

Chiral tertiary propargylic alcohols via Pd-catalyzed carboxylative kinetic resolution

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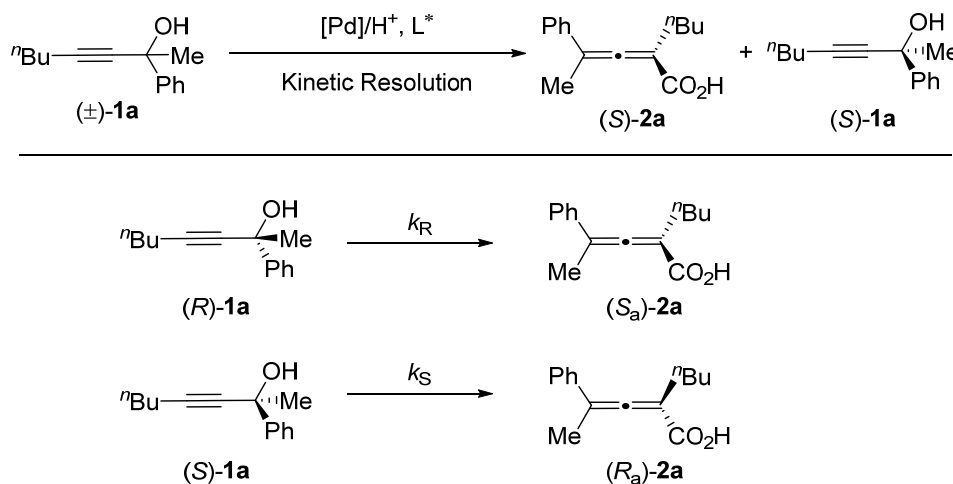
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General Information. NMR spectra were taken with a Bruker Avance III spectrometer (400 MHz for ^1H NMR, 100 MHz for ^{13}C NMR) in CDCl_3 . All ^1H NMR experiments were measured with tetramethylsilane (0 ppm) in CDCl_3 as the internal reference; ^{13}C NMR experiments were measured in relative to the signal of CDCl_3 (77.0 ppm). All reactions were carried out in Schlenk tubes. (*R*)-DTBM-SEGphos was purchased from Strem Chemicals Inc.; $(\text{PhO})_2\text{POOH}$ was purchased from Energy Chemical, acidified with 1 N HCl under stirring, and extracted with dichloromethane, then the solvent was removed under vacuum. Petroleum ether (b.p. 60~90°C) was purchased from Shanghai Titan Scientific Co., Ltd. Toluene was purchased from Shanghai Titan Scientific Co., Ltd and used as received without further purification. The reaction should be conducted in a hood working efficiently with a CO detector due to the toxicity of CO gas. All the temperatures are referred to the oil baths used. Recoveries of substrates were determined by ^1H NMR analysis using dibromomethane as the internal standard. The racemic propargylic alcohols were prepared according to the literature methods.¹

Calculation of selectivity factor s^2

In the kinetic resolution process, the selectivity factor s is related to the rate constants of the reaction of R - and S -enantiomers, k_R and k_S , respectively, by $s = k_R/k_S$, for $k_R > k_S$.



Basically, s can be established by the following equation for a first order reaction, in which C is the conversion and ee is the enantiomeric excess value of recovered substrate:

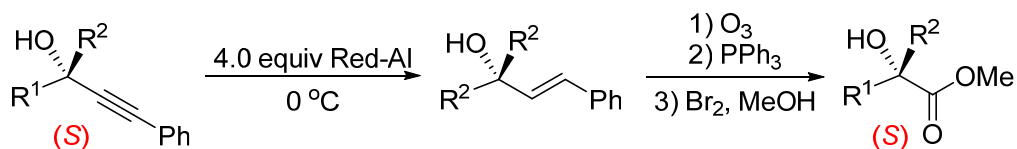
$$s = \frac{\ln [1-C(1+ee)]}{\ln [1-C(1-ee)]}$$

Besides, C can be calculated from the enantiomeric excess values of recovered substrate and product, ee and ee' , respectively, through the equation $C = ee/(ee+ee')$, if (R) -**1a** and (S) -**1a** were stereospecifically transferred to (S_a) -**2a** and (R_a) -**2a** in this kinetic resolution process. The conversion was determined by ^1H NMR analysis.

Determination of the absolute configuration

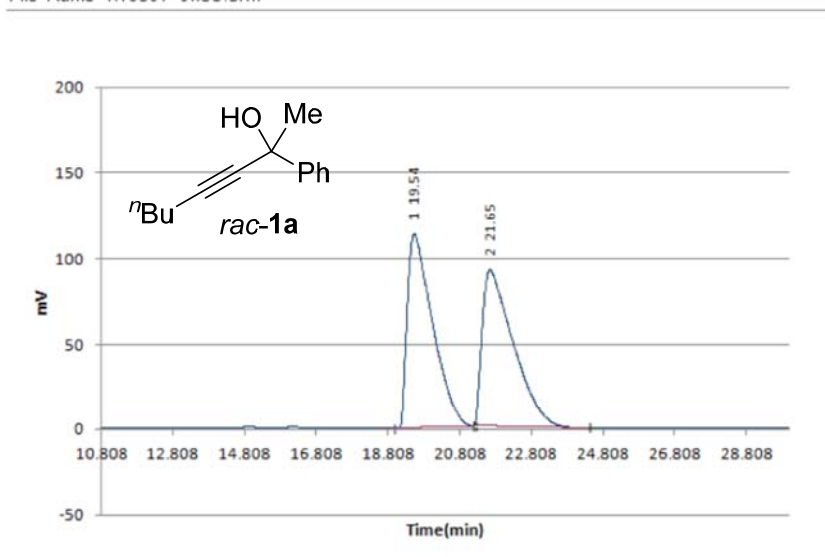
In principle, we could determine the absolute configuration of chiral propargylic alcohols by comparing the sign of optical rotation. However, the value of the optical rotation of this series of compounds is small, some confusion exists in the literatures regarding the relationship between the sign of optical rotation and the absolute configuration.³ The reported optical rotation of (*S*)-**1a** is $[\alpha]_D^{30} = -0.3$ [(*c* = 1.20, CHCl₃), 90% ee], which is too small.

Nakajima and coworkers determined the absolute configuration of chiral tertiary propargylic alcohols by transferring them into methyl esters.³ Then the absolute configuration of the obtained ester was unambiguously determined to be *S* by the sign of optical rotation,⁴ which suggested that the original propargylic alcohol had an *S*-configuration.



In their paper, the ee of (*S*)-**1a** (90%) was determined by HPLC analysis (HPLC condition: Daicel Chiralcel OD-H; eluent, hexane/*i*-PrOH = 200/1; flow rate: 1.0 mL/min, 254 nm, *t_R* (minor) = 20.7 min, *t_R* (major) = 22.5 min) and the HPLC spectra for *rac*- and (*S*)-**1a** reported by Nakajima are shown in Figure S1.

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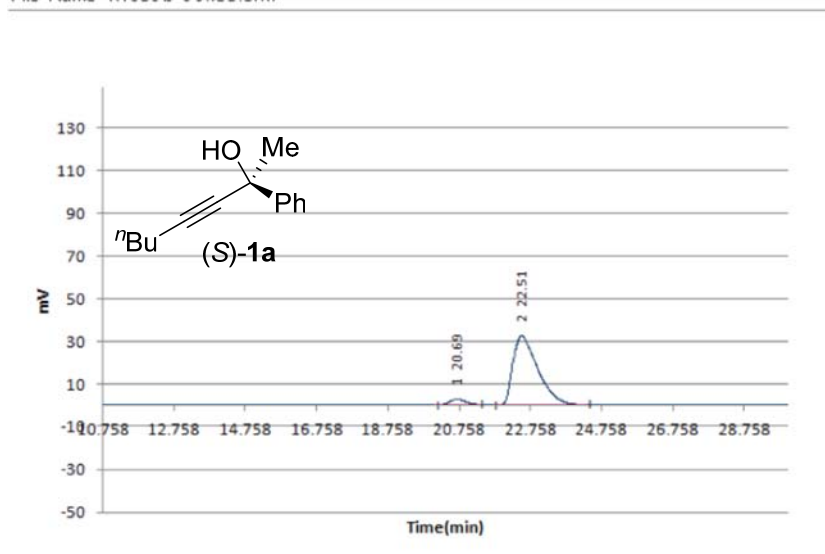


comment OD-H₂Hex/IPA=200/1_flow=1.0 mL/min_UL

Date 2013/6/3 12:20

No.	Rt	Peak Name	Area	Area(%)	Height	Amount	NTP	Tf	Resolution
1	19.54		5575289	50.1966	113604	----	3278.4	2.315	1.391
2	21.65		5531623	49.8034	92003	----	2678.4	2.588	----
			11106911	100	205607				

File Name k4085b-90%ee.crm



comment OD-H₂Hex/IPA=200/1_flow=1.0 mL/min_UL

Date 2013/6/3 11:40

No.	Rt	Peak Name	Area	Area(%)	Height	Amount	NTP	Tf	Resolution
1	20.69		80604	4.9267	2439	----	8762.6	1.144	1.65
2	22.51		1555458	95.0733	32250	----	4672.5	1.765	----
			1636062	100	34689				

Figure S1. The HPLC spectra of *rac*- and (*S*)-1a reported by Nakajima and coworkers

Then we determined the ee of **1a** prepared via our protocol with the same HPLC conditions (HPLC conditions: Daicel Chiralcel OD-H; eluent, hexane/*i*-PrOH = 200/1; flow rate: 1.0 mL/min, 214 nm, t_R (minor) = 19.0 min, t_R (major) = 20.8 min). After comparing the retention time (Figure S2), the absolute configuration of **1a** was determined to be *S*.

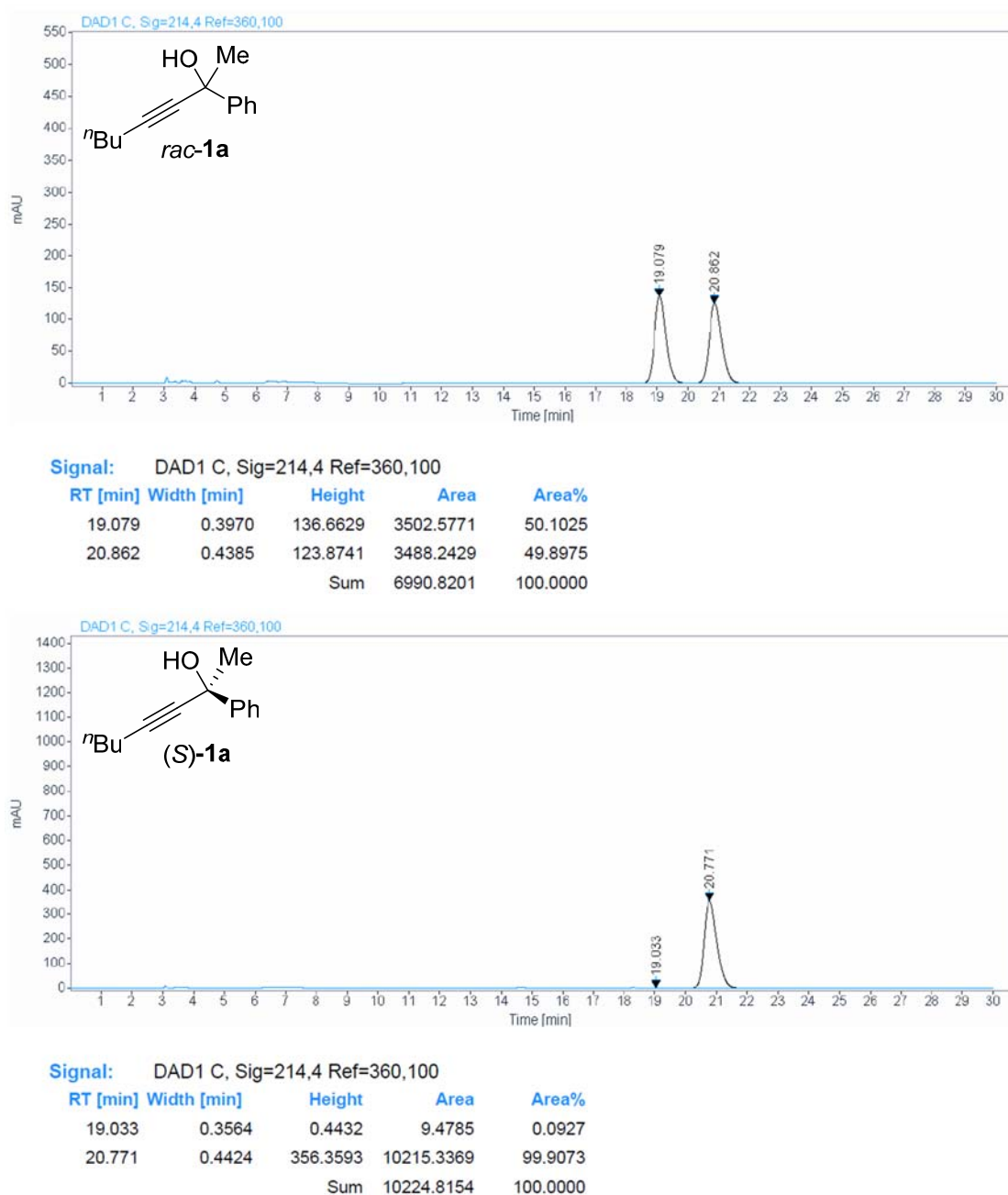
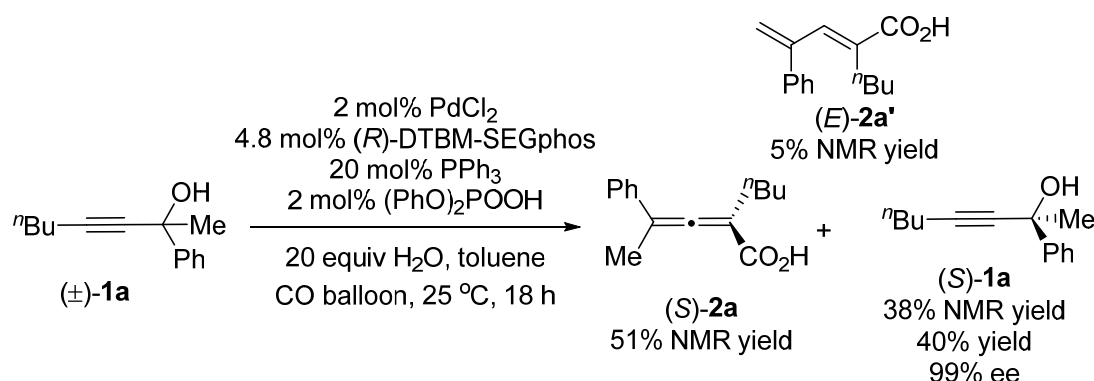


Figure S2. The HPLC spectra of *rac*- and (*S*)-**1a** synthesized via our protocol

Synthesis of chiral tertiary propargylic alcohols

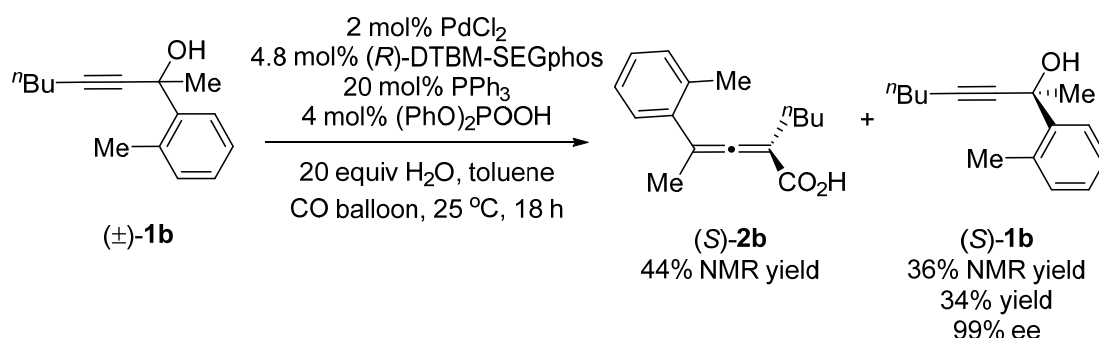
(1) Preparation of (*S*)-2-phenyloct-3-yn-2-ol ((*S*)-**1a**)



Typical Procedure: To a Schlenk flask (25 mL) were added PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (57.1 mg, 0.048 mmol), PPh₃ (52.5 mg, 0.2 mmol), and (PhO)₂POOH (5.0 mg, 0.02 mmol). The flask was then degassed and refilled with Ar for three times to ensure the complete exclusion of air. Then (\pm)-**1a** (201.3 mg, 1.0 mmol)/toluene (3 mL) and H₂O (360 μ L, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), toluene (2 mL) were added sequentially under Ar. After that, the Ar gas line was closed. The resulting mixture was then frozen with a liquid nitrogen bath, degassed to remove the argon inside completely, and refilled with CO by a balloon of CO (about 1 L) for three times. Then the liquid nitrogen bath was removed and the resulting mixture was allowed to stand until completely thawed, vigorously stirred at 25 °C with a balloon of CO for 18 h, treated with H₂O₂ (40 μ L, d = 1.13 g/mL, 30 wt. % in H₂O, 13.5 mg, 0.4 mmol), stirred for 30 min at room temperature, diluted with 5 mL of ethyl acetate, filtered through a short column silica gel (3 cm) eluted with ethyl acetate (20 mL), and concentrated. The crude product was analyzed with ¹H NMR with CH₂Br₂ (35 μ L) as the internal standard: 51% NMR yield of (*S*)-**2a** and 5% of (*E*)-**2a'**⁵ were formed with 38% of (*S*)-**1a** remained. The residue was purified by chromatography on silica gel to afford the pure product (*S*)-**1a**⁴ (81.1 mg, 40%) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 8/1 (360 mL)]; 99% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (minor) = 6.7 min, t_R (major) = 10.4 min); [α]_D²⁷ = +2.1 (c = 1.10, CHCl₃) [lit.³ [α]_D³⁰ = -0.3 (c = 1.20, CHCl₃)]; oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.64 (d, J

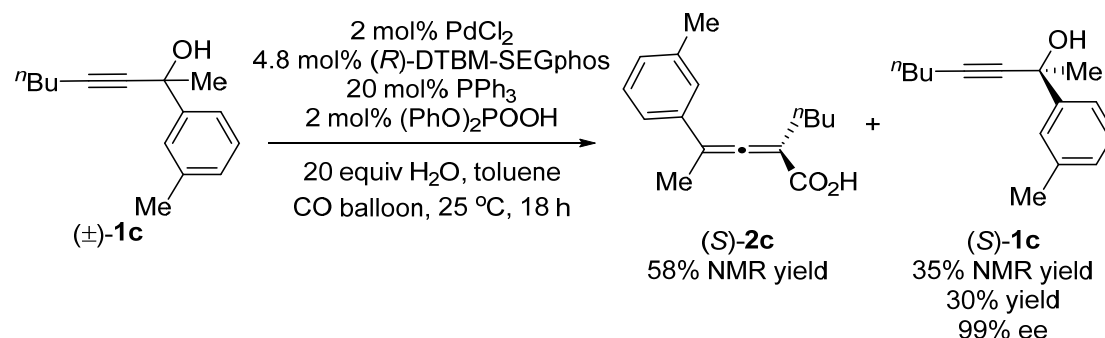
= 7.2 Hz, 2 H, Ar-H), 7.32 (t, $J = 7.6$ Hz, 2 H, Ar-H), 7.28-7.20 (m, 1 H, Ar-H), 2.64 (s, 1 H, OH), 2.25 (t, $J = 7.0$ Hz, 2 H, CH₂), 1.72 (s, 3 H, CH₃), 1.58-1.48 (m, 2 H, CH₂), 1.47-1.35 (m, 2 H, CH₂), 0.91 (t, $J = 7.2$ Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): $\delta = 146.2, 128.1, 127.4, 124.9, 85.6, 83.7, 70.0, 33.5, 30.7, 21.9, 18.3, 13.6$; IR (neat): $\nu = 3397, 2958, 2240, 1447, 1327, 1231, 1063$ cm⁻¹; MS (70 eV, EI) m/z (%): 202 (M⁺, 1.15), 187 (100).

(2) Preparation of (S)-2-(2-methylphenyl)oct-3-yn-2-ol ((S)-1b)



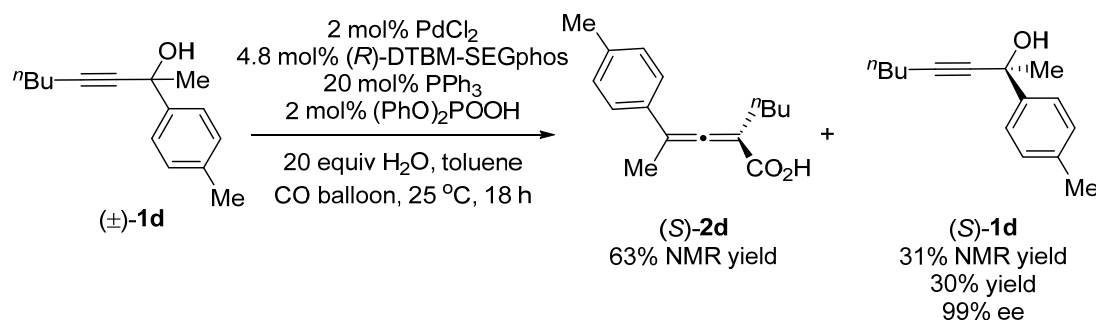
Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.5 mg, 0.048 mmol), PPh₃ (52.6 mg, 0.2 mmol), (PhO)₂POOH (10.0 mg, 0.04 mmol), (±)-1b (215.9 mg, 1.0 mmol), and H₂O (360 μL, $d = 1.0$ g/mL, 360.0 mg, 20.0 mmol) in toluene (5 mL) afforded (*S*)-1b (73.6 mg, 34%) (44% NMR yield of (*S*)-2b was formed and 36% of (*S*)-1b remained) [eluent: petroleum ether / diethyl ether / DCM = 50/1/1 (260 mL), to 20/1/1 (440 mL), to 12/1/1 (350 mL), then petroleum ether/ethyl acetate = 5/1 (300 mL)]: 99% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 95/5, 0.9 mL/min, $\lambda = 214$ nm, t_R (minor) = 5.3 min, t_R (major) = 6.4 min); $[\alpha]_D^{21} = -3.8$ ($c = 0.98$, CHCl₃); oil; ¹H NMR (400 MHz, CDCl₃): $\delta = 7.75$ -7.63 (m, 1 H, Ar-H), 7.22-7.13 (m, 3 H, Ar-H), 2.62 (s, 3 H, CH₃), 2.36 (s, 1 H, OH), 2.23 (t, $J = 7.0$ Hz, 2 H, CH₂), 1.80 (s, 3 H, CH₃), 1.57-1.45 (m, 2 H, CH₂), 1.45-1.32 (m, 2 H, CH₂), 0.90 (t, $J = 7.2$ Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): $\delta = 142.8, 135.6, 132.1, 127.4, 125.6, 124.9, 85.2, 84.0, 69.9, 31.1, 30.6, 22.0, 21.2, 18.4, 13.6$; IR (neat): $\nu = 3428, 2930, 2866, 2243, 1454, 1369, 1325, 1051$ cm⁻¹; MS (70 eV, EI) m/z (%): 216 (M⁺, 1.60), 201 (100); HRMS calcd. for C₁₅H₂₀O [M⁺]: 216.1514; Found: 216.1517.

(3) Preparation of (*S*)-2-(3-methylphenyl)oct-3-yn-2-ol ((*S*)-1c)



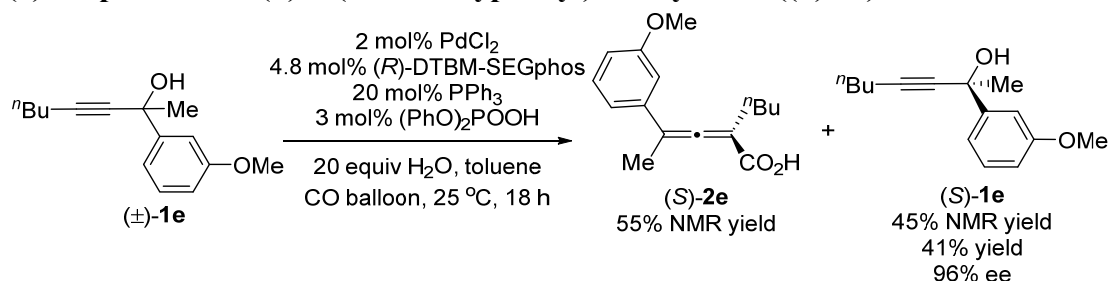
Following Typical Procedure, the reaction of PdCl₂ (3.8 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.7 mg, 0.048 mmol), PPh₃ (52.6 mg, 0.2 mmol), (PhO)₂POOH (5.1 mg, 0.02 mmol), (±)-1c (215.8 mg, 1.0 mmol), and H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol) in toluene (5 mL) afforded (*S*)-1c (63.9 mg, 30%) (58% NMR yield of (*S*)-2c was formed and 35% of (*S*)-1c remained) [eluent: petroleum ether / diethyl ether / DCM = 40/1/1 (1200 mL)]: 99% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 95/5, 1.3 mL/min, λ = 214 nm, *t*_R (minor) = 3.5 min, *t*_R (major) = 4.2 min); [α]_D²⁶ = +1.5 (*c* = 1.37, CHCl₃); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.50-7.40 (m, 2 H, Ar-H), 7.28-7.20 (m, 1 H, Ar-H), 7.09 (d, *J* = 7.2 Hz, 1 H, Ar-H), 2.37 (s, 3 H, CH₃), 2.32-2.22 (m, 3 H, CH₂ and OH) 1.74 (s, 3 H, CH₃), 1.58-1.50 (m, 2 H, CH₂), 1.49-1.39 (m, 2 H, CH₂), 0.93 (t, *J* = 7.2 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 146.2, 137.8, 128.2, 128.1, 125.6, 122.0, 85.5, 83.9, 70.0, 33.5, 30.7, 21.9, 21.5, 18.4, 13.6; IR (neat): ν = 3390, 2958, 2930, 2863, 2242, 1607, 1458, 1325, 1198, 1083 cm⁻¹; MS (70 eV, EI) *m/z* (%): 216 (M⁺, 2.67), 201 (100); HRMS: Calcd for C₁₅H₂₀O [M⁺]: 216.1514; Found: 216.1516.

(4) Preparation of (*S*)-2-(4-methylphenyl)oct-3-yn-2-ol ((*S*)-1d)



Following Typical Procedure, the reaction of PdCl₂ (3.7 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.6 mg, 0.048 mmol), PPh₃ (52.3 mg, 0.2 mmol), (PhO)₂POOH (5.0 mg, 0.02 mmol), (±)-**1d** (216.4 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1d**⁴ (64.7 mg, 30%) (63% NMR yield of (*S*)-**2d** was formed and 31% of (*S*)-**1d** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 10/1 (320 mL)]: 99% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, λ = 214 nm, *t*_R (minor) = 7.2 min, *t*_R (major) = 9.7 min); [α]_D²⁵ = -1.4 (*c* = 1.17, CHCl₃) [lit.⁶ [α]_D²³ = -0.4 (*c* = 0.96, CHCl₃)]; oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.53 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.15 (d, *J* = 8.0 Hz, 2 H, Ar-H), 2.40-2.30 (m, 4 H, OH and CH₃), 2.27 (t, *J* = 7.2 Hz, 2 H, CH₂), 1.72 (s, 3 H, CH₃), 1.57-1.46 (m, 2 H, CH₂), 1.46-1.35 (m, 2 H, CH₂), 0.92 (t, *J* = 7.4 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 143.4, 137.0, 128.8, 124.9, 85.3, 83.9, 69.8, 33.4, 30.7, 21.9, 20.9, 18.4, 13.5; IR (neat): ν = 3405, 2929, 2866, 2241, 1452, 1325, 1175, 1088 cm⁻¹; MS (70 eV, EI) *m/z* (%): 217 (M⁺+1, 1.08), 216 (M⁺, 2.23), 201 (100).

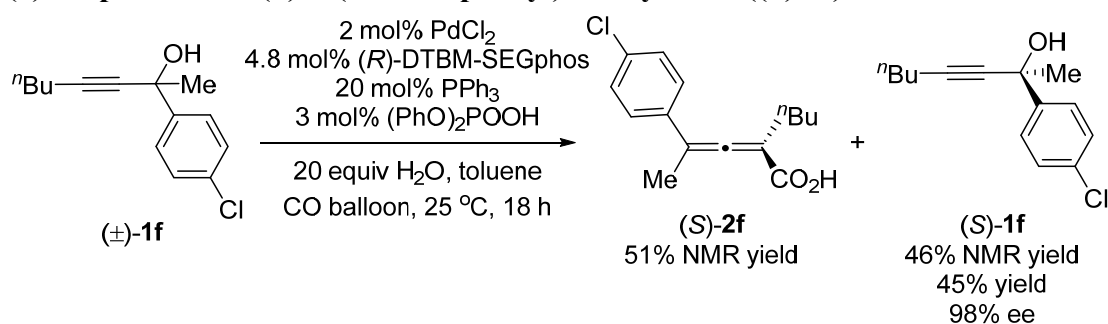
(5) Preparation of (*S*)-2-(3-methoxyphenyl)oct-3-yn-2-ol ((*S*)-**1e**)



Following Typical Procedure, the reaction of PdCl₂ (3.7 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.5 mg, 0.048 mmol), PPh₃ (52.7 mg, 0.2 mmol), (PhO)₂POOH (8.0 mg, 0.03 mmol), (±)-**1e** (231.0 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1e** (94.5 mg, 41%) (55% NMR yield of (*S*)-**2e** was formed and 45% of (*S*)-**1e** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 10/1 (275 mL)]: 96% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, λ = 214 nm, *t*_R (minor) = 12.1 min, *t*_R (major) = 18.8 min); [α]_D²⁶ = +2.9 (*c* = 1.00, CHCl₃); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.32-7.14 (m, 3 H, Ar-H), 6.80 (dt, *J*₁ =

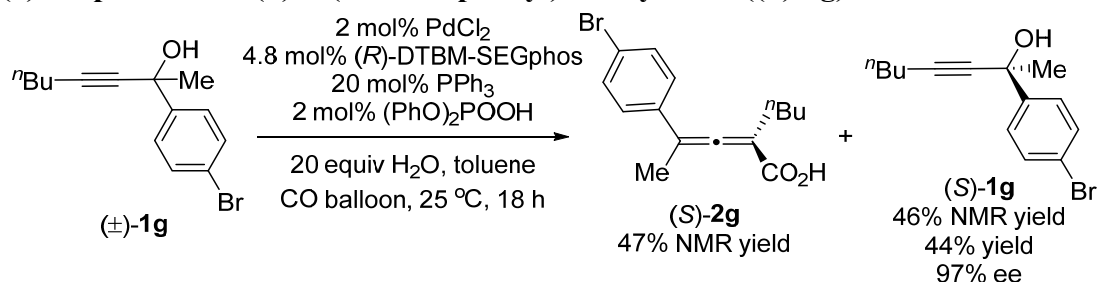
6.8 Hz, $J_2 = 2.2$ Hz, 1 H, Ar-H), 3.80 (s, 3 H, OCH₃), 2.57 (s, 1 H, OH), 2.26 (t, $J = 7.2$ Hz, 2 H, CH₂), 1.72 (s, 3 H, CH₃), 1.58-1.47 (m, 2 H, CH₂), 1.47-1.35 (m, 2 H, CH₂), 0.92 (t, $J = 7.2$ Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): $\delta = 159.3, 148.0, 129.1, 117.3, 112.9, 110.7, 85.4, 83.7, 69.8, 55.1, 33.4, 30.6, 21.9, 18.3, 13.5$; IR (neat): $\nu = 3431, 2932, 2240, 1596, 1480, 1432, 1254, 1041$ cm⁻¹; MS (70 eV, EI) m/z (%): 233 ($M^+ + 1$, 4.22), 232 (M^+ , 25.23), 217 (100); HRMS calcd for C₁₅H₂₀O₂ [M^+]: 232.1463, found: 232.1466.

(6) Preparation of (*S*)-2-(4-chlorophenyl)oct-3-yn-2-ol ((*S*)-1f)



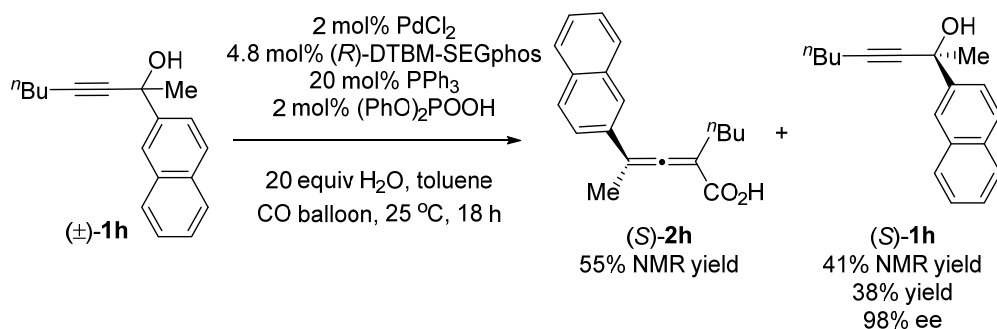
Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.6 mg, 0.048 mmol), PPh₃ (52.5 mg, 0.2 mmol), (PhO)₂POOH (7.8 mg, 0.03 mmol), (\pm)-1f (235.0 mg, 1.0 mmol), H₂O (360 μ L, $d = 1.0$ g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-1f⁴ (106.3 mg, 45%) (51% NMR yield of (*S*)-2f was formed and 46% of (*S*)-1f remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 15/1 (320 mL)]: 98% ee (HPLC conditions: AS-H column, hexane/^{*i*}PrOH = 98/2, 1.0 mL/min, $\lambda = 214$ nm, t_R (minor) = 7.2 min, t_R (major) = 9.8 min); $[\alpha]_D^{24} = -0.6$ ($c = 1.00$, CHCl₃) [lit.⁶ $[\alpha]_D^{20} = -0.6$ ($c = 1.20$, CHCl₃)]; oil; ¹H NMR (400 MHz, CDCl₃): $\delta = 7.56$ (d, $J = 8.8$ Hz, 2 H, Ar-H), 7.29 (d, $J = 8.8$ Hz, 2 H, Ar-H), 2.58 (s, 1 H, OH), 2.25 (t, $J = 7.0$ Hz, 2 H, CH₂), 1.70 (s, 3 H, CH₃), 1.58-1.47 (m, 2 H, CH₂), 1.47-1.34 (m, 2 H, CH₂), 0.92 (t, $J = 7.2$ Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): $\delta = 144.8, 133.2, 128.2, 126.5, 85.9, 83.3, 69.5, 33.6, 30.6, 21.9, 18.3, 13.5$; IR (neat): $\nu = 3371, 2931, 2240, 1486, 1364, 1228, 1088$ cm⁻¹; MS (70 eV, EI) m/z (%): 238 (M^+ (³⁷Cl), 0.52), 236 (M^+ (³⁵Cl), 1.65), 221 (100).

(7) Preparation of (*S*)-2-(4-bromophenyl)oct-3-yn-2-ol ((*S*)-1g)



Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (57.8 mg, 0.048 mmol), PPh₃ (52.5 mg, 0.2 mmol), (PhO)₂POOH (5.1 mg, 0.02 mmol), (±)-1g (281.3 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-1g (123.1 mg, 44%) (47% NMR yield of (*S*)-2g was formed and 46% of (*S*)-1g remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (~320 mL), to petroleum ether / ethyl ether / dichloromethane = 20/1/1 (~220 mL), then petroleum ether/ethyl acetate = 5/1 (~240 mL)]: 97% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, λ = 214 nm, *t*_R (minor) = 8.5 min, *t*_R (major) = 11.3 min); [α]_D²⁵ = -1.1 (c = 0.99, CHCl₃); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.52 (d, *J* = 8.8 Hz, 2 H, Ar-H), 7.46 (d, *J* = 8.0 Hz, 2 H, Ar-H), 2.37 (s, 1 H, OH), 2.26 (t, *J* = 7.2 Hz, 2 H, CH₂), 1.71 (s, 3 H, CH₃), 1.59-1.48 (m, 2 H, CH₂), 1.48-1.35 (m, 2 H, CH₂), 0.92 (t, *J* = 7.4 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 145.3, 131.2, 126.9, 121.4, 86.0, 83.2, 69.6, 33.6, 30.6, 21.9, 18.3, 13.5; IR (neat): ν = 3379, 2957, 2930, 2862, 2240, 1750, 1485, 1394, 1074, 1009 cm⁻¹; MS (70 eV, EI) *m/z* (%): 282 (M⁺(⁸¹Br), 2.75), 280 (M⁺(⁷⁹Br), 2.58), 265 (100); HRMS calcd for C₁₄H₁₇O⁷⁹Br [M⁺]: 280.0463, found: 280.0464.

