Supporting Information

Metalloradical Activation of In Situ-Generated α-Alkynyldiazomethanes for Asymmetric Radical Cyclopropanation of Alkenes

Jing Ke, Wan-Chen Cindy Lee, Xiaoxu Wang, Yong Wang, Xin Wen, and X. Peter Zhang*

*Department of Chemistry, Merkert Chemistry Center, Boston College

Chestnut Hill, Massachusetts 02467, United States

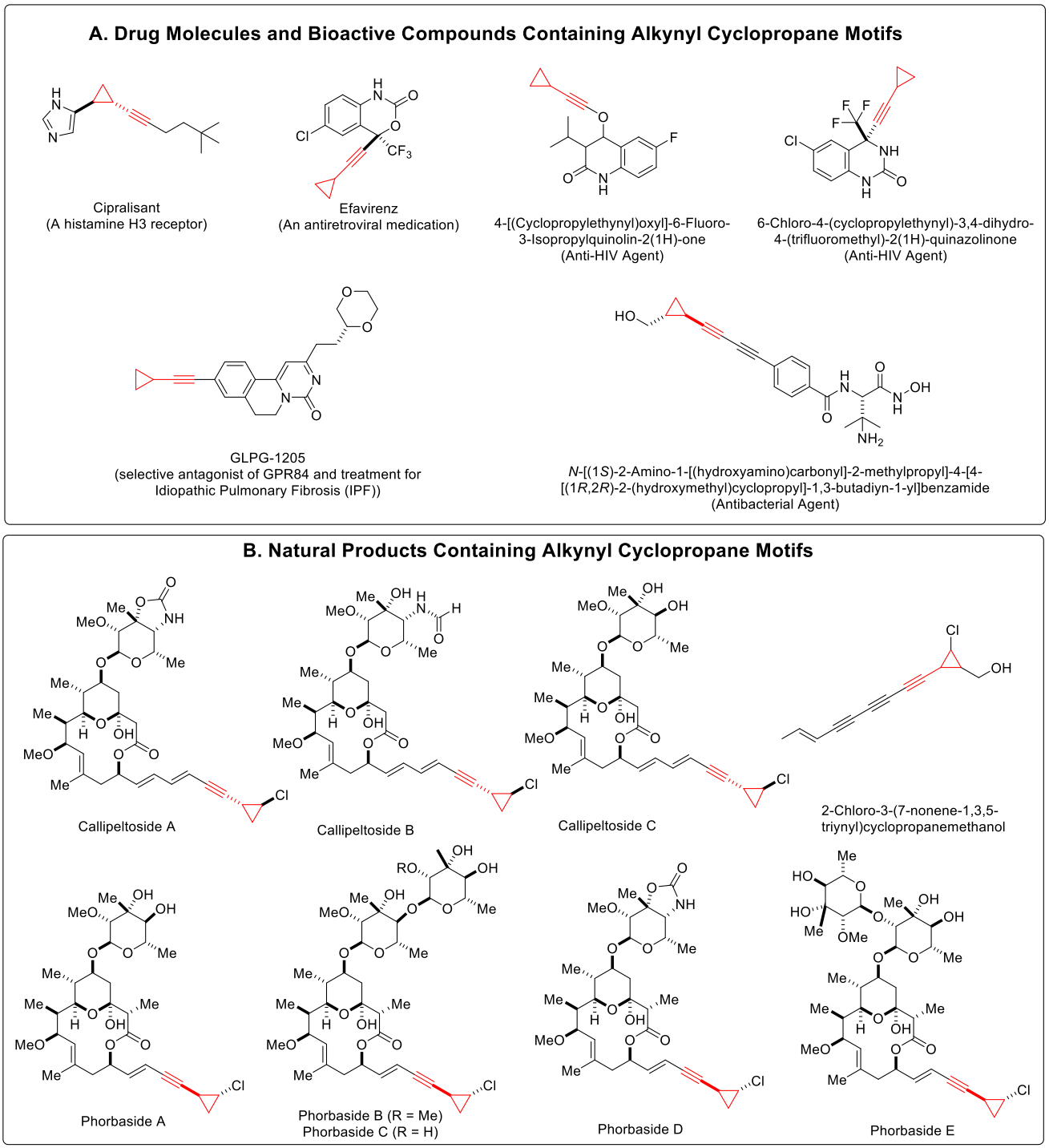
Corresponding author Email: peter.zhang@bc.edu

Table of Contents

1. General Considerations

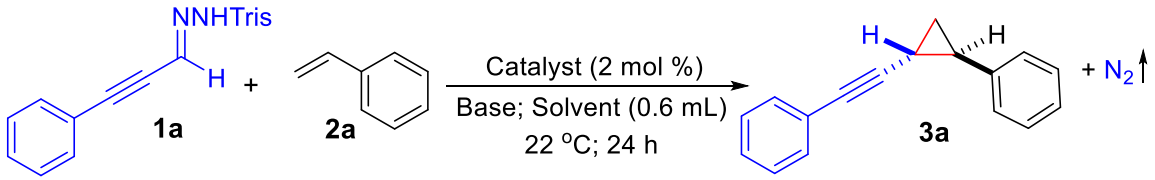
All cyclopropanation reactions were performed in anhydrous solvents under N_2 atmosphere in an oven-dried glassware following standard Schlenk techniques. Gas tight syringes were used to transfer liquid reagents and solvents in catalytic reactions. Solvent was freshly distilled/degassed prior to use unless otherwise noted. Thin layer chromatography was performed on Merck TLC plates (silica gel 60 F254). Flash column chromatography was performed with ICN silica gel (60 Å, 230-400 mesh, 32-63 μm). ^{1}H NMR spectra were acquired using Varian INOVA 400 (400 MHz), Bruker 500 (500 MHz), or Varian INOVA 600 (600 MHz) spectrometer. Chemical shifts were internally referenced to residual solvent peak ($CHCl_3$ δ = 7.26 ppm). Data were reported as follows: chemical shift (ppm), integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, hept = heptet, m = multiplet), and coupling constants *J* (Hz). ^{13}C NMR spectra were acquired using Bruker 500 (126 MHz), or INOVA 600 (151 MHz) spectrometer with complete proton decoupling. Chemical shifts were reported in ppm with residual solvent peak ($CDCl_3$ δ = 77.16 ppm) as the internal standard. ^{19}F NMR spectrum was acquired using Varian INOVA 600 (564 MHz) spectrometer. Infrared spectra were measured with a Nicolet Avatar 320 spectrometer with a Smart Miracle accessory. Optical rotations were measured on a Rudolph Research Analytical AUTOPOL® IV digital polarimeter. HPLC measurements were carried out on a Shimadzu HPLC system with Chiralcel OD-H, IA, IB, IC, ID, and IE columns. High-resolution mass spectrometry (DART and ESI) was performed at the Mass Spectrometry Facility, Boston College, Chestnut Hill, MA. The X-ray diffraction data were collected using Bruker-AXS SMART-APEXII CCD diffractometer. All reagents were purchased either from Aldrich, Alfa Aesar, Acros, Ak Sci, Oakwood Chemicals, Strem Chemicals or TCI and were used without further purification.

2. Figure S1: Selected Examples of Bioactive Compounds Containing Alkynyl Cyclopropanes



3. Scheme S1. Solvent and Base Effect on Radical Cyclopropanation

A 10 mL oven-dried Schlenk tube was charged with *N*-sulfonyl hydrazone **1a** (0.10 mmol, 1.0 equiv), [Co(Por)] (2 mol %) and Base. The Schlenk tube was capped with a Teflon screw cap, evacuated and backfilled with nitrogen 3 times. Under nitrogen atmosphere, styrene **2a** (0.20 mmol, 2.0 equiv) and anhydrous solvent (0.6 mL) were added. The Schlenk tube was then purged with nitrogen for 1 min and sealed with the Teflon screw cap. The reaction mixture was stirred at 22°C for 24 h. Following completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum and purified by flash column chromatography.



Catalyst	Base	Solvent	Yield (%)	dr	ee (%)
[Co(**P1**)]	Cs_2CO_3 (2.0 equiv)	Tetrahydrofuran	14	54:46	N/A
[Co(**P1**)]	Cs_2CO_3 (2.0 equiv)	1,4-Dioxane	5	57:43	N/A
[Co(**P1**)]	Cs_2CO_3 (2.0 equiv)	Benzene	19	54:46	N/A
[Co(**P1**)]	Cs_2CO_3 (2.0 equiv)	Toluene	26	52:48	N/A
[Co(**P1**)]	Cs_2CO_3 (2.0 equiv)	Methanol	25	56:44	N/A
[Co(**P3**)]	Cs_2CO_3 (2.0 equiv)	Methanol	38	77:23	53
[Co(**P3**)]	Na_2CO_3 (2.0 equiv)	Methanol	21	77:23	53
[Co(**P3**)]	K_2CO_3 (2.0 equiv)	Methanol	28	77:23	53
[Co(**P3**)]	Et_3N (2.0 equiv)	Methanol	32	72:26	51
[Co(**P3**)]	Hunnig's Base (2.0 equiv)	Methanol	16	72:28	51
[Co(**P3**)]	KO^tBu (2.0 equiv)	Methanol	33	77:23	53
[Co(**P3**)]	KH (2.0 equiv)	Methanol	46	77:23	53
[Co(**P3**)]	KH (2.0 equiv)	Ethyl Acetate	76	79:21	53
[Co(**P3**)]	KH (4.0 equiv)	Ethyl Acetate	98	79:21	53

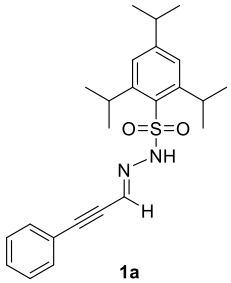
4. Synthesis and Characterization of *N*-Sulfonyl Hydrazones

4.1. Experimental Procedure for Preparation of *N*-2,4,6-Triisopropylbenzenesulfonyl Hydrazones

To a stirred solution of 2,4,6-triisopropylbenzenesulfonyl hydrazide (1.0 mmol) in THF (10.0 mL) at room temperature, aldehyde (1.0 equiv) was added dropwise (or portionwise if solid).[1] After the reaction was stirred overnight, the solvent was removed directly under reduced pressure, and the crude mixture was further purified by trituration.

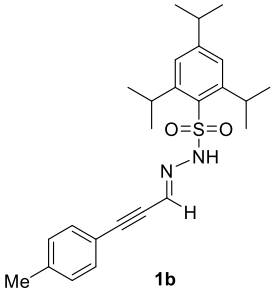
4.2. Characterization of *N*-2,4,6-Triisopropylbenzenesulfonyl Hydrazones

3-Phenylpropiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone (**1a**) Yield: 87%. R_f = 0.30 (Hexane/Ethyl Acetate: 7/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.78 (s, 1H), 7.51 (d, *J* = 7.9 Hz, 2H), 7.45 (t, *J* = 7.1 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.19 (s, 2H), 6.82 (s, 1H), 4.21 (hept, *J* = 6.7 Hz, 2H), 2.91 (hept, *J* = 6.9 Hz, 1H), 1.28 (d, *J* = 6.7 Hz, 12H), 1.26 (d, *J* = 6.7 Hz, 6H).^{13}C NMR (151 MHz, $CDCl_3$) δ 153.71, 151.27, 132.19, 131.32, 130.48, 128.86, 124.39, 124.05, 120.41, 103.24, 77.75, 34.33, 30.15, 24.92, 23.66. IR (neat, cm^{-1}): 3208.36, 2959.66, 2929.18, 2869.34, 2198.09, 1599.13, 1560.44, 1488.75, 1462.75, 1425.72, 1335.96, 1167.42, 1036.71, 923.23, 757.24, 669.57. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{24}H_{31}N_2O_2S^+$: 411.21008, found: 441.20865.



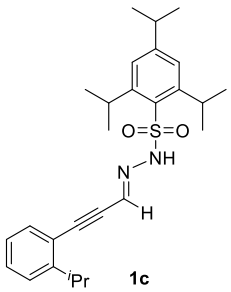
1a

3-(*p*-Tolyl)propiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone (**1b**) Yield: 79%. R_f = 0.3 (Hexane/Ethyl Acetate: 10/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.74 (s, 1H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.18 (s, 2H), 6.80 (s, 1H), 4.27 – 4.14 (m, 2H), 2.91 (dt, *J* = 13.8, 6.9 Hz, 1H), 2.40 (s, 3H), 1.27 (dd, *J* = 13.1, 6.8 Hz, 18H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.67, 151.26, 141.11, 132.13, 131.37, 129.66, 124.71, 124.04, 117.33, 103.74, 77.40, 34.34, 30.16, 24.93, 23.67, 21.84. IR (neat, cm^{-1}): 3211.65, 2959.77, 2869.33, 2361.17, 2188.25, 1599.64, 1560.02, 1462.85, 1425.73, 1363.41, 1335.65, 1167.63, 1036.70, 924.00, 726.73. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{25}H_{33}N_2O_2S^+$: 425.22573, found: 425.22601.



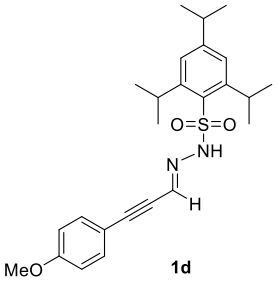
1b

3-(2-Isopropylphenyl)propiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone (**1c**) Yield: 90%. R_f = 0.3 (Hexane/Ethyl Acetate: 10/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.73 (s, 1H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.19 (s, 2H), 6.85 (s, 1H), 4.21 (hept, *J* = 6.7 Hz, 2H), 3.38 (hept, *J* = 6.9 Hz, 1H), 2.91 (hept, *J* = 6.9 Hz, 1H), 1.31 (d, *J* = 6.9 Hz, 6H), 1.28 (d, *J* = 6.8 Hz, 12H), 1.26 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.71, 151.32, 151.31, 133.14, 131.35, 130.97, 126.13, 125.46, 124.55, 124.05, 119.27, 102.41, 81.49, 34.34, 32.22, 30.18, 24.93, 23.67, 23.25. IR (neat, cm^{-1}): 3209.06, 2960.58, 2869.78, 2360.30, 2189.14, 1599.32, 1462.76, 1383.26, 1337.01, 1168.12, 1036.66, 758.10, 665.98. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{27}H_{37}N_2O_2S^+$: 453.25703, found: 453.25706.



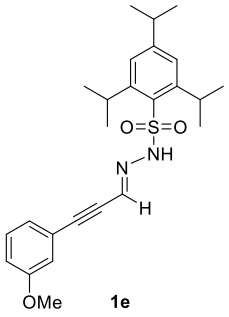
1c

3-(4-Methoxyphenyl)propiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone (**1d**) Yield: 85%. R_f = 0.3 (Hexane/Ethyl Acetate: 8/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.79 (s, 1H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.19 (s, 2H), 6.90 (d, *J* = 8.6 Hz, 2H), 6.80 (s, 1H), 4.22 (dt, *J* = 13.3, 6.7 Hz, 2H), 3.85 (s, 3H), 2.91 (dt, *J* = 13.8, 6.9 Hz, 1H), 1.27 (dd, *J* = 10.4, 7.0 Hz, 18H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.32, 153.62, 151.21, 133.91, 131.36, 124.95, 124.00, 114.53, 112.27, 103.84, 77.14, 55.54, 34.30, 30.11, 24.90, 23.63. IR (neat, cm^{-1}): 3209.86, 2959.06, 2869.51, 2359.98, 2193.19, 1598.06, 1463.31, 1425.28, 1336.01, 1291.42, 1121.29, 1167.09, 1037.64, 943.18, 726.20, 666.89. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{25}H_{33}N_2O_3S^+$: 441.22064, found: 441.22142.



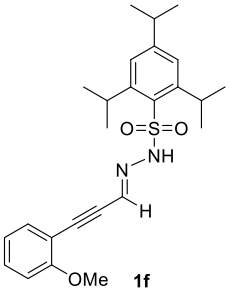
1d

3-(3-Methoxyphenyl)propiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone (**1e**) Yield: 85%. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.76 (s, 1H), 7.31 (td, *J* = 7.7, 0.9 Hz, 1H), 7.19 (s, 2H), 7.10 (dt, *J* = 7.6, 1.1 Hz, 1H), 7.05 – 6.97 (m, 2H), 6.81 (s, 1H), 4.20 (hept, *J* = 6.7 Hz, 2H), 3.84 (s, 3H), 2.92 (dq, *J* = 13.8, 6.9 Hz, 1H), 1.36 – 1.24 (m, 18H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.63, 153.73, 151.27, 131.30, 129.99, 124.73, 124.33, 124.06, 121.33, 117.12, 116.83, 103.15, 77.46, 55.57, 34.34, 30.16, 24.93, 23.66. IR (neat, cm^{-1}): 3212.24, 2959.37, 2868.99, 2360.27, 2188.31, 1603.09, 1508.39, 1296.65, 1252.94, 1167.55, 1035.00, 833.52, 750.11. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{25}H_{33}N_2O_3S^+$: 441.22064, found: 441.22163.



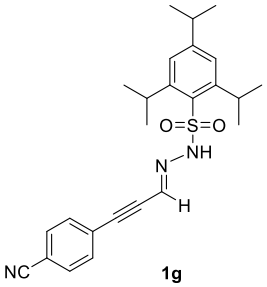
1e

3-(2-Methoxyphenyl)propiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone drazide (**1f**) Yield: 85%. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.66 (s, 1H), 7.46 – 7.43 (m, 1H), 7.40 (d, *J* = 7.5 Hz, 1H), 7.18 (s, 2H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.98 (t, *J* = 7.5 Hz, 1H), 6.74 (s, 1H), 4.31 – 4.24 (m, 2H), 4.10 (s, 3H), 2.94 – 2.87 (m, 1H), 1.26 (dd, *J* = 6.8, 3.7 Hz, 18H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.72, 153.38, 151.03, 132.33, 132.21, 131.81, 124.00, 123.90, 120.90, 110.64, 109.74, 101.19, 83.83, 55.99, 34.24, 29.93, 24.87, 23.61. IR (neat, cm^{-1}): 3213.01, 2959.30, 2869.23, 2359.28, 2187.85, 1598.14, 1487.99, 1464.79, 1337.88, 1266.21, 1166.70, 1035.71, 1019.62, 753.08, 668.66. HRMS (DART) ([M+H]$^+$) Calcd. for Calcd. for $C_{25}H_{33}N_2O_3S^+$: 441.22064, found: 441.22216.



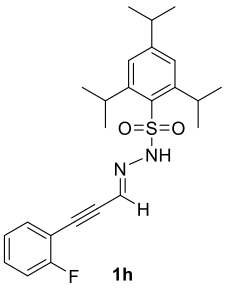
1f

4-(3-Oxoprop-1-yn-1-yl)benzonitrile 2,4,6-triisopropylbenzenesulfonyl hydrazone (**1g**) Yield: 90%. R_f = 0.3 (Hexane/Ethyl Acetate: 15/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.90 (s, 1H), 7.72 – 7.64 (m, 2H), 7.62 – 7.57 (m, 2H), 7.19 (s, 2H), 6.82 (s, 1H), 4.19 (hept, *J* = 6.7 Hz, 2H), 2.91 (hept, *J* = 6.9 Hz, 1H), 1.31 – 1.21 (m, 18H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.99, 151.36, 132.67, 132.44, 131.04, 125.17, 124.12, 122.99, 118.01, 113.82, 100.35, 80.98, 34.35, 30.14, 24.90, 23.66. IR (neat, cm^{-1}): 3207.45, 2962.26, 2229.10, 1598.26, 1380.52, 1332.57, 1219.45, 1166.34, 1037.44. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{25}H_{30}N_3O_2S^+$: 436.20532, found: 436.20638.

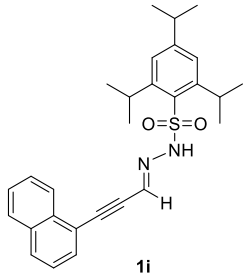


1g

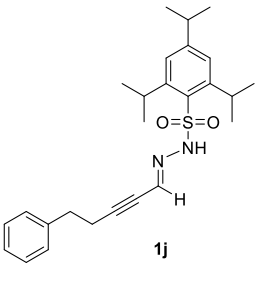
3-(2-Fluorophenyl)propiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone (**1h**) Yield: 91%. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 7.40 (t, *J* = 7.2 Hz, 1H), 7.35 – 7.29 (m, 2H), 7.22 (s, 2H), 7.06 (dt, *J* = 17.7, 8.2 Hz, 2H), 4.29 – 4.21 (m, 2H), 2.96 – 2.88 (m, 1H), 1.33 (d, *J* = 6.8 Hz, 12H), 1.27 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.89 (d, *J* = 253.6 Hz), 153.84, 151.69, 133.75, 131.30 (d, *J* = 8.0 Hz), 131.02, 128.89, 124.18 (d, *J* = 3.7 Hz), 124.15, 115.71 (d, *J* = 20.6 Hz), 110.47 (d, *J* = 15.5 Hz), 88.77 (d, *J* = 3.1 Hz), 87.26, 34.32, 30.20, 24.93, 23.62. ^{19}F NMR (564 MHz, $CDCl_3$): –113.83. IR (neat, cm^{-1}): 3202.62, 2960.19, 2870.09, 2197.93, 2078.94, 1599.11, 1489.80, 1459.77, 1426.07, 1363.70, 1336.84, 1260.07, 1167.91, 1058.83, 1036.83, 941.02, 821.70. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{24}H_{30}FN_2O_2S^+$: 429.20065, found: 429.19980.



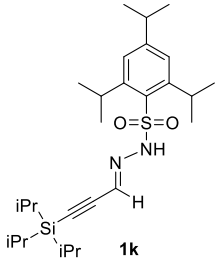
3-(Naphthalen-1-yl)propiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone (**1i**) Yield: 93%. R_f = 0.3 (Hexane/Ethyl Acetate: 15/1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.88 (s, 1H), 8.20 (d, *J* = 8.3 Hz, 1H), 7.97 (d, *J* = 8.3 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.78 (d, *J* = 7.0 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.59 (dd, *J* = 11.0, 4.0 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.20 (s, 2H), 6.98 (s, 1H), 4.25 (dt, *J* = 13.5, 6.7 Hz, 2H), 2.92 (dt, *J* = 13.8, 6.9 Hz, 1H), 1.29 (d, *J* = 6.8 Hz, 12H), 1.27 (d, *J* = 6.9 Hz, 6H).^{13}C NMR (151 MHz, $CDCl_3$) δ 153.75, 151.31, 133.25, 132.90, 132.11, 131.34, 131.21, 128.82, 127.84, 127.12, 125.51, 125.35, 124.45, 124.08, 117.99, 101.65, 82.29, 34.35, 30.21, 24.96, 23.67. IR (neat, cm^{-1}): 3210.51, 2959.06, 2868.68, 2184.79. 1599.00, 1461.98, 1425.64, 1334,26, 1166.76, 1105.60, 1035.93. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{28}H_{33}N_2O_2S^+$: 461.22573, found: 461.22563.



3-(Phenylethyl)propiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone (**1j**) Yield: 82%. R_f =0.3 (Hexanes/Ethyl Acetate = 10/1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (s, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.30 – 7.22 (m, 3H), 7.16 (s, 2H), 6.53 (d, *J* = 1.7 Hz, 1H), 4.12 (hept, *J* = 6.7 Hz, 2H), 2.96 – 2.84 (m, 3H), 2.77 (t, *J* = 7.2 Hz, 2H), 1.26 (s, 6H), 1.24 (d, *J* = 7.0 Hz, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.55, 151.21, 139.57, 131.40, 128.96, 128.40, 127.03, 124.73, 123.97, 104.84, 71.29, 34.30, 34.26, 30.00, 24.85, 23.64, 21.94. IR (neat, cm^{-1}): 3215.93, 2958.77, 2209.25, 1599.51, 1425.21, 1334.27, 1167.71, 1035.85. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{26}H_{35}N_2O_2S^+$: 439.2413, found: 439.2418.



3-(Triisopropylsilyl)propiolaldehyde 2,4,6-triisopropylbenzenesulfonyl hydrazone hydrazide (**1k**) Yield: 80%. R_f = 0.3 (Hexane/Ethyl Acetate: 25:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.72 (s, 1H), 7.18 (s, 2H), 6.60 (s, 1H), 4.25 – 4.12 (m, 2H), 2.90 (hept, *J* = 6.9 Hz, 1H), 1.26 (dd, *J* = 6.8, 5.4 Hz, 18H), 1.15 – 1.10 (m, 21H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.68, 151.32, 131.41, 124.03, 123.94, 108.69, 94.38, 34.35, 30.19, 24.99, 23.67, 18.68, 11.13. IR (neat, cm^{-1}): 3209.88, 2960.97, 2866.10, 2361.47, 2341.66, 1599.80, 1550.36, 1462.13, 1425.85, 1380.21, 1363.82, 1335.33,



1172.34, 1103.99, 1070.21, 1037.47, 1019.85, 941.06, 922.35, 882.85, 757.41, 730.62. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{27}H_{47}N_2O_2SSi^+$: 491.31220, found: 491.31171.

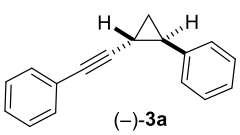
5. Synthesis and Characterization of Alkynyl Cyclopropanes

5.1. Experimental Procedure for [Co(Por)]-Catalyzed Asymmetric Cyclopropanation

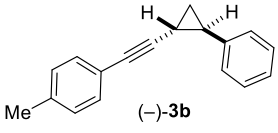
A 10 mL oven-dried Schlenk tube was charged with *N*-sulfonyl hydrazone (0.10 mmol, 1.0 equiv), [Co(Por)] (2 mol %) and KH (0.40 mmol, 4.0 equiv). The Schlenk tube was capped with a Teflon screw cap, evacuated and backfilled with nitrogen 3 times. Under nitrogen atmosphere, olefin (0.20 mmol, 2.0 equiv) and anhydrous ethyl acetate (0.6 mL) were added. The Schlenk tube was then purged with nitrogen for 1 min and sealed with the Teflon screw cap. The reaction mixture was stirred at 22°C for 24 h. Following completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum and purified by flash column chromatography.

5.2. Characterization of Alkynyl Cyclopropane Products

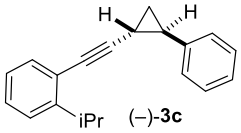
((1*R*,2*R*)-(2-Phenylcyclopropyl)ethynyl)benzene ((–)-**3a**) Yield: 90%. dr: 87:13. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-192.98° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.39 (m, 2H), 7.33 – 7.27 (m, 5H), 7.21 – 7.18 (m, 1H), 7.15 – 7.12 (m, 2H), 2.37 (ddd, *J* = 8.8, 6.1, 4.6 Hz, 1H), 1.72 (ddd, *J* = 8.7, 5.6, 4.6 Hz, 1H), 1.45 – 1.41 (m, 1H), 1.37 – 1.33 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.89, 131.76, 128.57, 128.35, 127.75, 126.38, 126.12, 123.86, 92.05, 77.19, 26.74, 18.18, 12.22. IR (neat, cm^{-1}): 3030.36, 2959.46, 2926.32, 2360.59, 2225.21, 1976.75, 1598.37, 1491.23, 1457.55, 1178.57, 1070.09, 911.31, 755.37, 691.47. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{17}H_{15}^+$: 219.11683, found 219.11631. HPLC analysis: ee = 96%. IC (100% hexanes, 0.8 mL/min): t_{major} = 14.56 min, t_{minor} = 17.34 min.



1-Methyl-4-(((1*R*,2*R*)-2-phenylcyclopropyl)ethynyl)benzene ((–)-**3b**) Yield: 90%. dr: 79:21. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-187.98° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 4H), 7.19 (t, J = 7.4 Hz, 1H), 7.14 – 7.09 (m, 4H), 2.41 – 2.35 (m, 1H), 2.34 (s, 3H), 1.70 (dt, J = 9.6, 5.0 Hz, 1H), 1.41 (dt, J = 9.9, 5.1 Hz, 1H), 1.33 (dt, J = 10.5, 5.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.98, 137.75, 131.64, 129.11, 128.56, 126.34, 126.11, 120.75, 91.22, 77.24, 26.70, 21.56, 18.17, 12.27. IR (neat, cm^{-1}): 3027.56, 2921.15, 2225.19, 2157.79, 1604.05, 1509.97, 1457.26, 1030.99, 948.51, 816.04, 747.88, 696.57. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{18}H_{17}^+$: 233.13248, found: 233.13261. HPLC analysis: ee = 97%. IC (100% hexanes, 0.8 mL/min): t_{major} = 20.35 min, t_{minor} = 26.07 min.

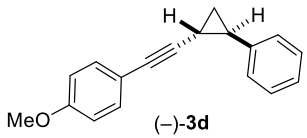


1-Isopropyl-2-(((1*R*,2*R*)-2-phenylcyclopropyl)ethynyl)benzene ((–)-**3c**) Yield: 90%. dr: 96:4. R_f = 0.3 (Hexane/Ethyl Acetate: 30/1). $[\alpha]_D^{20}$ = (–)-417.51° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (d, J = 7.6 Hz, 1H), 7.30 (t, J = 7.3 Hz, 2H), 7.25 (d, J = 4.3 Hz, 2H), 7.21 (t, J = 7.1 Hz, 1H), 7.14 – 7.09 (m, 3H), 3.49 – 3.40 (m, 1H),

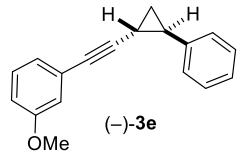


2.38 – 2.34 (m, 1H), 1.76 (dt, J = 9.4, 4.9 Hz, 1H), 1.45 – 1.42 (m, 1H), 1.39 – 1.35 (m, 1H), 1.27 (d, J = 6.8 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.53, 141.00, 132.46, 128.59, 128.09, 126.37, 126.08, 125.54, 124.94, 122.55, 95.65, 75.79, 31.61, 26.87, 23.20, 23.18, 18.40, 12.50. IR (neat, cm^{-1}): 3025.41, 2958.77, 2221.27, 1603.66, 1483.61, 1027.89, 947.56, 757.37, 696.75. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{20}H_{21}^+$: 261.16378, found: 261.16452. HPLC analysis: ee = 99%. IC (100% hexanes, 0.5 mL/min): t_{major} = 17.43 min, t_{minor} = 15.65 min.

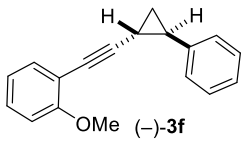
1-Methoxy-4-(((1*R*,2*R*)-2-phenylcyclopropyl)ethynyl)benzene ((–)-**3d**) Yield: 90%. dr: 85:15. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-151.56° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.25 (m, 2H), 7.19 (dd, *J* = 13.4, 7.0 Hz, 2H), 7.12 (d, *J* = 7.5 Hz, 2H), 7.00 (d, *J* = 7.5 Hz, 1H), 6.94 (s, 1H), 6.84 (d, *J* = 8.4 Hz, 1H), 3.80 (s, 3H), 2.37 (dd, *J* = 11.6, 7.3 Hz, 1H), 1.75 – 1.67 (m, 1H), 1.47 – 1.40 (m, 1H), 1.35 (dd, *J* = 12.7, 6.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.32, 132.86, 131.74, 129.53, 128.33, 127.70, 127.35, 114.03, 92.30, 77.06, 55.46, 26.09, 17.73, 11.71. IR (neat, cm^{-1}): 3004.01, 2832.88, 2222.28, 1735.61, 1596.76, 1573.47, 1490.18, 1458.41, 1426.86, 1285.02, 1214.10, 1161.09, 1044.51, 900.13, 785.39, 697.99 HRMS (DART) ($[M+H]^+$) Calcd. for $C_{18}H_{17}O^+$: 249.12739, found: 249.12800. HPLC analysis: ee = 98%. ID (99.5% hexanes: 0.5% isopropanol, 0.8 mL/min): t_{major} = 19.23 min, t_{minor} = 16.79 min.



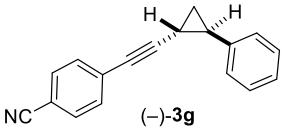
1-Methoxy-3-(((1*R*,2*R*)-2-phenylcyclopropyl)ethynyl)benzene ((–)-**3e**) Yield: 94%. dr: 90:10. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-90.93° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H), 7.23 – 7.11 (m, 4H), 7.03 – 6.99 (m, 1H), 6.94 (dd, *J* = 2.5, 1.4 Hz, 1H), 6.84 (ddd, *J* = 8.3, 2.6, 0.8 Hz, 1H), 3.80 (s, 3H), 2.37 (ddd, *J* = 8.8, 6.1, 4.6 Hz, 1H), 1.71 (ddd, *J* = 8.7, 5.6, 4.6 Hz, 1H), 1.43 (ddd, *J* = 8.8, 5.6, 4.9 Hz, 1H), 1.35 (ddd, *J* = 8.7, 6.2, 4.8 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.43, 140.85, 129.40, 128.58, 126.40, 126.13, 124.86, 124.33, 116.57, 114.47, 91.93, 77.13, 55.38, 26.75, 18.16, 12.19. IR (neat, cm^{-1}): 3029.78, 2931.66, 2835.34, 2225.55, 1605.33, 1510.25, 1457.81, 1288.71, 1248.50, 1173.27, 1029.39, 832.80, 749.26, 698.59. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{18}H_{17}O^+$: 249.12739, found: 249.12807. HPLC analysis: ee = 99%. IE (99.5% hexanes: 0.5% isopropanol, 0.8 mL/min): t_{major} = 19.52 min, t_{minor} = 16.54 min.



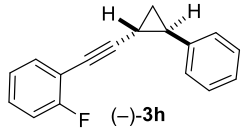
1-Methoxy-2-(((1*R*,2*R*)-2-phenylcyclopropyl)ethynyl)benzene ((–)-**3f**) Yield: 99%. dr: 94:6. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-120.65° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.38 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.29 – 2.23 (m, 3H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 7.5 Hz, 2H), 6.91 – 6.83 (m, 2H), 3.88 (s, 3H), 2.50 – 2.33 (m, 1H), 1.79 (dt, *J* = 8.8, 5.2 Hz, 1H), 1.46 (dt, *J* = 8.9, 5.3 Hz, 1H), 1.39 – 1.31 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.15, 141.04, 133.84, 129.15, 128.53, 126.31, 126.12, 120.55, 112.93, 110.67, 96.20, 73.24, 55.92, 26.89, 18.48, 12.60. IR (neat, cm^{-1}): 3026.46, 2933.30, 2224.21, 2144.80, 1595.45, 1574.20, 1494.20, 1461.81, 1434.12, 1262.24, 1025.21, 950.32, 752.69, 698.71. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{18}H_{17}O^+$: 249.12739, found: 249.12833. HPLC analysis: ee = 95%. IA (99% hexanes: 1% isopropanol, 0.8 mL/min): t_{major} = 7.84 min, t_{minor} = 7.35 min.



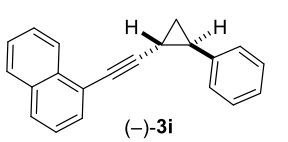
4-(((1*R*,2*R*)-2-Phenylcyclopropyl)ethynyl)benzonitrile ((–)-**3g**) Yield: 94%. dr: 90:10. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-96.44° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.59 – 7.55 (m, 2H), 7.48 – 7.45 (m, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.24 – 7.20 (m, 1H), 7.14 – 7.11 (m, 2H), 2.40 (ddd, *J* = 8.9, 6.3, 4.6 Hz, 1H), 1.72 (ddd, *J* = 8.7, 5.6, 4.6 Hz, 1H), 1.48 – 1.43 (m, 1H), 1.41 (ddd, *J* = 8.7, 6.3, 4.9 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.31, 132.22, 132.07, 128.96, 128.67, 126.64, 126.14, 118.76, 110.99, 97.27, 76.05, 27.04, 18.22, 12.11. IR (neat, cm^{-1}): 2960.52, 2916.60, 2224.00, 2171.15, 1602.59, 1500.30, 1458.90, 1344.91, 1219.35, 1178.01, 1105.49. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{18}H_{14}N^+$: 244.11208, found: 244.11371. HPLC analysis: ee = 90%. IA (99.2% hexanes: 0.8% isopropanol, 1.0 mL/min): t_{major} = 11.05 min, t_{minor} = 8.36 min.



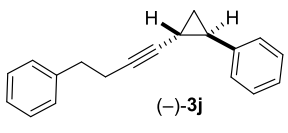
1-Fluoro-2-(((1*R*,2*R*)-2-phenylcyclopropyl)ethynyl)benzene ((–)-**3h**) Yield: 90%. dr: 93:7. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1); $[\alpha]_D^{20}$ = (–)-119.42° (*c* = 0.5, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (t, J = 7.4 Hz, 1H), 7.33 – 7.27 (m, 2H), 7.25 – 7.22 (m, 1H), 7.20 (t, J = 7.3 Hz, 1H), 7.13 (d, J = 7.6 Hz, 1H), 7.05 (dd, J = 17.5, 8.5 Hz, 2H), 2.42 – 2.38 (m, 1H), 1.77 – 1.74 (m, 1H), 1.48 – 1.44 (m, 1H), 1.38 (dt, J = 9.5, 5.5 Hz, 1H). ^{13}C NMR (151MHz, $CDCl_3$) δ 163.05 (d, *J* = 250.3 Hz), 140.71, 133.71 (d, *J* = 1.2 Hz), 129.34 (d, *J* = 7.8 Hz), 128.59, 126.45, 126.13, 123.94 (d, *J* = 3.7 Hz), 115.50 (d, *J* = 21.0 Hz), 112.37 (d, *J* = 15.8 Hz), 97.43 (d, *J* = 3.1 Hz), 70.47, 26.88, 18.29, 12.29. ^{19}F NMR (564MHz, $CDCl_3$) δ –110.86 (s, 1F). IR (neat, cm^{-1}): 3053.04, 2925.74, 2853.66, 2157.23, 1604.00, 1494.46, 1264.14, 895.94, 731.81, 703.27. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{17}H_{13}F^+$: 237.10741, found: 237.10823. HPLC analysis: ee = 98%. IC (100% hexanes, 0.8 mL/min): t_{major} = 17.56 min, t_{minor} = 15.84 min.



1-(((1*R*,2*R*)-2-phenylcyclopropyl)ethynyl)naphthalene ((–)-**3i**) Yield: 95%. dr: 80:20. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-94.31° (*c* = 0.5, $CHCl_3$) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.80 (d, *J* = 8.3 Hz, 1H), 7.66 (dd, *J* = 7.1, 1.1 Hz, 1H), 7.59 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.53 (ddd, *J* = 8.1, 6.9, 1.3 Hz, 1H), 7.42 (dd, *J* = 8.2, 7.2 Hz, 1H), 7.35 – 7.31 (m, 2H), 7.27 – 7.22 (m, 1H), 7.19 (dd, *J* = 8.1, 1.0 Hz, 2H), 2.51 (ddd, *J* = 8.9, 6.1, 4.5 Hz, 1H), 1.90 (ddd, *J* = 8.7, 5.6, 4.6 Hz, 1H), 1.57 (ddd, *J* = 8.9, 5.7, 4.9 Hz, 1H), 1.46 (ddd, *J* = 8.7, 6.2, 4.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.86, 133.69, 133.33, 130.29, 128.62, 128.37, 128.16, 126.67, 126.44, 126.40, 126.35, 126.14, 125.36, 121.53, 97.16, 75.25, 27.07, 18.52, 12.53. IR (neat, cm^{-1}): 3057.62, 2922.15, 2220.80, 1603.97, 1584.51, 1497.84, 1457.41, 1400.50, 1215.93, 1183.31, 1018.73. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{21}H_{17}^+$: 269.13248, found: 269.13270. HPLC analysis: ee = 90%. IA (100% hexanes, 0.8 mL/min): t_{major} = 16.42 min, t_{minor} = 20.87 min.

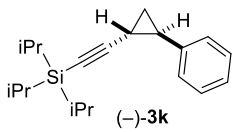


((1*R*,2*R*)-2-(4-phenylbut-1-yn-1-yl)cyclopropyl)benzene ((–)-**3j**) Yield: 41%. dr: 91:9. R_f =0.4 (Hexanes/Ethyl Acetate = 20/1).). $[\alpha]_D^{20}$ = (–)-253.30º (*c*=0.5, $CHCl_3$). ^{1}H NMR (500 MHz, $CHCl_3$) δ 7.29 (q, *J* = 6.6 Hz, 4H), 7.23 (t, *J* = 7.2 Hz, 3H), 7.17 (t, *J* = 7.4 Hz, 1H), 7.09 – 7.04 (m, 2H), 2.81 (t, *J* = 7.6 Hz, 2H), 2.45 (td, *J* = 7.6, 1.9 Hz, 2H), 2.14 (ddd, *J* = 8.7, 6.0, 4.5 Hz, 1H), 1.46 (dddt, *J* = 8.1, 6.3, 4.2, 1.9 Hz, 1H), 1.24 – 1.15 (m, 2H). ^{13}C NMR (151 MHz, $CHCl_3$) δ 141.29, 141.05, 128.63, 128.50, 128.45, 126.35,

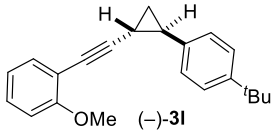


126.20, 126.02, 82.88, 76.42, 35.64, 26.15, 21.25, 17.80, 11.75. IR (neat, cm^{-1}): 3026.43, 2924.37, 1603.83, 1495.48, 1453.88, 1275.36, 1260.61, 749.58. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{19}H_{19}^+$: 247.1481, found: 247.1484. HPLC analysis: ee = 85%. IC (99.9% hexanes : 0.1% isopropanol, 0.8 mL/min): t_{major} = 6.50 min, t_{minor} = 7.19 min.

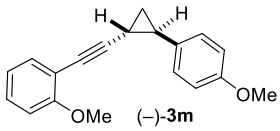
Triisopropyl(((1*R*,2*R*)-2-phenylcyclopropyl)ethynyl)silane ((–)-**3k**) Yield: 71%. dr: 96:4. R_f = 0.3 (Hexane/Ethyl Acetate: 30/1). $[\alpha]_D^{20}$ = (–)-62.18° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.27 (t, *J* = 7.6 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 7.2 Hz, 2H), 2.25 (ddd, *J* = 8.8, 6.0, 4.6 Hz, 1H), 1.59 – 1.55 (m, 1H), 1.34 – 1.30(m, 1H), 1.24 (ddd, *J* = 8.7, 6.1, 4.7 Hz, 1H), 1.09 – 1.04 (m, 21H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 141.01, 128.54, 126.33, 126.02, 110.70, 76.90, 27.08, 18.79, 18.73, 12.56, 11.47. IR (neat, cm^{-1}): 3029.62, 2941.29, 2863.78, 2158.44, 1731.59, 1604.88, 1461.55, 1382.49, 1126.08, 1072.72, 995.91, 883.40, 747.93, 696.28,677.48. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{20}H_{31}Si^+$: 299.21895, found: 299.21913. HPLC analysis: ee = 87%. IC (100% hexanes, 0.8 mL/min): t_{major} = 6.28 min, t_{minor} = 6.64 min.



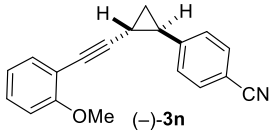
1-(((1*R*,2*R*)-2-(4-(*tert*-Butyl)phenyl)cyclopropyl)ethynyl)-2-methoxybenzene ((–)-**3l**) Yield: 94%. dr: 91:9. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-154.77° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.38 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.34 – 7.30 (m, 2H), 7.25 – 7.22 (m, 1H), 7.08 – 7.05 (m, 2H), 6.90 – 6.84 (m, 2H), 3.88 (s, 3H), 2.37 (ddd, *J* = 8.9, 6.1, 4.6 Hz, 1H), 1.76 (ddd, *J* = 8.7, 5.6, 4.6 Hz, 1H), 1.43 (ddd, *J* = 8.9, 5.5, 4.8 Hz, 1H), 1.36 – 1.31 (m, 10H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.14, 149.26, 137.99, 133.83, 129.09, 125.85, 125.44, 120.53, 113.01, 110.67, 96.40, 73.11, 55.91, 34.54, 31.50, 26.50, 18.30, 12.42. IR (neat, cm^{-1}): 3005.32, 2959.45, 2224.63, 1505.13, 1574.07, 1493.24, 1462.24, 1433.35, 1362.33, 1260.43, 1239.75, 1122.33, 1023.86, 913.75, 749.57. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{22}H_{25}O^+$: 305.18999, found: 305.19136. HPLC analysis: ee = 89%. IC (99% hexanes: 1% isopropanol, 0.8 mL/min): t_{major} = 7.35 min, t_{minor} = 19.02 min.



1-Methoxy-2-(((1*R*,2*R*)-2-(4-methoxyphenyl)cyclopropyl)ethynyl)benzene ((–)-**3m**) Yield: 89%. dr: 90:10. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-268.89° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.37 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.08 – 7.04 (m, 2H), 6.90 – 6.80 (m, 4H), 3.88 (s, 3H), 3.79 (s, 3H), 2.36 (ddd, *J* = 8.8, 6.1, 4.6 Hz, 1H), 1.70 (ddd, *J* = 8.7, 5.5, 4.6 Hz, 1H), 1.40 (ddd, *J* = 8.8, 5.5, 4.8 Hz, 1H), 1.28 (ddd, *J* = 8.7, 6.2, 4.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 160.12, 158.26, 133.81, 133.00, 129.08, 127.34, 120.52, 113.98, 112.99, 110.66, 96.45, 73.10, 55.90, 55.44, 26.22, 18.02, 12.07. IR (neat, cm^{-1}): 3004.06, 2834.59, 2221.30, 1712.67, 1595.27, 1514.93, 1493.71, 1246.07, 1032.57, 753.19. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{19}H_{19}O_2^+$: 279.13796, found: 279.13922. HPLC analysis: ee = 94%. IC (98% hexanes: 2% isopropanol, 0.8 mL/min): t_{major} = 12.62 min, t_{minor} = 26.52 min.

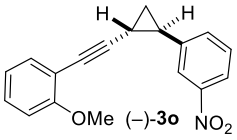


4-((1*R*,2*R*)-2-((2-Methoxyphenyl)ethynyl)cyclopropyl)benzonitrile ((–)-**3n**) Yield: 85%. dr: 81:19. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-166.32° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.37 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.28 – 7.24 (m, 1H), 7.18 (d, *J* = 8.3 Hz, 2H), 6.89 – 6.85 (m, 2H),

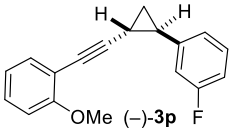


3.88 (s, 3H), 2.42 (ddd, *J* = 8.8, 6.0, 4.5 Hz, 1H), 1.85 (ddd, *J* = 8.8, 5.9, 4.5 Hz, 1H), 1.57 (ddd, *J* = 8.8, 5.8, 5.1 Hz, 1H), 1.40 (ddd, *J* = 8.8, 6.0, 5.1 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.16, 146.93, 133.82, 132.35, 129.47, 126.61, 120.57, 119.08, 112.44, 110.67, 109.91, 94.82, 74.14, 55.90, 26.94, 19.31, 13.91. IR (neat, cm^{-1}): 2958.79, 2924.59, 2852.88, 2360.28, 2342.02, 2225.74, 2158.90, 1718.70, 1607.79, 1595.93, 1493.62, 1463.86, 1434.85, 1262.91, 1241.84, 1122.93, 1023.71, 837.06, 752.98. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{19}H_{16}NO^+$: 274.12264, found: 274.12280. HPLC analysis: ee = 95%. IC (90% hexanes: 10% isopropanol, 1 mL/min): t_{major} = 26.22 min, t_{minor} = 45.85 min.

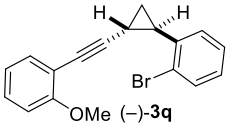
1-Methoxy-2-(((1*R*,2*R*)-2-(3-nitrophenyl)cyclopropyl)ethynyl)benzene ((–)-**3o**) Yield: 88%. dr: 78:22. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-144.58° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.04 (dd, *J* = 7.3, 2.1 Hz, 1H), 7.96 (s, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.38 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.27 (d, *J* = 15.8 Hz, 1H), 6.89 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 3.88 (s, 3H), 2.52 – 2.47 (m, 1H), 1.86 (dt, *J* = 10.1, 5.2 Hz, 1H), 1.58 (dt, *J* = 8.7, 5.4 Hz, 1H), 1.43 (dt, *J* = 8.8, 5.6 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.19, 143.34, 133.84, 132.49, 129.45, 129.41, 123.26, 121.37, 120.89, 120.57, 112.49, 110.68, 94.85, 74.07, 55.91, 26.43, 18.75, 13.38. IR (neat, cm^{-1}): 3074.86, 3008.02, 2933.88, 2835.38, 2223.53, 2155.68, 2045.47, 1698.41, 1595.06, 1528.15, 1493.62, 1463.66, 1348.20, 1263.54, 1241.89, 1024.19, 755.31. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{18}H_{16}NO_3^+$, 294.11247, found: 294.11214. HPLC analysis: ee = 81%. IC (90% hexanes: 10% isopropanol, 1 mL/min): t_{major} =17.66 min, t_{minor} =18.52 min.



1-(((1*R*,2*R*)-2-(3-Fluorophenyl)cyclopropyl)ethynyl)-2-methoxybenzene ((–)-**3p**) Yield: 96%. dr: 85:15. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-96.21° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.38 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.25 (ddd, *J* = 9.2, 6.4, 1.7 Hz, 1H), 7.11 – 7.07 (m, 2H), 6.97 (ddd, *J* = 8.7, 7.8, 4.6 Hz, 2H), 6.88 (ddd, *J* = 10.8, 8.6, 4.6 Hz, 2H), 3.88 (s, 3H), 2.38 (ddd, *J* = 8.9, 6.0, 4.7 Hz, 1H), 1.73 (ddd, *J* = 8.7, 5.5, 4.7 Hz, 1H), 1.47 – 1.42 (m, 1H), 1.30 (ddd, *J* = 8.7, 6.2, 4.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 161.59 (d, *J* = 244.2 Hz), 160.15, 136.62 (d, *J* = 3.3 Hz), 133.83, 130.06 (d, *J* = 7.8 Hz), 129.21, 127.70 (d, *J* = 8.0 Hz), 120.55, 115.41, 115.24, 112.84, 110.68, 95.94, 73.38, 55.91, 26.18, 18.27, 12.42. ^{19}F NMR (564MHz, $CDCl_3$) δ –108.26 (s, 1F). HRMS (DART) ($[M+H]^+$) Calcd. for $C_{18}H_{16}FO^+$: 267.11797, found: 267.11835. HPLC analysis: ee = 95%. IA (99.7% hexanes: 0.3% isopropanol, 1 mL/min): t_{major} =12.10 min, t_{minor} =10.75 min.

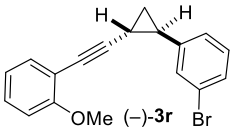


1-Bromo-2-((1*R*,2*R*)-2-((2-methoxyphenyl)ethynyl)cyclopropyl)benzene ((–)-**3q**) Yield: 91%. dr: 90:10. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-144.92° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.58 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.28 – 7.21 (m, 2H), 7.08 (td, *J* = 7.7, 1.6 Hz, 1H), 7.00 (dd, *J* = 11.6, 5.0 Hz, 1H), 6.88 (ddd, *J* = 12.0, 9.3, 4.7 Hz, 2H), 3.89 (s, 3H), 2.66 – 2.60 (m, 1H), 1.83 – 1.77 (m, 1H), 1.52 (ddd, *J* = 8.9, 5.5, 4.9 Hz, 1H), 1.33 – 1.26 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.23, 140.05, 133.92, 132.74, 131.55, 129.19, 127.95, 127.45, 127.22, 126.33, 120.54, 110.75, 95.87, 73.44, 55.96, 27.59, 17.77, 11.44. IR (neat, cm^{-1}): 2959.06, 1594.84, 1574.10, 1493.09, 1463.23, 1433.85,

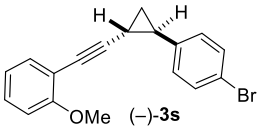


1261.01, 1240.02, 1219.52, 1180.38, 1161.43, 1121.33, 1046.77, 1023,44. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{18}H_{16}BrO^+$: 327.03790, found: 327.03886. HPLC analysis: ee = 94%. ODH (98% hexanes: 2% isopropanol, 1 mL/min): t_{major} = 36.73 min, t_{minor} = 50.38 min.

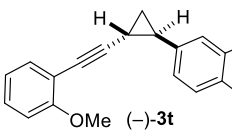
1-(((1*R*,2*R*)-2-(3-bBomophenyl)cyclopropyl)ethynyl)-2-methoxybenzene ((–)-**3r**) Yield: 88%. dr: 88:12. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-151.97° (*c* = 0.5, $CHCl_3$) ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.37 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.32 (d, *J* = 7.9 Hz, 1H), 7.26 – 7.21 (m, 2H), 7.14 (t, *J* = 7.8 Hz, 1H), 7.04 (d, *J* = 7.7 Hz, 1H), 6.84 – 6.70 (m, 2H), 3.88 (s, 3H), 2.39 – 2.33 (m, 1H), 1.78 – 1.75 (m, 1H), 1.47 (dt, *J* = 8.8, 5.3 Hz, 1H), 1.34 (ddd, *J* = 8.7, 6.0, 5.1 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.18, 143.49, 133.85, 130.05, 129.42, 129.30, 129.29, 124.88, 122.69, 120.56, 112.73, 110.68, 95.55, 73.62, 55.92, 26.48, 18.47, 12.85. IR (neat, cm^{-1}): 3052.53, 2928.16, 2221.82, 2035.47, 1951.20, 1596.77, 1566.35, 1493.96, 1265.16, 1024.68, 895.64, 746.09. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{18}H_{16}BrO^+$: 327.03790, found: 327.03788. HPLC analysis: ee = 94%. IC (99% hexanes : 1% isopropanol, 0.8 mL/min): t_{major} = 15.05 min, t_{minor} = 35.29 min.



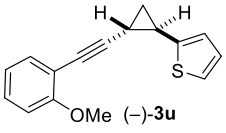
1-(((1*R*,2*R*)-2-(4-Bromophenyl)cyclopropyl)ethynyl)-2-methoxybenzene ((–)-**3s**) Yield: 93%. dr: 84:16. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-177.86° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.38 (dd, *J* = 14.3, 4.9 Hz, 2H), 7.25 – 7.18 (m, 2H), 6.99 (d, *J* = 8.4 Hz, 2H), 6.88 – 6.86 (m, 2H), 3.88 (s, 3H), 2.37 – 2.33 (m, 1H), 1.77 – 1.73 (m, 1H), 1.49 – 1.45 (m, 1H), 1.33 – 1.29 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.14, 140.11, 133.83, 131.56, 130.28, 129.27, 127.88, 120.56, 119.93, 110.67, 95.68, 73.55, 55.91, 26.38, 18.49, 12.74. IR (neat, cm^{-1}): 2915.93, 2848.44, 2361.23, 2181.48, 1596.50, 1565.70, 1493.74, 1463.52, 1434.28, 1261.97, 1240.71, 1179.48, 1024.49, 750.67. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{18}H_{16}BrO^+$: 327.03790, found: 327.03750. HPLC analysis: ee = 91%. IA (99.7% hexanes: 0.3% isopropanol, 1 mL/min): t_{major} = 17.36 min, t_{minor} = 13.36 min.



2-((1*R*,2*R*)-2-((2-Methoxyphenyl)ethynyl)cyclopropyl)naphthalene ((–)-**3t**) Yield: 96%. dr: 92:8. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-186.99° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.78 (dd, *J* = 17.6, 8.2 Hz, 3H), 7.58 (s, 1H), 7.47-7.40 (m, 3H), 7.27 – 7.24 (m, 2H), 6.91 – 6.86 (m, 2H), 3.89 (s, 3H), 2.57 (tt, *J* = 14.8, 7.2 Hz, 1H), 1.90 (dt, *J* = 8.9, 5.4 Hz, 1H), 1.54 – 1.52 (m, 1H), 1.50 – 1.46 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.17, 138.48, 133.86, 133.57, 132.33, 129.18, 128.19, 127.75, 127.53, 126.29, 125.43, 124.82, 124.51, 120.56, 112.91, 110.68, 96.18, 73.38, 55.93, 27.16, 18.41, 12.62. IR (neat, cm^{-1}): 3049.84, 2933.69, 2833.69, 2222.57, 1726.29, 1594.94, 1492.53, 1462.22, 1433.04, 1261.35, 1023.58, 974.27, 815.73, 750.18. HRMS (DART) ([M+H]$^+$) Calcd. for $C_{22}H_{19}O^+$: 299.14304, found: 299.14364. HPLC analysis: ee = 99%. IC (99% hexanes : 1% isopropanol, 0.8 mL/min): t_{major} = 19.71min, t_{minor} = 23.40 min.

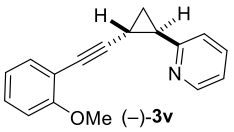


2-((1*R*,2*R*)-2-((2-Methoxyphenyl)ethynyl)cyclopropyl)thiophene ((–)-**3u**) Yield: 97%. dr: 96:4. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-212.02° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.38 (d, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 7.9 Hz, 1H), 7.08 (d, *J* = 5.1 Hz, 1H), 6.91 – 6.82 (m, 4H), 3.88 (s, 3H), 2.59 – 2.55 (m, 1H), 1.83

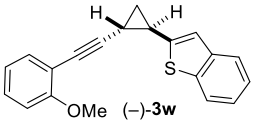


(dt, *J* = 9.7, 5.0 Hz, 1H), 1.49 (ddd, *J* = 9.7, 5.5, 0.7 Hz, 1H), 1.37 – 1.33 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.12, 145.24, 133.82, 129.24, 126.93, 123.64, 122.92, 120.53, 112.73, 110.64, 95.45, 73.78, 55.88, 22.24, 19.35, 13.44. IR (neat, cm^{-1}): 3004.51, 2958.93, 2834.69, 2359.94, 2342.06, 1733.86, 1595.14, 1493.32, 1463.04, 1434.12, 1261.58, 1241.27, 1023.74, 752.03, 696.87. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{16}H_{15}OS^+$: 255.08381, found: 255.08346. HPLC analysis: ee = 92%. IC (99.5% hexanes: 0.5% isopropanol, 0.8 mL/min): t_{major} = 17.45 min, t_{minor} = 28.64 min.

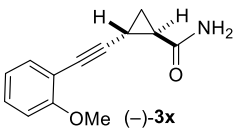
2-((1*R*,2*R*)-2-((2-Methoxyphenyl)ethynyl)cyclopropyl)pyridine ((–)-**3v**) Yield: 92%. dr: 90:10. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-309.74° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.43 (d, *J* = 4.6 Hz, 1H), 7.54 (td, *J* = 7.6, 1.1 Hz, 1H), 7.38 (d, *J* = 7.5 Hz, 1H), 7.25 – 7.22 (m, 2H), 7.05 (dd, *J* = 7.3, 5.0 Hz, 1H), 6.87 – 6.84 (m, 2H), 3.86 (s, 3H), 2.47 – 2.44 (m, 1H), 2.18 – 2.14 (m, 1H), 1.70 – 1.65 (m, 1H), 1.48 – 1.44 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.13, 159.60, 149.45, 135.94, 133.84, 129.13, 122.56, 121.07, 120.50, 112.87, 110.62, 96.10, 73.16, 55.86, 28.02, 19.06, 12.94. IR (neat, cm^{-1}): 2968.41, 2927.53, 2360.32, 1717.35, 1596.16, 1494.22, 1464.75, 1263.99, 1161.37, 1123.92, 1024.27, 950.53, 735.14, HRMS (DART) ($[M+H]^+$) Calcd. for $C_{17}H_{16}NO^+$: 250.12264, found: 250.12161. HPLC analysis: ee = 92%. IC (99.5% hexanes: 0.5% isopropanol, 1.0 mL/min): t_{major} = 47.91 min, t_{minor} = 62.80 min.



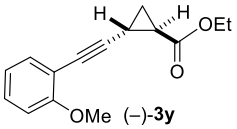
2-((1*R*,2*R*)-2-((2-Methoxyphenyl)ethynyl)cyclopropyl)benzo[b]thiophene ((–)-**3w**) Yield: 90%. dr: 88:12. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-174.25° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.02 (d, *J* = 8.0 Hz, 1H), 7.85 (t, *J* = 8.0 Hz, 1H), 7.43 (dd, *J* = 7.9, 7.2 Hz, 2H), 7.39 – 7.36 (m, 1H), 7.28 – 7.26 (m, 1H), 7.02 (s, 1H), 6.92 – 6.86 (m, 2H), 3.90 (s, 3H), 2.56 – 2.52 (m, 1H), 1.81 – 1.77 (m, 1H), 1.50 (dt, *J* = 9.6, 5.0 Hz, 1H), 1.38 (ddd, *J* = 8.6, 6.2, 4.9 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.22, 140.49, 139.61, 136.33, 133.85, 129.23, 124.71, 124.25, 122.92, 122.34, 120.91, 120.56, 112.91, 110.72, 96.10, 73.38, 55.94, 20.87, 16.42, 10.07. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{20}H_{17}OS^+$: 305.09946, found: 305.09874. HPLC analysis: ee = 93%. IC (99.5% hexanes: 0.5% isopropanol, 0.8 mL/min): t_{major} =17.74 min, t_{minor} = 29.07 min.



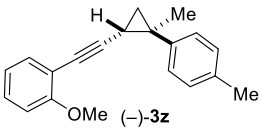
(1*R*,2*R*)-2-((2-Methoxyphenyl)ethynyl)cyclopropane-1-carboxamide ((–)-**3x**) Yield: 92%. dr: 98:2. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-96.32° (*c* = 0.5, $CHCl_3$) ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.31 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.22 (td, *J* = 8.4, 1.6 Hz, 1H), 6.84 (ddd, *J* = 11.1, 8.8, 4.6 Hz, 2H), 5.91 (s, 2H), 3.83 (s, 3H), 2.09 – 2.04 (m, 1H), 1.91 – 1.85 (m, 1H), 1.46 (ddd, *J* = 9.2, 5.3, 4.1 Hz, 1H), 1.22 (ddd, *J* = 8.4, 6.2, 4.1 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 173.20, 160.19, 133.89, 129.52, 120.58, 112.35, 110.68, 94.30, 73.74, 55.90, 24.57, 16.90, 10.95. IR (neat, cm^{-1}): 2964.37, 2934.13, 2361.03, 2342.20, 2158.68, 1724.96, 1596.50, 1494.77, 1334.80, 1261.55, 1192.09, 1180.94, 1124.56, 752.96. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{13}H_{14}NO_2^+$: 216.10191, found: 216.10149. HPLC analysis: ee = 89%. IC (99% hexanes: 1% isopropanol, 0.8 mL/min): t_{major} = 30.75 min, t_{minor} = 36.84 min.



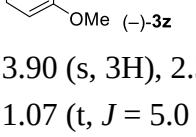
Ethyl-(1*R*,2*R*)-2-((2-methoxyphenyl)ethynyl)cyclopropane-1-carboxylate ((–)-**3y**) Yield: 89%. dr: 96:4. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-116.67° (*c* = 0.5, $CHCl_3$). ^1H NMR (600 MHz, $CDCl_3$): δ 7.34 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.25 (dd, *J* = 12.5, 5.0 Hz, 1H), 6.89 – 6.83 (m, 2H), 4.16 (ddd, *J* = 14.3, 7.2, 3.0 Hz, 2H), 3.87 (s, 3H), 2.13 (ddd, *J* = 9.1, 6.2, 4.1 Hz, 1H), 2.08 – 2.03 (m, 1H), 1.47 (ddd, *J* = 9.4, 5.5, 4.2 Hz, 1H), 1.34 – 1.31 (m, 1H), 1.30 – 1.23 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 172.51, 160.26, 133.90, 129.54, 120.54, 112.32, 110.67, 93.74, 73.97, 61.05, 55.90, 23.46, 17.44, 14.39, 11.53. IR (neat, cm^{-1}): 2979.80, 1723.87, 1596.21, 1575.23, 1494.51, 1464.14, 1405.49, 1324.14, 1261.27, 1179.78, 1025.69. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{15}H_{17}O_3^+$: 245.11722, found: 245.11754. HPLC analysis: ee = 88%. IA (99.7% hexanes: 0.3% isopropanol, 1 mL/min): t_{major} = 9.47 min, t_{minor} = 10.72 min.

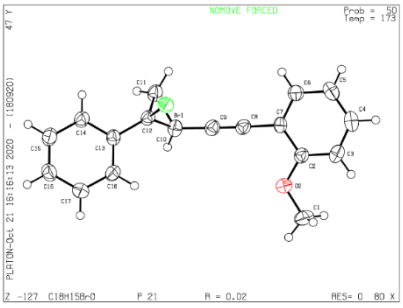


1-Methoxy-2-(((1*S*,2*R*)-2-Methyl-2-(p-tolyl)cyclopropyl)ethynyl)benzene ((–)-**3z**) Yield: 93%. dr: 96:4. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-240.41° (*c* = 0.5, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$): δ 7.42 (d, *J* = 7.5 Hz, 1H), 7.25 (dd, *J* = 18.3, 7.9 Hz, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.89 (dd, *J* = 17.1, 8.1 Hz, 2H), 3.90 (s, 3H), 2.34 (s, 3H), 1.88 (dd, *J* = 8.9, 5.6 Hz, 1H), 1.65 (s, 3H), 1.48 (dd, *J* = 8.7, 4.2 Hz, 1H), 1.07 (t, *J* = 5.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 160.19, 142.99, 135.91, 133.66, 129.17, 128.92, 127.35, 120.51, 113.36, 110.72, 94.98, 75.40, 55.91, 27.92, 23.64, 22.78, 21.11, 16.45. IR (neat, cm^{-1}): 2959.00, 2916.52, 2848.85, 2224.98, 1595.39, 1574,37, 1516,57, 1493.90, 1463.28, 1434,04, 1262.63, 1240.08, 1161.60, 1121.96, 1025.38. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{20}H_{21}O^+$: 277.15869, found: 277.15930. HPLC analysis: ee = 94%. IC (99.5% hexanes: 0.5% isopropanol, 0.8 mL/min): t_{major} = 14.22 min, t_{minor} = 16.97 min.

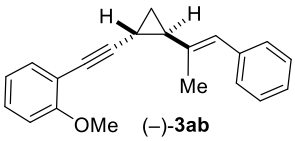


1-(((1*S*,2*S*)-2-Bromo-2-phenylcyclopropyl)ethynyl)-2-methoxybenzene ((–)-**3aa**) Yield: 91%. dr: 97:3. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-240.41° (*c* = 0.5, $CHCl_3$). ^1H NMR (600 MHz, $CDCl_3$): δ 7.53 – 7.50 (m, 3H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.28 (dd, *J* = 11.1, 4.3 Hz, 2H), 6.93 – 6.87 (m, 2H), 3.91 (s, 3H), 2.13 (dd, *J* = 9.7, 6.8 Hz, 1H), 1.91 (dd, *J* = 9.7, 6.0 Hz, 1H), 1.75 (t, *J* = 6.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.30, 142.92, 134.16, 129.51, 128.79, 128.76, 128.49, 120.60, 112.67, 110.82, 93.10, 77.24, 56.03, 39.46, 25.96, 17.92. IR (neat, cm^{-1}): 259.61, 2925.60, 2359.96, 2341.91, 2158.64, 2006.36, 1724.59, 1597.77, 1494.16, 1463.91, 1258.03, 1180.03, 1121.41, 1025.10, 752.20, 697.42. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{18}H_{16}OBr^+$: 327.03790, found: 327.03766. HPLC analysis: ee = 91%. IA (99.5% hexanes: 0.5% isopropanol, 0.8 mL/min): t_{major} = 18.84 min, t_{minor} = 17.84 min.



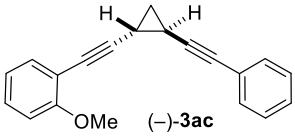


1-Methoxy-2-(((1*R*,2*R*)-2-((*E*)-1-phenylprop-1-en-2-yl)cyclopropyl)ethynyl)benzene ((–)-**3ab**) Yield: 79%. dr: 85:15. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-62.99° (*c* = 0.5, $CHCl_3$). ^1H NMR (600 MHz, $CDCl_3$): δ 7.38 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.24 – 7.18 (m, 4H), 6.89 – 6.84 (m,

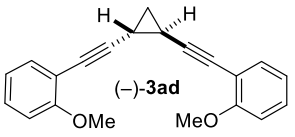


2H), 6.39 (s, 1H), 3.89 (s, 3H), 2.08 – 2.05 (m, 1H), 1.78 (s, 1H), 1.72 (dt, *J* = 8.8, 5.2 Hz, 1H), 1.23 – 1.19 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.13, 138.16, 136.81, 133.83, 129.08, 128.98, 128.22, 126.22, 125.30, 120.54, 113.00, 110.65, 96.66, 72.97, 55.94, 31.41, 15.73, 15.33, 8.52. IR (neat, cm^{-1}): 3444.24, 2925.13, 2360.20, 2341.42, 2204.65, 2158.56, 1717.77, 1596.20, 1493.40, 1456.63, 1260.50, 1023.79, 752.82. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{21}H_{21}O^+$: 289.15869, found: 289.15712. HPLC analysis: ee = 93%. IB (99.5% hexanes: 0.5% isopropanol, 0.8 mL/min): t_{major} = 34.07 min, t_{minor} = 22.47 min.

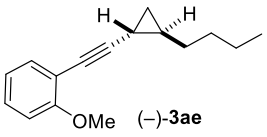
1-Methoxy-2-(((1*R*,2*R*)-2-(phenylethynyl)cyclopropyl)ethynyl)benzene ((–)-**3ac**) Yield: 93%. dr: 97:3. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-108.98° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.37 (ddd, *J* = 8.9, 7.4, 2.5 Hz, 3H), 7.28 – 7.24 (m, 4H), 6.87 (dd, *J* = 13.0, 5.4 Hz, 2H), 3.88 (s, 3H), 1.99 – 1.91 (m, 2H), 1.37 – 1.30 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 160.26, 133.90, 131.82, 129.42, 128.36, 127.95, 123.54, 120.55, 112.56, 110.69, 94.49, 90.55, 77.88, 74.06, 55.92, 18.62, 12.08, 11.88. IR (neat, cm^{-1}): 3009.91, 2922.50, 2834.60, 2229.39, 1722.14, 1595.33, 1573.80, 1492.27, 1463.11, 1433.89, 1264.86, 1024.60, 963.79, 756.20, 692.56. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{20}H_{17}O^+$: 273.12739, found: 273.12716. HPLC analysis: ee = 93%. IC (99% hexanes: 1% isopropanol, 0.8 mL/min): t_{major} = 7.83 min, t_{minor} = 10.68 min.



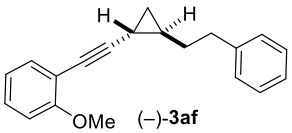
(1*R*,2*R*)-1,2-Bis((2-methoxyphenyl)ethynyl)cyclopropane ((–)-**3ad**) Yield: 93%. dr: 91:9. R_f = 0.3 (Hexane/Ethyl Acetate: 7/1). $[\alpha]_D^{20}$ = (–)-177.5° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.35 (dd, *J* = 7.6, 1.7 Hz, 2H), 7.25 (ddd, *J* = 9.2, 5.7, 1.8 Hz, 2H), 6.89 – 6.83 (m, 4H), 3.87 (s, 6H), 2.02 – 1.97 (m, 2H), 1.37 – 1.33 (m, 2H).^{13}C NMR (151 MHz, $CDCl_3$): δ 160.26, 133.90, 129.36, 120.54, 112.63, 110.69, 94.66, 73.98, 55.91, 18.79, 12.25. IR (neat, cm^{-1}): 3006.54, 2959.73, 2835.23, 2232.65, 1731.22, 1595.29, 1574.14, 1493.23, 1463.39, 1434.14, 1361.97, 1278.67, 1260.77, 1241.06, 1181.03, 1161.99, 1119.91, 1047.91, 1024.30, 935.74, 907.42, 826.31, 751.48. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{21}H_{19}O_2^+$: 303.13796, found: 303.13921. HPLC analysis: ee = 95%. IA (99.5% hexanes: 0.5% isopropanol, 1 mL/min): t_{major} = 12.22 min, t_{minor} = 17.06 min.



1-(((1*R*,2*R*)-2-Butylcyclopropyl)ethynyl)-2-methoxybenzene ((–)-**3ae**) Yield: 32%. dr: 86:14. R_f = 0.3 (Hexane/Ethyl Acetate: 20/1). $[\alpha]_D^{20}$ = (–)-82.6° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.33 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.21 (ddd, *J* = 8.3, 7.6, 1.7 Hz, 1H), 6.85 (ddt, *J* = 13.1, 8.3, 2.6 Hz, 3H), 3.85 (s, 4H), 1.63 – 1.57 (m, 2H), 1.56 – 1.49 (m, 4H), 1.46 – 1.34 (m, 5H), 1.09 – 0.97 (m, 3H), 0.91 (dd, *J* = 13.5, 6.3 Hz, 4H), 0.49 (dt, *J* = 9.9, 5.1 Hz, 1H).^{13}C NMR (151 MHz, $CDCl_3$): δ 160.21, 133.67, 128.74, 120.46, 113.56, 110.66, 95.62, 73.89, 55.87, 31.61, 30.04, 22.79, 19.25, 15.37, 14.31, 6.55. IR (neat, cm^{-1}): 2956.71, 2927.35, 2855.58, 2225.08, 1595.37, 1493.72, 1463.69, 1262.53, 1240.39, 1122.15, 1026.59. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{16}H_{21}O_1^+$: 229.15869, found: 229.15926. HPLC analysis: ee = 81%. IF (99.7% hexanes: 0.3% isopropanol, 0.8 mL/min): t_{major} = 19.15 min, t_{minor} = 18.58 min.

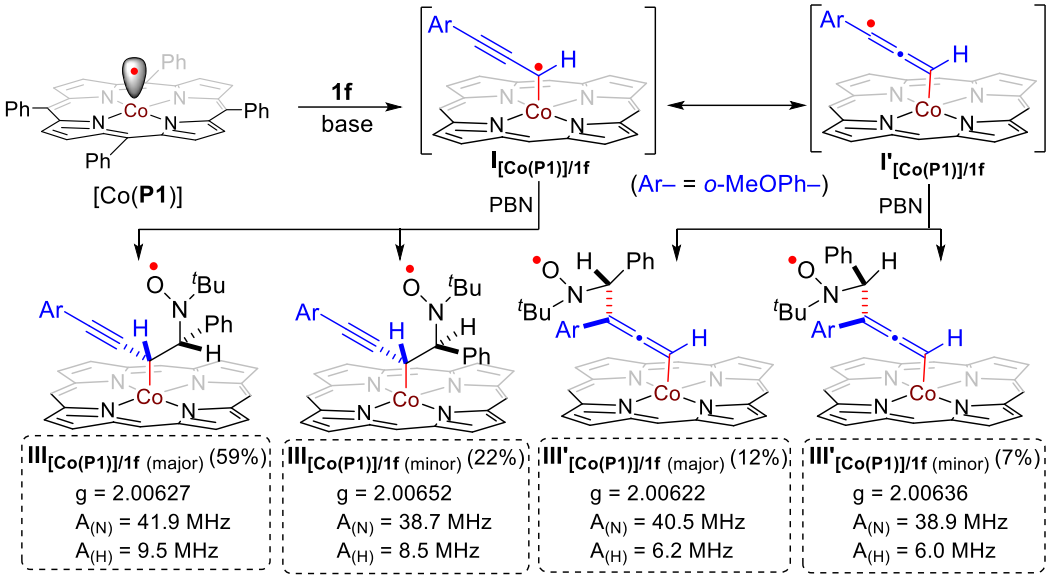


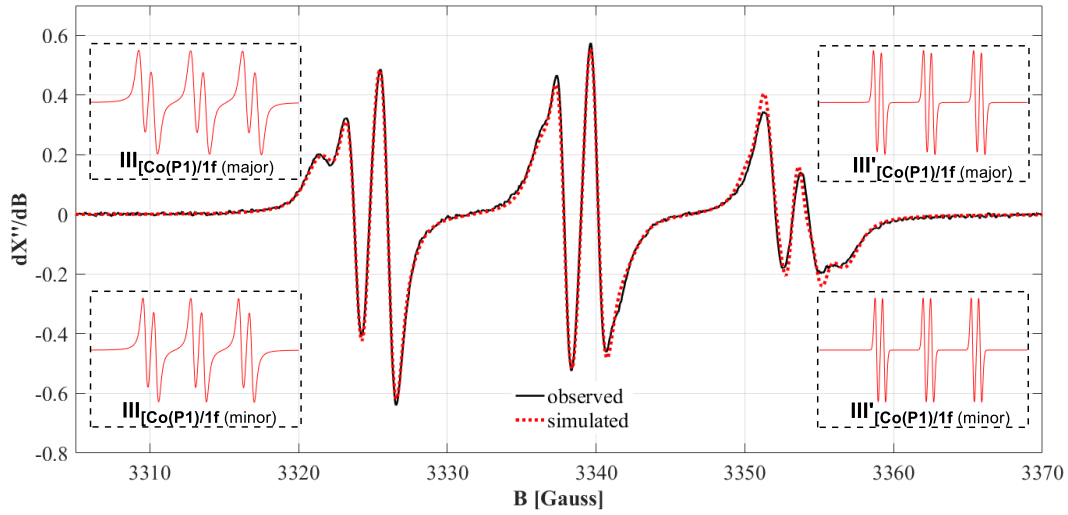
1-(((1*R*,2*R*)-2-Butylcyclopropyl)ethynyl)-2-methoxybenzene ((–)-**3af**) Yield: 40%. dr: 89:11. R_f = 0.3 (Hexane/Ethyl Acetate: 15:1). $[\alpha]_D^{20}$ = (–)-101.34° (*c* = 0.5, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$): δ 7.35 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.30 – 7.14 (m, 6H), 6.85 (dd, *J* = 16.8, 8.1 Hz, 2H), 3.80 (s, 3H), 2.97 – 2.87 (m, 1H), 2.77 (ddd, *J* = 13.6, 9.3, 6.6 Hz, 1H), 1.98 – 1.82 (m, 2H), 1.69 – 1.61 (m, 1H), 1.11 (dd, *J* = 14.1, 6.3 Hz, 1H), 1.04 (td, *J* = 8.3, 4.3 Hz, 1H), 0.55 (dd, *J* = 10.2, 5.4 Hz, 1H).^{13}C NMR (126 MHz, $CDCl_3$): δ 160.27, 142.74, 133.66, 128.84, 128.69, 128.56, 128.35, 125.75, 120.46, 110.62, 95.23, 74.12, 55.79, 35.62, 32.51, 18.83, 15.39, 6.59. IR (neat, cm^{-1}): 3025.09, 2923.97, 2333.48, 2032.88, 2005.85, 1595.32, 1493.34, 1453.99, 1241.32, 1116.57, 1026.87. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{20}H_{21}O^+$: 277.15869, found: 277.15789. HPLC analysis: ee = 85%. IF (99.9% hexanes: 0.1% isopropanol, 1 mL/min): t_{major} = 14.51 min, t_{minor} = 15.37 min.

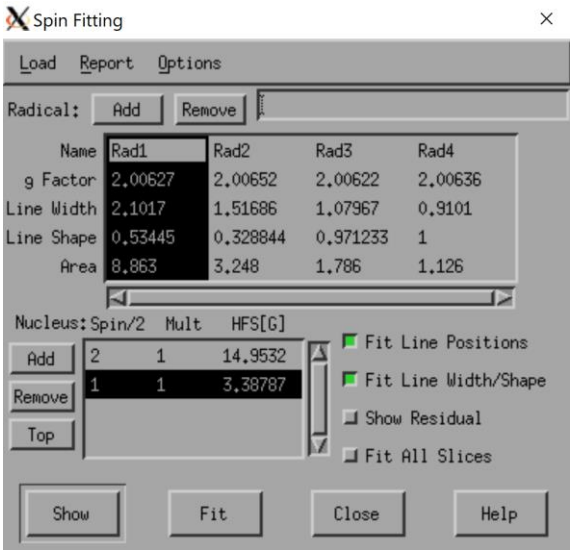


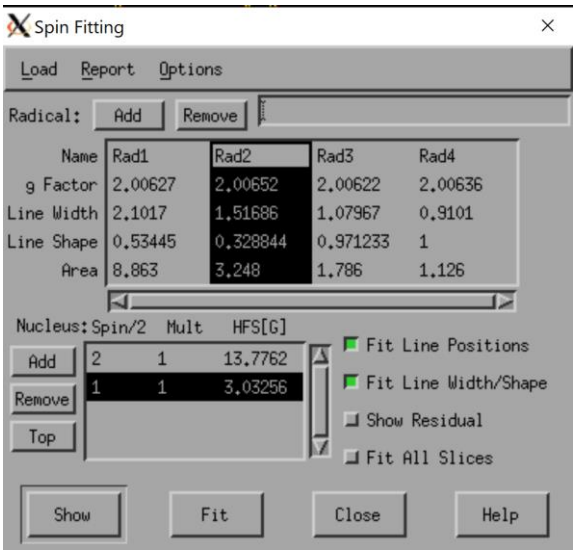
6. Mechanistic Studies of Stepwise Radical Mechanism

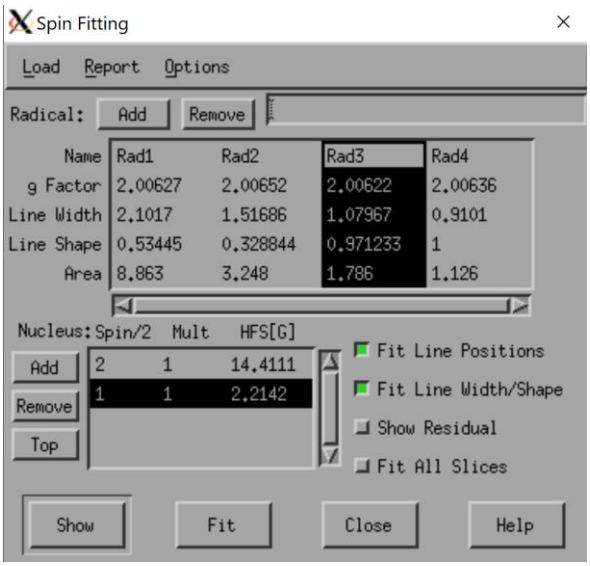
6.1. Characterization of α-Co(III)-Propargyl Radical and γ-Co(III)-Allenyl Radical Intermediates by EPR

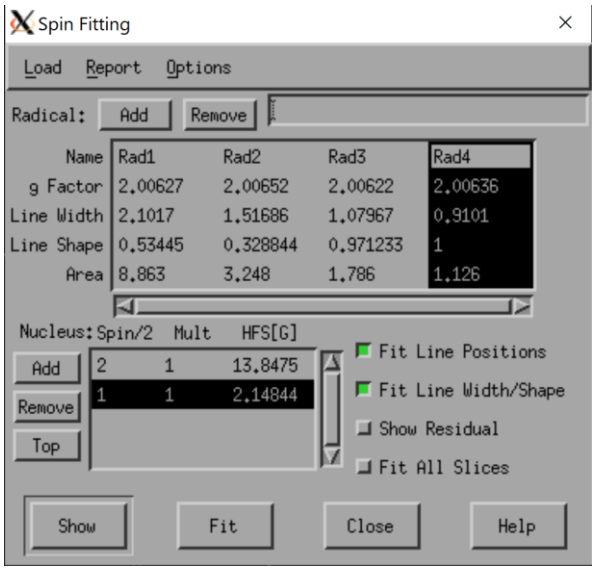












The resulting notable EPR signal (in black) has been simulated (in red) for:

III$_{\textbf{[Co(P1)]/1f (major)}}$ with g = 2.00627, $A_{(N)}$ = 41.9 MHz, $A_{(H)}$ = 9.5 MHz;

III$_{\textbf{[Co(P1)]/1f (minor)}}$ with g = 2.00652, $A_{(N)}$ = 38.7 MHz, $A_{(H)}$ = 8.5 MHz;

III'$_{\textbf{[Co(P1)]/1f (major)}}$ with g = 2.00622, $A_{(N)}$ = 40.5 MHz, $A_{(H)}$ = 6.2 MHz;

III'$_{\textbf{[Co(P1)]/1f (minor)}}$ with g = 2.00636, $A_{(N)}$ = 38.9 MHz, $A_{(H)}$ = 6.0 MHz.

[The simulation of the EPR spectrum was performed by iteration of the isotopic g-values and line widths using the EPR simulation program SpinFit Xenon]

Supplemental Experimental Procedure for EPR Experiment: A 10 mL oven-dried Schlenk tube was charged with *N*-sulfonyl hydrazone **1f** (0.10 mmol, 1.0 equiv), [Co(TPP)] (2 mol %) and PBN (0.12 mmol, 1.2 equiv). The Schlenk tube was capped with a Teflon screw cap, evacuated and backfilled with nitrogen 3 times. Under nitrogen atmosphere, Et_3N (0.20 mmol, 2.0 equiv) and anhydrous benzene (1.0 mL) were added via a syringe. The reaction mixture was stirred at 60 °C for 10 min. The reaction mixture was then transferred into a degassed EPR tube (filled with argon) through a syringe. The sample was then carried out for EPR experiment at room temperature.

EPR Simulation Details:

For **III**$_{[Co(P1)]/1f}$:

Major diastereomer (59%)

g = 2.00627

$A_{(N)}$ = 14.9532 × 2.00627 × 1.399611451 = 41.9 MHz

$A_{(H)}$ = 3.38787 × 2.00627 × 1.399611451 = 9.5 MHz

Minor diastereomer: (22%)

g = 2.00652

$A_{(N)}$ = 13.7762 × 2.00652 × 1.399611451 = 38.7 MHz

$A_{(H)}$ = 3.03256 × 2.00652 × 1.399611451 = 8.5 MHz

For **III'**$_{[Co(TPP)]/1f}$:

Major diastereomer: (12%)

g = 2.00622

$A_{(N)}$ = 14.4111 × 2.00622 × 1.399611451 = 40.5 MHz

$A_{(H)}$ = 2.21420 × 2.00622 × 1.399611451 = 6.2 MHz

Minor diastereomer: (7%)

g = 2.00636

$A_{(N)}$ = 13.8475 × 2.00636 × 1.399611451 = 38.9 MHz

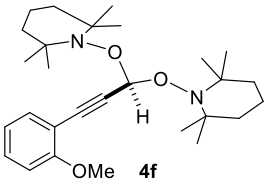
$A_{(H)}$ = 2.14844 × 2.00636 × 1.399611451 = 6.0 MHz

6.2. TEMPO Trapping Experiments

An oven-dried Schlenk tube was charged with sulfonyl hydrazone **1** (0.10 mmol, 1.0 equiv), [Co(**P1**)] (2 mol %) and KH (0.40 mmol, 4.0 equiv). The Schlenk tube was capped with a Teflon screw cap, evacuated and backfilled with nitrogen 3 times. Under nitrogen atmosphere, TEMPO (0.60 mmol, 6.0 equiv) and anhydrous ethyl acetate (0.6 mL) were added. The Schlenk tube was then purged with nitrogen for 1 min and sealed with the Teflon screw cap. The reaction mixture was stirred at 22 °C for

24 h. Following completion of the reaction, the reaction mixture was filtered through a pad of silica gel, concentrated under vacuum and purified by flash column chromatography.

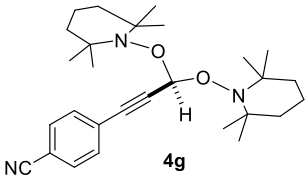
1,1'-((3-(2-Methoxyphenyl)prop-2-yne-1,1-diyl)bis(oxy))bis(2,2,6,6-tetramethylpipe-ridine) (**4f**)



4f

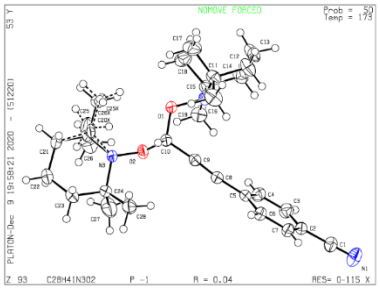
Yield: 40%. R_f = 0.3 (Hexane/Ethyl Acetate: 10/1). ^{1}H NMR (600 MHz, $CDCl_3$):δ 7.40 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.29 – 7.24 (m, 1H), 6.93 – 6.80 (m, 2H), 6.00 (s, 1H), 3.84 (s, 3H), 1.54 – 1.47 (m, 8H), 1.40 – 1.24 (m, 16H), 1.14 (d, *J* = 6.9 Hz, 12H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 132.15, 131.98, 128.52, 118.70, 111.57, 106.14, 91.61, 87.42, 60.12, 40.35, 40.25, 33.41, 33.35, 20.91, 17.38. IR (neat, cm^{-1}): 2930.21, 2362.19, 1596.22, 1493.89, 1464.28, 1376.14, 1361.67, 1326.42, 1292.09, 1261.43, 1181.67, 1132.22, 1046.59, 1027.98, 946.38, 749.46. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{28}H_{45}N_2O_3^+$: 457.34247, found: 457.34047.

1,1'-((3-(2-Methoxyphenyl)prop-2-yne-1,1-diyl)bis(oxy))bis(2,2,6,6-tetramethylpiper-idine) (**4g**)

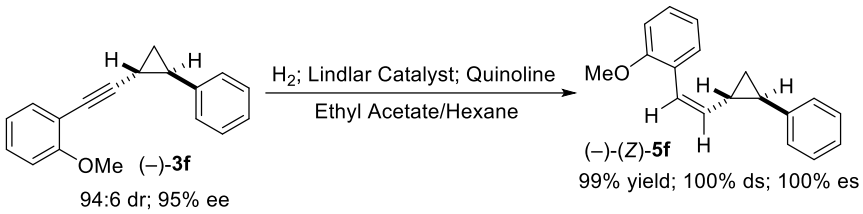


4g

Yield: 46%. R_f = 0.3 (Hexane/Ethyl Acetate: 10/1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.65 – 7.59 (m, 2H), 7.54 – 7.49 (m, 2H), 5.98 (s, 1H), 1.50 – 1.44 (m, 6H), 1.34 – 1.25 (m, 18H), 1.14 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 132.16, 131.99, 128.53, 118.70, 111.59, 106.16, 91.64, 87.44, 60.12, 40.37, 40.28, 33.42, 33.36, 20.92, 17.40. IR (neat, cm^{-1}): 2928.93, 2871.34, 2228.55, 1977.59, 1603.99, 1500.27, 1464.91, 1376.67, 1362.39, 1326.60, 1219.31, 1180.12, 1132.51. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{28}H_{42}N_3O_2^+$: 452.32715, found: 452.32842.

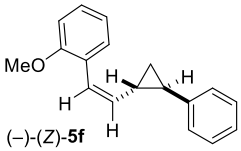


7. Further Transformations of Alkynyl-Substituted Cyclopropanes

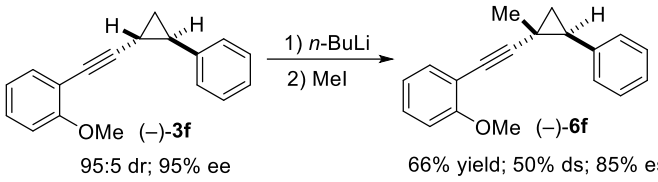


A round bottomed flask was charged with alkynylcyclopropane **3f** (0.1 mmol, 1.0 equiv), Lindlar Catalyst (0.12 mmol, 1.2 equiv), quinoline (0.2 mmol, 2.0 equiv), anhydrous hexane (1.0 mL) and anhydrous ethyl acetate (1.0 mL). The flask then was bubbled with hydrogen for 2 h. The mixture was then stirred at room temperature in hydrogen atmosphere. After 10 h, the reaction mixture was concentrated and purified by flash chromatography. The fractions containing product were collected and concentrated by rotary evaporation to afford the compound **5f**.

1-Methoxy-2-((*Z*)-2-((1*R*,2*S*)-2-phenylcyclopropyl)vinyl)benzene ((–)-(*Z*)-**5f**) Yield: 99%. dr: 94:6.

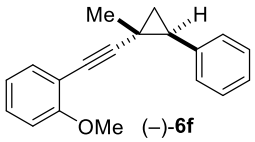


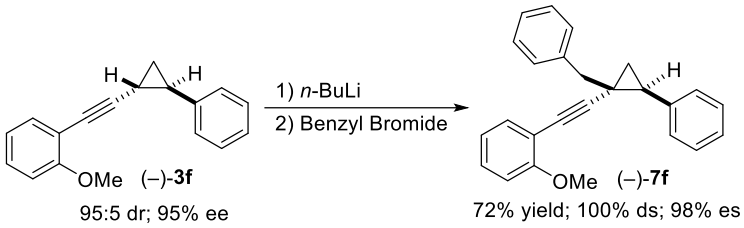
R_f = 0.3 (Hexane/Ethyl Acetate: 15/1). $[\alpha]_D^{20}$ = (–)-92.33° (*c* = 0.5, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$): δ 7.40 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.28 – 7.24 (m, 2H), 7.23 – 7.19 (m, 1H), 7.18 – 7.14 (m, 1H), 7.07 (dd, *J* = 8.0, 1.0 Hz, 2H), 6.86 (t, *J* = 8.3 Hz, 2H), 6.55 (d, *J* = 11.4 Hz, 1H), 5.32 (dd, *J* = 11.4, 9.5 Hz, 1H), 3.80 (s, 3H), 2.11 – 2.03 (m, 2H), 1.28 (ddd, *J* = 8.5, 5.7, 5.0 Hz, 1H), 1.19 – 1.14 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 157.05, 142.18, 134.95, 130.19, 129.27, 128.43, 128.14, 125.88, 125.70, 123.43, 120.23, 110.49, 55.49, 26.14, 24.19, 18.17. IR (neat, cm^{-1}): 3025.74, 3000.38, 2956.38, 2833.56, 1597.39, 1488.04, 1461.62, 1435.77, 1289.31, 1240.61, 1174.08, 1107.72, 1028.08. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{18}H_{19}O^+$: 251.14304, found: 251.14301. HPLC analysis: ee = 95%. IB (100% hexanes, 1 mL/min): t_{major} = 22.58 min, t_{minor} = 16.67 min.



A 10 mL oven-dried Schlenk tube was capped with a Teflon screw cap, evacuated and backfilled with nitrogen 3 times. Under nitrogen atmosphere, solution of alkynylcyclopropane **3f** (0.10 mmol, 1.0 equiv) in anhydrous THF (2.0 mL) was added followed by the addition of *n*-BuLi (0.16 mmol, 1.6 M in hexanes, 1.6 equiv) at −78 °C. After being warmed up naturally and stirred at 22°C for 1 h, methyl iodide (0.16 mmol, 1.6 equiv) was added. The reaction mixture was stirred at 22°C for 24 h. Following completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NH_4Cl, extracted with ether, drying over anhydrous $MgSO_4$, concentrated under vacuum and purified by flash column chromatography to afford the compound **6f**.[2]

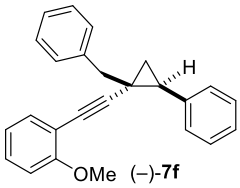
1-Methoxy-2-(((1S,2R)-1-methyl-2-phenylcyclopropyl)ethynyl)benzene ((–)-**6f**) Yield: 66%. dr: 72:28. R_f = 0.3 (Hexane/Ethyl Acetate: 10/1). $[\alpha]_D^{20}$ = (–)-133.98° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35 – 7.28 (m, 4H), 7.01 (dd, *J* = 7.7, 1.7 Hz, 1H), 6.89 (ddd, *J* = 12.6, 9.6, 4.6 Hz, 1H), 6.77 (ddd, *J* = 6.7, 3.3, 2.5 Hz, 2H), 3.78 (s, 3H), 2.18 (dd, *J* = 8.5, 6.7 Hz, 1H), 1.57 (s, 3H), 1.50 (dd, *J* = 6.6, 5.1 Hz, 1H), 1.28 (dd, *J* = 8.5, 5.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 159.97, 138.97, 133.72, 129.39, 128.36, 127.81, 126.07, 120.35, 113.23, 110.69, 96.88, 76.42, 55.84, 32.79, 25.74, 23.29, 17.97. IR (neat, cm^{-1}): 2960.12, 2930.36, 2344.24, 2222.81, 1737.47, 1595.78, 1574.03, 1494.12, 1433.30, 1365.31, 1275.51, 1249.43, 1114,76, 1025.64 HRMS (DART) ($[M+H]^+$) Calcd. for $C_{19}H_{19}O^+$: 263.14304, found: 263.14337. HPLC analysis: ee = 81%. ODH (99.7% hexanes : 0.3% isopropanol, 1 mL/min): t_{major} = 14.79 min, t_{minor} = 9.53 min.

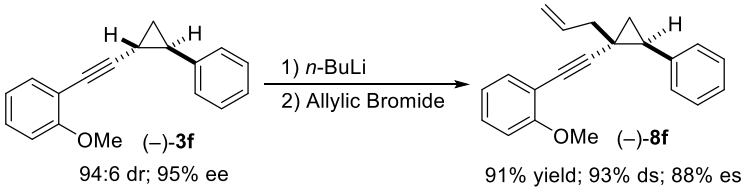




A 10 mL oven-dried Schlenk tube was capped with a Teflon screw cap, evacuated and backfilled with nitrogen 3 times. Under nitrogen atmosphere, solution of alkynylcyclopropane **3f** (0.10 mmol, 1.0 equiv) in anhydrous THF (2.0 mL) was added followed by the addition of *n*-BuLi (0.16 mmol, 1.6 M in hexanes, 1.6 equiv) at −78 °C. After being warmed up naturally and stirred at 22°C for 1 h, benzyl bromide (0.16 mmol, 1.6 equiv) was added. The reaction mixture was stirred at 22°C for 24 h. Following completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NH_4Cl, extracted with ether, drying over anhydrous $MgSO_4$, concentrated under vacuum and purified by flash column chromatography to afford the compound **7f**.[2]

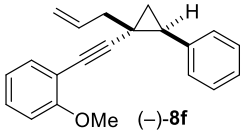
1-(((1*R*,2*R*)-1-Benzyl-2-phenylcyclopropyl)ethynyl)-2-methoxybenzene ((–)-**7f**) Yield: 72%. dr: 94:6. R_f = 0.3 (Hexane/Ethyl Acetate: 10/1). $[\alpha]_D^{20}$ = (–)-121.93° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.49 (d, J = 7.4 Hz, 2H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.31 (dd, *J* = 10.9, 5.8 Hz, 4H), 7.28 – 7.21 (m, 2H), 7.17 (t, *J* = 7.9 Hz, 1H), 7.00 – 6.97 (m, 1H), 6.78 (dd, *J* = 7.3, 6.5 Hz, 2H), 3.78 (s, 3H), 3.05 (s, 2H), 2.42 – 2.36 (m, 1H), 1.59 – 1.55 (m, 1H), 1.47 (dd, *J* = 8.7, 5.2 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.62, 141.88, 141.11, 135.98, 132.16, 131.25, 131.04, 130.78, 130.35, 129.07, 128.71, 122.84, 115.86, 113.29, 98.25, 80.81, 58.32, 47.32, 34.09, 26.39, 24.27. IR (neat, cm^{-1}): 3060.24, 3026.95, 2932.32, 2224.94, 1715.68, 1595.77, 1493.83, 1453.91, 1433,20 1250.54, 1113.19, 1027.36. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{25}H_{23}O^+$: 339.17434, found: 339.17432. HPLC analysis: ee = 93%. IA (99.5% hexanes: 0.5% isopropanol, 0.5 mL/min): t_{major} = 11.80 min, t_{minor} = 12.85 min.



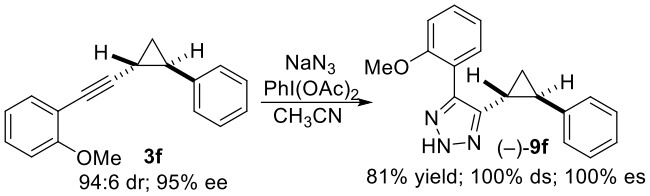


A 10 mL oven-dried Schlenk tube was capped with a Teflon screw cap, evacuated and backfilled with nitrogen 3 times. Under nitrogen atmosphere, solution of alkynylcyclopropane **3f** (0.10 mmol, 1.0 equiv) in anhydrous THF (2.0 mL) was added followed by the addition of *n*-BuLi (0.16 mmol, 1.6 M in hexanes, 1.6 equiv) at −78 °C. After being warmed up naturally and stirred at 22°C for 1 h, allylic bromide (0.16 mmol, 1.6 equiv) was added. The reaction mixture was stirred at 22°C for 24 h. Following completion of the reaction, the reaction mixture was quenched with saturated aqueous solution of NH_4Cl, extracted with ether, drying over anhydrous $MgSO_4$, concentrated under vacuum and purified by flash column chromatography to afford the compound **8f**.[2]

1-(((1*S*,2*R*)-1-Allyl-2-phenylcyclopropyl)ethynyl)-2-methoxybenzene ((–)-**8f**) Yield: 91%. dr: 91:9.

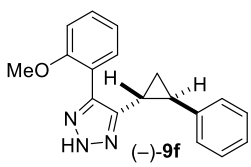


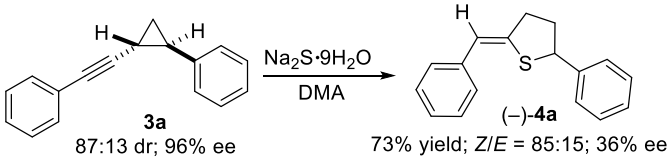
R_f = 0.3 (Hexane/Ethyl Acetate: 10/1). $[\alpha]_D^{20}$ = (–)-83.28° (*c* = 0.5, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$): δ 7.30 (dt, *J* = 13.2, 7.5 Hz, 4H), 7.21 – 7.12 (m, 2H), 7.00 – 6.96 (m, 1H), 6.77 – 6.70 (m, 2H), 6.07 (ddt, *J* = 17.0, 10.2, 6.8 Hz, 1H), 5.16 (ddd, *J* = 13.6, 11.0, 1.2 Hz, 2H), 3.75 (s, 3H), 2.42 (ddd, *J* = 81.5, 14.4, 6.8 Hz, 2H), 2.21 (dd, *J* = 8.5, 6.9 Hz, 1H), 1.49 (dd, *J* = 6.6, 5.3 Hz, 1H), 1.32 (dd, *J* = 8.7, 5.1 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 160.05, 138.70, 135.58, 133.62, 128.76, 128.47, 127.82, 126.14, 120.33, 116.85, 110.79, 107.50, 95.58, 77.68, 55.86, 43.42, 31.22, 22.61, 21.63. IR (neat, cm^{-1}): 3073.85, 3002.62, 2934.50, 2834.24, 2220.46, 1640.44, 1595.17, 1574.31, 1493.19, 1455.50, 1432.92, 1251.99, 1114.12, 1047.26, 1025.78. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{21}H_{21}O^+$: 289.15869, found: 289.15874. HPLC analysis: ee = 84%. IB (99.8% hexanes: 0.2% isopropanol, 0.5 mL/min): t_{major} = 14.06 min, t_{minor} = 13.74 min.



