
120.2168
118.3120
77.2791
77.0674
76.8555
64.5595
O
NO2
NH
OMe
O
1q
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

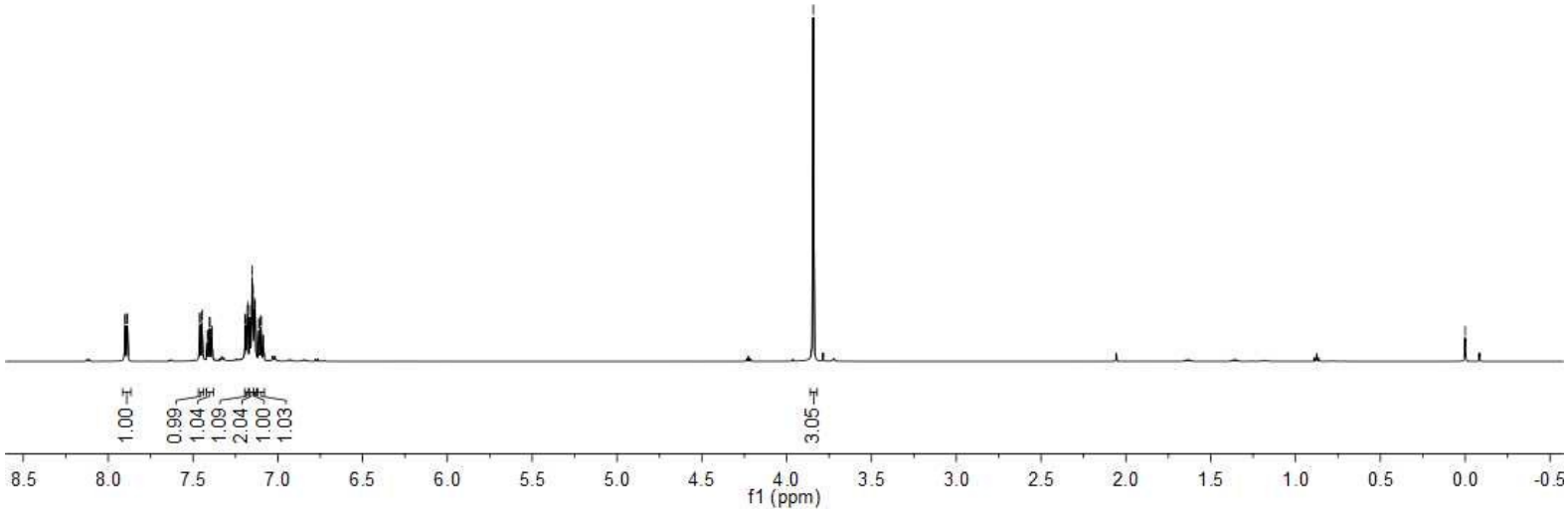

10.236
8.243
7.353
7.350
7.348
7.345
7.274
7.270
7.265
7.166
7.161
7.141
7.037
7.030
7.023
7.015
6.956
6.951
6.947
6.943
6.936
6.723
6.716
6.710
3.889
3.833
0.000
O
OMe
NH
O
OMe
1r
1.00
1.09
1.05
1.09
2.09
2.14
1.07
2.92
2.99
f1 (ppm)

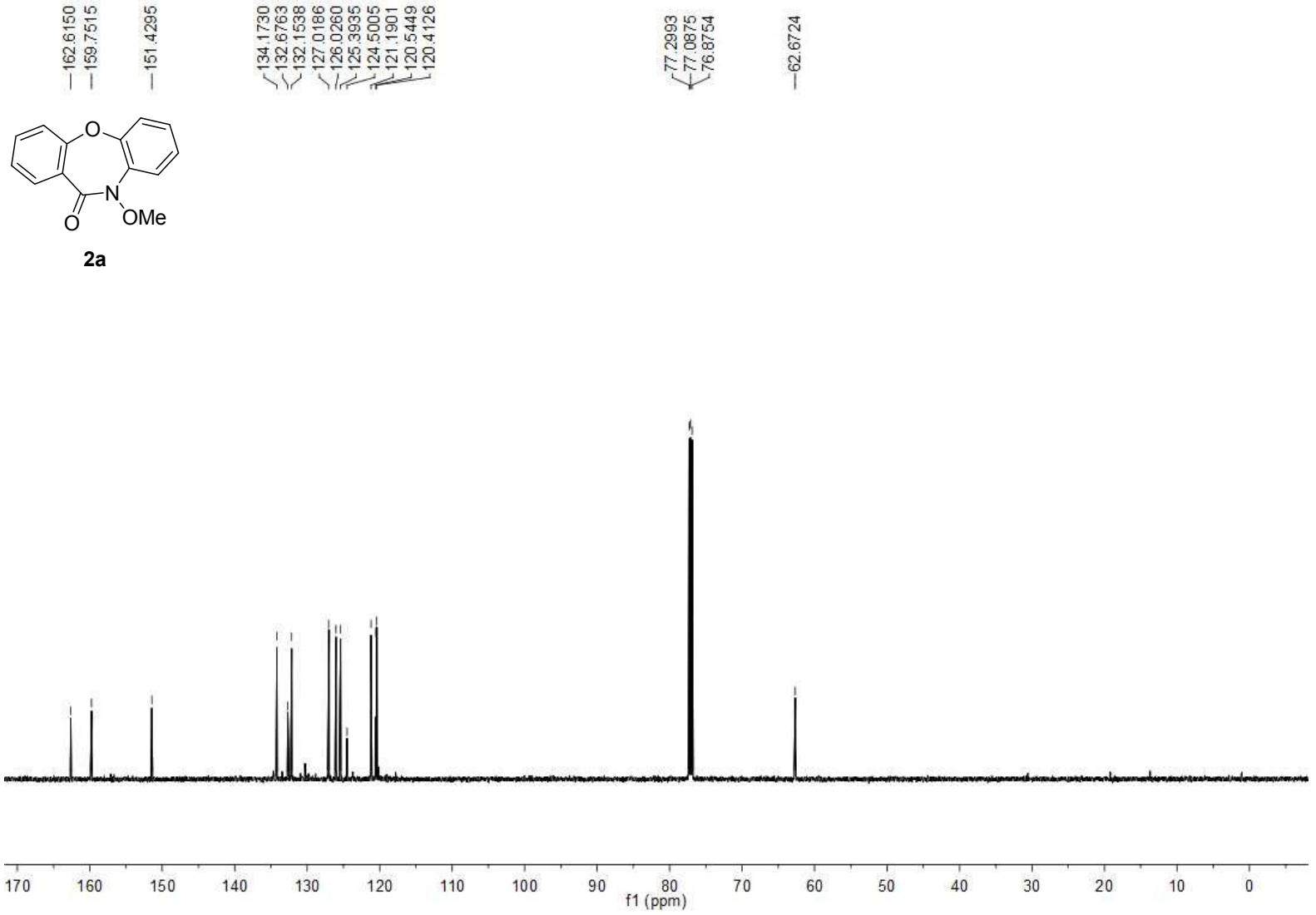

163.726
157.089
156.564
147.786
133.130
132.170
123.007
121.739
120.720
116.359
115.261
77.273
77.061
76.849
64.559
55.713
O
OMe
NH
O
OMe
1r
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.9012
7.8985
7.8883
7.8855
7.4605
7.4579
7.4471
7.4445
7.4158
7.4130
7.4024
7.4005
7.3901
7.3872
7.1929
7.1905
7.1852
7.1797
7.1773
7.1637
7.1612
7.1511
7.1466
7.1382
7.1352
7.1329
7.1122
7.1095
7.0992
7.0967
7.0867
7.0840
3.8431
0.0000

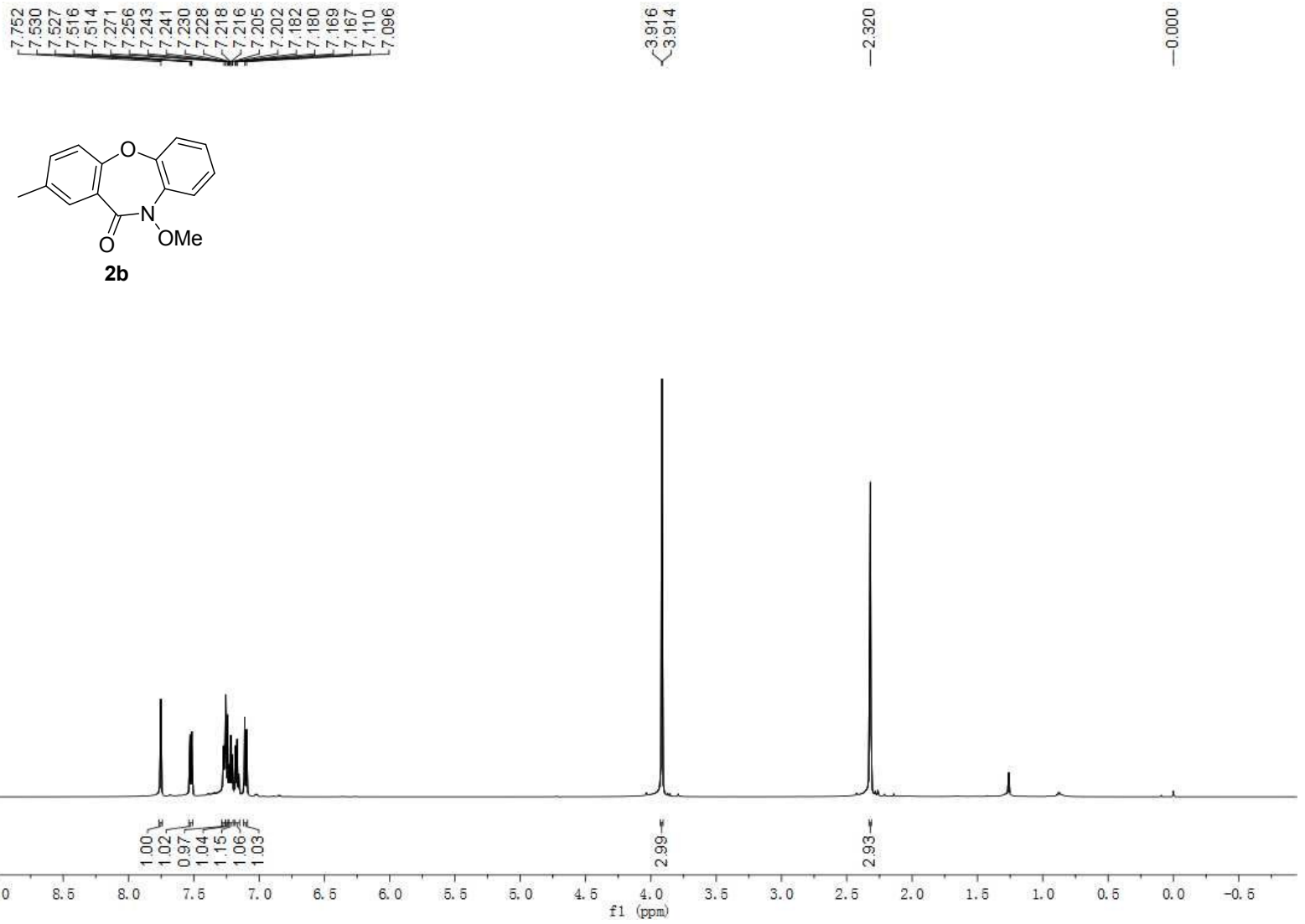

O
N
OMe
O

2a

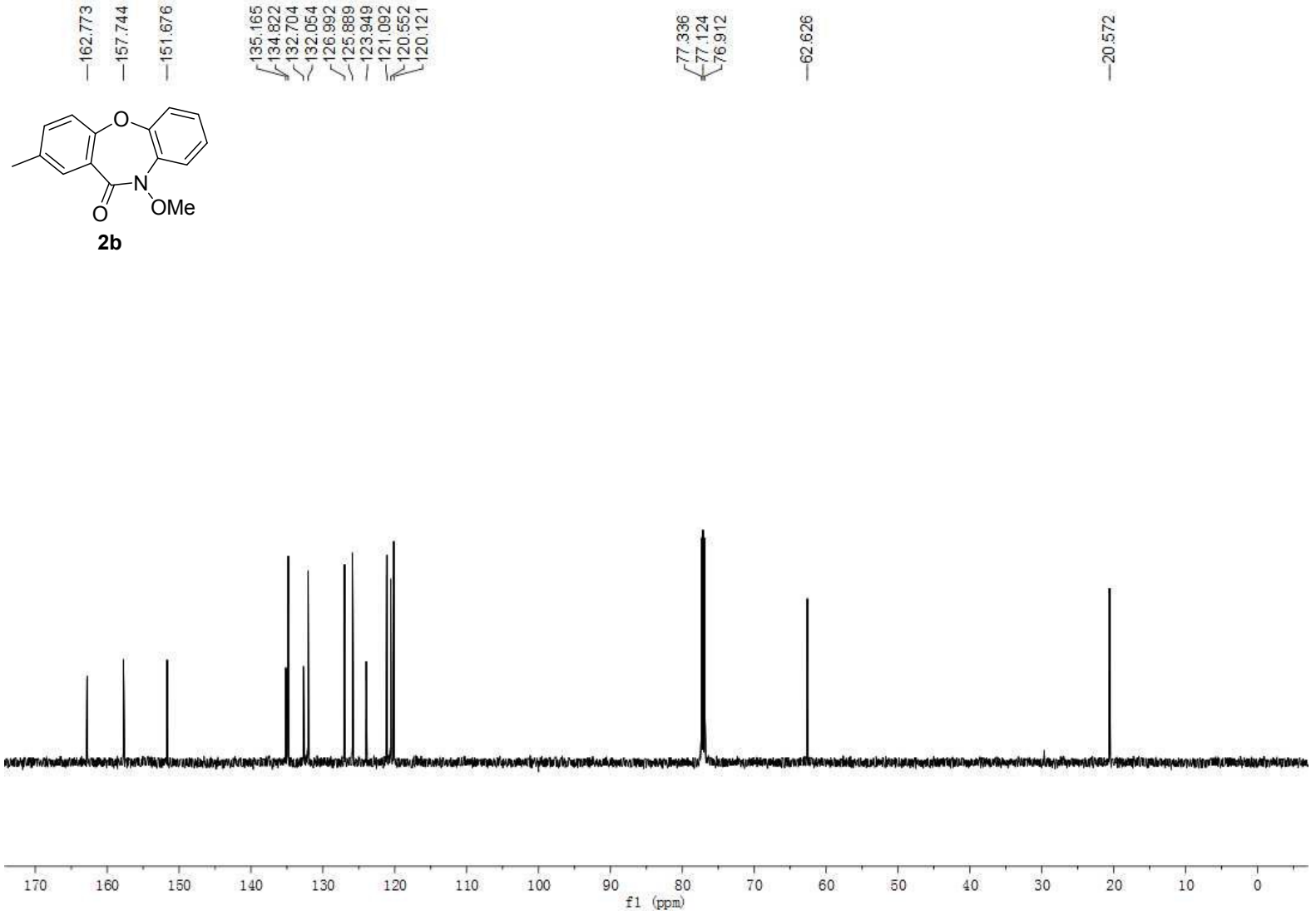

1.00
0.99
1.04
1.09
2.04
1.00
1.03
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

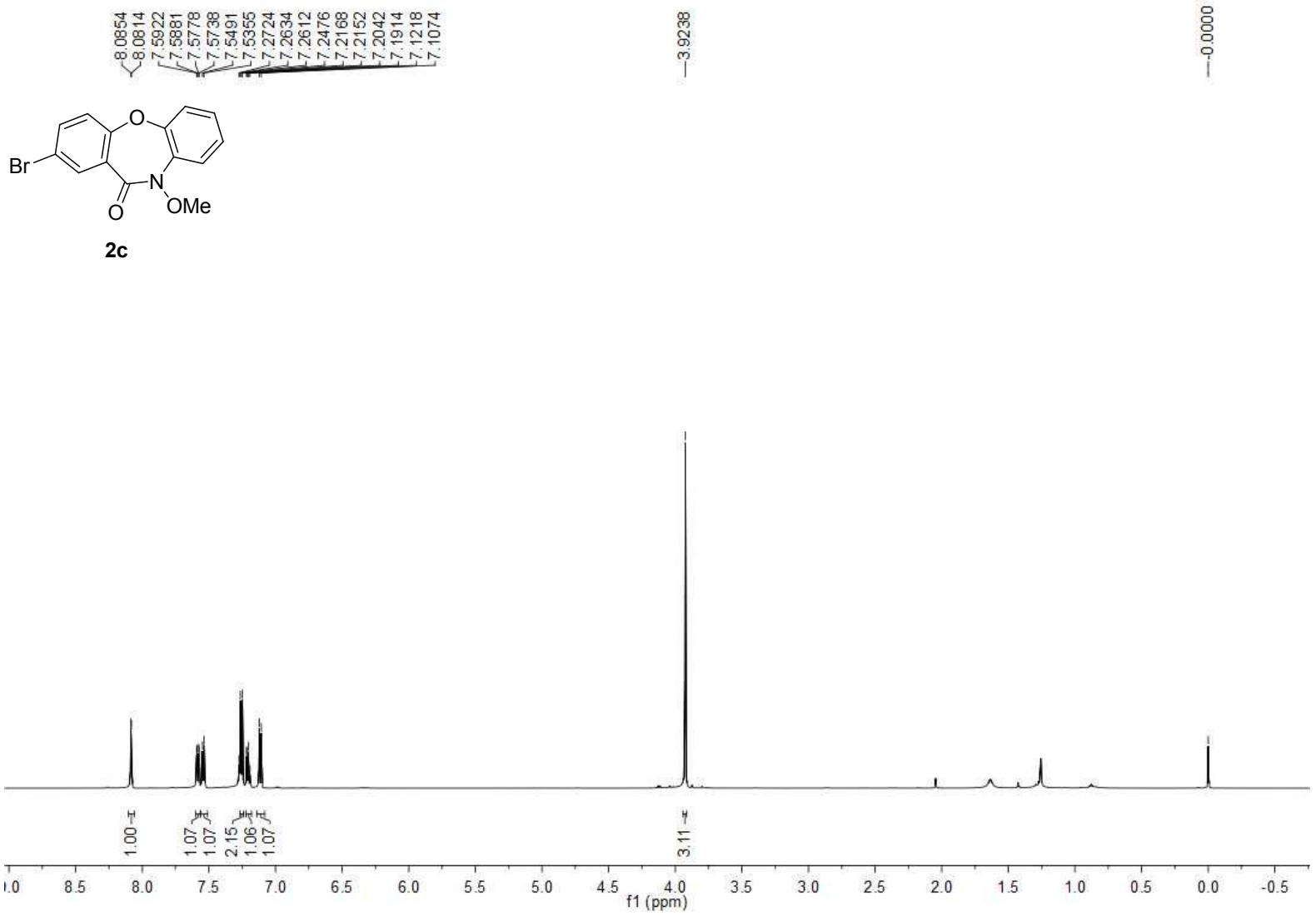

162.6150
159.7515
151.4295
134.1730
132.6763
132.1538
127.0186
126.0260
125.3935
124.5005
121.1901
120.5449
120.4126
77.2993
77.0875
76.8754
62.6724
O
N
OMe
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2a

