Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

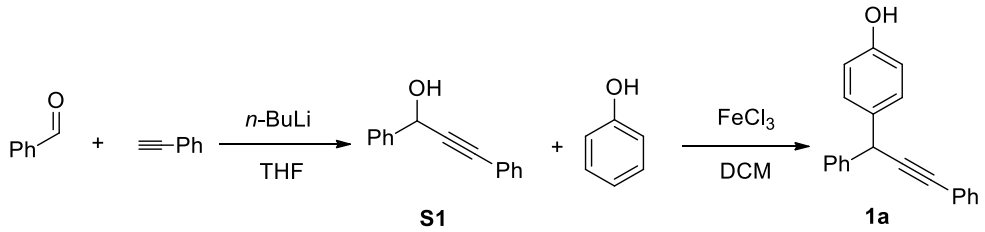
Supporting Information

General information

Proton (^{1}H NMR) and carbon (^{13}C NMR) nuclear magnetic resonance spectra were recorded at 500 MHz and 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: $CDCl_3$ = 7.26 ppm, for ^{13}C NMR: $CDCl_3$ = 77.23, 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. Optical rotations were measured using a 1.0 mL cell with a 10 cm path length on ANTON PAAR MCP 200 polarimeter and concentrations (c) were reported in g×(100 mL)$^{-1}$. Enantiomeric excesses were determined by HPLC using a Daicel Chiralpak AD-H, AS-H or OD-H column with hexane/*i*-PrOH as the eluent.

General procedure

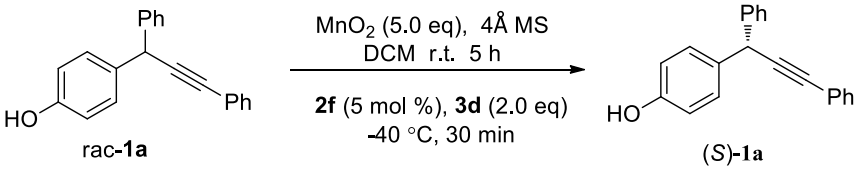
Procedure A: The synthesis of racemic 4-(1,3-diphenylprop-2-yn-1-yl)phenol (*rac*-1a)

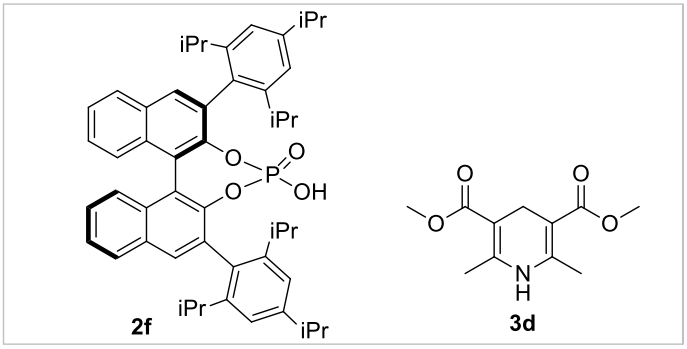


To a solution of phenylacetylene (14.0 mmol, 1.1 equiv) in THF (20 mL) at –78℃ was added *n*-BuLi (2.5 M in n-hexane 5.2 mL, 13.0 mmol, 1.0 equiv) dropwise. After stirring for 1 h at –78℃, benzaldehyde was added at the same temperature and stirred for an additional 0.5 h. After quenching with saturated aq NH_4Cl, the resulting solution was extracted with EtOAc. The organic layer was washed with saturated aq $NaHCO_3$ and brine. After drying over Na_2SO_4, the solvent was removed under vacuum, and the residue was purified by silica gel column chromatography (hexane-EtOAc, 5:1) to give **S1**.

To **S1** (10.0 mmol, 1.0 equiv) in CH_2Cl_2 (10 mL) at room temperature was added phenol (30.0 mmol, 3.0 equiv) and $FeCl_3$ (0.5 mmol, 5 mol %), and the mixture was stirred for 2 h. After concentration, the residue was purified by silica gel chromatography (hexane-EtOAc, 9:1) to give compound **1a**.

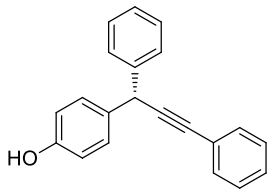
Procedure B: The synthesis of *(S)*-4-(1,3-Diphenylprop-2-yn-1-yl)phenol ((*S*)-1a)





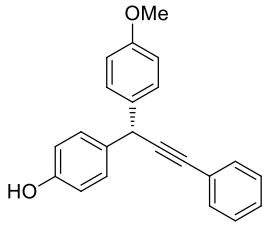
To a solution of rac-**1a** (0.1 mmol, 1.0 equiv.) in anhydrous CH_2Cl_2 (1.0 mL) was added MnO_2 (0.5 mmol, 5.0 eq) and 4 Å MS (20 mg) at room temperature. The reaction was monitored by TLC and upon starting material consumption completely, the mixture was cooled to -40℃, catalyst **2f** (5 mol %) and reductant **3d** (0.2 mol) were added. The mixture was stirred at -40℃ for 30 minutes. After concentration, the residue was purified by silica gel chromatography (hexane-EtOAc, 9:1) to give compound (*S*)-**1a**.

Analytical data



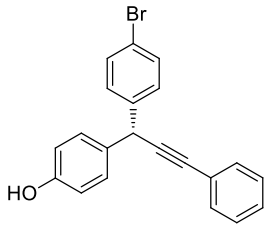
(*S*)-4-(1,3-Diphenylprop-2-yn-1-yl)phenol (1a)

Yield 24.9 mg (88%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-.44 (m, 2H), 7.43-.39 (m, 2H), 7.35-7.25 (m, 7H), 7.24-.20 (m, 1H), 6.76 (d, *J* = 8.6 Hz, 2H), 5.14 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.6, 142.2, 134.3, 131.9, 129.3, 128.8, 128.4, 128.2, 128.0, 127.0, 123.7, 115.6, 90.7, 84.9, 43.1. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 9.5 min (minor), 15.6 min (major). ee = 97%. HRMS (EI) Calcd for $C_{21}H_{17}O$ $(M + H)^+$: 285.1274, Found: 285.1282. $[\alpha]_D^{25}$: -36.3 (c = 1.0, $CHCl_3$).



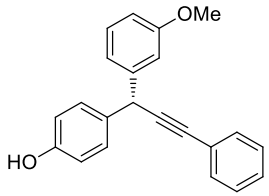
(*R*)-4-(1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-yl)phenol (1b)

Yield 28.2 mg (90%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.41 (m, 1H), 7.37-7.25 (m, 3H), 6.89-6.82 (m, 1H), 6.80-6.74 (m, 1H), 5.11 (s, 1H), 4.96 (s, 1H), 3.78 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.6, 154.6, 134.6, 134.5, 131.9, 129.2, 129.0, 128.4, 128.1, 123.8, 115.6, 114.2, 90.9, 84.8, 55.5, 42.3. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 12.2 min (minor), 22.6 min (major). ee = 94%. HRMS (EI) Calcd for $C_{22}H_{19}O_2$ $(M + H)^+$: 315.1380, Found: 315.1369. $[\alpha]_D^{25}$: -34.1(c = 1.0, $CHCl_3$).



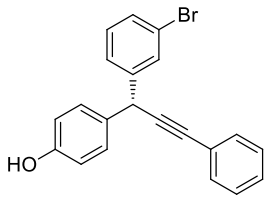
(*R*)-4-(1-(4-Bromophenyl)-3-phenylprop-2-yn-1-yl)phenol (1c)

Yield 31.4 mg (87%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49-7.40 (m, 4H), 7.34-7.22 (m, 7H), 6.78 (d, *J* = 8.4 Hz, 2H), 5.10 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.7, 141.3, 133.7, 131.9, 131.8, 129.7, 129.3, 128.5, 128.3, 123.4, 120.9, 115.7, 89.9, 85.3, 42.5. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 9.3 min (minor), 16.4 min (major). ee = 92%. HRMS (EI) Calcd for $C_{21}H_{16}BrO$ $(M + H)^+$: 363.0379, Found: 363.0378. $[\alpha]_D$ ^{25}: -36.3 (c = 1.0, $CHCl_3$).



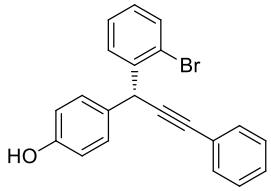
(*R*)-4-(1-(3-Methoxyphenyl)-3-phenylprop-2-yn-1-yl)phenol (1d)

Yield 26.6 mg (85%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 3.4 Hz, 2H), 7.34 (d, *J* = 7.5 Hz, 5H), 7.28 (t, *J* = 7.9 Hz, 1H), 7.05 (s, 2H), 6.82 (t, *J* = 7.9 Hz, 3H), 5.17 (s, 1H), 5.03 (s, 1H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 154.6, 143.8, 134.1, 131.8, 129.8, 129.3, 128.4, 128.2, 123.7, 120.5, 115.6, 114.0, 112.2, 90.5, 84.9, 55.4, 43.1. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.7 min (minor), 22.3 min (major). ee = 91%. HRMS (EI) Calcd for $C_{22}H_{19}O_2$ $(M + H)^+$: 315.1380, Found: 315.1386. $[\alpha]_D$ ^{25}: -30.9 (c = 1.0, $CHCl_3$).



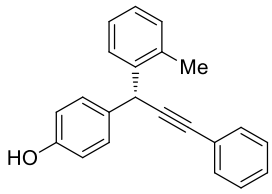
(*R*)-4-(1-(3-Bromophenyl)-3-phenylprop-2-yn-1-yl)phenol (1e)

Yield 29.3 mg (81%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (t, *J* = 1.7 Hz, 1H), 7.51-7.46 (m, 2H), 7.40-7.27 (m, 7H), 7.20 (t, *J* = 7.8 Hz, 1H), 6.83-6.77 (m, 2H), 5.13 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.8, 144.5, 133.5, 131.9, 131.0, 130.3, 130.2, 129.3, 128.5, 128.4, 126.7, 123.4, 122.8, 115.8, 89.7, 85.5, 42.7. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.7 min (minor), 24.4 min (major). ee = 92%. HRMS (EI) Calcd for $C_{21}H_{16}BrO$ (M + H): 363.0379, Found: 363.0366. $[\alpha]_D^{25}$: -39.2 (c = 1.0, $CHCl_3$).



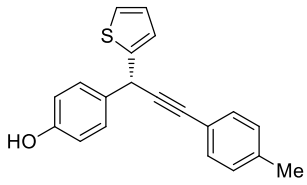
(*S*)-4-(1-(2-Bromophenyl)-3-phenylprop-2-yn-1-yl)phenol (1f)

Yield 30.7 mg (82%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.55 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.48-7.43 (m, 2H), 7.34-7.26 (m, 6H), 7.10 (td, *J* = 7.8, 1.7 Hz, 1H), 6.82-6.71 (m, 2H), 5.66 (s, 1H), 4.85 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.6, 141.4, 133.2, 132.9, 131.9, 130.5, 129.4, 128.8, 128.4, 128.3, 128.1, 124.0, 123.5, 115.6, 90.1, 84.7, 42.2. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.6 min (minor), 9.9 min (major). ee = 89%. HRMS (EI) Calcd for $C_{21}H_{16}BrO$ $(M + H)^+$: 363.0379, Found: 363.0370. $[\alpha]_D^{25}$: -29.3 (c = 1.0, $CHCl_3$).



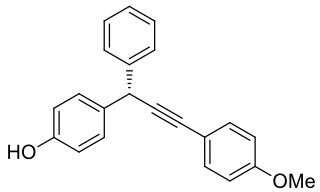
(*S*)-4-(3-Phenyl-1-(o-tolyl)prop-2-yn-1-yl)phenol (1g)

Yield 25.9 mg (87%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53-7.42 (m, 3H), 7.32-7.15 (m, 8H), 6.80-6.71 (m, 2H), 5.32 (s, 1H), 4.69 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.4, 139.8, 136.1, 133.3, 131.8, 130.9, 129.4, 128.9, 128.4, 128.1, 127.3, 126.5, 123.8, 115.5, 90.6, 84.6, 40.2, 19.8. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 7.5 min (minor), 14.2 min (major). ee = 86%. HRMS (EI) Calcd for $C_{22}H_{19}O$ $(M + H)^+$: 299.1430, Found: 299.1444. $[\alpha]_D^{25}$: -37.6(c = 1.0, $CHCl_3$).



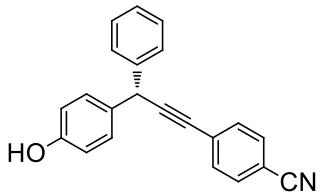
(*S*)-4-(1-(Thiophen-2-yl)-3-(p-tolyl)prop-2-yn-1-yl)phenol (1h)

Yield 26.4 mg (87%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32-7.25 (m, 4H), 7.11 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.04 (d, *J* = 7.9 Hz, 2H), 6.92-6.89 (m, 1H), 6.85 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.76-6.69 (m, 2H), 5.28 (s, 1H), 4.65 (s, 1H), 2.27 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 146.6, 138.4, 134.0, 131.8, 129.2, 126.8, 125.1, 124.9, 120.3, 115.7, 89.2, 84.5, 38.6, 21.7. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 15% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 12.0 min (minor), 25.6 min (major). ee = 79%. HRMS (EI) Calcd for $C_{20}H_{17}OS$ $(M + H)^+$: 305.0995, Found: 305.0998. $[\alpha]_D^{25}$: -29.3 (c = 1.0, $CHCl_3$).



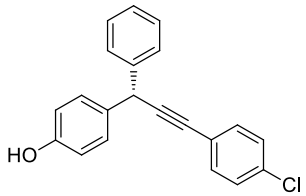
(*S*)-4-(3-(4-Methoxyphenyl)-1-phenylprop-2-yn-1-yl)phenol (1i)

Yield 28.2 mg (90%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45-7.41 (m, 4H), 7.34-7.28 (m, 4H), 7.25-7.21 (m, 1H), 6.86-6.82 (m, 2H), 6.81-6.77 (m, 2H), 5.14 (s, 1H), 4.95 (s, 1H), 3.81 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.5, 154.6, 142.4, 134.5, 133.2, 129.3, 128.8, 128.0, 127.0, 115.9, 115.6, 114.1, 89.1, 84.7, 55.5, 43.1. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 14.7 min (minor), 26.9 min (major). ee = 97%. HRMS (EI) Calcd for $C_{22}H_{19}O_2$ $(M + H)^+$: 315.1380, Found: 315.1378. $[\alpha]_D$ ^{25}: -38.3 (c = 1.0, $CHCl_3$).



(*S*)-4-(3-(4-Hydroxyphenyl)-3-phenylprop-1-yn-1-yl)benzonitrile (1j)

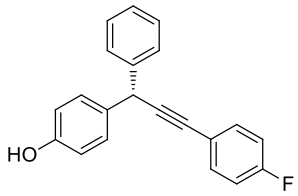
Yield 26.2 mg (85%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62-7.57 (m, 2H), 7.56-7.52 (m, 2H), 7.42-7.37 (m, 2H), 7.36-7.31 (m, 2H), 7.29-7.24 (m, 3H), 6.84-6.78 (m, 2H), 5.18 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 141.4, 133.4, 132.4, 132.2, 129.3, 128.9, 128.7, 127.9, 127.3, 118.7, 115.8, 111.4, 95.6, 83.4, 43.1. HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.4 min (major), 14.7 min (minor). ee = 95%. HRMS (EI) Calcd for $C_{22}H_{16}NO$ $(M + H)^+$: 310.1226, Found: 310.1233. $[\alpha]_D^{25}$: -35.4 (c = 1.0, $CHCl_3$).



(*S*)-4-(3-(4-Chlorophenyl)-1-phenylprop-2-yn-1-yl)phenol (1k)

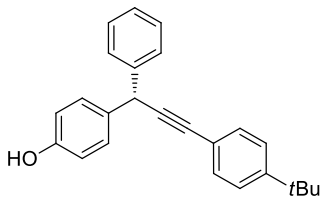
Yield 27.3 mg (86%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45-7.36 (m, 4H), 7.35-7.30 (m, 2H), 7.29-7.21 (m, 5H), 6.78 (d, *J* = 8.4 Hz, 2H), 5.14 (s, 1H), 4.85 (s, 1H).; ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.7, 142.0, 134.1, 134.0, 133.1, 129.3, 128.8, 128.7, 128.0, 127.1, 122.2, 115.7, 91.7, 83.8, 43.1. HPLC analysis of the product: Daicel

CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 10.9 min (minor), 21.1 min (major). ee = 96% HRMS (EI) Calcd for $C_{21}H_{16}ClO$ (M + H)$^+$: 319.0884, Found: 318.0888. $[\alpha]_D^{25}$: -38.3 (c = 1.0, $CHCl_3$).



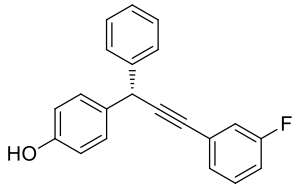
(*S*)-4-(3-(4-Fluorophenyl)-1-phenylprop-2-yn-1-yl)phenol (1l)

Yield 25.1 mg (83%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47-7.38 (m, 4H), 7.35-7.21 (m, 5H), 7.03-6.95 (m, 2H), 6.82-6.75 (m, 2H), 5.14 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.8, 161.3, 154.6, 142.1, 134.2, 133.7, 133.7, 129.3, 128.8, 128.0, 127.1, 119.8, 119.7, 115.8, 115.6, 115.6, 90.3, 83.9, 43.1. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.1 min (minor), 19.9 min (major). ee = 96%. HRMS (EI) Calcd for $C_{21}H_{16}FO$ (M + H)$^+$: 303.1180, Found: 303.1186. $[\alpha]_D^{25}$: -39.7 (c = 1.0, $CHCl_3$).



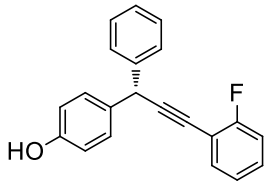
(*S*)-4-(3-(4-(tert-Butyl)phenyl)-1-phenylprop-2-yn-1-yl)phenol (1m)

Yield 29.9 mg (88%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.43 (m, 4H), 7.38-7.31 (m, 6H), 7.29-7.22 (m, 1H), 6.82-6.74 (m, 2H), 5.18 (s, 1H), 1.35 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.5, 151.4, 142.4, 134.5, 131.6, 129.3, 128.8, 128.0, 127.0, 125.4, 120.7, 115.6, 89.9, 85.0, 43.1, 34.9, 31.4. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 15% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 7.6 min (minor), 13.3 min (major). ee = 94%. HRMS (EI) Calcd for $C_{25}H_{25}O$ (M + H)$^+$: 341.1900, Found: 341.1907. $[\alpha]_D^{25}$: -32.3 (c = 1.0, $CHCl_3$).



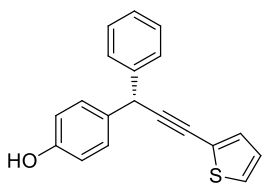
(*S*)-4-(3-(3-Fluorophenyl)-1-phenylprop-2-yn-1-yl)phenol (1n)

Yield 24.8 mg (82%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.3 Hz, 2H), 7.36-7.30 (m, 2H), 7.30-7.22 (m, 5H), 7.19-7.14 (m, 1H), 7.05-6.96 (m, 1H), 6.85-6.71 (m, 2H), 5.15 (s, 1H), 4.76 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.5, 161.6, 154.7, 141.9, 134.0, 130.0, 129.9, 129.3, 128.9, 128.0, 127.8, 127.7, 127.2, 125.6, 125.5, 118.8, 118.6, 115.7, 115.6, 115.5, 91.7, 83.8, 43.1. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 15% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.6 min (minor), 19.7 min (major). ee = 91%. HRMS (EI) Calcd for $C_{21}H_{16}FO$ $(M + H)^+$: 303.1180, Found: 302.1182. $[\alpha]_D^{25}$: -39.8 (c = 1.0, $CHCl_3$).



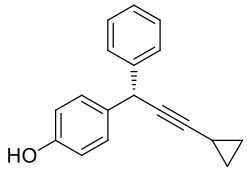
(*S*)-4-(3-(2-Fluorophenyl)-1-phenylprop-2-yn-1-yl)phenol (1o)

Yield 25.4 mg (84%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.32 (m, 1H), 7.28-7.21 (m, 1H), 7.20-7.12 (m, 1H), 7.05-6.96 (m, 1H), 6.76-6.63 (m, 1H), 5.11 (s, 1H), 4.75 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.2, 162.2, 154.6, 141.9, 134.1, 133.7, 129.9, 129.8, 129.3, 128.8, 128.0, 127.1, 124.0, 124.0, 115.7, 115.7, 115.5, 112.3, 112.2, 96.0, 96.0, 78.4, 43.3. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 15% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.5 min (minor), 17.4 min (major). ee = 96%. HRMS (EI) Calcd for $C_{21}H_{16}FO$ $(M + H)^+$: 303.1180, Found: 303.1184. $[\alpha]_D^{25}$: -30.1 (c = 1.0, $CHCl_3$).



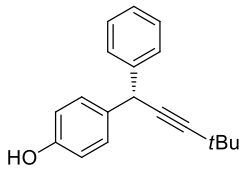
(*S*)-4-(1-Phenyl-3-(thiophen-2-yl)prop-2-yn-1-yl)phenol (1p)

Yield 25.5 mg (88%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43-7.37 (m, 2H), 7.36-7.30 (m, 2H), 7.30-7.23 (m, 4H), 7.23-7.18 (m, 2H), 6.96 (dd, *J* = 5.2, 3.6 Hz, 1H), 6.82-6.73 (m, 2H), 5.18 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.7, 141.8, 134.0, 131.8, 129.4, 128.8, 128.0, 127.1, 127.1, 126.7, 123.7, 115.6, 94.5, 78.1, 43.3. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 15% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.2 min (minor), 19.3 min (major). ee = 96%. HRMS (EI) Calcd for $C_{19}H_{15}OS$ $(M + H)^+$: 291.0838, Found: 291.0846. $[\alpha]_D^{25}$: -34.1 (c = 1.0, $CHCl_3$).



(*S*)-4-(3-Cyclopropyl-1-phenylprop-2-yn-1-yl)phenol (1q)

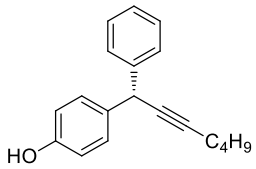
Yield 18.6 mg (75%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29-7.17 (m, 4H), 7.14-7.06 (m, 3H), 6.70-6.58 (m, 2H), 4.79 (s, 1H), 4.77 (s, 1H), 1.26-1.19 (m, 1H), 0.71-0.64 (m, 2H), 0.64-0.57 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.4, 142.8, 135.0, 129.2, 128.7, 127.9, 126.8, 115.5, 88.2, 76.3, 42.6, 8.4, -0.04. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 10% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 12.0 min (minor), 12.6 min (major). ee = 90%. HRMS (EI) Calcd for $C_{18}H_{17}O$ $(M + H)^+$: 249.1274, Found: 248.1273. $[\alpha]_D^{25}$: -27.8 (c = 1.0, $CHCl_3$).



(*S*)-4-(4,4-Dimethyl-1-phenylpent-2-yn-1-yl)phenol (1r)

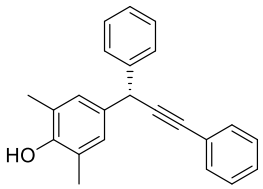
Yield 19.0 mg (72%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.4 Hz, 2H), 7.24-7.08 (m, 5H), 6.67 (d, *J* = 8.4 Hz, 2H), 4.80 (s, 1H), 4.58 (s, 1H), 1.20 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.3, 143.1, 135.3, 129.1, 128.6, 127.9, 126.7, 115.4, 93.7, 79.5, 42.5, 31.5, 27.8. HPLC analysis of the product: Daicel CHIRALPAK

AS-H column; 5% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 9.0 min (minor), 11.1 min (major). ee = 90%. HRMS (EI) Calcd for $C_{19}H_{21}O$ $(M + H)^+$: 265.1587, Found: 265.1585. $[\alpha]_D^{25}$: -25.3 (c = 1.0, $CHCl_3$).



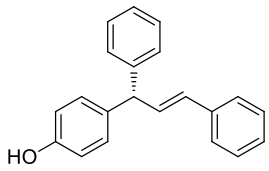
(*S*)-4-(1-Phenylhept-2-yn-1-yl)phenol (1s)

Yield 22.6 mg (79%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-6.98 (m, 7H), 6.68 (d, *J* = 8.4 Hz, 2H), 4.83 (s, 1H), 4.68 (s, 1H), 2.20 (t, *J* = 6.1 Hz, 2H), 1.51-1.42 (m, 2H), 1.42-1.32 (m, 2H), 0.85 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.4, 142.9, 135.1, 129.2, 128.7, 127.9, 126.8, 115.5, 85.2, 80.9, 42.6, 31.3, 22.2, 18.9, 13.8. HPLC analysis of the product: Daicel CHIRALPAK AS-H column; 10% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.8 min (minor), 7.5 min (major). ee = 92%. HRMS (EI) Calcd for $C_{19}H_{21}O$ $(M + H)^+$: 265.1587, Found: 264.1595. $[\alpha]_D^{25}$: -22.2 (c = 1.0, $CHCl_3$).



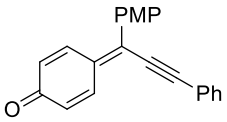
(*S*)-4-(1,3-Diphenylprop-2-yn-1-yl)-2,6-dimethylphenol (1t)

Yield 24.3 mg (78%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51-7.42 (m, 4H), 7.35-7.27 (m, 5H), 7.26-7.20 (m, 1H), 7.04 (s, 2H), 5.10 (s, 1H), 2.22 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.3, 142.4, 133.6, 131.9, 128.8, 128.4, 128.2, 128.1, 128.0, 126.9, 123.88, 123.3, 90.9, 84.8, 43.2, 16.2. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 5.9 min (major 6.4 min (minor),). ee = 80%. HRMS (EI) Calcd for $C_{23}H_{21}O$ $(M + H)^+$: 313.1587, Found: 313.1581. $[\alpha]_D^{25}$: -9.2 (c = 1.0, $CHCl_3$).



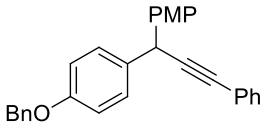
(*S*,*E*)-4-(1,3-Diphenylallyl)phenol (4)

Yield 22.8 mg (80%), ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31-7.27 (m, 2H), 7.26-7.18 (m, 4H), 7.17-7.10 (m, 4H), 7.06-6.97 (m, 2H), 6.73-6.64 (m, 2H), 6.56 (dd, *J* = 15.8, 7.5 Hz, 1H), 6.25 (d, *J* = 15.8 Hz, 1H), 4.76 (d, *J* = 7.5 Hz, 1H), 4.66 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.2, 143.9, 137.5, 136.0, 133.1, 131.4, 130.0, 128.8, 128.7, 128.7, 127.5, 126.6, 126.5, 115.5, 53.5. HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 10.6 min (minor), 14.2 min (major). ee = 90%. HRMS (EI) Calcd for $C_{21}H_{19}O$ $(M + H)^+$: 287.1430, Found: 286.1432. $[\alpha]_D^{25}$: -25.1 (c = 1.0, $CHCl_3$).