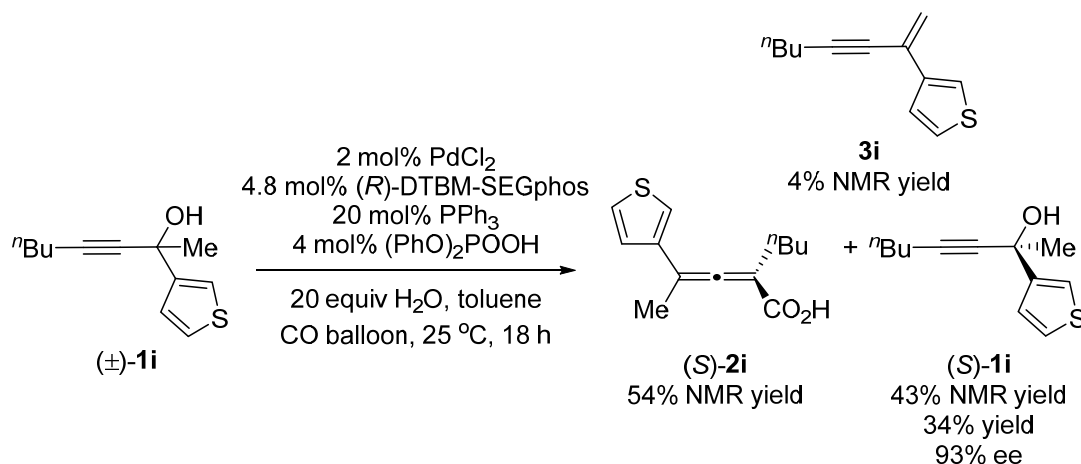
(8) Preparation of (*S*)-2-(2-naphthyl)oct-3-yn-2-ol ((*S*)-1h)



Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-

DTBM-SEGphos (57.9 mg, 0.048 mmol), PPh₃ (52.6 mg, 0.2 mmol), (PhO)₂POOH (5.0 mg, 0.02 mmol), (±)-**1h** (252.3 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1h**⁴ (95.9 mg, 38%) (55% NMR yield of (*S*)-**2h** was formed and 41% of (*S*)-**1h** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 20/1/1 (500 mL) to 10/1/ (500 mL), then petroleum ether / ethyl acetate = 5/1 (200 mL)]: 98% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 95/5, 1.3 mL/min, λ = 214 nm, *t*_R (minor) = 4.9 min, *t*_R (major) = 5.7 min); [α]_D²⁶ = -11.5 (*c* = 1.15, CHCl₃) [lit.⁶ [α]_D²³ = -11.8 (*c* = 1.55, CHCl₃)]; oil; ¹H NMR (400 MHz, CDCl₃): δ = 8.12 (s, 1 H, Ar-H), 7.90-7.78 (m, 3 H, Ar-H), 7.74 (dd, *J*₁ = 8.4 Hz, *J*₂ = 1.6 Hz, 1 H, Ar-H), 7.52-7.43 (m, 2 H, Ar-H), 2.45-2.38 (m, 1 H, OH), 2.32 (t, *J* = 7.0 Hz, 2 H, CH₂), 1.83 (s, 3 H, CH₃), 1.62-1.52 (m, 2 H, CH₂), 1.52-1.41 (m, 2 H, CH₂), 0.94 (t, *J* = 7.2 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 143.5, 133.0, 132.8, 128.3, 128.0, 127.5, 126.1, 126.0, 123.7, 123.3, 85.9, 83.7, 70.1, 33.4, 30.7, 22.0, 18.4, 13.6; IR (neat): ν = 3390, 2957, 2931, 2241, 1353, 1127, 1084 cm⁻¹; MS (70 eV, EI) *m/z* (%): 253 (M⁺+1, 4.68), 252 (M⁺, 22.51), 237 (100).

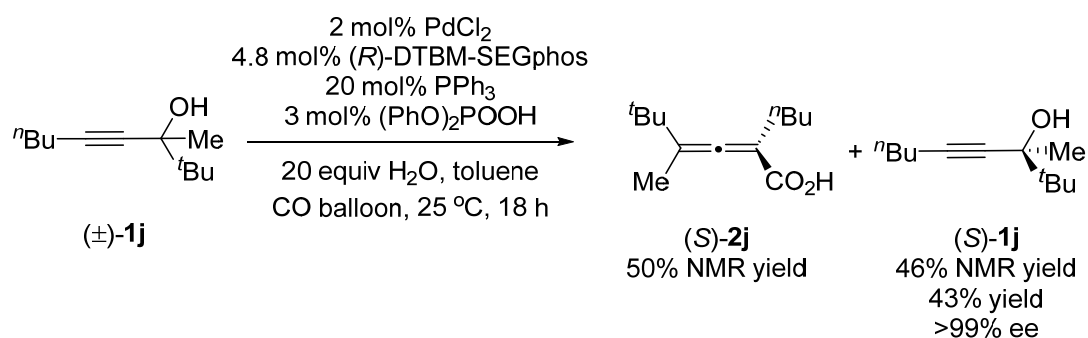
(9) Preparation of (*S*)-2-(thiophen-3-yl)oct-3-yn-2-ol ((*S*)-**1i**)



Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (57.0 mg, 0.048 mmol), PPh₃ (52.5 mg, 0.2 mmol), (PhO)₂POOH (10.1 mg, 0.04 mmol), (±)-**1i** (207.7 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol) in toluene (5 mL) afforded (*S*)-**1i** (70.1 mg, 34%) (54% NMR yield of (*S*)-**2i**, 4% NMR yield of **3i** were formed and 43% of (*S*)-**1i** remained) [eluent:

petroleum ether / diethyl ether / DCM = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 8/1 (270 mL)]: 93% ee (HPLC conditions: AS-H column, hexane/ⁱPrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (minor) = 8.7 min, t_R (major) = 12.1 min); $[\alpha]_D^{28}$ = -6.9 (c = 1.00, CHCl₃); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.41-7.31 (m, 1 H, one proton from thienyl), 7.30-7.22 (m, 1 H, one proton from thienyl), 7.22-7.14 (m, 1 H, one proton from thienyl), 2.62-2.48 (m, 1 H, OH), 2.25 (t, J = 6.8 Hz, 2 H, CH₂), 1.75 (s, 3 H, CH₃), 1.57-1.34 (m, 4 H, 2 x CH₂), 0.92 (t, J = 7.0 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 147.9, 125.9, 125.7, 120.5, 84.7, 83.6, 67.3, 32.3, 30.6, 21.9, 18.3, 13.5; IR (neat): ν = 3387, 2932, 2244, 1461, 1365, 1228, 1158, 1087 cm⁻¹; MS (70 eV, EI) m/z (%): 208 (M⁺, 4.20), 193 (100); HRMS calcd for C₁₂H₁₇OS [M+H]⁺: 209.0995, found: 209.1000.

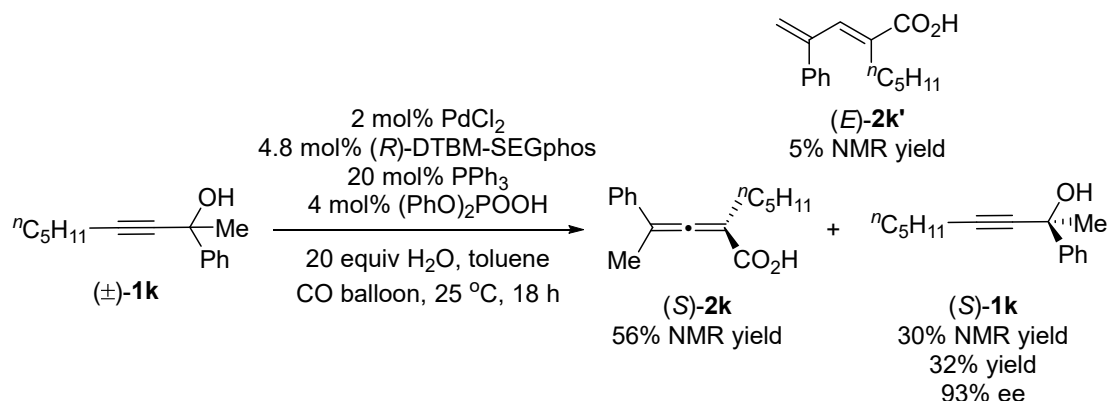
(10) Preparation of (S)-2,2,3-trimethylnon-4-yn-3-ol ((S)-1j)



Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (R)-DTBM-SEGphos (57.0 mg, 0.048 mmol), PPh₃ (52.6 mg, 0.2 mmol), (PhO)₂POOH (7.6 mg, 0.03 mmol), (±)-1j (181.8 mg, 1.0 mmol), H₂O (360 μ L, d = 1.0 g/mL, 360.0 mg, 20.0 mmol) in toluene (5 mL) afforded (S)-1j (77.4 mg, 43%) (50% NMR yield of (S)-2j was formed and 46% of (S)-1j remained) [eluent: petroleum ether / diethyl ether / DCM = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 5/1 (480 mL)]: >99% ee (HPLC conditions: IC column, hexane/ⁱPrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (major) = 4.7 min); $[\alpha]_D^{27}$ = +3.9 (c = 1.07, CHCl₃); oil; ¹H NMR (400 MHz, CDCl₃): δ = 2.20 (t, J = 6.8 Hz, 2 H, CH₂), 1.82 (s, 1 H, OH), 1.54-1.34 (m, 7 H, 2 x CH₂ and CH₃), 1.03 (s, 9 H, 3 x CH₃), 0.91 (t, J = 7.2 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 84.2, 83.7, 74.0, 38.2, 30.8, 25.1, 25.0, 21.9, 18.3, 13.6; IR (neat): ν = 3470,

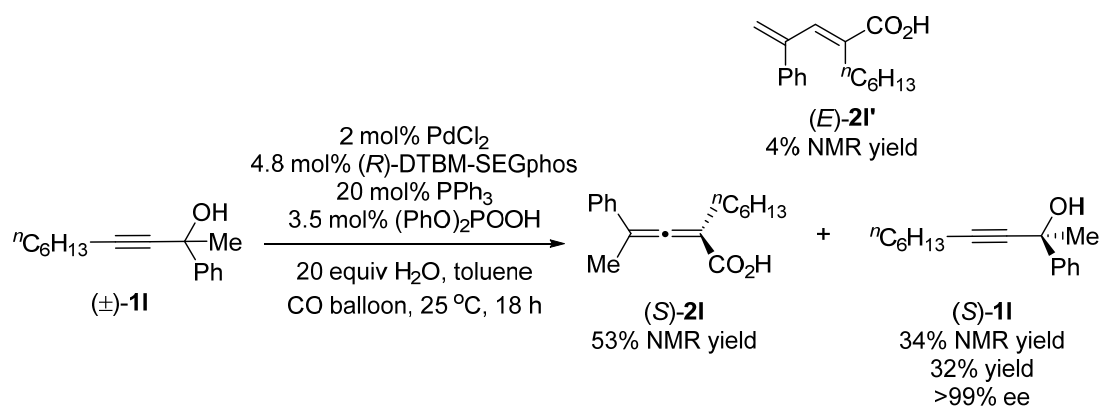
2960, 2242, 1460, 1367, 1324, 1087 cm^{-1} ; **MS** (ESI) m/z (%): 183 ($\text{M}+\text{H}^+$), 165 ($\text{M}-\text{OH}^+$); **HRMS** calcd for $\text{C}_{12}\text{H}_{23}\text{O}$ [$\text{M}+\text{H}^+$]: 183.1743, found: 183.1742.

(11) Preparation of (*S*)-2-phenylnon-3-yn-2-ol ((*S*)-1k)



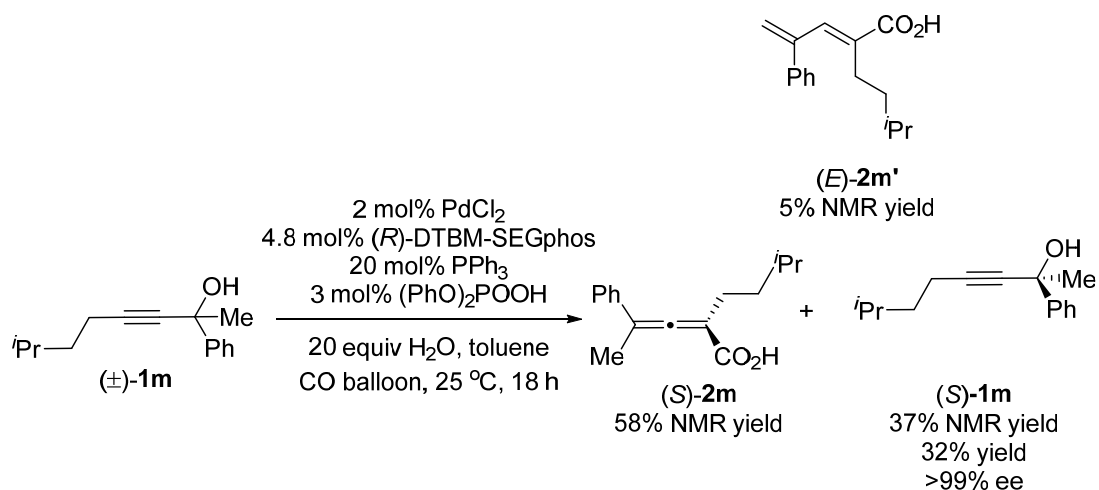
Following Typical Procedure, the reaction of PdCl_2 (3.8 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.5 mg, 0.048 mmol), PPh_3 (52.5 mg, 0.2 mmol), $(\text{PhO})_2\text{POOH}$ (9.8 mg, 0.04 mmol), (\pm)-**1k** (214.7 mg, 1.0 mmol), H_2O (360 μL , $d = 1.0 \text{ g/mL}$, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1k** (68.6 mg, 32%) (56% NMR yield of (*S*)-**2k**, 5% NMR yield of (*E*)-**2k'** were formed and 30% of (*S*)-**1k** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 10/1 (330 mL)]: 93% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, $\lambda = 214 \text{ nm}$, t_{R} (minor) = 6.8 min, t_{R} (major) = 9.9 min); $[\alpha]_{\text{D}}^{26} = +9.2$ ($c = 1.09$, CHCl_3); oil; **$^1\text{H NMR}$** (400 MHz, CDCl_3): $\delta = 7.64$ (d, $J = 6.8 \text{ Hz}$, 2 H, Ar-H), 7.33 (t, $J = 7.2 \text{ Hz}$, 2 H, Ar-H), 7.29-7.21 (m, 1 H, Ar-H), 2.56 (s, 1 H, OH), 2.25 (t, $J = 7.0 \text{ Hz}$, 2 H, CH_2), 1.73 (s, 3 H, CH_3), 1.60-1.47 (m, 2 H, CH_2), 1.45-1.24 (m, 4 H, 2 x CH_2), 0.90 (t, $J = 7.0 \text{ Hz}$, 3 H, CH_3); **$^{13}\text{C NMR}$** (100 MHz, CDCl_3): $\delta = 146.2, 128.0, 127.3, 124.9, 85.6, 83.7, 69.9, 33.5, 31.0, 28.2, 22.1, 18.6, 13.9$; **IR** (neat): $\nu = 3420, 2929, 2861, 2240, 1754, 1448, 1329, 1230, 1059 \text{ cm}^{-1}$; **MS** (70 eV, EI) m/z (%): 216 (M^+ , 1.24), 201 (100); **HRMS** calcd for $\text{C}_{15}\text{H}_{20}\text{O}$ [M^+]: 216.1514, found: 216.1511.

(12) Preparation of (*S*)-2-phenyldec-3-yn-2-ol ((*S*)-1l)



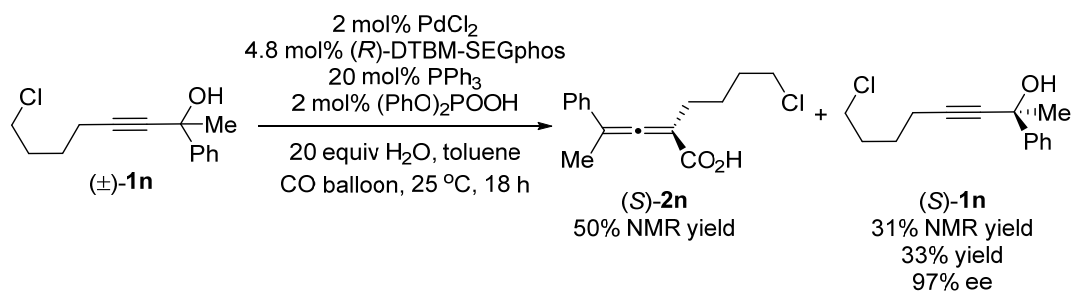
Following Typical Procedure, the reaction of PdCl₂ (3.7 mg, 0.02 mmol), (R)-DTBM-SEGphos (56.8 mg, 0.048 mmol), PPh₃ (52.3 mg, 0.2 mmol), (PhO)₂POOH (8.8 mg, 0.035 mmol), (±)-**11** (229.7 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (S)-**11** (73.7 mg, 32%) (53% NMR yield of (S)-**2I**, 4% NMR yield of (E)-**2I'** were formed and 34% of (S)-**11** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 8/1 (360 mL)]: >99% ee (HPLC conditions: AS-H column, hexane/ⁱPrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (major) = 8.0 min); [α]_D²⁶ = -1.9 (c = 1.10, CHCl₃); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.65 (d, J = 7.2 Hz, 2 H, Ar-H), 7.33 (t, J = 7.4 Hz, 2 H, Ar-H), 7.29-7.20 (m, 1 H, Ar-H), 2.53-2.37 (m, 1 H, OH), 2.26 (t, J = 7.0 Hz, 2 H, CH₂), 1.73 (s, 3 H, CH₃), 1.58-1.48 (m, 2 H, CH₂), 1.47-1.35 (m, 2 H, CH₂), 1.35-1.19 (m, 4 H, 2 x CH₂), 0.89 (t, J = 6.6 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 146.2, 128.1, 127.4, 124.9, 85.6, 83.8, 70.0, 33.5, 31.2, 28.6, 28.5, 22.5, 18.7, 14.0; IR (neat): ν = 3396, 2929, 2858, 2242, 1447, 1329, 1232, 1060 cm⁻¹; MS (70 eV, EI) m/z (%): 230 (M⁺, 1.20), 215 (100); HRMS calcd for C₁₆H₂₂O [M⁺]: 230.1671, found: 230.1668.

(13) Preparation of (S)-7-methyl-2-phenyloct-3-yn-2-ol ((S)-**1m**)



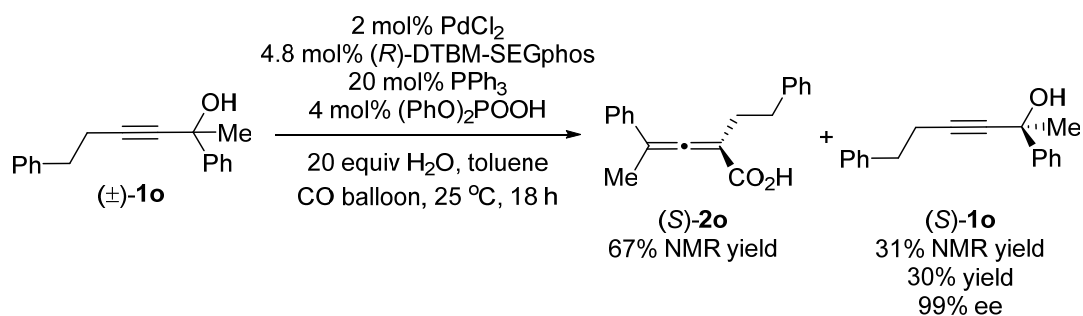
Following Typical Procedure, the reaction of PdCl₂ (3.8 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.8 mg, 0.048 mmol), PPh₃ (52.5 mg, 0.2 mmol), (PhO)₂POOH (7.7 mg, 0.03 mmol), (±)-**1m** (215.5 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1m** (69.1 mg, 32%) (58% NMR yield of (*S*)-**2m**, 5% (*E*)-**2m'** were formed and 37% of (*S*)-**1m** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 15/1 (320 mL)]: >99% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, λ = 214 nm, *t*_R (minor) = 6.3 min, *t*_R (major) = 9.9 min); [α]_D²⁶ = +4.2 (*c* = 1.00, CHCl₃); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.64 (d, *J* = 7.2 Hz, 2 H, Ar-H), 7.33 (t, *J* = 7.4 Hz, 2 H, Ar-H), 7.29-7.20 (m, 1 H, Ar-H), 2.60 (s, 1 H, OH), 2.26 (t, *J* = 7.6 Hz, 2 H, CH₂), 1.80-1.62 (m, 4 H, CH and CH₃), 1.44 (q, *J* = 7.3 Hz, 2 H, CH₂), 0.90 (d, *J* = 6.4 Hz, 6 H, 2 x CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 146.2, 128.1, 127.3, 124.9, 85.6, 83.6, 69.9, 37.5, 33.5, 27.2, 22.1, 16.7; IR (neat): ν = 3396, 2953, 2240, 1450, 1365, 1230, 1061 cm⁻¹; MS (70 eV, EI) *m/z* (%): 216 (M⁺, 1.00), 201 (100); HRMS calcd for C₁₅H₂₀O [M⁺]: 216.1514, found: 216.1516.

(14) Preparation of (*S*)-8-chloro-2-phenyloct-3-yn-2-ol ((*S*)-**1n**)



Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.5 mg, 0.048 mmol), PPh₃ (52.6 mg, 0.2 mmol), (PhO)₂POOH (5.3 mg, 0.02 mmol), (±)-**1n** (234.9 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1n**⁴ (77.7 mg, 33%) (50% NMR yield of (*S*)-**2n** was formed and 31% of (*S*)-**1n** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 10/1 (330 mL)]: 97% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 95/5, 1.3 mL/min, λ = 214 nm, *t*_R (minor) = 6.7 min, *t*_R (major) = 11.0 min); [α]_D²⁵ = +1.6 (*c* = 1.20, CHCl₃) [lit.⁶ [α]_D²⁴ = +0.7 (*c* = 1.69, CHCl₃)]; oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.68-7.60 (m, 2 H, Ar-H), 7.36 (t, *J* = 7.4 Hz, 2 H, Ar-H), 7.32-7.22 (m, 1 H, Ar-H), 3.57 (t, *J* = 6.6 Hz, 2 H, CH₂), 2.38-2.28 (m, 3 H, OH and CH₂), 1.96-1.85 (m, 2 H, CH₂), 1.78-1.66 (m, 5 H, CH₂ and CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 146.0, 128.2, 127.5, 124.9, 84.6, 84.5, 70.0, 44.5, 33.4, 31.6, 25.7, 18.0; IR (neat): ν = 3410, 2938, 2239, 1444, 1325, 1230, 1062 cm⁻¹; MS (ESI) *m/z*: 237 (M(³⁷Cl)+H⁺), 221 (M(³⁷Cl)-OH)⁺, 219 (M(³⁵Cl)-OH)⁺.

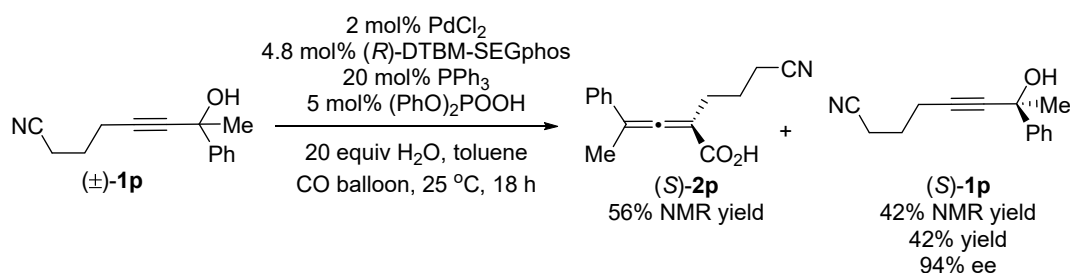
(15) Preparation of (*S*)-2,6-diphenylhex-3-yn-2-ol ((*S*)-**1o**)



Following Typical Procedure, the reaction of PdCl₂ (3.7 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.6 mg, 0.048 mmol), PPh₃ (52.7 mg, 0.2 mmol), (PhO)₂POOH (9.8 mg, 0.04 mmol), (±)-**1o** (247.3 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1o** (74.1 mg, 30%) (67% NMR yield of (*S*)-**2o** was formed and 31% of (*S*)-**1o** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 10/1 (220 mL)]: 99% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, λ = 214 nm, *t*_R (minor) = 12.8 min, *t*_R (major) = 16.3 min); [α]_D²⁵ = -0.8 (*c* = 1.50, CHCl₃);

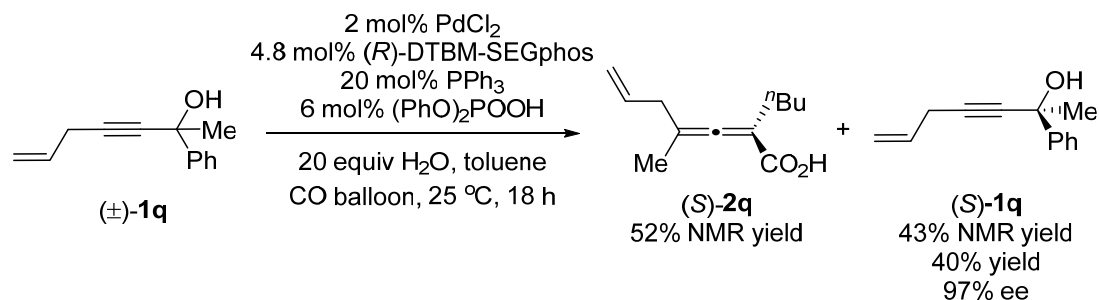
oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.54$ (d, $J = 7.6$ Hz, 2 H, Ar-H), 7.38-7.07 (m, 8 H, Ar-H), 2.82 (t, $J = 7.6$ Hz, 2 H, CH_2), 2.60-2.43 (m, 3 H, OH and CH_2), 1.69 (s, 3 H, CH_3); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta = 145.9, 140.4, 128.5, 128.3, 128.0, 127.3, 126.2, 124.9, 84.64, 84.59, 69.8, 34.8, 33.3, 20.8$; **IR** (neat): $\nu = 3409, 2984, 2241, 1492, 1446, 1331, 1229, 1064$ cm^{-1} ; **MS** (70 eV, EI) m/z (%): 250 (M^+ , 1.65), 91 (100); **HRMS** calcd for $\text{C}_{18}\text{H}_{18}\text{O}$ [M^+]: 250.1358, found: 250.1361.

(16) Preparation of (*S*)-7-cyano-2-phenylhept-3-yn-2-ol ((*S*)-1p)



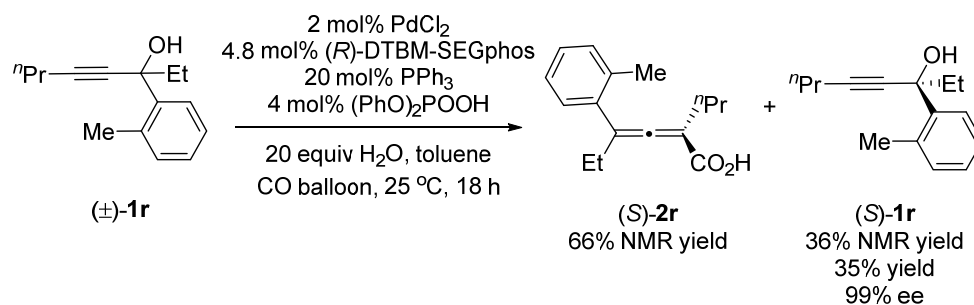
Following Typical Procedure, the reaction of PdCl_2 (3.8 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.5 mg, 0.048 mmol), PPh_3 (52.6 mg, 0.2 mmol), $(\text{PhO})_2\text{POOH}$ (12.7 mg, 0.05 mmol), (\pm)-**1p** (211.7 mg, 1.0 mmol), H_2O (360 μL , $d = 1.0$ g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1p** (88.9 mg, 42%) (56% NMR yield of (*S*)-**2p** was formed and 42% of (*S*)-**1p** remained) [eluent: petroleum ether / diethyl ether / DCM = 20/1/1 (220 mL) to 10/1/1 (480 mL), then petroleum ether / ethyl acetate = 5/1 (480 mL)]: 94% ee (HPLC conditions: Daicel Chiralpak AS-H column, hexane/*i*PrOH = 90/10, 1.3 mL/min, $\lambda = 214$ nm, t_R (minor) = 13.4 min, t_R (major) = 24.4 min); $[\alpha]_D^{26} = +0.9$ ($c = 1.00$, CHCl_3); oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.61$ (d, $J = 8.0$ Hz, 2 H, Ar-H), 7.35 (t, $J = 7.6$ Hz, 2 H, Ar-H), 7.31-7.23 (m, 1 H, Ar-H), 2.66 (br, 1 H, OH), 2.46 (q, $J = 6.8$ Hz, 4 H, 2 x CH_2), 1.88 (quintet, $J = 7.0$ Hz, 2 H, CH_2), 1.74 (s, 3 H, CH_3); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta = 145.7, 128.2, 127.5, 124.7, 119.1, 85.9, 82.2, 69.8, 33.3, 24.3, 17.8, 16.1$; **IR** (neat): $\nu = 3439, 2982, 2931, 2248, 1491, 1361, 1229, 1172, 1095, 1064, 1027$ cm^{-1} ; **MS** (70 eV, EI) m/z (%): 213 (M^+ , 1.19), 198 (100); **HRMS** calcd for $\text{C}_{14}\text{H}_{15}\text{NO}$ [M^+]: 213.1154, found: 213.1158.

(17) Preparation of (*S*)-2-phenylhept-6-en-3-yn-2-ol ((*S*)-1q)



Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.9 mg, 0.048 mmol), PPh₃ (52.4 mg, 0.2 mmol), (PhO)₂POOH (15.0 mg, 0.06 mmol), (±)-**1q** (186.1 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1q** (74.1 mg, 40%) (53% NMR yield of (*S*)-**2q** was formed and 43% of (*S*)-**1q** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL) to 20/1/1 (220 mL)]: 97% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, λ = 214 nm, *t*_R (minor) = 9.5 min, *t*_R (major) = 12.3 min); [α]_D²⁸ = +1.4 (c = 1.37, CHCl₃); oil; **¹H NMR** (400 MHz, CDCl₃): δ = 7.65 (d, *J* = 7.2 Hz, 2 H, Ar-H), 7.34 (t, *J* = 7.6 Hz, 2 H, Ar-H), 7.30-7.24 (m, 1 H, Ar-H), 5.92-5.75 (m, 1 H, =CH), 5.34 (dd, *J*₁ = 17.2 Hz, *J*₂ = 1.6 Hz, 1 H, one proton of =CH₂), 5.11 (dd, *J*₁ = 9.2 Hz, *J*₂ = 1.6 Hz, 1 H, one proton of =CH₂), 3.05 (dt, *J*₁ = 5.2 Hz, *J*₂ = 1.8 Hz, 2 H, CH₂), 2.58-2.50 (m, 1 H, OH), 1.76 (s, 3 H, CH₃); **¹³C NMR** (100 MHz, CDCl₃): δ = 145.9, 132.3, 128.2, 127.5, 124.9, 116.2, 86.2, 81.9, 70.0, 33.4, 23.0; **IR** (neat): ν = 3389, 2984, 2244, 1641, 1446, 1325, 1230, 1061 cm⁻¹; **MS** (70 eV, EI) *m/z* (%) 186 (M⁺, 1.53), 171 (100); **HRMS** calcd for C₁₃H₁₄O [M⁺]: 186.1045, found: 186.1046.

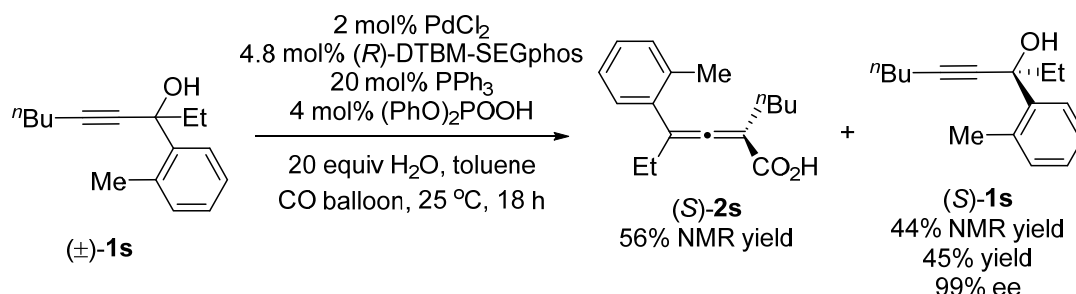
(18) Preparation of (*S*)-3-(2-methylphenyl)oct-4-yn-3-ol ((*S*)-**1r**)



Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-

DTBM-SEGphos (57.0 mg, 0.048 mmol), PPh₃ (52.4 mg, 0.2 mmol), (PhO)₂POOH (10.0 mg, 0.04 mmol), (±)-**1r** (216.1 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol) in toluene (5 mL) afforded (*S*)-**1r** (75.0 mg, 35%) (66% NMR yield of (*S*)-**2r** was formed and 36% of (*S*)-**1r** remained) [eluent: petroleum ether / diethyl ether / DCM = 30/1/1 (320 mL), then petroleum ether/ethyl acetate = 5/1 (480 mL)]: 99% ee (HPLC conditions: AS-H column, hexane/ⁱPrOH = 98/2, 1.0 mL/min, λ = 214 nm, *t*_R (minor) = 5.1 min, *t*_R (major) = 6.5 min); [α]_D²⁶ = +0.5 (c = 1.40, CHCl₃); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.72 (t, *J* = 4.4 Hz, 1 H, Ar-H), 7.23-7.08 (m, 3 H, Ar-H), 2.58 (s, 3 H, CH₃), 2.30-2.17 (m, 3 H, CH₂ and OH), 2.10-1.88 (m, 2 H, CH₂), 1.57 (sextet, *J* = 7.2 Hz, 2 H, CH₂), 1.05-0.91 (m, 6 H, 2 x CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 142.0, 135.4, 132.2, 127.3, 126.2, 125.4, 86.5, 83.1, 73.8, 35.3, 22.0, 21.3, 20.8, 13.6, 8.9; IR (neat): ν = 3453, 2964, 2933, 2873, 2236, 1456, 1328, 1161, 1050 cm⁻¹; MS (ESI) *m/z*: 217 (M+H⁺), 199 (M-OH)⁺; HRMS calcd *m/z* for C₁₅H₂₀O [M⁺]: 216.1509, found: 216.1512.