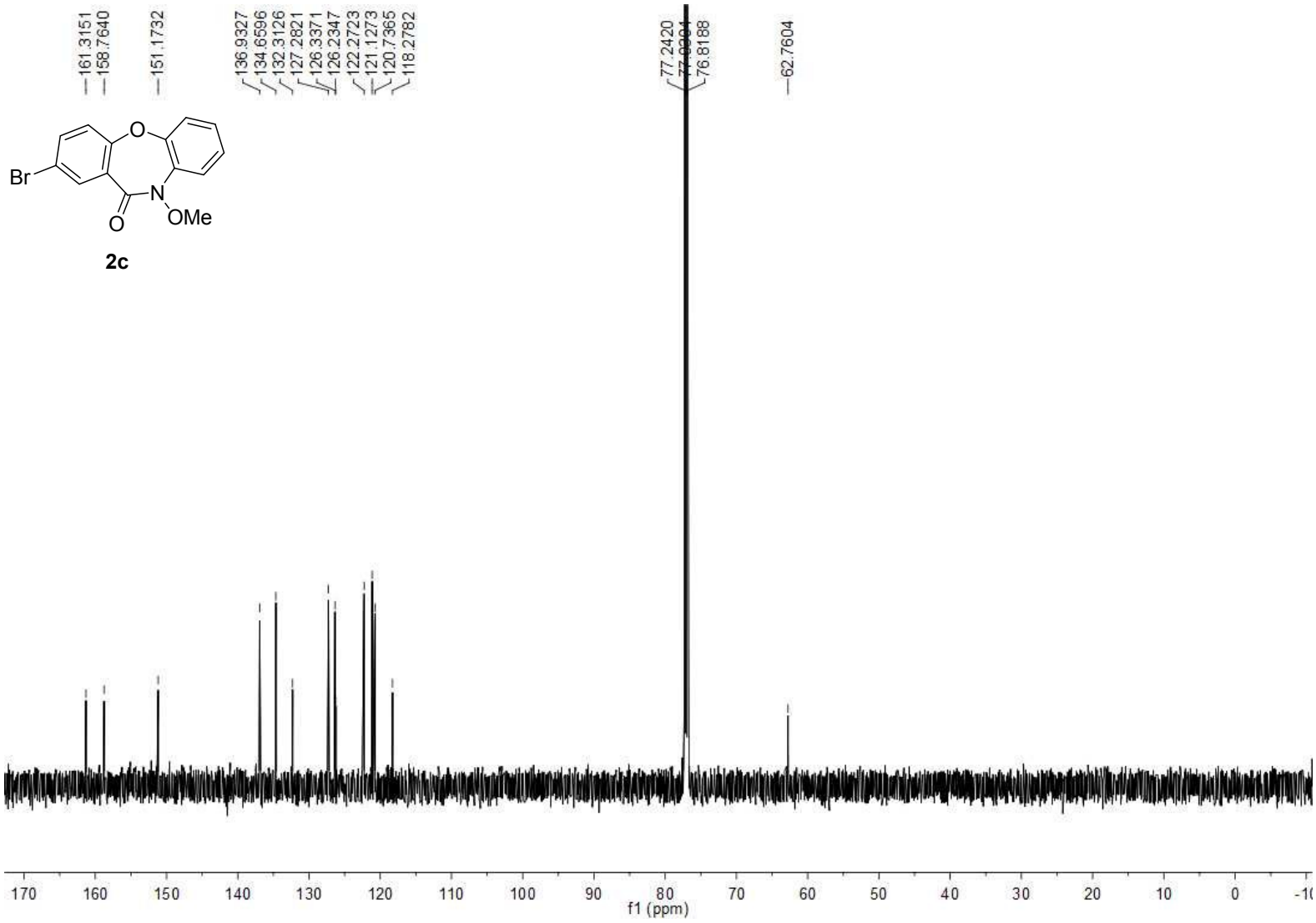

7.752
7.530
7.527
7.516
7.514
7.271
7.256
7.243
7.241
7.230
7.228
7.218
7.216
7.205
7.202
7.182
7.180
7.169
7.167
7.110
7.096
3.916
3.914
2.320
0.000
O
N
OMe
O
1.00
1.02
0.97
1.04
1.15
1.06
1.03
2.99
2.93
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

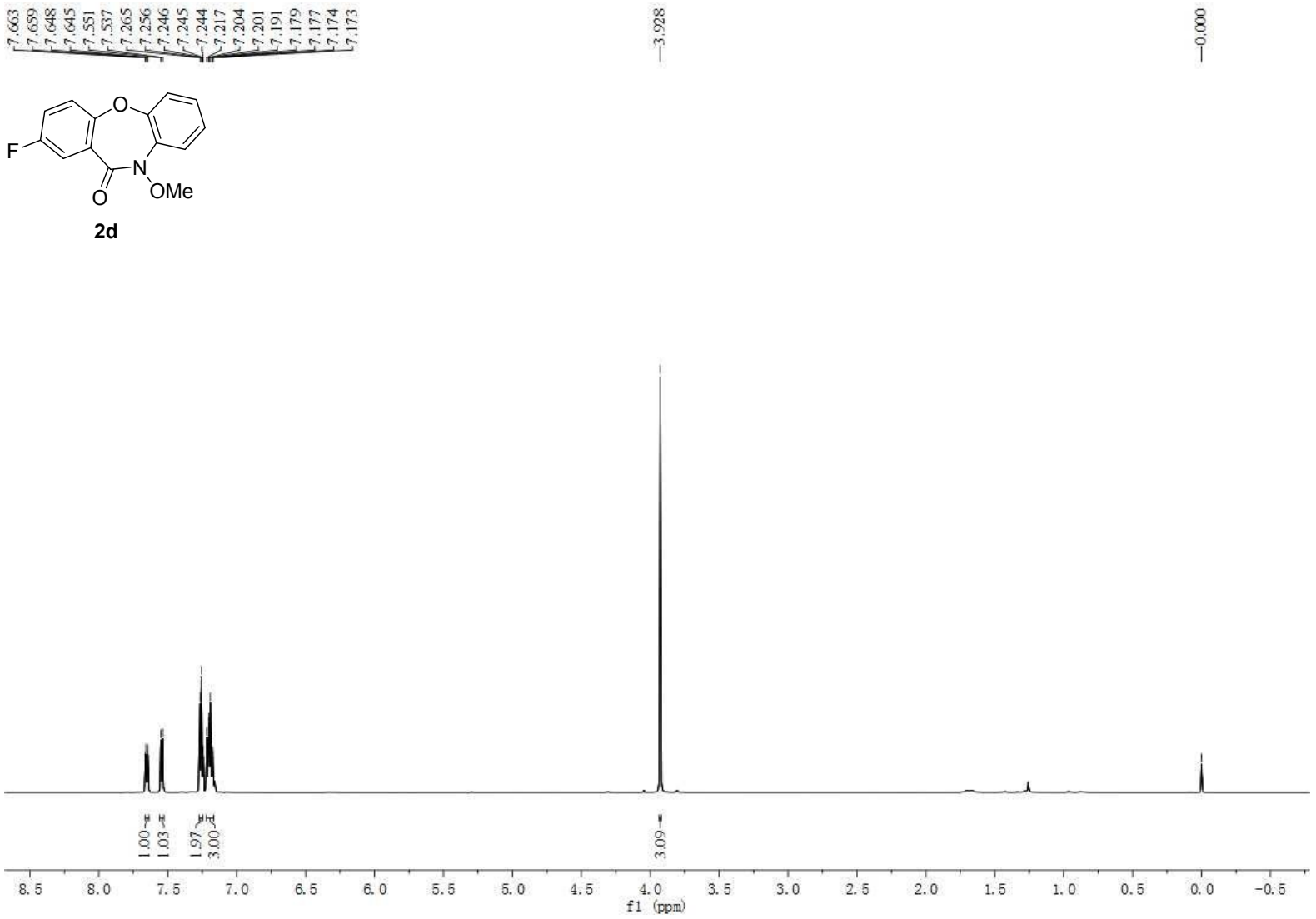
2b


162.773
157.744
151.676
135.165
134.822
132.704
132.054
126.992
125.889
123.949
121.092
120.552
120.121
77.336
77.124
76.912
62.626
20.572
O
N
OMe
O
2b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

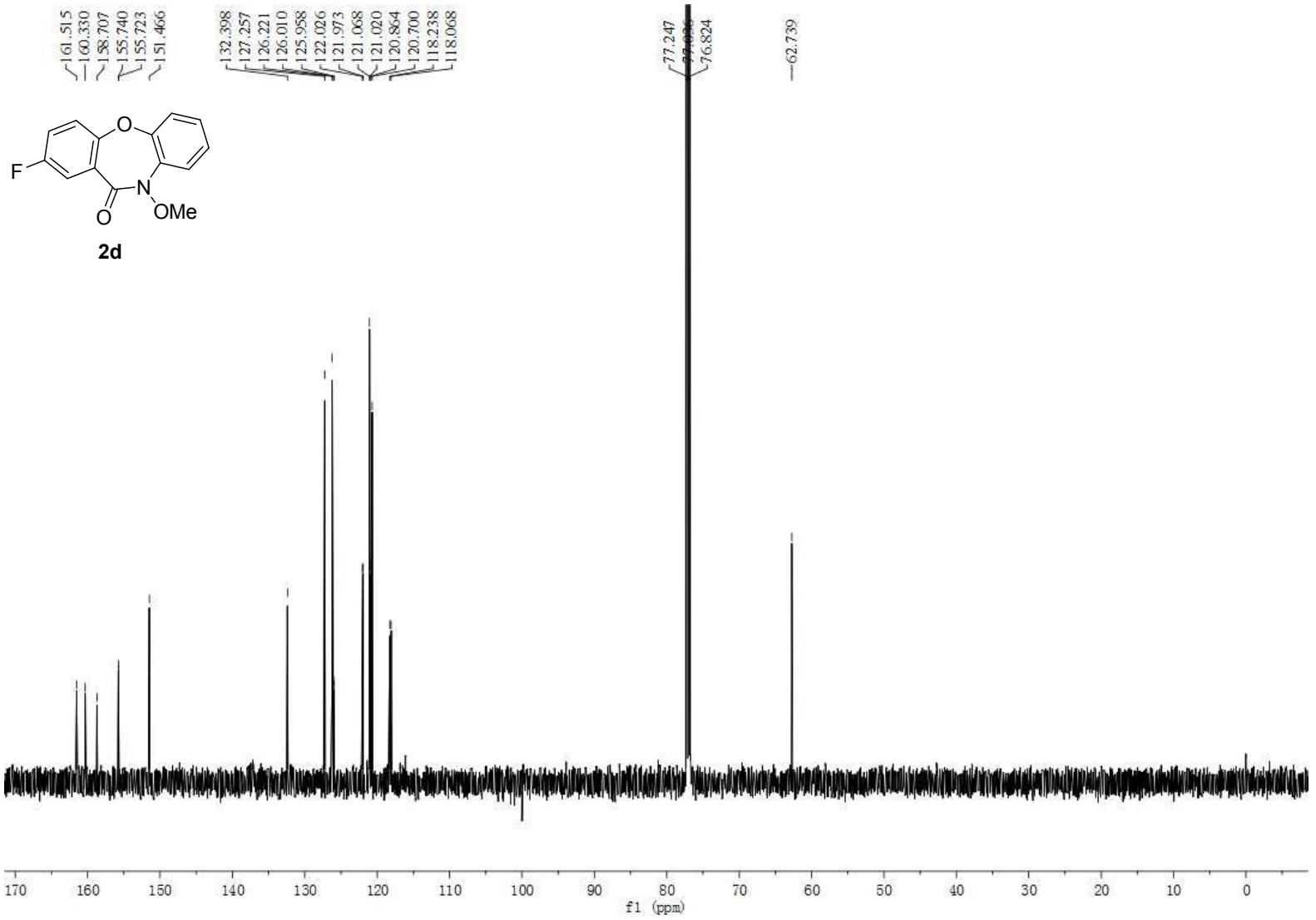

8.0854
8.0814
7.5922
7.5881
7.5778
7.5738
7.5491
7.5355
7.2724
7.2634
7.2612
7.2476
7.2168
7.2152
7.2042
7.1914
7.1218
7.1074
3.9238
0.0000
Br
O
N
OMe
O
1.00
1.07
1.07
2.15
1.06
1.07
3.11
f1 (ppm)

2c


161.3151
158.7640
151.1732
136.9327
134.6596
132.3126
127.2821
126.3371
126.2347
122.2723
121.1273
120.7365
118.2782
77.2420
77.0301
76.8188
62.7604
Br
O
N
OMe
O
2c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

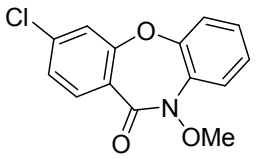

7.663
7.659
7.648
7.645
7.551
7.537
7.265
7.256
7.246
7.245
7.244
7.217
7.204
7.201
7.191
7.179
7.177
7.174
7.173
3.928
0.000
F
O
N
OMe
O
1.00
1.03
1.97
3.00
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

2d

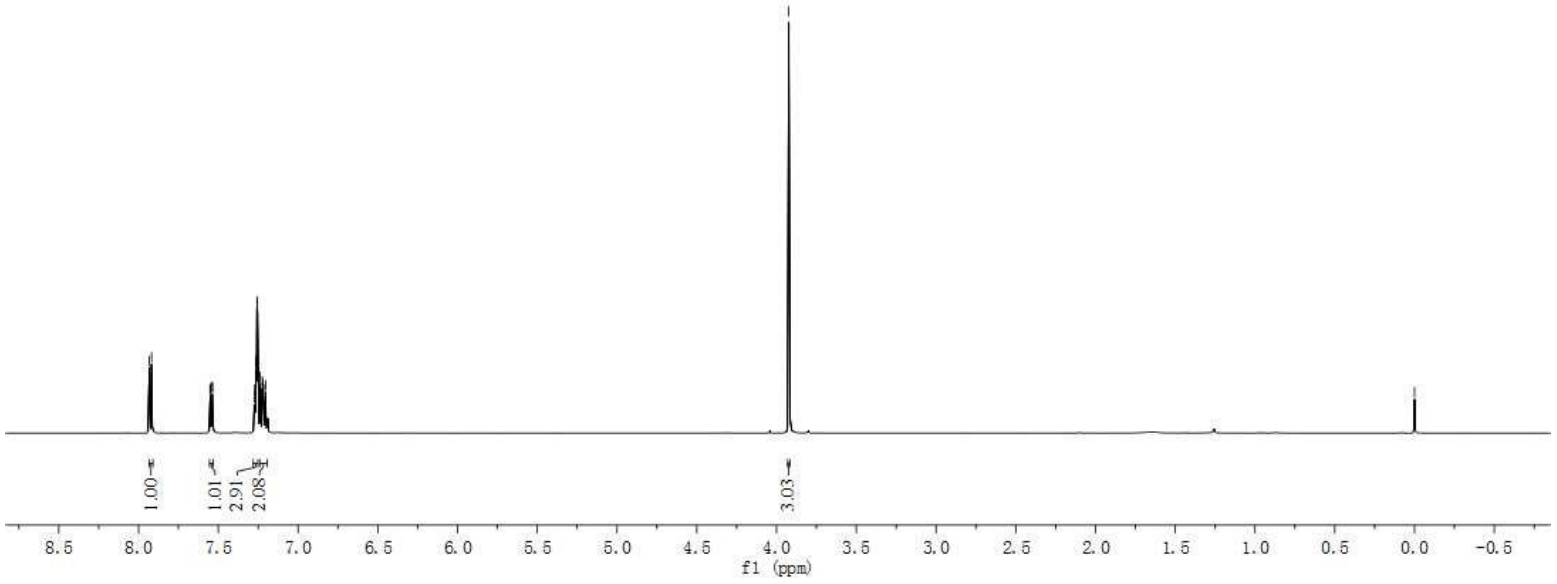

161.515
160.330
158.707
155.740
155.723
151.466
132.398
127.257
126.221
126.010
125.958
122.026
121.973
121.068
121.020
120.864
120.700
118.238
118.068
77.247
76.824
62.739
F
O
N
OMe
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

