Supporting Information:

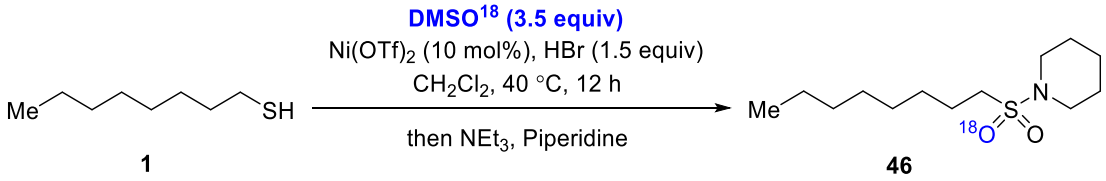
Table of Contents

General Remarks

All commercially available compounds were purchased from Sigma-Aldrich, Alfa-Aesar, Acros, Beijing Ouhe, and Beijing Chemical Works, Ltd. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. Analysis of crude reaction mixture was done on an Agilent 7890 GC System with an Agilent 5975 Mass Selective Detector. Products were purified by flash chromatography on silica gel. ^{1}H-NMR spectra were recorded on Bruker AVANCE III-400 spectrometers. Chemical shifts (in ppm) were referenced to the solvent peak of $CDCl_3$ (7.26 ppm) and DMSO-d_6 (2.50 ppm). ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.0 ppm) and DMSO-d_6 (39.5 ppm). Mass spectra were recorded using a PE SCLEX QSTAR spectrometer. High resolution mass spectra were obtained with a Bruker APEX IV Fourier transform ion cyclotron resonance mass spectrometer.

Mechanistic Studies

(1) ^{18}O labeling experiments



To a solution of $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), octane-1-thiol (0.50 mmol, 73.1 mg), **DMSO^{18}** (1.75 mmol, 120 μL) in DCM (2 mL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) was added. The mixture was stirred in anhydrous DCM (2 mL) at 40 °C for 12 h under N_2 atmosphere. Then the reaction mixture was added dropwise to the solution of piperidine (1.5 mmol, 127.8 mg) and NEt_3 (4 mmol, 404.8 mg) in anhydrous DCM (1 mL) with ice-salt bath. The mixture was stirred at ambient temperature for 8 h, washed by 1M HCl (4 mL × 2) and brine (4 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to afford **46** (55.3 mg, 42%) as a white solid. The

ratio of $^{16}O,^{16}O$-**46**:$^{16}O,^{18}O$-**46** was determined by ESI-HRMS as 3:1. The low ^{18}O-labled ratio may attribute to H_2O^{16} in reagents.

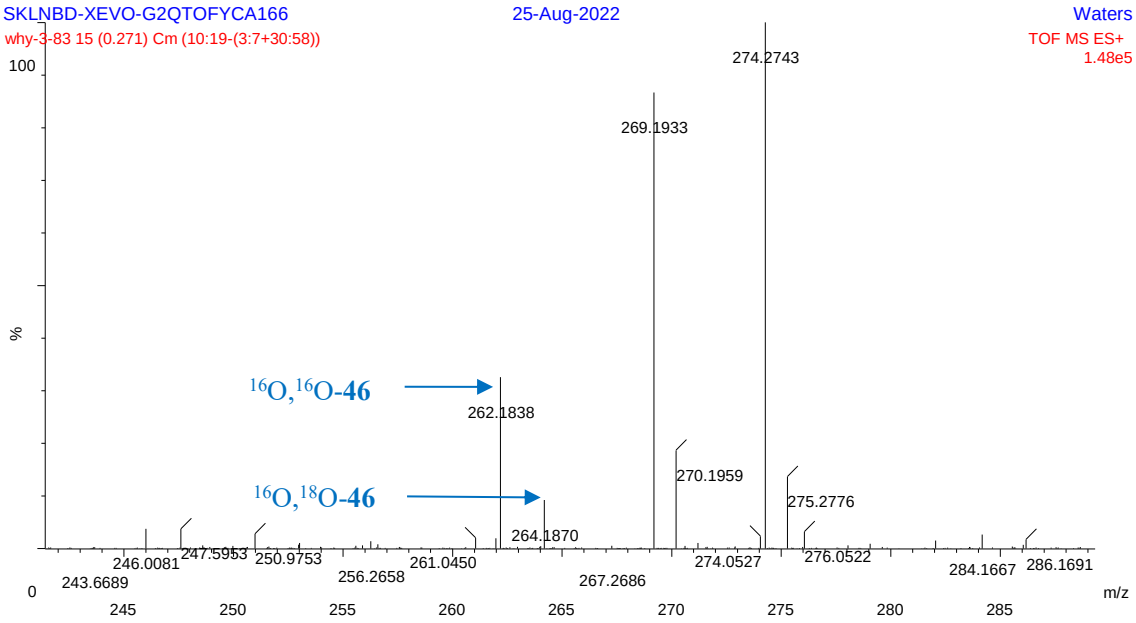
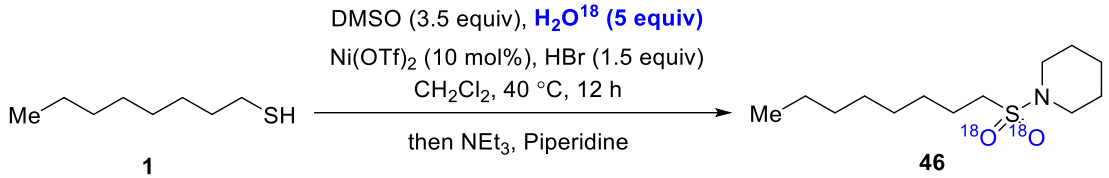


Figure S1. Analysis of 46 by HRMS.



To a solution of $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), **H_2O^{18}** (2.5 mmol, 45.0 mg) in DCM (2 mL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) was added at room temperature. The mixture was stirred in anhydrous DCM (2 mL) at 40 °C for 12 h under N_2 atmosphere. Then the reaction mixture was added dropwise to the solution of piperidine (1.5 mmol, 127.8 mg) and NEt_3 (4 mmol, 404.8 mg) in anhydrous DCM (1 mL) with ice-salt bath. The mixture was stirred at ambient temperature for 8 h, washed by 1N HCl (4 mL × 2) and brine (4 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to afford **46** (73.0 mg, 55%) as a white solid. The ratio of $^{16}O,^{16}O$-**46** : $^{16}O,^{18}O$-**46** : $^{18}O,^{18}O$-**46** was determined by ESI-HRMS as 10:9:2.

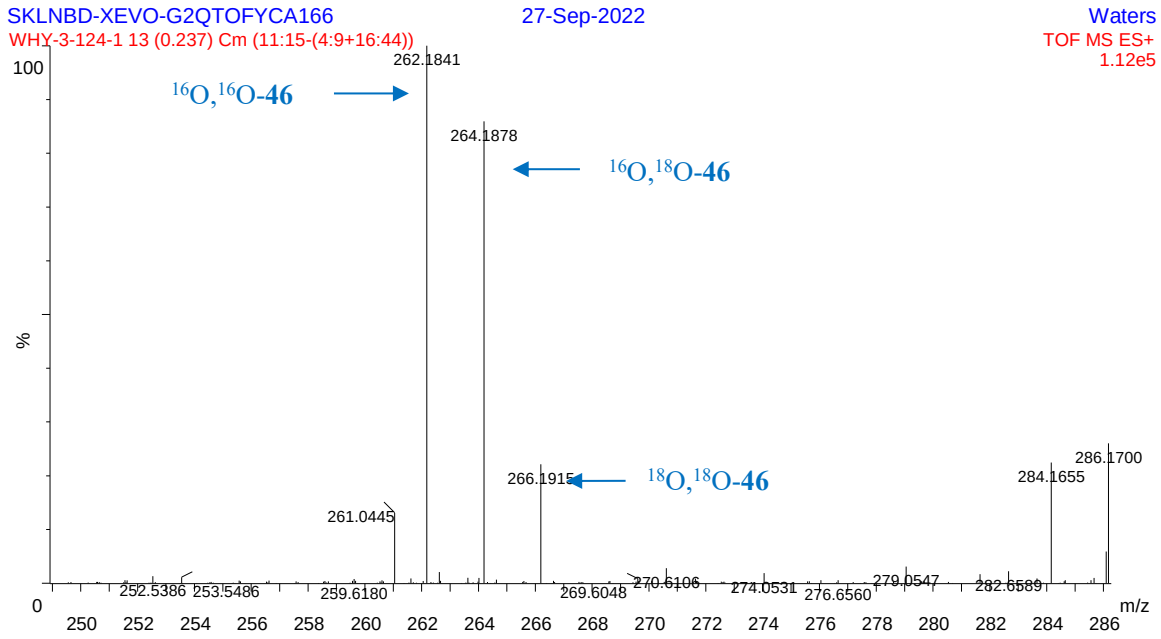
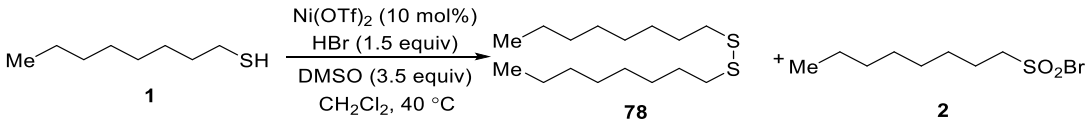


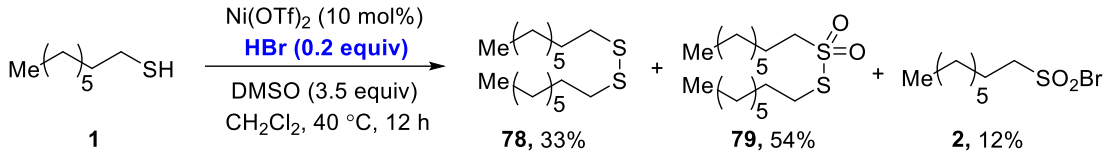
Figure S2. Analysis of 46 by HRMS.

(2) The kinetic experiments

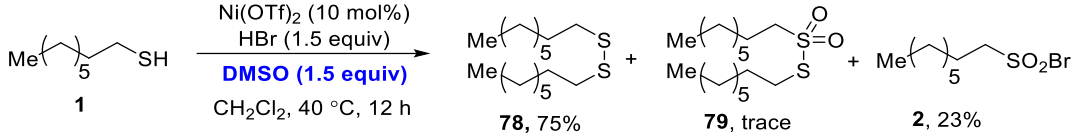


To a solution of $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), octane-1-thiol **1** (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL) in anhydrous DCM (2 mL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) was added at room temperature. The mixture was stirred at 40 °C for desired time. After cooling down to room temperature, the reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the crude product. 1,1,2,2-Tetrachloroethane (33.5 mg) was added into the crude product as internal standard to determine the yield by ^{1}H-NMR. 0.200 Mmol (40%) of **2** and 0.137 mmol (55%) of **77** were detected in 1 h. 0.250 Mmol (50%) of **2** and 0.110 mmol (44%) of **78** were afforded in 2 h. 0.410 Mmol (82%) of **2** and 0.030 mmol (12%) of **78** were afforded in 8 h.

(3) Control experiments

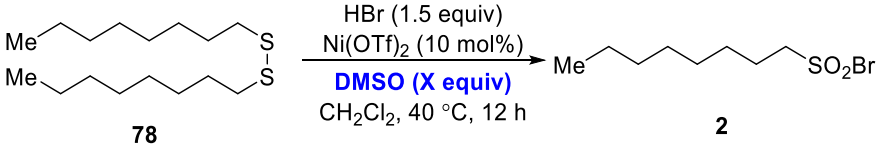


To a solution of $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), octane-1-thiol **1** (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL) in anhydrous DCM (2 mL), HBr (AcOH solution, 33% w/w, 0.01 mmol, 16 μL) was added at room temperature. The mixture was stirred at 40 °C for 12 h. After cooling down to room temperature, the reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the crude product. 1,1,2,2-Tetrachloroethane (33.5 mg) was added into the crude product as internal standard to determine the yield by ^{1}H-NMR. 0.100 Mmol (12%) of **2**, 0.082 mmol (33%) of **78**, and 0.135 mmol (54%) of **79** were detected.

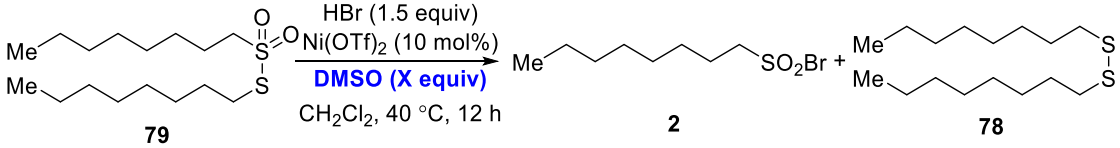


To a solution of $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), octane-1-thiol **1** (0.50 mmol, 73.1 mg), DMSO (0.75 mmol, 52 μL) in anhydrous DCM (2 mL), HBr (AcOH solution, 33% w/w, 0.01 mmol, 16 μL) was added at room temperature. The mixture was stirred at 40 °C for 12 h. After cooling down to room temperature, the reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the crude product. 1,1,2,2-Tetrachloroethane (33.5 mg) was added into the crude product as internal standard to determine the yield by ^{1}H-NMR. 0.115 mmol (23%) of **2** and 0.187 mmol (75%) of **78** were detected.

(4) Intermediate characterization



To a solution of $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), 1,2-dioctyldisulfane **78** (0.25 mmol, 72.6 mg), different equiv. of DMSO in anhydrous DCM (2 mL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) was added at room temperature. The mixture was stirred with at 40 °C for 12 h. After cooling down to room temperature, the reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the crude product. 1,1,2,2-Tetrachloroethane (33.5 mg) was added into the crude product as internal standard to determine the yield by ^{1}H-NMR. Only 0.250 mmol (100%) of **78** was detected without DMSO. 0.130 Mmol (26%) of **2** and 0.167 mmol (67%) of **78** were detected with 1 equiv. of DMSO (0.5 mmol, 34 μL). 0.295 Mmol of **2** (59%) and 0.082 mmol (33%) of **78** were detected with 2 equiv. of DMSO (1.0 mmol, 68 μL). 0.340 Mmol (68%) of **2** and 0.062 mmol (25%) of **78** were detected with 3 equiv. of DMSO (1.5 mmol, 103 μL).

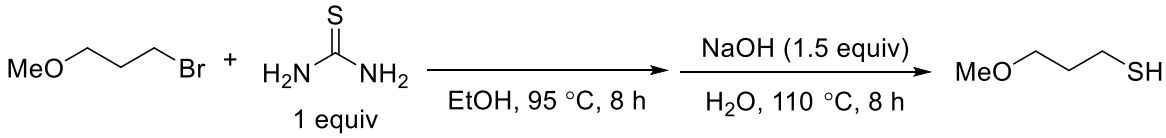


To a solution of $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), *S*-octyl octane-1-sulfonothioate **79** (0.25 mmol, 80.65 mg), different equiv. of DMSO in anhydrous DCM (2 mL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) was added at room temperature. The mixture was stirred with at 40 °C for 12 h. After cooling down to room temperature, the reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the crude product. 1,1,2,2-Tetrachloroethane (33.5 mg) was added into the crude product as internal standard to determine the yield by ^{1}H-NMR. 0.155 Mmol (31%) of **2** and 0.115 mmol (46%) of **78** were detected without DMSO. 0.295 Mmol (59%) of **2** and 0.067 mmol (27%) of **78** were detected with 1 equiv. of DMSO (0.5 mmol, 34 μL). 0.375 Mmol of **2** (75%) and 0.040 mmol (16%) of **78** were detected with 2 equiv. of DMSO (1.0 mmol, 68 μL), 0.345 mmol (69%) of **2** and 0 mmol (0%) of **78** were detected with 3 equiv. of DMSO (1.5 mmol, 103 μL).

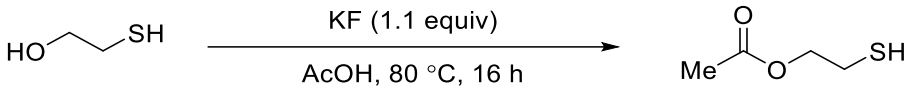
Experimental Section

1) Materials preparation

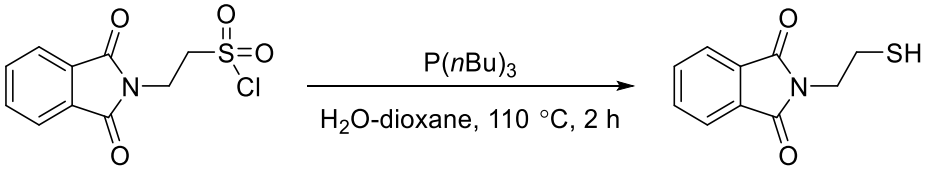
Method A: Substrate for **8** was prepared according to literature[1].



Method B: Substrate for **9** was prepared according to literature[2].



Method C: Substrate for **13** was prepared according to literature[3].



2) General procedure

Typical procedure for the oxidative bromination of primary thiols (1, 3-6, 8-12, 17, 23-24, 26-27, 30-33, 37-38, 41)

$Ni(OTf)_2$ (10 mol%, 17.8 mg, for **1**,**3-12**,**17**), thiol substrate (0.5 mmol), DMSO (3.5 equiv, 120 μL) and anhydrous DCM (2 mL) were added into a reaction tube with a magnetic stir bar at room temperature, then HBr (AcOH solution, 33% w/w, 1.5 equiv, 120 μL) was added. The reaction mixture was stirred at 40 ºC under N_2 atmosphere until the full consumption of substrate monitored by TLC. The reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the product. Some products (**26-27**,**38**) were purified by chromatography on silica gel.

Typical procedure for the oxidative bromination of secondary thiols (14-16)

$Ni(OTf)_2$ (10 mol%, 17.8 mg), thiol substrate (0.5 mmol), DMSO (6.4 equiv, 220 μL) and anhydrous DCM (2 mL) were added into a reaction tube with a magnetic stir bar at room temperature, then HBr (AcOH solution, 33% w/w, 2.5 equiv, 200 μL) was added.

The reaction mixture was stirred at 40 ºC under N_2 atmosphere until the full consumption of substrate monitored by TLC. The reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the product.

Typical procedure for the oxidative bromination of aromatic thiols (7, 18-22, 25, 28-29, 34-36)

$Ni(OTf)_2$ (10 mol%, 17.8 mg, for **18-21, 28, 34-35**), thiol substrate (0.5 mmol), DMSO (3.5 equiv, 120 μL) and anhydrous DCM (2 mL) were added into a reaction tube with a magnetic stir bar at room temperature, then HBr (AcOH solution, 33% w/w, 1.5 equiv, 120 μL) was added. The reaction mixture was stirred under 40 ºC under N_2 atmosphere for 12 h. DMSO (1.2 equiv, 40 μL) and HBr (AcOH solution, 33% w/w, 0.5 equiv, 40 μL) were added next, the mixture was stired until the full consumption of substrate monitored by TLC. The reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the product.

Typical procedure for the oxidative bromination of thiols with HBr sensitive groups (13, 39-40)

$Ni(OTf)_2$ (10 mol%, 17.8 mg, for **13**), thiol substrate (0.5 mmol), DMSO (3.5 equiv, 120 μL) and EA (2 mL) were added into a reaction tube with a magnetic stir bar at room temperature, then HBr (Aqueous, 48% w/w, 1.5 equiv, 84 μL) was added. The reaction mixture was stirred under 40 ºC until the full consumption of substrate monitored by TLC. The reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the product.

Typical procedure for the one-pot synthesis of sulfonyl derivatives

$Ni(OTf)_2$ (10 mol%, 17.8 mg), thiol substrate (0.5 mmol), DMSO (3.5 equiv, 120 μL) and anhydrous DCM (2 mL) were added into a reaction tube with a magnetic stir bar at room temperature, then HBr (AcOH solution, 33% w/w, 1.5 equiv, 120 μL) was added.

The reaction mixture was stirred at 40 ºC under N_2 atmosphere until the full consumption of substrate monitored by TLC.

For sulfonamide: The reaction mixture was added dropwise to a solution of amine (3 equiv) and NEt_3 (4 mmol, 404 mg) in DCM (1 mL) with ice-salt bath under N_2 atmosphere, then stirred at ambient temperature for 8 h. The resulting solution was washed by 1N HCl (4 mL × 2) and brine (4 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was purified by chromatography on a silica gel (petroleum ether/ethyl acetate) to afford the corresponding sulfonamides.

For sulfonate: The reaction mixture was added dropwise to a solution of alcohol (3 equiv) and NEt_3 (4 mmol, 404 mg) in DCM (1 mL) with ice-salt bath, then stirred at ambient temperature for 8 h. The resulting solution was washed by water (4 mL × 2) and brine (4 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was purified by chromatography on a silica gel (petroleum ether/ethyl acetate) to afford the corresponding sulfonamides.

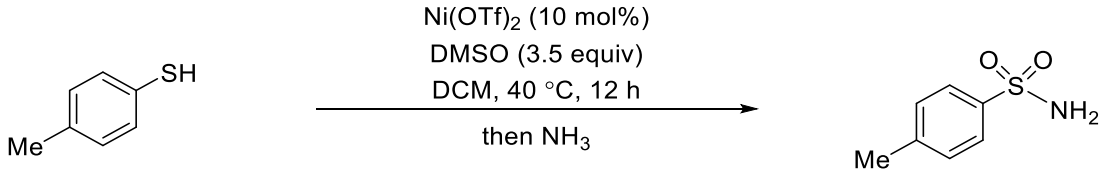
For sulfonyl fluoride: The reaction mixture was added dropwise to a solution of tetrabutylammonium fluoride (TBAF) (5 equiv, 653.7 mg) and NEt_3 (3.5 mmol, 353.5 mg) in DCM (1 mL) with ice-salt bath, then stirred at ambient temperature for 8 h. The resulting solution was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was dried over Na_2SO_4 and evaporated in vacuo to afford the corresponding sulfonyl fluoride.

For sulfonyl azide: The reaction mixture was added dropwise to a solution of $TMSN_3$ (3 equiv, 172.8 mg) and NEt_3 (4 mmol, 404 mg) in DCM (1 mL) with ice-salt bath, then stirred at ambient temperature for 8 h. The resulting solution was washed by water (4 mL × 2) and brine (4 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was purified by chromatography on a silica gel (petroleum ether/ethyl acetate) to afford the corresponding sulfonyl azide.

Typical procedure for the gram-scale synthesis of 18

$Ni(OTf)_2$ (10 mol%, 356.8 mg), 4-methylbenzenethiol (10 mmol), DMSO (3.5 equiv, 2.4 mL) and anhydrous DCM (40 mL) were added into a round-bottom flask with a magnetic stir bar at room temperature, then HBr (AcOH solution, 33% w/w, 1.5 equiv, 2.4 mL) was added. The flask was equipped with a condenser, then the reaction mixture was stirred under 40 ºC for 12 h. DMSO (1.2 equiv, 0.8 mL) and HBr (AcOH solution, 33% w/w, 0.5 equiv, 0.8 mL) were added next, the mixture was stired until the full consumption of substrate monitored by TLC. The reaction mixture was diluted with water (20 mL) and extracted with DCM (20 mL × 2). The combined organic extracts were washed with a saturated solution of NaCl (20 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was filtrated over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1), and the filtrate was evaporated in vacuo to afford the product (1.69 g, 72%).

Procedure for one-pot synthesis of pharmaceutical intermediate 77



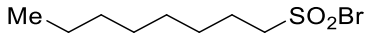
77, 71%

$Ni(OTf)_2$ (10 mol%, 16.84 mg), 4-methylbenzenethiol (0.5 mmol), DMSO (3.5 equiv, 120 μL) and anhydrous DCM (2 mL) were added into a reaction tube with a magnetic stir bar at room temperature, then HBr (AcOH solution, 33% w/w, 1.5 equiv, 120 μL) was added. The reaction mixture was stirred under 40 ºC under N_2 atmosphere for 12 h. DMSO (1.2 equiv, 40 μL) and HBr (AcOH solution, 33% w/w, 0.5 equiv, 40 μL) were added next, the mixture was stired until the full consumption of substrate monitored by TLC. The reaction mixture was filtered over a short pad of silica gel by a mixture of hexane and ethyl acetate (10:1). The filtrate was evaporated in vacuo. The residue and NEt_3 (1.2 equiv, 60.7 mg) was dissolved in DCM (2 mL), then NH_3 was bubbled into the solution in ice-salt bath for 1 h. The resulting solution was washed by water (2 mL × 2) and brine (2 mL), dried over Na_2SO_4, and evaporated in vacuo.

The residue was purified by chromatography on a silica gel (petroleum ether/ethyl acetate = 4:1) to afford the product (60.8 mg, 71%).

Analytical Data for Products

octane-1-sulfonyl bromide (2)[4] **:**



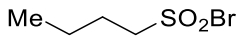
2

The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 110.6 mg (86%) of **2** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.73 (t, *J* = 7.6 Hz, 2H), 2.05 – 1.96 (m, 2H), 1.53 – 1.44 (m, 2H), 1.38 – 1.24 (m, 8H), 0.88 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 69.7, 31.6, 28.86, 28.82, 27.2, 24.6, 22.5, 14.0.

butane-1-sulfonyl bromide (3)[5] **:**



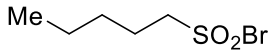
3

The reaction of butane-1-thiol (0.50 mmol, 45.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 81.4 mg (81%) of **3** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.74 (t, *J* = 8.0 Hz, 2H), 2.05 – 1.96 (m, 2H), 1.60 – 1.49 (m, 2H), 1.01 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 69.3, 26.5, 20.6, 13.4.

pentane-1-sulfonyl bromide (4) :



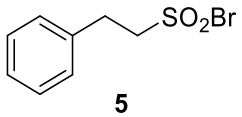
4

The reaction of pentane-1-thiol (0.50 mmol, 52.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 83.9 mg (78%) of **4** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.73 (t, *J* = 7.6 Hz, 2H), 2.06 – 1.97 (m, 2H), 1.52 – 1.34 (m, 4H), 0.94 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 69.6, 29.2, 24.2, 21.9, 13.5.

2-phenylethane-1-sulfonyl bromide (5) :



5

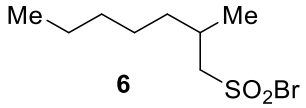
The reaction of 2-phenylethane-1-thiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 99.6 mg (80%) of **4** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (t, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 6.9 Hz, 1H), 7.28 (d, *J* = 7.4 Hz, 2H), 4.04 – 3.97 (m, 2H), 3.38 – 3.32 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 135.2, 129.0, 128.5, 127.5, 70.1, 30.6.

HRMS m/z (EI) calcd for C_8H_9Br $[M\text{-}SO_2]^+$ 183.9888, found: 183.9881.

2-ethylhexane-1-sulfonyl bromide (6) :



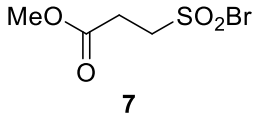
6

The reaction of 2-ethylhexane-1-thiol (0.50 mmol, 73.2 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 90.1 mg (78%) of **4** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.78 (d, *J* = 6.0 Hz, 2H), 2.21 – 2.13 (m, 1H), 1.63 – 1.55 (m, 2H), 1.55 – 1.47 (m, 2H), 1.34 – 1.28 (m, 4H), 0.98 – 0.85 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 74.3, 36.6, 31.7, 28.0, 25.1, 22.5, 13.9, 10.1.

methyl 3-(bromosulfonyl)propanoate (7) :



7

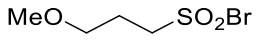
The reaction of methyl 3-mercaptopropanoate (0.50 mmol, 60.1 mg), DMSO (2.3 mmol, 160 μL), HBr (AcOH solution, 33% w/w, 1 mmol, 160 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL)

and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 66.9 mg (58%) of **7** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.06 (t, *J* = 7.6 Hz, 2H), 3.76 (s, 3H), 3.01 (t, *J* = 7.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.8, 63.9, 52.7, 29.1.

3-methoxypropane-1-sulfonyl bromide (8):



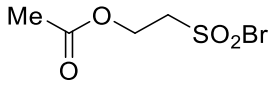
8

The reaction of 3-methoxypropane-1-thiol (0.50 mmol, 53.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 94.4 mg (87%) of **8** as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.86 (t, *J* = 7.6 Hz, 2H), 3.54 (t, *J* = 5.7 Hz, 2H), 3.35 (s, 3H), 2.30 – 2.21 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 68.6, 66.8, 58.7, 25.1.

2-(bromosulfonyl)ethyl acetate (9) :



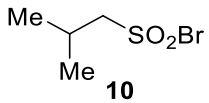
9

The reaction of 2-mercaptoethyl acetate (0.50 mmol, 60.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 6 h afforded 72.7 mg (63%) of **9** as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.58 (t, *J* = 5.8 Hz, 2H), 4.09 (t, *J* = 5.8 Hz, 2H), 2.11 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 170.2, 67.2, 57.5, 20.5.

2-methylpropane-1-sulfonyl bromide (10)[6] :



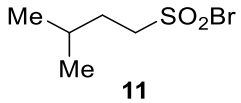
10

The reaction of 2-methylpropane-1-thiol (0.50 mmol, 45.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 59.3 mg (76%) of **10** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.76 (d, *J* = 6.4 Hz, 2H), 2.58 – 2.46 (m, 1H), 1.19 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 77.9, 26.4, 21.8.

3-methylbutane-1-sulfonyl bromide (11) :



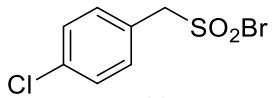
11

The reaction of 3-methylbutane-1-thiol (0.50 mmol, 52.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 57.1 mg (70%) of **11** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.78 – 3.70 (m, 2H), 1.95 – 1.86 (m, 2H), 1.85 – 1.73 (m, 1H), 0.99 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 68.2, 32.8, 26.6, 22.0.

(4-chlorophenyl)methanesulfonyl bromide (12)[7] :



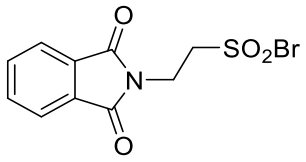
12

The reaction of (4-chlorophenyl)methanethiol (0.50 mmol, 79.0 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 56.6 mg (42%) of **12** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 (s, 4H), 4.91 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 136.8, 132.8, 129.5, 124.9, 73.9.

2-(1,3-dioxoisoindolin-2-yl)ethane-1-sulfonyl bromide (13) :



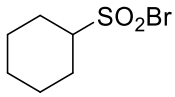
13

The reaction of 2-(2-mercaptoethyl)isoindoline-1,3-dione (0.50 mmol, 103.6 mg), DMSO (1.75 mmol, 120 μL), HBr (Aqueous, 48% w/w, 0.75 mmol, 84 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 119.3 mg (75%) of **13** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.76 (dd, *J* = 5.5, 3.1 Hz, 2H), 4.32 (t, *J* = 6.5 Hz, 2H), 4.15 (t, *J* = 6.5 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 167.3, 134.5, 131.6, 123.7, 65.0, 32.9.

cyclohexanesulfonyl bromide (14)[4] :



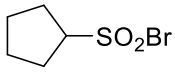
14

The reaction of cyclohexanethiol (0.50 mmol, 83.1 mg), DMSO (3.2 mmol, 220 μL), HBr (AcOH solution, 33% w/w, 1.25 mmol, 200 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 93.1 mg (82%) of **14** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.49 (tt, *J* = 11.9, 3.5 Hz, 1H), 2.49 – 2.34 (m, 2H), 2.02 – 1.95 (m, 2H), 1.77 – 1.67 (m, 3H), 1.46 – 1.22 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 78.8, 27.5, 24.9, 24.8.

cyclopentanesulfonyl bromide (15) :



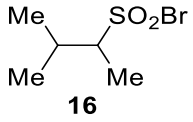
15

The reaction of cyclopentanethiol (0.50 mmol, 61.1 mg), DMSO (3.2 mmol, 220 μL), HBr (AcOH solution, 33% w/w, 1.25 mmol, 200 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 66.2 mg (77%) of **15** as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.14 (ddd, *J* = 15.0, 8.7, 6.4 Hz, 1H), 2.28 – 2.11 (m, 4H), 1.98 – 1.86 (m, 2H), 1.81 – 1.68 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 79.3, 29.2, 25.6.

3-methylbutane-2-sulfonyl bromide (16) :



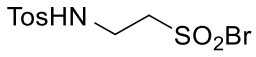
16

The reaction of 3-methylbutane-2-thiol (0.50 mmol, 52.1 mg), DMSO (3.2 mmol, 220 μL), HBr (AcOH solution, 33% w/w, 1.25 mmol, 200 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 68.8 mg (64%) of **16** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.77 – 3.69 (m, 1H), 2.77 – 2.63 (m, 1H), 1.52 (d, J = 7.0 Hz, 3H), 1.09 (dd, J = 6.9, 3.6 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 82.7, 29.1, 21.2, 17.1, 10.4.

2-((4-methylphenyl)sulfonamido)ethane-1-sulfonyl bromide (17) :



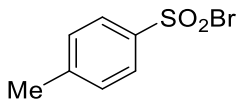
17

The reaction of *N*-(2-mercaptoethyl)-4-methylbenzenesulfonamide (0.50 mmol, 115.5 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h afforded 90.7 mg (53%) of **17** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.2 Hz, 2H), 7.34 (d, J = 8.1 Hz, 2H), 5.54 (t, J = 6.0 Hz, 1H), 3.96 (t, J = 6.2 Hz, 2H), 3.53 (q, J = 6.1 Hz, 2H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 144.3, 135.9, 130.0, 127.0, 68.2, 38.0, 21.5.

4-methylbenzenesulfonyl bromide (18)[4] :



18

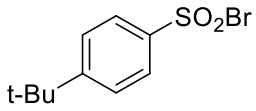
The reaction of 4-methylbenzenethiol (0.50 mmol, 62.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8

mg) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 90.4 mg (80%) of **18** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.3 Hz, 2H), 2.48 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 146.7, 144.5, 130.0, 126.4, 21.7.

4-(tert-butyl)benzenesulfonyl bromide (19)[5] :



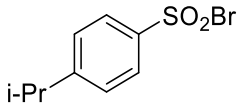
19

The reaction of 4-(tert-butyl)benzenethiol (0.50 mmol, 83.2 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 103.9 mg (75%) of **19** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.8 Hz, 2H), 7.61 (d, *J* = 8.7 Hz, 2H), 1.37 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 159.5, 144.3, 126.5, 126.3, 35.5, 30.9.

4-isopropylbenzenesulfonyl bromide (20)[4] :



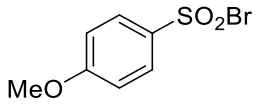
20

The reaction of 4-isopropylbenzenethiol (0.50 mmol, 76.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 86.8 mg (66%) of **20** as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 8.5 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 3.10 – 3. 01 (m, 1H), 1.32 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 157.2, 144.6, 127.6, 126.6, 34.3, 23.4.

4-methoxybenzenesulfonyl bromide (21)[4] :



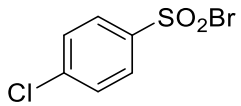
21

The reaction of 4-methoxybenzenethiol (0.50 mmol, 70.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 87.9 mg (70%) of **21** as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, J = 9.0 Hz, 2H), 7.03 (d, J = 9.0 Hz, 2H), 3.92 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 164.7, 139.1, 129.0, 114.5, 55.9.

4-chlorobenzenesulfonyl bromide (22)[4] :



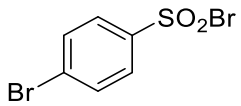
22

The reaction of 4-chlorobenzenethiol (0.50 mmol, 72.3 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40 μL) at 40 °C for 4 h afforded 102.2 mg (80%) of **22** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, J = 8.7 Hz, 2H), 7.59 (d, J = 8.7 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 145.3, 142.0, 129.8, 127.8.

4-bromobenzenesulfonyl bromide (23)[5] :



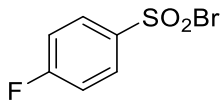
23

The reaction of 4-bromobenzenethiol (0.50 mmol, 94.6 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h afforded 88.5 mg (59%) of **23** as a yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, *J* = 8.8 Hz, 2H), 7.76 (d, *J* = 8.8 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 145.8, 132.9, 130.7, 127.8.

4-fluorobenzenesulfonyl bromide (24)[4] :



24

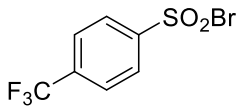
The reaction of 4-fluorobenzenethiol (0.50 mmol, 64.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h afforded 75.3 mg (63%) of **24** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 – 8.00 (m, 2H), 7.34 – 7.25 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 166.2 (d, *J* = 261.5 Hz), 143.0 (d, *J* = 1.8 Hz), 129.5 (d, *J* = 10.1 Hz), 116.9 (d, *J* = 23.2 Hz).

^{19}F NMR (376 MHz, $CDCl_3$): δ -99.56.

4-(trifluoromethyl)benzenesulfonyl bromide (25)[5] :



25

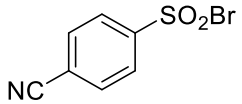
The reaction of 4-(trifluoromethyl)benzenethiol (0.50 mmol, 89.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40 μL) at 40 °C for 4 h afforded 80.9 mg (56%) of **25** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, *J* = 8.6 Hz, 2H), 7.90 (d, *J* = 8.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 149.5, 136.5 (q, *J* = 33.6 Hz), 127.0, 126.8 (q, *J* = 3.6 Hz), 122.6 (q, *J* = 274.4 Hz).

^{19}F NMR (376 MHz, $CDCl_3$): δ -63.35.

4-cyanobenzenesulfonyl bromide (26)[8] **:**



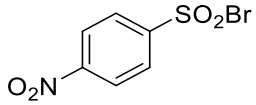
26

The reaction of 4-mercaptobenzonitrile (0.50 mmol, 67.6 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h afforded 22.1 mg (18%) of **26** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 (d, *J* = 8.6 Hz, 2H), 7.93 (d, *J* = 8.5 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 149.6, 133.4, 127.0, 118.7, 116.5.

4-nitrobenzenesulfonyl bromide (27)[5] **:**



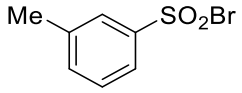
27

The reaction of 4-nitrobenzenethiol (0.50 mmol, 77.6 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h afforded 21.3 mg (16%) of **27** as a pale red solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (d, *J* = 9.1 Hz, 2H), 8.21 (d, *J* = 9.1 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 150.8, 127.9, 124.9.

3-methylbenzenesulfonyl bromide (28)[9] **:**



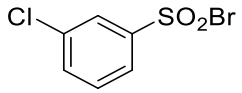
28

The reaction of 3-methylbenzenethiol (0.50 mmol, 62.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 82.3 mg (70%) of **28** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (s, 2H), 7.56 – 7.45 (m, 2H), 2.49 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 147.0, 140.1, 135.9, 129.3, 126.5, 123.5, 21.3.

3-chlorobenzenesulfonyl bromide (29)[9] **:**



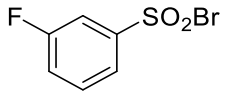
29

The reaction of 3-chlorobenzenethiol (0.50 mmol, 72.3 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 75.4 mg (59%) of **29** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (s, 1H), 7.89 (d, *J* = 8.6 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.57 (t, *J* = 8.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 147.9, 135.5, 135.2, 130.8, 126.4, 124.5.

3-fluorobenzenesulfonyl bromide (30)[10] **:**



30

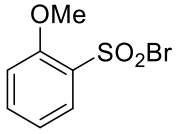
The reaction of 3-fluorobenzenethiol (0.50 mmol, 64.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h afforded 80.1 mg (67%) of **30** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.6 Hz, 1H), 7.70 (dt, *J* = 7.5, 2.0 Hz, 1H), 7.63 (td, *J* = 8.2, 5.2 Hz, 1H), 7.49 – 7.40 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.8 (d, *J* = 255.5 Hz), 148.1 (d, *J* = 7.4 Hz), 131.3 (d, *J* = 8.1 Hz), 122.5 (d, *J* = 21.2 Hz), 122.2 (d, *J* = 3.0 Hz), 113.9 (d, *J* = 113.9 Hz).

^{19}F NMR (376 MHz, $CDCl_3$): δ -107.19.

2-methoxybenzenesulfonyl bromide (31)[8] **:**



31

The reaction of 2-methoxybenzenethiol (0.50 mmol, 70.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h afforded 106.7 mg (85%) of **31** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 9.7 Hz, 1H), 7.71 (t, *J* = 8.7 Hz, 1H), 7.17 – 7.08 (m, 2H), 4.10 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 157.1, 137.1, 134.2, 129.1, 120.0, 113.3, 56.5.

2-fluorobenzenesulfonyl bromide (32)[4] :

32

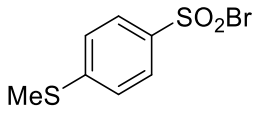
The reaction of 2-fluorobenzenethiol (0.50 mmol, 64.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h afforded 100.4 mg (84%) of **32** as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 – 7.89 (m, 1H), 7.80 – 7.72 (m, 1H), 7.39 – 7.29 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 158.4 (d, *J* = 264.6 Hz), 137.6 (d, *J* = 8.1 Hz), 134.4 (d, *J* = 12.1 Hz), 128.7, 124.5 (d, *J* = 4.0 Hz), 118.2 (d, *J* = 20.2 Hz).

^{19}F NMR (376 MHz, $CDCl_3$): δ -107.13.

4-(methylthio)benzenesulfonyl bromide (33) :



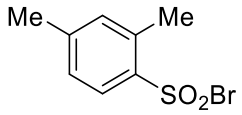
33

The reaction of 4-(methylthio)benzenethiol (0.50 mmol, 78.2 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h afforded 78.8 mg (59%) of **33** as a yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.7 Hz, 2H), 7.34 (d, *J* = 8.7 Hz, 2H), 2.55 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 149.9, 142.6, 126.6, 125.0, 14.6.

2,4-dimethylbenzenesulfonyl bromide (34)[4] :



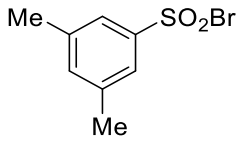
34

The reaction of 2,4-dimethylbenzenethiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 95.9 mg (77%) of **34** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 7.9 Hz, 1H), 7.24 – 7.14 (m, 2H), 2.73 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 146.6, 142.9, 137.4, 134.0, 128.3, 127.1, 21.5, 20.0.

3,5-dimethylbenzenesulfonyl bromide (35)[5] :



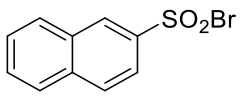
35

The reaction of 3,5-dimethylbenzenethiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 90.0 mg (65%) of **35** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (s, 2H), 7.34 (s, 1H), 2.44 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 146.9, 139.8, 136.8, 123.7, 21.2.

naphthalene-2-sulfonyl bromide (36)[4] :



36

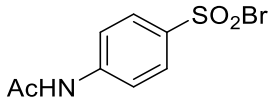
The reaction of 3,5-dimethylbenzenethiol (0.50 mmol, 80.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C

for 12 h, followed by adding DMSO (0.55 mmol, 40 μL) and HBr (AcOH solution, 33% w/w, 0.25 mmol, 40μL) at 40 °C for 4 h afforded 85.4 mg (63%) of **36** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.54 (d, *J* = 1.6 Hz, 1H), 8.08 – 7.92 (m, 4H), 7.79 – 7.64 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 143.8, 135.6, 131.4, 130.3, 130.1, 129.9, 128.3, 128.1, 128.1, 120.9.

4-acetamidobenzenesulfonyl bromide (37) :



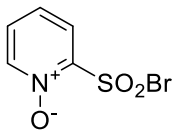
37

The reaction of *N*-(4-mercaptophenyl)acetamide (0.50 mmol, 83.6 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 6 h afforded 34.8 mg (25%) of **37** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 9.0 Hz, 2H), 7.85 – 7.59 (m, 3H), 2.25 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.7, 144.0, 141.6, 128.1, 119.1, 24.8.

2-(bromosulfonyl)pyridine 1-oxide (38) :



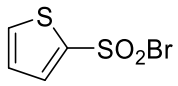
38

The reaction of 2-mercaptopyridine 1-oxide (0.50 mmol, 63.6 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in DCM (2 mL) at 40 °C for 12 h afforded 44.0 mg (37%) of **38** as a white solid.

^{1}H NMR (400 MHz, DMSO-d_6): δ 8.45 (d, *J* = 6.2 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.43 (t, *J* = 6.5 Hz, 1H), 7.23 (t, *J* = 7.7 Hz, 1H).

^{13}C NMR (101 MHz, DMSO-d_6): δ 140.3, 131.9, 131.1, 125.8, 125.7.

thiophene-3-sulfonyl bromide (39)[5] :



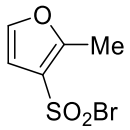
39

The reaction of thiophene-2-thiol (0.50 mmol, 58.1 mg), DMSO (1.75 mmol, 120 μL), HBr (Aqueous, 48% w/w, 0.75 mmol, 84 μL) in DCM (2 mL) at 40 °C for 12 h afforded 60.2 mg (53%) of **39** as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90 – 7.85 (m, 1H), 7.84 – 7.79 (m, 1H), 7.19 – 7.14 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 147.0, 135.3, 134.0, 127.5.

2-methylfuran-3-sulfonyl bromide (40) :



40

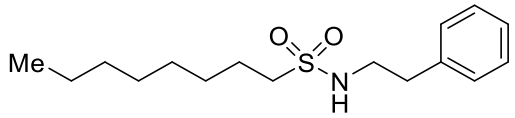
The reaction of 2-methylfuran-3-thiol (0.50 mmol, 57.1 mg), DMSO (1.75 mmol, 120 μL), HBr (Aqueous, 48% w/w, 0.75 mmol, 84 μL) in DCM (2 mL) at 40 °C for 12 h afforded 46.2 mg (41%) of **40** as a brown oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (s, 1H), 6.74 (s, 1H), 2.63 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 157.6, 141.1, 129.6, 108.9, 13.3.

HRMS m/z (EI) calcd for $C_5H_5BrO_3S$ $[M]^+$ 223.9137, found: 223.9135.

***N*-phenethyloctane-1-sulfonamide (41)**[11] **:**



41

The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 2-phenylethan-1-amine (1.5 mmol, 181.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-

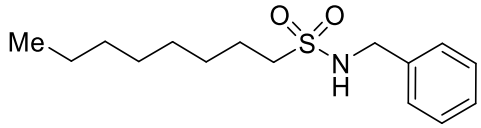
salt bath, then reacted at ambient temperature for 8 h afforded 93.7 mg (63%) of **41** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.27 (m, 2H), 7.27 – 7.19 (m, 3H), 4.55 (t, *J* = 6.1 Hz, 1H), 3.37 (q, *J* = 6.8 Hz, 2H), 2. 90 – 2. 83 (m, 4H), 1. 72 – 1. 62 (m, 2H), 1.26 (s, 10H), 0.89 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 137.9, 128.7, 128.6, 126.7, 52.5, 44.3, 36.5, 31.6, 28.9, 28.8, 28.1, 23.4, 22.5, 13.9.

MS m/z (ESI) calcd for $C_{16}H_{28}NO_2S$ $[M+H]^+$ 298.18, found: 298.18.

***N*-benzyloctane-1-sulfonamide (42) :**



42

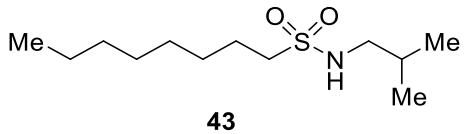
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of phenylmethanamine (1.5 mmol, 160.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 90.7 mg (64%) of **42** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.25 (m, 5H), 5.04 (t, *J* = 6.1 Hz, 1H), 4.26 (d, *J* = 6.2 Hz, 2H), 2.85 (t, *J* = 8.0 Hz, 2H), 1. 74 – 1. 64 (m, 2H), 1.24 (s, 10H), 0.88 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 137.0, 128.6, 127.8, 53.1, 46.9, 31.6, 28.9, 28.8, 28.1, 23.4, 22.5, 13.9.

HRMS m/z (ESI) calcd for $C_{15}H_{26}NO_2S$ $[M+H]^+$ 284.1684, found: 284.1689.

***N*-isobutyloctane-1-sulfonamide (43) :**



43

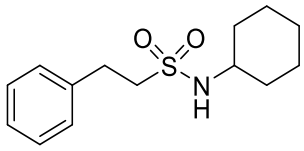
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 2-methylpropan-1-amine (1.5 mmol, 109.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 73.6 mg (59%) of **43** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.37 (s, 1H), 2.99 (t, *J* = 7.6 Hz, 2H), 2.91 (t, *J* = 5.8 Hz, 2H), 1.84 – 1. 74 (m, 3H), 1.45 – 1.35 (m, 2H), 1.34 – 1.21 (m, 8H), 0.94 (d, *J* = 6.7 Hz, 6H), 0.87 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 52.5, 50.6, 31.6, 29.0, 28.95, 28.93, 28.2, 23.6, 22.5, 19.8, 14.0.

HRMS m/z (ESI) calcd for $C_{12}H_{28}NO_2S$ $[M+H]^+$ 250.1841, found: 250.1842.

***N*-cyclohexyl-2-phenylethane-1-sulfonamide (44)[12] :**



44

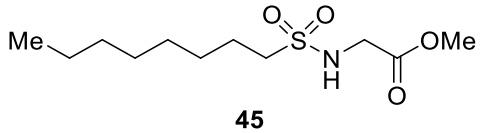
The reaction of 2-phenylethane-1-thiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of cyclohexanamine (1.5 mmol, 148.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 69.5 mg (52%) of **44** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.30 (m, 2H), 7.30 – 7.26 (m, 1H), 7.26 – 7.22 (m, 2H), 4.17 (d, *J* = 7.6 Hz, 1H), 3.37 – 3.23 (m, 3H), 3.20 – 3.10 (m, 2H), 1.97 – 1.93 (m, 2H), 1.78 – 1.60 (m, 2H), 1. 60 – 1.56 (m, 1H), 1. 40 – 1.16 (m, 5H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 138.0, 128.8, 128.4, 126.9, 55.4, 52.8, 34.5, 30.2, 25.1, 24.7.

MS m/z (ESI) calcd for $C_{14}H_{22}NO_2S$ $[M+H]^+$ 268.14, found: 268.14

methyl (octylsulfonyl)glycinate (45) :



45

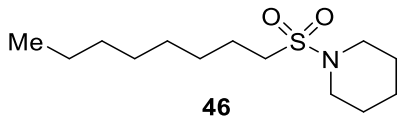
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of methyl glycinate hydrochloride (1.5 mmol, 188.3 mg) and NEt_3 (5.5 mmol, 556.1 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 66.3 mg (50%) of **45** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.91 (t, *J* = 5.5 Hz, 1H), 3.94 (d, *J* = 5.7 Hz, 2H), 3.77 (s, 3H), 3.05 (t, *J* = 8.0 Hz, 2H), 1. 88 – 1.76 (m, 2H), 1.47 – 1.36 (m, 2H), 1.35 – 1.22 (m, 8H), 0.87 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 170.2, 53.7, 52.6, 44.1, 31.6, 29.0, 28.9, 28.2, 23.5, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{11}H_{24}NO_4S$ $[M+H]^+$ 266.1426, found: 266.1430.

1-(octylsulfonyl)piperidine (46) :



46

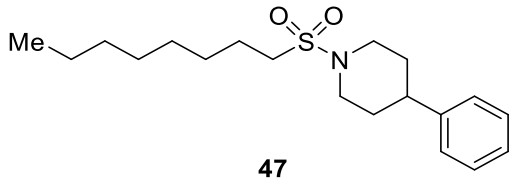
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of piperidine (1.5 mmol, 127.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 81.0 mg (62%) of **46** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.26 – 3.18 (m, 4H), 2.86 (t, *J* = 8.0 Hz, 2H), 1. 84 – 1.75 (m, 2H), 1.64 (s, 4H), 1.56 (s, 2H), 1.44 – 1.35 (m, 2H), 1.33 – 1.22 (m, 8H), 0.90 – 0.84 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 49.1, 46.6, 31.7, 29.0, 28.9, 28.5, 25.7, 23.8, 23.0, 22.6, 14.0.

HRMS m/z (ESI) calcd for $C_{13}H_{28}NO_2S$ $[M+H]^+$ 262.1841, found: 262.1844.

1-(octylsulfonyl)-4-phenylpiperidine (47) :



47

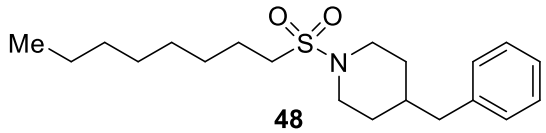
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 4-phenylpiperidine (1.5 mmol, 241.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 148.4 mg (71%) of **47** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.30 (m, 2H), 7. 25 – 7.19 (m, 3H), 3.94 (d, *J* = 12.1 Hz, 2H), 2.98 – 2.82 (m, 4H), 2.62 (t, *J* = 12.1 Hz, 1H), 1.95 – 1.92 (m, 2H), 1.89 – 1.74 (m, 4H), 1. 47 – 1.39 (m, 2H), 1.36 – 1.25 (m, 8H), 0.92 – 0.85 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 144.9, 128.6, 126.7, 126.6, 49.4, 46.5, 42.1, 33.1, 31.7, 29.1, 29.0, 28.5, 23.1, 22.6, 14.1.

HRMS m/z (ESI) calcd for $C_{19}H_{32}NO_2S$ $[M+H]^+$ 338.2154, found: 338.2156.

4-benzyl-1-(octylsulfonyl)piperidine (48) :



48

The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 4-benzylpiperidine (1.5 mmol, 262.9 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 131.7 mg (60%) of **48** as a white solid.

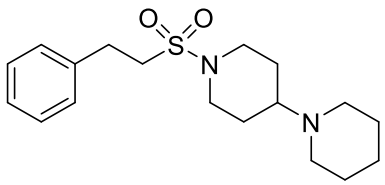
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28 (t, *J* = 7.4 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.13 (d, *J* = 7.5 Hz, 2H), 3.77 (d, *J* = 12.1 Hz, 2H), 2.89 – 2.82 (m, 2H), 2.68 (t, *J* = 11.6 Hz,

2H), 2.56 (d, *J* = 7.0 Hz, 2H), 1.81 – 1.69 (m, 4H), 1.65 (s, 1H), 1.38 (d, *J* = 7.8 Hz, 2H), 1.27 (s, 10H), 0.88 (t, *J* = 6.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 139.7, 129.0, 128.2, 126.0, 49.2, 46.0, 42.7, 37.6, 31.8, 31.6, 29.0, 28.9, 28.4, 23.0, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{20}H_{34}NO_2S$ $[M+H]^+$ 352.2310, found: 352.2307.

1'-(phenethylsulfonyl)-1,4'-bipiperidine (49) :



49

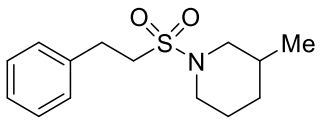
The reaction of 2-phenylethane-1-thiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 1,4'-bipiperidine (1.5 mmol, 252.5 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 94.2 mg (56%) of **49** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.30 (m, 2H), 7.26 – 7.18 (m, 3H), 3.86 (d, *J* = 12.2 Hz, 2H), 3.20 – 3.05 (m, 4H), 2.74 (t, *J* = 11.6 Hz, 2H), 2.55 – 2.44 (m, 4H), 2.34 (t, *J* = 11.4 Hz, 1H), 1.87 (d, *J* = 12.5 Hz, 2H), 1.65 – 1.54 (m, 6H), 1.48 – 1.39 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 138.1, 128.8, 128.3, 126.8, 61.9, 50.9, 50.1, 45.7, 29.3, 27.8, 26.3, 24.6.

HRMS m/z (ESI) calcd for $C_{18}H_{29}N_2O_2S$ $[M+H]^+$ 337.1950, found: 337.1953.

3-methyl-1-(phenethylsulfonyl)piperidine (50) :



50

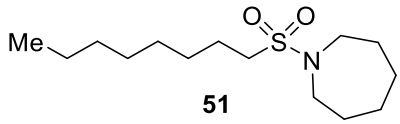
The reaction of 2-phenylethane-1-thiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 3-methylpiperidine (1.5 mmol, 148.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 82.9 mg (62%) of **50** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7. 34 – 7.28 (m, 2H), 7.29 – 7.21 (m, 3H), 3.72 (t, *J* = 13.2 Hz, 2H), 3.15 (s, 4H), 2.73 – 2.53 (m, 1H), 2.35 (t, *J* = 10.4Hz, 1H), 1.87 – 1.54 (m, 4H), 1.04 – 0.95 (m, 1H), 0.93 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 138.2, 128.8, 128.3, 126.8, 52.8, 50.7, 46.1, 32.3, 31.0, 29.3, 25.1, 18.8.

HRMS m/z (ESI) calcd for $C_{14}H_{22}NO_2S$ $[M+H]^+$ 268.1371, found: 268.1372.

1-(octylsulfonyl)azepane (51) :



51

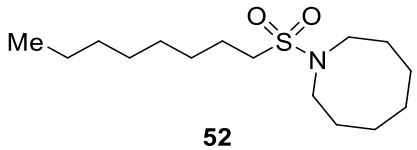
The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of hexamethyleneimine (1.5 mmol, 148.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted for another 8 h to afford 95.6 mg (69%) of **51** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.33 (t, *J* = 6.0 Hz, 4H), 2.97 – 2.84 (m, 2H), 1.80 – 1.70 (m, 6H), 1.66 – 1.58 (m, 4H), 1.40 – 1.35 (m, 2H), 1.26 (s, 8H), 0.86 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 50.7, 48.2, 31.6, 29.6, 29.0, 28.9, 28.4, 26.8, 23.3, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{14}H_{30}NO_2S$ $[M+H]^+$ 276.1997, found: 276.1996.

1-(octylsulfonyl)azocane (52) :



52

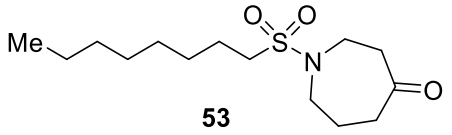
The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of azocane (1.5 mmol, 169.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted for another 8 h to afford 85.0 mg (59%) of **52** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.26 (t, *J* = 5.8 Hz, 4H), 2.98 – 2.83 (m, 2H), 1.82 – 1.67 (m, 6H), 1.64 (s, 6H), 1.42 – 1.34 (m, 2H), 1.33 – 1.19 (m, 8H), 0.87 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 49.4, 48.9, 31.6, 29.0, 28.9, 28.5, 28.0, 26.7, 24.8, 23.2, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{15}H_{32}NO_2S$ $[M+H]^+$ 290.2154, found: 290.2154.

1-(octylsulfonyl)azepan-4-one (53) :



53

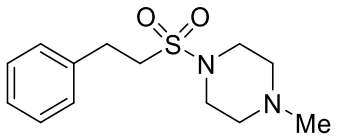
The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of 4-perhydroazepinone hydrochloride (1.5 mmol, 224.4 mg) and NEt_3 (4.5 mmol, 455.4 mg) in ice-salt bath, then reacted for another 8 h to afford 81.4 mg (56%) of **53** as a white oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.59 – 3.45 (m, 4H), 2.99 – 2.86 (m, 2H), 2.76 – 2.59 (m, 4H), 1.95 – 1.85 (m, 2H), 1.81 – 1.70 (m, 2H), 1.44 – 1.35 (m, 2H), 1.27 (s, 8H), 0.91 – 0.84 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 210.5, 51.6, 50.7, 45.5, 44.4, 42.5, 31.6, 29.0, 28.9, 28.3, 25.7, 23.3, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{14}H_{31}N_2O_3S$ $[M+NH_4]^+$ 307.2050, found *m/z*: 307.2055.

1-methyl-4-(phenethylsulfonyl)piperazine (54) :



54

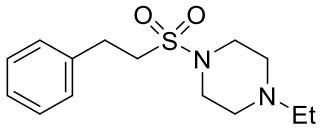
The reaction of 2-phenylethane-1-thiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 1-methylpiperazine (1.5 mmol, 150.3 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 92.6 mg (69%) of **54** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.30 (m, 2H), 7.26 (s, 1H), 7. 23 – 7.18 (m, 2H), 3.40 – 3.26 (m, 4H), 3.21 – 3.08 (m, 4H), 2.57 – 2.43 (m, 4H), 2.32 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 137.8, 128.7, 128.1, 126.7, 54.3, 50.5, 45.7, 45.4, 29.1.

HRMS m/z (ESI) calcd for $C_{13}H_{21}N_2O_2S$ $[M+H]^+$ 269.1324, found: 269.1328.

1-ethyl-4-(phenethylsulfonyl)piperazine (55) :



55

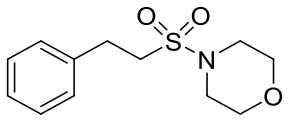
The reaction of 2-phenylethane-1-thiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 1-ethylpiperazine (1.5 mmol, 171.3 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 115.4 mg (68%) of **55** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7. 36 – 7.29 (m, 2H), 7.28 – 7.24 (m, 1H), 7. 23 – 7.18 (m, 2H), 3.33 (t, *J* = 4.3 Hz, 4H), 3. 23 – 3.08 (m, 4H), 2.52 (t, *J* = 4.3 Hz, 4H), 2.46 (q, *J* = 7.2 Hz, 2H), 1.09 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 137.9, 128.7, 128.1, 126.7, 52.1, 51.8, 50.3, 45.5, 29.1, 11.7.

HRMS m/z (ESI) calcd for $C_{14}H_{23}N_2O_2S$ $[M+H]^+$ 283.1480, found: 283.1480.

4-(phenethylsulfonyl)morpholine (56)[13] **:**



56

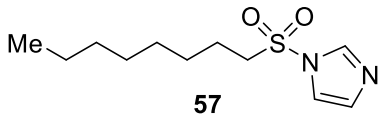
The reaction of 2-phenylethane-1-thiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of morpholine (1.5 mmol, 130.6 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 84.2 mg (66%) of **56** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.30 (m, 2H), 7.29 – 7.25 (m, 1H), 7.25 – 7.20 (m, 2H), 3.72 (t, *J* = 4.4 Hz, 4H), 3.24 (t, *J* = 4.4 Hz, 4H), 3.20 – 3.05 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 137.8, 128.8, 128.3, 126.9, 66.5, 50.2, 45.7, 29.1.

MS m/z (ESI) calcd for $C_{12}H_{18}NO_3S$ $[M+H]^+$ 256.10, found: 256.10.

1-(octylsulfonyl)-1*H*-imidazole (57) :



57

The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of 1*H*-

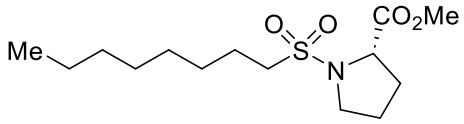
imidazole (1.5 mmol, 102.1 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted for another 8 h to afford 57.7 mg (47%) of **57** as an orange oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (s, 1H), 7.30 (s, 1H), 7.18 (s, 1H), 3.33 – 3.27 (m, 2H), 1.74 – 1.68 (m, 2H), 1.40 – 1.33 (m, 2H), 1.29 – 1.21 (m, 8H), 0.87 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 136.9, 131.3, 117.6, 56.0, 31.5, 28.7, 27.7, 23.1, 22.4, 13.9.

HRMS m/z (ESI) calcd for $C_{11}H_{21}N_2O_2S$ $[M+H]^+$ 245.1324, found: 245.1328.

methyl (octylsulfonyl)-*L*-prolinate (58) :



58

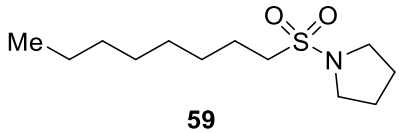
The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of methyl *L*-prolinate hydrochloride (1.5 mmol, 248.4 mg) and NEt_3 (4.5 mmol, 455.4 mg) in ice-salt bath, then reacted for another 8 h to afford 81.7 mg (53%) of **58** as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.50 (dd, *J* = 8.5, 3.8 Hz, 1H), 3.72 (s, 3H), 3.57 (q, *J* = 7.1 Hz, 1H), 3.45 – 3.38 (m, 1H), 3.08 (t, *J* = 7.1 Hz, 2H), 2.30 – 2.21 (m, 1H), 2.07 – 2.01 (m, 1H), 2.00 – 1.94 (m, 2H), 1.85 – 1.77 (m, 2H), 1.42 – 1.35 (m, 2H), 1.31 – 1.21 (m, 8H), 0.89 – 0.82 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 172.9, 60.2, 52.8, 52.2, 48.2, 31.6, 30.8, 29.0, 28.8, 28.3, 25.0, 23.0, 22.5, 13.9.

HRMS m/z (ESI) calc'd for $C_{14}H_{28}NO_4S$ $[M+H]^+$ 306.1739, found: 306.1743.

1-(octylsulfonyl)pyrrolidine (59) :



59

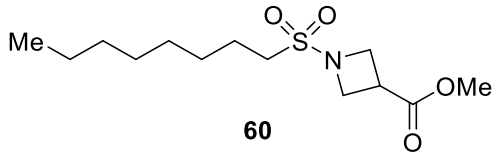
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of pyrrolidine (1.5 mmol, 106.6 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 73.0 mg (59%) of **59** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.35 (t, *J* = 6.7 Hz, 4H), 2.94 (t, *J* = 8.0 Hz, 2H), 2.00 – 1.86 (m, 4H), 1.86 – 1.74 (m, 2H), 1.43 – 1.37 (m, 2H), 1.35 – 1.22 (m, 8H), 0.87 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 49.5, 47.6, 31.7, 29.0, 28.9, 28.4, 25.8, 23.2, 22.5, 14.0.

HRMS m/z (ESI) calc'd for $C_{12}H_{26}NO_2S$ $[M+H]^+$ 248.1684, found: 248.1687.

methyl 1-(octylsulfonyl)azetidine-3-carboxylate (60) :



60

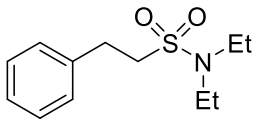
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of methyl azetidine-3-carboxylate hydrochloride (1.5 mmol, 227.4 mg) and NEt_3 (5.5 mmol, 556.1 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 93.3 mg (64%) of **60** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.11 (d, *J* = 8.5 Hz, 4H), 3.76 (s, 3H), 3. 44 – 3.35 (m, 1H), 2.93 (t, *J* = 8.0 Hz, 2H), 1. 82 – 1.74 (m, 2H), 1.46 – 1.34 (m, 2H), 1.34 – 1.22 (m, 8H), 0.87 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 172.0, 52.4, 52.0, 51.0, 31.6, 31.4, 28.97, 28.90, 28.3, 23.0, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{13}H_{26}NO_4S$ $[M+H]^+$ 292.1583, found: 292.1588.

***N,N*-diethyl-2-phenylethane-1-sulfonamide (61) :**



61

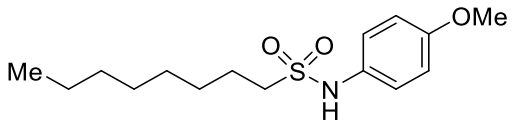
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of diethylamine (5 mmol, 365.5 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 49.5 mg (41%) of **61** as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7. 37 – 7.28 (m, 2H), 7.26 – 7.23 (m, 1H), 7. 23 – 7.18 (m, 2H), 3.31 (q, *J* = 7.1 Hz, 4H), 3.20 – 3.04 (m, 4H), 1.21 (t, *J* = 7.1 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 138.2, 128.7, 128.2, 126.7, 53.7, 41.4, 29.7, 14.4.

HRMS m/z (ESI) calcd for $C_{12}H_{20}NO_2S$ $[M+H]^+$ 242.1215, found: 242.1218.

***N*-(4-methoxyphenyl)octane-1-sulfonamide (62) :**



62

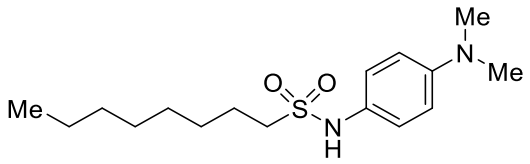
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of methyl 4-methoxyaniline (1.5 mmol, 184.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath under argon atmosphere, then reacted at ambient temperature for 8 h afforded 97.3 mg (65%) of **62** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.19 (d, *J* = 8.9 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 3H), 3.79 (s, 3H), 3.01 (t, *J* = 8.0 Hz, 2H), 1.84 - 1.75 (m, 2H), 1.42 – 1.16 (m, 10H), 0.86 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 157.6, 129.2, 124.1, 114.6, 55.4, 50.9, 31.6, 28.8, 28.1, 23.3, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{15}H_{24}NO_3S$ $[M-H]^-$ 298.1477, found: 298.1478.

***N*-(4-(dimethylamino)phenyl)octane-1-sulfonamide (63) :**



63

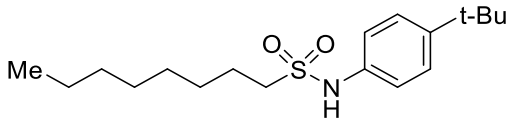
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of *N,N*-dimethylbenzene-1,4-diamine (1.5 mmol, 204.3 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath under argon atmosphere, then reacted at ambient temperature for 8 h afforded 90.6 mg (58%) of **63** as a yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.13 (d, *J* = 8.9 Hz, 2H), 6.67 (d, *J* = 8.9 Hz, 2H), 6.56 (s, 1H), 2.99 (t, *J* = 8.0 Hz, 2H), 2.94 (s, 6H), 1.84 – 1.76 (m, 2H), 1.39 – 1.31 (m, 2H), 1.24 (s, 8H), 0.86 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 149.1, 125.0, 112.9, 50.6, 40.6, 31.6, 28.9, 28.8, 28.1, 23.4, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{16}H_{29}N_2O_2S$ $[M+H]^+$ 313.1950, found: 313.1955.

***N*-(4-(tert-butyl)phenyl)octane-1-sulfonamide (64) :**



64

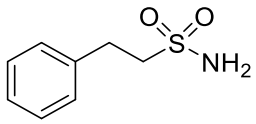
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 4-(tert-butyl)aniline (1.5 mmol, 223.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath under argon atmosphere, then reacted at ambient temperature for 8 h afforded 108 mg (54%) of **64** as a yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 (d, *J* = 7.9 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 6.74 (s, 1H), 3.07 (t, *J* = 8.0 Hz, 2H), 1.85 – 1.77 (m, 2H), 1.36 (s, 2H), 1.30 (s, 9H), 1.23 (s, 8H), 0.86 (t, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 148.2, 134.0, 126.4, 120.6, 51.4, 34.4, 31.6, 31.2, 28.9, 28.1, 23.4, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{18}H_{35}N_2O_2S$ $[M+H]^+$ 343.2419, found: 343.2422.

2-phenylethane-1-sulfonamide (65)[13] **:**



65

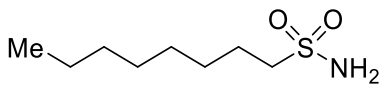
The reaction of 2-phenylethane-1-thiol (0.50 mmol, 69.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of NEt_3 (4 mmol, 404.8 mg) in ice-salt bath under NH_3(g) atmosphere, then reacted at ambient temperature for 8 h afforded 47.2 mg (51%) of **65** as a white solid.

^{1}H NMR (400 MHz, DMSO-d_6): δ 7.41 – 7.14 (m, 5H), 6.87 (s, 2H), 3.30 – 3.21 (m, 2H), 3.05 – 2.95 (m, 2H).

^{13}C NMR (101 MHz, DMSO-d_6): δ 139.1, 128.9, 128.7, 126.8, 55.9, 30.0.

MS m/z (ESI) calcd for $C_8H_{10}NO_2S$ $[M-H]^-$ 184.04, found: 184.04.

octane-1-sulfonamide (66)[14] **:**



66

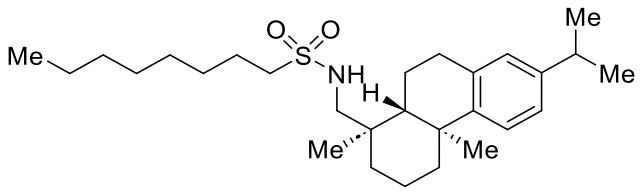
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of NEt_3 (4 mmol, 404.8 mg) in ice-salt bath under NH_3(g) atmosphere, then reacted at ambient temperature for 8 h afforded 59.0 mg (61%) of **66** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.97 (s, 2H), 3.10 (t, *J* = 8.0 Hz, 2H), 1.88 – 1.76 (m, 2H), 1.48 – 1.38 (m, 2H), 1.36 – 1.22 (m, 8H), 0.93 – 0.82 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 55.2, 31.6, 29.0, 28.9, 28.1, 23.8, 22.5, 14.0.

MS m/z (ESI) calcd for $C_8H_{18}NO_2S$ $[M-H]^-$ 192.11, found: 192.11.

***N*-(((1*R*,4a*S*,10a*R*)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-yl)methyl)octane-1-sulfonamide (67) :**



67

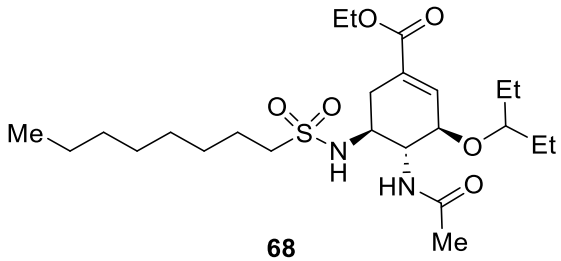
The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of dehydroabietylamine (1.5 mmol, 426.7 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted for another 8 h to afford 87.7 mg (38%) of **67** as a white solid.

^{1}H NMR (400 MHz, **$CDCl_3$**) δ 7.17 (d, *J* = 8.2 Hz, 1H), 7.00 (dd, *J* = 8.1, 2.0 Hz, 1H), 6.89 (d, *J* = 2.0 Hz, 1H), 4.22 (t, *J* = 6.9 Hz, 1H), 3.01 – 2.96 (m, 3H), 2.93 – 2.89 (m, 2H), 2.89 – 2.81 (m, 2H), 2.34 – 2.27 (m, 1H), 1.80 – 1.75 (m, 4H), 1.74 – 1.65 (m, 2H), 1.52 (dd, *J* = 10.9, 3.8 Hz, 1H), 1. 51 – 1.49 (m, 1H), 1.43 – 1.36 (m, 4H), 1.31 – 1.27 (m, 8H), 1.24 (s, 3H), 1.22 (d, *J* = 1.9 Hz, 6H), 0.97 (s, 3H), 0.92 – 0.88 (m, 3H).

^{13}C NMR (101 MHz, **$CDCl_3$**) δ 146.9, 145.6, 134.5, 126.8, 124.1, 123.8, 53.9, 52.5, 44.9, 38.2, 37.3, 37.0, 35.8, 33.4, 31.7, 29.8, 29.0, 28.9, 28.3, 25.2, 24.0, 23.9, 23.6, 22.6, 18.8, 18.5, 18.4, 14.0.

HRMS m/z (ESI) calcd for $C_{28}H_{51}N_2O_2S$ $[M+NH_4]^+$ 479.3671, found: 479.3677.

ethyl (3*R*,4*R*,5*S*)-4-acetamido-5-(octylsulfonamido)-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylate (68) :



68

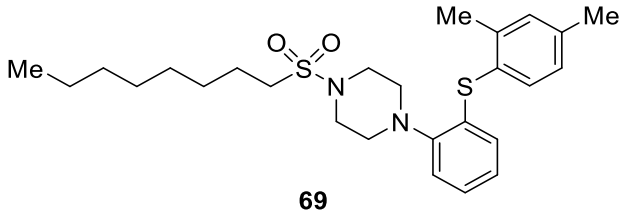
The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, solvent was recovered with reduced pressure, then the residuals were dissolved in THF (1.0 mL), and added dropwise into THF (1 mL) solution of oseltamivir (1.5 mmol, 468.6 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted for another 8 h to afford 87.2 mg (36%) of **68** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.76 (s, 1H), 6.30 (d, *J* = 8.8 Hz, 1H), 5.65 (d, *J* = 8.6 Hz, 1H), 4.19 (q, *J* = 7.1 Hz, 2H), 4.10 (d, *J* = 7.3 Hz, 1H), 3.97 (q, *J* = 8.7 Hz, 1H), 3.69 – 3.59 (m, 1H), 3.38 – 3.33 (m, 1H), 3.04 – 2.93 (m, 2H), 2.76 (dd, *J* = 17.8, 5.1 Hz, 1H), 2.43 (dd, *J* = 17.7, 9.6 Hz, 1H), 2.04 – 1.99 (m, 3H), 1.79 – 1.71 (m, 2H), 1.56 – 1.45 (m, 4H), 1.41 – 1.34 (m, 2H), 1.31 – 1.23 (m, 11H), 0.87 (q, *J* = 7.2 Hz, 9H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 172.0, 165.8, 137.3, 129.0, 82.3, 75.1, 61.0, 54.6, 54.2, 52.4, 32.2, 31.6, 29.0, 28.9, 28.2, 26.1, 25.6, 23.6, 23.3, 22.5, 14.1, 14.0, 9.4, 9.2.

HRMS m/z (ESI) calcd for $C_{24}H_{45}N_2O_6S$ $[M+H]^+$ 489.2998, found: 489.3003.

1-(2-((2,4-dimethylphenyl)thio)phenyl)-4-(octylsulfonyl)piperazine (69) :



69

The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of

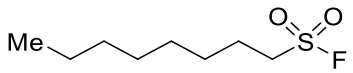
vortioxetine (1.5 mmol, 447.7 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted for another 8 h to afford 152.3 mg (64%) of **69** as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (d, *J* = 7.8 Hz, 1H), 7.16 (s, 1H), 7.12 – 7.06 (m, 1H), 7.06 – 6.99 (m, 2H), 6.93 – 6.86 (m, 1H), 6.52 (dd, *J* = 7.8, 1.0 Hz, 1H), 3.47 (t, *J* = 4.4 Hz, 4H), 3.14 (t, *J* = 4.6 Hz, 4H), 2.99 – 2.89 (m, 2H), 2.34 (d, *J* = 20.4 Hz, 6H), 1.91 – 1.79 (m, 2H), 1.47 – 1.38 (m, 2H), 1.34 – 1.25 (m, 8H), 0.88 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 148.2, 142.1, 139.2, 136.0, 134.4, 131.6, 127.7, 127.4, 126.2, 125.5, 124.9, 120.0, 51.3, 48.8, 46.2, 31.6, 28.9, 28.8, 28.4, 22.9, 22.5, 21.1, 20.4, 13.9.

HRMS m/z (ESI) calcd for $C_{26}H_{39}N_2O_2S_2$ $[M+H]^+$ 475.2453, found. 475.2457.

octane-1-sulfonyl fluoride (70)[15] **:**



70

The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of TBAF (2.5 mmol, 653.7 mg) and NEt_3 (3.5 mmol, 354.2 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 58.9 mg (60%) of **70** as a colorless oil.

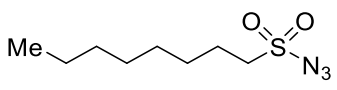
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.41 – 3.30 (m, 2H), 2.00 – 1.89 (m, 2H), 1.53 – 1.43 (m, 2H), 1.35 – 1.25 (m, 8H), 0.89 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 50.9 (d, *J* = 16.2 Hz), 31.6, 28.8, 28.7, 27.8, 23.3, 22.5, 14.0.

^{19}F NMR (376 MHz, $CDCl_3$): δ 53.27 .

MS m/z (EI) calcd for $C_8H_{17}FO_2S$ $[M]^+$ 196.09, found: 196.11.

octane-1-sulfonyl azide (71)[16] **:**



71

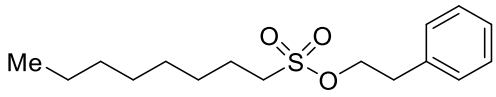
The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of azidotrimethylsilane (1.5 mmol, 172.8 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted for another 8 h to afford 84.8 mg (77%) of **71** as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.36 – 3.27 (m, 2H), 1.97 – 1.87 (m, 2H), 1.51 – 1.42 (m, 2H), 1.37 – 1.25 (m, 8H), 0.93 – 0.86 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 55.9, 31.5, 28.8, 27.9, 23.3, 22.5, 13.9.

MS m/z (EI) calcd for $C_8H_{17}N_3O_2S$ $[M]^+$ 219.10, found: 219.25.

phenethyl octane-1-sulfonate (72) :



72

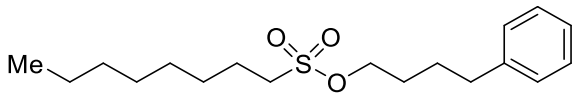
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 2-phenylethan-1-ol (1.5 mmol, 183.3 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 98.5 mg (66%) of **72** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 – 7.29 (m, 2H), 7.28 – 7.21 (m, 3H), 4.40 (t, J = 6.9 Hz, 2H), 3.04 (t, J = 6.9 Hz, 2H), 2.93 (t, J = 8.0 Hz, 2H), 1.76 – 1.63 (m, 2H), 1.35 – 1.21 (m, 10H), 0.88 (t, J = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 136.4, 128.9, 128.5, 126.9, 69.7, 50.3, 35.6, 31.6, 28.8, 28.0, 23.2, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{16}H_{30}NO_3S$ $[M+NH_4]^+$ 316.1946, found: 316.1949.

4-phenylbutyl octane-1-sulfonate (73) :



73

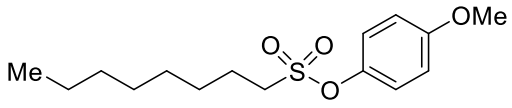
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 4-phenylbutan-1-ol (1.5 mmol, 225.3 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted at ambient temperature for 8 h afforded 112.6 mg (69%) of **73** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 – 7.23 (m, 2H), 7.23 – 7.12 (m, 3H), 4.21 (t, *J* = 5.1 Hz, 2H), 3.06 (t, *J* = 8.0 Hz, 2H), 2.66 (t, *J* = 6.3 Hz, 2H), 1.89 – 1.68 (m, 6H), 1.46 – 1.37 (m, 2H), 1.28 (s, 8H), 0.88 (t, *J* = 6.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 141.5, 128.4, 128.3, 125.9, 69.3, 50.4, 35.1, 31.6, 28.9, 28.9, 28.7, 28.1, 27.2, 23.4, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{18}H_{34}NO_3S$ $[M+NH_4]^+$ 344.2259, found: 344.2257.

4-methoxyphenyl octane-1-sulfonate (74):



74

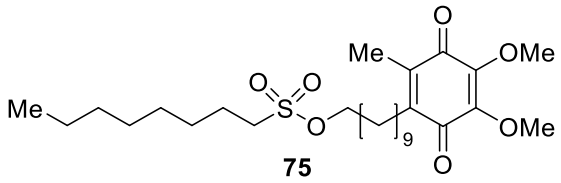
The reaction of octane-1-thiol (0.50 mmol, 73.1 mg), DMSO (1.75 mmol, 120 μL), HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg) in DCM (2 mL) at 40 °C for 12 h, followed by added dropwise into DCM (1 mL) solution of 4-methoxyphenol (1.5 mmol, 225.3 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath under N_2 atmosphere, then reacted at ambient temperature for 8 h afforded 105.1 mg (70%) of **74** as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.19 (d, *J* = 7.3 Hz, 2H), 6.90 (d, *J* = 7.3 Hz, 2H), 3.80 (s, 3H), 3.20 (t, *J* = 8.0 Hz, 2H), 2.01 – 1.89 (m, 2H), 1.51 – 1.40 (m, 2H), 1.40 – 1.20 (m, 8H), 0.89 (t, *J* = 6.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 158.3, 142.4, 123.0, 114.8, 55.6, 50.0, 31.6, 28.9, 28.8, 28.1, 23.4, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{15}H_{23}O_4S$ $[M-H]^-$ 299.1317, found: 299.1319.

10-(4,5-dimethoxy-2-methyl-3,6-dioxocyclohexa-1,4-dien-1-yl)decyloctane-1-sulfonate (75) :



75

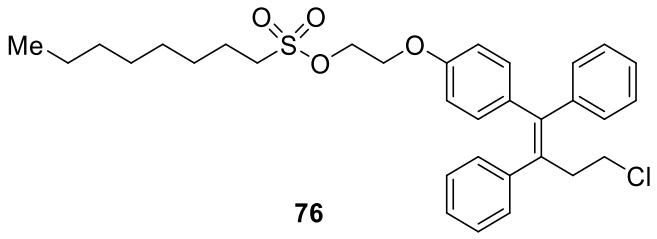
The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of 2-(10-hydroxydecyl)-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (1.5 mmol, 507.7 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted for another 8 h to afford 183.1 mg (71%) of **75** as an orange oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.20 (t, *J* = 6.6 Hz, 2H), 3.99 (d, *J* = 1.1 Hz, 6H), 3.11 – 3.04 (m, 2H), 2.47 – 2.42 (t, *J* = 7.4 Hz, 2H), 2.01 (s, 3H), 1.85 (m, 2H), 1.77 – 1.69 (m, 2H), 1.42 – 1.25 (m, 24H), 0.91 – 0.85 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 184.4, 183.9, 144.1, 144.0, 142.8, 138.4, 69.5, 60.9, 50.1, 31.5, 29.6, 29.1, 28.7, 28.5, 27.9, 26.1, 25.2, 23.3, 22.4, 13.8, 11.7.

HRMS m/z (ESI) calcd for $C_{27}H_{47}O_7S$ $[M+H]^+$ 515.3042, found: 515.3048.

(*Z*)-2-(4-(4-chloro-1,2-diphenylbut-1-en-1-yl)phenoxy)ethyl octane-1-sulfonate (76):



76

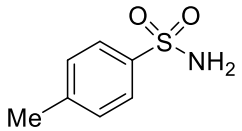
The solution of thiol **1** (0.50 mmol, 73.1 mg), $Ni(OTf)_2$ (0.05 mmol, 17.8 mg), DMSO (1.75 mmol, 136.7 mg) and HBr (AcOH solution, 33% w/w, 0.75 mmol, 120 μL) in anhydrous DCM (2.0 mL) was heated at 40 ℃ for 12 h. After the termination of the reaction, the reaction mixture was added dropwise into DCM (1 mL) solution of (*Z*)-2-(4-(4-chloro-1,2-diphenylbut-1-en-1-yl)phenoxy)ethan-1-ol (1.5 mmol, 568.3 mg) and NEt_3 (4 mmol, 404.8 mg) in ice-salt bath, then reacted for another 8 h to afford 172.6 mg (62%) of **76** as a white oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 – 7.34 (t, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 7.0 Hz, 3H), 7.23 – 7.17 (t, *J* = 7.4 Hz, 2H), 7.14 (t, *J* = 6.6 Hz, 3H), 6.80 (d, *J* = 8.7 Hz, 2H), 6.54 (d, *J* = 8.7 Hz, 2H), 4.50 – 4.39 (m, 2H), 4.12 – 4.03 (m, 2H), 3.41 (t, *J* = 7.4 Hz, 2H), 3.14 – 3.06 (m, 2H), 2.92 (t, *J* = 7.4 Hz, 2H), 1.89 – 1.73 (m, 2H), 1.42 – 1.33 (m, 2H), 1.30 – 1.18 (m, 8H), 0.87 (t, *J* = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 156.1, 142.6, 141.4, 140.8, 135.6, 135.5, 131.7, 129.4, 129.3, 128.3, 128.2, 126.9, 126.6, 113.4, 67.4, 65.5, 50.6, 42.7, 38.4, 31.6, 28.8, 28.7, 28.0, 23.3, 22.5, 14.0.

HRMS m/z (ESI) calcd for $C_{32}H_{43}ClNO_4S$ $[M+NH_4]^+$ 572.2601, found: 572.2609.

4-methylbenzenesulfonamide (77)[17] **:**



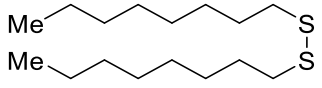
77

^{1}H NMR (400 MHz, DMSO-d_6): δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.27 (s, 2H), 2.37 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6): δ 141.8, 141.4, 129.2, 125.5, 20.8.

MS m/z (ESI) calcd for $C_7H_8NO_2S$ $[M-H]^-$ 170.03, found: 170.03.

1,2-dioctyldisulfane (78)[18] **:**

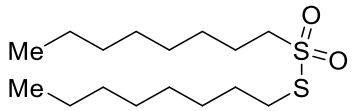


78

^{1}H NMR (400 MHz, $CDCl_3$): δ 2.68 (t, *J* = 7.6 Hz, 4H), 1.72 – 1.63 (m, 4H), 1.38 (s, 4H), 1.28 (s, 16H), 0.88 (t, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 39.2, 31.8, 29.22, 29.20, 29.1, 28.5, 22.6, 14.0.