4-(1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-ylidene)cyclohexa-2,5-dienone (8)

Yield 24.3 mg (80%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 9.9, 2.6 Hz, 1H), 7.60-7.53 (m, 4H), 7.52 (dd, *J* = 10.0, 2.7 Hz, 1H), 7.45-7.38 (m, 3H), 7.04-6.99 (m, 2H), 6.56 (dd, *J* = 9.9, 2.0 Hz, 1H), 6.41 (dd, *J* = 10.0, 2.0 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.4, 161.6, 139.1, 138.8, 136.8, 134.1, 132.5, 132.2, 130.2, 129.4, 129.1, 128.8, 128.5, 122.1, 114.3, 108.4, 90.3, 55.7. HRMS (EI) Calcd for $C_{22}H_{17}O_2$ $(M + H)^+$: 313.1223, Found: 313.1230.



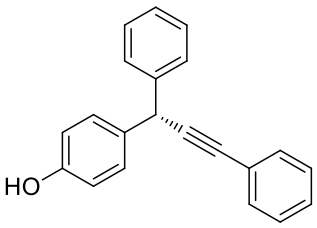
1-(Benzyloxy)-4-(1-(4-methoxyphenyl)-3-phenylprop-2-yn-1-yl)benzene (9)

Yield 37.2 mg (92%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53-7.49 (m, 2H), 7.47-7.43 (m, 2H), 7.43-7.30 (m, 10H), 6.97 (dd, *J* = 8.8, 2.3 Hz, 2H), 6.89 (dd, *J* = 8.8, 2.2 Hz, 2H),

5.16 (s, 1H), 5.07 (s, 2H), 3.81 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.6, 157.8, 137.2, 134.7, 134.4, 131.8, 129.0, 128.7, 128.4, 128.1, 128.0, 127.6, 123.7, 115.0, 114.1, 90.9, 84.7, 70.2, 55.4, 42.3. HRMS (EI) Calcd for $C_{29}H_{25}O_2$ $(M + H)^+$: 405.1849, Found: 405.1855.

Absolute stereochemistry determination

The absolute stereochemistry of the compound (**1a**) was determined by comparing with known compound.[1]

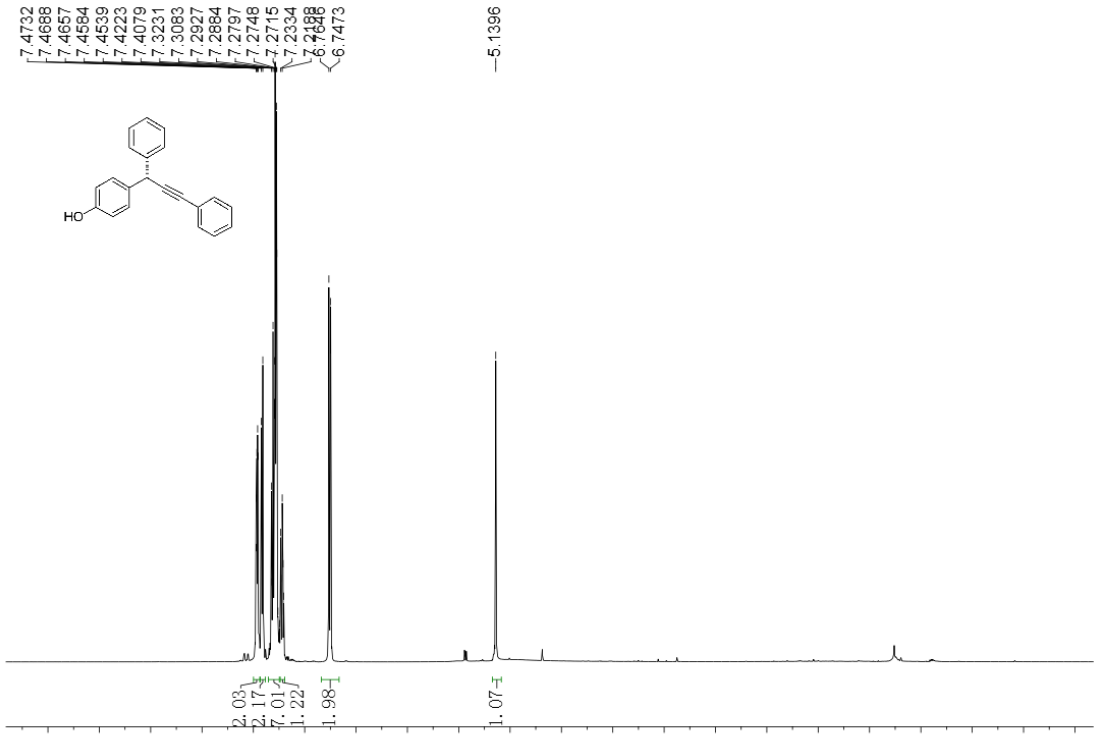


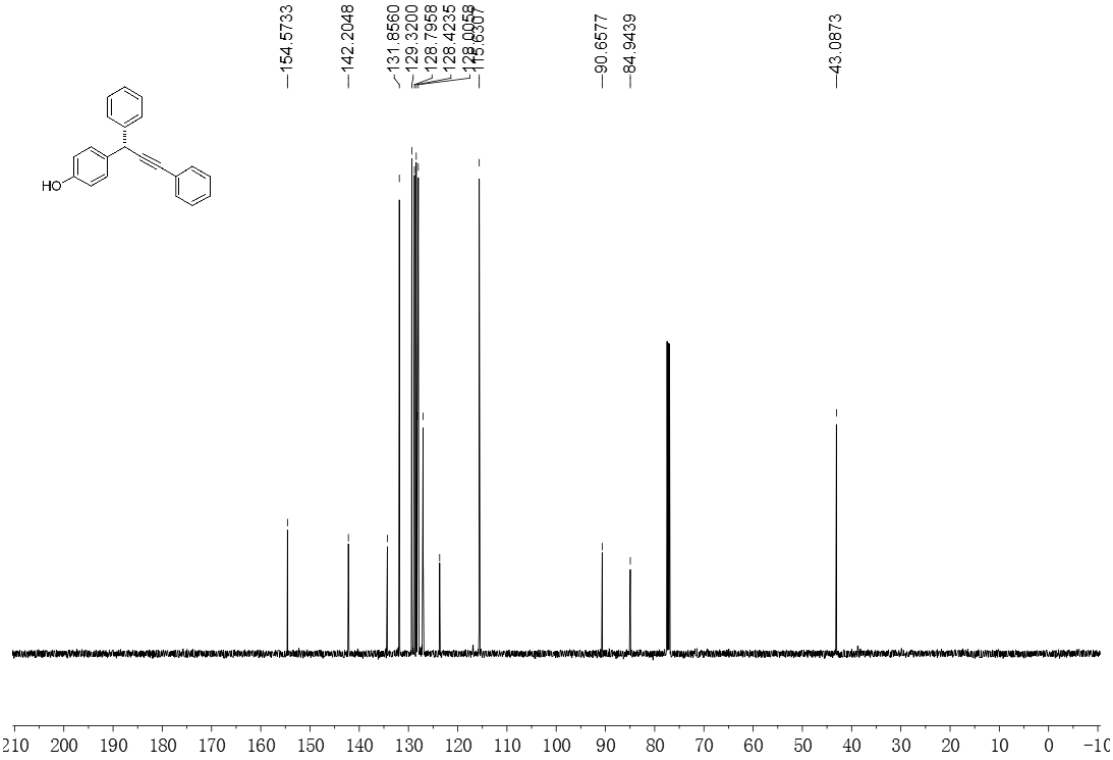
1a (*S*)-4-(1,3-diphenylprop-2-yn-1-yl)phenol

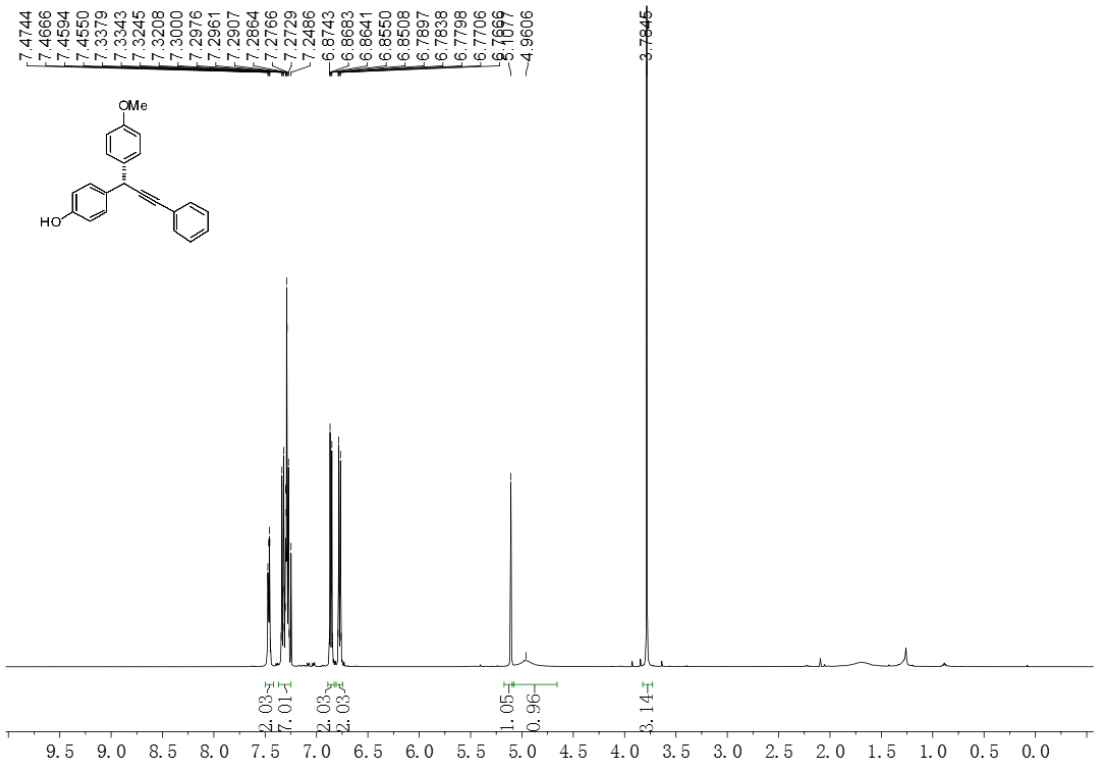
Reference

[1] M. Chen, J. Sun, *Angew. Chem. Int. Ed.* **2017**, *129*, 12128.