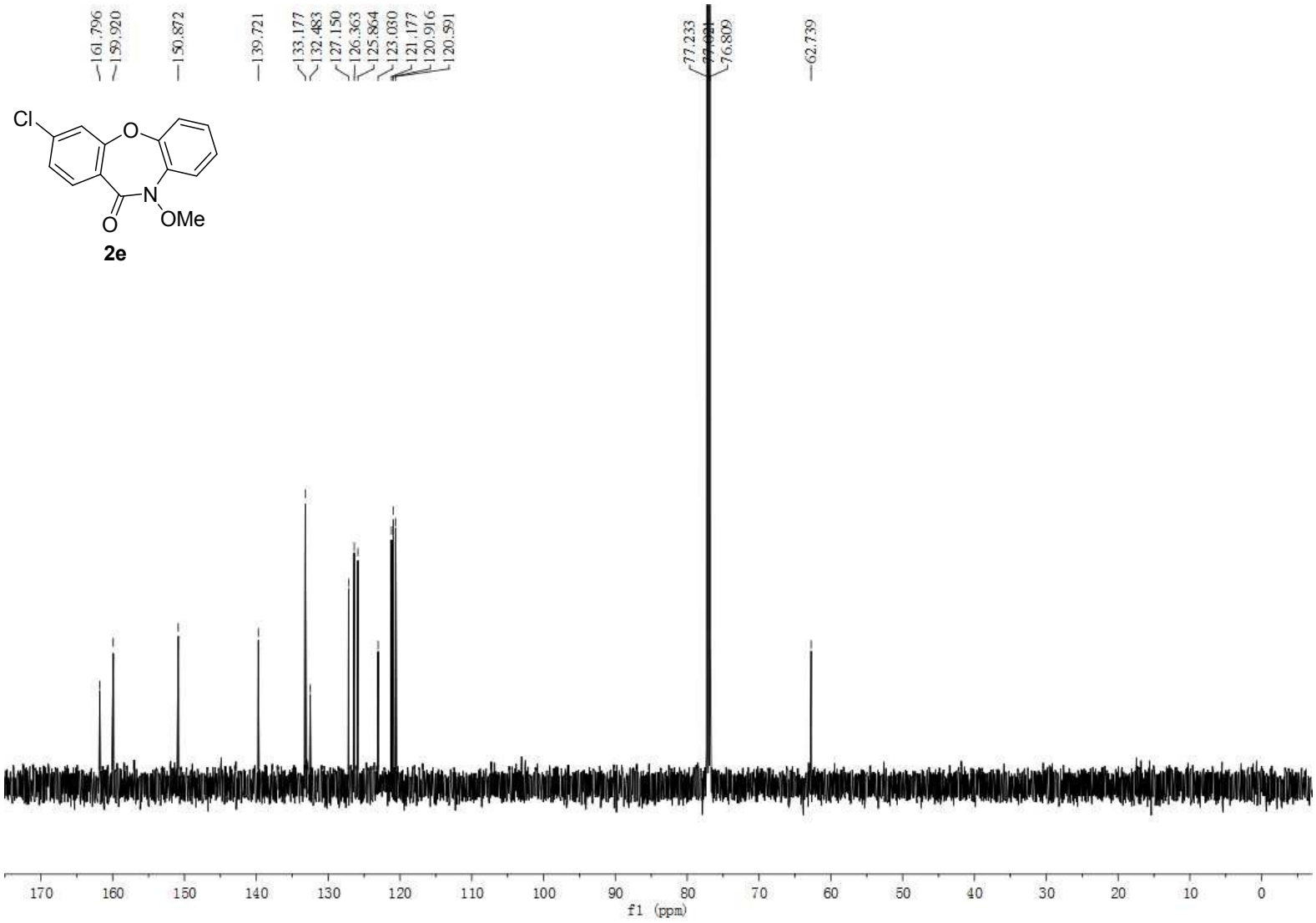
2d

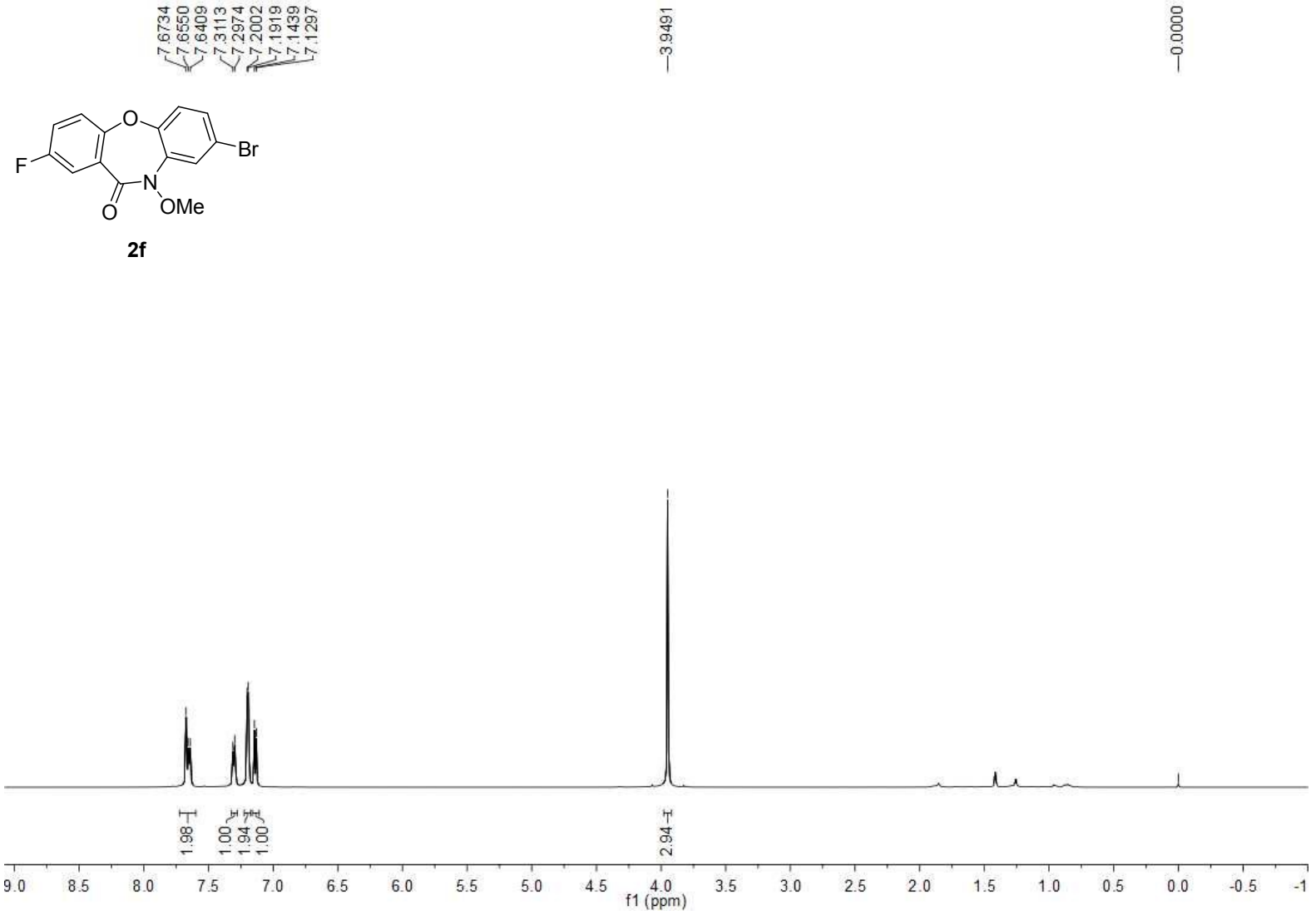

7.932
7.918
7.552
7.550
7.539
7.536
7.276
7.273
7.271
7.268
7.264
7.262
7.258
7.255
7.250
7.238
7.235
7.224
7.221
7.218
7.216
7.206
7.203
3.923
0.000

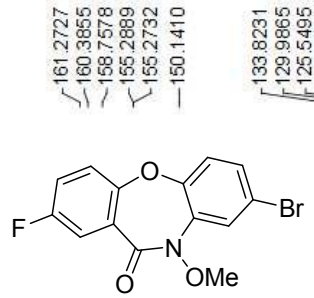

Cl
O
N
OMe
O

2e

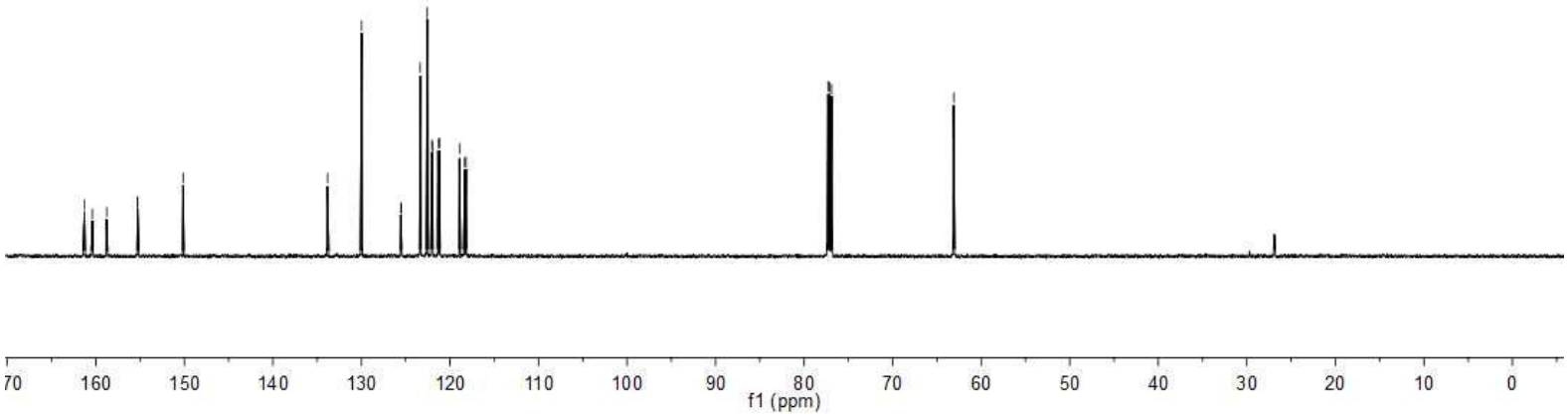

1.00
1.01
2.91
2.08
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

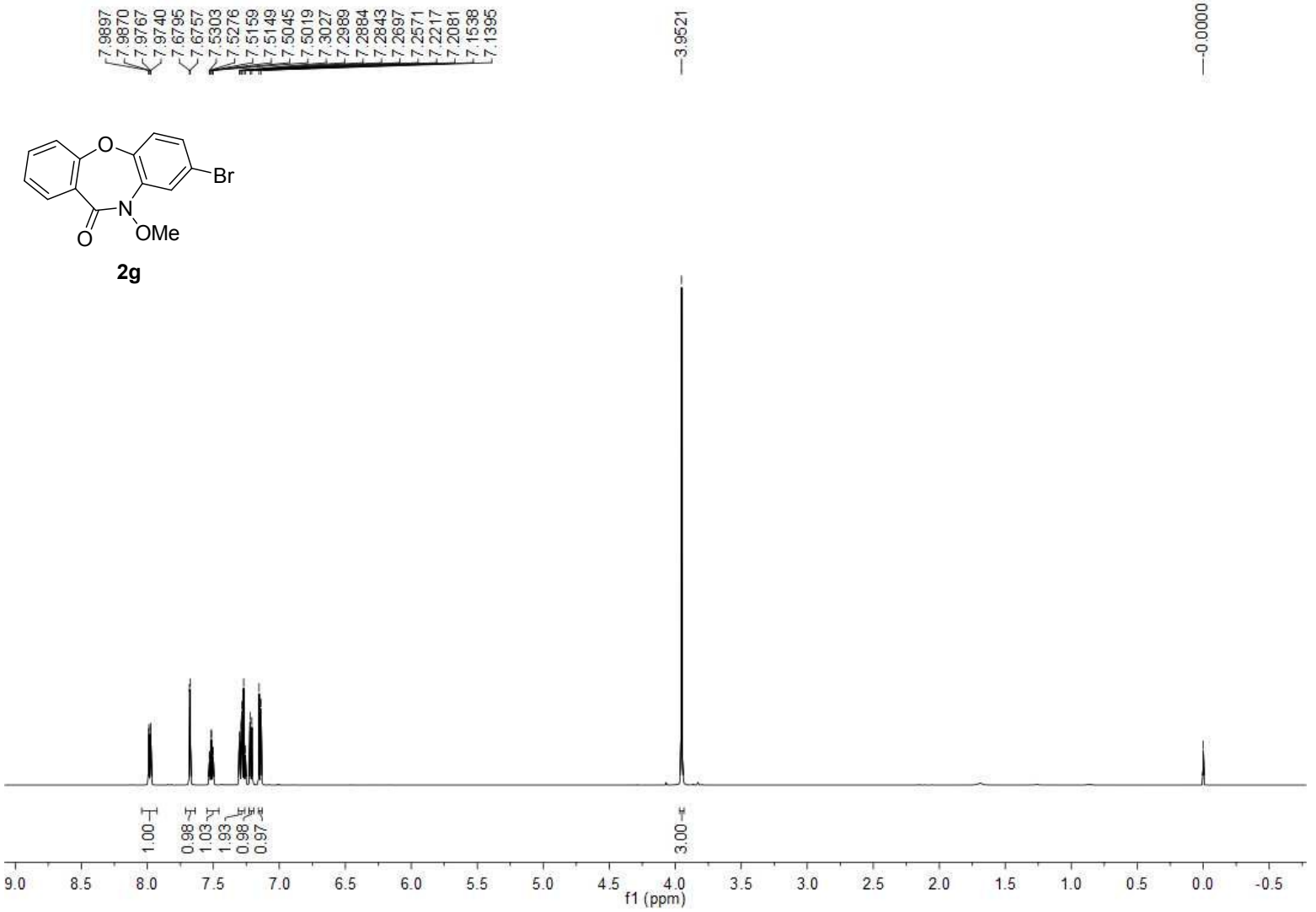

161.796
159.920
150.872
139.721
133.177
132.483
127.150
126.363
125.864
123.030
121.177
120.916
120.591
77.233
77.021
76.809
62.739
Cl
O
N
OMe
O
2e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

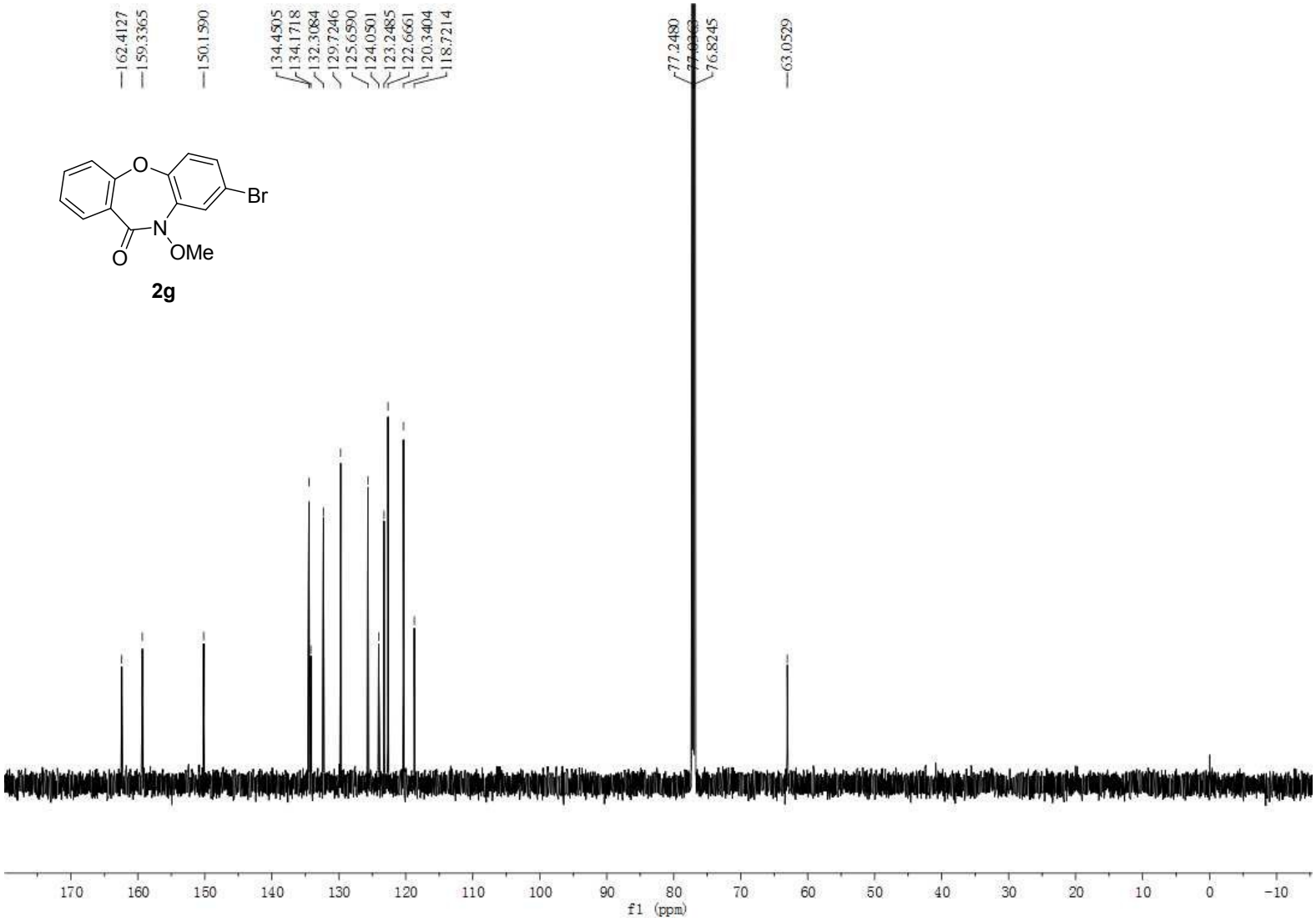

7.6734
7.6550
7.6409
7.3113
7.2974
7.2002
7.1919
7.1439
7.1297
3.9491
0.0000
O
Br
F
N
OMe
O
2f
1.98
1.00
1.94
1.00
2.94
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