***S*-octyl octane-1-sulfonothioate (79)**[19] **:**



79

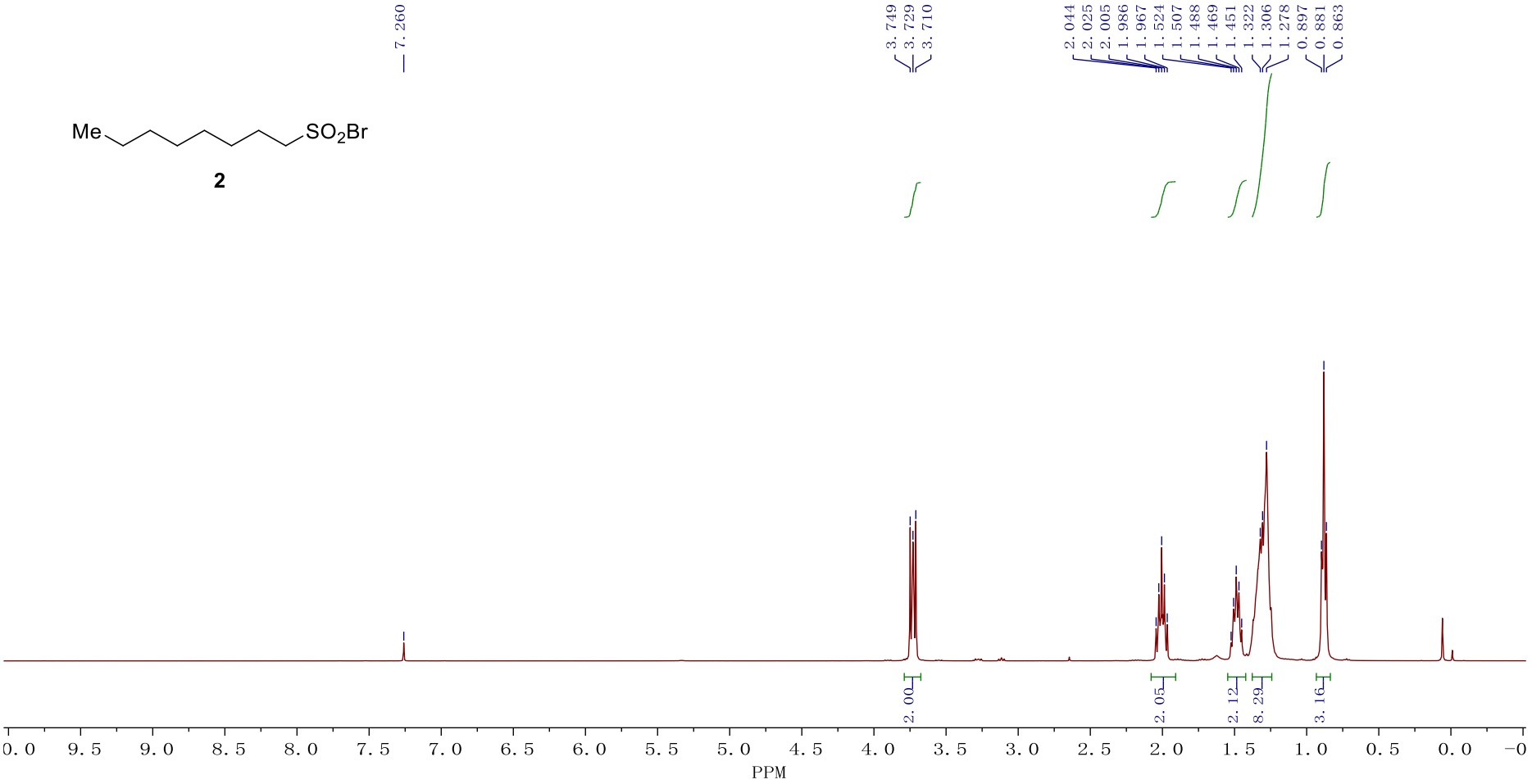
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.28 (t, *J* = 7.6 Hz, 2H), 3.12 (t, *J* = 7.4 Hz, 2H), 1.97 – 1.84 (m, 2H), 1.78 – 1.67 (m, 2H), 1.48 – 1.37 (m, 4H), 1.27 (s, 16H), 0.88 (t, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 62.7, 36.2, 31.7, 31.6, 29.6, 29.0, 28.98, 28.92, 28.89, 28.5, 27.9, 23.5, 22.59, 22.57, 14.05, 14.04.

References

1. M. Yuki, K. Sakata, S. Kikuchi, H. Kawai, T. Takahashi, M. Ando, K. Nakajima and Y. Nishibayashi, *Chem. - Eur. J.*, 2017, **23**, 1007-1012.
2. J. W. J. Bosco, B. R. Raju and A. K. Saikia, *Synth. Commun.*, 2004, **34**, 2849-2855.
3. A. Gayet, C. Bolea and P. G. Andersson, *Org. Biomol. Chem.*, 2004, **2**, 1887-1893.
4. M. Jereb and L. Hribernik, *Green. Chem.*, 2017, **19**, 2286-2295.
5. R. Chen, S. Xu, F. Shen, C. Xu, K. Wang, Z. Wang and L. Liu, *Molecules*, 2021, **26**, 5551.
6. T. Kataoka, T. Iwama, T. Setta and A. Takagi, *Synthesis*, 1998, **4**, 423-426.
7. J. F. King and D. J. H. Smith, *J. Am. Chem. Soc.*, 1967, **89**, 4803-4804.
8. C. Silva-Cuevas, C. Perez-Arrieta, L. A. Polindara-Garcia and J. Armando Lujan-Montelongo, *Tetrahedron Lett.*, 2017, **58**, 2244-2247.
9. S. Lee, O. Cil, P. M. Haggie and A. S. Verkman, *J. Med. Chem.*, 2019, **62**, 8330-8337.

10. S. Madabhushi, R. Jillella, V. Sriramoju and R. Singh, *Green. Chem.*, 2014, **16**, 3125-3131.
11. N. Shohji, T. Kawaji and S. Okamoto, *Org. Lett.*, 2011, **13**, 2626-2629.
12. R. A. Abramovitch, W. D. Holcomb and S. Wake, *J. Am. Chem. Soc.*, 1981, **103**, 1525-1533.
13. J. A. Andrews, L. R. E. Pantaine, C. F. Palmer, D. L. Poole and M. C. Willis, *Org. Lett.*, 2021, **23**, 8488-8493.
14. D. Zhong, D. Wu, Y. Zhang, Z. Lu, M. Usman, W. Liu, X. Lu and W.-B. Liu, *Org. Lett.*, 2019, **21**, 5808-5812.
15. P. Wang, H. Zhang, M. Zhao, S. Ji, L. Lin, N. Yang, X. Nie, J. Song and S. Liao, *Angew. Chem. Int. Ed.*, 2022, **61**, e202207684.
16. S. Azeez, P. Chaudhary, P. Sureshbabu, S. Sabiah and J. Kandasamy, *Org. Biomol. Chem.*, 2018, **16**, 8280-8285.
17. T. Q. Davies, M. J. Tilby, D. Skolc, A. Hall and M. C. Willis, *Org. Lett.*, 2020, **22**, 9495-9499.
18. E. Rattanangkool, W. Krailat, T. Vilaivan, P. Phuwapraisirisan, M. Sukwattanasinitt and S. Wacharasindhu, *Eur. J. Org. Chem.*, 2014, **2014**, 4795-4804.
19. T. X. T. Luu, T.-T. T. Nguyen, T. N. Le, J. Spanget-Larsen and F. Duus, *Journal of Sulfur Chemistry*, 2015, **36**, 340-350.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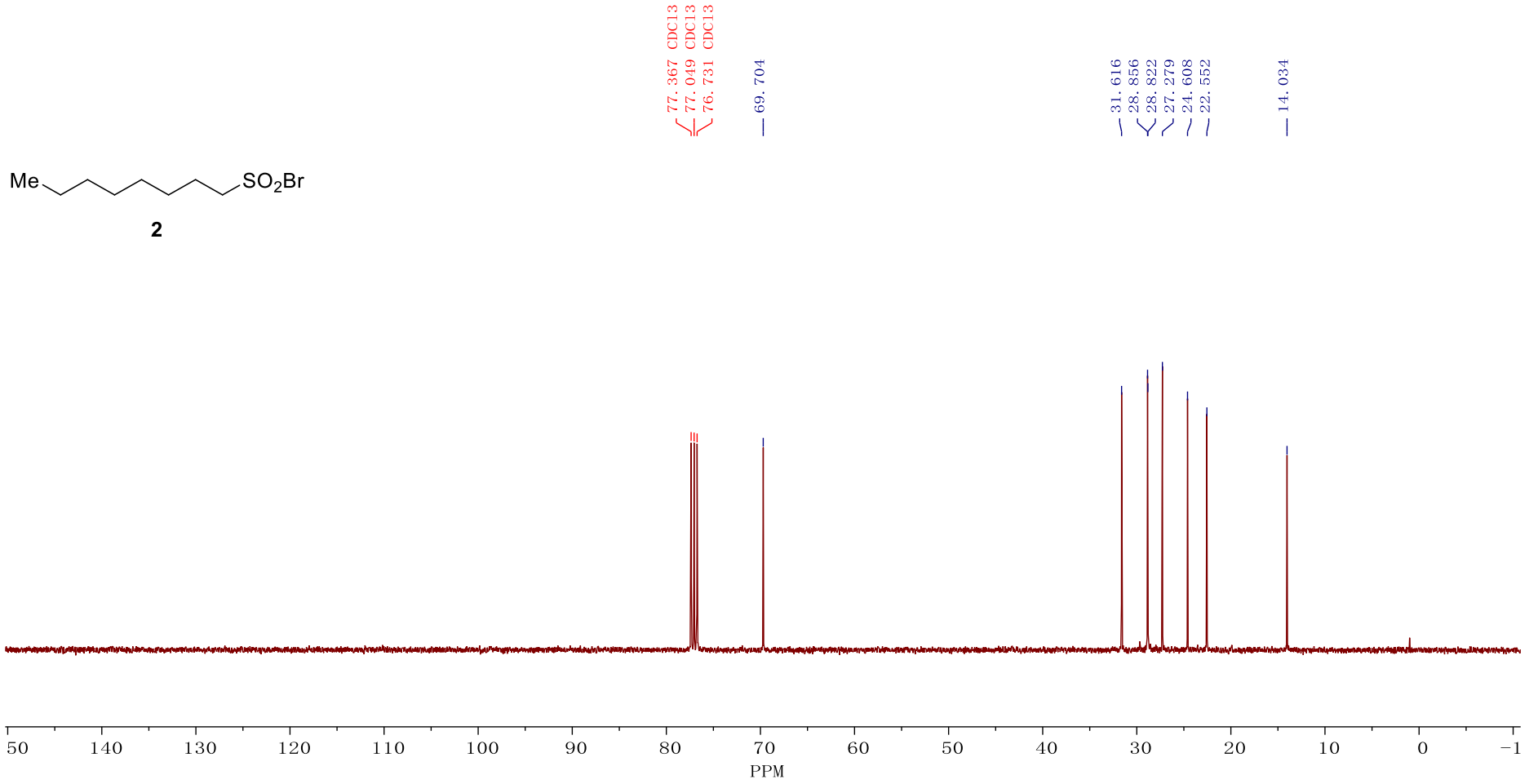
1.524
1.507
1.488
1.469
1.451
1.322
1.306
1.278
0.897
0.881
0.863
2.00
2.05
2.12
8.29
3.16
PPM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76.731 CDCl3
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28.822
27.279
24.608
22.552
14.034
Me
SO2Br
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50
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130
120
110
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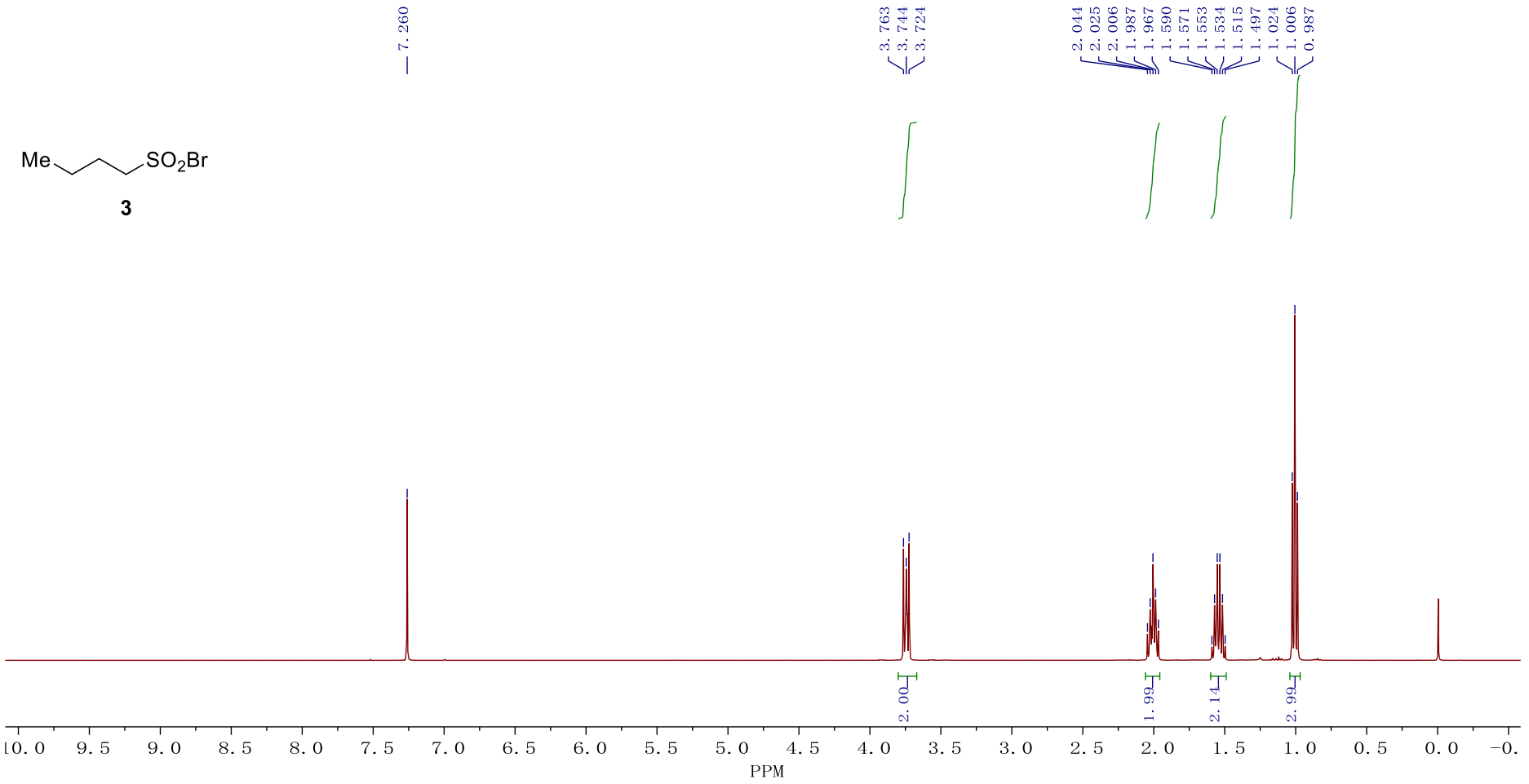
90
80
70
60
50
40
30
20
10
0
−1
PPM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1.99
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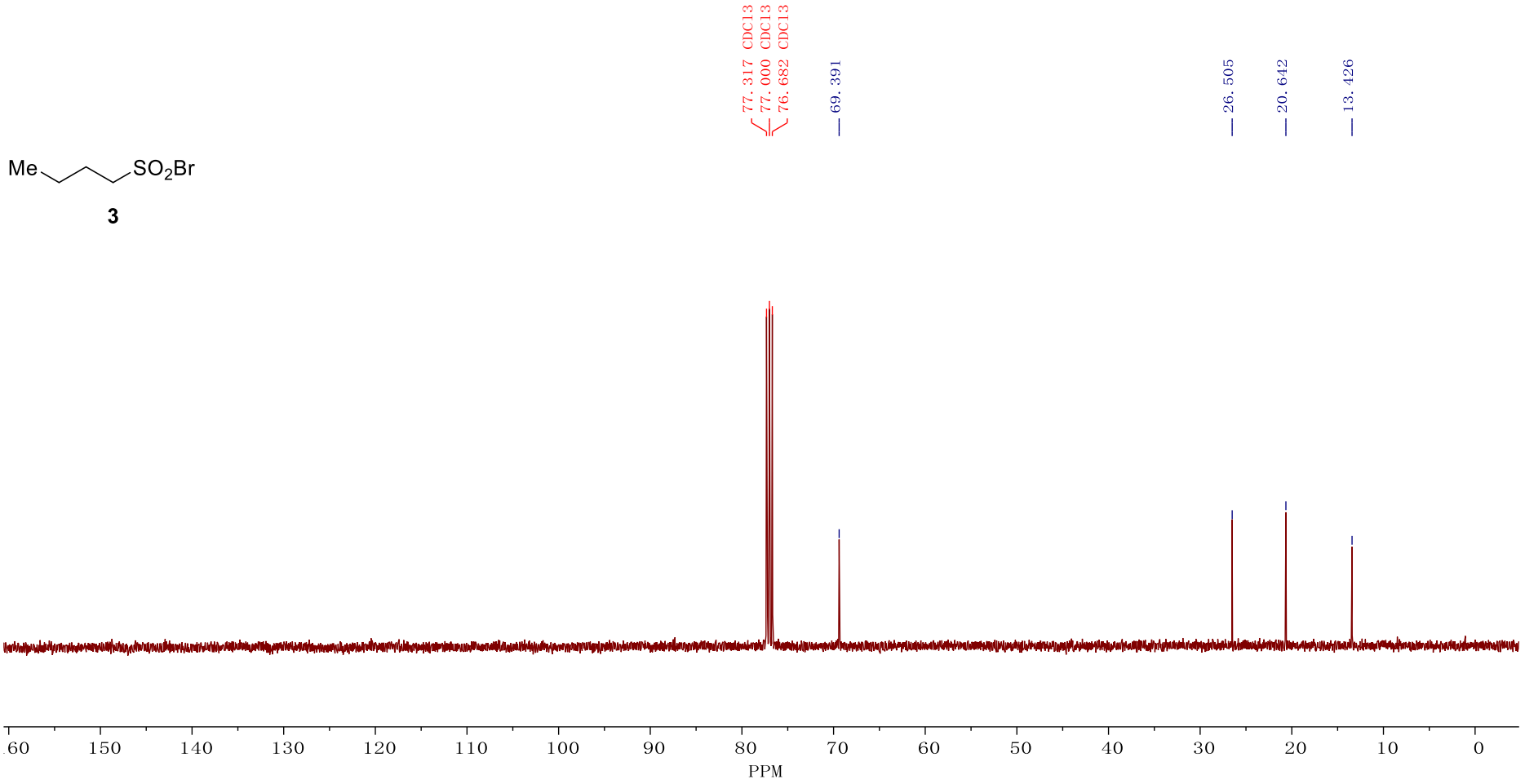
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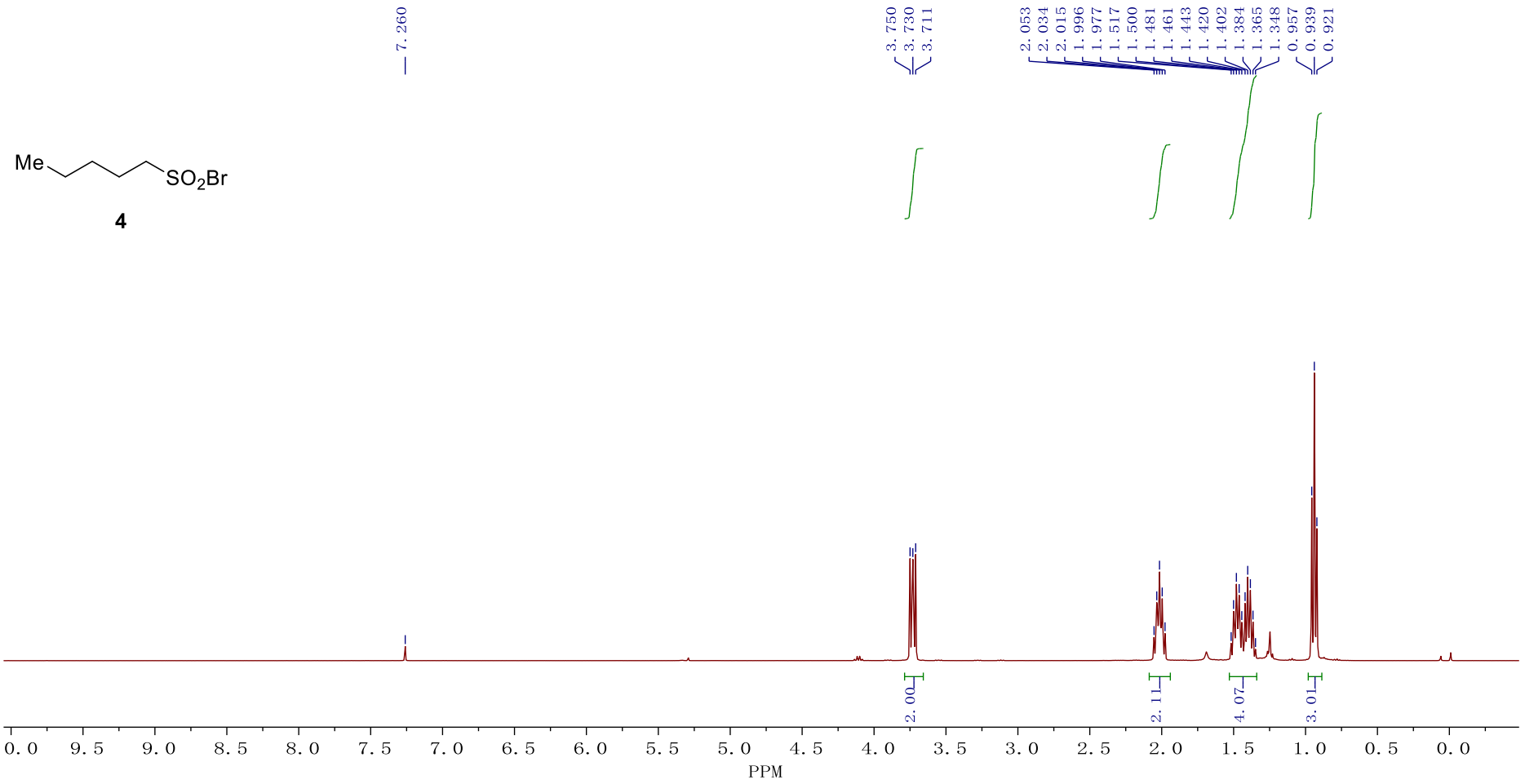
20
10
0
PPM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1.348
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3.01
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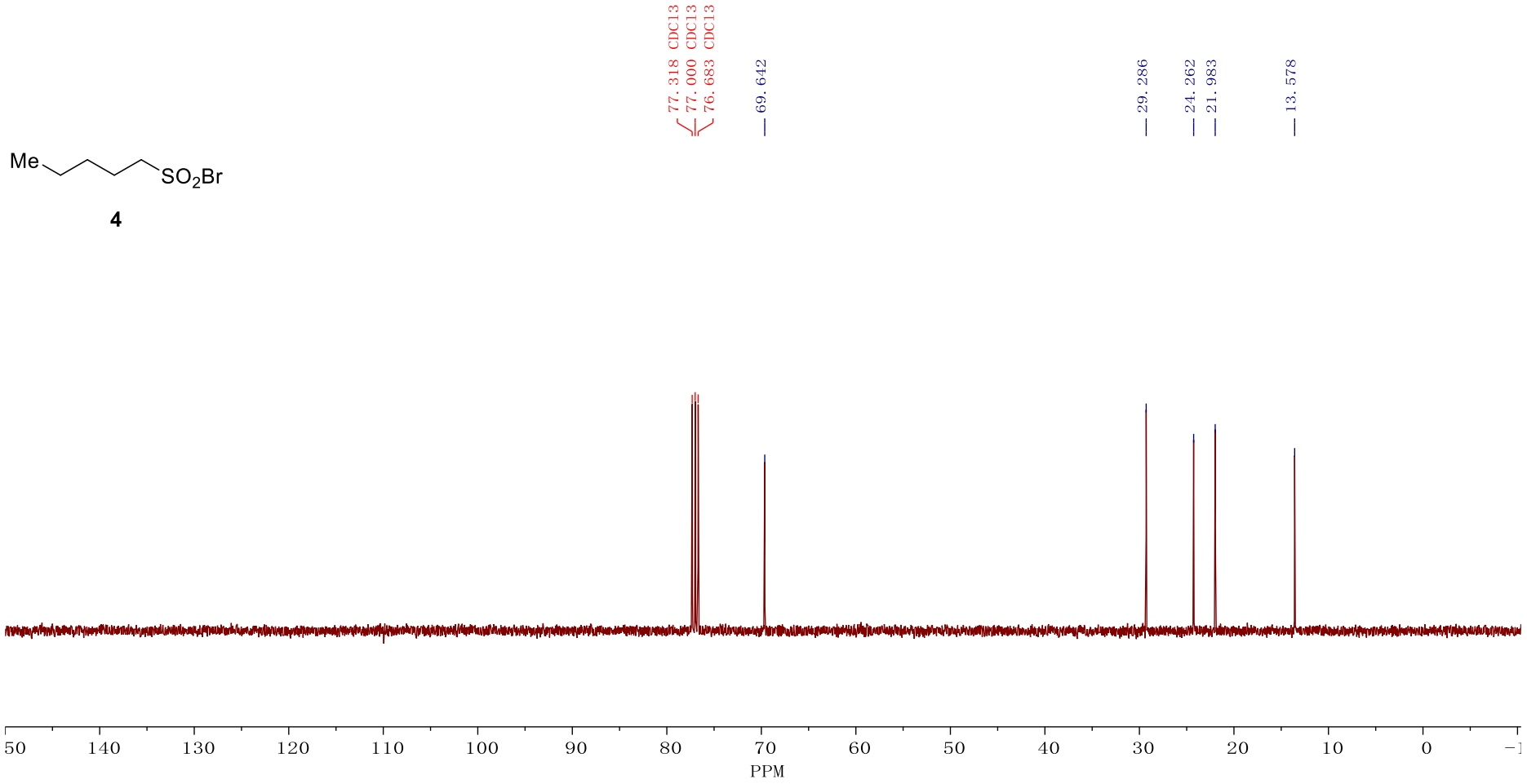
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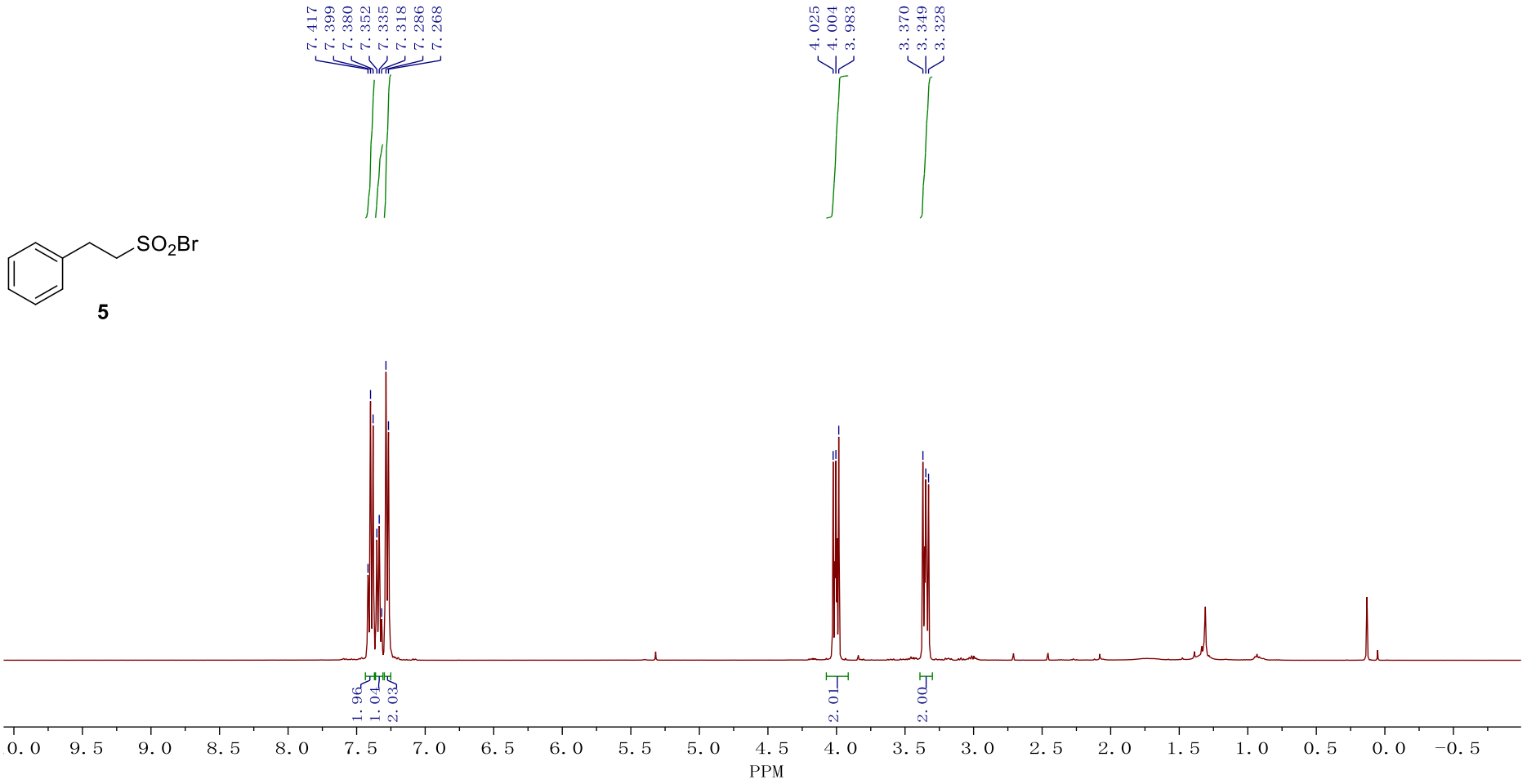
PPM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SO2Br
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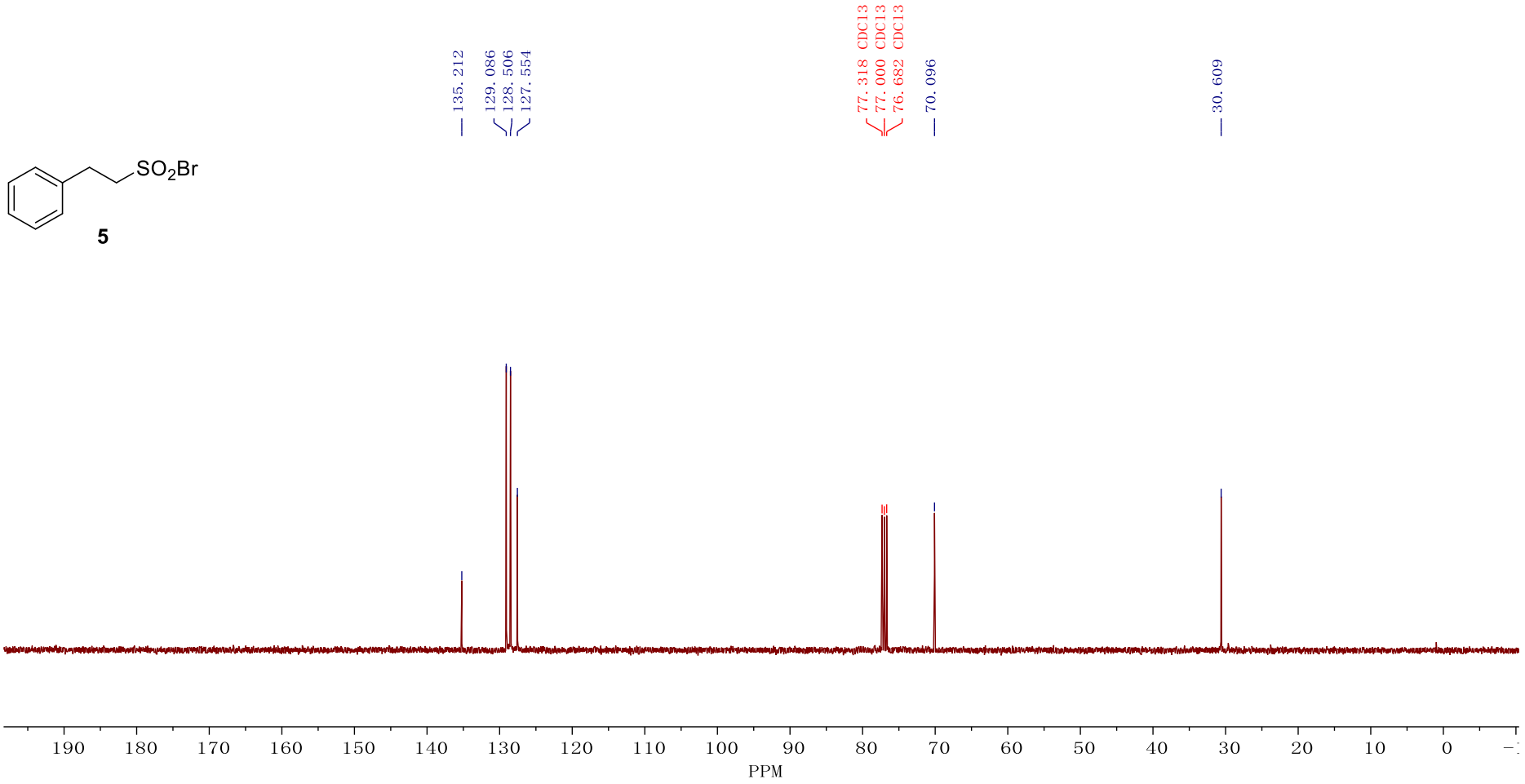
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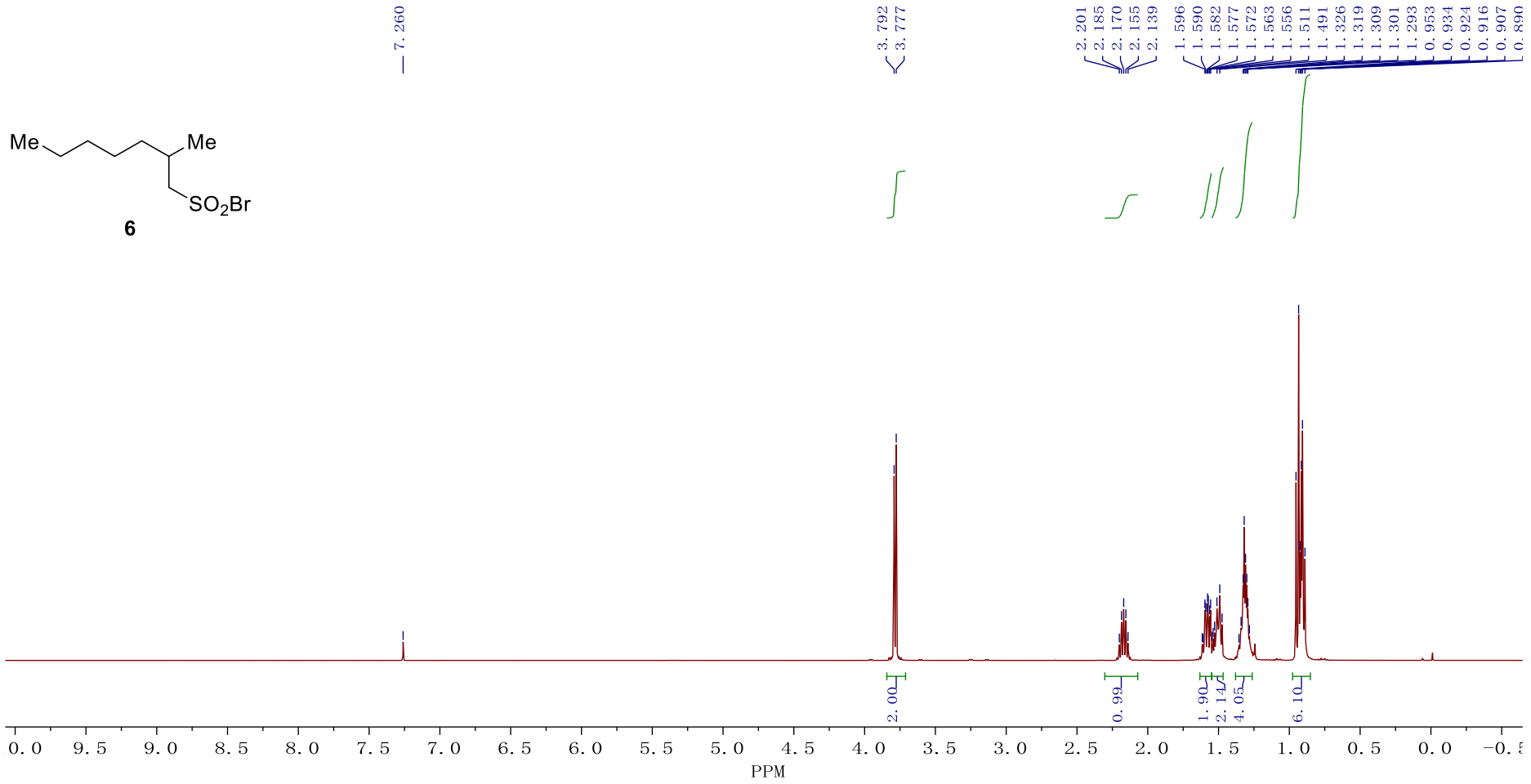
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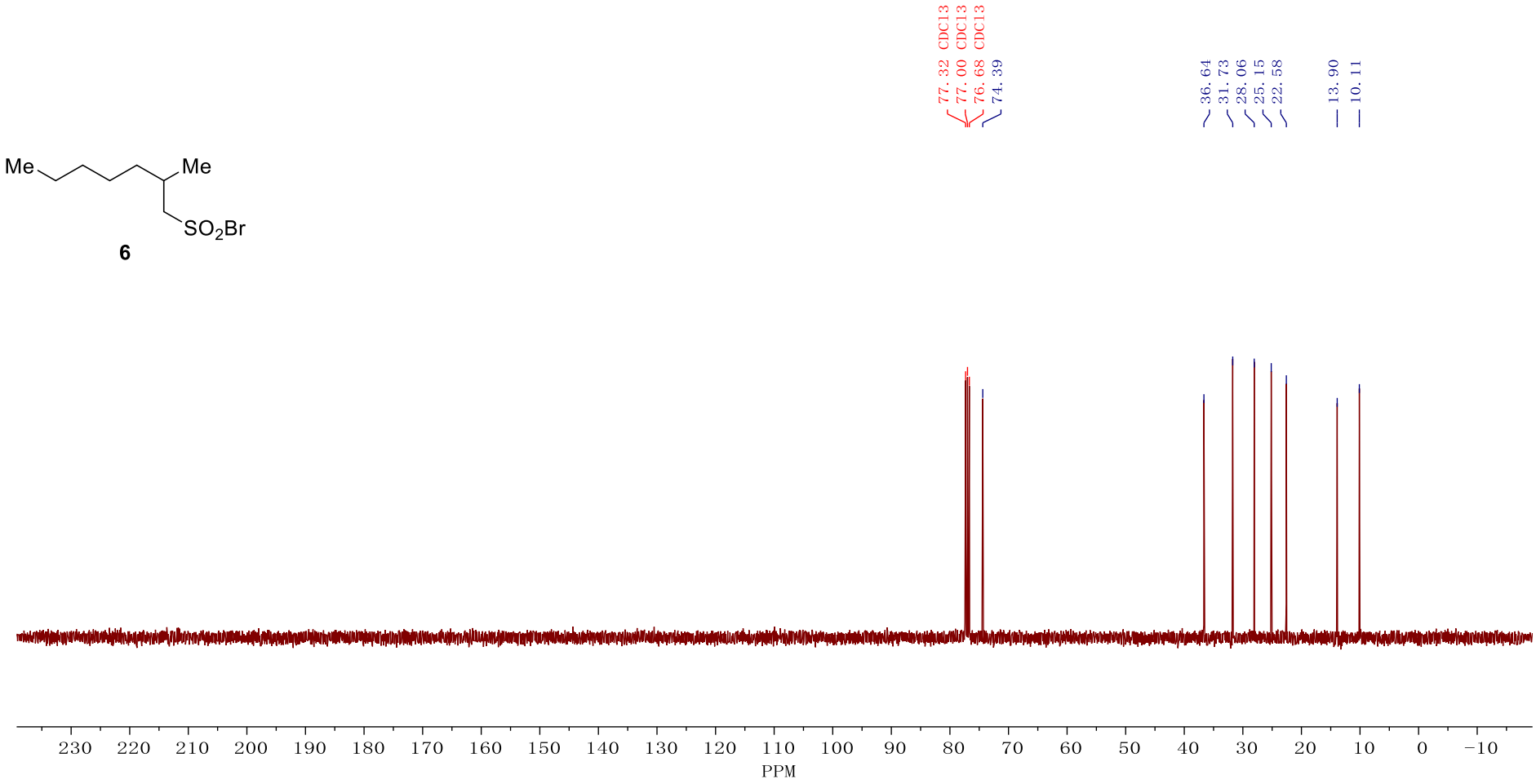
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10.11
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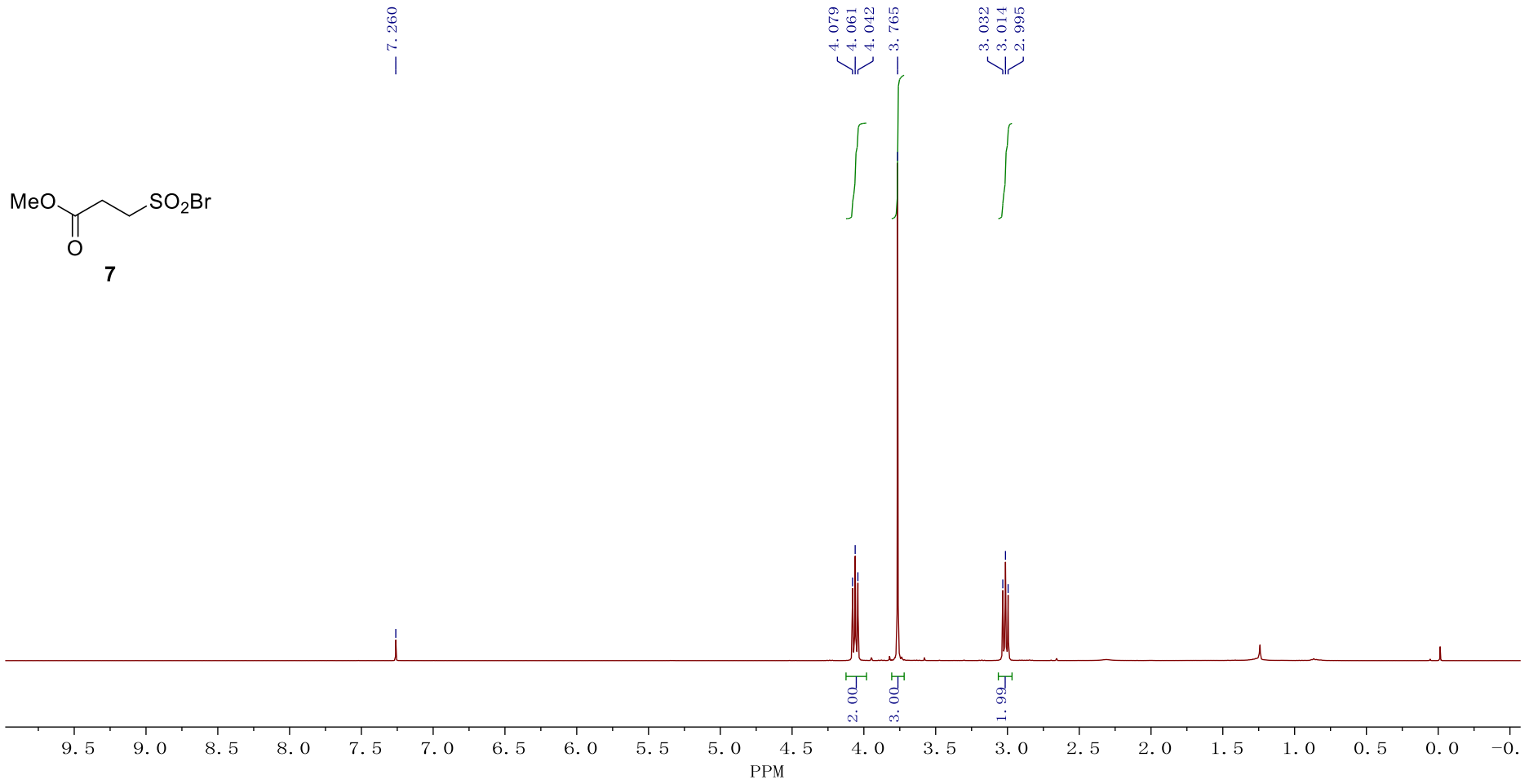
PPM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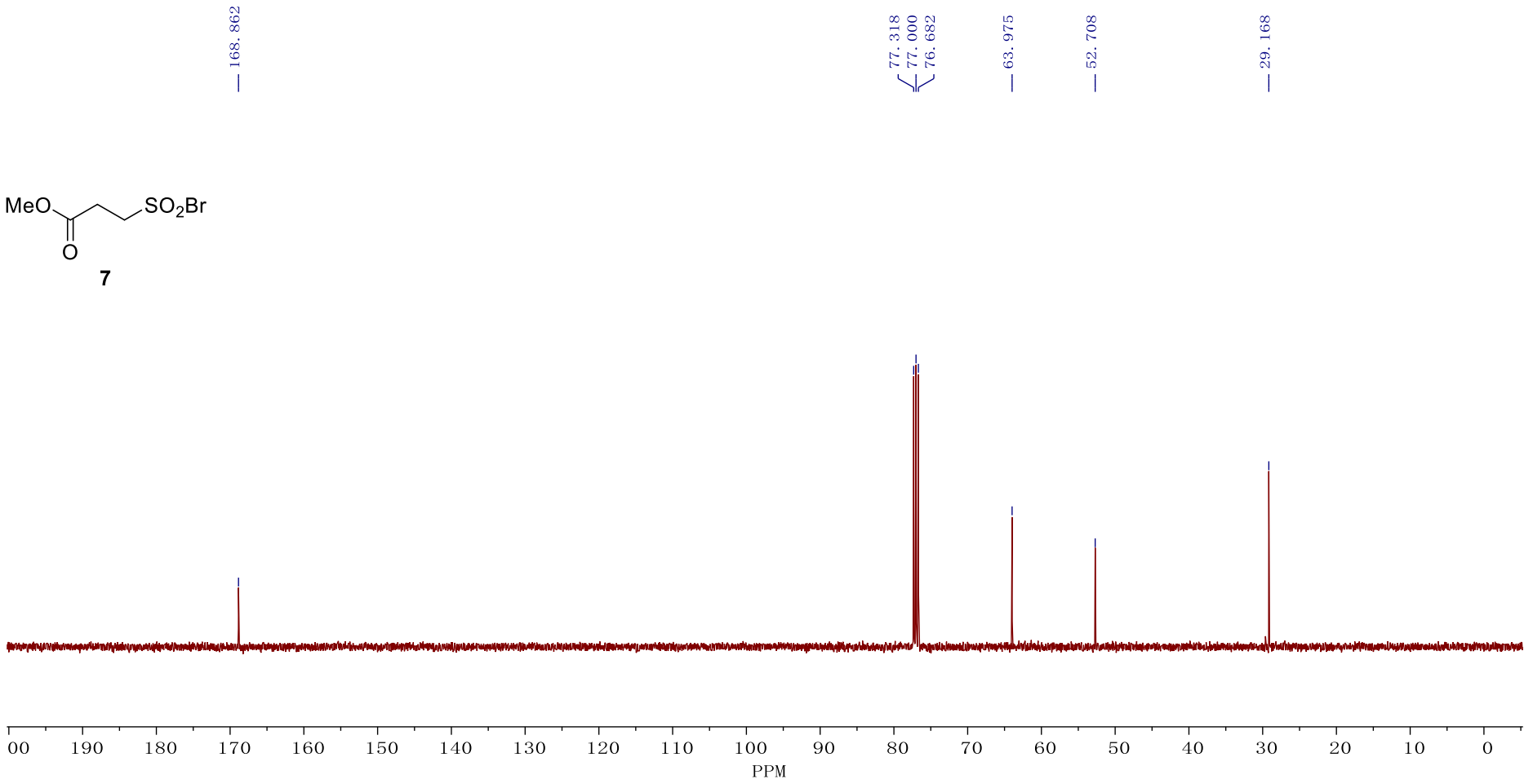
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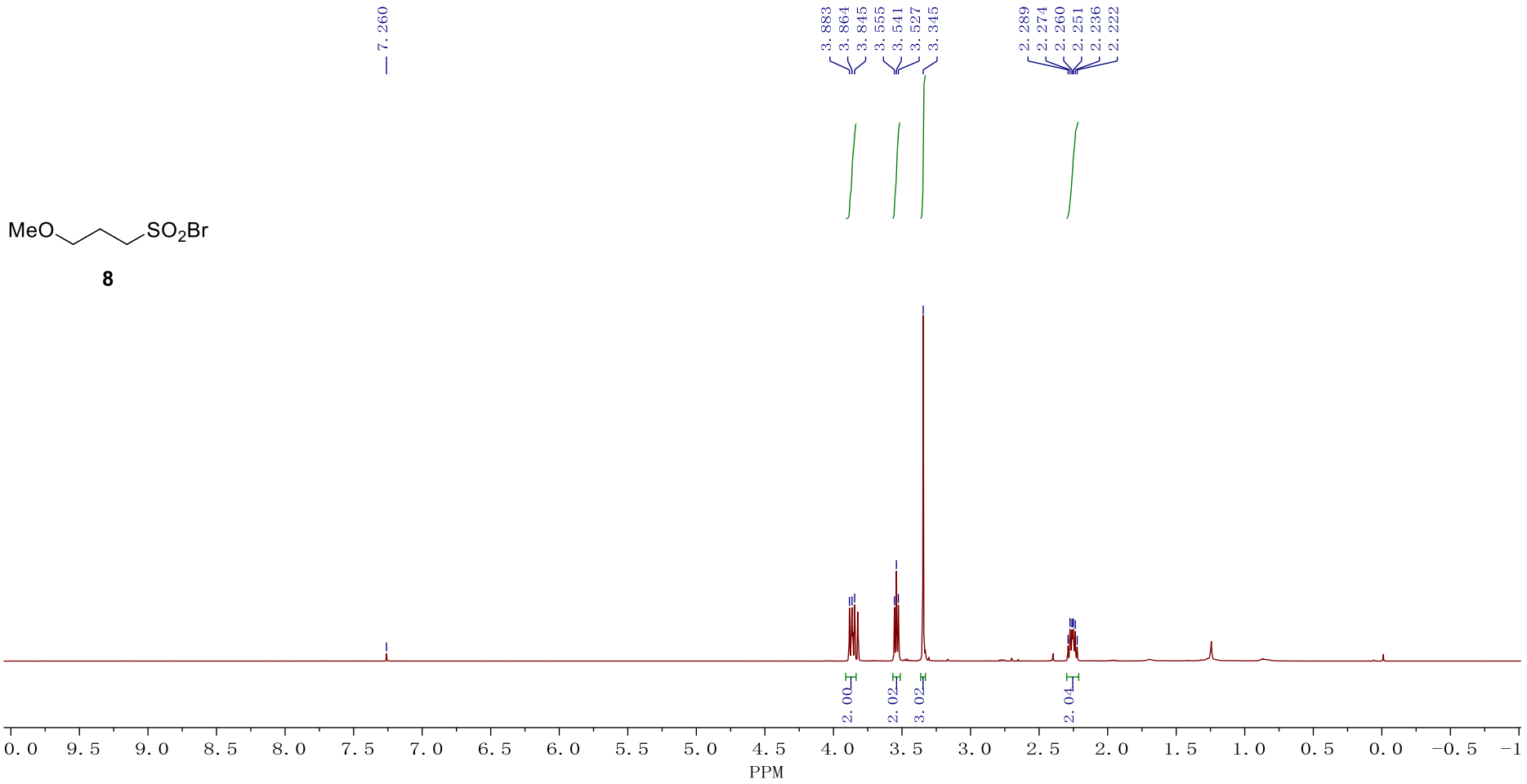
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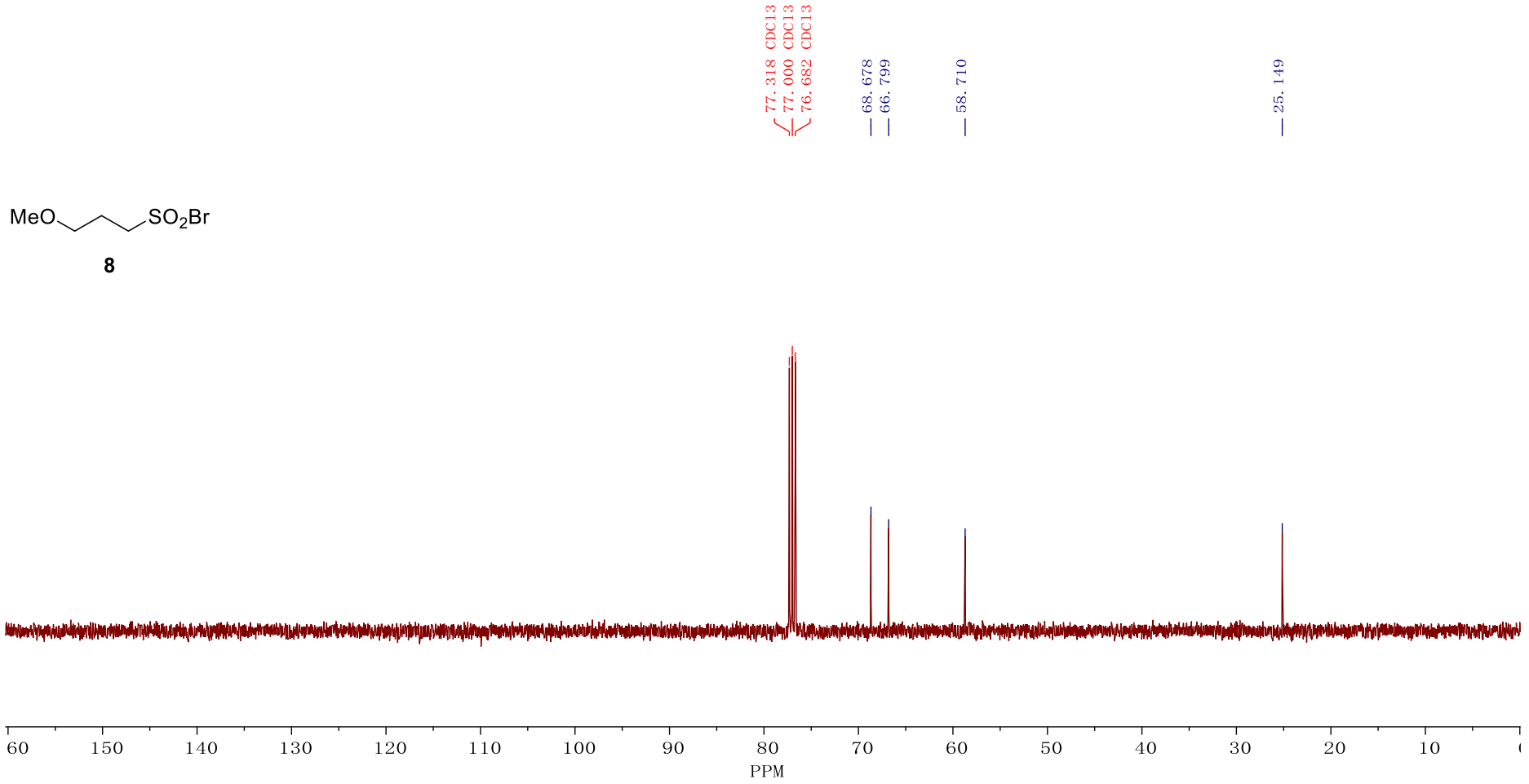
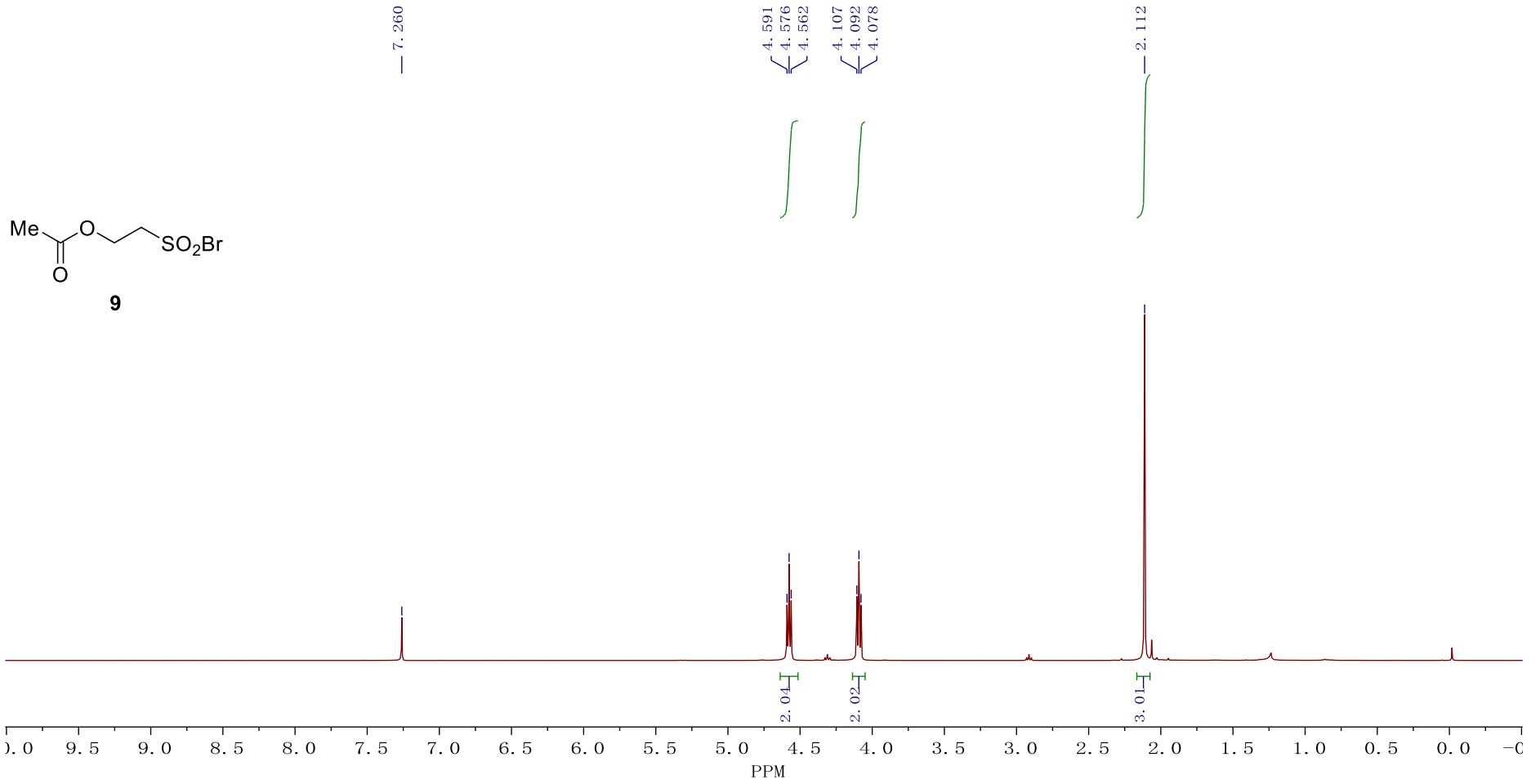
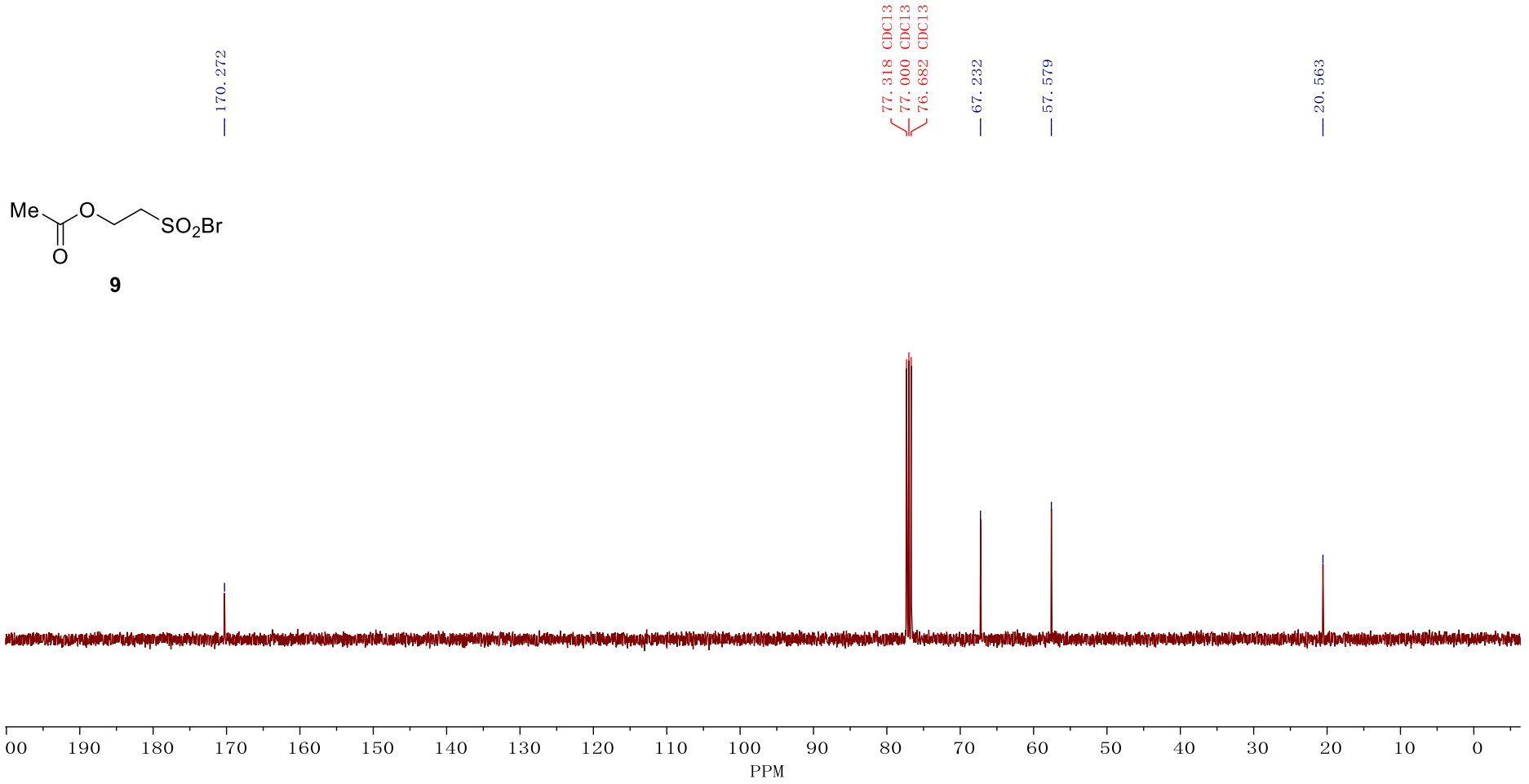
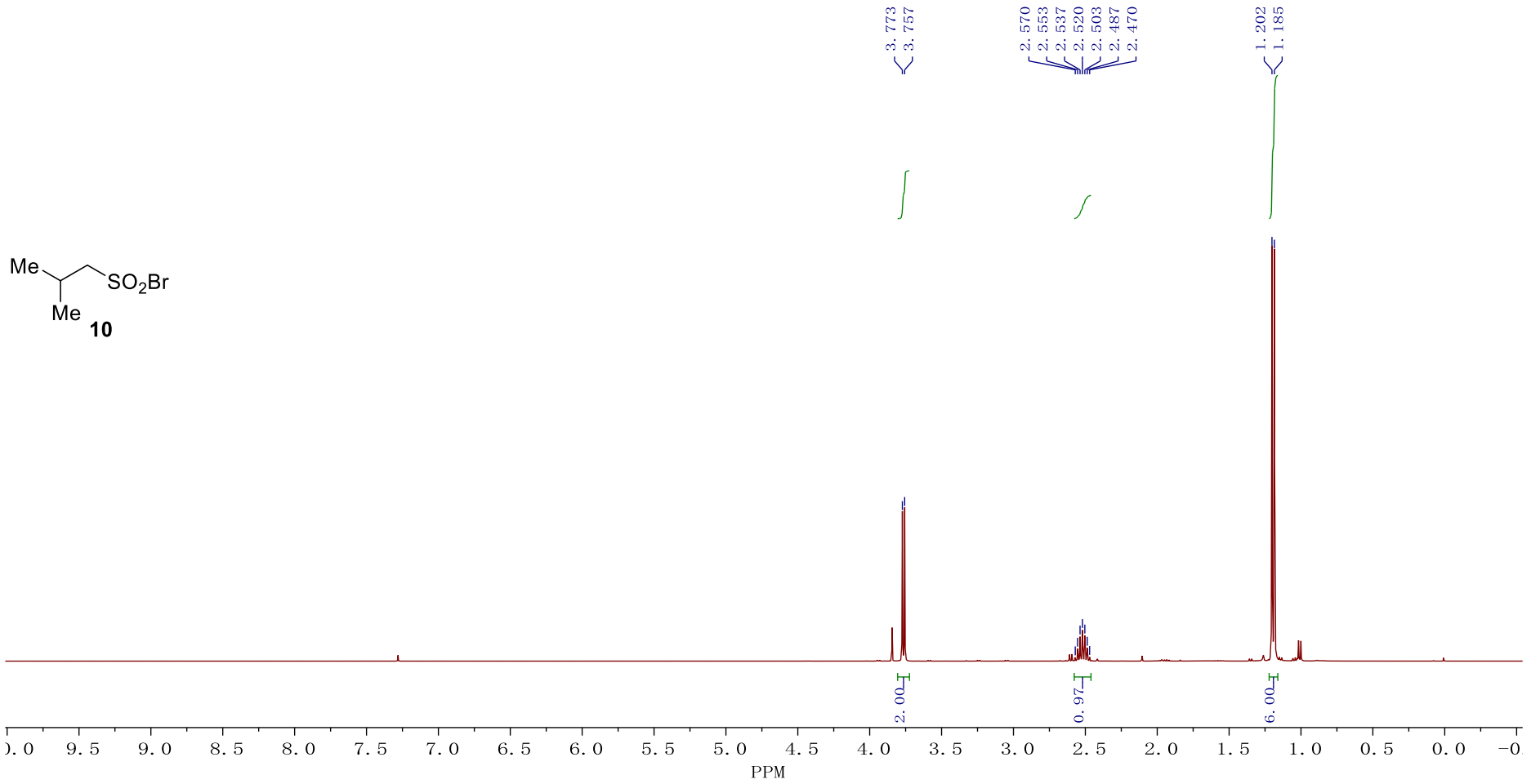
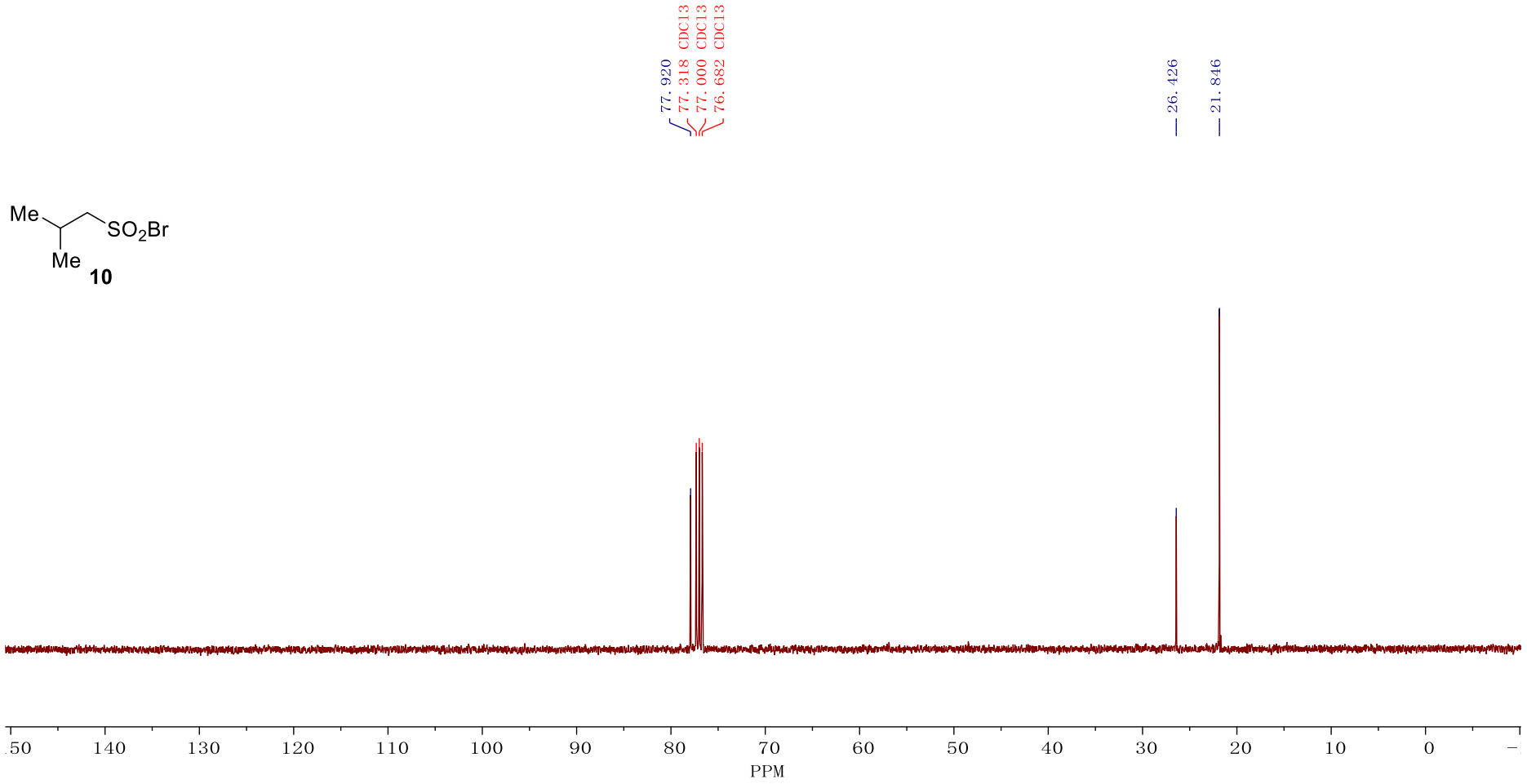
2.04
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
PPM


77.318 CDCl3
77.000 CDCl3
76.682 CDCl3
68.678
66.799
58.710
25.149
MeO
SO2Br
8
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
PPM


7.260
4.591
4.576
4.562
4.107
4.092
4.078
2.112
Me
O
O
SO2Br
9
2.04
2.02
3.01
PPM


170.272
77.318 CDC13
77.000 CDC13
76.682 CDC13
67.232
57.579
20.563
Me
O
O
SO2Br
9
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM


Me
SO2Br
Me
10
3.773
3.757
2.570
2.553
2.537
2.520
2.503
2.487
2.470
1.202
1.185
2.00
0.97
6.00
PPM


77.920
77.318 CDC13
77.000 CDC13
76.682 CDC13
26.426
21.846
Me
SO2Br
Me
10
150
140
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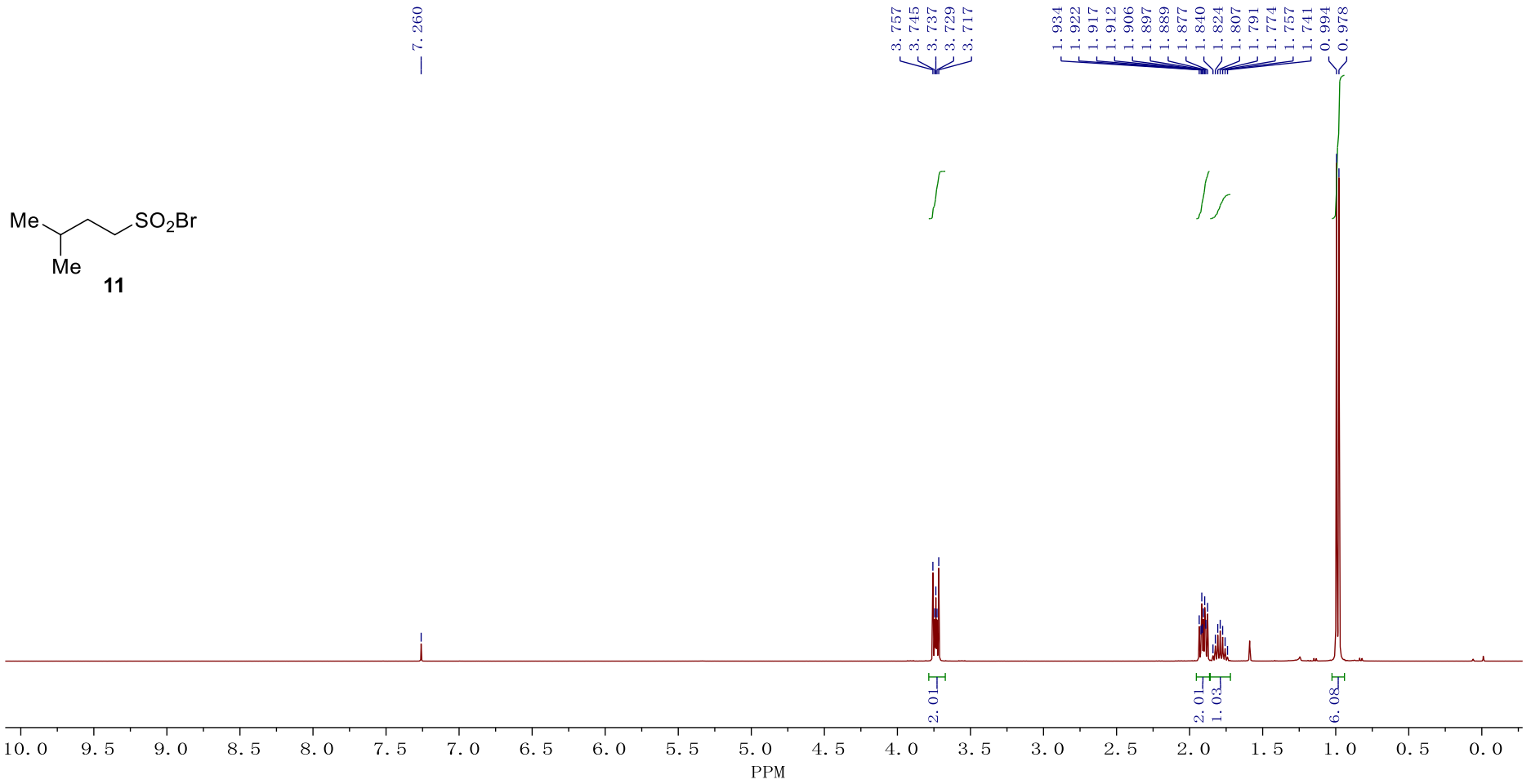
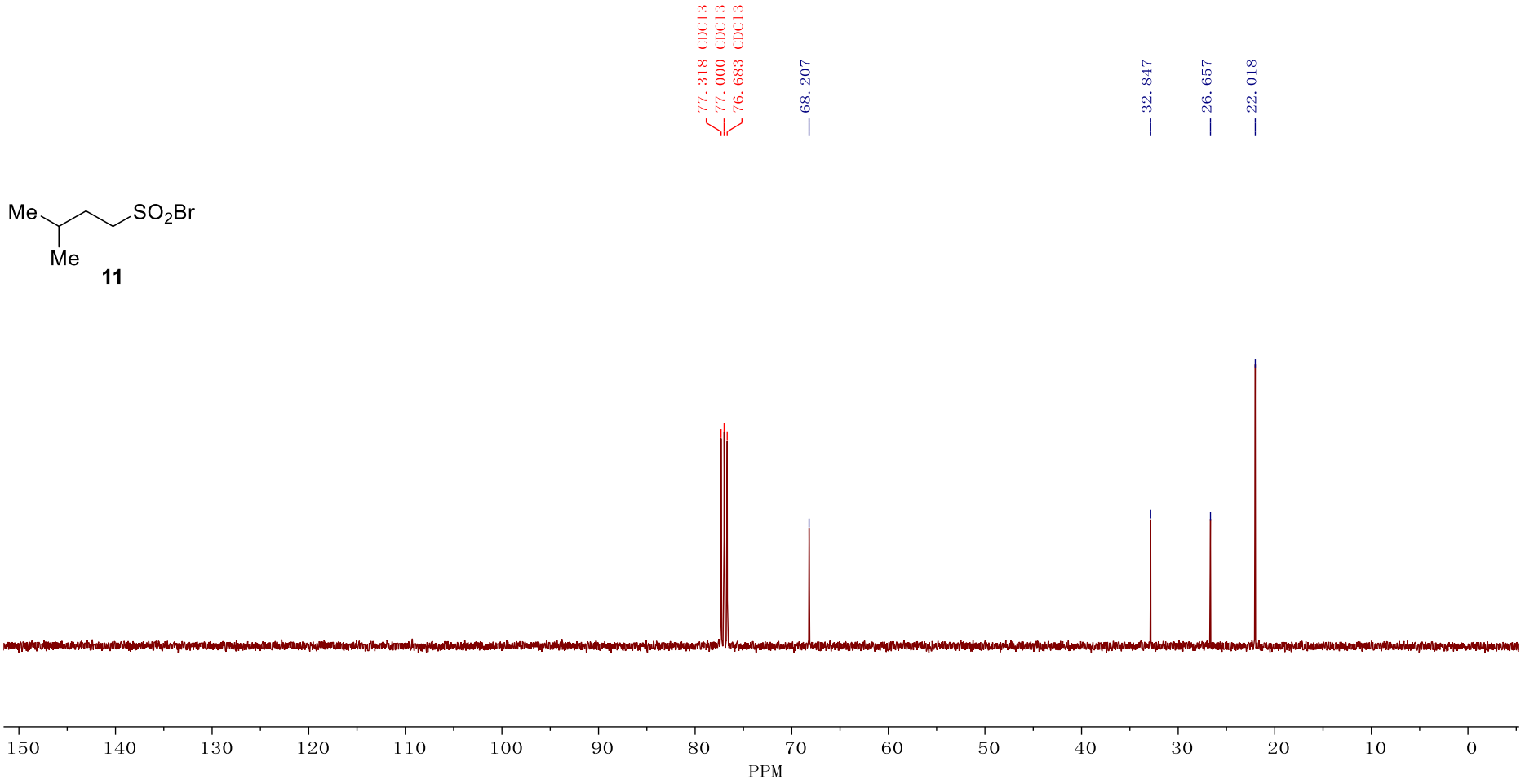
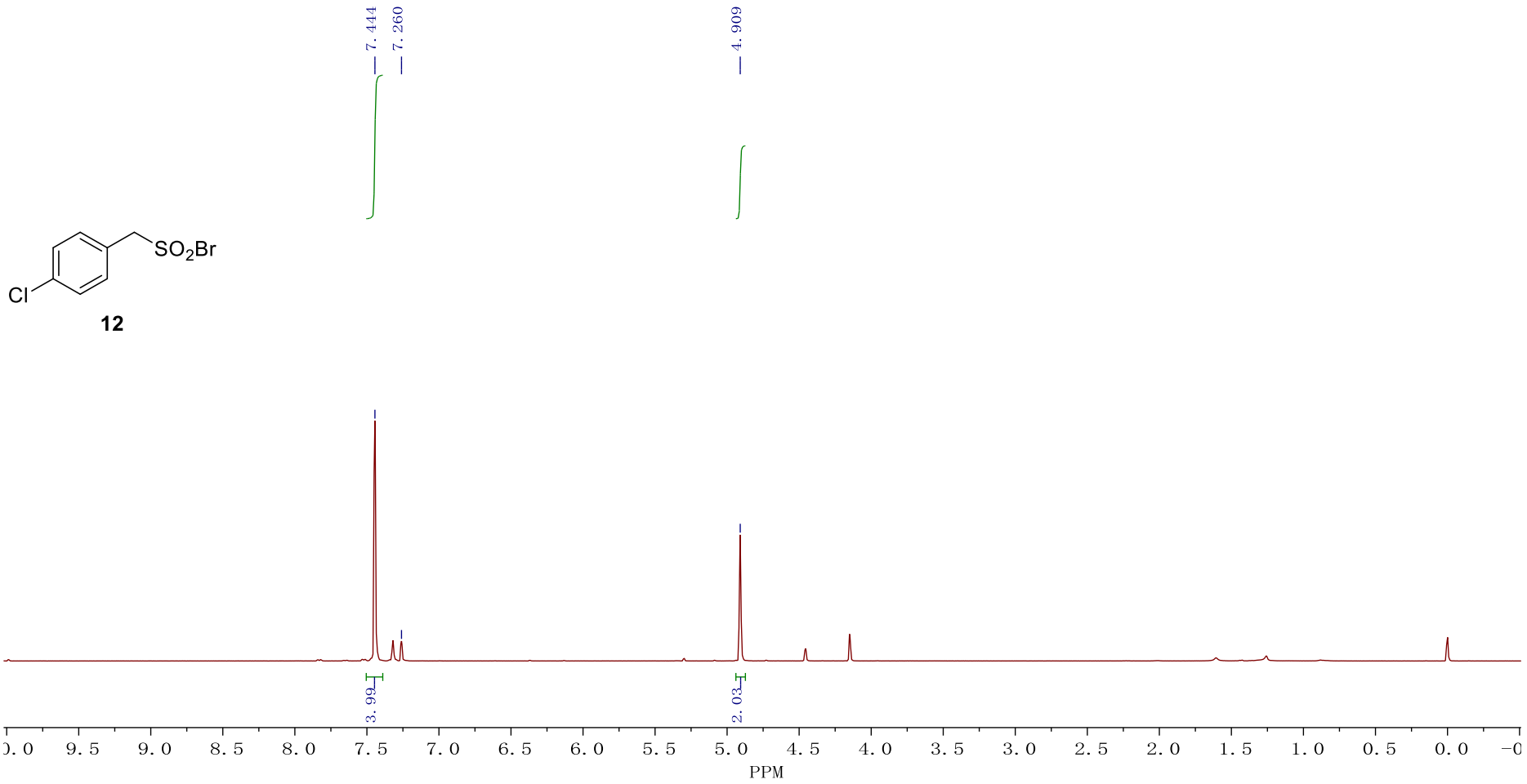
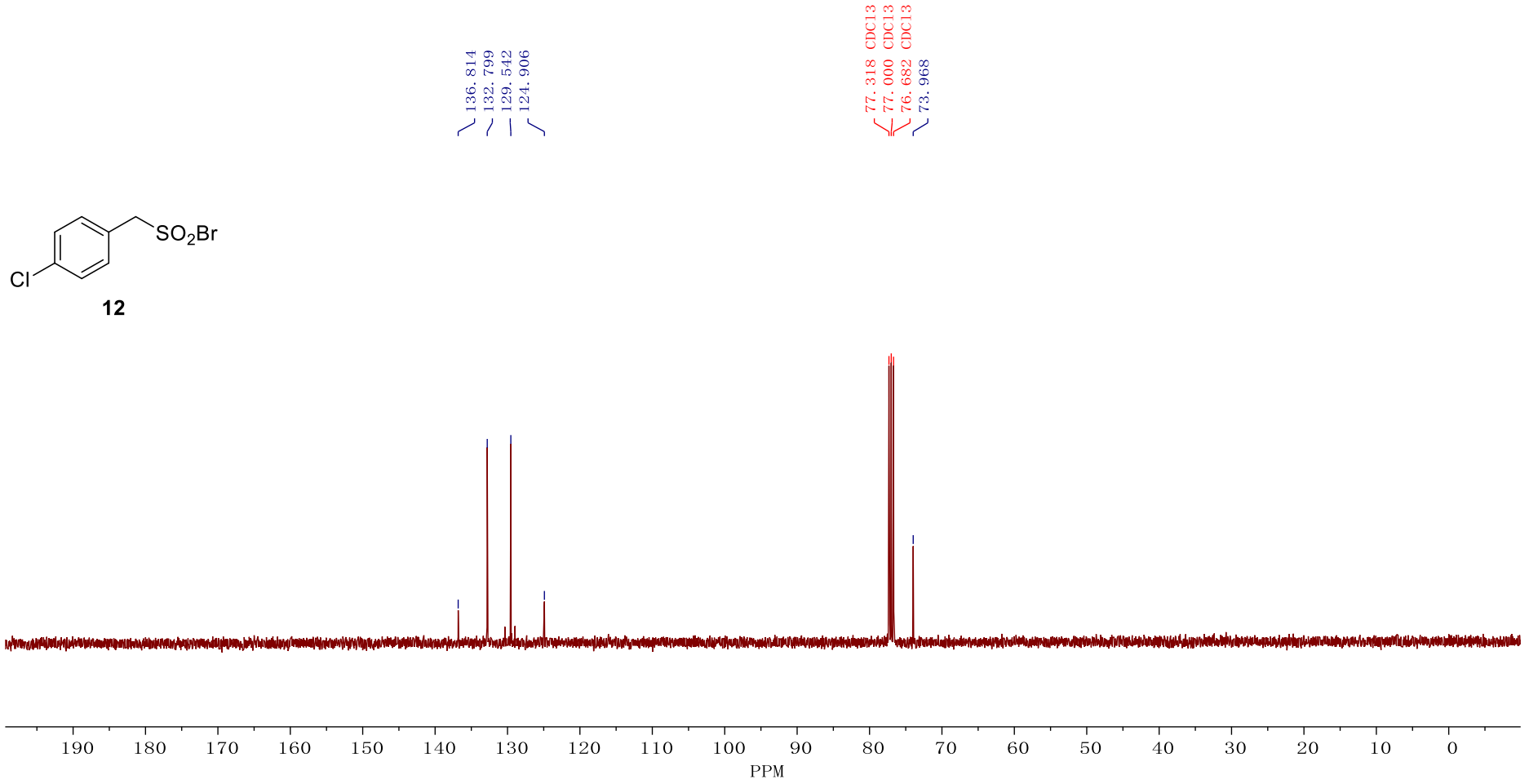
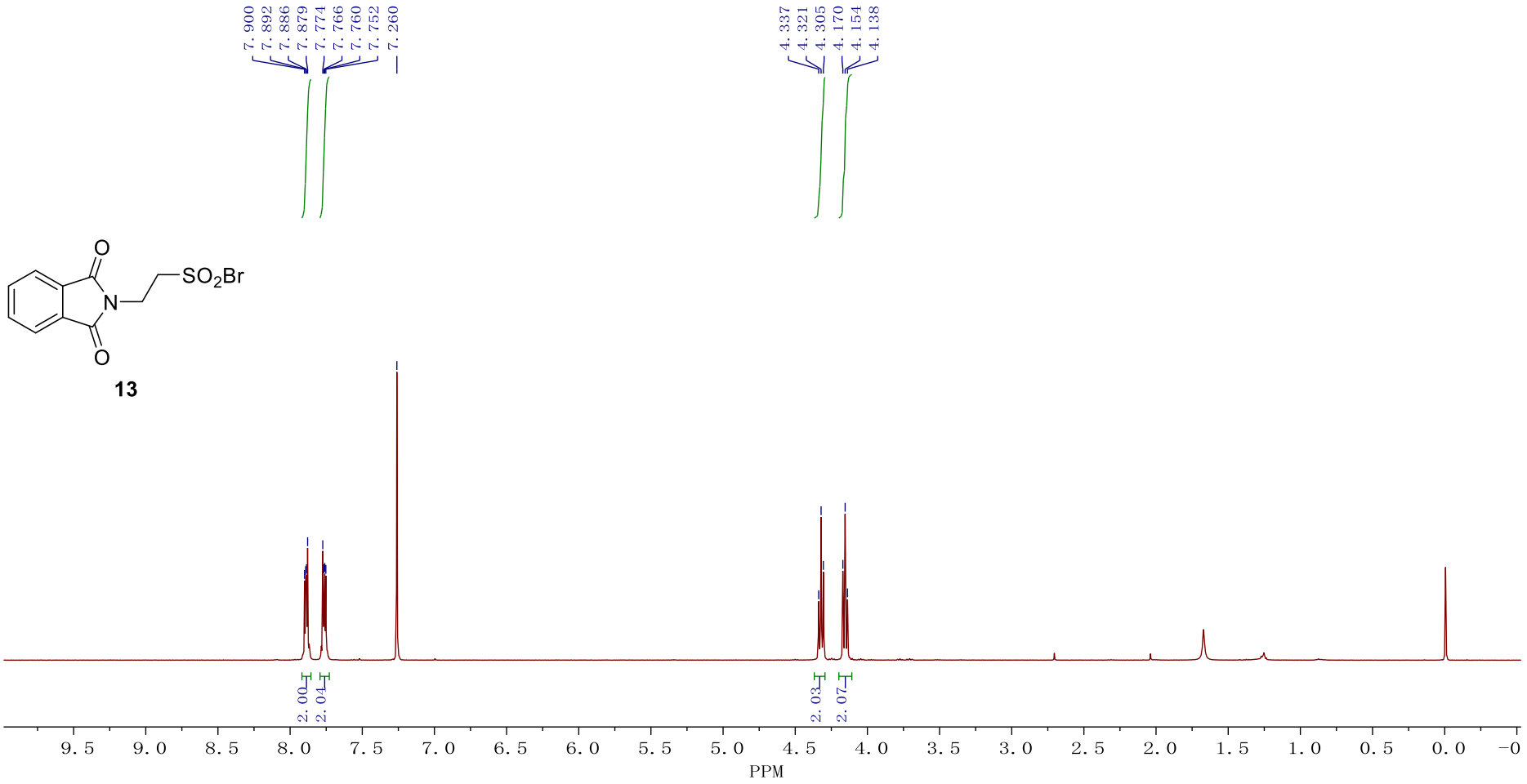
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM

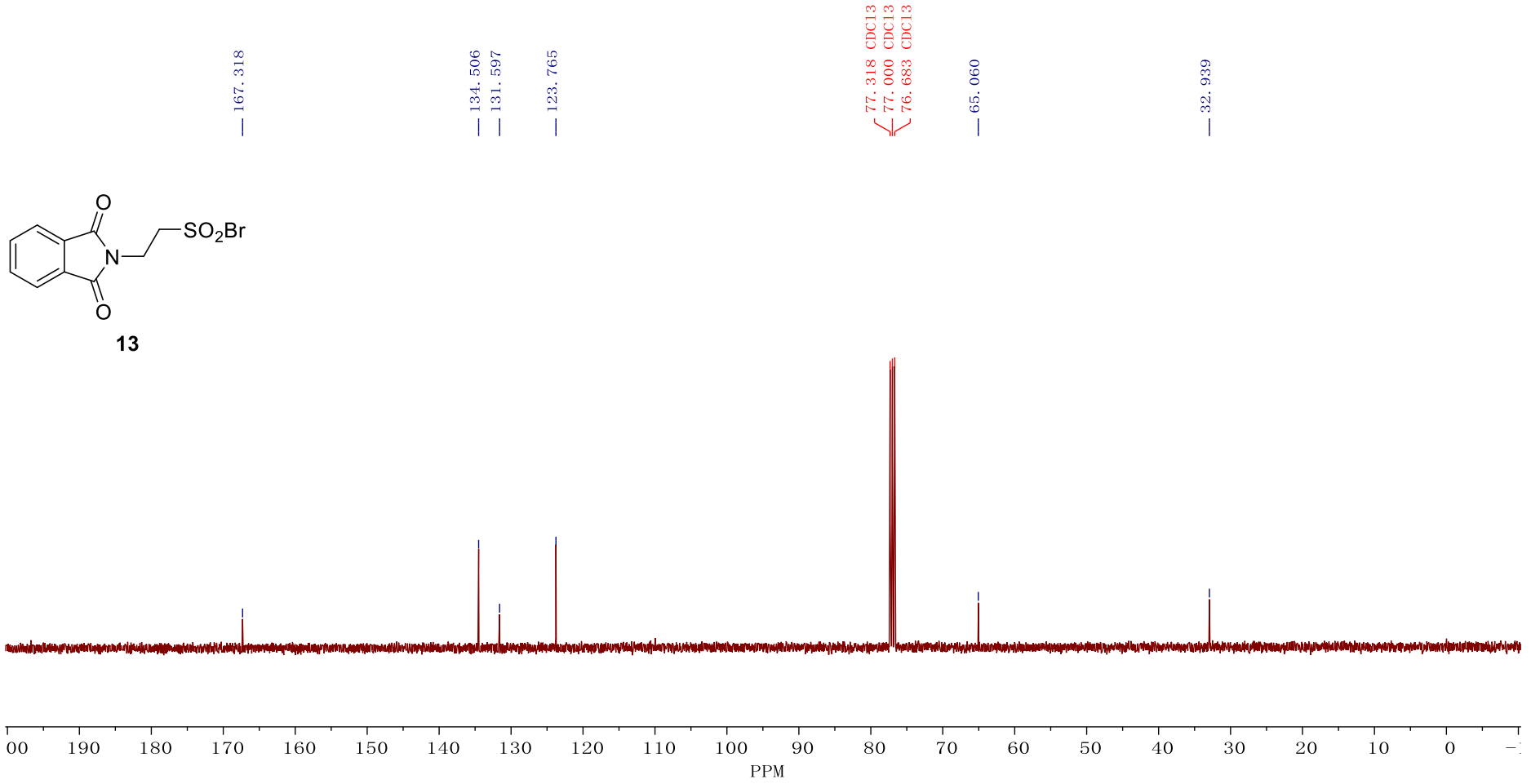

Me
SO2Br
Me
11
7.260
3.757
3.745
3.737
3.729
3.717
1.934
1.922
1.917
1.912
1.906
1.897
1.889
1.877
1.840
1.824
1.807
1.791
1.774
1.757
1.741
0.994
0.978
2.01
2.01
1.03
6.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
PPM

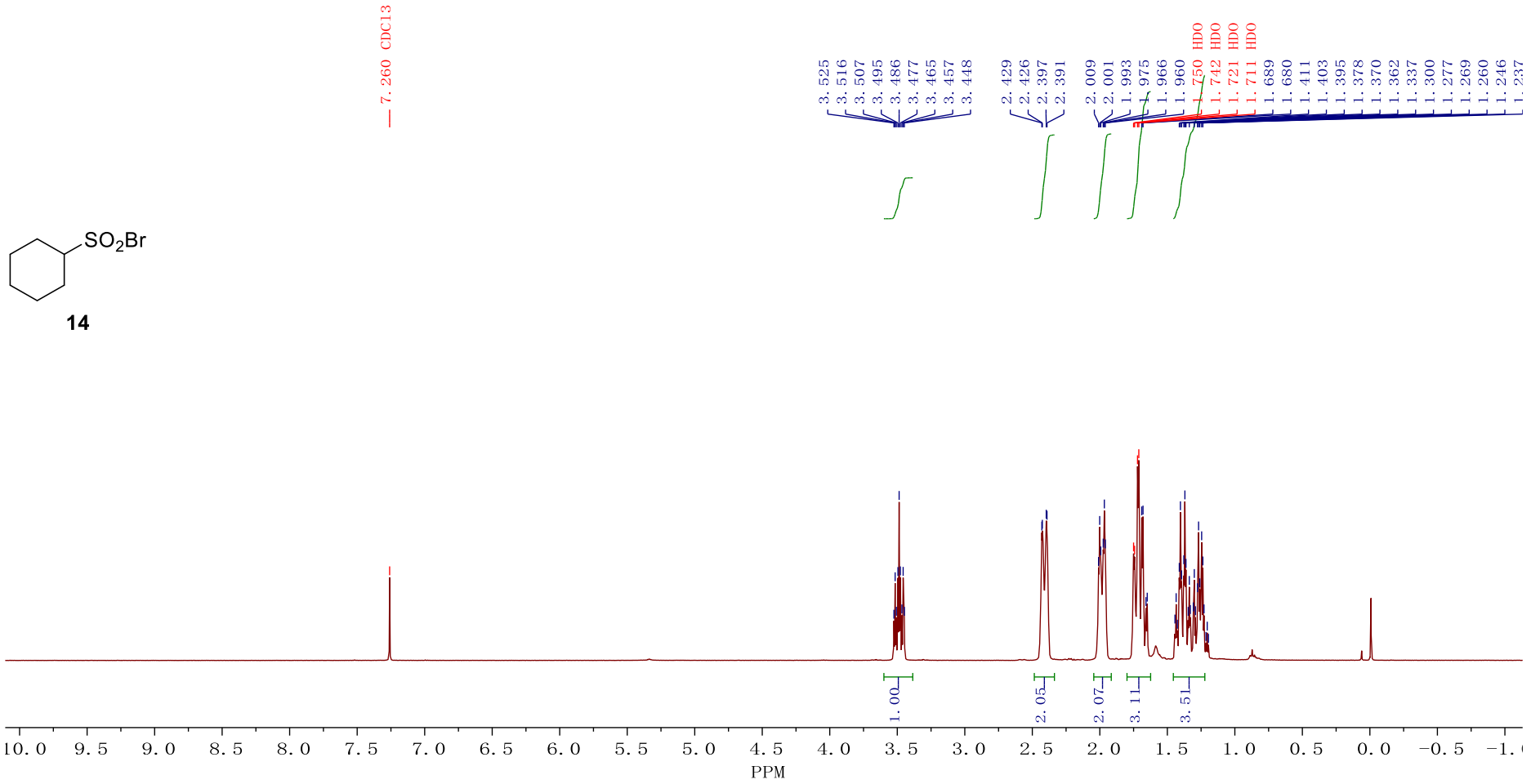

77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
68.207
32.847
26.657
22.018
Me
SO2Br
Me
11
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM

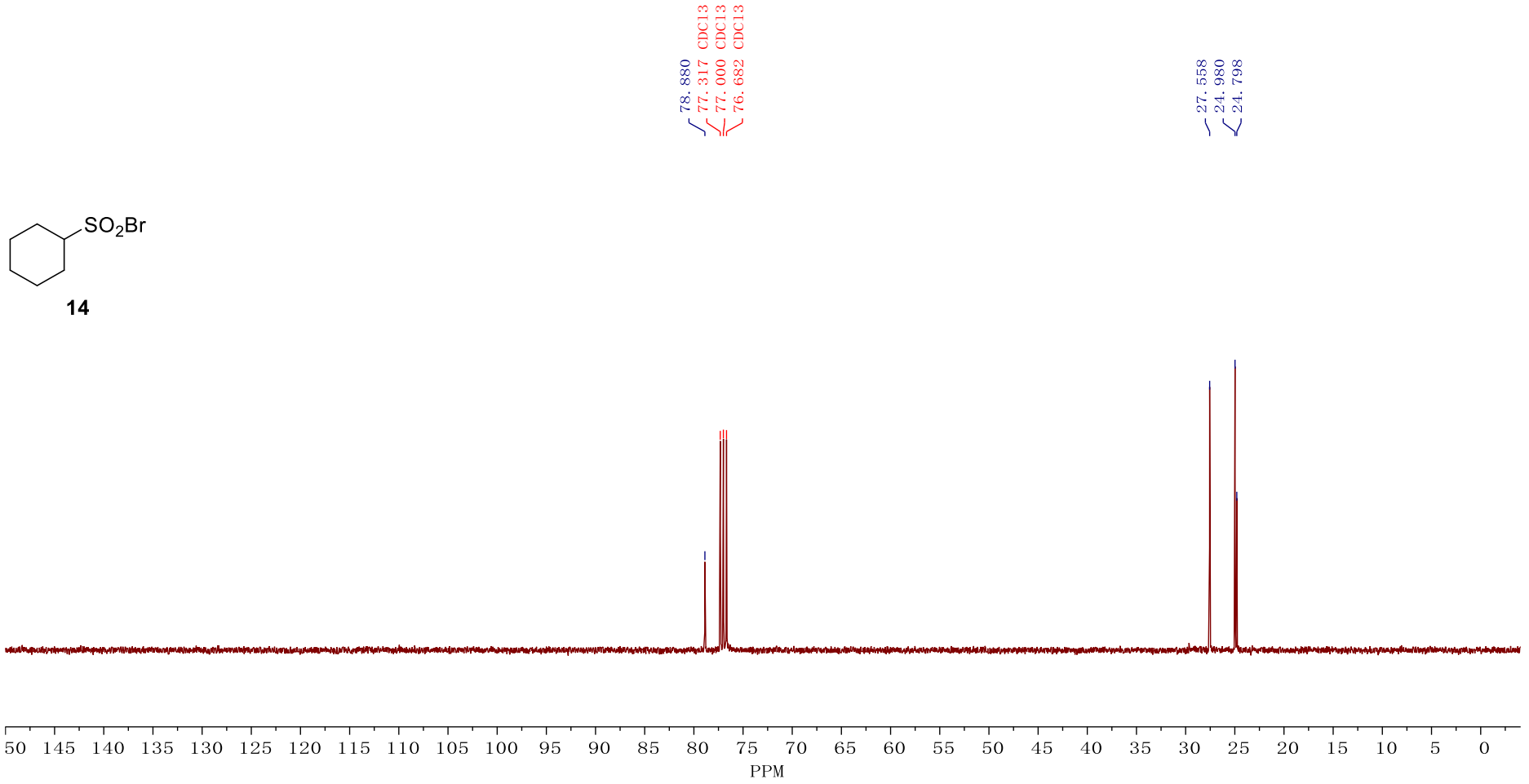

7.444
7.260
4.909
SO2Br
Cl
12
3.99
2.03
PPM


136.814
132.799
129.542
124.906
77.318 CDC13
77.000 CDC13
76.682 CDC13
73.968
SO2Br
Cl
12
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM


7.900
7.892
7.886
7.879
7.774
7.766
7.760
7.752
7.260
4.337
4.321
4.305
4.170
4.154
4.138
O
N
SO2Br
O
13
2.00
2.04
2.03
2.07
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
PPM


167.318
134.506
131.597
123.765
77.318 CDC13
77.000 CDC13
76.683 CDC13
65.060
32.939
O
N
SO2Br
O
13
PPM


7.260 CDCl3
3.525
3.516
3.507
3.495
3.486
3.477
3.465
3.457
3.448
2.429
2.426
2.397
2.391
2.009
2.001
1.993
1.975
1.966
1.960
1.750 HDO
1.742 HDO
1.721 HDO
1.711 HDO
1.689
1.680
1.411
1.403
1.395
1.378
1.370
1.362
1.337
1.300
1.277
1.269
1.260
1.246
1.237
SO2Br
14
1.00
2.05
2.07
3.11
3.51
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
PPM


78.880
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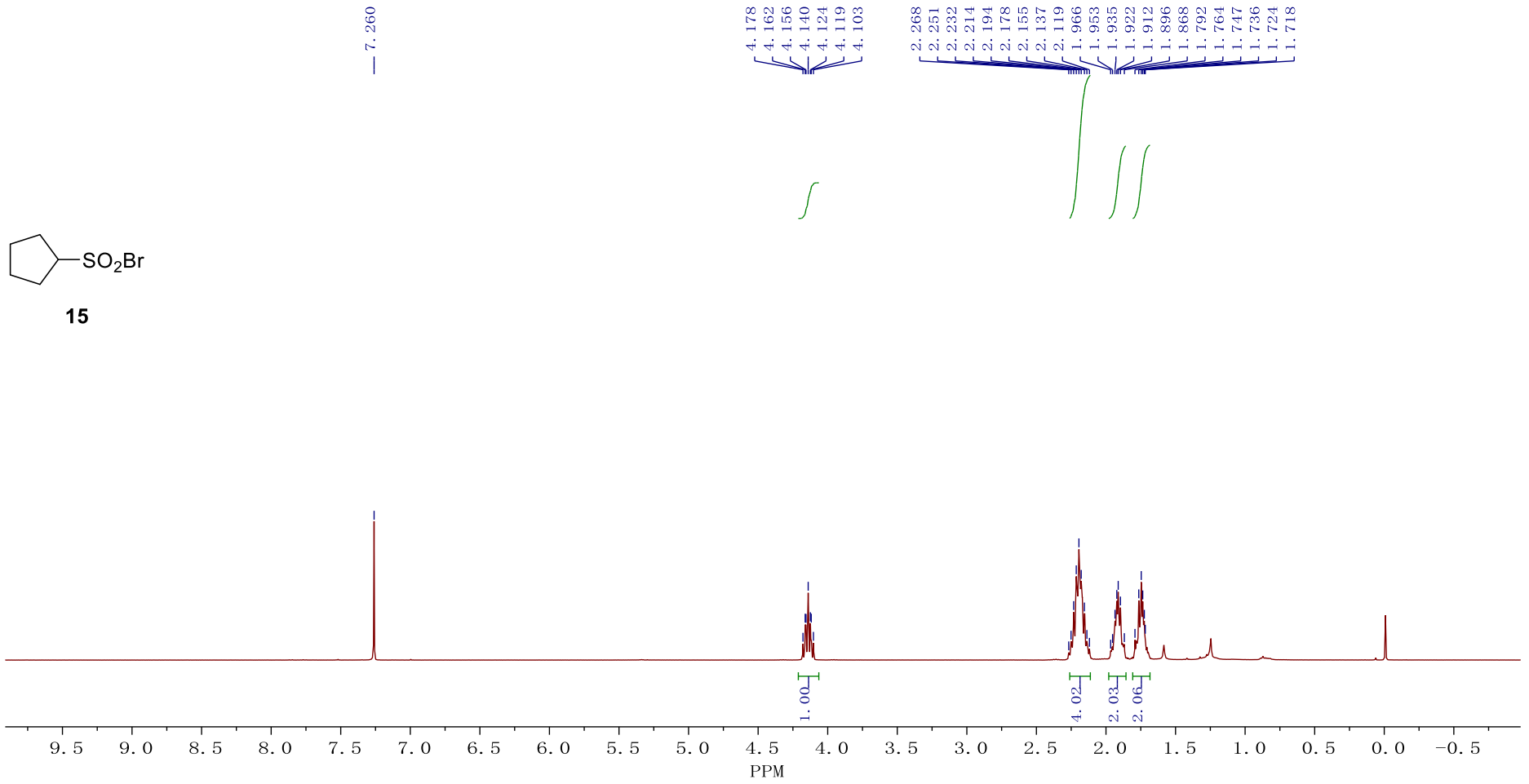
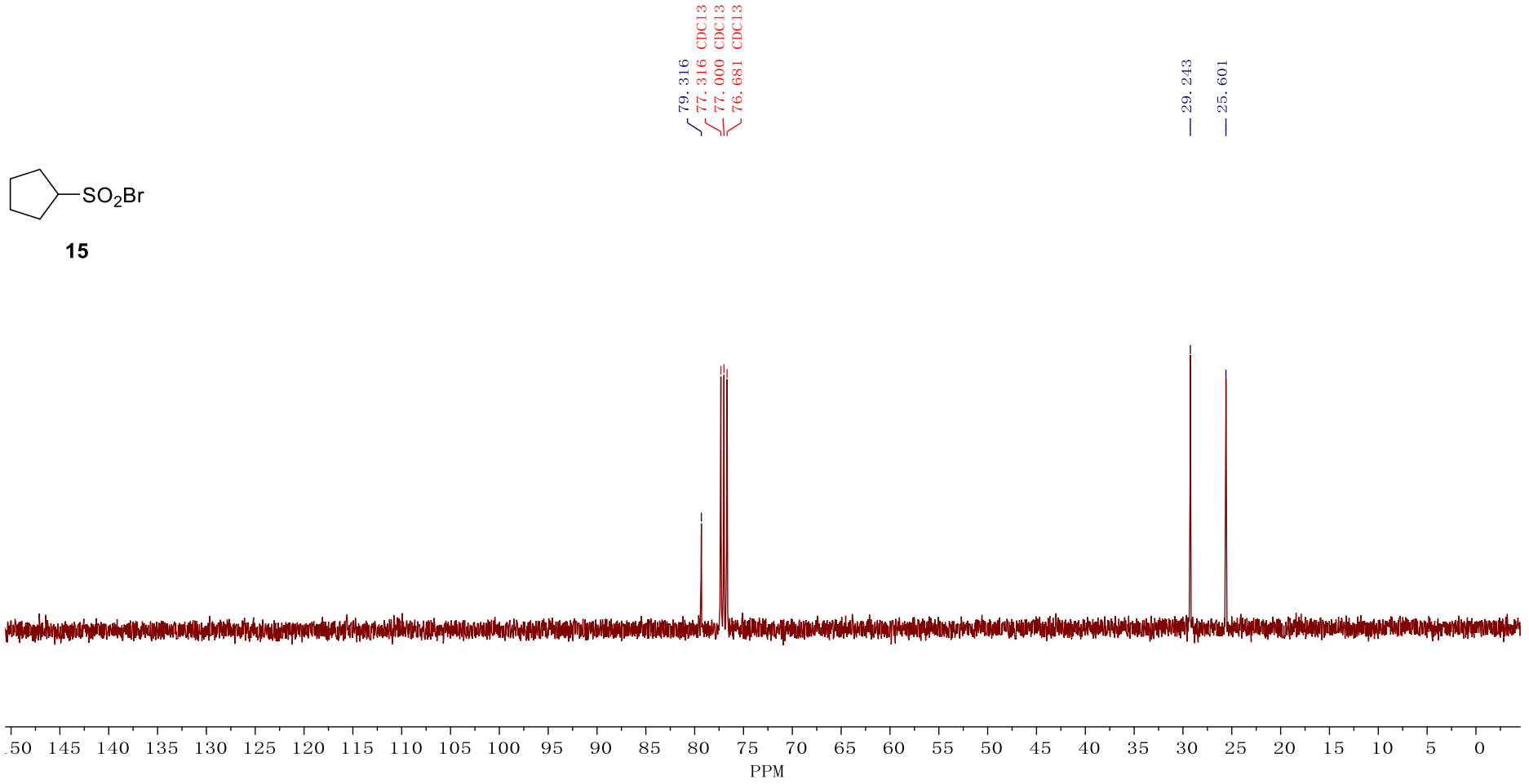
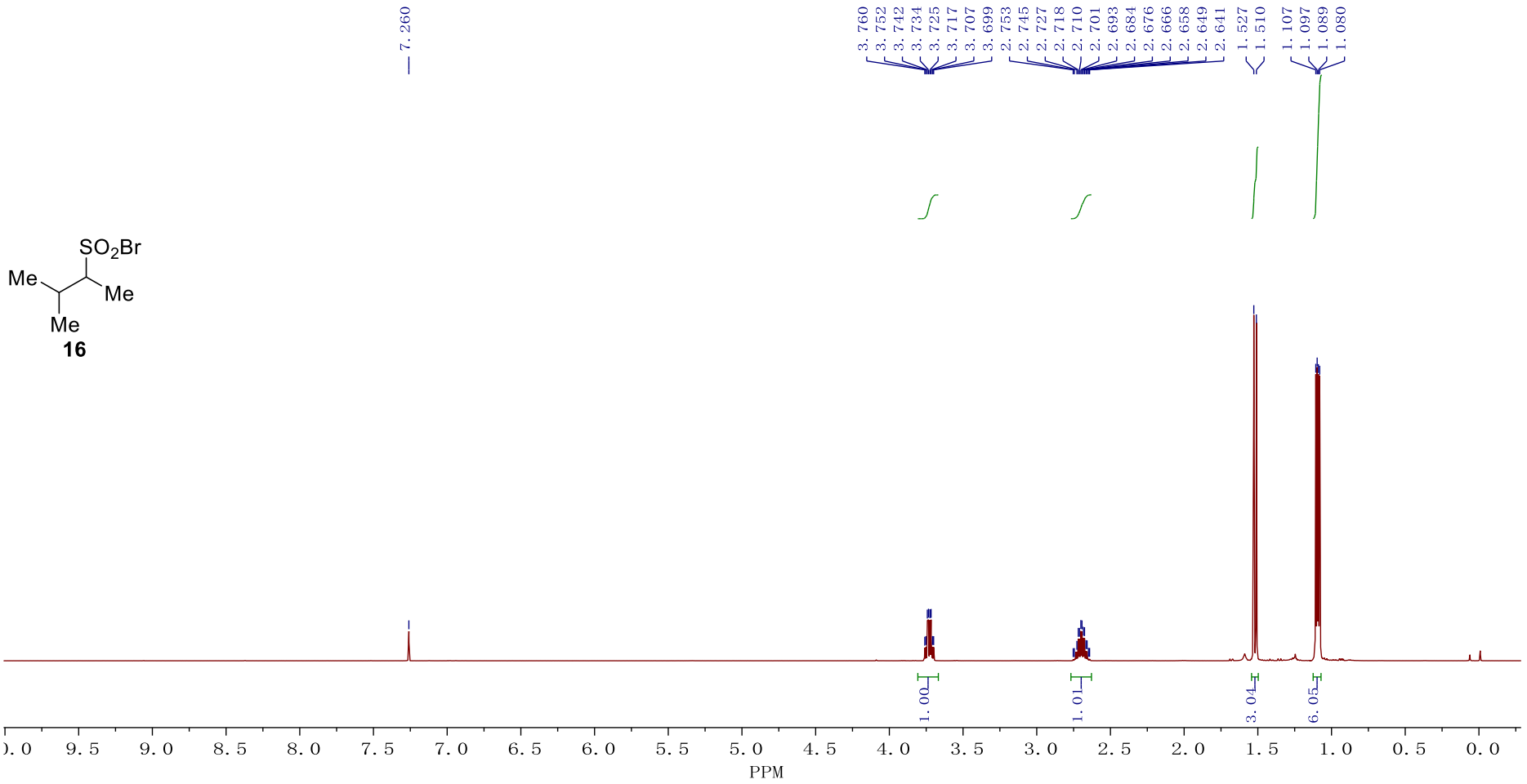
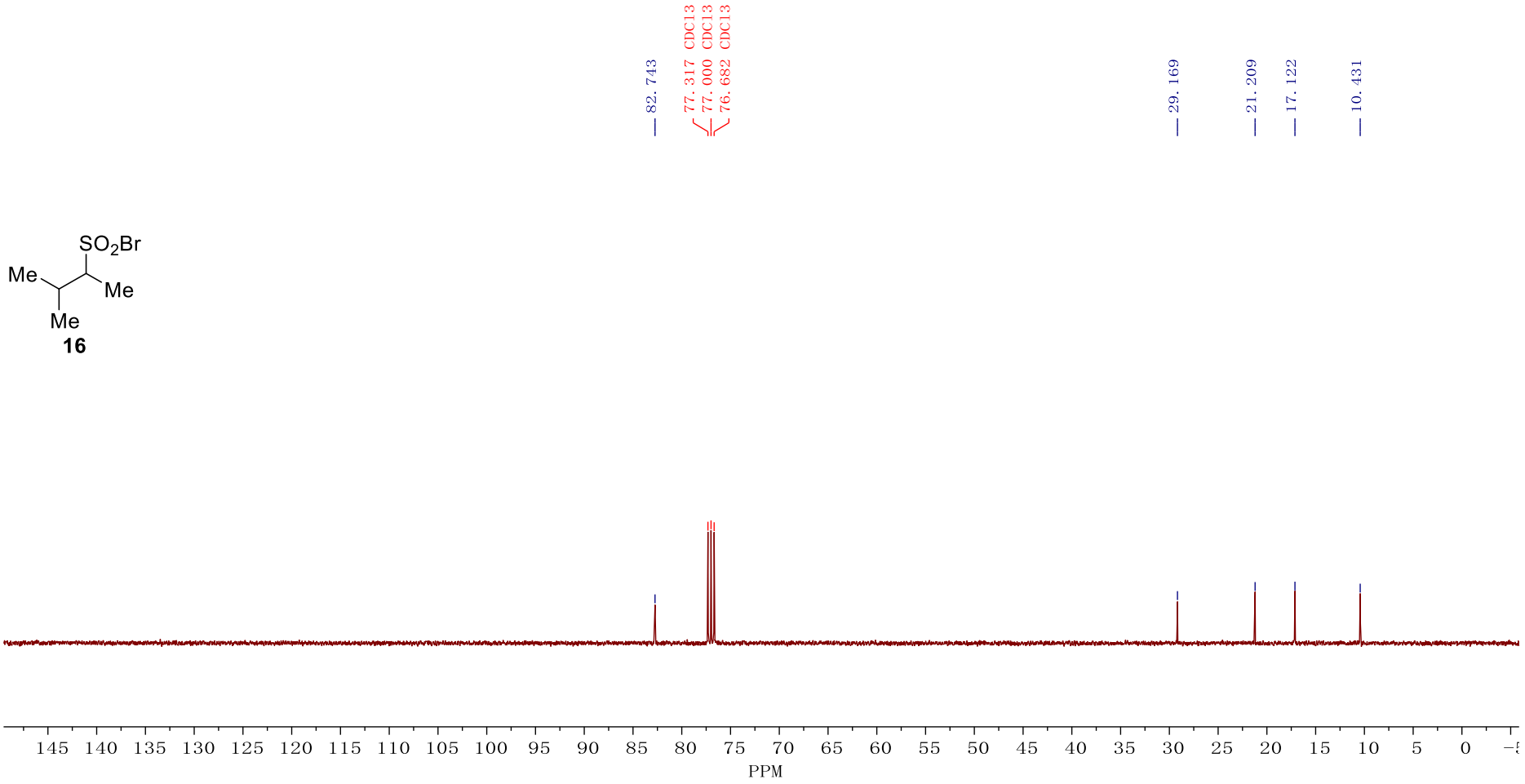
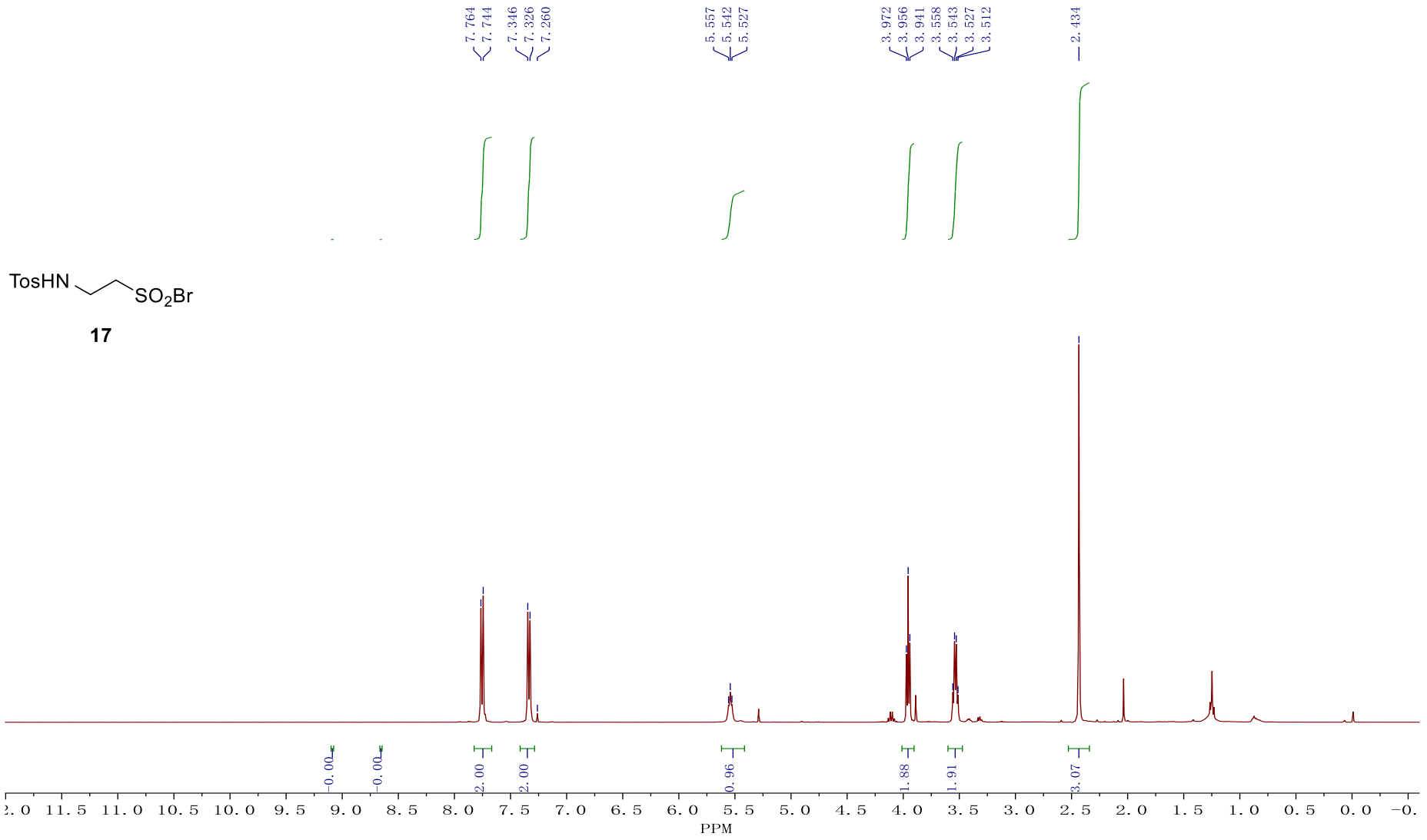
77.000 CDCl3
76.682 CDCl3
27.558
24.980
24.798
SO2Br
14
50 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
PPM

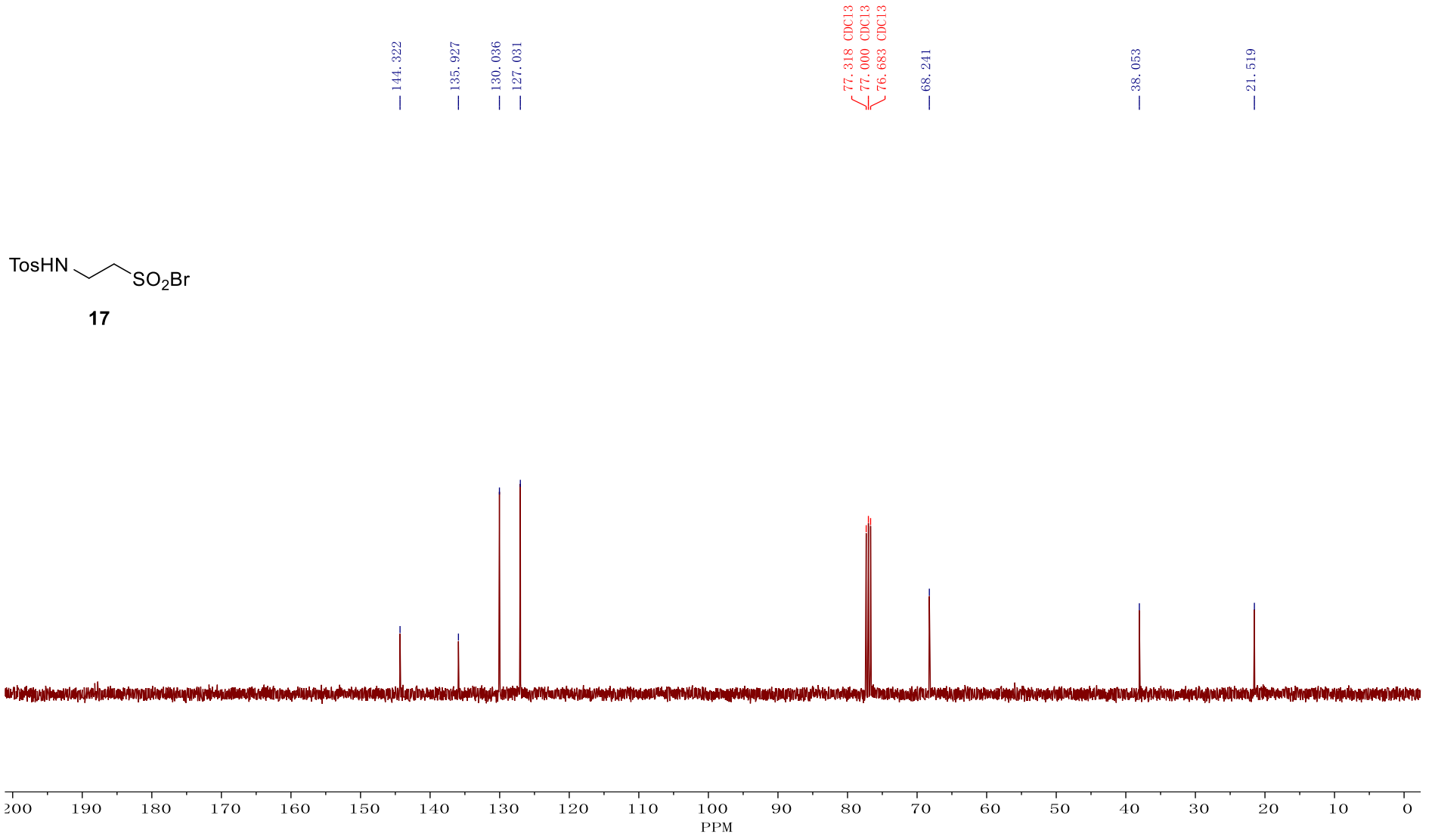

7.260
4.178
4.162
4.156
4.140
4.124
4.119
4.103
2.268
2.251
2.232
2.214
2.194
2.178
2.155
2.137
2.119
1.966
1.953
1.935
1.922
1.912
1.896
1.868
1.792
1.764
1.747
1.736
1.724
1.718
SO2Br
15
1.00
4.02
2.03
2.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
PPM

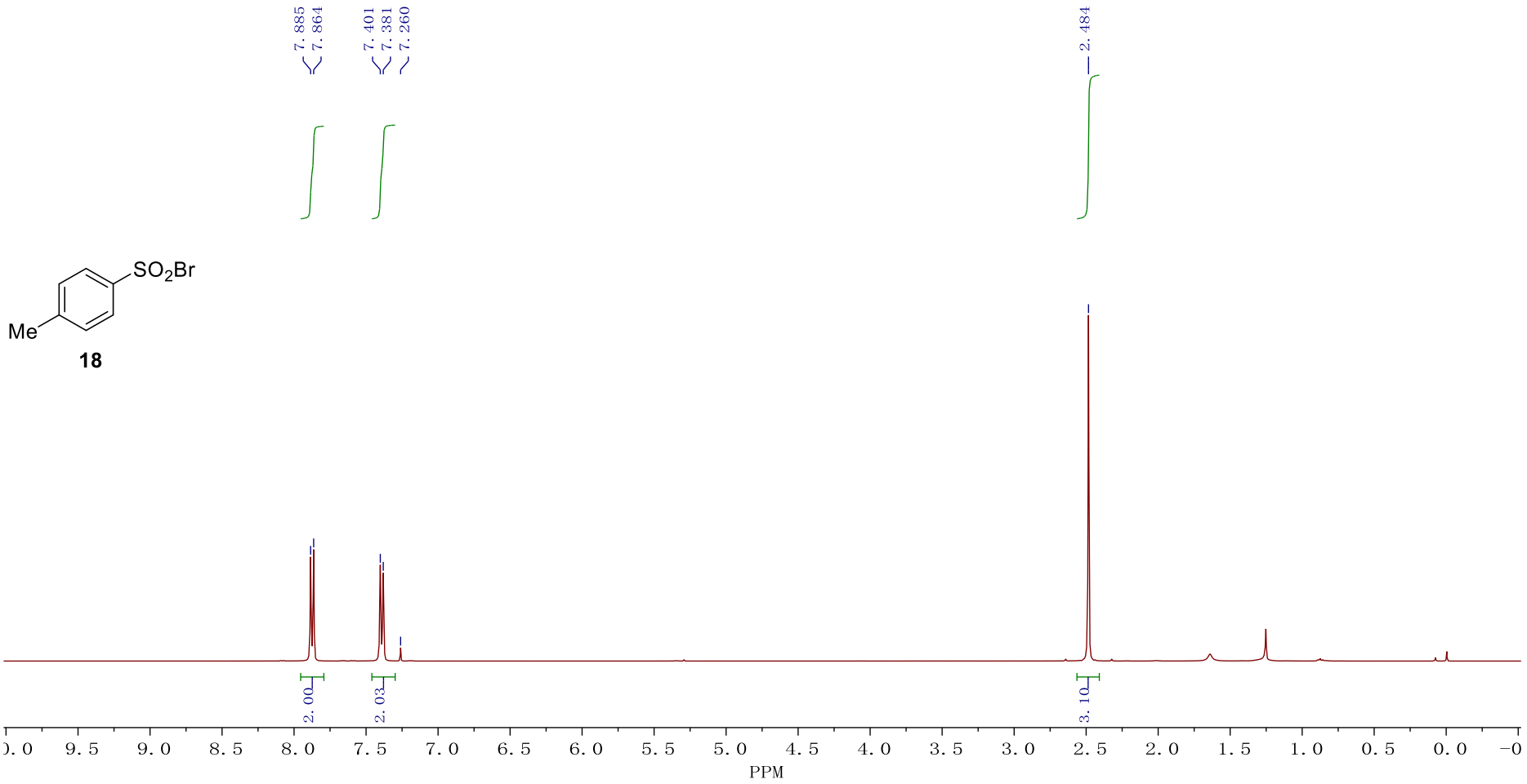

79.316
77.316 CDCl3
77.000 CDCl3
76.681 CDCl3
29.243
25.601
SO2Br
15
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
PPM

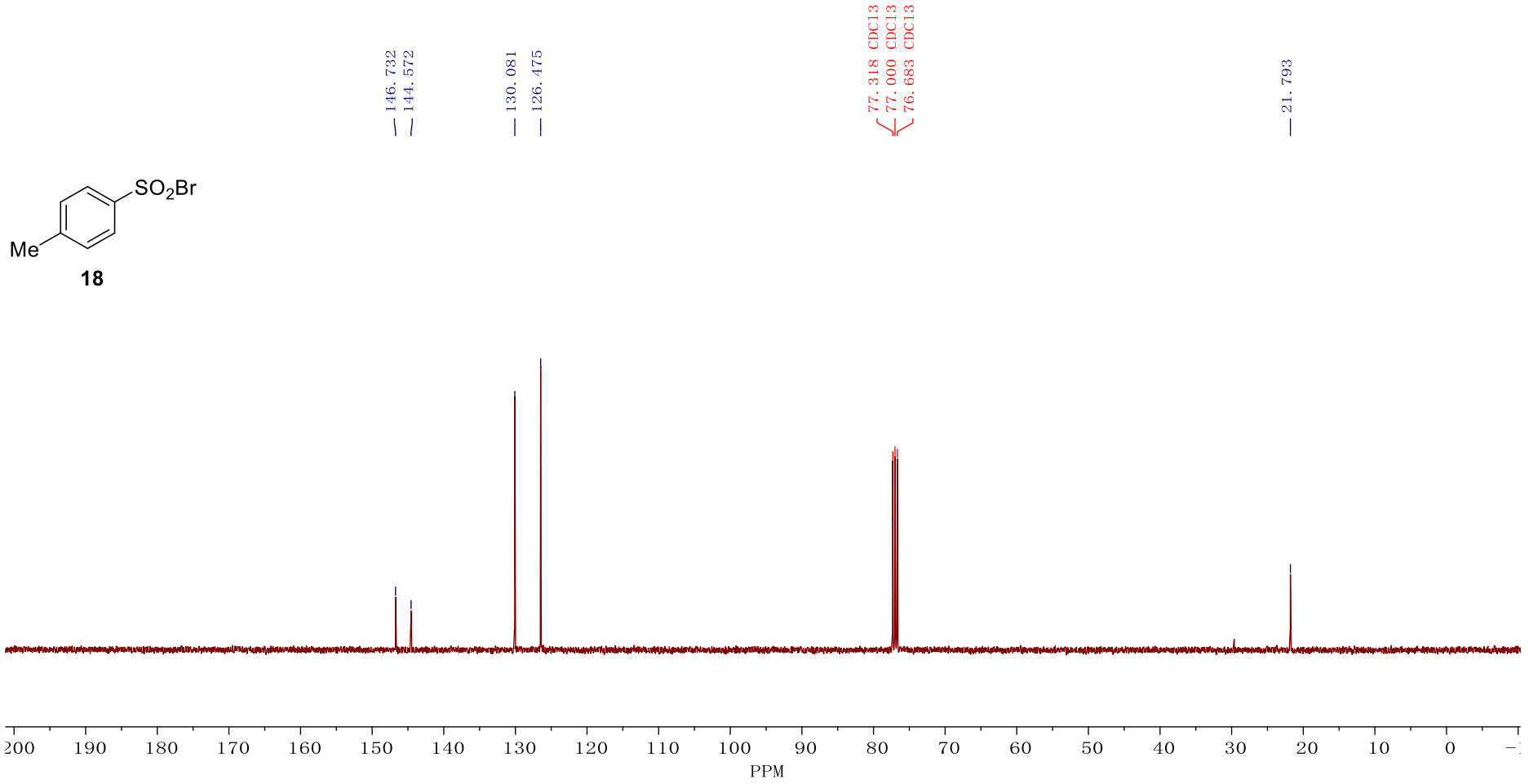

7.260
3.760
3.752
3.742
3.734
3.725
3.717
3.707
3.699
2.753
2.745
2.727
2.718
2.710
2.701
2.693
2.684
2.676
2.666
2.658
2.649
2.641
1.527
1.510
1.107
1.097
1.089
1.080
SO2Br
Me
Me
Me
16
1.00
1.01
3.04
6.05
PPM

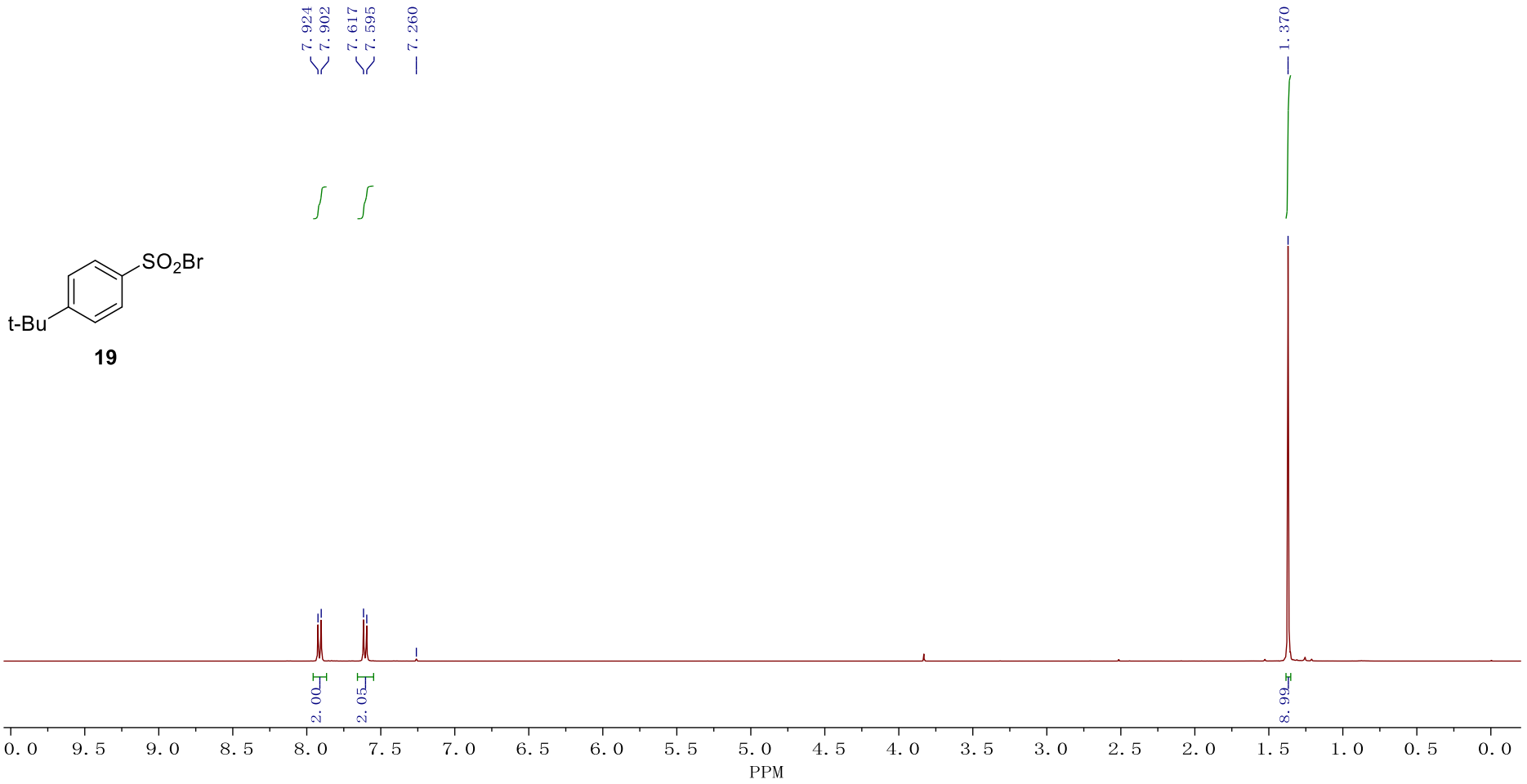

82.743
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
29.169
21.209
17.122
10.431
SO2Br
Me
Me
Me
16
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
PPM

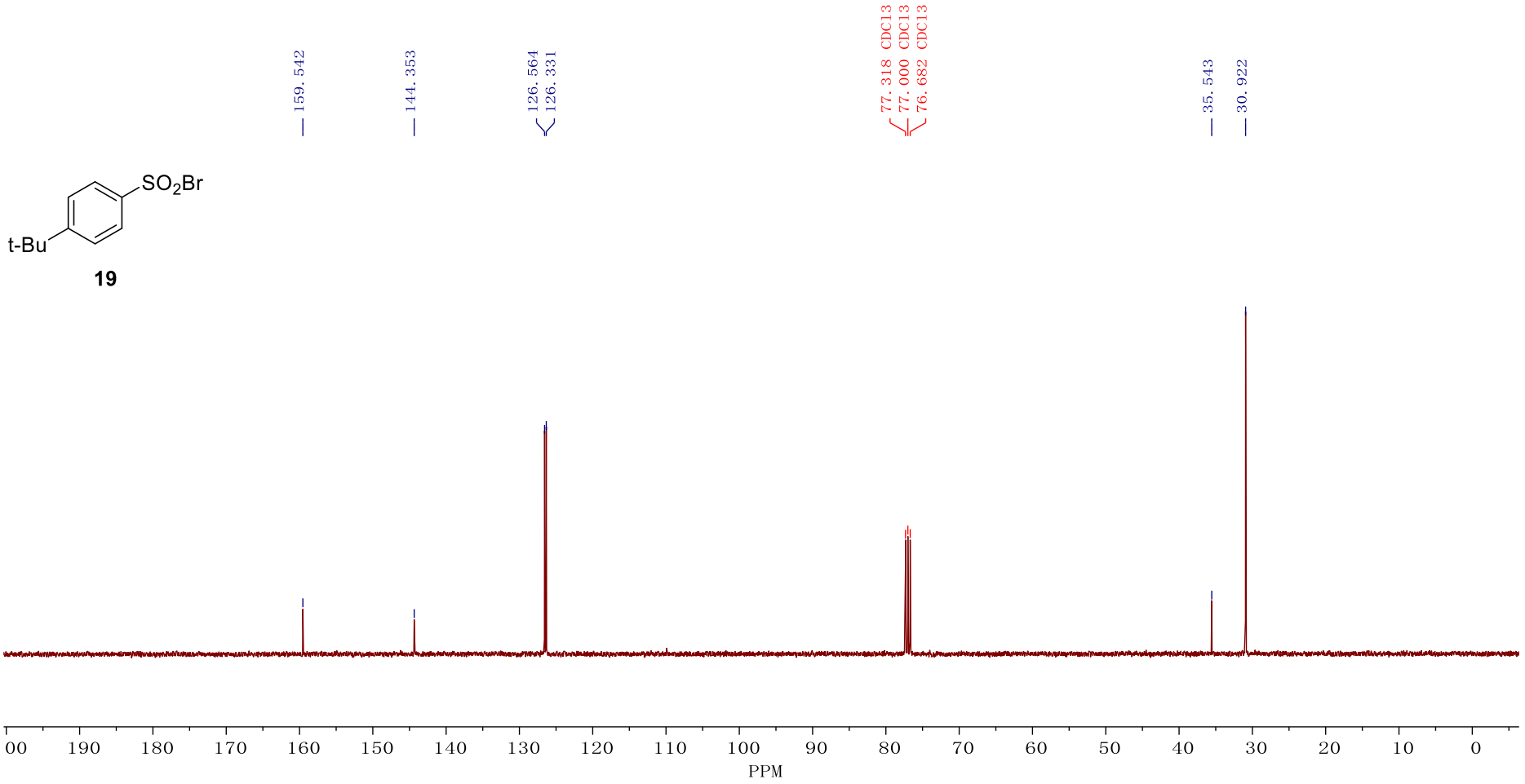

7.764
7.744
7.346
7.326
7.260
5.557
5.542
5.527
3.972
3.956
3.941
3.558
3.543
3.527
3.512
2.434
TosHN
SO2Br
17
0.00
0.00
2.00
2.00
0.96
1.88
1.91
3.07
PPM

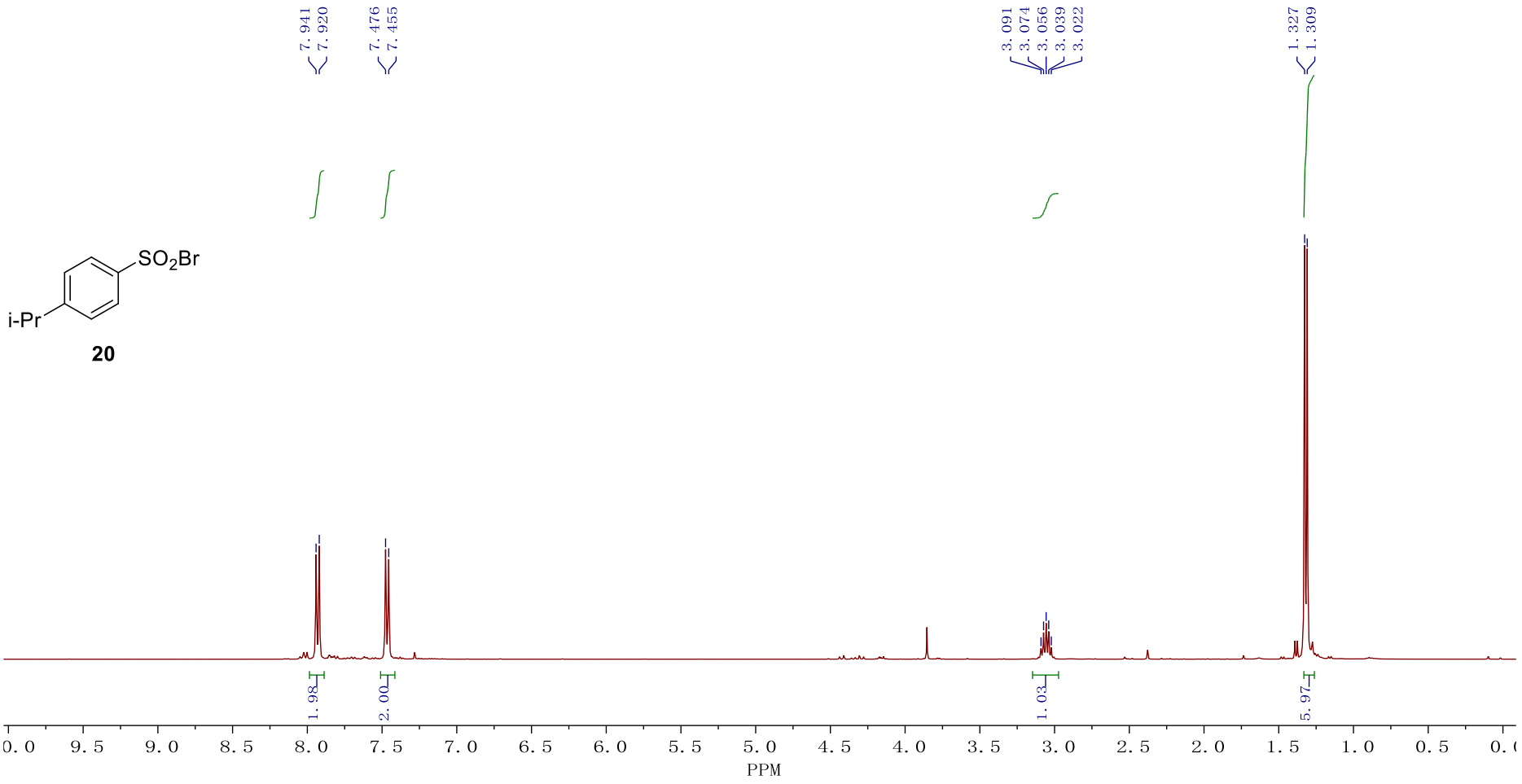

144.322
135.927
130.036
127.031
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
68.241
38.053
21.519
TosHN
SO2Br
17
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM

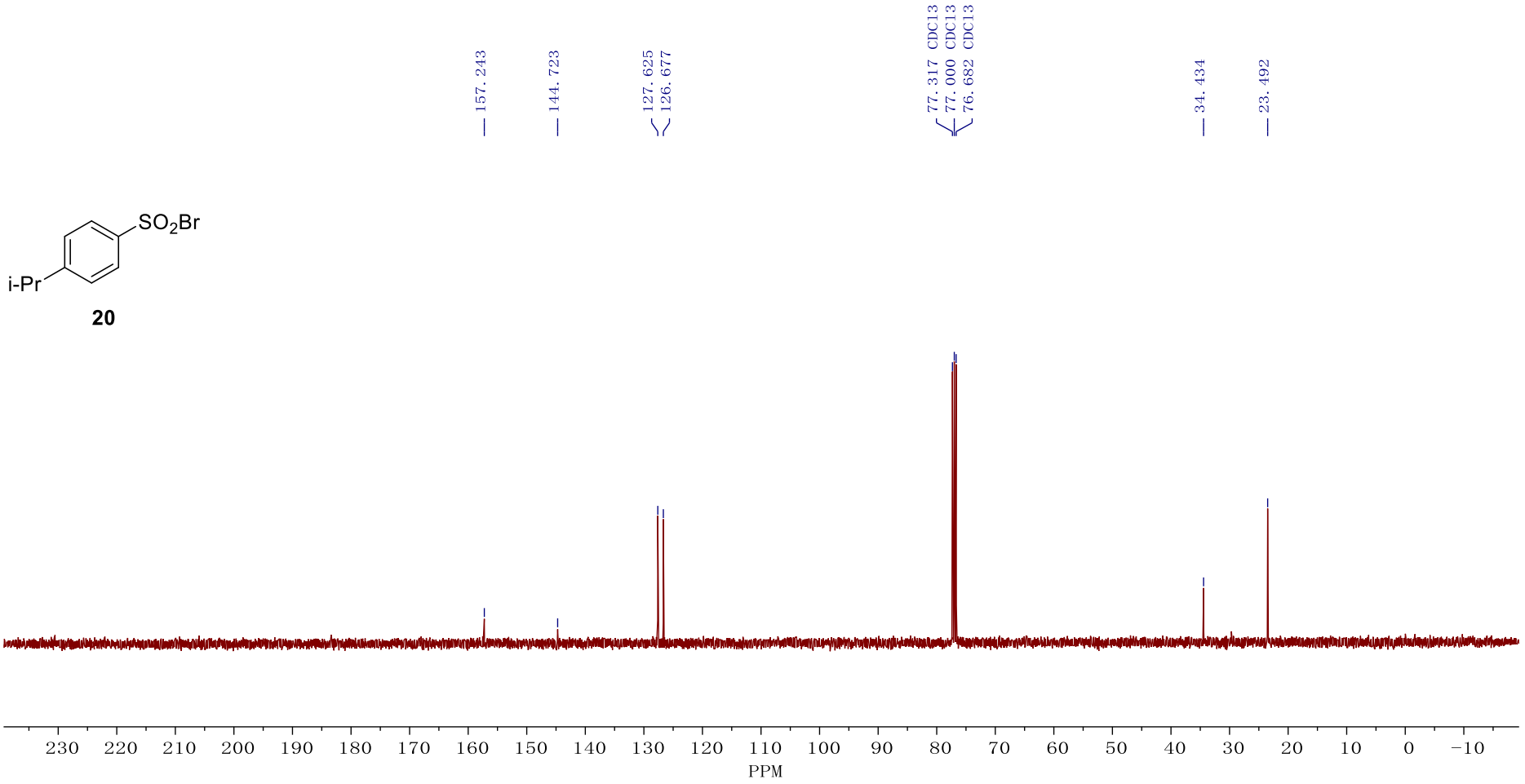

7.885
7.864
7.401
7.381
7.260
2.484
SO2Br
Me
18
2.00
2.03
3.10
PPM

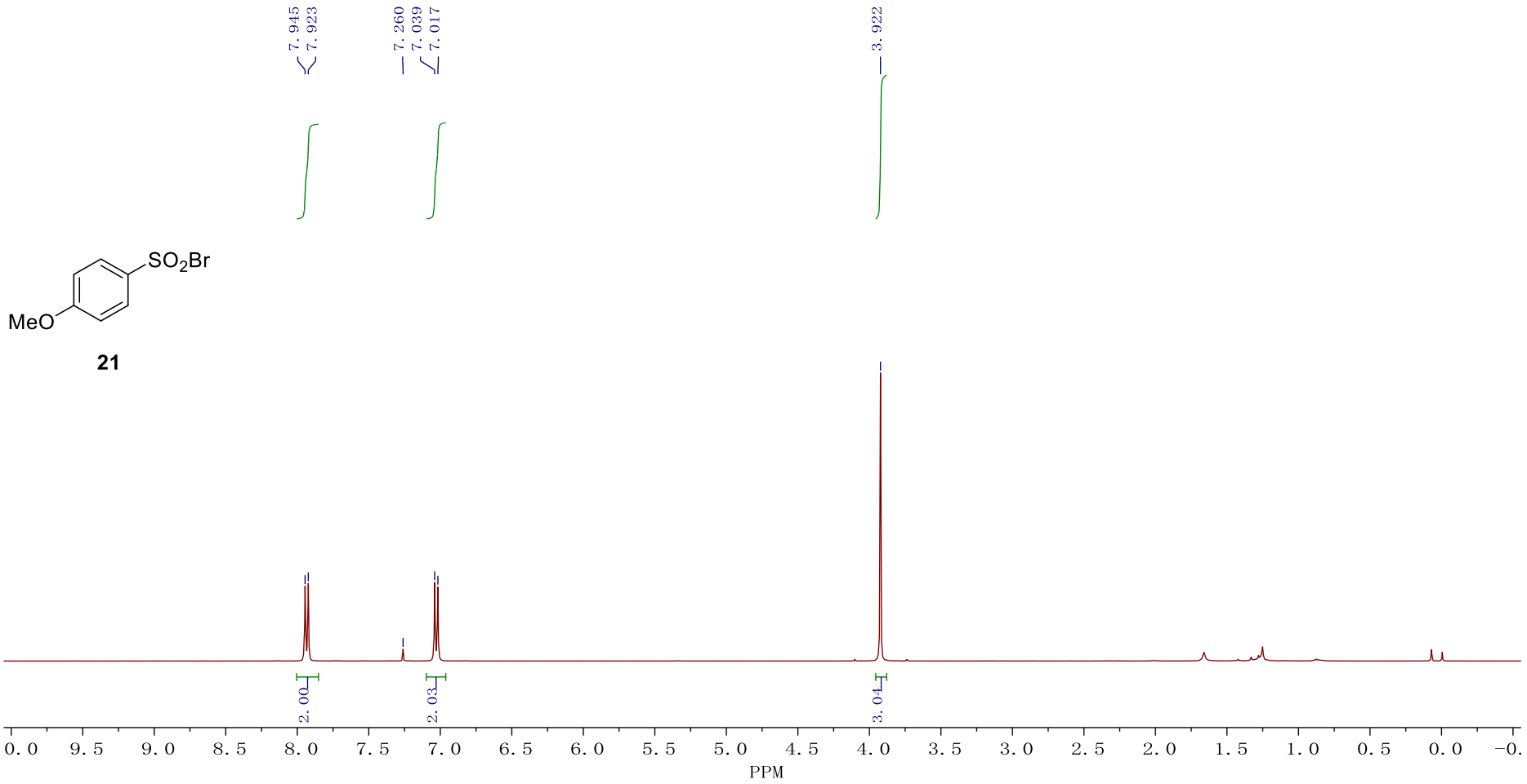

146.732
144.572
130.081
126.475
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
21.793
SO2Br
Me
18
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM

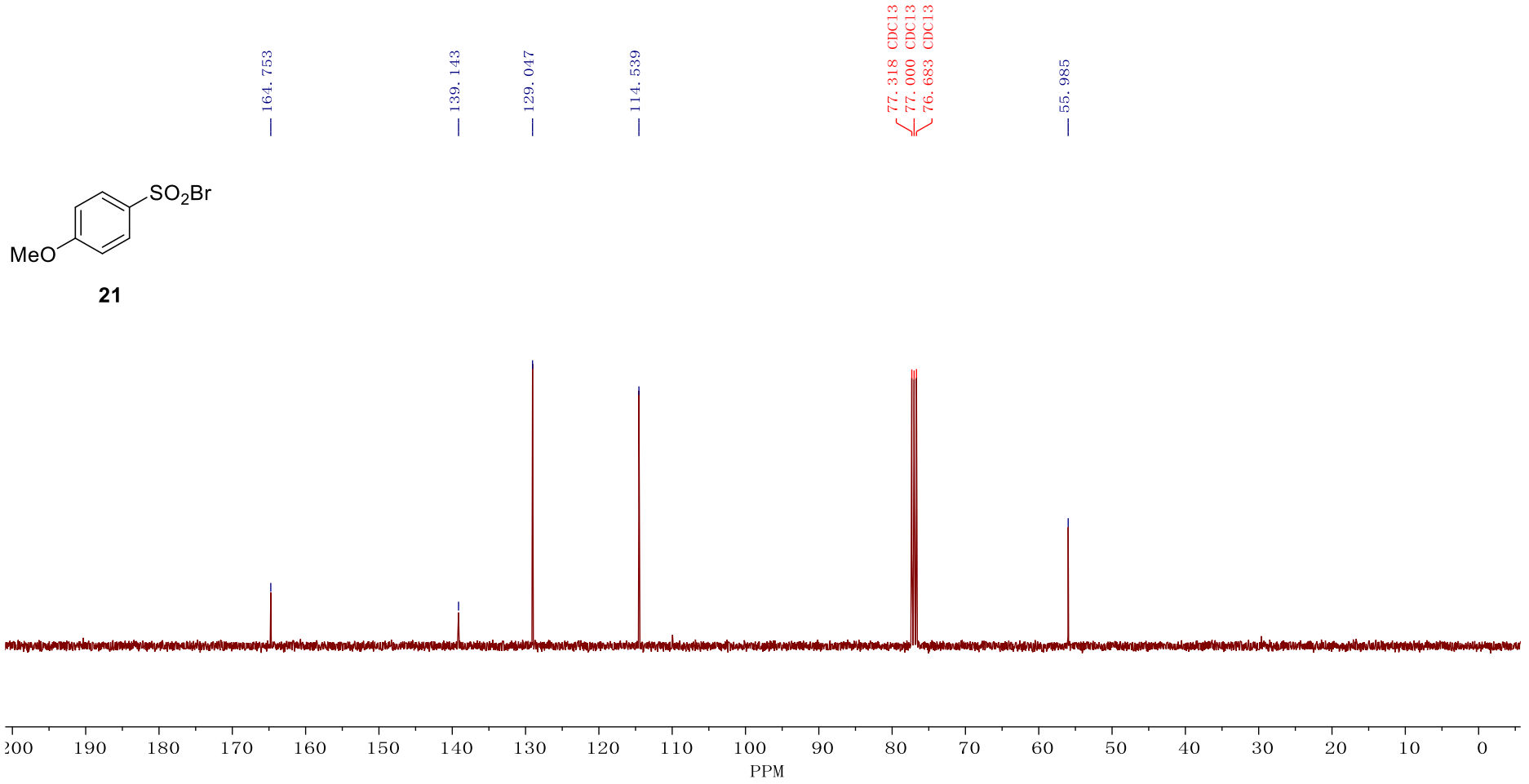

7.924
7.902
7.617
7.595
7.260
1.370
SO2Br
t-Bu
19
2.00
2.05
8.99
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
PPM

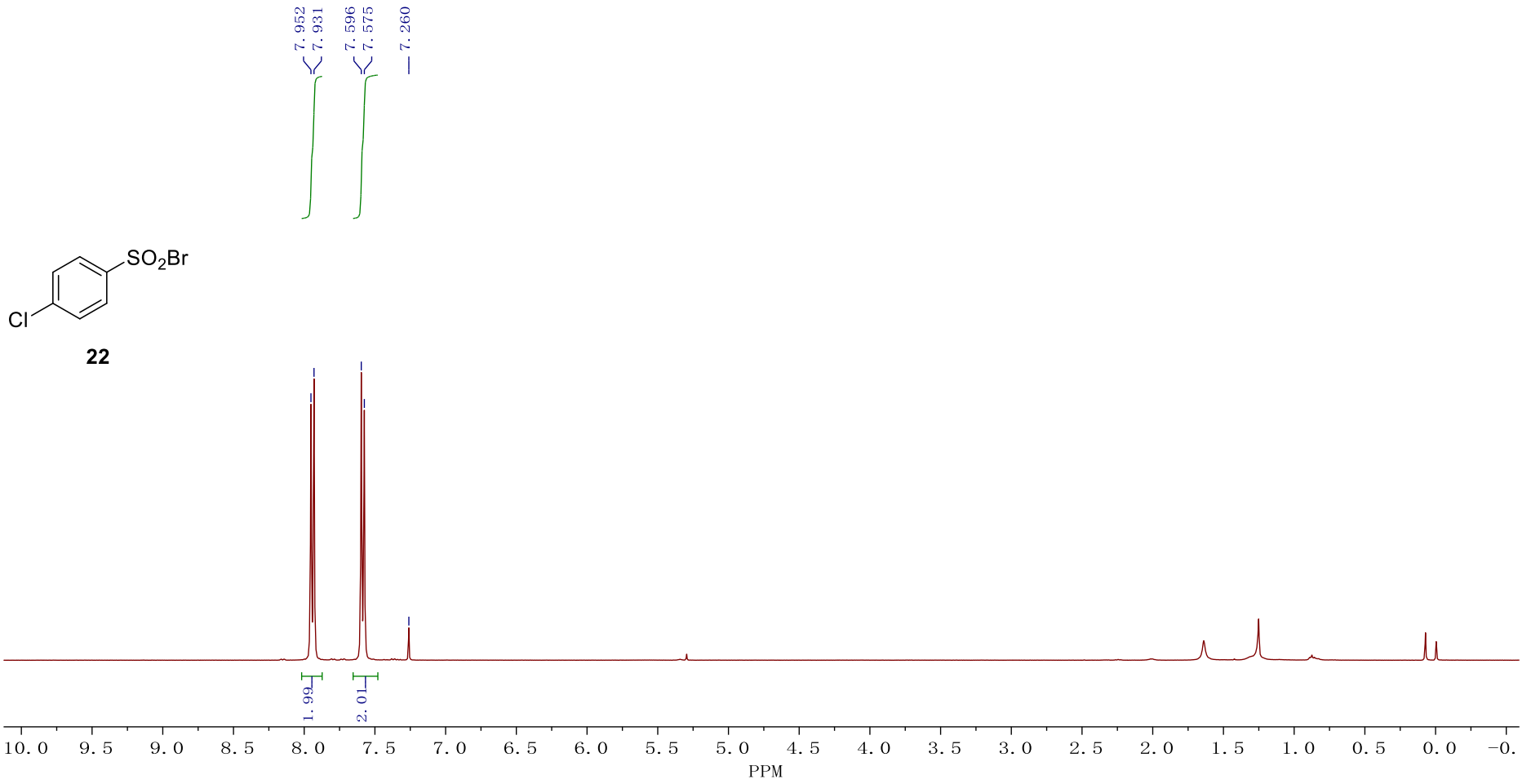

159.542
144.353
126.564
126.331
77.318 CDC13
77.000 CDC13
76.682 CDC13
35.543
30.922
SO2Br
t-Bu
19
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
PPM

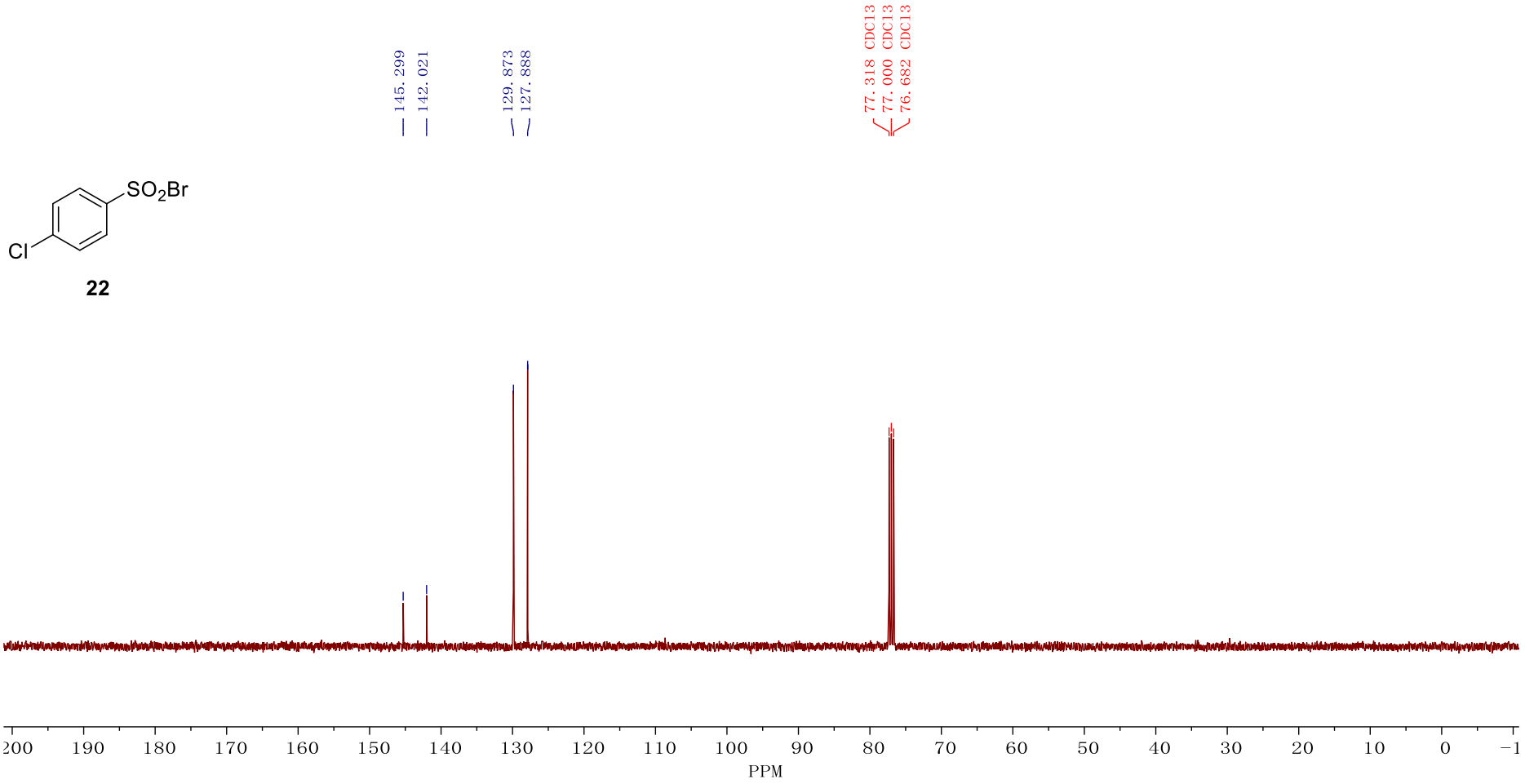

7.941
7.920
7.476
7.455
3.091
3.074
3.056
3.039
3.022
1.327
1.309
SO2Br
i-Pr
20
1.98
2.00
1.03
5.97
PPM

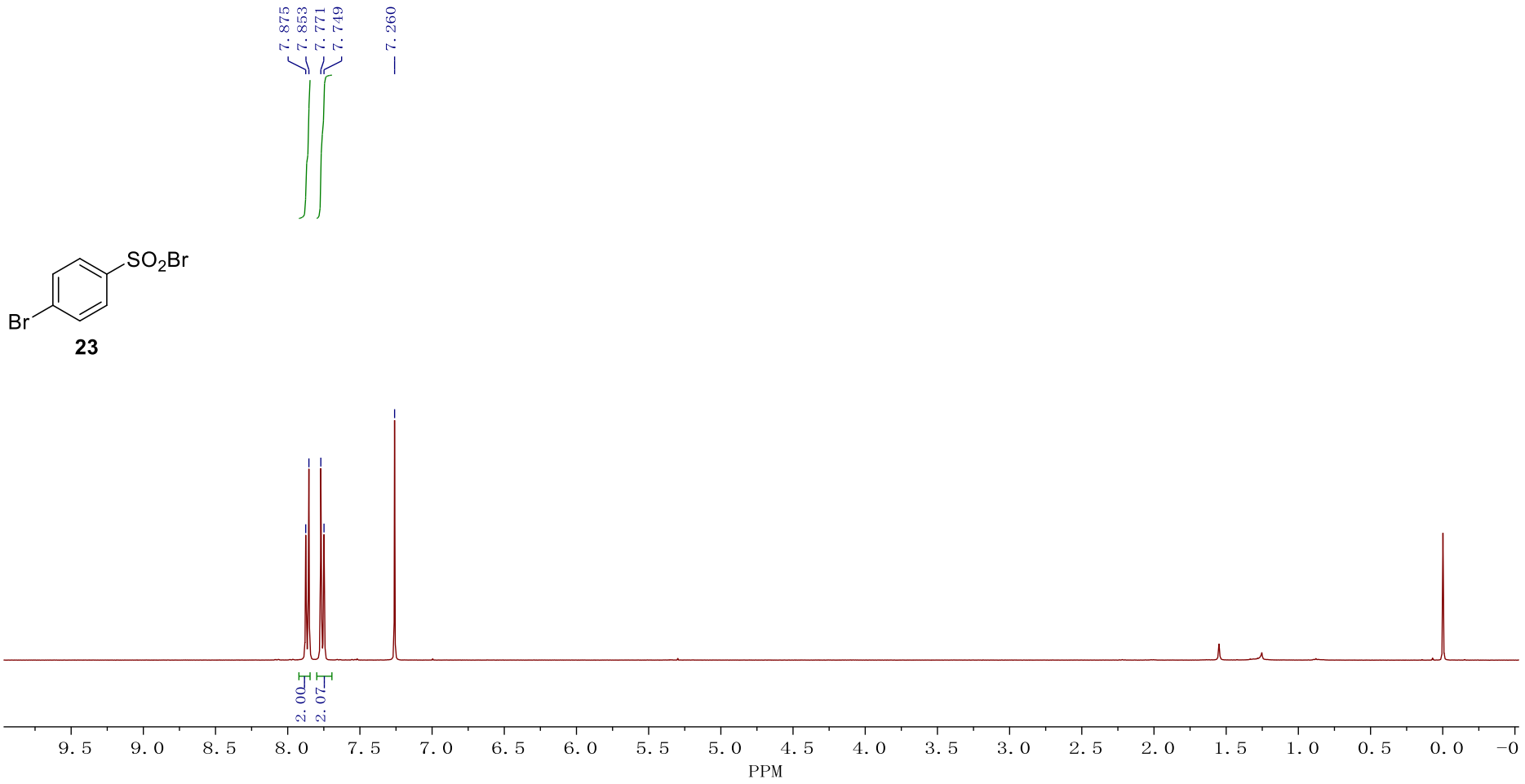

157.243
144.723
127.625
126.677
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
34.434
23.492
SO2Br
i-Pr
20
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
PPM

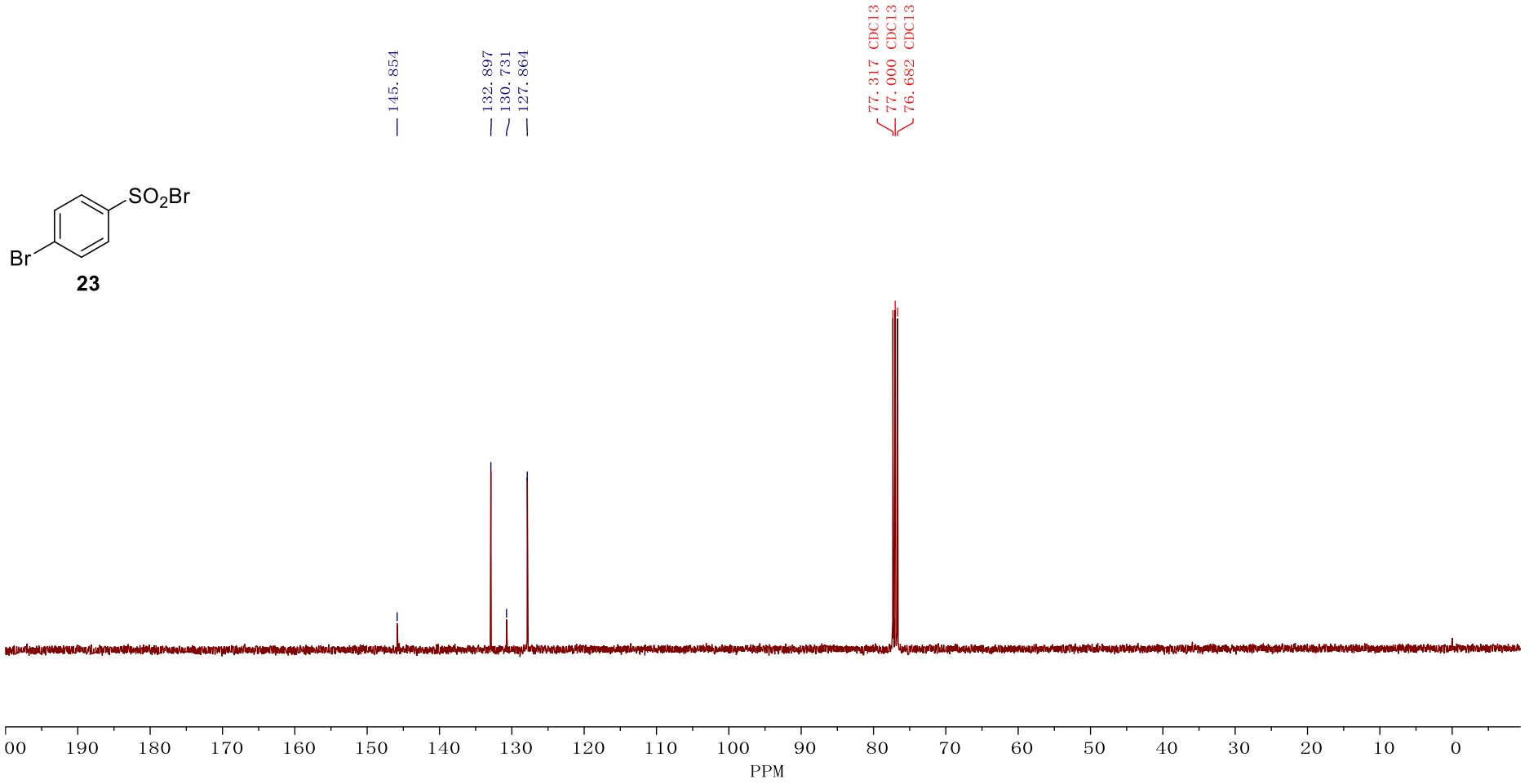

7.945
7.923
7.260
7.039
7.017
3.922
SO2Br
MeO
21
2.00
2.03
3.04
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.
PPM

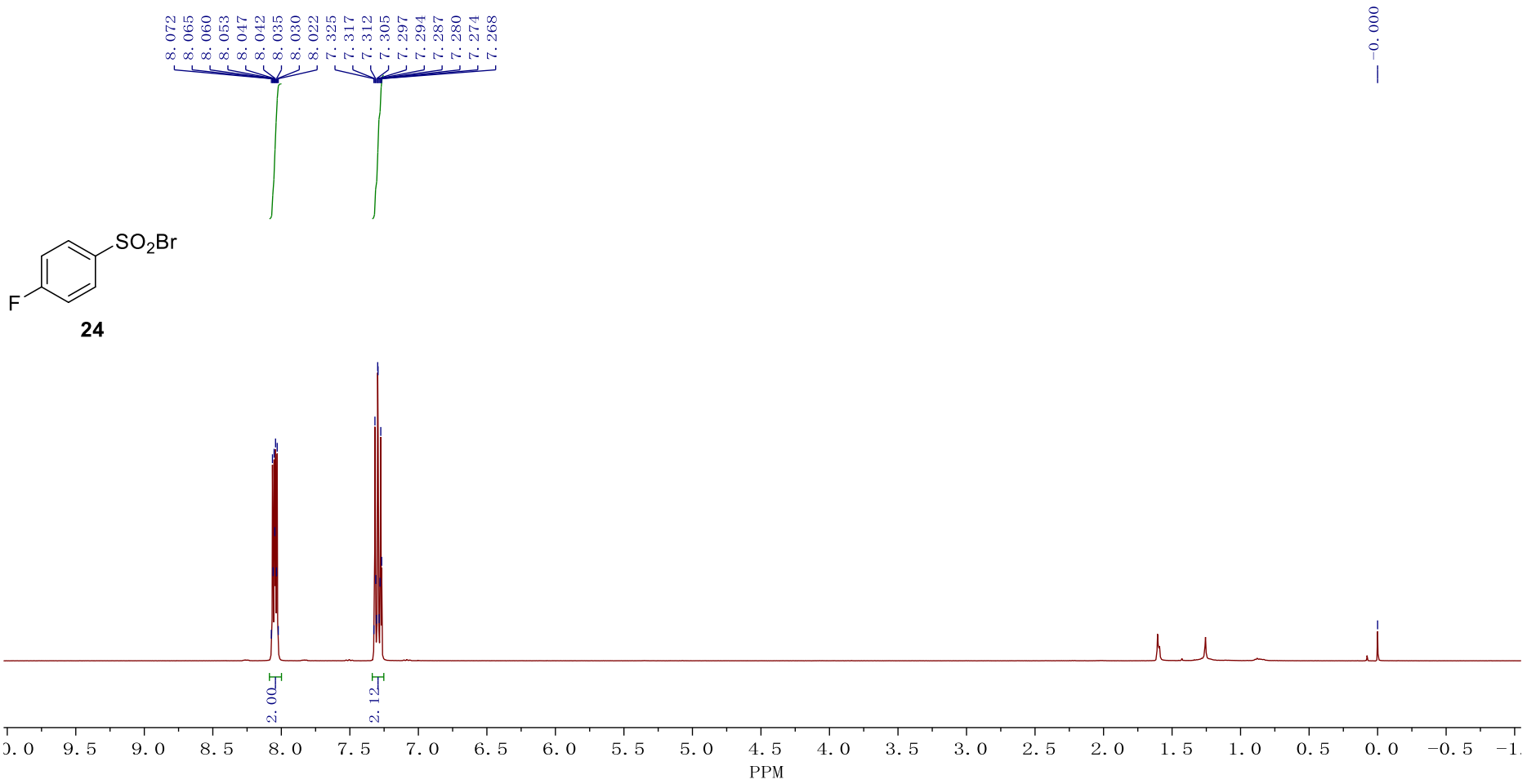

164.753
139.143
129.047
114.539
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
55.985
SO2Br
MeO
21
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM


7.952
7.931
7.596
7.575
7.260
SO2Br
Cl
22
1.99
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 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.
PPM


145.299
142.021
129.873
127.888
77.318 CDC13
77.000 CDC13
76.682 CDC13
SO2Br
Cl
22
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
PPM


7.875
7.853
7.771
7.749
7.260
SO2Br
Br
23
2.00
2.07
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
PPM