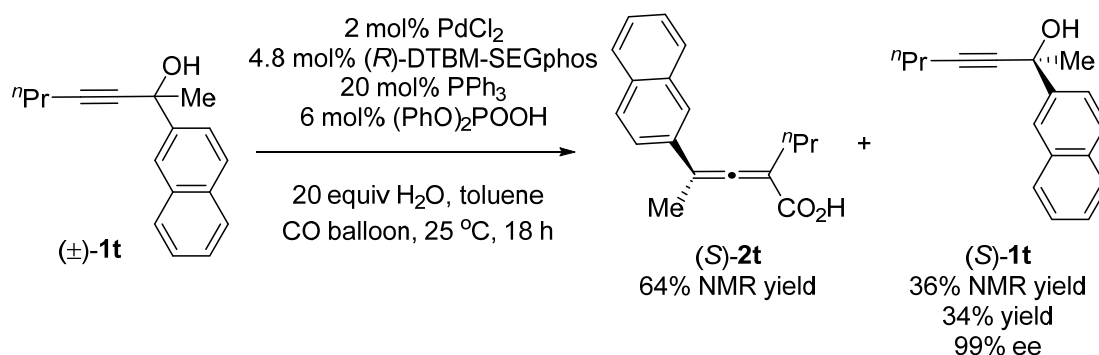
(19) Preparation of (*S*)-3-(2-methylphenyl)non-4-yn-3-ol ((*S*)-**1s**)



Following Typical Procedure, the reaction of PdCl₂ (3.7 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.8 mg, 0.048 mmol), PPh₃ (52.4 mg, 0.2 mmol), (PhO)₂POOH (10.2 mg, 0.04 mmol), (±)-**1s** (230.3 mg, 1.0 mmol), H₂O (360 μL, d = 1.0 g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1s** (103.3 mg, 45%) (56% NMR yield of (*S*)-**2s** was formed and 44% of (*S*)-**1s** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL), then petroleum ether / ethyl acetate = 8/1 (360 mL)]: 99% ee (HPLC conditions: AS-H column, hexane/ⁱPrOH = 98/2, 1.0 mL/min, λ = 214 nm, *t*_R (minor) = 5.1 min, *t*_R (major) = 6.1 min); [α]_D²⁸ = -0.9 (c = 1.10, CHCl₃);

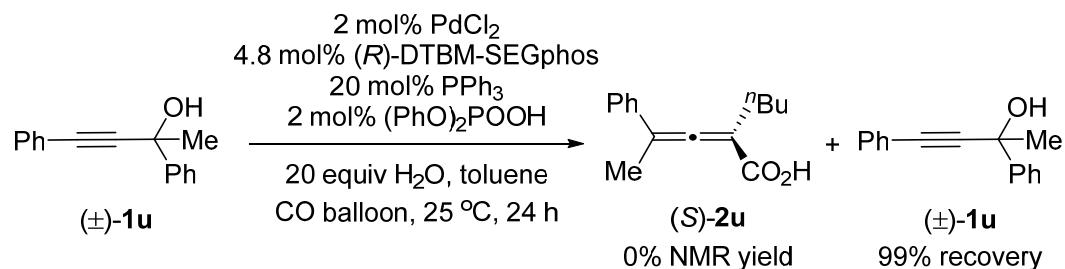
oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.75\text{-}7.67$ (m, 1 H, Ar-H), $7.20\text{-}7.09$ (m, 3 H, Ar-H), 2.57 (s, 3 H, CH_3), 2.32 (br, 1 H, OH), 2.26 (t, $J = 7.0$ Hz, 2 H, CH_2), $2.08\text{-}1.88$ (m, 2 H, CH_2), $1.57\text{-}1.47$ (m, 2 H, CH_2), $1.47\text{-}1.35$ (m, 2 H, CH_2), 0.98 (t, $J = 7.4$ Hz, 3 H, CH_3), 0.91 (t, $J = 7.2$ Hz, 3 H, CH_3); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta = 142.0, 135.4, 132.1, 127.3, 126.2, 125.4, 86.6, 82.9, 73.7, 35.2, 30.6, 22.0, 21.3, 18.4, 13.5, 8.9$; **IR** (neat): $\nu = 3454, 2930, 2238, 1456, 1326, 1046$ cm^{-1} ; **MS** (ESI) m/z : 231 ($\text{M}+\text{H}^+$), 213 ($\text{M}-\text{OH}$) $^+$; **HRMS** calcd for $\text{C}_{16}\text{H}_{23}\text{O}$ [$\text{M}+\text{H}^+$]: 231.1743, found: 231.1741.

(20) Preparation of (*S*)-2-(naphthalen-2-yl)hept-3-yn-2-ol ((*S*)-1t)



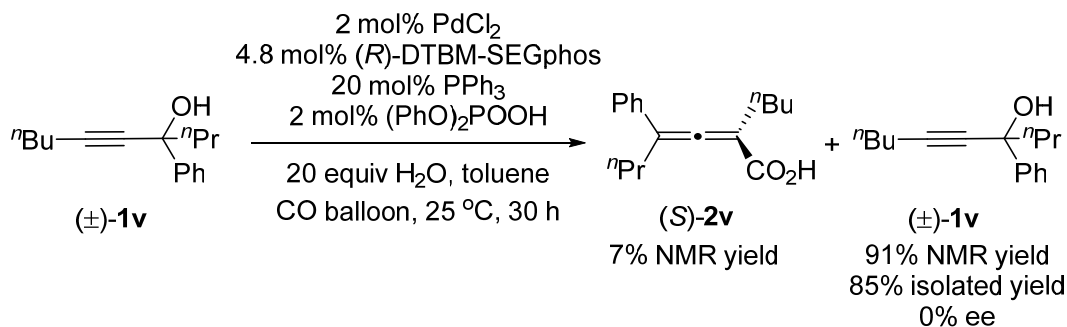
Following Typical Procedure, the reaction of PdCl_2 (3.6 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (57.1 mg, 0.048 mmol), PPh_3 (52.3 mg, 0.2 mmol), $(\text{PhO})_2\text{POOH}$ (15.0 mg, 0.06 mmol), (\pm)-**1t** (238.0 mg, 1.0 mmol), H_2O (360 μL , $d = 1.0$ g/mL, 360.0 mg, 20.0 mmol), and toluene (5 mL) afforded (*S*)-**1t** (80.6 mg, 34%) (64% NMR yield of (*S*)-**2t** was formed and 36% of (*S*)-**1t** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 20/1/1 (1760 mL)]: 99% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, $\lambda = 214$ nm, t_{R} (minor) = 12.1 min, t_{R} (major) = 15.8 min); $[\alpha]_{\text{D}}^{29} = +6.2$ ($c = 1.00$, CHCl_3); oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 8.11$ (s, 1 H, Ar-H), $7.88\text{-}7.76$ (m, 3 H, Ar-H), 7.73 (dd, $J_1 = 8.6$ Hz, $J_2 = 1.4$ Hz, 1 H, Ar-H), $7.52\text{-}7.37$ (m, 2 H, Ar-H), 2.62 (s, 1 H, OH), 2.26 (t, $J = 7.0$ Hz, 2 H, CH_2), 1.82 (s, 3 H, CH_3), $1.64\text{-}1.49$ (m, 2 H, CH_2), 1.02 (t, $J = 7.4$ Hz, 3 H, CH_3); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta = 143.5, 133.0, 132.7, 128.2, 127.9, 127.5, 126.0, 125.9, 123.6, 123.2, 85.7, 84.0, 70.1, 33.3, 22.0, 20.7, 13.5$; **IR** (neat): $\nu = 3418, 2964, 2931, 2871, 2240, 1752, 1358, 1085, 1052$ cm^{-1} ; **MS** (70 eV, EI) m/z (%): 239 (M^++1 , 5.39), 238 (M^+ , 27.03), 223 (100); **HRMS** calcd m/z for $\text{C}_{17}\text{H}_{18}\text{O}$ [M^+]: 238.1352, found: 238.1354.

(20) Preparation of (*S*)-2-(naphthalen-2-yl)hept-3-yn-2-ol ((*S*)-**1u**)



Following Typical Procedure, the reaction of PdCl₂ (3.6 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (57.0 mg, 0.048 mmol), PPh₃ (52.7 mg, 0.2 mmol), (PhO)₂POOH (5.0 mg, 0.02 mmol), (\pm)-**1u** (222.4 mg, 1.0 mmol)/toluene (3 mL), H₂O (360 μ L, d = 1.0 g/mL, 360.0 mg, 20.0 mmol)/toluene (2 mL), no desired product was formed with 99% NMR yield of (\pm)-**1u** recovered.

(22) Synthesis of 4-phenyldec-5-yn-4-ol (**2v**)

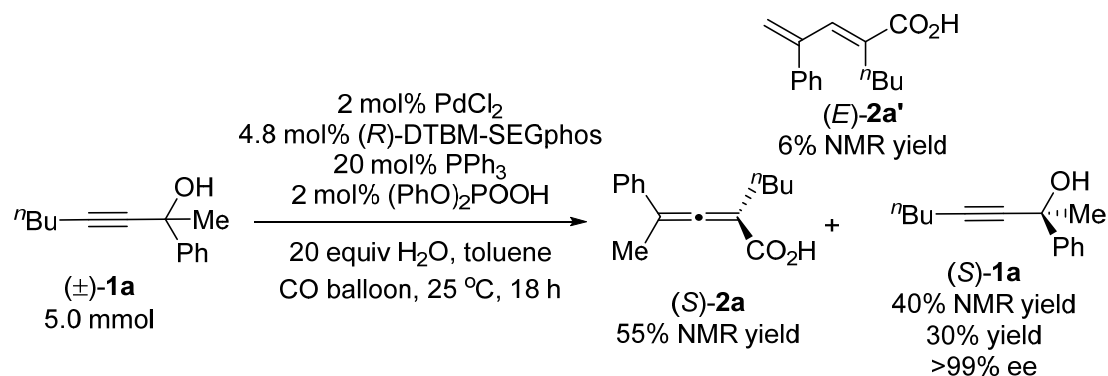


Following Typical Procedure, the reaction of PdCl₂ (3.7 mg, 0.02 mmol), (*R*)-DTBM-SEGphos (56.7 mg, 0.048 mmol), PPh₃ (52.5 mg, 0.2 mmol), and (PhO)₂POOH (5.1 mg, 0.02 mmol), (\pm)-**1v** (230.1 mg, 1.0 mmol)/toluene (3 mL) and H₂O (360 μ L, 20.0 mmol)/toluene (2 mL), recovered (\pm)-**1v** (195.4 mg, 85%) (7% NMR yield of (*S*)-**2v** was formed and 91% of (\pm)-**1v** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (320 mL)]: 0% ee (HPLC conditions: AS-H column, hexane/*i*-PrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_1 = 5.3 min, t_2 = 6.6 min); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.68-7.57 (m, 2 H, Ar-H), 7.39-7.31 (m, 2 H, Ar-H), 7.31-7.24 (m, 1 H, Ar-H), 2.38-2.22 (m, 3 H, CH₂ and OH), 1.96-1.73 (m, 2 H, CH₂), 1.60-1.24 (m, 6 H, 3 x CH₂), 0.93 (t, J = 7.2 Hz, 3 H, CH₃), 0.88 (t, J = 7.6 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 145.4, 128.0, 127.4, 125.5, 86.7, 82.6, 73.4,

47.8, 30.8, 22.0, 18.4, 18.1, 14.0, 13.6.

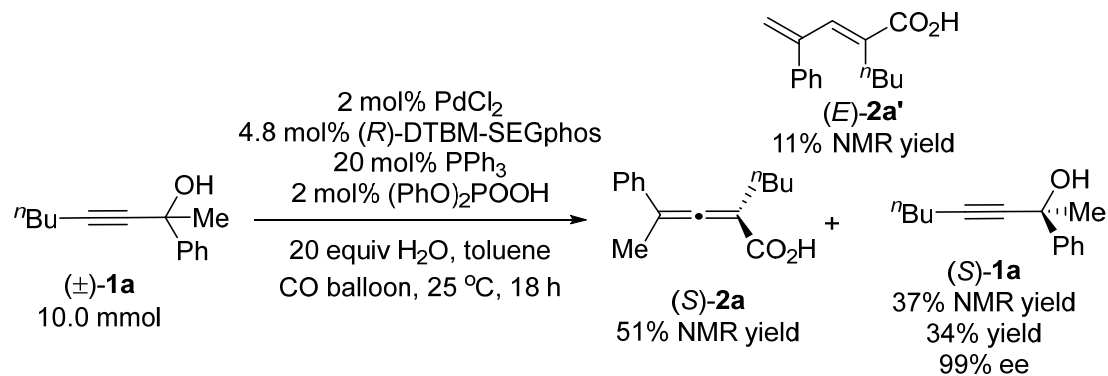
2. Gram-scale reactions

(1) Gram scale synthesis of (*S*)-2-phenyloct-3-yn-2-ol ((*S*)-**1a**)



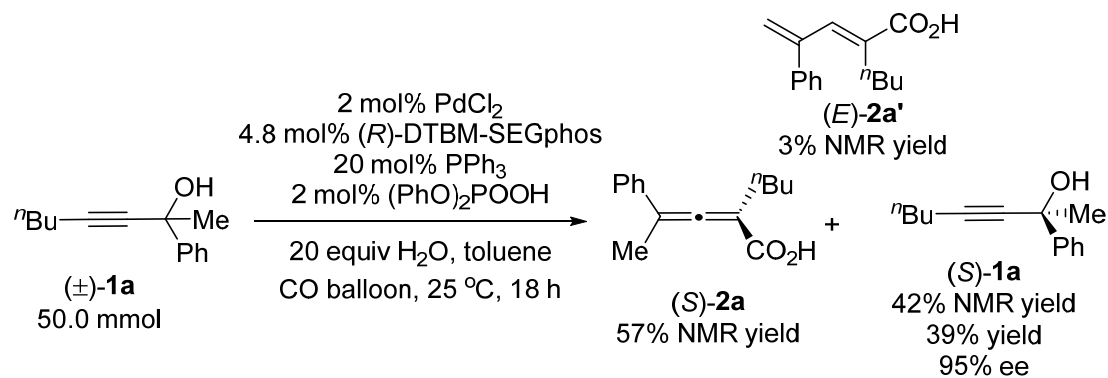
Following Typical Procedure, the reaction of PdCl₂ (17.8 mg, 0.1 mmol), (*R*)-DTBM-SEGphos (288.8 mg, 0.24 mmol), PPh₃ (262.1 mg, 1.0 mmol), and (PhO)₂POOH (25.3 mg, 0.1 mmol), (\pm)-**1a** (1.0112 g, 5.0 mmol)/toluene (15 mL) and H₂O (1.8051 g, 100.0 mmol)/toluene (10 mL), afforded **1a** (301.9 mg, 30%) (55% NMR yield of (*S*)-**2a** and 6% of (*E*)-**2a'** were formed and 40% of (*S*)-**1a** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (1280 mL), 10/1/1 (1200 mL), then petroleum ether / ethyl acetate = 8/1 (900 mL)]: >99% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (major) = 11.1 min); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.66 (d, J = 8.0 Hz, 2 H, Ar-H), 7.36 (t, J = 7.4 Hz, 2 H, Ar-H), 7.32-7.27 (m, 1 H, Ar-H), 2.35-2.20 (m, 3 H, OH and CH₂), 1.74 (s, 3 H, CH₃), 1.60-1.50 (m, 2 H, CH₂), 1.50-1.35 (m, 2 H, CH₂), 0.93 (t, J = 7.2 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 146.2, 128.1, 127.4, 124.9, 85.5, 83.7, 70.0, 33.5, 30.7, 21.9, 18.3, 13.5.

(2) Gram scale synthesis of (*S*)-2-phenyloct-3-yn-2-ol ((*S*)-**1a**)



Following Typical Procedure, the reaction of PdCl_2 (35.6 mg, 0.2 mmol), *(R)*-DTBM-SEGphos (577.9 mg, 0.48 mmol), PPh_3 (524.9 mg, 2.0 mmol), $(\text{PhO})_2\text{POOH}$ (50.1 mg, 0.2 mmol), **(±)-1a** (2.0234 g, 10.0 mmol), H_2O (3.6011 g, 200.0 mmol), and toluene (50 mL) afforded **(S)-1a** (684.5 mg, 34%) (51% NMR yield of **(S)-2a**, 11% **(E)-2a'** were formed and 37% of **(S)-1a** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (1280 mL), 10/1/1 (1080 mL), then petroleum ether / ethyl acetate = 8/1 (1800 mL)]: 99% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, $\lambda = 214 \text{ nm}$, t_R (minor) = 7.4 min, t_R (major) = 11.5 min); oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.65$ (d, $J = 7.6 \text{ Hz}$, 2 H, Ar-H), 7.35 (t, $J = 7.4 \text{ Hz}$, 2 H, Ar-H), 7.31-7.22 (m, 1 H, Ar-H), 2.45-2.15 (m, 3 H, OH and CH_2), 1.74 (s, 3 H, CH_3), 1.58-1.48 (m, 2 H, CH_2), 1.48-1.36 (m, 2 H, CH_2), 0.93 (t, $J = 7.2 \text{ Hz}$, 3 H, CH_3); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta = 146.2, 128.1, 127.4, 124.9, 85.5, 83.7, 70.0, 33.5, 30.7, 21.9, 18.3, 13.5$.

(3) Gram scale synthesis of *(S)*-2-phenyloct-3-yn-2-ol (**(S)-1a**)



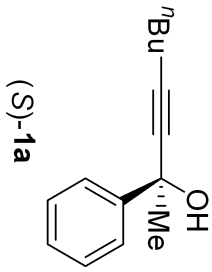
Following Typical Procedure, the reaction of PdCl_2 (177.4 mg, 1.0 mmol), *(R)*-DTBM-SEGphos (2830.5 mg, 2.4 mmol), PPh_3 (2630.2 mg, 10.0 mmol), $(\text{PhO})_2\text{POOH}$

(250.4 mg, 1.0 mmol), (\pm)-**1a** (10.1141 g, 50.0 mmol), H₂O (18 mL, 1000.0 mmol), and toluene (250 mL) afforded (*S*)-**1a** (3.9229 g, 39%) (57% NMR yield of (*S*)-**2a**, 3% (*E*)-**2a'** were formed and 42% of (*S*)-**1a** remained) [eluent: petroleum ether / ethyl ether / dichloromethane = 30/1/1 (4800 mL), then petroleum ether / ethyl acetate = 5/1 (1800 mL)]: 95% ee (HPLC conditions: AS-H column, hexane/*i*PrOH = 98/2, 1.0 mL/min, λ = 214 nm, t_R (minor) = 7.2 min, t_R (major) = 10.5 min); oil; ¹H NMR (400 MHz, CDCl₃): δ = 7.69-7.62 (m, 2 H, Ar-H), 7.39-7.32 (m, 2 H, Ar-H), 7.31-7.24 (m, 1 H, Ar-H), 2.35-2.23 (m, 3 H, OH and CH₂), 1.74 (s, 3 H, CH₃), 1.58-1.50 (m, 2 H, CH₂), 1.50-1.38 (m, 2 H, CH₂), 0.93 (t, J = 7.2 Hz, 3 H, CH₃); ¹³C NMR (100 MHz, CDCl₃): δ = 146.2, 128.2, 127.5, 124.9, 85.7, 83.7, 70.0, 33.5, 30.7, 22.0, 18.4, 13.6.

References:

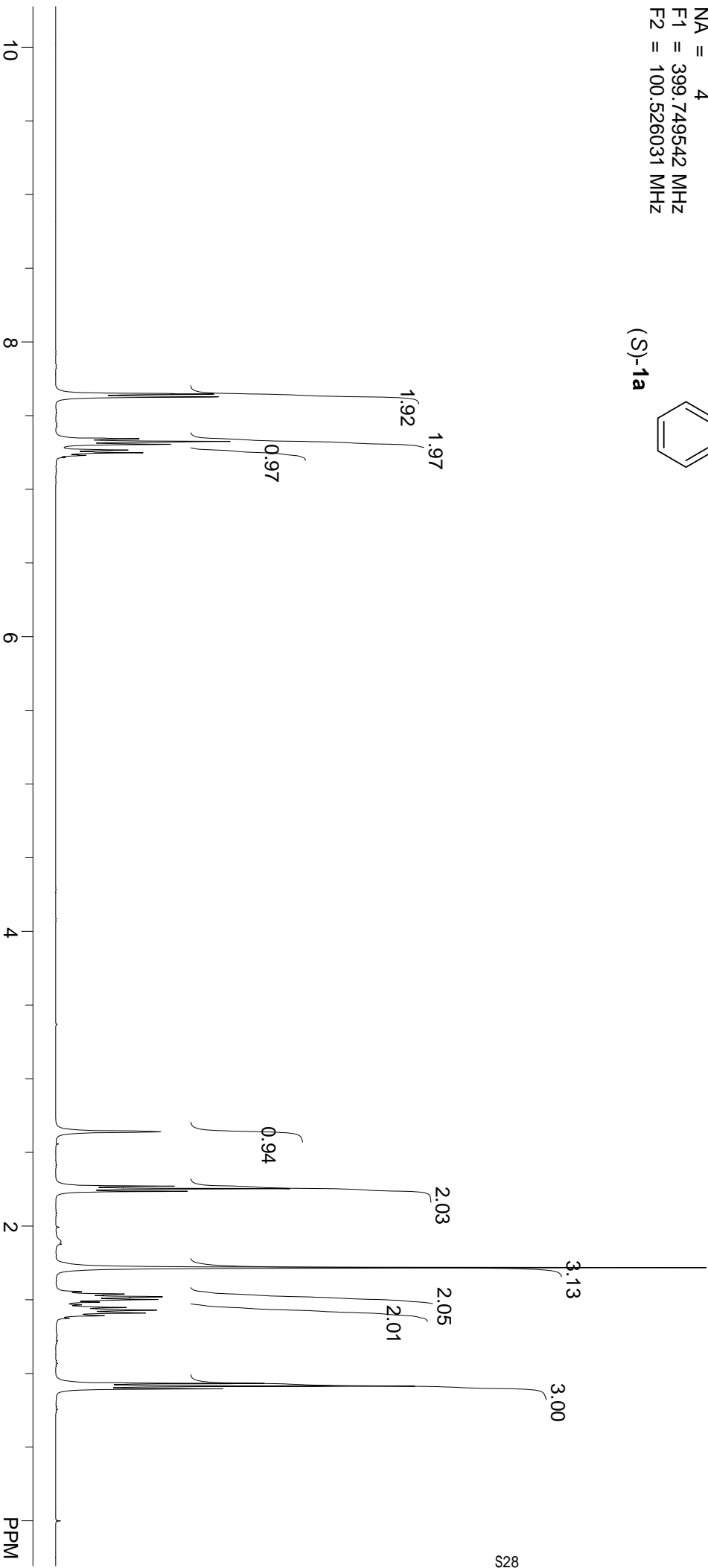
1. W. Zhang, C. Huang, Y. Yuan and S. Ma, *Chem. Commun.*, 2017, **53**, 12430.
2. H. B. Kagan and J. C. Fiaud, *Top. Stereochem.* 1988, **18**, 249.
3. S. Kotani, K. Kukita, K. Tanaka, T. Ichibakase and M. Nakajima, *J. Org. Chem.*, 2014, **79**, 4817.
4. H.-L. Wu, P.-Y. Wu, Y.-Y. Shen and B.-J. Uang, *J. Org. Chem.*, 2008, **73**, 6445.
5. W.-F. Zheng, W. Zhang, J. Huang, Y. Yu, H. Qian and S. Ma, *Org. Chem. Front.*, 2018, **5**, 1900.
6. W. Zhang, and S. Ma, *Chem. Commun.*, 2018, **54**, 6064.

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May 12 2018
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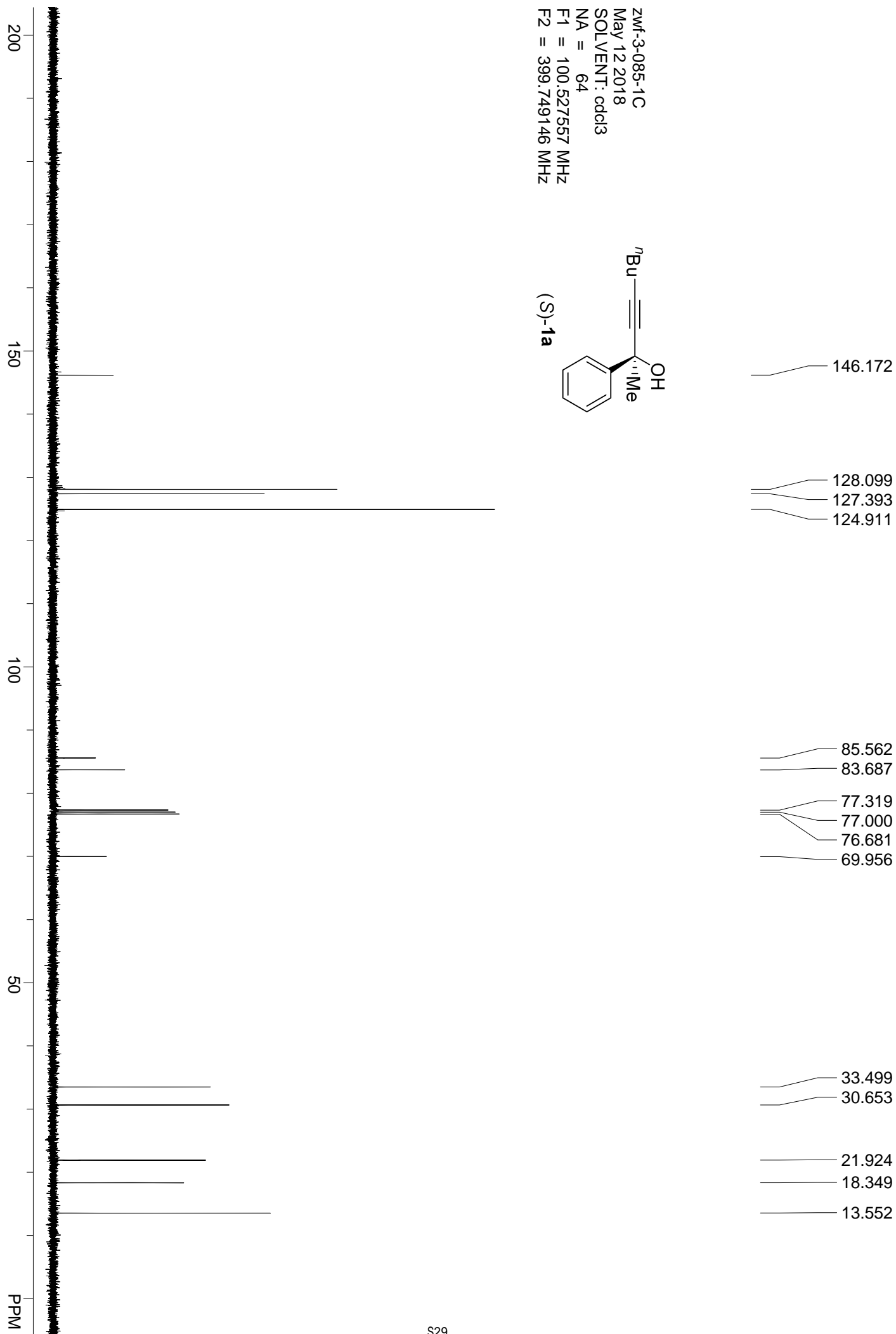
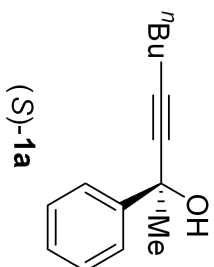


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zwf-3-085-1C
May 12 2018
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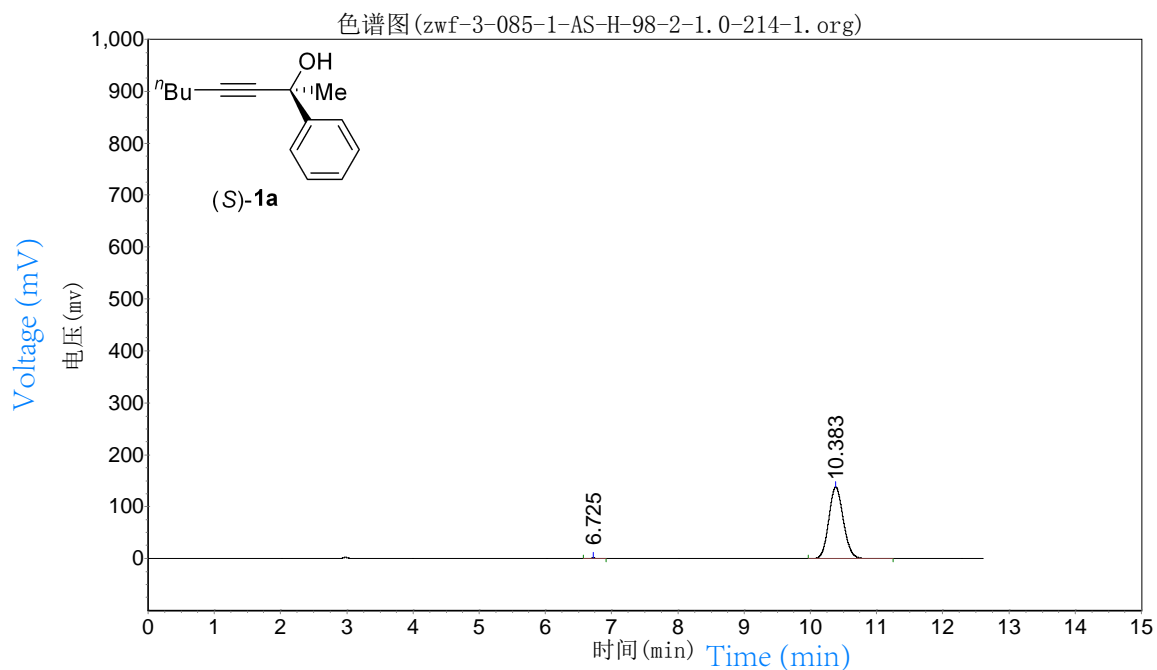
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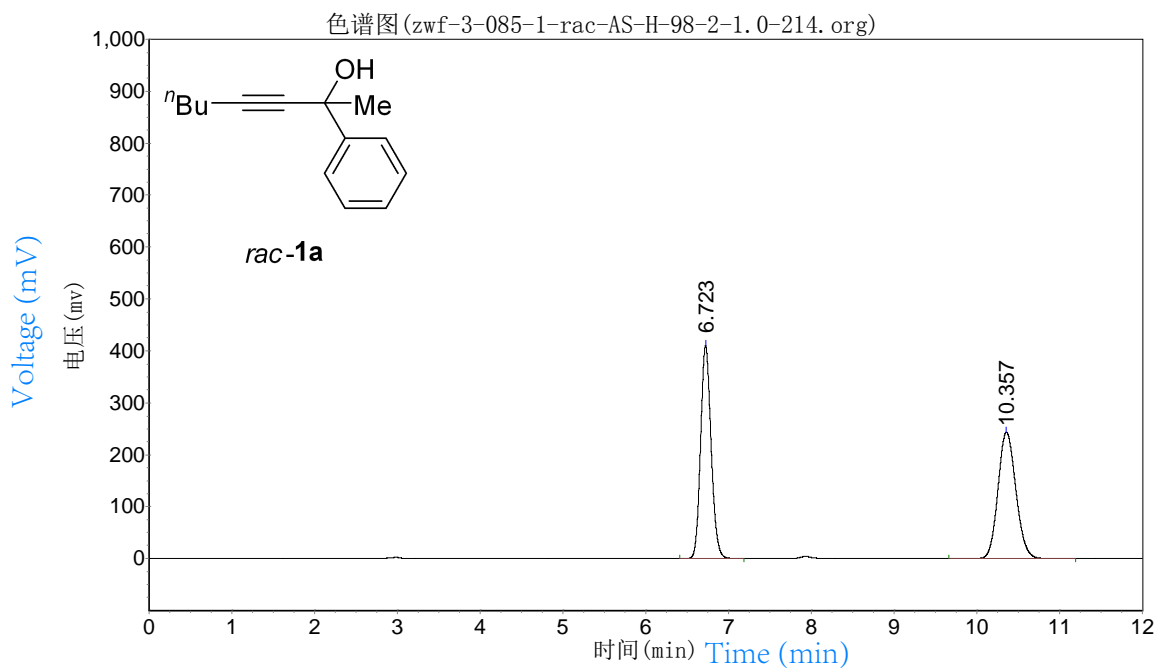
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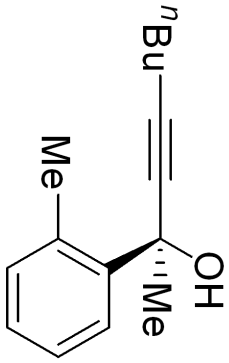
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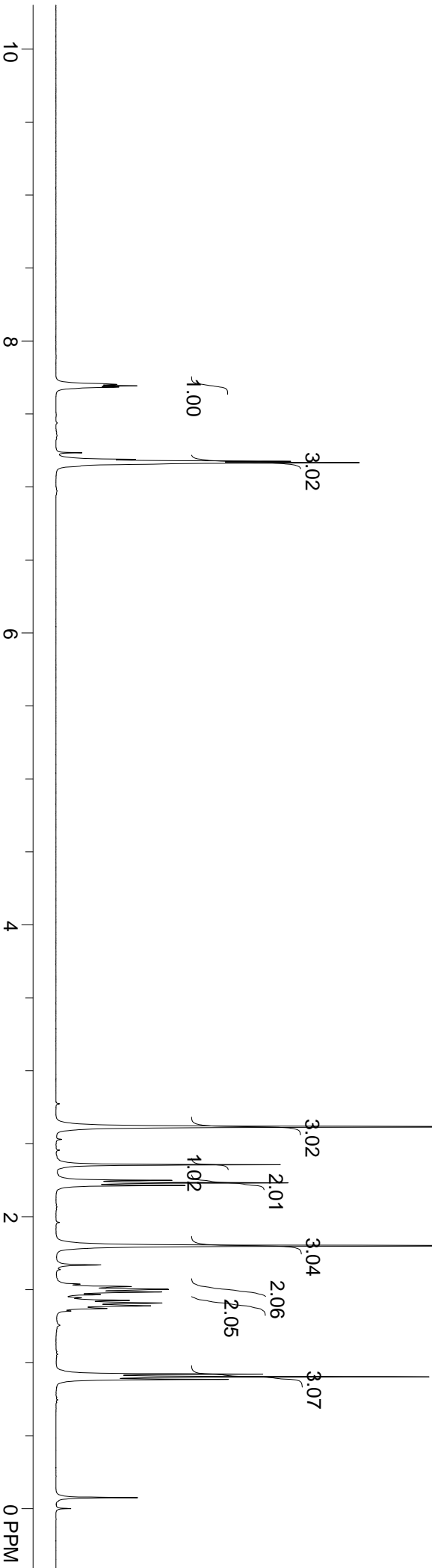
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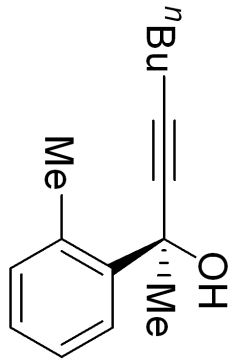
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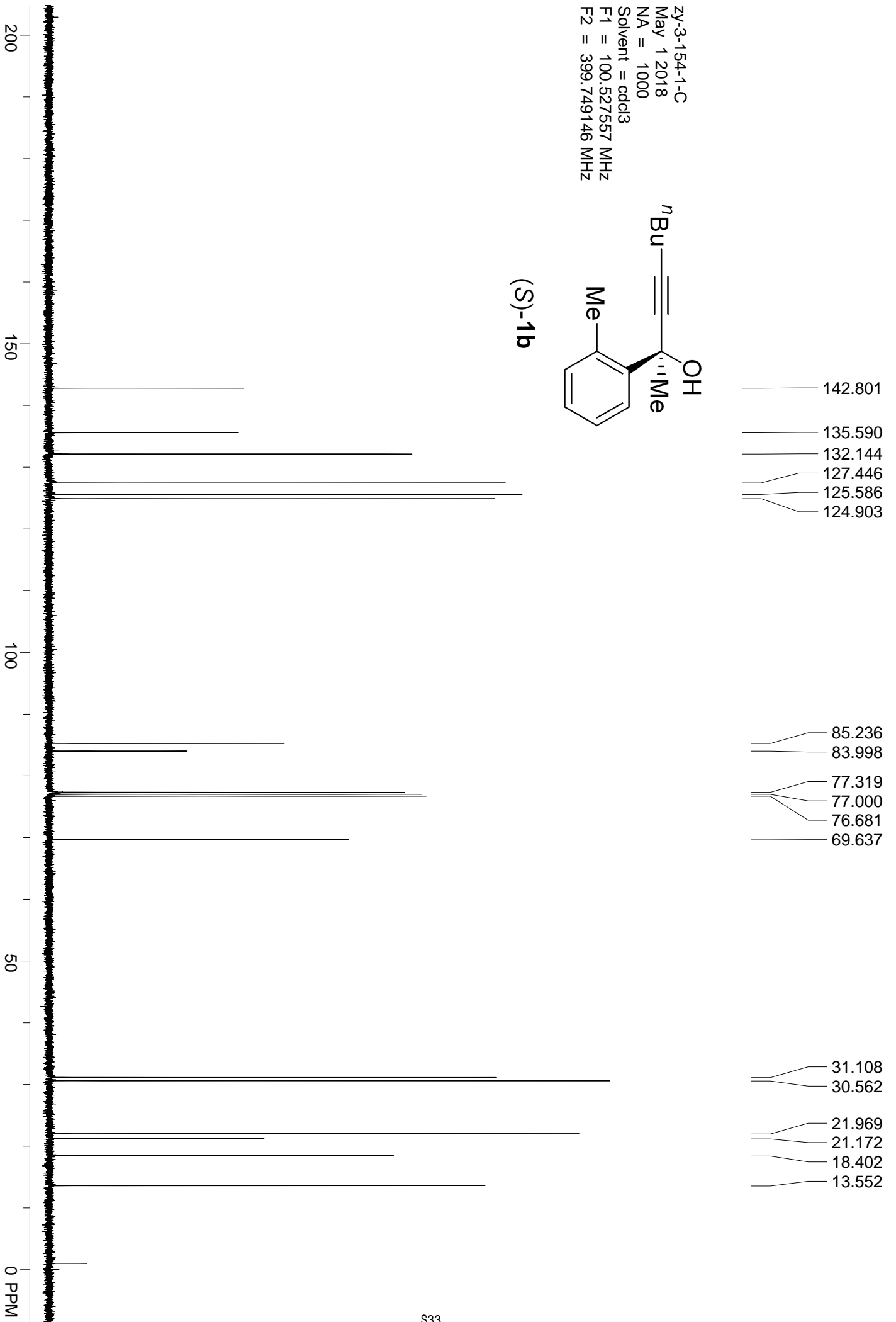
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May 1 2018
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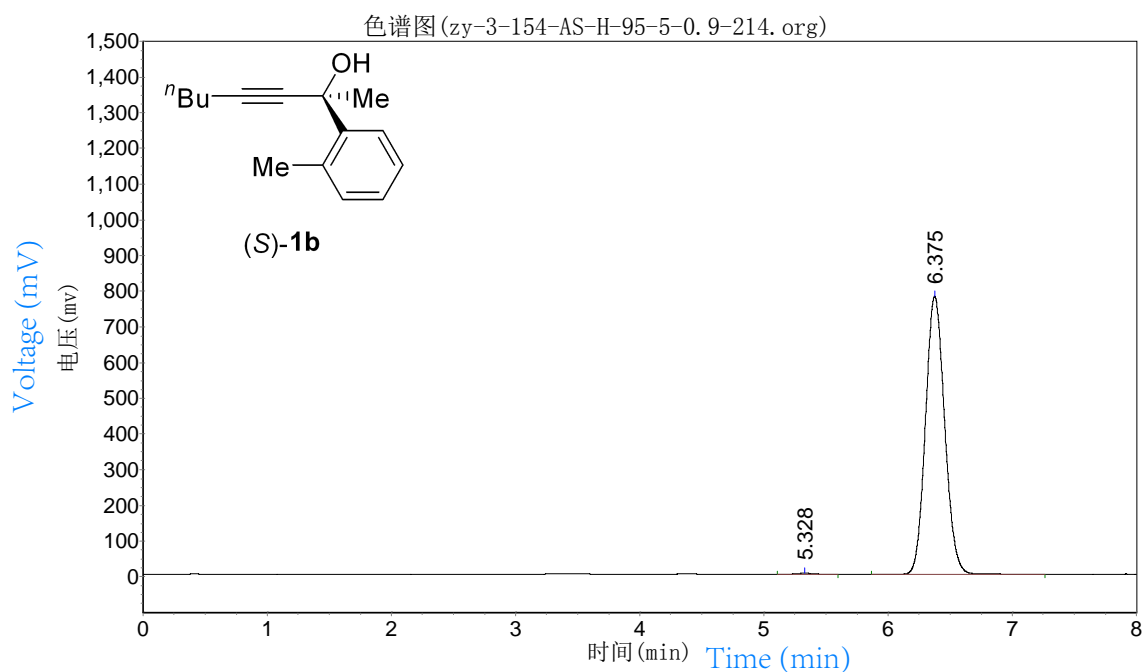