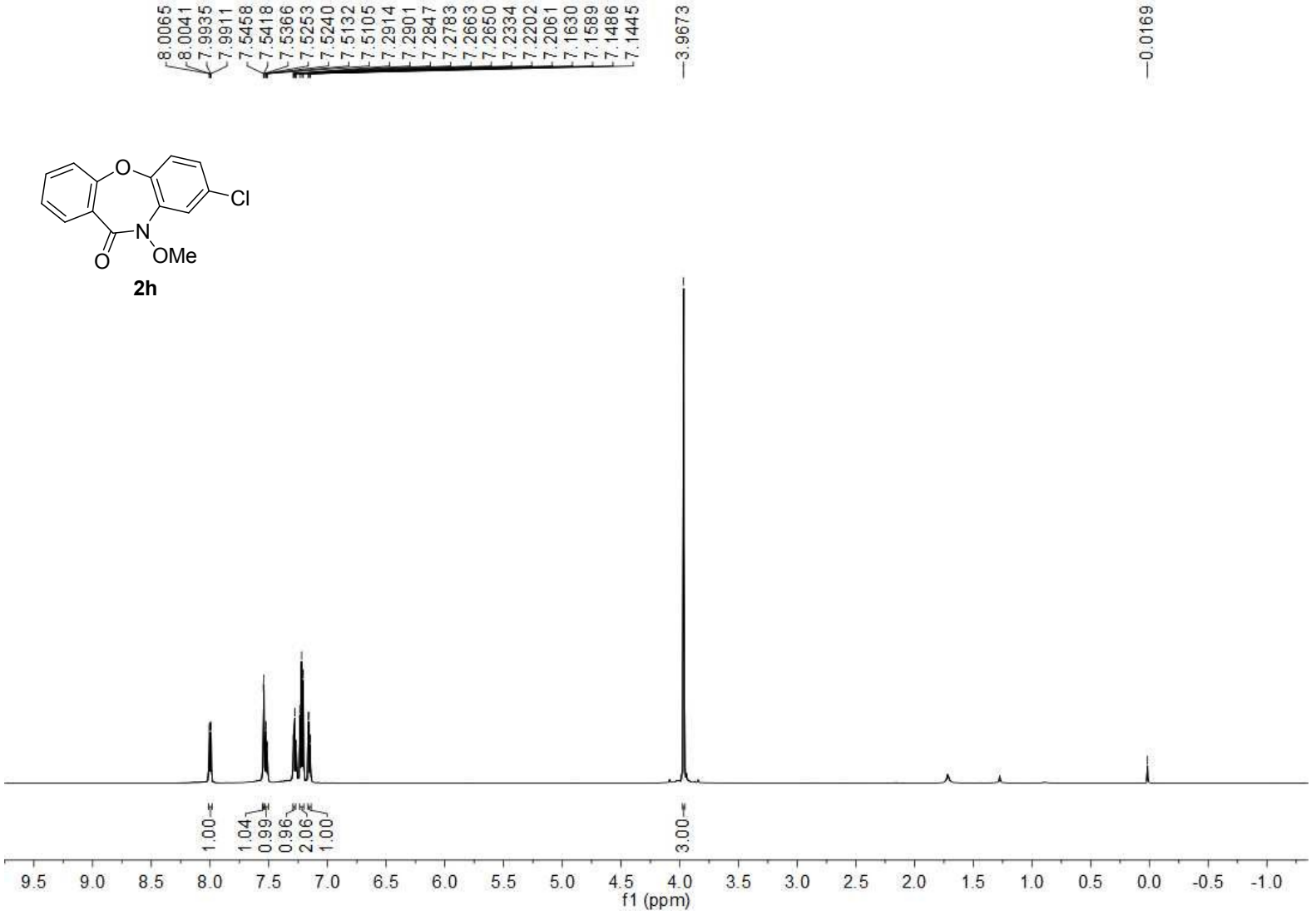

161.2727
160.3855
158.7578
155.2889
155.2732
150.1410
133.8231
129.9865
125.5495
125.4970
123.3609
122.5595
122.0319
121.9784
121.3339
121.1771
118.9154
118.3500
118.1807
77.3129
77.1010
76.8891
63.0958
O
Br
F
N
OMe
O

2f

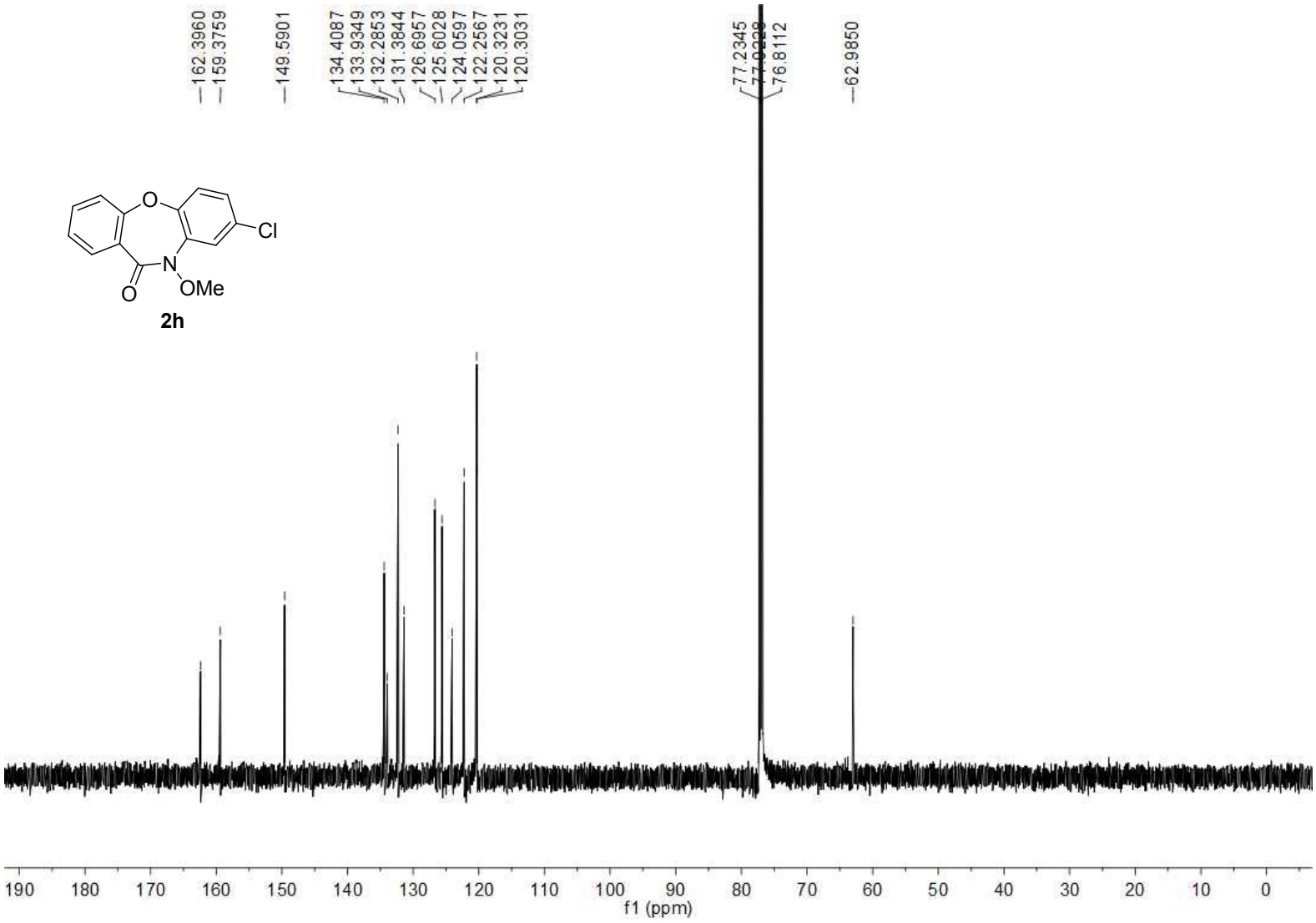

70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

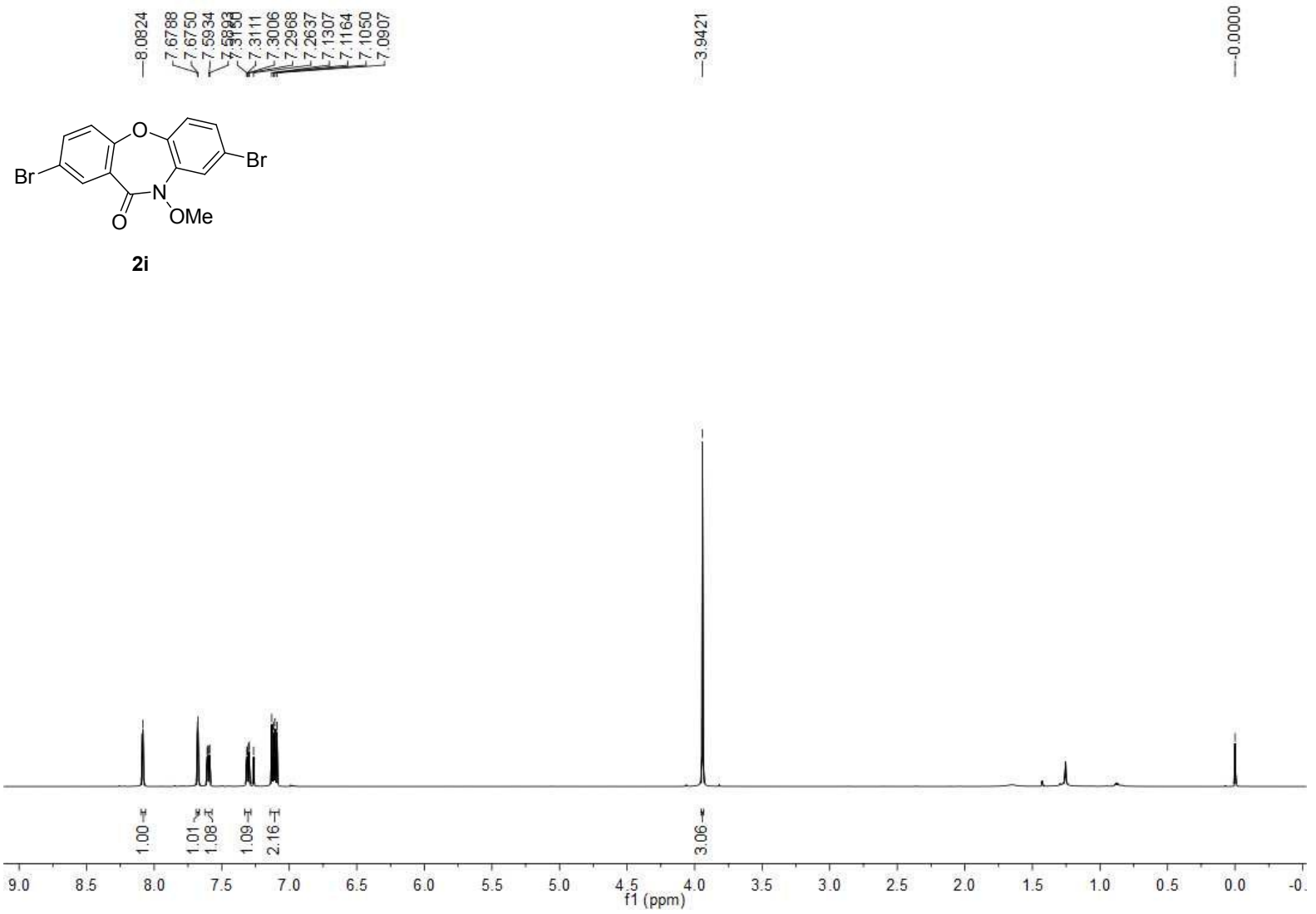

7.9897
7.9870
7.9767
7.9740
7.6795
7.6757
7.5303
7.5276
7.5159
7.5149
7.5045
7.5019
7.3027
7.2989
7.2884
7.2843
7.2697
7.2571
7.2217
7.2081
7.1538
7.1395
3.9521
-0.0000
O
Br
N
OMe
O
2g
1.00
0.98
1.03
1.93
0.98
0.97
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


162.4127
159.3365
150.1590
134.4505
134.1718
132.3084
129.7246
125.6590
124.0501
123.2485
122.6661
120.3404
118.7214
77.2480
76.8245
63.0529
O
Br
N
OMe
O
2g
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

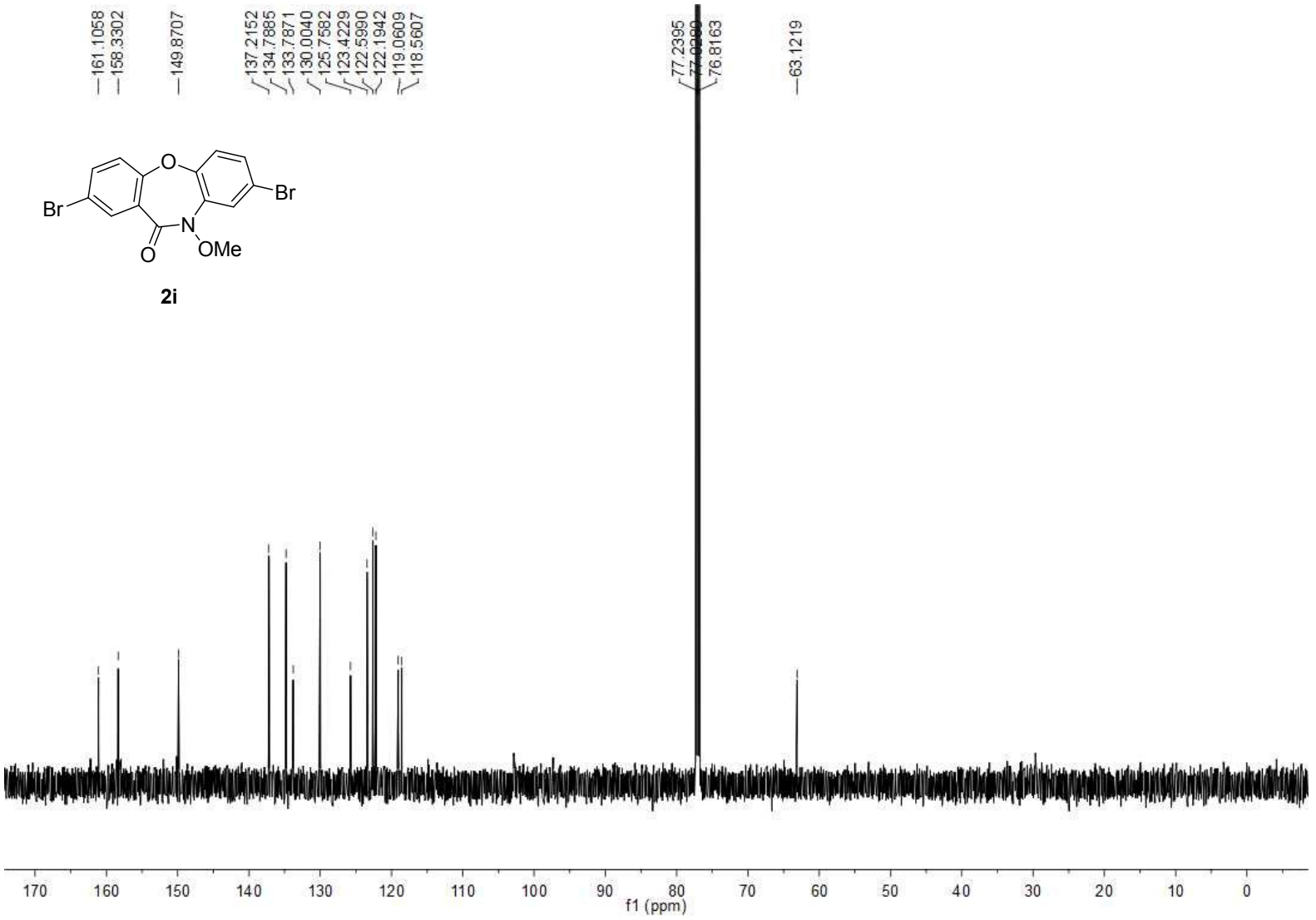

8.0065
8.0041
7.9935
7.9911
7.5458
7.5418
7.5366
7.5253
7.5240
7.5132
7.5105
7.2914
7.2901
7.2847
7.2783
7.2663
7.2650
7.2334
7.2202
7.2061
7.1630
7.1589
7.1486
7.1445
3.9673
0.0169
O
Cl
N
OMe
O
1.00
1.04
0.99
0.96
2.06
1.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

2h

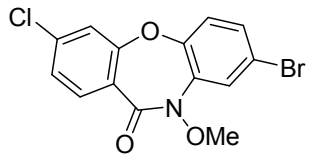

162.3960
159.3759
149.5901
134.4087
133.9349
132.2853
131.3844
126.6957
125.6028
124.0597
122.2567
120.3231
120.3031
77.2345
77.0228
76.8112
62.9850
O
Cl
N
OMe
O
2h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.0824
7.6788
7.6750
7.5934
7.3111
7.3006
7.2968
7.2637
7.1307
7.1164
7.1050
7.0907
3.9421
0.0000
Br
Br
O
N
OMe
O
1.00
1.01
1.08
1.09
2.16
3.06
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)