145.854
132.897
130.731
127.864
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
SO2Br
Br
23
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
PPM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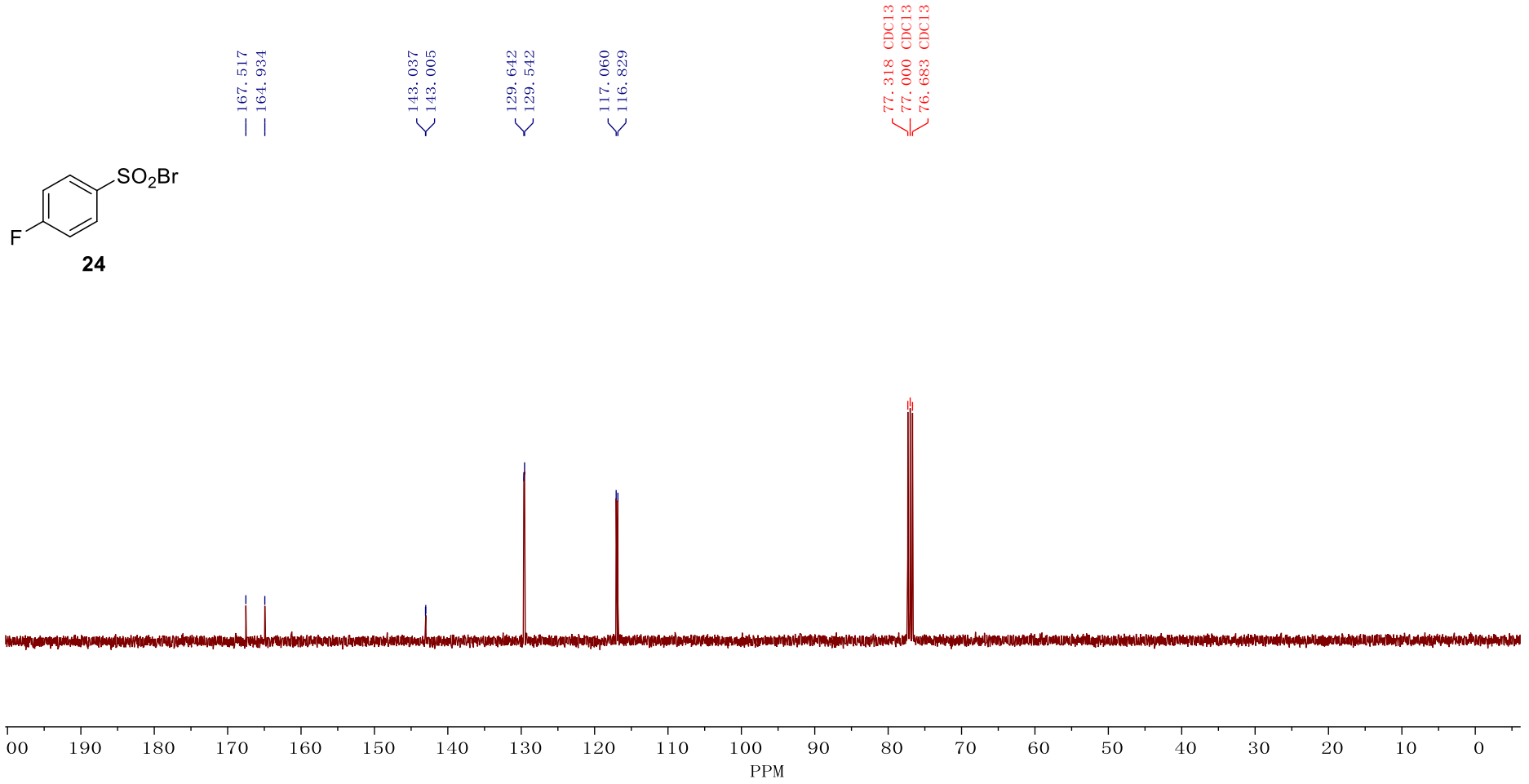
8.065
8.060
8.053
8.047
8.042
8.035
8.030
8.022
7.325
7.317
7.312
7.305
7.297
7.294
7.287
7.280
7.274
7.268
-0.000
SO2Br
F
24
2.00
2.12
PPM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143.037
143.005
129.642
129.542
117.060
116.829
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
SO2Br
F
24
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
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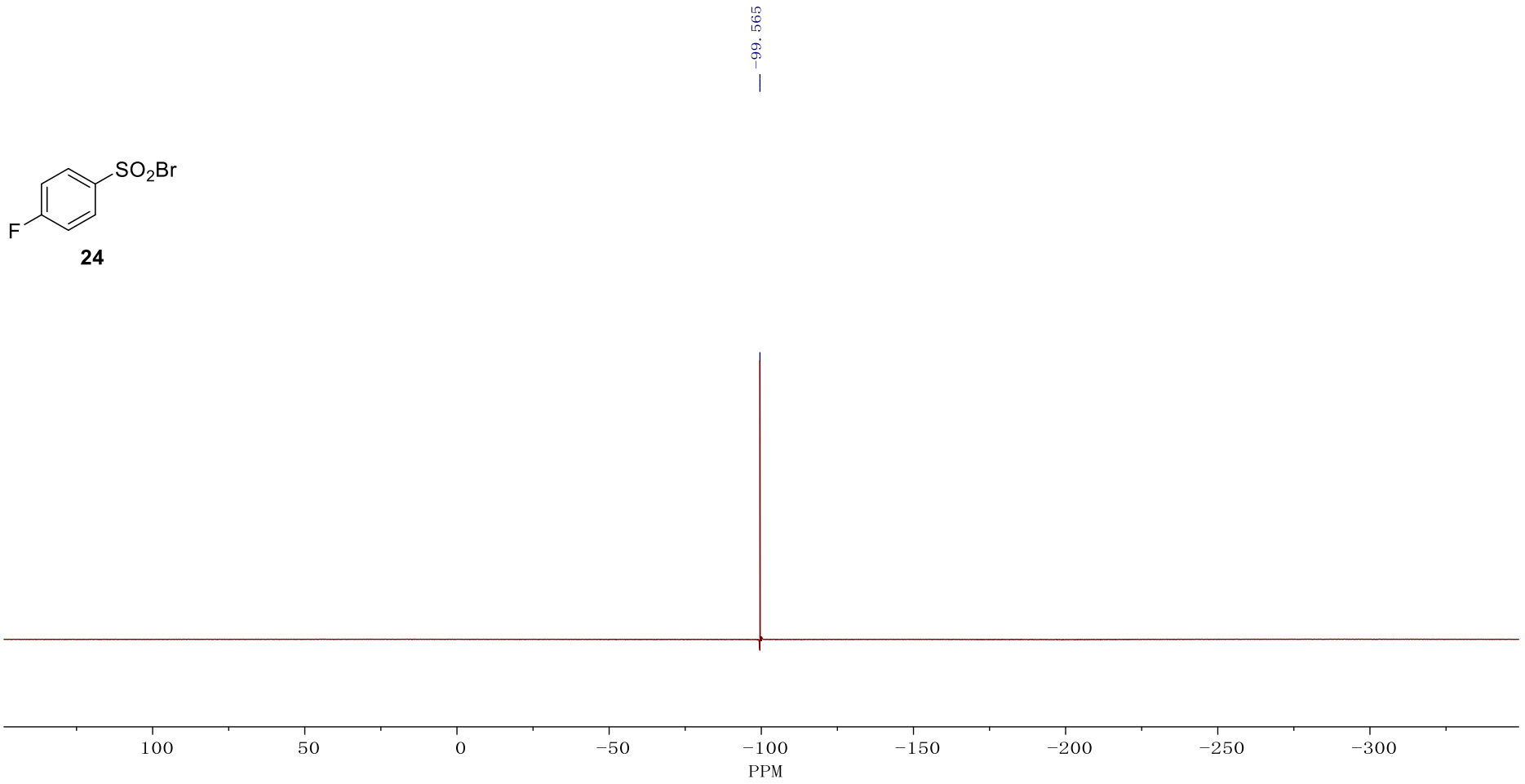
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-99.565
100
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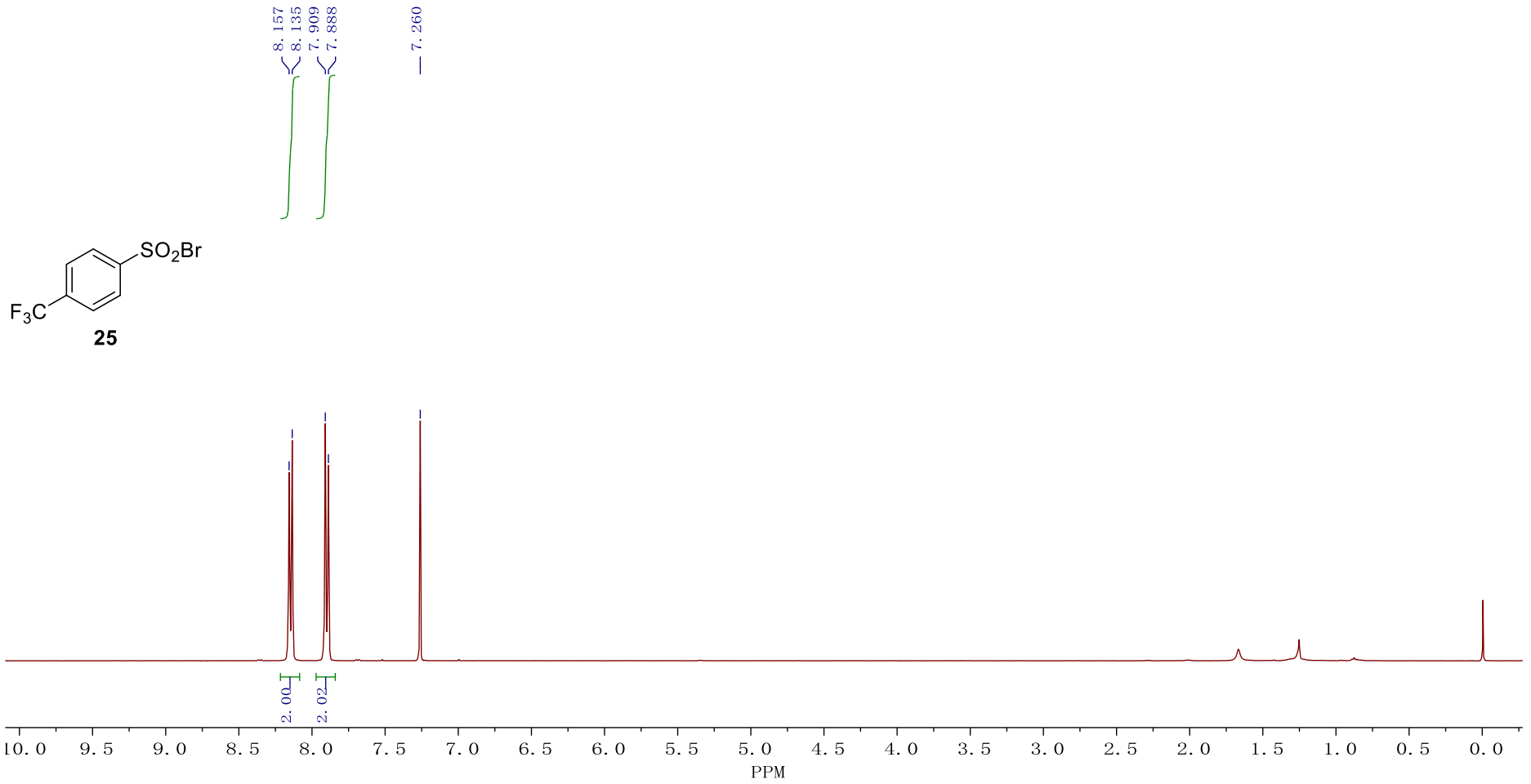
0
-50
-100
-150
-200
-250
-300
PPM


8.157
8.135
7.909
7.888
7.260
SO2Br
F3C
25
2.00
2.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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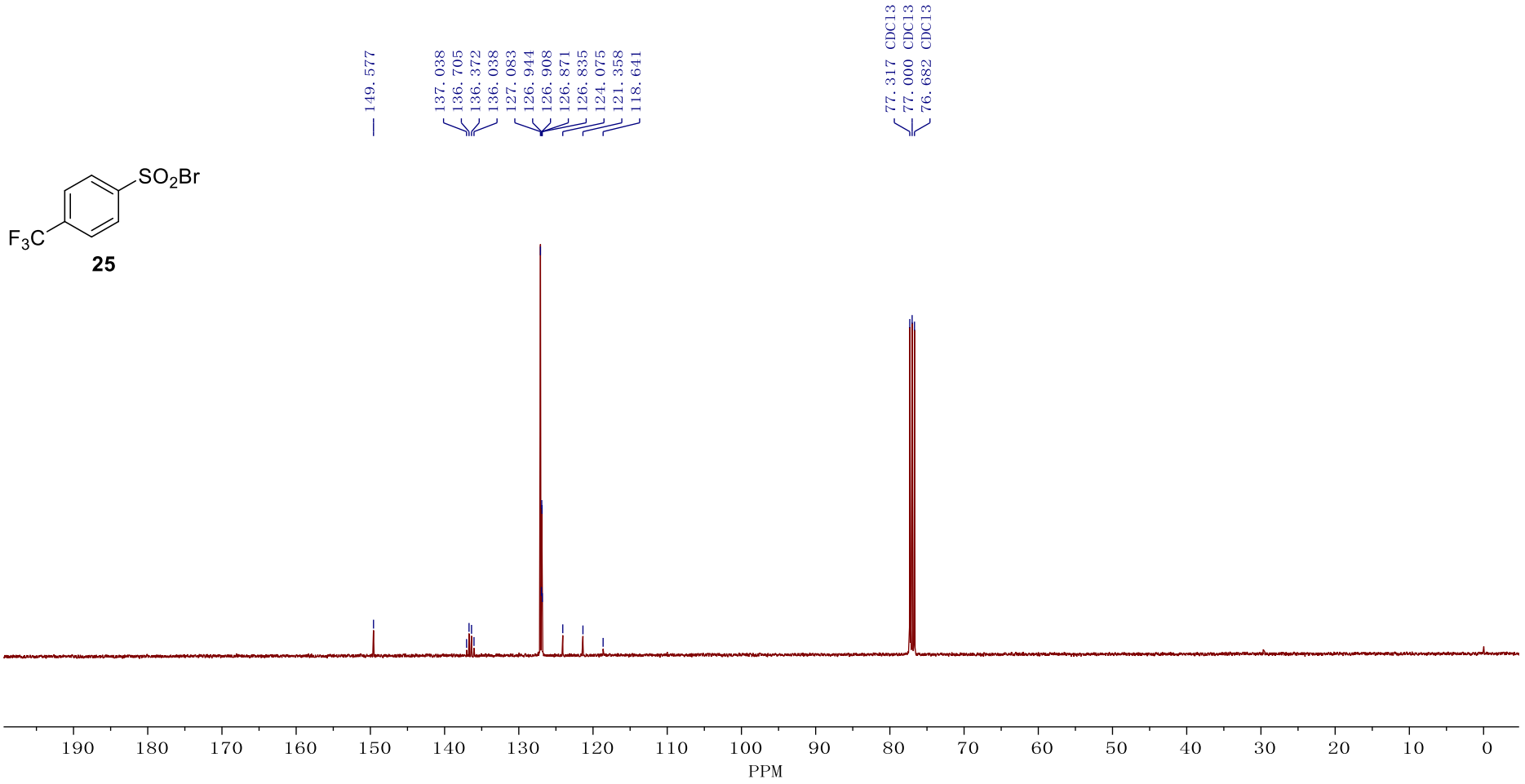
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
PPM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136.705
136.372
136.038
127.083
126.944
126.908
126.871
126.835
124.075
121.358
118.641
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
SO2Br
F3C
25
190
180
170
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150
140
130
120
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100
90
80
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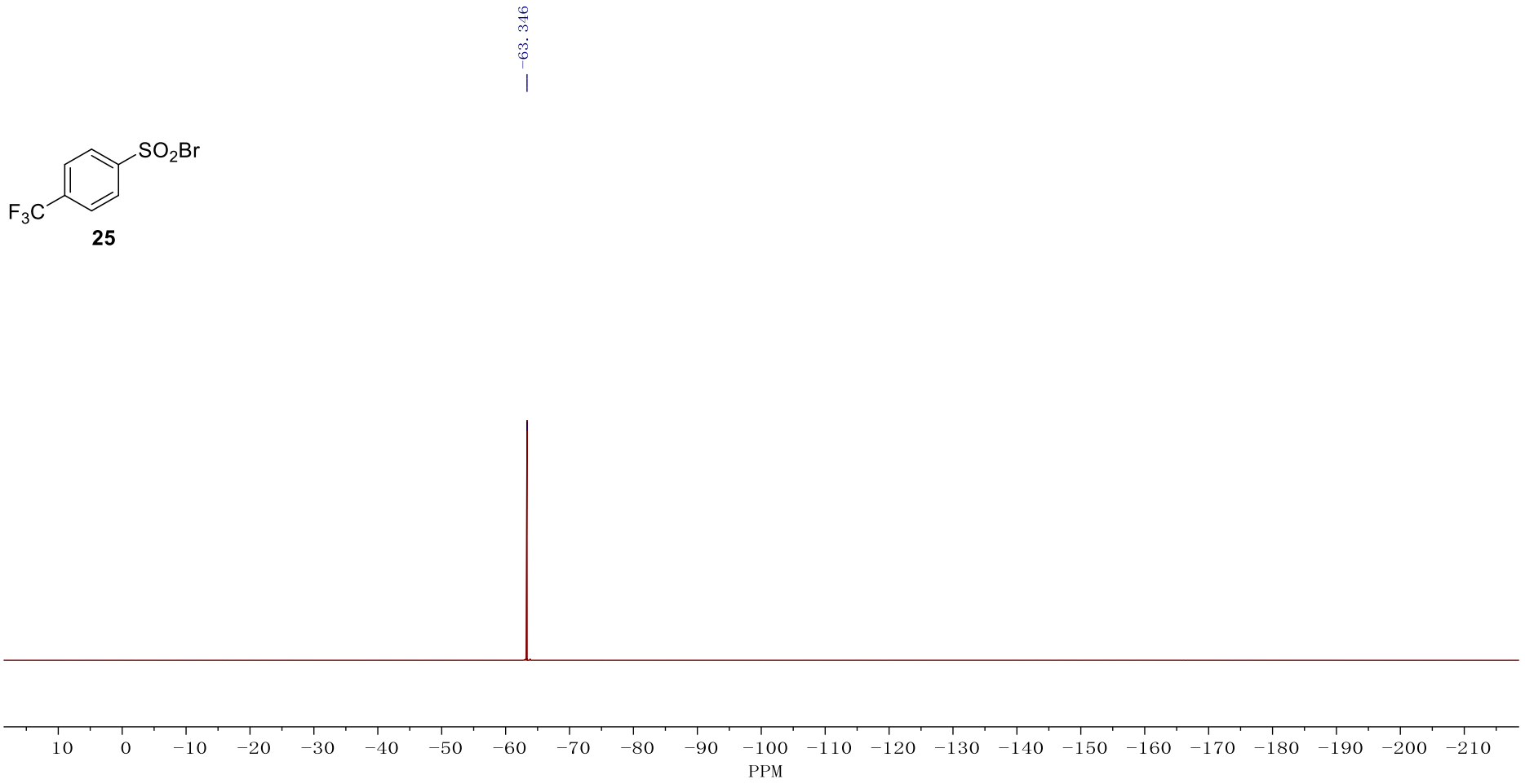
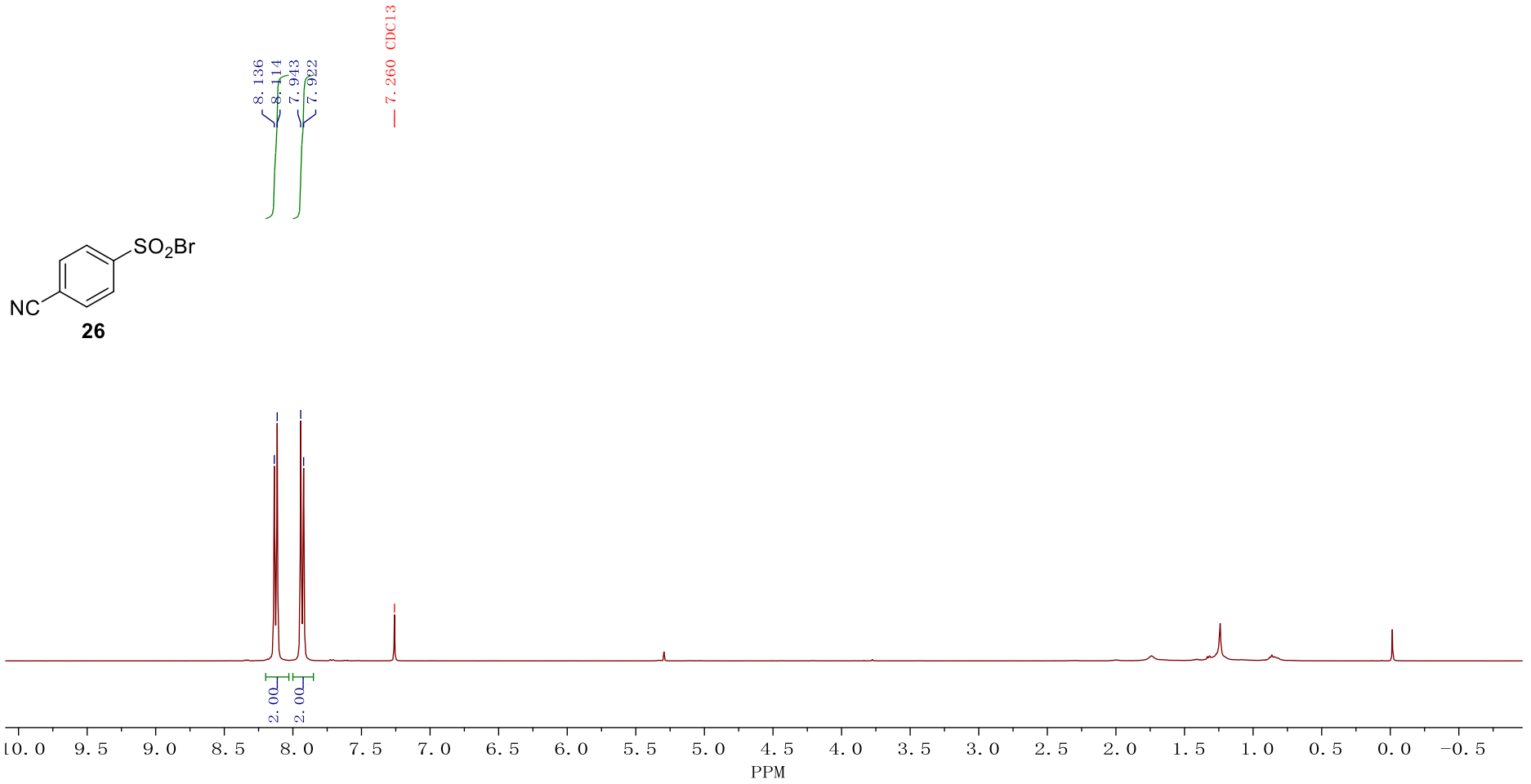
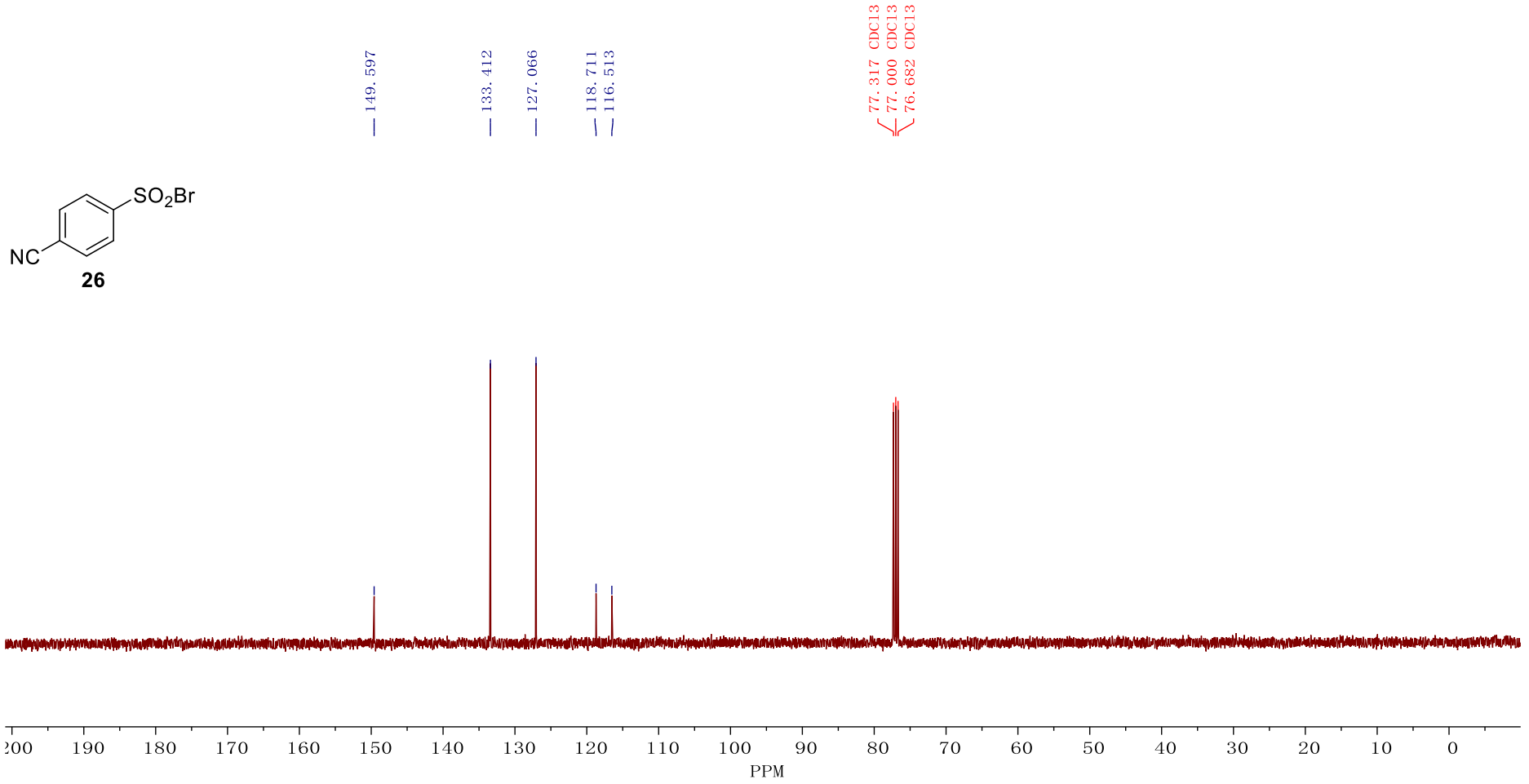
60
50
40
30
20
10
0
PPM


−63.346
SO2Br
F3C
25
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
PPM


8.136
8.114
7.943
7.922
7.260 CDC13
SO2Br
NC
26
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
PPM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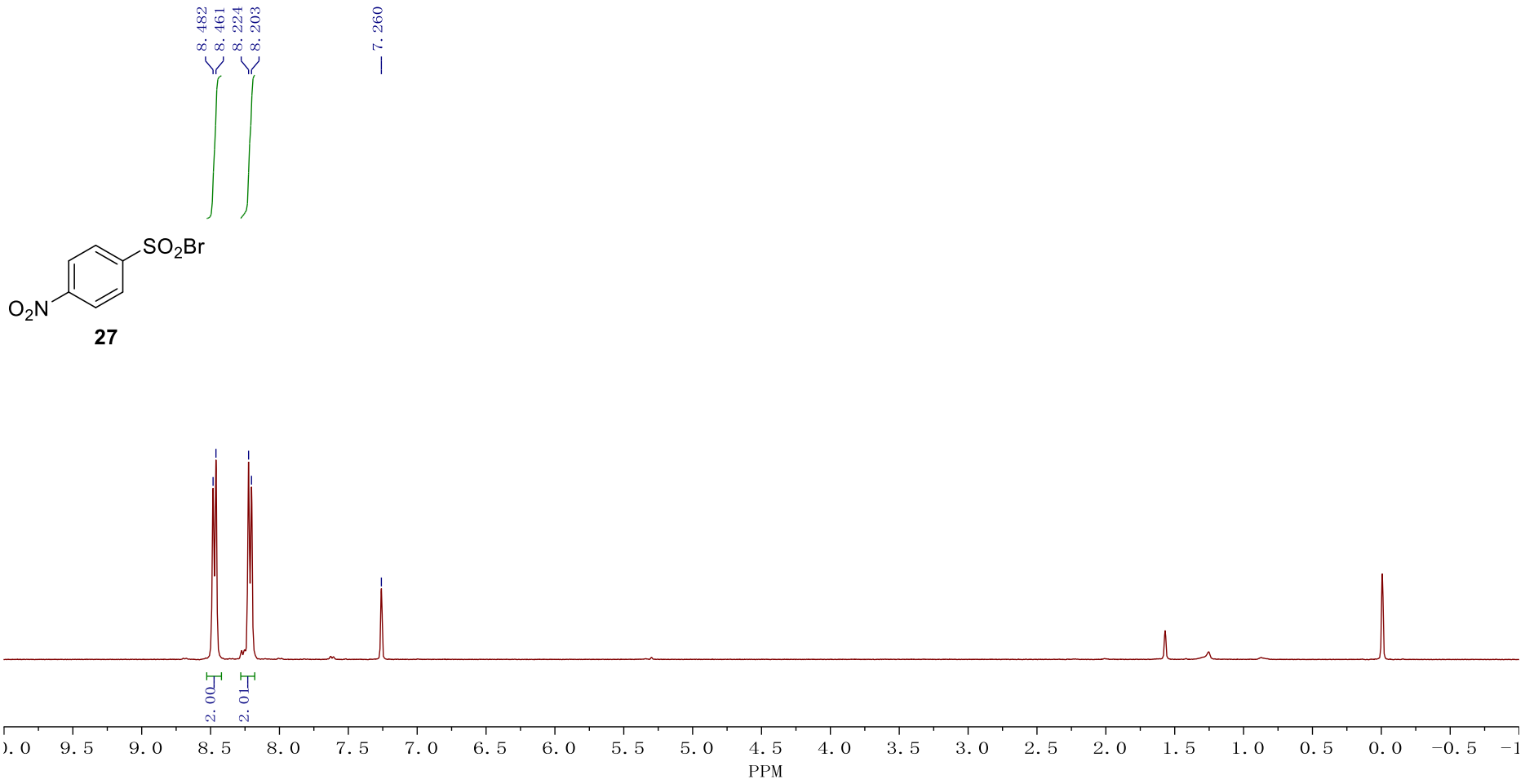
133.412
127.066
118.711
116.513
77.317 CDC13
77.000 CDC13
76.682 CDC13
SO2Br
NC
26
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM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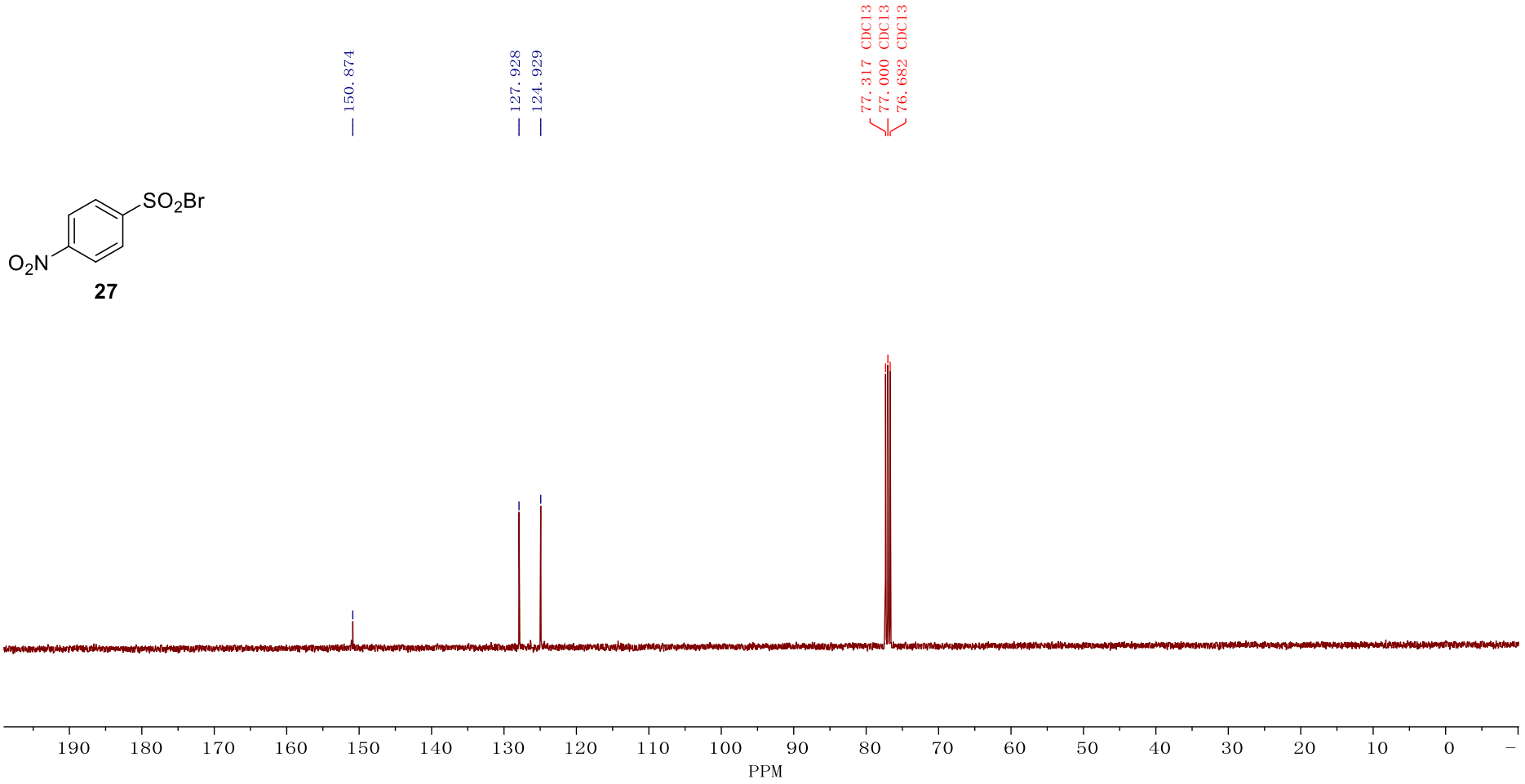
8.461
8.224
8.203
7.260
SO2Br
O2N
27
2.00
2.01
PPM


150.874
127.928
124.929
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
SO2Br
O2N
27
190
180
170
160
150
140
130
120
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100
90
80
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60
50
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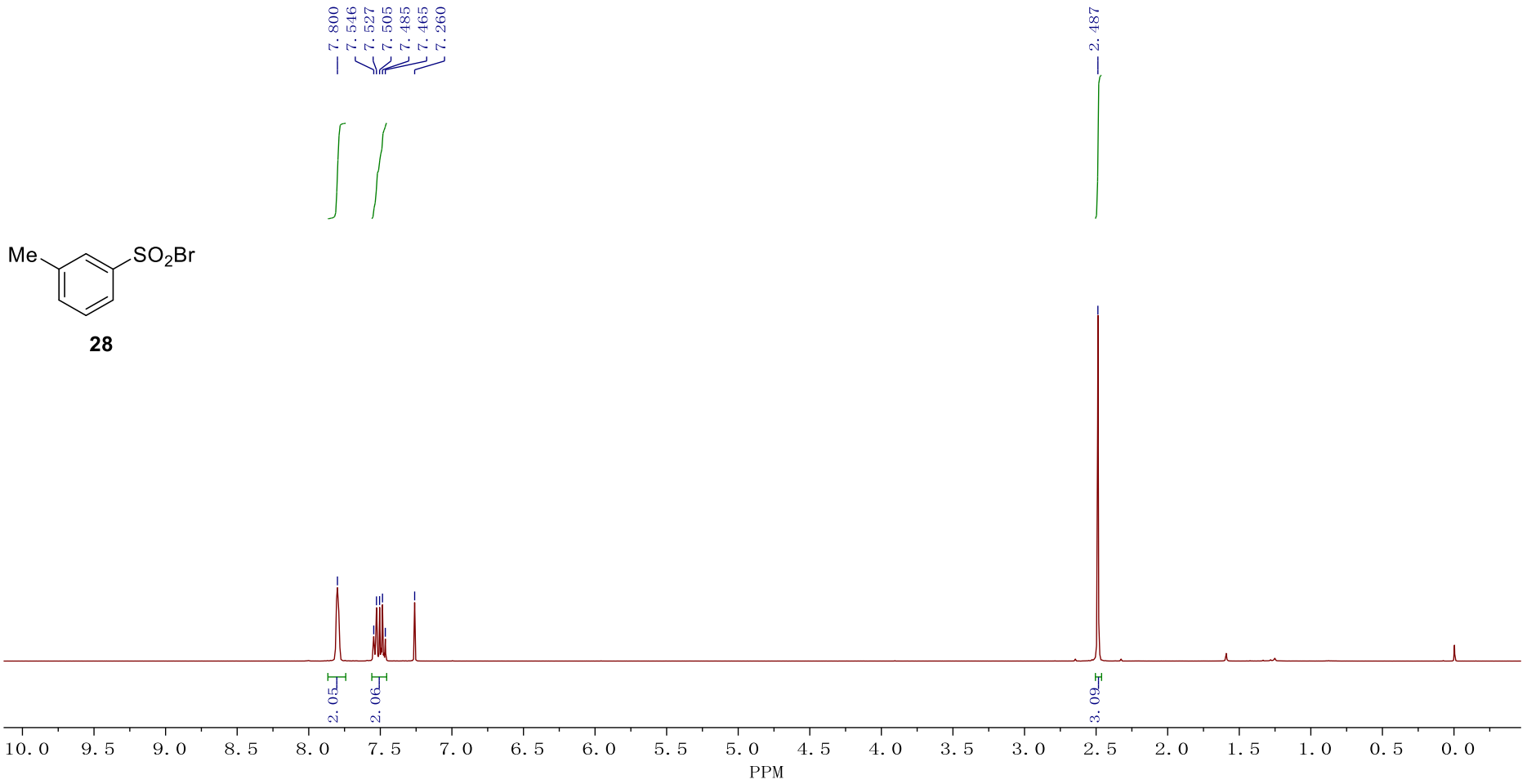
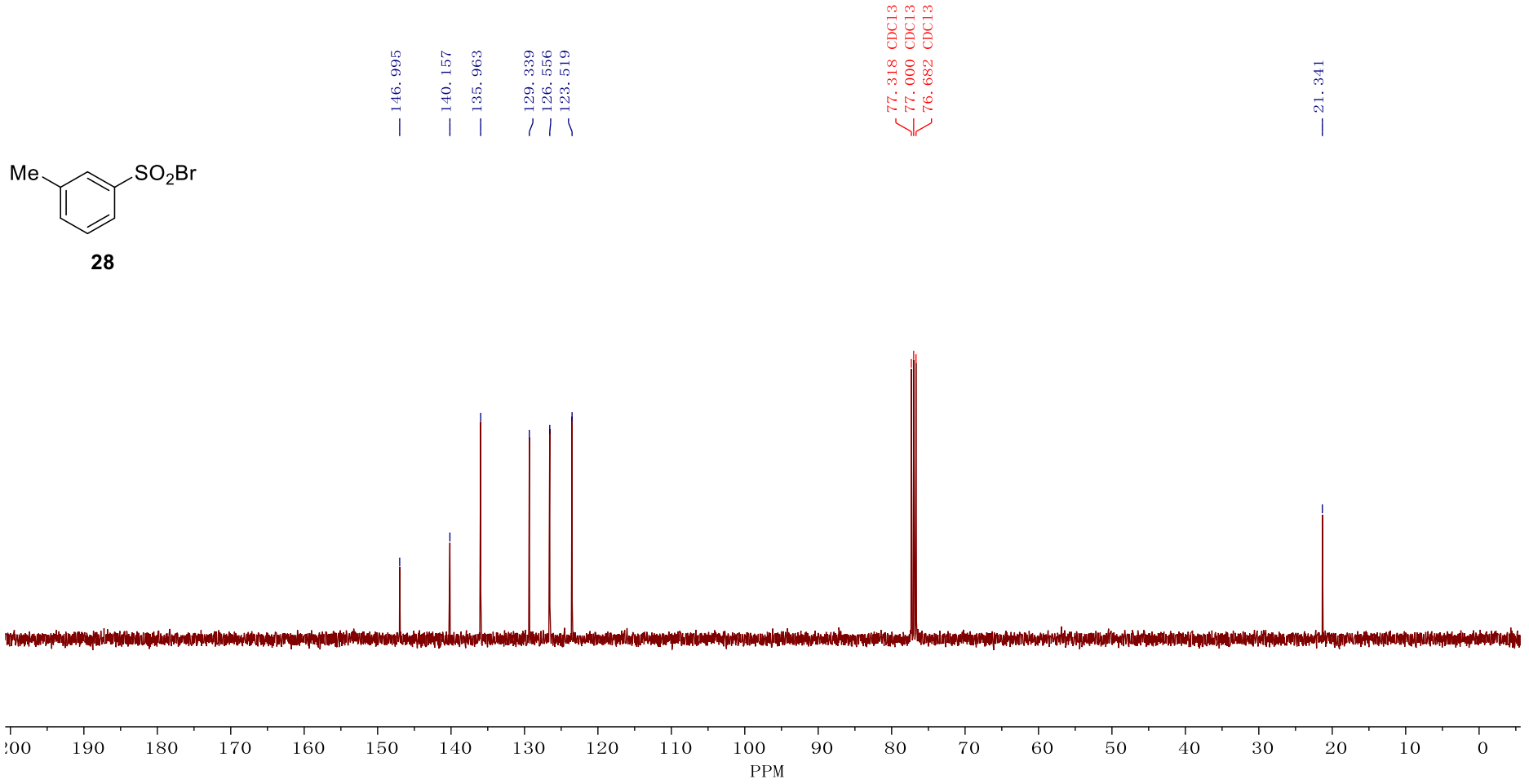
10
0
PPM


7.800
7.546
7.527
7.505
7.485
7.465
7.260
2.487
Me
SO2Br
28
2.05
2.06
3.09
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
PPM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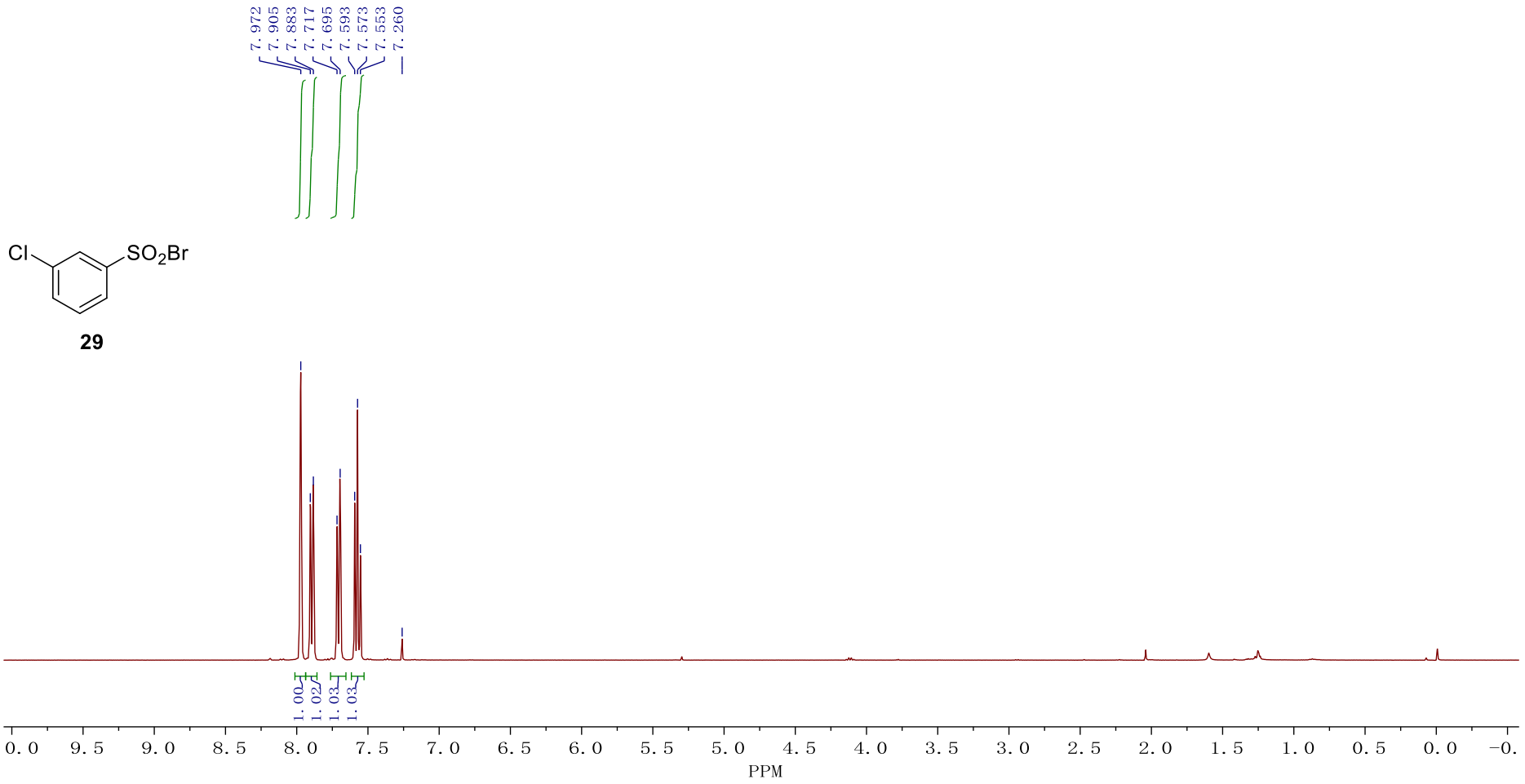
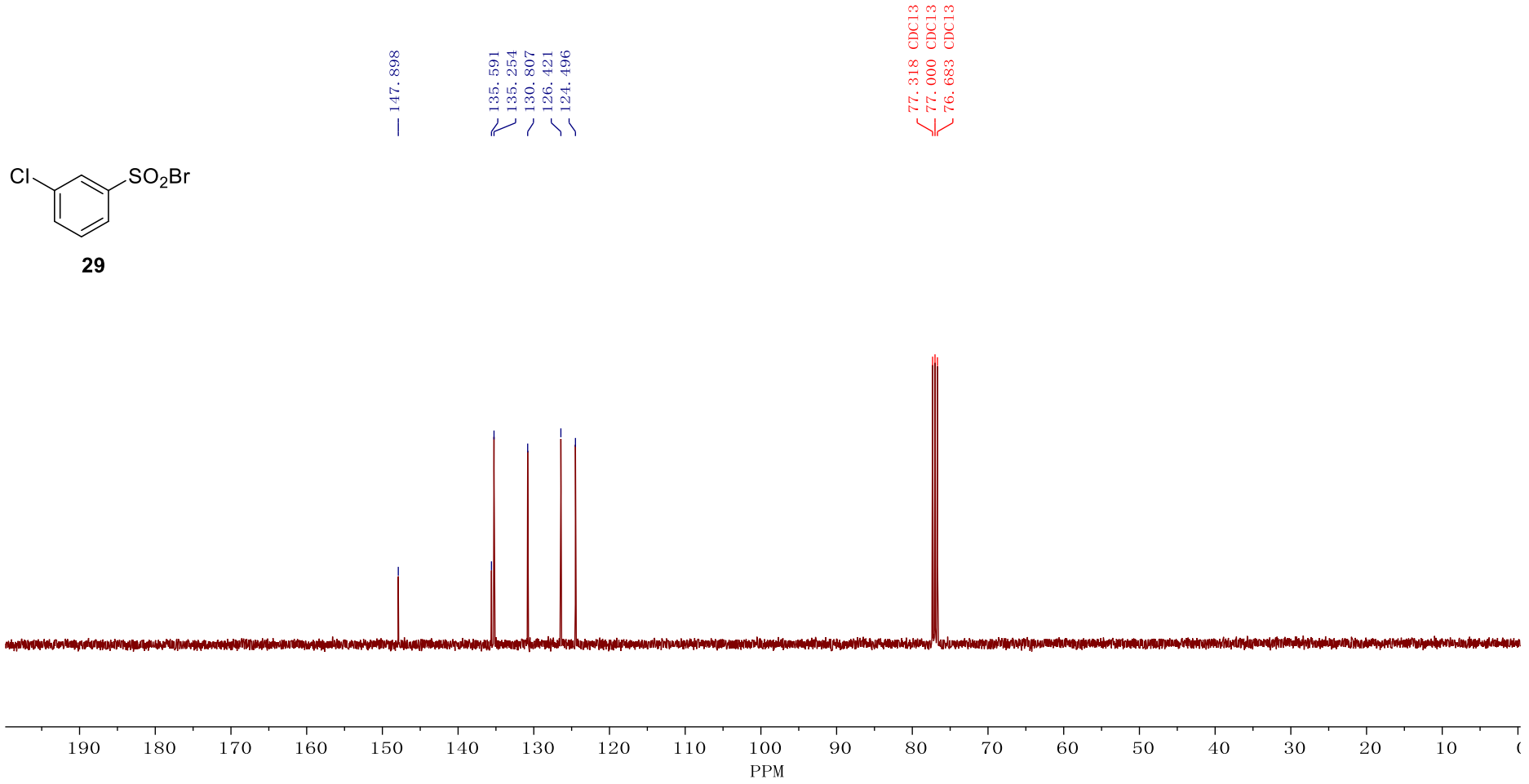
140.157
135.963
129.339
126.556
123.519
77.318 CDC13
77.000 CDC13
76.682 CDC13
21.341
Me
SO2Br
28
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM


7.972
7.905
7.883
7.717
7.695
7.593
7.573
7.553
7.260
Cl
SO2Br
29
1.00
1.02
1.03
1.03
0.0
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.
PPM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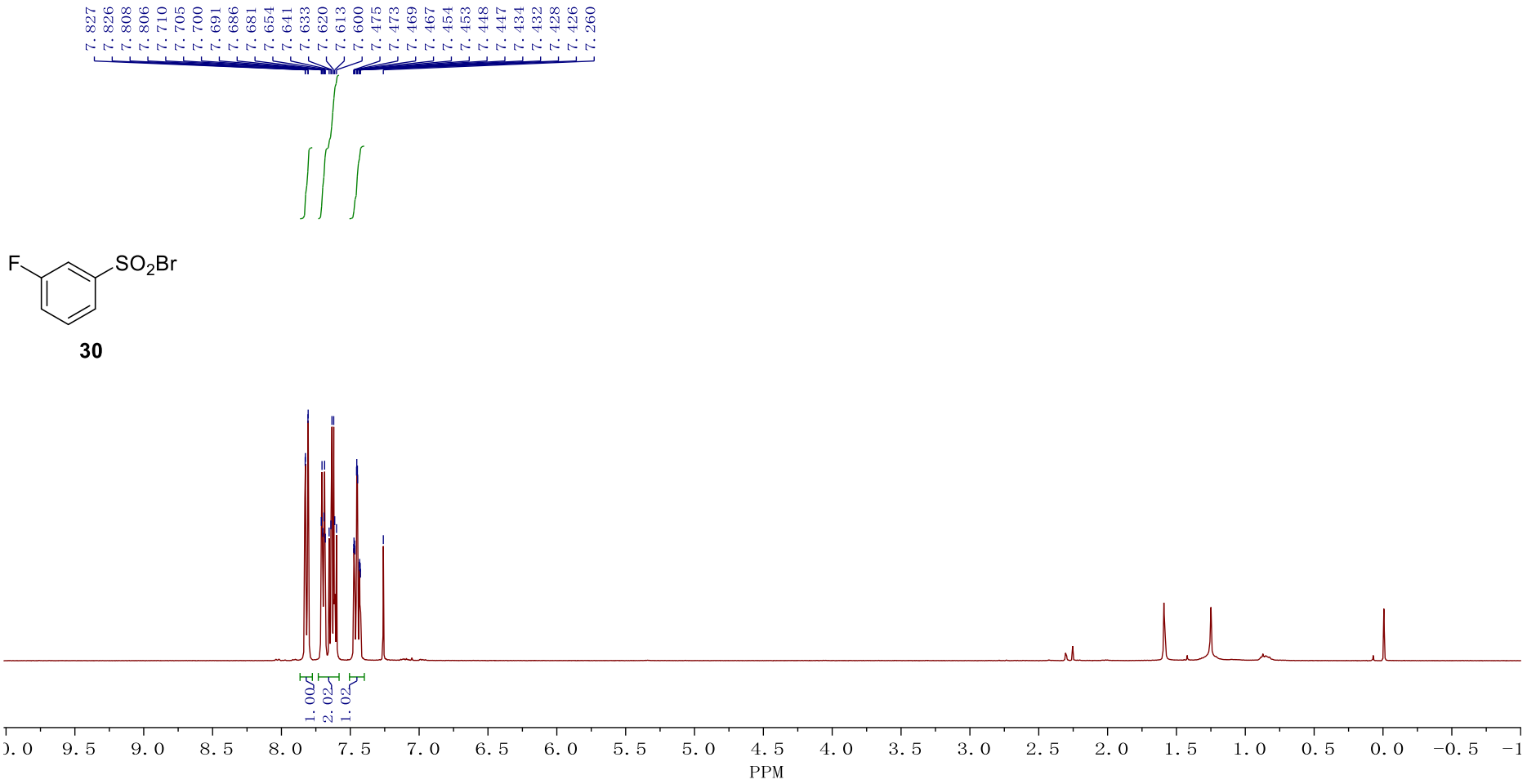
135.254
130.807
126.421
124.496
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
Cl
SO2Br
29
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
PPM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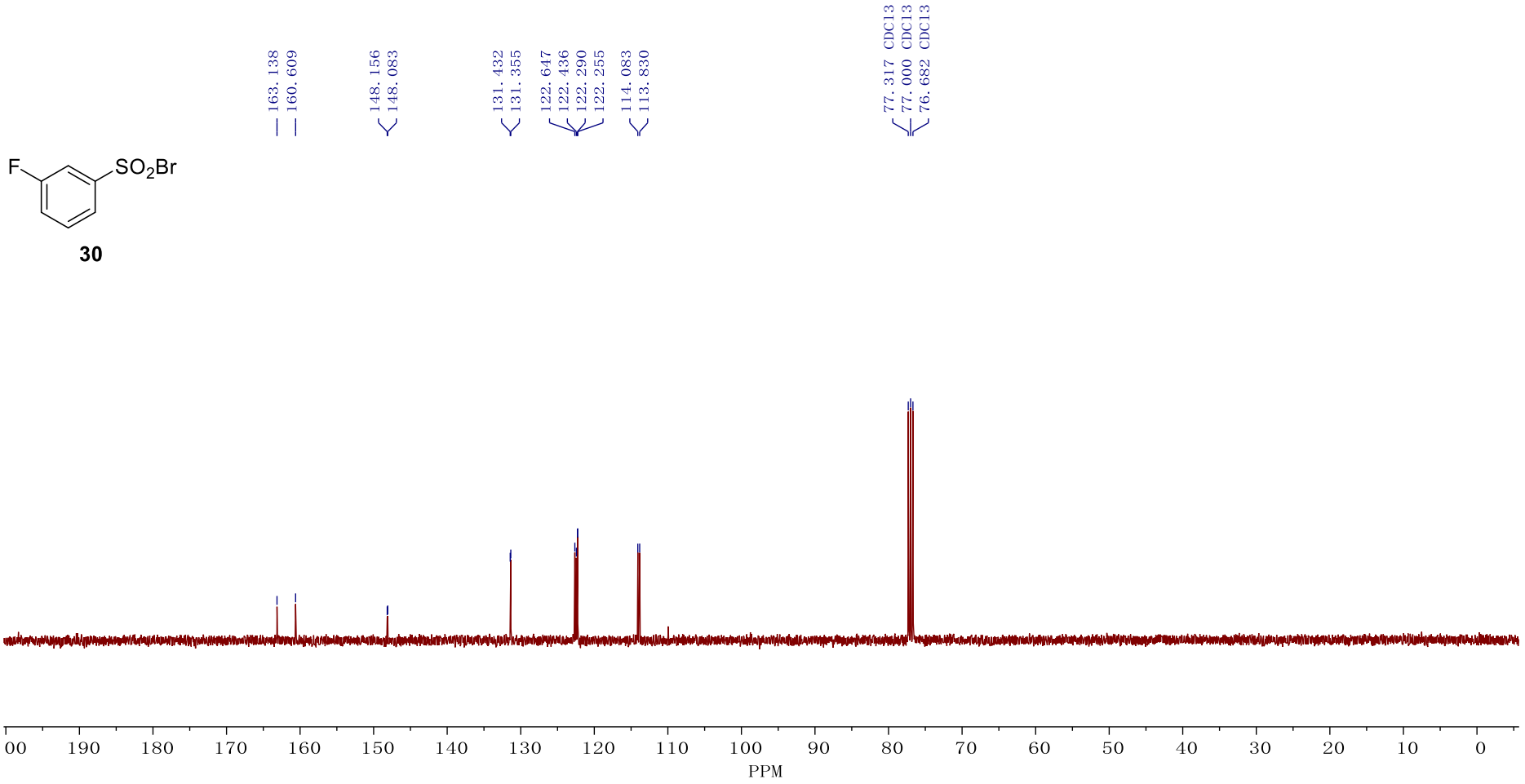
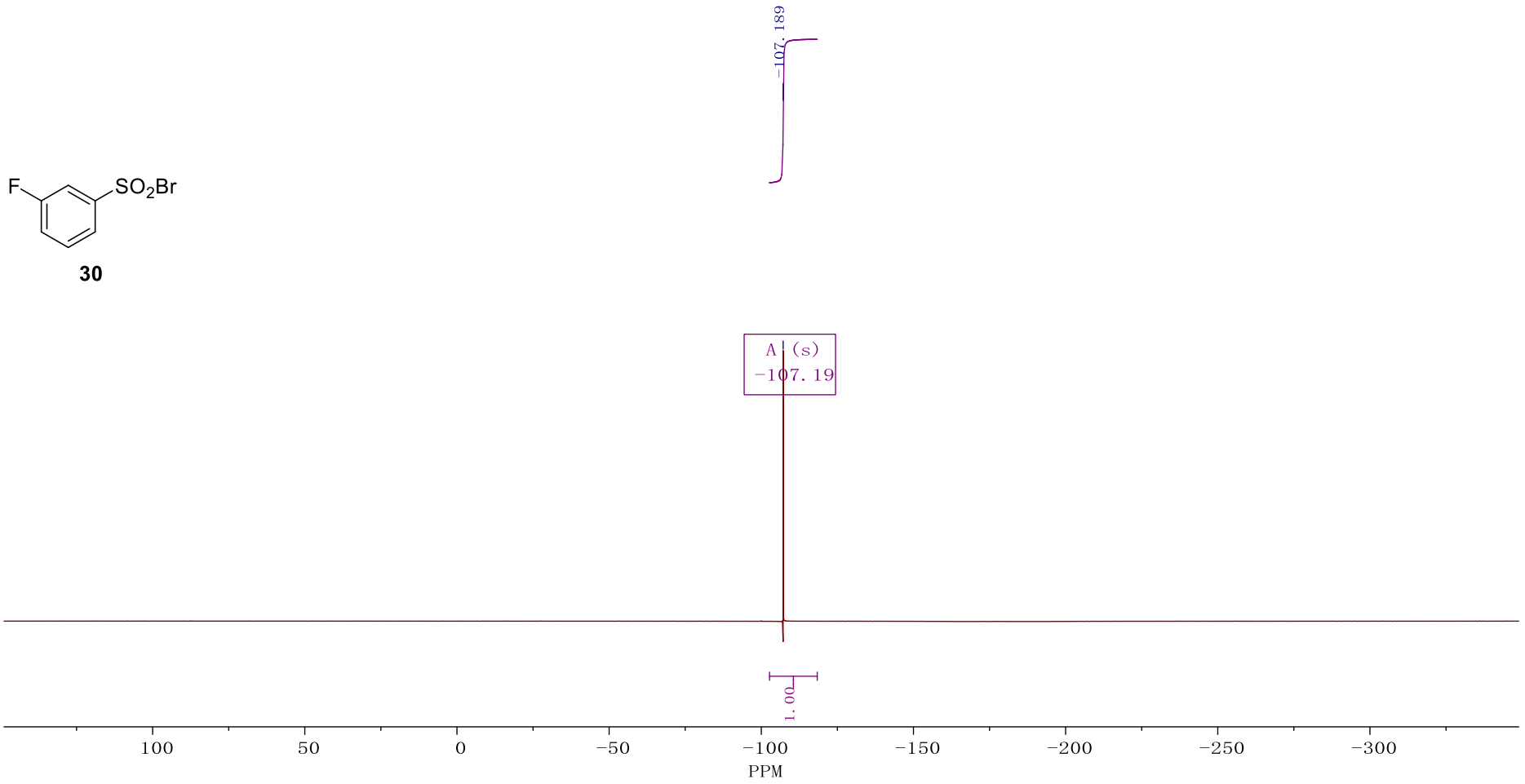
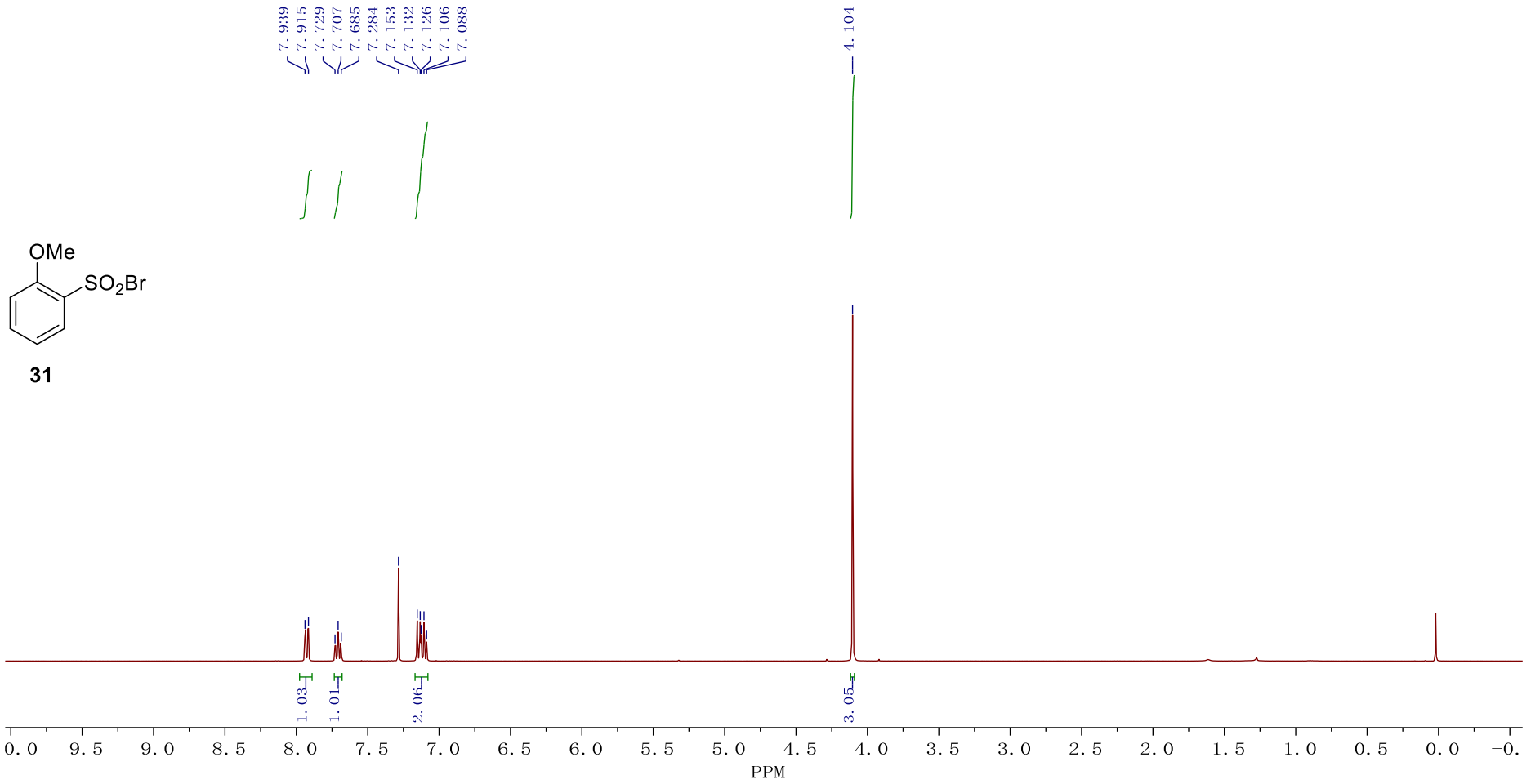
7.826
7.808
7.806
7.710
7.705
7.700
7.691
7.686
7.681
7.654
7.641
7.633
7.620
7.613
7.600
7.475
7.473
7.469
7.467
7.454
7.453
7.448
7.447
7.434
7.432
7.428
7.426
7.260
F
SO2Br
30
1.00
2.02
1.02
PPM


163.138
160.609
148.156
148.083
131.432
131.355
122.647
122.436
122.290
122.255
114.083
113.830
77.317 CDC13
77.000 CDC13
76.682 CDC13
F
SO2Br
30
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
PPM


F
SO2Br
30
-107.189
A (s)
-107.19
1.00
100
50
0
-50
-100
-150
-200
-250
-300
PPM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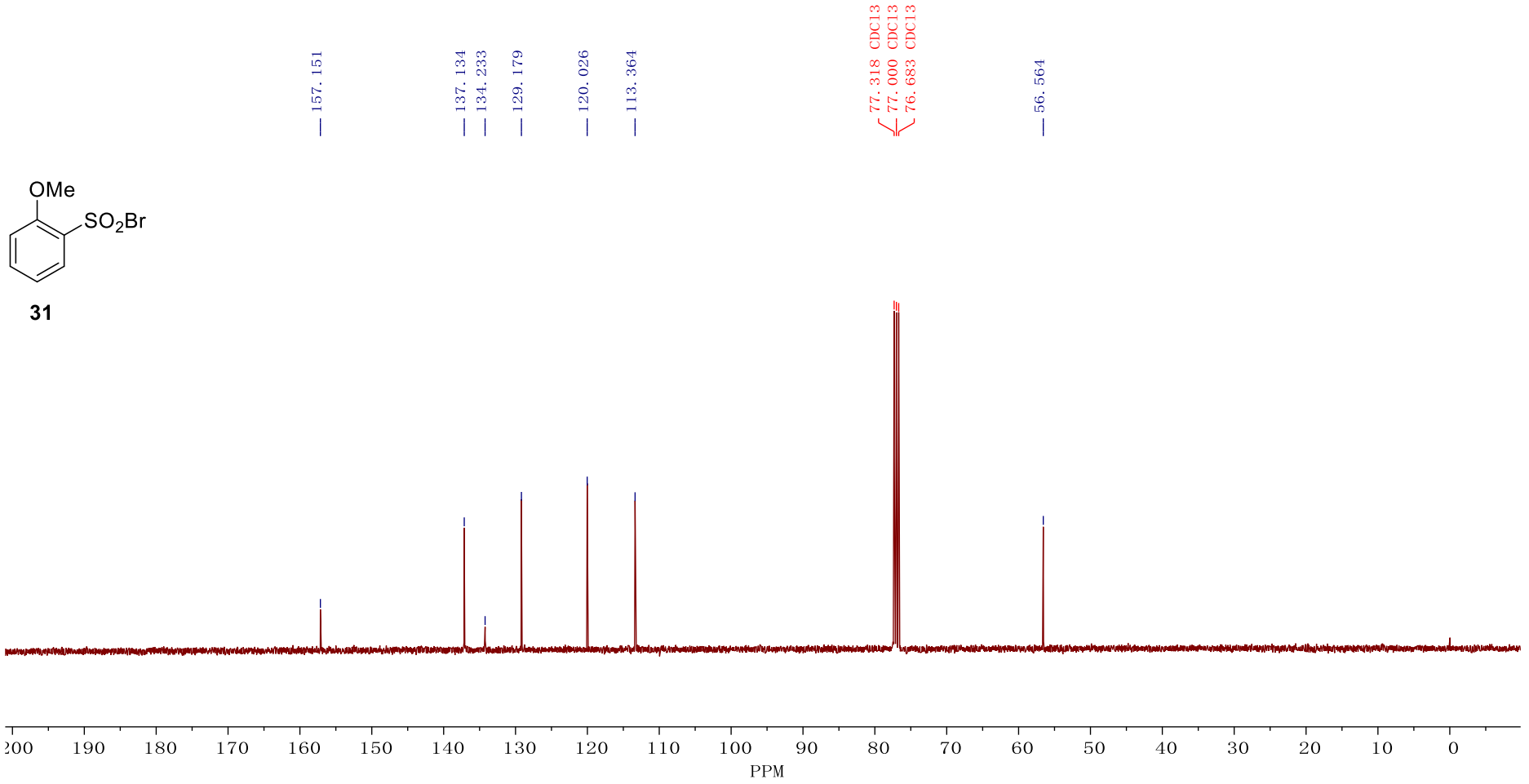
7.915
7.729
7.707
7.685
7.284
7.153
7.132
7.126
7.106
7.088
4.104
OMe
SO2Br
31
1.03
1.01
2.06
3.05
PPM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137.134
134.233
129.179
120.026
113.364
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
56.564
OMe
SO2Br
31
200
190
180
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160
150
140
130
120
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100
90
80
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60
50
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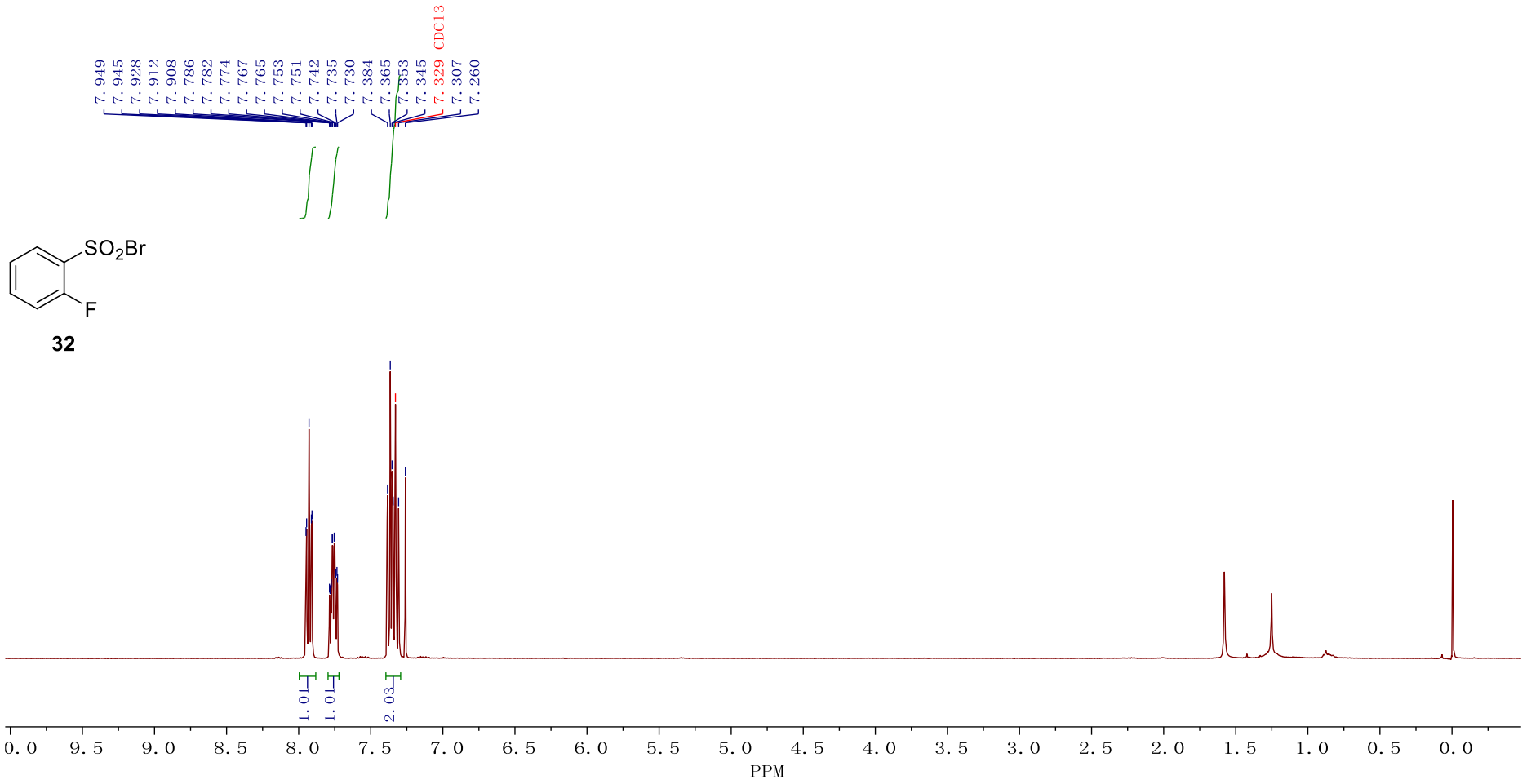
30
20
10
0
PPM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7.928
7.912
7.908
7.786
7.782
7.774
7.767
7.765
7.753
7.751
7.742
7.735
7.730
7.384
7.365
7.353
7.345
7.329 CDCl3
7.307
7.260
SO2Br
F
32
1.01
1.01
2.03
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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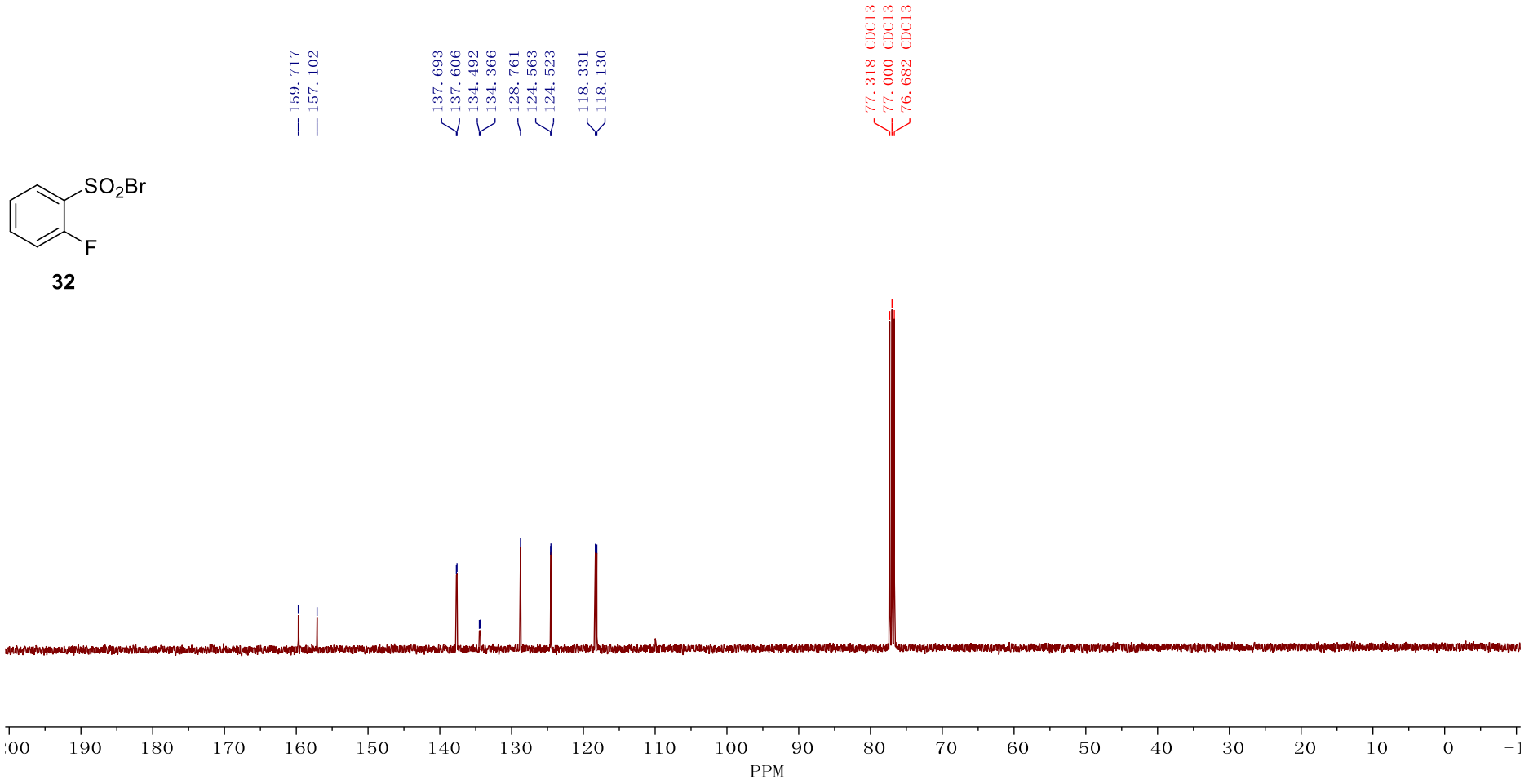
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
PPM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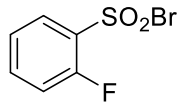
137.606
134.492
134.366
128.761
124.563
124.523
118.331
118.130
77.318 CDC13
77.000 CDC13
76.682 CDC13
SO2Br
F
32
PPM



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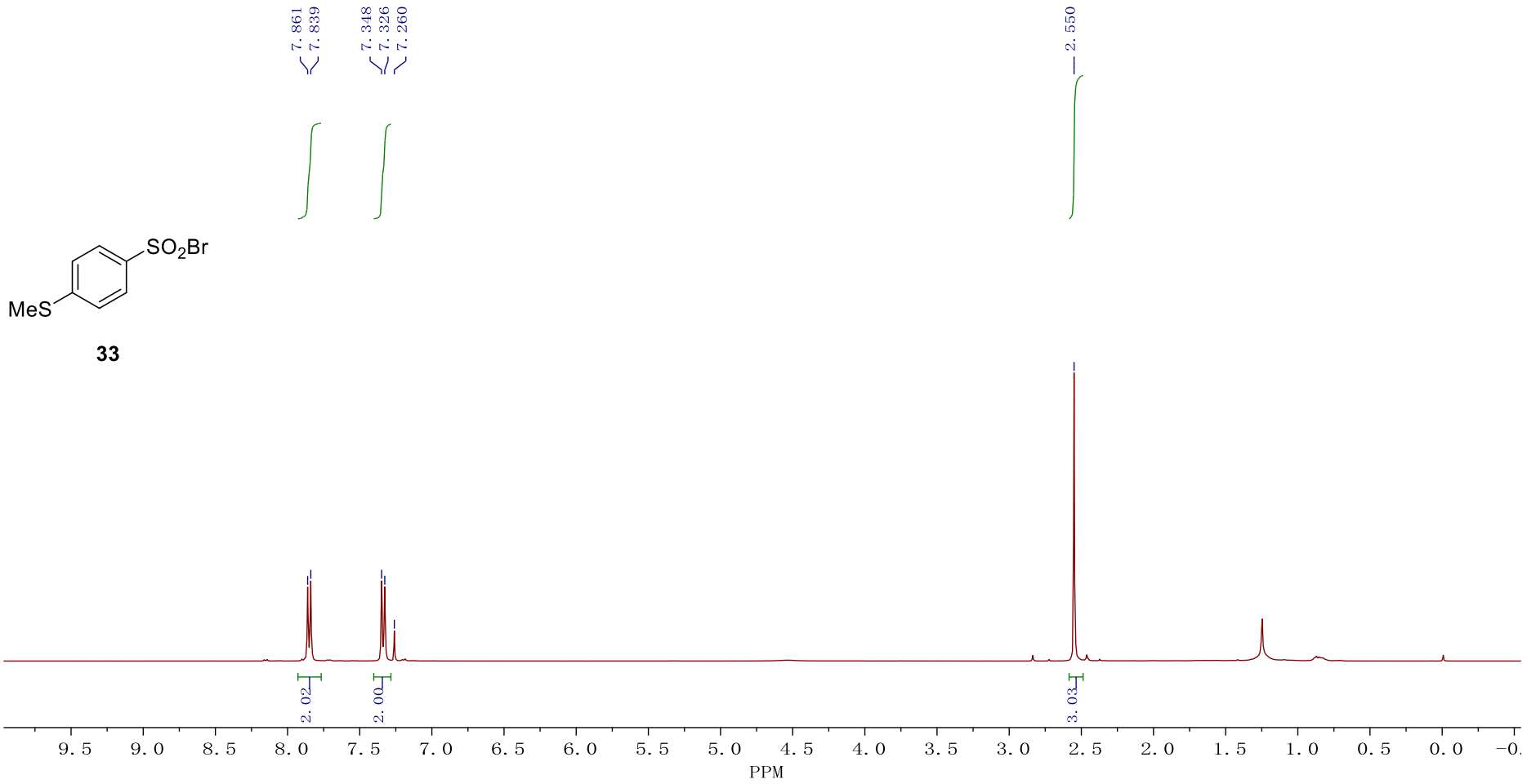
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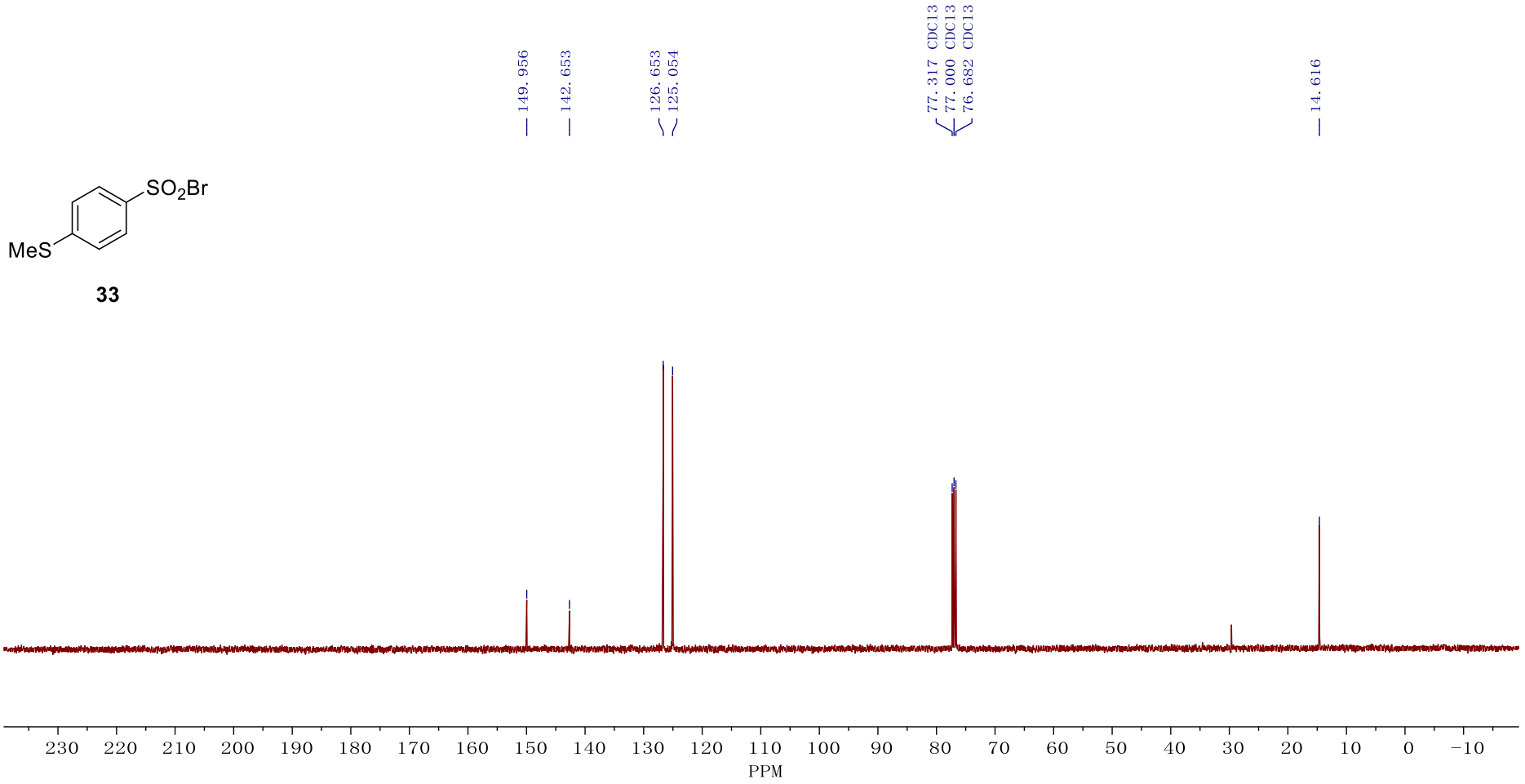
7.839
7.348
7.326
7.260
2.550
SO2Br
MeS
33
2.02
2.00
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
PPM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142.653
126.653
125.054
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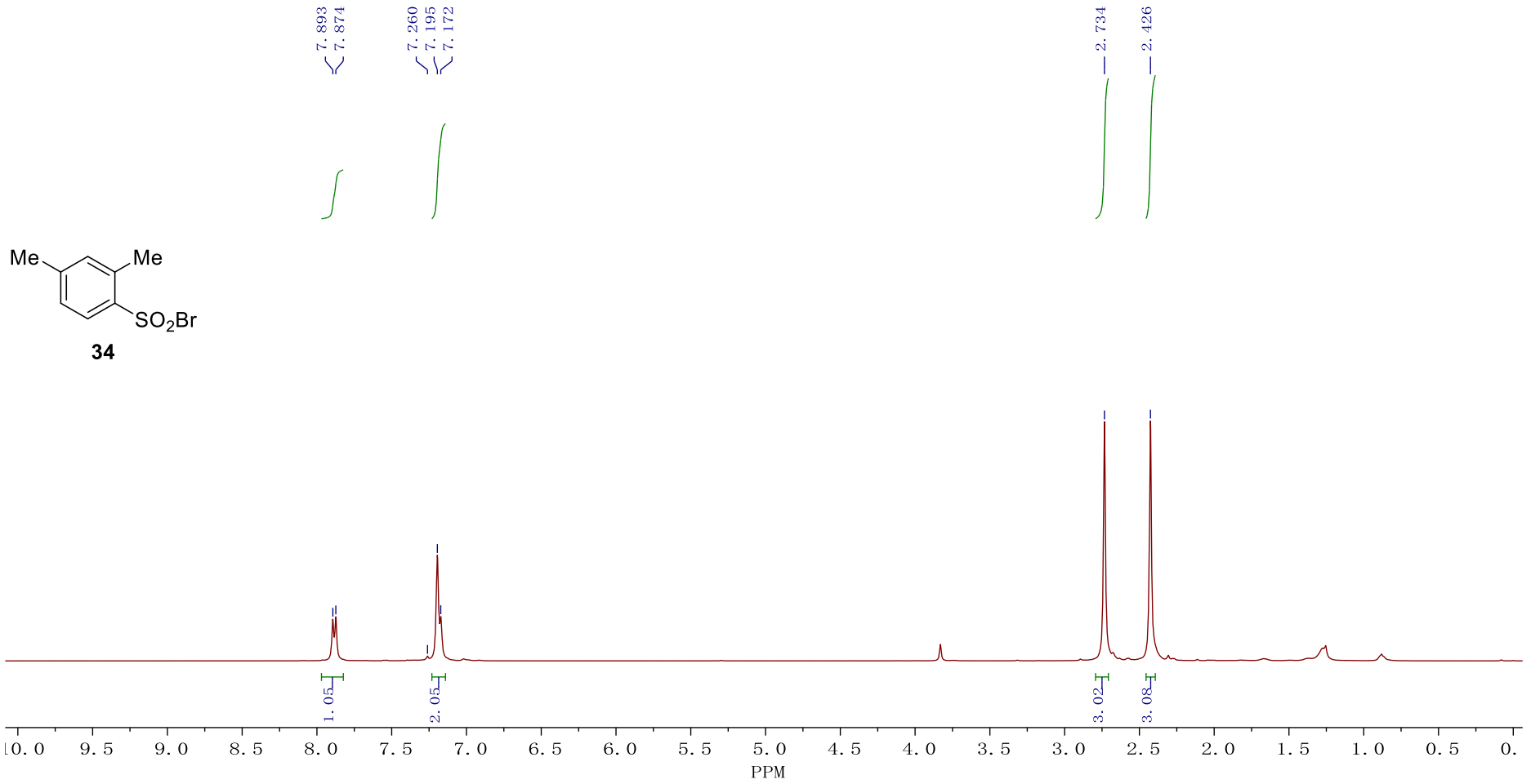
77.000 CDC13
76.682 CDC13
14.616
SO2Br
MeS
33
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
PPM


