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Supporting Information

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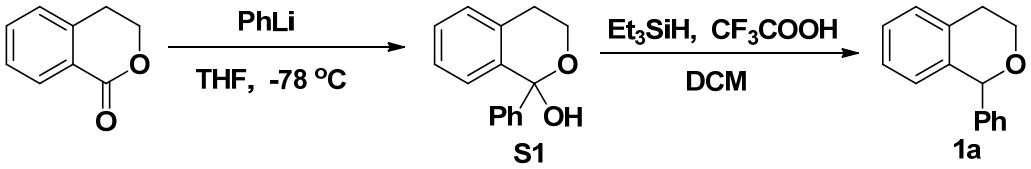
General information

Proton (^{1}H NMR) and carbon (^{13}C NMR) nuclear magnetic resonance spectra wererecorded at 400 or 500 MHz and 101 or 126 MHz, respectively. The chemical shifts are given in parts per million (ppm) on the delta (δ) scale. The solvent peak was used as a reference value, for ^{1}H NMR: $CDCl_3$ = 7.27 ppm; for ^{13}C NMR: $CDCl_3$ = 77.23 ppm. Analytical TLC was performed on precoated silica gel GF254 plates. Column chromatography was carried out on silica gel (200–300 mesh). HRMS were carried out on an Orbitrap analyzer.

General procedure

Procedure A for the synthesis of 1-phenylisochroman (1a)

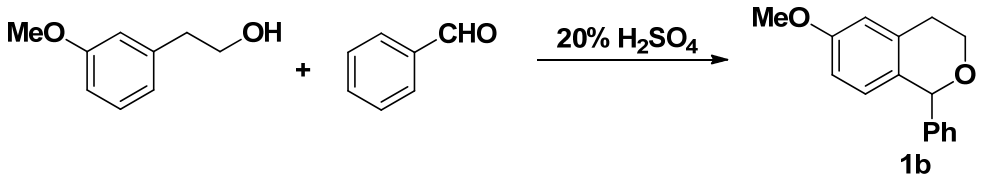


A solution of isochroman-1-one (0.74 g, 5.0 mmol, 1.0 equiv) and THF (10 mL) was cooled to –78 °C. PhLi (2.5 M in n-hexane 2.4 mL, 6.0 mmol, 1.2 equiv) was added dropwise. After being stirred for 1h. Cold water (10 mL) was added, and the aqueous phase was extracted with ethyl acetate (3×10 mL). The combined organic layers were washed with sat. brine (10 mL), dried ($MgSO_4$), filtered and concentrated. The resulting pale yellow oil was purified by silica gel chromatography (hexane-EtOAc, 4:1) to give hemiketal **S1** as an oil, which was directly used in the next step.

To a hemiketal **S1** in anhyd. CH_2Cl_2 (10 mL) at 0°C was added TFA (0.37 mL, 5 mmol) dropwise and the mixture was stirred for 15 min. Et_3SiH (0.75 mL, 5 mmol) was added dropwise to the reaction mixture at 0 °C and the mixture was stirred for 2 h then warmed to r.t. The reaction mixture was quenched with ice water (10 mL) and extracted with CH_2Cl_2 (3 × 10 mL). The combined organic extracts were washed with

sat. brine (10 mL) and dried (anhyd $MgSO_4$). After concentration, the residue was purified by flash chromatography (hexane-EtOAc, 9:1) to give compound **1a**.

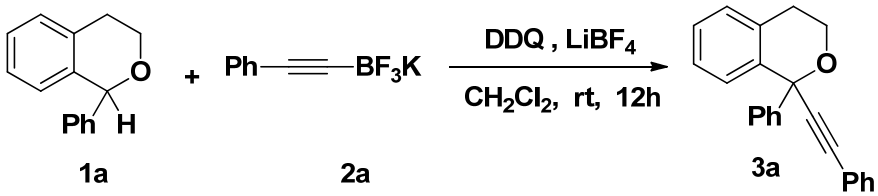
Procedure B for the synthesis of 6-methoxy-1-phenylisochroman (1b)



1b

General Procedure to get **6-methoxy-1-phenylisochroman (1b)** from 2-(3-methoxyphenyl)ethanol (2 mmol 1.0 eq) and H_2SO_4 (0.2 eq) were added successively to a solution of aldehyde (1.2 eq) in toluene (5 mL). The reaction mixture stirred for 2 h. The reaction mixture was quenched with water (2 mL) and extracted with EtOAc (3×10 mL). The combined organic extracts were washed with sat. brine (10 mL) and dried (anhyd. $MgSO_4$). After concentration, the residue was purified by flash chromatography (hexane-EtOAc, 9:1) to give compound **1b**.

Procedure C for the synthesis of 1-phenyl-1-(phenylethynyl)isochroman (3a)

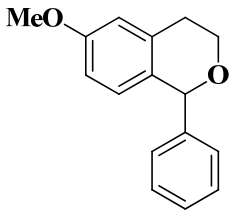


1a 2a 3a

General Procedure to get **1-phenyl-1-(phenylethynyl)isochroman (3a)**

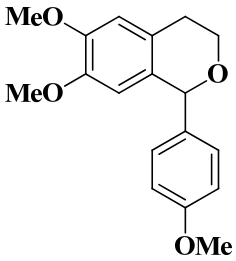
To a solution of **1a** (0.10 mmol, 1.0 eq) in CH_2Cl_2 (1 mL) was added **2a** (0.15 mmol, 1.5 eq), DDQ (0.12 mmol, 1.2 eq) and $LiBF_4$ (0.10 mmol, 1.0 eq) at room temperature for 12h. The reaction was quenched by saturated aqueous $NaHCO_3$, extracted with DCM (3×5 mL), and the combined organic layer was dried over $MgSO_4$, filtered and evaporated under vacuum. The residue waspurified by flash column chromatography to give the desired product **3a**.

Analytical data for products



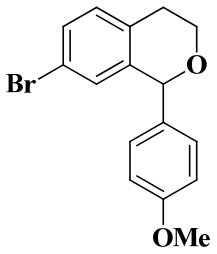
6-Methoxy-1-phenylisochroman (1b)

It was prepared following the general procedure B and purified by flashchromatography on silica gel by using hexane-EtOAc (9:1) as eluent to afford **1b** (393 mg, 82%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.28 (m, 5H), 6.71 (d, *J* = 1.0 Hz, 1H), 6.68–6.63 (m, 2H), 5.69 (s, 1H), 4.21–4.15 (m, 1H), 3.97–3.91 (m, 1H), 3.79 (s, 3H), 3.24–3.06 (m, 1H), 2.83–2.74 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.3, 142.6, 135.3, 129.9, 129.0, 128.6, 128.3, 128.2, 113.4, 112.5, 79.6, 64.0, 55.4, 29.4. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{16}H_{17}O_2$: 241.1223, found: 241.1226.



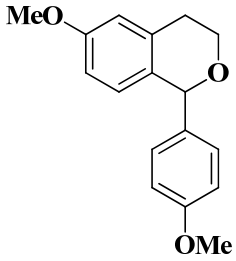
6,7-Dimethoxy-1-(4-methoxyphenyl)isochroman (1c)

It was prepared following the general procedure B and purified by flashchromatography on silica gel by using hexane-EtOAc (4:1) as eluent to afford **1c** (482 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25–7.19 (m, 2H), 6.90–6.84 (m, 2H), 6.65 (s, 1H), 6.24 (s, 1H), 5.64 (s, 1H), 4.15–4.08 (m, 1H), 3.91–3.83 (m, 4H), 3.80 (s, 3H), 3.66 (s, 3H), 3.10–2.95 (m, 1H), 2.76–2.68 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 147.9, 147.4, 134.7, 130.3, 129.4, 126.3, 113.9, 111.3, 109.9, 78.8, 63.6, 56.1, 56.1, 55.5, 28.6. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{18}H_{21}O_4$: 301.1434 found: 301.1431.



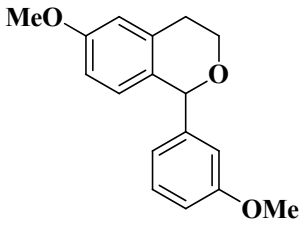
7-Bromo-1-(4-methoxyphenyl)isochroman (1d)

It was prepared following the general procedure A and purified by flashchromatography on silica gel by using hexane-EtOAc (9:1) as eluent to afford **1d** (630 mg, 41%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.21 (d, *J* = 8.6 Hz, 2H), 7.04 (d, *J* = 8.2 Hz, 1H), 6.95–6.84 (m, 3H), 5.63 (s, 1H), 4.21–4.12 (m, 1H), 3.95–3.85 (m, 1H), 3.82 (s, 3H), 3.18–2.94 (m, 1H), 2.81–2.69 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.8, 140.1, 133.8, 133.1, 130.6, 130.3, 129.9, 129.9, 119.7, 114.2, 78.9, 63.8, 55.5, 28.5. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{16}H_{16}BrO_2$: 319.0328, found: 319.0331.



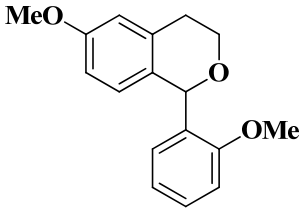
6-Methoxy-1-(4-methoxyphenyl)isochroman (1e)

It was prepared following the general procedure B and purified by flashchromatography on silica gel by using hexane-EtOAc (9:1) as eluent to afford **1e** (405 mg, 75%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24–7.19 (m, 2H), 6.90–6.83 (m, 2H), 6.72–6.60 (m, 3H), 5.65 (s, 1H), 4.19–4.11 (m, 1H), 3.95–3.85 (m, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.14–3.07 (m, 1H), 2.81–2.72 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.6, 158.3, 135.4, 134.9, 130.3, 130.2, 128.3, 113.9, 113.3, 112.5, 79.1, 63.9, 55.5, 55.4, 29.4. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{17}H_{19}O_3$: 271.1329, found: 271.1331.



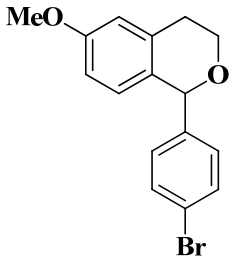
6-Methoxy-1-(3-methoxyphenyl)isochroman (1f)

It was prepared following the general procedure B and purified by flashchromatography on silica gel by using hexane-EtOAc (9:1) as eluent to afford **1f** (412 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.23 (m, 1H), 6.92 (d, *J* = 7.7 Hz, 1H), 6.90–6.83 (m, 2H), 6.68–6.68 (m, 3H), 5.68 (s, 1H), 4.22–4.13 (m, 1H), 3.98–3.87 (m, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.19–3.07 (m, 1H), 2.84–2.76 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.8, 158.3, 144.1, 135.2, 129.7, 129.5, 128.2, 121.4, 114.4, 113.8, 113.3, 112.5, 79.5, 63.9, 55.4, 29.3. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{17}H_{19}O_3$: 271.1329, found: 271.1325.



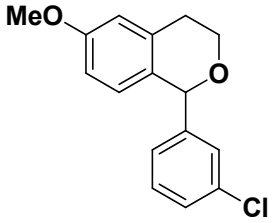
6-Methoxy-1-(2-methoxyphenyl)isochroman (1g)

It was prepared following the general procedure B and purified by flashchromatography on silica gel by using hexane-EtOAc (9:1) as eluent to afford **1g** (424 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.23 (m, 1H), 7.08 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.95 (d, *J* = 8.2 Hz, 1H), 6.89 (t, *J* = 7.5 Hz, 1H), 6.73–6.60 (m, 3H), 6.23(s, 1H), 4.19–4.12(m, 1H), 3.99–3.86 (m, 4H), 3.79 (s, 3H), 3.17–3.05 (m, 1H), 2.83–2.76 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 157.6, 135.6, 131.1, 130.2, 129.9, 129.2, 127.9, 120.8, 113.2, 112.5, 110.9, 72.3, 63.7, 55. 9, 55.4, 29.4. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{17}H_{19}O_3$: 271.1329, found: 271.1326.



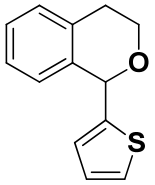
1-(4-Bromophenyl)-6-methoxyisochroman (1h)

It was prepared following the general procedure B and purified by flashchromatography on silica gel by using hexane-EtOAc (9:1) as eluent to afford **1h** (522 mg, 80%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 2.1 Hz, 1H), 6.68–6.62 (m, 2H), 5.64 (s, 1H), 4.19–4.10 (m, 1H), 3.93–3.83 (m, 1H), 3.79 (s, 3H), 3.19–2.99 (m, 1H), 2.85–2.75 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.5, 141.7, 135.3, 131.7, 130.7, 129.2, 128,1, 122.3, 113.5, 112.6, 78.9, 63.9, 55.4, 29.3. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{16}H_{16}BrO_2$: 319.0328, found: 319.0331.



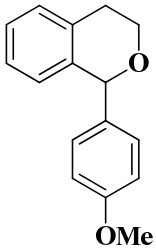
1-(3-Chlorophenyl)-6-methoxyisochroman (1i)

It was prepared following the general procedure B and purified by flashchromatography on silica gel by using hexane-EtOAc (9:1) as eluent to afford **1i** (427 mg, 78%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31–7.24 (m, 3H), 7.23–7.18 (m, 1H), 6.72–6.62 (m, 3H), 5.65 (s, 1H), 4.18–4.10 (m, 1H), 3.95–3.85 (m, 1H), 3.79 (s, 3H), 3.21–3.03 (m, 1H), 2.85–2.68 (m, 1H).^{13}C NMR (126 MHz, $CDCl_3$) δ 158.5, 144.7, 135.3, 134.5, 129.8, 129.1, 129.0, 128.4, 128.1, 127.2, 113.5, 112.7, 78.9, 64.0, 55.4, 29.2. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{16}H_{16}ClO_2$: 275.0833, found: 275.0836.



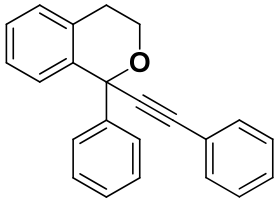
1-(Thiophen-2-yl)isochroman (1j)

It was prepared following the general procedure A and purified by flashchromatography on silica gel by using hexane-EtOAc (9:1) as eluent to afford **1j** (411 mg , 39%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.29 (m, 1H), 7.24–7.01 (m, 3H), 6.99–6.96 (m, 3H), 6.06 (s, 1H), 4.19–4.10 (m, 1H), 3.98–3.89 (m, 1H), 3.01–2.86 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.2, 136.5, 133.7, 129.0, 127.4, 127.2, 127.1, 126.5, 126.4, 126.1, 74.1, 62.6, 28.7. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{13}H_{13}OS$: 217.0682, found: 217.0684.



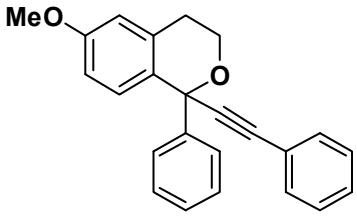
1-(4-Methoxyphenyl)isochroman (1k)

It was prepared following the general procedure A and purified by flashchromatography on silica gel by using hexane-EtOAc (9:1) as eluent to afford **1k** (732 mg , 62%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24–7.20 (m, 2H), 7.20–7.13 (m,2H), 7.11–7.04 (m, 1H), 6.91–6.84 (m, 2H), 6.76 (d, *J* = 7.7 Hz, 1H), 5.69（s, 1H）, 4.19–4.12 (m, 1H), 3.94–3.91 (m, 1H), 3.80 (s, 3H), 3.20–3.04 (m, 1H), 2.84–2.76 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.6, 137.9, 134.8, 134.1, 130.3, 128.9, 127.2, 126.75, 126.1, 113.9, 79.3, 63.9, 55.5, 29.1. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{16}H_{17}O_2$: 241.1223, found: 241.1220.



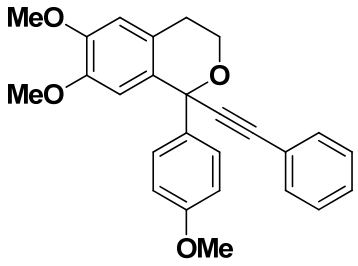
1-Phenyl-1-(phenylethynyl)isochroman (3a)

Colorless oil. Yield: 28.9 mg (93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 8.1, 1.4 Hz, 2H), 7.55–7.46 (m, 2H), 7.41–7.29 (m, 6H), 7.24–7.16 (m, 2H), 7.16–7.09 (m, 1H), 7.04 (d, *J* = 7.9 Hz, 1H), 4.48–4.41 (m, 1H), 4.22–4.15 (m, 1H), 3.27–3.20 (m, 1H), 2.87–2.81 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9, 139.3, 133.1, 132.0, 128.9, 128.7, 128.5, 128.4, 128.4, 128.3, 128.0, 127.2, 126.5, 122.9, 90.5, 88.8, 77.9, 62.1, 28.8. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{23}H_{19}O$: 311.1430, found: 311.1433.



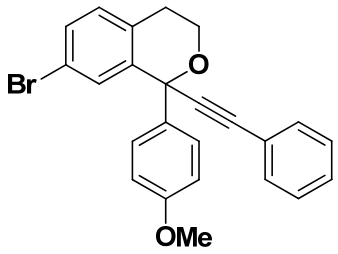
6-Methoxy-1-phenyl-1-(phenylethynyl)isochroman (3b)

Colorless oil. Yield: 31.9 mg (94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71–7.60 (m, 2H), 7.55–7.46 (m, 2H), 7.39–7.28 (m, 6H), 6.98–6.88 (m, 1H), 6.75–6.60 (m, 2H), 4.44–4.36 (m, 1H), 4.18–4.11 (m, 1H), 3.79 (s, 3H), 3.22–3.15 (m, 1H), 2.81–2.76 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5, 144.1, 134.5, 132.0, 131.6, 129.7, 128.7, 128.4, 128.4, 127.9, 122.9, 113.2, 113.1, 90.7, 88.5, 77.7, 61.9, 55.4, 29.1. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{24}H_{21}O_2$: 341.1536, found: 341.1533.



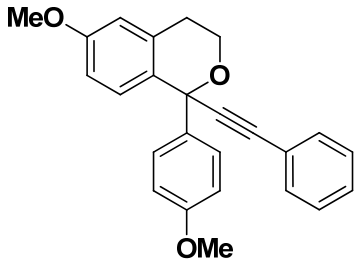
6,7-Dimethoxy-1-(4-methoxyphenyl)-1-(phenylethynyl)isochroman (3c)

Colorless oil. Yield: 36.5 mg (91%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57–7.52 (m, 2H), 7.52–7.47 (m, 2H), 7.35–7.29 (m, 3H), 6.90–6.83 (m, 2H), 6.63 (s, 1H), 6.50 (s, 1H), 4.41–4.22 (m, 1H), 4.17–4.00 (m, 1H), 3.89 (s, 3H), 3.81 (s, 3H), 3.70 (s, 3H), 3.15– 3.02 (m, 1H), 2.80–2.67 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.7, 148.5, 147.8, 136.3, 132.0, 131.0, 129.4, 128.7, 128.5, 125.7, 123.0, 113.7, 111.1, 111.0, 100.2, 90.9, 88.1, 61.9, 56.2, 56.1, 55.5, 28.4. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{26}H_{25}O_4$: 401.1747, found: 401.1744.



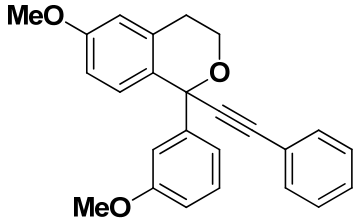
7-Bromo-1-(4-methoxyphenyl)-1-(phenylethynyl)isochroman (3d)

Colorless oil. Yield: 38.1 mg (91%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57–7.52 (m, 2H), 7.52–7.48 (m, 2H), 7.37–7.29 (m, 4H), 7.15 (d, J = 2.0 Hz, 1H), 7.04 (d, J = 8.2 Hz, 1H), 6.95–6.84 (m, 2H), 4.47–4.31 (m, 1H), 4.20–4.04 (m, 1H), 3.82 (s, 3H), 3.21–3.06 (m, 1H), 2.85–2.71 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 141.7, 135.5, 132.2, 132.0, 131.2, 130.7, 130.4, 129.3, 128.9 128.5, 122.6, 119.9, 113.8, 89.9, 89.2, 77.4, 61.8, 55.5, 28.3. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{24}H_{20}BrO_2$: 419.0641, found: 419.0644.



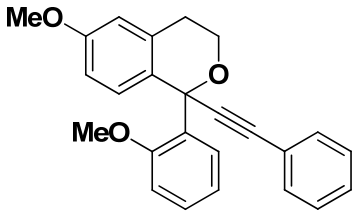
6-Methoxy-1-(4-methoxyphenyl)-1-(phenylethynyl)isochroman (3e)

Colorless oil. Yield: 33.5 mg (90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57–7.53 (m, 2H), 7.50–7.46 (m, 2H), 7.32–7.29 (m, 3H), 6.94 (d, *J* = 8.4 Hz, 1H), 6.91–6.82 (m, 2H), 6.74–6.62 (m, 2H), 4.41–4.32 (m, 1H), 4.21–4.10 (m, 1H), 3.81 (s, 3H), 3.80 (s, 3H), 3.23–3.11 (m, 1H), 2.83–2.75 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.6, 158.5, 136.5, 134.6, 131.9, 131.8, 129.7, 129.3, 128.6, 128.4, 123.0, 113.6, 113.2, 113.1, 90.9, 88.3, 77.3, 61.9, 55.5, 55.4, 29.2. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{25}H_{23}O_3$: 371.1642, found: 371.1644.



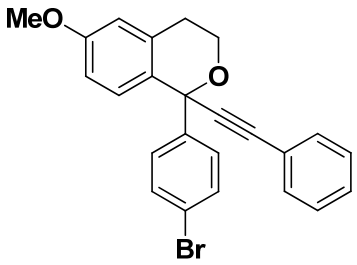
6-Methoxy-1-(3-methoxyphenyl)-1-(phenylethynyl)isochroman (3f)

Colorless oil. Yield: 32.7 mg (88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55–7.46 (m, 2H), 7.37–7.19 (m, 6H), 6.99 (d, *J* = 8.5 Hz, 1H), 6.87–6.85 (m, , 1H), 6.77–6.65 (m, 2H), 4.46–4.33 (m, 1H), 4.22–4.11 (m, 1H), 3.82 (s, 3H), 3.81 (s, 3H), 3.24–3.14 (m, 5.8 Hz, 1H), 2.85–2.74 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 158.6, 145.7, 134.4, 132.0, 131.4, 129.6, 129.3, 128.7, 128.4, 122.9, 120.5, 114.0, 113.6, 113.2, 113.1, 90.7, 88.4, 77.6, 61.9, 55.5, 55.4, 29.1. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{25}H_{23}O_3$: 371.1642, found: 371.1645.



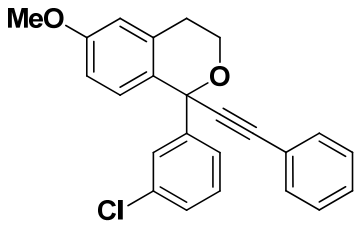
6-Methoxy-1-(2-methoxyphenyl)-1-(phenylethynyl)isochroman (3g)

Colorless oil. Yield: 26.2 mg (70%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.55–7.45 (m, 2H), 7.36–7.28 (m, 4H), 7.06–6.95 (m, 1H), 6.91–6.79 (m, 2H), 6.70–6.57 (m, 2H), 4.47–4.29 (m, 1H), 4.27–4.13 (m, 1H), 3.79 (s, 3H), 3.47 (s, 3H), 3.32–3.15 (m, 1H), 2.81–2.60 (m, 1H). ^{13}C NMR (126 MHz, CDCl3) δ 158.1, 157.9, 134.9, 132. 3, 131.9, 131.9, 130.2, 130.0, 128.5, 128.4, 127.7, 123.2, 120.3, 113.9, 112.7, 112.5, 90.7, 89.2, 77.3, 62.3, 56.3, 55.4, 29.0. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{25}H_{23}O_3$: 371.1642, found: 371.1640.



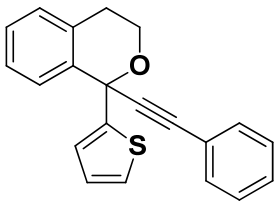
1-(4-Bromophenyl)-6-methoxy-1-(phenylethynyl)isochroman (3h)

Colorless oil. Yield: 36.6 mg (86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57–7.52 (m, 2H), 7.49–7.45 (m, 4H),7.34–7.30 (m, 3H), 6.91–6.88 (m, 1H), 6.75–6.63 (m, 2H), 4.46–4.33 (m, 1H), 4.21–4.10 (m, 1H), 3.80 (s, 3H), 3.23–3.15 (m, 1H), 2.83–2.74(m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 143.3 134.4, 131.9 , 131.4, 131.1, 129.8, 129.5, 128.8, 128.5 122.7, 122.5, 113.3, 113.2, 90.0, 88.8, 77.3, 61.9 55.4, 29.0. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{24}H_{20}BrO_2$: 419.0641, found: 419.0644.



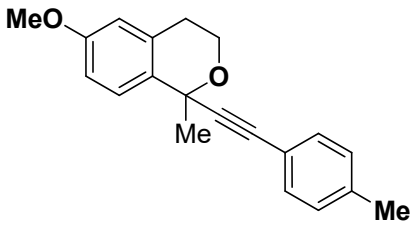
1-(3-Chlorophenyl)-6-methoxy-1-(phenylethynyl)isochroman (3i)

Colorless oil. Yield: 31.4 mg (82%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 – 7.53 (m, 1H), 7.51–7.45 (m, 1H), 7.43–7.36 (m, 2H), 7.27–7.17 (m, 5H), 6.83 (d, J = 8.5 Hz, 1H), 6.68–6.55 (m, 2H), 4.38–4.24 (m, 1H), 4.14–3.99 (m, 1H), 3.70 (s, 3H), 3.26–3.02 (m, 1H), 2.82–2.60 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.7, 146.2, 134.4, 134.3, 132.0, 130.9, 129.6, 129.5, 128.8, 128.5, 128.5, 128.2, 126.2, 122.6, 113.4, 113.2, 89.9, 88.9, 77.3, 62.0, 55.4, 29.0. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{24}H_{20}ClO_2$: 375.1146, found: 375.1149.