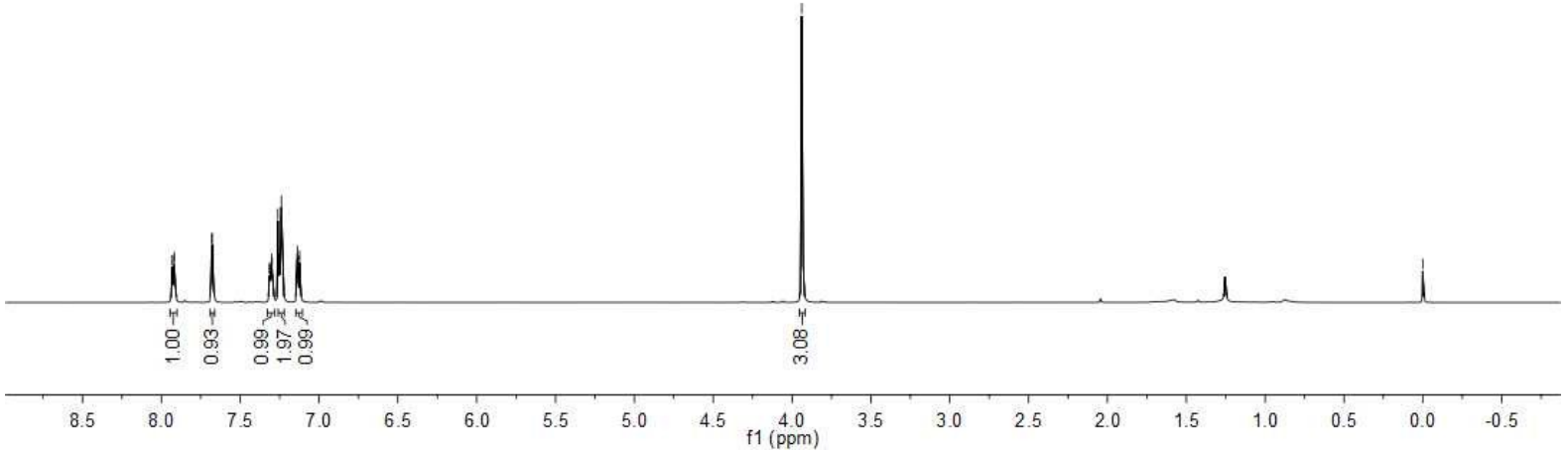
2i

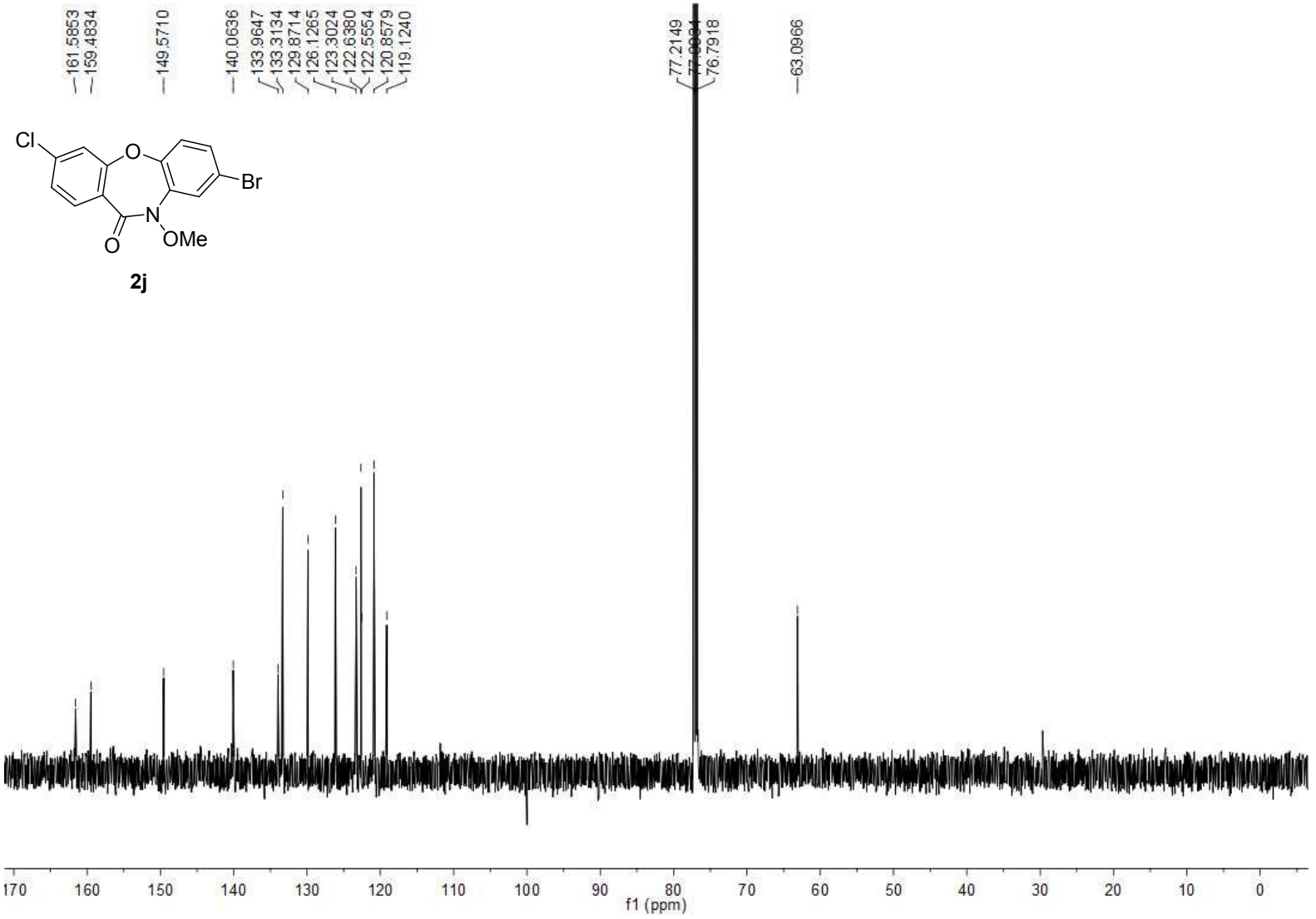

161.1058
158.3302
149.8707
137.2152
134.7885
133.7871
130.0040
125.7582
123.4229
122.5990
122.1942
119.0609
118.5607
77.2395
77.0280
76.8163
63.1219
Br
Br
O
N
OMe
O
2i
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

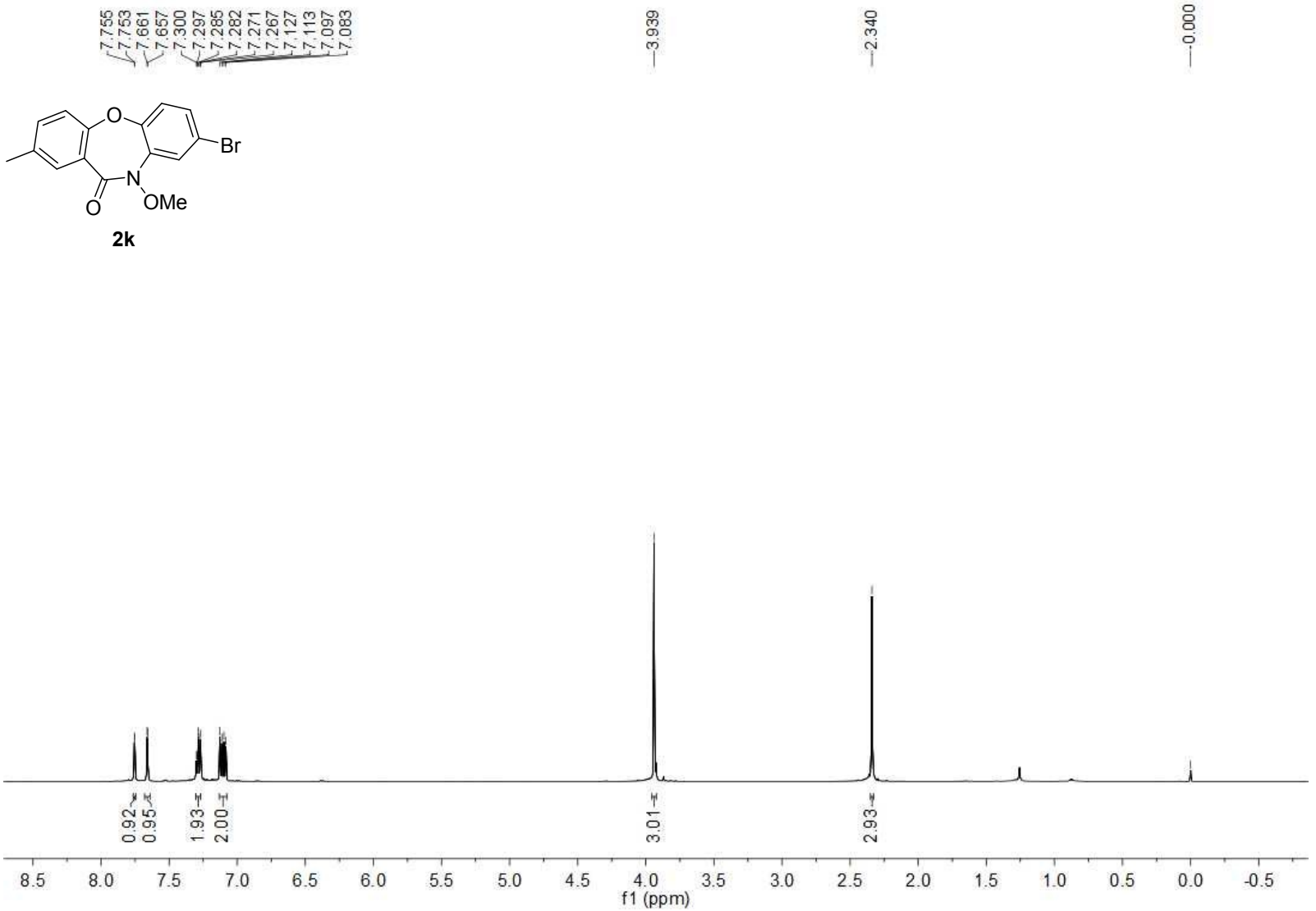

7.9322
7.9209
7.9185
7.6837
7.6803
7.6770
7.3184
7.3149
7.3115
7.3044
7.3007
7.2973
7.2614
7.2563
7.2530
7.2415
7.2391
7.2362
7.1401
7.1378
7.1258
7.1235
3.9391
0.0000