7.893
7.874
7.260
7.195
7.172
2.734
2.426
Me
Me
SO2Br
34
1.05
2.05
3.02
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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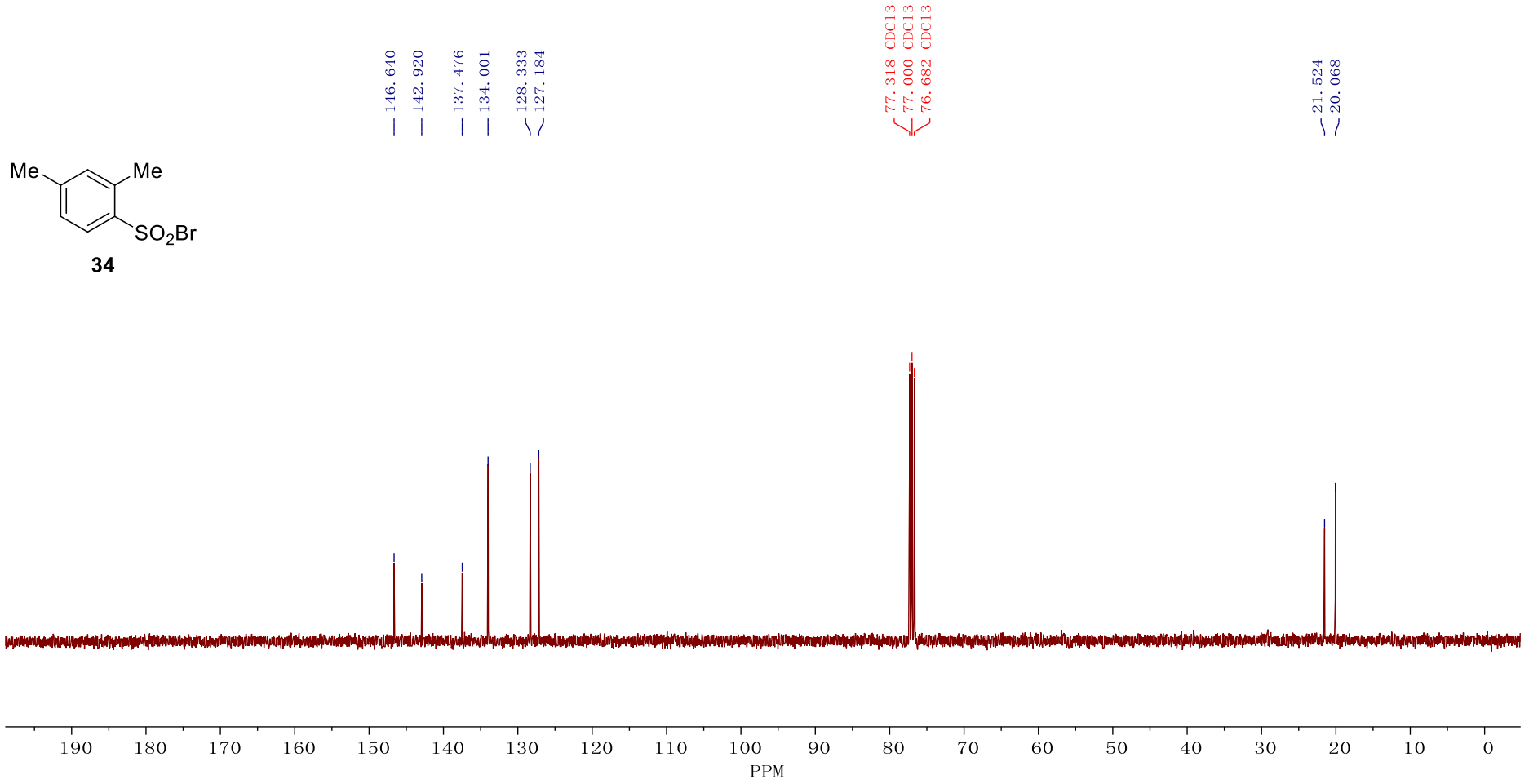
PPM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137.476
134.001
128.333
127.184
77.318 CDC13
77.000 CDC13
76.682 CDC13
21.524
20.068
Me
Me
SO2Br
34
190
180
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160
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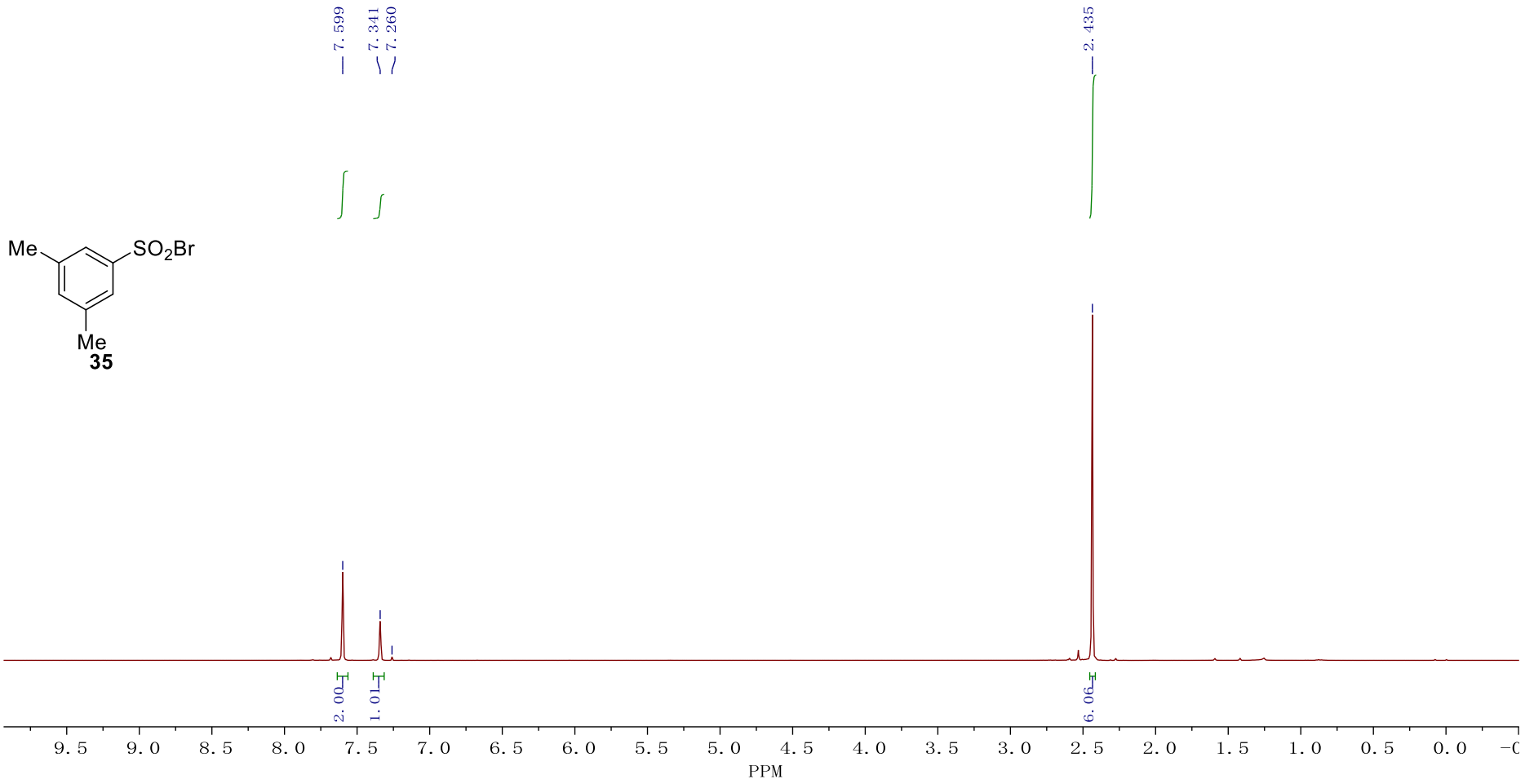
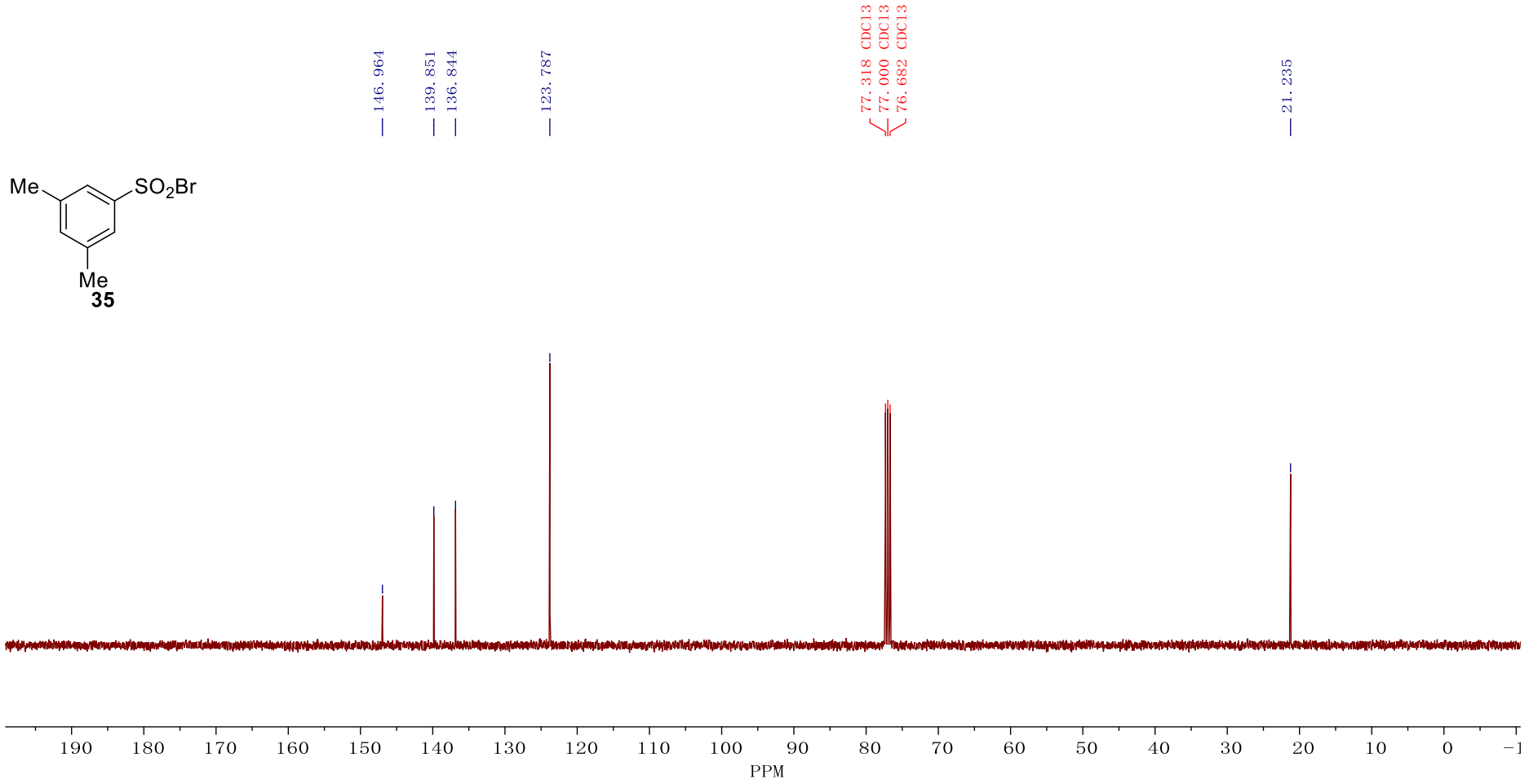
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM


7.599
7.341
7.260
2.435
Me
SO2Br
Me
35
2.00
1.01
6.06
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
PPM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136.844
123.787
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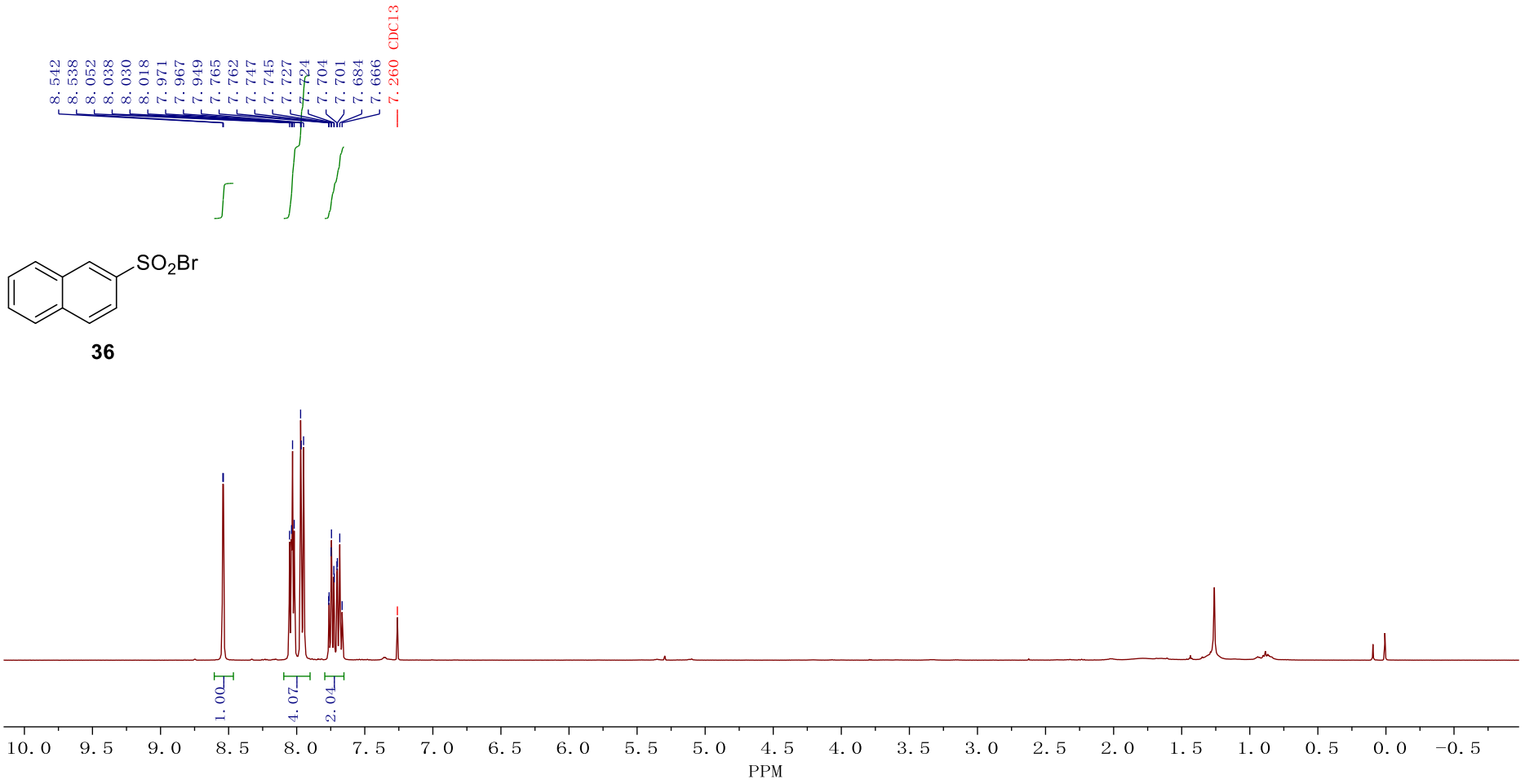
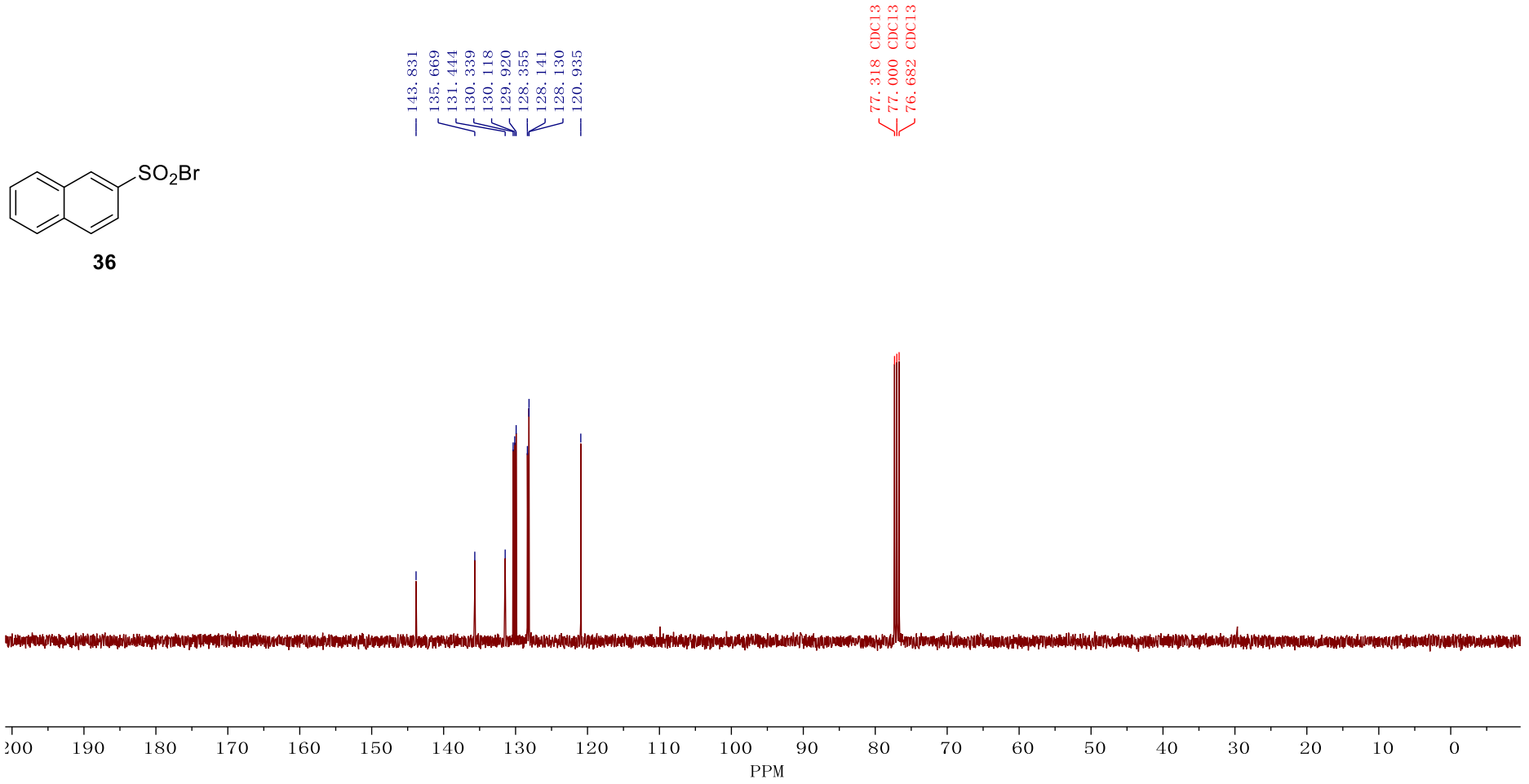
77.000 CDCl3
76.682 CDCl3
21.235
Me
SO2Br
Me
35
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
PPM


8.542
8.538
8.052
8.038
8.030
8.018
7.971
7.967
7.949
7.765
7.762
7.747
7.745
7.727
7.724
7.704
7.701
7.684
7.666
7.260 CDCl3
SO2Br
36
1.00
4.07
2.04
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
PPM


143.831
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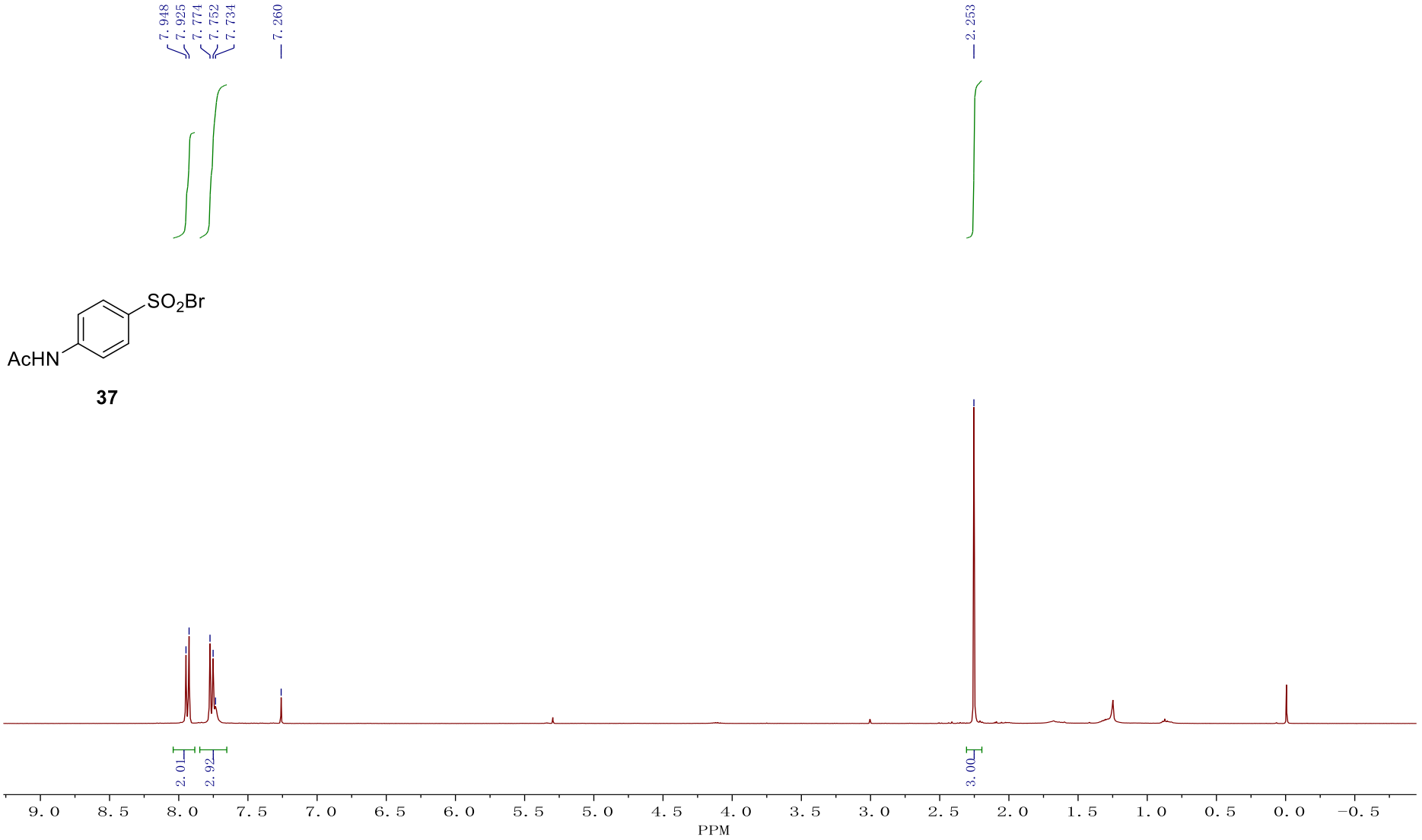
131.444
130.339
130.118
129.920
128.355
128.141
128.130
120.935
77.318 CDCl3
77.000 CDCl3
76.682 CDCl3
SO2Br
36
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM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7.925
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7.734
7.260
2.253
SO2Br
AcHN
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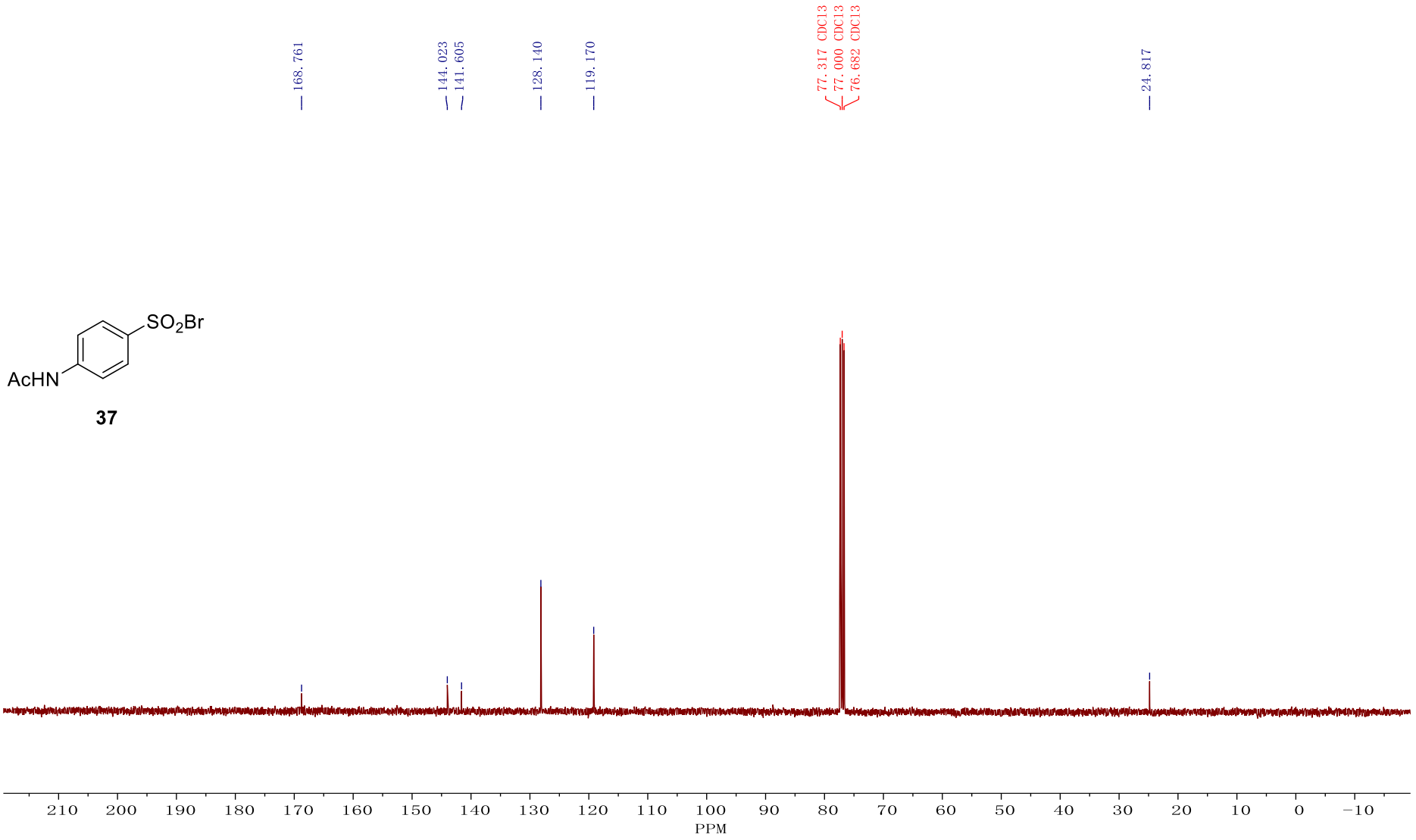
2.01
2.92
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
PPM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128.140
119.170
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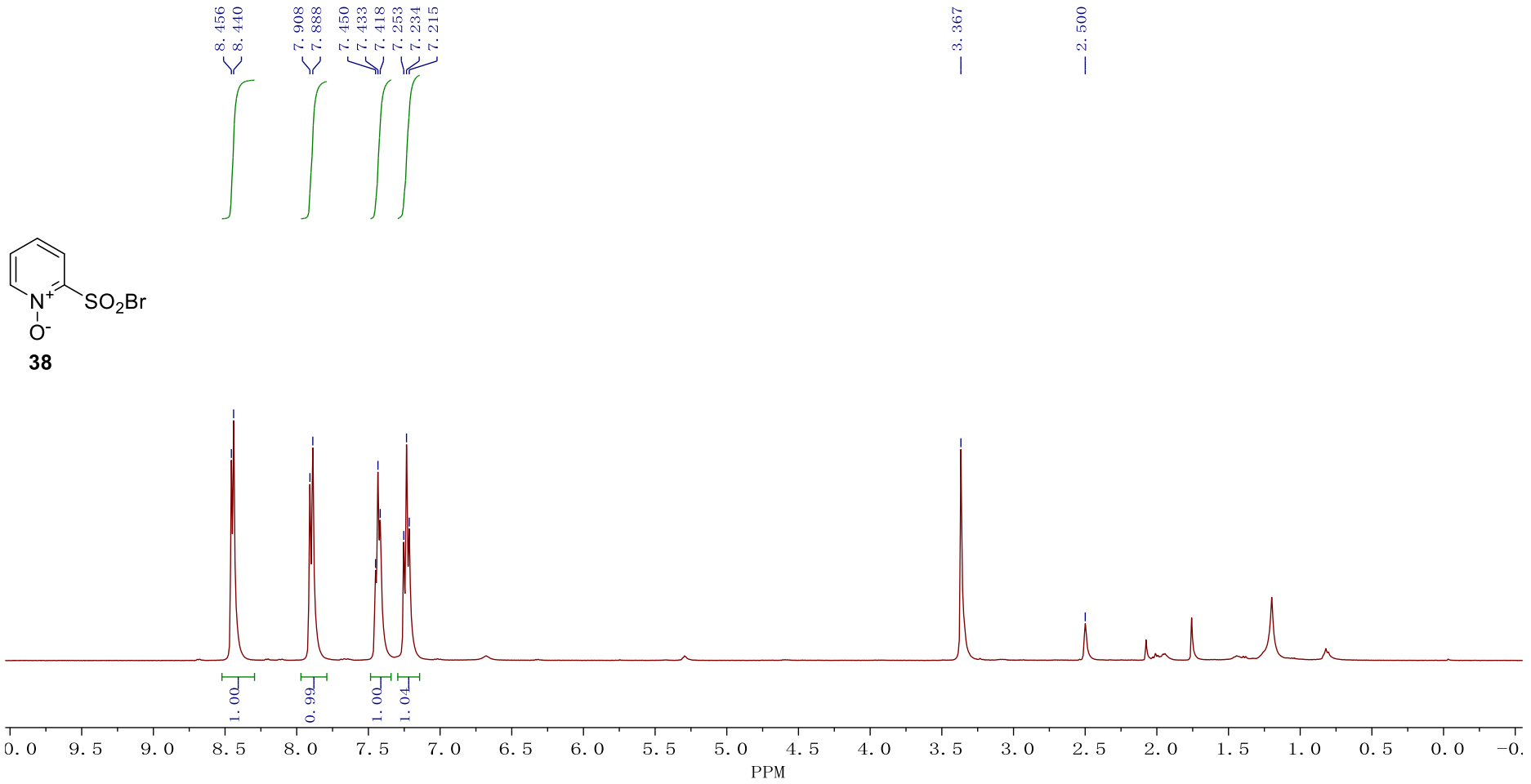
76.682 CDCl3
24.817
SO2Br
AcHN
37
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
PPM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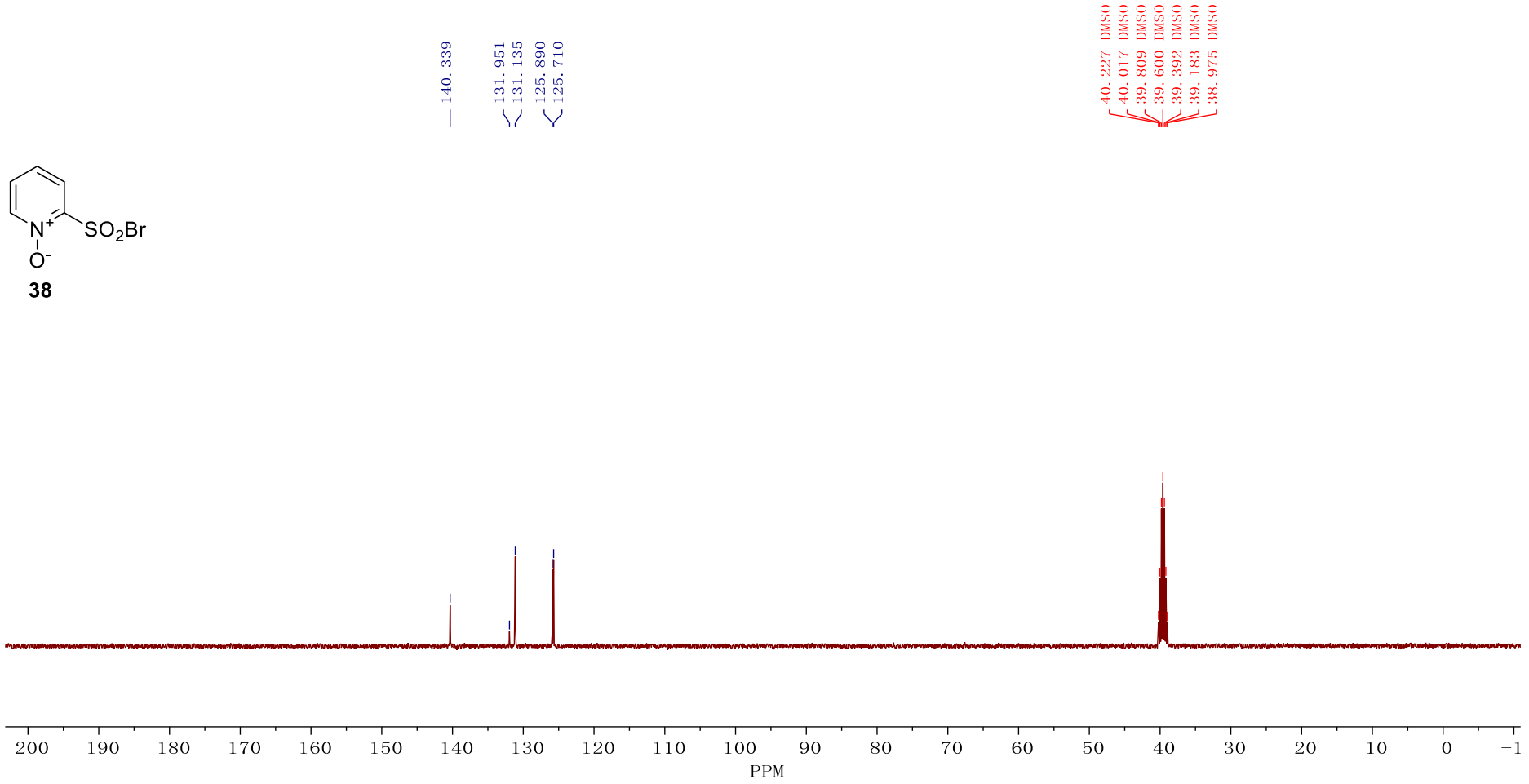
8.440
7.908
7.888
7.450
7.433
7.418
7.253
7.234
7.215
3.367
2.500
N+
O-
SO2Br
38
1.00
0.99
1.00
1.04
PPM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131.951
131.135
125.890
125.710
40.227 DMSO
40.017 DMSO
39.809 DMSO
39.600 DMSO
39.392 DMSO
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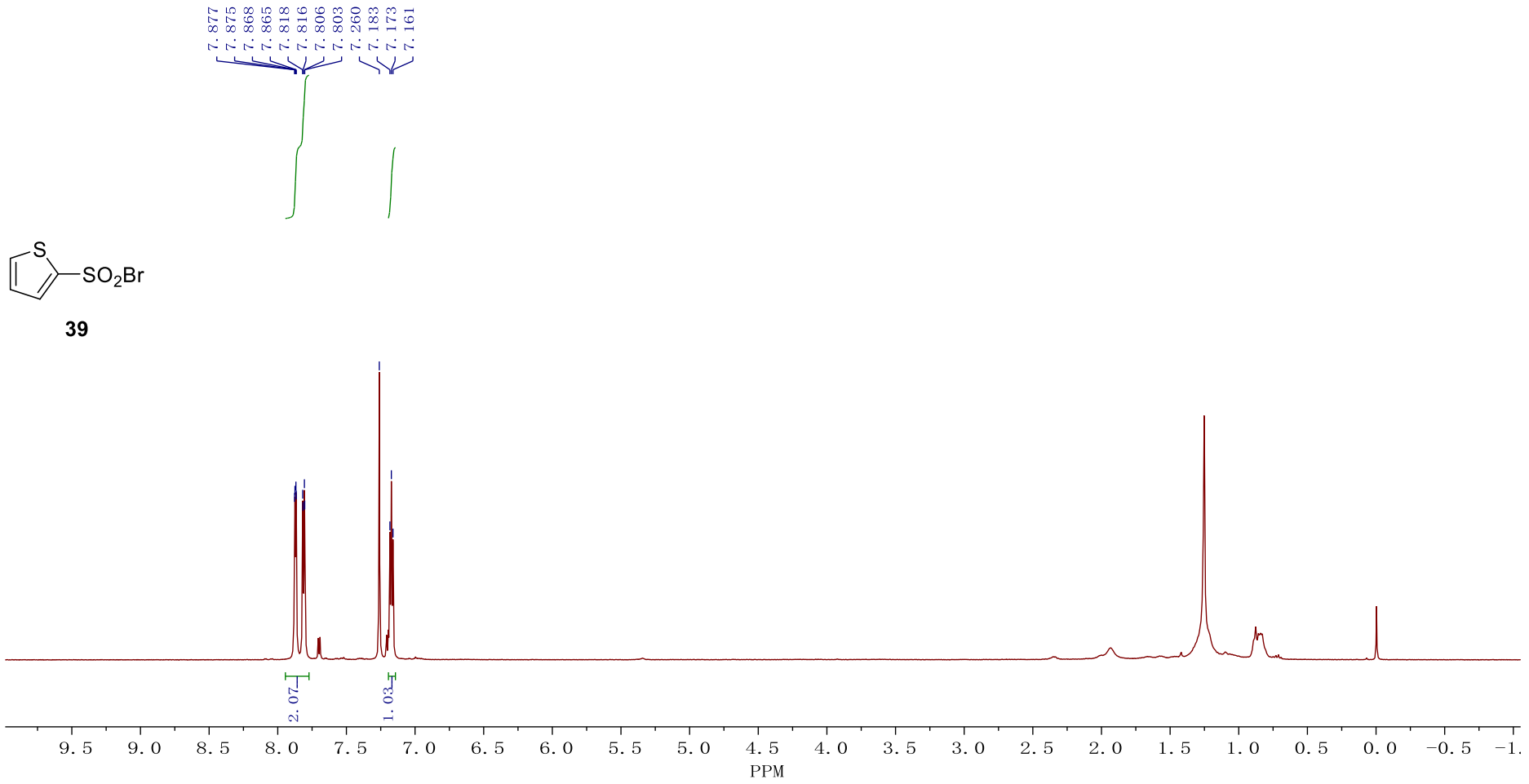
38.975 DMSO
N+
O-
SO2Br
38
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −1
PPM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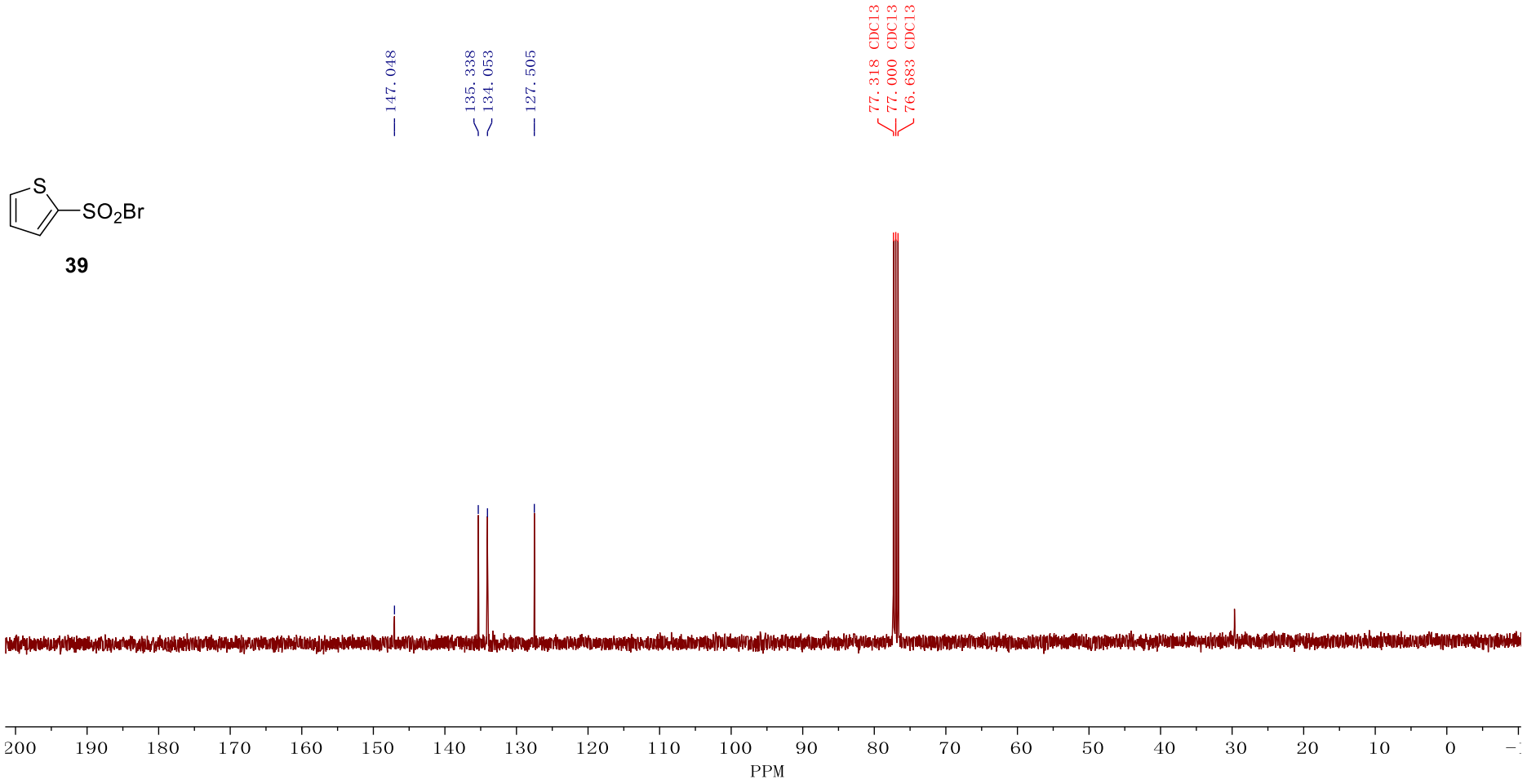
7.816
7.806
7.803
7.260
7.183
7.173
7.161
S
SO2Br
39
2.07
1.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
PPM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135.338
134.053
127.505
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
S
SO2Br
39
200
190
180
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150
140
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120
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100
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80
70
60
50
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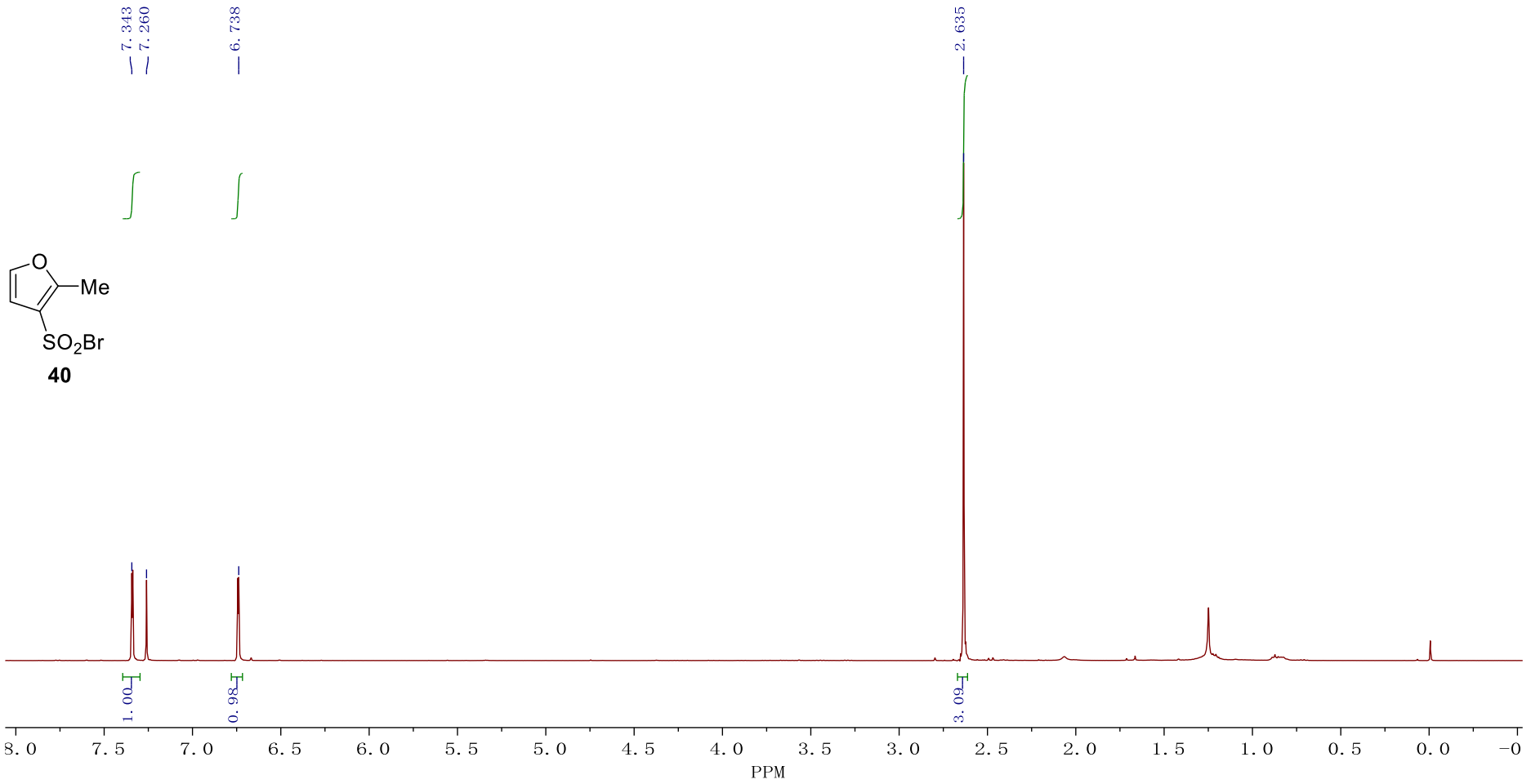
30
20
10
0
PPM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7.260
6.738
2.635
O
Me
SO2Br
40
1.00
0.98
3.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0
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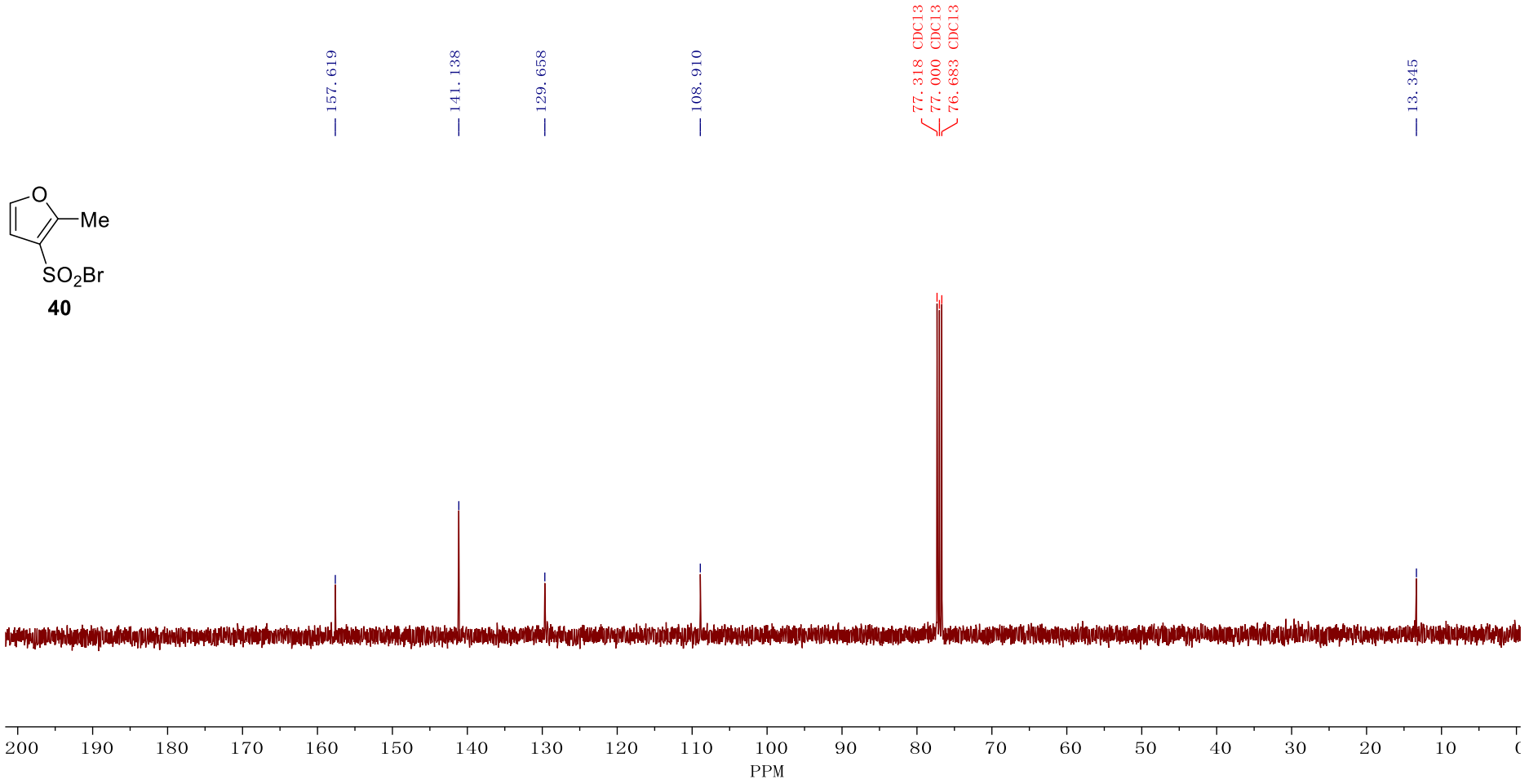
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141.138
129.658
108.910
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77.000 CDCl3
76.683 CDCl3
13.345
O
Me
SO2Br
40
200
190
180
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150
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130
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110
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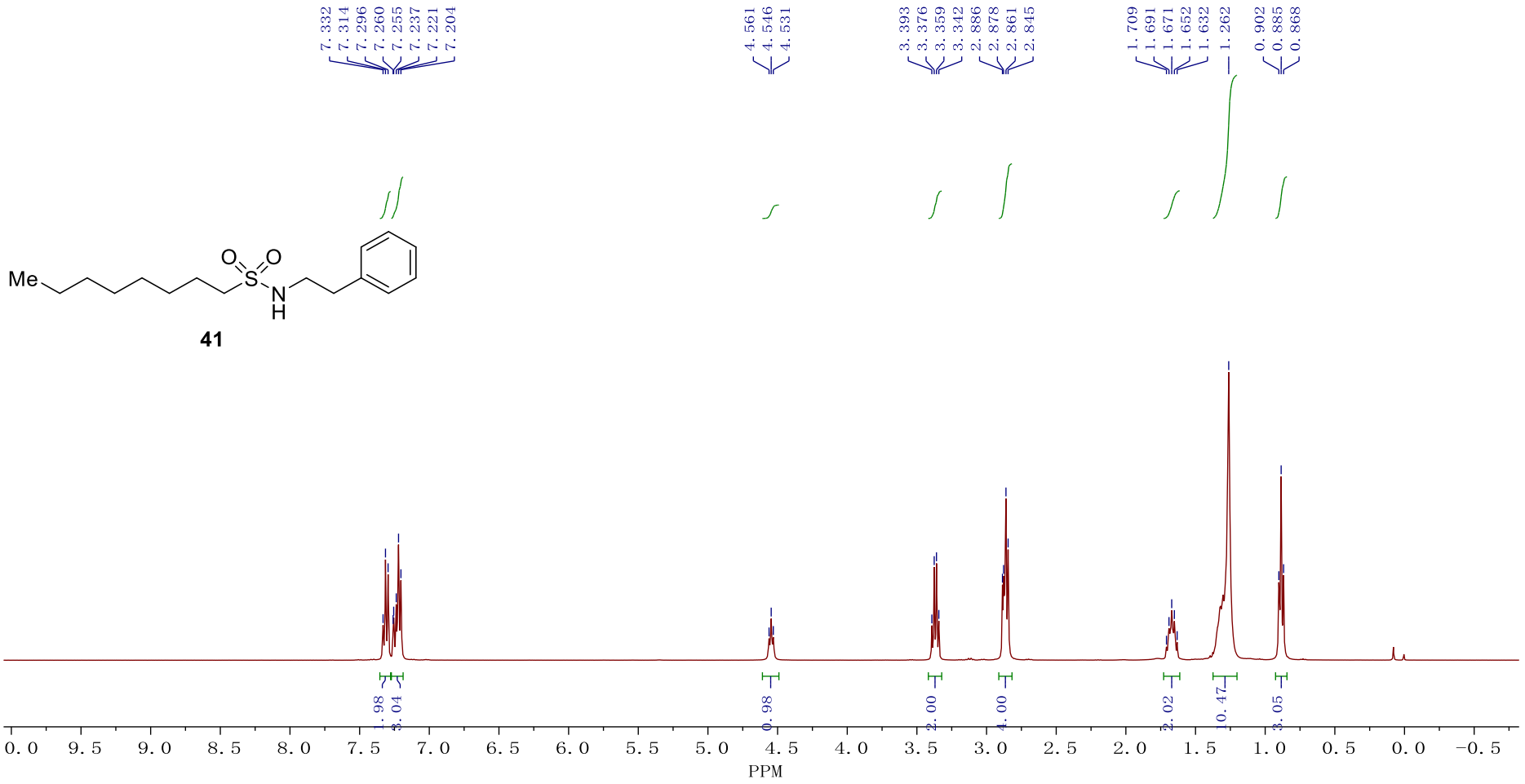
70
60
50
40
30
20
10
PPM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7.204
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4.546
4.531
3.393
3.376
3.359
3.342
2.886
2.878
2.861
2.845
1.709
1.691
1.671
1.652
1.632
1.262
0.902
0.885
0.868
Me
O
O
S
N
H
41
1.98
3.04
0.98
2.00
4.00
2.02
10.47
3.05
0.0
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
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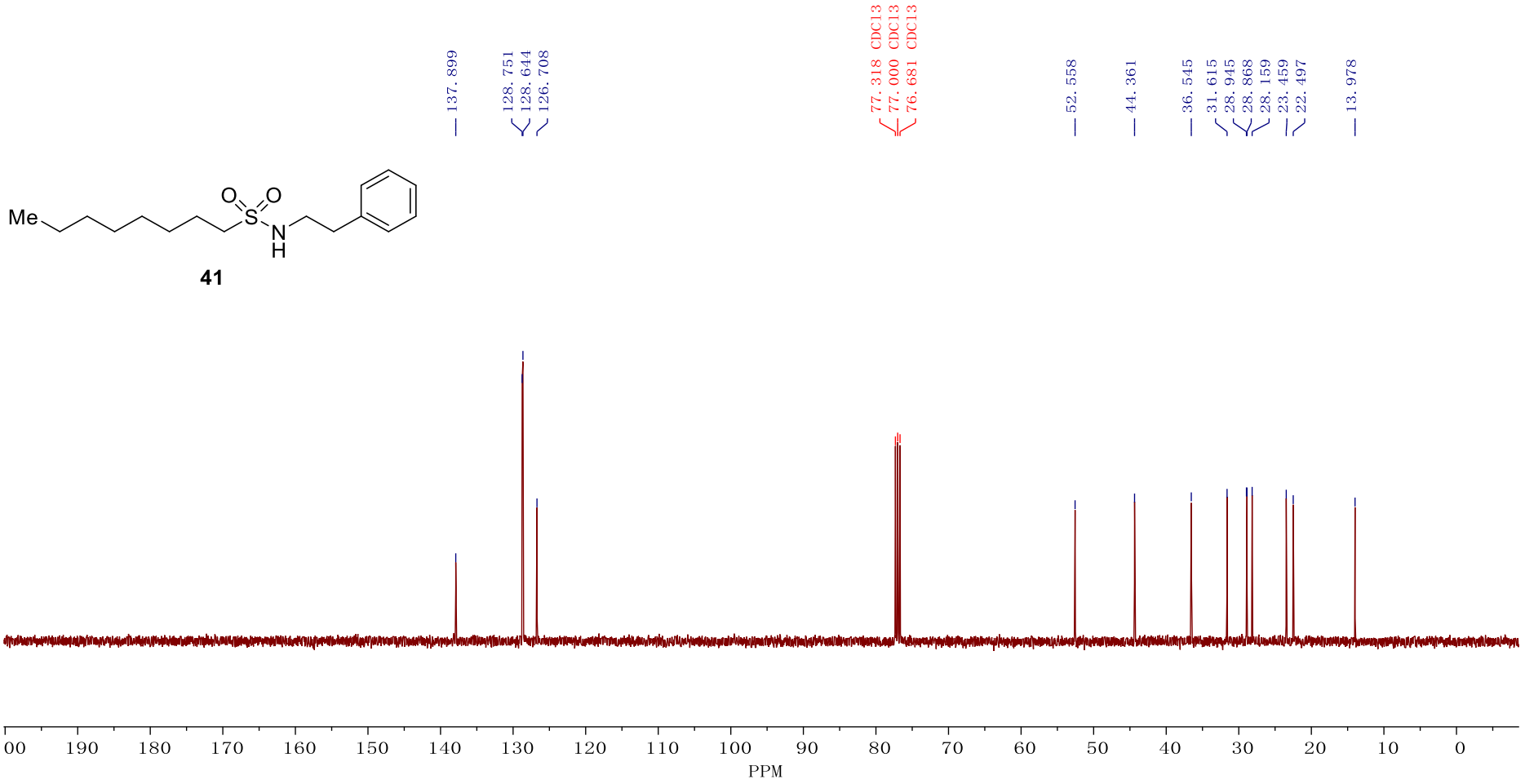
PPM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128.644
126.708
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77.000 CDCl3
76.681 CDCl3
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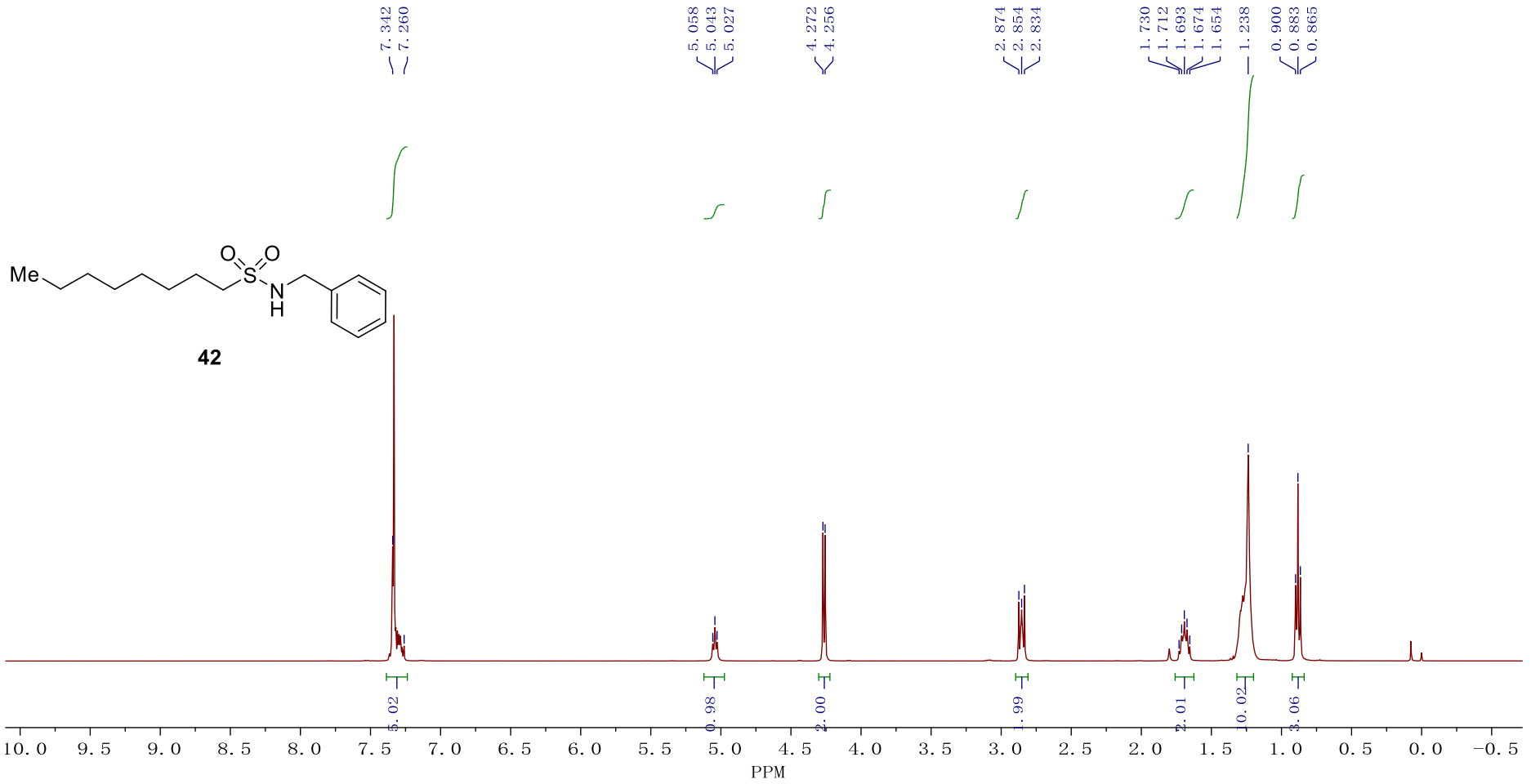
44.361
36.545
31.615
28.945
28.868
28.159
23.459
22.497
13.978
Me
O
O
S
N
H
41
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM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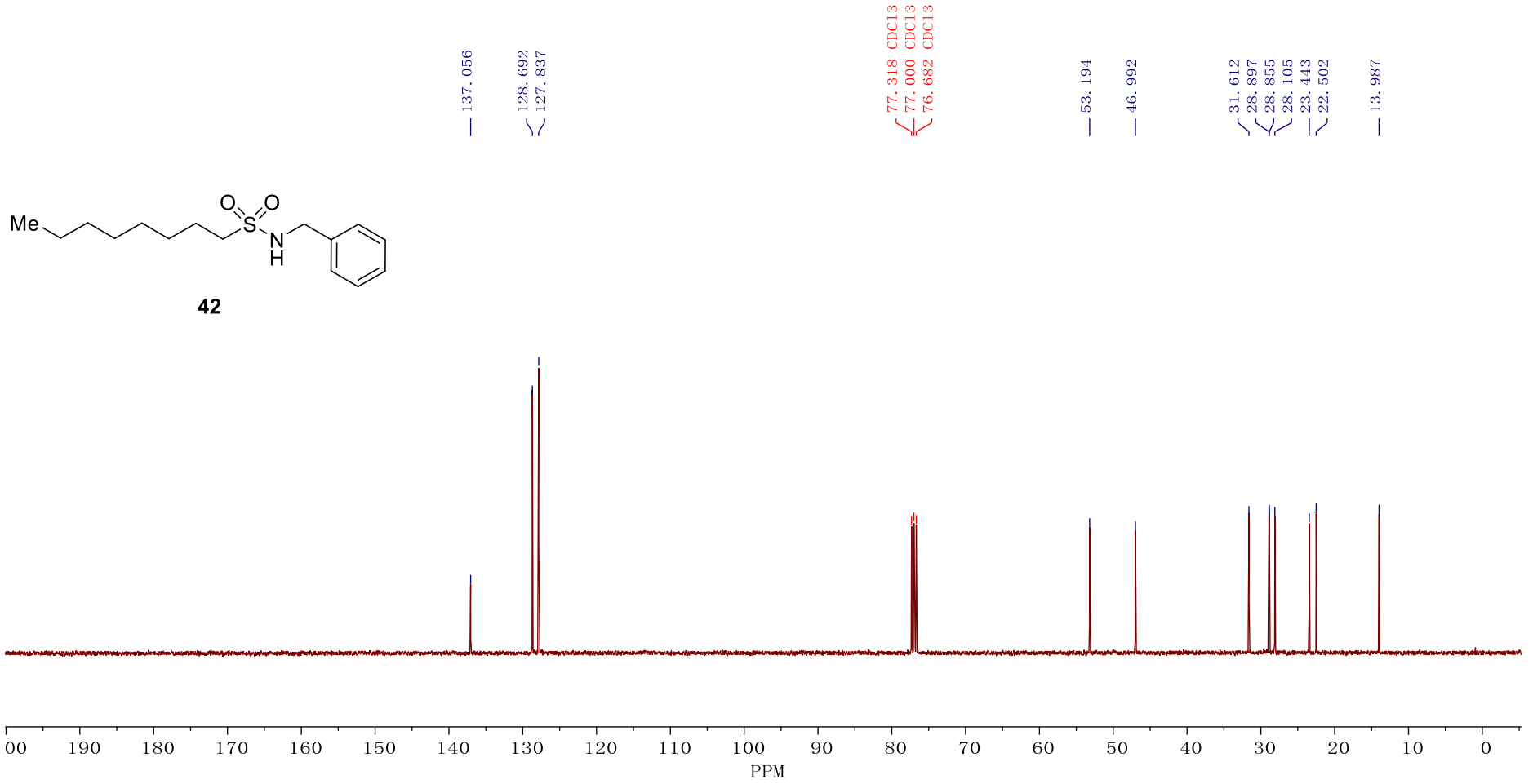
1.712
1.693
1.674
1.654
1.238
0.900
0.883
0.865
Me
O
O
S
N
H
42
5.02
0.98
2.00
1.99
2.01
10.02
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
PPM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127.837
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77.000 CDC13
76.682 CDC13
53.194
46.992
31.612
28.897
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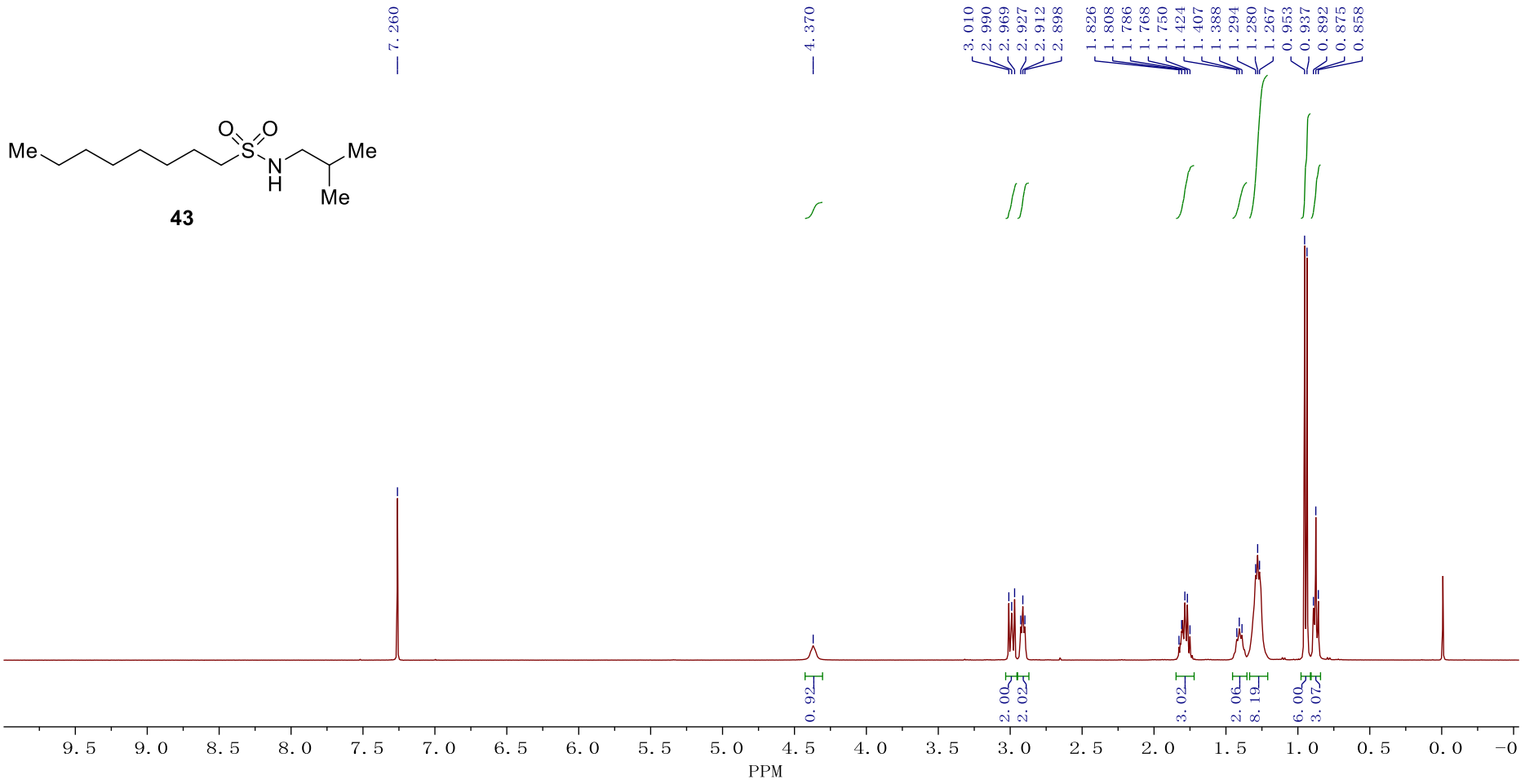
28.105
23.443
22.502
13.987
Me
O
O
S
N
H
42
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
PPM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2.898
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1.808
1.786
1.768
1.750
1.424
1.407
1.388
1.294
1.280
1.267
0.953
0.937
0.892
0.875
0.858
Me
O
O
S
N
H
Me
Me
43
0.92
2.00
2.02
3.02
2.06
8.19
6.00
3.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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1.0
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0.0
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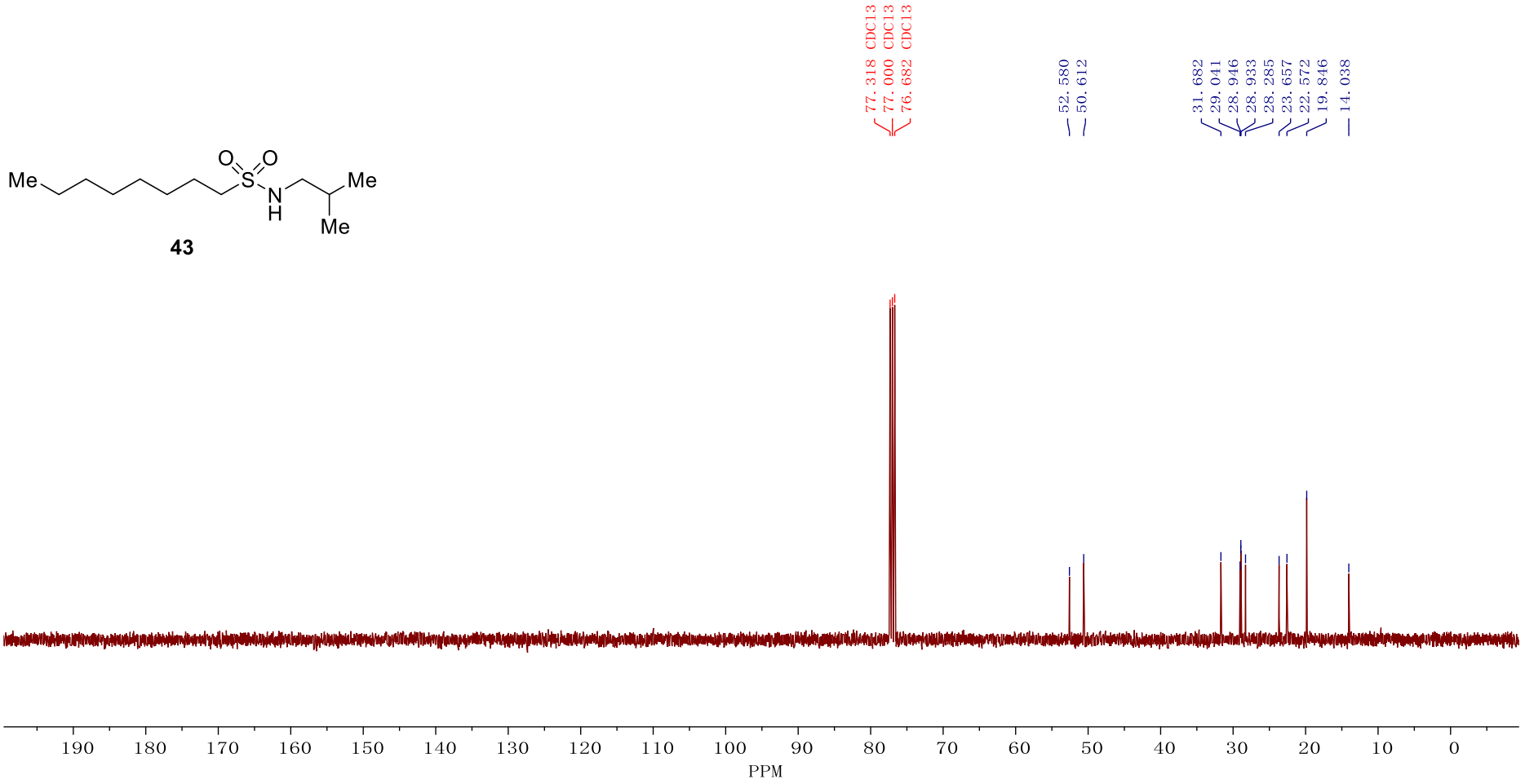
PPM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O
O
S
N
H
Me
Me
43
77.318 CDCl3
77.000 CDCl3
76.682 CDCl3
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50.612
31.682
29.041
28.946
28.933
28.285
23.657
22.572
19.846
14.038
190
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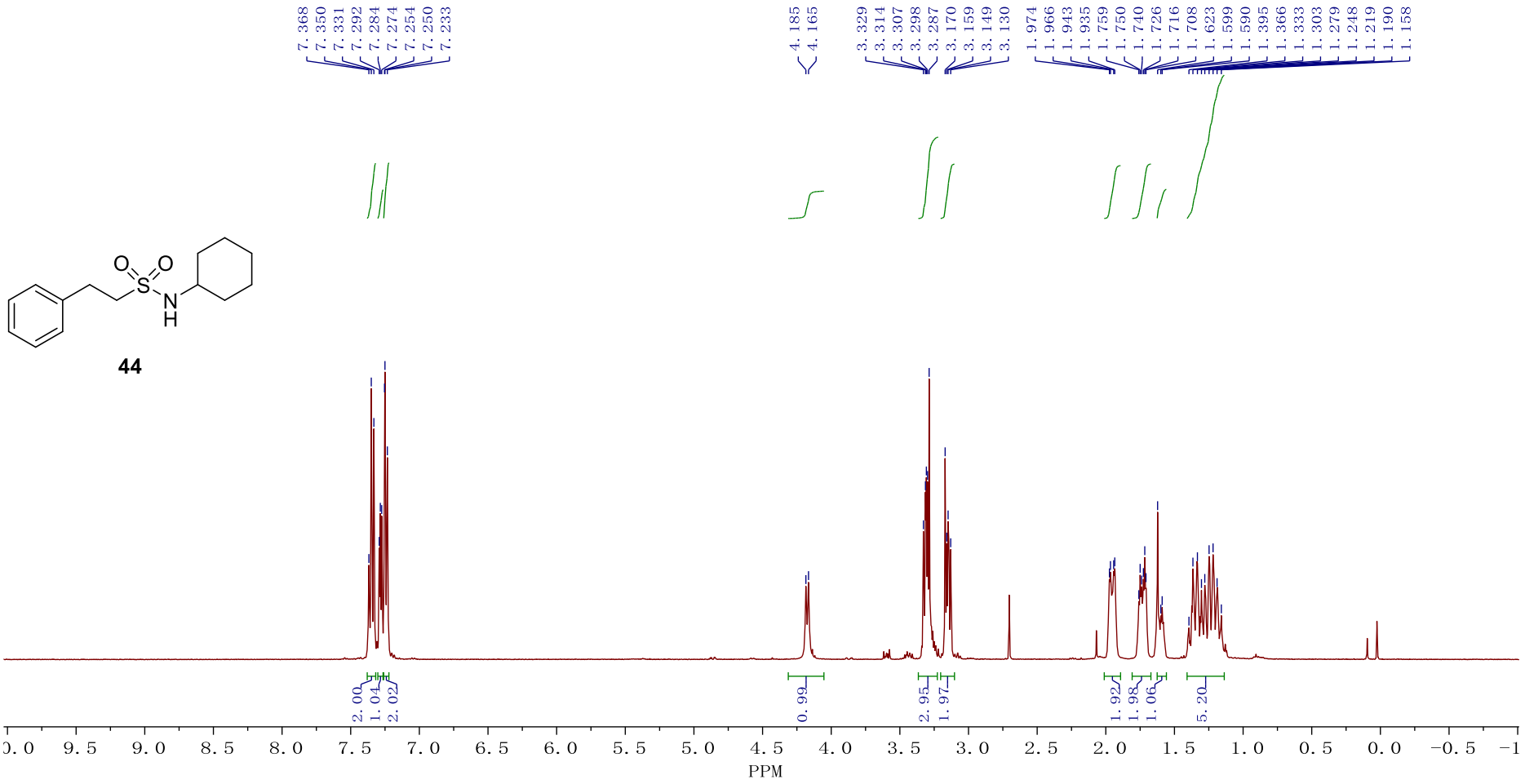
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM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3.307
3.298
3.287
3.170
3.159
3.149
3.130
1.974
1.966
1.943
1.935
1.759
1.750
1.740
1.726
1.716
1.708
1.623
1.599
1.590
1.395
1.366
1.333
1.303
1.279
1.248
1.219
1.190
1.158
O
O
S
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2.02
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1.92
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1.06
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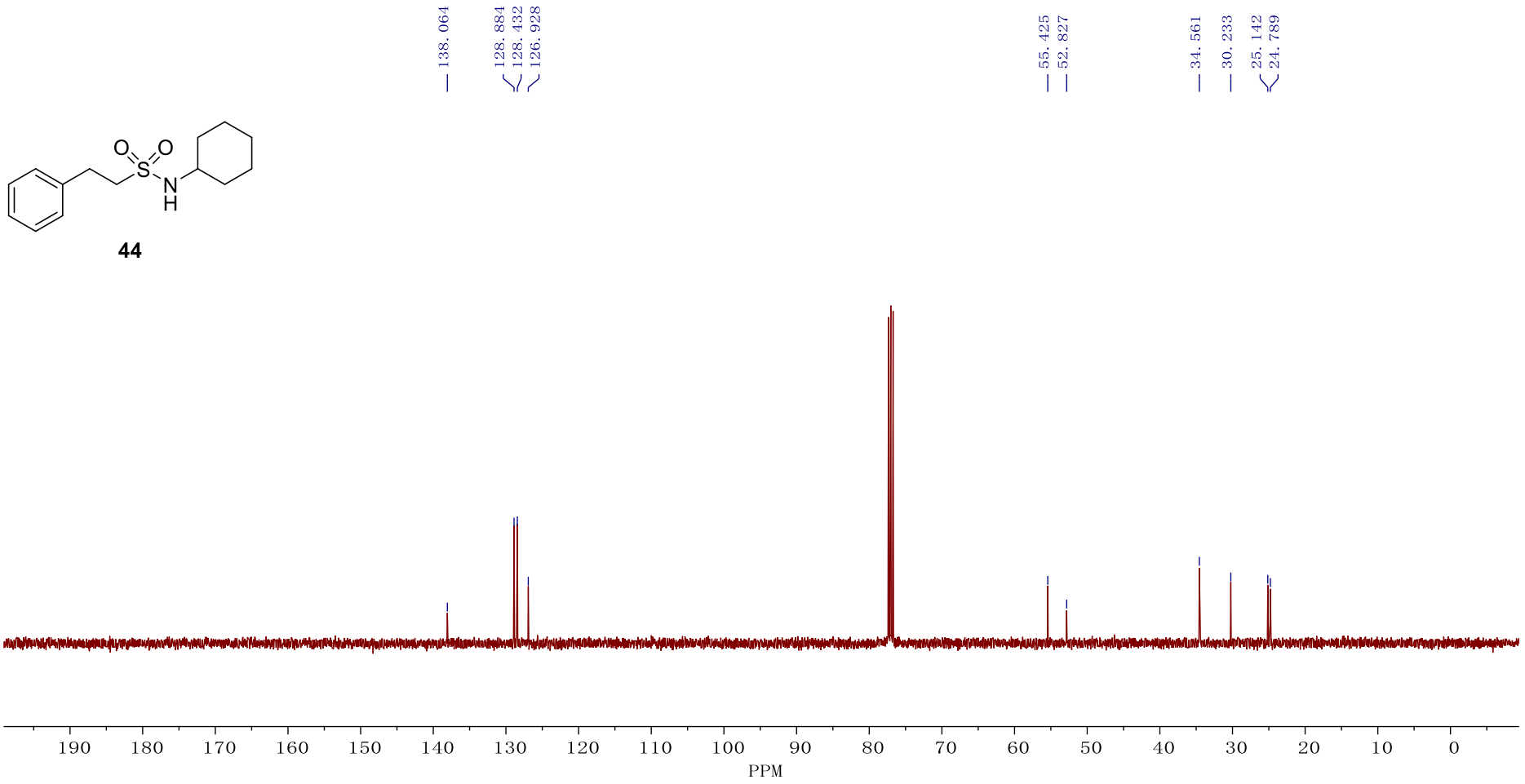
PPM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30.233
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24.789
O
O
S
N
H
44
190
180
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140
130
120
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100
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80
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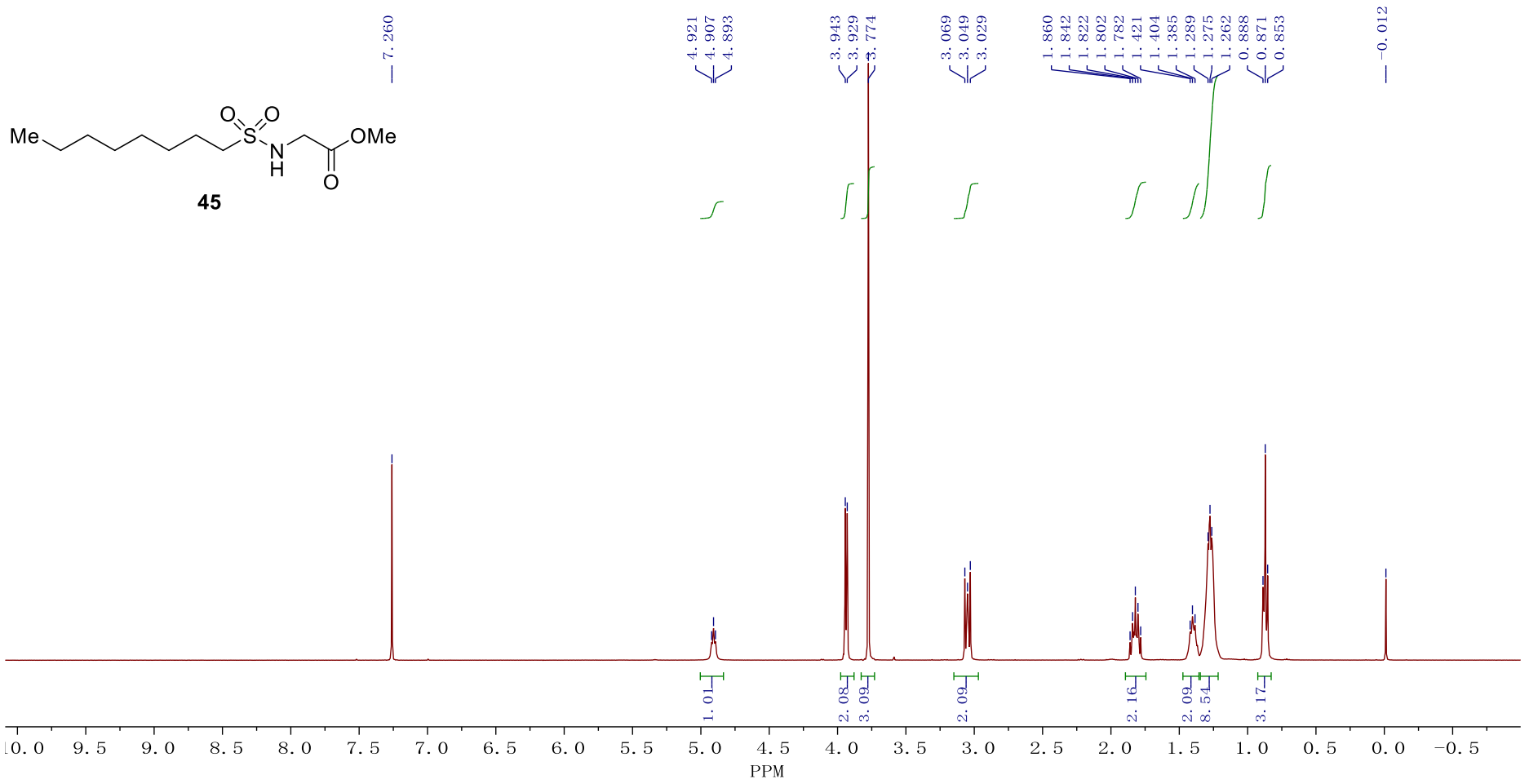
PPM