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实验内容简介:



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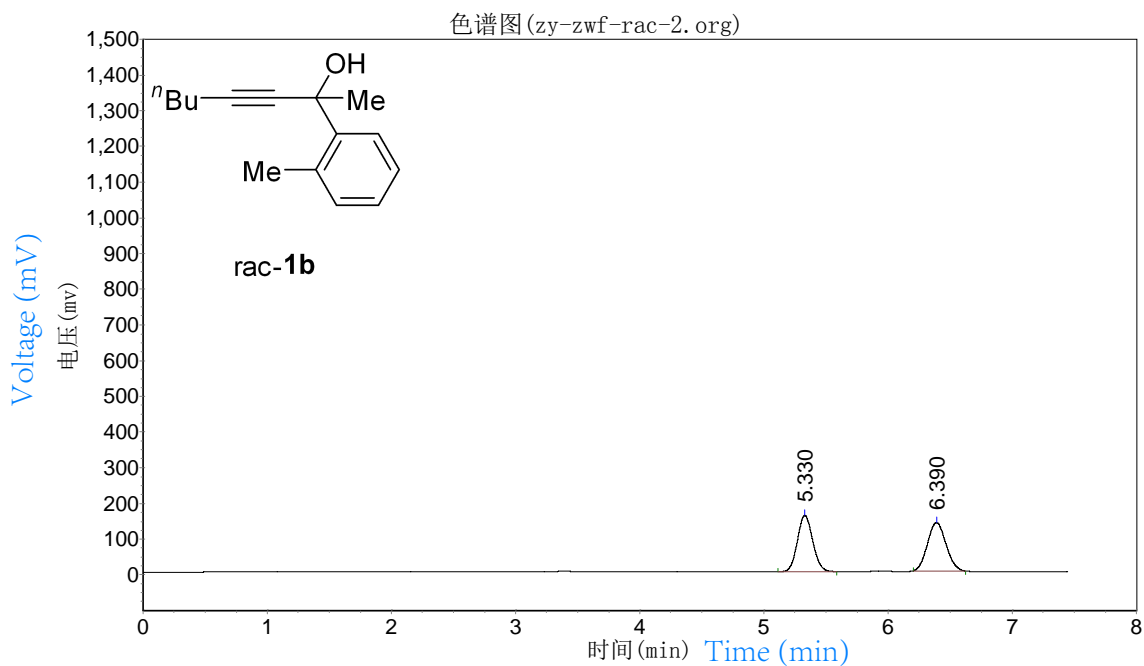
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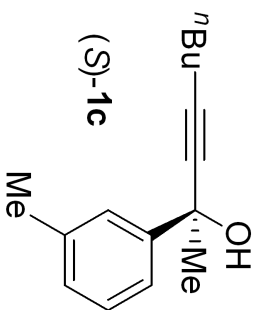
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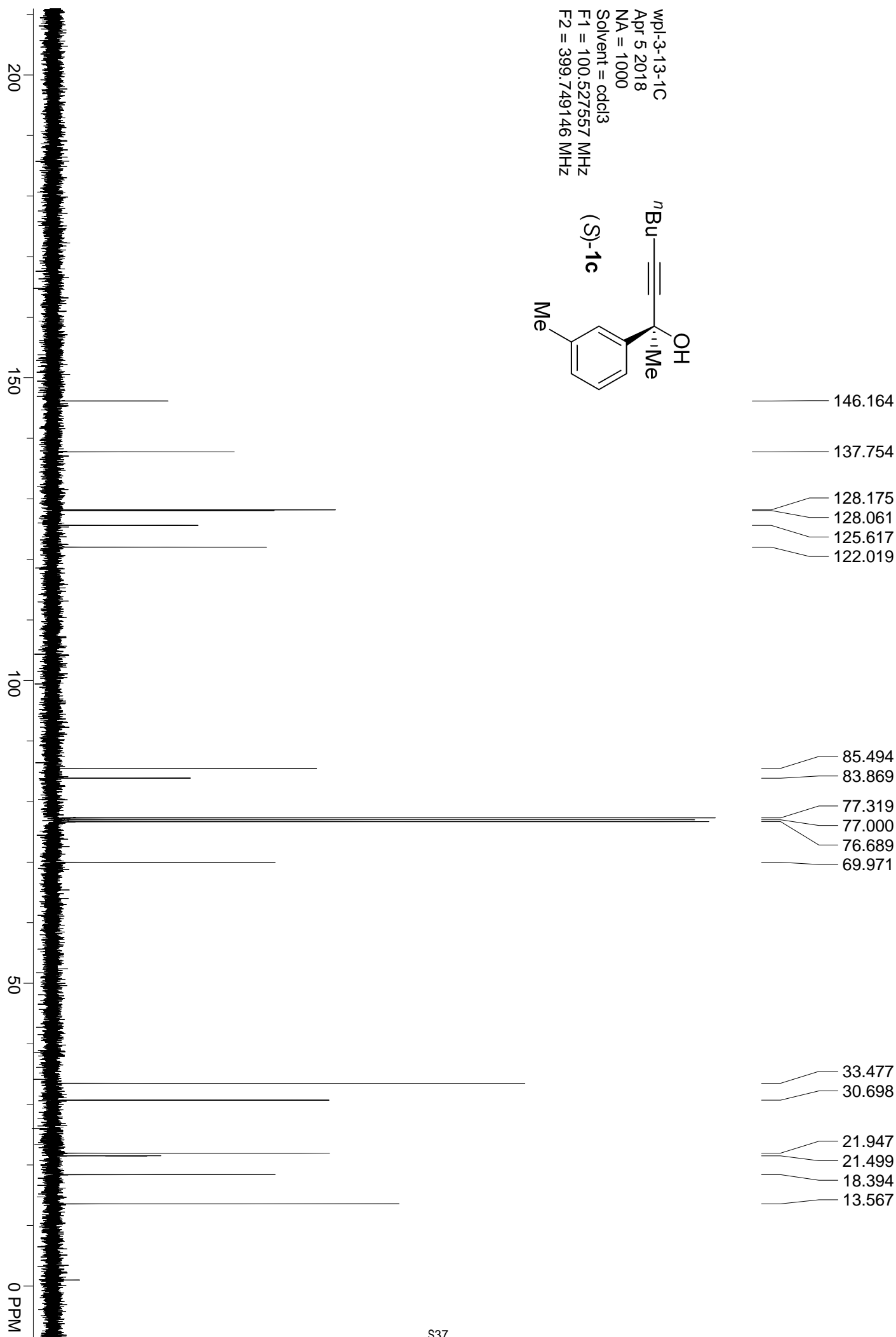
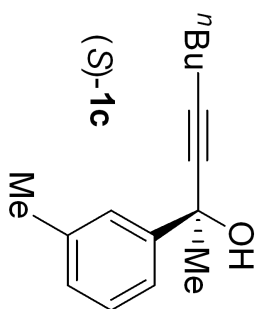


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Apr 4 2018
NA = 4
Solvent = cdcl3
F1 = 399.749542 MHz
F2 = 100.526031 MHz

2.373
2.298
2.282
2.264
2.249
1.735
1.562
1.542
1.524
1.506
1.470
1.453
1.433
1.414
0.947
0.929
0.911
0.000



wpl-3-13-1C
Apr 5 2018
NA = 1000
Solvent = cdcl3
F1 = 100.527557 MHz
F2 = 399.749146 MHz



wpl-3-013-1-as-h-95-5-1.3-214

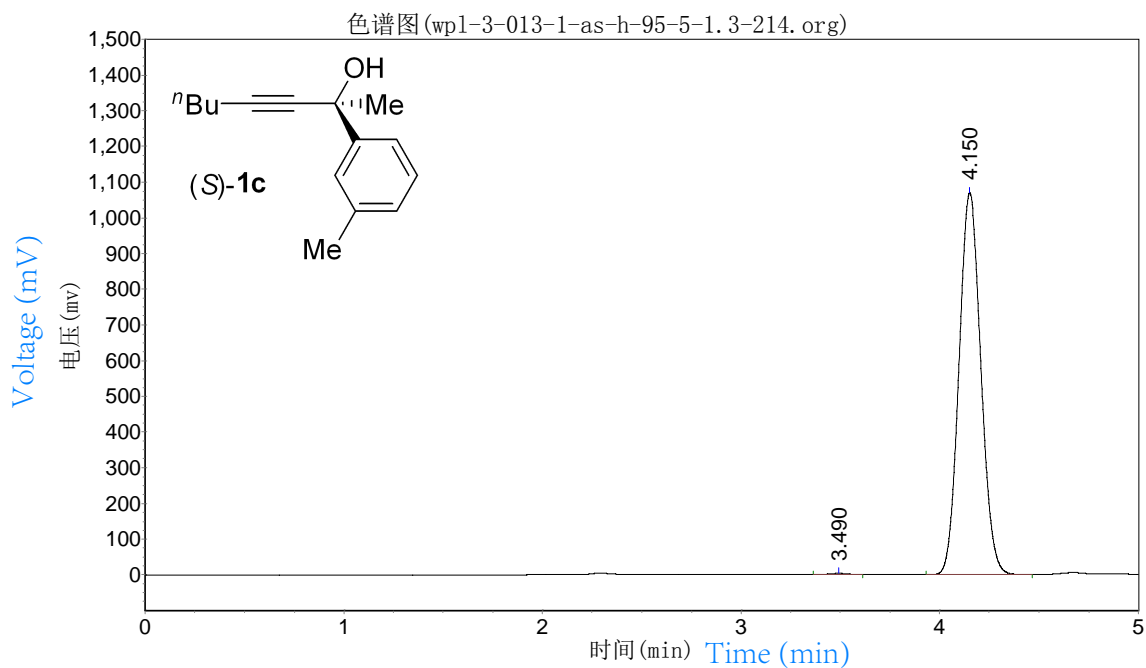
实验时间: 2018-04-06, 15:53:55

报告时间: 2018-07-17, 18:53:20

谱图文件: E:\data\zwf\other\wpl-3-013-1-as-h-95-5-1.3-214.org

方法文件: E:\data\zwf\zwf-method.mtd

实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		3.490	3659.800	23983.699	0.2921
2		4.150	1069736.625	8186462.000	99.7079
总计			1073396.425	8210445.699	100.0000

wpl-3-013-1-rac-as-h-95-5-1.3-214

实验时间: 2018-04-08, 17:04:30

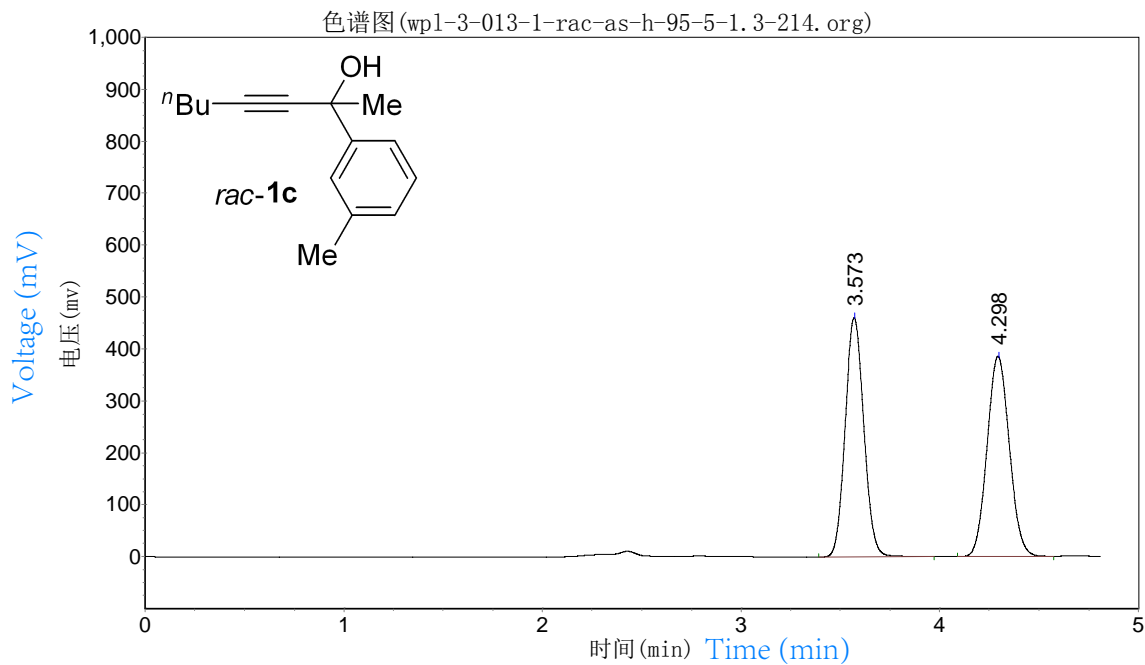
报告时间: 2018-07-17, 18:52:10

谱图文件: E:\data\zwf\other\wpl-3-013-1-rac-as-h-95-5-1.3-

214.org

方法文件: E:\data\zwf\zwf-method.mtd

实验内容简介:



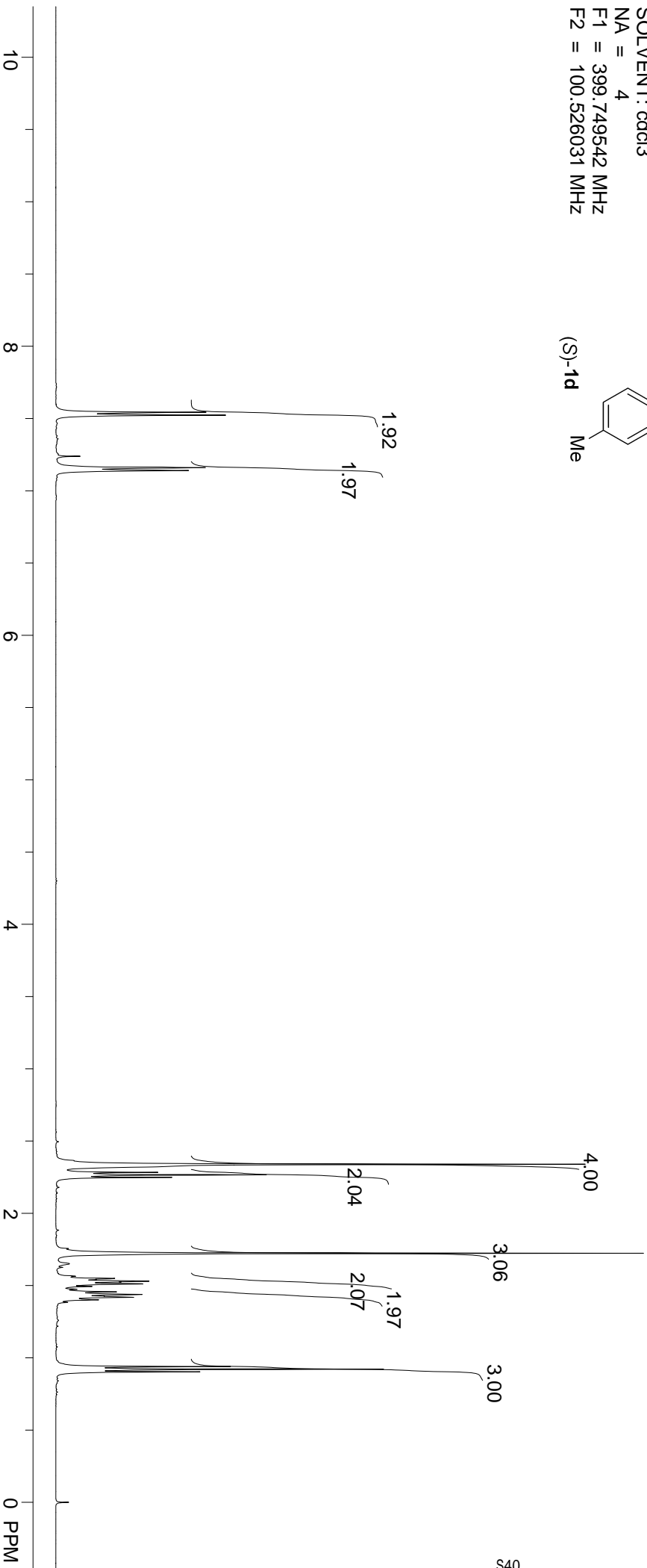
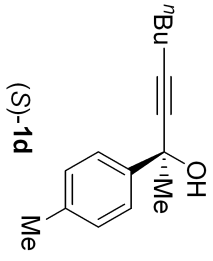
分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		3.573	460089.656	2991042.250	50.0341
2		4.298	384762.594	2986964.750	49.9659
总计			844852.250	5978007.000	100.0000

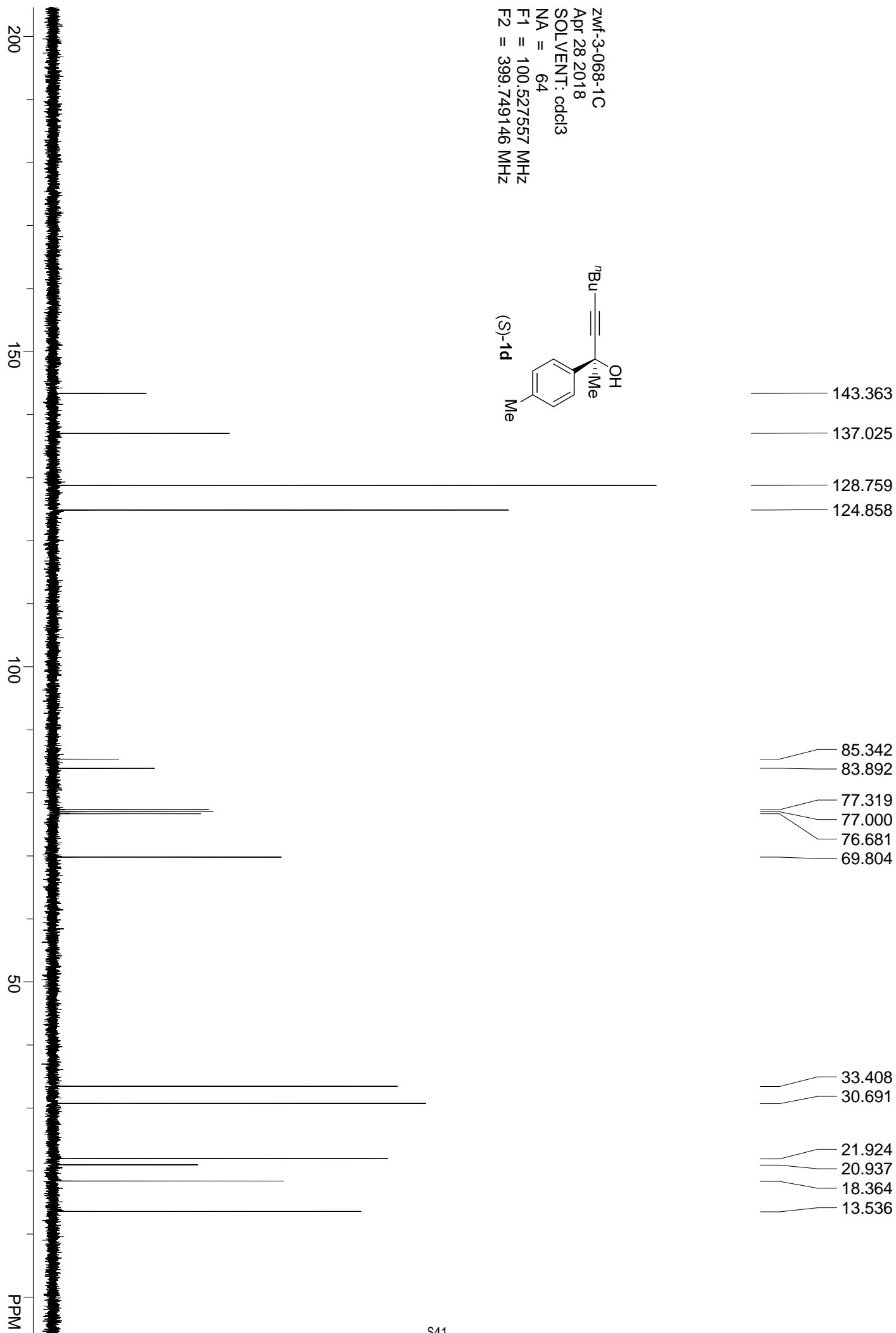
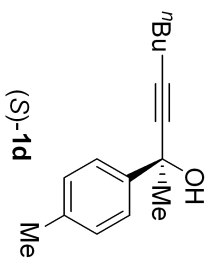
7.544
7.523
7.238
7.160
7.140

2.339
2.284
2.266
2.248
1.724
1.564
1.549
1.530
1.511
1.494
1.474
1.456
1.438
1.418
1.401
1.383
0.940
0.921
0.903
-0.000

zwf-3-068-1H
Apr 28 2018
SOLVENT: cdcl3
NA = 4
F1 = 399.749542 MHz
F2 = 100.526031 MHz



zwf-3-068-1C
Apr 28 2018
SOLVENT: cdcl3
NA = 64
F1 = 100.527557 MHz
F2 = 399.749146 MHz



zwf-3-068-1-AS-H-98-2-1.0-214

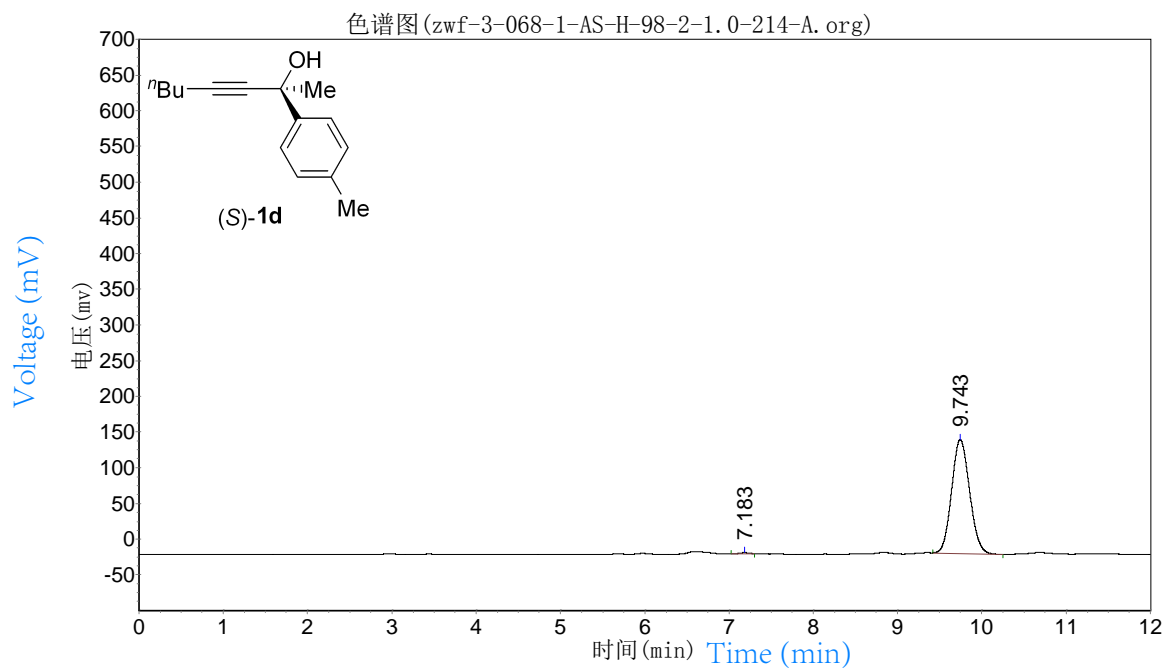
实验时间: 2018-04-27, 21:25:09

报告时间: 2018-04-27, 22:06:08

谱图文件: E:\data\zwf\zwf-3-068-1-AS-H-98-2-1.0-214-A.org

方法文件: E:\data\yaoyuan\0414.mtd

实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		7.183	1625.179	13089.509	0.5526
2		9.743	159608.438	2355492.500	99.4474
总计			161233.616	2368582.009	100.0000

zwf-3-068-1-rac-AS-H-98-2-1.0-214

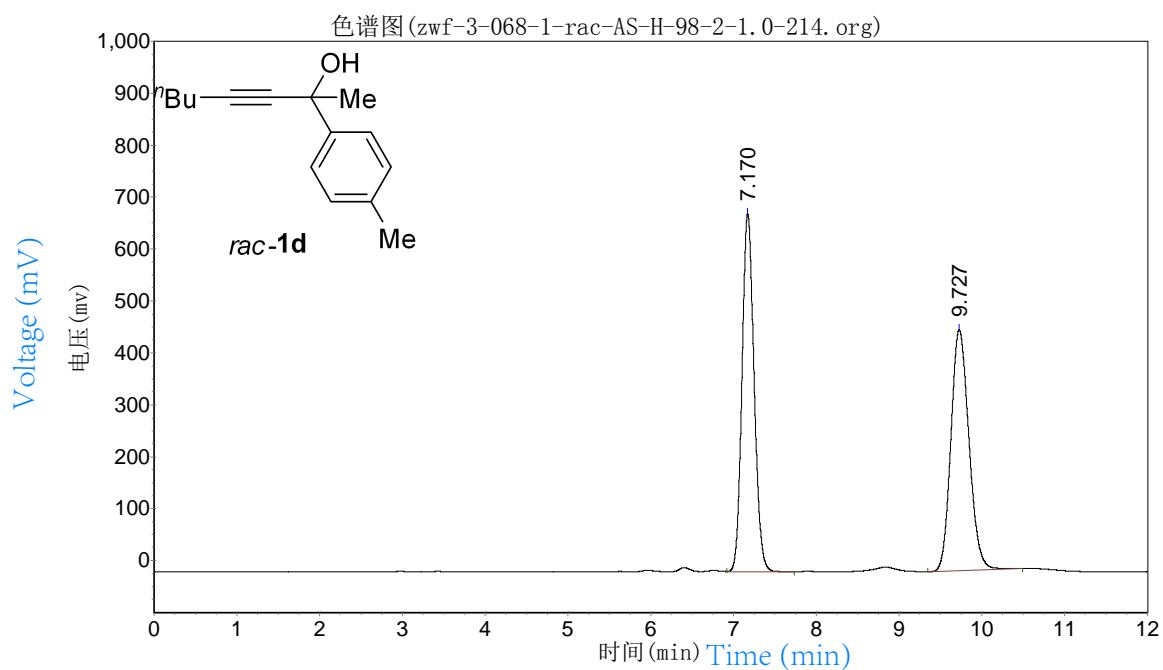
实验时间: 2018-04-27, 20:31:04

报告时间: 2018-04-27, 21:58:32

谱图文件: E:\data\zwf\zwf-3-068-1-rac-AS-H-98-2-1.0-214.org

方法文件: E:\data\yaoyuan\0414.mtd

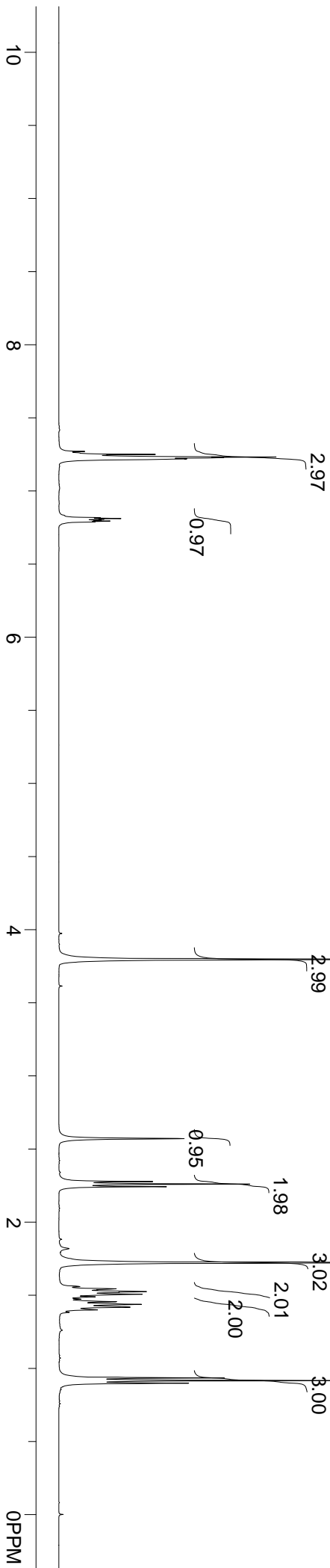
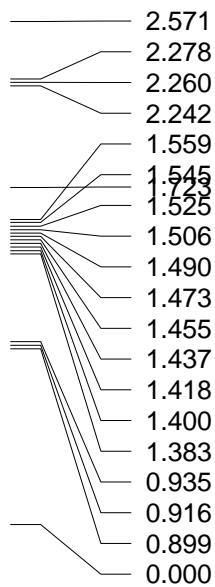
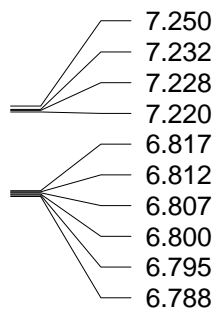
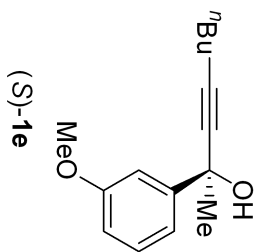
实验内容简介:



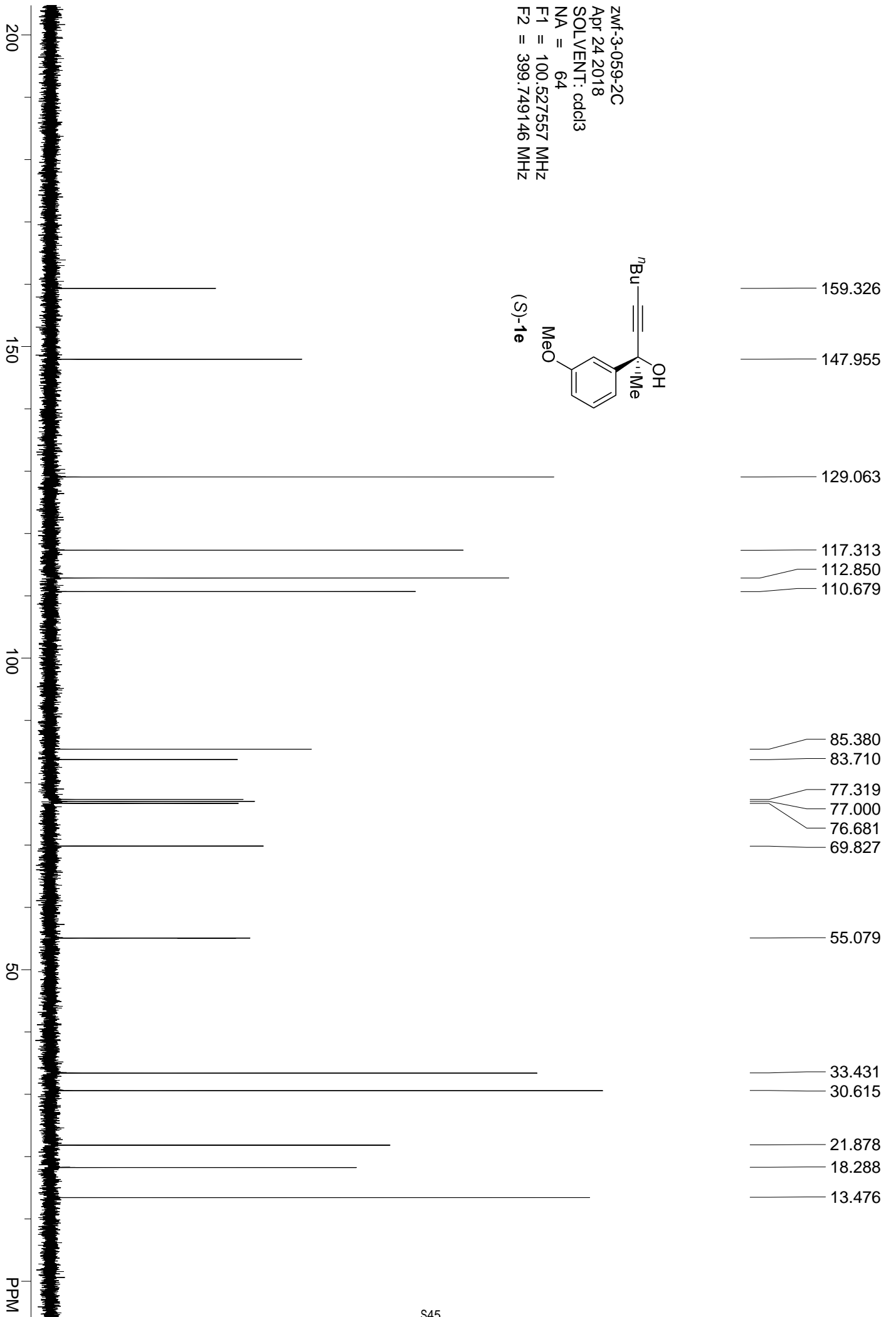
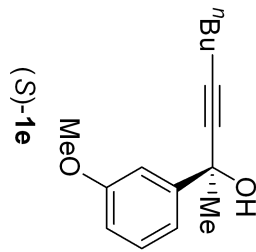
分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		7.170	689154.438	6978570.000	49.9152
2		9.727	463632.469	7002289.000	50.0848
总计			1152786.906	13980859.000	100.0000

zwf-3-059-1H
 Apr 24 2018
 SOLVENT: cdcl3
 NA = 4
 F1 = 399.749542 MHz
 F2 = 100.526031 MHz



zwf-3-059-2C
Apr 24 2018
SOLVENT: cdcl3
NA = 64
F1 = 100.527557 MHz
F2 = 399.749146 MHz