Cl
O
Br
N
OMe
O

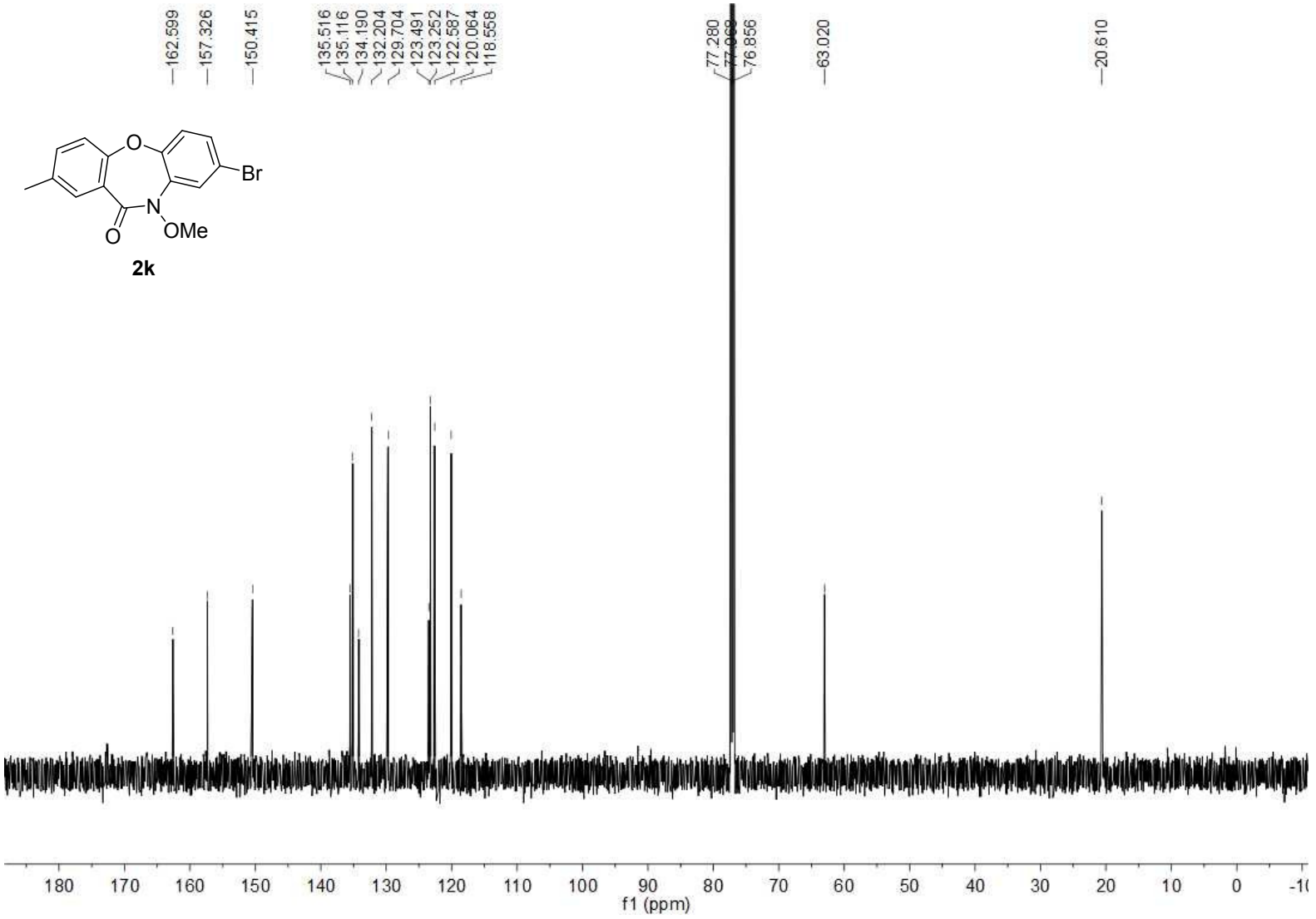
2j

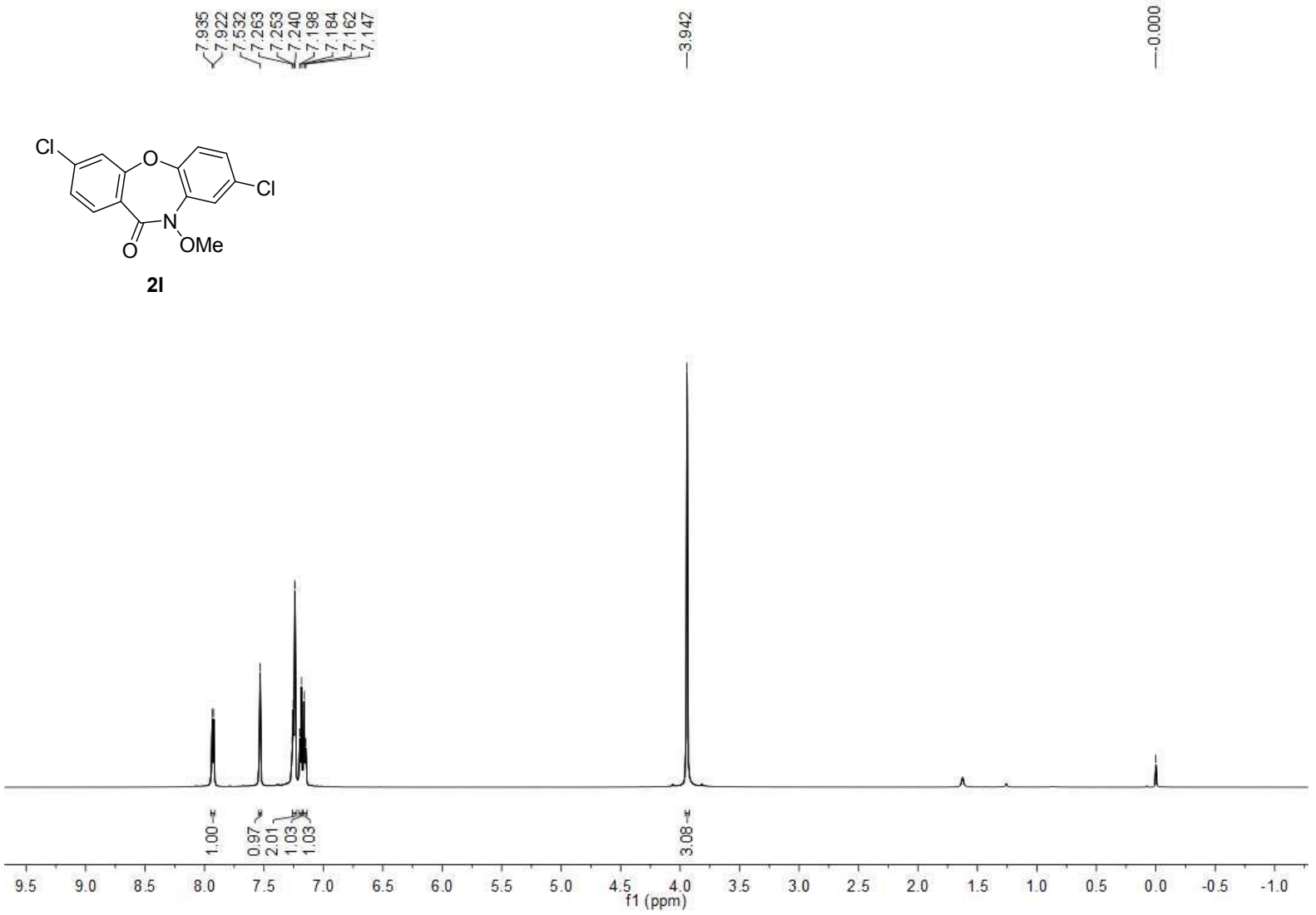

1.00
0.93
0.99
1.97
0.99
3.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

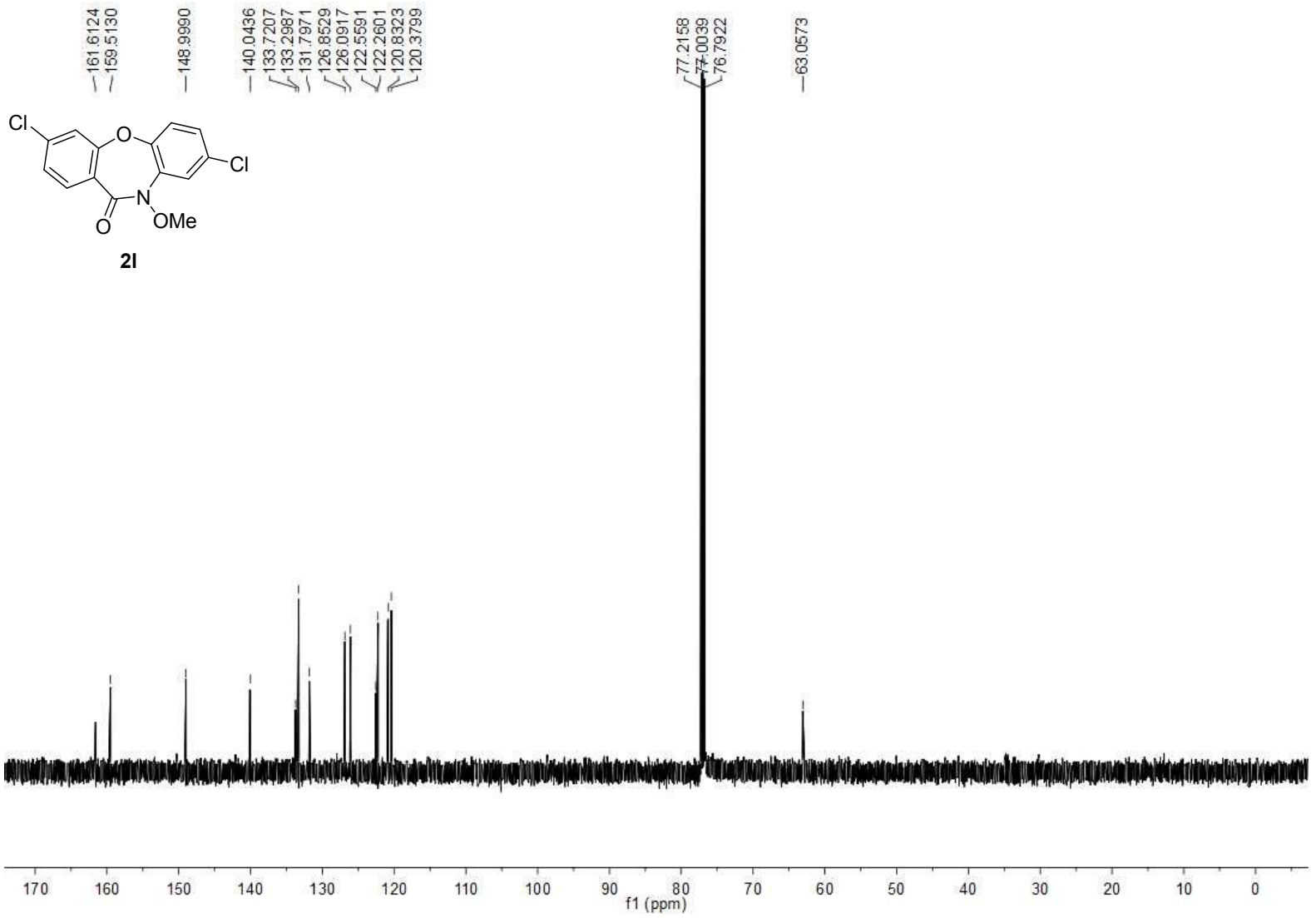

161.5853
159.4834
149.5710
140.0636
133.9647
133.3134
129.8714
126.1265
123.3024
122.6380
122.5554
120.8579
119.1240
77.2149
77.0031
76.7918
63.0966
Cl
O
Br
N
OMe
O
2j
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

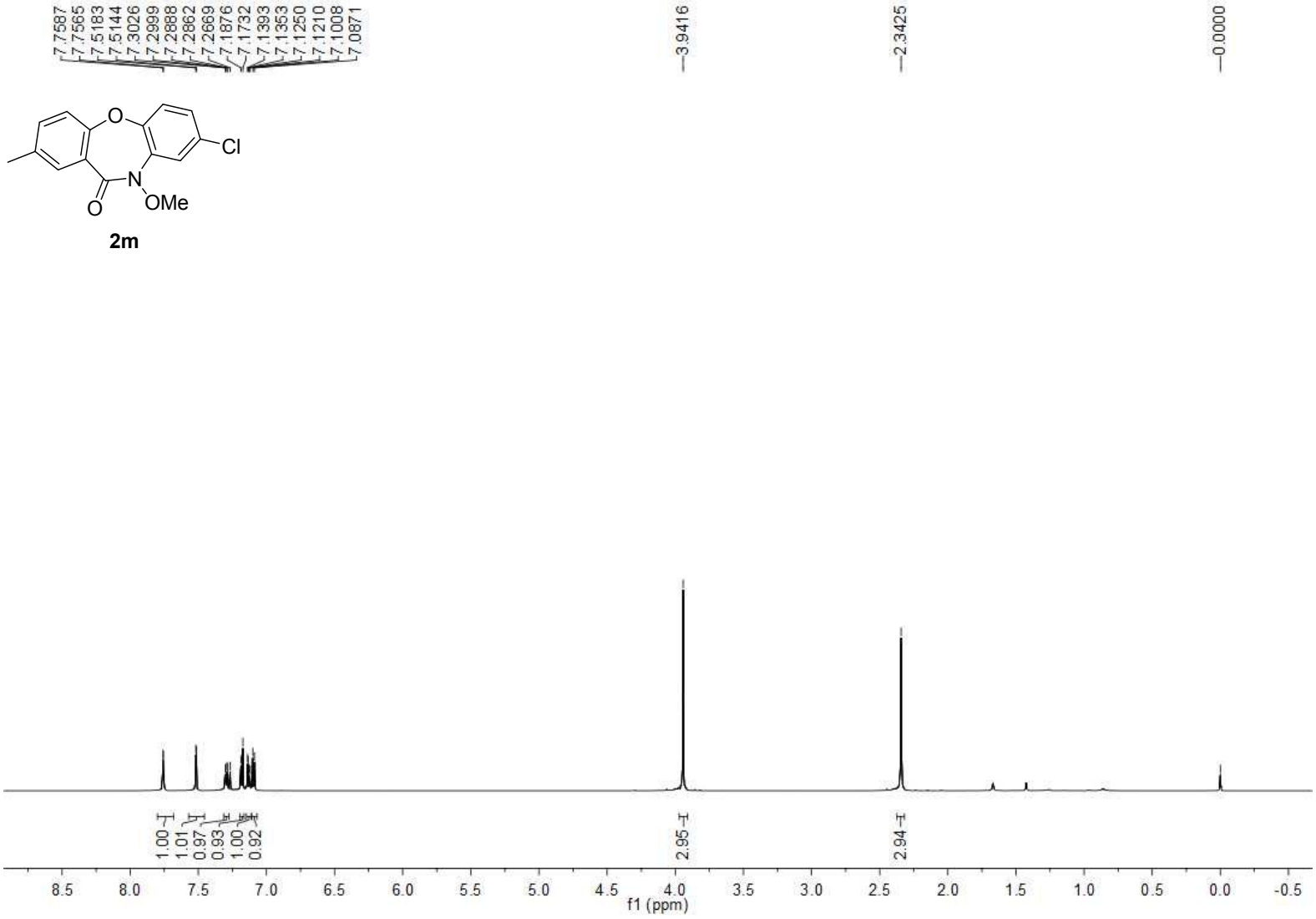

7.755
7.753
7.661
7.657
7.300
7.297
7.285
7.282
7.271
7.267
7.127
7.113
7.097
7.083
3.939
2.340
0.000
O
Br
N
OMe
O
0.92
0.95
1.93
2.00
3.01
2.93
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

2k

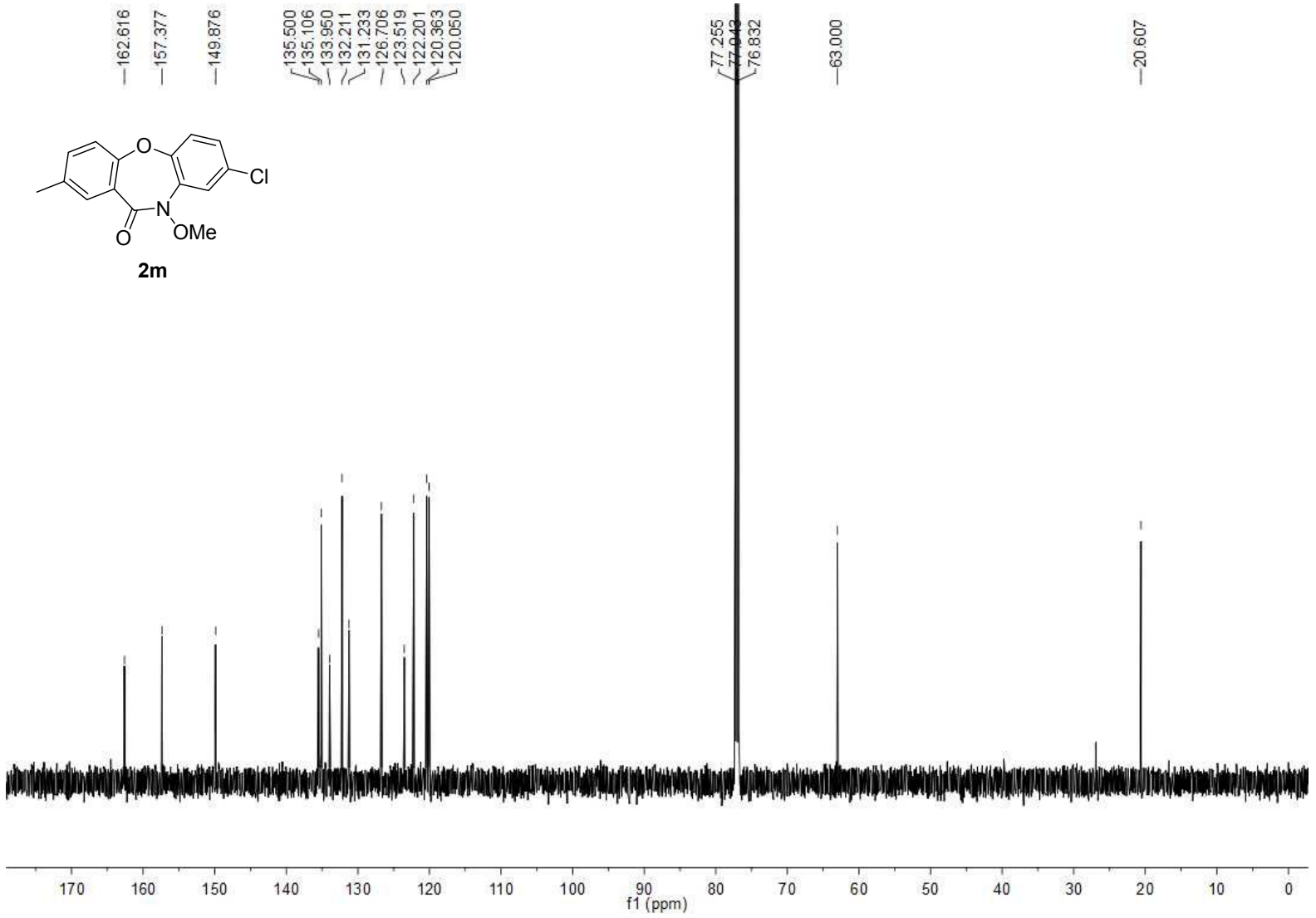

162.599
157.326
150.415
135.516
135.116
134.190
132.204
129.704
123.491
123.252
122.587
120.064
118.558
77.280
77.069
76.856
63.020
20.610
O
Br
N
OMe
O
2k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

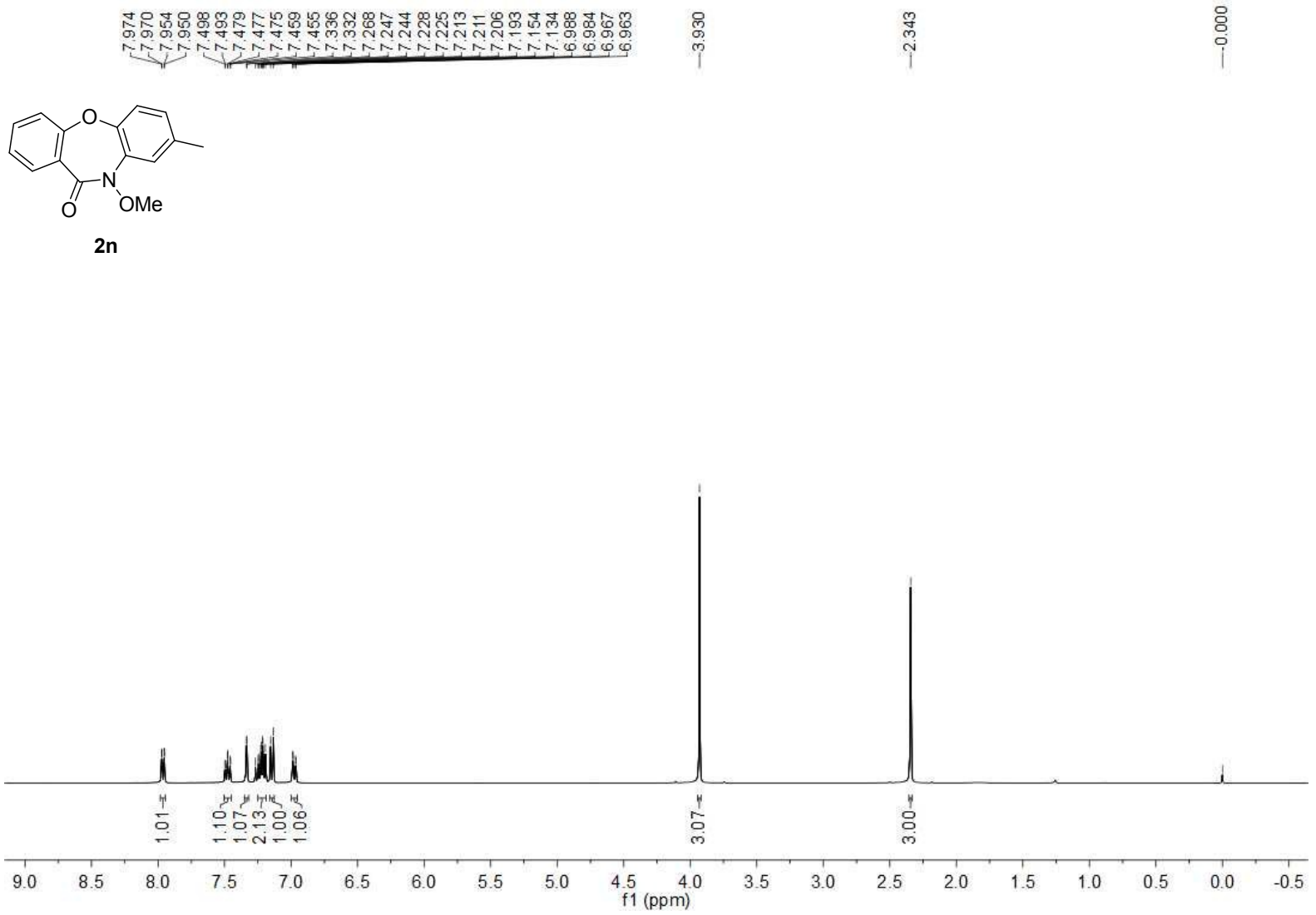

7.935
7.922
7.532
7.263
7.253
7.240
7.198
7.184
7.162
7.147
3.942
0.000
Cl
O
Cl
N
O
OMe
2l
1.00
0.97
2.01
1.03
1.03
3.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


161.6124
159.5130
148.9990
140.0436
133.7207
133.2987
131.7971
126.8529
126.0917
122.5591
122.2601
120.8323
120.3799
77.2158
77.0039
76.7922
63.0573
Cl
O
Cl
N
OMe
O
2l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