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



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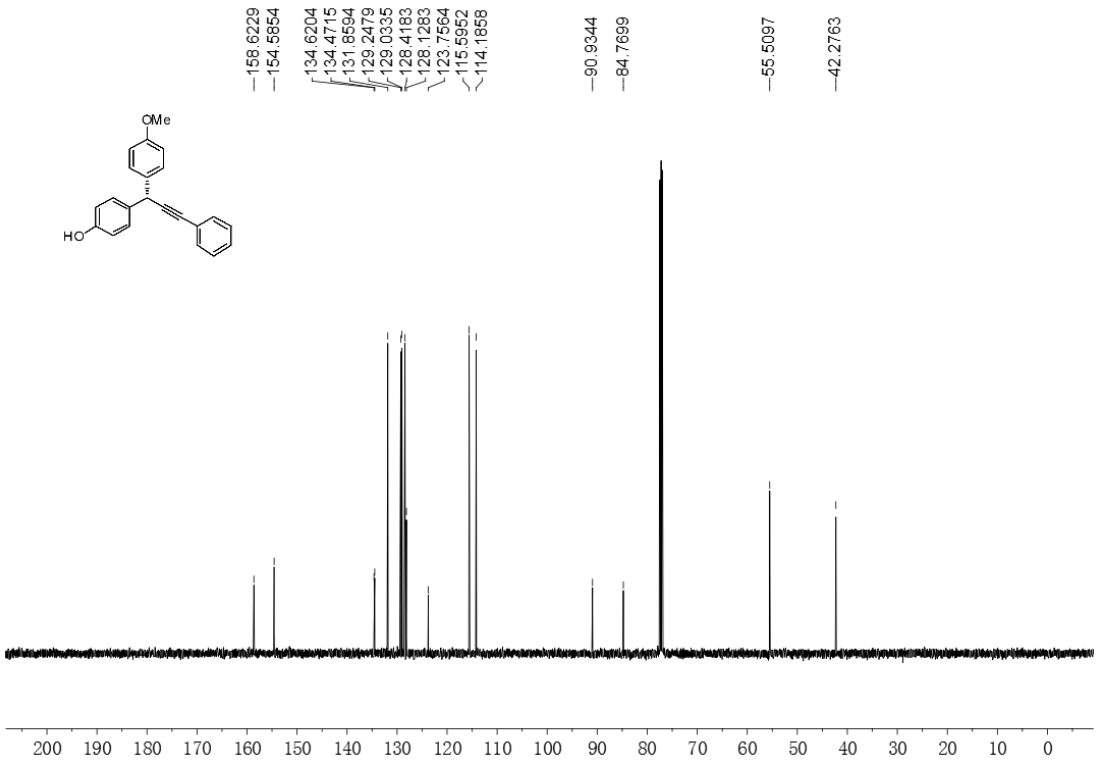
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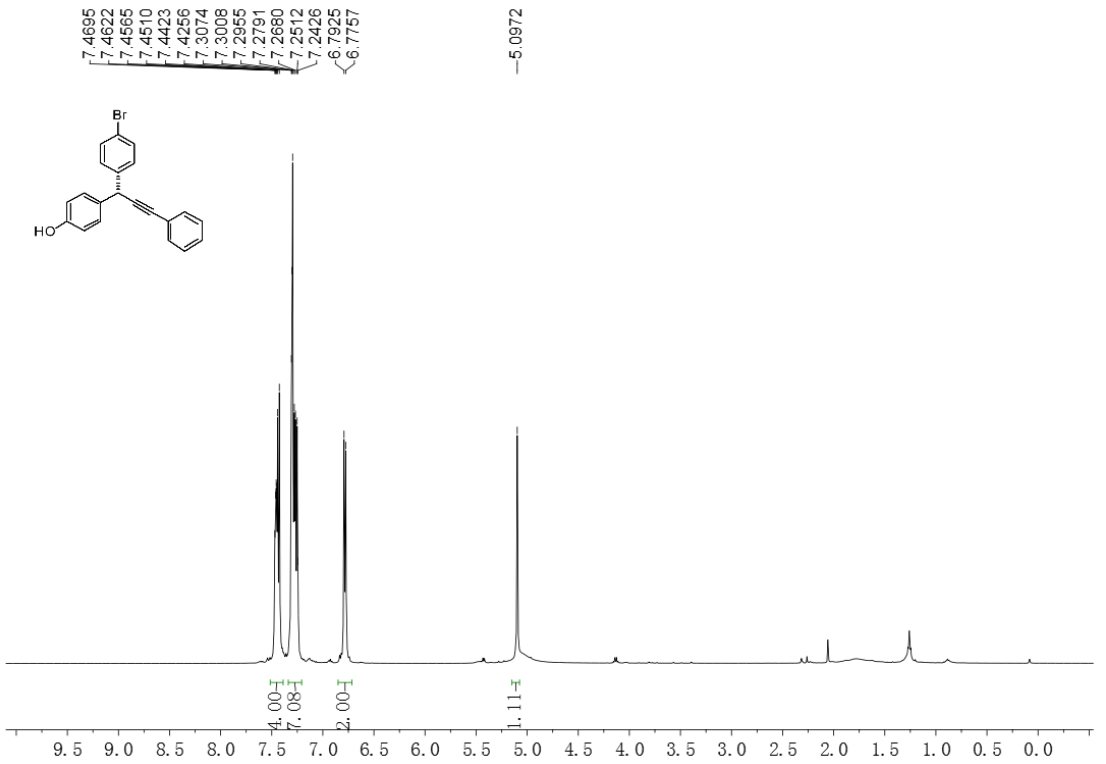
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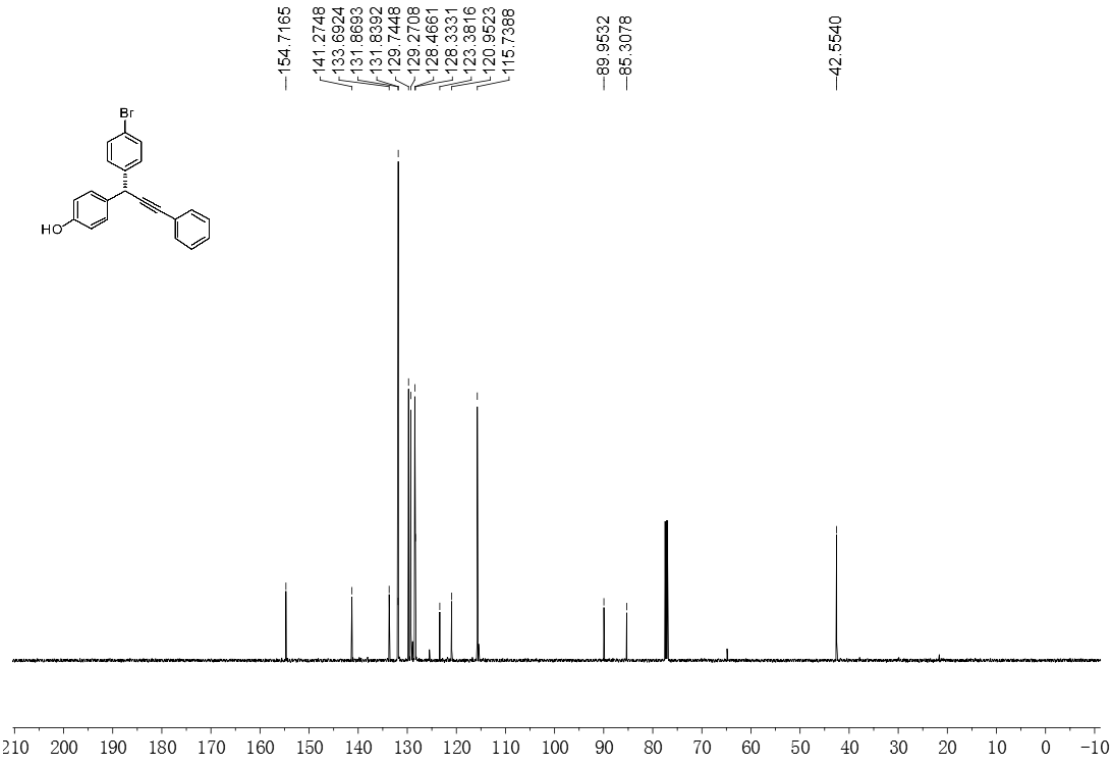
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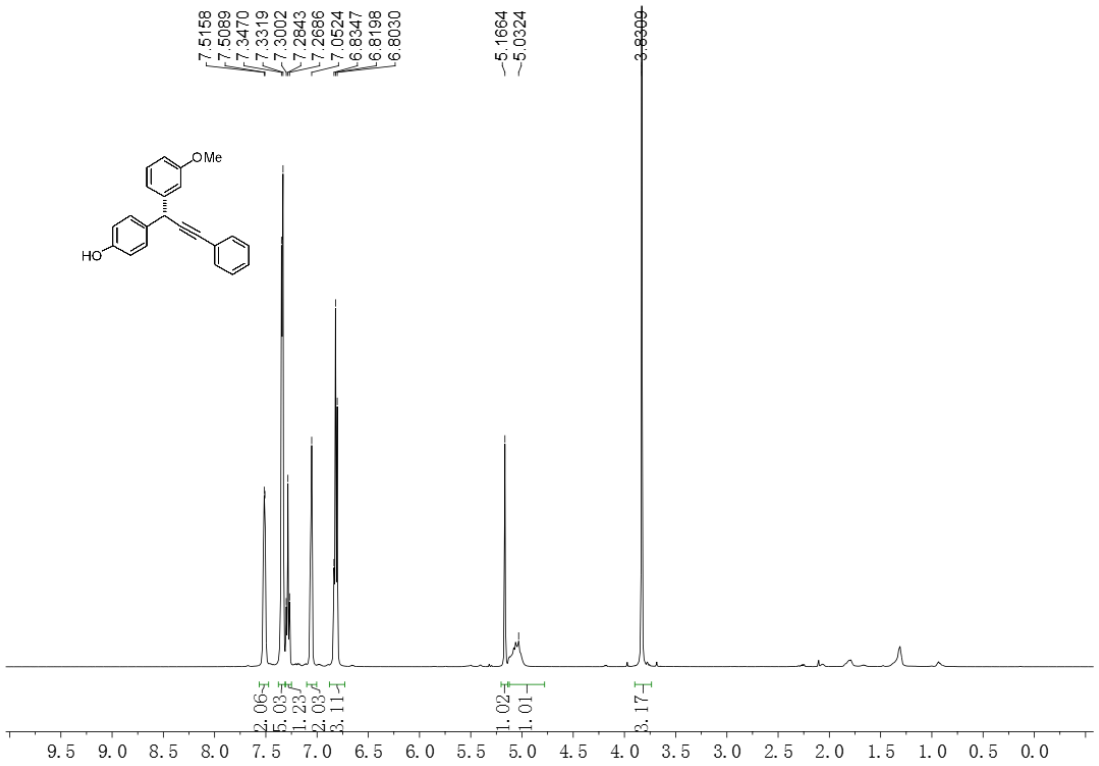
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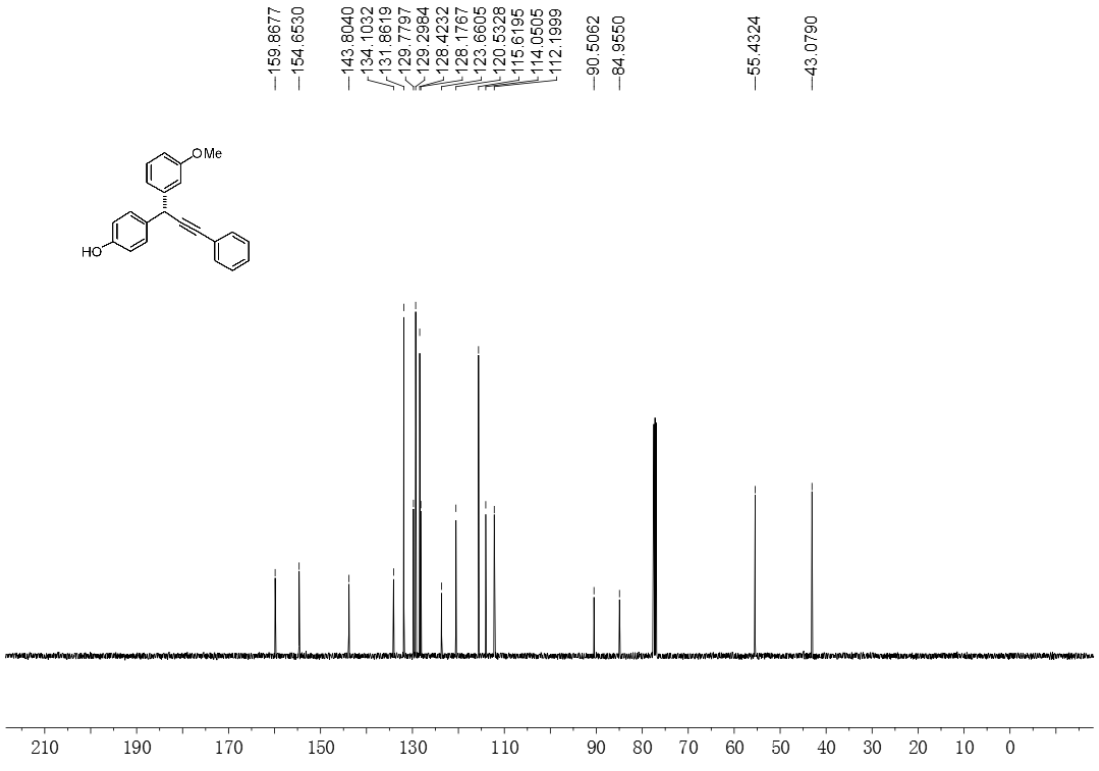
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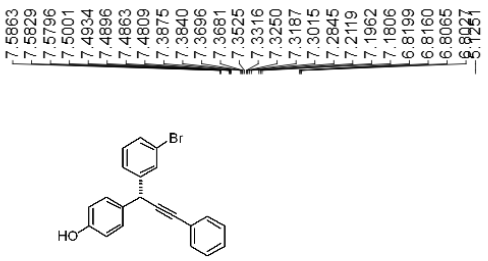
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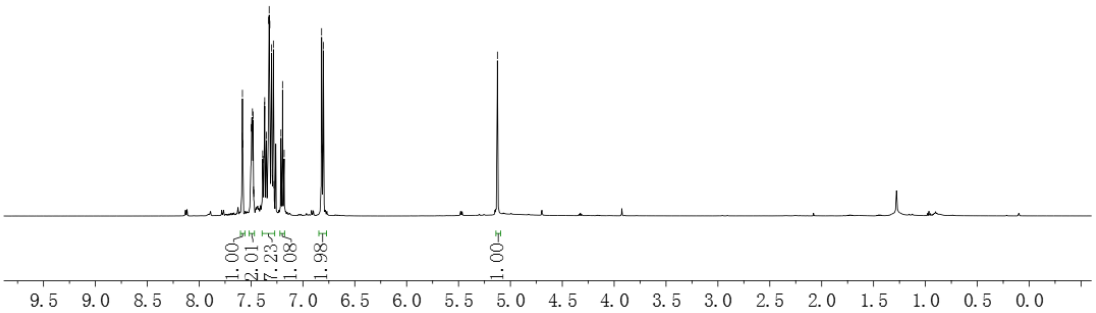
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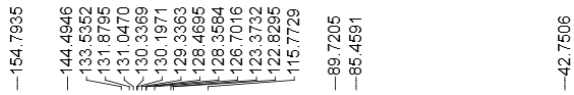
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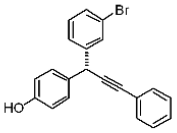
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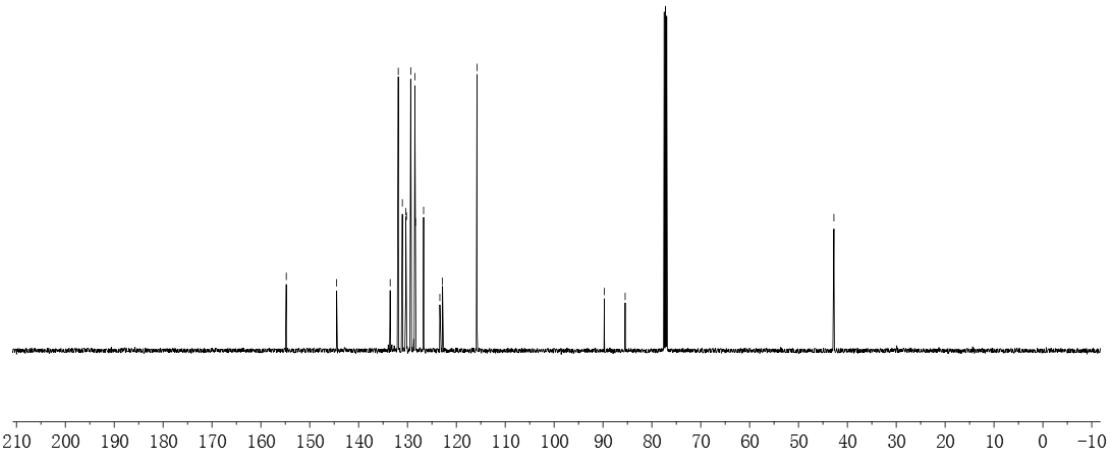
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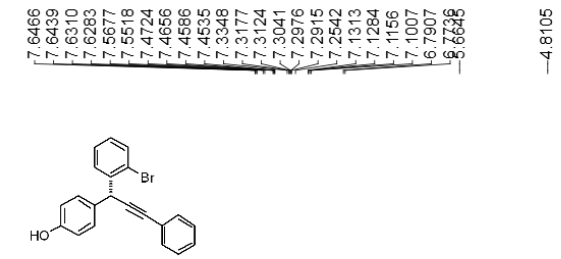
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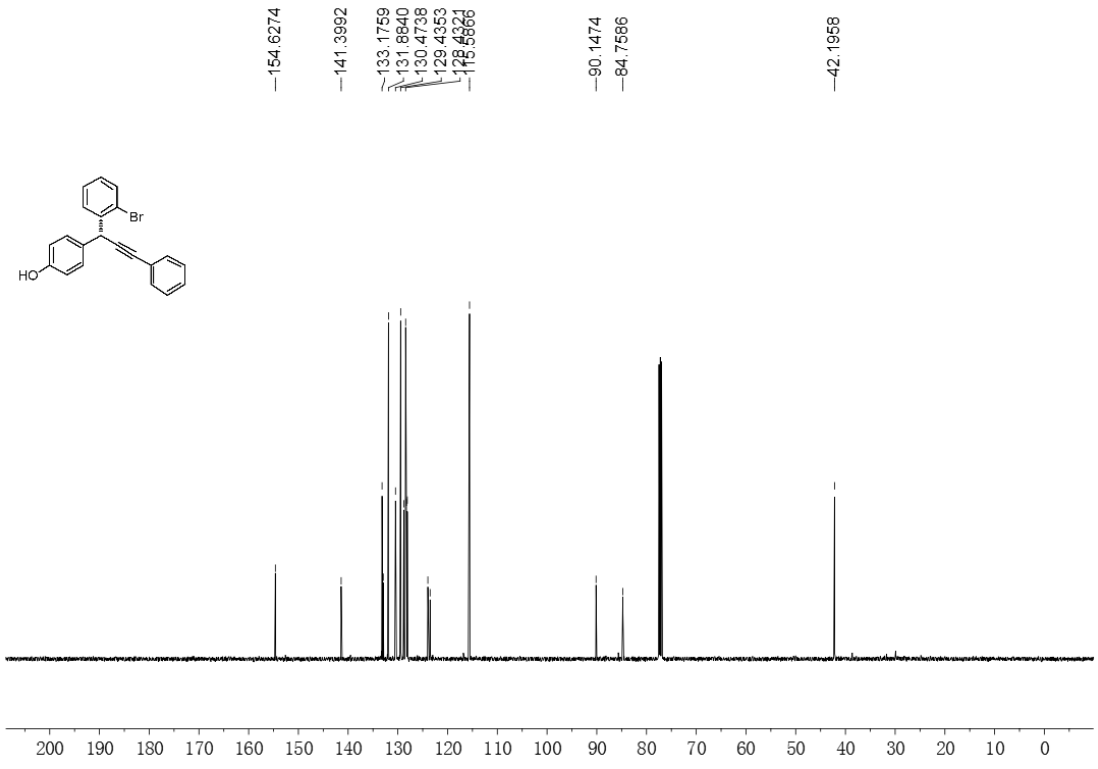
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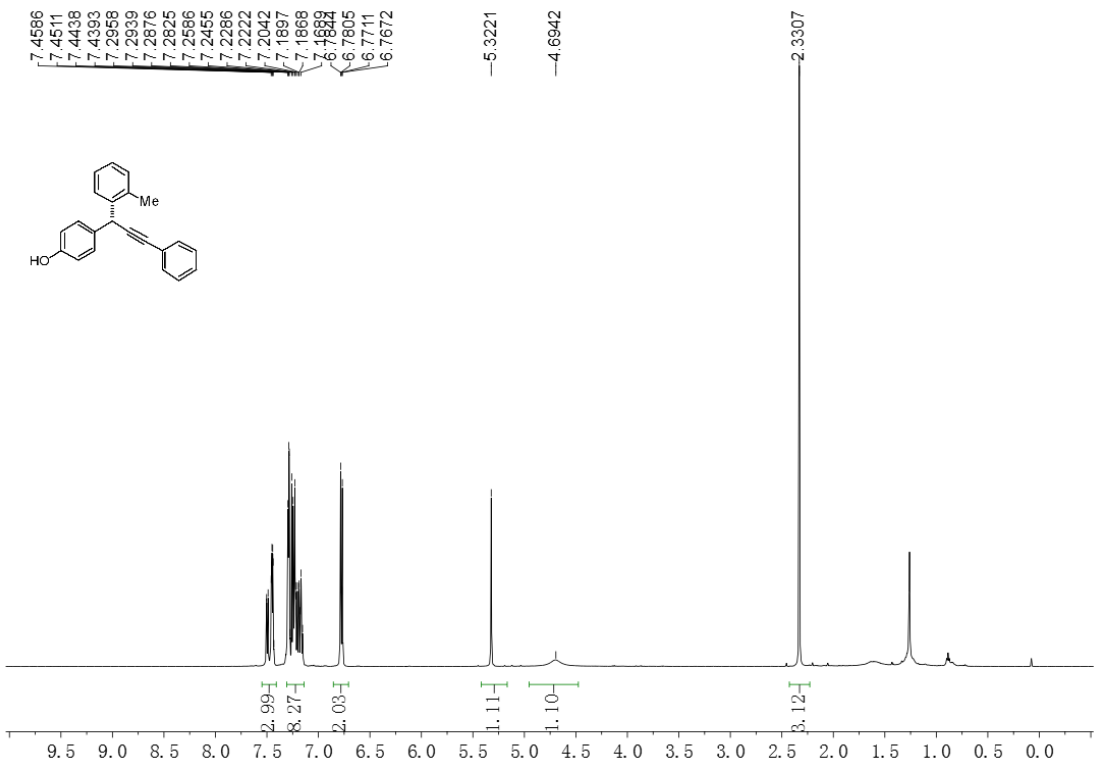
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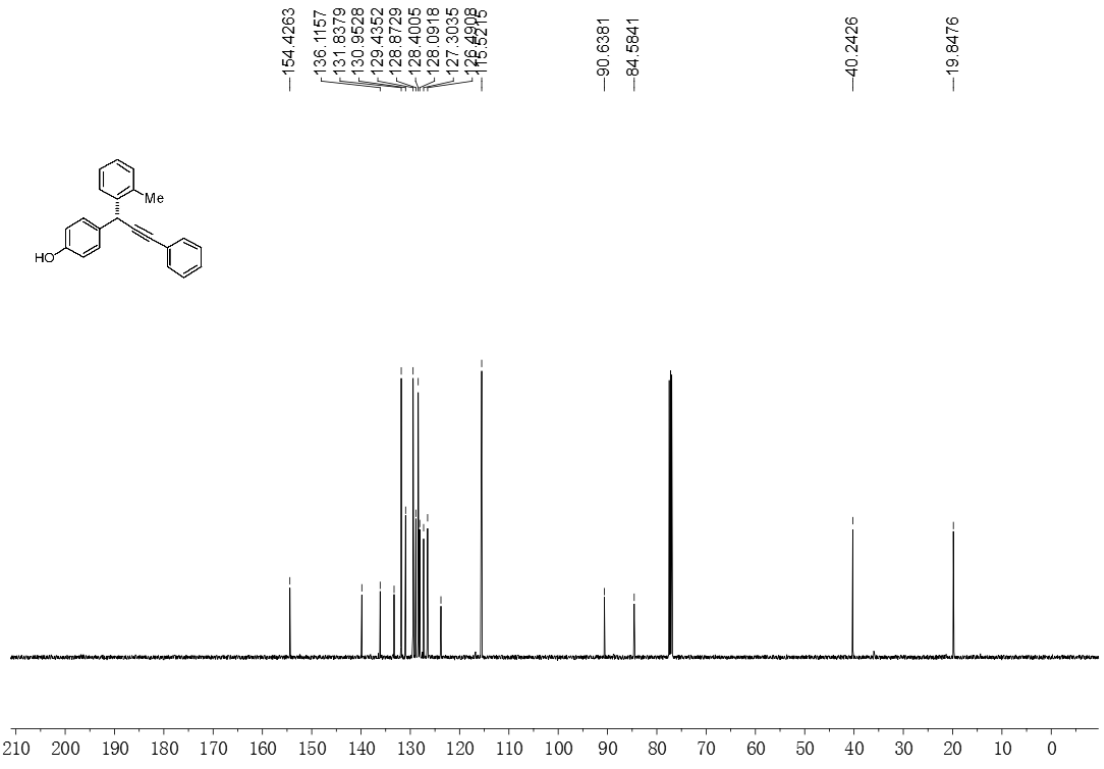
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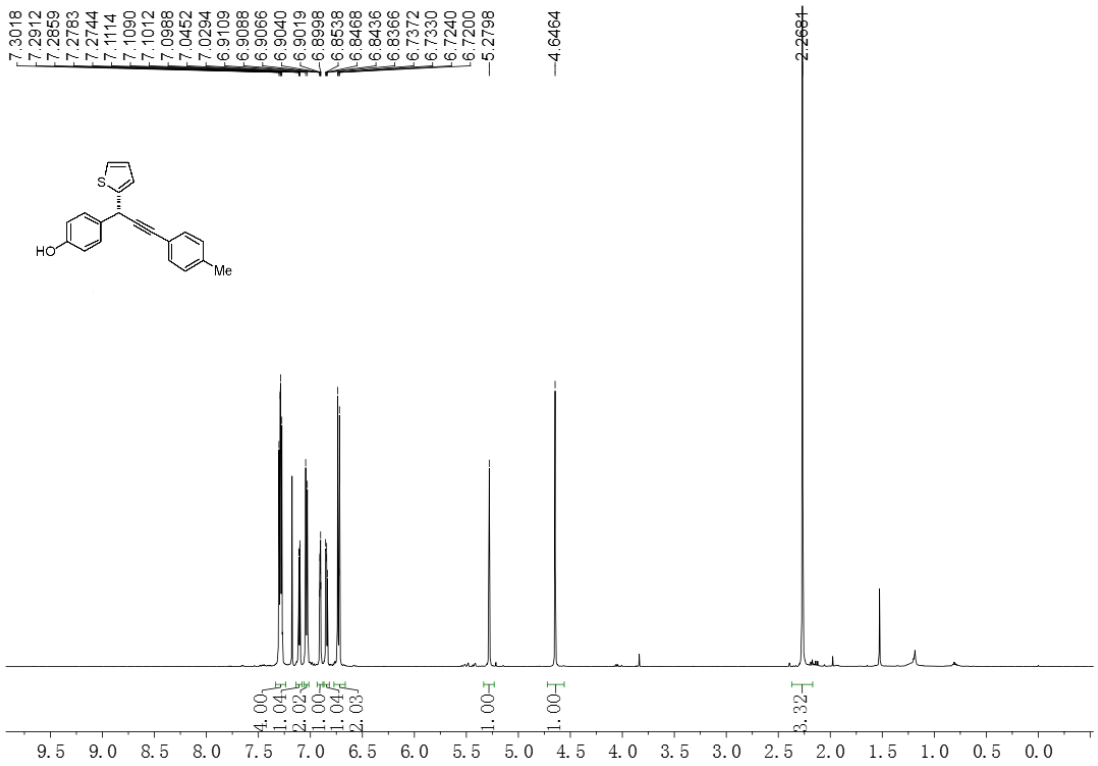
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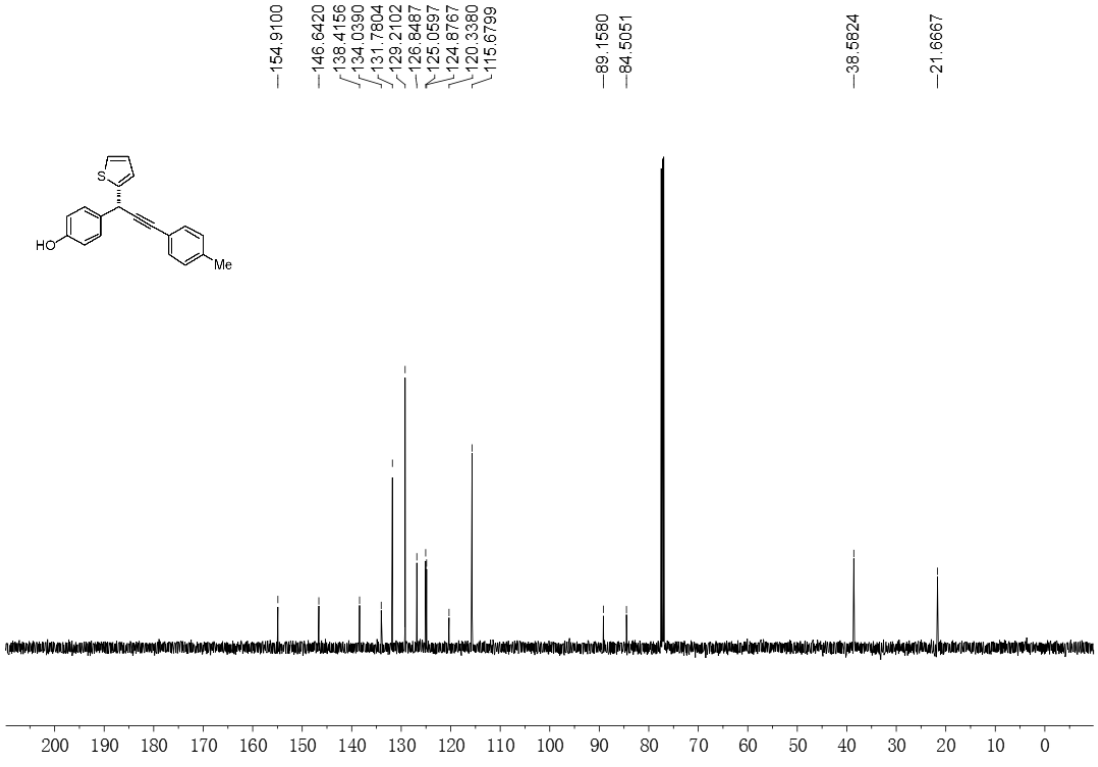
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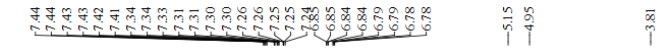
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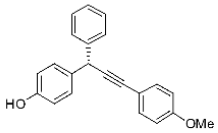
