Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Palladium-Catalyzed C(carbonyl)-C Bond Cleavage of Amides: A Facile Access to Phenylcarbamate Derivatives with Alcohols

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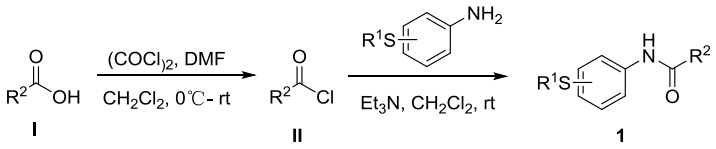
I. General remarks

NMR spectra were obtained on an Agilent 400-MR DD2 or a Bruker AV II-400 spectrometer. The ^{1}H NMR (400 MHz) chemical shifts were measured relative to $CDCl_3$ or DMSO-d_6 as the internal reference ($CDCl_3$: δ = 7.26 ppm, DMSO-d_6 : δ = 2.50 ppm). The ^{13}C NMR (100 MHz) chemical shifts were given using $CDCl_3$ or DMSO-d_6 as the internal standard ($CDCl_3$: δ = 77.16 ppm, DMSO-d_6 : δ = 39.52 ppm). High resolution mass spectra (HR-MS) were obtained with a Shimadzu LCMS-IT-TOF (ESI). Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Phenylamide derivatives were prepared according to the literature procedures.[1,2] Toluene, dichloroethane (DCE), acetonitrile (MeCN) and *N*,*N*-Dimethylformamide (DMF) were dried before used.

II. General procedures

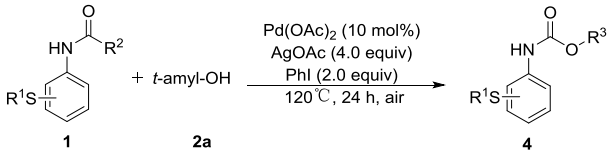
2.1 Synthesis of amides



Oxalyl chloride (1.75 mL, 20.0 mmol) was added slowly to a stirred solution of the carboxylic acid **I** (10.0 mmol) and DMF (0.1 mL) in CH_2Cl_2 (20 mL) at 0 ºC. The mixture was stirred at 0 ºC for 1 h and another 16 h at room temperature, and evaporated in vacuo to give the crude acid chloride **II**, which was used directly for the next step without further purification.

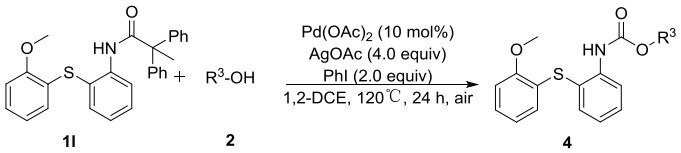
The acid chloride **II** was added dropwise to a solution of S-substitued aniline (8.0 mmol) and Et_3N (2.3 mL, 16.0 mmol) in CH_2Cl_2 (20 mL). The mixture was stirred overnight at room temperature, and then quenched with saturated $NaHCO_3$ (100 mL) solution. The mixture was extracted with CH_2Cl_2 (50 mL x 3). The combined organic layer was washed with saturated NaCl solution, dried over Na_2SO_4, filtrated and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to afford amide **1**.

2.2 Palladium-catalyzed C–C activation reaction



Procedure A:

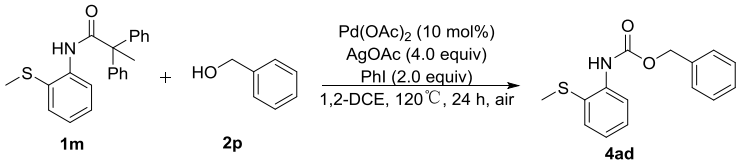
A Schlenk tube with a magnetic stir bar was charged with **1** (0.2 mmol), **2a** (1.0 mL), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol), AgOAc (133.0 mg, 0.8 mmol), iodobenzene (81.6 mg, 0.4 mmol). The Schlenk tube was then sealed with a Teflon lined cap and the mixture was heated at 120°C for 24 hours under air. The reaction solution was then cooled to ambient temperature, diluted with 5 mL of CH_2Cl_2, filtered through a celite pad and washed with 10-20 mL of CH_2Cl_2. The filtrate was collected and concentrated. The residue was purified by column chromatography on silica gel to provide the desired product **4.**



1l 2 4

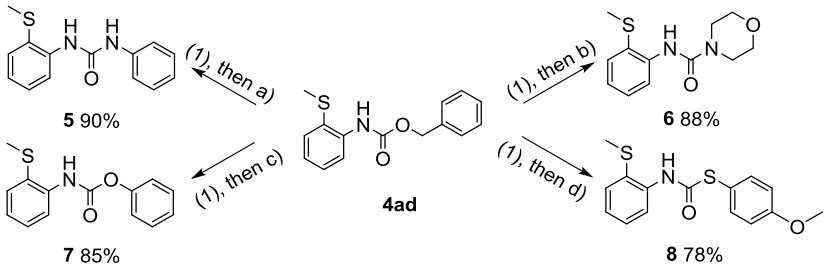
Procedure B:
A Schlenk tube with a magnetic stir bar was charged with **1l** (87.9 mg, 0.2 mmol), **2** (1.0 mmol), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol), AgOAc (133.0 mg, 0.8 mmol), iodobenzene (81.6 mg, 0.4 mmol) and 1,2-DCE (1.0 mL). The Schlenk tube was then sealed with a Teflon lined cap and the mixture was heated at 120°C for 24 hours under air. The reaction solution was then cooled to ambient temperature, diluted with 5 mL of CH_2Cl_2, filtered through a celite pad and washed with 10-20 mL of CH_2Cl_2. The filtrate was collected and concentrated. The residue was purified by column chromatography on silica gel to provide the desired product **4.**

III. Product transformations



1m 2p 4ad

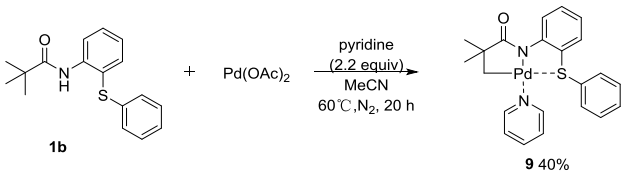
A Schlenk tube with a magnetic stir bar was charged with **1m** (70.0 mg, 0.2 mmol), **2p** (108.0 mg, 1.0 mmol), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol), AgOAc (133.0 mg, 0.8 mmol), iodobenzene (81.6 mg, 0.4 mmol) and 1,2-DCE (1.0 mL). The Schlenk tube was then sealed with a Teflon lined cap and the mixture was heated at 120°C for 24 hours under air. The reaction solution was then cooled to ambient temperature, diluted with 5 mL of CH_2Cl_2, filtered through a celite pad and washed with 10-20 mL of CH_2Cl_2. The filtrate was collected and concentrated. The residue was purified by column chromatography on silica gel to provide the desired product **4ad** as a white solid (62% yield).



A Schlenk tube with a magnetic stir bar was charged with **4ad** (55.0 mg, 0.2 mmol), 2-Cl pyridine (68.0 mg, 0.6 mmol), Tf_2O (50.0 μL, 0.3 mmol) and CH_2Cl_2 (1.0 mL). The Schlenk tube was then sealed with a Teflon lined cap and the mixture was stirred at room temperature for 1 hour under air. After that, nucleophiles (0.6 mmol) (for a=aniline, b=morpholine, c=phenol and d=*p*-OMe thiophenol) were added and the mixture was stirred for another 1 hour at r.t. under air. The reaction solution was then diluted with CH_2Cl_2, and filtered through a celite pad. The filtrate was collected and concentrated. The residue was purified by column chromatography on silica gel to provide the desired product **5, 6, 7** and **8.**

IV. Mechanistic studies

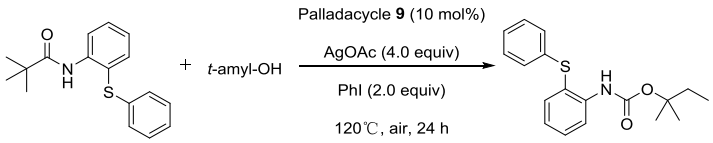
1. Preparation of Palladacycle **9**



1b 9 40%

A flame-dried Schlenk tube with a magnetic stirring bar was charged with **1b** (285.0 mg, 1.0 mmol), $Pd(OAc)_2$ (203.0 mg, 0.9 mmol) and pyridine (180.0 μL, 2.2 mmol). Then the Schlenk tube was evacuated and refilled with N_2 three times. Next, MeCN (3.0 mL) was added. The Schlenk tube was then sealed with a Teflon lined cap and the mixture was heated at 60 ℃ for 20 hours under N_2. After been cooled to room temperature, the mixture was filtered through a pad of celite, washed with 10-20 mL of CH_2Cl_2, and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography (petroleum ether/ethyl acetate = 1/1, v/v) on silica gel to afford the product **9** as a white solid in 40% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (d, *J* = 9.7 Hz, 1H), 8.40 – 8.31 (m, 2H), 7.78 (tt, *J* = 7.7, 1.6 Hz, 1H), 7.32 – 7.21 (m, 9H), 6.82 (t, *J* = 8.1 Hz, 1H), 1.93 (s, 2H), 1.29 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.69, 154.67, 151.86, 137.43, 135.86, 135.23, 130.79, 129.33, 128.96, 127.85, 125.30, 123.80, 121.43, 121.03, 49.58, 38.31, 30.30. HRMS (ESI$^+$): calcd for $C_{22}H_{23}N_2OPdS$ $[M+H]^+$ 469.0566, found 469.0570.

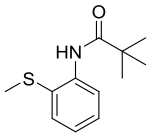
2. Catalytic C-C cleavage/C-O formation reaction with Palladacycle **9**



1b **2a** **4b** 40%

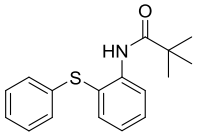
A Schlenk tube with a magnetic stir bar was charged with **1b** (57.0 mg, 0.2 mmol), **2a** (1.0 mL), palladacycle **9** (9.0 mg, 0.02 mmol), AgOAc (133.0 mg, 0.8 mmol) and iodobenzene (81.6 mg, 0.4 mmol). The Schlenk tube was then sealed with a Teflon lined cap and the mixture was heated at 120°C for 24 hours under air. The reaction solution was then cooled to ambient temperature, diluted with 5 mL of CH_2Cl_2, filtered through a celite pad and washed with 10-20 mL of CH_2Cl_2. The filtrate was collected and concentrated. The residue was purified by column chromatography on silica gel to provide the desired product **4b** as a white solid (40% yield).

V. Experimental data for the described substances



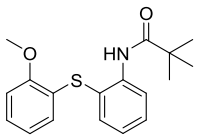
***N*-(2-(methylthio)phenyl)pivalamide (1a)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (s, 1H), 8.36 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.47 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.31 – 7.25 (m, 1H), 7.03 (td, *J* = 7.6, 1.4 Hz, 1H), 2.35 (s, 3H), 1.34 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.67, 138.72, 133.15, 129.08, 125.10, 124.01, 120.24, 40.18, 27.59, 18.88. HRMS (ESI$^+$): calcd for $C_{12}H_{17}NNaOS$ $[M+Na]^+$ 246.0929, found 246.0920.



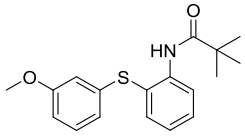
***N*-(2-(phenylthio)phenyl)pivalamide (1b)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.52 (d, *J* = 8.3 Hz, 1H), 7.61 (d, *J* = 9.2 Hz, 1H), 7.46 (t, *J* = 7.9 Hz, 1H), 7.25 – 7.18 (m, 2H), 7.16 – 7.09 (m, 2H), 7.03 (dt, *J* = 3.3, 1.9 Hz, 2H), 1.10 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.66, 140.13, 136.69, 135.48, 131.19, 129.26, 126.37, 126.04, 124.07, 120.54, 119.41, 40.01, 27.23. HRMS (ESI$^+$): calcd for $C_{17}H_{19}NNaOS$ $[M+Na]^+$ 308.1085, found 308.1080.



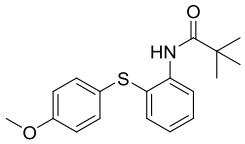
***N*-(2-((2-methoxyphenyl)thio)phenyl)pivalamide (1c)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (s, 1H), 8.49 (d, *J* = 8.3 Hz, 1H), 7.58 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.43 (t, *J* = 7.9 Hz, 1H), 7.16 – 7.02 (m, 2H), 6.84 (d, *J* = 8.2 Hz, 1H), 6.76 (t, *J* = 7.6 Hz, 1H), 6.62 (dd, *J* = 7.8, 1.3 Hz, 1H), 3.89 (s, 3H), 1.09 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.65, 155.88, 140.35, 136.81, 130.94, 127.22, 124.09, 123.76, 121.52, 120.44, 119.35, 110.58, 55.83, 39.99, 27.18. HRMS (ESI$^+$): calcd for $C_{18}H_{21}NNaO_2S$ $[M+Na]^+$ 338.1191, found 338.1187.



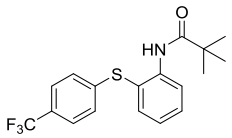
***N*-(2-((3-methoxyphenyl)thio)phenyl)pivalamide (1d)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.50 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.59 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.48 – 7.39 (m, 1H), 7.15 – 7.06 (m, 2H), 6.66 (ddd, *J* = 8.3, 2.4, 0.6 Hz, 1H), 6.60 (ddd, *J* = 7.8, 1.6, 0.8 Hz, 1H), 6.57 – 6.52 (m, 1H), 3.68 (s, 3H), 1.11 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.65, 160.21, 140.19, 136.79, 136.70, 131.26, 130.10, 124.07, 120.59, 119.30, 118.66, 111.91, 111.74, 55.21, 40.03, 27.25. HRMS (ESI$^+$): calcd for $C_{18}H_{21}NNaO_2S$ $[M+Na]^+$ 338.1191, found 338.1187.



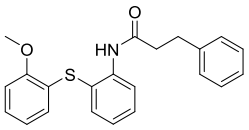
***N*-(2-((4-methoxyphenyl)thio)phenyl)pivalamide (1e)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H), 8.47 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.53 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.45 – 7.33 (m, 1H), 7.12 – 6.99 (m, 3H), 6.85 – 6.72 (m, 2H), 3.75 (s, 3H), 1.18 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.71, 158.75, 139.54, 135.76, 130.51, 129.45, 125.73, 124.06, 121.65, 120.62, 115.08, 55.40, 40.10, 27.41. HRMS (ESI$^+$): calcd for $C_{18}H_{21}NNaO_2S$ $[M+Na]^+$ 338.1191, found 338.1187.



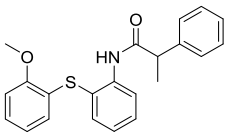
***N*-(2-((4-(trifluoromethyl)phenyl)thio)phenyl)pivalamide (1f)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.3 Hz, 1H), 8.47 (s, 1H), 7.60 (d, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 8.3 Hz, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.07 (d, *J* = 8.3 Hz, 2H), 1.08 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.62, 140.90 (d, *J* = 1.4 Hz), 140.32, 136.95, 131.95, 128.21, 127.88, 126.06 (q, *J* = 3.8 Hz), 125.79, 124.43, 120.91, 117.71, 40.01, 27.19.



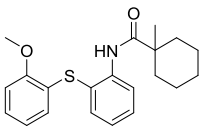
***N*-(2-((2-methoxyphenyl)thio)phenyl)-3-phenylpropanamide (1g)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.2 Hz, 1H), 8.41 (s, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.26 (dd, *J* = 11.1, 4.0 Hz, 2H), 7.17 (dd, *J* = 13.3, 4.4 Hz, 4H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.89 – 6.70 (m, 3H), 3.86 (s, 3H), 2.96 – 2.87 (m, 2H), 2.61 – 2.54 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.40, 156.18, 140.50, 140.21, 136.75, 130.84, 128.62, 128.53, 128.22, 127.75, 126.25, 124.36, 123.75, 121.62, 120.63, 119.67, 110.70, 55.89, 39.49, 31.22. HRMS (ESI$^+$): calcd for $C_{22}H_{21}NNaO_2S$ $[M+Na]^+$ 386.1191, found 386.1183.



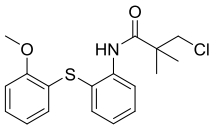
***N*-(2-((2-methoxyphenyl)thio)phenyl)-2-phenylpropanamide (1h)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.2 Hz, 1H), 8.36 (s, 1H), 7.49 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.45 – 7.38 (m, 1H), 7.23 – 7.08 (m, 6H), 7.05 (td, *J* = 7.6, 1.3 Hz, 1H), 6.83 (dd, *J* = 8.1, 0.8 Hz, 1H), 6.71 (td, *J* = 7.6, 1.1 Hz, 1H), 6.43 (dd, *J* = 7.8, 1.4 Hz, 1H), 3.87 (s, 3H), 3.62 (q, *J* = 7.2 Hz, 1H), 1.48 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.49, 155.61, 140.56, 140.10, 136.93, 130.98, 128.80, 127.46, 127.22, 127.00, 126.92, 124.35, 123.93, 121.39, 120.18, 118.90, 110.36, 55.68, 48.39, 17.86. HRMS (ESI$^+$): calcd for $C_{22}H_{21}NNaO_2S$ $[M+Na]^+$ 386.1191, found 386.1185.



***N*-(2-((2-methoxyphenyl)thio)phenyl)-1-methylcyclohexane-1-carboxamide (1i)**

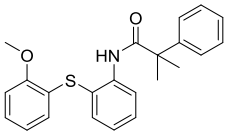
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 8.53 (d, *J* = 8.3 Hz, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.9 Hz, 1H), 7.09 (dt, *J* = 15.3, 4.5 Hz, 2H), 6.83 (d, *J* = 8.2 Hz, 1H), 6.74 (t, *J* = 7.6 Hz, 1H), 6.58 (d, *J* = 7.8 Hz, 1H), 3.88 (s, 3H), 1.87 – 1.75 (m, 2H), 1.40 (d, *J* = 7.5 Hz, 4H), 1.23 (d, *J* = 8.8 Hz, 4H), 1.00 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.07, 155.78, 140.49, 136.97, 131.03, 127.15, 127.07, 124.02, 123.91, 121.55, 120.41, 119.05, 110.50, 55.83, 44.10, 35.46, 25.70, 23.11, 22.77. HRMS (ESI$^+$): calcd for $C_{21}H_{25}NNaO_2S$ $[M+Na]^+$ 378.1504, found 378.1502.



3-chloro-*N*-(2-((2-methoxyphenyl)thio)phenyl)-2,2-dimethylpropanamide (1j)

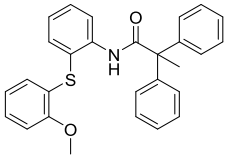
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (s, 1H), 8.48 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.59 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.48 – 7.39 (m, 1H), 7.18 – 7.06 (m, 2H), 6.86 (dd, *J* = 8.2, 0.9 Hz, 1H), 6.77 (td, *J* = 7.6, 1.1 Hz, 1H), 6.65 (dd, *J* = 7.8, 1.6 Hz, 1H), 3.90 (s, 3H), 3.54 (s, 2H), 1.18 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.99, 155.97, 139.79, 136.81, 130.91, 127.52, 127.41, 124.57, 123.65, 121.57, 120.63, 119.89, 110.63, 55.85, 52.43, 45.49, 23.07.

HRMS (ESI$^+$): calcd for $C_{18}H_{20}ClNNaO_2S$ $[M+Na]^+$ 372.0801, found 372.0800.



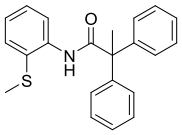
***N*-(2-((2-methoxyphenyl)thio)phenyl)-2-methyl-2-phenylpropanamide (1k)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (dd, *J* = 8.3, 1.1 Hz, 1H), 8.21 (s, 1H), 7.48 – 7.43 (m, 1H), 7.40 (dd, *J* = 8.0, 6.5 Hz, 1H), 7.21 – 7.16 (m, 2H), 7.16 – 7.07 (m, 4H), 7.04 (td, *J* = 7.6, 1.3 Hz, 1H), 6.80 (dd, *J* = 8.1, 0.8 Hz, 1H), 6.70 (td, *J* = 7.6, 1.1 Hz, 1H), 6.33 (dd, *J* = 7.8, 1.5 Hz, 1H), 3.84 (s, 3H), 1.50 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.65, 155.45, 143.89, 140.80, 136.99, 130.99, 128.51, 126.86, 126.70, 126.32, 126.07, 124.20, 124.18, 121.29, 120.04, 118.71, 110.26, 55.58, 48.12, 26.54. HRMS (ESI$^+$): calcd for $C_{23}H_{23}NNaO_2S$ $[M+Na]^+$ 400.1347, found 400.1341.



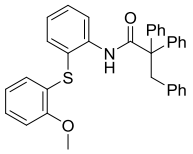
***N*-(2-((2-methoxyphenyl)thio)phenyl)-2,2-diphenylpropanamide (1l)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 8.3 Hz, 1H), 8.57 (s, 1H), 7.46 (dd, *J* = 13.3, 4.8 Hz, 2H), 7.19 – 7.05 (m, 12H), 6.77 (dd, *J* = 8.1, 0.8 Hz, 1H), 6.71 (td, *J* = 7.6, 1.1 Hz, 1H), 6.31 (dd, *J* = 7.8, 1.5 Hz, 1H), 3.82 (s, 3H), 1.97 (s, 3H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.64, 155.26, 144.19, 140.87, 137.21, 131.08, 128.36, 127.92, 126.81, 126.55, 126.00, 124.61, 124.43, 121.24, 120.11, 118.88, 110.18, 58.09, 55.49, 26.93. HRMS (ESI$^+$): calcd for $C_{28}H_{25}NNaO_2S$ $[M+Na]^+$ 462.1504, found 462.1500.



***N*-(2-(methylthio)phenyl)-2,2-diphenylpropanamide (1m)**

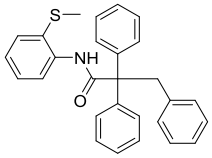
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.53 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.42 – 7.27 (m, 12H), 7.01 (td, *J* = 7.6, 1.3 Hz, 1H), 2.10 (s, 3H), 1.90 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.49, 144.68, 138.87, 133.91, 129.34, 128.69, 128.21, 127.15, 125.06, 124.23, 119.70, 58.29, 27.18, 19.00. HRMS (ESI$^+$): calcd for $C_{22}H_{21}NNaOS$ $[M+Na]^+$ 370.1242, found 370.1236.



***N*-(2-((2-methoxyphenyl)thio)phenyl)-2,2,3-triphenylpropanamide (1n)**

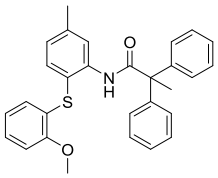
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 8.57 (d, *J* = 8.3 Hz, 1H), 7.53 – 7.37 (m, 2H), 7.13 – 7.01 (m, 13H), 6.97 (t, *J* = 7.4 Hz, 2H), 6.69 (dt, *J* = 23.1, 7.5 Hz, 4H), 6.28 (dd, *J* = 7.8, 1.3 Hz, 1H), 3.75 (s, 2H), 3.72 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.10, 155.48, 141.57, 141.02, 137.77, 137.37, 131.13, 131.07, 129.40, 127.93, 127.36, 126.90, 126.67, 126.49, 126.04, 124.62, 124.29, 121.38, 119.99,

118.85, 110.35, 64.27, 55.62, 44.34. HRMS (ESI$^+$): calcd for $C_{34}H_{29}NNaO_2S$ [M+Na]$^+$ 538.1817, found 538.1810.



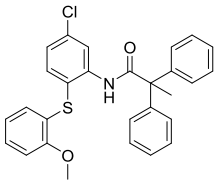
***N*-(2-(methylthio)phenyl)-2,2,3-triphenylpropanamide (1o)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 8.43 (d, *J* = 8.3 Hz, 1H), 7.40 (d, *J* = 9.2 Hz, 1H), 7.35 – 7.26 (m, 11H), 7.10 – 6.97 (m, 4H), 6.79 (d, *J* = 7.1 Hz, 2H), 3.85 (s, 2H), 1.90 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.14, 141.72, 139.00, 137.71, 133.89, 131.18, 129.59, 129.27, 128.16, 127.37, 127.18, 126.09, 125.03, 124.02, 119.72, 64.20, 44.48, 19.23. HRMS (ESI$^+$): calcd for $C_{28}H_{25}NNaOS$ [M+Na]$^+$ 446.1555, found 446.1548.



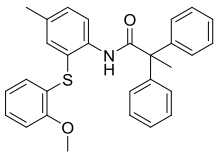
***N*-(2-((2-methoxyphenyl)thio)-5-methylphenyl)-2,2-diphenylpropanamide (1p)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 1.4 Hz, 2H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.15 (q, *J* = 3.7 Hz, 6H), 7.09 (ddd, *J* = 10.4, 6.6, 2.6 Hz, 5H), 6.92 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.76 (dd, *J* = 8.1, 0.9 Hz, 1H), 6.70 (td, *J* = 7.6, 1.1 Hz, 1H), 6.27 (dd, *J* = 7.8, 1.5 Hz, 1H), 3.83 (s, 3H), 2.41 (s, 3H), 1.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.73, 155.07, 144.16, 141.88, 140.68, 137.16, 128.35, 127.90, 126.79, 126.26, 125.56, 125.53, 124.85, 121.21, 120.67, 115.07, 110.05, 58.08, 55.48, 26.90, 21.82. HRMS (ESI$^+$): calcd for $C_{29}H_{27}NNaO_2S$ [M+Na]$^+$ 476.1660, found 476.1656.



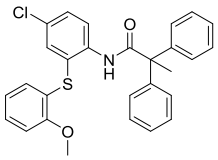
***N*-(5-chloro-2-((2-methoxyphenyl)thio)phenyl)-2,2-diphenylpropanamide (1q)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 2.3 Hz, 1H), 8.59 (s, 1H), 7.39 (d, *J* = 8.3 Hz, 1H), 7.20 – 7.15 (m, 6H), 7.14 – 7.08 (m, 5H), 7.06 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.80 – 6.68 (m, 2H), 6.32 (dd, *J* = 7.8, 1.5 Hz, 1H), 3.80 (s, 3H), 1.98 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.80, 155.37, 145.81, 143.91, 141.52, 137.86, 137.08, 128.44, 127.88, 126.94, 126.18, 124.62, 123.75, 121.26, 120.07, 117.23, 110.28, 58.14, 55.50, 26.91. HRMS (ESI$^+$): calcd for $C_{28}H_{24}ClNNaO_2S$ [M+Na]$^+$ 496.1114, found 496.1110.



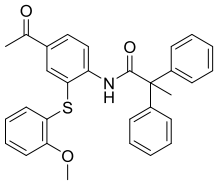
***N*-(2-((2-methoxyphenyl)thio)-4-methylphenyl)-2,2-diphenylpropanamide (1r)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.3 Hz, 1H), 8.47 (s, 1H), 7.28 (dd, *J* = 11.9, 3.5 Hz, 2H), 7.17 – 7.12 (m, 6H), 7.12 – 7.06 (m, 5H), 6.80 – 6.67 (m, 2H), 6.30 (dd, *J* = 7.8, 1.5 Hz, 1H), 3.82 (s, 3H), 2.27 (s, 3H), 1.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.48, 155.13, 144.27, 138.42, 137.53, 134.40, 131.77, 128.35, 127.92, 126.78, 126.40, 125.77, 124.59, 121.24, 120.00, 118.43, 110.11, 58.01, 55.50, 26.89, 20.62. HRMS (ESI$^+$): calcd for $C_{29}H_{27}NNaO_2S$ $[M+Na]^+$ 476.1660, found 476.1656.



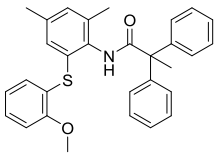
***N*-(4-chloro-2-((2-methoxyphenyl)thio)phenyl)-2,2-diphenylpropanamide (1s)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 8.9 Hz, 1H), 8.53 (s, 1H), 7.47 – 7.36 (m, 2H), 7.21 – 7.16 (m, 6H), 7.12 (dt, *J* = 5.6, 2.3 Hz, 5H), 6.82 – 6.70 (m, 2H), 6.41 (dd, *J* = 7.7, 1.5 Hz, 1H), 3.78 (s, 3H), 1.98 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.68, 155.61, 144.04, 139.17, 136.02, 130.74, 128.93, 128.45, 128.13, 128.01, 127.91, 127.35, 126.94, 123.23, 121.29, 121.10, 110.41, 58.10, 55.51, 26.92. HRMS (ESI$^+$): calcd for $C_{28}H_{24}ClNNaO_2S$ $[M+Na]^+$ 496.1114, found 496.1109.



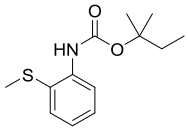
***N*-(4-acetyl-2-((2-methoxyphenyl)thio)phenyl)-2,2-diphenylpropanamide (1t)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (s, 1H), 8.78 (d, *J* = 8.7 Hz, 1H), 8.10 (d, *J* = 2.1 Hz, 1H), 8.05 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.22 – 7.16 (m, 6H), 7.15 – 7.08 (m, 5H), 6.81 – 6.75 (m, 1H), 6.72 (td, *J* = 7.6, 1.1 Hz, 1H), 6.31 (dd, *J* = 7.8, 1.5 Hz, 1H), 3.81 (s, 3H), 2.53 (s, 3H), 1.99 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.15, 174.05, 155.47, 144.72, 143.80, 137.67, 133.05, 131.43, 128.49, 127.87, 127.68, 127.13, 127.01, 126.37, 123.45, 121.27, 119.16, 110.37, 58.30, 55.52, 26.97, 26.40. HRMS (ESI$^+$): calcd for $C_{30}H_{27}NNaO_3S$ $[M+Na]^+$ 504.1609, found 504.1602.



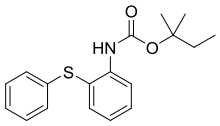
***N*-(2-((2-methoxyphenyl)thio)-4,6-dimethylphenyl)-2,2-diphenylpropanamide (1u)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (s, 1H), 7.26 – 7.14 (m, 11H), 7.06 (d, *J* = 10.0 Hz, 2H), 6.89 – 6.77 (m, 2H), 6.71 (dd, *J* = 7.7, 1.6 Hz, 1H), 3.83 (s, 3H), 2.24 (s, 3H), 2.20 (s, 3H), 1.93 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.05, 156.02, 144.69, 137.19, 136.32, 135.29, 133.42, 132.62, 128.38, 128.27, 127.81, 127.13, 126.71, 124.89, 121.54, 110.37, 109.99, 57.29, 55.67, 27.01, 20.74, 19.27. HRMS (ESI$^+$): calcd for $C_{30}H_{29}NNaO_2S$ $[M+Na]^+$ 490.1817, found 490.1811.



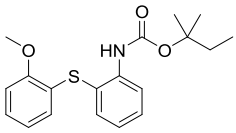
***tert*-pentyl (2-(methylthio)phenyl)carbamate (4a)**

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4a** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.2 Hz, 1H), 7.58 (s, 1H), 7.45 (d, *J* = 9.2 Hz, 1H), 7.26 (t, *J* = 7.8 Hz, 1H), 6.98 (t, *J* = 6.9 Hz, 1H), 2.36 (s, 3H), 1.86 (q, *J* = 7.5 Hz, 2H), 1.50 (s, 6H), 0.94 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.71, 138.98, 133.15, 128.89, 124.21, 123.02, 118.92, 83.06, 33.53, 25.82, 18.92, 8.31. HRMS (ESI^+): calcd for $C_{13}H_{19}NNaO_2S$ $[M+Na]^+$ 276.1034, found 276.1030.



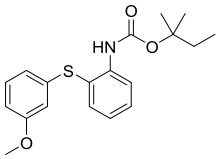
***tert*-pentyl (2-(phenylthio)phenyl)carbamate (4b)**

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4b** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.3 Hz, 1H), 7.53 (d, *J* = 9.3 Hz, 2H), 7.39 (t, *J* = 7.9 Hz, 1H), 7.26 – 7.19 (m, 2H), 7.13 (dd, *J* = 8.4, 6.3 Hz, 1H), 7.08 (d, *J* = 7.2 Hz, 2H), 7.02 (t, *J* = 8.2 Hz, 1H), 1.76 (q, *J* = 7.5 Hz, 2H), 1.40 (s, 6H), 0.82 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.50, 140.59, 136.55, 136.10, 130.82, 129.14, 127.30, 126.06, 123.14, 119.27, 109.99, 83.11, 33.50, 25.68, 8.18. HRMS (ESI^+): calcd for $C_{18}H_{21}NNaO_2S$ $[M+Na]^+$ 338.1191, found 338.1183.



***tert*-pentyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4c)**

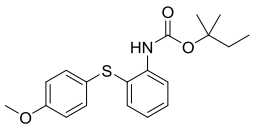
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4c** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.2 Hz, 1H), 7.81 (s, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.15 (s, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.78 (s, 2H), 3.92 (s, 3H), 1.79 (q, *J* = 7.4 Hz, 2H), 1.42 (s, 6H), 0.84 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.31, 152.65, 141.15, 136.96, 130.74, 128.96, 127.58, 124.23, 123.05, 121.47, 119.00, 118.90, 110.53, 83.03, 55.86, 33.40, 25.79, 8.26. HRMS (ESI^+): calcd for $C_{19}H_{23}NNaO_3S$ $[M+Na]^+$ 368.1296, found 368.1290.



***tert*-pentyl (2-((3-methoxyphenyl)thio)phenyl)carbamate (4d)**

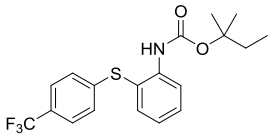
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4d** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.3 Hz, 1H), 7.53 (dd, *J* = 7.6, 1.5 Hz, 2H), 7.39 (t, *J* = 7.9 Hz, 1H), 7.13 (t, *J* = 8.0 Hz, 1H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.66 (t, *J* = 8.2 Hz, 2H), 6.61 (s, 1H), 3.70 (s, 3H), 1.77 (q, *J* = 7.5 Hz, 2H), 1.41 (s, 6H), 0.83 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.09, 152.49,

140.66, 137.43, 136.63, 130.91, 129.96, 123.14, 119.48, 119.33, 119.02, 112.64, 111.80, 83.11, 55.16, 33.50, 25.68, 8.18. HRMS (ESI$^+$): calcd for $C_{19}H_{23}NNaO_3S$ $[M+Na]^+$ 368.1296, found 368.1290.



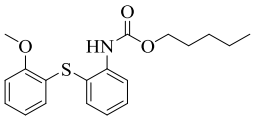
***tert*-pentyl (2-((4-methoxyphenyl)thio)phenyl)carbamate (4e)**

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4e** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.2 Hz, 1H), 7.53 (s, 1H), 7.45 (d, *J* = 9.3 Hz, 1H), 7.34 – 7.30 (m, 1H), 7.15 (d, *J* = 8.9 Hz, 2H), 6.98 (t, *J* = 8.2 Hz, 1H), 6.80 (d, *J* = 8.9 Hz, 2H), 3.75 (s, 3H), 1.79 (q, *J* = 7.5 Hz, 2H), 1.44 (s, 6H), 0.87 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.96, 152.60, 139.66, 135.21, 130.99, 130.00, 125.96, 123.14, 122.02, 119.45, 114.99, 83.05, 55.36, 33.61, 25.76, 8.25. HRMS (ESI$^+$): calcd for $C_{19}H_{23}NNaO_3S$ $[M+Na]^+$ 368.1296, found 368.1290.



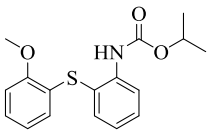
***tert*-pentyl (2-((4-(trifluoromethyl)phenyl)thio)phenyl)carbamate (4f)**

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4f** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.3 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.51 – 7.38 (m, 4H), 7.09 (dd, *J* = 13.8, 7.7 Hz, 3H), 1.75 (q, *J* = 7.5 Hz, 2H), 1.40 (s, 6H), 0.80 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.37, 141.53, 140.88, 136.95, 131.63, 128.07, 127.75, 126.23, 125.91 (q, *J* = 3.8 Hz), 123.49, 119.75, 117.34, 83.40, 33.40, 25.64, 8.08. HRMS (ESI$^+$): calcd for $C_{19}H_{20}F_3NNaO_2S$ $[M+Na]^+$ 406.1065, found 406.1063.



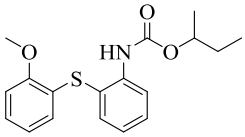
pentyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4g)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4g** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.3 Hz, 1H), 8.01 (s, 1H), 7.56 (d, *J* = 8.9 Hz, 1H), 7.39 (t, *J* = 8.4 Hz, 1H), 7.16 (t, *J* = 8.6 Hz, 1H), 7.02 (t, *J* = 8.1 Hz, 1H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.84 – 6.77 (m, 2H), 4.10 (t, *J* = 6.8 Hz, 2H), 3.92 (s, 3H), 1.62 (dd, *J* = 14.0, 7.0 Hz, 2H), 1.37 – 1.27 (m, 4H), 0.89 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.45, 153.59, 140.82, 136.96, 130.82, 129.36, 127.81, 124.00, 123.28, 121.48, 119.26, 118.85, 110.59, 65.38, 55.83, 28.56, 27.91, 22.31, 13.94. HRMS (ESI$^+$): calcd for $C_{19}H_{23}NNaO_3S$ $[M+Na]^+$ 368.1296, found 368.1290.



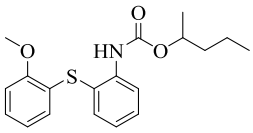
isopropyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4h)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4h** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.3 Hz, 1H), 8.01 (s, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 1H), 7.22 – 7.12 (m, 1H), 7.03 (t, *J* = 8.2 Hz, 1H), 6.90 – 6.83 (m, 2H), 6.83 – 6.78 (m, 1H), 5.04 – 4.92 (m, 1H), 3.94 (s, 3H), 1.27 (d, *J* = 6.3 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.49, 153.12, 140.95, 136.95, 130.80, 129.57, 127.85, 124.05, 123.19, 121.48, 119.27, 118.81, 110.57, 68.69, 55.84, 22.04. HRMS (ESI^+): calcd for $C_{17}H_{19}NNaO_3S$ $[M+Na]^+$ 340.0983, found 340.0980.



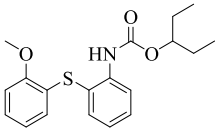
***sec*-butyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4i)**

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4i** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.3 Hz, 1H), 7.98 (s, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.39 (t, *J* = 8.6 Hz, 1H), 7.19 – 7.12 (m, 1H), 7.01 (t, *J* = 8.2 Hz, 1H), 6.82 (dt, *J* = 14.8, 8.0 Hz, 3H), 4.92 – 4.67 (m, 1H), 3.92 (s, 3H), 1.62 – 1.51 (m, 2H), 1.22 (d, *J* = 6.3 Hz, 3H), 0.88 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.48, 153.33, 140.94, 136.92, 130.78, 129.50, 127.84, 124.00, 123.19, 121.48, 119.30, 118.88, 110.58, 73.28, 55.83, 28.97, 19.67, 9.69. HRMS (ESI^+): calcd for $C_{18}H_{21}NNaO_3S$ $[M+Na]^+$ 354.1140, found 354.1134.



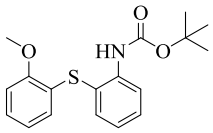
pentan-2-yl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4j)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4j** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.3 Hz, 1H), 7.98 (s, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 1H), 7.17 (t, *J* = 8.5 Hz, 1H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.91 – 6.76 (m, 3H), 4.93 – 4.83 (m, 1H), 3.93 (s, 3H), 1.55 – 1.28 (m, 4H), 1.23 (d, *J* = 6.3 Hz, 3H), 0.90 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.46, 153.32, 140.94, 136.92, 130.79, 129.45, 127.81, 124.00, 123.19, 121.48, 119.27, 118.89, 110.57, 71.86, 55.83, 38.24, 20.21, 18.61, 13.90. HRMS (ESI^+): calcd for $C_{19}H_{23}NNaO_3S$ $[M+Na]^+$ 368.1296, found 368.1290.



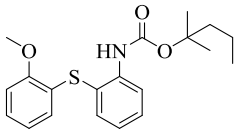
pentan-3-yl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4k)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4k** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.3 Hz, 1H), 7.97 (s, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 7.15 (t, *J* = 8.4 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 6.82 (dt, *J* = 14.8, 7.9 Hz, 3H), 4.73 – 4.64 (m, 1H), 3.92 (s, 3H), 1.56 (dd, *J* = 14.2, 7.4 Hz, 4H), 0.86 (t, *J* = 7.4 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.45, 153.65, 140.94, 136.89, 130.78, 129.39, 127.81, 123.94, 123.19, 121.48, 119.30, 118.95, 110.58, 77.82, 55.82, 26.65, 9.58. HRMS (ESI^+): calcd for $C_{19}H_{23}NNaO_3S$ $[M+Na]^+$ 368.1296, found 368.1290.



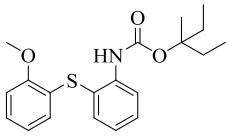
***tert*-butyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4l)**

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4l** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.3 Hz, 1H), 7.85 (s, 1H), 7.56 (d, *J* = 9.1 Hz, 1H), 7.39 (t, *J* = 8.5 Hz, 1H), 7.17 (t, *J* = 8.6 Hz, 1H), 7.01 (t, *J* = 8.1 Hz, 1H), 6.87 (d, *J* = 8.1 Hz, 1H), 6.80 (d, *J* = 3.3 Hz, 2H), 3.94 (s, 3H), 1.48 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.34, 152.70, 141.20, 137.00, 130.76, 129.07, 127.61, 124.31, 123.06, 121.48, 118.92, 118.89, 110.53, 80.55, 55.87, 28.28. HRMS (ESI$^+$): calcd for $C_{18}H_{21}NNaO_3S$ $[M+Na]^+$ 354.1140, found 354.1133.



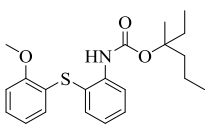
2-methylpentan-2-yl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4m)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4m** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.2 Hz, 1H), 7.78 (s, 1H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.37 (t, *J* = 7.1 Hz, 1H), 7.19 – 7.12 (m, 1H), 7.00 (t, *J* = 8.2 Hz, 1H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.81 – 6.76 (m, 2H), 3.92 (s, 3H), 1.73 (t, *J* = 7.3 Hz, 2H), 1.43 (s, 6H), 1.31 – 1.24 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.36, 152.63, 141.13, 136.91, 130.70, 129.01, 127.57, 124.25, 123.03, 121.47, 119.05, 118.99, 110.57, 82.80, 55.86, 43.07, 26.29, 17.16, 14.39. HRMS (ESI$^+$): calcd for $C_{20}H_{25}NNaO_3S$ $[M+Na]^+$ 382.1453, found 382.1446.



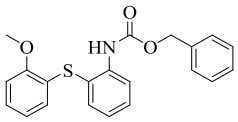
3-methylpentan-3-yl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4n)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4n** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.3 Hz, 1H), 7.80 (s, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.14 (dd, *J* = 8.4, 4.3 Hz, 1H), 7.00 (t, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 8.2 Hz, 1H), 6.79 (d, *J* = 4.3 Hz, 2H), 3.92 (s, 3H), 1.88 (dd, *J* = 14.2, 7.4 Hz, 2H), 1.74 (dd, *J* = 14.2, 7.4 Hz, 2H), 1.36 (s, 3H), 0.82 (t, *J* = 7.5 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.36, 152.54, 141.10, 136.89, 130.70, 129.00, 127.60, 124.15, 123.04, 121.48, 119.07, 119.04, 110.57, 85.62, 55.85, 30.58, 22.98, 7.96. HRMS (ESI$^+$): calcd for $C_{20}H_{25}NNaO_3S$ $[M+Na]^+$ 382.1453, found 382.1446.



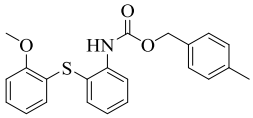
3-methylhexan-3-yl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4o)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4o** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.3 Hz, 1H), 7.79 (s, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.19 – 7.13 (m, 1H), 7.01 (t, *J* = 8.2 Hz, 1H), 6.86 (d, *J* = 8.2 Hz, 1H), 6.80 (d, *J* = 4.2 Hz, 2H), 3.93 (s, 3H), 1.92 – 1.70 (m, 4H), 1.38 (s, 3H), 1.26 (dd, *J* = 16.1, 7.9 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H), 0.83 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.36, 152.54, 141.10, 136.88, 130.68, 130.03, 128.98, 127.58, 124.16, 123.03, 121.47, 119.11, 110.59, 85.39, 55.85, 40.35, 31.11, 23.48, 16.87, 14.46, 8.00. HRMS (ESI$^+$): calcd for $C_{21}H_{27}NNaO_3S$ $[M+Na]^+$ 396.1609, found 396.1604.



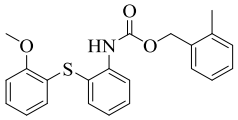
benzyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4p)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4p** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.3 Hz, 1H), 8.15 (s, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 7.9 Hz, 1H), 7.38 – 7.32 (m, 5H), 7.16 (t, *J* = 6.6 Hz, 1H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.81 (dd, *J* = 10.6, 7.8 Hz, 3H), 5.16 (s, 2H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.54, 153.29, 140.66, 137.03, 136.04, 130.90, 129.66, 128.59, 128.42, 128.34, 127.99, 123.84, 123.52, 121.51, 119.61, 118.92, 110.62, 67.00, 55.81. HRMS (ESI$^+$): calcd for $C_{21}H_{19}NNaO_3S$ $[M+Na]^+$ 388.0983, found 388.0977.



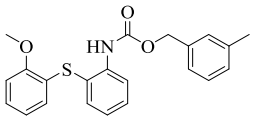
4-methylbenzyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4q)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4q** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.2 Hz, 1H), 8.13 (s, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 1H), 7.25 (d, *J* = 7.3 Hz, 2H), 7.16 (d, *J* = 7.2 Hz, 3H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.80 (dd, *J* = 16.9, 10.2 Hz, 3H), 5.12 (s, 2H), 3.83 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.43, 153.30, 140.69, 138.17, 137.02, 132.93, 130.87, 129.46, 129.23, 128.49, 127.87, 123.84, 123.42, 121.44, 119.40, 118.83, 110.54, 66.94, 55.78, 21.23. HRMS (ESI$^+$): calcd for $C_{22}H_{21}NNaO_3S$ $[M+Na]^+$ 402.1140, found 402.1135.



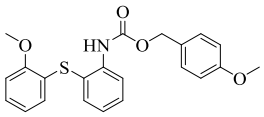
2-methylbenzyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4r)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4r** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.2 Hz, 1H), 8.11 (s, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 8.6 Hz, 1H), 7.30 (d, *J* = 7.0 Hz, 1H), 7.24 (t, *J* = 7.4 Hz, 1H), 7.16 (dd, *J* = 16.6, 8.1 Hz, 3H), 7.04 (t, *J* = 8.2 Hz, 1H), 6.80 (t, *J* = 8.8 Hz, 3H), 5.17 (s, 2H), 3.80 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.43, 153.26, 140.61, 137.07, 136.98, 133.86, 130.87, 130.36, 129.46, 129.34, 128.61, 127.90, 126.02, 123.72, 123.47, 121.44, 119.51, 118.87, 110.54, 65.39, 55.71, 18.90. HRMS (ESI$^+$): calcd for $C_{22}H_{21}NNaO_3S$ $[M+Na]^+$ 402.1140, found 402.1135.



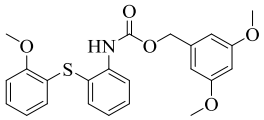
3-methylbenzyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4s)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4s** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.3 Hz, 1H), 8.14 (s, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 7.1 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.15 (dd, *J* = 12.6, 6.0 Hz, 4H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.85 – 6.76 (m, 3H), 5.13 (s, 2H), 3.84 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.43, 153.27, 140.68, 138.26, 137.02, 135.85, 130.87, 129.44, 129.06, 129.05, 128.46, 127.87, 125.38, 123.84, 123.45, 121.45, 119.39, 118.83, 110.54, 67.03, 55.77, 21.37. HRMS (ESI$^+$): calcd for $C_{22}H_{21}NNaO_3S$ $[M+Na]^+$ 402.1140, found 402.1135.



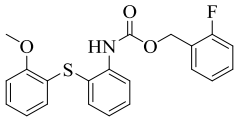
4-methoxybenzyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4t)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4t** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.2 Hz, 1H), 8.11 (s, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 8.7 Hz, 2H), 7.19 – 7.12 (m, 1H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.84 – 6.76 (m, 3H), 5.09 (s, 2H), 3.83 (s, 3H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.65, 156.45, 153.33, 140.70, 137.00, 130.84, 130.20, 129.52, 128.06, 127.88, 123.84, 123.40, 121.44, 118.82, 113.90, 110.54, 109.99, 66.80, 55.76, 55.29. HRMS (ESI$^+$): calcd for $C_{22}H_{21}NNaO_4S$ $[M+Na]^+$ 418.1089, found 418.1080.



3,5-dimethoxybenzyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4u)

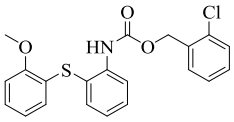
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4u** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.2 Hz, 1H), 8.15 (s, 1H), 7.57 (d, *J* = 8.9 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 1H), 7.18 – 7.12 (m, 1H), 7.04 (t, *J* = 7.8 Hz, 1H), 6.81 (dd, *J* = 14.0, 6.9 Hz, 3H), 6.50 (s, 2H), 6.41 (s, 1H), 5.09 (s, 2H), 3.85 (s, 3H), 3.77 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.87, 156.43, 153.16, 140.60, 138.21, 137.02, 130.86, 129.42, 127.90, 123.82, 123.52, 121.44, 119.47, 118.86, 110.56, 105.93, 100.23, 66.89, 55.79, 55.37. HRMS (ESI$^+$): calcd for $C_{23}H_{23}NNaO_5S$ $[M+Na]^+$ 448.1195, found 448.1188.



2-fluorobenzyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4v)

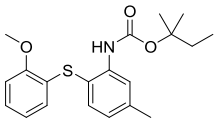
Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4v** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.17 (m, 2H), 7.60 (d, *J* = 9.2 Hz, 1H), 7.40 (q, *J* = 7.4 Hz, 2H), 7.33 (dd, *J* = 15.4, 7.4 Hz, 1H), 7.20 – 7.02 (m, 4H), 6.90 – 6.77 (m, 3H), 5.25 (s, 2H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.22, 159.75, 156.57, 153.07, 140.52, 136.97, 130.83 (d, *J* = 2.2 Hz), 130.78, 130.30 (d,

J = 8.2 Hz), 130.01, 128.11, 124.16 (d, *J* = 3.8 Hz), 123.57 (d, *J* = 14.0 Hz), 123.19 (d, *J* = 14.6 Hz), 121.46, 119.77, 118.83, 115.45 (d, *J* = 21.1 Hz), 110.57, 60.73 (d, *J* = 4.3 Hz), 55.74. HRMS (ESI$^+$): calcd for $C_{21}H_{18}FNNaO_3S$ $[M+Na]^+$ 406.0889, found 406.0882.



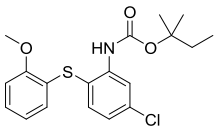
2-chlorobenzyl (2-((2-methoxyphenyl)thio)phenyl)carbamate (4w)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4w** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.17 (m, 2H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.40 (dd, *J* = 14.9, 7.5 Hz, 3H), 7.28 – 7.24 (m, 2H), 7.20 – 7.15 (m, 1H), 7.05 (t, *J* = 8.2 Hz, 1H), 6.83 (ddd, *J* = 19.4, 12.9, 6.9 Hz, 3H), 5.29 (s, 2H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.56, 153.02, 140.47, 136.96, 133.75, 133.60, 130.86, 129.91, 129.84, 129.52, 128.09, 126.89, 123.64, 123.56, 121.48, 119.79, 118.92, 117.55, 110.60, 64.15, 55.79. HRMS (ESI$^+$): calcd for $C_{21}H_{18}ClNNaO_3S$ $[M+Na]^+$ 422.0594, found 422.0588.



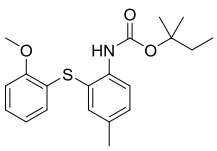
tert-pentyl (2-((2-methoxyphenyl)thio)-5-methylphenyl)carbamate (4x)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4x** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.80 (s, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.14 (ddd, *J* = 8.2, 7.3, 1.8 Hz, 1H), 6.88 – 6.83 (m, 2H), 6.79 (td, *J* = 7.5, 1.1 Hz, 1H), 6.74 (dd, *J* = 7.8, 1.8 Hz, 1H), 3.94 (s, 3H), 2.37 (s, 3H), 1.80 (q, *J* = 7.5 Hz, 2H), 1.43 (s, 6H), 0.85 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.12, 152.71, 141.46, 141.00, 136.97, 128.41, 127.25, 124.78, 124.06, 121.45, 119.45, 115.15, 110.44, 82.98, 55.85, 33.39, 25.81, 21.79, 8.25. HRMS (ESI$^+$): calcd for $C_{20}H_{25}NNaO_3S$ $[M+Na]^+$ 382.1453, found 382.1450.



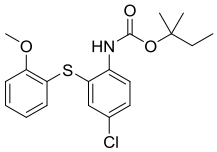
tert-pentyl (5-chloro-2-((2-methoxyphenyl)thio)phenyl)carbamate (4y)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4y** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 1.7 Hz, 1H), 7.89 (s, 1H), 7.48 (d, *J* = 8.3 Hz, 1H), 7.20 (ddd, *J* = 8.2, 6.9, 2.2 Hz, 2H), 6.98 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.87 (dd, *J* = 5.8, 2.5 Hz, 1H), 6.85 (dd, *J* = 2.8, 1.6 Hz, 1H), 3.93 (s, 3H), 1.82 (q, *J* = 7.5 Hz, 2H), 1.45 (s, 6H), 0.87 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.58, 152.30, 141.97, 137.62, 136.76, 129.62, 128.14, 123.53, 123.02, 121.52, 118.82, 117.45, 110.68, 83.57, 55.87, 33.35, 25.76, 8.26. HRMS (ESI$^+$): calcd for $C_{19}H_{22}ClNNaO_3S$ $[M+Na]^+$ 402.0907, found 402.0900.



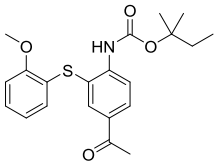
tert-pentyl (2-((2-methoxyphenyl)thio)-4-methylphenyl)carbamate (4z)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4z** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.4 Hz, 1H), 7.70 (s, 1H), 7.38 (d, *J* = 1.7 Hz, 1H), 7.22 – 7.13 (m, 2H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.83 – 6.75 (m, 2H), 3.94 (s, 3H), 2.28 (s, 3H), 1.79 (q, *J* = 7.5 Hz, 2H), 1.42 (s, 6H), 0.85 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.19, 152.76, 138.65, 137.22, 132.66, 131.46, 128.71, 127.39, 124.48, 121.47, 119.03, 118.53, 110.48, 82.83, 55.86, 33.43, 25.80, 20.48, 8.26. HRMS (ESI^+): calcd for $C_{20}H_{25}NNaO_3S$ $[M+Na]^+$ 382.1453, found 382.1448.



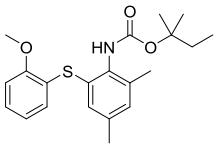
tert-pentyl (4-chloro-2-((2-methoxyphenyl)thio)phenyl)carbamate (4aa)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4aa** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.9 Hz, 1H), 7.82 (s, 1H), 7.53 (d, *J* = 2.5 Hz, 1H), 7.32 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.22 (ddd, *J* = 8.3, 7.5, 1.7 Hz, 1H), 6.95 (dd, *J* = 7.7, 1.7 Hz, 1H), 6.90 – 6.83 (m, 2H), 3.92 (s, 3H), 1.81 (q, *J* = 7.5 Hz, 2H), 1.44 (s, 6H), 0.87 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.83, 152.50, 139.51, 135.65, 130.42, 130.36, 128.56, 128.48, 127.28, 122.93, 121.58, 120.01, 110.80, 83.35, 55.87, 33.41, 25.77, 8.27. HRMS (ESI^+): calcd for $C_{19}H_{22}ClNNaO_3S$ $[M+Na]^+$ 402.0907, found 402.0901.