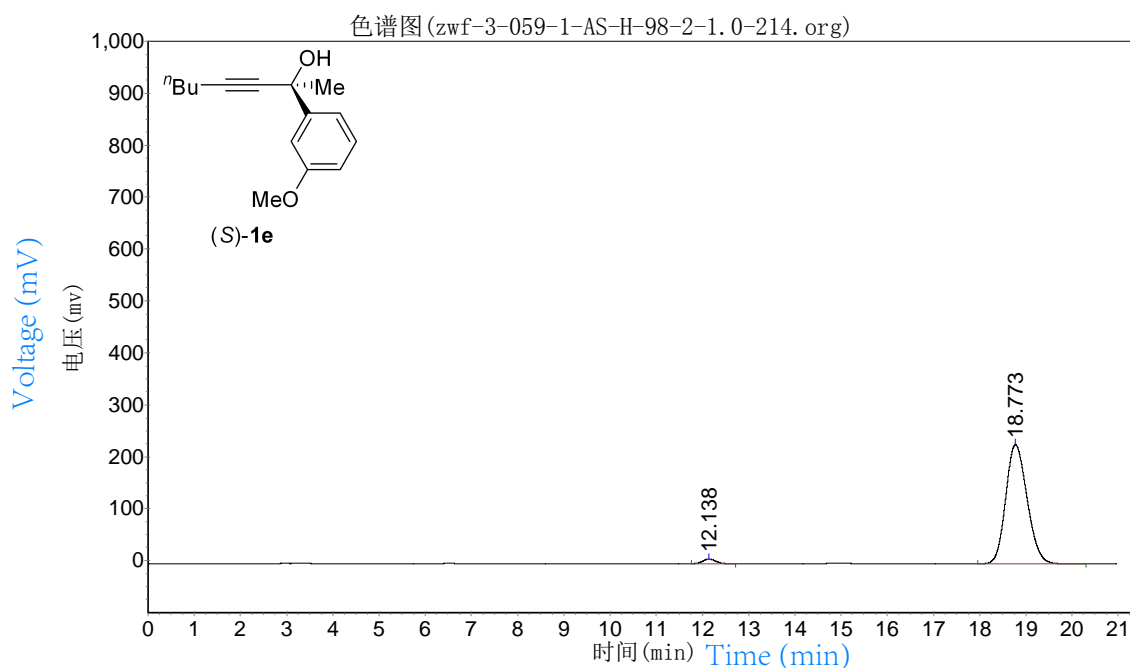


zwf-3-059-1-AS-H-98-2-1.0-214

实验时间: 2018-04-24, 11:03:07
谱图文件: E:\data\zwf\zwf-3-059-1-AS-H-98-2-1.0-214.org
方法文件: E:\data\yaoyuan\0414.mtd

报告时间: 2018-04-24, 11:27:00

实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		12.138	8985.907	167726.438	2.2317
2		18.773	229401.469	7347846.500	97.7683
总计			238387.376	7515572.938	100.0000

zwf-3-059-1-rac-AS-H-98-2-1.0-214

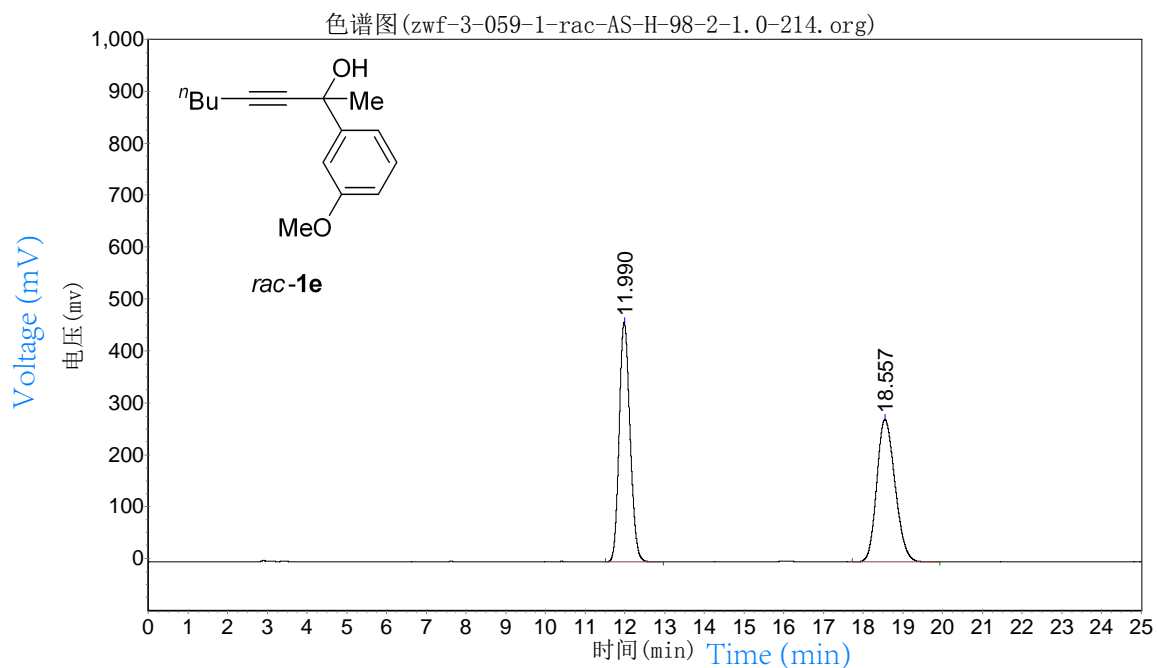
实验时间: 2018-04-24, 11:24:45

报告时间: 2018-04-24, 11:54:41

谱图文件: E:\data\zwf\zwf-3-059-1-rac-AS-H-98-2-1.0-214.org

方法文件: E:\data\yaoyuan\0414.mtd

实验内容简介:



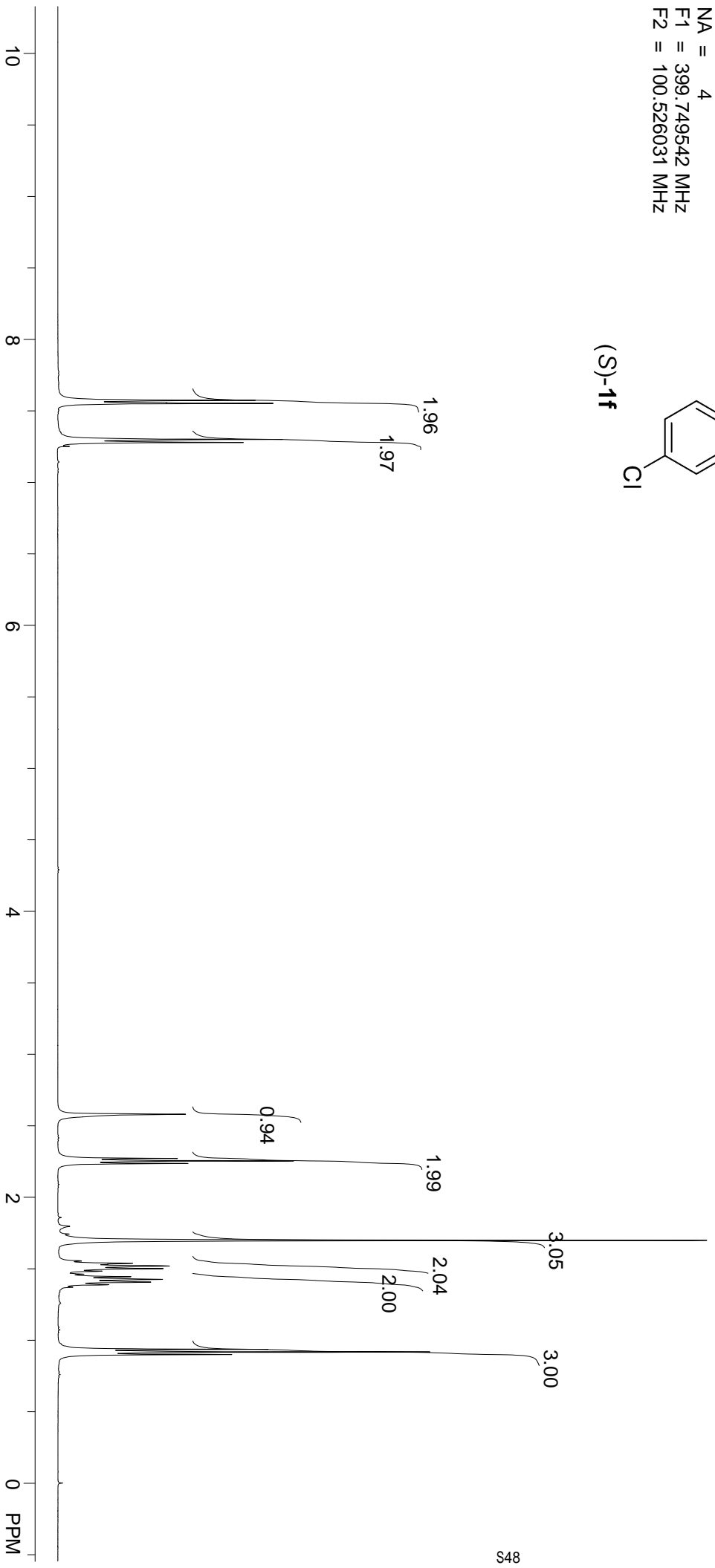
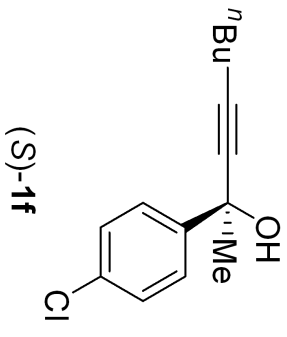
分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		11.990	461343.125	8738462.000	49.9666
2		18.557	274084.594	8750151.000	50.0334
总计			735427.719	17488613.000	100.0000

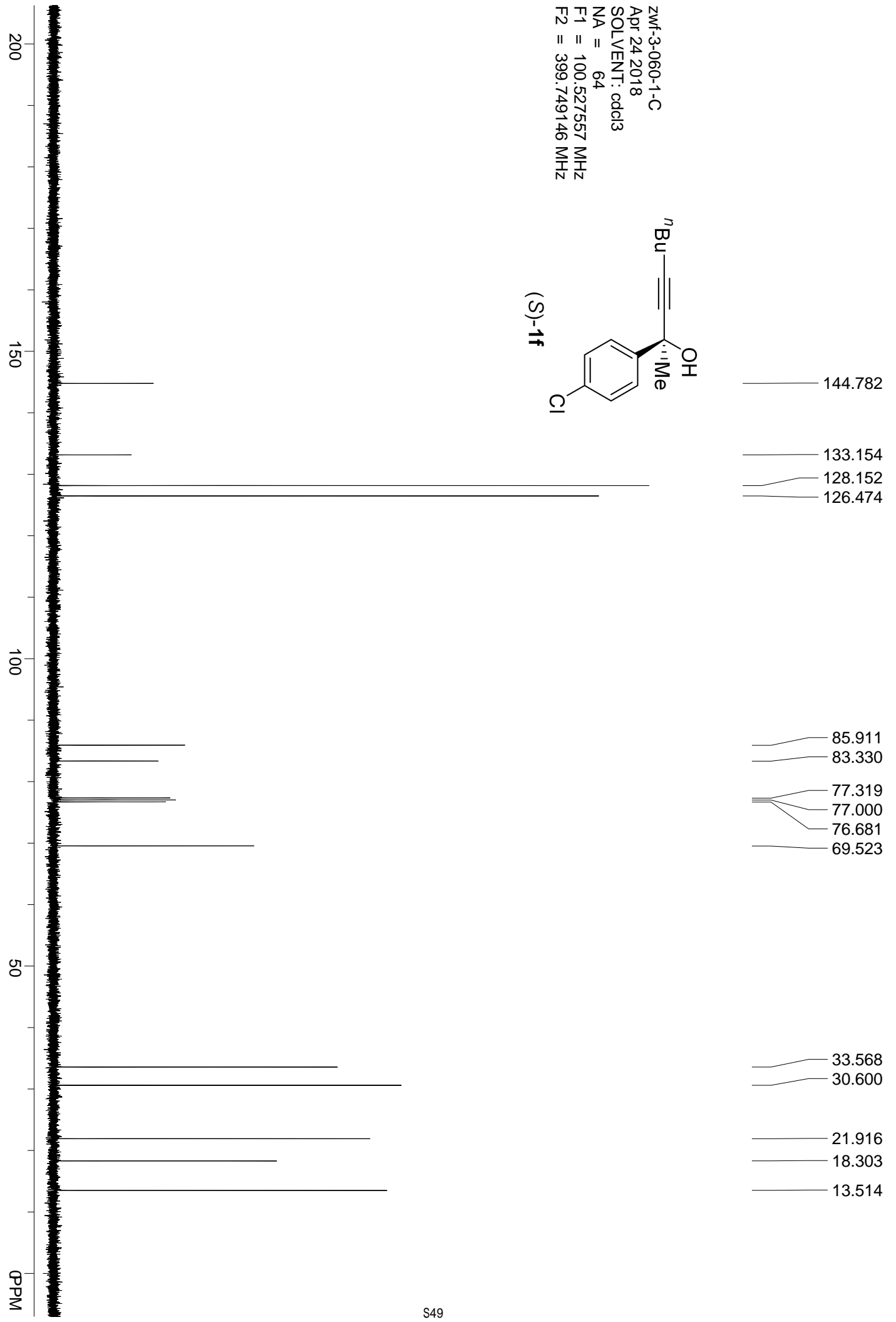
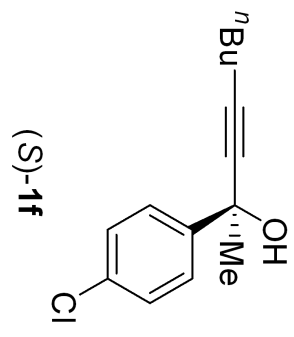
7.574
7.557
7.552
7.301
7.279

2.271
2.254
2.580
2.236
1.698
1.553
1.538
1.531
1.518
1.501
1.483
1.461
1.444
1.425
1.406
1.388
0.936
0.917
0.900
-0.000

zmf-3-060-1H
Apr 24 2018
SOLVENT: cdcl3
NA = 4
F1 = 399.749542 MHz
F2 = 100.526031 MHz



Zwf-3-060-1-C
Apr 24 2018
SOLVENT: cdcl3
NA = 64
F1 = 100.527557 MHz
F2 = 399.749146 MHz



zwf-3-060-1-AS-H-98-2-1.0-214

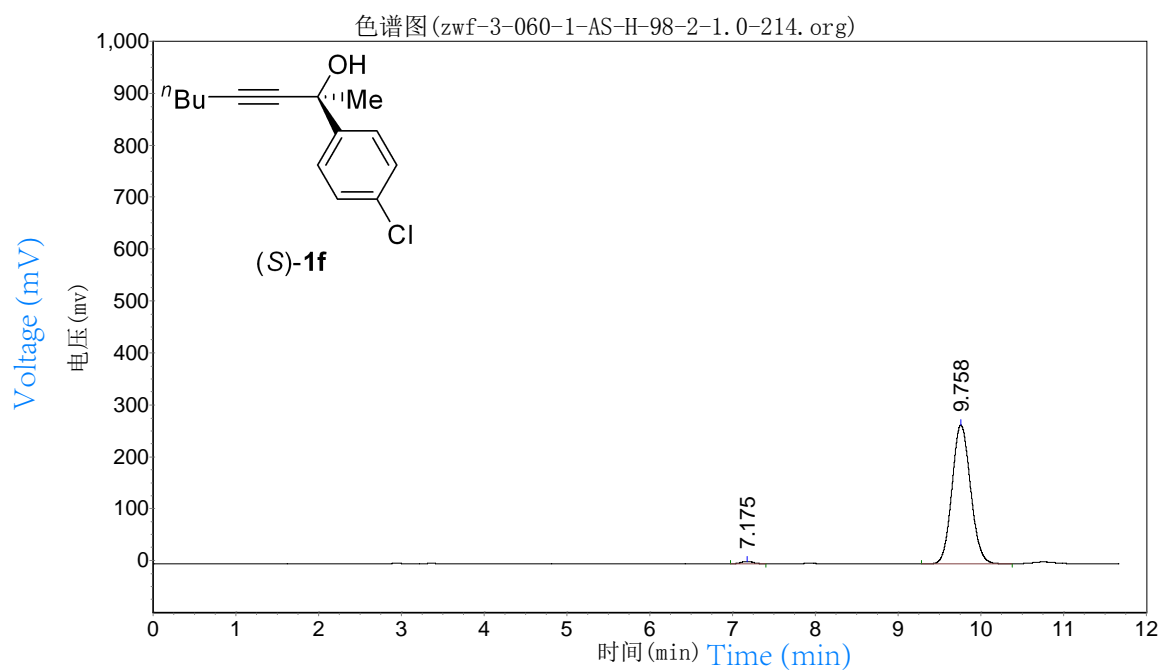
实验时间: 2018-04-24, 11:52:54

报告时间: 2018-04-24, 12:20:34

谱图文件: E:\data\zwf\zwf-3-060-1-AS-H-98-2-1.0-214.org

方法文件: E:\data\yaoyuan\0414.mtd

实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		7.175	4275.595	43203.250	1.0291
2		9.758	267504.875	4154805.000	98.9709
总计			271780.470	4198008.250	100.0000

zwf-3-060-1-rac-AS-H-98-2-1.0-214

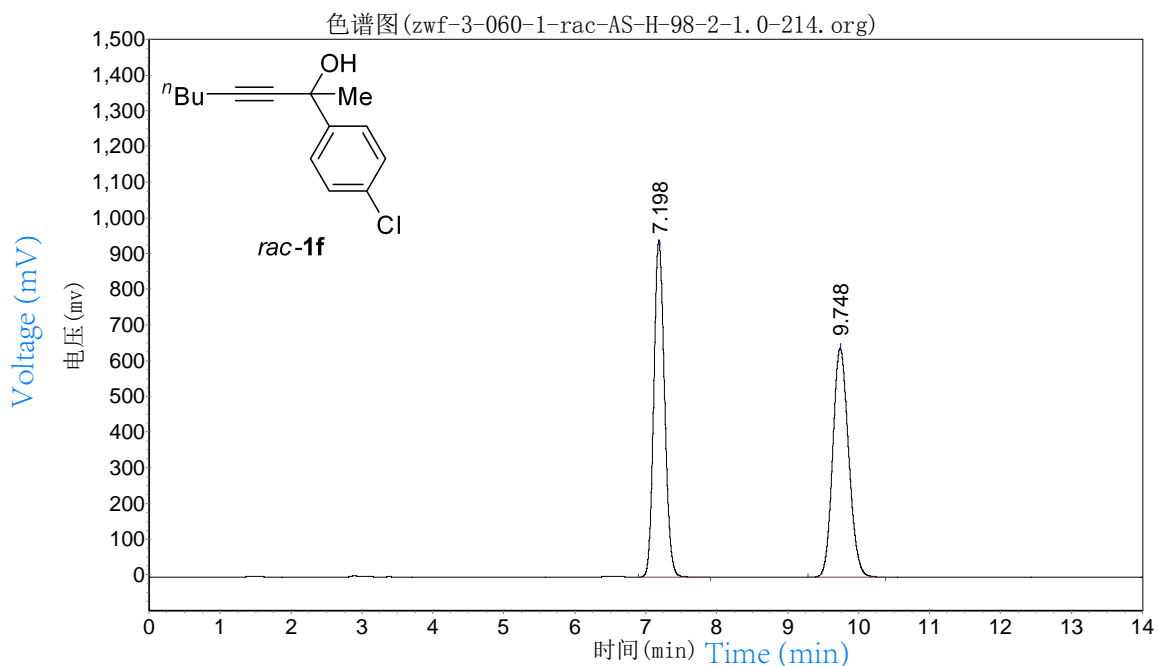
实验时间: 2018-04-24, 12:05:09

报告时间: 2018-04-24, 12:21:19

谱图文件: E:\data\zwf\zwf-3-060-1-rac-AS-H-98-2-1.0-214.org

方法文件: E:\data\yaoyuan\0414.mtd

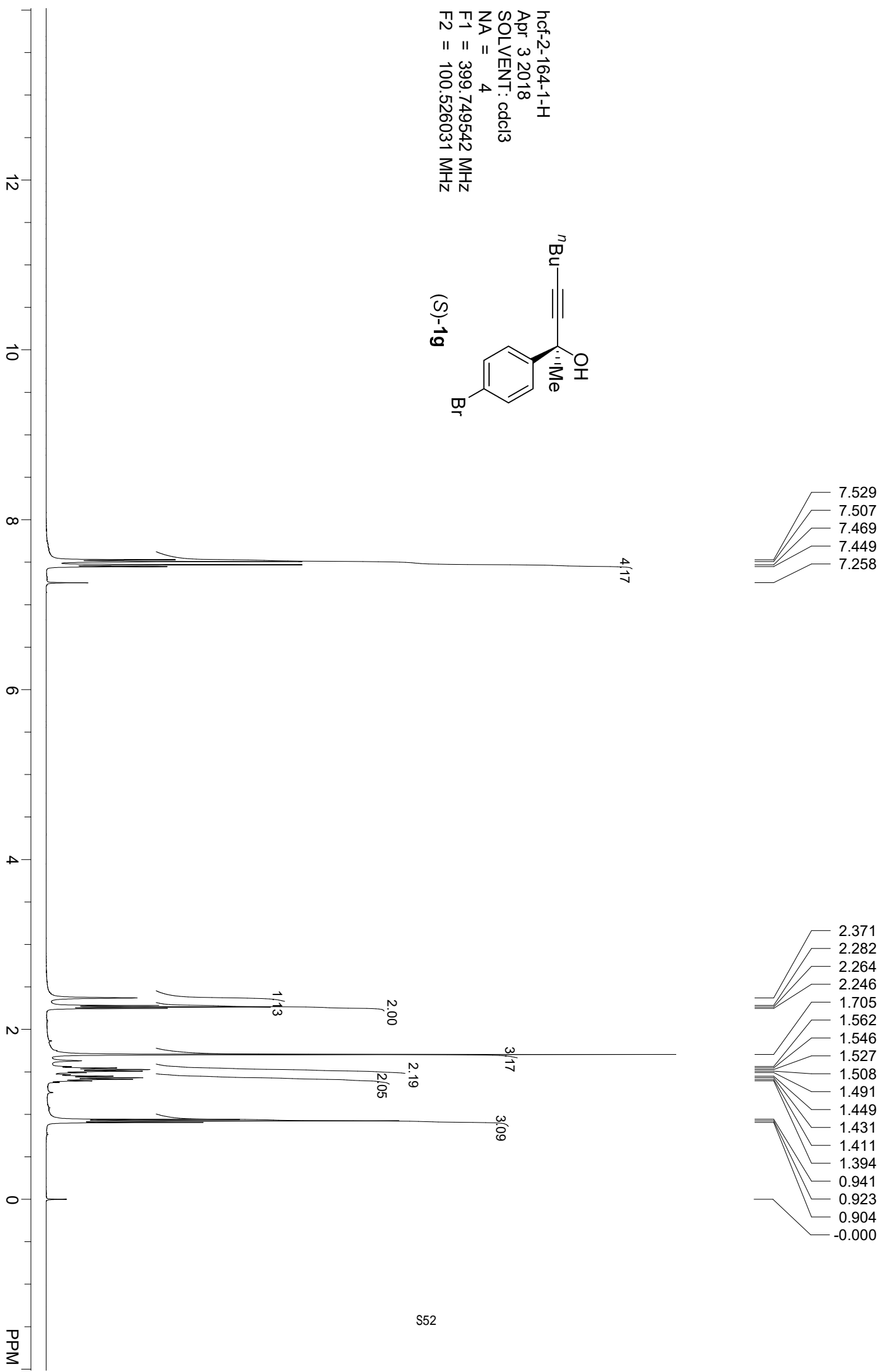
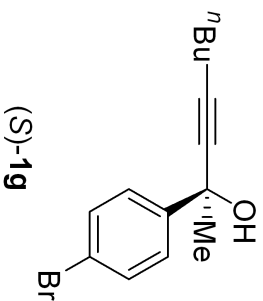
实验内容简介:



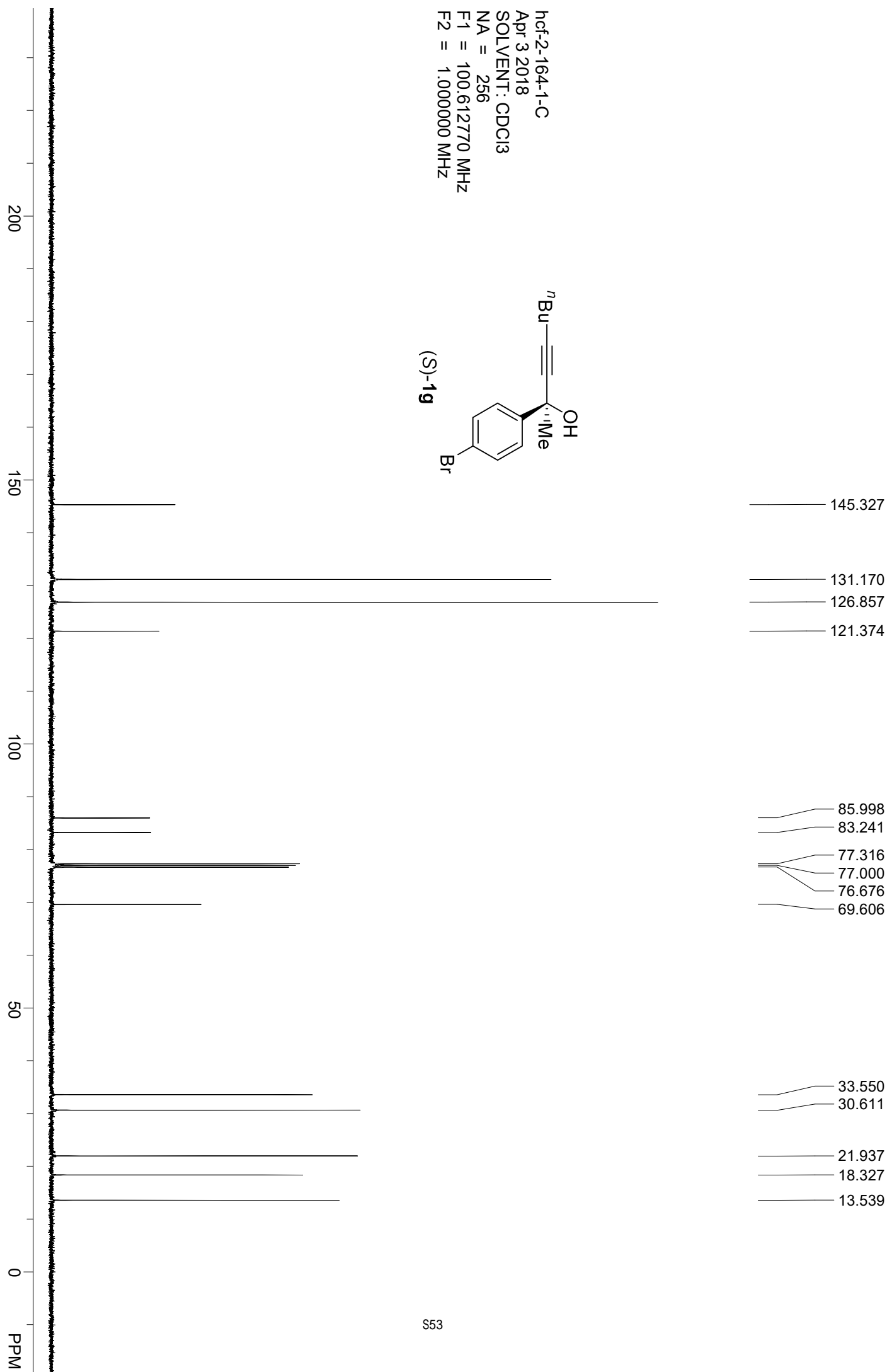
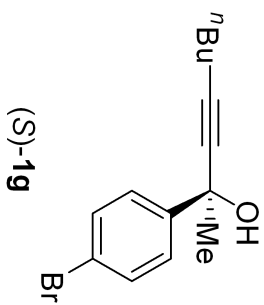
分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		7.198	937231.813	9895886.000	49.8592
2		9.748	639910.625	9951757.000	50.1408
总计			1577142.438	19847643.000	100.0000

hcf-2-164-1-H
Apr 3 2018
SOLVENT: cdcl3
NA = 4
F1 = 399.749542 MHz
F2 = 100.526031 MHz



hcf-2-164-1-C
Apr 3 2018
SOLVENT: CDCI3
NA = 256
F1 = 100.612770 MHz
F2 = 1.000000 MHz



hcf-2-164-1

实验时间: 2018-04-03, 13:50:12

报告时间: 2018-04-03, 14:10:49

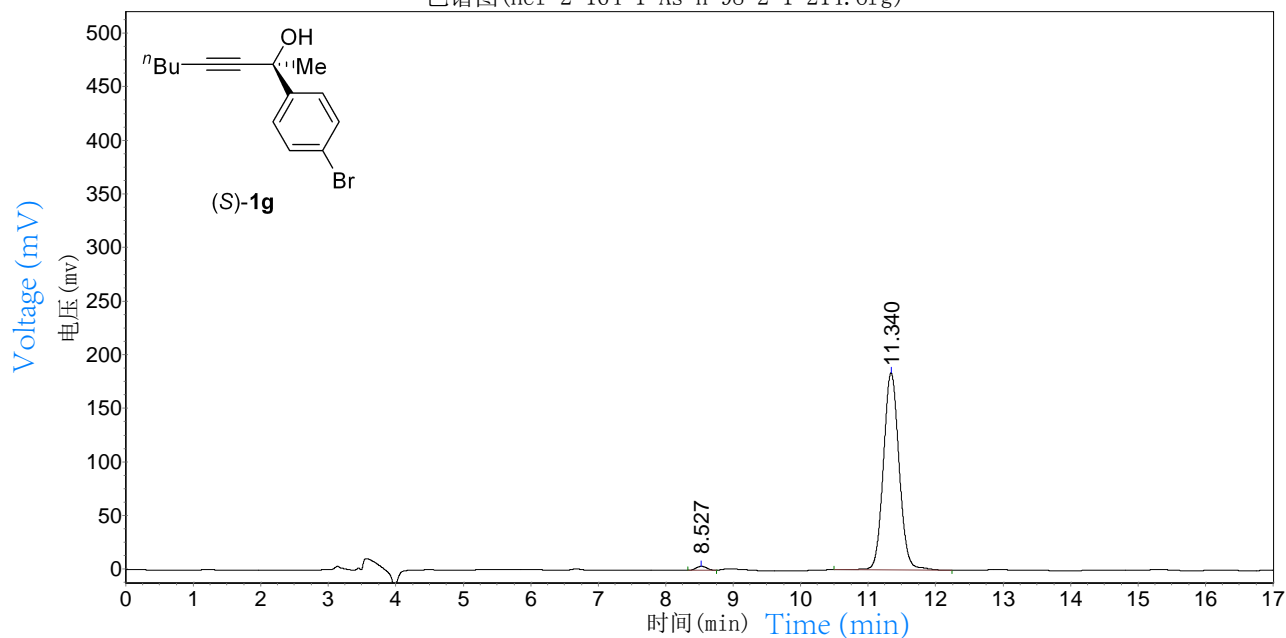
谱图文件: D:\HPLC\s1f\zwf-2018-04-02\hcf-2-164-1-As-h-98-2-1-214.org

实验内容简介:

As-h 98:2

214nm 1.0ml/min

色谱图 (hcf-2-164-1-As-h-98-2-1-214.org)



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		8.527	3716.220	39677.426	1.3138
2		11.340	183960.844	2980311.500	98.6862
总计			187677.063	3019988.926	100.0000

zwf-1-68

实验时间: 2018-04-03, 13:34:01

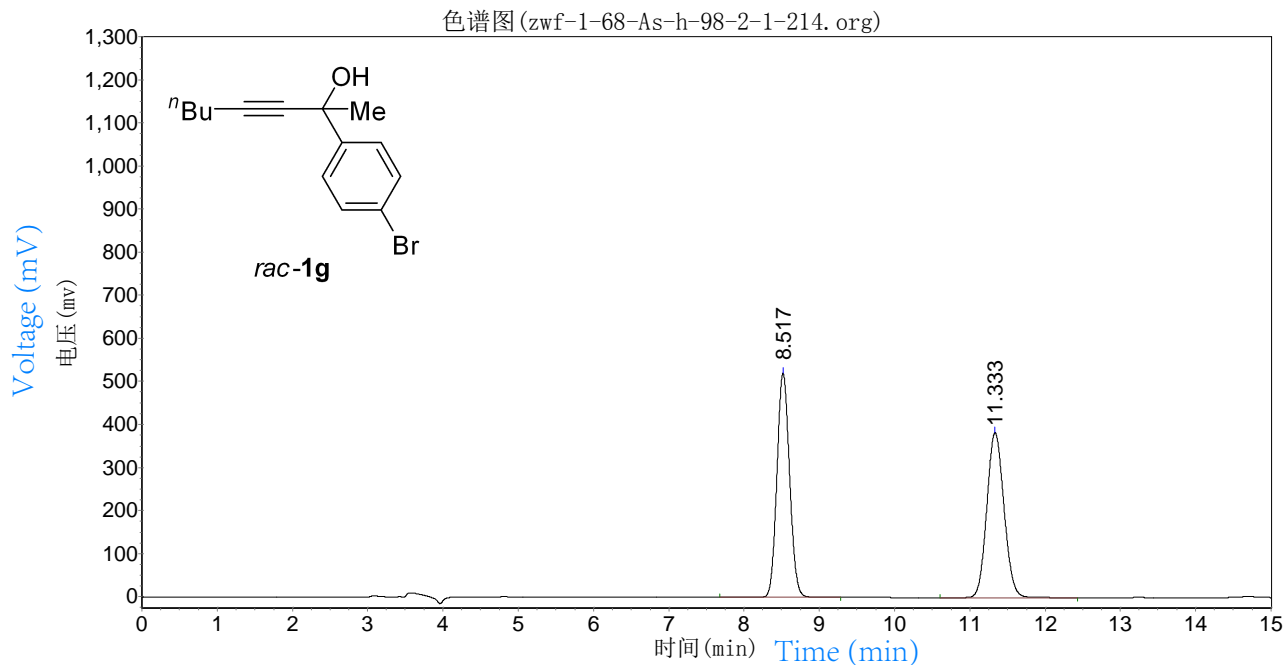
报告时间: 2018-04-03, 13:51:29

谱图文件: D:\HPLC\s1f\zwf-2018-04-02\zwf-1-68-As-h-98-2-1-214.org

实验内容简介:

As-h 98:2

214nm 1.0ml/min

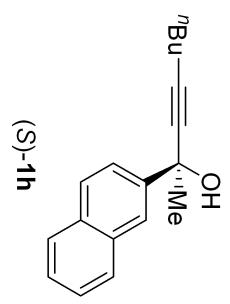


分析结果表

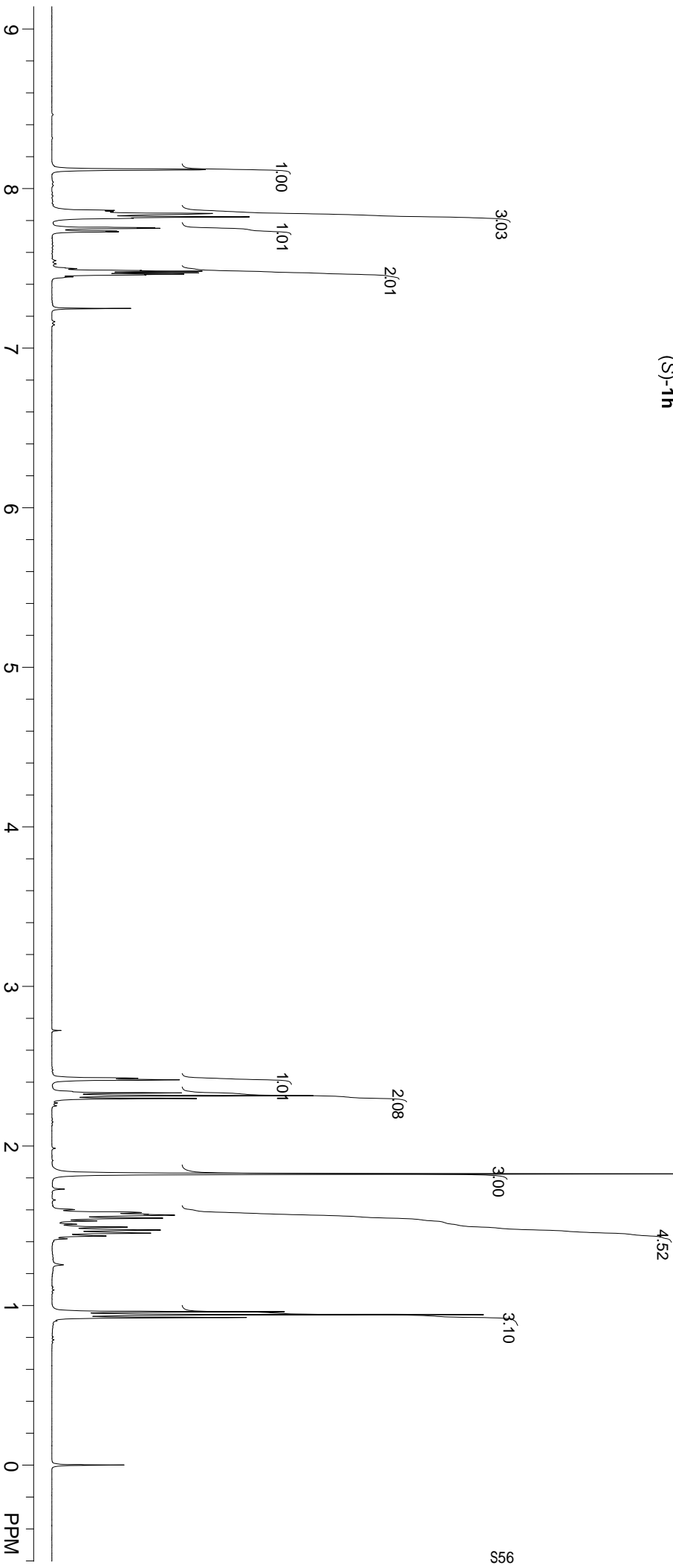
峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		8.517	521300.813	6087377.000	50.0528
2		11.333	383455.000	6074537.500	49.9472
总计			904755.813	12161914.500	100.0000