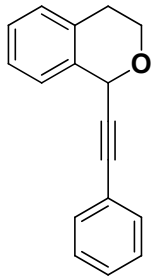
1-(Phenylethynyl)-1-(thiophen-2-yl)isochroman (3j)

Colorless oil. Yield: 28.9 mg (83%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53–7.45 (m, 2H), 7.35–7.27 (m, 5H), 7.25–7.20 (m, 2H), 7.17 (t, *J* = 8.4 Hz, 2H), 6.95 (dd, *J* = 5.0, 3.6 Hz, 1H), 4.39–4.28 (m, 1H), 4.20–4.08 (m, 1H), 3.19–3.07 (m, 1H), 2.94–2.80 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.0, 138.5, 132.8, 132.1, 129.0, 128.9, 128.5, 128.3, 127.7, 127.3, 126.8, 126.5, 126.2, 122.6, 90.7, 87.0, 74.6, 61.9, 28.6. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{21}H_{17}OS$: 317.0995, found: 317.0997.



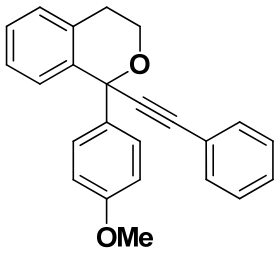
6-Methoxy-1-methyl-1-(p-tolylethynyl)isochroman (3k)

Colorless oil. Yield:15.1 mg (51%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31–7.23 (m, 3H), 7.07 (d, J = 7.9 Hz, 2H), 6.83–6.76 (m, 1H), 6.63 (d, J = 2.5 Hz, 1H), 4.27–4.17 (m, 1H), 4.14–4.04 (m, 1H), 3.80 (s, 3H), 3.15–2.97 (m, 1H), 2.74–2.52 (m, 1H), 2.32 (s, 3H), 1.86 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.4, 138.4, 134.1, 132.5, 131.8, 129.0, 127.3, 119.9, 113.3, 113.1, 91.8, 84.6, 71.8, 61.5, 55.4, 31.0, 29.3, 21.6. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{20}H_{21}O_2$: 293.1536, found: 293.1539.



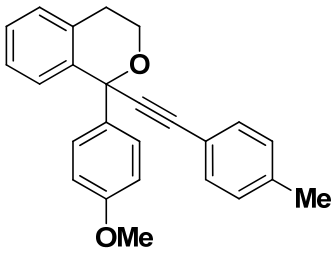
1-(Phenylethynyl)isochroman (3l)

Colorless oil. Yield: 15.2 mg (65%) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49–7.45 (m, 2H), 7.40–7.35 (m, 1H), 7.35–7.28 (m, 3H), 7.26–7.21 (m, 2H), 7.19–7.13 (m, 1H), 5.80 (s, 1H), 4.32–4.27 (m, 1H), 4.09–4.00 (m, 1H), 3.01–2.84 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.1, 133.0, 132.1, 129.2, 128.7, 128.4, 127.4, 126.6, 126.2, 122.7, 88.3, 85.9, 67.5, 62.9, 28.2; HRMS (EI) m/z $[M + H]^+$ calculated for $C_{17}H_{15}O$: 235.1117, found: 235.1115.



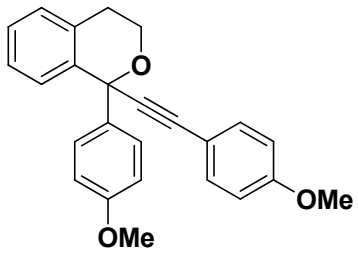
1-(4-Methoxyphenyl)-1-(phenylethynyl)isochroman (4a)

Colorless oil. Yield: 31.2 mg (91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60–7.53 (m, 2H), 7.52–7.45 (m, 2H), 7.36–7.27 (m, 3H), 7.23–7.09 (m, 3H), 7.04 (d, *J* = 7.9 Hz, 1H), 6.94–6.78 (m, 2H), 4.46–4.35 (m, 1H), 4.20–4.11 (m, 1H), 3.81 (s, 3H), 3.23–3.17 (m, 1H), 2.87–2.78 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 139.5, 136.3, 133.2, 131.9, 129.4, 128.9, 128.7, 128.5, 128.4, 127.2, 126.5, 122.9, 113.6, 90.8, 88.5, 77.5, 62.0, 55.5, 28.8. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{24}H_{21}O_2$: 341.1536, found:341.1539.



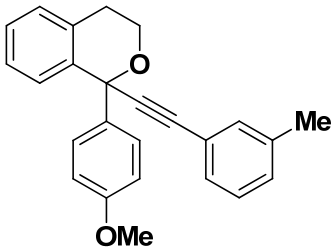
1-(4-Methoxyphenyl)-1-(p-tolylethynyl)isochroman (4b)

Colorless oil. Yield: 32.6 mg (92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.52 (m, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.22–7.08 (m, 5H), 7.03 (d, *J* = 7.7 Hz, 1H), 6.93–6.81 (m, 2H), 4.43–4.36 (m, 1H), 4.18–4.09(m, 1H), 3.80 (s, 3H), 3.25–3.16 (m, 1H), 2.86–2.77 (m, 1H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 139.6, 138.8, 136.4, 133.2, 131.9, 129.4, 129.2, 128.9, 128.6, 127.1, 126.5, 119.8, 113.6, 90.0, 88.7, 77.4, 61.9, 55.5, 28.8, 21.7. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{25}H_{23}O_2$: 355.1693, found: 355.1695.



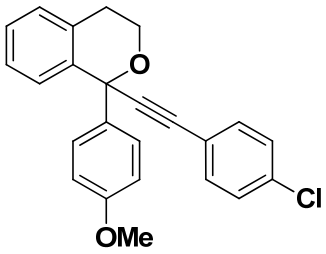
1-(4-Methoxyphenyl)-1-((4-methoxyphenyl)ethynyl)isochroman (4c)

Colorless oil. Yield: 35.2 mg (95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61–7.51 (m, 2H), 7.48–7.35 (m, 2H), 7.22–7.08 (m, 3H), 7.03 (d, *J* = 7.5 Hz, 1H), 6.91–6.79 (m, 4H), 4.45–4.34 (m, 1H), 4.18–4.09 (m, 1H), 3.81 (s, 3H), 3.80 (s, 3H), 3.24–3.15 (m, 1H), 2.86–2.77 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 159.6, 139.7, 136.5, 133.5, 133.2, 129.4, 128.9, 128.6, 127.1, 126.5, 115.1, 114.0, 113.6, 89.4, 88.4, 77.2, 61.9, 55.5, 28.8. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{25}H_{23}O_3$: 371.1642, found: 371.1645.



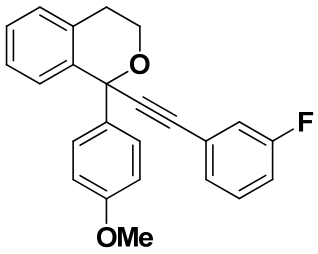
1-(4-Methoxyphenyl)-1-(m-tolylethynyl)isochroman (4d)

Colorless oil. Yield: 32.9 mg (93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63–7.48 (m, 2H), 7.31 (dd, *J* = 6.2, 5.3 Hz, 2H), 7.25–7.08 (m, 5H), 7.06–6.97 (m, 1H), 6.92–6.79 (m, 2H), 4.46–4.36 (m, 1H), 4.19–4.12 (m, 1H), 3.81 (s, 3H), 3.26–3.20 (m, 1H), 2.86–2.78 (m, 1H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 139.6, 138.1, 136.4, 133.2, 132.6, 129.5, 129.34, 129.1, 128.9, 128.5, 128.3, 127.1, 126.5, 122.7, 113.6, 90.4, 88.7, 77.4, 62.0, 55.5, 28.8, 21.4. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{25}H_{23}O_2$: 355.1693, found: 355.1696.



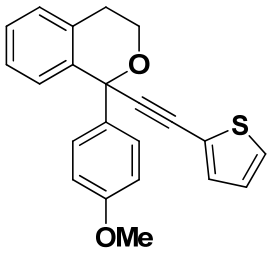
1-((4-Chlorophenyl)ethynyl)-1-(4-methoxyphenyl)isochroman (4e)

Colorless oil. Yield: 33.7 mg (90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58–7.50 (m, 2H), 7.47–7.37 (m, 2H), 7.34–7.27 (m, 2H), 7.24–7.07 (m, 3H), 7.03 (d, *J* = 7.8 Hz, 1H), 6.93–6.81 (m, 2H), 4.43–4.31 (m, 1H), 4.18–4.09 (m, 1H), 3.80 (s, 3H), 3.24–3.18 (m, 1H), 2.86–2.77 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 139.2, 136.1, 134.7, 133.2, 129.3, 129.0, 128.8, 128.5, 127.3, 126.5, 121.4, 113.7, 91.8, 87.3, 77.5, 62.0, 55.5, 28.8. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{24}H_{20}ClO_2$: 375.1146 found: 375.1142.



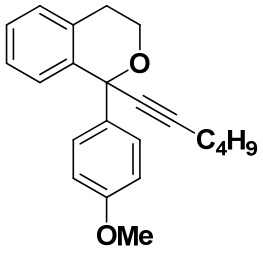
1-((3-Fluorophenyl)ethynyl)-1-(4-methoxyphenyl)isochroman (4f)

Colorless oil. Yield: 32.9 mg (92%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58–7.48 (m, 2H), 7.34–7.24 (m, 2H), 7.24–7.08 (m, 4H), 7.08–6.96 (m, 2H), 6.95–6.77 (m, 2H), 4.43–4.29 (m, 1H), 4.19–4.10 (m, 1H), 3.81 (s, 3H), 3.24–3.17 (m, 1H), 2.87–2.78 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.5 (d, $J_{C\text{-}F}$ = 246.6 Hz), 159.7, 139.2, 136.1, 133.3, 130.1 (d, $J_{C\text{-}F}$ = 8.6 Hz), 129.3, 129.0, 128.5, 127.9 (d, $J_{C\text{-}F}$ = 3.1 Hz), 127.3, 126.6, 124.8 (d, $J_{C\text{-}F}$ =9.4 Hz), 118.9 (d, $J_{C\text{-}F}$ = 22.8 Hz), 116.1 (d, $J_{C\text{-}F}$ = 21.1 Hz), 113.7, 91.8, 87.2, 77.5, 62.1, 55.5, 28.8. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{24}H_{20}FO_2$: 359.1442, found: 359.1445.



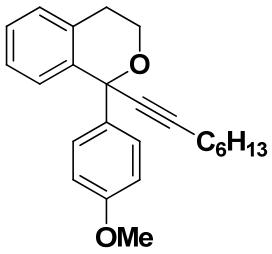
1-(4-Methoxyphenyl)-1-(thiophen-2-ylethynyl)isochroman (4g)

Colorless oil. Yield: 30.5 mg (88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56–7.46 (m, 2H), 7.29–7.24 (m, 2H), 7.22–7.08 (m, 3H), 7.04–6.95 (m, 2H), 6.91–6.82 (m, 2H), 4.42–4.31 (m, 1H), 4.18–4.09 (m, 1H), 3.80 (s, 3H), 3.24–3.18 (m, 1H), 2.86–2.77 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 139.1, 136.1, 133.3, 132.6, 129.3, 129.0, 128.6, 127.6, 127.3, 127.1, 126.6, 122.8, 113.7, 94.5, 81.7, 77.7, 62.1, 55.5, 28.8. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{22}H_{19}O_2S$: 347.1100, found: 347.1103.



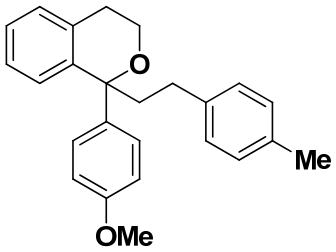
1-(Hex-1-yn-1-yl)-1-(4-methoxyphenyl)isochroman (4h)

Colorless oil. Yield: 26.7 mg (83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55–7.42 (m, 2H), 7.20–7.04 (m, 3H), 6.94 (d, *J* = 7.8 Hz, 1H), 6.88–6.77 (m, 2H), 4.37–4.26 (m, 1H), 4.11–4.02 (m, 1H), 3.79 (s, 3H), 3.20–3.11 (m, 1H), 2.82–2.74(m, 1H), 2.35–2.28 (m, 2H), 1.62–1.50 (m, 2H), 1.47–1.37 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.5, 140.2, 136.8, 133.0, 129.3, 128.8, 128.4, 126.9, 126.3, 113.5, 89.5, 81.7, 77.2, 61.6, 55.5, 30.9, 28.8, 22.3, 18.9, 13.8. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{22}H_{24}O_2$: 321.1849, found: 321.1846.



1-(4-Methoxyphenyl)-1-(oct-1-yn-1-yl)isochroman (4i)

Colorless oil. Yield: 29.9 mg (86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53–7.42 (m, 2H), 7.21–7.04 (m, 3H), 6.94 (d, *J* = 7.7 Hz, 1H), 6.87–6.76 (m, 2H), 4.36–4.23 (m, 1H), 4.11–4.02 (m, 1H), 3.79 (s, 3H), 3.19–3.10 (m, 1H), 2.82–2.73 (m, 1H), 2.31 (t, *J* = 7.1 Hz, 2H), 1.62–1.51 (m, 2H), 1.49–1.37 (m, 2H), 1.34–1.23 (m, 4H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.5, 140.2, 136.8, 133.0, 129.4, 128.8, 128.4, 126.9, 126.3, 113.5, 89.6, 81.8, 77.2, 61.6, 55.5, 31.5, 28.8, 28.8, 22.8, 19.2, 14.2. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{24}H_{29}O_2$: 349.2162, found: 349.2159.



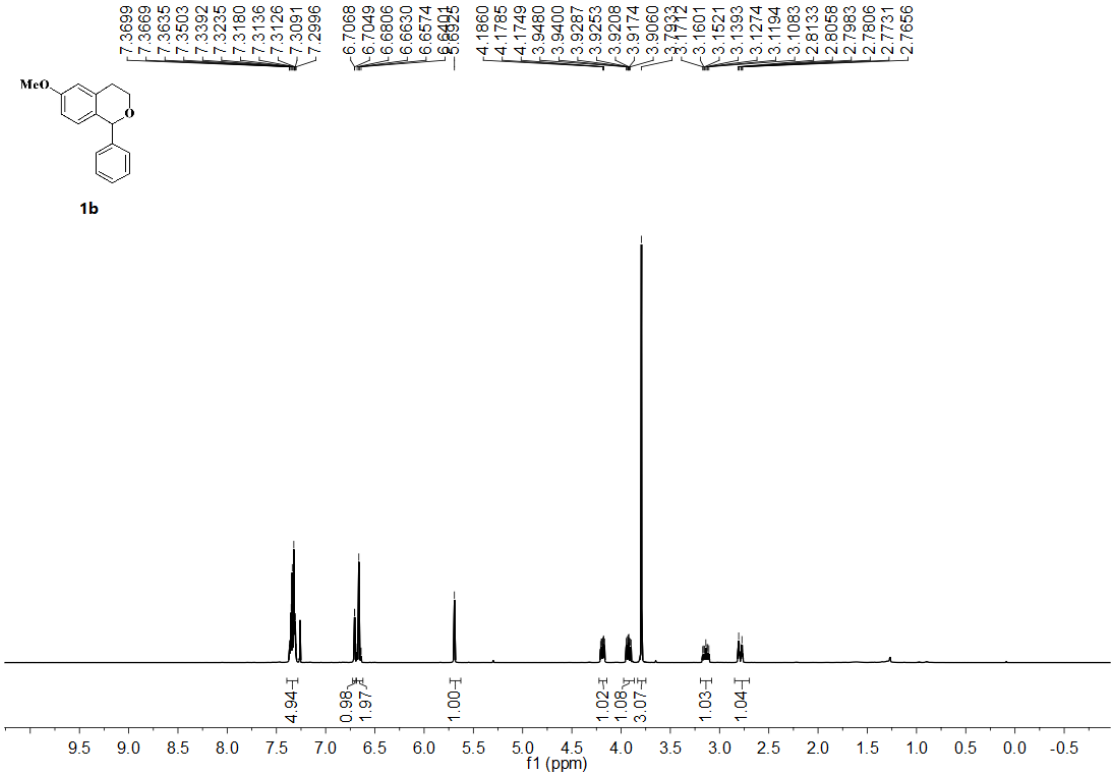
1-(4-Methoxyphenyl)-1-(4-methylphenethyl)isochroman (5)

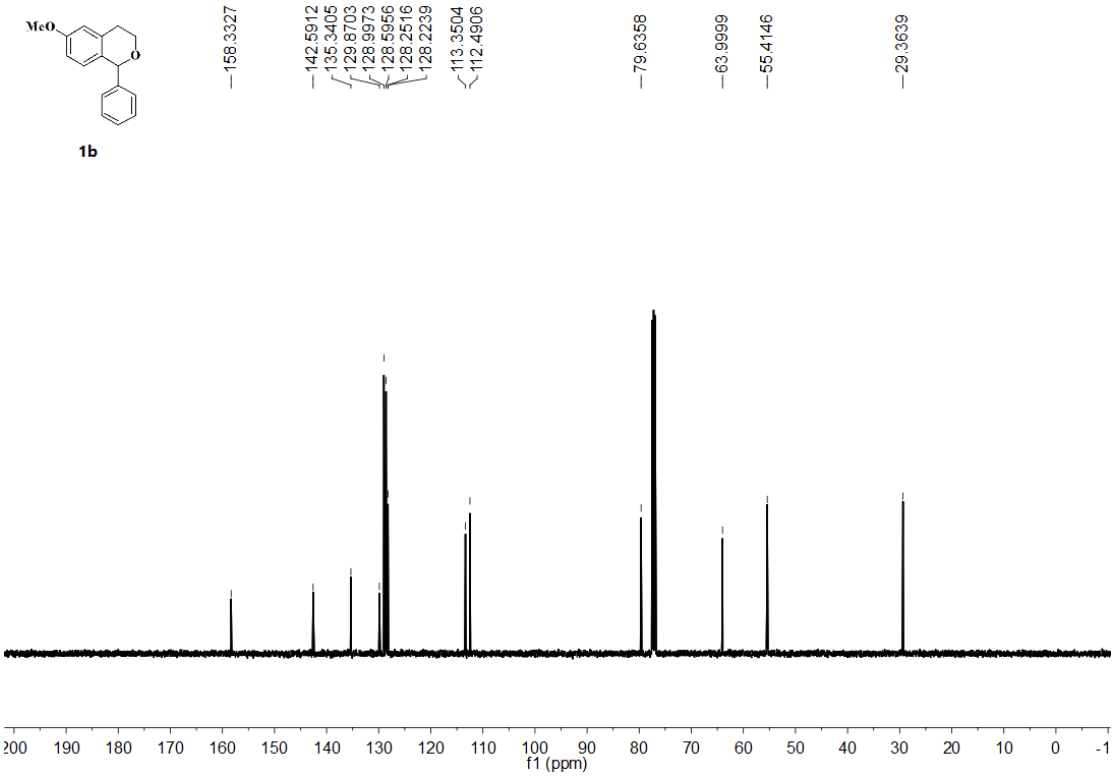
Colorless oil. Yield: 28.7 mg (90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33–7.16 (m, 6H), 7.12–6.94 (m, 4H), 6.87–6.73 (m, 2H), 3.94–3.83 (m, 1H), 3.78 (s, 3H), 3.70–3.58 (m, 1H), 3.21–3.02 (m, 1H), 2.88–2.72 (m, 1H), 2.71–2.60 (m, 1H), 2.59–2.44 (m, 1H), 2.42–2.19 (m, 5H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.8, 139.9, 138.4, 138.2, 135.2, 135.2, 129.5, 129.2, 128.8, 128.5, 127.6, 126.7, 125.9, 113.4, 80.9, 59.9, 55.4, 45.4, 30.5, 29.3, 21.2. HRMS (EI) m/z $[M + H]^+$ calculated for $C_{25}H_{27}O_2$: 359.2006, found: 359.2002.

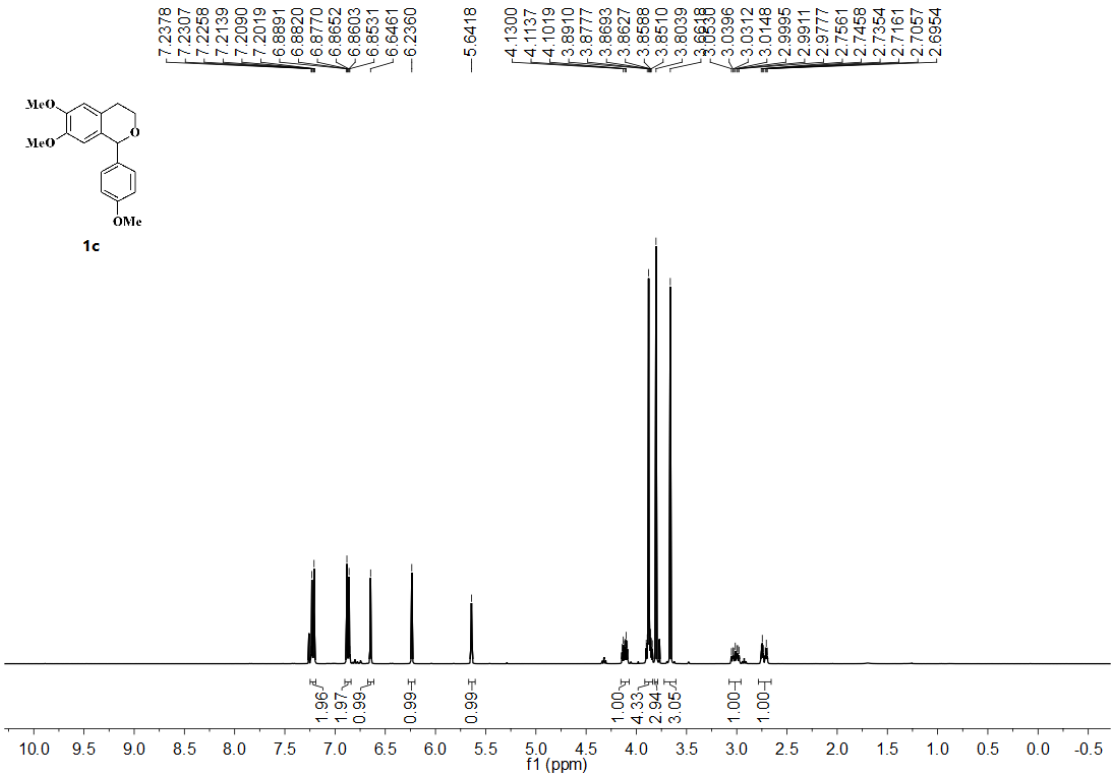
Reference:

1. Srimoyee Dasgupta, Thomas Rivas, and Mary P. Watson, *Angew. Chem. Int. Ed.* **2015**, *54*, 14154–14158.
2. Benaissa Bouguerne, Pascal Hoffmann, and Christian Lherbet, *Synthetic Communications*. **2010**, *40,* 915–926.