A 10 mL oven-dried Schlenk tube was capped with a Teflon screw cap, evacuated and backfilled with nitrogen 3 times. Under nitrogen atmosphere, solution of alkynylcyclopropane **3f** (0.10 mmol, 1.0 equiv) in anhydrous acetonitrile (2.0 mL) was added followed by the addition of NaN_3 (0.15 mmol, 1.5 equiv) and $PhI(OAc)_2$ (0.1 mmol, 1.0 equiv). The reaction mixture was stirred at 22°C for 12 h. Following completion of the reaction, the reaction mixture was concentrated under vacuum and purified by flash column chromatography to afford the compound **9f**.[3]

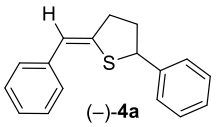
4-(2-Methoxyphenyl)-5-((1*R*,2*R*)-2-phenylcyclopropyl)-2H-1,2,3-triazole ((–)-**9f**) Yield: 81%. dr: 94:6. R_f = 0.3 (Hexane/Ethyl Acetate: 1/1). $[\alpha]_D^{20}$ = (–)-79.31° (*c* = 0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.64 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.36 (ddd, *J* = 8.5, 7.7, 1.7 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 2H), 7.18 (dd, *J* = 10.5, 4.2 Hz, 1H), 7.13 (d, *J* = 7.2 Hz, 2H), 6.97 (ddd, *J* = 8.4, 7.0, 3.1 Hz, 2H), 3.78 (s, 3H), 2.61 – 2.43 (m, 1H), 2.22 (ddd, *J* = 8.8, 5.8, 4.7 Hz, 1H), 1.81 (dt, *J* = 8.8, 5.4 Hz, 1H), 1.64 – 1.42 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 156.42, 144.67, 142.08, 130.32, 130.04, 129.97, 128.51, 125.99, 125.92, 121.25, 116.96, 111.39, 55.70, 26.33, 19.59, 17.50. IR (neat, cm^{-1}): 2933.53, 2836.57, 2103.14, 1604.31, 1489.90, 1462.88, 1434.70, 1117.48, 1024.70. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{18}H_{18}N_3O^+$: 292.14444, found: 292.14493. HPLC analysis: ee = 95%. IB (85% hexanes: 15% isopropanol, 1 mL/min): t_{major} = 5.87 min, t_{minor} = 5.30 min.





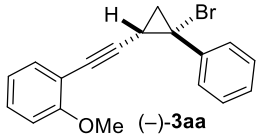
A 10 mL oven-dried Schlenk tube was capped with a Teflon screw cap, evacuated and backfilled with nitrogen 3 times. Under nitrogen atmosphere, solution of alkynylcyclopropane **3a** (0.10 mmol, 1.0 equiv) and $Na_2S·9H_2O$ (0.60 mmol, 6.0 equiv) in DMA (0.5 mL) was added. The reaction mixture was stirred at 150 °C for 12 h. Following completion of the reaction, ethyl acetate (2.0 mL) was added. The solution was washed with water (3 × 3.0 mL) and extracted with ethyl acetate (3 × 3.0 mL). The organic layers were combined, dried over sodium sulfate, concentrated under vacuum and purified by flash column chromatography to afford the compound **4a**.[4]

4-(2-Methoxyphenyl)-5-((1*R*,2*R*)-2-phenylcyclopropyl)-2H-1,2,3-triazole ((–)-**9f**) Yield: 73%. *Z*/*E*: 85:15. R_f =0.3 (Hexane/Ethyl Acetate = 20/1). $[\alpha]_D^{20}$ = (–)-17.49º (*c*=0.5, $CHCl_3$). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (t, *J* = 7.9 Hz, 4H), 7.34 (ddd, *J* = 8.3, 6.2, 1.6 Hz, 5H), 7.17 (q, *J* = 6.8 Hz, 1H), 6.48 (s, 1H), 4.84 (dd, *J* = 10.0, 5.3 Hz, 1H), 3.12 – 3.02 (m, 1H), 2.96 (dddd, *J* = 13.9, 11.7, 6.3, 2.2 Hz, 1H), 2.45 (dtd, *J* = 11.4, 5.7, 2.3 Hz, 1H), 2.10 (tddd, *J* = 11.4, 10.0, 6.3, 1.3 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.17, 140.70, 137.74, 128.73, 128.45, 127.90, 127.85, 127.24, 125.90, 116.89, 56.38, 46.87, 46.73, 40.44, 37.61. IR (neat, cm^{-1}): 3023.86, 2926.98, 1614.26, 1490.68, 1444.63, 1262.85, 1088.98, 750.35. HRMS (DART) ($[M+H]^+$) Calcd. for $C_{17}H_{17}S^+$: 253.1045, found: 253.1045. HPLC analysis: ee = 36%. ID (99.9% hexanes : 0.1% isopropanol, 0.8 mL/min): t_{major} = 13.41 min, t_{minor} = 12.17 min.



8. X-Ray Crystallography

The X-ray diffraction data were collected using Bruker-AXS SMART-APEXII CCD diffractometer (CuKα, λ = 1.54178 Å). Indexing was performed using *APEX2*[5] (Difference Vectors method). Data integration and reduction were performed using SaintPlus.[6] Absorption correction was performed by multi-scan method implemented in SADABS.[7] Space groups were determined using XPREP implemented in APEX2.[5] The structure was solved using SHELXS-97 (direct methods) and refined using SHELXL97 contained in WinGX v1.70.01[8,9,10] program.



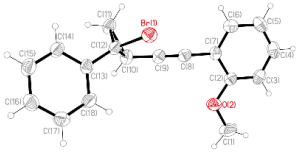
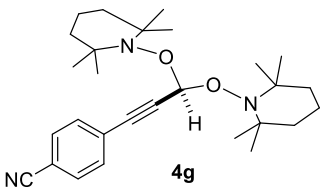


Table S1. Crystal data and structure refinement for (–)-3aa

Identification code	C18H15BrO	
Empirical formula	C18 H15 Br O	
Formula weight	327.21	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 8.4438(8) Å	α= 90°.
	b = 5.8701(6) Å	β= 100.634(3)°.
	c = 15.4882(15) Å	γ = 90°.
Volume	754.50(13) $Å^3$	
Z	2	
Density (calculated)	1.440 Mg/m^3	
Absorption coefficient	3.640 mm^{-1}	
F(000)	332	
Crystal size	0.380 x 0.080 x 0.060 mm^3	
Theta range for data collection	2.903 to 66.379°.	
Index ranges	-9<=h<=9, -6<=k<=6, -18<=l<=18	
Reflections collected	8320	
Independent reflections	2577 [R(int) = 0.0332]	
Completeness to theta = 66.380°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.5569	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2577 / 1 / 181	
Goodness-of-fit on F2	1.077	
Final R indices [I>2sigma(I)]	R1 = 0.0205, wR2 = 0.0546	
R indices (all data)	R1 = 0.0275, wR2 = 0.0553	
Absolute structure parameter	-0.038(14)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.215 and -0.219 e.Å-3	



4g

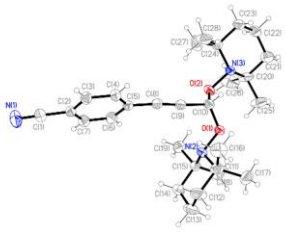


Table S2. Crystal data and structure refinement for 4g

dentification code	C28H41N3O2	
Empirical formula	C28 H41 N3 O2	
Formula weight	451.64	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P_{-1}	
Unit cell dimensions	a = 7.6884(2) Å	α= 107.9050(10)°.
	b = 12.6896(3) Å	β= 90.1750(10)°.
	c = 14.6933(4) Å	γ = 99.4080(10)°.
Volume	1343.57(6) $Å^3$	
Z	2	
Density (calculated)	1.116 Mg/m^3	
Absorption coefficient	0.546 mm-1	
F(000)	492	
Crystal size	0.160 x 0.120 x 0.060 mm3	
Theta range for data collection	3.166 to 66.545°.	
Index ranges	-9<=h<=9, -15<=k<=15, -17<=l<=17	
Reflections collected	22818	
Independent reflections	4588 [R(int) = 0.0282]	
Completeness to theta = 66.545°	96.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.7131	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4588 / 21 / 336	
Goodness-of-fit on F2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.1093	
R indices (all data)	R1 = 0.0498, wR2 = 0.1195	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.184 and -0.180 $e.Å^{-3}$	

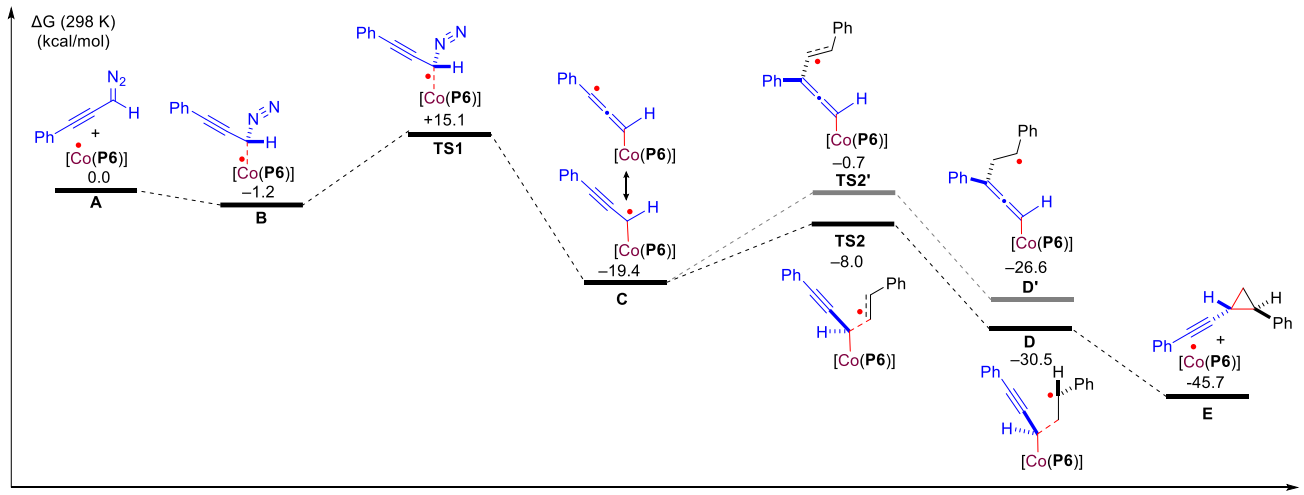
9. DFT Calculations

Considering the cost of time and computing resources for the large system with [Co(**P6**)], the geometry optimizations were performed with the Gaussian 16[11] at the BP86[12.13]/lanl2dz[14,15] level of theory in the gas phase at room temperature. Gas-phase Hessian matrix calculations were applied to the characterization of all minima (without imaginary frequency) and transition states (with only one imaginary frequency).

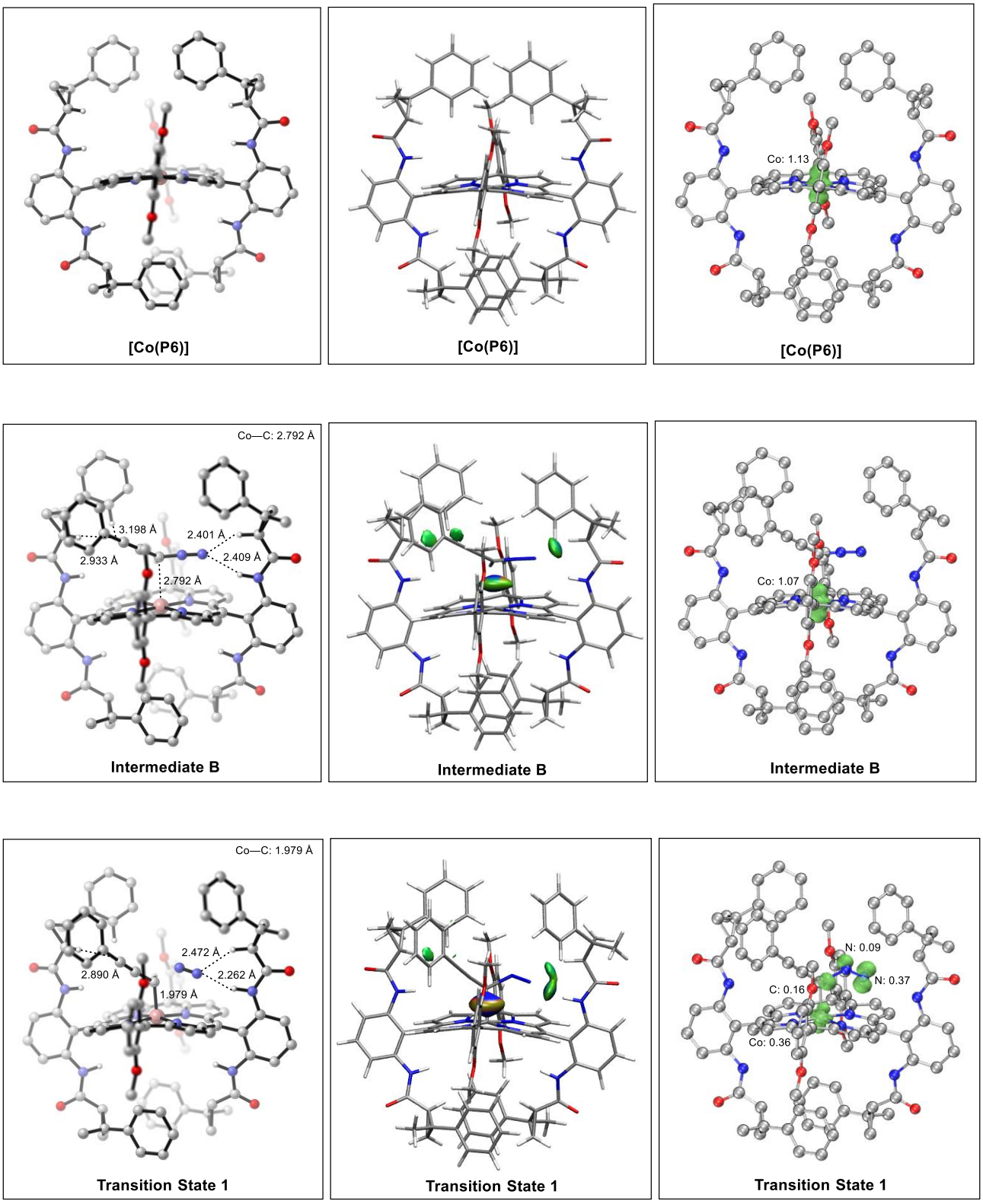
Thermochemical parameters such as internal energy, enthalpy, entropy, Gibbs free energy and thermal corrections (entropy and enthalpy, 298.15 K, 1 Atm) were obtained from these calculations. To further improve the accuracy of energies, single point energies were carried out at the B3LYP[16]/def2-tzvp[14,15] level of theory along with Grimme's dispersion correction[17] (D3BJ) and SMD[18] solvation model (in ethyl acetate).

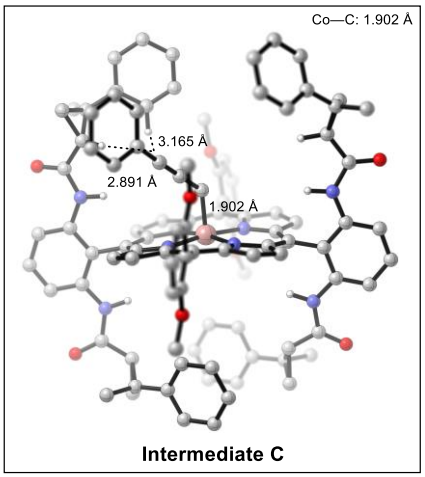
Independent Gradient Model (IGM)[19] analysis was performed with Multiwfn[20] software package using high quality grid option to generate files for further plotting. The visualization of IGM analysis results were presented with VMD[21] visualization software. As shown in Scheme S2, the 3D diagrams of optimized structures were generated with CYLview software.[22] The NCI (noncovalent interaction) and the spin density visual representations of optimized structures were generated with VMD and rendered with Tachyon.[23]

9.1. Scheme S2: Calculated Energy Diagram for [Co(P6)]-Catalyzed Radical Cyclopropanation of Styrene (2a) with Alkynyl Diazomethane (1a')

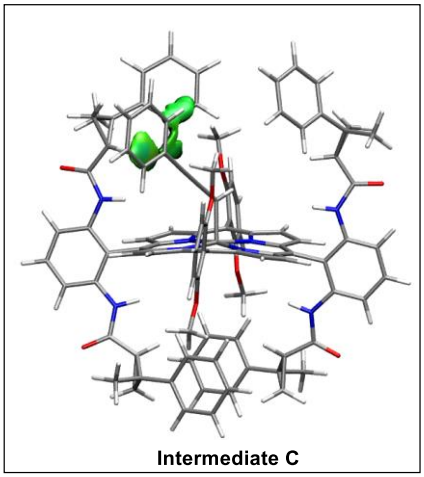


9.2. Scheme S3: Optimized Structure Models, NCI Plot and Spin Density Representations of Intermediates and Transition States

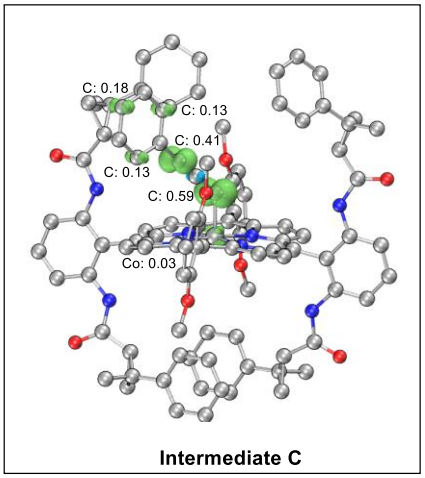




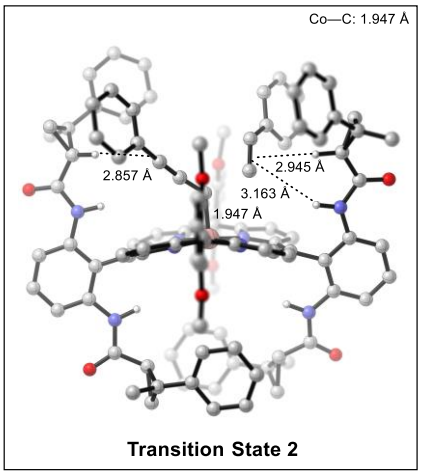
Intermediate C



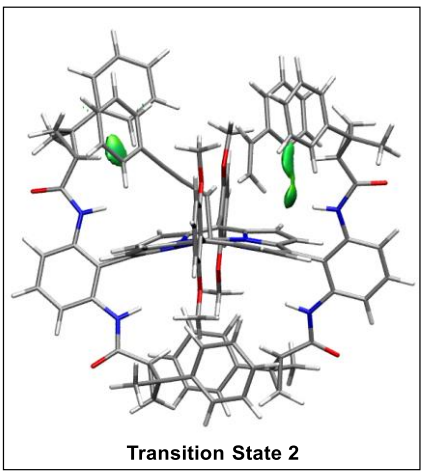
Intermediate C



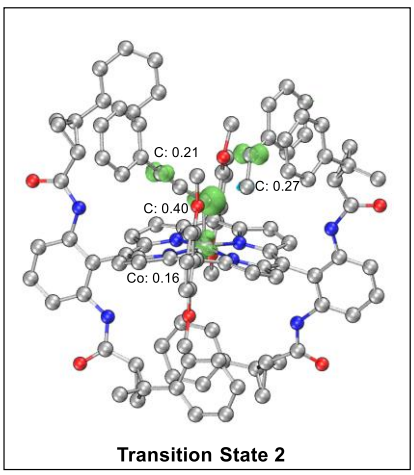
Intermediate C



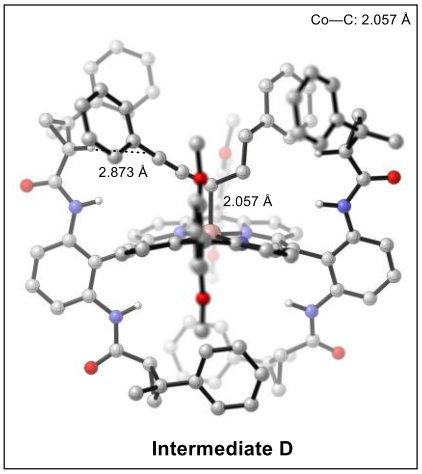
Transition State 2



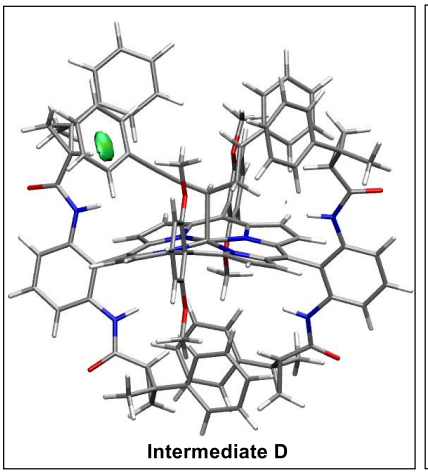
Transition State 2



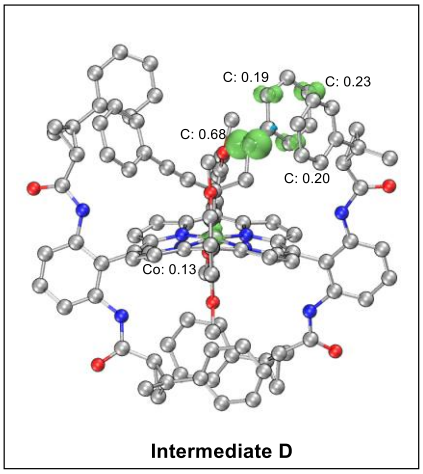
Transition State 2



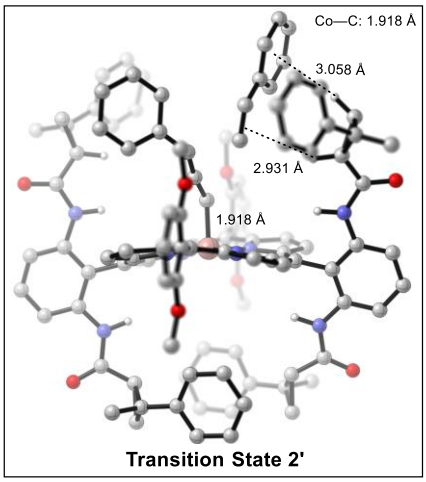
Intermediate D



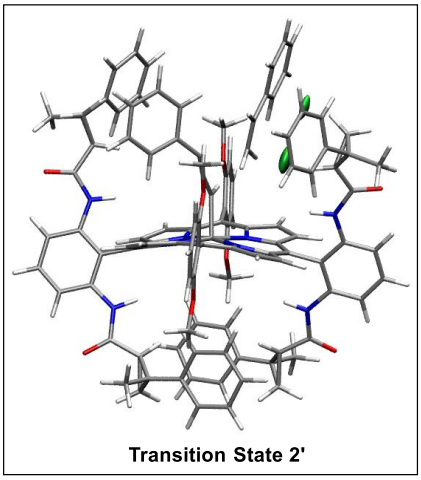
Intermediate D

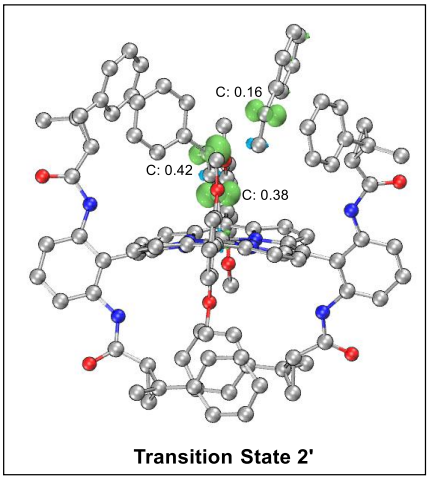


Intermediate D

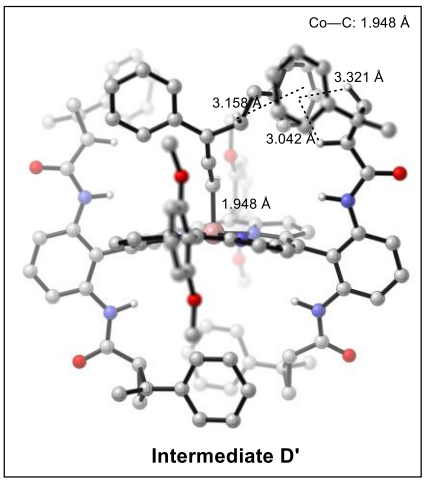


Transition State 2'

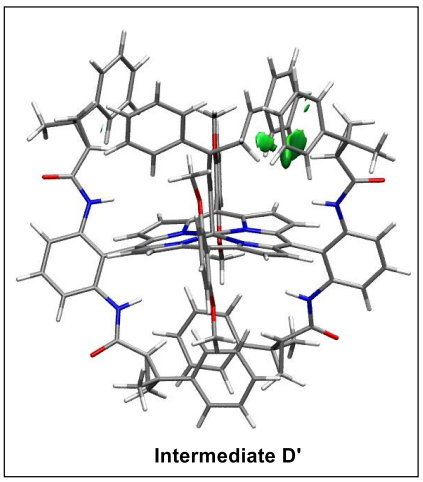

Transition State 2'

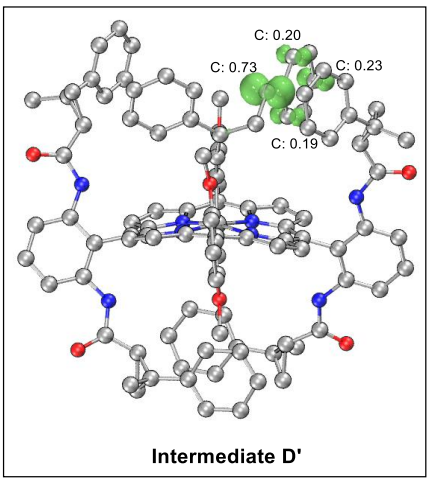


Transition State 2'



Intermediate D'


Intermediate D'



Intermediate D'

Intermediate A

$A_{[Co(II)(P6)]}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.333865 Hartree

H_corr: 1.583795 Hartree

SCF: -4738.422006 Hartree

S: 526.023 Cal/Mol-Kelvin

H: -4736.838211 Hartree

G: -4737.088141 Hartree

Cartesian Coordinates:

Co	0.03934800	-0.00003300	0.00001000
O	3.08077300	7.33946200	0.26140600
O	-4.90023900	5.62002500	1.06249500
O	-1.78130800	-0.18595100	5.26643800
O	2.87722900	-0.86170600	4.48060600
N	0.05983900	1.24476900	1.53516800
N	0.01209800	-1.52989400	1.24959600
N	1.80702300	5.36918900	0.47554800
H	1.88057400	4.34710300	0.51694300
N	-2.95133500	4.36821100	0.62192900
H	-2.61075500	3.41062600	0.48572700
C	-0.29835800	3.43626100	0.35821500
C	-0.10254700	2.64686000	1.51000200
C	0.01093100	3.20182300	2.85253800

H	-0.08367500	4.26113300	3.08888000
C	0.26773900	2.14634300	3.70288600
H	0.41994300	2.16532200	4.78094400
C	0.26458100	0.93413100	2.89779400
C	0.34462300	-0.35788700	3.44409600
C	0.15853700	-1.50440100	2.65343200
C	0.02778800	-2.84446900	3.20543700
H	0.10321600	-3.07975500	4.26613500
C	-0.22242800	-3.69797100	2.15125300
H	-0.38252200	-4.77521800	2.16925200
C	-0.20362500	-2.89041200	0.93846000
C	-0.58298200	4.91134200	0.50847100
C	0.47456000	5.87233200	0.52250800
C	0.18725800	7.26155900	0.61306500
H	1.01024100	7.97775900	0.59745300
C	-1.15796200	7.67423200	0.71884400
H	-1.38022800	8.74510400	0.79364300
C	-2.22526300	6.75156000	0.73678200
H	-3.26416600	7.07108400	0.83412000
C	-1.93495600	5.36467500	0.62602500
C	3.01217200	6.07589000	0.40158400
C	4.23191000	5.19991800	0.51179200
H	4.07399900	4.22650200	0.99334800
C	5.58751000	5.88633800	0.78549700
H	6.25549000	5.40469300	1.50692700
H	5.54816300	6.98021800	0.82483300

C	5.36253100	5.22663500	-0.57706900
C	6.06524200	3.90716900	-0.84527700
C	7.48530200	3.86253800	-0.88261500
H	8.05460800	4.77809500	-0.67720700
C	8.16521200	2.65518100	-1.16671100
H	9.26158400	2.63731200	-1.18856300
C	7.43264700	1.46785400	-1.41263500
H	7.95535700	0.52601400	-1.61638600
C	6.01727800	1.50223500	-1.38162700
H	5.44321900	0.58382300	-1.55490800
C	5.34041900	2.71522500	-1.10812900
H	4.24346700	2.73443800	-1.09289600
C	5.19559300	6.11807800	-1.81578400
H	6.18833300	6.37704000	-2.23019500
H	4.66492900	7.05187700	-1.56257000
H	4.62625500	5.59078400	-2.60443900
C	-4.32833300	4.50521800	0.83688600
C	-5.06448900	3.19454400	0.79893700
H	-4.56995500	2.38644300	0.24515900
C	-6.60477700	3.20018200	0.74228800
H	-7.06809200	4.19248100	0.76748200
H	-7.07237800	2.46842900	0.07582200
C	-5.92641800	2.71772600	2.02541400
C	-5.89825800	1.22917200	2.32110200
C	-4.67466600	0.56547200	2.60389400
H	-3.73188600	1.12559000	2.56223000

C	-4.65476800	-0.81117500	2.93220600
H	-3.69803300	-1.30409400	3.14192200
C	-5.86628800	-1.54350000	2.99209900
H	-5.85356900	-2.61124700	3.24091600
C	-7.09315400	-0.88891200	2.72090200
H	-8.03476400	-1.44944800	2.76916200
C	-7.10708200	0.48664100	2.38824600
H	-8.05750700	0.99072700	2.17175200
C	-6.00510000	3.60240400	3.27825400
H	-6.93984800	3.38707100	3.82997300
H	-5.99131700	4.67272100	3.01013500
H	-5.15597500	3.39898000	3.95811500
C	0.55830100	-0.51798100	4.92373700
C	-0.52329300	-0.42191500	5.84550400
C	-0.31790500	-0.56588900	7.24392000
H	-1.15099700	-0.49072800	7.94782000
C	0.98655300	-0.81411600	7.72143700
H	1.15152900	-0.92601700	8.79931900
C	2.08233900	-0.92275900	6.83916600
H	3.08352100	-1.11474400	7.23414500
C	1.85922900	-0.77455400	5.44389400
C	-2.93434700	-0.04071500	6.17099300
C	4.23897400	-1.16179400	4.95137500
O	3.08104600	-7.33945400	-0.26115800
O	-4.90002400	-5.62015500	-1.06252300
O	-1.78143200	0.18583700	-5.26634000

O	2.87710100	0.86173400	-4.48066300
N	0.05990500	-1.24483600	-1.53514700
N	0.01199500	1.52982500	-1.24958000
N	1.80724200	-5.36923600	-0.47551300
H	1.88077000	-4.34715100	-0.51698300
N	-2.95111900	-4.36833300	-0.62197700
H	-2.61054700	-3.41074500	-0.48577700
C	-0.29817600	-3.43634700	-0.35819200
C	-0.10240900	-2.64693600	-1.50997900
C	0.01104900	-3.20189000	-2.85252100
H	-0.08351000	-4.26120400	-3.08886300
C	0.26776600	-2.14639300	-3.70287500
H	0.41992200	-2.16535400	-4.78094100
C	0.26457500	-0.93418500	-2.89777900
C	0.34454600	0.35783600	-3.44408200
C	0.15843000	1.50434400	-2.65341500
C	0.02763400	2.84440900	-3.20541500
H	0.10306900	3.07970300	-4.26611200
C	-0.22261400	3.69789700	-2.15122700
H	-0.38274500	4.77513900	-2.16922100
C	-0.20378300	2.89033300	-0.93843800
C	-0.58276900	-4.91143300	-0.50844600
C	0.47479100	-5.87240400	-0.52245100
C	0.18751100	-7.26163800	-0.61297100
H	1.01050400	-7.97782600	-0.59733500
C	-1.15770100	-7.67433700	-0.71876500

H	-1.37994300	-8.74521500	-0.79354700
C	-2.22501700	-6.75168200	-0.73674900
H	-3.26391300	-7.07122300	-0.83411000
C	-1.93473300	-5.36479000	-0.62601500
C	3.01241000	-6.07590300	-0.40151000
C	4.23212200	-5.19990100	-0.51176400
H	4.07420000	-4.22655900	-0.99346500
C	5.58776600	-5.88631400	-0.78529000
H	6.25576200	-5.40475100	-1.50676200
H	5.54845800	-6.98020000	-0.82446900
C	5.36268700	-5.22641700	0.57716000
C	6.06531800	-3.90687500	0.84520500
C	7.48537400	-3.86210100	0.88244500
H	8.05475500	-4.77762200	0.67708400
C	8.16518200	-2.65465000	1.16639600
H	9.26155300	-2.63666600	1.18817000
C	7.43251400	-1.46737700	1.41226900
H	7.95514300	-0.52546700	1.61590200
C	6.01714400	-1.50190100	1.38135500
H	5.44300600	-0.58352900	1.55458700
C	5.34039100	-2.71498100	1.10800300
H	4.24344000	-2.73430300	1.09281400
C	5.19569800	-6.11766600	1.81600600
H	6.18841800	-6.37650600	2.23053700
H	4.66509500	-7.05153000	1.56290200
H	4.62626800	-5.59027400	2.60453000

C	-4.32810500	-4.50533900	-0.83699200
C	-5.06426400	-3.19466200	-0.79901000
H	-4.56972400	-2.38658300	-0.24520500
C	-6.60455200	-3.20029900	-0.74235400
H	-7.06787000	-4.19259500	-0.76757500
H	-7.07214900	-2.46855400	-0.07587900
C	-5.92618300	-2.71781400	-2.02547100
C	-5.89802600	-1.22925000	-2.32111900
C	-4.67444200	-0.56550000	-2.60381200
H	-3.73164300	-1.12558200	-2.56210400
C	-4.65457700	0.81115700	-2.93209000
H	-3.69785100	1.30412000	-3.14174800
C	-5.86611800	1.54343900	-2.99204500
H	-5.85341900	2.61119400	-3.24082900
C	-7.09298100	0.88879900	-2.72094700
H	-8.03460800	1.44930200	-2.76925500
C	-7.10687700	-0.48676200	-2.38832900
H	-8.05729600	-0.99089200	-2.17191200
C	-6.00487300	-3.60246300	-3.27832900
H	-6.93962400	-3.38712100	-3.83003800
H	-5.99108900	-4.67278600	-3.01023100
H	-5.15575100	-3.39903000	-3.95819000
C	0.55817900	0.51794000	-4.92373000
C	-0.52345100	0.42185400	-5.84545300
C	-0.31811500	0.56583800	-7.24387600
H	-1.15122900	0.49066400	-7.94774800

C	0.98632300	0.81409500	-7.72143600
H	1.15125900	0.92600300	-8.79932400
C	2.08214000	0.92275700	-6.83920700
H	3.08330500	1.11476100	-7.23422100
C	1.85908100	0.77454200	-5.44392700
C	-2.93450200	0.04056600	-6.17084900
C	4.23882600	1.16185500	-4.95146300
H	4.84822200	-1.22351100	4.03848200
H	4.27196200	-2.13048600	5.48642700
H	4.61994500	-0.35558600	5.60810700
H	-3.79131200	0.14062400	5.50680200
H	-2.79575200	0.81735100	6.85675200
H	-3.10180900	-0.96675600	6.75447300
H	4.84808900	1.22361200	-4.03858100
H	4.27177800	2.13054400	-5.48652400
H	4.61980800	0.35565200	-5.60819200
H	-3.79143200	-0.14081600	-5.50662300
H	-2.79590300	-0.81748800	-6.85662400
H	-3.10202300	0.96660600	-6.75431400

$A_{1a'}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.084648 Hartree

H_corr: 0.131982 Hartree

SCF: -456.153645Hartree

S: 99.622 Cal/Mol-Kelvin

H: -455.757252 Hartree

G: -455.804586 Hartree

Cartesian Coordinates:

N	-4.85027900	1.00185300	0.00083100
N	-4.03063300	0.14431500	0.00015400
H	-3.51793700	-1.84750100	-0.00032800
C	-3.11657000	-0.82960100	-0.00020700
C	-1.73064700	-0.55419000	-0.00054500
C	-0.50204000	-0.35992600	-0.00065000
H	0.74035900	2.04581800	-0.00083600
C	0.91075500	-0.13281600	-0.00047000
C	1.43475200	1.19816300	-0.00048400
C	1.82602100	-1.23196800	0.00022600
H	1.43273300	-2.25473400	0.00043100
C	2.82854400	1.41628400	0.00001400
H	3.21576200	2.44188900	-0.00007400
C	3.21786700	-1.00166000	0.00045500
C	3.72769200	0.32074800	0.00037600
H	3.90752200	-1.85383800	0.00089600
H	4.80971100	0.49498500	0.00071900

Intermediate B

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.440962 Hartree

H_corr: 1.717747 Hartree

SCF: -5194.313943 Hartree

S: 582.542 Cal/Mol-Kelvin

H: -5192.596196 Hartree

G: -5192.872981 Hartree

Cartesian Coordinates:

N	2.30173200	1.68473800	0.71295300
N	2.21064600	2.86133900	0.66789400
Co	-0.36358800	0.05943400	0.13176100
O	3.30091400	-7.03292600	0.69027800
O	-4.49869500	-6.03228700	-1.48989300
O	-1.73735700	0.13111000	-5.31783200
O	2.79514800	0.88770900	-4.04922700
N	-0.10072000	-1.21552400	-1.35325600
N	-0.46938100	1.54833400	-1.16640700
N	1.97320500	-5.15598100	0.18414700
H	1.98569400	-4.13290700	0.11074000
N	-2.78646000	-4.59363800	-0.74169600
H	-2.57251400	-3.60765900	-0.55945400
C	-0.30083700	-3.40575800	-0.13314900
C	-0.11199200	-2.62517800	-1.29320200
C	0.14644500	-3.19672600	-2.60859500
H	0.17224600	-4.26557600	-2.81860200
C	0.34780200	-2.13972400	-3.47313300

H	0.55630100	-2.16679000	-4.54199500
C	0.17428000	-0.91581900	-2.70404400
C	0.19050300	0.36668400	-3.27882600
C	-0.17527900	1.50867600	-2.54578200
C	-0.39474800	2.81334600	-3.15359500
H	-0.23198600	3.03334300	-4.20782700
C	-0.86270300	3.65126900	-2.16266100
H	-1.15169600	4.69915900	-2.23473000
C	-0.88331700	2.87795300	-0.92758600
C	-0.41742600	-4.90543600	-0.26099000
C	0.70758300	-5.76676800	-0.06741300
C	0.55664700	-7.17834200	-0.15906000
H	1.42301700	-7.81725200	0.01560900
C	-0.71028400	-7.71477600	-0.46873100
H	-0.82164800	-8.80269500	-0.54506000
C	-1.83672500	-6.89439900	-0.68419400
H	-2.81473000	-7.30829600	-0.93478700
C	-1.68990700	-5.48565000	-0.57115100
C	3.18917400	-5.77874000	0.49502400
C	4.37188300	-4.84906700	0.54797200
H	4.22871600	-3.86445100	0.08729700
C	5.76492800	-5.49557100	0.35560500
H	6.47384500	-4.96190000	-0.28526300
H	5.75461200	-6.58699500	0.26467000
C	5.41162400	-4.90427500	1.72301800
C	6.09408900	-3.59973100	2.10003300

C	7.48017400	-3.61799200	2.42111700
H	8.03042700	-4.56576800	2.36161900
C	8.15562400	-2.43484900	2.79721400
H	9.22481900	-2.46901900	3.03902100
C	7.45562500	-1.20330200	2.85095500
H	7.97948600	-0.28088000	3.12864000
C	6.07704300	-1.17409200	2.53346800
H	5.53114400	-0.22240900	2.54606900
C	5.40071800	-2.36512100	2.17163700
H	4.33258900	-2.32985800	1.92851300
C	5.16850600	-5.85086700	2.90718500
H	6.13042700	-6.11015300	3.38882100
H	4.67828400	-6.78084800	2.57350200
H	4.52868500	-5.36670400	3.66901500
C	-4.09096100	-4.86889700	-1.17091100
C	-4.96360800	-3.64644600	-1.23796200
H	-4.65719300	-2.80673200	-0.60157400
C	-6.48291100	-3.82749800	-1.42420900
H	-6.81802000	-4.86483400	-1.53152400
H	-7.12924700	-3.17265200	-0.83144100
C	-5.67462600	-3.23519200	-2.57933800
C	-5.77720800	-1.74547100	-2.85046300
C	-4.61209100	-0.93782300	-2.93736300
H	-3.62602400	-1.38653600	-2.76282400
C	-4.70663500	0.44081700	-3.24388000
H	-3.79388400	1.04493000	-3.30564900

C	-5.97358400	1.03042000	-3.47809800
H	-6.05026900	2.09973500	-3.70747200
C	-7.14132500	0.23162900	-3.40355000
H	-8.12471600	0.68203400	-3.58543300
C	-7.04185500	-1.14543300	-3.09239300
H	-7.94740200	-1.76225600	-3.02931100
C	-5.45459700	-4.08608000	-3.83868100
H	-6.31112700	-3.96213100	-4.52833600
H	-5.35834400	-5.15536200	-3.58353500
H	-4.53964900	-3.76786600	-4.37370400
C	0.54526300	0.51286700	-4.73310400
C	-0.43053100	0.38903000	-5.76234100
C	-0.07903600	0.52162400	-7.13303400
H	-0.83174800	0.42663400	-7.92018800
C	1.26551600	0.78223200	-7.47330200
H	1.54151500	0.88655700	-8.52903500
C	2.26100100	0.91260000	-6.48155100
H	3.29611700	1.11559600	-6.76916700
C	1.89089300	0.77733200	-5.11690100
C	-2.78468500	-0.04429600	-6.33856100
C	4.21234300	1.10882900	-4.36984800
O	1.25540100	8.00568700	0.82088800
O	-6.15876100	4.68168900	0.63961400
O	-2.65977900	-0.33570000	5.22757200
O	2.09424000	-0.21665800	4.84704200
N	-0.69307100	1.33327600	1.61327200

N	-0.36654300	-1.43774000	1.42563700
N	0.50102900	5.79031500	0.52108100
H	0.81890600	4.81551300	0.44667300
N	-3.97790300	3.83558900	0.33307100
H	-3.45160300	2.96205900	0.22847300
C	-1.20238800	3.43261700	0.32836500
C	-1.03852600	2.69906900	1.52180200
C	-1.15091800	3.29034100	2.84828700
H	-1.41299400	4.33103900	3.03512500
C	-0.84256400	2.30039900	3.75844500
H	-0.81137300	2.36449600	4.84506900
C	-0.59196400	1.08349100	3.00085800
C	-0.38877300	-0.17413600	3.59554900
C	-0.35652700	-1.35747700	2.83621900
C	-0.37769400	-2.68855700	3.42365900
H	-0.37711600	-2.88615900	4.49469200
C	-0.42674100	-3.59294100	2.38277700
H	-0.46421600	-4.68066500	2.42679300
C	-0.38740000	-2.82144800	1.14710700
C	-1.75440800	4.83579800	0.40332900
C	-0.91279400	5.98962300	0.49216100
C	-1.48999400	7.28962100	0.56279400
H	-0.83167600	8.15597600	0.63239500
C	-2.89310100	7.42489600	0.55742400
H	-3.32908000	8.42911500	0.61525000
C	-3.75074000	6.30858400	0.48511900

H	-4.83706500	6.41006500	0.49600700
C	-3.17728100	5.01158700	0.40725500
C	1.49996800	6.76022500	0.69937000
C	2.89778800	6.21330800	0.75844400
H	2.98688900	5.12629200	0.84479500
C	3.95950200	7.04744600	1.51767200
H	4.64803000	6.49680700	2.16744300
H	3.60243500	8.00748700	1.90481100
C	4.08770900	6.91464500	0.00317000
C	5.16438900	5.99692800	-0.54762800
C	6.50938100	6.12301500	-0.10932900
H	6.74929400	6.85009500	0.67665600
C	7.53417900	5.32786700	-0.67503700
H	8.56794500	5.43825000	-0.32567800
C	7.22737500	4.39370100	-1.69370500
H	8.02002700	3.77736600	-2.13468000
C	5.88884600	4.26084300	-2.13749100
H	5.64302900	3.54022100	-2.92641600
C	4.86694300	5.05670900	-1.56981400
H	3.83133800	4.94895700	-1.91666200
C	3.82013200	8.14125900	-0.88179600
H	4.74154200	8.74892700	-0.96226000
H	3.01363800	8.76377900	-0.46032800
H	3.52986500	7.83205100	-1.90376600
C	-5.36615600	3.70145100	0.45914100
C	-5.83230400	2.27388300	0.38435300

H	-5.16003100	1.57881000	-0.13421500
C	-7.33892500	1.98696500	0.23423700
H	-7.98195000	2.87374900	0.22520200
H	-7.61726600	1.18535300	-0.45706600
C	-6.66144100	1.63522200	1.55920600
C	-6.36897900	0.17803100	1.86605700
C	-5.07017700	-0.23377900	2.26834700
H	-4.25670300	0.50140300	2.31298800
C	-4.81013600	-1.58253400	2.60983600
H	-3.80058400	-1.87665200	2.91989000
C	-5.85324500	-2.54033000	2.56050500
H	-5.65362800	-3.58709900	2.81832300
C	-7.15411000	-2.13855500	2.16880600
H	-7.96600600	-2.87518400	2.13203000
C	-7.40836000	-0.78921900	1.82543900
H	-8.41542800	-0.47939600	1.51854100
C	-6.98242300	2.48224100	2.79937700
H	-7.89048900	2.08977500	3.29543700
H	-7.15683700	3.53681400	2.52538200
H	-6.15206000	2.44162000	3.52986400
C	-0.28021900	-0.26648800	5.09146300
C	-1.43768100	-0.33971200	5.91785900
C	-1.33169000	-0.41719900	7.33235500
H	-2.22296800	-0.47096300	7.96325200
C	-0.04949700	-0.42666800	7.92176600
H	0.03957100	-0.48567300	9.01266700

C	1.12067300	-0.36318000	7.13532100
H	2.10178500	-0.37205600	7.61739900
C	0.99506000	-0.28454200	5.72266100
C	-3.89841800	-0.38960200	6.02228800
C	3.43904400	-0.27671500	5.44263600
H	4.71962400	1.12231900	-3.39475200
H	4.35711600	2.07522000	-4.89208400
H	4.61620600	0.28229800	-4.98518500
H	-3.70157100	-0.24519100	-5.76659500
H	-2.55371000	-0.90071000	-7.00115900
H	-2.91079500	0.87598500	-6.94120300
H	4.13140600	-0.26043900	4.58934800
H	3.58095900	-1.21419700	6.01353600
H	3.62357200	0.59683100	6.09743900
H	-4.70743000	-0.38442500	5.27812700
H	-3.98311100	0.49286600	6.68543600
H	-3.94639400	-1.31919300	6.62181800
C	3.16204600	-0.36999300	-0.16345700
C	5.05620800	-3.11154200	-3.85811300
C	4.74728800	-1.72241900	-1.84819100
C	4.20505500	-2.41246400	-2.97489700
C	6.45647400	-3.13023200	-3.63951300
C	3.88847100	-1.00288600	-0.94675000
C	7.00320900	-2.44843200	-2.52374500
C	2.34388300	0.34881800	0.74861100
C	6.15926800	-1.75314100	-1.63024500

H	6.57565900	-1.23725100	-0.75803400
H	8.08492200	-2.46406900	-2.34715400
H	7.11352400	-3.67467100	-4.32777400
H	3.12268400	-2.38971100	-3.14119700
H	4.62845100	-3.64383900	-4.71551000
H	1.88755200	-0.10440500	1.63636700

Transition State TS1

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -367.2223 cm-1

G_corr: 1.440841 Hartree

H_corr: 1.71512 Hartree

SCF: -5194.303944 Hartree

S: 577.269 Cal/Mol-Kelvin

H: -5192.588824 Hartree

G: -5192.863103 Hartree

Cartesian Coordinates:

N	2.62527600	1.31534700	0.68567000
N	2.44061600	2.42454100	0.31906800
Co	-0.19089100	0.06699100	0.17177000
O	2.16242300	-7.41637700	0.76345900
O	-5.36407500	-5.31515400	-1.61969000
O	-1.55536000	0.37034900	-5.31742200
O	3.00809700	0.52437000	-3.95421500

N	-0.26262400	-1.19232900	-1.34845100
N	-0.12245600	1.56920500	-1.11131700
N	1.13507800	-5.38419200	0.16371600
H	1.30099500	-4.37584100	0.07170200
N	-3.47613500	-4.14242700	-0.83287100
H	-3.12516500	-3.19854700	-0.63992000
C	-0.85040100	-3.33345000	-0.16650500
C	-0.52826300	-2.57798600	-1.31201200
C	-0.38122400	-3.16429800	-2.63693400
H	-0.55939700	-4.21447600	-2.86597900
C	0.01721400	-2.14929200	-3.48293300
H	0.21281700	-2.19490200	-4.55348900
C	0.07844300	-0.93014200	-2.69175700
C	0.34909000	0.33409200	-3.24120600
C	0.17875200	1.50769800	-2.48880700
C	0.15533600	2.83653300	-3.08043800
H	0.35360600	3.04257200	-4.13139700
C	-0.20399400	3.71905400	-2.08304600
H	-0.34765900	4.79720300	-2.14399700
C	-0.34325700	2.94266800	-0.85926000
C	-1.18736300	-4.79651900	-0.31441500
C	-0.19938500	-5.80943100	-0.10772500
C	-0.54885100	-7.18437900	-0.20888100
H	0.21343500	-7.94163300	-0.02139800
C	-1.87436700	-7.53220300	-0.54270800
H	-2.13956400	-8.59258500	-0.62653700

C	-2.86812800	-6.55822500	-0.77382300
H	-3.89053300	-6.82780400	-1.04329800
C	-2.52363600	-5.18521300	-0.65028600
C	2.23841800	-6.16646400	0.53011100
C	3.53633200	-5.40782100	0.59953400
H	3.55148200	-4.44094200	0.08304200
C	4.83691600	-6.24077200	0.52551600
H	5.64274800	-5.84554400	-0.10111500
H	4.68614700	-7.32517000	0.49352200
C	4.49642700	-5.52569800	1.83584000
C	5.31735100	-4.29443200	2.18131900
C	6.68540700	-4.45402000	2.53711700
H	7.12695800	-5.45880600	2.52621300
C	7.48111700	-3.33843500	2.88490600
H	8.53501100	-3.48084700	3.15301700
C	6.92181600	-2.03591400	2.87602600
H	7.53986000	-1.16674800	3.13083200
C	5.56085500	-1.86572900	2.52549400
H	5.12297300	-0.86036100	2.49269700
C	4.76405400	-2.98852300	2.19087100
H	3.71182300	-2.84486700	1.91953700
C	4.06737700	-6.35977500	3.05113900
H	4.95945900	-6.71404100	3.60185900
H	3.47505500	-7.23612800	2.73773600
H	3.45893200	-5.75194100	3.74721100
C	-4.79919900	-4.22405800	-1.28555000

C	-5.48596200	-2.88848600	-1.35670000
H	-5.06899000	-2.10280700	-0.71418100
C	-7.01392100	-2.84988300	-1.55834100
H	-7.49250900	-3.82845400	-1.67338500
H	-7.56606300	-2.11097700	-0.96913900
C	-6.11772700	-2.37552100	-2.70288500
C	-6.00529300	-0.88524700	-2.96783700
C	-4.73729200	-0.24887600	-3.03468800
H	-3.82704000	-0.83206800	-2.84649900
C	-4.63321800	1.13030800	-3.33550200
H	-3.64446300	1.60222400	-3.37750500
C	-5.80127500	1.89265600	-3.58463200
H	-5.72375200	2.96272000	-3.81030800
C	-7.07045900	1.26547400	-3.52954900
H	-7.97837500	1.84969600	-3.72280900
C	-7.16955100	-0.11270200	-3.22340500
H	-8.15359100	-0.59613500	-3.17477000
C	-6.00874500	-3.24459700	-3.96428100
H	-6.83252400	-2.99811900	-4.66086100
H	-6.06726200	-4.31755300	-3.71321000
H	-5.05303900	-3.05721000	-4.48982000
C	0.74630800	0.43879600	-4.68720500
C	-0.21651600	0.44781700	-5.73568300
C	0.17768800	0.53235800	-7.09839300
H	-0.56442900	0.53994000	-7.90112700
C	1.55211900	0.60941100	-7.41016400

H	1.86122600	0.67343200	-8.45992500
C	2.53562200	0.60809600	-6.39812000
H	3.59449100	0.66849400	-6.66365500
C	2.12318900	0.52661300	-5.04132200
C	-2.59715300	0.34717700	-6.35842300
C	4.44987800	0.56711300	-4.23777500
O	2.61182800	7.53611100	1.17484600
O	-5.26323600	5.60254300	0.67830100
O	-2.71970300	0.04267200	5.17163300
O	1.98190800	-0.73027300	4.95006600
N	-0.42121900	1.35899200	1.65840400
N	-0.58798700	-1.41068400	1.42586800
N	1.49463000	5.54019100	0.59590800
H	1.64562500	4.54021300	0.40685500
N	-3.25403000	4.40062100	0.39031600
H	-2.88400500	3.45249300	0.26729700
C	-0.58754900	3.52514500	0.39912100
C	-0.54635900	2.76241400	1.58312000
C	-0.58004900	3.34778900	2.91645200
H	-0.67915600	4.41421500	3.11490500
C	-0.43974000	2.31107700	3.81514800
H	-0.41452700	2.35500600	4.90283900
C	-0.37600200	1.07995900	3.04196100
C	-0.40727600	-0.20114300	3.61893400
C	-0.58133000	-1.35667700	2.83745500
C	-0.85923400	-2.66894500	3.39950200

H	-0.91904100	-2.87776800	4.46666000
C	-1.05139600	-3.53361700	2.34187200
H	-1.28892600	-4.59634200	2.36471300
C	-0.84878800	-2.76425600	1.12181000
C	-0.89368100	4.99894700	0.49391200
C	0.13807000	5.98327600	0.60920600
C	-0.20403800	7.36009900	0.73227200
H	0.59455600	8.09492800	0.83793600
C	-1.56228400	7.73799100	0.73865000
H	-1.81655000	8.79996400	0.83587000
C	-2.60225700	6.79235200	0.62645600
H	-3.65409100	7.08226600	0.64066600
C	-2.26377500	5.41858000	0.50415700
C	2.64356800	6.29843600	0.86983700
C	3.92841800	5.52431000	0.79328600
H	3.82722200	4.43962100	0.67815600
C	5.11740400	6.01442600	1.65753900
H	5.69900900	5.24590700	2.17771100
H	4.93188600	6.93489300	2.22103000
C	5.22261800	6.13915100	0.14065500
C	6.12671300	5.17063800	-0.60071200
C	7.46777600	4.97022900	-0.17858800
H	7.82309500	5.47307100	0.72964600
C	8.34378700	4.13873900	-0.91608100
H	9.37685200	3.99527200	-0.57677500
C	7.89026200	3.49740900	-2.09389300

H	8.56850600	2.85588400	-2.66933900
C	6.55394200	3.69049100	-2.52232400
H	6.19579800	3.20057700	-3.43580500
C	5.68049400	4.52001300	-1.78175300
H	4.64484600	4.66253800	-2.11533500
C	5.17394900	7.53385200	-0.50175600
H	6.18777900	7.97765800	-0.49997100
H	4.48675000	8.19792900	0.04771200
H	4.83606200	7.46965000	-1.55340600
C	-4.64707600	4.50493100	0.48553200
C	-5.34929800	3.18144700	0.35737800
H	-4.78565400	2.38939900	-0.15178200
C	-6.87545000	3.16238800	0.13989900
H	-7.35548200	4.14697400	0.12904600
H	-7.25732600	2.43389100	-0.58229700
C	-6.32607700	2.67388700	1.48077300
C	-6.30306000	1.18244700	1.76094800
C	-5.10817200	0.53820300	2.17954600
H	-4.17770300	1.11512000	2.25458700
C	-5.10090400	-0.84109400	2.49738300
H	-4.16716700	-1.31703100	2.81911800
C	-6.29660600	-1.59599200	2.40809200
H	-6.29302900	-2.66569900	2.64843300
C	-7.49546200	-0.96140200	1.99910600
H	-8.42488400	-1.54001000	1.93158500
C	-7.49692400	0.41718600	1.67908000

H	-8.42502400	0.90689300	1.35789800
C	-6.55147900	3.53952300	2.72920800
H	-7.53397100	3.29925400	3.17825400
H	-6.53063100	4.61336800	2.47633900
H	-5.77297300	3.34276200	3.49076400
C	-0.36480400	-0.33217600	5.11546200
C	-1.54458400	-0.19671600	5.90175400
C	-1.50561800	-0.30741600	7.31732100
H	-2.41306700	-0.19972600	7.91748100
C	-0.26933900	-0.56257500	7.94837400
H	-0.23161400	-0.64788200	9.04053000
C	0.91896000	-0.71182100	7.20213600
H	1.86360900	-0.90920200	7.71559200
C	0.86156800	-0.59719000	5.78719900
C	-3.97360400	0.21244100	5.92505300
C	3.27388700	-1.03420500	5.58775100
H	4.93005200	0.55809500	-3.24940500
H	4.72092900	1.49227800	-4.78367900
H	4.76693600	-0.32152600	-4.81622600
H	-3.54450400	0.27624000	-5.80540400
H	-2.47700600	-0.53135500	-7.02143400
H	-2.58037400	1.27755700	-6.95847500
H	3.98490200	-1.13980400	4.75669900
H	3.22457300	-1.98379200	6.15443400
H	3.58948300	-0.21028000	6.25669900
H	-4.74186800	0.37512000	5.15590900

H	-3.91581800	1.08854500	6.59939600
H	-4.21405000	-0.69784300	6.50764600
C	2.51622400	-1.01902600	-0.24852000
C	4.58905800	-3.68110700	-3.91324100
C	4.16141900	-2.38991700	-1.85893500
C	3.69822000	-2.97282200	-3.07911900
C	5.95501400	-3.81327300	-3.55744200
C	3.26926100	-1.66072500	-1.00506500
C	6.42412100	-3.23614800	-2.35072300
C	1.73175300	-0.15649900	0.58371300
C	5.53939500	-2.53654400	-1.50229600
H	5.89795500	-2.10132500	-0.56314800
H	7.47814600	-3.33751700	-2.06731900
H	6.64339700	-4.36377700	-4.20922300
H	2.64346600	-2.86358900	-3.35124500
H	4.21890300	-4.13166200	-4.84151700
H	1.75721600	-0.41634600	1.65881500

Intermediate C

$C_{[Co(III)(P6)]}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.434835 Hartree

H_corr: 1.705227 Hartree

SCF: -6325.50188201 Hartree

S: 569.087 Cal/Mol-Kelvin

H: -6323.796655 Hartree

G: -6324.067047 Hartree

Cartesian Coordinates:

Co	-0.21374200	0.10003500	0.14770900
O	2.68689800	-7.11820800	1.10494100
O	-5.13740600	-5.73513500	-0.84532600
O	-1.85809100	-0.14473700	-5.26259100
O	2.76036800	0.34977000	-4.19791200
N	-0.29462300	-1.28312900	-1.26404300
N	-0.21625000	1.49450000	-1.26147000
N	1.45134700	-5.20941600	0.49210300
H	1.52796900	-4.19784200	0.33891800
N	-3.28329300	-4.37929300	-0.31391900
H	-2.98512000	-3.40141800	-0.23576100
C	-0.69086000	-3.34236700	0.12129200
C	-0.46829800	-2.67344600	-1.09731600
C	-0.34516300	-3.36672500	-2.37217300
H	-0.46129400	-4.44251000	-2.49863200
C	-0.05586500	-2.40928300	-3.32164400
H	0.09925500	-2.53827000	-4.39185700
C	-0.03316800	-1.12371600	-2.64173400
C	0.15843000	0.09599800	-3.30950300
C	0.01807700	1.32280300	-2.64303800
C	-0.00379400	2.60328300	-3.33267200

H	0.14412600	2.72283500	-4.40499700
C	-0.27647600	3.56968700	-2.38782200
H	-0.39201300	4.64454400	-2.52263100
C	-0.37932900	2.88895400	-1.10376100
C	-0.92942000	-4.83187400	0.11319500
C	0.14260700	-5.75176400	0.33437100
C	-0.10879500	-7.15152500	0.36257500
H	0.71887500	-7.83542800	0.55543400
C	-1.42278200	-7.61628300	0.14468500
H	-1.61282800	-8.69583000	0.16139000
C	-2.49904800	-6.73636800	-0.09626700
H	-3.51297500	-7.09776400	-0.27525500
C	-2.25026400	-5.33752400	-0.10490100
C	2.63921600	-5.87788900	0.81890700
C	3.86266900	-5.00357100	0.78355900
H	3.76110000	-4.06304100	0.22898000
C	5.23258600	-5.71119800	0.67488800
H	5.96301100	-5.26742300	-0.00889400
H	5.18852900	-6.80550900	0.69380600
C	4.88676000	-4.97584300	1.97264300
C	5.59506600	-3.65730500	2.23398400
C	6.98531200	-3.66925800	2.53486400
H	7.52359500	-4.62581200	2.53625500
C	7.67973600	-2.46970400	2.81277000
H	8.75264400	-2.49861100	3.03869200

C	6.99333800	-1.22972500	2.78858800
H	7.53131900	-0.29554800	2.98955700
C	5.60956300	-1.20685700	2.49111900
H	5.07209600	-0.25159000	2.44802400
C	4.91491500	-2.41258600	2.22480300
H	3.84391000	-2.37913700	1.99348300
C	4.59958100	-5.79617600	3.23837400
H	5.54723900	-6.03583100	3.75721100
H	4.08558300	-6.73987300	2.98863800
H	3.96493900	-5.22278100	3.94039600
C	-4.62401400	-4.58458400	-0.66200700
C	-5.39834800	-3.30458300	-0.81951300
H	-4.99243300	-2.43243300	-0.29124500
C	-6.93541200	-3.37241600	-0.91913200
H	-7.35895800	-4.38246600	-0.90105100
H	-7.49565300	-2.60555400	-0.37492100
C	-6.14208000	-2.97277600	-2.16445000
C	-6.14089300	-1.51504600	-2.58782300
C	-4.92437900	-0.80352600	-2.76197100
H	-3.97008500	-1.29910100	-2.54355100
C	-4.92748400	0.53933000	-3.20940800
H	-3.97653300	1.07103600	-3.33293300
C	-6.15303900	1.18790700	-3.50069800
H	-6.15776900	2.22926300	-3.84398900
C	-7.37205800	0.48392900	-3.33910500

H	-8.32445100	0.97907400	-3.56462200
C	-7.36377100	-0.85648000	-2.88576100
H	-8.30908600	-1.39804800	-2.75348700
C	-6.05859000	-3.96308100	-3.33526900
H	-6.93724900	-3.83658300	-3.99596000
H	-6.03609300	-5.00511500	-2.97289500
H	-5.15045400	-3.78075000	-3.94075900
C	0.46908600	0.09104200	-4.78068500
C	-0.55016300	-0.04076800	-5.76552700
C	-0.23833400	-0.06031500	-7.15187900
H	-1.02387800	-0.16053900	-7.90553200
C	1.11023100	0.05467700	-7.55234800
H	1.35580400	0.03874500	-8.62057200
C	2.14766200	0.19202400	-6.60577600
H	3.18536600	0.27937300	-6.93884800
C	1.81768200	0.21276800	-5.22432900
C	-2.95049700	-0.32544100	-6.23397700
C	4.18256700	0.40805800	-4.56609100
O	2.72894900	7.50999700	0.69402100
O	-5.21082700	5.75121500	0.15960200
O	-2.65074400	0.47924300	5.16945200
O	2.05498800	-0.28480400	4.97749300
N	-0.41431800	1.50407000	1.53640700
N	-0.50573400	-1.27547000	1.53769200
N	1.53443200	5.53742000	0.21633900

H	1.63283100	4.52385800	0.09478600
N	-3.22107500	4.49330700	0.01538200
H	-2.86731200	3.53166900	-0.01663500
C	-0.56713600	3.57016700	0.11404100
C	-0.52076500	2.89992200	1.35166600
C	-0.53898000	3.59161500	2.63323200
H	-0.62760200	4.67131500	2.74633000
C	-0.40527100	2.62868200	3.61068500
H	-0.37183800	2.75821000	4.69127500
C	-0.35217900	1.33985200	2.93872700
C	-0.34827200	0.11359400	3.62233900
C	-0.47350800	-1.10614700	2.93949800
C	-0.65564500	-2.38117100	3.61495700
H	-0.68185500	-2.50191600	4.69689200
C	-0.80411200	-3.34202700	2.63801500
H	-0.96849900	-4.41252800	2.75241600
C	-0.68068900	-2.66409300	1.35457000
C	-0.85302600	5.05228000	0.10161100
C	0.19381200	6.02233900	0.16919300
C	-0.11260900	7.41103100	0.18892000
H	0.70129800	8.13378400	0.25744500
C	-1.46329200	7.81536900	0.14125700
H	-1.69731900	8.88619800	0.15753000
C	-2.52139200	6.88475900	0.07729600
H	-3.56664100	7.19731100	0.05192500

C	-2.21332200	5.49781800	0.06003500
C	2.70981200	6.25460700	0.47787100
C	3.95209300	5.40972000	0.50195000
H	3.79826300	4.32364400	0.46559700
C	5.13886100	5.89839700	1.37056400
H	5.65993300	5.14150200	1.96609700
H	4.98389100	6.86576300	1.85978000
C	5.30036800	5.90413200	-0.14601900
C	6.17348700	4.83666700	-0.78126900
C	7.48006200	4.58553200	-0.28503500
H	7.82827500	5.12630500	0.60393800
C	8.33247600	3.65597600	-0.92687800
H	9.33922500	3.47387100	-0.53184500
C	7.88948200	2.96538300	-2.08042900
H	8.54849100	2.24559200	-2.58029900
C	6.58773400	3.20925300	-2.58268200
H	6.23877800	2.67995100	-3.47721200
C	5.73795900	4.13774300	-1.93848100
H	4.72946900	4.32110700	-2.33079600
C	5.34478300	7.24749700	-0.88999500
H	6.38024100	7.63758200	-0.88436700
H	4.67759800	7.98584700	-0.41583700
H	5.03794700	7.12154800	-1.94539500
C	-4.61365300	4.62959000	0.08266100
C	-5.33560000	3.31077000	0.08124500

H	-4.78035100	2.46275600	-0.33961900
C	-6.86119100	3.28810500	-0.13946200
H	-7.32990200	4.27169300	-0.25275000
H	-7.25058300	2.49283300	-0.78315000
C	-6.32233400	2.93231100	1.24680200
C	-6.31720400	1.47702800	1.67811400
C	-5.12783100	0.86194200	2.15205900
H	-4.18917400	1.43034400	2.16109600
C	-5.13617400	-0.47772400	2.60860200
H	-4.20562800	-0.93226600	2.96855200
C	-6.34292200	-1.22032900	2.60602500
H	-6.35198600	-2.25946900	2.95584100
C	-7.53657700	-0.61330600	2.14329100
H	-8.47501800	-1.18127800	2.14340900
C	-7.52192700	0.72491100	1.68330800
H	-8.44575500	1.19149000	1.31859200
C	-6.54081200	3.92339000	2.39946300
H	-7.52794700	3.74217400	2.86559100
H	-6.50543700	4.96578700	2.03939700
H	-5.76817100	3.79487500	3.18121200
C	-0.29313300	0.10920400	5.12472700
C	-1.46792900	0.30340200	5.90635000
C	-1.41915500	0.30588200	7.32599400
H	-2.32329800	0.45629600	7.92183300
C	-0.17816000	0.10565600	7.96737100

H	-0.13347600	0.10665900	9.06260000
C	1.00583400	-0.09728700	7.22727500
H	1.95509200	-0.24917800	7.74776300
C	0.93940700	-0.09489900	5.80799500
C	-3.89671900	0.71194500	5.91942800
C	3.34779800	-0.56347100	5.62501100
H	4.71441500	0.47620600	-3.60689000
H	4.39580200	1.29886300	-5.18976200
H	4.49336300	-0.51210800	-5.09608500
H	-3.86078200	-0.40015500	-5.62233200
H	-2.81043700	-1.25329100	-6.82156400
H	-3.02473800	0.54439500	-6.91510900
H	4.04956200	-0.73667800	4.79716900
H	3.28892900	-1.47018600	6.25731400
H	3.68168300	0.29969300	6.23316500
H	-4.67238000	0.81838900	5.14786100
H	-3.82956400	1.63728700	6.52349700
H	-4.13427700	-0.14950700	6.57316700
C	2.53204200	-0.72055400	-0.36177200
C	4.77124900	-3.61515300	-3.75461400
C	4.27550900	-2.11944800	-1.84870900
C	3.83888900	-2.91007200	-2.96934600
C	6.15900800	-3.55742900	-3.45778400
C	3.34454200	-1.40371500	-1.05766300
C	6.60386600	-2.78393000	-2.35315300

C	1.67169400	0.02005500	0.38433100
C	5.68413400	-2.07638600	-1.55416200
H	6.02892000	-1.48949500	-0.69574800
H	7.67277400	-2.73862700	-2.11248200
H	6.87913800	-4.11104000	-4.07135800
H	2.76852000	-2.95293700	-3.19749300
H	4.41830400	-4.21787200	-4.60005300
H	1.97646400	0.61102900	1.25892100

$C_{[N2]}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: -0.013594 Hartree

H_corr: 0.008229 Hartree

SCF: -109.490074 Hartree

S: 45.93 Cal/Mol-Kelvin

H: -109.481845 Hartree

G: -109.503668 Hartree

Cartesian Coordinates:

N	0.00000000	0.00000000	0.57307000
N	0.00000000	0.00000000	-0.57307000

$C_{[2a]}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.099513 Hartree

H_corr: 0.138461 Hartree

SCF: -309.600539 Hartree

S: 81.974 Cal/Mol-Kelvin

H: -309.462078 Hartree

G: -309.501026 Hartree

Cartesian Coordinates:

C	-1.80367300	-1.06029300	0.00000000
C	-0.41103500	-1.30025800	0.00000000
C	0.52368900	-0.22415100	0.00000000
C	-2.29347400	0.26752500	0.00000000
C	0.01393200	1.10796100	0.00000000
C	-1.37608400	1.34941800	0.00000000
H	-2.50370300	-1.90413500	0.00000000
H	-3.37285400	0.45913400	0.00000000
H	-0.03630000	-2.33249700	0.00000000
H	0.70708900	1.95750300	0.00000000
H	-1.74926300	2.38061400	0.00000000
C	1.97164800	-0.53998900	0.00000000
C	3.01280800	0.33989400	0.00000000
H	2.20893300	-1.61528500	0.00000000
H	2.86955800	1.42734700	-0.00000100
H	4.04967000	-0.01332600	0.00000000

Transition State TS2

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -315.3313 cm-1

G_corr: 1.557 Hartree

H_corr: 1.844644 Hartree

SCF: -6635.302918 Hartree

S: 605.398 Cal/Mol-Kelvin

H: -6633.458274 Hartree

G: -6633.745918 Hartree

Cartesian Coordinates:

Co	0.39503800	0.00765600	0.06756300
O	-0.59689000	7.95663300	-0.53101300
O	6.27534600	3.96422600	-2.37493100
O	1.44993400	-1.21877400	-5.38664800
O	-2.96377100	-0.34864900	-3.83527000
N	0.57616500	1.06462800	-1.57973500
N	0.19630100	-1.61769400	-1.04457100
N	-0.00174700	5.67890100	-0.61930400
H	-0.36864500	4.72819100	-0.49885200
N	4.22083600	3.35363700	-1.39017300
H	3.69324300	2.54452600	-1.04701500
C	1.50425100	3.21103600	-0.66366000
C	1.04430400	2.38729500	-1.71169000
C	0.92579900	2.83791300	-3.09241900
H	1.24648900	3.81658000	-3.44799600

C	0.33331300	1.81146400	-3.79995800
H	0.09024200	1.76974900	-4.86101700
C	0.14230600	0.70641800	-2.87188300
C	-0.27982400	-0.57284200	-3.26898600
C	-0.15471800	-1.67681000	-2.40788000
C	-0.24369200	-3.05811000	-2.85645700
H	-0.49076300	-3.35830100	-3.87380900
C	0.09271700	-3.85652700	-1.78084000
H	0.17069100	-4.94251700	-1.73538100
C	0.31923500	-2.96769100	-0.64809700
C	2.12857100	4.54360900	-0.99696700
C	1.38180100	5.76241300	-0.95372500
C	2.01087300	7.00052600	-1.26358100
H	1.42584400	7.91932700	-1.20883000
C	3.37143800	7.00646100	-1.63416800
H	3.85032700	7.96177600	-1.87880900
C	4.13317400	5.82169500	-1.70140100
H	5.18244700	5.82445700	-2.00069400
C	3.51014600	4.58755700	-1.37420600
C	-0.91978400	6.72636600	-0.45477000
C	-2.32991000	6.27547000	-0.20112400
H	-2.54428400	5.22222000	-0.41689600
C	-3.46021400	7.28033900	-0.53056700
H	-4.34341500	6.87653700	-1.03551100
H	-3.11638900	8.26412500	-0.86758100

C	-3.20717900	6.91727800	0.93255000
C	-4.21187000	6.00182900	1.60952000
C	-5.54884900	6.44926600	1.79186900
H	-5.84233300	7.42993400	1.39582600
C	-6.49807800	5.64511400	2.46385900
H	-7.52565700	6.00551300	2.59544000
C	-6.12334500	4.37320600	2.96377000
H	-6.85854500	3.74452100	3.48055000
C	-4.79419400	3.91910800	2.78681300
H	-4.49555200	2.93276200	3.15841300
C	-3.84497300	4.73033900	2.12021200
H	-2.81825000	4.36826500	1.98753700
C	-2.59383100	7.96711000	1.87032800
H	-3.39114800	8.61672000	2.27899200
H	-1.86248600	8.59533300	1.33455800
H	-2.08537300	7.47969600	2.72361100
C	5.51095600	3.08307800	-1.86469600
C	5.89749600	1.63652900	-1.73262300
H	5.36489600	1.07145100	-0.95758800
C	7.36425800	1.23154500	-1.97099800
H	8.03121100	2.05048000	-2.26124100
H	7.78600500	0.49417100	-1.28091800
C	6.31693700	0.79372100	-2.99490400
C	5.86281700	-0.65424500	-3.00549100
C	4.47933300	-0.97671900	-3.04654500

H	3.73306000	-0.17240000	-3.02555500
C	4.05026100	-2.32361200	-3.11021100
H	2.97792000	-2.54889400	-3.14413600
C	5.00433900	-3.37128800	-3.13880600
H	4.67492000	-4.41617600	-3.18046200
C	6.38583100	-3.06088300	-3.10575200
H	7.12840100	-3.86770700	-3.12723300
C	6.81011700	-1.71179400	-3.04142900
H	7.88079000	-1.47238900	-3.01688900
C	6.31364400	1.46246100	-4.37722500
H	7.01870600	0.93640900	-5.04863900
H	6.61632000	2.52133600	-4.30672700
H	5.30773100	1.41421000	-4.83602700
C	-0.78004300	-0.78565700	-4.66880700
C	0.09569100	-1.10846000	-5.74234700
C	-0.39490600	-1.29915900	-7.06203200
H	0.28084400	-1.54413900	-7.88597800
C	-1.78030300	-1.16713000	-7.30108200
H	-2.16481200	-1.31315500	-8.31724600
C	-2.68036900	-0.85230300	-6.25999900
H	-3.74920500	-0.75629200	-6.46972700
C	-2.17118600	-0.66380500	-4.94717000
C	2.41938100	-1.53305900	-6.44910800
C	-4.40581400	-0.14126400	-4.04624900
O	-3.06082400	-7.08189200	1.48078600

O	4.96871000	-5.70982700	1.76802400
O	2.81815700	0.87143700	5.10945200
O	-1.91786700	0.99467600	4.60890100
N	0.50318600	-1.12069200	1.67931300
N	0.94550800	1.55790700	1.14151000
N	-1.69631400	-5.29844400	0.76519900
H	-1.72636300	-4.35890500	0.35560000
N	3.10910400	-4.46529000	1.02232000
H	2.83460000	-3.53596300	0.68799800
C	0.51802400	-3.42432400	0.67068500
C	0.52405600	-2.53010100	1.76307500
C	0.50401000	-2.95865800	3.15563800
H	0.53269700	-3.99879700	3.47796400
C	0.42994100	-1.81717100	3.92815300
H	0.39879800	-1.73336500	5.01355500
C	0.45695500	-0.68179500	3.01897200
C	0.56482100	0.65394500	3.44665100
C	0.87422400	1.68690700	2.54518900
C	1.27944700	3.02321500	2.95375100
H	1.31101000	3.36532500	3.98690600
C	1.63947200	3.70758800	1.81059100
H	2.01292500	4.72646500	1.71564000
C	1.39151900	2.81602300	0.68470200
C	0.71077400	-4.89455300	0.95050400
C	-0.39268000	-5.79944700	1.05528900

C	-0.17552400	-7.15591500	1.42480200
H	-1.03445300	-7.81971000	1.53083900
C	1.14036400	-7.60143400	1.66659100
H	1.30251100	-8.64660200	1.95483700
C	2.25356400	-6.74446900	1.54305600
H	3.27239500	-7.08821300	1.72871700
C	2.03665900	-5.38800800	1.18070700
C	-2.93591900	-5.93622400	0.93848700
C	-4.10290900	-5.14594200	0.42401400
H	-3.89583800	-4.10690900	0.13868900
C	-5.49866000	-5.40133800	1.03954700
H	-6.10562200	-4.51491100	1.24967700
H	-5.53545800	-6.19231100	1.79593000
C	-5.25740800	-5.83502000	-0.40226600
C	-5.86152100	-5.01750800	-1.52961300
C	-7.22034800	-4.60840600	-1.48493100
H	-7.81603900	-4.82726500	-0.59006800
C	-7.81072000	-3.93480800	-2.58101500
H	-8.86303100	-3.62952600	-2.53215500
C	-7.04885900	-3.66392600	-3.74316800
H	-7.50949600	-3.15315700	-4.59758600
C	-5.69018700	-4.06400000	-3.79605000
H	-5.09179700	-3.86345200	-4.69354700
C	-5.10412500	-4.73424400	-2.69791000
H	-4.05126200	-5.04056600	-2.74304700

C	-5.17747900	-7.33569400	-0.72257900
H	-6.19772400	-7.73136600	-0.88762300
H	-4.70330700	-7.89221000	0.10242200
H	-4.59483300	-7.51198700	-1.64651700
C	4.47149000	-4.63435900	1.30204900
C	5.29002700	-3.40726500	1.01379100
H	4.85368700	-2.70291600	0.29449000
C	6.82670600	-3.52286000	0.99239400
H	7.22181700	-4.51630800	1.23051700
H	7.34702500	-2.97962400	0.19723200
C	6.17415100	-2.74334400	2.13408100
C	6.23948600	-1.22722100	2.11721800
C	5.06648800	-0.44983800	2.31395700
H	4.09719900	-0.94991200	2.43426100
C	5.13210600	0.96314000	2.35768500
H	4.21527700	1.54296800	2.51557500
C	6.37909300	1.62026100	2.21013100
H	6.43186000	2.71500900	2.23531000
C	7.55566100	0.85458200	2.02126400
H	8.52298800	1.35820400	1.90542600
C	7.48475900	-0.55850700	1.97680800
H	8.39690500	-1.15098800	1.83053100
C	6.18386000	-3.35333000	3.54337900
H	7.12797200	-3.09041000	4.05735100
H	6.09845800	-4.45266600	3.50099900

H	5.34621300	-2.95815700	4.14891500
C	0.44384000	0.96089800	4.91187000
C	1.58645400	1.07137500	5.75336400
C	1.45679300	1.35397400	7.13944300
H	2.33663100	1.43751200	7.78310000
C	0.16567200	1.52572500	7.68395500
H	0.05925700	1.74780400	8.75210300
C	-0.99058700	1.41678700	6.88212700
H	-1.97953700	1.55802900	7.32620600
C	-0.84188900	1.13124900	5.49871200
C	4.04086600	0.93378700	5.92741800
C	-3.27936100	1.04236000	5.16670400
H	-4.79007800	0.16477100	-3.06333300
H	-4.89749700	-1.07915500	-4.36765200
H	-4.58753800	0.66529300	-4.78158500
H	3.39082500	-1.57426100	-5.93595600
H	2.43017900	-0.74206700	-7.22369100
H	2.19759200	-2.51327500	-6.91381300
H	-3.93923600	0.79330100	4.32340400
H	-3.51143700	2.05213300	5.55749600
H	-3.40884600	0.28563300	5.96287400
H	4.85913300	0.73922400	5.21945300
H	4.02911600	0.15886500	6.71803400
H	4.16506800	1.93555200	6.38246500
C	-2.11712100	1.45420100	-0.32983100

C	-4.01043500	4.18940700	-4.04248700
C	-3.61893800	3.02810600	-1.89856900
C	-3.18700300	3.39850900	-3.21543400
C	-5.28288200	4.62410800	-3.58966300
C	-2.80137500	2.21372500	-1.06105500
C	-5.72056400	4.26690000	-2.28841900
C	-1.45943500	0.48334500	0.42473100
C	-4.90172600	3.48627100	-1.44634300
H	-5.23390100	3.22611900	-0.43520900
H	-6.69904800	4.60451100	-1.92704200
H	-5.91979700	5.23723500	-4.23782500
H	-2.20629100	3.05744700	-3.56358700
H	-3.66084400	4.47037200	-5.04309000
H	-1.61935500	0.46694100	1.51558600
C	-5.41950500	-2.16491600	4.69504000
C	-6.24849900	-1.45606700	3.78867300
C	-4.10218900	-2.51754300	4.30078400
C	-3.61848000	-2.17595500	3.02218600
C	-4.44508700	-1.47372900	2.08657800
C	-5.76765300	-1.11706600	2.50570100
H	-2.59620000	-2.45967100	2.74705200
H	-5.79442600	-2.44487000	5.68651100
H	-3.45434800	-3.06844200	4.99285300
H	-6.41862300	-0.57881700	1.80378200
H	-7.26896000	-1.17872400	4.07992400

C	-4.02110500	-1.14499800	0.72202200
C	-2.77593800	-1.38202800	0.14559500
H	-2.01202100	-1.96941500	0.66754100
H	-2.64362400	-1.27126200	-0.93417500
H	-4.77468400	-0.63189000	0.10625100

Intermediate D

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.560918 Hartree

H_corr: 1.847566 Hartree

SCF: -6635.34275100 Hartree

S: 603.302 Cal/Mol-Kelvin

H: -6633.455352 Hartree

G: -6633.742 Hartree

Cartesian Coordinates:

Co	0.34131200	0.00130900	0.04502300
O	-0.59700200	7.99426400	-0.74827900
O	6.14440300	3.80548300	-2.62110400
O	1.47897800	-1.54803600	-5.31160000
O	-2.94828100	-0.54166200	-3.88827500
N	0.50839400	0.98273400	-1.64953900
N	0.20644900	-1.67272300	-0.98322800
N	-0.08381800	5.69714900	-0.87348200

H	-0.47677000	4.75916400	-0.73698100
N	4.09827000	3.27008100	-1.57672800
H	3.57025500	2.48744900	-1.17760400
C	1.38094300	3.19420100	-0.83415500
C	0.96129400	2.30328100	-1.84491500
C	0.87039300	2.67418400	-3.25130300
H	1.18581400	3.63628900	-3.65376500
C	0.30815600	1.60163000	-3.91410300
H	0.09058700	1.49814200	-4.97655000
C	0.11180300	0.54720900	-2.93019300
C	-0.27851300	-0.76005900	-3.26377100
C	-0.13616600	-1.81360400	-2.34387400
C	-0.18539100	-3.21858000	-2.71857900
H	-0.41809400	-3.57877500	-3.71969000
C	0.17208400	-3.94939000	-1.60212000
H	0.28504600	-5.02863900	-1.50132100
C	0.37147800	-2.99619900	-0.51717000
C	2.01939400	4.50313100	-1.23101000
C	1.29560700	5.73662300	-1.23230500
C	1.93904900	6.94854000	-1.60814800
H	1.37088100	7.87909700	-1.58337400
C	3.29318600	6.91565000	-1.99900800
H	3.78323300	7.85025000	-2.29592300
C	4.03477800	5.71672200	-2.01889700
H	5.08009100	5.68849600	-2.33038400

C	3.39826000	4.50946000	-1.62416300
C	-0.95804100	6.77473700	-0.67141800
C	-2.37041200	6.36884100	-0.36270200
H	-2.63955400	5.33642600	-0.61431900
C	-3.47851300	7.42648300	-0.56970000
H	-4.40456800	7.08047300	-1.03963400
H	-3.12023300	8.41433700	-0.87848000
C	-3.15204900	6.98108700	0.85532800
C	-4.13502500	6.05650600	1.55048100
C	-5.47192900	6.48428400	1.77217300
H	-5.78890400	7.46452400	1.39368400
C	-6.39106400	5.66079600	2.46363700
H	-7.41966500	6.00528600	2.62623400
C	-5.98497900	4.39090300	2.94331000
H	-6.69777200	3.74832500	3.47428800
C	-4.65430200	3.95661000	2.72814900
H	-4.32897500	2.97298400	3.08395200
C	-3.73640200	4.78651200	2.04224500
H	-2.70820500	4.44105100	1.87895900
C	-2.44317100	7.96129100	1.80084900
H	-3.18917700	8.61670000	2.28935400
H	-1.72370800	8.59078300	1.25024600
H	-1.90110100	7.41582200	2.59635400
C	5.38394300	2.96429800	-2.04157600
C	5.77587700	1.53310900	-1.80307300

H	5.24292500	1.02377200	-0.99069400
C	7.24823000	1.12463000	-2.00145200
H	7.90913100	1.92625300	-2.34835000
H	7.67218400	0.44628000	-1.25453900
C	6.21185200	0.60080900	-2.99504400
C	5.77285000	-0.84855000	-2.89598200
C	4.39389400	-1.18999800	-2.93879900
H	3.63856300	-0.39646500	-3.00215400
C	3.98068800	-2.54272400	-2.89777400
H	2.91183200	-2.78321800	-2.93518500
C	4.94599500	-3.57750700	-2.81842900
H	4.62834600	-4.62612500	-2.77926800
C	6.32312700	-3.24876700	-2.78339000
H	7.07439900	-4.04531800	-2.72131200
C	6.73160100	-1.89390200	-2.82349800
H	7.79892200	-1.64015800	-2.79760400
C	6.21054400	1.16154100	-4.42444600
H	6.92591800	0.59372200	-5.04938600
H	6.50090300	2.22614100	-4.43323600
H	5.20821500	1.06691100	-4.88387700
C	-0.75759900	-1.05529000	-4.65605700
C	0.13118400	-1.45140200	-5.69377800
C	-0.34099600	-1.72030600	-7.00669600
H	0.34516900	-2.02133300	-7.80302700
C	-1.72109300	-1.59153500	-7.27581800

H	-2.09127600	-1.79774700	-8.28687500
C	-2.63379900	-1.20284000	-6.27117400
H	-3.69817100	-1.10942900	-6.50384800
C	-2.14253500	-0.93614200	-4.96506200
C	2.46168900	-1.93699600	-6.33629600
C	-4.38544000	-0.34029600	-4.13223100
O	-2.92251700	-7.05934500	1.75473100
O	5.07223500	-5.47081300	2.14846500
O	2.65105400	1.29513100	5.02106900
O	-2.08782100	1.05382900	4.55591800
N	0.48123200	-1.02868200	1.71300500
N	0.78889300	1.63542500	1.04139800
N	-1.57057600	-5.29287100	0.97702000
H	-1.60398600	-4.38117300	0.50947500
N	3.20466600	-4.33553300	1.26245900
H	2.91489600	-3.43919100	0.85792500
C	0.59137300	-3.37708500	0.82270600
C	0.56924800	-2.42957000	1.86939100
C	0.56558700	-2.78648000	3.28204600
H	0.64484200	-3.80555900	3.65856300
C	0.42936700	-1.61186400	3.99451400
H	0.38686200	-1.47504200	5.07412600
C	0.40007100	-0.52462400	3.02848600
C	0.41817200	0.83622900	3.38656400
C	0.68408700	1.83705800	2.43486400

C	1.03715900	3.20648500	2.78022200
H	1.03187700	3.60511900	3.79338900
C	1.41831700	3.83505700	1.61222300
H	1.77315500	4.85554600	1.47317400
C	1.22636300	2.87641900	0.53066700
C	0.81995400	-4.82510200	1.18074000
C	-0.26348300	-5.74906600	1.32024900
C	-0.02413600	-7.07585400	1.77255200
H	-0.86979600	-7.75242600	1.90312900
C	1.29753800	-7.47504900	2.06134500
H	1.47863300	-8.49722900	2.41364400
C	2.39302800	-6.60068500	1.90422100
H	3.41592300	-6.90887100	2.12661600
C	2.15211700	-5.27290700	1.45928300
C	-2.80093800	-5.94393300	1.15205400
C	-3.96612100	-5.20900200	0.55515400
H	-3.77194300	-4.17896700	0.23095600
C	-5.38065100	-5.47503300	1.11926000
H	-6.02184400	-4.59907900	1.26033000
H	-5.43011800	-6.23218800	1.90880900
C	-5.06229500	-5.96550700	-0.28975500
C	-5.63595100	-5.21616000	-1.47857200
C	-7.01615100	-4.88696600	-1.53072900
H	-7.65348600	-5.11353600	-0.66694900
C	-7.57302200	-4.28175200	-2.68258700

H	-8.64188500	-4.03736900	-2.70884000
C	-6.75521000	-4.00017900	-3.80363600
H	-7.18938300	-3.54312700	-4.70125600
C	-5.37519700	-4.31972200	-3.75953700
H	-4.73276600	-4.10836400	-4.62335700
C	-4.82282800	-4.92234700	-2.60587700
H	-3.75346900	-5.16744500	-2.57611000
C	-4.92708800	-7.47590600	-0.53762600
H	-5.92740400	-7.90824000	-0.73005100
H	-4.47688500	-7.98167200	0.33234800
H	-4.29792600	-7.67511500	-1.42566400
C	4.56151500	-4.44508800	1.59353000
C	5.35312900	-3.21509500	1.24784700
H	4.92946500	-2.58543600	0.45544500
C	6.89111700	-3.27159400	1.31095400
H	7.30907000	-4.22757500	1.64439200
H	7.43288200	-2.77012400	0.50278000
C	6.15363400	-2.43397800	2.35595100
C	6.16333900	-0.92200200	2.22692700
C	4.95554100	-0.18075300	2.33331000
H	4.00318000	-0.70975000	2.46459300
C	4.96498000	1.23301800	2.27398600
H	4.02231200	1.78509800	2.36469700
C	6.18954600	1.92795700	2.11124800
H	6.19890800	3.02282600	2.05613700

C	7.39987100	1.19925600	2.01127500
H	8.34989900	1.73201300	1.88341200
C	7.38529900	-0.21510300	2.07060900
H	8.32391300	-0.77868300	1.99457000
C	6.11197200	-2.93741400	3.80621300
H	7.01803400	-2.59994700	4.34455000
H	6.06900200	-4.03947300	3.84316100
H	5.23035800	-2.53258900	4.33844600
C	0.27504200	1.20566700	4.83571900
C	1.41068900	1.43609900	5.66357200
C	1.26808000	1.76984800	7.03684900
H	2.14294900	1.94606000	7.66845300
C	-0.02888200	1.86872400	7.58503800
H	-0.14590100	2.12847600	8.64353400
C	-1.17758100	1.63867800	6.79845800
H	-2.17168900	1.72400800	7.24520100
C	-1.01609100	1.30610800	5.42692100
C	3.86933400	1.47990700	5.82676900
C	-3.44105700	1.00708600	5.13409200
H	-4.78104600	0.02895600	-3.17573300
H	-4.87865400	-1.29402500	-4.40047600
H	-4.55320300	0.41814700	-4.92050800
H	3.42457900	-1.95294800	-5.80591300
H	2.49149300	-1.19706200	-7.15935500
H	2.23867100	-2.94313300	-6.74121200

H	-4.09220500	0.69139500	4.30634500
H	-3.74678300	2.00336300	5.50878700
H	-3.49856800	0.26081900	5.94872300
H	4.69633300	1.30766500	5.12317000
H	3.91394200	0.74441500	6.65311400
H	3.92599900	2.50834200	6.23325800
C	-2.21683900	1.33046700	-0.45072900
C	-3.87945000	4.13002300	-4.21991500
C	-3.55920800	3.01945500	-2.04209500
C	-3.12551100	3.28409500	-3.37777300
C	-5.08007000	4.72247400	-3.75522000
C	-2.81486600	2.13689000	-1.18491100
C	-5.51768800	4.46830900	-2.43168400
C	-1.66376200	0.29564200	0.39511100
C	-4.76591000	3.63114500	-1.57838800
H	-5.09955300	3.44444200	-0.55149100
H	-6.44375600	4.92423800	-2.06209800
H	-5.66279300	5.37777500	-4.41312100
H	-2.19857000	2.82234900	-3.73360300
H	-3.52902700	4.32989300	-5.23946000
H	-1.59334300	0.61924000	1.44946600
C	-5.53035500	-2.38135200	4.50200900
C	-6.30272200	-1.57287300	3.62233400
C	-4.17720700	-2.66884000	4.17544700
C	-3.59865800	-2.17024700	2.99457200

C	-4.36464800	-1.35946400	2.07759700
C	-5.73517300	-1.07065800	2.43830100
H	-2.54798800	-2.39455000	2.78030500
H	-5.97531800	-2.78205500	5.42006900
H	-3.57542500	-3.29034200	4.84888700
H	-6.33859300	-0.45475500	1.75841500
H	-7.34771400	-1.34507300	3.86572200
C	-3.84827400	-0.85886000	0.83727800
C	-2.45891300	-1.05631900	0.29009700
H	-1.90804100	-1.83093200	0.84739400
H	-2.50421400	-1.35328600	-0.77385100
H	-4.51858800	-0.23037500	0.23298400

Intermediate E

$E_{[Co(II)(P6)]}$=$A_{[Co(II)(P6)]}$

$E_{[3a]}$

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 0.203217 Hartree

H_corr: 0.263701 Hartree

SCF: -656.05379 Hartree

S: 127.3 Cal/Mol-Kelvin

H: -655.790089 Hartree

G: -655.850573 Hartree

Cartesian Coordinates:

H	7.08964000	-0.93150700	0.19645900
C	6.02993400	-0.66768500	0.10154900
H	5.91657500	0.27931200	2.06376100
H	5.81903100	-1.53397100	-1.88981500
C	5.36773400	0.01416700	1.15235800
C	5.31293500	-1.00617100	-1.07285200
C	4.00342700	0.35644500	1.03363900
C	3.94803700	-0.66916900	-1.19870300
C	3.27090200	0.01921900	-0.14563500
H	3.49168400	0.88545800	1.84566900
H	3.39258700	-0.93221400	-2.10596600
C	1.88178900	0.36412000	-0.27115900
C	0.68400900	0.66392100	-0.38460400
C	-0.71374200	1.00154100	-0.51681400
H	-0.69948900	2.62554500	1.06127200
C	-1.34991100	2.11424700	0.34608600
C	-1.72748600	0.65726300	0.64314500
H	-2.94648200	-1.42612500	1.88627100
C	-3.56202400	-1.01653100	1.07489200
C	-3.07437500	0.08641500	0.32021600
H	-2.09999800	2.75512800	-0.12851900
C	-4.82345000	-1.59013900	0.79482800
H	-5.18030300	-2.43851100	1.39092100
C	-3.88918500	0.59703100	-0.72944100
H	-3.54591200	1.45016800	-1.32916300

C	-5.62415800	-1.07304600	-0.25172500
C	-5.14945400	0.02345300	-1.01230900
H	-6.60241800	-1.51625000	-0.47108400
H	-5.76301600	0.43174500	-1.82438600
H	-1.25006600	0.22122400	1.52779900
H	-1.13171800	0.87950700	-1.52403900

Transition State TS2

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

Imaginary Frequency: -349.5155 cm-1

G_corr: 1.554791 Hartree

H_corr: 1.844453 Hartree

SCF: -6635.28914366 Hartree

S: 609.644 Cal/Mol-Kelvin

H: -6633.444691 Hartree

G: -6633.734353 Hartree

Cartesian Coordinates:

Co	0.56340200	-0.02682400	0.11565000
O	-0.00147900	7.47241400	-2.32879000
O	6.55566600	2.77142400	-3.56674600
O	1.10013700	-2.13703100	-4.91024900
O	-3.29629200	-0.70550400	-3.71958300
N	0.62122000	0.74542600	-1.69513000
N	-0.07147900	-1.73250700	-0.66039300

N	0.72221500	5.41600000	-1.43717100
H	0.43117100	4.63070500	-0.84539900
N	4.58296500	2.56993200	-2.29072900
H	4.04647500	1.90737400	-1.72109900
C	1.96809800	2.82681700	-1.27717900
C	1.21433700	1.96147900	-2.09589100
C	0.93797500	2.23042200	-3.50119900
H	1.29638800	3.10623100	-4.04046200
C	0.15891100	1.19083200	-3.96372500
H	-0.23786800	1.03291500	-4.96567300
C	-0.01158900	0.25768000	-2.85947400
C	-0.59031400	-1.01323400	-3.00818600
C	-0.53853000	-1.96183300	-1.97218700
C	-0.86288900	-3.36698700	-2.16466500
H	-1.22847100	-3.78797900	-3.10012900
C	-0.57038300	-4.01816000	-0.98379500
H	-0.64937600	-5.08014300	-0.75246800
C	-0.11894300	-3.00335200	-0.03986200
C	2.65355000	4.00657700	-1.92160300
C	2.00144800	5.27194800	-2.04916600
C	2.63308600	6.33784500	-2.74757700
H	2.10552400	7.28593200	-2.86013800
C	3.91654100	6.13252000	-3.29600800
H	4.39981600	6.95422100	-3.83735300
C	4.59869200	4.90432800	-3.16628900

H	5.59070100	4.74548100	-3.59231800
C	3.96379300	3.83882500	-2.47318400
C	-0.18895700	6.47589200	-1.55755800
C	-1.40727900	6.32901400	-0.69331400
H	-1.52247400	5.36357900	-0.18497200
C	-2.72410700	7.00919300	-1.13691300
H	-3.63859100	6.41804100	-1.02524800
H	-2.65393500	7.60326600	-2.05412600
C	-2.01130900	7.55798300	0.09397300
C	-2.57671300	7.26441600	1.47193900
C	-3.97131500	7.34017300	1.72558300
H	-4.65707300	7.54839800	0.89530700
C	-4.48092900	7.16206100	3.03431500
H	-5.56103500	7.22647100	3.21285200
C	-3.59940800	6.91124300	4.11287000
H	-3.99285000	6.78669500	5.12910100
C	-2.20524100	6.82965800	3.86997000
H	-1.51205400	6.64383400	4.70004400
C	-1.70115400	7.00344500	2.56097800
H	-0.62085900	6.93803800	2.37887800
C	-1.33009500	8.93239300	0.00202600
H	-2.07405300	9.72446600	0.21110400
H	-0.89886000	9.09475400	-0.99919500
H	-0.52102300	9.02457200	0.75086400
C	5.79548100	2.09264500	-2.80363400

C	6.10363700	0.68487900	-2.37436400
H	5.60729300	0.34806200	-1.45545900
C	7.51873800	0.12308500	-2.61451600
H	8.20778300	0.80134600	-3.12926800
H	7.95042000	-0.47641900	-1.80681000
C	6.36189200	-0.44663000	-3.43619200
C	5.82457400	-1.82229500	-3.08646200
C	4.43317900	-2.02935500	-2.88685800
H	3.74455300	-1.17640800	-2.93842700
C	3.92388800	-3.32212500	-2.61714000
H	2.84628700	-3.45984200	-2.46840400
C	4.80281700	-4.43152300	-2.54978300
H	4.41190400	-5.43302000	-2.33510800
C	6.19102300	-4.23688200	-2.75394900
H	6.87606900	-5.09197700	-2.70447000
C	6.69598800	-2.94194100	-3.02143500
H	7.77197000	-2.79208800	-3.17660300
C	6.28265600	-0.10502600	-4.93128600
H	6.89250200	-0.82299300	-5.51196300
H	6.65647500	0.91487800	-5.12557400
H	5.23989700	-0.17184100	-5.29597500
C	-1.11289700	-1.43226100	-4.35617900
C	-0.23557300	-2.00477800	-5.32330400
C	-0.70289100	-2.40584100	-6.60325900
H	-0.02407300	-2.84115800	-7.34136100