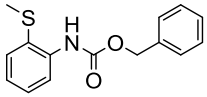
tert-pentyl (4-acetyl-2-((2-methoxyphenyl)thio)phenyl)carbamate (4ab)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 10/1, v/v) afforded **4ab** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.8 Hz, 1H), 8.22 (d, *J* = 2.1 Hz, 1H), 8.18 (s, 1H), 7.97 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.21 (ddd, *J* = 8.2, 7.4, 1.7 Hz, 1H), 6.95 – 6.80 (m, 3H), 3.93 (s, 3H), 2.55 (s, 3H), 1.83 (q, *J* = 7.5 Hz, 2H), 1.47 (s, 6H), 0.88 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.25, 156.79, 152.15, 145.30, 137.51, 131.68, 131.08, 130.22, 128.48, 123.09, 121.59, 119.64, 117.81, 110.78, 83.88, 55.89, 33.35, 26.36, 25.74, 8.28.HRMS (ESI^+): calcd for $C_{21}H_{25}NNaO_4S$ $[M+Na]^+$ 410.1402, found 410.1401.



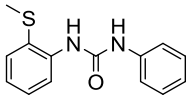
tert-pentyl (2-((2-methoxyphenyl)thio)-4,6-dimethylphenyl)carbamate (4ac)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 50/1, v/v) afforded **4ac** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (t, *J* = 7.8 Hz, 1H), 7.07 (d, *J* = 16.2 Hz, 2H), 6.86 (d, *J* = 7.8 Hz, 2H), 6.81 (t, *J* = 7.4 Hz, 1H), 6.55 (s, 1H), 3.89 (s, 3H), 2.29 (s, 3H), 2.25 (s, 3H), 1.68 (q, *J* = 7.4 Hz, 2H), 1.31 (s, 6H), 0.79 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.57, 153.47, 136.49, 136.34, 135.05, 132.69, 132.47, 129.75, 127.58, 127.56, 124.32, 121.59, 110.68, 82.19, 55.92, 33.57, 25.63, 20.78, 18.84, 8.11.HRMS (ESI^+): calcd for $C_{21}H_{27}NNaO_3S$ $[M+Na]^+$ 396.1609, found 396.1602.



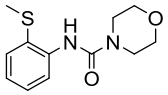
benzyl (2-(methylthio)phenyl)carbamate (4ad)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1, v/v) afforded **4ad** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.1 Hz, 1H), 7.84 (s, 1H), 7.47 – 7.32 (m, 6H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 5.21 (s, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.32, 138.53, 136.05, 133.37, 129.07, 128.82, 128.61, 128.36, 124.49, 123.52, 118.95, 67.08, 19.03. HRMS (ESI^+): calcd for $C_{15}H_{15}NNaO_2S$ $[M+Na]^+$ 296.0721, found 296.0715.



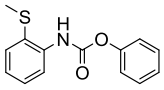
1-(2-(methylthio)phenyl)-3-phenylurea (5)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 5/1, v/v) afforded **5** as a white solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.40 (s, 1H), 8.13 (s, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 2H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.22 (dt, *J* = 16.8, 8.0 Hz, 3H), 6.97 (dt, *J* = 14.7, 7.0 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 152.91, 140.18, 138.35, 130.36, 129.26, 127.34, 127.18, 123.72, 122.28, 121.71, 118.47, 17.15. HRMS (ESI^+): calcd for $C_{14}H_{15}N_2OS$ $[M+H]^+$ 259.0905, found 259.0900.



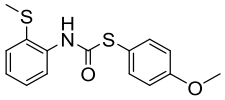
N-(2-(methylthio)phenyl)morpholine-4-carboxamide (6)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 5/1, v/v) afforded **6** as a white solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.10 (s, 1H), 7.33 – 7.24 (m, 2H), 7.13 (dt, *J* = 6.9, 4.9 Hz, 2H), 3.61 – 3.54 (m, 4H), 3.40 – 3.34 (m, 4H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 155.84, 137.24, 134.48, 127.19, 126.50, 125.88, 125.70, 66.39, 44.61, 15.74. HRMS (ESI^+): calcd for $C_{12}H_{17}N_2O_2S$ $[M+H]^+$ 253.1001, found 253.1008.



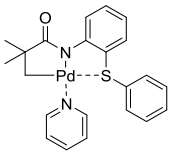
phenyl (2-(methylthio)phenyl)carbamate (7)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 10/1, v/v) afforded **7** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.5 Hz, 2H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.43 – 7.38 (m, 2H), 7.31 (t, *J* = 8.5 Hz, 1H), 7.27 – 7.20 (m, 3H), 7.06 (t, *J* = 8.2 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.62, 150.51, 133.49, 129.42, 129.21, 128.68, 128.55, 125.74, 123.93, 121.66, 121.02, 19.22. HRMS (ESI^+): calcd for $C_{14}H_{14}NO_2S$ $[M+H]^+$ 260.0745, found 260.0741.

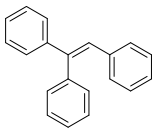


S-(4-methoxyphenyl) (2-(methylthio)phenyl)carbamothioate (8)

Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 10/1, v/v) afforded **8** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.20 (d, *J* = 9.3 Hz, 1H), 7.59 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 7.7 Hz, 1H), 7.26 (t, *J* = 7.9 Hz, 1H), 7.07 – 6.94 (m, 3H), 3.86 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.80, 161.40, 138.32, 137.76, 133.76, 129.36, 124.38, 119.55, 118.72, 115.35, 109.99, 55.51, 19.28. HRMS (ESI$^+$): calcd for $C_{15}H_{16}NO_2S_2$ $[M+H]^+$ 306.0622, found 306.0616.



Purification by column chromatography on silica gel (petroleum ether/ethyl acetate = 1/1, v/v) afforded **9** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (d, *J* = 9.7 Hz, 1H), 8.40 – 8.31 (m, 2H), 7.78 (tt, *J* = 7.7, 1.6 Hz, 1H), 7.32 – 7.21 (m, 9H), 6.82 (t, *J* = 8.1 Hz, 1H), 1.93 (s, 2H), 1.29 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.69, 154.67, 151.86, 137.43, 135.86, 135.23, 130.79, 129.33, 128.96, 127.85, 125.30, 123.80, 121.43, 121.03, 49.58, 38.31, 30.30. HRMS (ESI$^+$): calcd for $C_{22}H_{23}N_2OPdS$ $[M+H]^+$ 469.0566, found 469.0570 .



ethene-1,1,2-triyltribenzene

Purification by column chromatography on silica gel (petroleum ether) afforded ethene-1,1,2-triyltribenzene as colorless liquid.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.27 (m, 8H), 7.23 – 7.17 (m, 2H), 7.14 – 7.08 (m, 3H), 7.02 (d, *J* = 7.5 Hz, 2H), 6.96 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.44, 142.59, 140.37, 137.38, 130.41, 129.57, 128.66, 128.23, 128.19, 127.99, 127.63, 127.53, 127.43, 126.77.

VI. Crystal Data and Structure Refinement

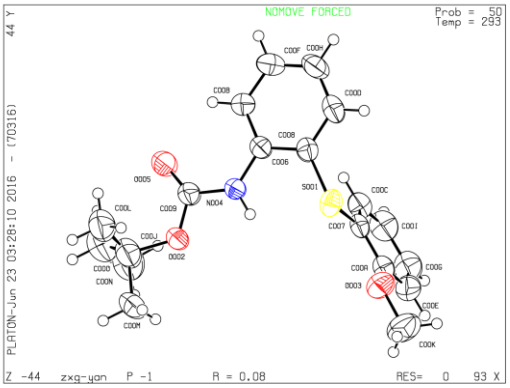


Table 1 Crystal data and structure refinement for **4c.**

Empirical formula	$C_{19}H_{23}NO_3S$
Formula weight	345.44
Temperature/K	293(2)
Crystal system	triclinic

Space group	P-1
a/Å	9.1466(5)
b/Å	10.0450(6)
c/Å	11.2749(6)
α/°	78.594(5)
β/°	69.193(5)
γ/°	70.534(6)
Volume/Å^3	909.28(10)
Z	2
ρ_{calc}g/cm^3	1.262
μ/mm^{-1}	1.711
F(000)	368.0
Crystal size/mm^3	0.4 × 0.4 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.424 to 145.278
Index ranges	-7 ≤ h ≤ 11, -12 ≤ k ≤ 12, -13 ≤ l ≤ 13
Reflections collected	10019
Independent reflections	3541 [R_{int} = 0.0373, R_{sigma} = 0.0288]
Data/restraints/parameters	3541/14/221
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	R_1 = 0.0837, wR_2 = 0.2340
Final R indexes [all data]	R_1 = 0.0880, wR_2 = 0.2403
Largest diff. peak/hole / e Å^{-3}	1.50/-0.51

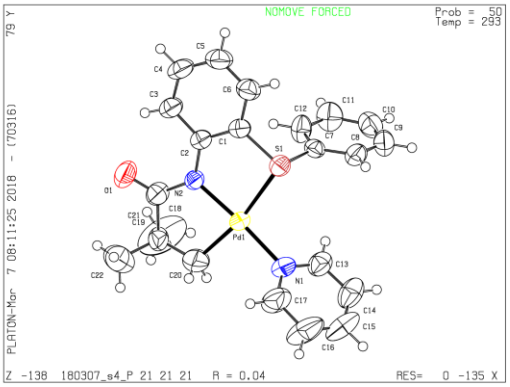


Table 1 Crystal data and structure refinement for **9**

Empirical formula	$C_{22}H_{22}N_2OPdS$
Formula weight	468.87
Temperature/K	293.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.4594(3)
b/Å	11.2077(4)
c/Å	19.4065(6)
α/°	90
β/°	90
γ/°	90

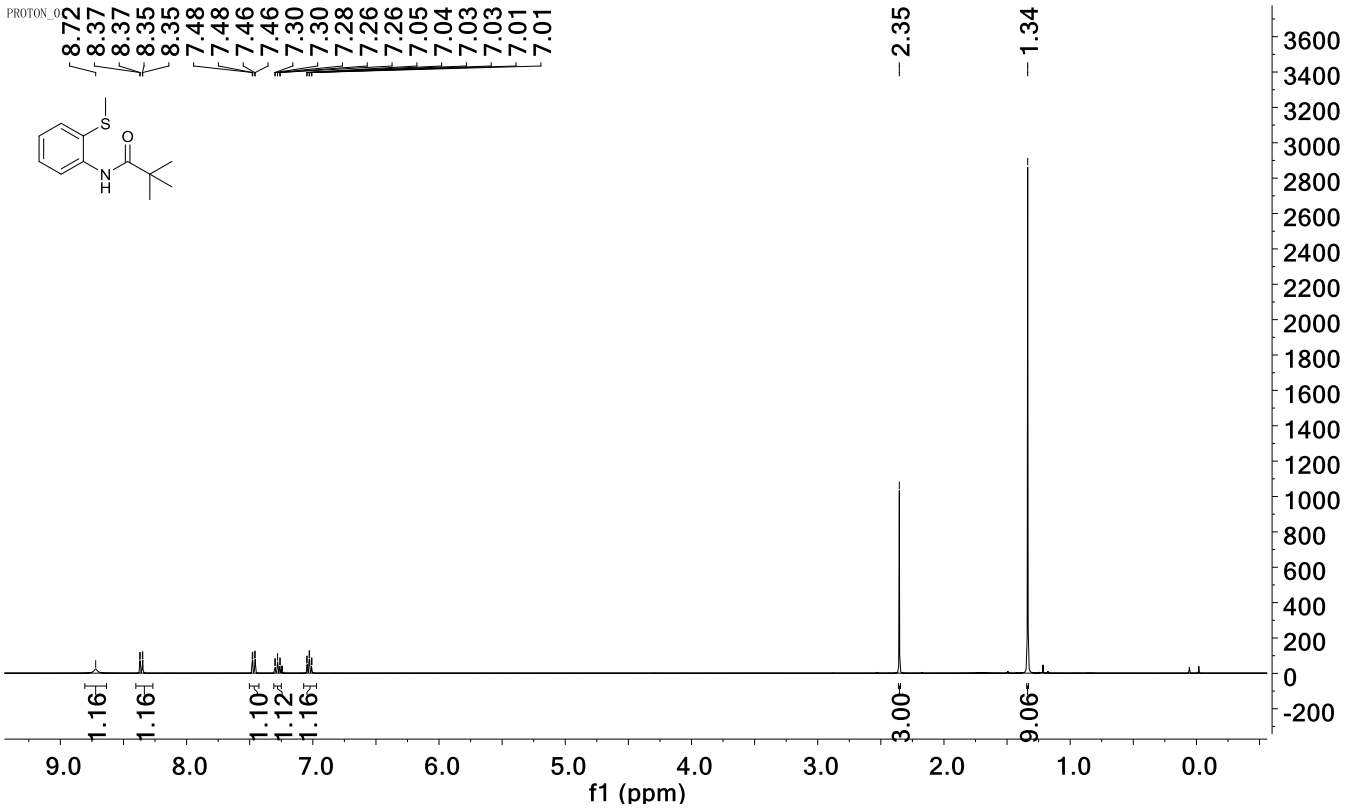
Volume/Å^3	2057.44(12)
Z	4
ρ_{calc}g/cm^3	1.514
μ/mm^{-1}	1.017
F(000)	952.0
Crystal size/mm^3	0.35 × 0.3 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.014 to 52.734
Index ranges	-11 ≤ h ≤ 10, -13 ≤ k ≤ 11, -23 ≤ l ≤ 24
Reflections collected	10241
Independent reflections	4056 [R_{int} = 0.0226, R_{sigma} = 0.0364]
Data/restraints/parameters	4056/0/246
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0356, wR_2 = 0.0744
Final R indexes [all data]	R_1 = 0.0522, wR_2 = 0.0825
Largest diff. peak/hole / e Å^{-3}	0.37/-0.58
Flack parameter	-0.032(15)