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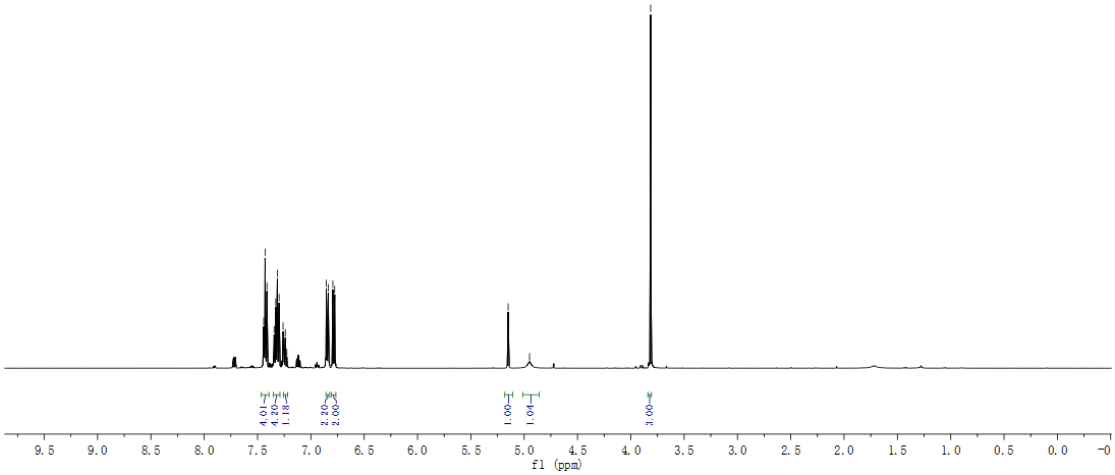
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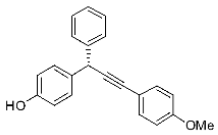
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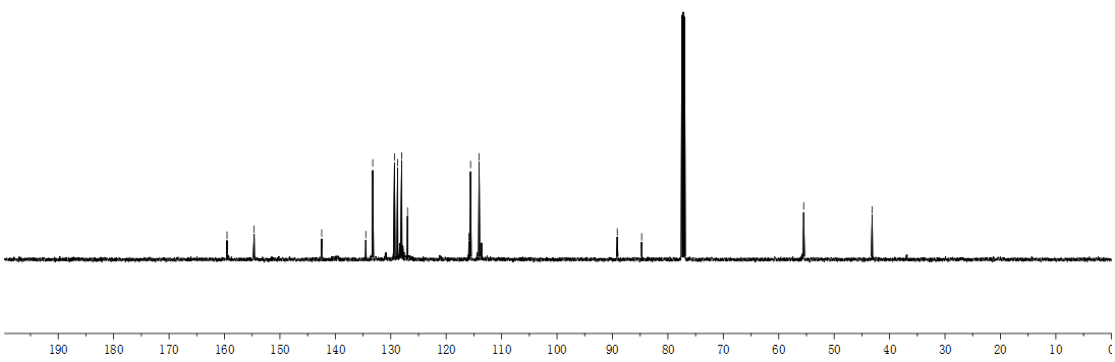
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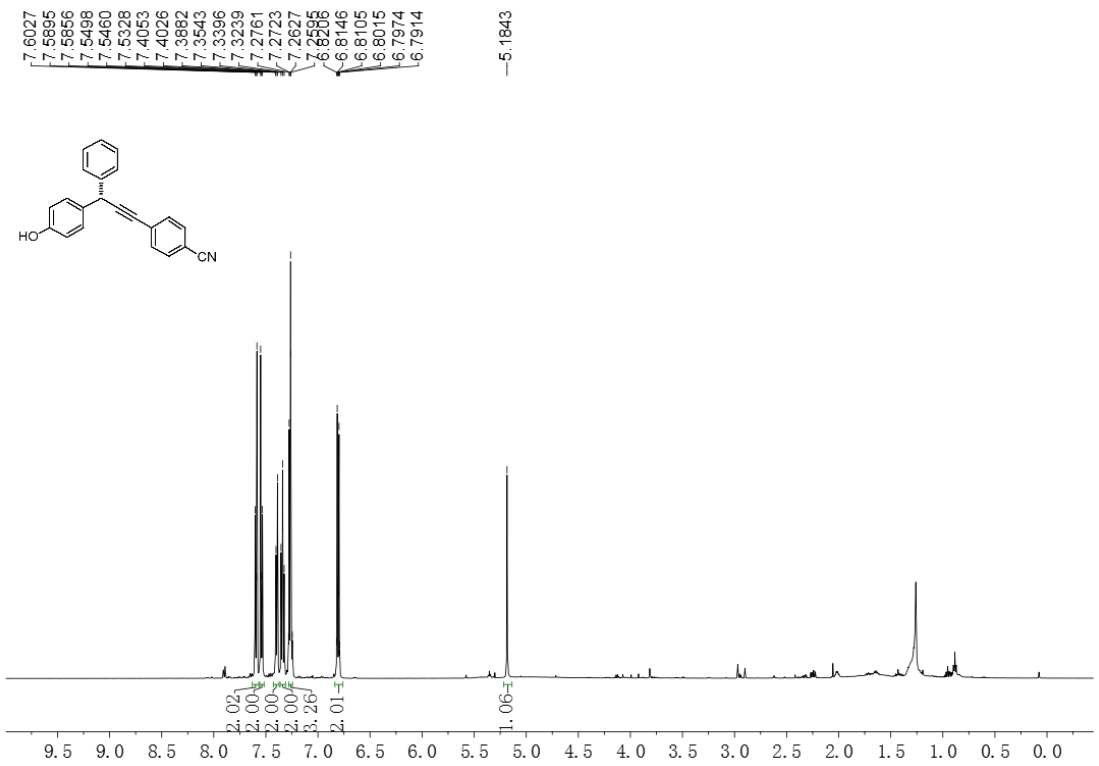
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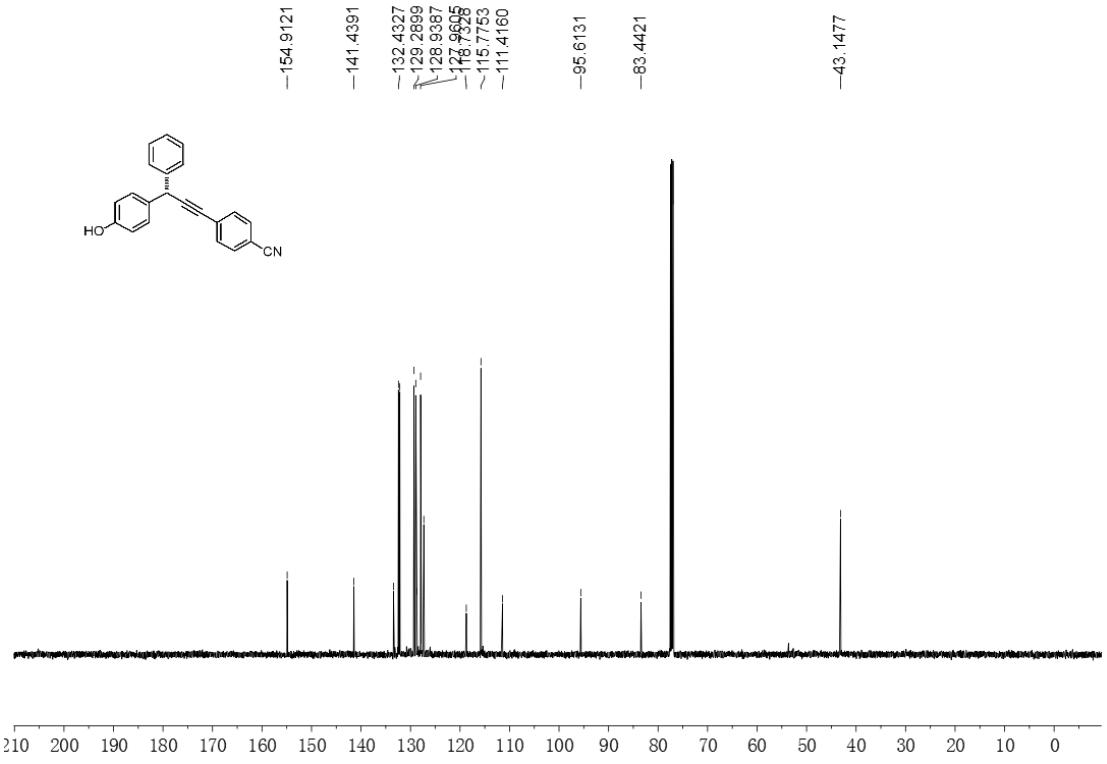
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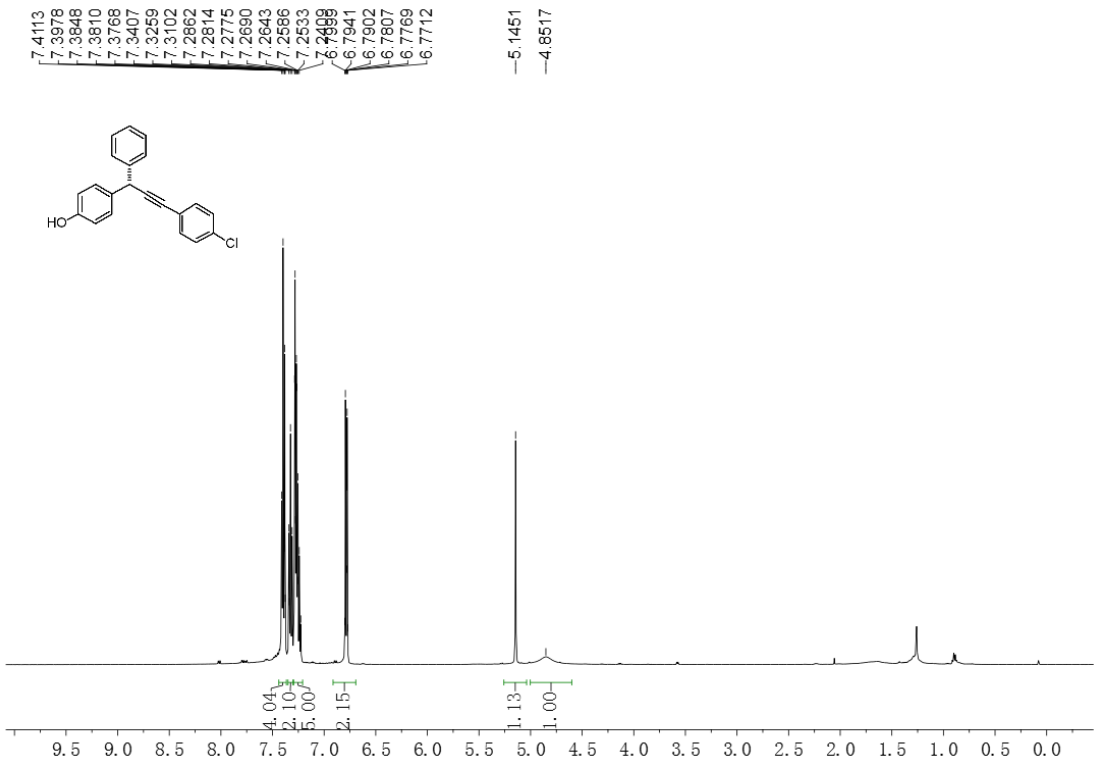
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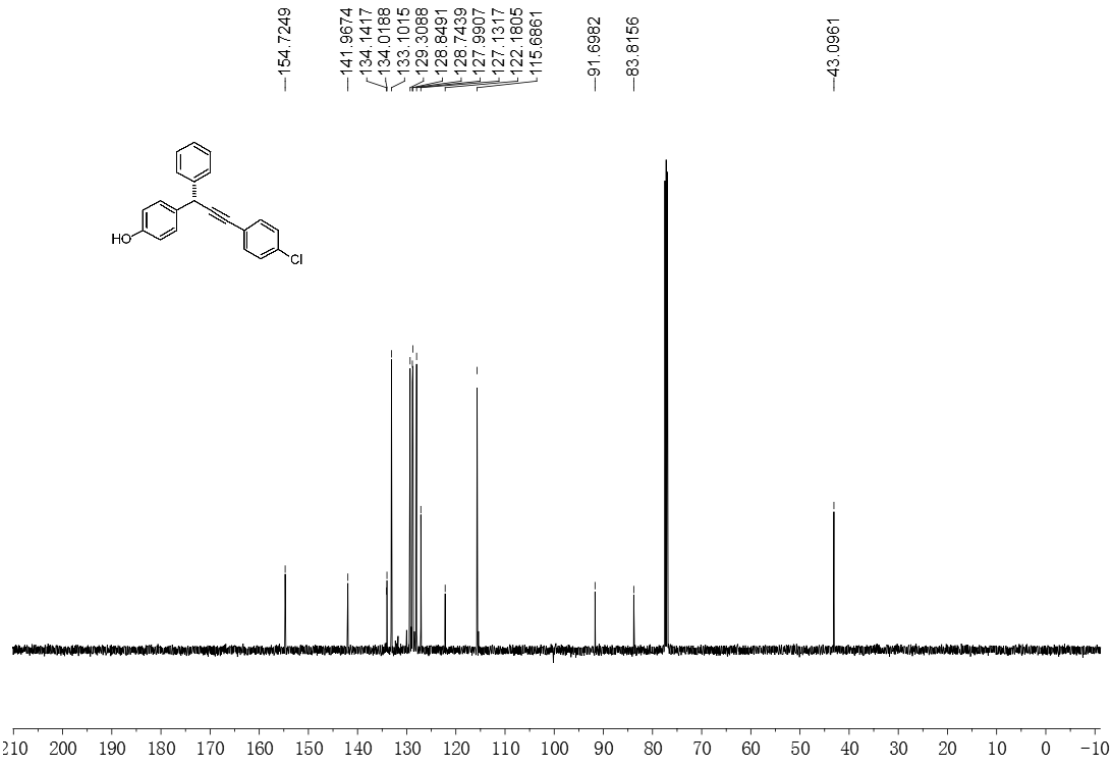
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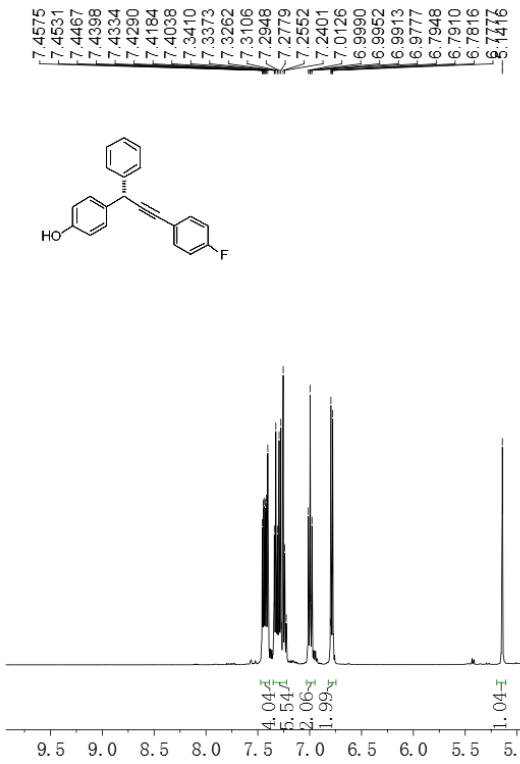
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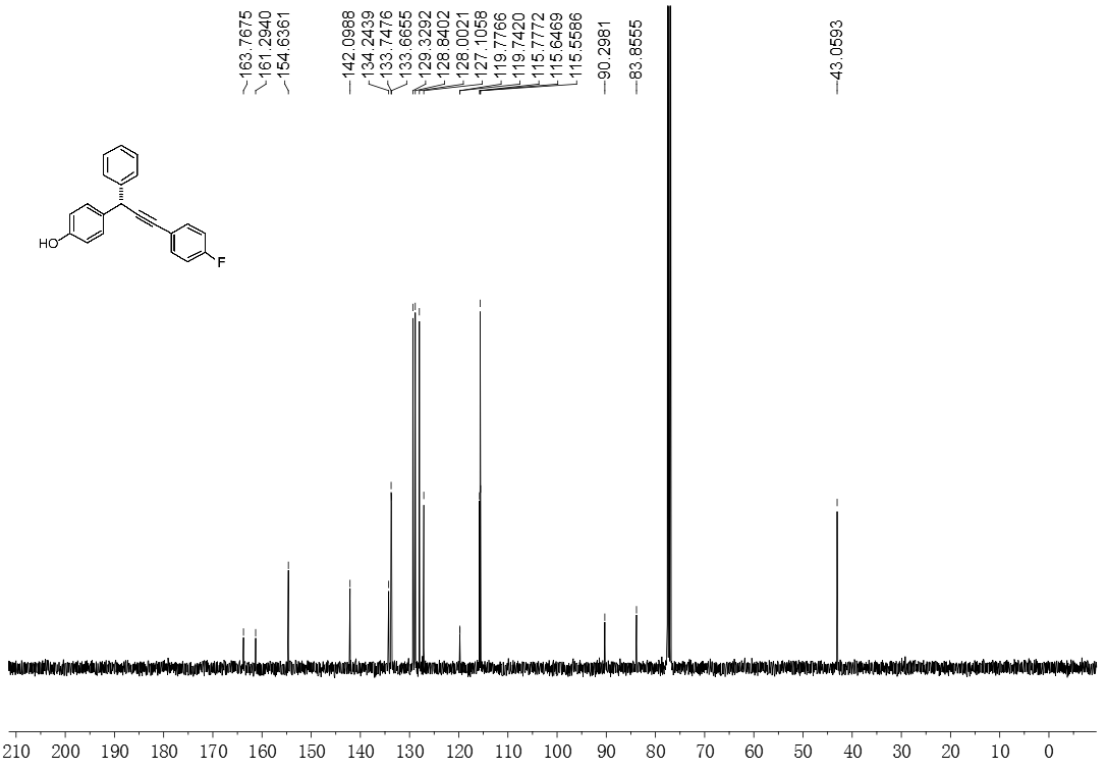
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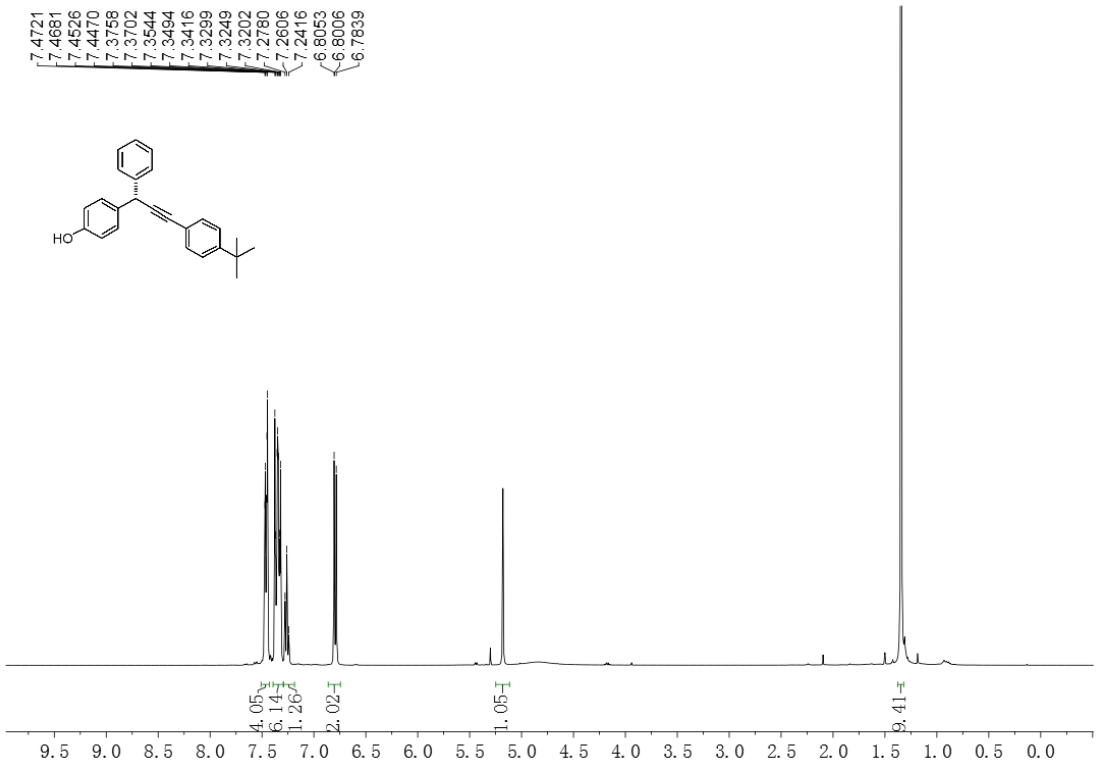
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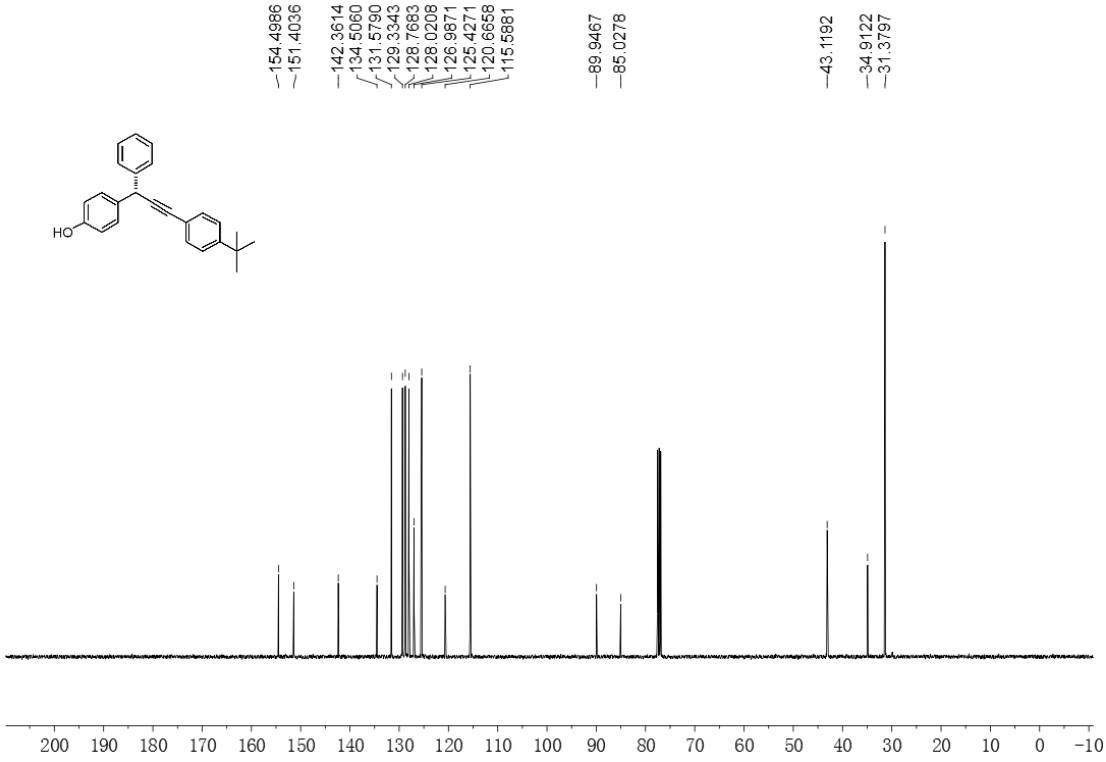
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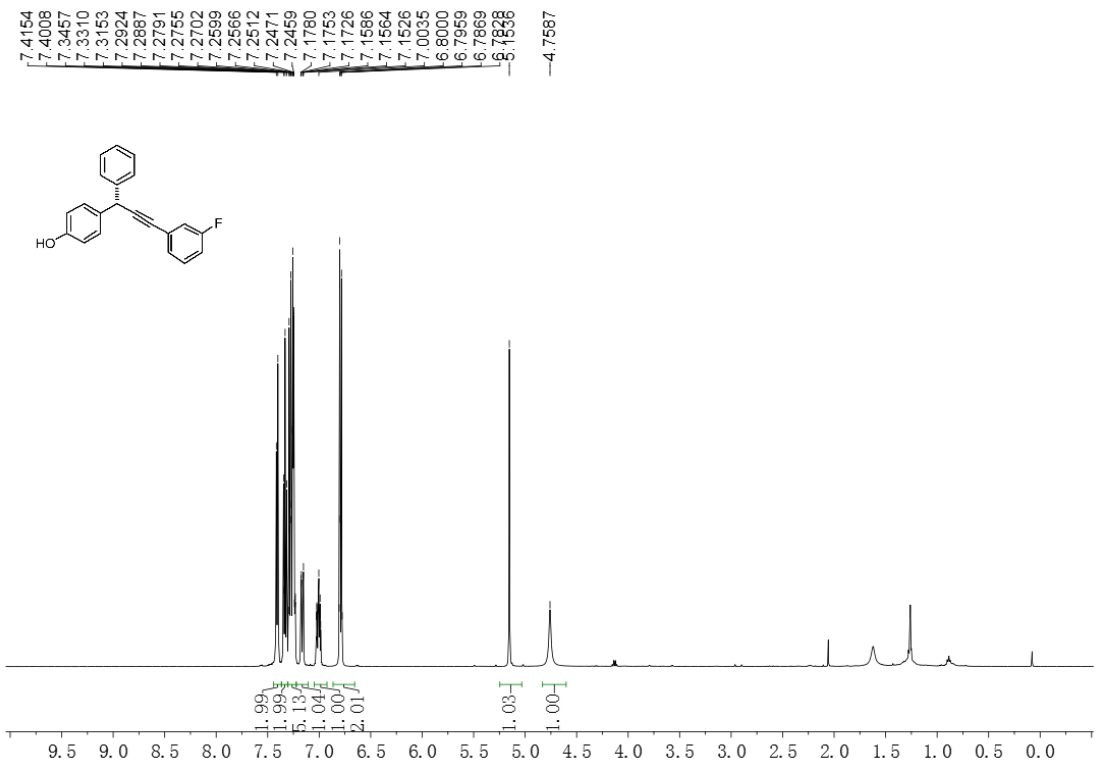
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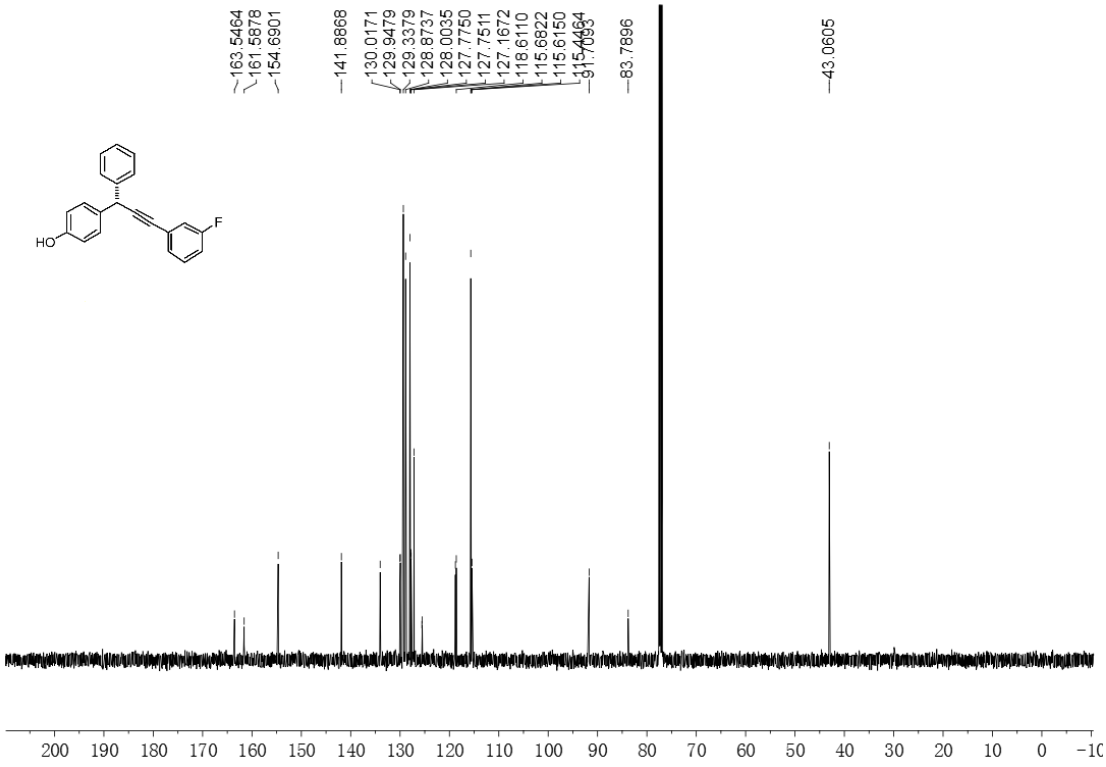
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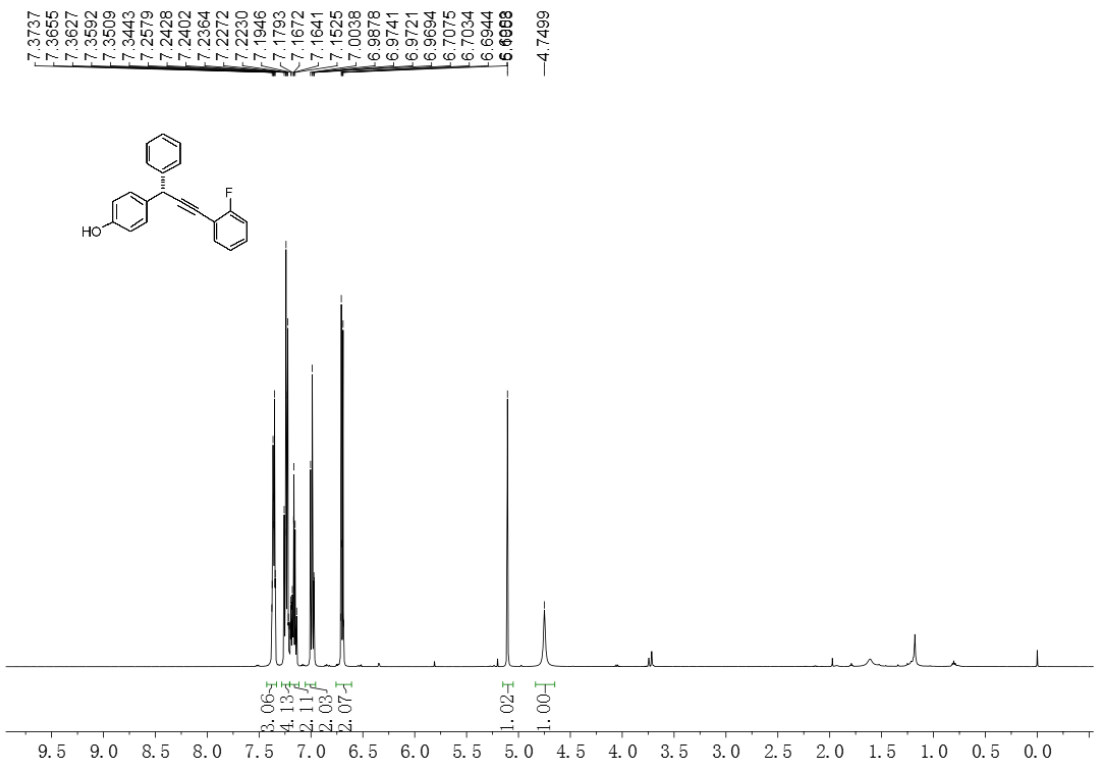
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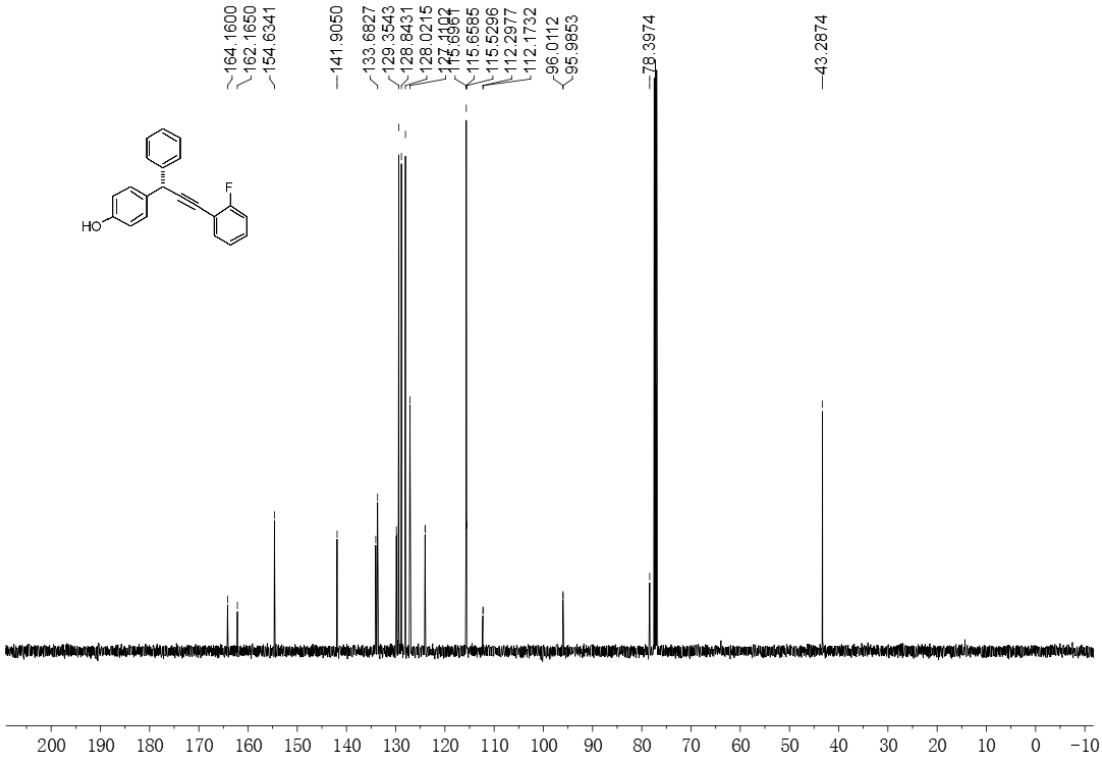
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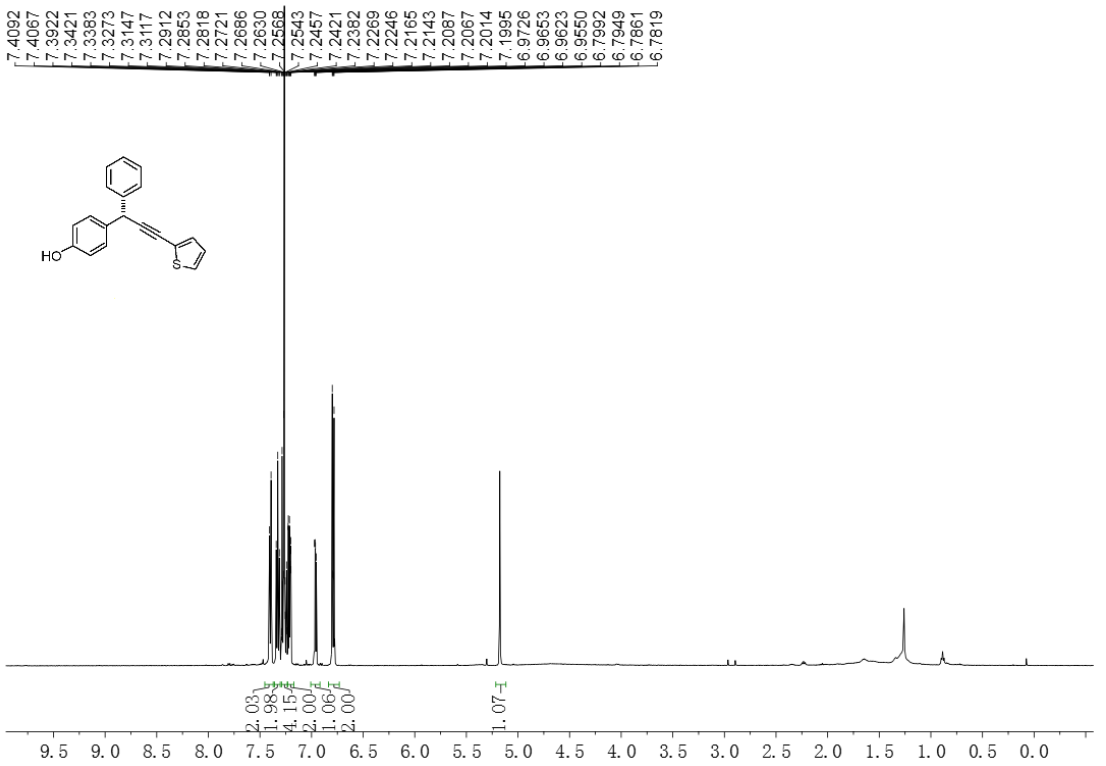
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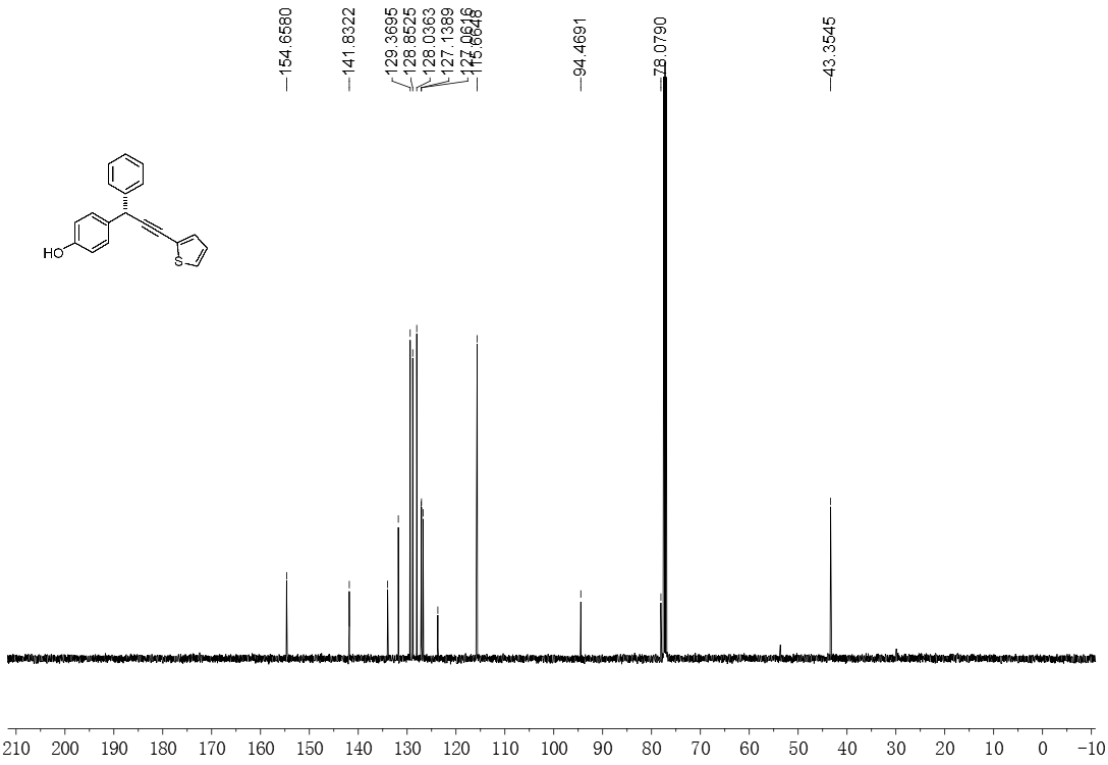
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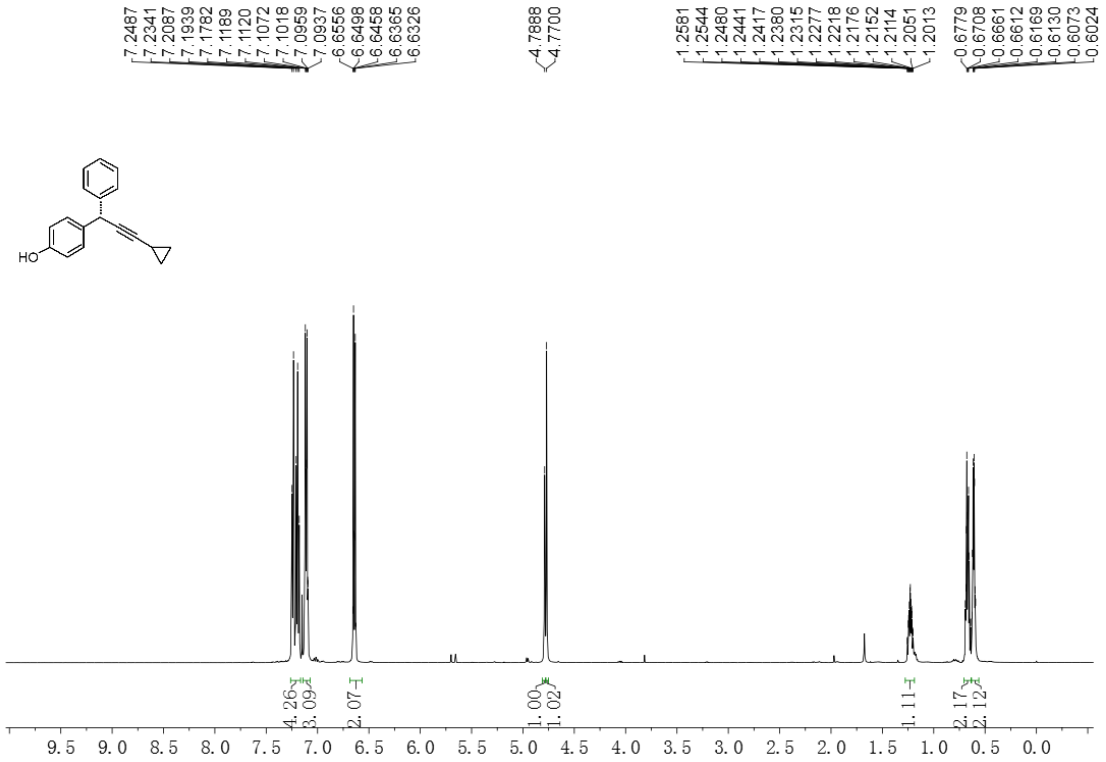
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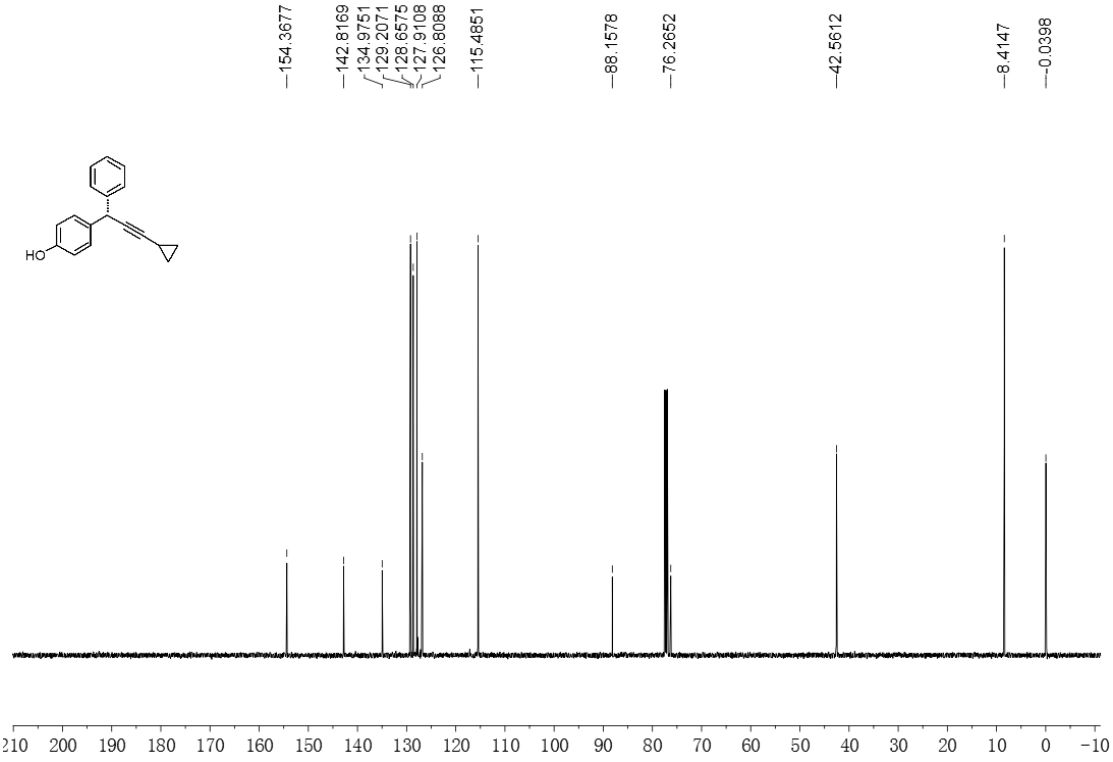