Me
O
O
S
N
H
OMe
O
45
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4.907
4.893
3.943
3.929
3.774
3.069
3.049
3.029
1.860
1.842
1.822
1.802
1.782
1.421
1.404
1.385
1.289
1.275
1.262
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0.871
0.853
-0.012
1.01
2.08
3.09
2.09
2.16
2.09
8.54
3.17
10.0
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9.0
8.5
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6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
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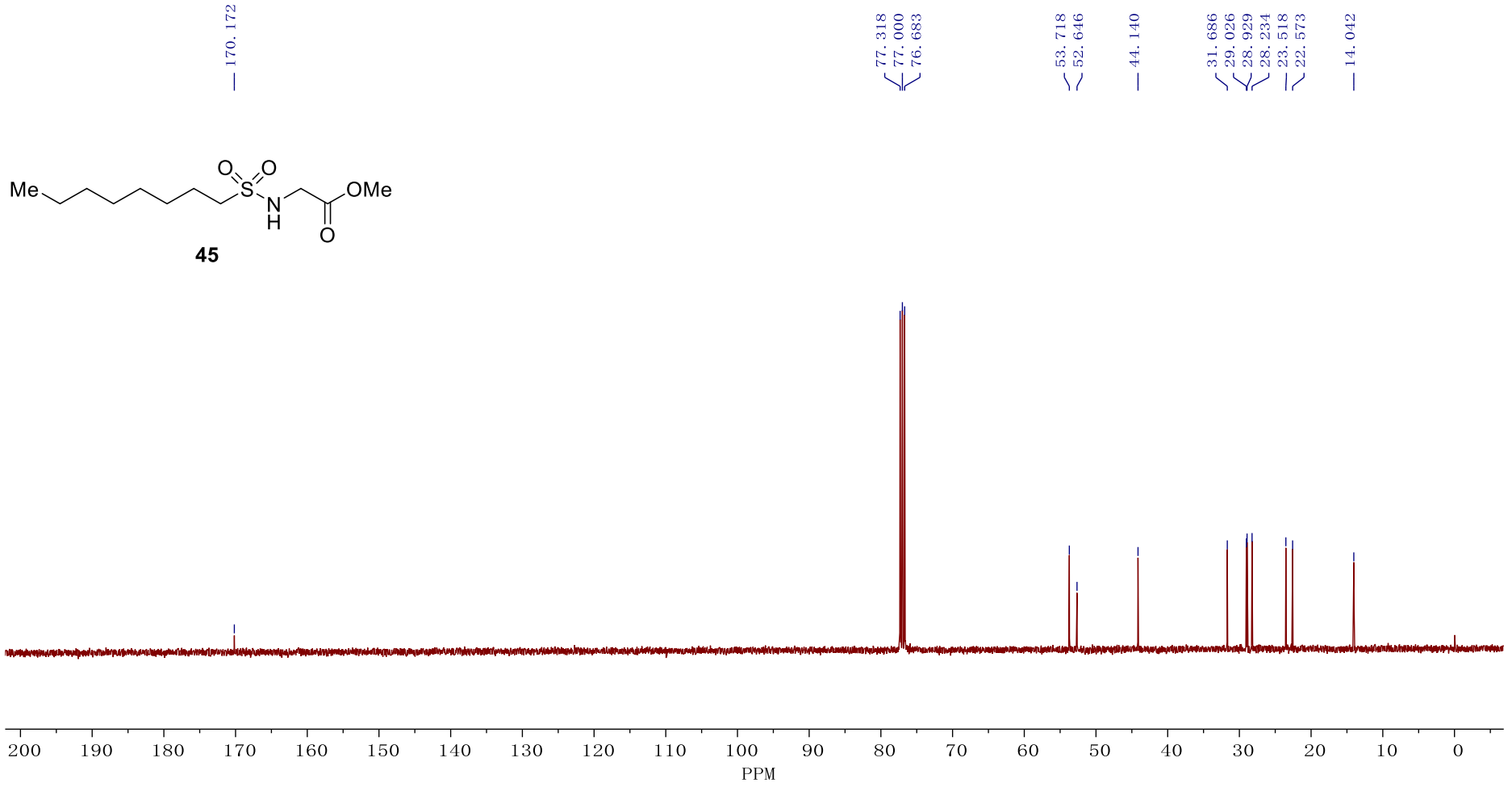
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22.573
14.042
Me
O
O
S
N
H
O
OMe
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200
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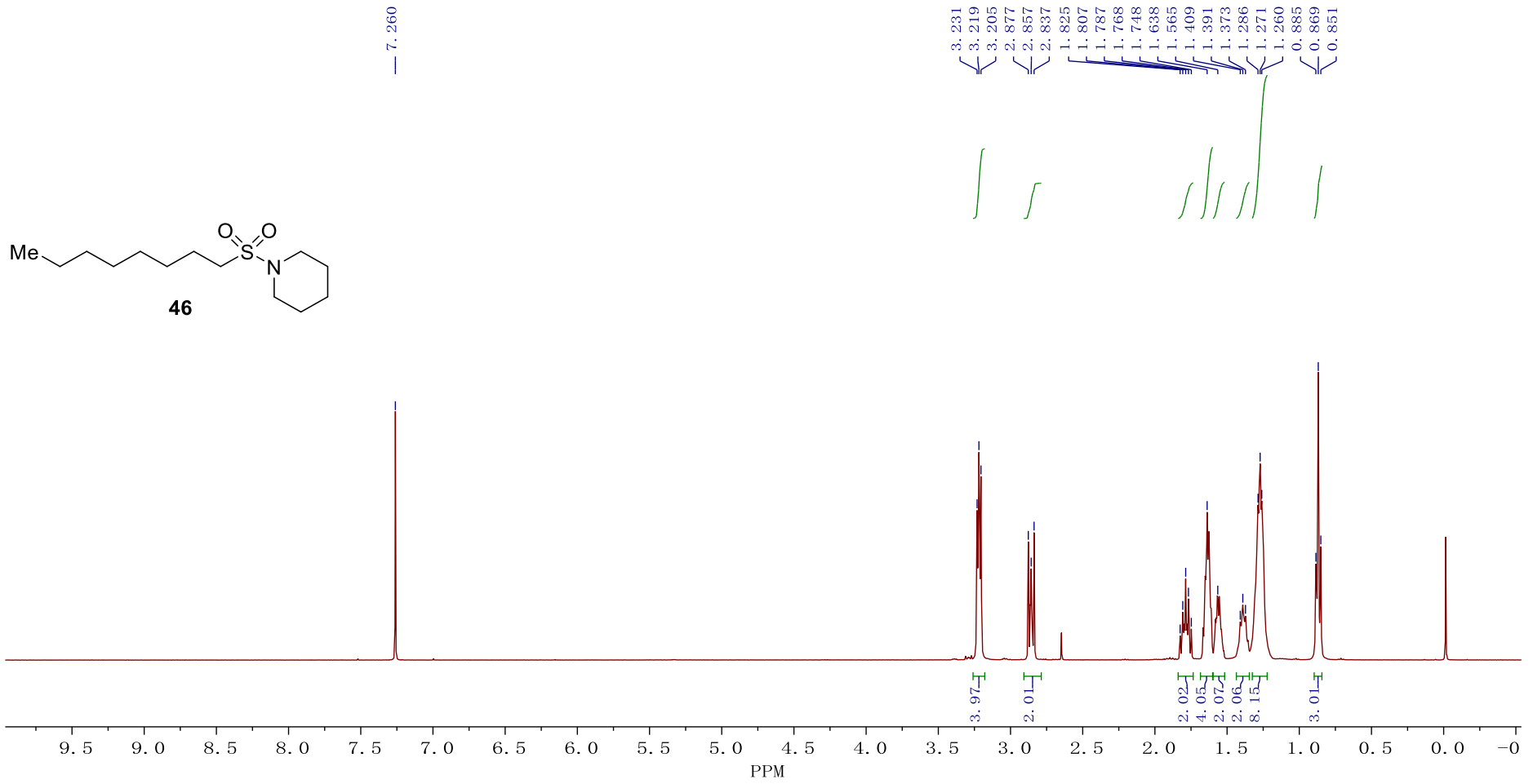
PPM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1.825
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1.768
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1.638
1.565
1.409
1.391
1.373
1.286
1.271
1.260
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0.869
0.851
Me
O
O
S
N
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2.02
4.05
2.07
2.06
8.15
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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1.0
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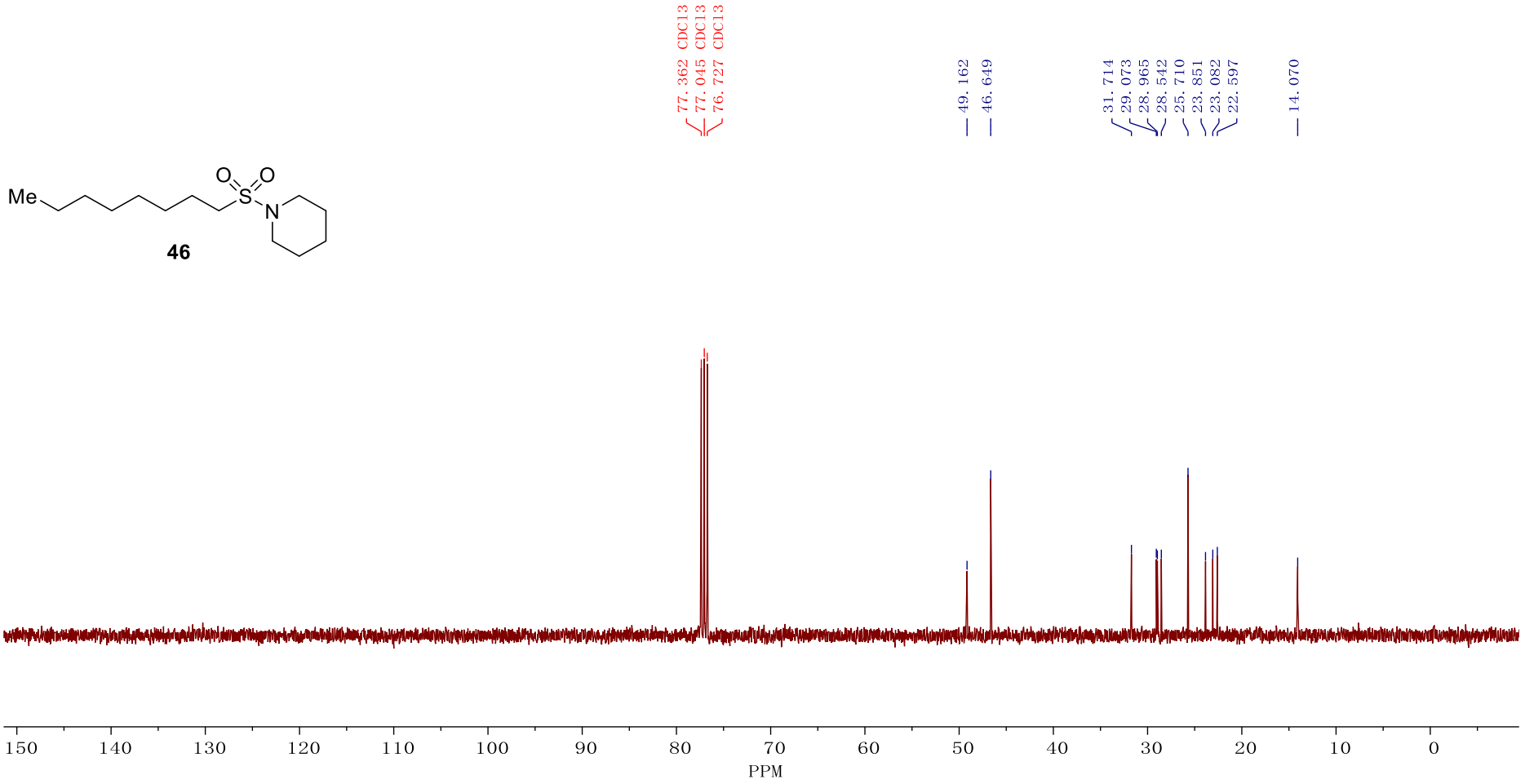
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23.082
22.597
14.070
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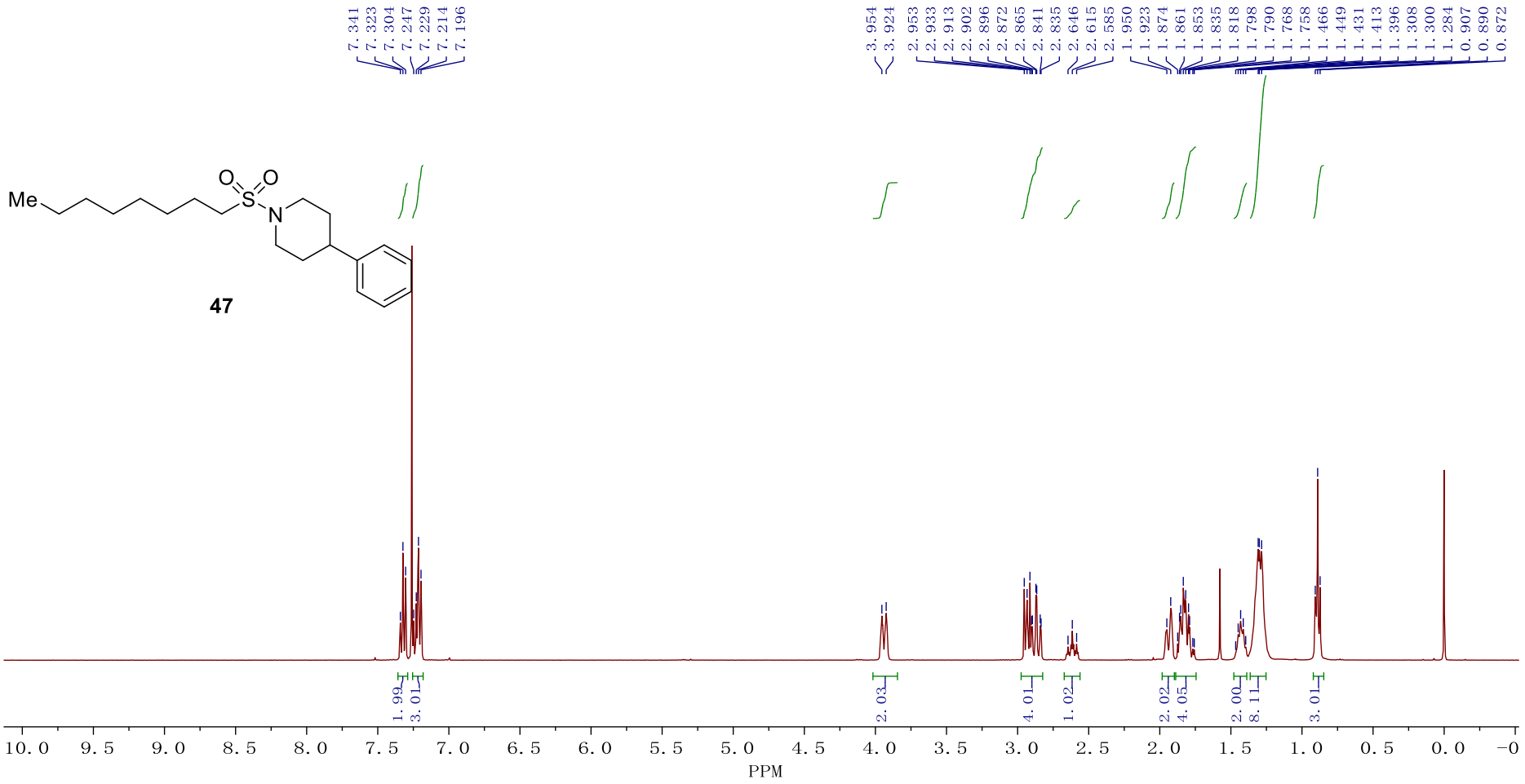
PPM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1.413
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0.907
0.890
0.872
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S
O
N
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2.03
4.01
1.02
2.02
4.05
2.00
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7.0
6.5
6.0
5.5
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1.0
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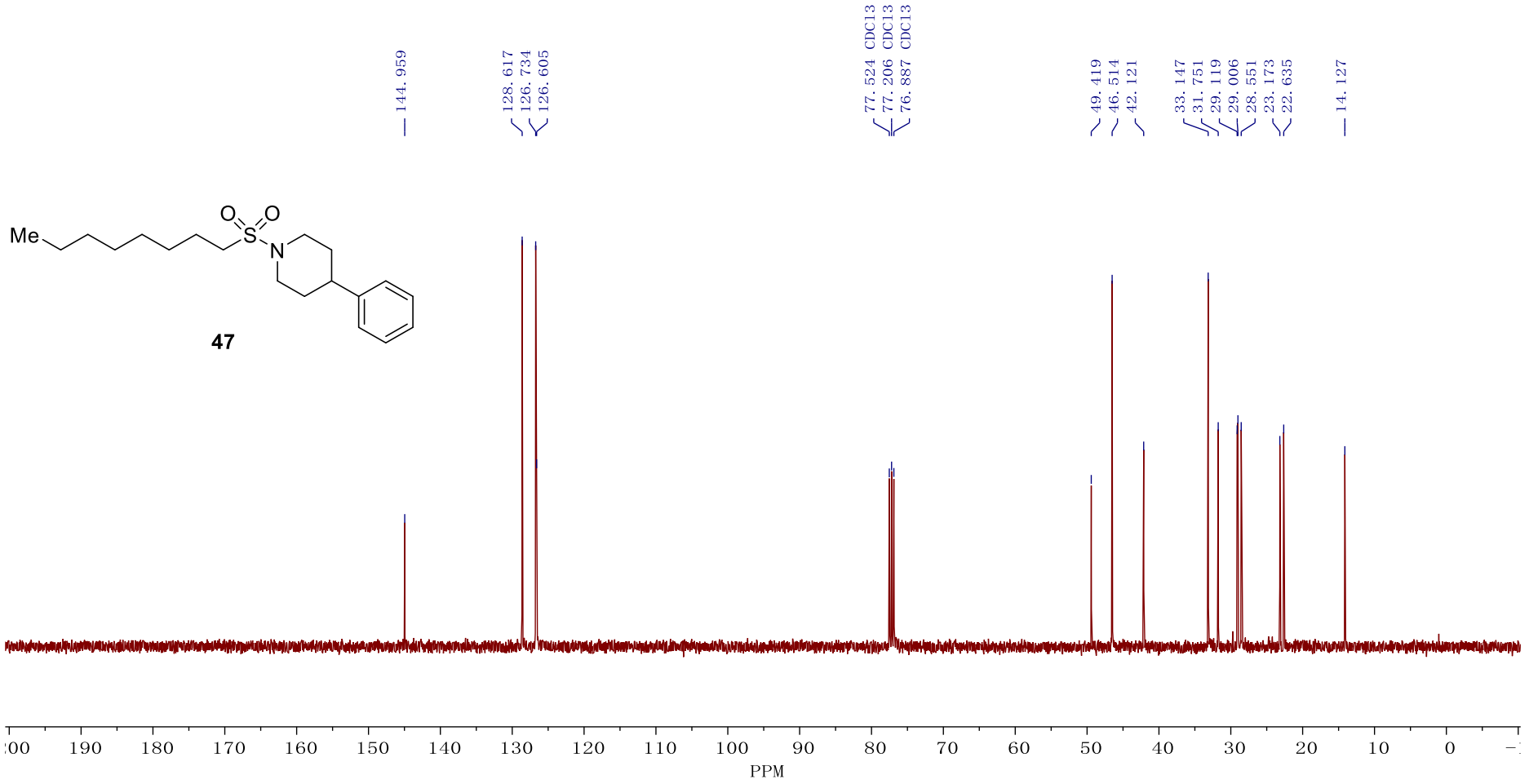
PPM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31.751
29.119
29.006
28.551
23.173
22.635
14.127
Me
O
O
S
N
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190
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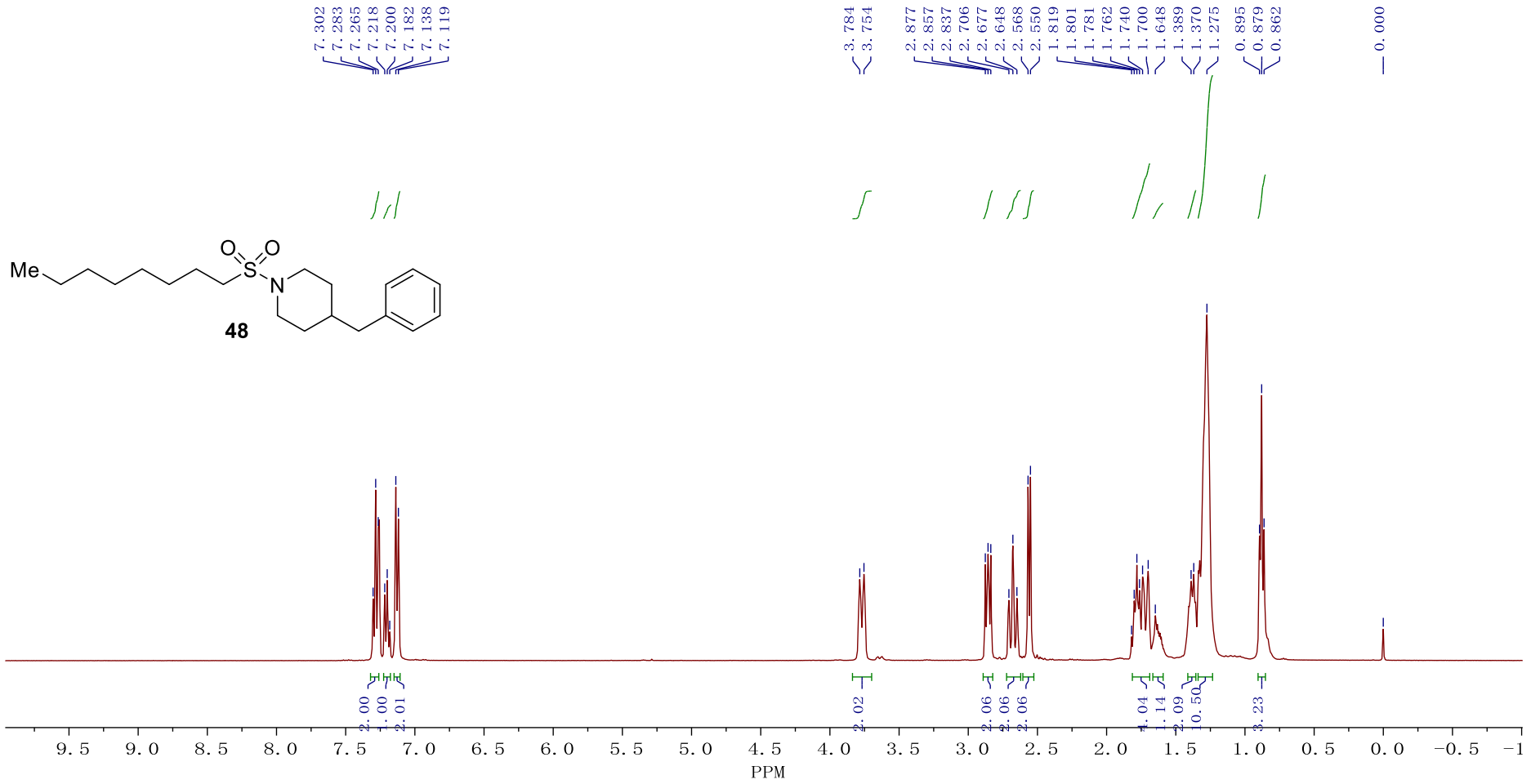
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2.706
2.677
2.648
2.568
2.550
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1.801
1.781
1.762
1.740
1.700
1.648
1.389
1.370
1.275
0.895
0.879
0.862
0.000
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O
O
S
N
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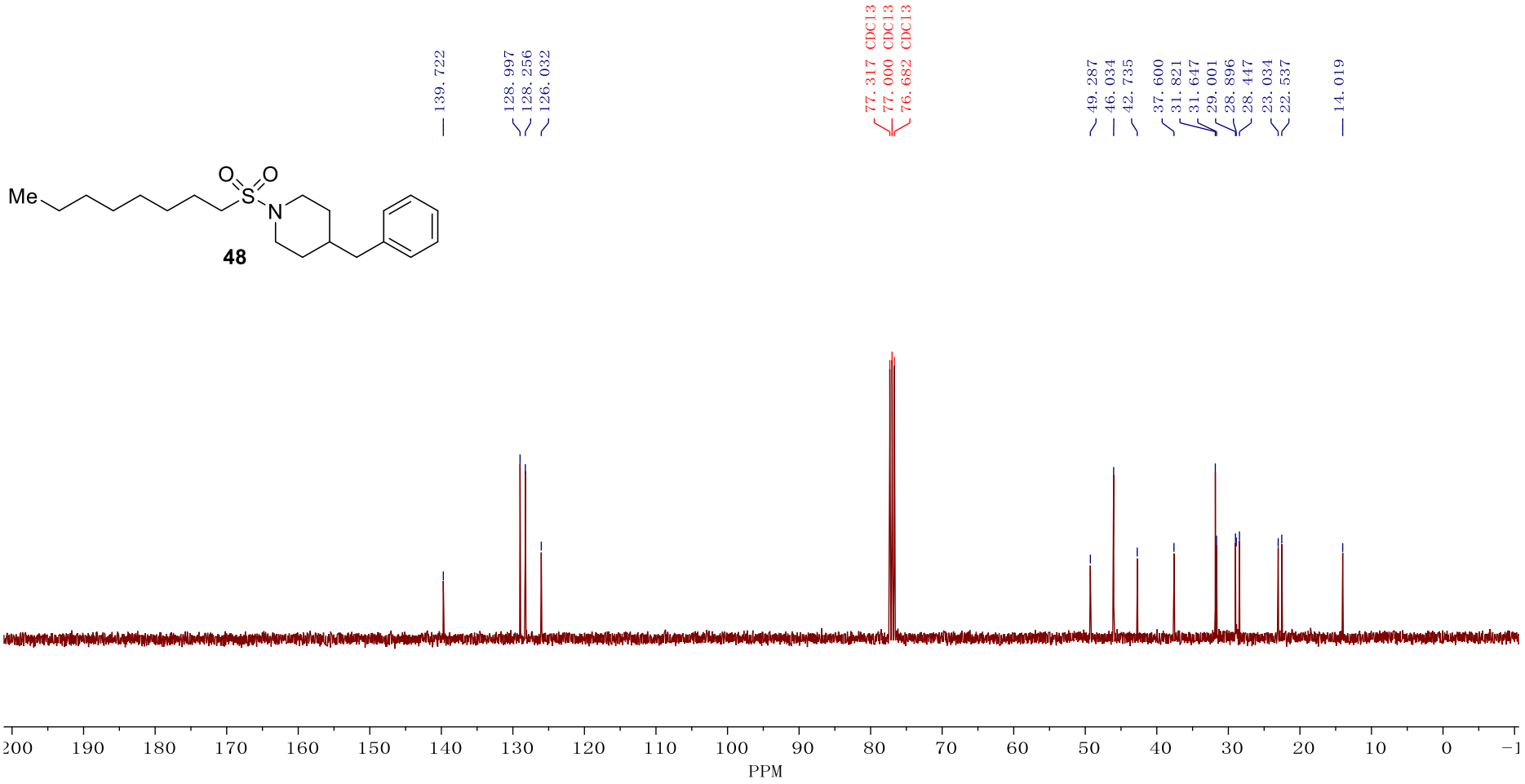
1.00
2.01
2.02
2.06
2.06
2.06
4.04
1.14
2.09
10.50
3.23
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
PPM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76.682 CDCl3
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46.034
42.735
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31.821
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28.896
28.447
23.034
22.537
14.019
Me
O
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S
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200
190
180
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0
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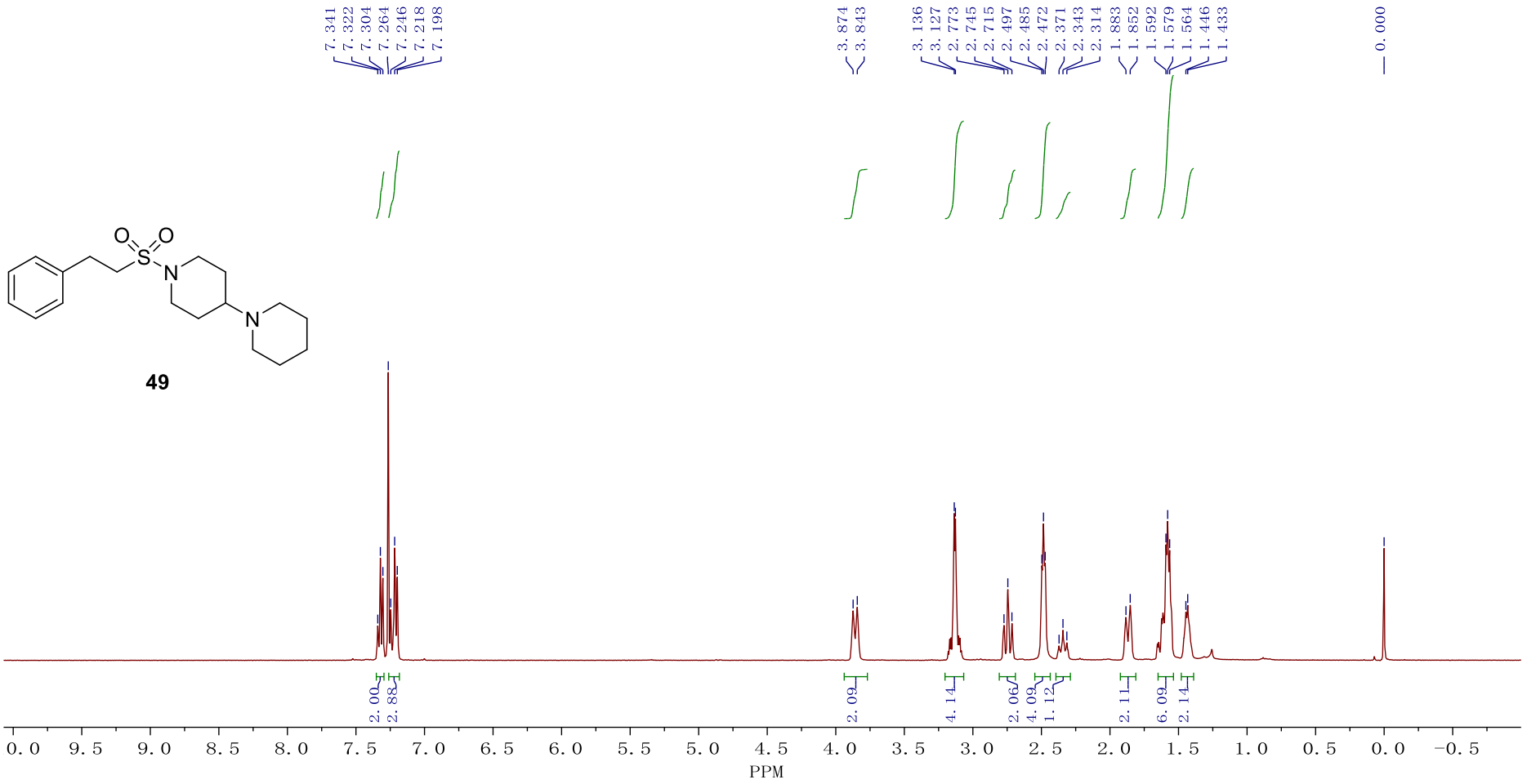
PPM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2.00
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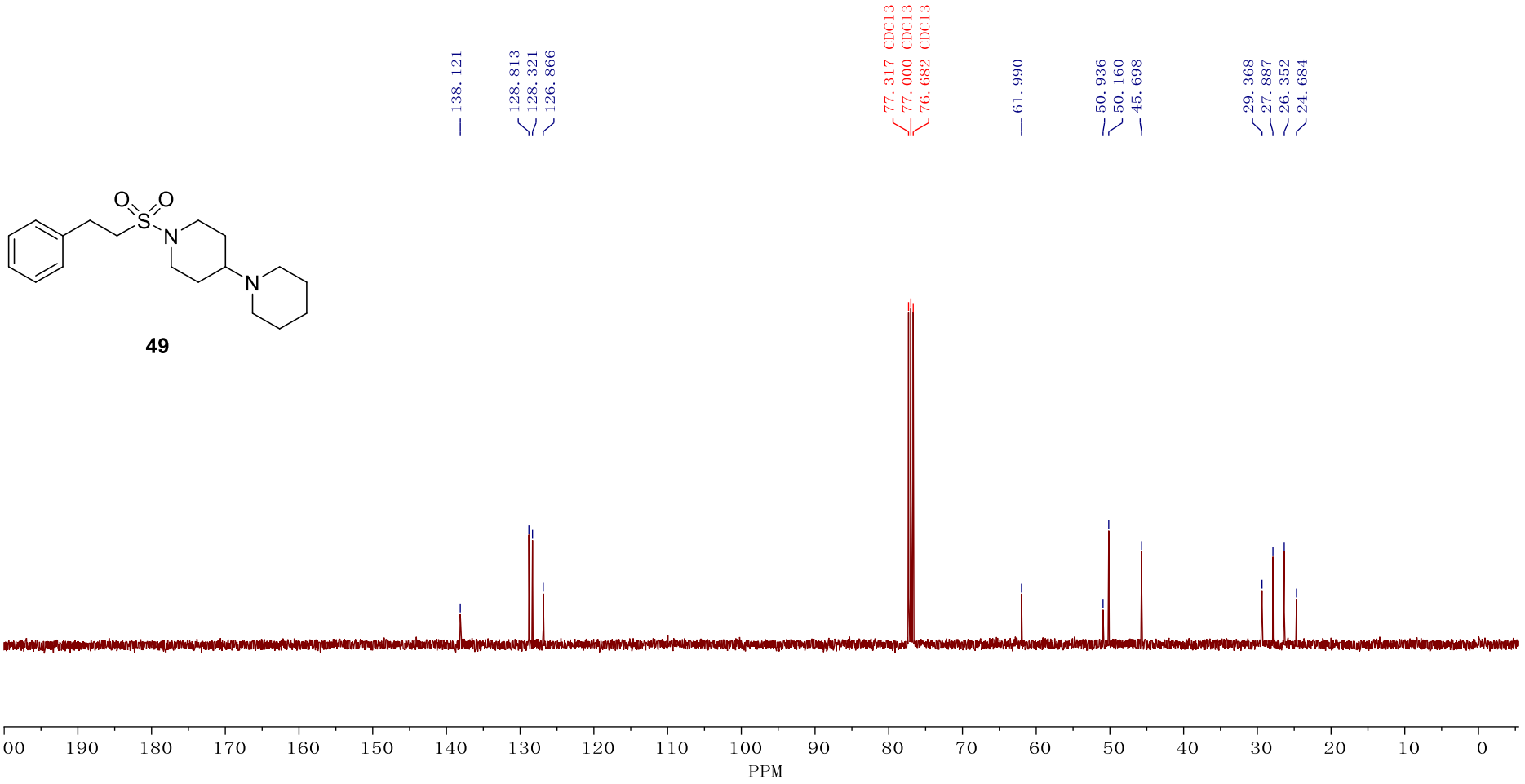
4.14
2.06
4.09
1.12
2.11
6.09
2.14
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
PPM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76.682 CDC13
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45.698
29.368
27.887
26.352
24.684
O
O
S
N
N
49
00
190
180
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150
140
130
120
110
100
90
80
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60
50
40
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20
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0
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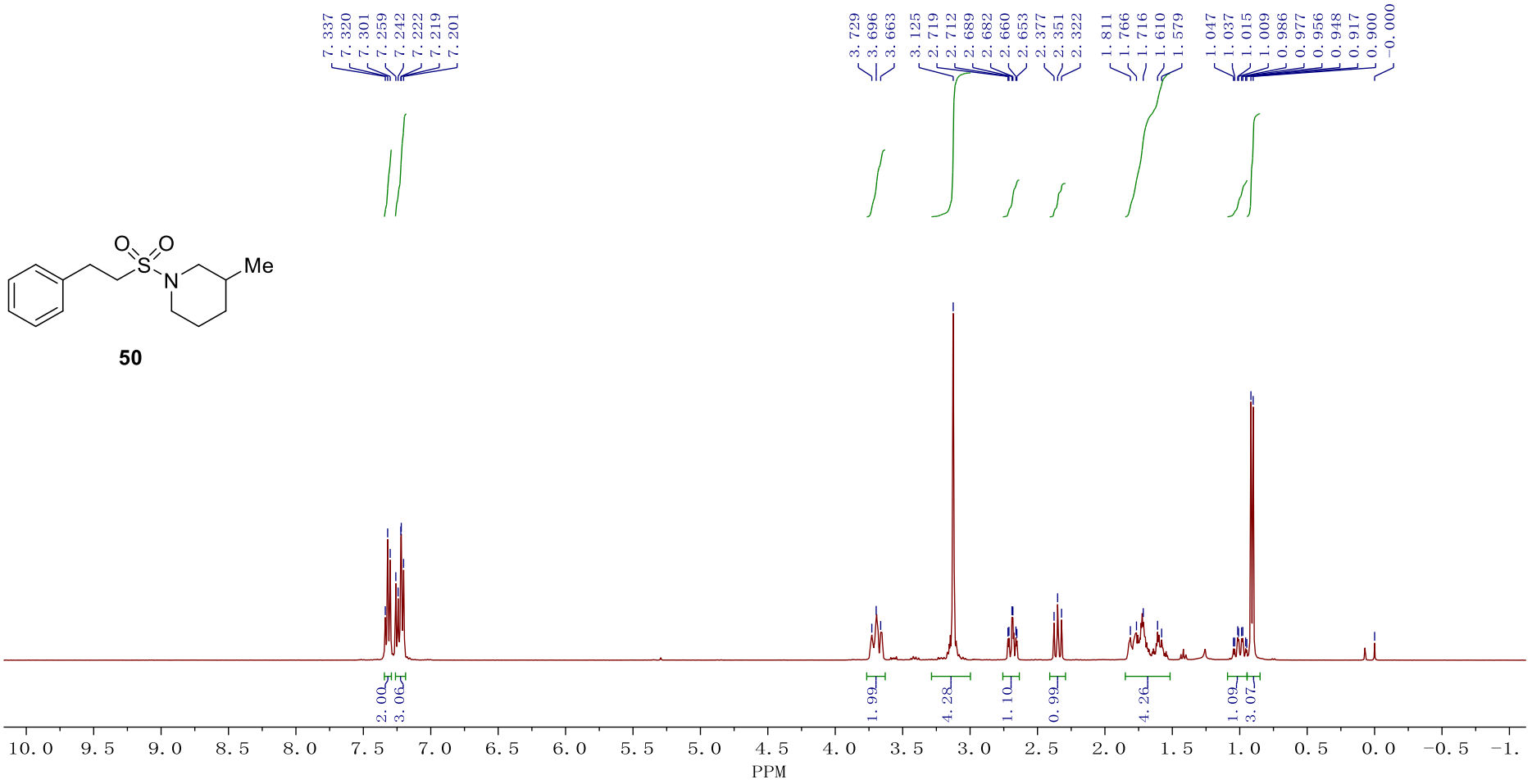
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7.201
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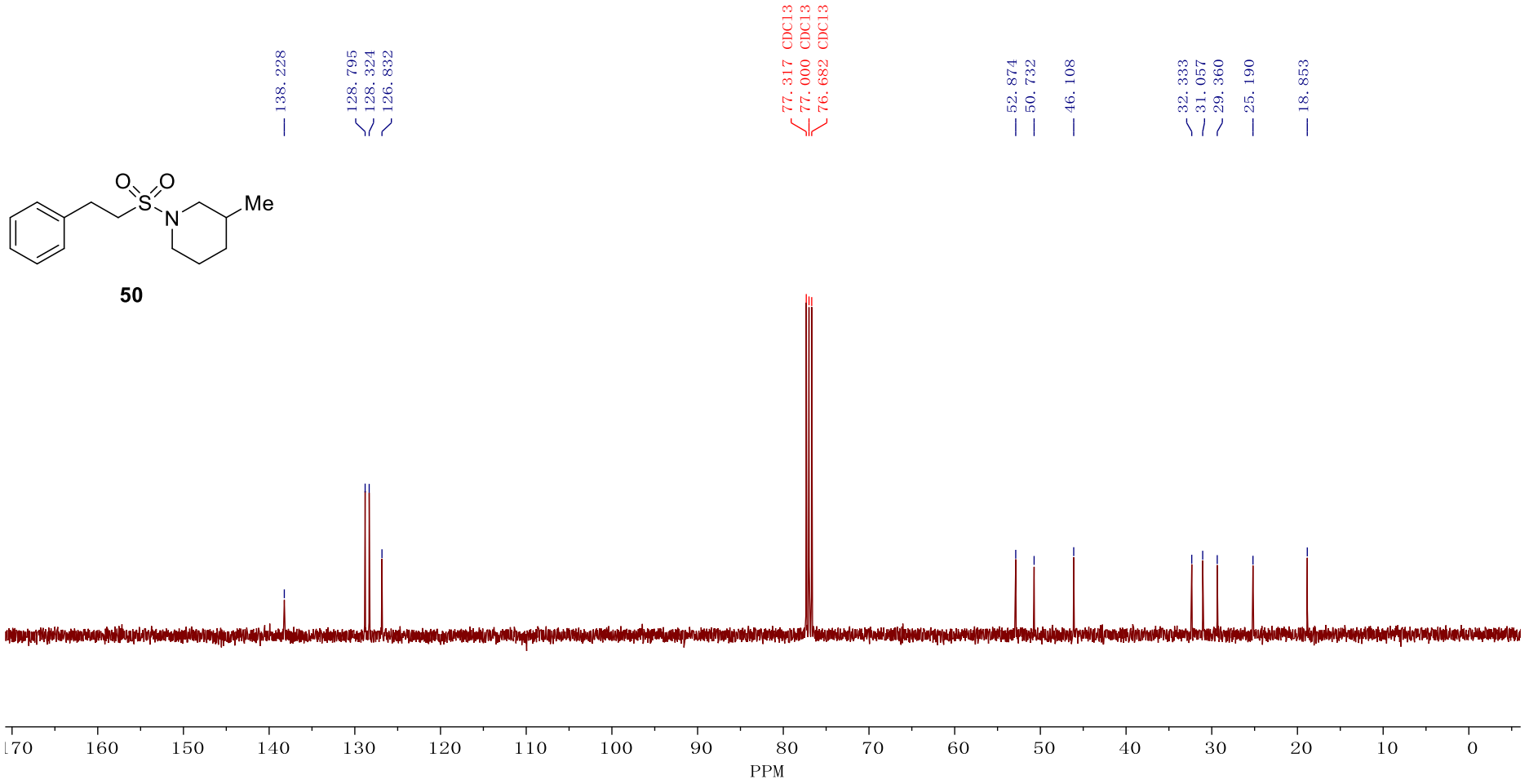
3.663
3.125
2.719
2.712
2.689
2.682
2.660
2.653
2.377
2.351
2.322
1.811
1.766
1.716
1.610
1.579
1.047
1.037
1.015
1.009
0.986
0.977
0.956
0.948
0.917
0.900
-0.000
O
O
S
N
Me
50
2.00
3.06
1.99
4.28
1.10
0.99
4.26
1.09
3.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
PPM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76.682 CDC13
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25.190
18.853
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O
S
N
Me
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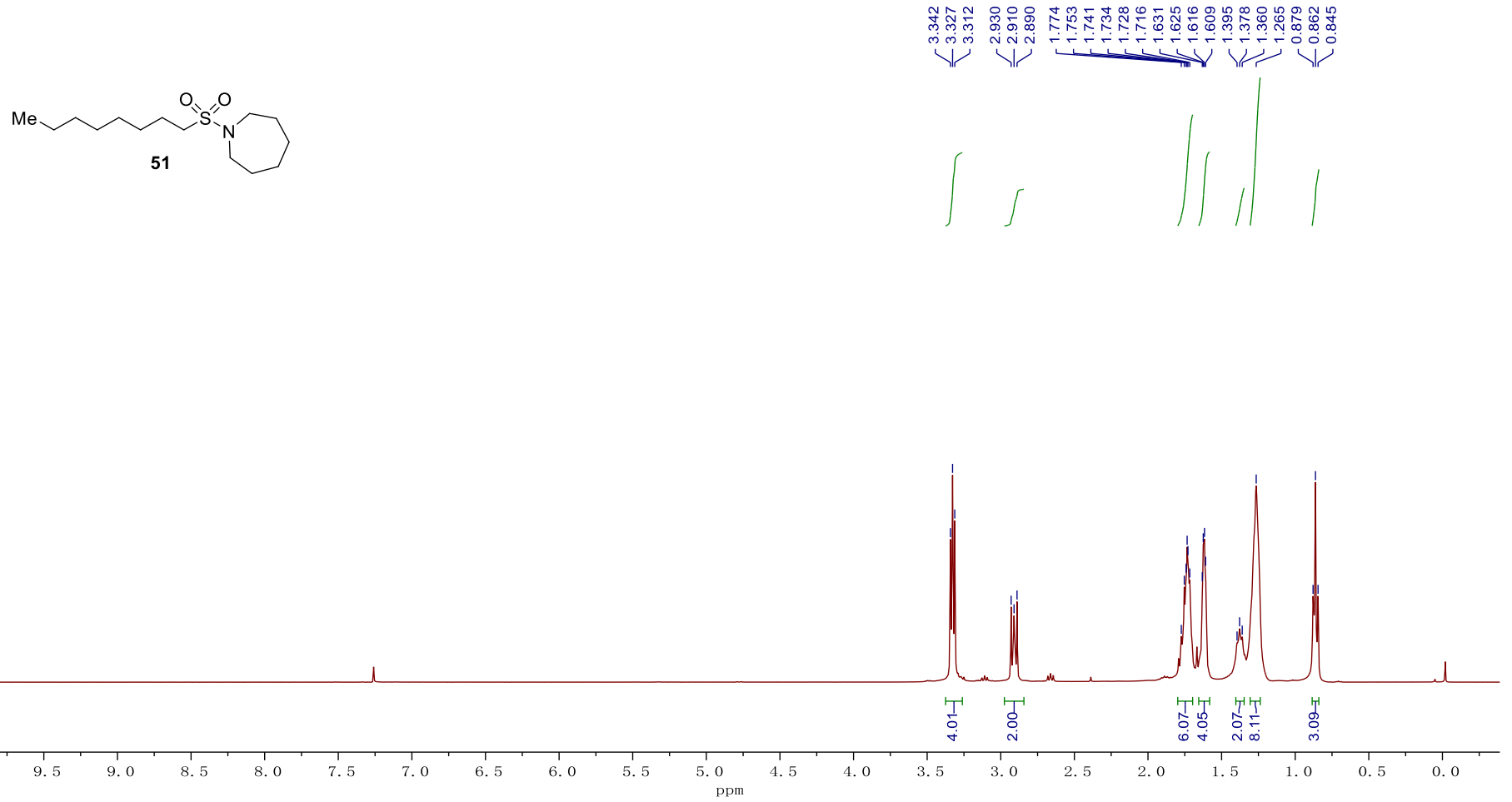
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1.631
1.625
1.616
1.609
1.395
1.378
1.360
1.265
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0.845
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2.00
6.07
4.05
2.07
8.11
3.09
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9.5
9.0
8.5
8.0
7.5
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6.5
6.0
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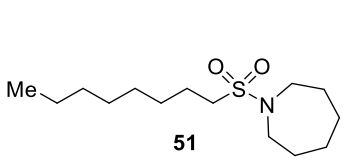
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N