C	-2.06824700	-2.23477600	-6.91602300
H	-2.43649900	-2.54286900	-7.90147000
C	-2.96782300	-1.67554900	-5.98471300
H	-4.02151400	-1.55448000	-6.24887000
C	-2.48329600	-1.27626600	-4.70924900
C	2.06155400	-2.70211300	-5.87205500
C	-4.70460700	-0.43783000	-4.06364900
O	-3.95610200	-6.04712600	2.85696100
O	4.19450500	-6.09988000	2.69019600
O	3.62529300	1.06114600	4.87215500
O	-0.95484200	2.24597700	4.33938600
N	0.70794700	-0.89429100	1.88153000
N	1.52733000	1.53670400	0.82733900
N	-2.35329100	-4.71417100	1.75739200
H	-2.24808600	-3.89234900	1.15394300
N	2.53614000	-4.68140600	1.79408300
H	2.40750800	-3.78865800	1.30725400
C	0.14142900	-3.27352800	1.31800100
C	0.44041000	-2.23471000	2.22436900
C	0.47143300	-2.41048800	3.67060000
H	0.30613200	-3.36036300	4.17708700
C	0.71556100	-1.16980900	4.22209300
H	0.80610100	-0.90002100	5.27329200
C	0.88905500	-0.23891100	3.11792300
C	1.29670700	1.09510300	3.28079500

C	1.68888400	1.88275700	2.18443600
C	2.37254300	3.16059500	2.30824100
H	2.62582400	3.63051300	3.25743100
C	2.64595800	3.60149700	1.02832100
H	3.15917800	4.50962100	0.71320900
C	2.07206200	2.62331500	0.11244800
C	0.09617800	-4.68437700	1.85142900
C	-1.13656100	-5.35326600	2.13896600
C	-1.13036300	-6.63071500	2.76510700
H	-2.08149900	-7.10294400	3.01390700
C	0.10183600	-7.24383400	3.06998500
H	0.10054600	-8.22706500	3.55473200
C	1.33509400	-6.63296500	2.76255200
H	2.28993300	-7.10905400	2.99094000
C	1.33079700	-5.35139900	2.15000800
C	-3.67129600	-5.10482600	2.04880700
C	-4.71717300	-4.32387600	1.30871300
H	-4.36852000	-3.43894500	0.76181300
C	-6.14025200	-4.21931400	1.90706200
H	-6.62297800	-3.23891300	1.84531400
H	-6.29309500	-4.76818700	2.84237000
C	-5.95133500	-5.05164200	0.64383200
C	-6.42862800	-4.49909000	-0.68694100
C	-7.72922500	-3.94617000	-0.81947100
H	-8.36150300	-3.84588600	0.07131100

C	-8.21513000	-3.53416900	-2.08341500
H	-9.22634300	-3.11812900	-2.17060100
C	-7.40476100	-3.67040700	-3.23666300
H	-7.78642000	-3.36407000	-4.21840600
C	-6.10210300	-4.21538800	-3.11369500
H	-5.46677800	-4.32800600	-4.00097300
C	-5.62189700	-4.62700400	-1.84917000
H	-4.61324900	-5.04992600	-1.75862800
C	-6.07976100	-6.58032600	0.73483200
H	-7.14431200	-6.86502700	0.63287100
H	-5.69614900	-6.95398200	1.69817800
H	-5.51999000	-7.07353900	-0.08229700
C	3.86362300	-5.05024100	2.04947900
C	4.86626100	-4.07681500	1.49644600
H	4.50429400	-3.42295900	0.69307100
C	6.34289700	-4.51094000	1.39208500
H	6.56052000	-5.51241600	1.77861300
H	6.87256300	-4.22457100	0.47796500
C	5.97388900	-3.43713900	2.41446400
C	6.32969200	-1.99272100	2.11288900
C	5.36388000	-0.96217300	2.26716300
H	4.33940100	-1.21683700	2.56643500
C	5.70542700	0.39151000	2.03646200
H	4.94383600	1.16962200	2.16396600
C	7.02583200	0.73494900	1.65299300

H	7.29175700	1.78236500	1.46743700
C	7.99877700	-0.28398200	1.50505700
H	9.02340300	-0.02385000	1.21246000
C	7.65170500	-1.63696000	1.73485700
H	8.40566500	-2.42573300	1.61826400
C	6.00997300	-3.79320400	3.90761800
H	7.03425300	-3.64902100	4.30100700
H	5.71107300	-4.84238900	4.07286400
H	5.32901700	-3.13883200	4.48436500
C	1.33563800	1.68340000	4.66151300
C	2.50682900	1.66644900	5.46748400
C	2.51020100	2.22868900	6.77239000
H	3.41086000	2.21233900	7.39209100
C	1.32465400	2.81433200	7.26717000
H	1.32160400	3.24983400	8.27312900
C	0.14271700	2.84947400	6.49549200
H	-0.76336200	3.30652600	6.90259300
C	0.15752300	2.27916700	5.19525200
C	4.86752600	0.98327600	5.65889100
C	-2.20605700	2.86522300	4.80462300
H	-5.10840600	0.10041100	-3.19536300
H	-5.25804700	-1.38362200	-4.21855600
H	-4.77692500	0.20661700	-4.95992400
H	3.02066300	-2.71443900	-5.33528400
H	2.13775200	-2.06765100	-6.77614600

H	1.77912100	-3.73392900	-6.15756000
H	-2.91660100	2.72031400	3.97837700
H	-2.06988000	3.94774300	4.98653500
H	-2.58085800	2.36642900	5.71941300
H	5.58517500	0.47950400	4.99571200
H	4.71698900	0.38846800	6.58038900
H	5.23897400	1.99364300	5.91809600
C	-2.13179900	1.08514600	-0.10147100
C	-4.03994800	3.53871600	-3.62661000
C	-3.99270300	2.13728700	-1.59432500
C	-3.34910000	2.66433300	-2.76155400
C	-5.38362800	3.90563900	-3.35652100
C	-3.26829200	1.24946000	-0.70923700
C	-6.03027000	3.38762200	-2.20593800
C	-1.07958300	0.79428700	0.66964800
C	-5.34804600	2.50997600	-1.33505000
H	-5.84562200	2.12208000	-0.44057600
H	-7.06593200	3.67225700	-1.98437200
H	-5.91580400	4.58769300	-4.03016900
H	-2.31436900	2.37461400	-2.97317800
H	-3.52897300	3.94088600	-4.50958900
H	-1.01399200	1.06323700	1.73455700
C	-8.06279300	0.23109000	3.42546300
C	-8.70444500	0.02541300	2.17803600
C	-6.64593300	0.18376500	3.49384300

C	-5.87875800	-0.06595000	2.33756400
C	-6.50897200	-0.28326100	1.06961700
C	-7.93909000	-0.22680700	1.02010700
H	-4.78519400	-0.09181900	2.41066400
H	-8.65433200	0.42482200	4.32779700
H	-6.14303700	0.34088900	4.45589100
H	-8.44082900	-0.38884900	0.05681200
H	-9.79861200	0.06152000	2.11243100
C	-5.76236400	-0.56328900	-0.16077200
C	-4.37950500	-0.70064700	-0.28222600
H	-3.74920500	-0.81095200	0.60686400
H	-3.94817400	-1.07384400	-1.21763400
H	-6.37350300	-0.65244700	-1.07102700

Intermediate E

Temperature: 298.15 Kelvin

Pressure: 1.0 Atm

G_corr: 1.559943 Hartree

H_corr: 1.846928 Hartree

SCF: -6635.33554801 Hartree

S: 604.009 Cal/Mol-Kelvin

H: -6633.48862 Hartree

G: -6633.775605 Hartree

Cartesian Coordinates:

Co	-0.40814900	-0.06844200	0.01878600
O	0.06203100	7.46535500	2.38455500
O	-6.68120800	2.89800300	3.07615200
O	-1.67927700	-2.53791500	4.72620200
O	2.68004800	-0.59063500	4.55217000
N	-0.68593500	0.68816800	1.81329600
N	0.05612100	-1.80576800	0.84410000
N	-0.62482300	5.40571000	1.46987100
H	-0.31649400	4.62700400	0.87816200
N	-4.60310000	2.64269800	1.99238000
H	-4.03830900	1.97148800	1.46155400
C	-1.88903700	2.82513500	1.24929200
C	-1.28826400	1.92126400	2.14933400
C	-1.21539500	2.15501100	3.58605900
H	-1.61403100	3.03671300	4.08592300
C	-0.56244100	1.07361200	4.13666300
H	-0.32515100	0.88547100	5.18258100
C	-0.25997200	0.15366600	3.04968000
C	0.24231100	-1.14231700	3.25782200
C	0.32962500	-2.06933200	2.20412300
C	0.60715300	-3.48367900	2.40766400
H	0.84014800	-3.92868700	3.37383100
C	0.46674200	-4.10750600	1.18563300
H	0.56741500	-5.16515200	0.94384200
C	0.15774200	-3.06807600	0.21104300

C	-2.60729400	4.02490900	1.81685700
C	-1.94549600	5.27954900	1.99381800
C	-2.60738000	6.35658000	2.64504900
H	-2.07148200	7.29378400	2.80123500
C	-3.93420500	6.17716800	3.08937700
H	-4.44121700	7.00670400	3.59590300
C	-4.63119200	4.96639000	2.89374800
H	-5.65972300	4.82964000	3.23165500
C	-3.96538700	3.88909800	2.24926500
C	0.27813300	6.46731600	1.62253900
C	1.52472400	6.32880800	0.79666500
H	1.68480500	5.35105600	0.32495900
C	2.80349100	7.07485800	1.24312800
H	3.74407000	6.51980600	1.16730000
H	2.68981200	7.69928400	2.13578000
C	2.09759500	7.55108600	-0.02220200
C	2.70877100	7.23334700	-1.37486200
C	4.09104300	7.44764000	-1.61768900
H	4.73552900	7.77652600	-0.79310200
C	4.63835400	7.25134200	-2.90820500
H	5.70752800	7.42459100	-3.08013000
C	3.80705200	6.84086900	-3.97813100
H	4.22835000	6.70151400	-4.98118700
C	2.42668100	6.61839700	-3.74499200
H	1.77347500	6.30138600	-4.56727100

C	1.88489300	6.81364300	-2.45381000
H	0.81571200	6.63926300	-2.27820600
C	1.36044400	8.89915400	0.00321400
H	2.07634400	9.71288900	-0.21999600
H	0.90128200	9.08234500	0.98848400
H	0.56626800	8.92937400	-0.76638700
C	-5.87914500	2.20639300	2.36939000
C	-6.20829600	0.82985100	1.86134800
H	-5.63328700	0.49502400	0.98882700
C	-7.67186300	0.34752300	1.92553800
H	-8.37313900	1.05100500	2.38718700
H	-8.04535500	-0.20165800	1.05538800
C	-6.64527100	-0.31563700	2.84478100
C	-6.15969600	-1.71206100	2.50143600
C	-4.77364000	-1.99426900	2.37368200
H	-4.04254300	-1.18311000	2.48030000
C	-4.32358200	-3.31040400	2.11056000
H	-3.24893600	-3.50720900	2.01722900
C	-5.25735000	-4.36793000	1.97954100
H	-4.91118700	-5.38635200	1.76805400
C	-6.64174600	-4.09827200	2.11296400
H	-7.36965300	-4.91248200	2.01272700
C	-7.08726000	-2.78032400	2.37227500
H	-8.16024900	-2.57162900	2.47038600
C	-6.70959700	-0.02871000	4.35204400

H	-7.41947800	-0.72599300	4.83625400
H	-7.04275200	1.00546200	4.54479700
H	-5.71815100	-0.17232700	4.82208400
C	0.51877100	-1.59804300	4.66657200
C	-0.47211700	-2.30932800	5.40623100
C	-0.23825100	-2.73637600	6.74085400
H	-1.00230000	-3.28247500	7.30015600
C	1.00017100	-2.44006200	7.34751000
H	1.18693800	-2.76655100	8.37712200
C	2.00014100	-1.72757600	6.65415300
H	2.95086800	-1.50503300	7.14558500
C	1.75124000	-1.30941900	5.31849800
C	-2.75468800	-3.22659800	5.46041200
C	3.91170200	-0.14642700	5.22439000
O	4.11966300	-6.38722500	-2.21818000
O	-3.98350100	-5.94900000	-2.93111500
O	-2.71320900	1.25207600	-5.12591700
O	1.78377300	2.15681800	-3.86516100
N	-0.34198300	-0.90839000	-1.76713300
N	-1.20367200	1.54384400	-0.79234300
N	2.50944600	-4.83679400	-1.46799900
H	2.39838100	-3.93194500	-0.99932100
N	-2.35548200	-4.59705900	-1.88770600
H	-2.22808700	-3.69485900	-1.41823200
C	0.05147500	-3.31459300	-1.17264800

C	-0.09768100	-2.25667900	-2.09442900
C	0.03958400	-2.41882200	-3.53621500
H	0.21180800	-3.37303300	-4.03270300
C	-0.06926200	-1.16109200	-4.09461600
H	-0.02026000	-0.87713800	-5.14501900
C	-0.33287300	-0.23302600	-3.00590800
C	-0.65127500	1.12114200	-3.19779200
C	-1.16097100	1.91156200	-2.15273800
C	-1.77536100	3.21484100	-2.35133800
H	-1.87820500	3.70273500	-3.31948100
C	-2.21394300	3.64963200	-1.11566800
H	-2.74120000	4.56914800	-0.86249900
C	-1.80750900	2.64104200	-0.14466200
C	0.07678600	-4.72702600	-1.70656400
C	1.29487100	-5.45784700	-1.88286000
C	1.27747100	-6.76059100	-2.45412700
H	2.22157800	-7.28762100	-2.59701300
C	0.04505700	-7.32686000	-2.83854100
H	0.03620600	-8.32949200	-3.28169700
C	-1.17532400	-6.64174300	-2.66942400
H	-2.12940700	-7.07641100	-2.97145700
C	-1.15887600	-5.33979300	-2.10064900
C	3.82472300	-5.30395800	-1.61607900
C	4.86237000	-4.41151400	-1.00085200
H	4.51384700	-3.42629600	-0.66872900

C	6.30010900	-4.44686500	-1.56987500
H	6.79282000	-3.47808900	-1.70071600
H	6.46436200	-5.17710300	-2.36917600
C	6.06562200	-4.99837200	-0.16735300
C	6.51849800	-4.18073100	1.02847000
C	7.81284700	-3.59855000	1.06403500
H	8.46404800	-3.68821200	0.18578400
C	8.26905500	-2.91626900	2.21727700
H	9.27430900	-2.47757800	2.23055200
C	7.43485400	-2.80872100	3.35641600
H	7.79061500	-2.28788600	4.25367400
C	6.14034400	-3.38505200	3.33017400
H	5.48604500	-3.31017400	4.20722800
C	5.68899800	-4.06556500	2.17607800
H	4.68531400	-4.50915500	2.16162400
C	6.16704700	-6.51398000	0.06311500
H	7.22296500	-6.78833500	0.24861100
H	5.79673400	-7.07282200	-0.81196400
H	5.57930000	-6.81894800	0.94951400
C	-3.66563300	-4.89910100	-2.28410200
C	-4.66608300	-3.85493500	-1.87617900
H	-4.36366300	-3.20109700	-1.04884600
C	-6.16725400	-4.20297900	-1.94086600
H	-6.39476500	-5.20078500	-2.33122900
H	-6.78302900	-3.86520200	-1.10145200

C	-5.61864700	-3.17870900	-2.93272400
C	-5.92307300	-1.70959400	-2.70193200
C	-4.89040900	-0.73633700	-2.77403800
H	-3.85590500	-1.05259500	-2.95798700
C	-5.17764100	0.63888100	-2.60562900
H	-4.36410700	1.37121700	-2.66426900
C	-6.50940600	1.06196700	-2.36909200
H	-6.73394600	2.12643000	-2.23183300
C	-7.54796500	0.10087100	-2.30486500
H	-8.58120800	0.42262300	-2.12584600
C	-7.25509400	-1.27404100	-2.47130300
H	-8.05995300	-2.01810100	-2.41914200
C	-5.49841200	-3.57109600	-4.41219200
H	-6.45961700	-3.38312800	-4.92742000
H	-5.24141700	-4.63875100	-4.51989800
H	-4.71915000	-2.96909600	-4.91699100
C	-0.45258000	1.73431800	-4.55323800
C	-1.48444200	1.80196100	-5.52785900
C	-1.25520300	2.38743000	-6.80214600
H	-2.04866100	2.43564200	-7.55296100
C	0.02372400	2.91154700	-7.09255700
H	0.20602000	3.36483800	-8.07395800
C	1.07244000	2.86379100	-6.14808400
H	2.05449400	3.27557000	-6.39648400
C	0.82577600	2.27101000	-4.88129600

C	-3.82221100	1.25913100	-6.09390300
C	3.14418300	2.66129800	-4.12403200
H	4.43529400	0.46445500	4.47686200
H	4.53881500	-1.01083100	5.51941200
H	3.67796000	0.46984300	6.11371000
H	-3.59425500	-3.27068300	4.75265700
H	-3.04822500	-2.65486600	6.36191500
H	-2.44775200	-4.25128000	5.74673000
H	3.71432200	2.40273500	-3.22089300
H	3.13587200	3.75834900	-4.26595000
H	3.59354500	2.15660300	-5.00004300
H	-4.65946600	0.78636000	-5.56064800
H	-3.56525400	0.67212800	-6.99674000
H	-4.09436800	2.29326700	-6.38137400
C	2.41020100	0.68840100	0.46333200
C	3.47236800	3.80579900	3.31386600
C	4.01814700	1.77000000	2.02317000
C	3.07863900	2.75038200	2.46699900
C	4.81943200	3.91456200	3.74663400
C	3.59006000	0.66442200	1.12612600
C	5.76304600	2.94940600	3.32049800
C	1.35891400	0.68012100	-0.31441200
C	5.36730500	1.88893400	2.47275500
H	6.11748100	1.15905200	2.15139200
H	6.80816600	3.02328300	3.64499200

H	5.12443700	4.73619700	4.40518200
H	2.03297100	2.65779200	2.15164900
H	2.73016000	4.54110200	3.64559300
H	1.34102900	1.12387800	-1.32205800
C	5.38366500	-0.76488300	-4.40112300
C	6.60021000	-0.36219600	-3.78263800
C	4.23147100	-0.98007800	-3.59817700
C	4.28511700	-0.80991800	-2.20271900
C	5.51147100	-0.41802500	-1.54870200
C	6.66501800	-0.18887500	-2.38957600
H	3.37678600	-0.95367500	-1.60737600
H	5.33726100	-0.91135000	-5.48654300
H	3.28610600	-1.27905600	-4.06598300
H	7.60756600	0.11998600	-1.91812700
H	7.49339800	-0.19027400	-4.39576800
C	5.63219700	-0.26970600	-0.12892100
C	4.53798700	-0.54319200	0.88382100
H	3.91008400	-1.39032200	0.55300900
H	4.99451300	-0.84443700	1.84545900
H	6.60864800	0.05857300	0.25483600

10. References

(1) Wang, Y.; Wen, X.; Cui, X.; Wojtas, L.; Zhang, X. P. *J. Am. Chem. Soc.* **2017**, *139*, 1049–1052.

(2) Ma, S.; He, Q., *Tetrahedron* **2006**, *62*, 2769–2778.

(3) Hiroki, H.; Ogata, K.; Fukuzawa, S.-i., *Synlett* **2013**, *24*, 843–846.

(4) Li, J.-H.; Huang, Q.; Wang, S.-Y.; Ji, S.-J., *Org. Lett.* **2018**, *20*, 4704–4708.

(5) Bruker (**2012**). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.

(6) Bruker (**2012**). SAINT. Data Reduction Software.

(7) Sheldrick, G. M. (**1996**). *SADABS. Program for Empirical Absorption Correction.* University of Gottingen, Germany.

(8) Farrugia, L. J. *J. Appl. Cryst.* **1999**, *32*, 837–838.

(9) Sheldrick, G. M. (**2012** Beta) SHELXL-97. Program for the Refinement of Crystal.

(10) Sheldrick, G. M. *Acta Cryst.* **1990**, *A46*, 467–473.

(11) Frisch, M. J. *et al.*, *Gaussian 16*, *Revision A.03*, Gaussian, Inc., Wallingford CT, **2016**

(12) Schultz, N. E.; Zhao, Yan; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 11127.

(13) Suarez, A. I. O.; Jiang, H.-L.; Zhang, X. P.; de Bruin, B. *Dalton Trans.* **2011**, *40*, 5697–5705.

(14) Lang, K.; Torker, S.; Wojtas, L.; Zhang, X. P. *J. Am. Chem. Soc.* **2019**, *141*, 12388–12396.

(15) Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. *Theor. Chem. Acc.* **1997**, *97*, 119–124.

(16) Furche, F.; Perdew, J. P. *J. Chem. Phys.* **2006**, *124*, 044103.

(17) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys*. **2010**, *132*, 154104.

(18) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378–6396.

(19) Lefebvre, C.; Rubez, G.; Khartabil, H.; Boisson, J.-C.; Contreras-García, J.; Hénon, E. *Phys. Chem. Chem. Phys.* **2017**, *19*, 17928–17936.

(20) Lu, T.; Chen, F. *J. Comput. Chem.* **2012**, *33*, 580–592.

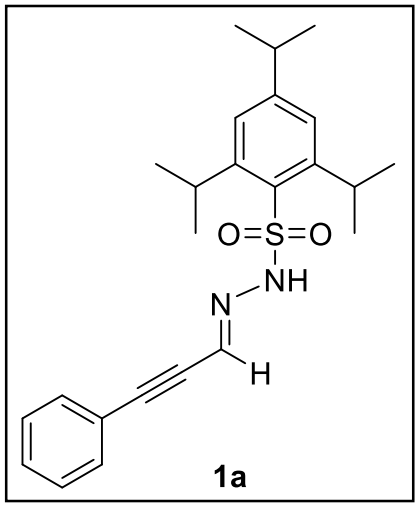
(21) Humphrey, W.; Dalke, A.; Schulten, K. *J. Mol. Graph.* **1996**, *14*, 33–38.

(22) Legault, C. Y. CYLview, 1.0b (Université de Sherbrooke, Québec, Montreal, Canada, **2009**).

(23) Stone, J.E. An Efficient Library for Parallel Ray Tracing and Animation. Master's Thesis, University of Missouri, **1998**.

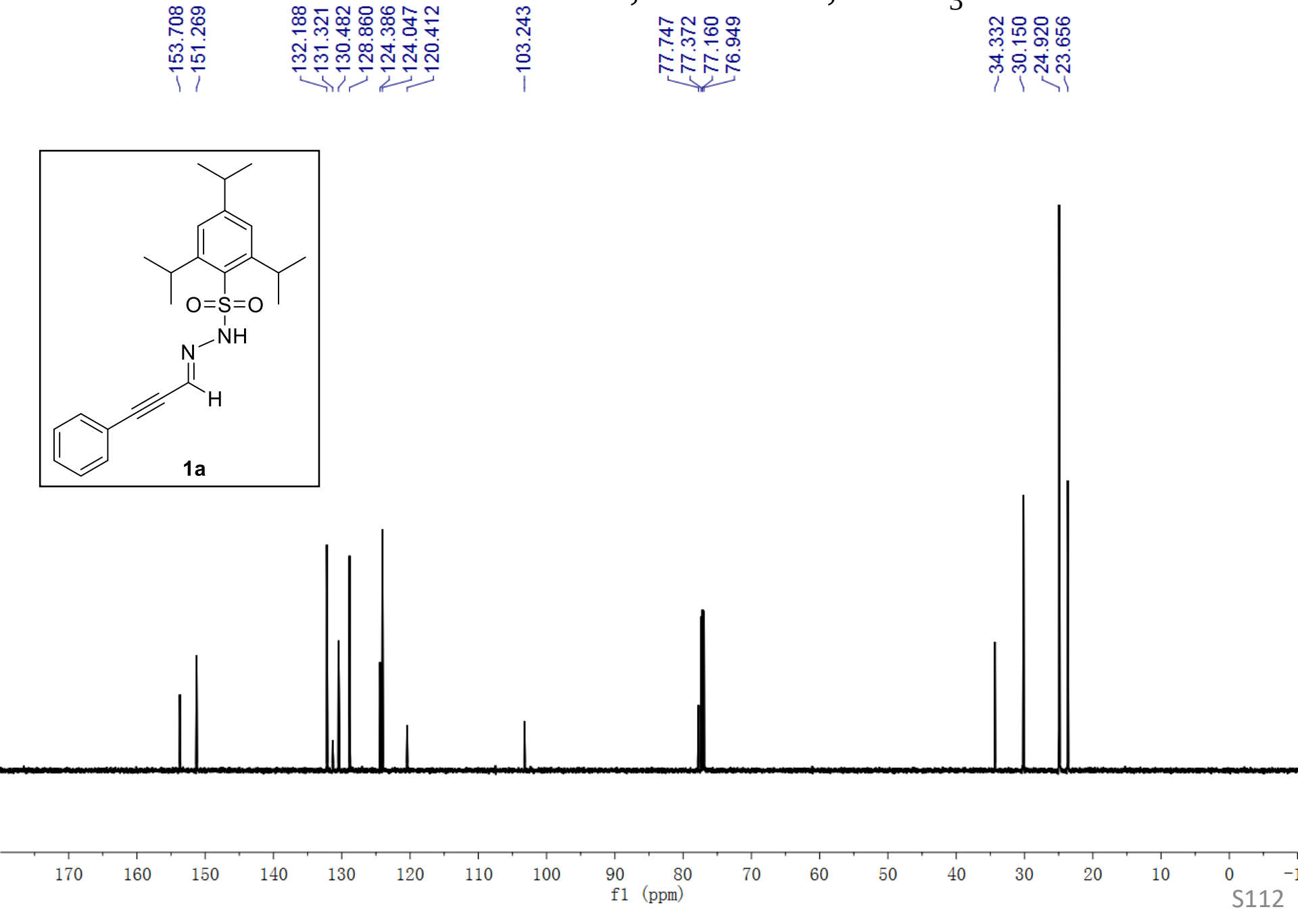
11. NMR/HPLC Spectral Data

^{1}H NMR of **1a**, 600 MHz, $CDCl_3$

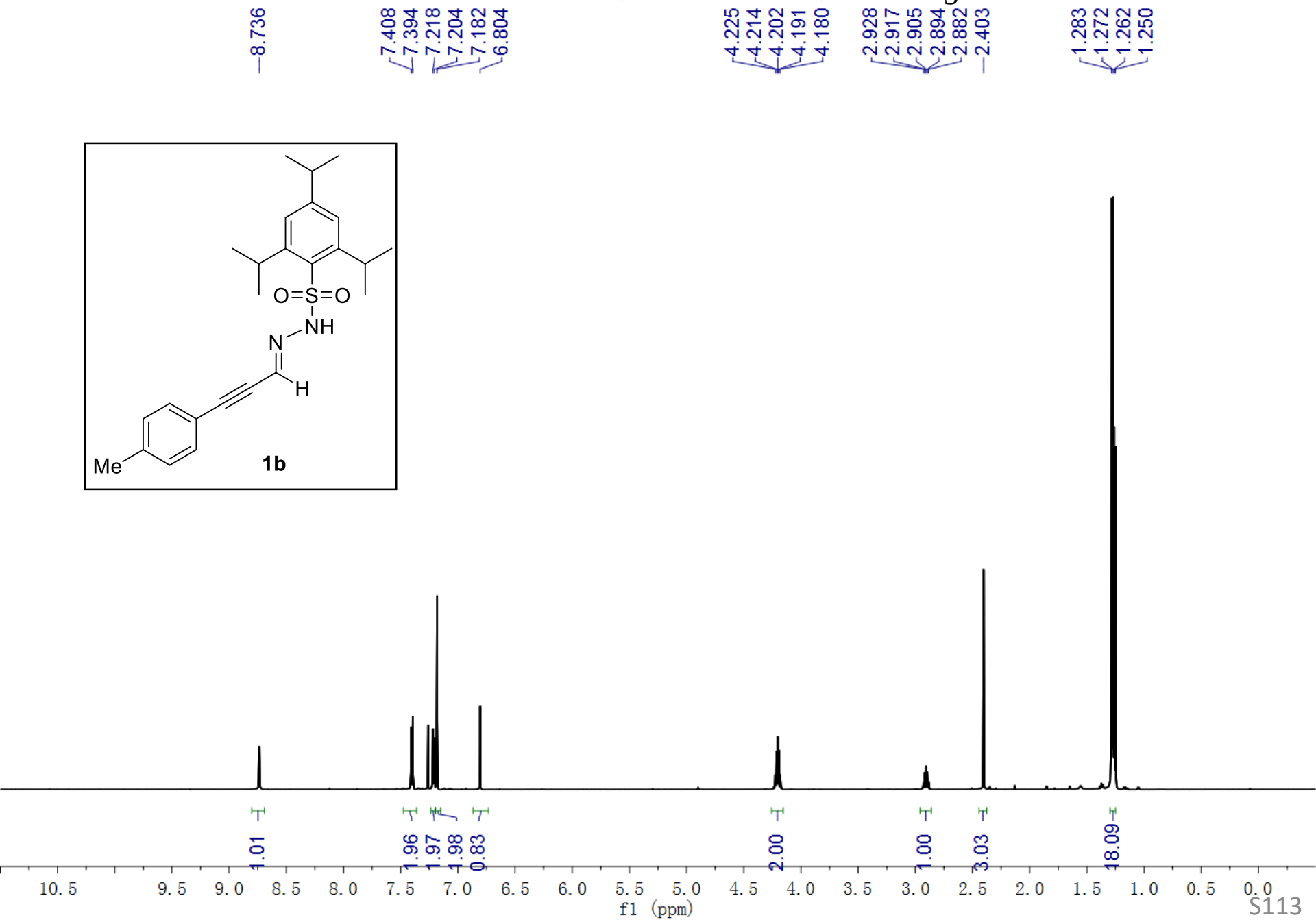


1a

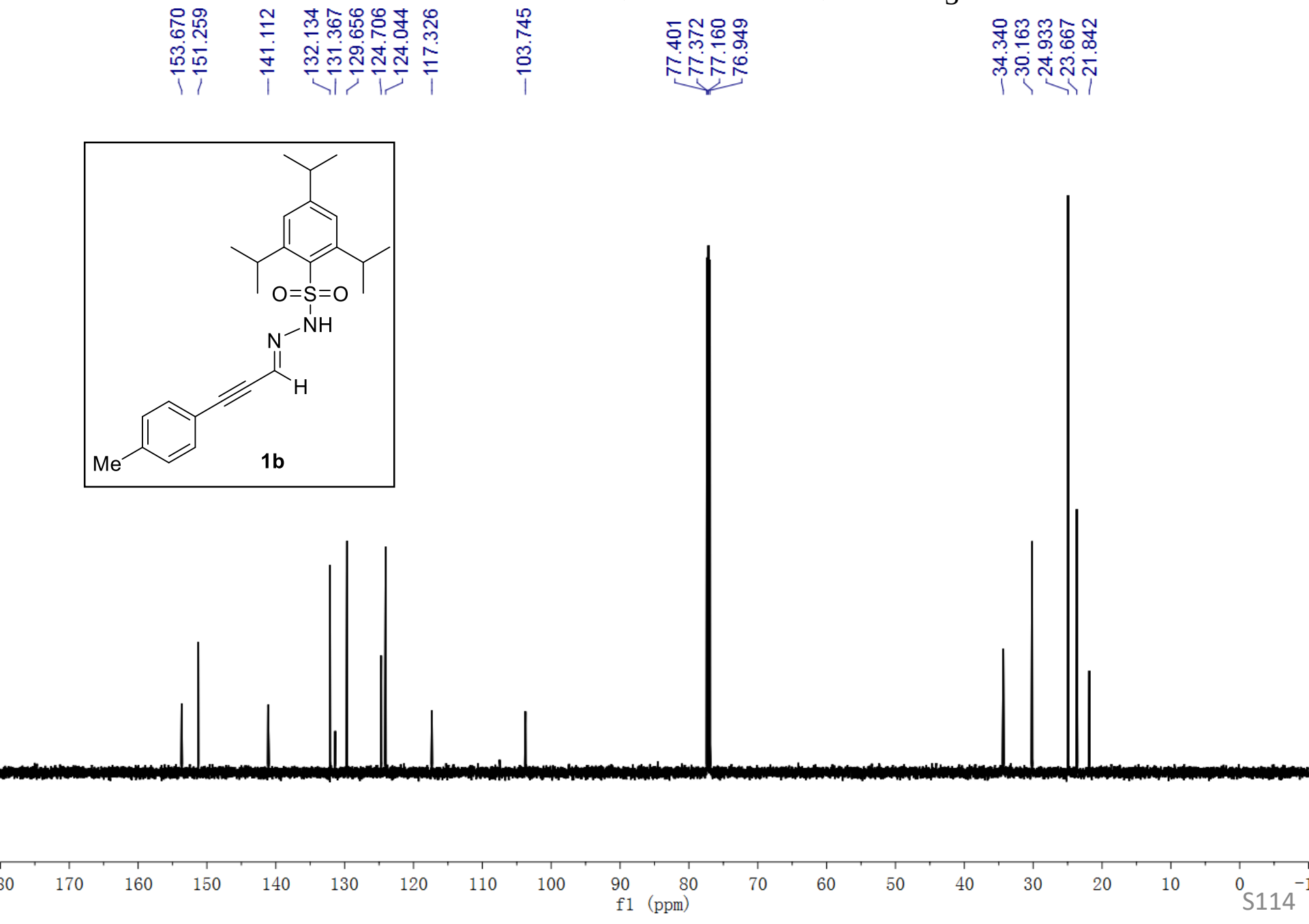
^{13}C NMR of **1a**, 151 MHz, $CDCl_3$



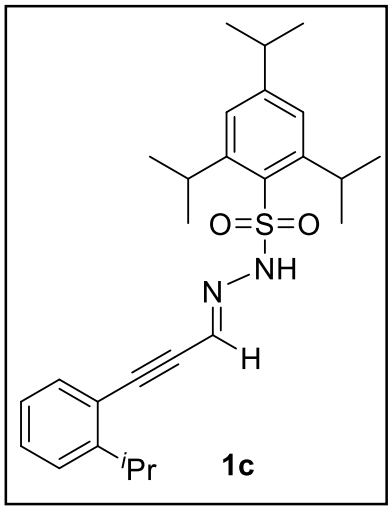
^{1}H NMR of **1b**, 600 MHz, $CDCl_3$



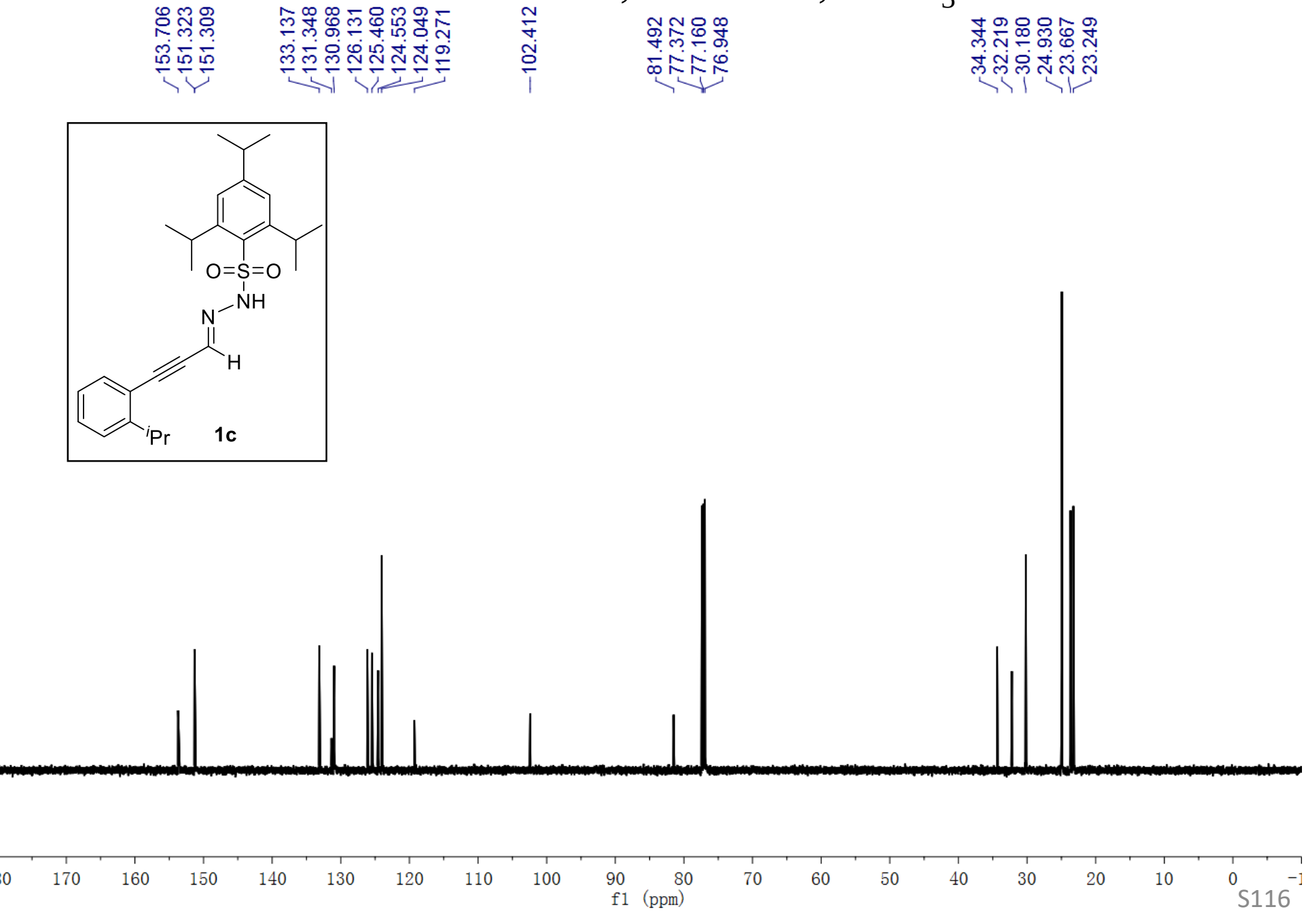
^{13}C NMR of **1b**, 151 MHz, $CDCl_3$



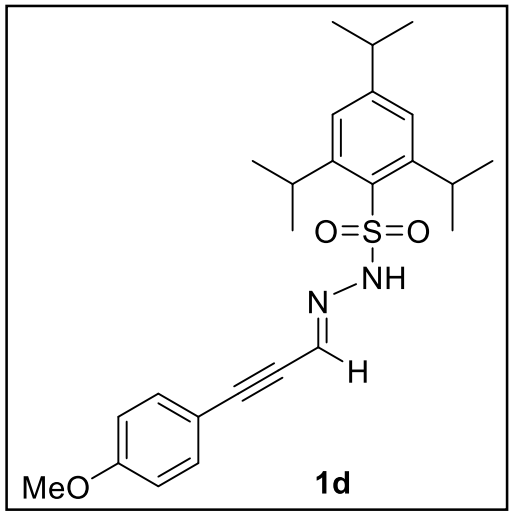
^{1}H NMR of **1c**, 600 MHz, $CDCl_3$



^{13}C NMR of **1c**, 151 MHz, $CDCl_3$

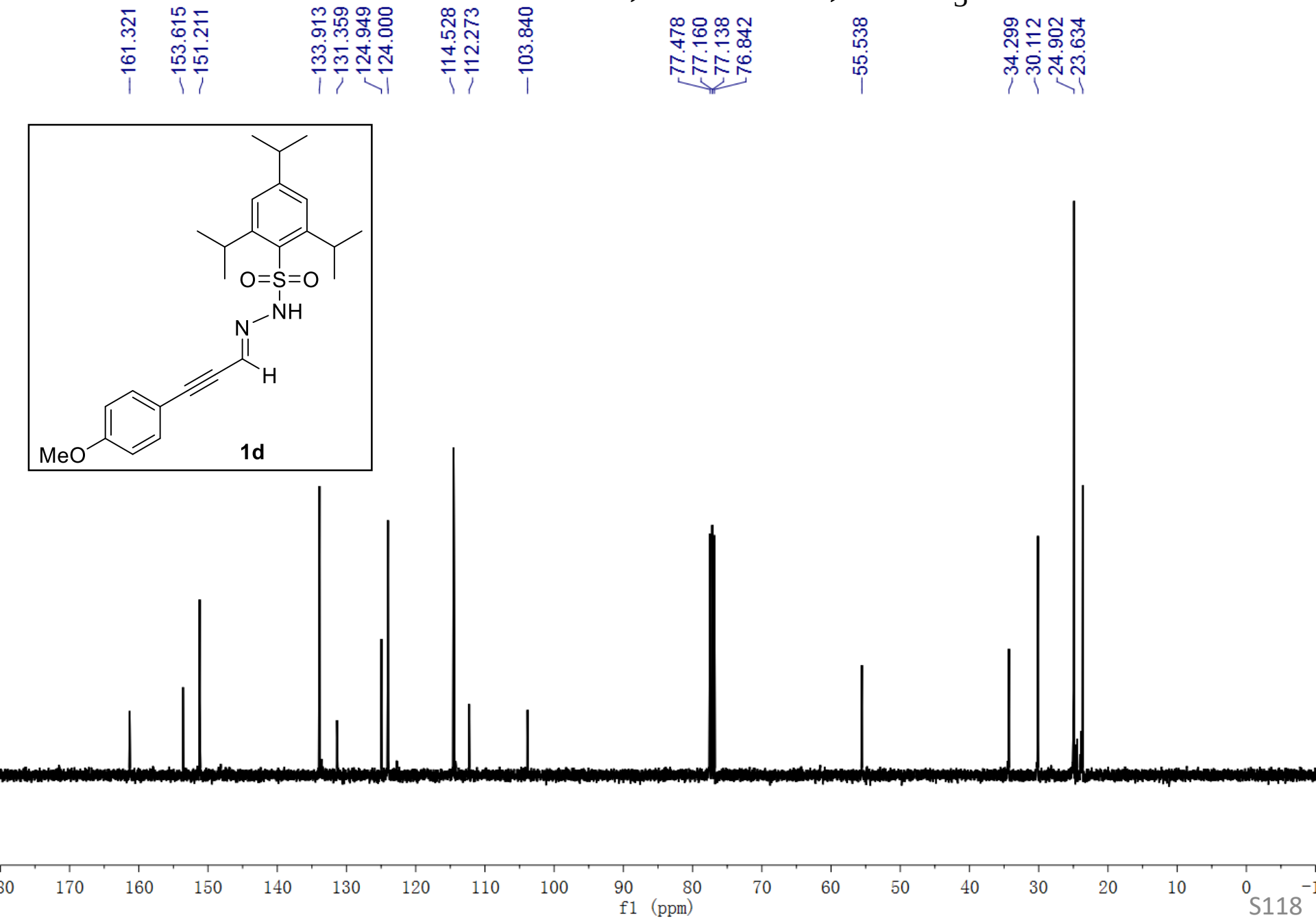


^{1}H NMR of **1d**, 400 MHz, $CDCl_3$

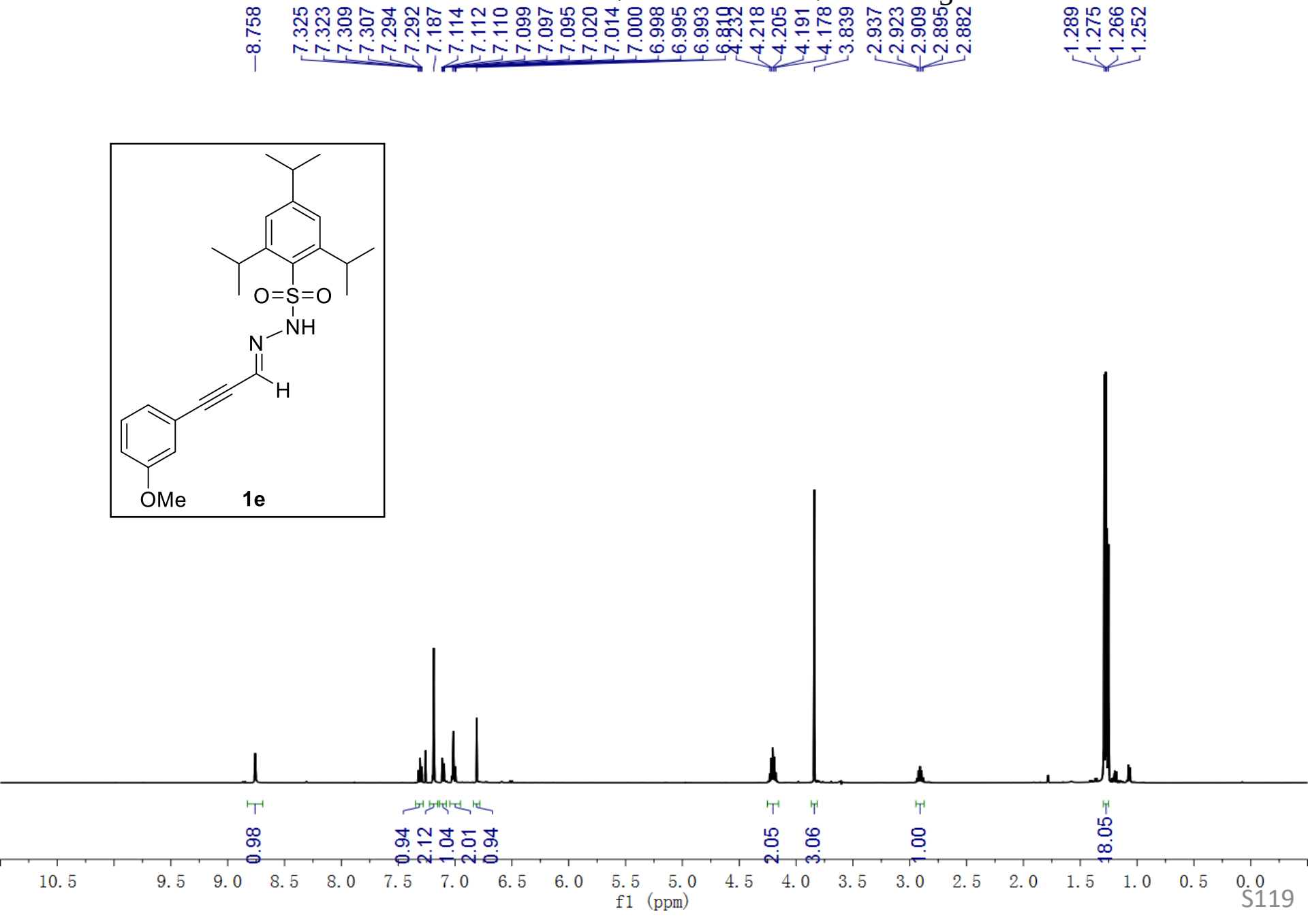


1d

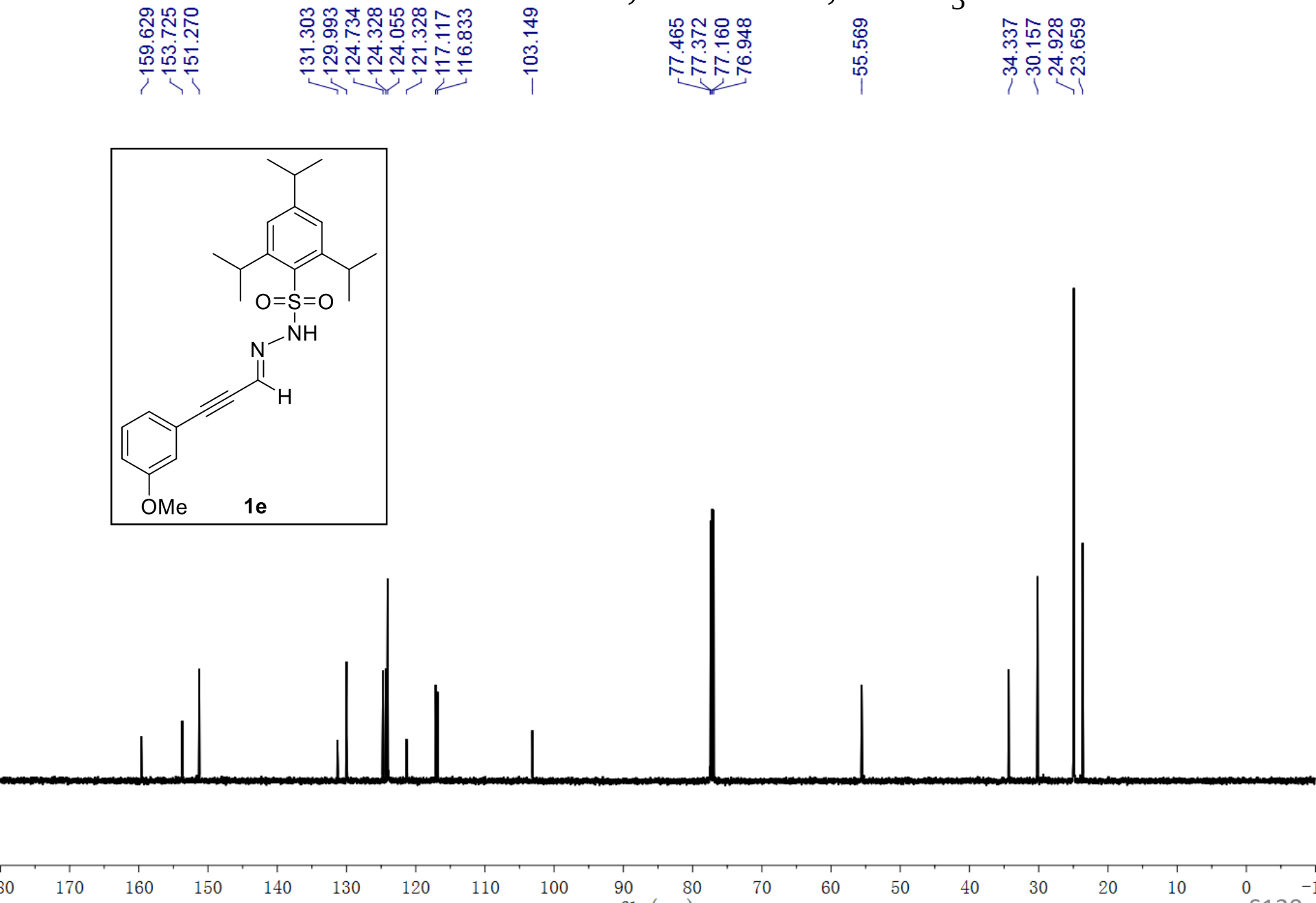
^{13}C NMR of **1d**, 101 MHz, $CDCl_3$



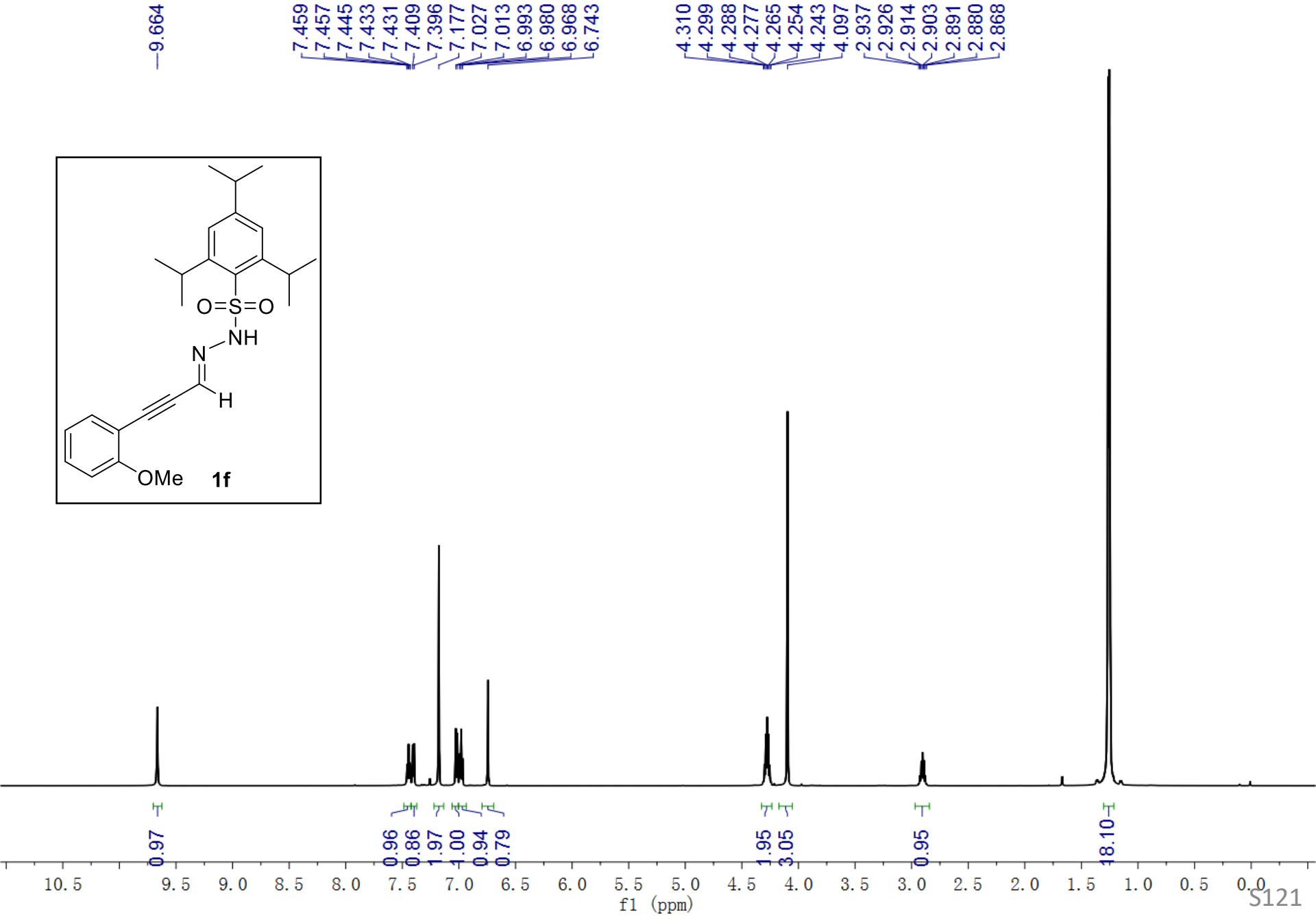
^{1}H NMR of **1e**, 600 MHz, $CDCl_3$



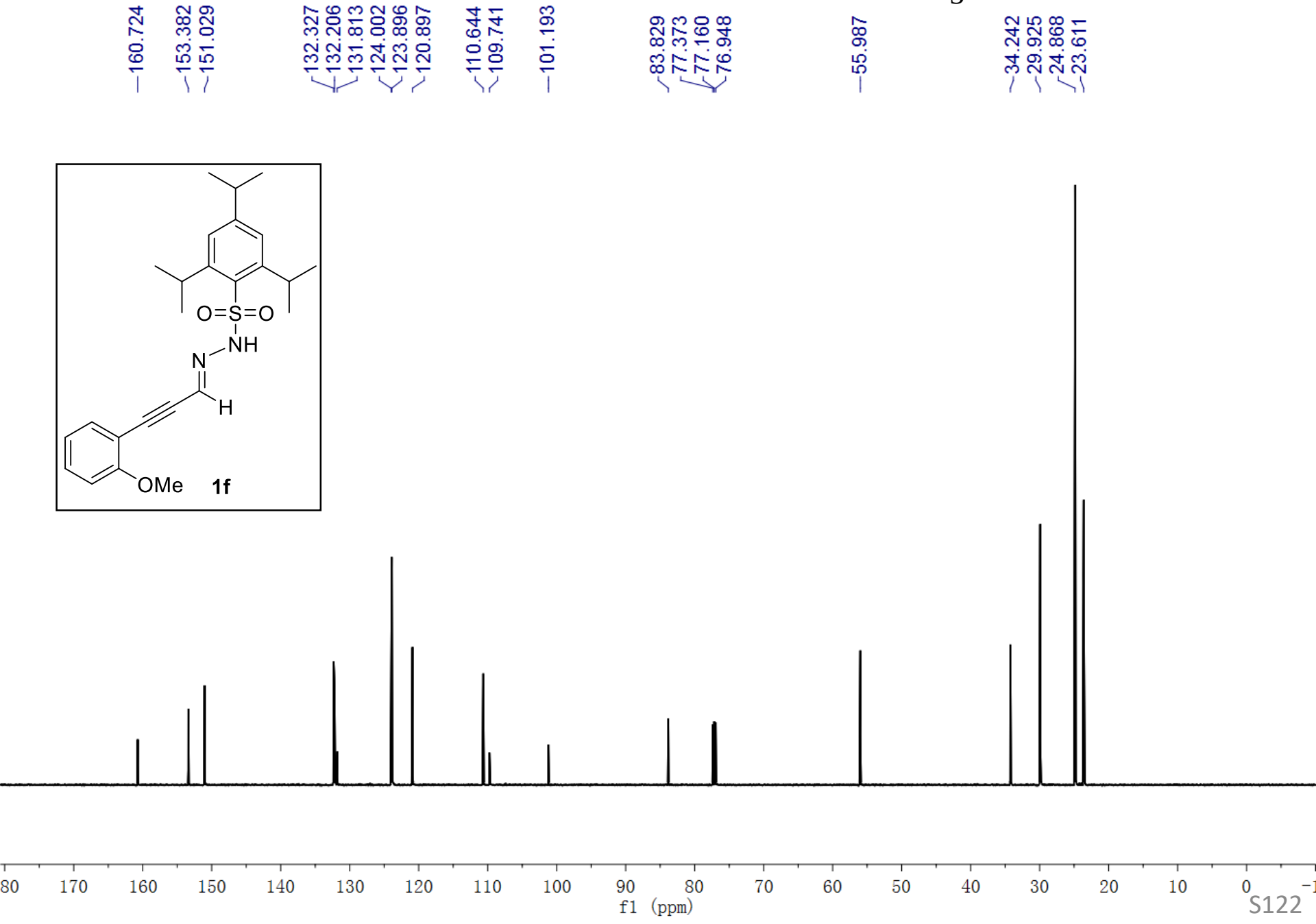
^{13}C NMR of **1e**, 151 MHz, $CDCl_3$



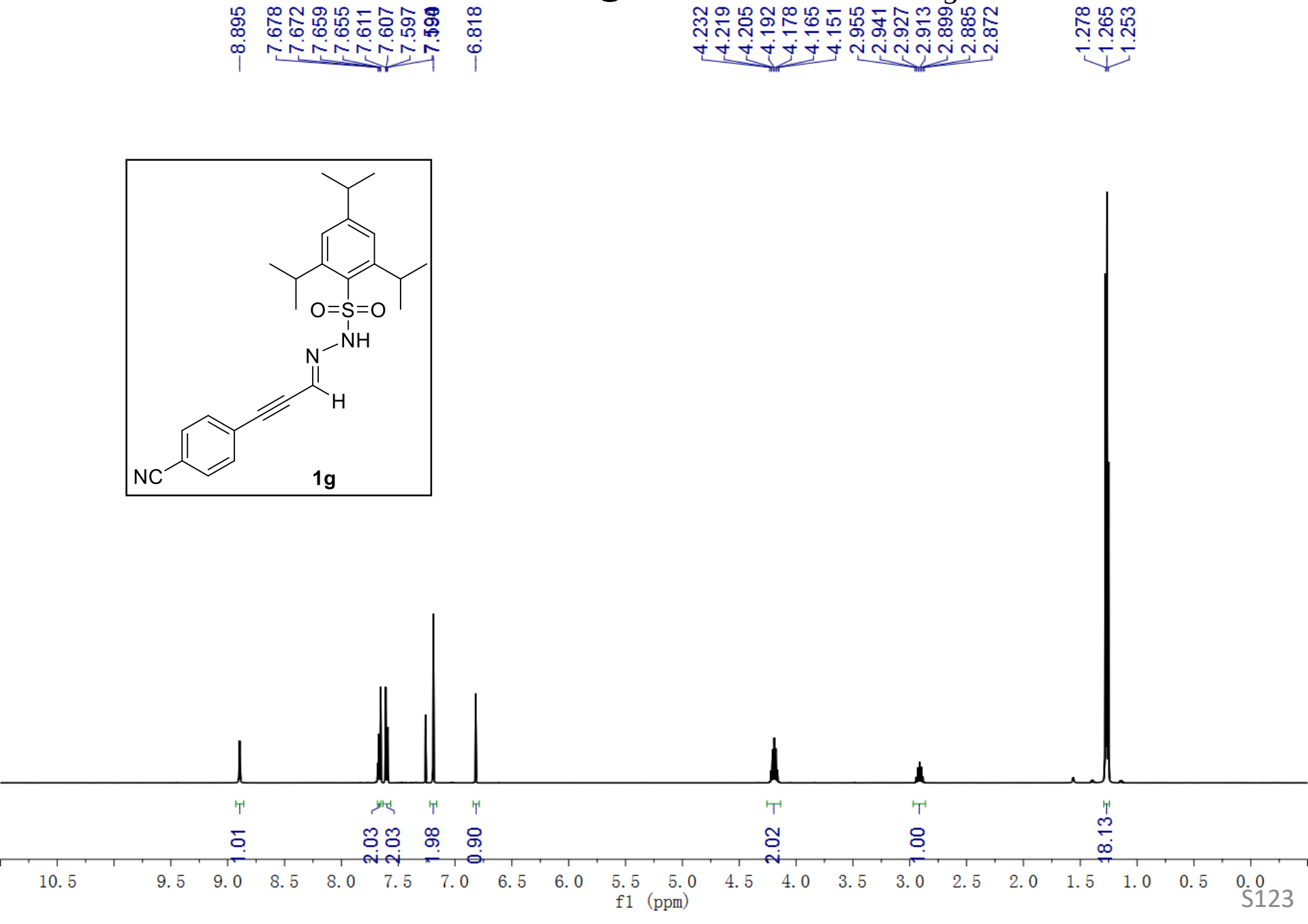
^{1}H NMR of **1f**, 600 MHz, $CDCl_3$



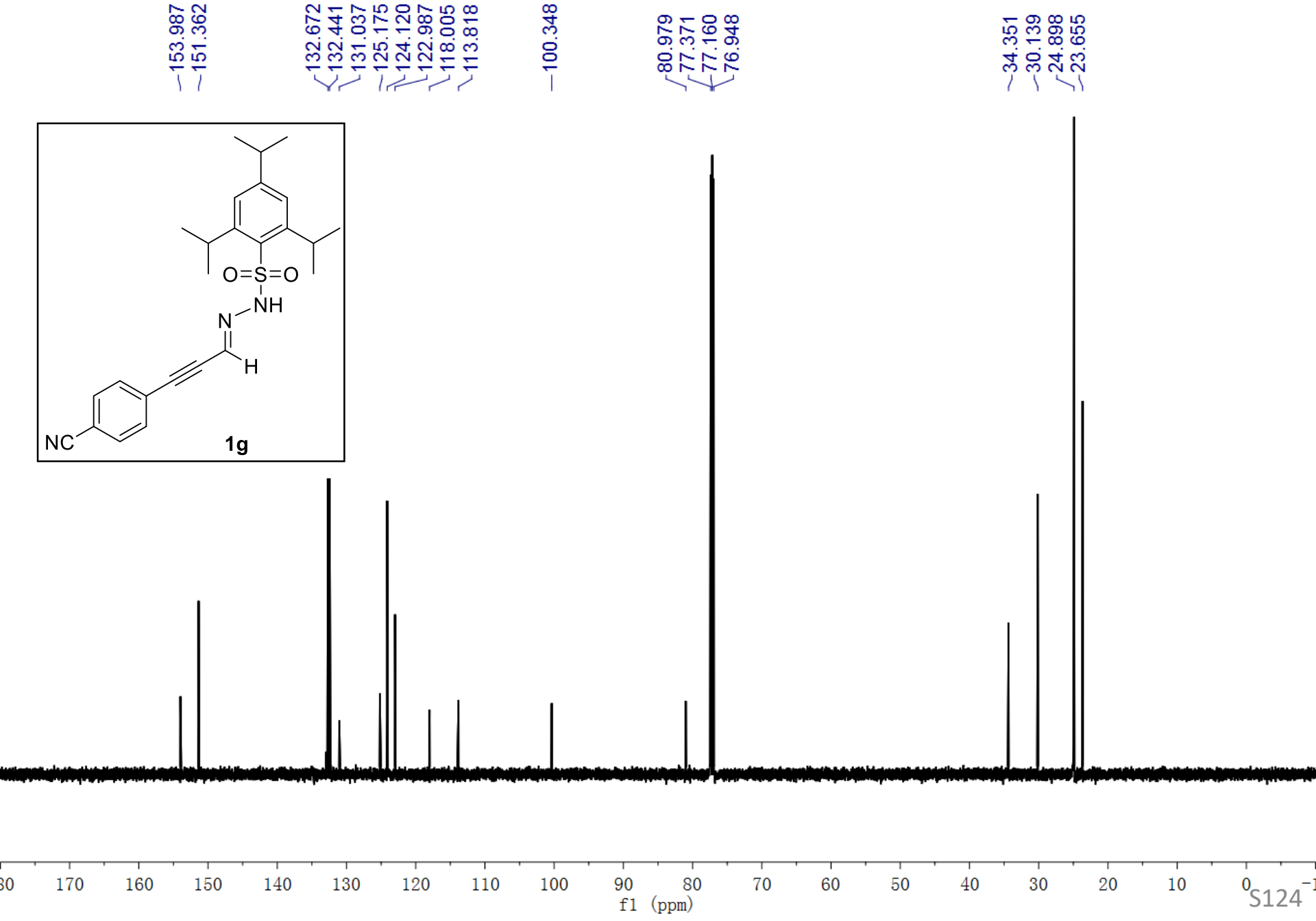
^{13}C NMR of **1f**, 151 MHz, $CDCl_3$



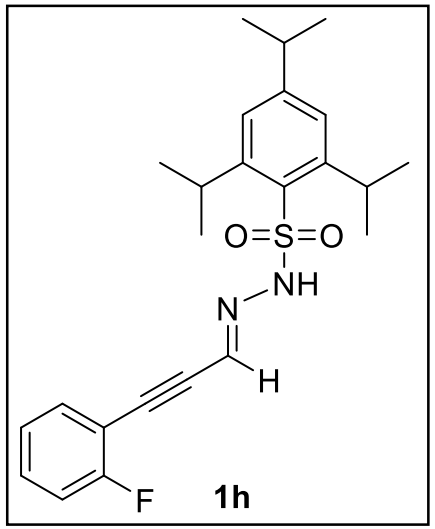
^{1}H NMR of **1g**, 600 MHz, $CDCl_3$



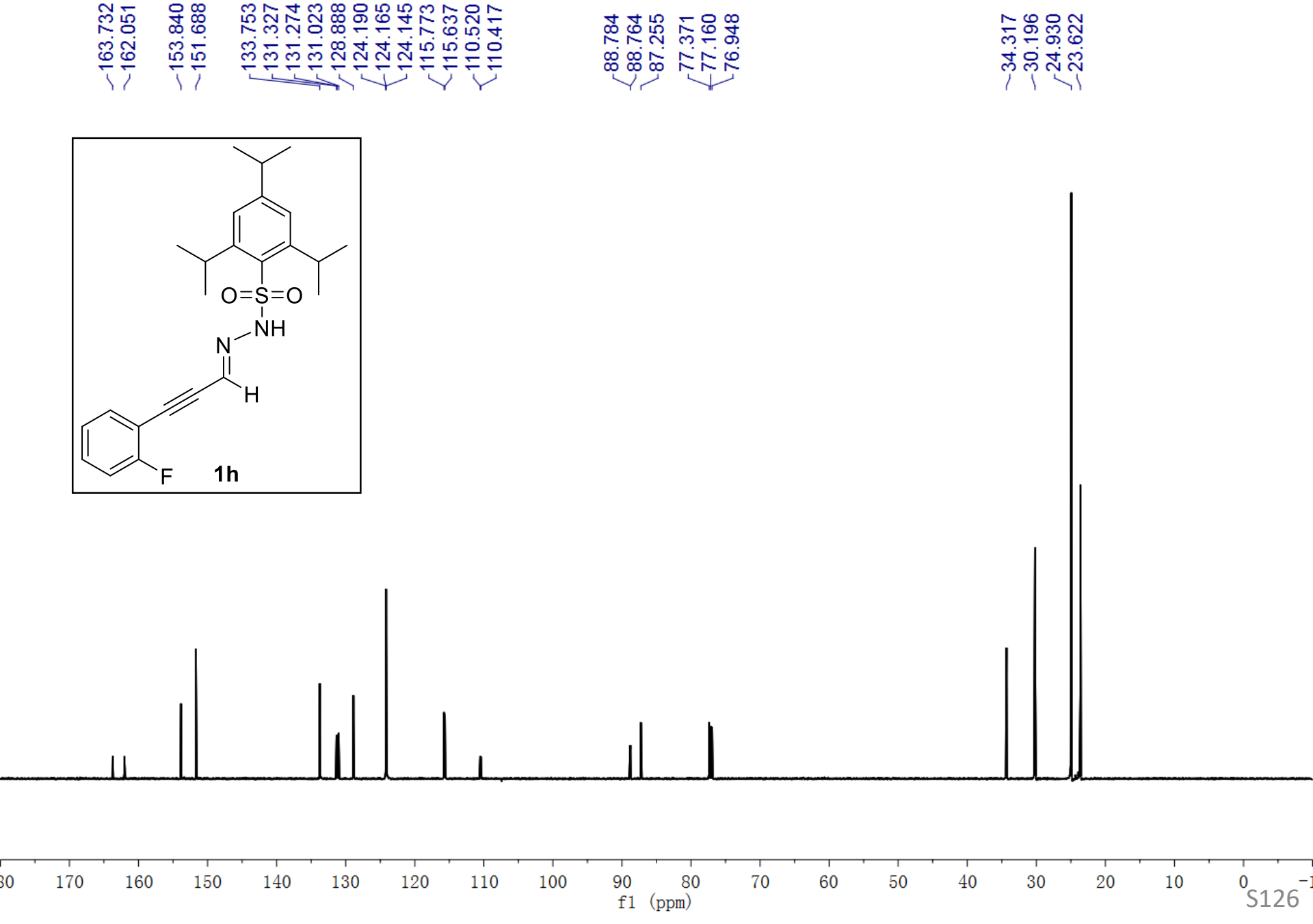
^{13}C NMR of **1g**, 151 MHz, $CDCl_3$



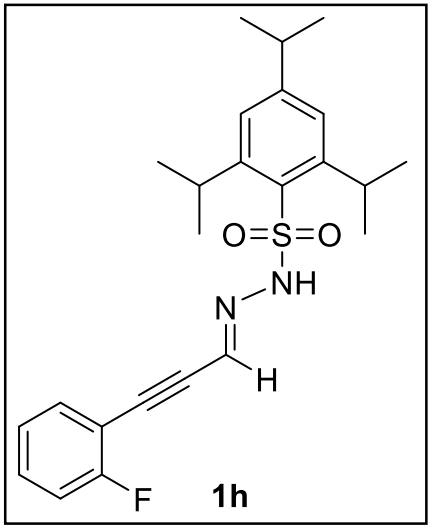
^{1}H NMR of **1h**, 600 MHz, $CDCl_3$



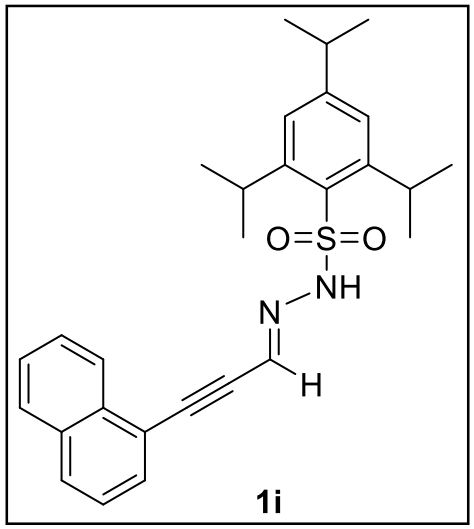
^{13}C NMR of **1h**, 151 MHz, $CDCl_3$



^{19}F NMR of **1h**, 564 MHz, $CDCl_3$

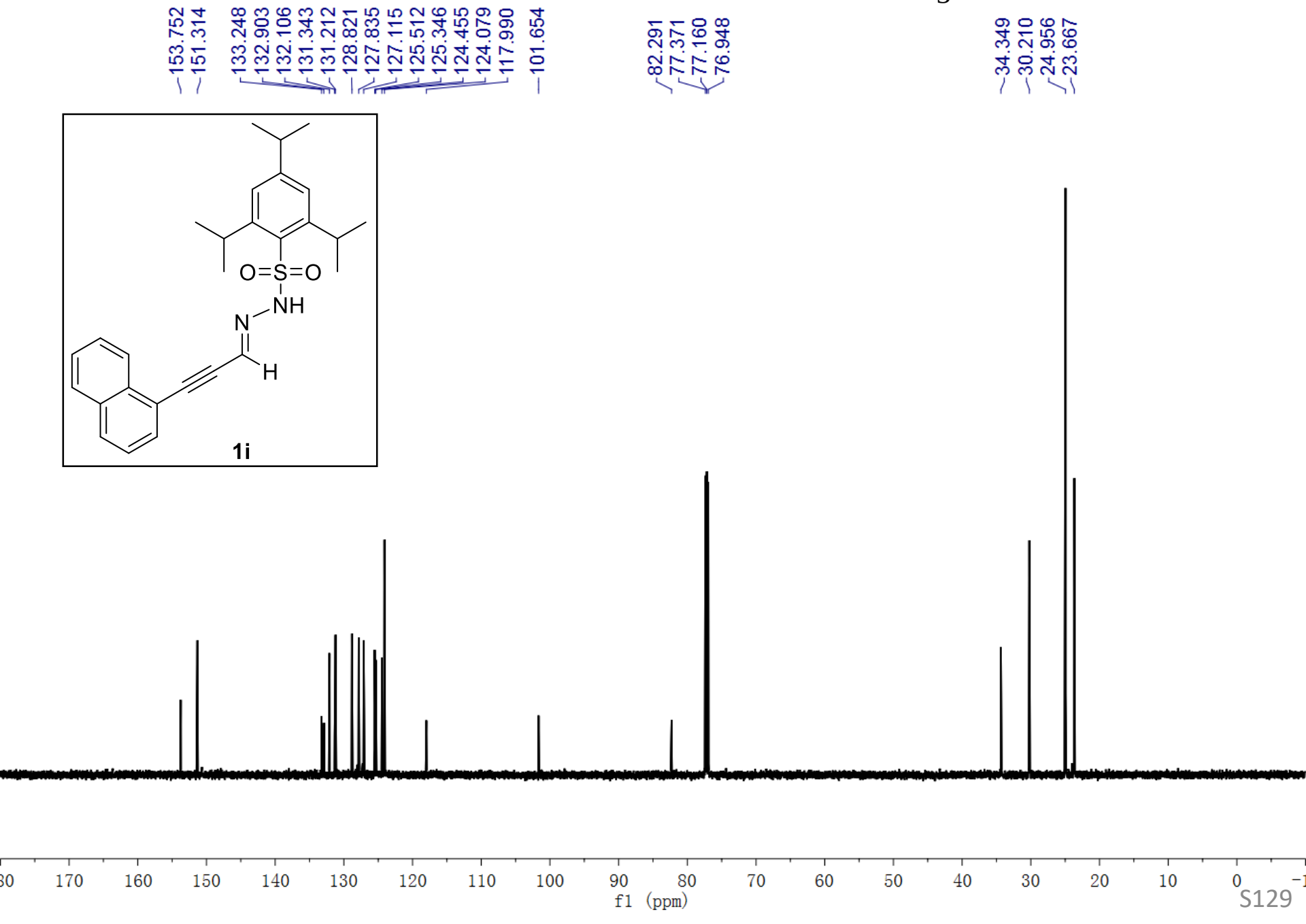


^{1}H NMR of **1i**, 600 MHz, $CDCl_3$

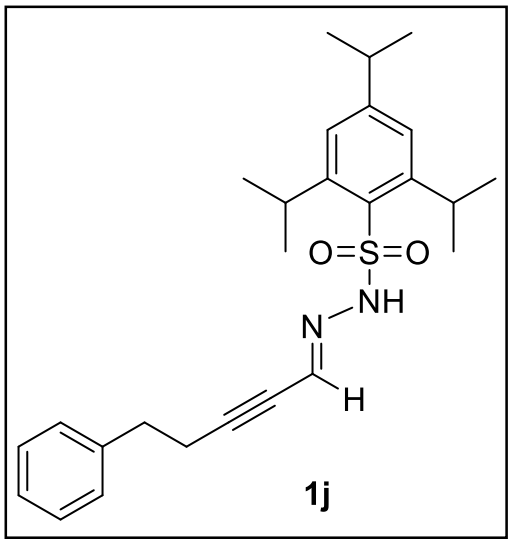


1i

^{13}C NMR of **1i**, 151 MHz, $CDCl_3$

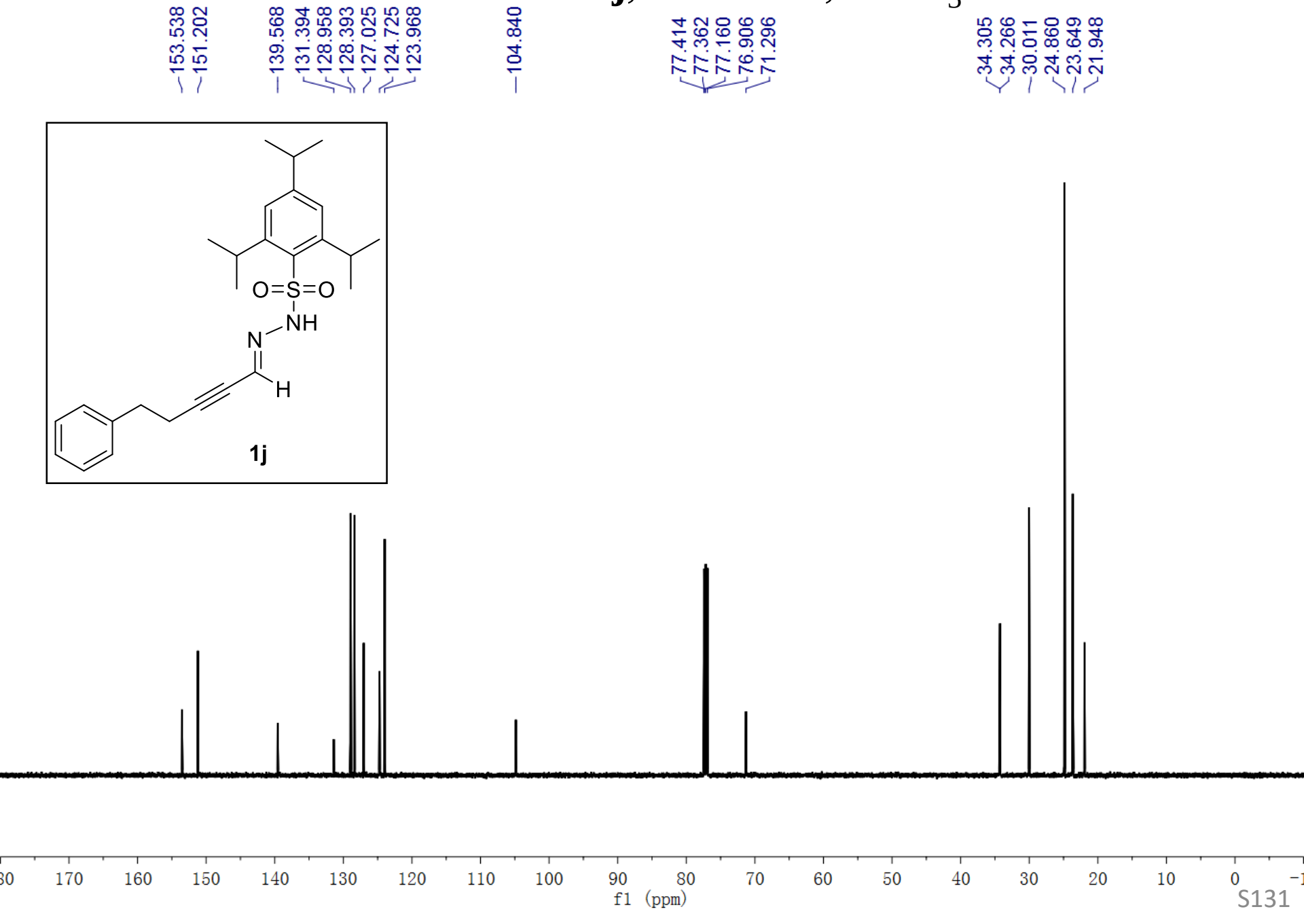


^{1}H NMR of **1j**, 500 MHz, $CDCl_3$

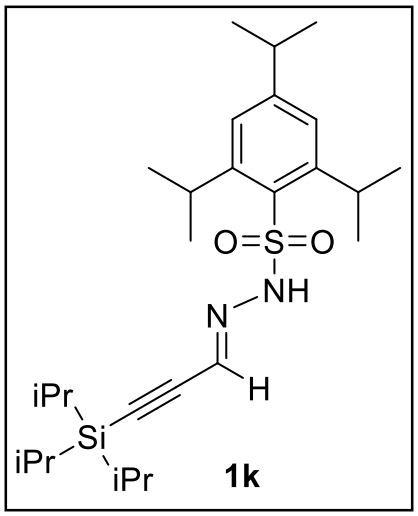


1j

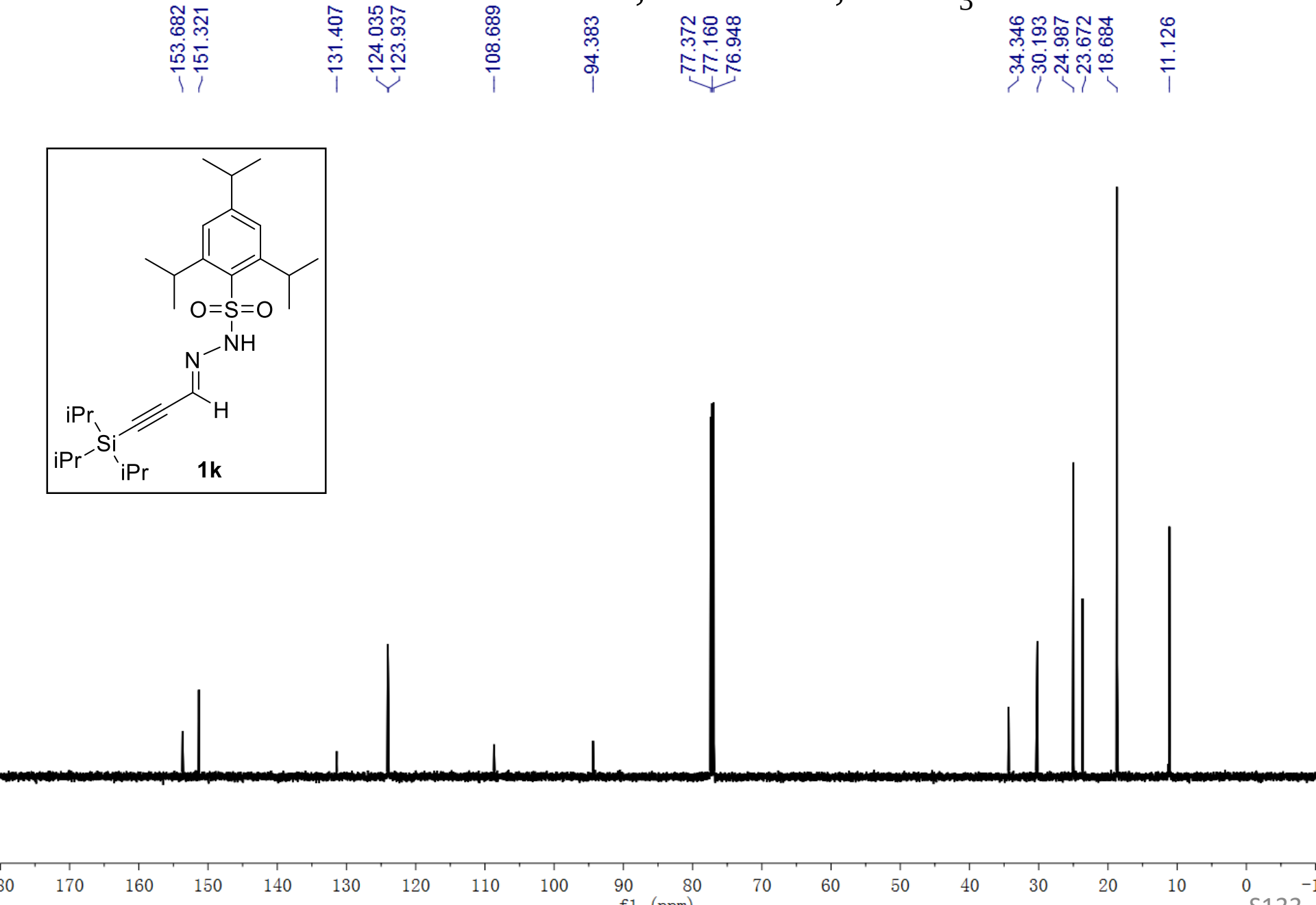
^{13}C NMR of **1j**, 126 MHz, $CDCl_3$



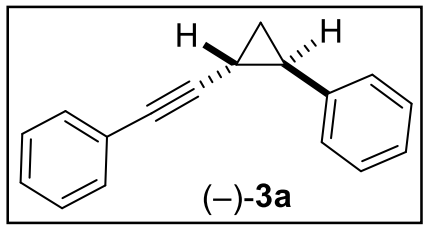
^{1}H NMR of **1k**, 600 MHz, $CDCl_3$



^{13}C NMR of **1k**, 151 MHz, $CDCl_3$

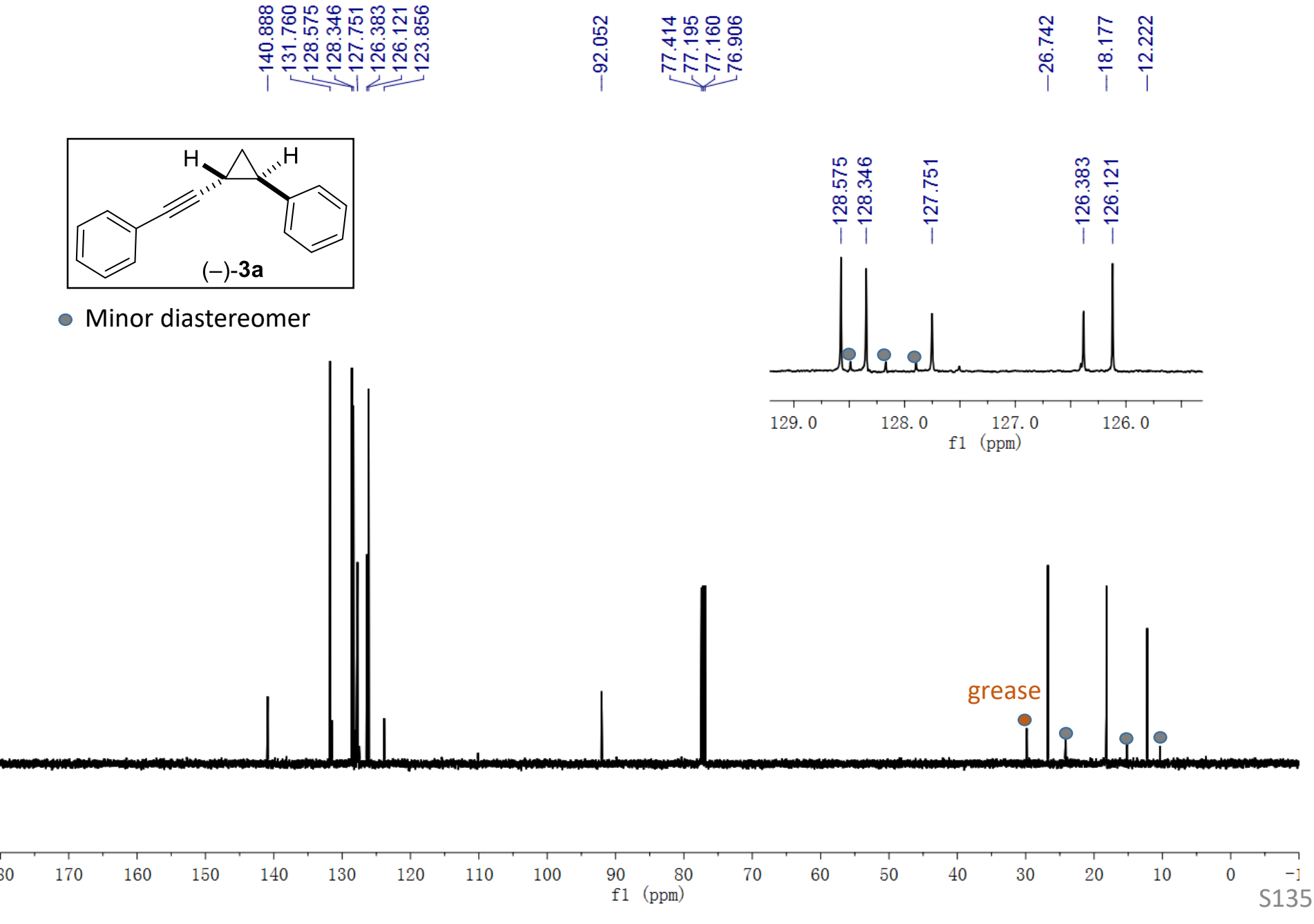


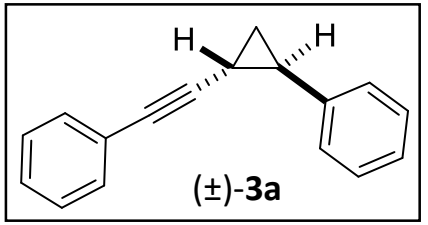
^{1}H NMR of **3a**, 500 MHz, $CDCl_3$



- Minor diastereomer

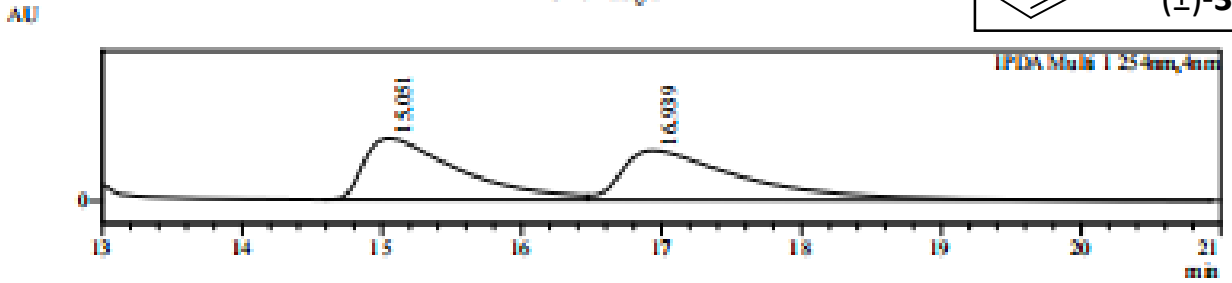
^{13}C NMR of **3a**, 126 MHz, $CDCl_3$



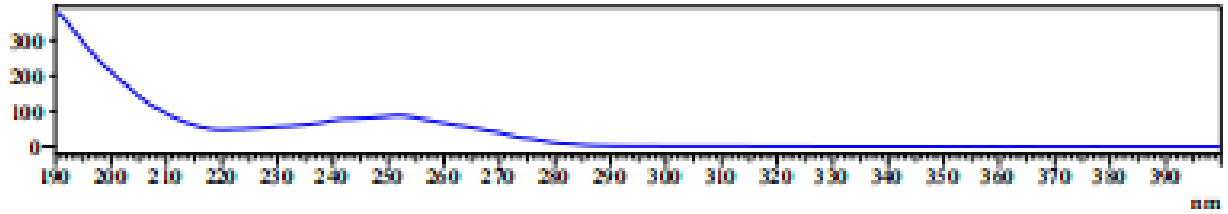


Data File : J0K-0070-4C-0%-0.8ML-isopropanol-solvent004.lcd
Sample Name : J0K-0070-4C-0%-0.8ML-isopropanol-solvent004
Sample ID : J0K-0070-4C-0%-0.8ML-isopropano
Method File : JK-0%-0.8ml.lcm

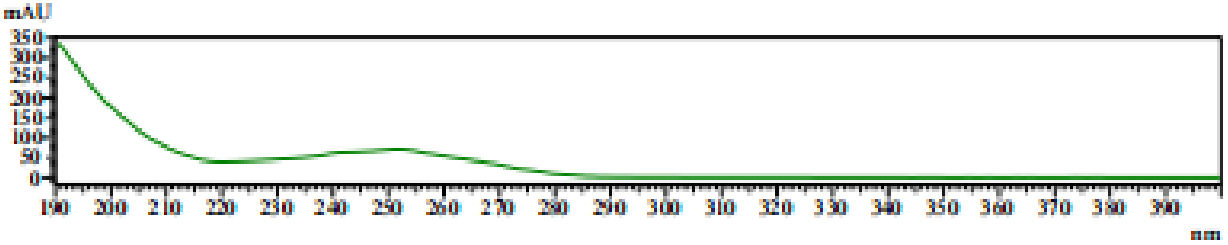
Chromatogram



UV Spectrum
Retention time= 15.051



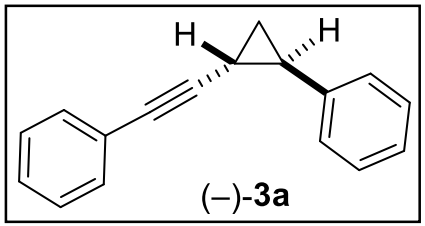
UV Spectrum
Retention time= 16.939



Peak Table

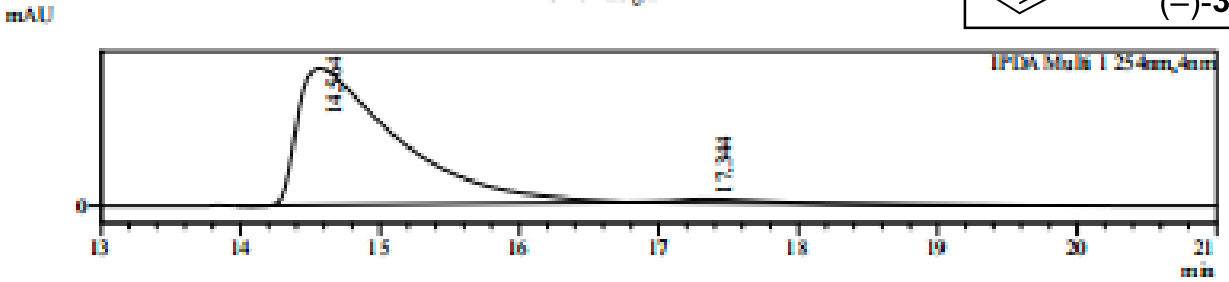
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	15.051	3817557	49.333
2	16.939	3920860	50.667
Total		7738417	100.000

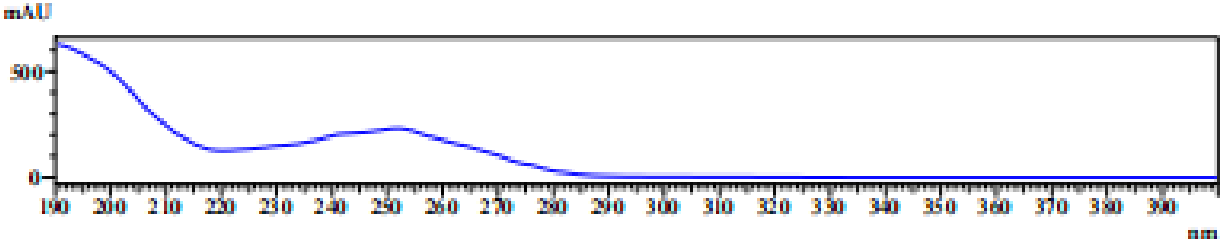


Data File : J0K-0068-4C-0%-0.8ML-isopropanol-solvent005.lcd
Sample Name : J0K-0068-4C-0%-0.8ML-isopropanol-solvent005
Sample ID : J0K-0068-4C-0%-0.8ML-isopropano
Method File : JK-0%-0.8ml.lcm

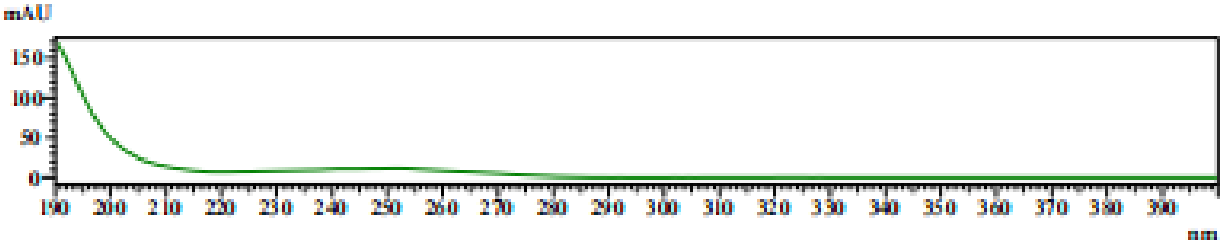
Chromatogram



UV Spectrum
Retention time = 14.564



UV Spectrum
Retention time = 17.344

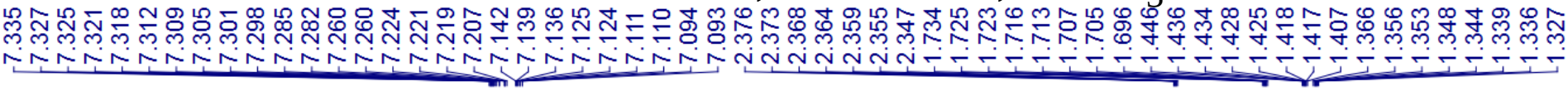


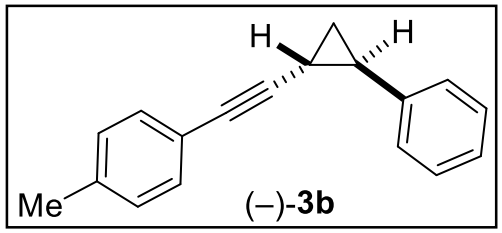
Peak Table

PDA Ch1 254nm

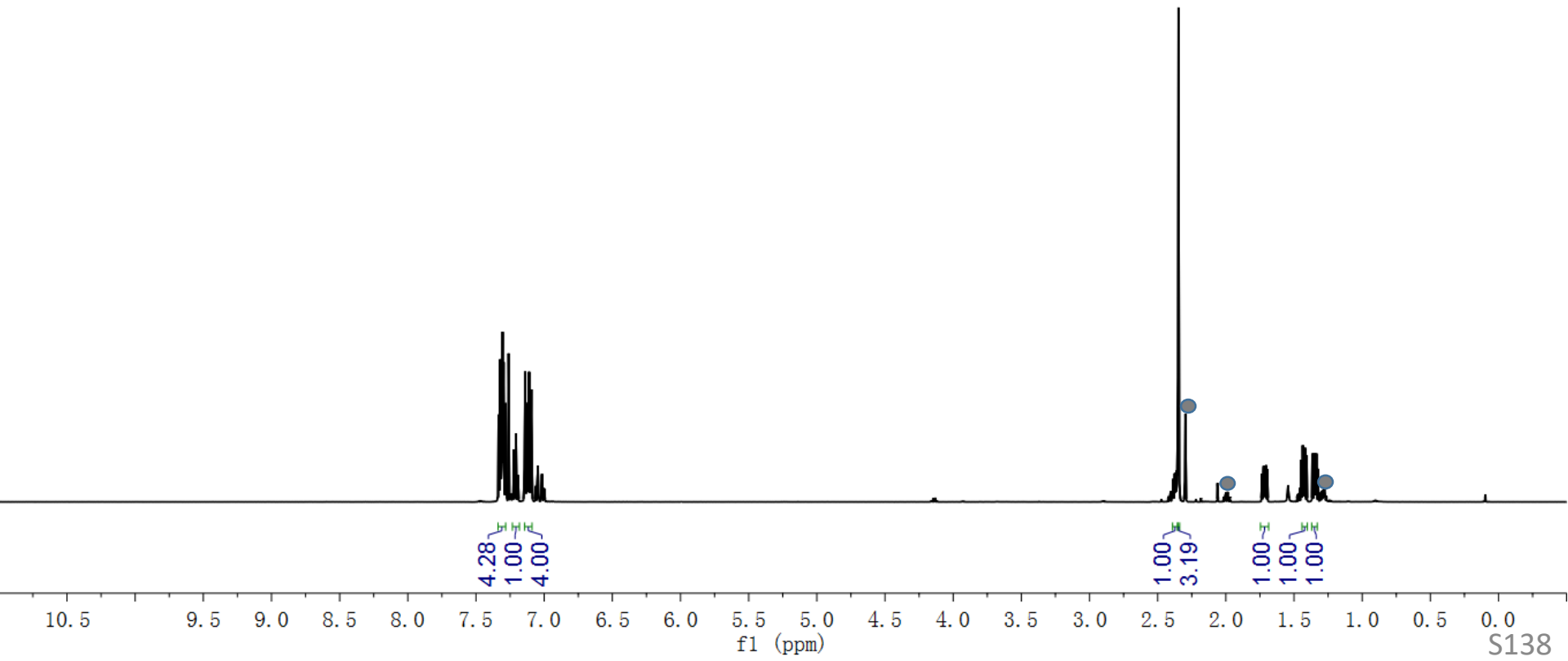
Peak#	Ret. Time	Area	Area%
1	14.564	10795024	97.917
2	17.344	229635	2.083
Total		11024660	100.000