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



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OMe
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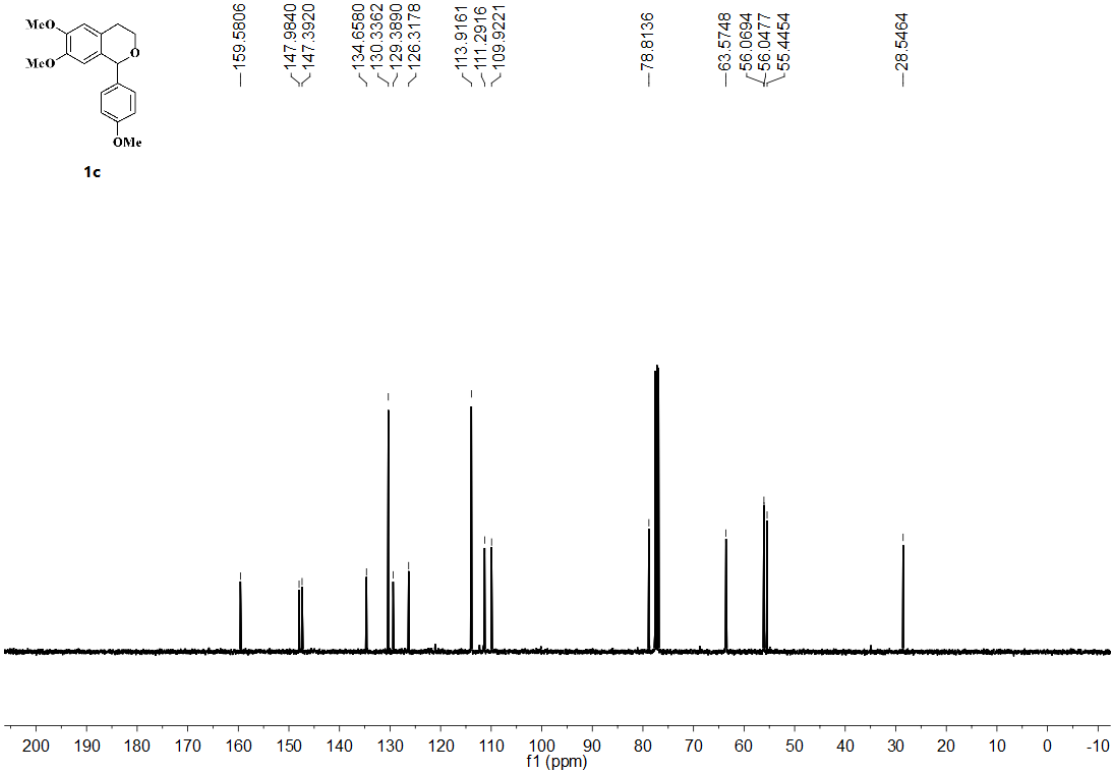
f1 (ppm)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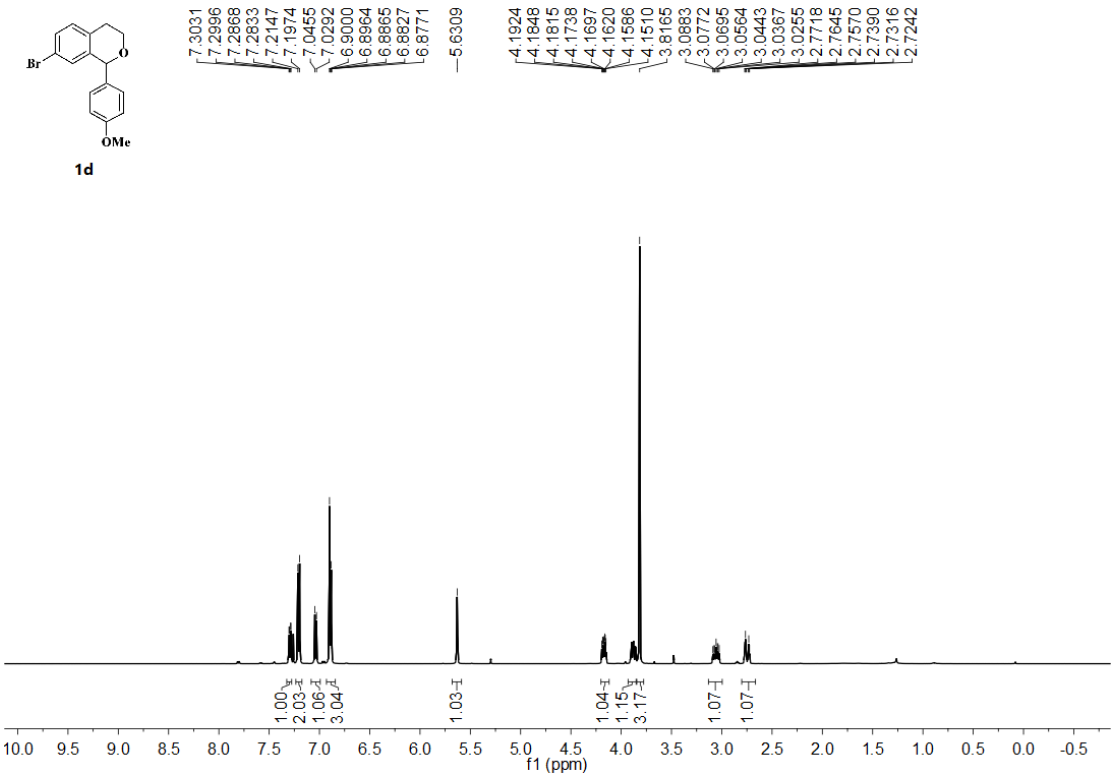
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OMe
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1.06
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1.03
1.04
1.15
3.17
1.07
1.07
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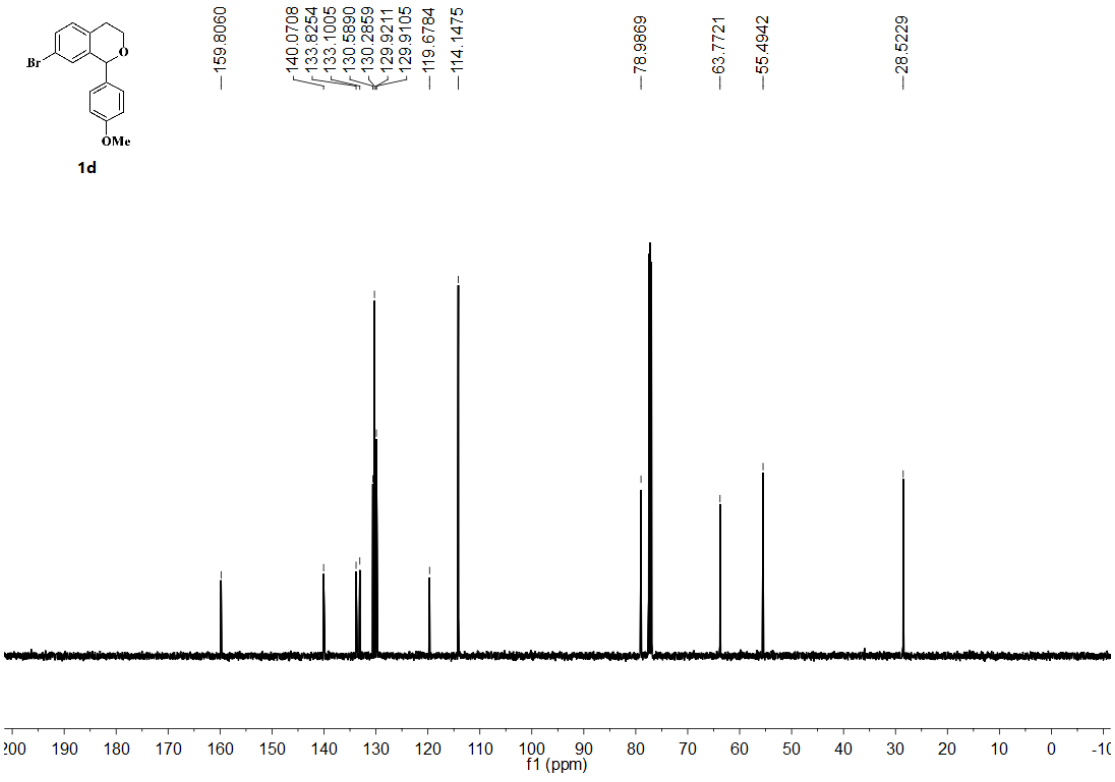
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O
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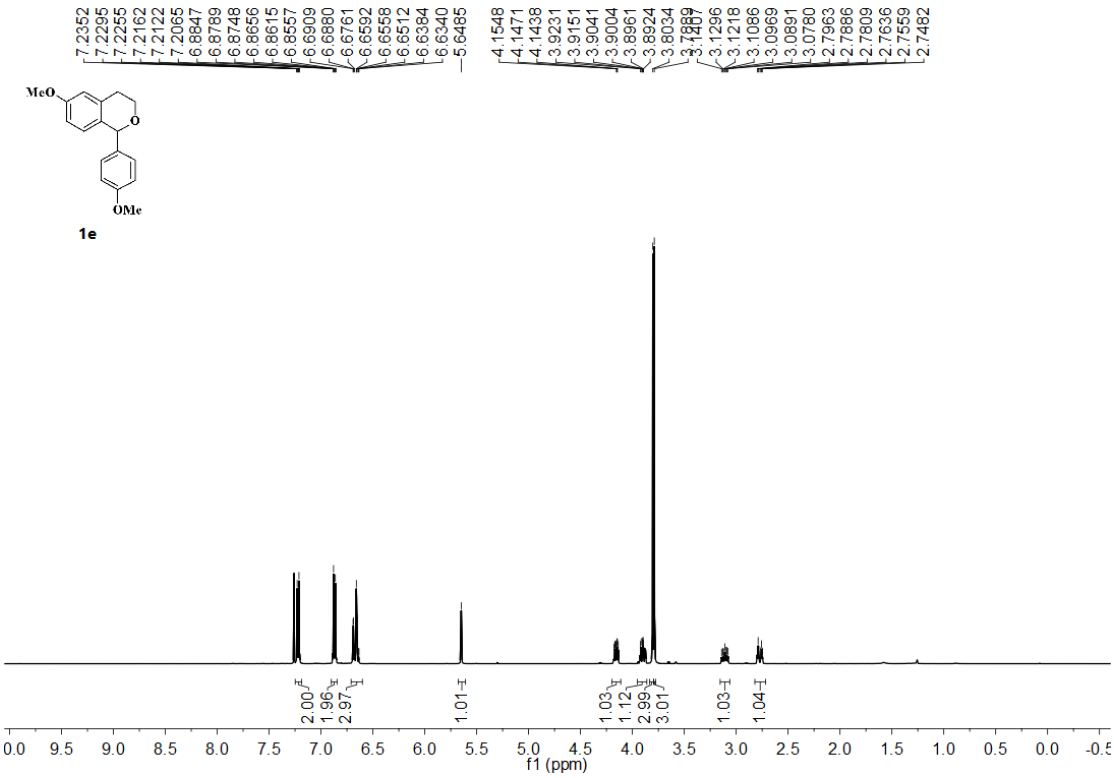
f1 (ppm)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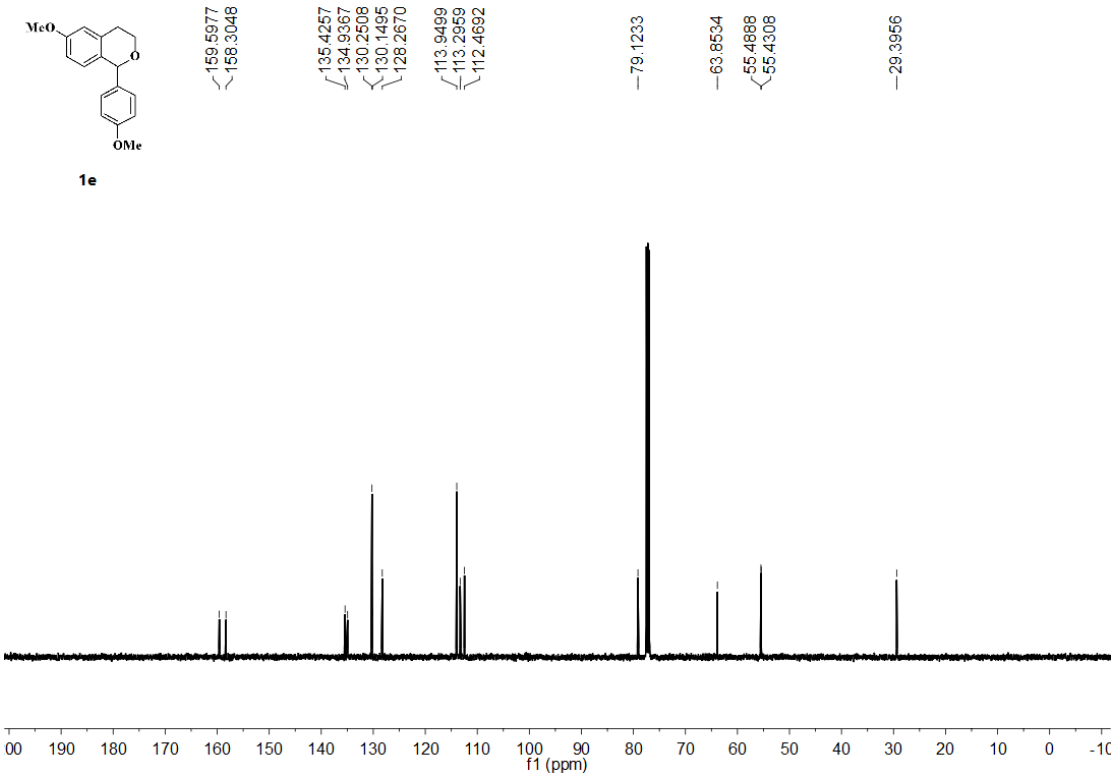
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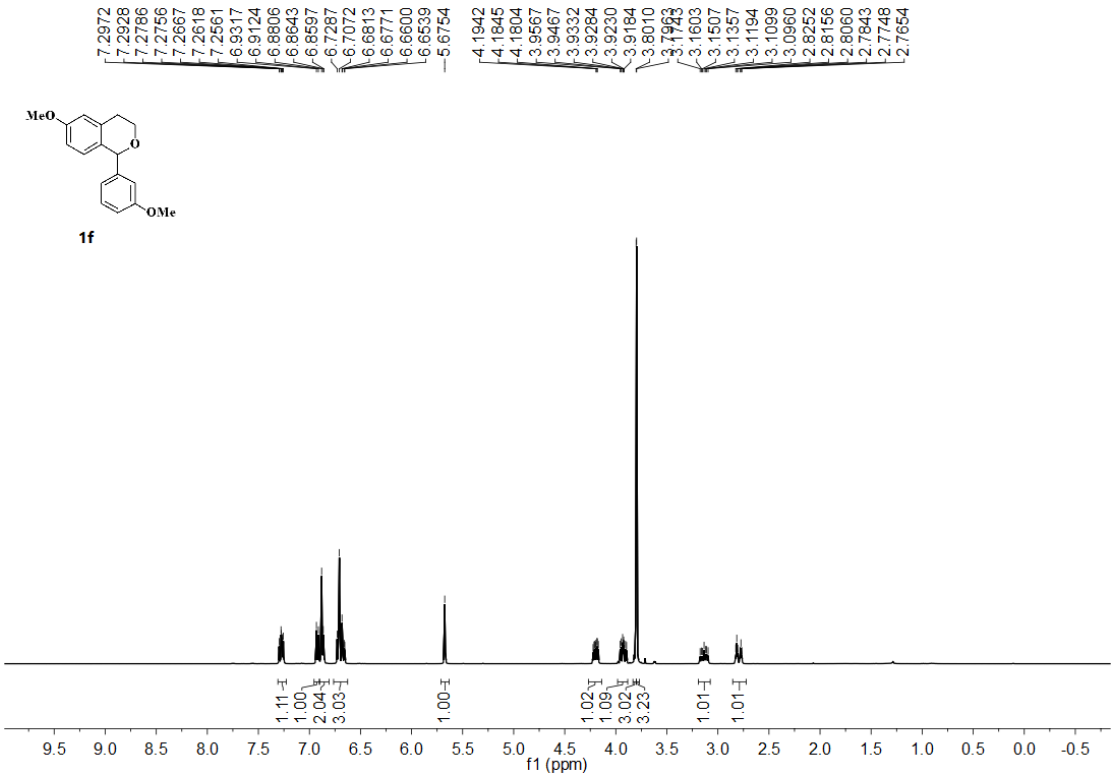
f1 (ppm)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1.00
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3.23
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1.01
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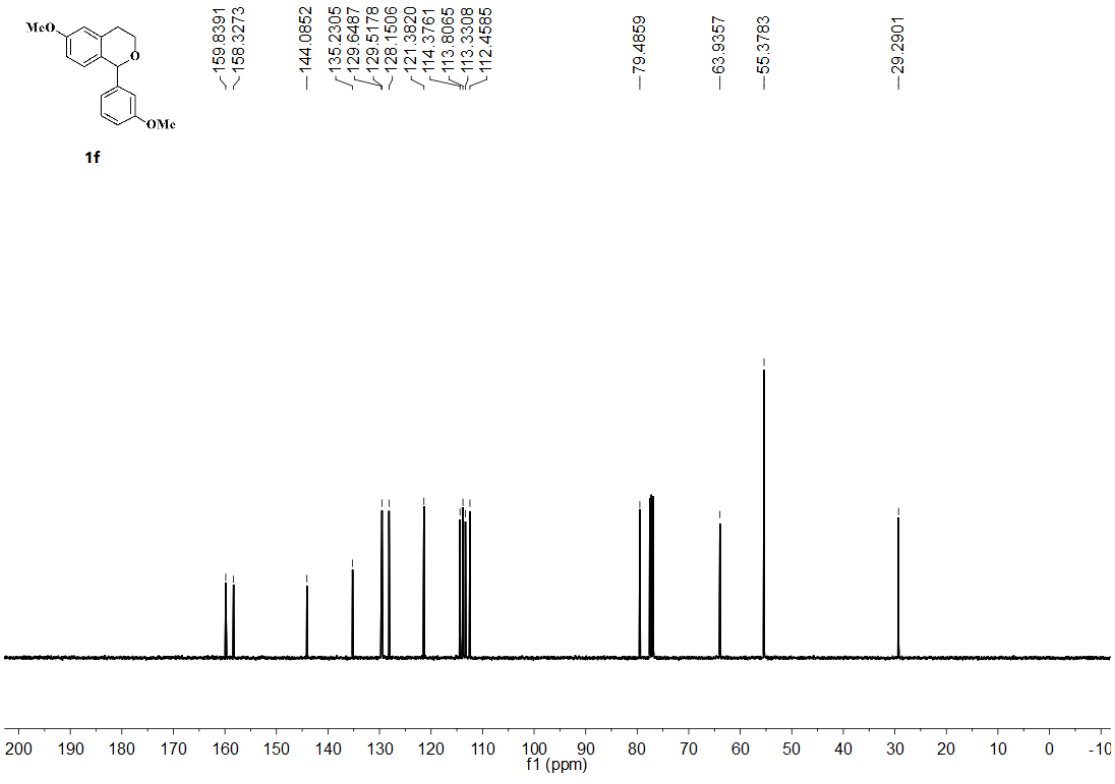
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1f
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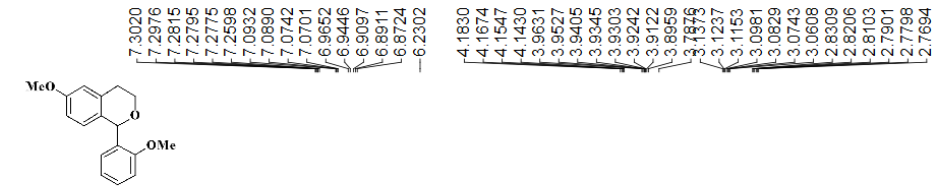
f1 (ppm)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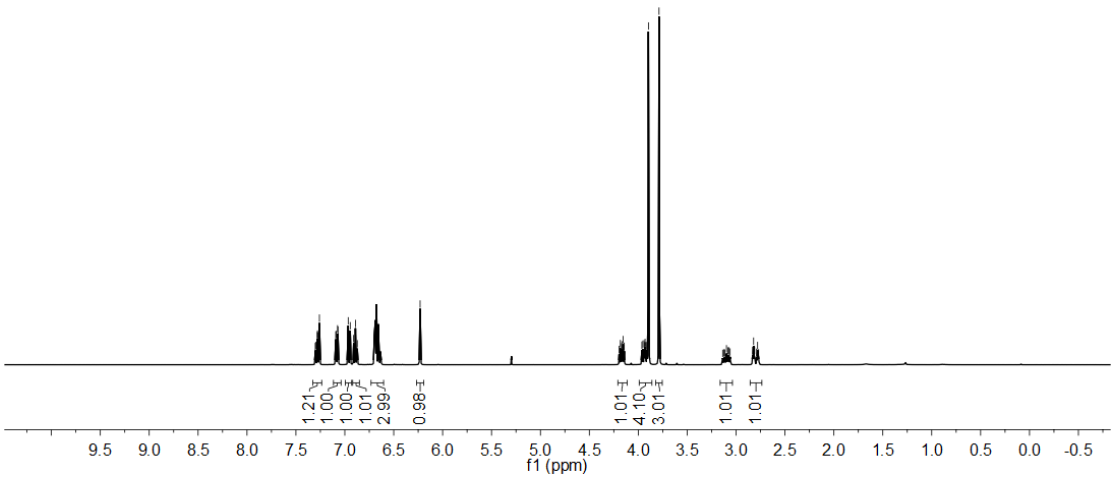
OMe

1g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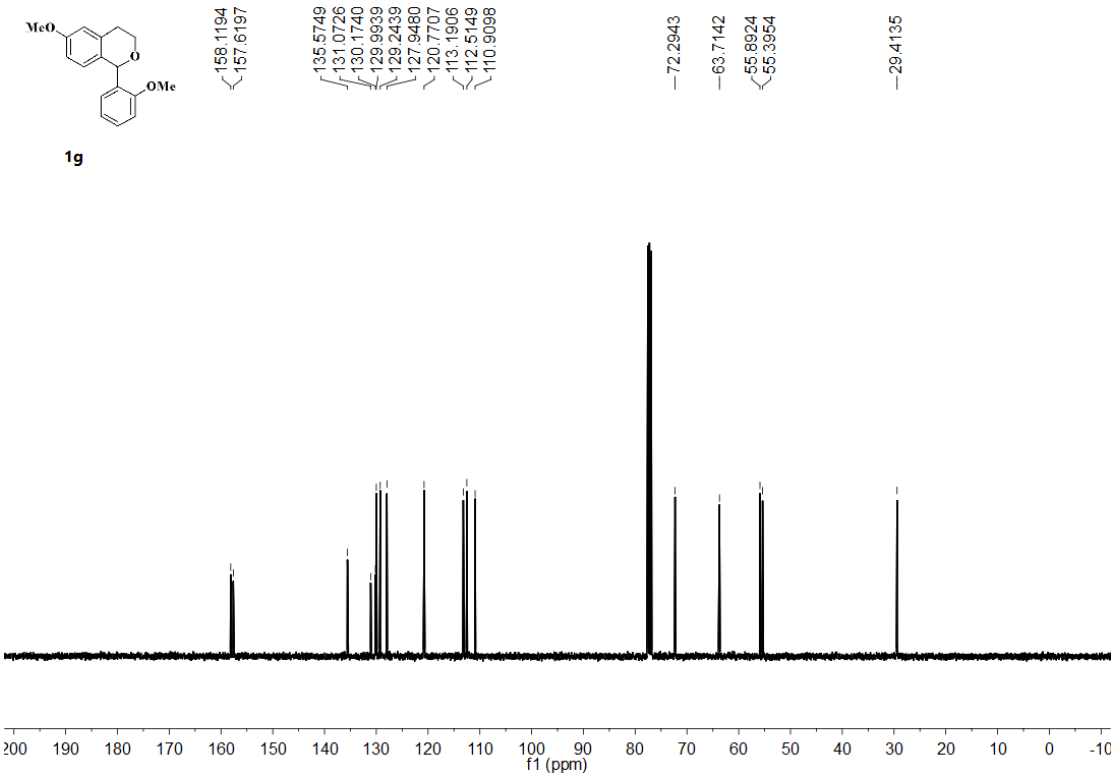
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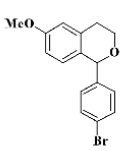
OMe
f1 (ppm)