- 8.118
- 7.864
- 7.857
- 7.854
- 7.844
- 7.823
- 7.814
- 7.755
- 7.751
- 7.734
- 7.730
- 7.499
- 7.487
- 7.482
- 7.472
- 7.463
- 7.459
- 7.249

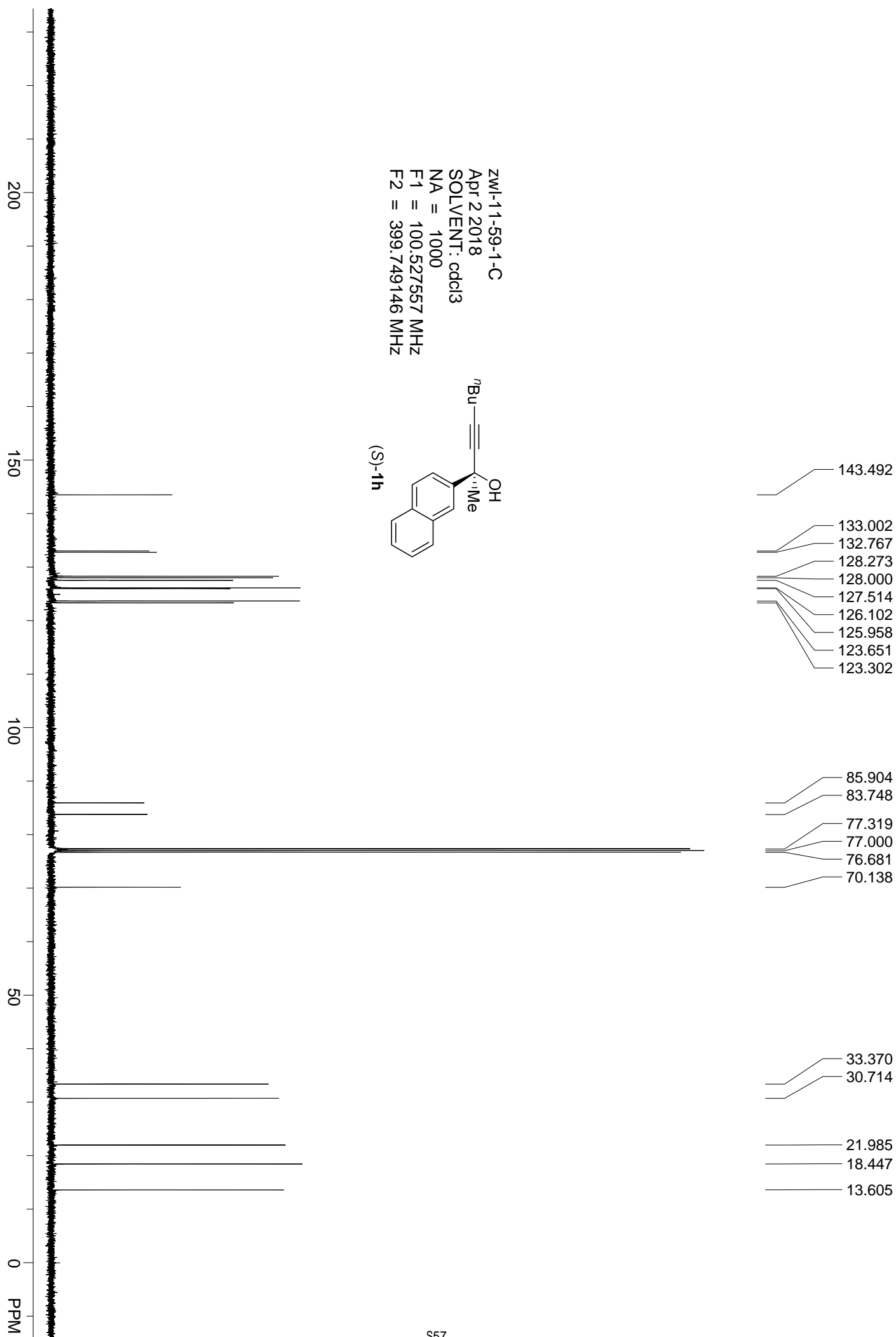
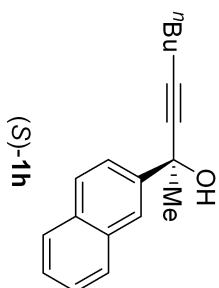
ZWI-11-59-1-H
 Apr 2 2018
 SOLVENT: cdcl3
 NA = 8
 F1 = 399.749542 MHz
 F2 = 100.526031 MHz



- 2.425
- 2.415
- 2.332
- 2.315
- 2.297
- 1.825
- 1.583
- 1.573
- 1.566
- 1.547
- 1.530
- 1.509
- 1.492
- 1.473
- 1.454
- 1.436
- 0.961
- 0.943
- 0.925
- 0.000



zwl-11-59-1-C
Apr 2 2018
SOLVENT: cdcl3
NA = 1000
F1 = 100.527557 MHZ
F2 = 399.749146 MHZ

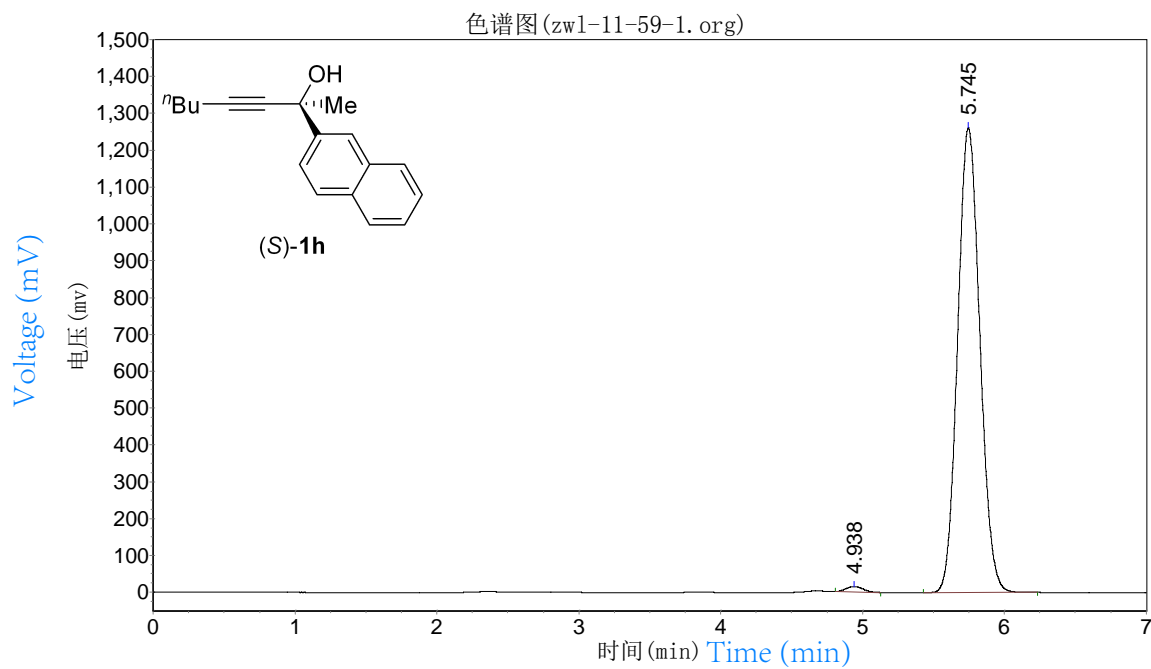


zw1-11-59-1-AS-H-95-5-1.3-214

实验时间: 2018-04-06, 16:58:27
谱图文件: E:\data\zwf\zw1-11-59-1.org

报告时间: 2018-04-06, 17:07:48

实验内容简介:



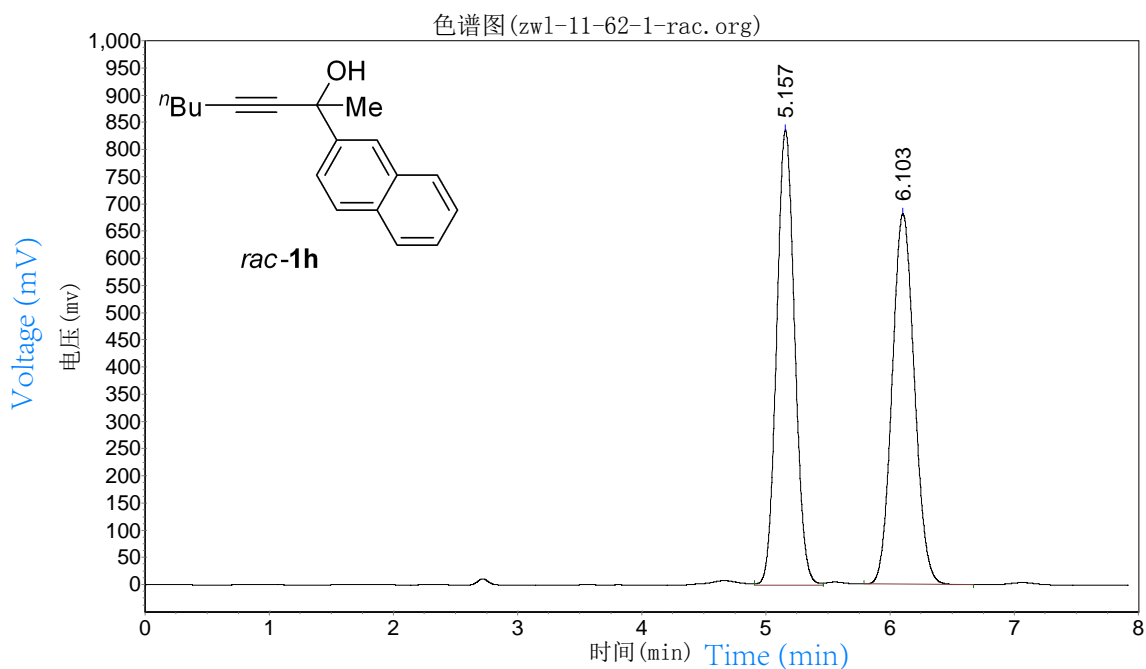
分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		4.938	14837.720	122513.195	0.8860
2		5.745	1260740.625	13704575.000	99.1140
总计			1275578.345	13827088.195	100.0000

zw1-11-62-1-rac-AS-H-95-5-1.3-214

实验时间: 2018-04-13, 13:24:34
谱图文件: E:\data\zwf\zw1-11-62-1-rac.org

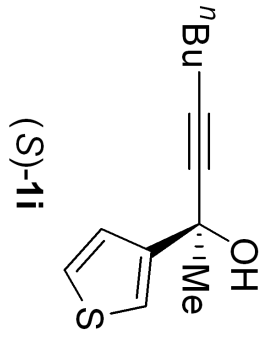
实验者:
报告时间: 2018-04-13, 14:16:18
积分方法: 面积归一法



分析结果表

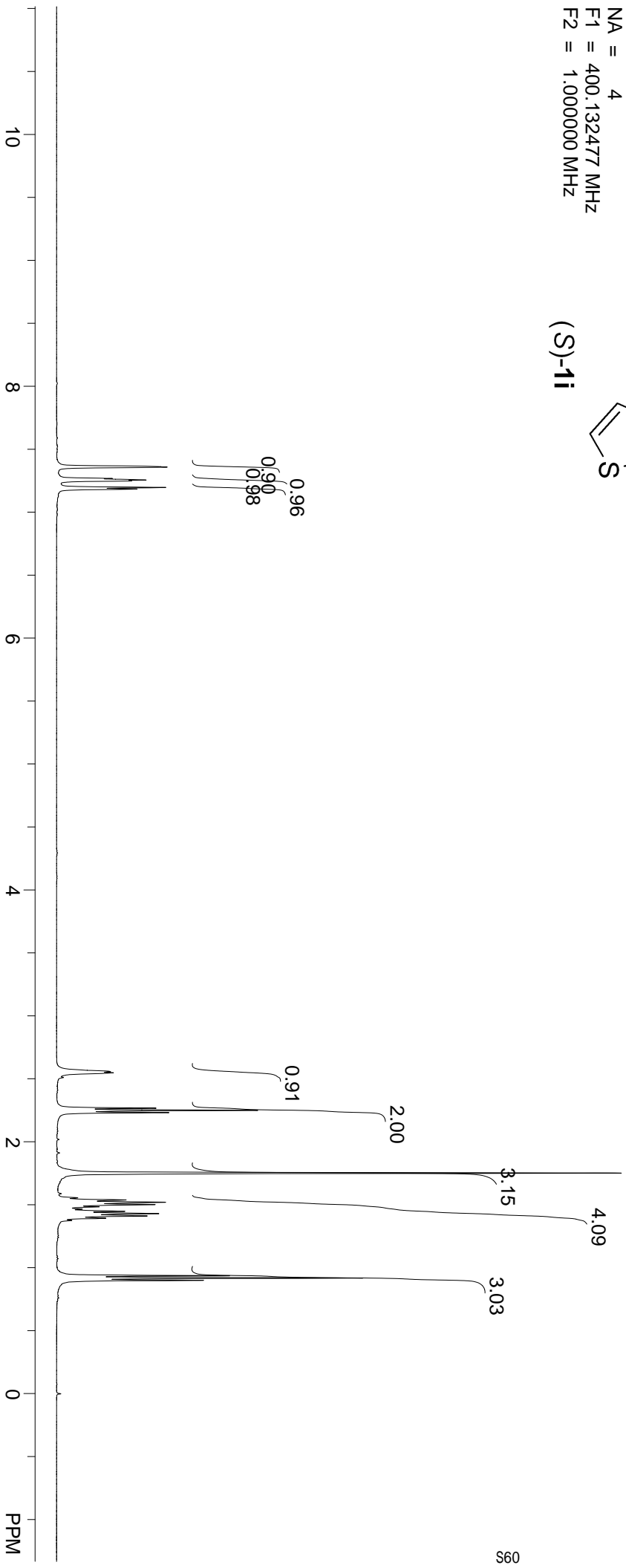
峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		5.157	836917.063	8474005.000	50.0051
2		6.103	681487.188	8472274.000	49.9949
总计			1518404.250	16946279.000	100.0000

zwf-5-025-1
Dec 14 2018
SOLVENT: CDCI3
NA = 4
F1 = 400.132477 MHz
F2 = 1.000000 MHz

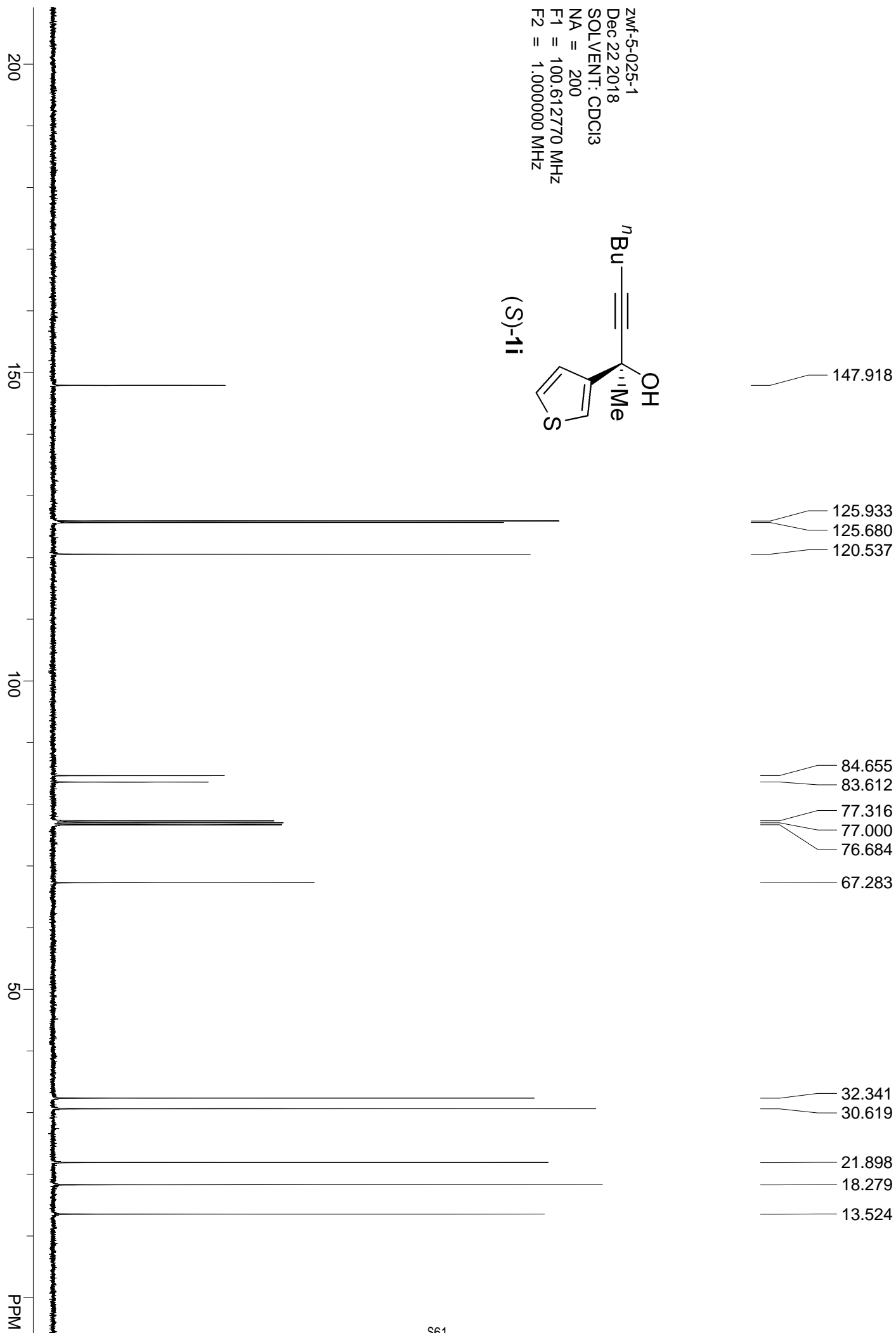
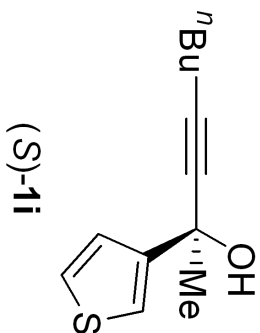


- 7.361
- 7.358
- 7.267
- 7.255
- 7.248
- 7.196
- 7.183

- 2.267
- 2.250
- 2.558
- 2.233
- 1.752
- 1.556
- 1.539
- 1.521
- 1.502
- 1.484
- 1.466
- 1.448
- 1.430
- 1.412
- 1.393
- 0.936
- 0.919
- 0.901
- 0.000



Zwf-5-025-1
Dec 22 2018
SOLVENT: CDCl3
NA = 200
F1 = 100.612770 MHz
F2 = 1.000000 MHz



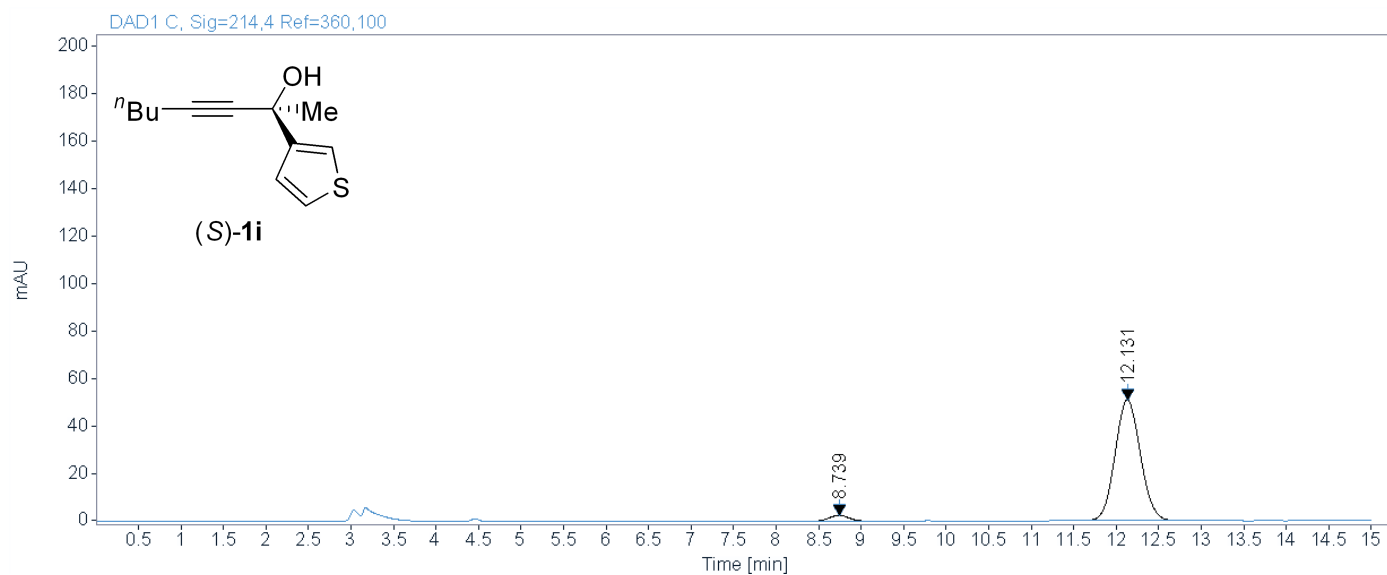
Area Percent Report



Agilent Technologies

Sample name: zwf-5-025-1-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\zwf-allenioc acid_LC 2018-12-22 17-24-32\003-P1-C1-zwf-5-025-1.D



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
8.739	0.2567	2.4698	40.7896	3.7103
12.131	0.3227	50.8951	1058.5587	96.2897
Sum			1099.3483	100.0000

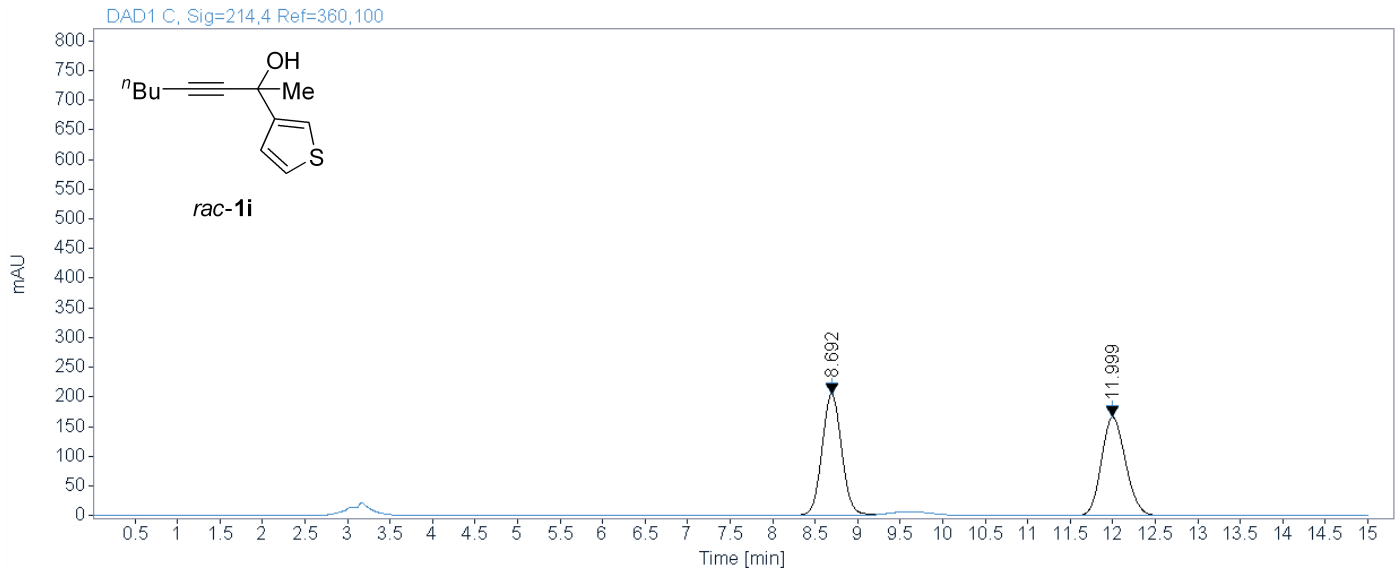
Area Percent Report



Agilent Technologies

Sample name: zwf-5-025-1-rac-AS-H-98-2-1.0-214

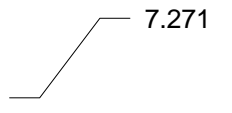
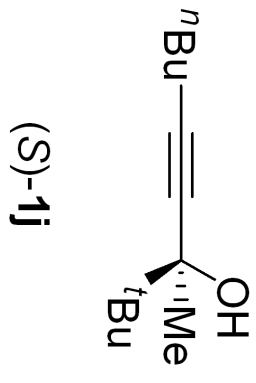
Data file: C:\Users\Public\Documents\ChemStation\1\Data\zwf-allenioc acid_LC 2018-12-22 17-24-32\004-P1-C2-zwf-5-025-1-rac.D



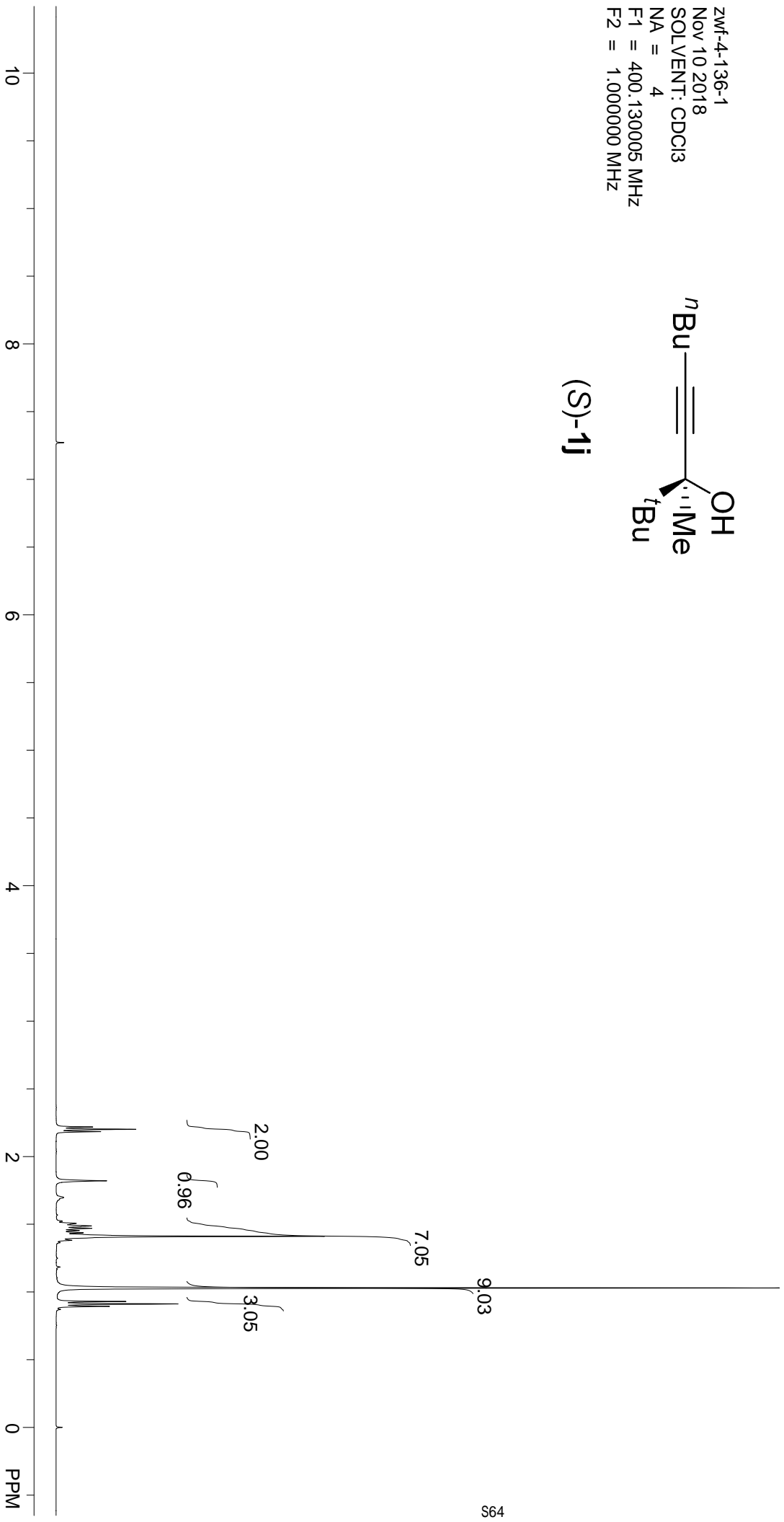
Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
8.692	0.2707	205.2032	3332.5664	50.3005
11.999	0.3091	166.2543	3292.7439	49.6995
Sum			6625.3103	100.0000

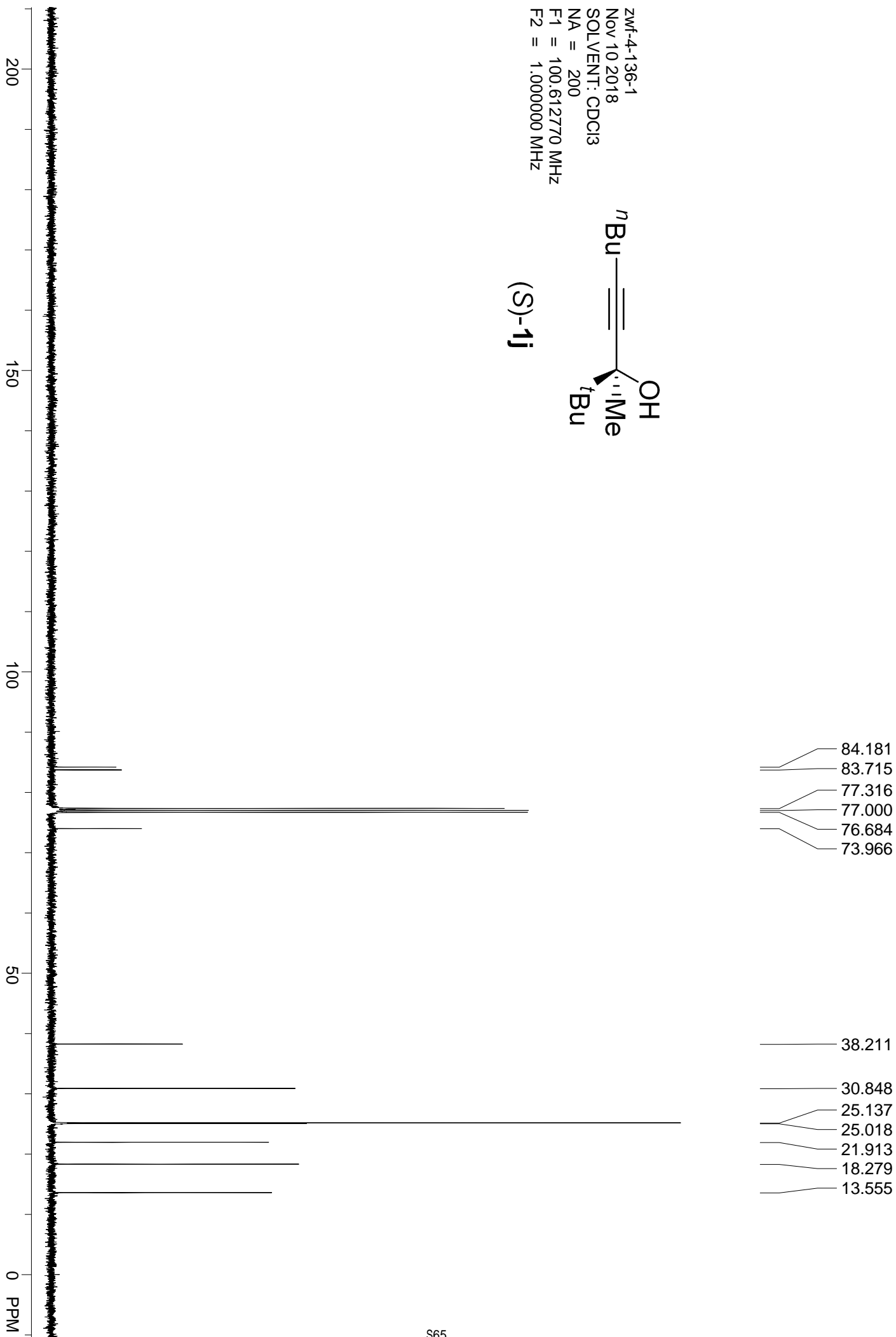
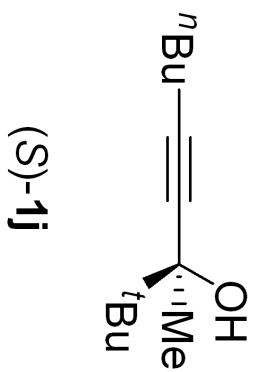
Zwf-4-136-1
Nov 10 2018
SOLVENT: CDCl3
NA = 4
F1 = 400.130005 MHz
F2 = 1.000000 MHz



- 2.219
- 2.203
- 2.185
- 1.822
- 1.508
- 1.488
- 1.471
- 1.454
- 1.437
- 1.412
- 1.382
- 1.030
- 0.930
- 0.912
- 0.894
- 0.000



Zwf-4-136-1
Nov 10 2018
SOLVENT: CDCl3
NA = 200
F1 = 100.612770 MHz
F2 = 1.000000 MHz



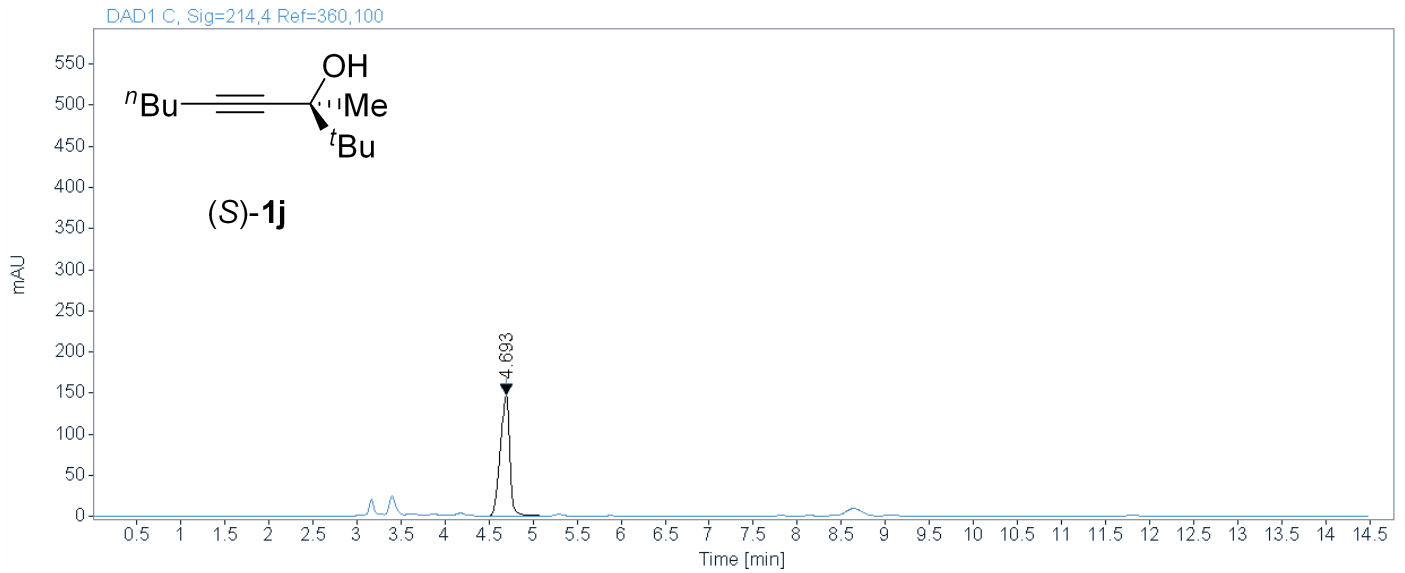
Area Percent Report



Agilent Technologies

Sample name: zwf-4-136-1-IC-98-1.0-214

Data file: C:\USERS\PUBLIC\DOCUMENTS\CHEMSTATION\1\DATA\ZWF\zwf-4-136-1-IC-98-2-1.0-214.D



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
4.693	0.1245	148.0412	1106.2639	100.0000
Sum			1106.2639	100.0000