^{1}H NMR of **3b**, 500 MHz, $CDCl_3$

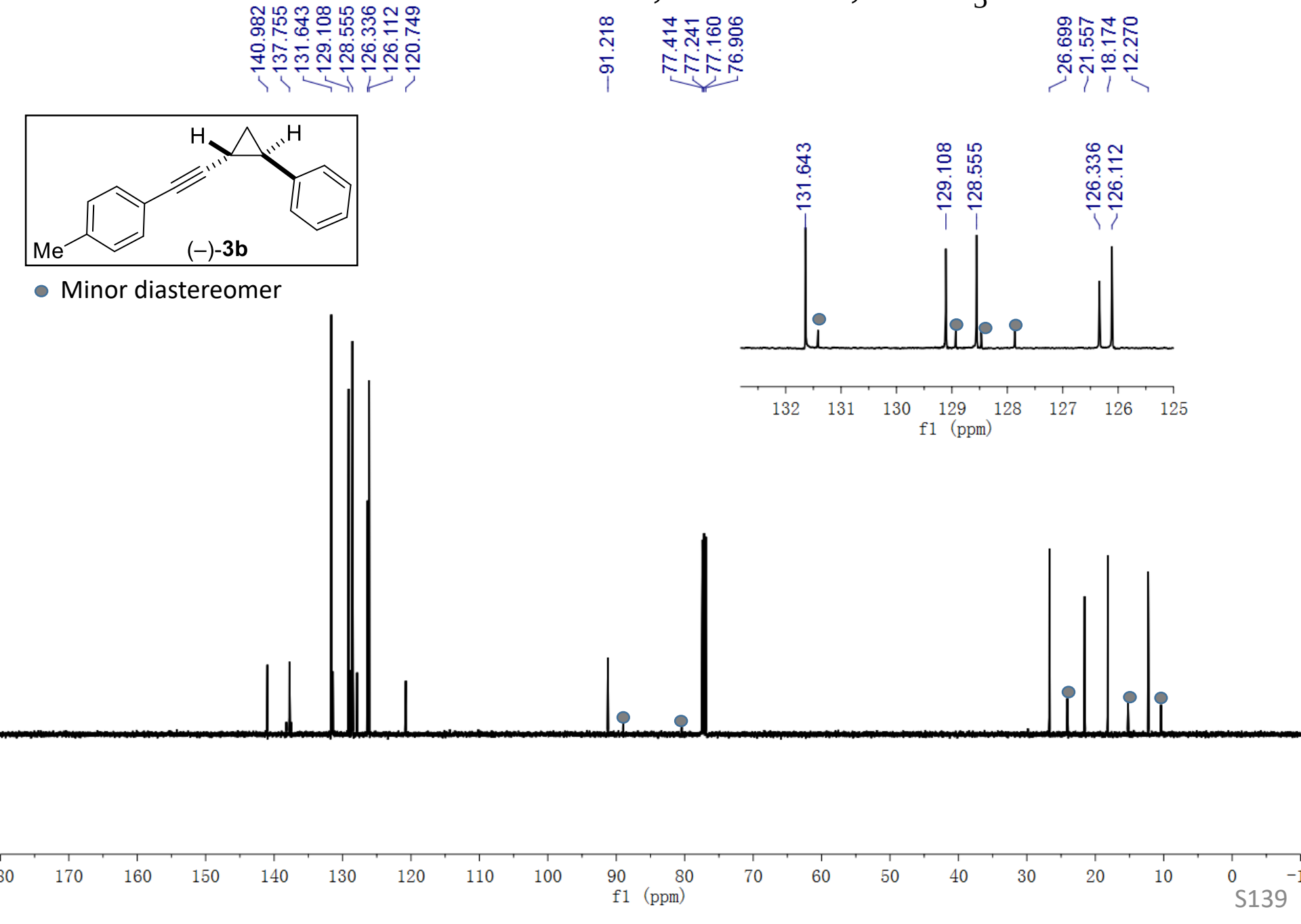


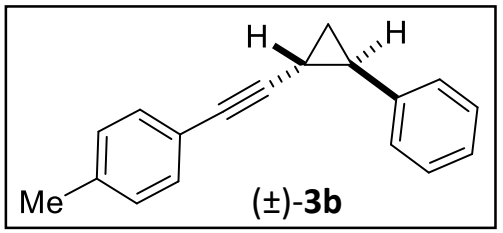


- Minor diastereomer



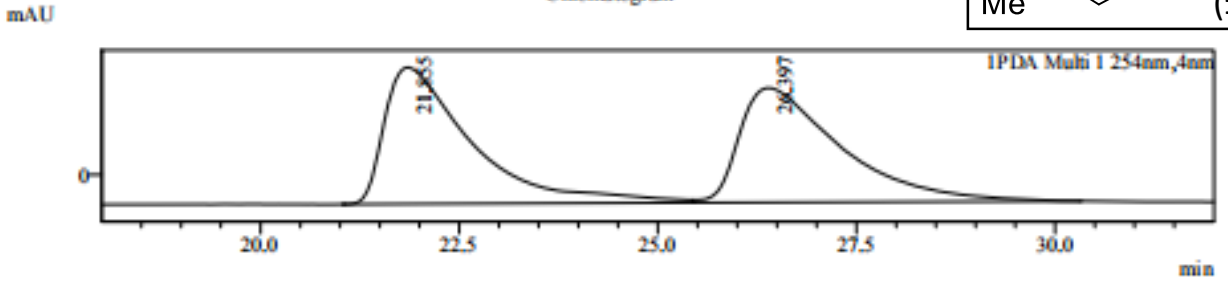
^{13}C NMR of **3b**, 126 MHz, $CDCl_3$



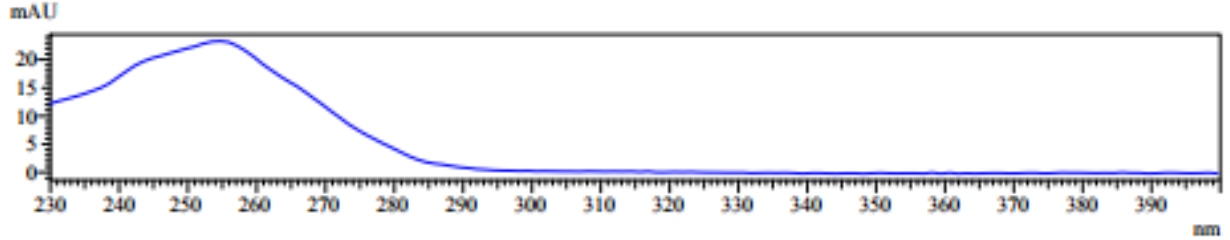


Data File : J0K-0097-IC-0%-0.8ML-isopropanol-solvent003.lcd
Sample Name : J0K-0097-IC-0%-0.8ML-isopropanol-solvent003
Sample ID : J0K-0097-IC-0%-0.8ML-isopropano
Method File : JK-0%-0.8ml.lcm

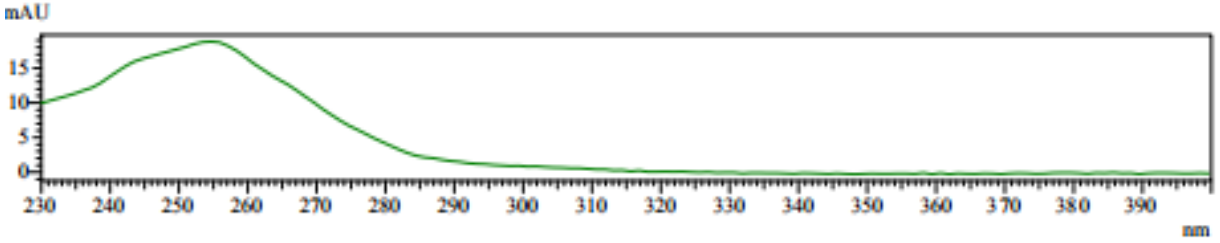
Chromatogram



UV Spectrum
Retention time = 21.855



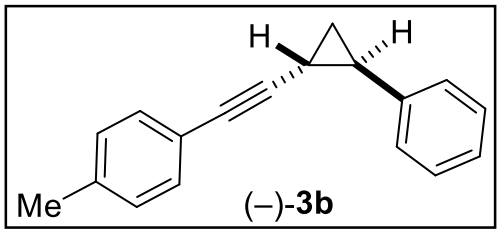
Retention time = 26.397



Peak Table

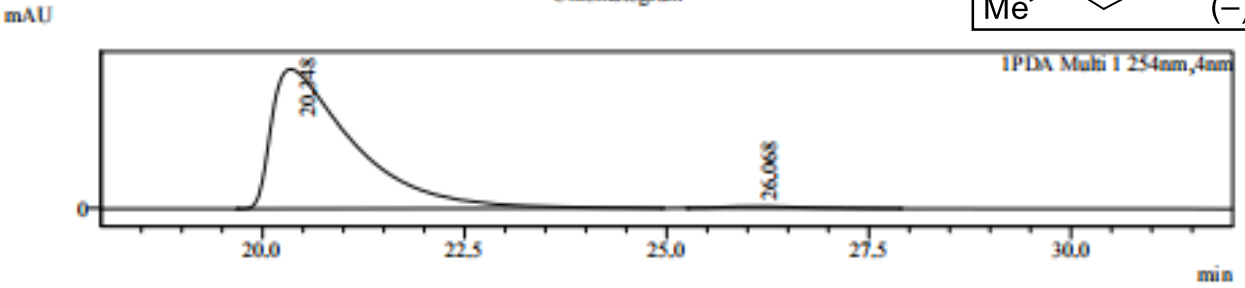
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	21.855	2215993	50.737
2	26.397	2151617	49.263
Total		4367610	100.000

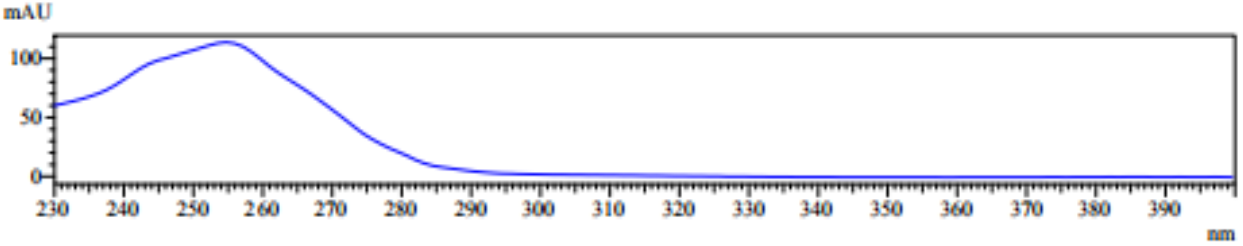


Data File : J0K-0115-IC-0%-0.8ML-isopropanol-solvent004.lcd
Sample Name : J0K-0115-IC-0%-0.8ML-isopropanol-solvent004
Sample ID : J0K-0115-IC-0%-0.8ML-isopropano
Method File : JK-0%-0.8ml.lcm

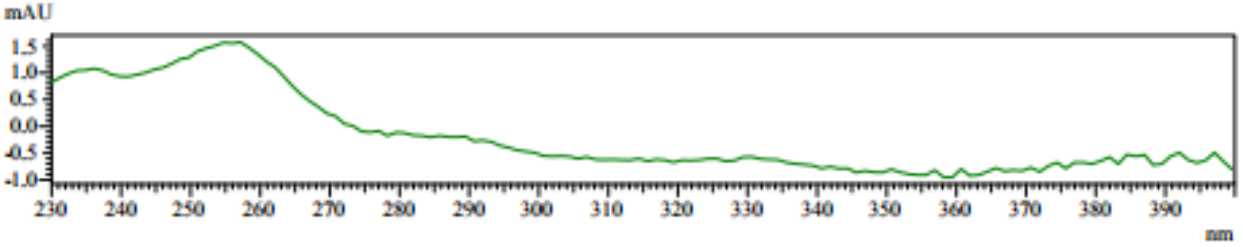
Chromatogram



UV Spectrum
Retention time = 20.348



t
Retention time = 26.068

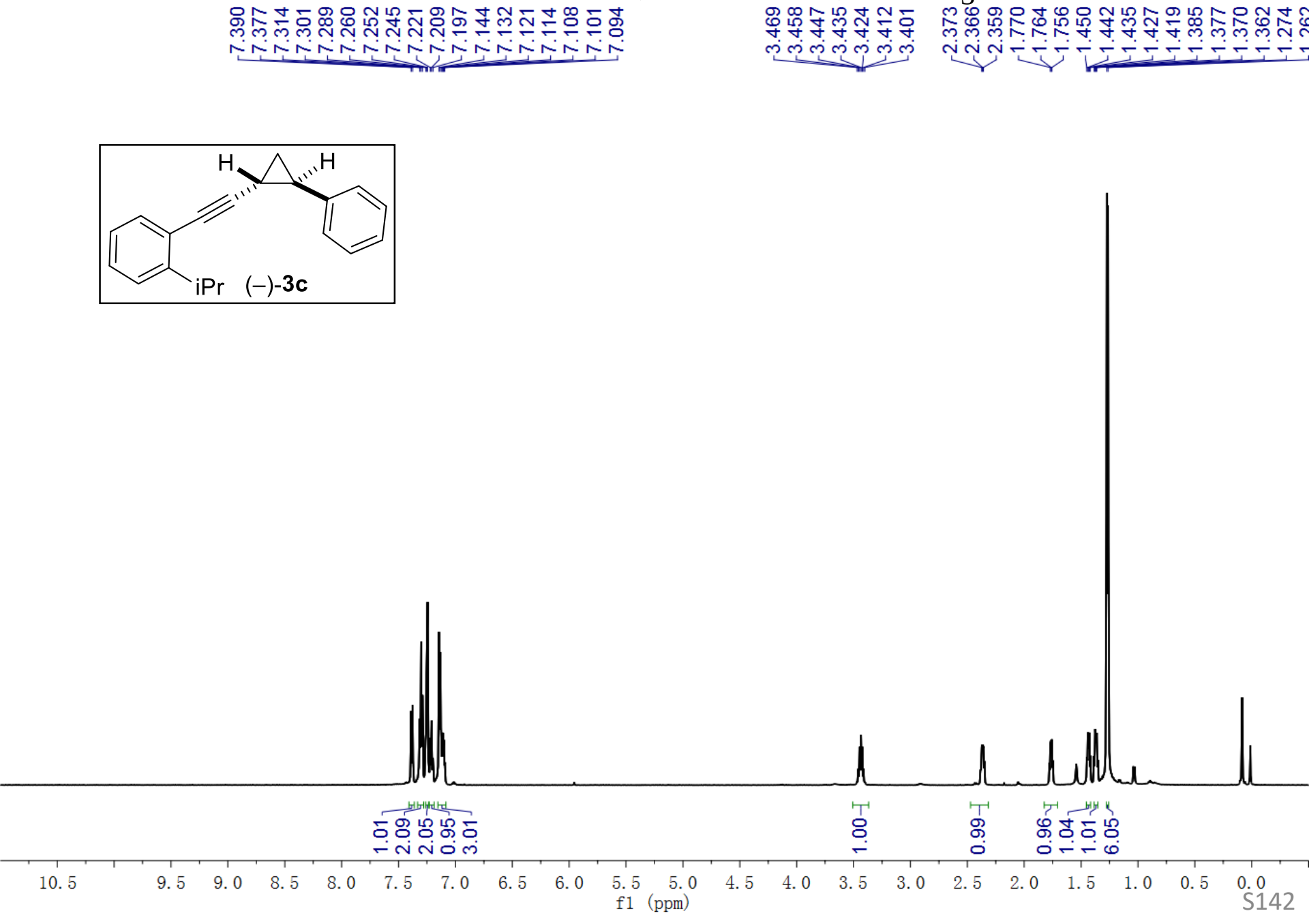


Peak Table

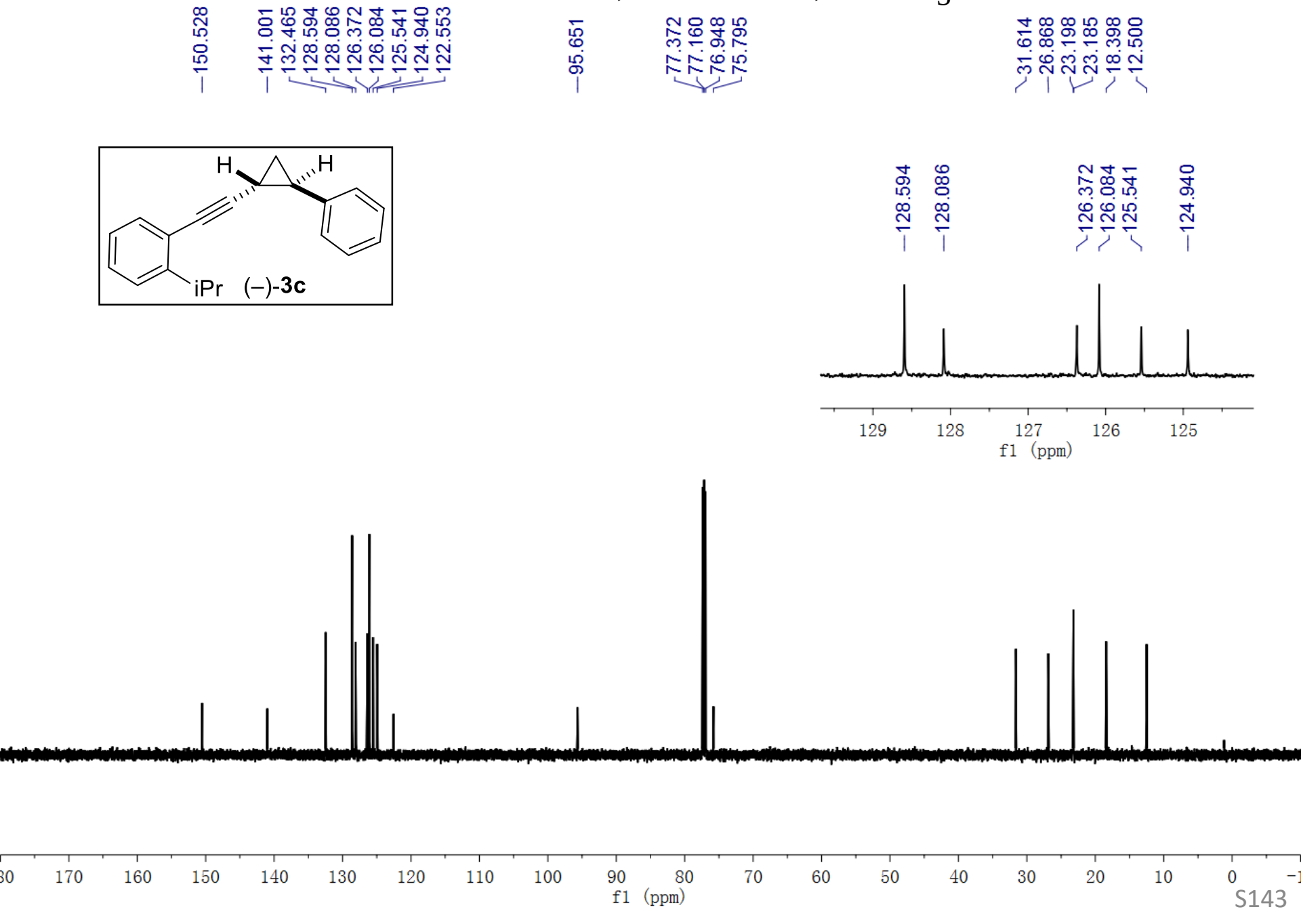
PDA Ch1 254nm

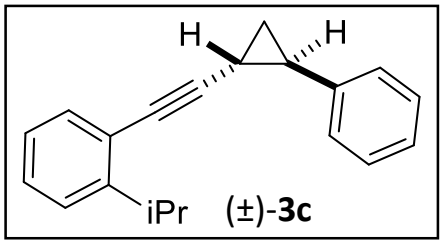
Peak#	Ret. Time	Area	Area%
1	20.348	7849014	98.625
2	26.068	109463	1.375
Total		7958477	100.000

^{1}H NMR of **3c**, 600 MHz, $CDCl_3$



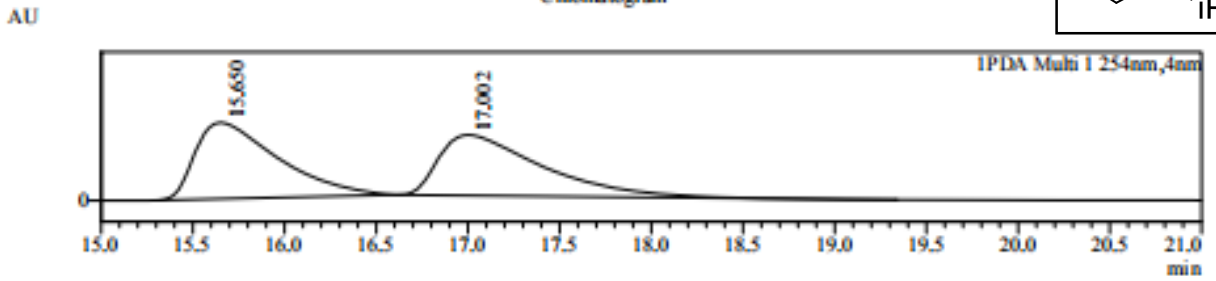
^{13}C NMR of **3c**, 151 MHz, $CDCl_3$



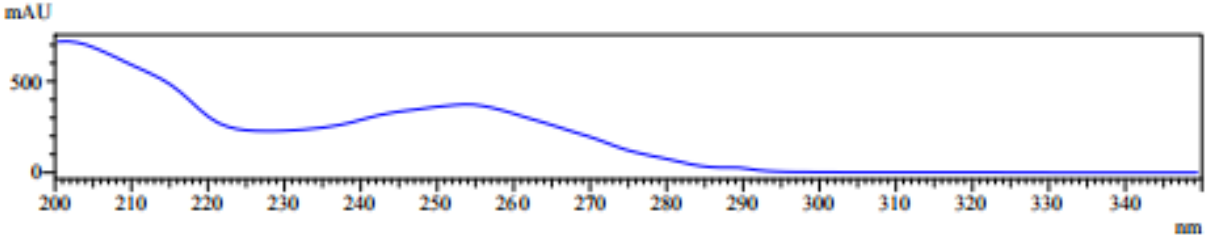


Data File : J0K-0241-12-IC-0%-0.5ML-isopropanol-solvent006-modified.lcd
Sample Name : J0K-0241-12-IC-0%-0.5ML-isopropanol-solvent006
Sample ID : J0K-0241-12-IC-0%-0.5ML-isoprop
Method File : J0K-0%-0.5ml.lcm

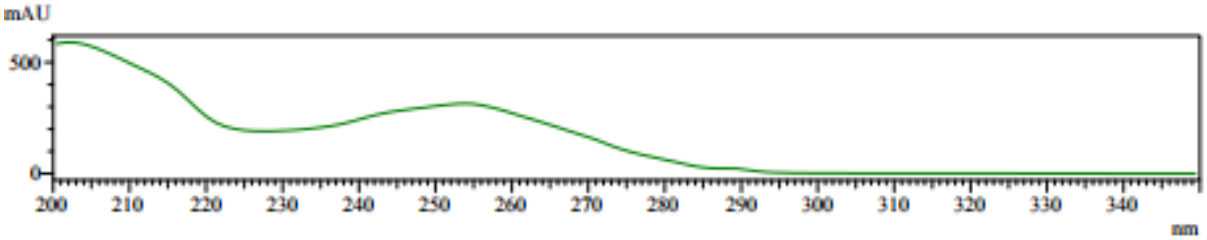
Chromatogram



UV Spectrum
Retention time = 15.650



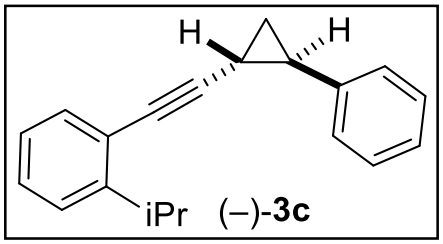
Retention time = 17.002



Peak Table

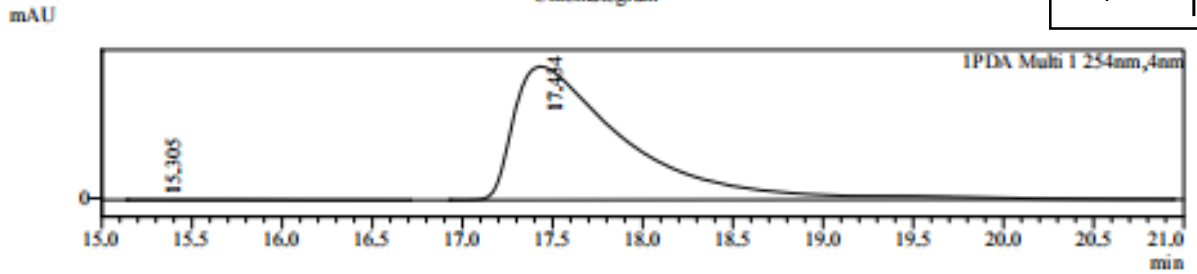
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	15.650	11294352	50.388
2	17.002	11120560	49.612
Total		22414912	100.000

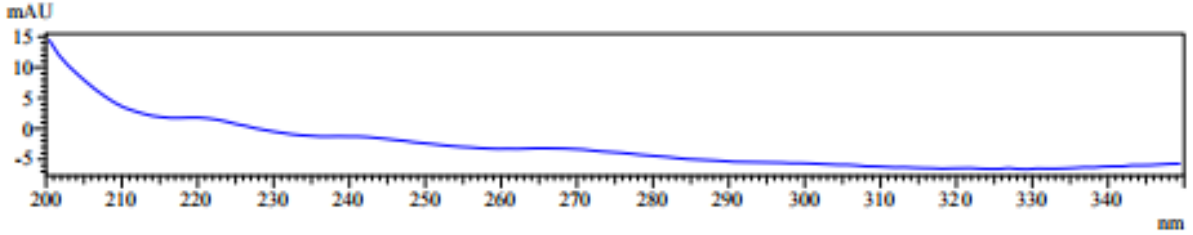


Data File : J0K-0242-13-IC-0%-0.5ML-isopropanol-solvent005-modified.lcd
Sample Name : J0K-0242-13-IC-0%-0.5ML-isopropanol-solvent005
Sample ID : J0K-0242-13-IC-0%-0.5ML-isoprop
Method File : J0K-0%-0.5ml.lcm

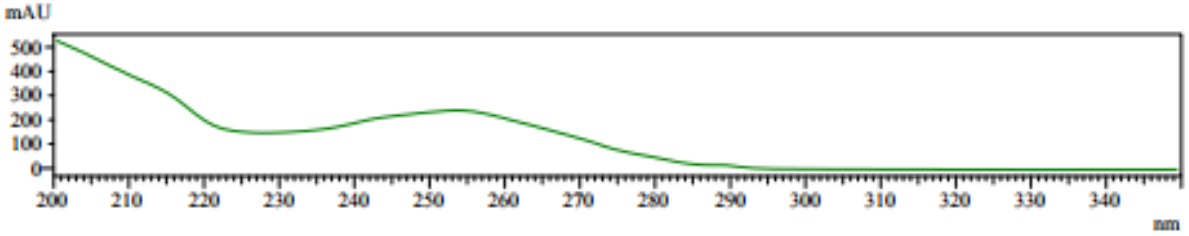
Chromatogram



UV Spectrum
Retention time = 15.305



Retention time = 17.434

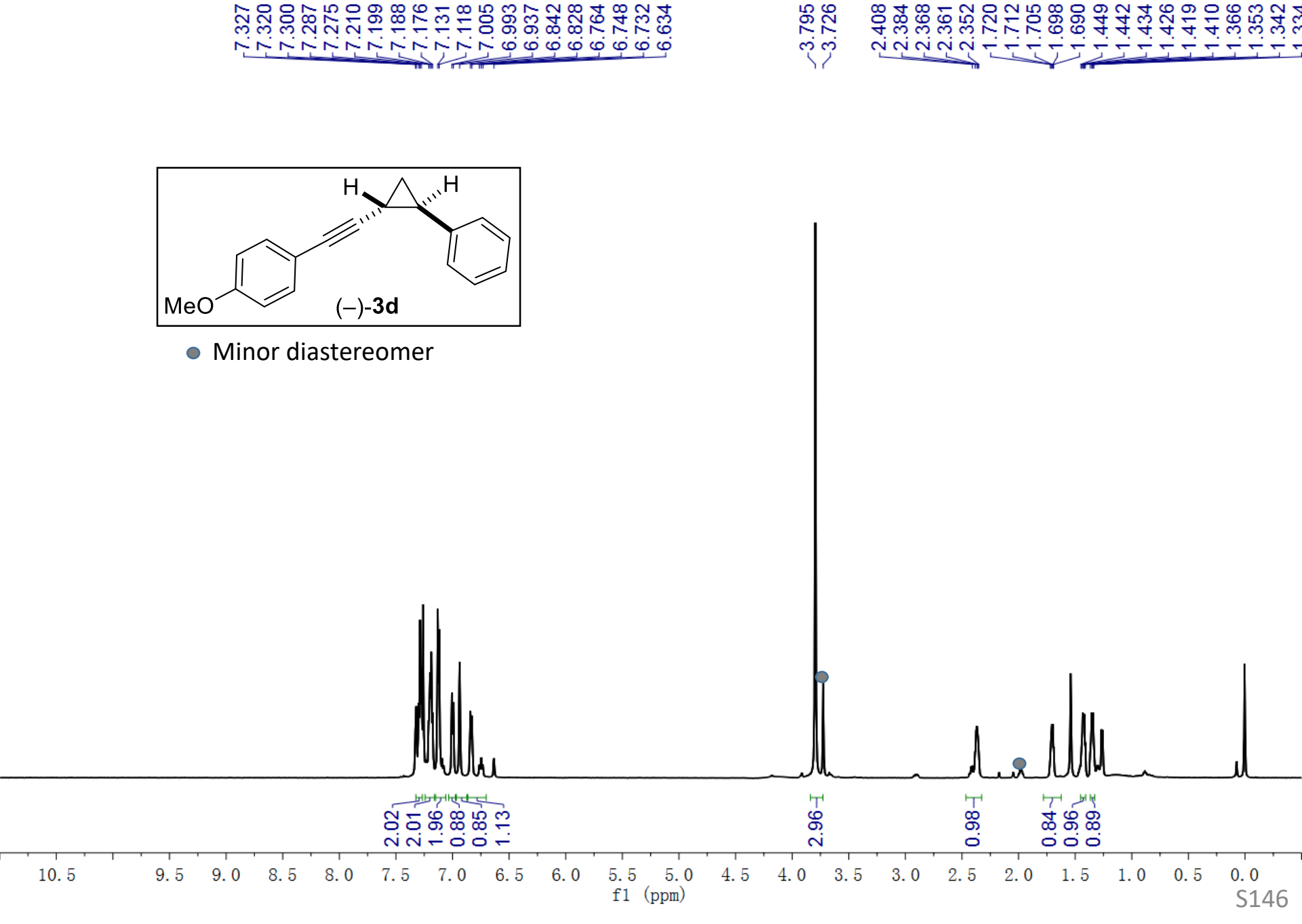


Peak Table

PDA Ch1 254nm

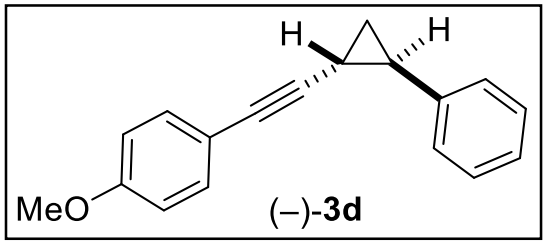
Peak#	Ret. Time	Area	Area%
1	15.305	21830	0.213
2	17.434	10222096	99.787
Total		10243926	100.000

^{1}H NMR of **3d**, 500 MHz, $CDCl_3$



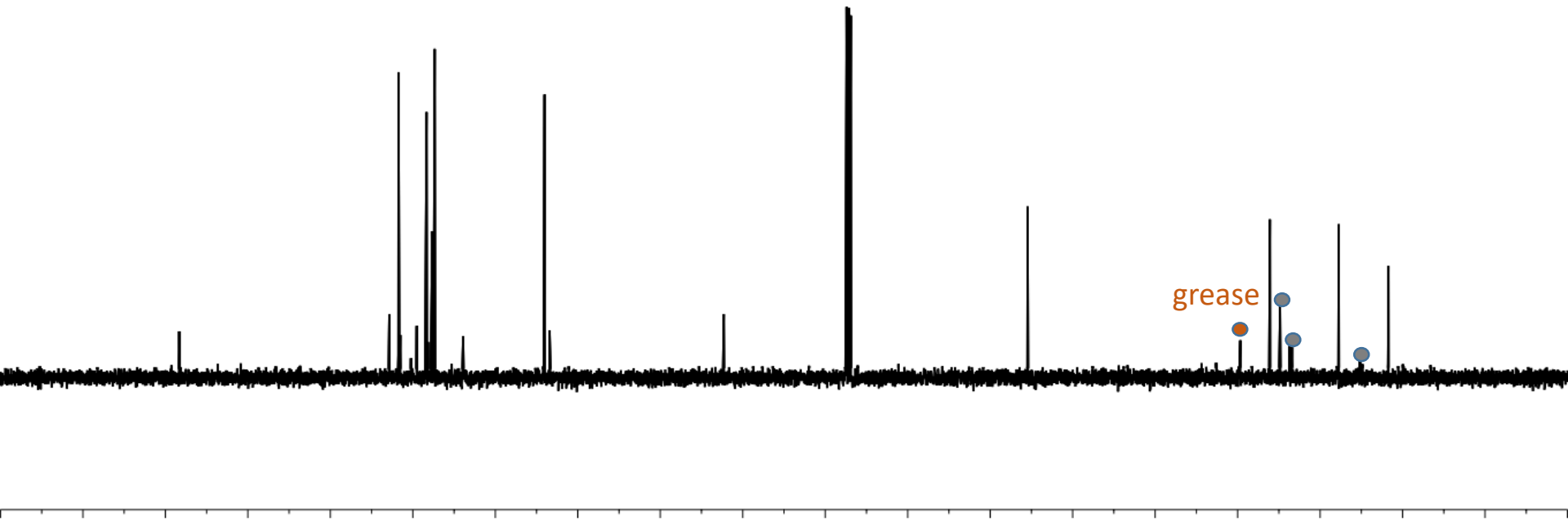
^{13}C NMR of **3d**, 126 MHz, $CDCl_3$

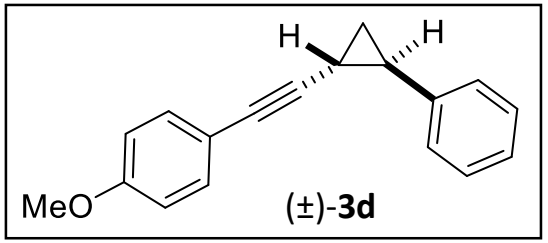
158.318
132.859
131.736
129.532
128.334
127.700
127.353
114.027
92.297
77.415
77.160
77.056
76.907
55.459
26.087
17.734
11.705



(–)-**3d**

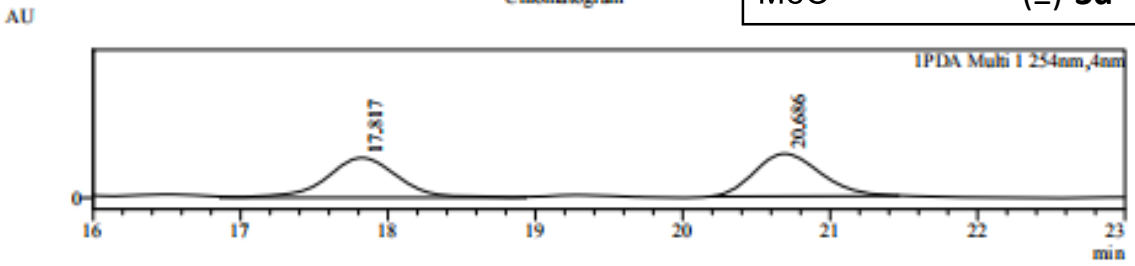
● Minor diastereomer



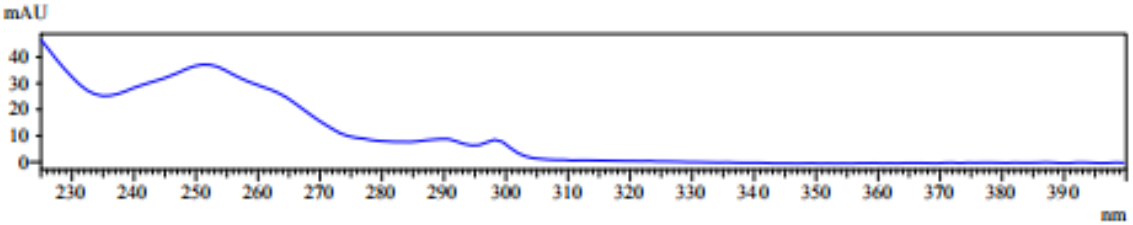


Data File : J0K-0608-ID-0.5%-0.8ML.lcd
Sample Name : J0K-0608-ID-0.5%-0.8ML
Sample ID : J0K-0608-ID-0.5%-0.8ML
Method File : J0K-0.5%--35min-0.8ml.lcm

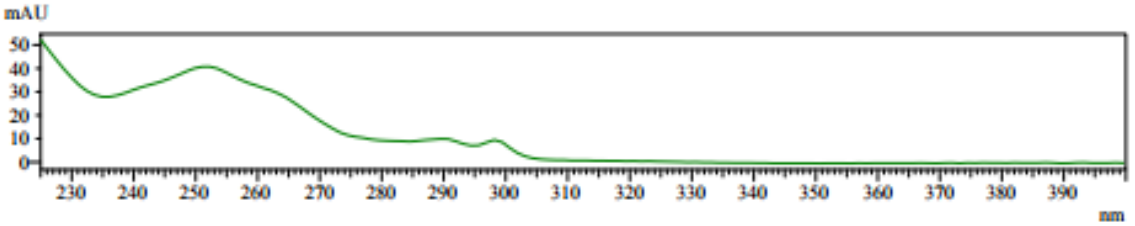
Chromatogram



UV Spectrum
Retention time = 17.817



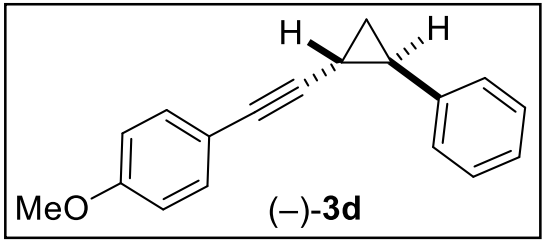
Retention time = 20.686



Peak Table

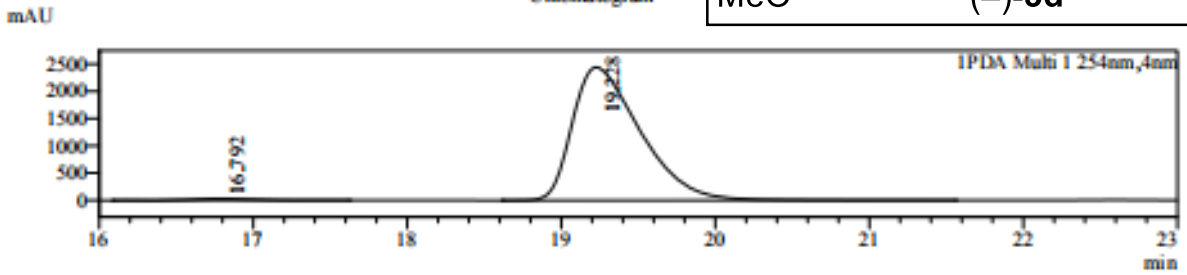
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	17.817	1175582	50.070
2	20.686	1172308	49.930
Total		2347890	100.000

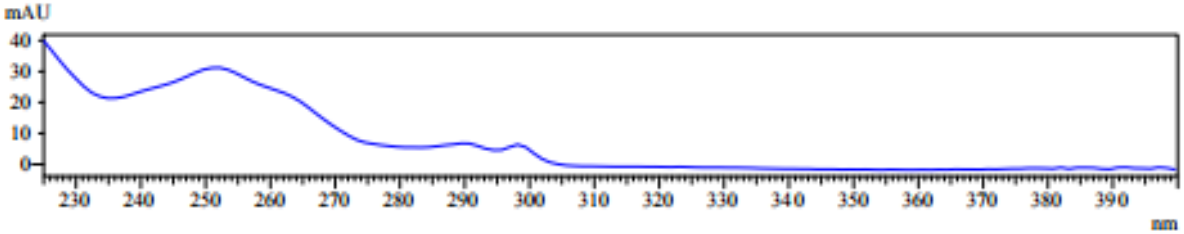


Data File : J0K-0607-ID-3-0.5%-0.8ML.lcd
Sample Name : J0K-0607-ID-3-0.5%-0.8ML
Sample ID : J0K-0607-ID-3-0.5%-0.8ML
Method File : J0K-0.5%--35min-0.8ml.lcm

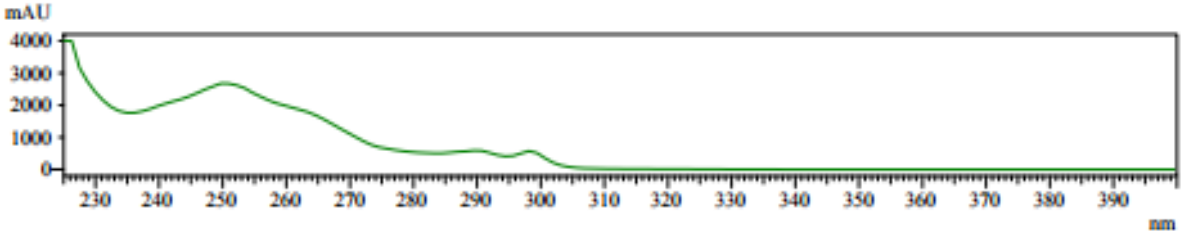
Chromatogram



UV Spectrum
Retention time = 16.792



Retention time = 19.228

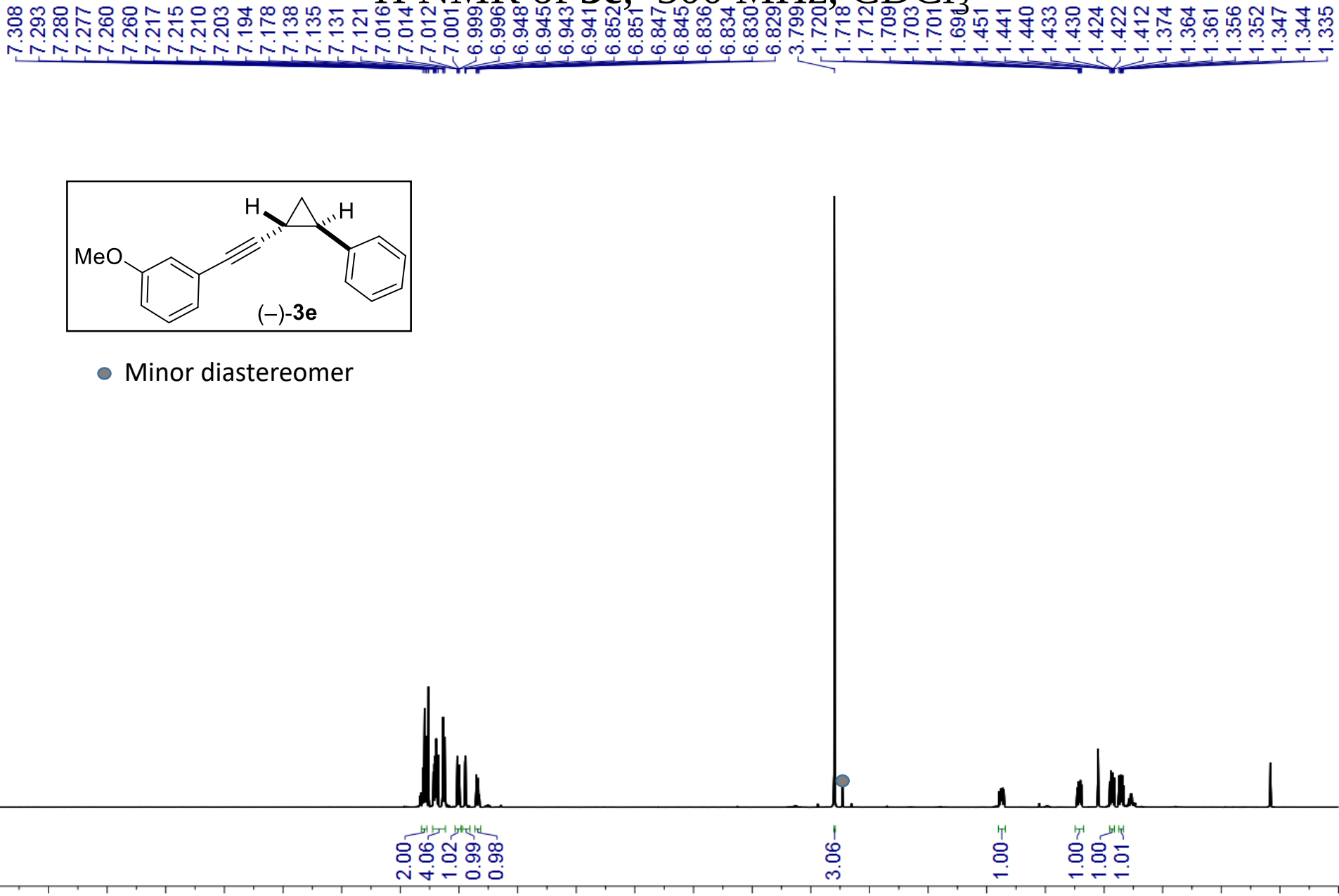


Peak Table

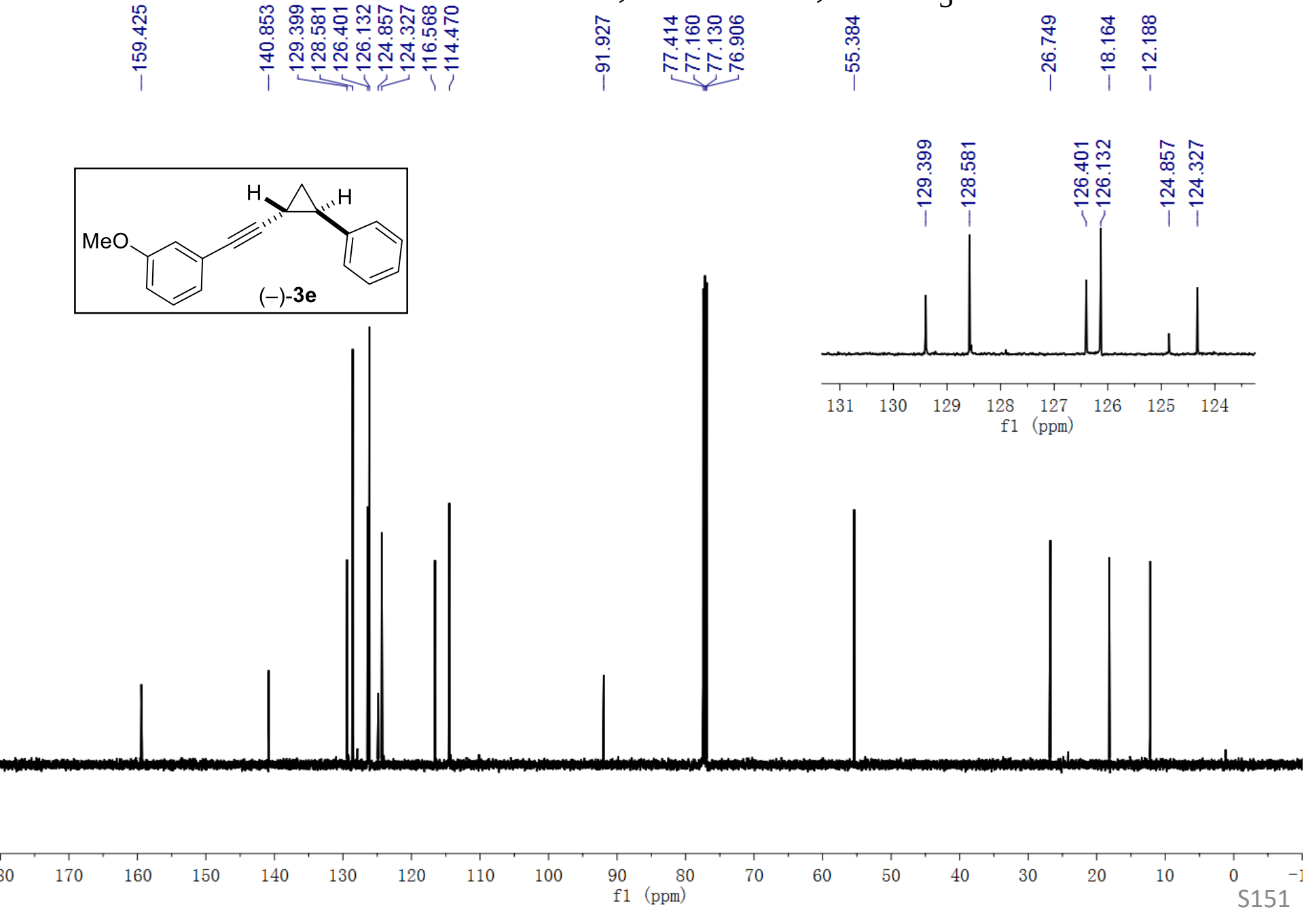
PDA Ch1 254nm

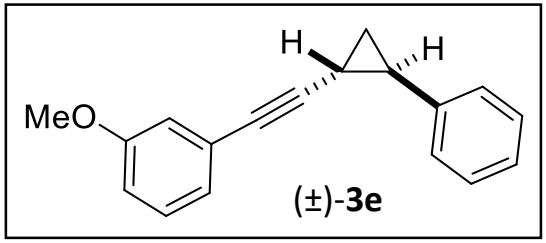
Peak#	Ret. Time	Area	Area%
1	16.792	866540	1.151
2	19.228	74413811	98.849
Total		75280351	100.000

^{1}H NMR of **3e**, 500 MHz, $CDCl_3$



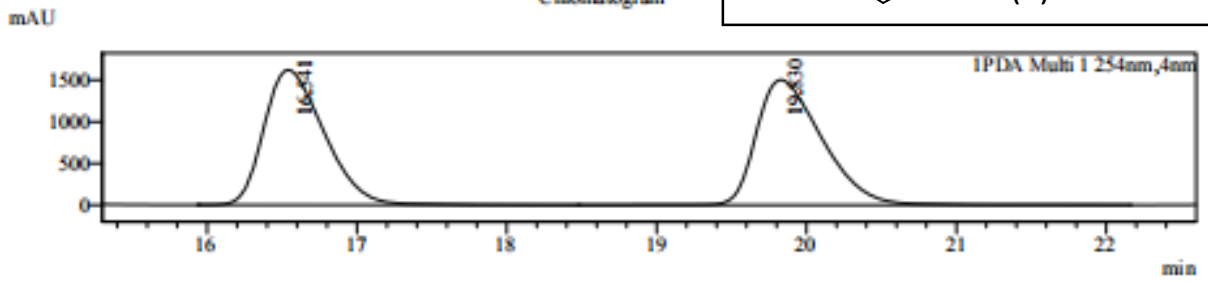
^{13}C NMR of **3e**, 126 MHz, $CDCl_3$



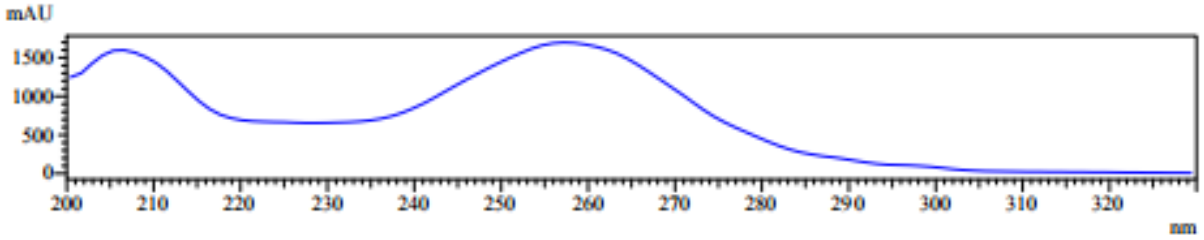


Data File : J0K-0606-IE-0.5%-0.8ML.lcd
Sample Name : J0K-0606-IE-0.5%-0.8ML
Sample ID : J0K-0606-IE-0.5%-0.8ML
Method File : J0K-0.5%--35min-0.8ml.lcm

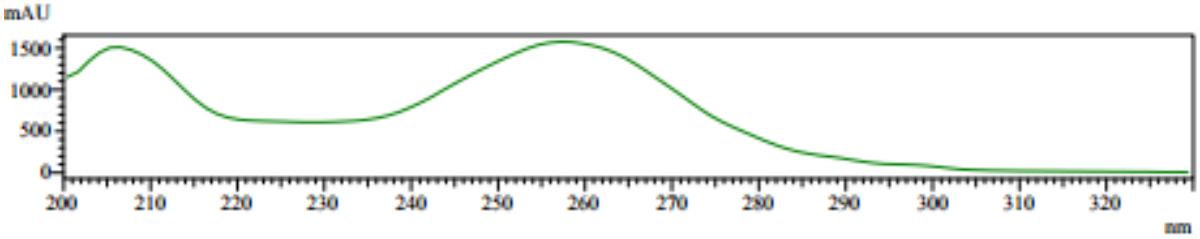
Chromatogram



UV Spectrum
Retention time = 16.541



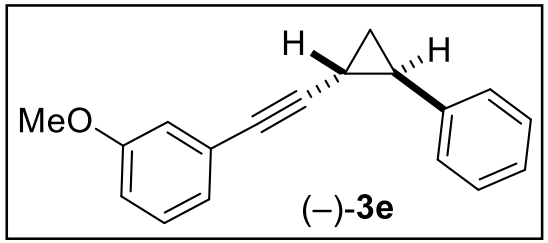
t
Retention time = 19.830



Peak Table

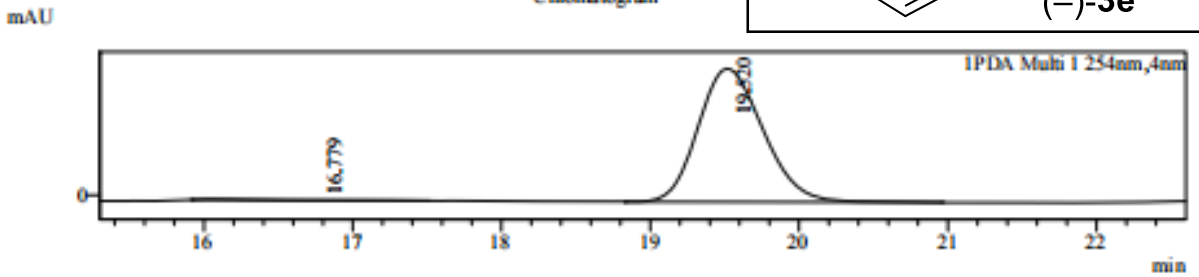
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	16.541	45091963	49.821
2	19.830	45416294	50.179
Total		90508257	100.000

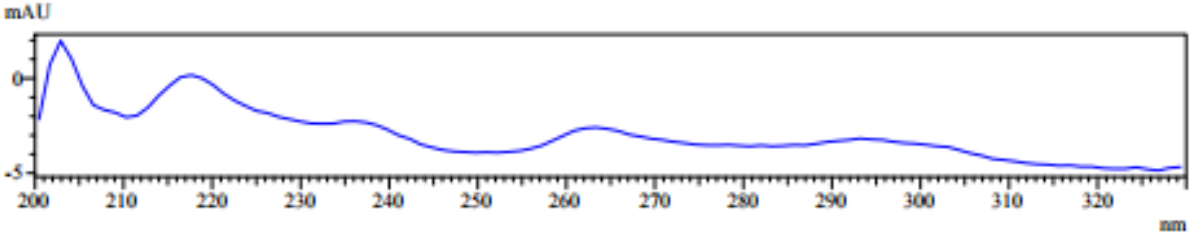


Data File : J0K-0605-IE-2-0.5%-0.8ML.lcd
Sample Name : J0K-0605-IE-2-0.5%-0.8ML
Sample ID : J0K-0605-IE-2-0.5%-0.8ML
Method File : J0K-0.5%--35min-0.8ml.lcm

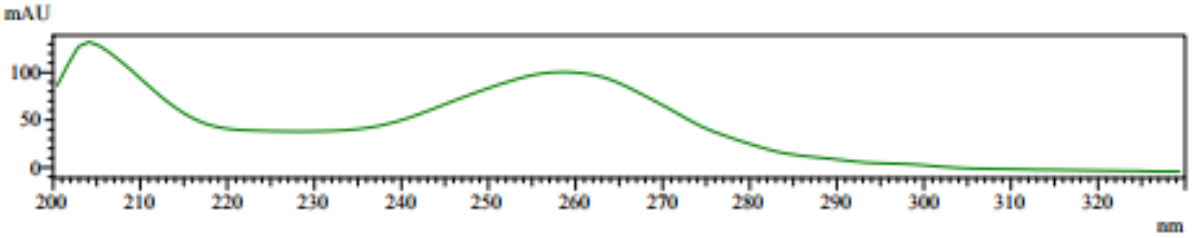
Chromatogram



UV Spectrum
Retention time = 16.779



Retention time = 19.520

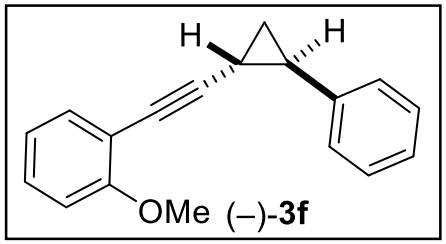


Peak Table

PDA Ch1 254nm

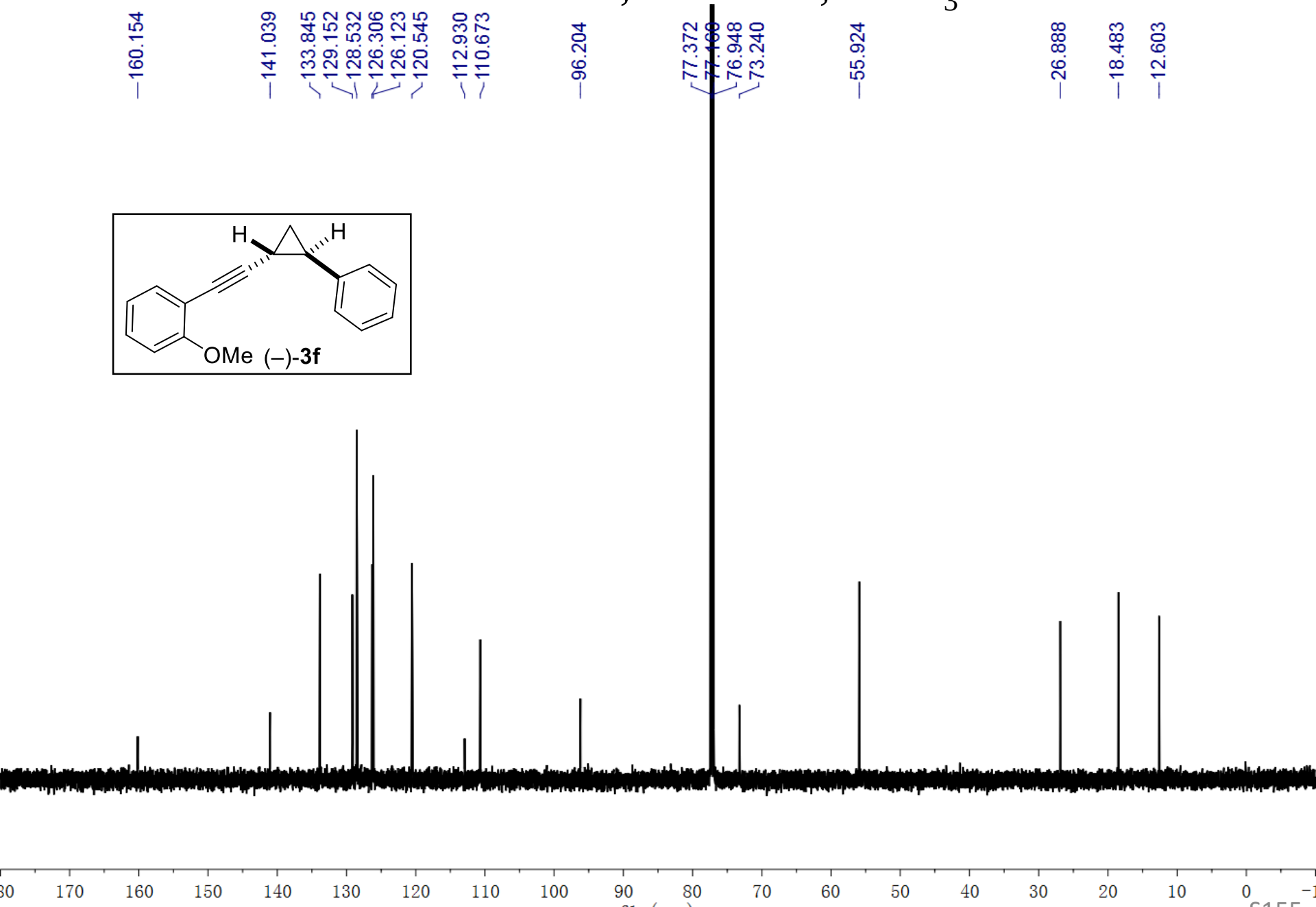
Peak#	Ret. Time	Area	Area%
1	16.779	10536	0.348
2	19.520	3013872	99.652
Total		3024408	100.000

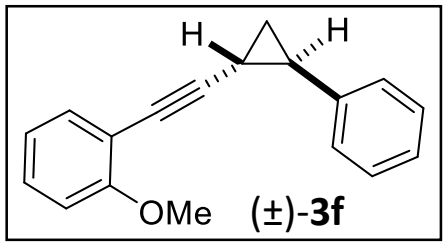
^{1}H NMR of **3f**, 600 MHz, $CDCl_3$



- Minor diastereomer

^{13}C NMR of **3f**, 151 MHz, $CDCl_3$

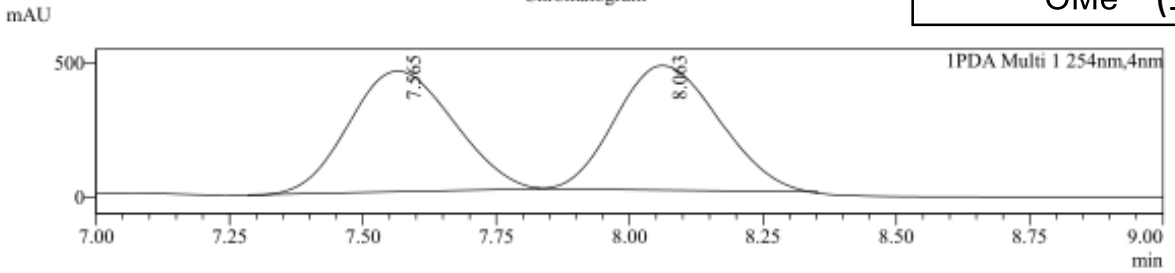




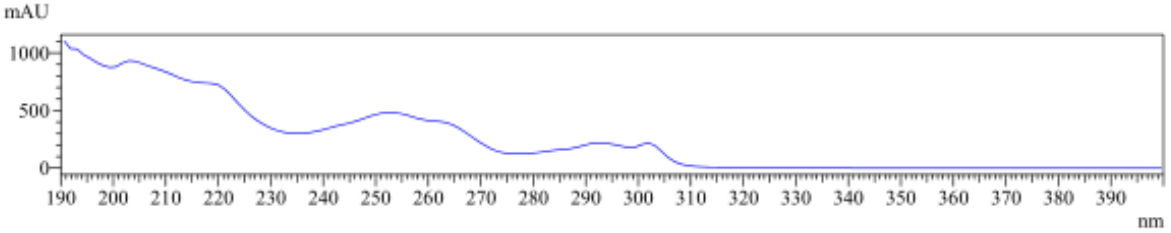
(±)-**3f**

Data File : J0K-0143-IA-1%-0.8ML-isopropanol-solvent005.lcd
Sample Name : J0K-0143-IA-1%-0.8ML-isopropanol-solvent005
Sample ID : J0K-0143-IA-1%-0.8ML-isopropano
Method File : J0K-1%-0.8ml.lcm

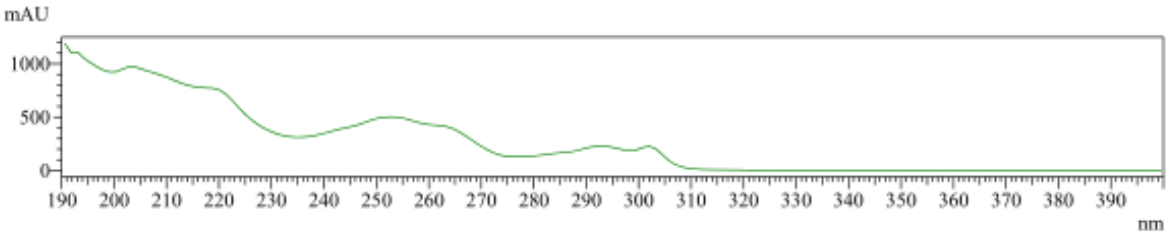
Chromatogram



UV Spectrum
Retention time = 7.565



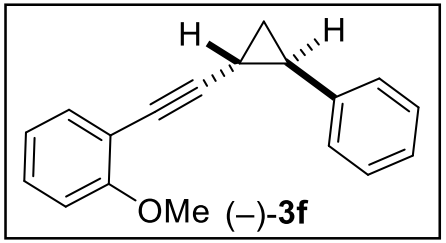
UV Spectrum
Retention time = 8.063



Peak Table

PDA Ch1 254nm

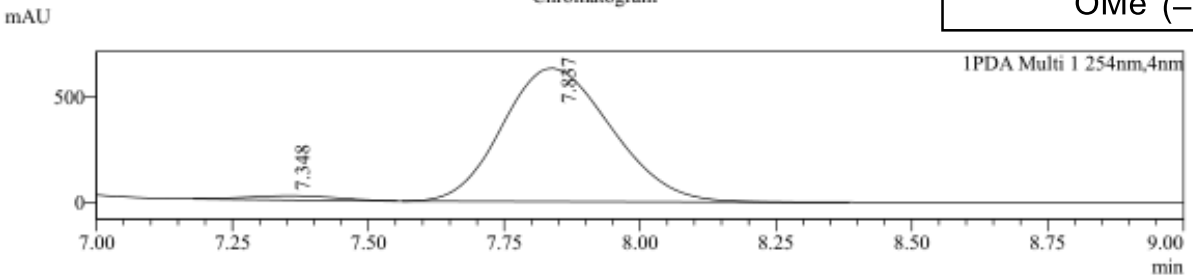
Peak#	Ret. Time	Area	Area%
1	7.565	6121948	49.586
2	8.063	6224168	50.414
Total		12346117	100.000



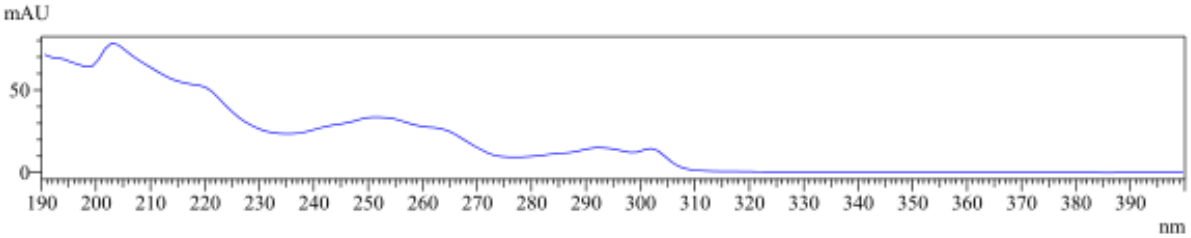
(–)-**3f**

Data File : J0K-0153-IA-6-1%-0.8ML-isopropanol-solvent005.lcd
Sample Name : J0K-0153-IA-6-1%-0.8ML-isopropanol-solvent005
Sample ID : J0K-0153-IA-6-1%-0.8ML-isopropa
Method File : J0K-1%--15min-0.8ml.lcm

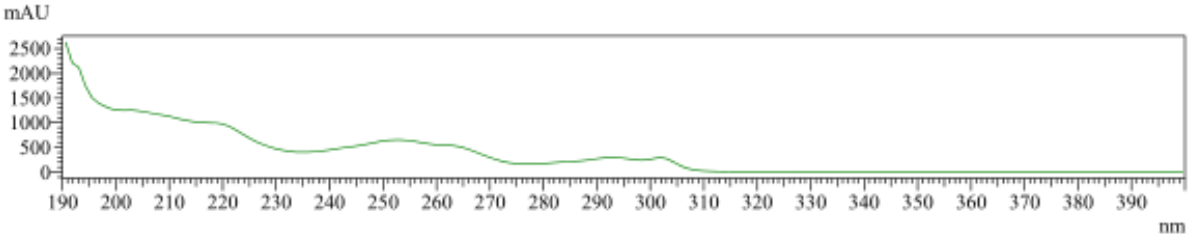
Chromatogram



UV Spectrum
Retention time = 7.348



UV Spectrum
Retention time = 7.837

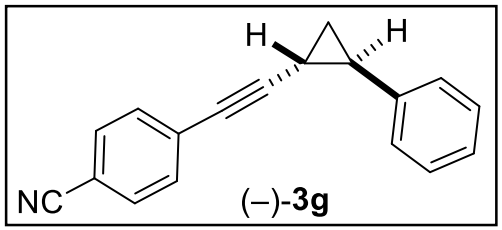


Peak Table

PDA Ch1 254nm

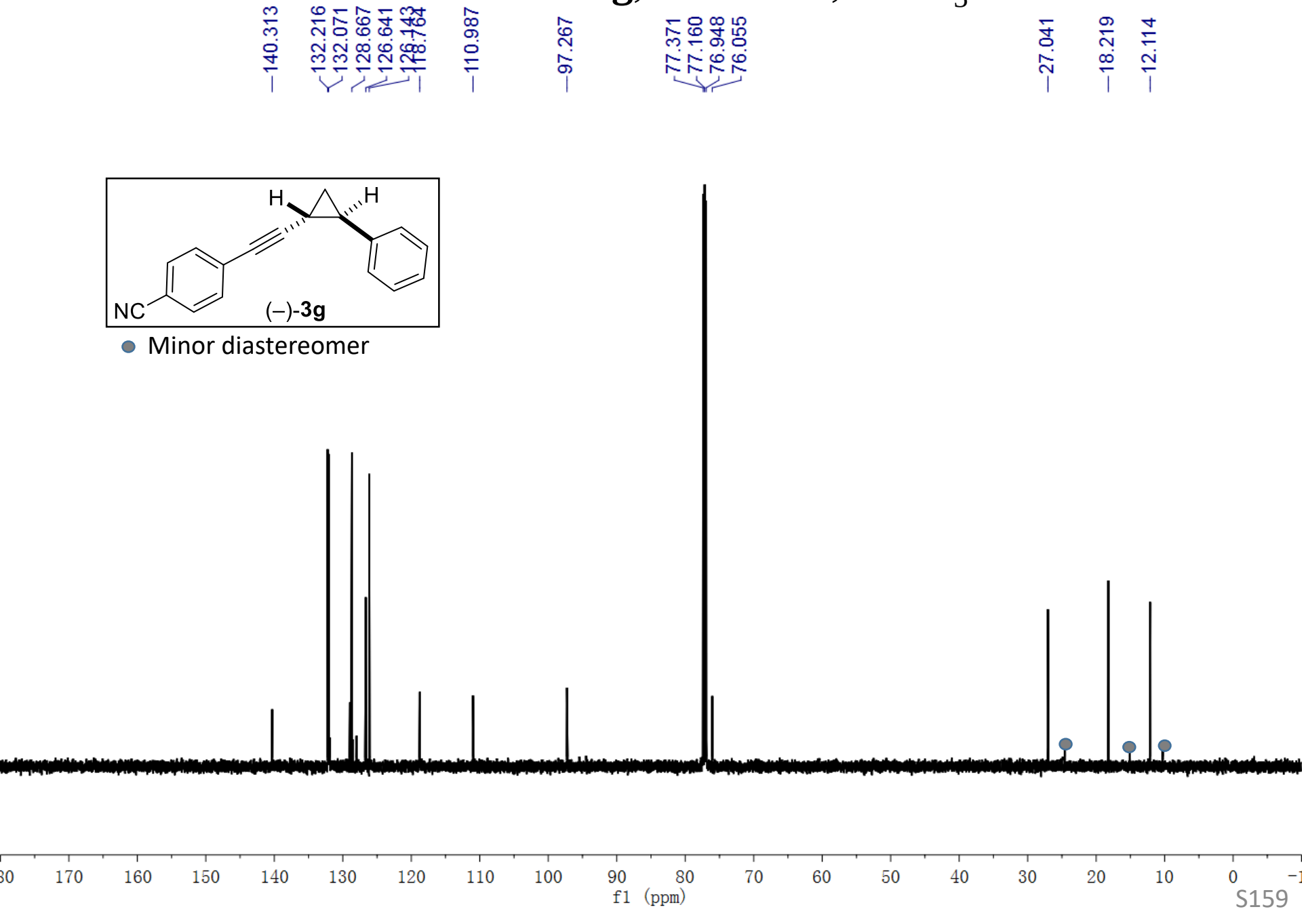
Peak#	Ret. Time	Area	Area%
1	7.348	224745	2.487
2	7.837	8812566	97.513
Total		9037311	100.000

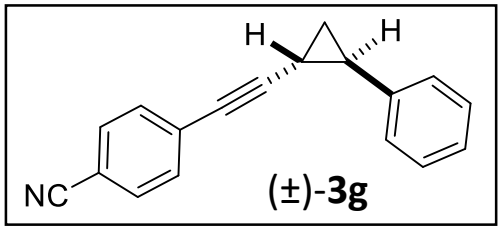
^{1}H NMR of **3g**, 600 MHz, $CDCl_3$



- Minor diastereomer

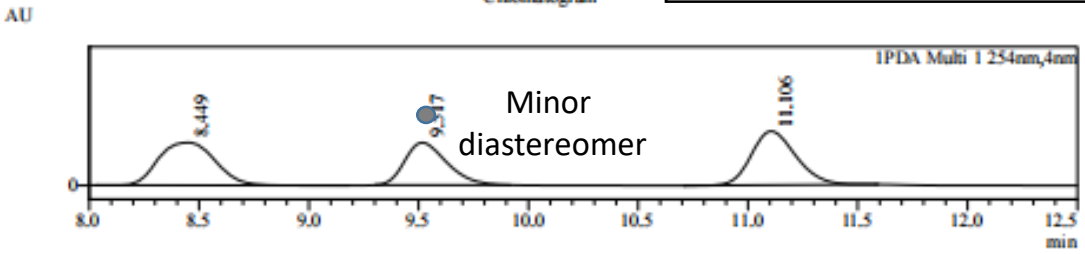
^{13}C NMR of **3g**, 151 MHz, $CDCl_3$



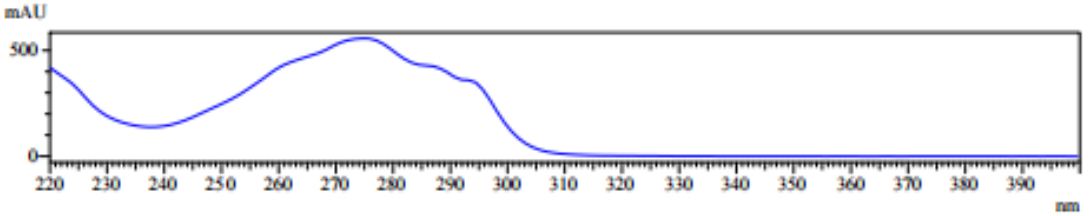


Data File : J0K-1474-IA--0.8%-1ML.lcd
Sample Name : J0K-1474-IA--0.8%-1ML
Sample ID : J0K-1474-IA--0.8%-1ML
Method File : J0K-0.8%-50min-1ml.lcm

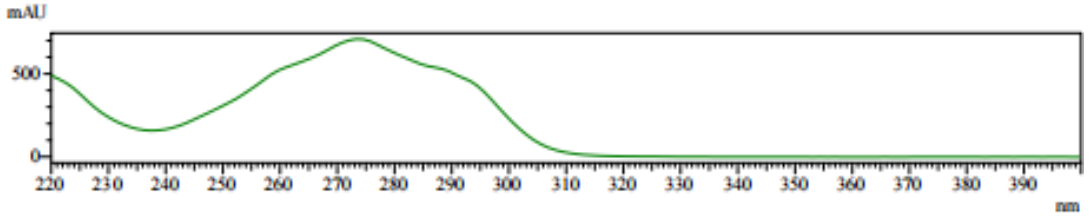
Chromatogram



UV Spectrum
Retention time = 8.449



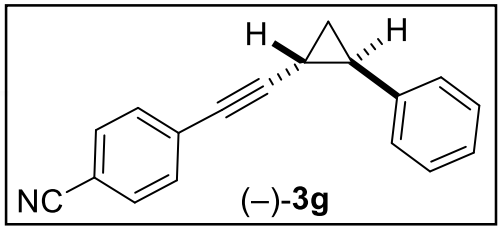
UV Spectrum
Retention time = 11.106



Peak Table

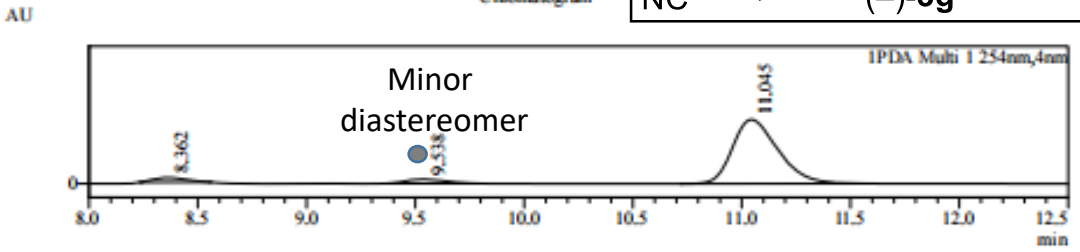
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	8.449	5520988	36.621
2	9.517	4073960	27.023
3	11.106	5480991	36.356
Total		15075939	100.000

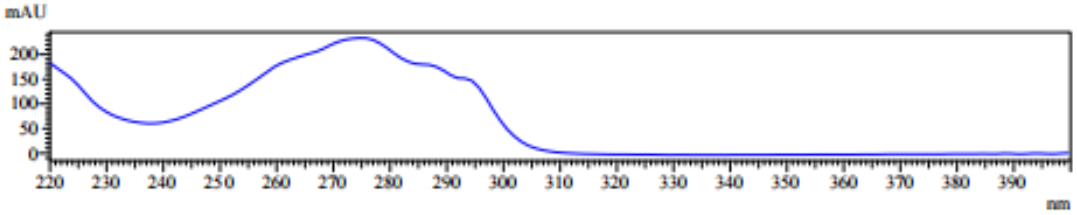


Data File : J0K-1473-IA--0.8%-1ML.lcd
Sample Name : J0K-1473-IA--0.8%-1ML
Sample ID : J0K-1473-IA--0.8%-1ML
Method File : J0K-0.8%-50min-1ml.lcm

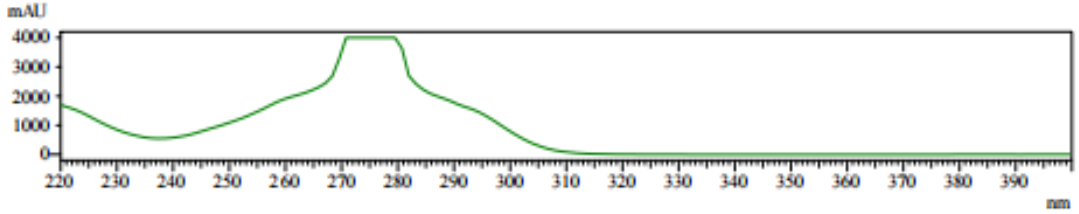
Chromatogram



UV Spectrum
Retention time = 8.362



UV Spectrum
Retention time = 11.045

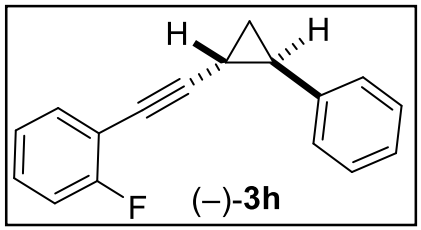


Peak Table

PDA Ch1 254nm

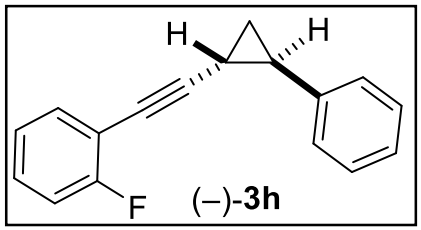
Peak#	Ret. Time	Area	Area%
1	8.362	1045994	4.641
2	9.538	1171121	5.196
3	11.045	20321950	90.163
Total		22539065	100.000

^{1}H NMR of **3h**, 400 MHz, $CDCl_3$



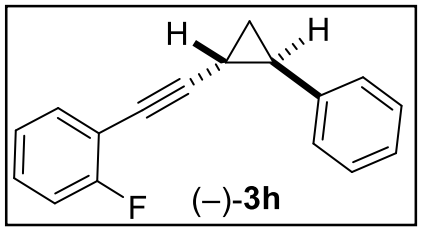
- Minor diastereomer

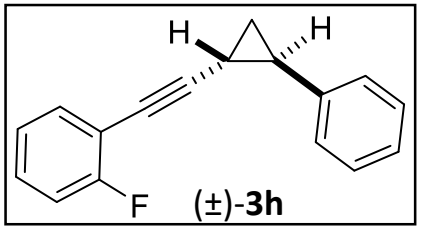
^{13}C NMR of **3h**, 151 MHz, $CDCl_3$



- Minor diastereomer

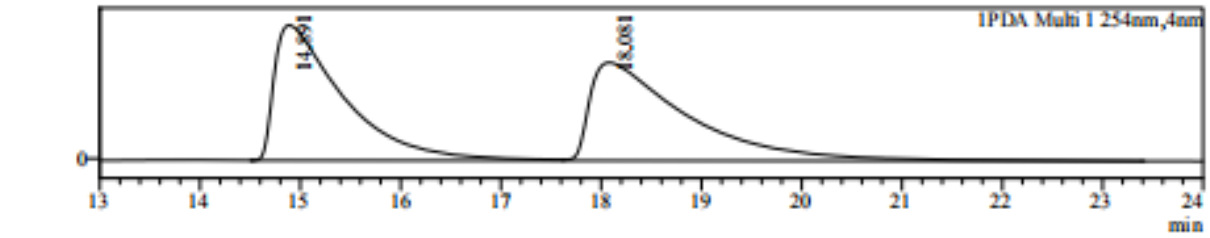
^{19}F NMR of **3h**, 564 MHz, $CDCl_3$



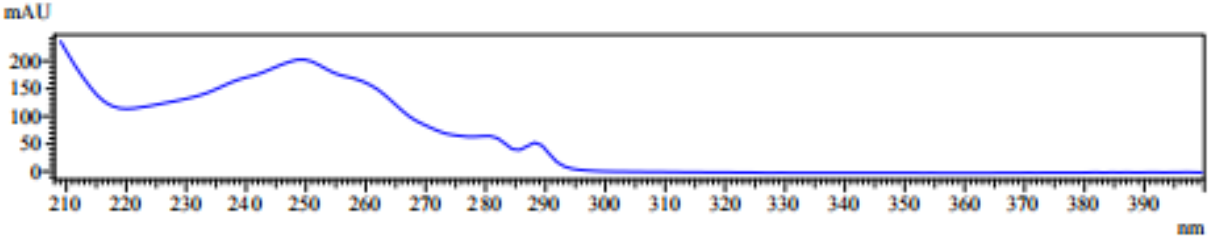


Data File : J0K-0222-4-IC-0%-0.8ML-isopropanol-solvent003.lcd
Sample Name : J0K-0222-4-IC-0%-0.8ML-isopropanol-solvent003
Sample ID : J0K-0222-4-IC-0%-0.8ML-isopropa
Method File : J0K-0%-0.8ml.lcm

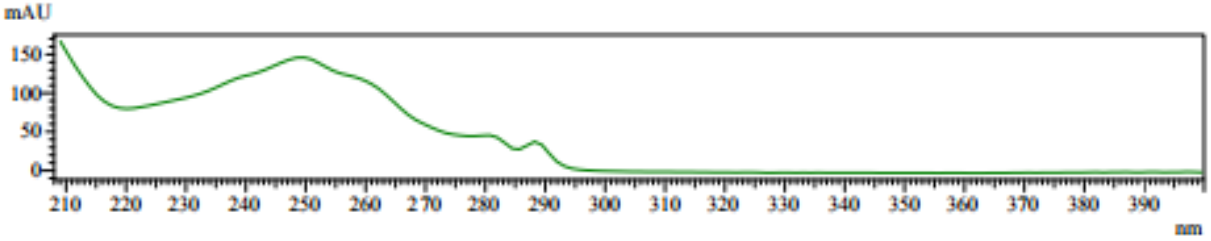
Chromatogram



UV Spectrum
Retention time = 14.891



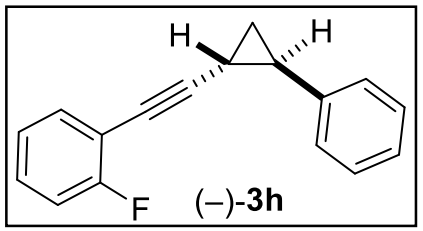
Retention time = 18.081



Peak Table

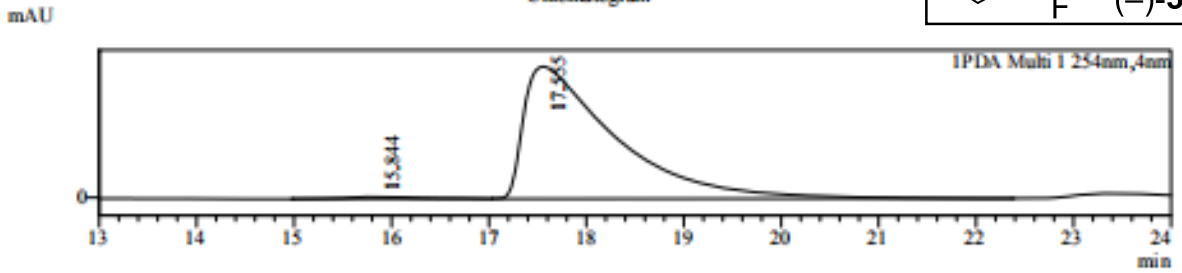
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	14.891	8882879	49.608
2	18.081	9023178	50.392
Total		17906056	100.000

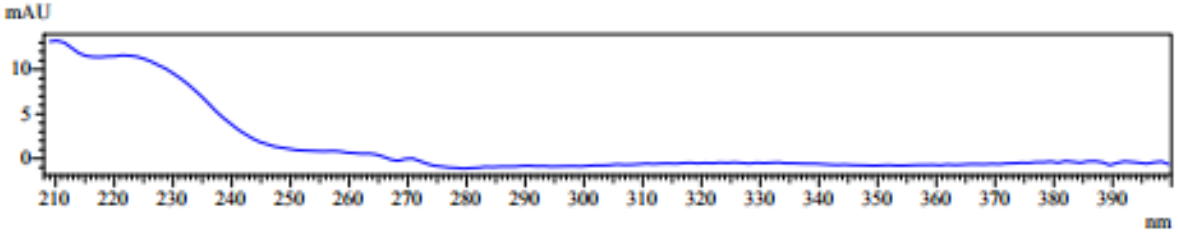


Data File : J0K-0223-4-IC-0%-0.8ML-isopropanol-solvent004.lcd
Sample Name : J0K-0223-4-IC-0%-0.8ML-isopropanol-solvent004
Sample ID : J0K-0223-4-IC-0%-0.8ML-isopropa
Method File : J0K-0%-0.8ml.lcm

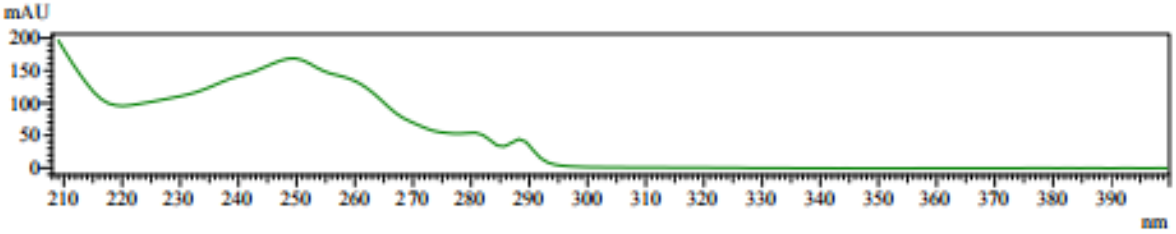
Chromatogram



UV Spectrum
Retention time = 15.844



1
Retention time = 17.555

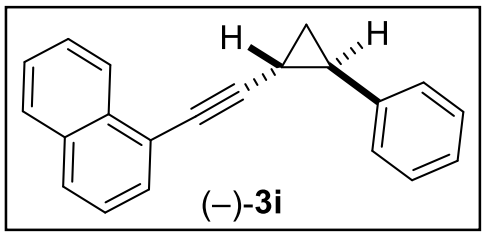


Peak Table

PDA Ch1 254nm

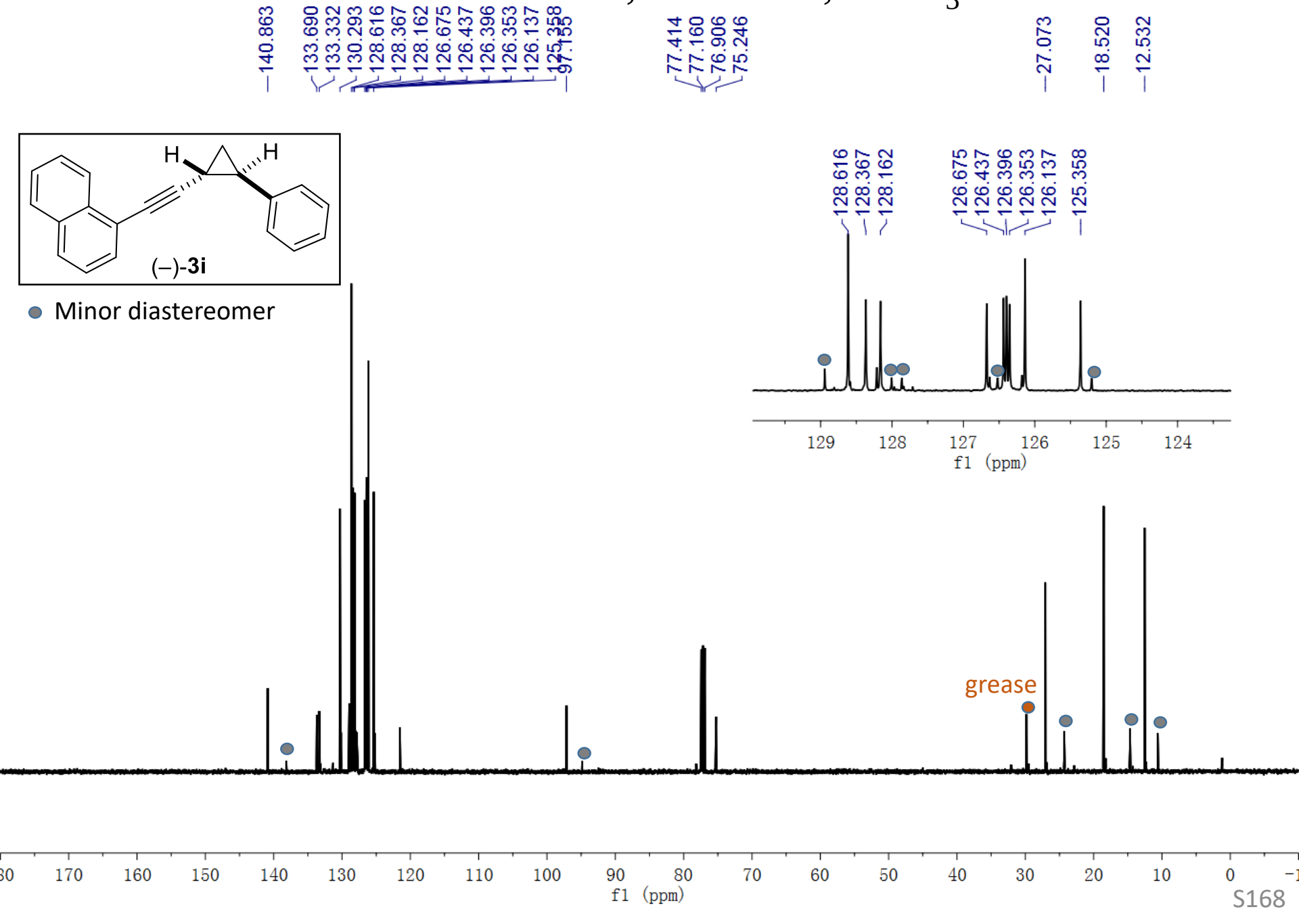
Peak#	Ret. Time	Area	Area%
1	15.844	125202	1.231
2	17.555	10045730	98.769
Total		10170931	100.000

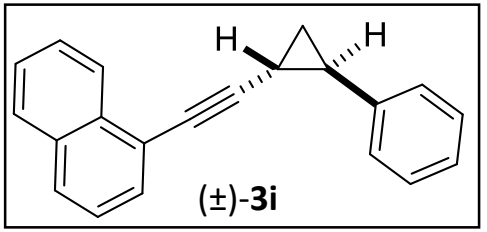
^{1}H NMR of **3i**, 500 MHz, $CDCl_3$



- Minor diastereomer

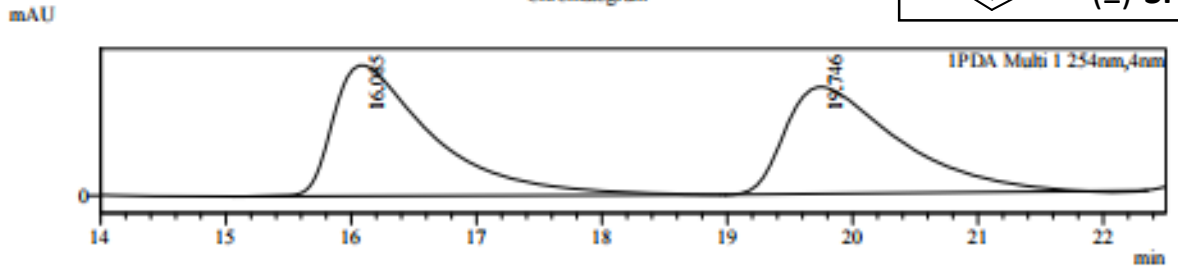
^{13}C NMR of **3i**, 126 MHz, $CDCl_3$



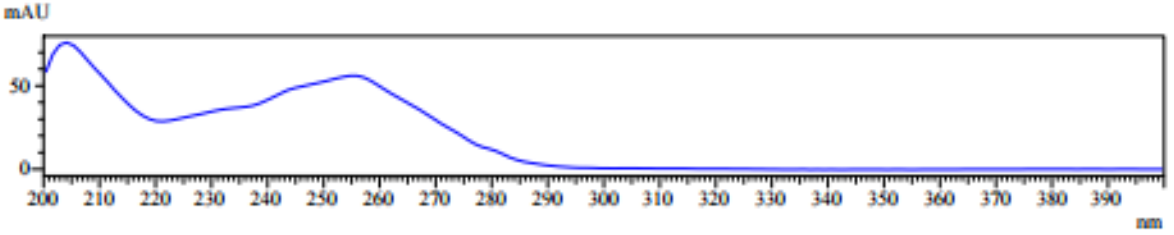


Data File : J0K-0119-IC-0%-0.8ML-isopropanol-solvent004.lcd
Sample Name : J0K-0119-IC-0%-0.8ML-isopropanol-solvent004
Sample ID : J0K-0119-IC-0%-0.8ML-isopropano
Method File : JK-0%-0.8ml.lcm

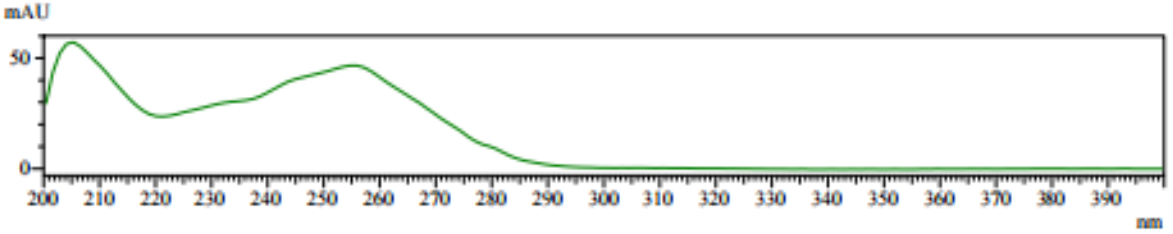
Chromatogram



UV Spectrum
Retention time = 16.085



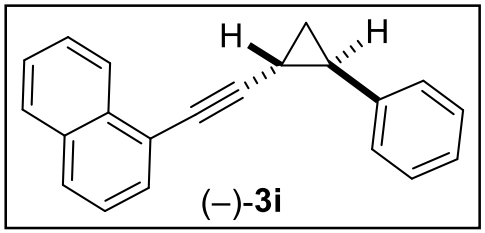
U
Retention time = 19.746



Peak Table

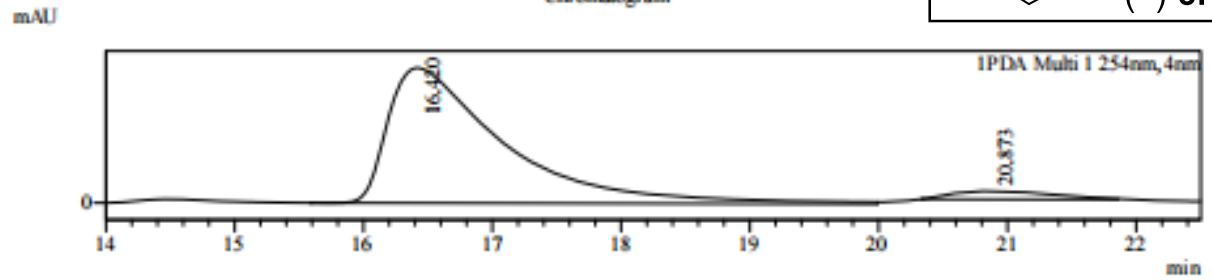
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	16.085	3026512	51.835
2	19.746	2812184	48.165
Total		5838697	100.000

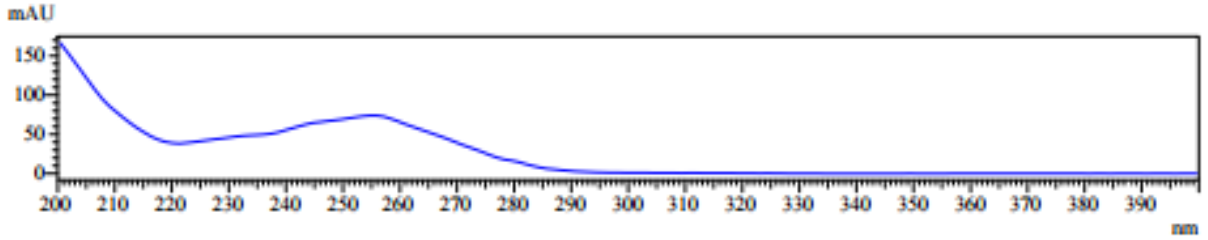


Data File : J0K-0120-IC-0%-0.8ML-isopropanol-solvent005.lcd
Sample Name : J0K-0120-IC-0%-0.8ML-isopropanol-solvent005
Sample ID : J0K-0120-IC-0%-0.8ML-isopropano
Method File : JK-0%-0.8ml.lcm

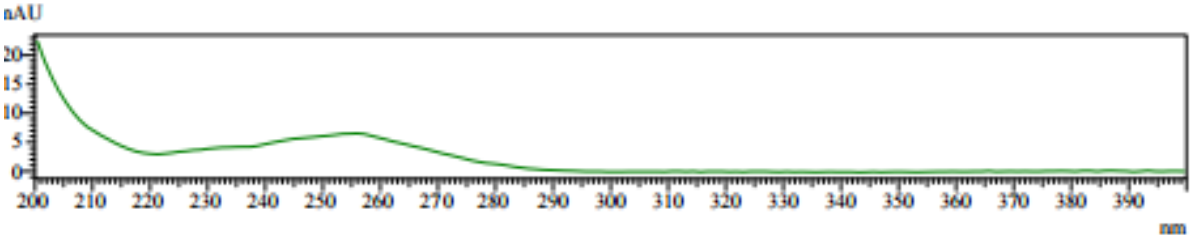
Chromatogram



UV Spectrum
Retention time = 16.420



Retention time = 20.873

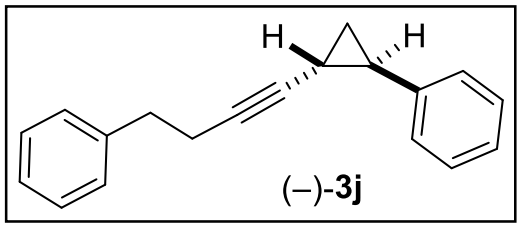


Peak Table

PDA Ch1 254nm

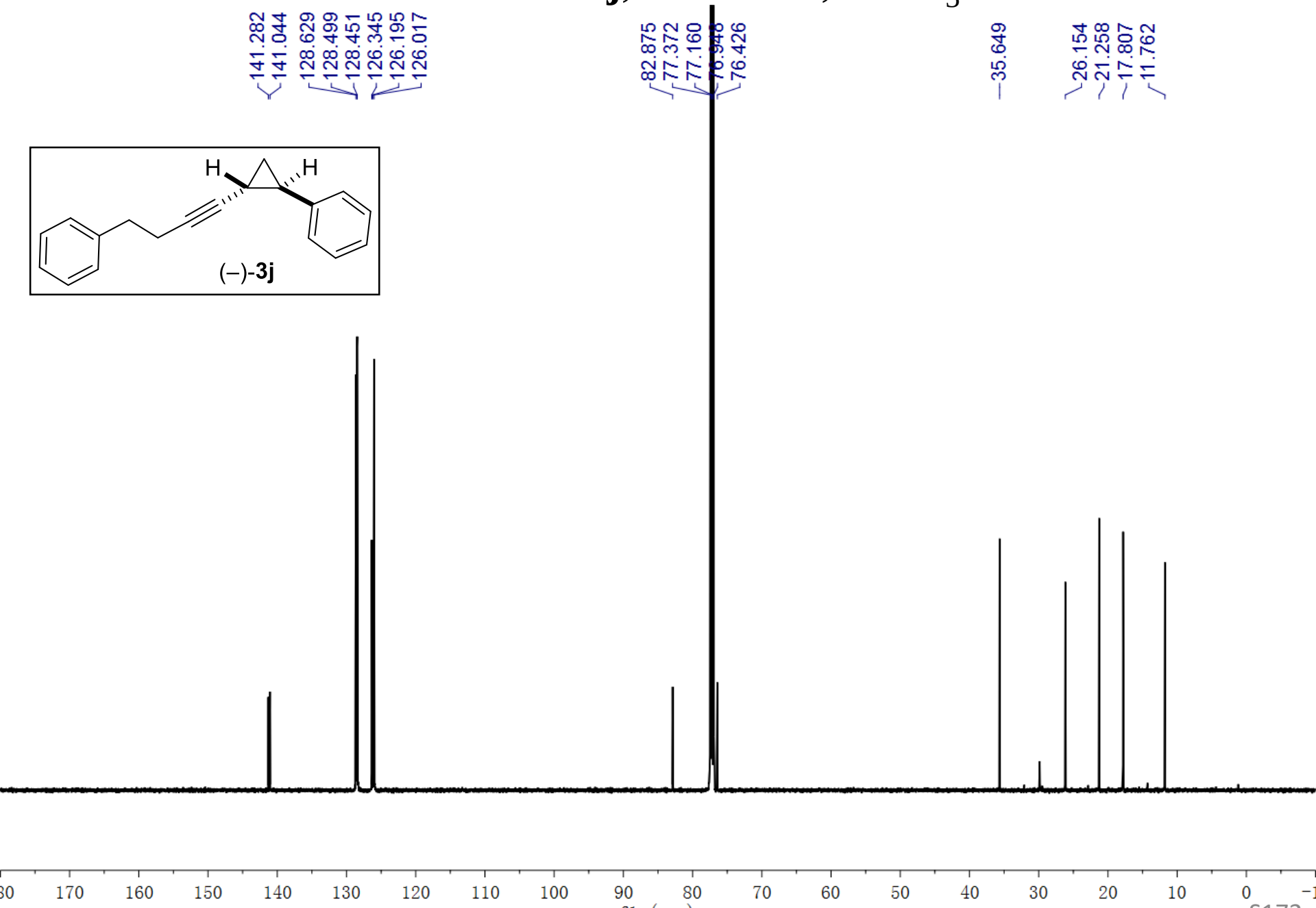
Peak#	Ret. Time	Area	Area%
1	16.420	4527761	95.035
2	20.873	236566	4.965
Total		4764327	100.000