1g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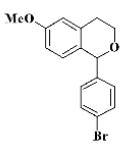
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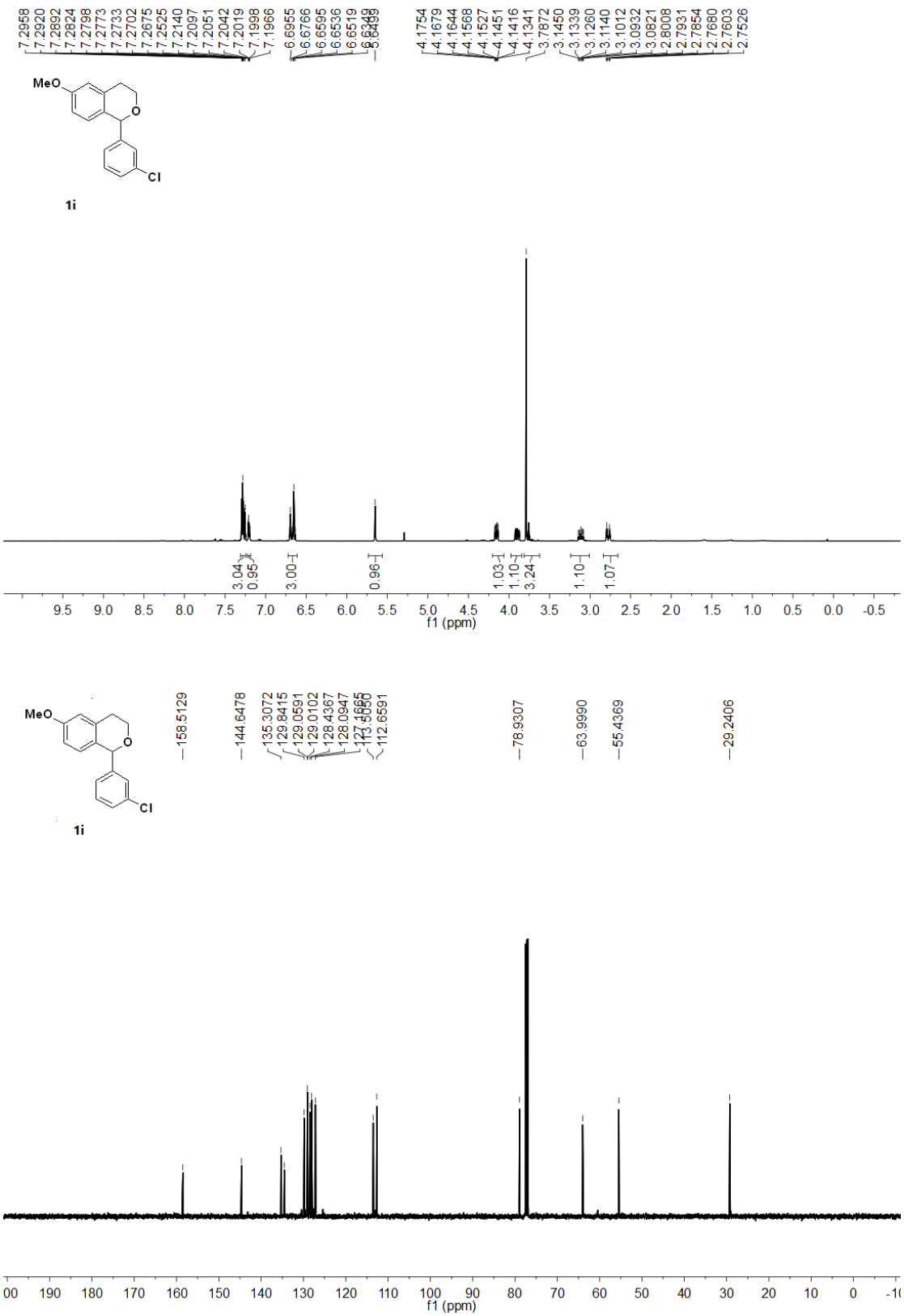
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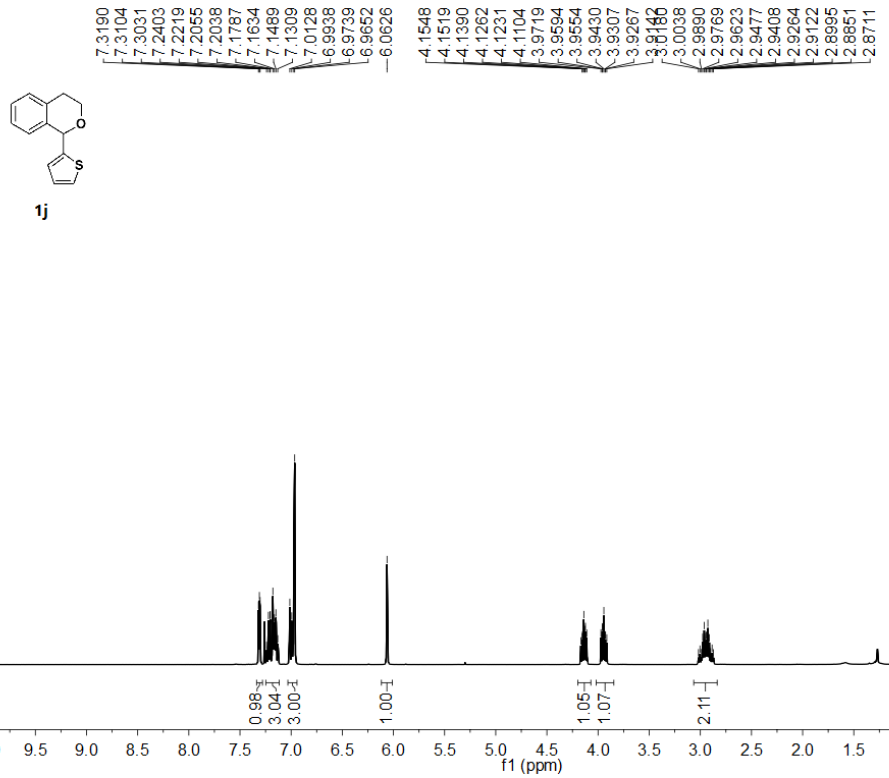
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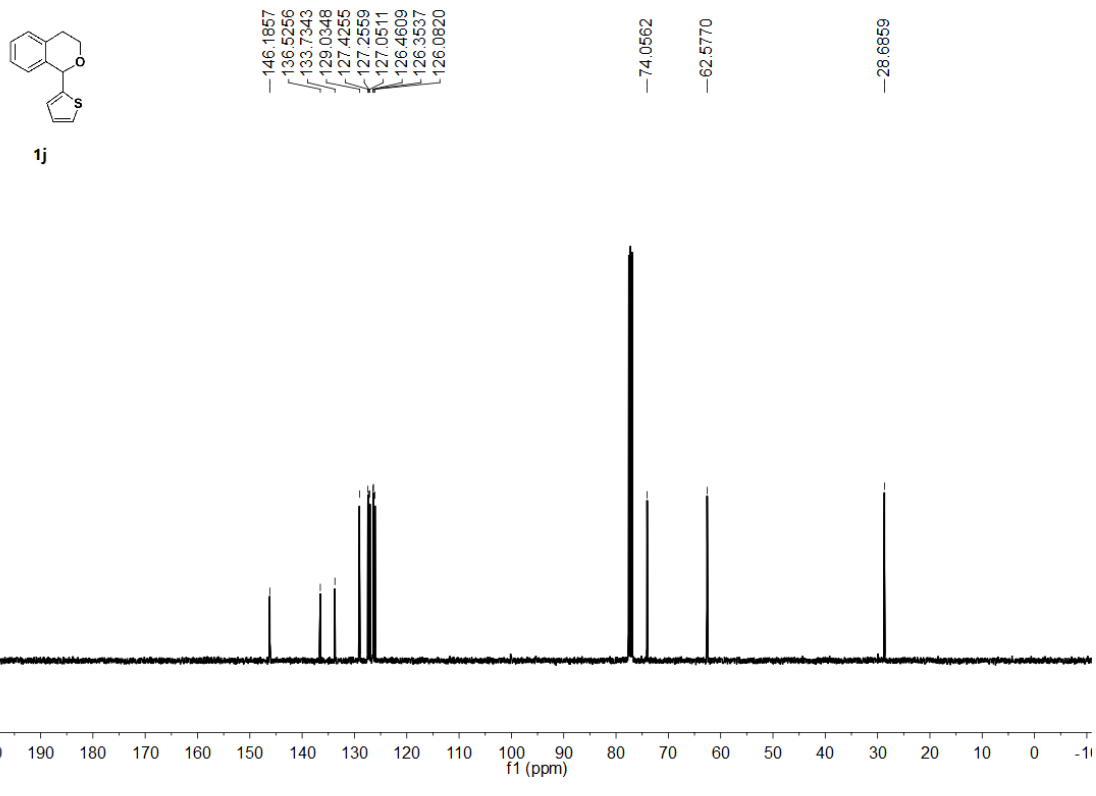
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1j
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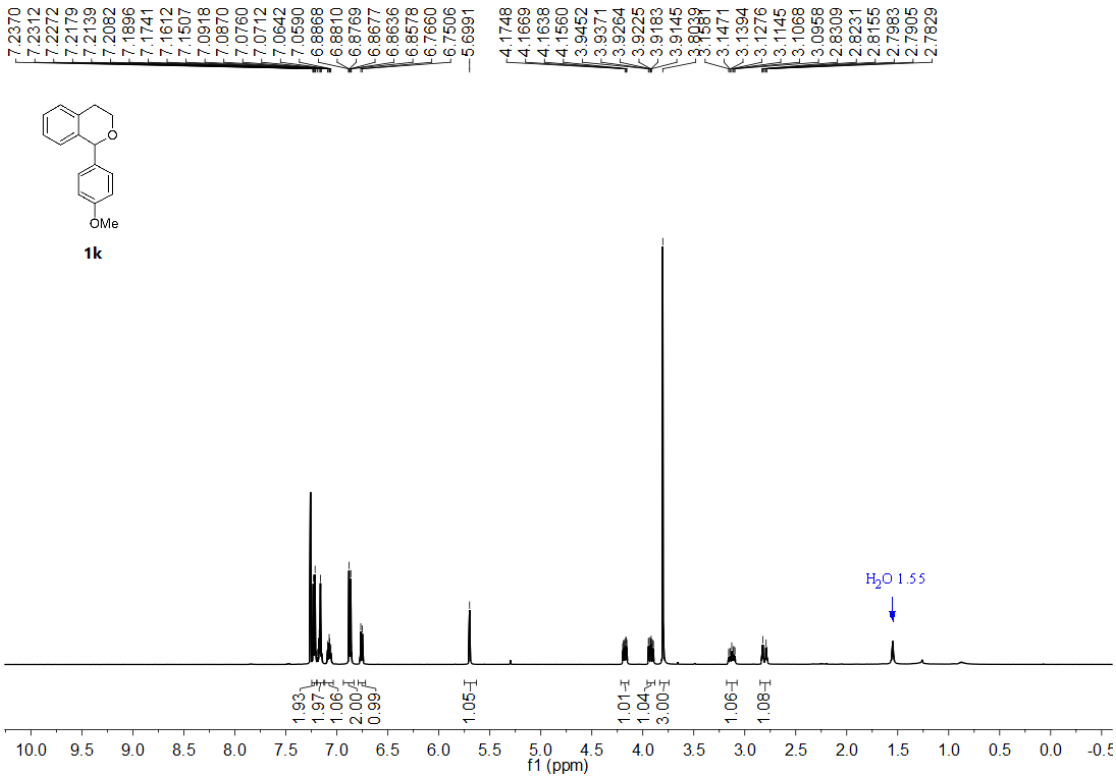
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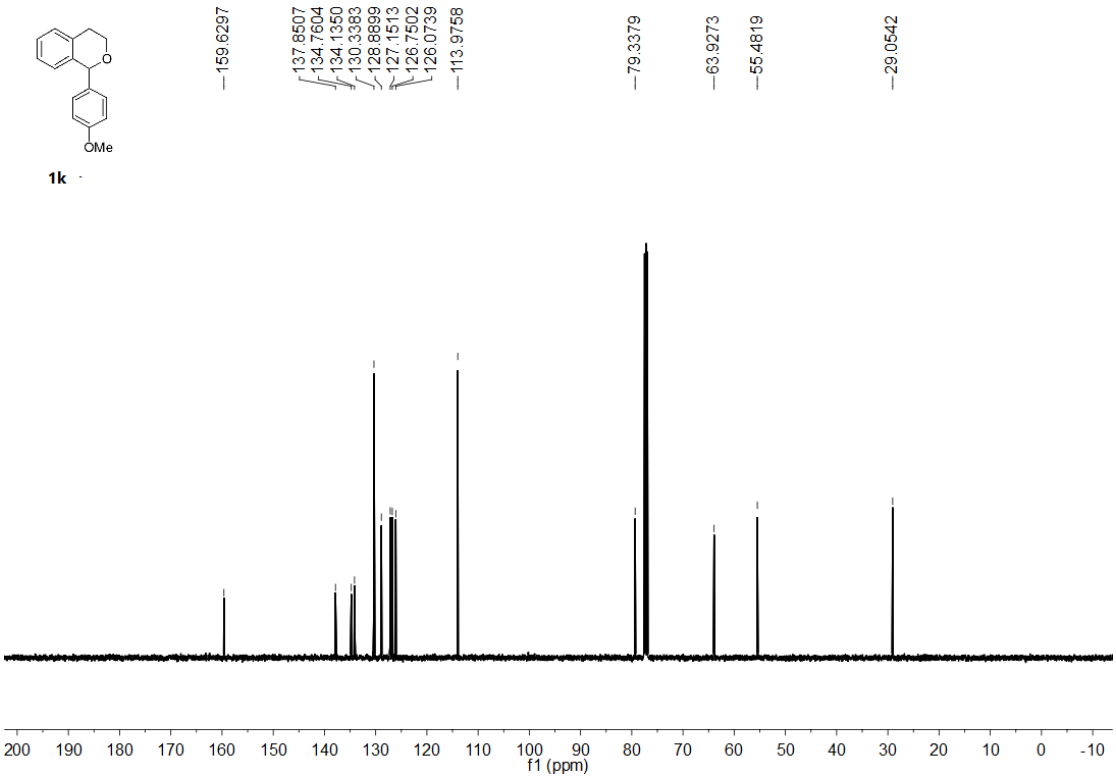
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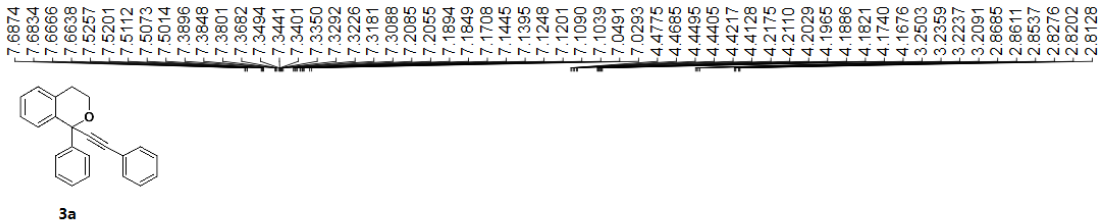
1k
f1 (ppm)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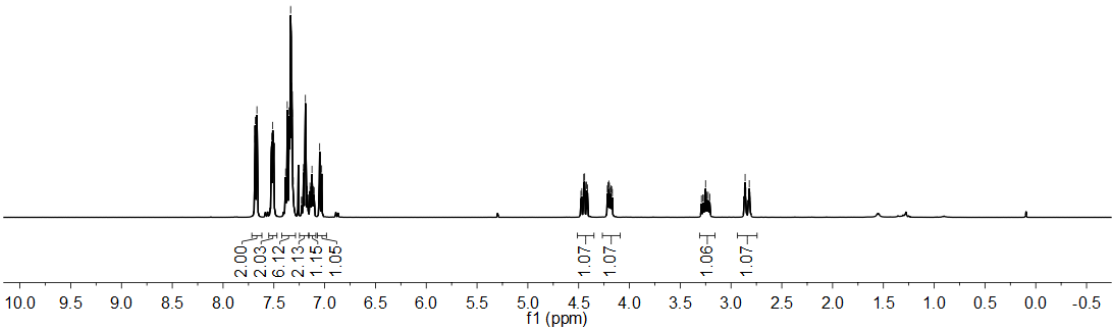
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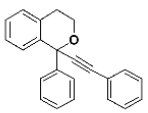
1.06
1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



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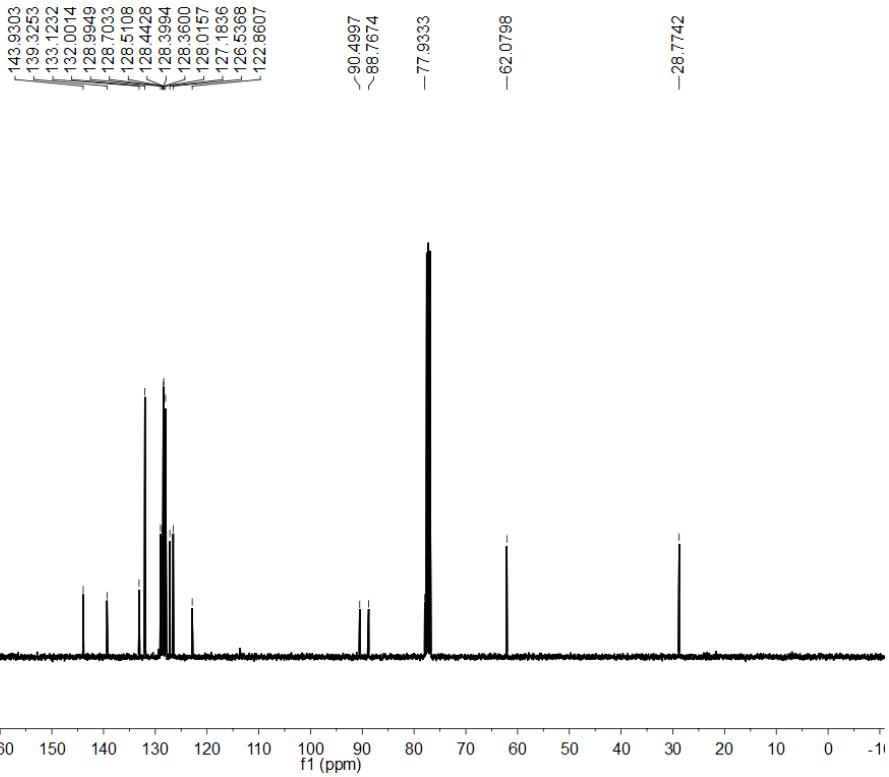
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132.0014
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128.5108
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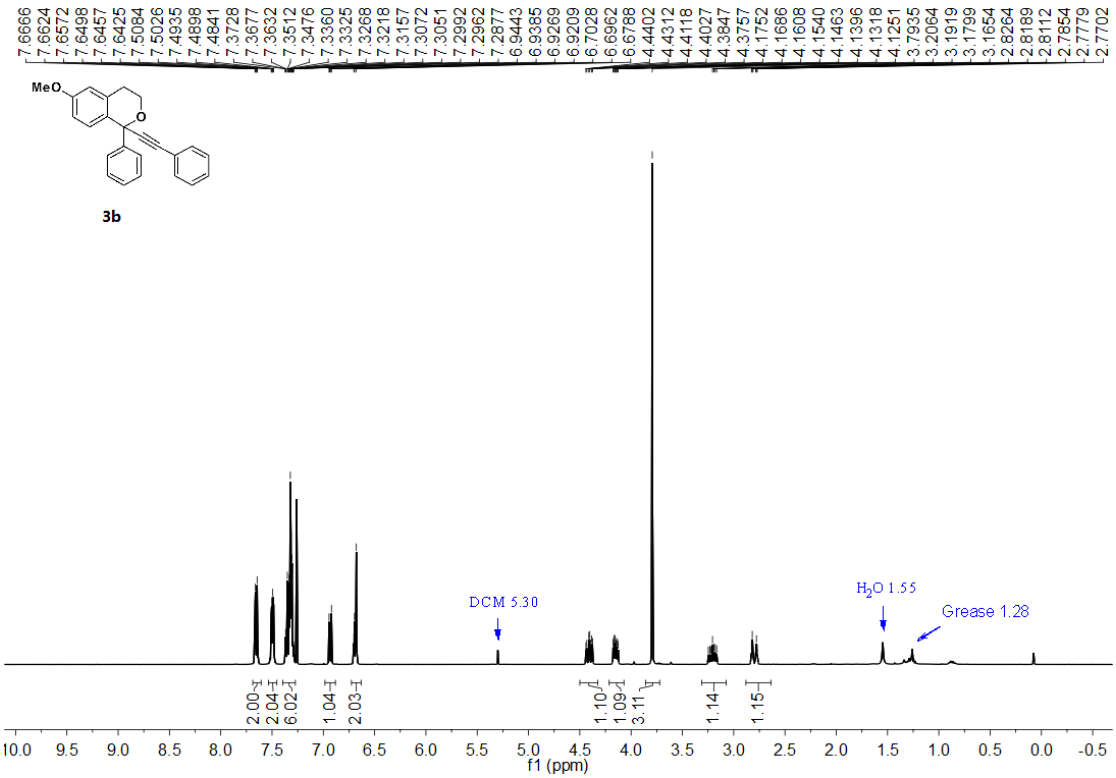
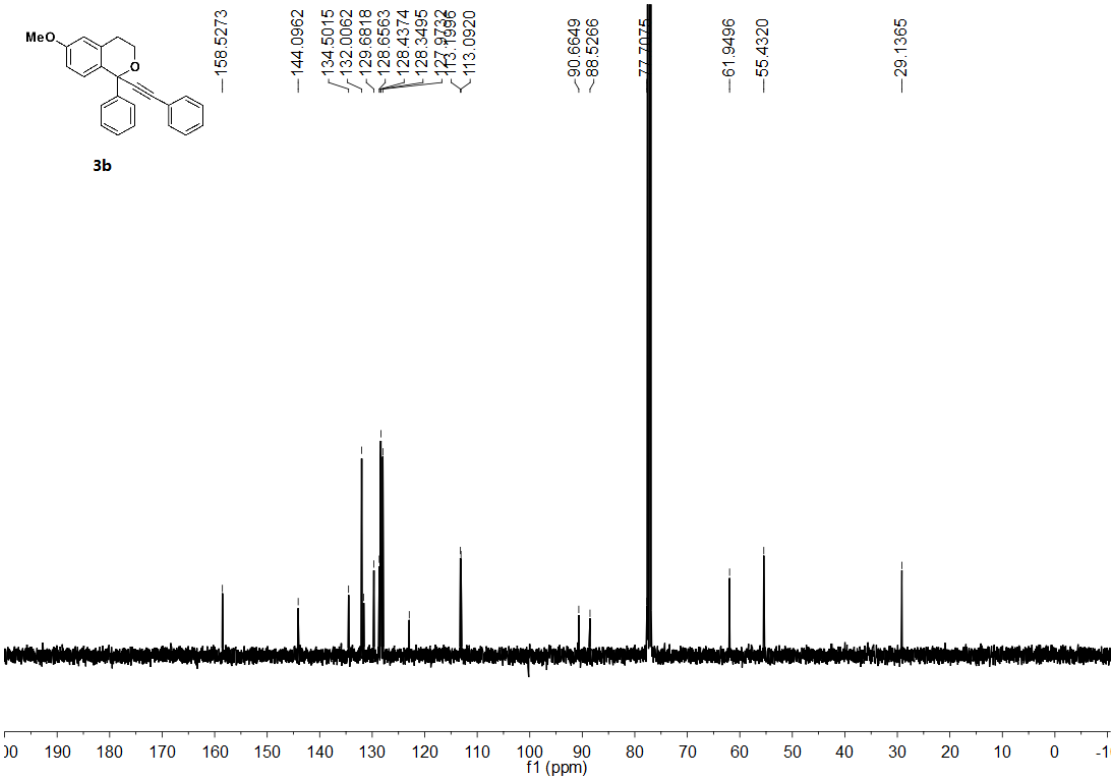
128.3994
128.3600
128.0157
127.1836
126.5368
122.8607
90.4997
88.7674
77.9333
62.0798
28.7742
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