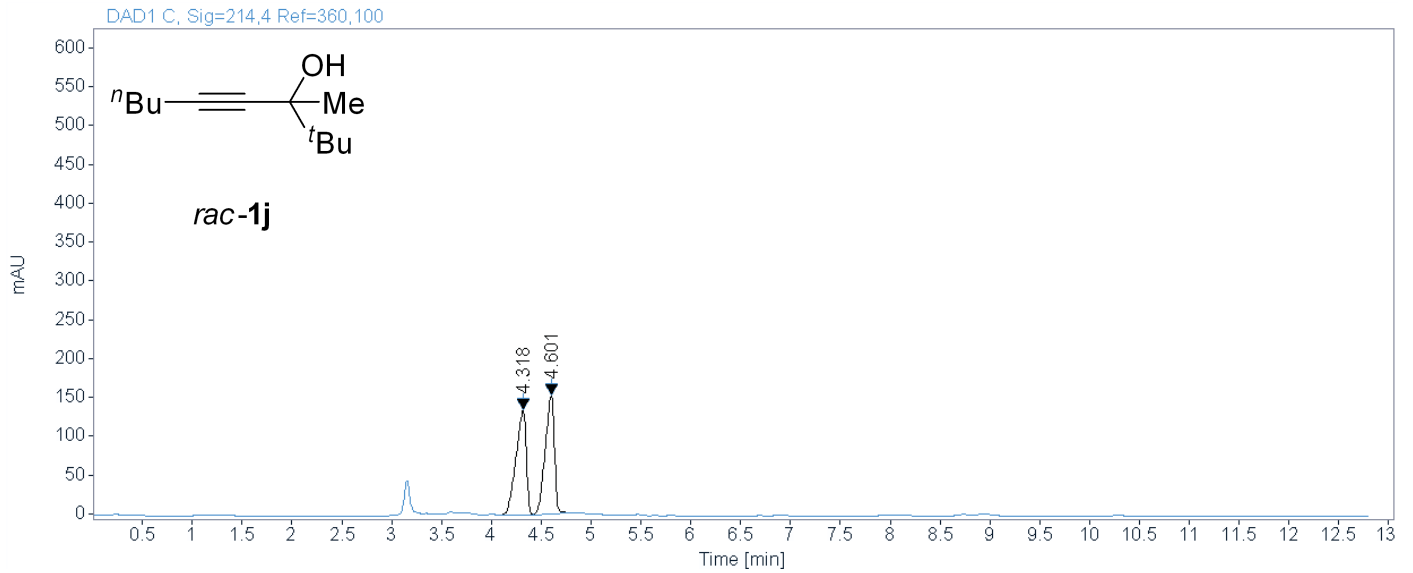
Area Percent Report



Agilent Technologies

Sample name: zwf-4-136-1-rac-IC-98-1.0-214

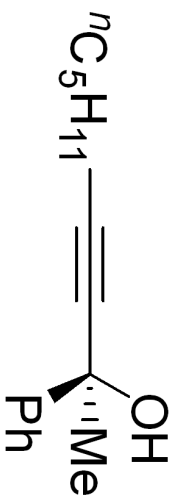
Data file: C:\USERS\PUBLIC\DOCUMENTS\CHEMSTATION\1\DATA\ZWF\zwf-4-136-1-rac-IC-98-2-1.0-214.D



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
4.318	0.1202	136.0092	980.8727	49.7126
4.601	0.1072	154.2787	992.2144	50.2874
Sum			1973.0872	100.0000

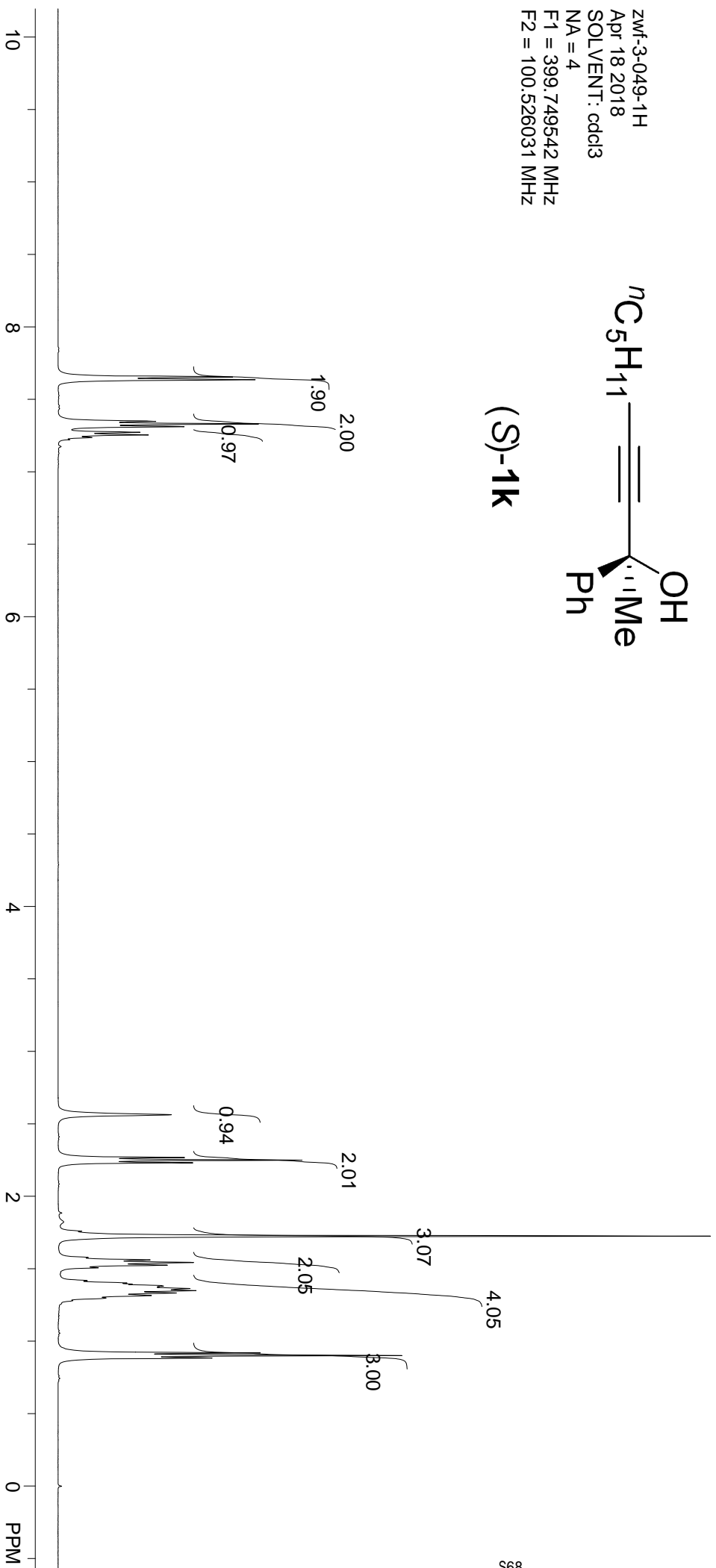
zwf-3-049-1H
Apr 18 2018
SOLVENT: cdcl3
NA = 4
F1 = 399.749542 MHz
F2 = 100.526031 MHz



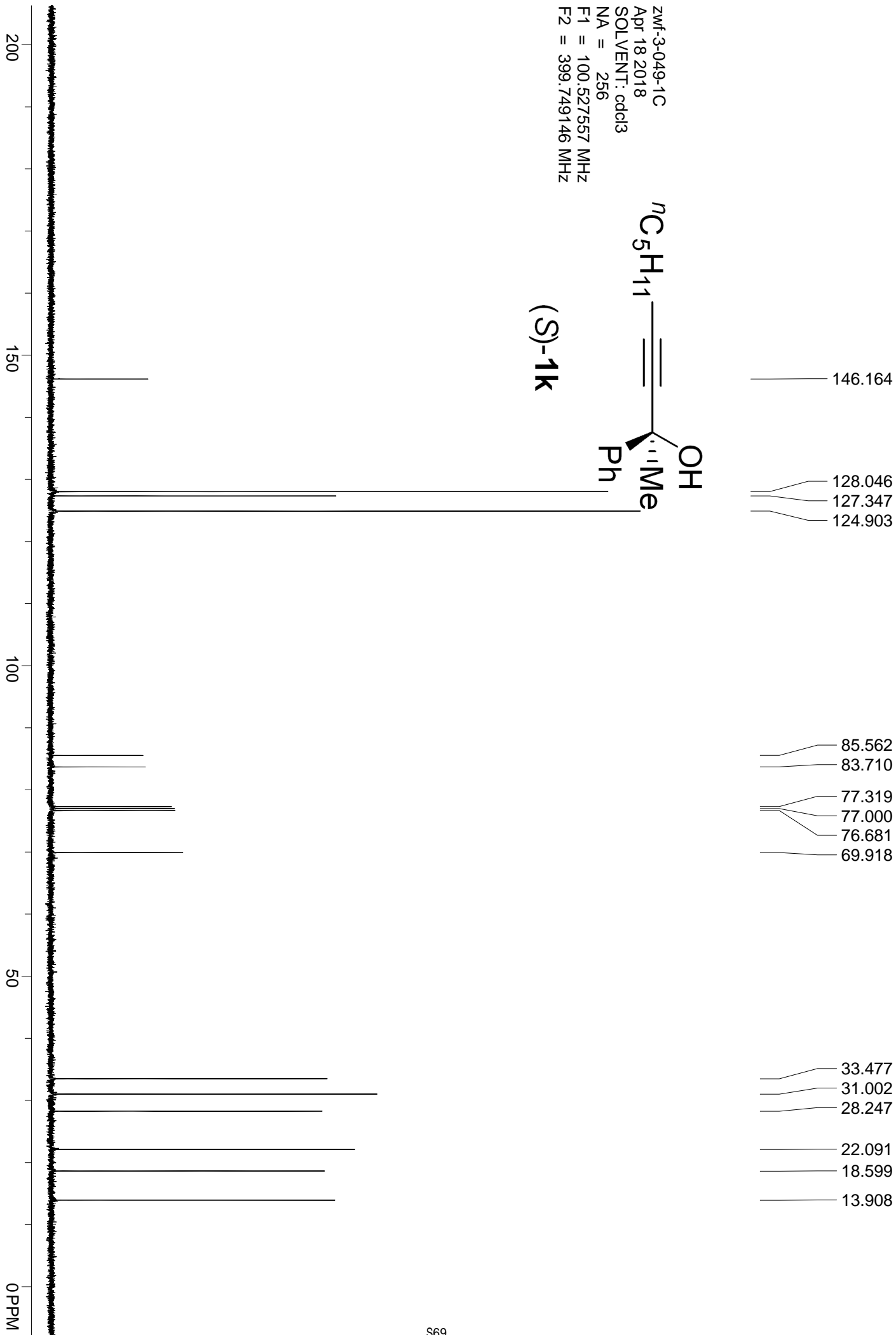
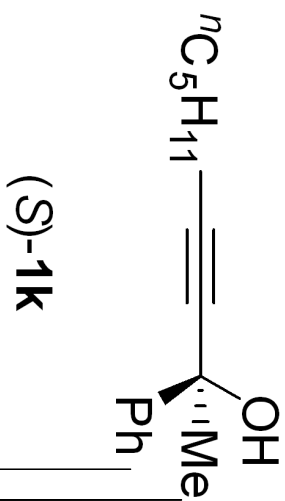
(S)-1k

7.653
7.636
7.348
7.330
7.312
7.273
7.254
7.236

2.267
2.249
2.232
2.563
1.726
1.578
1.561
1.544
1.525
1.507
1.417
1.402
1.380
1.363
1.350
1.333
1.316
1.298
0.919
0.901
0.884
0.000



zwf-3-049-1C
Apr 18 2018
SOLVENT: cdcl3
NA = 256
F1 = 100.527557 MHz
F2 = 399.749146 MHz

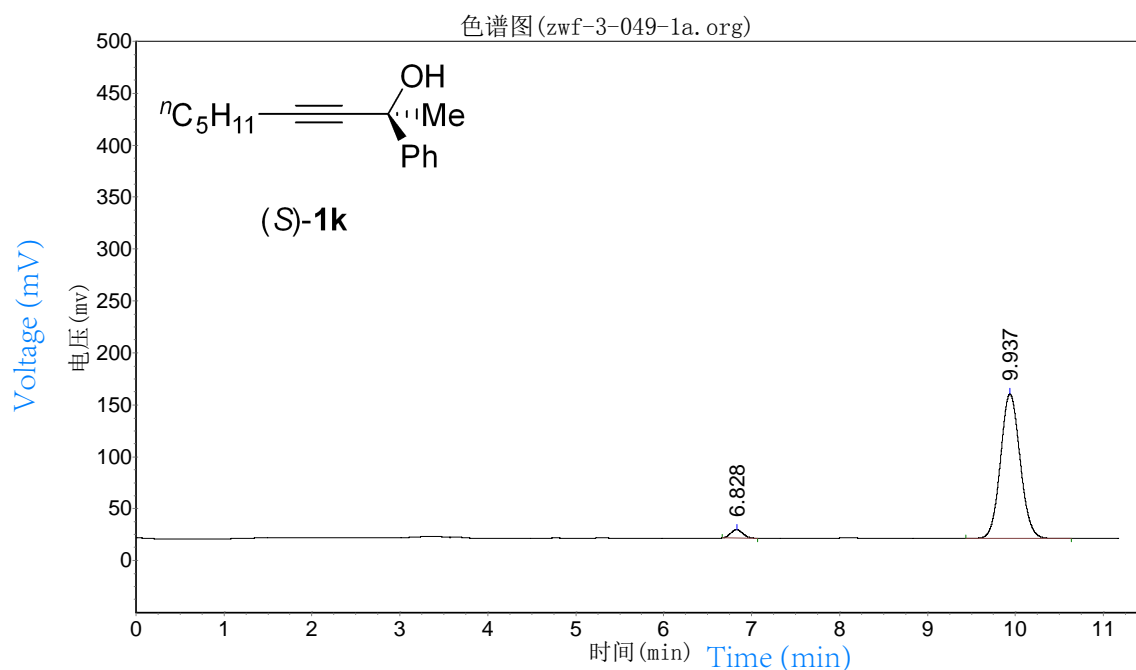


zwf-3-049-1-AS-H-98-2-1.0-214

实验时间: 2018-04-18, 21:26:05
谱图文件: E:\data\zwf\zwf-3-049-1a.org
方法文件: E:\data\yaoyuan\0414.mtd

报告时间: 2018-04-18, 21:41:17

实验内容简介:



分析结果表

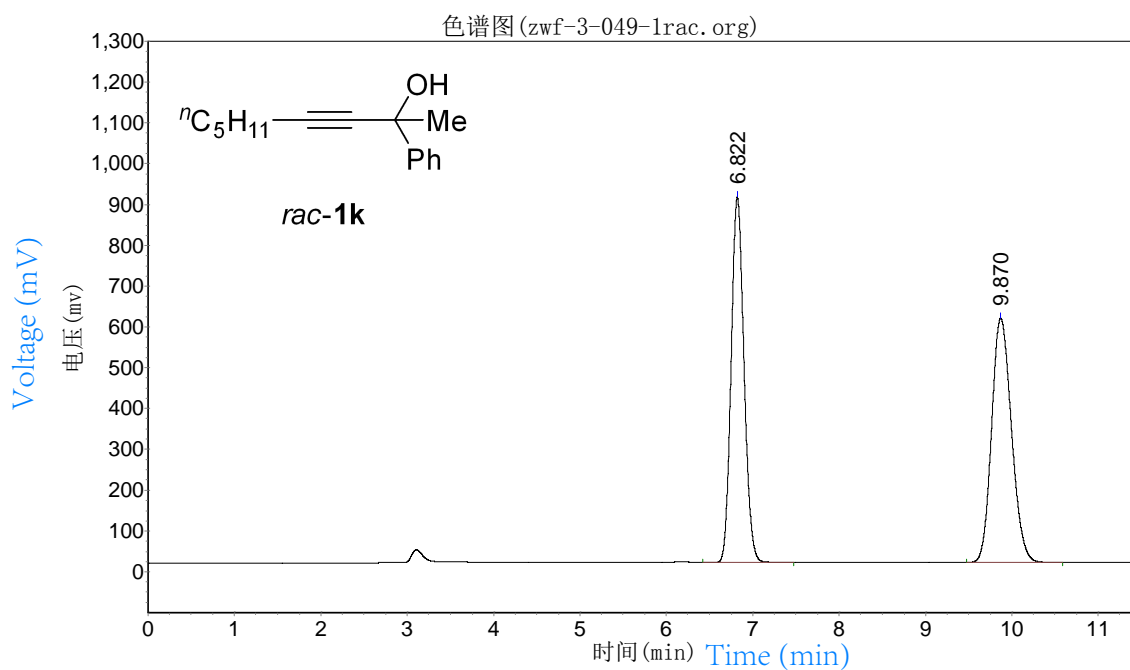
峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		6.828	8095.054	78488.320	3.5182
2		9.937	139246.141	2152453.750	96.4818
总计			147341.194	2230942.070	100.0000

zwf-3-049-1rac-AS-H-98-2-1.0-214

实验时间: 2018-04-18, 21:13:09
谱图文件: E:\data\zwf\zwf-3-049-1rac.org
方法文件: E:\data\yaoyuan\0414.mtd

报告时间: 2018-04-18, 21:27:31

实验内容简介:



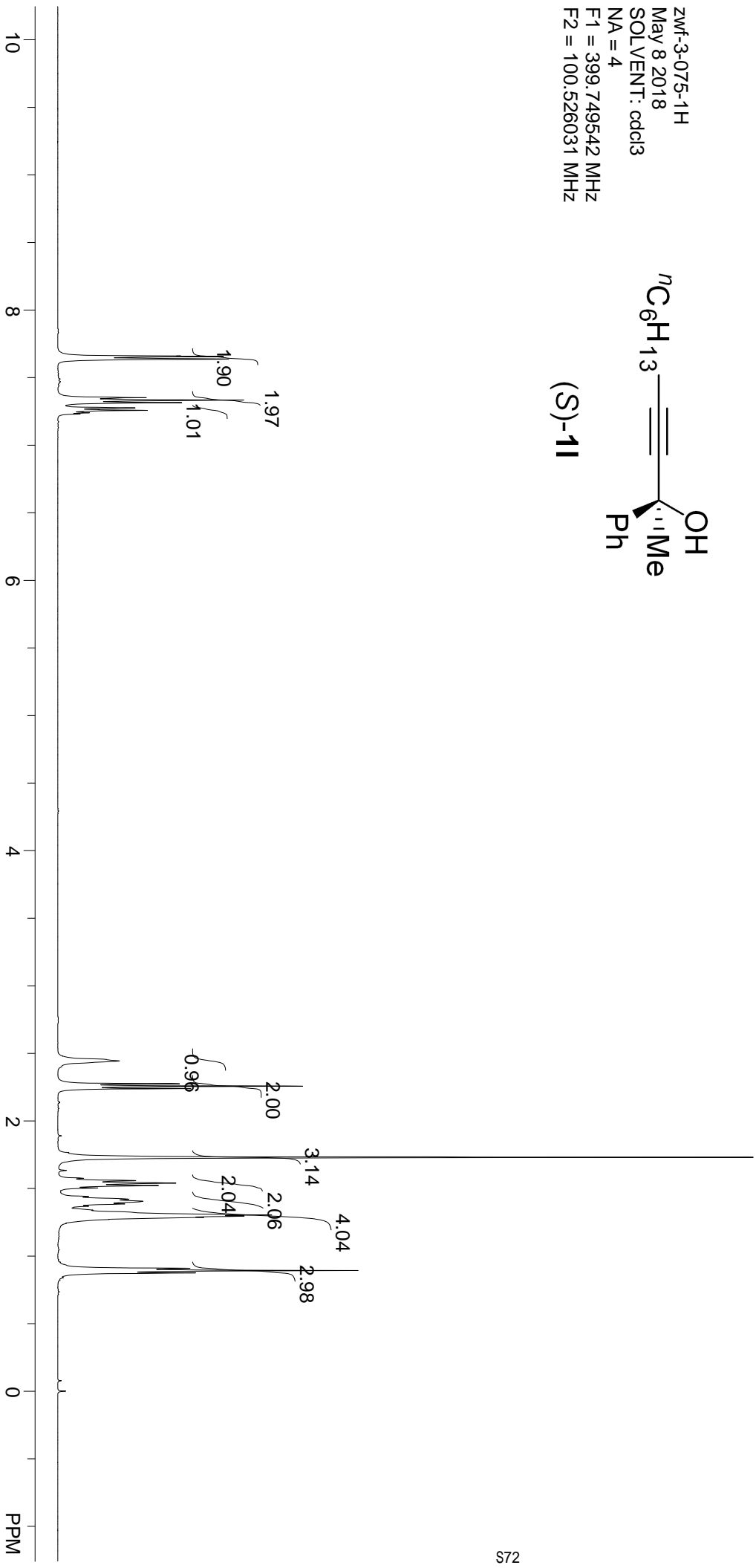
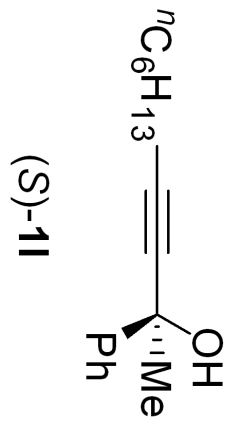
分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		6.822	896229.875	9276932.000	49.2526
2		9.870	598705.750	9558496.000	50.7474
总计			1494935.625	18835428.000	100.0000

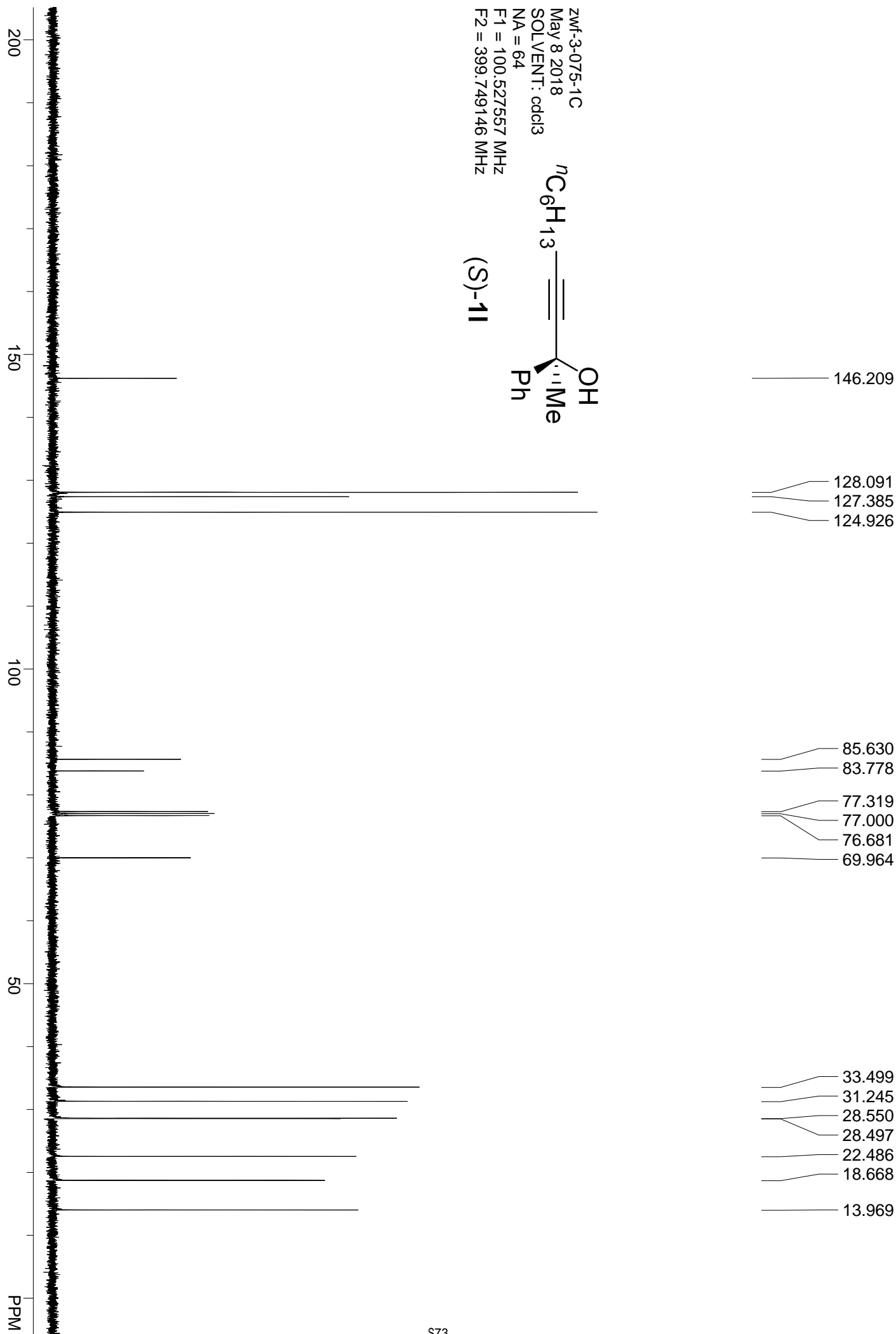
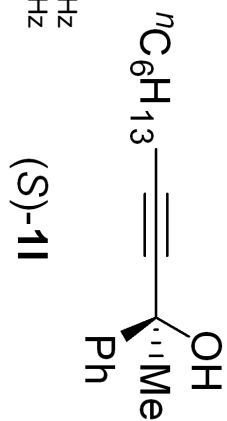
7.656
7.638
7.352
7.334
7.315
7.277
7.258
7.240
7.231

2.275
2.257
2.240
2.444
1.731
1.575
1.558
1.540
1.521
1.504
1.441
1.420
1.406
1.386
1.368
1.304
1.296
1.286
0.908
0.893
0.875
0.000

zwf-3-075-1H
May 8 2018
SOLVENT: cdcl3
NA = 4
F1 = 399.749542 MHz
F2 = 100.526031 MHz



zwtf-3-075-1C
May 8 2018
SOLVENT: cdcl3
NA = 64
F1 = 100.527557 MHz
F2 = 399.749146 MHz



zwf-3-075-1-AS-H-98-2-1.0-214

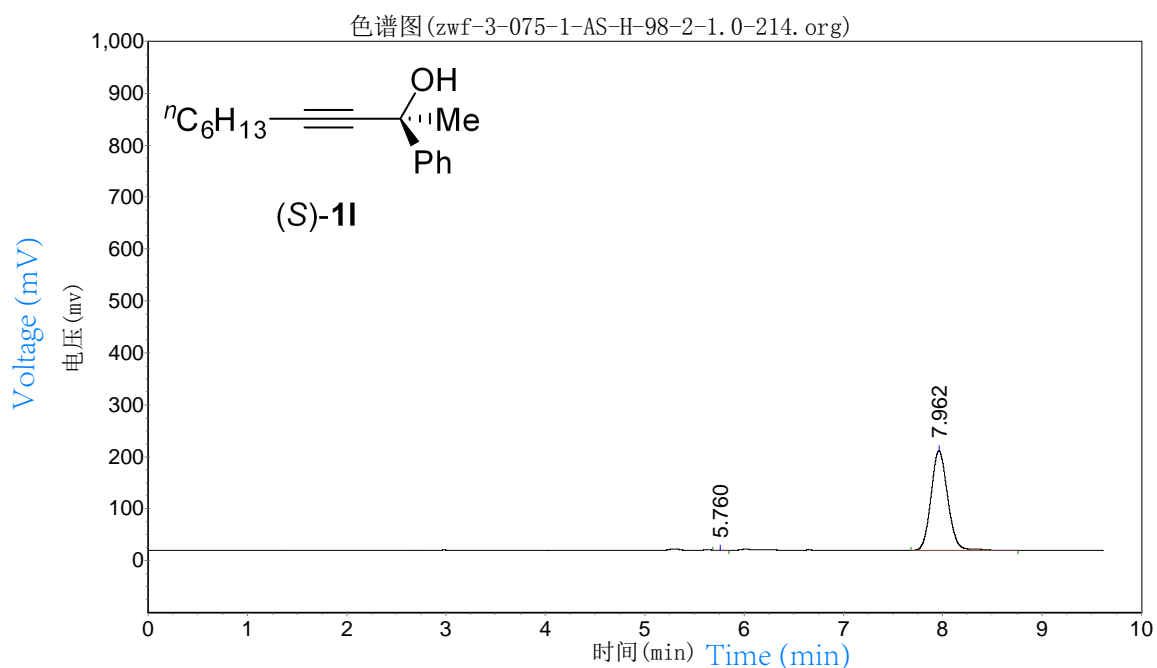
实验时间: 2018-05-08, 17:14:32

报告时间: 2018-05-08, 17:27:48

谱图文件: E:\data\zwf\zwf-3-075-1-AS-H-98-2-1.0-214.org

方法文件: E:\data\yaoyuan\0414.mtd

实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		5.760	283.889	1292.553	0.0575
2		7.962	191921.219	2248376.250	99.9425
总计			192205.108	2249668.803	100.0000

zwf-3-075-1-rac-AS-H-98-2-1.0-214

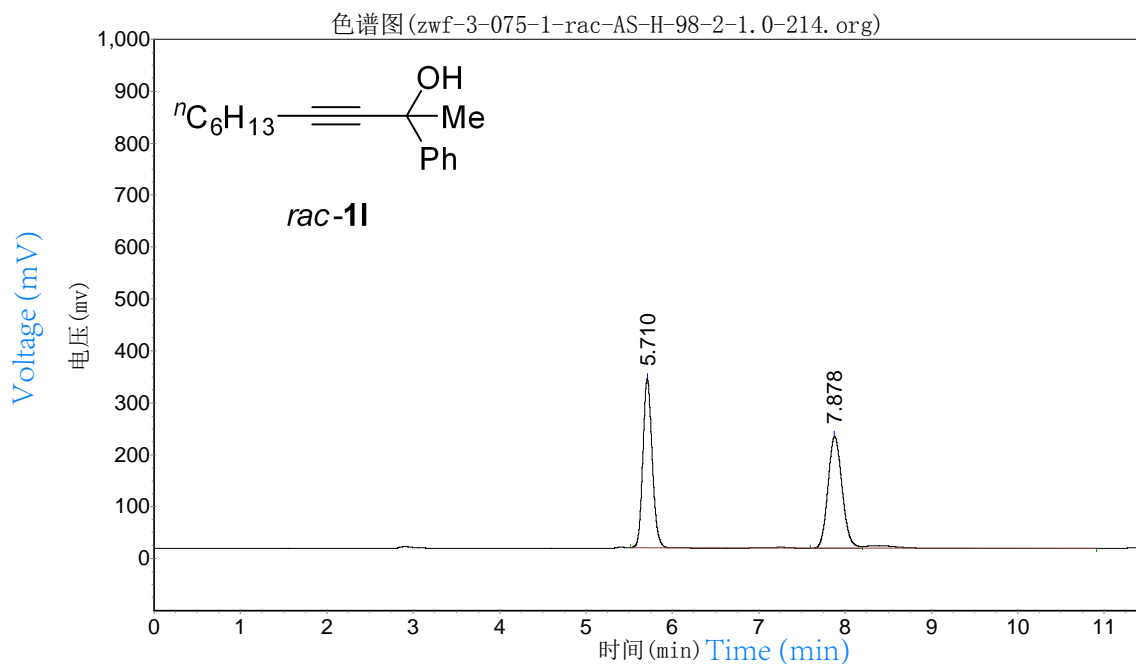
实验时间: 2018-05-08, 16:55:49

报告时间: 2018-05-08, 17:17:31

谱图文件: E:\data\zwf\zwf-3-075-1-rac-AS-H-98-2-1.0-214.org

方法文件: E:\data\yaoyuan\0414.mtd

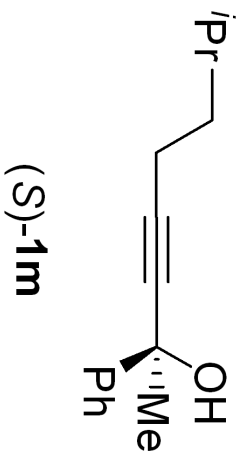
实验内容简介:



分析结果表

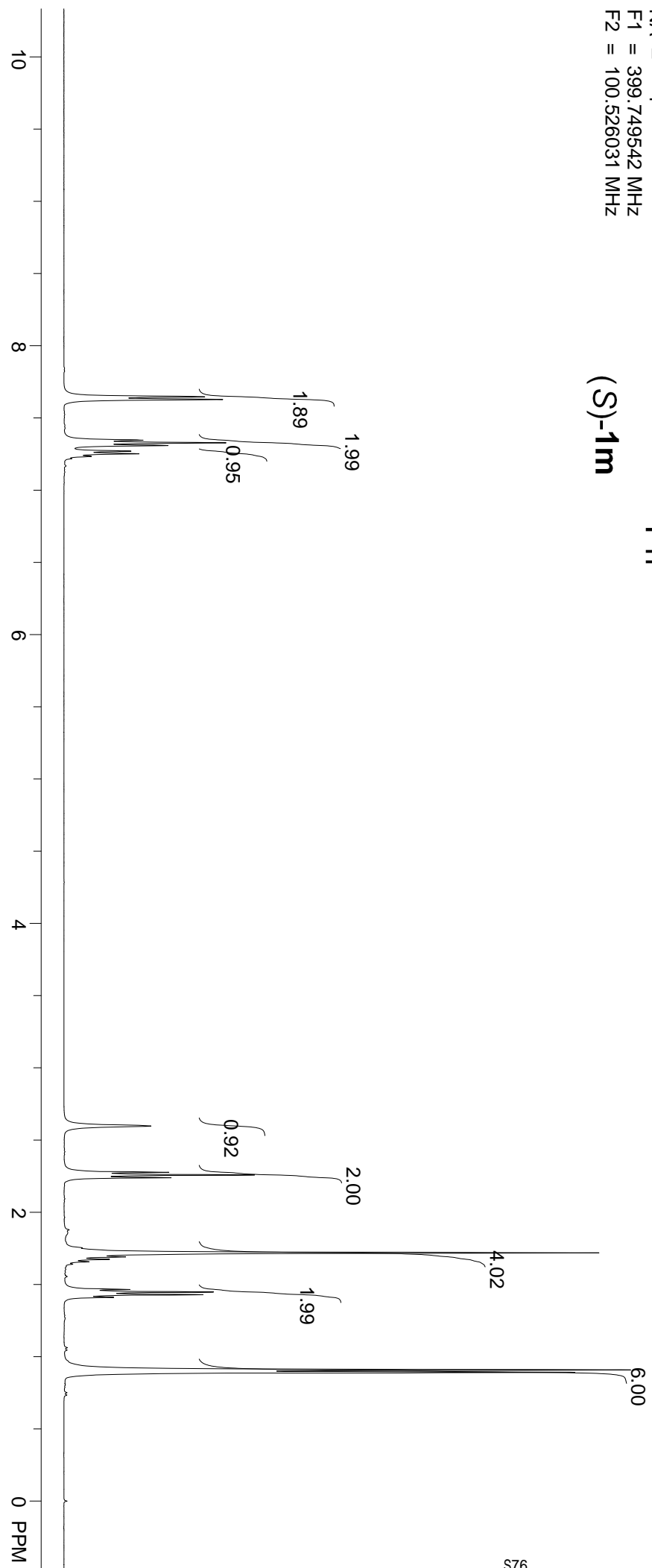
峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		5.710	325666.500	2562523.250	50.8096
2		7.878	215890.078	2480862.250	49.1904
总计			541556.578	5043385.500	100.0000

ZWF-3-057-1H
Apr 24 2018
SOLVENT: cdcl3
NA = 4
F1 = 399.749542 MHz
F2 = 100.526031 MHz