^{1}H NMR of **3j**, 500 MHz, $CDCl_3$



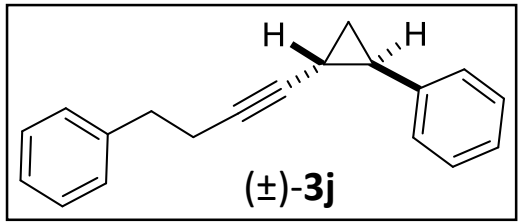
(–)-**3j**

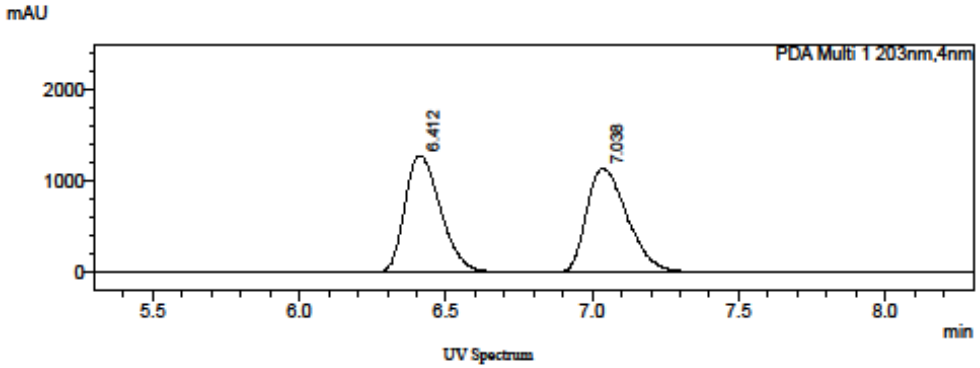
^{13}C NMR of **3j**, 151 MHz, $CDCl_3$



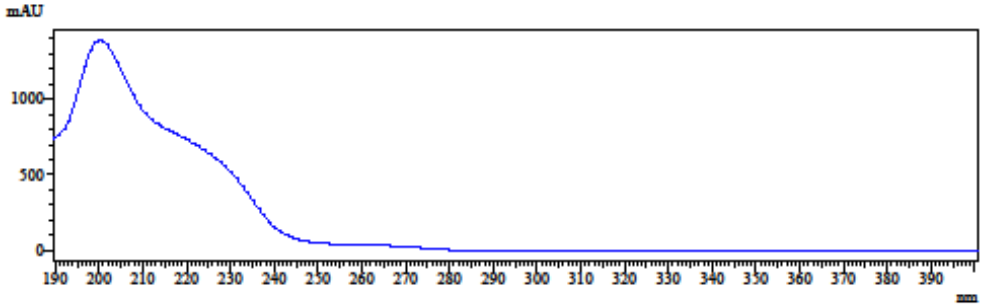
==== Shimadzu LabSolutions Analysis Report ====

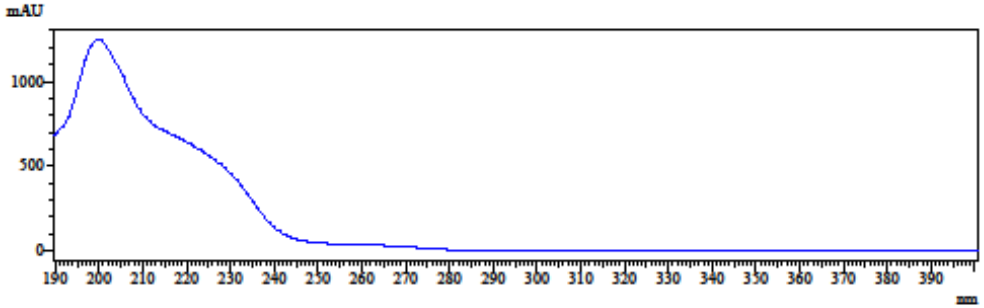
WCL-1844-2-IC-0.1%0.8mL
WCL-0.1%-20min0.8mL.lcm





UV Spectrum



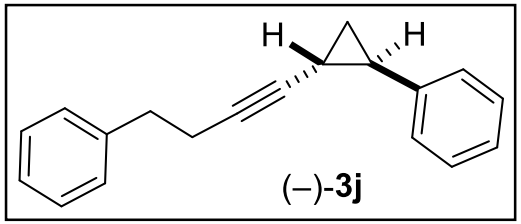


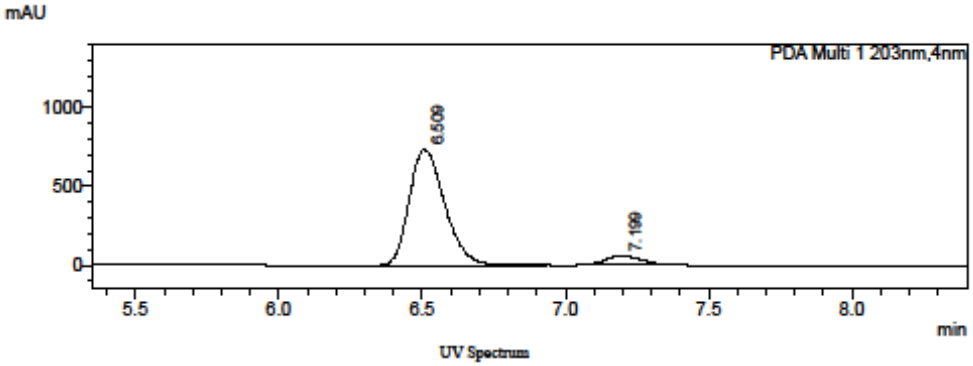
Peak Table
PDA Ch1 203nm

Peak#	Ret. Time	Area%
1	6.412	49.969
2	7.038	50.031
Total		100.000

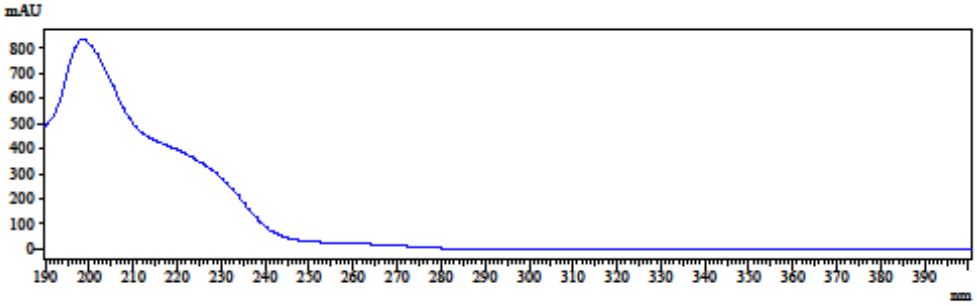
==== Shimadzu LabSolutions Analysis Report ====

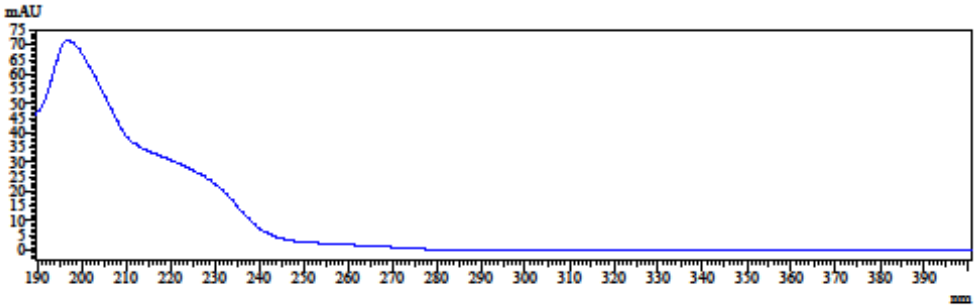
WCL-1845-1-IC-0.1%0.8mL
WCL-0.1%-20min0.8mL.lcm





UV Spectrum



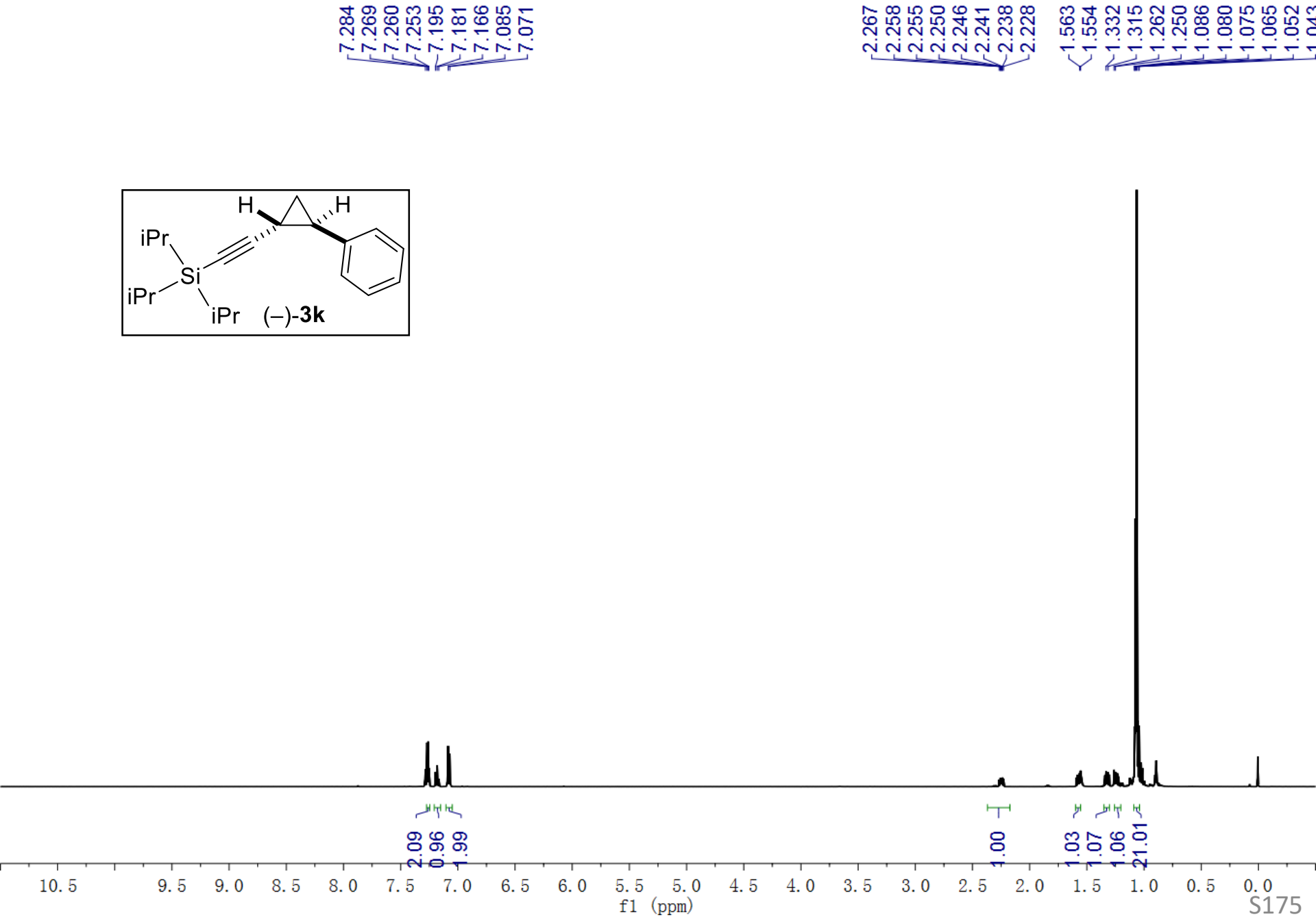


Peak Table

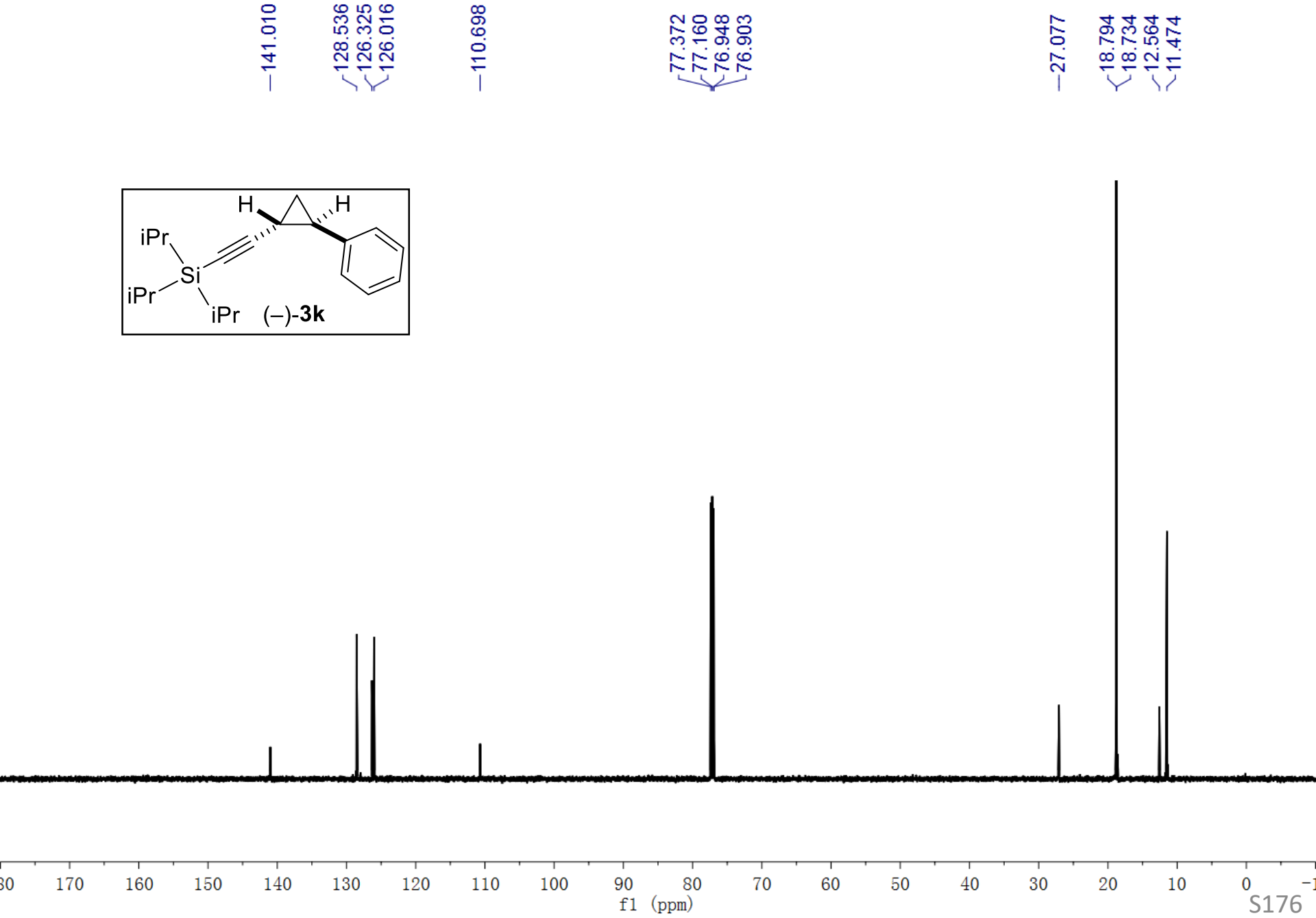
PDA Ch1 203nm

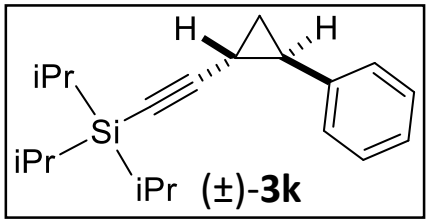
Peak#	Ret. Time	Area%
1	6.509	92.506
2	7.199	7.494
Total		100.000

^{1}H NMR of **3k**, 600 MHz, $CDCl_3$



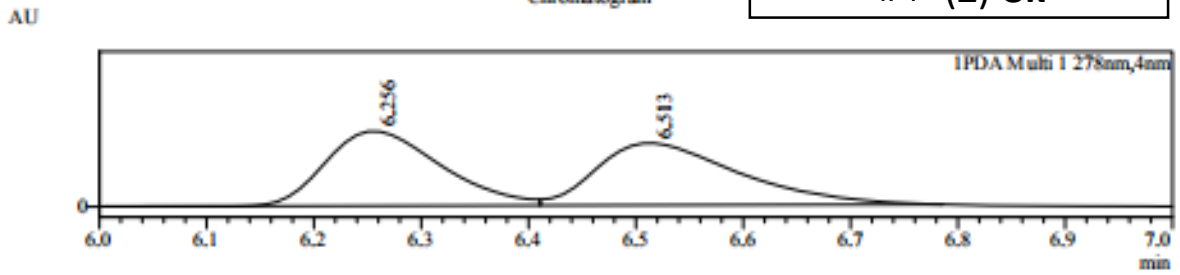
^{13}C NMR of **3j**, 151 MHz, $CDCl_3$



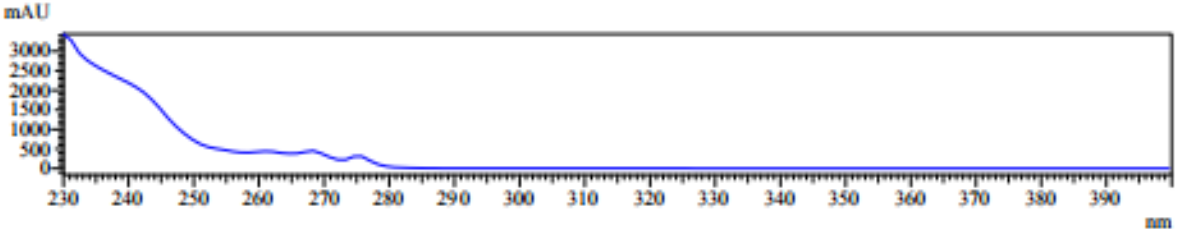


Data File : J0K-1401-IC-0%-0.8ML001.lcd
Sample Name : J0K-1401-IC-0%-0.8ML
Sample ID : J0K-1401-IC-0%-0.8ML
Method File : J0K-0%--25min-0.6ml.lcm

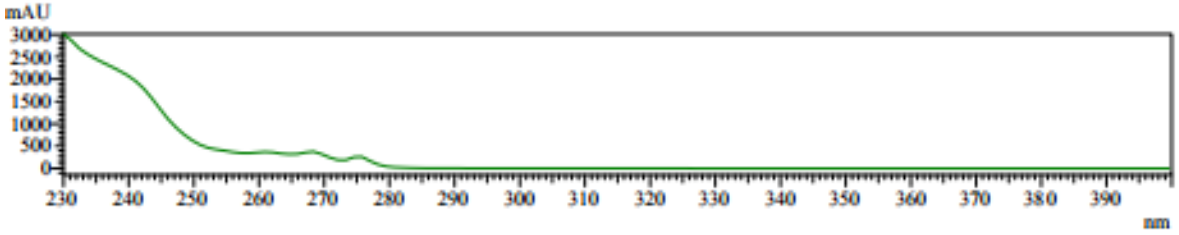
Chromatogram



UV Spectrum
Retention time = 6.256



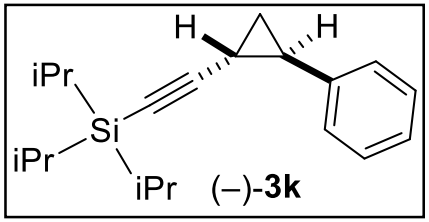
l.
Retention time = 6.513



Peak Table

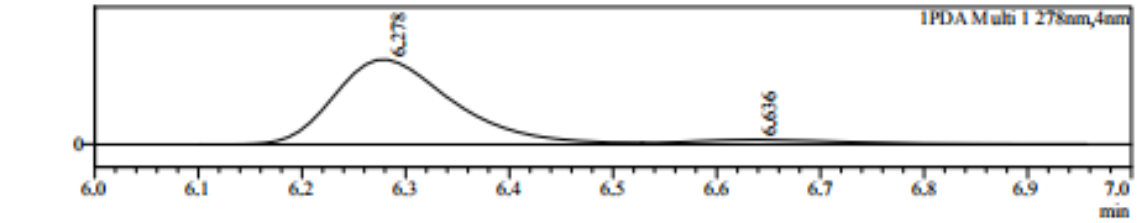
PDA Ch1 278nm

Peak#	Ret. Time	Area	Area%
1	6.256	1083124	49.482
2	6.513	1105802	50.518
Total		2188926	100.000

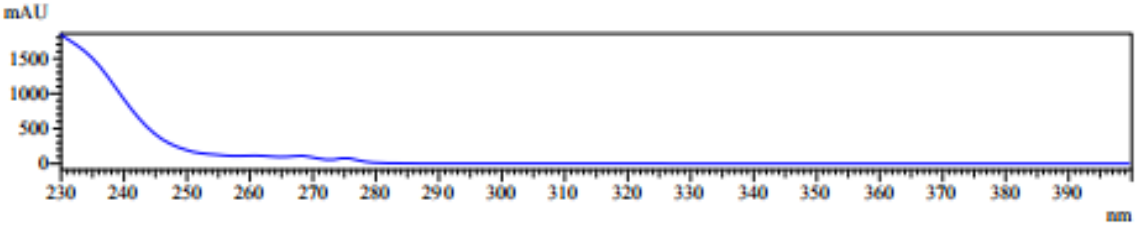


Data File : J0K-1402-IC-0%-0.8ML-3.lcd
Sample Name : J0K-1402-IC-0%-0.8ML-3
Sample ID : J0K-1402-IC-0%-0.8ML-3
Method File : J0K-0%--25min-0.6ml.lcm

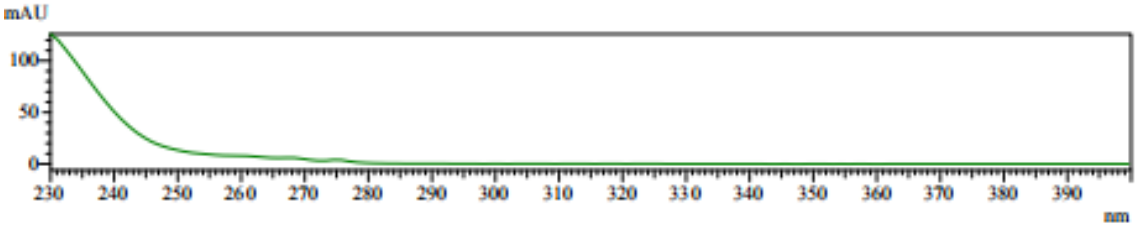
Chromatogram



UV Spectrum
Retention time = 6.278



Retention time = 6.636

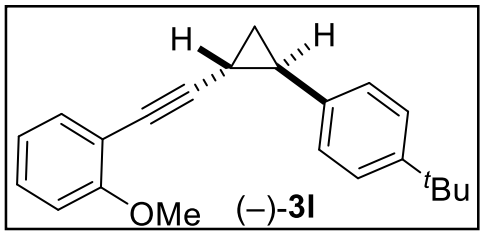


Peak Table

PDA Ch1 278nm

Peak#	Ret. Time	Area	Area%
1	6.278	296817	93.309
2	6.636	21284	6.691
Total		318101	100.000

^{1}H NMR of **3l**, 600 MHz, $CDCl_3$



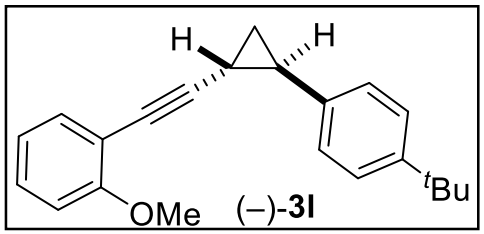
Minor diastereomer

water

f1 (ppm)

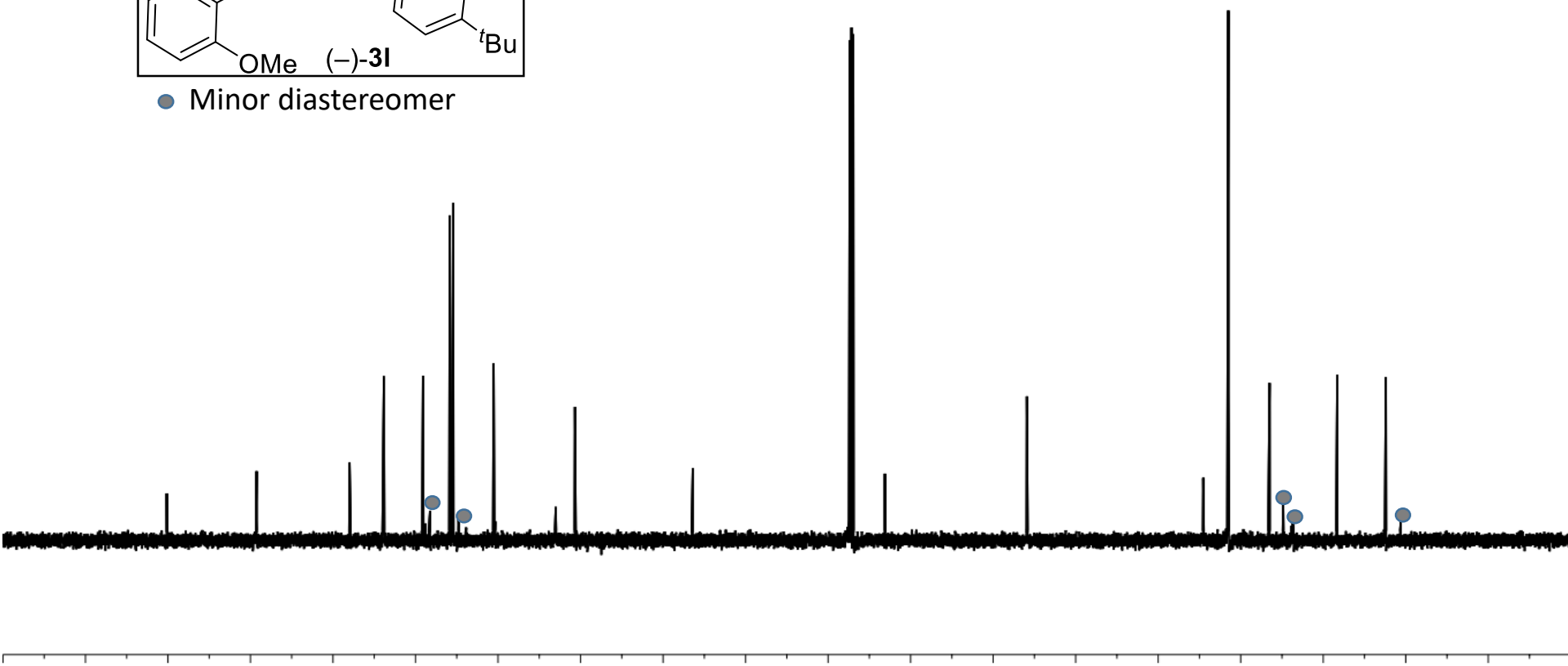
^{13}C NMR of **3l**, 151 MHz, $CDCl_3$

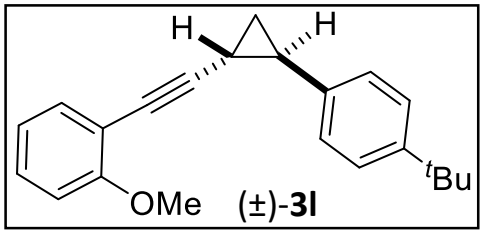
160.142
149.259
137.986
133.826
129.087
125.850
125.439
120.527
113.006
110.671
96.401
77.372
77.160
76.948
73.114
55.910
34.543
31.503
26.496
18.301
12.416



(–)-**3l**

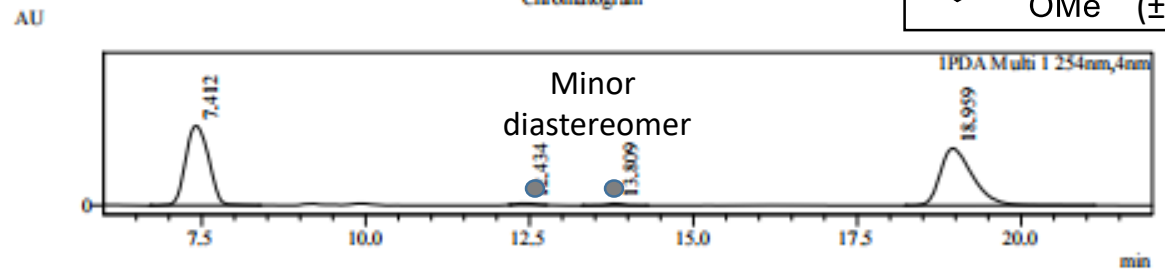
● Minor diastereomer



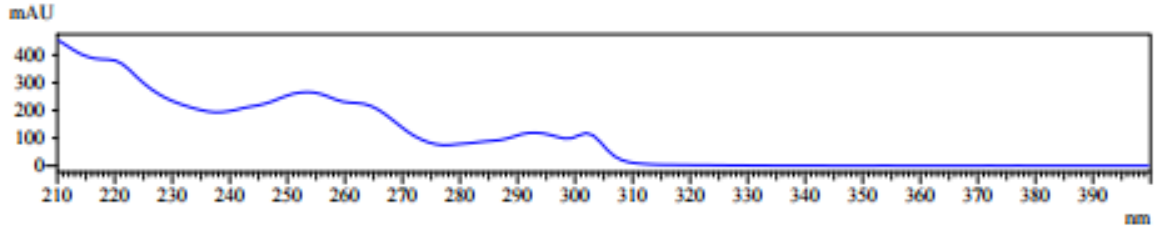


Data File : J0K-0169-2-IC-1%-0.8ML-isopropanol-solvent003.lcd
Sample Name : J0K-0169-2-IC-1%-0.8ML-isopropanol-solvent003
Sample ID : J0K-0169-2-IC-1%-0.8ML-isopropa
Method File : J0K-1%-0.8ml.lcm

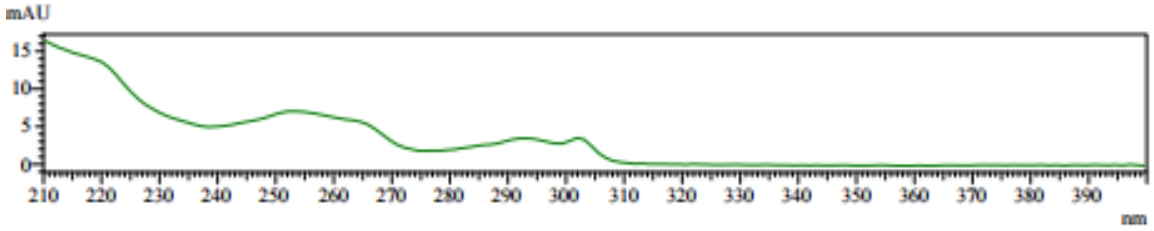
Chromatogram



UV Spectrum
Retention time = 7.412



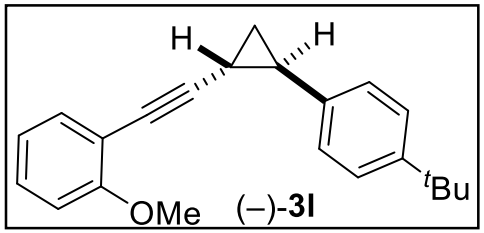
U
Retention time = 12.434



Peak Table

PDA Ch1 254nm

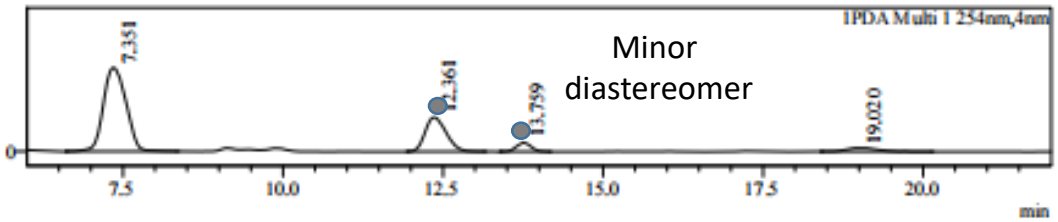
Peak#	Ret. Time	Area	Area%
1	7.412	6343268	49.007
2	12.434	99943	0.772
3	13.809	101856	0.787
4	18.959	6398503	49.434
Total		12943570	100.000



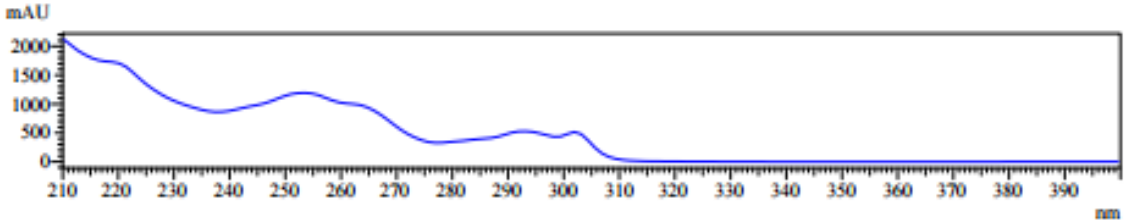
Data File : J0K-0170-IC-1%-0.8ML-isopropanol-solvent003.lcd
Sample Name : J0K-0170-IC-1%-0.8ML-isopropanol-solvent003
Sample ID : J0K-0170-IC-1%-0.8ML-isopropano
Method File : J0K-1%-0.8ml.lcm

Chromatogram

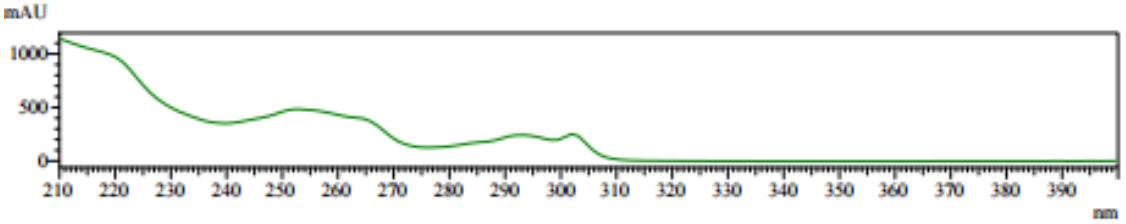
AU



UV Spectrum
Retention time = 7.351



U
Retention time = 12.361

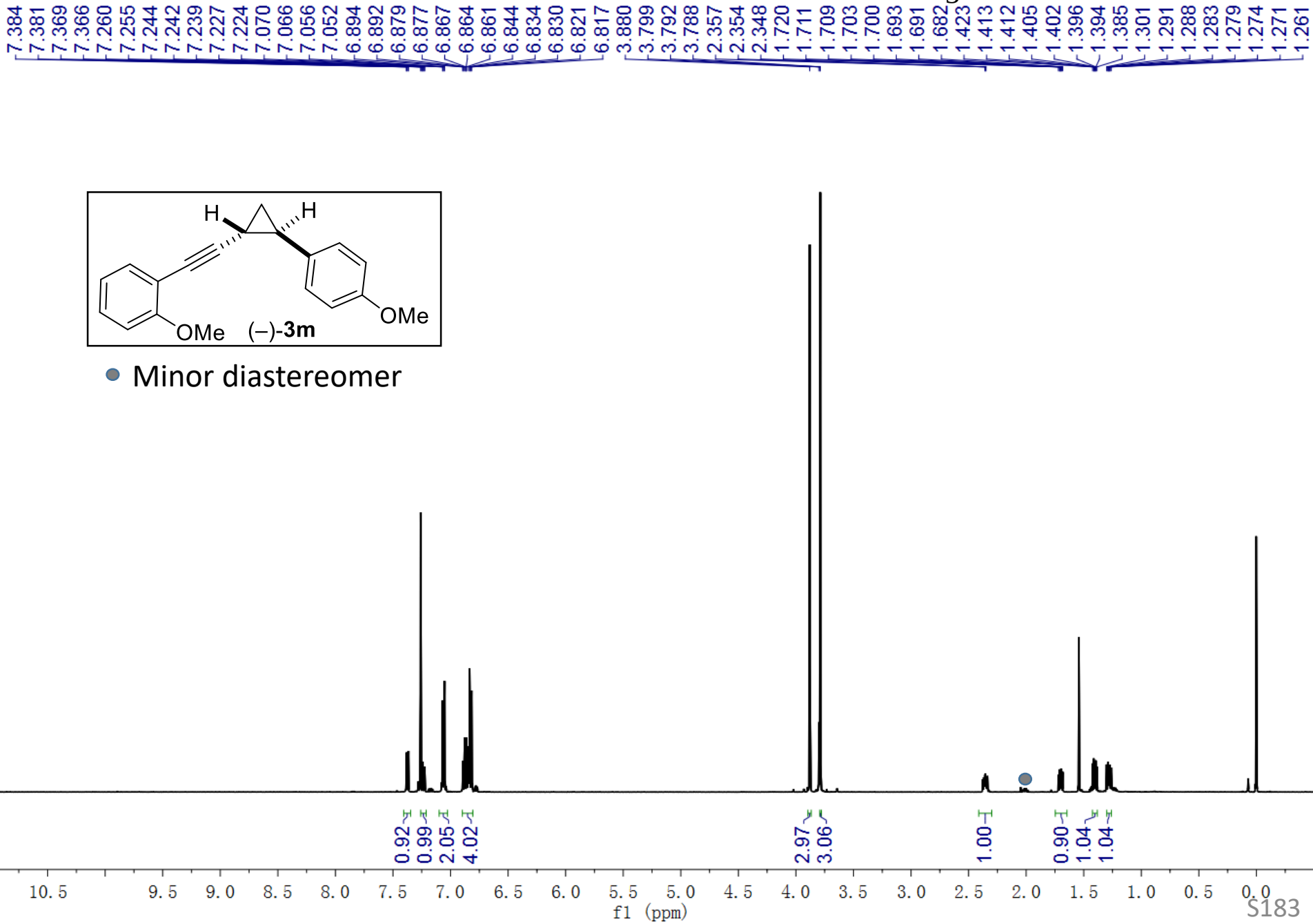


Peak Table

PDA Ch1 254nm

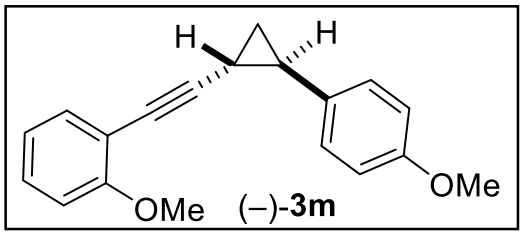
Peak#	Ret. Time	Area	Area%
1	7.351	28725643	66.428
2	12.361	10836399	25.059
3	13.759	1966955	4.549
4	19.020	1714331	3.964
Total		43243327	100.000

^{1}H NMR of **3m**, 500 MHz, $CDCl_3$

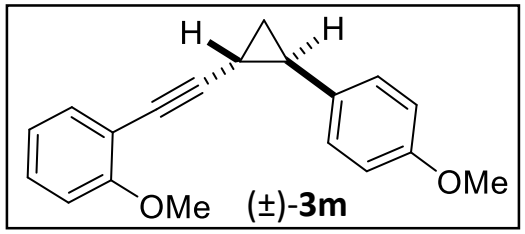


- Minor diastereomer

^{13}C NMR of **3m**, 126 MHz, $CDCl_3$

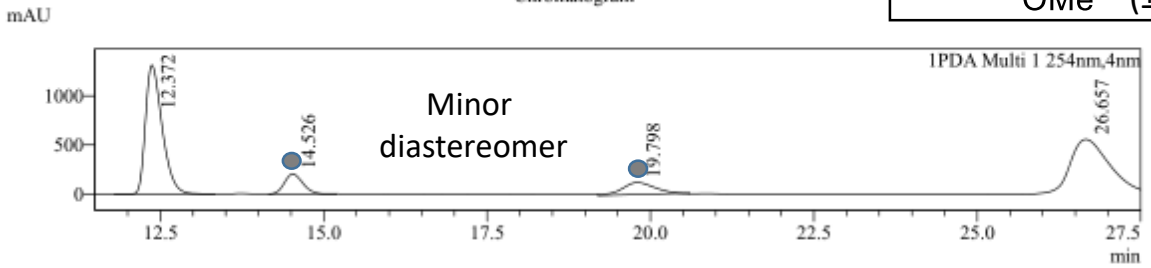


- Minor diastereomer

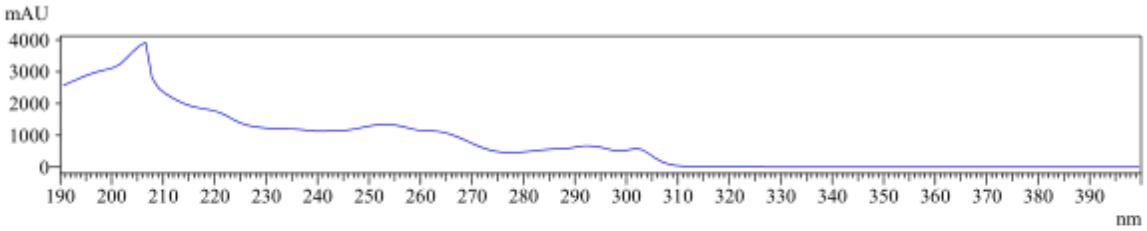


Data File : J0K-0171-IC-2%-0.8ML-isopropanol-solvent004.lcd
Sample Name : J0K-0171-IC-2%-0.8ML-isopropanol-solvent004
Sample ID : J0K-0171-IC-2%-0.8ML-isopropano
Method File : J0K-2%-0.8ml.lcm

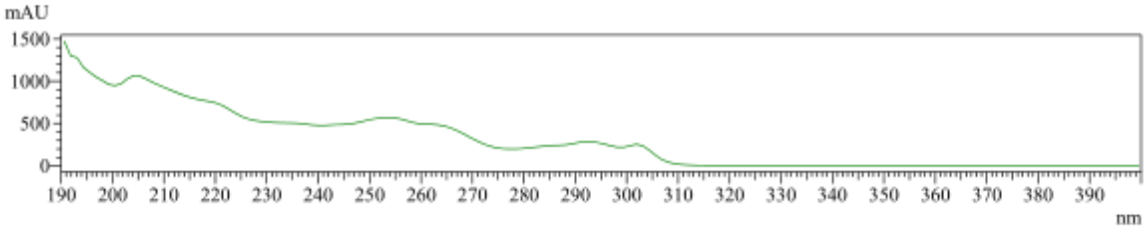
Chromatogram



UV Spectrum
Retention time = 12.372



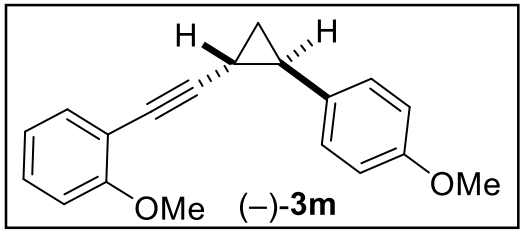
UV Spectrum
Retention time = 26.657



Peak Table

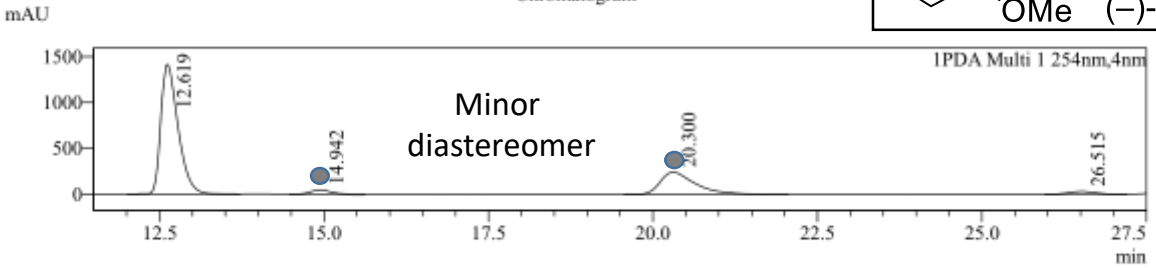
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	12.372	23278478	41.919
2	14.526	4205933	7.574
3	19.798	4184760	7.536
4	26.657	23862693	42.971
Total		55531864	100.000

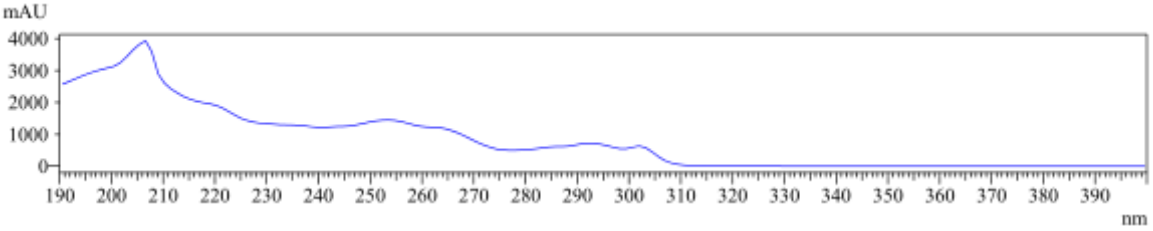


Data File : J0K-0172-IC-2%-0.8ML-isopropanol-solvent004.lcd
Sample Name : J0K-0172-IC-2%-0.8ML-isopropanol-solvent004
Sample ID : J0K-0172-IC-2%-0.8ML-isopropano
Method File : J0K-2%-0.8ml.lcm

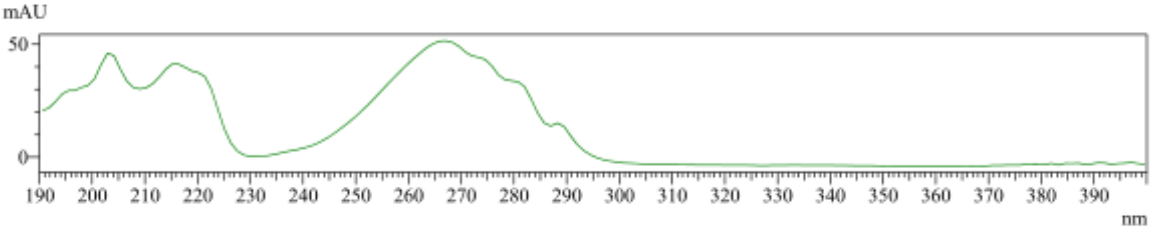
Chromatogram



UV Spectrum
Retention time = 12.619



UV Spectrum
Retention time = 26.515

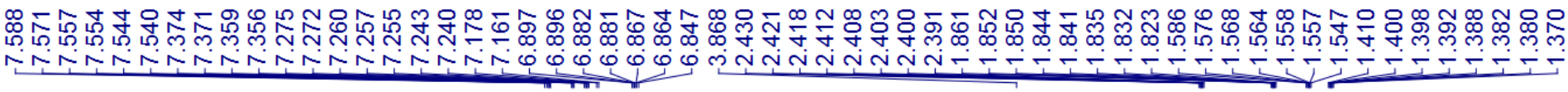


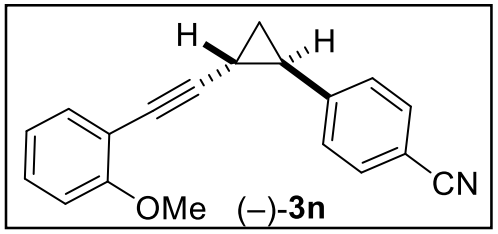
Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	12.619	25840960	70.332
2	14.942	1295076	3.525
3	20.300	8808180	23.973
4	26.515	797214	2.170
Total		36741431	100.000

^{1}H NMR of **3n**, 600 MHz, $CDCl_3$

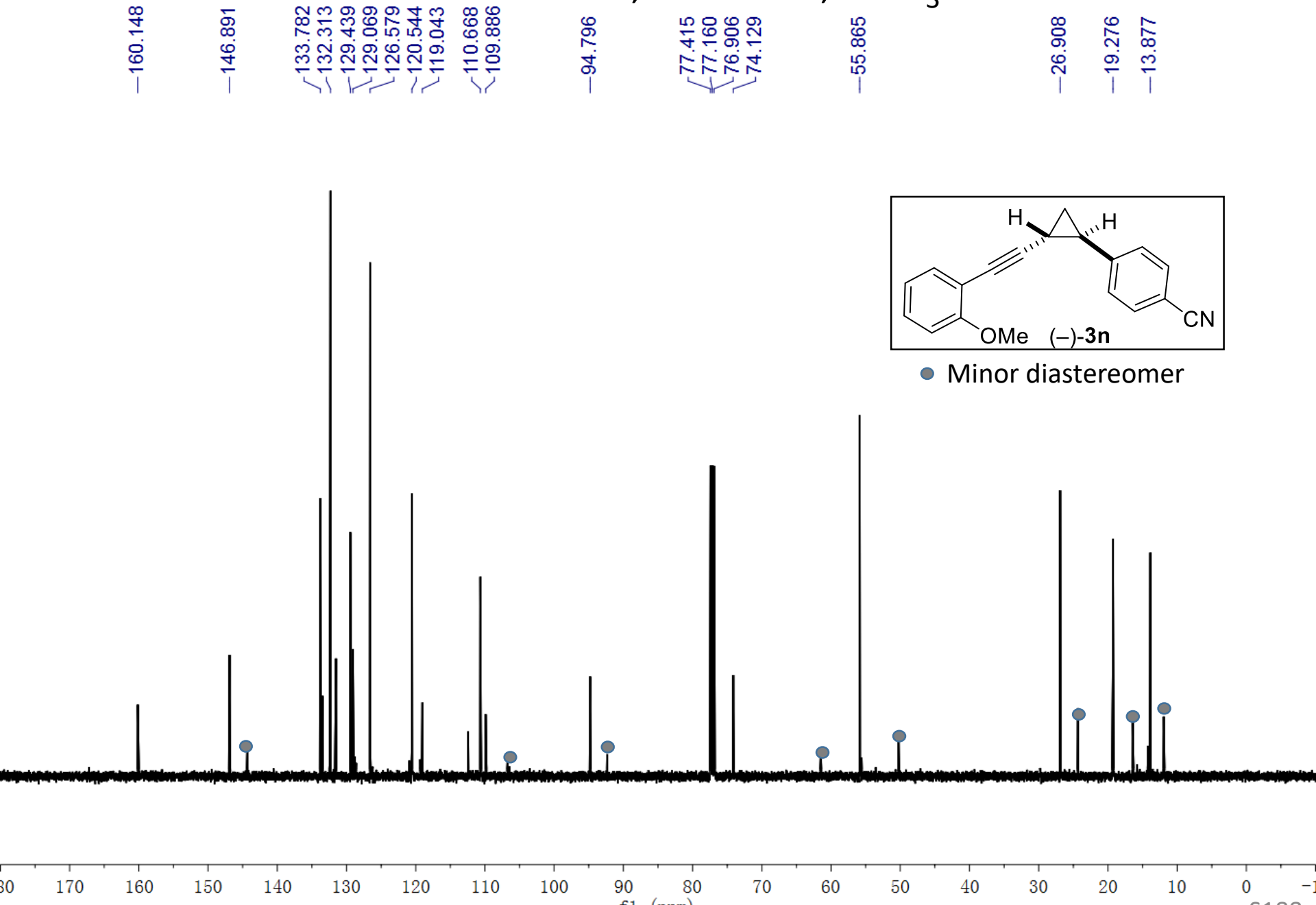




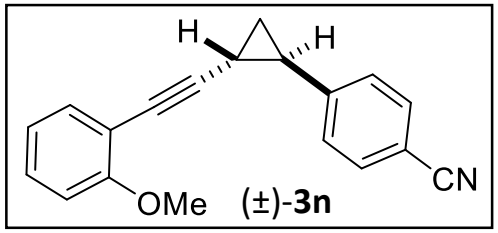
(–)-**3n**

- Minor diastereomer

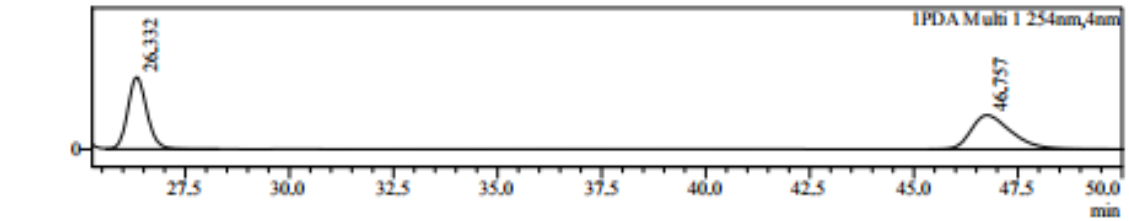
^{13}C NMR of **3n**, 151 MHz, $CDCl_3$



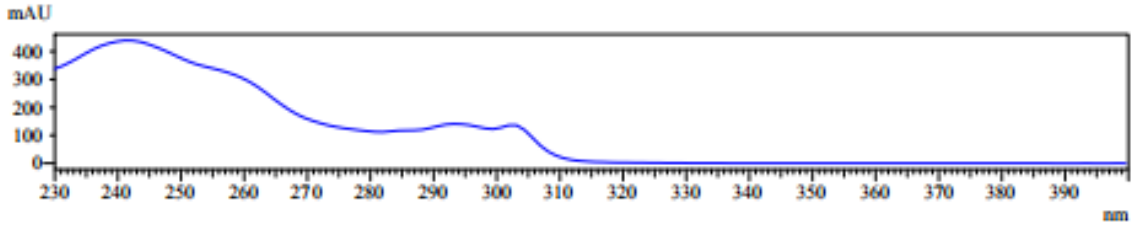
Data File : J0K-0631-IC--10%-1ML.lcd
Sample Name : J0K-0631-IC--10%-1ML
Sample ID : J0K-0631-IC--10%-1ML
Method File : J0K-10%--50min-1ml.lcm



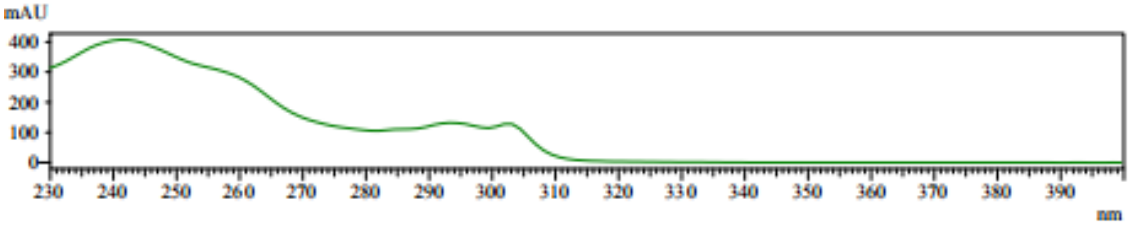
Chromatogram



UV Spectrum
Retention time = 23.718



Retention time = 24.752

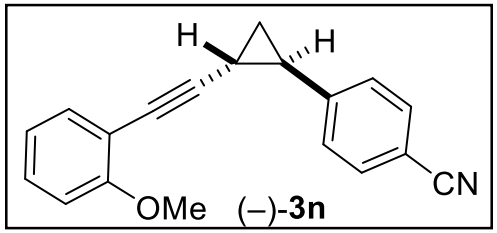


Peak Table

PDA Ch1 254nm

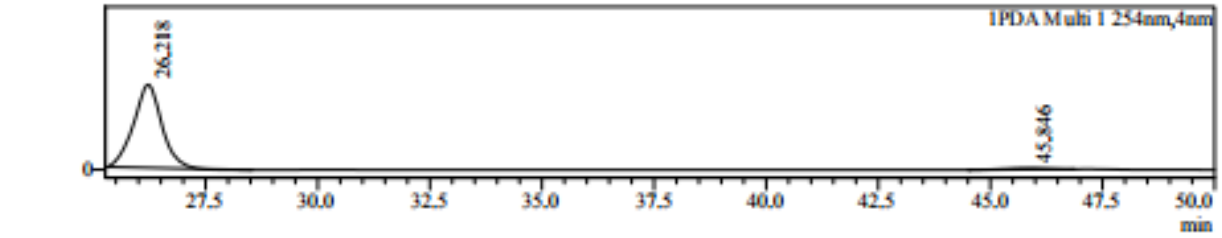
Peak#	Ret. Time	Area	Area%
1	23.718	9570289	21.223
2	24.752	9632285	21.361
3	26.332	12974775	28.773
4	46.757	12916100	28.643
Total		45093449	100.000

Data File : J0K-0630-IC--10%-1ML.lcd
Sample Name : J0K-0630-IC--10%-1ML
Sample ID : J0K-0630-IC--10%-1ML
Method File : J0K-10%--50min-1ml.lcm

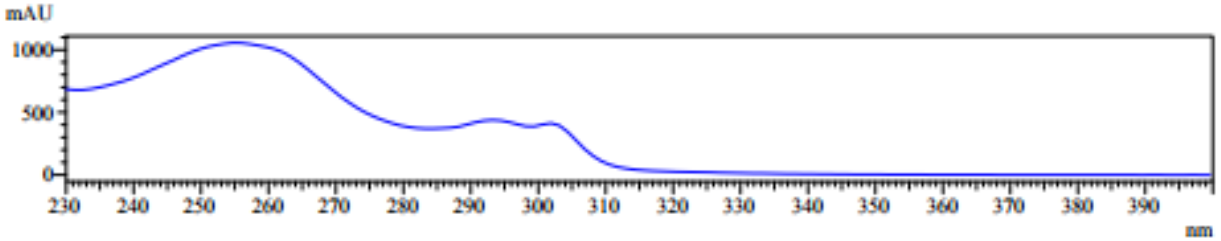


(–)-**3n**

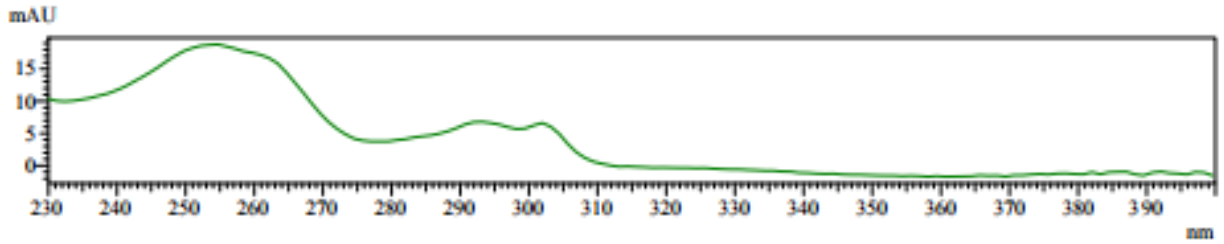
Chromatogram



UV Spectrum
Retention time = 26.218



L
Retention time = 45.846

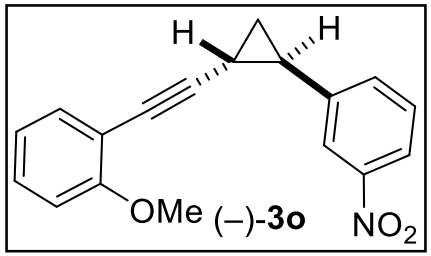


Peak Table

PDA Ch1 254nm

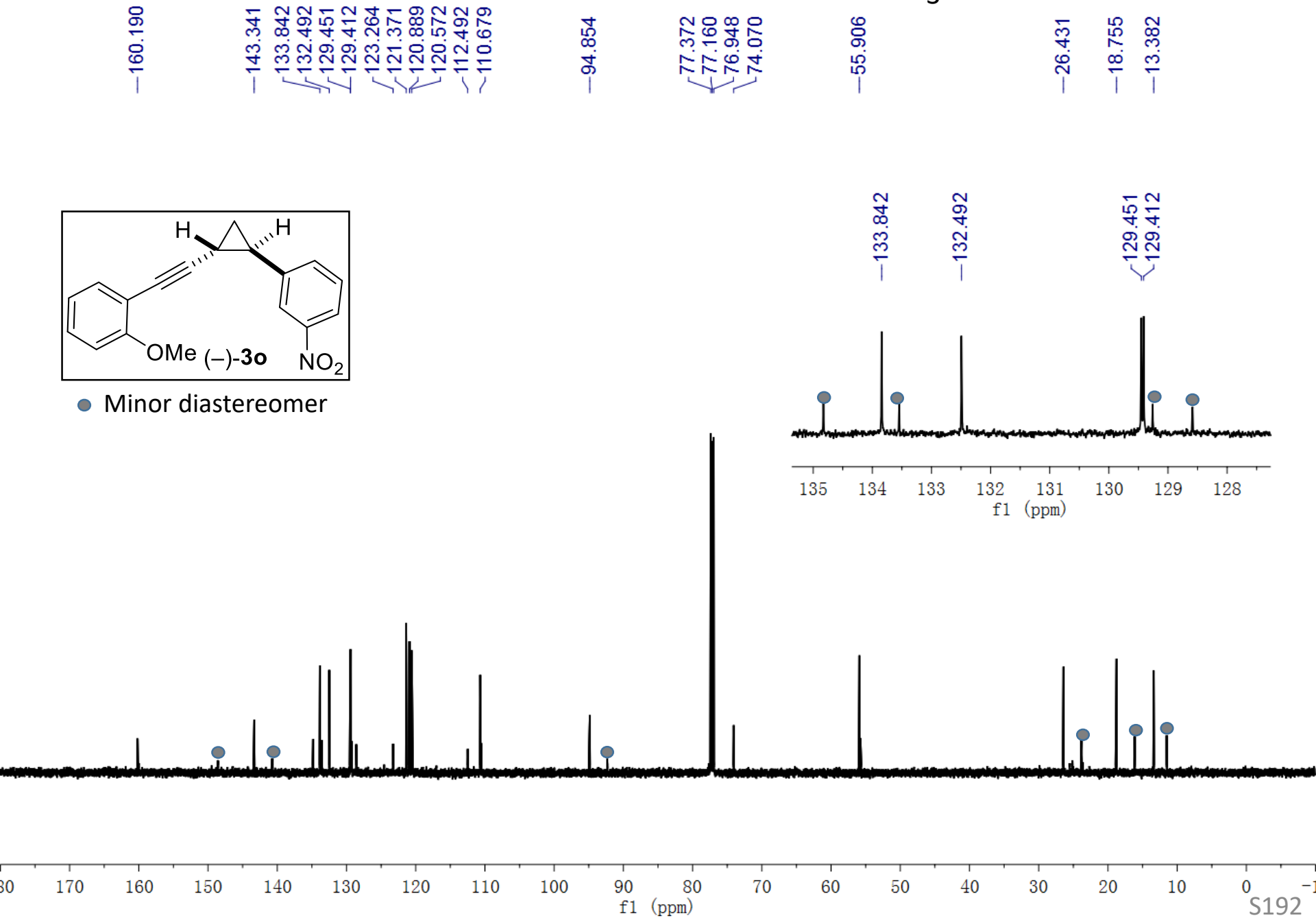
Peak#	Ret. Time	Area	Area%
1	26.218	44689706	97.722
2	45.846	1041945	2.278
Total		45731651	100.000

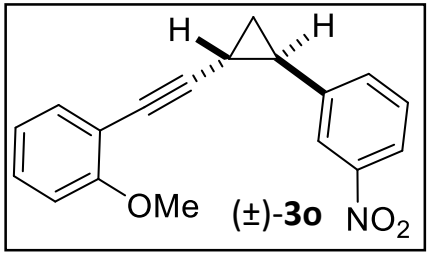
^{1}H NMR of **3o**, 600 MHz, $CDCl_3$



- Minor diastereomer

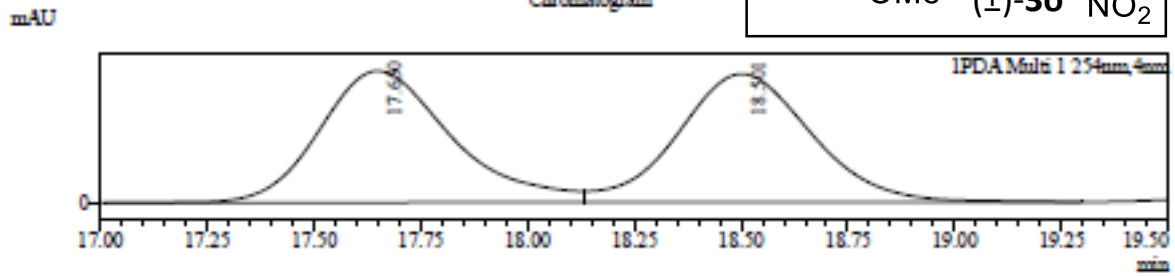
^{13}C NMR of **3o**, 151 MHz, $CDCl_3$



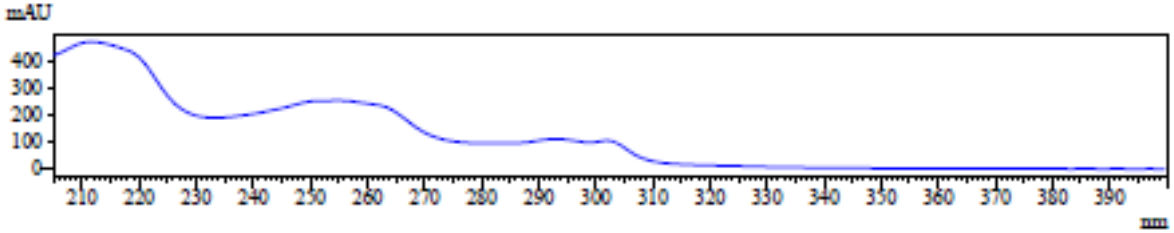


Data File : J0K-0629-IC--10%-1ML.lcd
Sample Name : J0K-0629-IC--10%-1ML
Sample ID : J0K-0629-IC--10%-1ML
Method File : J0K-10%--50min-1ml.lcm

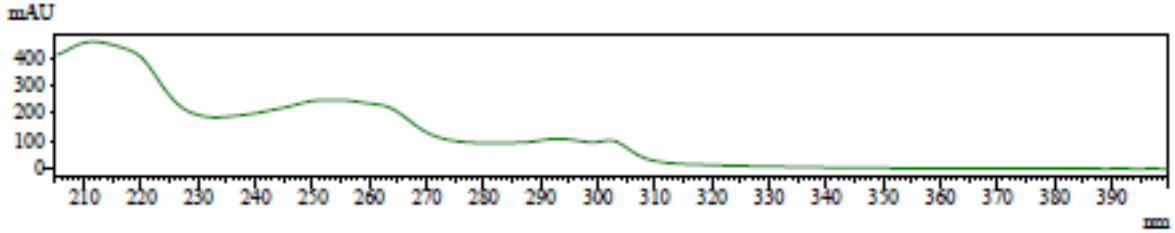
Chromatogram



UV Spectrum
Retention time = 17.650



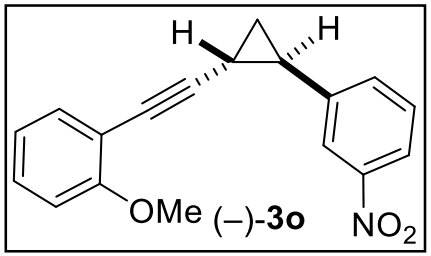
UV Spectrum
Retention time = 18.501



Peak Table

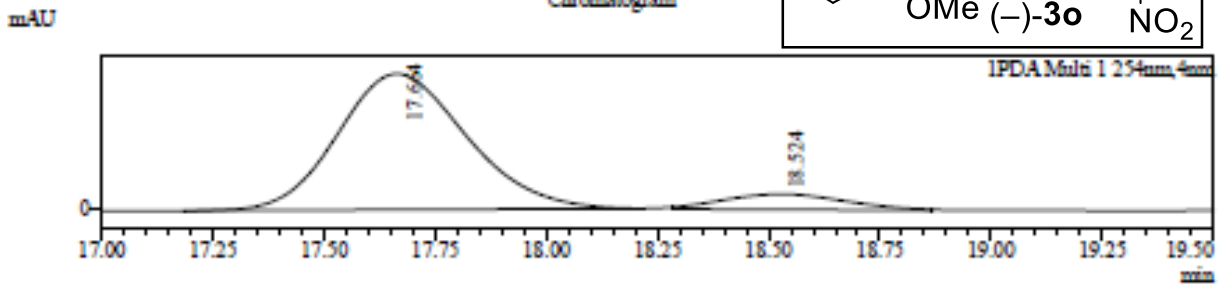
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	17.650	5392862	50.364
2	18.501	5314868	49.636
Total		10707730	100.000

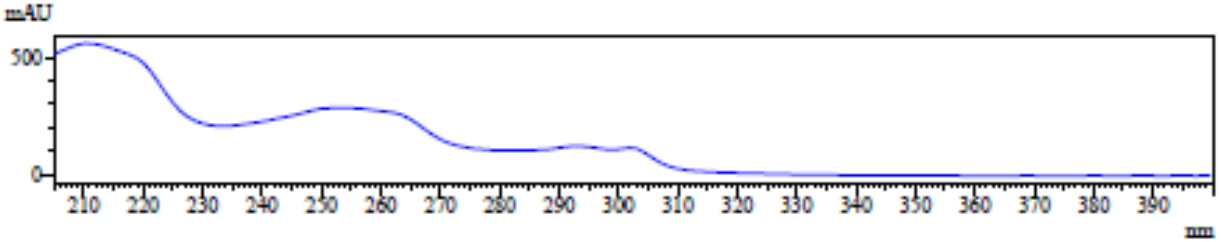


Data File : J0K-0628-IC--10%-1ML.lcd
Sample Name : J0K-0628-IC--10%-1ML
Sample ID : J0K-0628-IC--10%-1ML
Method File : J0K-10%--50min-1ml.lcm

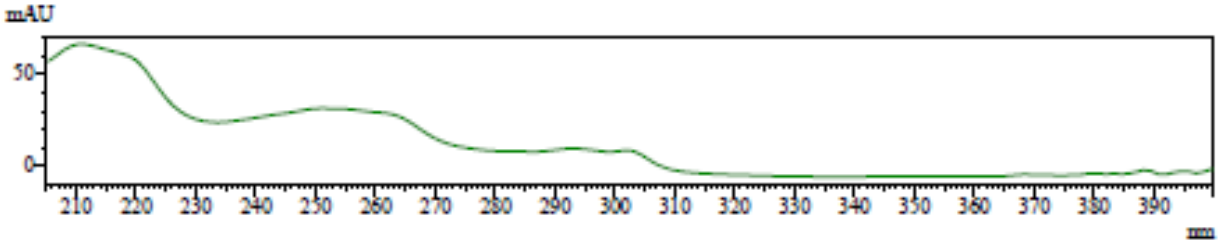
Chromatogram



UV Spectrum
Retention time = 17.664



UV Spectrum
Retention time = 18.524

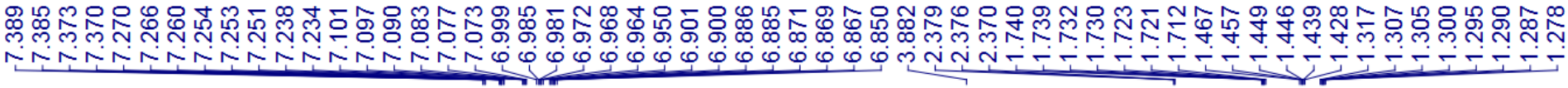


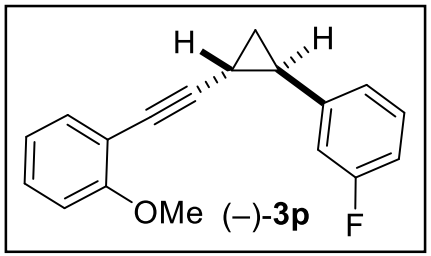
Peak Table

PDA Ch1 254nm

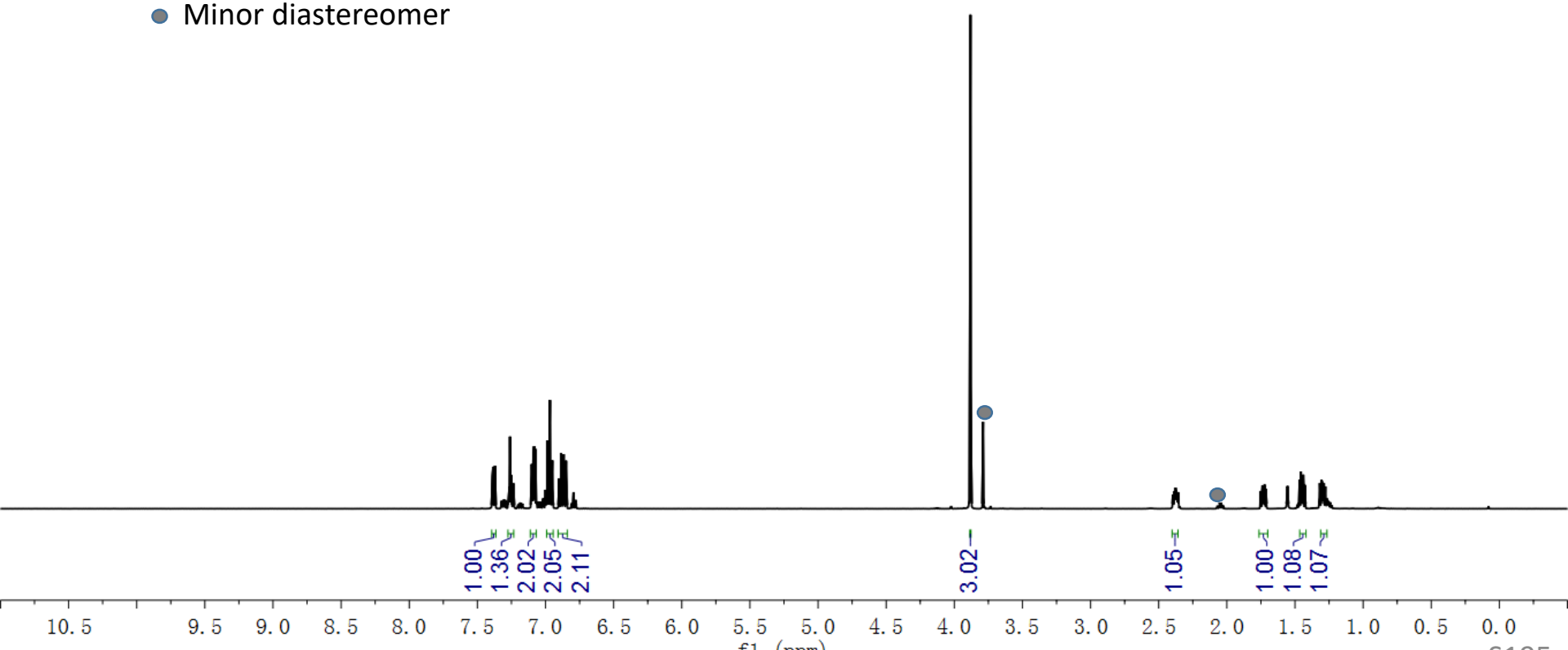
Peak#	Ret. Time	Area	Area%
1	17.664	5722100	90.281
2	18.524	616010	9.719
Total		6338110	100.000

^{1}H NMR of **3p**, 500 MHz, $CDCl_3$

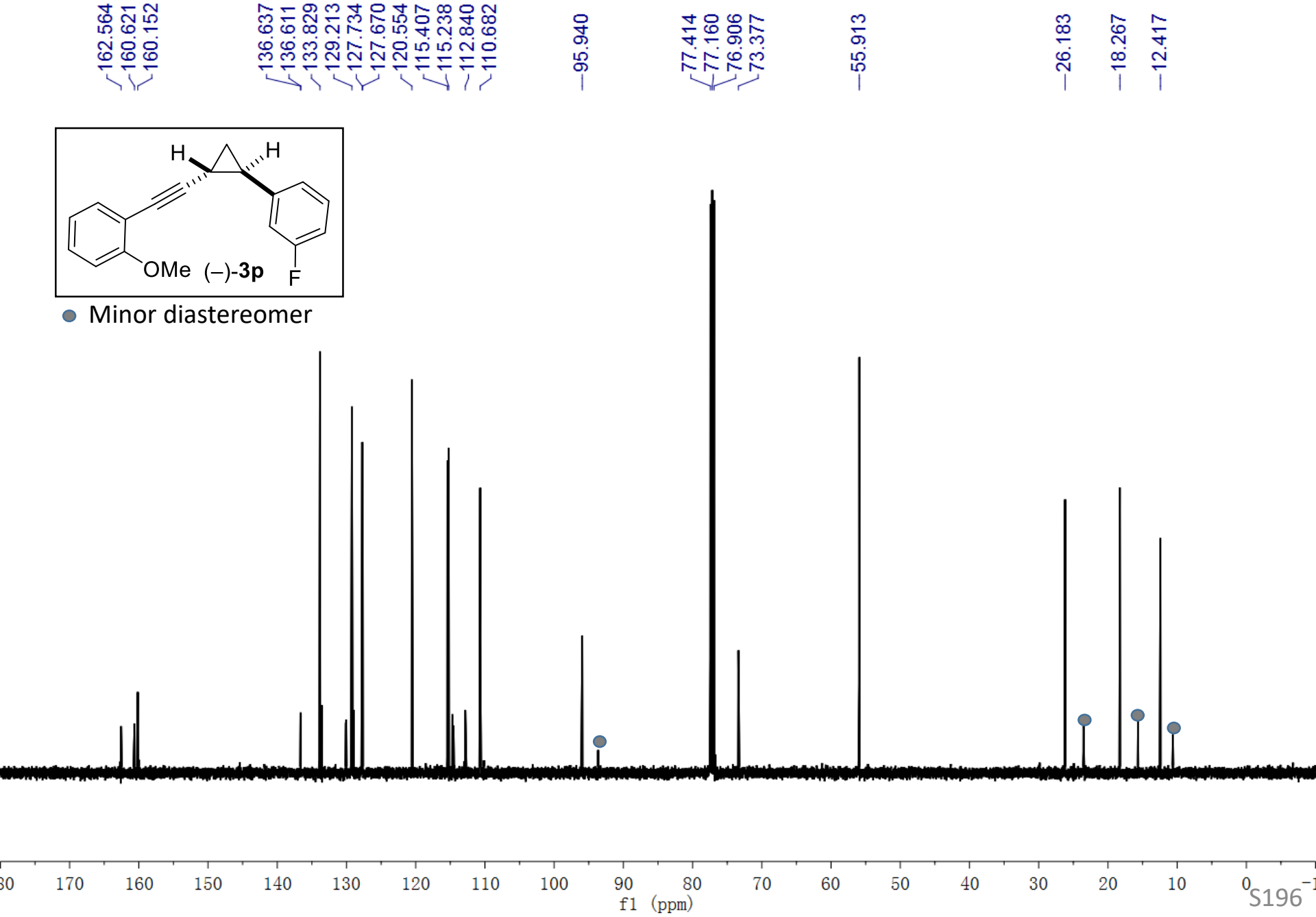




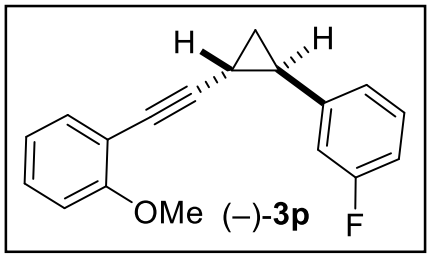
- Minor diastereomer

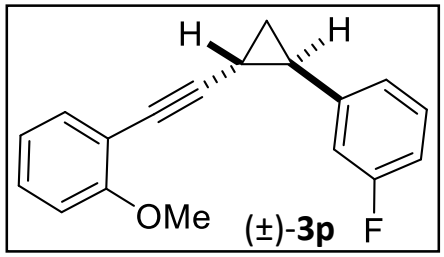


^{13}C NMR of **3p**, 126 MHz, $CDCl_3$



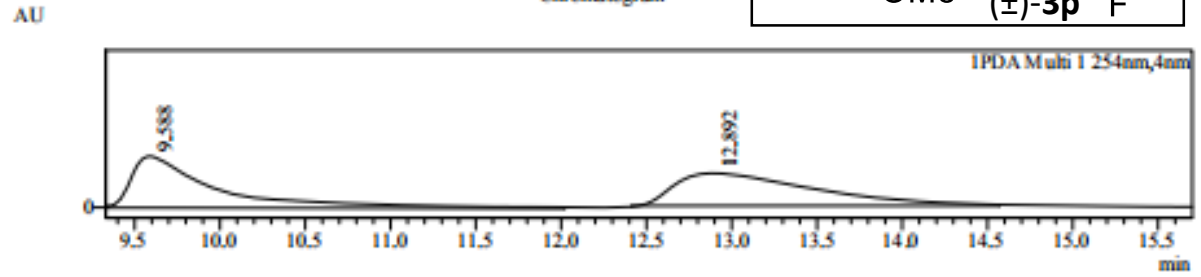
^{19}F NMR of **3p**, 564 MHz, $CDCl_3$



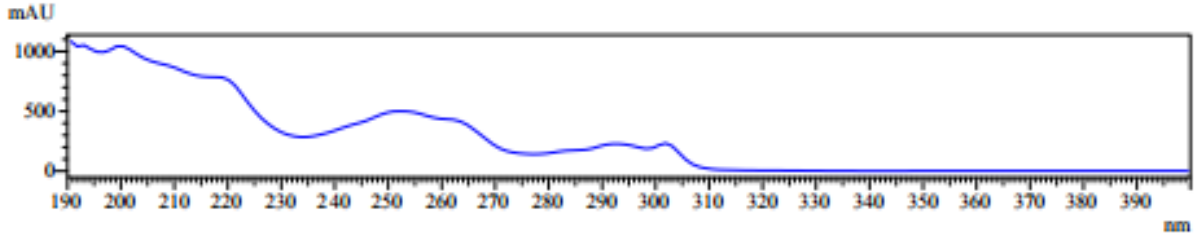


Data File : J0K-1512-new-IA--0.3%-1ML.lcd
Sample Name : J0K-1512-new-IA--0.3%-1ML
Sample ID : J0K-1512-new-IA--0.3%-1ML
Method File : J0K-0.3%--45min-1ml.lcm

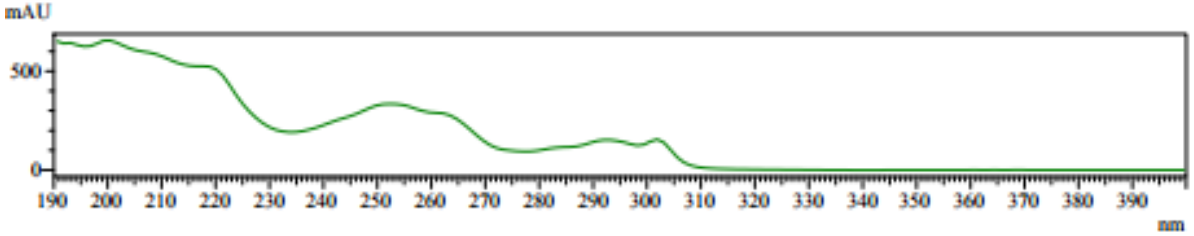
Chromatogram



UV Spectrum
Retention time = 9.588



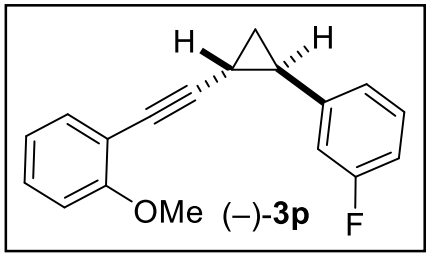
Retention time = 12.892



Peak Table

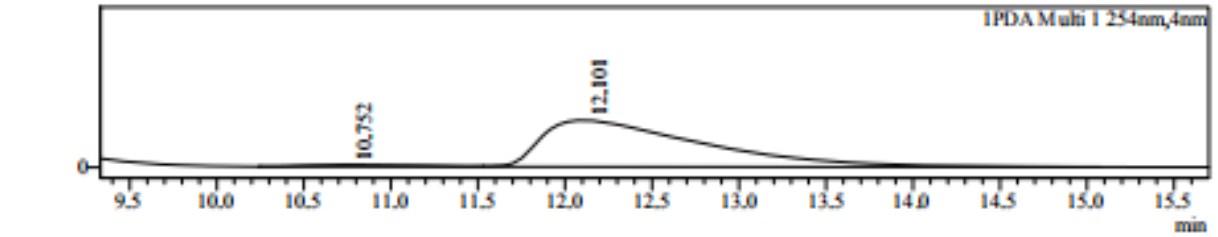
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	9.588	17225820	49.482
2	12.892	17586782	50.518
Total		34812602	100.000

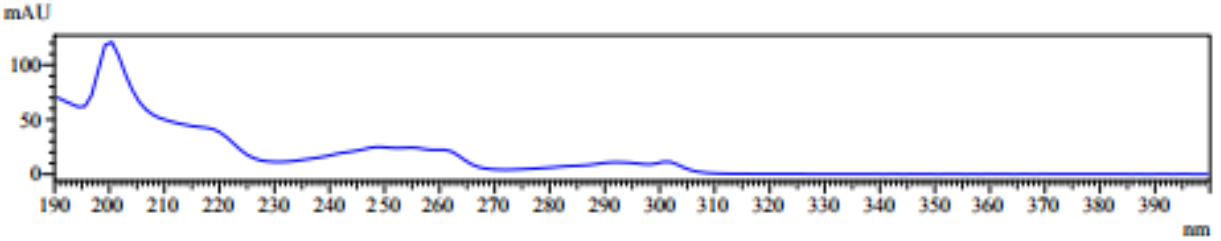


Data File : J0K-1511-IA--0.3%-1ML.lcd
Sample Name : J0K-1511-IA--0.3%-1ML
Sample ID : J0K-1511-IA--0.3%-1ML
Method File : J0K-0.3%--25min-1ml.lcm

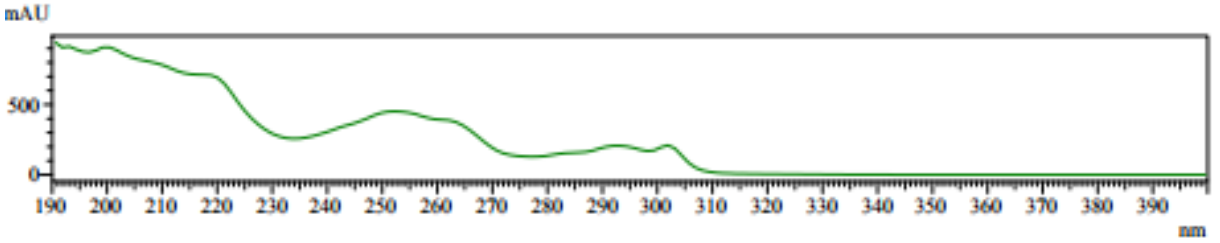
Chromatogram



UV Spectrum
Retention time = 10.752



Retention time = 12.101

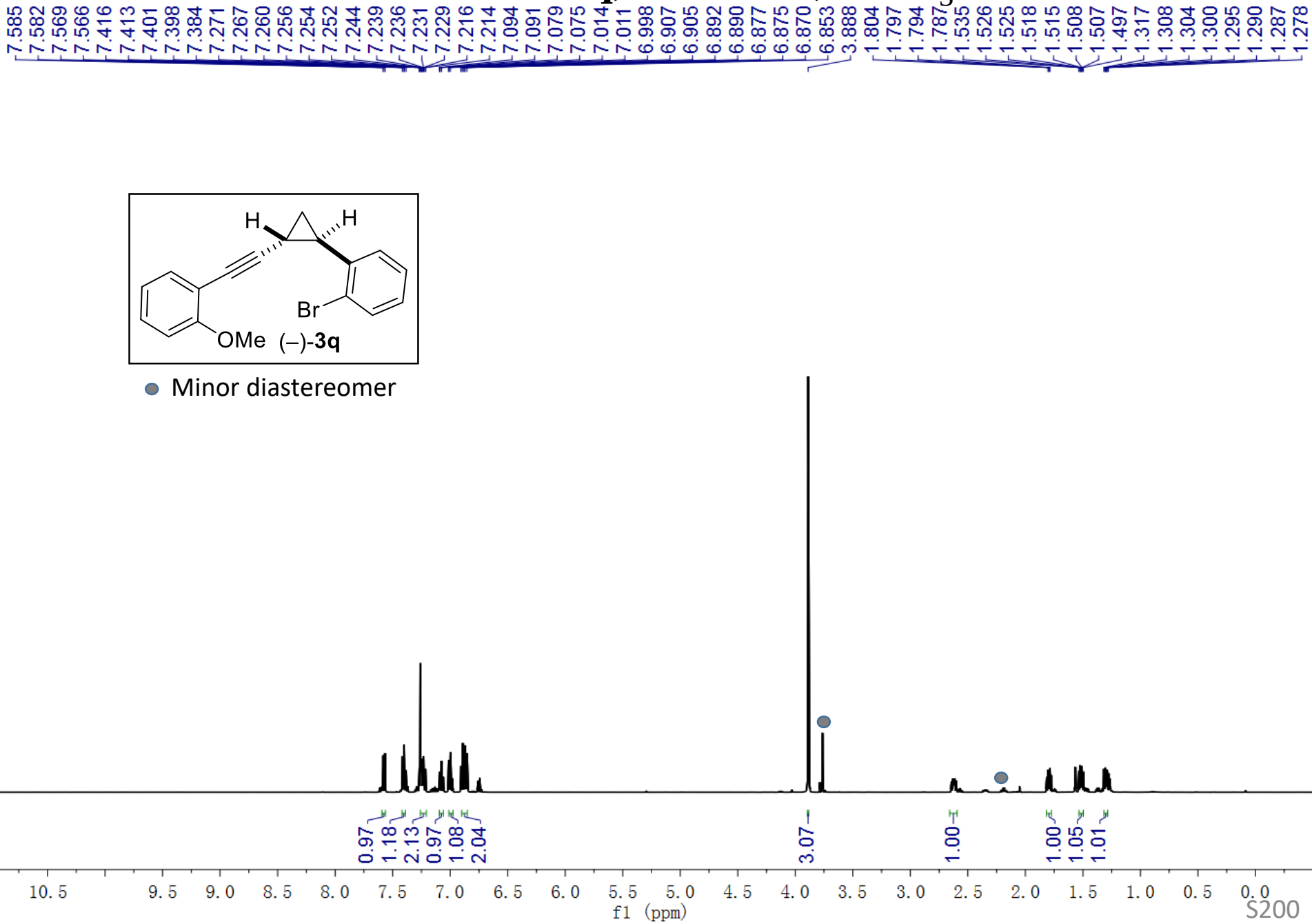


Peak Table

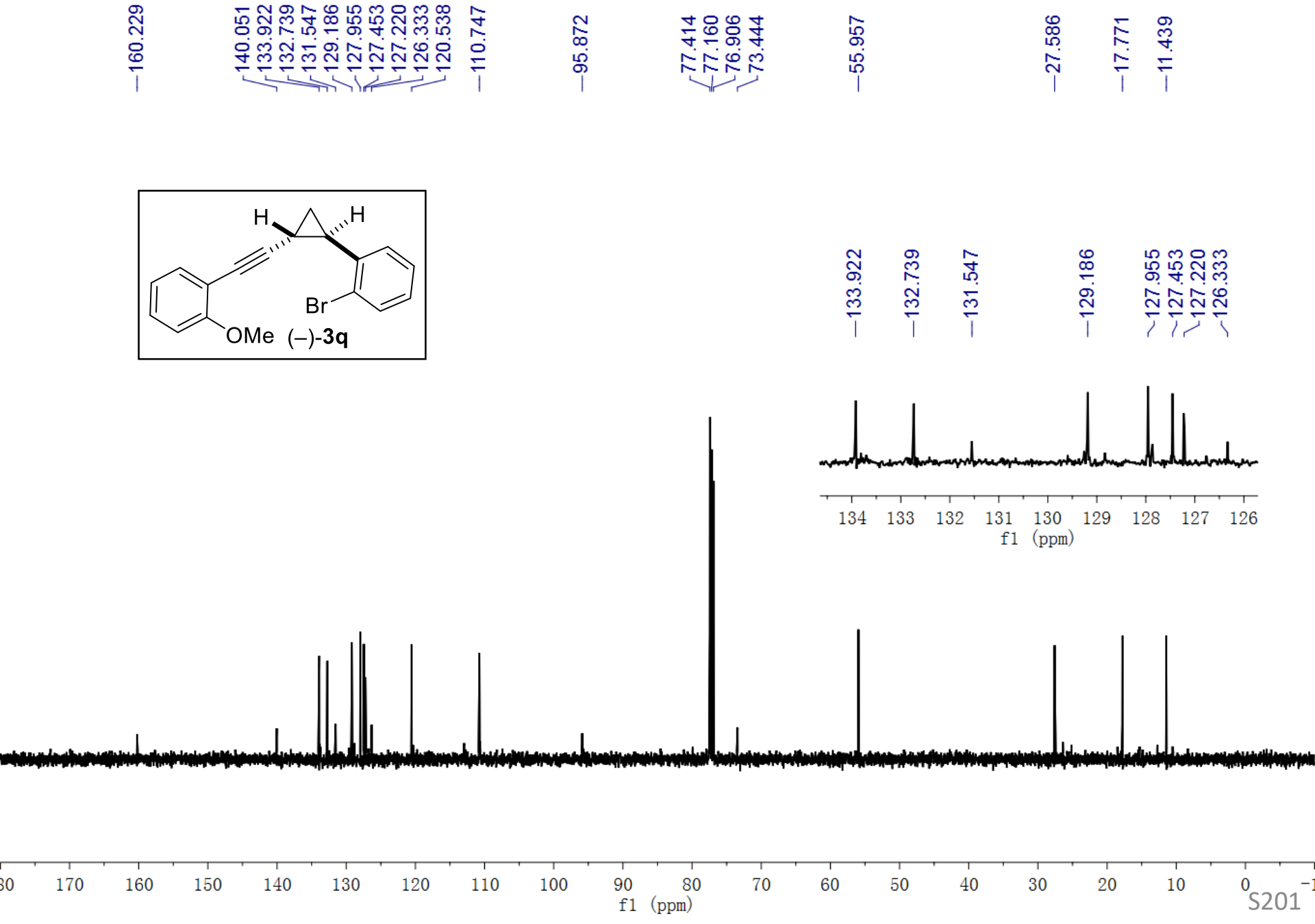
PDA Ch1 254nm

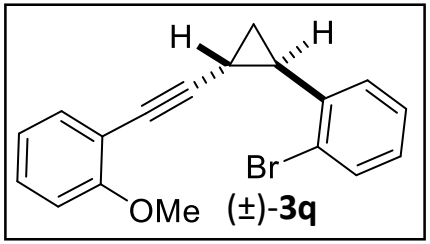
Peak#	Ret. Time	Area	Area%
1	10.752	770306	2.706
2	12.101	27700720	97.294
Total		28471026	100.000

^{1}H NMR of **3q**, 500 MHz, $CDCl_3$



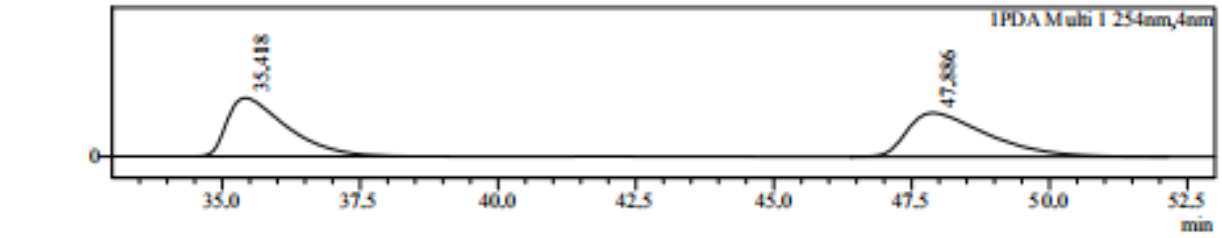
^{13}C NMR of **3q**, 151 MHz, $CDCl_3$



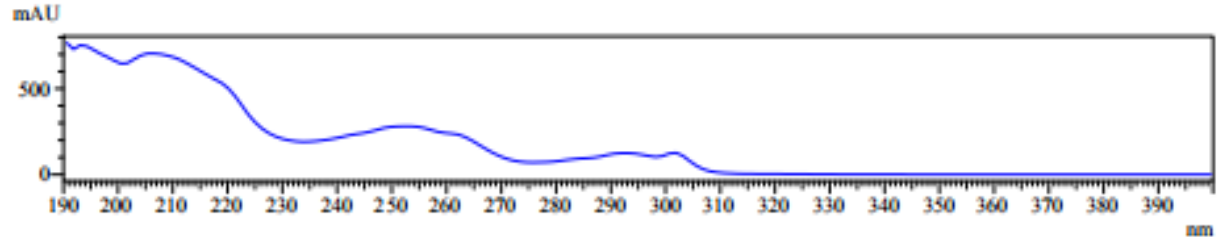


Data File : J0K-1451-ODH-2%-1ML-2.lcd
Sample Name : J0K-1451-ODH-2%-1ML-2
Sample ID : J0K-1451-ODH-2%-1ML-2
Method File : J0K-2%-40min-1mL.lcm

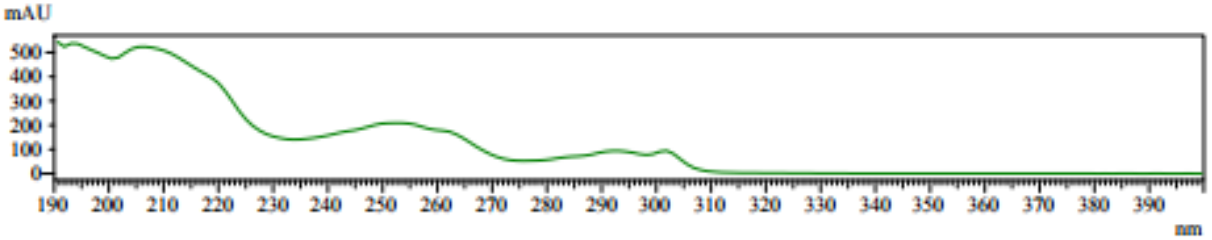
Chromatogram



UV Spectrum
Retention time = 35.418



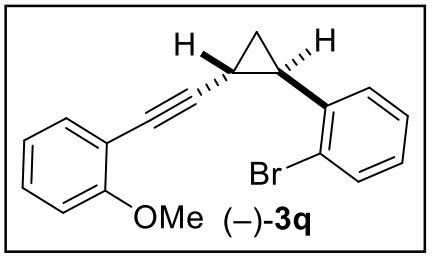
1
Retention time = 47.886



Peak Table

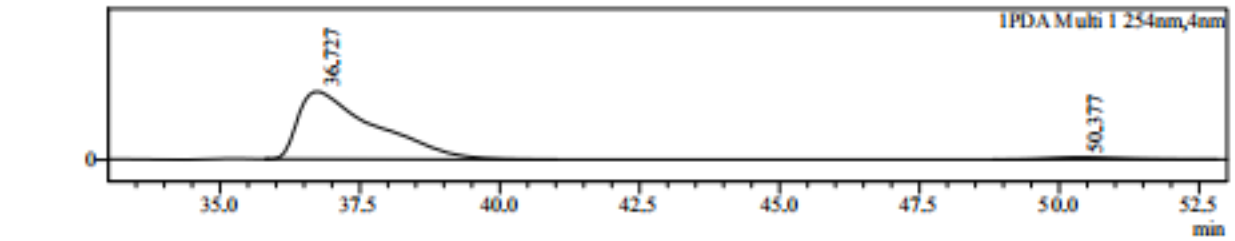
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	35.418	20668199	50.095
2	47.886	20589932	49.905
Total		41258131	100.000

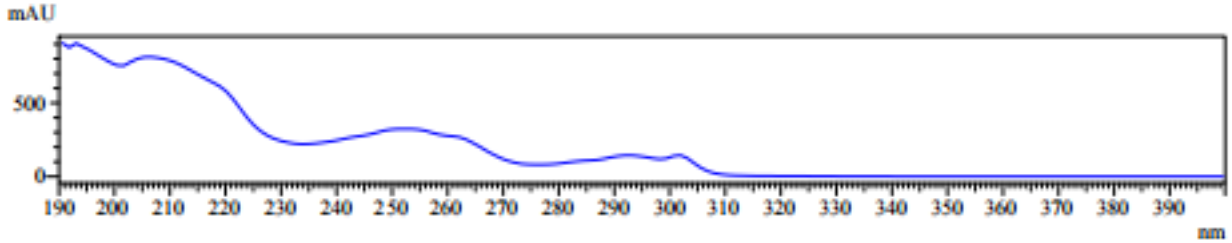


Data File : J0K-1449-ODH-2%-1ML-2.lcd
Sample Name : J0K-1449-ODH-2%-1ML-2
Sample ID : J0K-1449-ODH-2%-1ML-2
Method File : J0K-2%-40min-1ml.lcm