VII. References

1 E. Sperotto, G. P. M. van Klink, J. G. de Vries, G. van Koten, *J. Org. Chem.* **2008**, *73*, 5625-5628.

2 N. Barsu, S. K. Bolli, B. Sundararaju, *Chem. Sci.* **2017**, *8*, 2431-2435.

VIII. Copies of ^{1}H and ^{13}C spectra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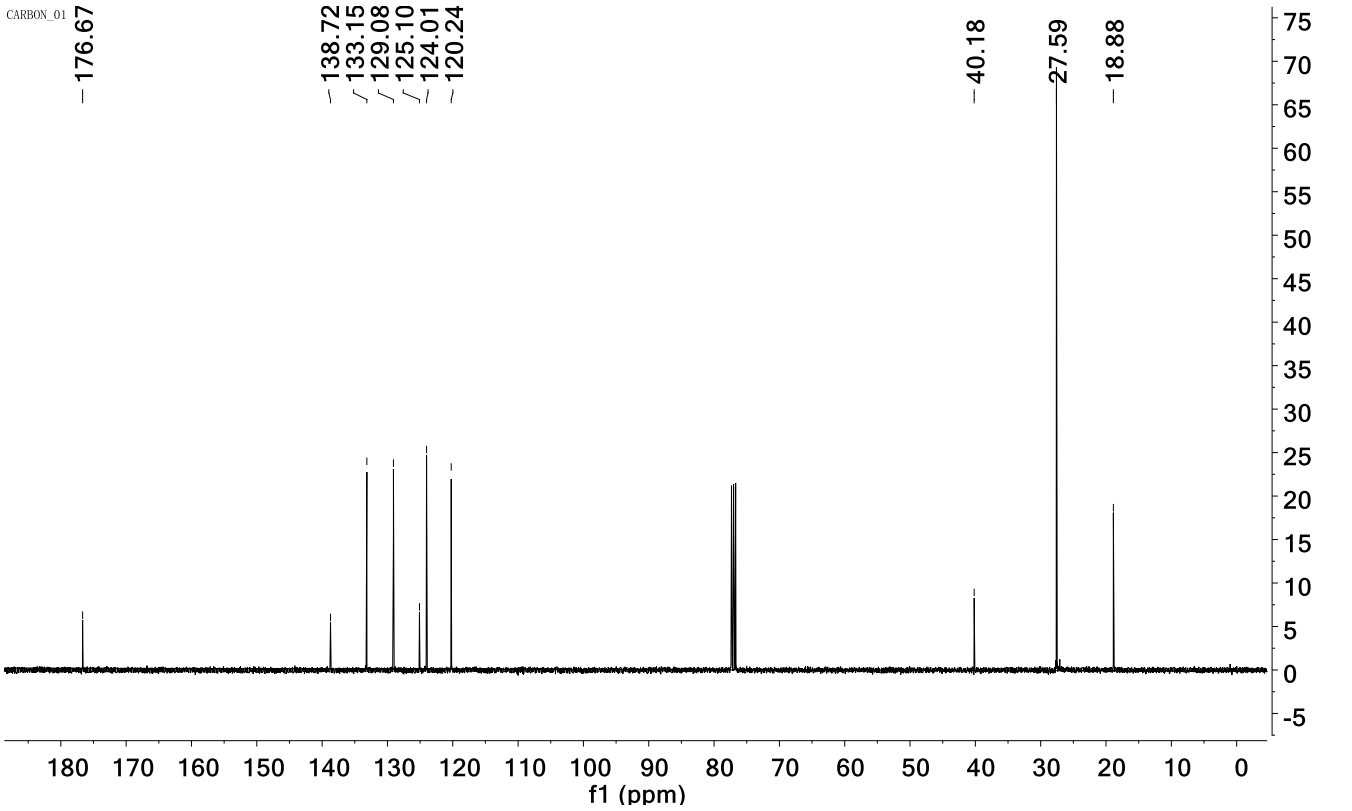
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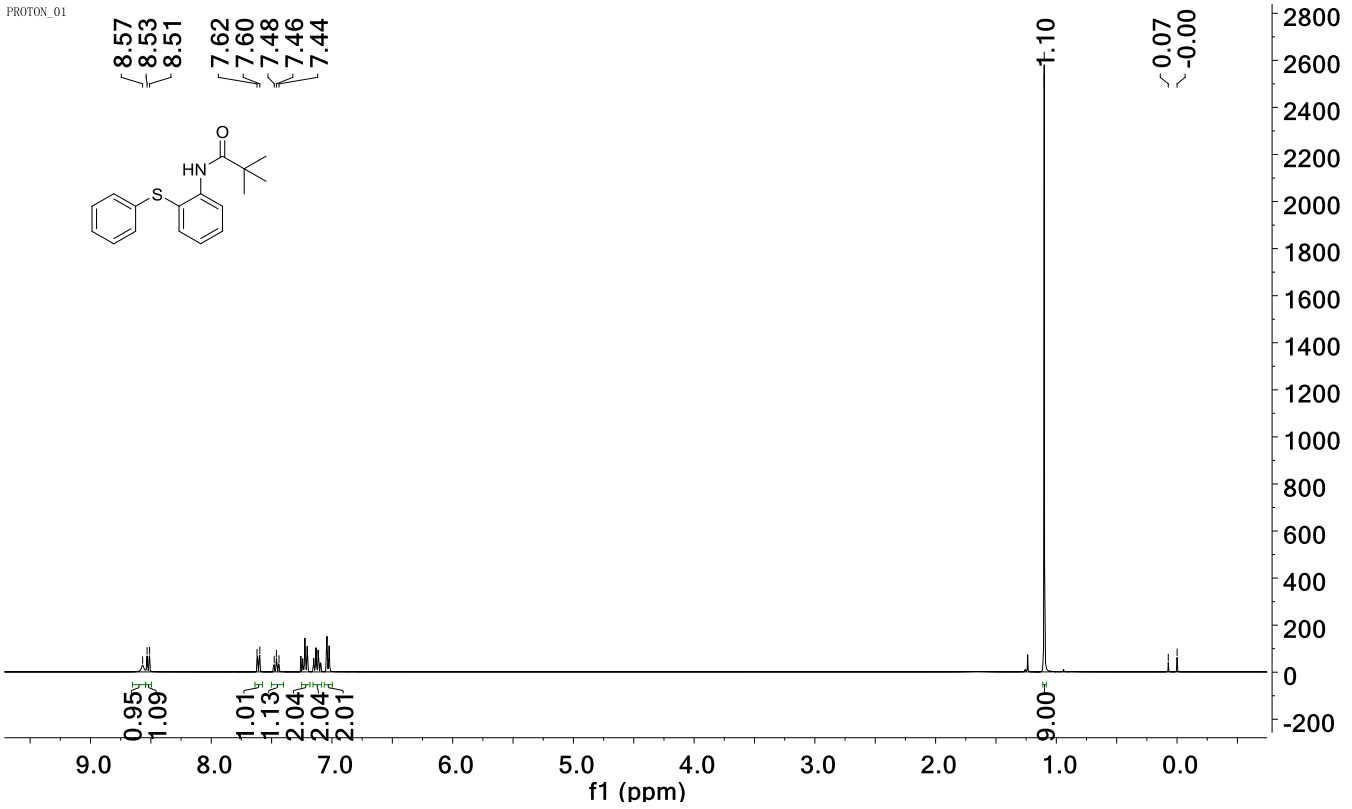
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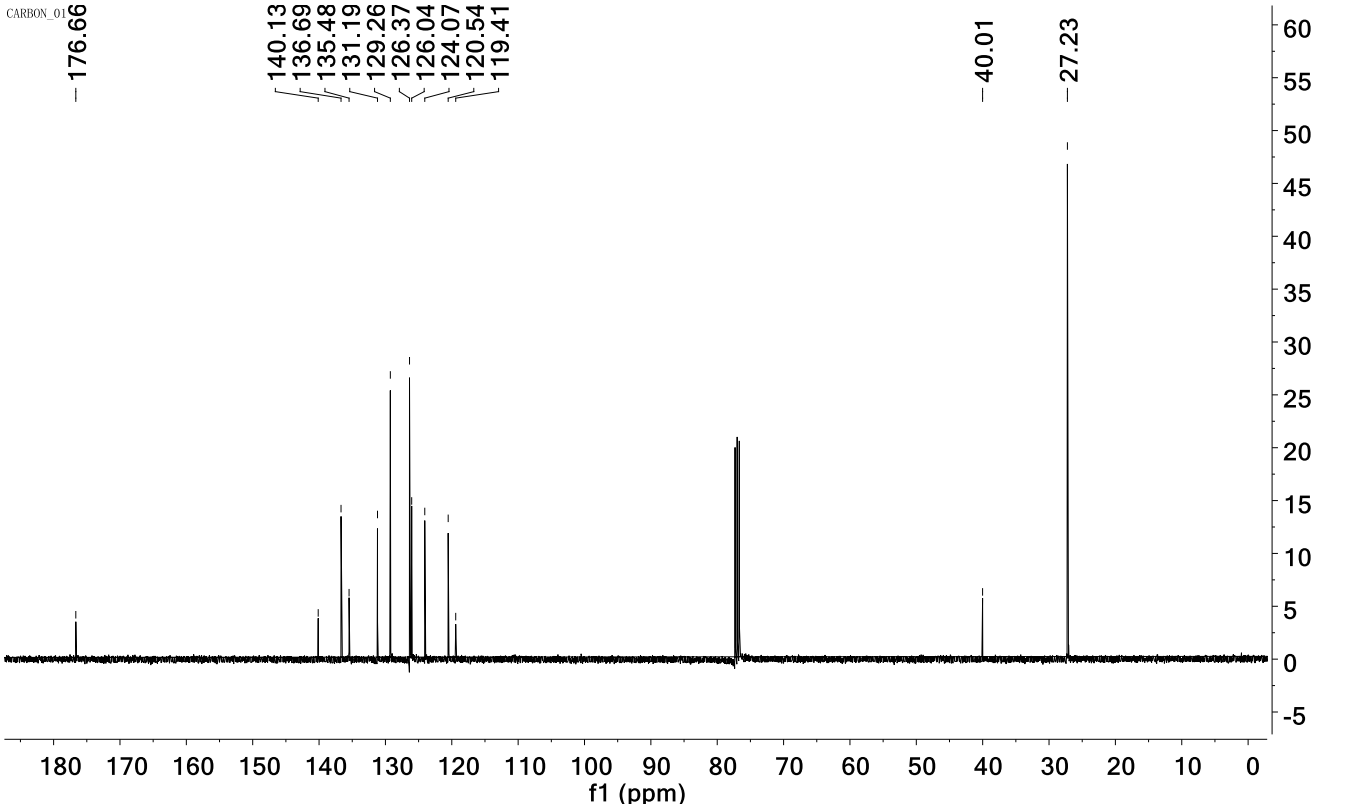
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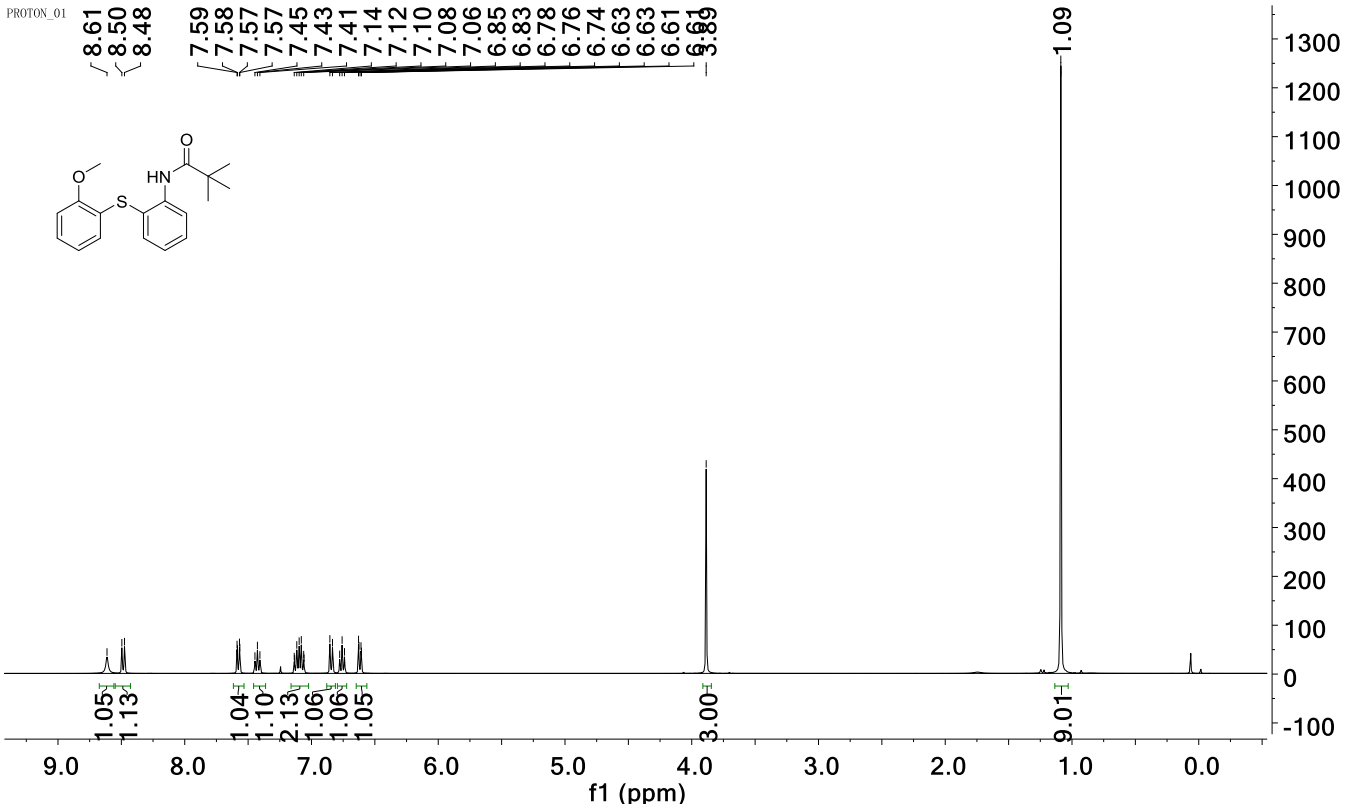
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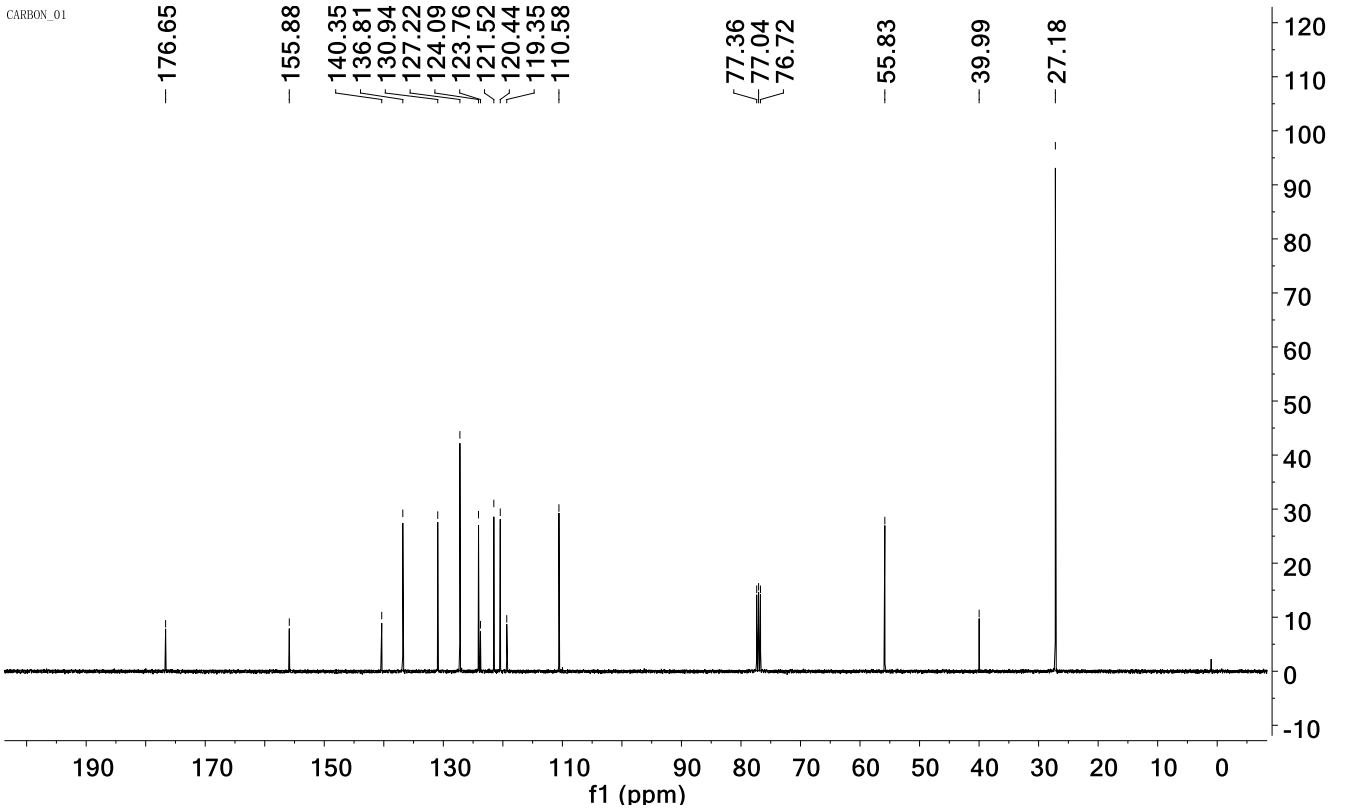
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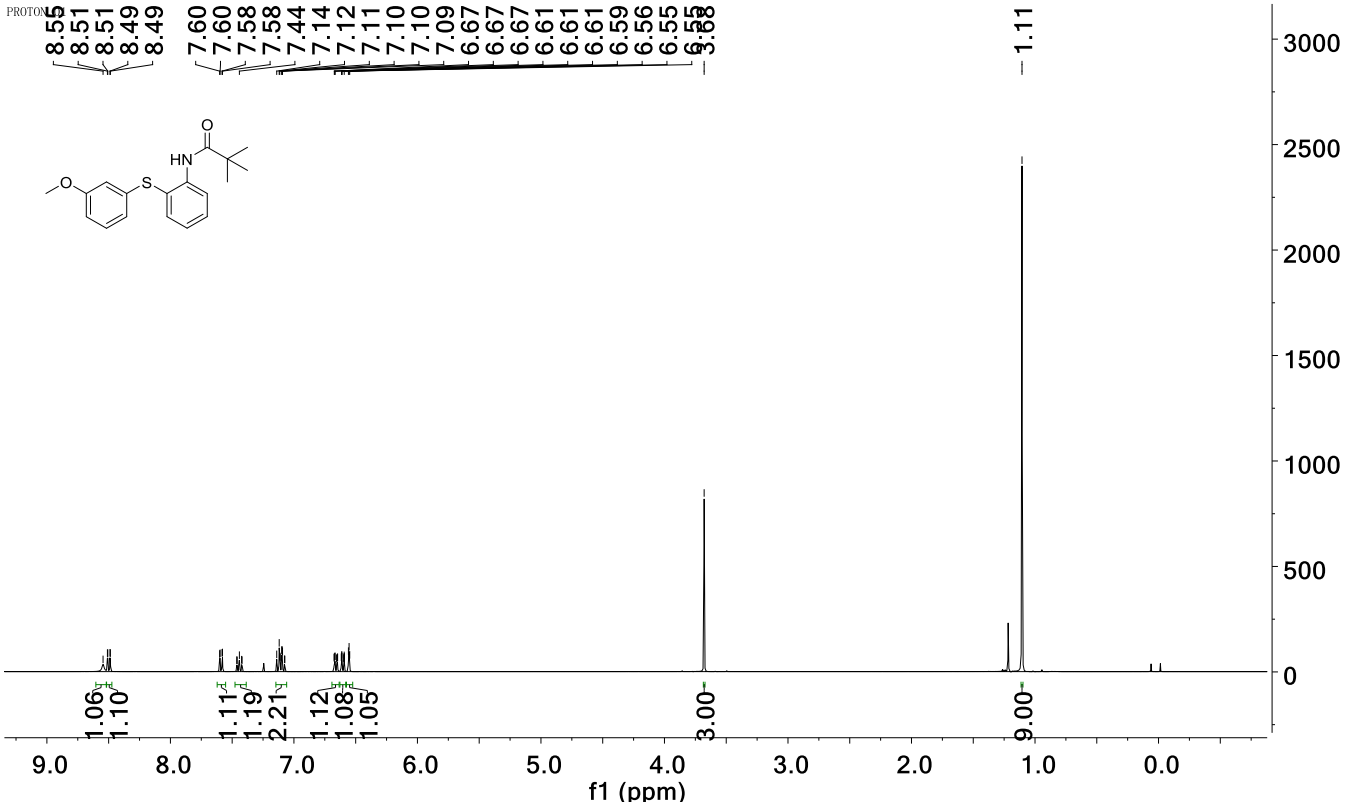
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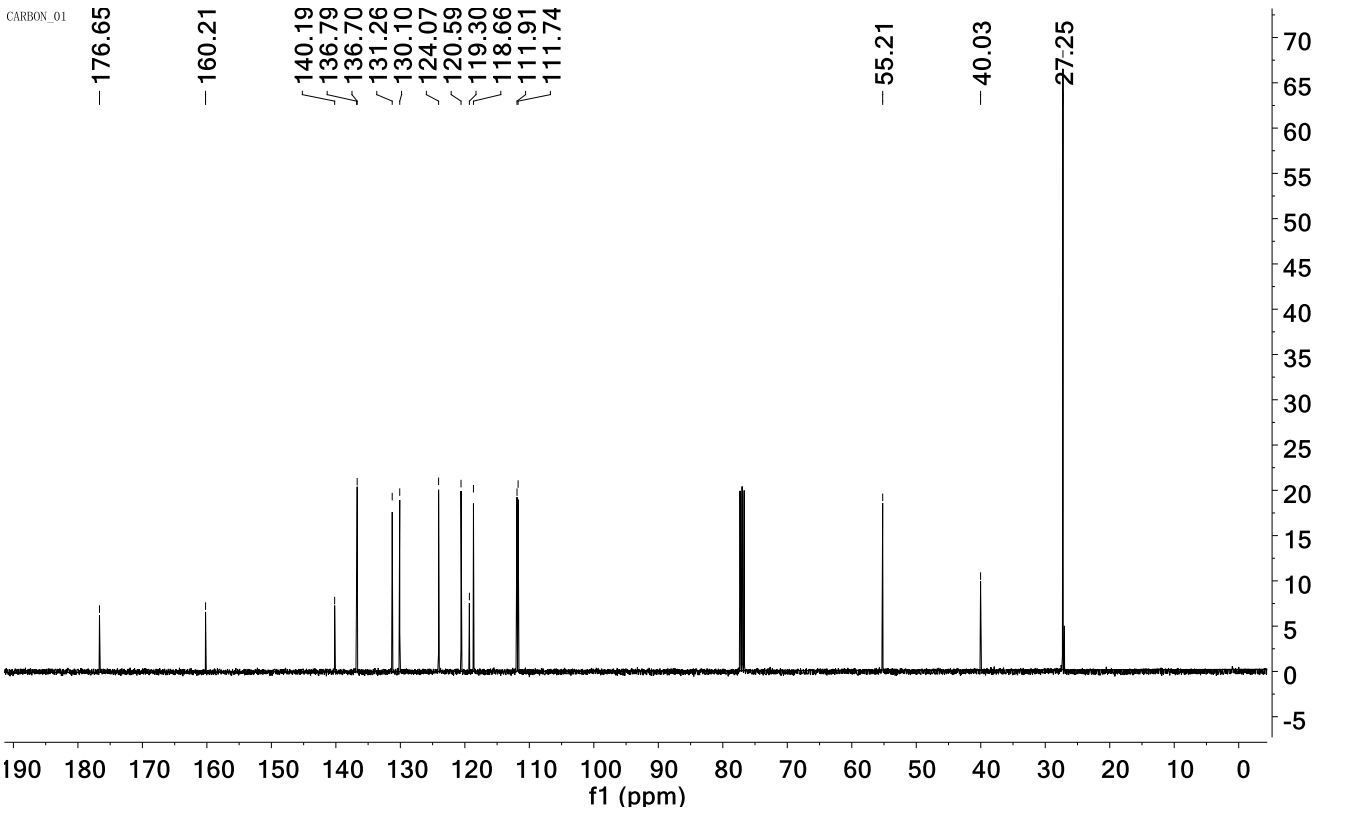
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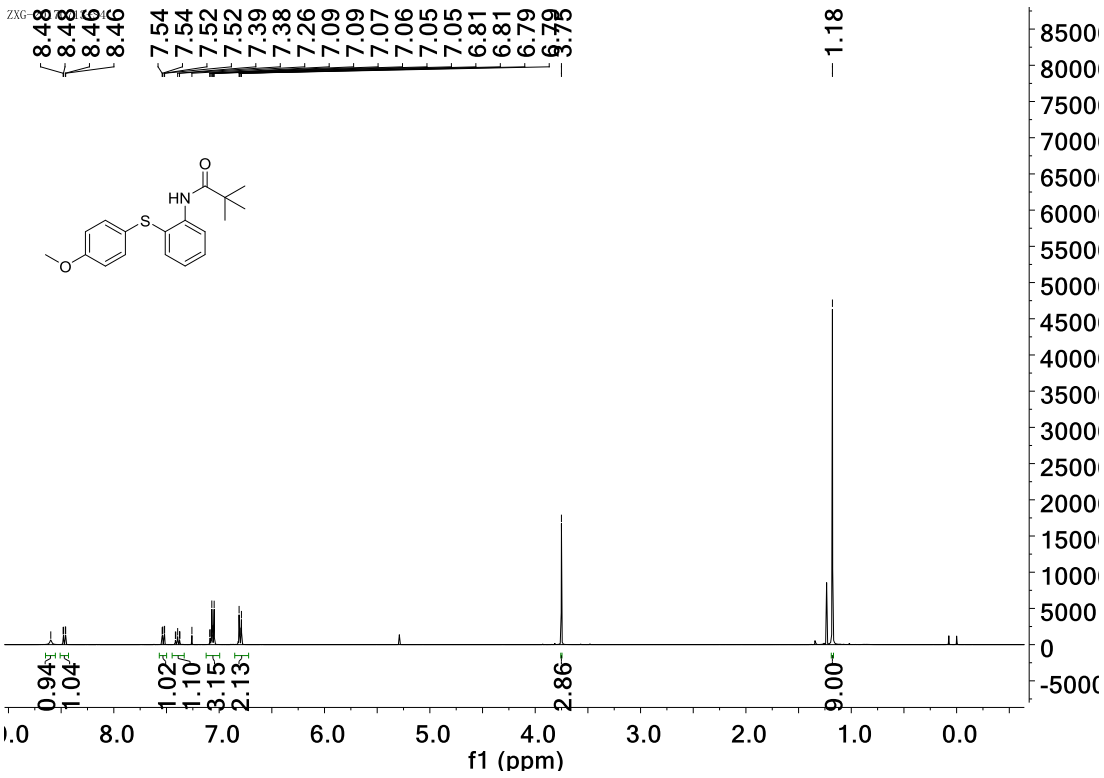
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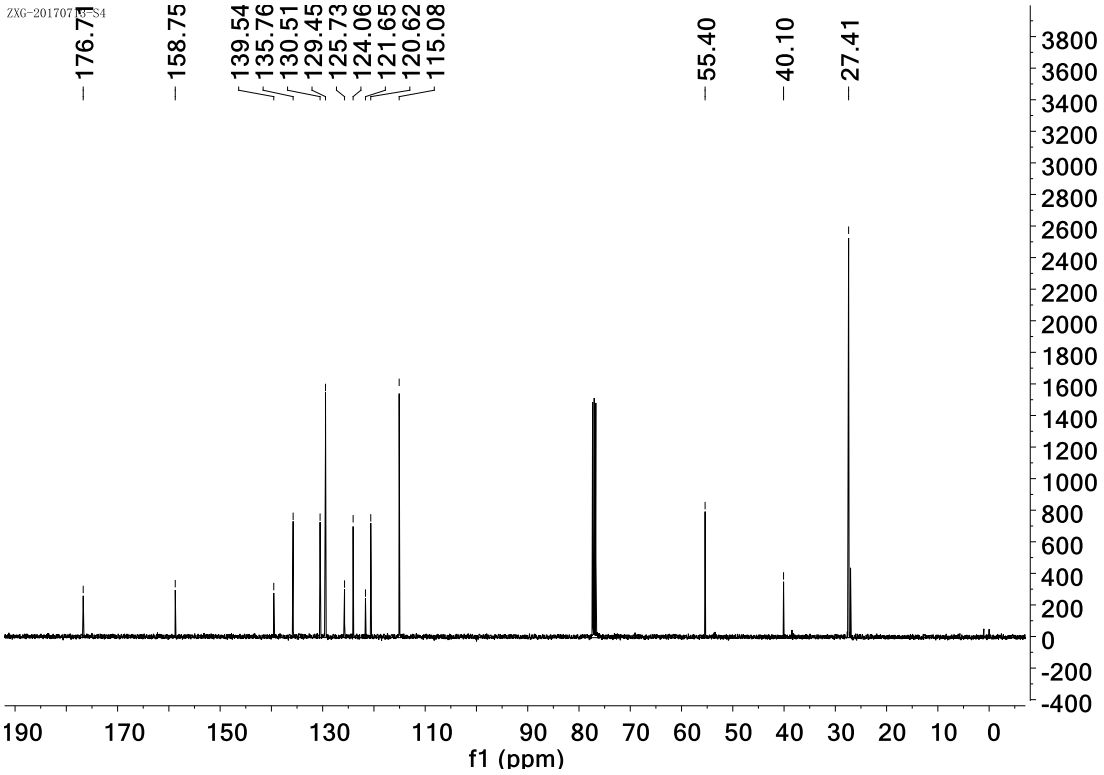
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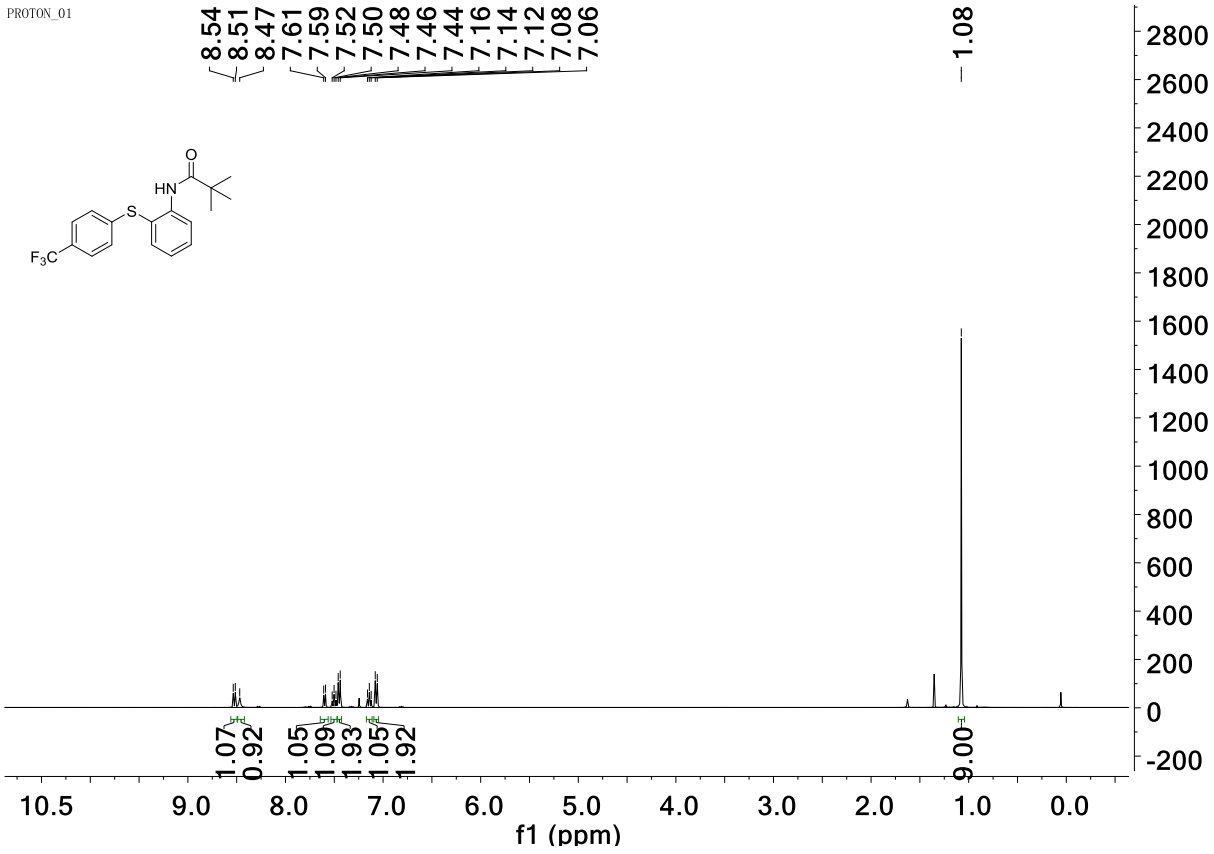
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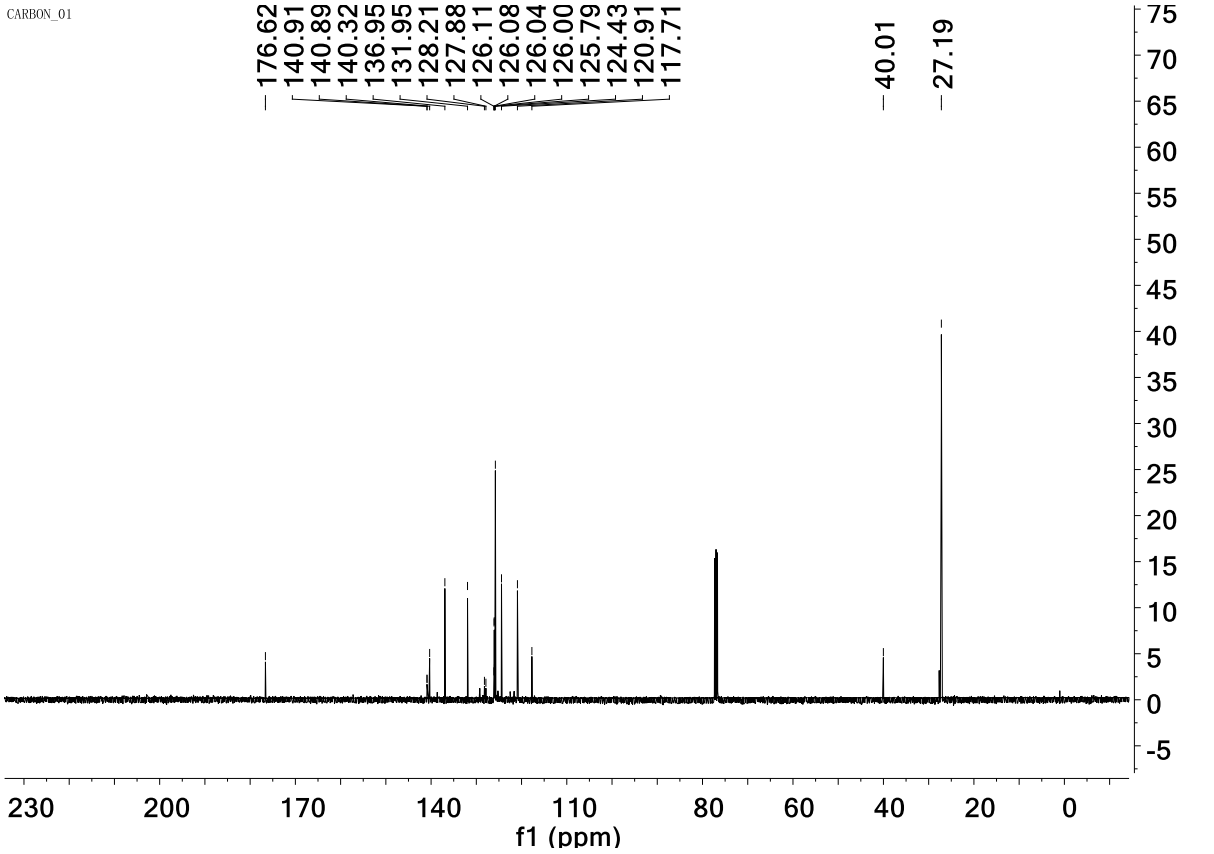
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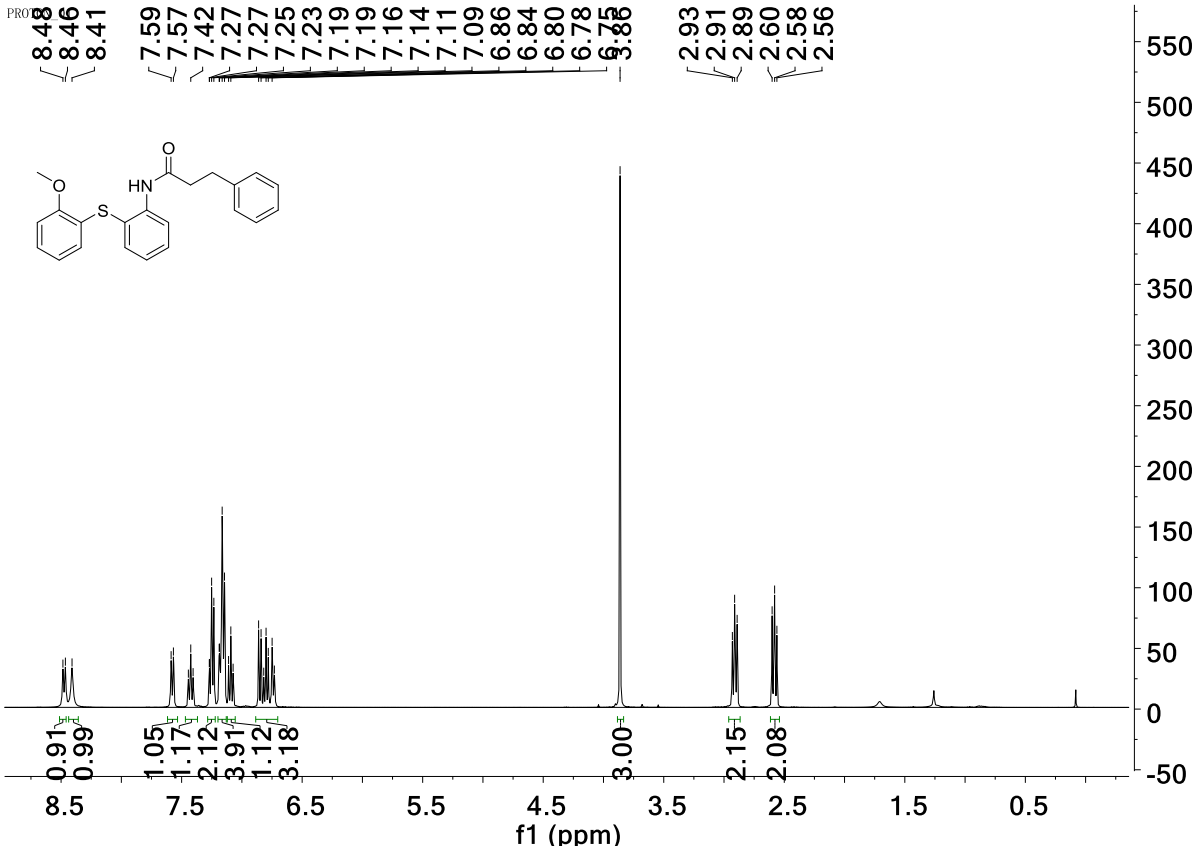
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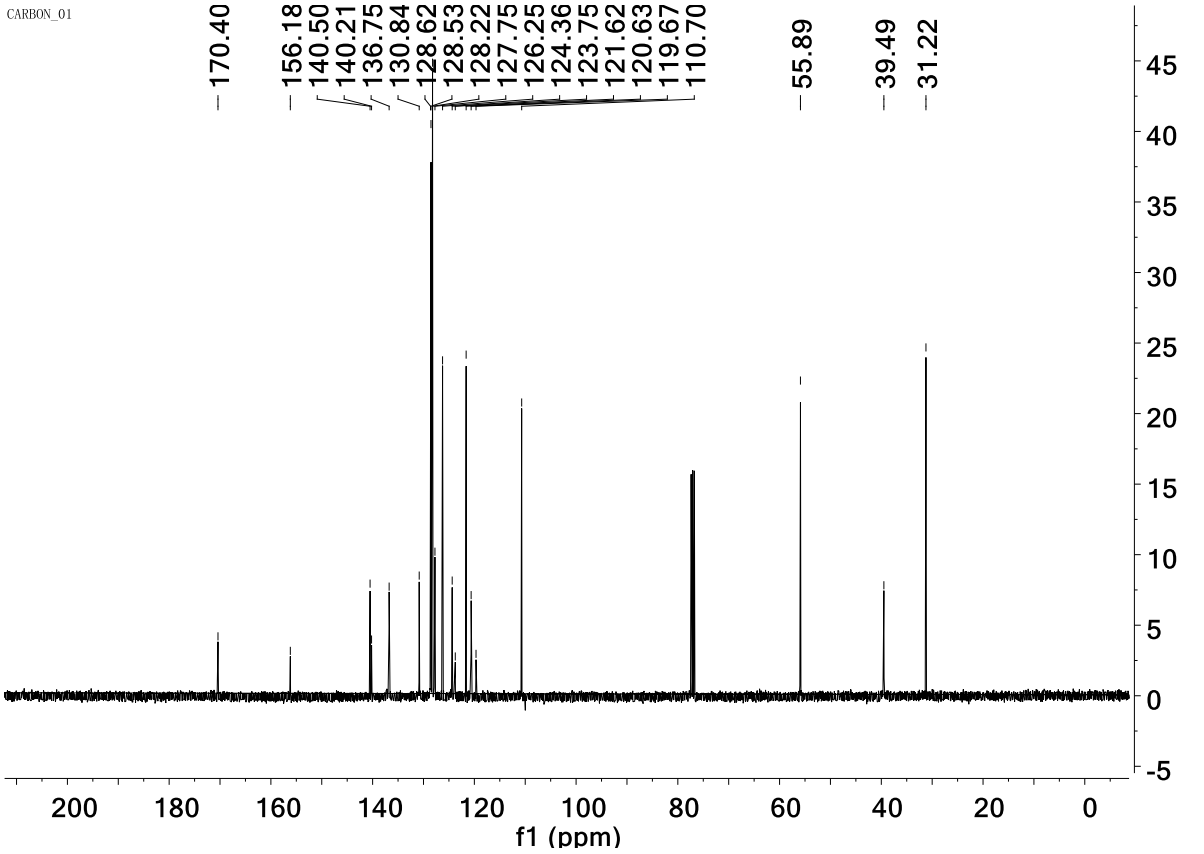
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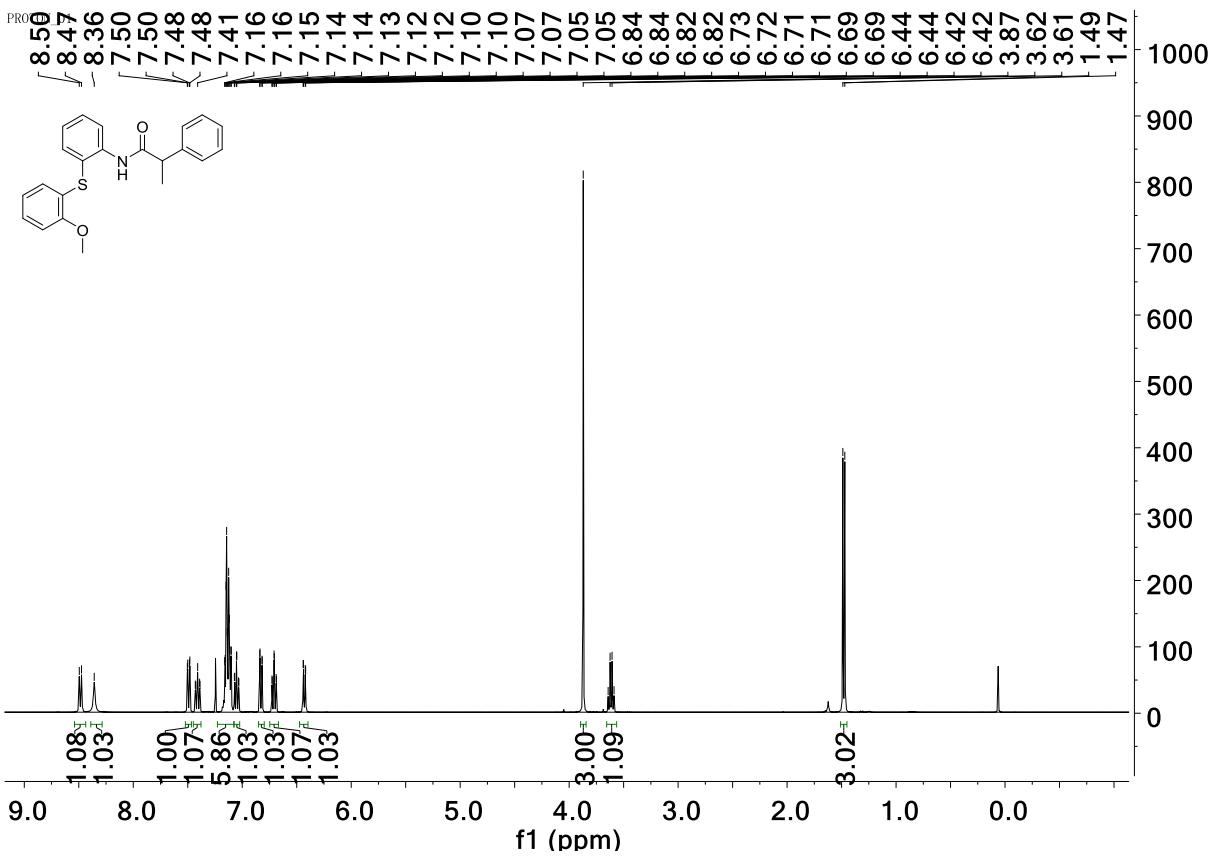
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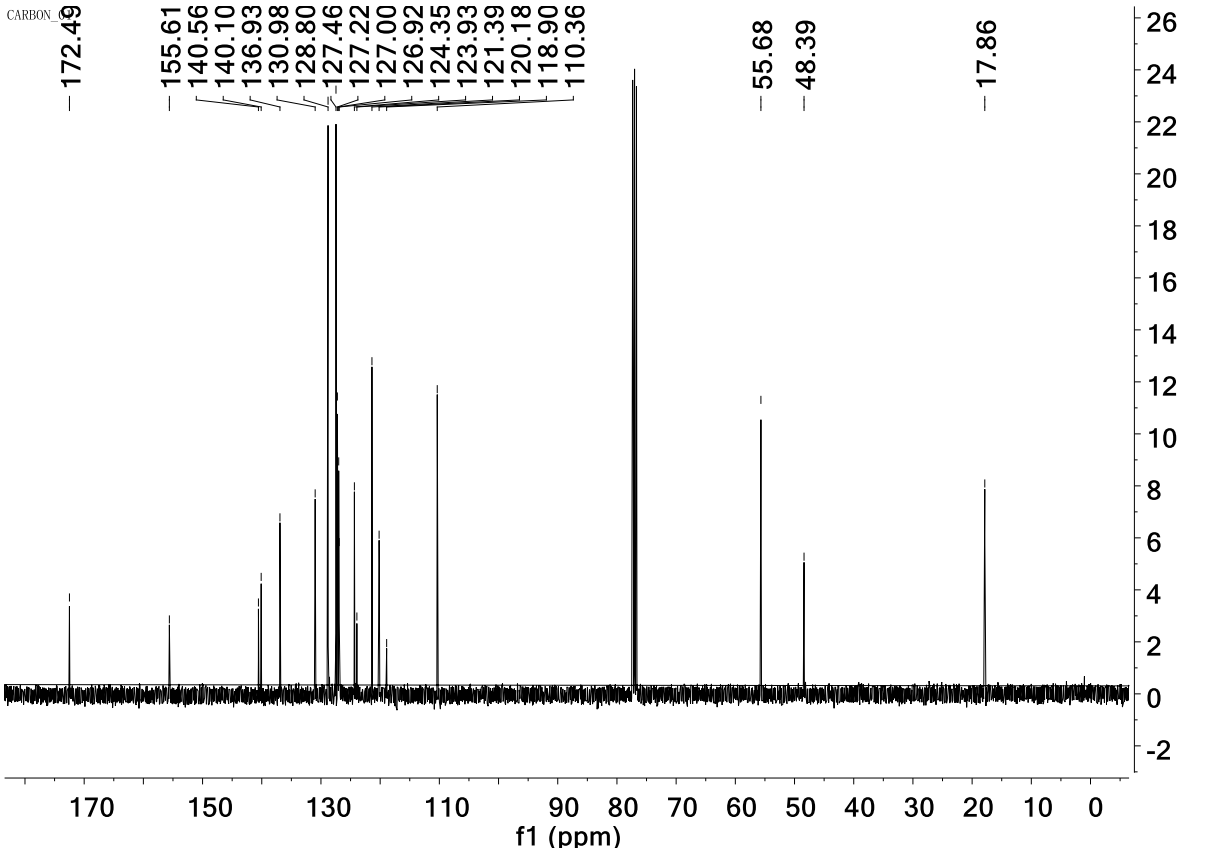
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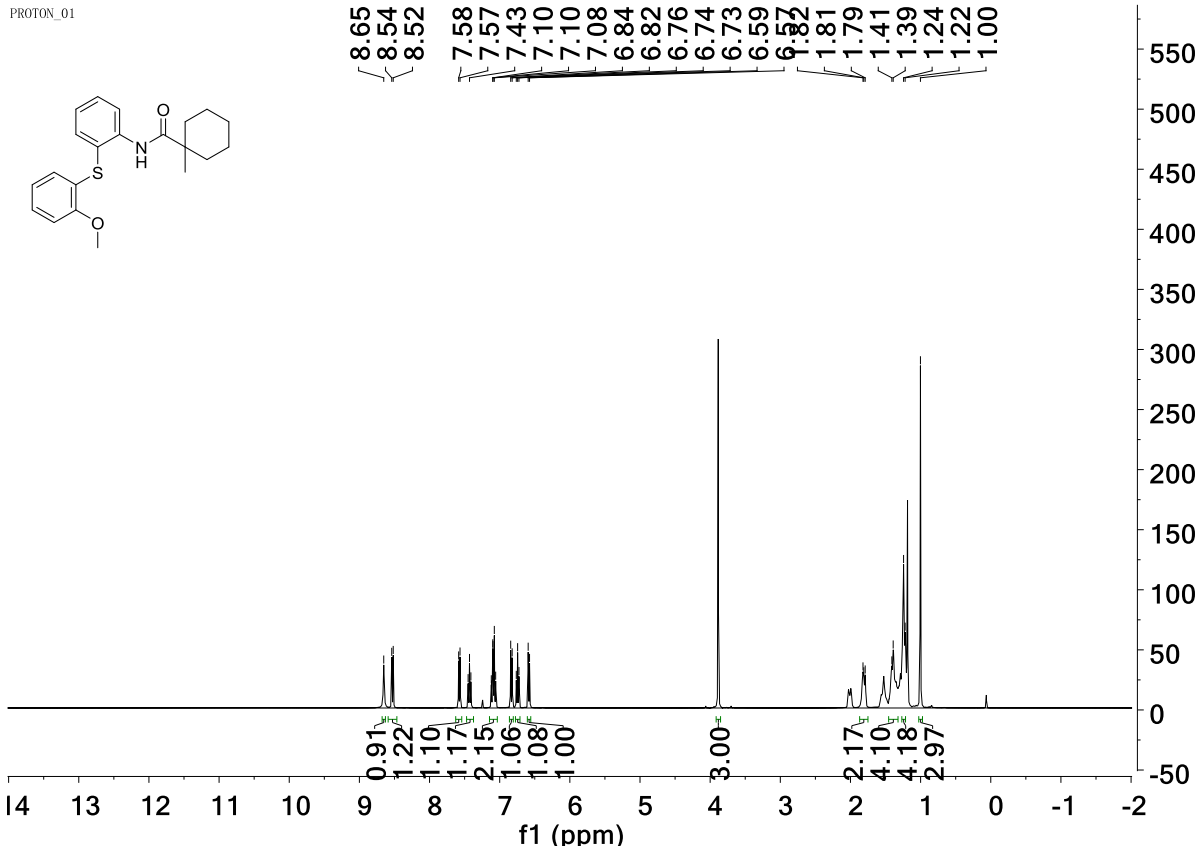
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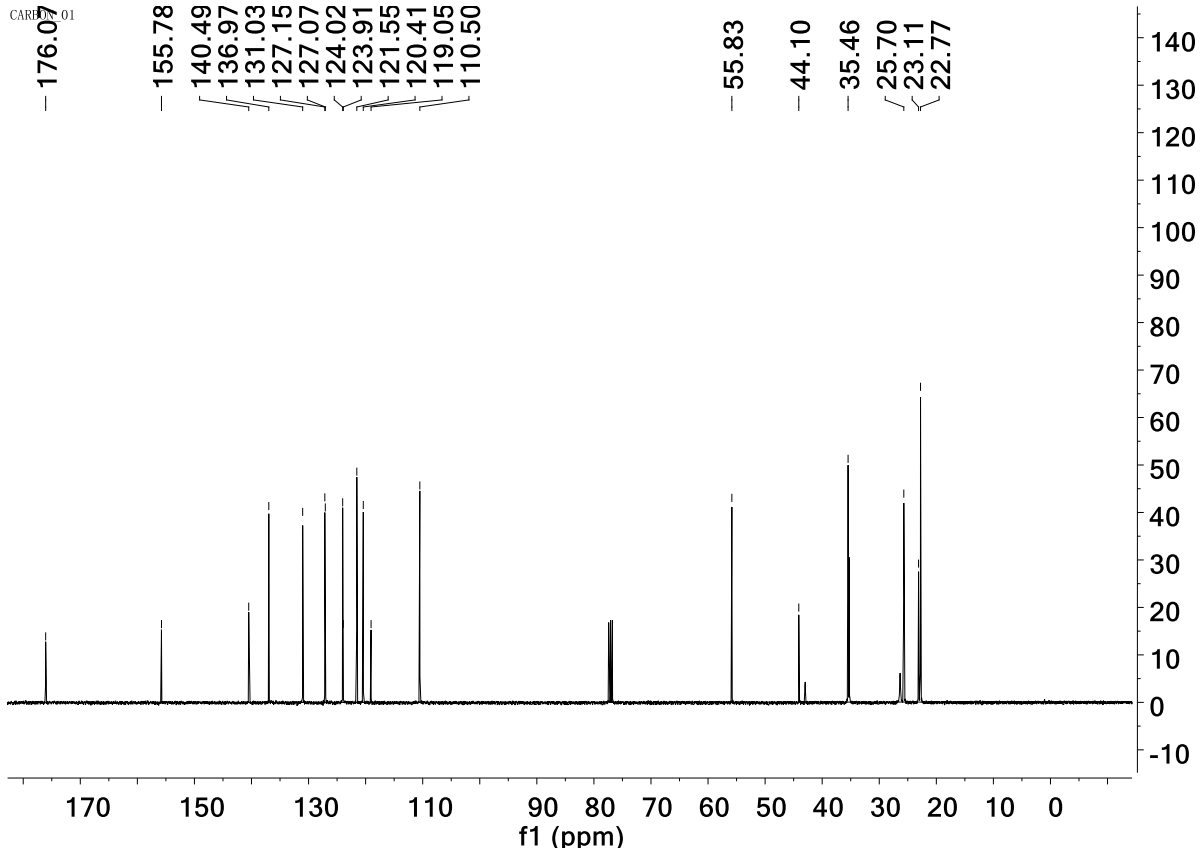
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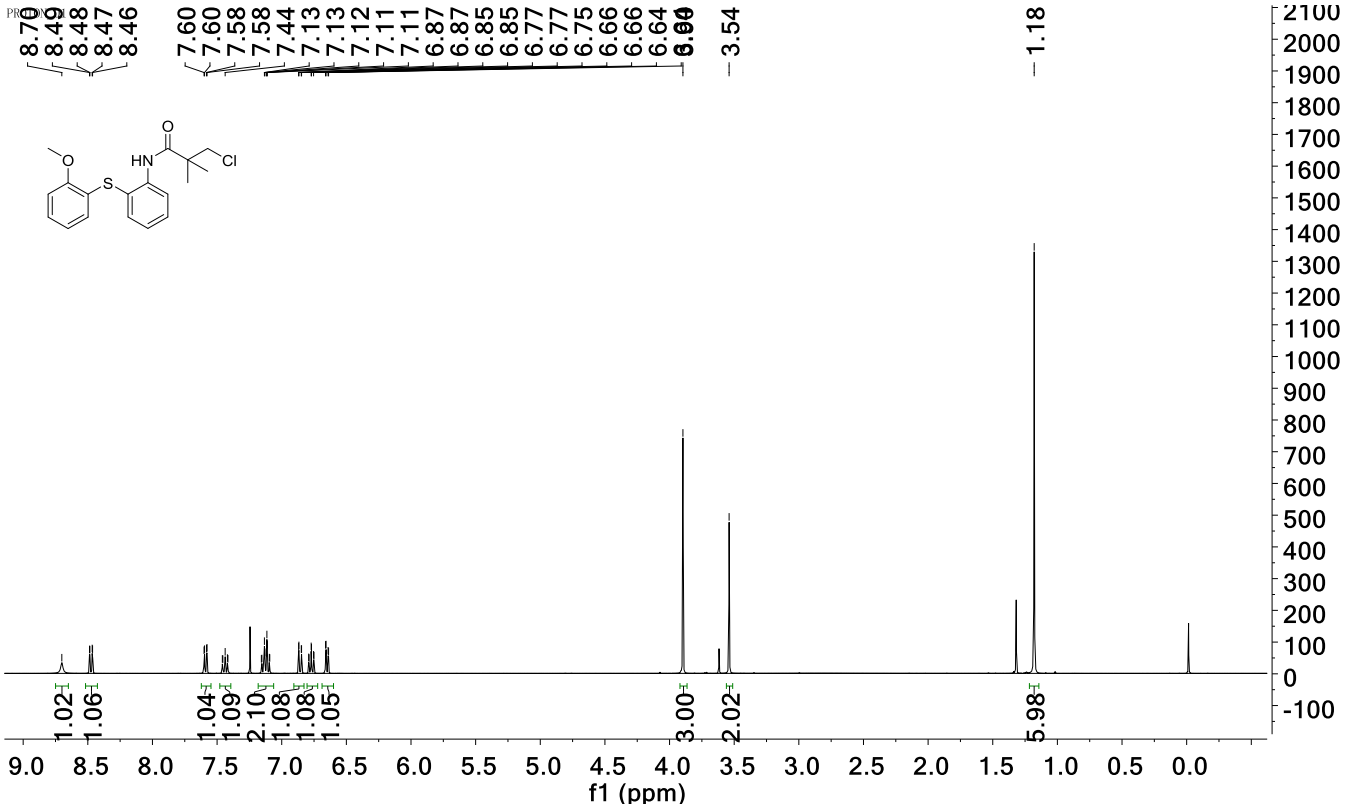
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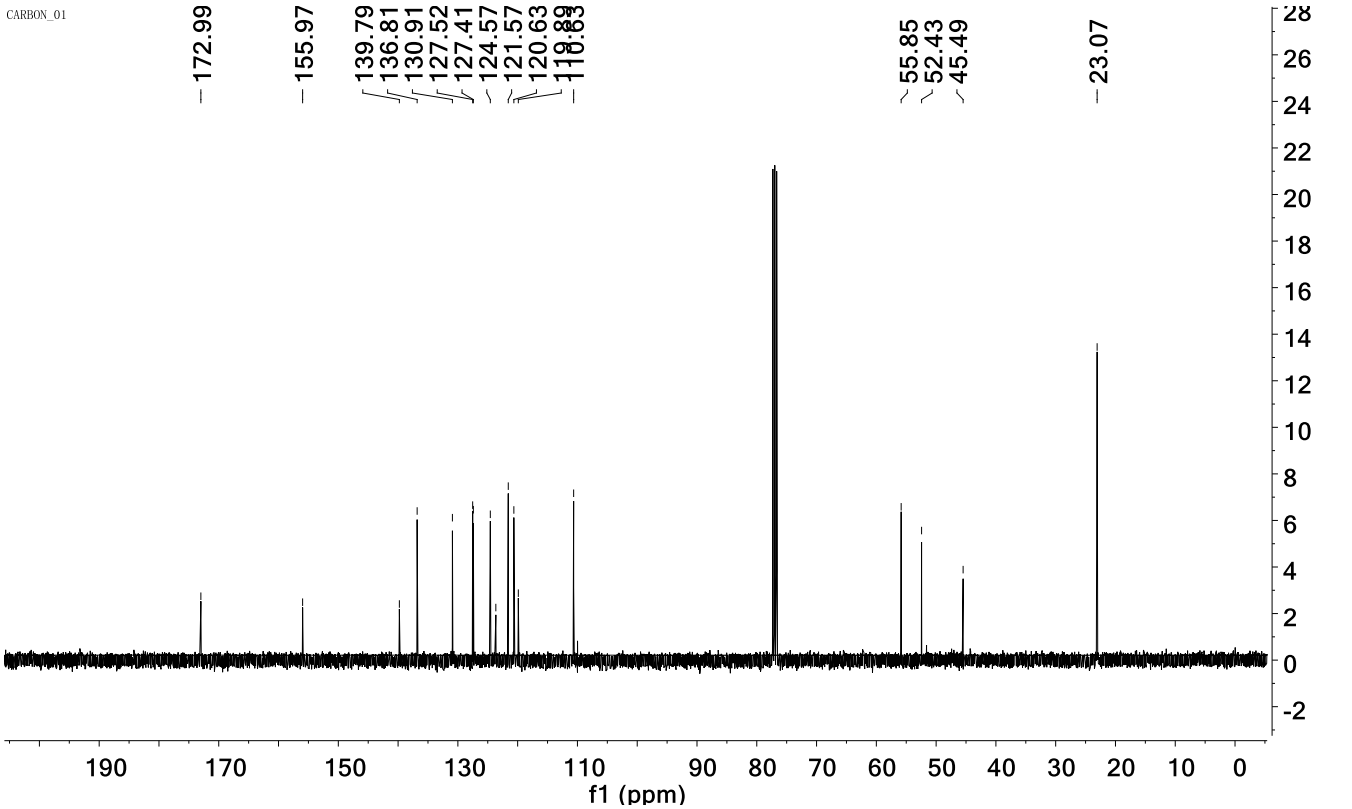
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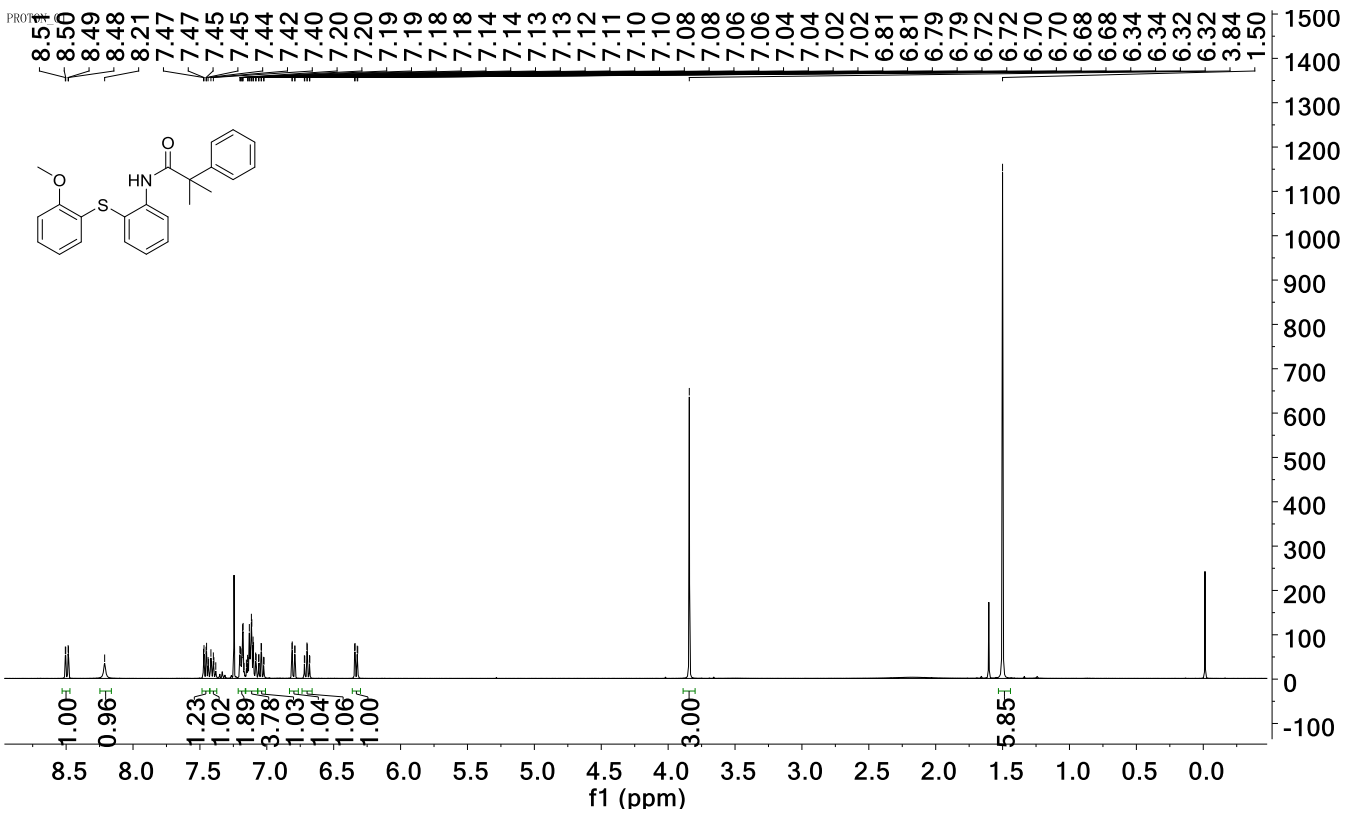
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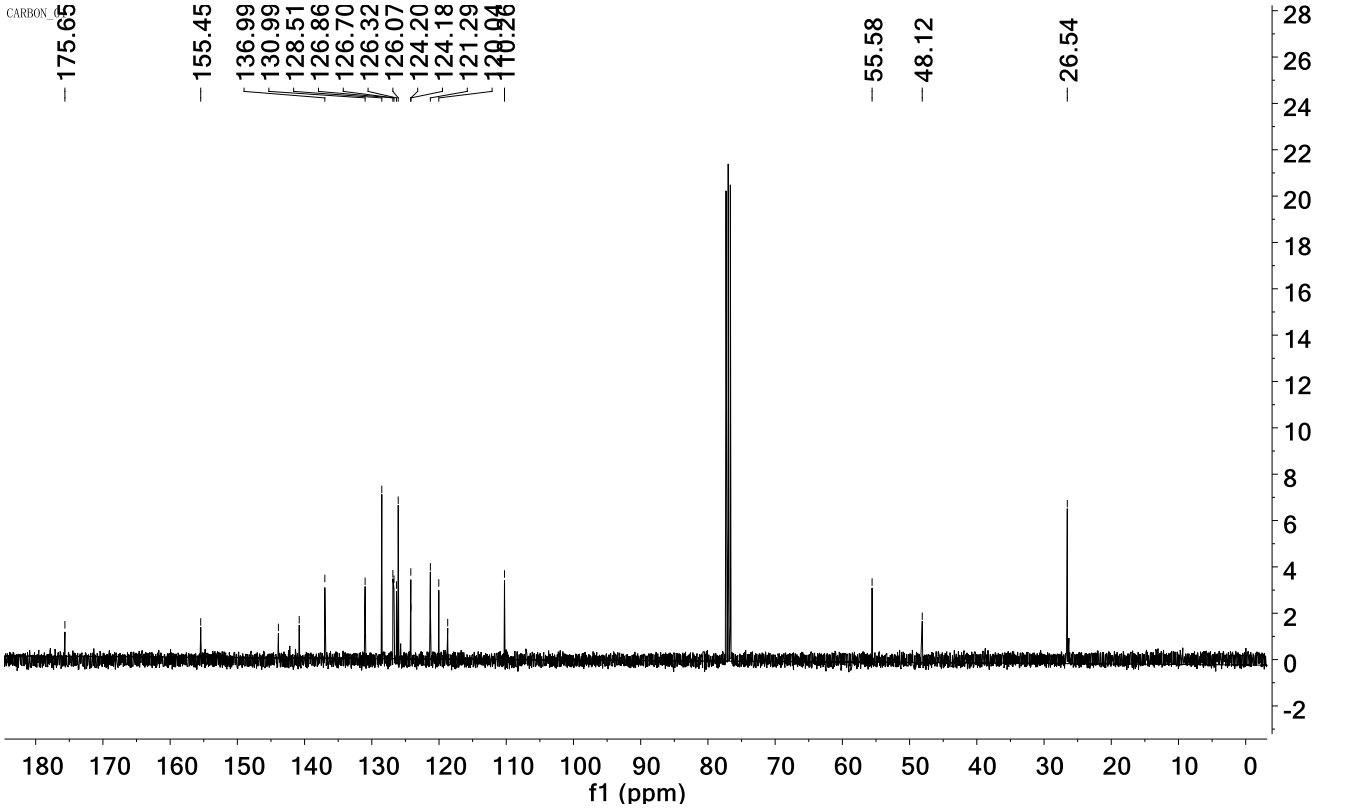
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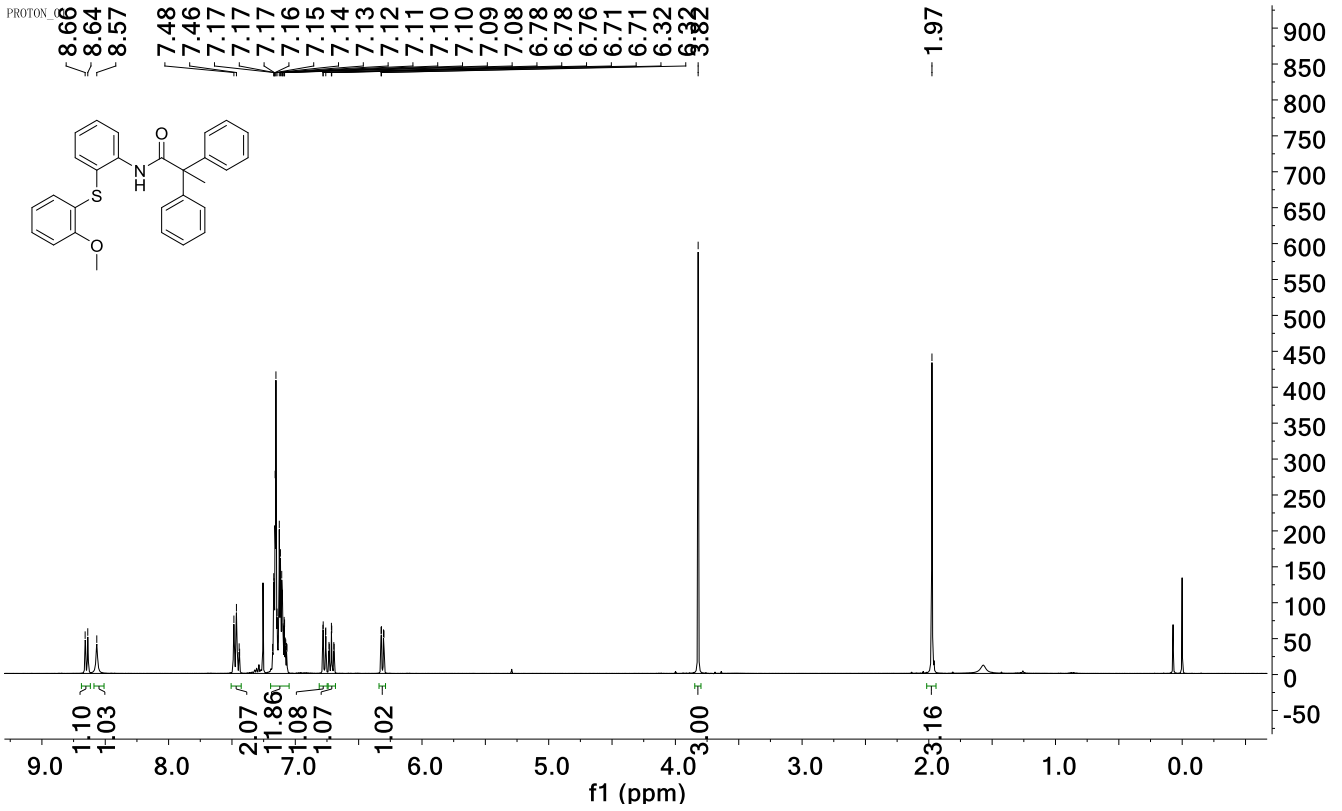
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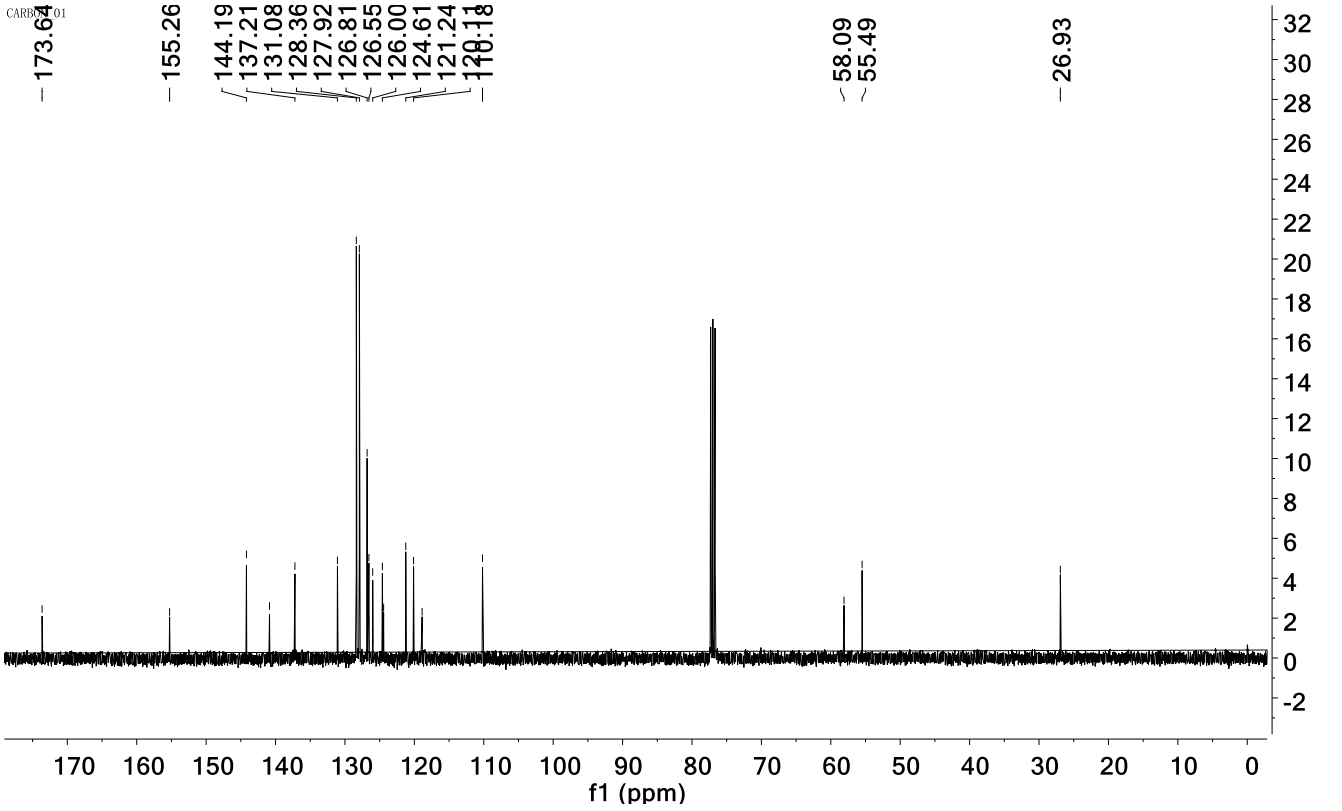
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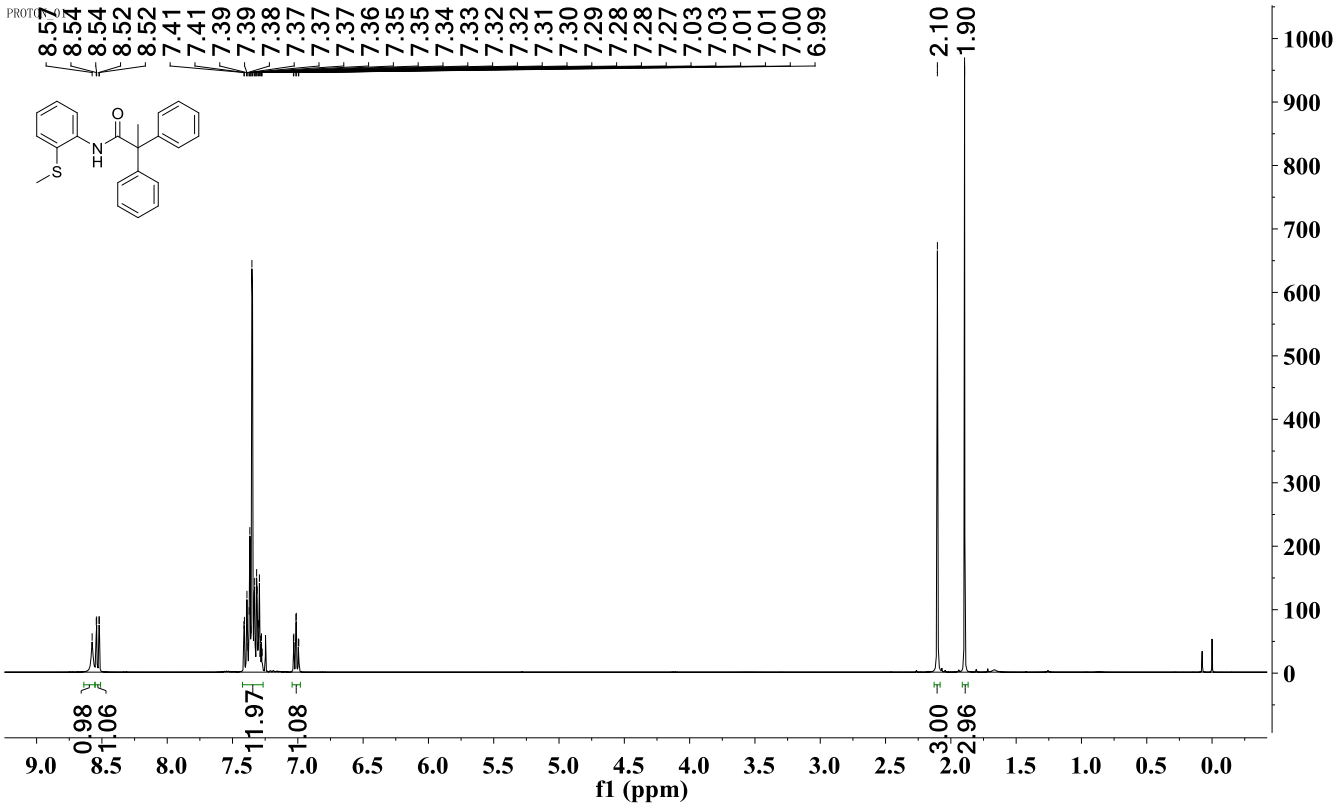
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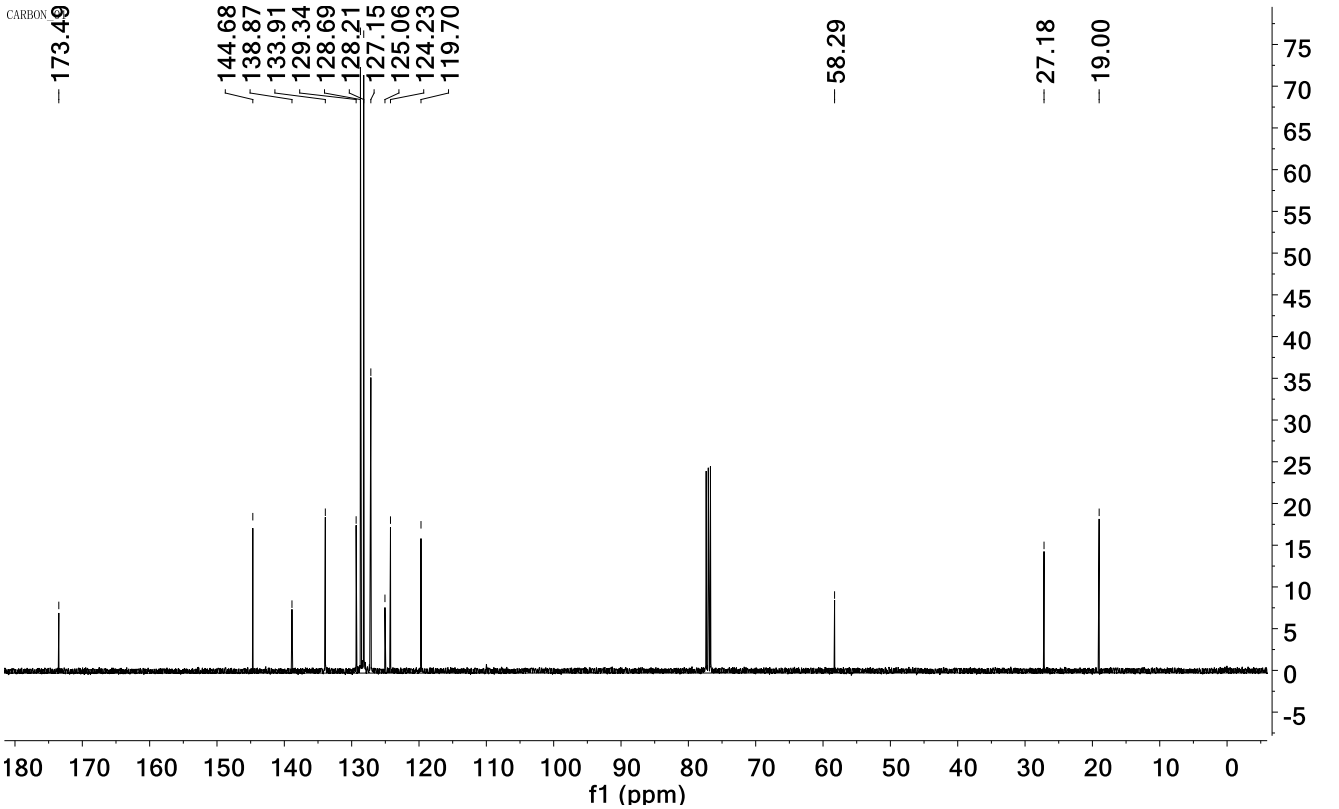
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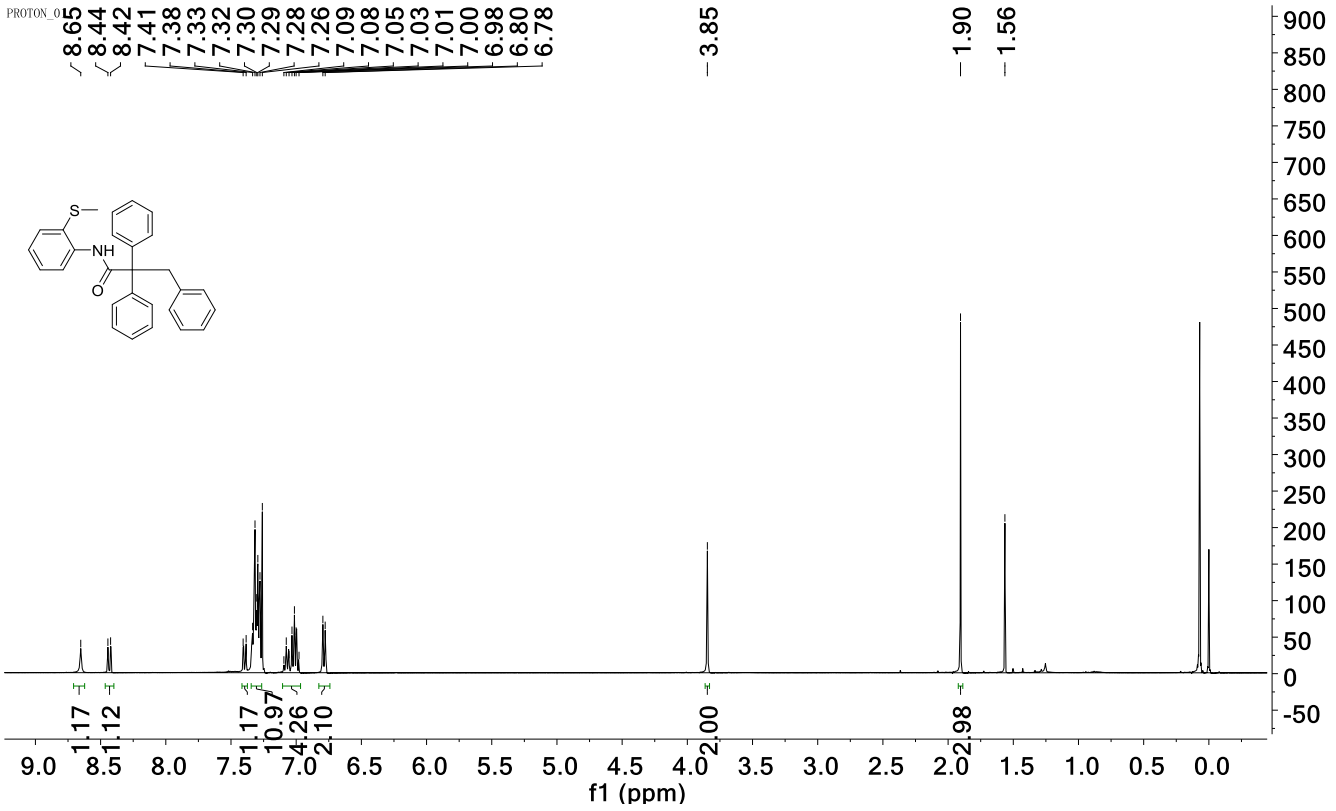
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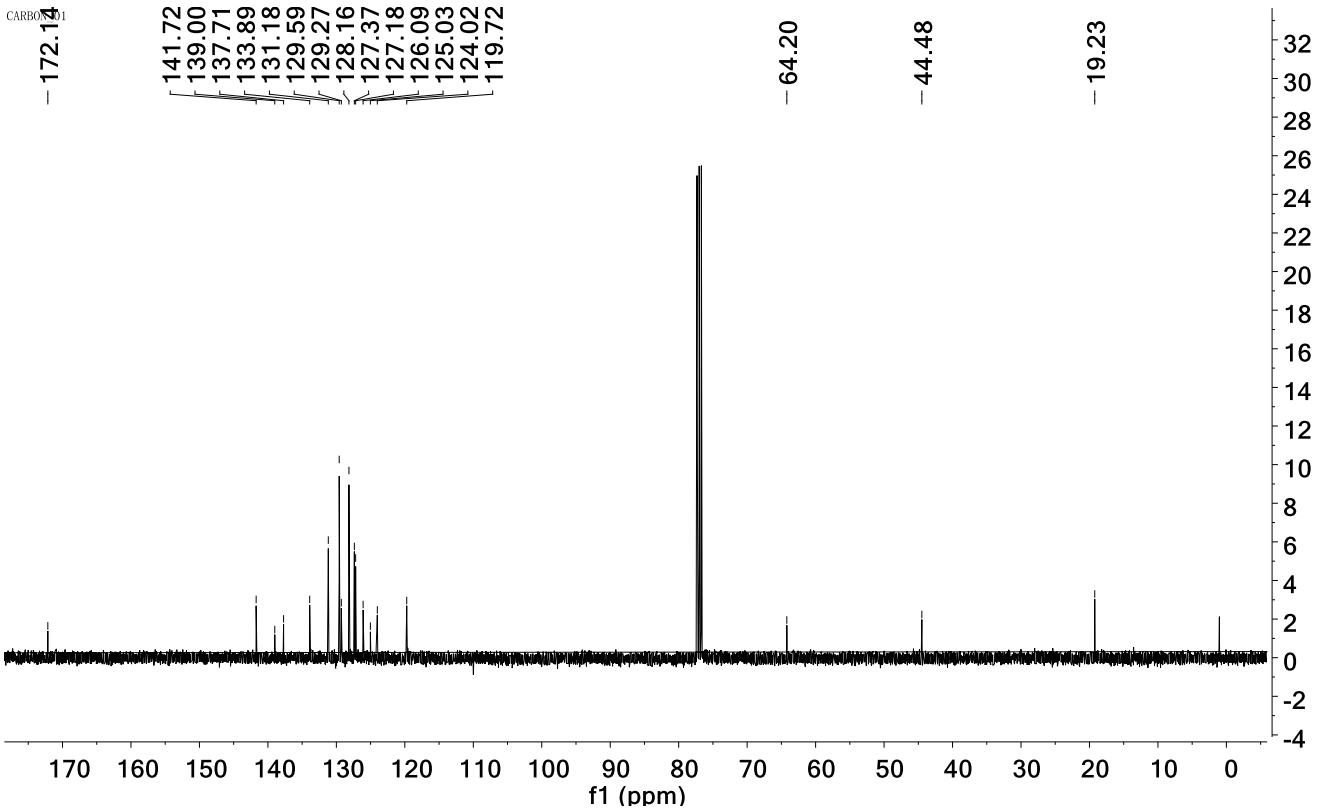
2.00
2.98
f1 (ppm)


CARBON_01
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129.59
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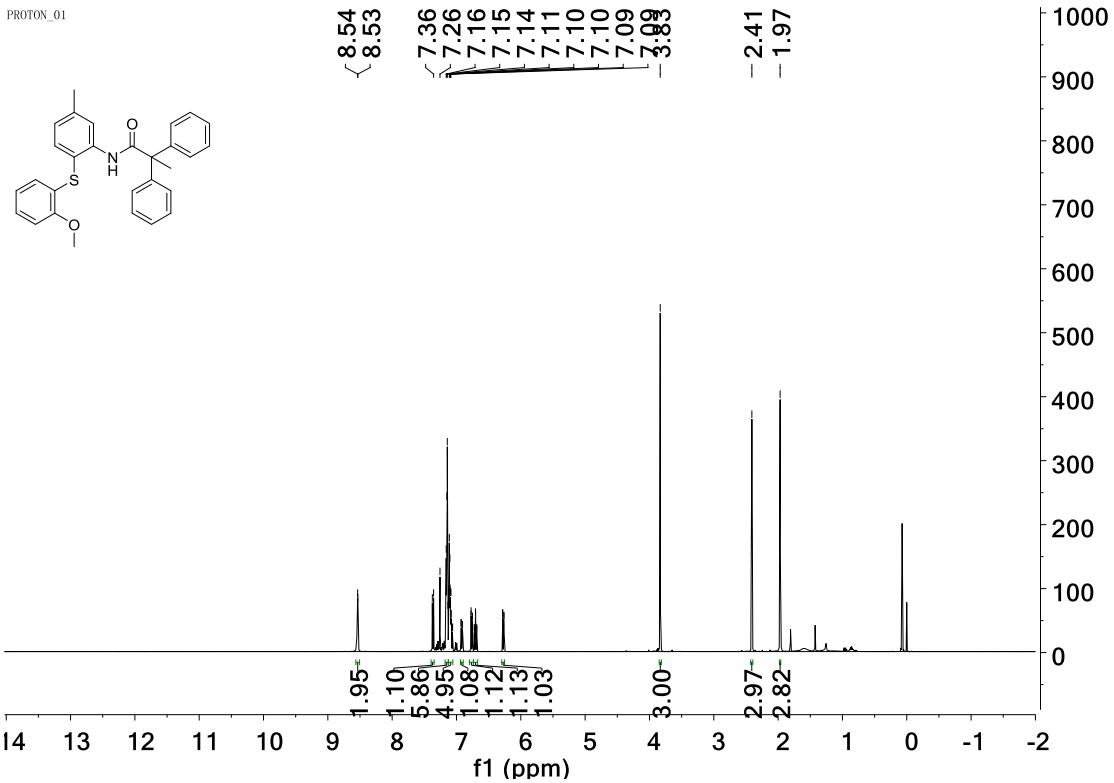
127.18
126.09
125.03
124.02
119.72
64.20
44.48
19.23
f1 (ppm)


PROTON_01
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7.15
7.14
7.11
7.10
7.10
7.09
7.04
3.83
2.41
1.97
1.95
1.10
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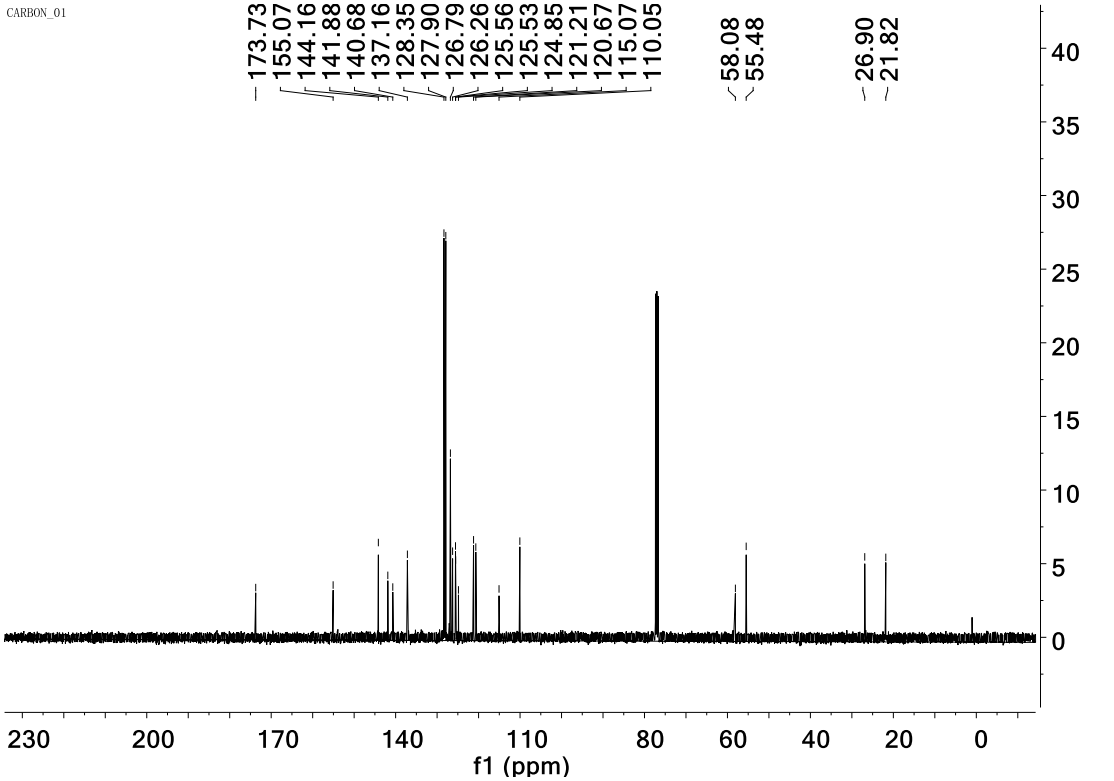
4.95
1.08
1.12
1.13
1.03
3.00
2.97
2.82
f1 (ppm)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140.68
137.16
128.35
127.90
126.79
126.26
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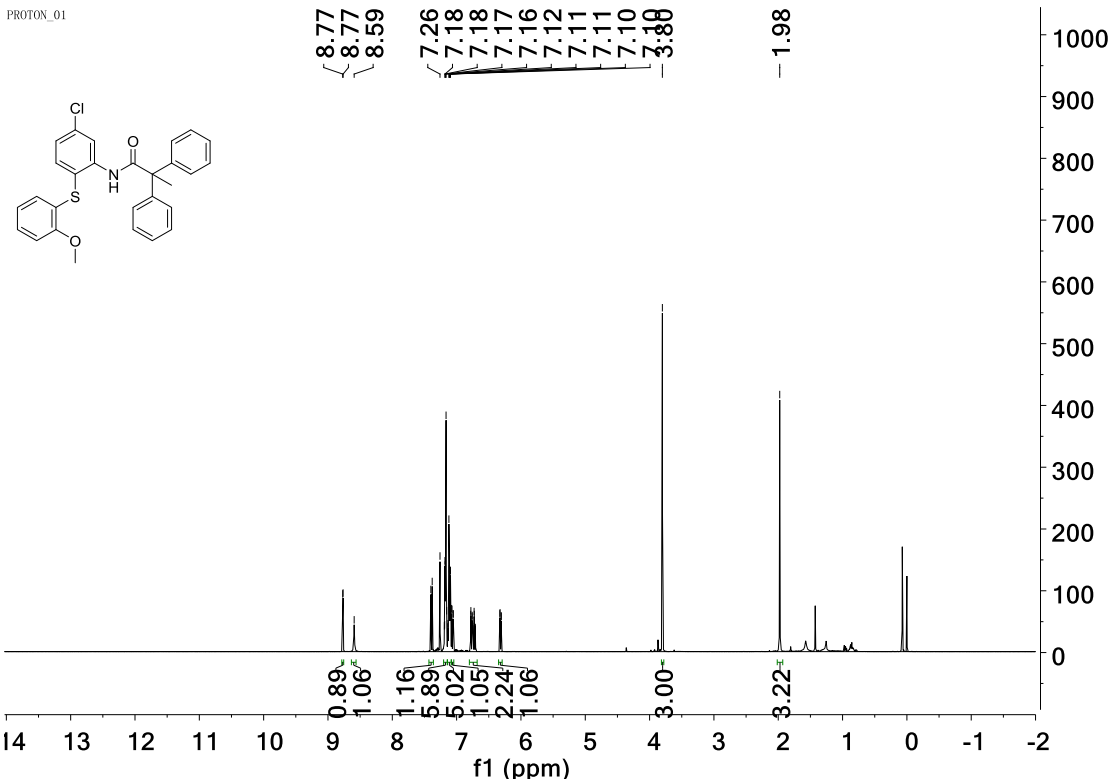
115.07
110.05
58.08
55.48
26.90
21.82
f1 (ppm)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7.18
7.17
7.16
7.12
7.11
7.11
7.10
3.80
1.98
Cl
O
N
H
S
O
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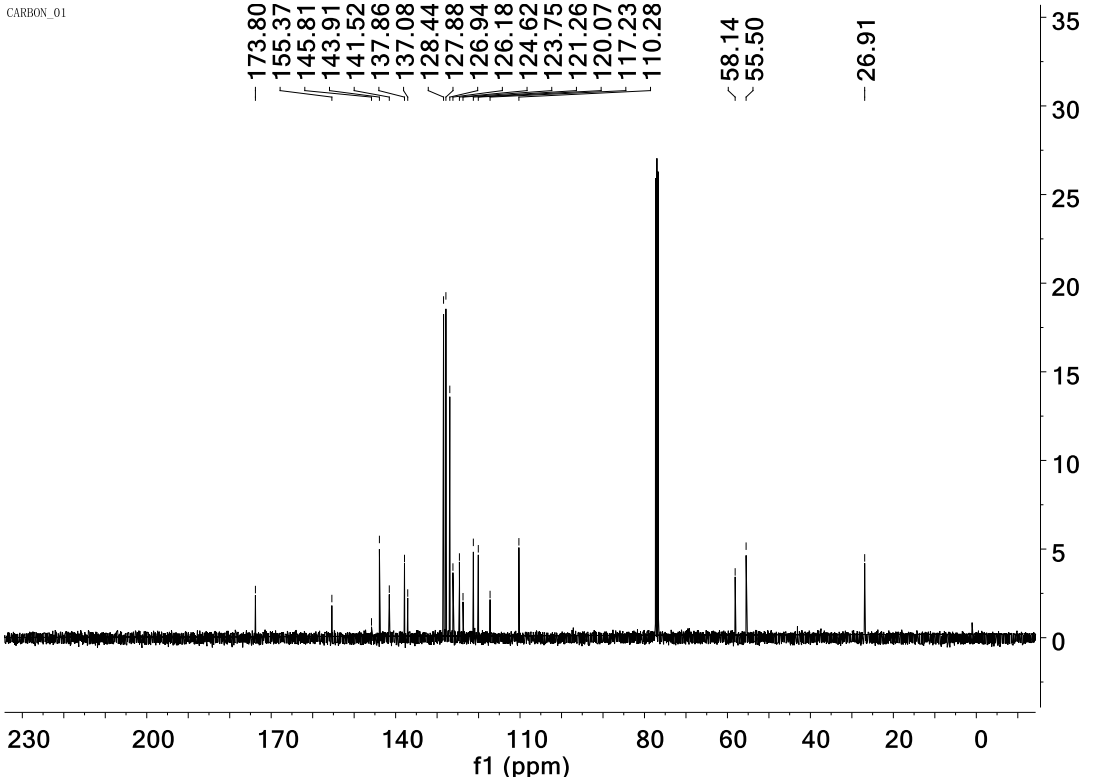
1.16
5.89
5.02
1.05
2.24
1.06
3.00
3.22
f1 (ppm)