MeO
O
3b
DCM 5.30
H2O 1.55
Grease 1.28
f1 (ppm)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O
3b
158.5273
144.0962
134.5015
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129.6818
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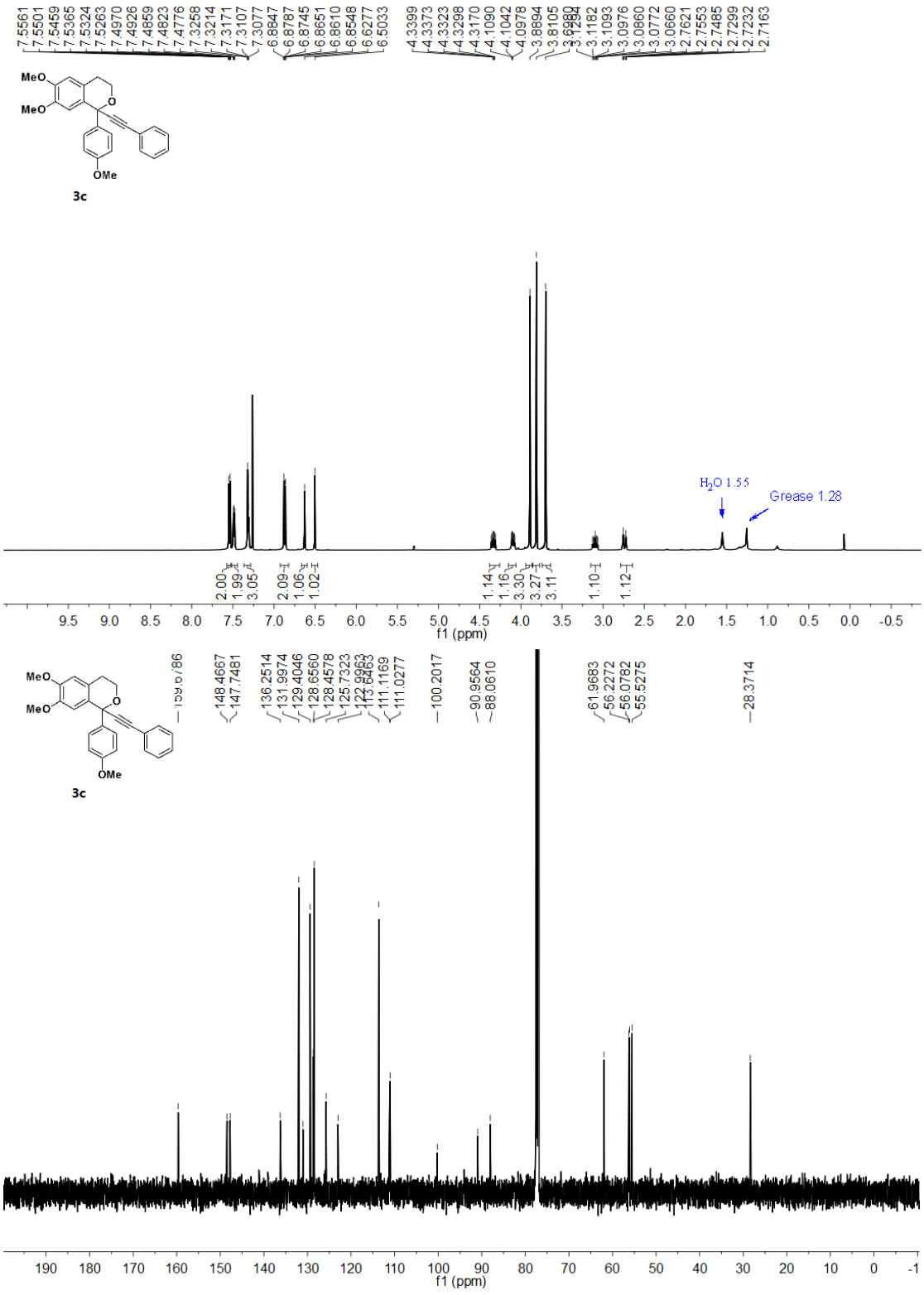
113.0920
90.6649
88.5266
77.7075
61.9496
55.4320
29.1365
f1 (ppm)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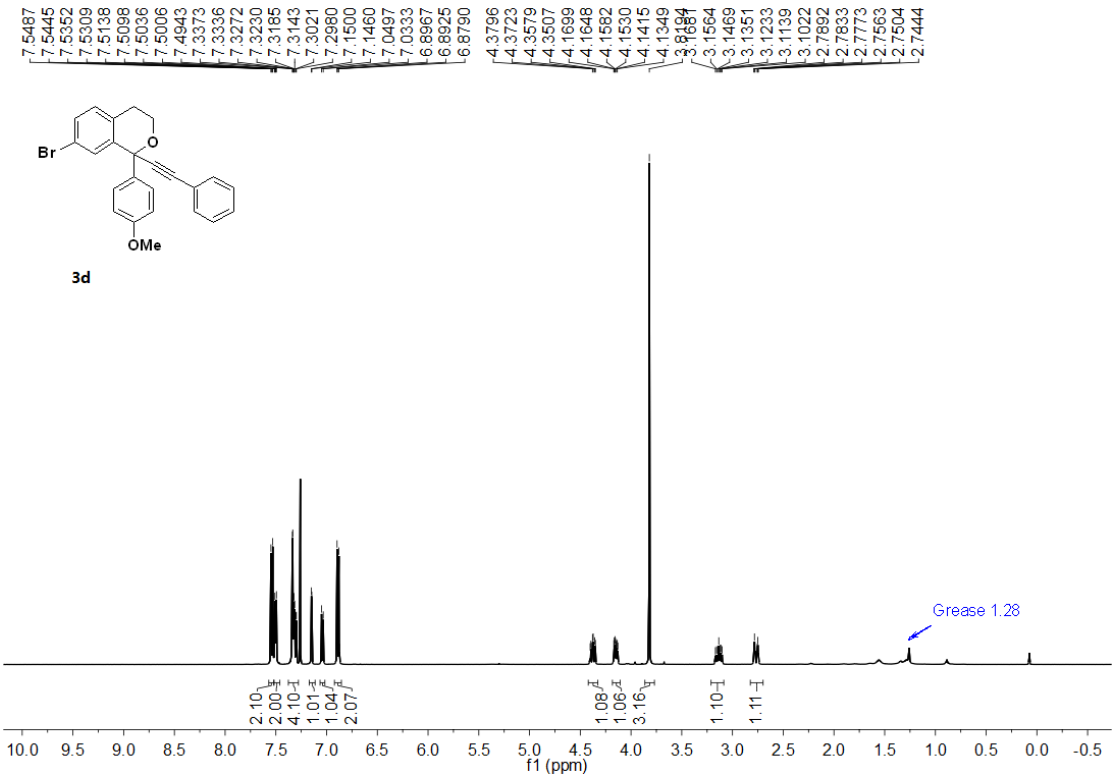
7.4776
7.3258
7.3214
7.3171
7.3107
7.3077
6.8847
6.8787
6.8745
6.8651
6.8610
6.8548
6.6277
6.5033
4.3399
4.3373
4.3323
4.3298
4.3170
4.1090
4.1042
4.0978
3.8894
3.8105
3.1182
3.1093
3.0976
3.0860
3.0772
3.0660
2.7621
2.7553
2.7485
2.7299
2.7232
2.7163
MeO
MeO
O
OMe
3c
H2O 1.55
Grease 1.28
2.00
1.99
3.05
2.09
1.06
1.02
1.14
1.16
3.30
3.27
3.11
1.10
1.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
MeO
MeO
O
OMe
3c
159.0786
148.4667
147.7481
136.2514
131.9974
129.4046
128.6560
128.4578
125.7323
122.9963
113.6483
111.1169
111.0277
100.2017
90.9564
88.0610
61.9683
56.2272
56.0782
55.5275
28.3714
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)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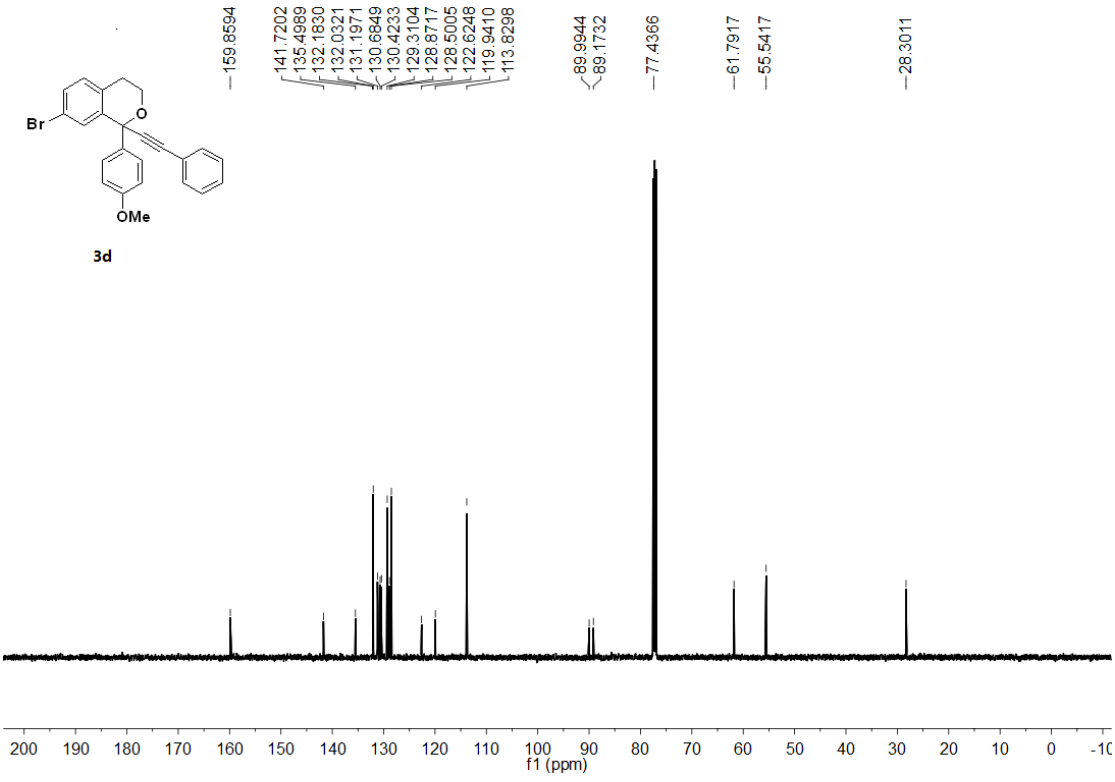
7.3373
7.3336
7.3272
7.3230
7.3185
7.3143
7.3021
7.2980
7.1500
7.1460
7.0497
7.0333
6.8967
6.8925
6.8790
4.3796
4.3723
4.3579
4.3507
4.1699
4.1648
4.1582
4.1530
4.1415
4.1349
3.1564
3.1469
3.1351
3.1233
3.1139
3.1022
2.7892
2.7833
2.7773
2.7563
2.7504
2.7444
Br
O
OMe
3d
Grease 1.28
2.10
2.00
4.10
1.01
1.04
2.07
1.08
1.06
3.16
1.10
1.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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132.0321
131.1971
130.6849
130.4233
129.3104
128.8717
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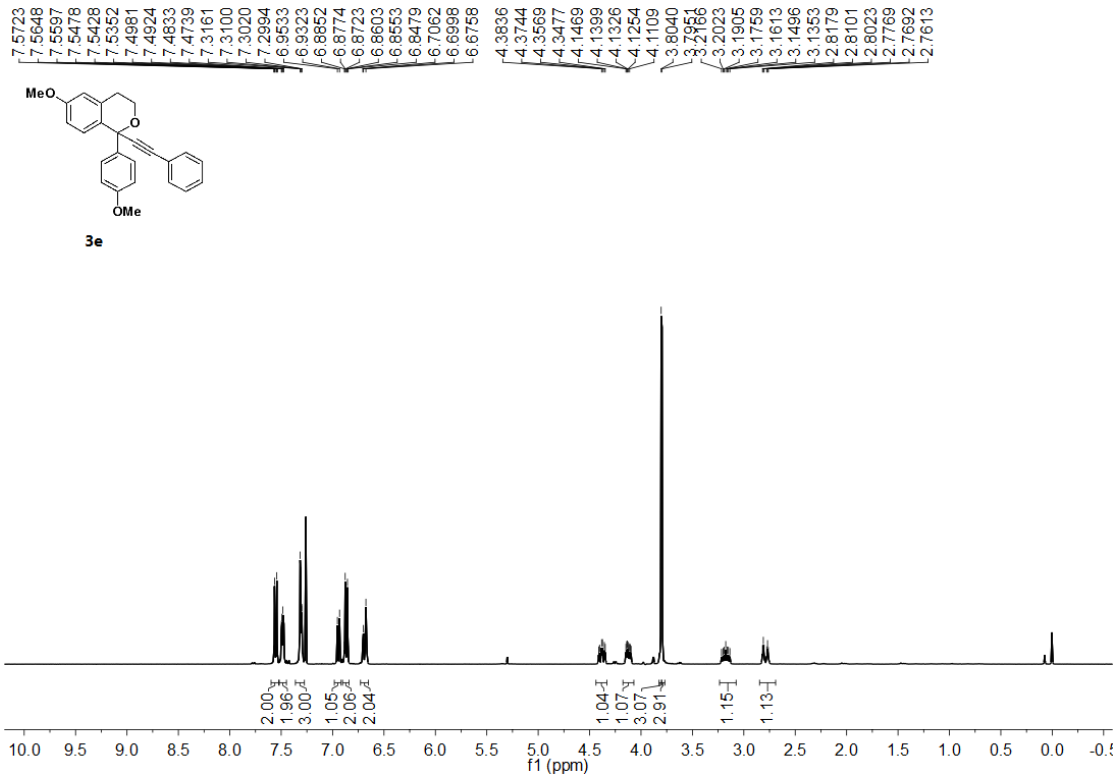
122.6248
119.9410
113.8298
89.9944
89.1732
77.4366
61.7917
55.5417
28.3011
Br
O
OMe
3d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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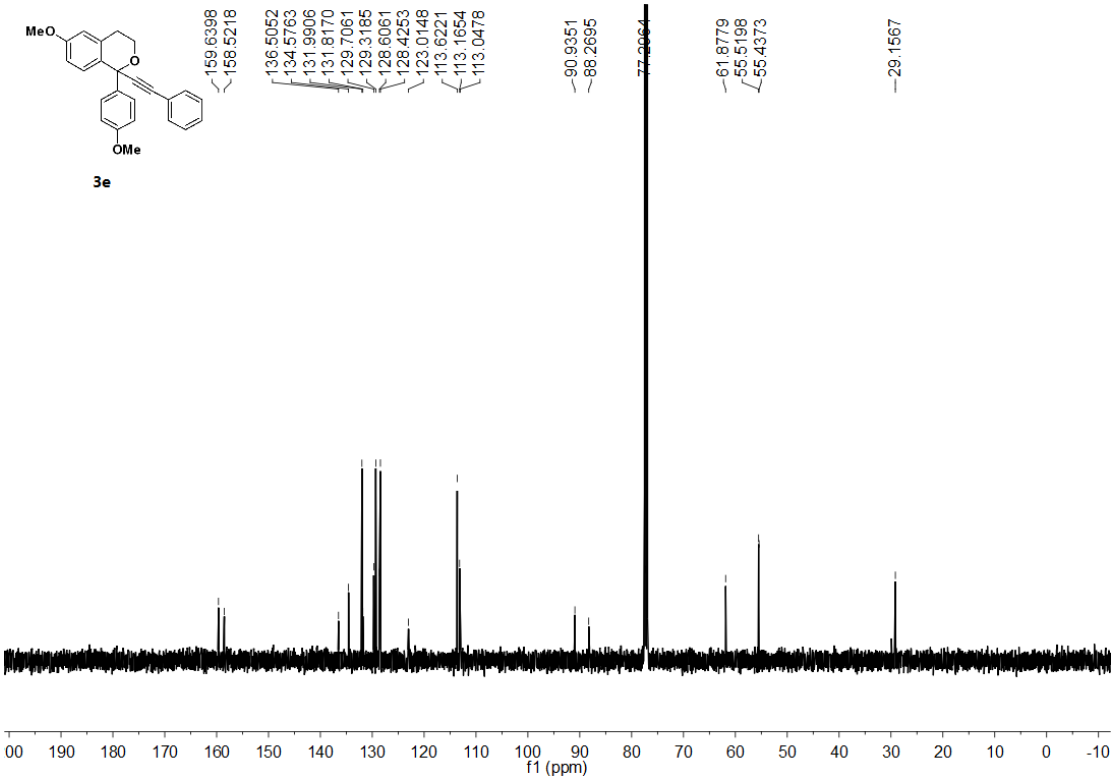
7.4924
7.4833
7.4739
7.3161
7.3100
7.3020
7.2994
6.9533
6.9323
6.8852
6.8774
6.8723
6.8603
6.8553
6.8479
6.7062
6.6998
6.6758
4.3836
4.3744
4.3569
4.3477
4.1469
4.1399
4.1326
4.1254
4.1109
3.8040
3.2766
3.2023
3.1905
3.1759
3.1613
3.1496
3.1353
2.8179
2.8101
2.8023
2.7769
2.7692
2.7613
MeO
O
OMe
3e
2.00
1.96
3.00
1.05
2.06
2.04
1.04
1.07
3.07
2.91
1.15
1.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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O
OMe
3e
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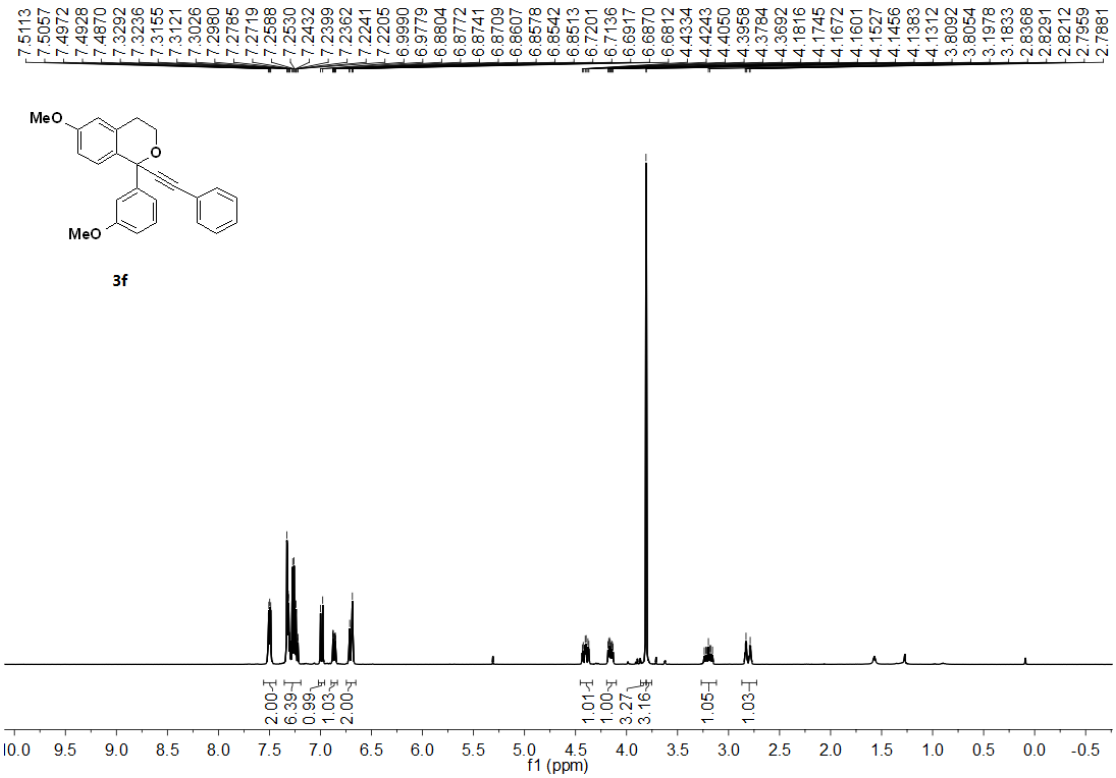
128.6061
128.4253
123.0148
113.6221
113.1654
113.0478
90.9351
88.2695
77.2964
61.8779
55.5198
55.4373
29.1567
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.2719
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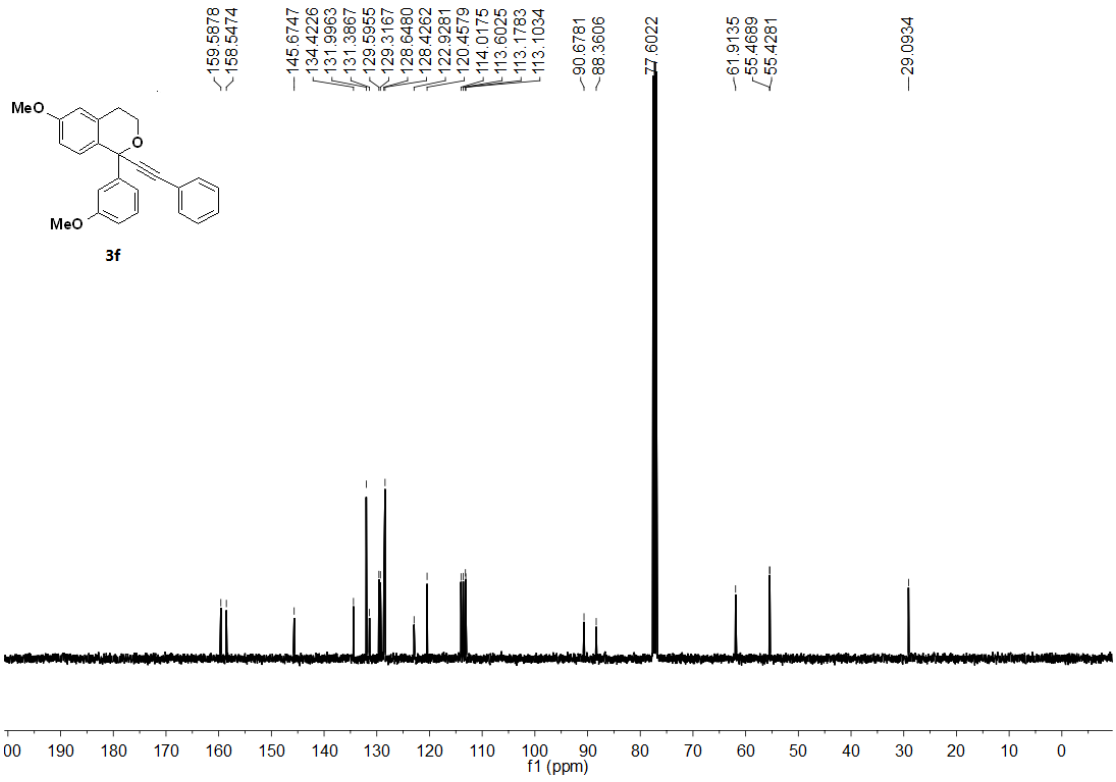
7.2530
7.2432
7.2399
7.2362
7.2241
7.2205
6.9990
6.9779
6.8804
6.8772
6.8741
6.8709
6.8607
6.8578
6.8542
6.8513
6.7201
6.7136
6.6917
6.6870
6.6812
4.4334
4.4243
4.4050