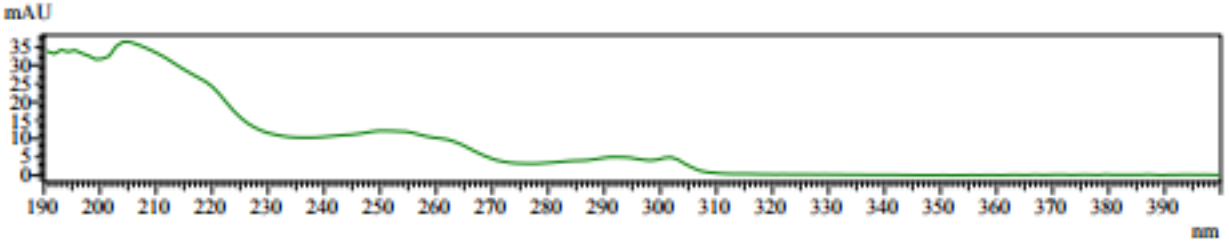
Chromatogram



UV Spectrum
Retention time = 36.727



1
Retention time = 50.377

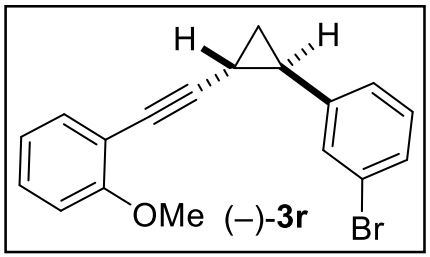


Peak Table

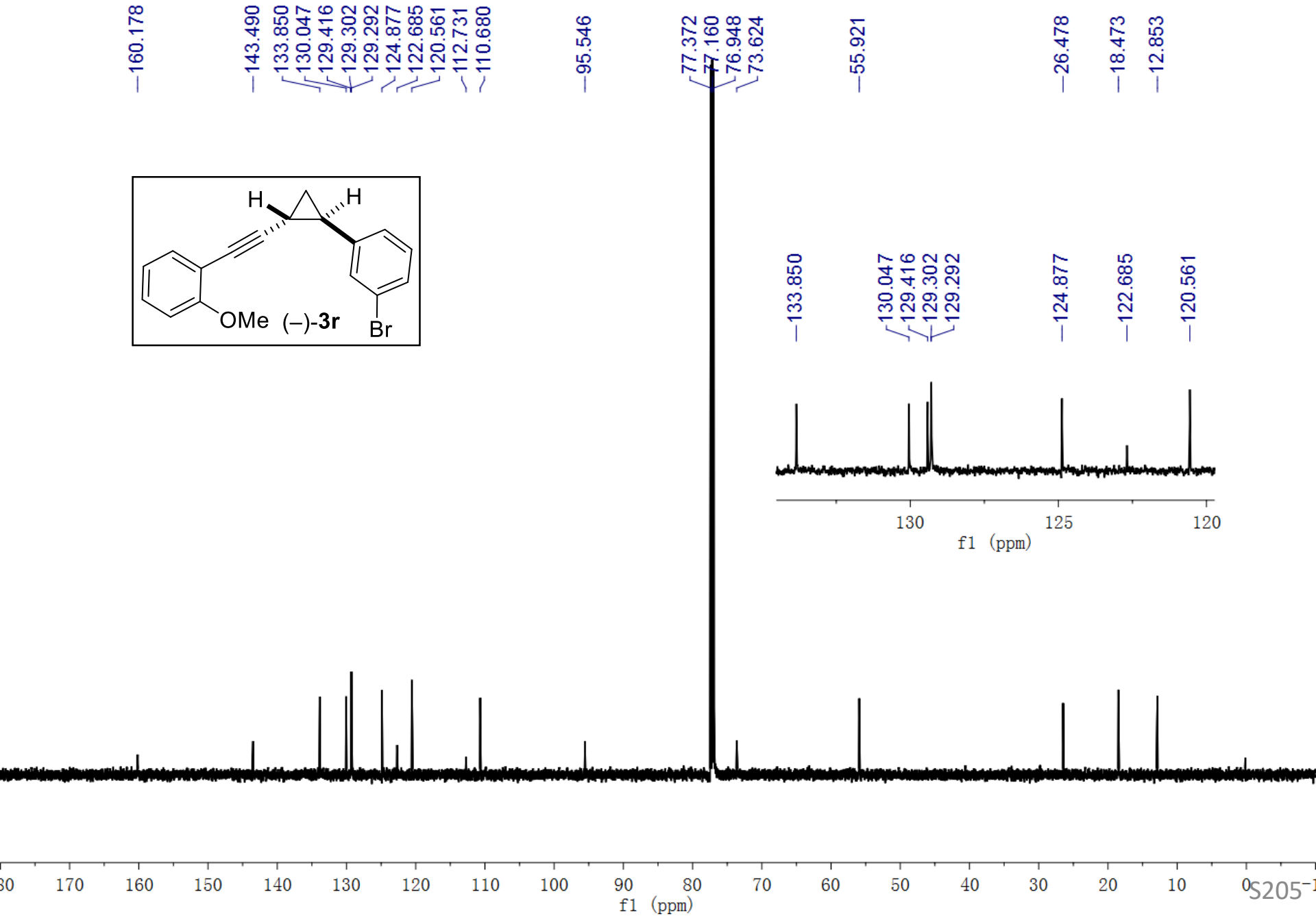
PDA Ch1 254nm

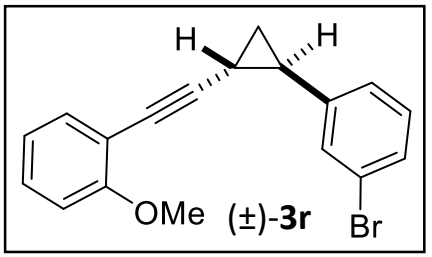
Peak#	Ret. Time	Area	Area%
1	36.727	29767184	97.041
2	50.377	907689	2.959
Total		30674873	100.000

^{1}H NMR of **3r**, 600 MHz, $CDCl_3$



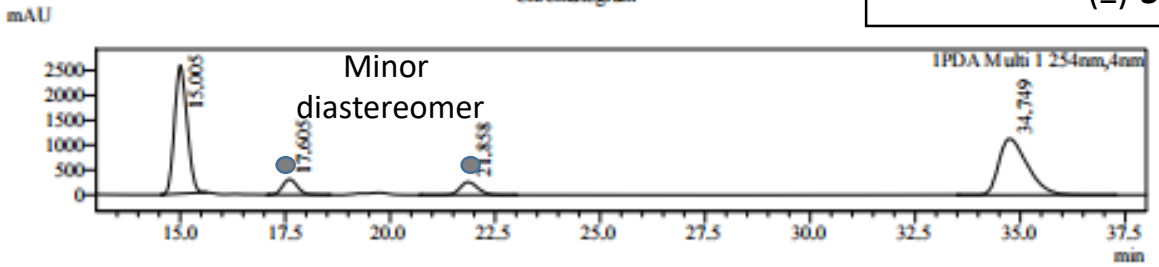
^{13}C NMR of **3r**, 151 MHz, $CDCl_3$



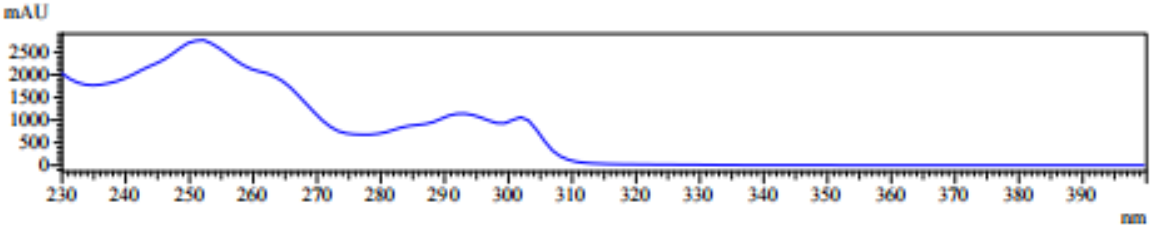


Data File : J0K-0341-IC-1%-0.8ML-isopropanol-solvent005.lcd
Sample Name : J0K-0341-IC-1%-0.8ML-isopropanol-solvent005
Sample ID : J0K-0341-IC-1%-0.8ML-isopropano
Method File : J0K-1%-0.8ml-50min.lcm

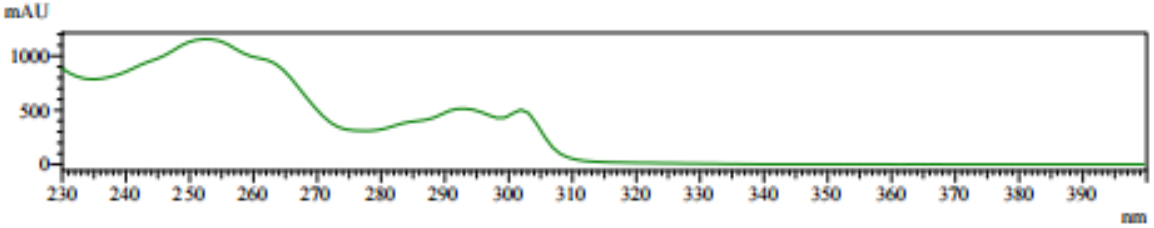
Chromatogram



UV Spectrum
Retention time = 15.005



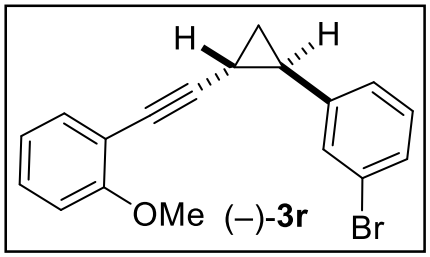
U
Retention time = 34.749



Peak Table

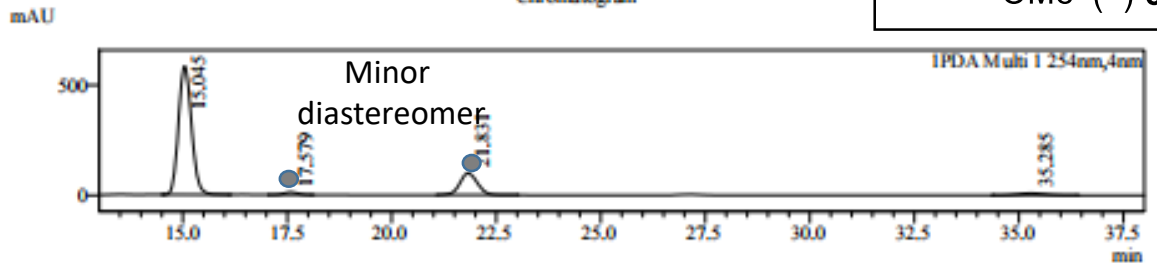
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	15.005	53369617	43.836
2	17.605	7481137	6.145
3	21.858	7551737	6.203
4	34.749	53346423	43.817
Total		121748915	100.000

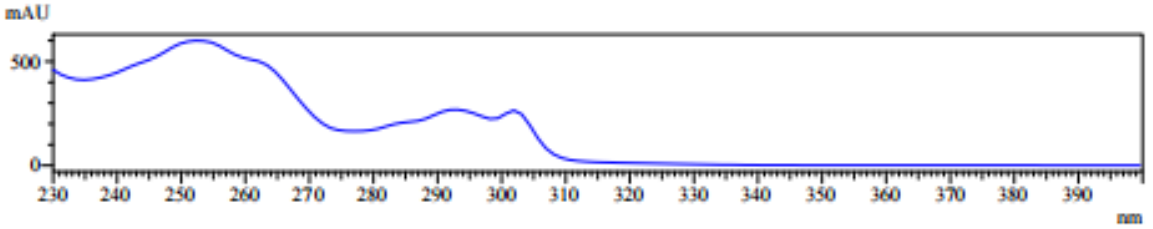


Data File : J0K-0297-IC-1%-0.8ML-isopropanol-solvent017.lcd
Sample Name : J0K-0297-IC-1%-0.8ML-isopropanol-solvent017
Sample ID : J0K-0297-IC-1%-0.8ML-isopropano
Method File : J0K-1%-0.8m-50MIN1.lcm

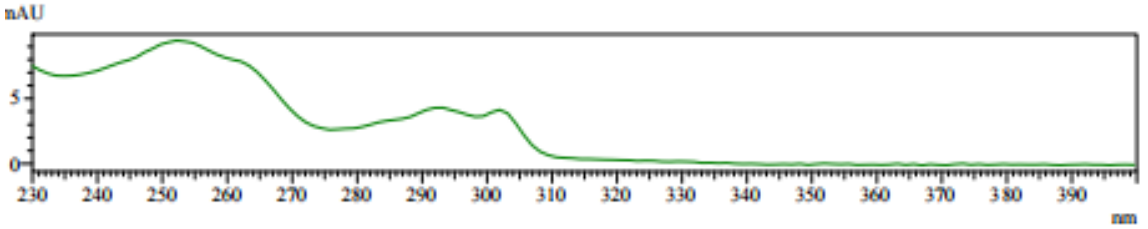
Chromatogram



UV Spectrum
Retention time = 15.045



Retention time = 35.285

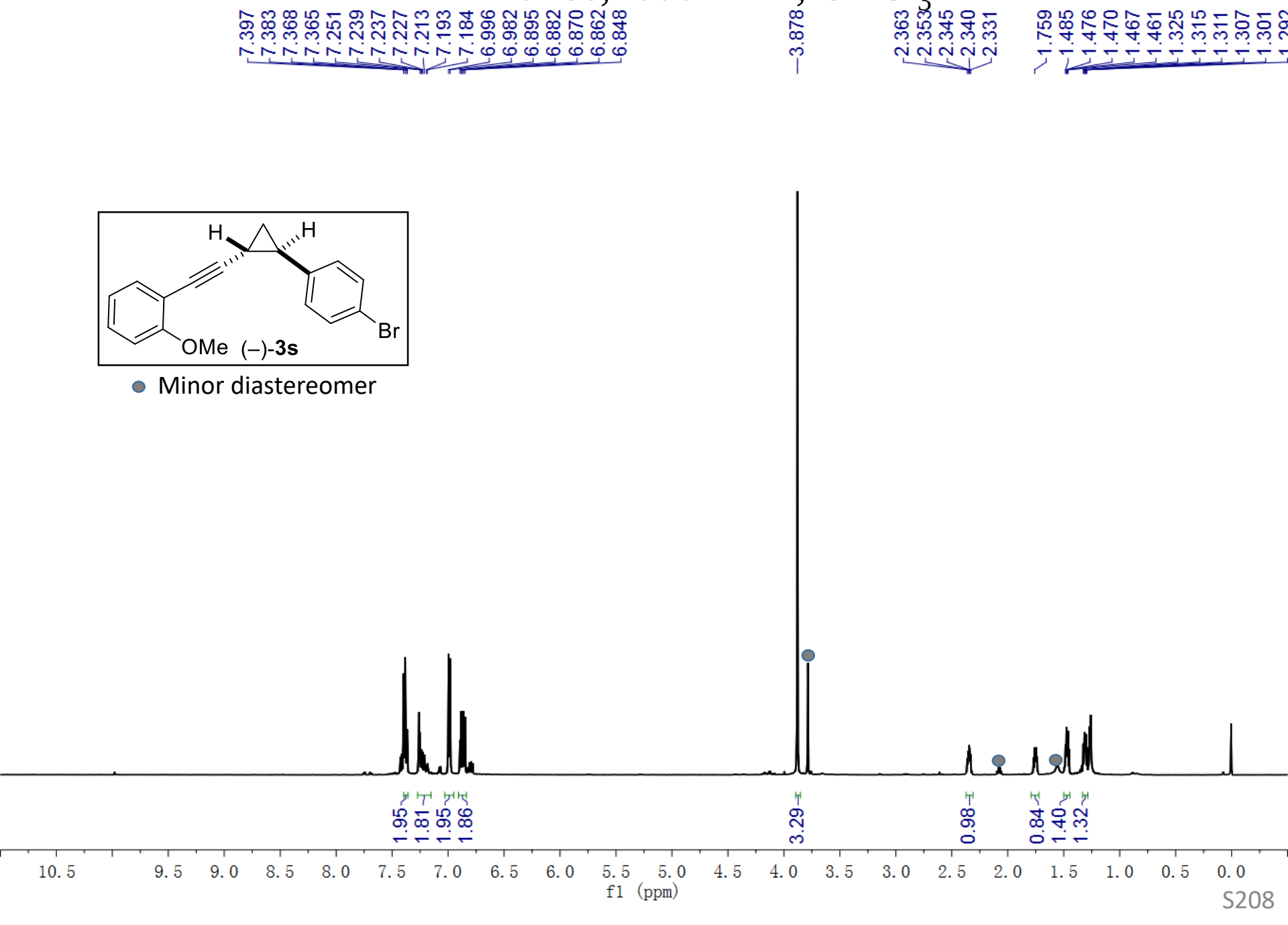


Peak Table

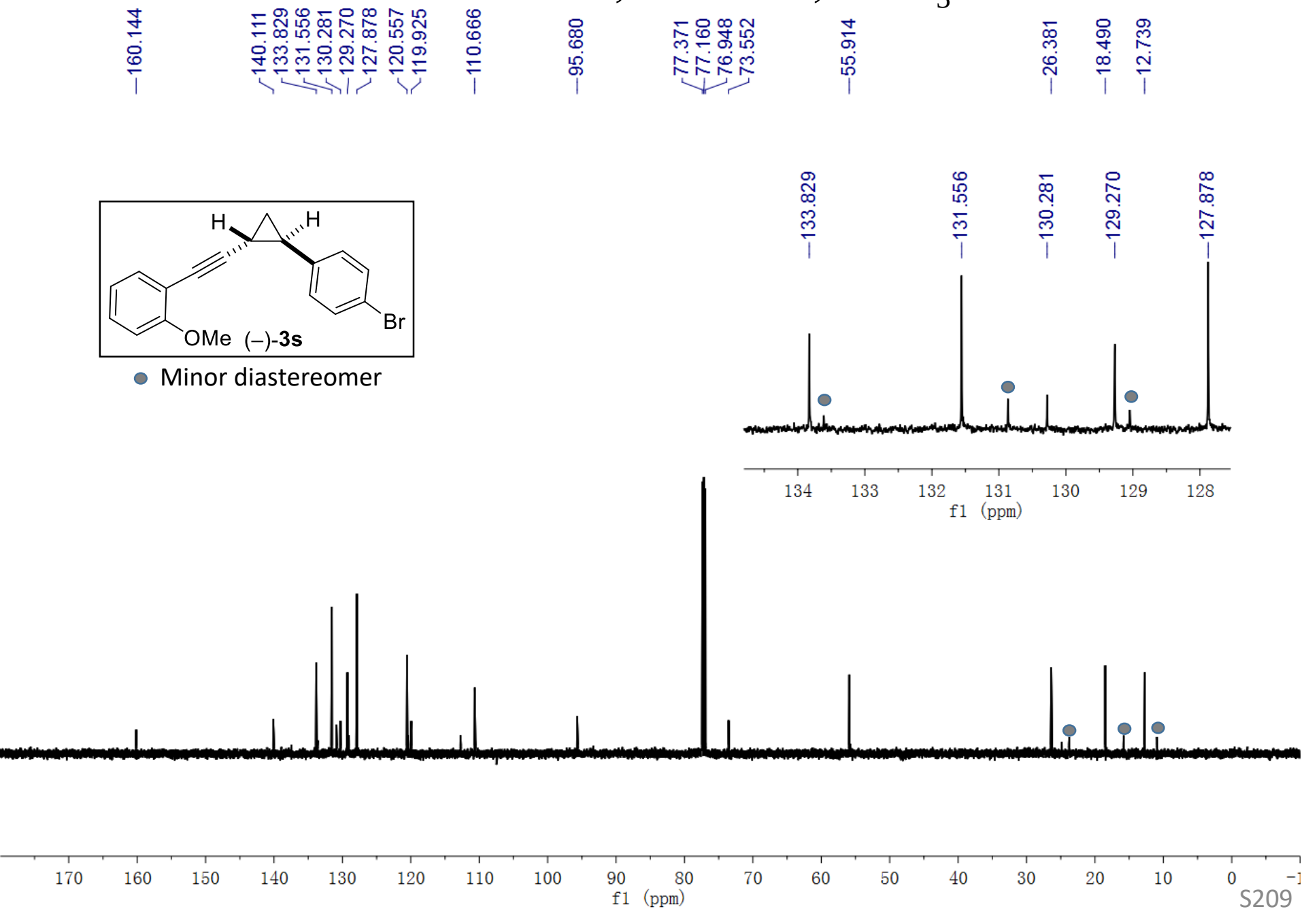
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	15.045	12643137	78.594
2	17.579	267298	1.662
3	21.831	2776700	17.261
4	35.285	399426	2.483
Total		16086561	100.000

^{1}H NMR of **3s**, 600 MHz, $CDCl_3$

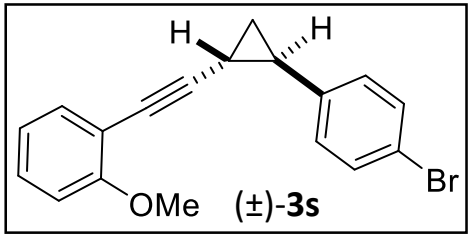


^{13}C NMR of **3s**, 151 MHz, $CDCl_3$



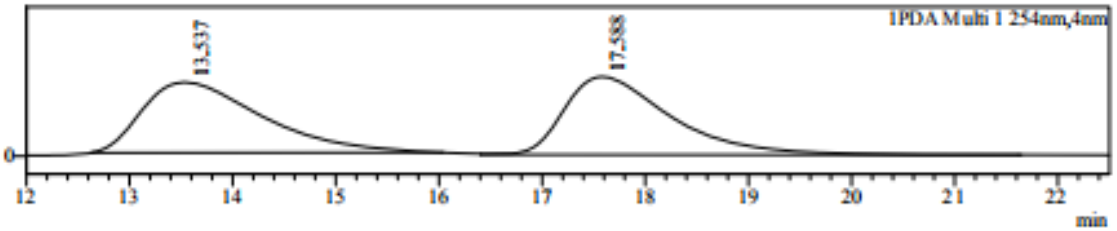
Data File : J0K-1452-IA--0.3%-1ML.lcd
Sample Name : J0K-1452-IA--0.3%-1ML
Sample ID : J0K-1452-IA--0.3%-1ML
Method File : J0K-0.3%--45min-1ml.lcm

Chromatogram



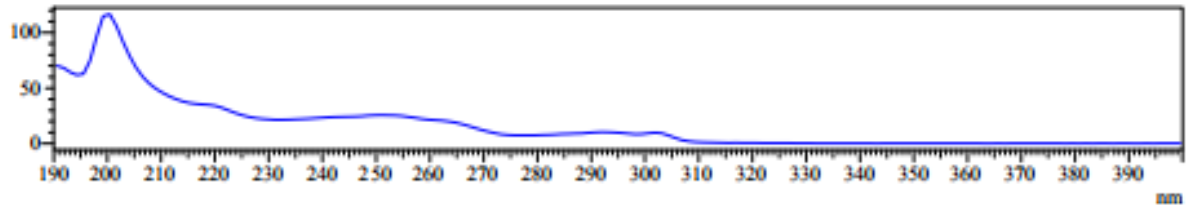
(±)-**3s**

AU



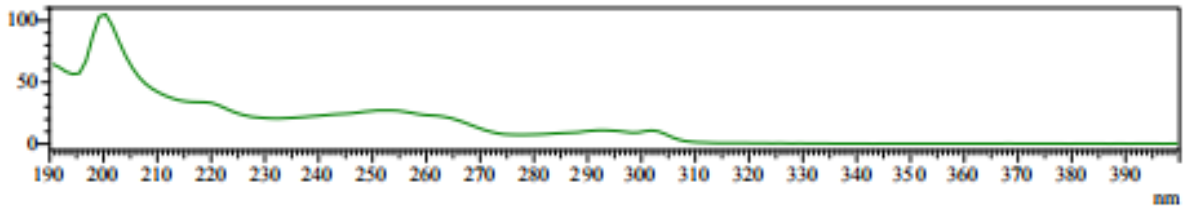
UV Spectrum
Retention time = 13.537

mAU



U
Retention time = 17.588

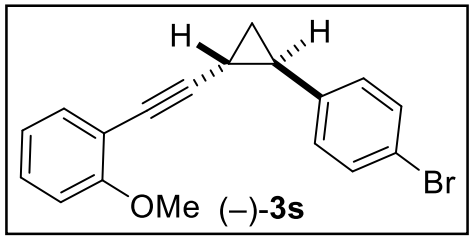
mAU



Peak Table

PDA Ch1 254nm

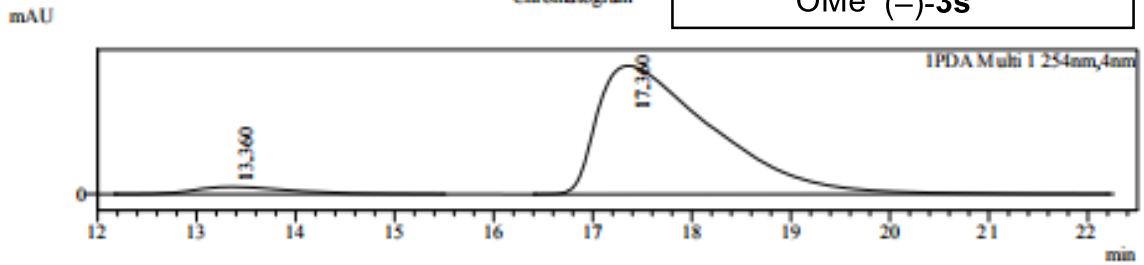
Peak#	Ret. Time	Area	Area%
1	13.537	1903237	50.331
2	17.588	1878235	49.669
Total		3781472	100.000



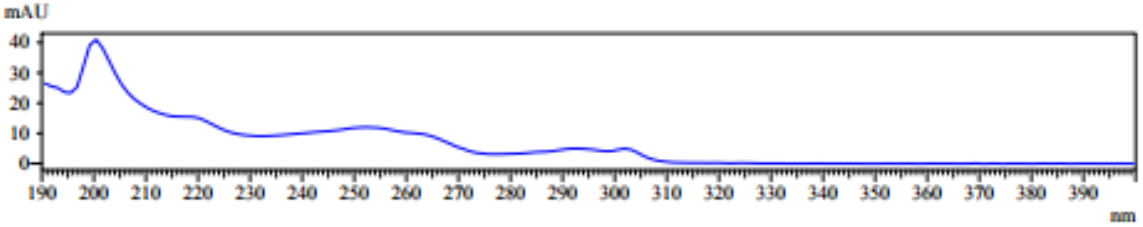
(–)-**3s**

Data File : J0K-1450-IA--0.3%-1ML.lcd
Sample Name : J0K-1450-IA--0.3%-1ML
Sample ID : J0K-1450-IA--0.3%-1ML
Method File : J0K-0.3%--25min-1ml.lcm

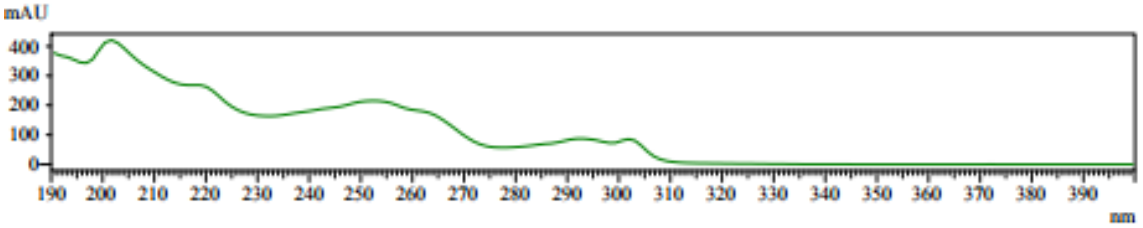
Chromatogram



UV Spectrum
Retention time = 13.360



U
Retention time = 17.360

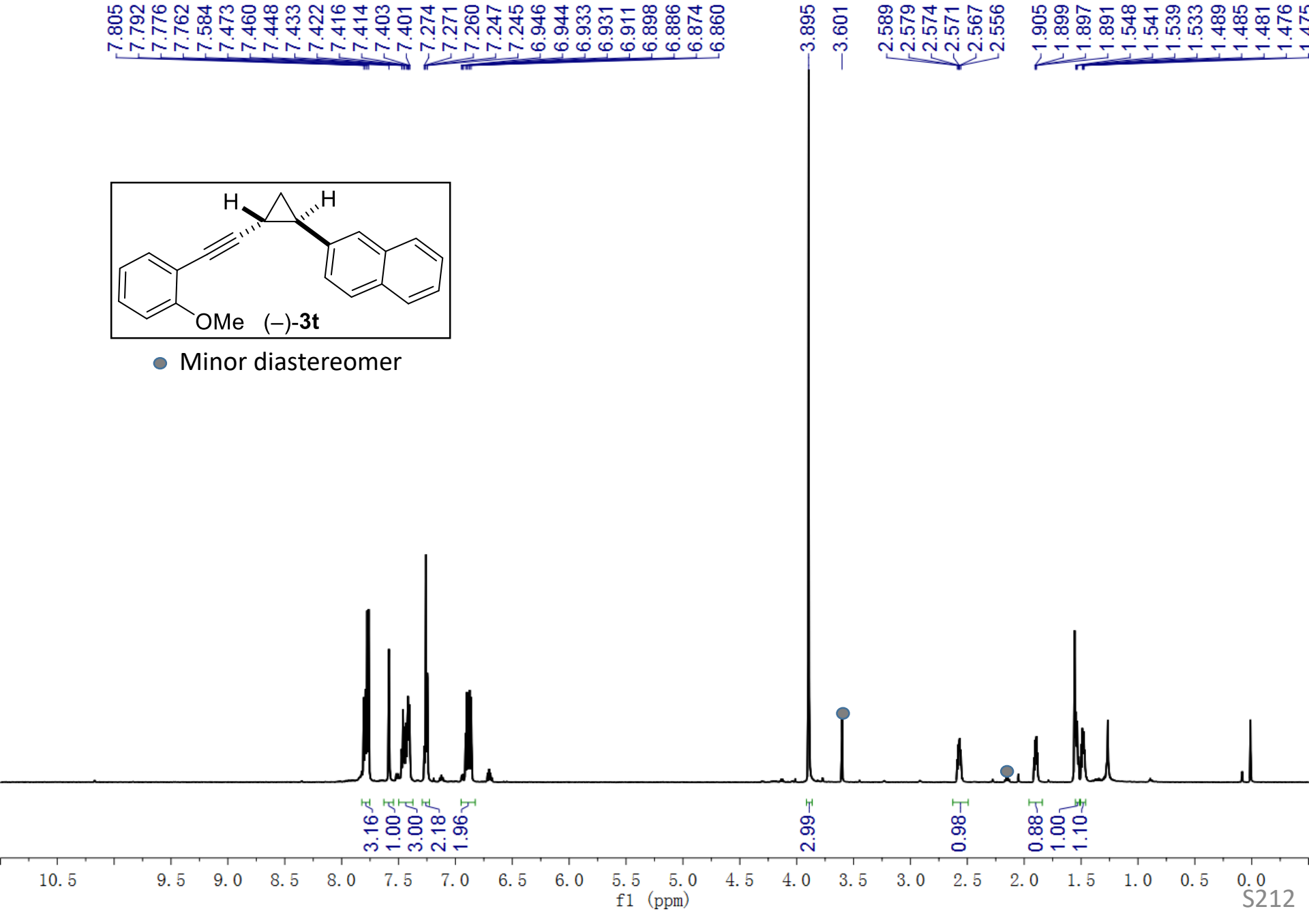


Peak Table

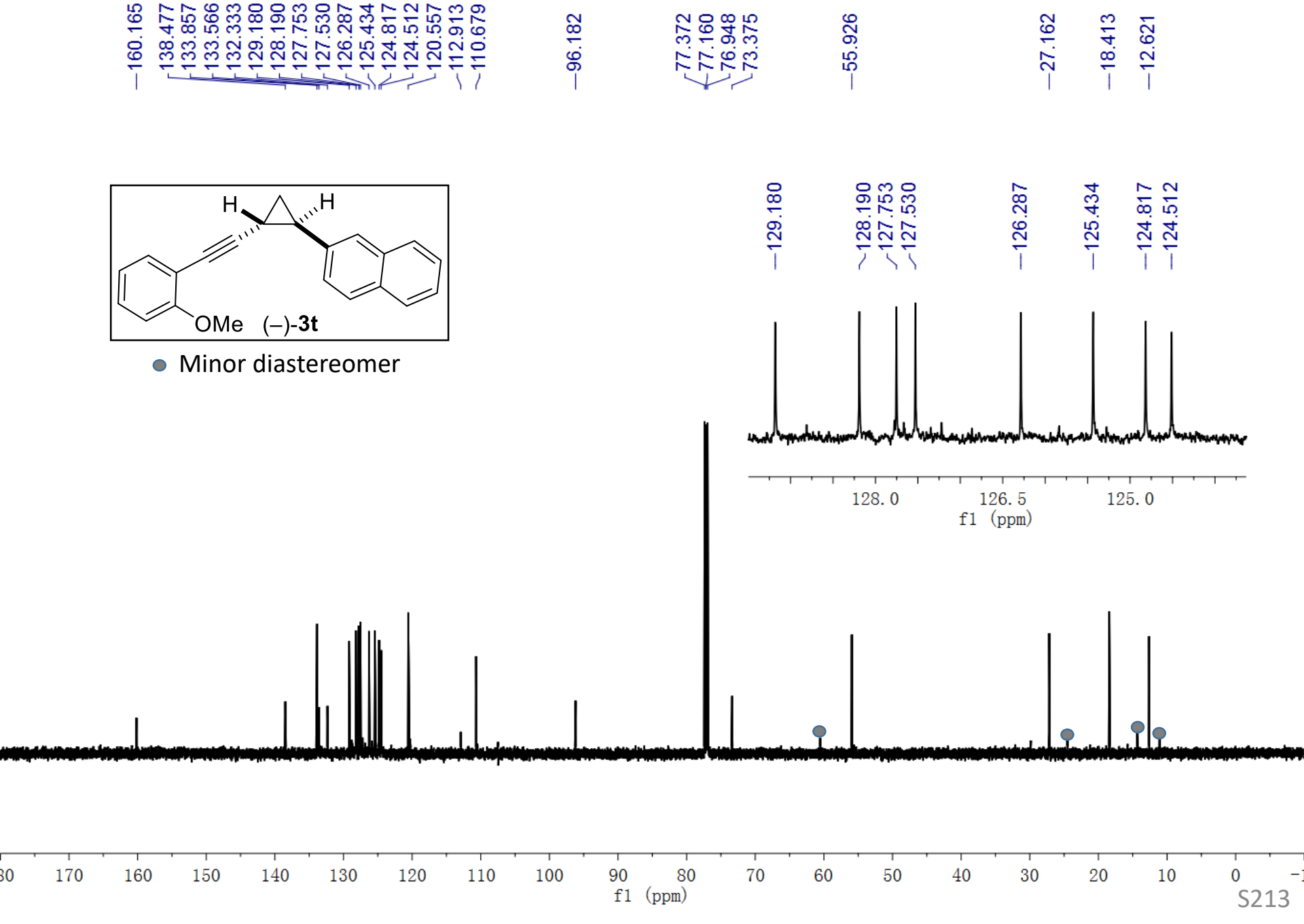
PDA Ch1 254nm

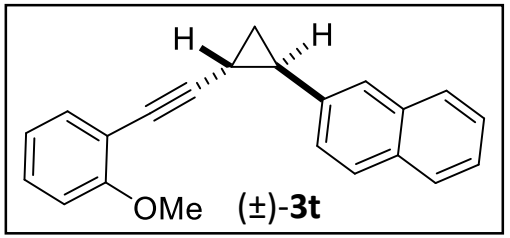
Peak#	Ret. Time	Area	Area%
1	13.360	804698	4.515
2	17.360	17019920	95.485
Total		17824619	100.000

^{1}H NMR of **3t**, 600 MHz, $CDCl_3$



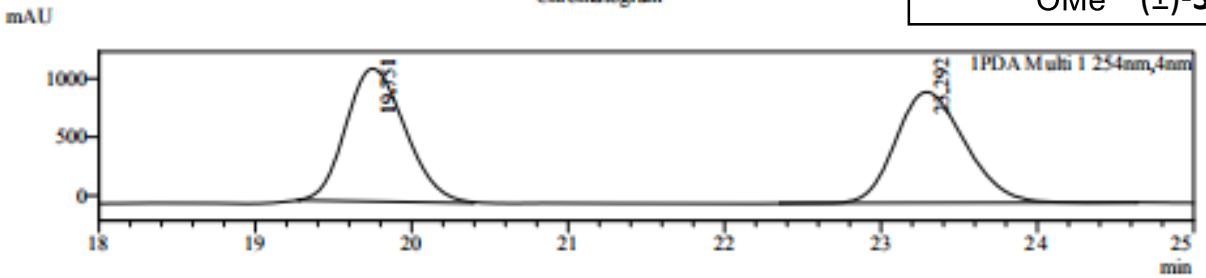
^{13}C NMR of **3t**, 151 MHz, $CDCl_3$



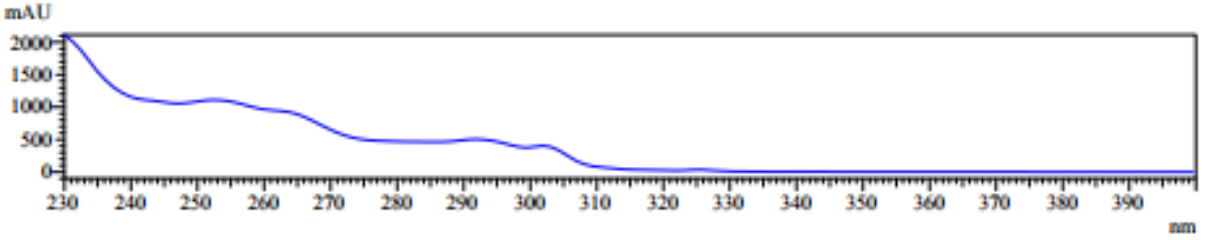


Data File : J0K-0340-IC-1%-0.8ML-isopropanol-solvent005.lcd
Sample Name : J0K-0340-IC-1%-0.8ML-isopropanol-solvent005
Sample ID : J0K-0340-IC-1%-0.8ML-isopropano
Method File : J0K-1%-0.8ml-50min.lcm

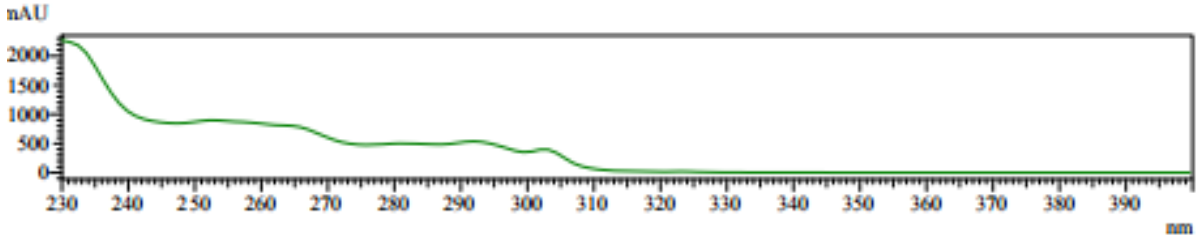
Chromatogram



UV Spectrum
Retention time = 19.751



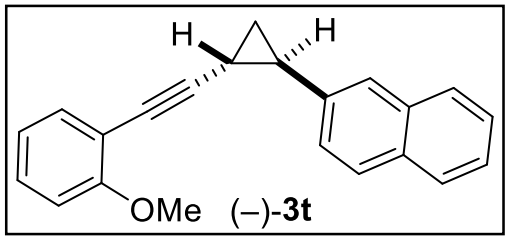
Retention time = 23.292



Peak Table

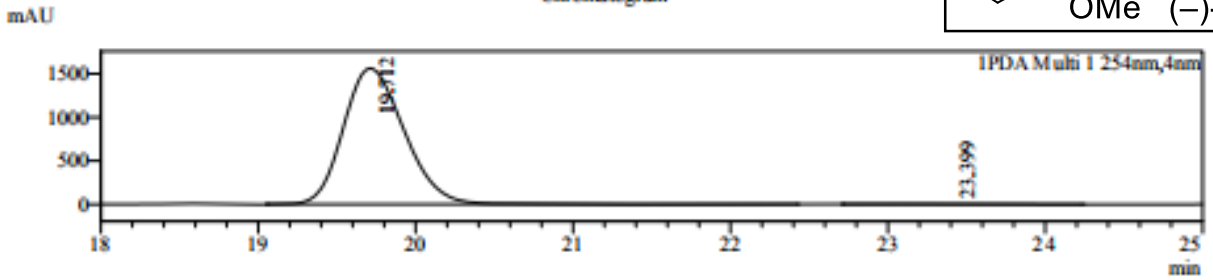
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	19.751	29870447	50.717
2	23.292	29025910	49.283
Total		58896357	100.000

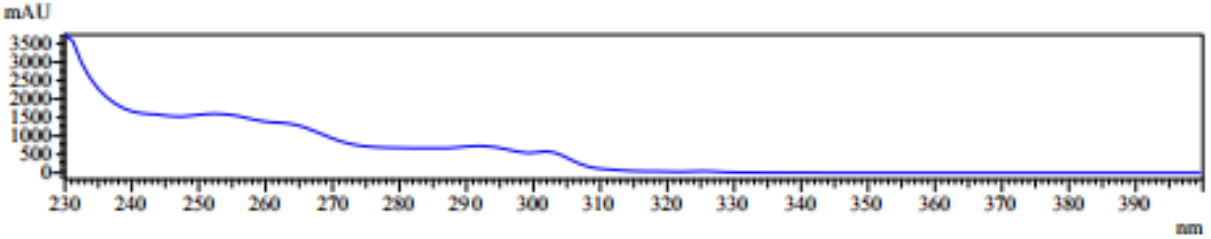


Data File : J0K-0336-2-IC-1%-0.8ML-isopropanol-solvent005.lcd
Sample Name : J0K-0336-2-IC-1%-0.8ML-isopropanol-solvent005
Sample ID : J0K-0336-2-IC-1%-0.8ML-isopropa
Method File : J0K-1%-0.8ml-50min.lcm

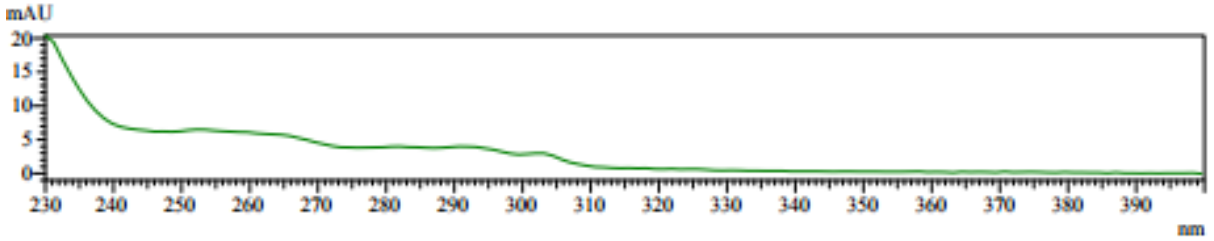
Chromatogram



UV Spectrum
Retention time = 19.712



U
Retention time = 23.399

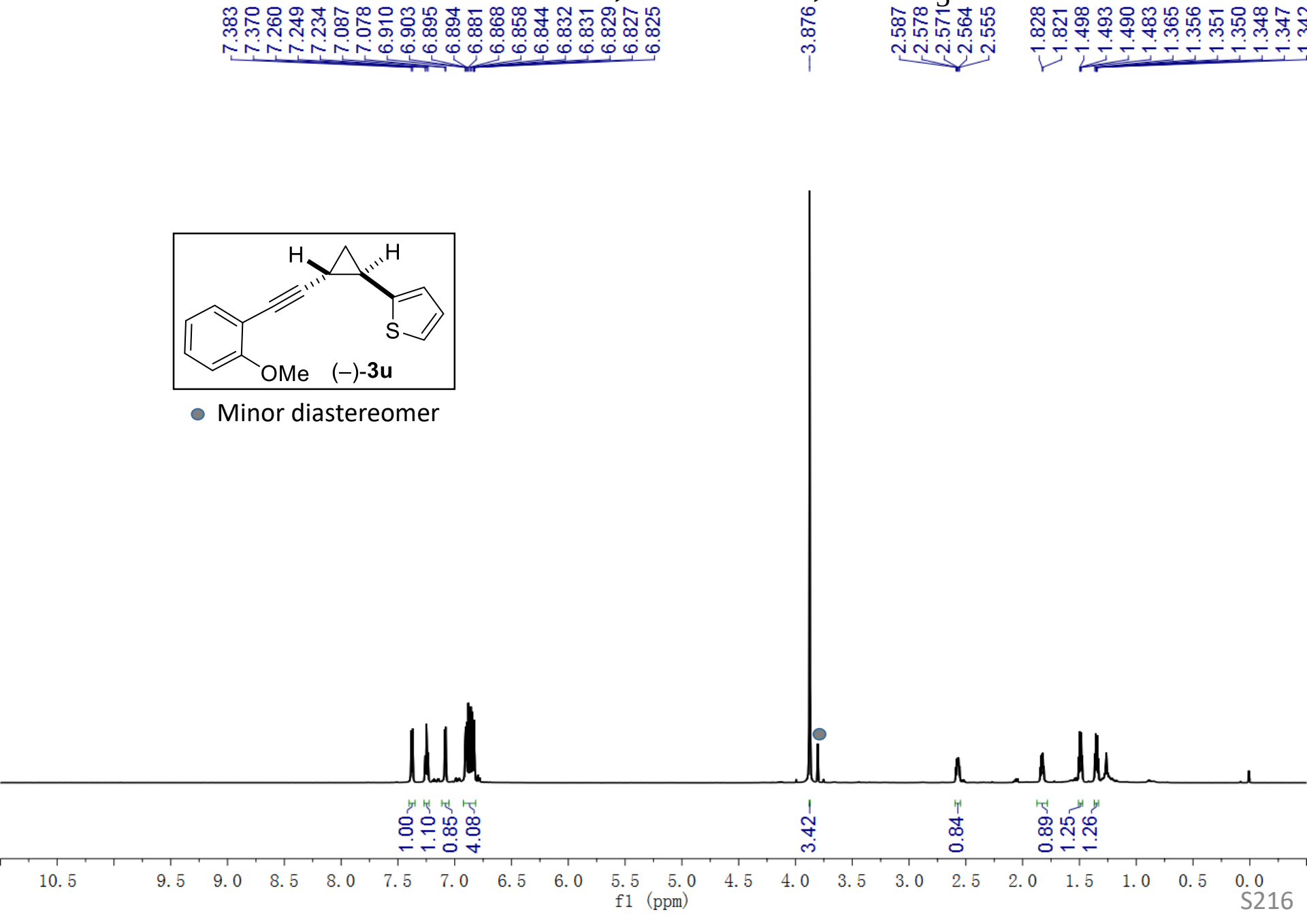


Peak Table

PDA Ch1 254nm

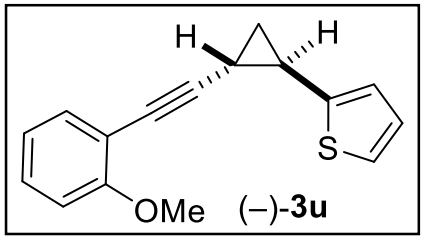
Peak#	Ret. Time	Area	Area%
1	19.712	41874366	99.587
2	23.399	173574	0.413
Total		42047940	100.000

^{1}H NMR of **3u**, 600 MHz, $CDCl_3$



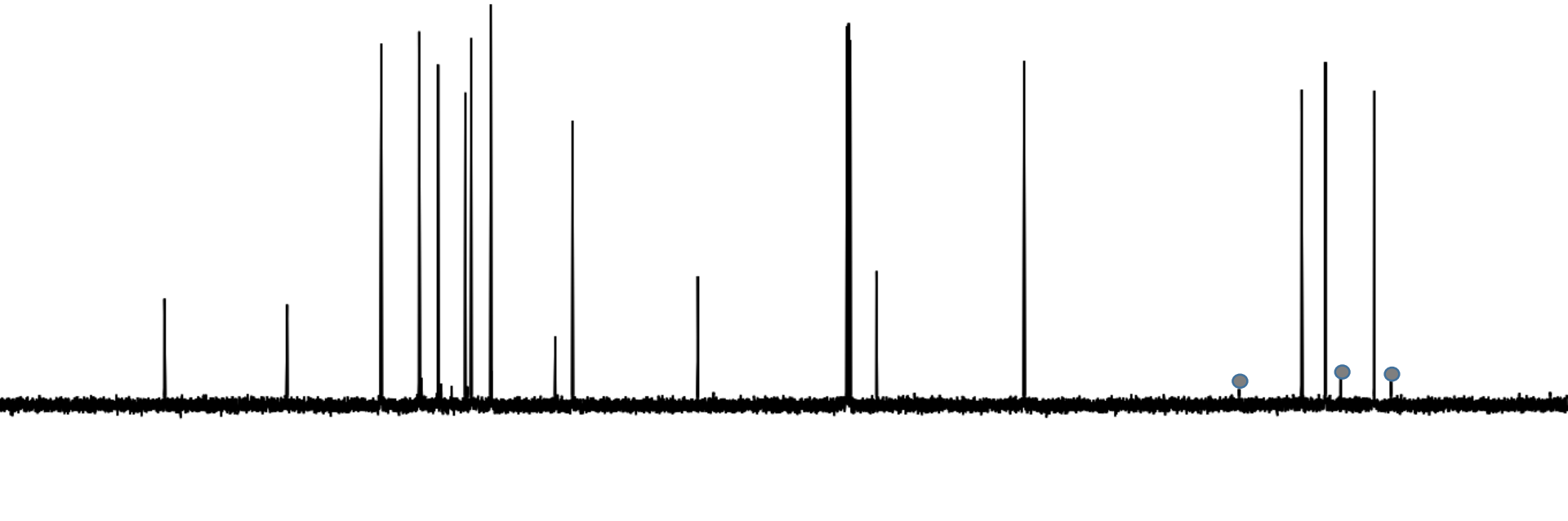
^{13}C NMR of **3u**, 151 MHz, $CDCl_3$

160.117
145.236
133.817
129.237
126.934
123.638
122.921
120.526
112.728
110.640
95.448
77.371
77.160
76.948
73.782
55.879
22.243
19.347
13.437



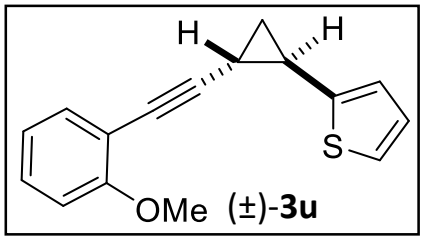
(–)-**3u**

● Minor diastereomer



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

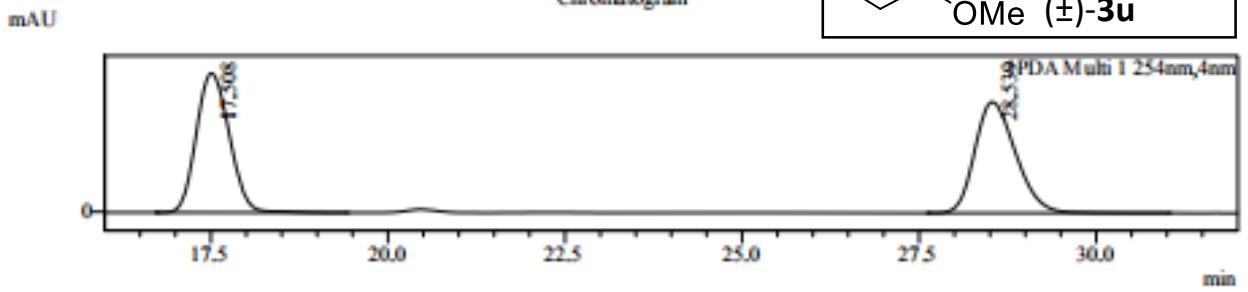
f1 (ppm)



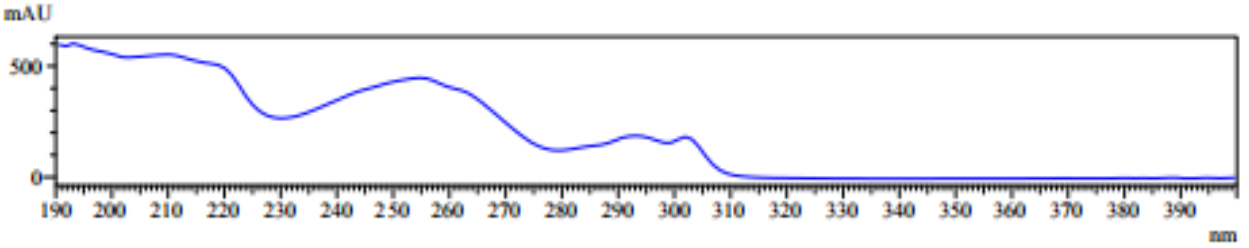
(±)-**3u**

Data File : J0K-0589-4-IC-0.5%-0.8ML.lcd
Sample Name : J0K-0589-4-IC-0.5%-0.8ML
Sample ID : J0K-0589-4-IC-0.5%-0.8ML
Method File : J0K-0.5%--60min-0.8ml.lcm

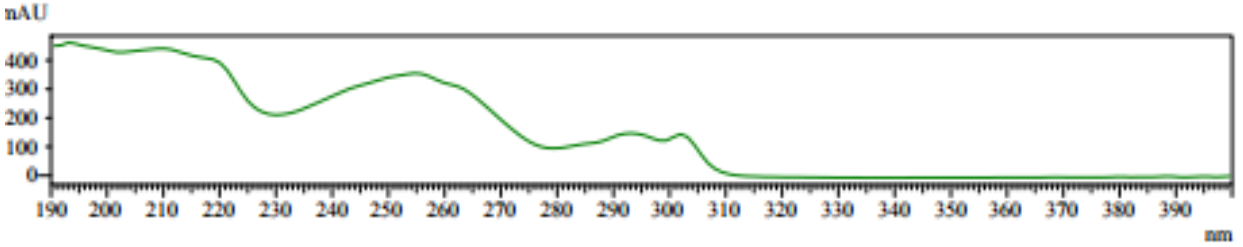
Chromatogram



UV Spectrum
Retention time = 17.508



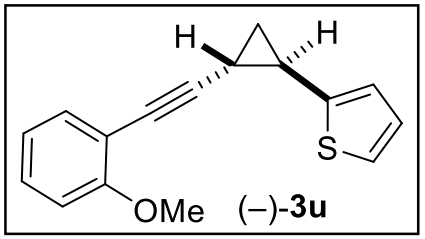
Retention time = 28.539



Peak Table

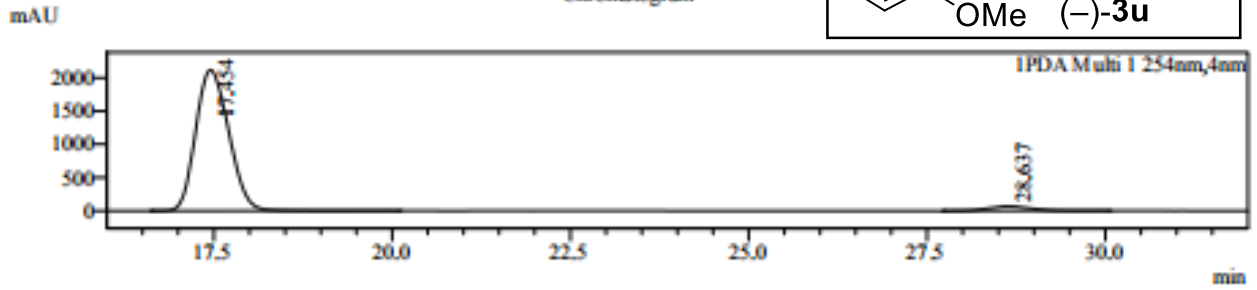
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	17.508	14384167	50.400
2	28.539	14155965	49.600
Total		28540132	100.000

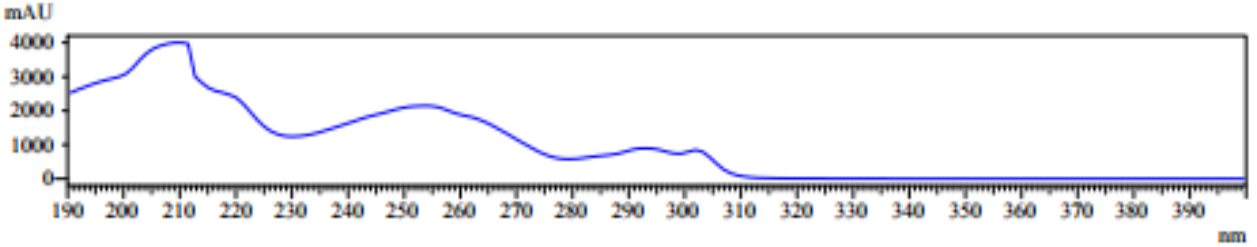


Data File : J0K-0588-4-IC-0.5%-0.8ML.lcd
Sample Name : J0K-0588-4-IC-0.5%-0.8ML
Sample ID : J0K-0588-4-IC-0.5%-0.8ML
Method File : J0K-0.5%--60min-0.8ml.lcm

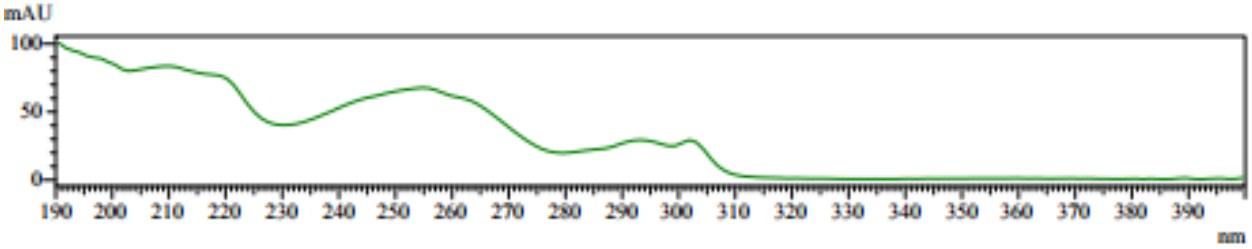
Chromatogram



UV Spectrum
Retention time = 17.454



U
Retention time = 28.637

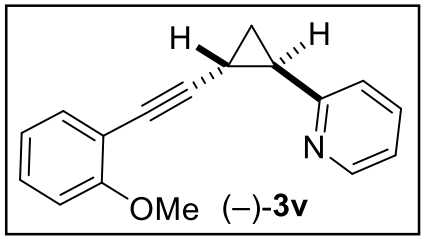


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	17.454	68120738	96.222
2	28.637	2674806	3.778
Total		70795544	100.000

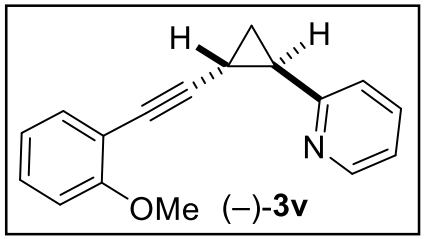
^{1}H NMR of **3v**, 600 MHz, $CDCl_3$



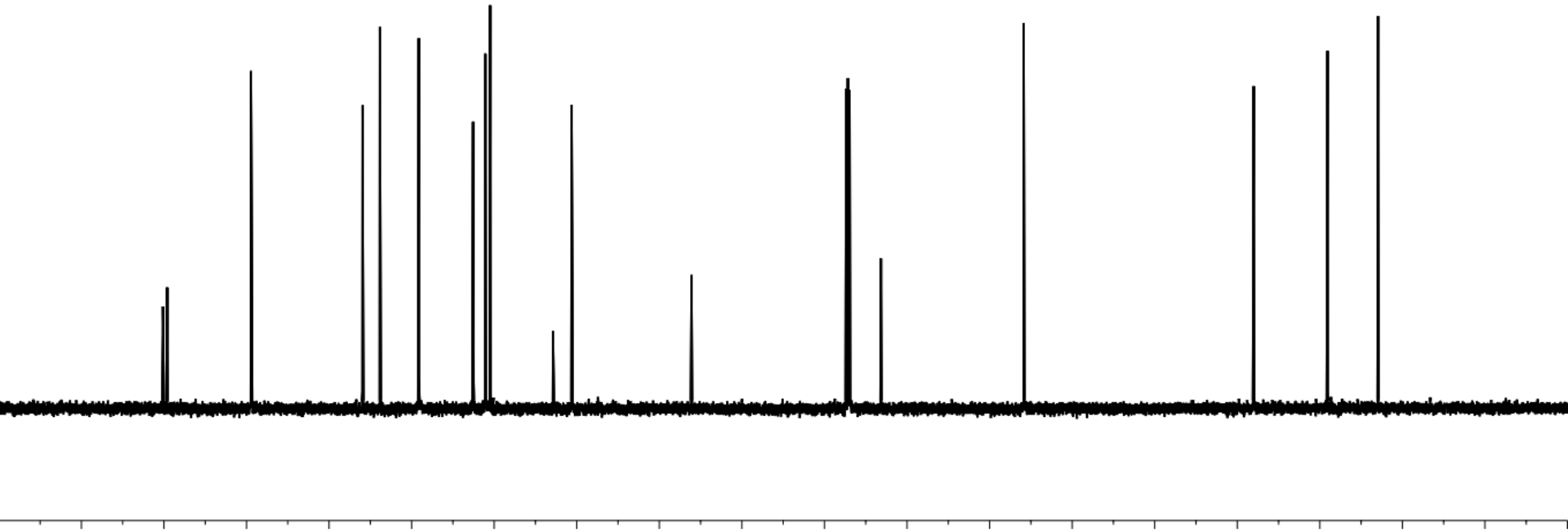
(–)-**3v**

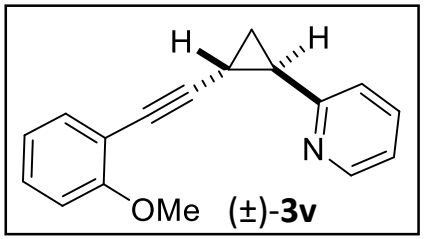
^{13}C NMR of **3v**, 151 MHz, $CDCl_3$

160.126
159.602
149.451
135.942
133.845
129.126
122.555
121.065
120.495
112.872
110.622
96.103
77.371
77.160
76.948
73.159
55.862
28.015
19.063
12.944



(–)-**3v**

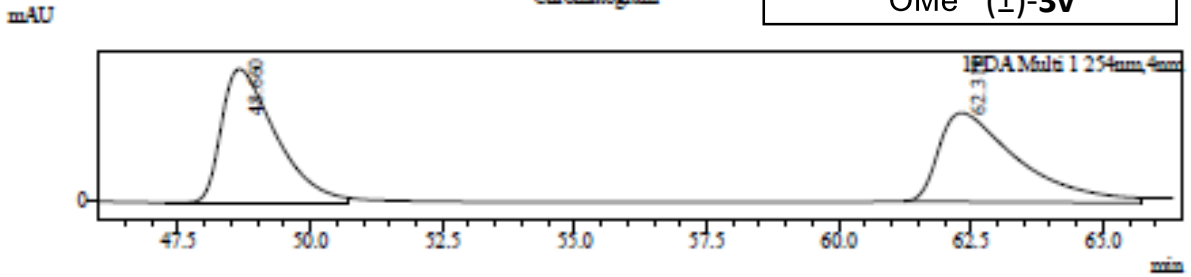




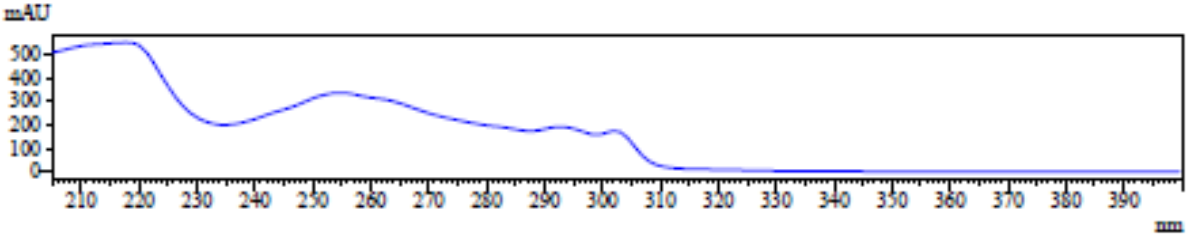
(±)-**3v**

Data File : J0K-0600-2-IC--0.5%-1ML.lcd
Sample Name : J0K-0600-2-IC--0.5%-1ML
Sample ID : J0K-0600-2-IC--0.5%-1ML
Method File : J0K-0.5%--80min-1ml.lcm

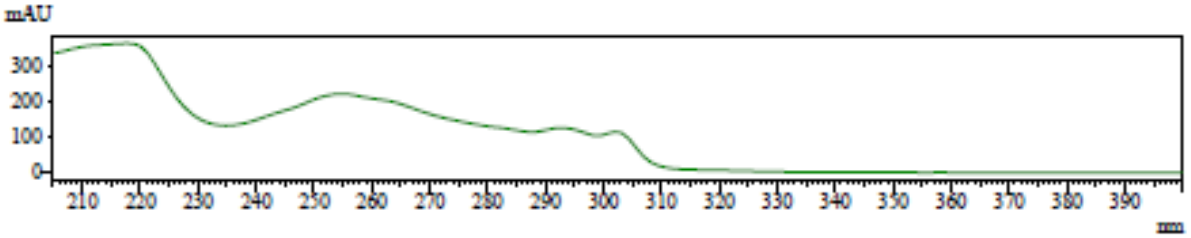
Chromatogram



UV Spectrum
Retention time = 48.660



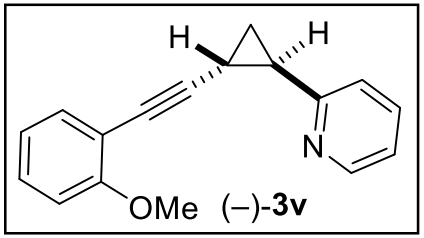
UV Spectrum
Retention time = 62.317



Peak Table

PDA Ch1 254nm

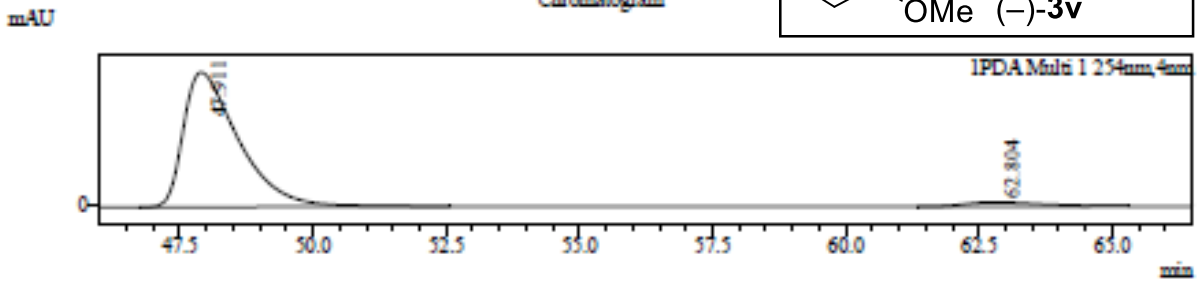
Peak#	Ret. Time	Area	Area%
1	48.660	24316400	50.828
2	62.317	23524334	49.172
Total		47840733	100.000



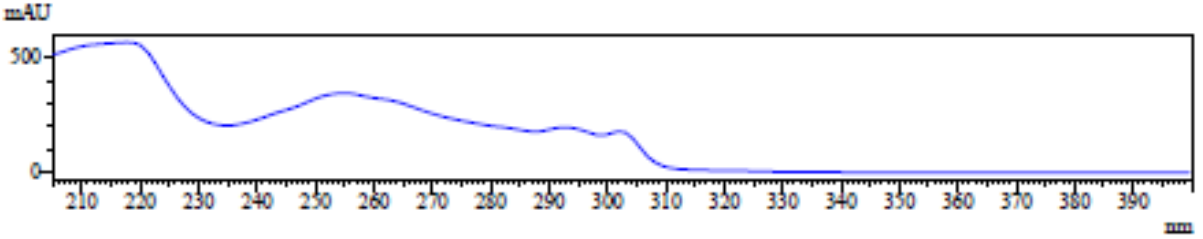
(−)-**3v**

Data File : J0K-0599--2-IC--0.5%-1ML.lcd
Sample Name : J0K-0599--2-IC--0.5%-1ML
Sample ID : J0K-0599--2-IC--0.5%-1ML
Method File : J0K-0.5%--80min-1ml.lcm

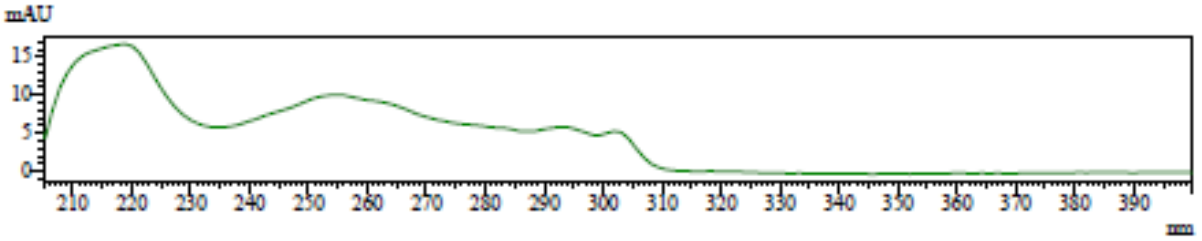
Chromatogram



UV Spectrum
Retention time = 47.911



UV Spectrum
Retention time = 62.804

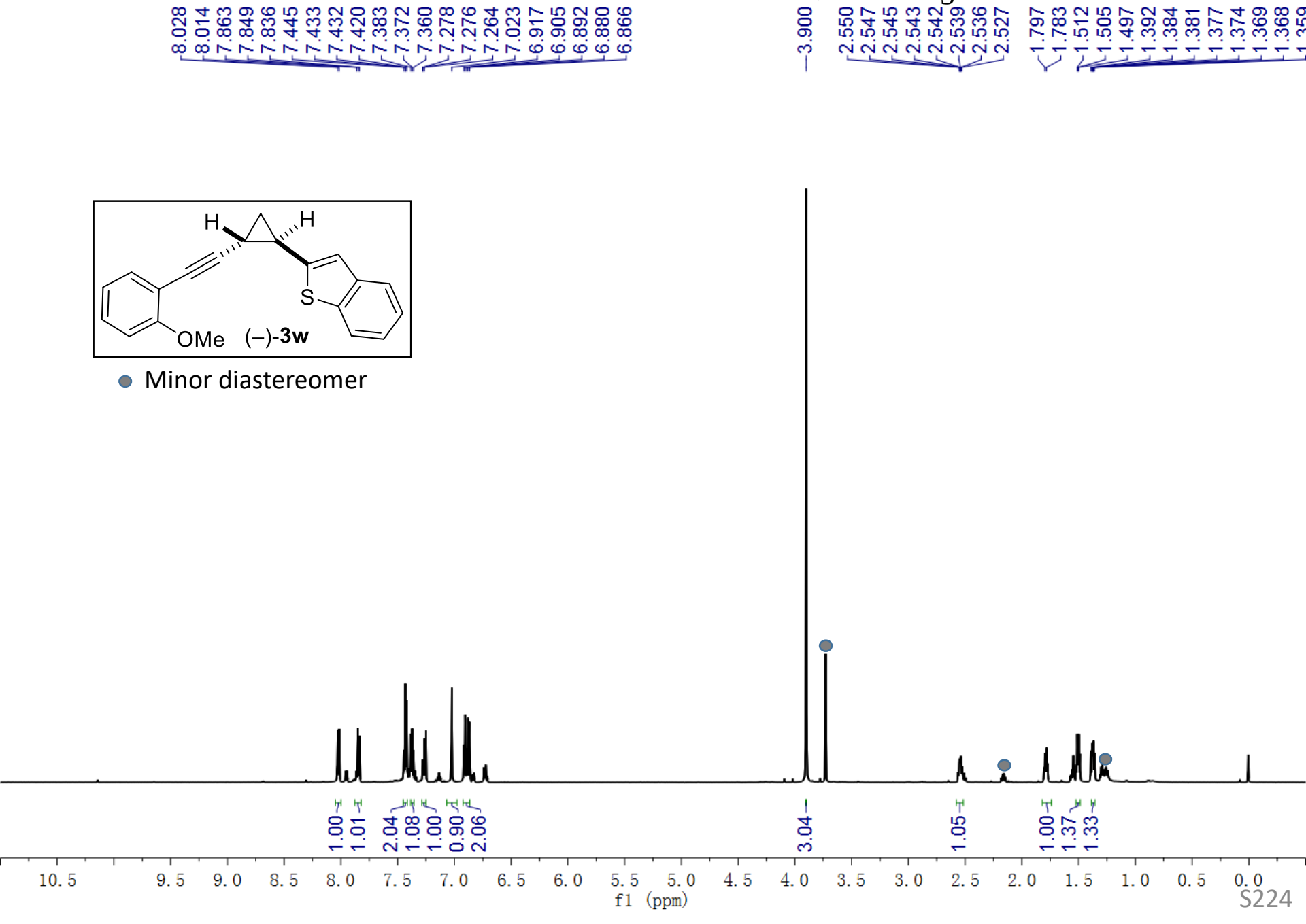


Peak Table

PDA Ch1 254nm

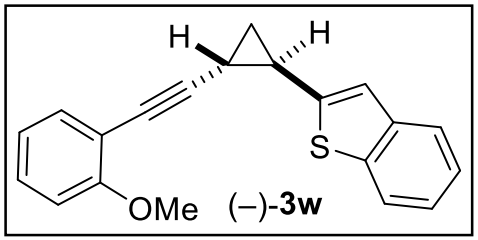
Peak#	Ret. Time	Area	Area%
1	47.911	24636457	95.788
2	62.804	1083431	4.212
Total		25719888	100.000

^{1}H NMR of **3w**, 600 MHz, $CDCl_3$



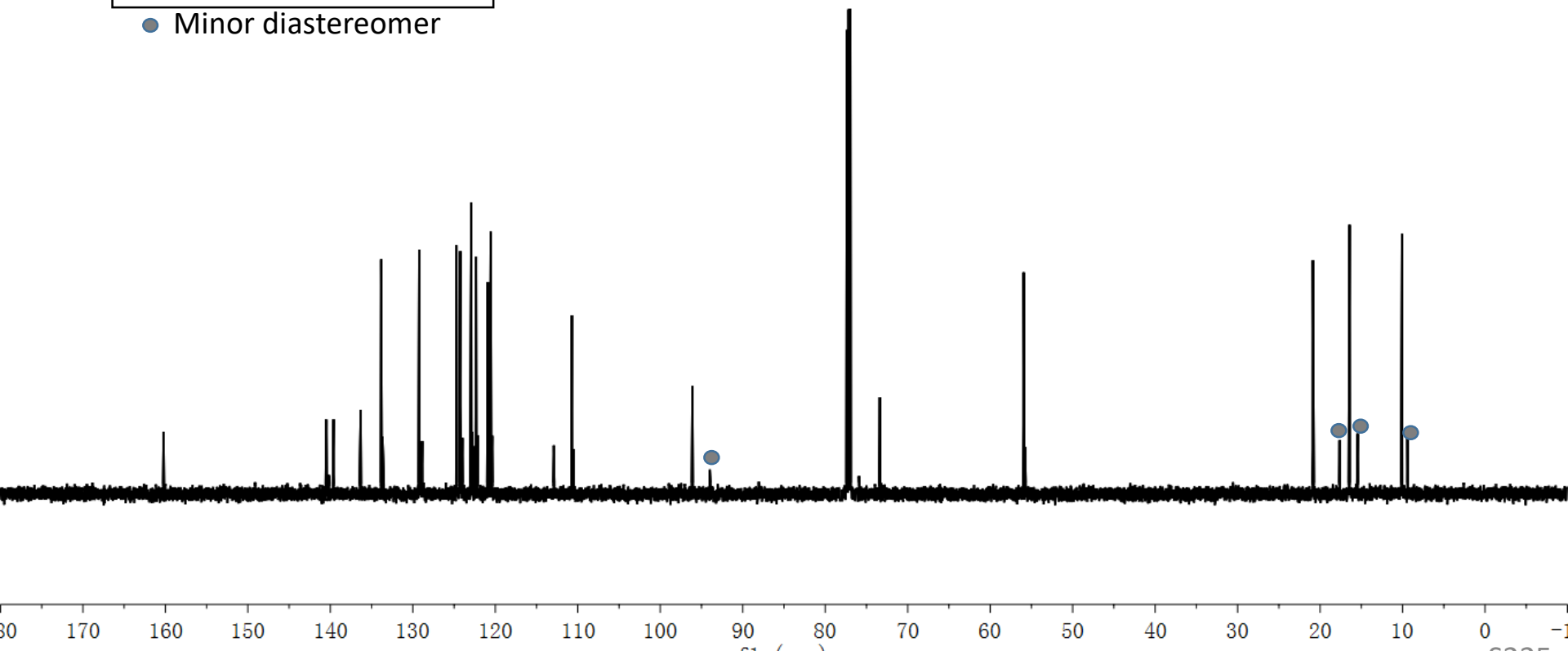
^{13}C NMR of **3w**, 151 MHz, $CDCl_3$

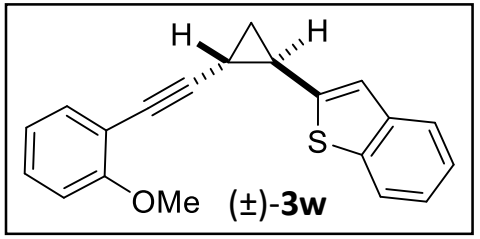
160.221
140.486
139.614
136.328
133.853
129.226
124.711
124.248
122.918
122.337
120.906
120.561
112.905
110.717
96.105
77.372
77.160
76.949
73.381
55.937
20.874
16.424
10.073



(–)-**3w**

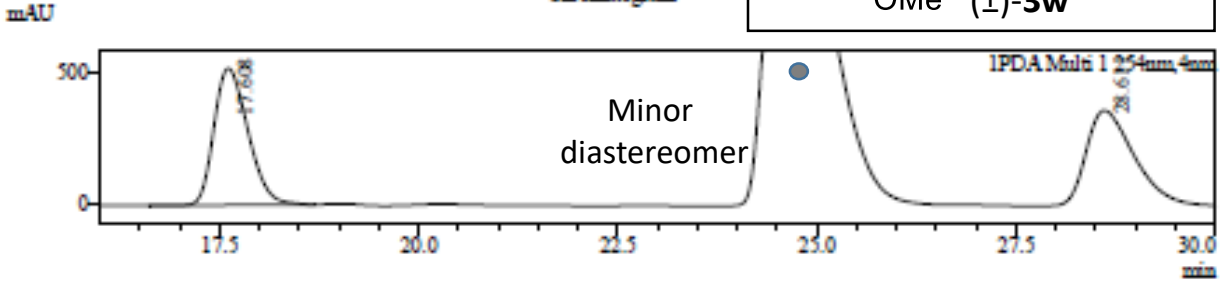
● Minor diastereomer



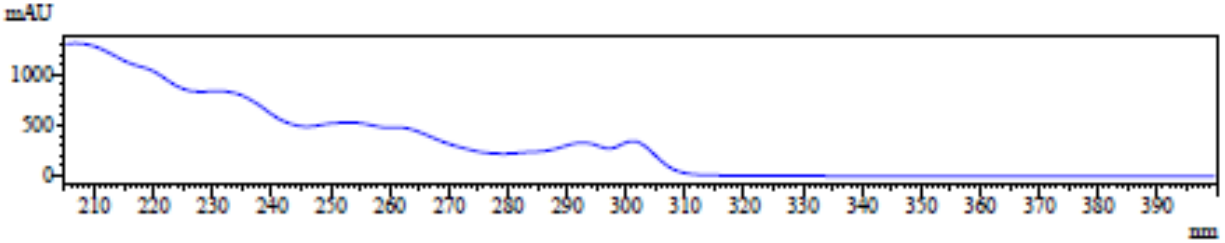


Data File : J0K-0587-3-IC-0.5%-0.8ML.lcd
Sample Name : J0K-0587-3-IC-0.5%-0.8ML
Sample ID : J0K-0587-3-IC-0.5%-0.8ML
Method File : J0K-0.5%--60min-0.8ml.lcm

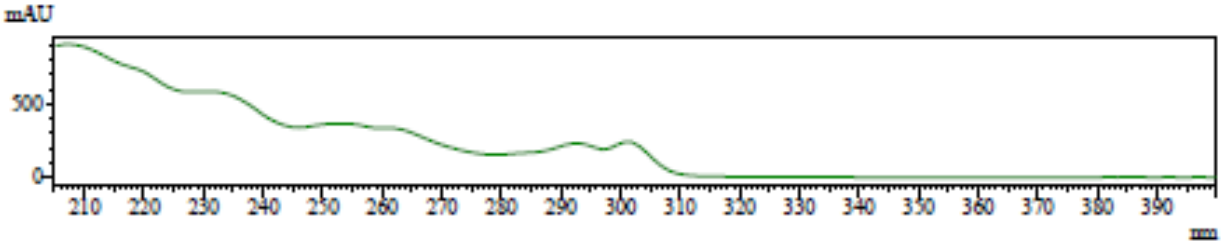
Chromatogram



UV Spectrum
Retention time = 17.608



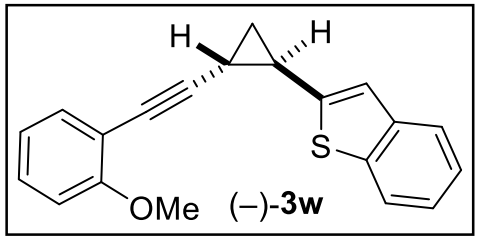
UV Spectrum
Retention time = 28.611



Peak Table

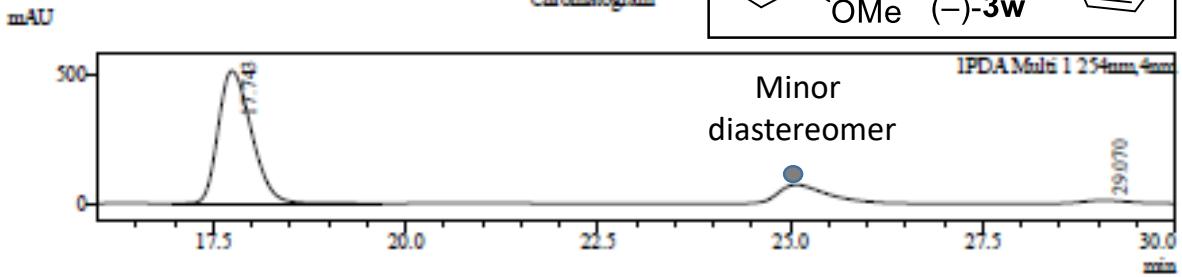
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	17.608	15423522	50.194
2	28.611	15304308	49.806
Total		30727830	100.000

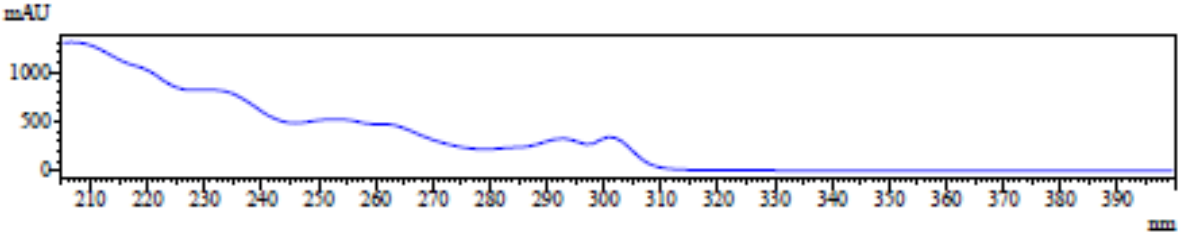


Data File : J0K-0586-IC-0.5%-0.8ML.lcd
Sample Name : J0K-0586-IC-0.5%-0.8ML
Sample ID : J0K-0586-IC-0.5%-0.8ML
Method File : J0K-0.5%--60min-0.8ml.lcm

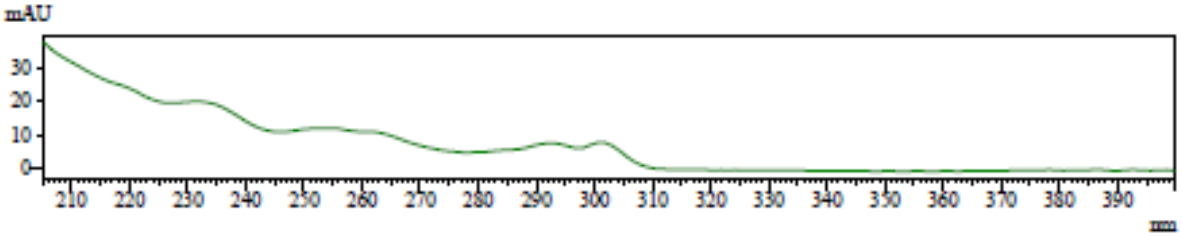
Chromatogram



UV Spectrum
Retention time = 17.743



UV Spectrum
Retention time = 29.070

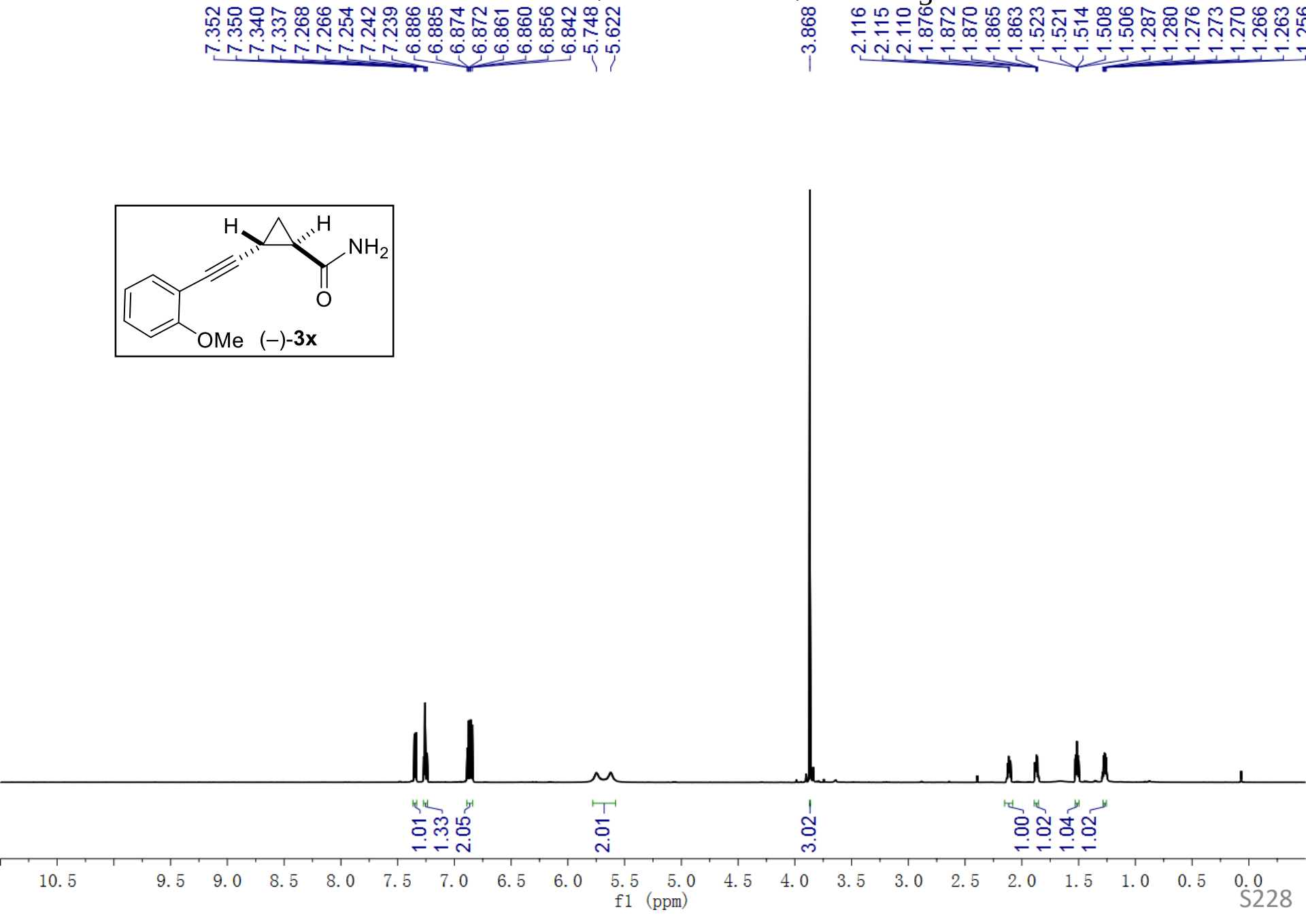


Peak Table

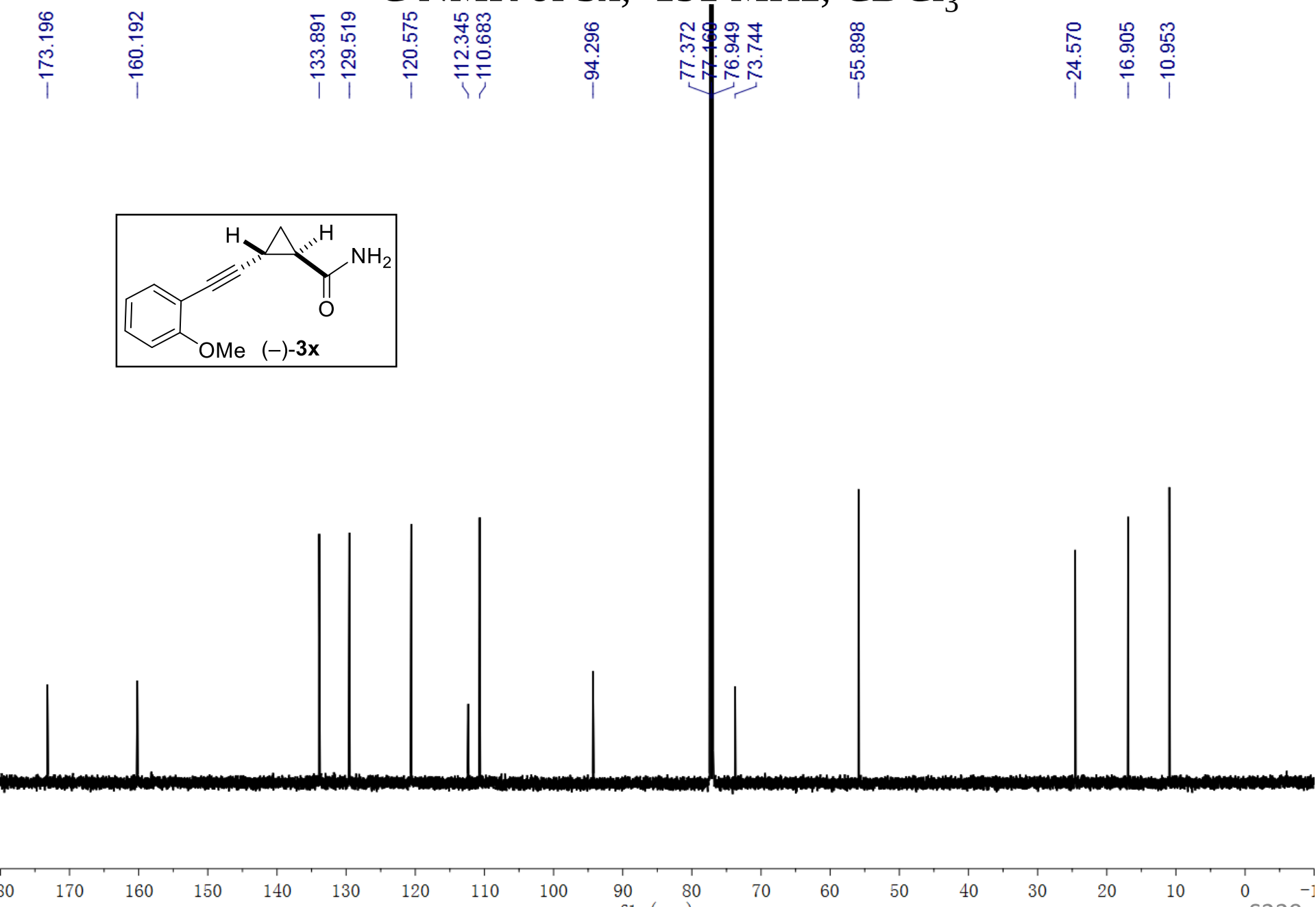
PDA Ch1 254nm

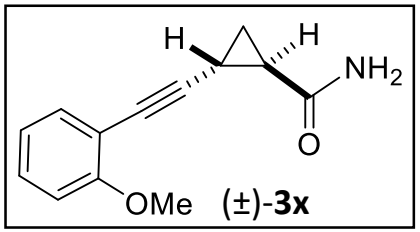
Peak#	Ret. Time	Area	Area%
1	17.743	15440731	96.643
2	29.070	536357	3.357
Total		15977089	100.000

^{1}H NMR of **3x**, 600 MHz, $CDCl_3$



^{13}C NMR of **3x**, 151 MHz, $CDCl_3$

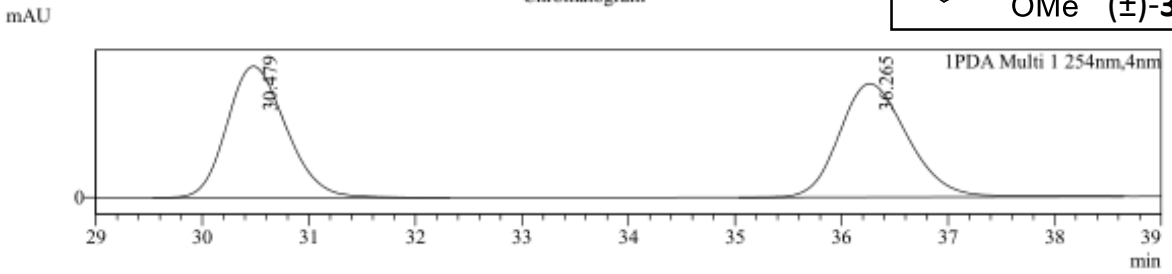




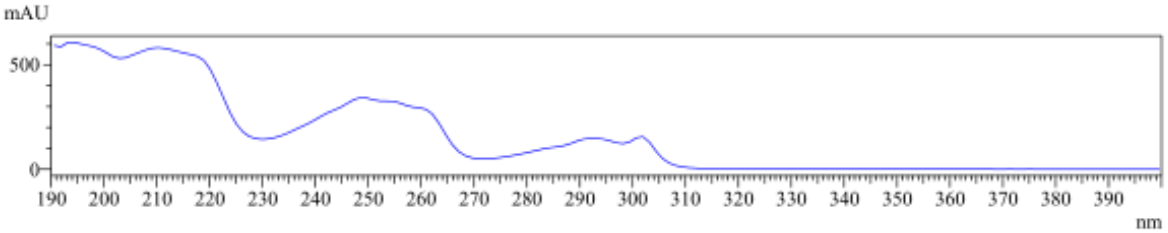
(±)-**3x**

Data File : J0K-0342-IC-1%-0.8ML-isopropanol-solvent005.lcd
Sample Name : J0K-0342-IC-1%-0.8ML-isopropanol-solvent005
Sample ID : J0K-0342-IC-1%-0.8ML-isopropano
Method File : J0K-1%-0.8ml-50min.lcm

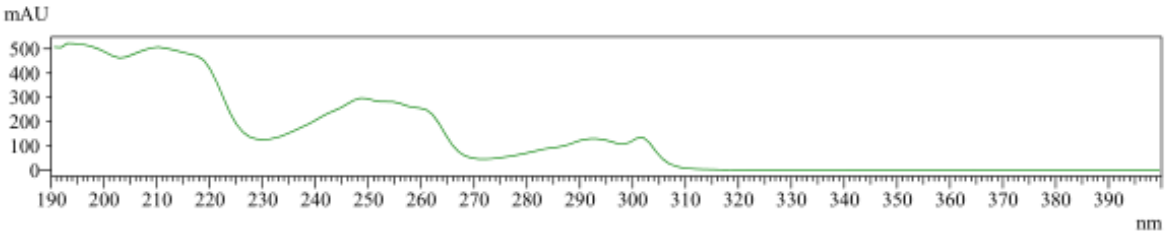
Chromatogram



UV Spectrum
Retention time = 30.479



UV Spectrum
Retention time = 36.265

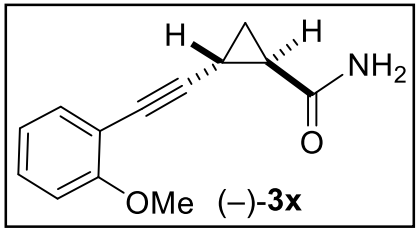


Peak Table

PDA Ch1 254nm

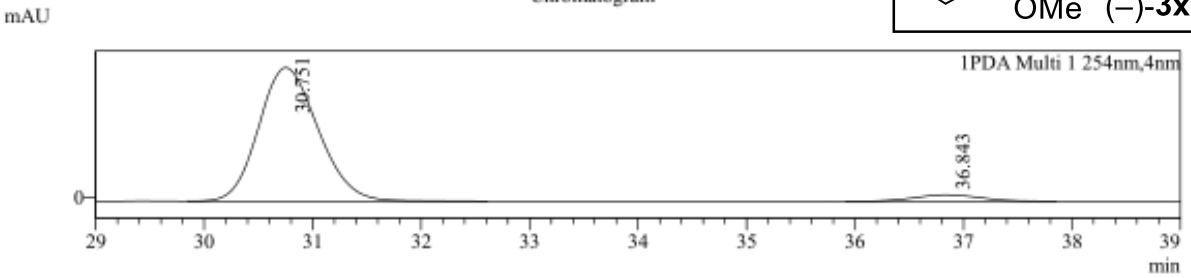
Peak#	Ret. Time	Area	Area%
1	30.479	12463706	50.047
2	36.265	12440286	49.953
Total		24903992	100.000

Data File : J0K-0310-IC-1%-0.8ML-isopropanol-solvent008.lcd
Sample Name : J0K-0310-IC-1%-0.8ML-isopropanol-solvent008
Sample ID : J0K-0310-IC-1%-0.8ML-isopropano
Method File : J0K-1%-0.8m-50MINl.lcm

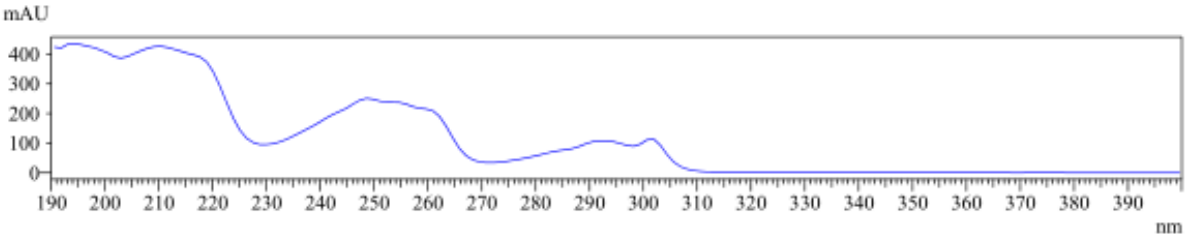


(–)-**3x**

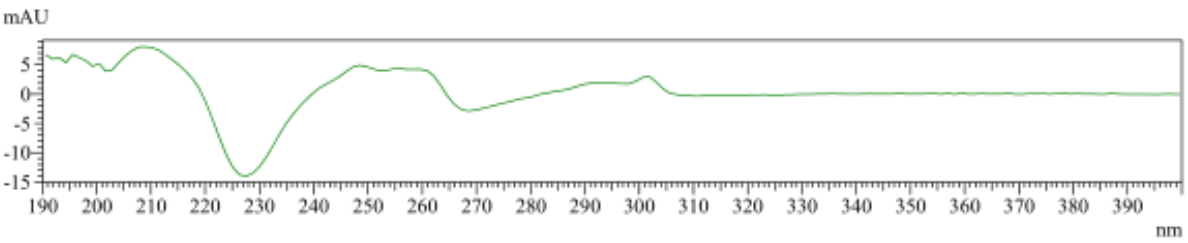
Chromatogram



UV Spectrum
Retention time = 30.751



UV Spectrum
Retention time = 36.843

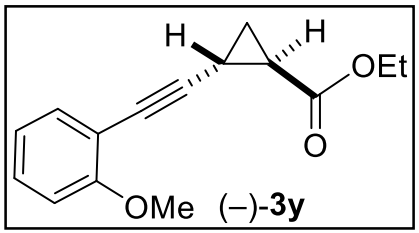


Peak Table

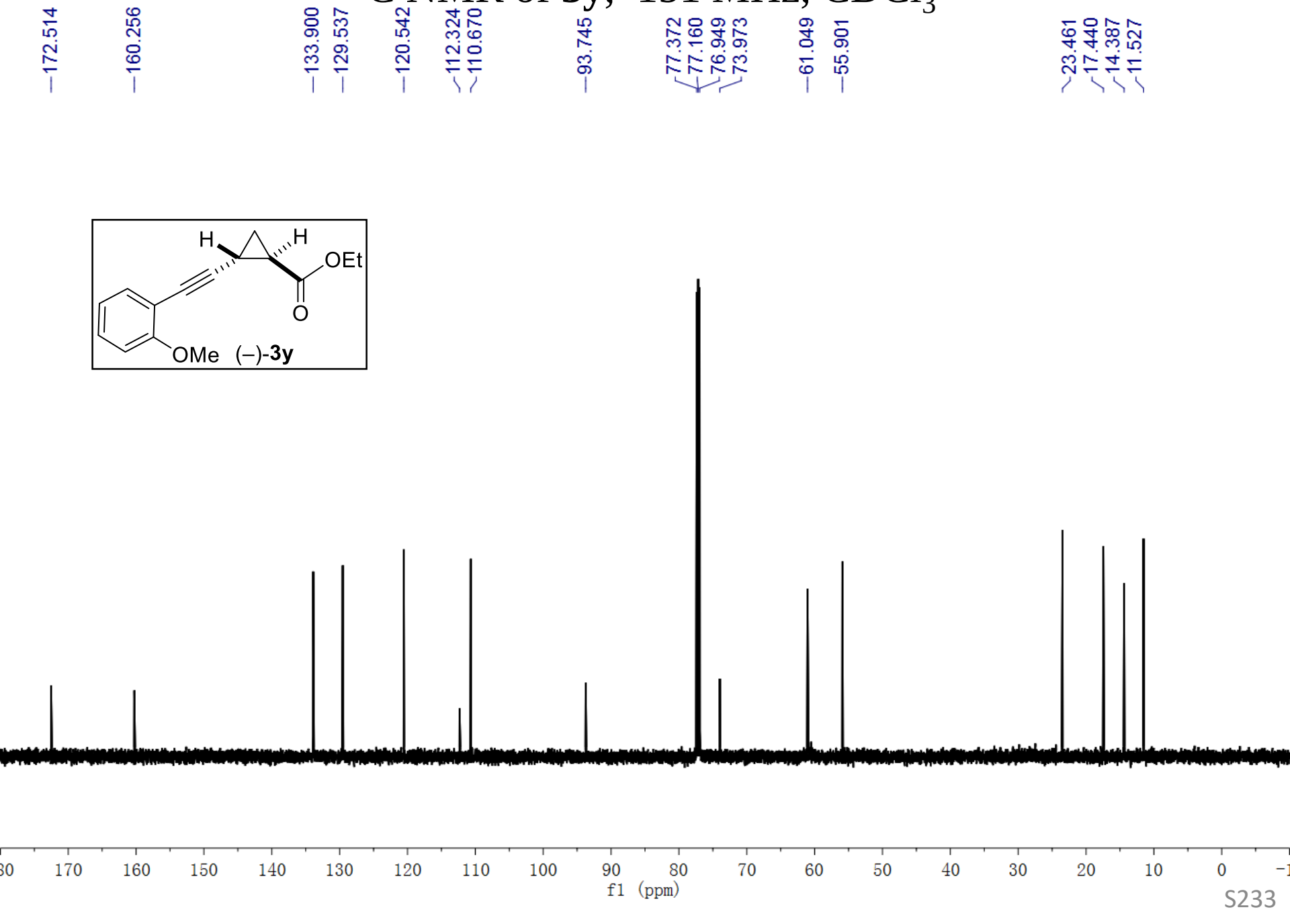
PDA Ch1 254nm

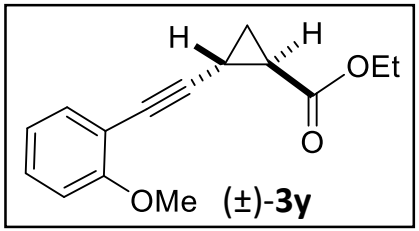
Peak#	Ret. Time	Area	Area%
1	30.751	9217551	94.697
2	36.843	516187	5.303
Total		9733738	100.000