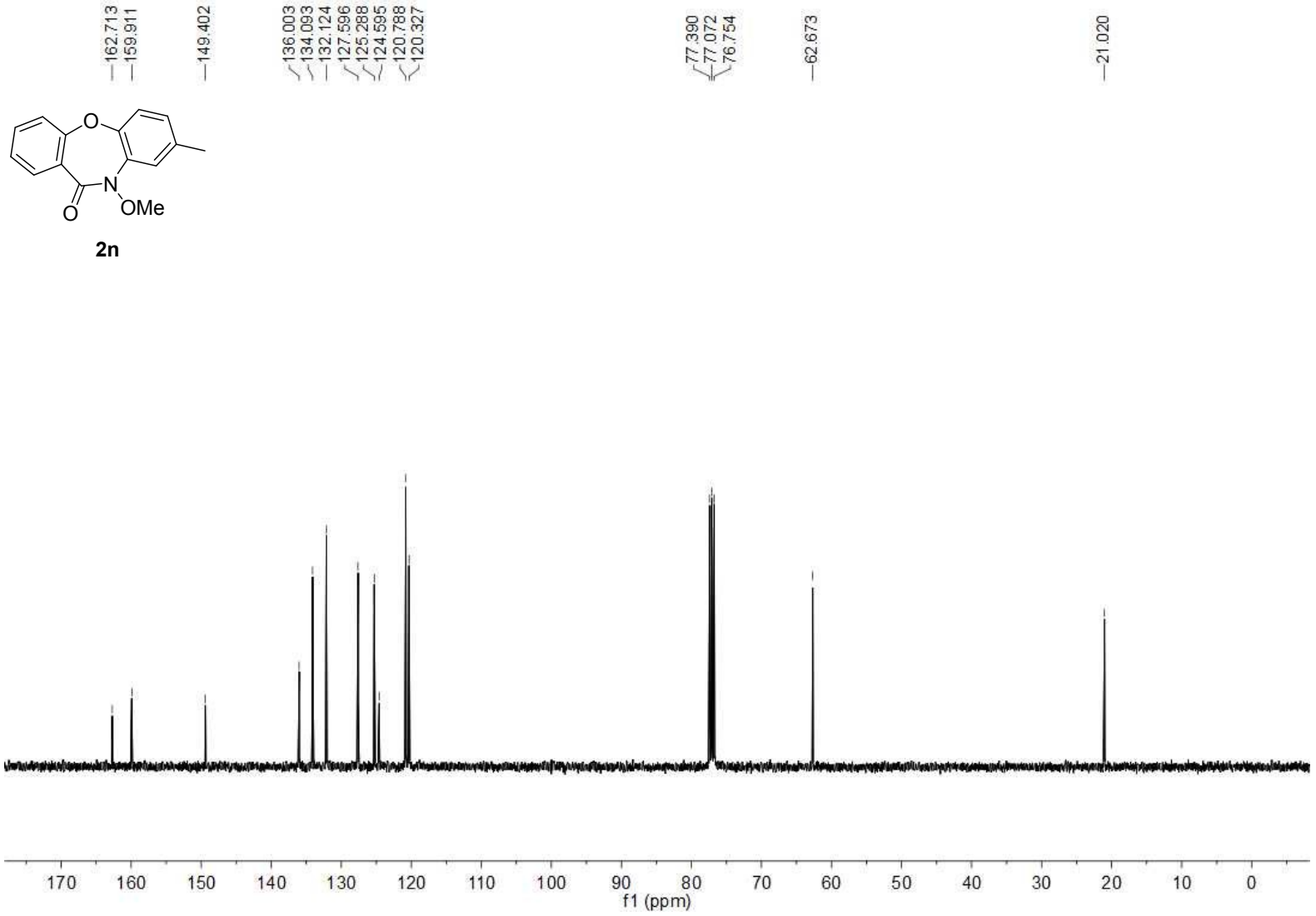

7.7587
7.7565
7.5183
7.5144
7.3026
7.2999
7.2888
7.2862
7.2669
7.1876
7.1732
7.1393
7.1353
7.1250
7.1210
7.1008
7.0871
3.9416
2.3425
0.0000
O
Cl
N
OMe
O
1.00
1.01
0.97
0.93
1.00
0.92
2.95
2.94
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

2m

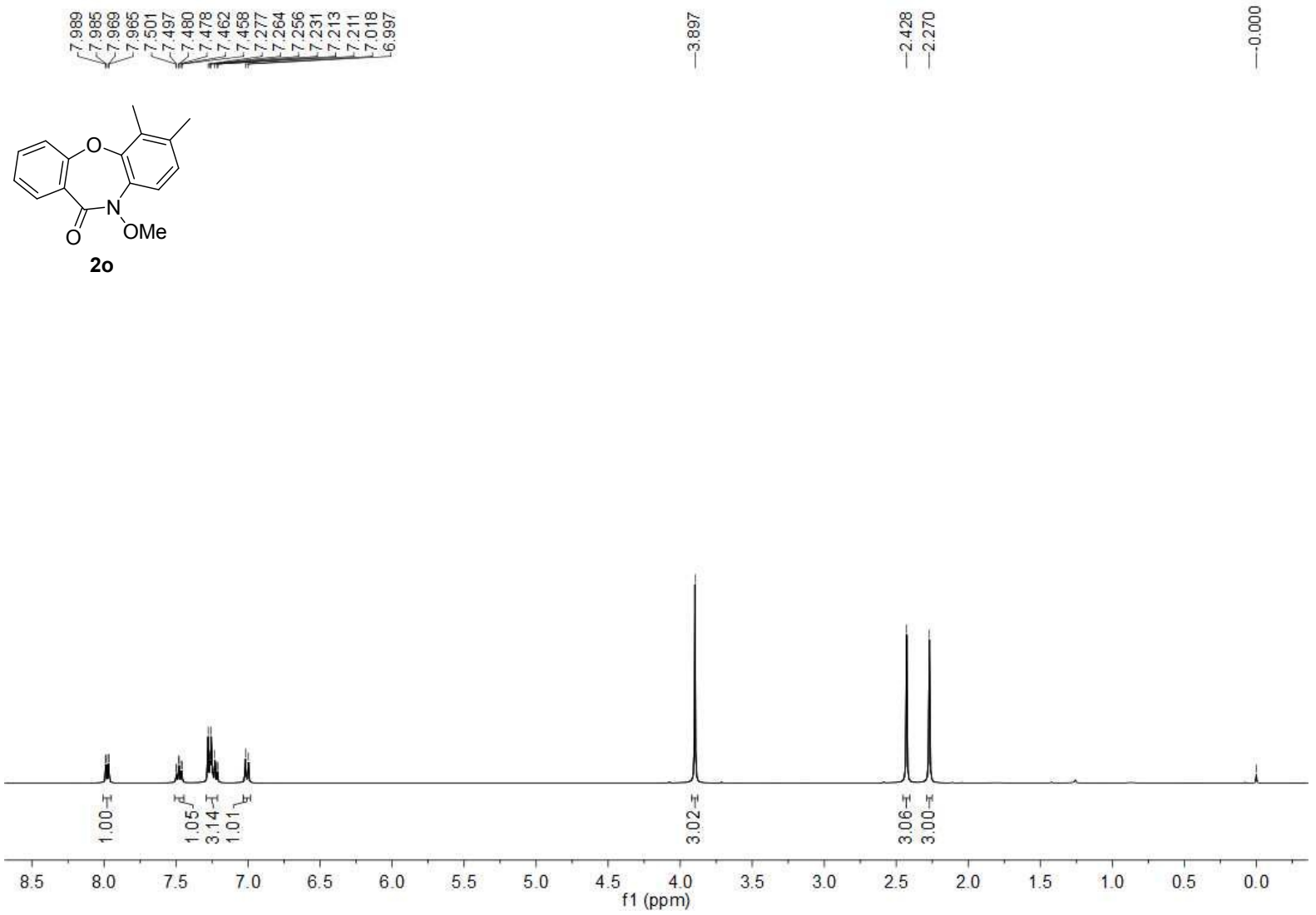

162.616
157.377
149.876
135.500
135.106
133.950
132.211
131.233
126.706
123.519
122.201
120.363
120.050
77.255
77.043
76.832
63.000
20.607
O
Cl
N
OMe
O
2m
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.974
7.970
7.954
7.950
7.498
7.493
7.479
7.477
7.475
7.459
7.455
7.336
7.332
7.268
7.247
7.244
7.228
7.225
7.213
7.211
7.206
7.193
7.154
7.134
6.988
6.984
6.967
6.963
3.930
2.343
0.000
O
N
OMe
O
1.01
1.10
1.07
2.13
1.00
1.06
3.07
3.00
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)

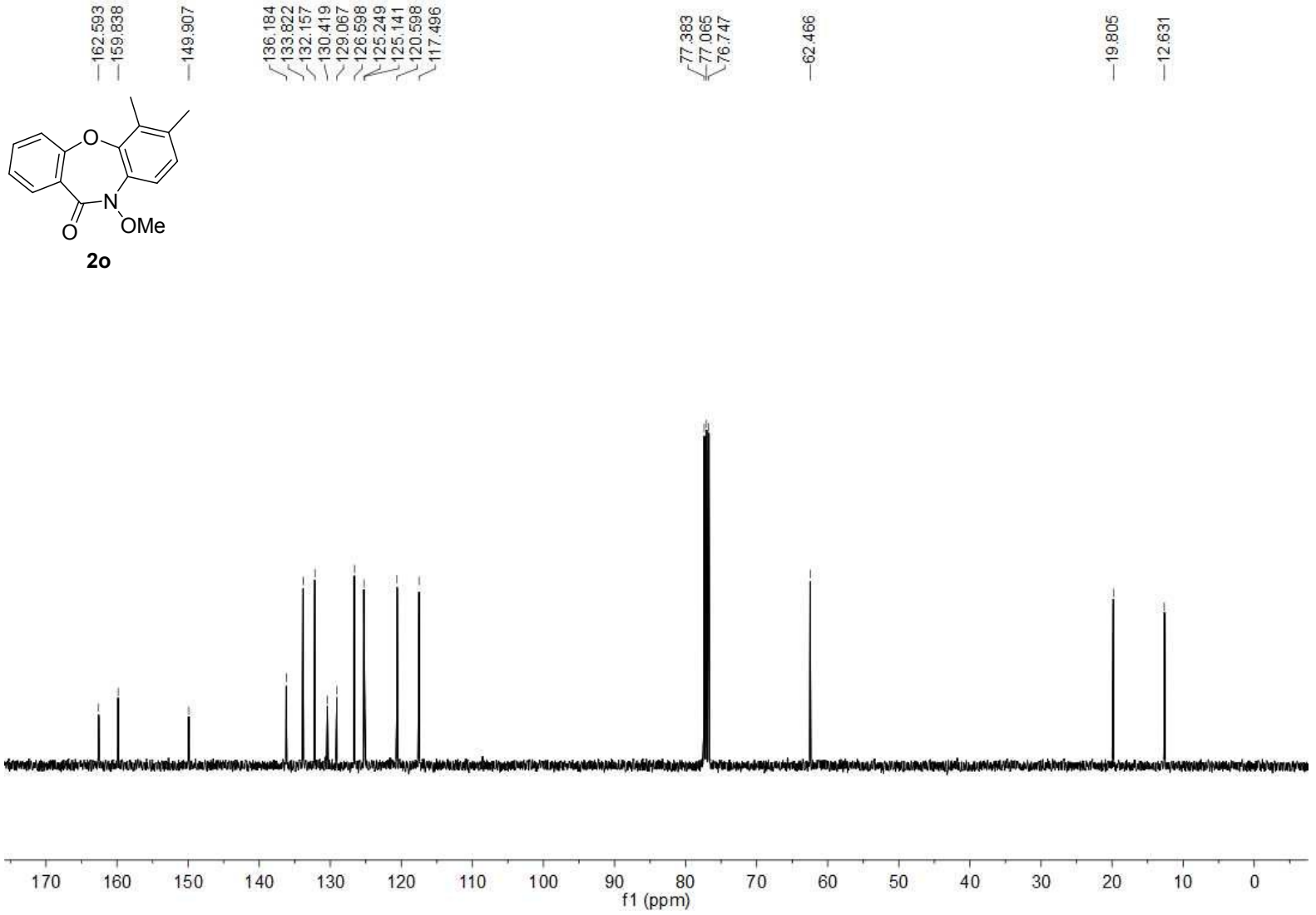
2n


162.713
159.911
149.402
136.003
134.093
132.124
127.596
125.288
124.595
120.788
120.327
77.390
77.072
76.754
62.673
21.020
O
N
OMe
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

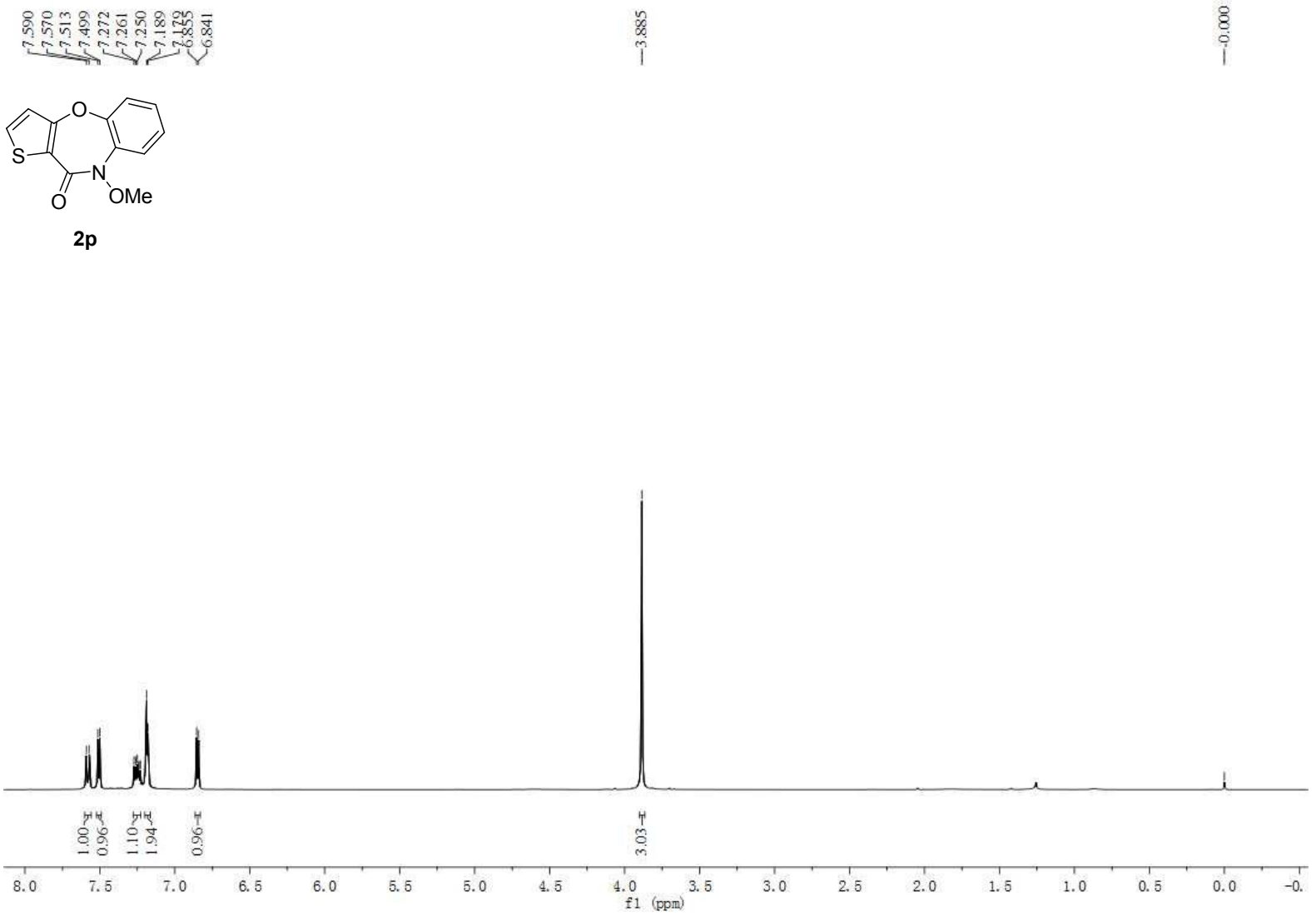
2n


7.989
7.985
7.969
7.965
7.501
7.497
7.480
7.478
7.462
7.458
7.277
7.264
7.256
7.231
7.213
7.211
7.018
6.997
3.897
2.428
2.270
0.000
O
N
OMe
O
1.00
1.05
3.14
1.01
3.02
3.06
3.00
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)

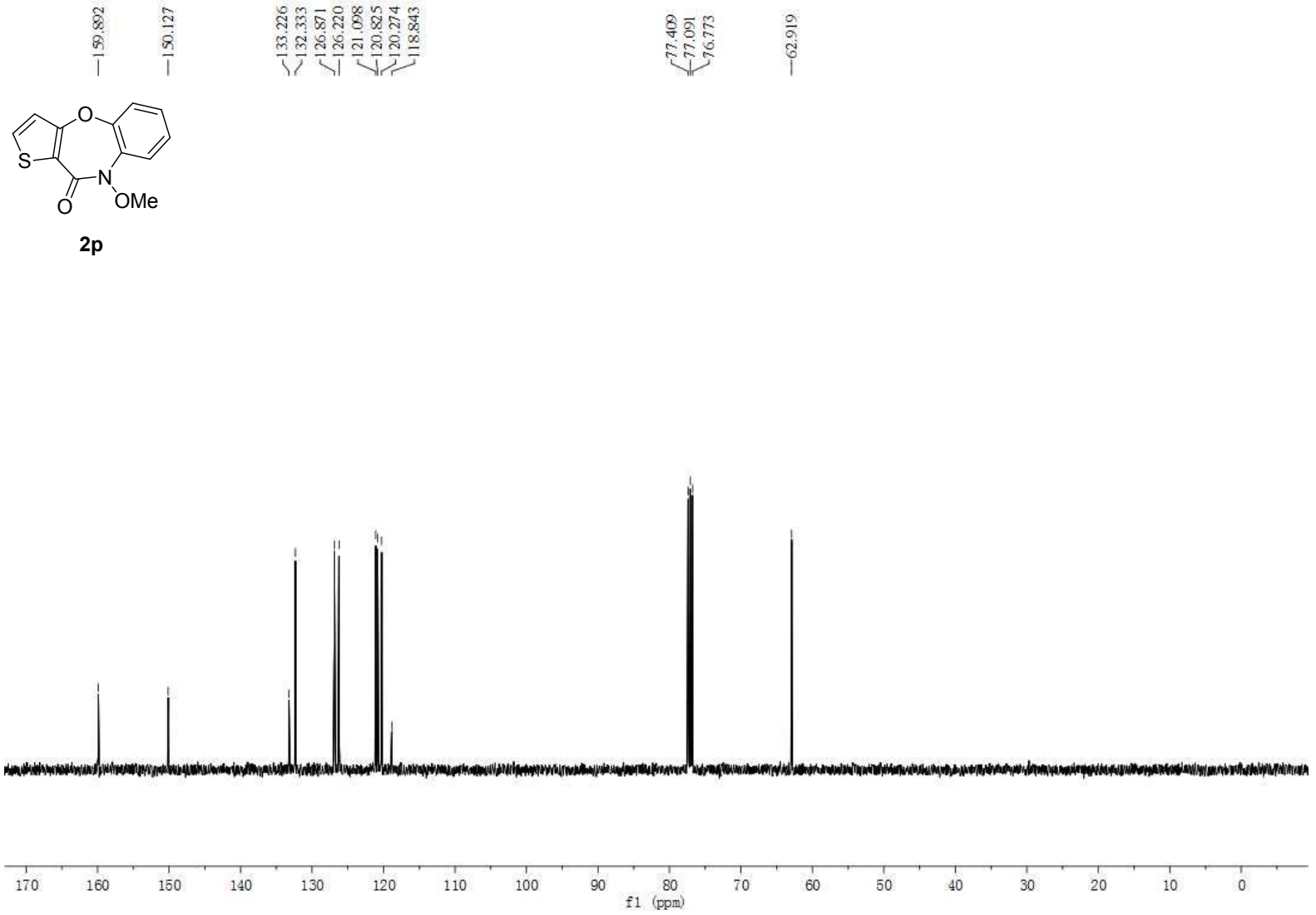
2o


162.593
159.838
149.907
136.184
133.822
132.157
130.419
129.067
126.598
125.249
125.141
120.598
117.496
77.383
77.065
76.747
62.466
19.805
12.631
O
N
OMe
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