4.3958
4.3784
4.3692
4.1816
4.1745
4.1672
4.1601
4.1527
4.1456
4.1383
4.1312
3.8092
3.8054
3.1978
3.1833
2.8368
2.8291
2.8212
2.7959
2.7881
MeO
O
MeO
3f
2.00
6.39
0.99
1.03
2.00
1.01
1.00
3.27
3.16
1.05
1.03
f1 (ppm)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128.6480
128.4262
122.9281
120.4579
114.0175
113.6025
113.1783
113.1034
90.6781
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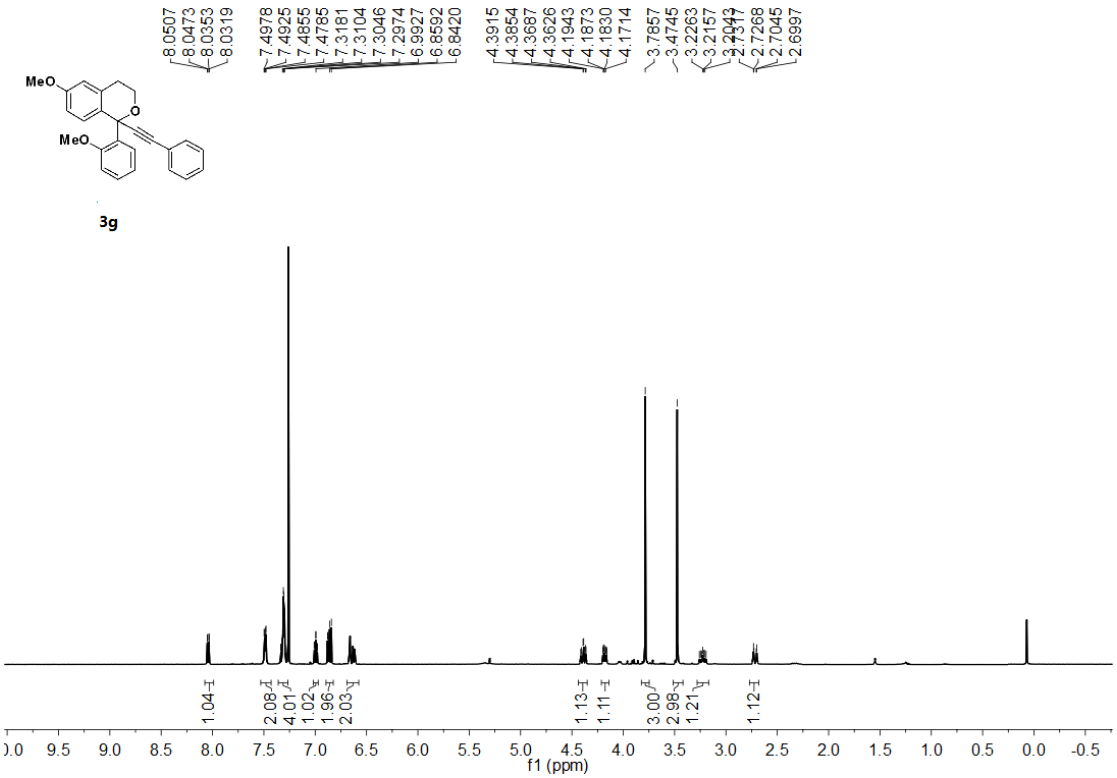
61.9135
55.4689
55.4281
29.0934
MeO
O
MeO
3f
f1 (ppm)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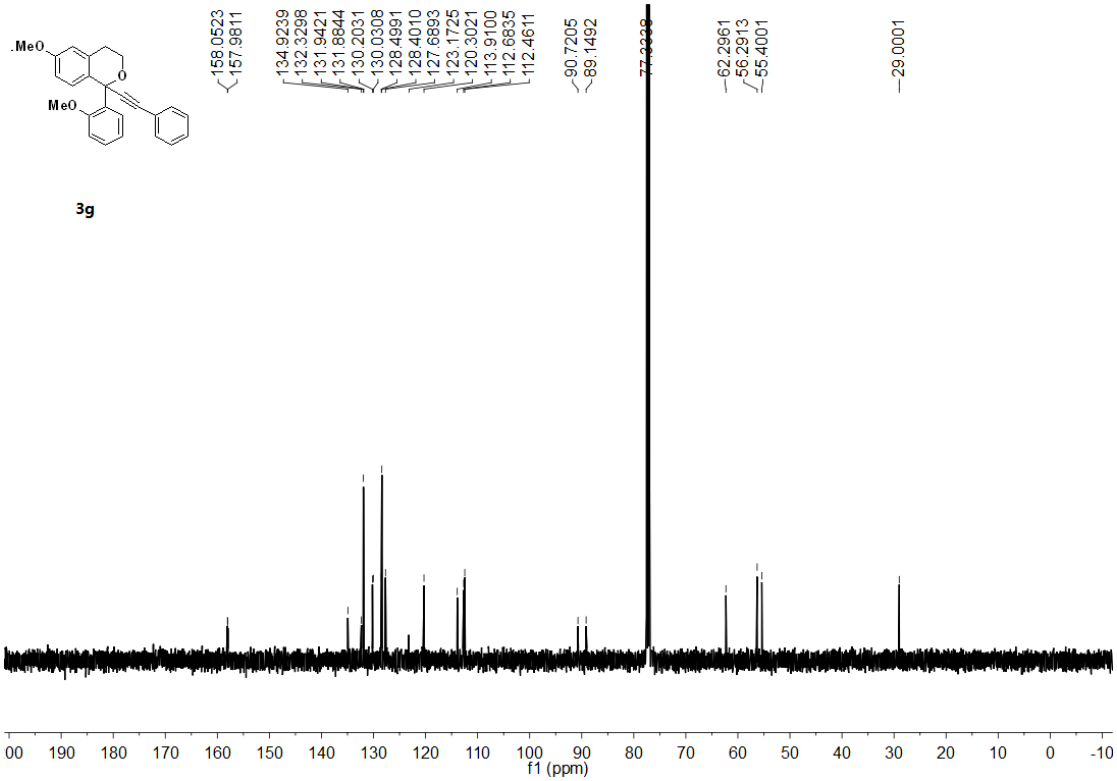
8.0353
8.0319
7.4978
7.4925
7.4855
7.4785
7.3181
7.3104
7.3046
7.2974
6.9927
6.8592
6.8420
4.3915
4.3854
4.3687
4.3626
4.1943
4.1873
4.1830
4.1714
3.7857
3.4745
3.2263
3.2157
2.7317
2.7268
2.7045
2.6997
MeO
MeO
O
3g
1.04
2.08
4.01
1.02
1.96
2.03
1.13
1.11
3.00
2.98
1.21
1.12
f1 (ppm)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130.2031
130.0308
128.4991
128.4010
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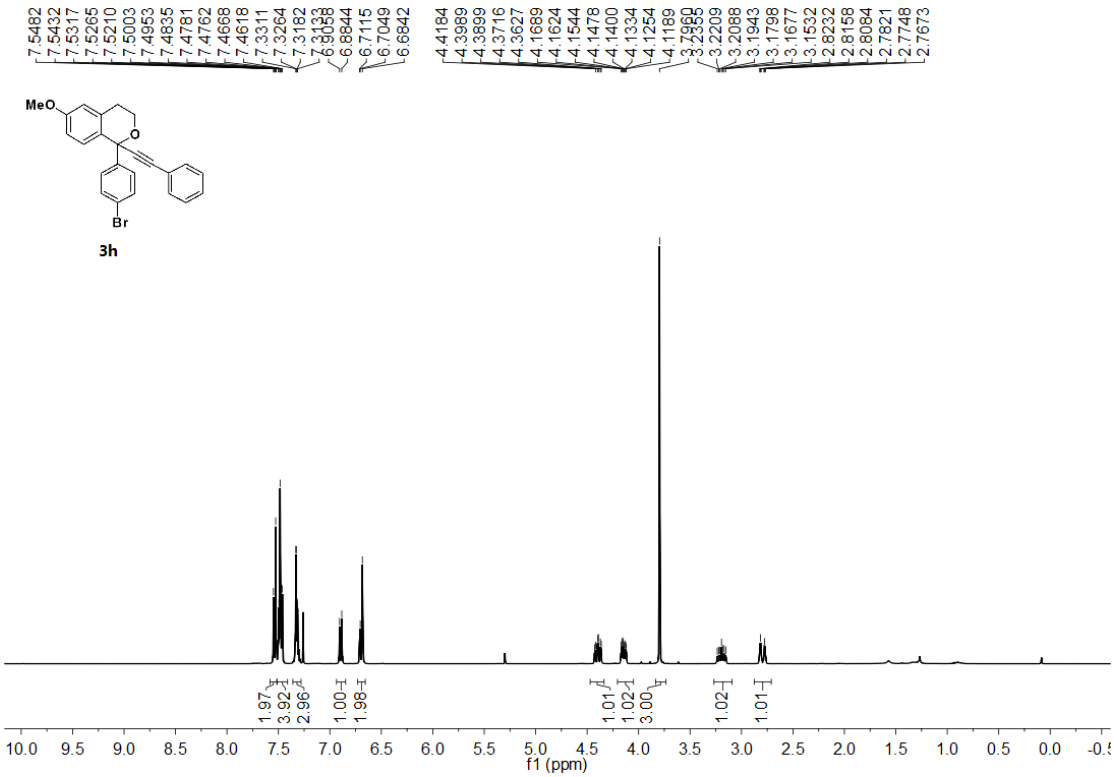
123.1725
120.3021
113.9100
112.6835
112.4611
90.7205
89.1492
77.3339
62.2961
56.2913
55.4001
29.0001
MeO
MeO
O
3g
f1 (ppm)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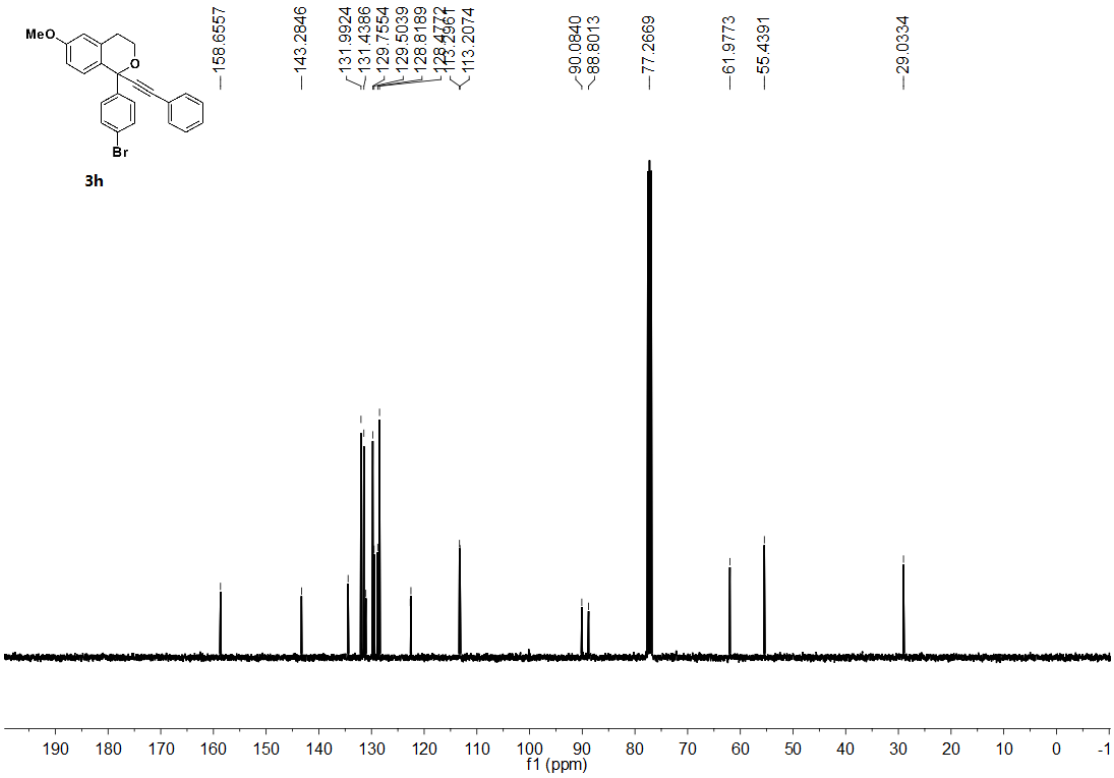
7.4762
7.4668
7.4618
7.3311
7.3264
7.3182
7.3133
6.9058
6.8844
6.7115
6.7049
6.6842
4.4184
4.3989
4.3899
4.3716
4.3627
4.1689
4.1624
4.1544
4.1478
4.1400
4.1334
4.1254
4.1189
3.2209
3.2088
3.1943
3.1798
3.1677
3.1532
2.8232
2.8158
2.8084
2.7821
2.7748
2.7673
MeO
O
Br
3h
1.97
3.92
2.96
1.00
1.98
1.01
1.02
3.00
1.02
1.01
f1 (ppm)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128.8189
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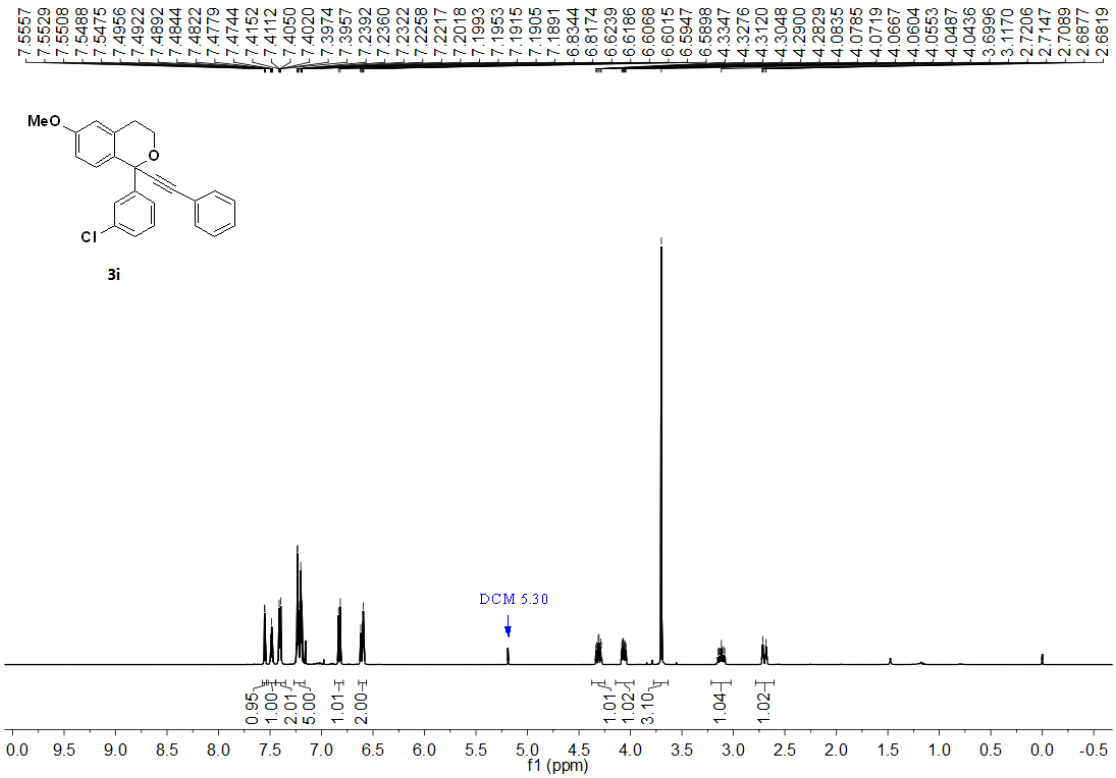
88.8013
77.2669
61.9773
55.4391
29.0334
MeO
O
Br
3h
f1 (ppm)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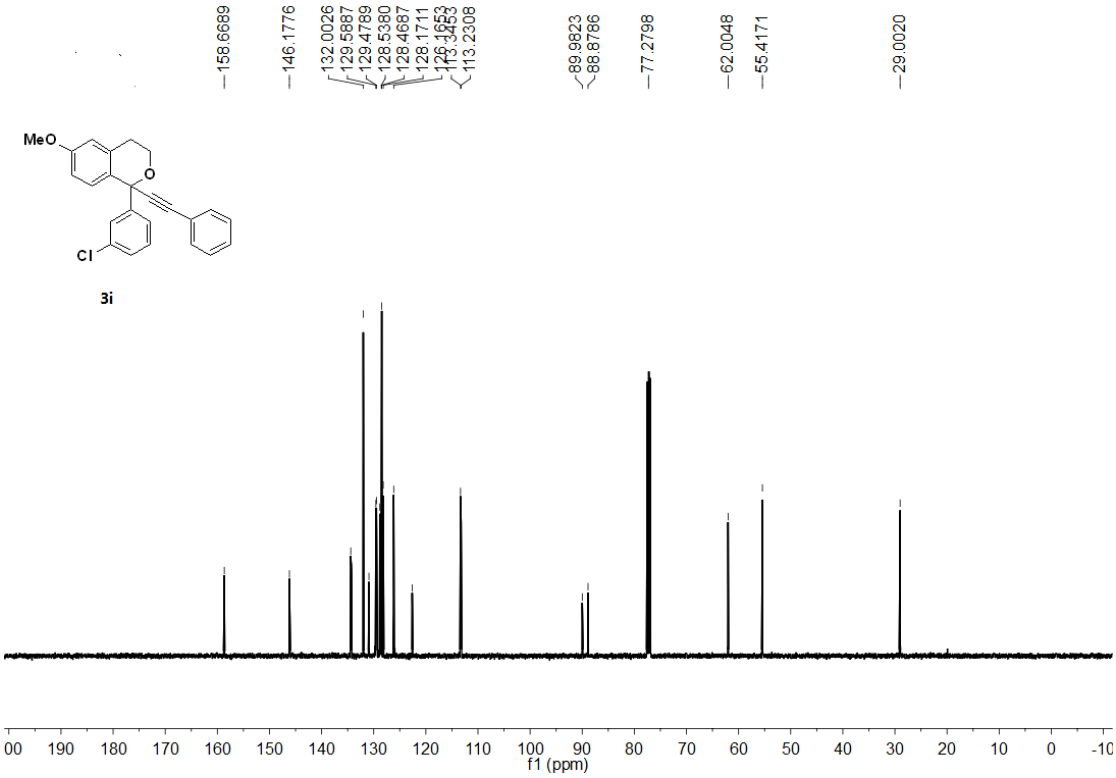
7.489
7.484
7.482
7.477
7.474
7.415
7.411
7.405
7.402
7.397
7.395
7.239
7.236
7.232
7.225
7.221
7.201
7.199
7.195
7.191
7.189
6.834
6.817
6.623
6.618
6.606
6.601
6.594
6.589
4.334
4.327
4.312
4.304
4.290
4.282
4.083
4.078
4.071
4.066
4.060
4.055
4.048
4.043
3.699
3.117
2.720
2.714
2.708
2.687
2.681
MeO
O
Cl
3i
DCM 5.30
0.95
1.00
2.01
5.00
1.01
2.00
1.01
1.02
3.10
1.04
1.02
f1 (ppm)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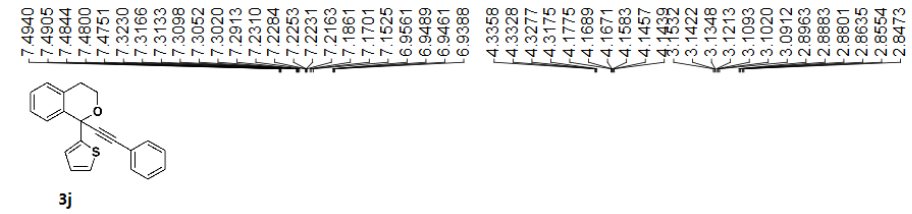
77.2798
62.0048
55.4171
29.0020
MeO
O
Cl
3i
f1 (ppm)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7.4800
7.4751
7.3230
7.3166
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7.3098
7.3052
7.3020
7.2913
7.2310
7.2284
7.2253
7.2231
7.2163
7.1861
7.1701
7.1525
6.9561
6.9489
6.9461
6.9388
4.3358
4.3328
4.3277
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4.1775
4.1689
4.1671
4.1583
4.1457
3.1422
3.1348
3.1213
3.1093
3.1020
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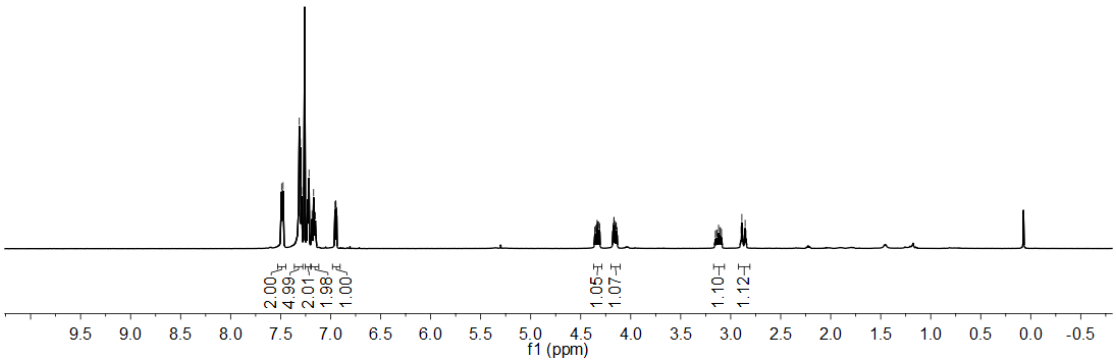
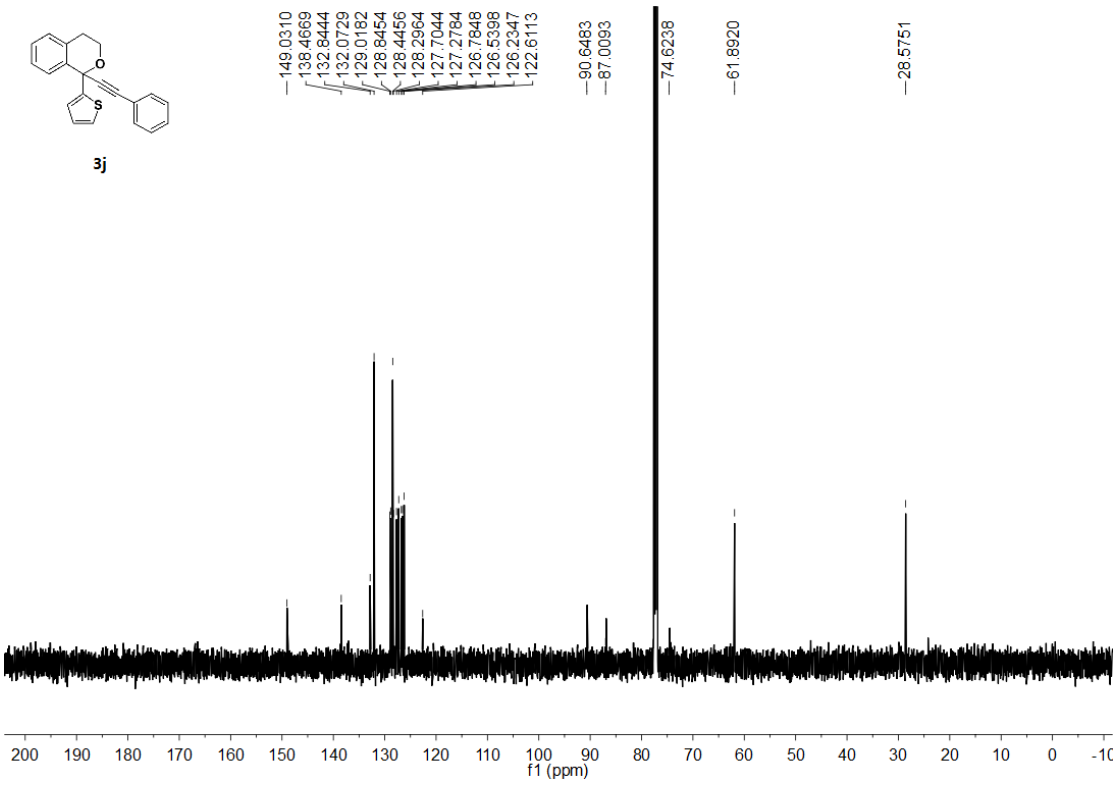
2.8963
2.8883
2.8801
2.8635
2.8554
2.8473
O
S