^{1}H NMR of **3y**, 600 MHz, $CDCl_3$



^{13}C NMR of **3y**, 151 MHz, $CDCl_3$

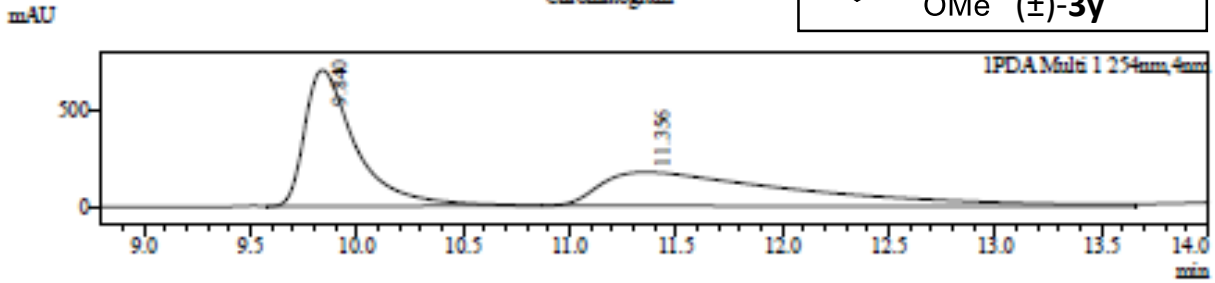




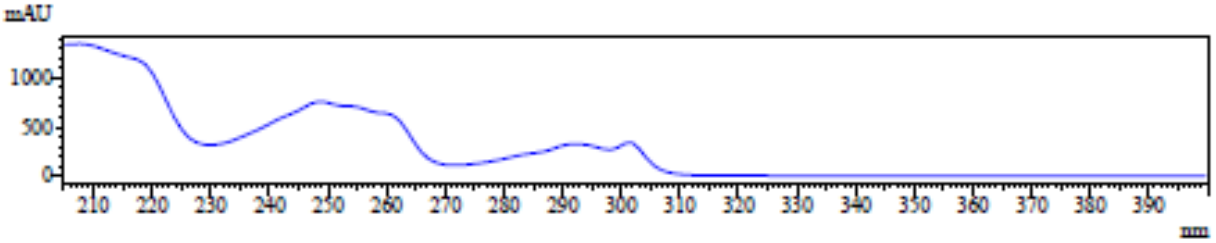
(±)-**3y**

Data File : J0K-1514-new-LA--0.3%-1ML.lcd
Sample Name : J0K-1514-new-LA--0.3%-1ML
Sample ID : J0K-1514-new-LA--0.3%-1ML
Method File : J0K-0.3%--45min-1ml.lcm

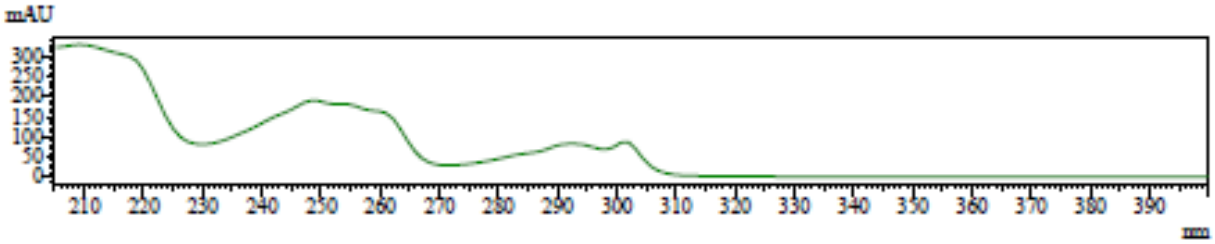
Chromatogram



UV Spectrum
Retention time = 9.840



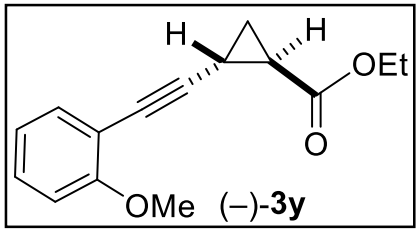
UV Spectrum
Retention time = 11.356



Peak Table

PDA Ch1 254nm

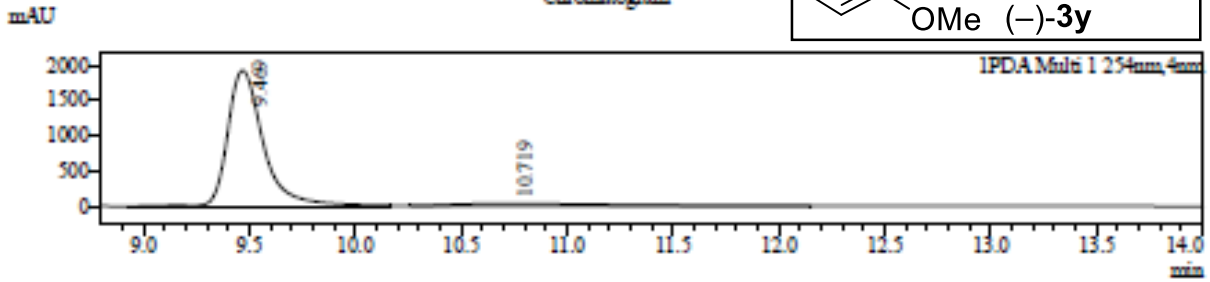
Peak#	Ret. Time	Area	Area%
1	9.840	11607489	50.875
2	11.356	11208328	49.125
Total		22815817	100.000



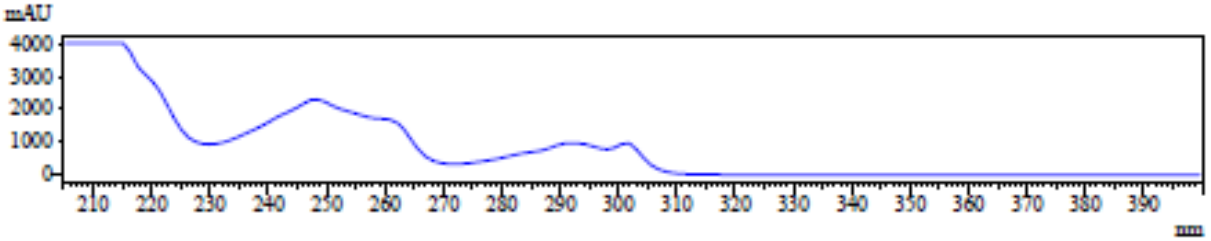
(–)-**3y**

Data File : J0K-1513-IA--0.3%-1ML.lcd
Sample Name : J0K-1513-IA--0.3%-1ML
Sample ID : J0K-1513-IA--0.3%-1ML
Method File : J0K-0.3%--25min-1ml.lcm

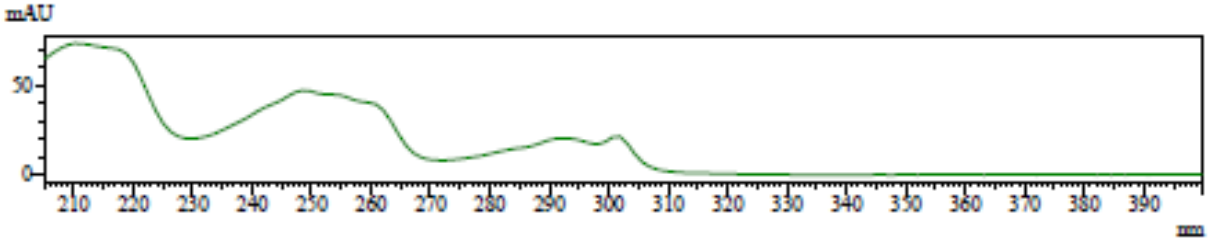
Chromatogram



UV Spectrum
Retention time = 9.469



UV Spectrum
Retention time = 10.719

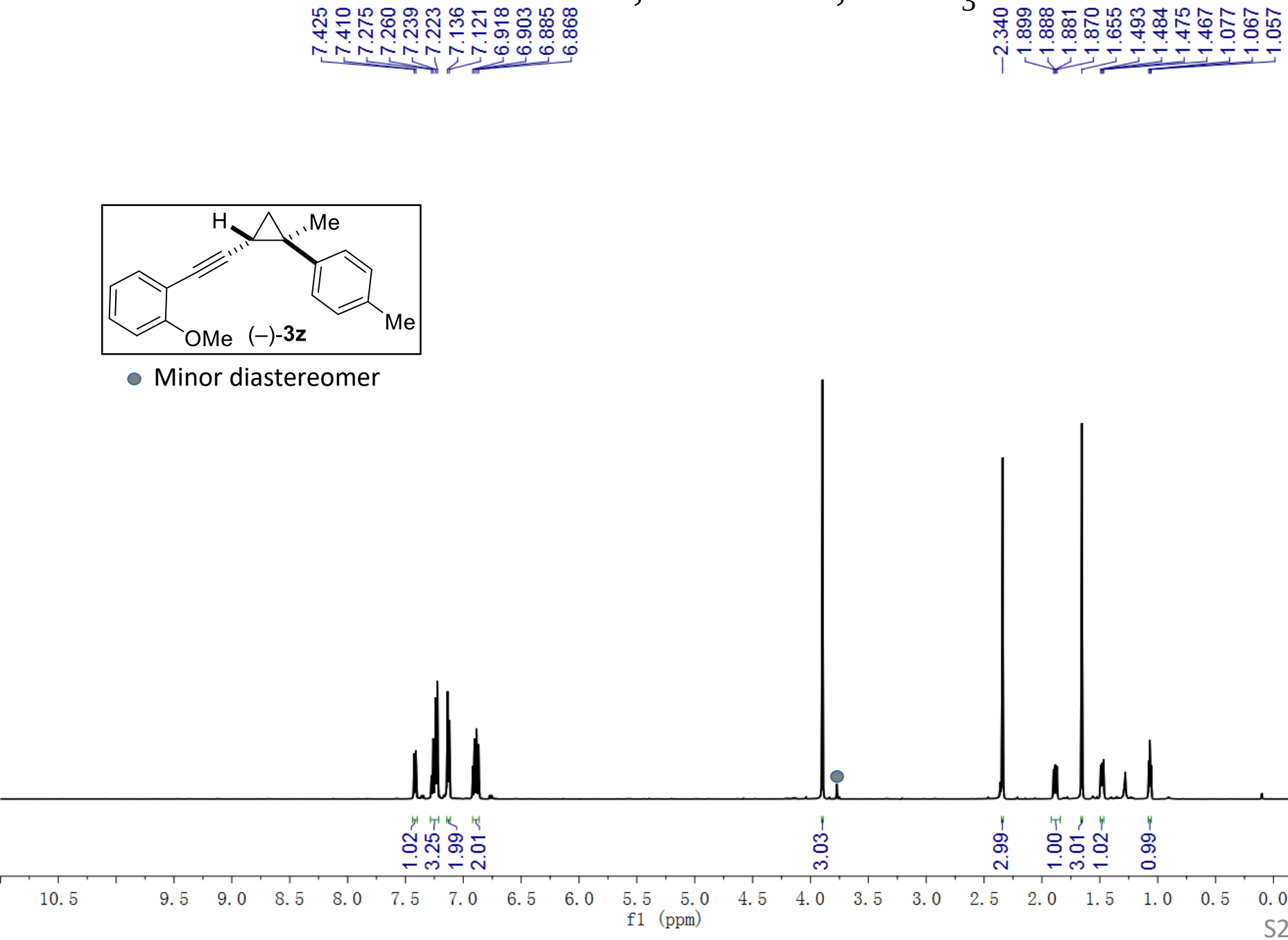


Peak Table

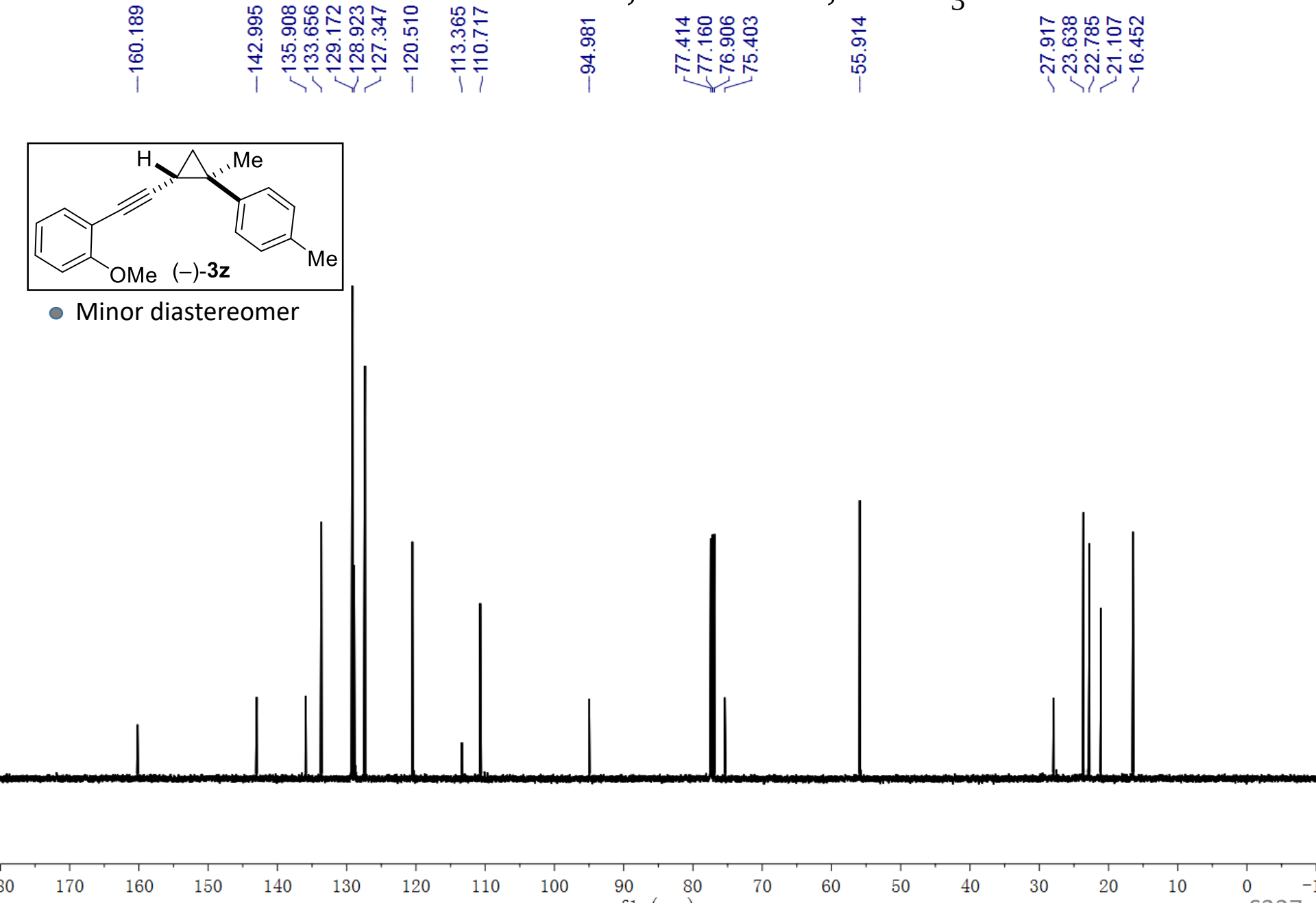
PDA Ch1 254nm

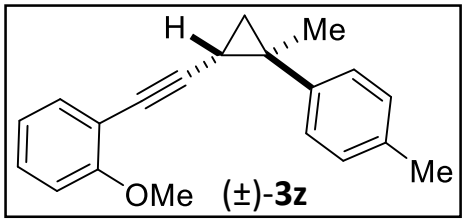
Peak#	Ret. Time	Area	Area%
1	9.469	22666700	93.877
2	10.719	1478374	6.123
Total		24145074	100.000

^{1}H NMR of **3z**, 500 MHz, $CDCl_3$



^{13}C NMR of **3z**, 126 MHz, $CDCl_3$

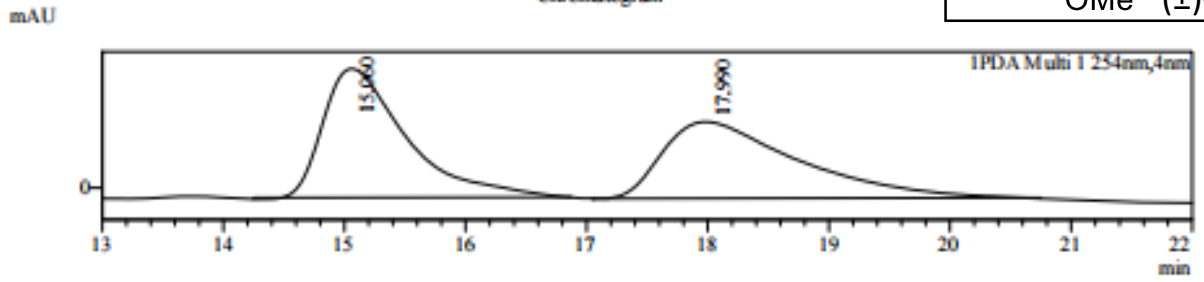




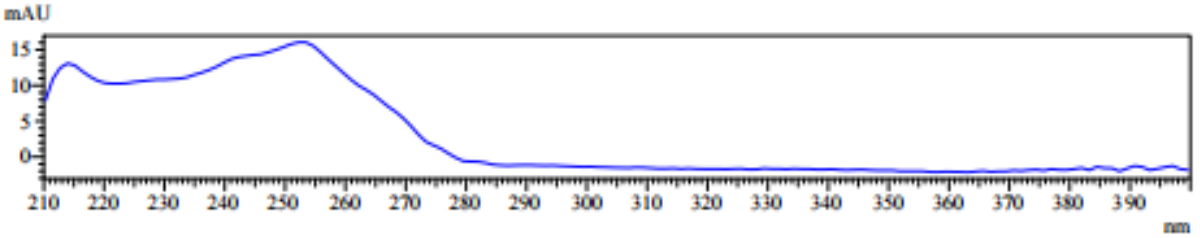
(±)-**3z**

Data File : J0K-0106-IC-0.5%-0.8ML-isopropanol-solvent003.lcd
Sample Name : J0K-0106-IC-0.5%-0.8ML-isopropanol-solvent003
Sample ID : J0K-0106-IC-0.5%-0.8ML-isopropa
Method File : JK-0%-0.8ml.lcm

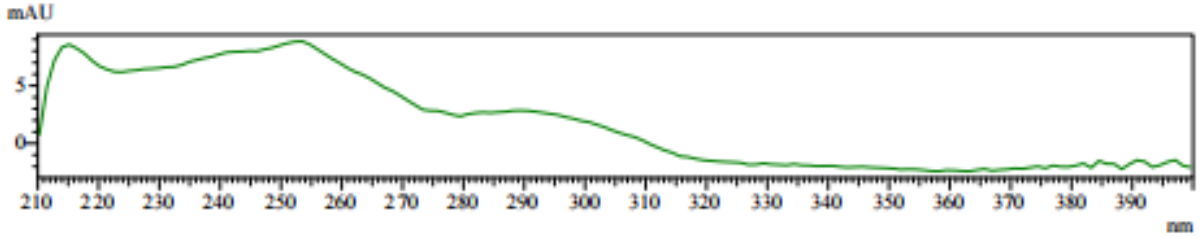
Chromatogram



UV Spectrum
Retention time = 15.060



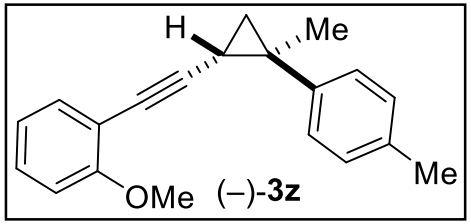
U
Retention time = 17.990



Peak Table

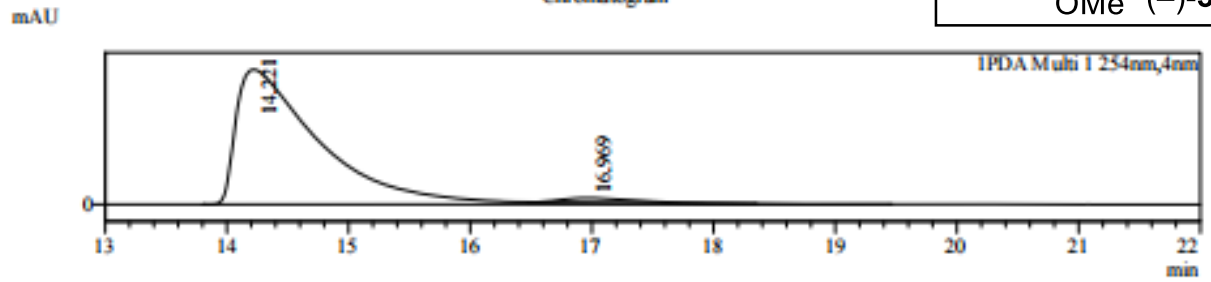
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	15.060	780497	50.719
2	17.990	758360	49.281
Total		1538857	100.000

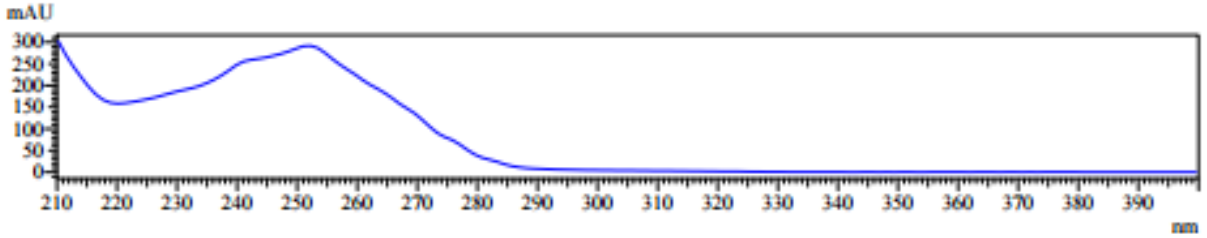


Data File : J0K-0108-IC-0.5%-0.8ML-isopropanol-solvent004.lcd
Sample Name : J0K-0108-IC-0.5%-0.8ML-isopropanol-solvent004
Sample ID : J0K-0108-IC-0.5%-0.8ML-isopropa
Method File : JK-0%-0.8ml.lcm

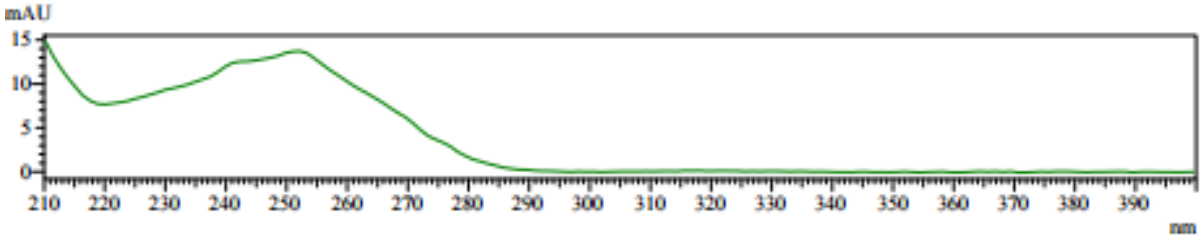
Chromatogram



UV Spectrum
Retention time = 14.221



U
Retention time = 16.969

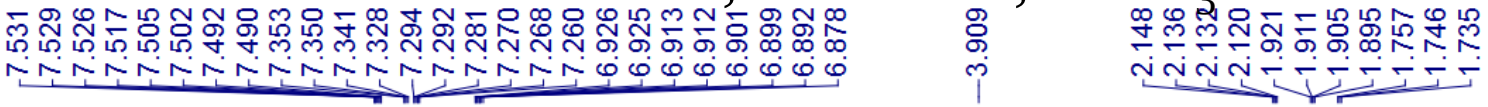


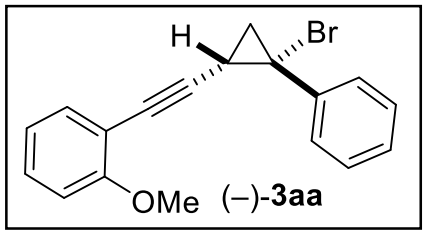
Peak Table

PDA Ch1 254nm

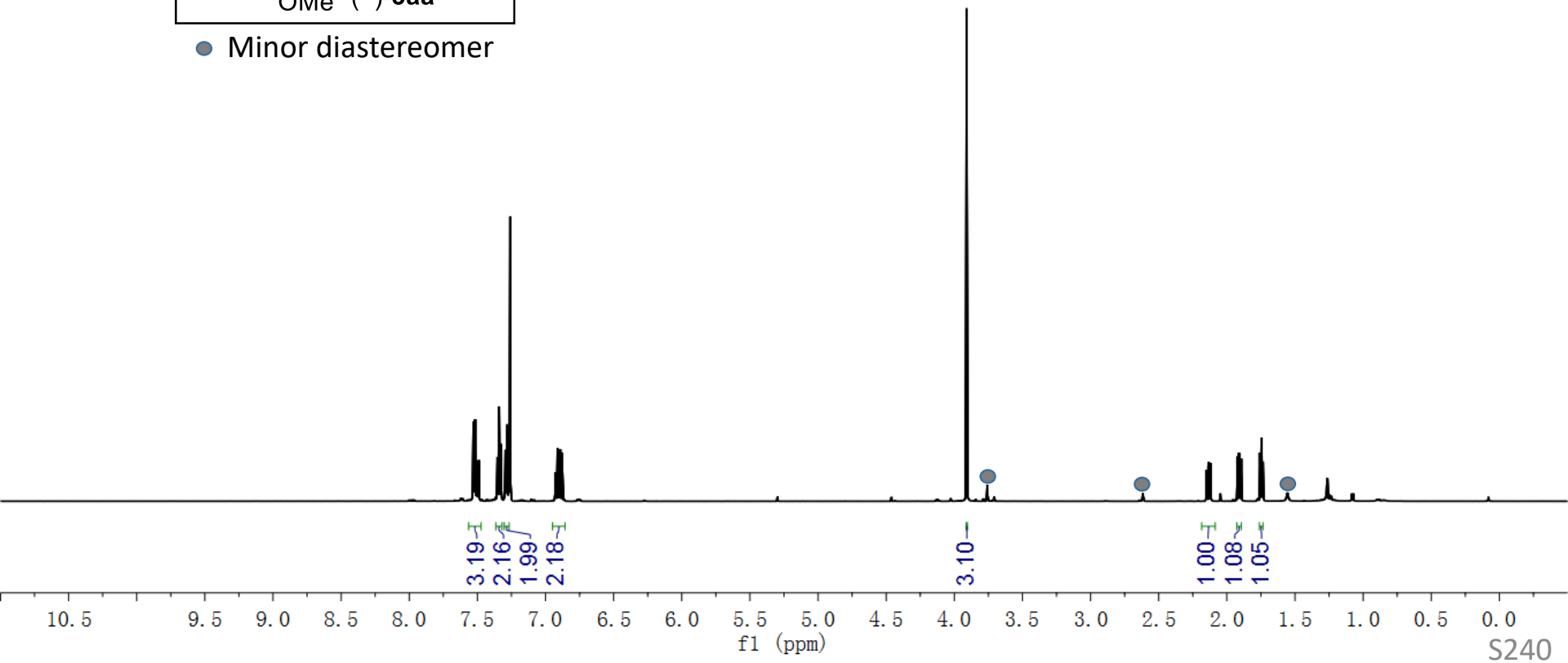
Peak#	Ret. Time	Area	Area%
1	14.221	13283795	97.162
2	16.969	388070	2.838
Total		13671865	100.000

^{1}H NMR of **3aa**, 600 MHz, $CDCl_3$



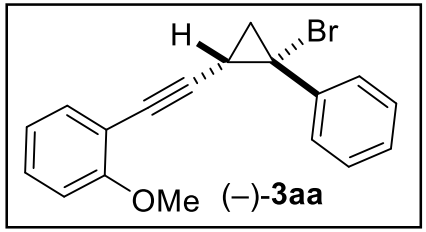


● Minor diastereomer



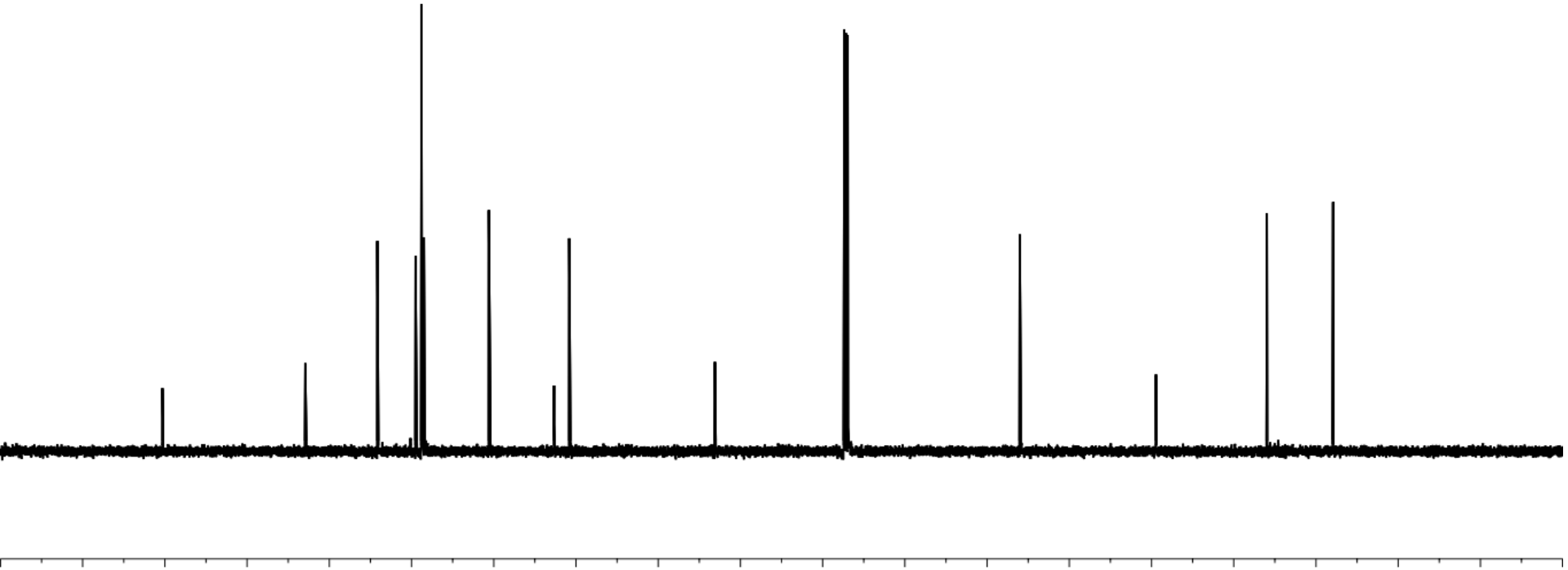
^{13}C NMR of **3ab**, 151 MHz, $CDCl_3$

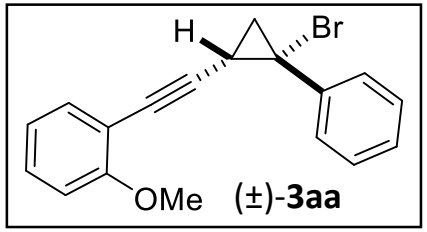
160.295
142.924
134.158
129.512
128.788
128.764
128.487
120.602
112.669
110.821
93.102
77.371
77.242
77.160
76.948
56.030
39.463
25.960
17.918



(–)-**3aa**

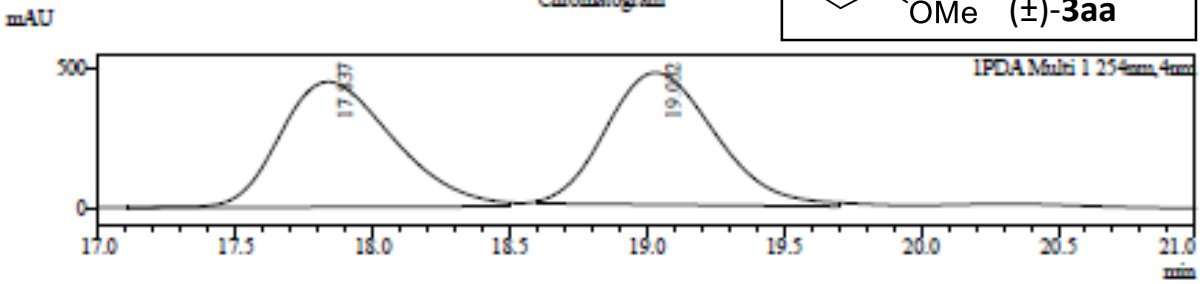
- Minor diastereomer



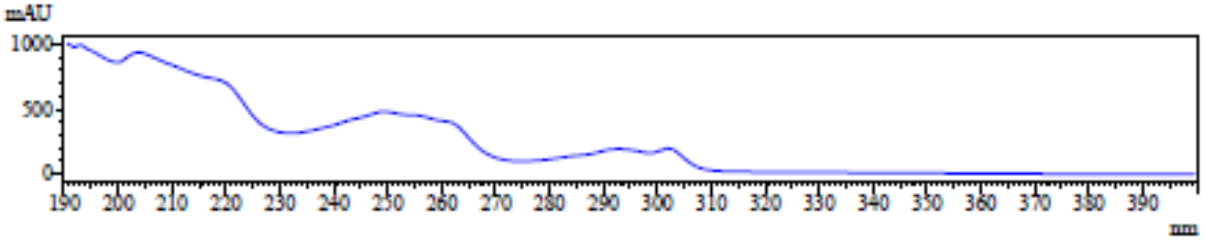


Data File : J0K-0620-IA-0.5%-0.8ML.lcd
Sample Name : J0K-0620-IA-0.5%-0.8ML
Sample ID : J0K-0620-IA-0.5%-0.8ML
Method File : J0K-0.5%--35min-0.8ml.lcm

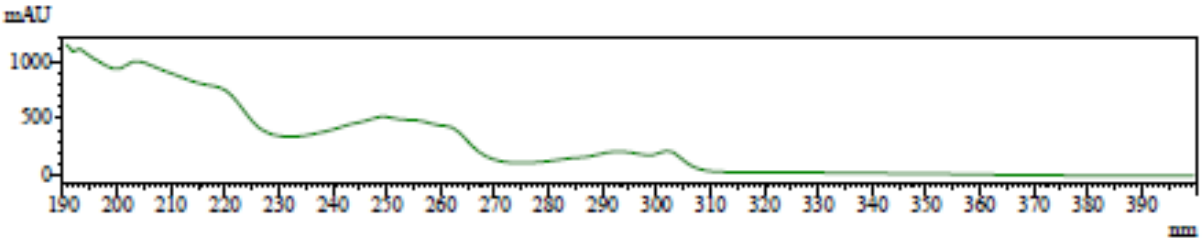
Chromatogram



UV Spectrum
Retention time = 17.837



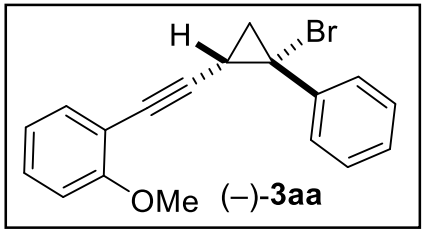
UV Spectrum
Retention time = 19.032



Peak Table

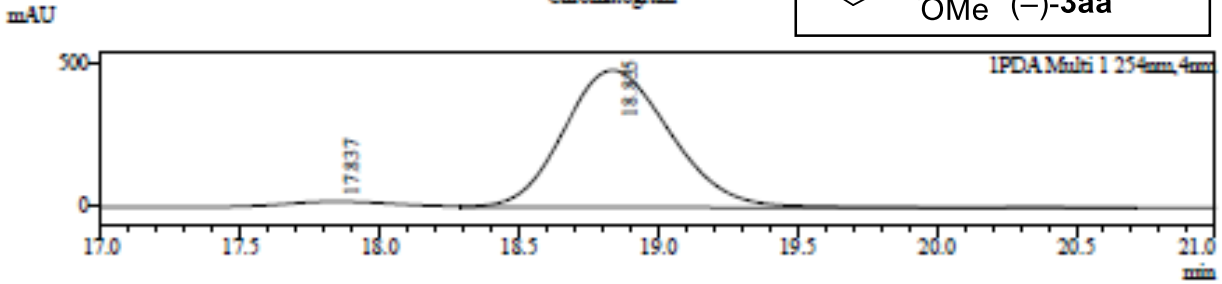
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	17.837	12883307	49.717
2	19.032	13030156	50.283
Total		25913463	100.000

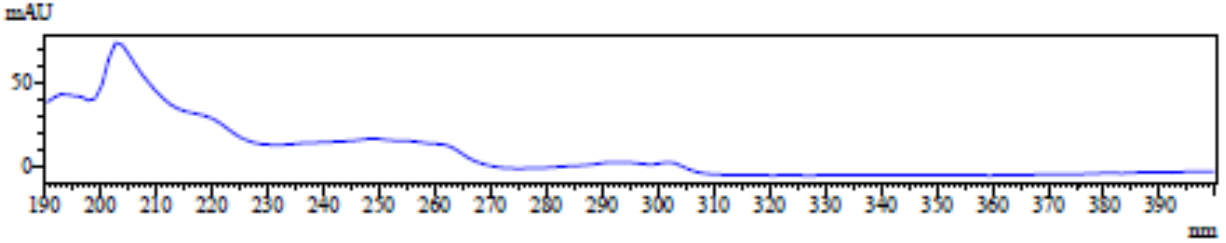


Data File : J0K-0619-IA-0.5%-0.8ML.lcd
Sample Name : J0K-0619-IA-0.5%-0.8ML
Sample ID : J0K-0619-IA-0.5%-0.8ML
Method File : J0K-0.5%--35min-0.8ml.lcm

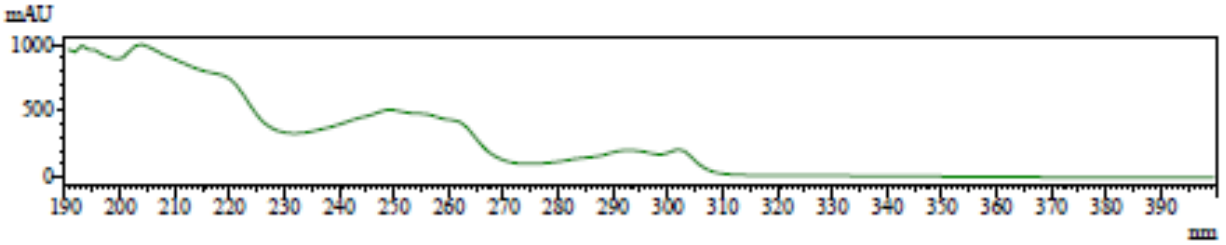
Chromatogram



UV Spectrum
Retention time = 17.837



UV Spectrum
Retention time = 18.835

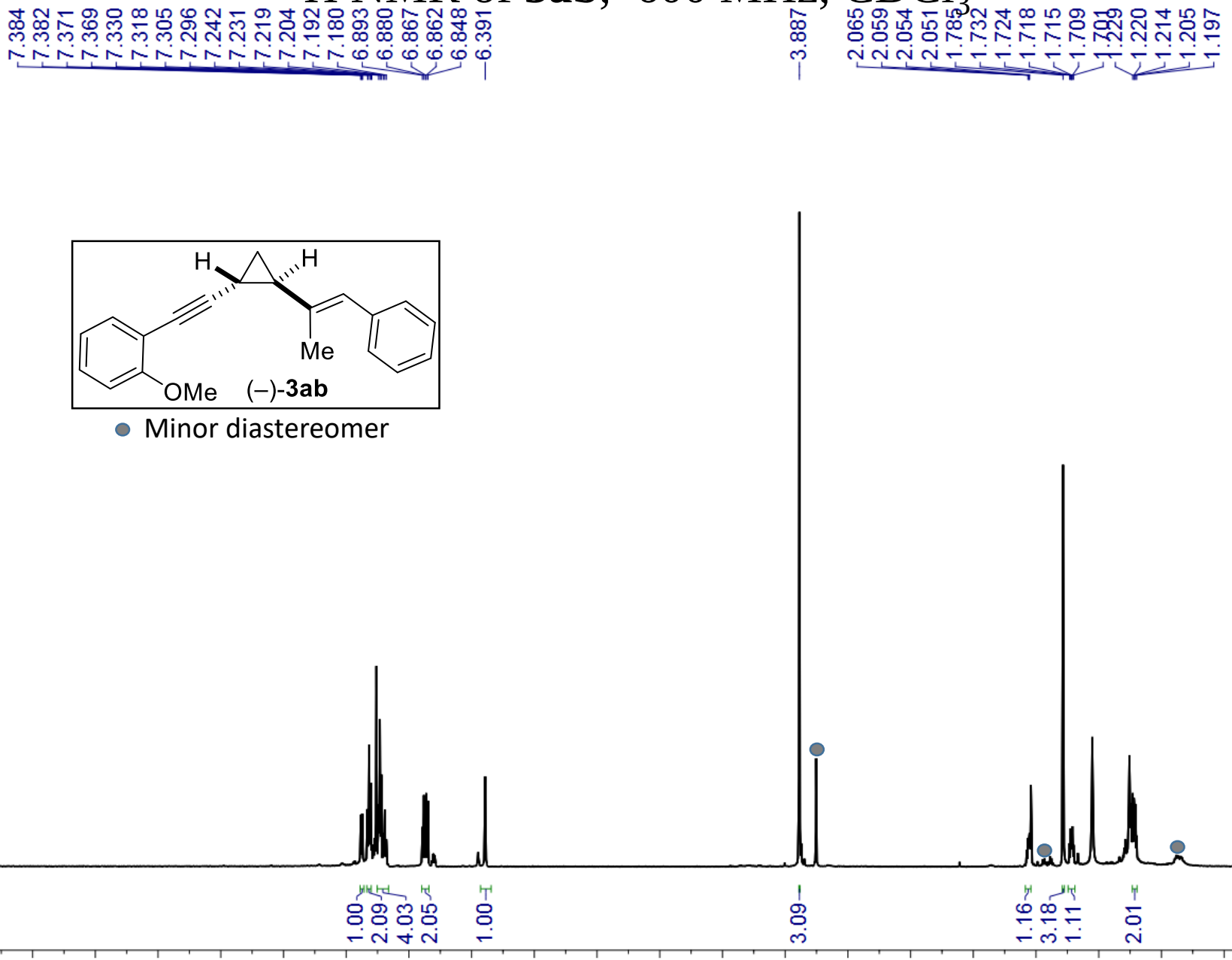


Peak Table

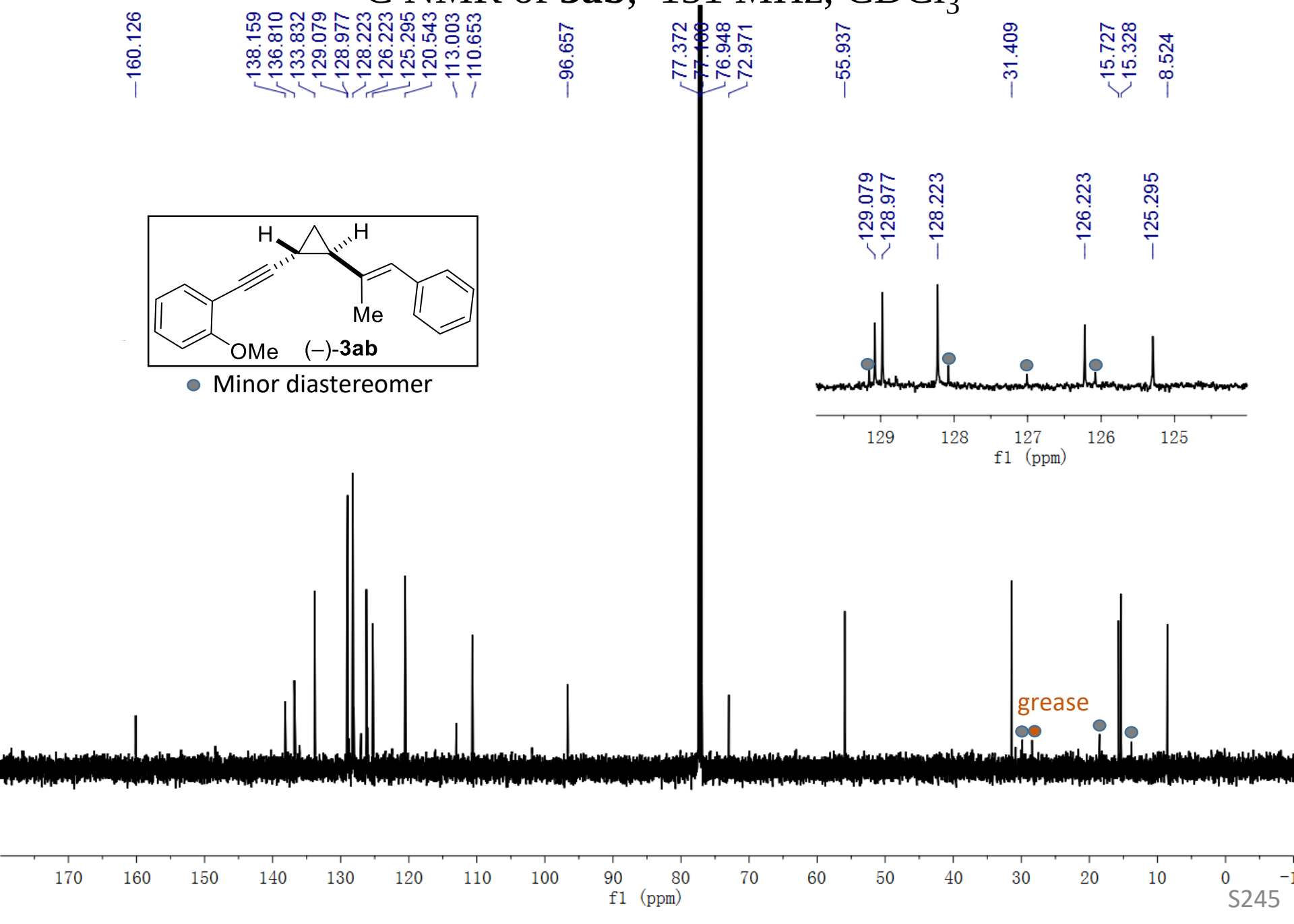
PDA Ch1 254nm

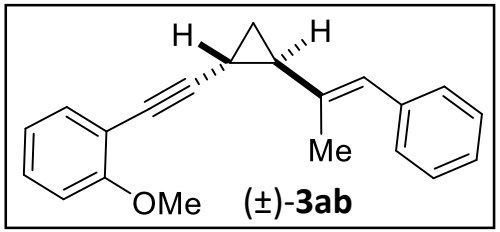
Peak#	Ret. Time	Area	Area%
1	17.837	580094	4.292
2	18.835	12935914	95.708
Total		13516008	100.000

^{1}H NMR of **3ab**, 600 MHz, $CDCl_3$



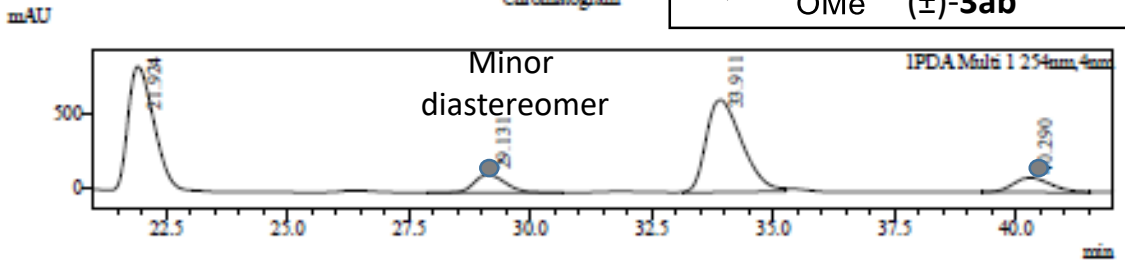
^{13}C NMR of **3ab**, 151 MHz, $CDCl_3$



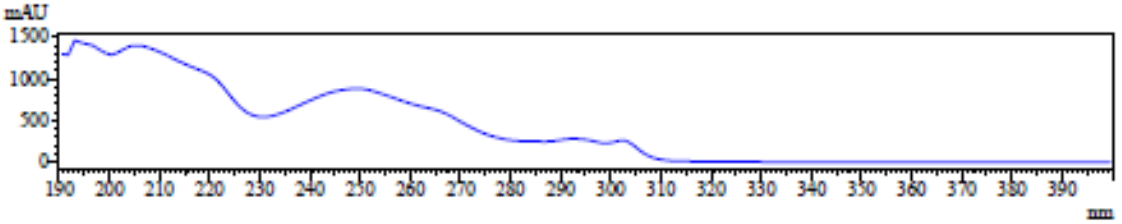


Data File : J0K-0572-IB-2-0.5%-0.8ML.lcd
Sample Name : J0K-0572-IB-2-0.5%-0.8ML
Sample ID : J0K-0572-IB-2-0.5%-0.8ML
Method File : J0K-0.5%--50min-0.8ml.lcm

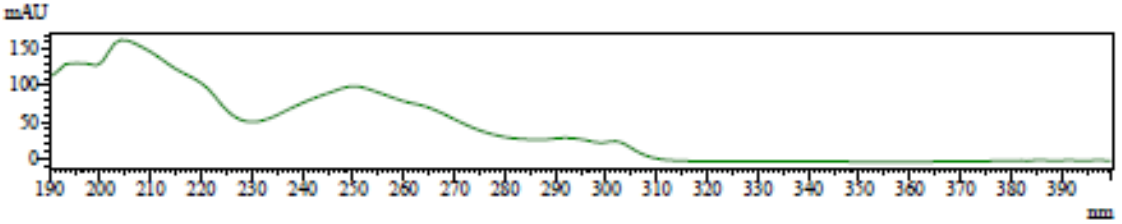
Chromatogram



UV Spectrum
Retention time = 21.924



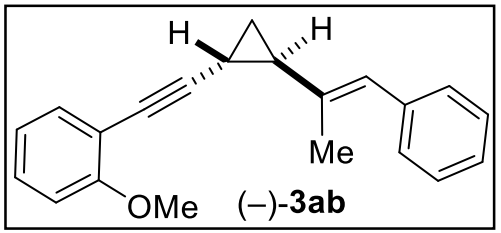
UV Spectrum
Retention time = 29.131



Peak Table

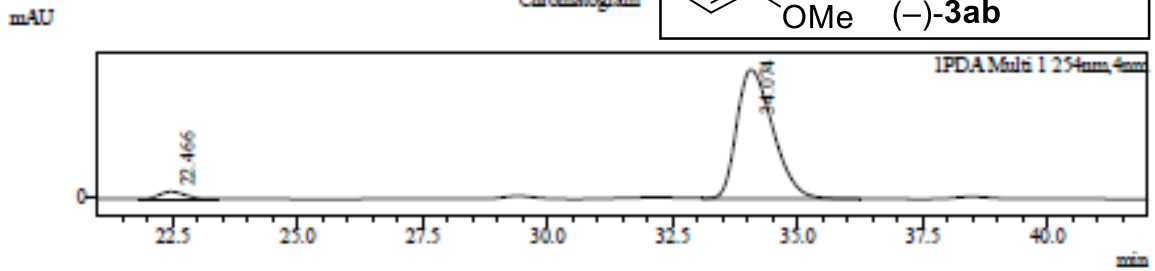
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	21.924	32295768	43.019
2	29.131	5296135	7.055
3	33.911	32148350	42.822
4	40.290	5333635	7.105
Total		75073888	100.000

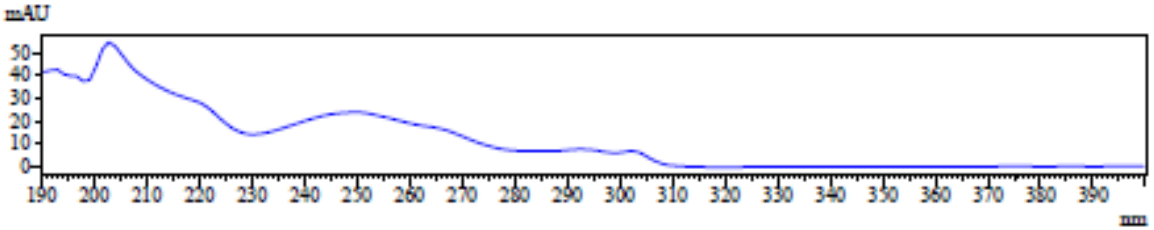


Data File : J0K-0571-IB-0.5%-0.8ML.lcd
Sample Name : J0K-0571-IB-0.5%-0.8ML
Sample ID : J0K-0571-IB-0.5%-0.8ML
Method File : J0K-0.5%--50min-0.8ml.lcm

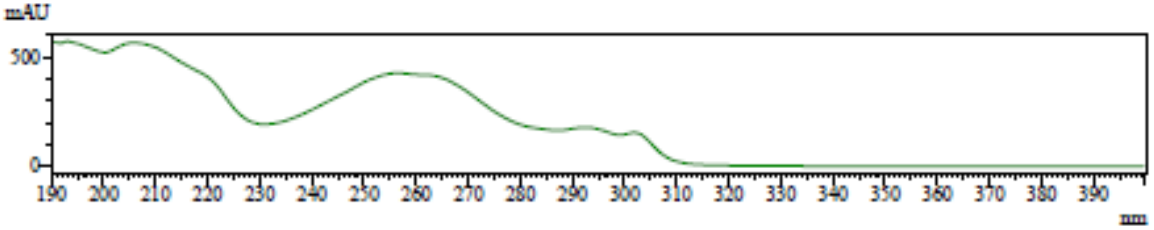
Chromatogram



UV Spectrum
Retention time = 22.466



UV Spectrum
Retention time = 34.074

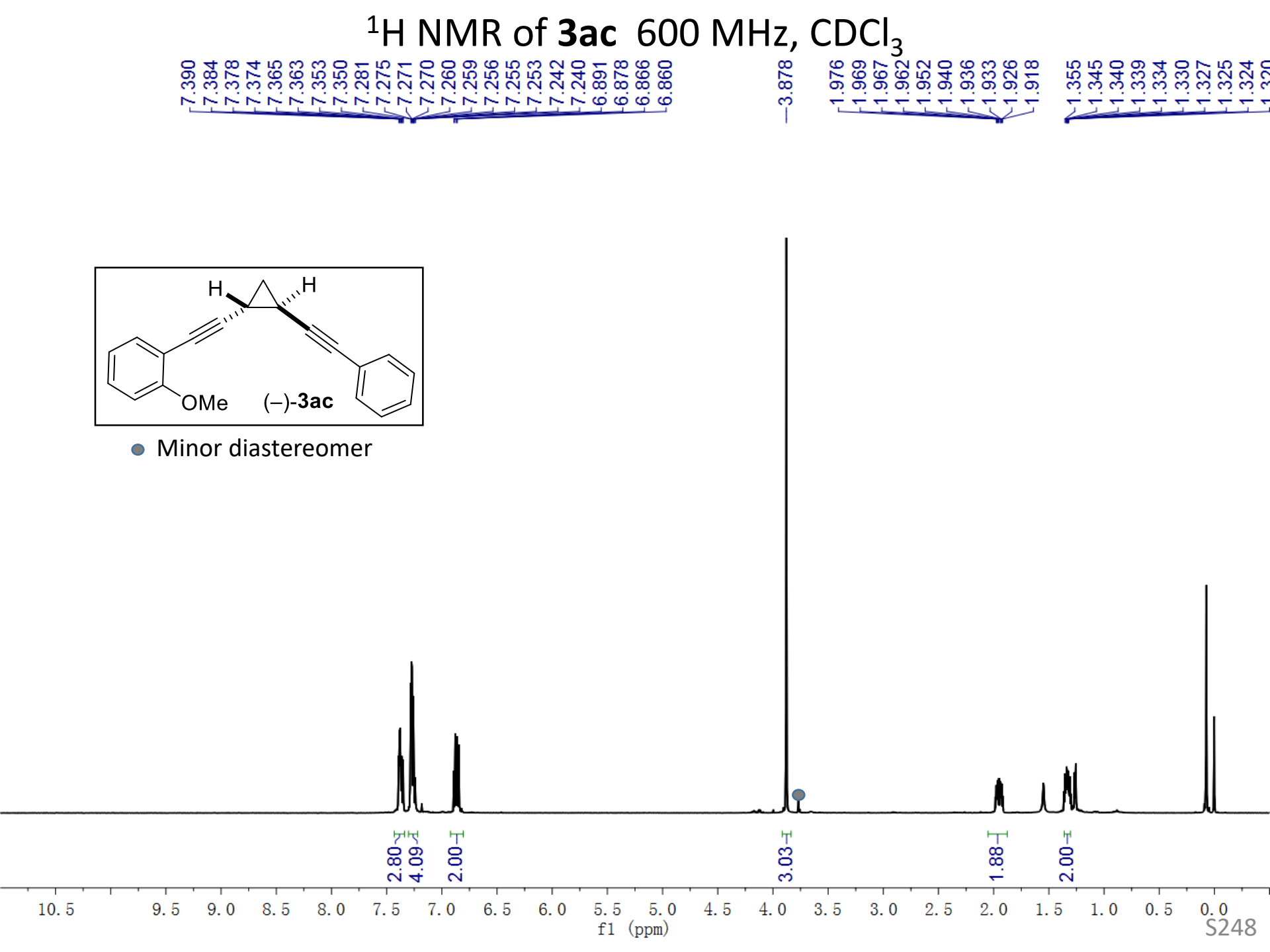


Peak Table

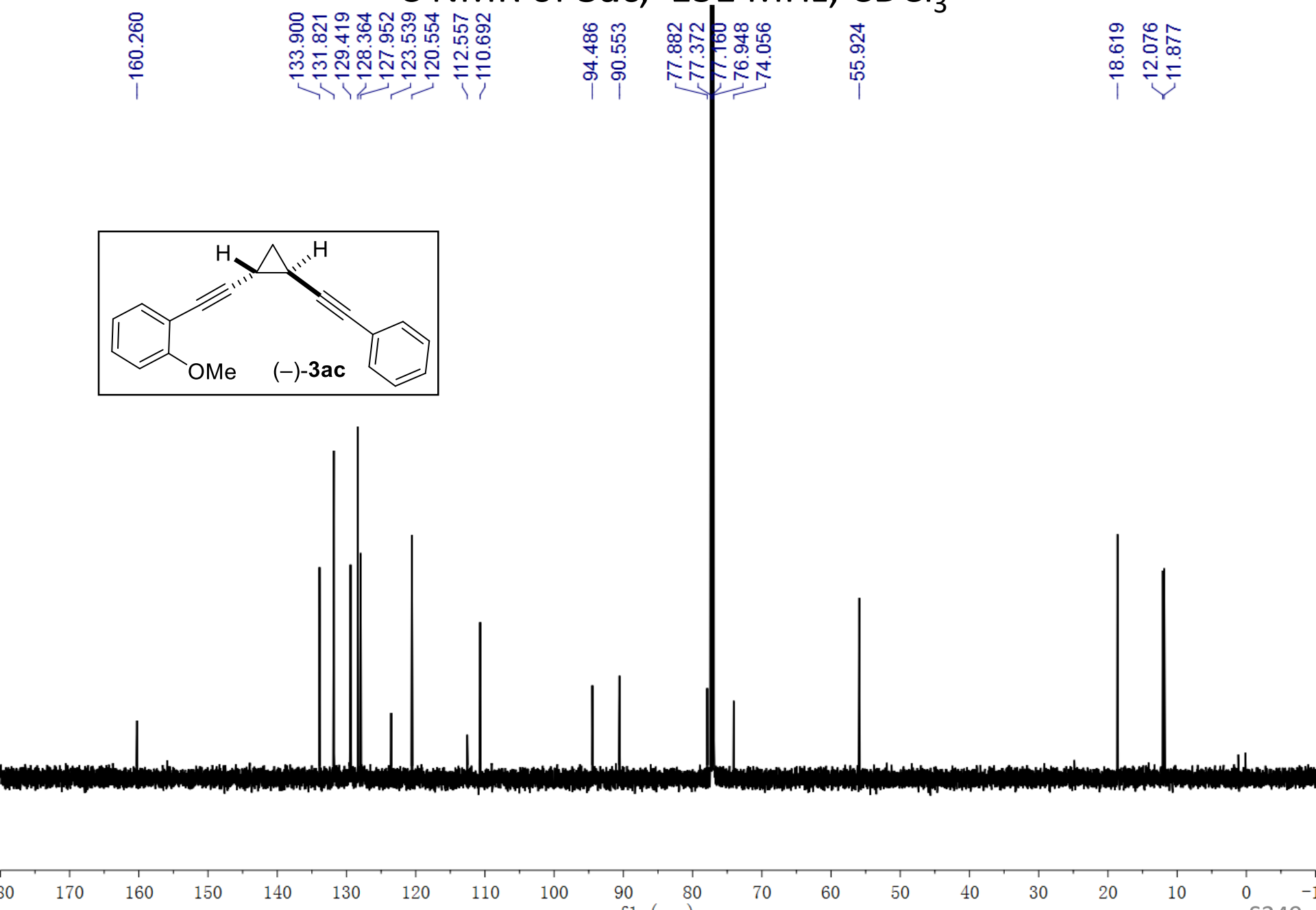
PDA Ch1 254nm

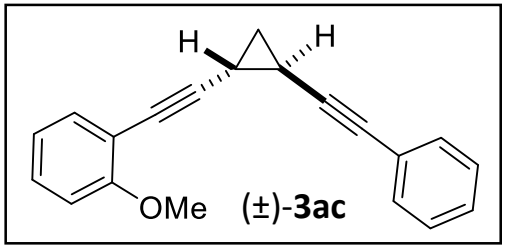
Peak#	Ret. Time	Area	Area%
1	22.466	796063	3.676
2	34.074	20857854	96.324
Total		21653917	100.000

^{1}H NMR of **3ac** 600 MHz, $CDCl_3$



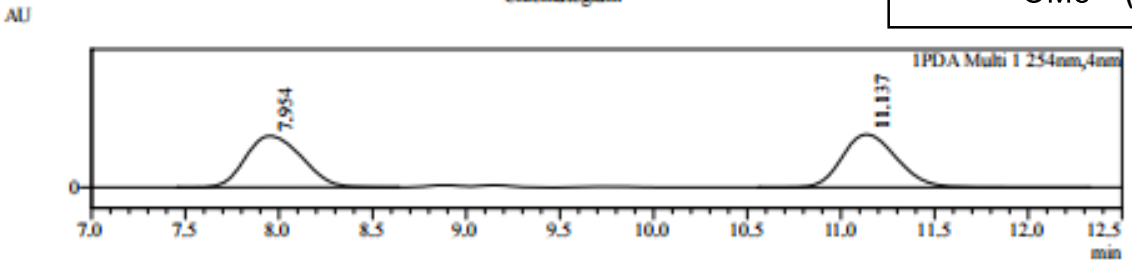
^{13}C NMR of **3ac**, 151 MHz, $CDCl_3$



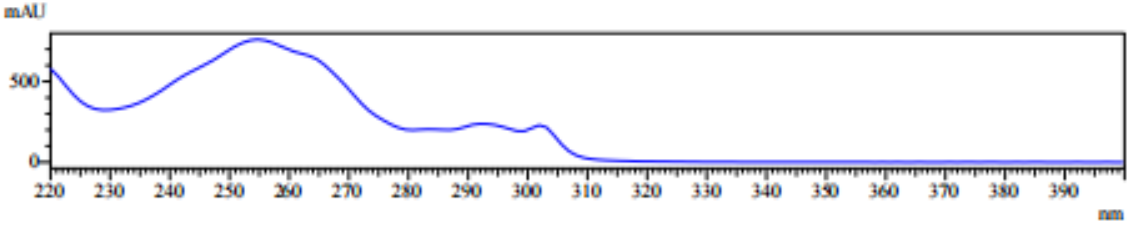


Data File : J0K-0168-IC-1%-0.8ML-isopropanol-solvent003.lcd
Sample Name : J0K-0168-IC-1%-0.8ML-isopropanol-solvent003
Sample ID : J0K-0168-IC-1%-0.8ML-isopropano
Method File : J0K-1%-0.8ml.lcm

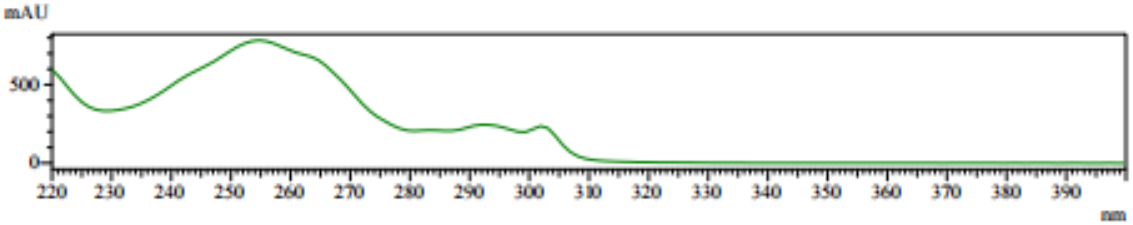
Chromatogram



UV Spectrum
Retention time = 7.954



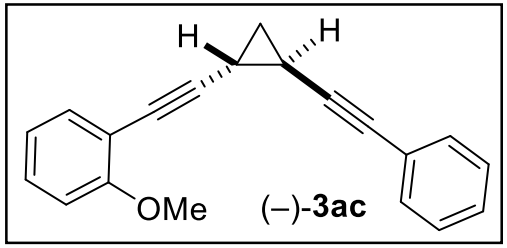
UV Spectrum
Retention time = 11.137



Peak Table

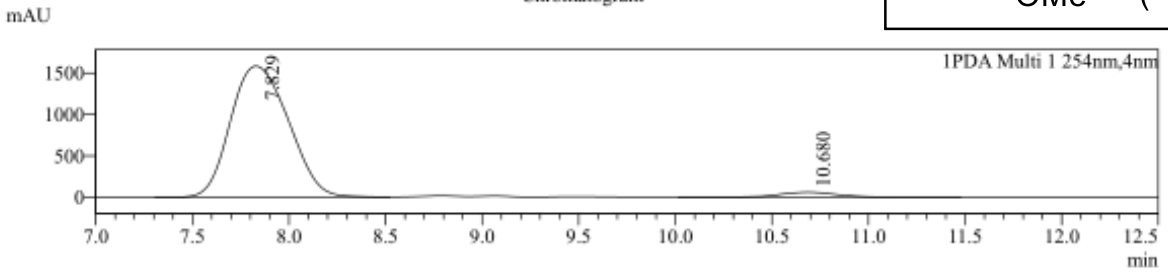
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	7.954	15546478	50.007
2	11.137	15542218	49.993
Total		31088696	100.000

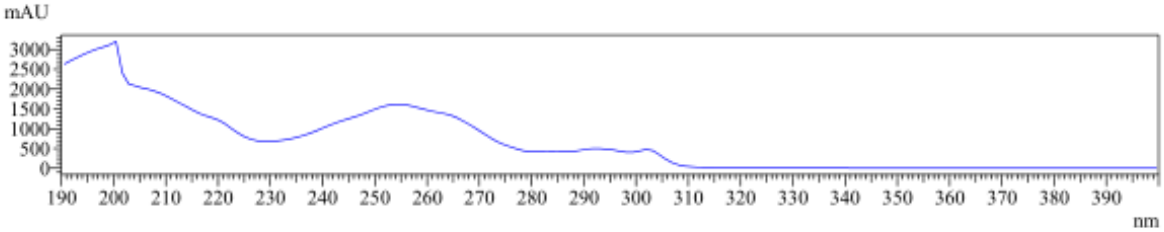


Data File : J0K-0167-IC-1%-0.8ML-isopropanol-solvent003.lcd
Sample Name : J0K-0167-IC-1%-0.8ML-isopropanol-solvent003
Sample ID : J0K-0167-IC-1%-0.8ML-isopropano
Method File : J0K-1%-0.8ml.lcm

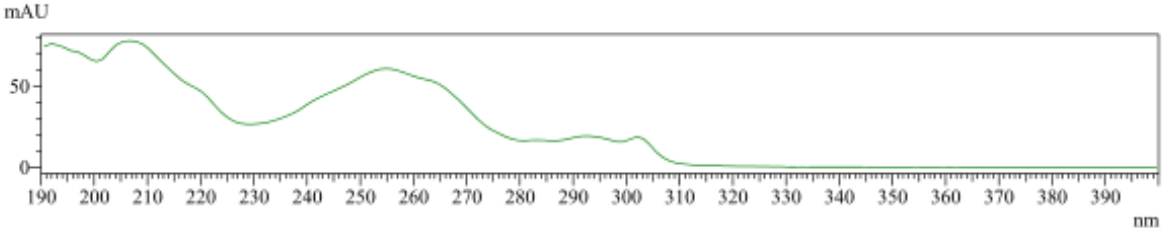
Chromatogram



UV Spectrum
Retention time = 7.829



UV Spectrum
Retention time = 10.680

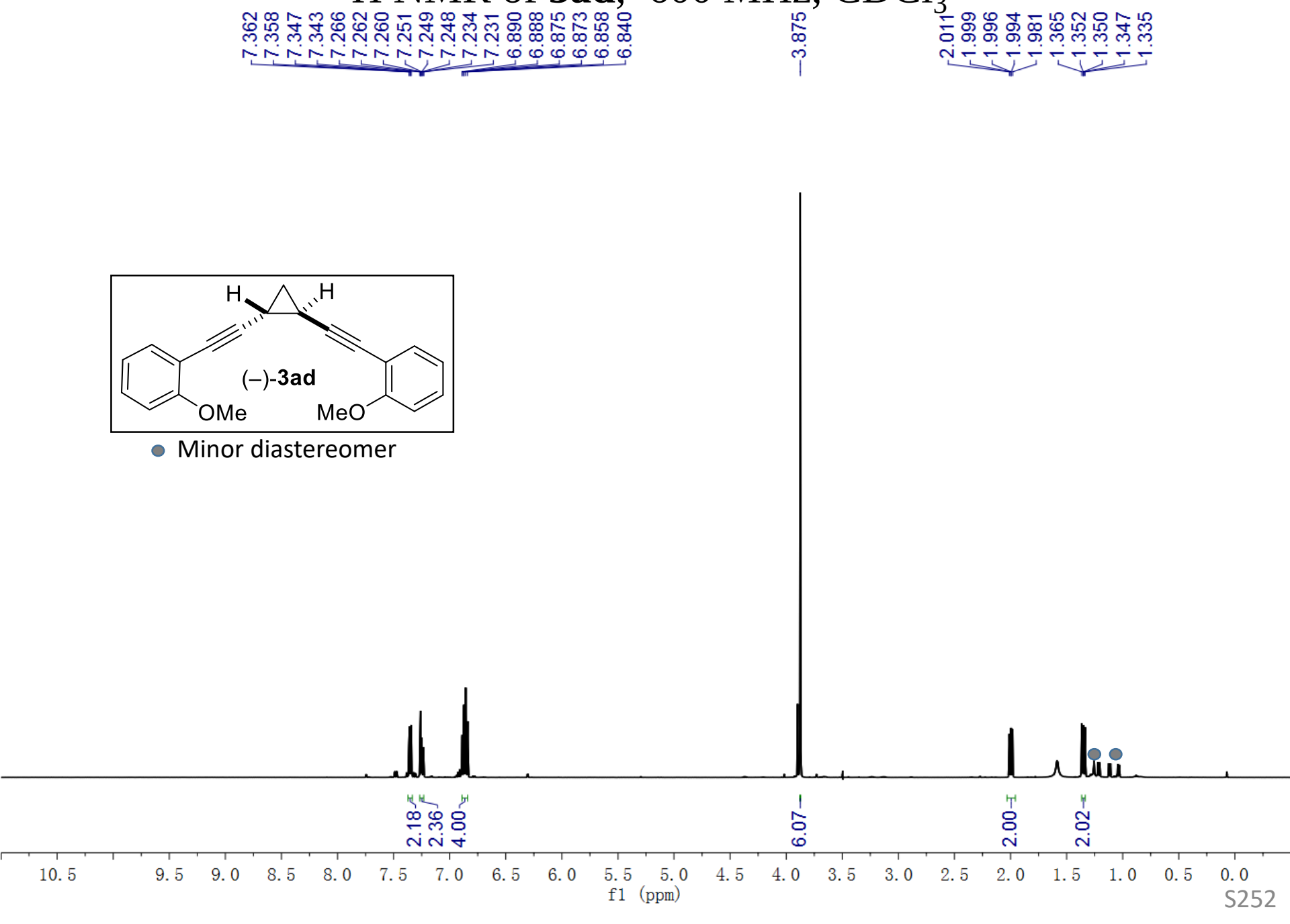


Peak Table

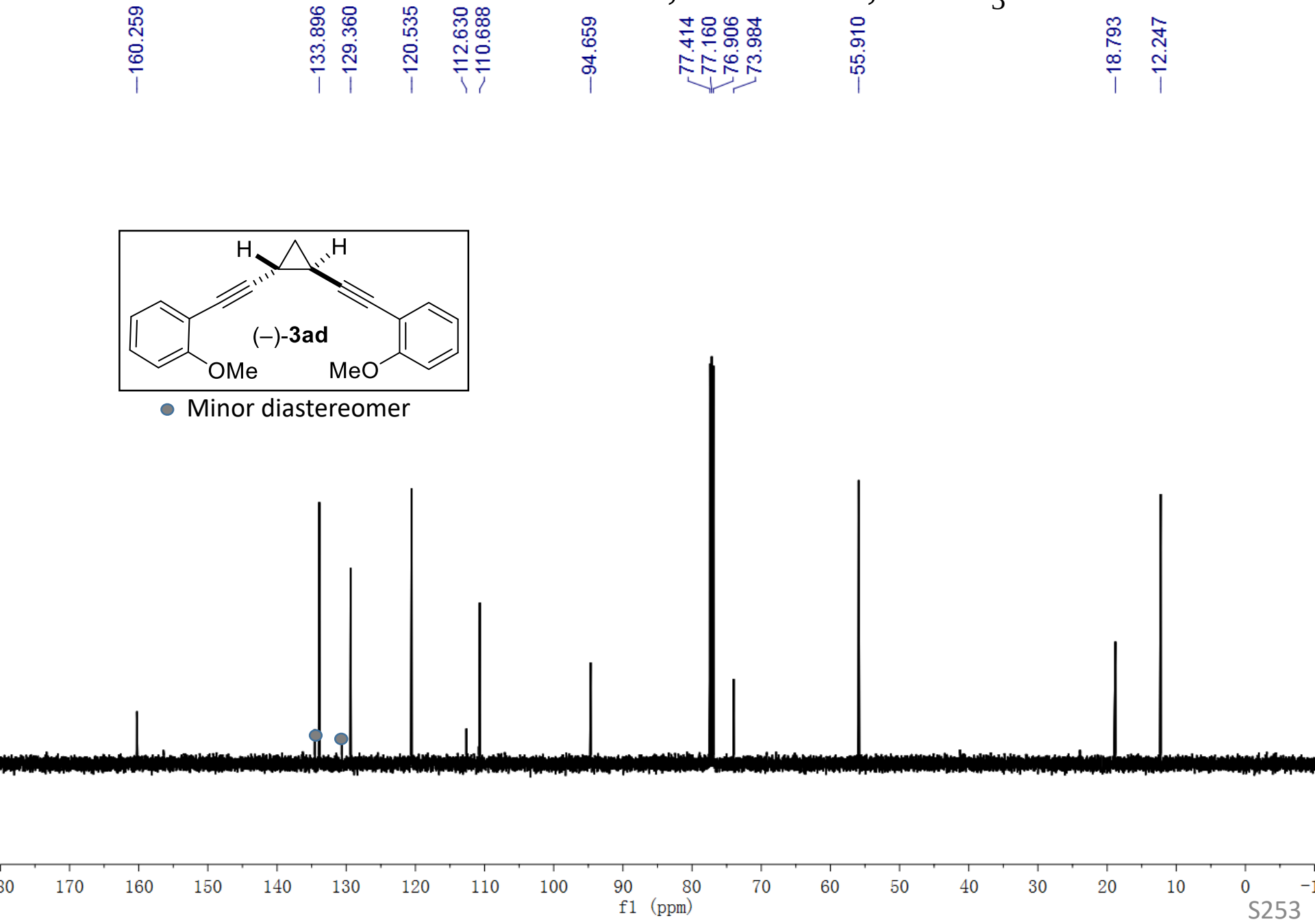
PDA Ch1 254nm

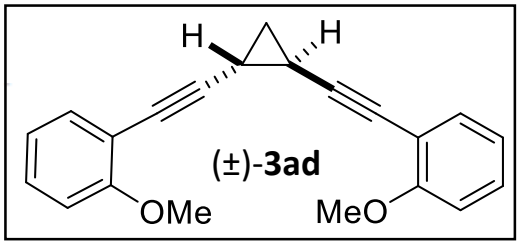
Peak#	Ret. Time	Area	Area%
1	7.829	32959040	96.411
2	10.680	1227035	3.589
Total		34186075	100.000

^{1}H NMR of **3ad**, 600 MHz, $CDCl_3$

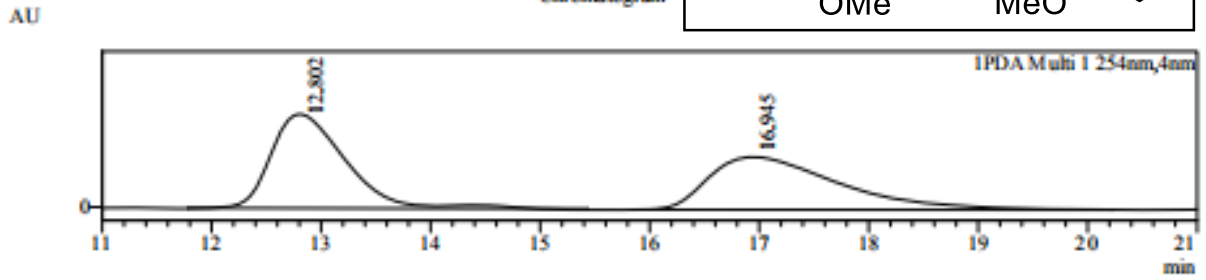


^{13}C NMR of **3ad**, 151 MHz, $CDCl_3$

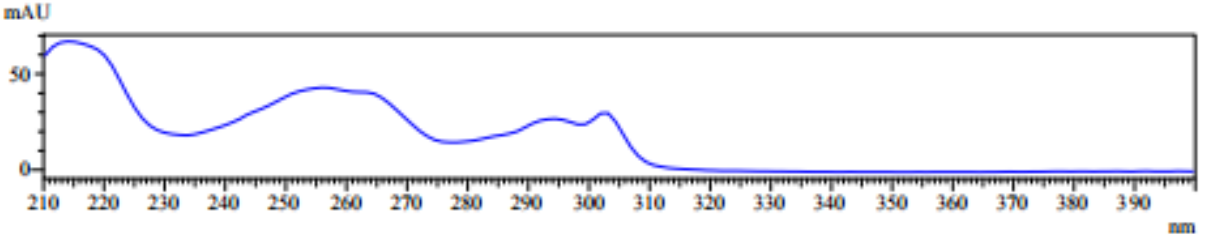




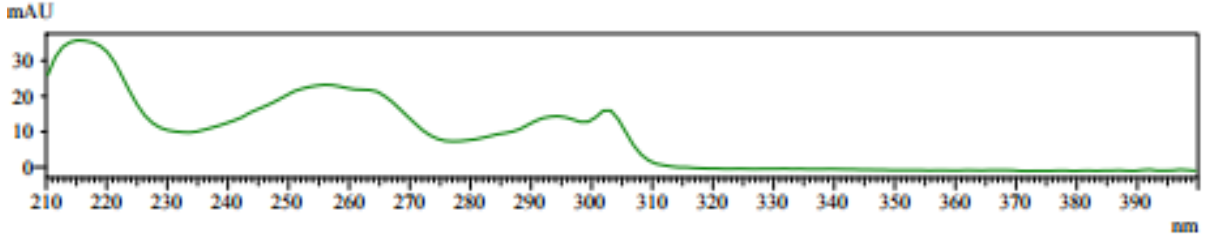
Data File : J0K-0831-IA--0.5%-1ML.lcd
Sample Name : J0K-0831-IA--0.5%-1ML
Sample ID : J0K-0831-IA--0.5%-1ML
Method File : J0K-0.5%--35min-1ml.lcm
Chromatogram



UV Spectrum
Retention time = 12.802



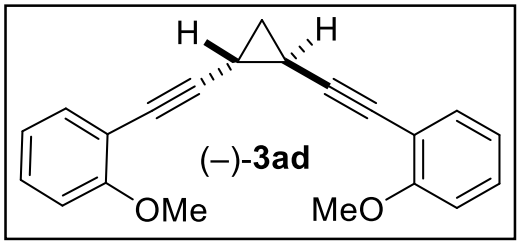
U
Retention time = 16.945



Peak Table

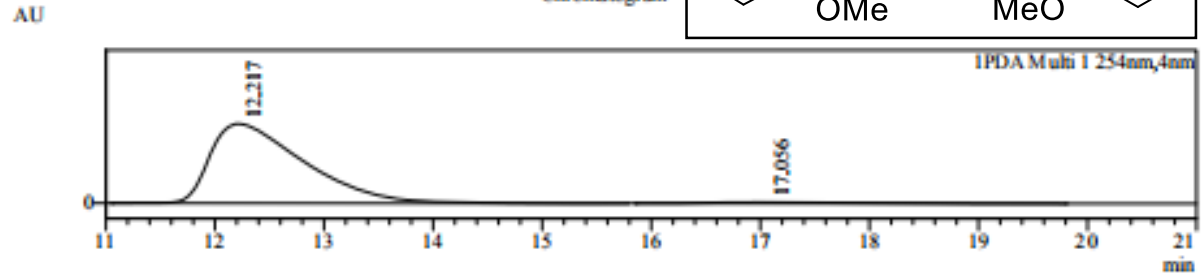
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	12.802	1979132	50.313
2	16.945	1954522	49.687
Total		3933655	100.000

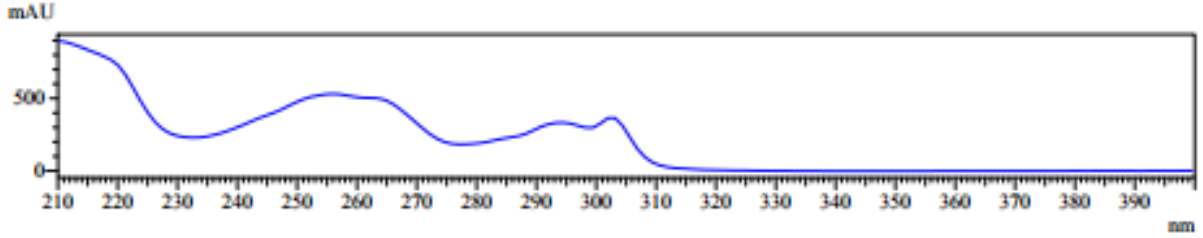


Data File : J0K-0830-2-IA--0.5%-1ML.lcd
Sample Name : J0K-0830-2-IA--0.5%-1ML
Sample ID : J0K-0830-2-IA--0.5%-1ML
Method File : J0K-0.5%--35min-1ml.lcm

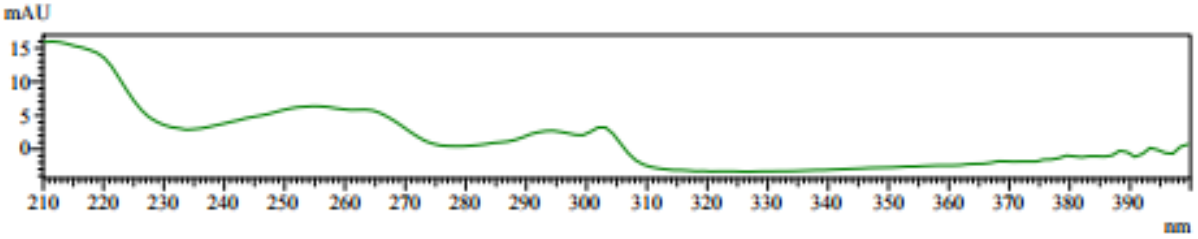
Chromatogram



UV Spectrum
Retention time = 12.217



U
Retention time = 17.056

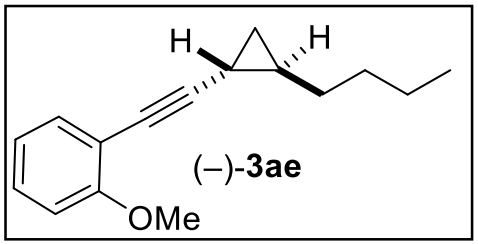


Peak Table

PDA Ch1 254nm

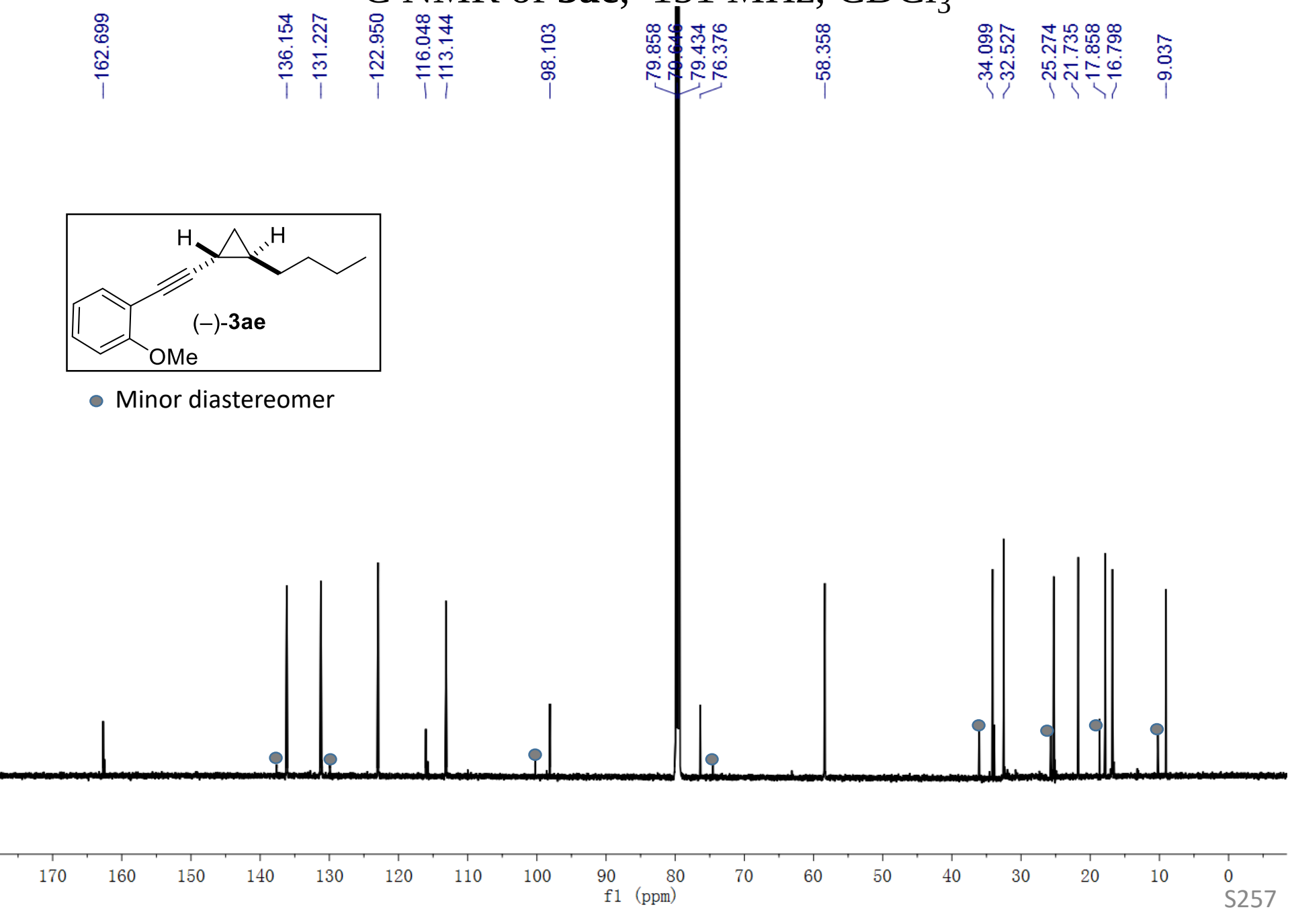
Peak#	Ret. Time	Area	Area%
1	12.217	31115081	97.598
2	17.056	765709	2.402
Total		31880790	100.000

^{1}H NMR of **3ae**, 600 MHz, $CDCl_3$

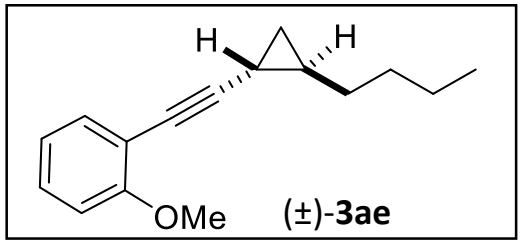


- Minor diastereomer

^{13}C NMR of **3ae**, 151 MHz, $CDCl_3$

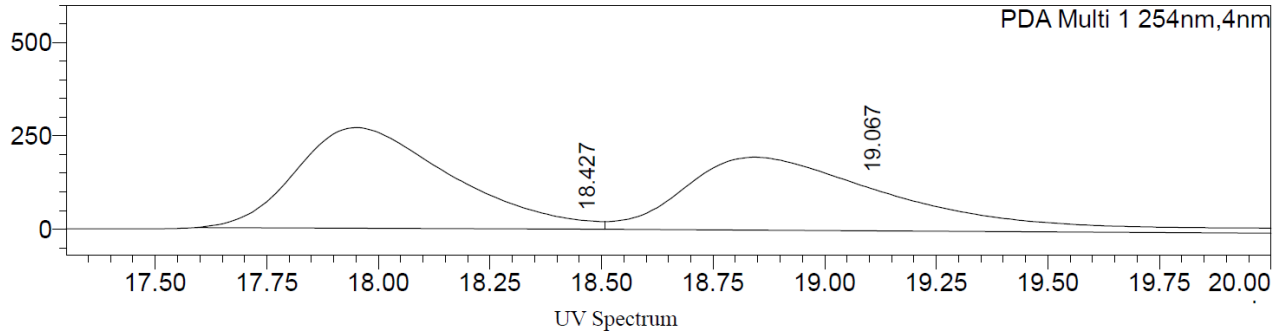


==== Shimadzu LabSolutions Analysis Report ====



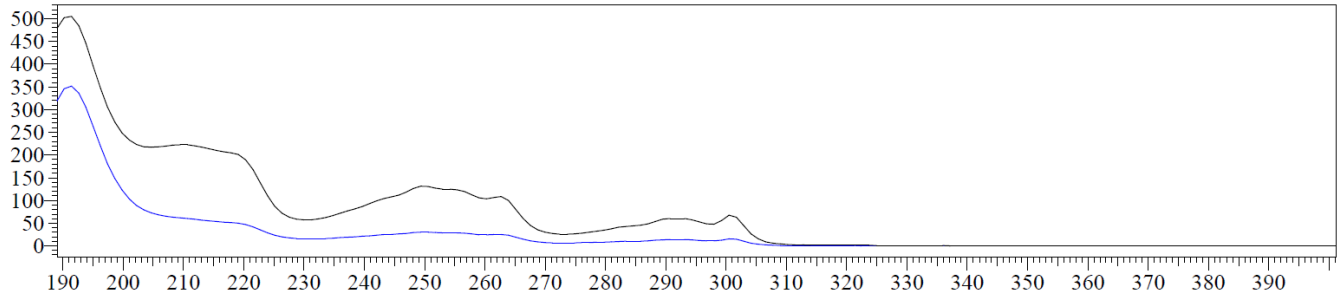
JK-1857-IF-0.3%-0.8mL
JK-0.3%-40min-0.8mL.lcm

mAU



JK-1857-IF-0.3%-0.8mL_002.lcd

mAU

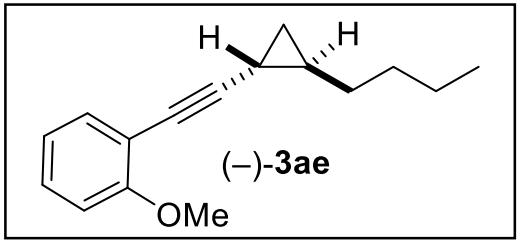


Peak Table

PDA Ch1 254nm

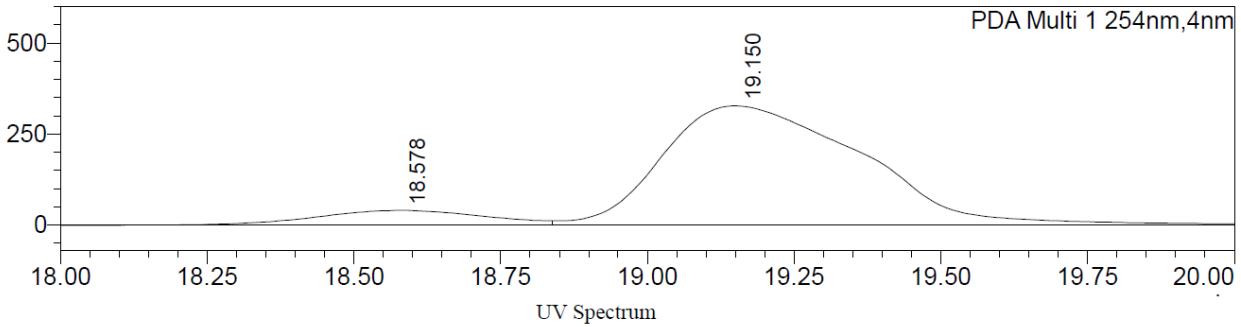
Peak#	Ret. Time	Area%
1	18.427	50.164
2	19.067	49.836
Total		100.000

==== Shimadzu LabSolutions Analysis Report ====



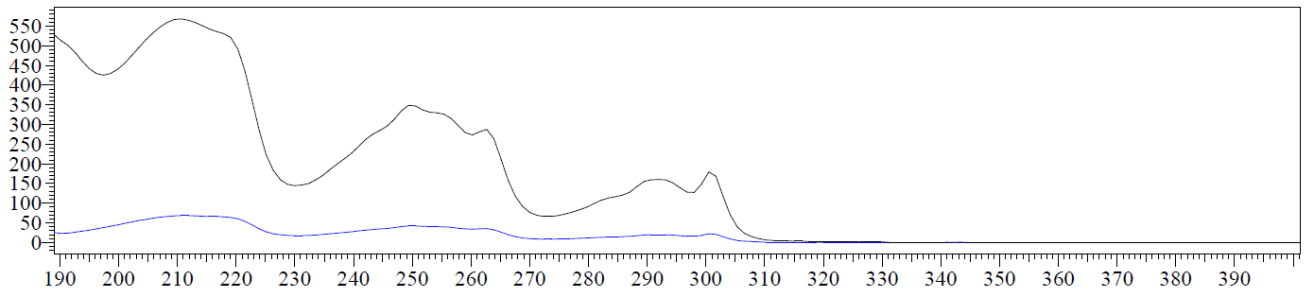
JK-1856-IF-0.3%-0.8mL
JK-0.3%-40min-0.8mL.lcm

mAU



JK-1856-IF-0.3%-0.8mL_001.lcd

mAU

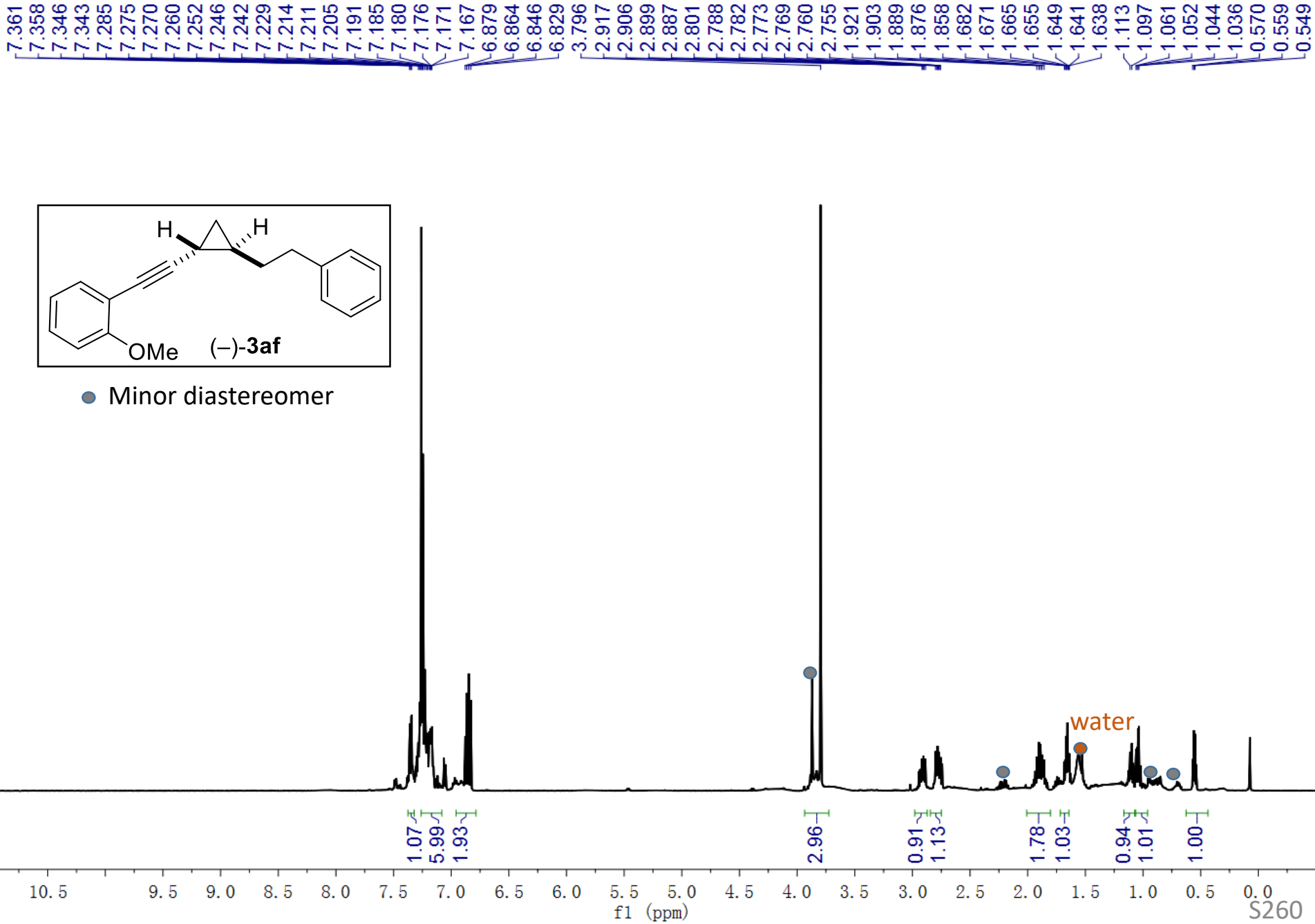


Peak Table

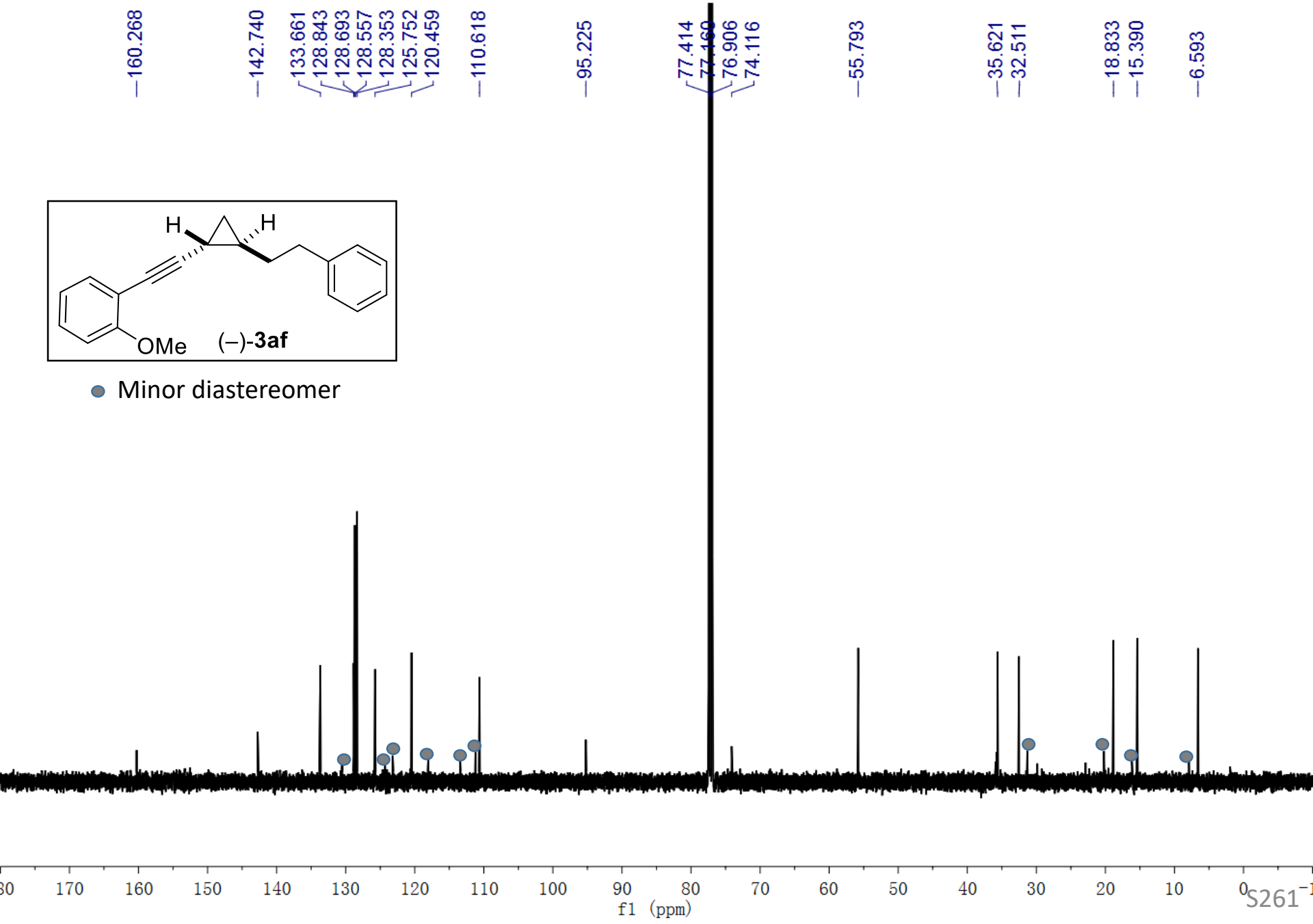
PDA Ch1 254nm

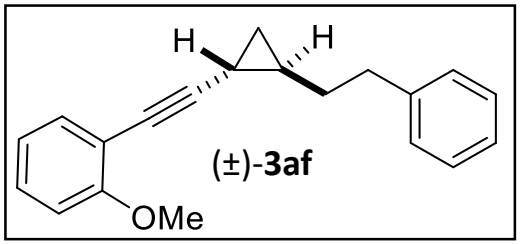
Peak#	Ret. Time	Area%
1	18.578	9.502
2	19.150	90.498
Total		100.000