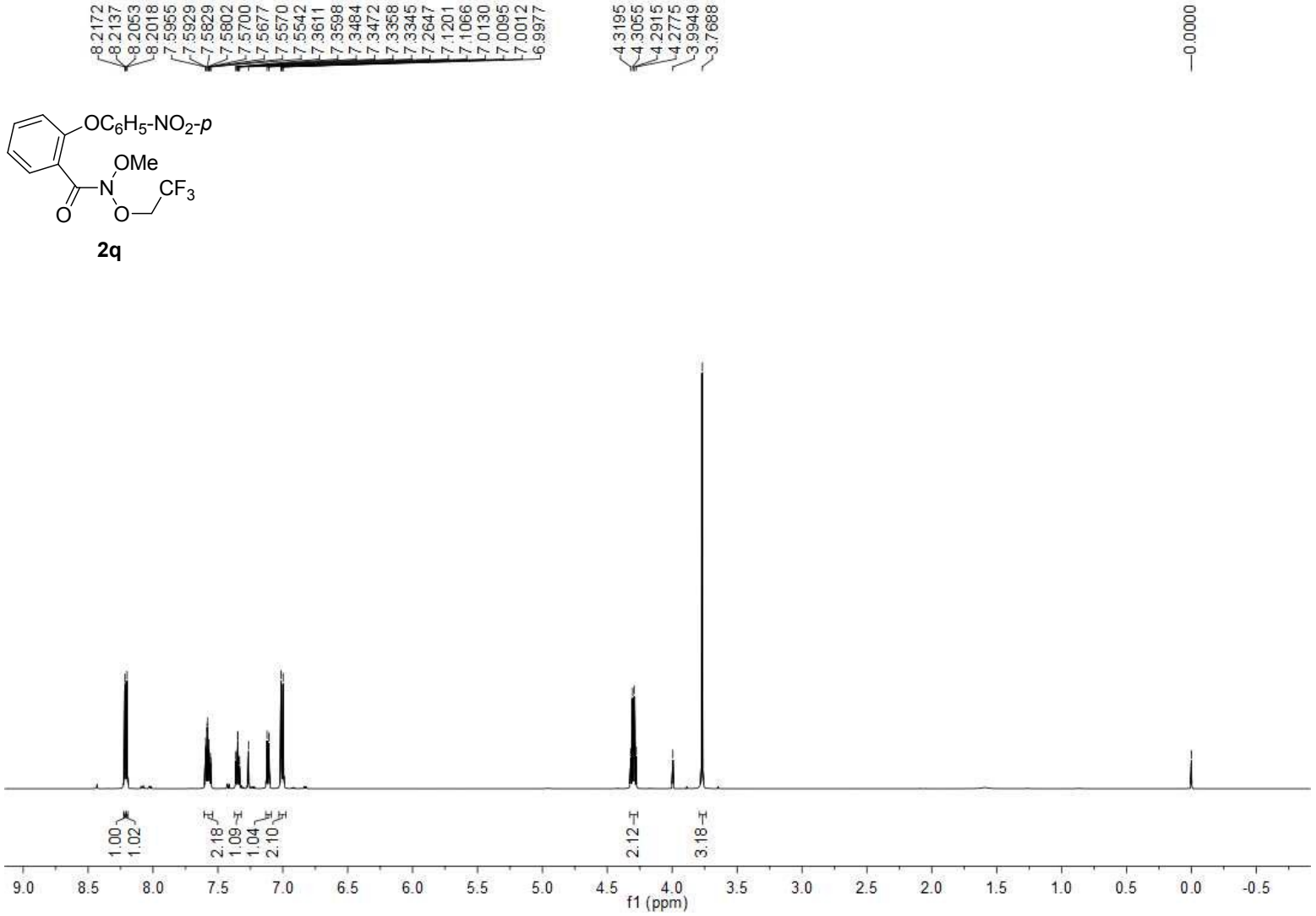
2o

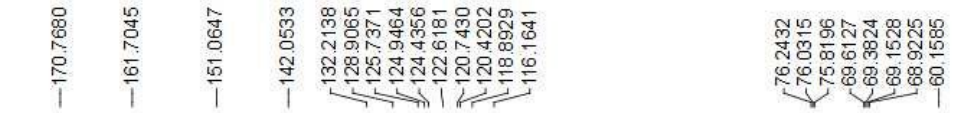

7.590
7.570
7.513
7.499
7.272
7.261
7.250
7.189
7.179
6.855
6.841
3.885
0.000
O
S
N
O
OMe
1.00
0.96
1.10
1.94
0.96
3.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

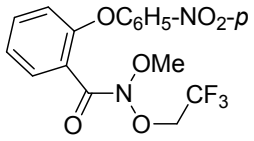
2p


159.892
150.127
133.226
132.333
126.871
126.220
121.098
120.825
120.274
118.843
77.409
77.091
76.773
62.919
O
S
N
O
OMe
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

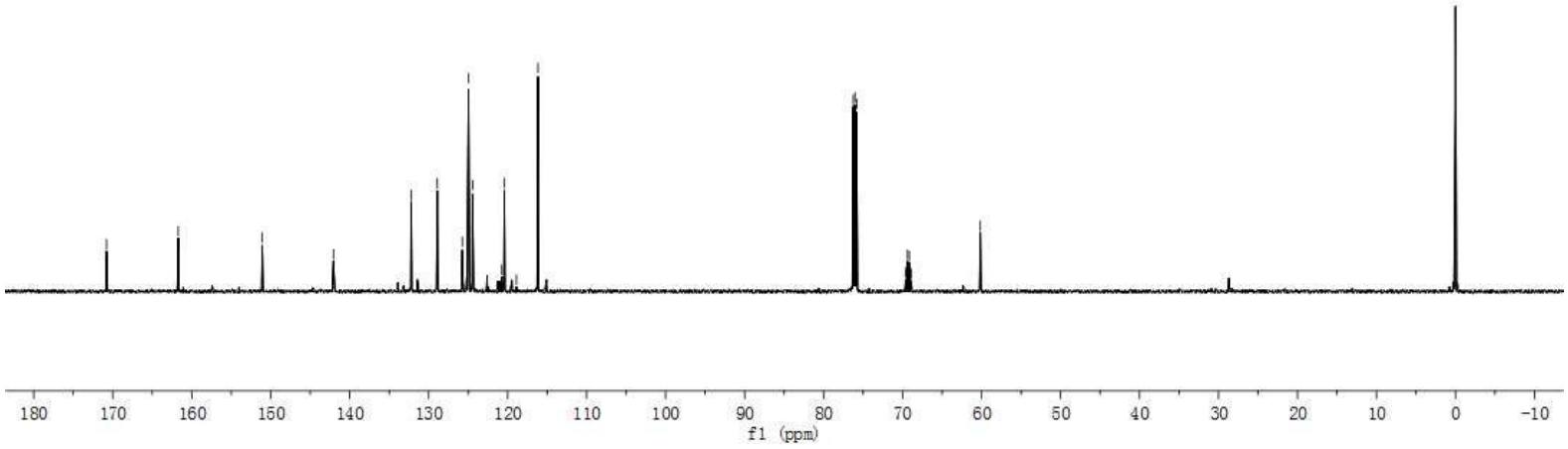
2p

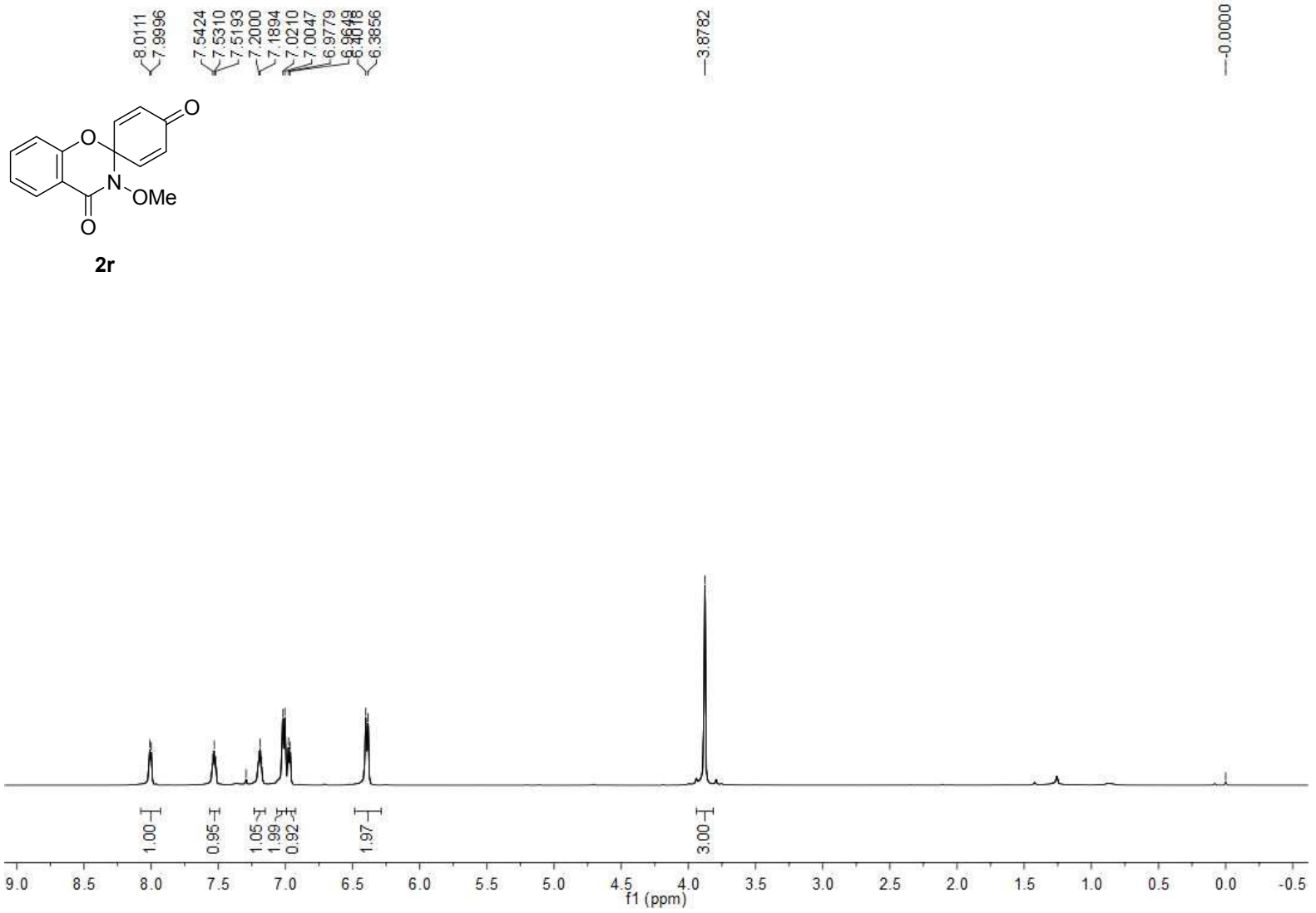

8.2172
8.2137
8.2053
8.2018
7.5955
7.5929
7.5829
7.5802
7.5700
7.5677
7.5570
7.5542
7.3611
7.3598
7.3484
7.3472
7.3358
7.3345
7.2647
7.1201
7.1066
7.0130
7.0095
7.0012
6.9977
4.3195
4.3055
4.2915
4.2775
3.9949
3.7688
0.0000
OC6H5-NO2-p
OMe
N
O
O
CF3
2q
1.00
1.02
2.18
1.09
1.04
2.10
2.12
3.18
9.0
8.5
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)


170.7680
161.7045
151.0647
142.0533
132.2138
128.9065
125.7371
124.9464
124.4356
122.6181
120.7430
120.4202
118.8929
116.1641
76.2432
76.0315
75.8196
69.6127
69.3824
69.1528
68.9225
60.1585

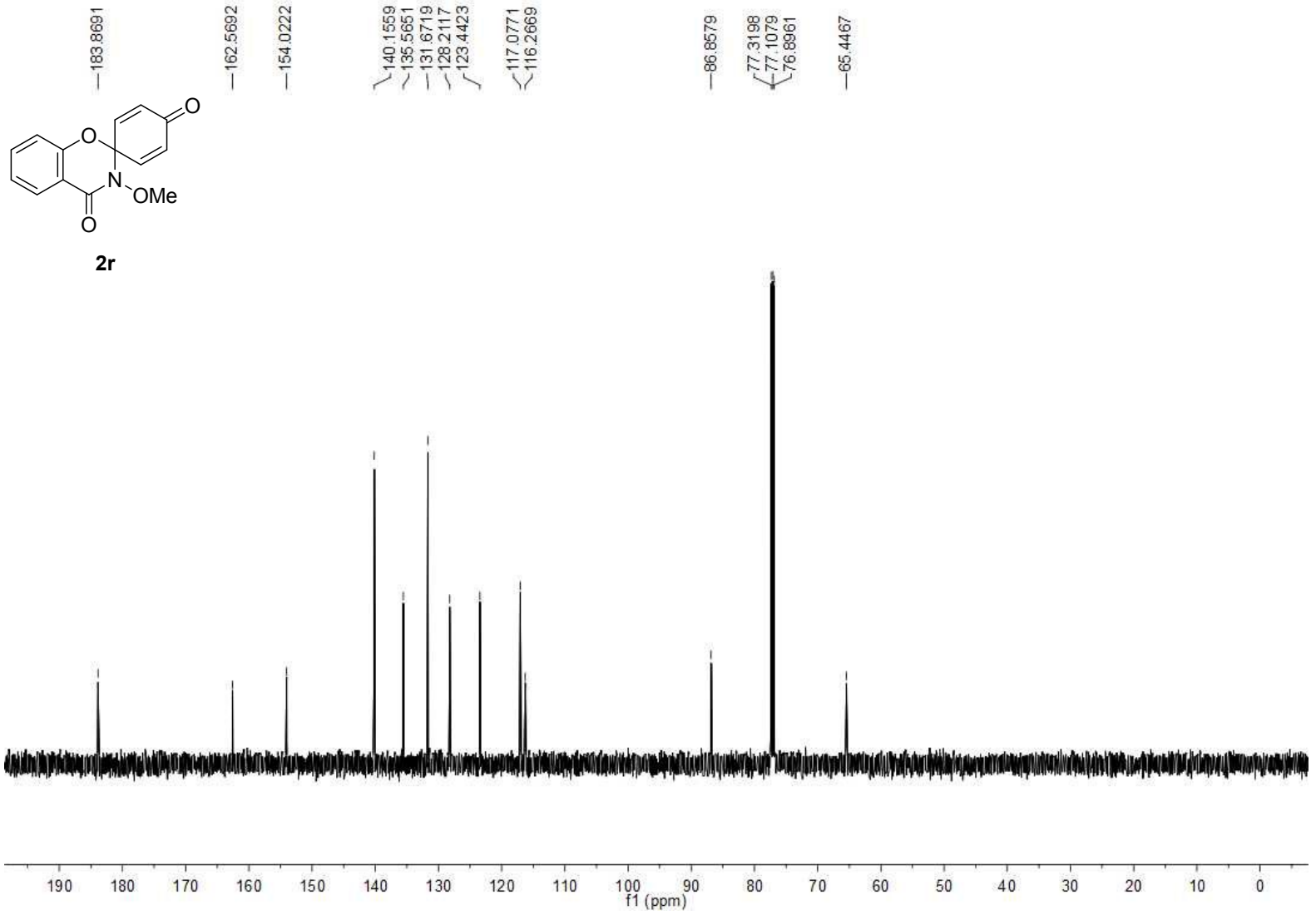

OC6H5-NO2-p
OMe
N
O
O
CF3

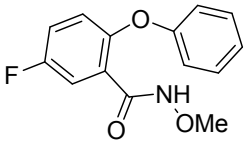
2q


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.0111
7.9996
7.5424
7.5310
7.5193
7.2000
7.1894
7.0210
7.0047
6.9779
6.3856
3.8782
0.0000
O
O
N
OMe
O
1.00
0.95
1.05
1.99
0.92
1.97
3.00
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)

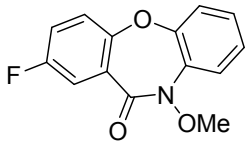
2r


183.8691
162.5692
154.0222
140.1559
135.5651
131.6719
128.2117
123.4423
117.0771
116.2669
86.8579
77.3198
77.1079
76.8961
65.4467
O
O
N
OMe
O
2r
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


F
O
NH
O
OMe

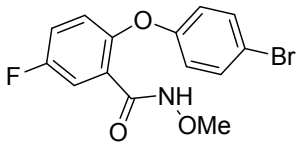
1d

-118.4792
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


F
O
N
O
OMe

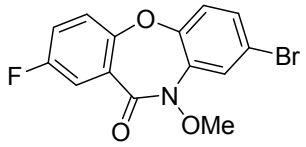
2d

-116.5353
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


O
Br
F
NH
O
OMe

1f

-117.4649
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


O
F
Br
N
O
OMe

2f

-115.9403
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)