CARBON_01
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141.52
137.86
137.08
128.44
127.88
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120.07
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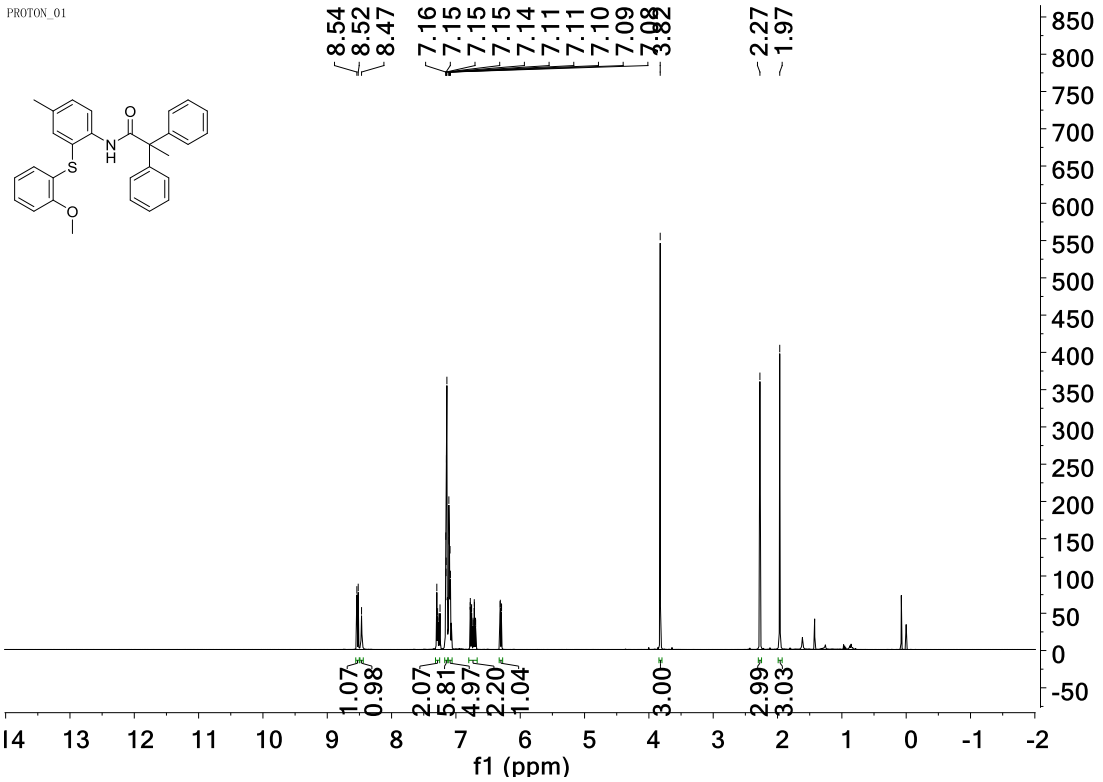
58.14
55.50
26.91
f1 (ppm)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7.15
7.14
7.11
7.11
7.10
7.09
3.82
2.27
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2.07
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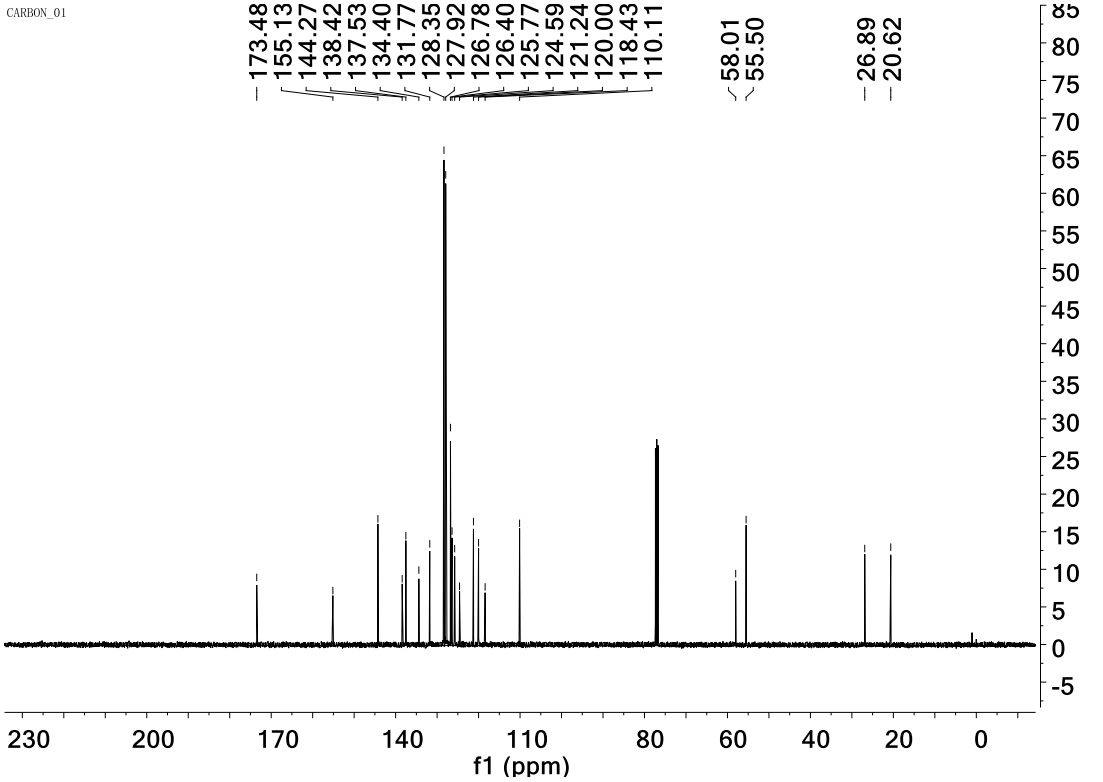
4.97
2.20
1.04
3.00
2.99
3.03
f1 (ppm)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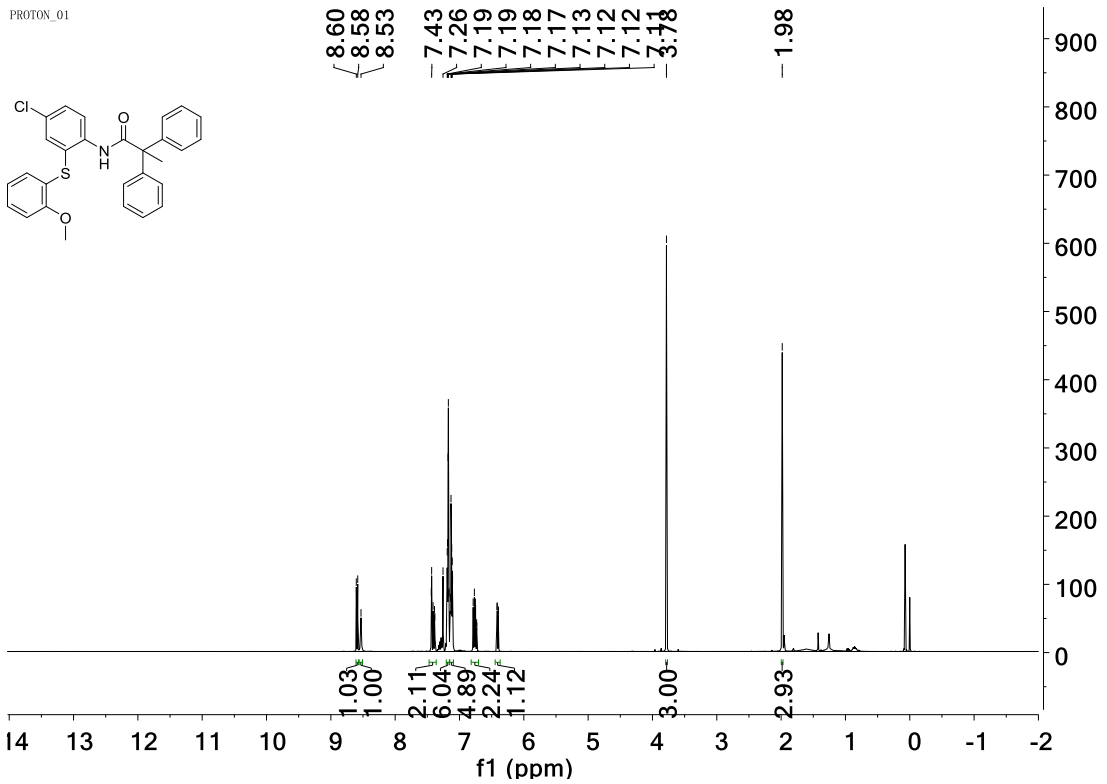
58.01
55.50
26.89
20.62
f1 (ppm)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7.17
7.13
7.12
7.12
7.11
3.78
1.98
Cl
O
N
H
S
O
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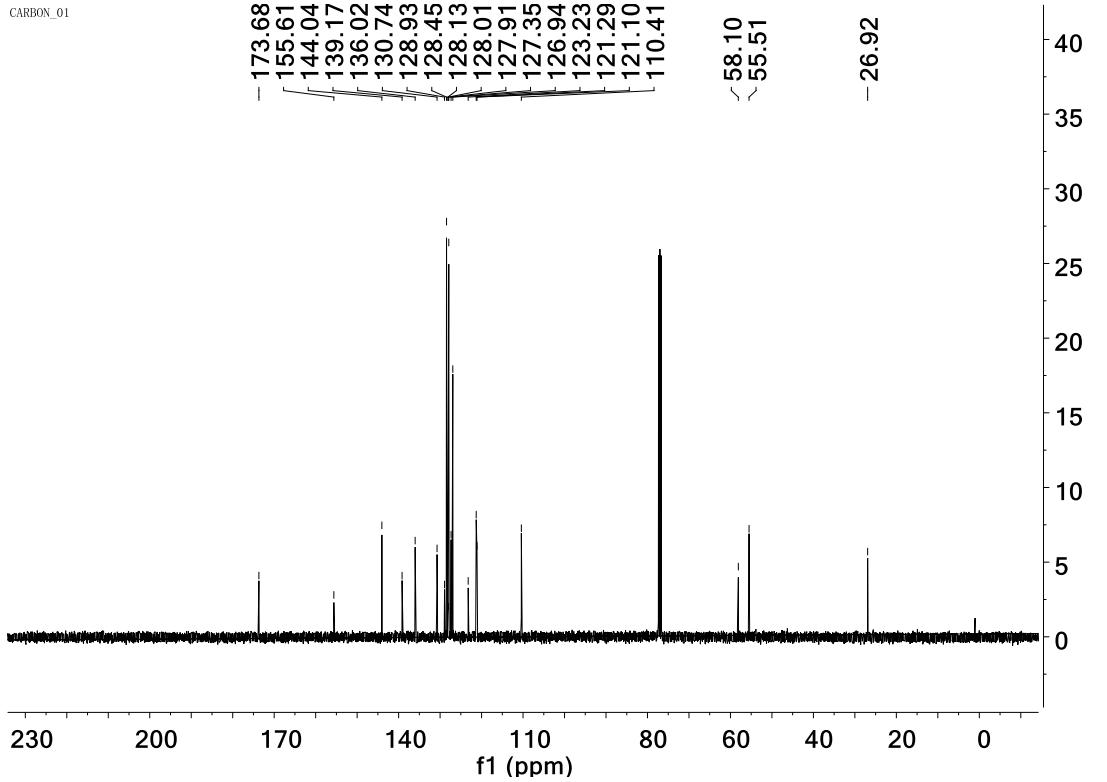
1.00
2.11
6.04
4.89
2.24
1.12
3.00
2.93
f1 (ppm)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130.74
128.93
128.45
128.13
128.01
127.91
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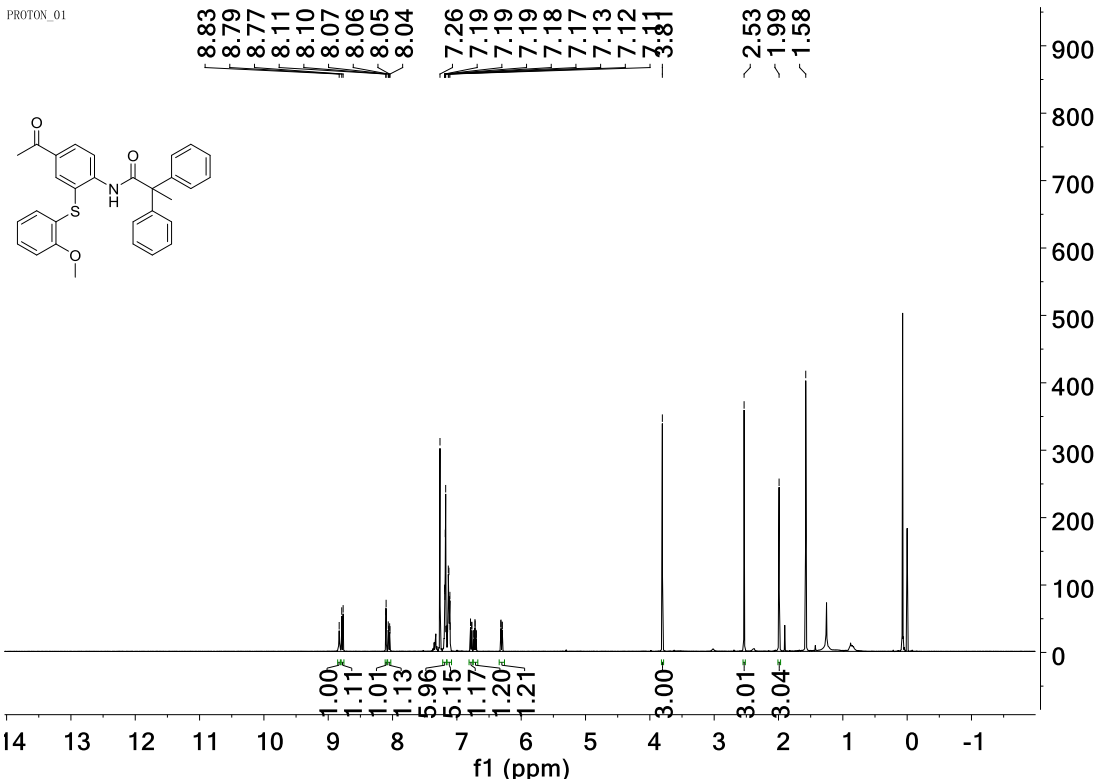
126.94
123.23
121.29
121.10
110.41
58.10
55.51
26.92
f1 (ppm)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8.07
8.06
8.05
8.04
7.26
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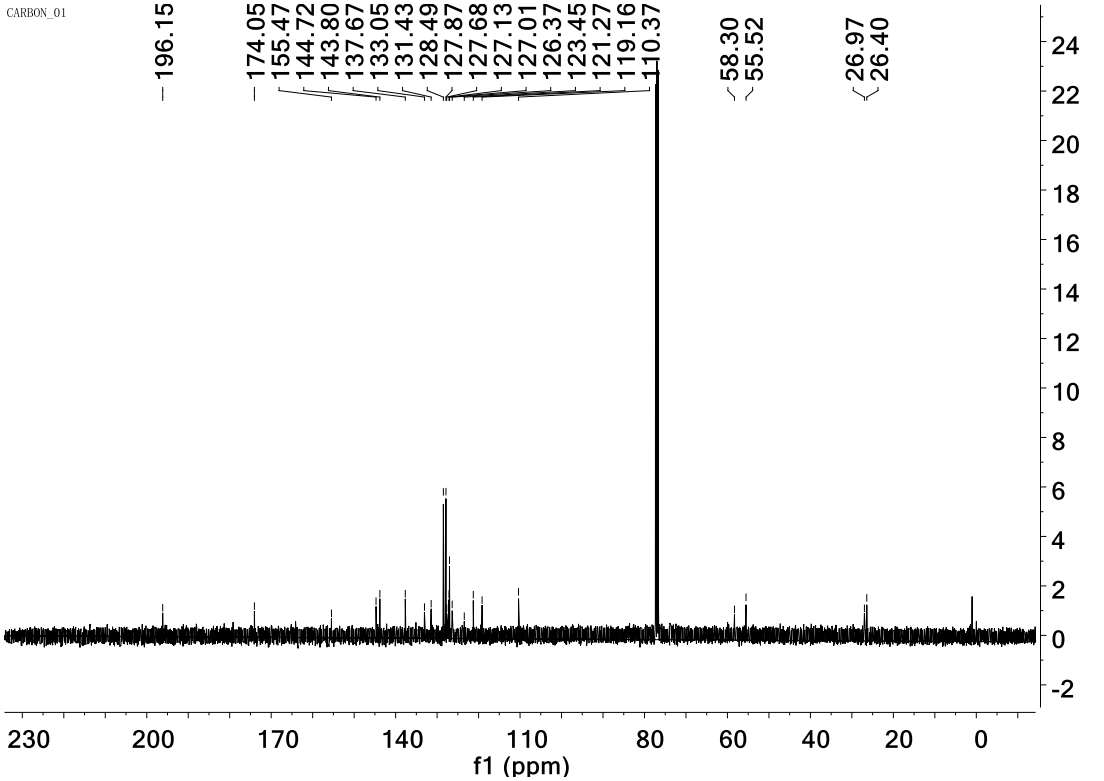
7.19
7.19
7.18
7.17
7.13
7.12
7.11
3.81
2.53
1.99
1.58
1.00
1.11
1.01
1.13
5.96
5.15
1.17
1.20
1.21
3.00
3.01
3.04
f1 (ppm)


CARBON_01
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133.05
131.43
128.49
127.87
127.68
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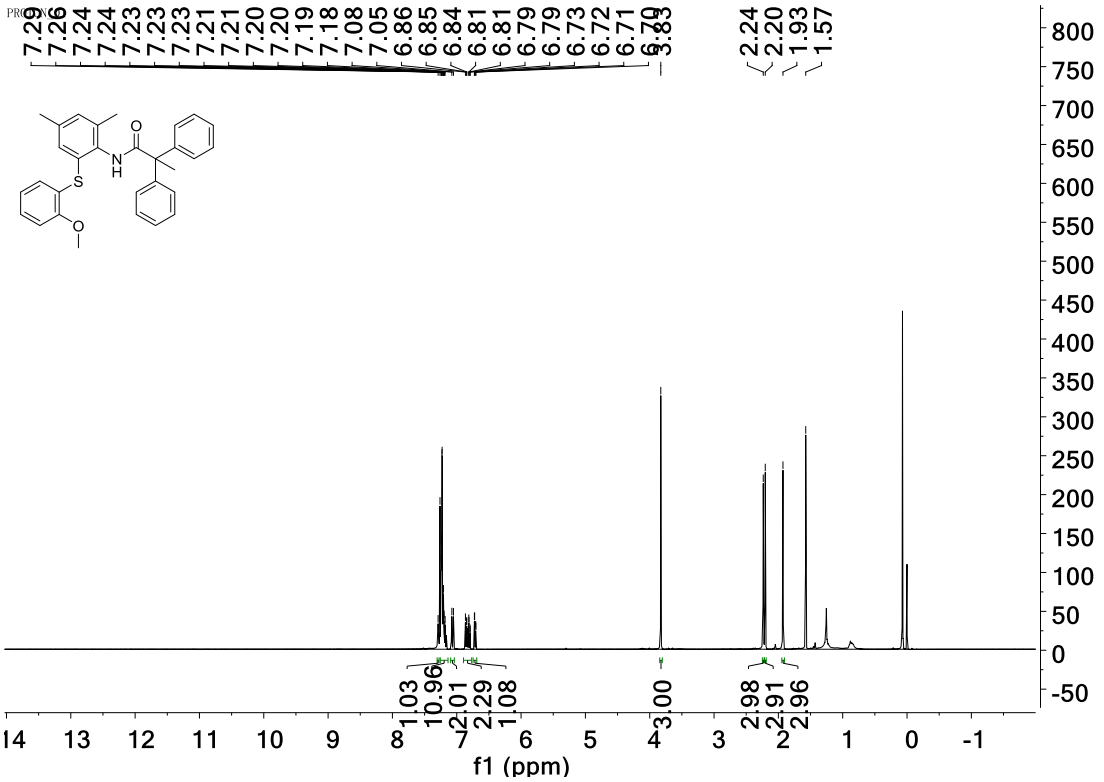
123.45
121.27
119.16
110.37
58.30
55.52
26.97
26.40
f1 (ppm)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7.24
7.23
7.23
7.23
7.21
7.21
7.20
7.20
7.19
7.18
7.08
7.05
6.86
6.85
6.84
6.81
6.81
6.79
6.79
6.73
6.72
6.71
6.70
3.83
2.24
2.20
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1.57
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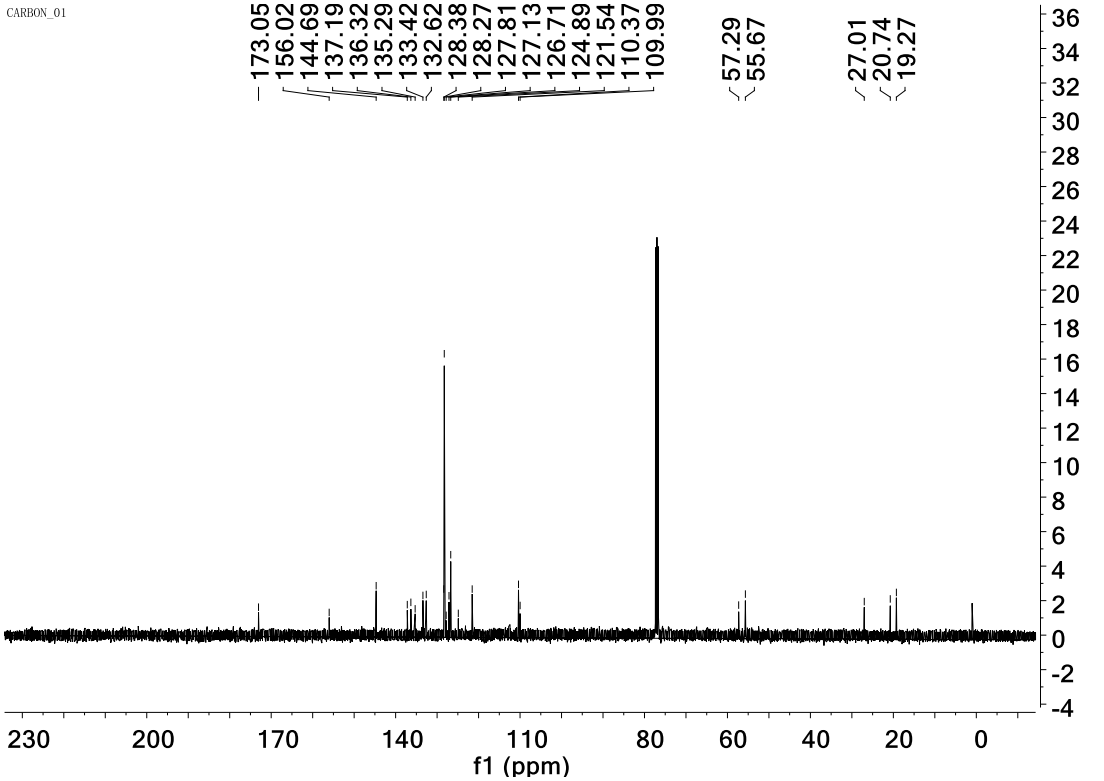
2.29
1.08
3.00
2.98
2.91
2.96
f1 (ppm)


CARBON_01
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135.29
133.42
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128.38
128.27
127.81
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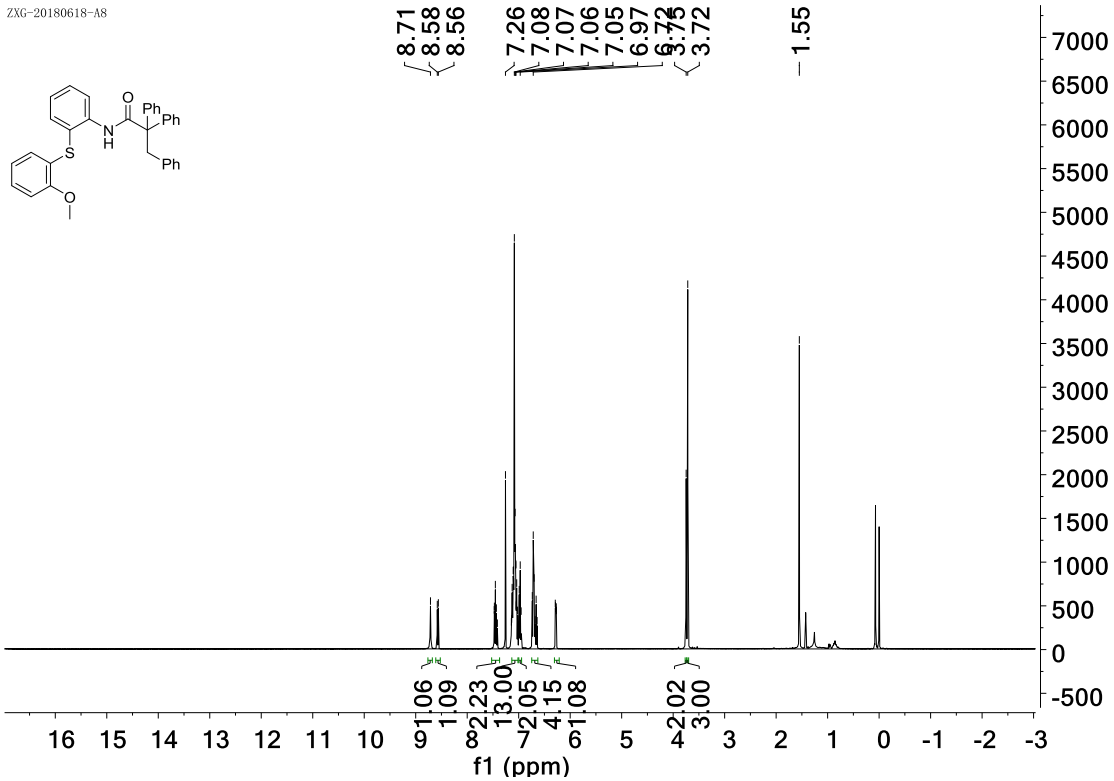
109.99
57.29
55.67
27.01
20.74
19.27
f1 (ppm)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7.07
7.06
7.05
6.97
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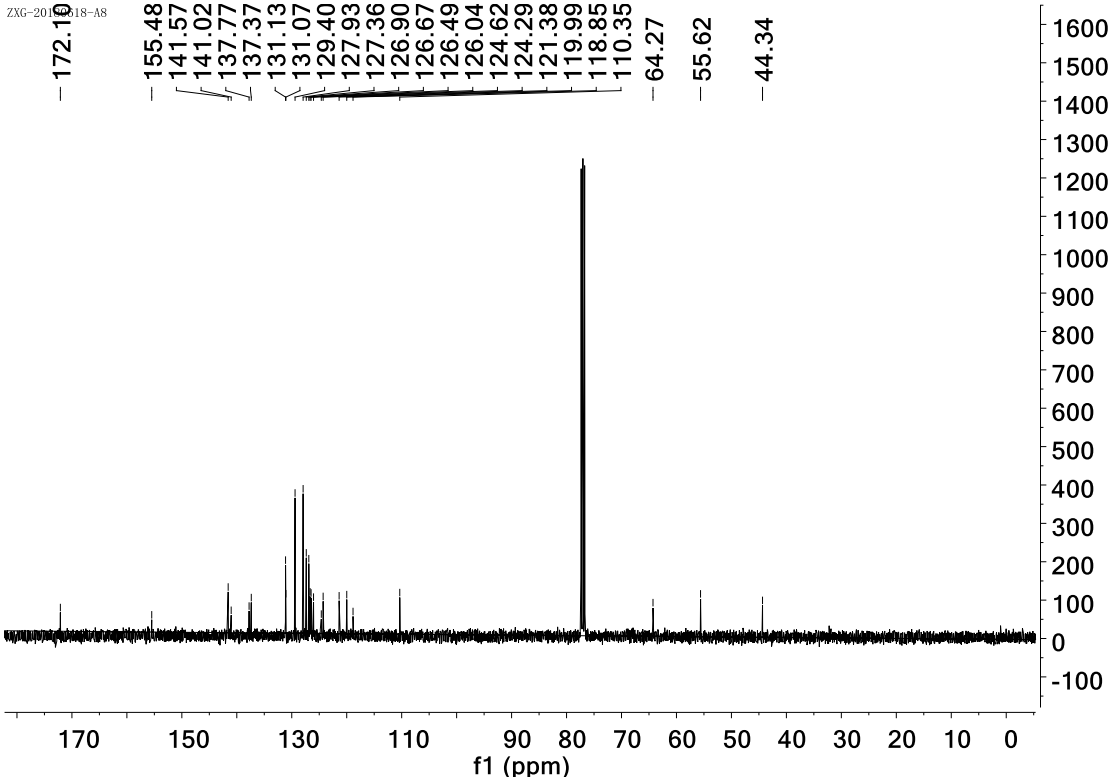
1.09
2.23
13.00
2.05
4.15
1.08
2.02
3.00
f1 (ppm)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124.29
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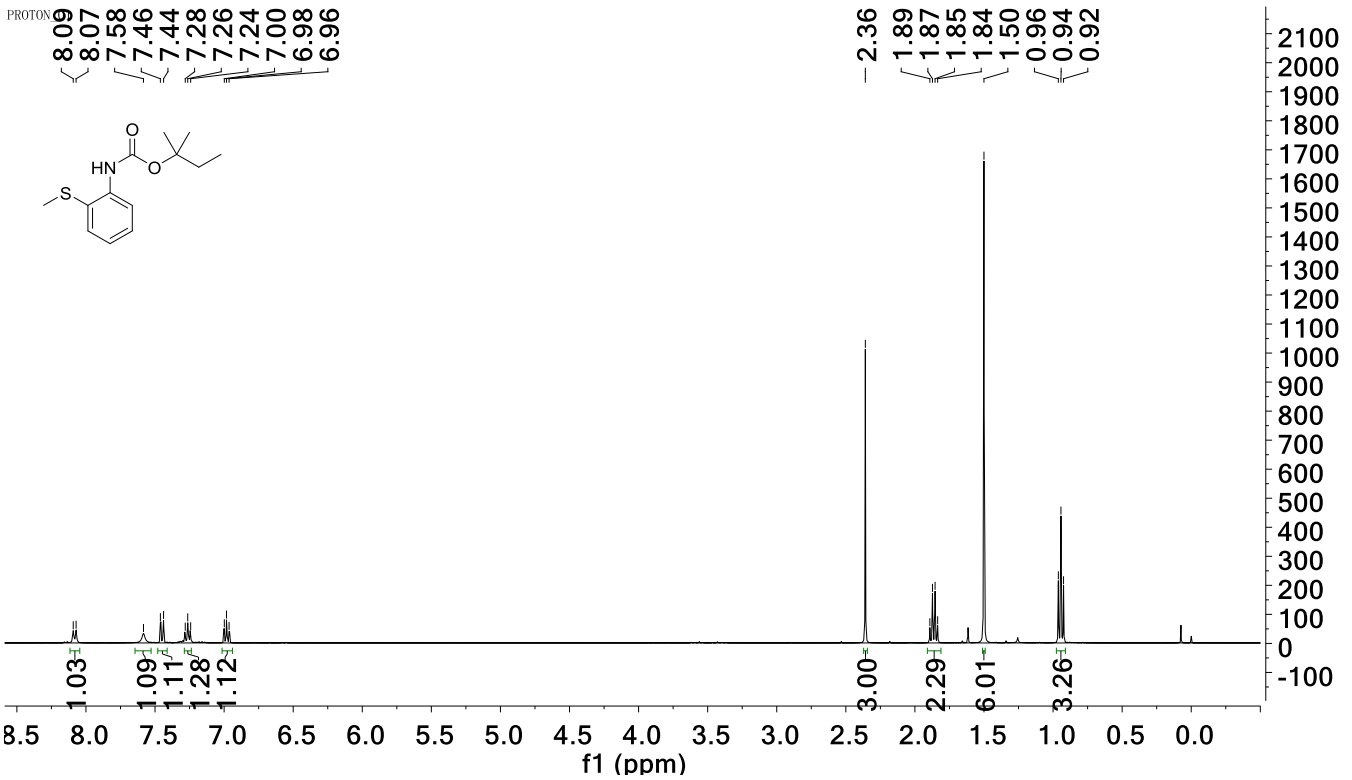
64.27
55.62
44.34
f1 (ppm)


PROTON
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7.26
7.24
7.00
6.98
6.96
2.36
1.89
1.87
1.85
1.84
1.50
0.96
0.94
0.92
HN
O
O
S
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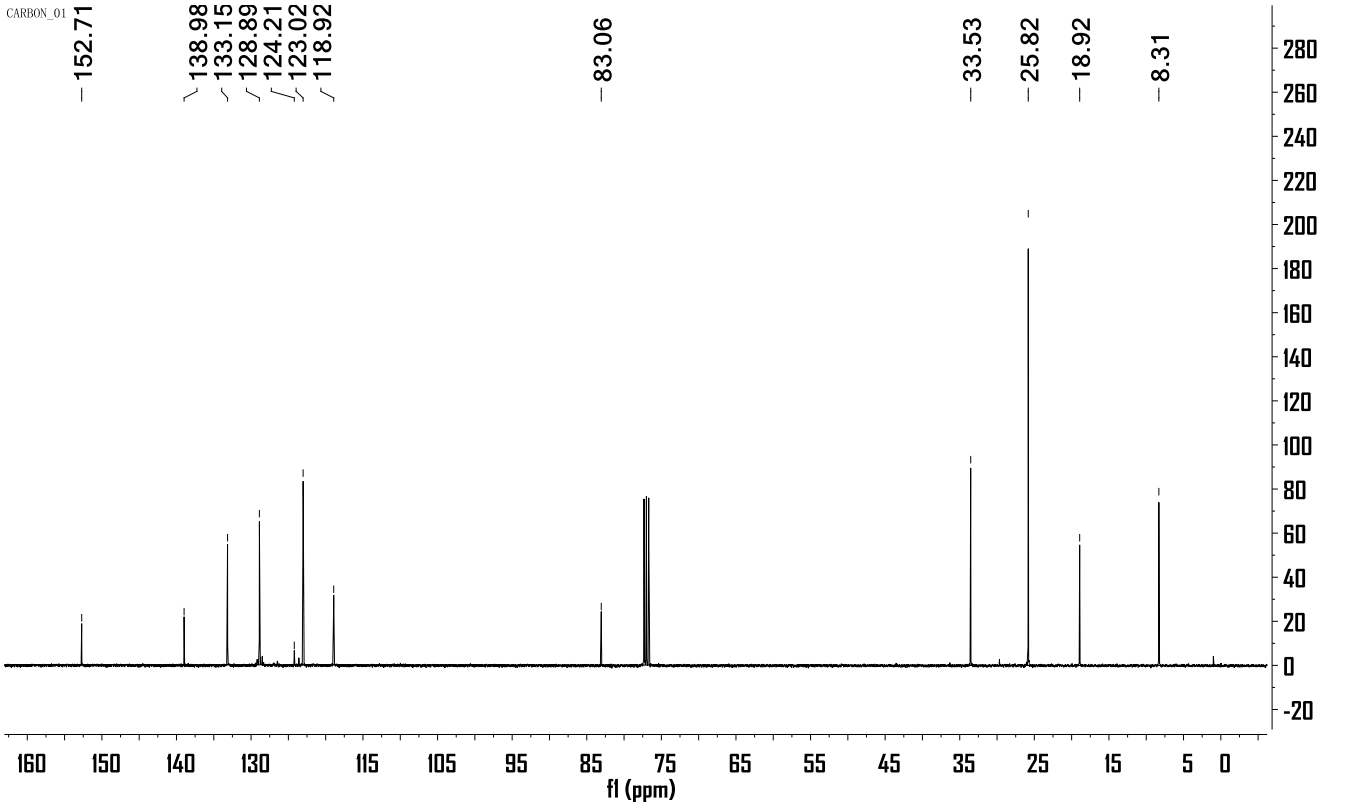
1.09
1.11
1.28
1.12
3.00
2.29
6.01
3.26
f1 (ppm)


CARBON_01
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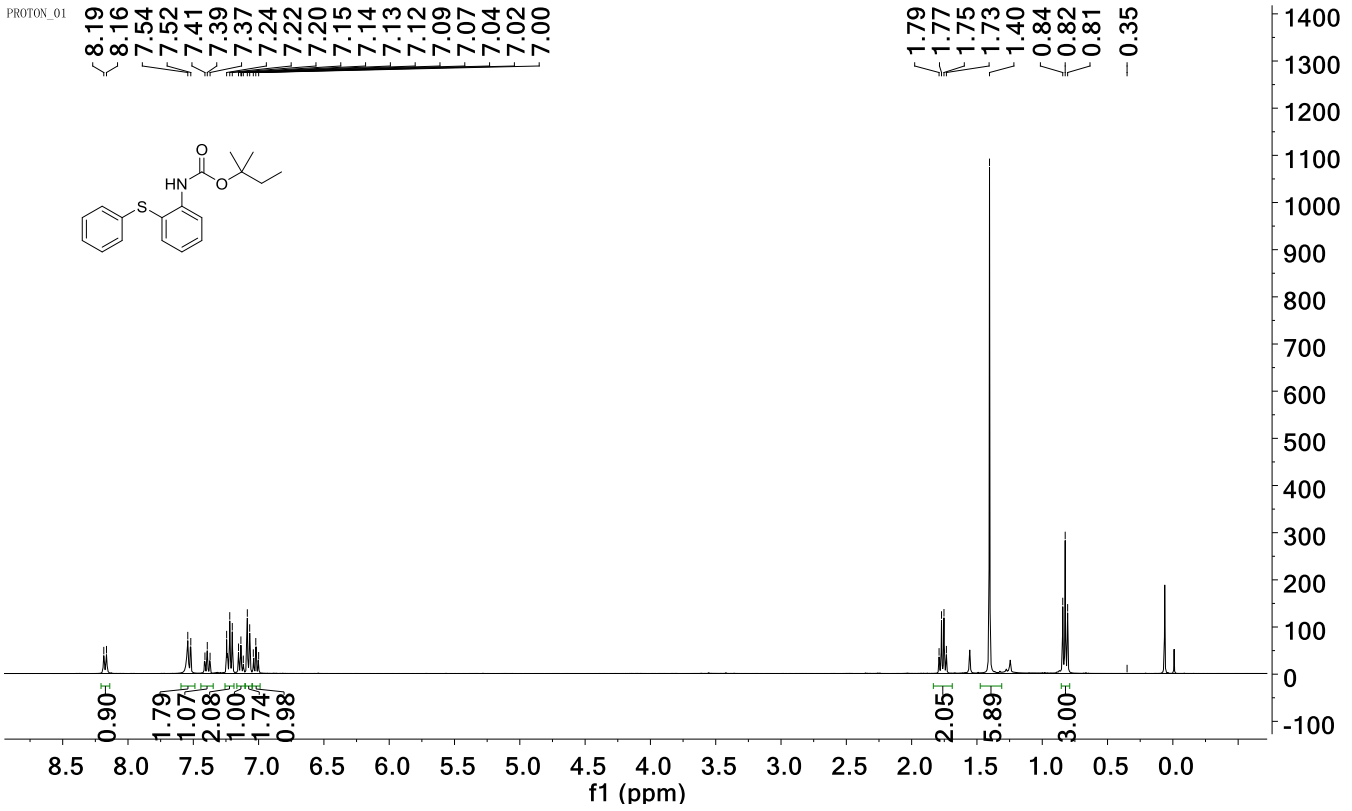
124.21
123.02
118.92
83.06
33.53
25.82
18.92
8.31
f1 (ppm)


PROTON_01
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7.22
7.20
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7.12
7.09
7.07
7.04
7.02
7.00
1.79
1.77
1.75
1.73
1.40
0.84
0.82
0.81
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0.90
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1.07
2.08
1.00
1.74
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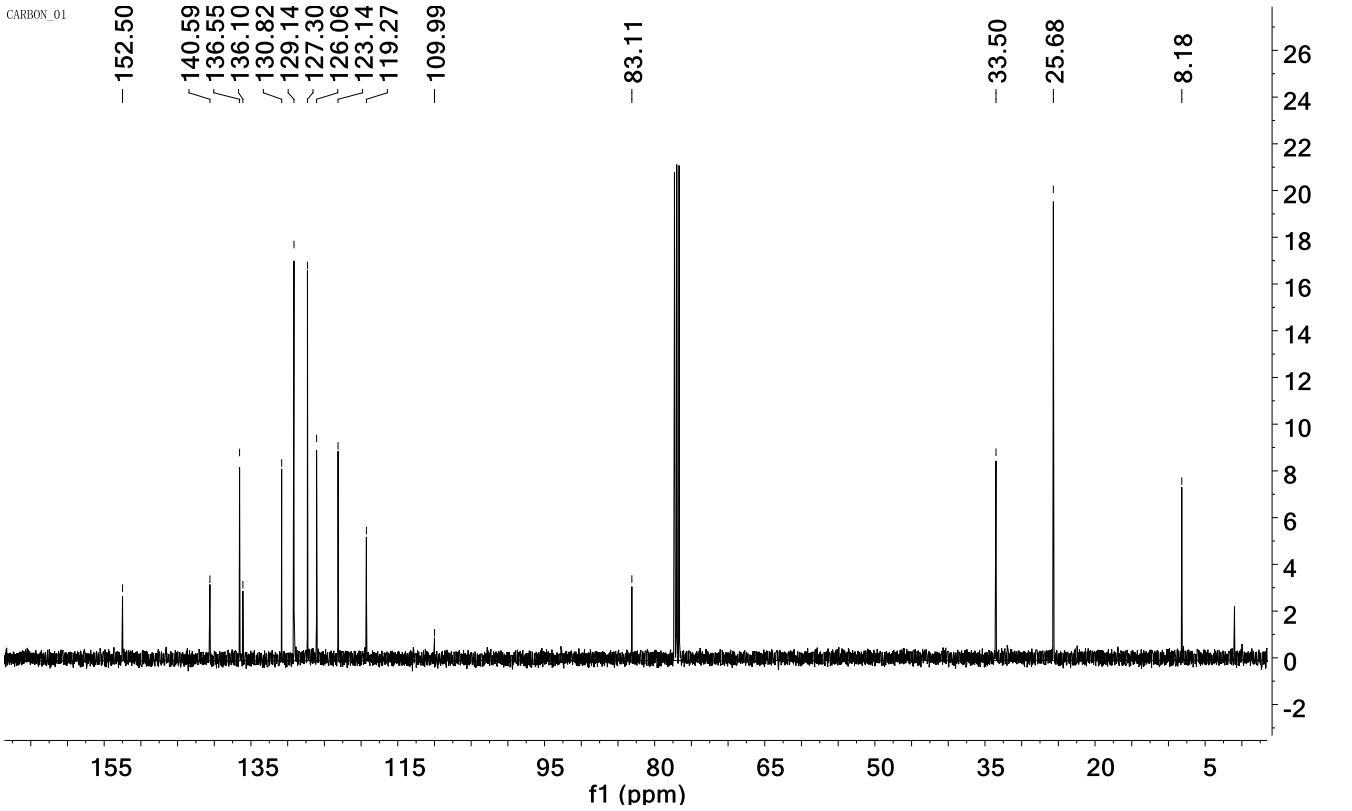
2.05
5.89
3.00
f1 (ppm)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123.14
119.27
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83.11
33.50
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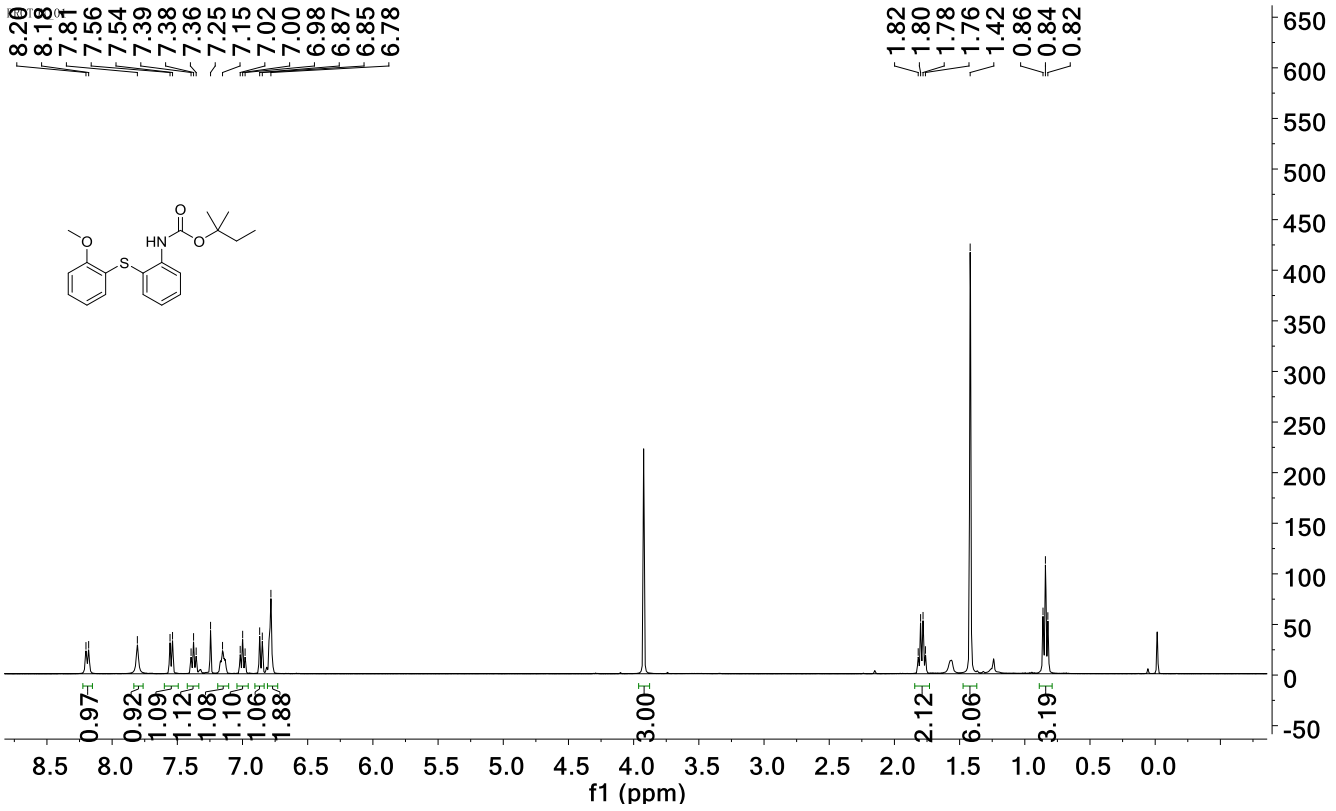
8.18
f1 (ppm)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7.15
7.02
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6.87
6.85
6.78
1.82
1.80
1.78
1.76
1.42
0.86
0.84
0.82
O
HN
O
O
S
0.97
0.92
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1.08
1.10
1.06
1.88
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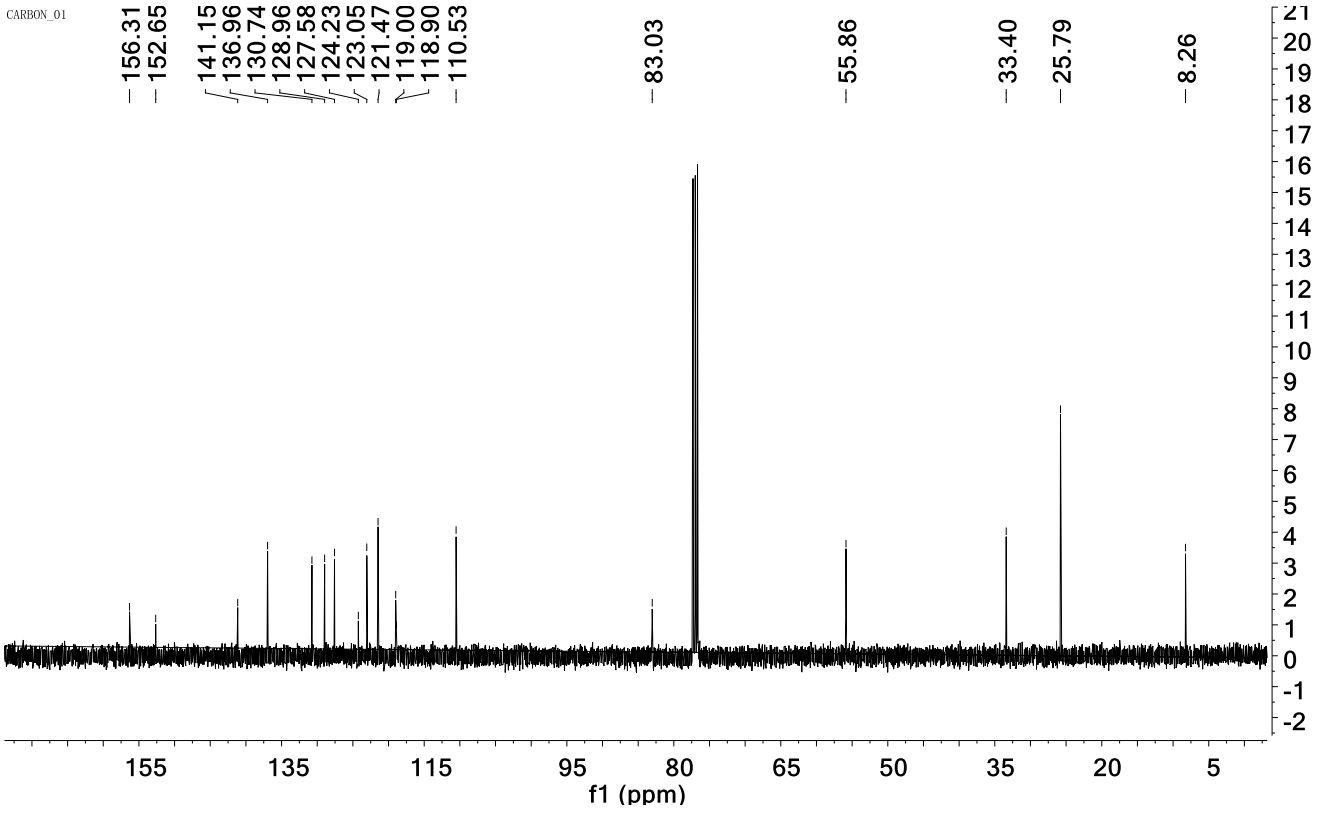
f1 (ppm)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110.53
83.03
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33.40
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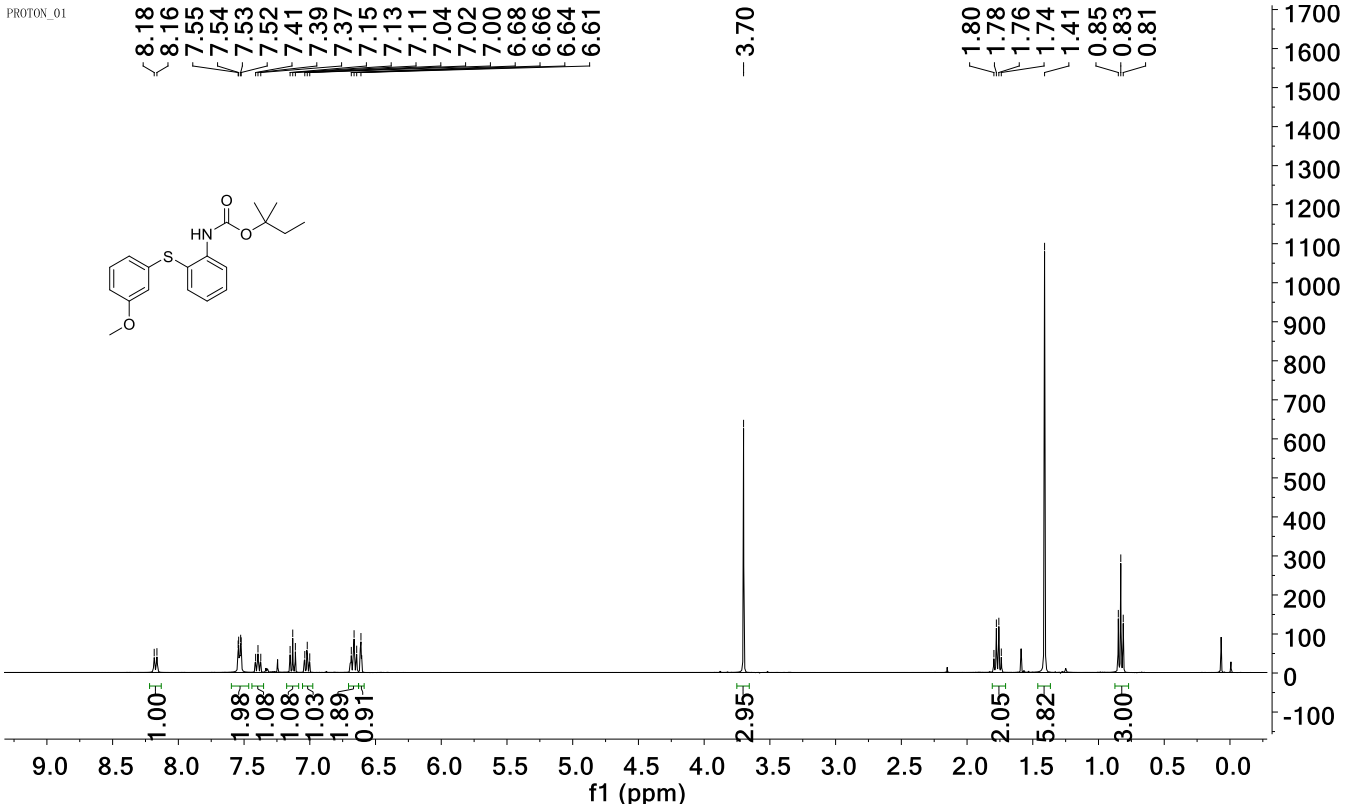
8.26
f1 (ppm)


PROTON_01
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7.41
7.39
7.37
7.15
7.13
7.11
7.04
7.02
7.00
6.68
6.66
6.64
6.61
3.70
1.80
1.78
1.76
1.74
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0.83
0.81
HN
O
O
S
O
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1.98
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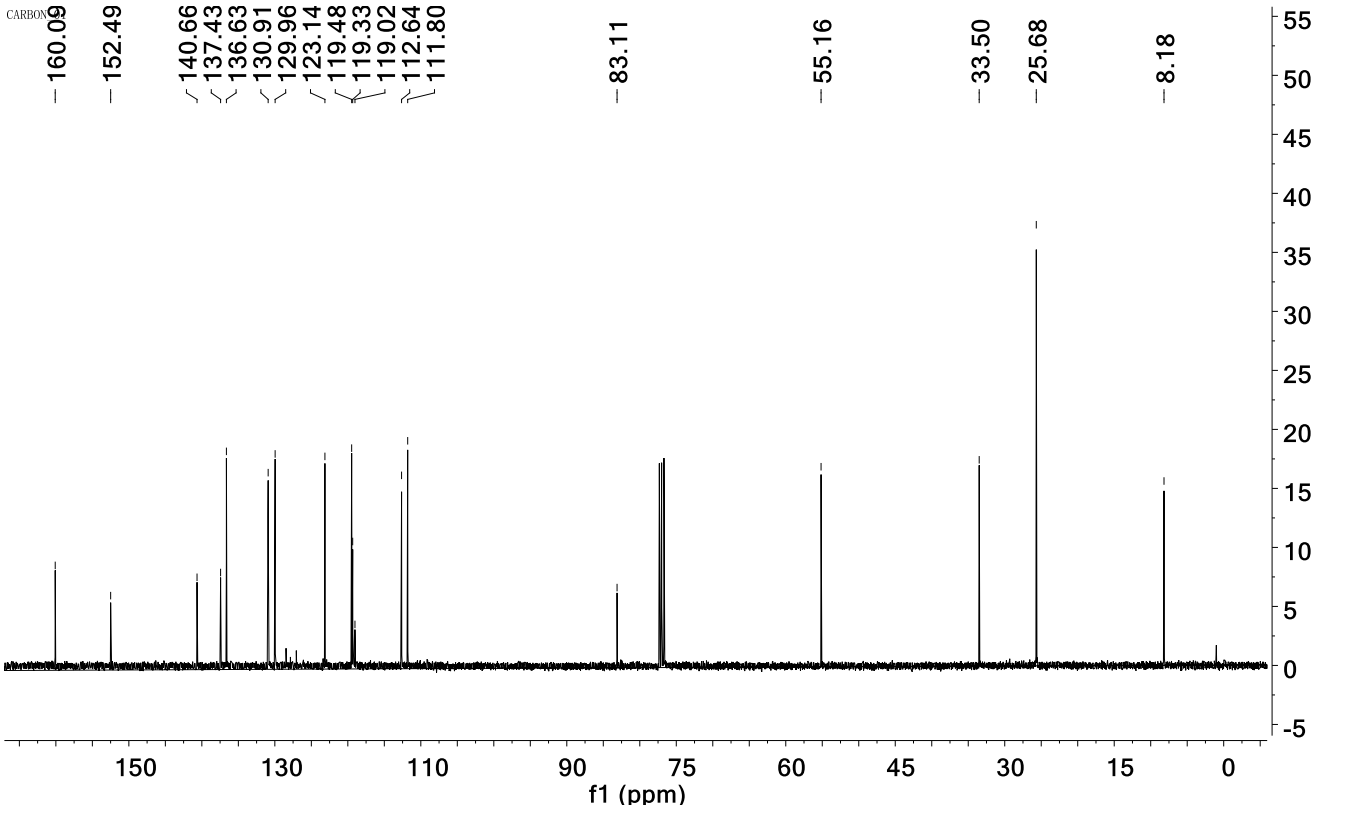
1.08
1.03
1.89
0.91
2.95
2.05
5.82
3.00
f1 (ppm)


CARBON
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83.11
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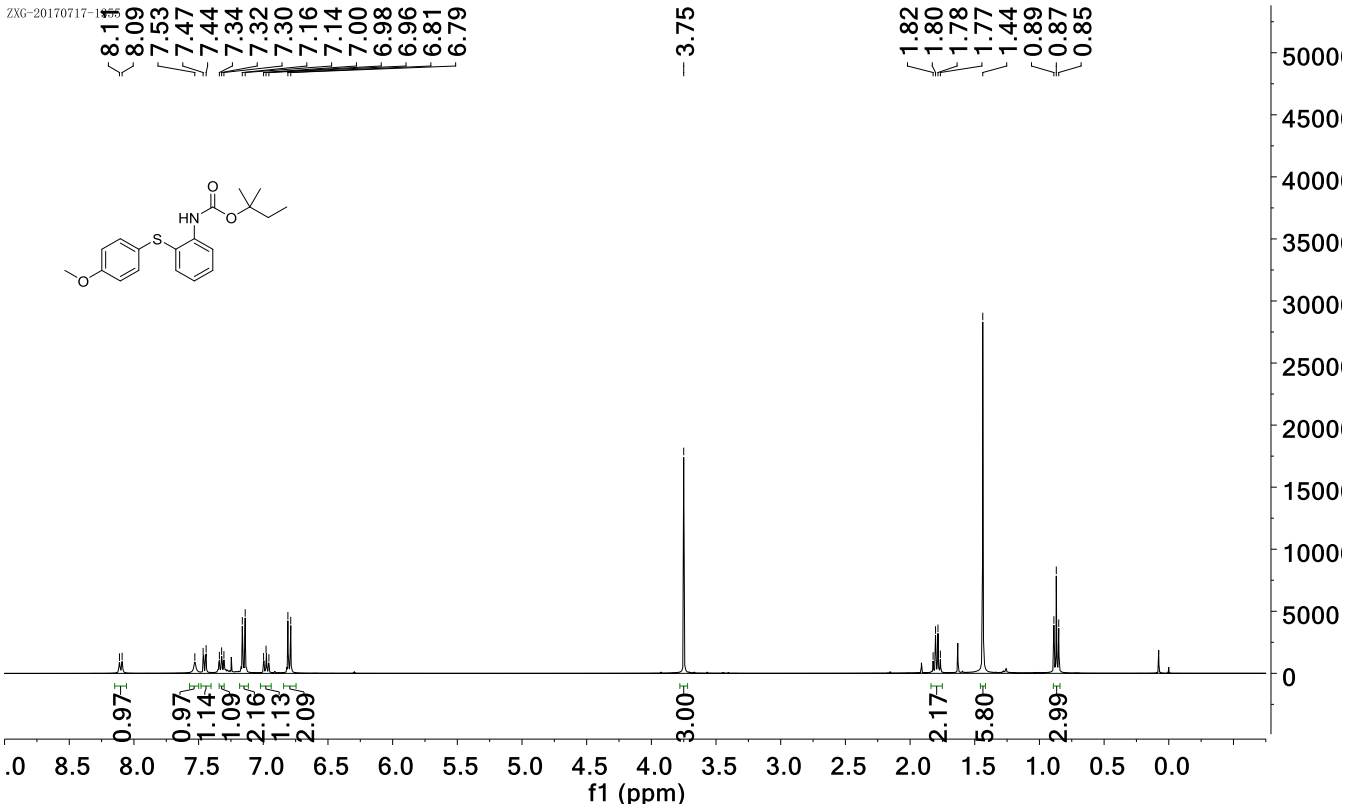
33.50
25.68
8.18
f1 (ppm)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6.81
6.79
3.75
1.82
1.80
1.78
1.77
1.44
0.89
0.87
0.85
HN
O
O
S
O
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0.97
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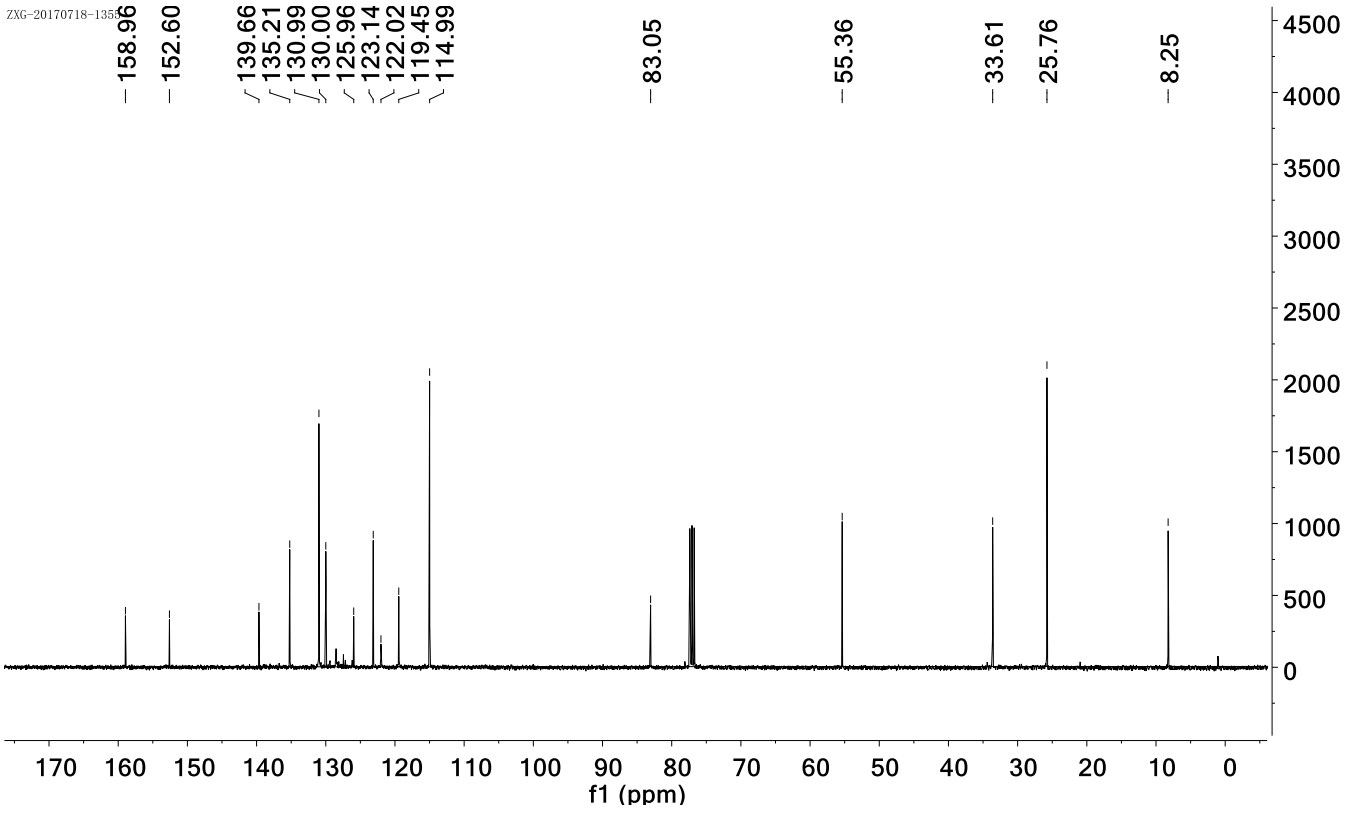
1.13
2.09
3.00
2.17
5.80
2.99
f1 (ppm)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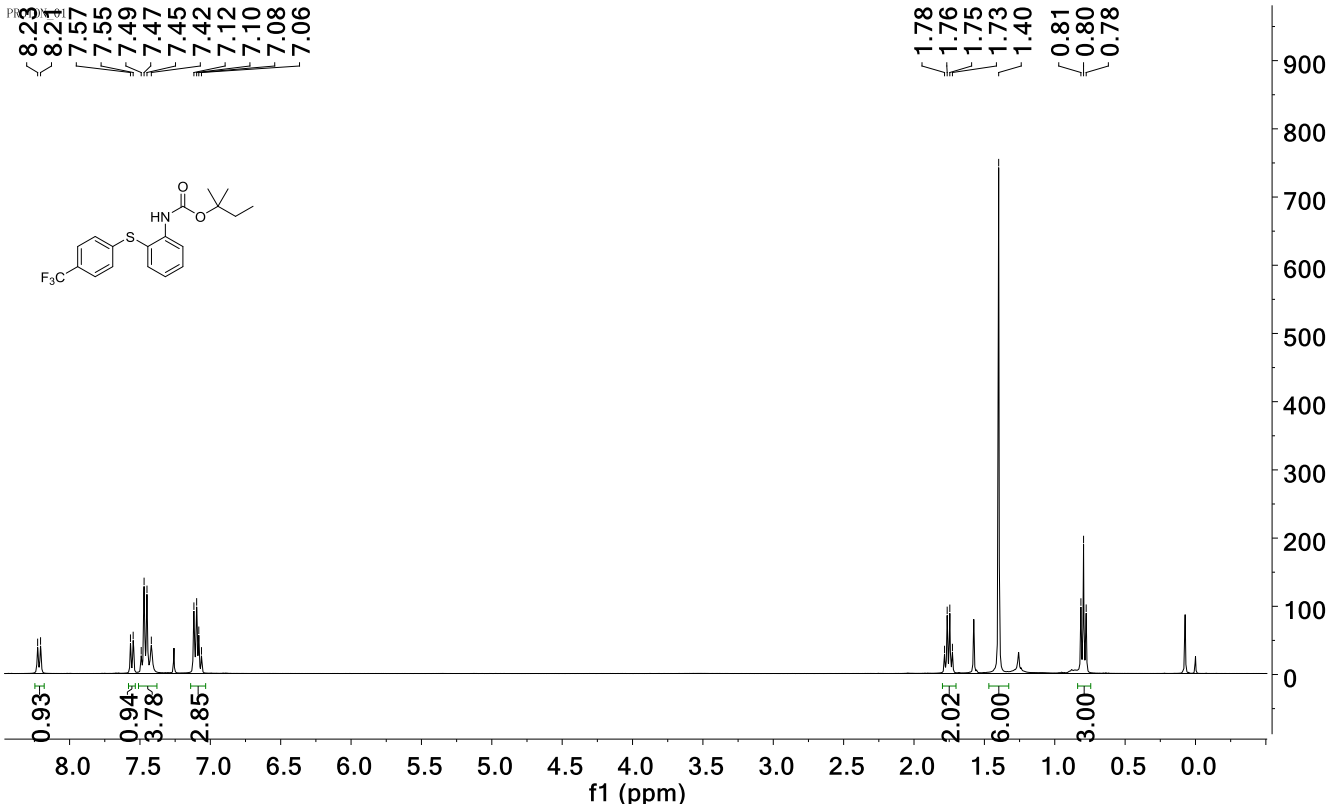
f1 (ppm)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7.06
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1.76
1.75
1.73
1.40
0.81
0.80
0.78
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S
F3C
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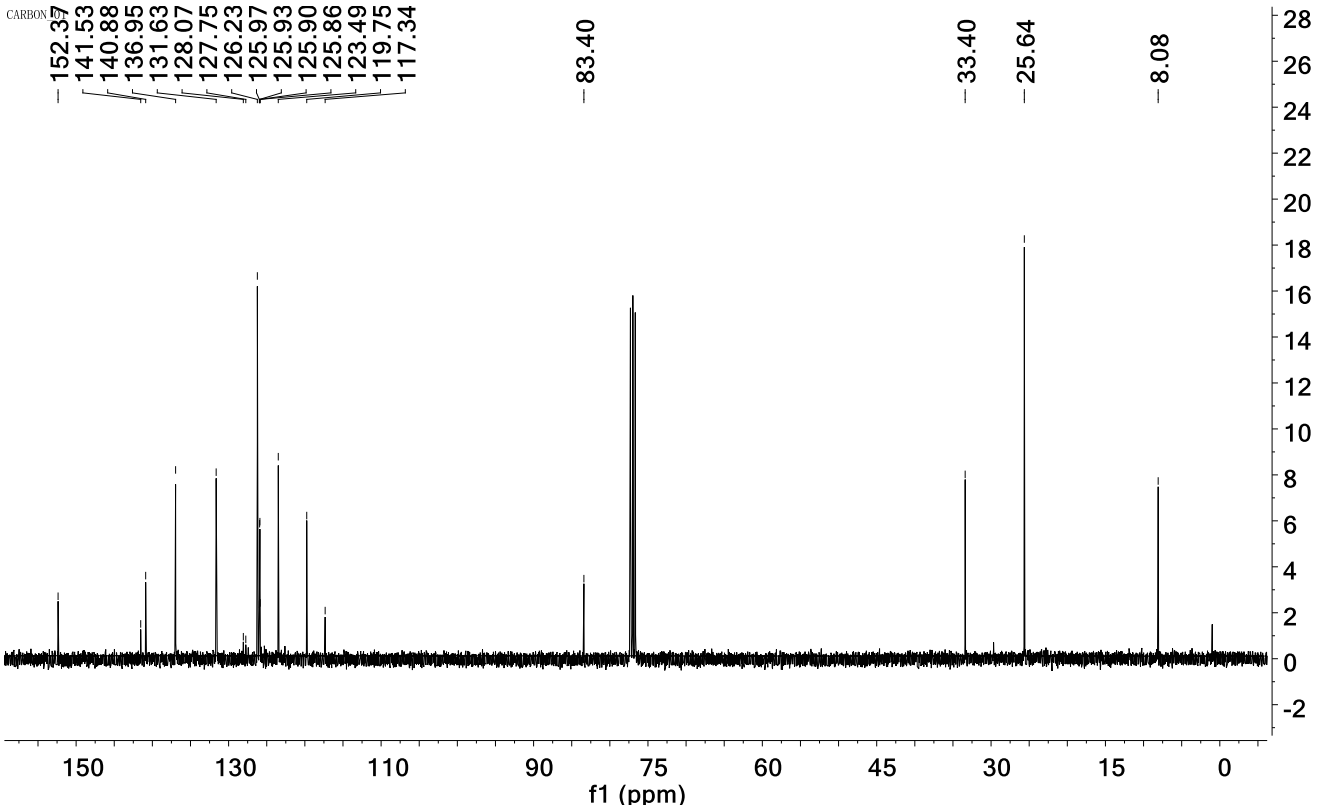
0.94
3.78
2.85
2.02
6.00
3.00
f1 (ppm)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127.75
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119.75
117.34
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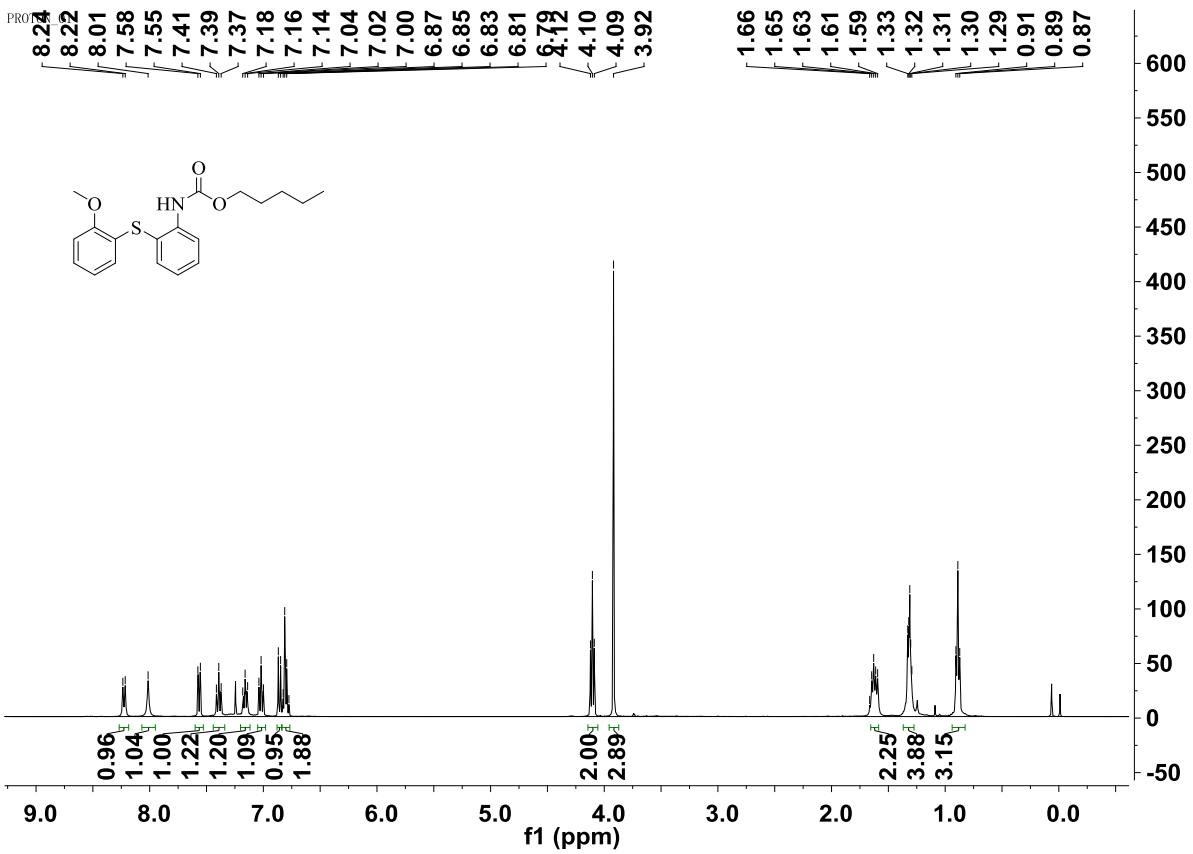
33.40
25.64
8.08
f1 (ppm)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7.14
7.04
7.02
7.00
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6.85
6.83
6.81
6.79
4.12
4.10
4.09
3.92
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1.65
1.63
1.61
1.59
1.33
1.32
1.31
1.30
1.29
0.91
0.89
0.87
O
HN
O
O
S
0.96
1.04
1.00
1.22
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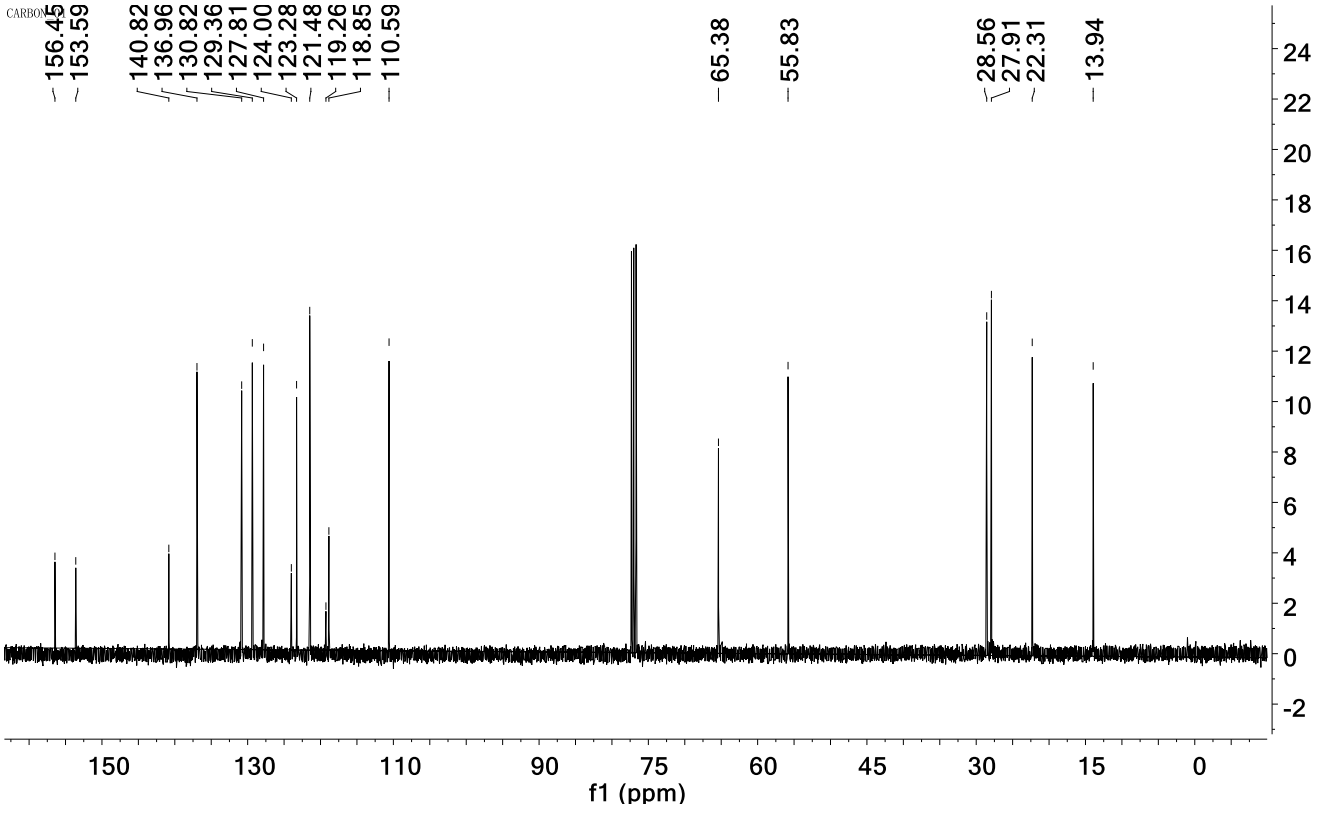
1.09
0.95
1.88
2.00
2.89
2.25
3.88
3.15
f1 (ppm)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136.96
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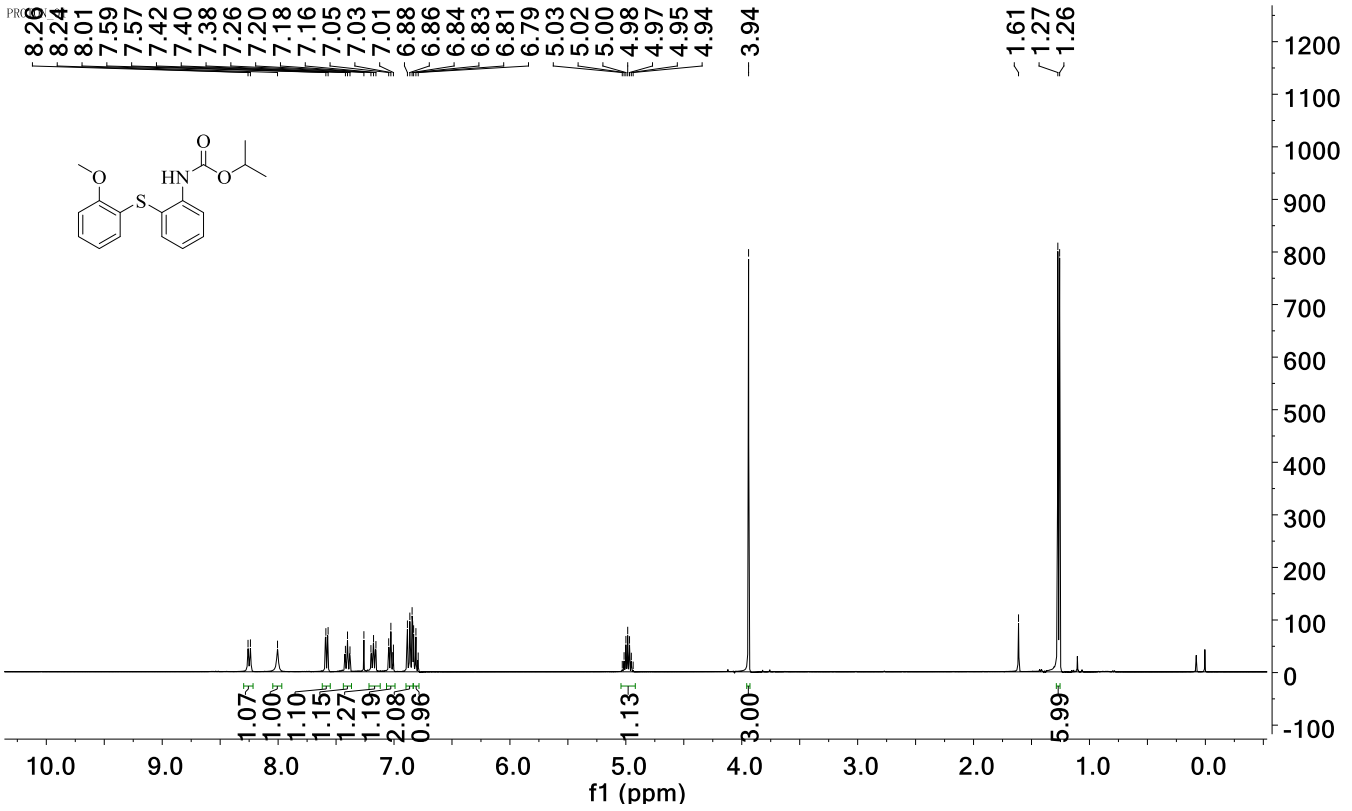
28.56
27.91
22.31
13.94
f1 (ppm)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7.03
7.01
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6.86
6.84
6.83
6.81
6.79
5.03
5.02
5.00
4.98
4.97
4.95
4.94
3.94
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1.27
1.26
O
HN
O
O
S
1.07
1.00
1.10
1.15
1.27
1.19
2.08
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1.13
3.00
5.99
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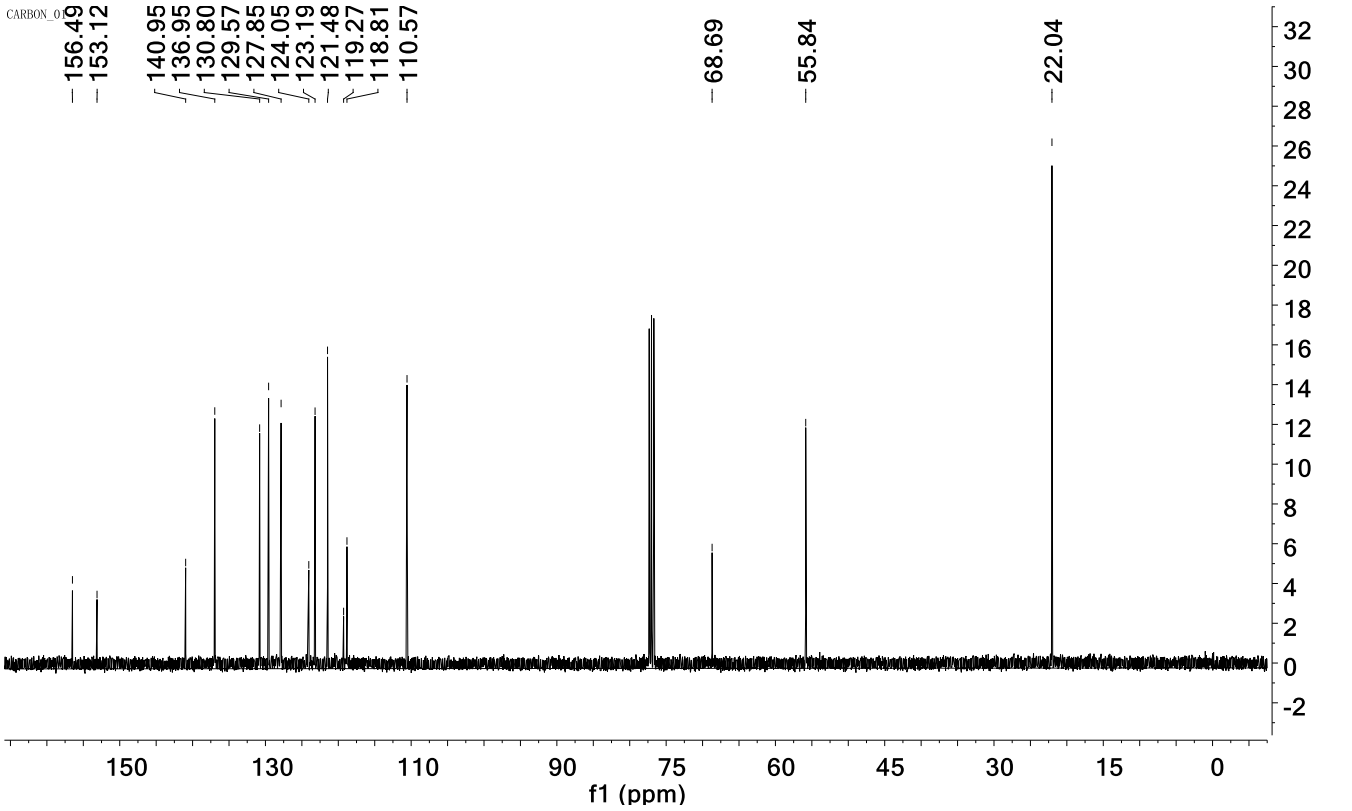
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110
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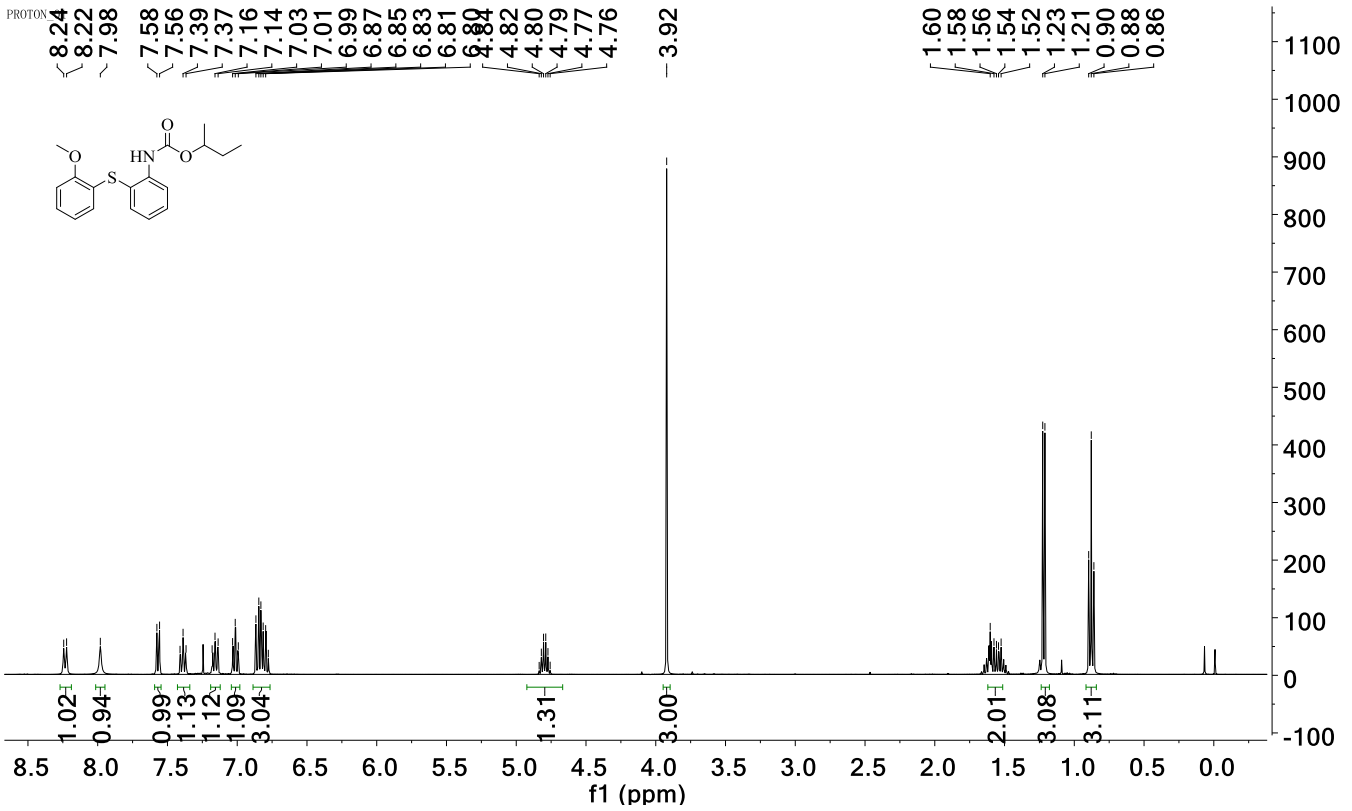
0
f1 (ppm)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6.85
6.83
6.81
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4.80
4.79
4.77
4.76
3.92
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1.58
1.56
1.54
1.52
1.23
1.21
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0.88
0.86
O
HN
O
O
S
1.02
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1.31
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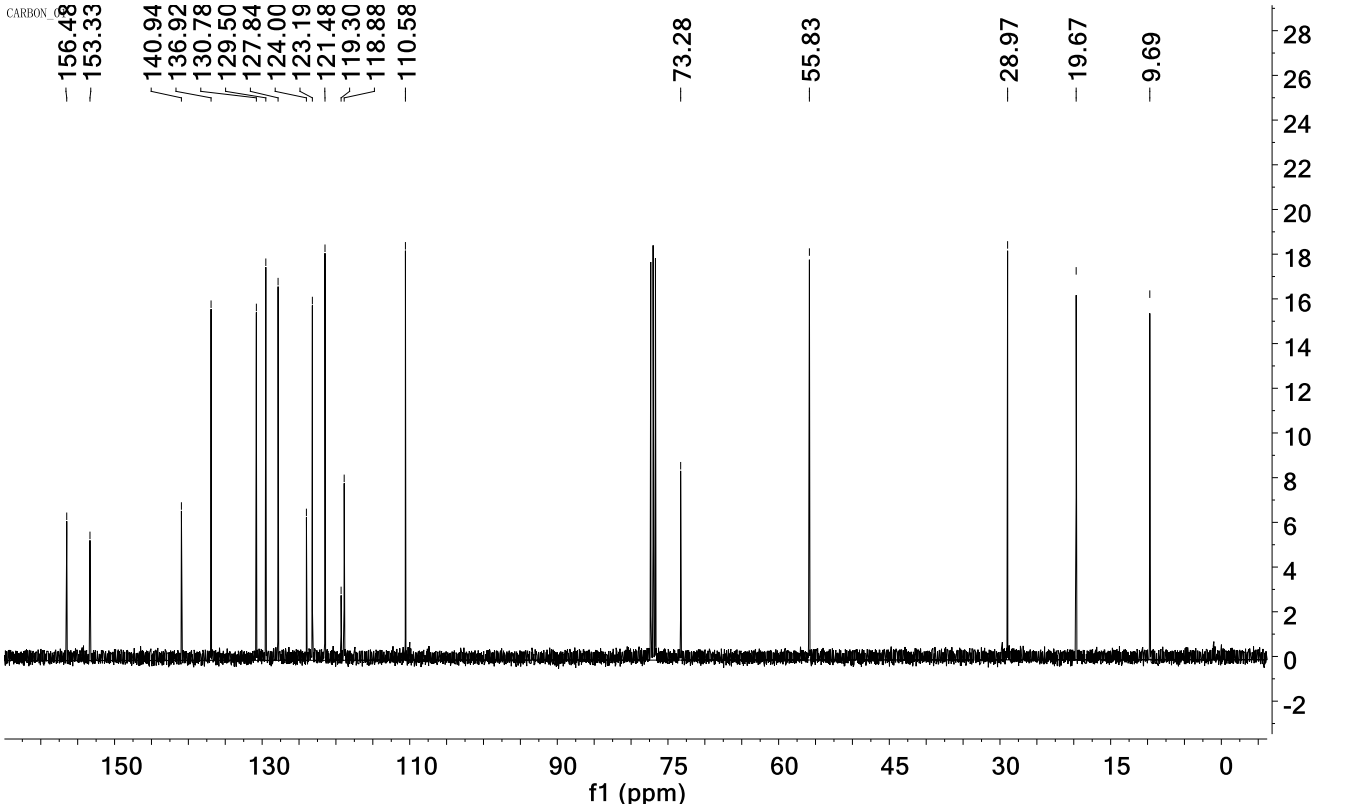
3.08
3.11
f1 (ppm)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28.97
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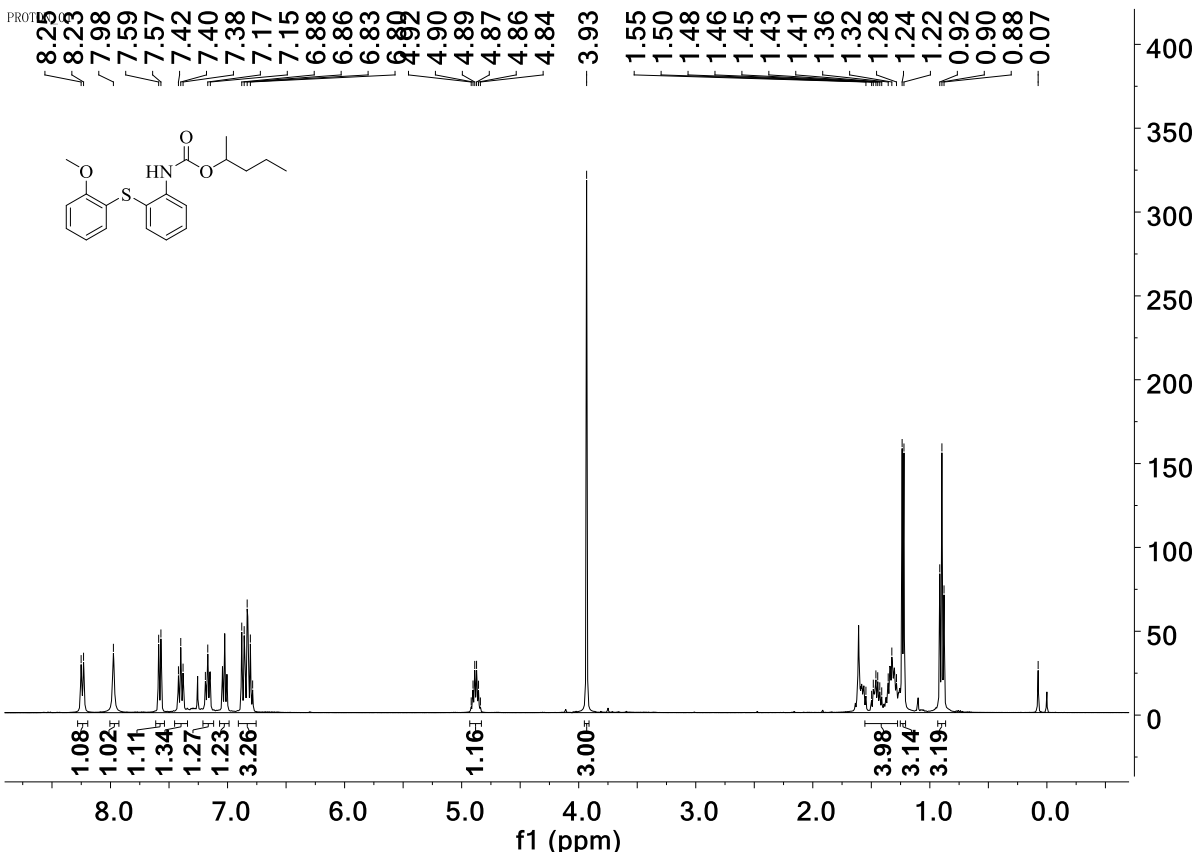
9.69
f1 (ppm)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4.89
4.87
4.86
4.84
3.93
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1.50
1.48
1.46
1.45
1.43
1.41
1.36
1.32
1.28
1.24
1.22
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0.07
O
HN
O
O
S
1.08
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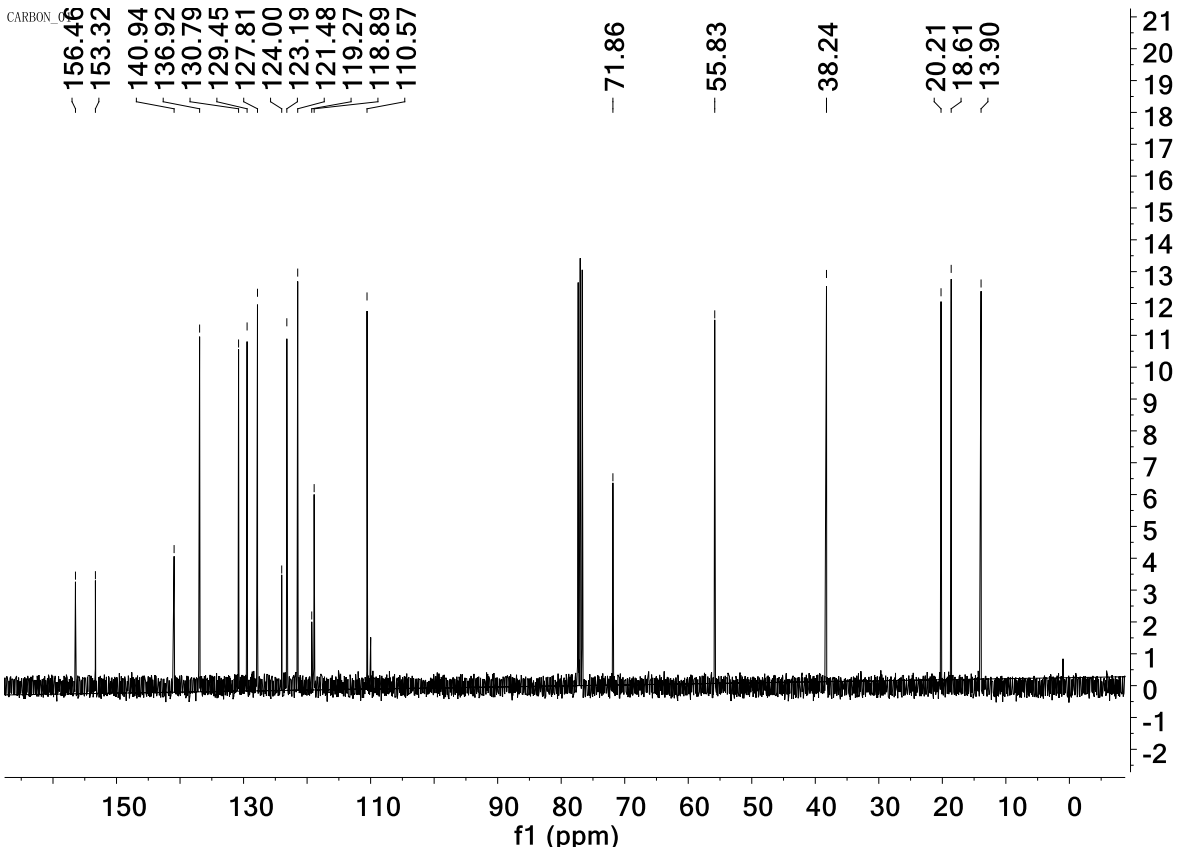
f1 (ppm)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38.24
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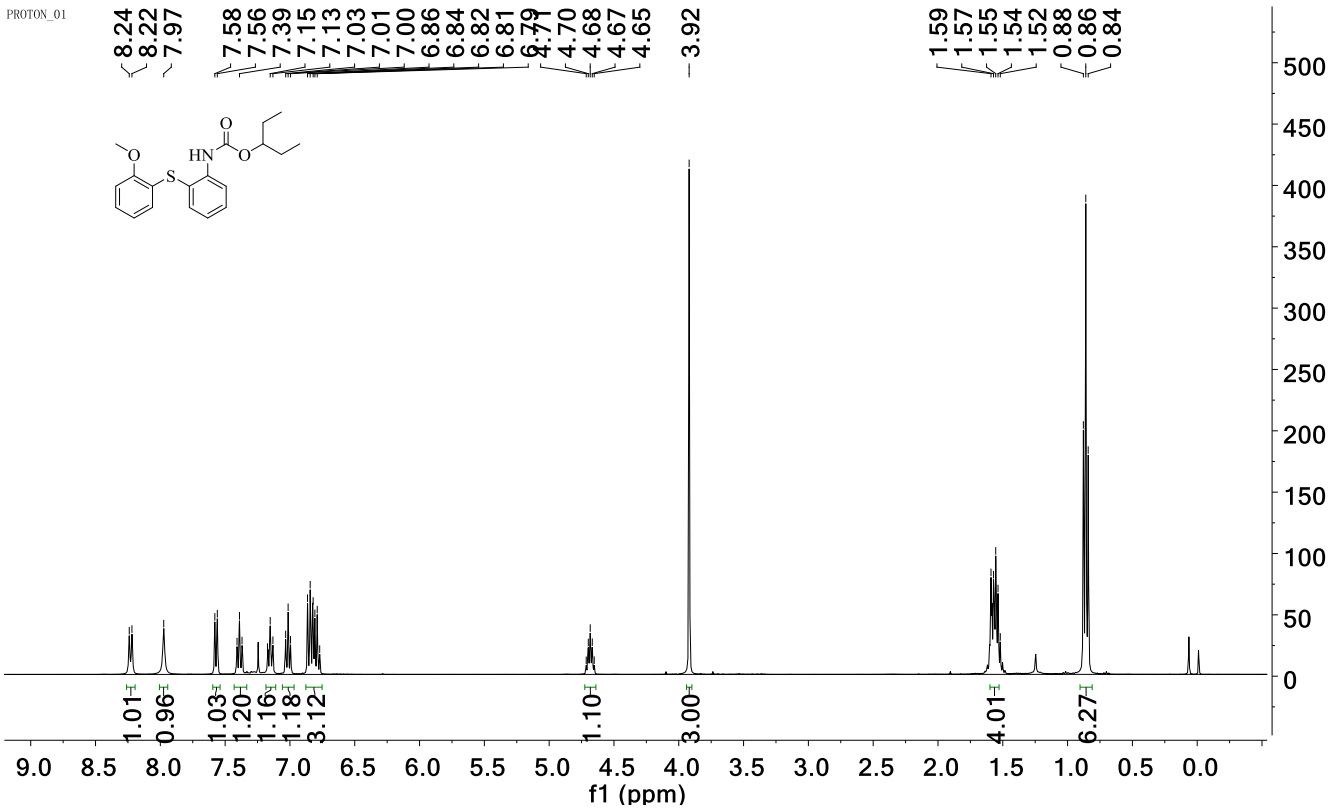
13.90
f1 (ppm)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6.79
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4.70
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1.55
1.54
1.52
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0.86
0.84
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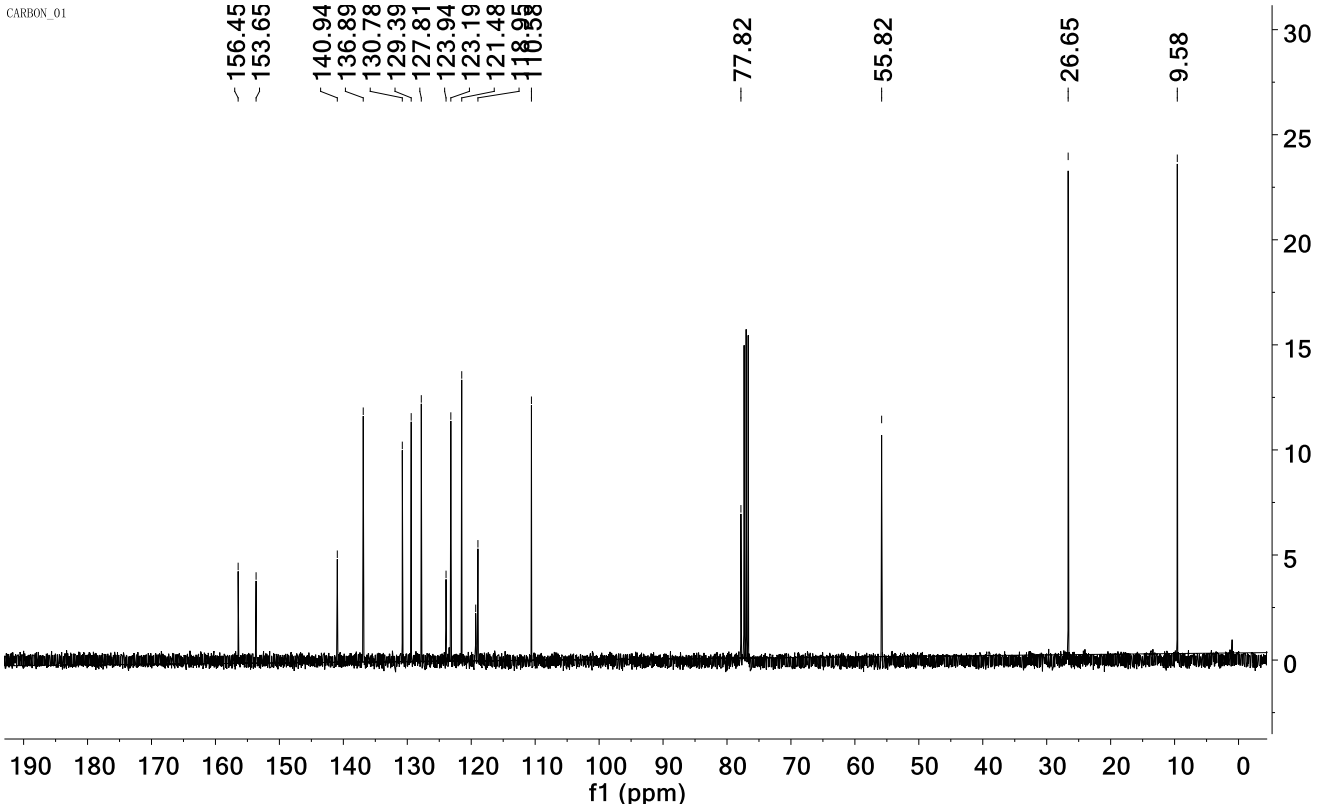
1.20
1.16
1.18
3.12
1.10
3.00
4.01
6.27
f1 (ppm)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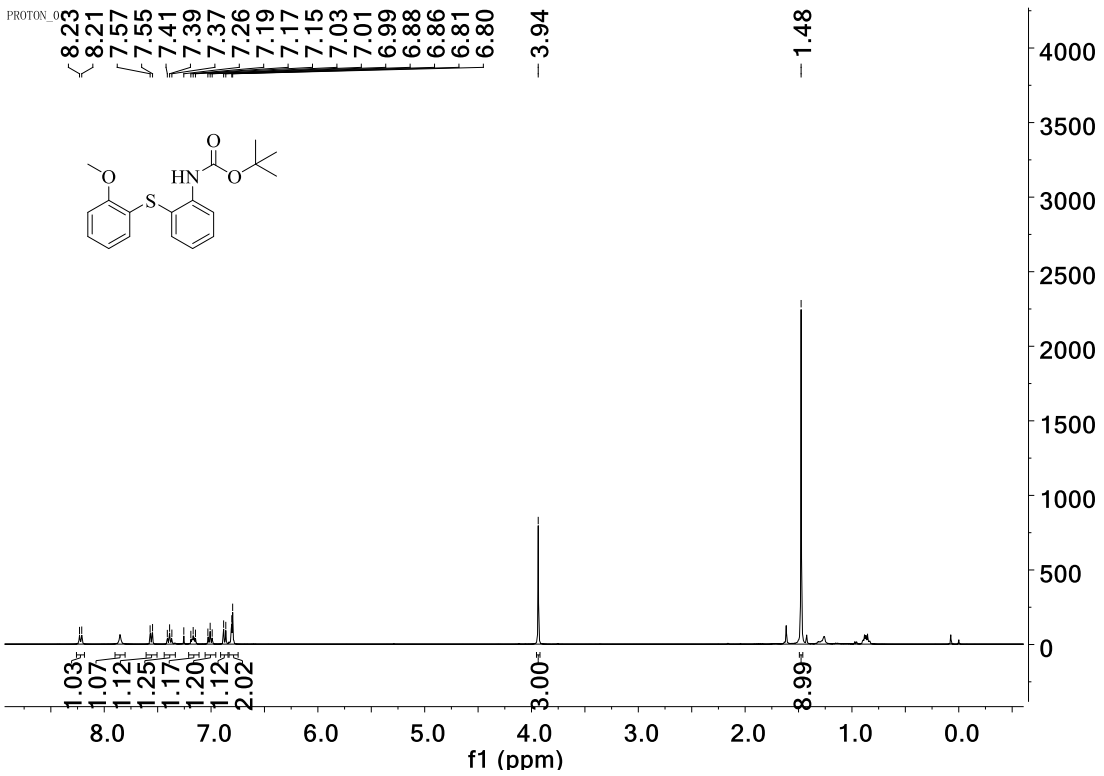
9.58
f1 (ppm)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7.17
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7.03
7.01
6.99
6.88
6.86
6.81
6.80
3.94
1.48
O
HN
O
O
S
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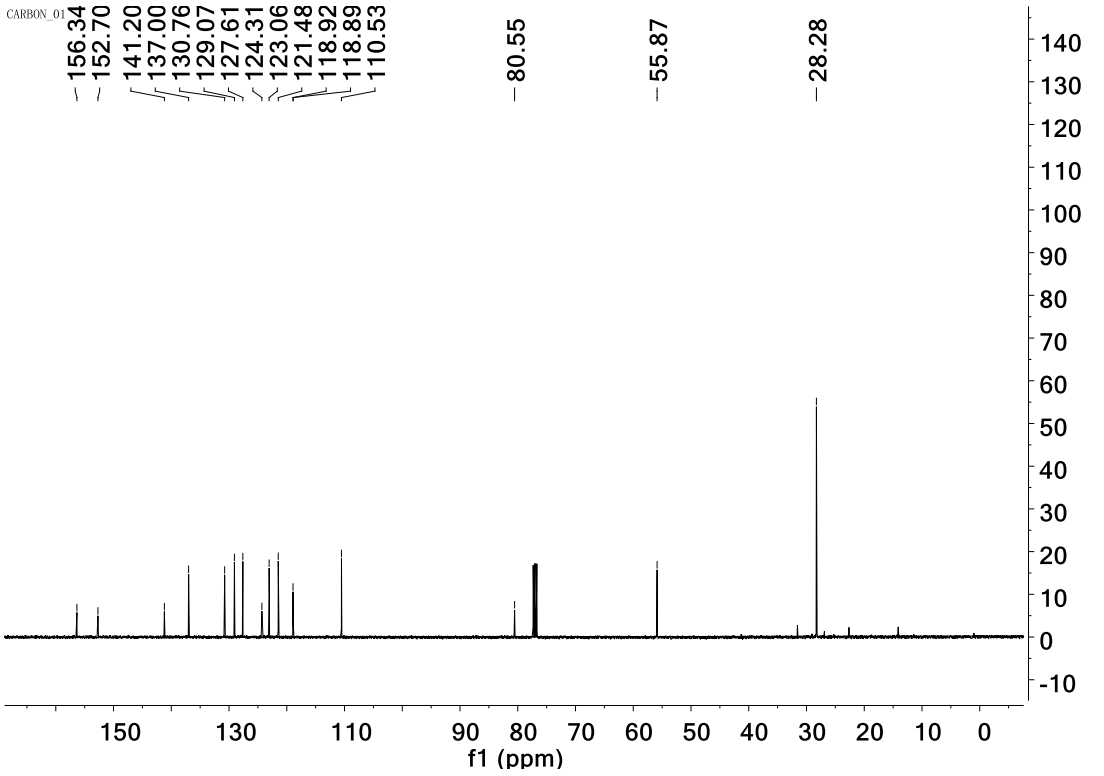
1.07
1.12
1.25
1.17
1.20
1.12
2.02
3.00
8.99
f1 (ppm)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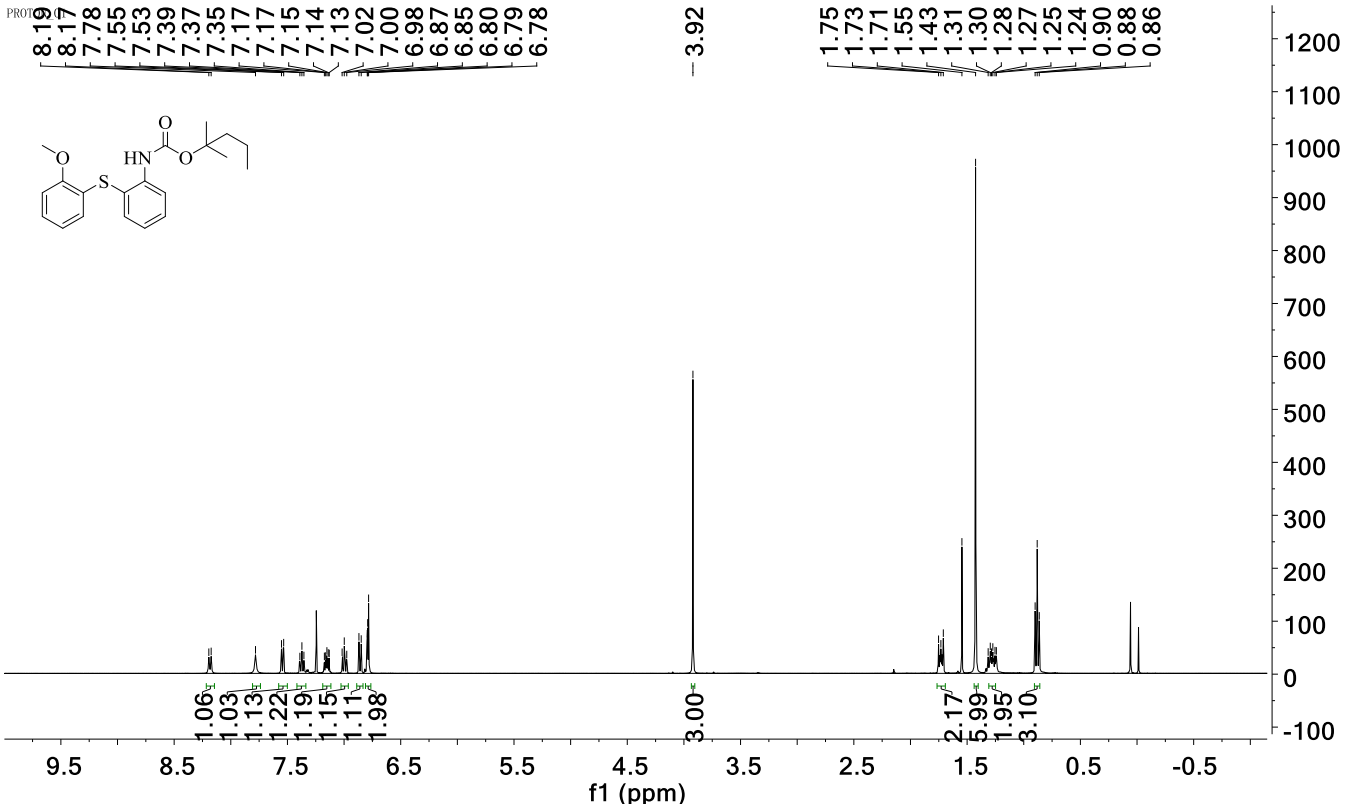
28.28
f1 (ppm)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7.15
7.14
7.13
7.02
7.00
6.98
6.87
6.85
6.80
6.79
6.78
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1.73
1.71
1.55
1.43
1.31
1.30
1.28
1.27
1.25
1.24
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0.88
0.86
O
HN
O
O
S
1.06
1.03
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1.11
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5.99
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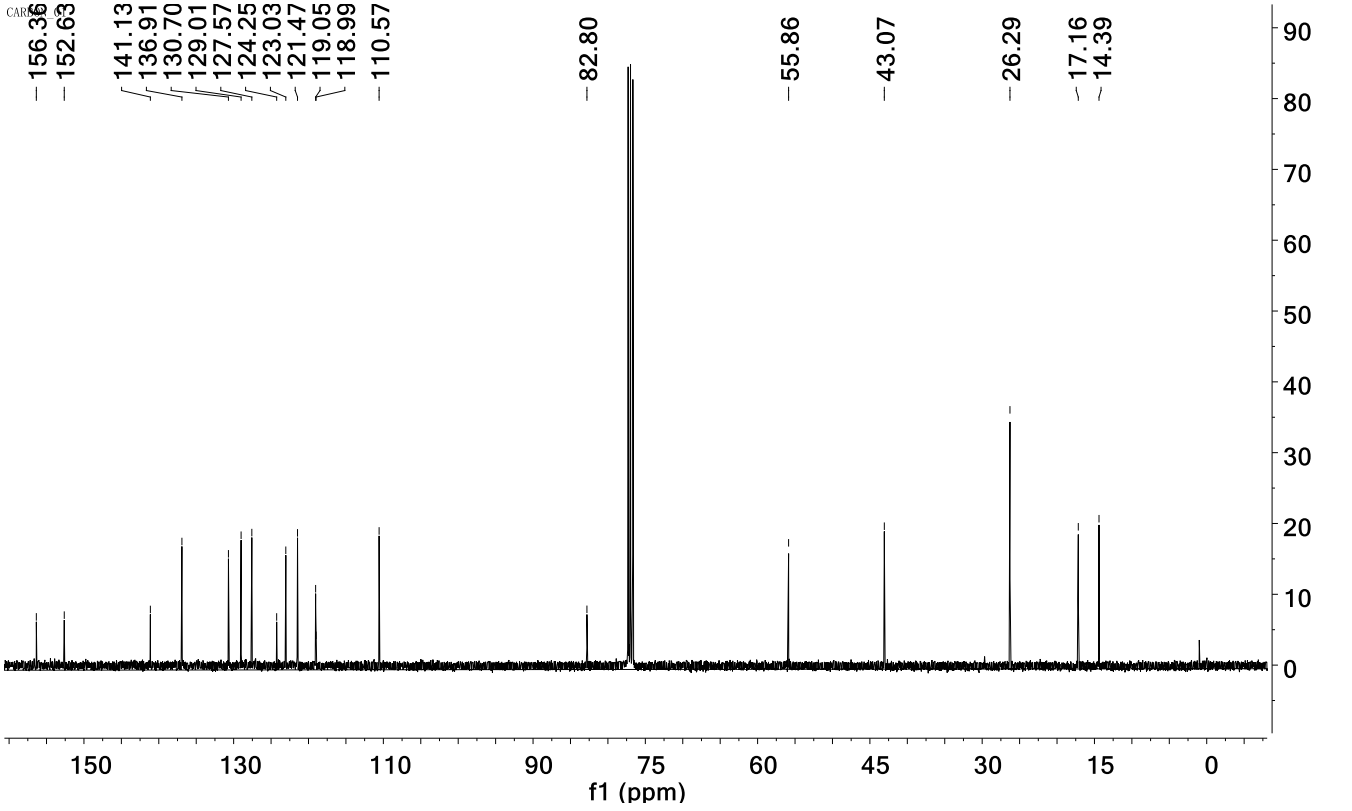
3.10
f1 (ppm)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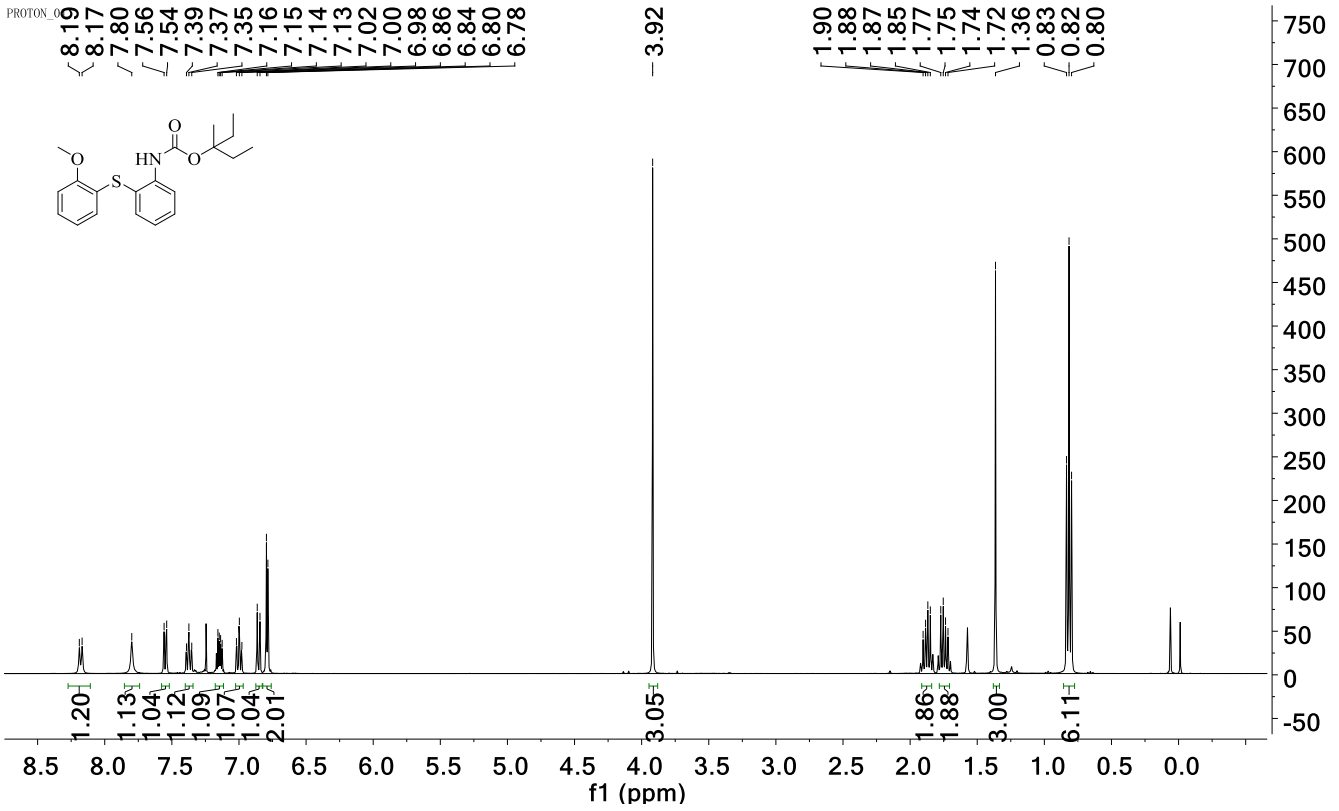
14.39
f1 (ppm)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7.16
7.15
7.14
7.13
7.02
7.00
6.98
6.86
6.84
6.80
6.78
3.92
1.90
1.88
1.87
1.85
1.77
1.75
1.74
1.72
1.36
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0.82
0.80
1.20
1.13
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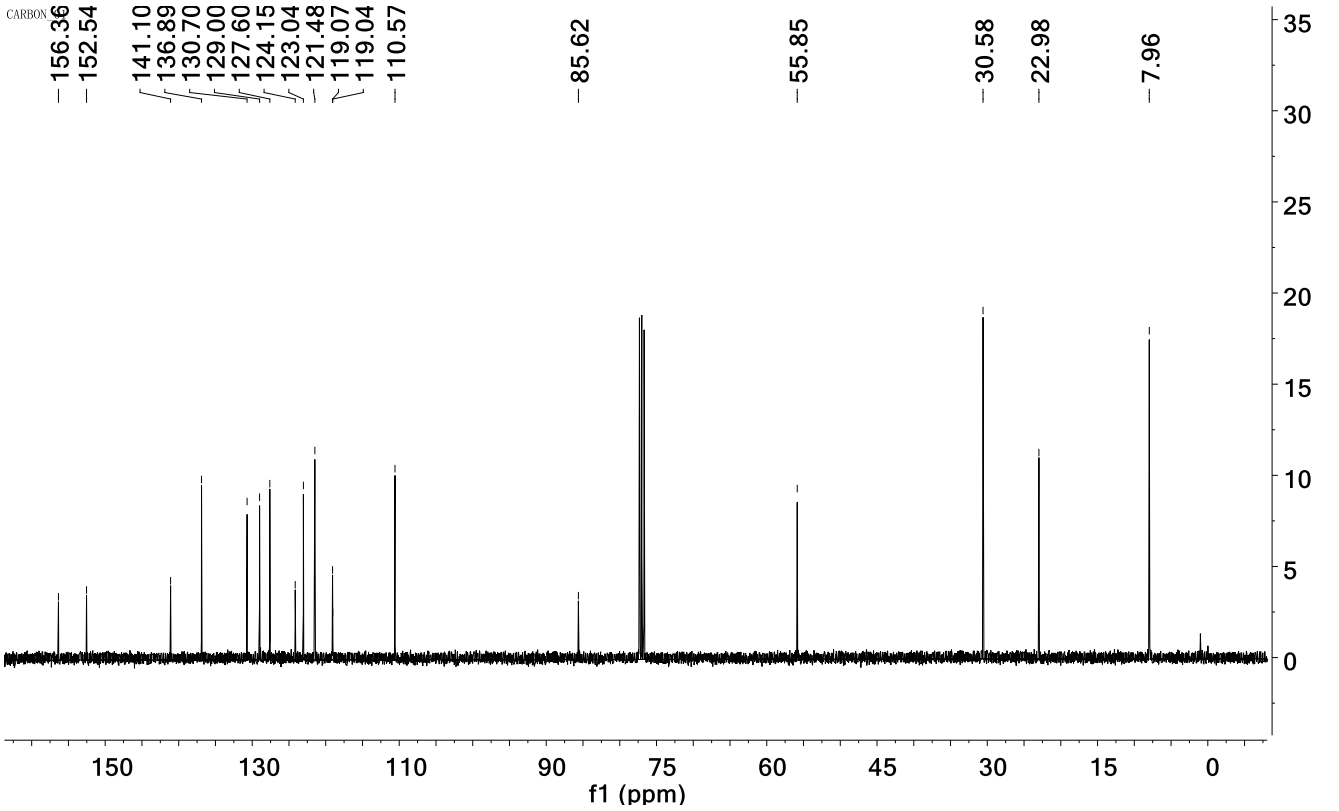
1.07
1.04
2.01
3.05
1.86
1.88
3.00
6.11
f1 (ppm)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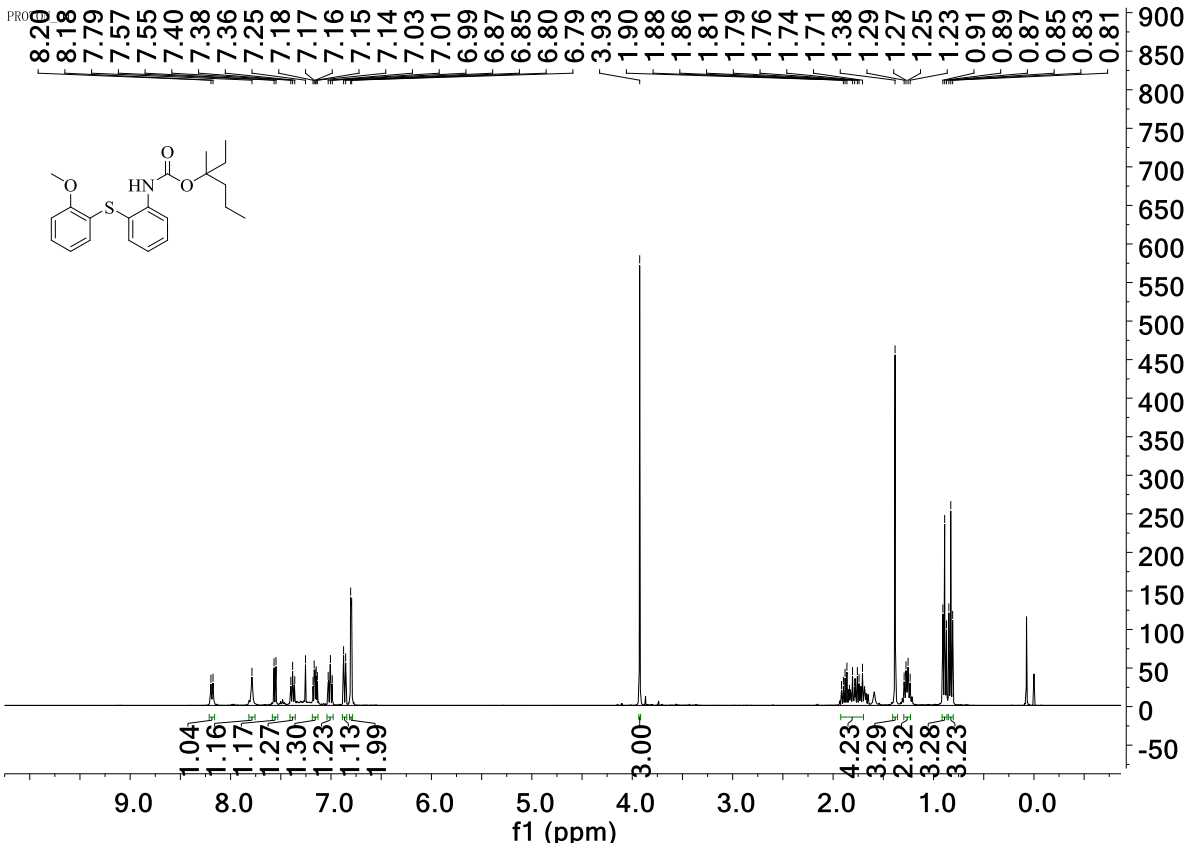
30.58
22.98
7.96
f1 (ppm)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7.14
7.03
7.01
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6.87
6.85
6.80
6.79
3.93
1.90
1.88
1.86
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1.74
1.71
1.38
1.29
1.27
1.25
1.23
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0.89
0.87
0.85
0.83
0.81
O
HN
O
O
S
1.04
1.16
1.17
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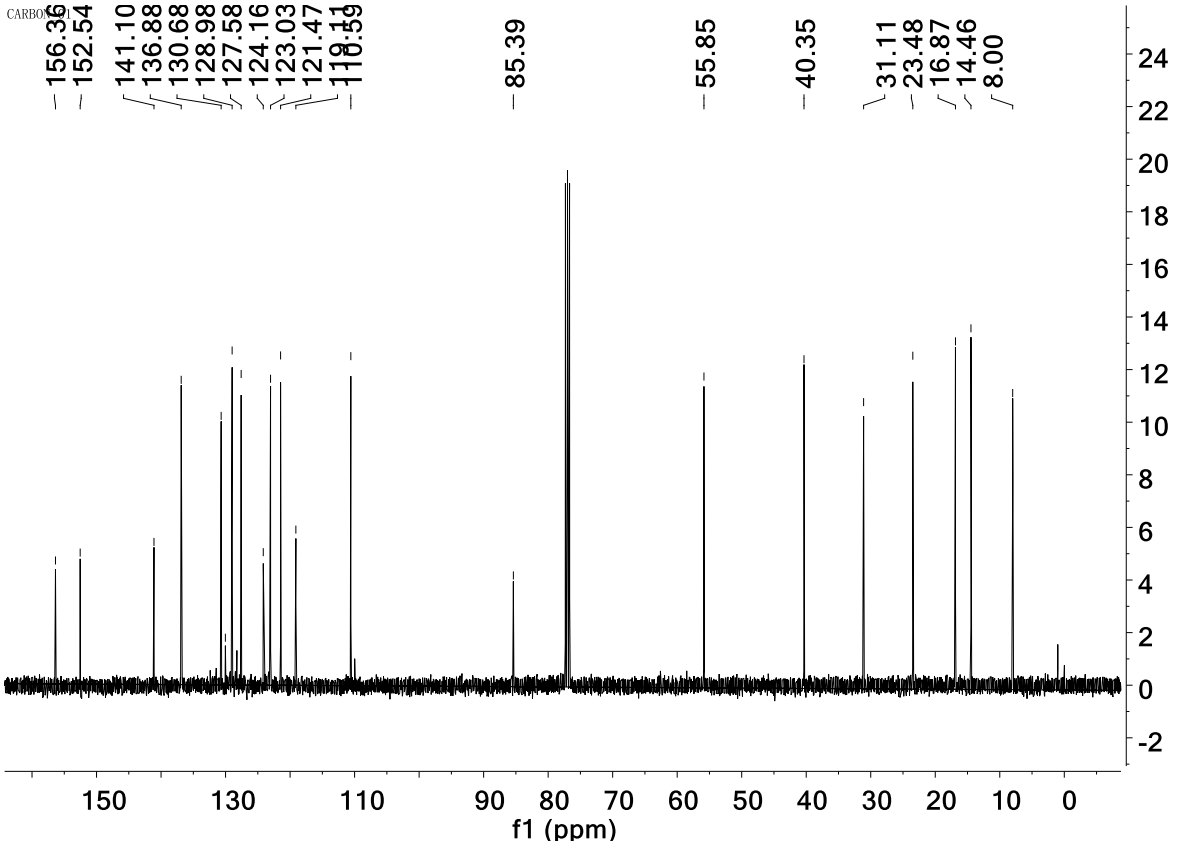
3.23
f1 (ppm)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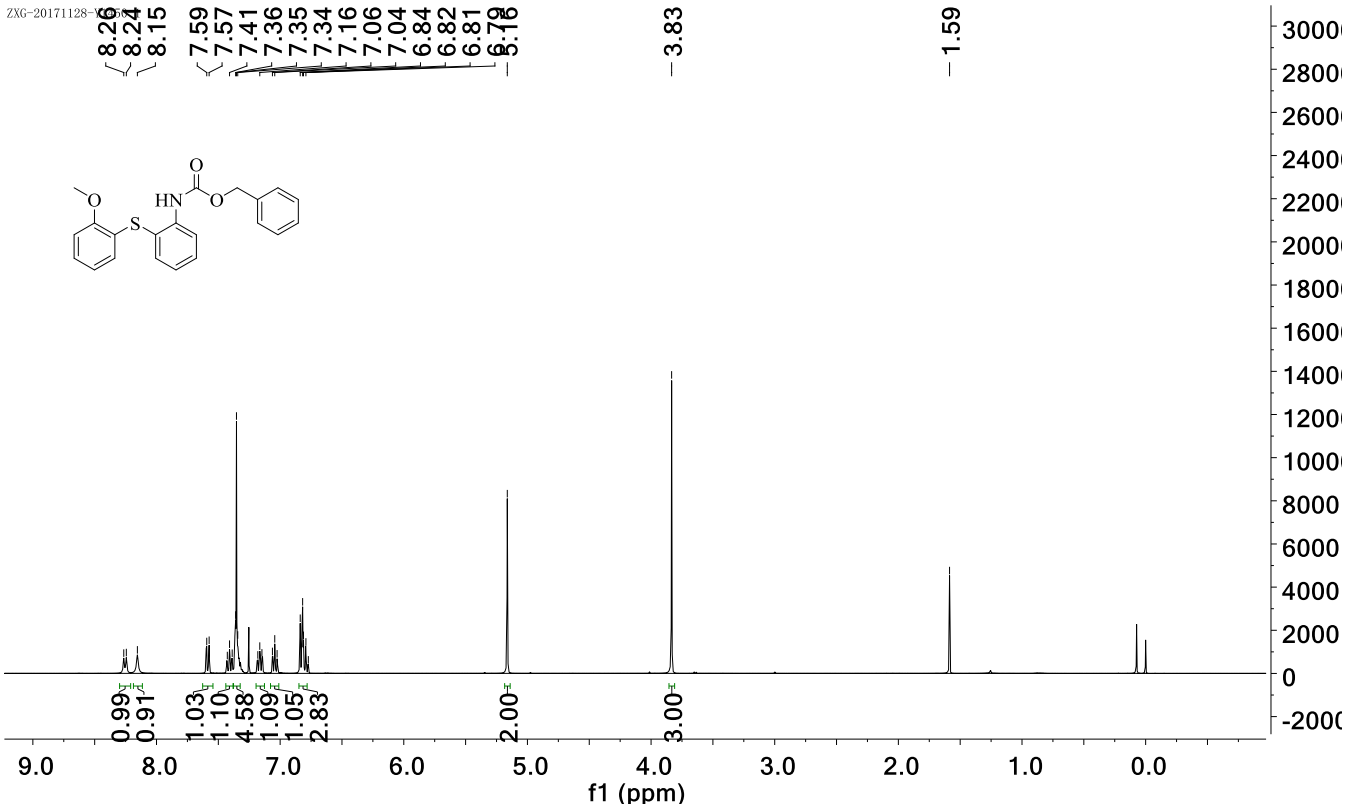
8.00
f1 (ppm)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6.82
6.81
3.83
1.59
O
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O
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4.58
1.09
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2.83
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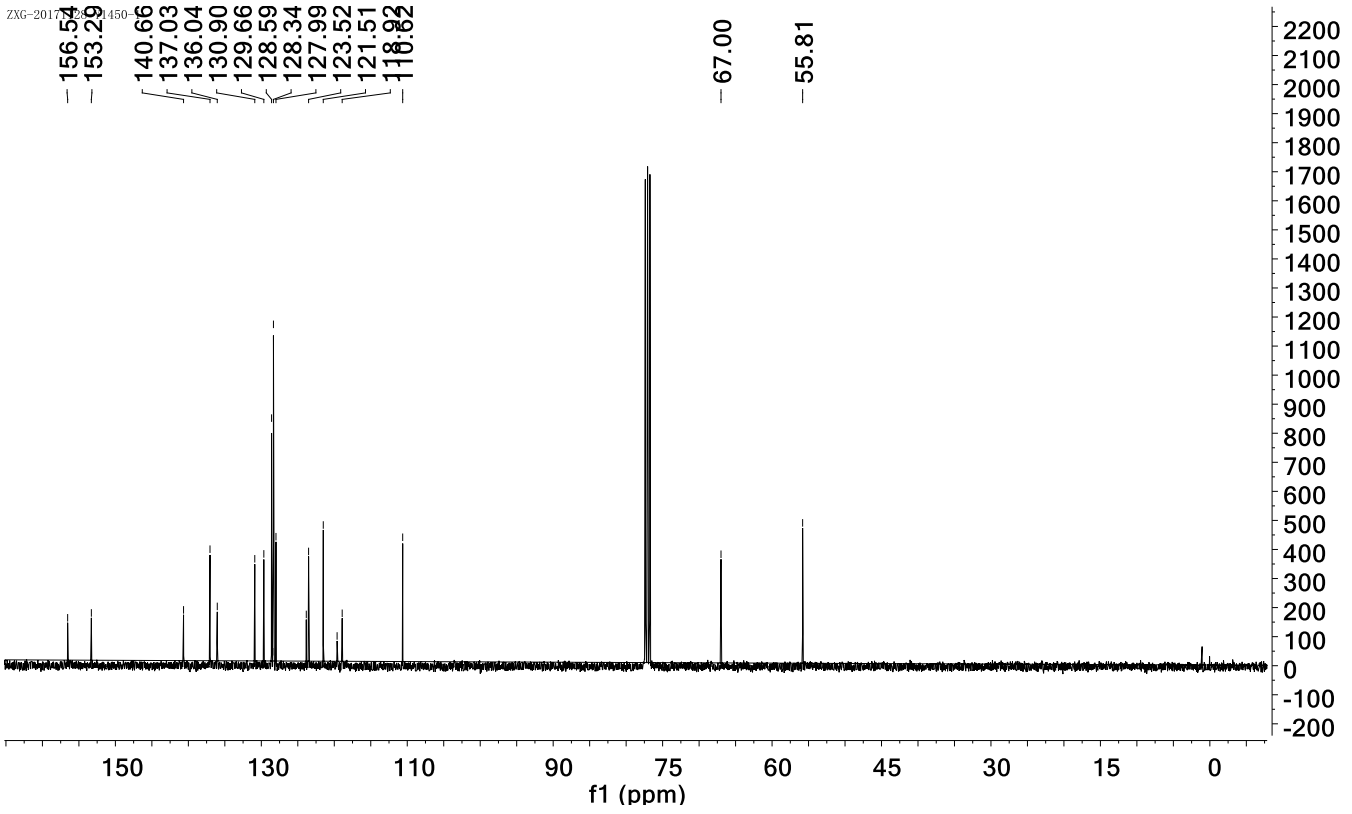
3.00
f1 (ppm)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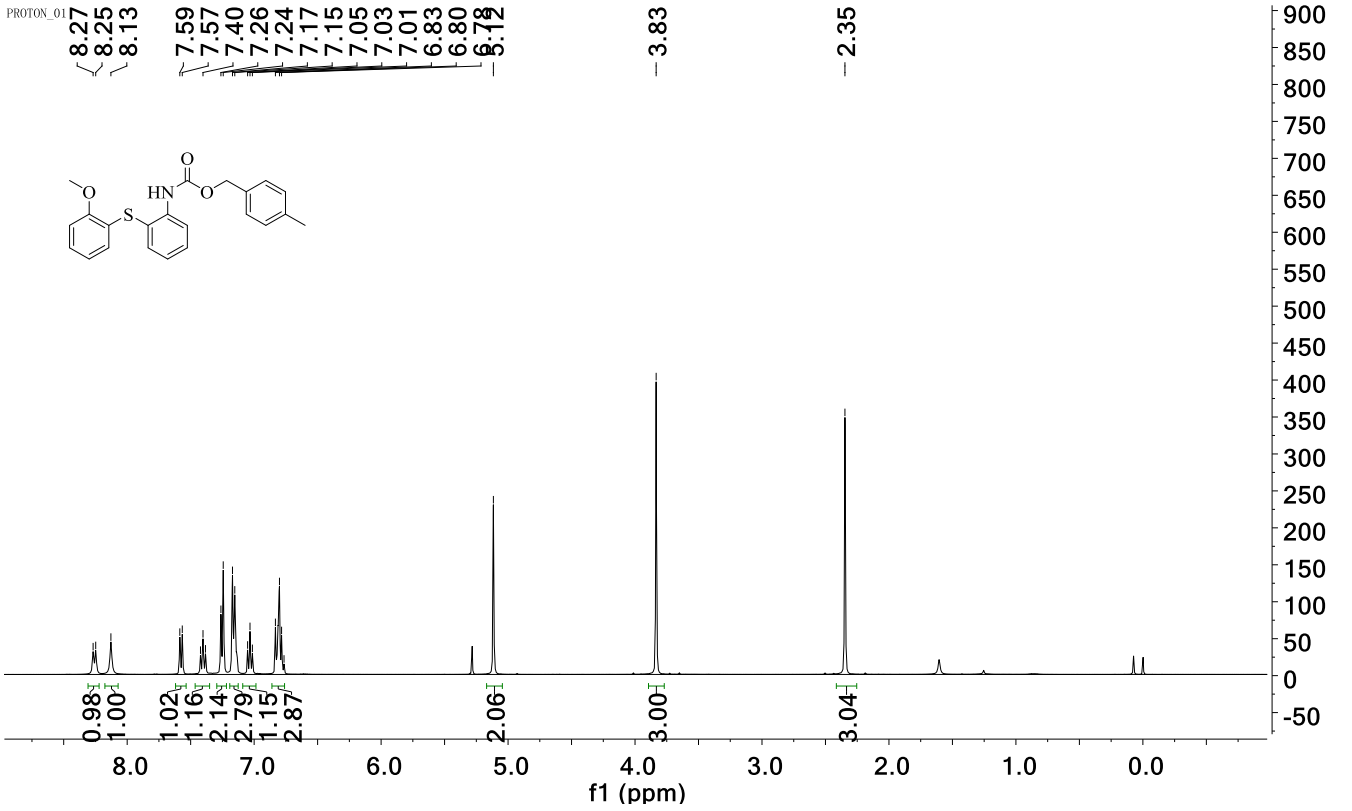
f1 (ppm)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7.17
7.15
7.05
7.03
7.01
6.83
6.80
3.83
2.35
O
HN
O
O
S
0.98
1.00
1.02
1.16
2.14
2.79
1.15
2.87
2.06
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3.04
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6.0
5.0
4.0
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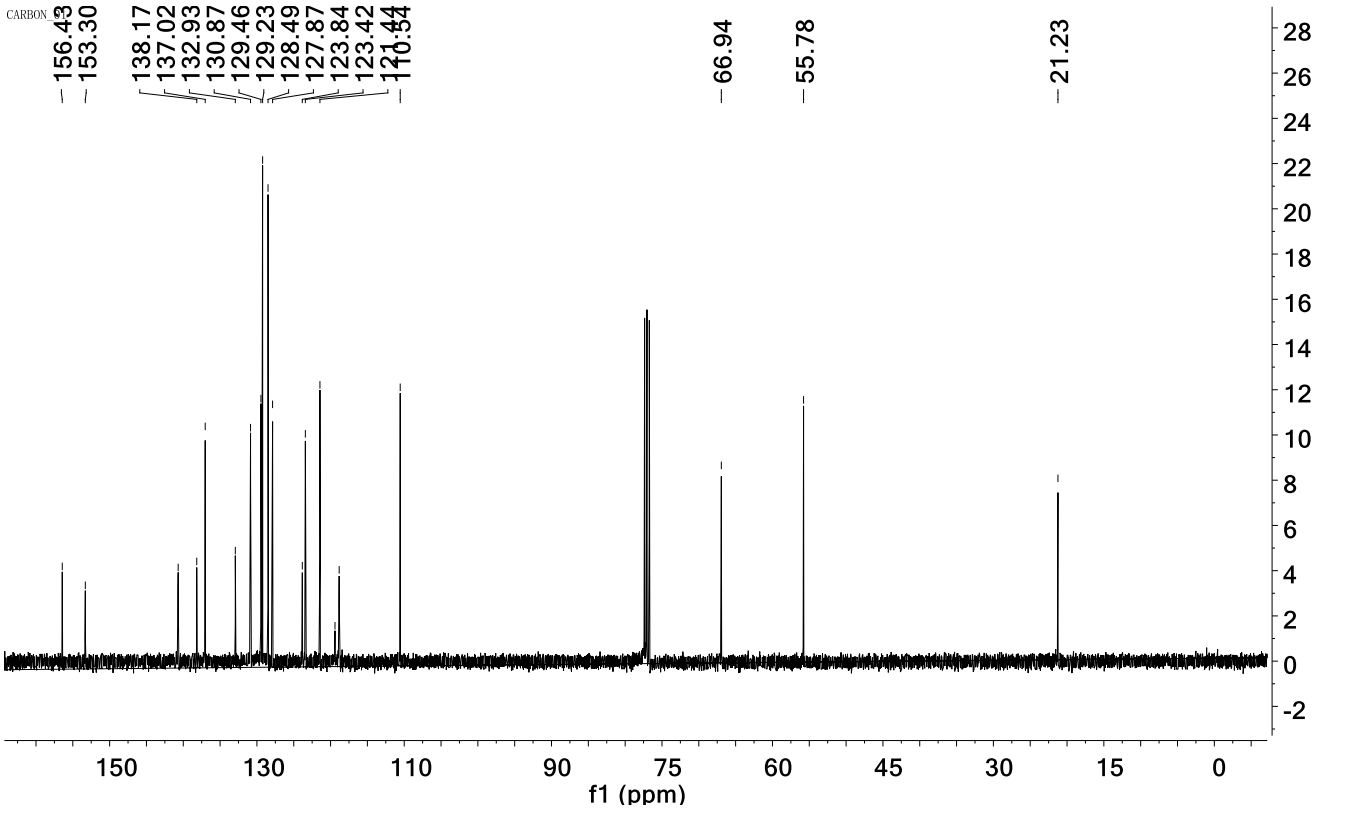
0.0
f1 (ppm)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110
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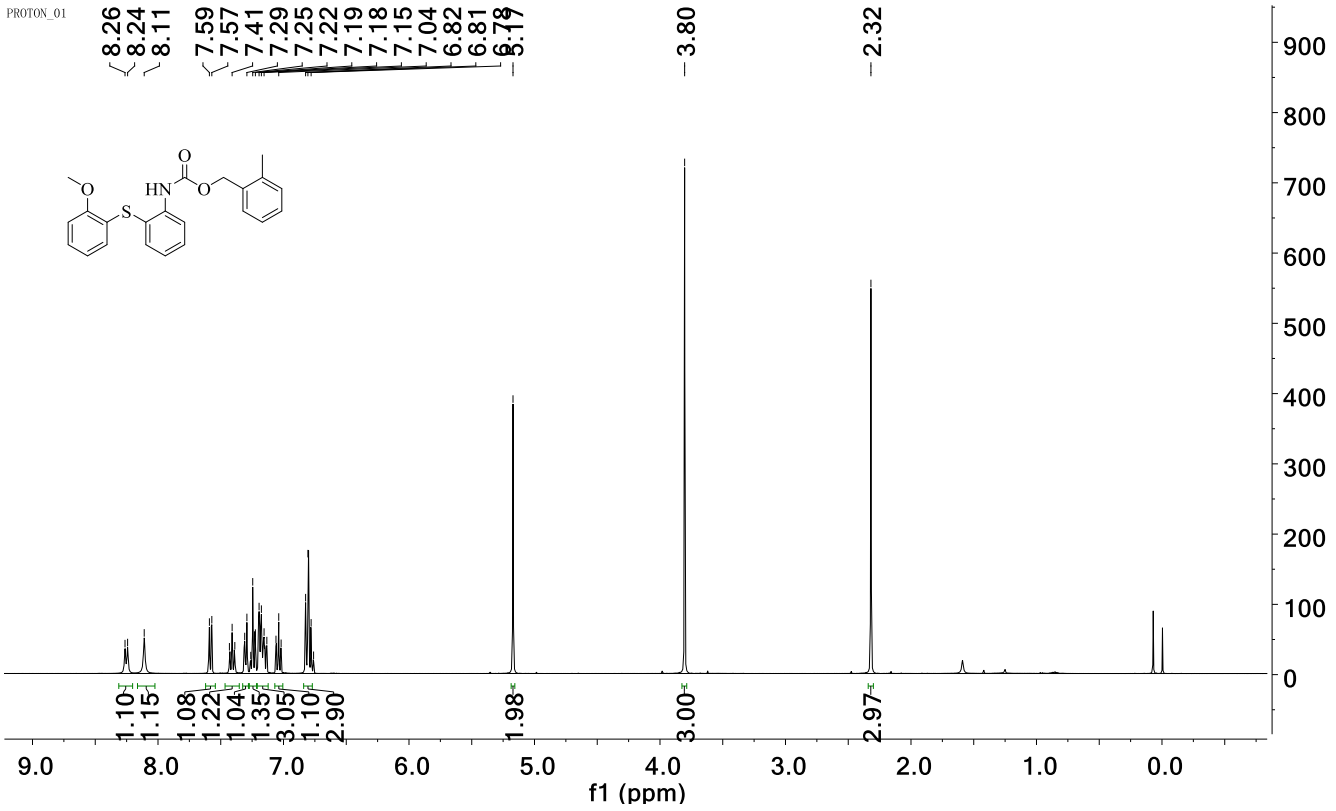
75
60
45
30
15
0
f1 (ppm)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7.25
7.22
7.19
7.18
7.15
7.04
6.82
6.81
3.80
2.32
1.10
1.15
1.08
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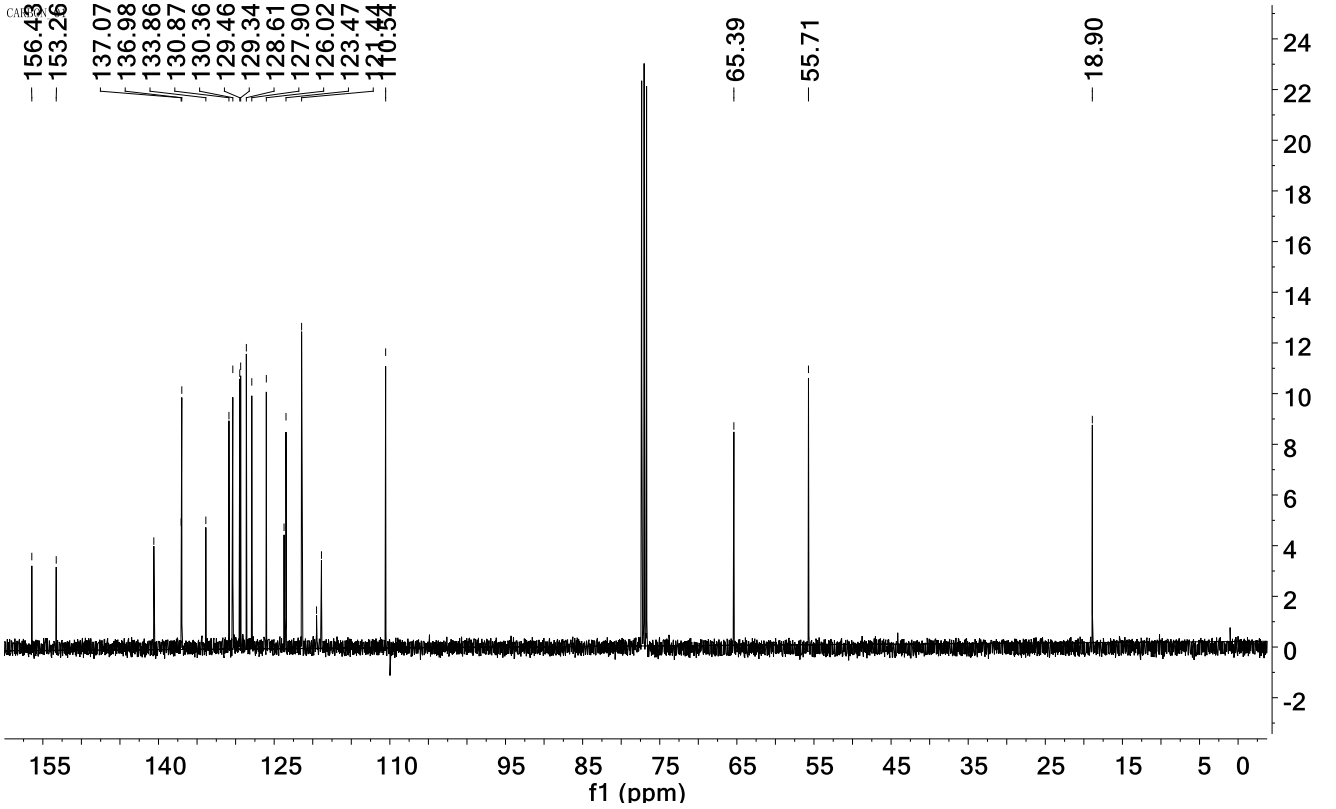
1.04
1.35
3.05
1.10
2.90
1.98
3.00
2.97
f1 (ppm)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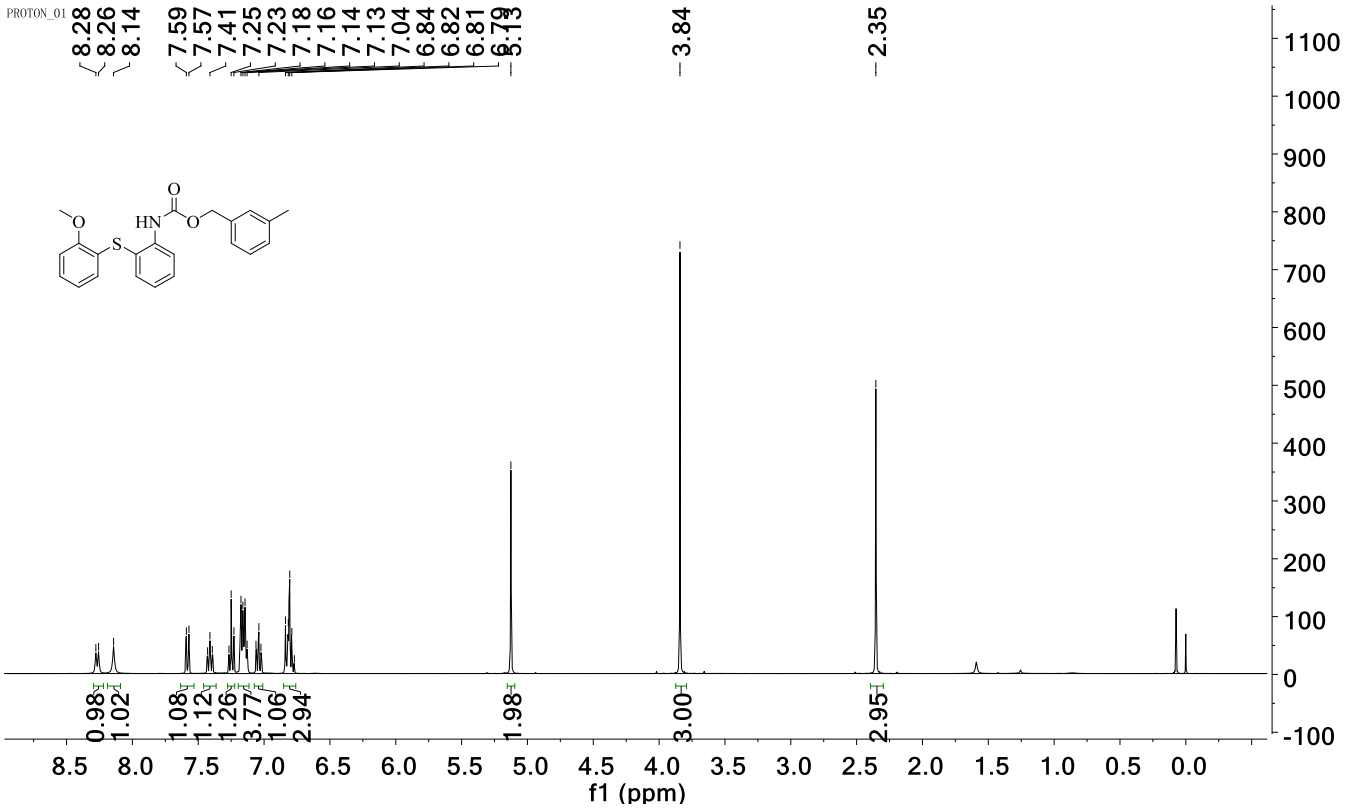
127.90
126.02
123.47
65.39
55.71
18.90
f1 (ppm)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7.13
7.04
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6.82
6.81
6.79
5.13
3.84
2.35
O
HN
O
O
S
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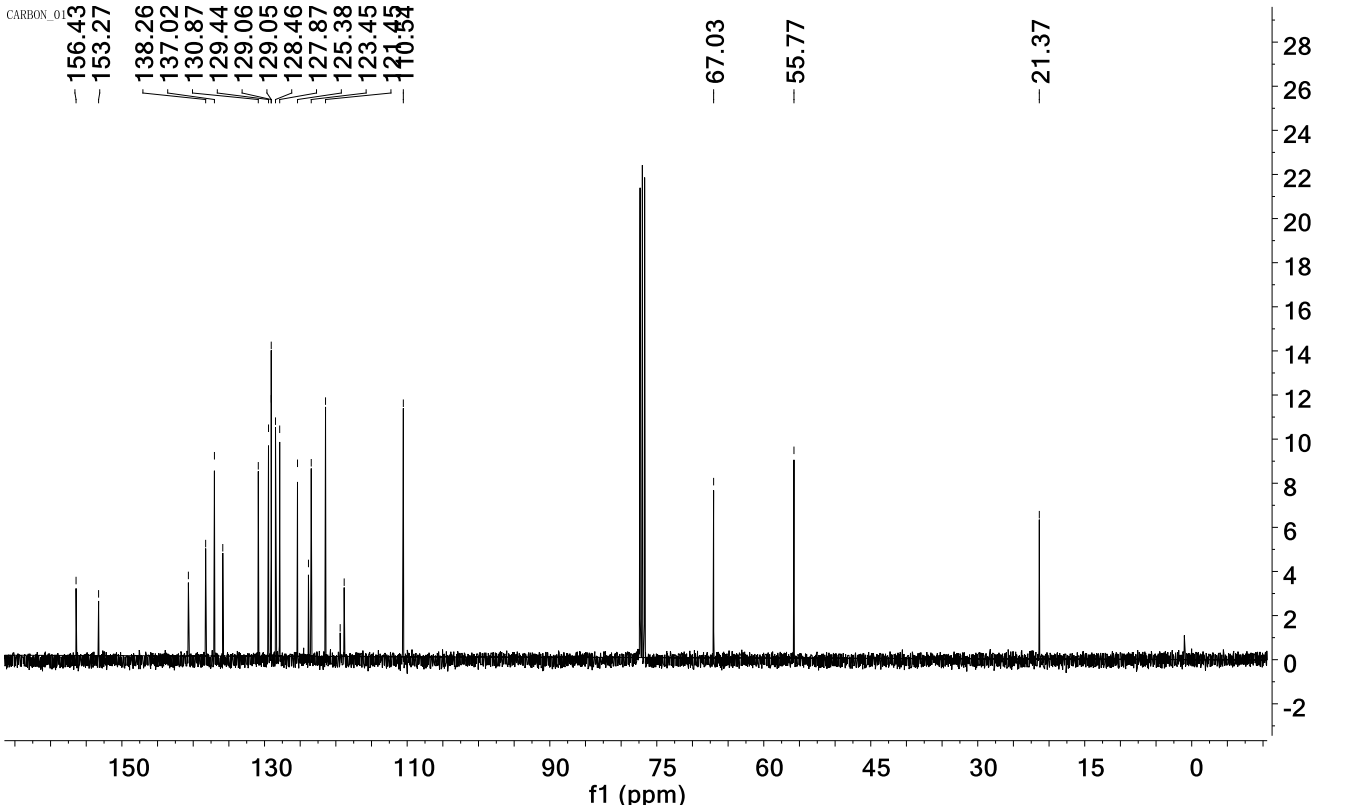
2.95
f1 (ppm)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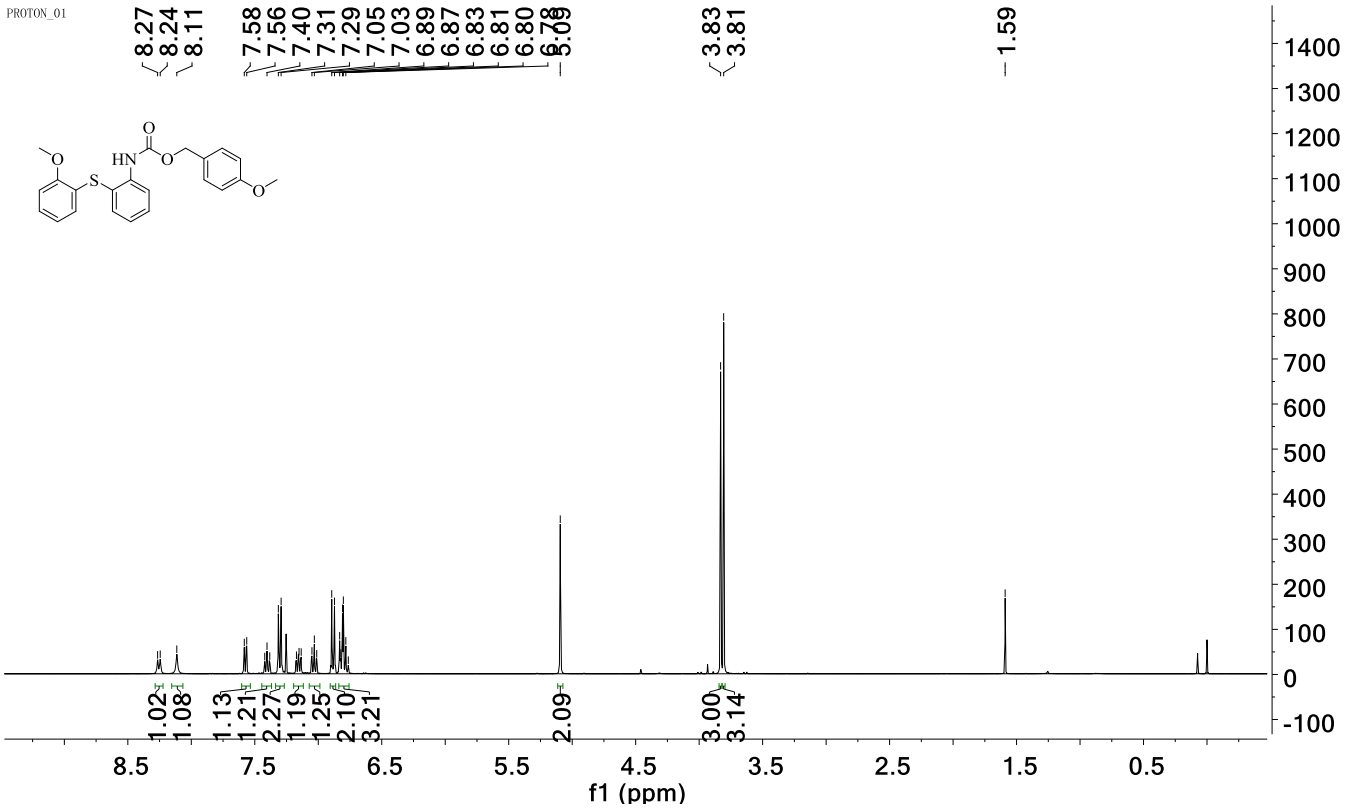
f1 (ppm)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3.81
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2.09
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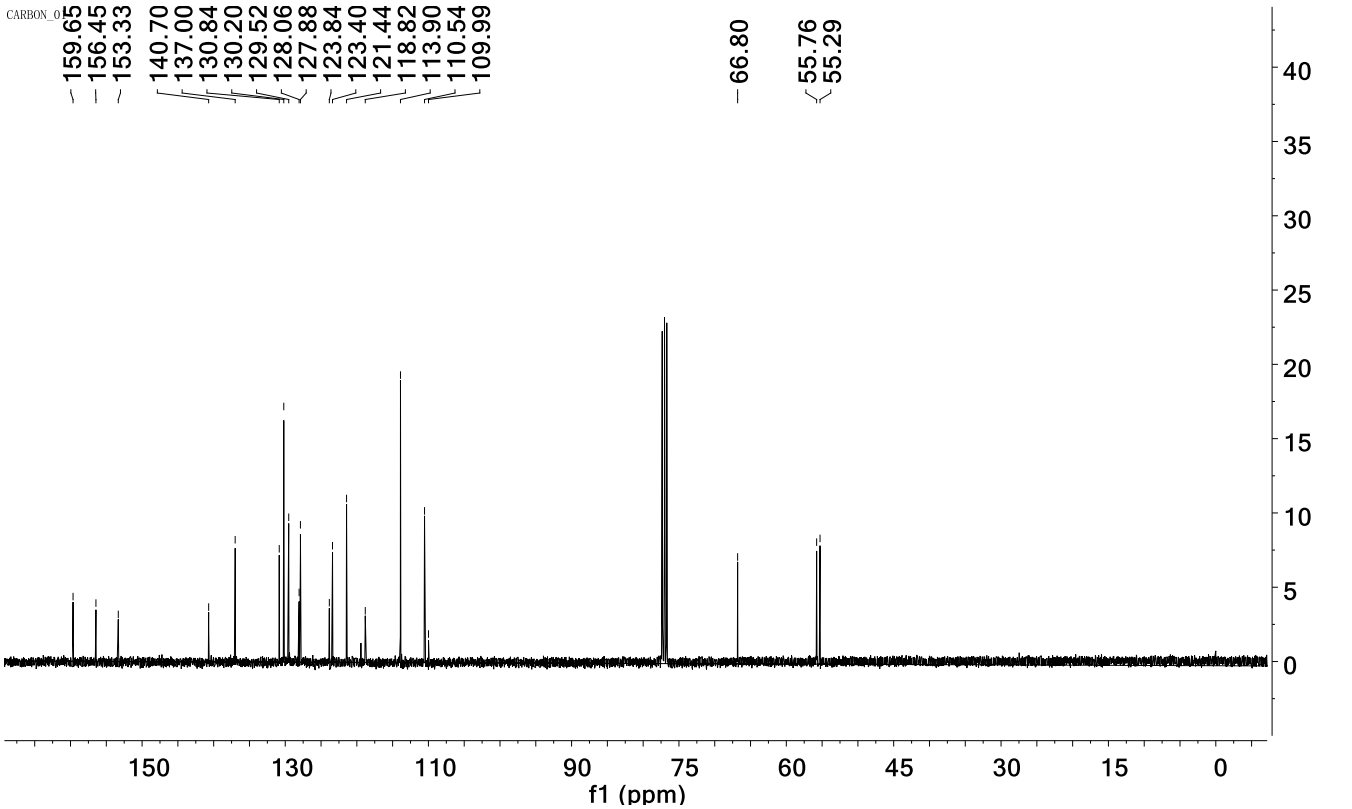
3.14
f1 (ppm)


CARBON_01
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109.99
66.80
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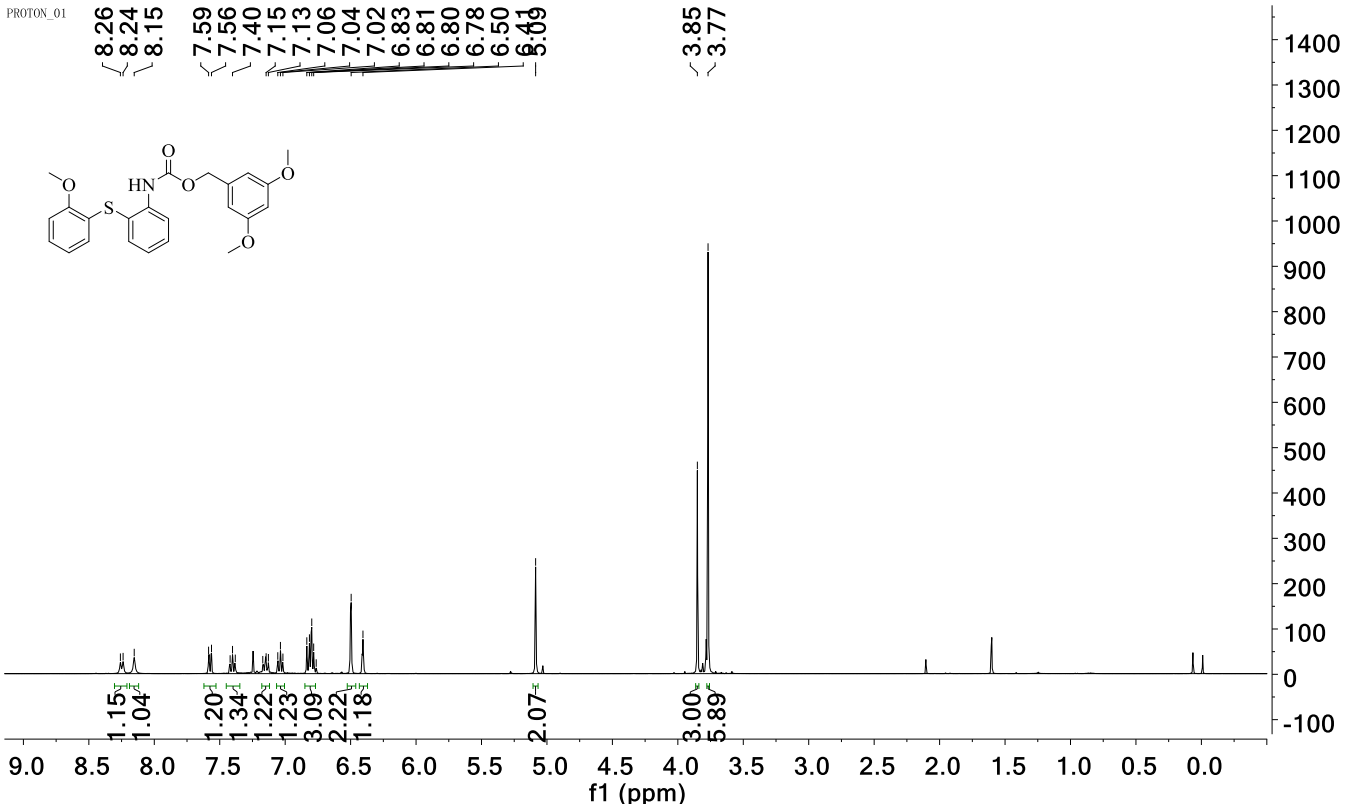
55.29
f1 (ppm)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7.06
7.04
7.02
6.83
6.81
6.80
6.78
6.50
6.41
5.09
3.85
3.77
1.15
1.04
1.20
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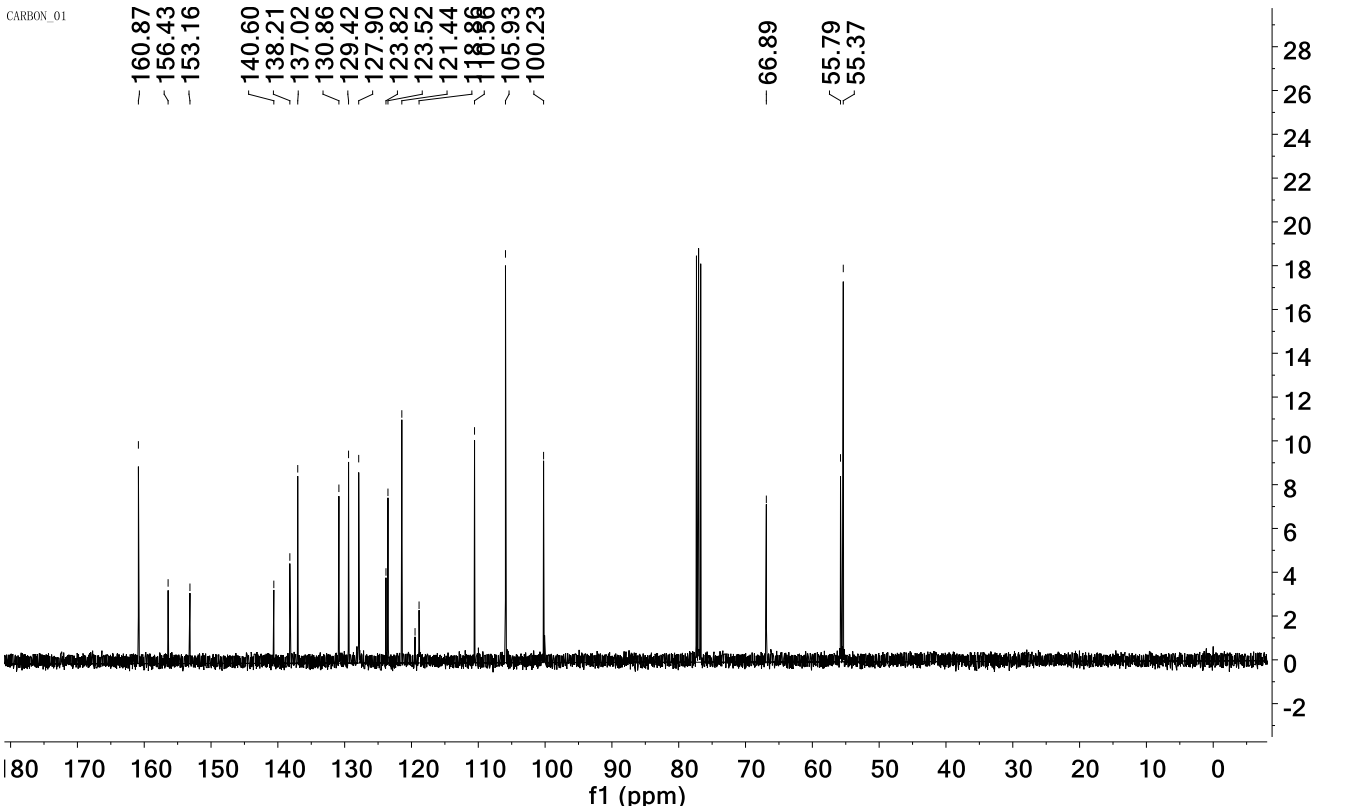
1.22
1.23
3.09
2.22
1.18
2.07
3.00
5.89
f1 (ppm)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66.89
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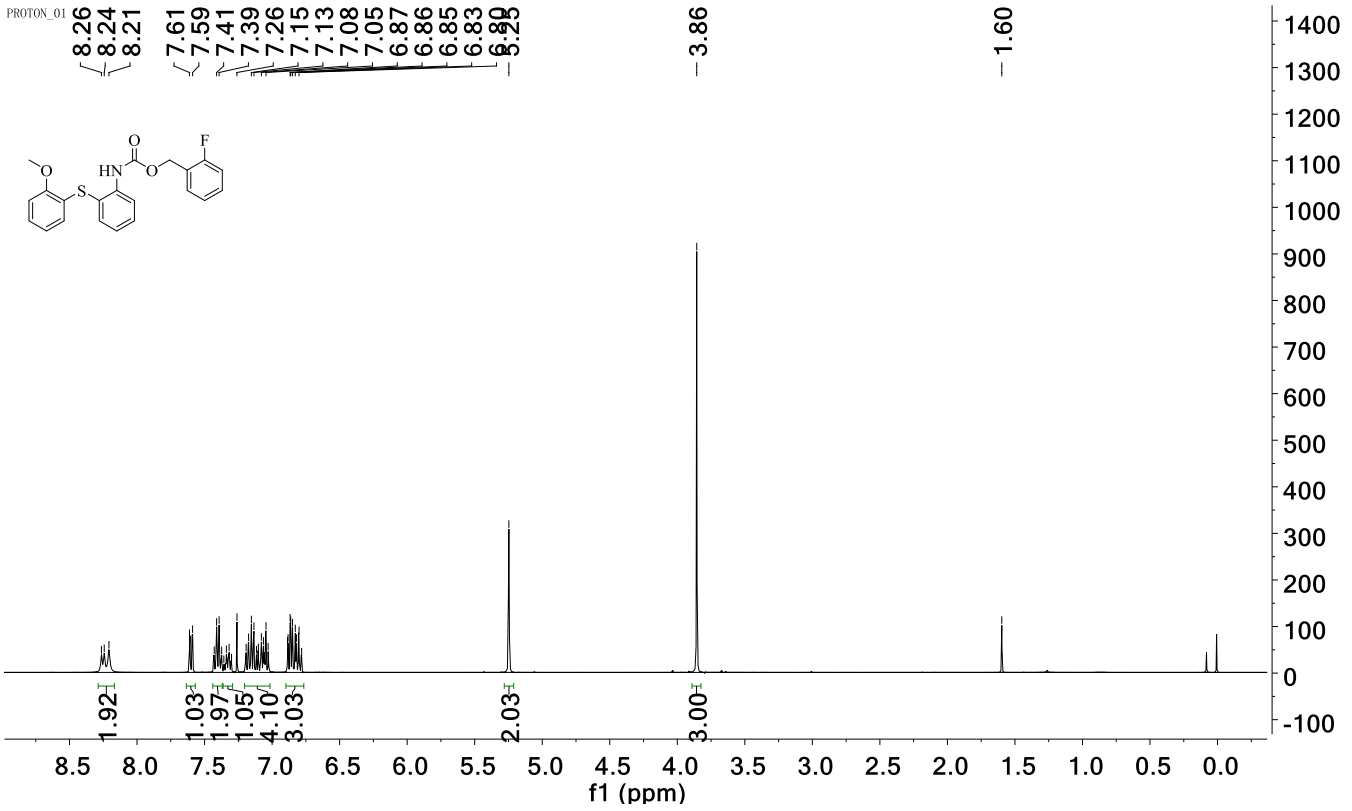
55.37
f1 (ppm)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6.85
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1.03
1.97
1.05
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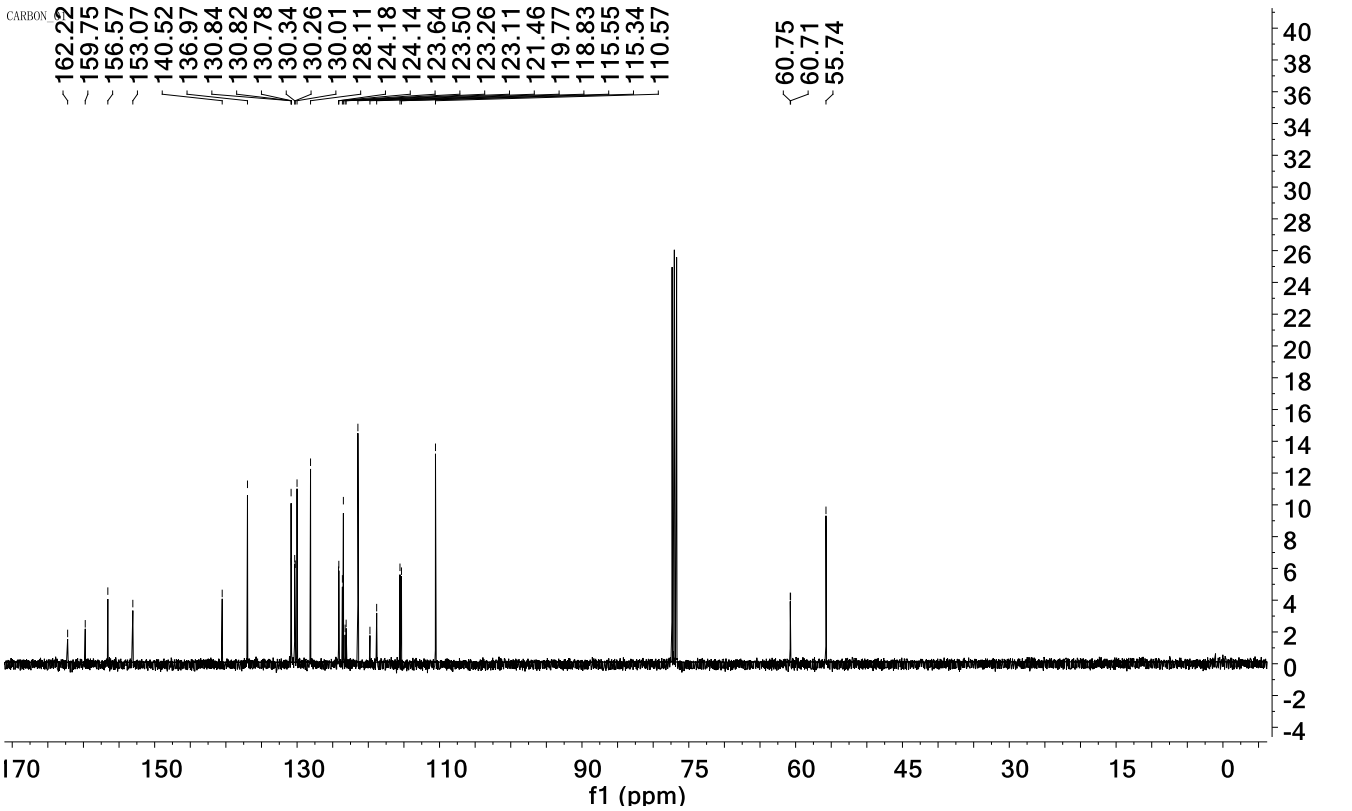
2.03
3.00
f1 (ppm)


CARBON_01
162.22
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130.82
130.78
130.34
130.26
130.01
128.11
124.18
124.14
123.64
123.50
123.26
123.11
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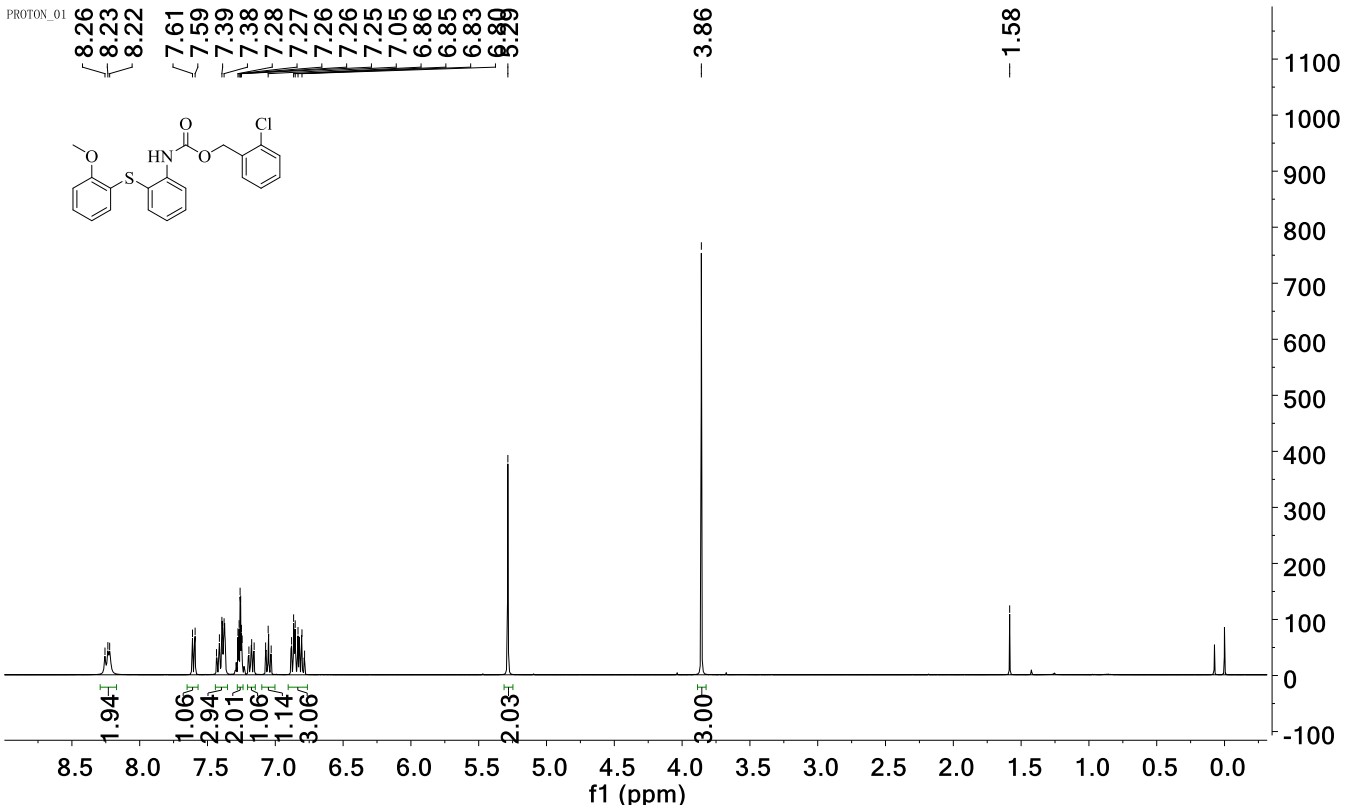
119.77
118.83
115.55
115.34
110.57
60.75
60.71
55.74
f1 (ppm)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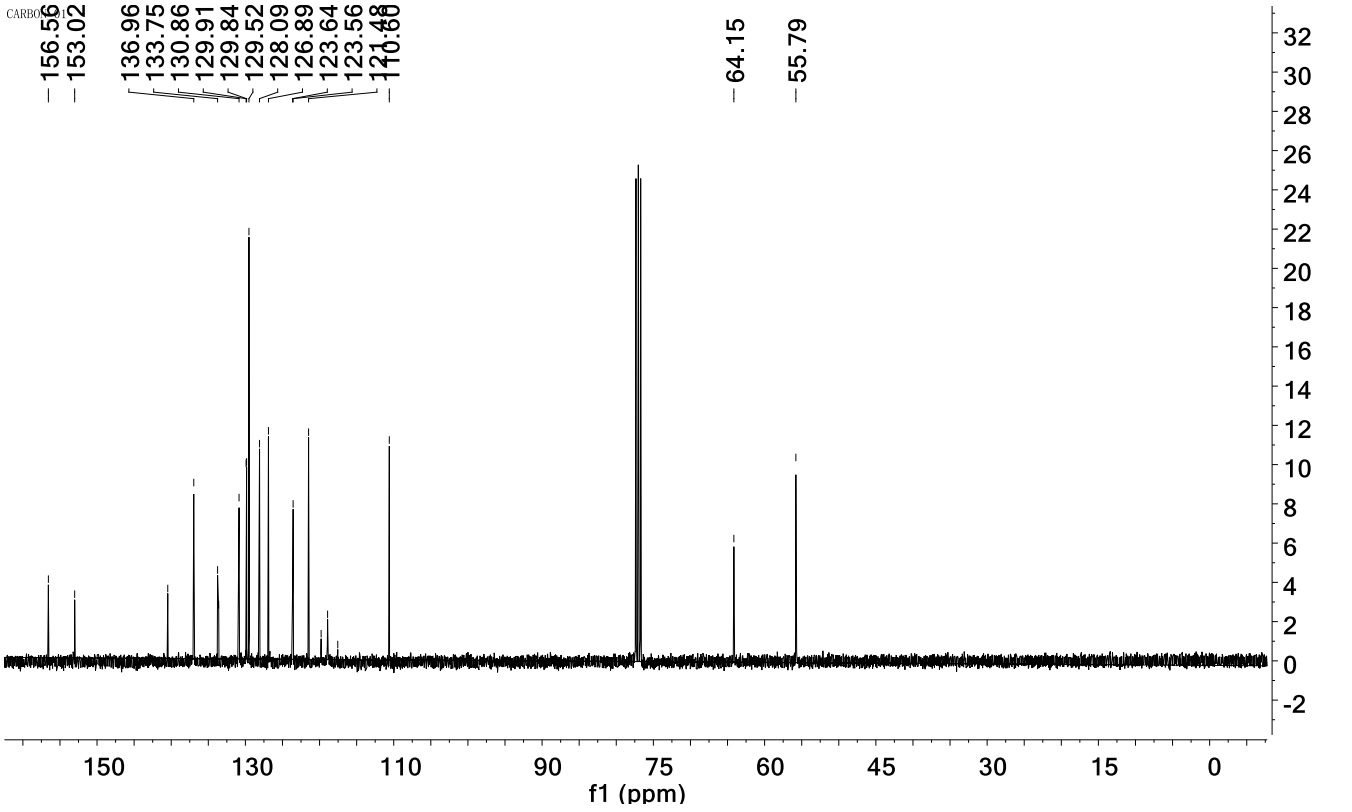
7.38
7.28
7.27
7.26
7.26
7.25
7.05
6.86
6.85
6.83
5.29
3.86
1.58
O
HN
O
Cl
O
S
1.94
1.06
2.94
2.01
1.06
1.14
3.06
2.03
3.00
f1 (ppm)


CARBON_01
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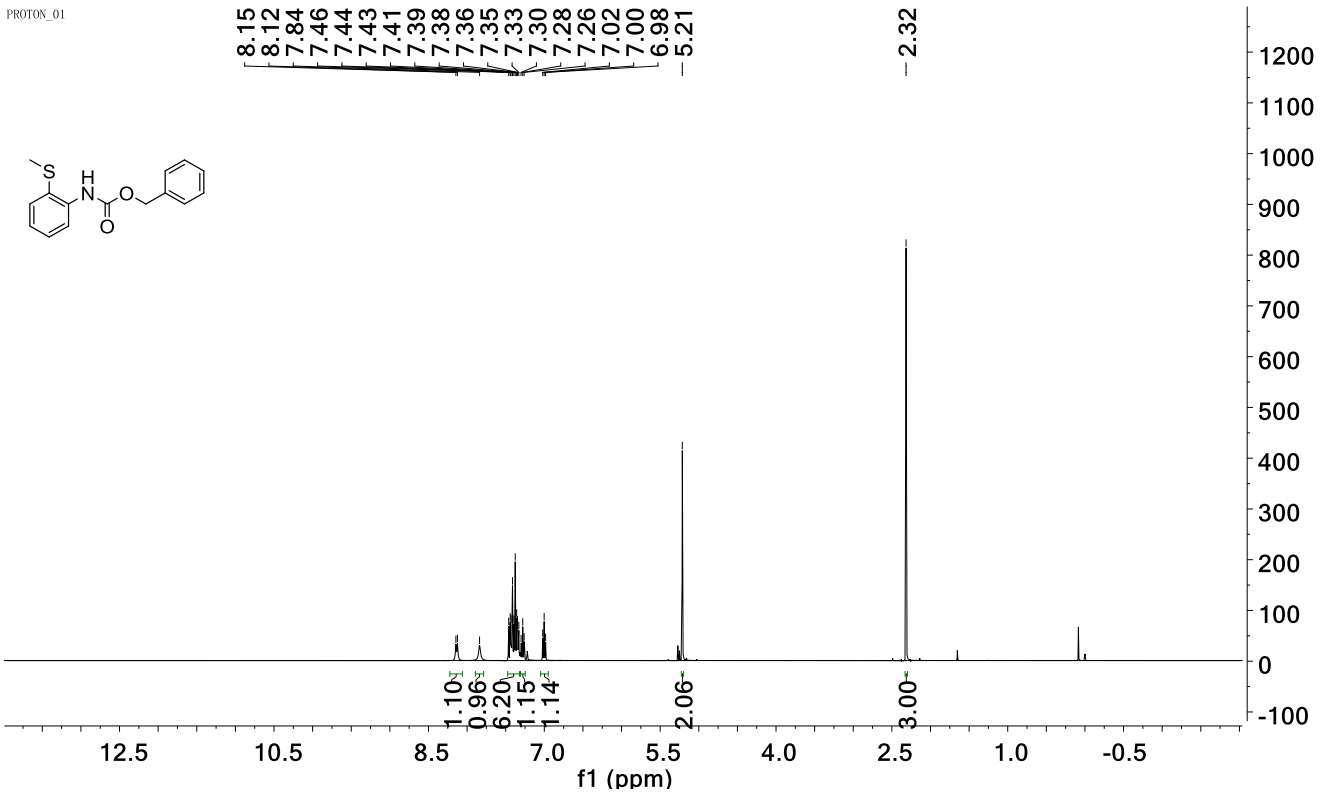
128.09
126.89
123.64
123.56
64.15
55.79
f1 (ppm)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7.41
7.39
7.38
7.36
7.35
7.33
7.30
7.28
7.26
7.02
7.00
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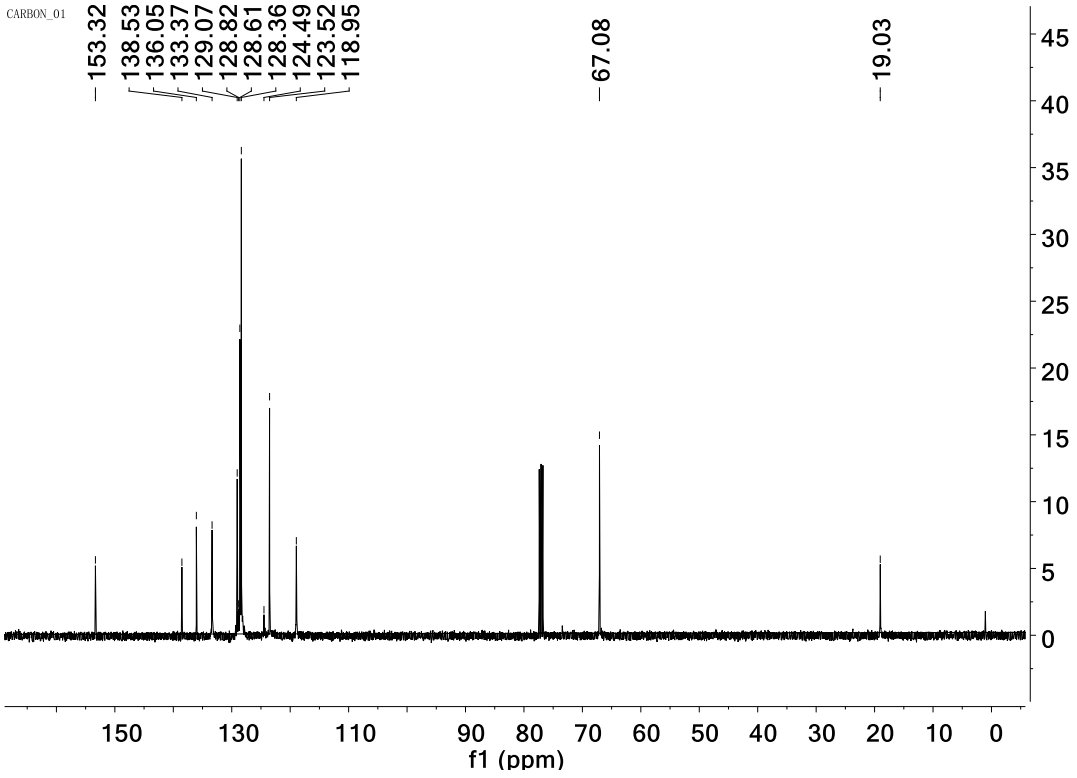
2.32
1.10
0.96
6.20
1.15
1.14
2.06
3.00
f1 (ppm)


CARBON_01
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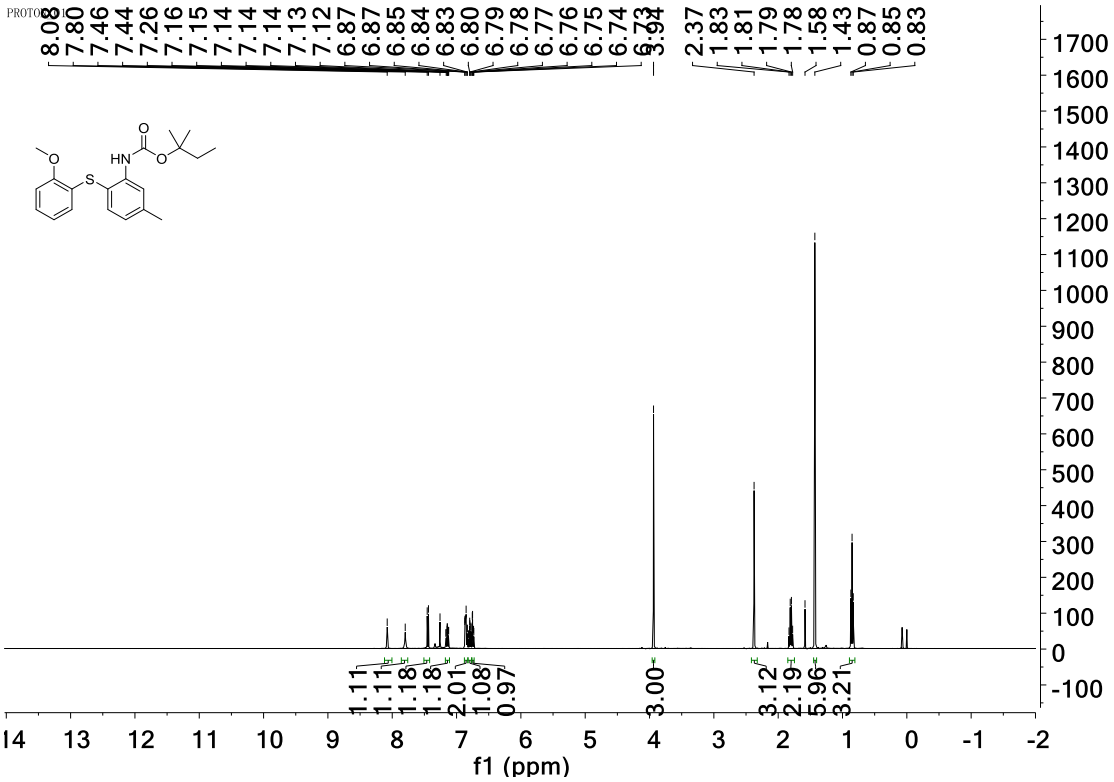
128.61
128.36
124.49
123.52
118.95
67.08
19.03
f1 (ppm)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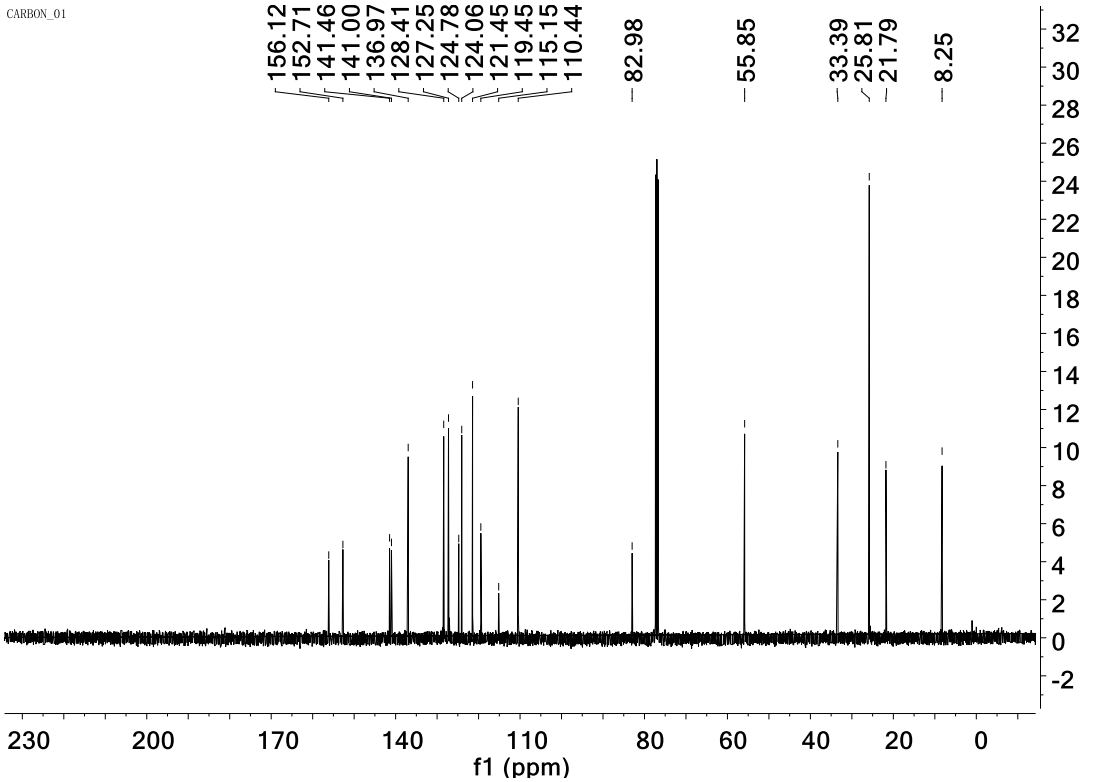
7.26
7.16
7.15
7.14
7.14
7.14
7.13
7.12
6.87
6.87
6.85
6.84
6.83
6.80
6.79
6.78
6.77
6.76
6.75
6.74
6.73
3.94
2.37
1.83
1.81
1.79
1.78
1.58
1.43
0.87
0.85
0.83
O
HN
O
O
S
1.11
1.11
1.18
1.18
2.01
1.08
0.97
3.00
3.12
2.19
5.96
3.21
f1 (ppm)


CARBON_01
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152.71
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128.41
127.25
124.78
124.06
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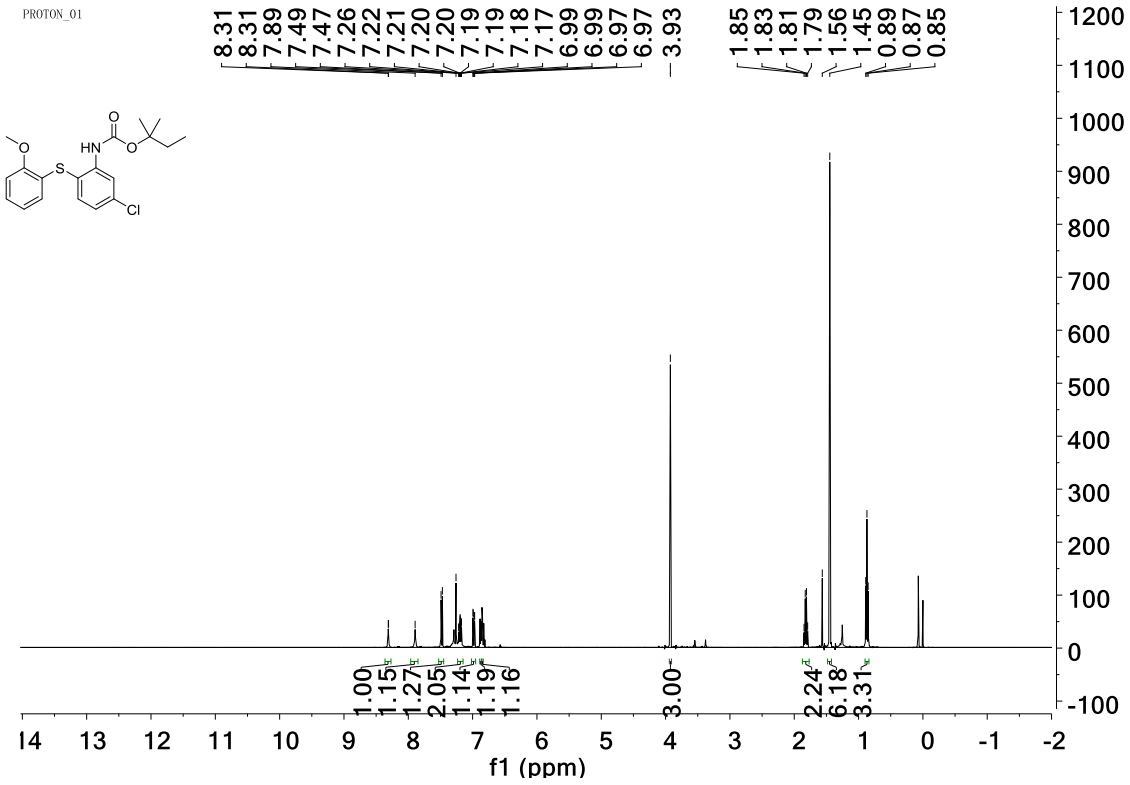
115.15
110.44
82.98
55.85
33.39
25.81
21.79
8.25
f1 (ppm)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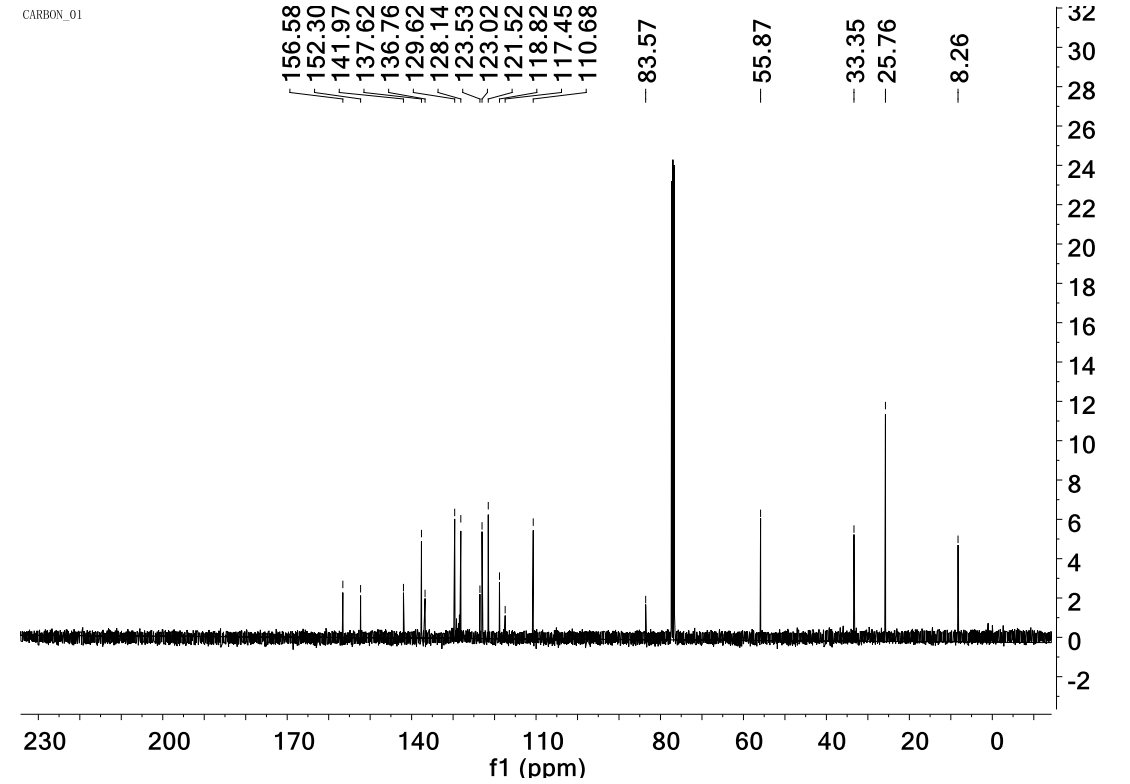
7.47
7.26
7.22
7.21
7.20
7.20
7.19
7.19
7.18
7.17
6.99
6.99
6.97
6.97
3.93
1.85
1.83
1.81
1.79
1.56
1.45
0.89
0.87
0.85
O
HN
O
O
S
Cl
1.00
1.15
1.27
2.05
1.14
1.19
1.16
3.00
2.24
6.18
3.31
f1 (ppm)


CARBON_01
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152.30
141.97
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136.76
129.62
128.14
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123.02
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118.82
117.45
110.68
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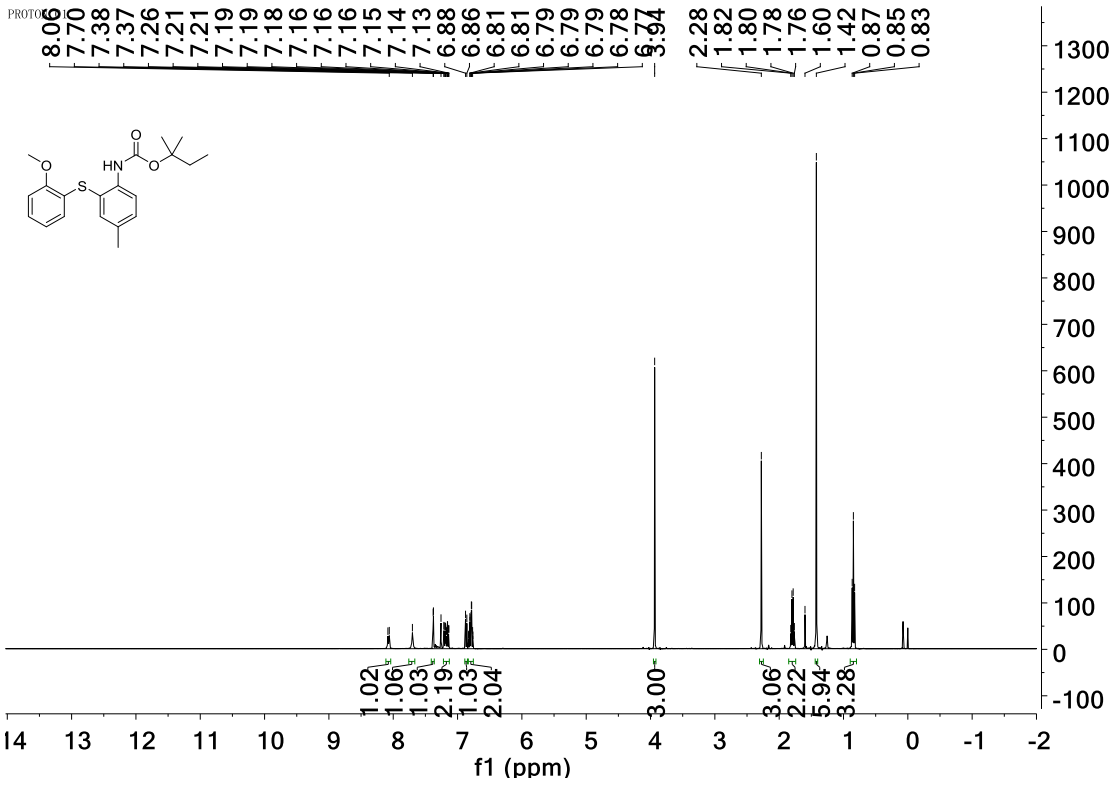
55.87
33.35
25.76
8.26
f1 (ppm)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7.19
7.19
7.18
7.16
7.16
7.16
7.15
7.14
7.13
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6.86
6.81
6.81
6.79
6.79
6.79
6.78
6.77
3.94
2.28
1.82
1.80
1.78
1.76
1.60
1.42
0.87
0.85
0.83
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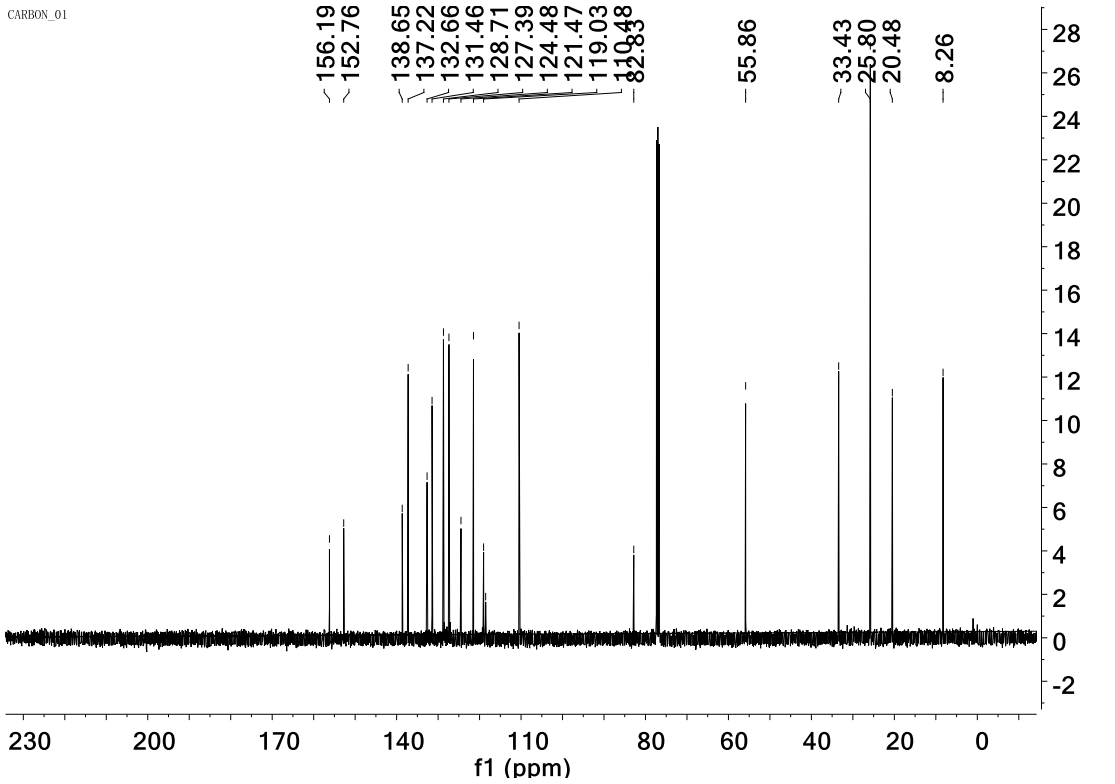
1.06
1.03
2.19
1.03
2.04
3.00
3.06
2.22
5.94
3.28
f1 (ppm)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132.66
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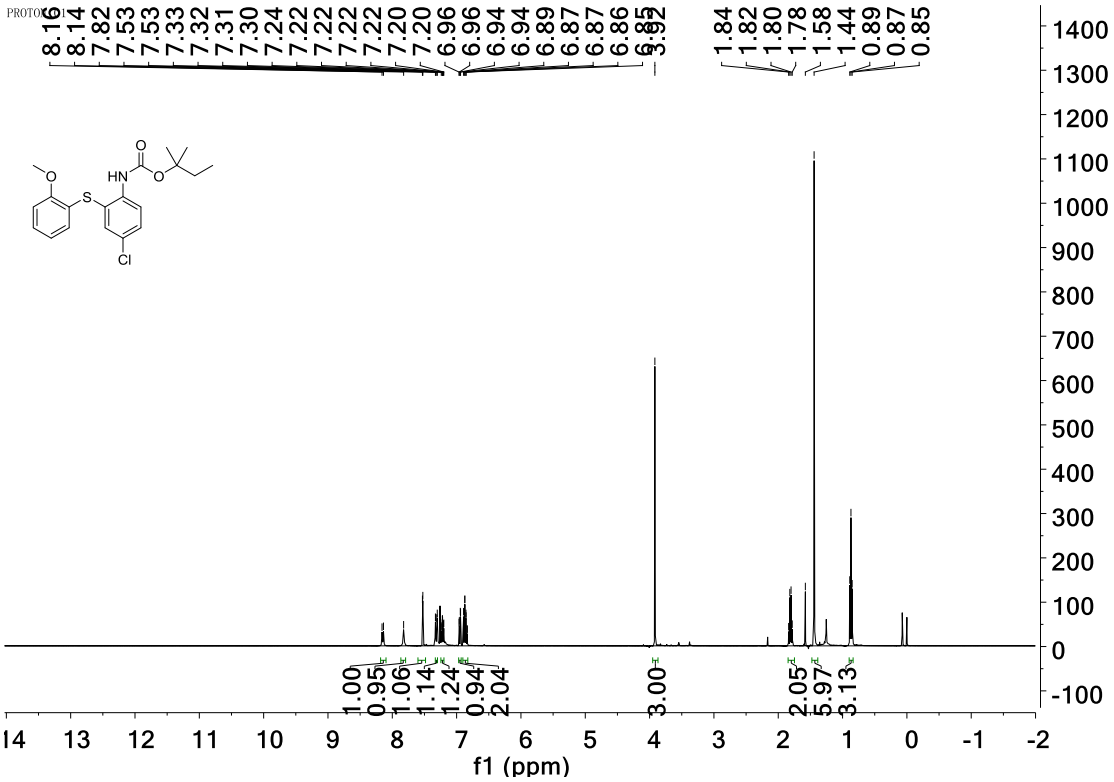
127.39
124.48
121.47
119.03
82.83
55.86
33.43
25.80
20.48
8.26
f1 (ppm)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7.32
7.31
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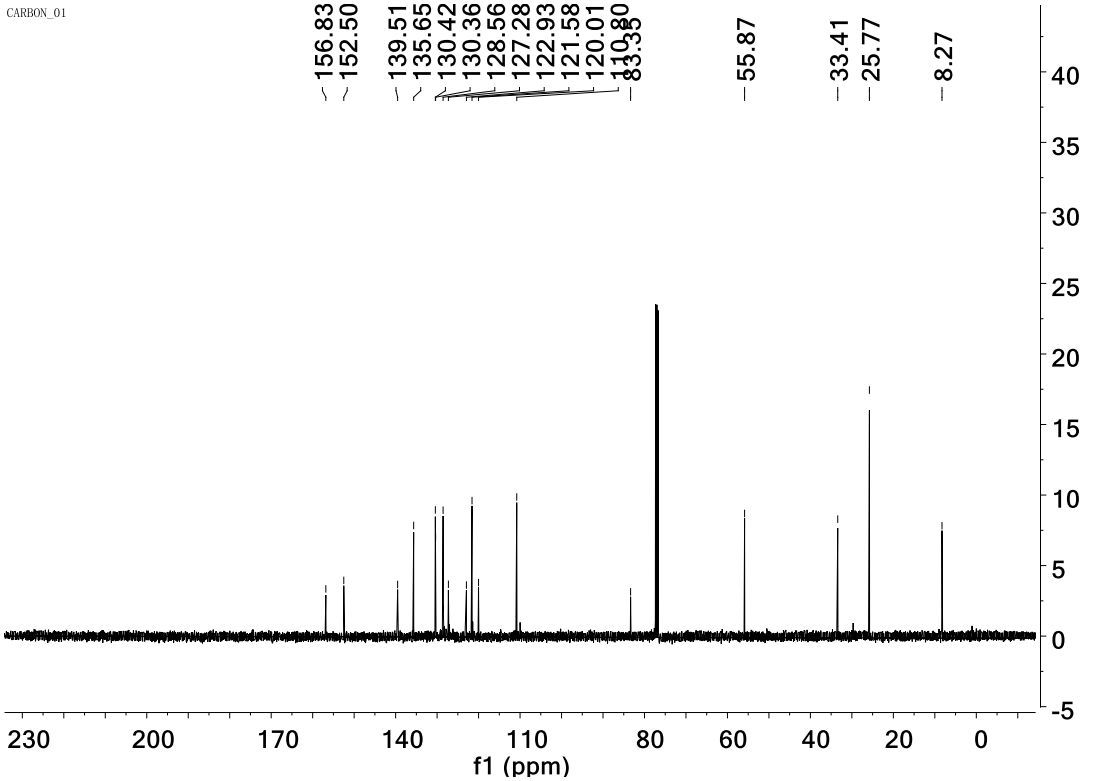
7.24
7.22
7.22
7.22
7.20
7.20
6.96
6.96
6.94
6.94
6.89
6.87
6.87
6.86
3.92
1.84
1.82
1.80
1.78
1.58
1.44
0.89
0.87
0.85
1.00
0.95
1.06
1.14
1.24
0.94
2.04
3.00
2.05
5.97
3.13
f1 (ppm)


CARBON_01
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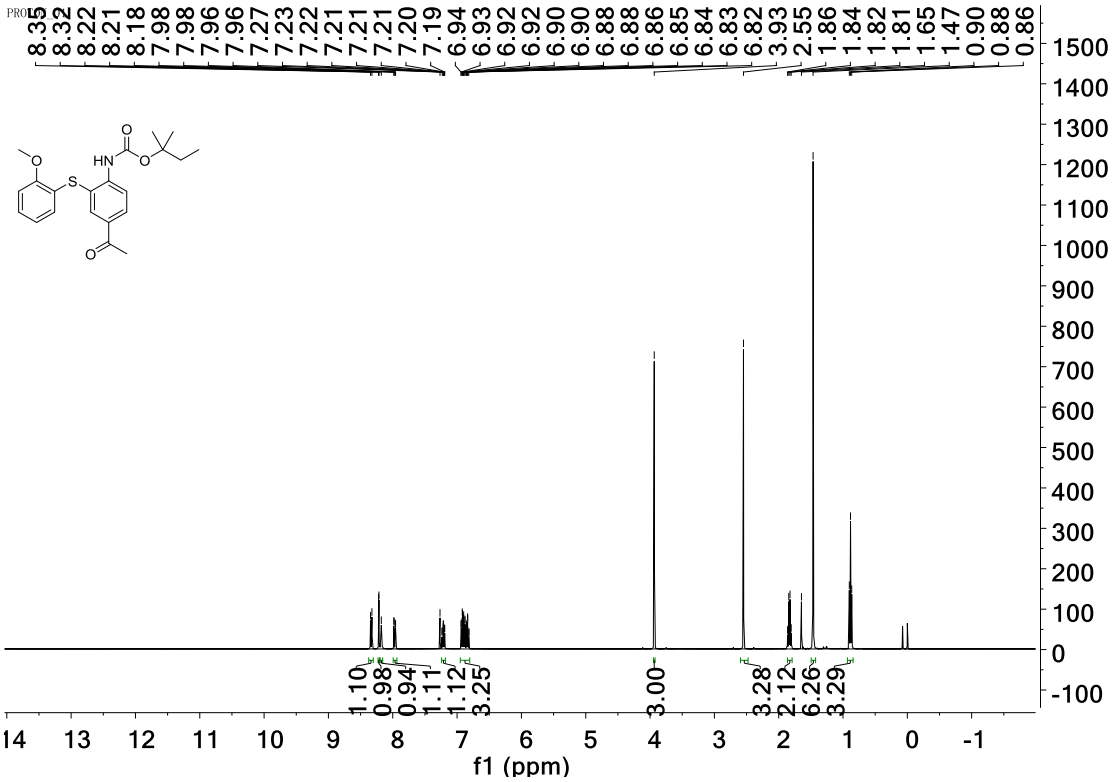
8.27
f1 (ppm)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7.96
7.96
7.27
7.23
7.22
7.21
7.21
7.21
7.20
7.19
6.94
6.93
6.92
6.92
6.90
6.90
6.88
6.88
6.86
6.85
6.84
6.83
6.82
3.93
2.55
1.86
1.84
1.82
1.81
1.65
1.47
0.90
0.88
0.86
1.10
0.98
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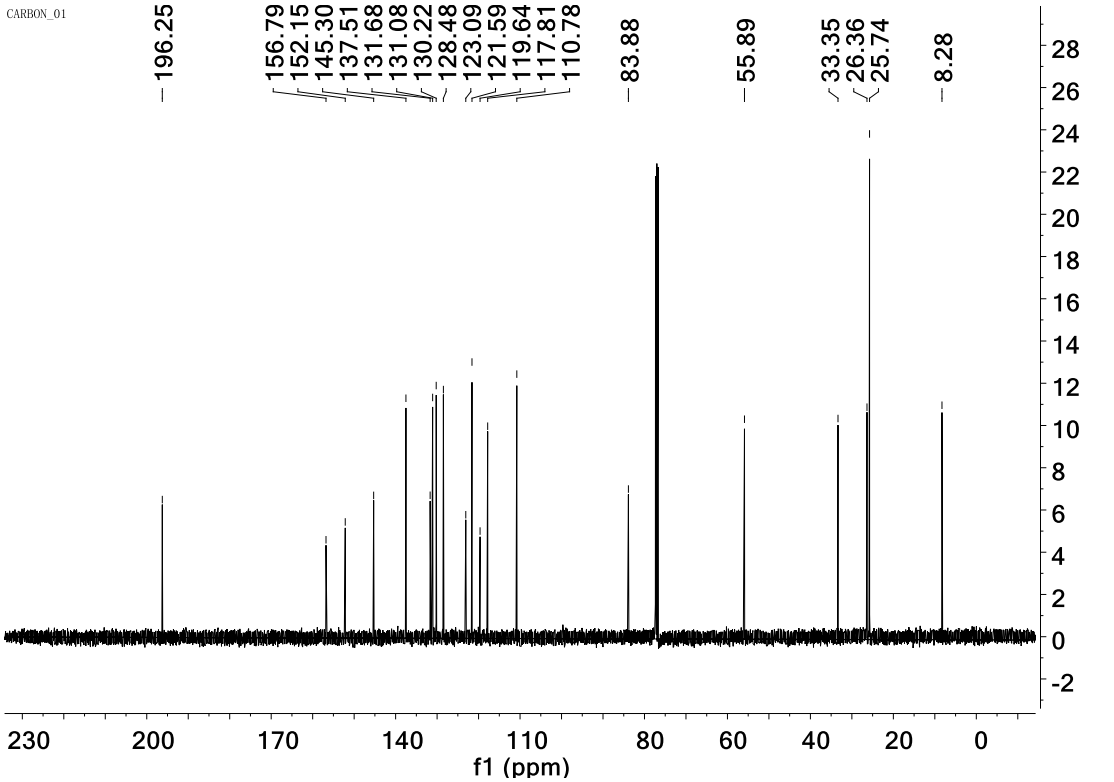
3.25
3.00
3.28
2.12
6.26
3.29
f1 (ppm)


CARBON_01
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131.68
131.08
130.22
128.48
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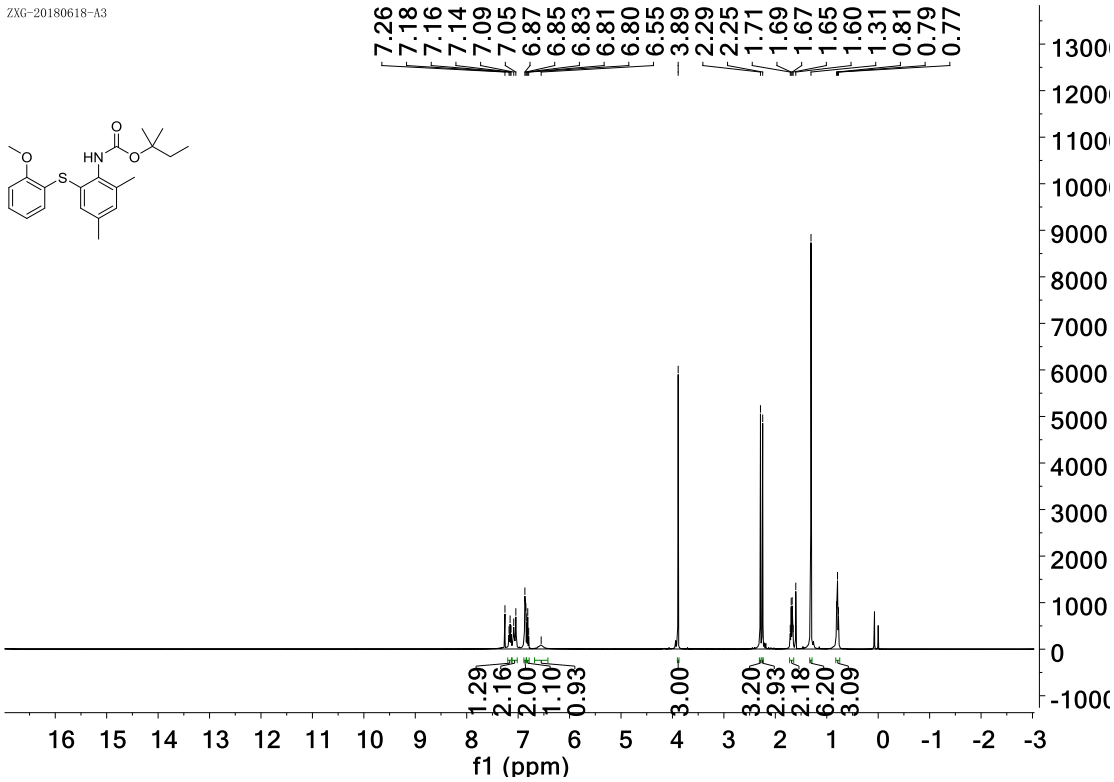
117.81
110.78
83.88
55.89
33.35
26.36
25.74
8.28
f1 (ppm)


ZXG-20180618-A3
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7.14
7.09
7.05
6.87
6.85
6.83
6.81
6.80
6.55
3.89
2.29
2.25
1.71
1.69
1.67
1.65
1.60
1.31
0.81
0.79
0.77
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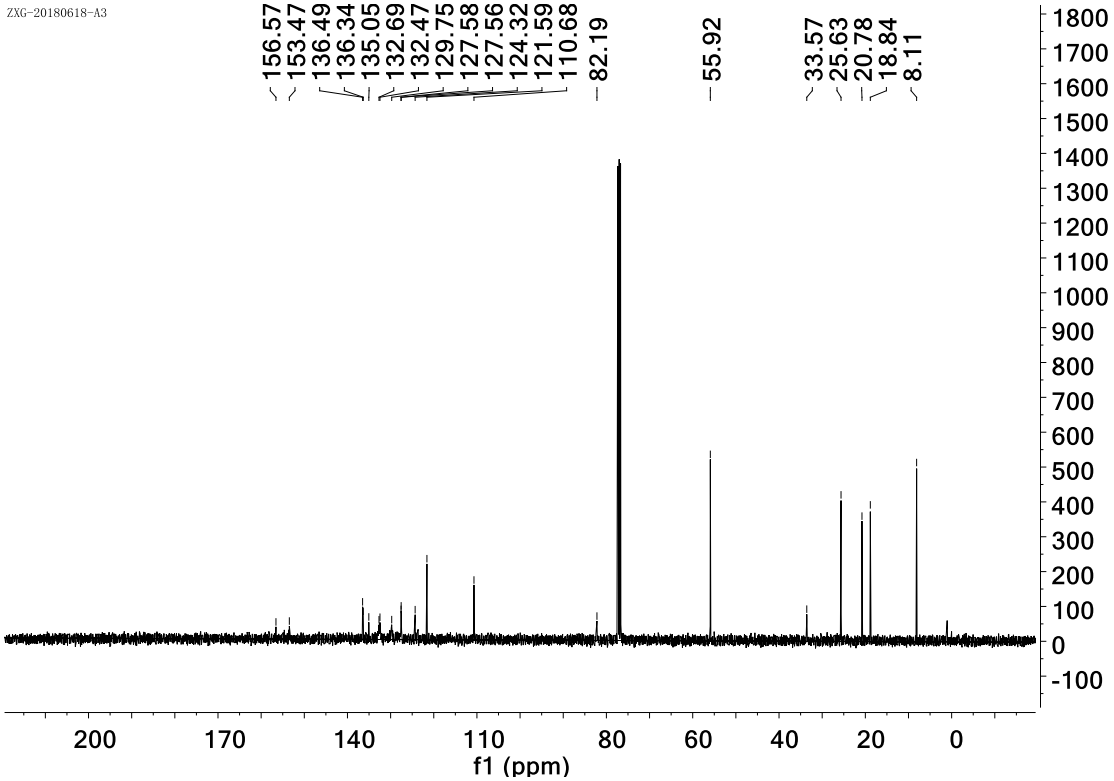
1.10
0.93
3.00
3.20
2.93
2.18
6.20
3.09
f1 (ppm)


ZXG-20180618-A3
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132.69
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129.75
127.58
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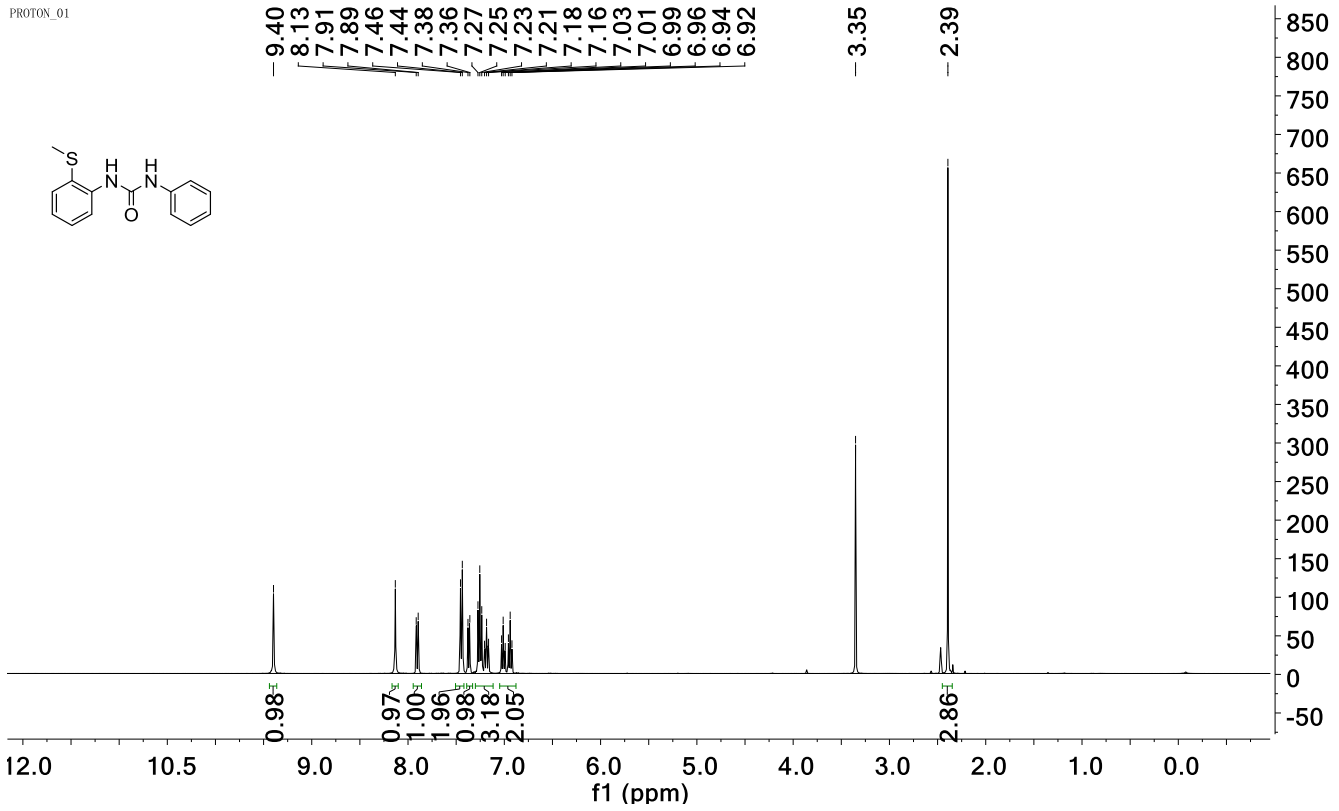
110.68
82.19
55.92
33.57
25.63
20.78
18.84
8.11
f1 (ppm)


PROTON_01
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7.36
7.27
7.25
7.23
7.21
7.18
7.16
7.03
7.01
6.99
6.96
6.94
6.92
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0.97
1.00
1.96
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3.18
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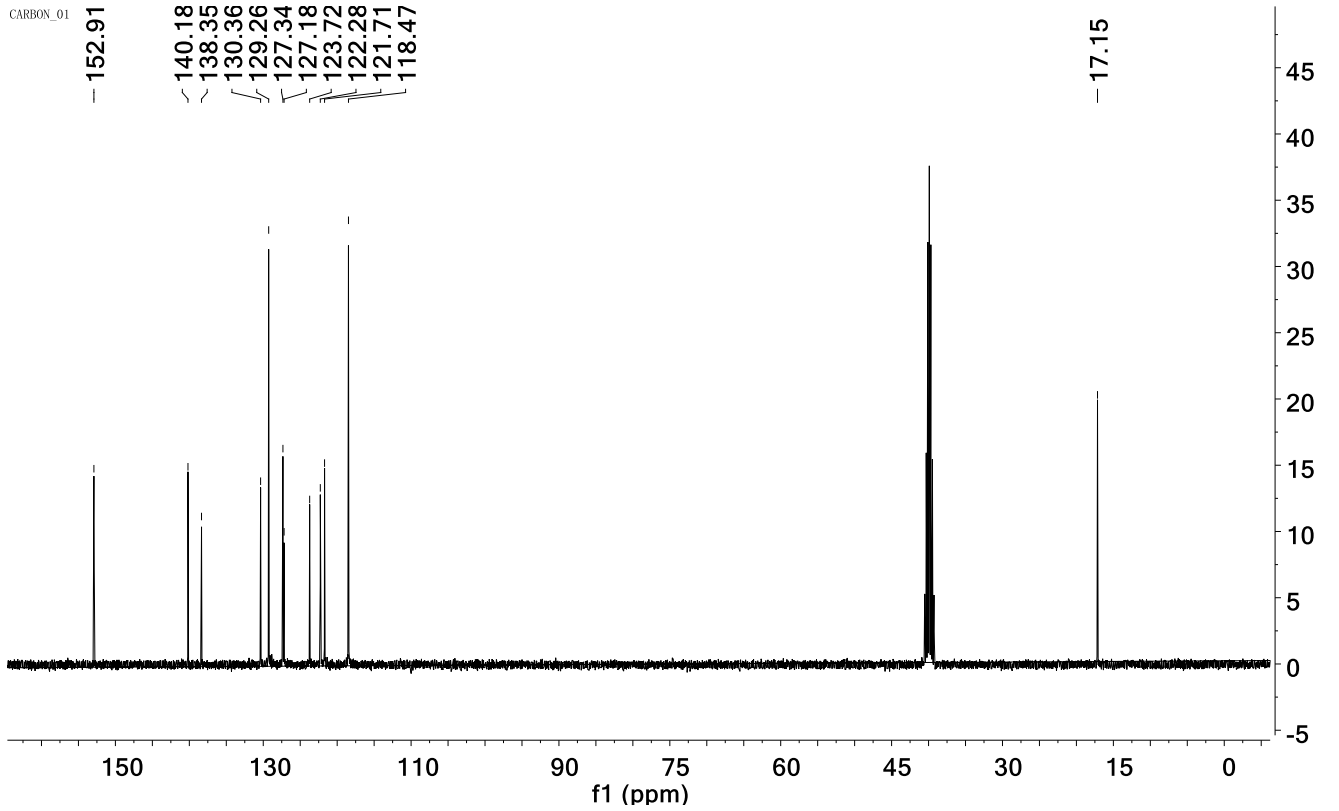
2.86
f1 (ppm)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127.18
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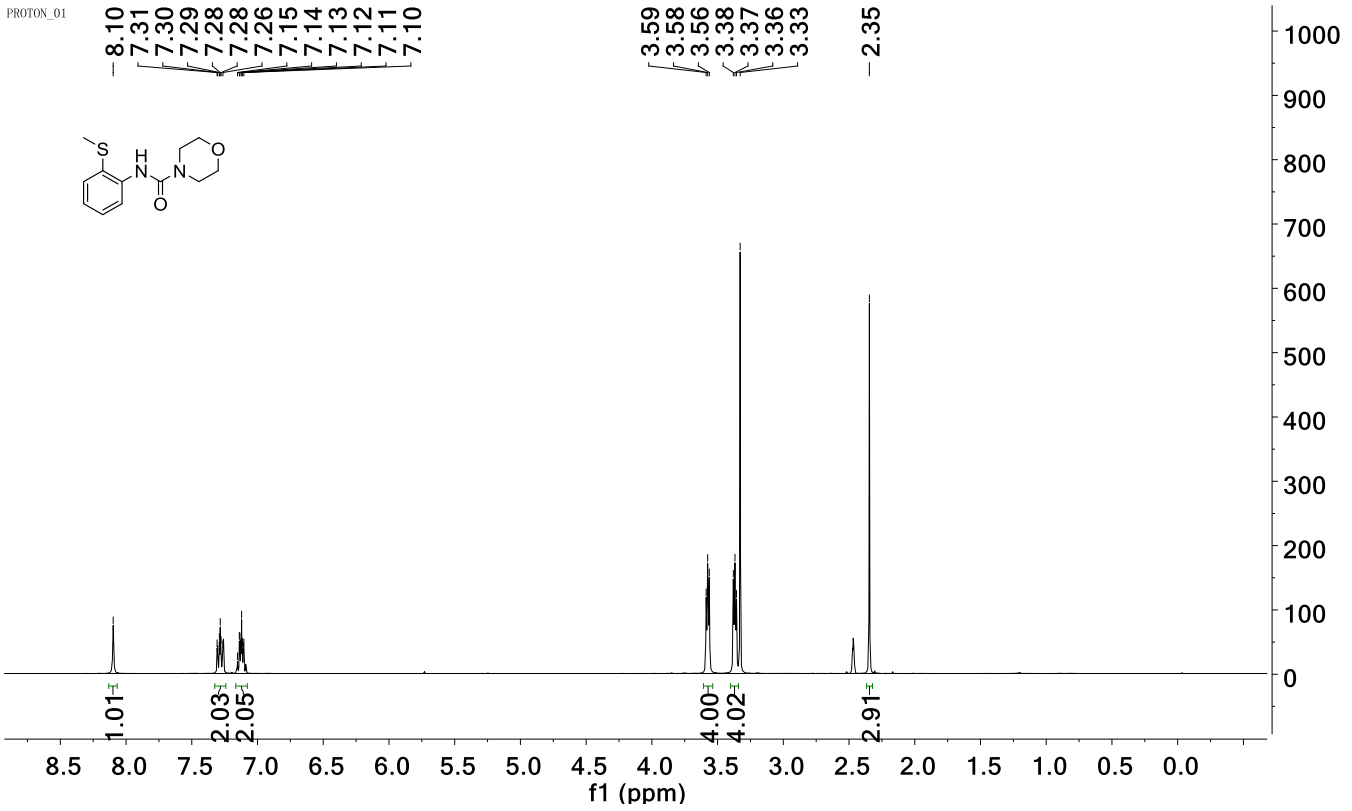
118.47
17.15
f1 (ppm)


PROTON_01
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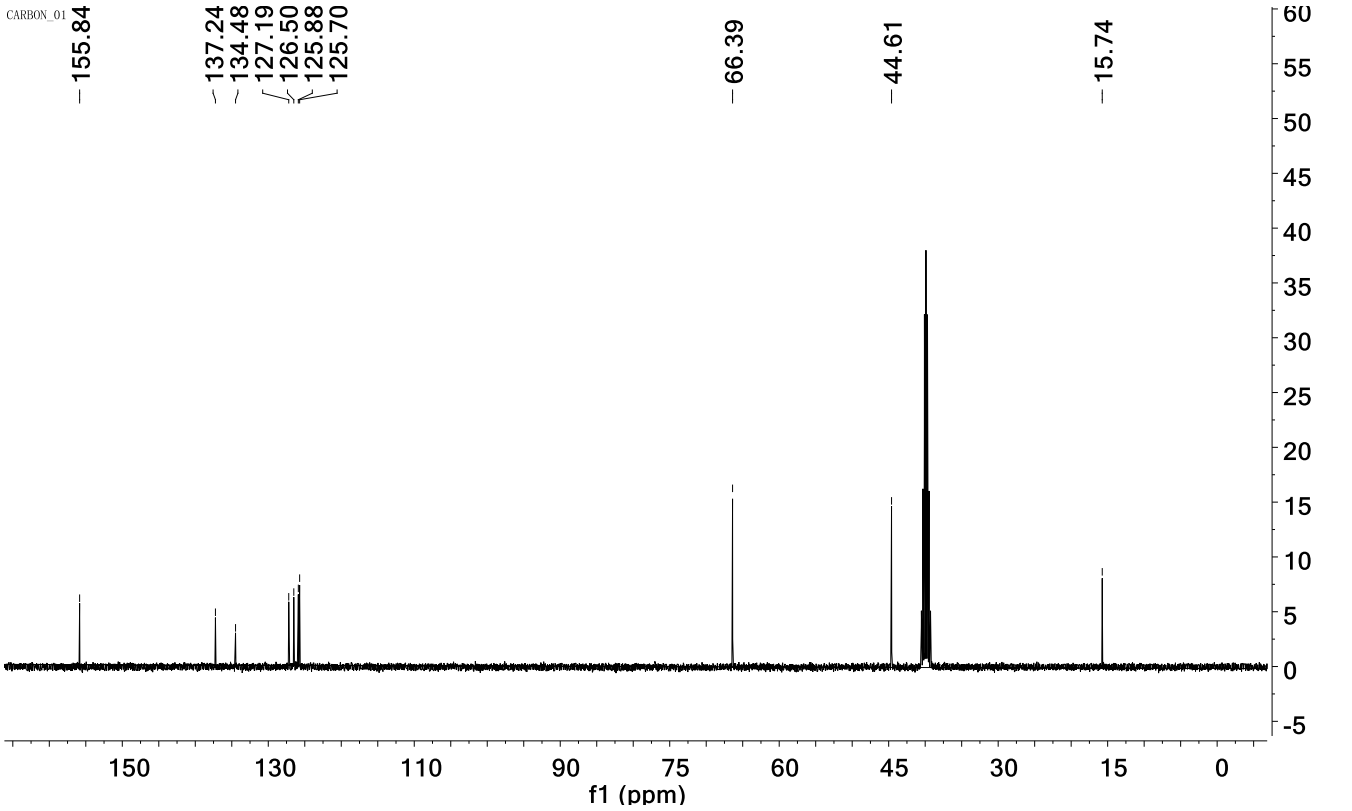
7.28
7.26
7.15
7.14
7.13
7.12
7.11
7.10
3.59
3.58
3.56
3.38
3.37
3.36
3.33
2.35
1.01
2.03
2.05
4.00
4.02
2.91
f1 (ppm)


CARBON_01
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125.88
125.70
66.39
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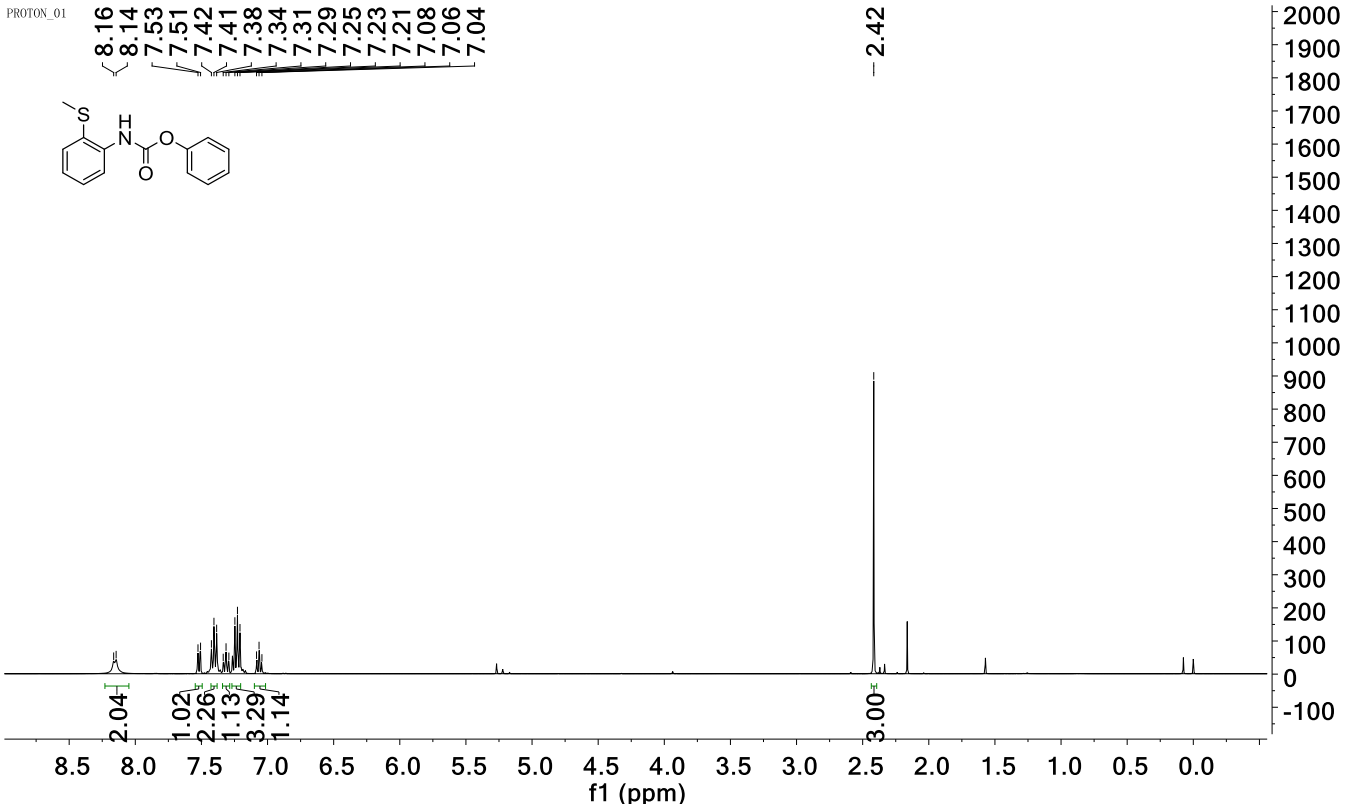
15.74
f1 (ppm)


PROTON_01
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7.31
7.29
7.25
7.23
7.21
7.08
7.06
7.04
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S
H
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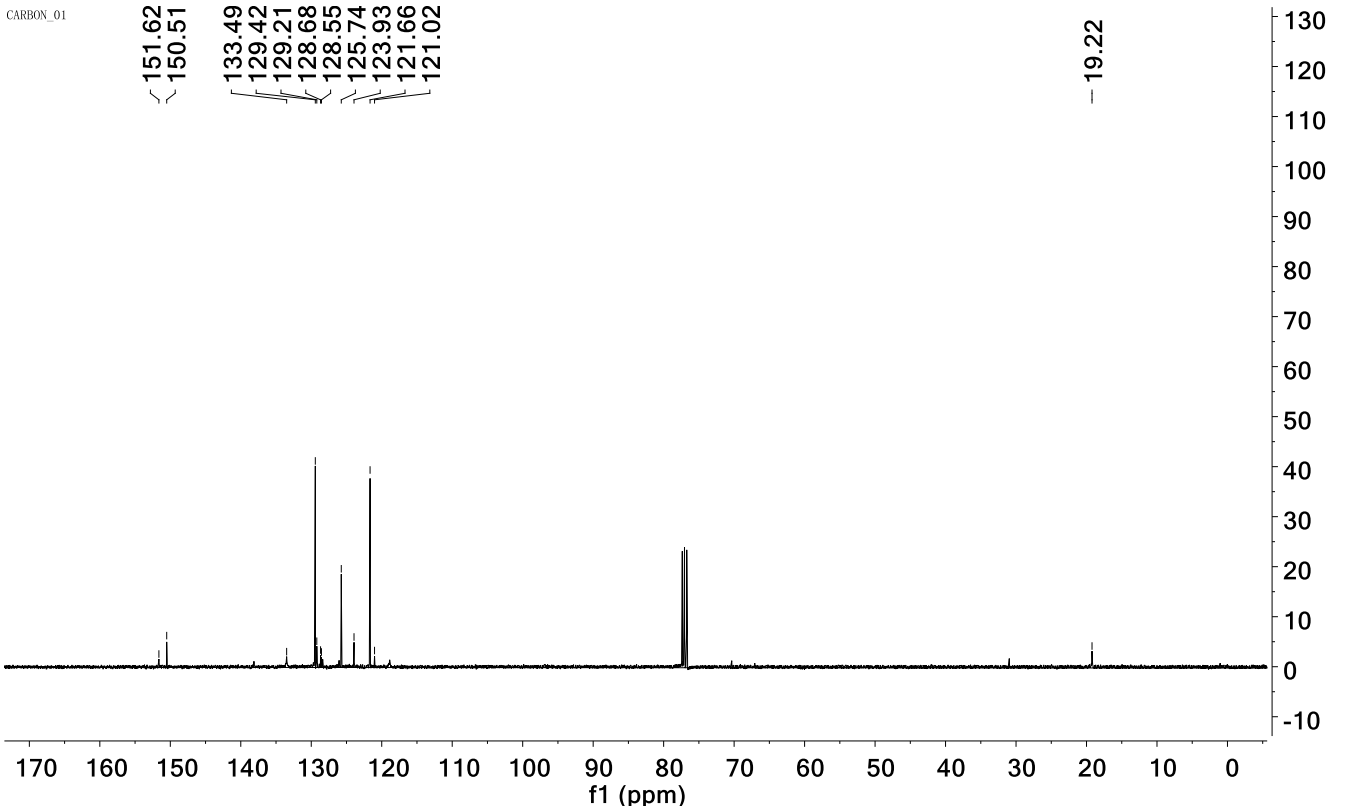
O
O
2.04
1.02
2.26
1.13
3.29
1.14
3.00
f1 (ppm)


CARBON_01
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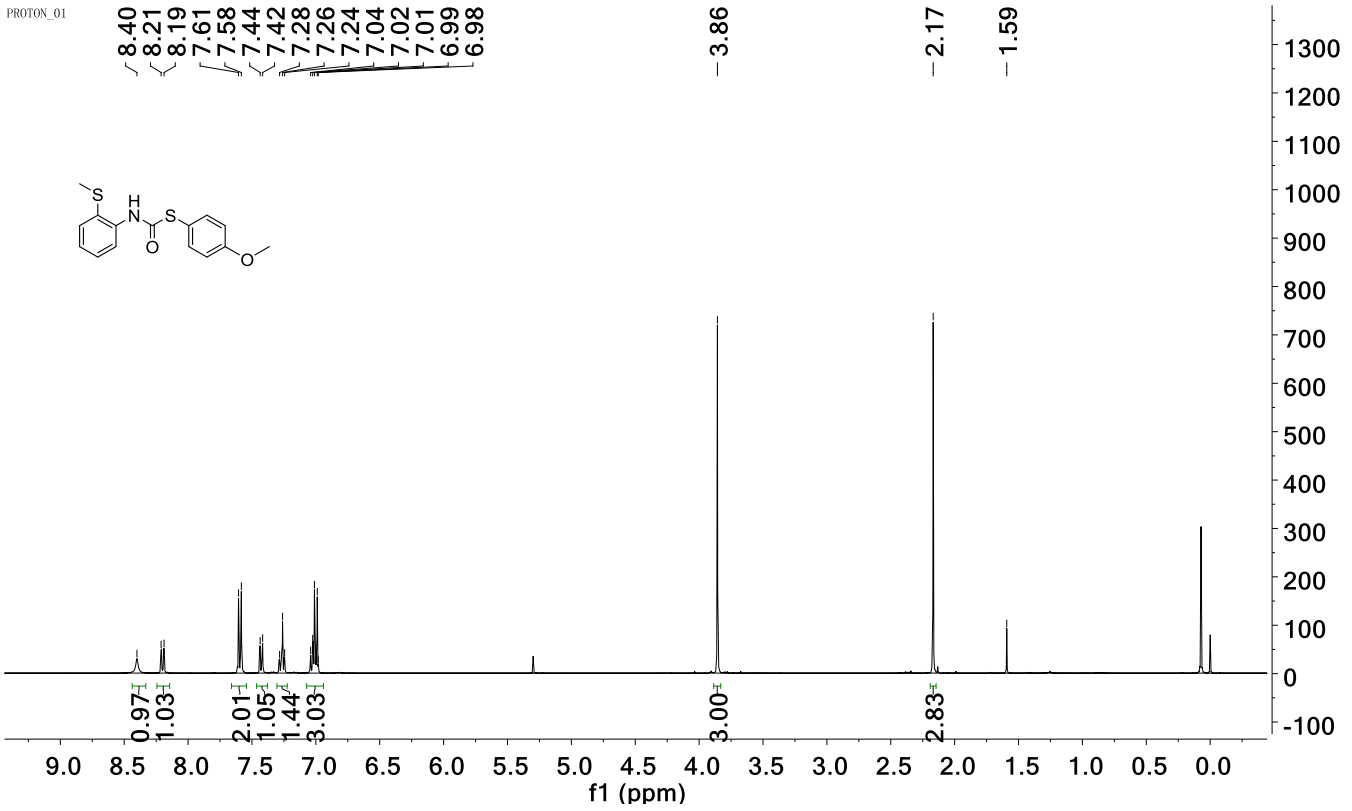
128.68
128.55
125.74
123.93
121.66
121.02
19.22
f1 (ppm)


PROTON_01
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7.58
7.44
7.42
7.28
7.26
7.24
7.04
7.02
7.01
6.99
6.98
3.86
2.17
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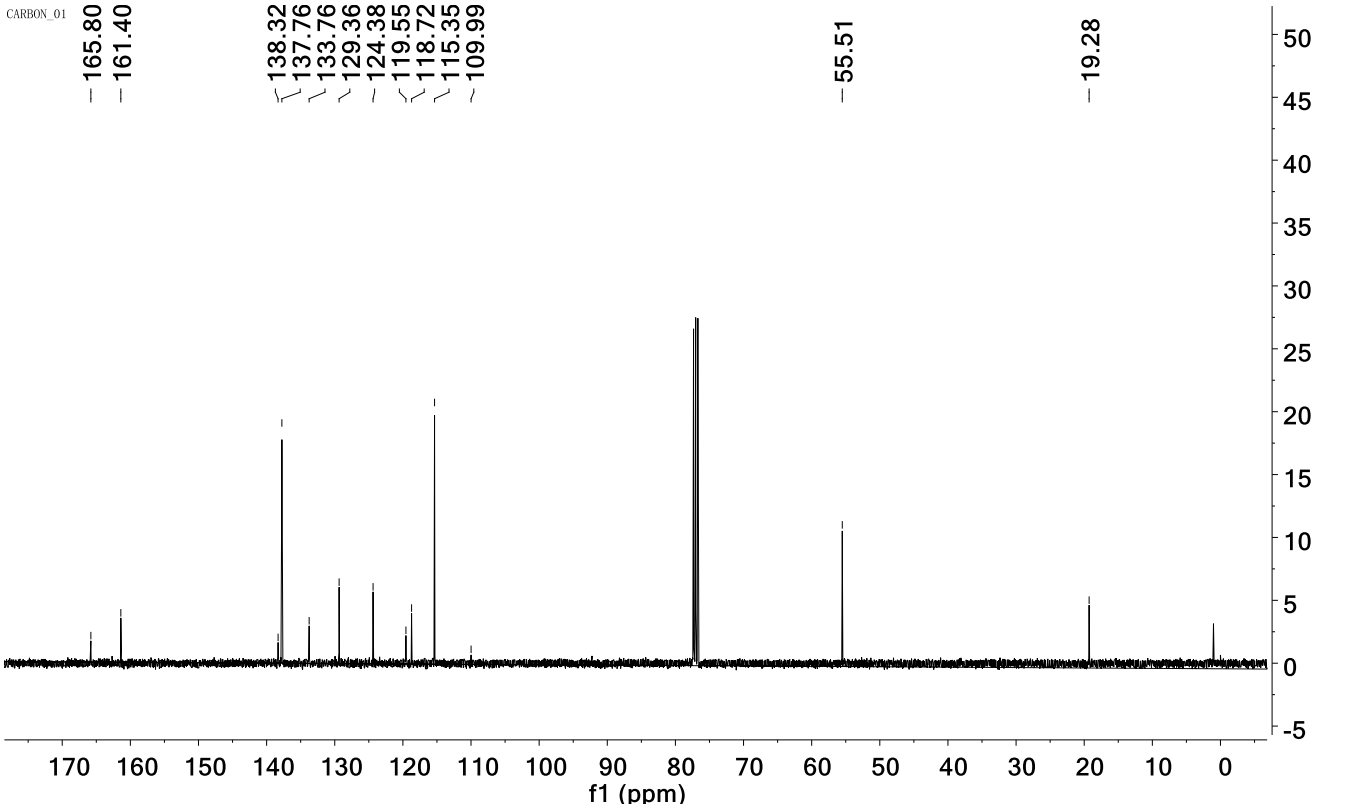
0.97
1.03
2.01
1.05
1.44
3.03
3.00
2.83
f1 (ppm)


CARBON_01
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129.36
124.38
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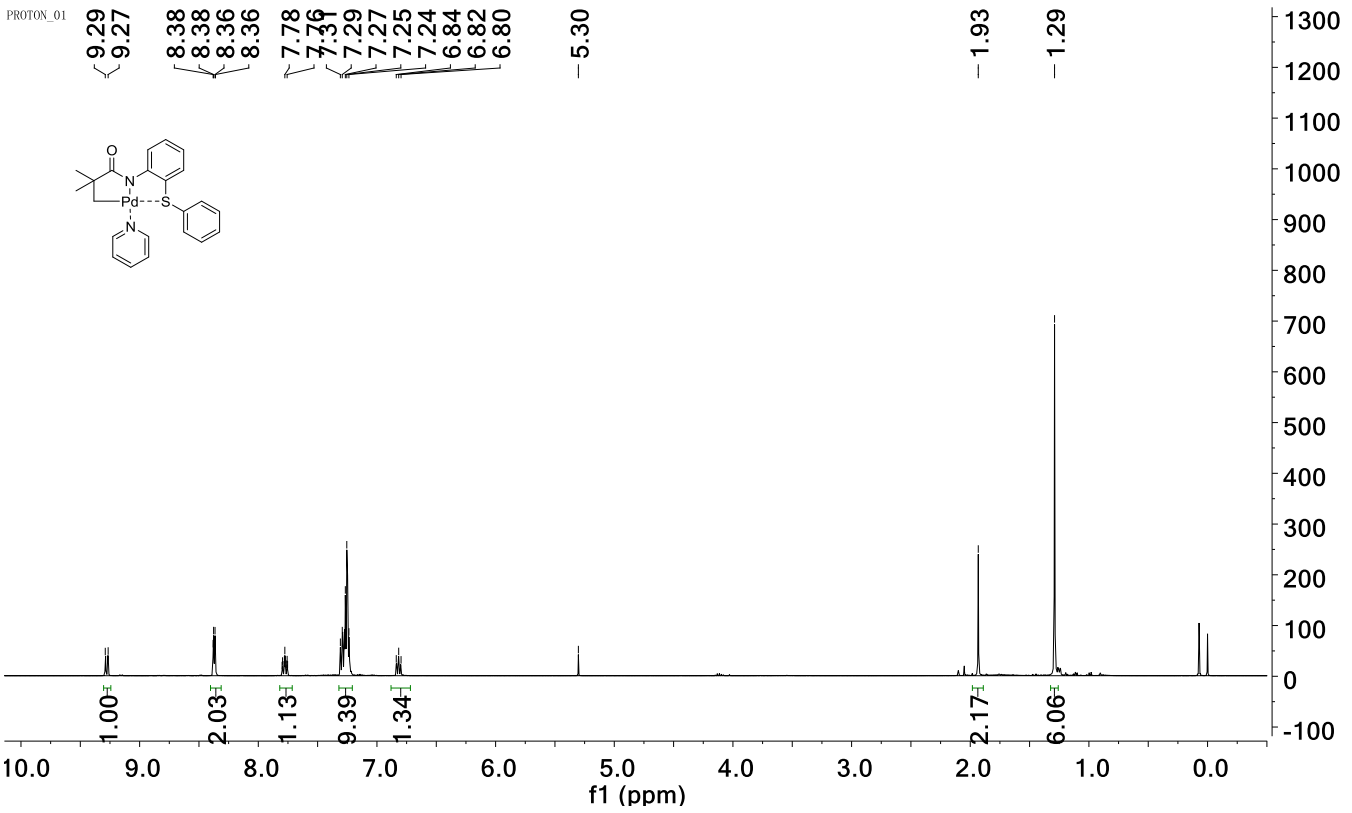
118.72
115.35
109.99
55.51
19.28
f1 (ppm)


PROTON_01
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9.27
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8.38
8.36
8.36
7.78
7.76
7.31
7.29
7.27
7.25
7.24
6.84
6.82
6.80
5.30
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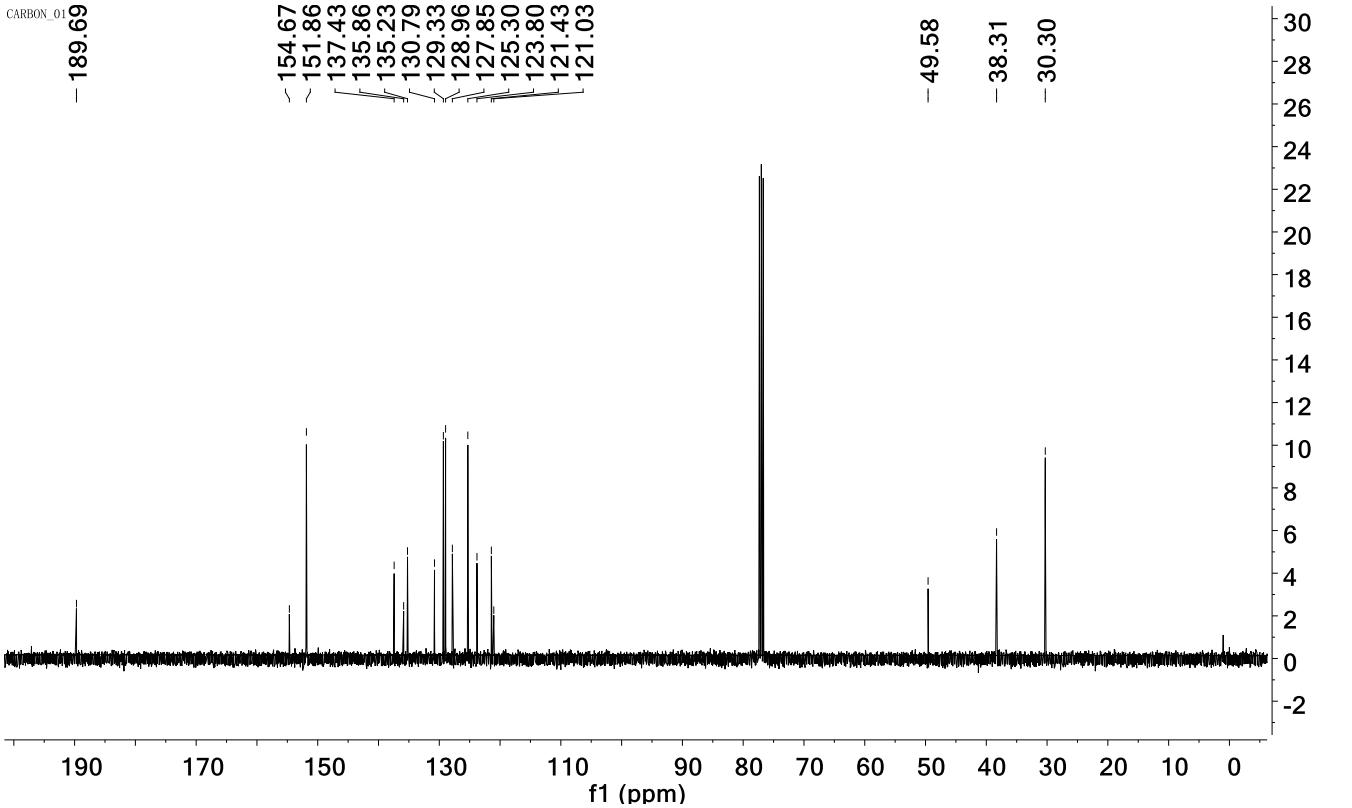
1.29
1.00
2.03
1.13
9.39
1.34
2.17
6.06
f1 (ppm)


CARBON_01
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135.23
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127.85
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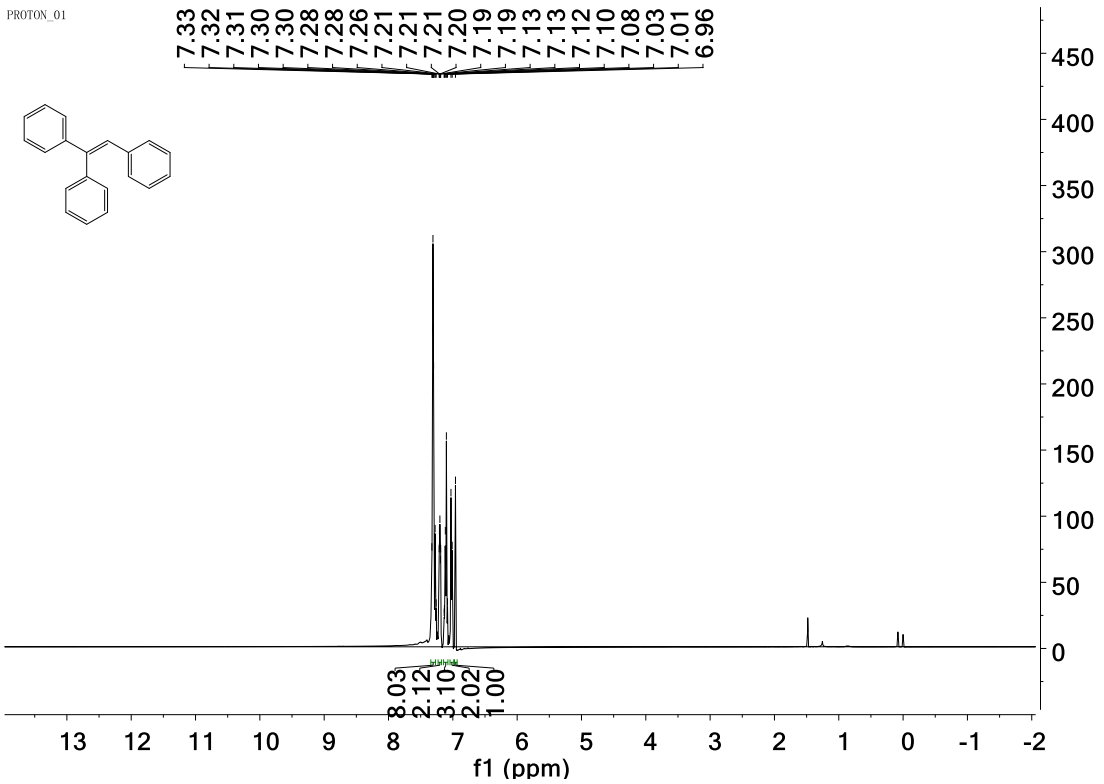
123.80
121.43
121.03
49.58
38.31
30.30
f1 (ppm)


PROTON_01
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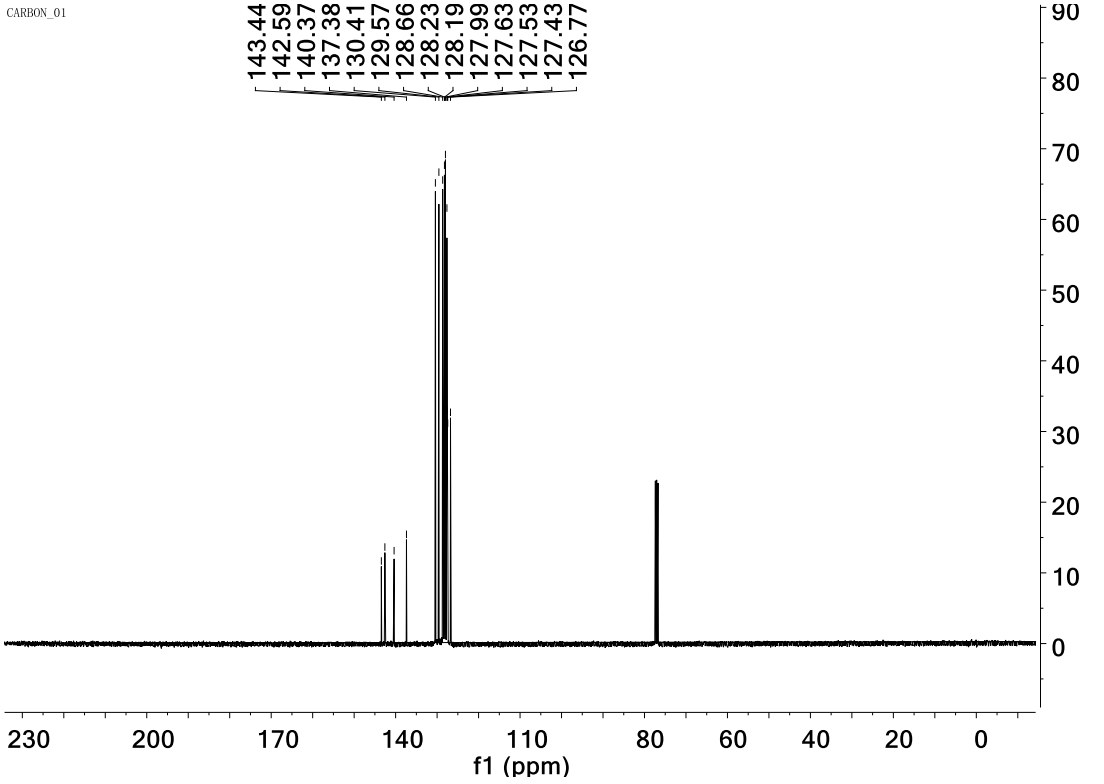
7.20
7.19
7.19
7.13
7.12
7.10
7.08
7.03
7.01
6.96
8.03
2.12
3.10
2.02
1.00
f1 (ppm)


CARBON_01
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128.23
128.19
127.99
127.63
127.53
127.43
126.77
f1 (ppm)