^{1}H NMR of **3af**, 500 MHz, $CDCl_3$



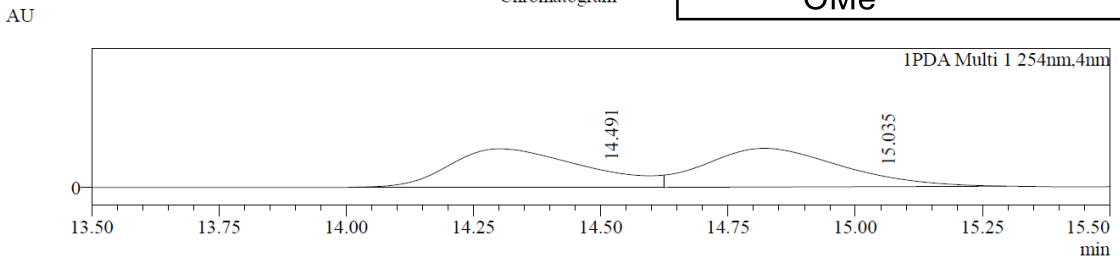
^{13}C NMR of **3af**, 126 MHz, $CDCl_3$



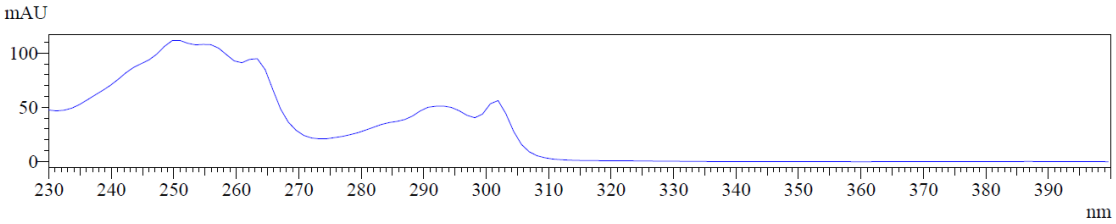


Data File : J0K-1843--IF-0.1%-1ML-3.lcd
Sample Name : J0K-1843--IF-0.1%-1ML-3
Sample ID : J0K-1843--IF-0.1%-1ML-3
Method File : J0K-0.1%--40min-1ml.lcm

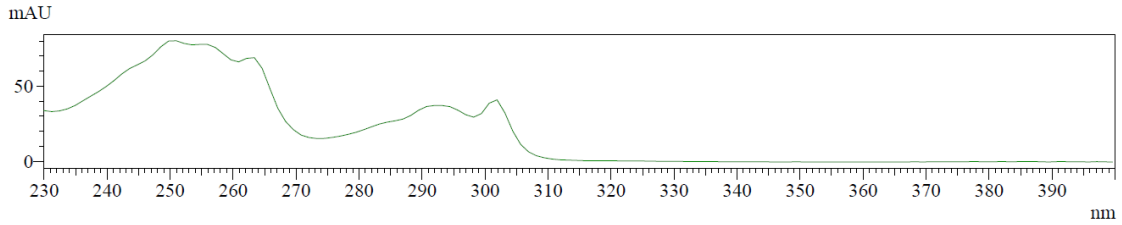
Chromatogram



UV Spectrum
Retention time = 14.491



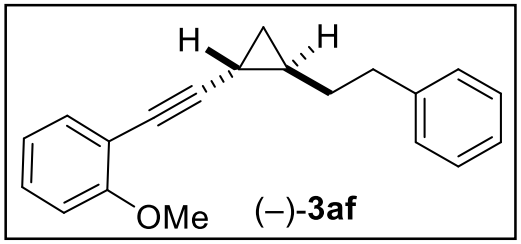
UV Spectrum
Retention time = 15.035



Peak Table

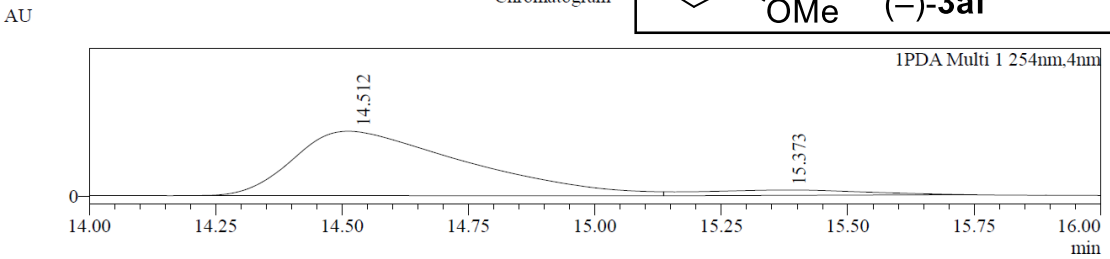
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	14.491	4118530	49.946
2	15.035	4127418	50.054
Total		8245948	100.000

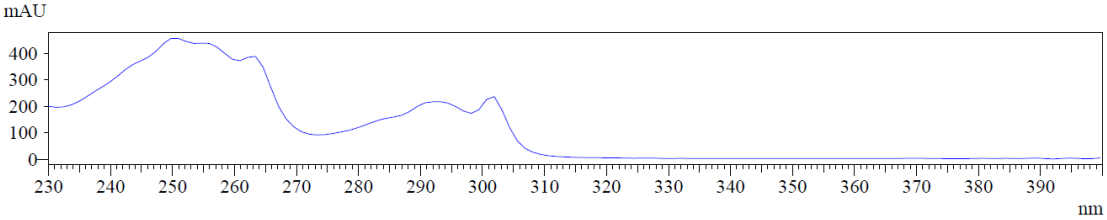


Data File : J0K-1842--IF-0.1%-1ML-2.lcd
Sample Name : J0K-1842--IF-0.1%-1ML-2
Sample ID : J0K-1842--IF-0.1%-1ML-2
Method File : J0K-0.1%--40min-1ml.lcm

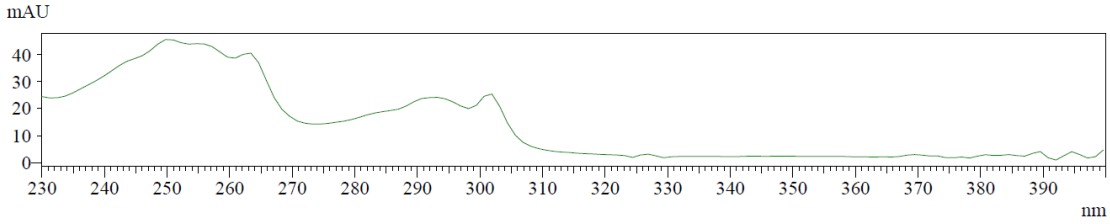
Chromatogram



UV Spectrum
Retention time = 14.512



UV Spectrum
Retention time = 15.373

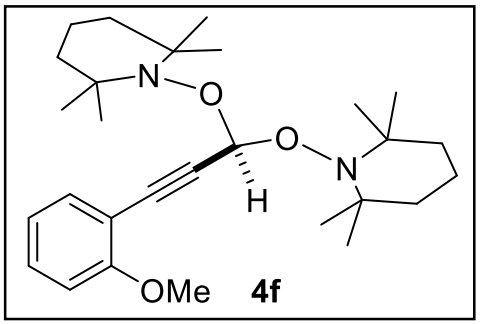


Peak Table

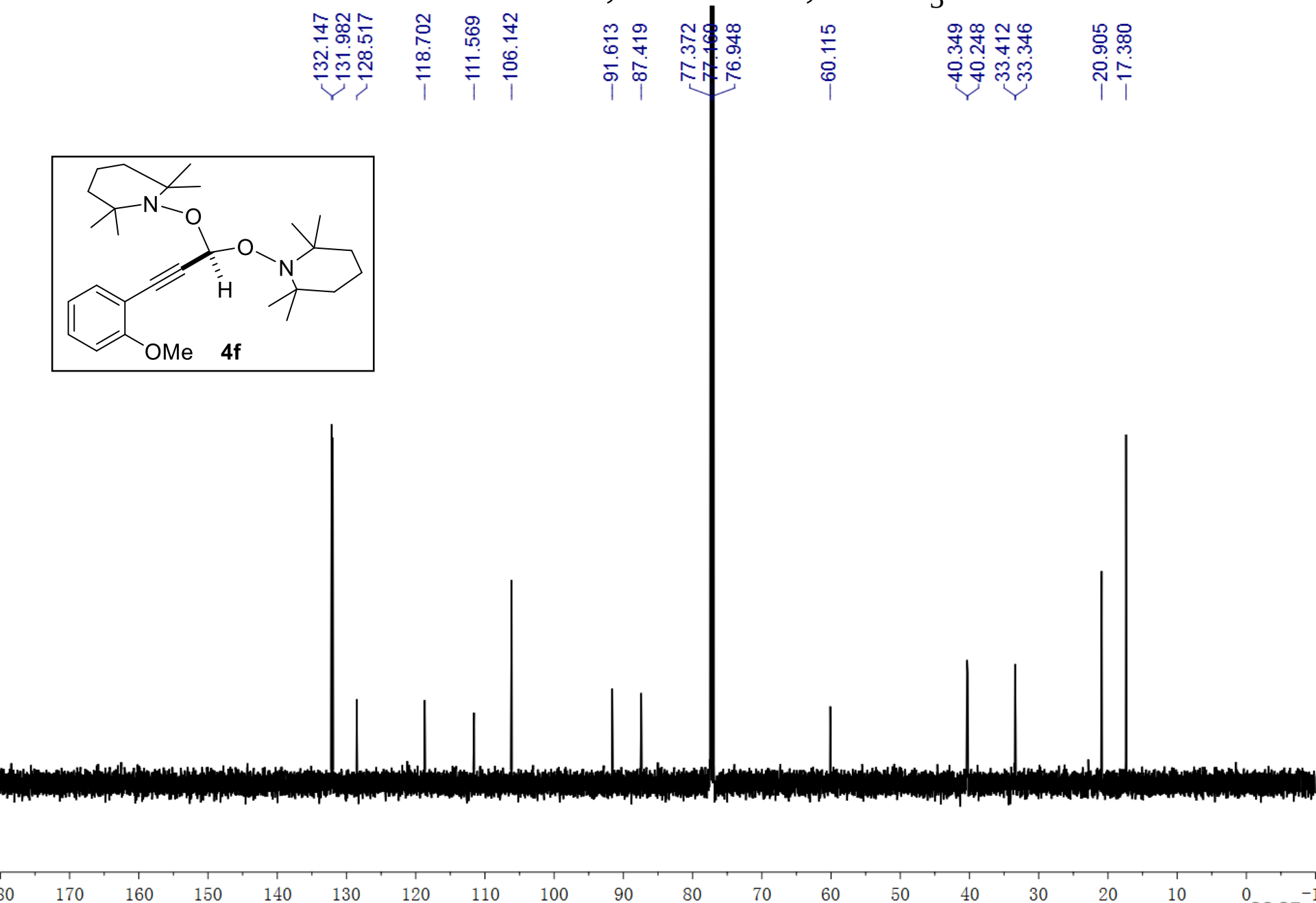
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	14.512	10300218	92.536
2	15.373	830833	7.464
Total		11131051	100.000

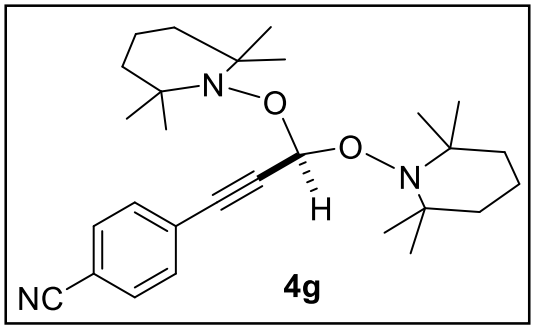
^{1}H NMR of **4f**, 600 MHz, $CDCl_3$



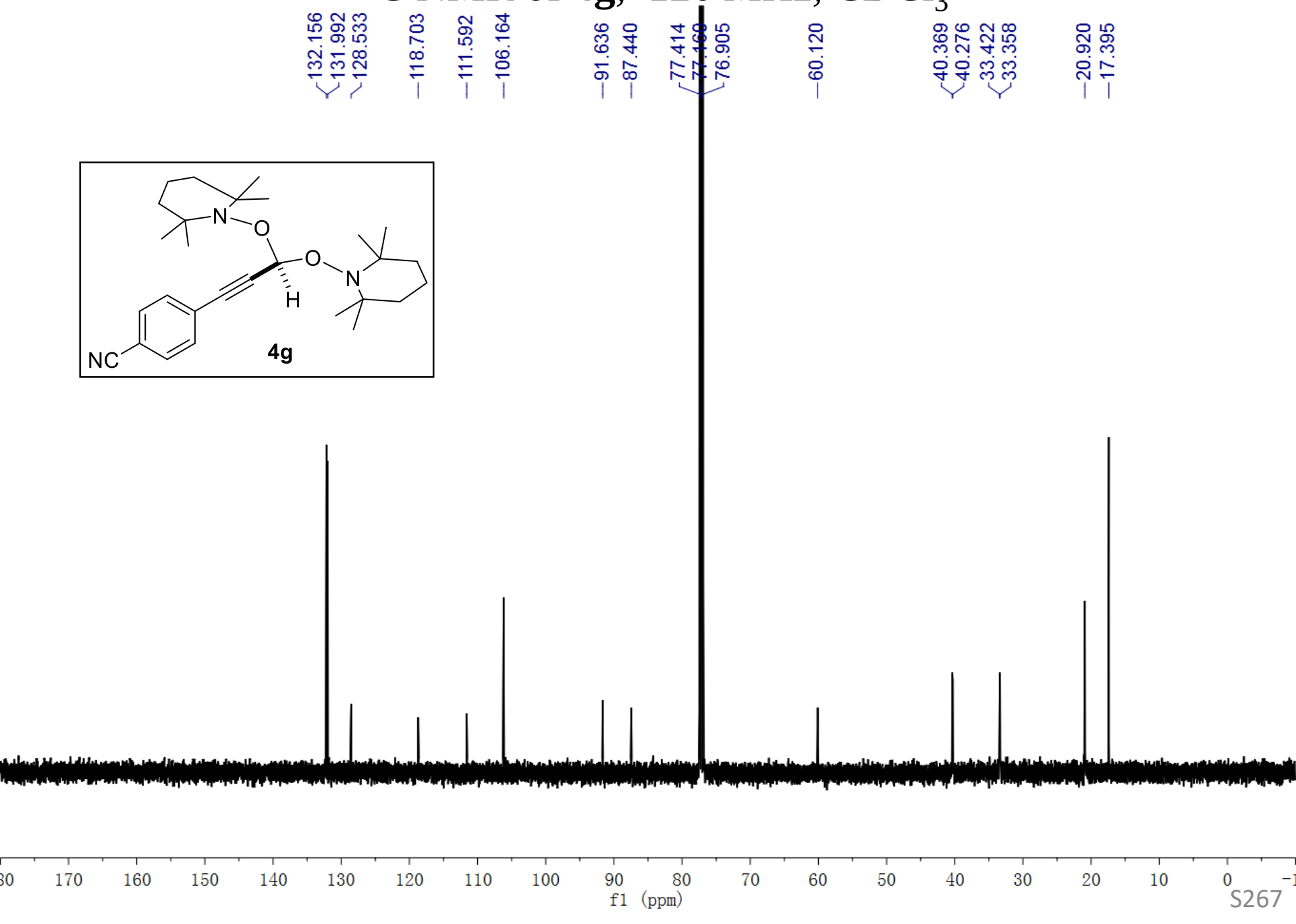
^{13}C NMR of **4f**, 151 MHz, $CDCl_3$



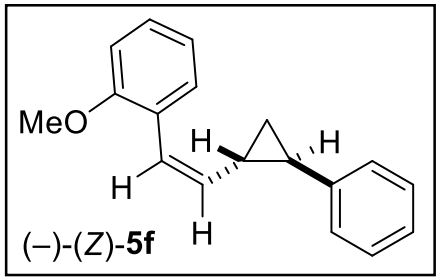
^{1}H NMR of **4g**, 500 MHz, $CDCl_3$



^{13}C NMR of **4g**, 126 MHz, $CDCl_3$

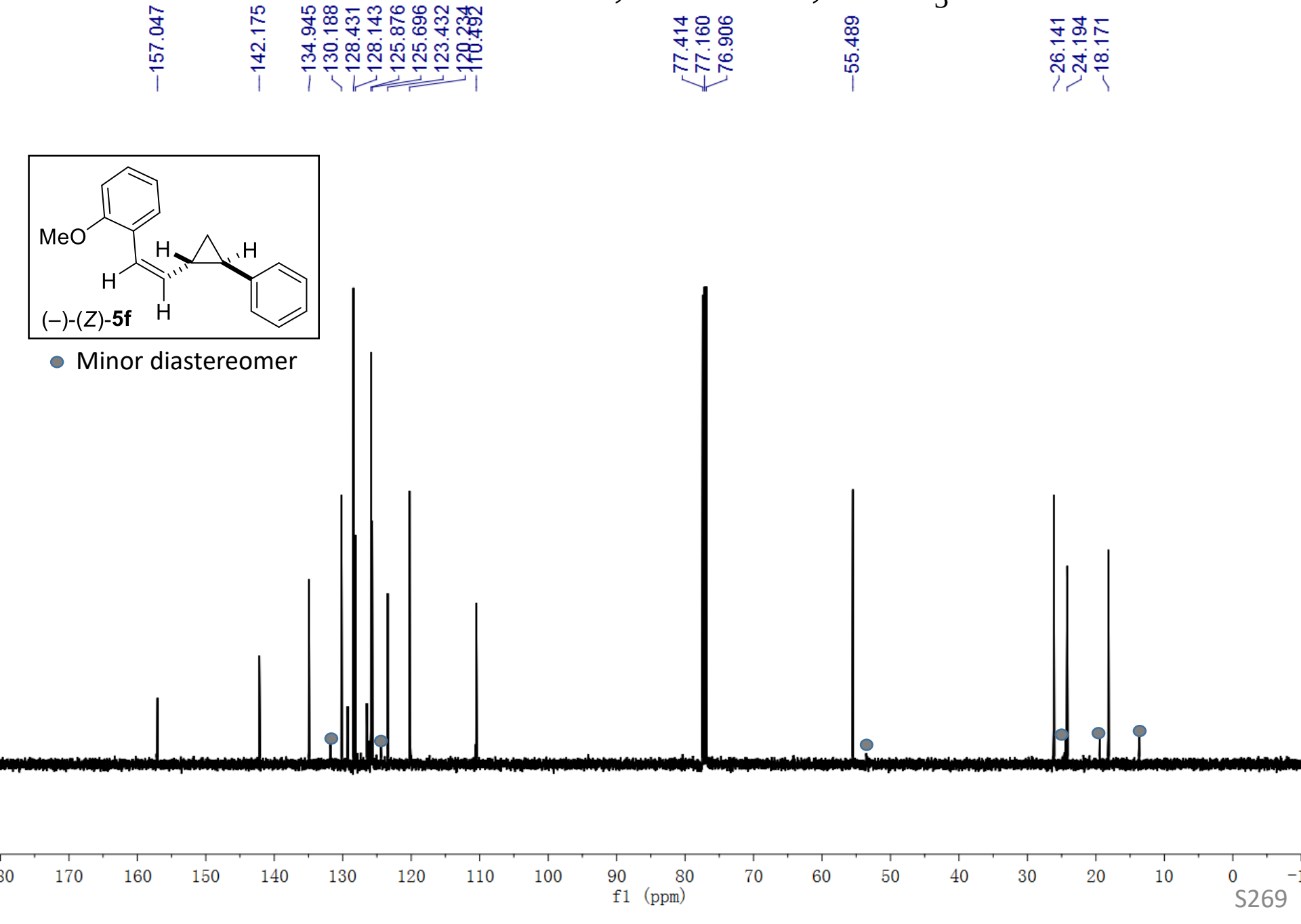


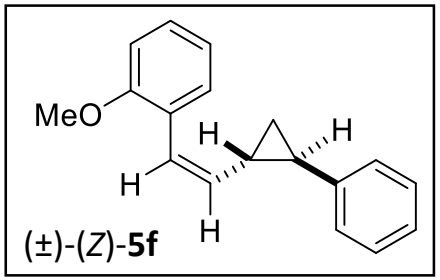
^{1}H NMR of **5f**, 500 MHz, $CDCl_3$



- Minor diastereomer

^{13}C NMR of 5**f**, 126 MHz, $CDCl_3$

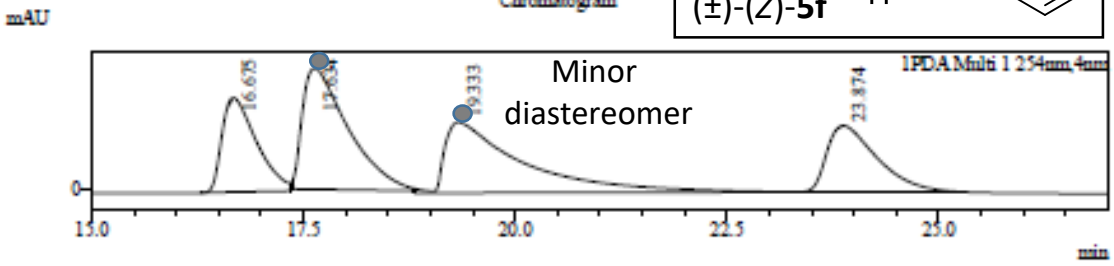




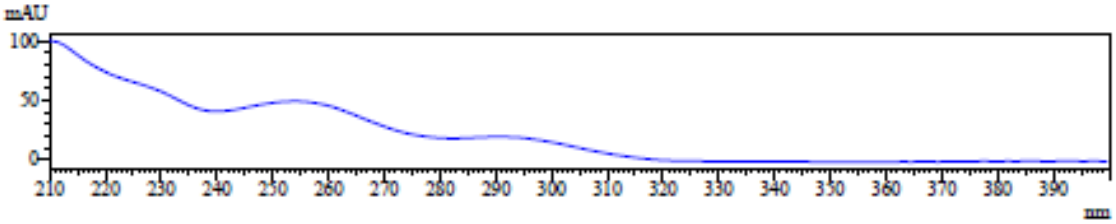
(±)-(*Z*)-**5f**

Data File : J0K-1000-IB-0%-1ML.lcd
Sample Name : J0K-1000-IB-0%-1ML
Sample ID : J0K-1000-IB-0%-1ML
Method File : J0K-0%--45min-1ml.lcm

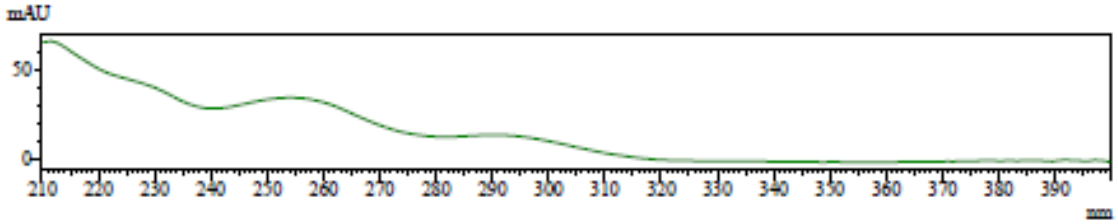
Chromatogram



UV Spectrum
Retention time = 16.675



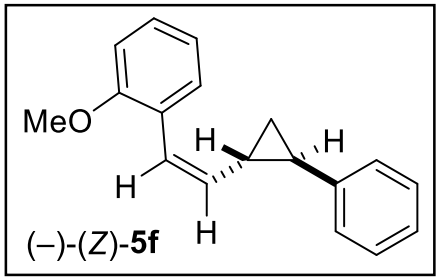
UV Spectrum
Retention time = 23.874



Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	16.675	1401565	18.515
2	17.634	2380278	31.444
3	19.333	2366946	31.268
4	23.874	1421163	18.774
Total		7569951	100.000

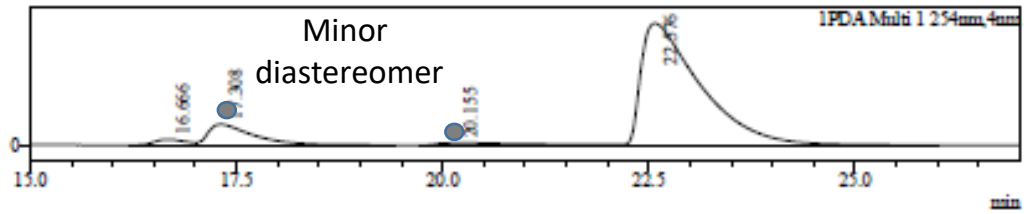


(–)-(*Z*)-**5f**

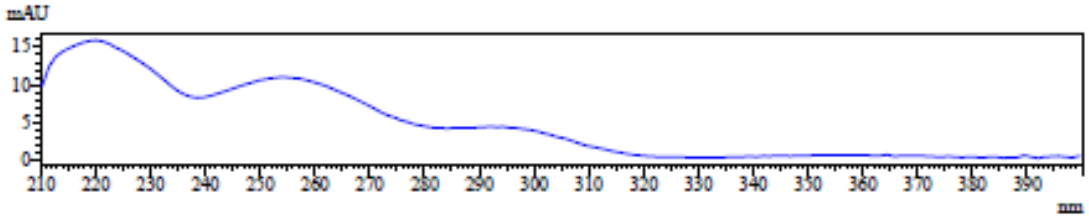
Data File : J0K-1003-IB-0%-1ML-6.lcd
Sample Name : J0K-1003-IB-0%-1ML-5
Sample ID : J0K-1003-IB-0%-1ML-5
Method File : J0K-0%--45min-1ml.lcm

Chromatogram

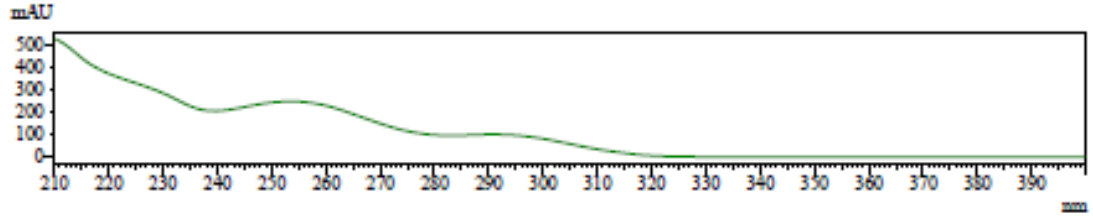
mAU



UV Spectrum
Retention time = 16.666



UV Spectrum
Retention time = 22.576

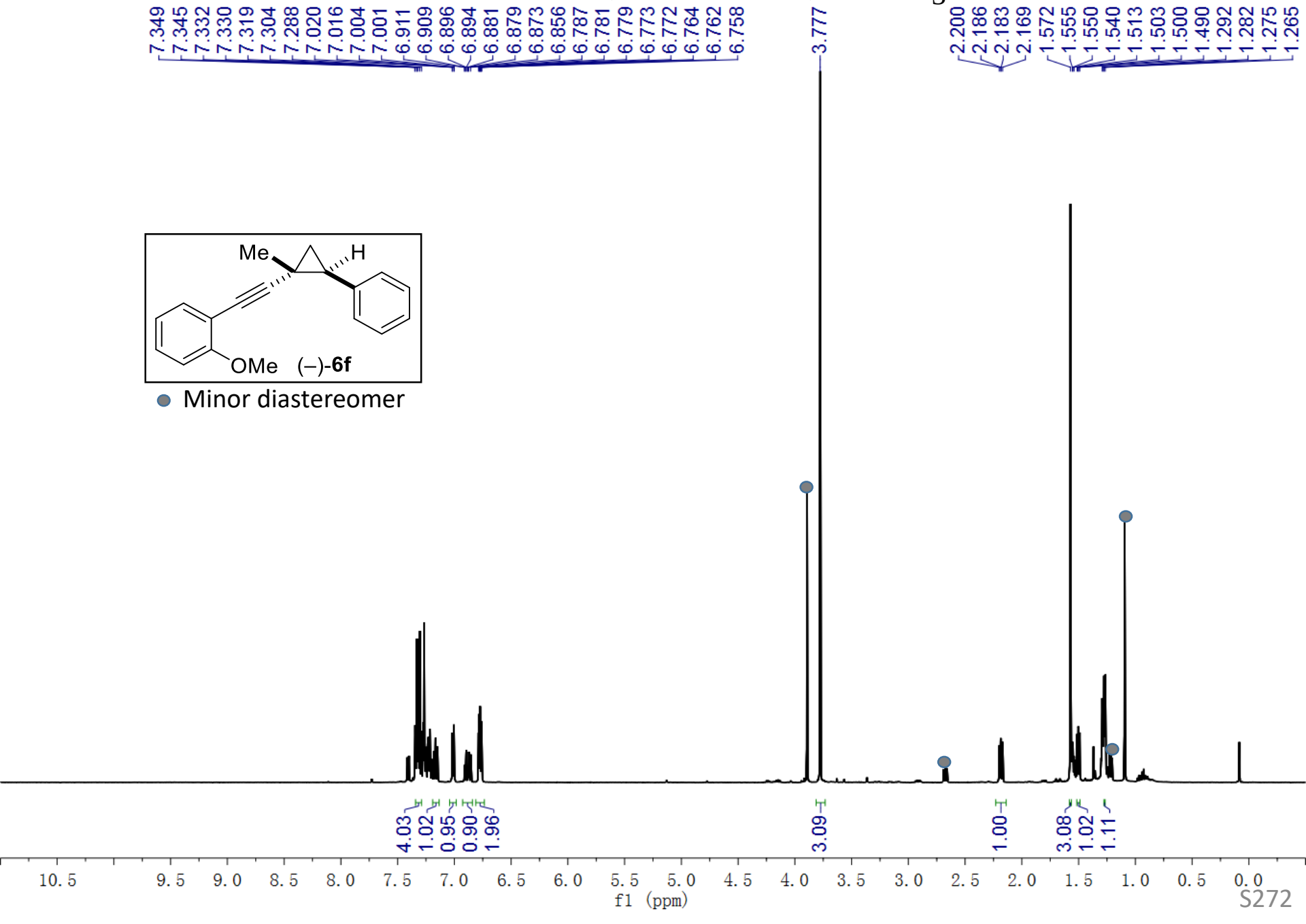


Peak Table

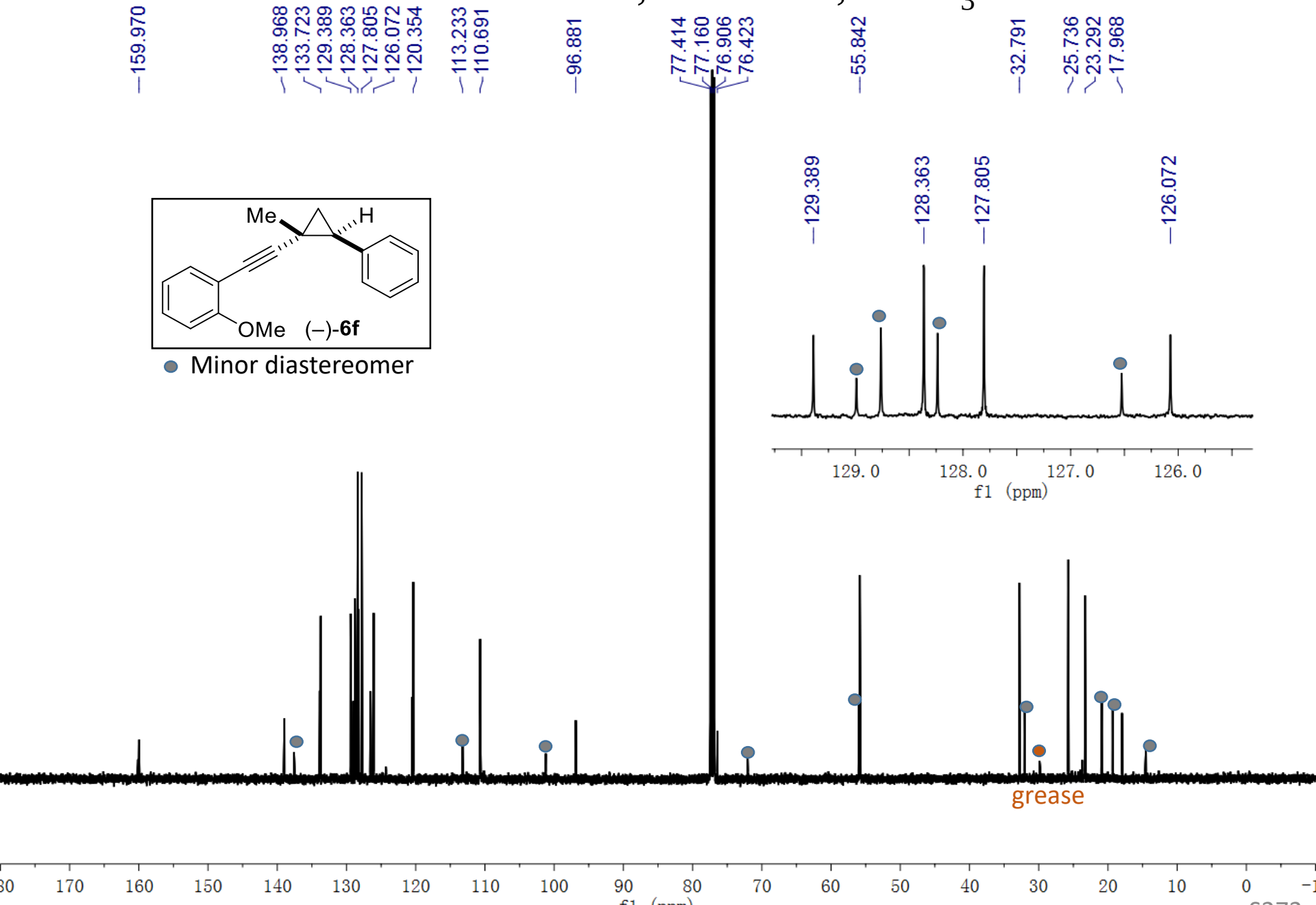
PDA Ch1 254nm

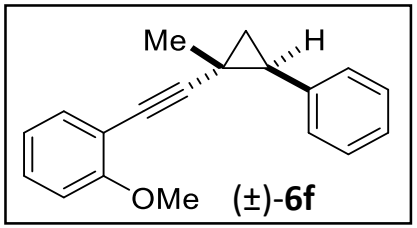
Peak#	Ret. Time	Area	Area%
1	16.666	288690	1.983
2	17.308	1599163	10.982
3	20.155	311844	2.142
4	22.576	12362128	84.894
Total		14561825	100.000

^{1}H NMR of **6f**, 500 MHz, $CDCl_3$



^{13}C NMR of **6f**, 126 MHz, $CDCl_3$

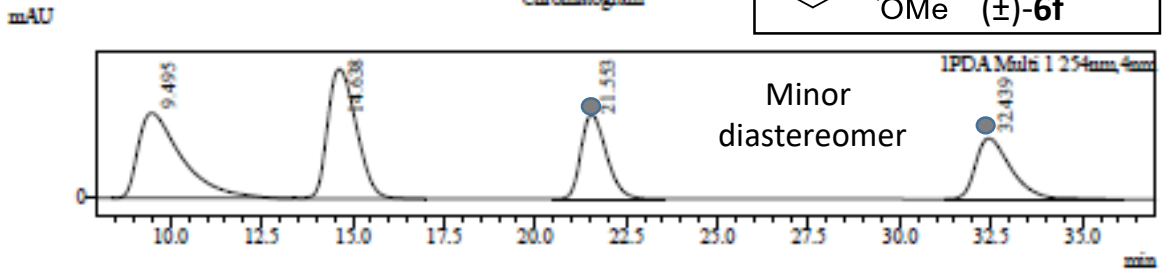




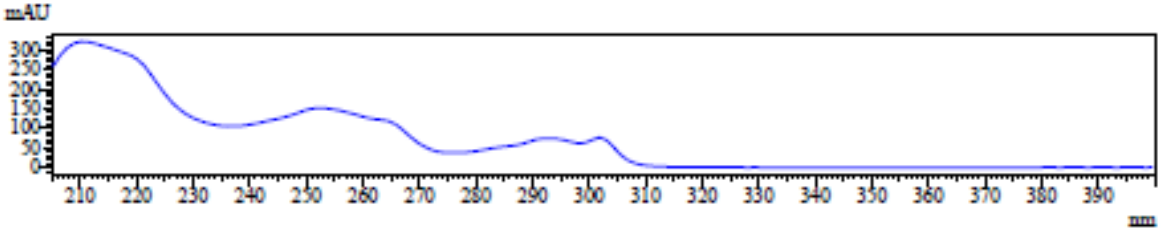
(±)-**6f**

Data File : J0K-1538-ODH--0.3%-1ML.lcd
Sample Name : J0K-1538-ODH--0.3%-1ML
Sample ID : J0K-1538-ODH--0.3%-1ML
Method File : J0K-0.3%--45min-1ml.lcm

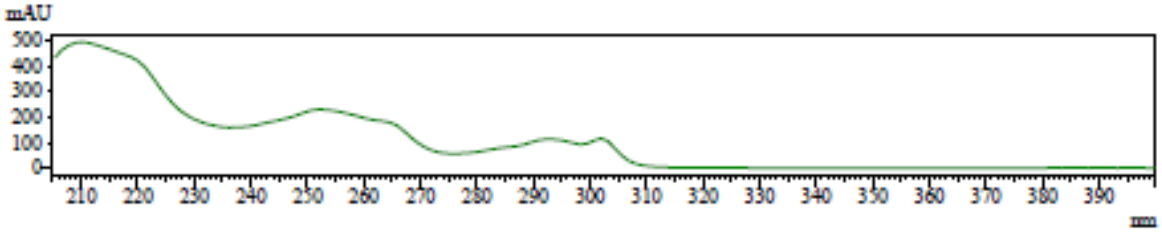
Chromatogram



UV Spectrum
Retention time = 9.495



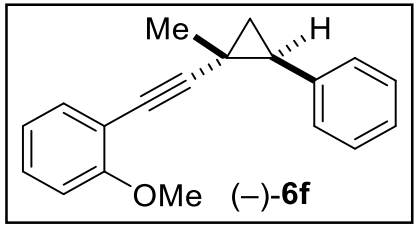
UV Spectrum
Retention time = 14.638



Peak Table

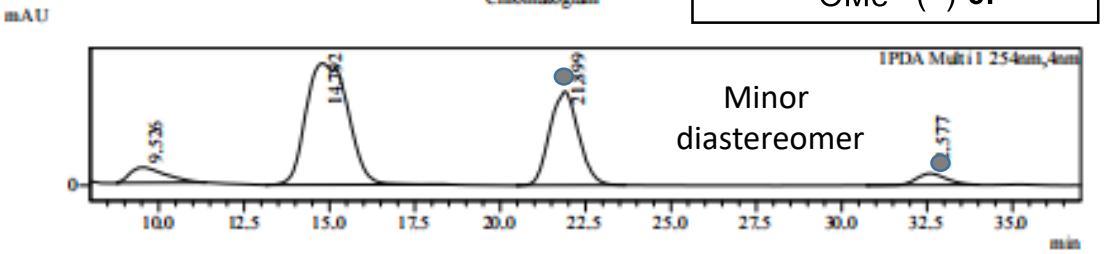
PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	9.495	12369764	31.724
2	14.638	12353166	31.682
3	21.553	7090460	18.185
4	32.439	7178261	18.410
Total		38991652	100.000

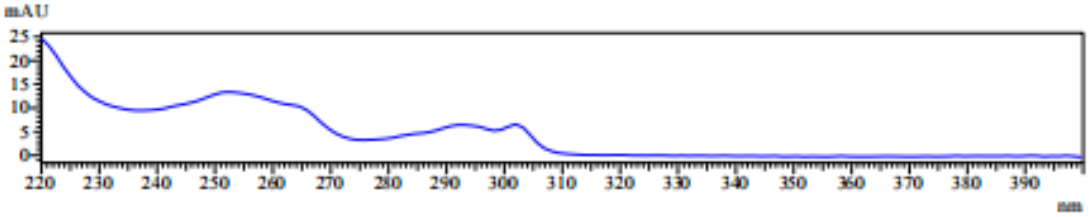


(–)-**6f**

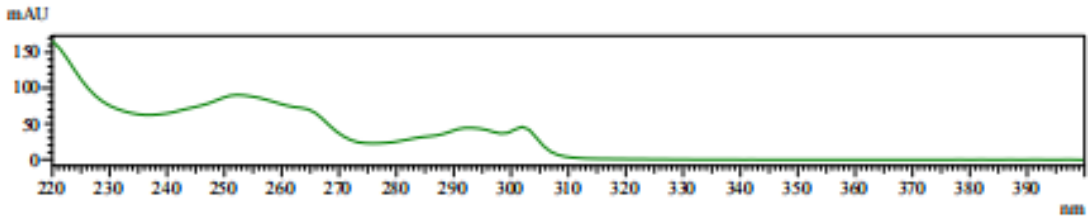
Data File : J0K-1539-ODH--0.3%-1ML.lcd
Sample Name : J0K-1539-ODH--0.3%-1ML
Sample ID : J0K-1539-ODH--0.3%-1ML
Method File : J0K-0.3%--45min-1ml.lcm
Chromatogram



UV Spectrum
Retention time = 9.526



UV Spectrum
Retention time = 14.792

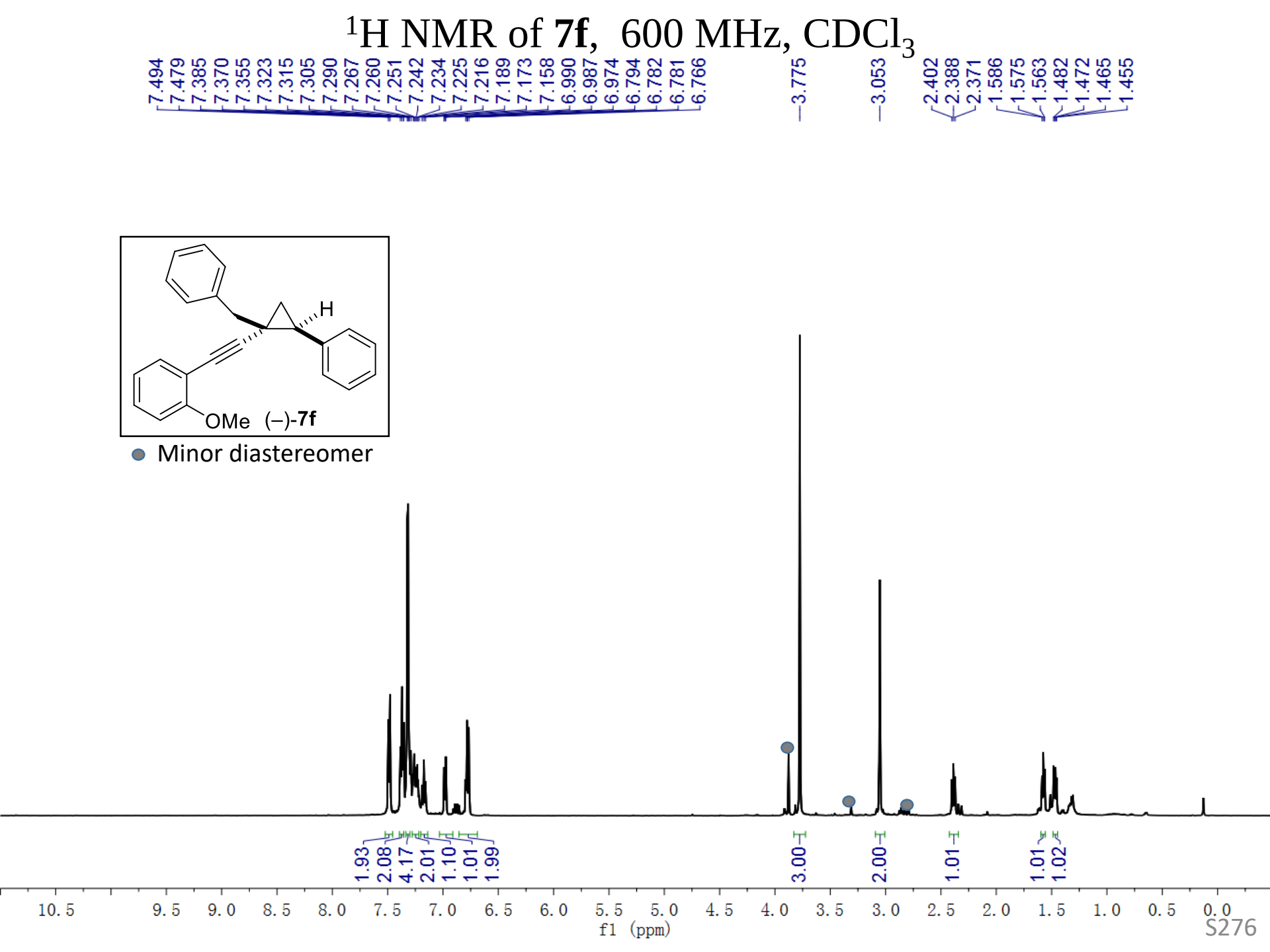


Peak Table

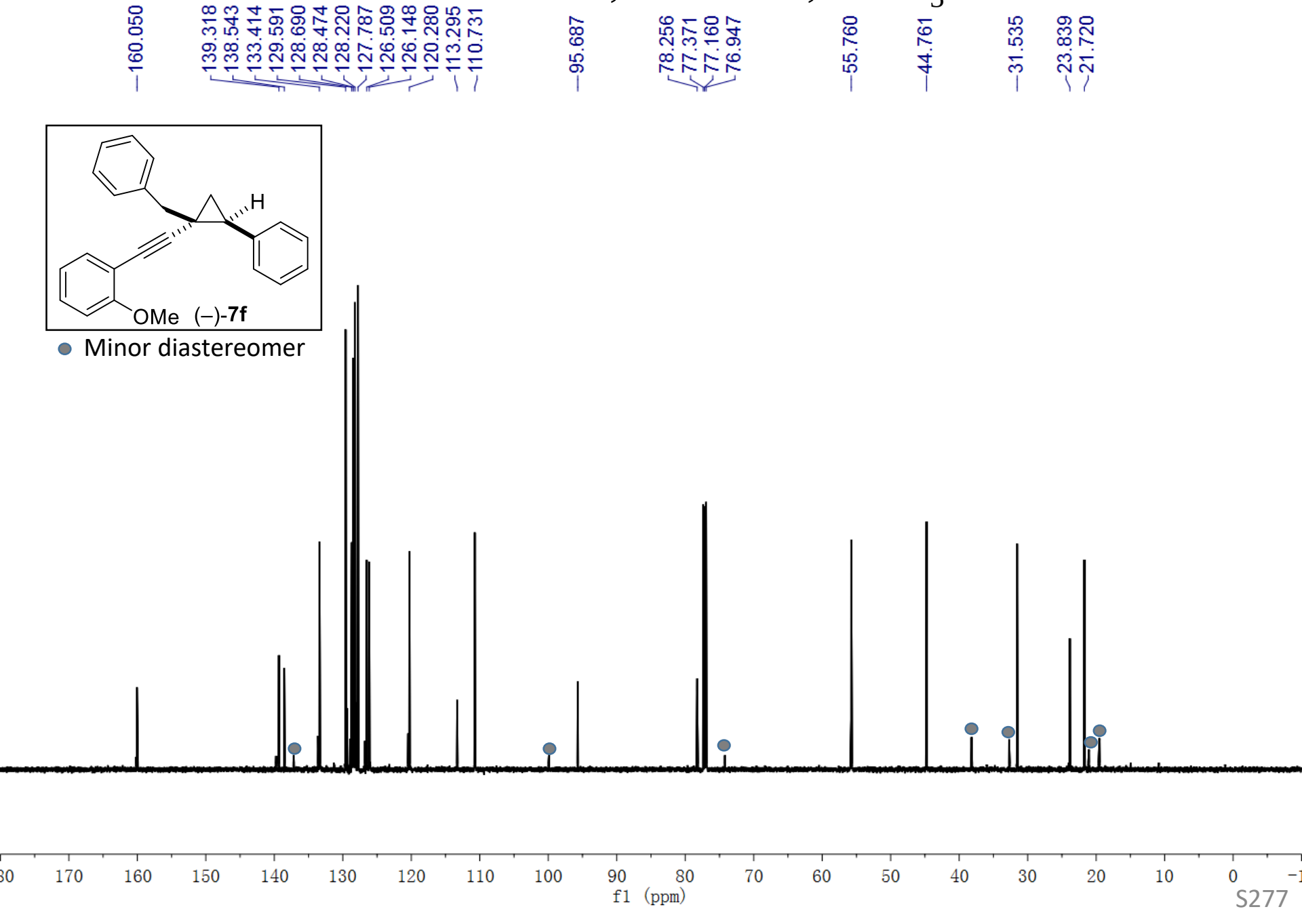
PDA Ch1 254nm

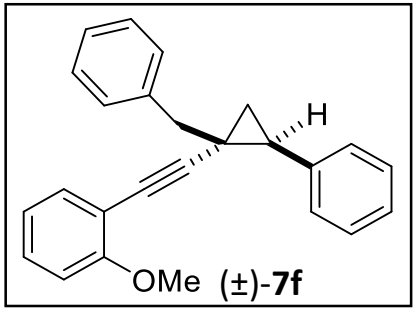
Peak#	Ret. Time	Area	Area%
1	9.526	793506	6.221
2	14.792	7495637	58.764
3	21.899	3969097	31.117
4	32.577	497335	3.899
Total		12755575	100.000

^{1}H NMR of **7f**, 600 MHz, $CDCl_3$



^{13}C NMR of **7f**, 151 MHz, $CDCl_3$

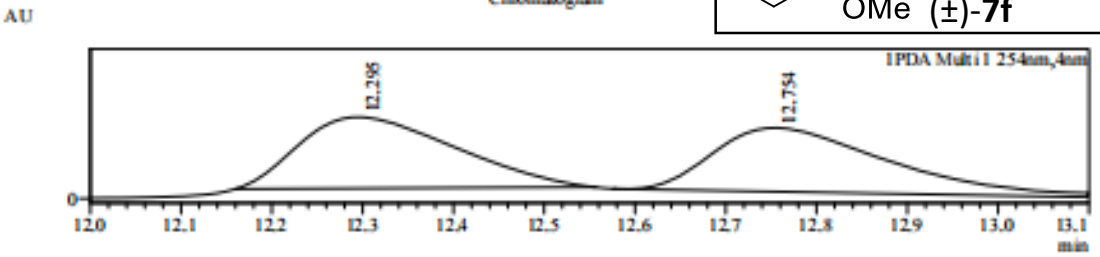




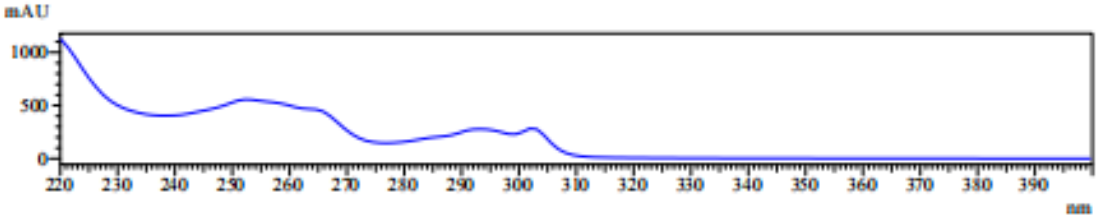
(±)-**7f**

Data File : J0K-1476-IA-NEW--0.5%-0.5Ml.lcd
Sample Name : J0K-1476-IA-NEW--0.5%-0.5Ml
Sample ID : J0K-1476-IA-NEW--0.5%-0.5Ml
Method File : J0K-0.5%--35min-0.5ml.lcm

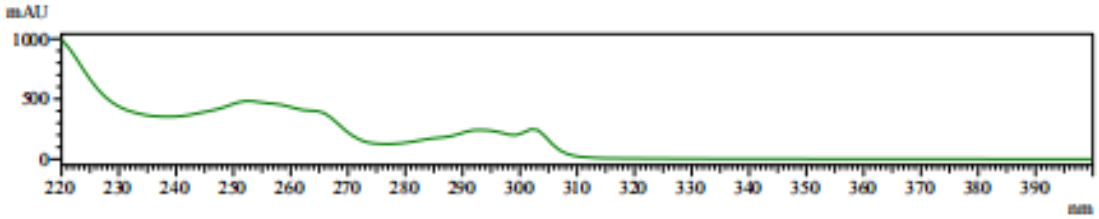
Chromatogram



UV Spectrum
Retention time = 12.295



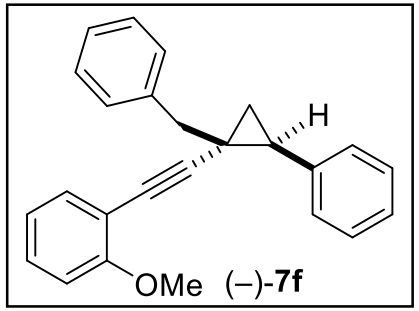
UV Spectrum
Retention time = 12.754



Peak Table

PDA Ch1 254nm

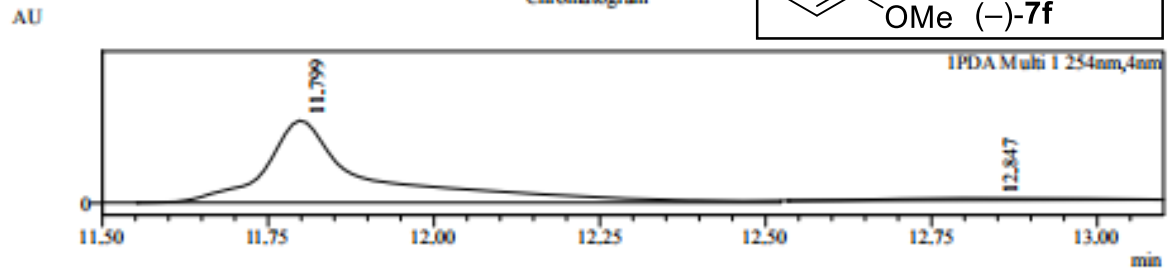
Peak#	Ret. Time	Area	Area%
1	12.295	5702969	50.172
2	12.754	5663776	49.828
Total		11366745	100.000



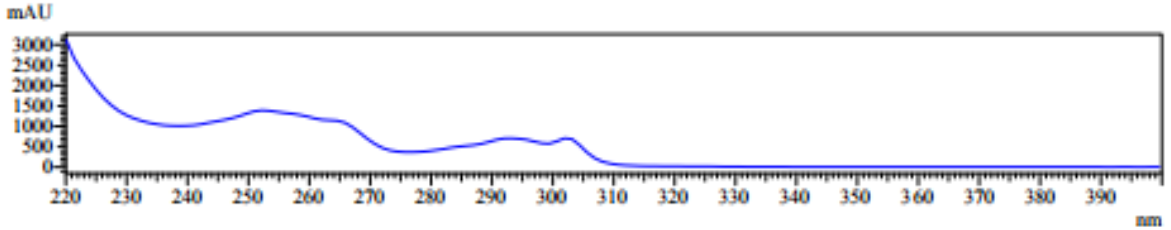
(–)-**7f**

Data File : J0K-1462-IA-0.5%-0.5ML.lcd
Sample Name : J0K-1462-IA-0.5%-0.5ML
Sample ID : J0K-1462-IA-0.5%-0.5ML
Method File : J0K-0.5%--35min-0.5ml.lcm

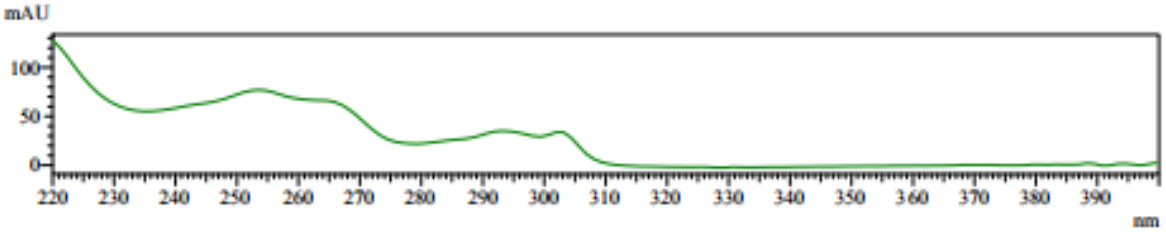
Chromatogram



UV Spectrum
Retention time = 11.799



U
Retention time = 12.847

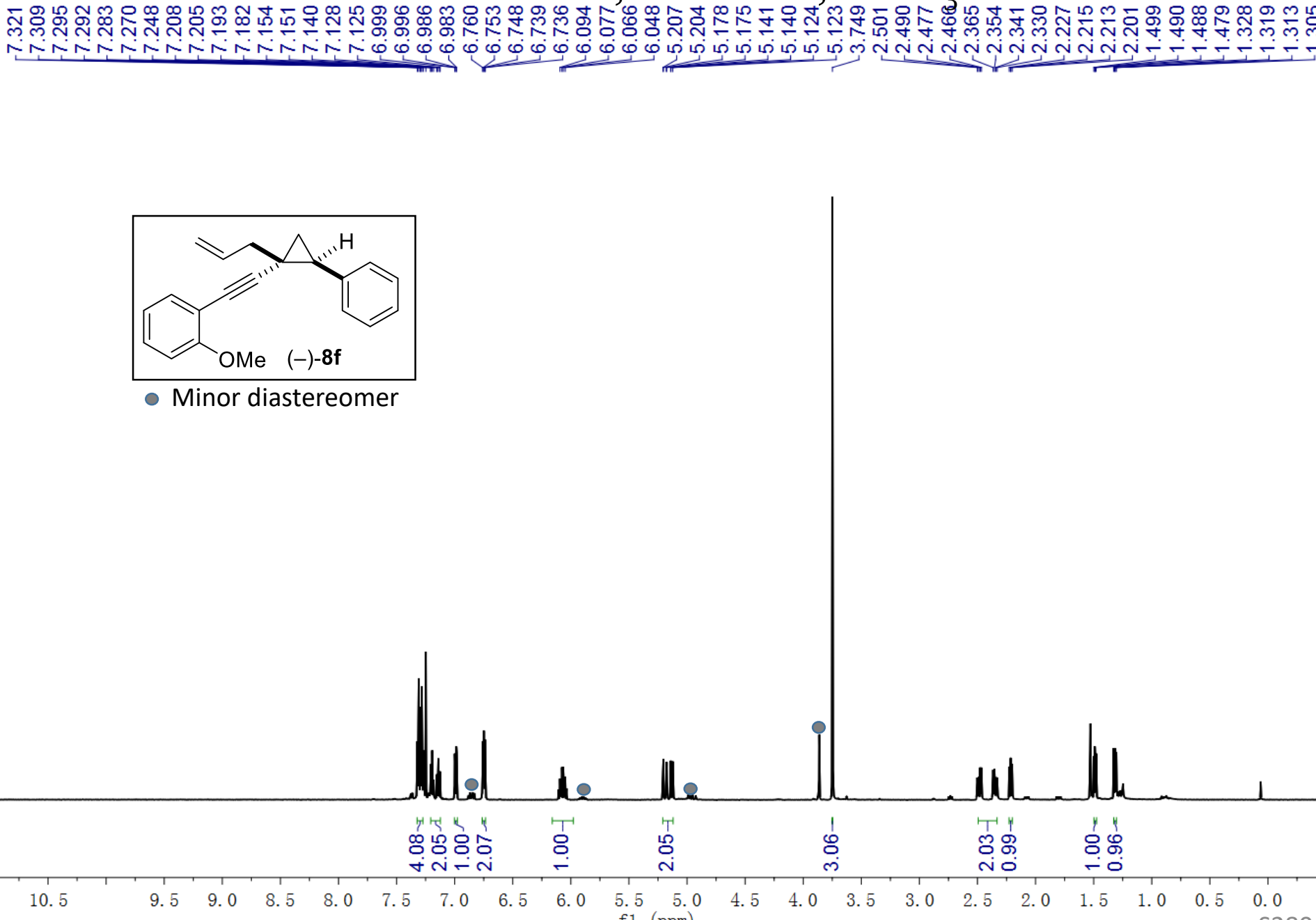


Peak Table

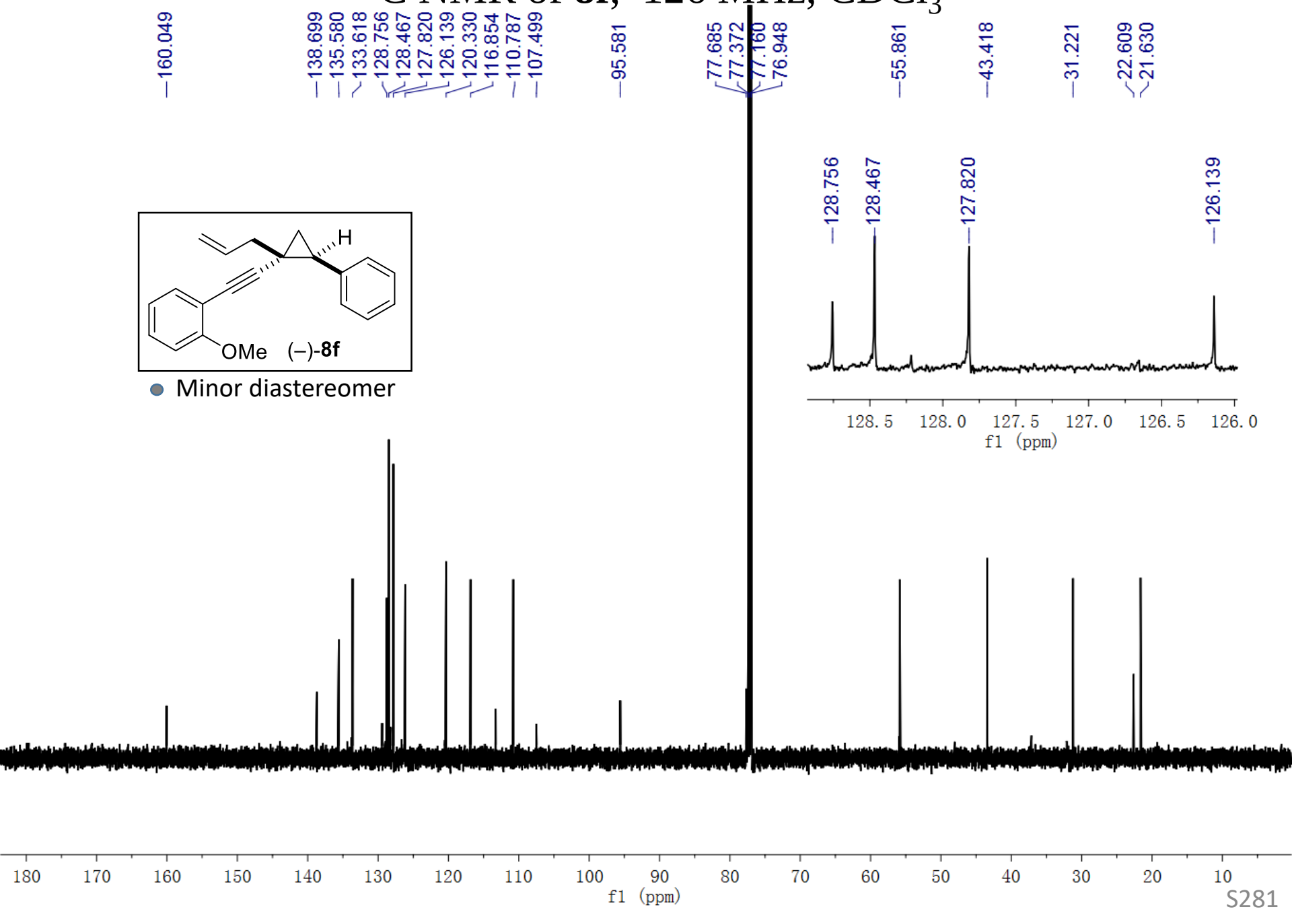
PDA Ch1 254nm

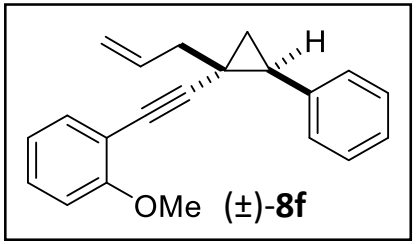
Peak#	Ret. Time	Area	Area%
1	11.799	14758228	96.142
2	12.847	592161	3.858
Total		15350389	100.000

^{1}H NMR of **8f**, 500 MHz, $CDCl_3$



^{13}C NMR of **8f**, 126 MHz, $CDCl_3$

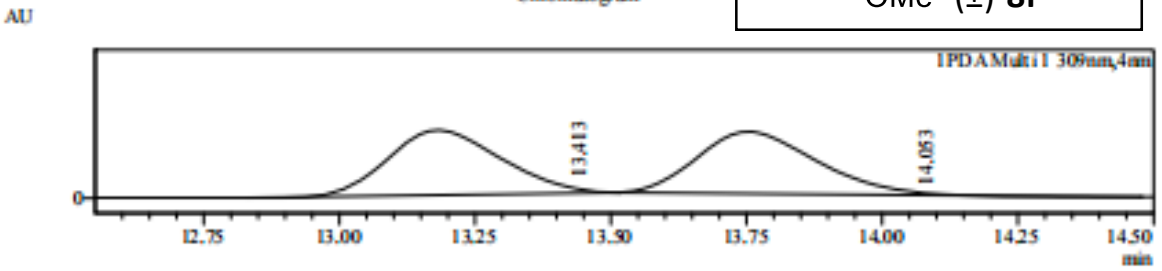




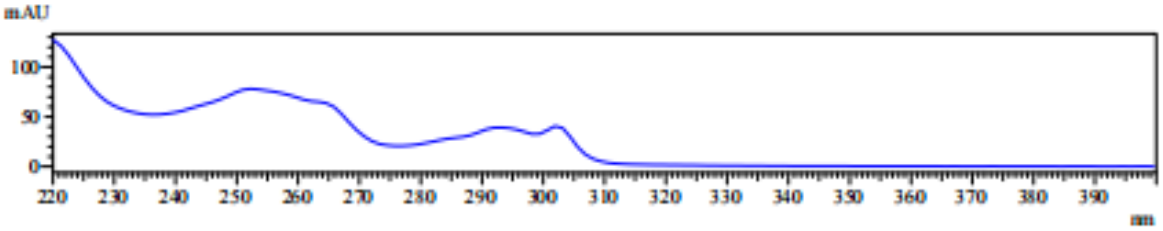
(±)-**8f**

Data File : J0K-1549-IB--0.2%-0.5ML-2.lcd
Sample Name : J0K-1549-IB--0.2%-0.5ML-2
Sample ID : J0K-1549-IB--0.2%-0.5ML-2
Method File : J0K-0.2%--40min-0.5ml.lcm

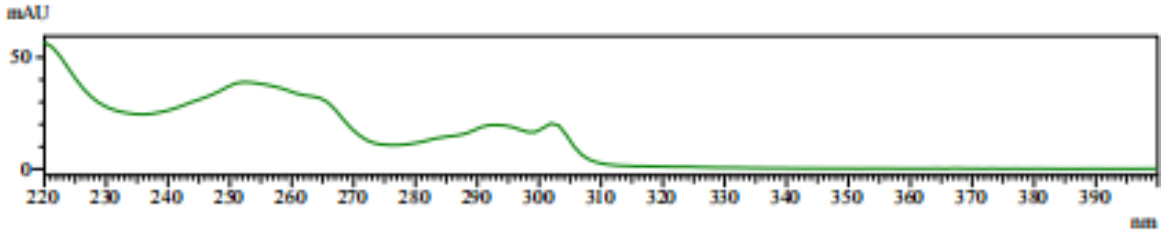
Chromatogram



UV Spectrum
Retention time = 13.413



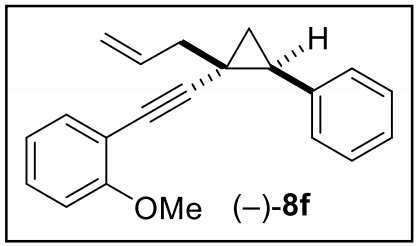
UV Spectrum
Retention time = 14.053



Peak Table

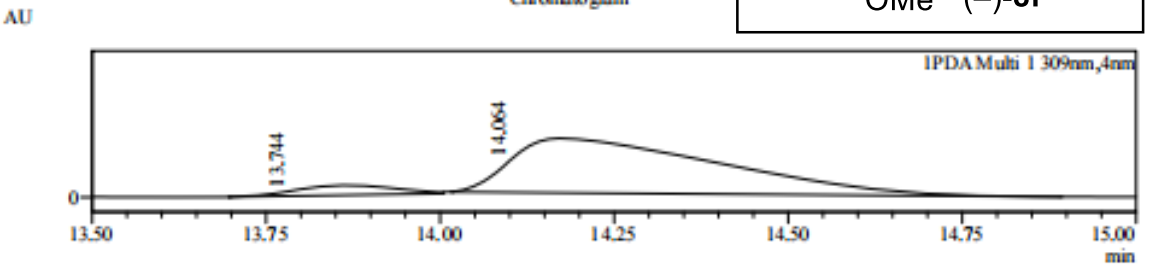
PDA Ch1 309nm

Peak#	Ret. Time	Area	Area%
1	13.413	631887	49.937
2	14.053	633470	50.063
Total		1265357	100.000

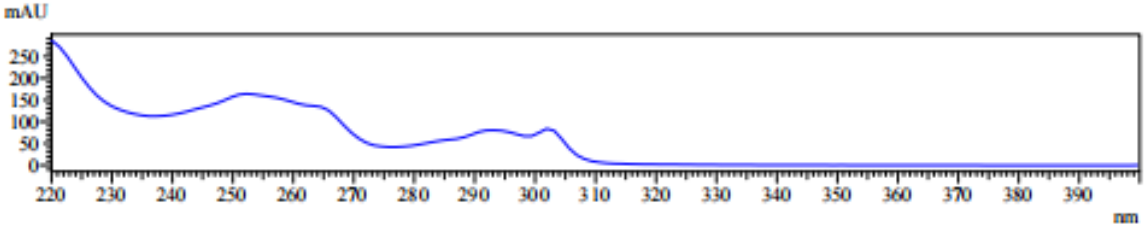


Data File : J0K-1560-IB--0.2%-0.5ML-3.lcd
Sample Name : J0K-1560-IB--0.2%-0.5ML-3
Sample ID : J0K-1560-IB--0.2%-0.5ML-3
Method File : J0K-0.2%--40min-0.5ml.lcm

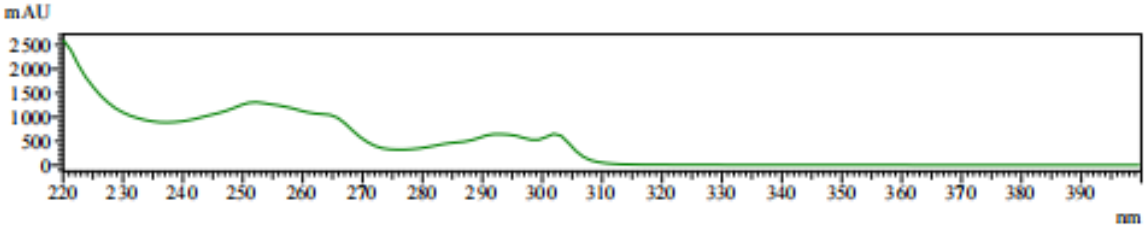
Chromatogram



UV Spectrum
Retention time = 13.744



UV Spectrum
Retention time = 14.064

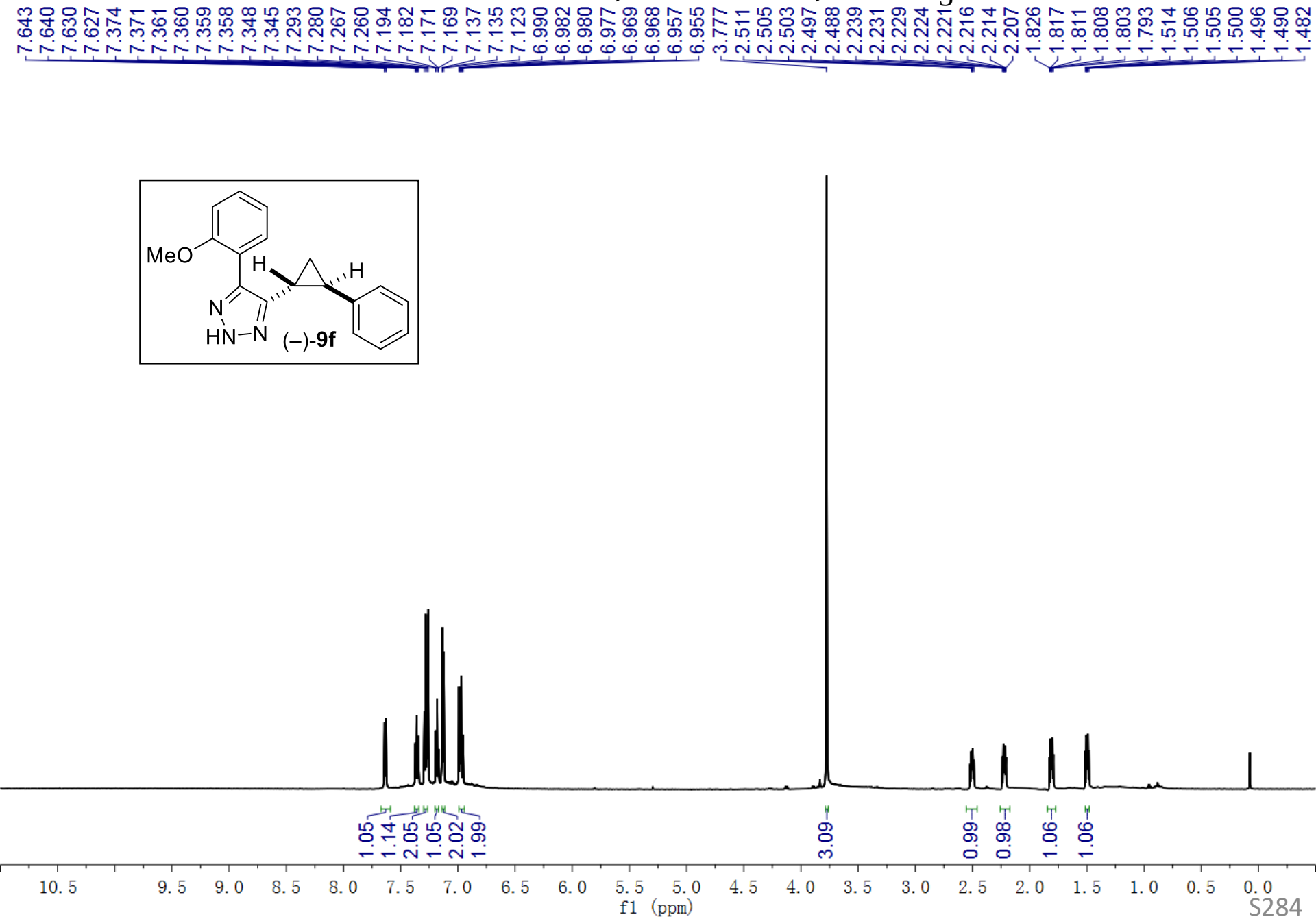


Peak Table

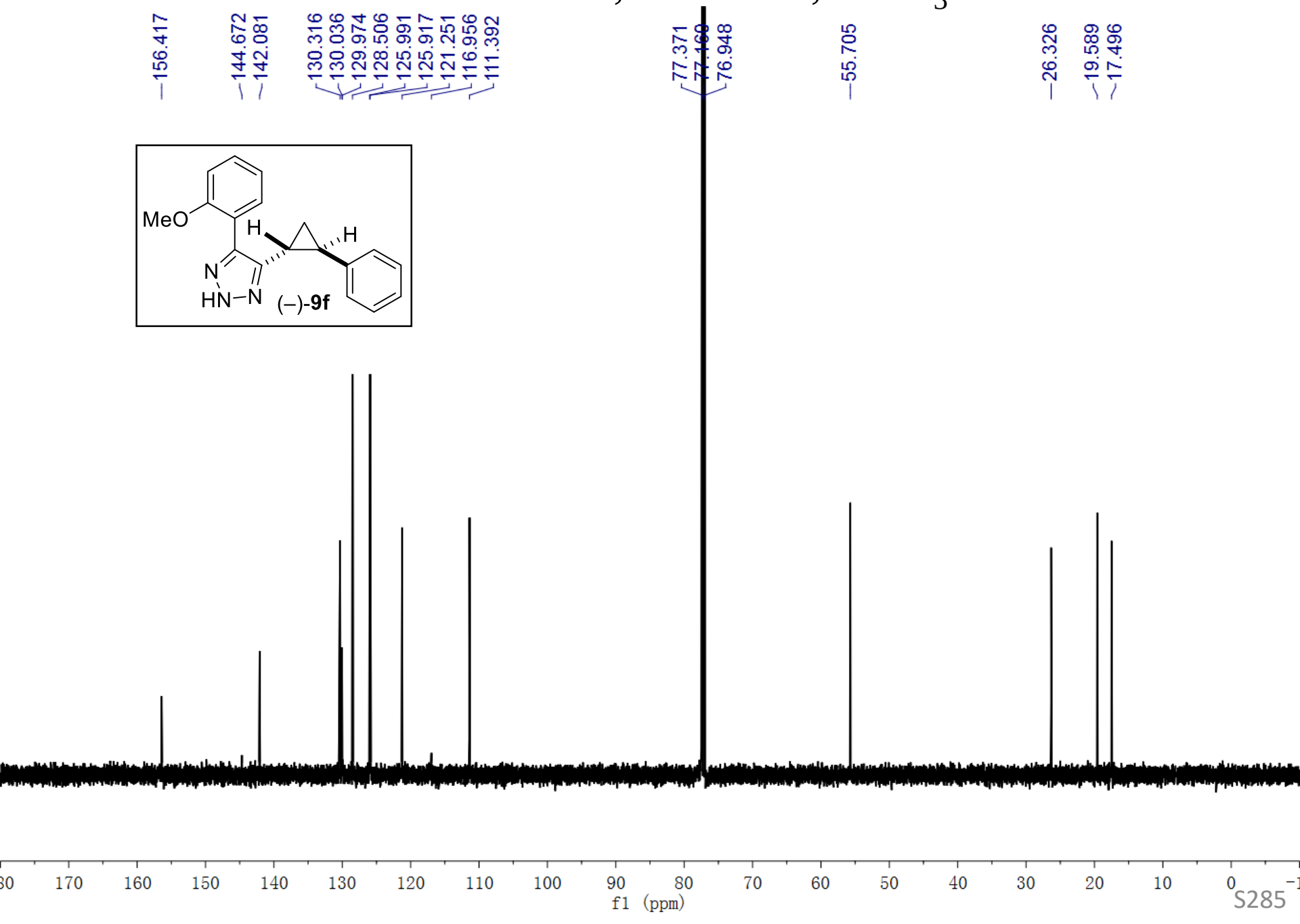
PDA Ch1 309nm

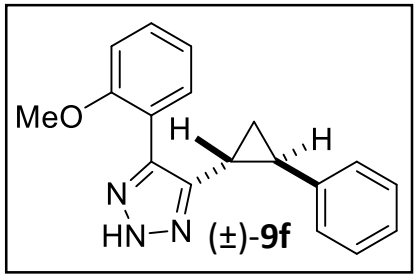
Peak#	Ret. Time	Area	Area%
1	13.744	673967	8.053
2	14.064	7695259	91.947
Total		8369226	100.000

^{1}H NMR of **9f**, 600 MHz, $CDCl_3$



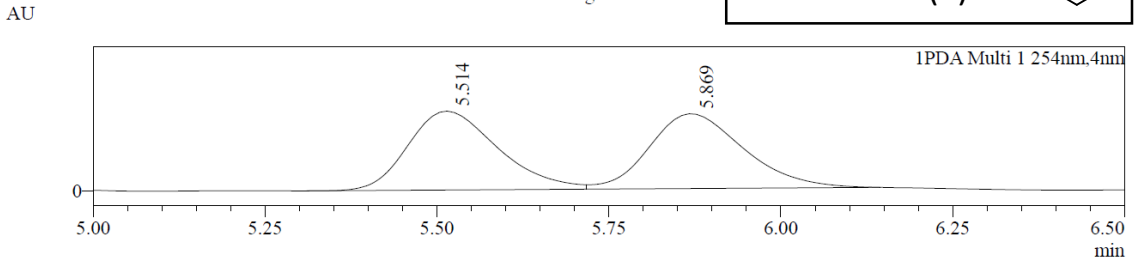
^{13}C NMR of **9f**, 151 MHz, $CDCl_3$



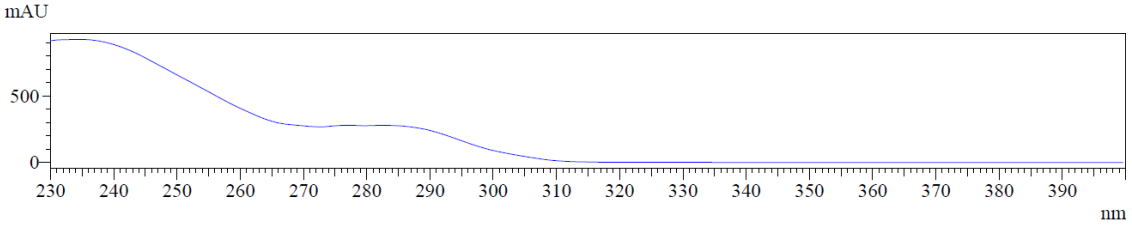


Data File : J0K-1852--IB-15%-1ML-3.lcd
Sample Name : J0K-1852--IB-15%-1ML-3
Sample ID : J0K-1852--IB-15%-1ML-3
Method File : J0K-15%--40min-1ml.lcm

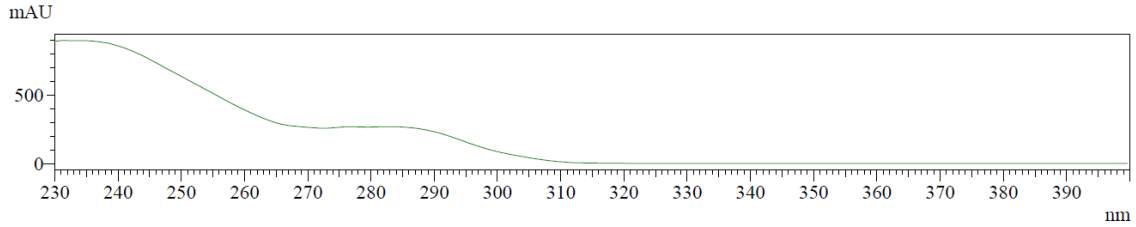
Chromatogram



UV Spectrum
Retention time = 5.514



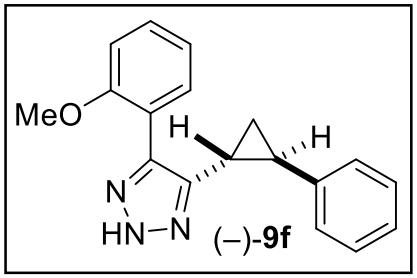
UV Spectrum
Retention time = 5.869



Peak Table

PDA Ch1 254nm

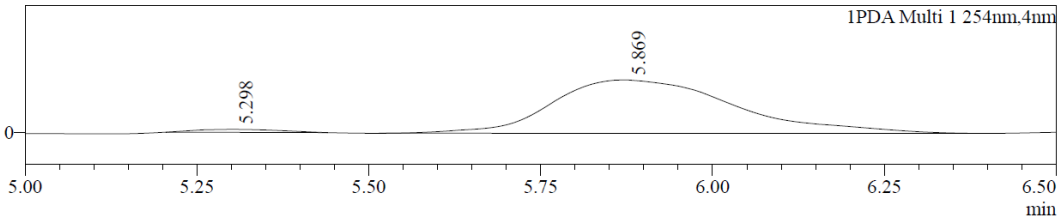
Peak#	Ret. Time	Area	Area%
1	5.514	4977612	50.153
2	5.869	4947185	49.847
Total		9924797	100.000



Data File : J0K-1853--IB-15%-1ML.lcd
Sample Name : J0K-1853--IB-15%-1ML
Sample ID : J0K-1853--IB-15%-1ML
Method File : J0K-15%--40min-1ml.lcm

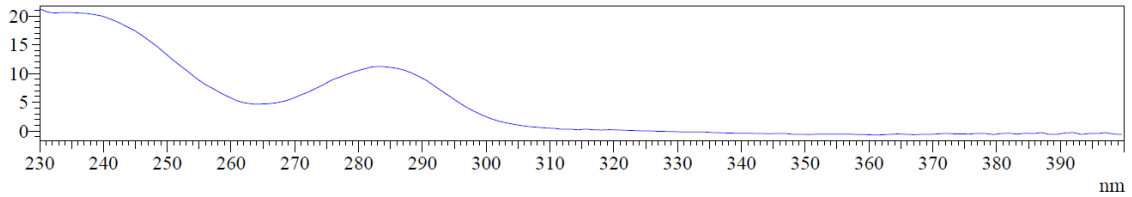
Chromatogram

AU



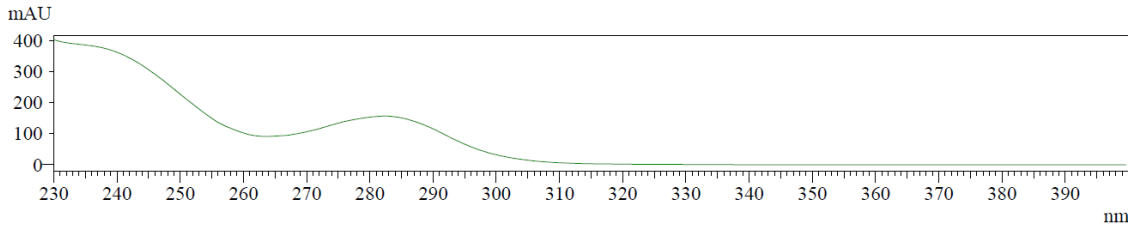
UV Spectrum
Retention time = 5.298

mAU



UV Spectrum
Retention time = 5.869

mAU

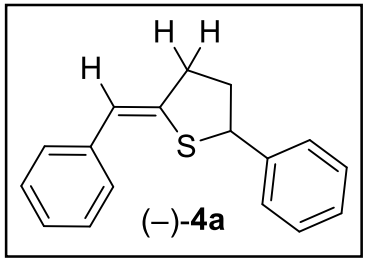


Peak Table

PDA Ch1 254nm

Peak#	Ret. Time	Area	Area%
1	5.298	80413	2.527
2	5.869	3101211	97.473
Total		3181624	100.000

^{1}H NMR of **4a**, 600 MHz, $CDCl_3$

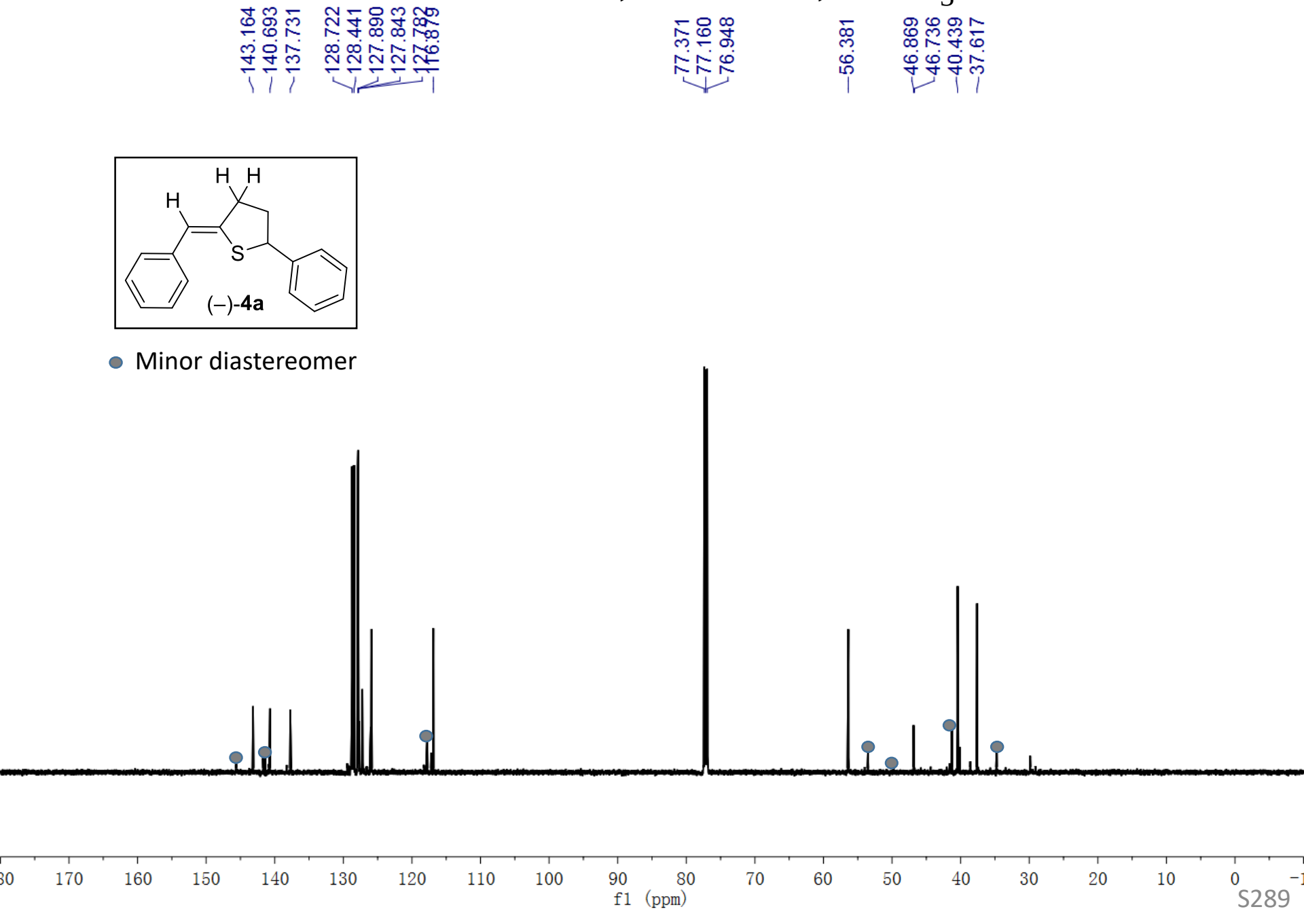


- Minor diastereomer

grease

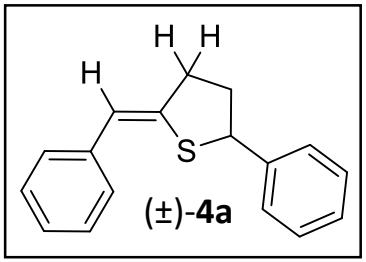
f1 (ppm)

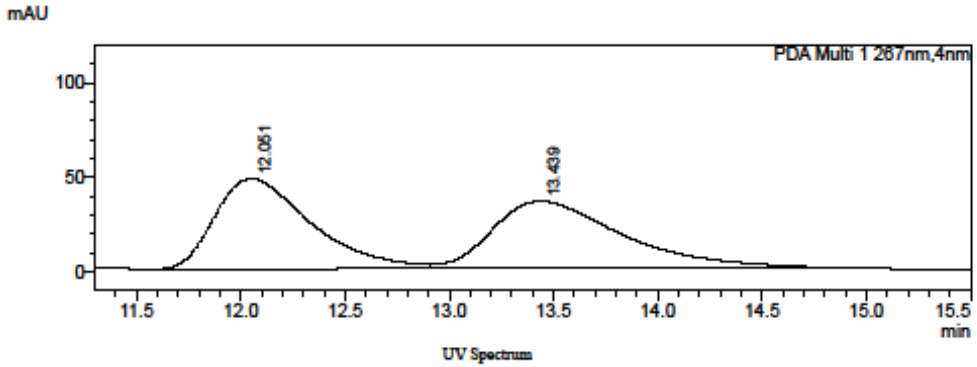
^{13}C NMR of **4a**, 151 MHz, $CDCl_3$



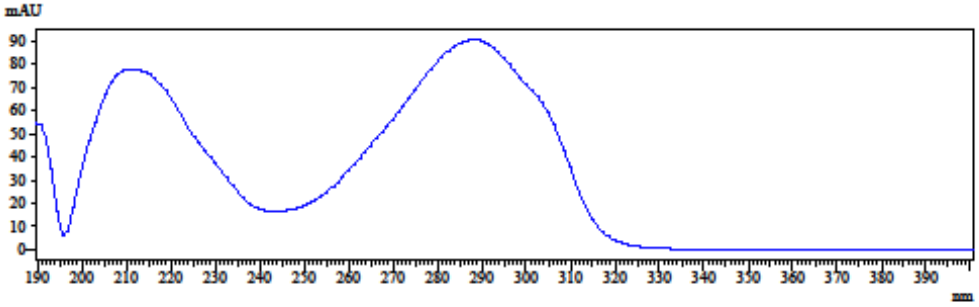
==== Shimadzu LabSolutions Analysis Report ====

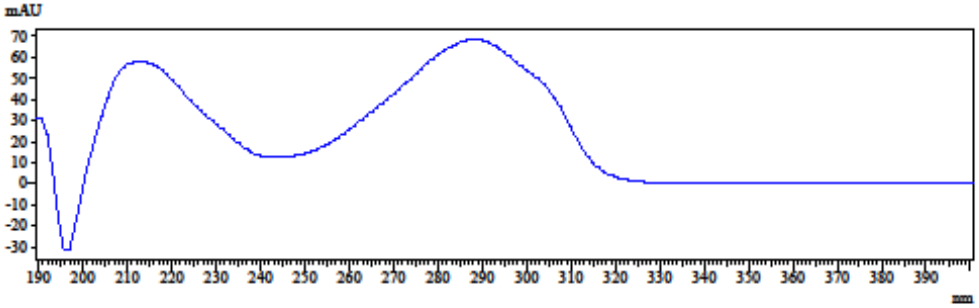
WCL1848-ID-0.1%0.8mL
WCL-0.1%-30min0.8mL.lcm





UV Spectrum



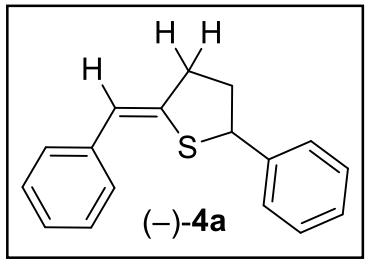


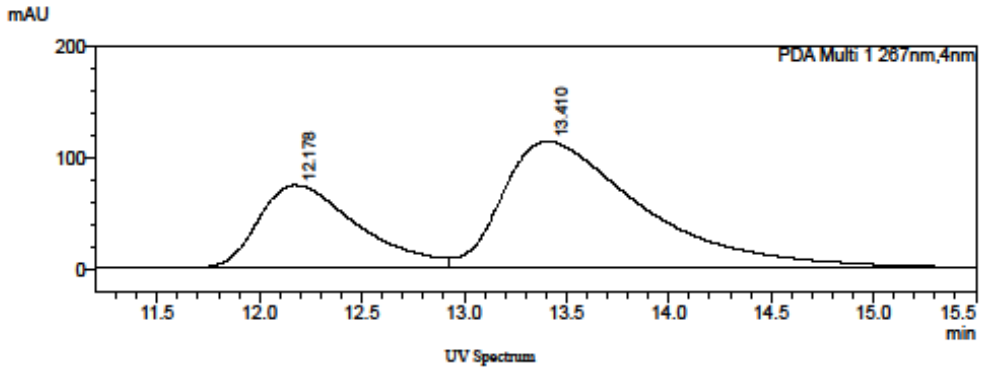
Peak Table
PDA Ch1 267nm

Peak#	Ret. Time	Area%
1	12.051	49.191
2	13.439	50.809
Total		100.000

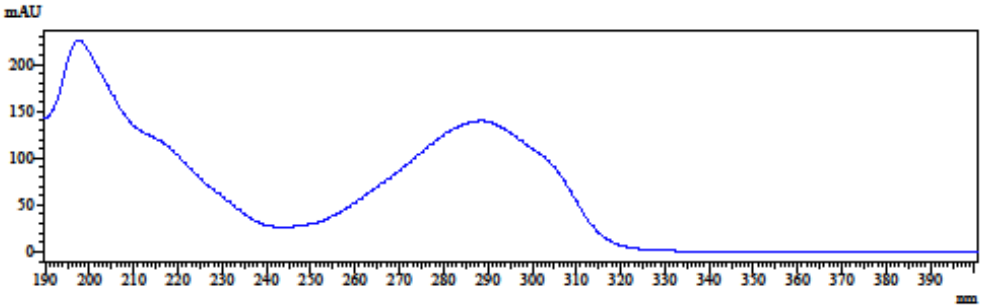
==== Shimadzu LabSolutions Analysis Report ====

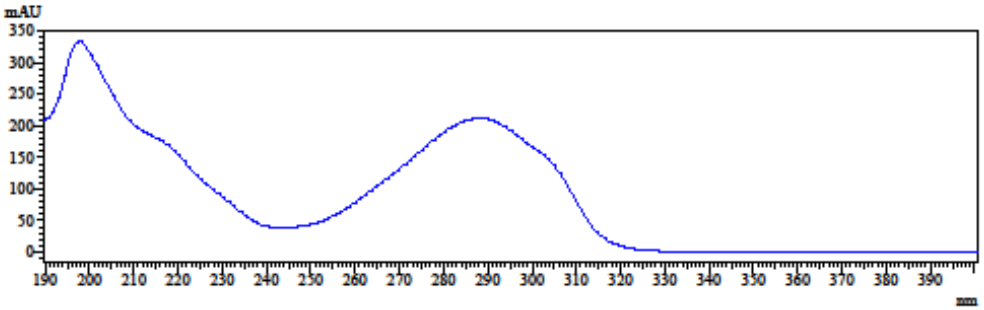
WCL1851-ID-0.1%0.8mL
WCL-0.1%-30min0.8mL.lcm





UV Spectrum





Peak Table

PDA Ch1 267nm

Peak#	Ret. Time	Area%
1	12.178	31.810
2	13.410	68.190
Total		100.000