51

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28.91
28.42
26.85
23.34
22.53
13.99
200
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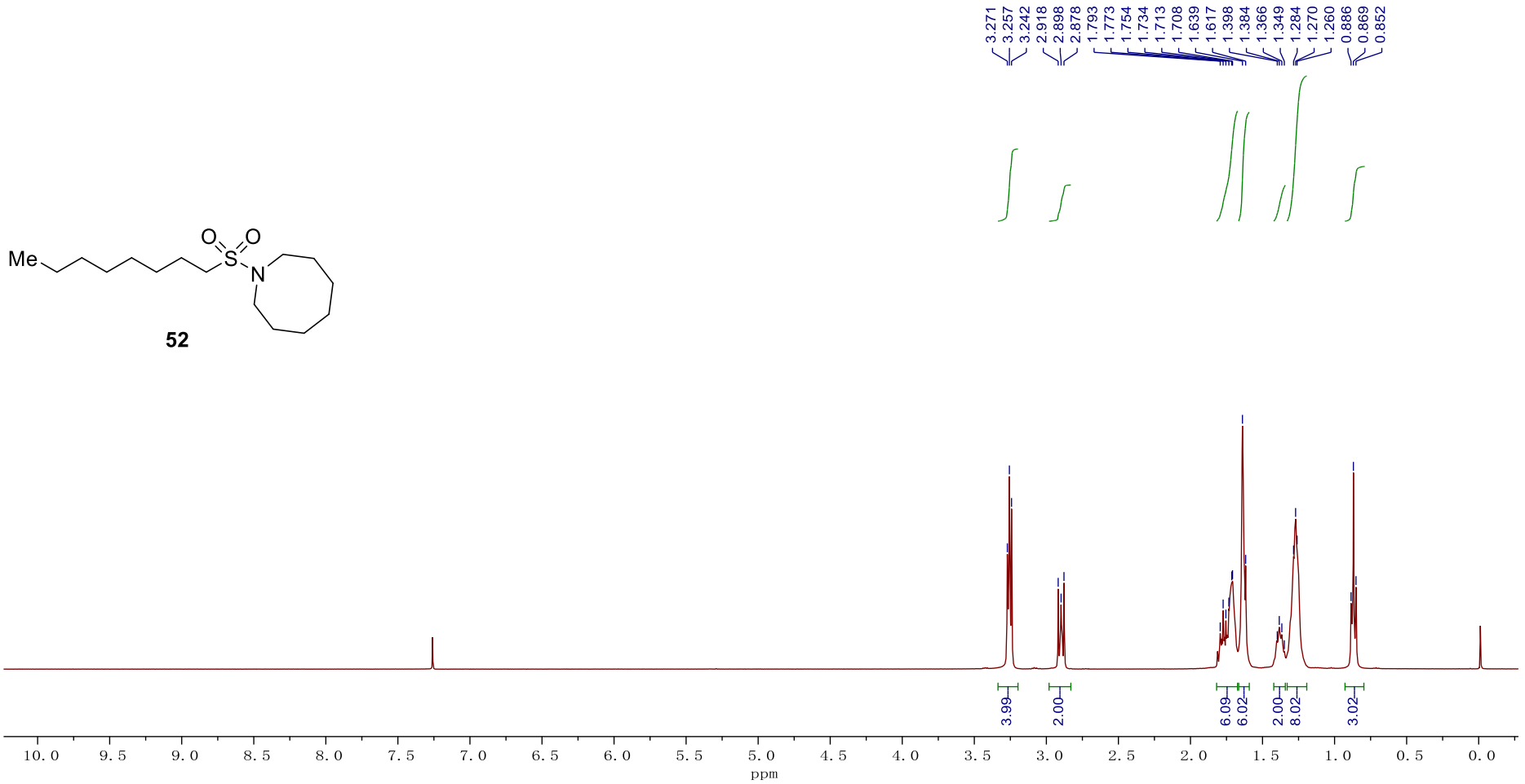
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1.349
1.284
1.270
1.260
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0.869
0.852
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O
S
N
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3.99
2.00
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6.02
2.00
8.02
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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3.0
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1.5
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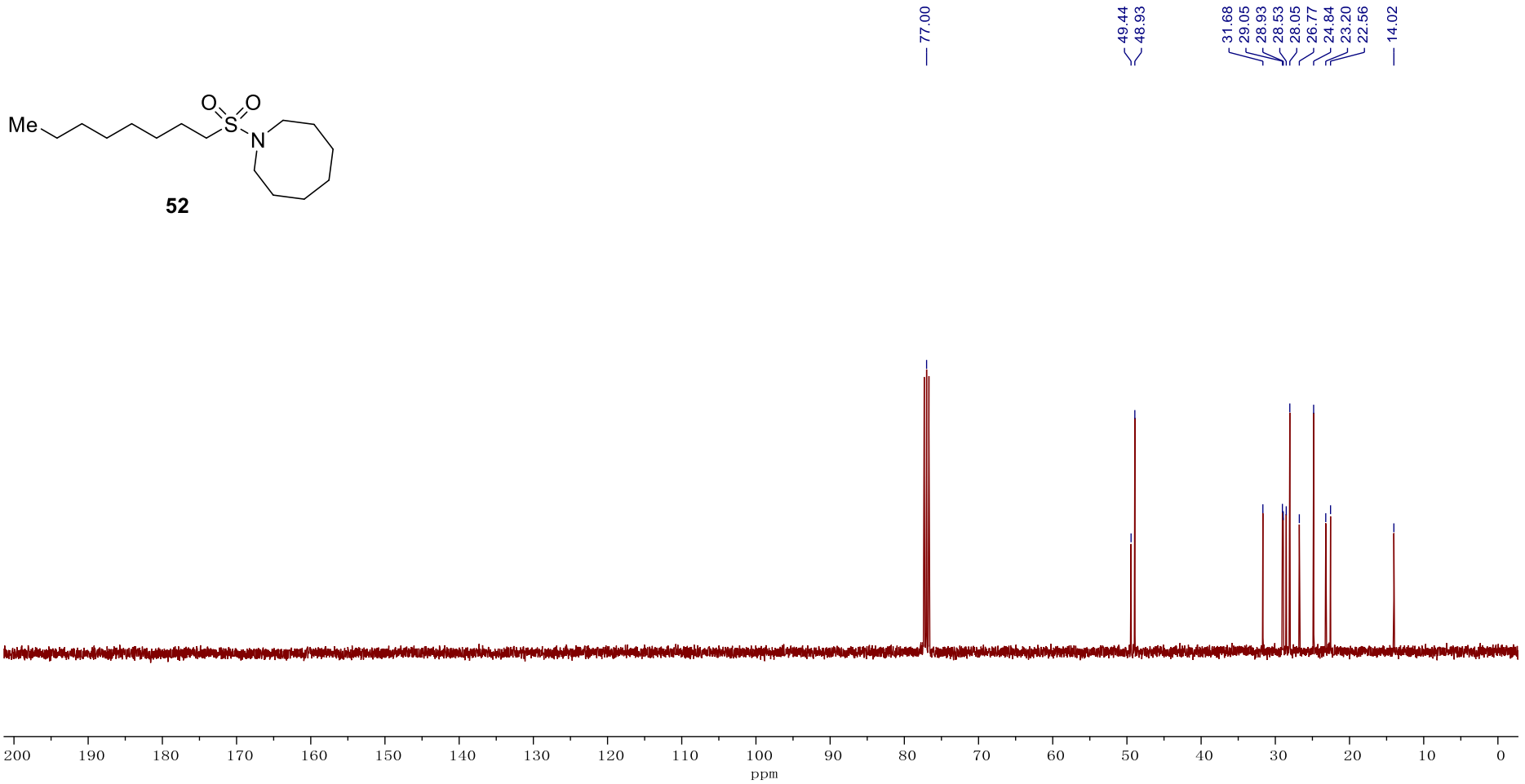
0.5
0.0
ppm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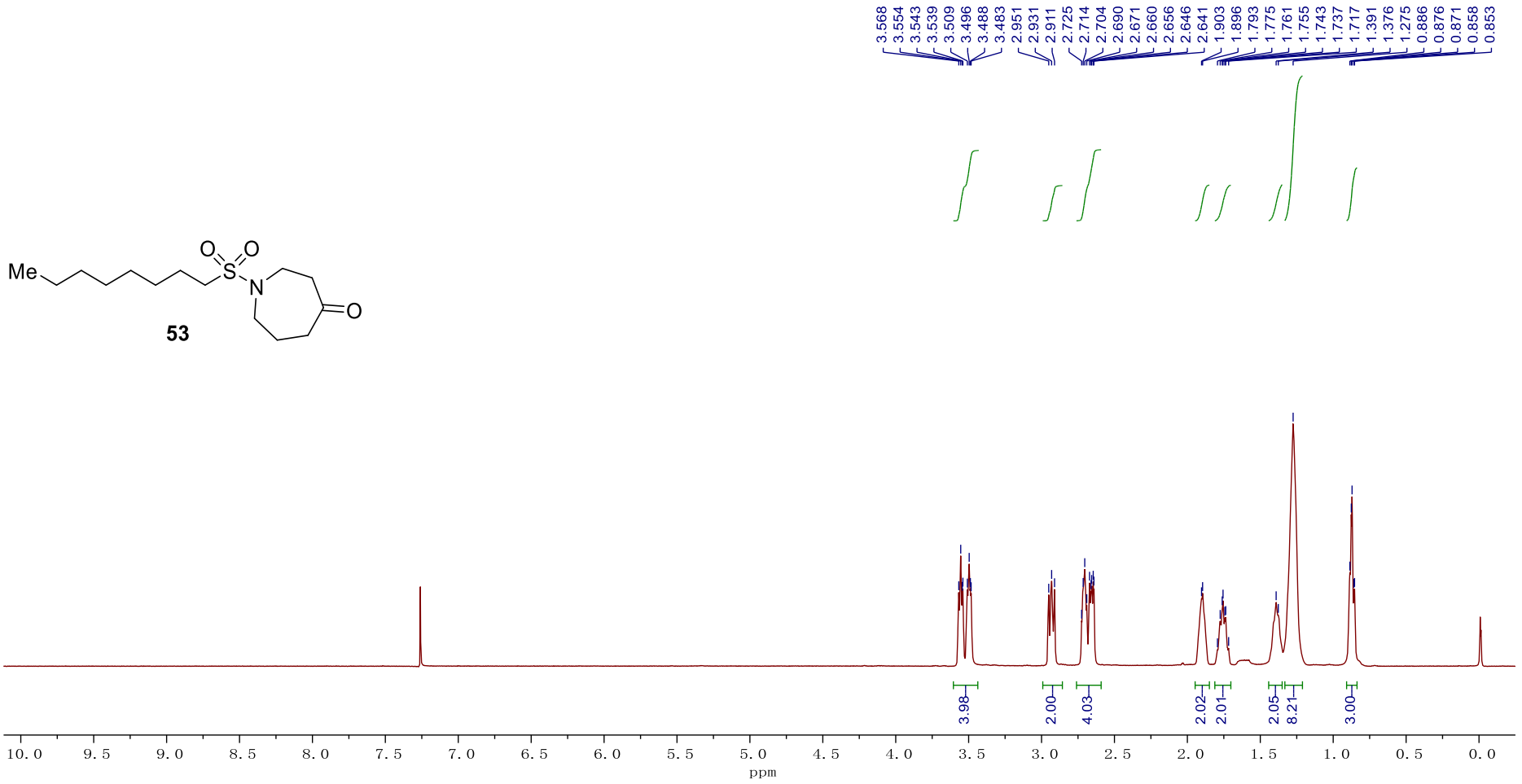
31.68
29.05
28.93
28.53
28.05
26.77
24.84
23.20
22.56
14.02
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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3.483
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2.911
2.725
2.714
2.704
2.690
2.671
2.660
2.656
2.646
2.641
1.903
1.896
1.793
1.775
1.761
1.755
1.743
1.737
1.717
1.391
1.376
1.275
0.886
0.876
0.871
0.858
0.853
Me
O
O
S
N
O
53
3.98
2.00
4.03
2.02
2.01
2.05
8.21
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
3.5
3.0
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1.5
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0.5
0.0
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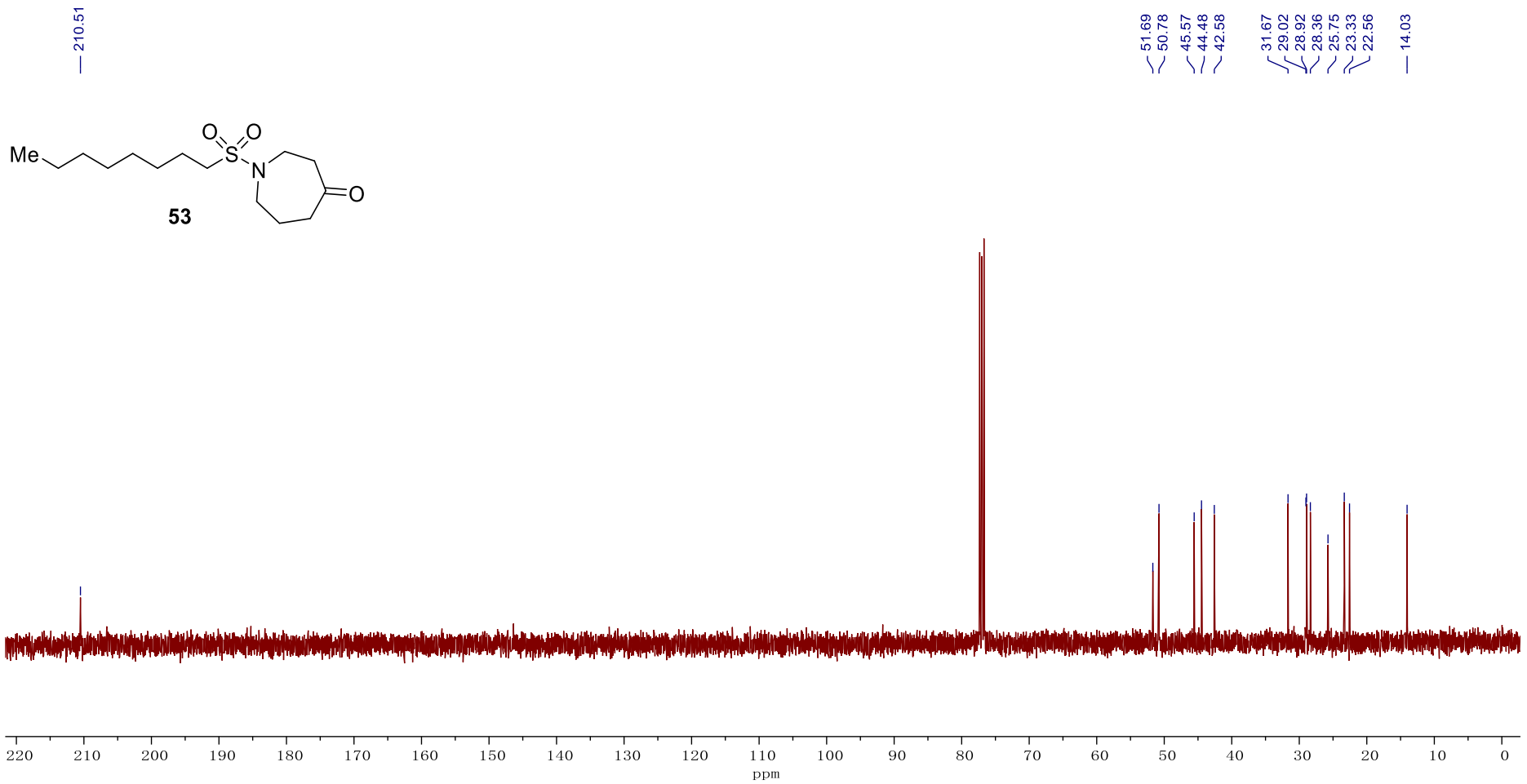
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42.58
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29.02
28.92
28.36
25.75
23.33
22.56
14.03
Me
O
O
S
N
O
53
220
210
200
190
180
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150
140
130
120
110
100
90
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60
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20
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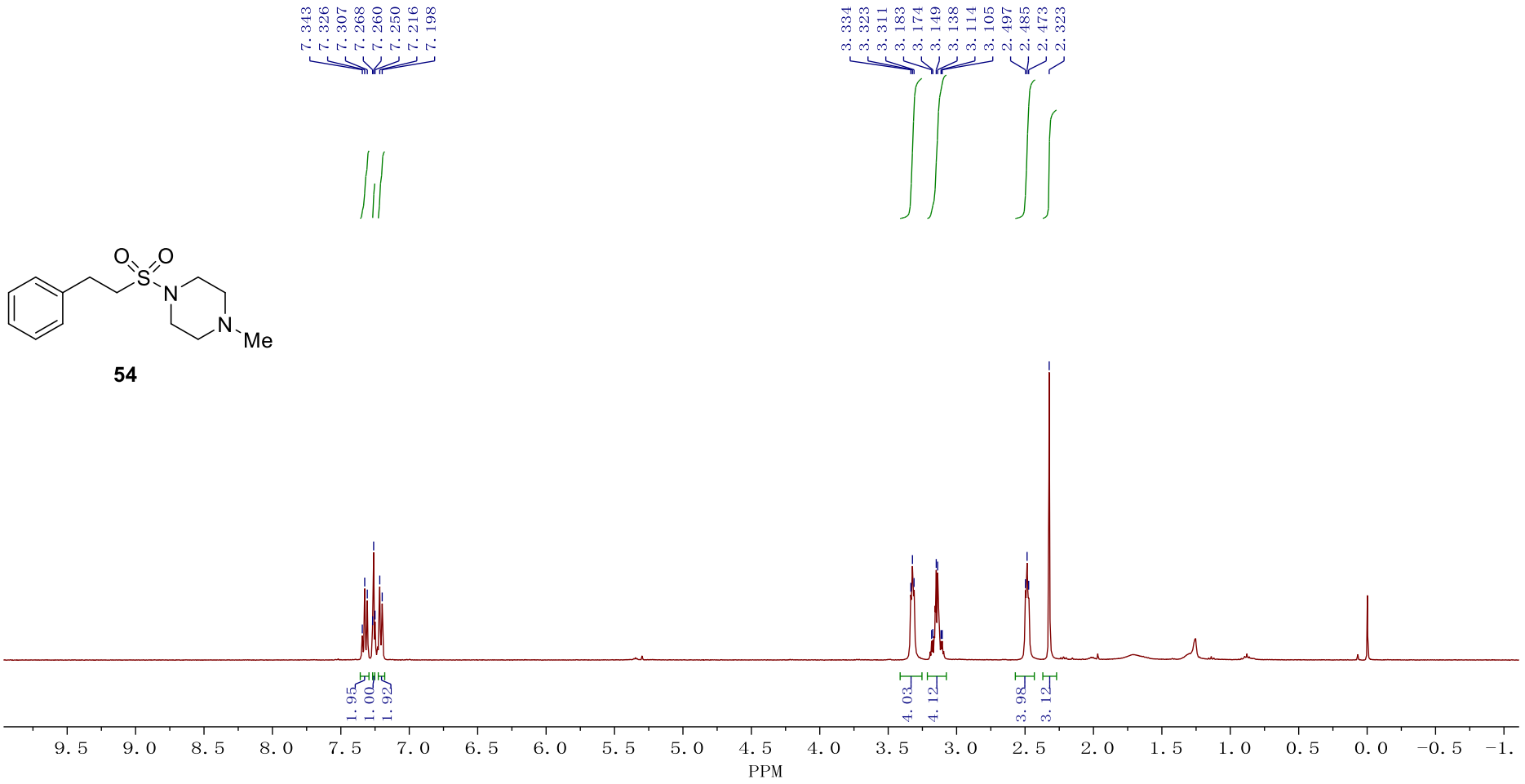
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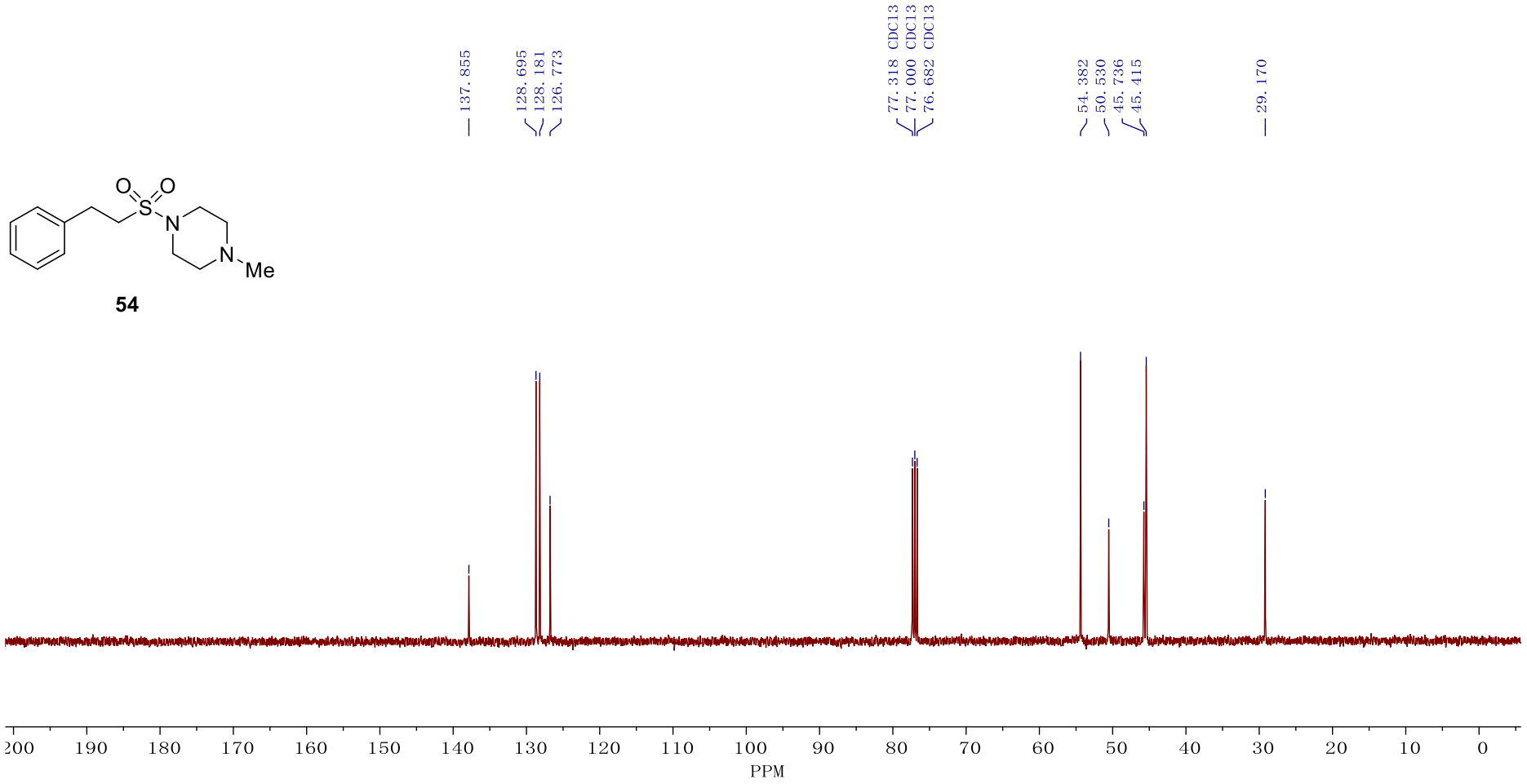
3.183
3.174
3.149
3.138
3.114
3.105
2.497
2.485
2.473
2.323
O
O
S
N
N
Me
54
1.95
1.00
1.92
4.03
4.12
3.98
3.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
PPM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77.000 CDC13
76.682 CDC13
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45.736
45.415
29.170
O
O
S
N
N
Me
54
200
190
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100
90
80
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50
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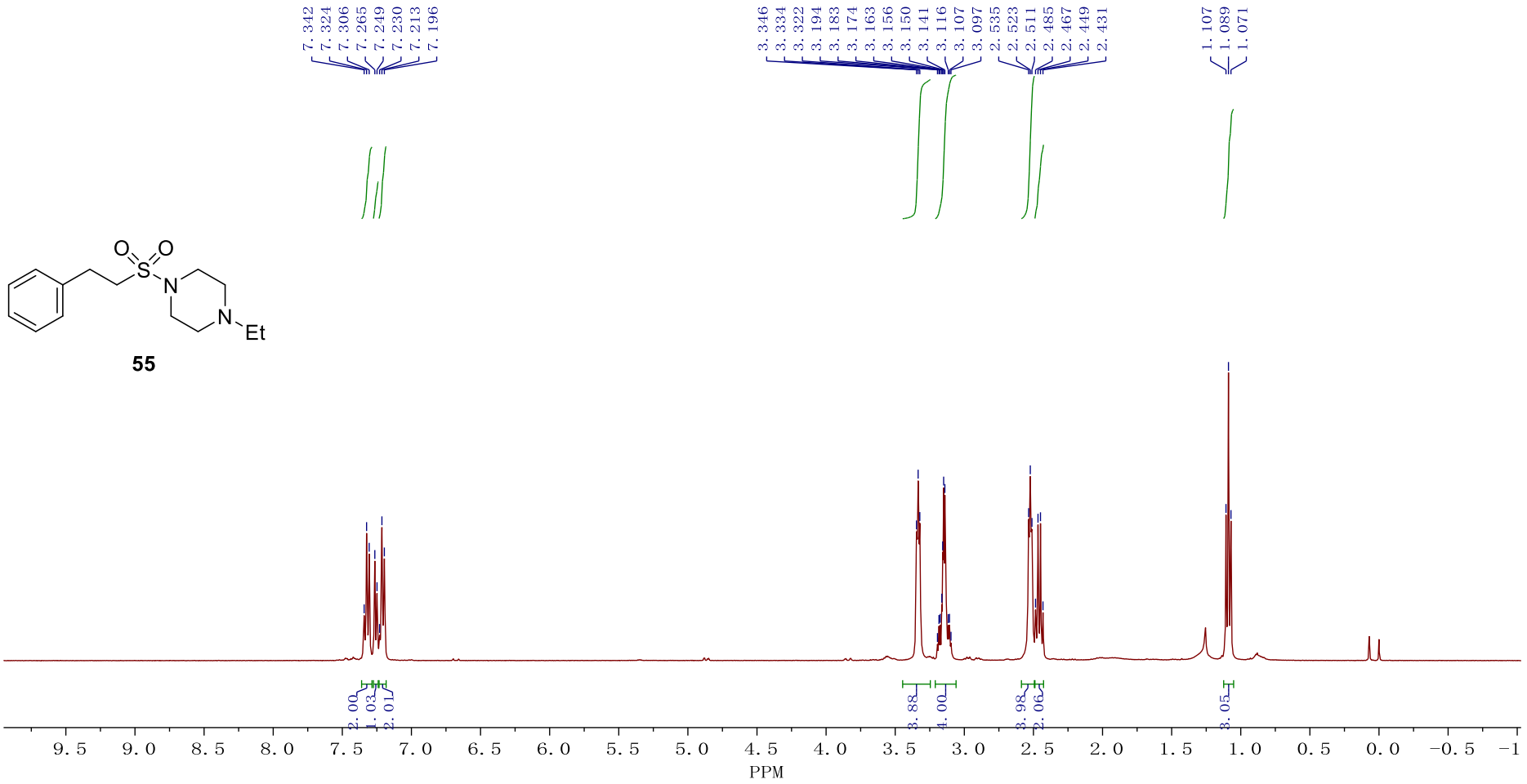
PPM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7.196
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3.334
3.322
3.194
3.183
3.174
3.163
3.156
3.150
3.141
3.116
3.107
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2.535
2.523
2.511
2.485
2.467
2.449
2.431
1.107
1.089
1.071
O
O
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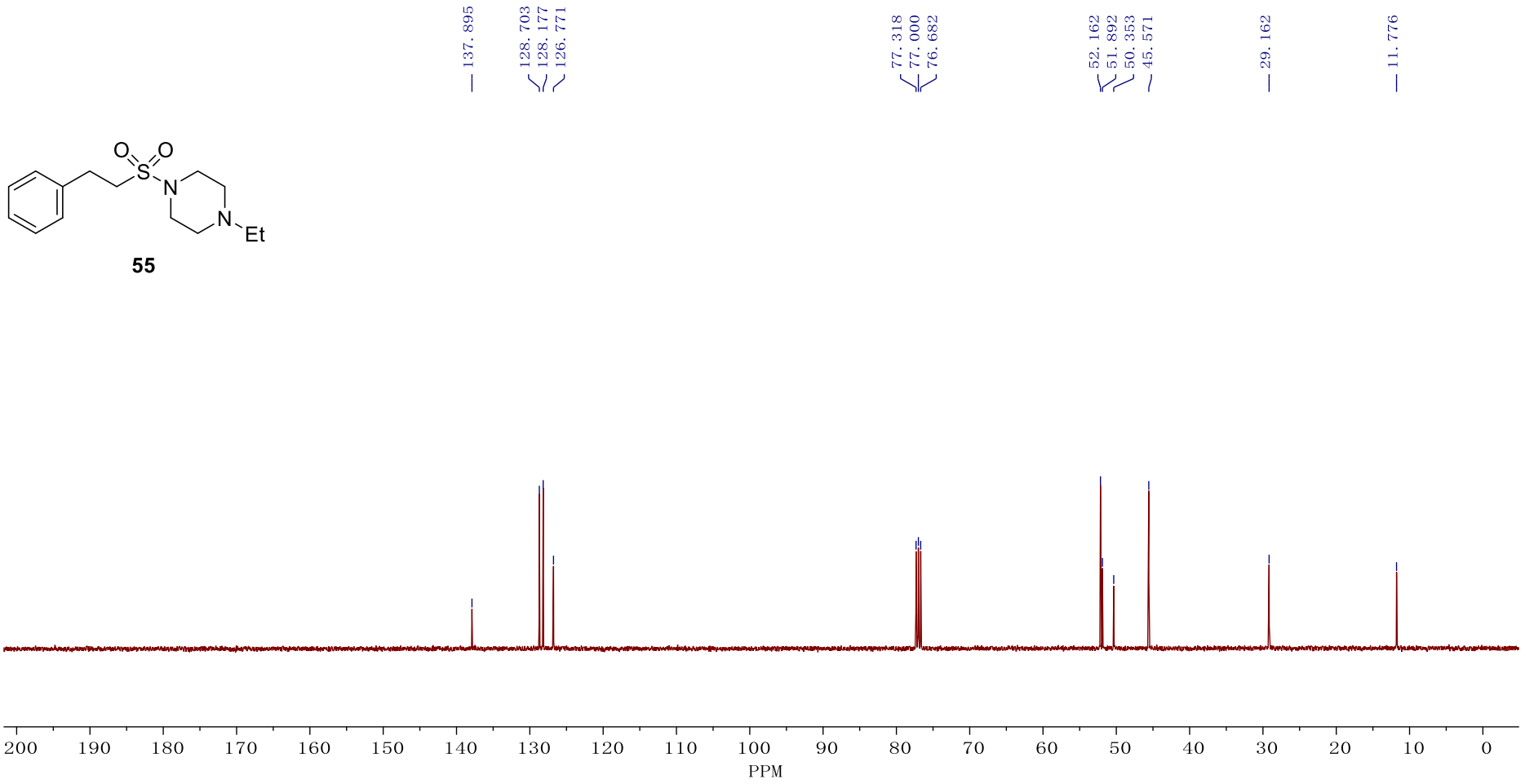
N
N
Et
55
2.00
1.03
2.01
3.88
4.00
3.98
2.06
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
PPM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50.353
45.571
29.162
11.776
O
O
S
N
N
Et
55
200
190
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140
130
120
110
100
90
80
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60
50
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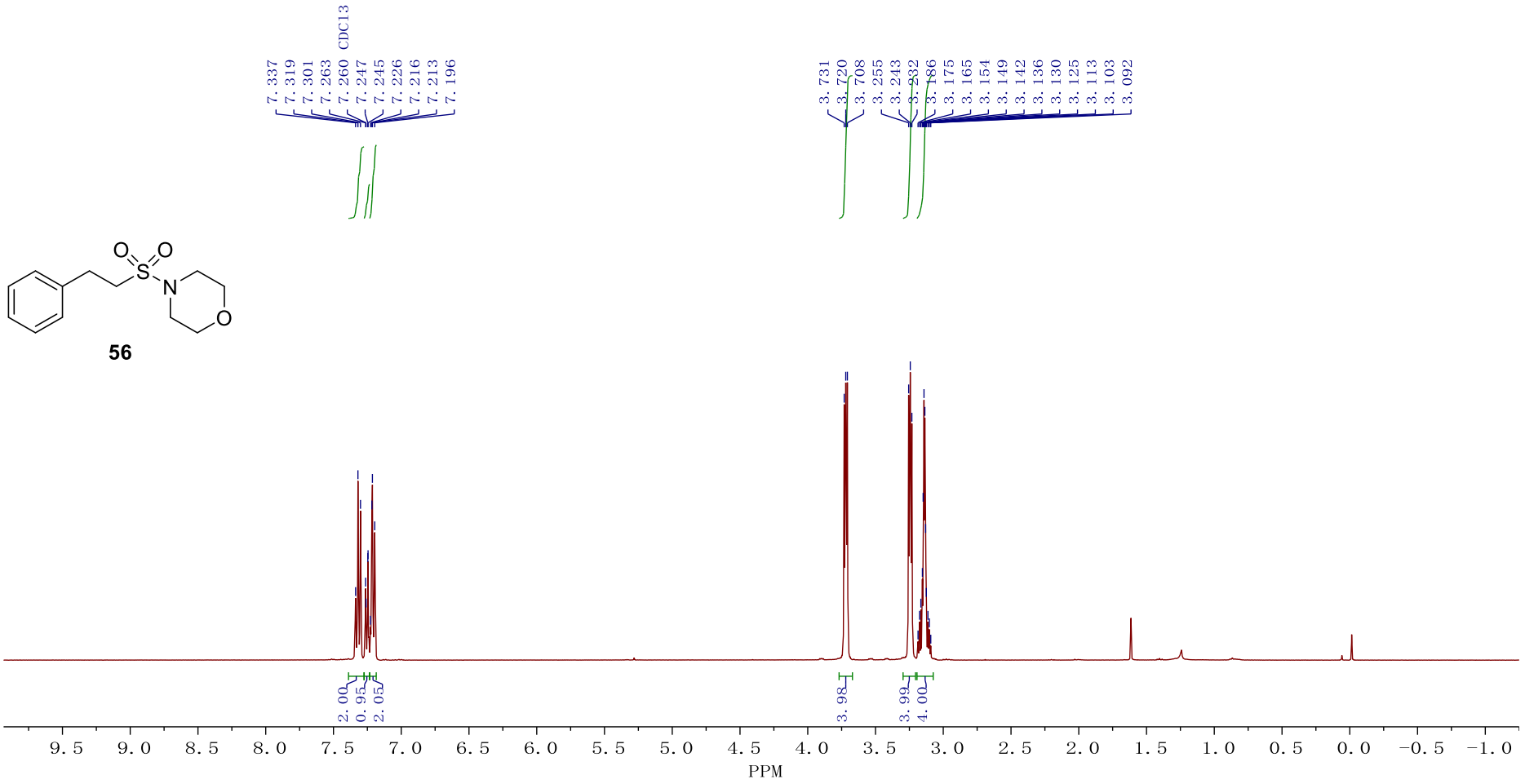
10
0
PPM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7.213
7.196
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3.720
3.708
3.255
3.243
3.232
3.186
3.175
3.165
3.154
3.149
3.142
3.136
3.130
3.125
3.113
3.103
3.092
O
O
S
N
O
56
2.00
0.95
2.05
3.98
3.99
4.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 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
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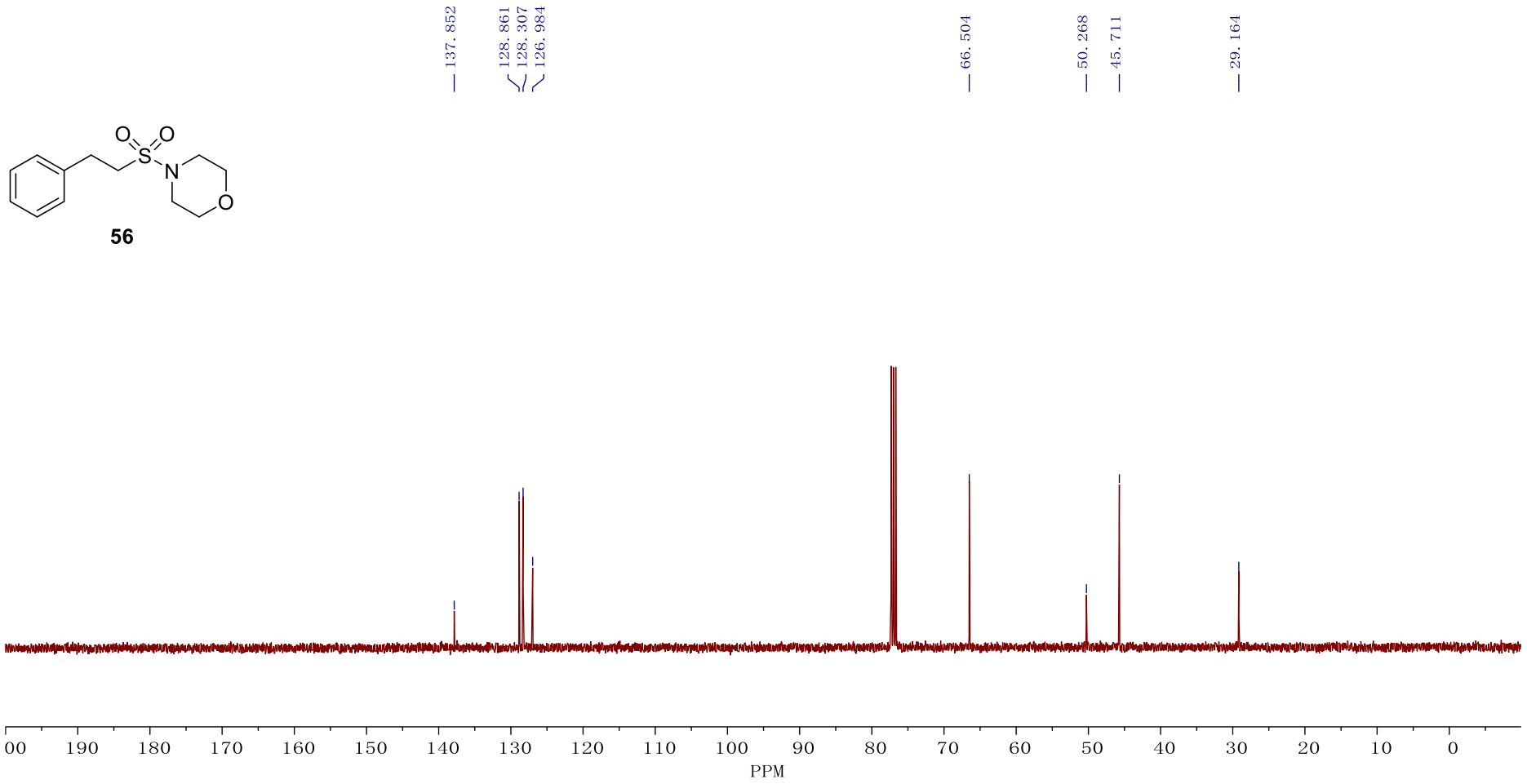
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O
S
N
O
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00
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120
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100
90
80
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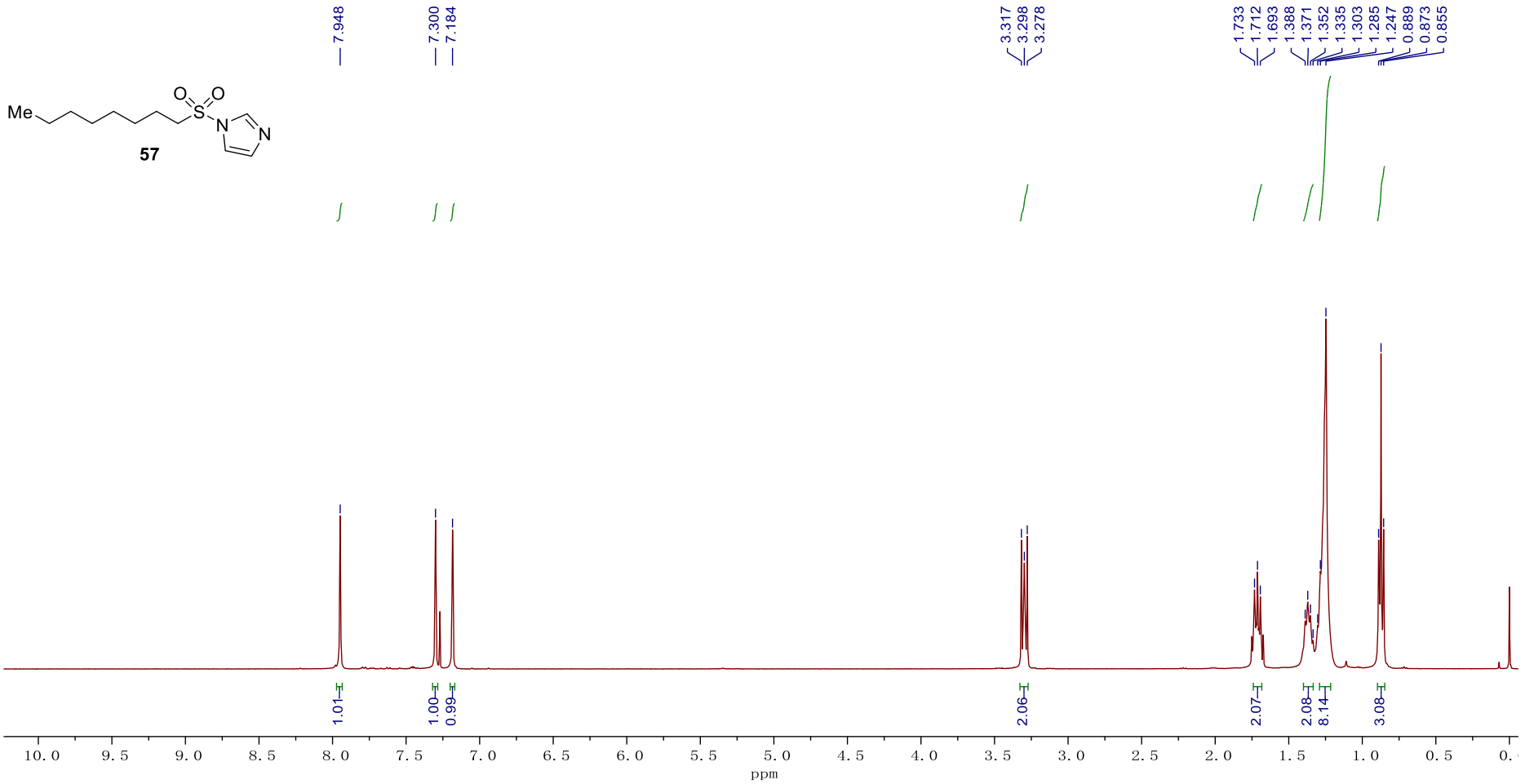
PPM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1.335
1.303
1.285
1.247
0.889
0.873
0.855
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O
S
N
N
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1.01
1.00
0.99
2.06
2.07
2.08
8.14
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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4.0
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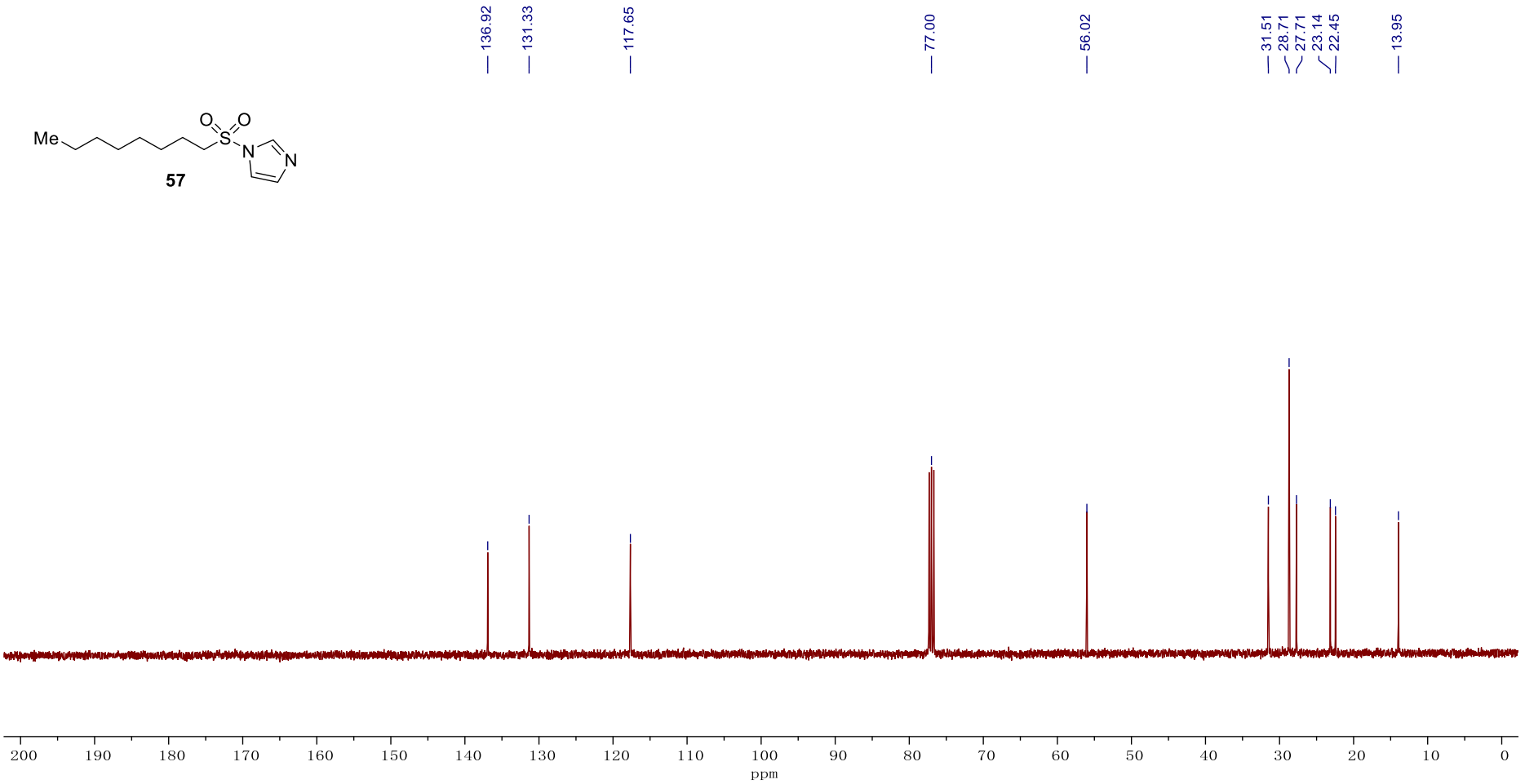
2.0
1.5
1.0
0.5
ppm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22.45
13.95
Me
O
O
S
N
N
57
200
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120
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100
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60
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20
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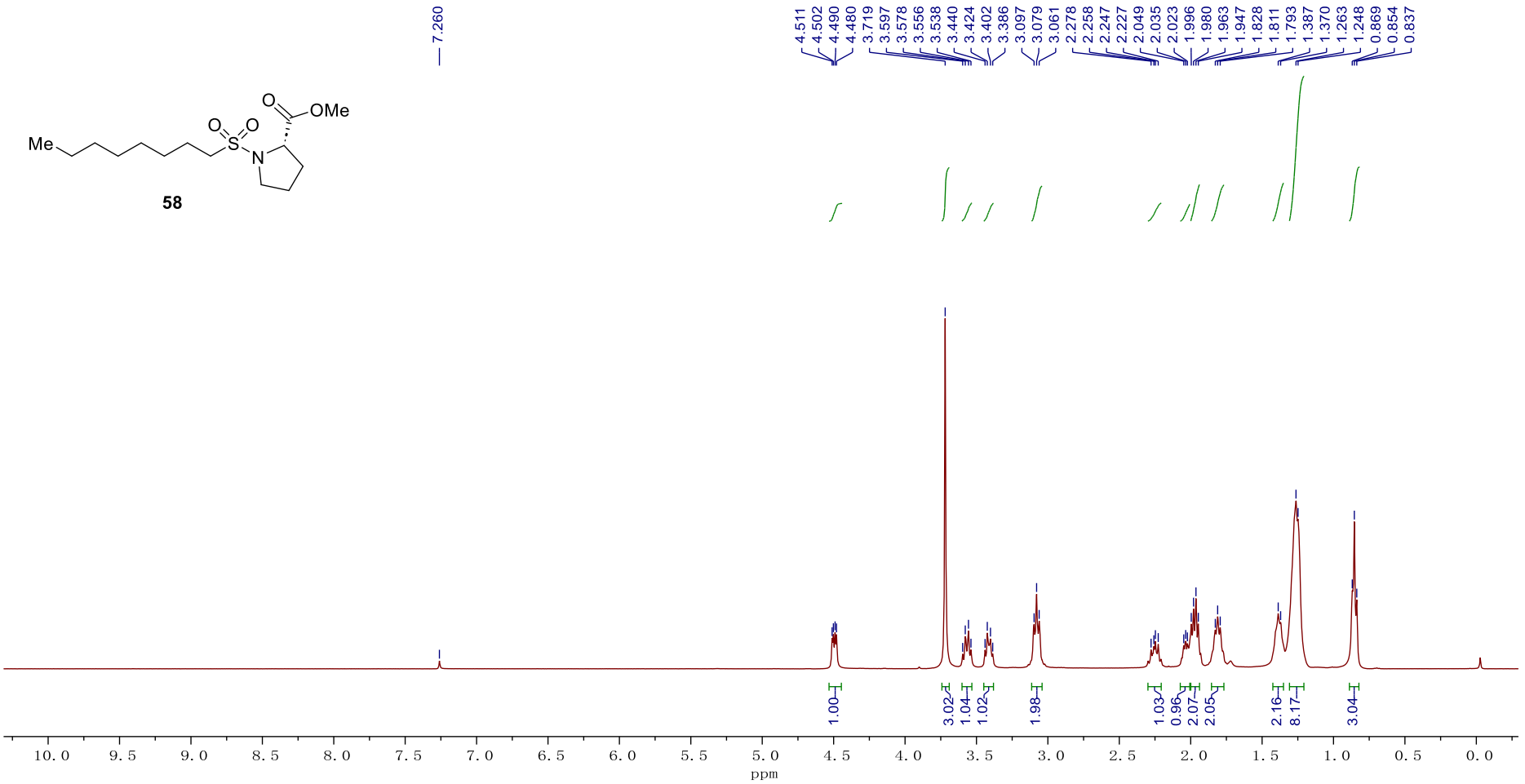
ppm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O
OMe
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4.480
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3.597
3.578
3.556
3.538
3.440
3.424
3.402
3.386
3.097
3.079
3.061
2.278
2.258
2.247
2.227
2.049
2.035
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1.98
1.03
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8.17
3.04
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6.0
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1.5
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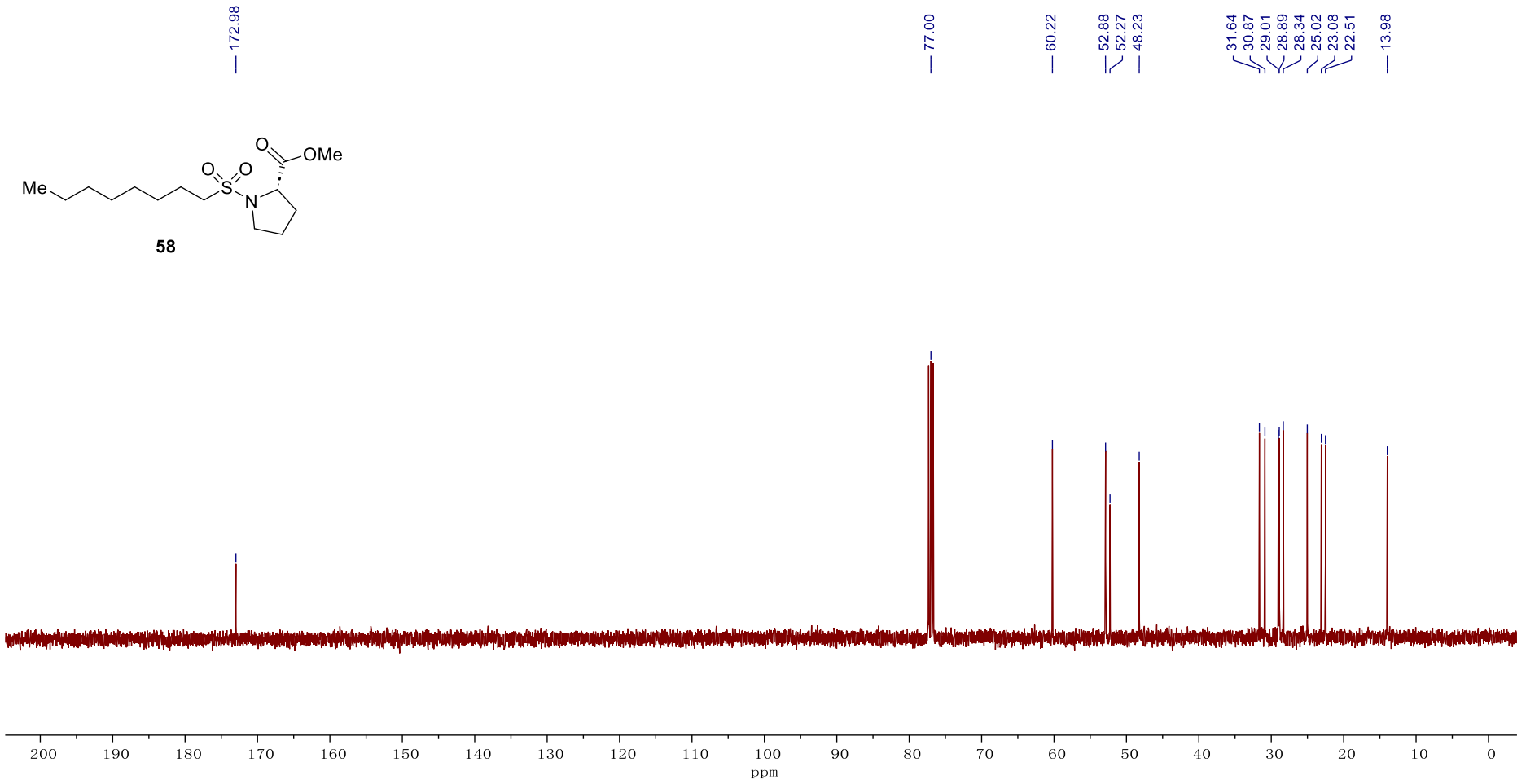
0.5
0.0
ppm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22.51
13.98
Me
O
OMe
O
O
S
N
58
200
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130
120
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100
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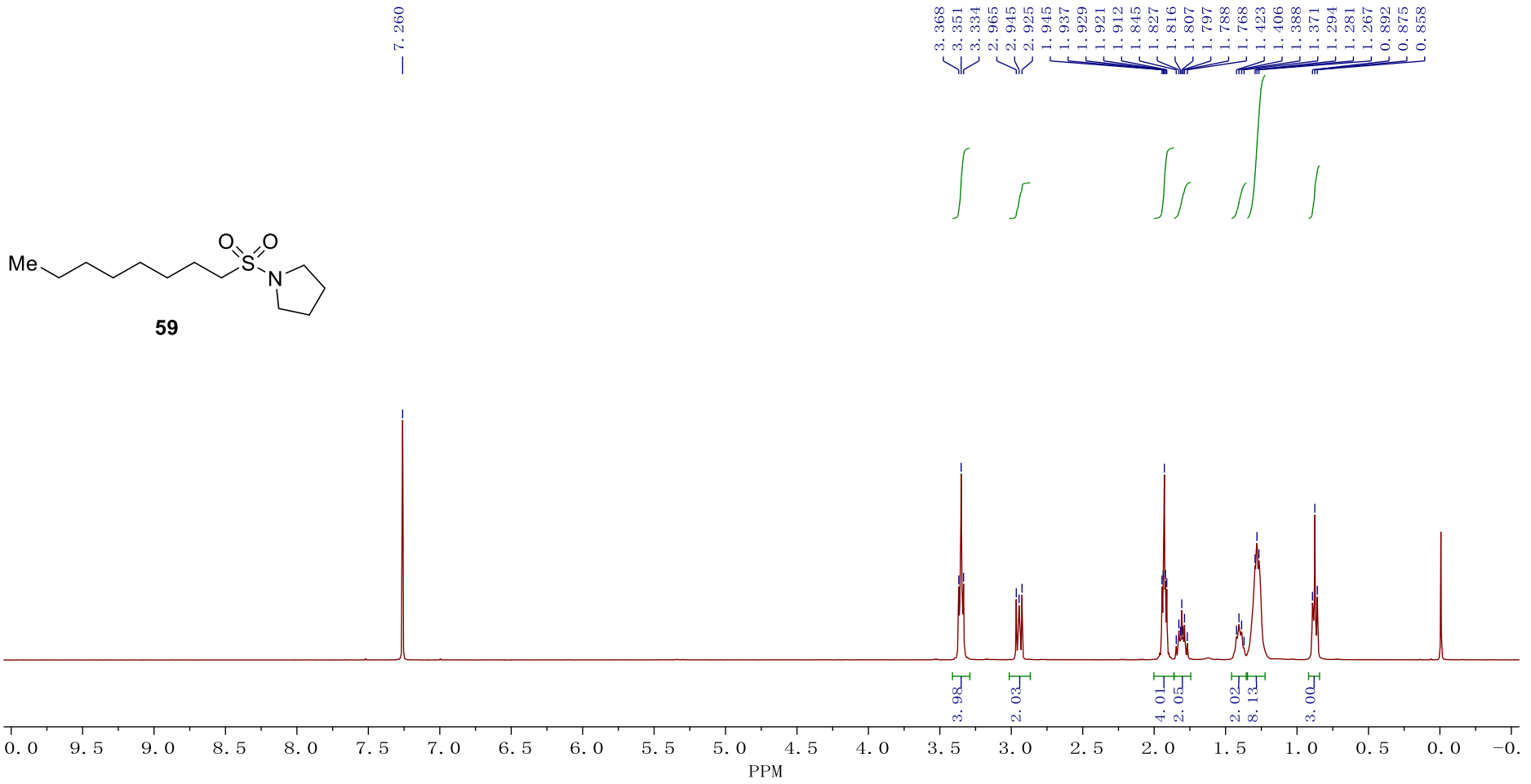
ppm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1.937
1.929
1.921
1.912
1.845
1.827
1.816
1.807
1.797
1.788
1.768
1.423
1.406
1.388
1.371
1.294
1.281
1.267
0.892
0.875
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N
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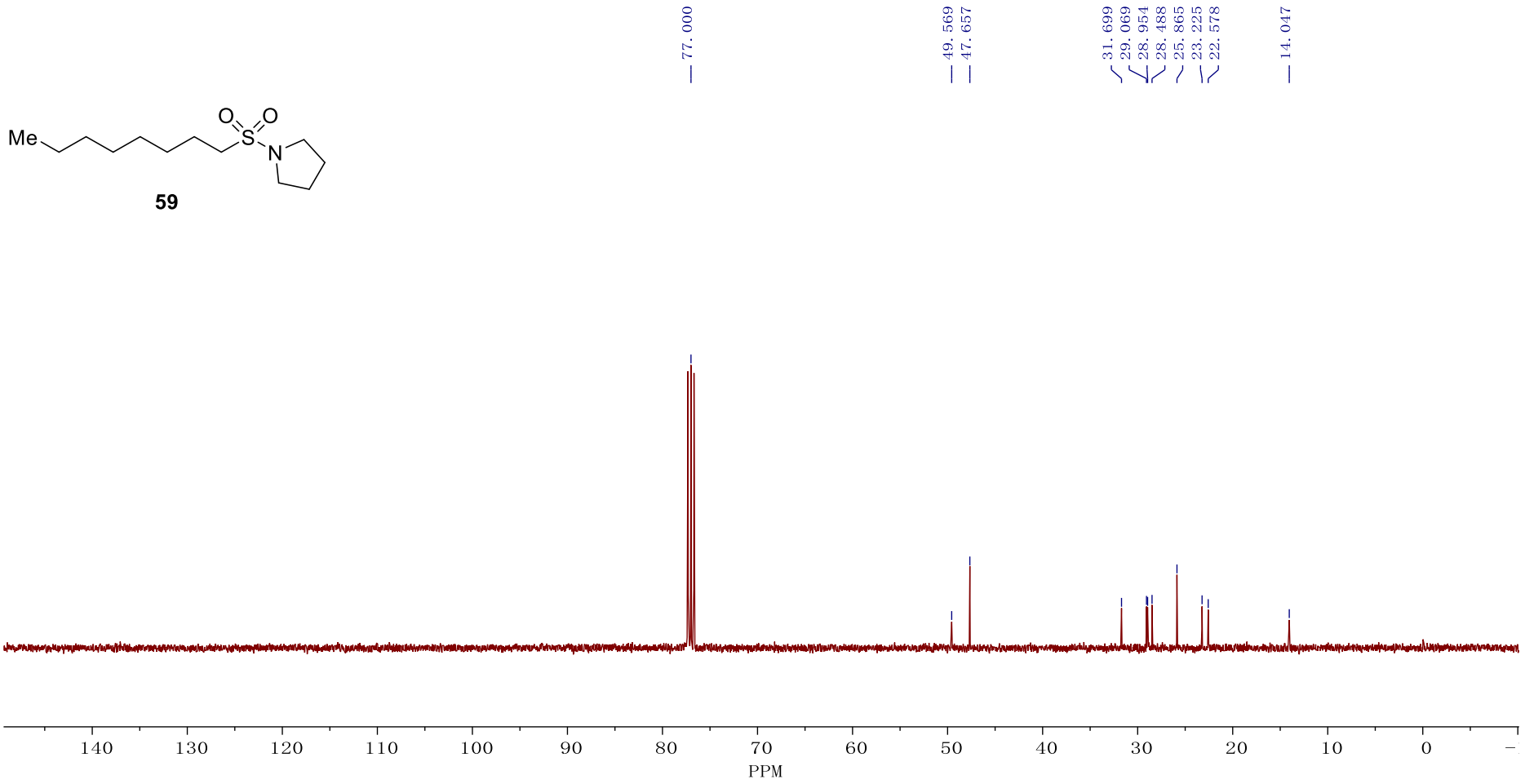
4.01
2.05
2.02
8.13
3.00
PPM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22.578
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Me
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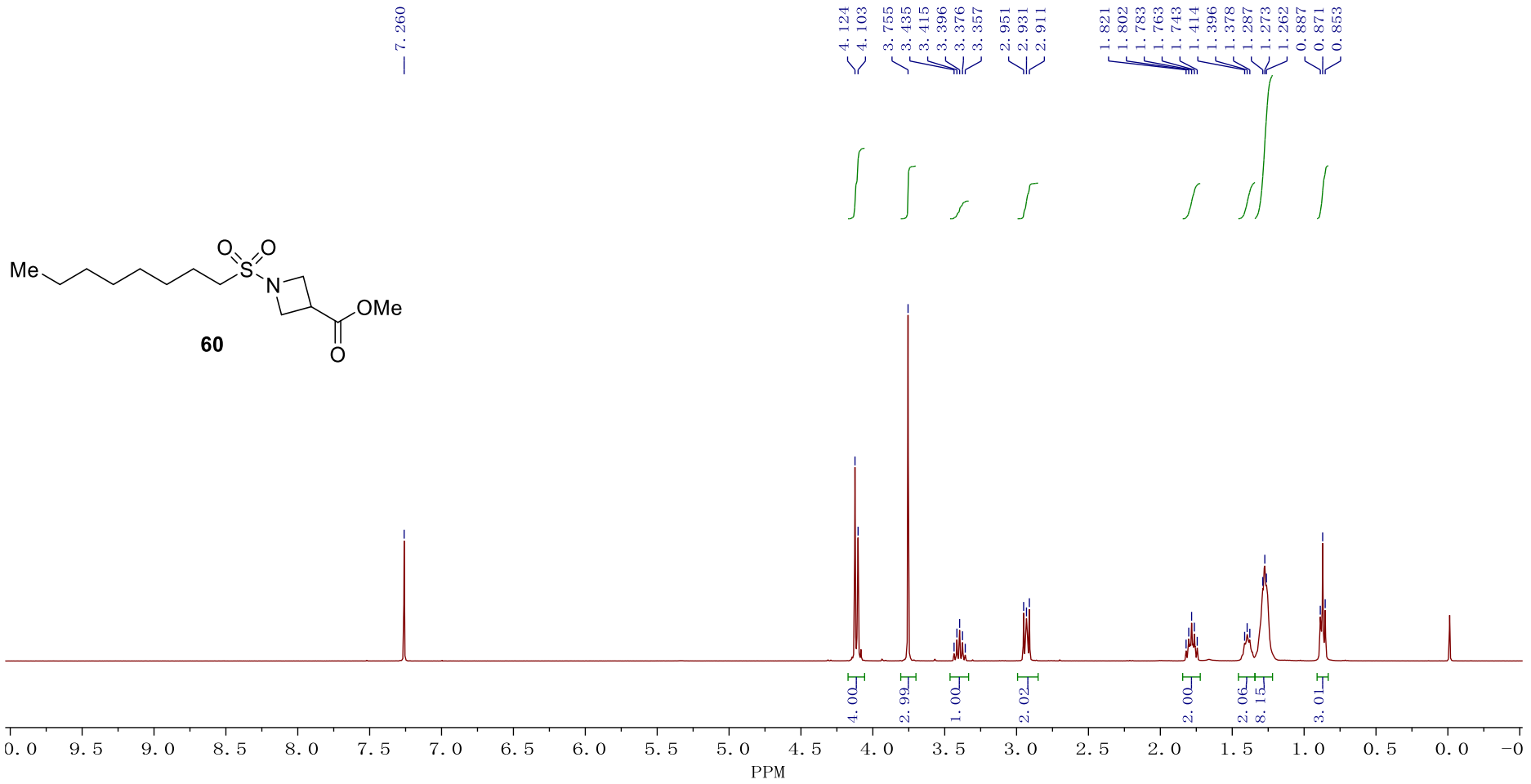
PPM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3.376
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2.951
2.931
2.911
1.821
1.802
1.783
1.763
1.743
1.414
1.396
1.378
1.287
1.273
1.262
0.887
0.871
0.853
Me
O
O
S
N
OMe
O
60
4.00
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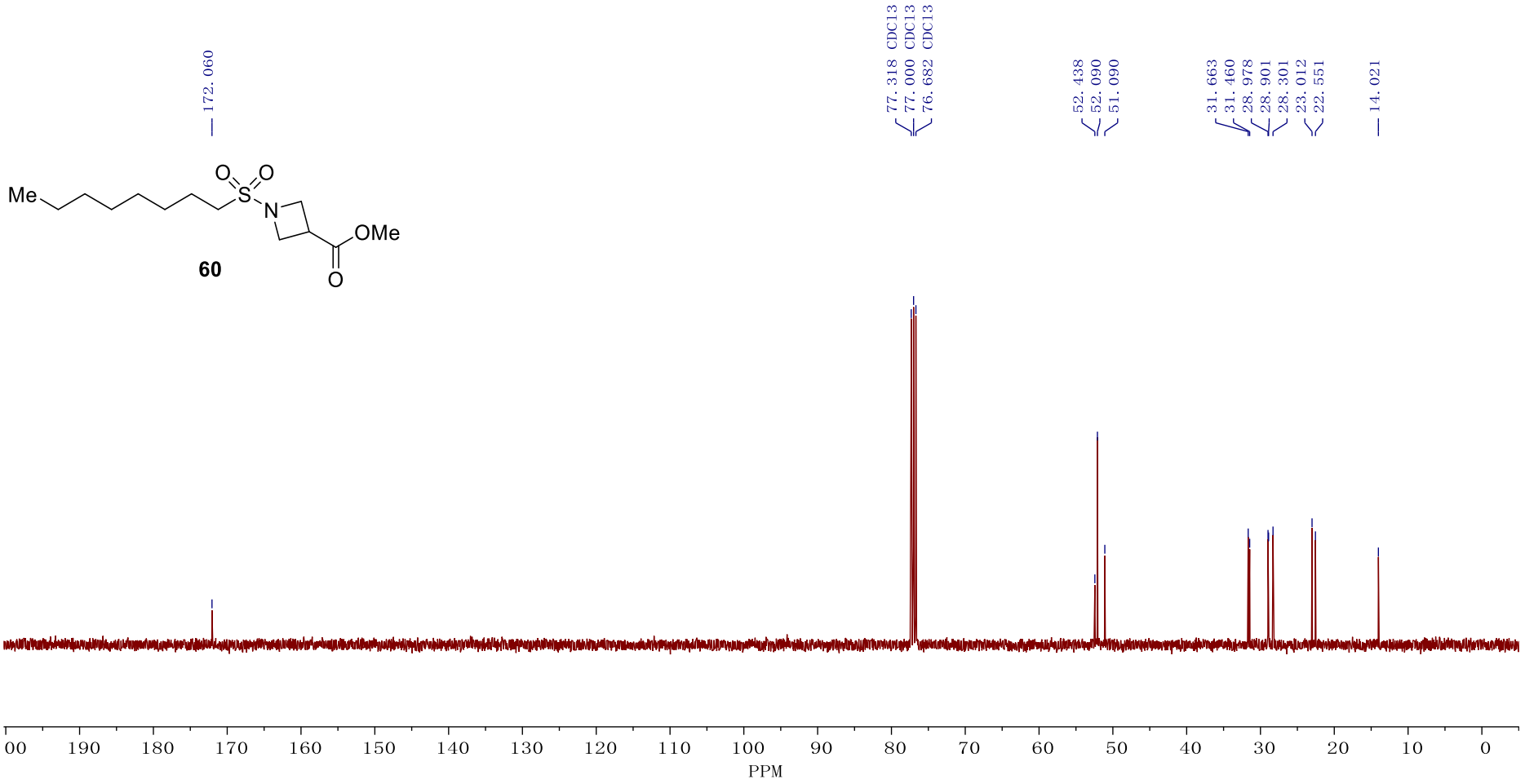
1.00
2.02
2.00
2.06
8.15
3.01
PPM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76.682 CDCl3
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51.090
31.663
31.460
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28.901
28.301
23.012
22.551
14.021
Me
O
O
S
N
OMe
O
60
00
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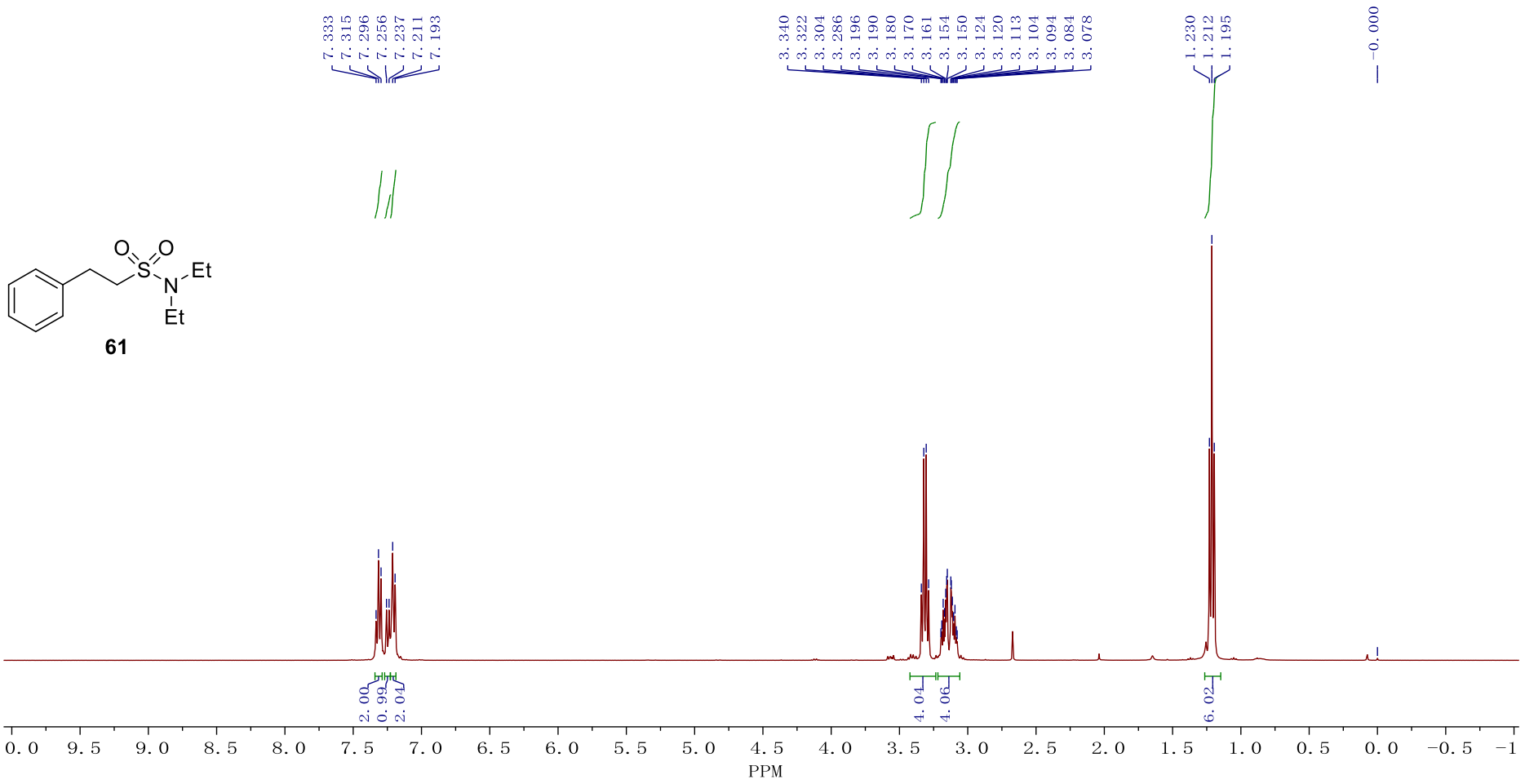
0
PPM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7.237
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3.154
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3.120
3.113
3.104
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3.078
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1.212
1.195
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O
O
S
N
Et
Et
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4.04
4.06
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8.5
8.0
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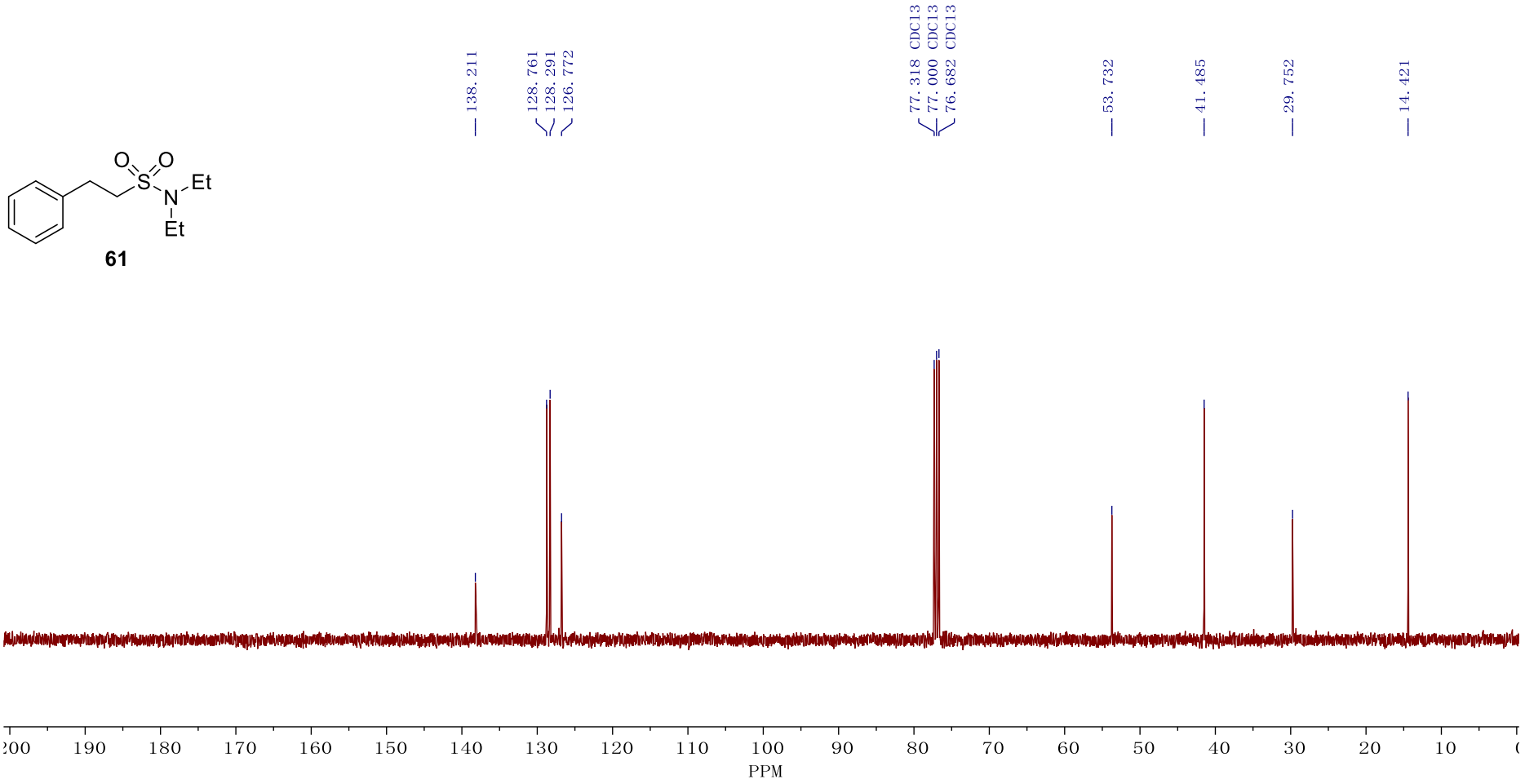
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N
Et
Et
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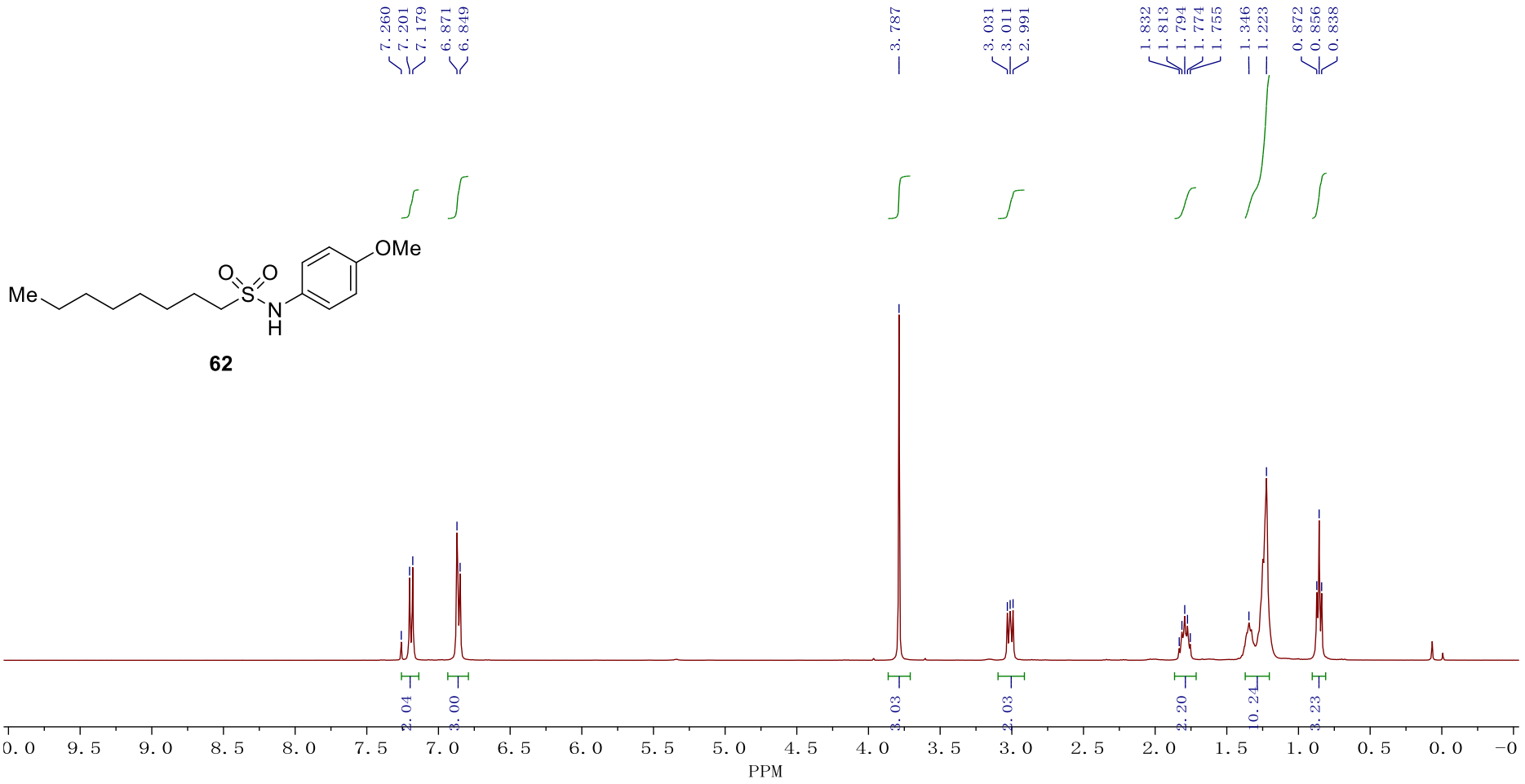
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OMe
Me
O
O
S
N
H
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6.0
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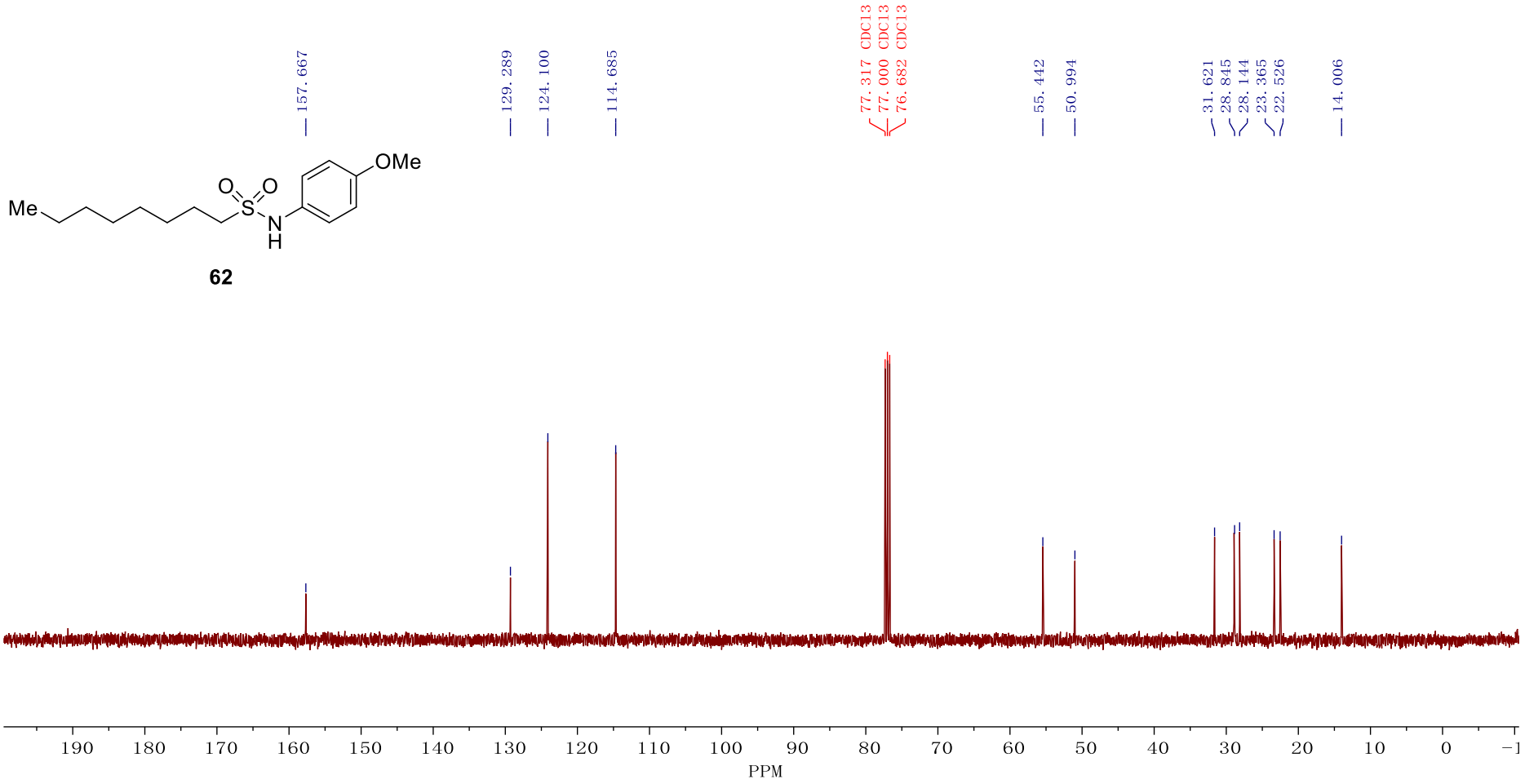
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OMe
Me
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N
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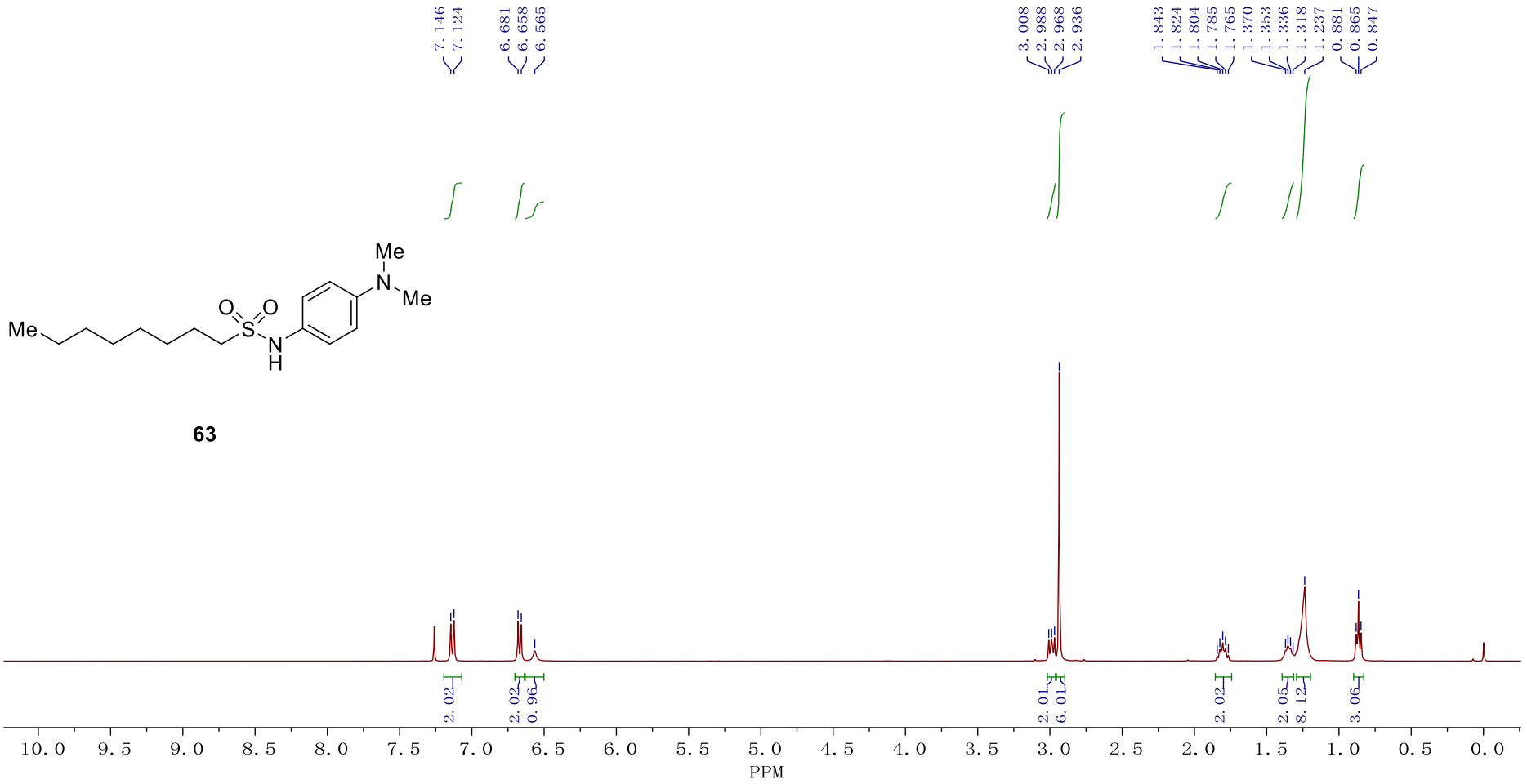
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N
Me
O
S
O
Me
N
H
63
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7.0
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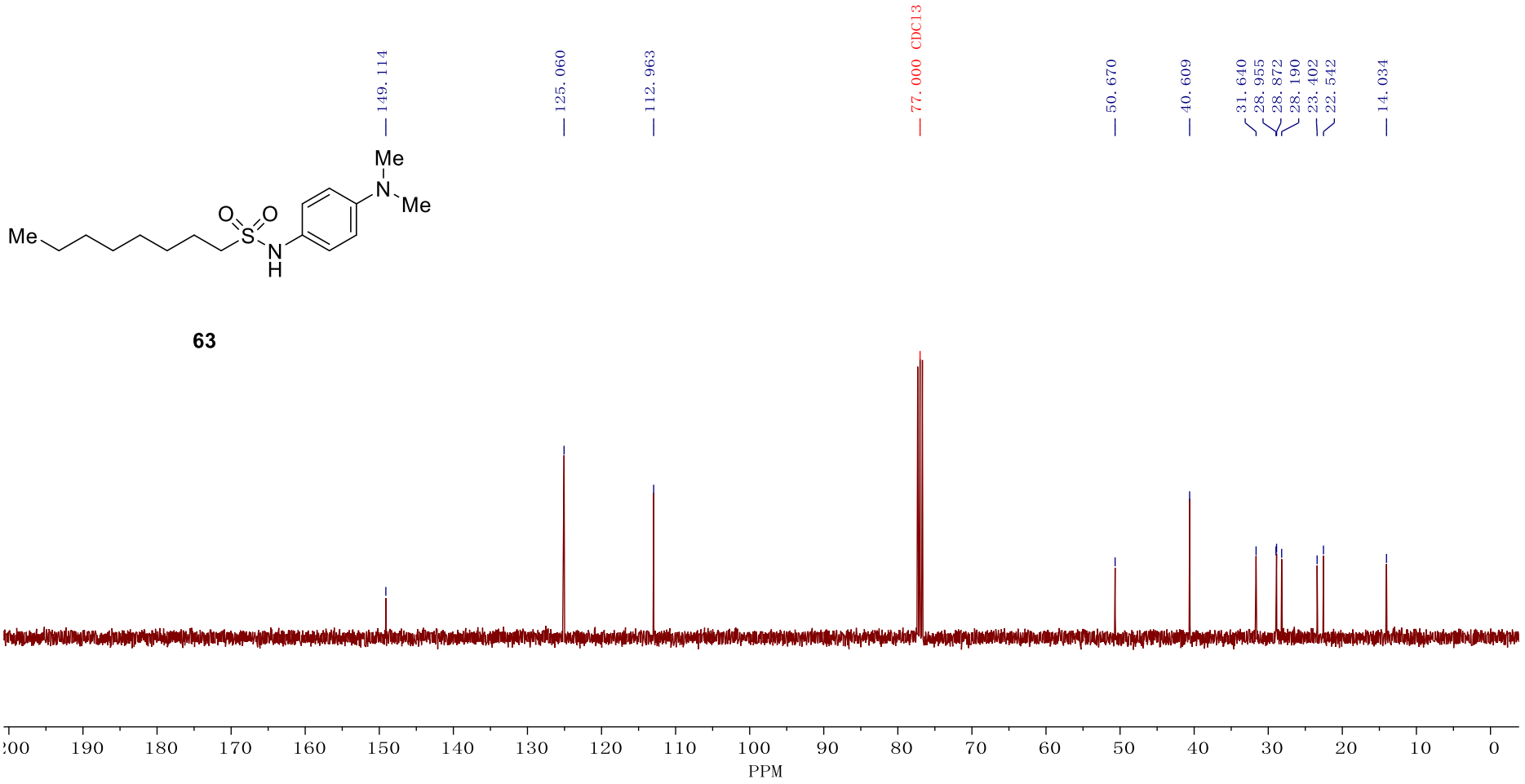
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N
Me
Me
O
O
S
N
H
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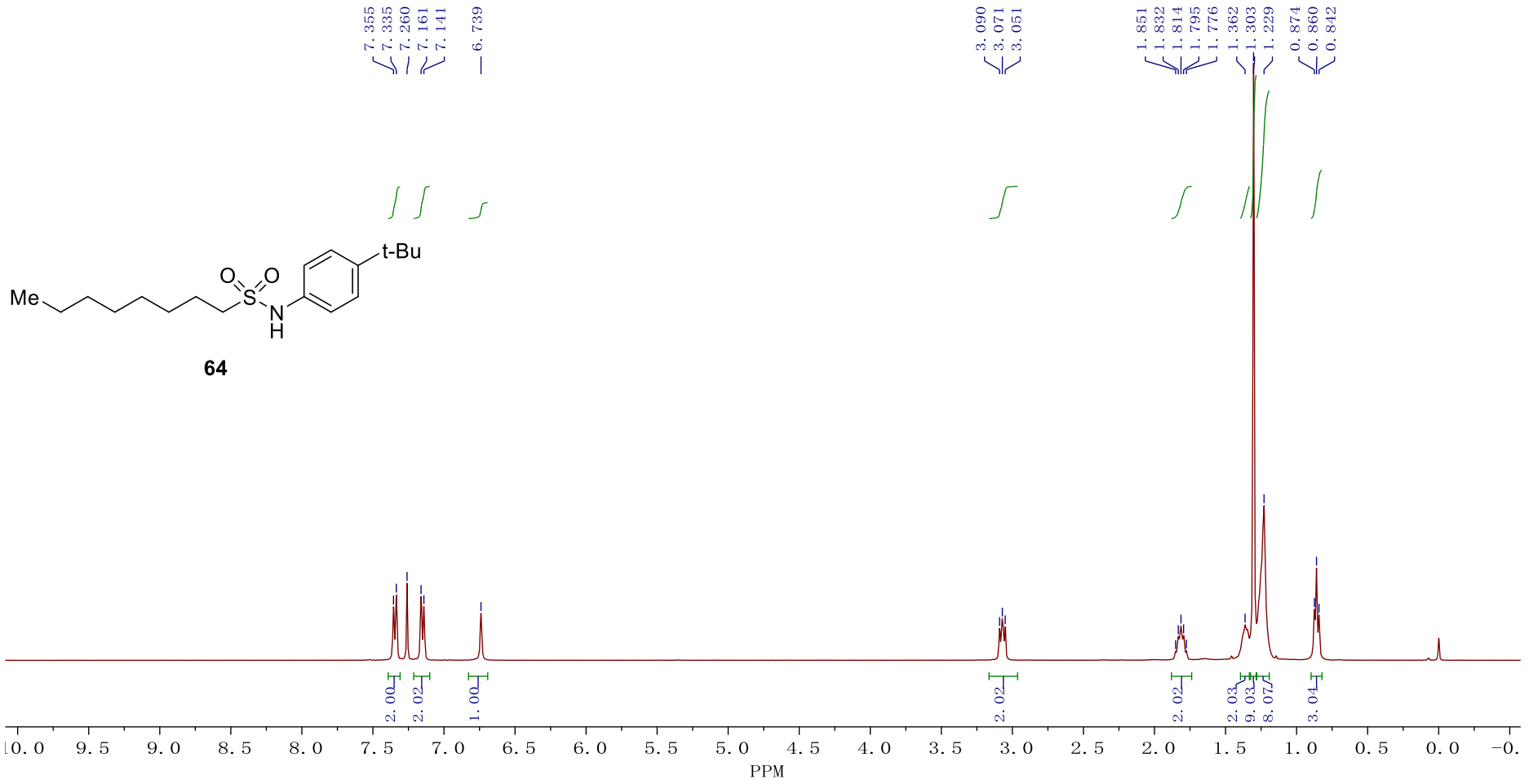
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1.229
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0.860
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O
O
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2.03
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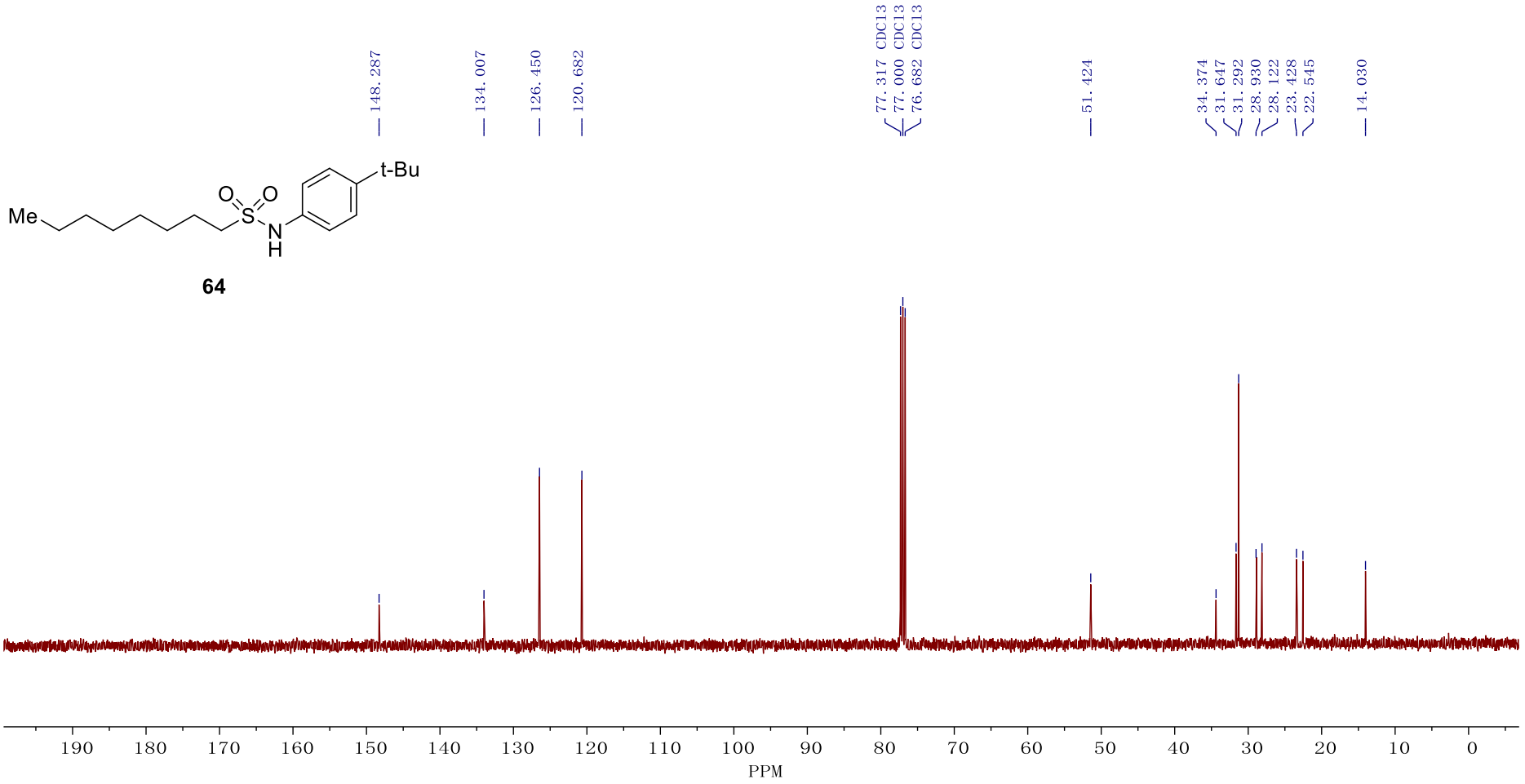
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28.930
28.122
23.428
22.545
14.030
t-Bu
O
O
S
N
H
Me
64
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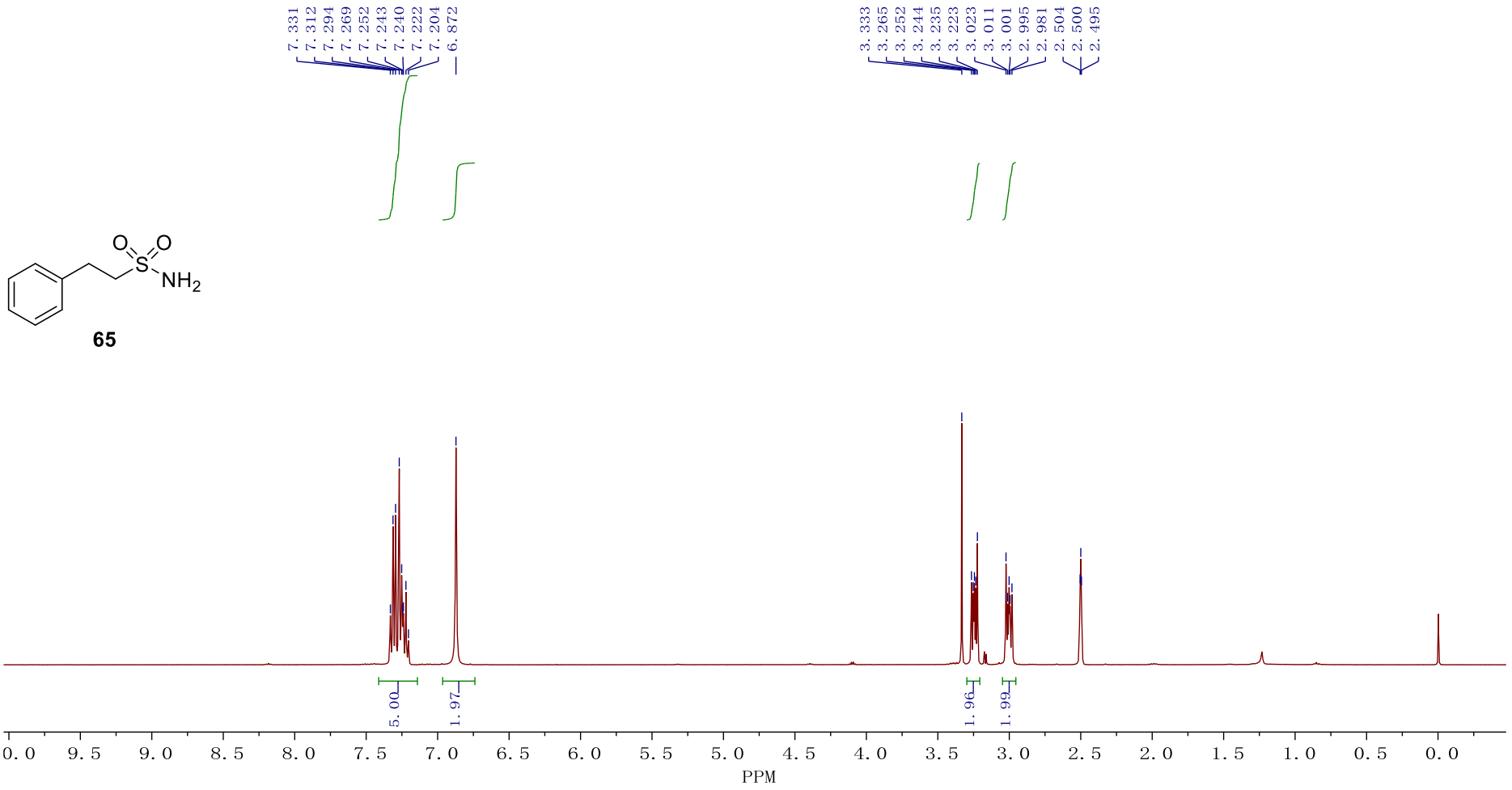
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7.222
7.204
6.872
3.333
3.265
3.252
3.244
3.235
3.223
3.023
3.011
3.001
2.995
2.981
2.504
2.500
2.495
O
O
S
NH2
65
5.00
1.97
1.96
1.99
0.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
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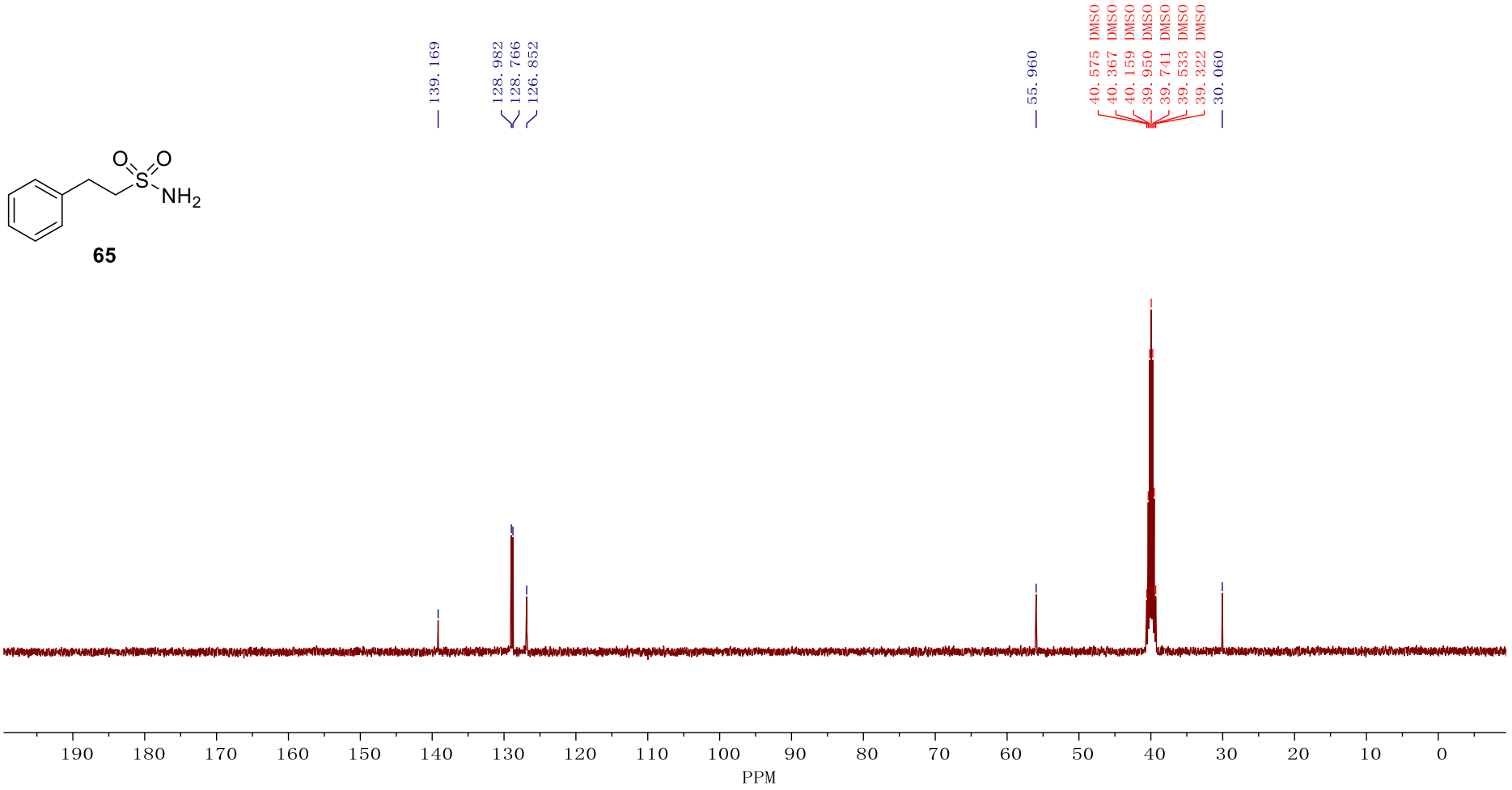
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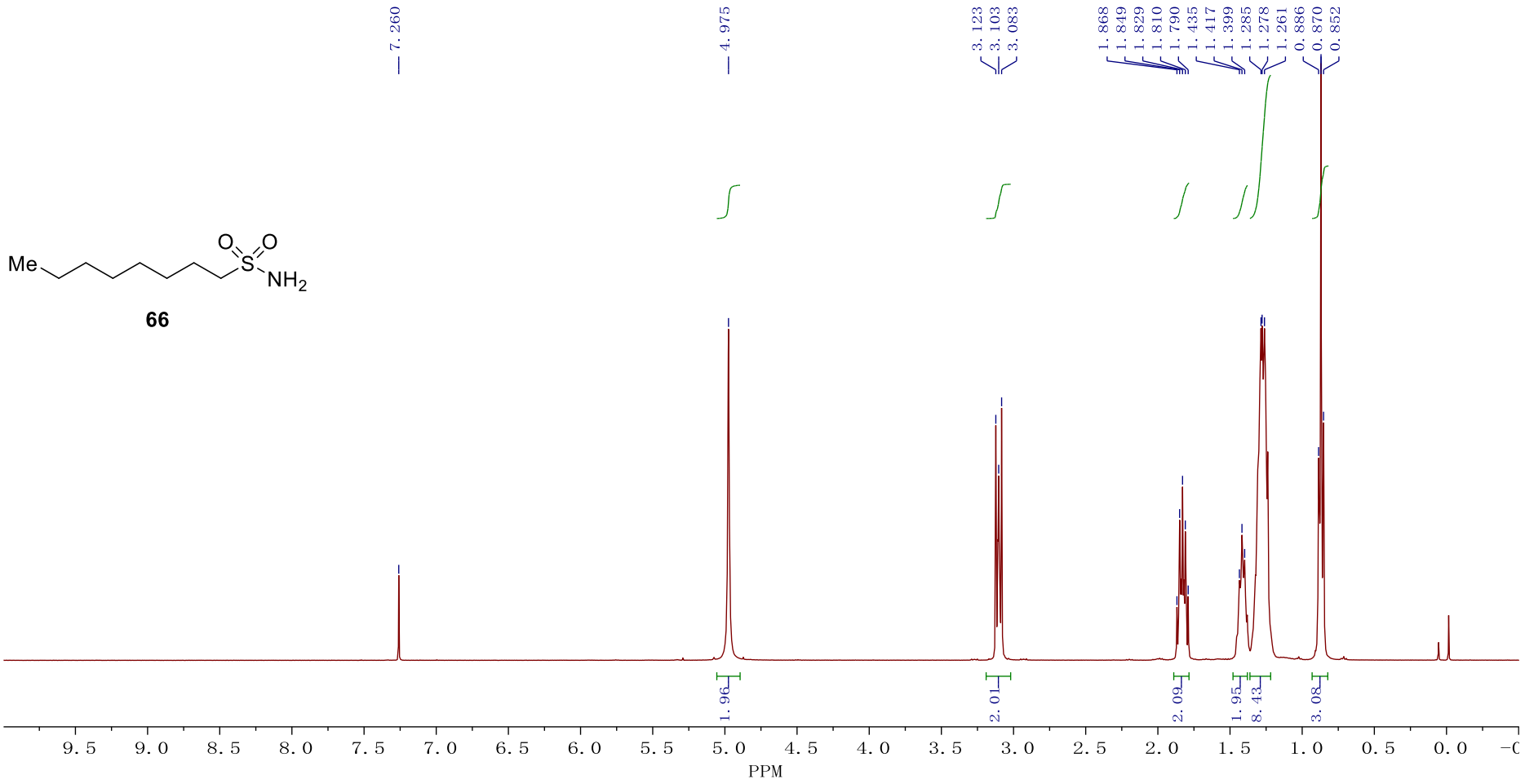
PPM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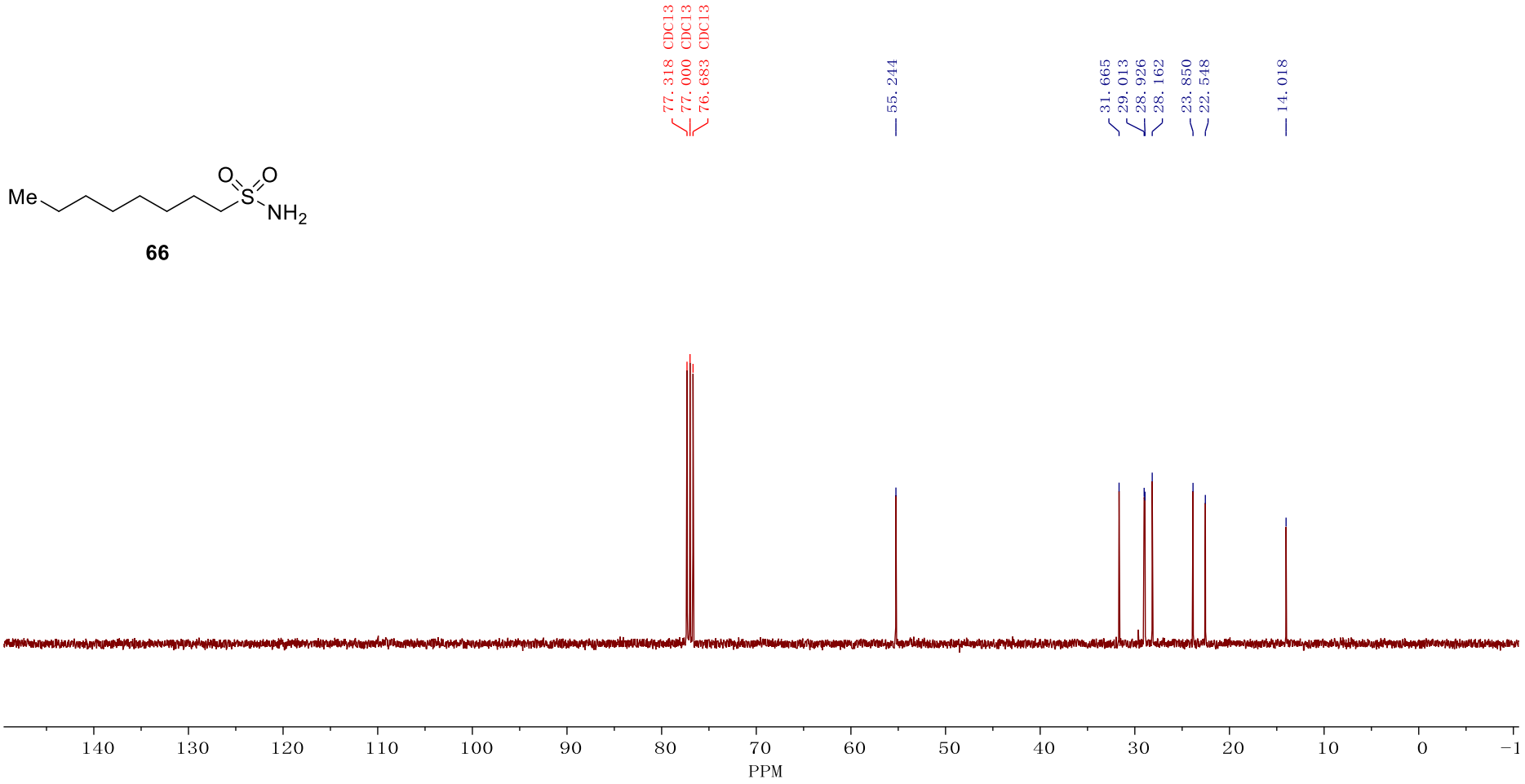
1.417
1.399
1.285
1.278
1.261
0.886
0.870
0.852
Me
O
S
O
NH2
66
1.96
2.01
2.09
1.95
8.43
3.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
PPM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22.548
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O
O
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110
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80
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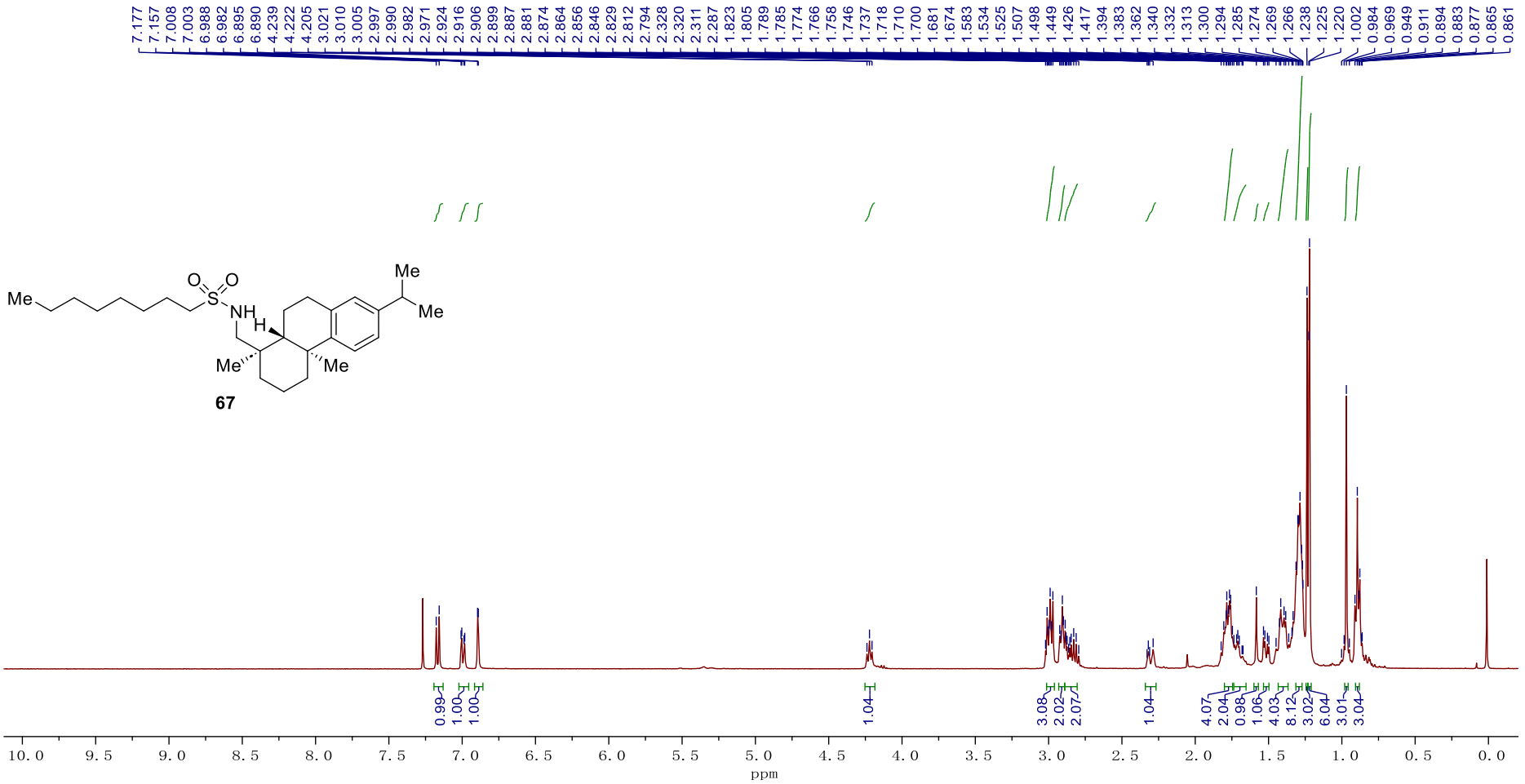
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3.010
3.005
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2.982
2.971
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2.916
2.906
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2.874
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2.856
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2.829
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1.774
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0.949
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0.877
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0.861
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S
NH
H
Me
Me
Me
Me
67
0.99
1.00
1.00
1.04
3.08
2.02
2.07
1.04
4.07
2.04
0.98
1.06
4.03
8.12
3.02
6.04
3.01
3.04
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9.0
8.5
8.0
7.5
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6.5
6.0
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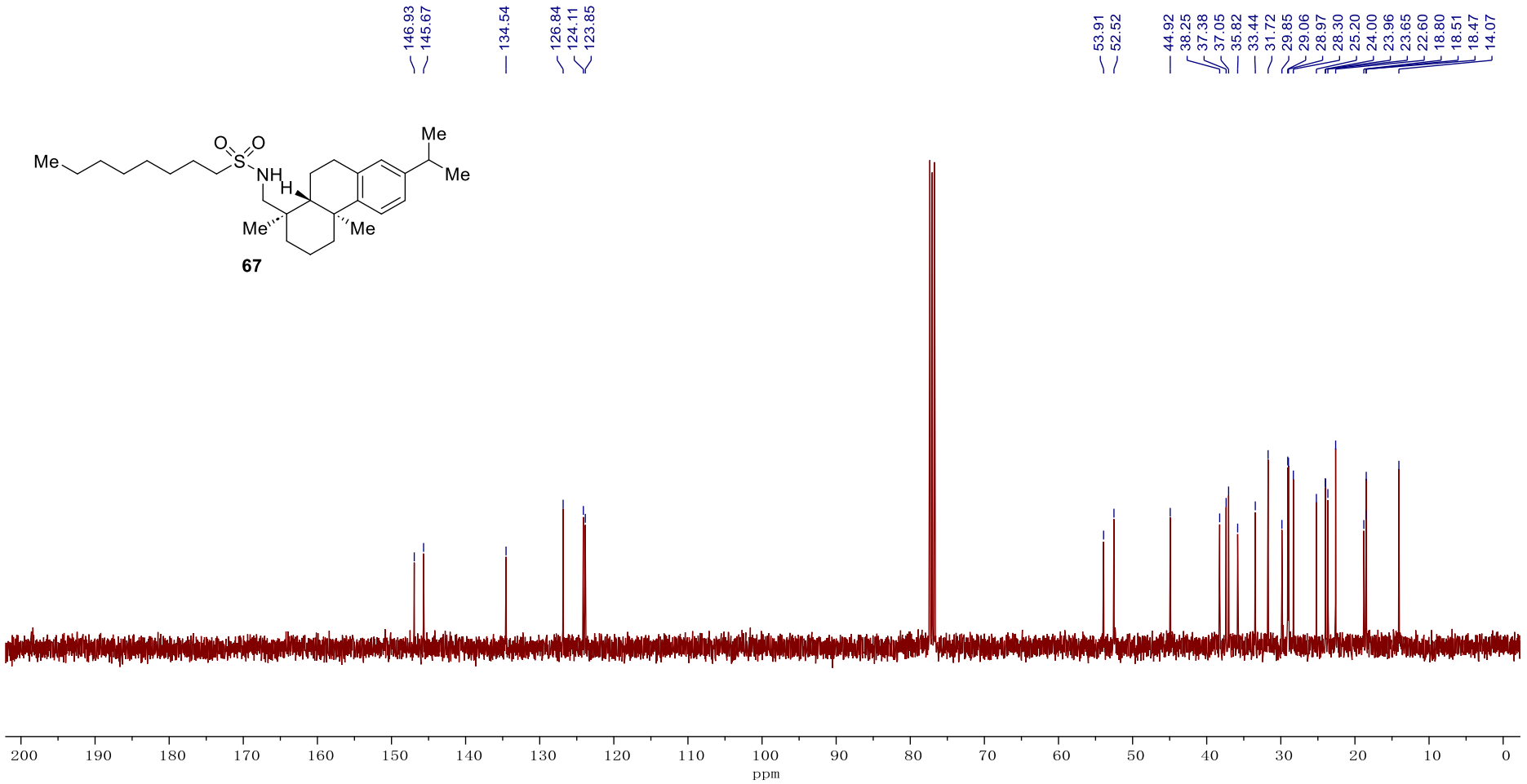
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29.06
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28.30
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24.00
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23.65
22.60
18.80
18.51
18.47
14.07
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O
O
S
NH
H
Me
Me
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Me
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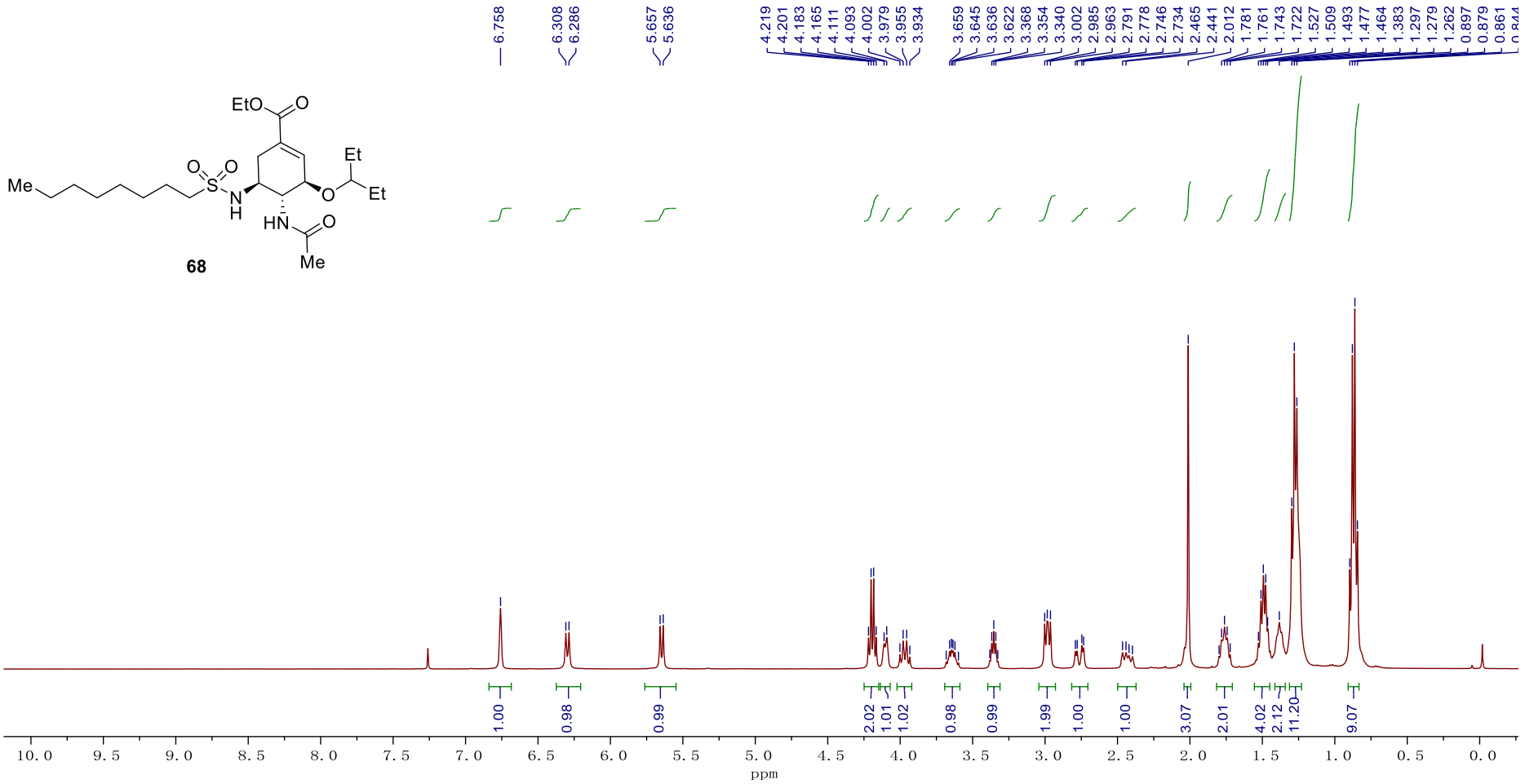
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Et
Me
O
O
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N
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HN
O
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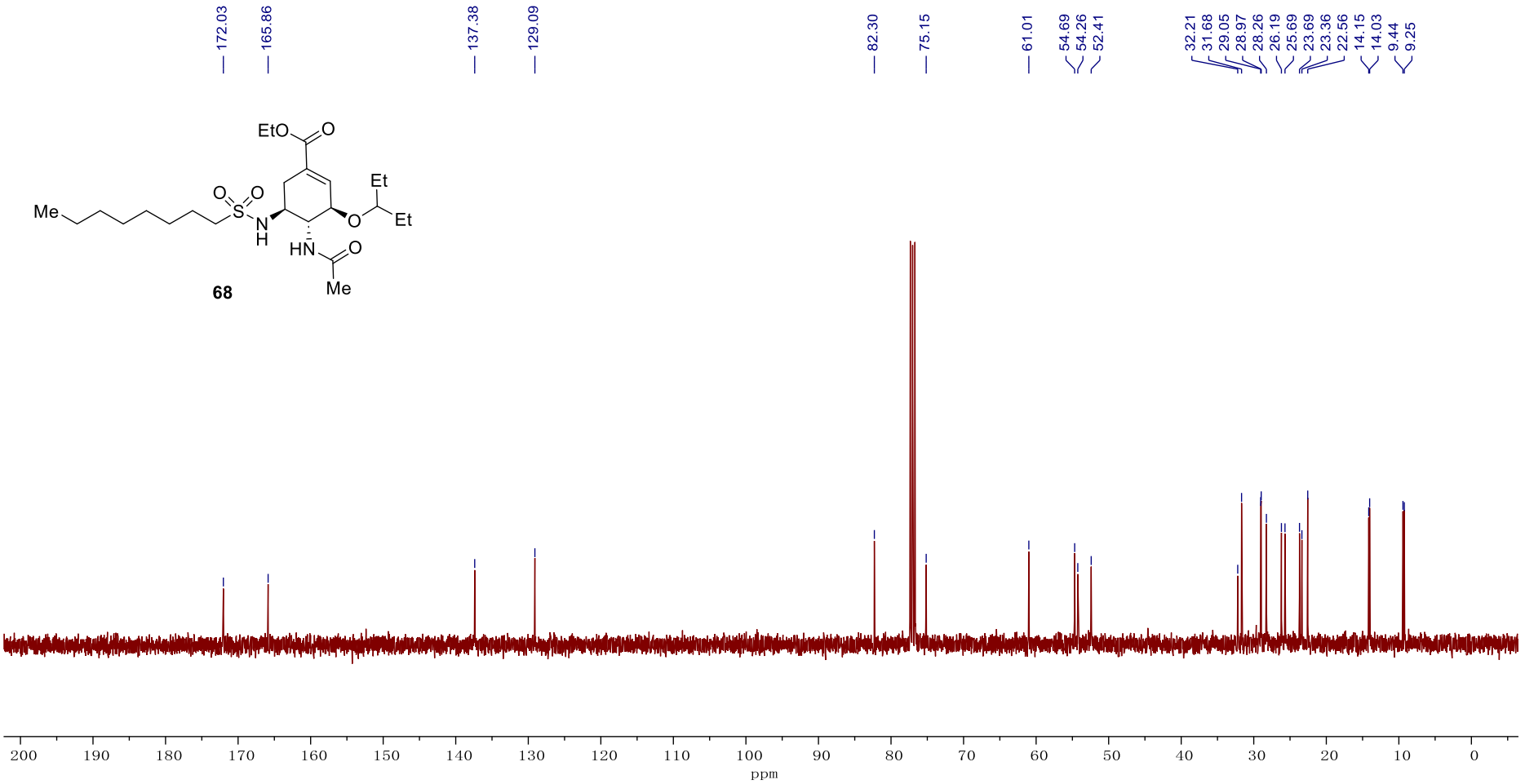
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28.26
26.19
25.69
23.69
23.36
22.56
14.15
14.03
9.44
9.25
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O
Et
Me
O
S
O
N
H
O
Et
HN
O
Me
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200
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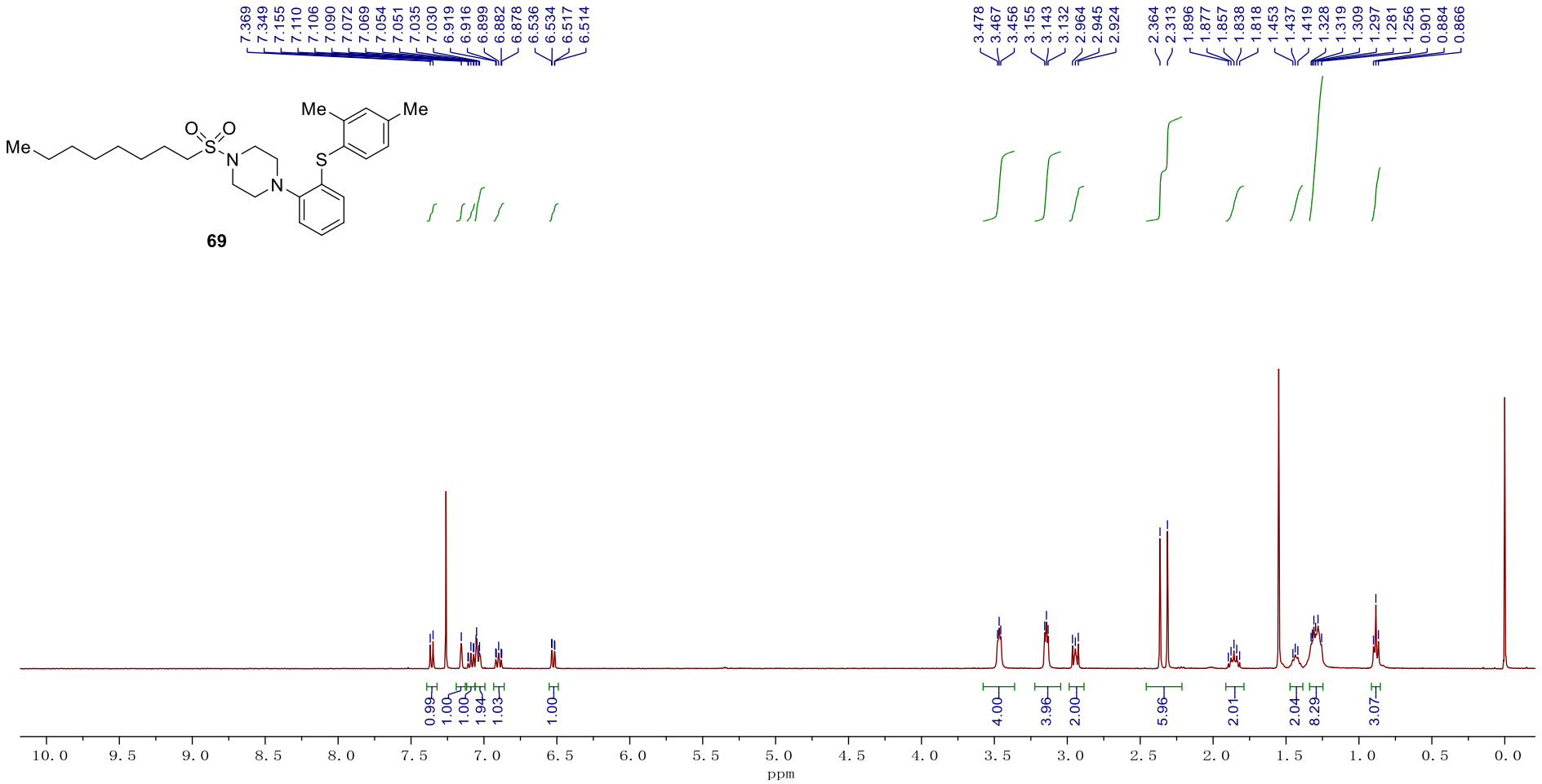
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Me
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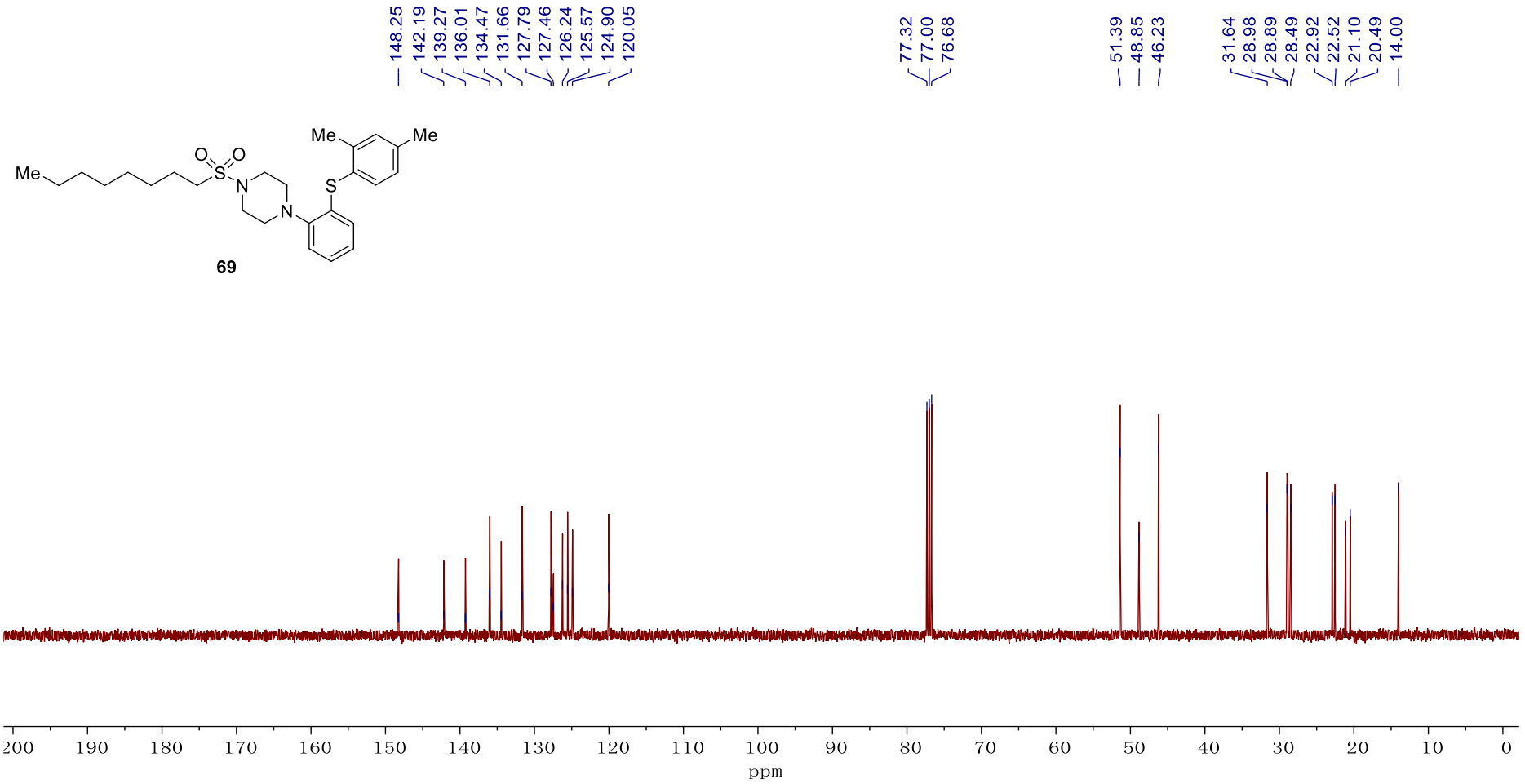
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77.00
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51.39
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21.10
20.49
14.00
Me
O
O
S
N
N
S
Me
Me
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120
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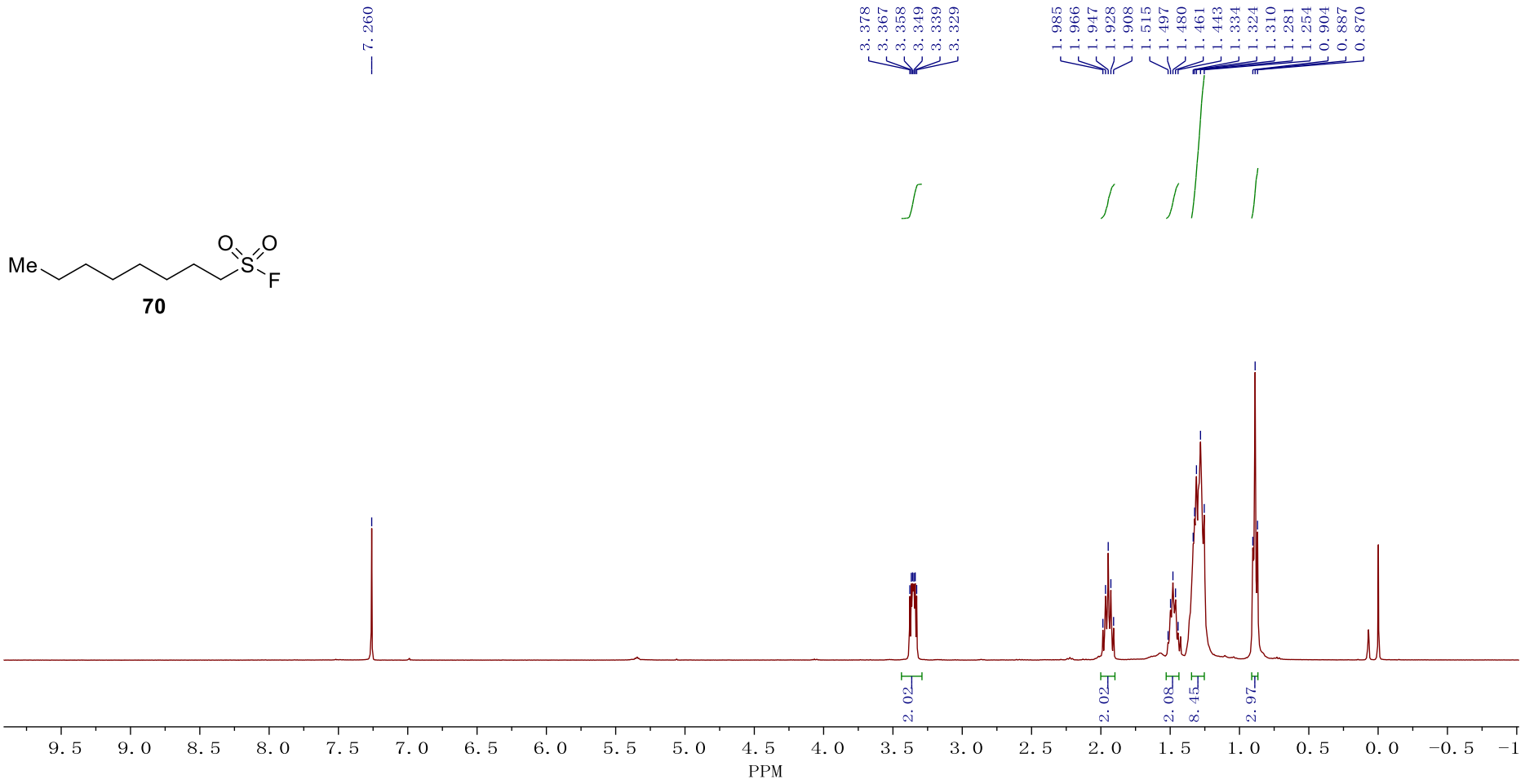
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1.310
1.281
1.254
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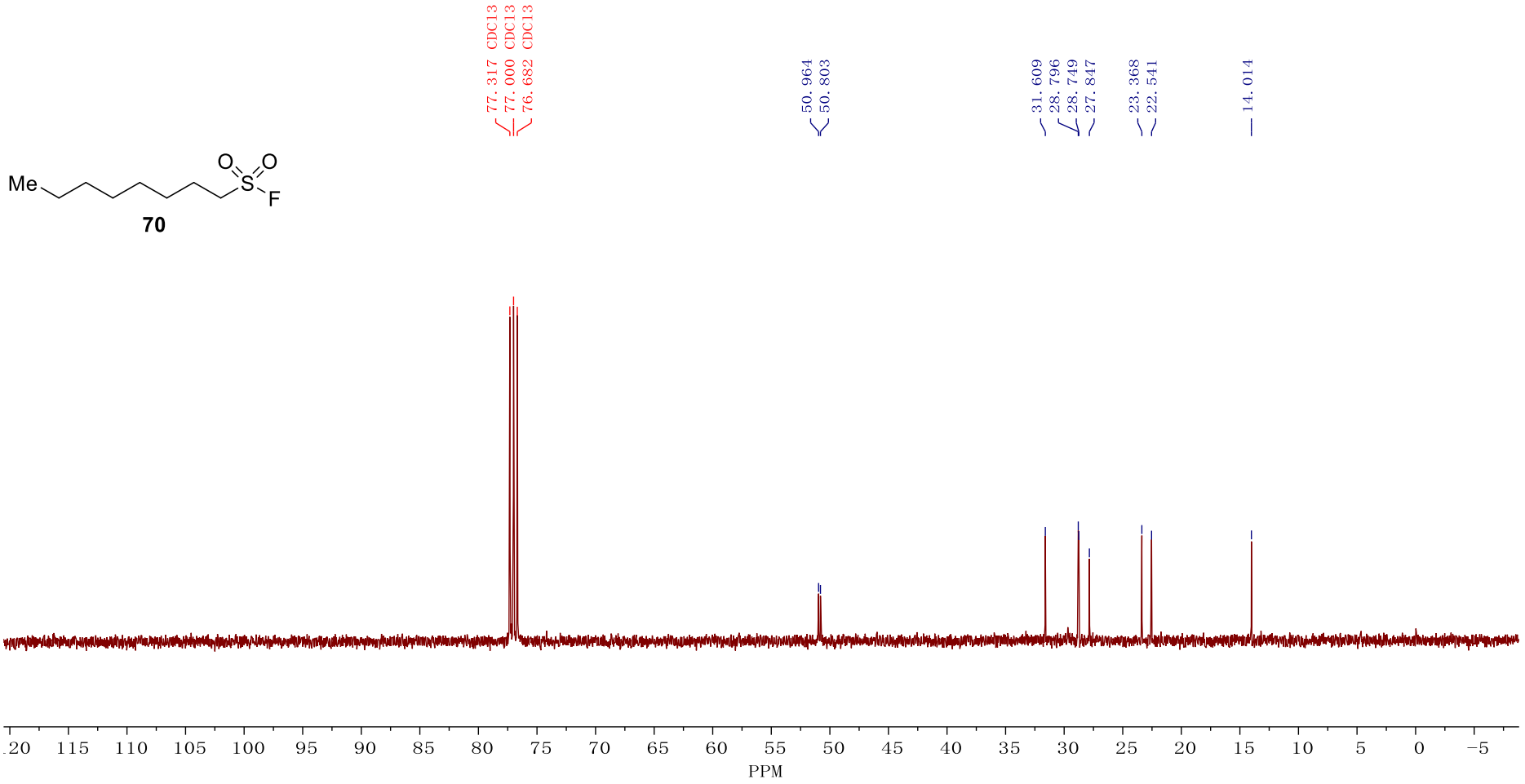
0.887
0.870
Me
O
O
S
F
70
2.02
2.02
2.08
8.45
2.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
PPM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77.000 CDC13
76.682 CDC13
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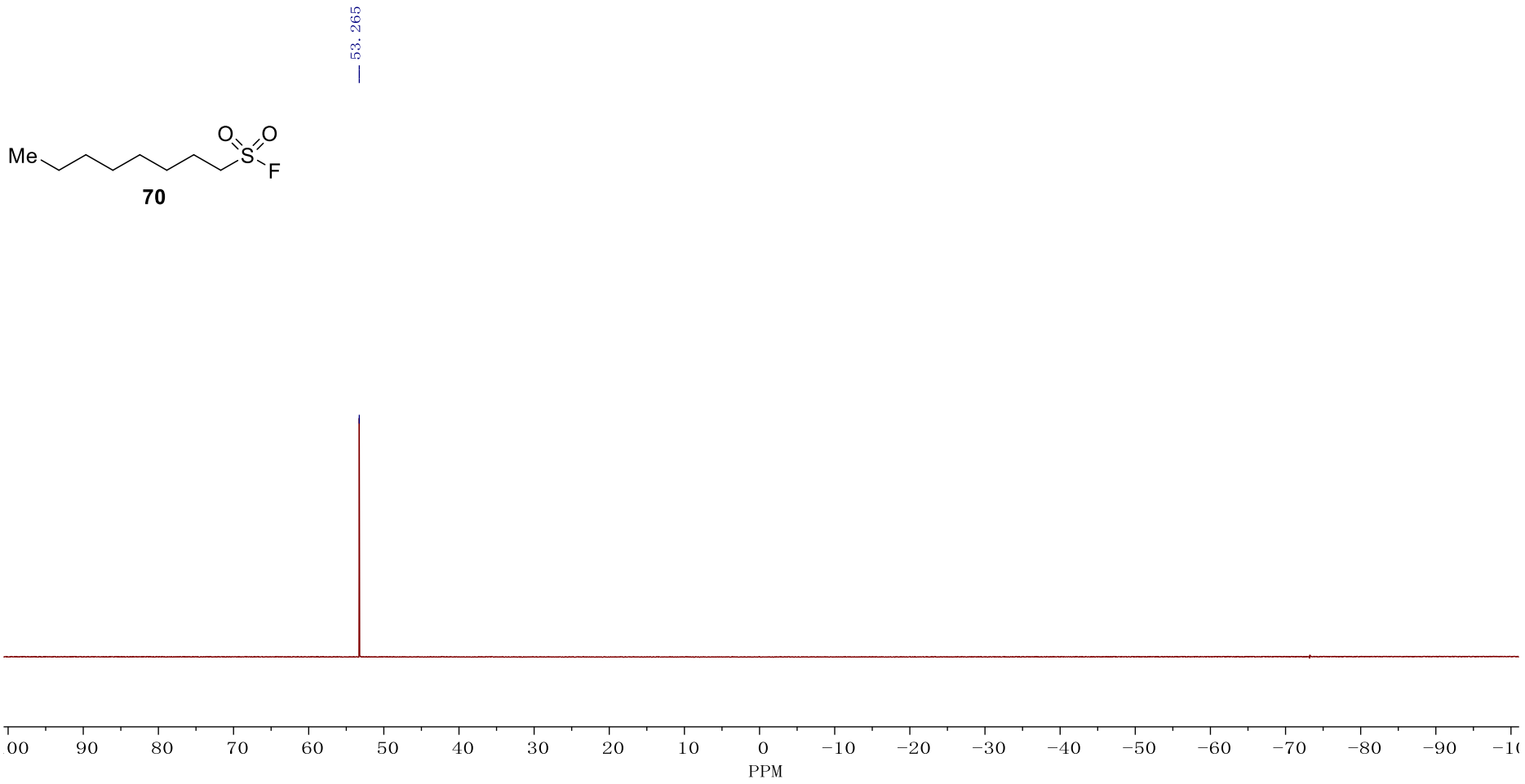
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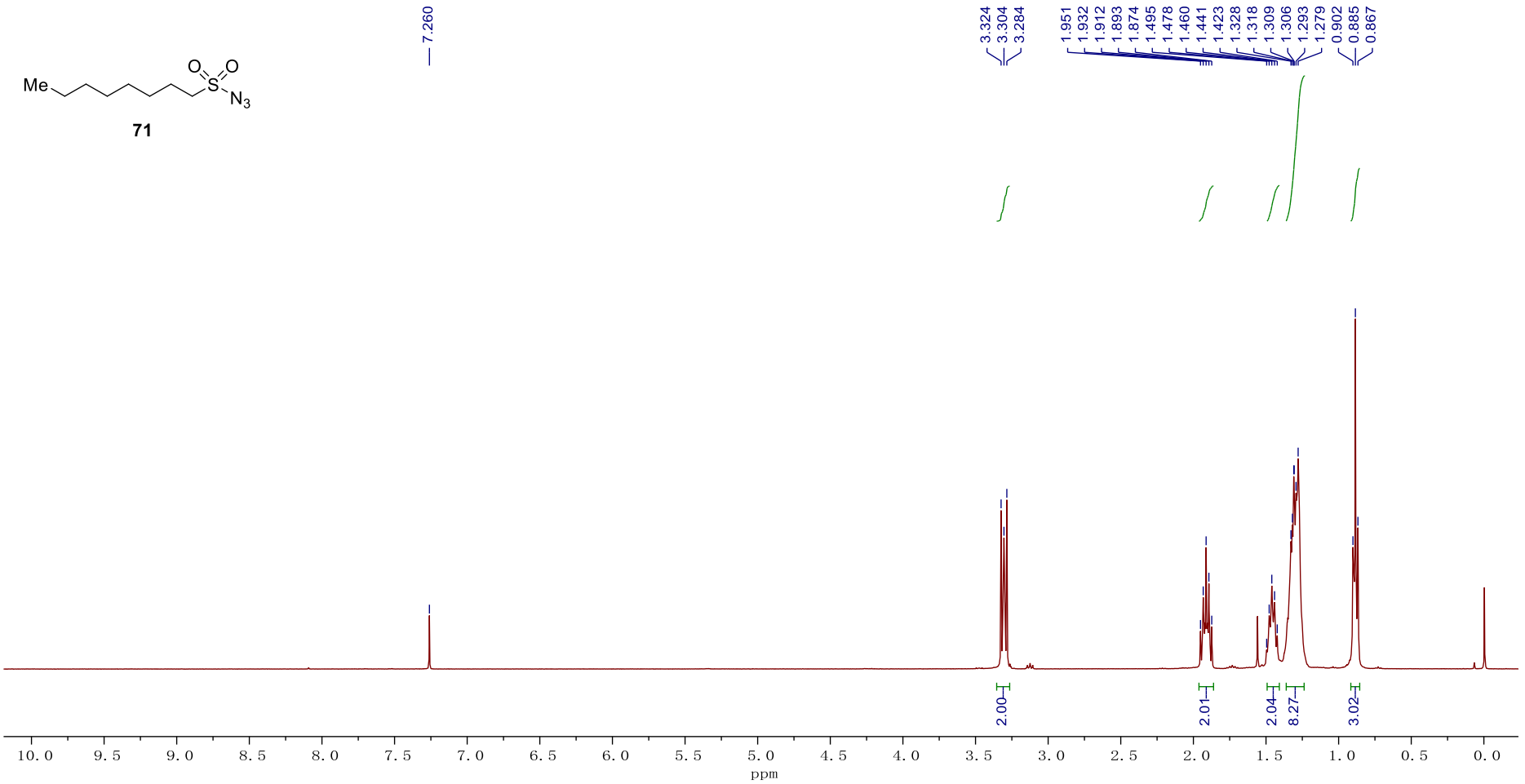
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2.5
2.0
1.5
1.0
0.5
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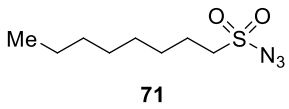
Me
O
O
S
N3