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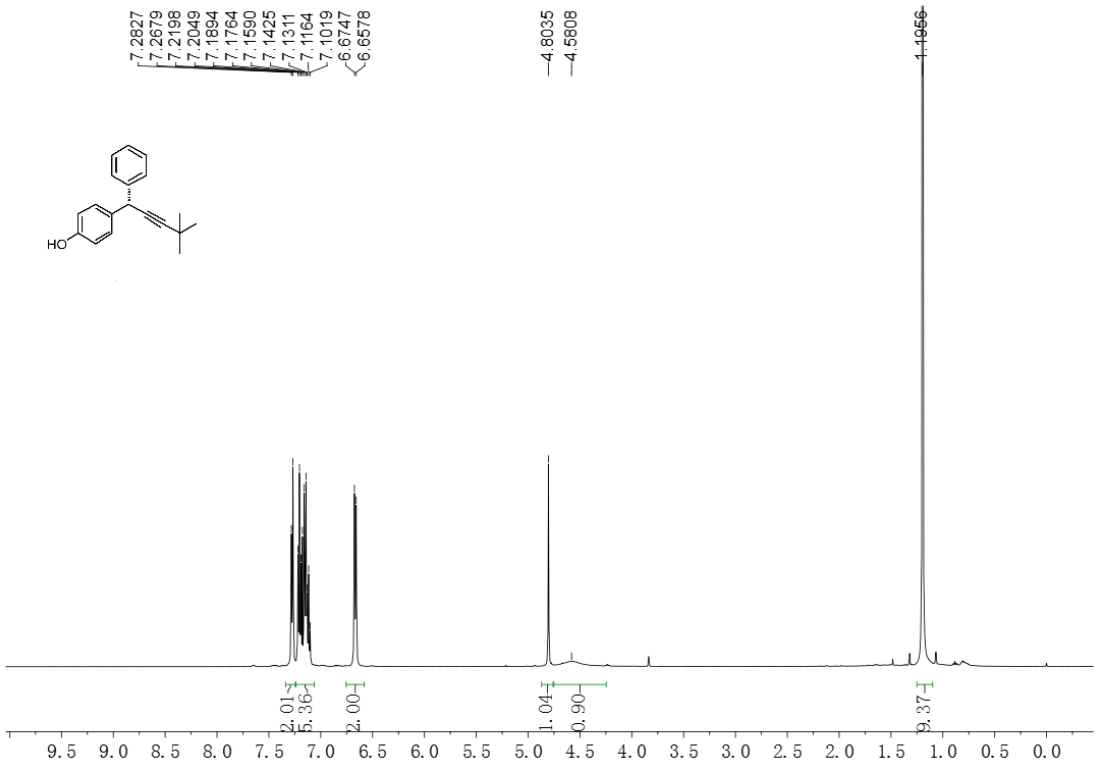
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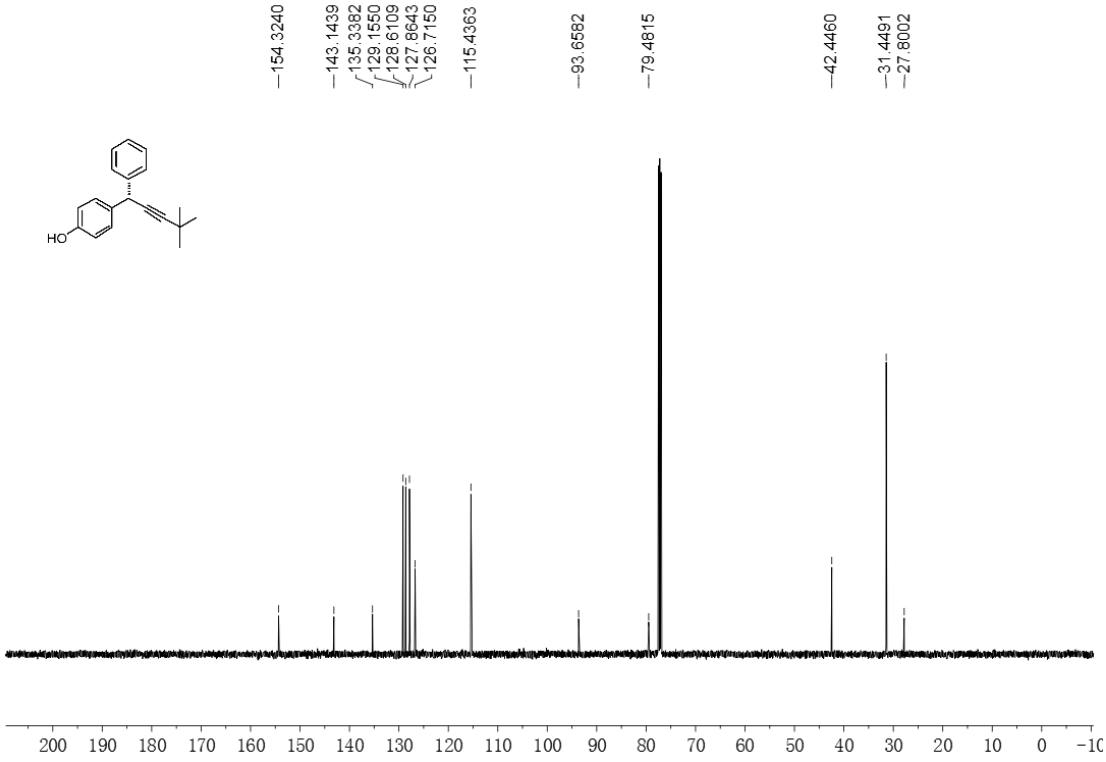
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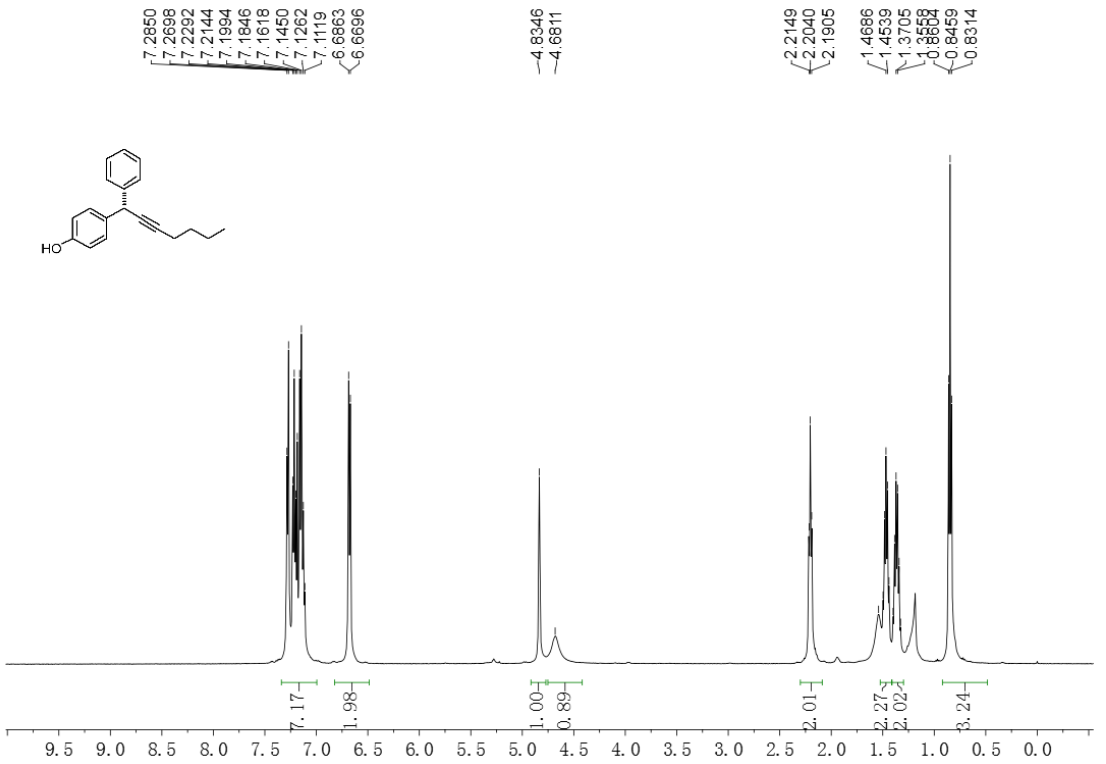
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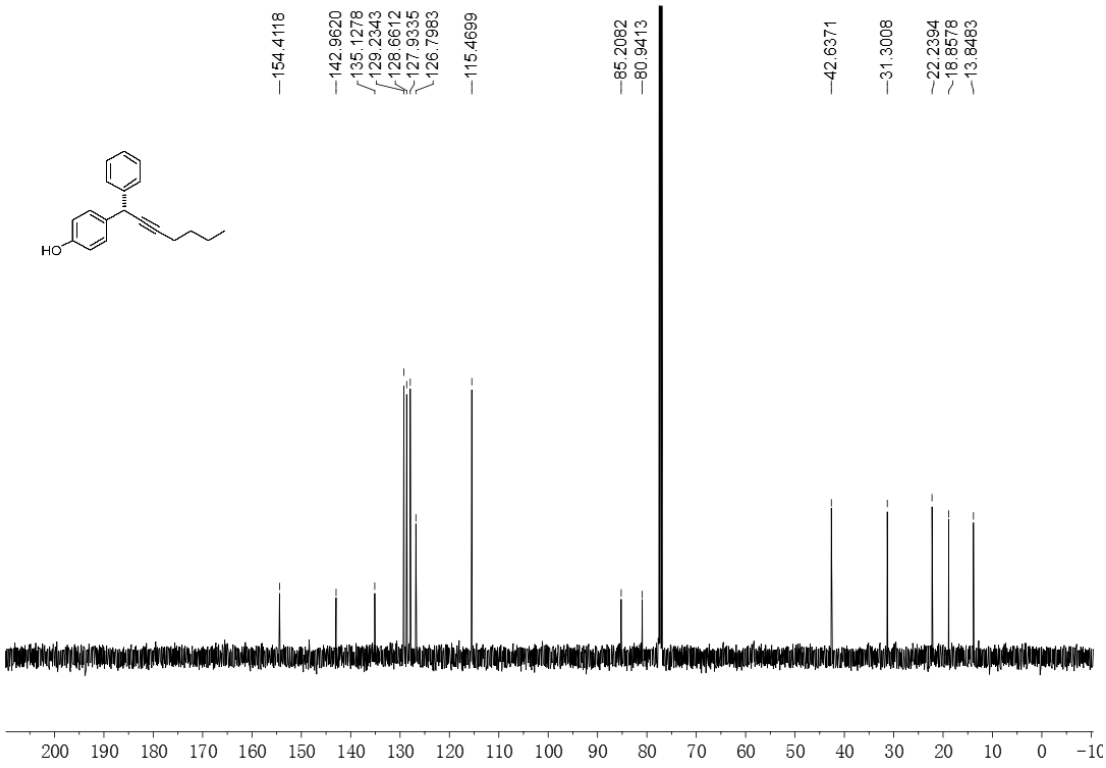
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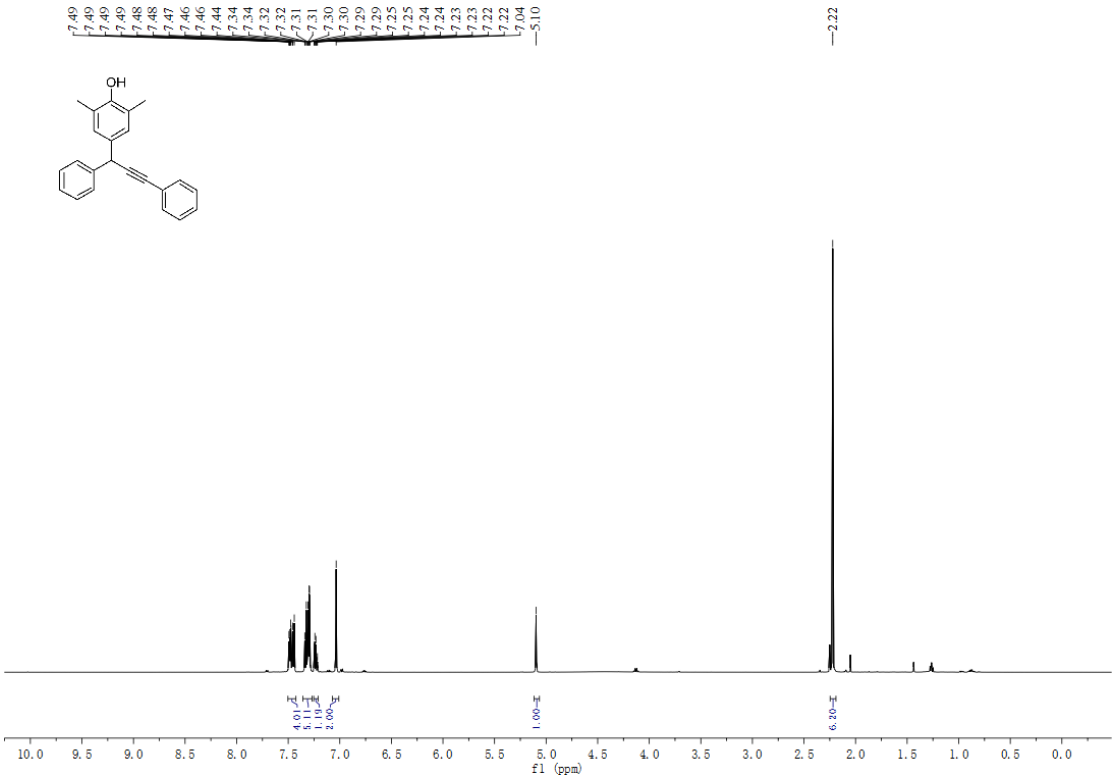
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7.22
7.04
5.10
2.22
OH
4.01
5.11
1.19
2.06
1.00
6.20
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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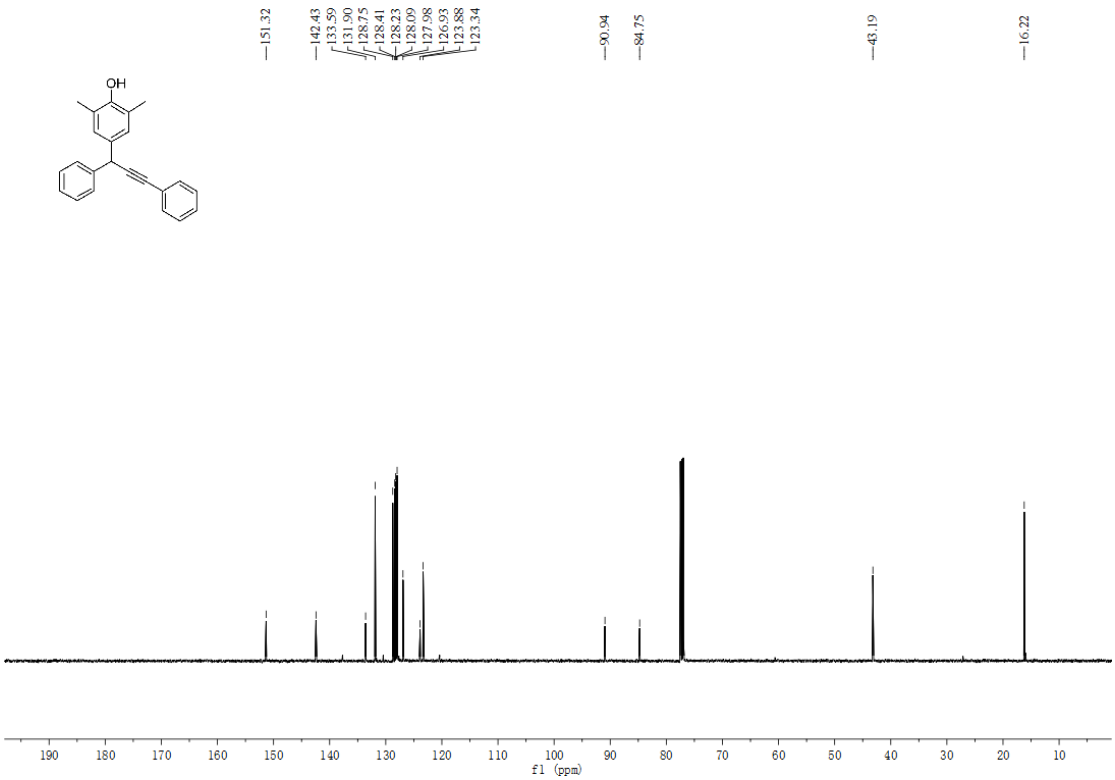
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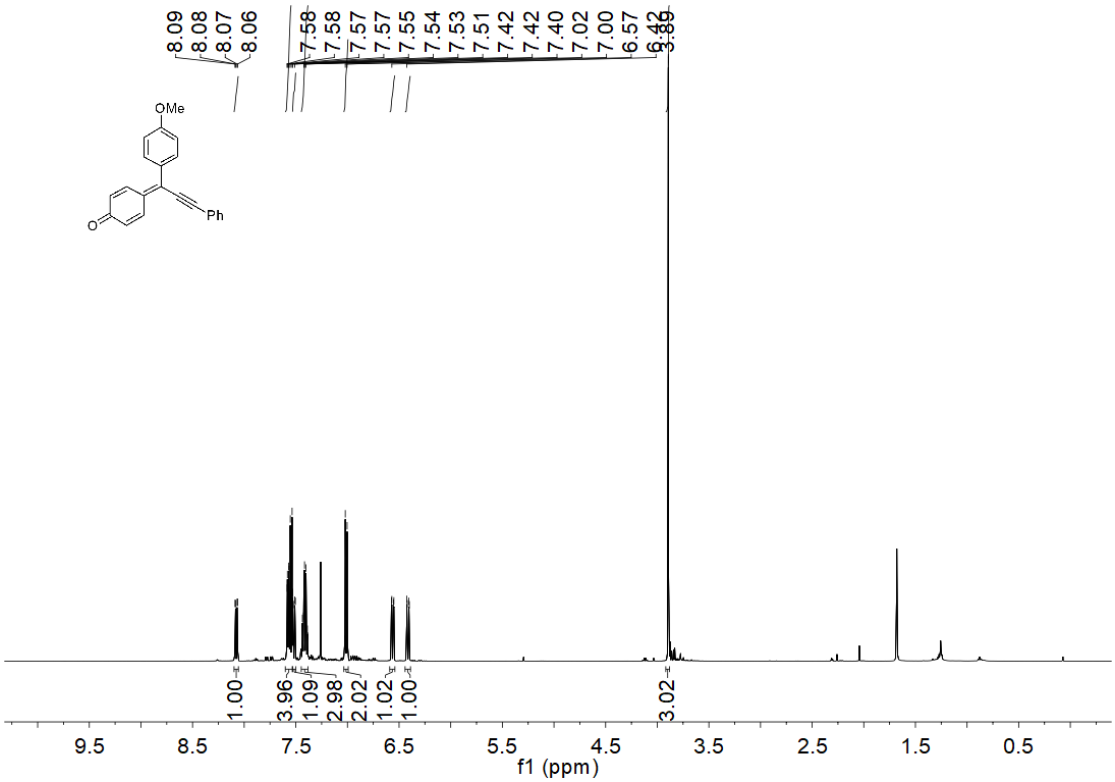
f1 (ppm)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7.00
6.57
6.42
3.89
OMe
Ph
O
1.00
3.96
1.09
2.98
2.02
1.02
1.00
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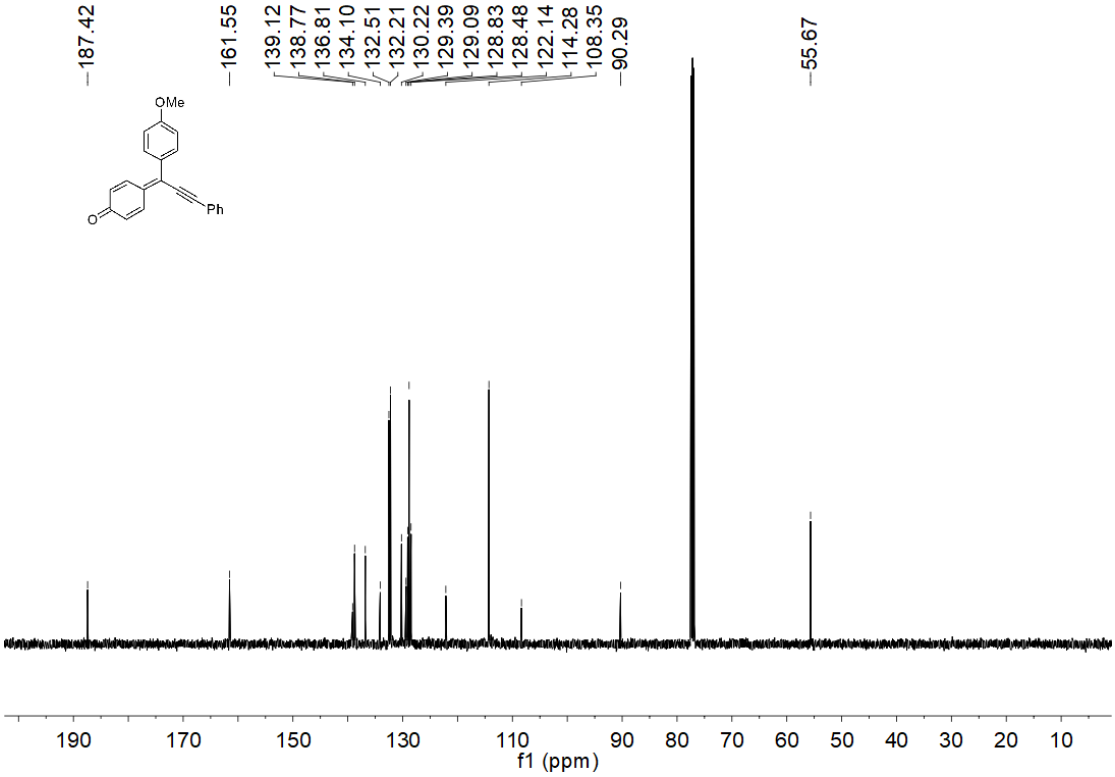
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108.35
90.29
55.67
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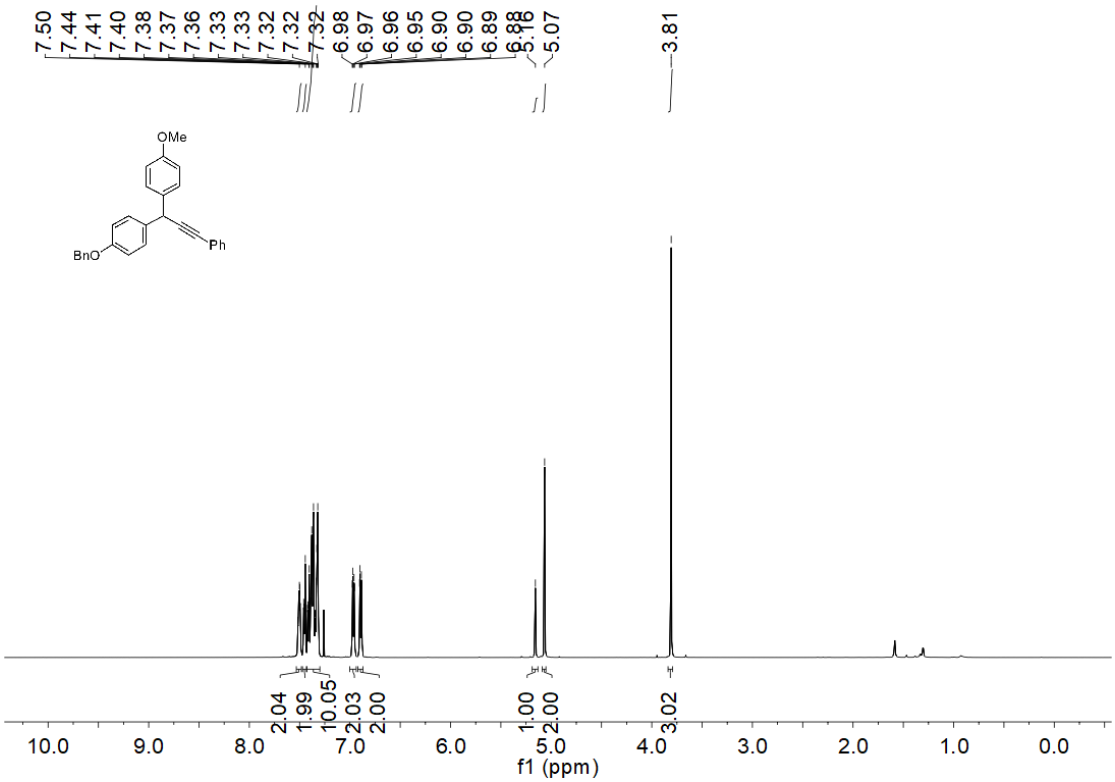
f1 (ppm)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6.97
6.96
6.95
6.90
6.90
6.89
5.07
3.81
OMe
BnO
Ph
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1.99
10.05
2.03
2.00
1.00
2.00
3.02
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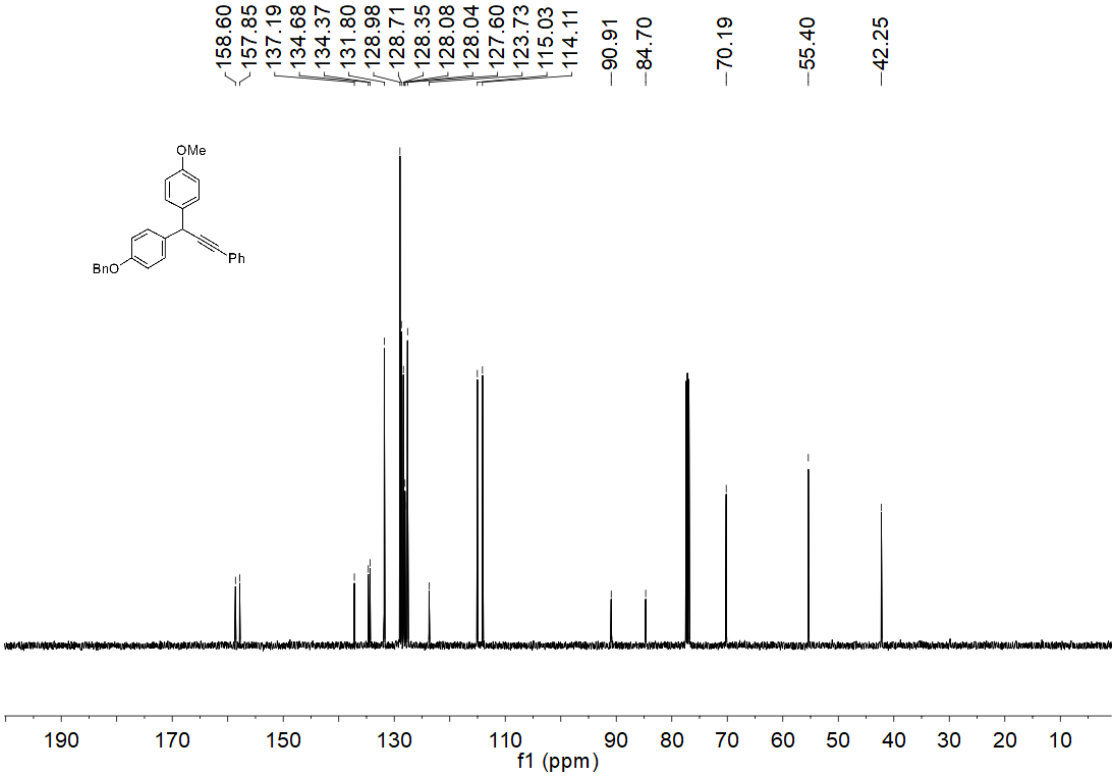
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55.40
42.25
OMe
BnO
Ph
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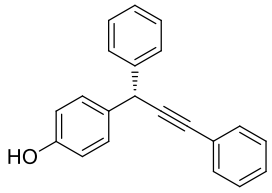
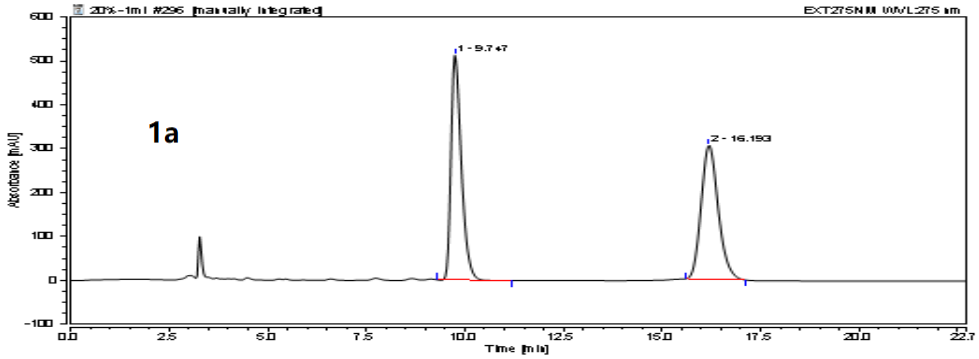
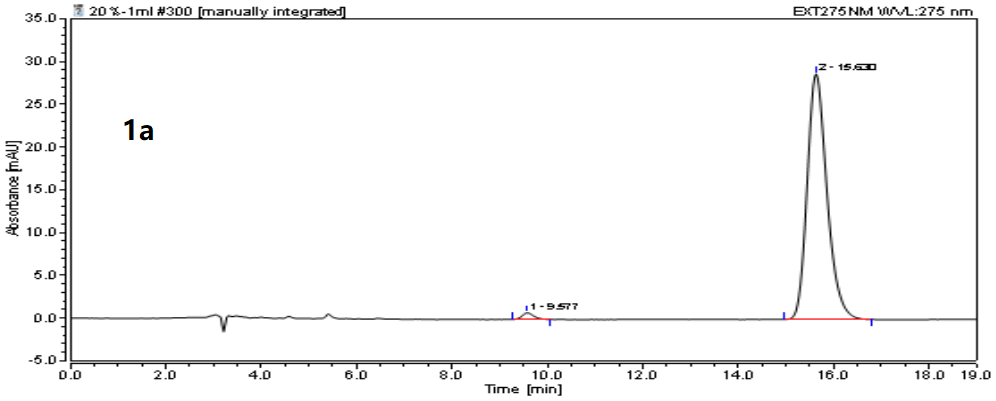
f1 (ppm)

HPLC traces

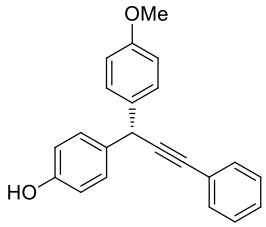


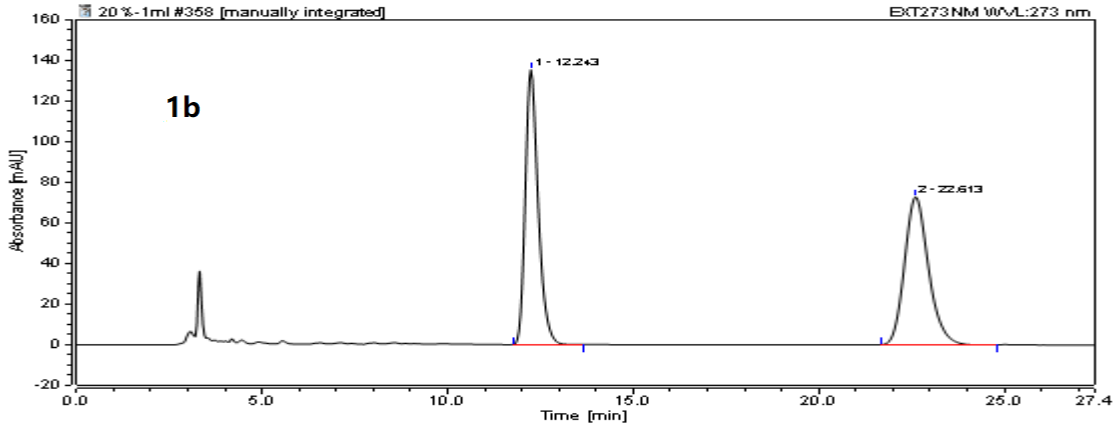


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	9.747	155.025	50.19	n.a.
2	n.a.	16.193	153.865	49.81	n.a.
Total:			**308.890**	**100.00**	

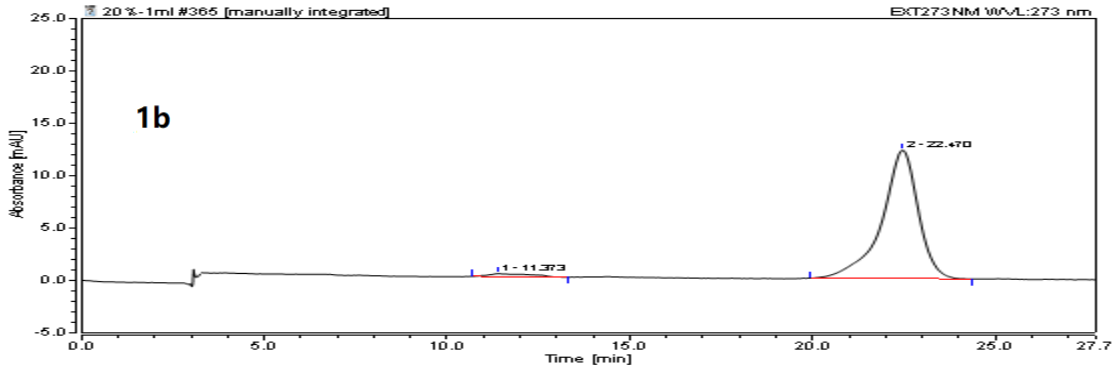


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	9.577	0.218	1.55	n.a.
2	n.a.	15.630	13.826	98.45	n.a.
Total:			**14.043**	**100.00**	

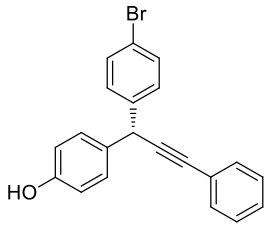


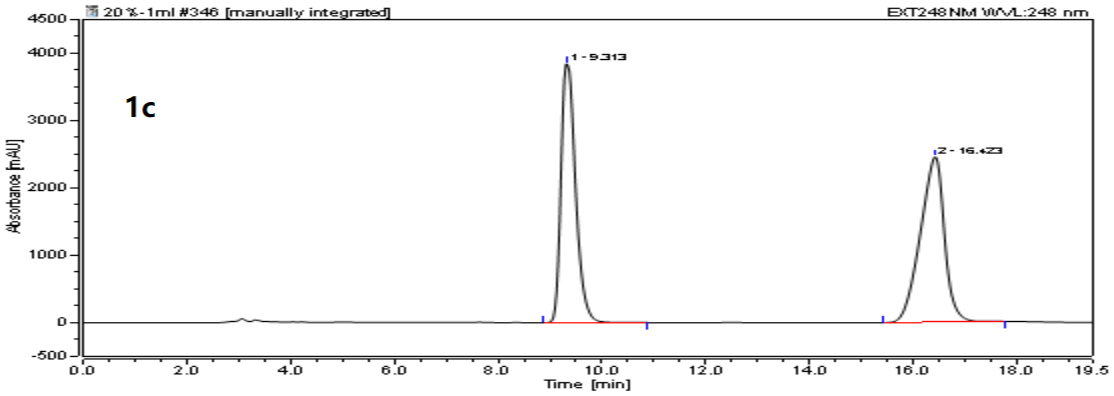


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1		12.243	54.227	49.95	n.a.
2		22.613	54.332	50.05	n.a.
Total:			**108.559**	**100.00**	

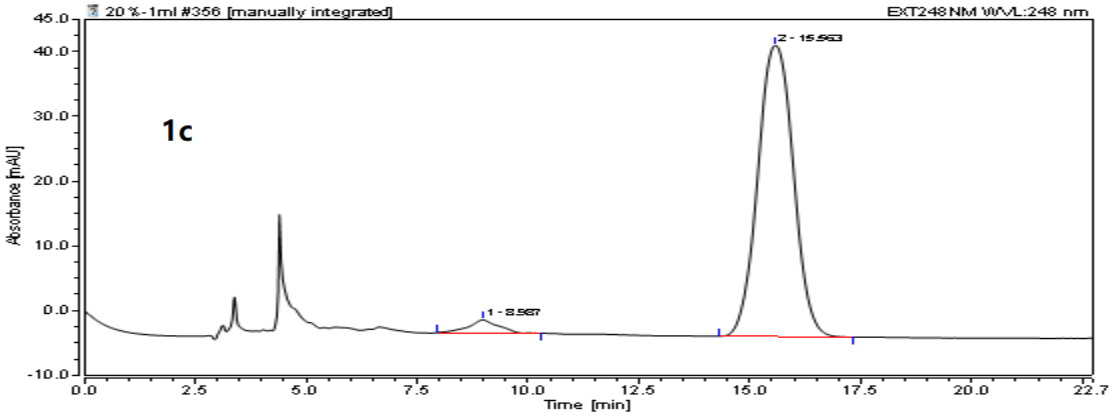


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.373	0.385	2.65	n.a.
2	n.a.	22.470	14.127	97.35	n.a.
Total:			**14.511**	**100.00**	

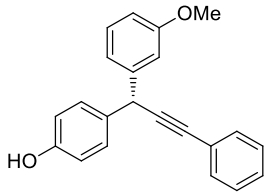


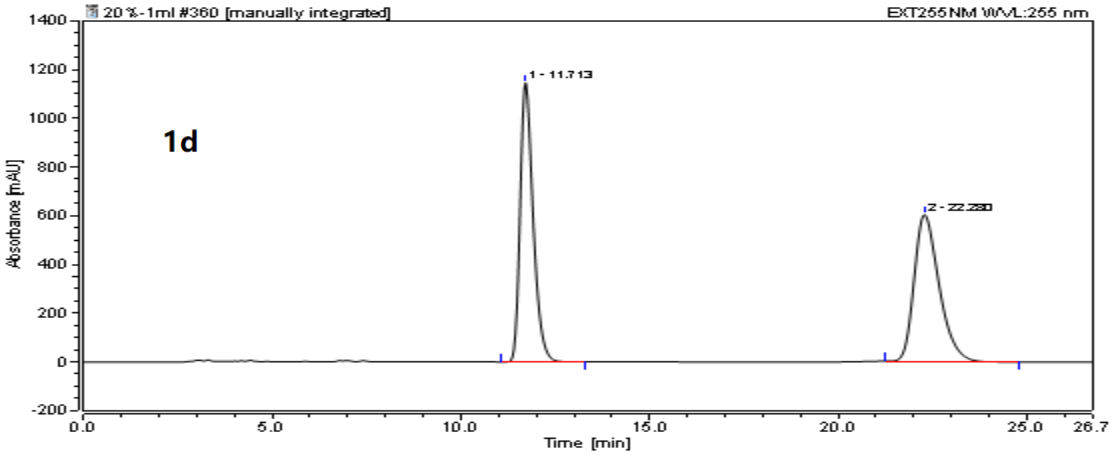


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	9.313	1251.119	48.75	n.a.
2	n.a.	16.423	1315.029	51.25	n.a.
Total:			**2566.148**	**100.00**	

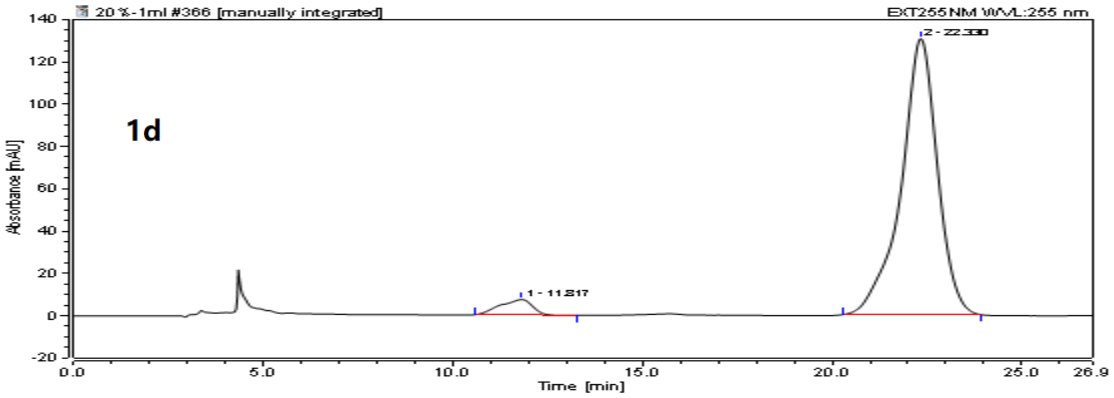


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	8.987	1.573	3.63	n.a.
2	n.a.	15.563	41.804	96.37	n.a.
Total:			**43.377**	**100.00**	

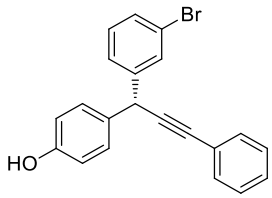


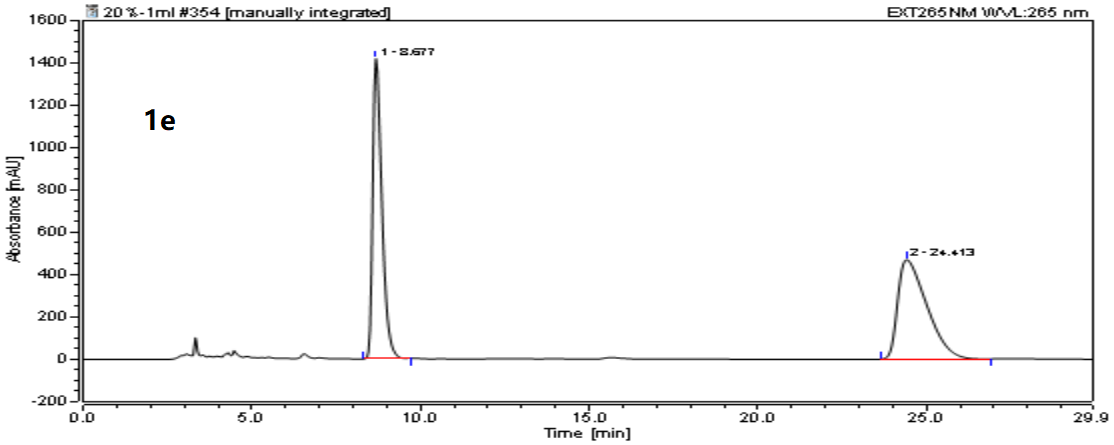


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.713	458.229	49.93	n.a.
2	n.a.	22.280	459.581	50.07	n.a.
Total:			**917.810**	**100.00**	

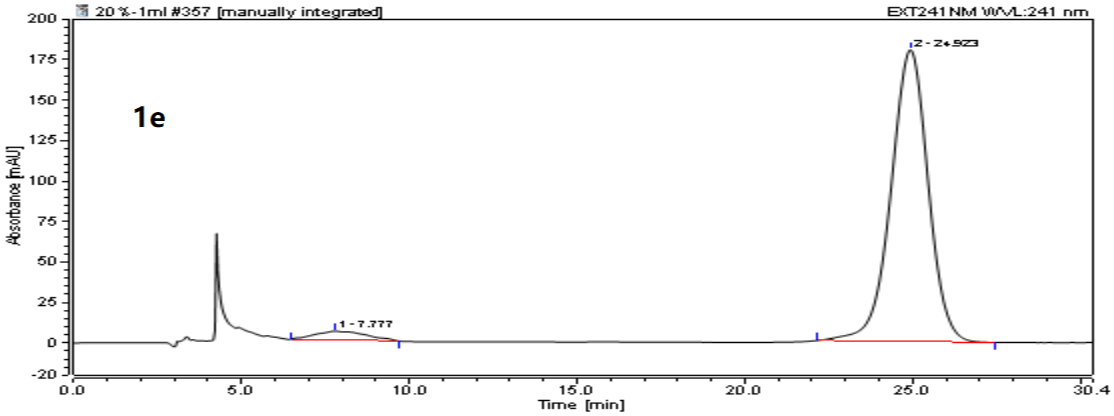


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.817	7.145	4.70	n.a.
2	n.a.	22.330	144.737	95.30	n.a.
Total:			**151.883**	**100.00**	

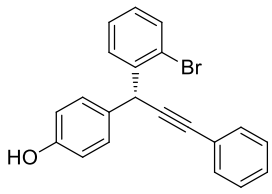


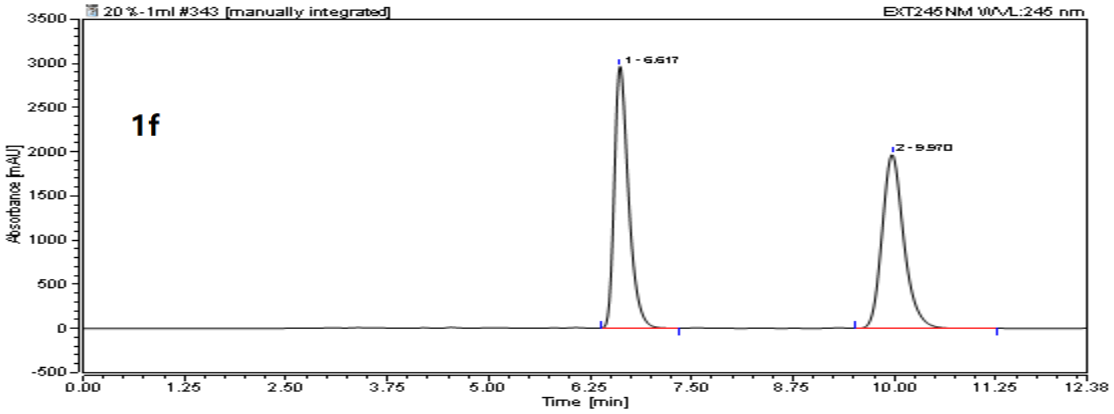


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	8.677	445.634	48.83	n.a.
2	n.a.	24.413	466.899	51.17	n.a.
Total:			**912.534**	**100.00**	

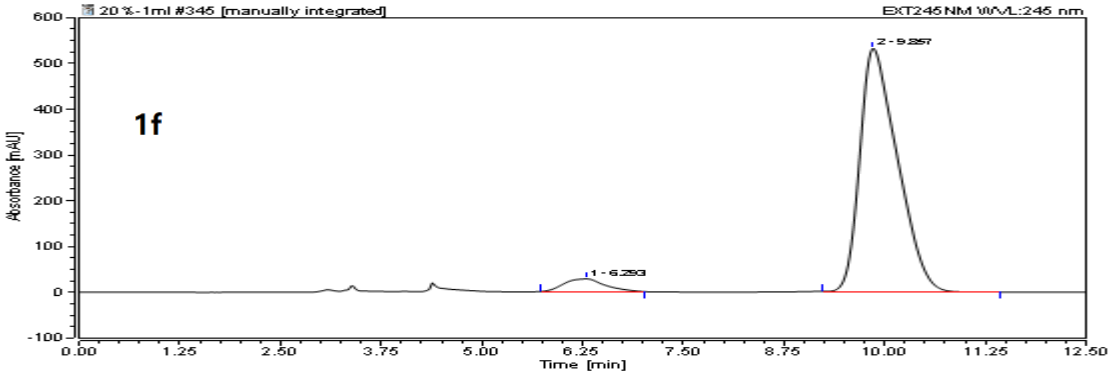


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	7.777	9.723	4.03	n.a.
2	n.a.	24.923	231.254	95.97	n.a.
Total:			**240.977**	**100.00**	

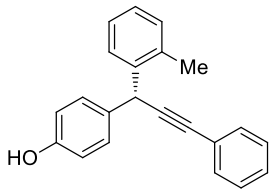


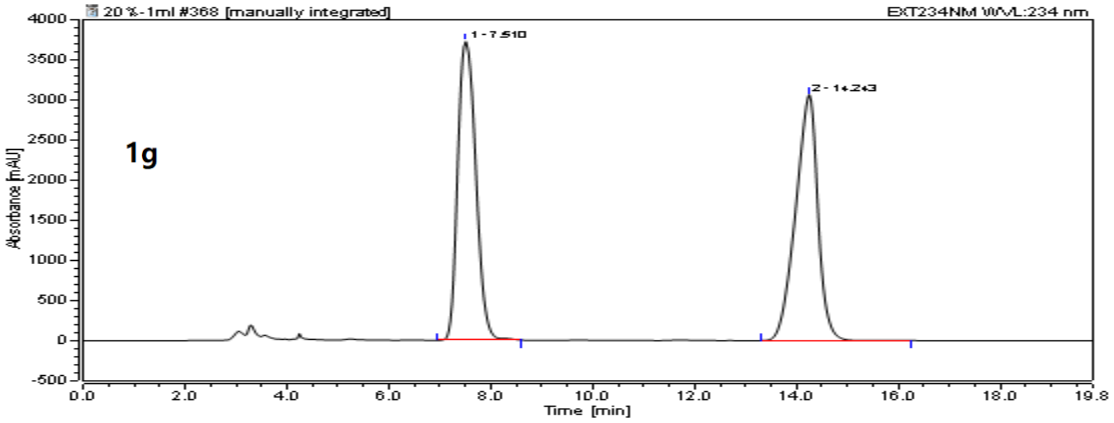


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	6.617	603.854	49.76	n.a.
2	n.a.	9.970	609.672	50.24	n.a.
Total:			**1213.526**	**100.00**	

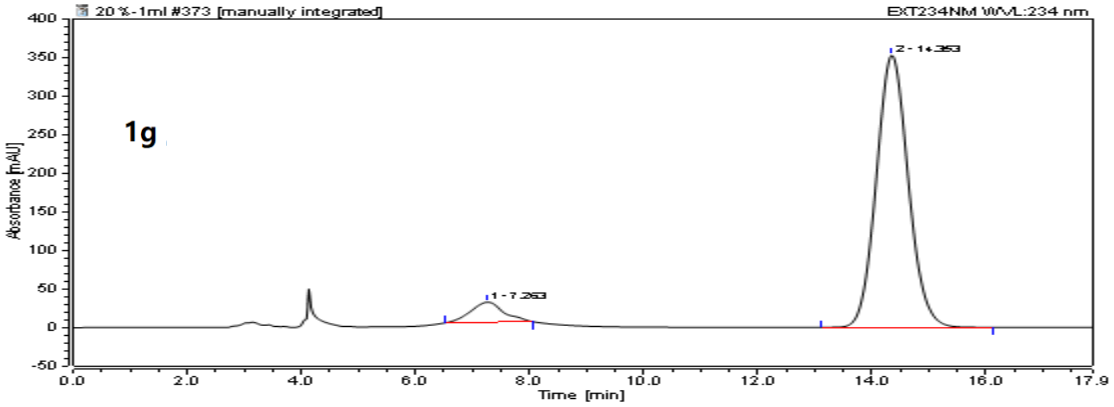


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	6.293	16.177	5.34	n.a.
2	n.a.	9.857	287.017	94.66	n.a.
Total:			**303.194**	**100.00**	

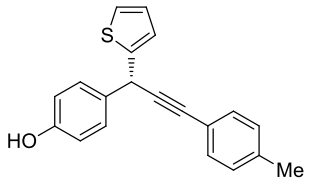


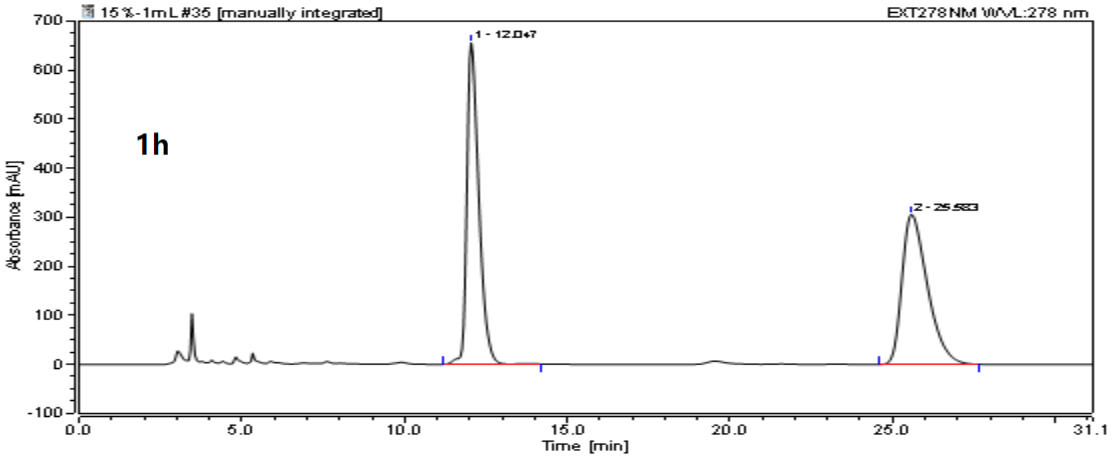


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	7.510	1533.863	49.76	n.a.
2	n.a.	14.243	1548.503	50.24	n.a.
Total:			**3082.365**	**100.00**	

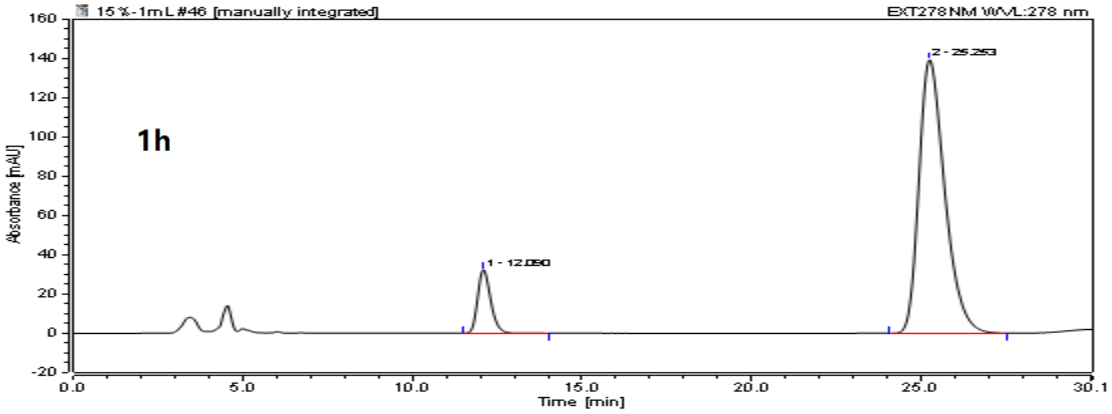


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	7.263	17.707	7.17	n.a.
2	n.a.	14.353	229.332	92.83	n.a.
Total:			**247.039**	**100.00**	

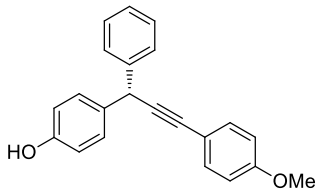


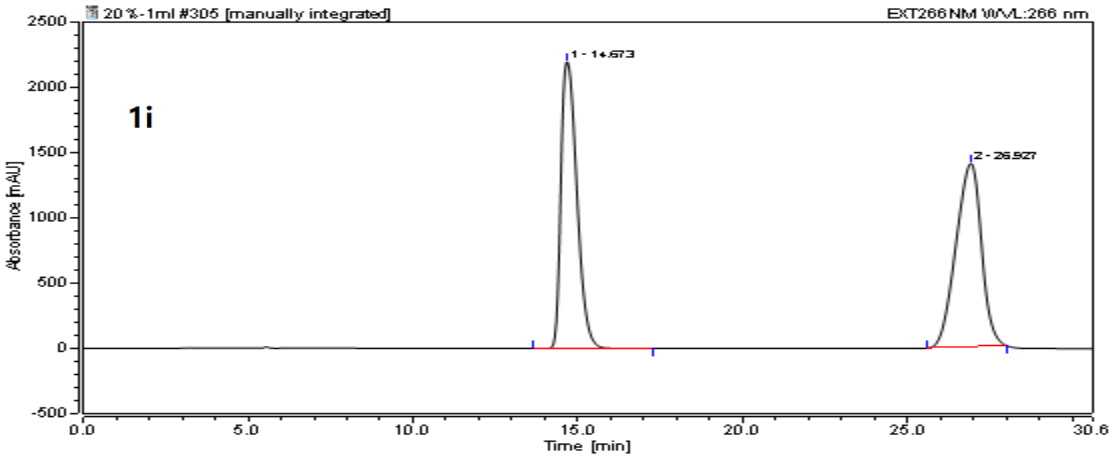


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	12.047	278.679	50.17	n.a.
2	n.a.	25.583	276.824	49.83	n.a.
Total:			**555.503**	**100.00**	

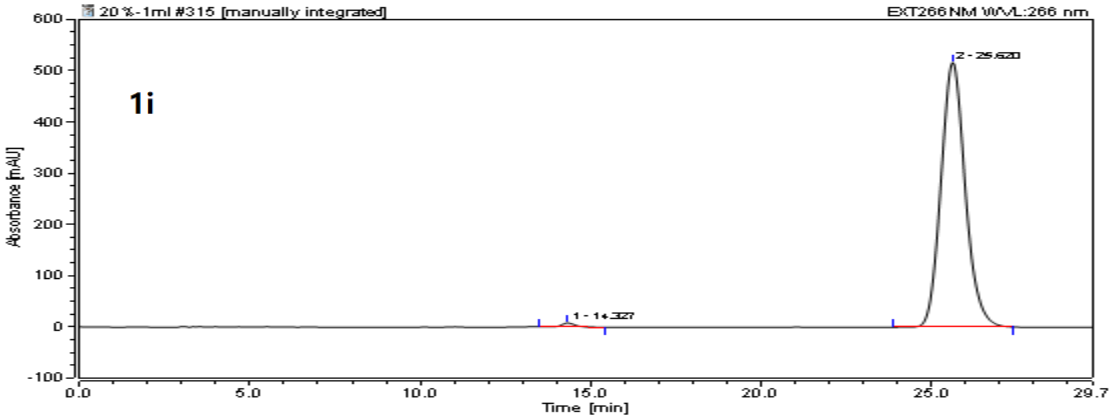


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	12.090	14.302	10.41	n.a.
2	n.a.	25.253	123.085	89.59	n.a.
Total:			**137.387**	**100.00**	

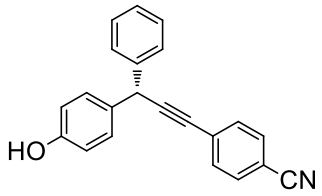


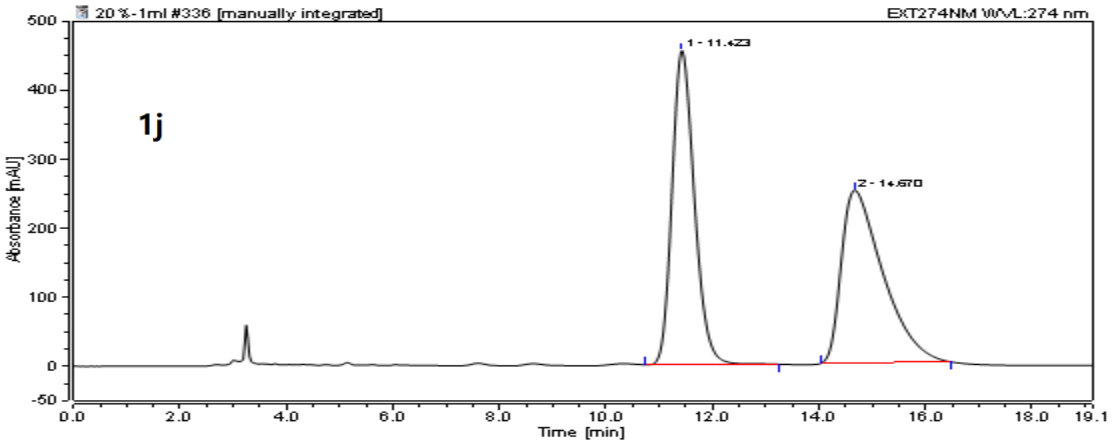


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	14.673	1228.653	49.43	n.a.
2	n.a.	26.927	1256.901	50.57	n.a.
Total:			**2485.554**	**100.00**	

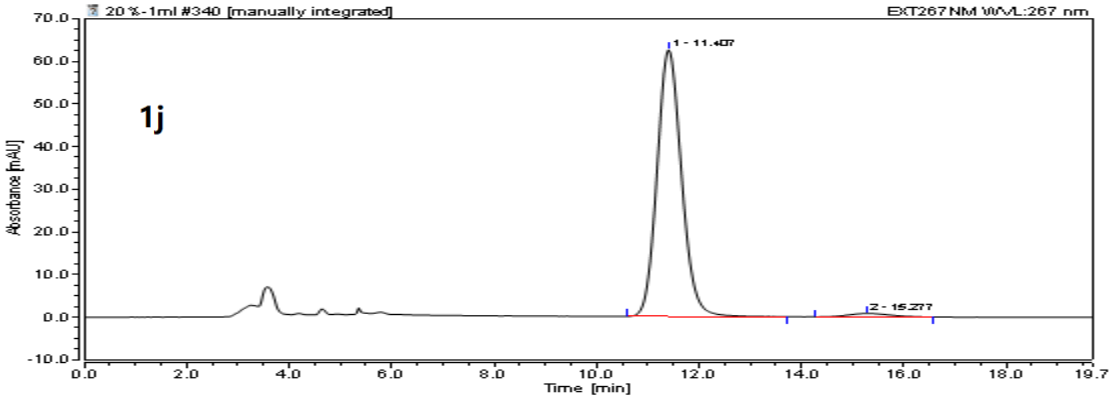


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	14.327	3.455	0.80	n.a.
2	n.a.	25.620	426.016	99.20	n.a.
Total:			**429.471**	**100.00**	

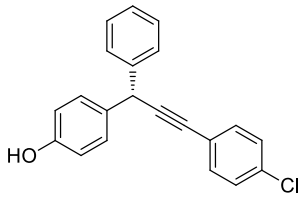


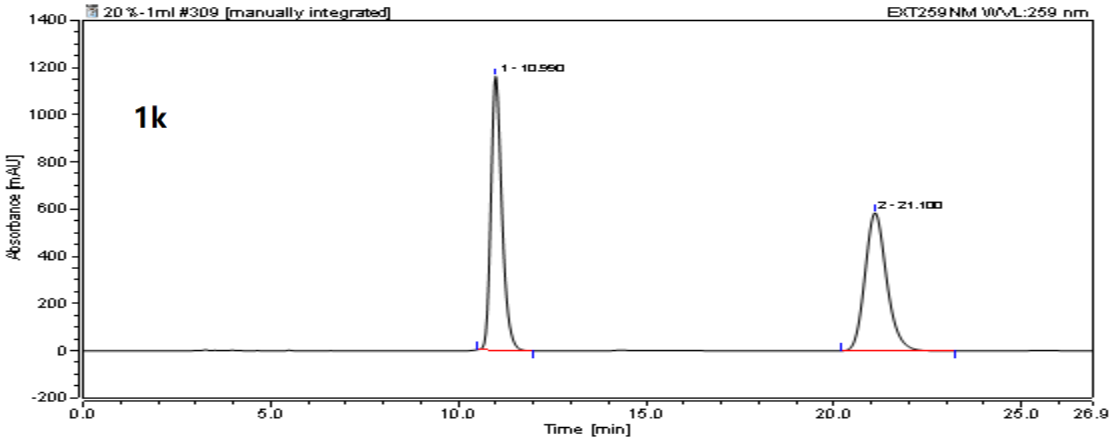


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.423	220.879	49.43	n.a.
2	n.a.	14.670	226.013	50.57	n.a.
Total:			**446.892**	**100.00**	

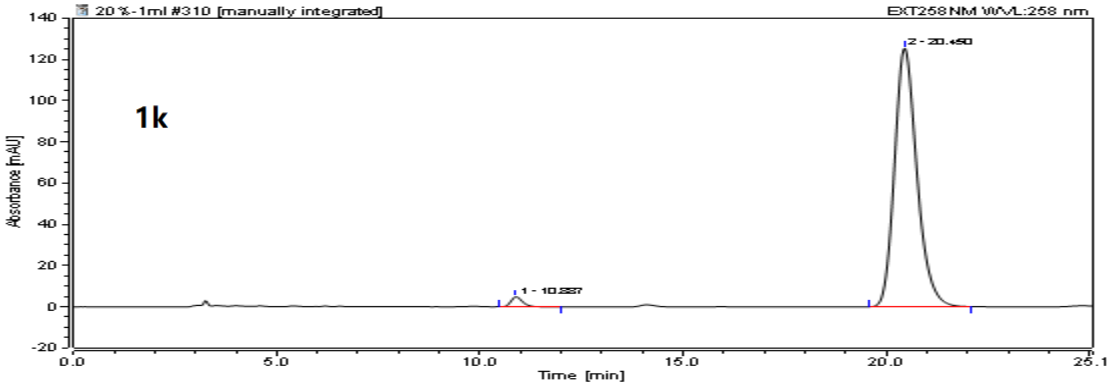


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.407	34.593	97.72	n.a.
2	n.a.	15.277	0.806	2.28	n.a.
Total:			**35.398**	**100.00**	

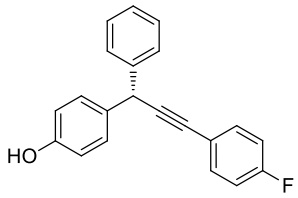


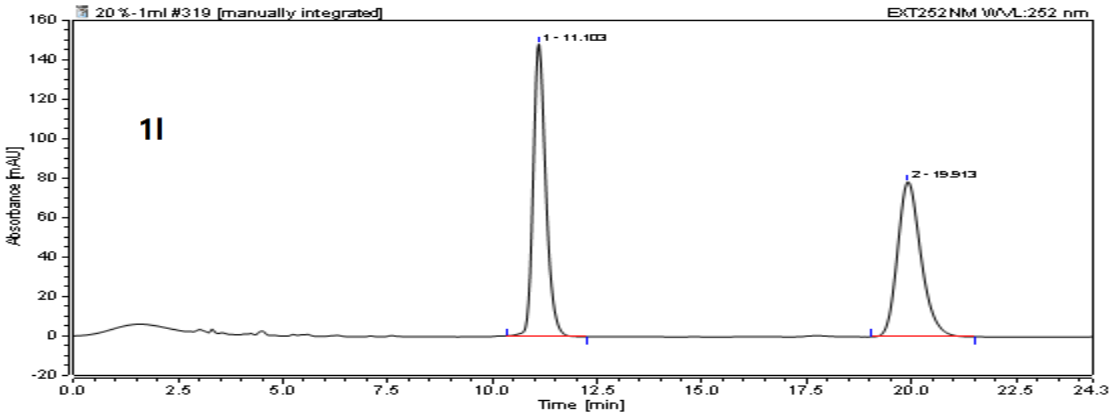


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	10.990	392.785	50.10	n.a.
2	n.a.	21.100	391.263	49.90	n.a.
Total:			**784.047**	**100.00**	

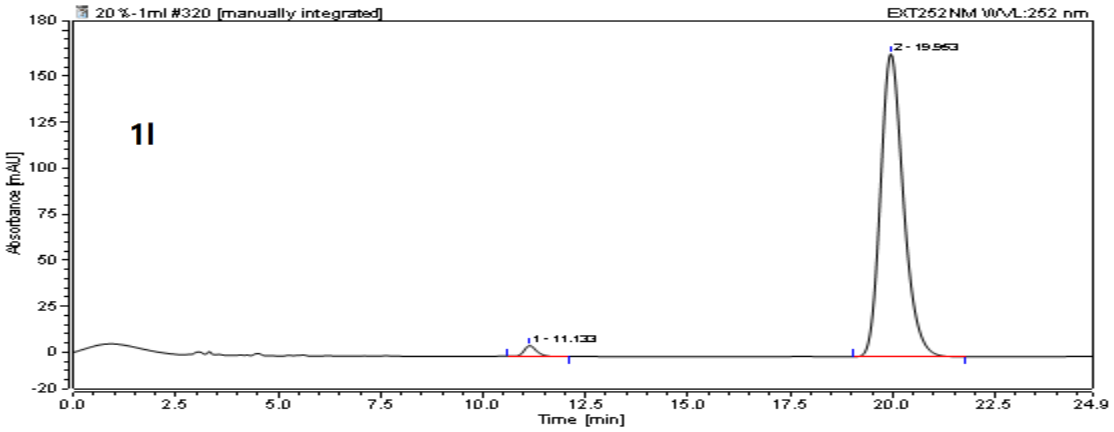


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	10.887	1.568	1.92	n.a.
2	n.a.	20.450	80.140	98.08	n.a.
Total:			**81.708**	**100.00**	

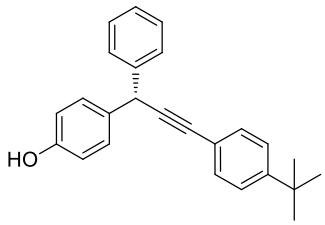


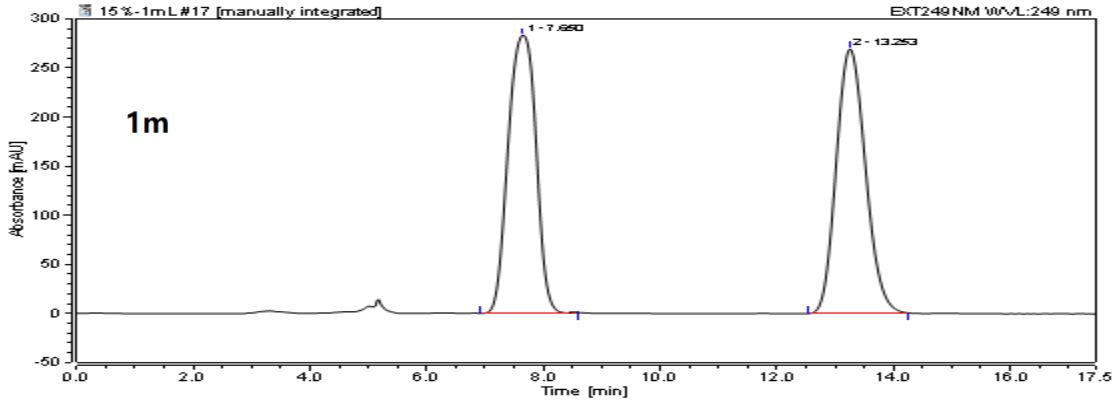


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.103	51.555	50.28	n.a.
2	n.a.	19.913	50.988	49.72	n.a.
Total:			**102.544**	**100.00**	

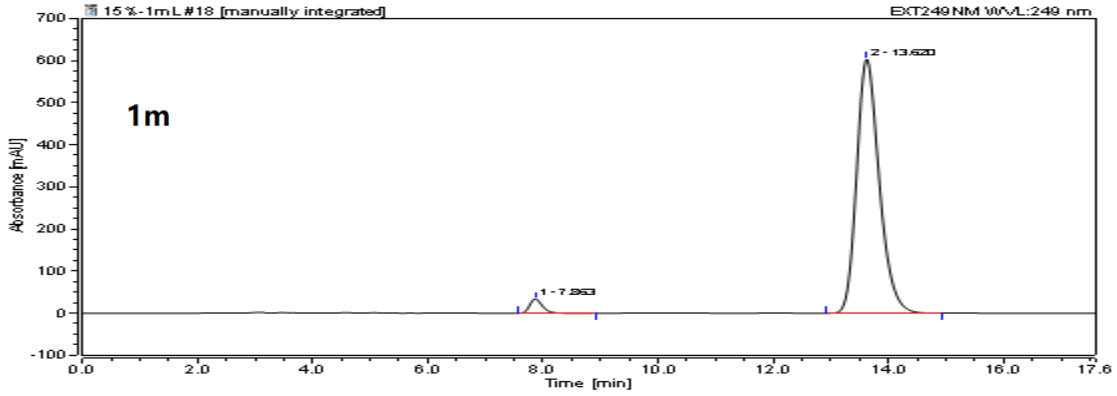


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.133	1.990	1.83	n.a.
2	n.a.	19.953	106.923	98.17	n.a.
Total:			**108.913**	**100.00**	

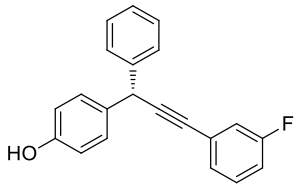


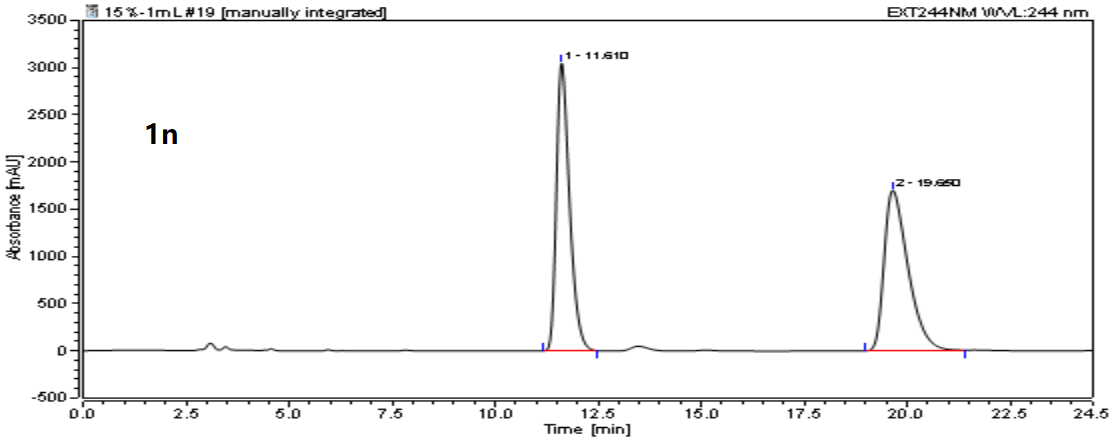


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	7.650	155.937	49.98	n.a.
2	n.a.	13.253	156.048	50.02	n.a.
Total:			**311.985**	**100.00**	

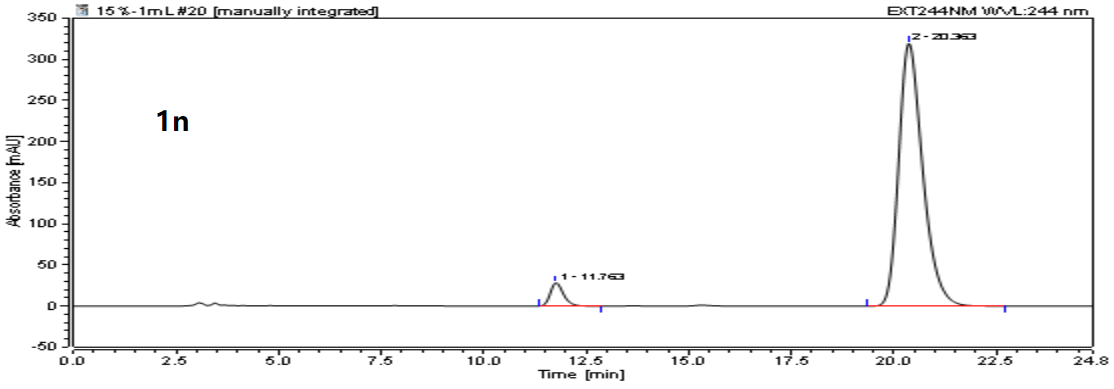


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	7.863	8.603	3.04	n.a.
2	n.a.	13.620	274.493	96.96	n.a.
Total:			**283.095**	**100.00**	

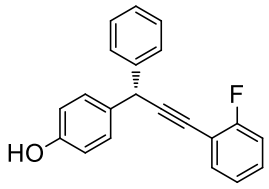


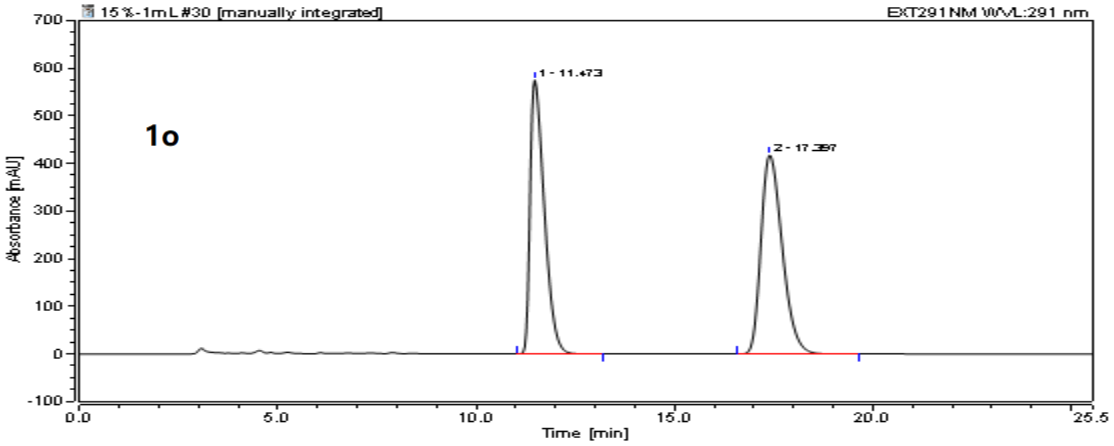


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.610	1130.669	49.84	n.a.
2	n.a.	19.650	1138.090	50.16	n.a.
Total:			**2268.758**	**100.00**	

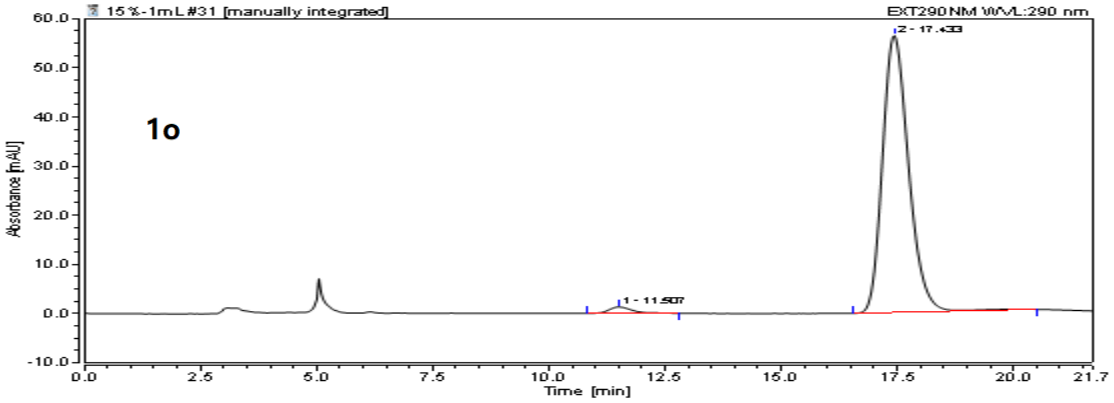


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.763	10.391	4.57	n.a.
2	n.a.	20.363	216.890	95.43	n.a.
Total:			**227.281**	**100.00**	

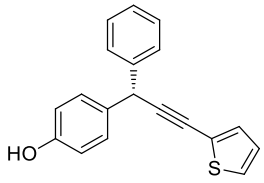


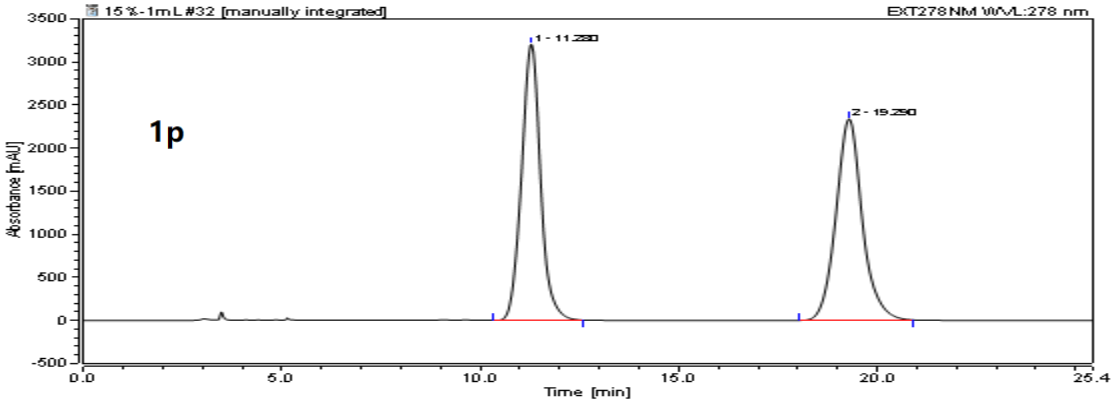


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.473	247.534	49.89	n.a.
2	n.a.	17.397	249.107	50.11	n.a.
Total:			**496.641**	**100.00**	

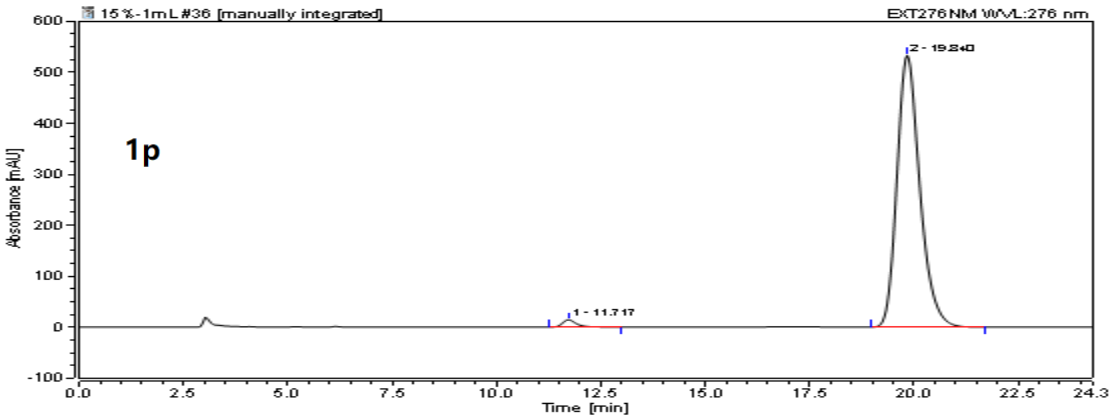


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.507	0.735	1.96	n.a.
2	n.a.	17.433	36.718	98.04	n.a.
Total:			**37.453**	**100.00**	

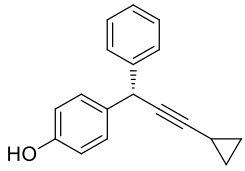


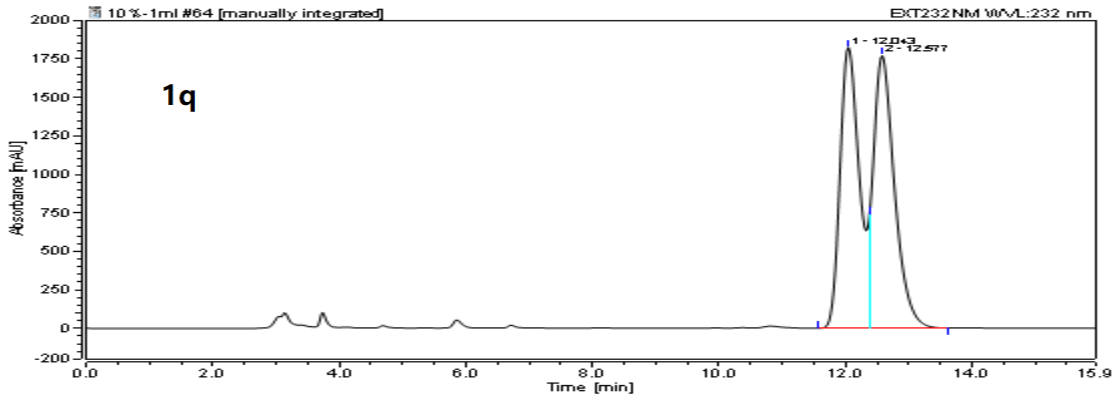


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.280	1775.439	49.76	n.a.
2	n.a.	19.290	1792.699	50.24	n.a.
Total:			**3568.138**	**100.00**	

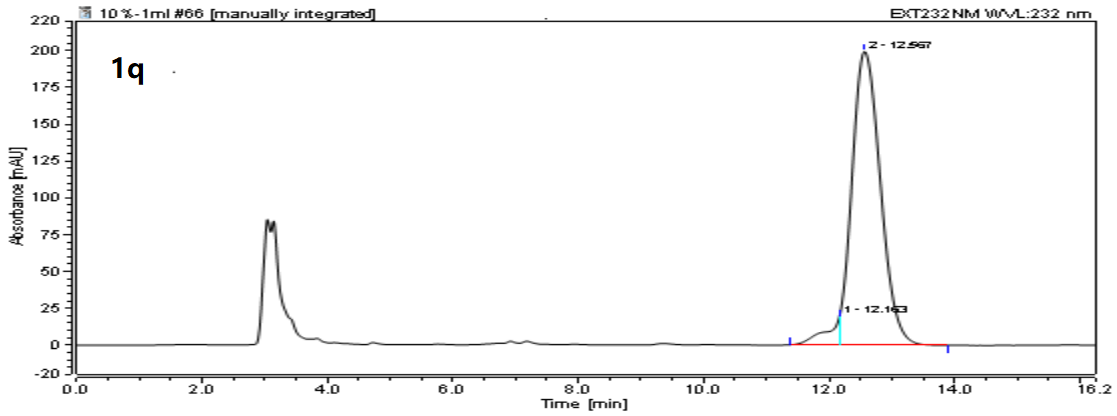


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	11.717	5.650	1.64	n.a.
2	n.a.	19.840	338.288	98.36	n.a.
Total:			**343.939**	**100.00**	

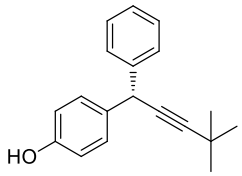


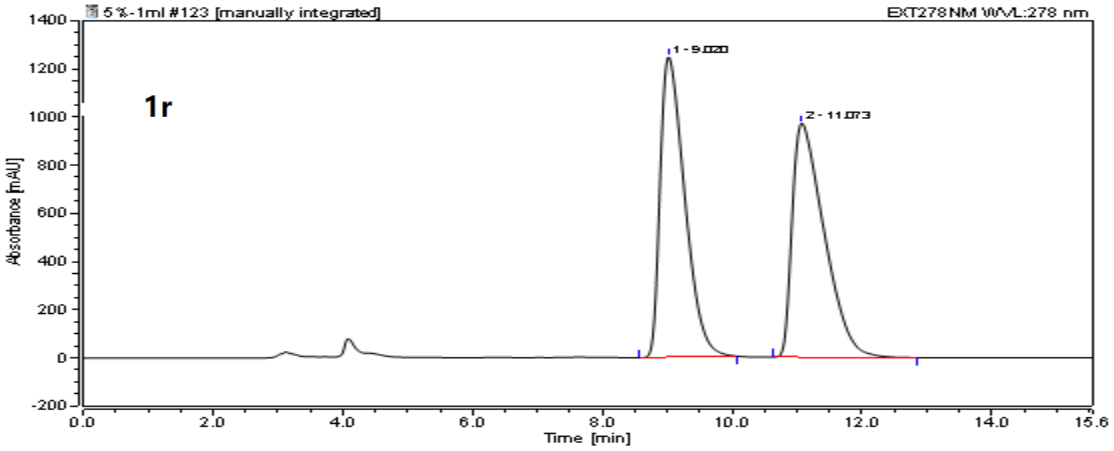


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	12.043	649.729	49.13	n.a.
2	n.a.	12.577	672.641	50.87	n.a.
Total:			**1322.370**	**100.00**	

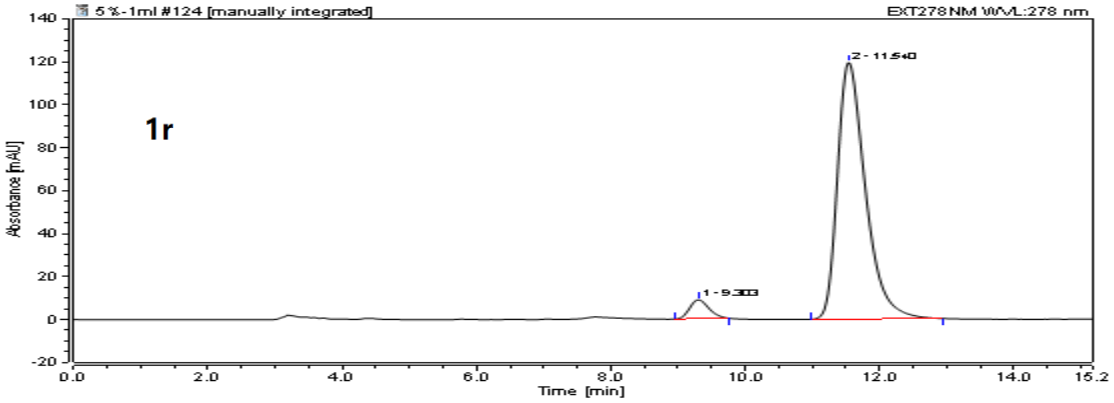


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	12.163	4.728	4.34	n.a.
2	n.a.	12.567	104.261	95.66	n.a.
Total:			**108.990**	**100.00**	

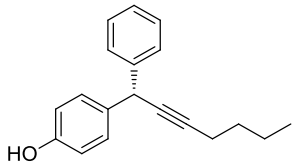


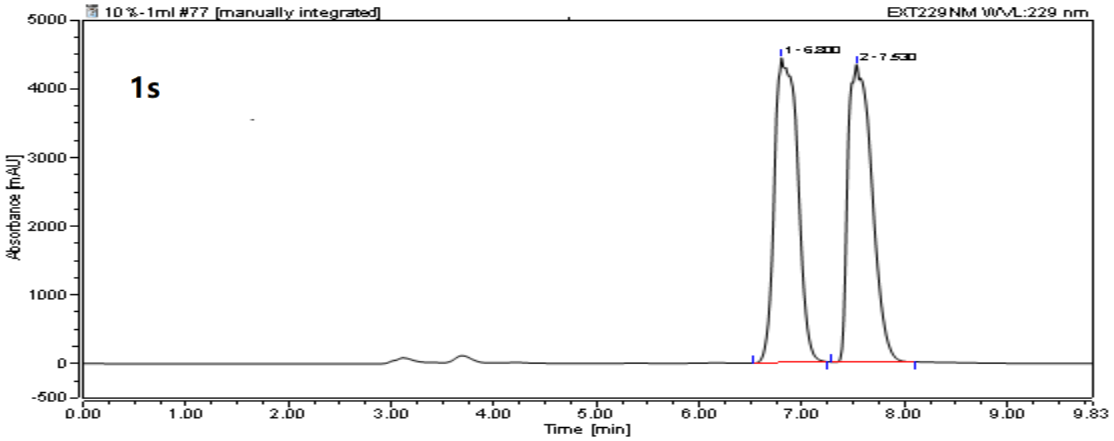


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	9.020	546.513	49.70	n.a.
2	n.a.	11.073	553.155	50.30	n.a.
Total:			**1099.669**	**100.00**	

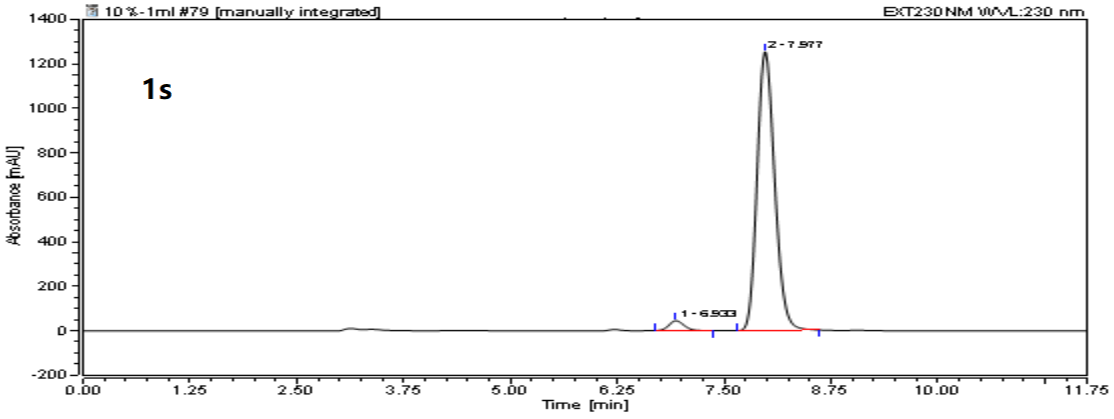


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	9.303	2.949	4.88	n.a.
2	n.a.	11.540	57.498	95.12	n.a.
Total:			**60.446**	**100.00**	

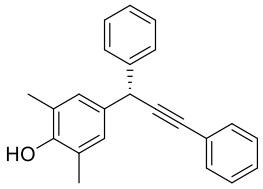


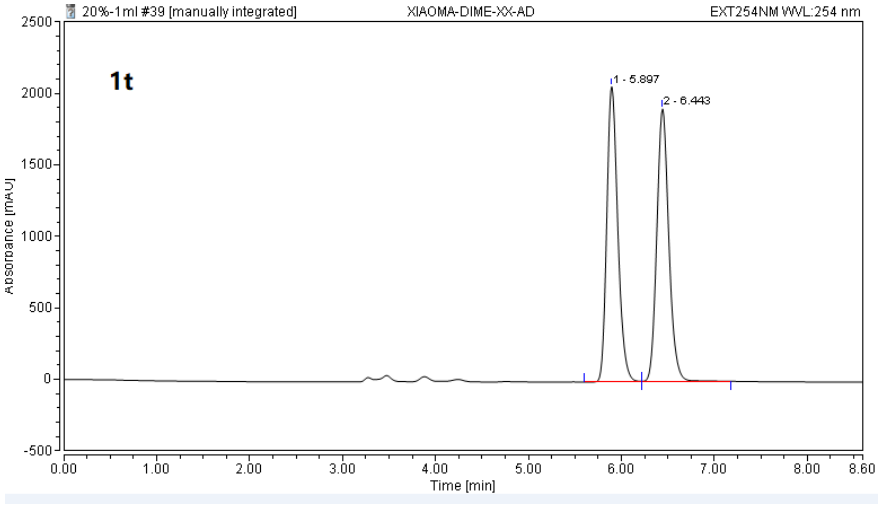


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	6.800	1160.141	49.84	n.a.
2	n.a.	7.530	1167.778	50.16	n.a.
Total:			**2327.919**	**100.00**	

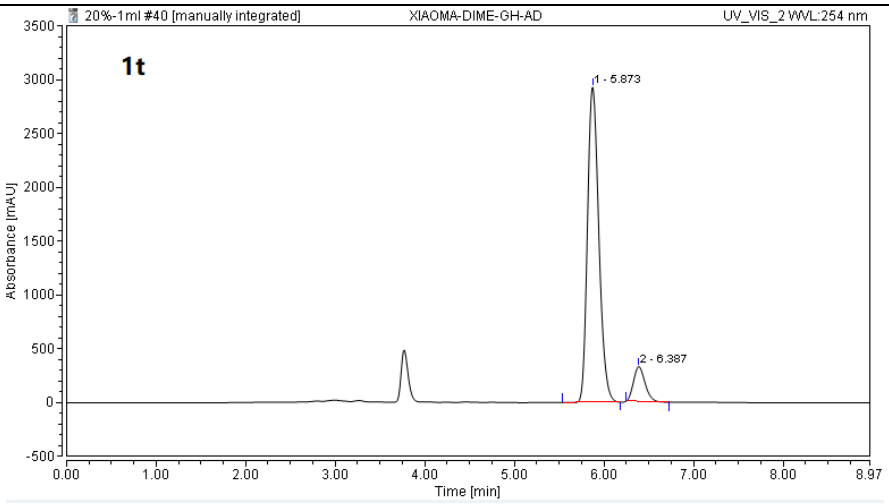


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	6.933	9.079	2.95	n.a.
2	n.a.	7.977	298.353	97.05	n.a.
Total:			**307.432**	**100.00**	

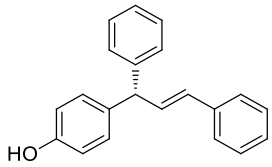


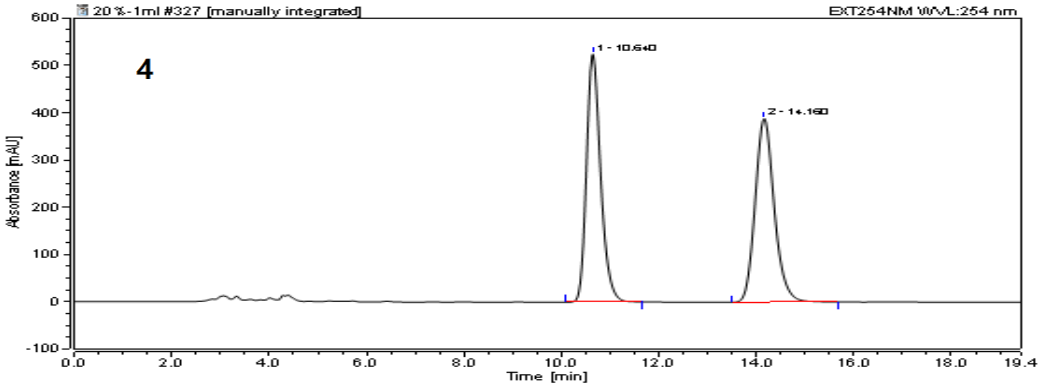


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	5.897	283.009	49.68	n.a.
2	n.a.	6.443	286.616	50.32	n.a.
Total:			**569.625**	**100.00**	

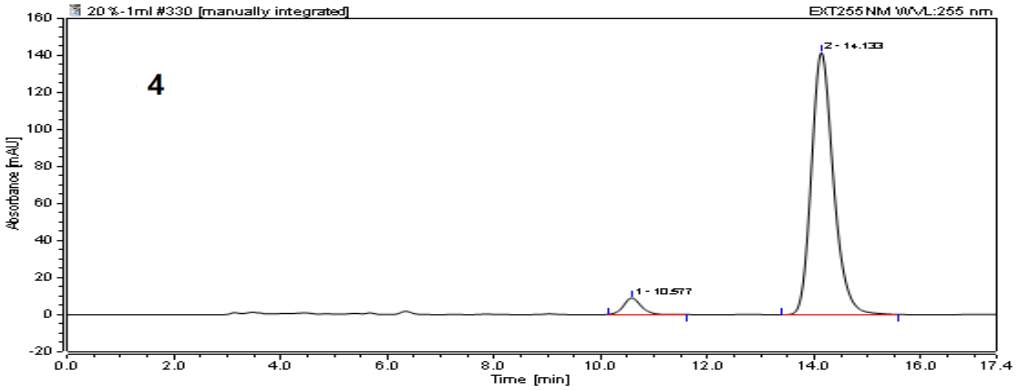


Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	5.873	429.298	90.03	n.a.
2	n.a.	6.387	47.538	9.97	n.a.
Total:			**476.837**	**100.00**	





Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	10.640	176.179	49.98	n.a.
2	n.a.	14.160	176.294	50.02	n.a.
Total:			**352.473**	**100.00**	



Integration Results					
No.	Peak Name	Retention Time min	Area mAU*min	Relative Area %	Amount n.a.
1	n.a.	10.577	3.353	4.72	n.a.
2	n.a.	14.133	67.609	95.28	n.a.
Total:			**70.961**	**100.00**	