3j


2.00
4.99
2.01
1.98
1.00
1.05
1.07
1.10
1.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.4456
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127.7044
127.2784
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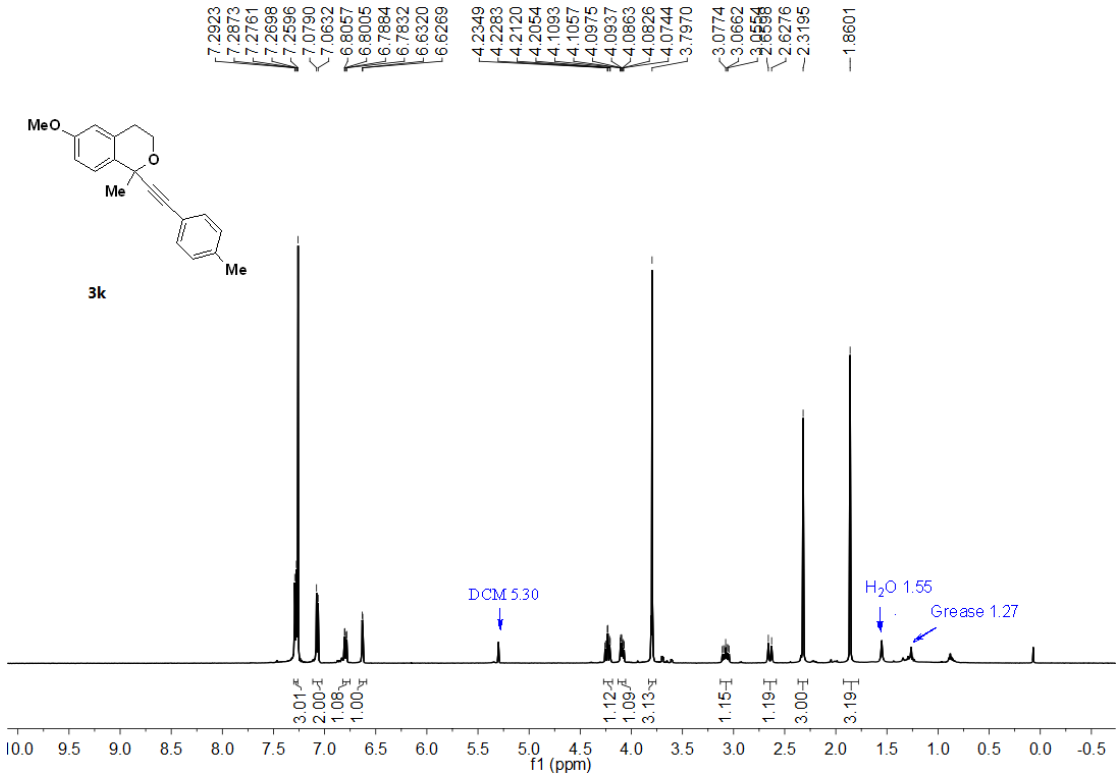
126.5398
126.2347
122.6113
90.6483
87.0093
74.6238
61.8920
28.5751
O
S
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3j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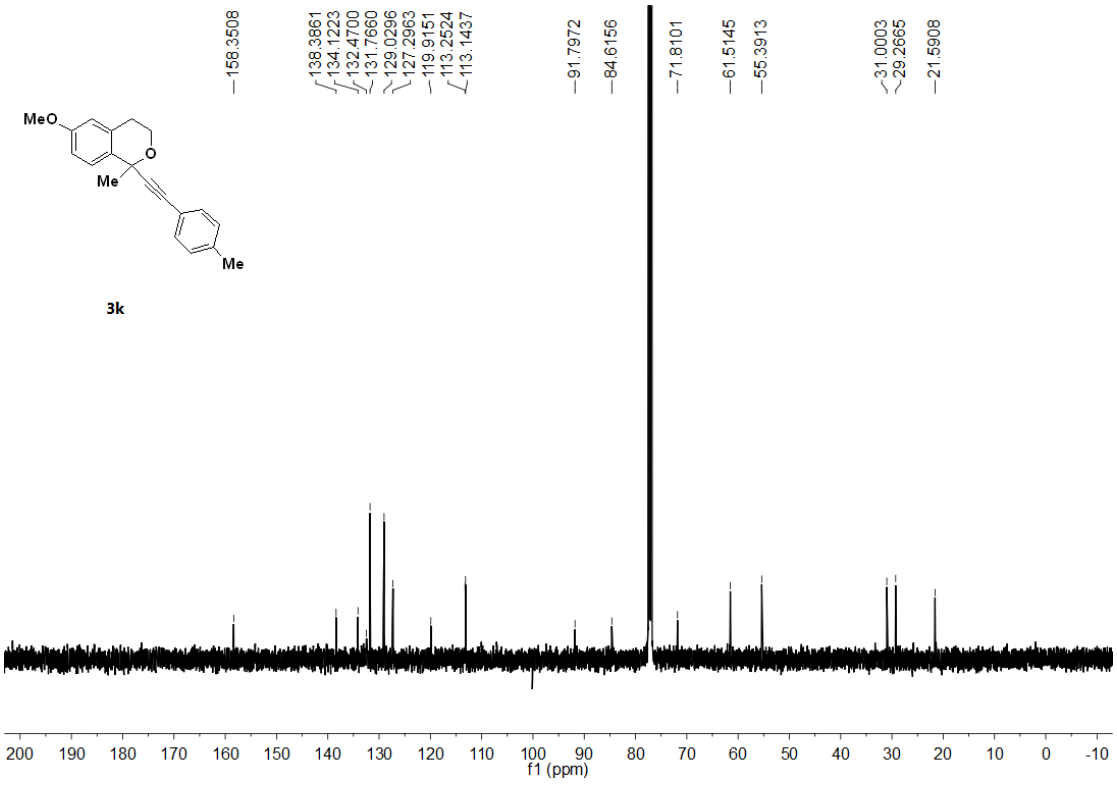
6.6320
6.6269
4.2349
4.2283
4.2120
4.2054
4.1093
4.1057
4.0975
4.0937
4.0863
4.0826
4.0744
3.7970
3.0774
3.0662
2.6276
2.3195
1.8601
MeO
O
Me
Me
3k
DCM 5.30
H2O 1.55
Grease 1.27
3.01
2.00
1.08
1.00
1.12
1.09
3.13
1.15
1.19
3.00
3.19
f1 (ppm)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127.2963
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113.2524
113.1437
91.7972
84.6156
71.8101
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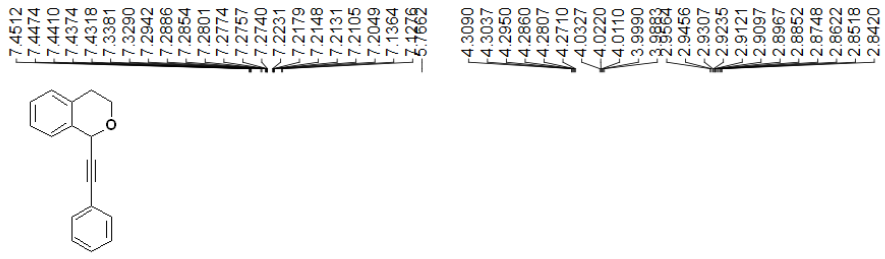
55.3913
31.0003
29.2665
21.5908
MeO
O
Me
Me
3k
f1 (ppm)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7.2740
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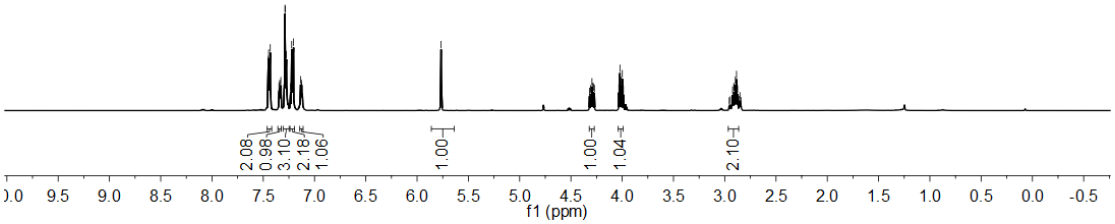
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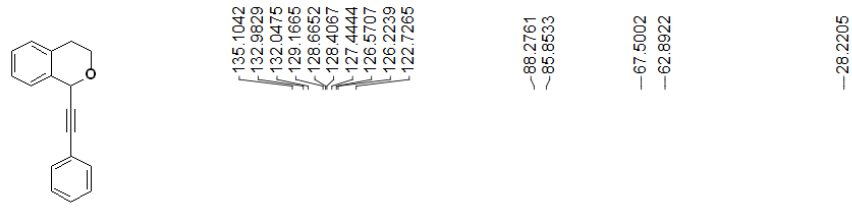
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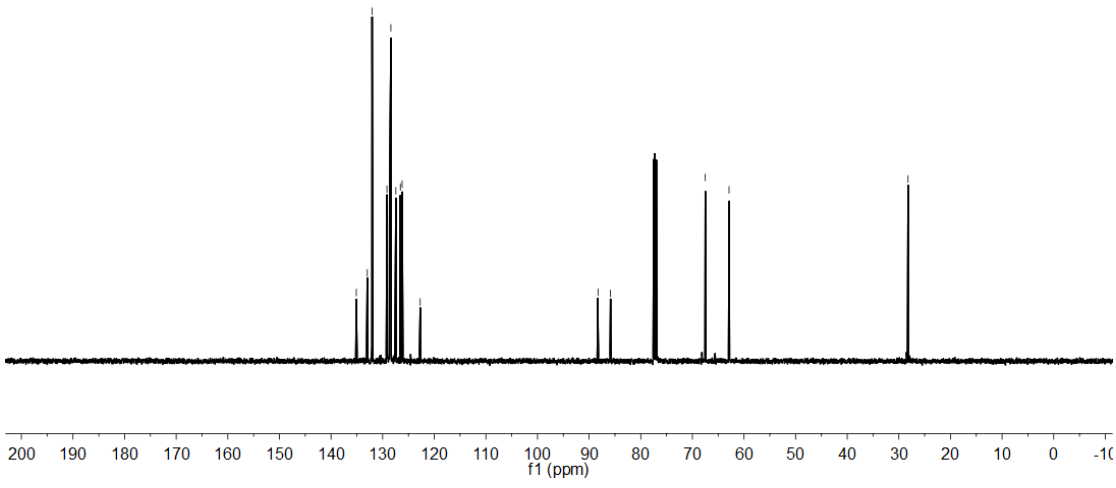
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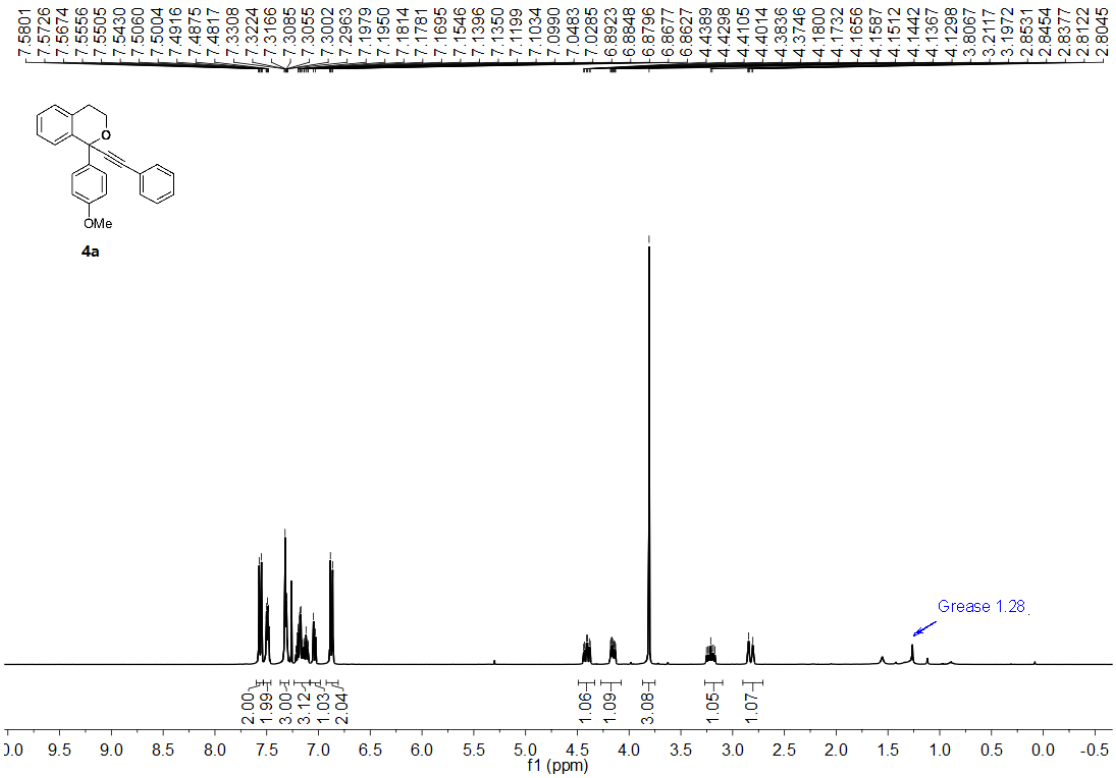
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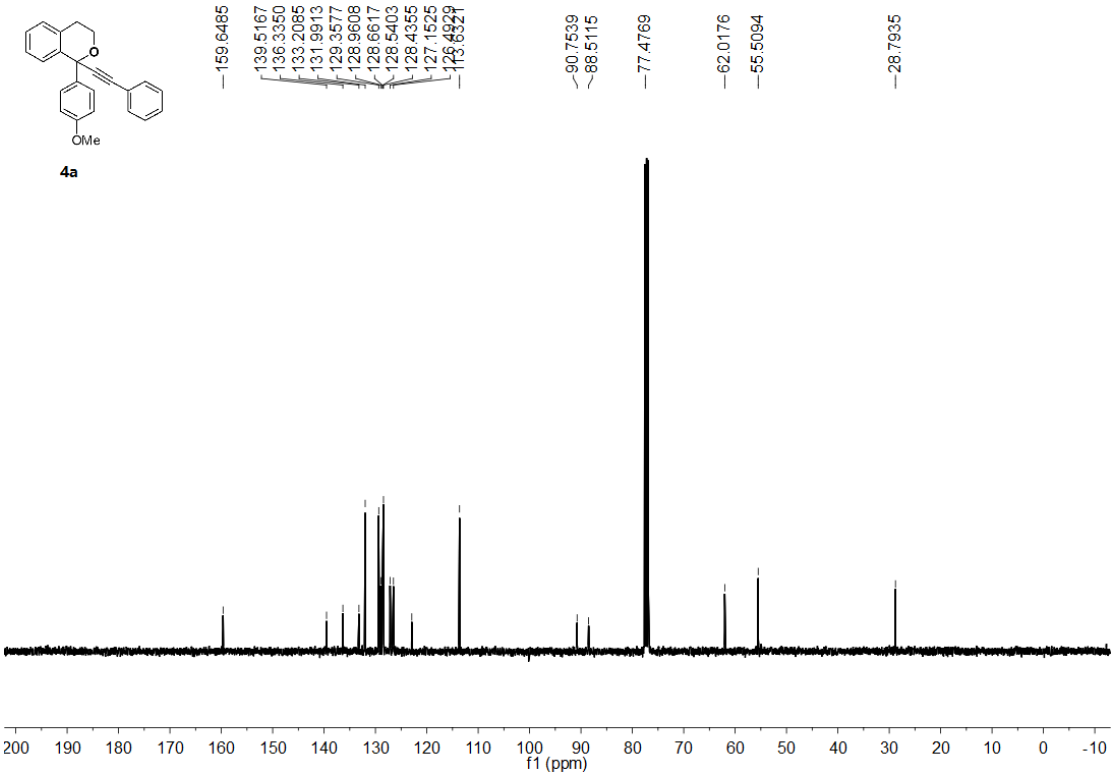
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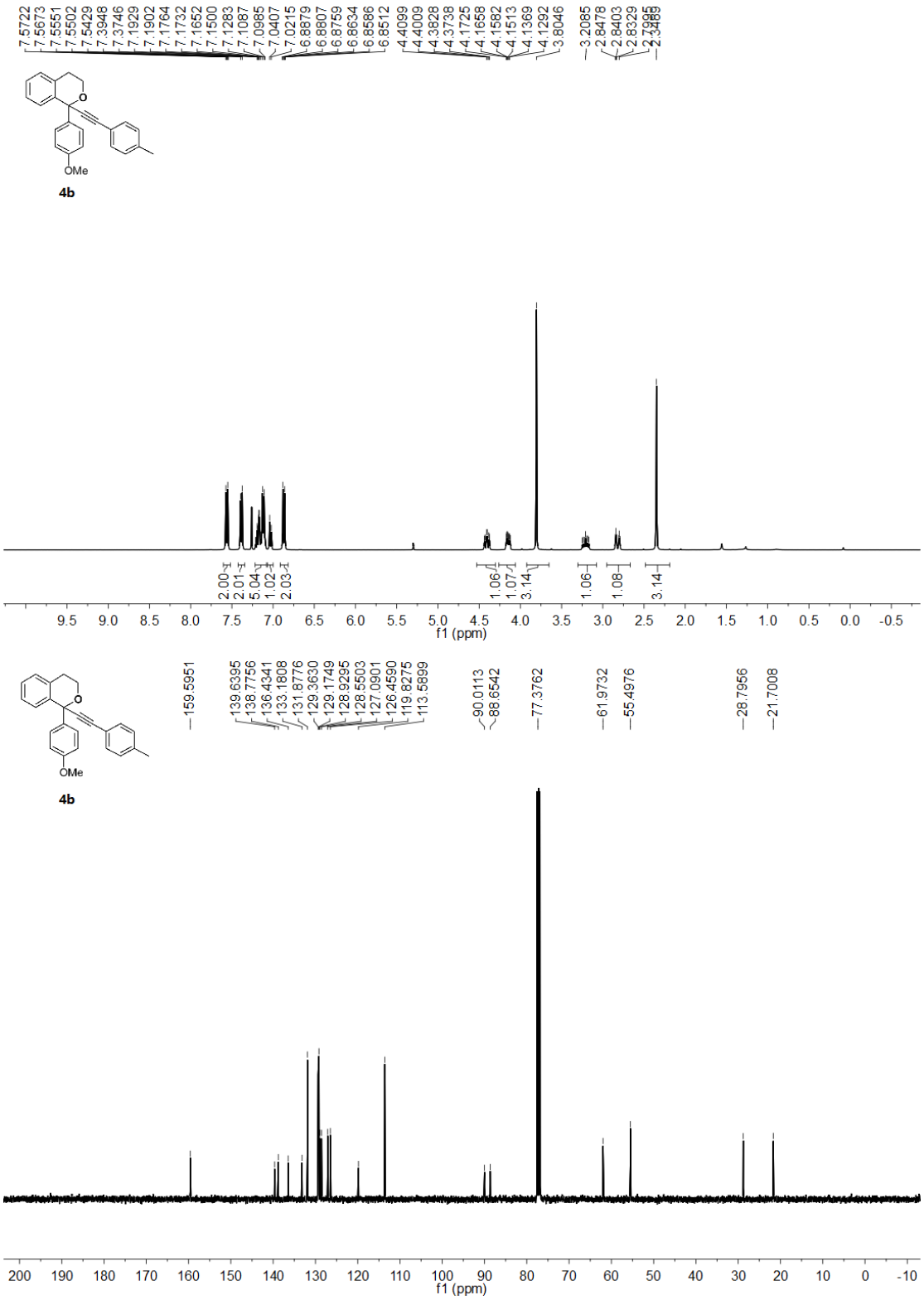
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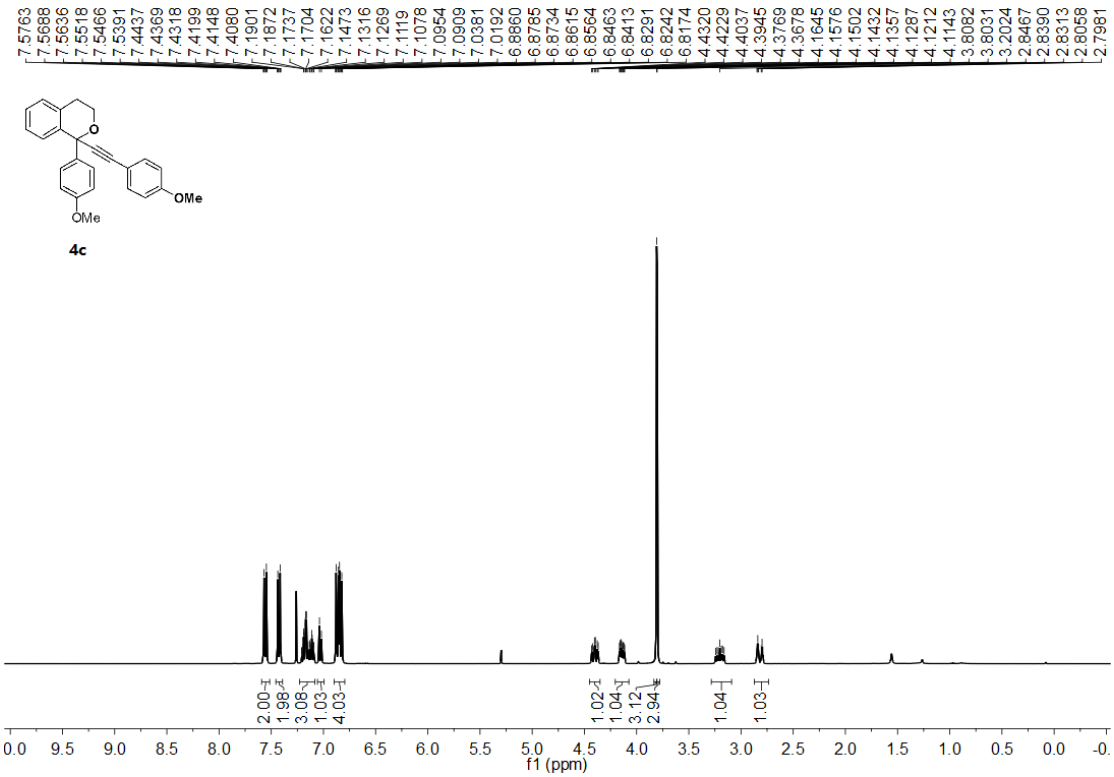
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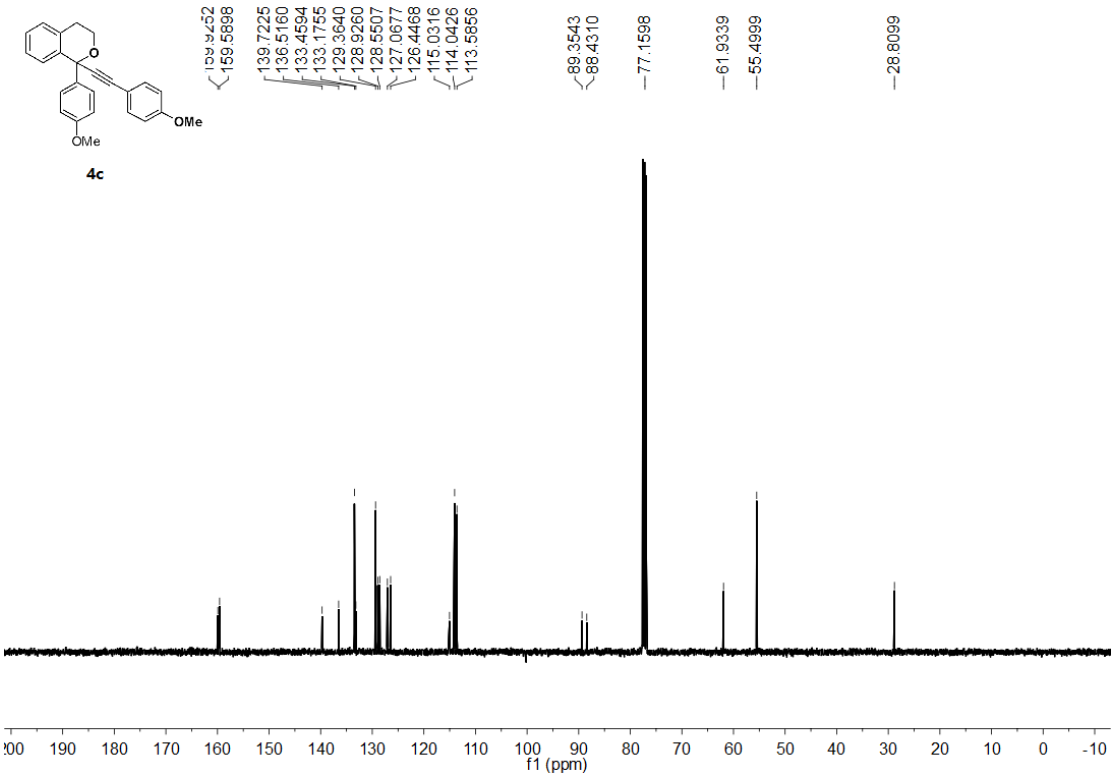
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OMe
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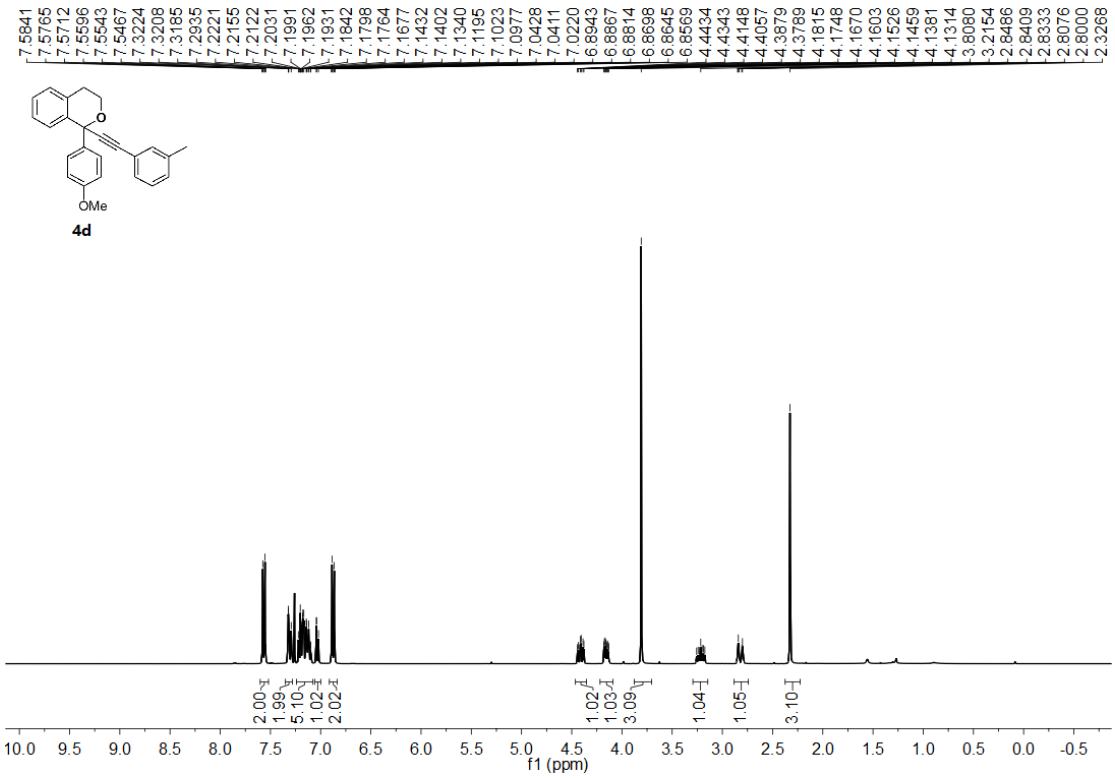
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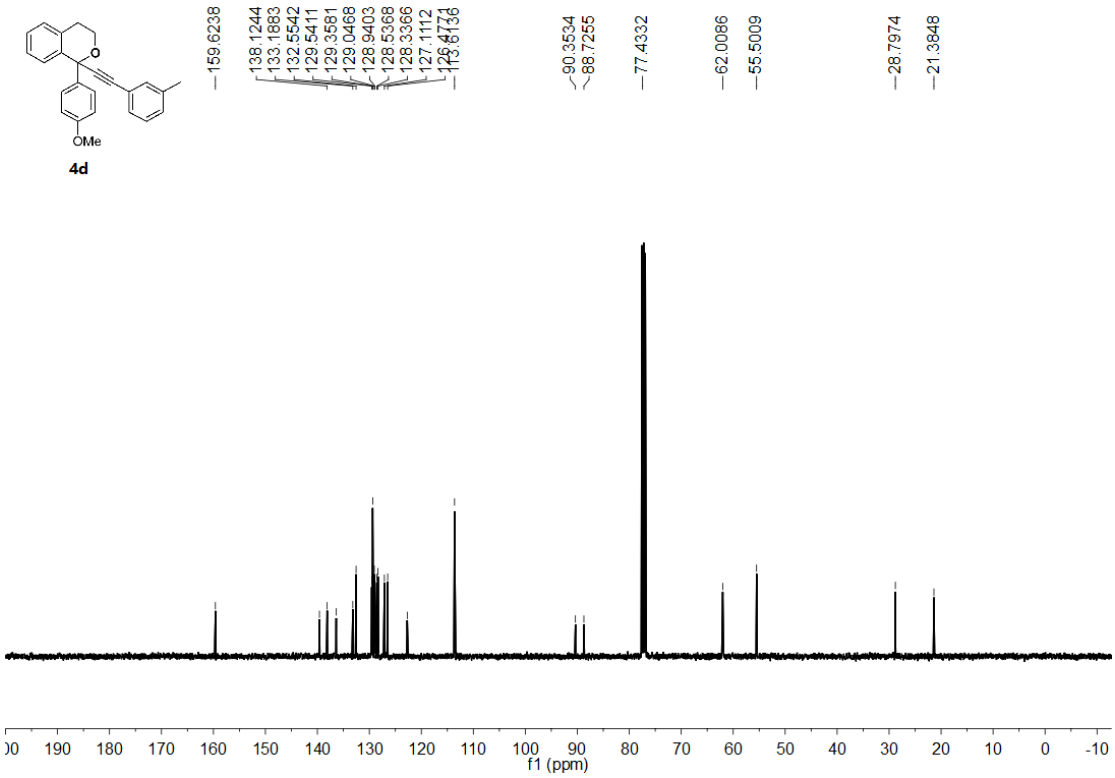
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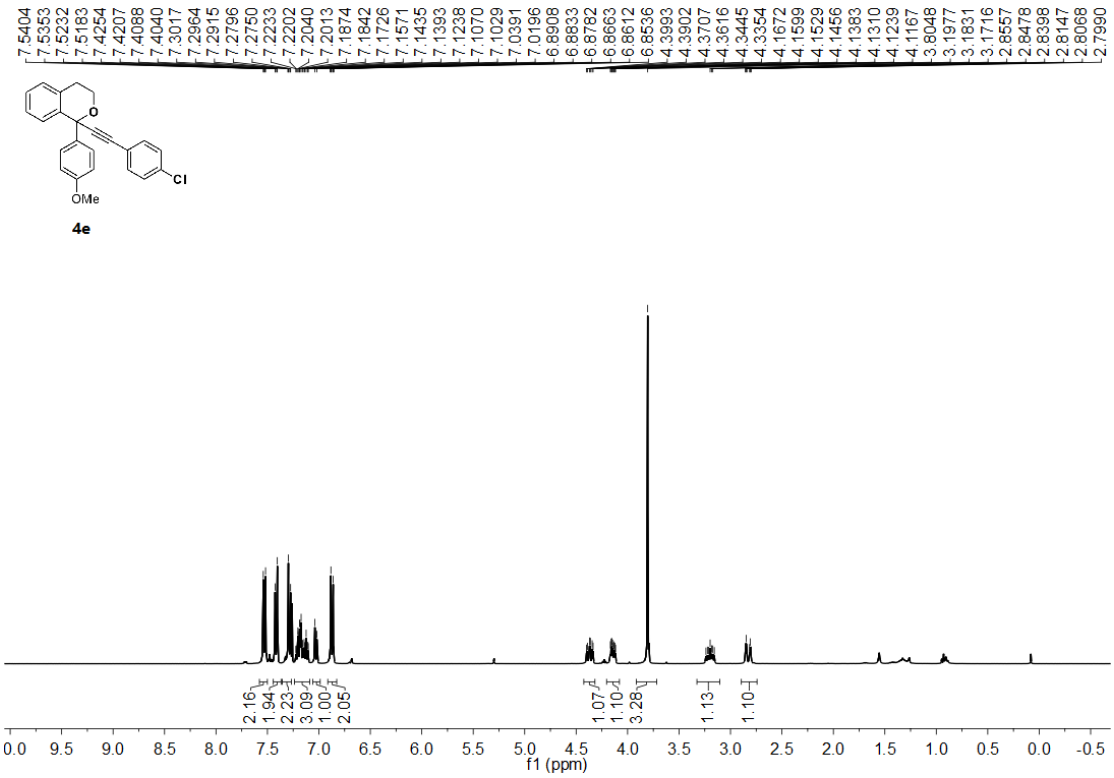
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Cl
OMe
4e
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1.10
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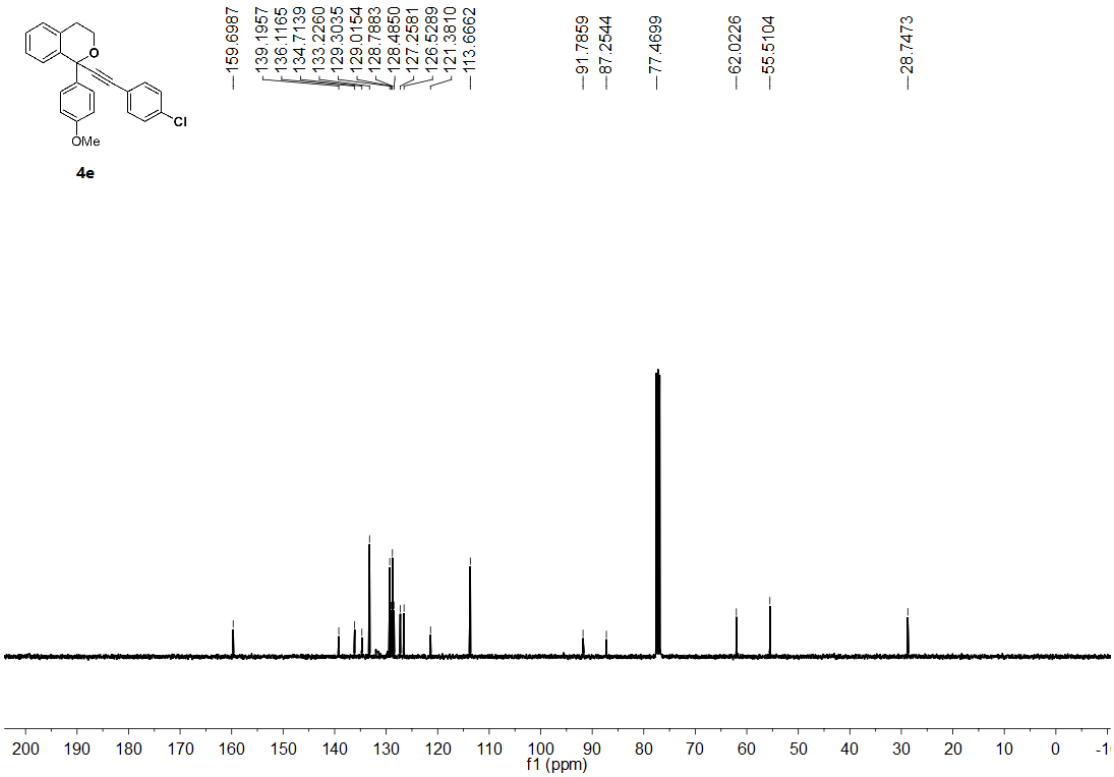
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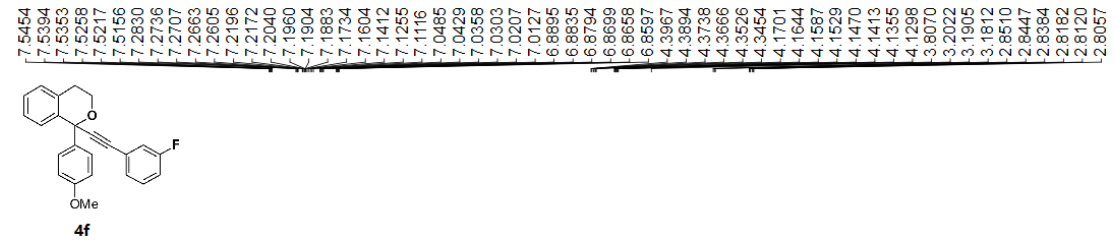
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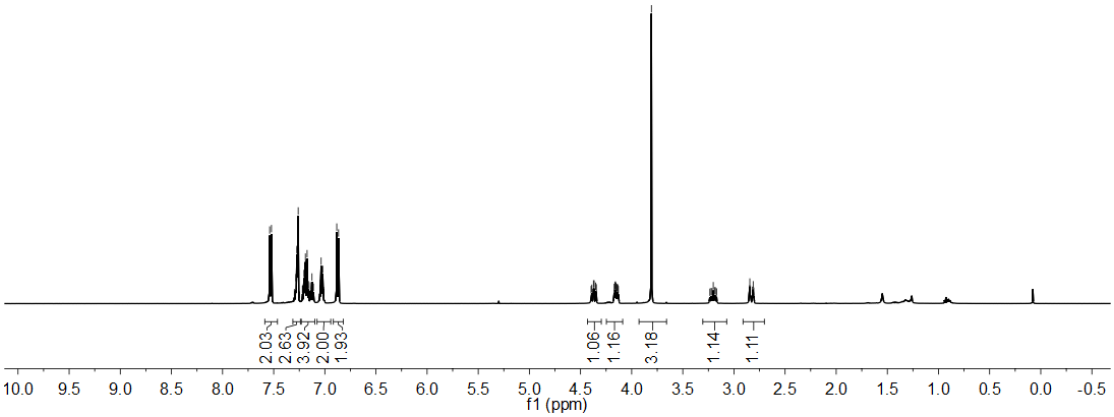
O
F
OMe

4f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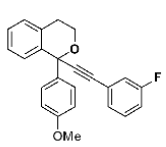
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OMe

4f

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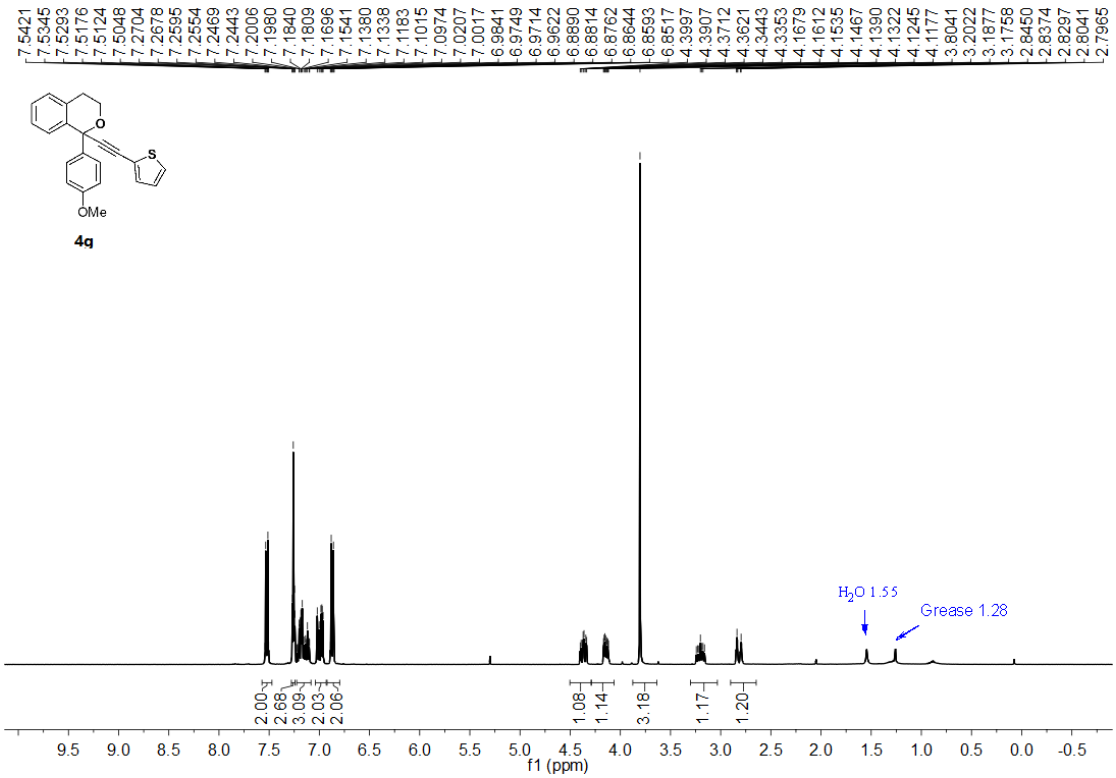
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S
OMe
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H2O 1.55
Grease 1.28
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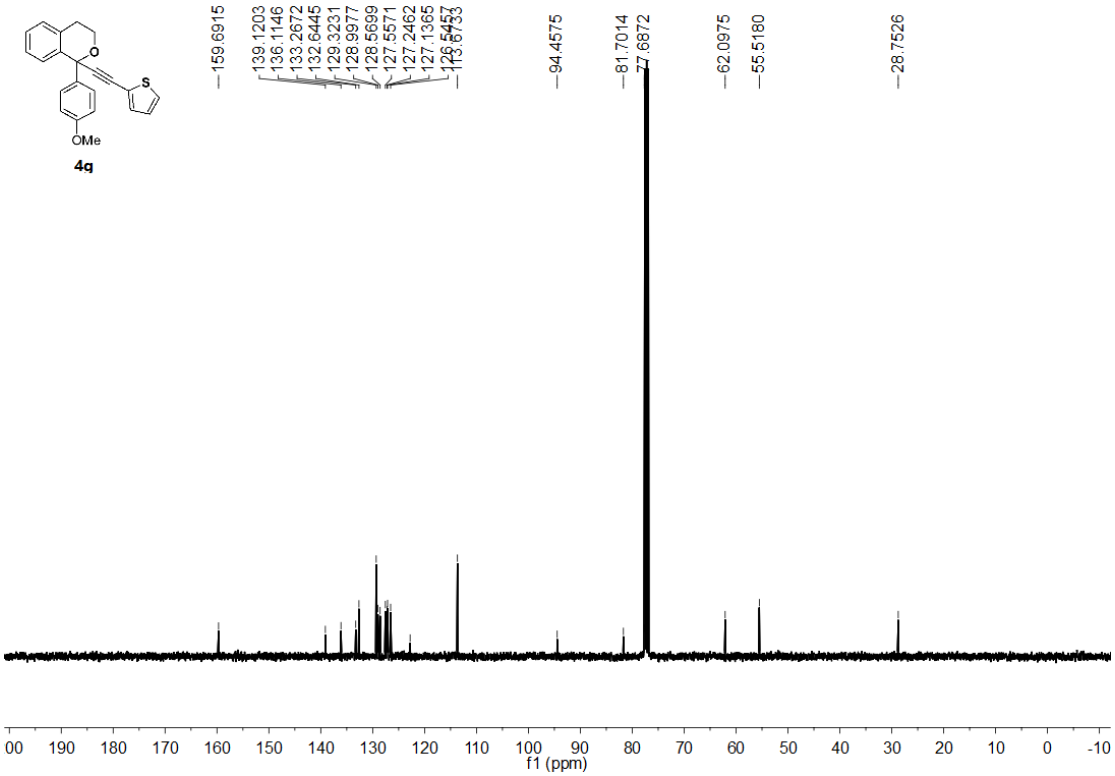
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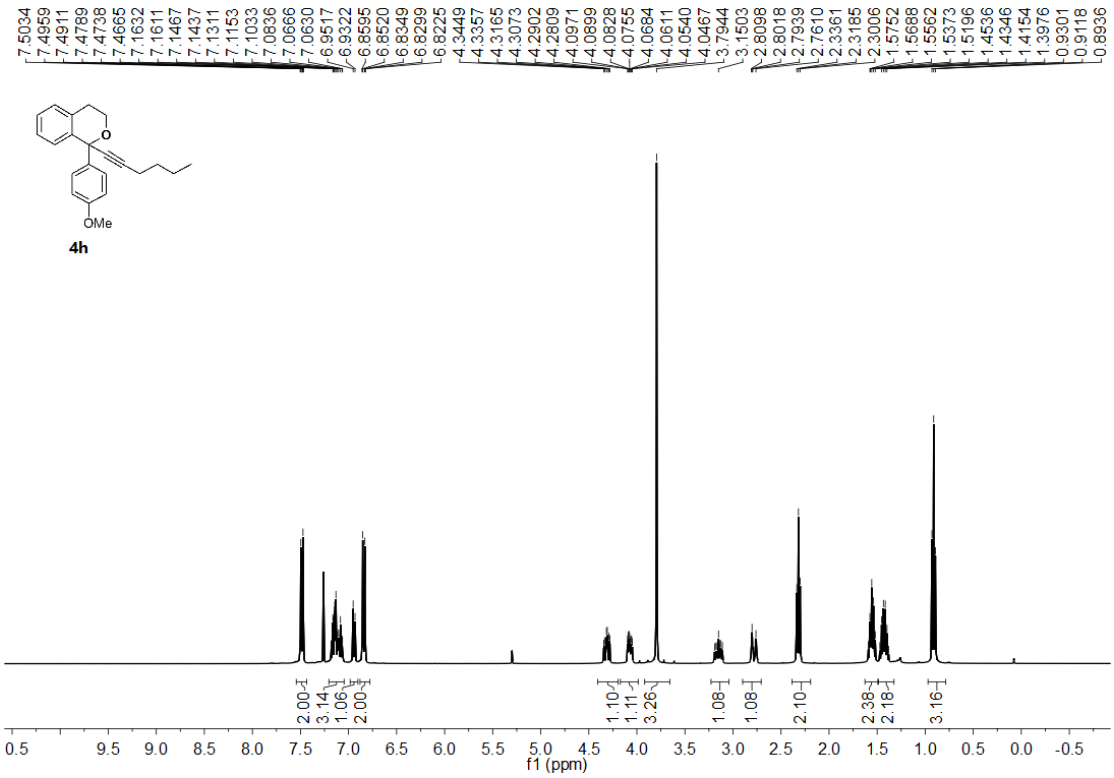
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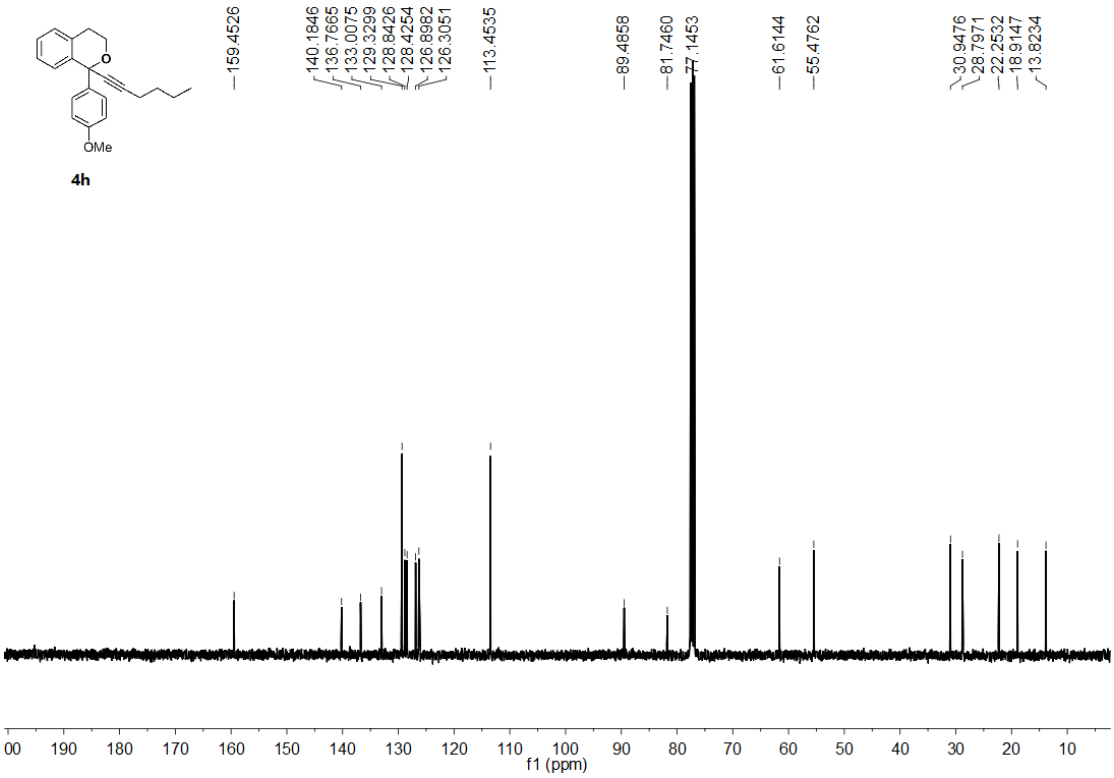
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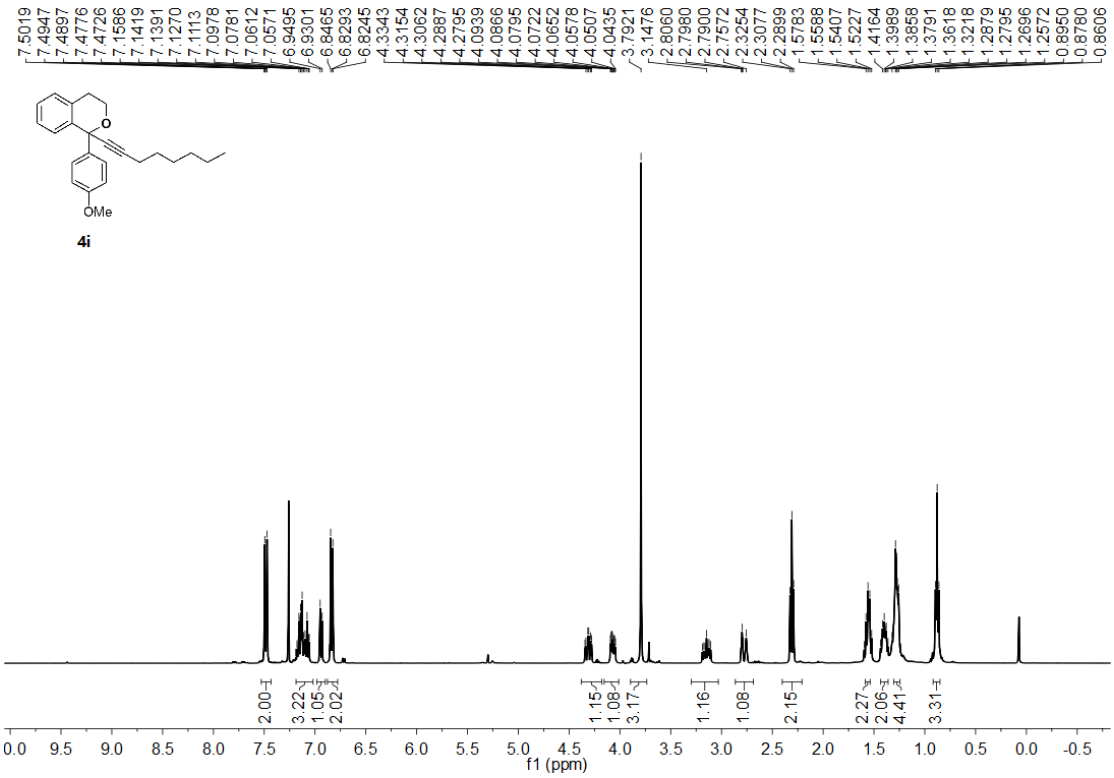
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OMe
4i
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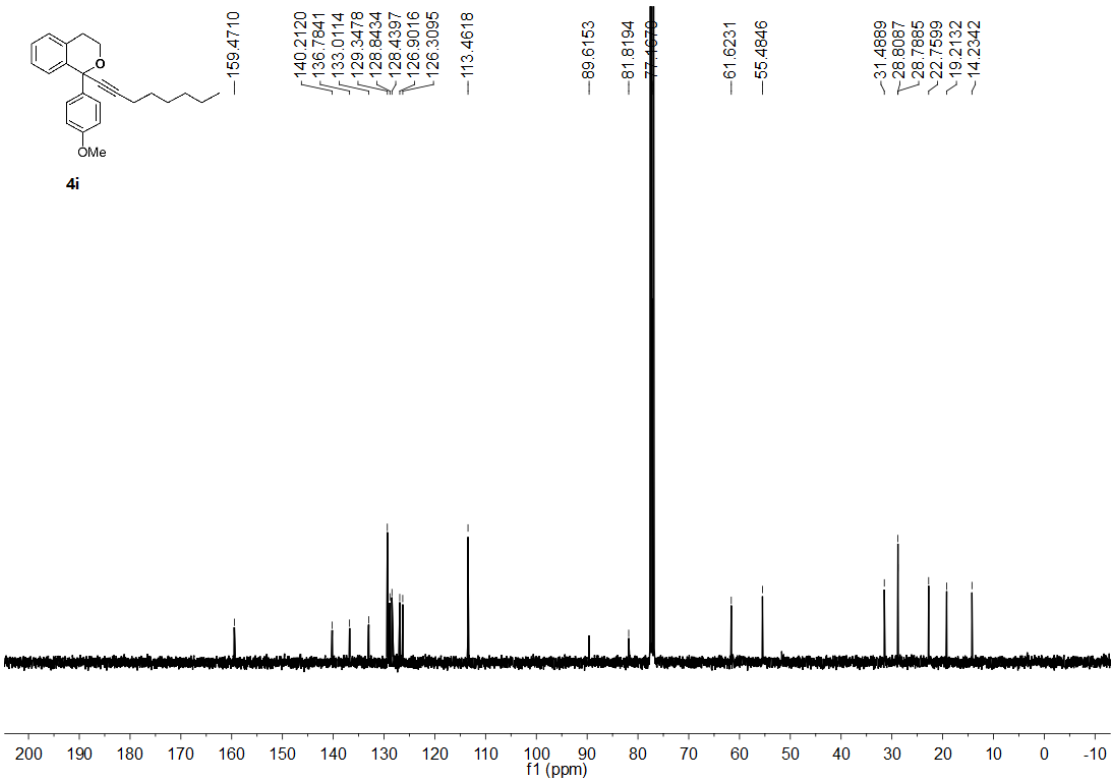
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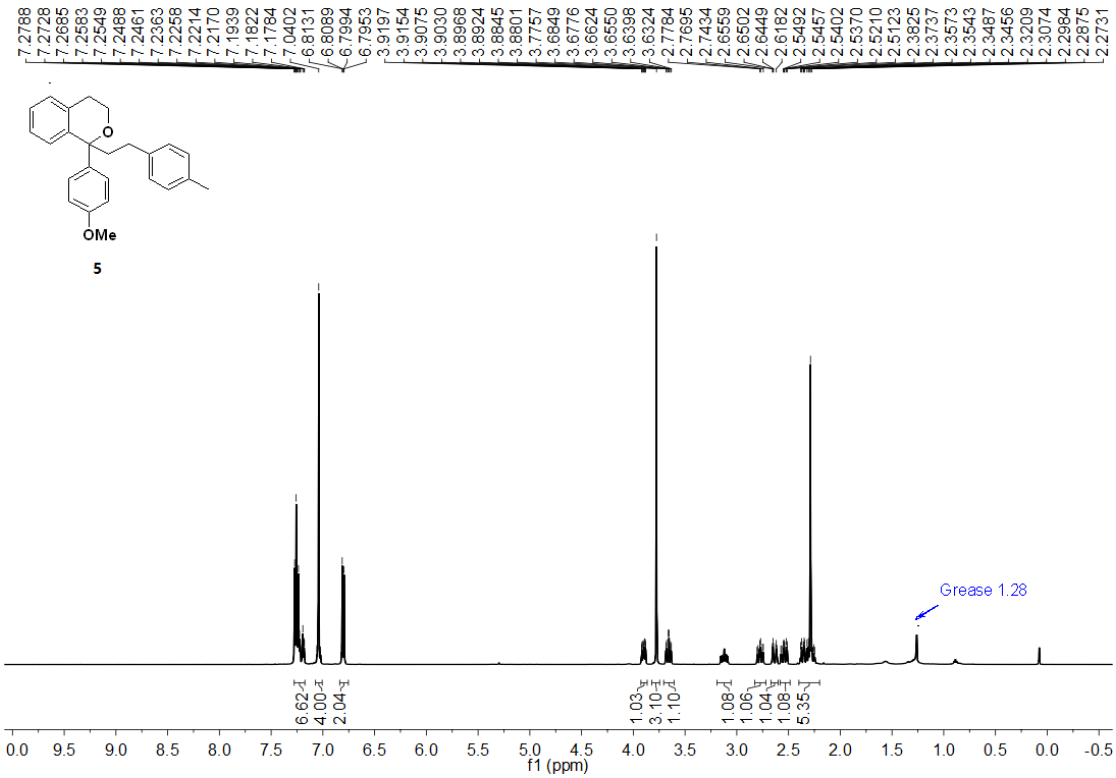
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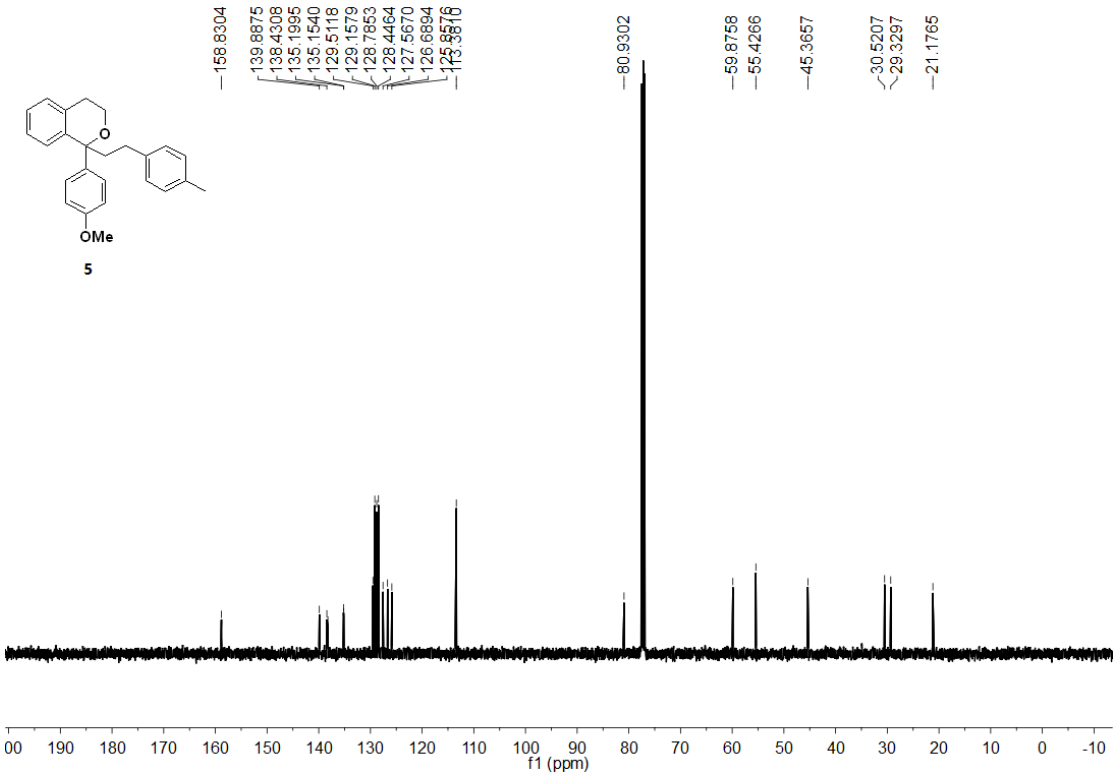
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