71

77.00
55.94
31.59
28.81
27.91
23.30
22.51
13.98
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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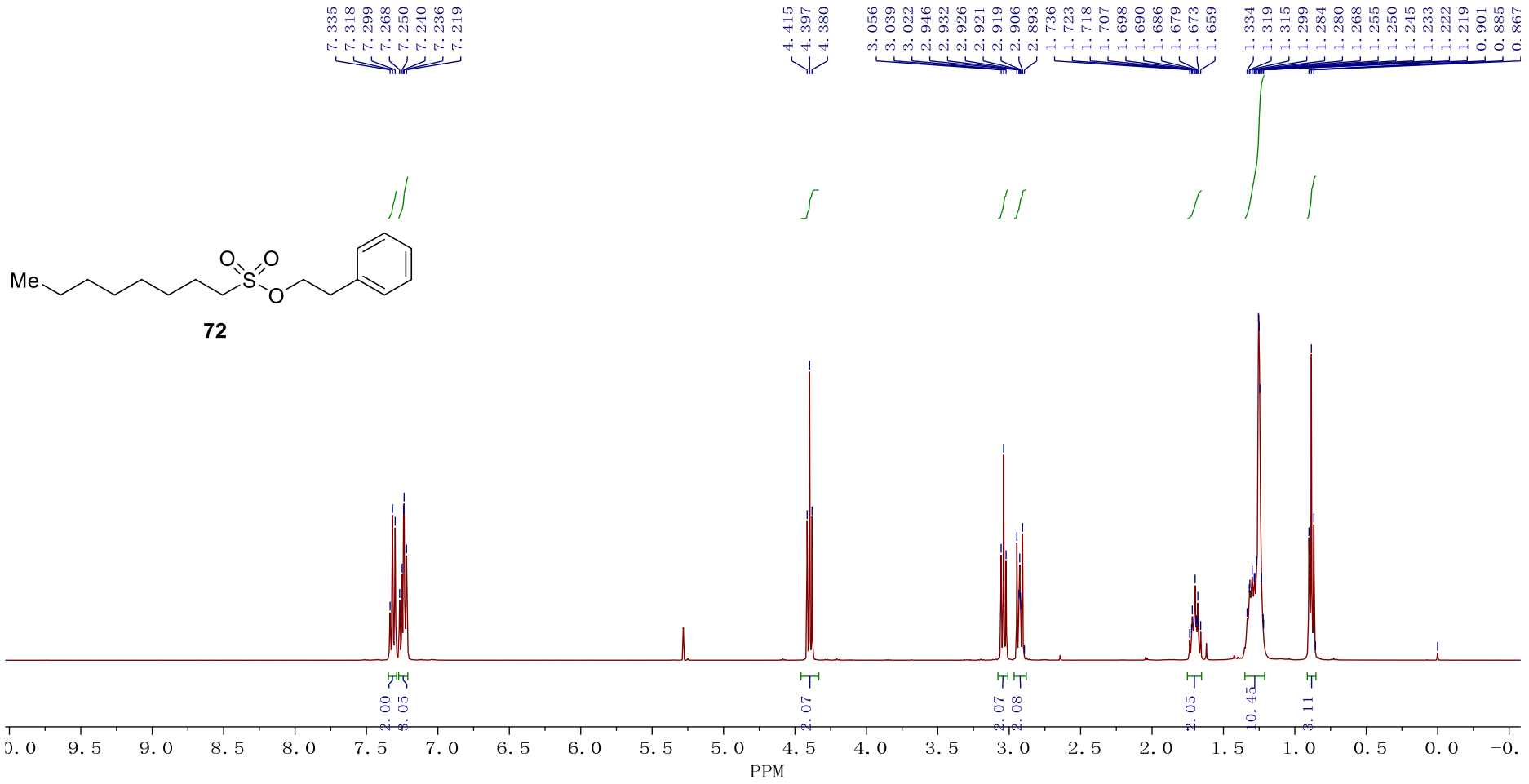
20
10
0
ppm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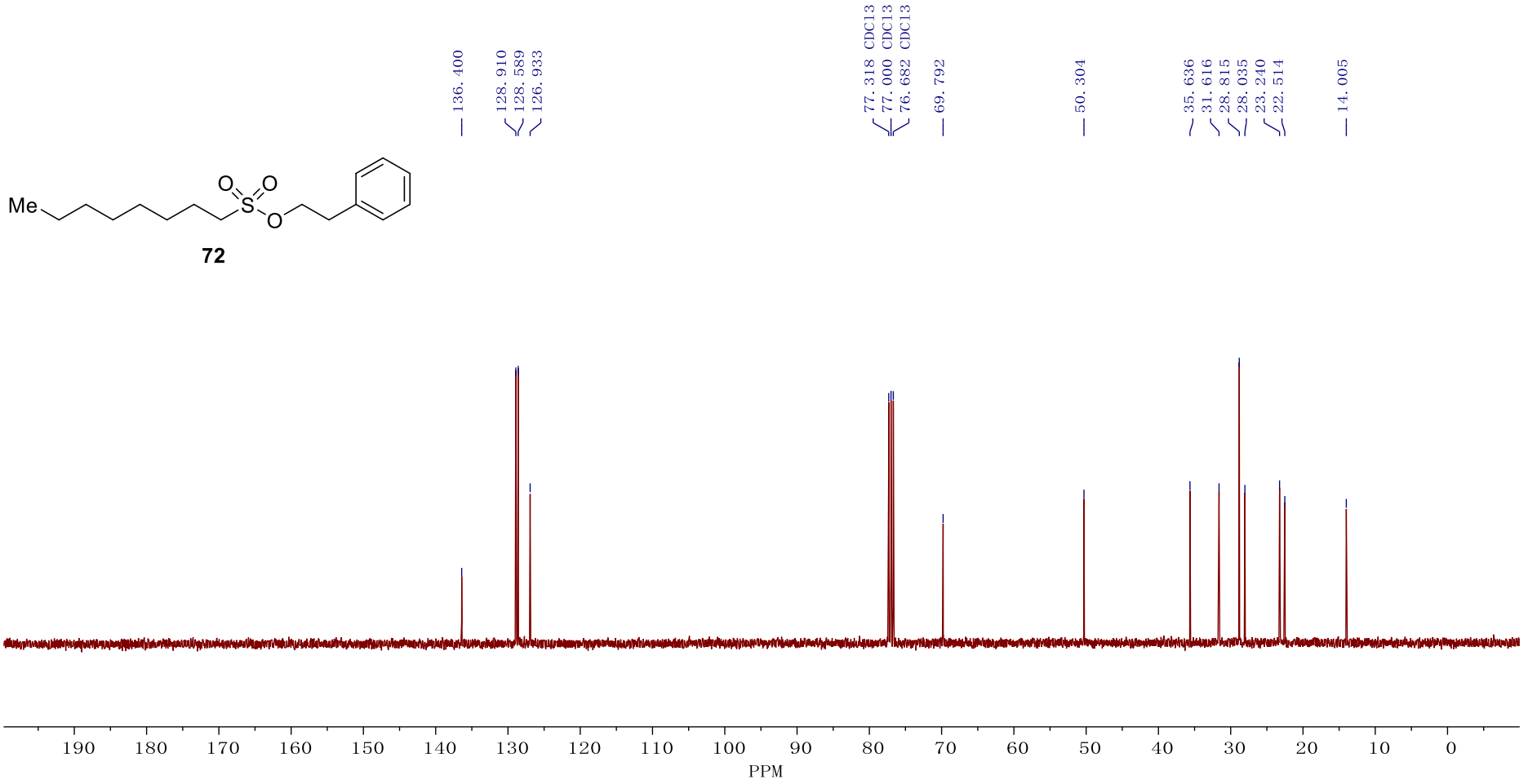
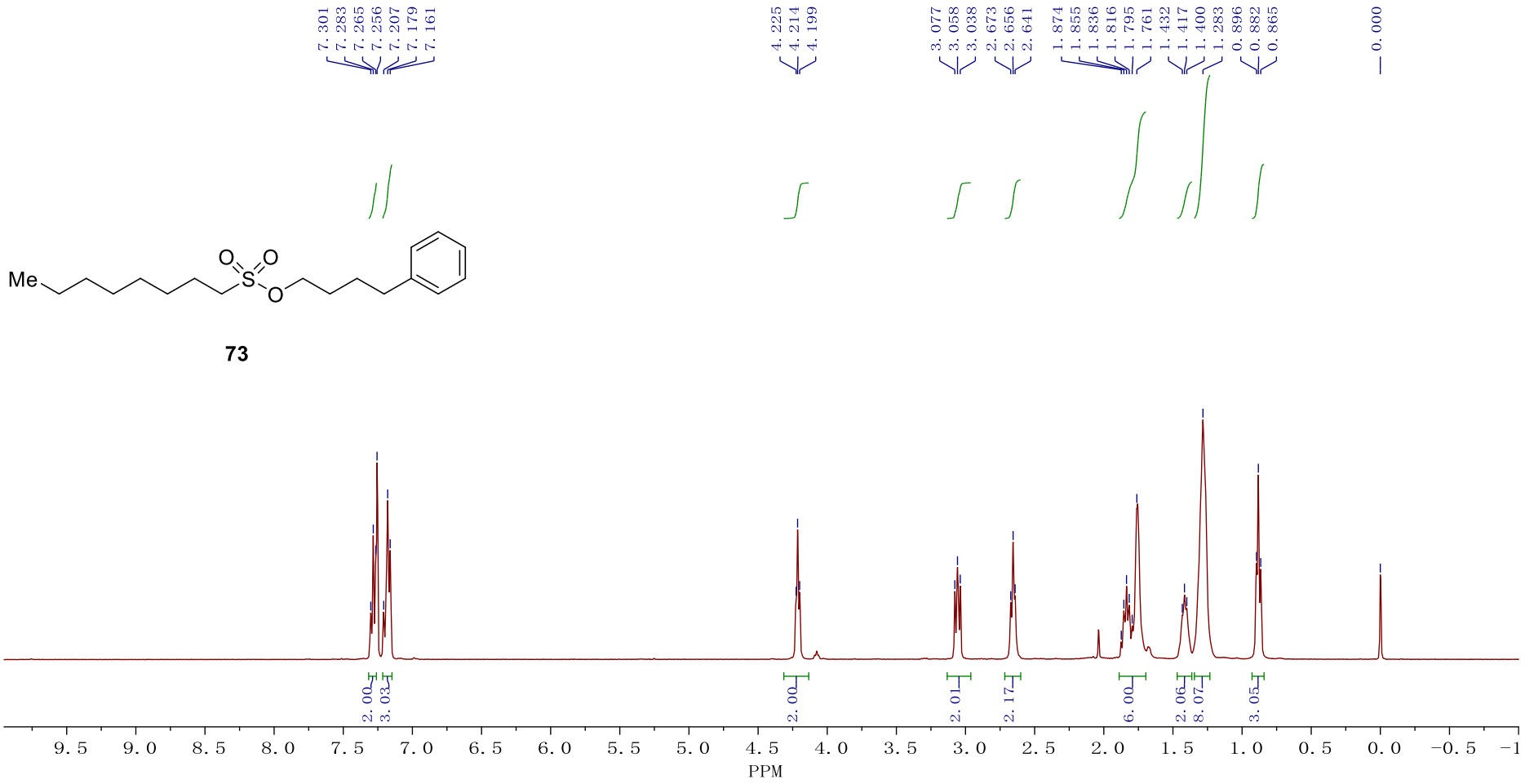
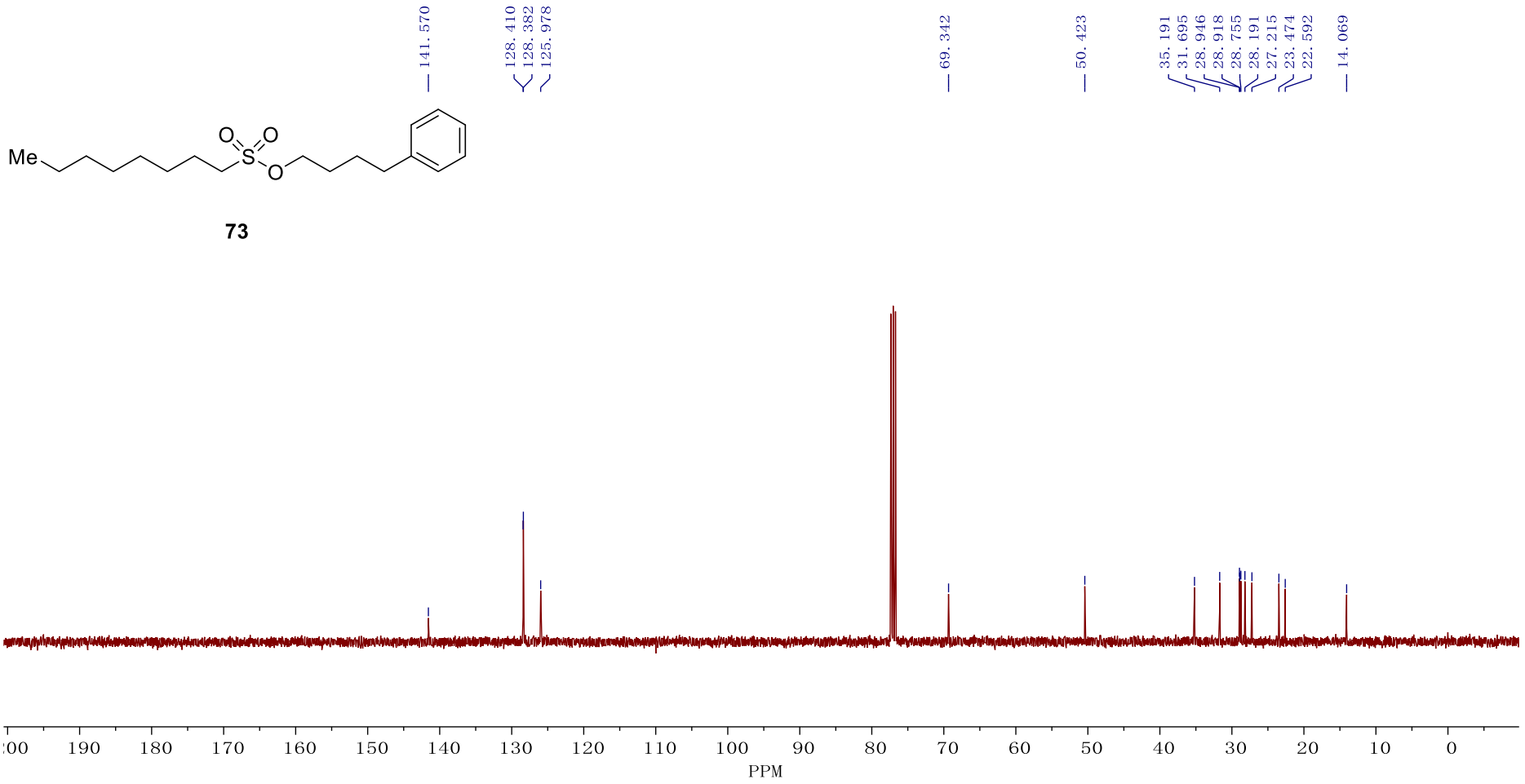
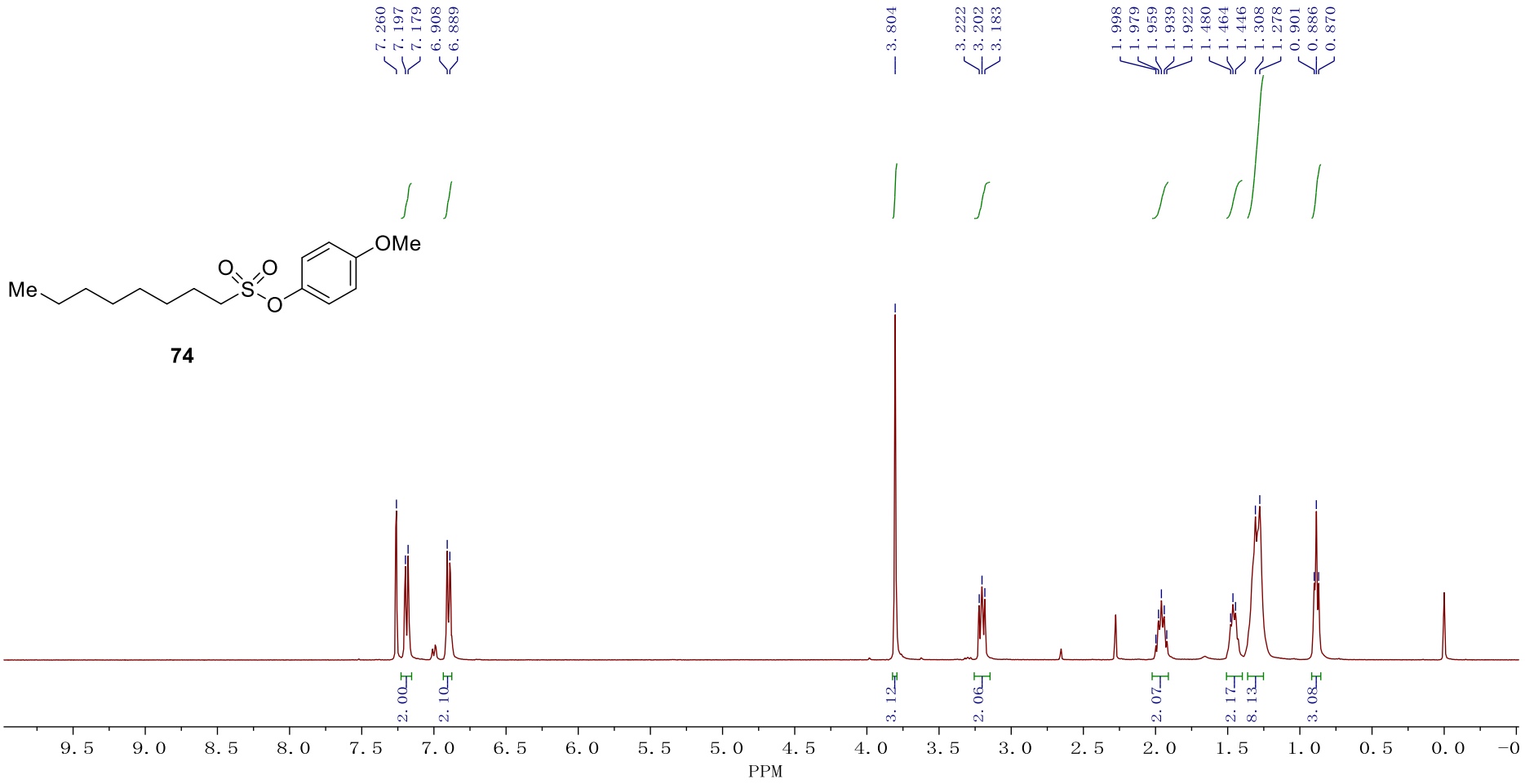
7.318
7.299
7.268
7.250
7.240
7.236
7.219
4.415
4.397
4.380
3.056
3.039
3.022
2.946
2.932
2.926
2.921
2.919
2.906
2.893
1.736
1.723
1.718
1.707
1.698
1.690
1.686
1.679
1.673
1.659
1.334
1.319
1.315
1.299
1.284
1.280
1.268
1.255
1.250
1.245
1.233
1.222
1.219
0.901
0.885
0.867
Me
O
O
S
O
72
2.00
3.05
2.07
2.07
2.08
2.05
10.45
3.11
PPM

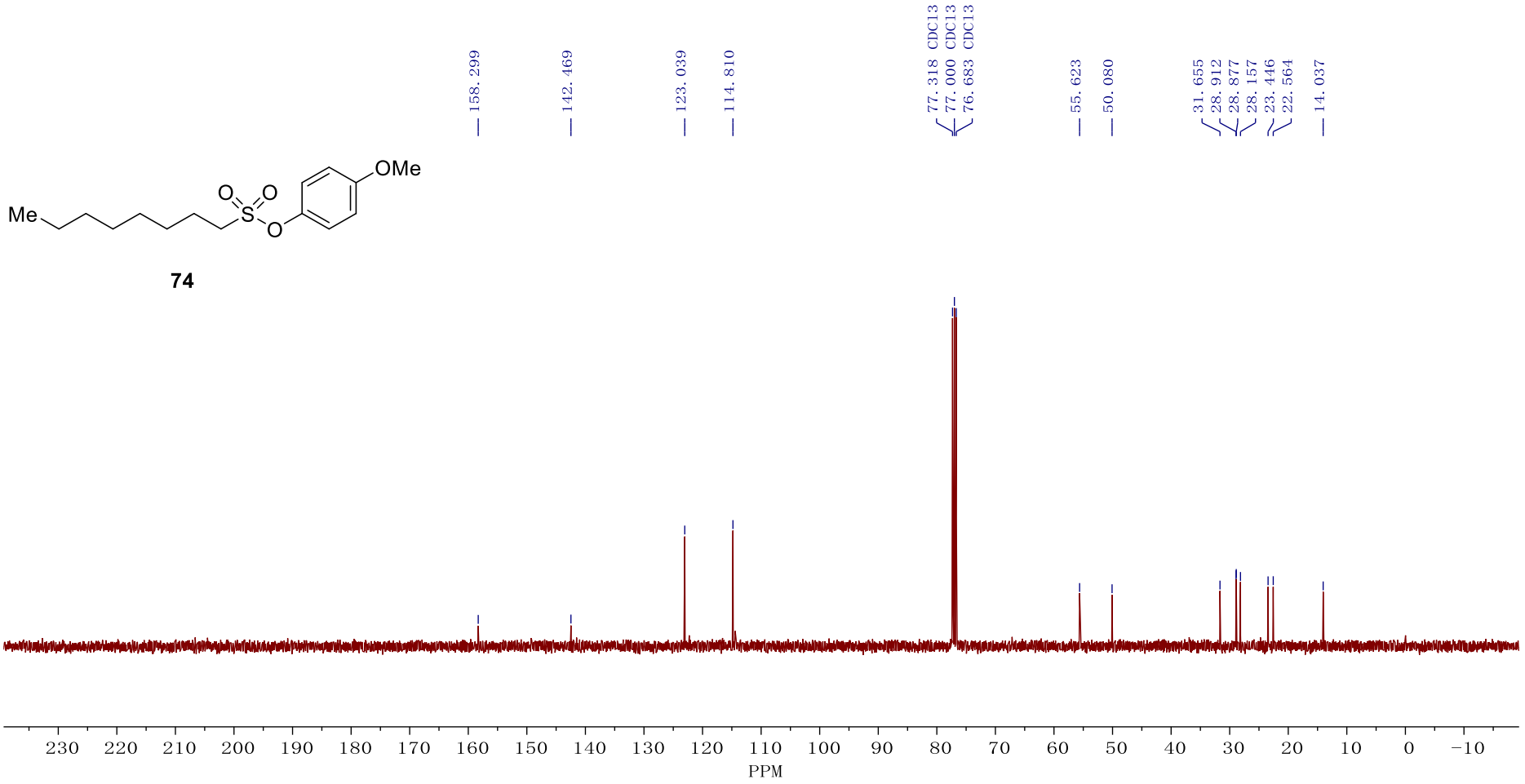

136.400
128.910
128.589
126.933
77.318 CDCl3
77.000 CDCl3
76.682 CDCl3
69.792
50.304
35.636
31.616
28.815
28.035
23.240
22.514
14.005
Me
O
O
S
O
72
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM

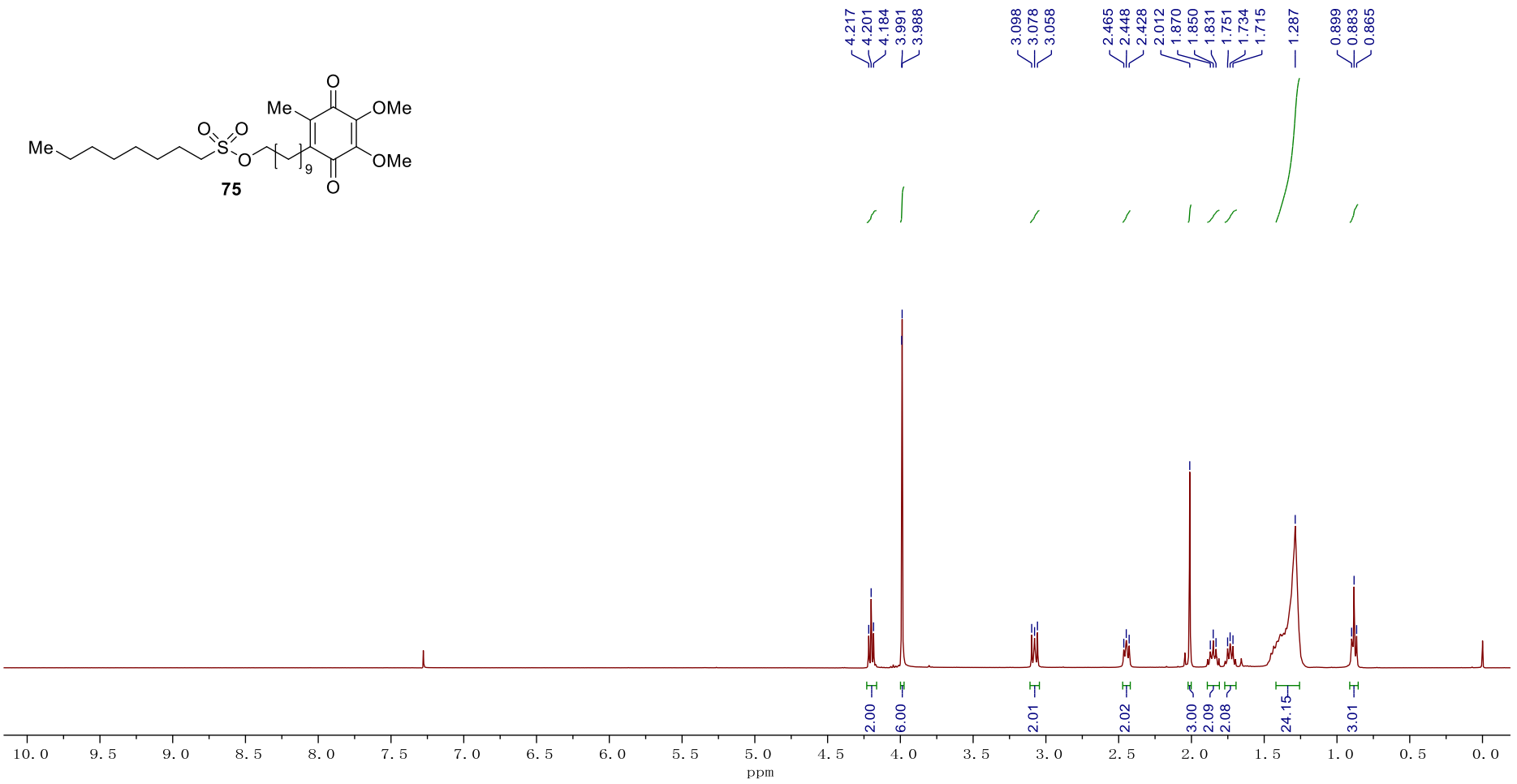

7.301
7.283
7.265
7.256
7.207
7.179
7.161
4.225
4.214
4.199
3.077
3.058
3.038
2.673
2.656
2.641
1.874
1.855
1.836
1.816
1.795
1.761
1.432
1.417
1.400
1.283
0.896
0.882
0.865
0.000
Me
O
O
S
O
2.00
3.03
2.00
2.01
2.17
6.00
2.06
8.07
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
PPM

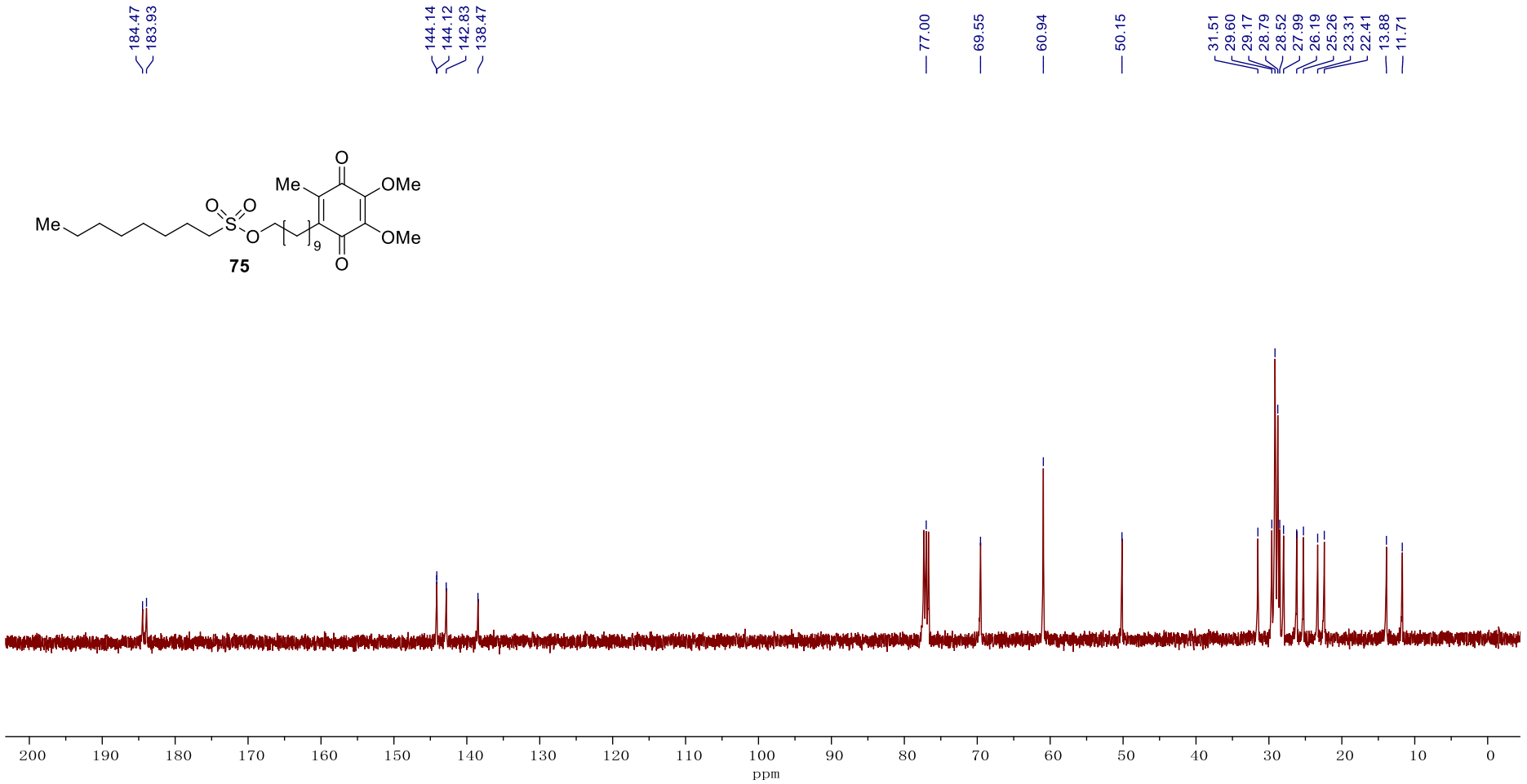
73

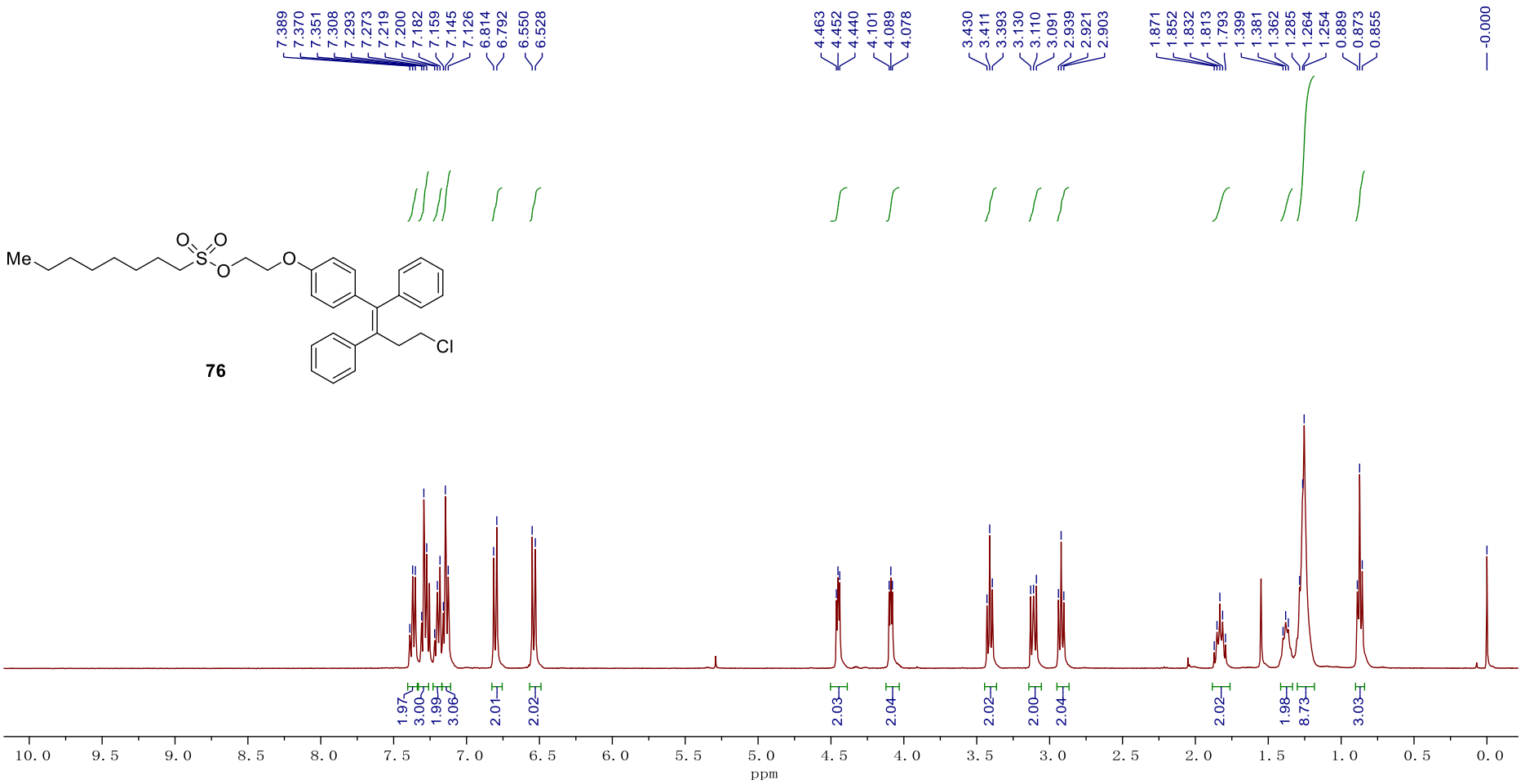

141.570
128.410
128.382
125.978
69.342
50.423
35.191
31.695
28.946
28.918
28.755
28.191
27.215
23.474
22.592
14.069
Me
O
O
S
O
73
PPM


7.260
7.197
7.179
6.908
6.889
3.804
3.222
3.202
3.183
1.998
1.979
1.959
1.939
1.922
1.480
1.464
1.446
1.308
1.278
0.901
0.886
0.870
OMe
Me
O
S
O
O
74
2.00
2.10
3.12
2.06
2.07
2.17
8.13
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
PPM


158.299
142.469
123.039
114.810
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
55.623
50.080
31.655
28.912
28.877
28.157
23.446
22.564
14.037
OMe
Me
O
S
O
O
74
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
PPM


Me
O
S
O
O
O
9
Me
O
OMe
OMe
O
75
4.217
4.201
4.184
3.991
3.988
3.098
3.078
3.058
2.465
2.448
2.428
2.012
1.870
1.850
1.831
1.751
1.734
1.715
1.287
0.899
0.883
0.865
2.00
6.00
2.01
2.02
3.00
2.09
2.08
24.15
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
ppm


184.47
183.93
144.14
144.12
142.83
138.47
77.00
69.55
60.94
50.15
31.51
29.60
29.17
28.79
28.52
27.99
26.19
25.26
23.31
22.41
13.88
11.71
Me
O
Me
OMe
O
S
O
O
9
OMe
O
Me
75
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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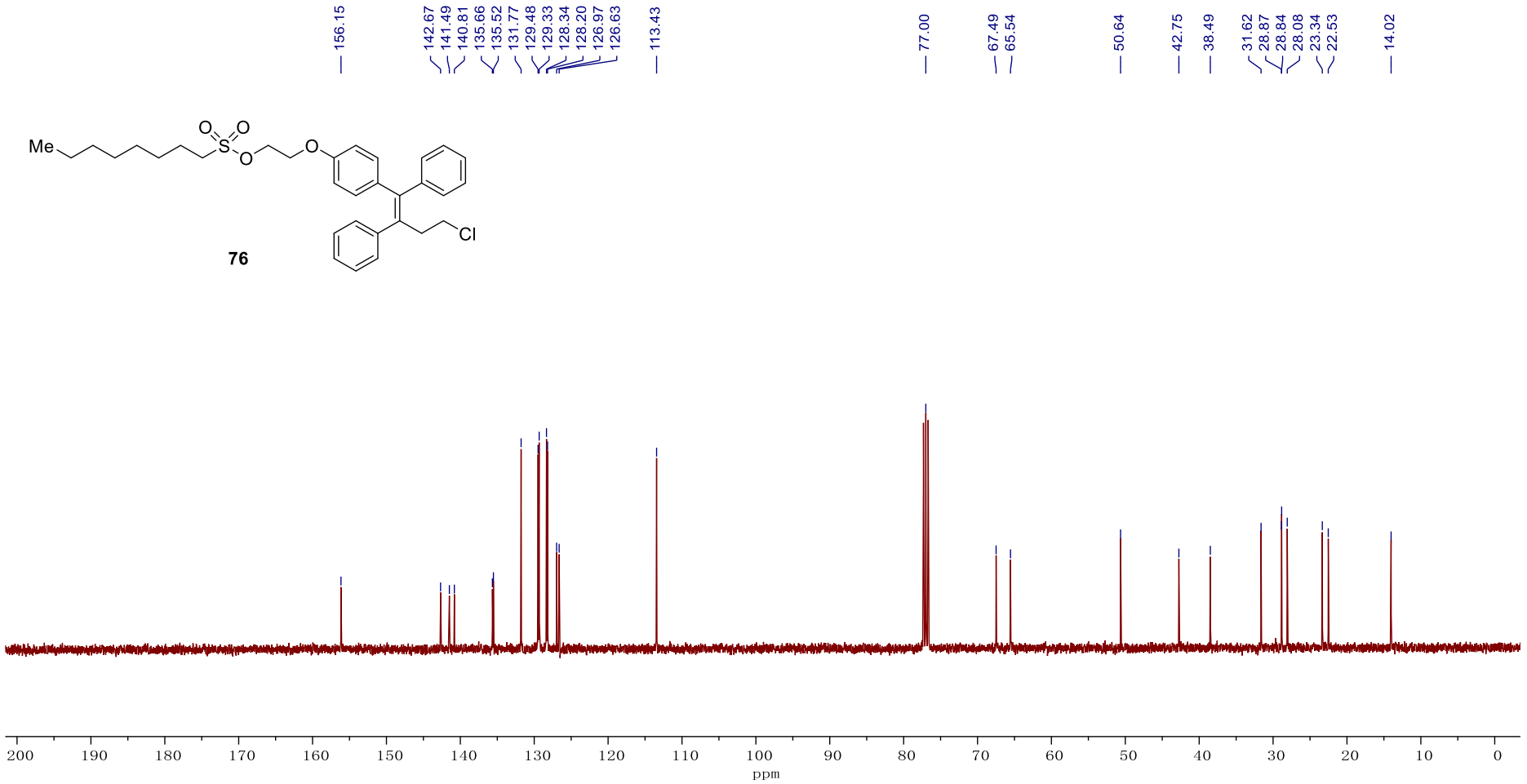
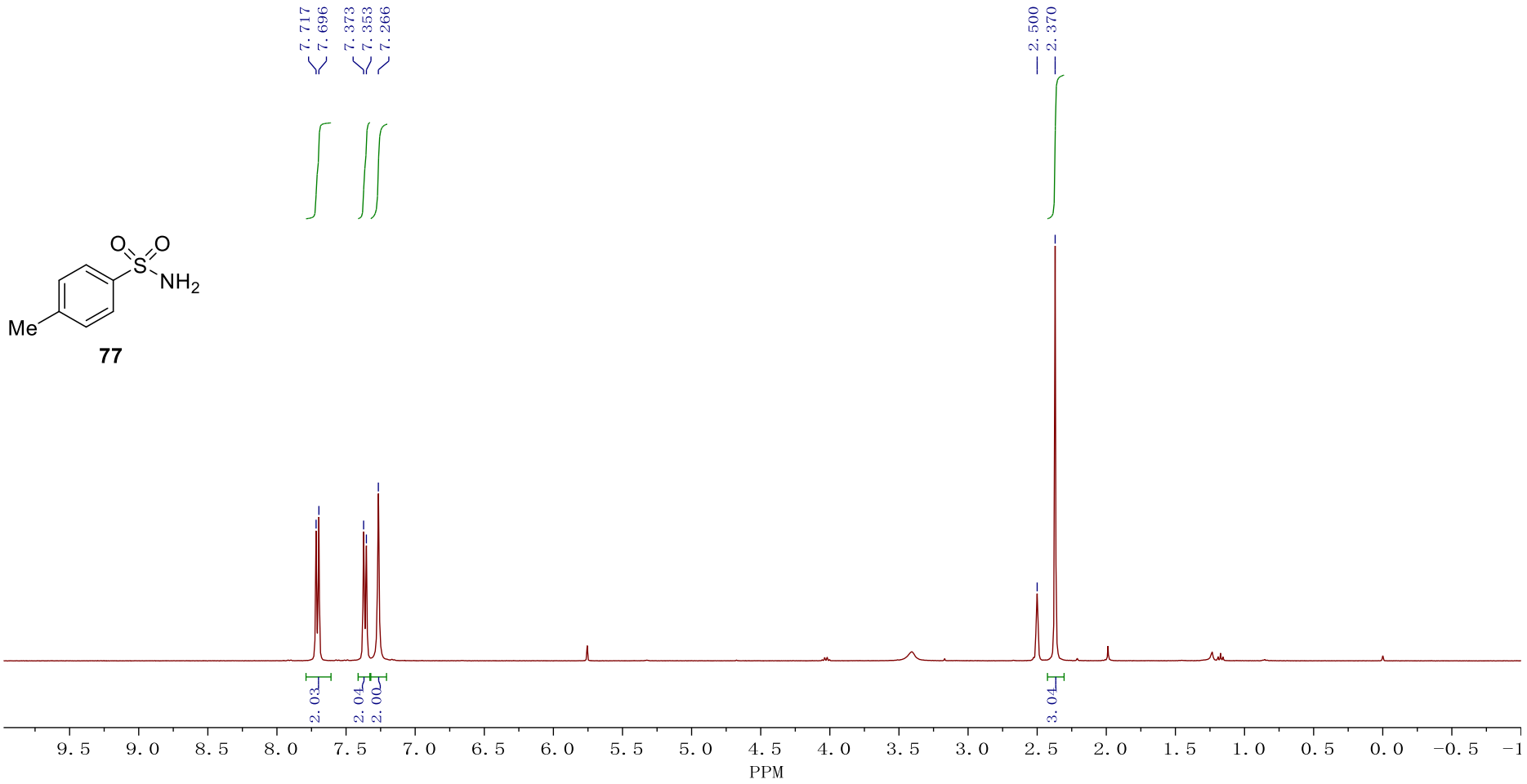
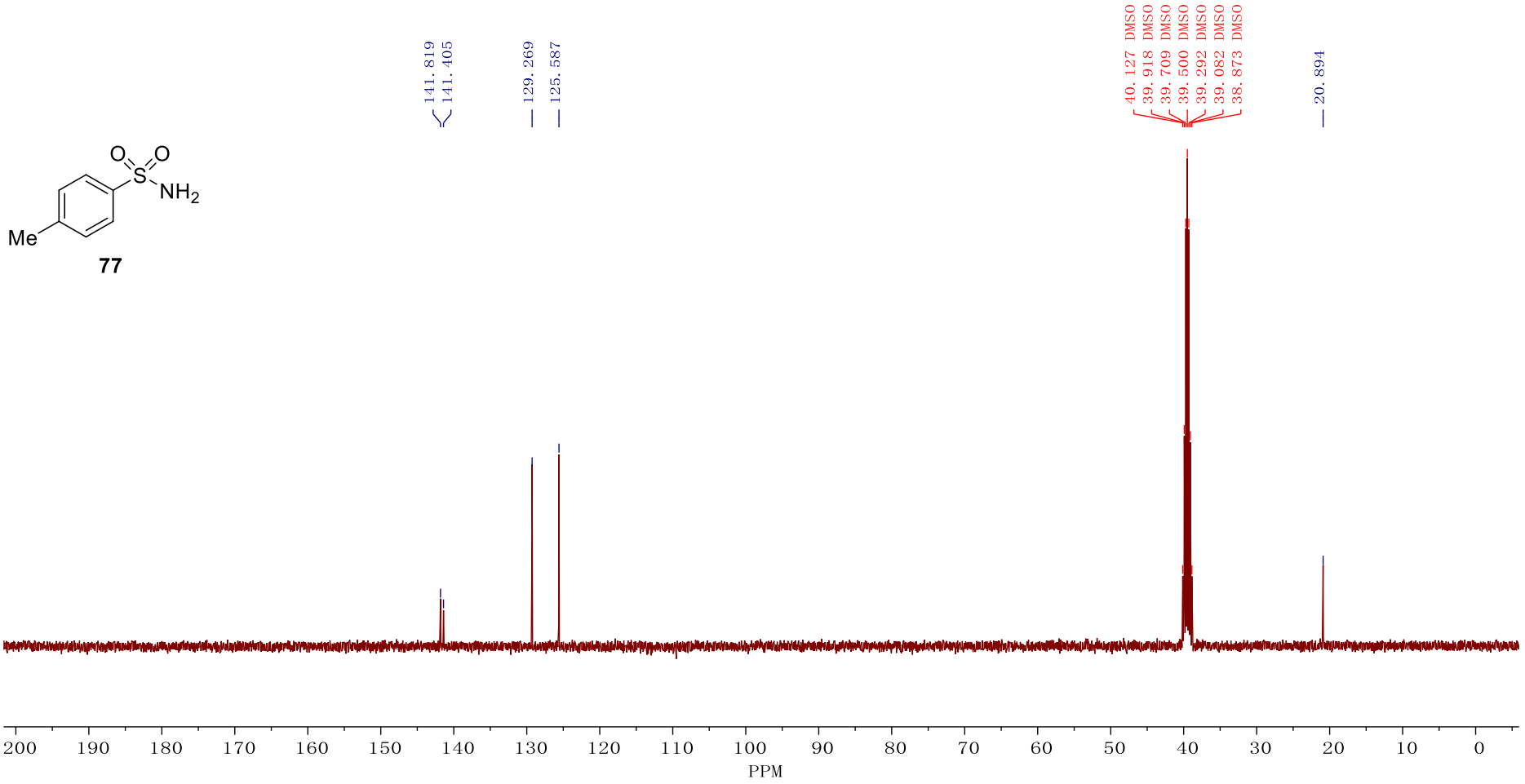
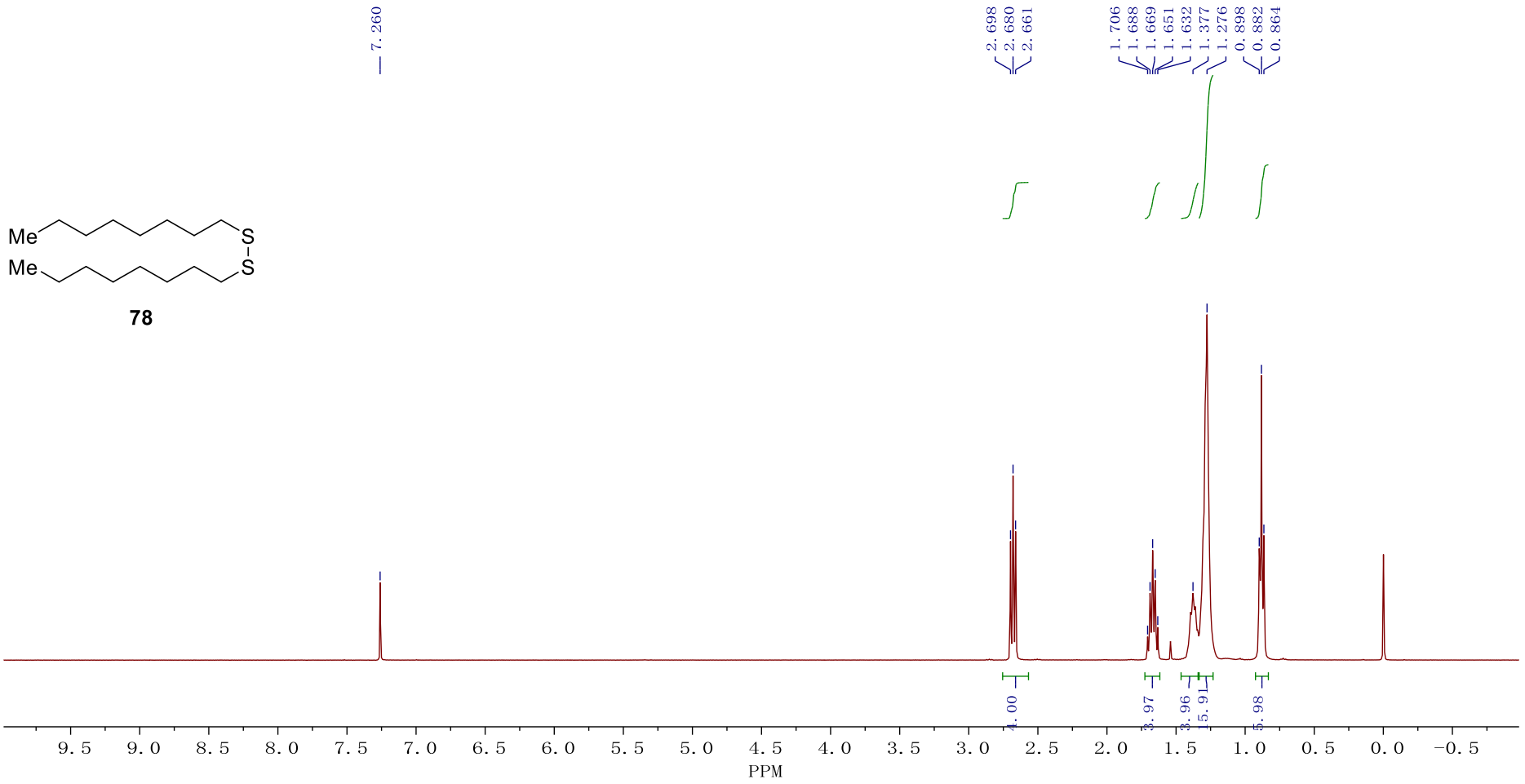
7.370
7.351
7.308
7.293
7.273
7.219
7.200
7.182
7.159
7.145
7.126
6.814
6.792
6.550
6.528
4.463
4.452
4.440
4.101
4.089
4.078
3.430
3.411
3.393
3.130
3.110
3.091
2.939
2.921
2.903
1.871
1.852
1.832
1.813
1.793
1.399
1.381
1.362
1.285
1.264
1.254
0.889
0.873
0.855
-0.000
Me
O
S
O
O
O
Cl
76
1.97
3.00
1.99
3.06
2.01
2.02
2.03
2.04
2.02
2.00
2.04
2.02
1.98
8.73
3.03
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
ppm


156.15
142.67
141.49
140.81
135.66
135.52
131.77
129.48
129.33
128.34
128.20
126.97
126.63
113.43
77.00
67.49
65.54
50.64
42.75
38.49
31.62
28.87
28.84
28.08
23.34
22.53
14.02
Me
O
O
S
O
O
Cl
76
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.717
7.696
7.373
7.353
7.266
2.500
2.370
O
O
S
NH2
Me
77
2.03
2.04
2.00
3.04
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
PPM


141.819
141.405
129.269
125.587
40.127 DMSO
39.918 DMSO
39.709 DMSO
39.500 DMSO
39.292 DMSO
39.082 DMSO
38.873 DMSO
20.894
O
O
S
NH2
Me
77
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
PPM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2.698
2.680
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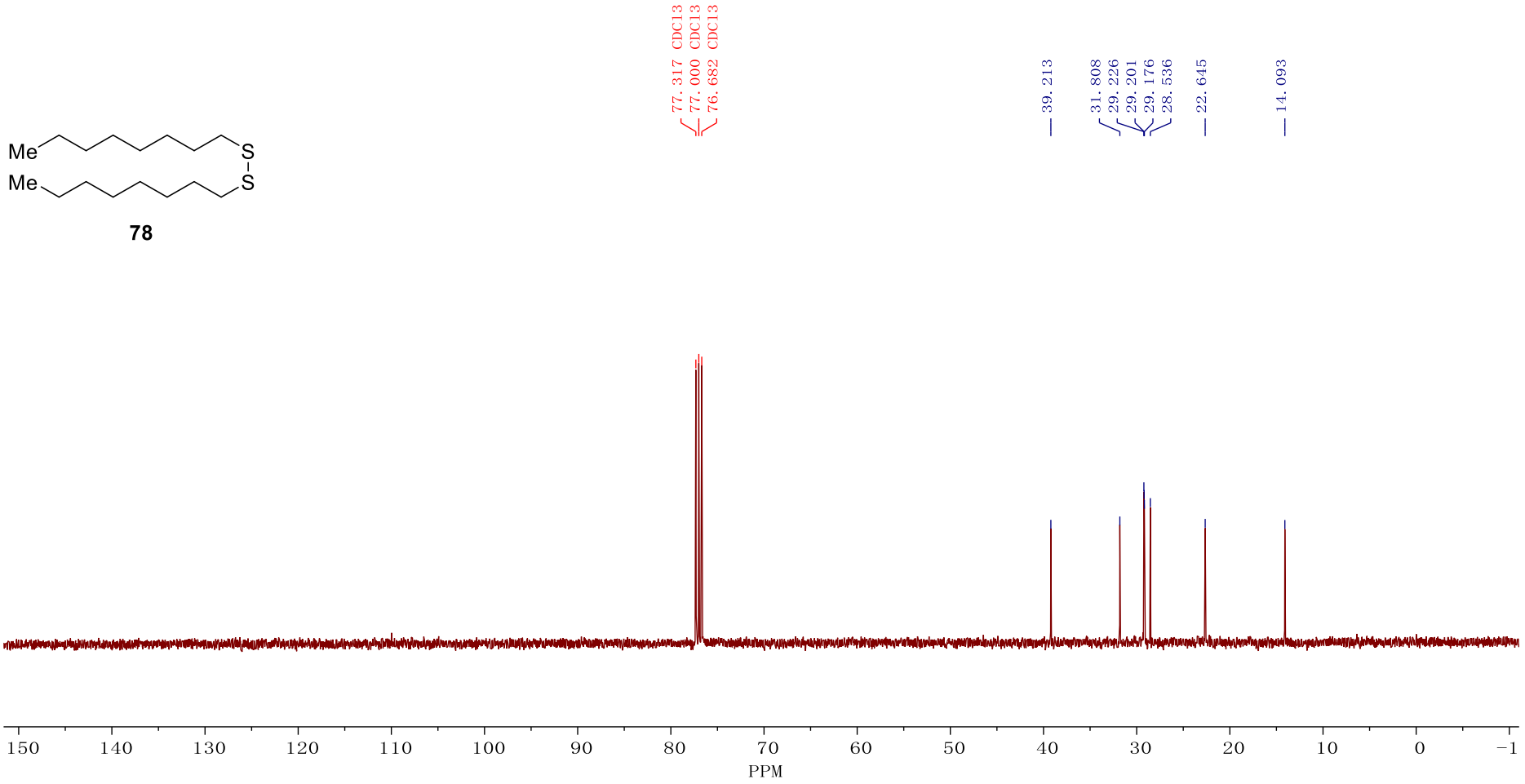
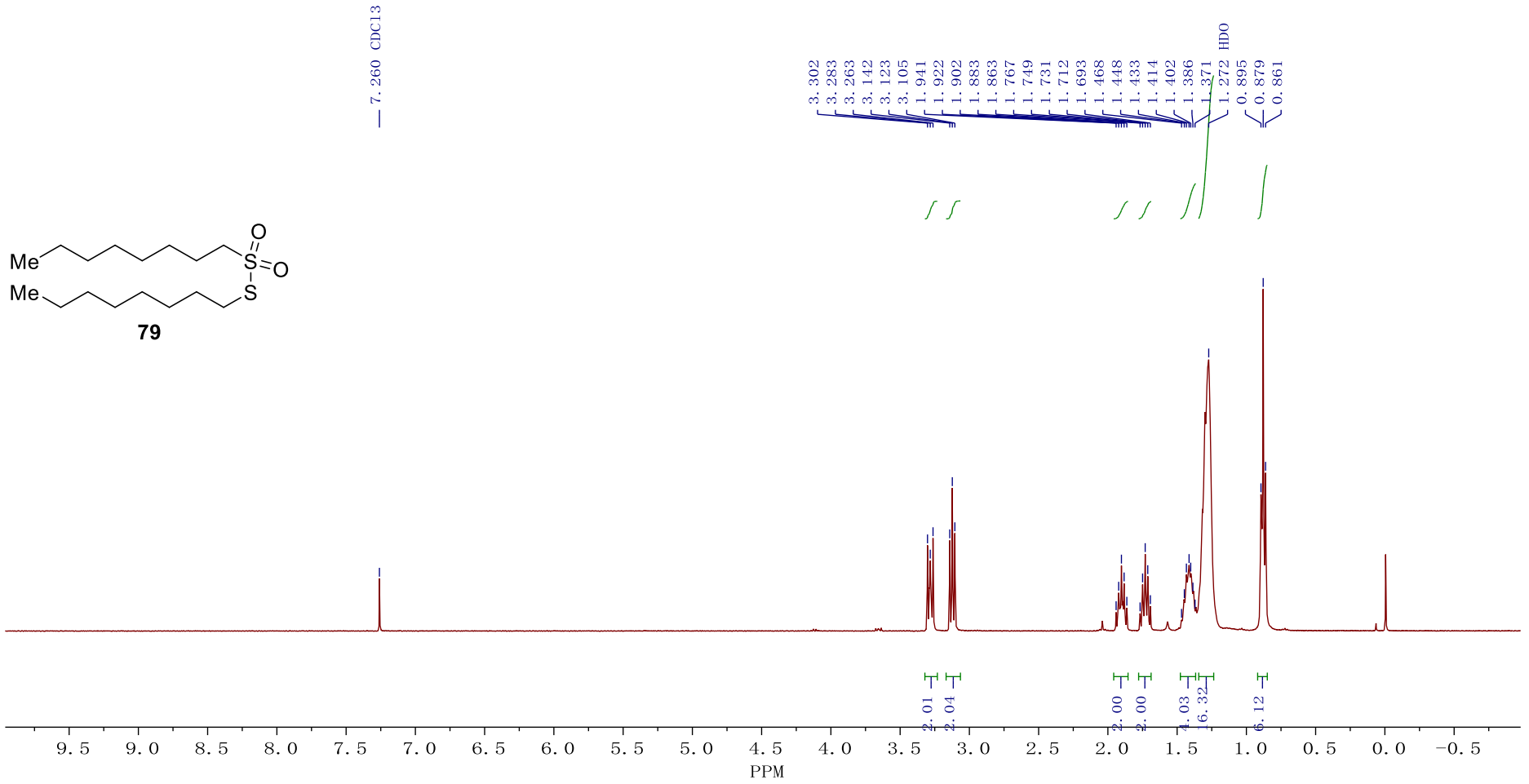
1.688
1.669
1.651
1.632
1.377
1.276
0.898
0.882
0.864
Me
S
Me
S
78
4.00
3.97
3.96
15.91
5.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
PPM


Me
S
Me
S
78
77.317 CDCl3
77.000 CDCl3
76.682 CDCl3
39.213
31.808
29.226
29.201
29.176
28.536
22.645
14.093
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
PPM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3.302
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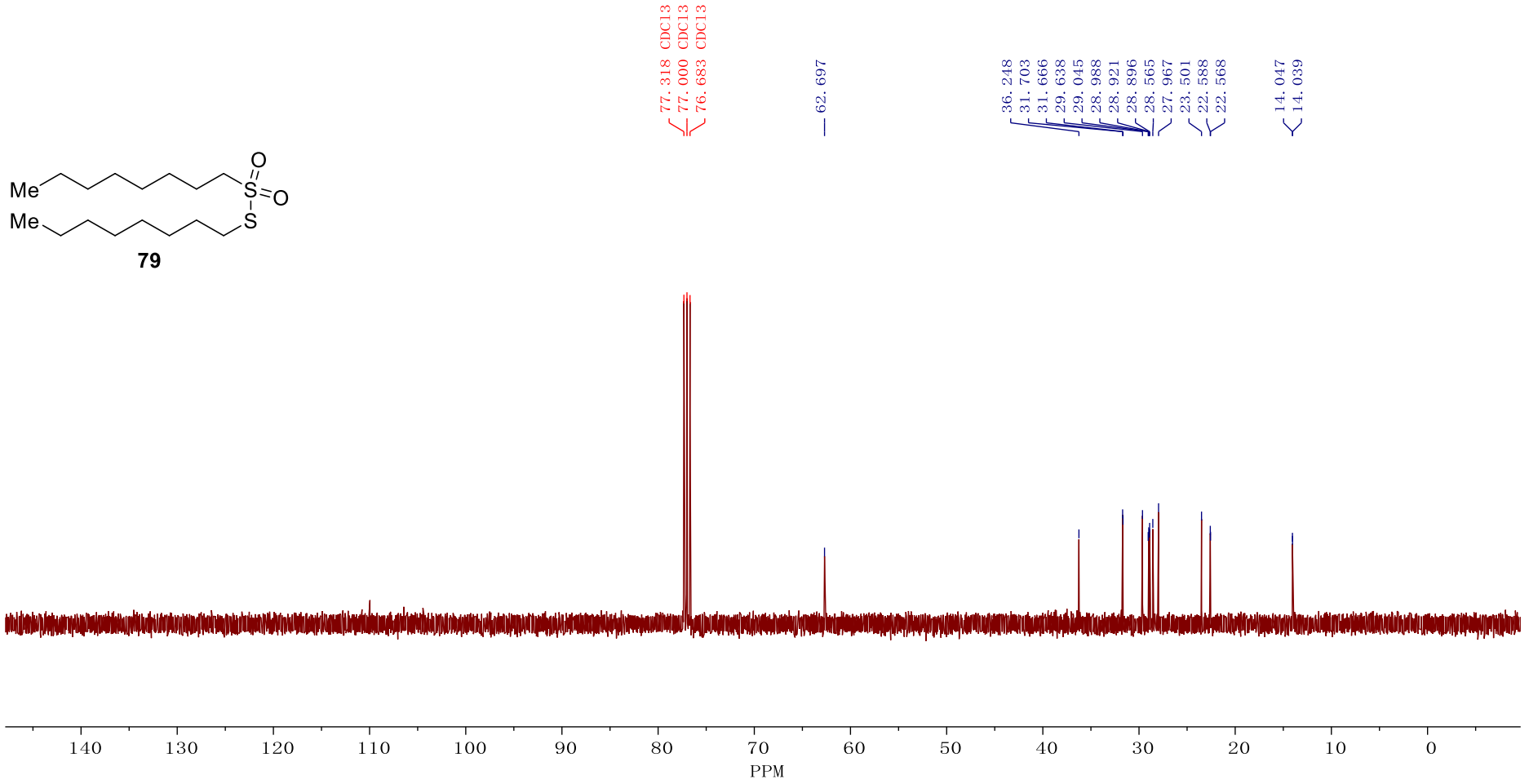
3.142
3.123
3.105
1.941
1.922
1.902
1.883
1.863
1.767
1.749
1.731
1.712
1.693
1.468
1.448
1.433
1.414
1.402
1.386
1.371
HDO
1.272
0.895
0.879
0.861
Me
Me
O
O
S
S
79
2.01
2.04
2.00
2.00
4.03
16.32
6.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
PPM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77.000 CDC13
76.683 CDC13
62.697
36.248
31.703
31.666
29.638
29.045
28.988
28.921
28.896
28.565
27.967
23.501
22.588
22.568
14.047
14.039
Me
Me
O
O
S
S
79
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM