Supporting Information I (SI-I)

Gold-Catalyzed Atom-Economic Synthesis of Sulfone-Containing Pyrrolo[2,1-*a*] Isoquinolines from Diynamides: Evidence for Consecutive Sulfonyl Migration

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Table of Content

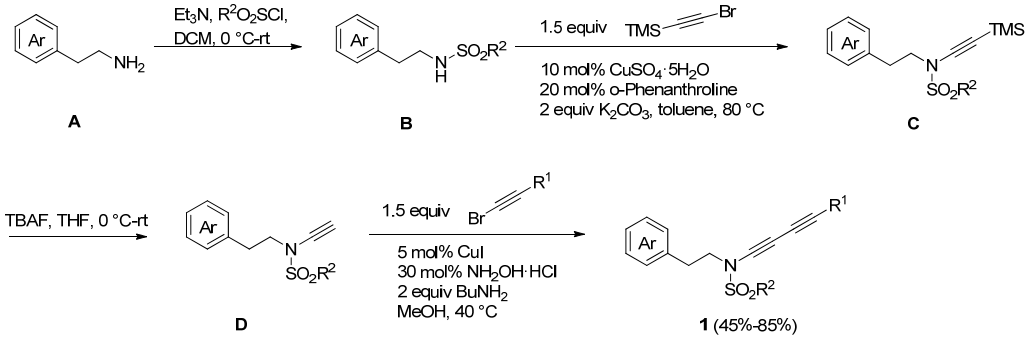
General information

Unless otherwise indicated, all glassware was dried by a heat gun before use and all reactions were performed under an atmosphere of Argon. All solvents were distilled from appropriate drying agents prior to use. All reagents were used as received from commercial suppliers unless otherwise stated. Several aryl ethylamines, bromocetylenes, and (Bromobuta-1,3-diyn-1-yl)benzene were prepared according to the procedures reported in the literatures. Reaction progress was monitored by thin layer chromatography (TLC). Visualization was achieved by ultraviolet light (254 nm). Flash column chromatography was performed using silica gel 60 (200-300 mesh, Merck and co.). Pressed KBr Disks for infra-red spectra were recorded using a Bruker-VERTEX 70 FT-IR spectrometer. Wavelengths (ν) are reported in cm^{-1}. Melting points were recorded using a SGW Melting Point thermometer (X-4). All ^{1}H NMR, ^{13}C NMR spectra were recorded on Bruker AV-III 400 in $CDCl_3$, CD_3CN or DMSO-d_6. Chemical shifts were given in parts per million (ppm, δ), referenced to the peak of tetramethylsilane, defined at δ = 0.00 (^{1}H NMR), or the solvent peak of $CDCl_3$, defined at δ = 77.0 (^{13}C NMR); the peak of CD_3CN, defined at δ = 1.94 (^{1}H NMR), defined at δ = 1.32 (^{13}C NMR); the peak of DMSO-d_6, defined at δ = 2.50 (^{1}H NMR), defined at δ = 40.0 (^{13}C NMR). Coupling constants were quoted in Hz (*J*). ^{1}H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q), pentet (p), septet (se), octet (o). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br).

General procedure for preparation of 1,3-Diynamides

Representative synthetic procedures A for the preparation of 1,3-diynamides 1 (1a-1j, 1s-1ac):

All bromocetylenes were synthesized according to known procedures reported in the literatures. [1]



Choose 1a as an example:

Synthesis of B: A solution of N-(3-methoxyphenethyl)methanesulfonamide (3.78 g, 25 mmol) in DCM (100 mL) at 0 °C was added Et_3N (6.7 mL, 50 mmol). Then methylsulfonyl chloride (2.13 mL, 27.5 mmol) was added drop-wise via syringe at this temperature. The mixture was allowed to warm up to room temperature and stirred for 2 hours. The reaction was diluted with DCM (60 mL) and water (60 mL), the organic layer was separated and the aqueous layer was extracted with DCM (3 × 60 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo to furnish the desired N-methyl indole. Recrystallization from PE/EA gave the product (5.55 g, 97%). R_f = 0.40 (petroleum ether : ethyl acetate = 1 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.21 (m, 1H), 6.81-6.75 (m, 3H), 4.51-4.39 (m, 1H), 3.80 (d, J = 1.6 Hz, 3H), 3.41-3.39 (m, 2H), 2.87-2.83 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 139.4, 129.8, 121.0, 114.6, 112.1, 55.1, 44.3, 40.2, 36.4.

Synthesis of C: To a sealed tube was added N-(3-methoxyphenethyl)methanesulfonamide (2.27 g, 10 mmol), $CuSO_4 \cdot 5H_2O$ (500 mg, 2.0 mmol), 1,10-phenanthroline (720 mg, 4.0 mmol) and K_2CO_3 (2.76 g, 20.0 mmol), and this mixture was treated with toluene (40 mL) and (bromoethynyl)trimethylsilane (2.65 g, 15 mmol) under argon. The solution was heated at 80 °C for 14 h. The resulting solution was cooled to room temperatures, filtered through celite, and concentrated in vacuo. Purification of the crude residue with silica flash chromatography gave the ynamide (2.30 g, 70 %). R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.01 (t, J = 8.0 Hz, 1H), 6.63 (d, J = 7.6 Hz, 1H), 6.58 (dt, J_1 = 8.0 Hz, J_2 = 2.4 Hz, 2H), 3.58 (s, 3H), 3.50 (t, J = 7.2 Hz, 2H), 2.76 (t, J = 7.2 Hz, 2H), 2.48 (s, 3H), 0.00 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 139.1, 129.6, 121.3, 114.7, 112.3, 93.7, 74.5, 55.0, 52.2, 38.0, 34.2. 0.1; IR (KBr) 2963, 2165, 1597, 1496, 1363, 125, 1163, 1044, 964, 852, 760, 701, 515 cm^{-1}; HRMS-(ESI) (m/z): $[M+Na]^+$ calcd for $C_{15}H_{23}NNaO_3SSi$, 348.1060; found 348.1060.

Synthesis of D: A solution of N-(3-methoxyphenethyl)-2-(trimethylsilyl)ethyn-1-amine (3.60 g, 11 mmol) in THF (80 mL) was cooled to 0 °C before drop-wise addition of TBAF (14.3 mL, 1 M in THF). The mixture was allowed to warm up to room temperature and stirred for 2 hours. The reaction mixture was diluted with ethyl acetate and washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by column chromatography (petroleum: ethyl acetate = 6 : 1) to give N-(3-methoxyphenethyl)ethynamine (2.22 g, 80%) as a yellow oil. R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (t, J = 8.0 Hz, 1H), 6.85 (d, J = 7.6 Hz, 1H), 6.81-6.77 (m, 2H), 3.79 (s, 3H), 3.72 (t, J = 7.2 Hz, 2H), 3.00 (t, J =

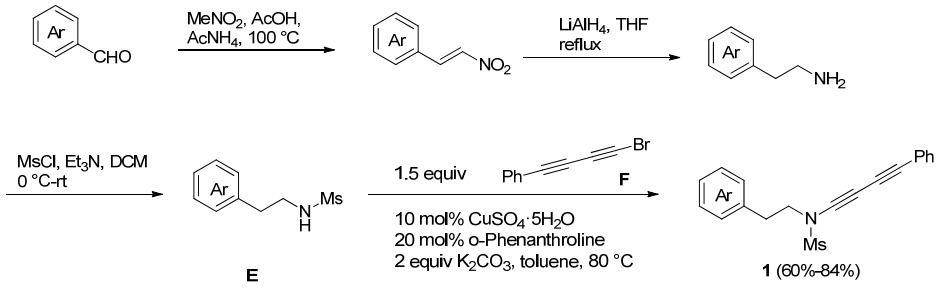
7.2 Hz, 2H), 2.92 (s, 1H), 2.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 139.0, 129.6, 121.2, 114.7, 112.3, 74.9, 60.5, 55.1, 52.1, 38.1, 34.1; IR (KBr) 3282, 2939, 2837, 2133, 1597, 1492, 1356, 1163, 1044, 964, 781, 515 cm^{-1}; HRMS-(ESI) (m/z): $[M+Na]^+$ calcd for $C_{12}H_{15}NNaO_3S$, 276.0665; found 276.0665.[2]

Synthesis of 1,3-diynamide 1a: To a sealed tube was added CuI (15 mg, 0.075 mmol), hydroxylamine hydrochloride (31 mg, 0.45 mmol), MeOH (15 mL), N-(3-methoxyphenethyl)ethynamine (380 mg, 1.5 mmol), n-$BuNH_2$ (0.30 mL, 3.0 mmol) and 1-bromopropyne (407 mg, 0.23 mmol) under argon. The reaction mixture was stirred at 40 °C. Upon completion, the suspension was cooled to room temperature, diluted with ethyl acetate (30 mL) and water (20 mL), the organic layer was separated and the aqueous layer was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography to give N-(3-methoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (392 mg, 74%). [3]

Representative synthetic procedures B for the preparation of 1,3-diynamides 1 (1k-1p, 1r, 1ad-1ah):

Aryl ethylamines were received from commercial suppliers or synthesized according to known procedures reported in the literatures. [4]

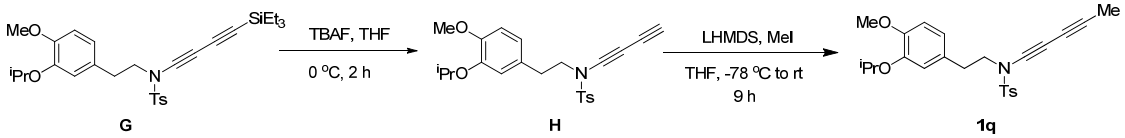
(Bromobuta-1,3-diyn-1-yl)benzene **F** was synthesized according to known procedures reported in the literature. [5]



Choose 1k as an example:

Synthesis of 1,3-diynamide 1k (same procedure as D to 1a): To a sealed tube was added N-(2,3-dimethoxyphenethyl)methanesulfonamide (390 mg, 1.5 mmol), $CuSO_4 \cdot 5H_2O$ (38 mg, 0.15 mmol), 1,10-phenanthroline (54 mg, 0.30 mmol) and K_2CO_3 (621 mg, 4.5 mmol), and this mixture was treated with toluene (15 mL) and (bromobuta-1,3-diyn-1-yl)benzene (460 mg, 2.25 mmol) under argon. The solution was heated at 80 °C for 14 h. The resulting solution was cooled to room temperatures, filtered through celite, and concentrated in vacuo. Purification of the crude residue with silica flash chromatography gave N-(2,3-dimethoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (426 mg, 74%).[3]

Synthetic procedures for the preparation of 1,3-diynamides 1q: [6]



N-(3-isopropoxy-4-methoxyphenethyl)-4-methyl-N-((triethylsilyl)buta-1,3-diyn-1-yl)benzenesulfonamide (G)

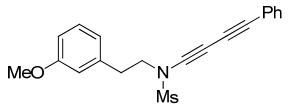
Compound **G** was obtained according to the general procedure A outlined above as a yellow oil (748 mg, 95%); R_f = 0.7 (Petroleum ether : ethyl acetate = 4 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.60 (d, *J* = 8.0 Hz, 1H,) 6.52 (d, *J* = 10.8 Hz, 2H), 4.35-4.29 (m, 1H), 3.66 (s, 3H), 3.40 (t, *J* = 7.2 Hz,

2H), 2.69 (t, *J* = 7.2 Hz, 2H), 2.28 (s, 3H), 1.19 (d, *J* = 6.0 Hz, 6H), 0.86 (t, *J* = 8.0 Hz, 9H), 0.49 (q, *J* = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 147.0, 144.8, 134.2, 129.7, 129.2, 127.3, 121.1, 116.5, 111.9, 88.3, 88.0, 71.2, 68.2, 59.7, 55.7, 52.6, 33.6, 21.9, 21.4, 7.2, 4.0; IR (KBr) ν 2953, 2918, 2851, 2221, 1510, 1471, 1377, 1261, 1170, 1023, 809, 676, 578, 543 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{29}H_{39}NNaO_4SSi$, 548.2261; found 548.2258.

***N*-(buta-1,3-diyn-1-yl)-*N*-(3-isopropoxy-4-methoxyphenethyl)-4-methylbenzenesulfonamide (H)**

To a solution of **G** (1.30 g, 2.47 mmol) in THF (15 mL), TBAF (4.9 mL, 1M in THF, 4.94 mmol) was added dropwise at 0 °C. The solution was stirred for 2 h during which the temperature gradually increased to room temperature. The reaction was quenched by water and extracted with ethyl acetate (3 × 20 mL). The combined extracts was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residual mass was purified by silica gel column chromatography using petroleum ether : ethyl acetate (5 : 1) as eluent to get **H** as a yellow oil (822 mg, 81%); R_f = 0.5 (petroleum ether : ethyl acetate = 3 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.68 (d, *J* = 8.0 Hz, 1H), 6.61-6.58 (m, 2H), 4.45-4.36 (m, 1H), 3.73 (s, 3H), 3.50 (t, *J* = 7.2 Hz, 2H), 2.76 (t, *J* = 7.2 Hz, 2H), 2.46 (s, 1H), 2.35 (s, 3H), 1.26 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.1, 146.9, 144.9, 134.0, 129.7, 129.1, 127.1, 121.1, 116.4, 111.9, 71.6, 71.1, 67.4, 58.7, 55.6, 52.4, 33.4, 21.8, 21.3; IR (KBr) ν 2942, 2354, 1636, 1464, 1257, 753, 417 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{23}H_{25}NNaO_4S$, 434.1396; found 434.1397.[2]

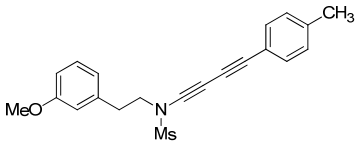
Synthesis of 1,3-diynamide 1q: To a solution of **H** (400 mg, 0.97 mmol) in THF (10 mL), LHMDS (1.5 mL, 1M in THF, 1.5 equiv.) was added dropwise at -78 °C. The temperature was increased to -60 °C and stirred for one hour after which the temperature was again maintained at -78 °C. Then MeI (1.94 mmol, 2 equiv.) was added slowly and the temperature was gradually increased to room temperature. It was stirred for another 9 h after which it was diluted by adding 10 mL of ethyl acetate and carefully quenched by saturated NH_4Cl solution. The reaction mixture was partitioned in a separating flask and the aqueous layer was extracted by ethyl acetate (3 × 15 mL). The combined extracts was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residual mass was purified by silica gel column chromatography using petroleum ether : ethyl acetate (5 : 1) as eluent to get **1q** as a yellow oil (256 mg, 62%).



1a

N-(3-methoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1a)

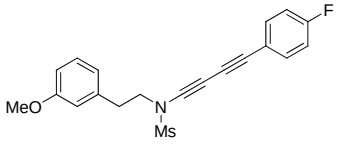
Compound **1a** was obtained according to the general procedure A outlined above as a yellow oil; R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 2H), 7.37-7.31 (m, 3H), 7.25 (t, J = 8.0 Hz, 1H), 6.88 (d, J = 7.6 Hz, 1H), 6.84-6.83 (m, 1H), 6.82-6.79 (m, 1H), 3.81 (s, 3H), 3.80 (t, J = 7.2 Hz, 2H), 3.04 (t, J = 7.2 Hz, 2H), 2.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 138.8, 132.4, 129.8, 129.1, 128.4, 121.9, 121.4, 114.7, 112.6, 81.8, 73.2, 72.7, 59.7, 55.2, 52.7, 39.0, 34.4; IR (KBr) 3170, 1643, 1570, 1412, 1163, 1016, 803, 645, 526 cm^{-1}; HRMS-(ESI) (m/z): $[M+Na]^+$ calcd for $C_{20}H_{19}NNaO_3S$, 376.0978; found 376.0976.



1b

N-(3-methoxyphenethyl)-N-(p-tolylbuta-1,3-diyn-1-yl)methanesulfonamide (1b)

Compound **1b** was obtained according to the general procedure A outlined above as a yellow oil (297 mg, 54%); R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.0 Hz, 2H), 7.25-7.22 (m, 1H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.83 (s, 1H), 6.79 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 3.80 (s, 3H), 3.79 (t, *J* = 7.2 Hz, 2H), 3.02 (t, *J* = 7.2 Hz, 2H), 2.72 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 139.5, 138.8, 132.3, 129.8, 129.2, 121.4, 118.7, 114.7, 112.6, 82.0, 72.5, 72.4, 59.8, 55.2, 52.7, 38.9, 34.4, 21.6; IR (KBr) ν 2890, 2217, 1619, 1492, 1405, 1244, 1167, 768, 614 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_3S$, 390.1134; found 390.1134.

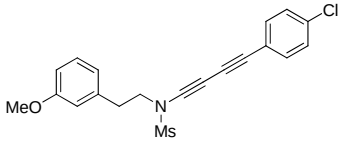


1c

N-((4-fluorophenyl)buta-1,3-diyn-1-yl)-N-(3-ethoxyphenethyl)methanesulfonamide (1c)

Compound **1c** was obtained according to the general procedure A outlined above as a yellow oil (395 mg, 71%); R_f = 0.50 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.47 (m, 2H), 7.25 (t, *J* = 8.0 Hz, 1H), 7.03 (t, *J* = 8.0 Hz, 2H), 6.88 (d, *J* = 7.6 Hz, 1H), 6.83-6.79 (m, 2H), 3.82 (s, 3H), 3.81 (t, *J* = 7.2 Hz, 2H), 3.04 (t, *J* = 7.2 Hz, 2H), 2.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, $J_{C\text{-}F}$ = 249.9 Hz), 159.9, 138.8, 134.4 (d, $J_{C\text{-}F}$ = 8.5 Hz), 129.8, 121.4, 118.0 (d, $J_{C\text{-}F}$ = 3.6 Hz), 115.8 (d, $J_{C\text{-}}$

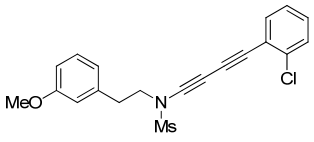
$_F$ = 22.1 Hz), 114.8, 112.6, 80.7, 73.0, 72.7, 59.6, 55.2, 52.7, 39.0, 34.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.8; IR (KBr) ν 2886, 1622, 1517, 1401, 1209, 620 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{18}FNNaO_3S$, 394.0884; found 394.0882.



1d

N-((4-chlorophenyl)buta-1,3-diyn-1-yl)-N-(3-ethoxyphenethyl)methanesulfonamide (1d)

Compound **1d** was obtained according to the general procedure A outlined above as a yellow oil (273 mg, 47%); R_f = 0.50 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 6.4 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.25 (t, *J* = 8.0 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.83-3.79 (m, 2H), 3.81 (s, 3H), 3.80 (t, *J* = 7.2 Hz, 2H), 3.03 (t, *J* = 7.2 Hz, 2H), 2.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 138.7, 135.2, 133.5, 129.8, 128.8, 121.3, 120.4, 114.8, 112.6, 80.6, 74.2, 73.3, 59.5, 55.2, 52.7, 39.0, 34.4; IR (KBr) ν 3002, 2354, 1618, 1401, 1160, 620, 466 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{18}ClNNaO_3S$, 410.0588; found 410.0588.

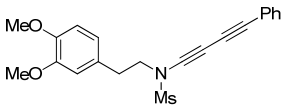


1e

N-((2-chlorophenyl)buta-1,3-diyn-1-yl)-N-(3-ethoxyphenethyl)methanesulfonamide (1e)

Compound **1e** was obtained according to the general procedure A outlined above as a yellow oil (336 mg, 58%); R_f = 0.45 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR

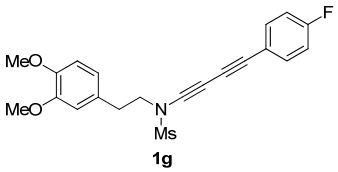
(400 MHz, $CDCl_3$) δ 7.52 (dd, J_1= 7.2 Hz, J_2= 1.6 Hz, 1H), 7.40 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.31-7.27 (m, 1H), 7.26-7.24 (m, 1H), 7.21 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 6.87 (d, J = 7.6 Hz, 1H), 6.83 (t, J = 2.0 Hz, 1H), 6.81 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 3.81 (s, 3H), 3.82 (t, J = 4.8 Hz, 2H), 3.04 (t, J = 7.2 Hz, 2H), 2.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 138.8, 136.7, 134.3, 130.1, 129.9, 129.34, 126.6, 122.1, 121.4, 114.8, 112.8, 78.3, 78.1, 74.3, 59.6, 55.3, 52.8, 39.1, 34.5; IR (KBr) ν 2935, 2231, 2150, 1590, 1478, 1370, 1268, 1167, 957, 897, 757, 508 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{18}ClNNaO_3S$, 410.0588; found 410.0585.



1f

N-(3,4-dimethoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1f)

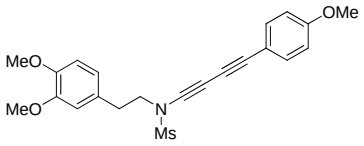
Compound **1f** was obtained according to the general procedure A outlined above as a yellow solid (356 mg, 62%); R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1); mp: 120-123 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 2H), 7.39-7.31 (m, 3H), 6.84 (appeared as a singlet, 2H), 6.81 (s, 1H), 3.91 (s, 3H), 3.86 (s, 3H), 3.79 (t, J = 8.0 Hz, 2H), 3.01 (t, J = 8.0 Hz, 2H), 2.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.1, 148.1, 132.4, 129.7, 129.1, 128.4, 121.8, 121.2, 112.3, 111.4, 81.8, 73.1, 72.8, 59.7, 55.94, 55.93, 52.8, 39.0, 34.0; IR (KBr) ν 2834, 2361, 2235, 2158, 1513, 1398, 1349, 1156, 967, 746, 617, 512 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_4S$, 406.1083; found 406.1083.



1g

N-(3,4-dimethoxyphenethyl)-N-((4-fluorophenyl)buta-1,3-diyn-1-yl)methanesulfonamide (1g)

Compound **1g** was obtained according to the general procedure A outlined above as a yellow oil (391 mg, 65%); R_f = 0.20 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, J_1 = 8.4 Hz, J_2 = 5.2 Hz, 2H), 7.03 (t, J = 8.8 Hz, 2H), 6.82 (d, J = 9.6 Hz, 3H), 3.90 (s, 3H), 3.86 (s, 3H), 3.79 (t, J = 7.2 Hz, 2H), 3.00 (t, J = 7.2 Hz, 2H), 2.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, $J_{C\text{-}F}$ = 249.9 Hz), 149.1, 148.1, 134.4 (d, $J_{C\text{-}F}$ = 8.5 Hz), 129.6, 121.1, 117.9 (d, $J_{C\text{-}F}$ = 3.6 Hz), 115.8 (d, $J_{C\text{-}F}$ = 22.1 Hz), 112.2, 111.3, 80.7, 72.9, 72.8, 59.5, 55.89 , 55.88, 52.8, 39.0, 34.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.7; IR (KBr) ν 3415, 2235, 2151, 1615, 1492, 1398, 1363, 1247, 1163, 1037, 764, 613 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{20}FNNaO_4S$, 424.0989; found 424.0989.

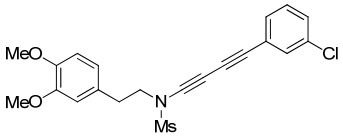


1h

N-(3,4-dimethoxyphenethyl)-N-((4-methoxyphenyl)buta-1,3-diyn-1-yl)methanesulfonamide (1h)

Compound **1h** was obtained according to the general procedure A outlined above as a yellow oil (316 mg, 51%); R_f = 0.15 (petroleum ether : ethyl acetate = 3 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dt, J_1 = 9.2 Hz, J_2 = 2.0 Hz, 2H), 6.87-6.83 (m, 4H), 6.81 (d, J = 0.8 Hz, 1H), 3.90 (s, 1H), 3.86 (s, 3H), 3.82 (s, 3H), 3.78 (t, J = 7.2 Hz, 2H), 3.00 (t, J = 7.2 Hz, 2H), 2.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 149.0, 148.0, 134.1, 129.7, 121.1, 114.1, 113.6, 112.2, 111.3, 81.9, 72.3,

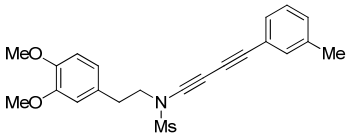
71.9, 59.8, 55.87, 55.86, 55.3, 52.8, 38.9, 33.9, 30.8; IR (KBr) ν 3105, 1644, 1528, 1417, 1165, 1028, 626 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{23}NNaO_5S$, 436.1189; found 436.1189.



1i

N-((3-chlorophenyl)buta-1,3-diyn-1-yl)-N-(3,4-dimethoxyphenethyl)methanesulfonamide (1i)

Compound **1i** was obtained according to the general procedure A outlined above as a yellow oil (394 mg, 63%); R_f = 0.20 (petroleum ether : ethyl acetate = 5 : 1); ^1H NMR (400 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.35-7.32 (m, 2H), 7.28-7.24 (m, 1H), 6.82 (d, *J* = 9.6 Hz, 3H), 3.90 (s, 3H), 3.86 (s, 3H), 3.79 (t, *J* = 7.2 Hz, 2H), 3.00 (t, *J* = 6.8 Hz, 2H), 2.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 148.1, 134.2, 131.9, 130.3, 129.6, 129.5, 129.3, 123.5, 121.1, 112.1, 111.3, 80.1, 74.3, 73.6, 59.3, 55.84, 55.82, 52.8, 39.0, 33.9; IR (KBr) ν 3005, 2357, 1615, 1405, 1170, 624, 473 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{20}ClNNaO_4S$, 440.0694; found 440.0688.

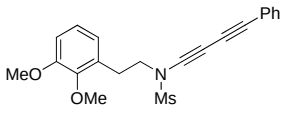


1j

N-(3,4-dimethoxyphenethyl)-N-(m-tolylbuta-1,3-diyn-1-yl)methanesulfonamide (1j)

Compound **1j** was obtained according to the general procedure A outlined above as a yellow solid (425 mg, 72%); R_f = 0.30 (petroleum ether : ethyl acetate = 5 : 1); mp: 128-130 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.31-7.27 (m, 2H), 7.21 (t, *J* = 7.8 Hz, 1H), 6.16 (d, *J* = 7.8 Hz, 1H), 6.82 (appeared as a

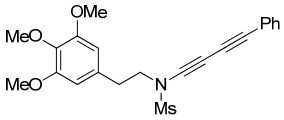
singlet, 2H), 6.81 (s, 1H), 3.89 (s, 3H), 3.87 (s, 3H), 3.77 (t, *J* = 6.8 Hz, 2H), 3.00 (t, *J* = 6.8 Hz, 2H), 2.75 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.1, 148.1, 138.1, 132.8, 130.1, 129.7, 129.4, 128.3, 121.6, 121.1, 112.2, 111.3, 82.0, 72.7, 72.6, 59.7 55.90, 55.89, 52.8, 38.9, 34.0, 21.2; IR (KBr) ν 3137, 2237, 1589, 1512, 1393, 1260, 1238, 1155, 1028, 965, 851, 687, 520 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{23}NNaO_4S$, 420.1240; found 420.1239.



1k

N-(2,3-dimethoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1k)

Compound **1k** was obtained according to the general procedure B outlined above as a yellow oil (426 mg, 74%); R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.48 (m, 2H), 7.36-7.31 (m, 3H), 7.01 (t, *J* = 7.8 Hz, 1H), 6.87-6.84 (m, 2H), 3.90 (s, 3H), 3.86 (s, 3H), 3.79 (t, *J* = 6.8 Hz, 2H), 3.07 (t, *J* = 7.2 Hz, 2H), 2.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 147.6, 132.3, 130.8, 129.0, 128.4, 124.0, 122.7, 122.0, 111.7, 81.5, 73.3, 73.1, 60.7, 59.3, 55.7, 51.8, 39.1, 29.6; IR (KBr) ν 2928, 2834, 2235, 2151, 1583, 1485, 1359, 1163, 963, 893, 753, 680, 515 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_4S$, 406.1083; found 406.1079.

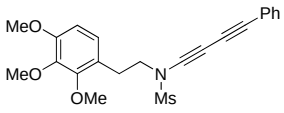


1l

N-(phenylbuta-1,3-diyn-1-yl)-N-(3,4,5-trimethoxyphenethyl)methanesulfonamide (1l)

Compound **1l** was obtained according to the general procedure B outlined above as a yellow solid (405 mg, 65%); R_f = 0.55 (petroleum ether : ethyl acetate = 3 : 1); mp: 116-

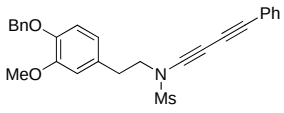
118 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.48 (m, 2H), 7.37-7.33 (m, 3H), 6.51 (s, 2H), 3.88 (s, 6H), 3.82 (s, 3H), 3.80 (t, *J* = 7.2 Hz, 2H), 3.00 (t, *J* = 7.2 Hz, 2H), 2.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 136.7, 132.6, 132.0, 128.9, 128.2, 121.4, 105.8, 81.6. 72.9, 72.8, 60.5, 59.3, 55.8, 52.3, 38.6, 34.5; IR (KBr) ν 3022, 2923, 2232, 2145, 1494, 1365, 1172, 752, 570, 512 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{23}NNaO_5S$, 436.1189; found 436.1187.



1m

N-(phenylbuta-1,3-diyn-1-yl)-N-(2,3,4-trimethoxyphenethyl)methanesulfonamide (1m)

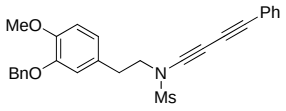
Compound **1m** was obtained according to the general procedure B outlined above as a yellow oil (371 mg, 60%); R_f = 0.75 (petroleum ether : ethyl acetate = 3 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.47 (m, 2H), 7.36-7.27 (m, 3H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.60 (d, *J* = 8.4 Hz, 1H), 3.93 (s, 3H), 3.84 (s, 3H), 3.82 (s, 3H), 3.75 (t, *J* = 7.2 Hz, 2H), 2.97 (t, *J* = 6.8 Hz, 2H), 2.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 151.9, 141.9, 132.0, 128.8, 128.2, 124.8, 122.5, 121.6, 106.8, 81.3, 73.2, 73.1, 60.6, 60.4, 58.8, 55.7, 51.6, 38.8, 29.3; IR (KBr) ν 2939, 2827, 2231, 2158, 1563, 1496, 1370, 1170, 1104, 1013, 967, 761, 698, 551 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{23}NNaO_5S$, 436.1189; found 436.1187.



1n

N-(4-(benzyloxy)-3-methoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1n)

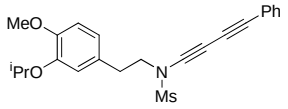
Compound **1n** was obtained according to the general procedure B outlined above as a yellow oil (427 mg, 62%); R_f = 0.25 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.45 (m, 2H), 7.40-7.38 (m, 2H), 7.34-7.26 (m, 6H), 6.83-6.81 (m, 2H), 6.72 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 5.10 (s, 2H), 3.87 (s, 3H), 3.73 (t, J = 6.8 Hz, 2H), 2.94 (t, J = 6.8 Hz, 2H), 2.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 146.9, 136.8, 132.1, 130.2, 129.0, 128.32, 128.29, 127.7, 127.1, 121.6, 121.0, 114.2, 112.7, 81.6, 73.1, 72.8, 70.2, 59.4, 55.8, 52.6, 38.7, 33.7; IR (KBr) ν 2921, 2231, 1646, 1510, 1366, 1160, 1012, 764, 536 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{27}H_{25}NNaO_4S$, 482.1396; found 482.1394.



1o

N-(3-(benzyloxy)-4-methoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1o)

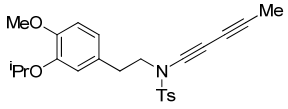
Compound **1o** was obtained according to the general procedure B outlined above as a yellow oil (309 mg, 45%); R_f = 0.50 (petroleum ether : ethyl acetate = 3 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.46 (m, 4H), 7.38-7.30 (m, 6H), 6.85-6.84 (m, 3H), 5.18 (s, 2H), 3.86 (s, 3H), 3.73 (t, J = 6.8 Hz, 2H), 2.93 (t, J = 6.8 Hz, 2H), 2.54 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 148.0, 136.9, 132.3, 129.7, 129.1, 128.6, 128.4, 127.9, 127.4, 121.8, 121.7, 115.2, 112.0, 81.8, 73.3, 72.8, 70.9, 59.7, 56.0, 52.8, 38.9, 33.8; IR (KBr) ν 3026, 2932, 2371, 2224, 2158, 1513, 1394, 1352, 1261, 1167, 1009, 697, 519 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{27}H_{25}NNaO_4S$, 482.1396; found 482.1393.



1p

N-(3-isopropoxy-4-methoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1p)

Compound **1p** was obtained according to the general procedure B outlined above as a yellow oil (460 mg, 75%); R_f = 0.50 (petroleum ether : ethyl acetate = 3 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 2H), 7.37-7.33 (m, 3H), 6.84 (s, appeared as a singlet, 3H), 4.60-4.51 (m, 1H), 3.83 (s, 3H), 3.78 (t, J = 7.2 Hz, 2H), 2.98 (t, J = 7.2 Hz, 2H), 2.71 (s, 3H), 1.38 (d, J = 6.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 147.4, 132.3, 129.6, 129.1, 128.4, 121.8, 121.6, 116.8, 112.1, 81.7, 73.2, 72.8, 71.5, 59.6, 56.0, 52.9, 38.9, 33.8, 22.1; IR (KBr) ν 2928, 2230, 2155, 1647, 1509, 1362, 1260, 1168, 958, 754 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{23}H_{25}NNaO_4S$, 434.1396; found 434.1397.

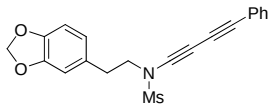


1q

N-(3-isopropoxy-4-methoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1q)

Compound **1q** was obtained according to the general procedure outlined above as a yellow oil (256 mg, 62%); R_f = 0.5 (petroleum ether : ethyl acetate = 3 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 6.75 (d, J = 8.0 Hz, 1H), 6.69-6.66 (m, 2H), 4.50-4.44 (m, 1H), 3.80 (s, 3H), 3.53 (t, J = 8.0 Hz, 2H), 2.83 (t, J = 7.6 Hz, 2H), 2.41 (s, 3H), 1.96 (s, 3H), 1.34 (d, J = 6.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.1, 147.0, 144.7, 134.2, 129.6, 129.4, 127.2, 121.1, 116.5, 111.9,

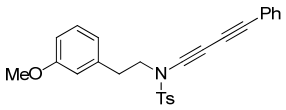
79.6, 71.2, 66.3, 63.5, 59.0, 55.7, 52.5, 33.5, 21.9, 21.4, 4.3; IR (KBr) ν 2925, 2848, 2372, 2168, 1699, 1506, 1366, 1167, 1027, 655, 575, 417 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{24}H_{27}NNaO_4S$, 448.1553; found 448.1552.



1r

N-(2-(benzo[d][1,3]dioxol-5-yl)ethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1r)

Compound **1r** was obtained according to the general procedure B outlined above as a yellow oil (462 mg, 84%); R_f = 0.35 (petroleum ether : ethyl acetate = 3 : 1); ^1H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 2H), 7.36-7.31 (m, 3H), 6.78-6.72 (m, 3H), 5.93 (s, 2H), 3.74 (t, J = 7.2 Hz, 2H), 2.97 (t, J = 7.2 Hz, 2H), 2.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 146.6, 132.3, 130.8, 129.1, 128.4, 122.1, 121.8, 109.4, 108.5, 101.0, 87.8, 73.1, 72.7, 59.6, 52.9, 39.1, 34.2; IR (KBr) ν 3135, 3112, 1639, 1619, 1402, 617 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{17}NNaO_4S$, 390.0770; found 390.0767.

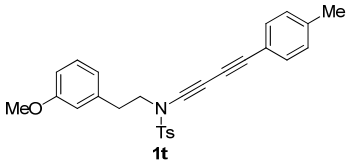


1s

N-(3-methoxyphenethyl)-4-methyl-N-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide (1s)

Compound **1s** was obtained according to the general procedure A outlined above as a yellow oil (373 mg, 58%); R_f = 0.60 (petroleum ether : ethyl acetate = 5 : 1); ^1H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.4 Hz, 2H), 7.49 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 2H), 7.35-7.30 (m, 5H), 7.18 (t, J = 8.0 Hz, 1H), 6.76 (dd, J_1 = 8.0 Hz, J_2 = 2.4 Hz, 2H), 6.69

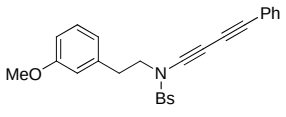
(d, J = 1.6 Hz, 1H), 3.76 (s, 3H), 3.61 (t, J = 8.0 Hz, 2H), 2.93 (t, J = 8.0 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 145.0, 138.6, 134.4, 132.3, 129.9, 129.6, 129.0, 128.4, 127.5, 122.0, 121.1, 114.4, 112.3, 81.3, 73.7, 73.5, 58.9, 55.1, 52.6, 34.4, 21.6; IR (KBr) ν 2991, 2364, 1618, 1401, 1167, 617, 480 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{26}H_{23}NNaO_3S$, 452.1291; found 452.1290.



1t

N-(3-methoxyphenethyl)-4-methyl-N-(p-tolylbuta-1,3-diyn-1-yl)benzenesulfonamide (1t)

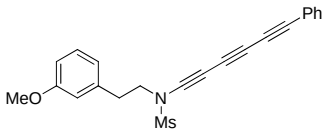
Compound **1t** was obtained according to the general procedure A outlined above as a yellow solid (435 mg, 67%); R_f = 0.60 (petroleum ether : ethyl acetate = 5 : 1); mp: 136-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 8.4 Hz, 2H), 7.18 (t, J = 8.0 Hz, 1H), 7.13 (d, J = 8.0 Hz, 2H), 6.77-6.75 (m, 2H), 6.69 (d, J = 2.0 Hz, 1H), 3.77 (s, 3H), 3.61 (t, J = 8.0 Hz, 2H), 2.93 (t, J = 8.0 Hz, 2H), 2.44 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 145.0, 139.4, 138.7, 134.5, 132.3, 129.9, 129.6, 129.2, 127.5, 121.1, 118.9, 114.4, 112.4, 81.6, 73.4, 72.9, 59.1, 55.1, 52.7, 34.4, 21.7, 21.6; IR (KBr) ν 2837, 2235, 2154, 1580, 1370, 1265, 1174, 1030, 771, 680, 547 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{27}H_{25}NNaO_3S$, 466.1447; found 466.1448.



1u

N-(3-methoxyphenethyl)-N-(phenylbuta-1,3-diyn-1-yl)benzenesulfonamide (1u)

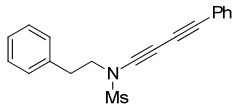
Compound **1u** was obtained according to the general procedure A outlined above as a yellow solid (510 mg, 82%); R_f = 0.50 (petroleum ether : ethyl acetate = 5 : 1); mp: 113-115 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.83 (m, 2H), 7.65-7.61 (m, 1H), 7.53-7.47 (m, 4H), 7.36-7.28 (m, 3H), 7.17 (t, *J* = 8.0 Hz, 1H), 6.76-6.73 (m, 2H), 6.69 (t, *J* = 2.0 Hz, 1H), 3.75 (s, 3H), 3.63 (t, *J* = 7.6 Hz, 2H), 2.92 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 138.4, 137.3, 133.8, 132.3, 129.6, 129.3, 129.0, 128.3, 127.4, 121.8, 121.0, 114.4, 112.3, 81.3, 73.5, 73.4, 59.0, 55.0, 52.6, 34.3; IR (KBr) ν 2949, 2837, 2224, 2151, 1612, 1492, 1398, 1258, 1044, 887, 733, 694, 603, 452 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{21}NNaO_3S$, 438.1134; found 438.1134.



1v

N-(3-methoxyphenethyl)-N-(phenylhexa-1,3,5-triyn-1-yl)methanesulfonamide (1v)

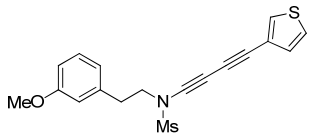
Compound **1v** was obtained according to the general procedure A outlined above as a yellow oil (306 mg, 51%); R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.2 Hz, 2H), 7.38 (d, *J* = 7.2 Hz, 1H), 7.33 (t, *J* = 7.2 Hz, 2H), 7.27-7.23 (m, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 6.81 (d, *J* = 6.4 Hz, 2H), 3.81 (s, 3H), 3.80 (t, *J* = 7.2 Hz, 2H), 3.01 (t, *J* = 7.2 Hz, 2H), 2.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 138.6, 132.9, 129.8, 129.6, 128.5, 121.3, 121.0, 114.7, 112.7, 79.0, 74.4, 69.9, 67.5, 65.8, 61.3, 55.2, 52.7, 39.2, 34.4; IR (KBr) ν 2939, 2368, 2200, 1688, 1366, 1261, 1167, 957, 757, 687, 505 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{19}NNaO_3S$, 400.0978; found 400.0968.



1w

N-phenethyl-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1w)

Compound **1w** was obtained according to the general procedure A outlined above as a yellow oil (363 mg, 75%); R_f = 0.50 (petroleum ether : ethyl acetate = 3 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.49 (m, 2H), 7.36-7.25 (m, 8H), 3.79 (t, *J* = 7.2 Hz, 2H), 3.04 (t, *J* = 7.2 Hz, 2H), 2.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.3, 132.3, 129.10, 129.05, 128.7, 128.4, 127.1, 121.8, 81.7, 73.2, 72.7, 59.6, 52.7, 38.8, 34.3; IR (KBr) ν 3303, 3016, 2932, 2228, 2161, 823, 753, 687 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{17}NNaO_2S$, 346.0872; found 346.0872.

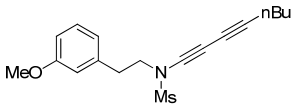


1x

N-(3-methoxyphenethyl)-N-(thiophen-3-ylbuta-1,3-diyn-1-yl)methanesulfonamide (1x)

Compound **1x** was obtained according to the general procedure A outlined above as a yellow solid (340 mg, 63%); R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1), mp: 155-158 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, J_1 = 2.8 Hz, J_2 = 1.2 Hz, 1H), 7.28-7.25 (m, 1H), 7.25-7.22 (m, 1H), 7.15 (dd, J_1 = 5.2 Hz, J_2 = 1.2 Hz, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 6.82-6.78 (m, 2H), 3.80 (s, 3H), 3.78 (t, *J* = 7.2 Hz, 2H), 3.02 (t, *J* = 7.2 Hz, 2H), 2.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 138.8, 131.2, 130.1, 129.8, 125.6, 121.4, 120.9, 114.7, 112.6, 76.9 , 72.8, 72.6, 59.7, 55.2, 52.7, 38.9, 34.4; IR (KBr) ν 2911,

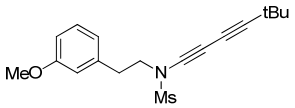
2224, 2154, 1597, 1513, 1366, 1223, 1167, 964, 834, 767, 515 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{17}NNaO_3S_2$, 382.0542; found 382.0542.



1y

N-(3-methoxyphenethyl)-N-(octa-1,3-diyn-1-yl)methanesulfonamide (1y)

Compound **1y** was obtained according to the general procedure A outlined above as a yellow oil (370 mg, 74%); R_f = 0.50 (petroleum ether : ethyl acetate = 5 : 1) ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (t, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 7.6 Hz, 1H), 6.80-6.78 (m, 2H), 3.81 (s, 3H), 3.74 (t, *J* = 7.2 Hz, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 2.71 (s, 3H), 2.34 (t, *J* = 7.2 Hz, 2H), 1.59-1.51 (m, 2H), 1.48-1.41 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 138.9, 129.7, 121.3, 114.7, 112.6, 84.8, 66.0, 64.1, 60.0, 55.2, 52.5, 38.7, 34.4, 30.3, 21.9, 19.2, 13.5; IR (KBr) ν 3005, 2364, 2168, 1622, 1405, 1160, 960, 624, 477 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{23}NNaO_3S$, 356.1291; found 356.1292.

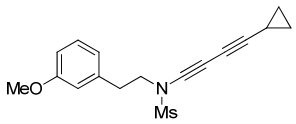


1z

N-(5,5-dimethylhexa-1,3-diyn-1-yl)-N-(3-methoxyphenethyl)methanesulfonamide (1z)

Compound **1z** was obtained according to the general procedure A outlined above as a yellow oil (275 mg, 55%); R_f = 0.50 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (t, *J* = 8.0 Hz, 1H), 6.85 (d, *J* = 7.2 Hz, 1H), 6.79 (d, *J* = 10.0 Hz, 2H), 3.80 (s, 3H), 3.73 (t, *J* = 7.2 Hz, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 2.71 (s, 3H), 1.27

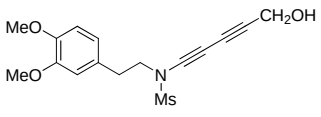
(s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 138.9, 129.7, 121.3, 114.7, 112.5, 92.0, 67.2, 62.8, 59.6, 55.2, 52.5, 38.7, 34.4, 30.5, 28.2; IR (KBr) ν 2970, 2252, 2154, 1604, 1359, 1265, 1163, 1044, 767, 501 cm^{-1}; $[M+Na]^+$ calcd for $C_{18}H_{23}NNaO_3S$, 356.1291; found 356.1288.



1aa

N-(cyclopropylbuta-1,3-diyn-1-yl)-N-(3-methoxyphenethyl)methanesulfonamide (1aa)

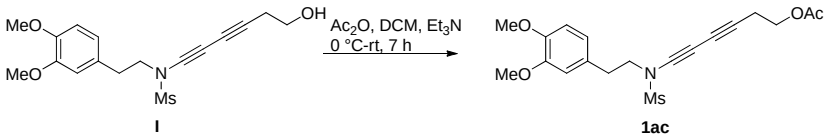
Compound **1aa** was obtained according to the general procedure A outlined above as a yellow solid (328 mg, 69%); R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1), mp: 118-120 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (t, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 7.6 Hz, 1H), 6.80-6.78 (m, 2H), 3.81 (s, 3H), 3.73 (t, *J* = 7.2 Hz, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 2.70 (s, 3H), 1.42-1.35 (m, 1H), 0.87-0.85 (m, 2H), 0.83-0.80 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 138.9, 129.7, 121.3, 114.7, 112.5, 88.1, 65.7, 60.4, 59.6, 55.2, 52.5, 38.7, 34.3, 9.0, 0.3; IR (KBr) ν 2939, 2833, 2343, 2238, 2158, 1615, 1580, 1492, 1398, 1254, 1156, 1068, 943, 747, 687, 634, 515, 463 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO_3S$, 340.0978; found 340.0979.



1ab

N-(3,4-dimethoxyphenethyl)-N-(5-hydroxypenta-1,3-diyn-1-yl)methanesulfonamide (1ab)

Compound **1ab** was obtained according to the general procedure A outlined above as a yellow oil (430 mg, 85%); R_f = 0.3 (petroleum ether : ethyl acetate = 2 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82-6.77 (m, 3H), 4.38 (s, 2H), 3.88 (s, 3H), 3.84 (s, 3H), 3.74 (t, *J* = 7.2 Hz, 2H), 2.95 (t, *J* = 7.2 Hz, 2H), 2.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 147.8, 129.4, 121.0, 112.0, 111.2, 81.5, 69.8, 69.1, 59.0, 55.7, 52.5, 51.1, 38.7, 33.7; IR (KBr) ν 2914, 2245, 1643, 1517, 1363, 1160, 1023, 757, 526 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{19}NNaO_5S$, 360.0876; found 360.0873.



I 1ac

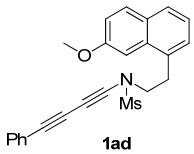
N-(3,4-dimethoxyphenethyl)-N-(6-hydroxyhexa-1,3-diyn-1-yl)methanesulfonamide (I)

Compound **I** was obtained according to the general procedure A outlined above as a yellow oil (253 mg, 50%); R_f = 0.20 (petroleum ether : ethyl acetate = 1 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.83-6.79 (m, 3H), 3.88 (s, 3H), 3.84 (s, 3H), 3.75 (t, *J* = 6.4 Hz, 2H), 3.71 (t, *J* = 7.2 Hz, 2H), 2.94 (t, *J* = 7.2 Hz, 2H), 2.74 (s, 3H), 2.60 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.0, 148.0, 129.6, 121.1, 112.2, 111.3, 81.2, 66.7, 65.8, 60.6, 59.6, 55.8, 52.6, 38.8, 33.9, 23.9; IR (KBr) ν 2932, 2256, 2172, 1643, 1517, 1359, 1261, 1170, 1026, 960, 771, 536 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{21}NNaO_5S$, 374.1033; found 374.1033.

6-(N-(3,4-dimethoxyphenethyl)methylsulfonamido)hexa-3,5-diyn-1-yl acetate (1ac)

A solution of **I** (425 mg, 1.26 mmol) in DCM (15 mL) at 0 °C was added Et_3N (0.70 mL, 5.0 mmol). Then acetic anhydride (257 mg, 2.52 mmol) was added drop-wise via syringe at this temperature. The mixture was allowed to warm up to room temperature and stirred

for 7 h. The reaction was diluted with DCM (20 mL) and water (20 mL), the organic layer was separated and the aqueous layer was extracted with DCM (3 × 20 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo to furnish the product as a yellow oil (255 mg, 59%); R_f = 0.35 (petroleum ether : ethyl acetate = 1 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84-6.79 (m, 3H), 4.18 (t, *J* = 6.8 Hz, 2H), 3.88 (s, 3H), 3.85 (s, 3H), 3.72 (t, *J* = 6.8 Hz, 2H), 2.96 (t, *J* = 6.8 Hz, 2H), 2.73 (s, 3H), 2.69 (t, *J* = 6.8 Hz, 2H), 2.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 148.8, 147.9, 129.5, 120.9, 112.0, 111.2, 79.8, 66.8, 65.5, 61.5, 59.4, 55.7, 52.4, 38.6, 33.7, 20.6, 19.8; IR (KBr) ν 3170, 2537, 2252, 2165, 1739, 1517, 1400, 1240, 1026 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{23}NNaO_6S$, 416.1138; found 416.1138.[7]

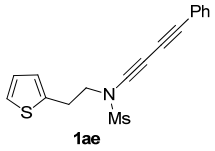


1ad

N-(2-(7-methoxynaphthalen-1-yl)ethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1ad)

Compound **1ad** was obtained according to the general procedure B outlined above as a yellow solid (210 mg, 70%); R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1), mp: 105-108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.8 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.51 (d, *J* = 7.2 Hz, 2H), 7.41-7.25 (m, 6H), 7.18-7.16 (m, 1H), 3.99 (s, 3H), 3.87 (d, *J* = 8.0 Hz, 2H), 3.51 (d, *J* = 8.0 Hz, 2H), 2.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 132.8, 132.4, 131.5, 130.4, 129.24, 129.18, 128.5, 128.0, 127.7, 123.2, 121.8, 118.8, 101.4, 81.9, 73.2, 73.1, 59.3, 55.4, 52.3, 39.3, 32.6; IR (KBr) ν 2921, 2361, 1468, 1307,

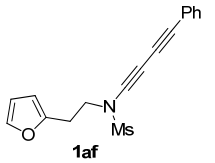
1146, 964, 768, 554 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{21}NNaO_3S$, 426.1134; found 426.1135.



1ae

N-(phenylbuta-1,3-diyn-1-yl)-N-(2-(thiophen-2-yl)ethyl)methanesulfonamide (1ae)

Compound **1ae** was obtained according to the general procedure B outlined above as a yellow solid (576 mg, 87%); R_f = 0.50 (petroleum ether : ethyl acetate = 5 : 1), mp: 90-93 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.52-7.49 (m, 2H), 7.38-7.30 (m, 3H), 7.21-7.19 (m, 1H), 6.98-6.96 (m, 2H), 3.82 (t, *J* = 7.2 Hz, 2H), 3.28 (t, *J* = 7.2 Hz, 2H), 2.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 132.4, 129.1, 128.4, 127.2, 126.5, 124.6, 121.8, 81.8, 73.1, 72.4, 59.8, 52.7, 39.0, 28.5; IR (KBr) ν 2925, 2364, 2221, 1594, 1493, 1366, 1156, 964, 761, 547, 512 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{15}NNaO_2S_2$, 352.0436; found 352.0439.

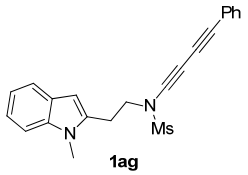


1af

N-(2-(furan-2-yl)ethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1af)

Compound **1af** was obtained according to the general procedure B outlined above as a yellow oil (253 mg, 67%); R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1); ^1H NMR (400 MHz, $CDCl_3$) δ 7.50-7.47 (m, 2H), 7.37-7.30 (m, 4H), 6.33-6.31 (m, 1H), 6.22-6.21 (m, 1H), 3.82 (t, *J* = 6.8 Hz, 2H), 3.09 (t, *J* = 6.8 Hz, 2H), 2.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.8, 141.8, 132.3, 129.1, 128.4, 121.8, 110.6, 107.8, 81.7, 73.1, 72.4, 59.3, 49.9, 39.1, 27.0; IR (KBr) ν 3026, 2231, 1769, 1493, 1317, 1146, 1076, 970, 764,

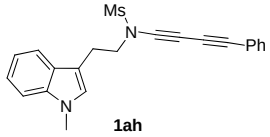
522 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{15}NNaO_3S$, 336.0665; found 336.0664.



1ag

N-(2-(1-methyl-1H-indol-2-yl)ethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1ag)

Compound **1ag** was obtained according to the general procedure B outlined above as a yellow oil (328 mg, 67%); R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1); ^1H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.6 Hz, 1H), 7.50-7.48 (m, 2H), 7.38-7.29 (m, 4H), 7.21-7.17 (m, 1H), 7.10-7.06 (m, 1H), 6.39 (s, 1H), 3.86 (t, *J* = 7.2 Hz, 2H), 3.71 (s, 3H), 3.22 (t, *J* = 7.2 Hz, 2H), 2.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 135.3, 132.4, 129.2, 128.4, 127.5, 121.7, 121.4, 120.1, 119.7, 109.1, 100.9, 81.9, 73.0, 72.6, 59.6, 50.7, 39.2, 29.6, 26.0; IR (KBr) ν 2983, 2883, 2399, 2207, 1482, 1388, 1179, 991, 724, 512 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{20}N_2NaO_2S$, 399.1138; found 399.1138.



1ah

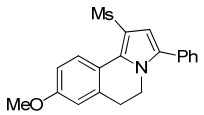
N-(2-(1-methyl-1H-indol-3-yl)ethyl)-N-(phenylbuta-1,3-diyn-1-yl)methanesulfonamide (1ah)

Compound **1ah** was obtained according to the general procedure B outlined above as a yellow oil (563 mg, 83%); R_f = 0.40 (petroleum ether : ethyl acetate = 5 : 1); ^1H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 1H), 7.42-7.28 (m, 6H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.09 (t, *J* = 7.2 Hz, 1H), 6.40 (s, 1H), 3.88 (t, *J* = 7.2 Hz, 2H), 3.73 (s, 3H), 3.24 (t, *J* =

7.2 Hz, 2H), 2.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 135.33, 135.28, 133.6, 128.8, 127.5, 121.5, 120.3, 120.2, 119.7, 109.1, 101.0, 80.8, 74.0, 73.1, 59.5, 50.7, 39.3, 29.7, 26.1; IR (KBr) ν 2983, 2883, 2399, 2207, 1482, 1388, 1179, 991, 724, 512, 463 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{20}N_2NaO_2S$, 399.1138; found 399.1137.

General procedure for the synthesis of Pyrrolo [2,1-a] isoquinolines

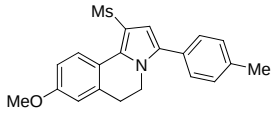
A dry Schlenk tube was charged with gold catalyst (5 mol %) and evacuated and back filled with argon. To this tube was added the solution of 1,3-diynamide (0.15 mmol) in DCM (1 mL). The reaction mixture was stirred at 30 °C or 40 °C and the progress of the reaction was monitored by TLC. The reaction typically took 4 h. Upon completion, the mixture was then quenched with small amount of water, diluted with DCM, washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by chromatography on silica gel (eluent : petroleum ether/DCM) to afford the desired pyrrolo [2, 1-a] isoquinolines **2**.



2a

8-methoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (2a)

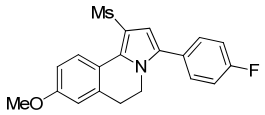
Compound **2a** was obtained as a white solid, 45.8 mg, in 87% yield; R_f = 0.50 (petroleum ether : ethyl acetate = 3 : 1); mp: 212-214 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, J = 8.8 Hz, 1H), 7.47-7.43 (m, 2H), 7.39-7.36 (m, 3H), 6.92 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 6.81 (d, J = 2.4 Hz, 1H), 6.77 (s, 1H), 4.08 (t, J = 6.4 Hz, 2H), 3.85 (s, 3H), 3.10 (s, 3H), 2.96 (t, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 135.4, 132.6, 130.9, 130.2, 128.9, 128.62，128.57, 127.9, 120.2, 119.1, 113.7, 112.7, 110.9, 55.3, 43.8, 42.2, 30.0; IR (KBr) ν 2932, 2231, 2154, 1601, 1493, 1370, 1265, 1170, 964, 764, 694, 512 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{19}NNaO_3S$, 376.0978; found 376.0976.



2b

8-methoxy-1-(methylsulfonyl)-3-(p-tolyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2b)

Compound **2b** was obtained as a white solid, 46.0 mg, in 83% yield; R_f = 0.60 (petroleum ether : ethyl acetate = 3 : 1); mp: 216-218 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, J = 8.8 Hz, 1H), 7.26 (appeared as a singlet, 4H), 6.92 (dd, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 1H), 6.81 (s, 1H), 6.74 (s, 1H), 4.07 (t, J = 6.4 Hz, 2H), 3.85 (s, 3H), 3.10 (s, 3H), 2.95 (t, J = 6.4 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 138.0, 135.4, 132.8, 130.0, 129.4, 128.9, 128.6, 128.0, 120.3, 119.1, 113.8, 112.7, 110.6, 55.3, 43.9, 42.2, 30.0, 21.2; IR (KBr) ν 2837, 2361, 1902, 1608, 1496, 1394, 1132, 946, 827, 767, 543 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_3S$, 390.1134; found 390.1129.

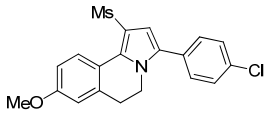


2c

3-(4-fluorophenyl)-8-methoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2c)

Compound **2c** was obtained as a white solid, 49.5 mg, in 89% yield; R_f = 0.50 (petroleum ether : ethyl acetate = 3 : 1); mp: 211-213 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, J = 8.4 Hz, 1H), 7.34 (dd, J_1 = 8.0 Hz, J_2 = 5.6 Hz, 2H), 7.14 (t, J = 8.4 Hz, 2H), 6.93 (dd, J_1 = 8.4 Hz, J_2 = 2.0 Hz, 1H), 6.82 (s, 1H), 6.74 (s, 1H), 4.04 (t, J = 6.4 Hz, 2H), 3.85 (s, 3H), 3.10 (s, 3H), 2.97 (t, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5 (d, J_{C-F} = 123.5 Hz), 159.5, 135.3, 131.6, 130.8 (d, J_{C-F} = 8.2 Hz), 130.2, 128.7, 127.1 (d, J_{C-F} = 3.3 Hz), 120.1, 119.1, 115.7 (d, J_{C-F} = 21.6 Hz), 113.81, 112.7, 111.0, 55.3, 43.8, 42.1,

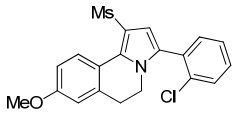
30.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.2; IR (KBr) ν 2921, 2368, 1611, 1496, 1391, 1135, 953, 837, 767, 655, 526, 480 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{18}FNNaO_3S$, 394.0884; found 394.0887.



2d

3-(4-chlorophenyl)-8-methoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2d)

Compound **2d** was obtained as a white solid, 41.8 mg, in 72% yield; R_f = 0.80 (petroleum ether : ethyl acetate = 3 : 1); mp: 211-213 ^oC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.8 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 6.93 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 6.82 (d, *J* = 2.4 Hz, 1H), 6.78 (s, 1H), 4.06 (t, *J* = 6.4 Hz, 2H), 3.86 (s, 3H), 3.10 (s, 3H), 2.97 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 135.3, 134.0, 131.4, 130.5, 130.1, 129.3, 128.9, 128.6, 120.0, 119.3, 113.8, 112.7, 111.2, 55.3, 43.8, 42.2, 29.9; IR (KBr) ν 3009, 2364, 1615, 1394, 1296, 1146, 816, 617, 484 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{18}ClNNaO_3S$, 410.0588; found 410.0588.

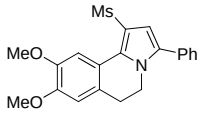


2e

3-(2-chlorophenyl)-8-methoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2e)

Compound **2e** was obtained as a white solid, 37.2 mg, in 64% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 195-197 ^oC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.8 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.40-7.35 (m, 3H), 6.93 (dd, J_1 = 8.4 Hz, J_2 = 2.4

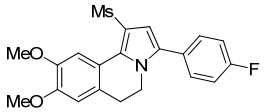
Hz, 1H), 6.81 (d, J = 2.4 Hz, 1H), 6.72 (s, 1H), 3.85 (appeared as a singlet, 5H), 3.12 (s, 3H), 2.98 (t, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 135.4, 135.0, 132.9, 130.24, 130.25, 130.0, 129.7, 129.4, 128.7, 127.0, 120.1, 118.7, 113.9, 112.7, 112.0, 55.3, 43.9, 42.4, 29.8; IR (KBr) ν 3117, 2960, 2837, 1604, 1520, 1468, 1293, 1237, 1132, 1030, 981, 844, 760, 554 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{18}ClNNaO_3S$, 410.0588; found 410.0588.



2f

8,9-dimethoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (2f)

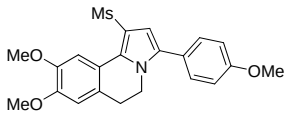
Compound **2f** was obtained as a white solid, 48.8 mg, in 85% yield; R_f = 0.60 (petroleum ether : ethyl acetate = 3 : 1); mp: 224-226 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.48-7.44 (m, 2H), 7.41-7.38 (m, 3H), 6.78 (d, J = 1.6 Hz, 2H), 4.10 (t, J = 6.4 Hz, 2H), 3.98 (s, 3H), 3.93 (s, 3H), 3.10 (s, 3H), 2.94 (t, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 148.3, 132.7, 130.9, 130.2, 129.0, 128.7, 128.0, 126.2, 120.0, 119.2, 111.1, 110.8, 110.4, 56.2, 55.9, 44.0, 42.5, 29.2; IR (KBr) ν 2834, 2364, 1615, 1394, 1132, 890, 768, 610, 463 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_4S$, 406.1083; found 406.1083.



2g

3-(4-fluorophenyl)-8,9-dimethoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2g)

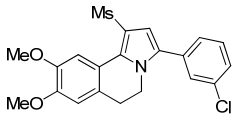
Compound **2g** was obtained as a white solid, 42.1 mg, in 70% yield; R_f = 0.60 (petroleum ether : ethyl acetate = 3 : 1); mp: 228-230 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.35 (dd, J_1 = 8.4 Hz, J_2 = 5.6 Hz, 2H), 7.15 (t, J = 8.8 Hz, 2H), 6.76 (d, J = 14.0 Hz, 2H), 4.05 (t, J = 6.8 Hz, 2H), 3.97 (s, 3H), 3.93 (s, 3H), 3.10 (s, 3H), 2.95 (t, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6 (d, J_{C-F} = 246.9 Hz), 148.8, 148.4, 131.6, 130.8 (d, J_{C-F} = 8.2 Hz), 130.2, 127.0 (d, J_{C-F} = 3.4 Hz), 126.1, 119.9, 119.2, 115.8 (d, J_{C-F} = 21.6 Hz), 111.1, 110.9, 110.4, 56.2, 56.0, 44.0, 42.4, 29.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.2; IR (KBr) ν 2837, 2361, 1615, 1499, 1394, 1265, 995, 837, 795, 557, 456 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{20}FNNaO_4S$, 424.0989; found 424.0988.



2h

8,9-dimethoxy-3-(4-methoxyphenyl)-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2h)

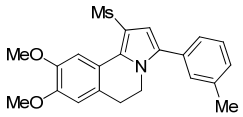
Compound **2h** was obtained as a white solid, 34.1 mg, in 55% yield; R_f = 0.45 (petroleum ether : ethyl acetate = 3 : 1); mp: 243-245 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.30 (t, J = 8.4 Hz, 2H), 6.77 (s, 1H), 6.71 (s, 1H), 4.05 (t, J = 6.4 Hz, 2H), 3.97 (s, 3H), 3.93 (s, 3H), 3.86 (s, 3H), 3.10 (s, 3H), 2.93 (t, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 148.6, 148.3, 132.6, 130.3, 129.8, 126.1, 123.3, 120.1, 119.0, 114.1, 110.8, 110.5, 110.4, 56.2, 55.9, 55.4, 44.0, 42.3, 29.2; IR (KBr) ν 3137, 2923, 1549, 1499, 1402, 1278, 1127, 891, 806, 762, 550 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{23}NNaO_5S$, 436.1189; found 436.1187.



2i

3-(3-chlorophenyl)-8,9-dimethoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2i)

Compound **2i** was obtained as a white solid, 45.7 mg, in 73% yield; R_f = 0.60 (petroleum ether : ethyl acetate = 3 : 1); mp: 213-215 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.41-7.36 (m, 3H), 7.27 (d, *J* = 4.4 Hz, 1H), 6.79 (d, *J* = 6.4 Hz, 2H), 4.09 (t, *J* = 6.4 Hz, 2H), 3.97 (s, 3H), 3.94 (s, 3H), 3.09 (s, 3H), 2.96 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 148.4, 134.6, 132.7, 131.2, 130.7, 130.0, 128.9, 128.1, 127.1, 126.1, 119.8, 119.5, 111.8, 110.8, 110.5, 56.3, 56.0, 44.0, 42.6, 29.2; IR (KBr) ν 3002, 2354, 1611, 1398, 1131, 1002, 620, 557 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{20}ClNNaO_4S$, 440.0694; found 440.0694.

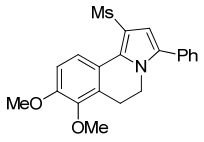


2j

8,9-dimethoxy-1-(methylsulfonyl)-3-(m-tolyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2j)

Compound **2j** was obtained as a white solid, 46.4 mg, in 78% yield; R_f = 0.60 (petroleum ether : ethyl acetate = 3 : 1); mp: 237-239 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.21-7.19 (m, 2H), 7.17 (d, *J* = 7.8 Hz, 1H), 6.78 (s, 1H), 6.76 (s, 1H), 4.09 (t, *J* = 7.2 Hz, 2H), 3.97 (s, 3H), 3.93 (s, 3H), 3.10 (s, 3H), 2.93 (t, *J* = 6.8 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 148.3, 138.4, 129.7, 128.8, 128.5, 126.2, 126.0, 120.0, 119.1, 111.1, 110.8, 110.4, 56.2, 55.9, 44.0, 42.5, 29.2, 21.4;

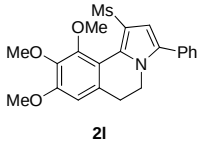
IR (KBr) ν 3122, 1532, 1402, 1190, 1133, 983 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{23}NNaO_4S$, 420.1240; found 420.1241.



2k

7,8-dimethoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (2k)

Compound **2k** was obtained as a white solid, 50.6 mg, in 88% yield; R_f = 0.75 (petroleum ether : ethyl acetate = 3 : 1); mp: 238-240 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.8 Hz, 1H), 7.48-7.44 (m, 2H), 7.41-7.37 (m, 3H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.78 (s, 1H), 4.07 (t, *J* = 6.4 Hz, 2H), 3.93 (s, 3H), 3.84 (s, 3H), 3.11 (s, 3H), 3.05 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 145.5, 132.7, 130.9, 130.0, 128.9, 128.6, 127.92, 127.85, 123.4, 120.7, 119.3, 111.0, 110.9, 60.7, 55.7, 43.7, 42.1, 22.8; IR (KBr) ν 2924, 2851, 2357, 1601, 1489, 1272, 1139, 957, 806, 767, 694, 564, 449 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{21}H_{21}NNaO_4S$, 406.1083; found 406.1084.

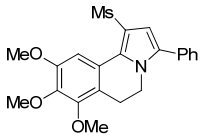


2l

8,9,10-trimethoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (2l)

Compound **2l** was obtained as a white solid, 50.2 mg, in 81% yield, R_f = 0.40 (petroleum ether : ethyl acetate = 3 : 1); mp: 243-245 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.47-7.40 (m, 4H), 7.39-7.37 (m, 1H), 6.78 (s, 1H), 6.59 (s, 1H), 4.00 (t, *J* = 6.0 Hz, 2H), 3.95 (s, 3H), 3.88 (s, 3H), 3.85 (s, 3H), 3.31 (s, 3H), 2.75 (t, *J* = 6.0 Hz, 2H); ^{13}C NMR (100

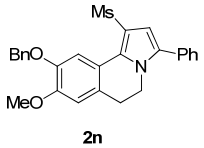
MHz, $CDCl_3$) δ 153.6, 151.5, 140.9, 134.0, 131.9, 130.9, 128.9, 128.7, 128.6, 127.8, 121.3, 114.7, 110.3, 106.4, 61.3, 60.7, 56.1, 43.1, 42.4, 31.0; IR (KBr) ν 2930, 1599, 1484, 1420, 1293, 996, 846, 762, 550 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{23}NNaO_5S$, 436.1189; found 436.1191.



2m

7,8,9-trimethoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-*a*]isoquinoline (2m)

Compound **2m** was obtained as a white solid, 21.1 mg, in 34% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 259-261 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.48-7.44 (m, 2H), 7.41-7.38 (m, 3H), 6.80 (s, 1H), 4.07 (t, *J* = 6.4 Hz, 2H), 3.95 (s, 3H), 3.94 (s, 3H), 3.89 (s, 3H), 3.12 (s, 3H), 2.97 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.7, 150.3, 142.0, 133.0, 130.8, 129.7, 129.0, 128.7, 128.1, 123.0, 120.0, 119.6, 111.4, 106.8, 61.1, 61.0, 56.3, 44.0, 42.4, 22.3; IR (KBr) ν 2921, 2858, 2368, 1720, 1601, 1461, 1293, 1139, 1111, 767, 561, 512 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{23}NNaO_5S$, 436.1189; found 436.1188.

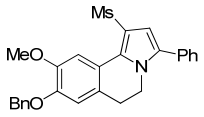


2n

9-(benzyloxy)-8-methoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-*a*]isoquinoline (2n)

Compound **2n** was obtained as a white solid, 47.5 mg, in 69% yield; R_f = 0.75 (petroleum ether : ethyl acetate = 3 : 1); mp: 262-264 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H),

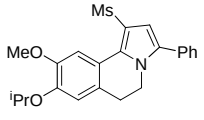
7.51 (d, *J* = 3.2 Hz, 2H), 7.45-7.42 (m, 2H), 7.39-7.34 (m, 5H), 7.28-7.26 (m, 1H), 6.79 (s, 1H), 6.73 (s, 1H), 5.32 (s, 2H), 4.05 (t, *J* = 6.4 Hz, 2H), 3.94 (s, 3H), 3.90 (t, *J* = 6.4 Hz, 2H), 2.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 147.0, 137.0, 132.7, 130.9, 130.0, 128.9, 128.6, 128.4, 127.9, 127.6, 127.2, 126.5, 119.9, 119.3, 112.0, 111.3, 111.0, 70.1, 56.0, 43.4, 42.4, 29.2; IR (KBr) ν 2921, 2851, 1527, 1494, 1293, 1270, 1133, 879, 759, 702, 550 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{27}H_{25}NNaO_4S$, 482.1397; found 482.1396.



2o

8-(benzyloxy)-9-methoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (2o)

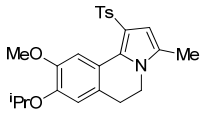
Compound **2o** was obtained as a white solid, 42.0 mg, in 61% yield; R_f = 0.80 (petroleum ether : ethyl acetate = 3 : 1); mp: 259-261 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.47-7.32 (m, 10H), 6.78 (d, *J* = 6.0 Hz, 2H), 5.20 (s, 2H), 4.06 (t, *J* = 6.4 Hz, 2H), 3.98 (s, 3H), 3.10 (s, 3H), 2.87 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 147.8, 136.7, 132.8, 130.9, 130.2, 128.9, 128.64, 128.58, 128.0, 127.9, 127.2, 126.0, 120.5, 119.3, 113.3, 111.1, 110.8, 71.0, 56.3, 44.0, 42.5, 29.1; IR (KBr) ν 2925, 1652, 1494, 1295, 1130, 803, 763, 697, 550 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{27}H_{25}NNaO_4S$, 482.1397; found 482.1393.



2p

8-isopropoxy-9-methoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (2p)

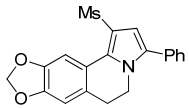
Compound **2p** was obtained as a white solid, 49.3 mg, in 80% yield; R_f = 0.60 (petroleum ether : ethyl acetate = 3 : 1); mp: 187-189 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.46-7.43 (m, 2H), 7.43-7.36 (m, 3H), 6.78 (d, *J* = 9.6 Hz, 2H), 4.60 (dt, J_1 = 12.0 Hz, J_2 = 6.0 Hz, 1H), 4.08 (t, *J* = 6.4 Hz, 2H), 3.94 (s, 3H), 3.10 (s, 3H), 2.91 (t, *J* = 6.4 Hz, 2H), 1.41 (d, *J* = 6.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 147.0, 132.6, 130.9, 130.3, 128.9, 128.6, 127.9, 126.0, 120.1, 119.1, 114.7, 111.0, 110.9, 71.4, 56.2, 43.9, 42.5, 29.1, 22.0; IR (KBr) ν 3135, 3019, 2840, 1608, 1517, 1436, 1335, 1289, 1125, 887, 757, 690, 561, 515, 470 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{23}H_{25}NNaO_4S$, 434.1396; found 434.1395.



2q

8-isopropoxy-9-methoxy-3-methyl-1-tosyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (2q)

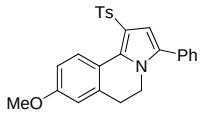
Compound **2q** was obtained as a white solid, 37.0 mg, in 58% yield; R_f = 0.40 (petroleum ether : ethyl acetate= 3 : 1); mp: 209-211 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 6.67 (s, 1H), 6.40 (s, 1H), 4.55-4.49 (m, 1H), 3.85-3.83 (m, 5H (O-CH_3 and N-CH_2 overlapped)), 2.85 (t, *J* = 6.4 Hz, 2H), 2.33 (s, 3H), 2.21 (s, 3H), 1.35 (d, *J* = 6.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.1, 146.5, 142.8, 141.0, 130.0, 129.2, 127.3, 126.3, 124.9, 120.3, 117.2, 114.6, 111.4, 110.6, 71.3, 56.1, 41.1, 28.7, 22.0, 21.4, 11.8; IR (KBr) ν 3135, 3019, 2840, 1608, 1517, 1436, 1335, 1289, 1125, 887, 757, 690, 561, 515 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{27}NNaO_4S$, 448.1553; found 448.1551.



2r

1-(methylsulfonyl)-3-phenyl-5,6-dihydro-[1,3]dioxolo[4,5-g]pyrrolo[2,1-a]isoquinoline (2r)

Compound **2r** was obtained as a white solid, 40.2 mg, in 73% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 251-253 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.44-7.36 (m, 5H), 6.76 (d, *J* = 11.2 Hz, 2H), 5.99 (s, 2H), 4.05 (t, *J* = 7.2 Hz, 2H), 3.11 (s, 3H), 2.88 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 147.2, 132.7, 130.8, 130.0, 128.9, 128.6, 128.1, 128.0, 121.0, 119.5, 111.0, 108.3, 107.6, 101.3, 44.1, 42.3, 29.8; IR (KBr) ν 3127, 1611, 1489, 1400, 1288, 1133, 781, 704 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{17}NNaO_4S$, 390.0770; found 390.0764.

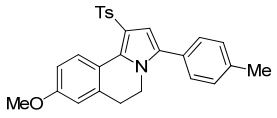


2s

8-methoxy-3-phenyl-1-tosyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (2s)

Compound **2s** was obtained as a white solid, 47.0 mg, in 73% yield; R_f = 0.40 (petroleum ether : ethyl acetate = 3 : 1); mp: 218-220 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 2H), 7.46-7.42 (m, 2H), 7.39-7.36 (m, 3H), 7.23 (d, *J* = 8.0 Hz, 2H), 6.85 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 6.75 (s, 1H), 6.72 (d, *J* = 2.4 Hz, 1H), 4.04 (t, *J* = 6.4 Hz, 2H), 3.83 (s, 3H), 2.88 (t, *J* = 6.4 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 143.1, 140.5, 135.1, 132.7, 131.1, 130.9, 129.40, 129.35, 129.0, 128.6, 127.9, 126.9, 120.1, 119.2, 113.4, 112.2, 111.8, 55.3, 42.3, 30.0, 21.5; IR

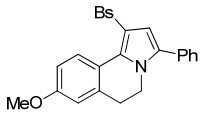
(KBr) ν 3002, 2357, 1615, 1394, 1307, 1149, 1096, 1033, 764, 676, 582, 480 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{26}H_{23}NNaO_3S$, 452.1291; found 452.1291.



2t

8-methoxy-3-(p-tolyl)-1-tosyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (2t)

Compound **2t** was obtained as a white solid, 42.9 mg, in 66% yield; R_f = 0.40 (petroleum ether : ethyl acetate = 3 : 1); mp: 223-225 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.8 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 2H), 7.26-7.21 (m, 6H), 6.84 (dd, J_1= 8.8 Hz, J_2= 2.4 Hz, 1H), 6.71 (s, 2H), 4.01 (t, *J* = 6.4 Hz, 2H), 3.82 (s, 3H), 2.86 (t, *J* = 6.4 Hz, 2H), 2.40 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 143.0, 140.5, 137.9, 135.1, 132.8, 130.7, 129.4, 129.3, 128.9, 128.1, 126.9, 120.2, 119.0, 113.3, 112.1, 111.5, 55.3, 42.2, 30.0, 21.5, 21.2; IR (KBr) ν 2935, 1611, 1496, 1244, 1146, 1030, 830, 683, 540 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{27}H_{25}NNaO_3S$, 466.1447; found 466.1450.

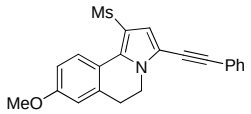


2u

8-methoxy-3-phenyl-1-(phenylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2u)

Compound **2u** was obtained as a white solid, 51.7 mg, in 83% yield; R_f = 0.40 (petroleum ether : ethyl acetate = 3 : 1); mp: 220-222 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.8 Hz, 1H), 7.96-7.94 (m, 2H), 7.50-7.43 (m, 5H), 7.39-7.36 (m, 3H), 6.84 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 6.78 (s, 1H), 6.72 (d, *J* = 2.4 Hz, 1H), 4.04 (t, *J* = 8.0 Hz, 2H), 3.82 (s, 3H), 2.88 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 143.4, 135.2, 132.9, 132.4, 131.2, 131.0, 129.4, 129.0, 128.8, 128.7, 127.9, 126.8, 120.1, 118.7, 113.4,

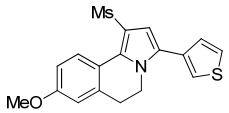
112.2, 111.9, 55.3, 42.3, 30.0; IR (KBr) ν 2834, 2354, 2035, 1611, 1405, 1289, 1146, 1030, 831, 732, 592, 484 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{21}NNaO_3S$, 438.1134; found 438.1128.



2v

8-methoxy-1-(methylsulfonyl)-3-(phenylethynyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2v)

Compound **2v** was obtained as a white solid, 31.1 mg, in 55% yield; R_f = 0.50 (petroleum ether : ethyl acetate = 3 : 1); mp: 179-181 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.8 Hz, 1H), 7.53-7.51 (m, 2H), 7.37-7.36 (m, 3H), 7.01 (s, 1H), 6.91 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 6.83 (d, *J* = 2.4 Hz, 1H), 4.22 (t, *J* = 6.4 Hz, 2H), 3.85 (s, 3H), 3.07 (t, *J* = 6.4 Hz, 2H), 3.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 135.2, 131.3, 130.8, 128.75, 128.67, 128.4, 122.3, 119.5, 119.2, 117.2, 114.13, 114.09, 112.8, 95.2, 78.9, 55.3, 43.9, 42.2, 29.5; IR (KBr) ν 3019, 2203, 1604, 1517, 1457, 1296, 1135, 1026, 942, 753, 690, 557, 508 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{19}NNaO_3S$, 400.0978; found 400.0977.

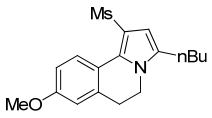


2x

8-methoxy-1-(methylsulfonyl)-3-(thiophen-3-yl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2x)

Compound **2x** was obtained as a white solid, 44.7 mg, in 83% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 214-216 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* =

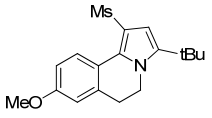
8.4 Hz, 1H), 7.42 (dd, J_1 = 4.8 Hz, J_2 = 4.0 Hz, 1H), 7.26-7.25 (m, 1H), 7.16 (d, J = 4.0 Hz, 1H), 6.92 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 6.81 (d, J = 2.0 Hz, 1H), 6.78 (s, 1H), 4.12 (t, J = 6.4 Hz, 2H), 3.85 (s, 3H), 3.09 (s, 3H), 2.98 (t, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 135.2, 131.4, 130.0, 128.6, 128.0, 127.8, 126.3, 123.2, 120.1, 119.0, 113.8, 112.7, 110.9, 55.3, 43.9, 41.9, 29.9; IR (KBr) ν 3019, 2841, 2357, 1611, 1576, 1471, 1398, 1132, 1030, 946, 859, 816, 760, 550 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{17}NNaO_3S_2$, 382.0542; found 382.0535.



2y

3-butyl-8-methoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2y)

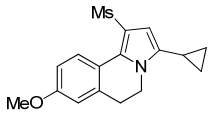
Compound **2y** was obtained as a white solid, 35.0 mg, in 70% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 203-205 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, J = 8.8 Hz, 1H), 6.89 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 6.79 (d, J = 2.4 Hz, 1H), 6.43 (s, 1H), 3.93 (t, J = 6.4 Hz, 2H), 3.84 (s, 3H), 3.04 (s, 3H), 3.00 (t, J = 6.4 Hz, 2H), 2.56 (t, J = 7.6 Hz, 2H), 1.61 (dt, J_1 = 15.2 Hz, J_2 = 7.2 Hz, 2H), 1.42 (dq, J_1 = 14.8 Hz, J_2 = 7.2 Hz, 2H), 0.95 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 134.6, 131.9, 129.1, 128.3, 120.3, 117.7, 113.7, 112.6, 108.6, 55.3, 43.9, 40.8, 30.3, 29.7, 25.7, 22.3, 13.8; IR (KBr) ν 2928, 2361, 1608, 1517, 1408, 1247, 1142, 1037, 949, 830, 757, 564, 480 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{23}NNaO_3S$, 356.1291; found 356.1290.



2z

3-(tert-butyl)-8-methoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2z)

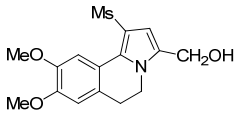
Compound **2z** was obtained as a white solid, 31.0 mg, in 62% yield; R_f = 0.60 (petroleum ether : ethyl acetate = 3 : 1); mp: 181-183 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.8 Hz, 1H), 6.78 (d, *J* = 8.4 Hz, 1H), 6.68 (s, 1H), 6.08 (s, 1H), 3.83 (s, 3H), 3.80 (t, *J* = 6.0 Hz, 2H), 2.91 (t, *J* = 6.0 Hz, 2H), 2.78 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 139.3, 136.4, 128.9, 123.9, 113.1, 111.9, 107.1, 104.5, 55.3, 45.6, 38.5, 30.6, 29.7, 28.2; IR (KBr) ν 2960, 2851, 1608, 1492, 1342, 1160, 1020, 963, 869, 736, 578 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{18}H_{23}NNaO_3S$, 356.1291; found 356.1292.



2aa

3-cyclopropyl-8-methoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (2aa)

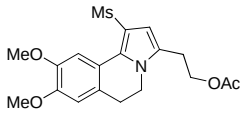
Compound **2aa** was obtained as a white solid, 38.0 mg, in 80% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 204-206 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.8 Hz, 1H), 6.89 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 6.80 (d, *J* = 2.4 Hz, 1H), 6.34 (d, *J* = 0.4 Hz, 1H), 4.13 (t, *J* = 6.4 Hz, 2H), 3.84 (s, 3H), 3.04 (s, 3H), 3.02 (t, *J* = 6.4 Hz, 2H), 1.71-1.64 (m, 1H), 0.94-0.89 (m, 2H), 0.69-0.65 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 134.8, 133.7, 129.3, 128.3, 120.3, 117.4, 113.9, 112.6, 108.3, 55.3, 43.9, 41.0, 29.7, 6.4, 5.8; IR (KBr) ν 3002, 2837, 2361, 1615, 1577, 1524, 1524, 1293, 1090, 984, 823, 767, 645, 543, 508, 435 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO_3S$, 340.0978; found 340.0978.



2ab

(8,9-dimethoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinolin-3-yl)methanol (2ab)

Compound **2ab** was obtained as a white solid (21.2 mg, 42%); R_f = 0.30 (petroleum ether : ethyl acetate = 3 : 1); mp: 249-251 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 6.75 (s, 1H), 6.60 (s, 1H), 4.61 (s, 2H), 4.12 (t, *J* = 6.8 Hz, 2H), 3.91 (appeared as doublet as O-*CH*$_3$ protons overlapped, *J* = 2.4 Hz, 6H), 3.01-2.96 (appeared as multiplet as Ar-*CH*$_2$ and –SO_2-*CH*$_3$ overlapped, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 148.3, 131.1, 130.1, 126.0, 119.5, 117.7, 111.5, 111.0, 110.3, 56.2, 55.9, 44.0, 41.7, 28.7; IR (KBr) ν 2914, 2354, 1643, 715, 424 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{16}H_{19}NNaO_5S$, 360.0876; found 360.0876.

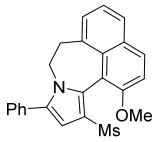


2ac

2-(8,9-dimethoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-a]isoquinolin-3-yl)ethyl acetate (2ac)

Compound **2ac** was obtained as a white solid, 38.9 mg, in 66% yield; R_f = 0.22 (petroleum ether : ethyl acetate = 3 : 1); mp: 239-241 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 6.77 (s, 1H), 6.52 (s, 1H), 4.27 (t, *J* = 6.8 Hz, 2H), 4.00 (t, *J* = 6.8 Hz, 2H), 3.94 (s, 3H), 3.92 (s, 3H), 3.04 (s, 3H), 3.00 (t, *J* = 6.4 Hz, 2H), 2.94 (t, *J* = 7.2 Hz, 2H), 2.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 148.6, 148.3, 129.8, 127.3, 125.4, 119.8, 118.2, 110.8, 110.2, 110.1, 62.6, 56.1, 55.9, 44.0, 41.4, 28.9, 25.6, 20.9; IR (KBr)

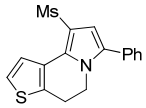
ν 3130, 1741, 1529, 1397, 1233, 1233, 1138, 891, 806, 552 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{23}NNaO_6S$, 416.1138; found 416.1137.



2ad

12-methoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydronaphtho[1,8-cd]pyrrolo[1,2-a]azepine (2ad)

Compound **2ad** was obtained as a white solid, 39.0 mg, in 65% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 178-180 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.4 Hz, 1H), 7.80 (t, *J* = 8.4 Hz, 2H), 7.50-7.39 (m, 5H), 7.25 (s, 1H), 7.19 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 6.88 (s, 1H), 4.22 (t, *J* = 6.4 Hz, 2H), 3.95 (s, 3H), 3.33 (t, *J* = 6.4 Hz, 2H), 3.11 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 133.0, 132.0, 130.8, 130.3, 130.2, 128.9, 128.7, 128.5, 128.14, 128.11, 127.5, 125.4, 122.2, 121.2, 118.5, 111.7, 102.3, 55.3, 44.2, 41.9, 25.1; IR (KBr) ν 2921, 2361, 1468, 1307, 1146, 964, 768, 554, 508, 435 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{21}NNaO_3S$, 426.1134; found 426.1135.

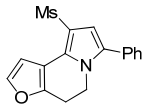


2ae

9-(methylsulfonyl)-7-phenyl-4,5-dihydrothieno[2,3-g]indolizine (2ae)

Compound **2ae** was obtained as a white solid, 35.0 mg, in 72% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 120-122 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 5.2 Hz, 1H), 7.48-7.44 (m, 2H), 7.41-7.37 (m, 3H), 7.23 (d, *J* = 5.6 Hz, 1H), 6.68 (s, 1H), 4.19 (t, *J* = 6.8 Hz, 2H), 3.13 (t, *J* = 6.8 Hz, 2H), 3.12 (s, 3H); ^{13}C NMR

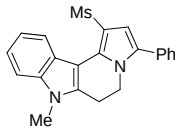
(100 MHz, $CDCl_3$) δ 133.9, 133.4, 131.1, 129.1, 128.7, 128.2, 128.1, 126.3, 123.7, 118.1, 110.2, 44.9, 43.0, 24.5; IR (KBr) ν 2914, 2368, 1293, 1139, 869, 767, 561, 515, 435 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{15}NNaO_2S_2$, 352.0436; found 352.0436.



2af

9-(methylsulfonyl)-7-phenyl-4,5-dihydrofuro[2,3-g]indolizine (2af)

Compound **2af** was obtained as a white oil, 15.0 mg, in 25% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); ^1H NMR (400 MHz, $CDCl_3$) δ 7.47-7.37 (m, 6H), 7.21 (s, 1H), 6.58 (s, 1H), 4.23 (t, *J* = 7.2 Hz, 2H), 3.11 (s, 3H), 3.09 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6, 142.5, 133.9, 131.2, 129.0, 128.7, 128.2, 117.8, 112.1, 109.7, 108.9, 45.3, 43.2, 22.8; IR (KBr) ν 2928, 1758, 1478, 1310, 1135, 764, 561, 522, 435 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{17}H_{15}NNaO_3S$, 336.0665; found 336.0665.

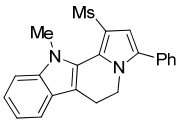


2ag

7-methyl-1-(methylsulfonyl)-3-phenyl-6,7-dihydro-5H-indolizino[7,8-b]indole (2ag)

Compound **2ag** was obtained as a white solid, 36.6 mg, in 65% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 237-239 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.65 (dd, J_1 = 6.4, J_2 = 2.4 Hz, 1H), 7.47-7.37 (m, 5H), 7.34-7.26 (m, 3H), 6.77 (s, 1H), 4.14 (t, *J* = 6.4 Hz, 2H), 3.74 (s, 3H), 3.16 (s, 3H), 3.02 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 136.9, 132.2, 131.3, 129.2, 128.9, 128.5, 127.7, 123.6, 121.8, 121.4, 120.8, 117.5, 109.3, 109.2, 103.9, 44.4, 41.7, 29.7, 21.6; IR (KBr) ν 2925, 2368,

2329, 2035, 1398, 1356, 1212, 991, 687, 494 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{20}N_2NaO_2S$, 399.1138; found 399.1138.

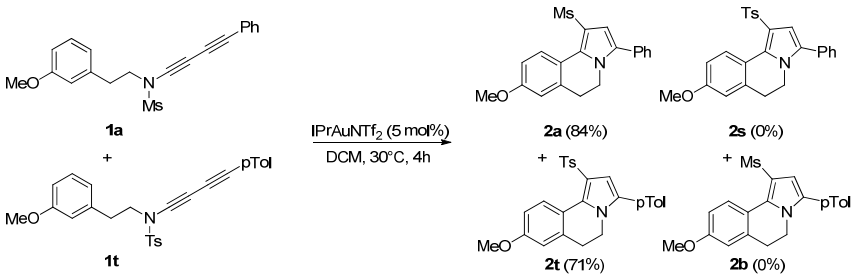


2ah

11-methyl-1-(methylsulfonyl)-3-phenyl-6,11-dihydro-5H-indolizino[8,7-b]indole (2ah)

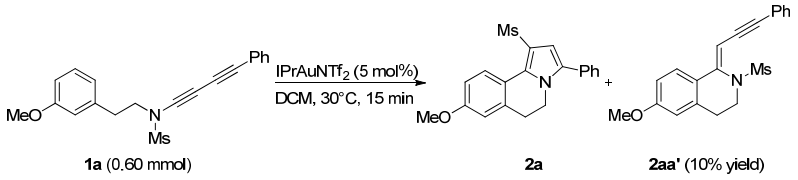
Compound **2ah** was obtained as a white solid, 24.7 mg, in 45% yield; R_f = 0.70 (petroleum ether : ethyl acetate = 3 : 1); mp: 235-237 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 1H), 7.50-7.46 (m, 2H), 7.43-7.41 (m, 4H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.17 (t, *J* = 7.2 Hz, 1H), 6.70 (s, 1H), 4.08 (t, *J* = 6.4 Hz, 2H), 3.98 (s, 3H), 3.20 (s, 3H), 2.99 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 135.8, 130.9, 130.4, 129.1, 128.7, 128.3, 125.5, 124.8, 122.9, 120.3, 119.1, 118.6, 112.6, 110.8, 109.3, 45.2, 43.6, 34.5, 21.9; IR (KBr) ν 2935, 2848, 2364, 1566, 1457, 1349, 1293, 1132, 1019, 767, 708, 547 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{22}H_{20}N_2NaO_2S$, 399.1138; found 399.1137.

Crossover experiments



A dry Schlenk tube was charged with gold catalyst (5 mol %) and evacuated and back filled with argon. To this tube was added the solution of **1a** (0.15 mmol) and **1t** (0.15 mmol) in DCM. The reaction mixture was stirred at 30 °C for 4 h. Upon completion, the mixture was then quenched with small amount of water, diluted with DCM, washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was checked by ^1H NMR using as an internal standard.

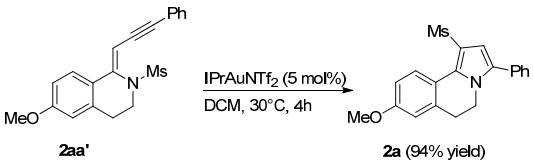
Separation of the intermediate 2aa'



1a (0.60 mmol) **2a** **2aa'** (10% yield)

A dry Schlenk tube was charged with gold catalyst (26 mg, 5 mol %) and evacuated and back filled with argon. To this tube was added the solution of **1a** (212 mg, 0.60 mmol) in DCM (4 mL). The reaction mixture was stirred at 30 °C for 15 min. Then the mixture was then quenched with small amount of water, diluted with DCM, washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by chromatography on silica gel (eluent: petroleum ether/DCM) and recrystallized (petroleum ether/DCM) to afford **2aa'** (21 mg, 10%). R_f = 0.35 (petroleum ether : ethyl acetate = 3 : 1); mp: 164-166 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, J = 8.8 Hz, 1H), 7.47-7.44 (m, 2H), 7.34-7.32 (m, 3H), 6.78 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 6.63 (d, J = 2.8 Hz, 1H), 6.35 (s, 1H), 3.82 (t, J = 6.0 Hz, 2H), 3.81 (s, 3H), 3.26 (s, 3H), 3.09 (t, J = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 142.6, 135.6, 131.3, 128.5, 125.4, 124.0, 123.2, 113.7, 113.6, 101.8, 96.9, 87.7, 55.3, 46.0, 42.2, 28.9; IR (KBr) ν 2916,

1664, 1607, 1342, 1330, 1148, 1108, 970, 759, 520 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{19}NNaO_3S$, 376.0978; found 376.0979.

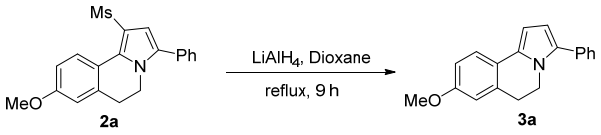


2aa' **2a** (94% yield)

A dry Schlenk tube was charged with gold catalyst (2.6 mg, 5 mol %) and evacuated and back filled with argon. To this tube was added the solution of **2aa'** (21 mg, 0.06 mmol) in DCM (1 mL). The reaction mixture was stirred at 30 °C for 4 h. Then the mixture was then quenched with small amount of water, diluted with DCM, washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by chromatography on silica gel (eluent: petroleum ether/DCM) to afford **2a** (19.7 mg, 94%).

Transformations of the products

a)



2a **3a**

8-methoxy-3-phenyl-5,6-dihydropyrrolo[2,1-*a*]isoquinoline (3a)

In a two-neck RB, $LiAlH_4$ (40 mg, 0.98 mmol, 7 equiv.) was weighed and 5 mL of dioxane (previously degassed with argon) was added under inert atmosphere. To this suspension solid **2a** (50 mg, 0.14 mmol) was added at room temperature. The mixture was then refluxed for 9 h. The reaction mixture was cooled to 0 °C, diluted by adding 5 mL of ethyl acetate and carefully quenched by saturated NH_4Cl solution. It was then filtered using a short pad of celite and filtrate was then extracted by ethyl acetate (3 × 10 mL). The combined extracts was washed with brine and dried over Na_2SO_4. The solvent

was removed under reduced pressure and the residual mass was purified by silica gel column chromatography using petroleum ether : ethylacetate (10 : 1) as eluent to afford the pure product **3a** (27.7 mg, 72%); R_f = 0.70 (petroleum ether : ethyl acetate = 5 : 1); mp: 231-233 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.4 Hz, 1H), 7.43-7.33 (m, 4H), 7.32-7.29 (m, 1H), 6.82 (d, *J* = 8.4 Hz, 1H), 6.76 (s, 1H), 6.50 (d, *J* = 3.6 Hz, 1H), 6.32 (d, *J* = 3.6 Hz, 1H), 4.14 (t, *J* = 6.4 Hz, 2H), 3.83 (s, 3H), 3.01 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 133.6, 133.0, 132.4, 131.1, 128.5, 128.4, 126.6, 123.9, 123.1, 113.2, 112.8, 109.2, 102.8, 55.3, 42.0, 30.0; IR (KBr) ν 2960, 2364, 1646, 1247, 1034, 806, 536 cm^{-1}; HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{19}H_{18}NO$, 276.1383; found 276.1383.[8]

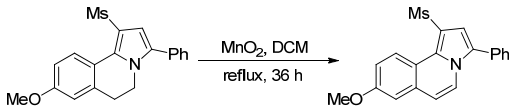
b)

2-bromo-8-methoxy-1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-*a*]isoquinoline (3b)

To a solution of **2a** (40 mg, 0.11 mmol) in 2 mL of THF, a THF (1 mL) solution of NBS (1.2 equiv.) was added at 0 $^\circ C$ and stirred for 12 h during which the temperature raised to room temperature. The reaction was quenched with water and extracted with DCM (3 × 10 mL). The organic layers were combined, washed with brine and dried over sodium sulfate. The pure product **3b** (45.6 mg, 95%) was obtained by flash column chromatography on silica gel (petroleum ether : DCM = 1 : 1); R_f = 0.40 (petroleum ether : DCM= 1 : 1); mp: 237-239 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.8 Hz, 1H), 7.51-7.45 (m, 3H), 7.40 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 2H), 6.90 (dd, J_1 = 8.8 Hz, J_2 =

2.8 Hz, 1H), 6.76 (d, *J* = 2.4 Hz, 1H), 3.84 (appeared as triplet, *J* = 6.4 Hz, 5H), 3.30 (s, 3H), 2.87 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 136.2, 132.7, 132.5, 131.3, 130.7, 129.04, 129.00, 128.5, 119.1, 116.7, 113.3, 111.9, 96.2, 55.3, 44.9, 43.0, 30.0; IR (KBr) ν 2921, 2844, 2368, 1608, 1454, 1303, 1146, 1030, 953.31, 708, 561 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{20}H_{18}BrNNaO_3S$, 454.0083; found 454.0081.[9]

c)

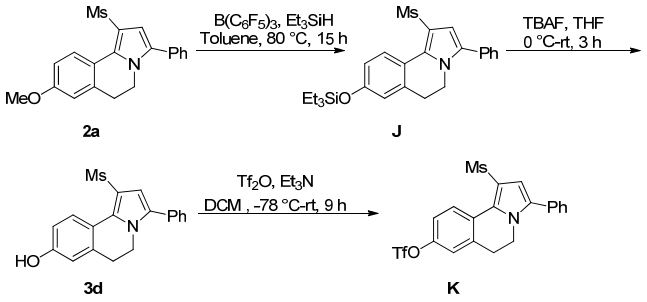


2a **3c** (59%)

8-methoxy-1-(methylsulfonyl)-3-phenylpyrrolo[2,1-a]isoquinoline (3c)

A mixture of **2a** (71 mg, 0.20 mmol) and activated MnO_2 (869 mg, 10 mmol) in dichloromethane (15 mL) was refluxed for 36 h. After cooling to room temperature, the mixture was passed through a pad of Celite and evaporated. The residue was purified by column chromatography eluted by petroleum ether/DCM to give **3c** as a yellow solid (41.7 mg, 59%). R_f = 0.25 (petroleum ether : ethyl acetate = 3 : 1); mp: 187-189 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (d, *J* = 9.2 Hz, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.53 (appeared as a singlet, 2H), 7.52 (appeared as a singlet, 2H), 7.48-7.43 (m, 1H), 7.29-7.25 (m, 2H), 7.10 (d, *J* = 2.8 Hz, 1H), 6.94 (d, *J* = 7.2 Hz, 1H), 3.94 (s, 3H), 3.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 130.8, 130.4, 129.4, 129.2, 129.1, 128.5, 127.8, 127.4, 122.3, 118.5, 117.8, 115.3, 114.7, 113.7, 108.8, 55.4, 44.3; IR (KBr) ν 2923, 1647, 1539, 1135, 766 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{17}NNaO_3S$, 374.0821; found 374.0822.[10]

d)



1-(methylsulfonyl)-3-phenyl-8-((triethylsilyl)oxy)-5,6-dihydropyrrolo[2,1-a]isoquinoline (J)

To a mixture of **2a** (150 mg, 0.42 mmol) and $B(C_6F_5)_3$ (10 mol%) in toluene (6 mL, degassed with argon), Et_3SiH (5 equiv.) was added at room temperature (immediate bubbling from the reaction mixture observed). It was then refluxed for 7 h during which the initial heterogeneous mixture turned into a yellow solution. The reaction was cooled to rt, diluted by adding 10 mL of ethyl acetate and quenched by saturated NH_4Cl solution. The reaction mixture was partitioned in a separating flask and the aqueous layer was extracted by ethyl acetate (3 × 15 mL). The combined extracts was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residual mass was purified by silica gel column chromatography using petroleum ether : ethyl acetate (5 : 1) as eluent to give **J** as a yellow oil (138.0 mg, 74%). R_f = 0.60 (petroleum ether : ethyl acetate = 5 : 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.4 Hz, 1H), 7.47-7.43 (m, 2H), 7.39-7.37 (m, 3H), 6.88 (d, *J* = 8.4 Hz, 1H), 6.80-6.77 (m, 2H), 4.09 (t, *J* = 6.0 Hz, 2H), 3.11 (s, 3H), 2.93 (t, *J* = 6.0 Hz, 2H), 1.03 (t, *J* = 8.0 Hz, 9H), 0.78 (dd, J_1 = 15.6 Hz, J_2 = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 135.3, 132.7, 131.0, 130.3, 129.0, 128.7, 128.6, 127.9, 120.7, 119.4, 119.2, 118.9, 111.0, 43.9, 42.3, 31.6, 29.9, 22.6, 14.1, 6.6, 5.0; IR (KBr) ν 2960, 2872, 2350, 1608, 1457, 1300, 1135, 953, 816, 757,

547 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{31}NNaO_3SSi$, 476.1686; found 476.1685.

1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-a]isoquinolin-8-ol (3d)

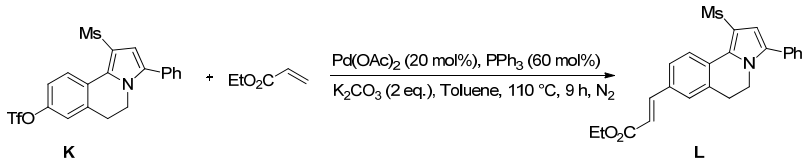
To a solution of **J** (120 mg, 0.26 mmol) in THF (5 mL), TBAF (0.52 mL, 1M in THF, 0.52 mmol) was added dropwise at 0 °C. The solution was stirred for 2 h during which the temperature gradually increased to room temperature. The reaction was quenched by water and extracted with ethyl acetate (3 × 10 mL). The combined extracts was washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure and the residual mass was purified by silica gel column chromatography using petroleum ether : ethyl acetate (3 : 1) as eluent to give **3d** as a yellow solid (81.2 mg, 92%). R_f = 0.70 (petroleum ether : ethyl acetate = 5 : 1); mp: 199-201 ^oC; ^1H NMR (400 MHz, $(CD_3)_2SO$) δ 9.77 (broad singlet, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.47 (appeared as doublet, *J* = 4.4 Hz, 4H), 7.42-7.36 (m, 1H), 6.78-6.76 (m, 2H), 6.62 (s, 1H), 4.07 (t, *J* = 6.4 Hz, 2H), 3.11 (s, 3H), 2.89 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ 158.0, 136.6, 132.5, 131.1, 130.5, 129.2, 128.7, 128.3, 119.2, 118.6, 115.3, 114.5, 110.2, 44.2, 42.5, 29.6; IR (KBr) ν 3348, 2364, 1611, 1457, 1264, 1132, 985, 767, 550 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{19}H_{17}NNaO_3S$, 362.0821; found 362.0820.

1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-a]isoquinolin-8-yl trifluoromethanesulfonate (K)

3d (80 mg, 0.24 mmol) was dissolved in DCM (3.0 mL) and then cooled to -78 ^oC. Triethylamine (TEA, 70.0 μL, 0.50 mmol) was added, followed by addition of trifluoromethanesulfonic anhydride (Tf_2O, 60.0 μL, 0.53 mmol) within 3 minutes via a syringe. The resulting solution was gradually warmed to room temperature and stirred for

2 h until **3d** had been completely consumed as determined by TLC. The solvent was then removed under reduced pressure to get the crude product, which was purified by flash column chromatography on silica gel, eluted by petroleum ether/DCM to afford the pure product **K** as a yellow solid (100.0 mg, 90% yield). R_f = 0.50 (petroleum ether : ethyl acetate = 5 : 1); mp: 161-163 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, J = 8.8 Hz, 1H), 7.50-7.46 (m, 2H), 7.44-7.42 (m, 1H), 7.41-7.37 (m, 2H), 7.29 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 7.22 (d, J = 2.4 Hz, 1H), 6.83 (s, 1H), 4.15 (t, J = 6.4 Hz, 2H), 3.12 (s, 3H), 3.04 (t, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 135.9, 134.1, 130.4, 129.1, 129.0, 128.8, 128.5, 127.8, 127.7, 121.7, 120.8, 120.6, 118.7 (q, $J_{C\text{-}F}$ = 319.1 Hz), 111.8, 44.3, 42.0, 29.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.8; IR (KBr) ν 2361, 1636, 1422, 1212, 1135, 932, 757, 606 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{20}H_{16}F_3NNaO_5S_2$, 494.0314; found 494.0313. [11]

e)

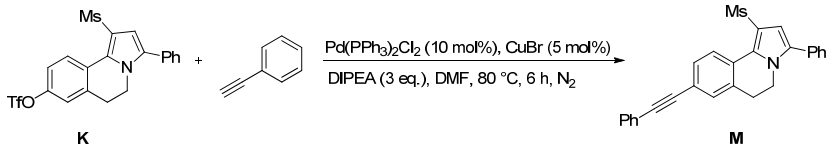


Ethyl (E)-3-(1-(methylsulfonyl)-3-phenyl-5,6-dihydropyrrolo[2,1-a]isoquinolin-8-yl)acrylate (L)

K (48.0 mg, 0.1 mmol), ethyl acrylate (106.4 μL, 1.0 mmol), palladium(II) aceate ($Pd(OAc)_2$, 4.4 mg, 0.02 mmol), triphenylphosphine (PPh_3, 15.7 mg, 0.06 mmol), potassium carbonate (K_2CO_3, 27.6 mg, 0.2 mmol), and toluene (1.0 mL) were added to a pressure tube. The reaction mixture was heated at 110 °C under N_2 condition for 9 h until **K** had been completely consumed as determined by TLC. The reaction mixture was cooled to room temperature and the solvent was removed under reduced pressure to get

the crude product, which was purified by flash column chromatography on silica gel, eluted by petroleum ether/DCM to afford the pure product **L** as a white solid (36.2 mg, 86% yield). R_f = 0.50 (petroleum ether : ethyl acetate = 5 : 1); mp: 162-164 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 16.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.49-7.45 (m, 2H), 7.43-7.38 (m, 4H), 6.84 (s, 1H), 6.47 (d, *J* = 15.6 Hz, 1H), 4.28 (q, *J* = 7.2 Hz, 2H), 4.14 (t, *J* = 6.4 Hz, 2H), 3.13 (s, 3H), 3.02 (t, *J* = 6.4 Hz, 2H), 1.35 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 143.5, 133.9, 133.8, 130.6, 129.03, 128.97, 128.9, 128.8, 128.3, 127.5, 127.4, 121.5, 118.8, 111.9, 60.6, 44.0, 42.4, 29.7, 14.3; IR (KBr) ν 2918, 2364, 1713, 1268, 1135, 754, 561 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{24}H_{23}NNaO_4S$, 444.1240; found 444.1242. [12]

f)

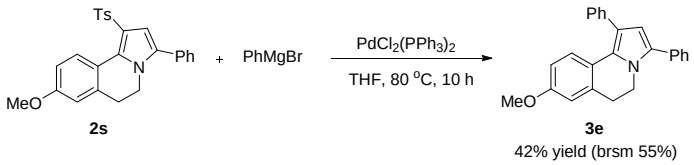


1-(methylsulfonyl)-3-phenyl-8-(phenylethynyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline (M)

K (48.0mg, 0.1mmol), phenylacetylene (33.0 μL, 0.3mmol), bis(triphenylphosphine)palladium(II) dichloride ($Pd(PPh_3)_2Cl_2$, 7.0 mg, 0.01 mmol), copper(I) bromide (CuBr, 0.7 mg, 0.005 mmol), diisopropylethylamine (DIPEA, 52.0 μL, 0.3 mmol), and DMF (1.0 mL) were added to a pressure tube. The reaction mixture was heated to 80 °C under N_2 condition for 6 h until **K** had been completely consumed as determined by TLC. The reaction mixture was cooled down to room temperature and then diluted with ethyl acetate (50 mL). The organic phase was washed with brine (4 × 10 mL) and dried with Na_2SO_4. The solvent was removed under reduced pressure to get the

crude product, which was purified by flash column chromatography on silica gel, eluted by petroleum ether/DCM to afford the product **M** as a white solid (38.0 mg, 90% yield). R_f = 0.50 (petroleum ether : ethyl acetate = 5 : 1); mp: 209-211 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 8.0 Hz, 1H), 7.55-7.53 (m, 3H), 7.48-7.35 (m, 9H), 6.83 (s, 1H), 4.12 (t, *J* = 6.4 Hz, 2H), 3.12 (s, 3H), 2.99 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.7, 133.3, 131.6, 131.0, 130.8, 130.6, 129.1, 129.0, 128.7, 128.5, 128.4, 128.2, 127.1, 126.9, 123.0, 122.8, 121.2, 111.7, 90.9, 89.0, 43.9, 42.3, 29.5; IR (KBr) ν 2361, 1485, 1300, 1135, 985, 767, 701, 550 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{27}H_{21}NNaO_2S$, 446.1185; found 446.1183.[12]

g)

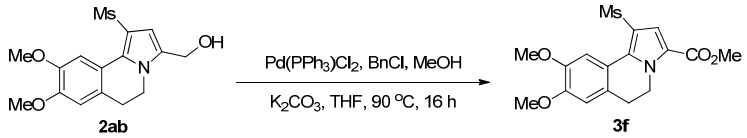


8-methoxy-1,3-diphenyl-5,6-dihydropyrrolo[2,1-a]isoquinoline (3e)

Under argon atmosphere, **2s** (43.0 mg 0.1mmol), $PdCl_2(PPh_3)_2$ (7.02mg, 10 mol%), dehydrated THF 1.0 mL were charged in a flask and cooled to 0 °C. Phenyl magnesium bromide (1M in THF, 0.4 mL, 4.0 equiv.) was added dropwise and stirred for 10 hours at 80 °C, water 2 mL were added and then filtered. The organic layer of the filtrate was dried over magnesium sulfate. Concentration and flash chromatography on a silica column (PE : EA = 100 : 1) afforded compound **3e** as yellow oil (14.7 mg, 42% yield). R_f = 0.50 (petroleum ether : ethyl acetate = 100 : 1); ^1H NMR (400 MHz, $CDCl_3$) δ 8.18-8.16 (m, 1H), 7.46-7.40 (m, 4H), 7.36-7.30 (m, 1H), 7.24-7.18 (m, 4H), 7.09-7.04 (m, 1H), 6.76-6.74 (m, 2H), 6.41 (s, 1H), 4.16 (t, *J* = 6.4 Hz, 2H), 3.78 (s, 3H), 2.98 (t, *J* = 6.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 140.0, 134.2, 133.4, 132.6, 132.0,

128.8, 128.6, 128.5, 127.1, 126.3, 125.7, 124.5, 122.2, 116.4, 113.4, 112.2, 103.7, 55.2, 42.3, 30.4; IR (KBr) ν 2830, 2375, 2333, 1772, 1608, 1580, 1485, 1433, 1433, 1314, 1240, 1037, 813, 764, 694, 512 cm^{-1}; HRMS-(ESI) (*m/z*): $[M+Na]^+$ calcd for $C_{25}H_{21}NNaO$, 374.1515; found 374.1511.[13]

h)



Methyl 8,9-dimethoxy-1-(methylsulfonyl)-5,6-dihydropyrrolo[2,1-*a*] isoquinoiline-3-carboxylate (3f)

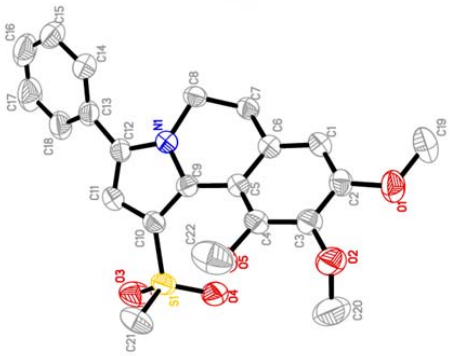
$PdCl_2(PPh_3)_2$ (17.5 mg, 0.025 mmol) and K_2CO_3 (139.0 mg, 1.0 mmol) were placed in a Shlenck tube, which was filled with argon by using standard Schlenk techniques. THF (2.0 mL), benzyl chloride (126.6 mg, 1.0 mmol), alcohol **2ab** (0.50 mmol) and methanol (5.0 mmol) were consequently added to the reaction tube. The reaction mixture was stirred at 90 °C for 16 h. Then the resulting mixture was quenched with saturated NH_4Cl solution and suspension was extracted by ethyl acetate (3 × 5 mL). The organic layers were combined, washed with brine and dried over sodium sulfate. The pure product **3f** (141 mg, 85%) was obtained by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 2 : 1); R_f= 0.60 (petroleum ether : ethyl acetate = 1 : 1); ^1H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.47 (s, 1H), 6.78 (s, 1H), 4.64 (t, *J* = 6.8 Hz, 2H), 3.92 (appeared as doublet as O-*CH*$_3$ protons overlapped, *J* = 3.6 Hz, 6H), 3.85 (s, 3H), 3.04 (s, 3H), 2.99 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 149.8, 148.4, 134.6, 127.2, 120.6, 120.2, 119.8, 118.5, 110.8, 56.2, 55.9, 51.6, 43.8, 42.6, 28.5; IR

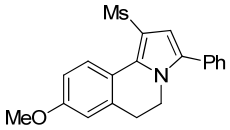
(KBr) ν 3075, 2074, 1636, 1132, 621, 477 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{17}H_{19}NNaO_6S$, 388.0825; found 388.0822.[14]

Crystal structures

General procedure for preparation of the crystals: The product (20 mg) was dissolved in DCM and filtered through a pad of filter paper. The filtrate was then transferred into several test-tubes by different volumes. Then to these solutions was added hexane in dropwise. These samples were allowed to be evaporated slowly at room temperature, which would eventually give colorless crystals on the surface of the tubes.

Crystal data of product 2a





2a

Bond precision: C-C = 0.0020 A Wavelength=0.71073

Cell: a=8.2877(17) b=14.334(3) c=14.903(3)

alpha=90 beta=103.09(3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	1724.4(6)	1724.4(6)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C20 H19 N O3 S	?

Sum formula	C20 H19 N O3 S	C20 H19 N O3 S
Mr	353.42	353.42
Dx,g cm-3	1.361	1.361
Z	4	4
Mu (mm-1)	0.207	0.207
F000	744.0	744.0
F000’	744.82	
h,k,lmax	10,18,19	10,18,19
Nref	3953	3939
Tmin,Tmax	0.959, 0.959	
Tmin’	0.959	

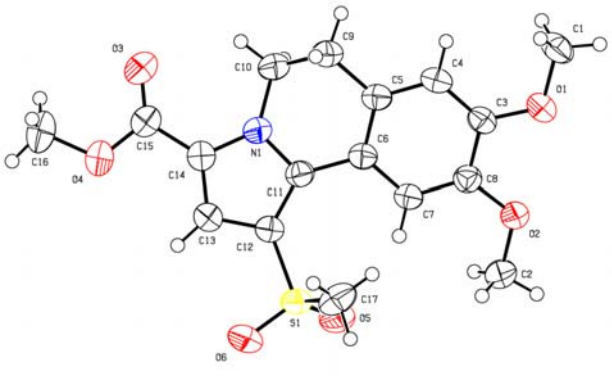
Correction method = Not given

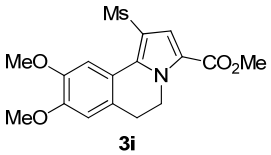
Data completeness = 0.996 Theta(max) = 27.480

R(reflections) = 0.0387(3200) wR2(reflections) = 0.1131(3939)

S = 1.060 Npar = 228

Crystal data of product 3i





3i

Identification code	d
Empirical formula	C_{17} H_{19} N O_6 S
Formula weight	365.39
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	?, ? P21/c
Unit cell dimensions	a = 7.5531(15) **Å** alpha = 90 **°**.
	b = 28.802(6) **Å** beta = 113.57(3) **°**.
	c = 8.5314(17) **Å** gamma = 90 **°**.
Volume	1701.2(6) $Å^3$
Z, Calculated density	4, 1.427 Mg/m^3
Absorption coefficient	0.224 mm^{-1}
F(000)	768
Crystal size	? x ? x ? mm
Theta range for data collection	2.70 to 27.48 **°**.
Limiting indices	-9<=h<=9, -37<=k<=37, -10<=l<=11

Reflections collected / unique	13063 / 3843 [R(int) = 0.0277]
Completeness to theta =	27.48 98.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3843 / 0 / 230
Goodness-of-fit on F^2	1.084
Final R indices [I>2sigma(I)]	R1 = 0.0468, wR2 = 0.1165
R indices (all data)	R1 = 0.0573, wR2 = 0.1232
Largest diff. peak and hole	0.219 and -0.289 $e.A^{-3}$

Reference

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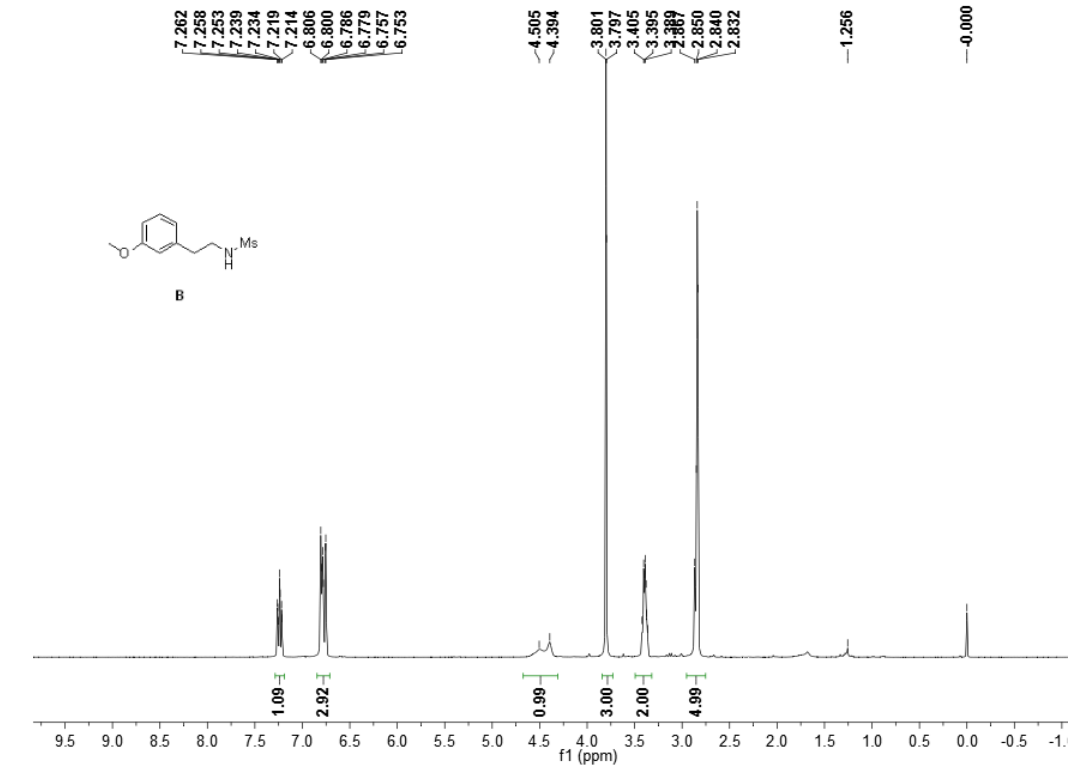
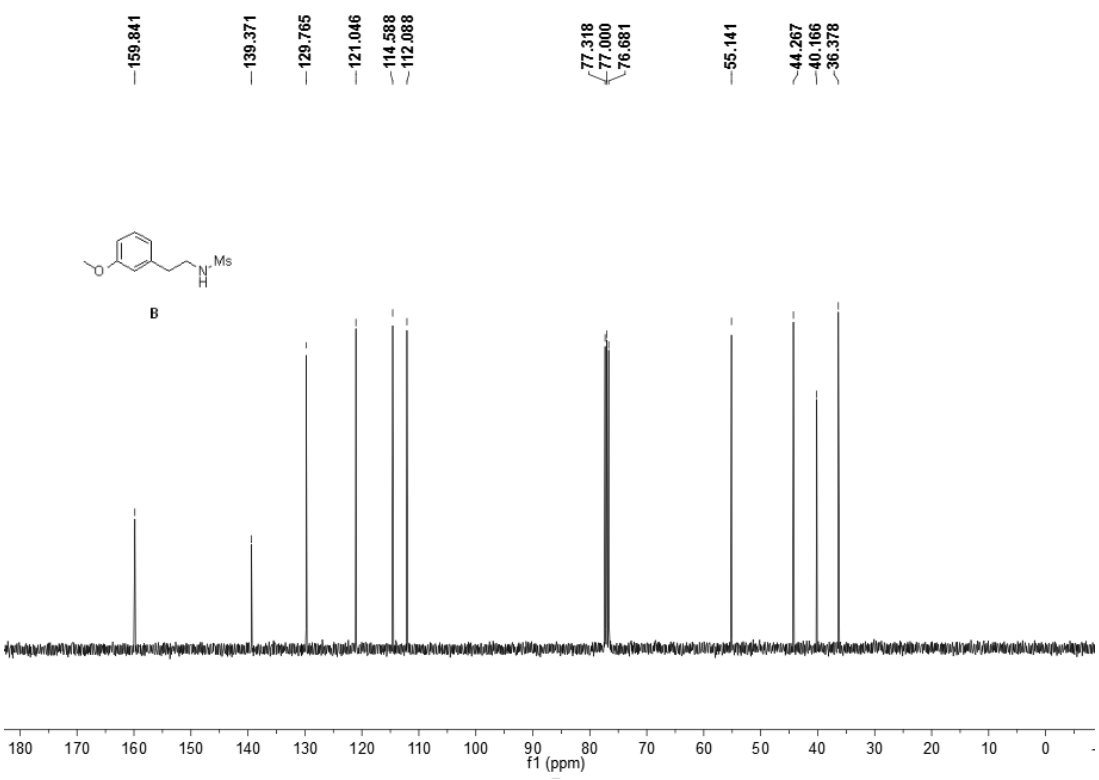
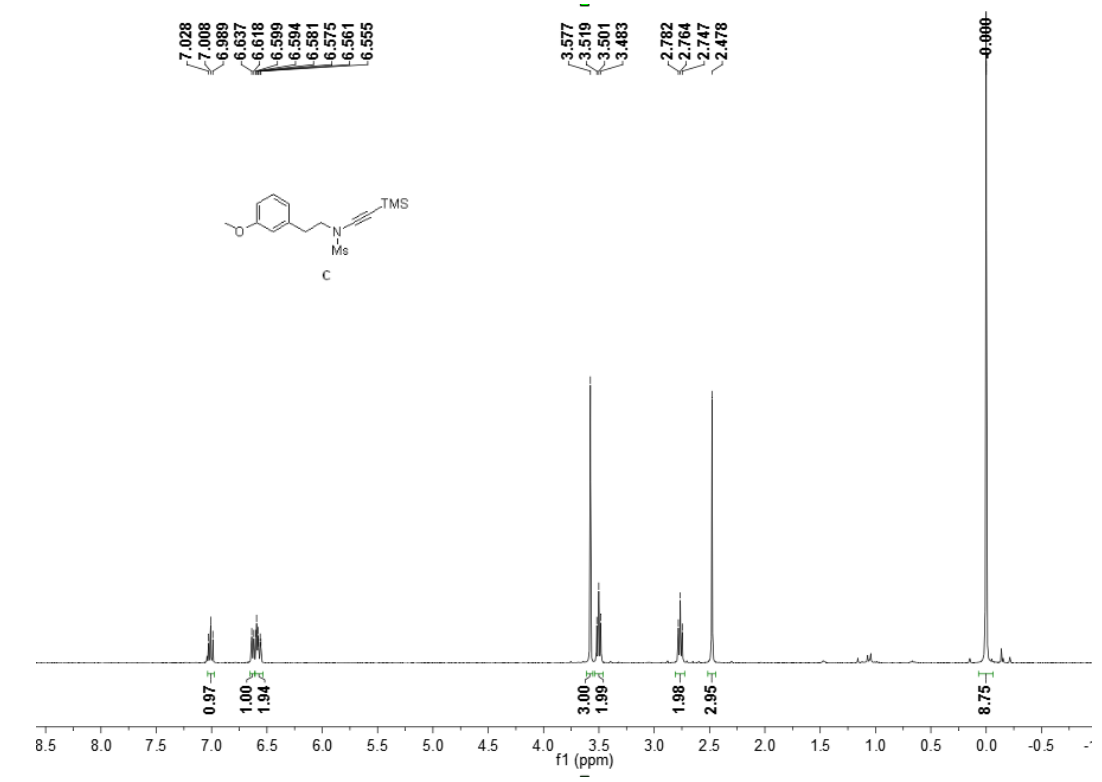
Copy of ^{1}H NMR and ^{13}C NMR spectra



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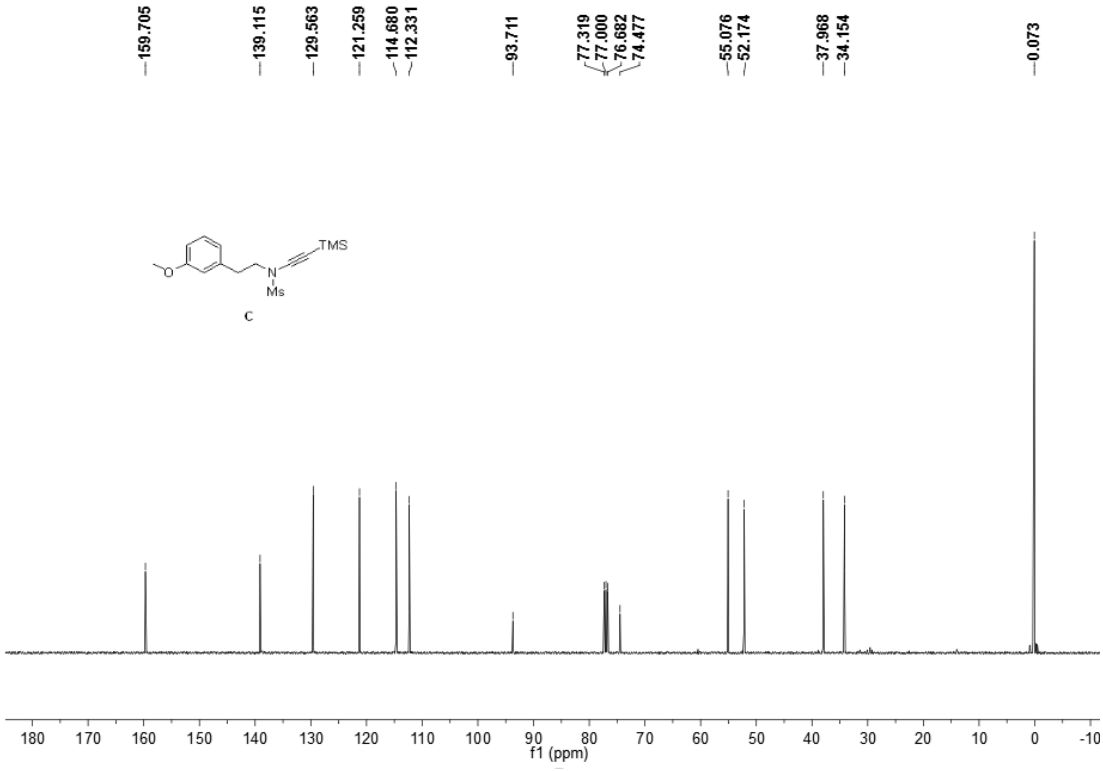
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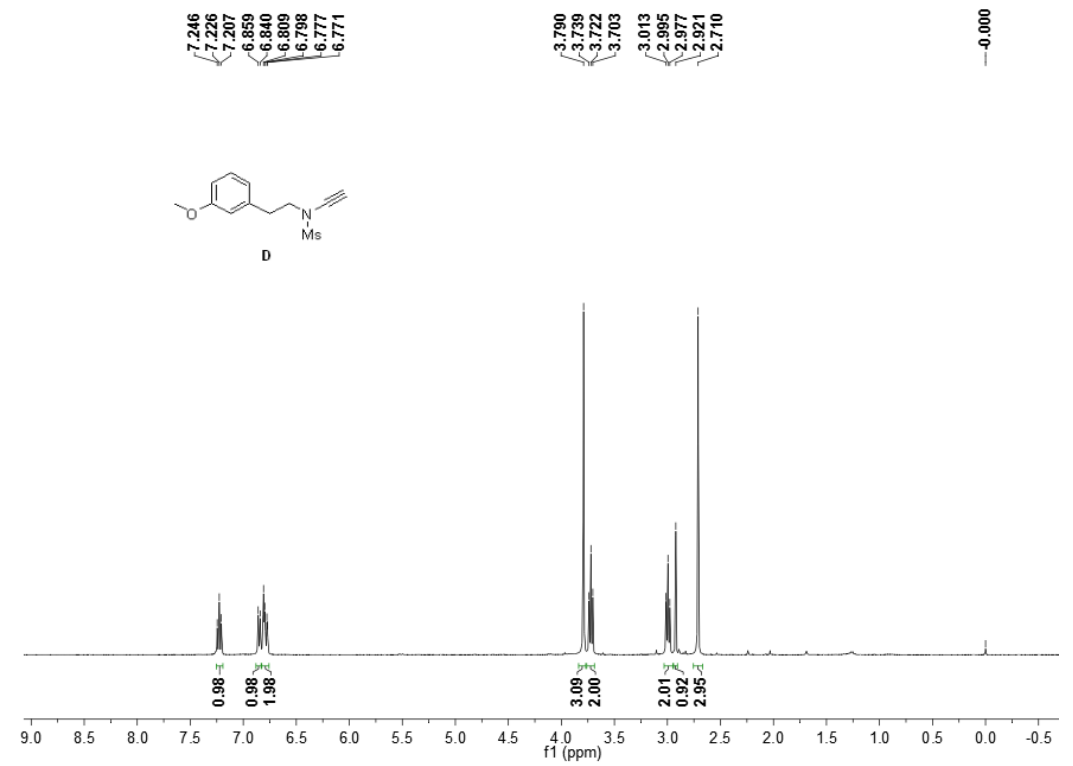
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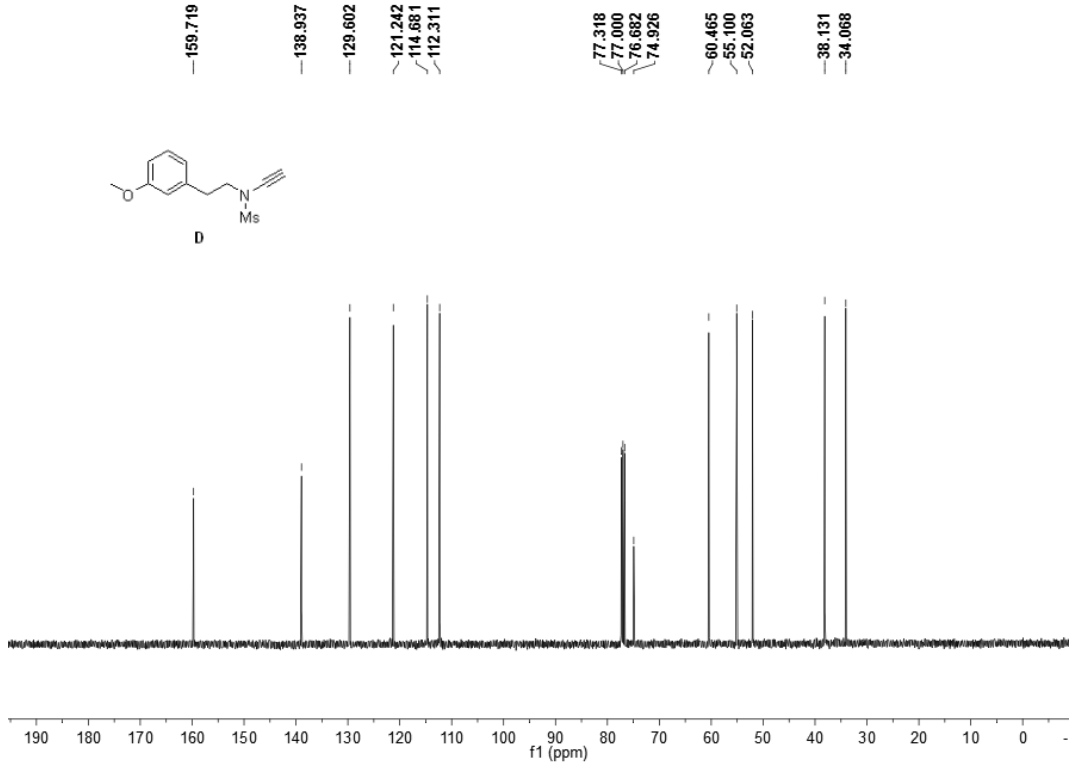
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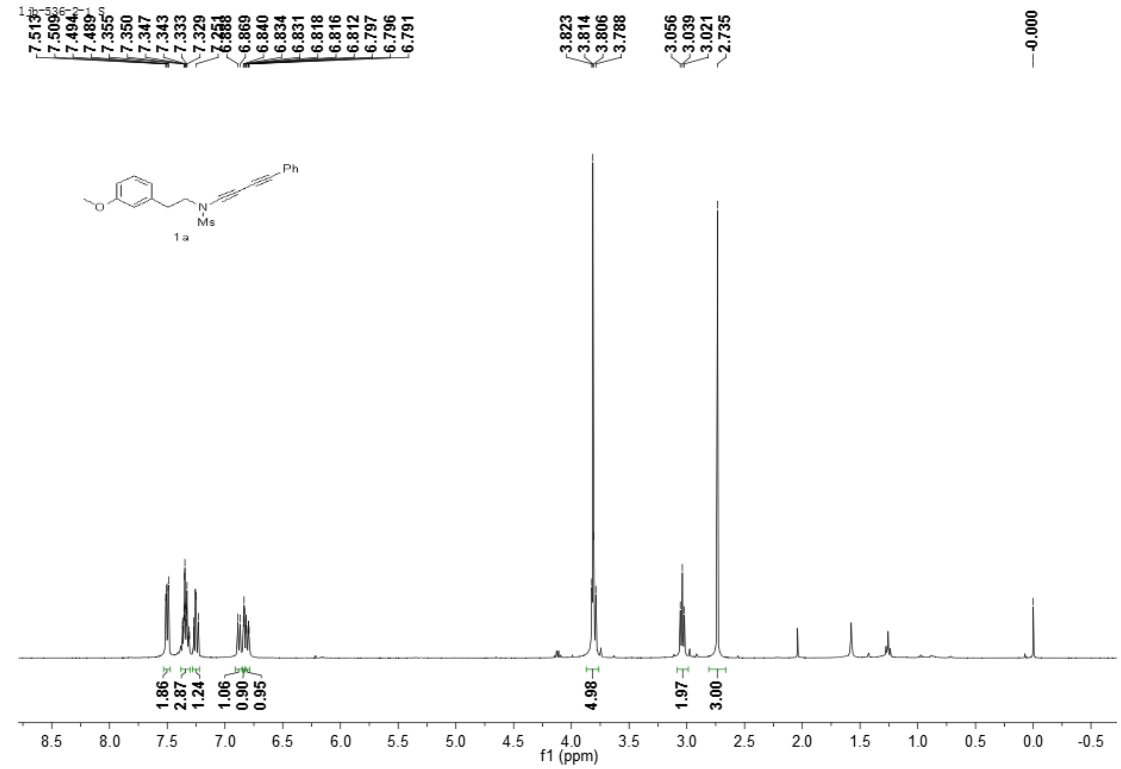
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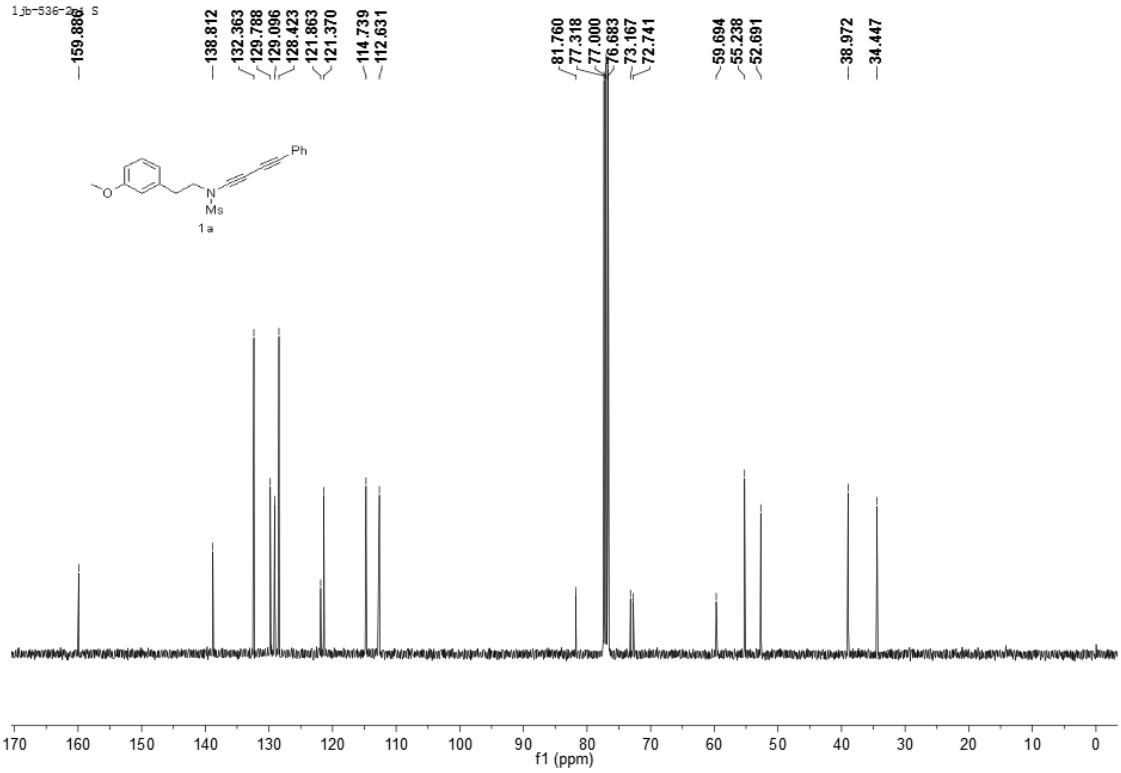
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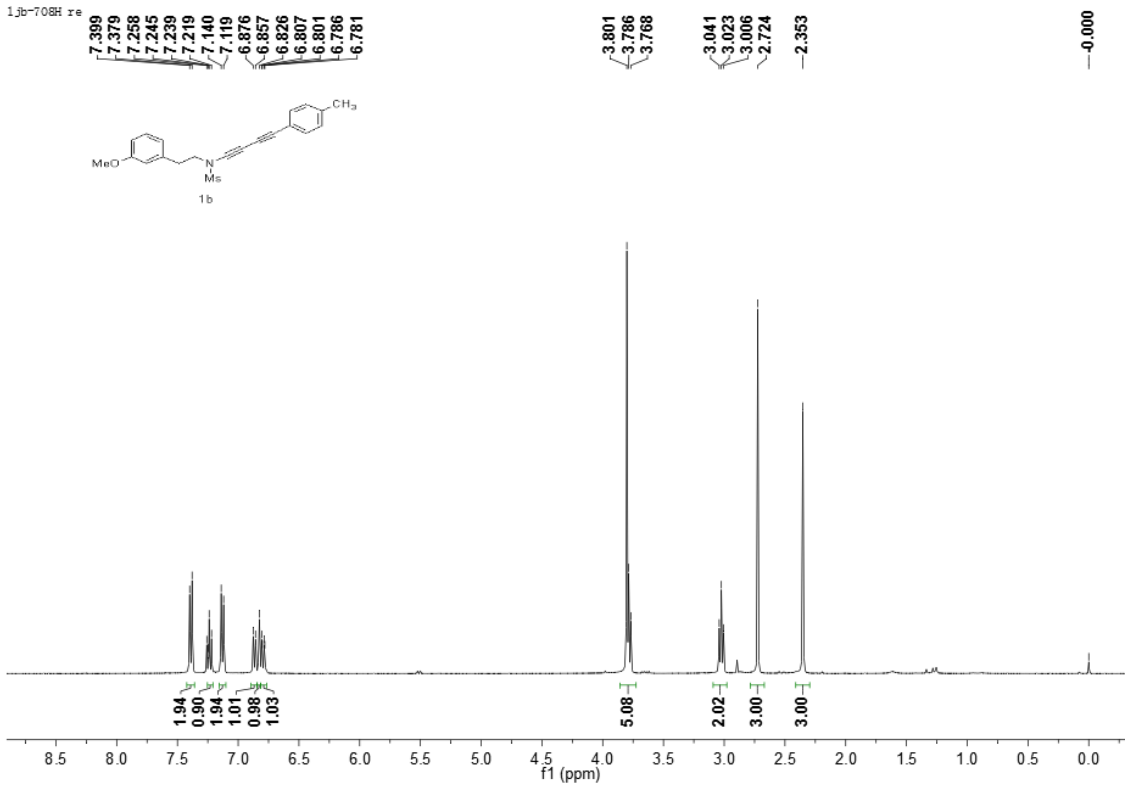
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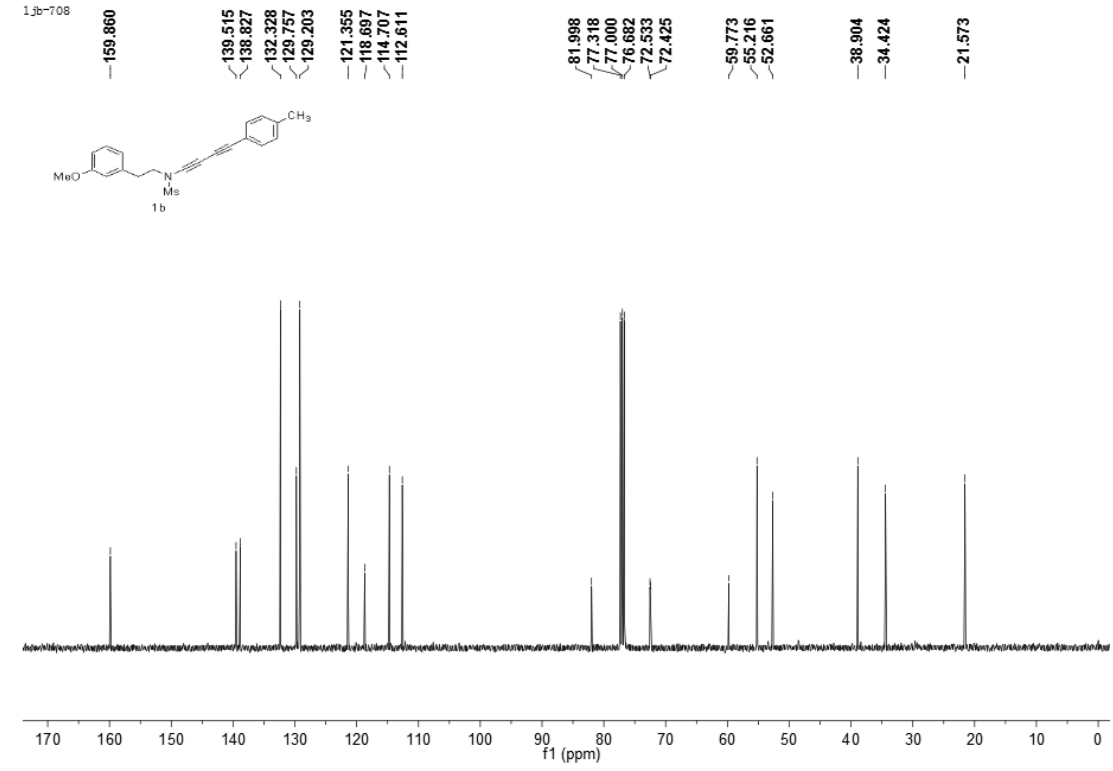
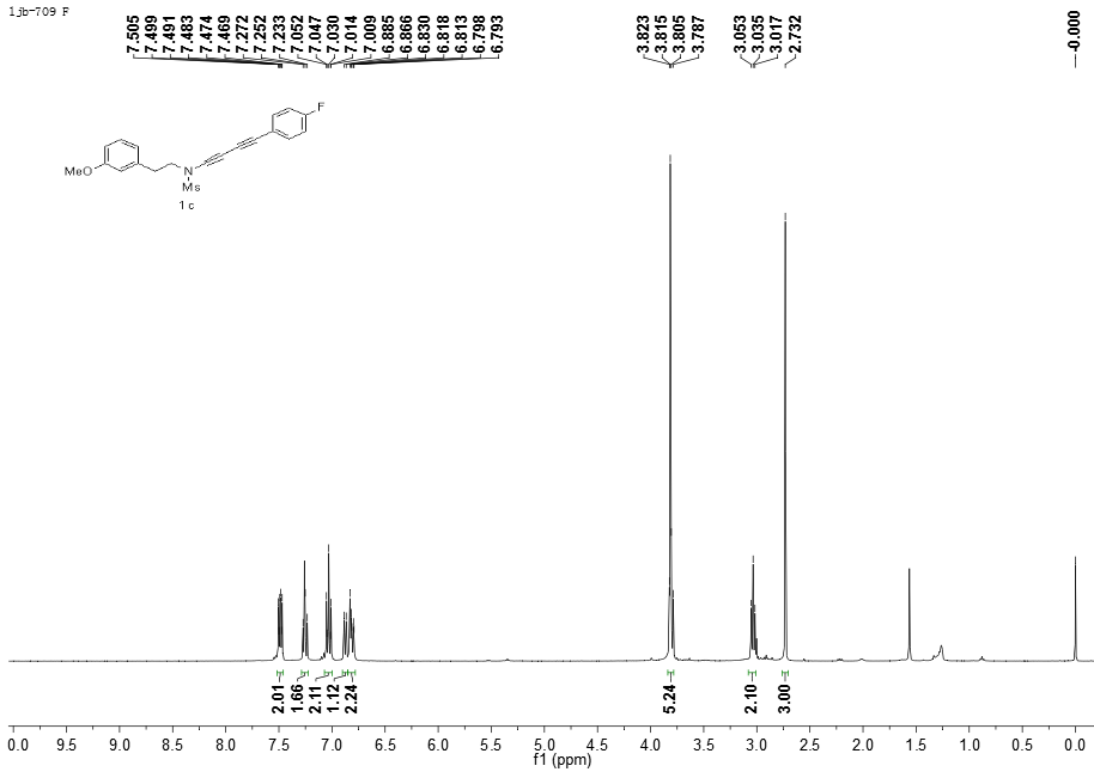
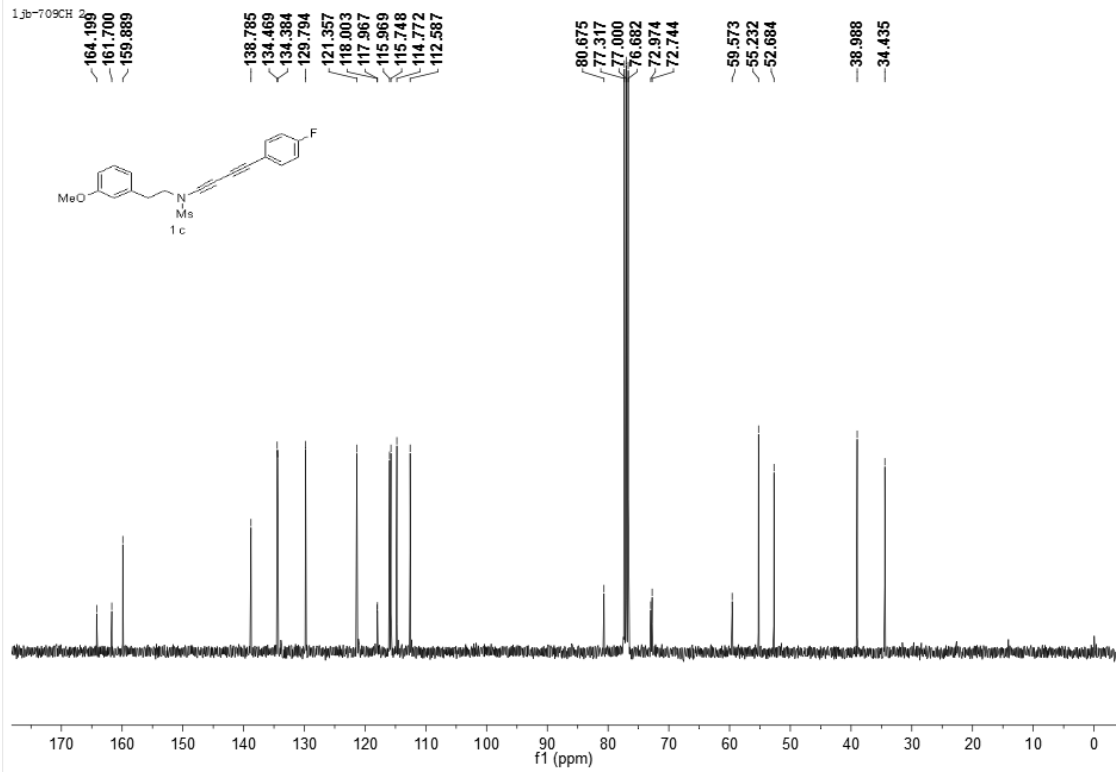
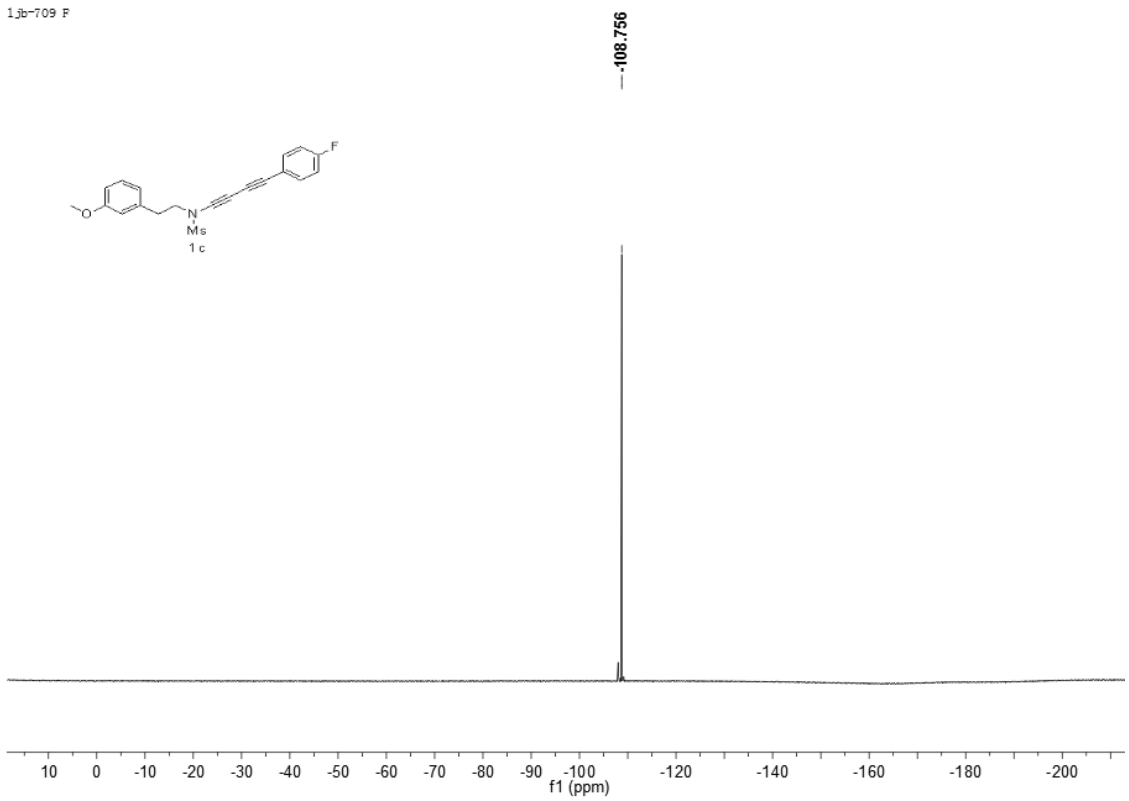
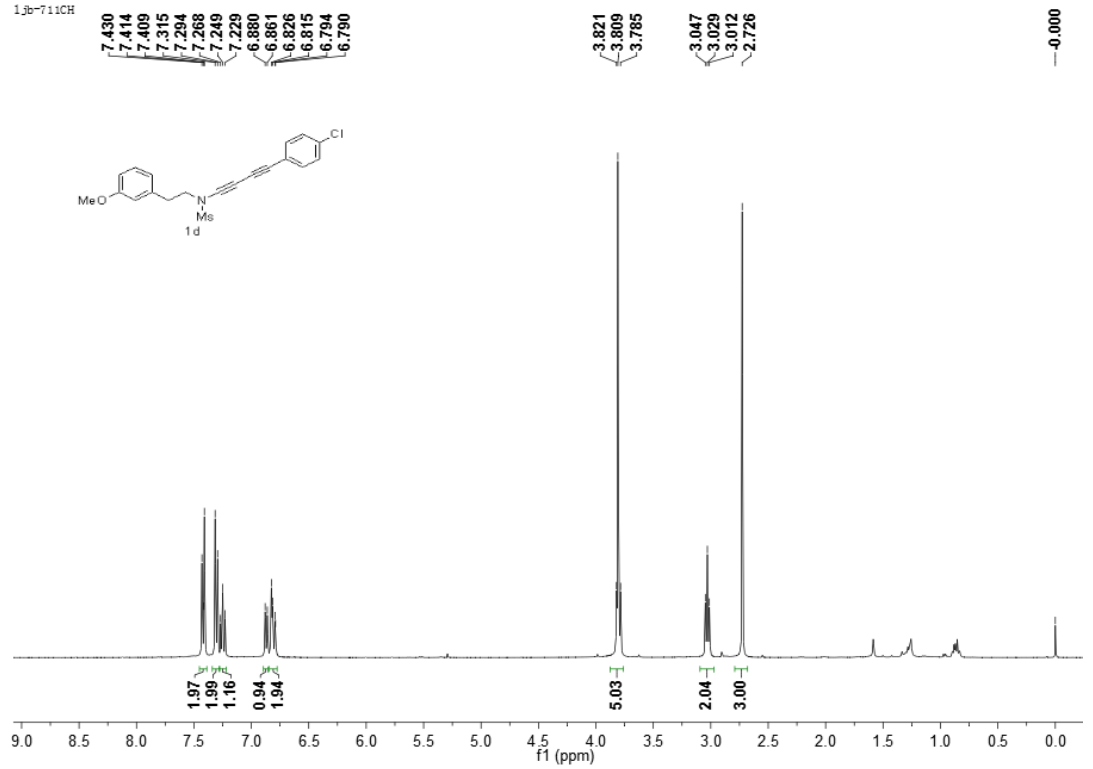
MeO
N
Ms
CH3
1b
1.94
0.90
1.94
1.01
0.98
1.03
5.08
2.02
3.00
3.00
f1 (ppm)

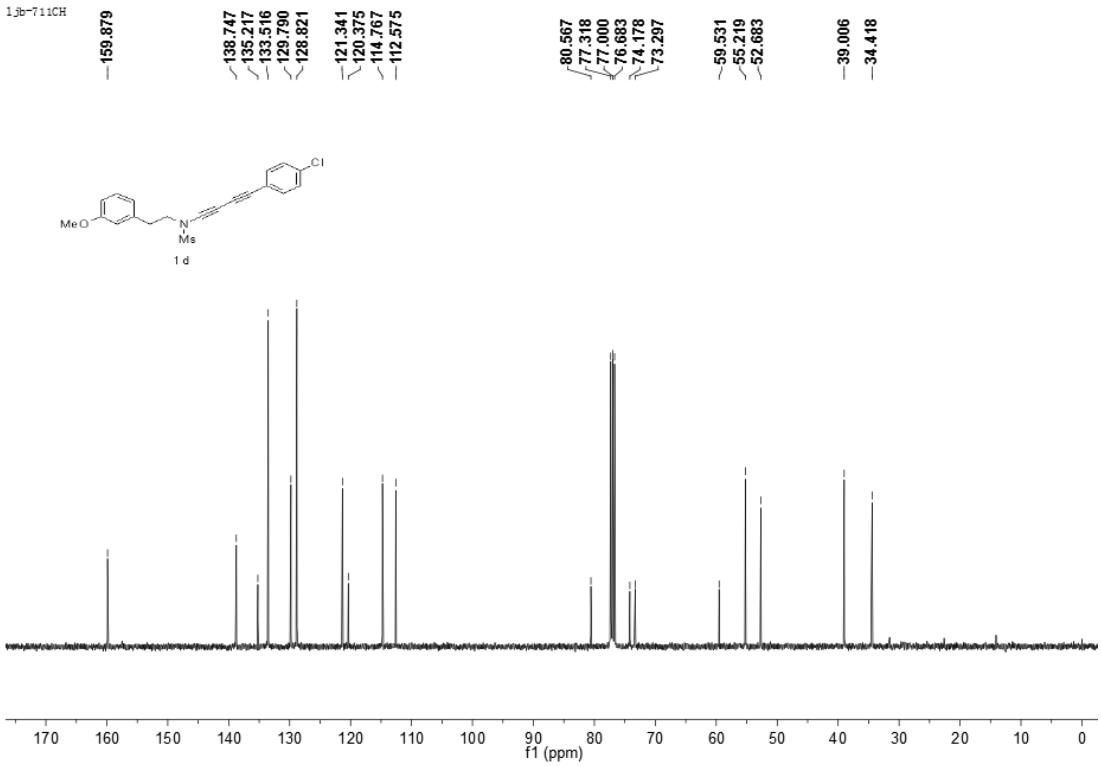

1jb-708
159.860
139.515
138.827
132.328
129.757
129.203
121.355
118.697
114.707
112.611
81.998
77.318
77.000
76.682
72.533
72.425
59.773
55.216
52.661
38.904
34.424
21.573
MeO
N
Ms
CH3
1b
f1 (ppm)

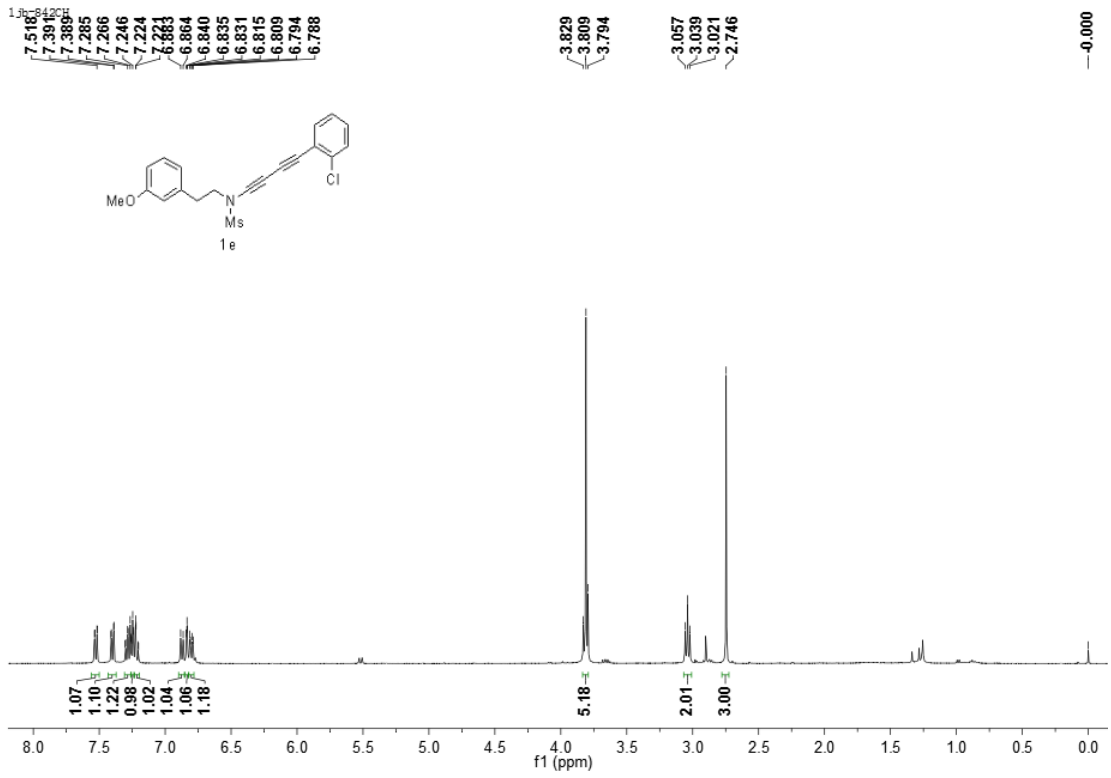

1jb-709 F
7.505
7.499
7.491
7.483
7.474
7.469
7.272
7.252
7.233
7.052
7.047
7.030
7.014
7.009
6.885
6.866
6.830
6.818
6.813
6.798
6.793
3.823
3.815
3.805
3.787
3.053
3.035
3.017
2.732
0.000
MeO
N
Ms
F
1c
2.01
1.66
2.11
1.12
2.24
5.24
2.10
3.00
f1 (ppm)

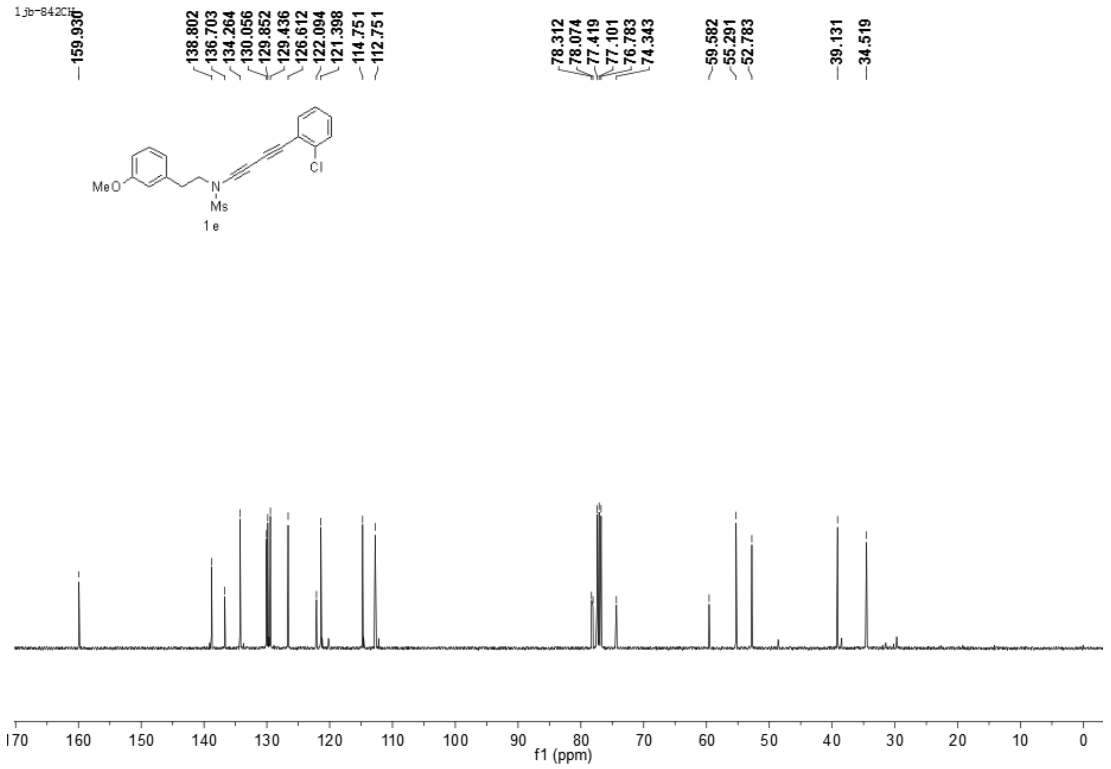

1jb-709CH 2
164.199
161.700
159.889
138.785
134.469
134.384
129.794
121.357
118.003
117.967
115.969
115.748
114.772
112.587
80.675
77.317
77.000
76.682
72.974
72.744
59.573
55.232
52.684
38.988
34.435
MeO
N
Ms
F
1c
f1 (ppm)

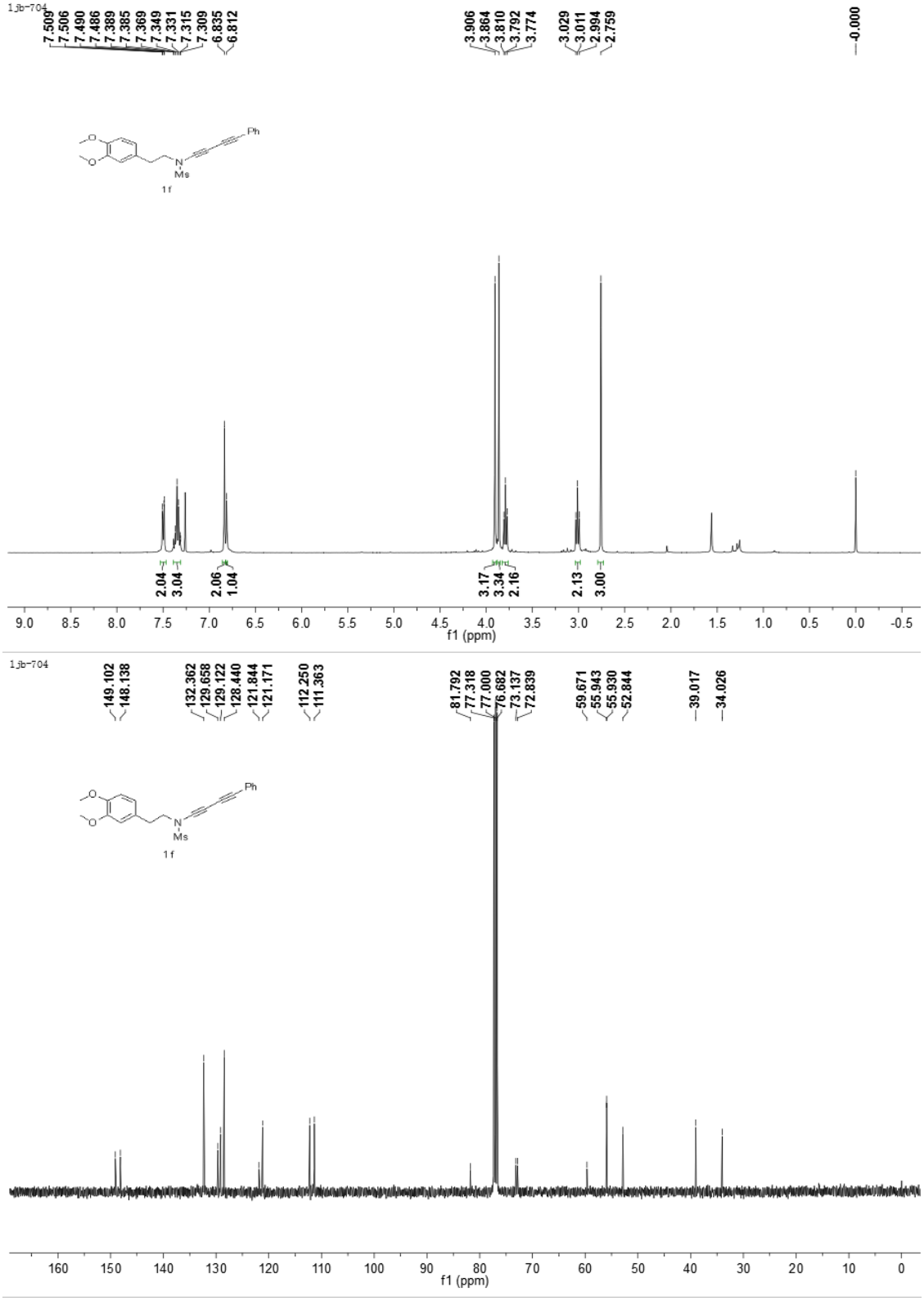

1jb-709 F
-108.756
F
O
N
Ms
1 c
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

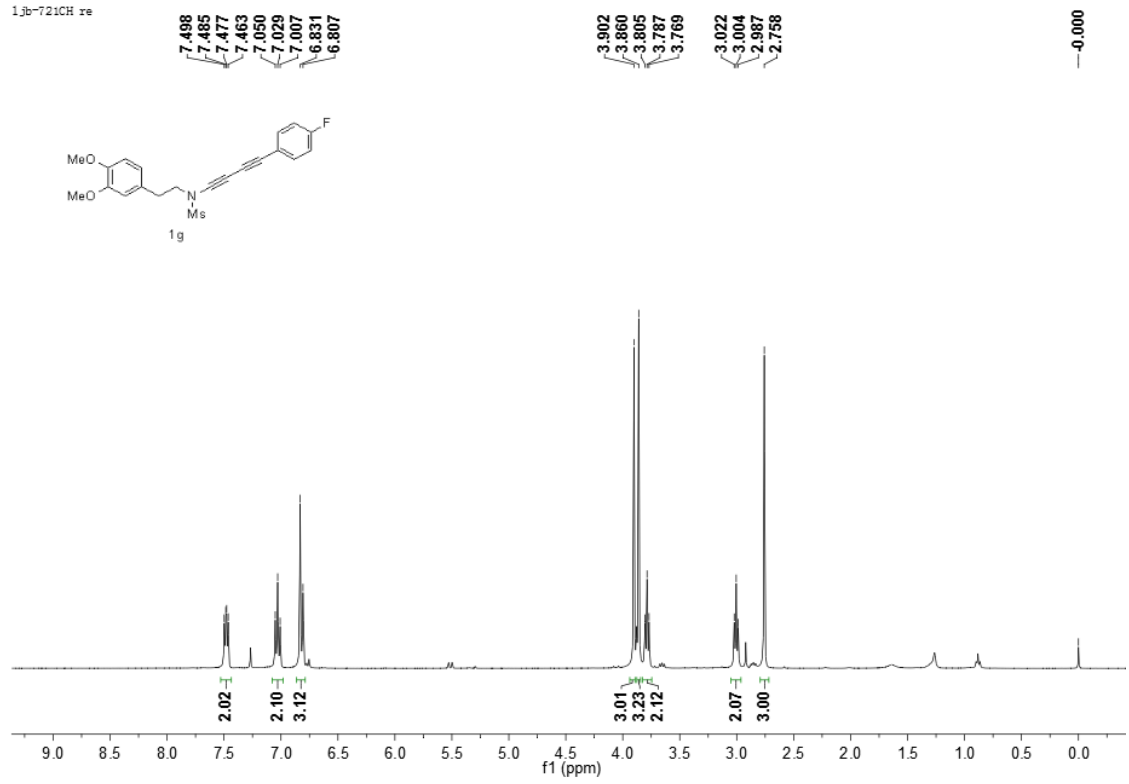

ljb-711CH
7.430
7.414
7.409
7.315
7.294
7.268
7.249
7.229
6.880
6.861
6.826
6.815
6.794
6.790
3.821
3.809
3.785
3.047
3.029
3.012
2.726
0.000
Cl
MeO
N
Ms
1d
1.97
1.99
1.16
0.94
1.94
5.03
2.04
3.00
f1 (ppm)

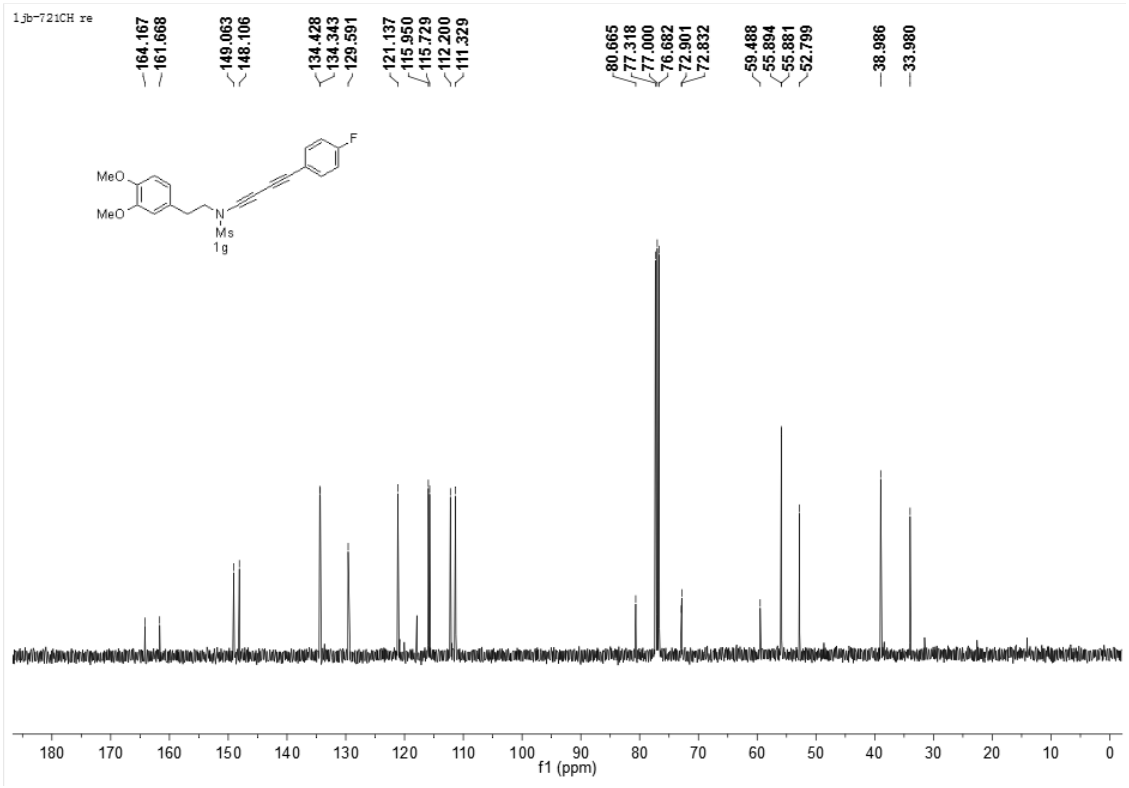

ljb-711CH
159.879
138.747
135.217
133.516
129.790
128.821
121.341
120.375
114.767
112.575
80.567
77.318
77.000
76.683
74.178
73.297
59.531
55.219
52.683
39.006
34.418
Cl
MeO
N
Ms
1d
f1 (ppm)

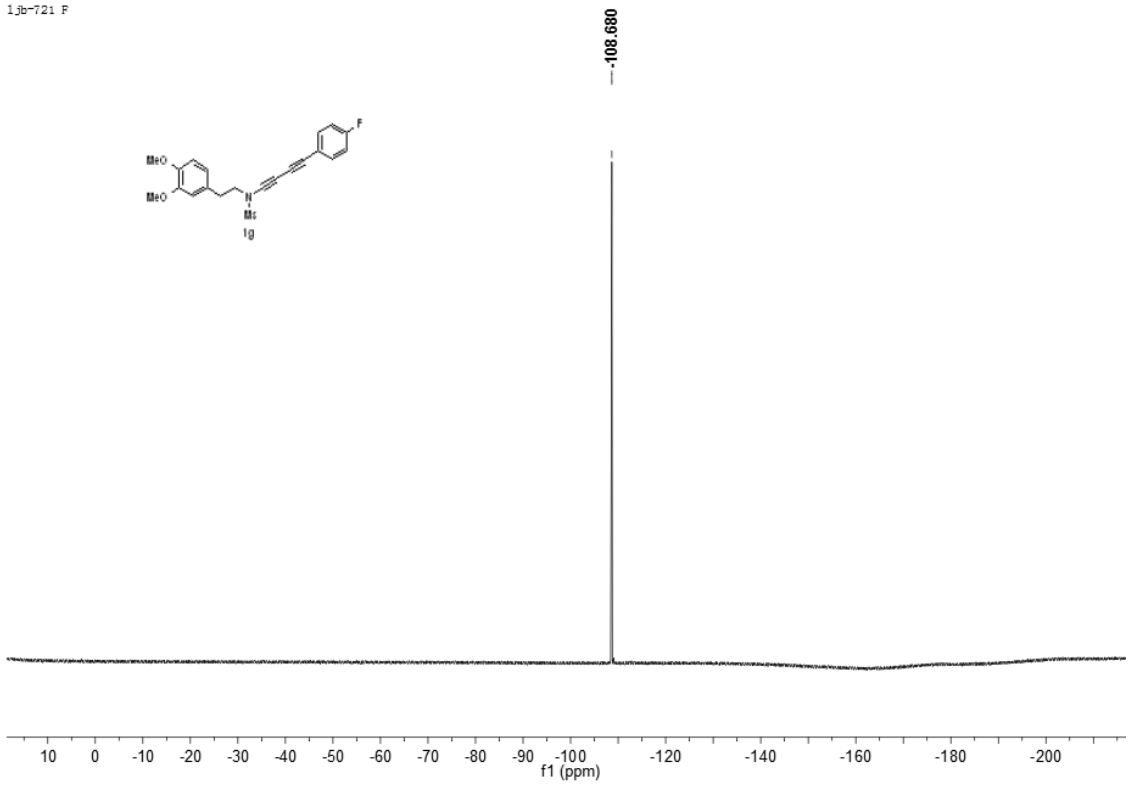

7.518
7.391
7.389
7.285
7.266
7.246
7.224
6.864
6.840
6.835
6.831
6.815
6.809
6.794
6.788
3.829
3.809
3.794
3.057
3.039
3.021
2.746
0.000
MeO
N
Ms
Cl
1e
1.07
1.10
1.22
0.98
1.02
1.04
1.06
1.18
5.18
2.01
3.00
f1 (ppm)

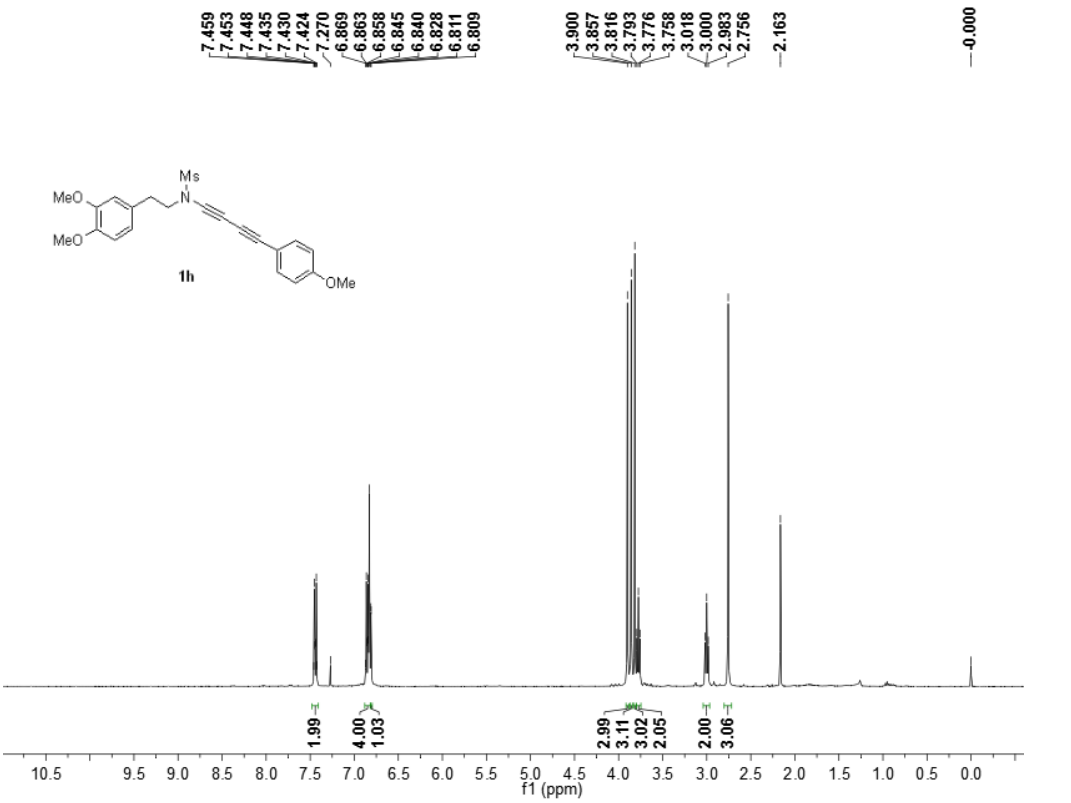

159.930
138.802
136.703
134.264
130.056
129.852
129.436
126.612
122.094
121.398
114.751
112.751
78.312
78.074
77.419
77.101
76.783
74.343
59.582
55.291
52.783
39.131
34.519
MeO
N
Ms
Cl
1e
f1 (ppm)


1jb-704
7.509
7.506
7.490
7.486
7.389
7.385
7.369
7.349
7.331
7.315
7.309
6.835
6.812
3.906
3.864
3.810
3.792
3.774
3.029
3.011
2.994
2.759
0.000
Ph
N
Ms
1f
2.04
3.04
2.06
1.04
3.17
3.34
2.16
2.13
3.00
f1 (ppm)
1jb-704
149.102
148.138
132.362
129.658
129.122
128.440
121.844
121.171
112.250
111.363
81.792
77.318
77.000
76.682
73.137
72.839
59.671
55.943
55.930
52.844
39.017
34.026
Ph
N
Ms
1f
f1 (ppm)


1jb-721CH re
7.498
7.485
7.477
7.463
7.050
7.029
7.007
6.831
6.807
3.902
3.860
3.805
3.787
3.769
3.022
3.004
2.987
2.758
0.000
MeO
MeO
N
Ms
F
1g
2.02
2.10
3.12
3.01
3.23
2.12
2.07
3.00
f1 (ppm)


1jb-721CH re
164.167
161.668
149.063
148.106
134.428
134.343
129.591
121.137
115.950
115.729
112.200
111.329
80.665
77.318
77.000
76.682
72.901
72.832
59.488
55.894
55.881
52.799
38.986
33.980
MeO
MeO
N
Ms
F
1g
f1 (ppm)


1jb-721 F
-108.680
MeO
MeO
N
Ms
1g
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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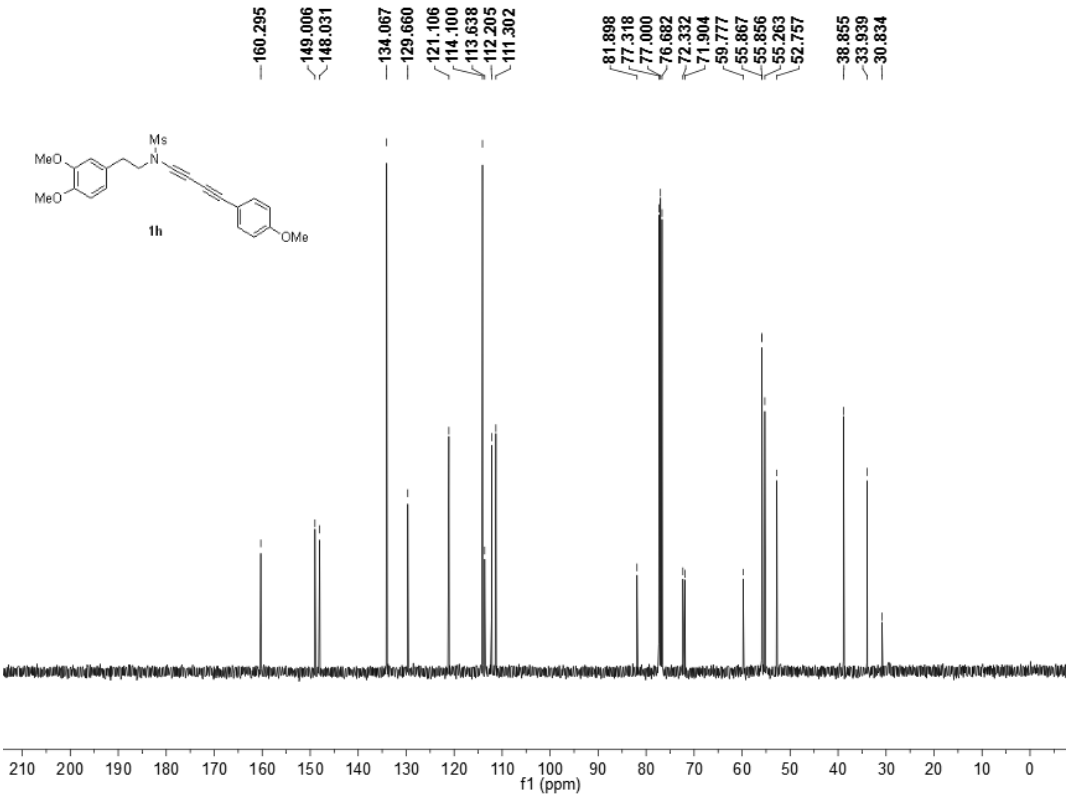
7.453
7.448
7.435
7.430
7.424
7.270
6.869
6.863
6.858
6.845
6.840
6.828
6.811
6.809
3.900
3.857
3.816
3.793
3.776
3.758
3.018
3.000
2.983
2.756
2.163
0.000
Ms
MeO
MeO
OMe
1h
1.99
4.00
1.03
2.99
3.11
3.02
2.05
2.00
3.06
f1 (ppm)


160.295
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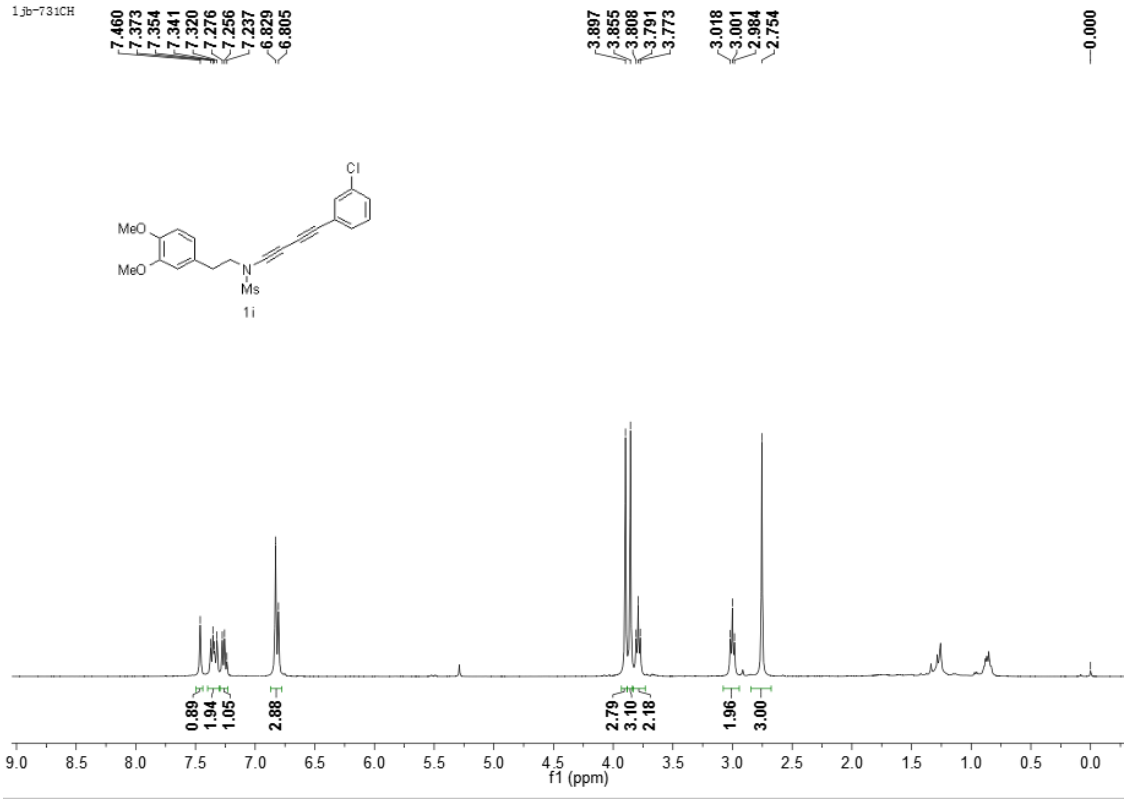
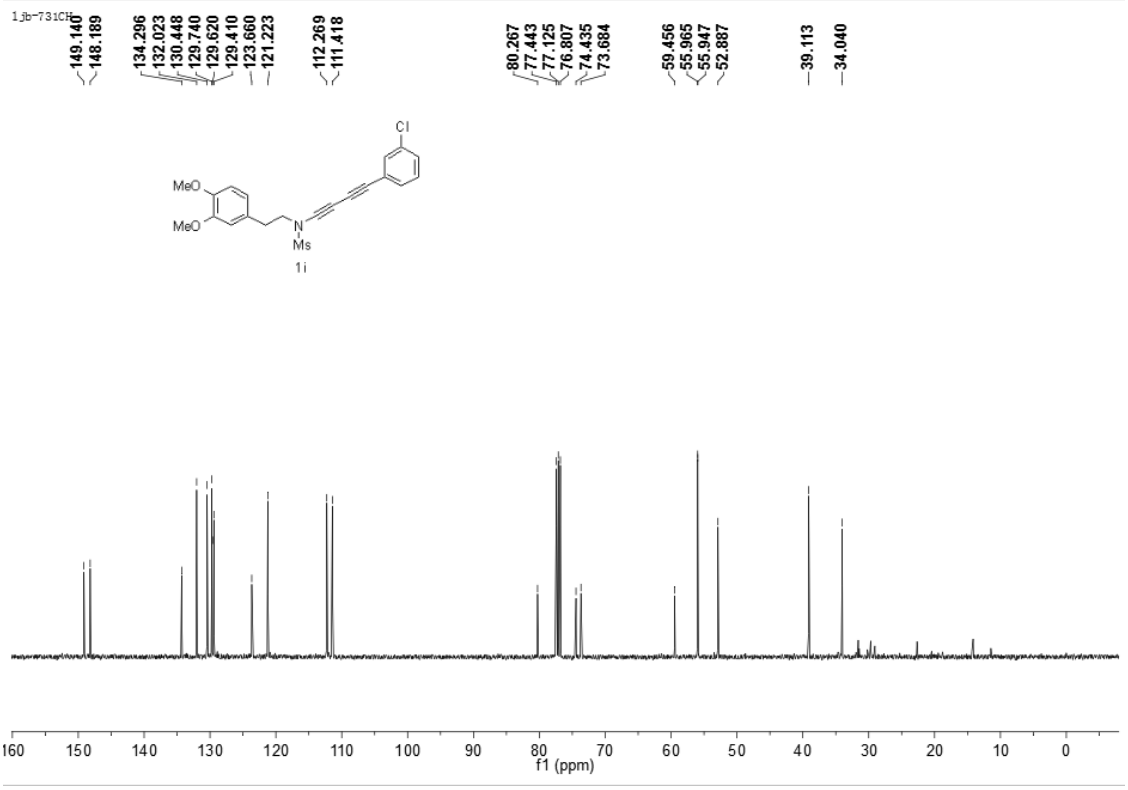
148.031
134.067
129.660
121.106
114.100
113.638
112.205
111.302
81.898
77.318
77.000
76.682
72.332
71.904
59.777
55.867
55.856
55.263
52.757
38.855
33.939
30.834
Ms
MeO
MeO
OMe
1h
f1 (ppm)


1jb-731CH
7.460
7.373
7.354
7.341
7.320
7.276
7.256
7.237
6.829
6.805
3.897
3.855
3.808
3.791
3.773
3.018
3.001
2.984
2.754
0.000
Cl
MeO
MeO
N
Ms
1i
0.89
1.94
1.05
2.88
2.79
3.10
2.18
1.96
3.00
f1 (ppm)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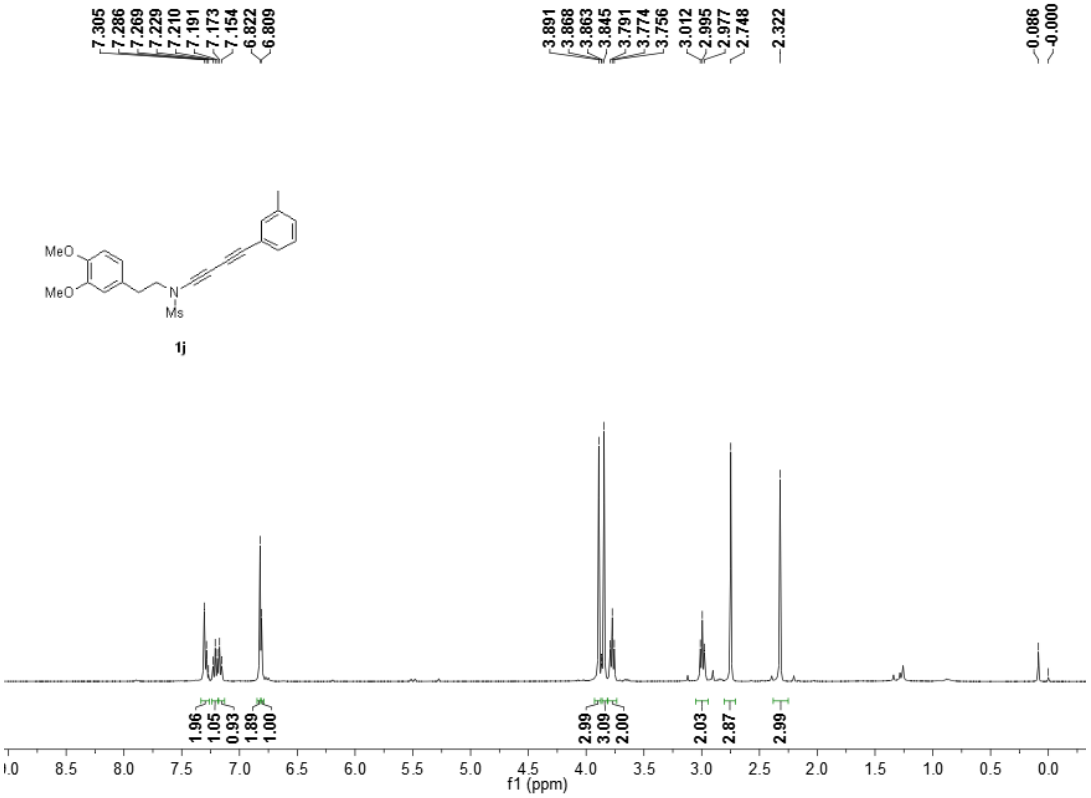
148.189
134.296
132.023
130.448
129.740
129.620
129.410
123.660
121.223
112.269
111.418
80.267
77.443
77.125
76.807
74.435
73.684
59.456
55.965
55.947
52.887
39.113
34.040
Cl
MeO
MeO
N
Ms
1i
f1 (ppm)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7.269
7.229
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7.191
7.173
7.154
6.822
6.809
3.891
3.868
3.863
3.845
3.791
3.774
3.756
3.012
2.995
2.977
2.748
2.322
0.086
-0.000
MeO
MeO
N
Ms
1j
1.96
1.05
0.93
1.89
1.00
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3.09
2.00
2.03
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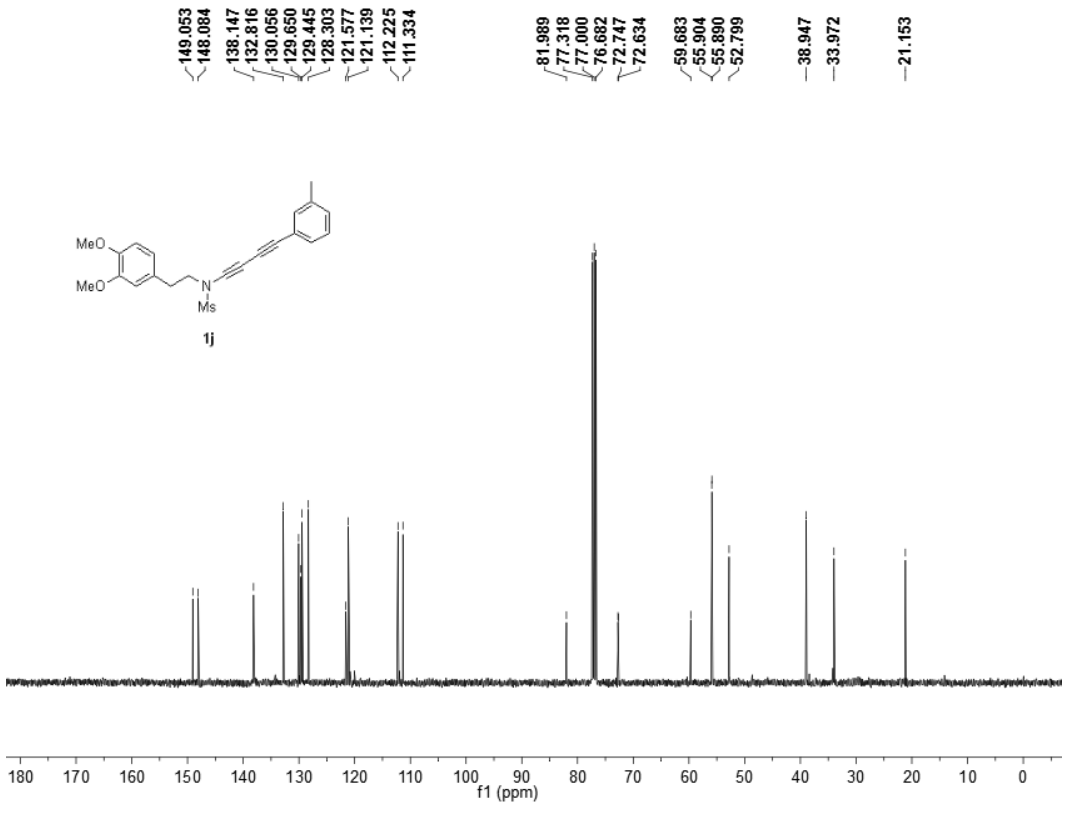
2.99
f1 (ppm)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129.445
128.303
121.577
121.139
112.225
111.334
81.989
77.318
77.000
76.682
72.747
72.634
59.683
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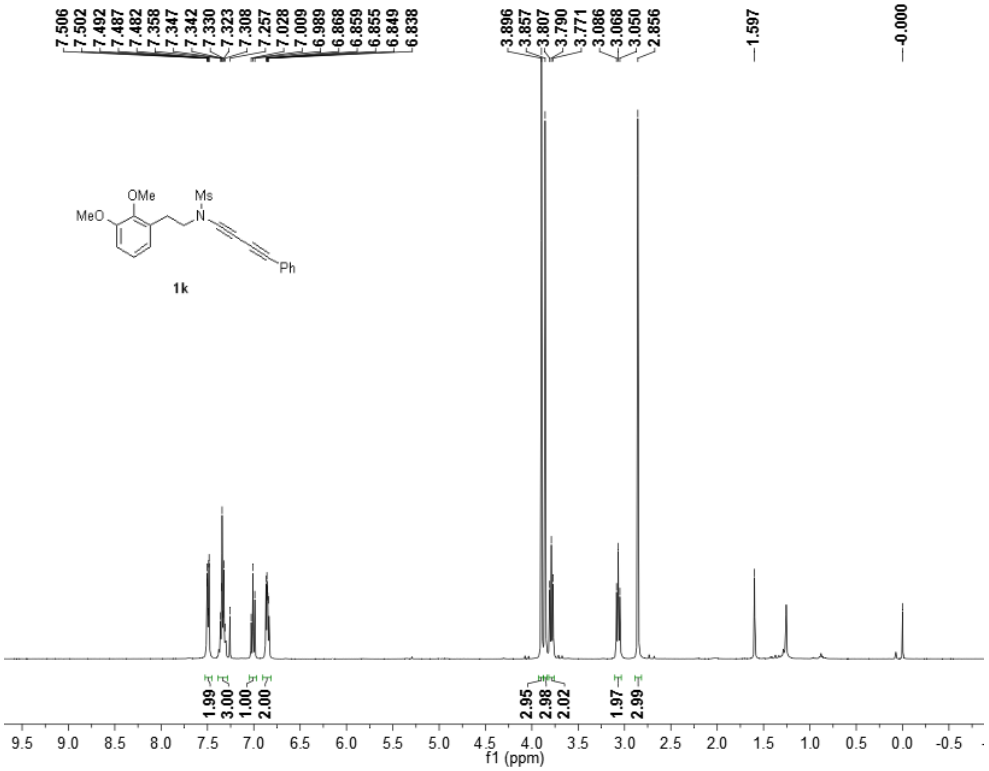
52.799
38.947
33.972
21.153
MeO
MeO
N
Ms
1j
f1 (ppm)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7.502
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7.487
7.482
7.358
7.347
7.342
7.330
7.323
7.308
7.257
7.028
7.009
6.989
6.868
6.859
6.855
6.849
6.838
3.896
3.857
3.807
3.790
3.771
3.086
3.068
3.050
2.856
1.597
0.000
OMe
Ms
MeO
N
Ph
1k
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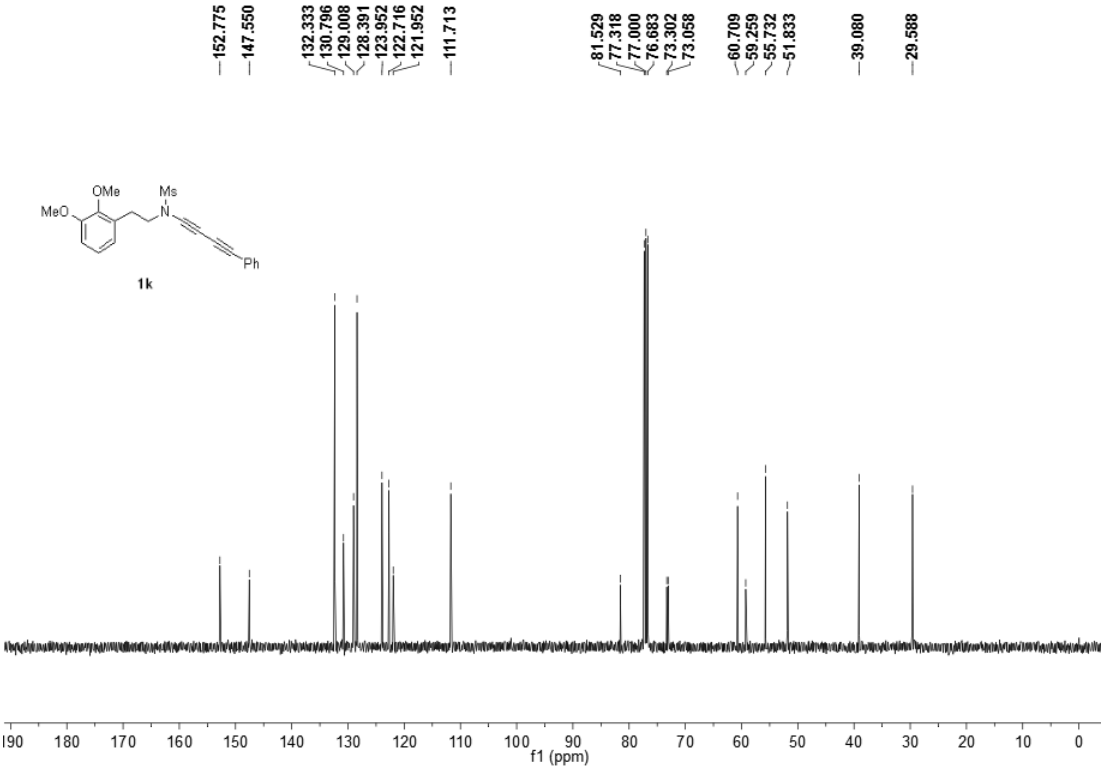
3.00
1.00
2.00
2.95
2.98
2.02
1.97
2.99
f1 (ppm)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132.333
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129.008
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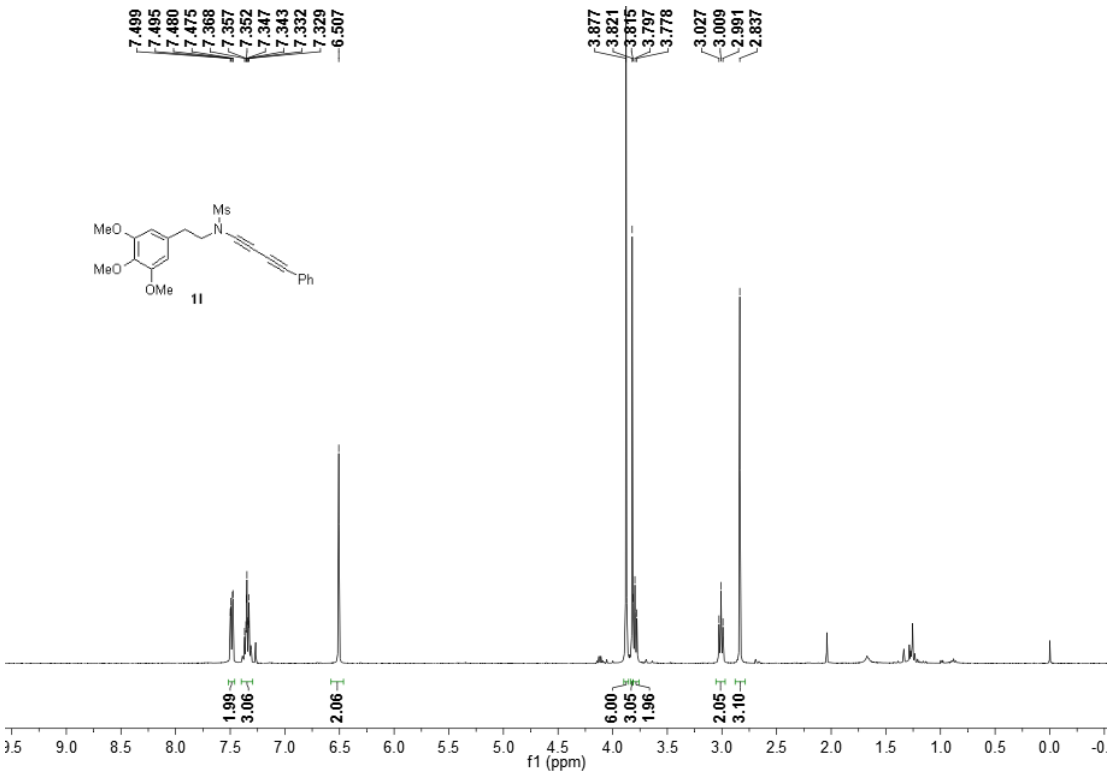
122.716
121.952
111.713
81.529
77.318
77.000
76.683
73.302
73.058
60.709
59.259
55.732
51.833
39.080
29.588
OMe
Ms
MeO
N
Ph
1k
f1 (ppm)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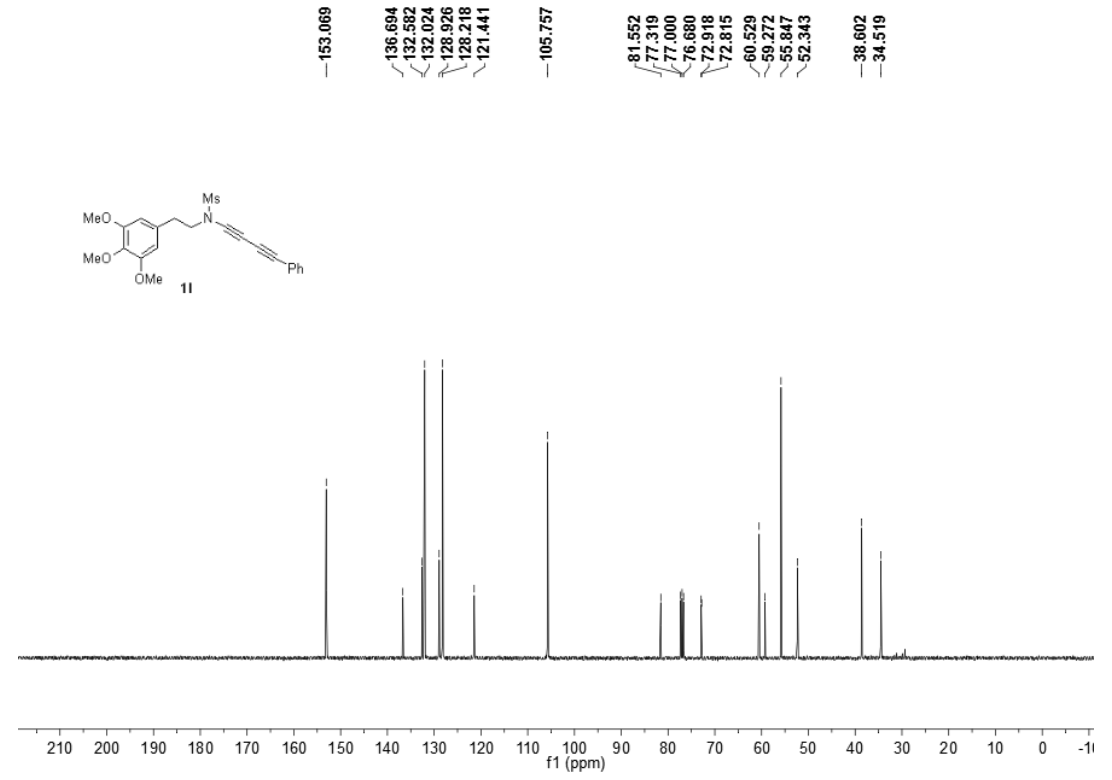
7.480
7.475
7.368
7.357
7.352
7.347
7.343
7.332
7.329
6.507
3.877
3.821
3.815
3.797
3.778
3.027
3.009
2.991
2.837
Ms
N
MeO
MeO
OMe
Ph
1l
1.99
3.06
2.06
6.00
3.05
1.96
2.05
3.10
f1 (ppm)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105.757
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77.319
77.000
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72.918
72.815
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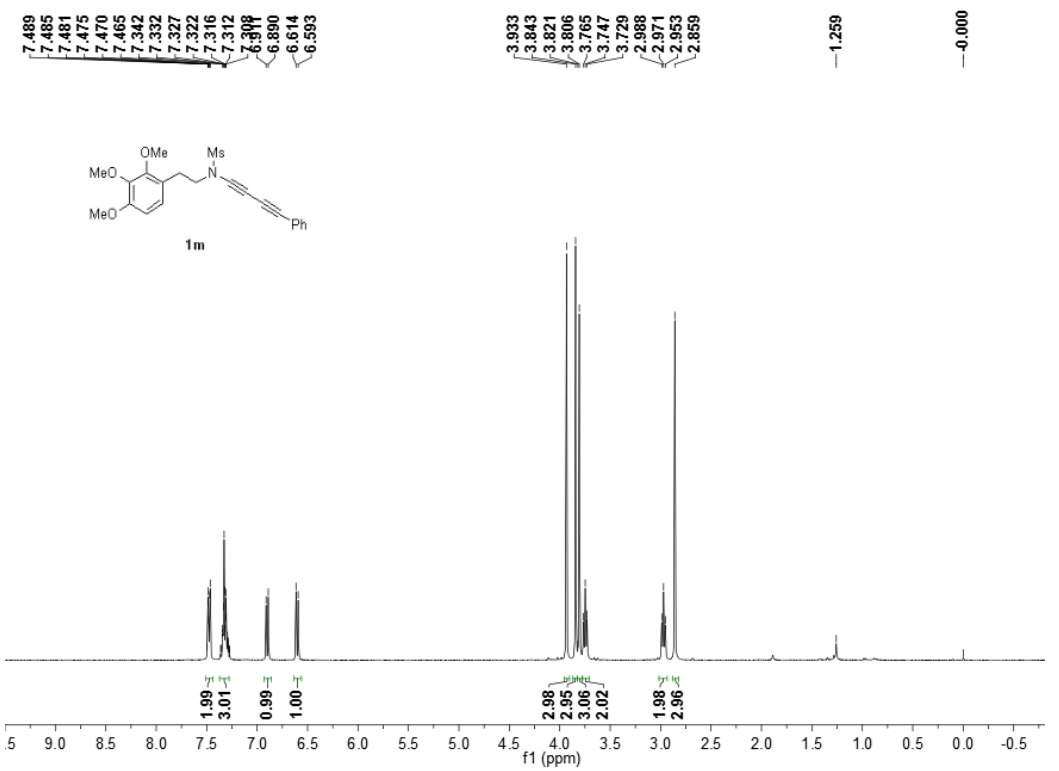
59.272
55.847
52.343
38.602
34.519
Ms
N
MeO
MeO
OMe
Ph
1l
f1 (ppm)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7.465
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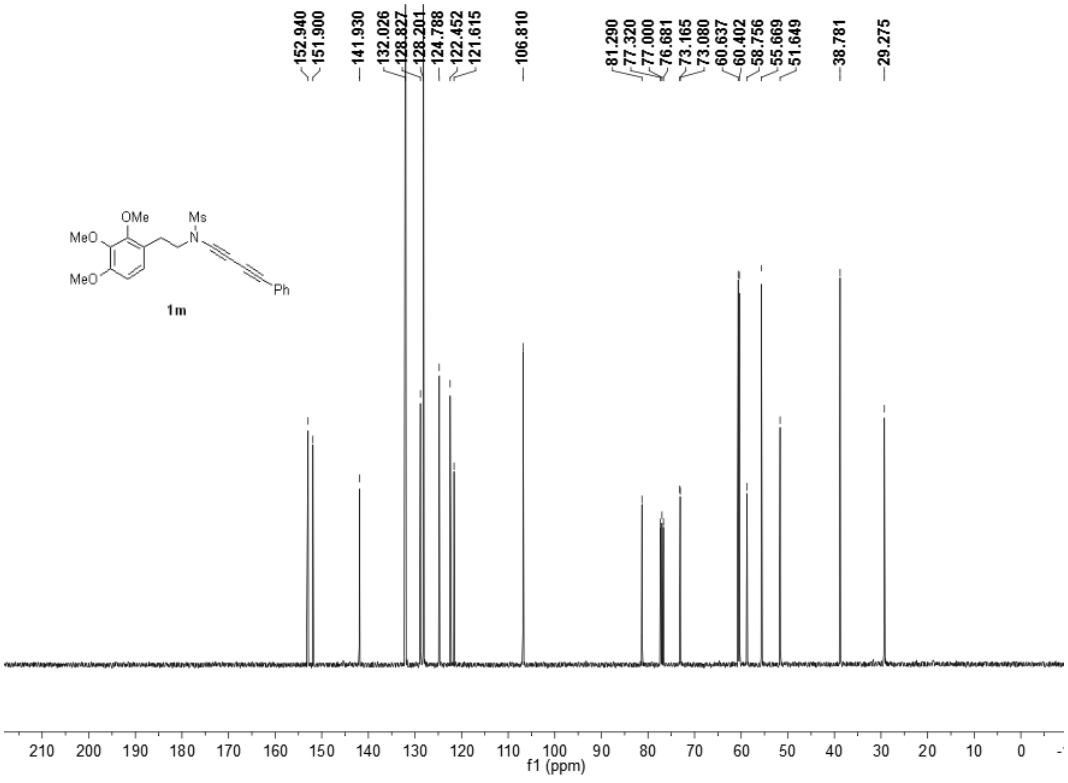
7.332
7.327
7.322
7.316
7.312
6.890
6.614
6.593
3.933
3.843
3.821
3.806
3.765
3.747
3.729
2.988
2.971
2.953
2.859
1.259
0.000
OMe
Ms
MeO
MeO
N
Ph
1m
1.99
3.01
0.99
1.00
2.98
2.95
3.06
2.02
1.98
2.96
f1 (ppm)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122.452
121.615
106.810
81.290
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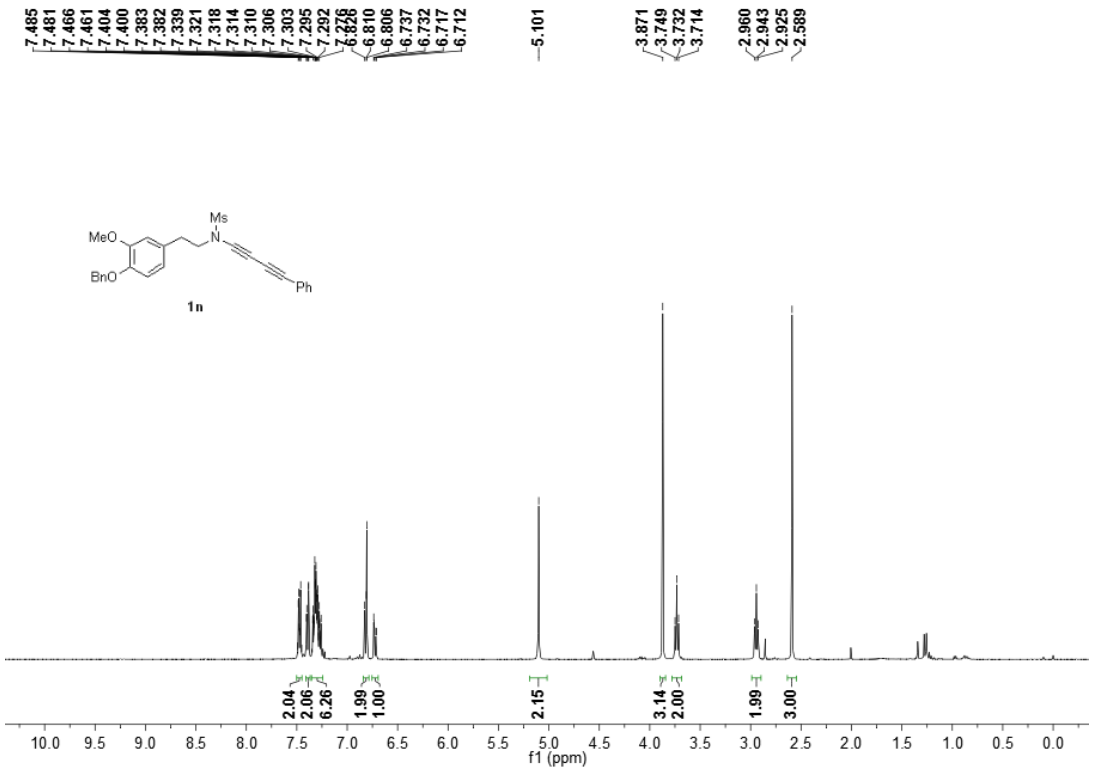
77.000
76.681
73.165
73.080
60.637
60.402
58.756
55.669
51.649
38.781
29.275
OMe
Ms
MeO
MeO
N
Ph
1m
f1 (ppm)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7.321
7.318
7.314
7.310
7.306
7.303
7.295
7.292
7.276
6.828
6.810
6.806
6.737
6.732
6.717
6.712
5.101
3.871
3.749
3.732
3.714
2.960
2.943
2.925
2.589
MeO
BnO
Ms
N
Ph
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2.06
6.26
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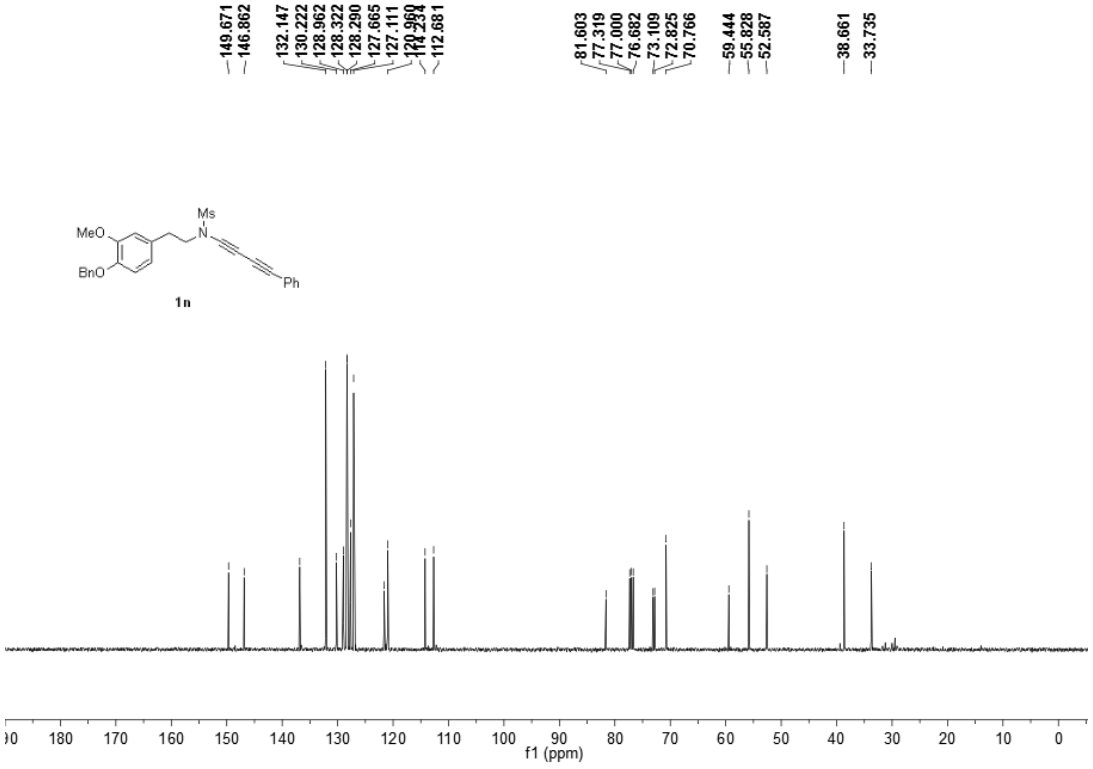
2.15
3.14
2.00
1.99
3.00
f1 (ppm)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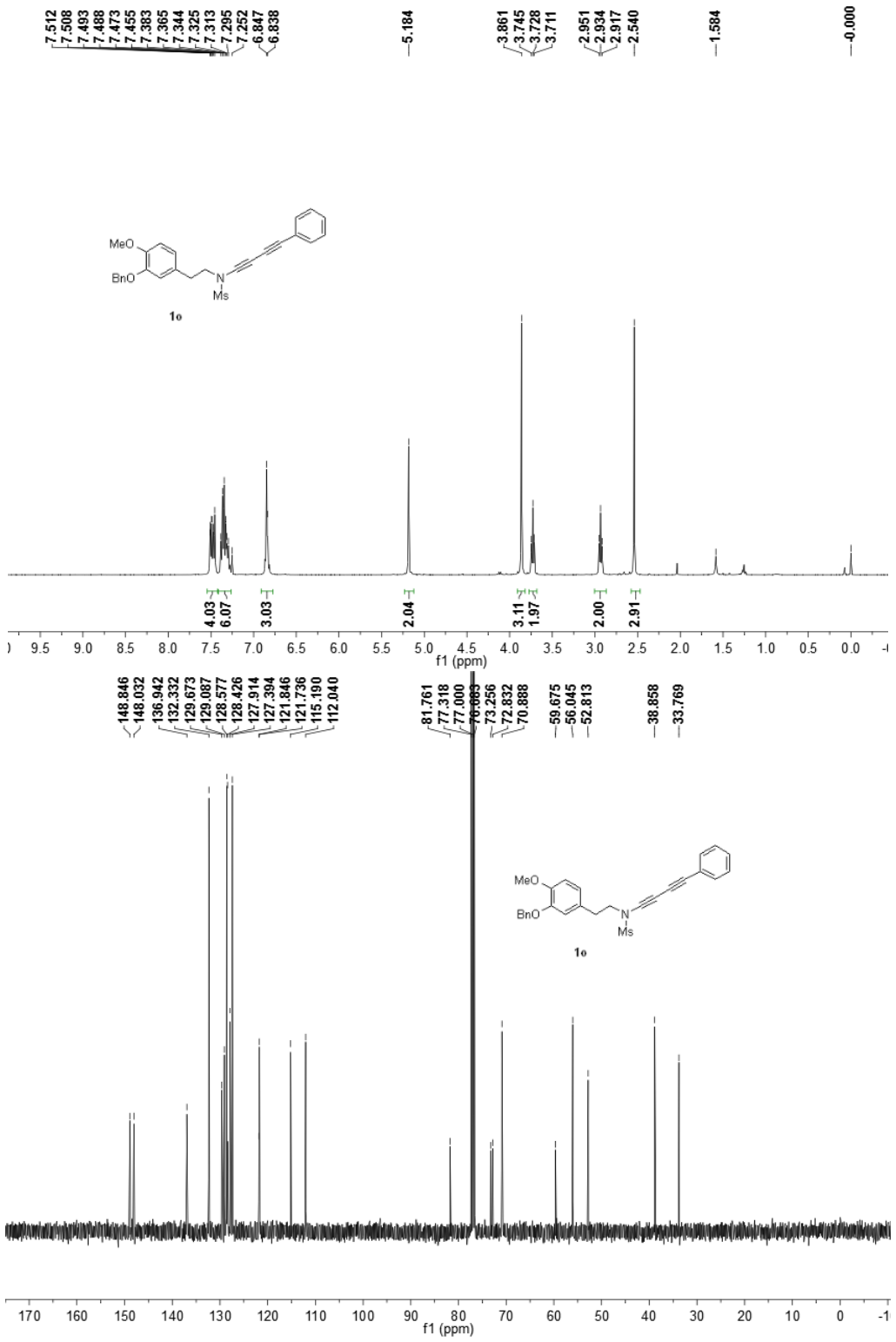
130.222
128.962
128.322
128.290
127.665
127.111
120.960
112.681
81.603
77.319
77.000
76.682
73.109
72.825
70.766
59.444
55.828
52.587
38.661
33.735
MeO
BnO
Ms
N
Ph
1n
f1 (ppm)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7.493
7.488
7.473
7.455
7.383
7.365
7.344
7.325
7.313
7.295
7.252
6.847
6.838
5.184
3.861
3.745
3.728
3.711
2.951
2.934
2.917
2.540
1.584
0.000
MeO
BnO
N
Ms
1o
4.03
6.07
3.03
2.04
3.11
1.97
2.00
2.91
f1 (ppm)
148.846
148.032
136.942
132.332
129.673
129.087
128.577
128.426
127.914
127.394
121.846
121.736
115.190
112.040
81.761
77.318
77.000
76.683
73.256
72.832
70.888
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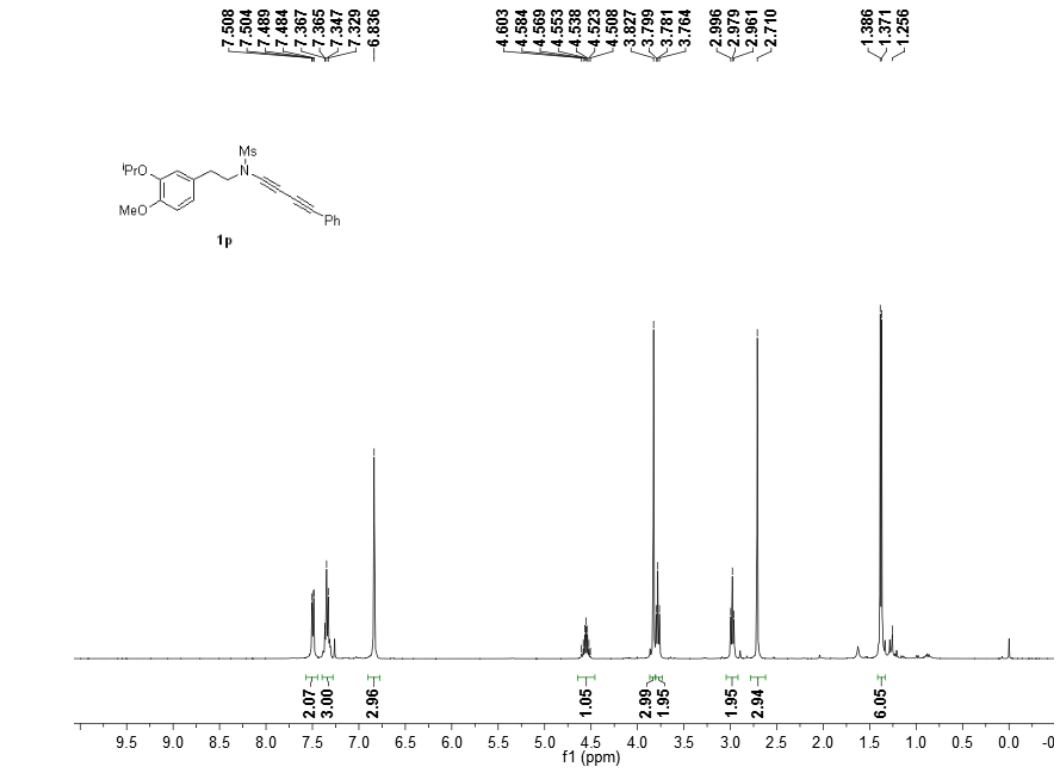
56.045
52.813
38.858
33.769
MeO
BnO
N
Ms
1o
f1 (ppm)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7.329
6.836
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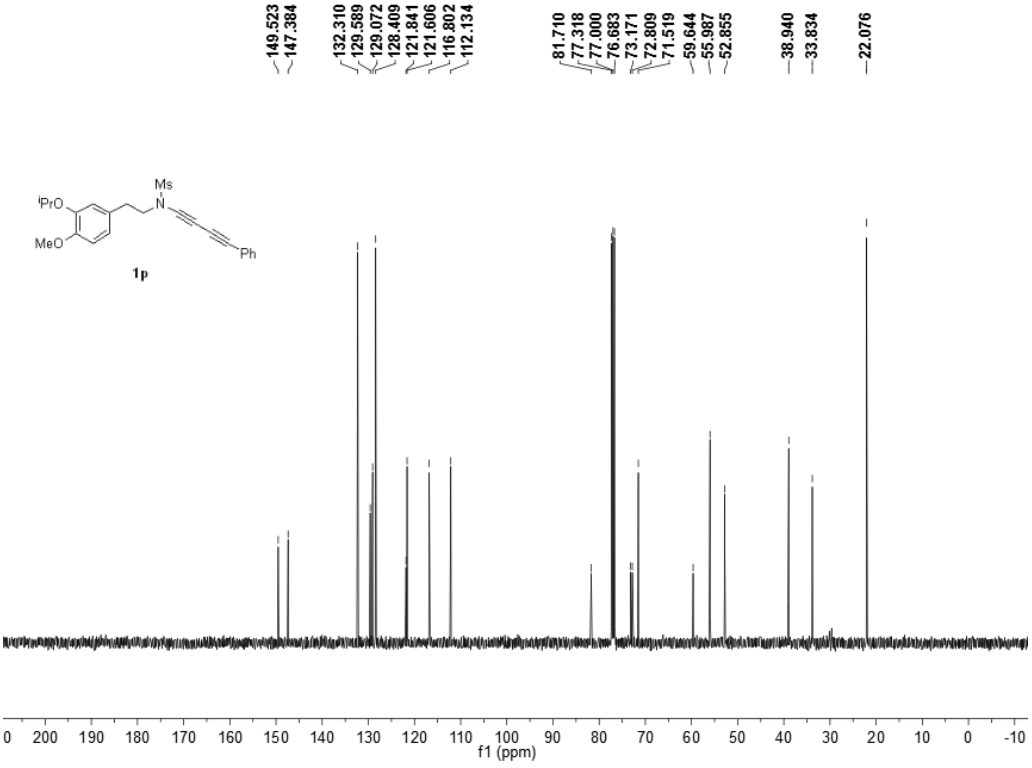
4.584
4.569
4.553
4.538
4.523
4.508
3.827
3.799
3.781
3.764
2.996
2.979
2.961
2.710
1.386
1.371
1.256
Ms
N
iPrO
MeO
Ph
1p
2.07
3.00
2.96
1.05
2.99
1.95
1.95
2.94
6.05
f1 (ppm)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128.409
121.841
121.606
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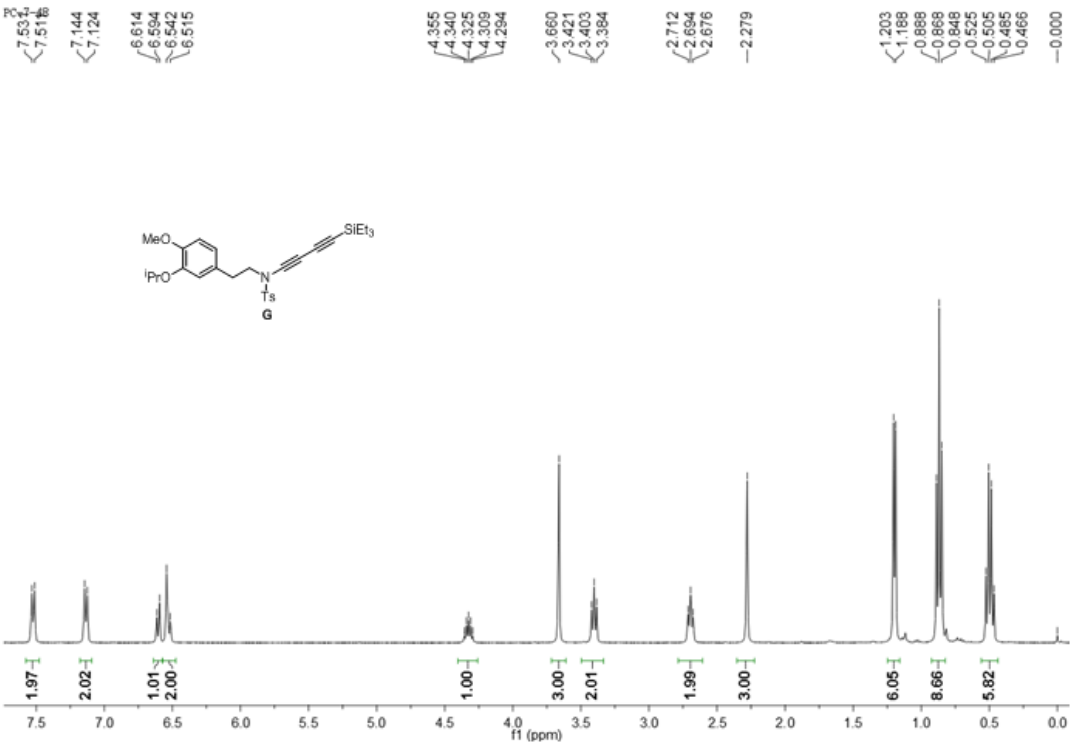
112.134
81.710
77.318
77.000
76.683
73.171
72.809
71.519
59.644
55.987
52.855
38.940
33.834
22.076
Ms
N
iPrO
MeO
Ph
1p
f1 (ppm)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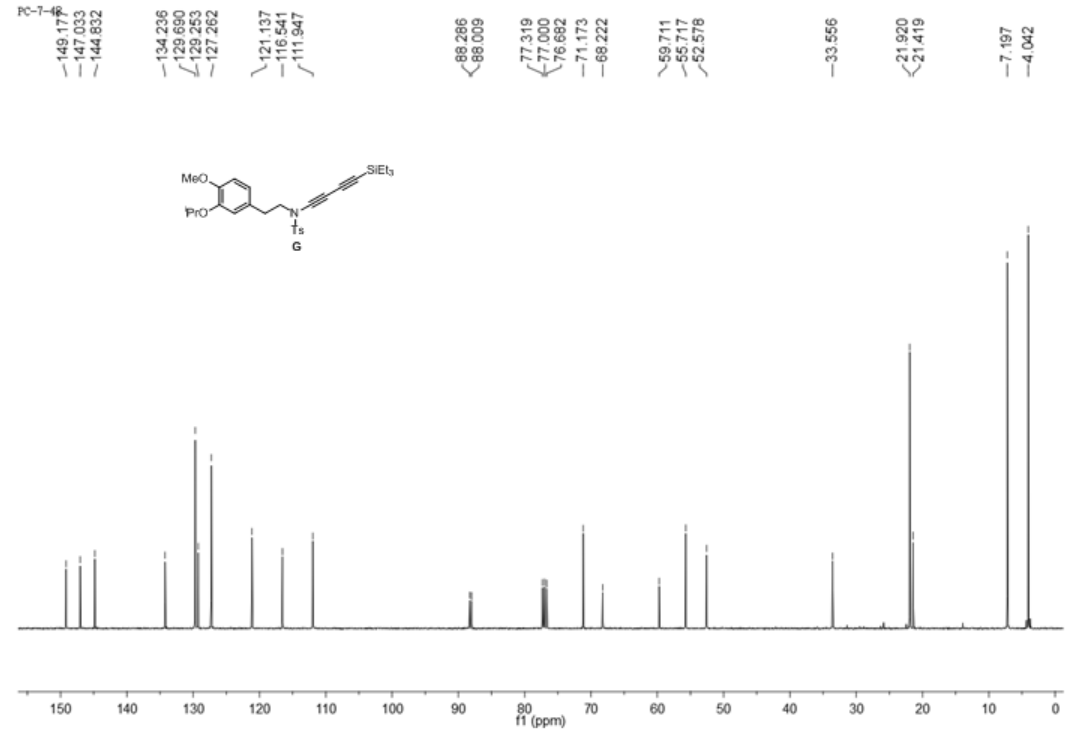
7.516
7.144
7.124
6.614
6.594
6.542
6.515
4.355
4.340
4.325
4.309
4.294
3.660
3.421
3.403
3.384
2.712
2.694
2.676
2.279
1.203
1.188
0.888
0.868
0.848
0.525
0.505
0.485
0.466
0.000
MeO
iPrO
N
Ts
SiEt3
G
1.97
2.02
1.01
2.00
1.00
3.00
2.01
1.99
3.00
6.05
8.66
5.82
f1 (ppm)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121.137
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88.009
77.319
77.000
76.682
71.173
68.222
59.711
55.717
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21.920
21.419
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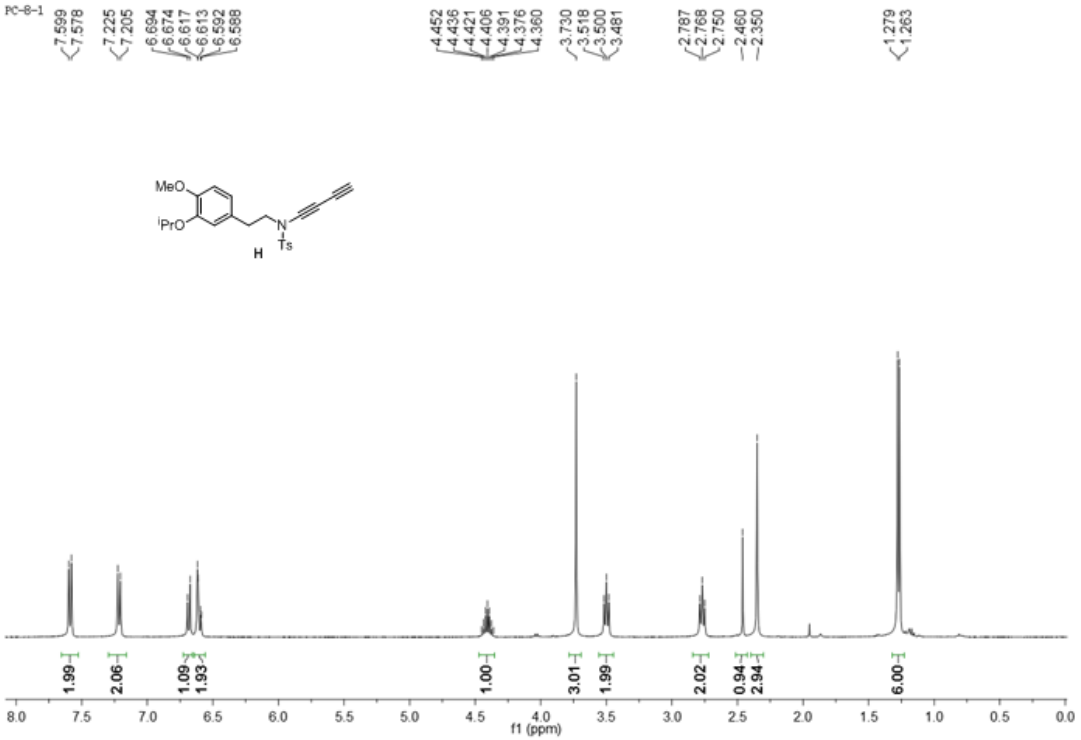
4.042
MeO
iPrO
N
Ts
SiEt3
G
f1 (ppm)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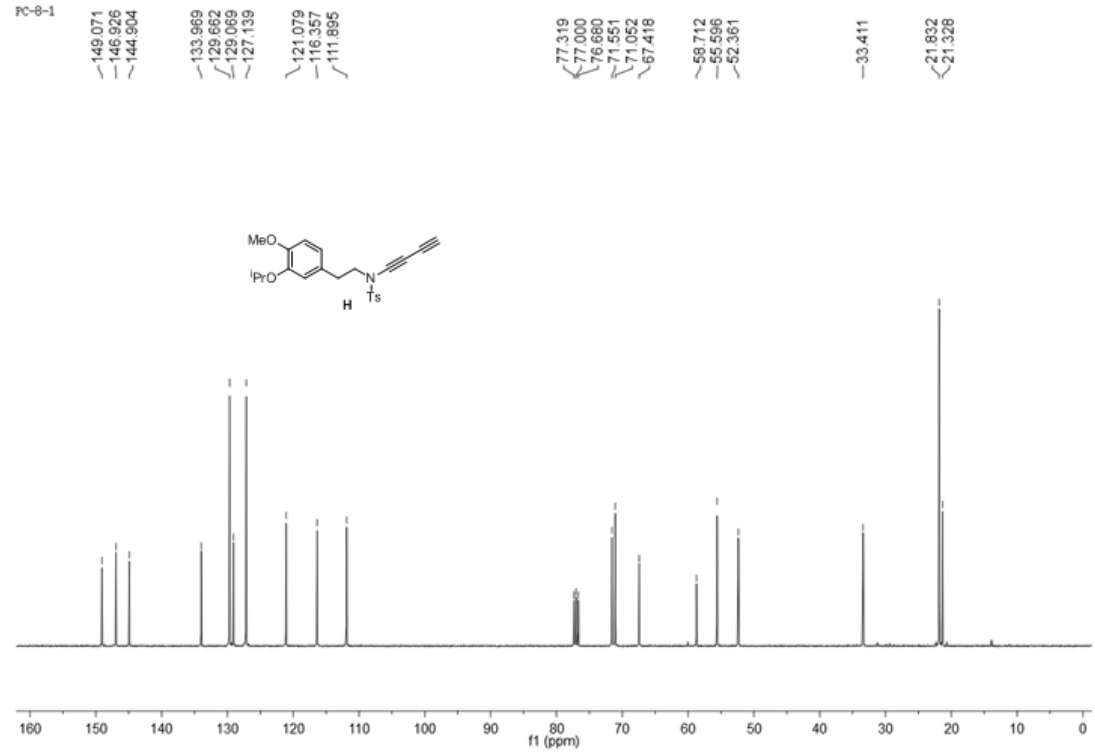
7.578
7.225
7.205
6.694
6.674
6.617
6.613
6.592
6.588
4.452
4.436
4.421
4.406
4.391
4.376
4.360
3.730
3.518
3.500
3.481
2.787
2.768
2.750
2.460
2.350
1.279
1.263
MeO
iPrO
N
Ts
H
1.99
2.06
1.09
1.93
1.00
3.01
1.99
2.02
0.94
2.94
6.00
f1 (ppm)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77.319
77.000
76.680
71.551
71.052
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52.361
33.411
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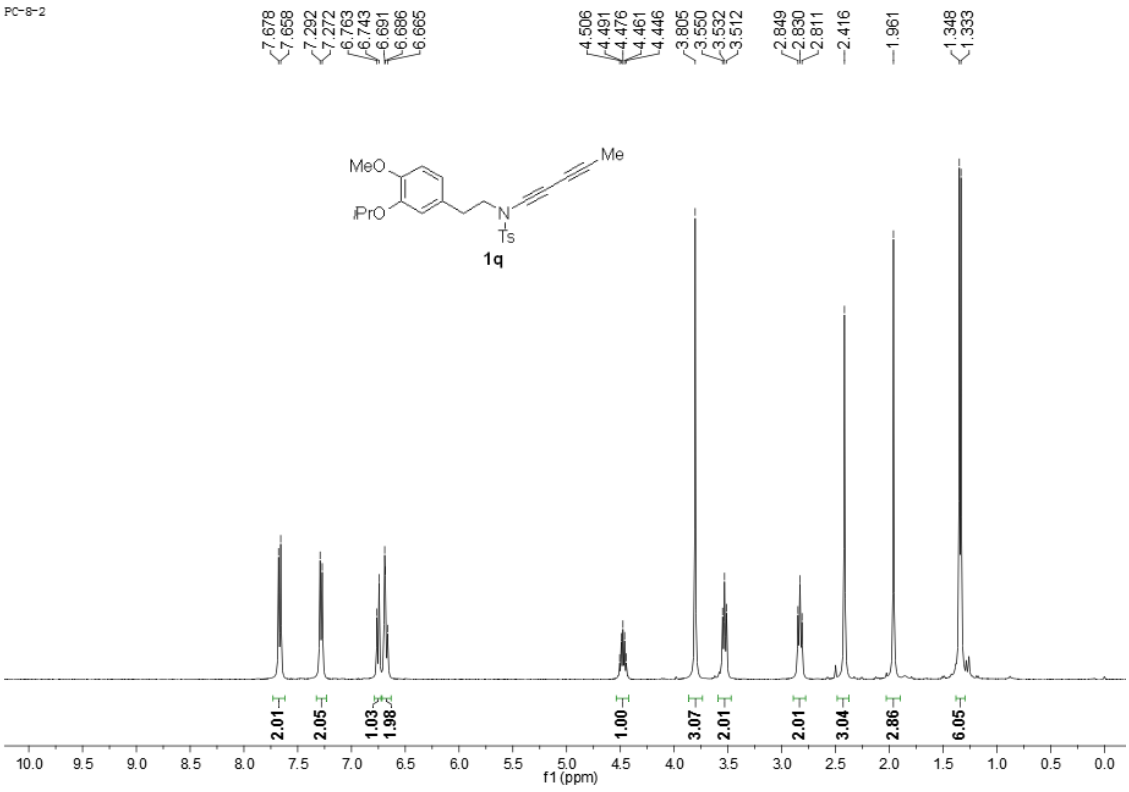
21.328
MeO
iPrO
N
Ts
H
f1 (ppm)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7.292
7.272
6.763
6.743
6.691
6.686
6.665
4.506
4.491
4.476
4.461
4.446
3.805
3.550
3.532
3.512
2.849
2.830
2.811
2.416
1.961
1.348
1.333
MeO
iPrO
Me
N
Ts
1q
2.01
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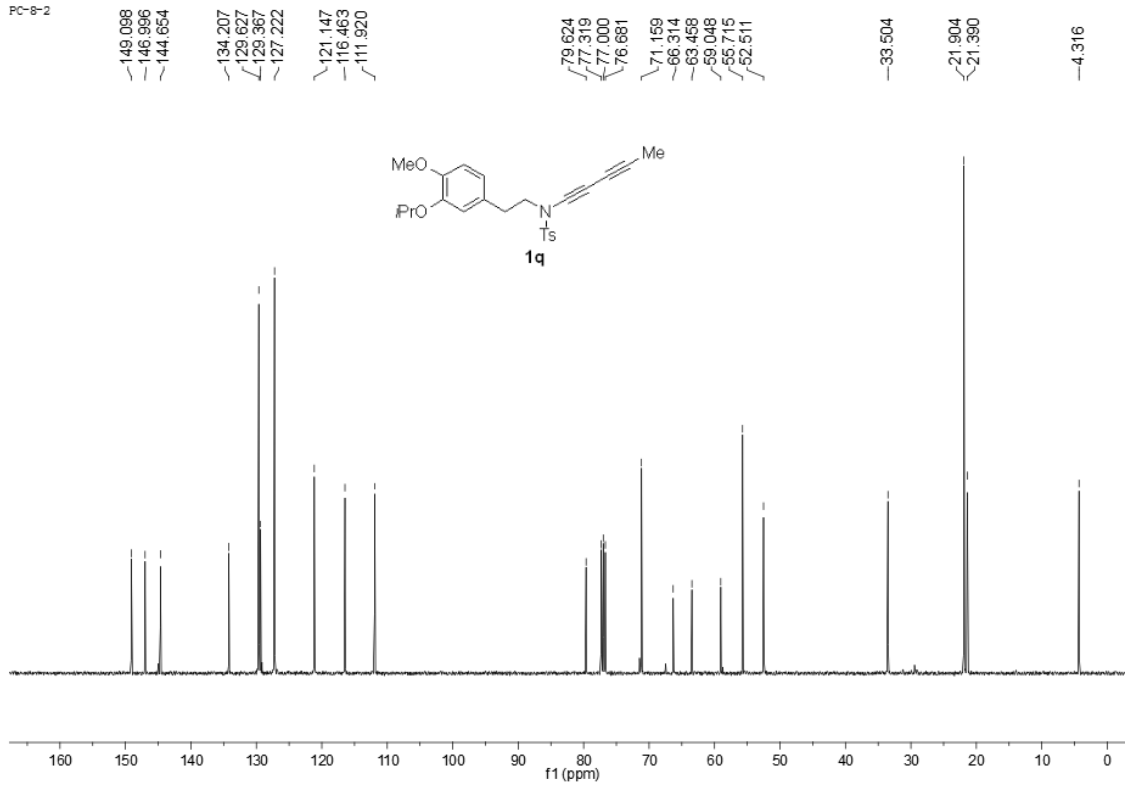
1.98
1.00
3.07
2.01
2.01
3.04
2.86
6.05
f1 (ppm)


PC-8-2
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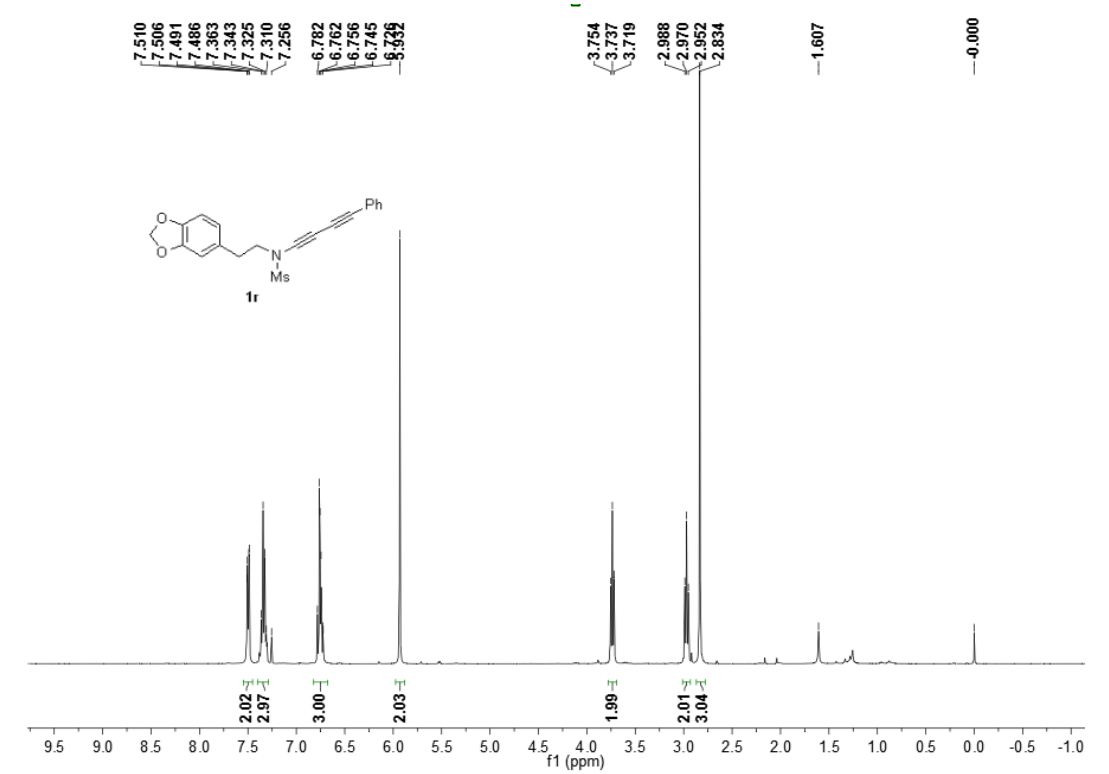
129.367
127.222
121.147
116.463
111.920
79.624
77.319
77.000
76.681
71.159
66.314
63.458
59.048
55.715
52.511
33.504
21.904
21.390
4.316
MeO
iPrO
Me
N
Ts
1q
f1 (ppm)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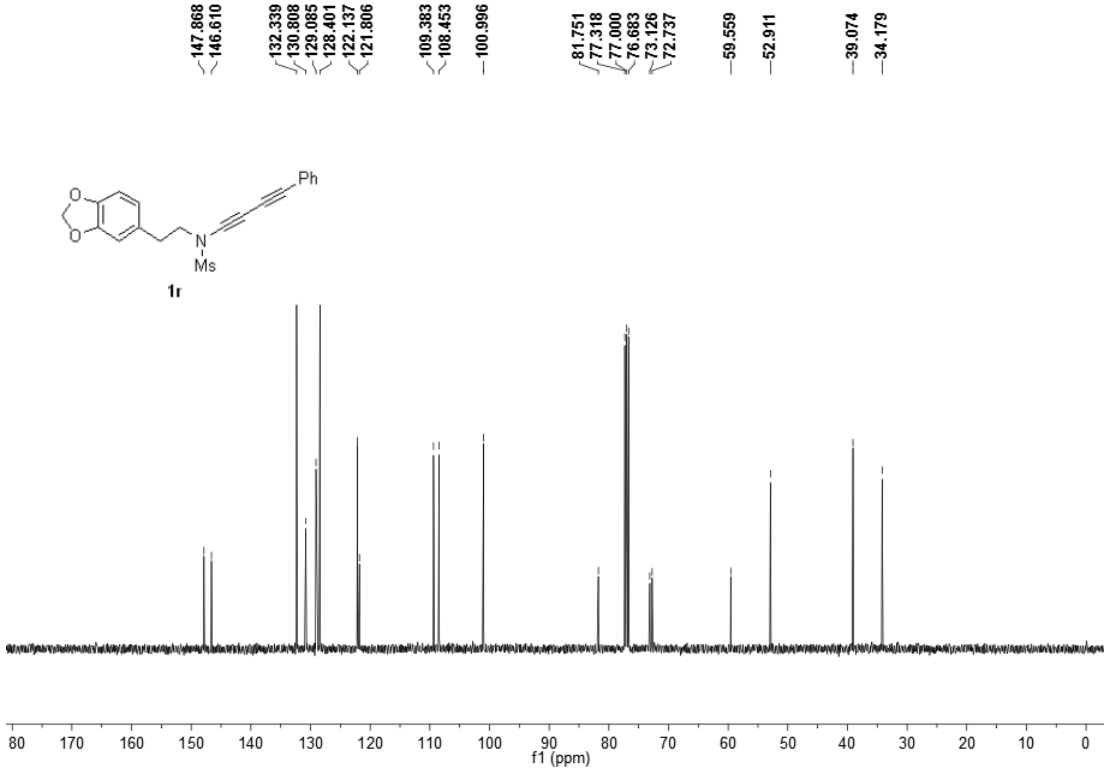
7.506
7.491
7.486
7.363
7.343
7.325
7.310
7.256
6.782
6.762
6.756
6.745
3.754
3.737
3.719
2.988
2.970
2.952
2.834
1.607
-0.000
Ph
O
O
N
Ms
1r
2.02
2.97
3.00
2.03
1.99
2.01
3.04
f1 (ppm)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108.453
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81.751
77.318
77.000
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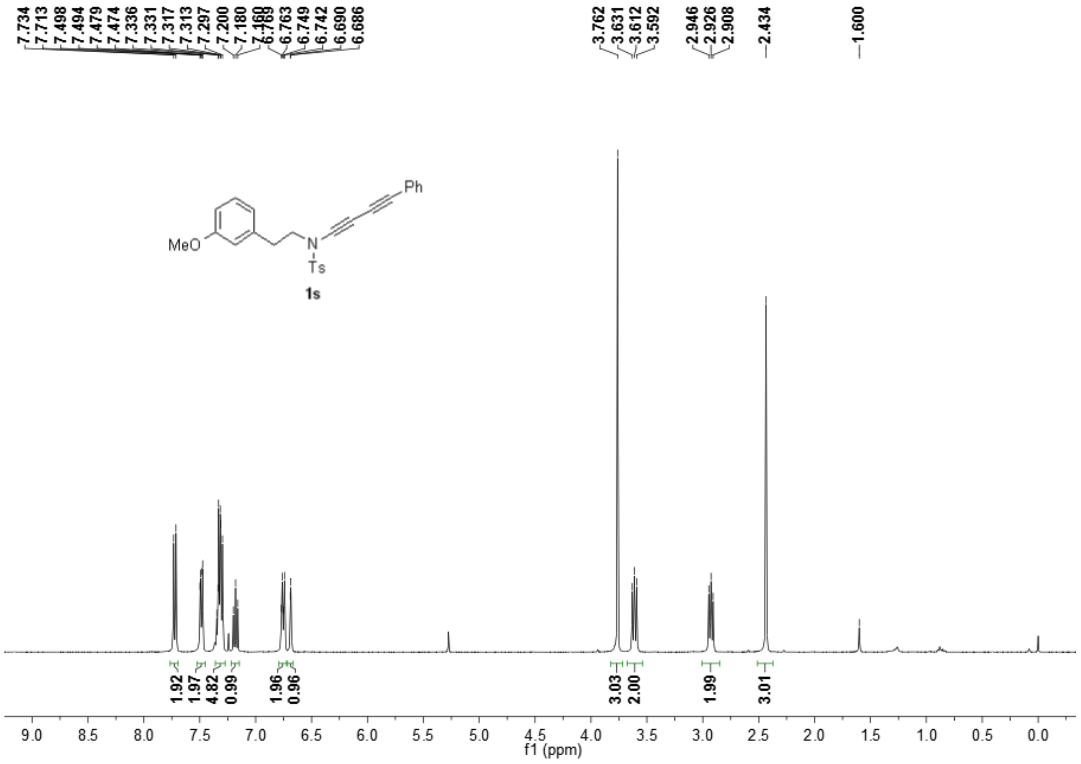
59.559
52.911
39.074
34.179
Ph
O
O
N
Ms
1r
f1 (ppm)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7.479
7.474
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7.331
7.317
7.313
7.297
7.200
7.180
7.169
6.763
6.749
6.742
6.690
6.686
3.762
3.631
3.612
3.592
2.946
2.926
2.908
2.434
1.600
Ph
MeO
N
Ts
1s
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4.82
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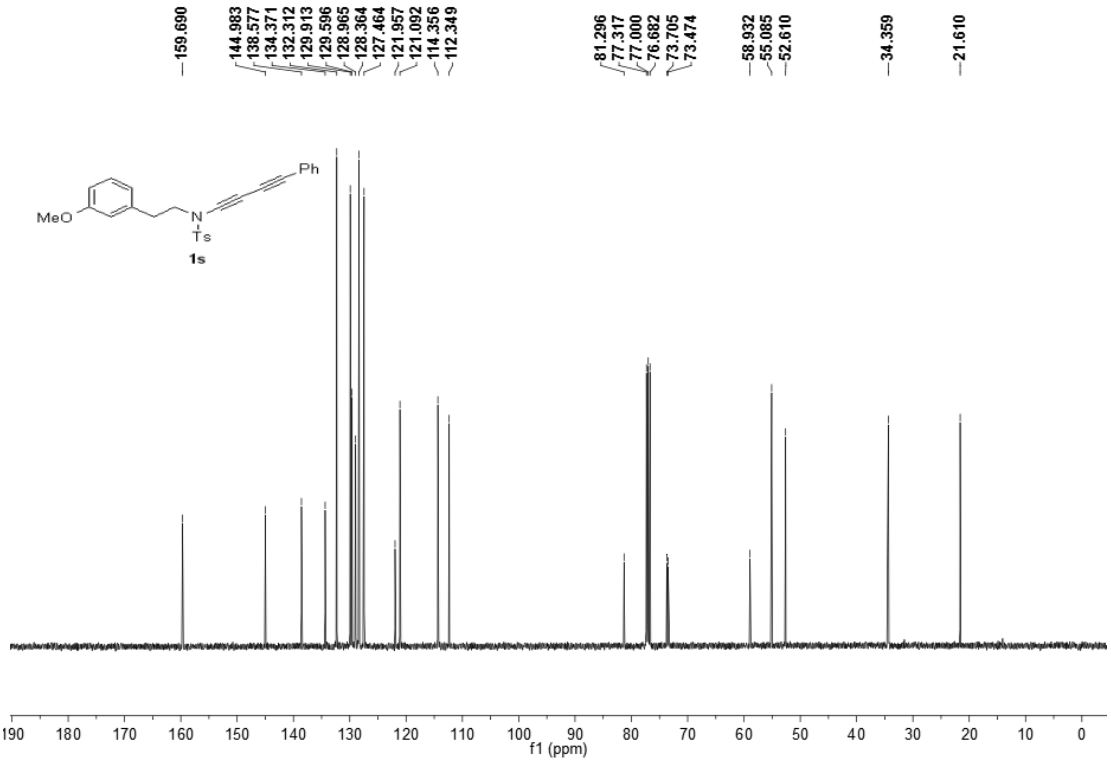
1.96
0.96
3.03
2.00
1.99
3.01
f1 (ppm)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114.356
112.349
81.296
77.317
77.000
76.682
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55.085
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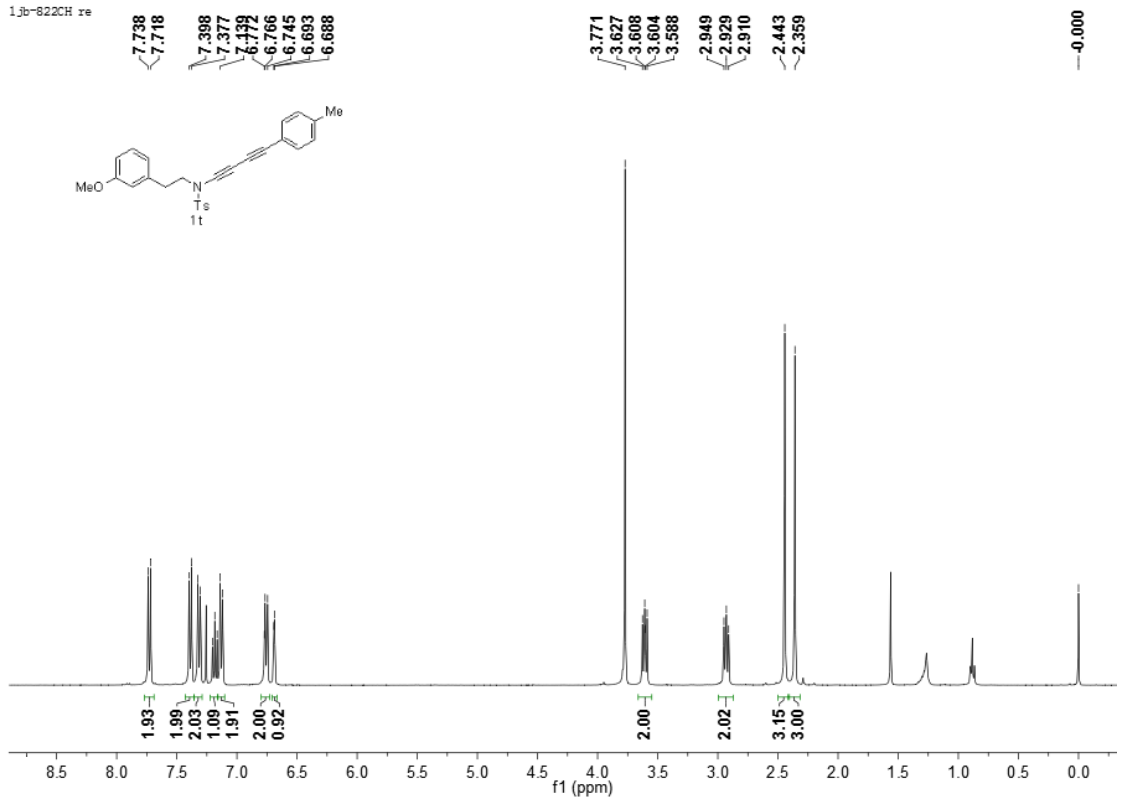
Ph
MeO
N
Ts
1s
f1 (ppm)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7.398
7.377
7.139
6.766
6.745
6.693
6.688
3.771
3.627
3.608
3.604
3.588
2.949
2.929
2.910
2.443
2.359
0.000
Me
MeO
N
Ts
1t
1.93
1.99
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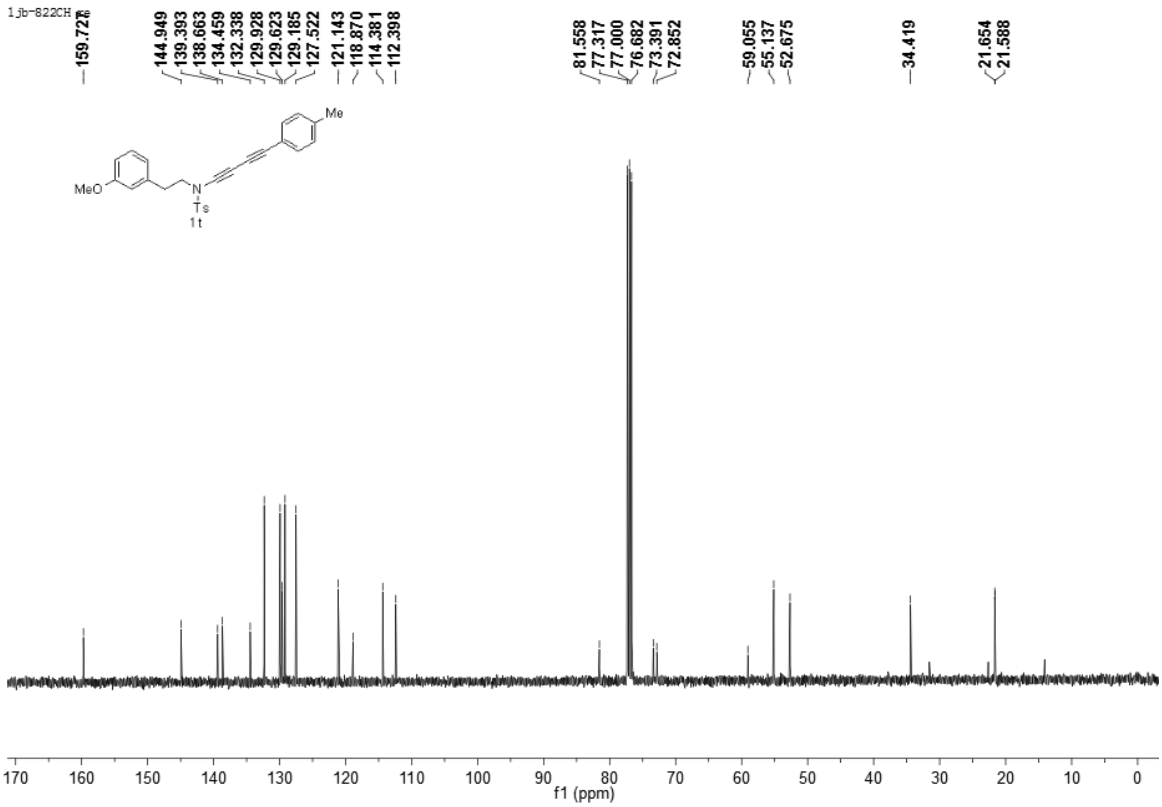
1.09
1.91
2.00
0.92
2.00
2.02
3.15
3.00
f1 (ppm)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138.663
134.459
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129.623
129.185
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121.143
118.870
114.381
112.398
81.558
77.317
77.000
76.682
73.391
72.852
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55.137
52.675
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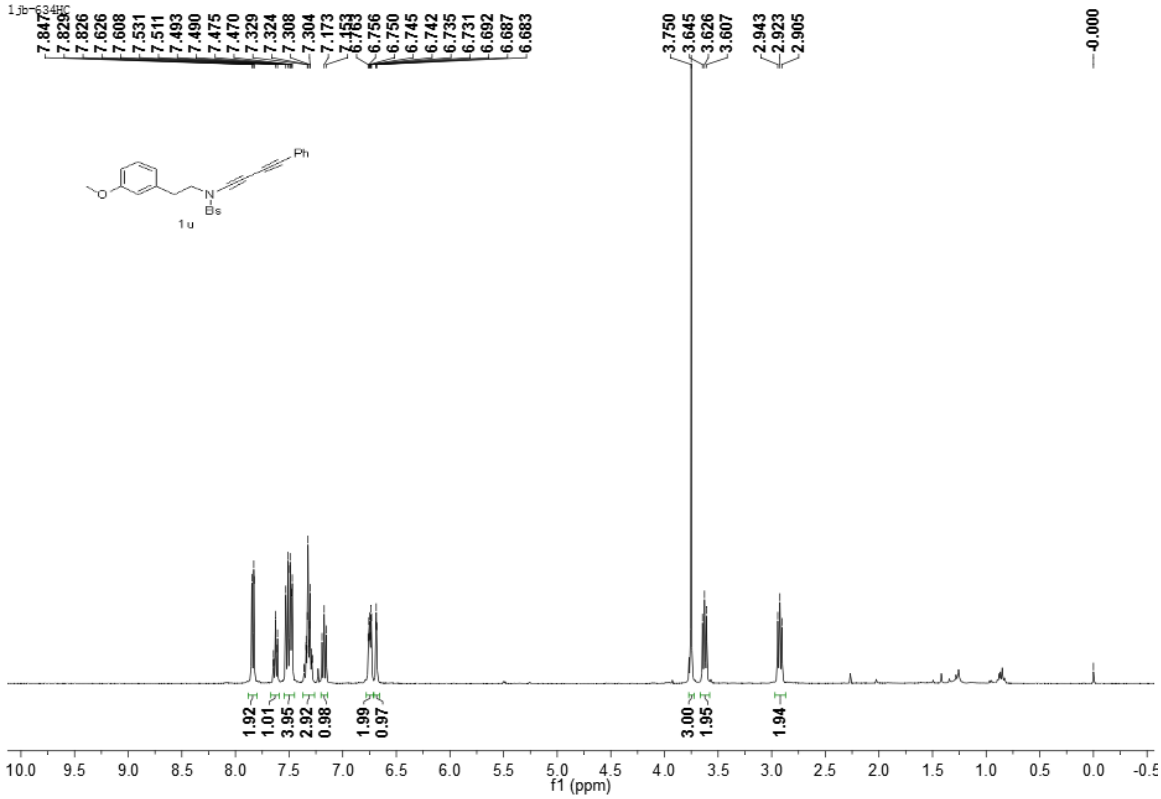
21.588
Me
MeO
N
Ts
1t
f1 (ppm)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7.608
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7.490
7.475
7.470
7.329
7.324
7.308
7.304
7.173
6.763
6.756
6.750
6.745
6.742
6.735
6.731
6.692
6.687
6.683
3.750
3.645
3.626
3.607
2.943
2.923
2.905
-0.000
Ph
O
N
Bs
1u
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3.95
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1.99
0.97
3.00
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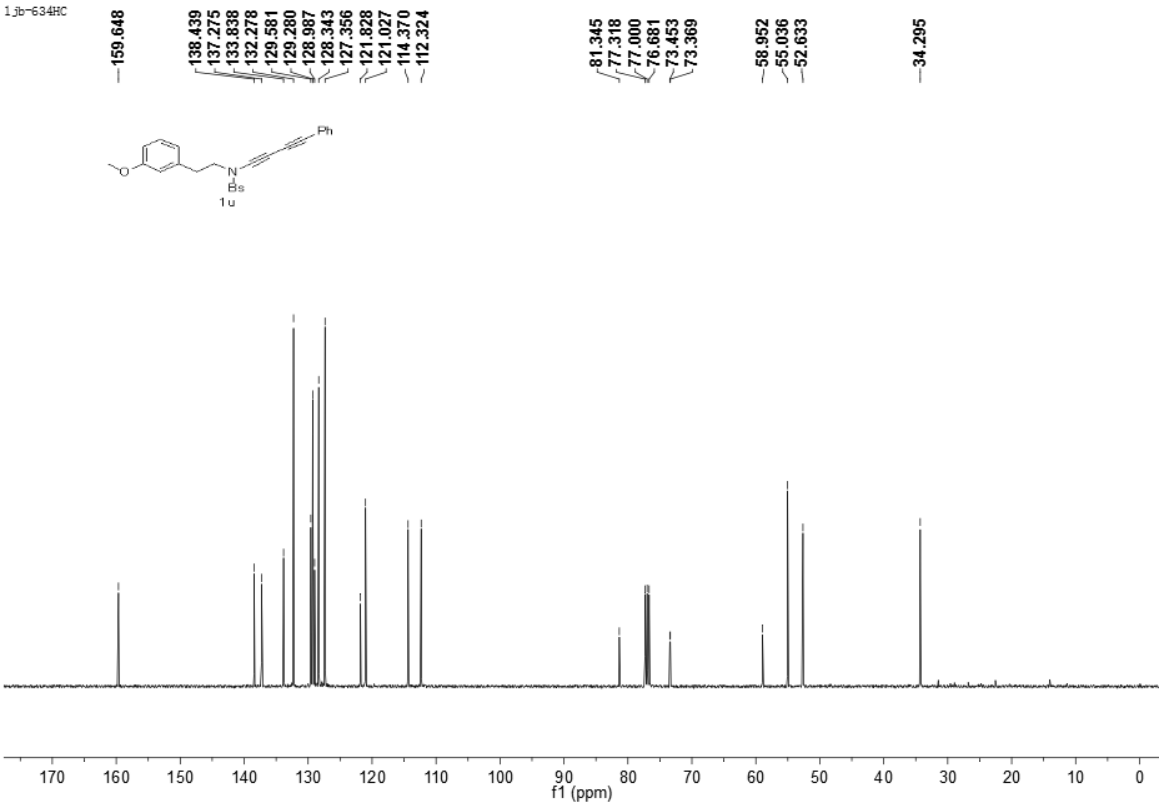
1.94
f1 (ppm)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121.027
114.370
112.324
81.345
77.318
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55.036
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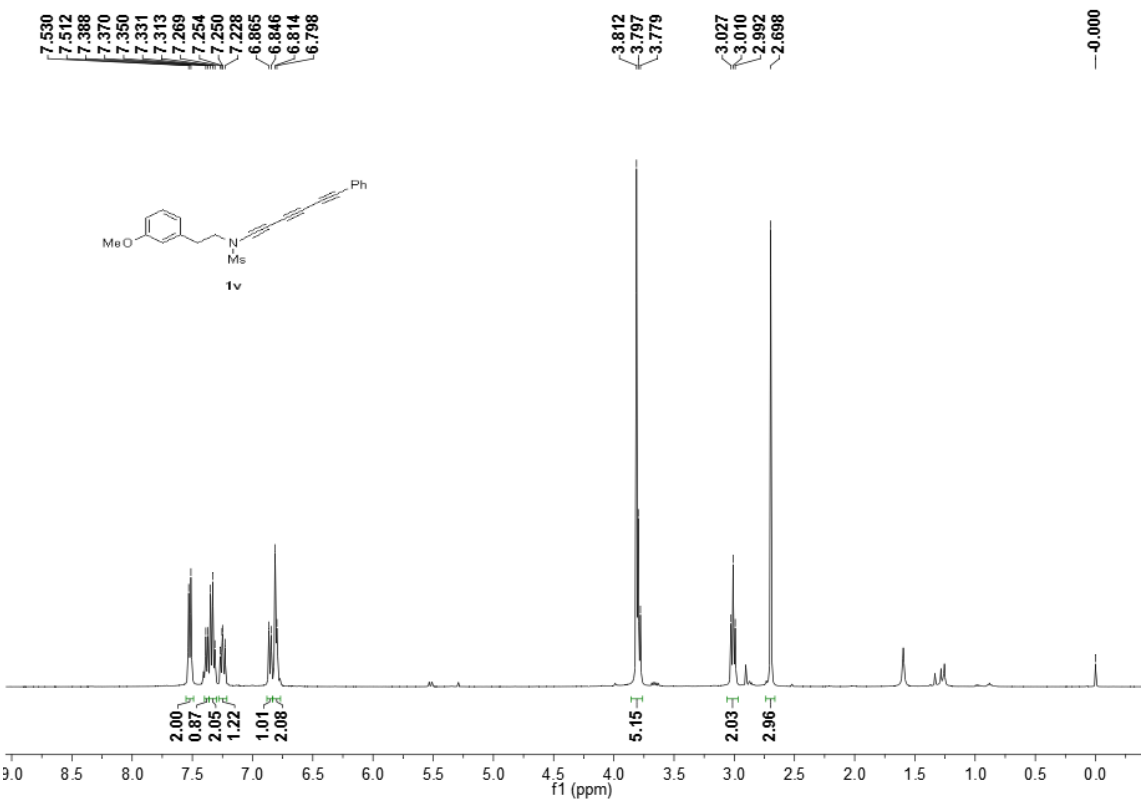
34.295
Ph
O
N
Bs
1u
f1 (ppm)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7.331
7.313
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7.254
7.250
7.228
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6.846
6.814
6.798
3.812
3.797
3.779
3.027
3.010
2.992
2.698
0.000
Ph
MeO
N
Ms
1v
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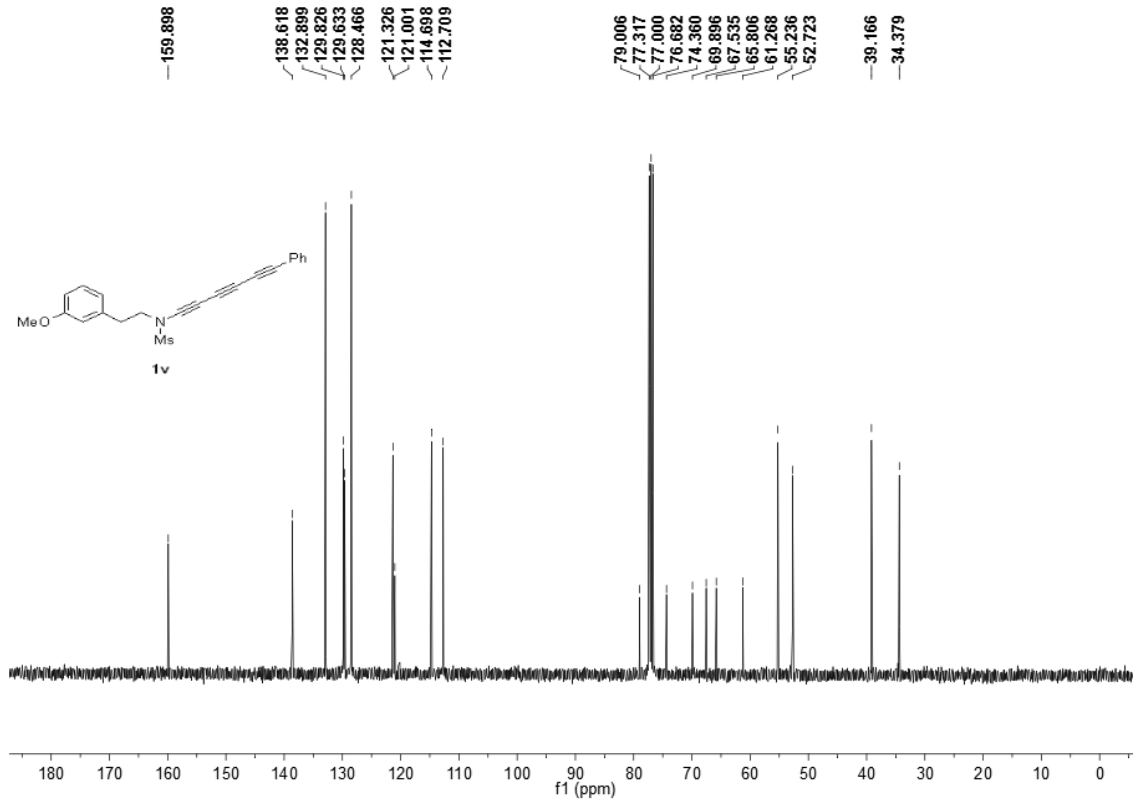
0.87
2.05
1.22
1.01
2.08
5.15
2.03
2.96
f1 (ppm)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77.317
77.000
76.682
74.360
69.896
67.535
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55.236
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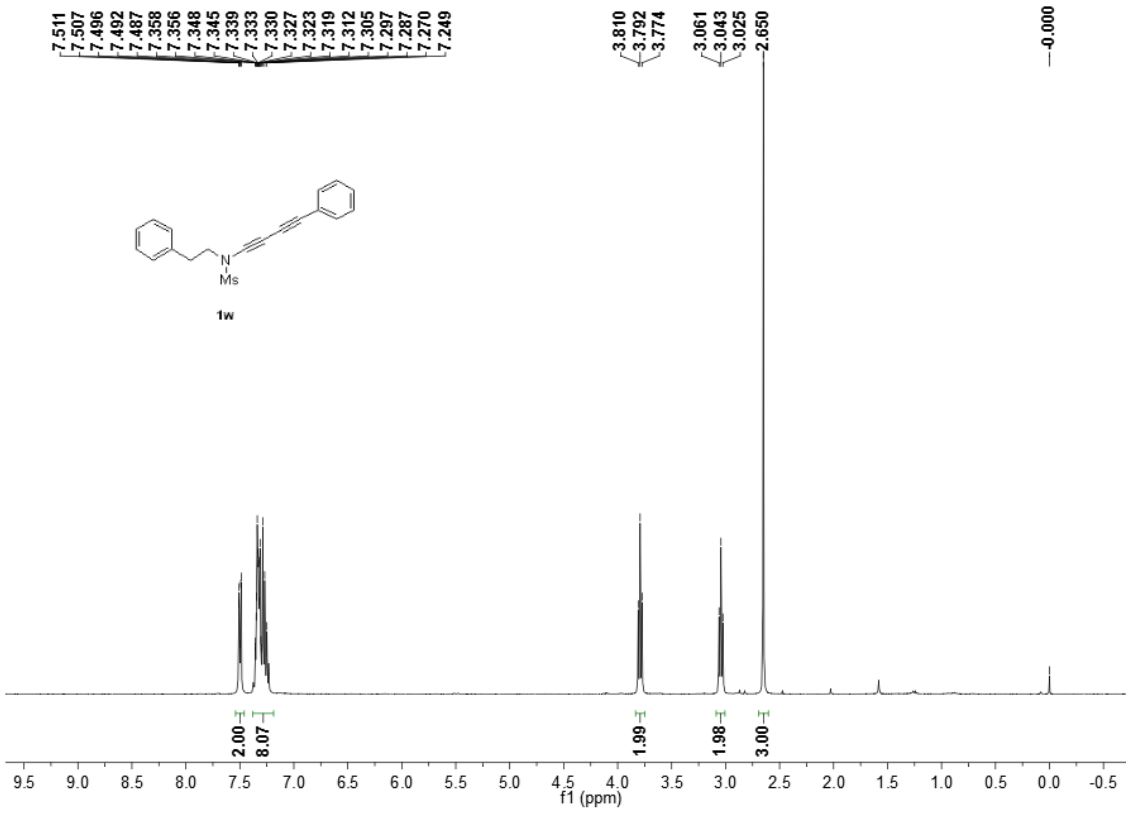
Ph
MeO
N
Ms
1v
f1 (ppm)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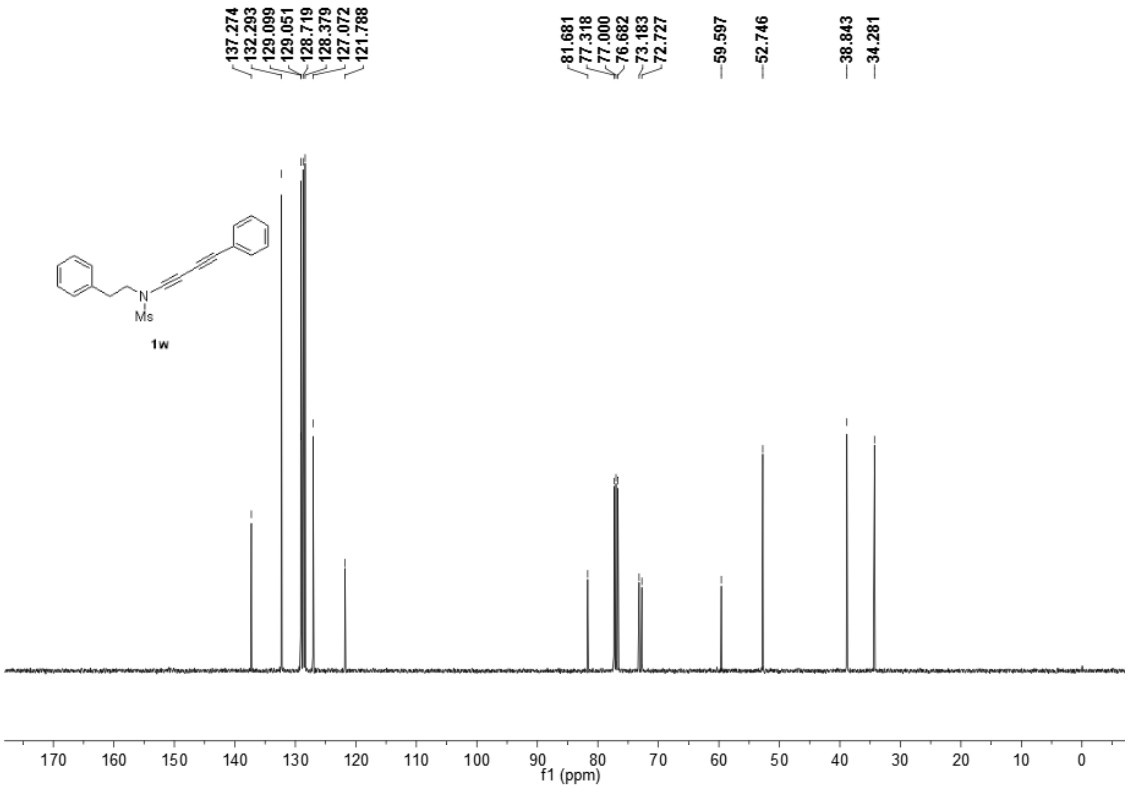
7.323
7.319
7.312
7.305
7.297
7.287
7.270
7.249
3.810
3.792
3.774
3.061
3.043
3.025
2.650
0.000
N
Ms
1w
2.00
8.07
1.99
1.98
3.00
f1 (ppm)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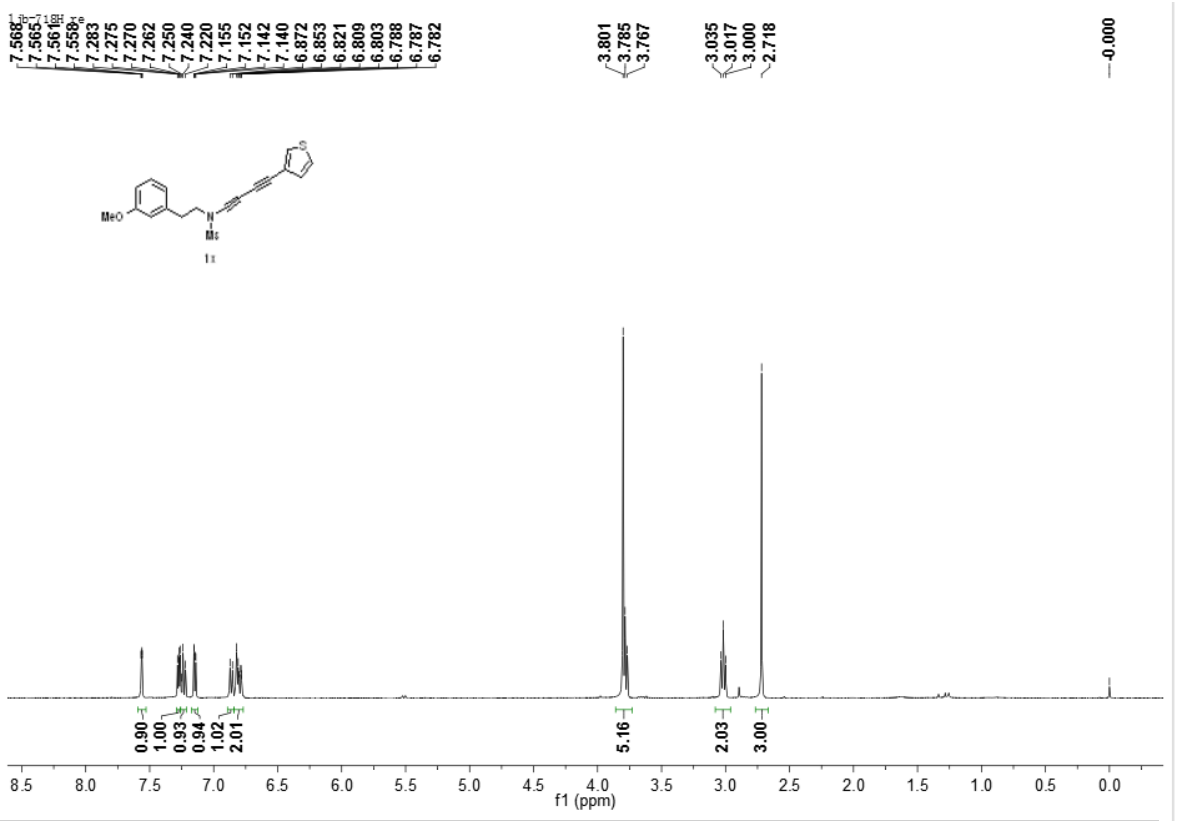
Ms
1w
f1 (ppm)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7.240
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7.152
7.142
7.140
6.872
6.853
6.821
6.809
6.803
6.788
6.787
6.782
3.801
3.785
3.767
3.035
3.017
3.000
2.718
-0.000
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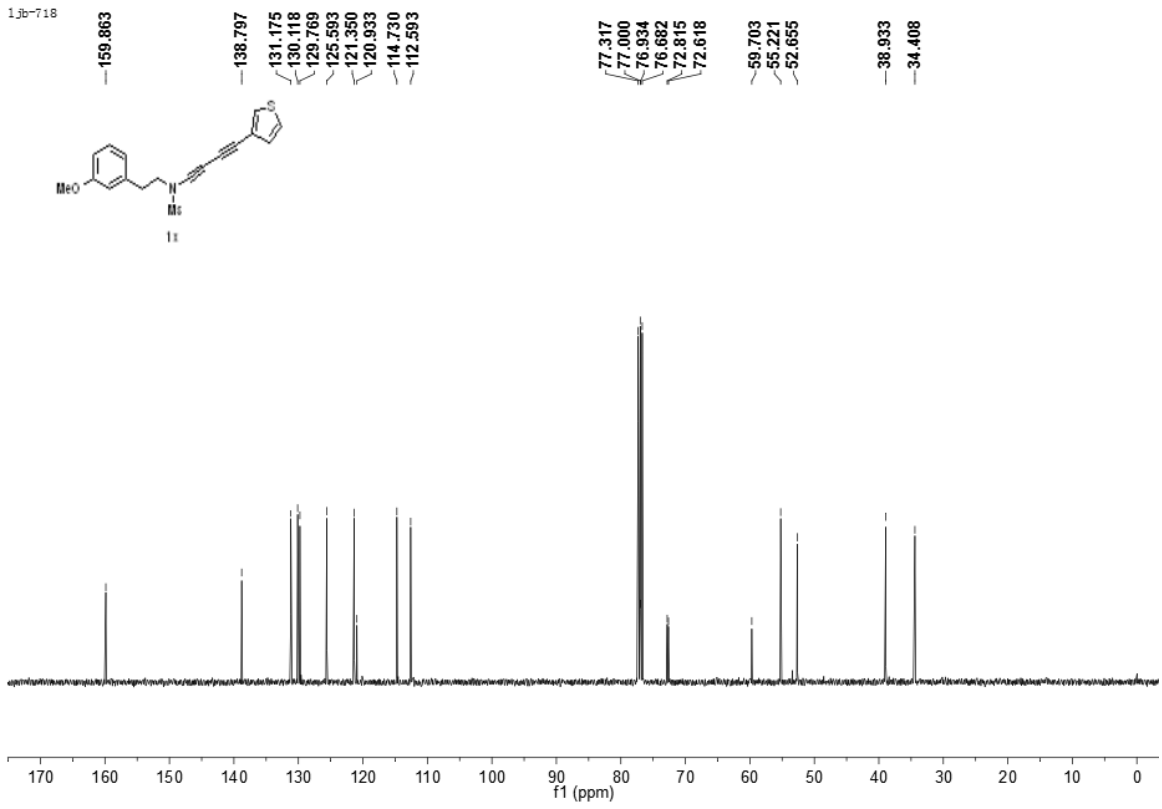
5.16
2.03
3.00
f1 (ppm)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77.000
76.934
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72.618
59.703
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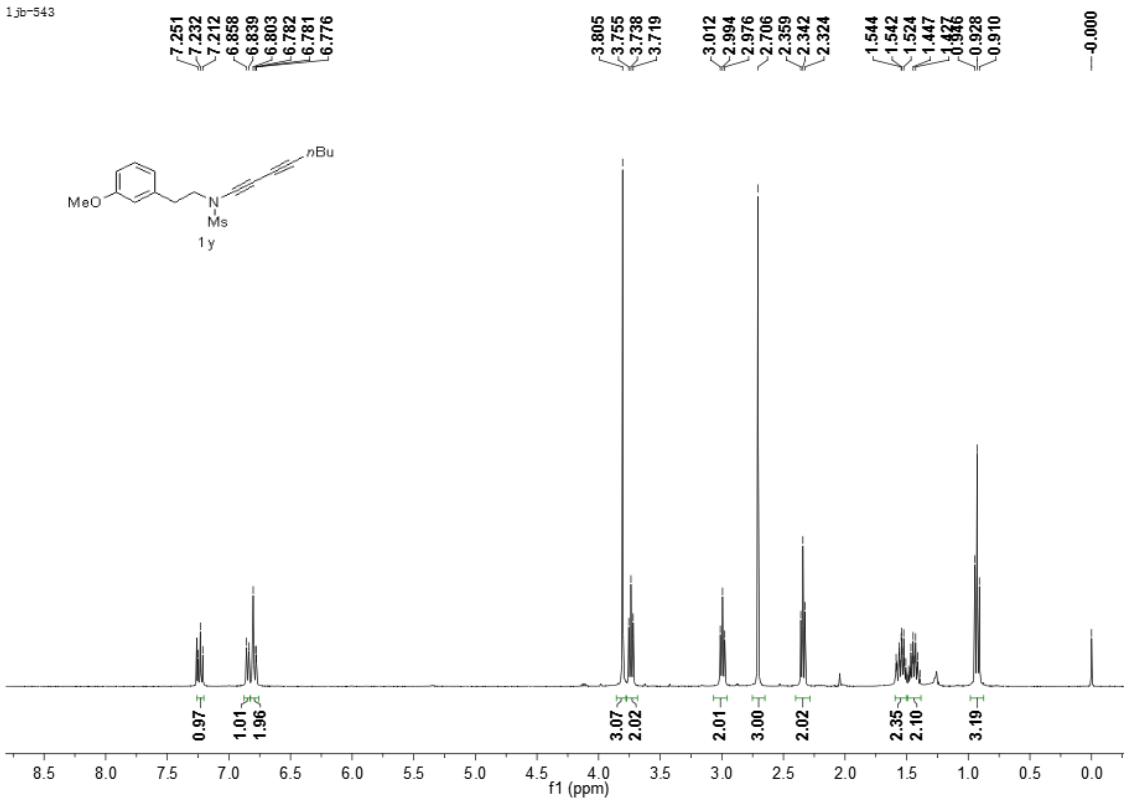
38.933
34.408
MeO
Ms
1x
f1 (ppm)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6.782
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3.738
3.719
3.012
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2.976
2.706
2.359
2.342
2.324
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1.542
1.524
1.447
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0.000
nBu
MeO
N
Ms
1y
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2.01
3.00
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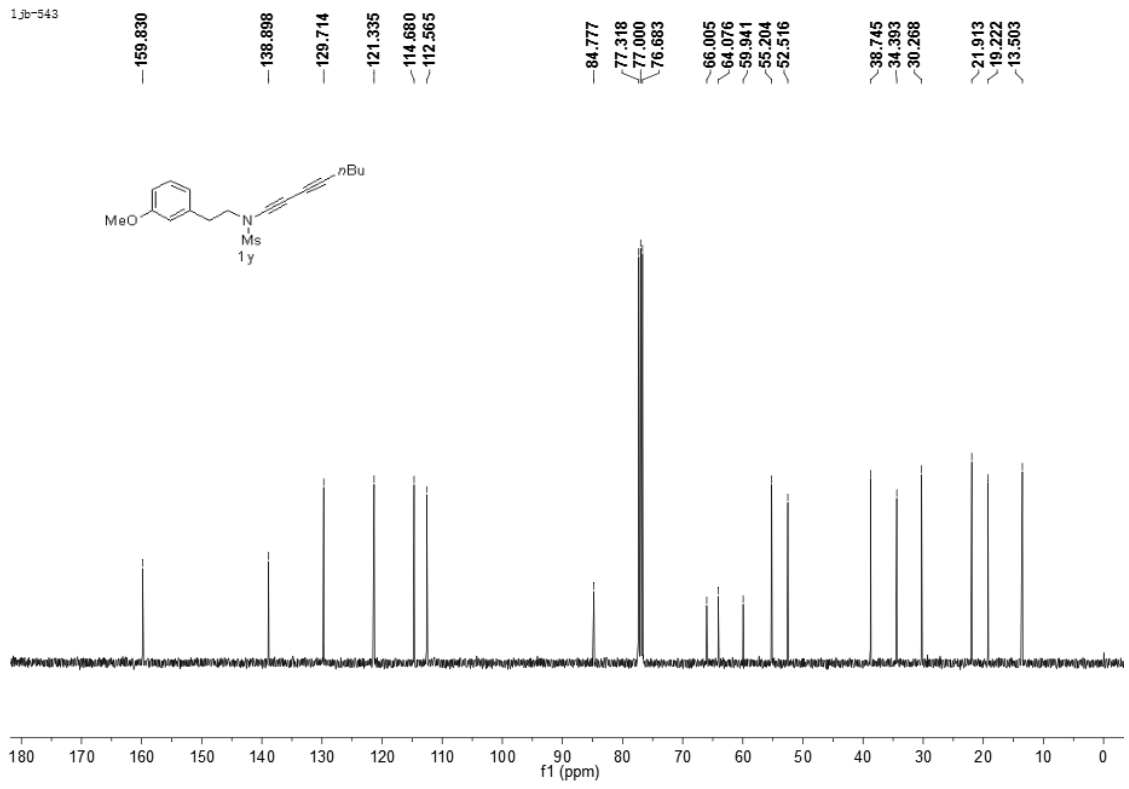
3.19
f1 (ppm)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77.000
76.683
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64.076
59.941
55.204
52.516
38.745
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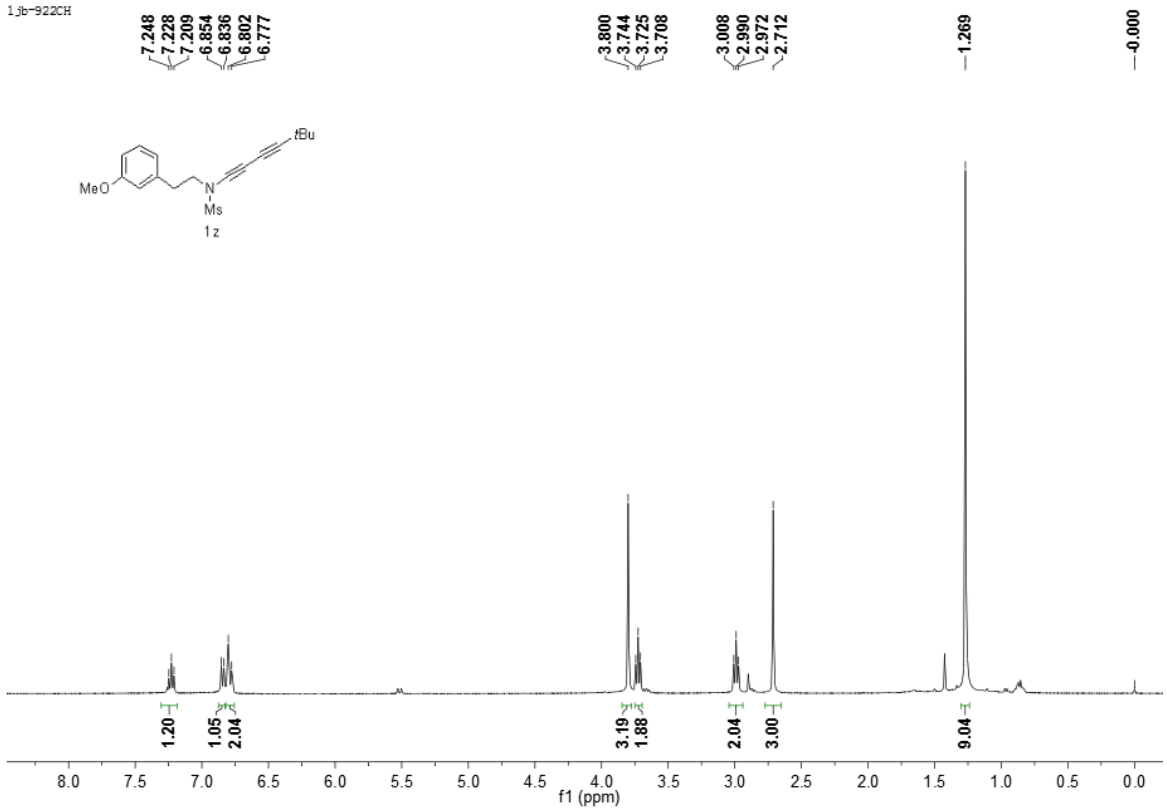
30.268
21.913
19.222
13.503
nBu
MeO
N
Ms
1y
f1 (ppm)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6.802
6.777
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3.744
3.725
3.708
3.008
2.990
2.972
2.712
1.269
0.000
tBu
MeO
N
Ms
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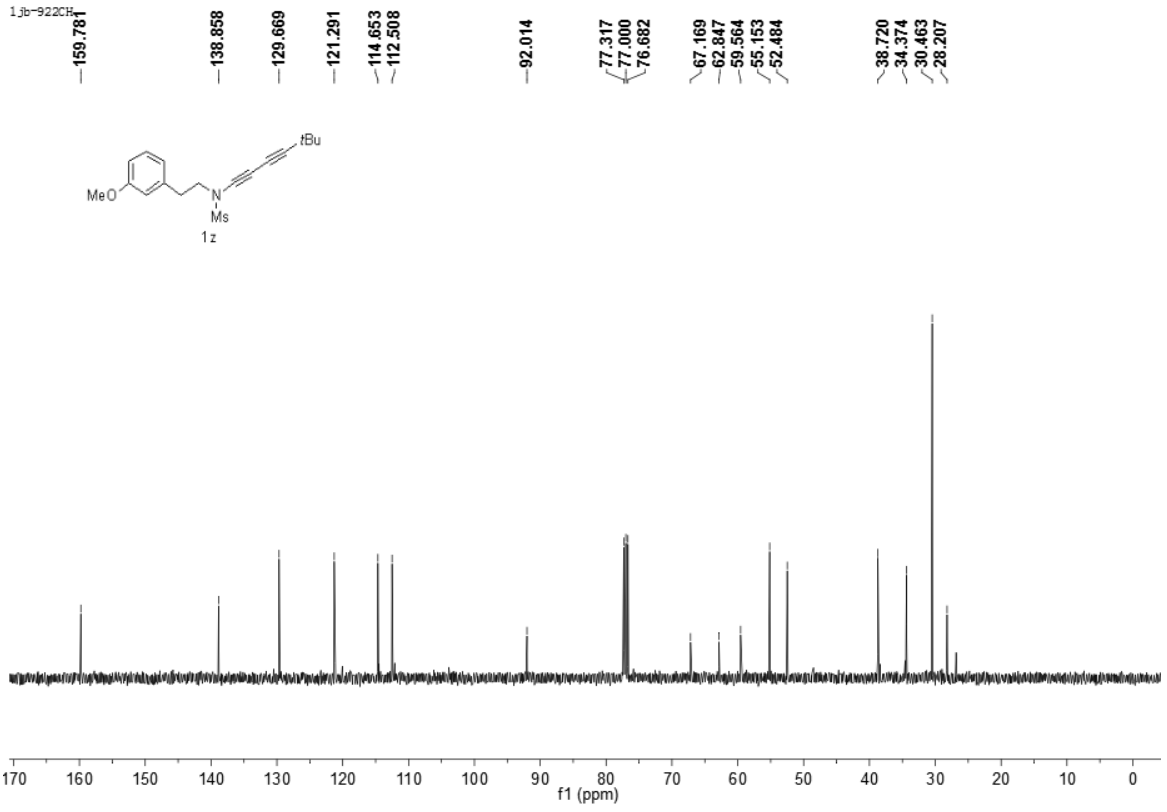
2.04
3.00
9.04
f1 (ppm)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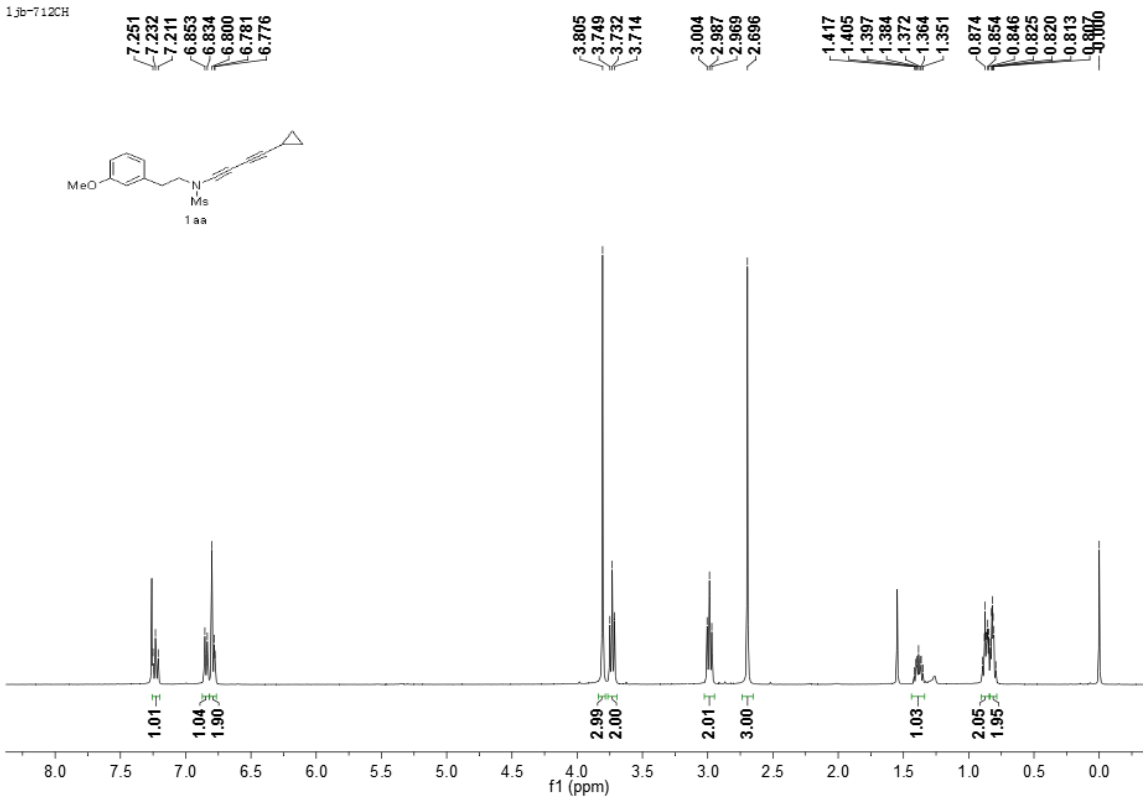
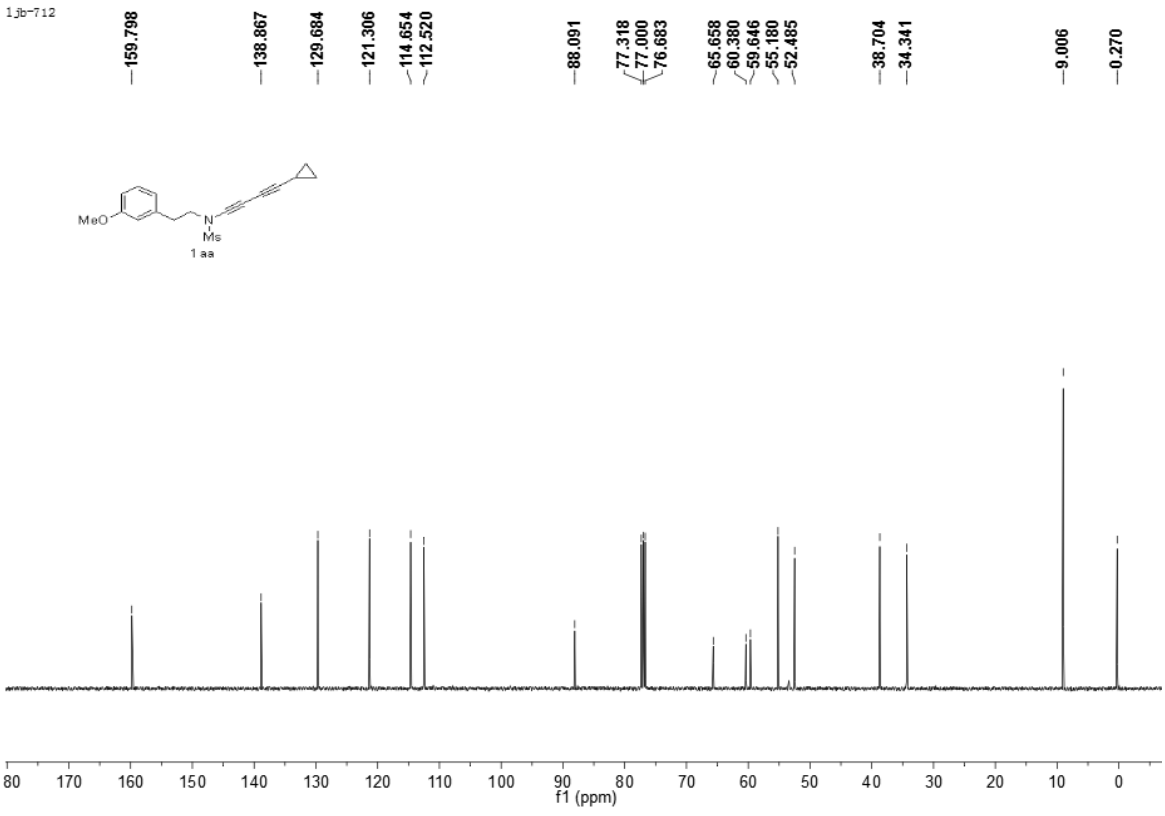
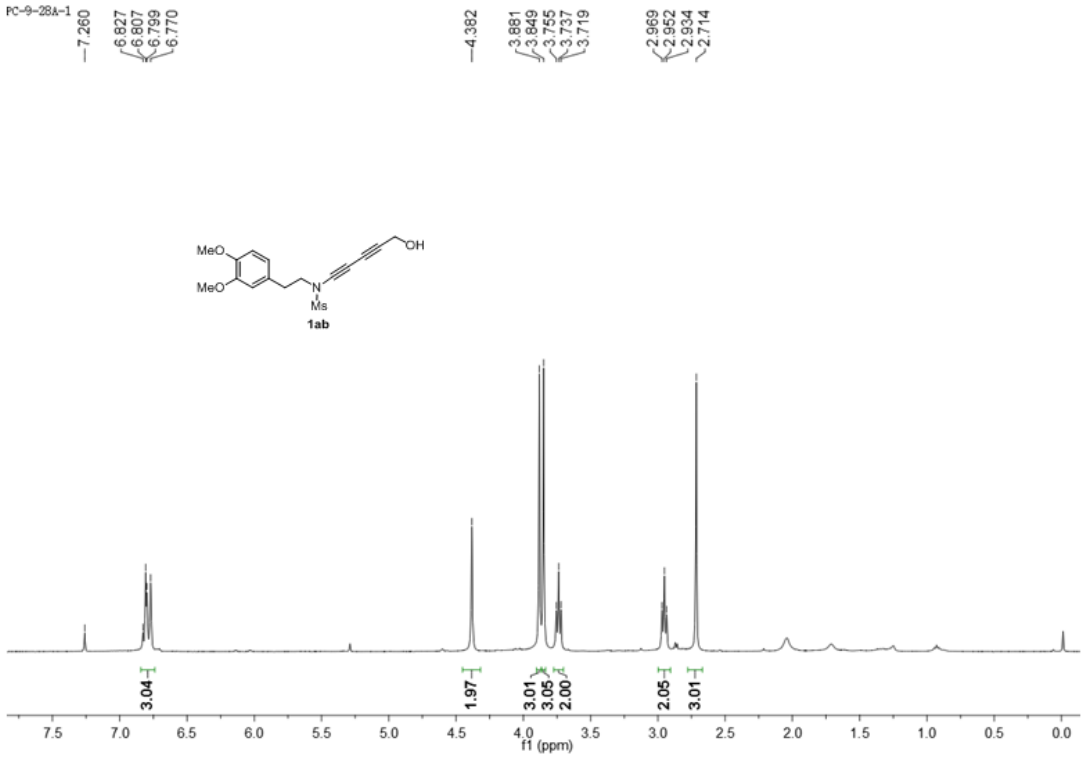
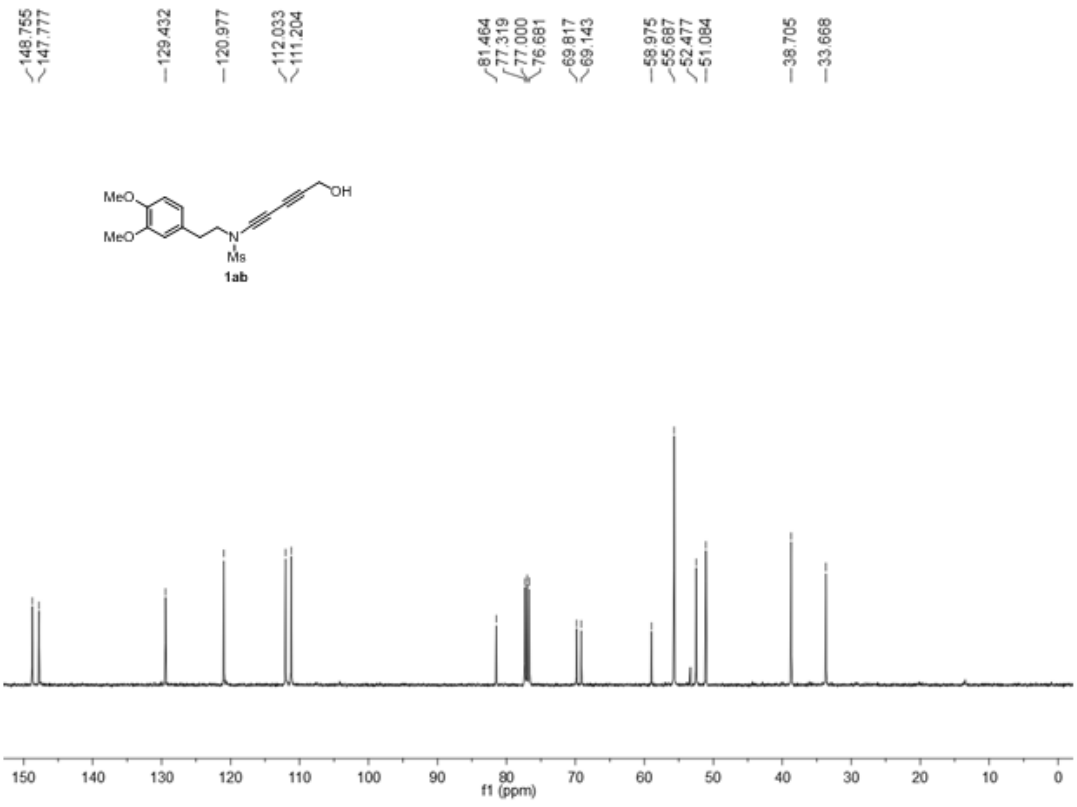
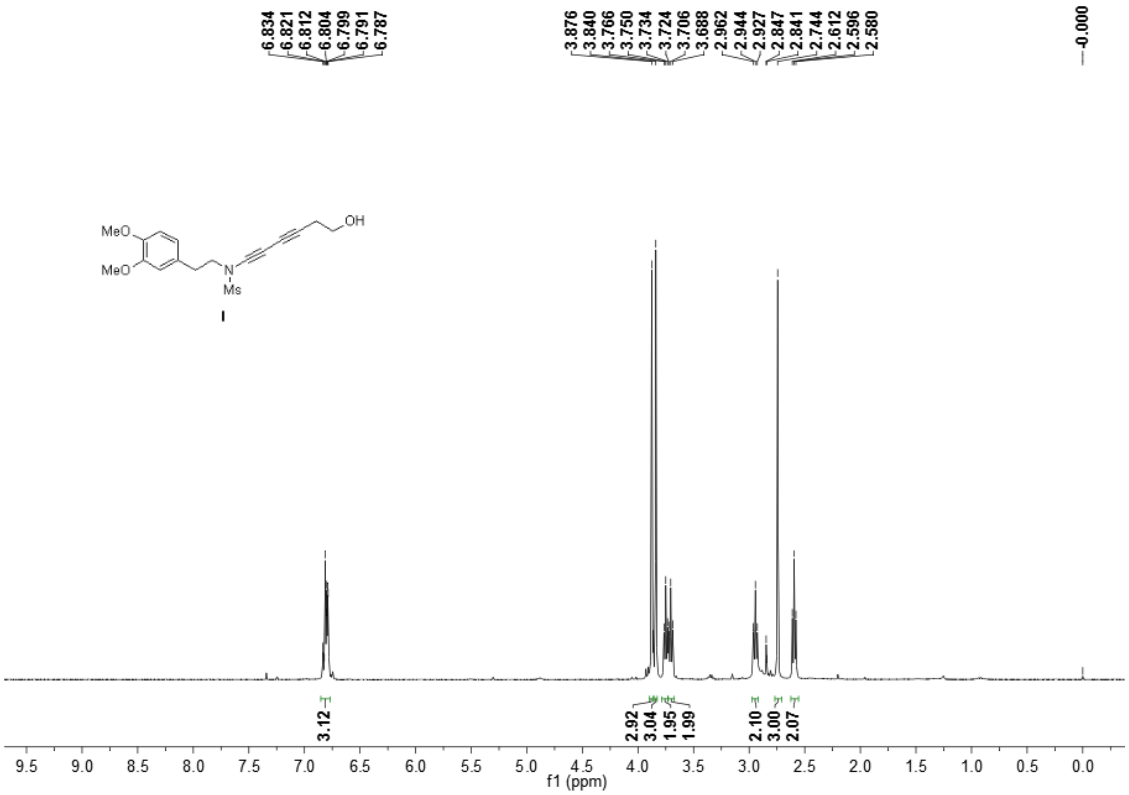
77.317
77.000
76.682
67.169
62.847
59.564
55.153
52.484
38.720
34.374
30.463
28.207
tBu
MeO
N
Ms
1z
f1 (ppm)

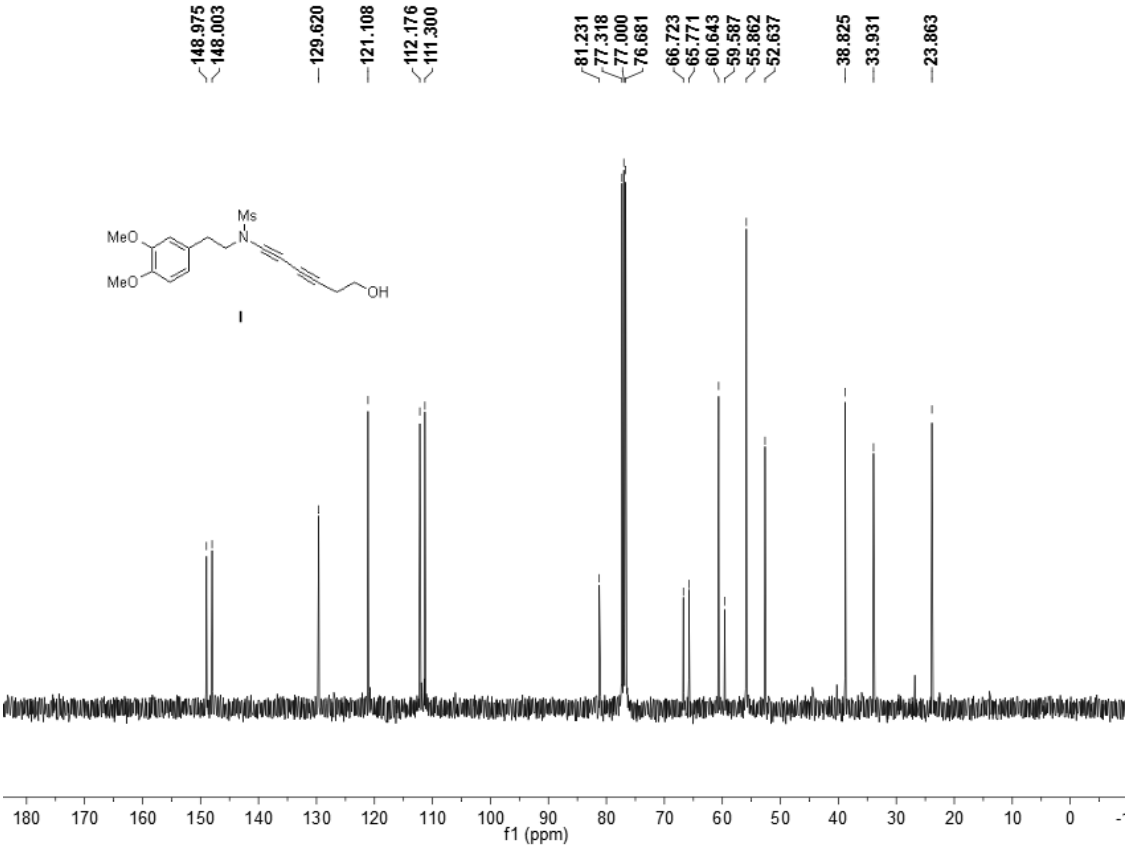

1jb-712CH
7.251
7.232
7.211
6.853
6.834
6.800
6.781
6.776
3.805
3.749
3.732
3.714
3.004
2.987
2.969
2.696
1.417
1.405
1.397
1.384
1.372
1.364
1.351
0.874
0.854
0.846
0.825
0.820
0.813
0.000
MeO
N
Ms
1aa
1.01
1.04
1.90
2.99
2.00
2.01
3.00
1.03
2.05
1.95
f1 (ppm)

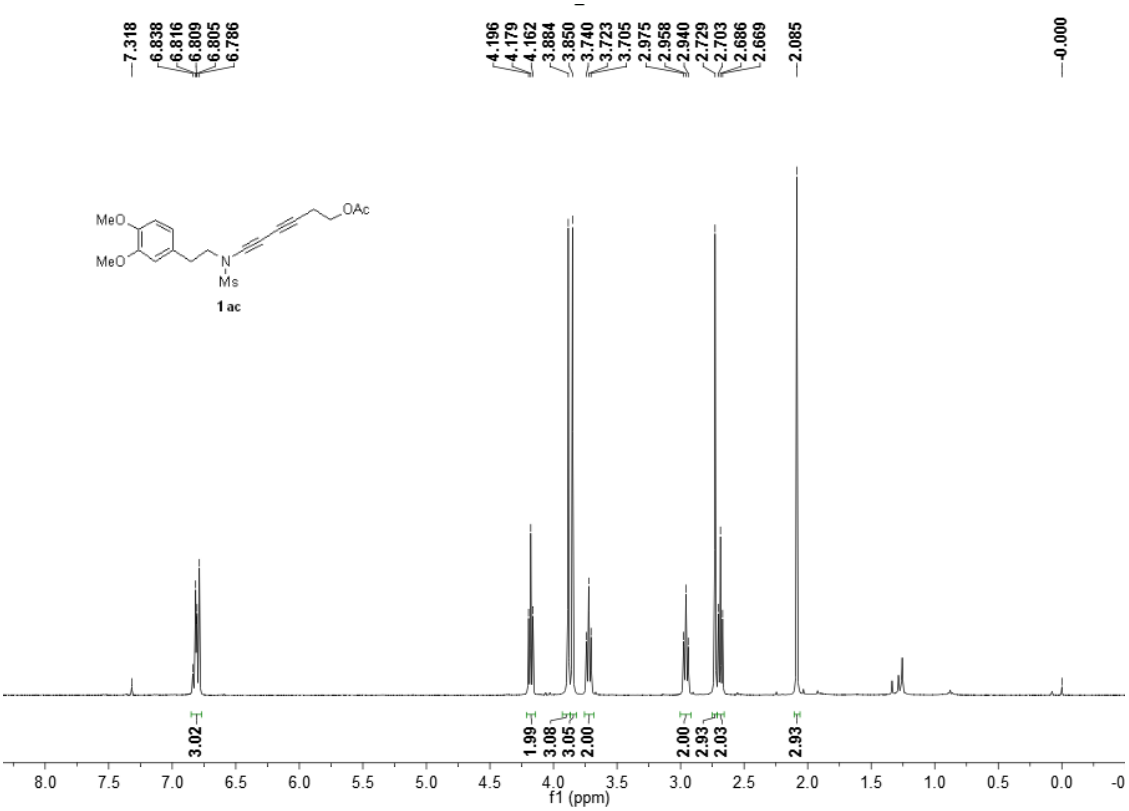

1jb-712
159.798
138.867
129.684
121.306
114.654
112.520
88.091
77.318
77.000
76.683
65.658
60.380
59.646
55.180
52.485
38.704
34.341
9.006
0.270
MeO
N
Ms
1aa
f1 (ppm)

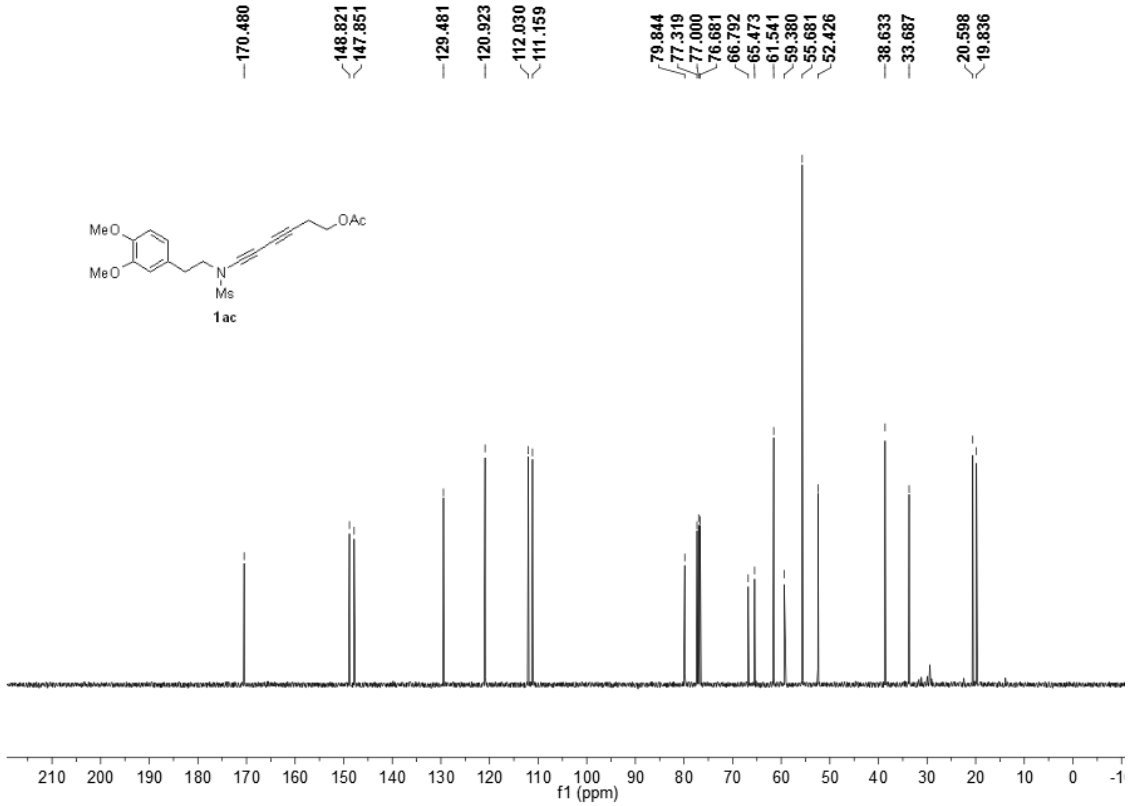

PC-9-28A-1
7.260
6.827
6.807
6.799
6.770
4.382
3.881
3.849
3.755
3.737
3.719
2.969
2.952
2.934
2.714
MeO
MeO
N
Ms
OH
1ab
3.04
1.97
3.01
3.05
2.00
2.05
3.01
f1 (ppm)

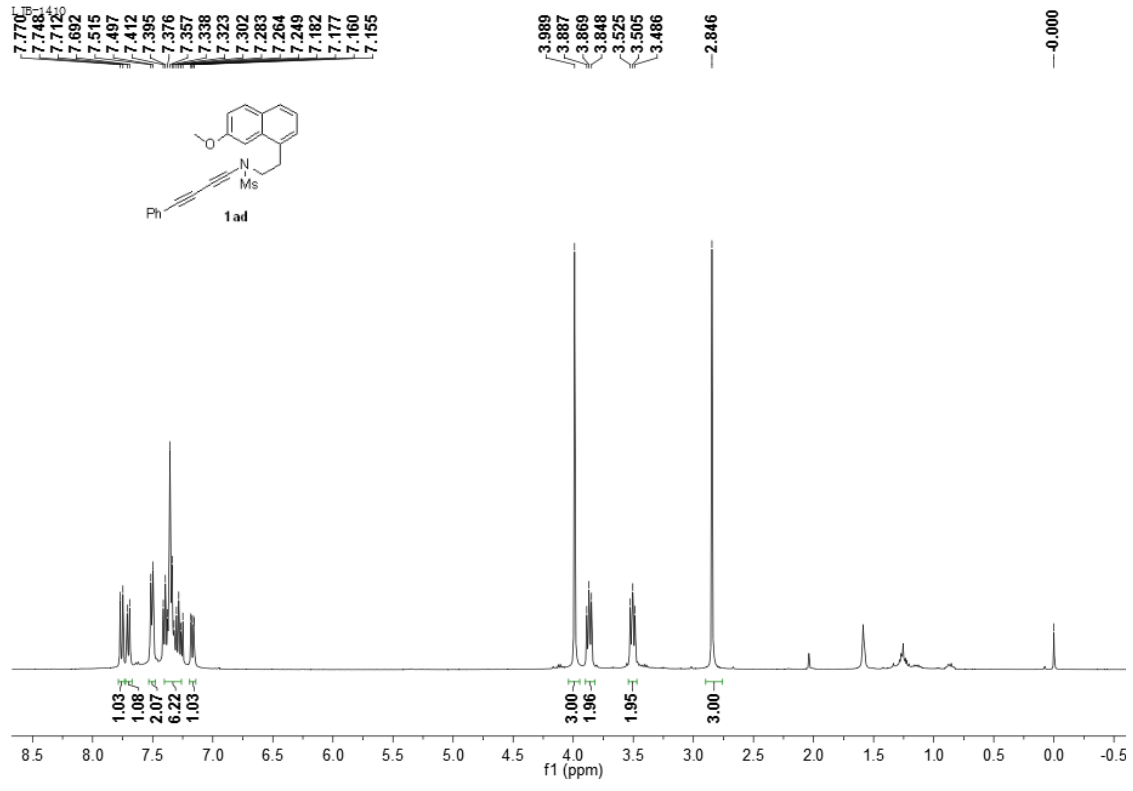

148.755
147.777
129.432
120.977
112.033
111.204
81.464
77.319
77.000
76.681
69.817
69.143
58.975
55.687
52.477
51.084
38.705
33.668
MeO
MeO
N
Ms
OH
1ab
f1 (ppm)

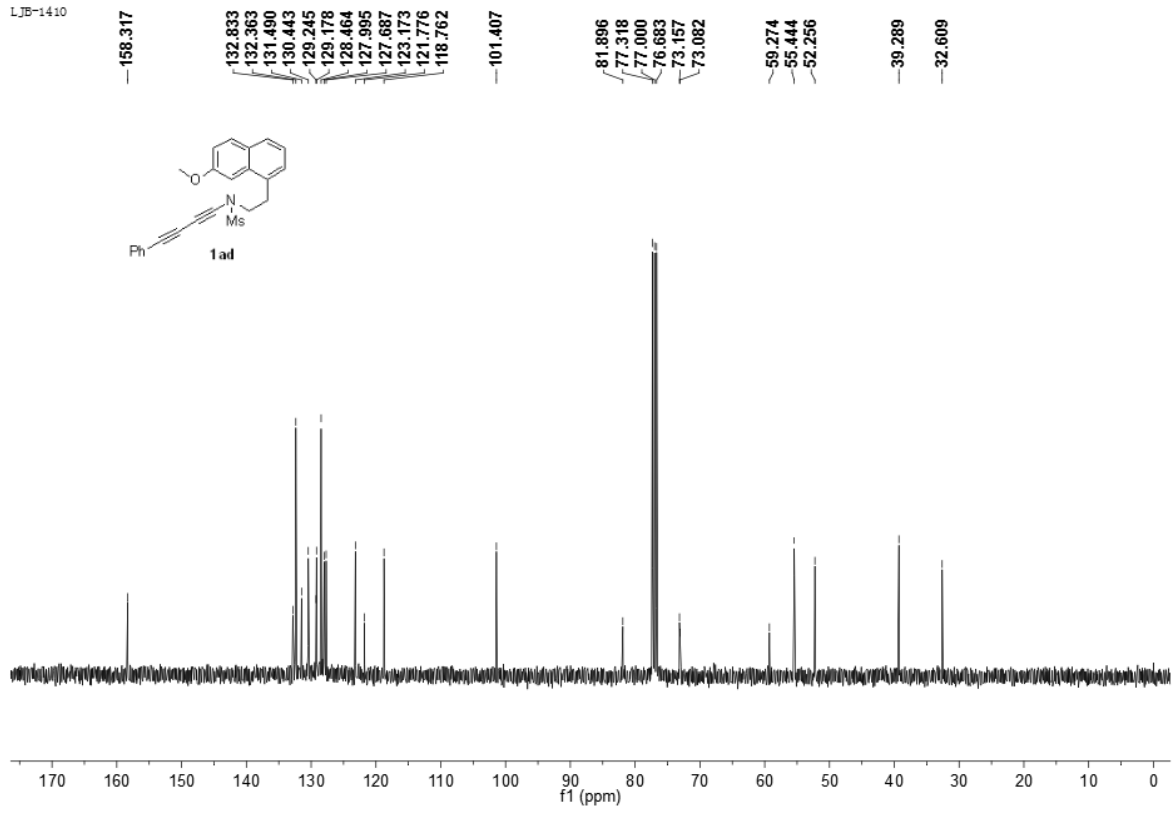

6.834
6.821
6.812
6.804
6.799
6.791
6.787
3.876
3.840
3.766
3.750
3.734
3.724
3.706
3.688
2.962
2.944
2.927
2.847
2.841
2.744
2.612
2.596
2.580
0.000
MeO
MeO
N
Ms
OH
I
3.12
2.92
3.04
1.95
1.99
2.10
3.00
2.07
f1 (ppm)

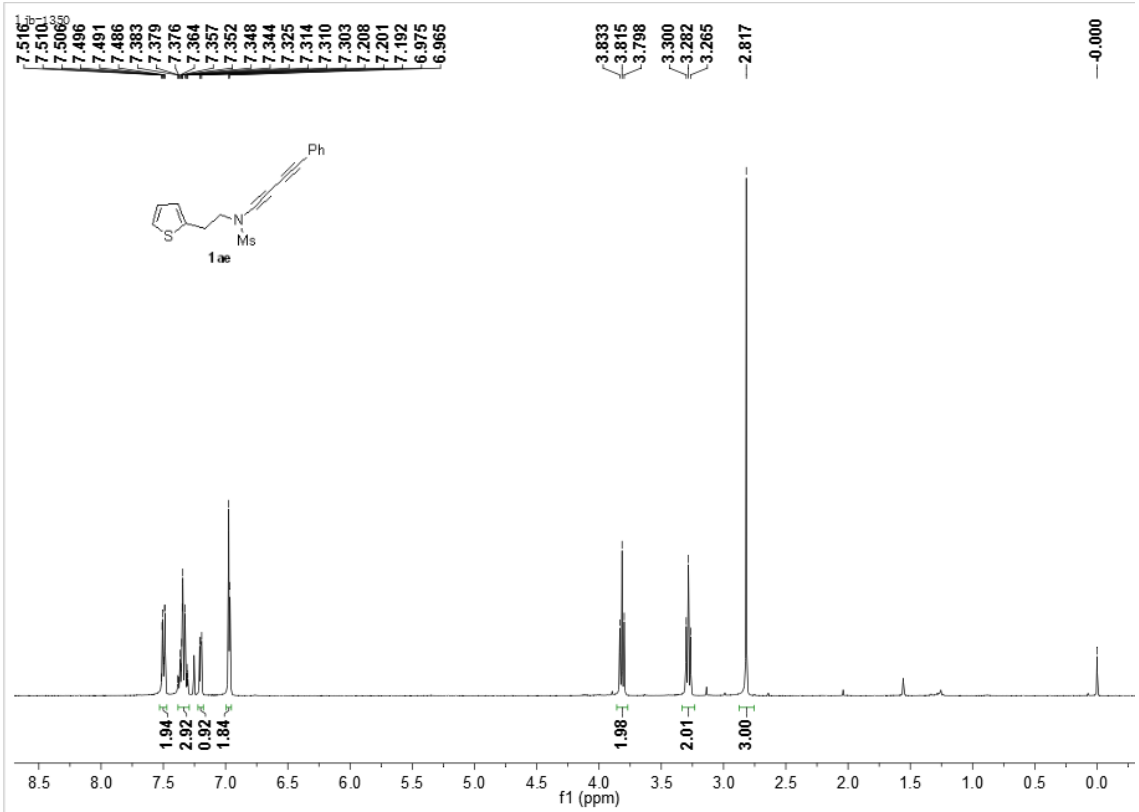

148.975
148.003
129.620
121.108
112.176
111.300
81.231
77.318
77.000
76.681
66.723
65.771
60.643
59.587
55.862
52.637
38.825
33.931
23.863
Ms
N
MeO
MeO
OH
I
f1 (ppm)

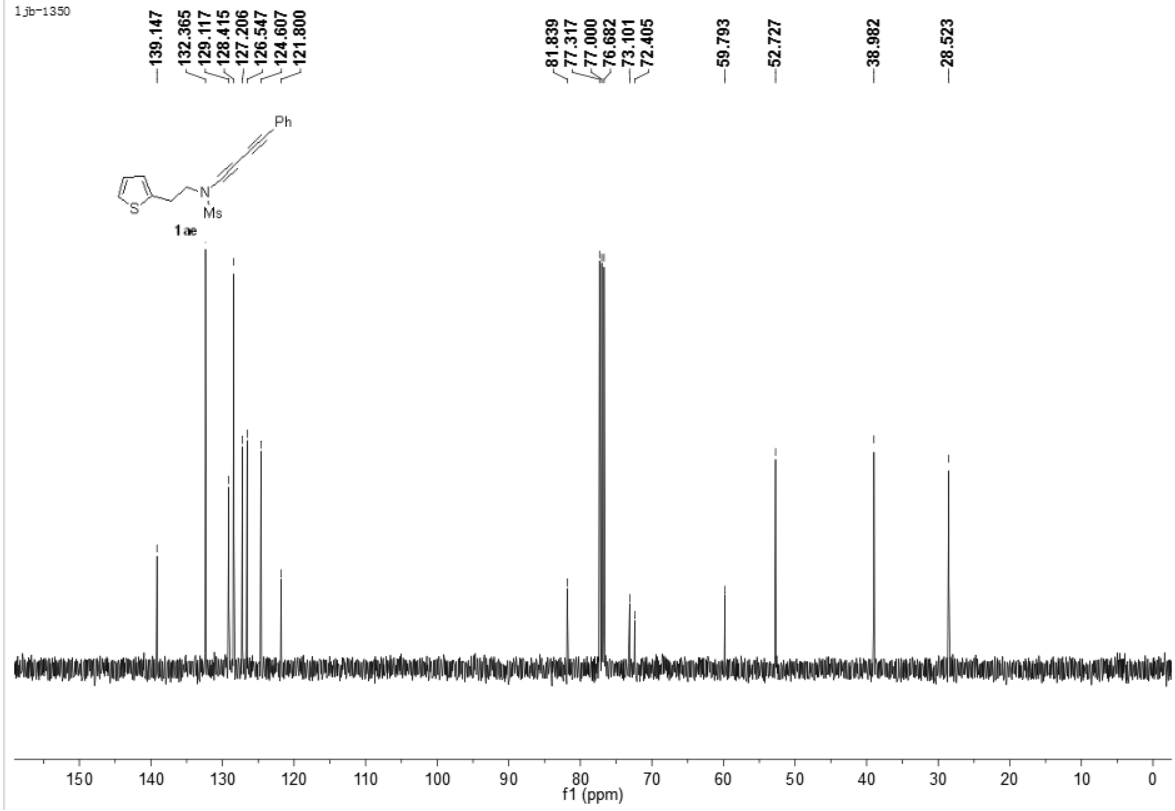

7.318
6.838
6.816
6.809
6.805
6.786
4.196
4.179
4.162
3.884
3.850
3.740
3.723
3.705
2.975
2.958
2.940
2.729
2.703
2.686
2.669
2.085
0.000
MeO
MeO
N
Ms
OAc
1ac
3.02
1.99
3.08
3.05
2.00
2.00
2.93
2.03
2.93
f1 (ppm)

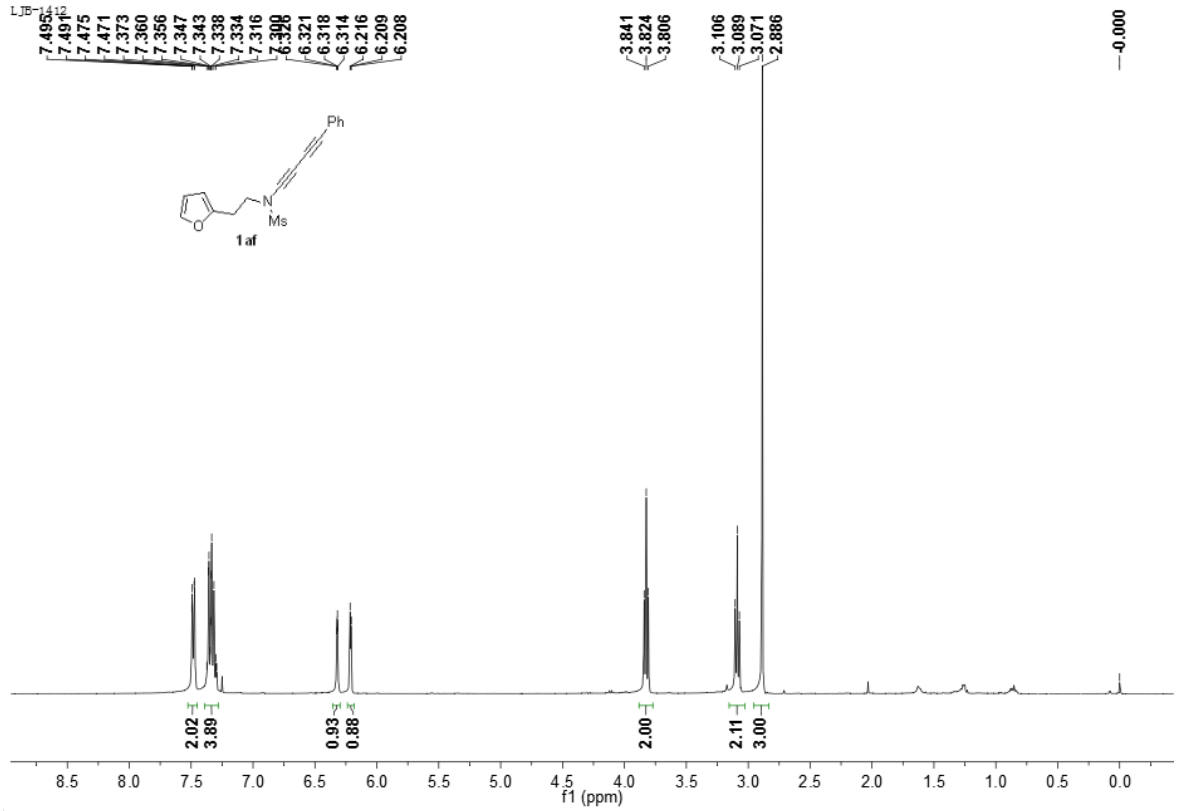

170.480
148.821
147.851
129.481
120.923
112.030
111.159
79.844
77.319
77.000
76.681
66.792
65.473
61.541
59.380
55.681
52.426
38.633
33.687
20.598
19.836
MeO
MeO
N
Ms
OAc
1ac
f1 (ppm)

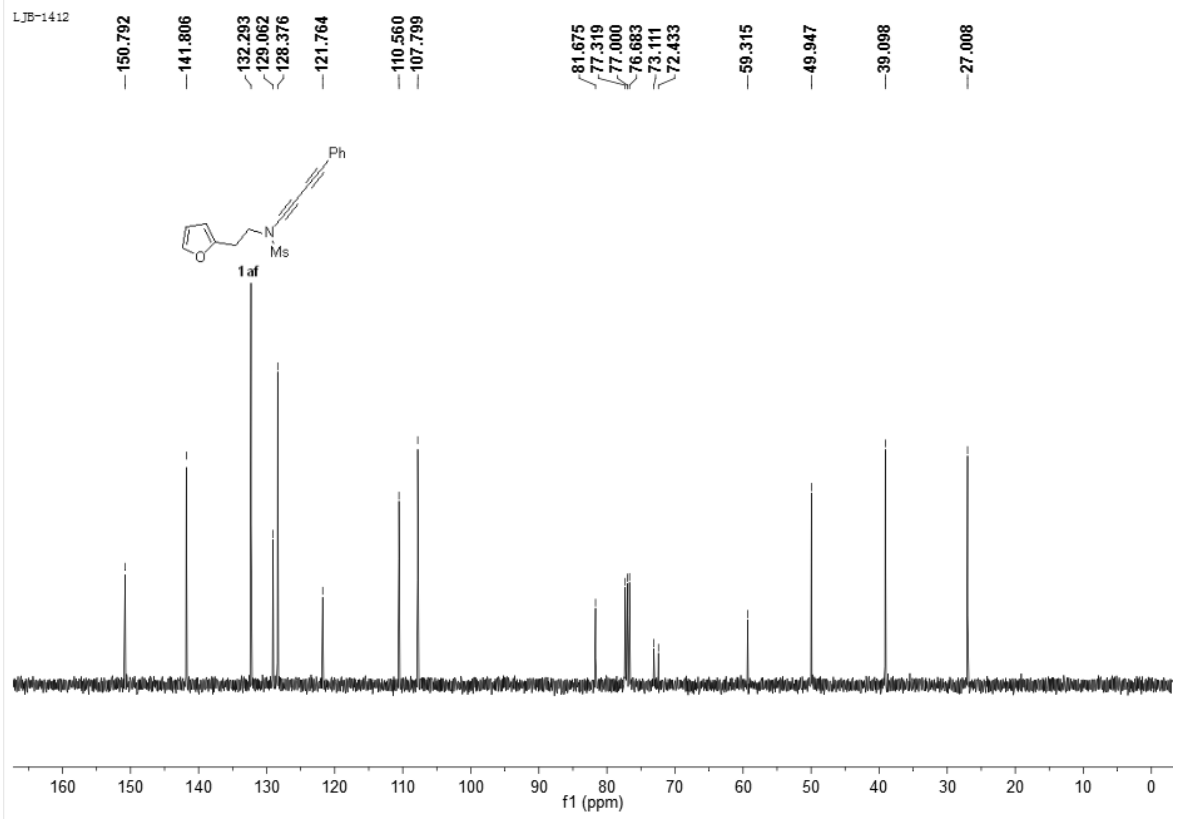

LJB-1410
7.770
7.748
7.712
7.692
7.515
7.497
7.412
7.395
7.376
7.357
7.338
7.323
7.302
7.283
7.264
7.249
7.182
7.177
7.160
7.155
3.989
3.887
3.869
3.848
3.525
3.505
3.486
2.846
0.000
O
N
Ms
Ph
1ad
1.03
1.08
2.07
6.22
1.03
3.00
1.96
1.95
3.00
f1 (ppm)

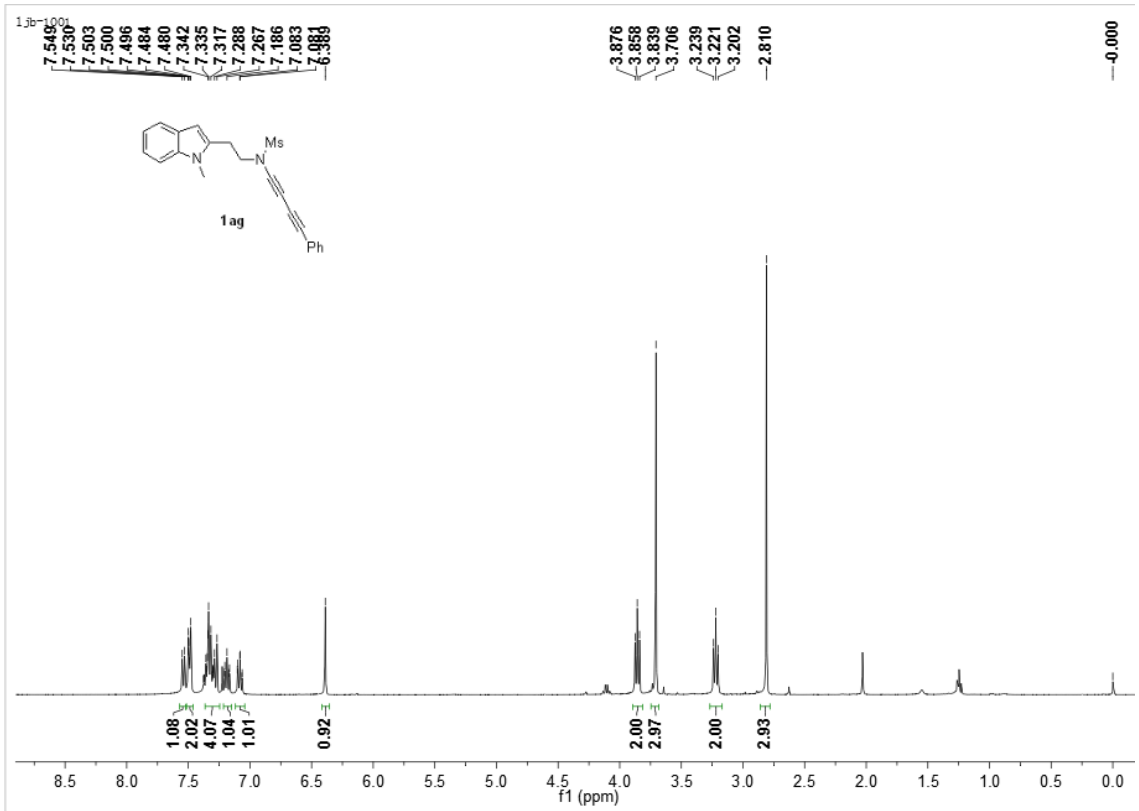

LJB-1410
158.317
132.833
132.363
131.490
130.443
129.245
129.178
128.464
127.995
127.687
123.173
121.776
118.762
101.407
81.896
77.318
77.000
76.683
73.157
73.082
59.274
55.444
52.256
39.289
32.609
O
N
Ms
Ph
1ad
f1 (ppm)

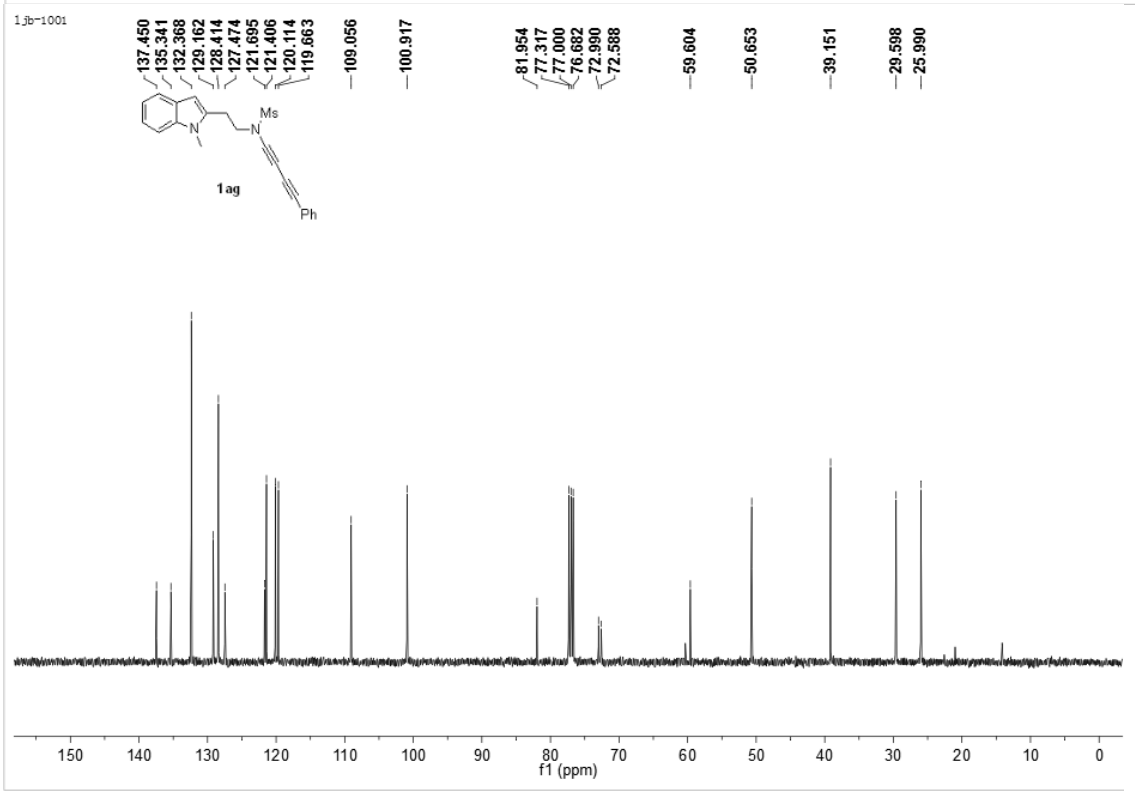

1jb-1350
7.516
7.510
7.506
7.496
7.491
7.486
7.383
7.379
7.376
7.364
7.357
7.352
7.348
7.344
7.325
7.314
7.310
7.303
7.208
7.201
7.192
6.975
6.965
3.833
3.815
3.798
3.300
3.282
3.265
2.817
0.000
Ph
N
Ms
S
1ae
1.94
2.92
0.92
1.84
1.98
2.01
3.00
f1 (ppm)

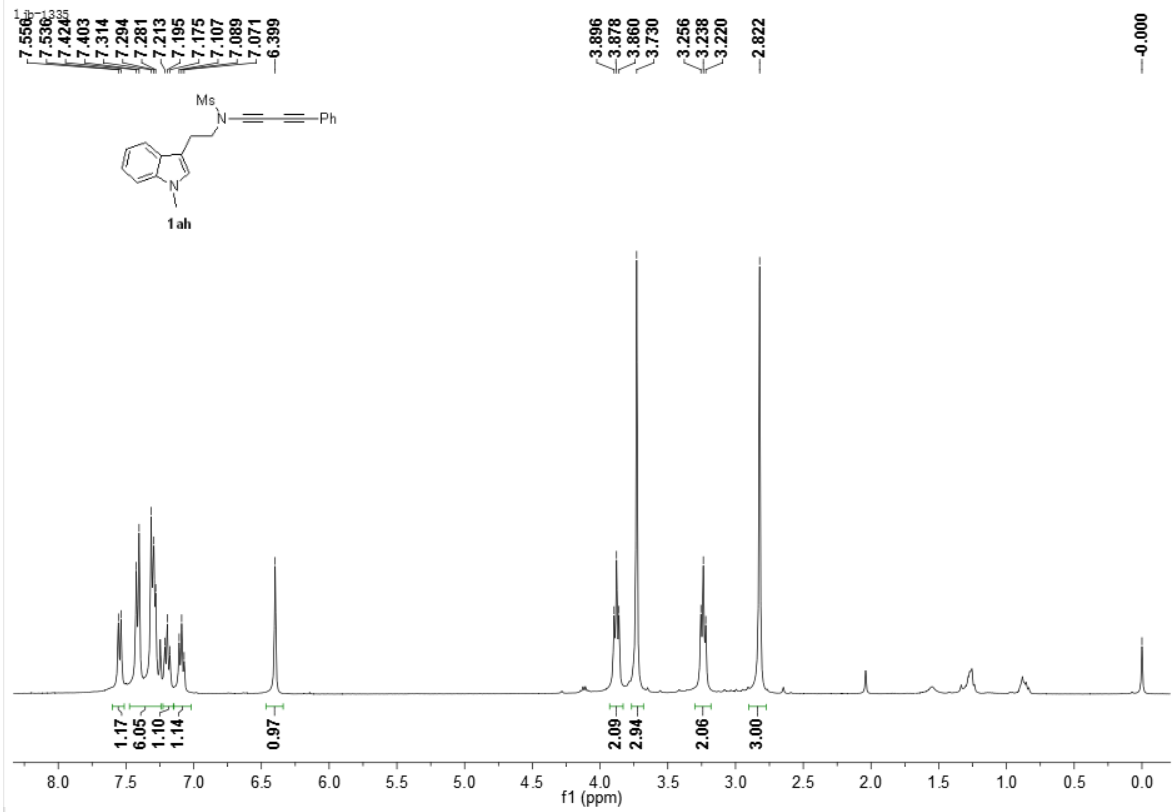

1jb-1350
139.147
132.365
129.117
128.415
127.206
126.547
124.607
121.800
81.839
77.317
77.000
76.682
73.101
72.405
59.793
52.727
38.982
28.523
Ph
N
Ms
S
1ae
f1 (ppm)

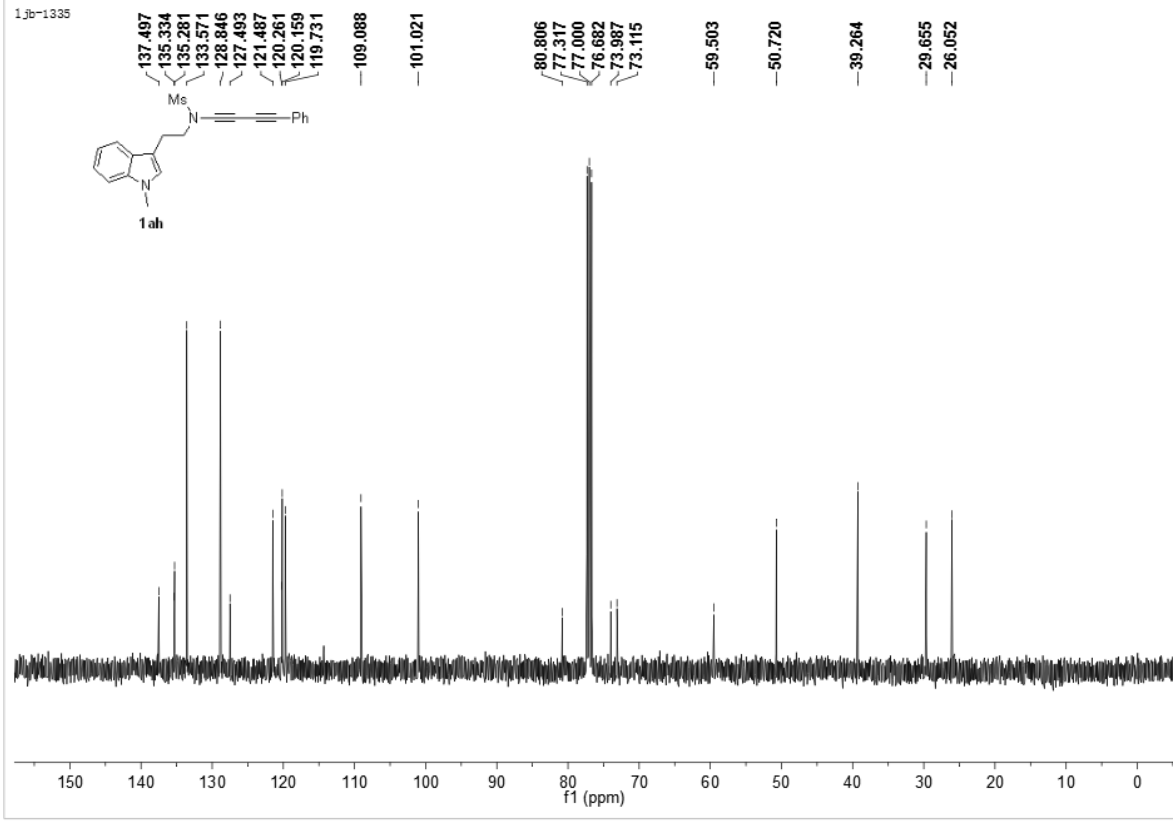

LJB-1412
7.495
7.491
7.475
7.471
7.373
7.360
7.356
7.347
7.343
7.338
7.334
7.316
6.321
6.318
6.314
6.216
6.209
6.208
3.841
3.824
3.806
3.106
3.089
3.071
2.886
-0.000
Ph
N
Ms
O
1af
2.02
3.89
0.93
0.88
2.00
2.11
3.00
f1 (ppm)

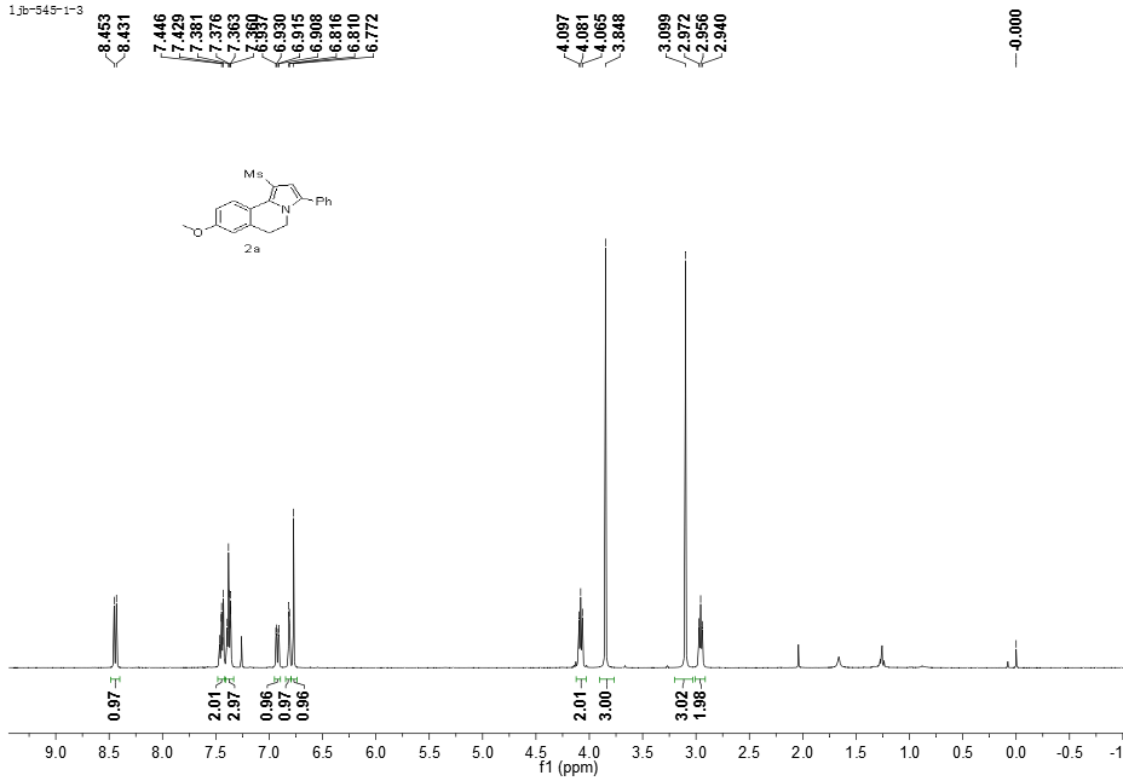

LJB-1412
150.792
141.806
132.293
129.062
128.376
121.764
110.560
107.799
81.675
77.319
77.000
76.683
73.111
72.433
59.315
49.947
39.098
27.008
Ph
N
Ms
O
1af
f1 (ppm)

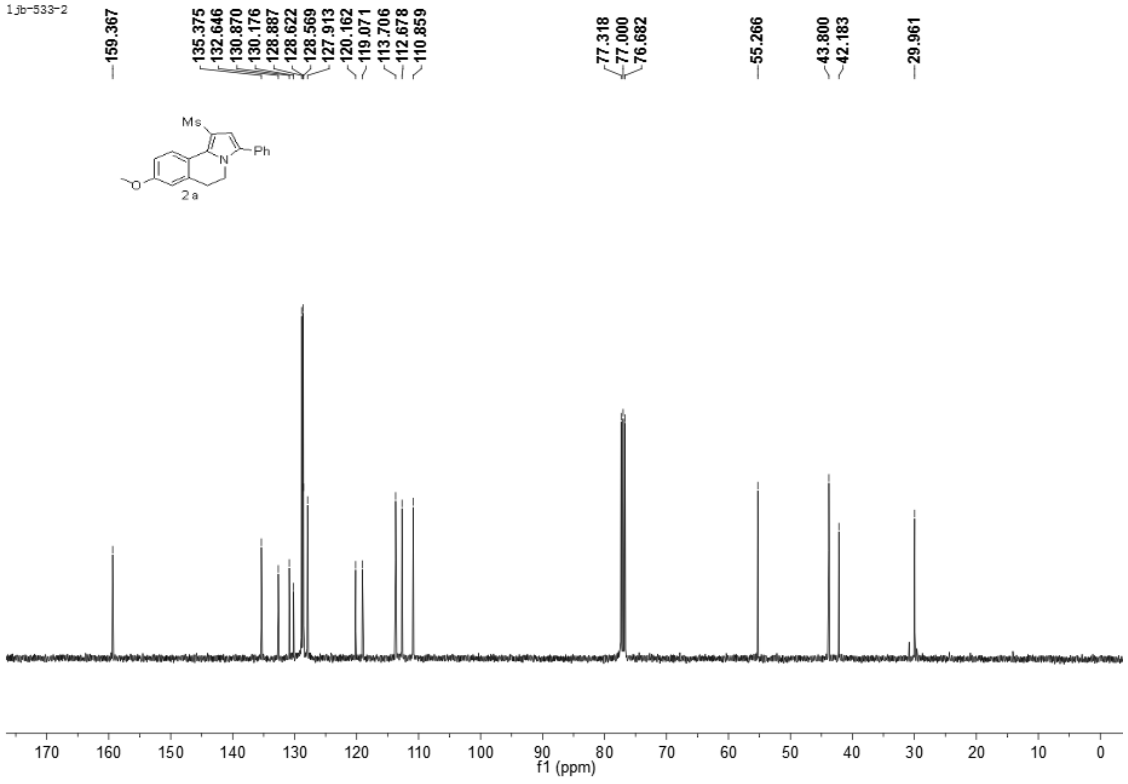

1jb-1001
7.549
7.530
7.503
7.500
7.496
7.484
7.480
7.342
7.335
7.317
7.288
7.267
7.186
7.083
3.876
3.858
3.839
3.706
3.239
3.221
3.202
2.810
0.000
Ms
N
1ag
Ph
1.08
2.02
4.07
1.04
1.01
0.92
2.00
2.97
2.00
2.93
f1 (ppm)

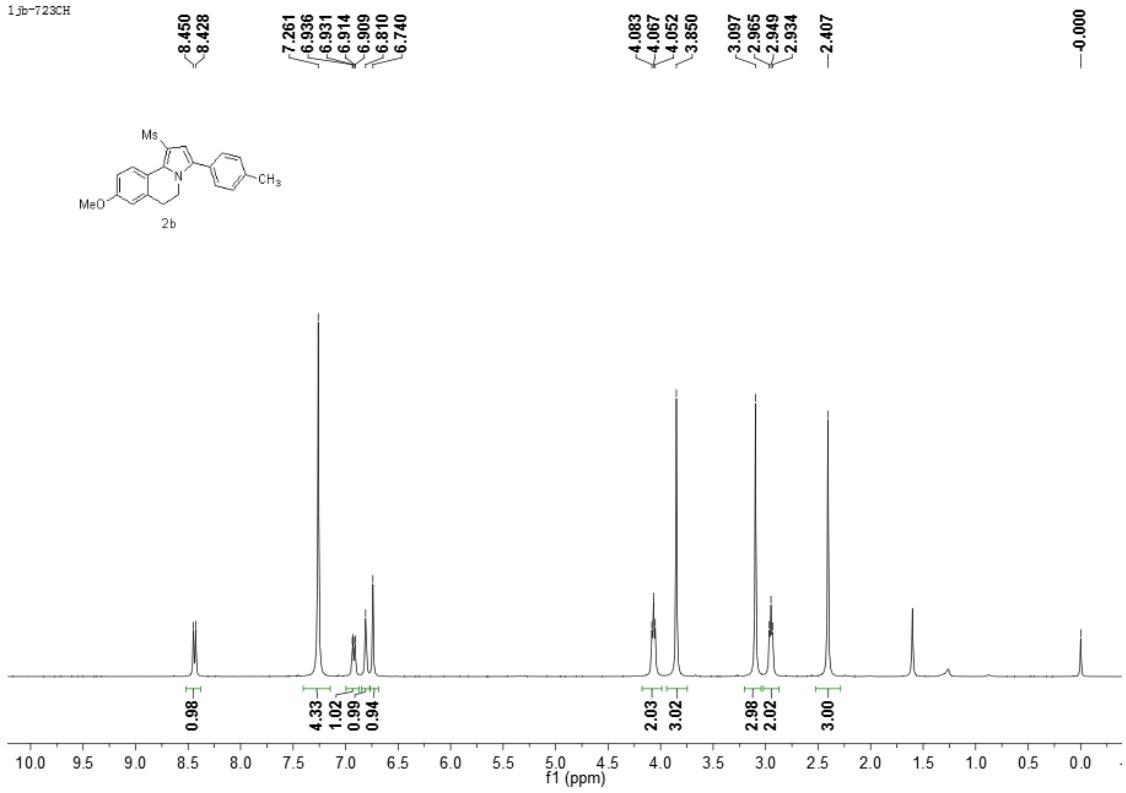

1jb-1001
137.450
135.341
132.368
129.162
128.414
127.474
121.695
121.406
120.114
119.663
109.056
100.917
81.954
77.317
77.000
76.682
72.990
72.588
59.604
50.653
39.151
29.598
25.990
Ms
N
1ag
Ph
f1 (ppm)

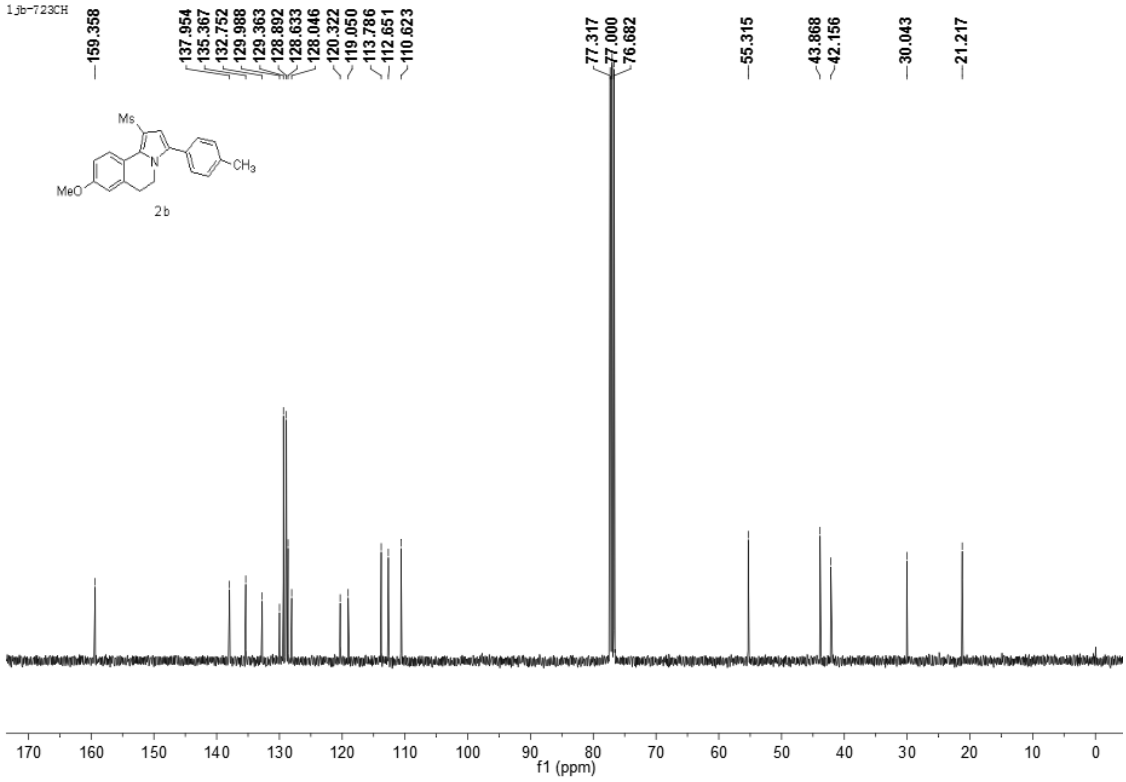

1jb-1335
7.556
7.536
7.424
7.403
7.314
7.294
7.281
7.213
7.195
7.175
7.107
7.089
7.071
6.399
3.896
3.878
3.860
3.730
3.256
3.238
3.220
2.822
0.000
Ms
N
Ph
N
1ah
1.17
6.05
1.10
1.14
0.97
2.09
2.94
2.06
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

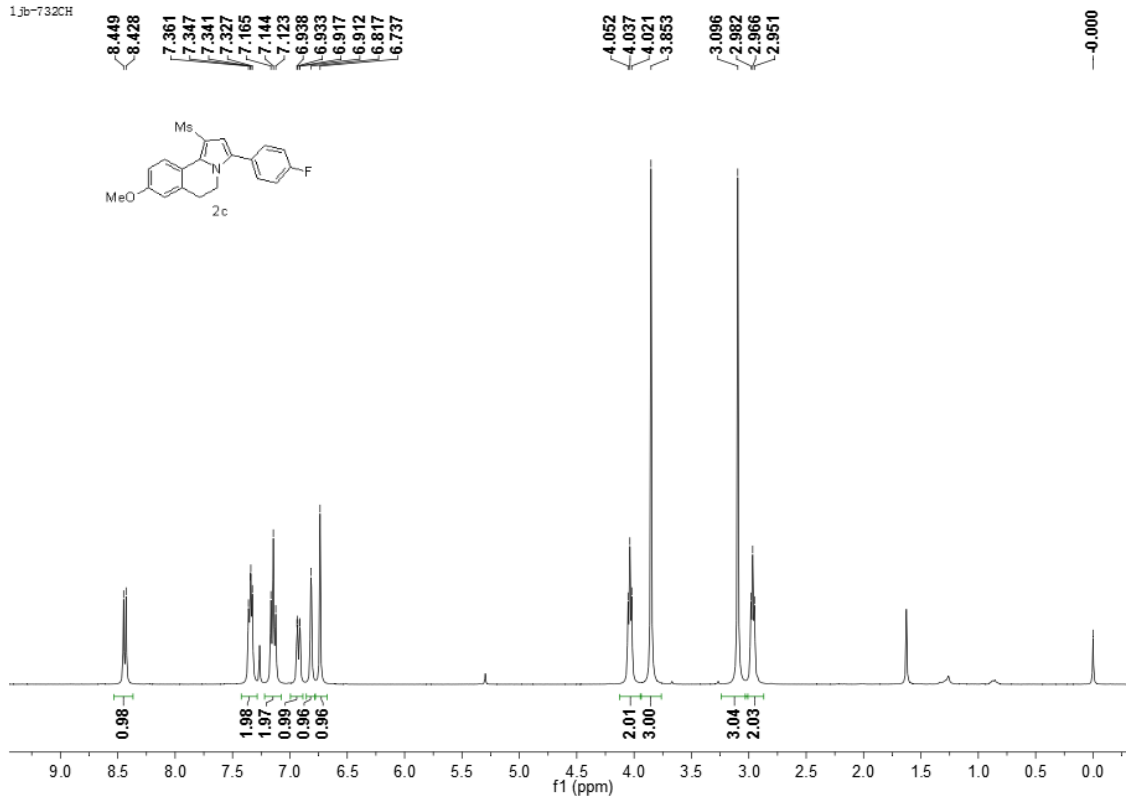

1jb-1335
137.497
135.334
135.281
133.571
128.846
127.493
121.487
120.261
120.159
119.731
109.088
101.021
80.806
77.317
77.000
76.682
73.987
73.115
59.503
50.720
39.264
29.655
26.052
Ms
N
Ph
N
1ah
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

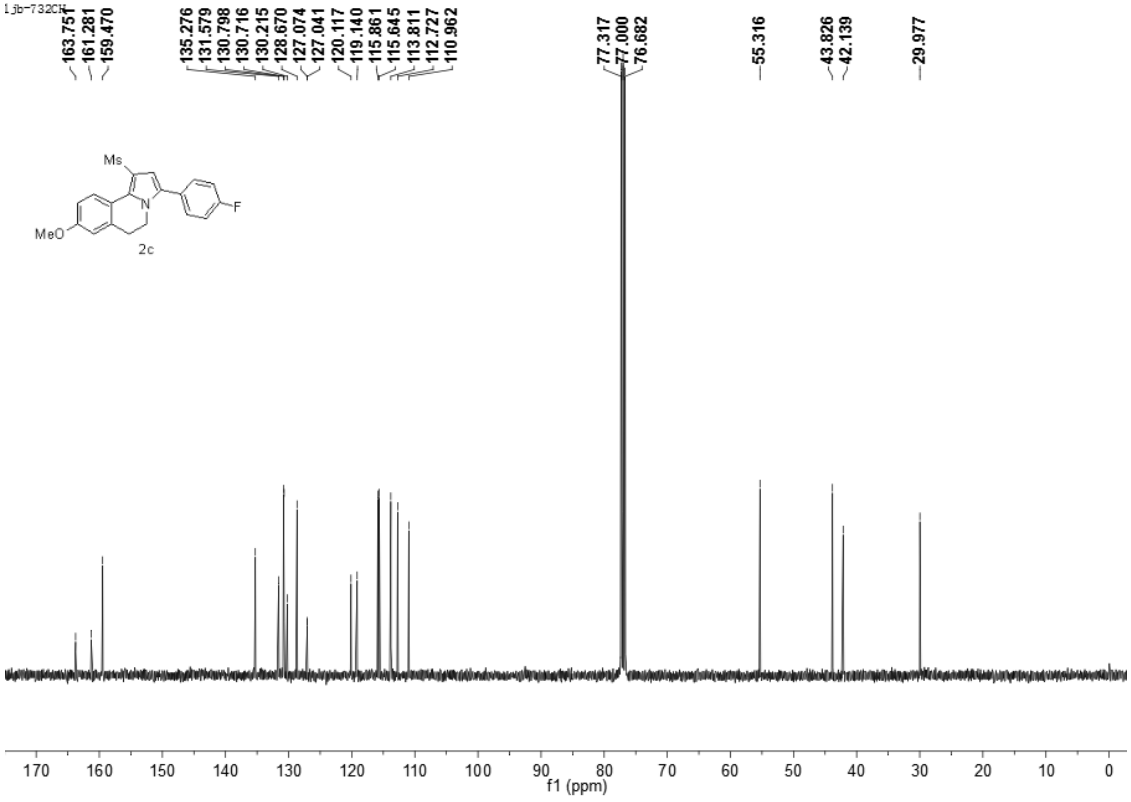

1jb-545-1-3
8.453
8.431
7.446
7.429
7.381
7.376
7.363
6.930
6.915
6.908
6.816
6.810
6.772
4.097
4.081
4.065
3.848
3.099
2.972
2.956
2.940
0.000
Ms
Ph
N
O
2a
0.97
2.01
2.97
0.96
0.97
0.96
2.01
3.00
3.02
1.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

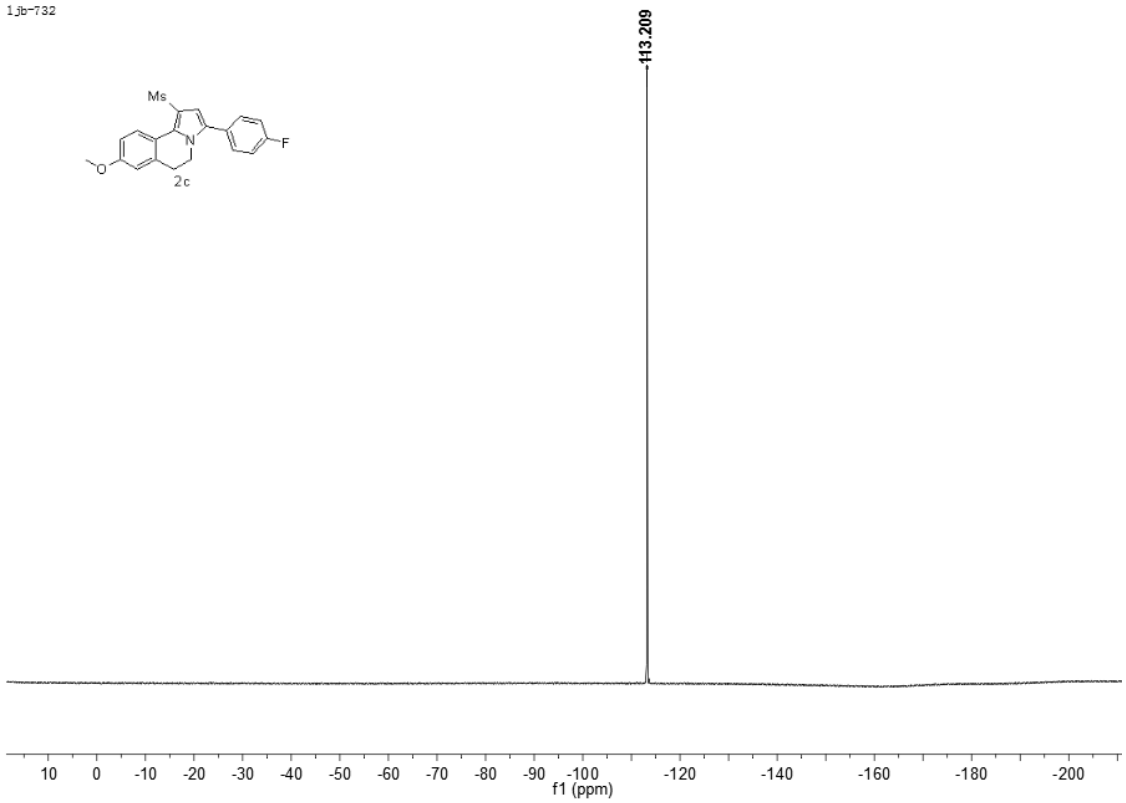

1jb-533-2
159.367
135.375
132.646
130.870
130.176
128.887
128.622
128.569
127.913
120.162
119.071
113.706
112.678
110.859
77.318
77.000
76.682
55.266
43.800
42.183
29.961
Ms
Ph
N
O
2a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

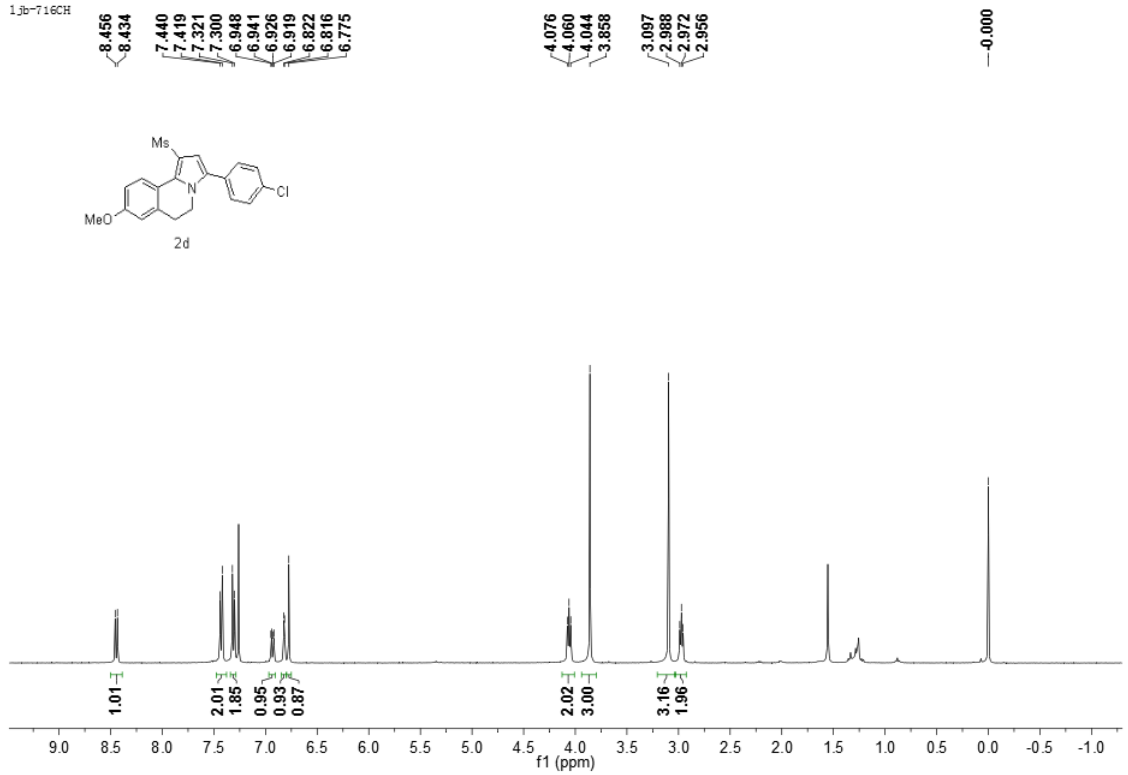

1jb-723CH
8.450
8.428
7.261
6.936
6.931
6.914
6.909
6.810
6.740
4.083
4.067
4.052
3.850
3.097
2.965
2.949
2.934
2.407
0.000
Ms
MeO
CH3
2b
0.98
4.33
1.02
0.99
0.94
2.03
3.02
2.98
2.02
3.00
f1 (ppm)

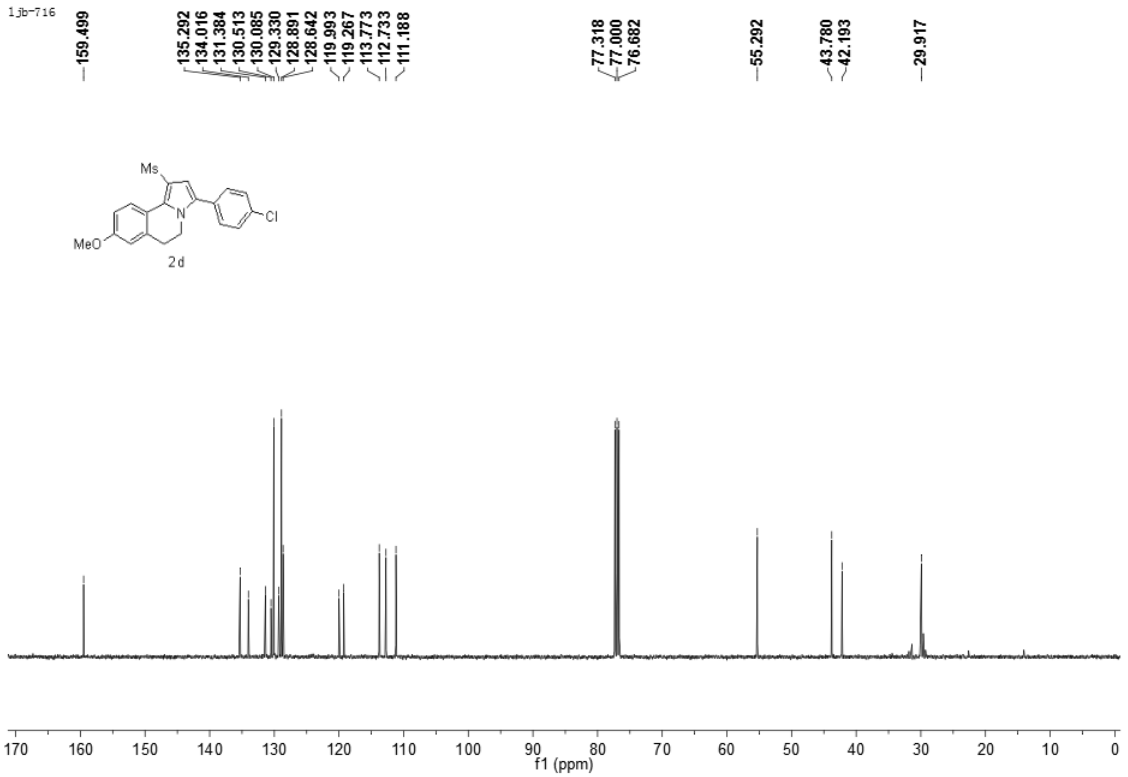

1jb-723CH
159.358
137.954
135.367
132.752
129.988
129.363
128.892
128.633
128.046
120.322
119.050
113.786
112.651
110.623
77.317
77.000
76.682
55.315
43.868
42.156
30.043
21.217
Ms
MeO
CH3
2b
f1 (ppm)

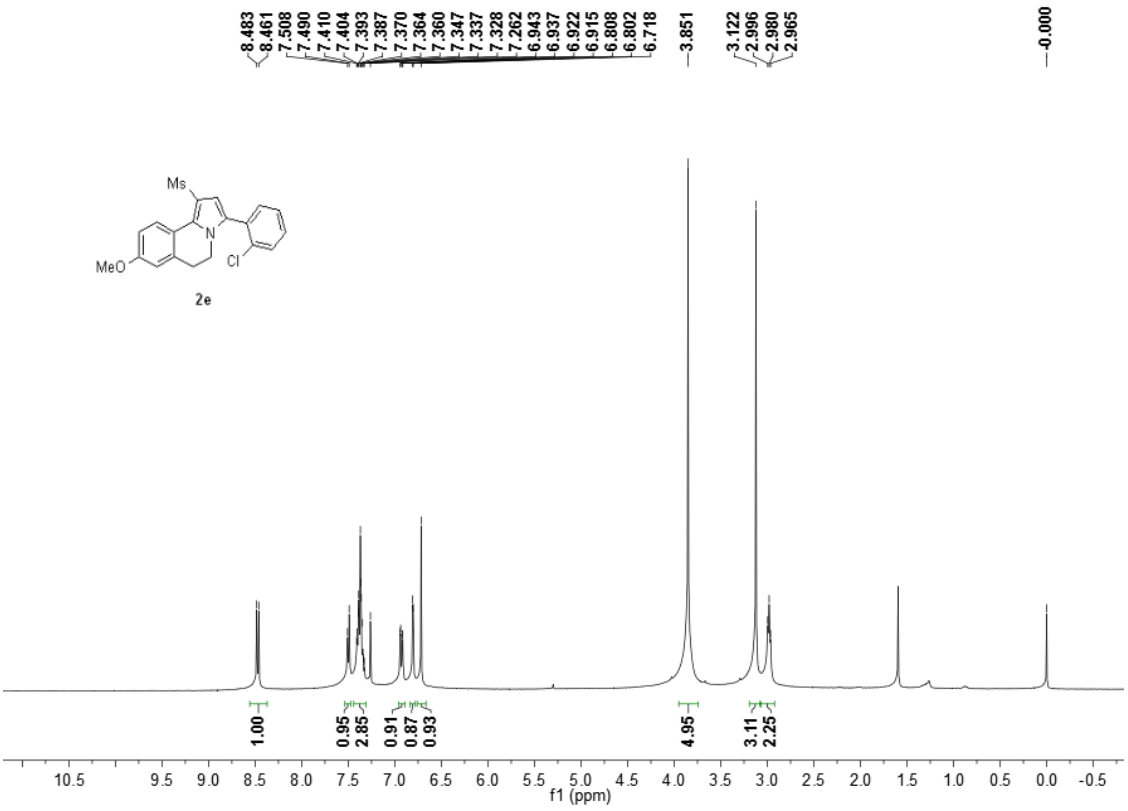

1jb-732CH
8.449
8.428
7.361
7.347
7.341
7.327
7.165
7.144
7.123
6.938
6.933
6.917
6.912
6.817
6.737
4.052
4.037
4.021
3.853
3.096
2.982
2.966
2.951
0.000
Ms
MeO
F
N
2c
0.98
1.98
1.97
0.99
0.96
0.96
2.01
3.00
3.04
2.03
f1 (ppm)

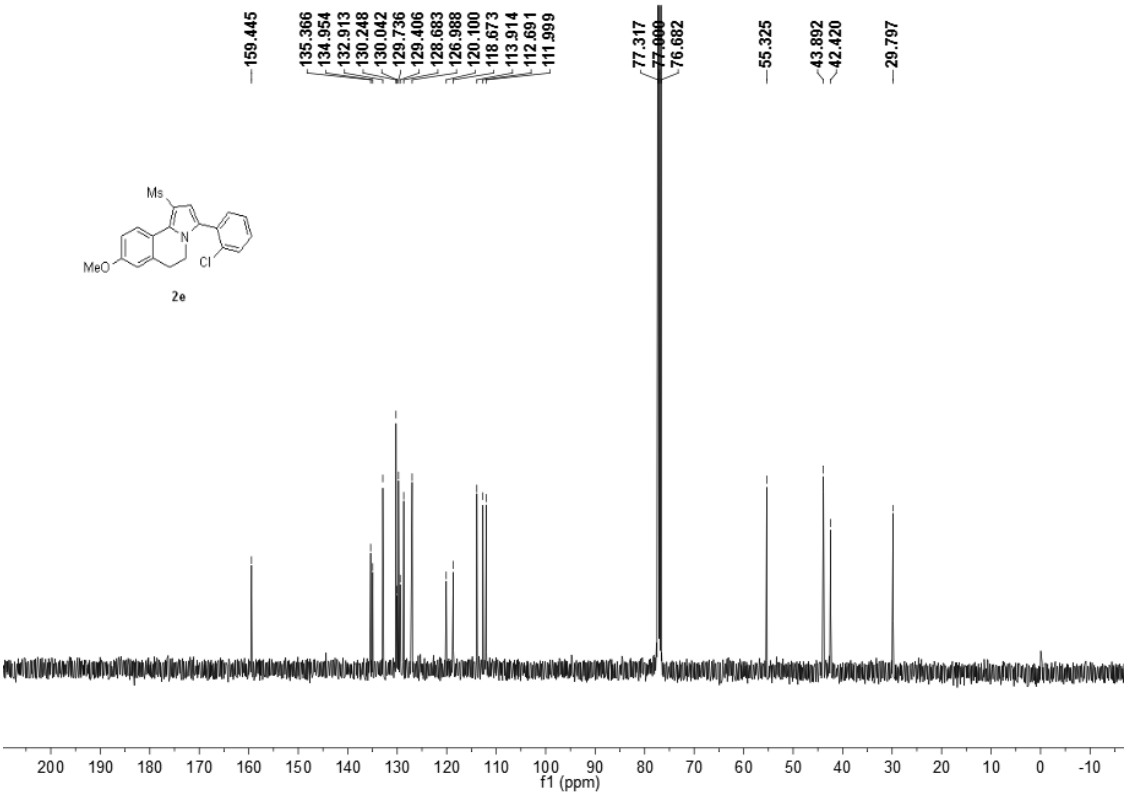

1jb-732CH
163.751
161.281
159.470
135.276
131.579
130.798
130.716
130.215
128.670
127.074
127.041
120.117
119.140
115.861
115.645
113.811
112.727
110.962
77.317
77.000
76.682
55.316
43.826
42.139
29.977
Ms
MeO
F
N
2c
f1 (ppm)

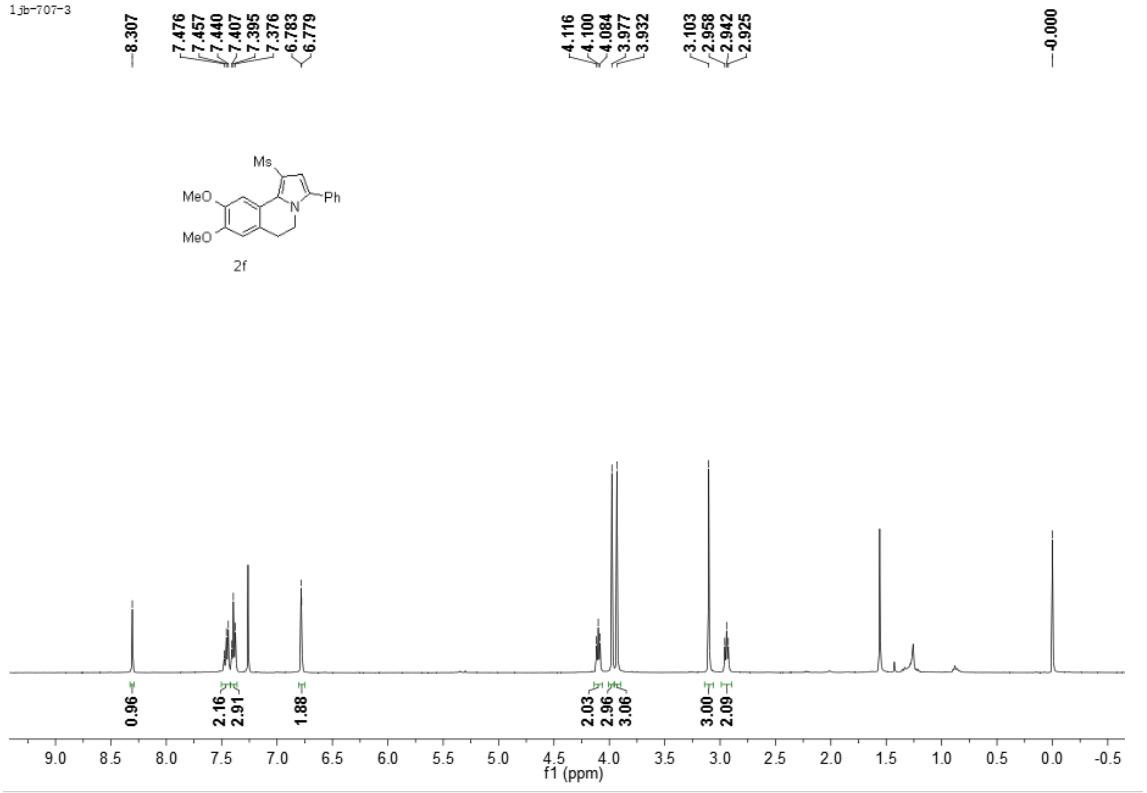

1jb-732
113.209
Ms
F
O
2c
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

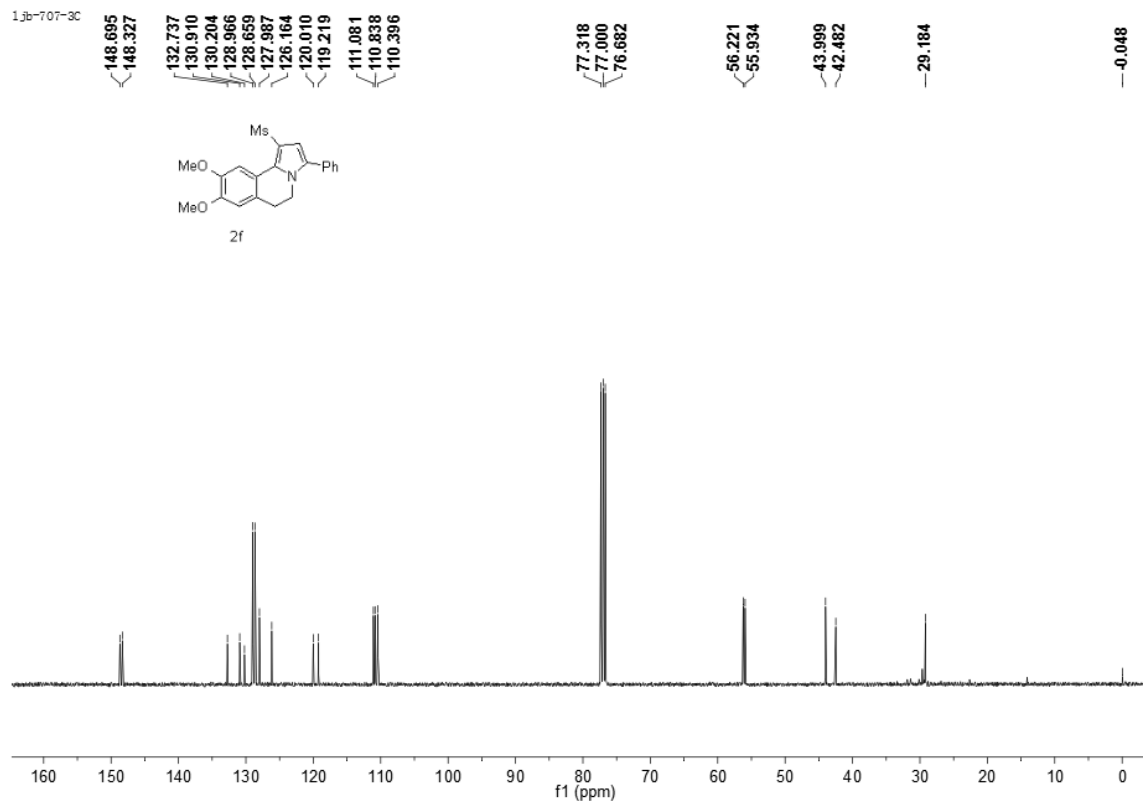

1jb-716CH
8.456
8.434
7.440
7.419
7.321
7.300
6.948
6.941
6.926
6.919
6.822
6.816
6.775
4.076
4.060
4.044
3.858
3.097
2.988
2.972
2.956
0.000
Ms
Cl
MeO
2d
1.01
2.01
1.85
0.95
0.93
0.87
2.02
3.00
3.16
1.96
f1 (ppm)


1jb-716
159.499
135.292
134.016
131.384
130.513
130.085
129.330
128.891
128.642
119.993
119.267
113.773
112.733
111.188
77.318
77.000
76.682
55.292
43.780
42.193
29.917
Ms
Cl
MeO
2d
f1 (ppm)


8.483
8.461
7.508
7.490
7.410
7.404
7.393
7.387
7.370
7.364
7.360
7.347
7.337
7.328
7.262
6.943
6.937
6.922
6.915
6.808
6.802
6.718
3.851
3.122
2.996
2.980
2.965
0.000
Ms
MeO
Cl
2e
1.00
0.95
2.85
0.91
0.87
0.93
4.95
3.11
2.25
f1 (ppm)


159.445
135.366
134.954
132.913
130.248
130.042
129.736
129.406
128.683
126.988
120.100
118.673
113.914
112.691
111.999
77.317
77.000
76.682
55.325
43.892
42.420
29.797
Ms
MeO
Cl
2e
f1 (ppm)


1jb-707-3
8.307
7.476
7.457
7.440
7.407
7.395
7.376
6.783
6.779
4.116
4.100
4.084
3.977
3.932
3.103
2.958
2.942
2.925
0.000
Ms
MeO
MeO
N
Ph
2f
0.96
2.16
2.91
1.88
2.03
2.96
3.06
3.00
2.09
f1 (ppm)


1jb-707-3C
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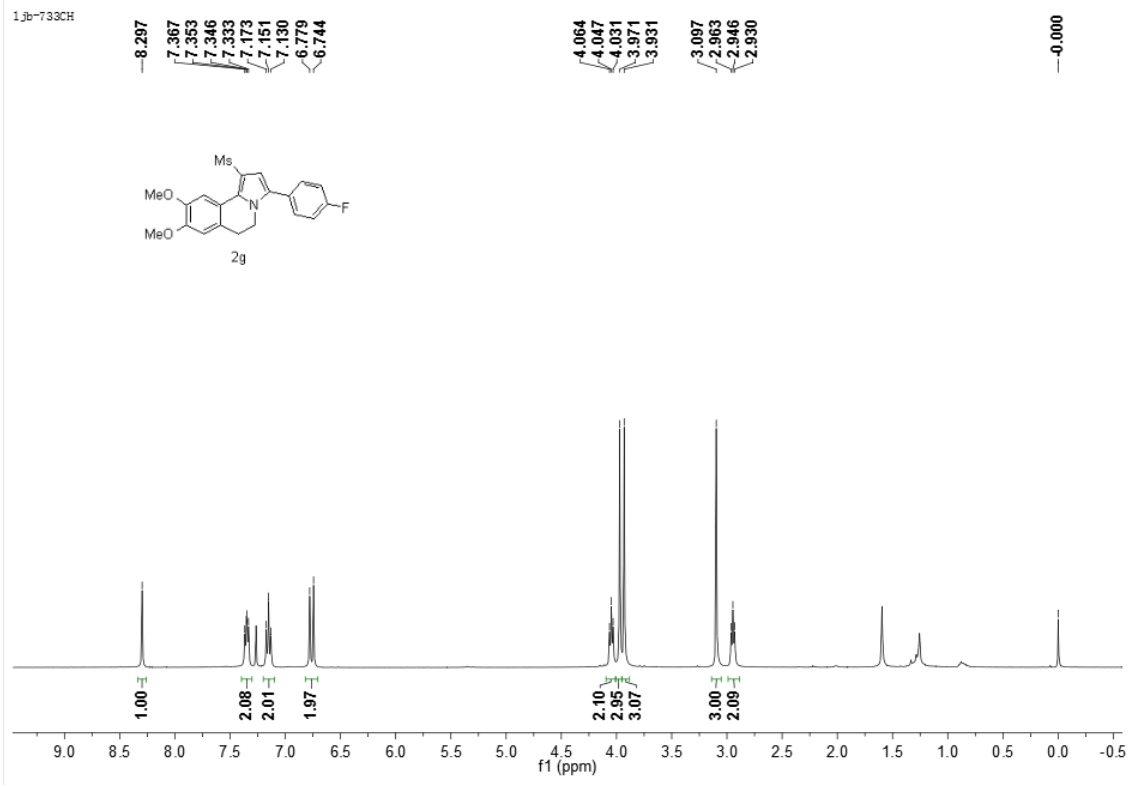
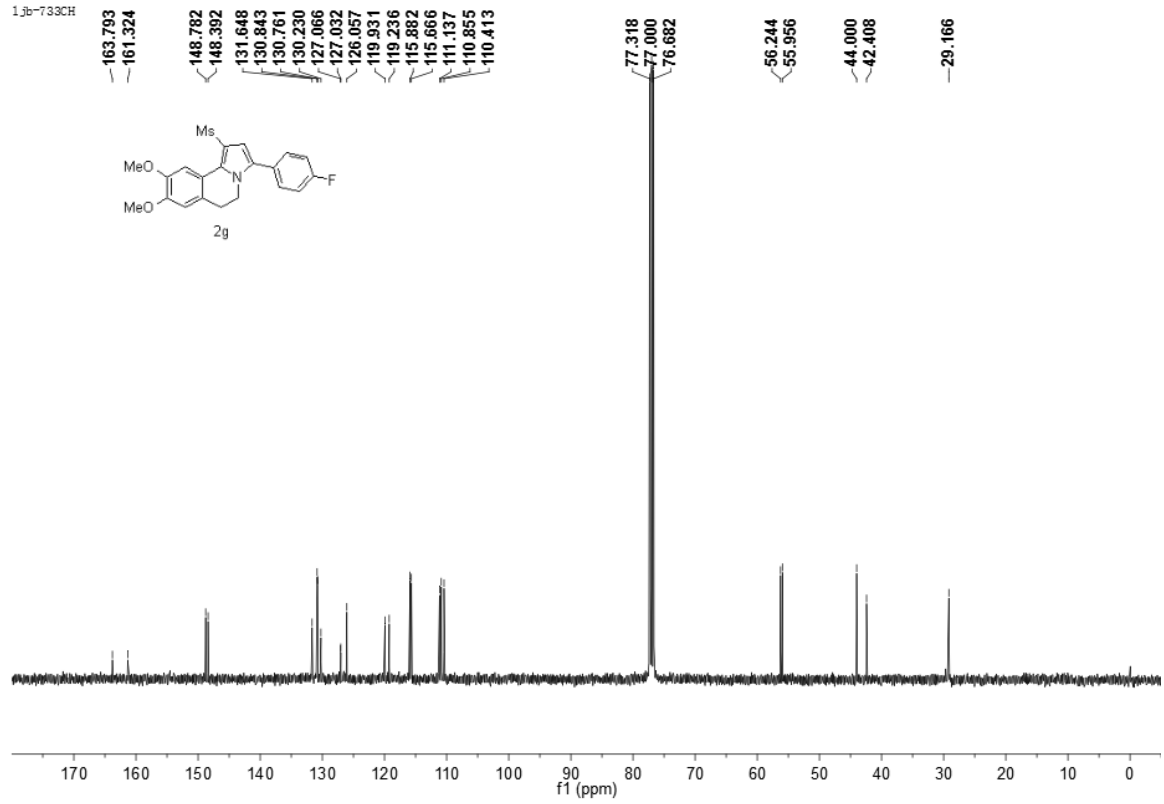
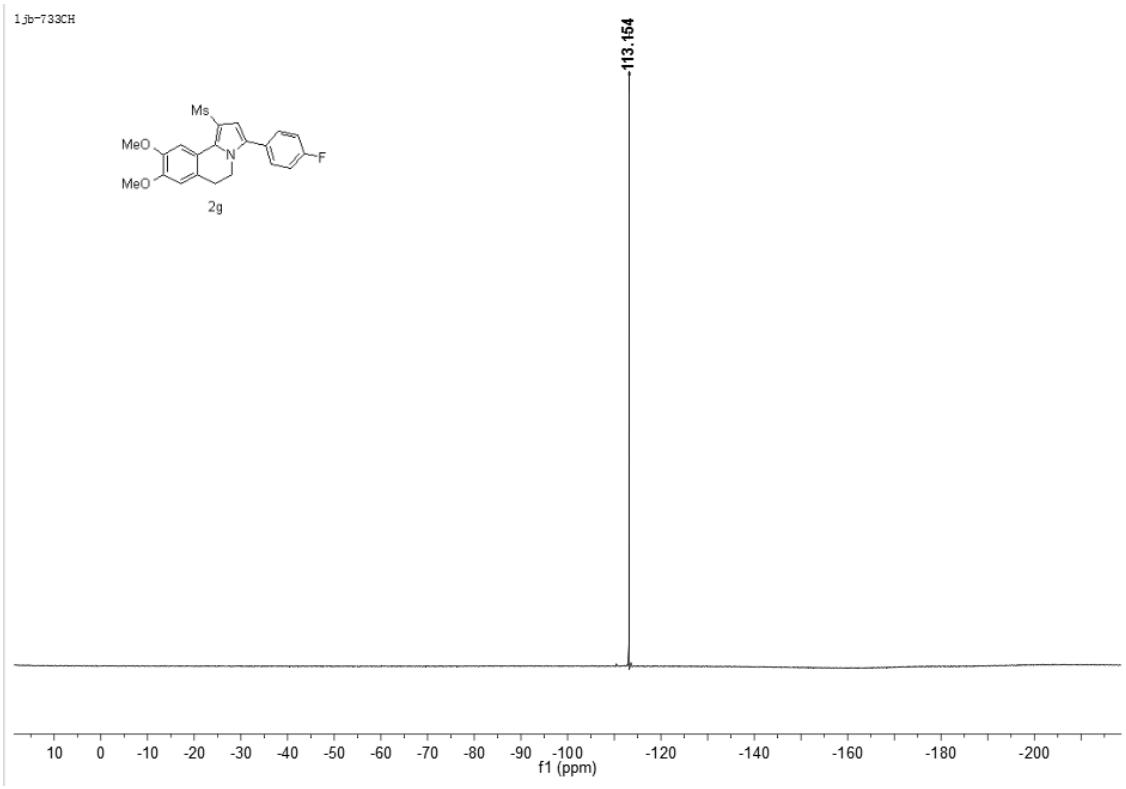
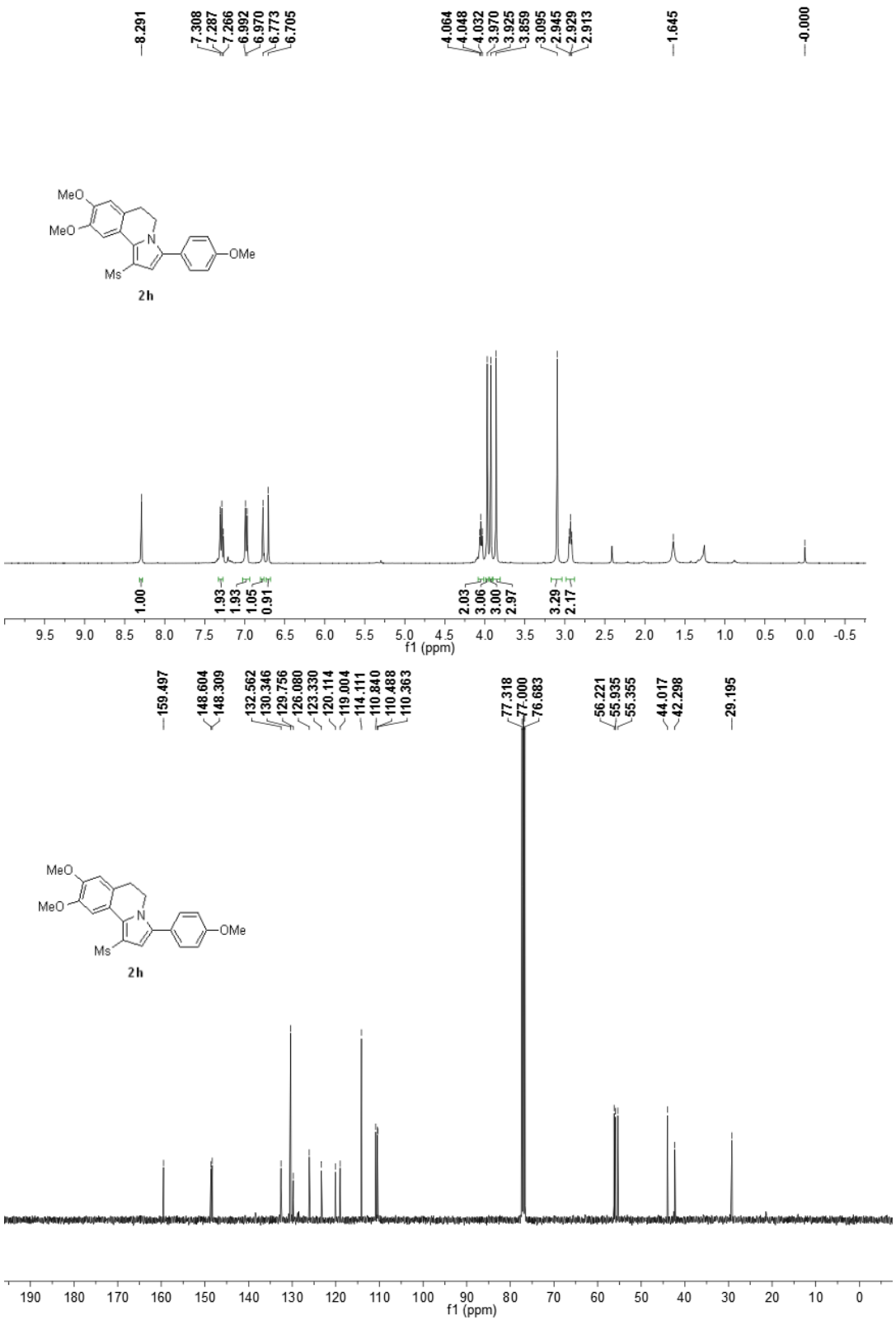
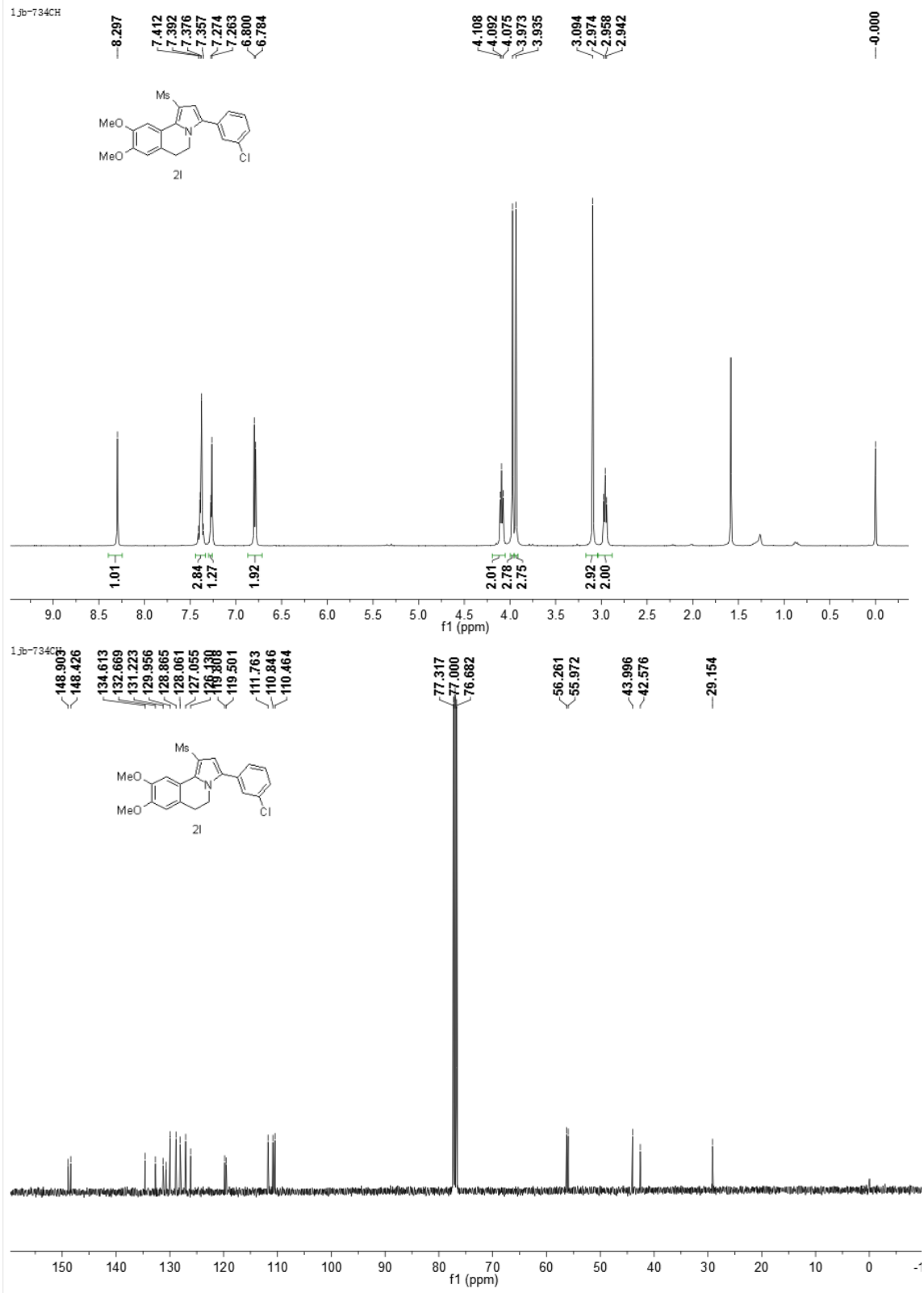
132.737
130.910
130.204
128.966
128.659
127.987
126.164
120.010
119.219
111.081
110.838
110.396
77.318
77.000
76.682
56.221
55.934
43.999
42.482
29.184
0.048
Ms
MeO
MeO
N
Ph
2f
f1 (ppm)

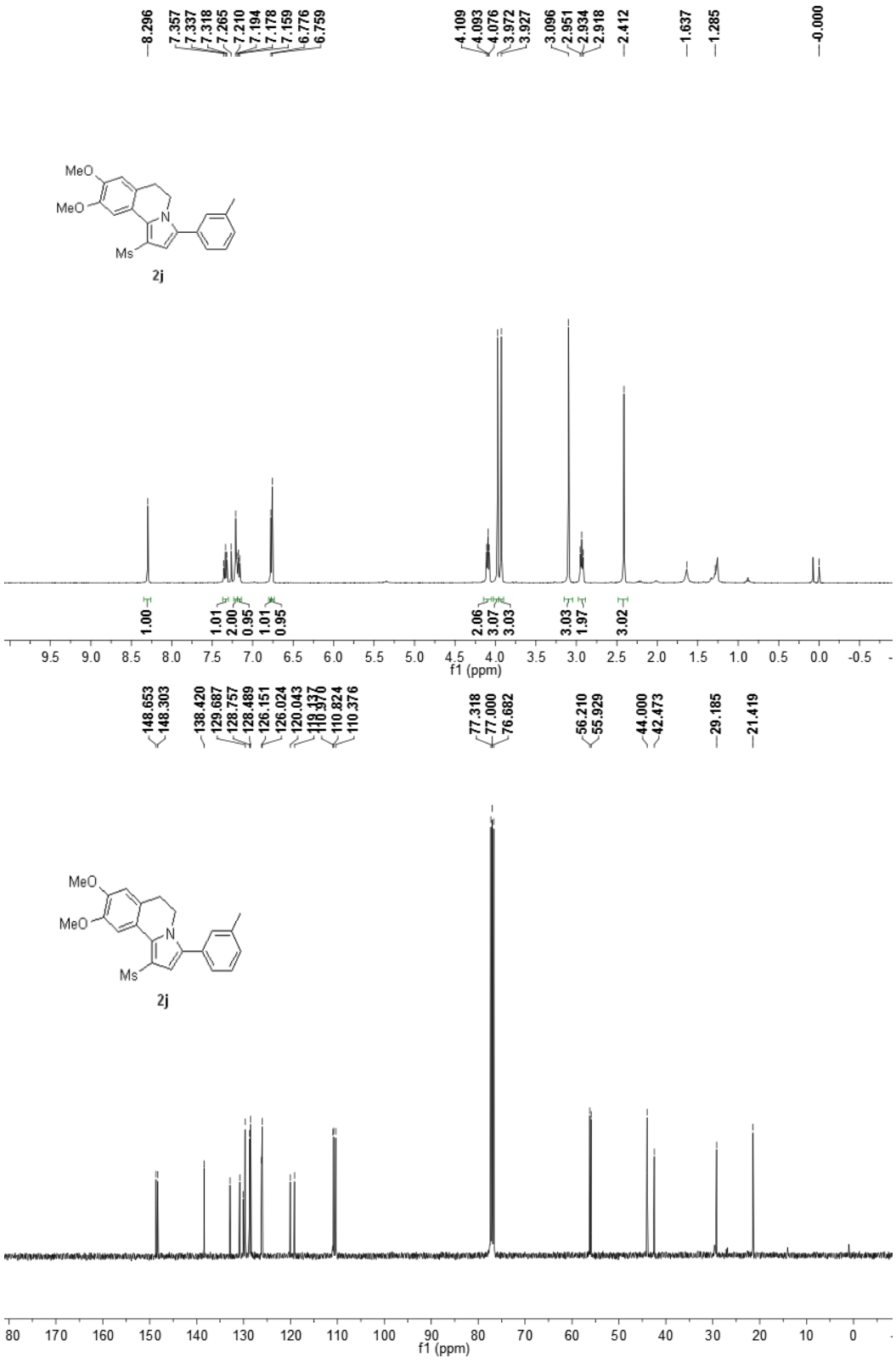

1jb-733CH
8.297
7.367
7.353
7.346
7.333
7.173
7.151
7.130
6.779
6.744
4.064
4.047
4.031
3.971
3.931
3.097
2.963
2.946
2.930
0.000
Ms
MeO
MeO
N
F
2g
1.00
2.08
2.01
1.97
2.10
2.95
3.07
3.00
2.09
f1 (ppm)

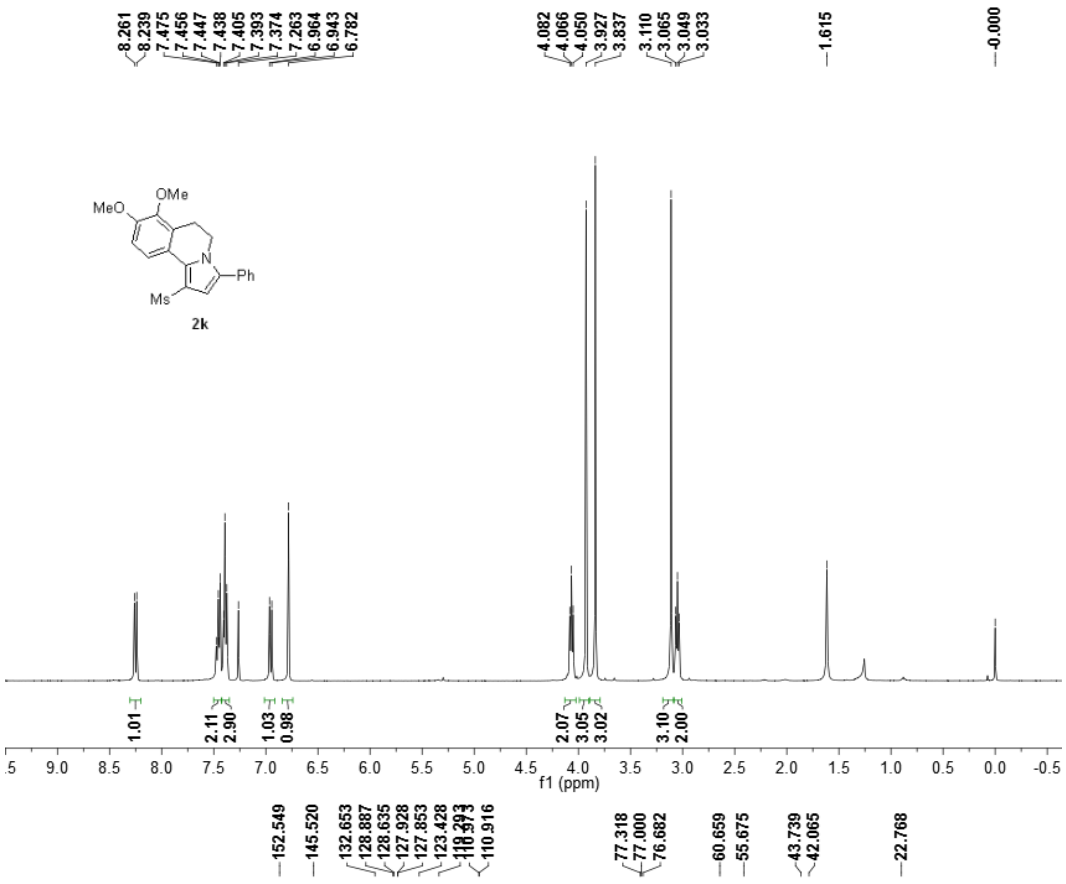

1jb-733CH
163.793
161.324
148.782
148.392
131.648
130.843
130.761
130.230
127.066
127.032
126.057
119.931
119.236
115.882
115.666
111.137
110.855
110.413
77.318
77.000
76.682
56.244
55.956
44.000
42.408
29.166
Ms
MeO
MeO
N
F
2g
f1 (ppm)

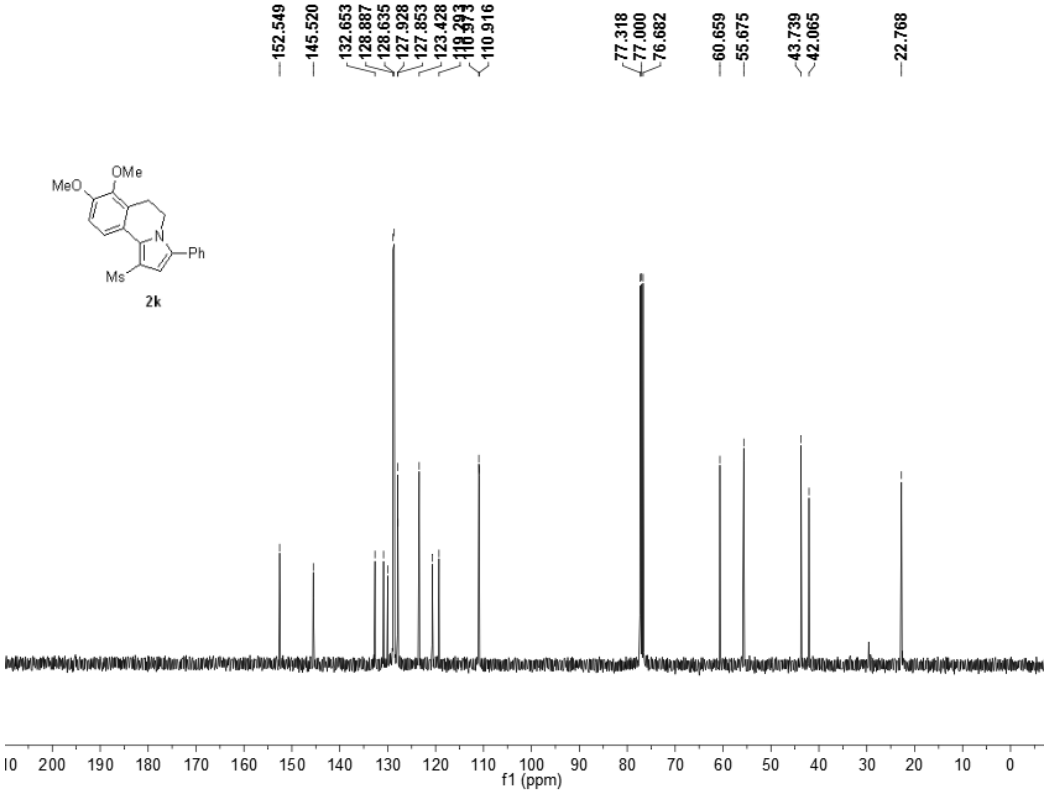

1jb-733CH
113.154
Ms
MeO
MeO
N
F
2g
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

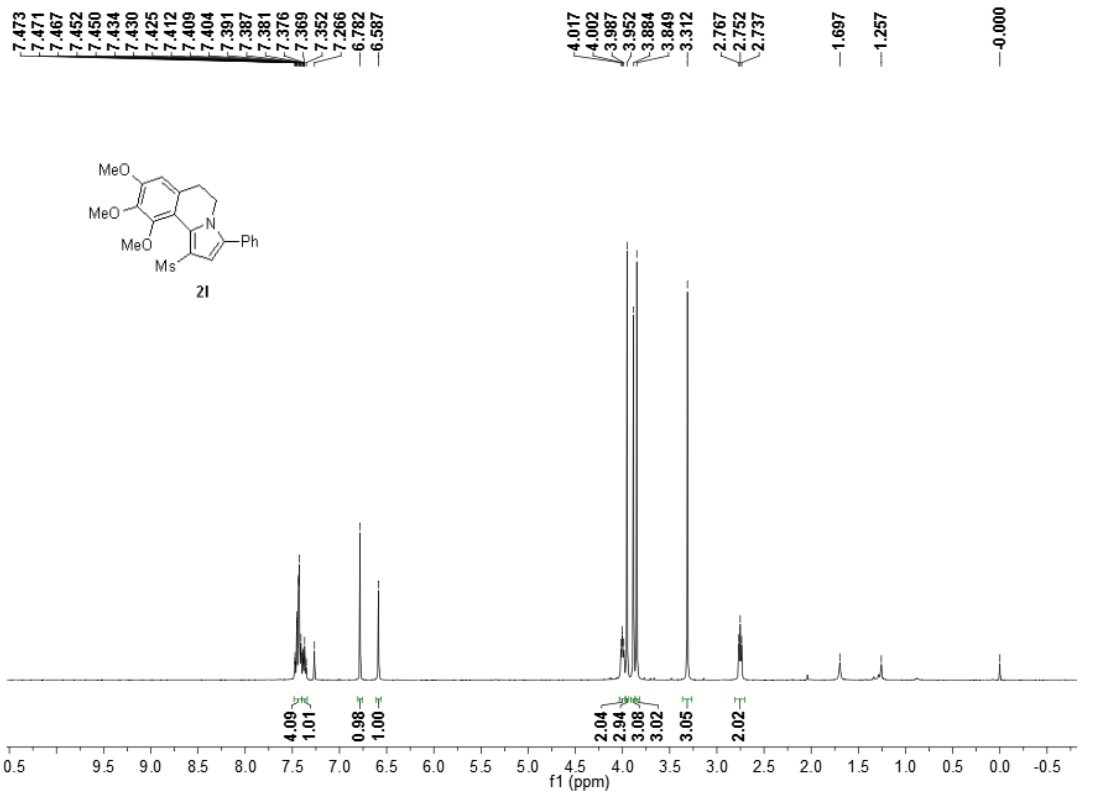

8.291
7.308
7.287
7.266
6.992
6.970
6.773
6.705
4.064
4.048
4.032
3.970
3.925
3.859
3.095
2.945
2.929
2.913
1.645
0.000
MeO
MeO
OMe
Ms
2h
1.00
1.93
1.93
1.05
0.91
2.03
3.06
3.00
2.97
3.29
2.17
f1 (ppm)
159.497
148.604
148.309
132.562
130.346
129.756
126.080
123.330
120.114
119.004
114.111
110.840
110.488
110.363
77.318
77.000
76.683
56.221
55.935
55.355
44.017
42.298
29.195
MeO
MeO
OMe
Ms
2h
f1 (ppm)

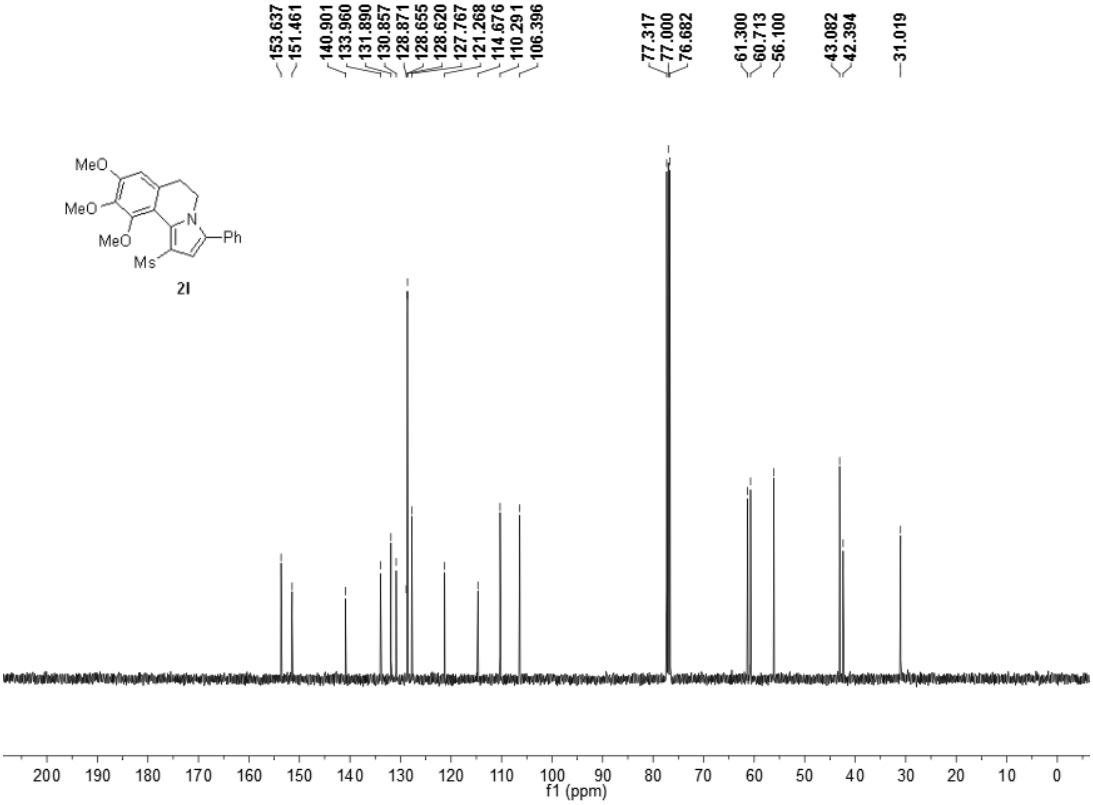

1jb-734CH
8.297
7.412
7.392
7.376
7.357
7.274
7.263
6.800
6.784
4.108
4.092
4.075
3.973
3.935
3.094
2.974
2.958
2.942
0.000
Ms
MeO
MeO
Cl
2l
1.01
2.84
1.27
1.92
2.01
2.78
2.75
2.92
2.00
f1 (ppm)
148.903
148.426
134.613
132.669
131.223
129.956
128.865
128.061
127.055
119.501
111.763
110.846
110.464
77.317
77.000
76.682
56.261
55.972
43.996
42.576
29.154
f1 (ppm)

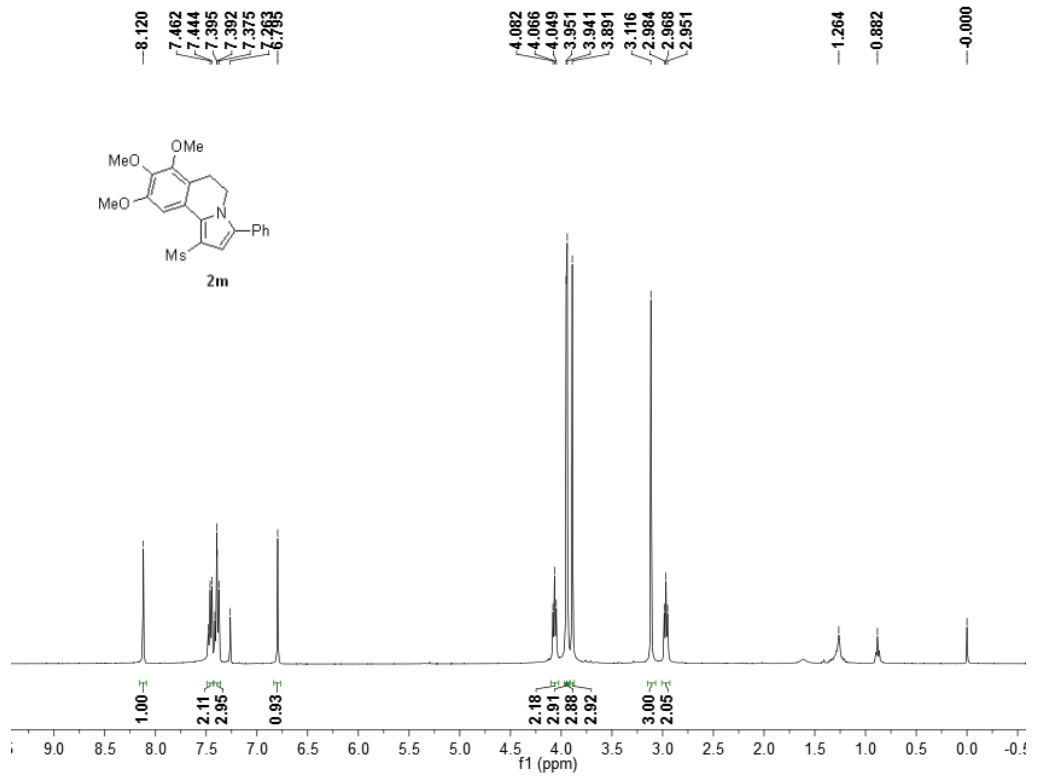

8.296
7.357
7.337
7.318
7.265
7.210
7.194
7.178
7.159
6.776
6.759
4.109
4.093
4.076
3.972
3.927
3.096
2.951
2.934
2.918
2.412
1.637
1.285
0.000
MeO
MeO
N
Ms
2j
1.00
1.01
2.00
0.95
1.01
0.95
2.06
3.07
3.03
3.03
1.97
3.02
f1 (ppm)
148.653
148.303
138.420
129.687
128.757
128.489
126.151
126.024
120.043
110.437
110.370
110.824
110.376
77.318
77.000
76.682
56.210
55.929
44.000
42.473
29.185
21.419
MeO
MeO
N
Ms
2j
f1 (ppm)

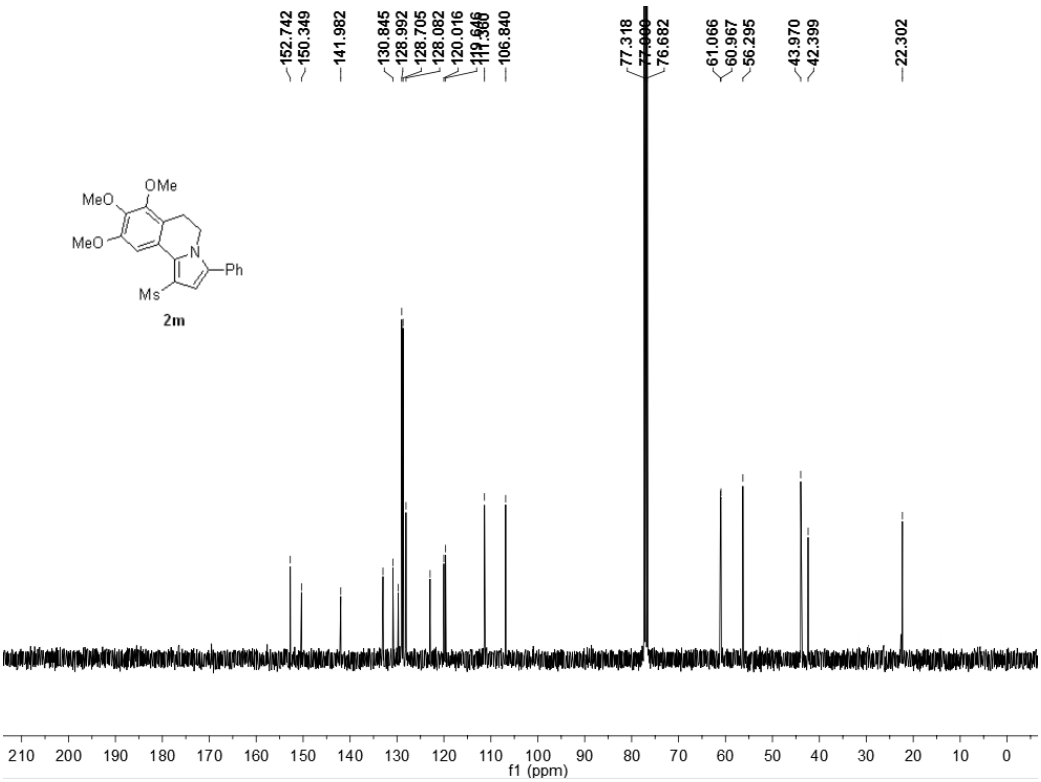

8.261
8.239
7.475
7.456
7.447
7.438
7.405
7.393
7.374
7.263
6.964
6.943
6.782
4.082
4.066
4.050
3.927
3.837
3.110
3.065
3.049
3.033
1.615
0.000
MeO
OMe
N
Ph
Ms
2k
1.01
2.11
2.90
1.03
0.98
2.07
3.05
3.02
3.10
2.00
f1 (ppm)

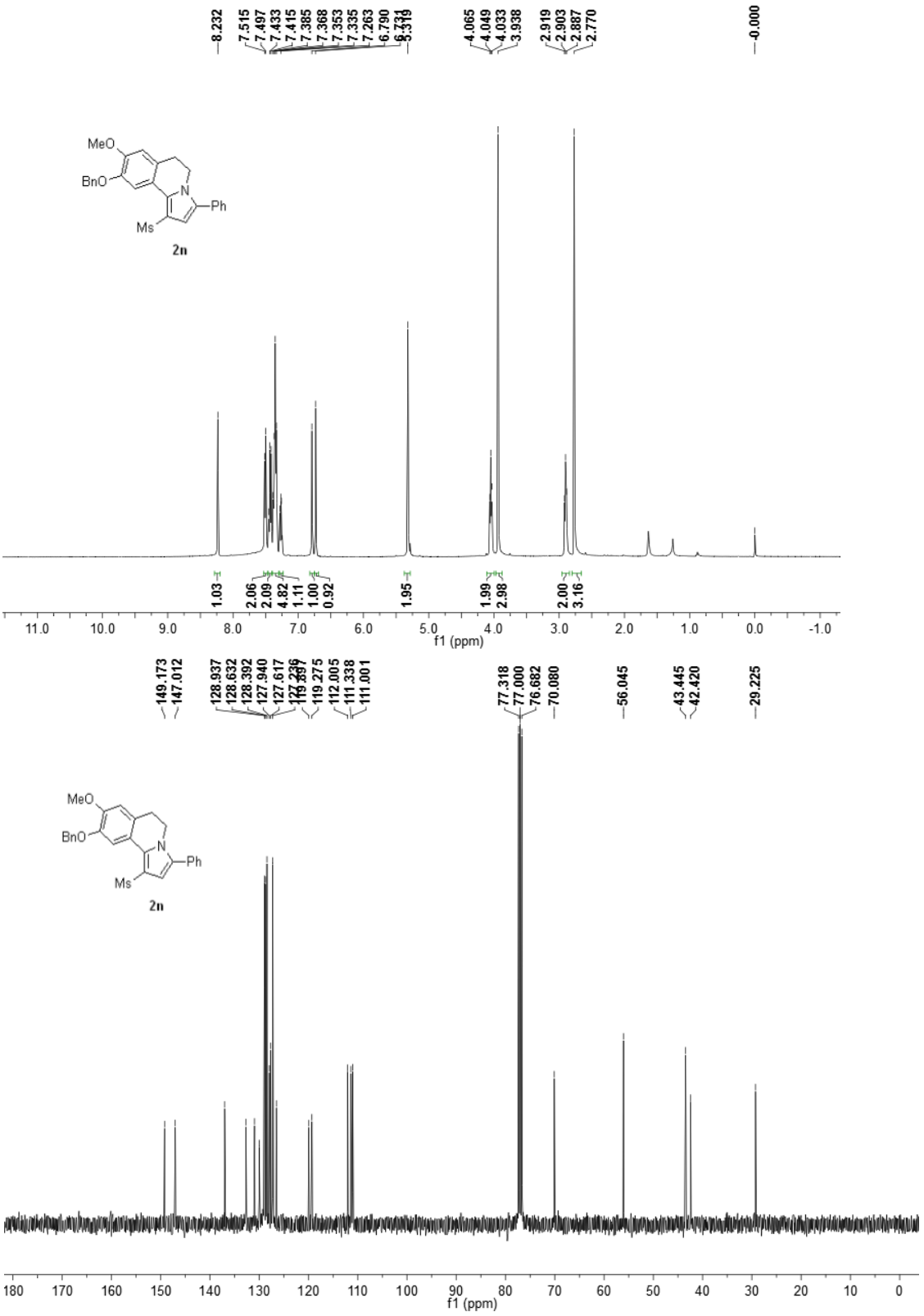

152.549
145.520
132.653
128.887
128.635
127.928
127.853
123.428
110.916
77.318
77.000
76.682
60.659
55.675
43.739
42.065
22.768
MeO
OMe
N
Ph
Ms
2k
f1 (ppm)

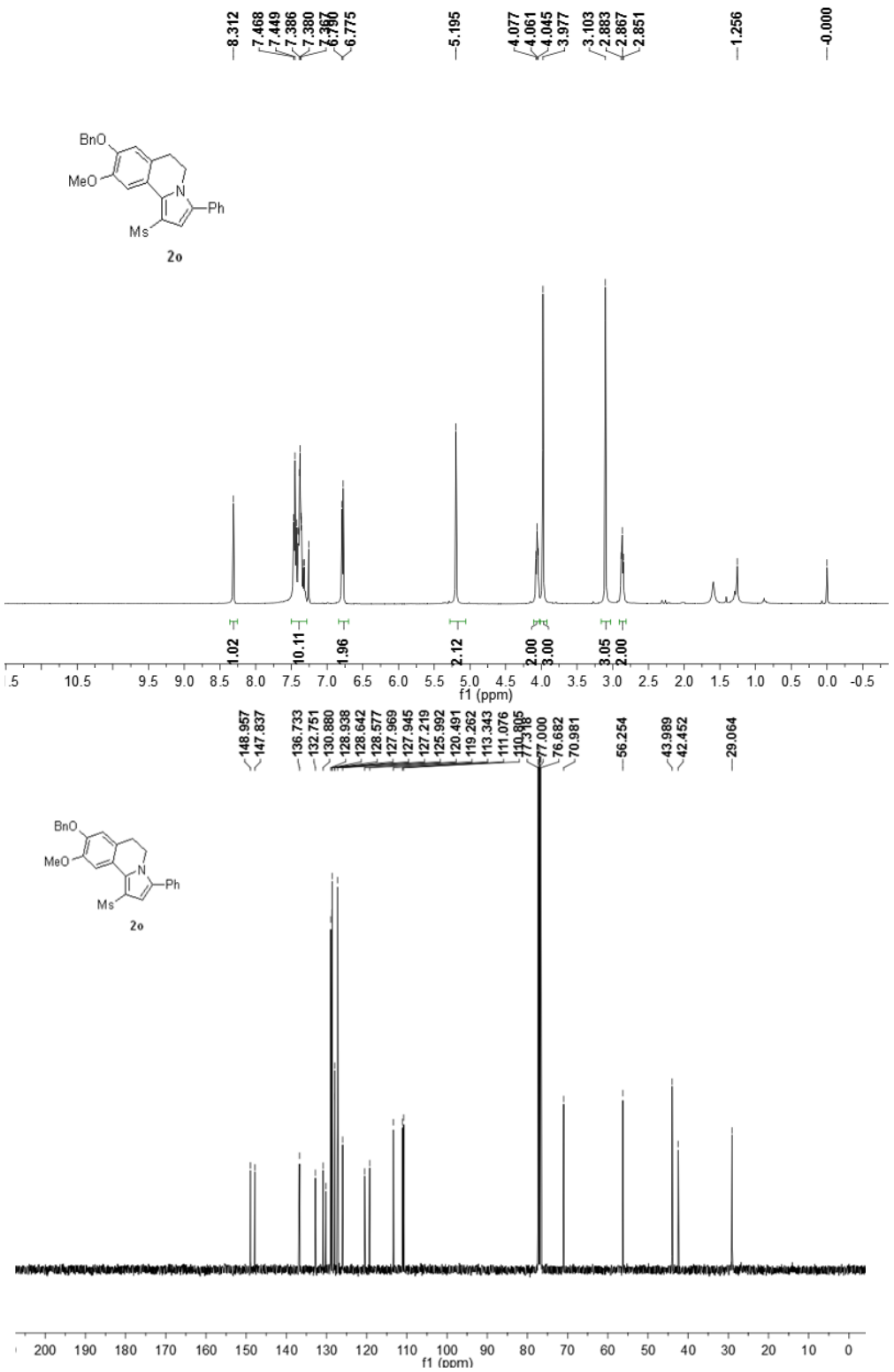

7.473
7.471
7.467
7.452
7.450
7.434
7.430
7.425
7.412
7.409
7.404
7.391
7.387
7.381
7.376
7.369
7.352
7.266
6.782
6.587
4.017
4.002
3.987
3.952
3.884
3.849
3.312
2.767
2.752
2.737
1.697
1.257
-0.000
MeO
MeO
MeO
N
Ph
Ms
2l
4.09
1.01
0.98
1.00
2.04
2.94
3.08
3.02
3.05
2.02
f1 (ppm)

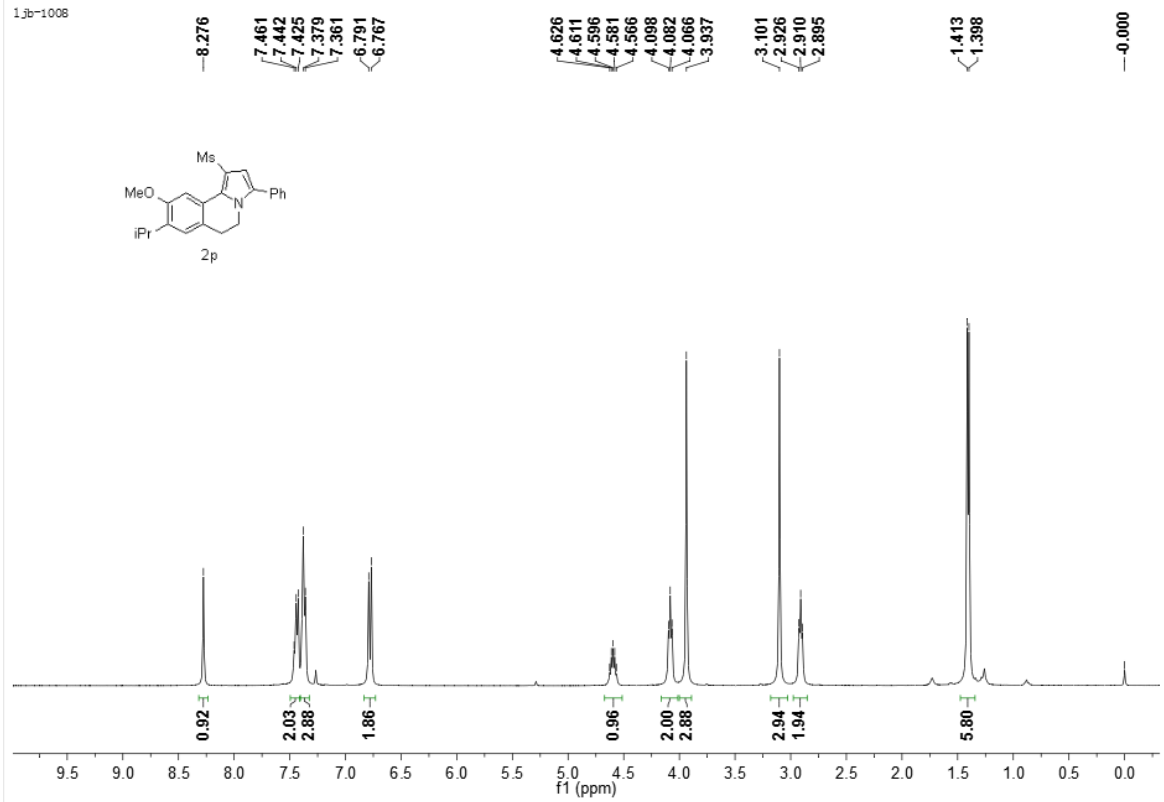

153.637
151.461
140.901
133.960
131.890
130.857
128.871
128.655
128.620
127.767
121.268
114.676
110.291
106.396
77.317
77.000
76.682
61.300
60.713
56.100
43.082
42.394
31.019
MeO
MeO
MeO
N
Ph
Ms
2l
f1 (ppm)

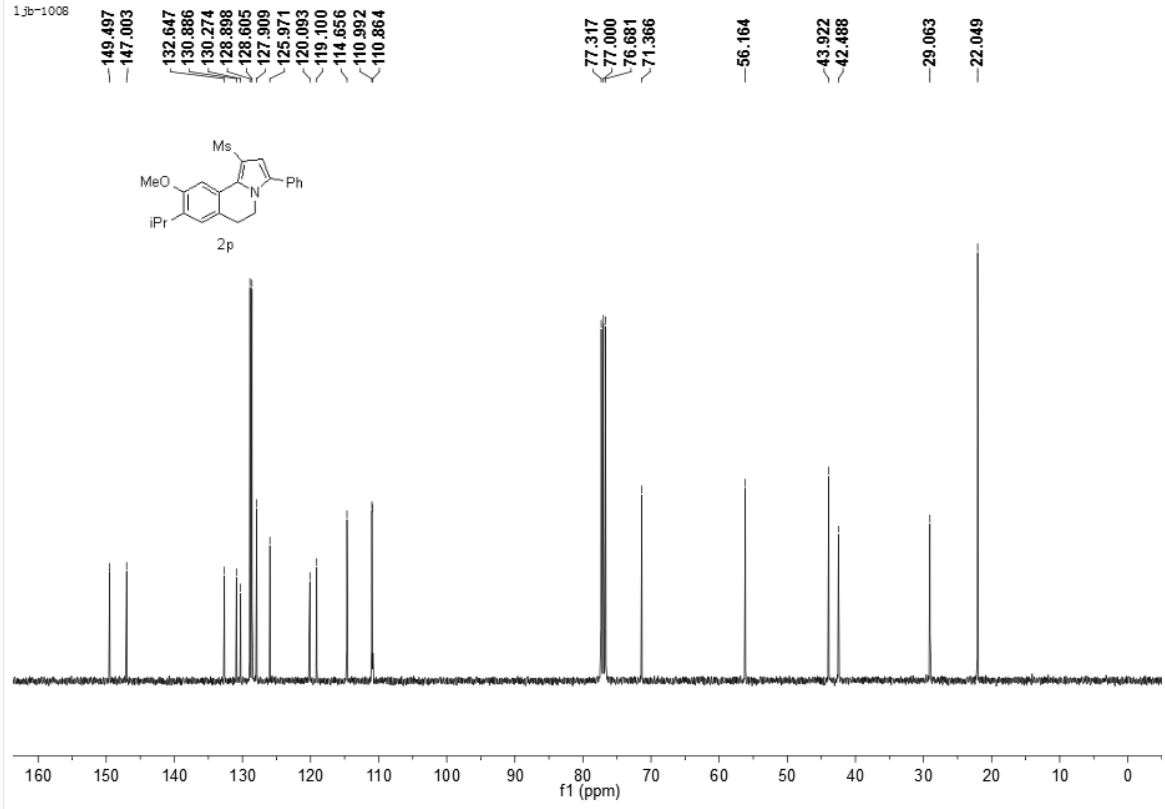

8.120
7.462
7.444
7.395
7.392
7.375
7.263
6.795
4.082
4.066
4.049
3.951
3.941
3.891
3.116
2.984
2.968
2.951
1.264
0.882
0.000
MeO
OMe
MeO
N
Ph
Ms
2m
1.00
2.11
2.95
0.93
2.18
2.91
2.88
2.92
3.00
2.05
f1 (ppm)

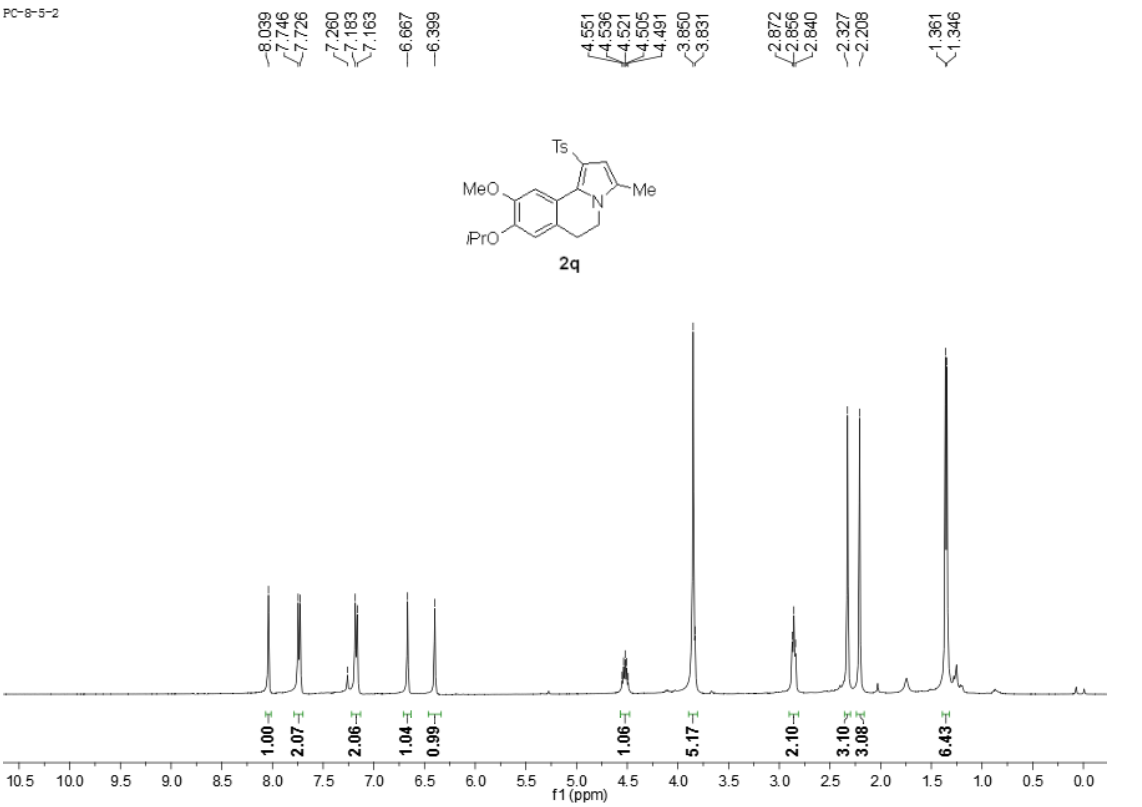

152.742
150.349
141.982
130.845
128.992
128.705
128.082
120.016
106.840
77.318
76.682
61.066
60.967
56.295
43.970
42.399
22.302
MeO
OMe
MeO
N
Ph
Ms
2m
f1 (ppm)

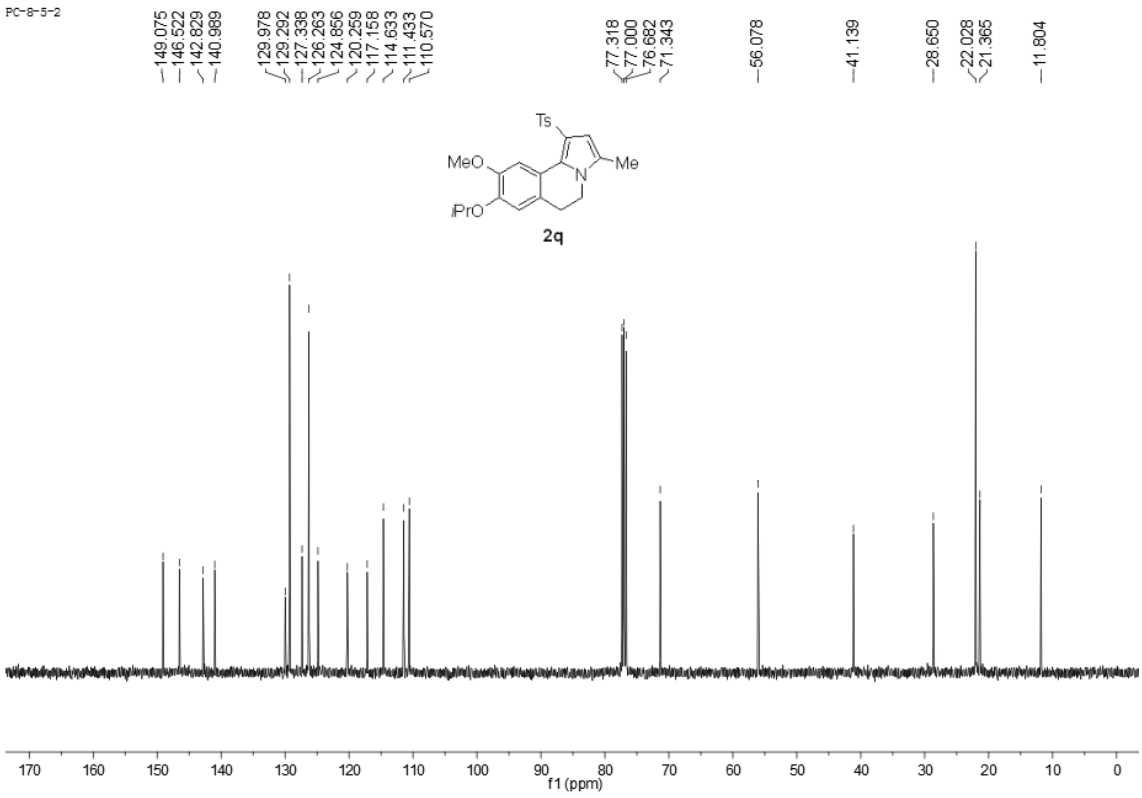

8.232
7.515
7.497
7.433
7.415
7.385
7.368
7.353
7.335
7.263
6.790
4.065
4.049
4.033
3.938
2.919
2.903
2.887
2.770
0.000
MeO
BnO
N
Ph
Ms
2n
1.03
2.06
2.09
4.82
1.11
1.00
0.92
1.95
1.99
2.98
2.00
3.16
f1 (ppm)
149.173
147.012
128.937
128.632
128.392
127.940
127.617
119.275
112.005
111.338
111.001
77.318
77.000
76.682
70.080
56.045
43.445
42.420
29.225
f1 (ppm)

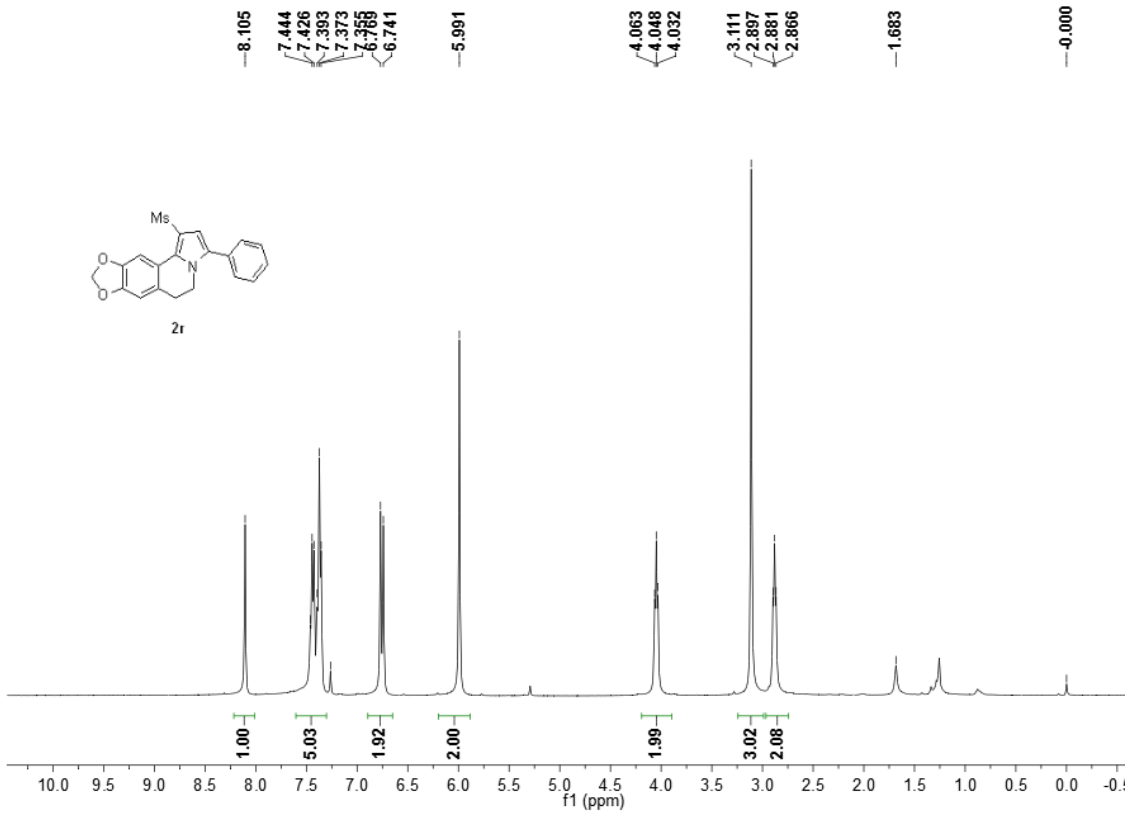

8.312
7.468
7.449
7.386
7.380
6.775
5.195
4.077
4.061
4.045
3.977
3.103
2.883
2.867
2.851
1.256
0.000
BnO
MeO
N
Ph
Ms
2o
1.02
10.11
1.96
2.12
2.00
3.00
3.05
2.00
f1 (ppm)
148.957
147.837
136.733
132.751
130.880
128.938
128.642
128.577
127.969
127.945
127.219
125.992
120.491
119.262
113.343
111.076
77.000
76.682
70.981
56.254
43.989
42.452
29.064
f1 (ppm)

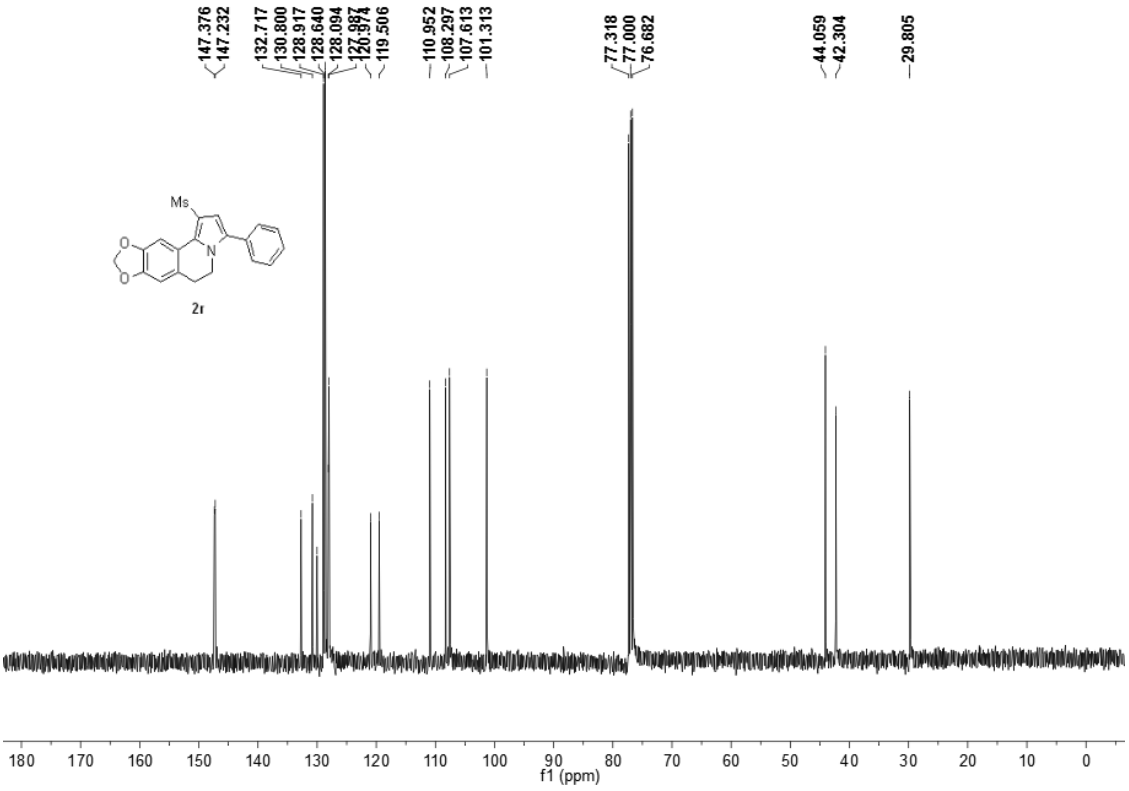

1jb-1008
8.276
7.461
7.442
7.425
7.379
7.361
6.791
6.767
4.626
4.611
4.596
4.581
4.566
4.098
4.082
4.066
3.937
3.101
2.926
2.910
2.895
1.413
1.398
0.000
Ms
MeO
Ph
iPr
2p
0.92
2.03
2.88
1.86
0.96
2.00
2.88
2.94
1.94
5.80
f1 (ppm)

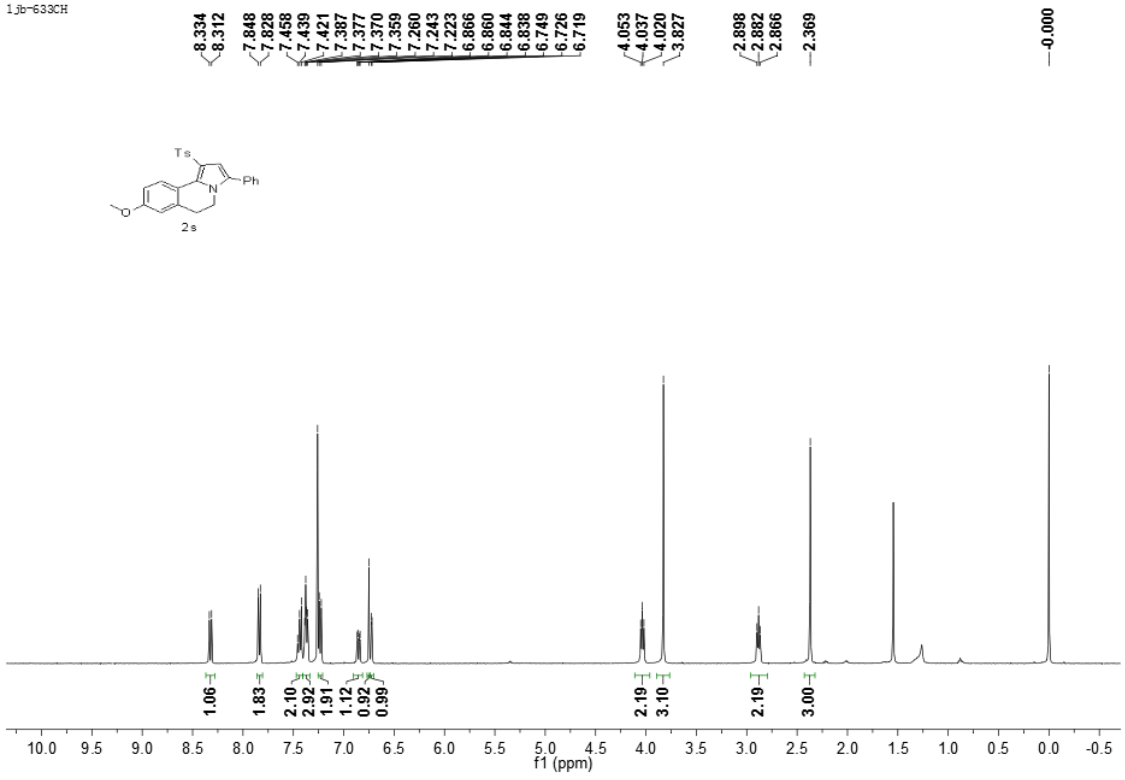

1jb-1008
149.497
147.003
132.647
130.886
130.274
128.898
128.605
127.909
125.971
120.093
119.100
114.656
110.992
110.864
77.317
77.000
76.681
71.366
56.164
43.922
42.488
29.063
22.049
Ms
MeO
Ph
iPr
2p
f1 (ppm)

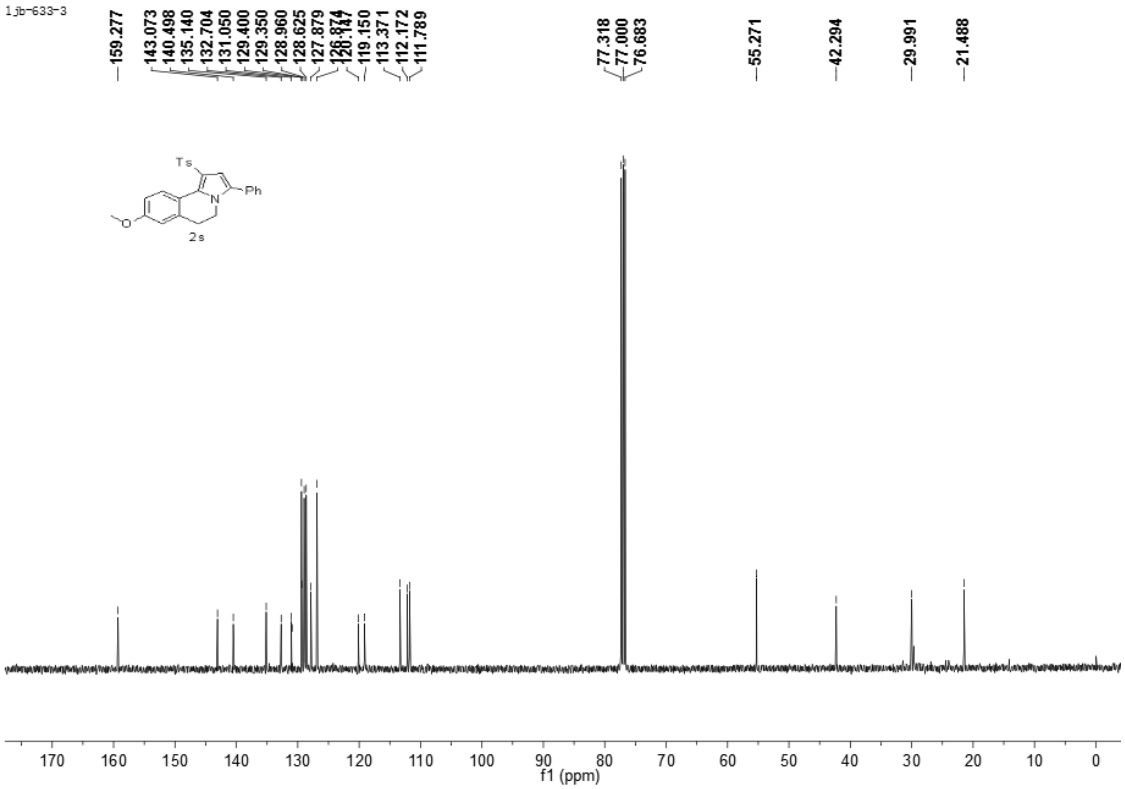

PC-8-5-2
8.039
7.746
7.726
7.260
7.183
7.163
6.667
6.399
4.551
4.536
4.521
4.505
4.491
3.850
3.831
2.872
2.856
2.840
2.327
2.208
1.361
1.346
Ts
MeO
Me
N
iPrO
2q
1.00
2.07
2.06
1.04
0.99
1.06
5.17
2.10
3.10
3.08
6.43
f1 (ppm)

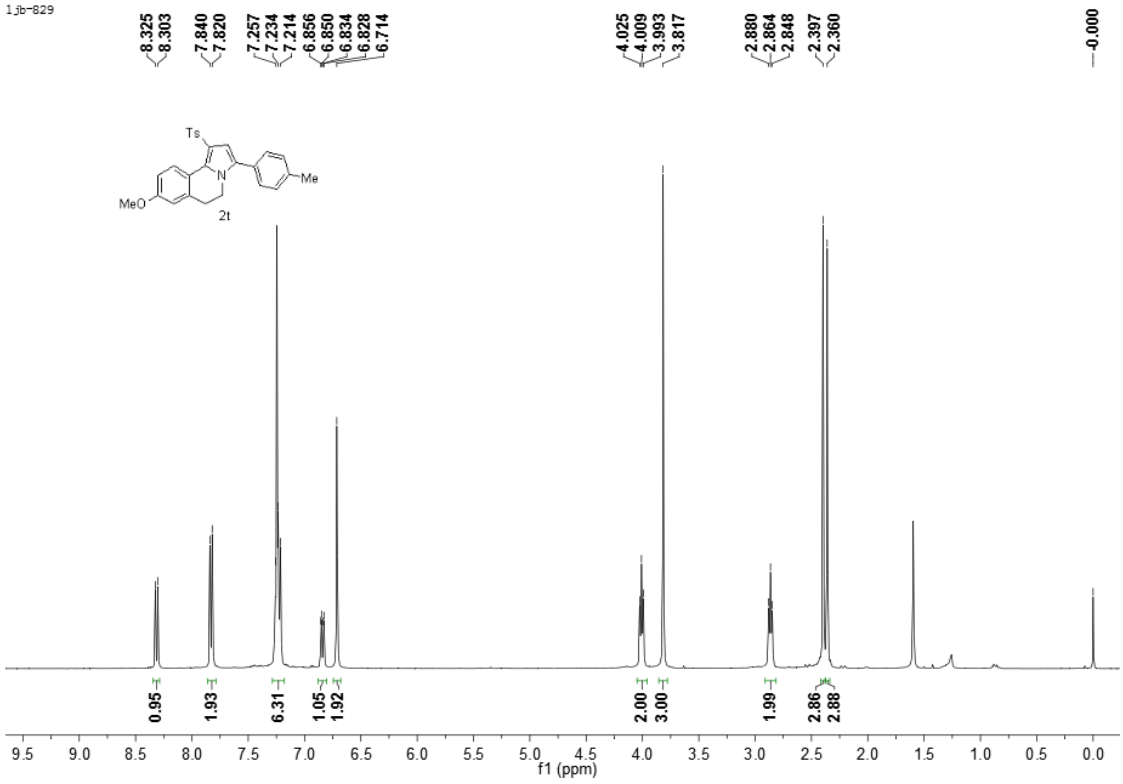

PC-8-5-2
149.075
146.522
142.829
140.989
129.978
129.292
127.338
126.263
124.856
120.259
117.158
114.633
111.433
110.570
77.318
77.000
76.682
71.343
56.078
41.139
28.650
22.028
21.365
11.804
Ts
MeO
Me
N
iPrO
2q
f1 (ppm)

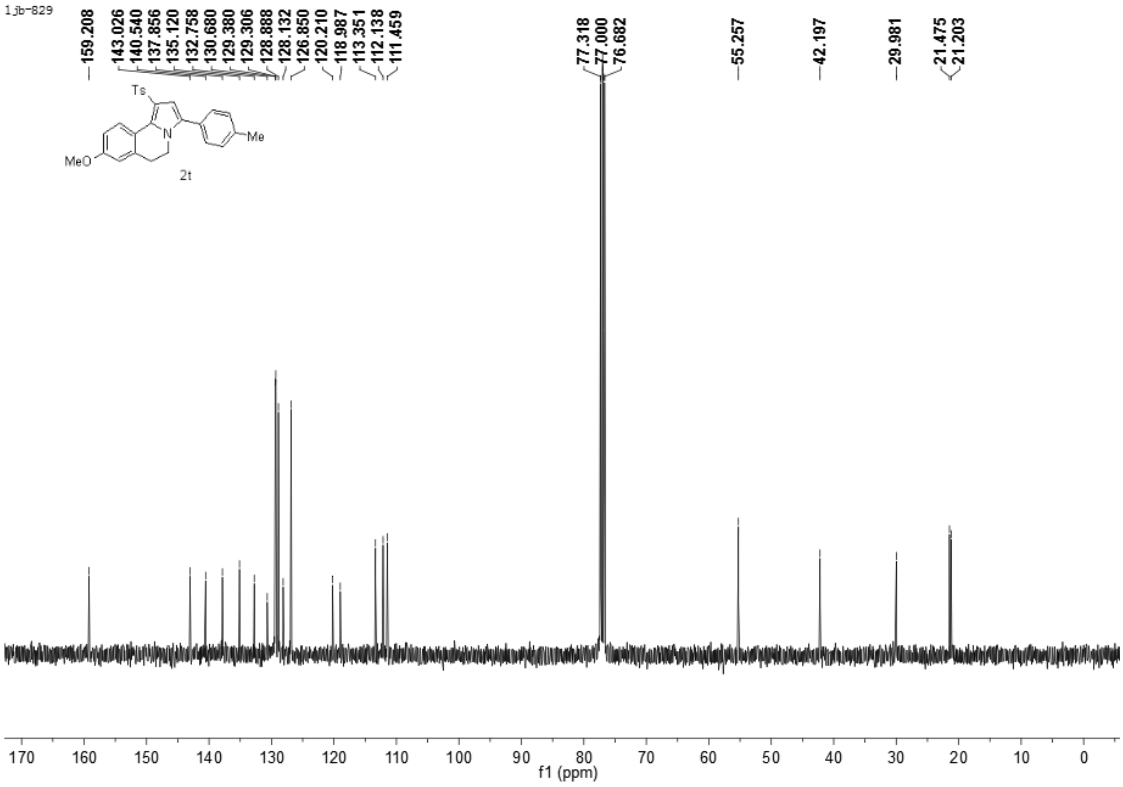

8.105
7.444
7.426
7.393
7.373
6.741
5.991
4.063
4.048
4.032
3.111
2.897
2.881
2.866
1.683
0.000
Ms
2r
1.00
5.03
1.92
2.00
1.99
3.02
2.08
f1 (ppm)

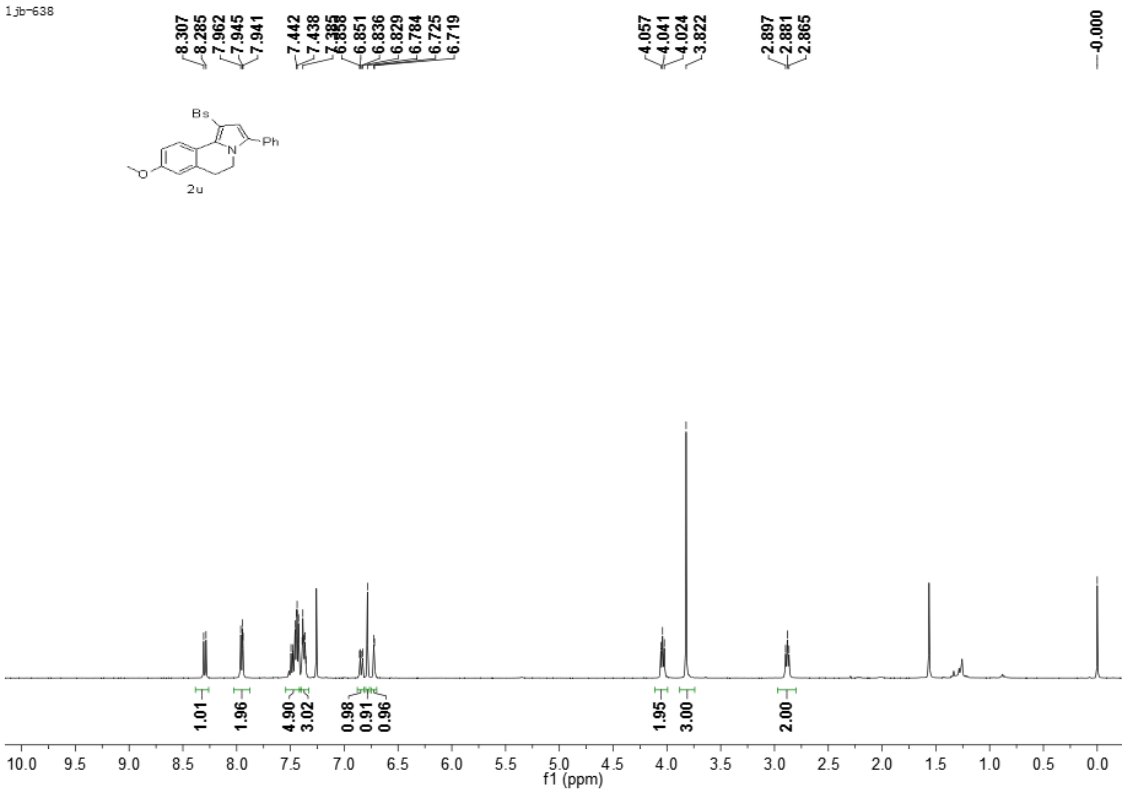

147.376
147.232
132.717
130.800
128.917
128.640
128.094
119.506
110.952
108.297
107.613
101.313
77.318
77.000
76.682
44.059
42.304
29.805
Ms
2r
f1 (ppm)

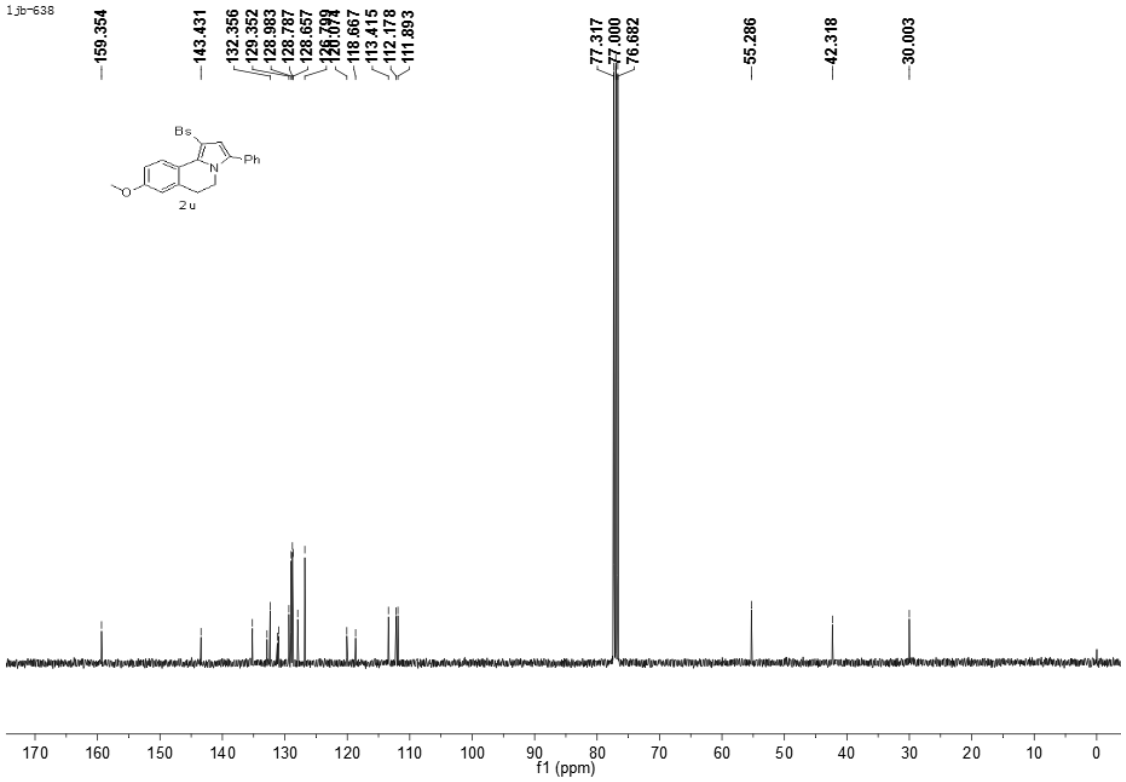

1jb-633CH
8.334
8.312
7.848
7.828
7.458
7.439
7.421
7.387
7.377
7.370
7.359
7.260
7.243
7.223
6.866
6.860
6.844
6.838
6.749
6.726
6.719
4.053
4.037
4.020
3.827
2.898
2.882
2.866
2.369
0.000
Ts
Ph
N
O
2s
1.06
1.83
2.10
2.92
1.91
1.12
0.92
0.99
2.19
3.10
2.19
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

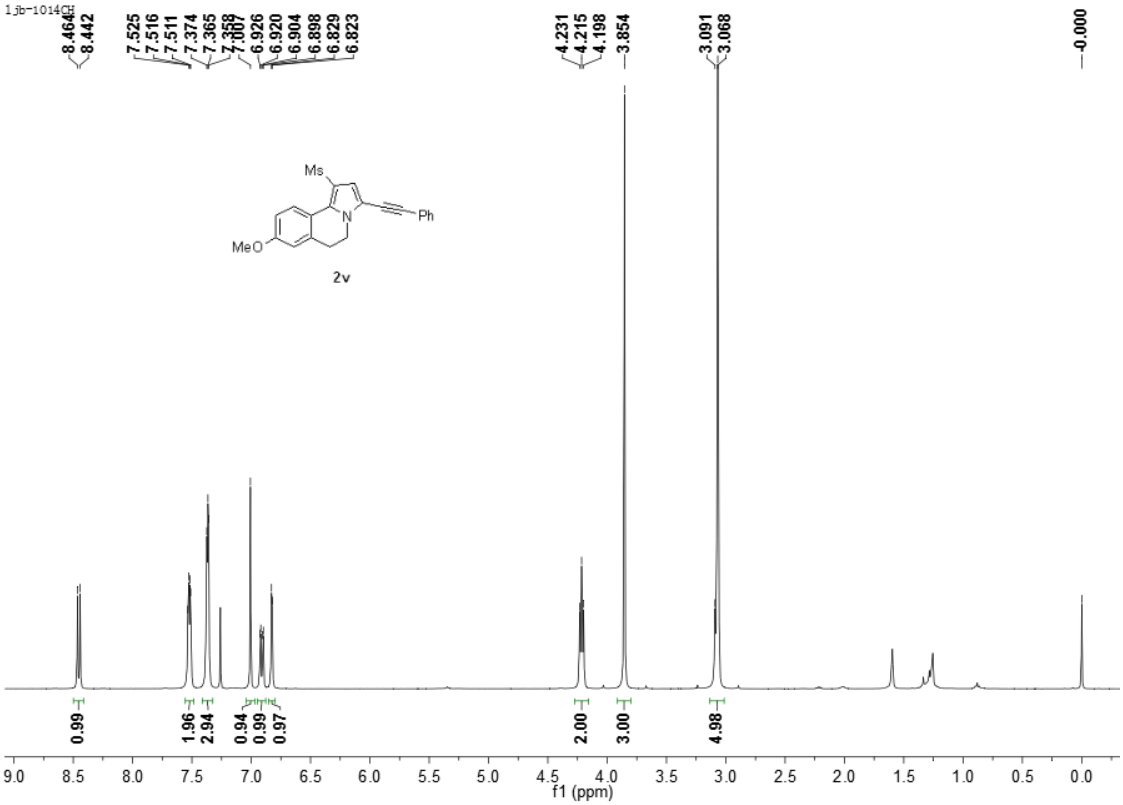

1jb-633-3
159.277
143.073
140.498
135.140
132.704
131.050
129.400
129.350
128.960
128.625
127.879
126.874
120.147
119.150
113.371
112.172
111.789
77.318
77.000
76.683
55.271
42.294
29.991
21.488
Ts
Ph
N
O
2s
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

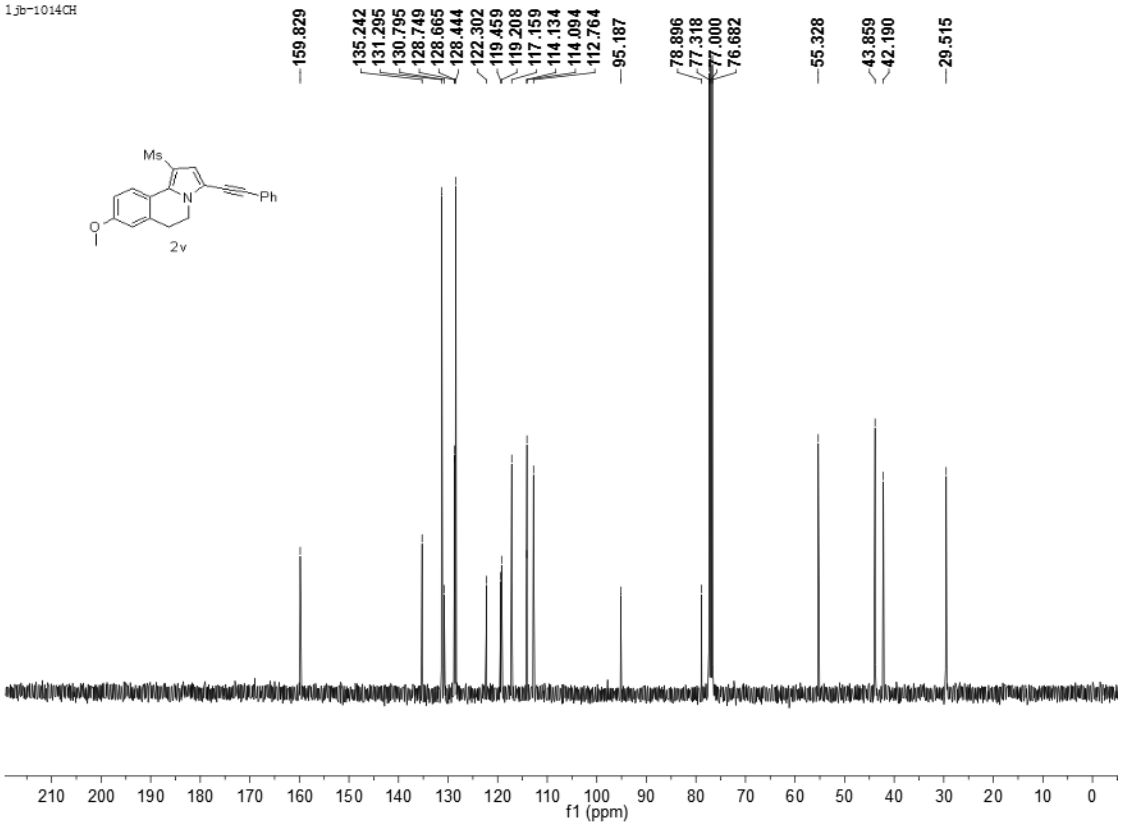

1jb-829
8.325
8.303
7.840
7.820
7.257
7.234
7.214
6.856
6.850
6.834
6.828
6.714
4.025
4.009
3.993
3.817
2.880
2.864
2.848
2.397
2.360
-0.000
Ts
Me
MeO
2t
0.95
1.93
6.31
1.05
1.92
2.00
3.00
1.99
2.86
2.88
f1 (ppm)

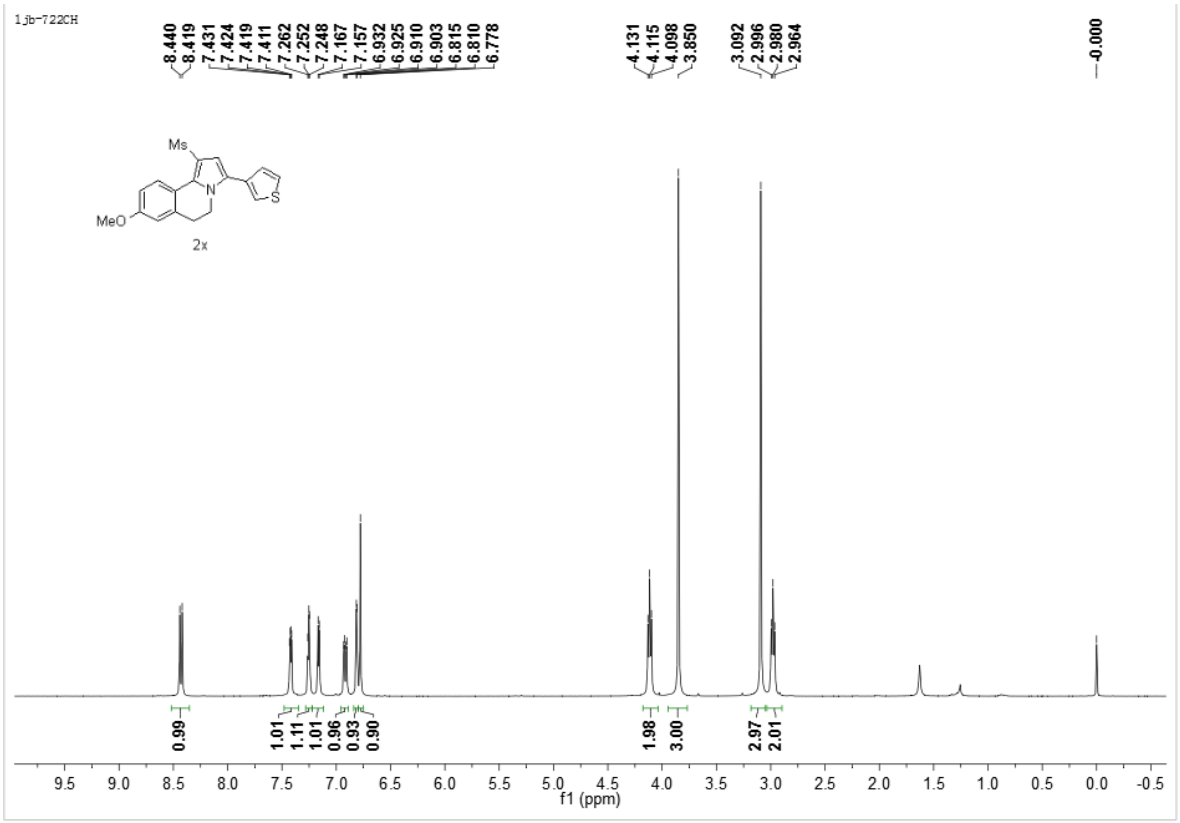

1jb-829
159.208
143.026
140.540
137.856
135.120
132.758
130.680
129.380
129.306
128.888
128.132
126.850
120.210
118.987
113.351
112.138
111.459
77.318
77.000
76.682
55.257
42.197
29.981
21.475
21.203
Ts
Me
MeO
2t
f1 (ppm)

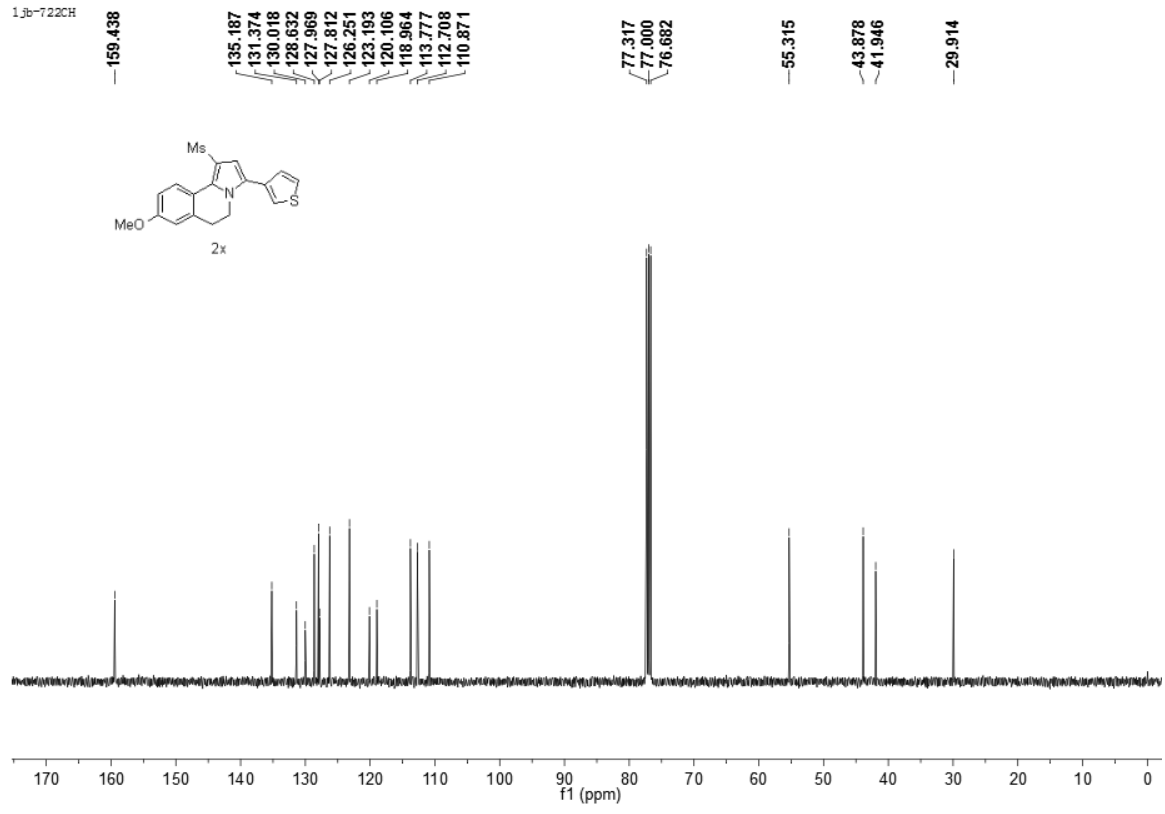

1jb-638
8.307
8.285
7.962
7.945
7.941
7.442
7.438
6.851
6.836
6.829
6.784
6.725
6.719
4.057
4.041
4.024
3.822
2.897
2.881
2.865
0.000
Bs
Ph
N
O
2u
1.01
1.96
4.90
3.02
0.98
0.91
0.96
1.95
3.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

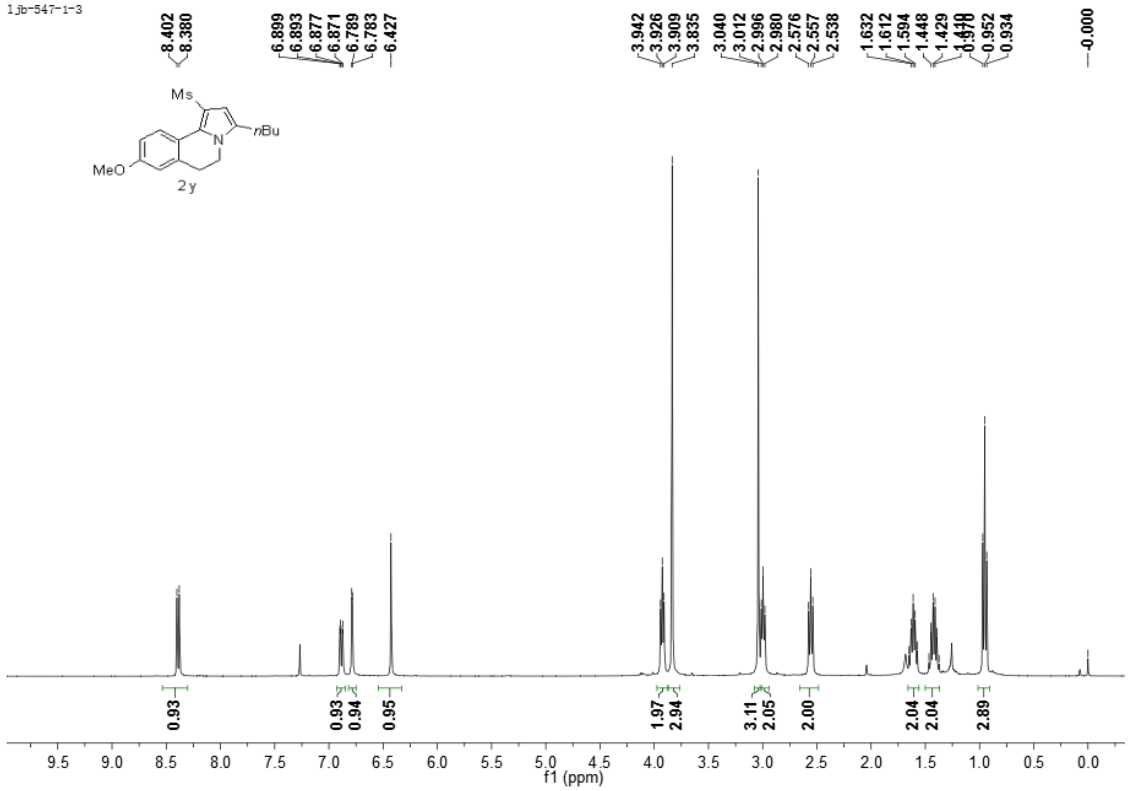

1jb-638
159.354
143.431
132.356
129.352
128.983
128.787
128.657
118.667
113.415
112.178
111.893
77.317
77.000
76.682
55.286
42.318
30.003
Bs
Ph
N
O
2u
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

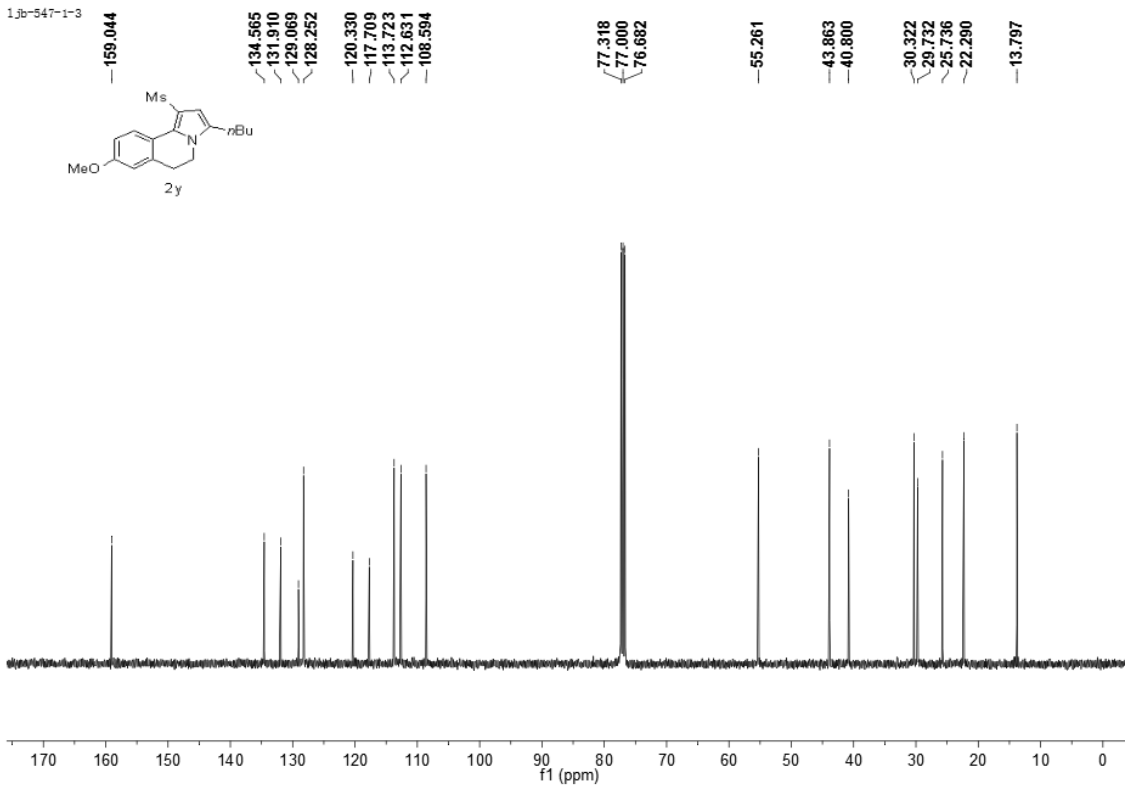

1jb-1014CH
8.464
8.442
7.525
7.516
7.511
7.374
7.365
6.926
6.920
6.904
6.898
6.829
6.823
4.231
4.215
4.198
3.854
3.091
3.068
0.000
Ms
Ph
MeO
2v
0.99
1.96
2.94
0.94
0.99
0.97
2.00
3.00
4.98
f1 (ppm)

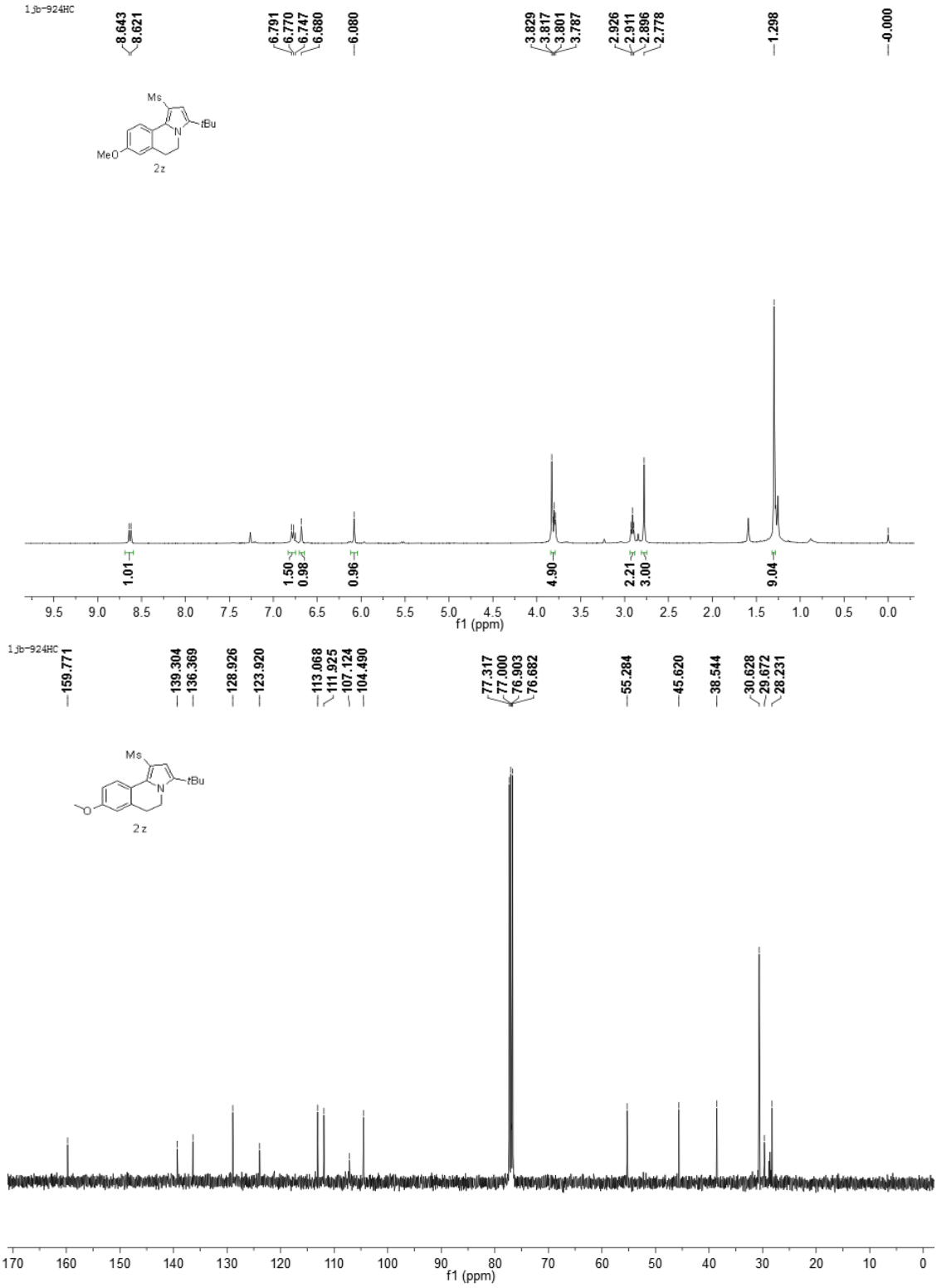

1jb-1014CH
159.829
135.242
131.295
130.795
128.749
128.665
128.444
122.302
119.459
119.208
117.159
114.134
114.094
112.764
95.187
78.896
77.318
77.000
76.682
55.328
43.859
42.190
29.515
Ms
Ph
O
2v
f1 (ppm)

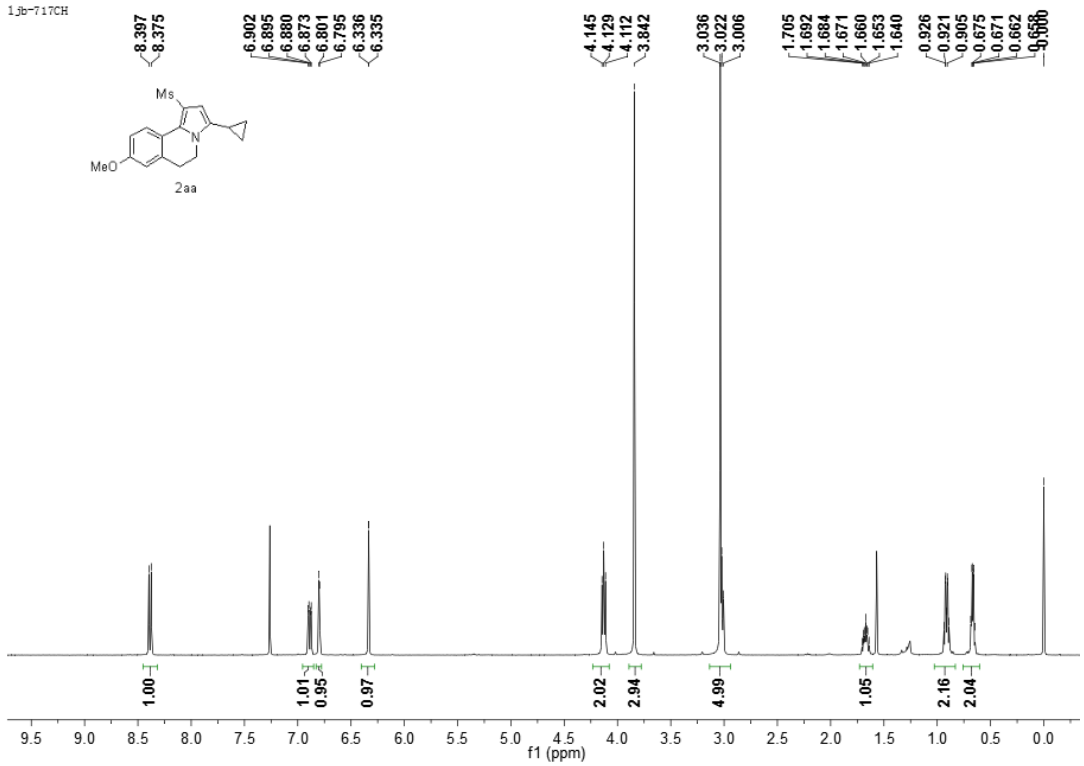

1jb-722CH
8.440
8.419
7.431
7.424
7.419
7.411
7.262
7.252
7.248
7.167
7.157
6.932
6.925
6.910
6.903
6.815
6.810
6.778
4.131
4.115
4.098
3.850
3.092
2.996
2.980
2.964
-0.000
Ms
MeO
2x
0.99
1.01
1.11
1.01
0.96
0.93
0.90
1.98
3.00
2.97
2.01
f1 (ppm)

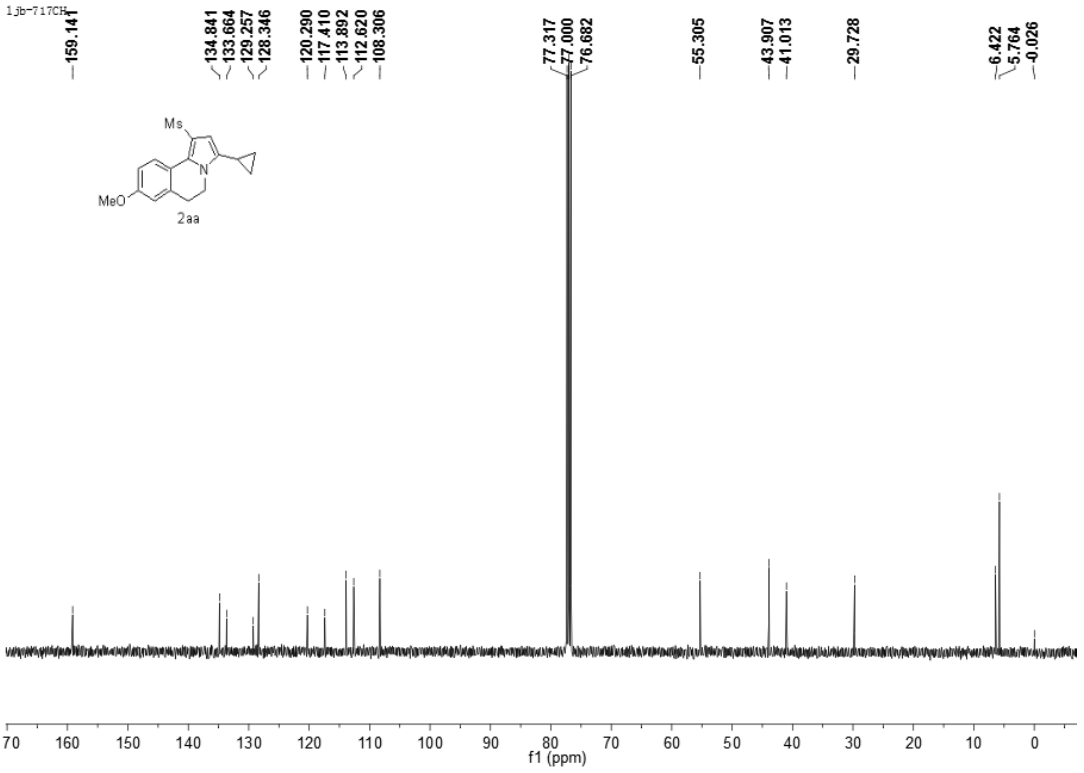

1jb-722CH
159.438
135.187
131.374
130.018
128.632
127.969
127.812
126.251
123.193
120.106
118.964
113.777
112.708
110.871
77.317
77.000
76.682
55.315
43.878
41.946
29.914
Ms
MeO
2x
f1 (ppm)

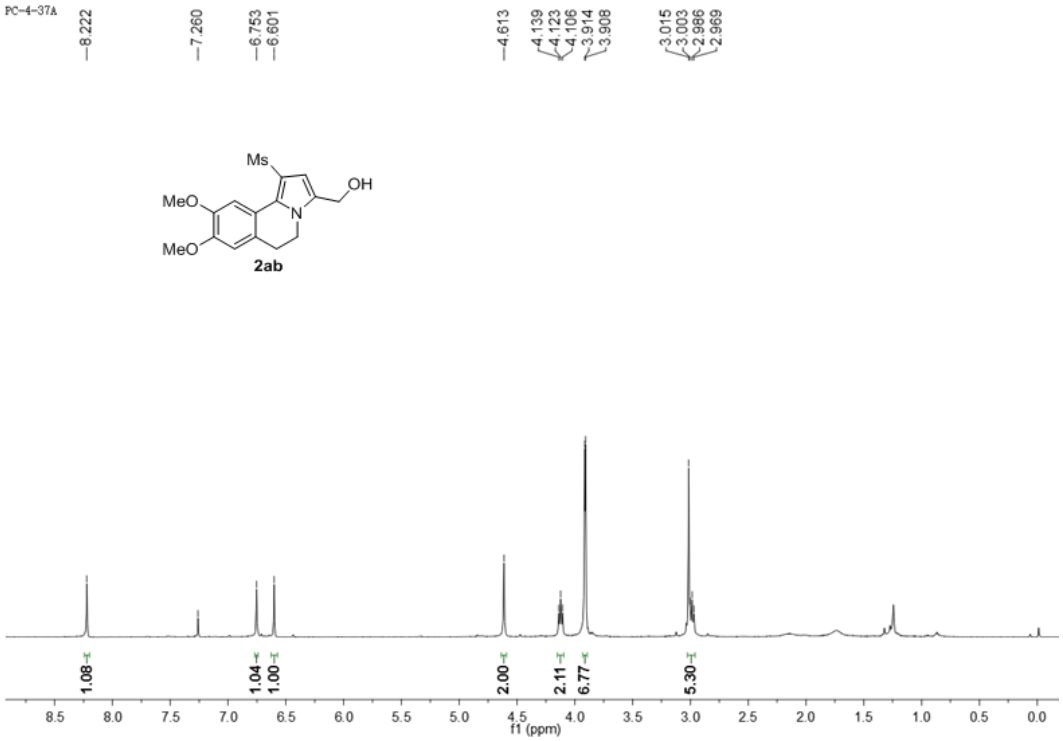

1jb-547-i-3
8.402
8.380
6.899
6.893
6.877
6.871
6.789
6.783
6.427
3.942
3.926
3.909
3.835
3.040
3.012
2.996
2.980
2.576
2.557
2.538
1.632
1.612
1.594
1.448
1.429
1.410
0.952
0.934
0.000
Ms
nBu
N
MeO
2y
0.93
0.93
0.94
0.95
1.97
2.94
3.11
2.05
2.00
2.04
2.04
2.89
f1 (ppm)

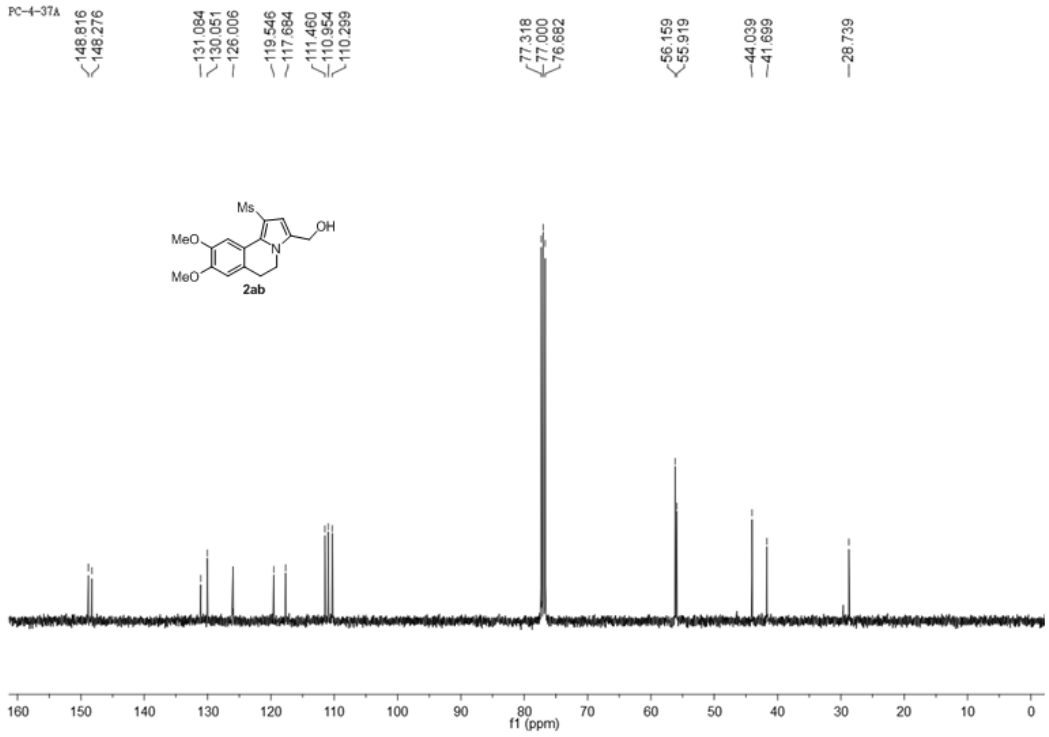

1jb-547-i-3
159.044
134.565
131.910
129.069
128.252
120.330
117.709
113.723
112.631
108.594
77.318
77.000
76.682
55.261
43.863
40.800
30.322
29.732
25.736
22.290
13.797
Ms
nBu
N
MeO
2y
f1 (ppm)

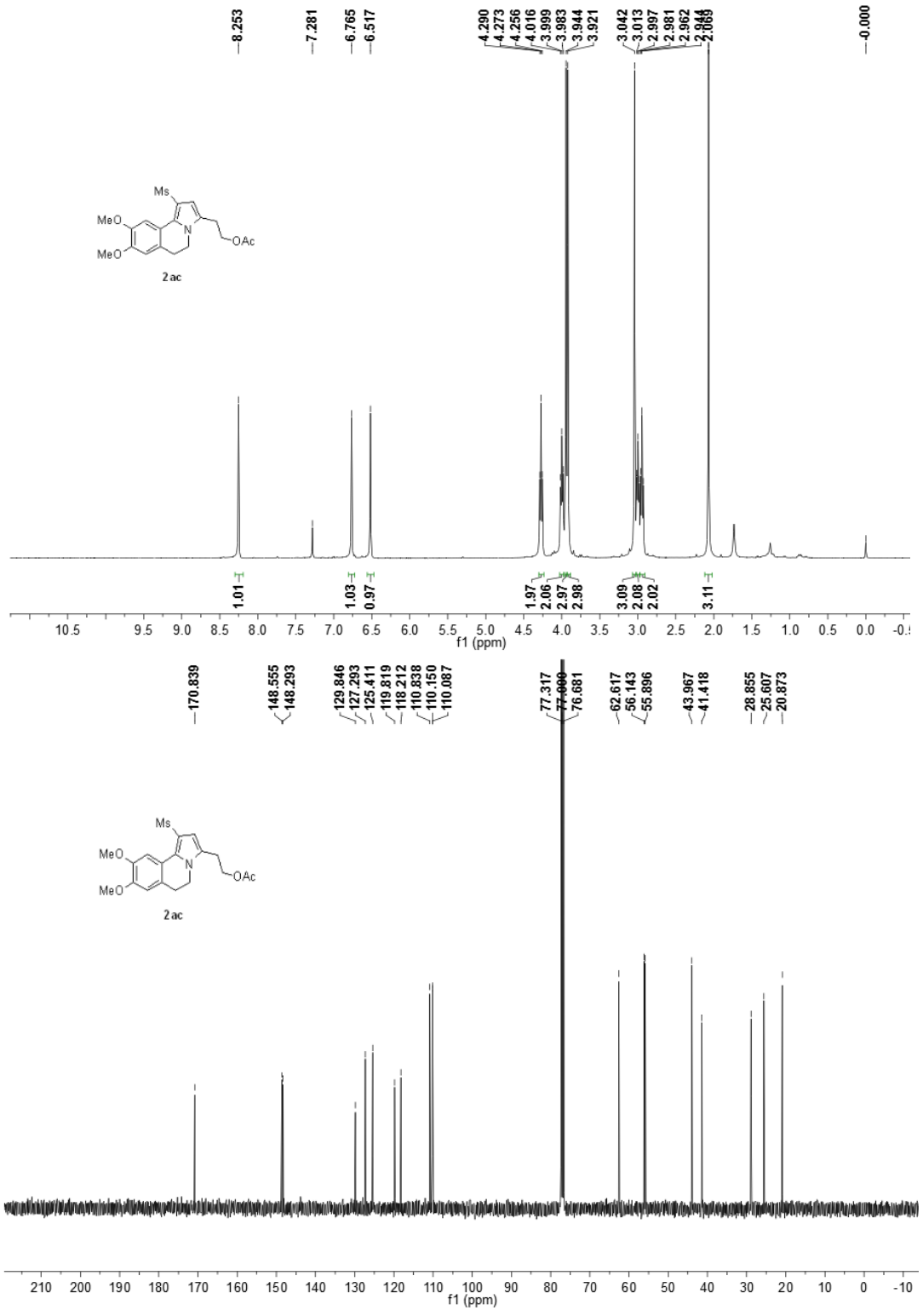

1jb-924HC
8.643
8.621
6.791
6.770
6.747
6.680
6.080
3.829
3.817
3.801
3.787
2.926
2.911
2.896
2.778
1.298
0.000
Ms
tBu
MeO
2z
1.01
1.50
0.98
0.96
4.90
2.21
3.00
9.04
f1 (ppm)
1jb-924HC
159.771
139.304
136.369
128.926
123.920
113.068
111.925
107.124
104.490
77.317
77.000
76.903
76.682
55.284
45.620
38.544
30.628
29.672
28.231
Ms
tBu
O
2z
f1 (ppm)

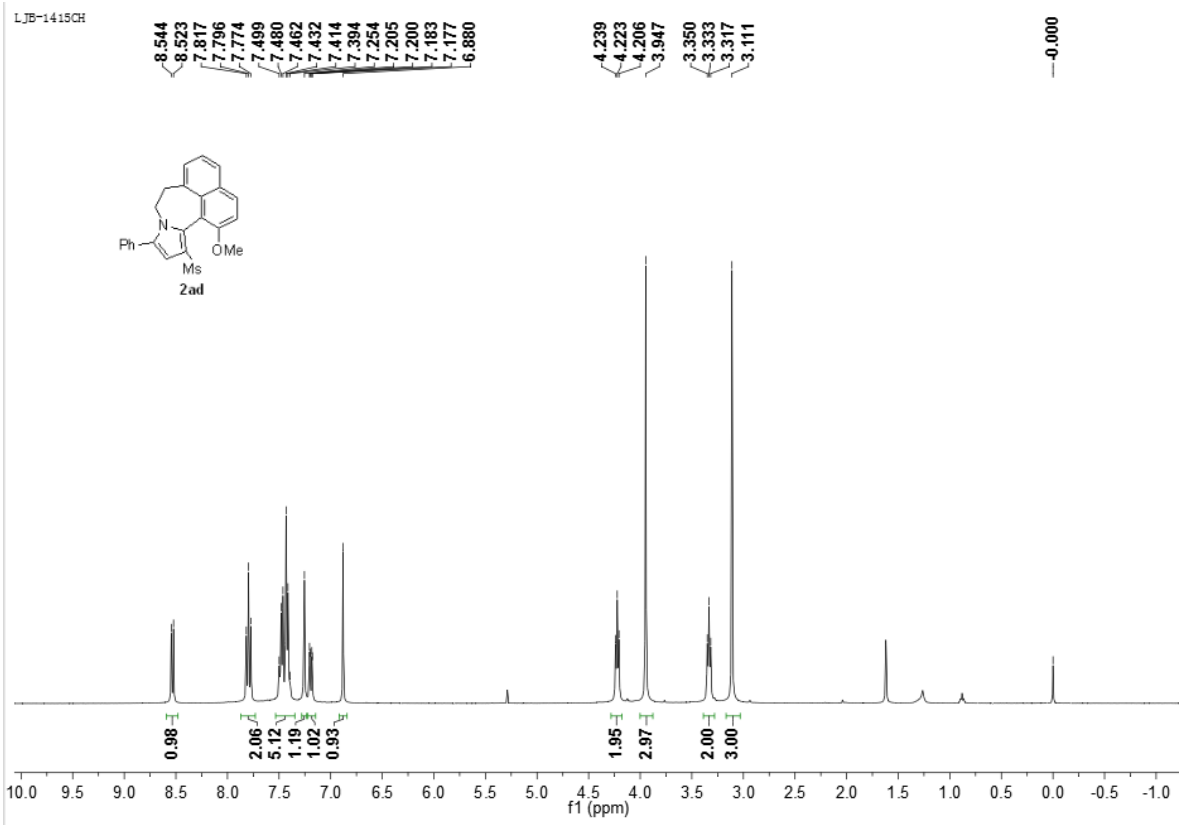

ljb-717CH
8.397
8.375
6.902
6.895
6.880
6.873
6.801
6.795
6.336
6.335
4.145
4.129
4.112
3.842
3.036
3.022
3.006
1.705
1.692
1.684
1.671
1.660
1.653
1.640
0.926
0.921
0.905
0.675
0.671
0.662
0.658
0.000
Ms
MeO
2aa
1.00
1.01
0.95
0.97
2.02
2.94
4.99
1.05
2.16
2.04
f1 (ppm)

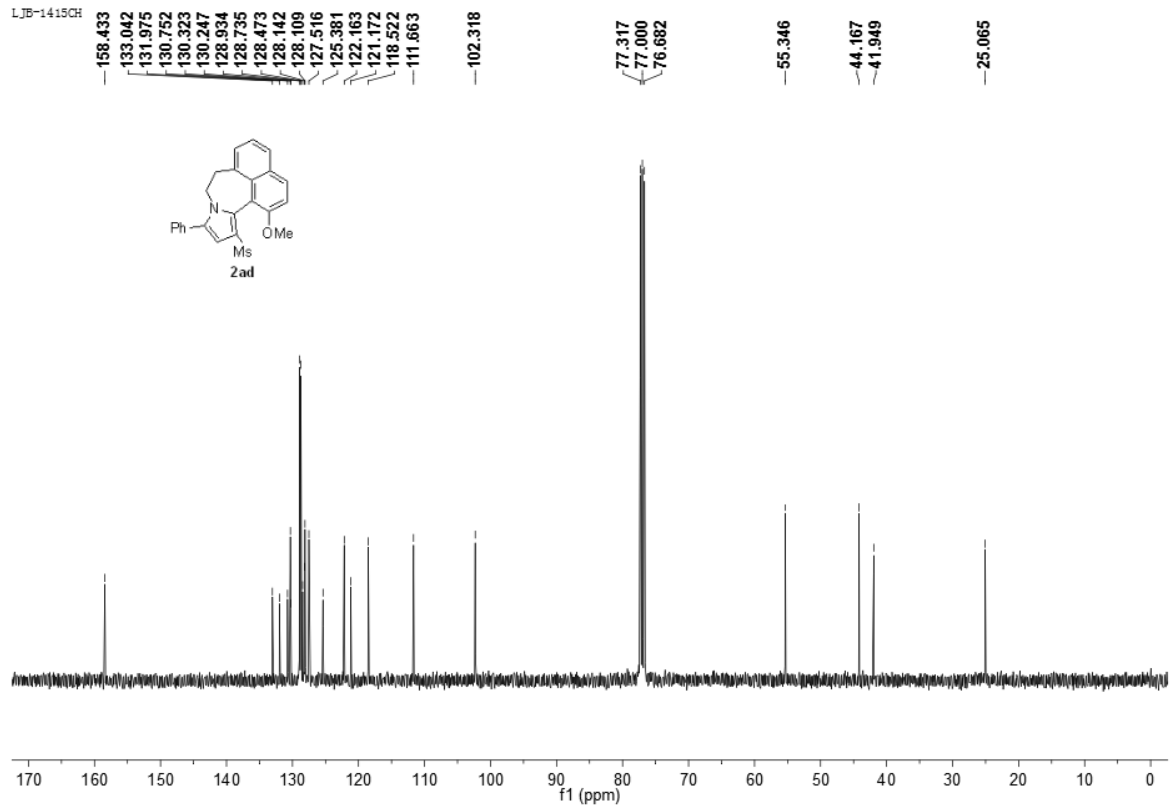

ljb-717CH
159.141
134.841
133.664
129.257
128.346
120.290
117.410
113.892
112.620
108.306
77.317
77.000
76.682
55.305
43.907
41.013
29.728
6.422
5.764
-0.026
Ms
MeO
2aa
f1 (ppm)

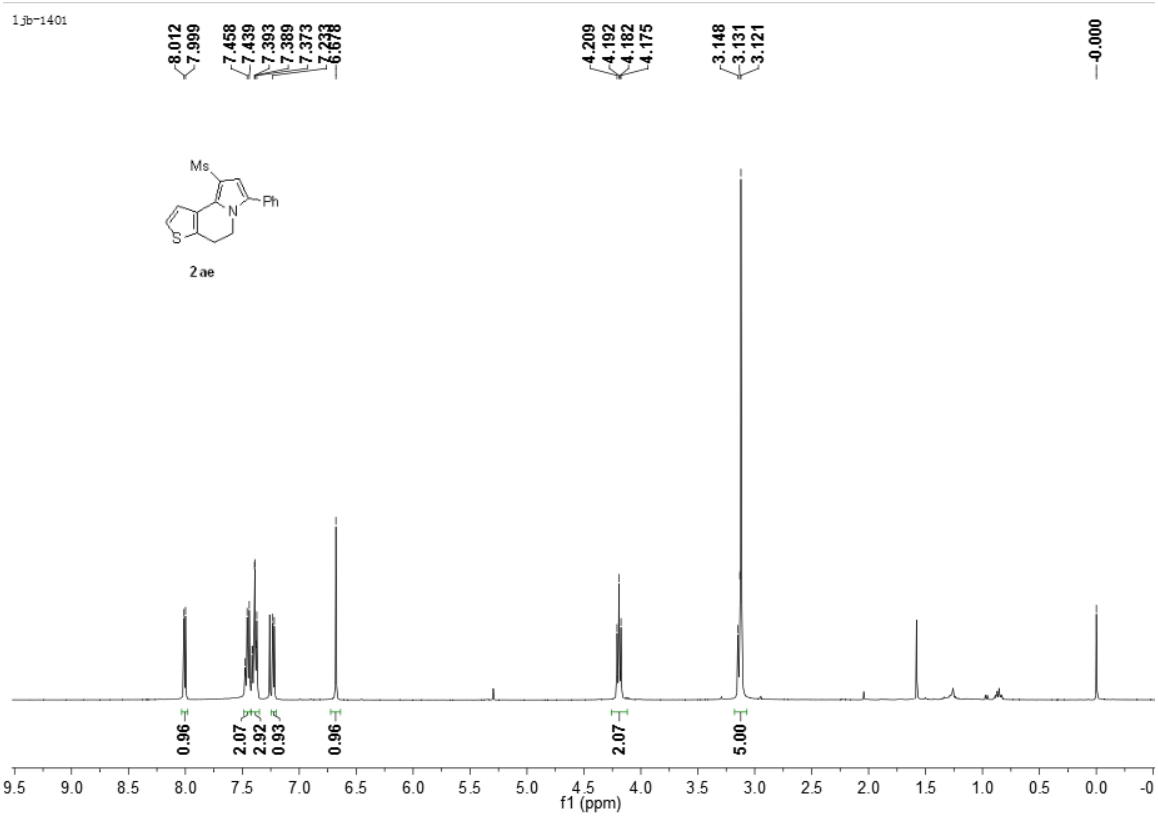

PC-4-37A
8.222
7.260
6.753
6.601
4.613
4.139
4.123
4.106
3.914
3.908
3.015
3.003
2.986
2.969
Ms
OH
MeO
MeO
N
2ab
1.08
1.04
1.00
2.00
2.11
6.77
5.30
f1 (ppm)

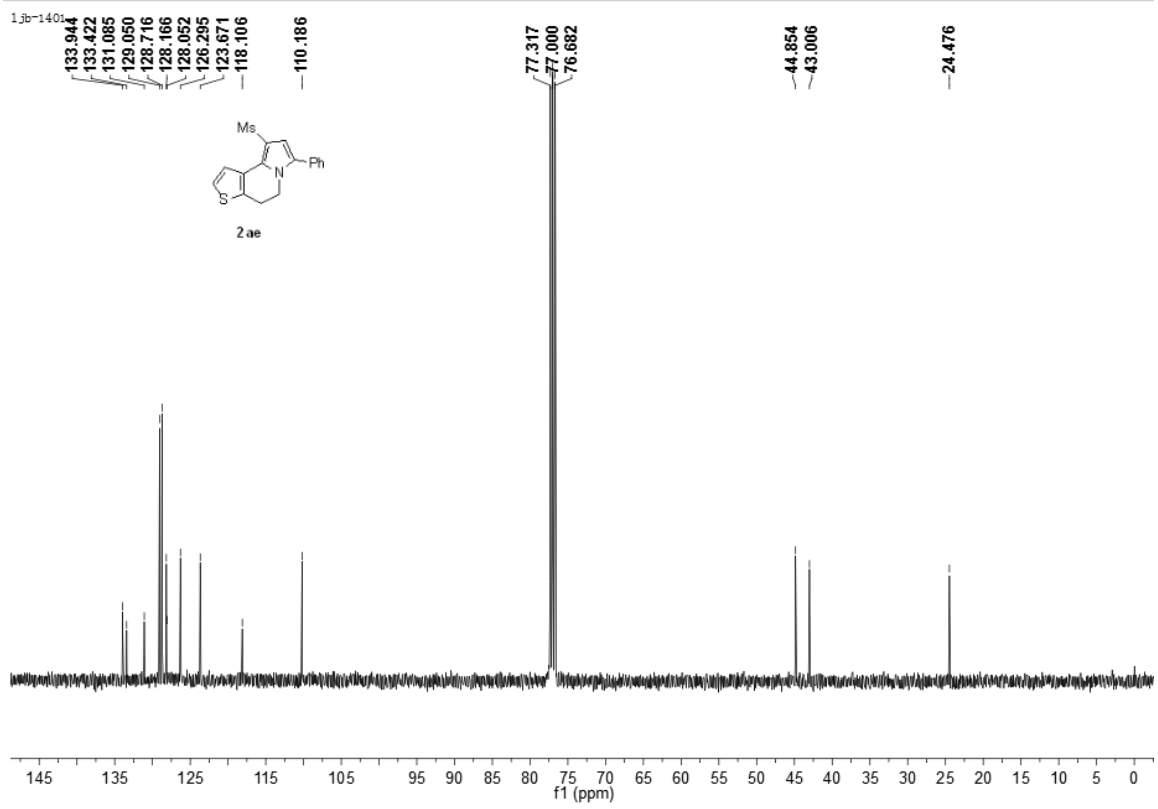

PC-4-37A
148.816
148.276
131.084
130.051
126.006
119.546
117.684
111.460
110.954
110.299
77.318
77.000
76.682
56.159
55.919
44.039
41.699
28.739
Ms
OH
MeO
MeO
N
2ab
f1 (ppm)

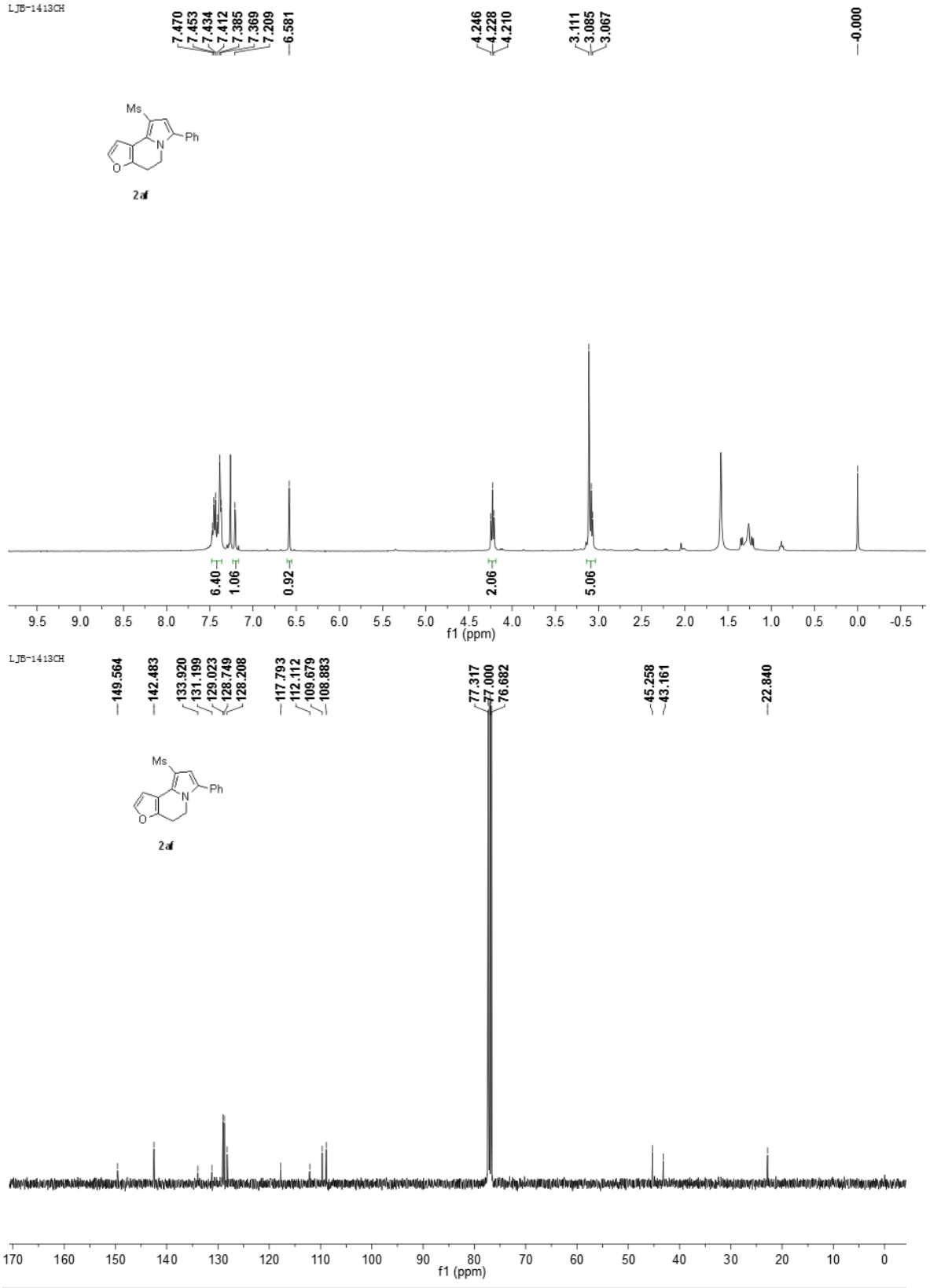

8.253
7.281
6.765
6.517
4.290
4.273
4.256
4.016
3.999
3.983
3.944
3.921
3.042
3.013
2.997
2.981
2.962
-0.000
Ms
MeO
MeO
N
OAc
2ac
1.01
1.03
0.97
1.97
2.06
2.97
2.98
3.09
2.08
2.02
3.11
f1 (ppm)
170.839
148.555
148.293
129.846
127.293
125.411
119.819
118.212
110.838
110.150
110.087
77.317
77.000
76.681
62.617
56.143
55.896
43.967
41.418
28.855
25.607
20.873
f1 (ppm)

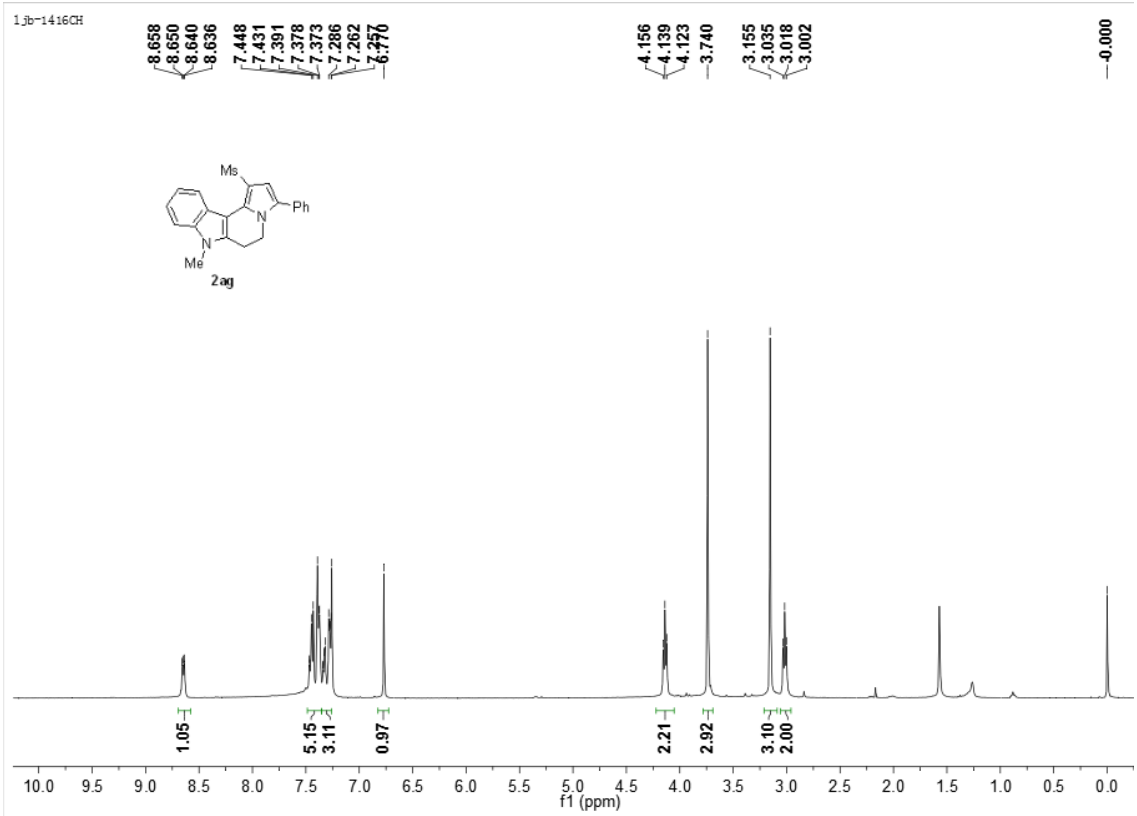

LJB-1415CH
8.544
8.523
7.817
7.796
7.774
7.499
7.480
7.462
7.432
7.414
7.394
7.254
7.205
7.200
7.183
7.177
6.880
4.239
4.223
4.206
3.947
3.350
3.333
3.317
3.111
0.000
Ph
OMe
Ms
2ad
0.98
2.06
5.12
1.19
1.02
0.93
1.95
2.97
2.00
3.00
f1 (ppm)

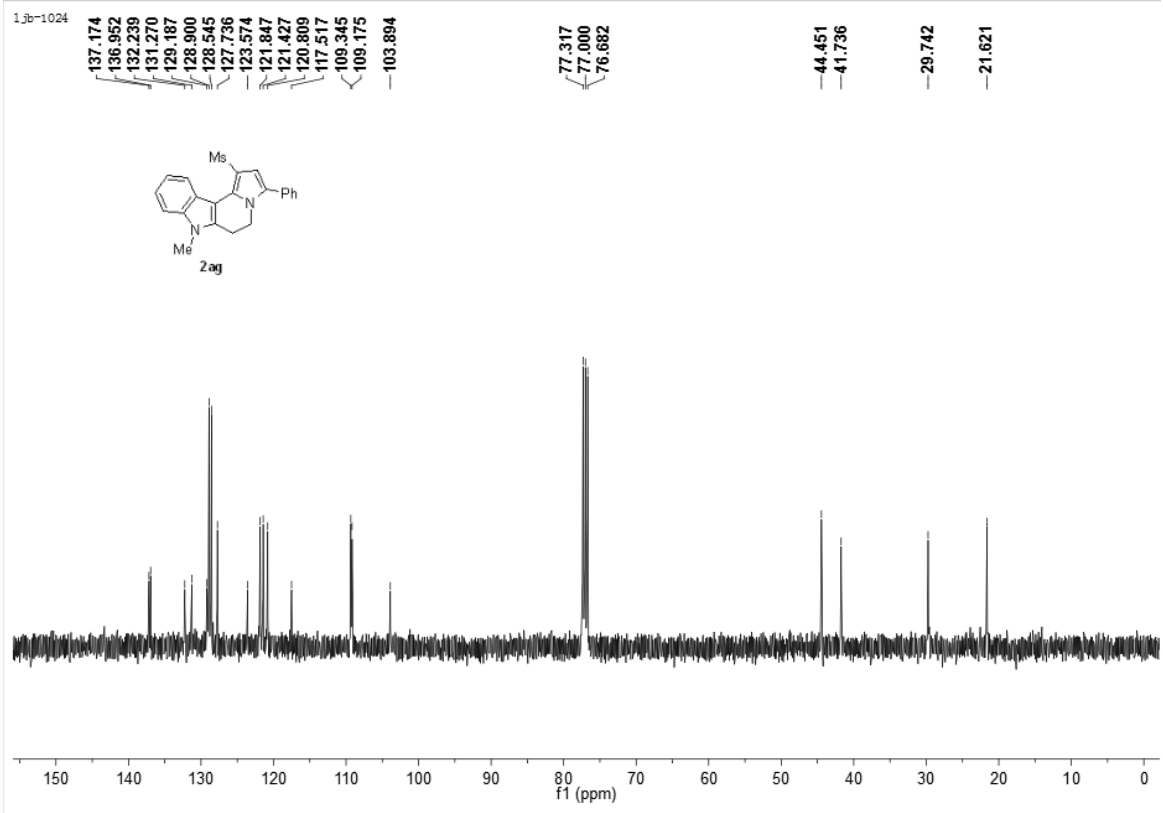

LJB-1415CH
158.433
133.042
131.975
130.752
130.323
130.247
128.934
128.735
128.473
128.142
128.109
127.516
125.381
122.163
121.172
118.522
111.663
102.318
77.317
77.000
76.682
55.346
44.167
41.949
25.065
Ph
OMe
Ms
2ad
f1 (ppm)

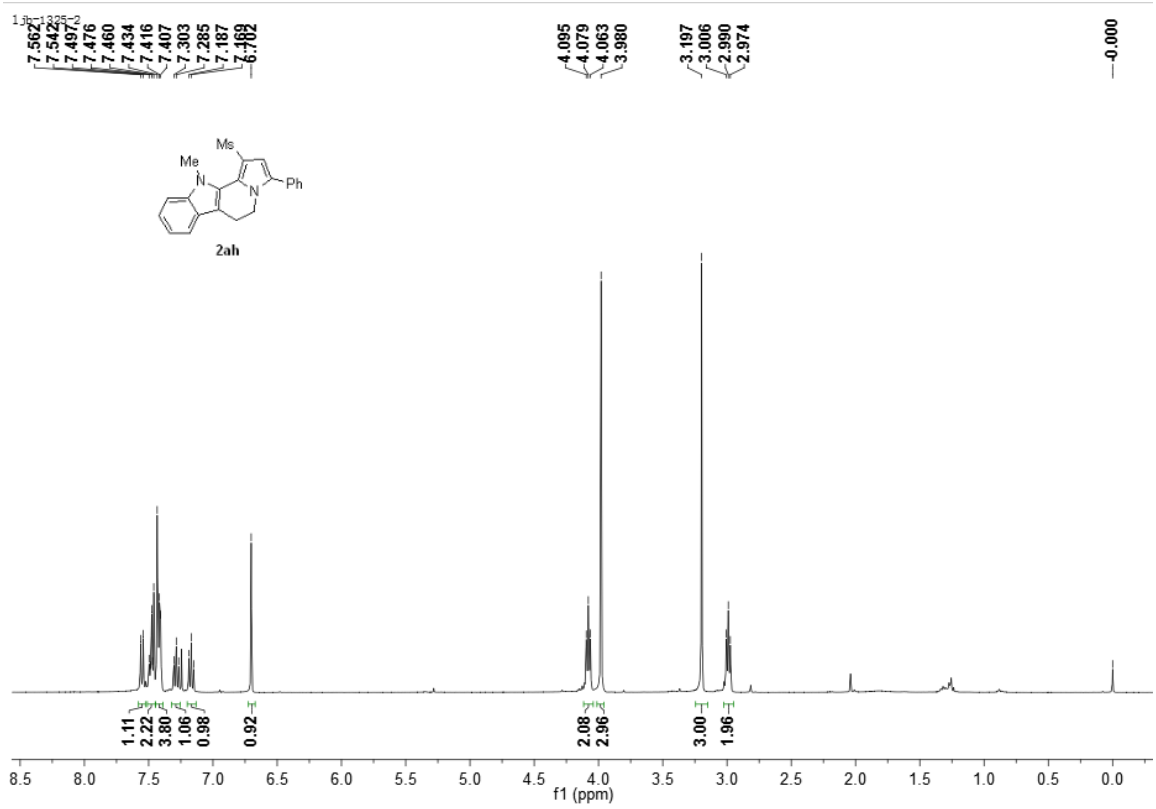

1jb-1401
8.012
7.999
7.458
7.439
7.393
7.389
7.373
7.233
6.678
4.209
4.192
4.182
4.175
3.148
3.131
3.121
0.000
Ms
Ph
N
S
2ae
0.96
2.07
2.92
0.93
0.96
2.07
5.00
f1 (ppm)

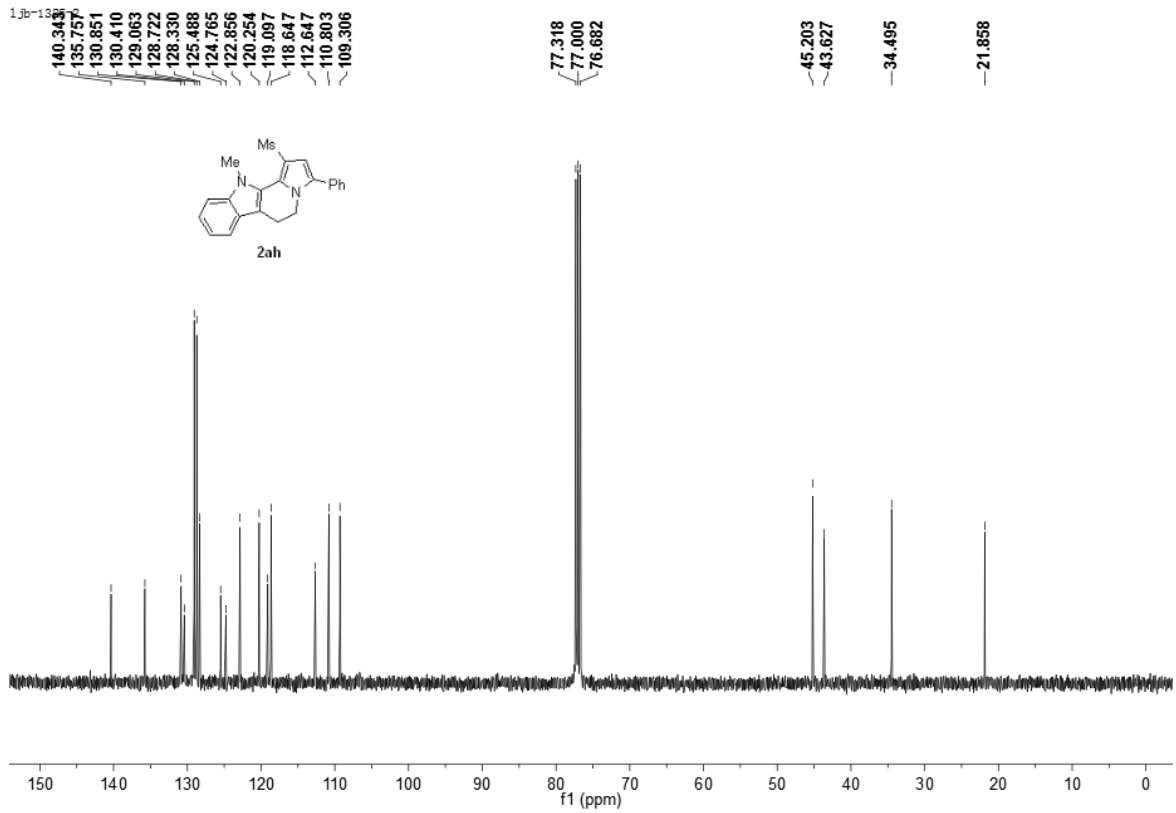

1jb-1401
133.944
133.422
131.085
129.050
128.716
128.166
128.052
126.295
123.671
118.106
110.186
77.317
77.000
76.682
44.854
43.006
24.476
Ms
Ph
N
S
2ae
f1 (ppm)

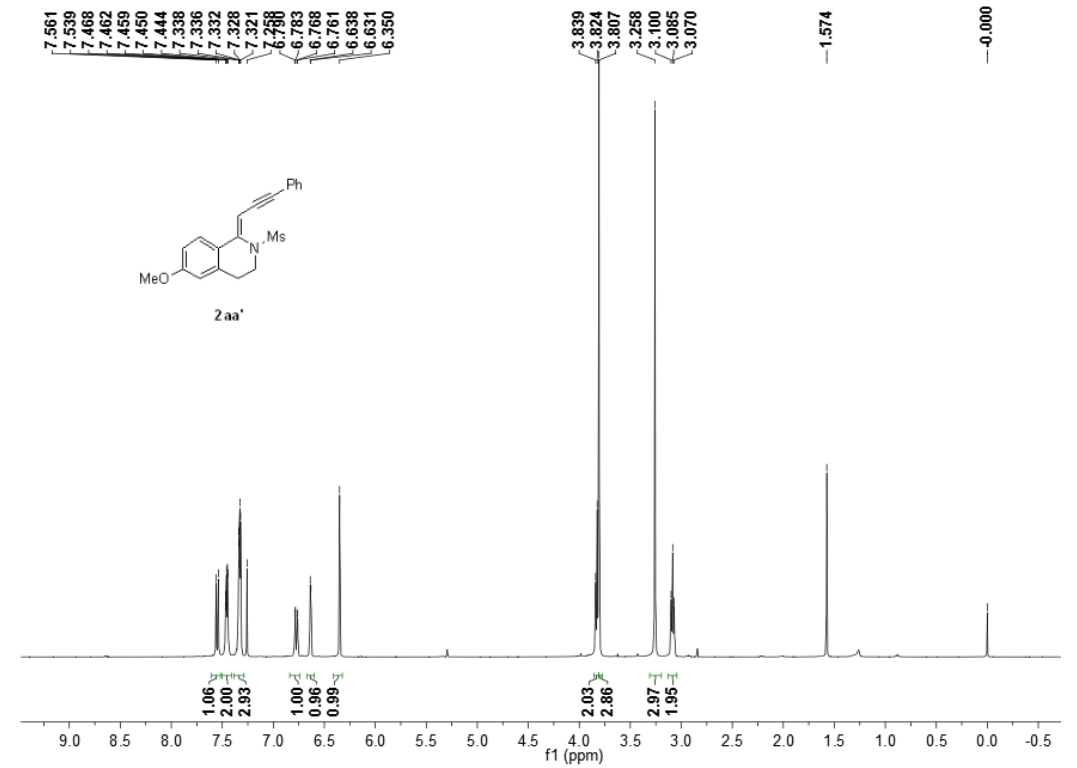

LJB-1413CH
7.470
7.453
7.434
7.412
7.385
7.369
7.209
6.581
4.246
4.228
4.210
3.111
3.085
3.067
0.000
Ms
Ph
N
O
2af
6.40
1.06
0.92
2.06
5.06
f1 (ppm)
LJB-1413CH
149.564
142.483
133.920
131.199
129.023
128.749
128.208
117.793
112.112
109.679
108.883
77.317
77.000
76.682
45.258
43.161
22.840
Ms
Ph
N
O
2af
f1 (ppm)

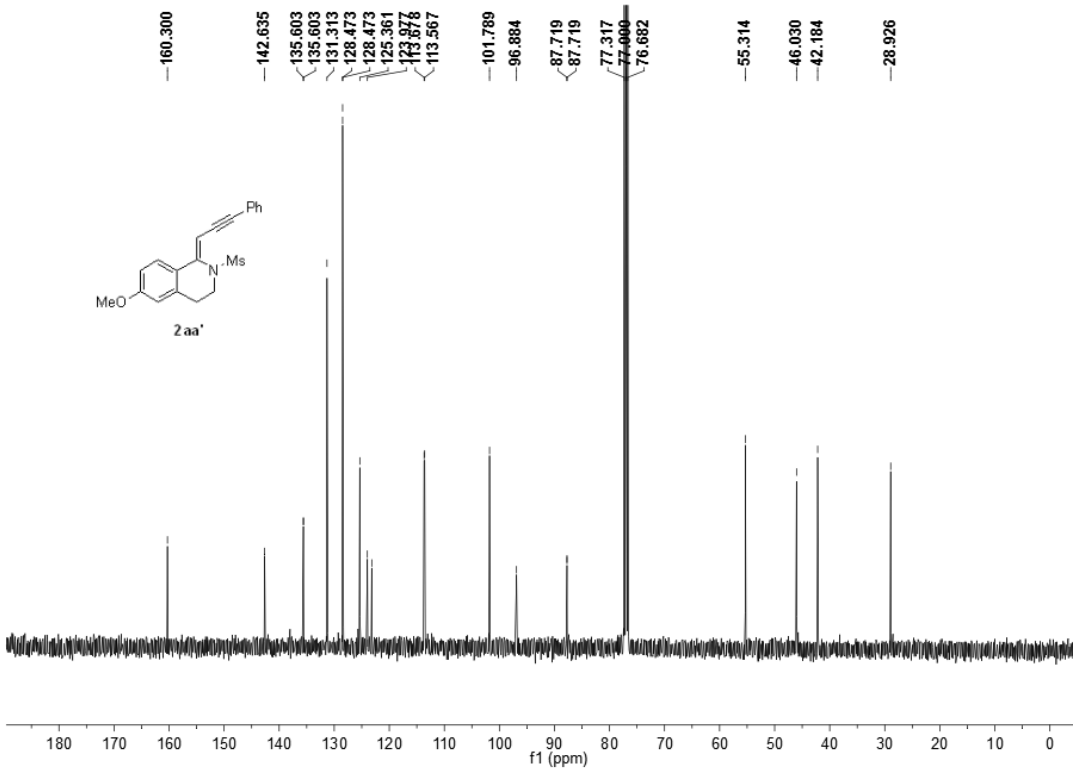

1jb-1416CH
8.658
8.650
8.640
8.636
7.448
7.431
7.391
7.378
7.373
7.286
7.262
4.156
4.139
4.123
3.740
3.155
3.035
3.018
3.002
0.000
Ms
Ph
N
N
Me
2ag
1.05
5.15
3.11
0.97
2.21
2.92
3.10
2.00
f1 (ppm)

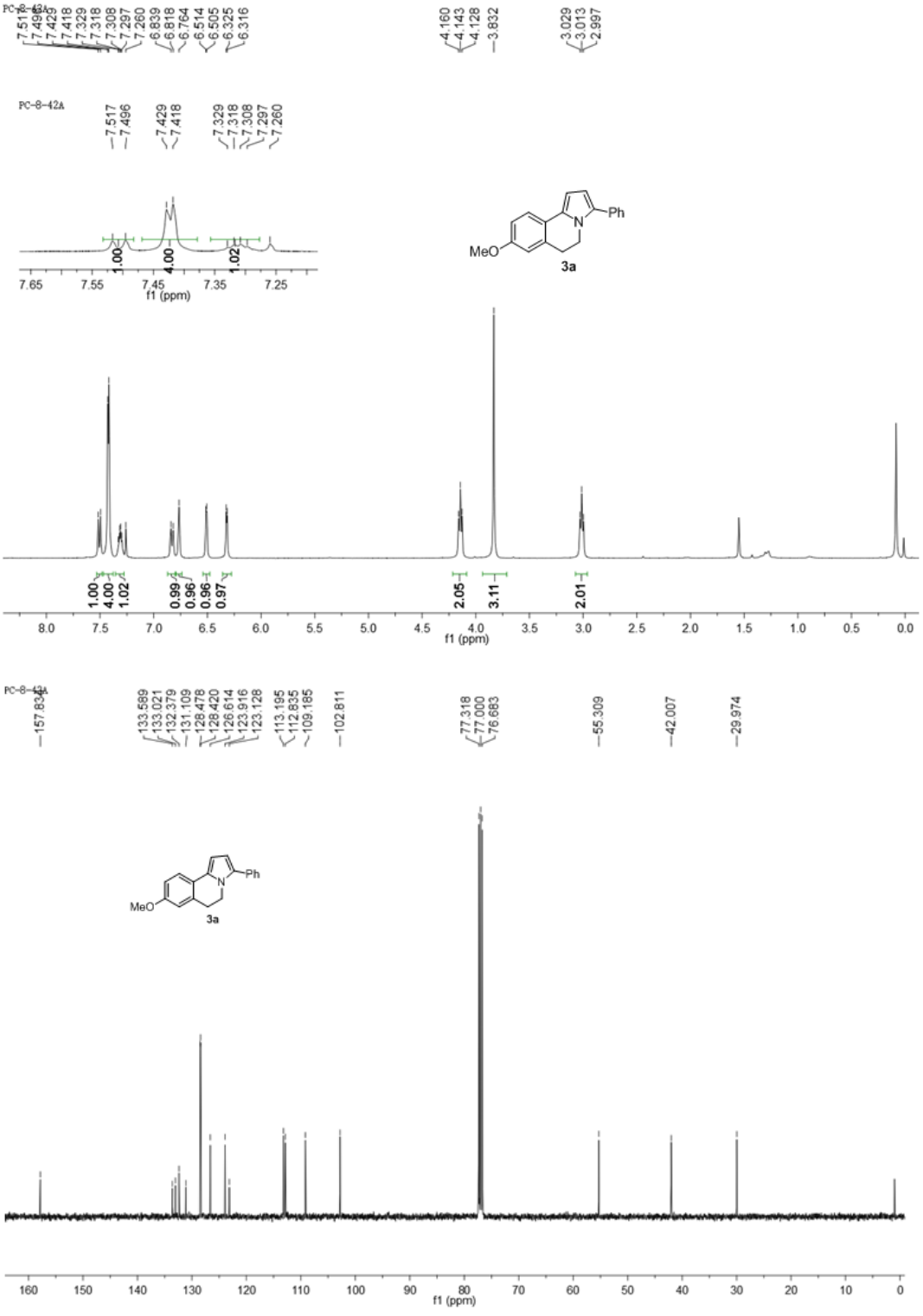

1jb-1024
137.174
136.952
132.239
131.270
129.187
128.900
128.545
127.736
123.574
121.847
121.427
120.809
117.517
109.345
109.175
103.894
77.317
77.000
76.682
44.451
41.736
29.742
21.621
Ms
Ph
N
N
Me
2ag
f1 (ppm)

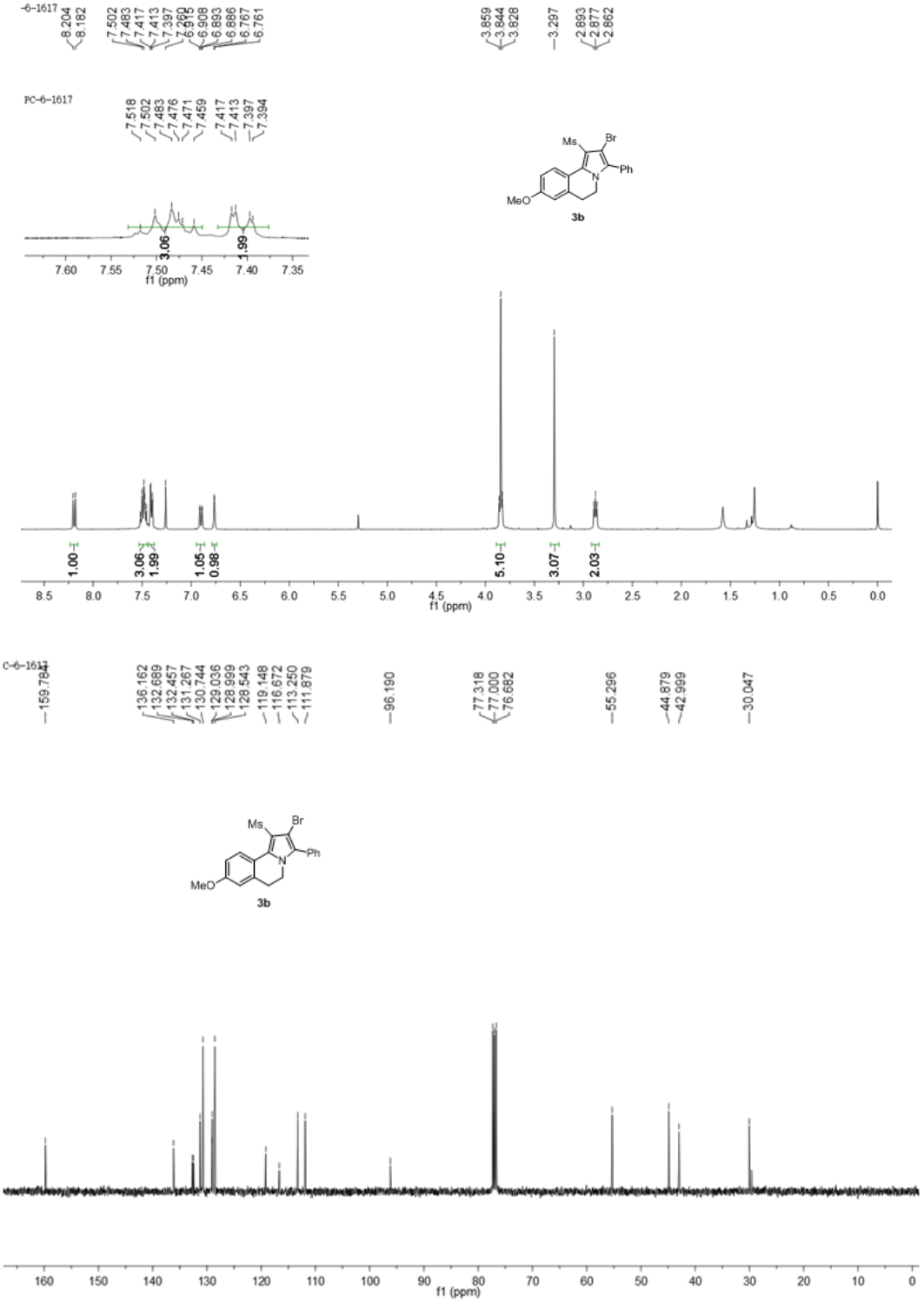

7.562
7.542
7.497
7.476
7.460
7.434
7.416
7.407
7.303
7.285
7.187
6.702
4.095
4.079
4.063
3.980
3.197
3.006
2.990
2.974
0.000
Ms
Me
N
Ph
N
2ah
1.11
2.22
3.80
1.06
0.98
0.92
2.08
2.96
3.00
1.96
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

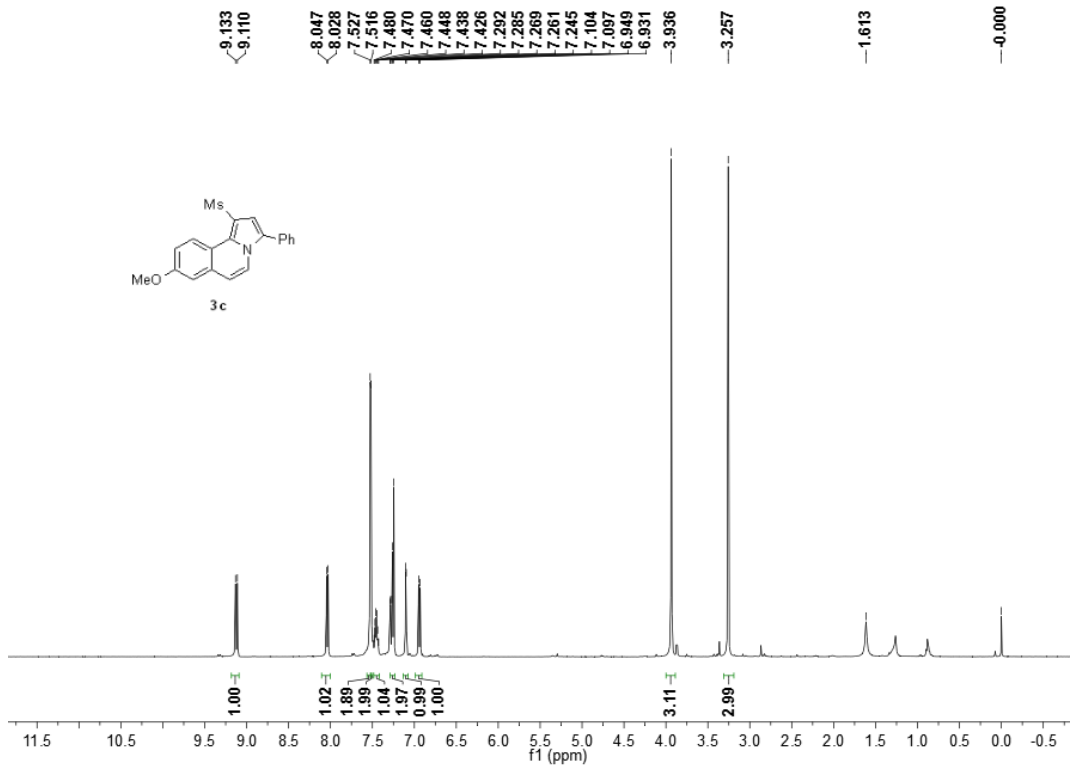

140.343
135.757
130.851
130.410
129.063
128.722
128.330
125.488
124.765
122.856
120.254
119.097
118.647
112.647
110.803
109.306
77.318
77.000
76.682
45.203
43.627
34.495
21.858
Ms
Me
N
Ph
N
2ah
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

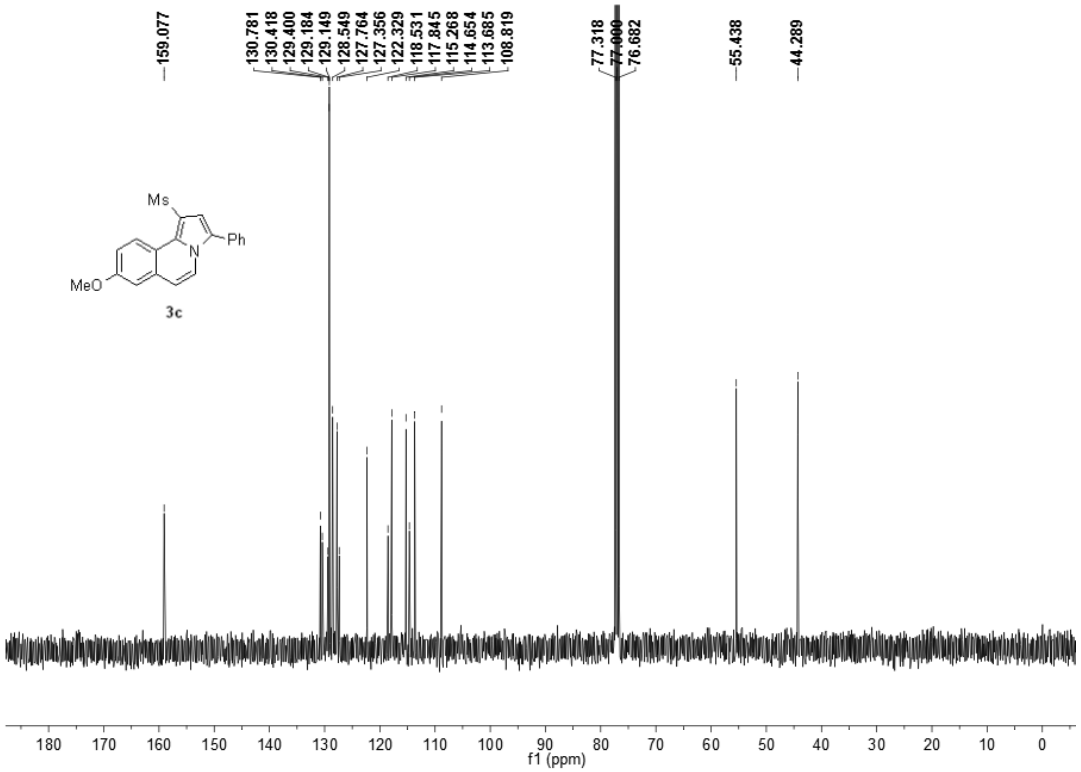

7.561
7.539
7.468
7.462
7.459
7.450
7.444
7.338
7.336
7.332
7.328
7.321
6.790
6.783
6.768
6.761
6.638
6.631
6.350
3.839
3.824
3.807
3.258
3.100
3.085
3.070
1.574
0.000
Ph
Ms
N
MeO
2aa'
1.06
2.00
2.93
1.00
0.96
0.99
2.03
2.86
2.97
1.95
f1 (ppm)

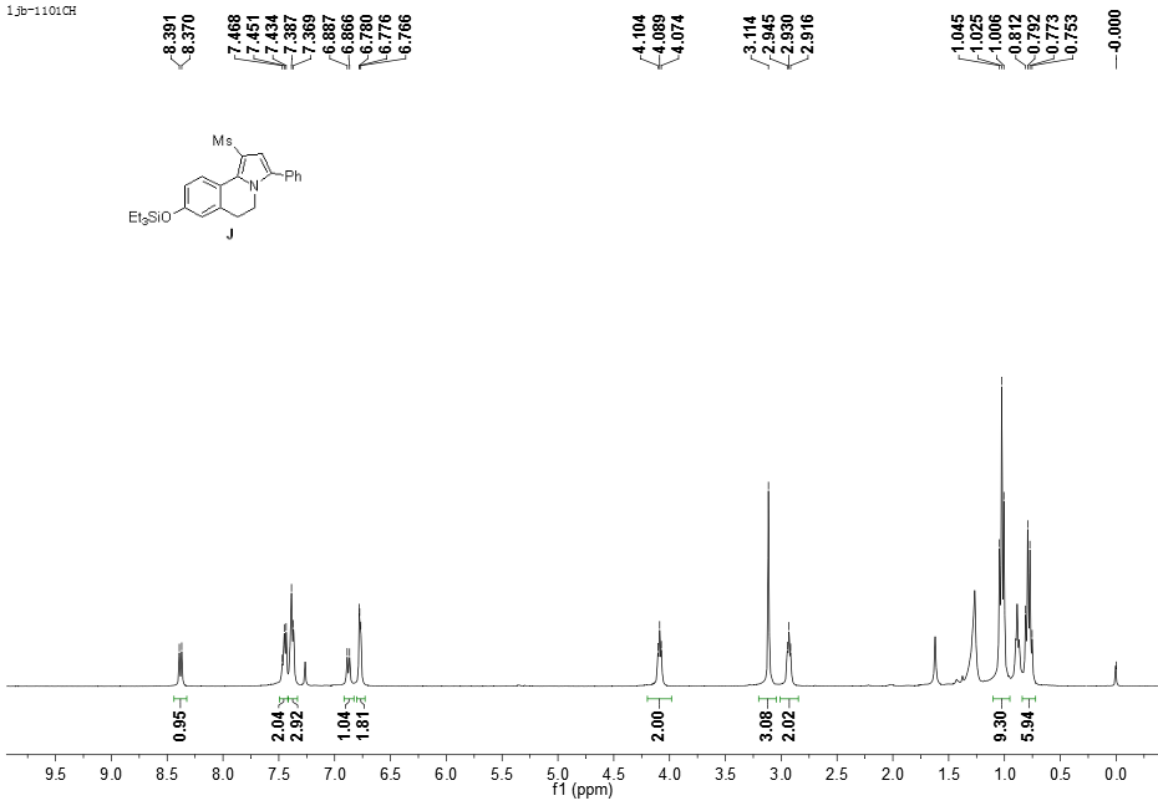

160.300
142.635
135.603
135.603
131.313
128.473
128.473
125.361
113.567
101.789
96.884
87.719
87.719
77.317
77.000
76.682
55.314
46.030
42.184
28.926
Ph
Ms
N
MeO
2aa'
f1 (ppm)

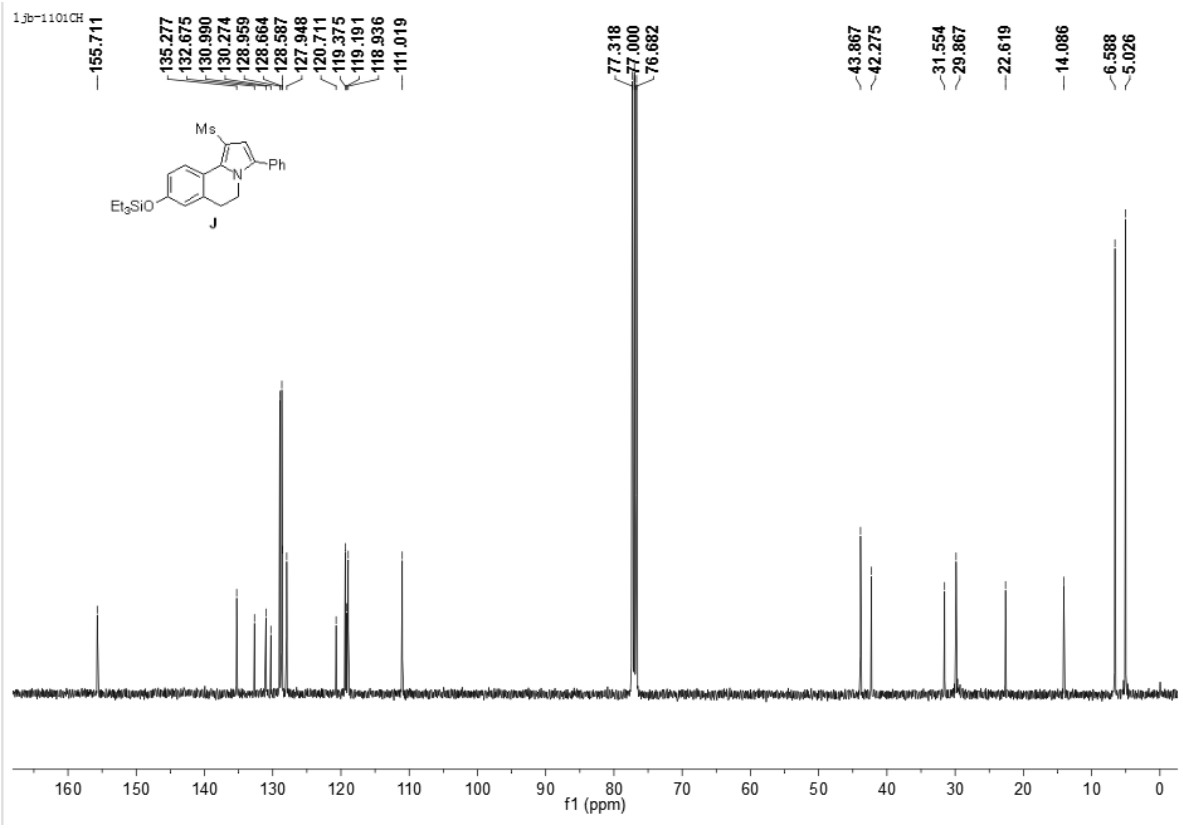

PC-8-42A
7.517
7.496
7.429
7.418
7.329
7.318
7.308
7.297
7.260
6.839
6.818
6.764
6.514
6.505
6.325
6.316
4.160
4.143
4.128
3.832
3.029
3.013
2.997
1.00
4.00
1.02
0.99
0.96
0.96
0.97
2.05
3.11
2.01
f1 (ppm)
MeO
Ph
N
3a
133.589
133.021
132.379
131.109
128.478
128.420
126.614
123.916
123.128
113.195
112.835
109.185
102.811
77.318
77.000
76.683
55.309
42.007
29.974

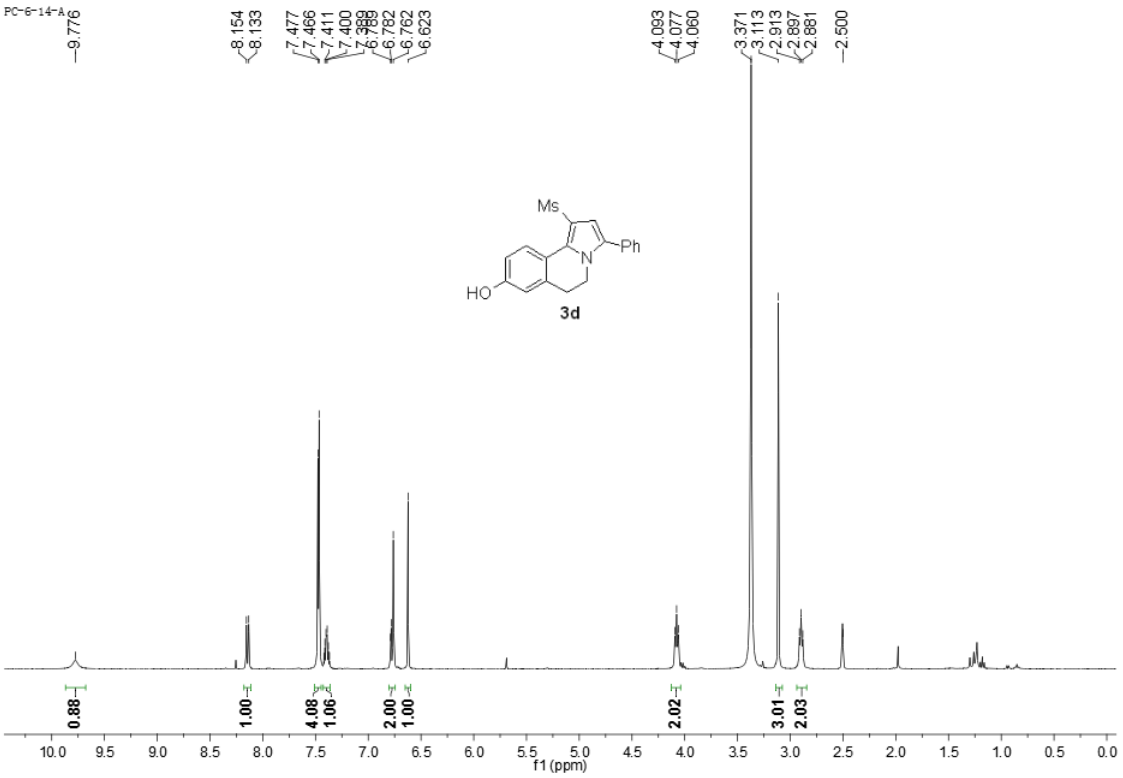

-6-1617
8.204
8.182
7.502
7.483
7.417
7.413
7.397
7.260
6.915
6.908
6.893
6.886
6.767
6.761
3.859
3.844
3.828
3.297
2.893
2.877
2.862
PC-6-1617
7.518
7.502
7.483
7.476
7.471
7.459
7.417
7.413
7.397
7.394
Ms
Br
Ph
N
MeO
3b
3.06
1.99
7.60
7.55
7.50
7.45
7.40
7.35
f1 (ppm)
1.00
3.06
1.99
1.05
0.98
5.10
3.07
2.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
C-6-1617
159.784
136.162
132.689
132.457
131.267
130.744
129.036
128.999
128.543
119.148
116.672
113.250
111.879
96.190
77.318
77.000
76.682
55.296
44.879
42.999
30.047
Ms
Br
Ph
N
MeO
3b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

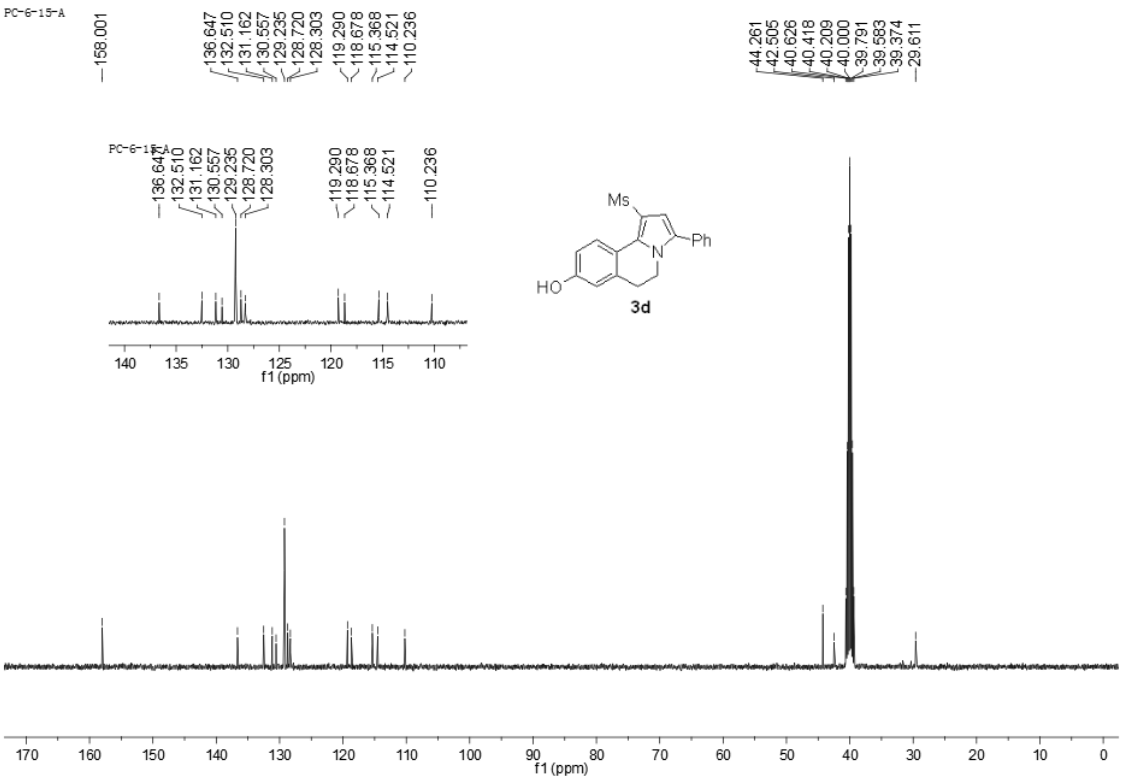

9.133
9.110
8.047
8.028
7.527
7.516
7.480
7.470
7.460
7.448
7.438
7.426
7.292
7.285
7.269
7.261
7.245
7.104
7.097
6.949
6.931
3.936
3.257
1.613
0.000
Ms
Ph
N
MeO
3c
1.00
1.02
1.89
1.99
1.04
1.97
0.99
1.00
3.11
2.99
f1 (ppm)

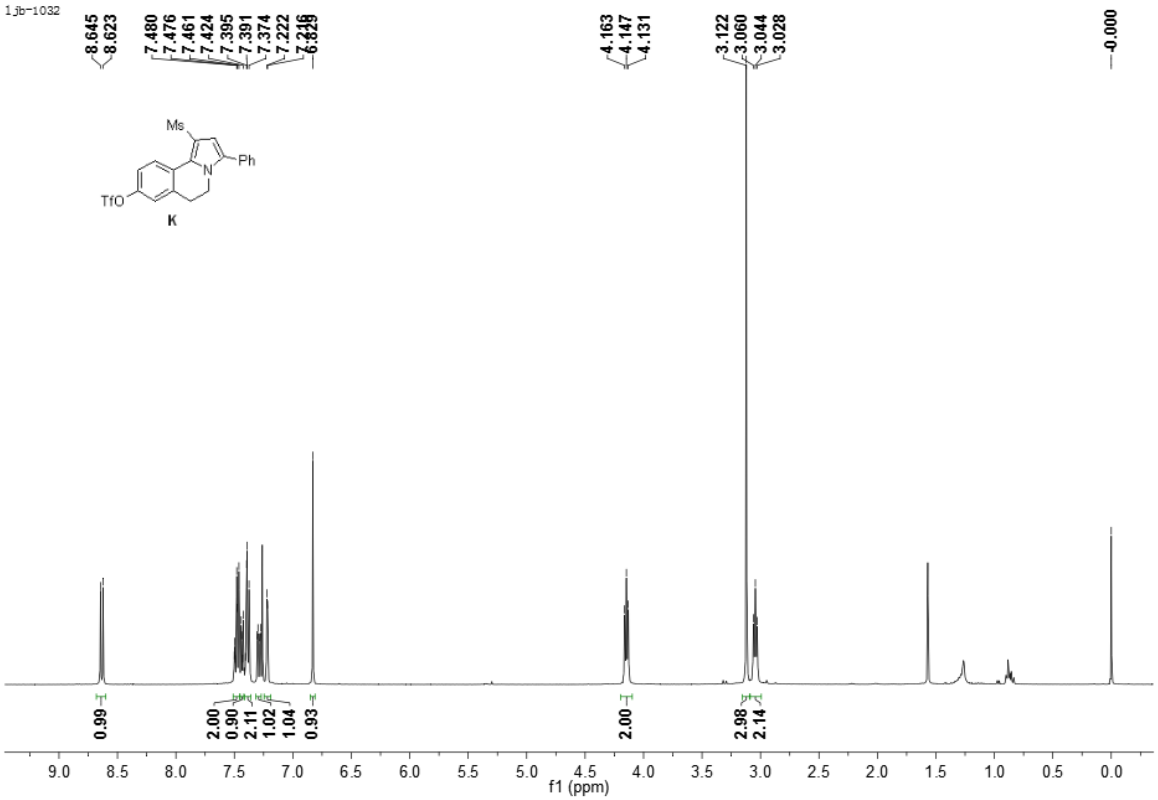

159.077
130.781
130.418
129.400
129.184
129.149
128.549
127.764
127.356
122.329
118.531
117.845
115.268
114.654
113.685
108.819
77.318
77.000
76.682
55.438
44.289
Ms
Ph
N
MeO
3c
f1 (ppm)

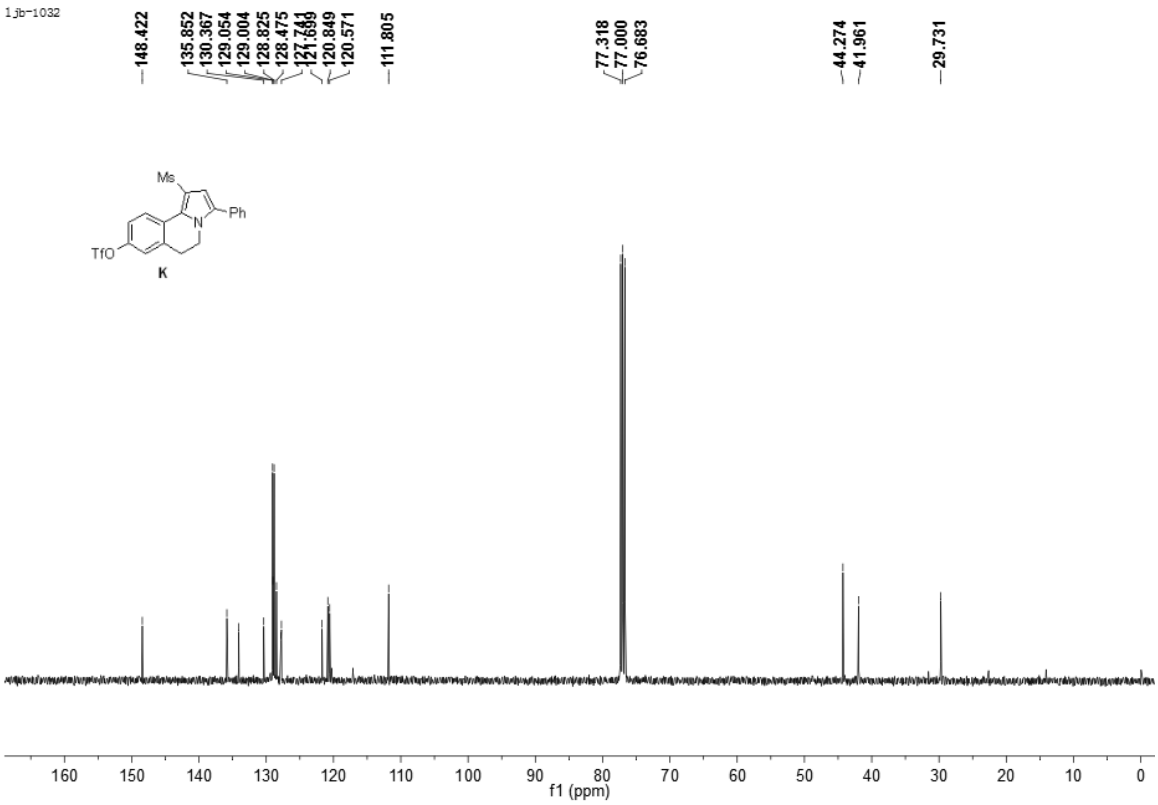

1jb-1101CH
8.391
8.370
7.468
7.451
7.434
7.387
7.369
6.887
6.866
6.780
6.776
6.766
4.104
4.089
4.074
3.114
2.945
2.930
2.916
1.045
1.025
1.006
0.812
0.792
0.773
0.753
0.000
Ms
Ph
N
Et3SiO
J
0.95
2.04
2.92
1.04
1.81
2.00
3.08
2.02
9.30
5.94
f1 (ppm)

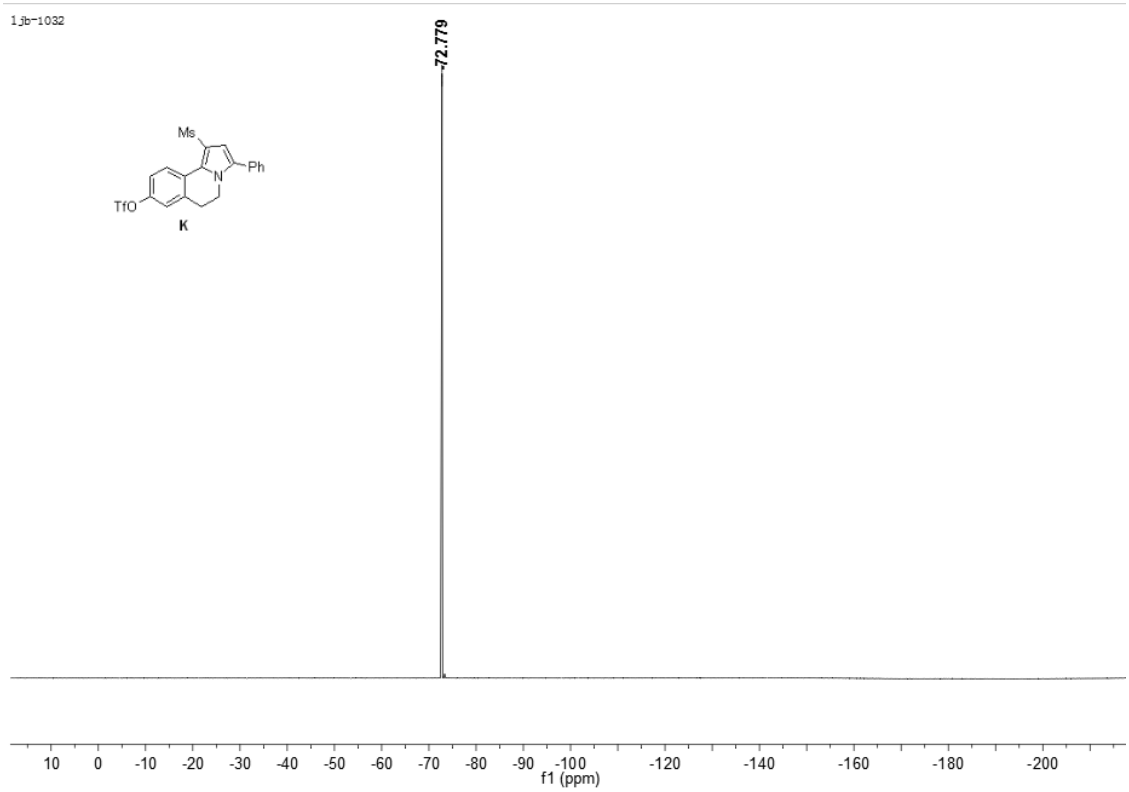

1jb-1101CH
155.711
135.277
132.675
130.990
130.274
128.959
128.664
128.587
127.948
120.711
119.375
119.191
118.936
111.019
77.318
77.000
76.682
43.867
42.275
31.554
29.867
22.619
14.086
6.588
5.026
Ms
Ph
N
Et3SiO
J
f1 (ppm)

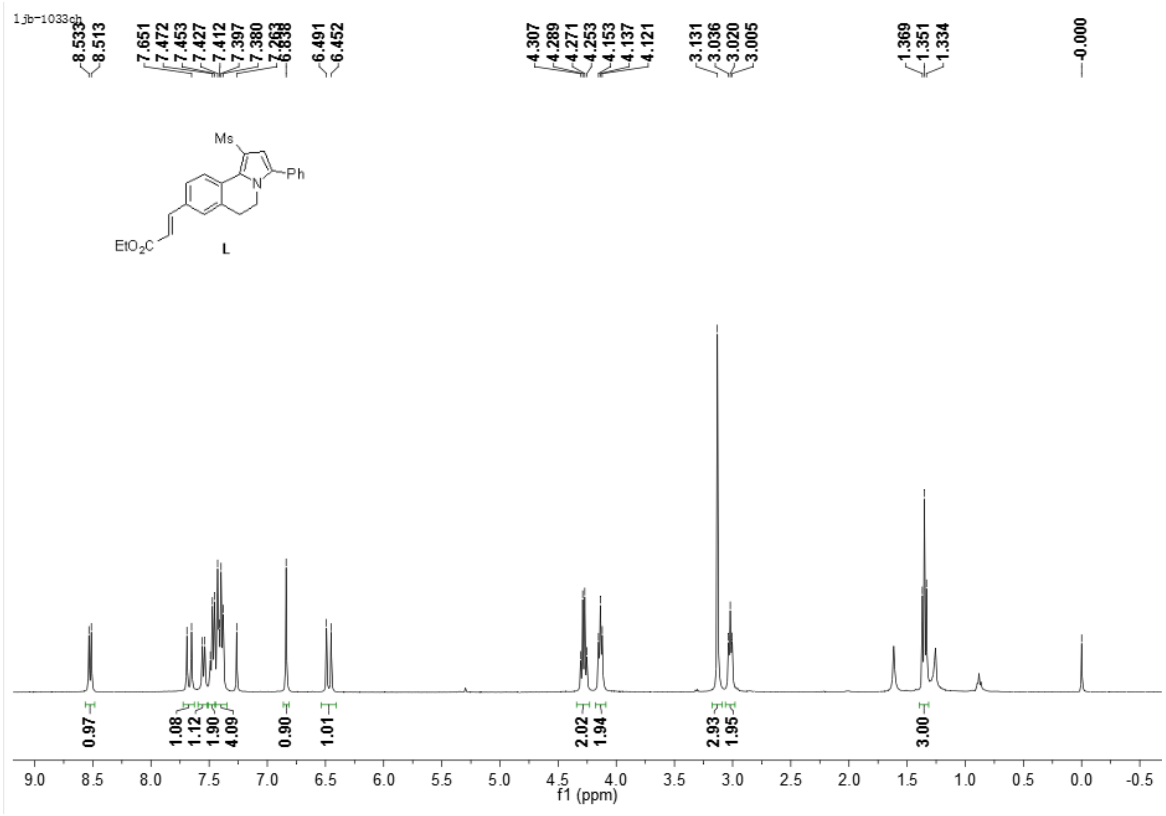

PC-6-14-A
9.776
8.154
8.133
7.477
7.466
7.411
7.400
6.782
6.762
6.623
4.093
4.077
4.060
3.371
3.113
2.913
2.897
2.881
2.500
Ms
Ph
N
HO
3d
0.88
1.00
4.08
1.06
2.00
1.00
2.02
3.01
2.03
f1 (ppm)

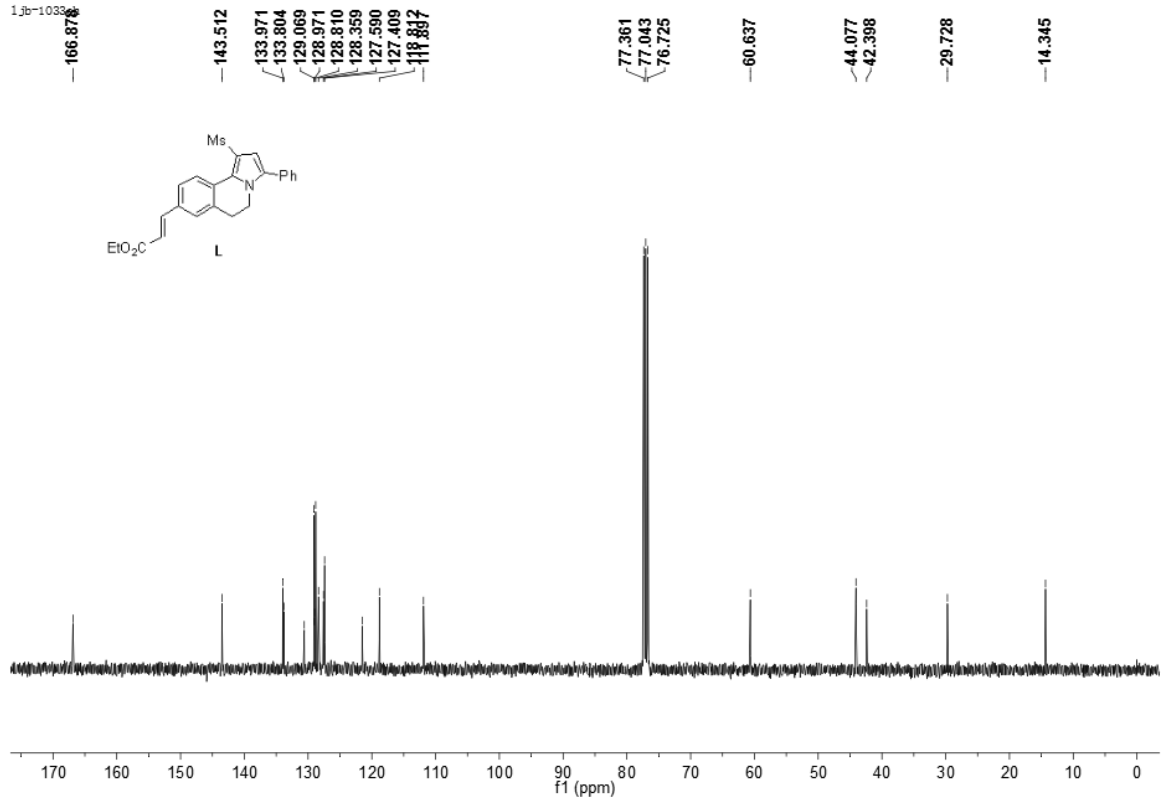

PC-6-15-A
158.001
136.647
132.510
131.162
130.557
129.235
128.720
128.303
119.290
118.678
115.368
114.521
110.236
44.261
42.505
40.626
40.418
40.209
40.000
39.791
39.583
39.374
29.611
Ms
Ph
N
HO
3d
f1 (ppm)

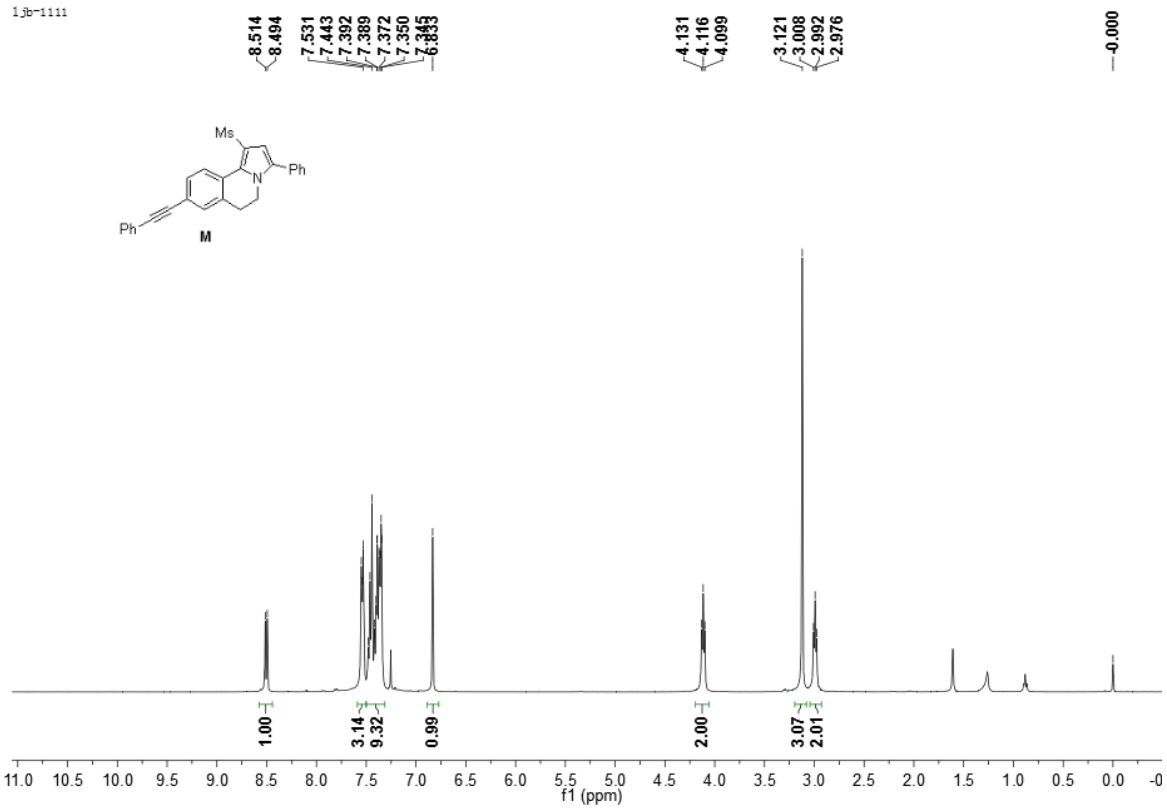

1jb-1032
8.645
8.623
7.480
7.476
7.461
7.424
7.395
7.391
7.374
7.222
4.163
4.147
4.131
3.122
3.060
3.044
3.028
0.000
Ms
Ph
TfO
K
0.99
2.00
0.90
2.11
1.02
1.04
0.93
2.00
2.98
2.14
f1 (ppm)

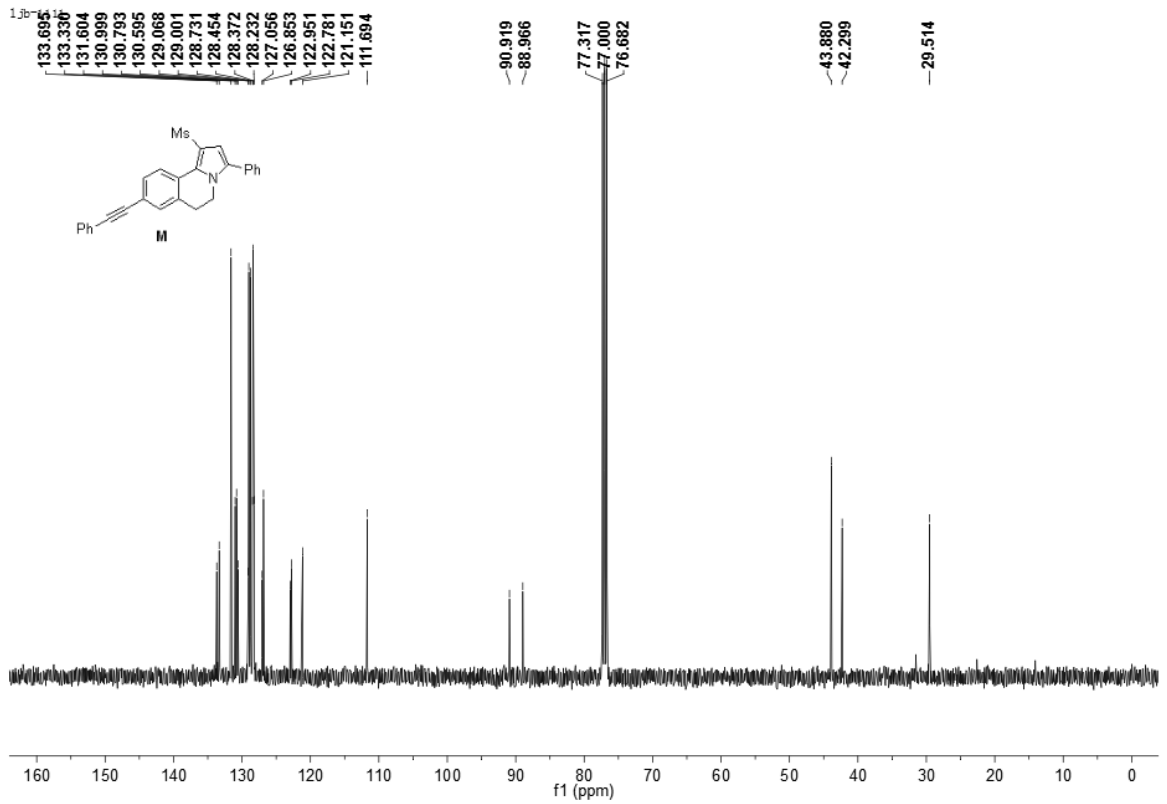

1jb-1032
148.422
135.852
130.367
129.054
129.004
128.825
128.475
120.849
120.571
111.805
77.318
77.000
76.683
44.274
41.961
29.731
Ms
Ph
TfO
K
f1 (ppm)

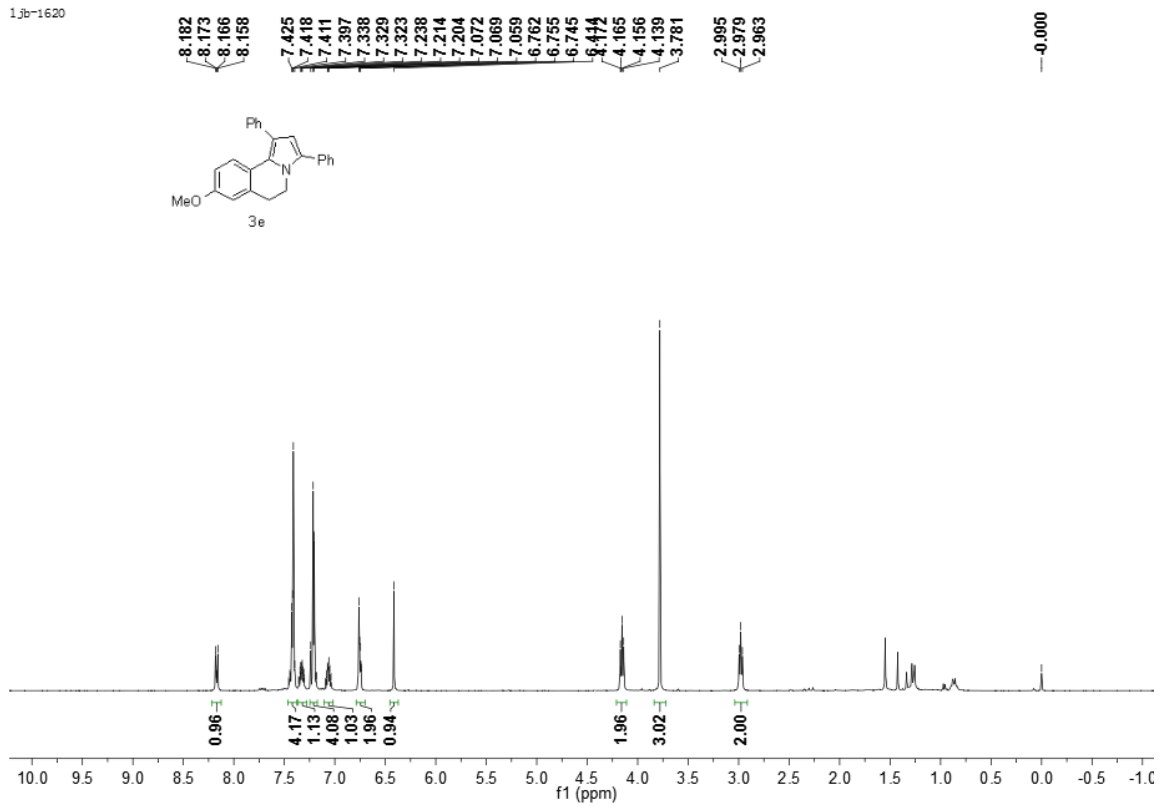

1jb-1032
-72.779
Ms
Ph
N
TfO
K
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

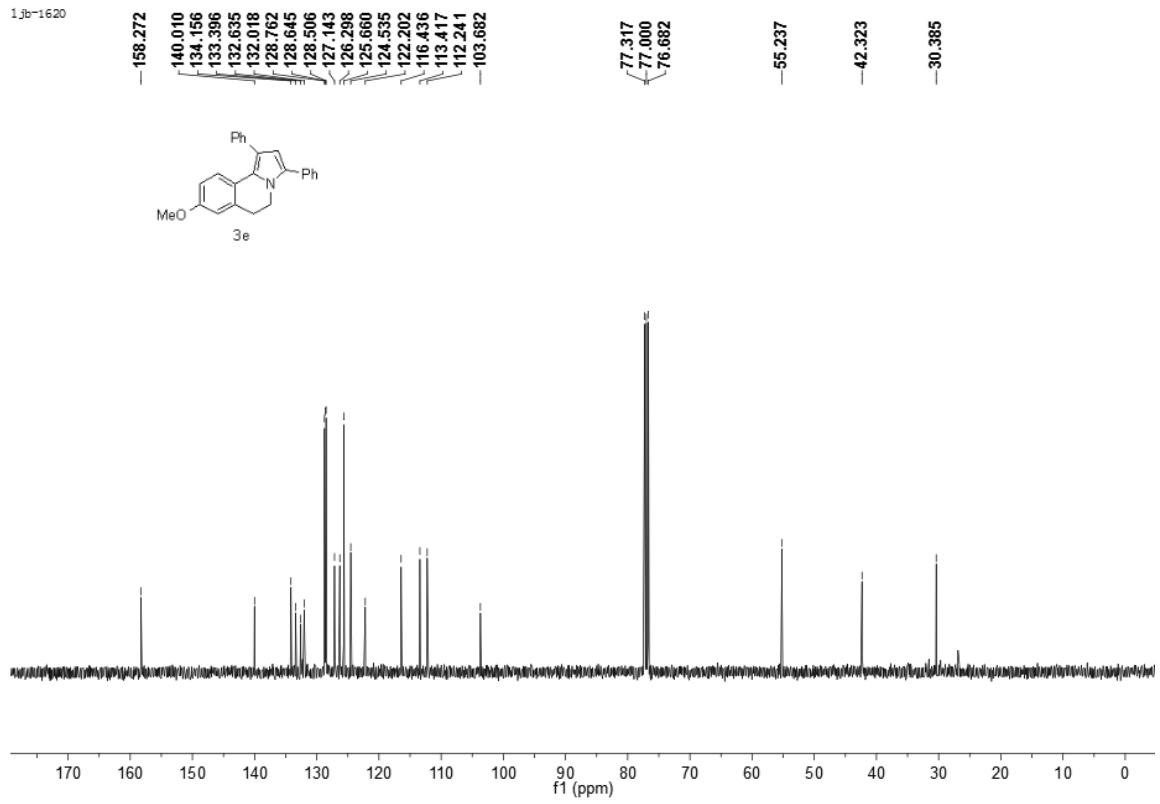

8.533
8.513
7.651
7.472
7.453
7.427
7.412
7.397
7.380
6.491
6.452
4.307
4.289
4.271
4.253
4.153
4.137
4.121
3.131
3.036
3.020
3.005
1.369
1.351
1.334
0.000
Ms
Ph
N
EtO2C
L
0.97
1.08
1.12
1.90
4.09
0.90
1.01
2.02
1.94
2.93
1.95
3.00
f1 (ppm)

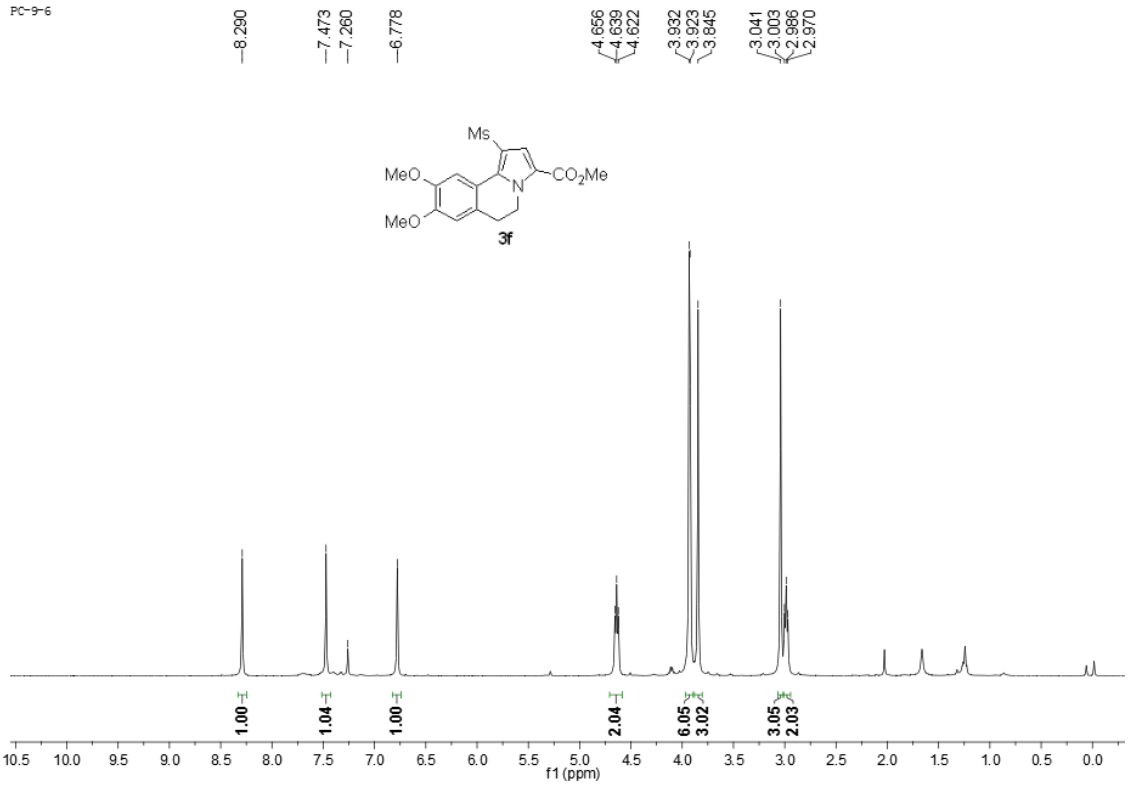

166.878
143.512
133.971
133.804
129.069
128.971
128.810
128.359
127.590
127.409
77.361
77.043
76.725
60.637
44.077
42.398
29.728
14.345
Ms
Ph
N
EtO2C
L
f1 (ppm)

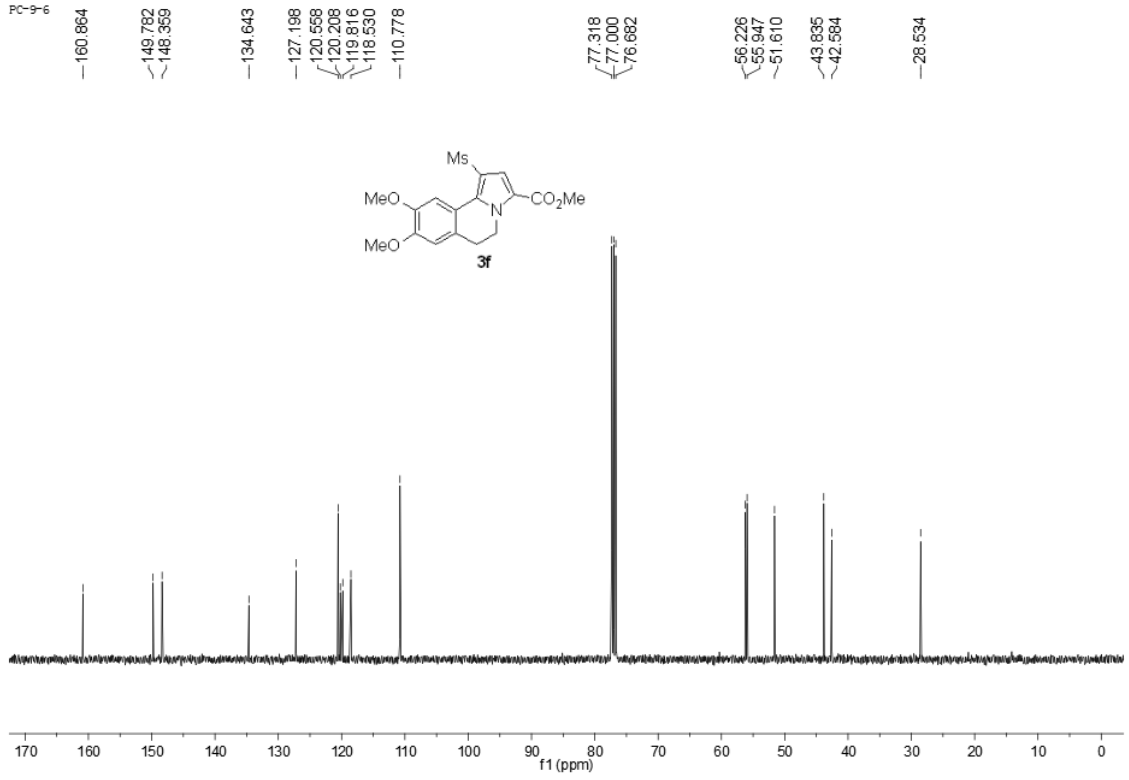

1jb-1111
8.514
8.494
7.531
7.443
7.392
7.389
7.372
7.350
4.131
4.116
4.099
3.121
3.008
2.992
2.976
-0.000
Ms
Ph
Ph
M
1.00
3.14
9.32
0.99
2.00
3.07
2.01
f1 (ppm)


133.695
133.330
131.604
130.999
130.793
130.595
129.068
129.001
128.731
128.454
128.372
128.232
127.056
126.853
122.951
122.781
121.151
111.694
90.919
88.966
77.317
77.000
76.682
43.880
42.299
29.514
Ms
Ph
Ph
M
f1 (ppm)


1jb-1620
8.182
8.173
8.166
8.158
7.425
7.418
7.411
7.397
7.338
7.329
7.323
7.238
7.214
7.204
7.072
7.069
7.059
6.762
6.755
6.745
4.165
4.156
4.139
3.781
2.995
2.979
2.963
0.000
Ph
Ph
MeO
3e
0.96
4.17
1.13
4.08
1.03
1.96
0.94
1.96
3.02
2.00
f1 (ppm)


1jb-1620
158.272
140.010
134.156
133.396
132.635
132.018
128.762
128.645
128.506
127.143
126.298
125.660
124.535
122.202
116.436
113.417
112.241
103.682
77.317
77.000
76.682
55.237
42.323
30.385
Ph
Ph
MeO
3e
f1 (ppm)


PC-9-6
8.290
7.473
7.260
6.778
4.656
4.639
4.622
3.932
3.923
3.845
3.041
3.003
2.986
2.970
Ms
MeO
MeO
CO2Me
N
3f
1.00
1.04
1.00
2.04
6.05
3.02
3.05
2.03
f1 (ppm)


PC-9-6
160.864
149.782
148.359
134.643
127.198
120.556
120.208
119.816
118.530
110.778
77.318
77.000
76.682
56.226
55.947
51.610
43.835
42.584
28.534
Ms
MeO
MeO
CO2Me
N
3f
f1 (ppm)