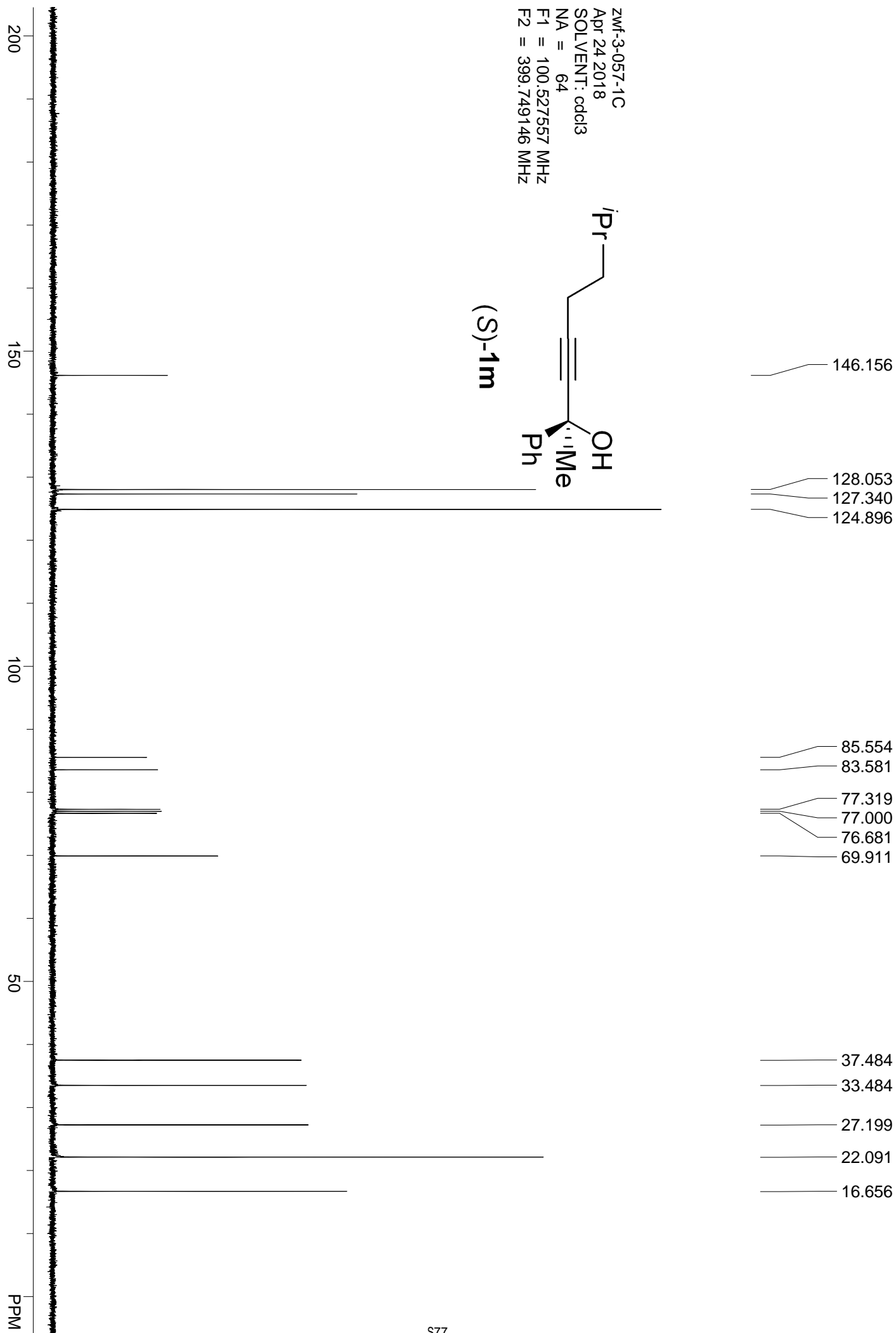
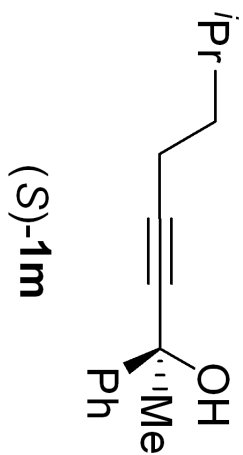


- 7.646
- 7.628
- 7.346
- 7.327
- 7.309
- 7.270
- 7.252
- 7.233

- 2.597
- 2.277
- 2.258
- 2.239
- 1.719
- 1.690
- 1.674
- 1.657
- 1.465
- 1.448
- 1.429
- 1.410
- 0.908
- 0.892
- 0.000



Zwf-3-057-1C
Apr 24 2018
SOLVENT: cdcl3
NA = 64
F1 = 100.527557 MHz
F2 = 399.749146 MHz



zwf-3-057-1-AS-H-98-2-1.0-214

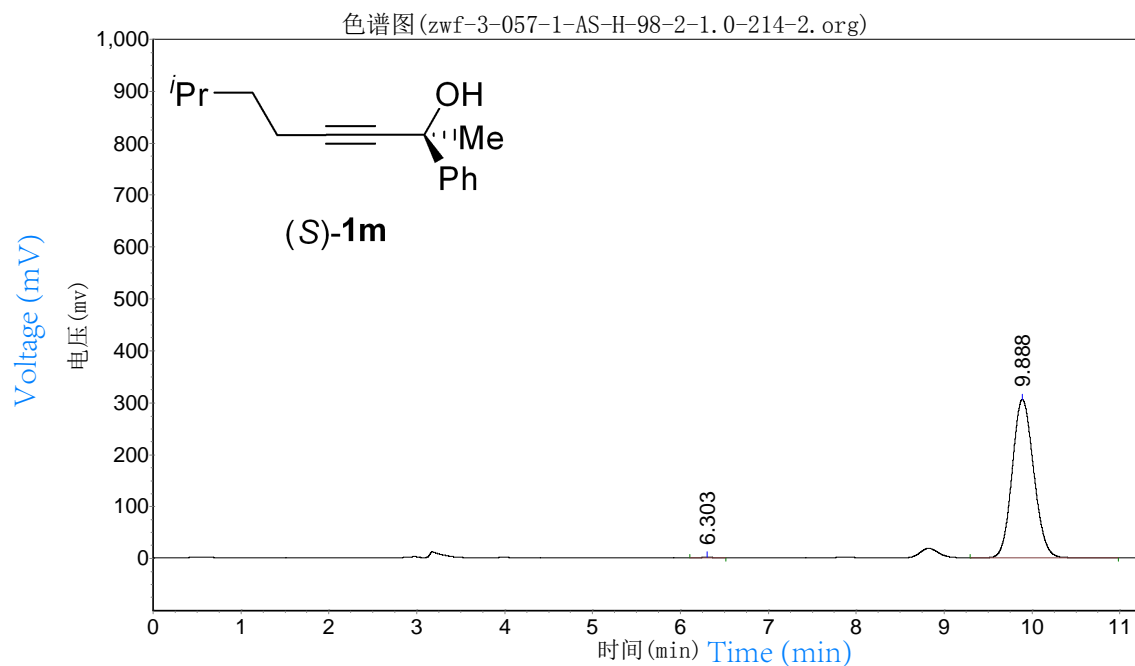
实验时间: 2018-04-24, 14:00:11

报告时间: 2018-04-24, 14:15:41

谱图文件: E:\data\zwf\zwf-3-057-1-AS-H-98-2-1.0-214-2.org

方法文件: E:\data\yaoyuan\0414.mtd

实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		6.303	848.246	8848.999	0.1705
2		9.888	304907.313	5180251.000	99.8295
总计			305755.558	5189099.999	100.0000

zwf-3-057-1-rac-AS-H-98-2-1.0-214

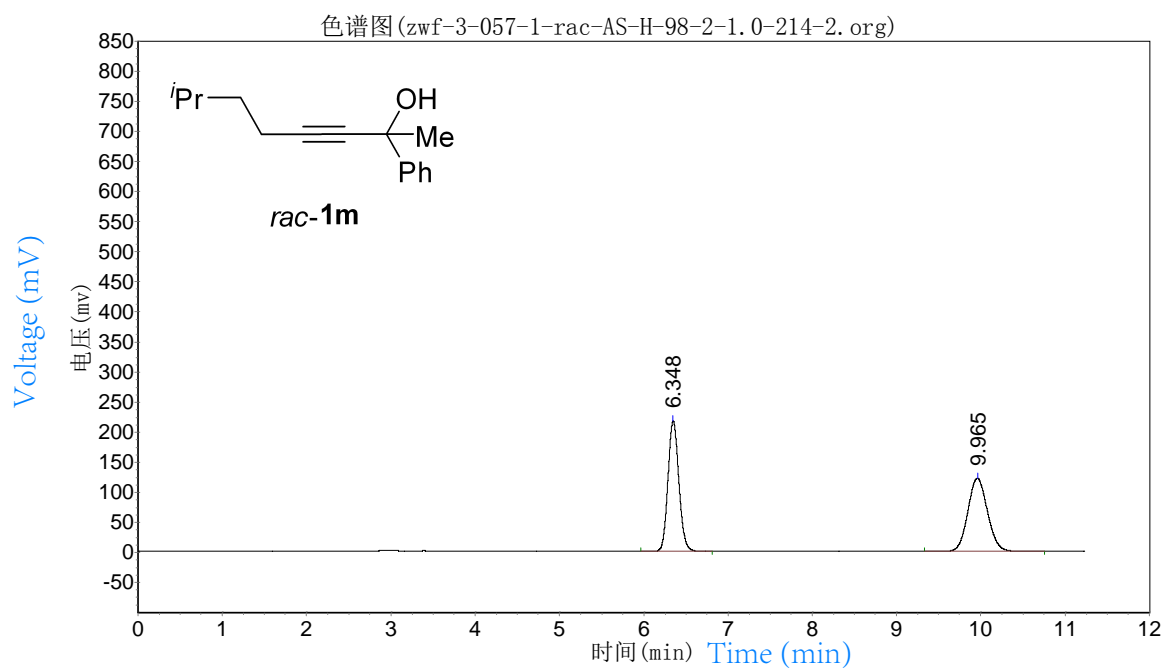
实验时间: 2018-04-24, 14:24:57

报告时间: 2018-04-24, 14:39:25

谱图文件: E:\data\zwf\zwf-3-057-1-rac-AS-H-98-2-1.0-214-2.org

方法文件: E:\data\yaoyuan\0414.mtd

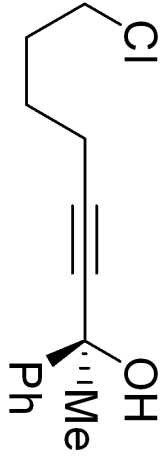
实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		6.348	216354.641	1939244.500	49.8360
2		9.965	121371.891	1952005.750	50.1640
总计			337726.531	3891250.250	100.0000

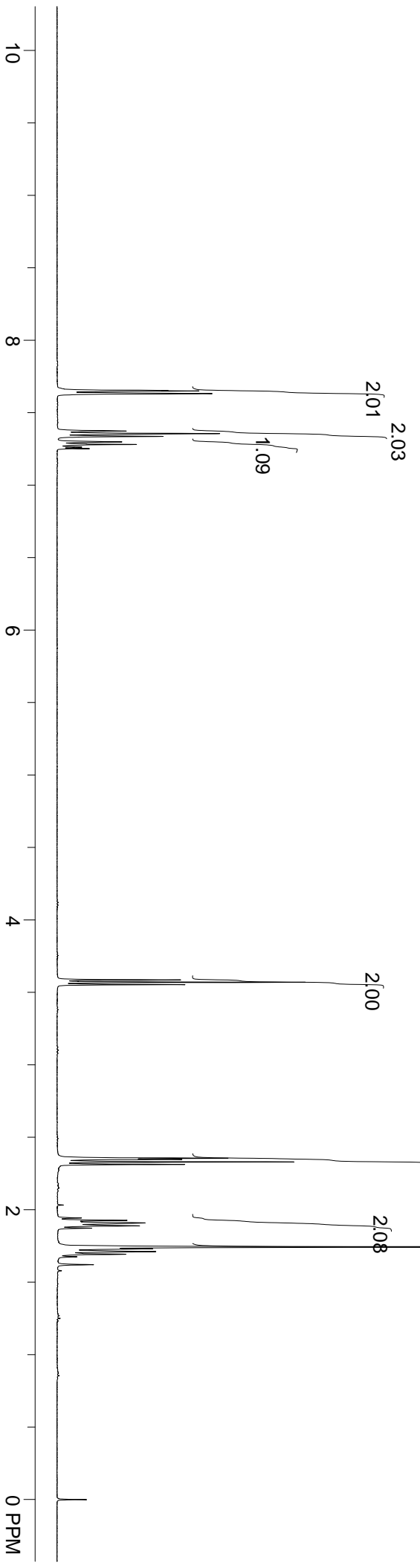
zwf-3-070-1H
Apr 28 2018
SOLVENT: CDCl3
NA = 4
F1 = 400.132477 MHz
F2 = 1.000000 MHz



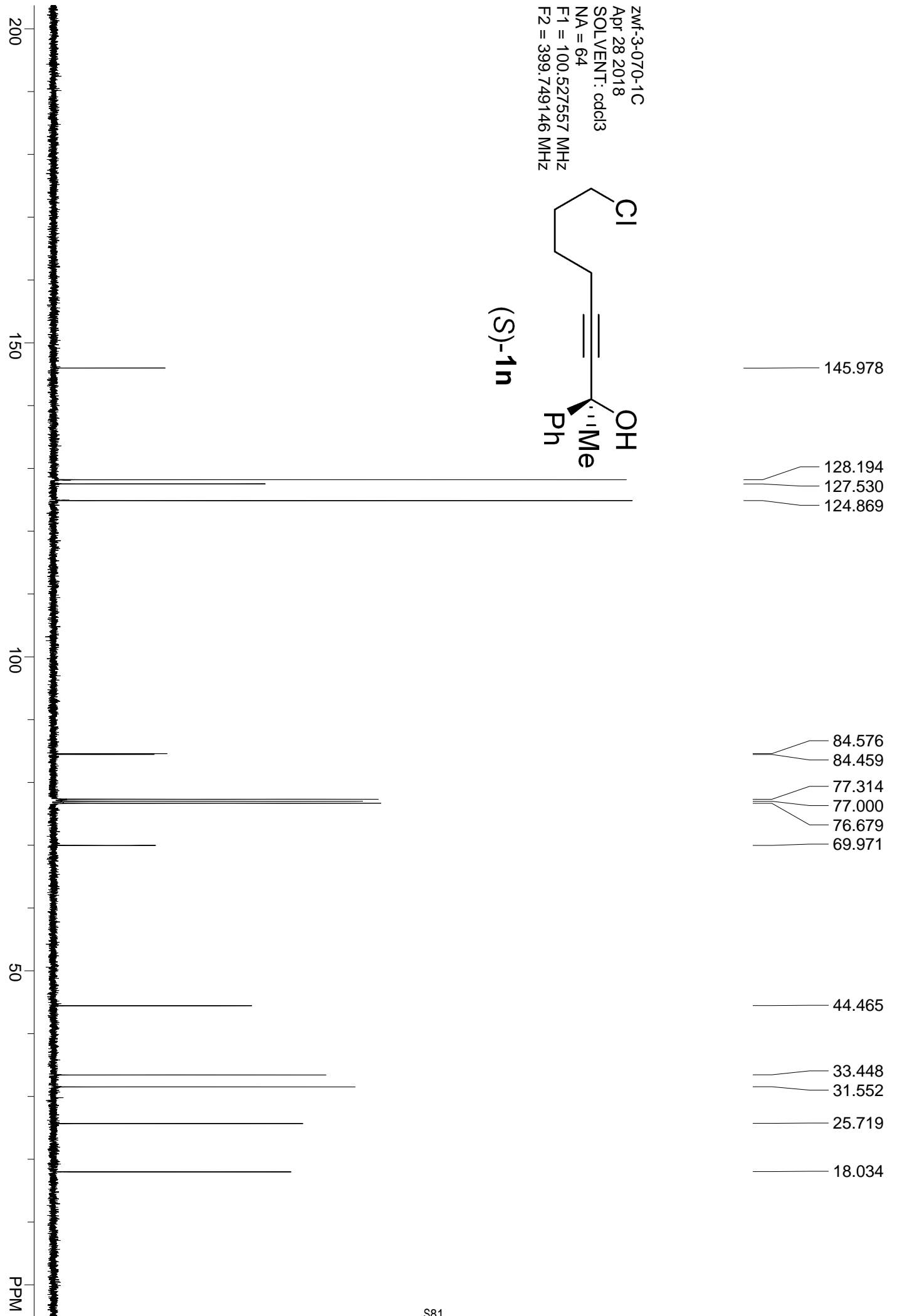
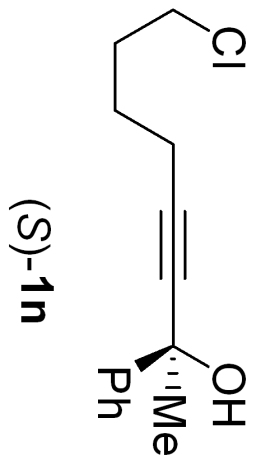
- 7.653
- 7.650
- 7.631
- 7.373
- 7.355
- 7.336
- 7.298
- 7.285
- 7.280
- 7.262
- 7.251

- 3.586
- 3.570
- 3.553

- 2.355
- 2.347
- 2.330
- 2.313
- 1.943
- 1.926
- 1.919
- 1.909
- 1.889
- 1.873
- 1.743
- 1.731
- 1.711
- 1.693
- 1.676
- 1.621
- 0.000



ZWF-3-070-1C
Apr 28 2018
SOLVENT: cdcl3
NA = 64
F1 = 100.527557 MHz
F2 = 399.749146 MHz

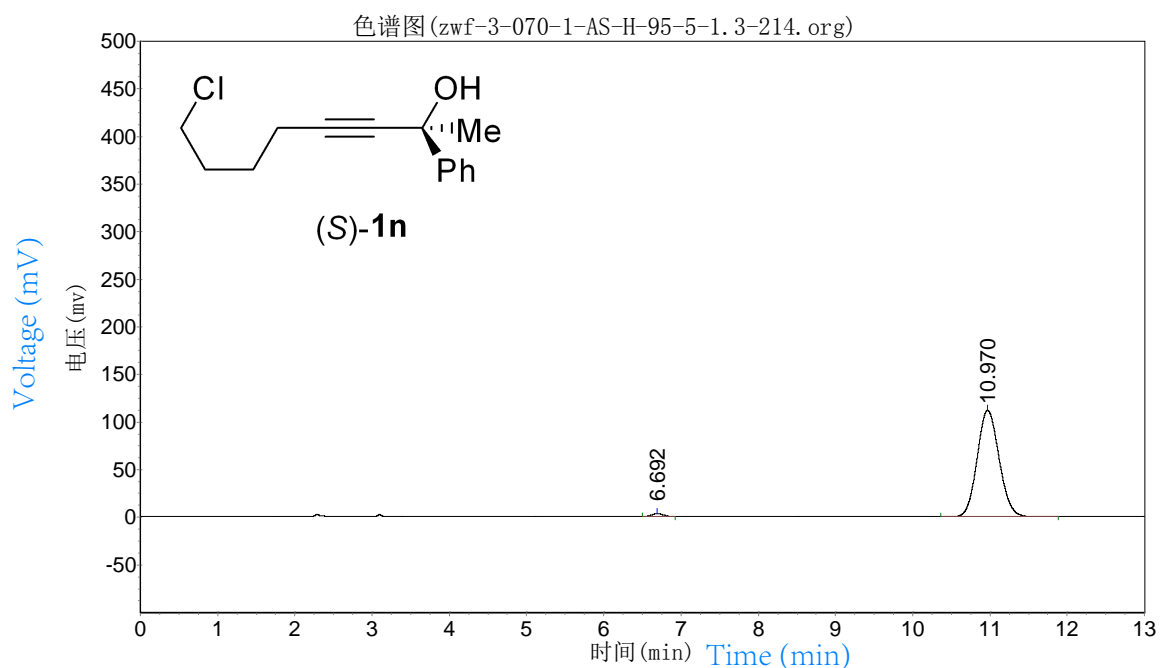


zwf-3-070-1-AS-H-95-5-1.3-214

实验时间: 2018-04-28, 10:32:56
谱图文件: E:\data\zwf\zwf-3-070-1-AS-H-95-5-1.3-214.org
方法文件: E:\data\yaoyuan\0414.mtd

报告时间: 2018-04-28, 10:49:35

实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		6.692	2978.383	30816.500	1.3805
2		10.970	111792.617	2201448.000	98.6195
总计			114771.000	2232264.500	100.0000

zwf-3-070-1-rac-AS-H-95-5-1.3-214

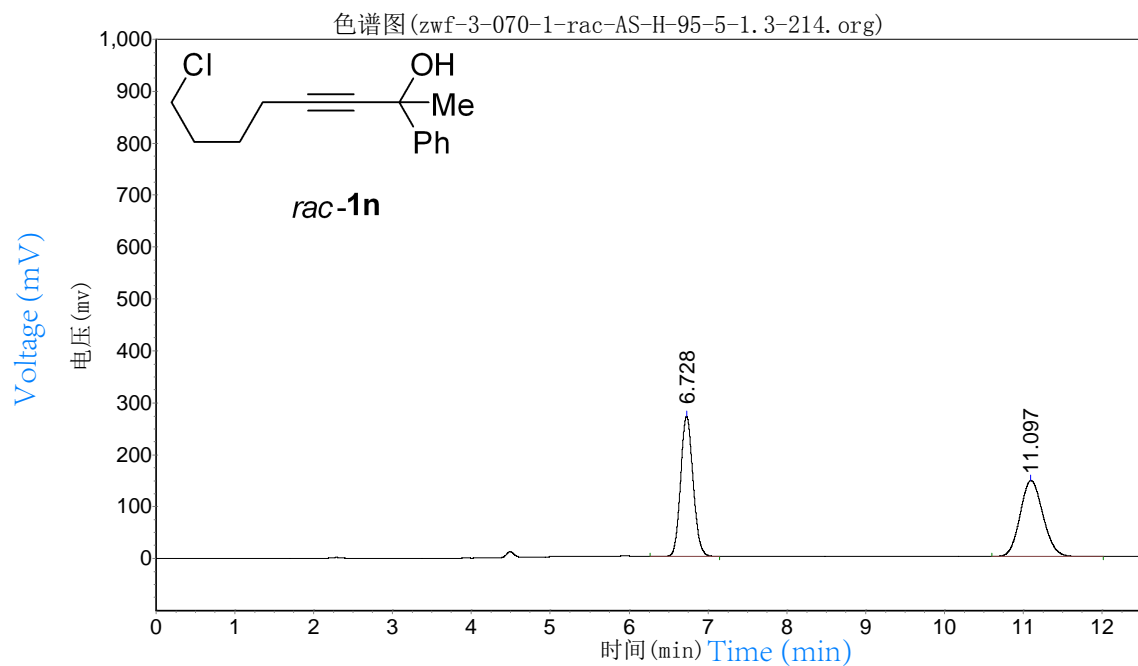
实验时间: 2018-04-28, 10:19:08

报告时间: 2018-04-28, 10:35:13

谱图文件: E:\data\zwf\zwf-3-070-1-rac-AS-H-95-5-1.3-214.org

方法文件: E:\data\yaoyuan\0414.mtd

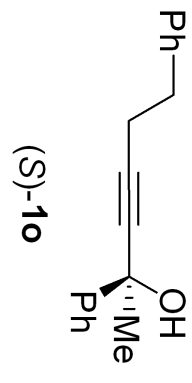
实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		6.728	269807.063	2967686.750	50.2455
2		11.097	146205.141	2938686.250	49.7545
总计			416012.203	5906373.000	100.0000

zwf-3-050-1H
Apr 18 2018
SOLVENT: cdcl3
NA = 4
F1 = 399.749542 MHz
F2 = 100.526031 MHz

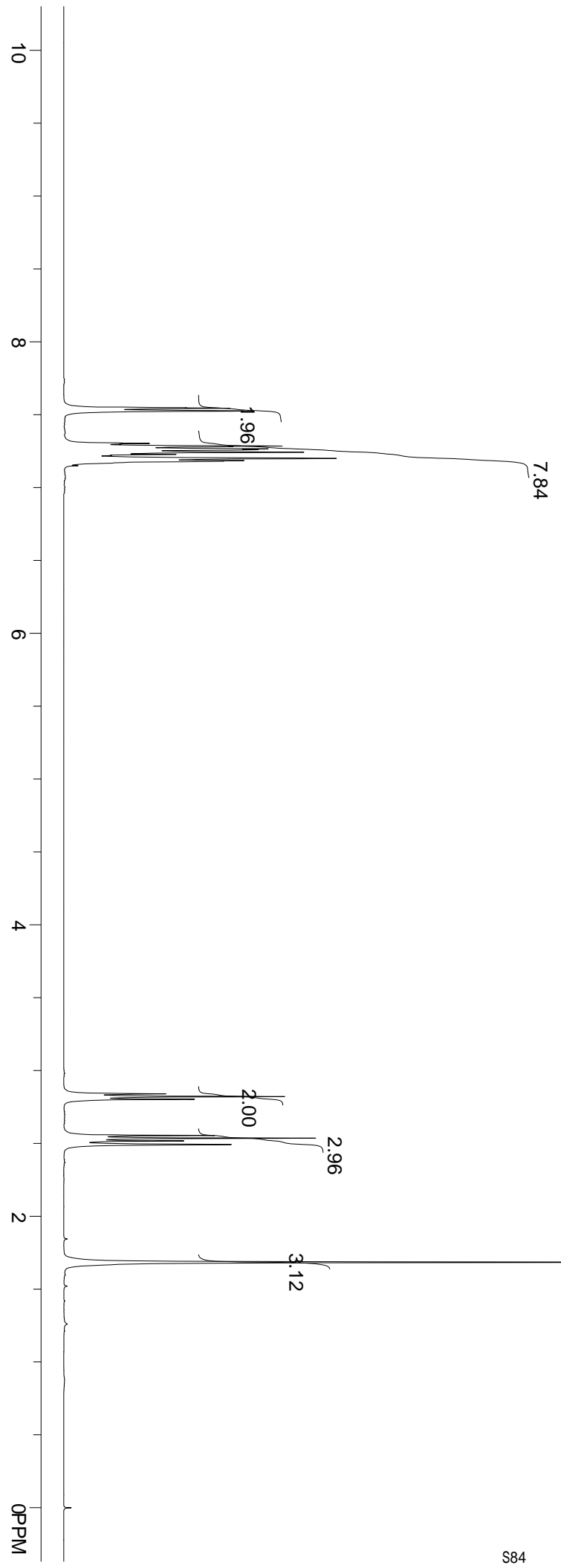


- 7.545
- 7.526
- 7.303
- 7.285
- 7.266
- 7.261
- 7.242
- 7.228
- 7.200
- 7.185

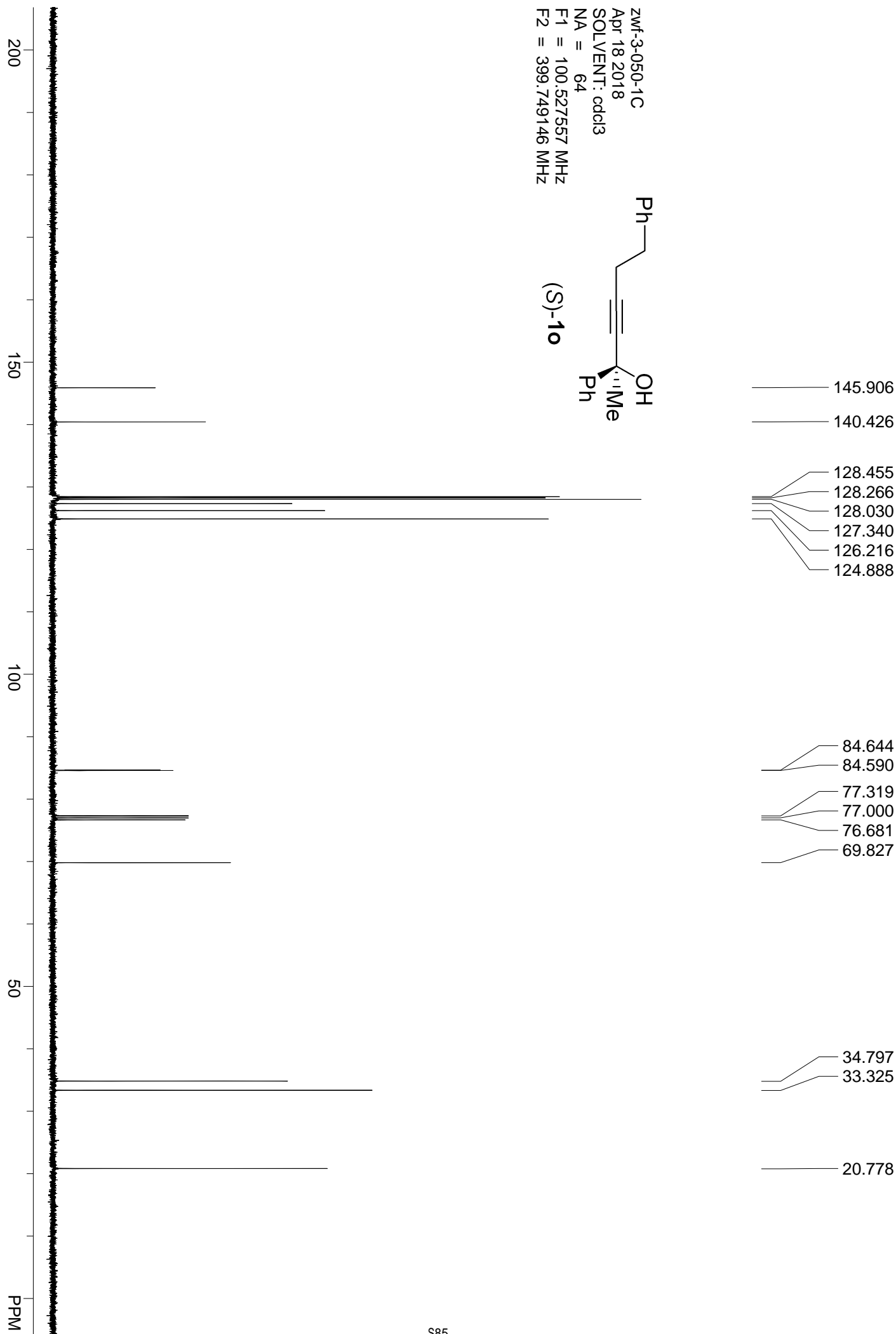
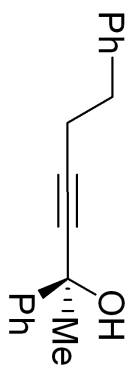
- 2.840
- 2.821
- 2.802
- 2.554
- 2.535
- 2.517
- 2.492

1.685

0.000



zwf-3-050-1C
Apr 18 2018
SOLVENT: cdcl3
NA = 64
F1 = 100.527557 MHz
F2 = 399.749146 MHz

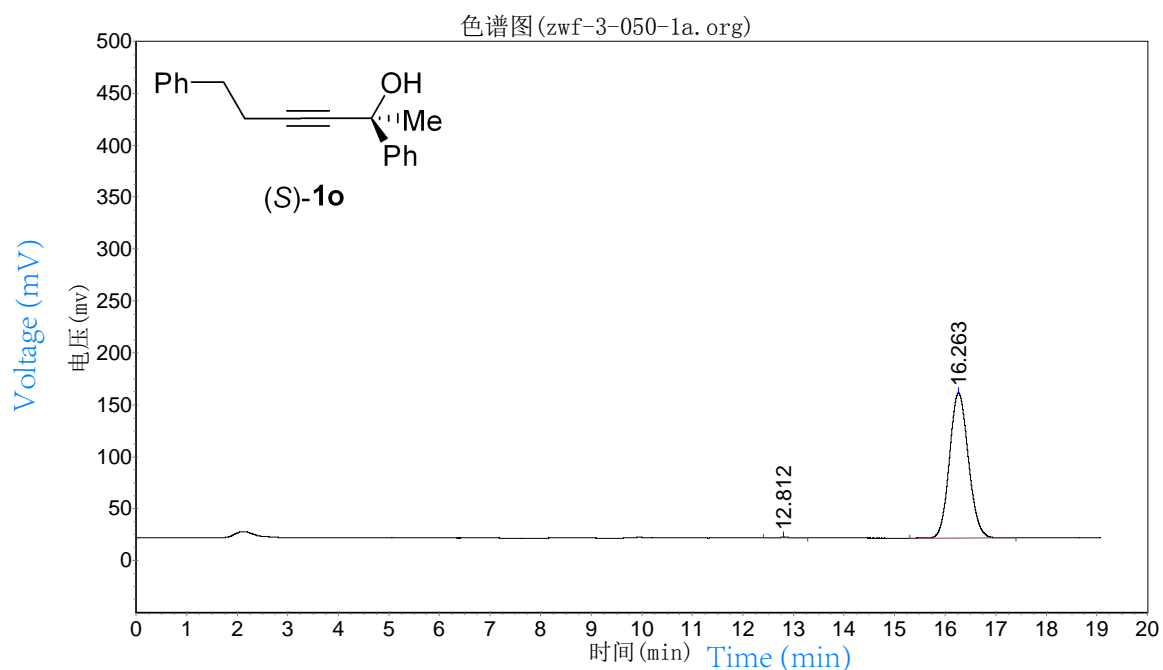


zwf-3-050-1-AS-H-98-2-1.0-214

实验时间: 2018-04-18, 21:39:45
谱图文件: E:\data\zwf\zwf-3-050-1a.org
方法文件: E:\data\yaoyuan\0414.mtd

报告时间: 2018-04-18, 22:03:51

实验内容简介:



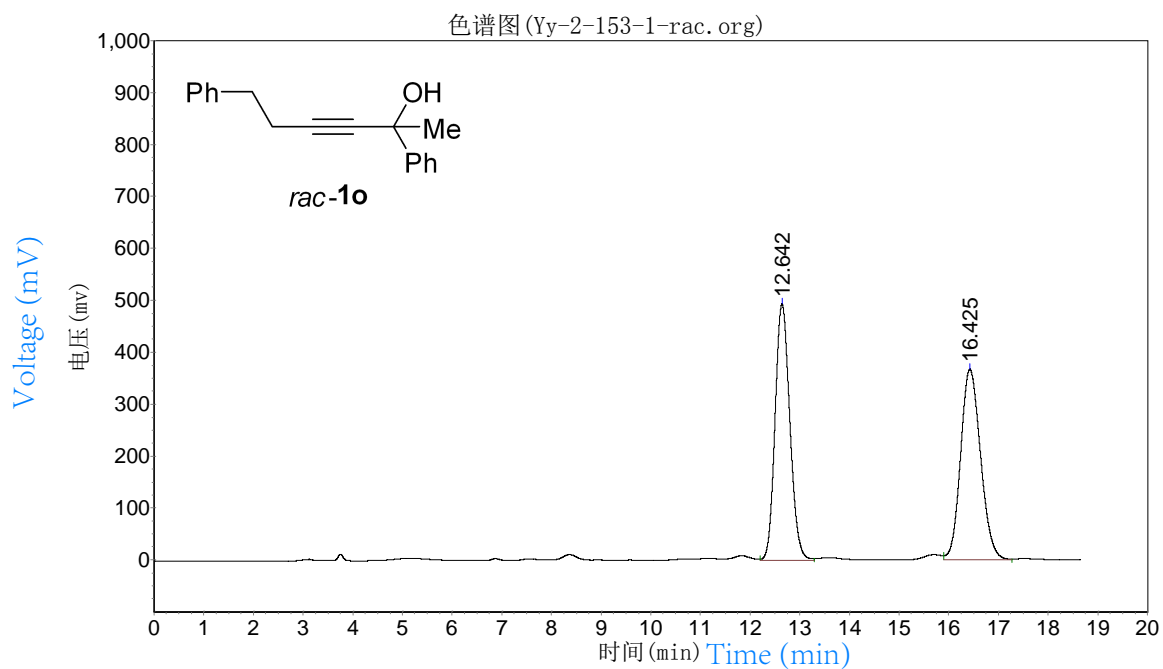
分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		12.812	729.064	14020.701	0.3850
2		16.263	139980.406	3627492.750	99.6150
总计			140709.470	3641513.451	100.0000

zwf-3-050-1-rac-AS-H-98-2-1.0-214

实验时间: 2018-04-14, 11:10:48
谱图文件: E:\data\zwf\other\Yy-2-153-1-rac.org
方法文件: E:\data\yaoyuan\0414.mtd

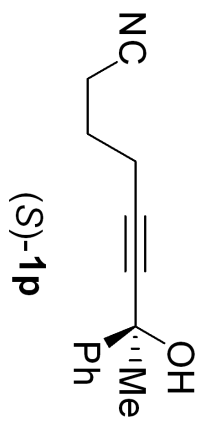
实验者:
报告时间: 2018-04-18, 22:22:34
积分方法: 面积归一法



分析结果表

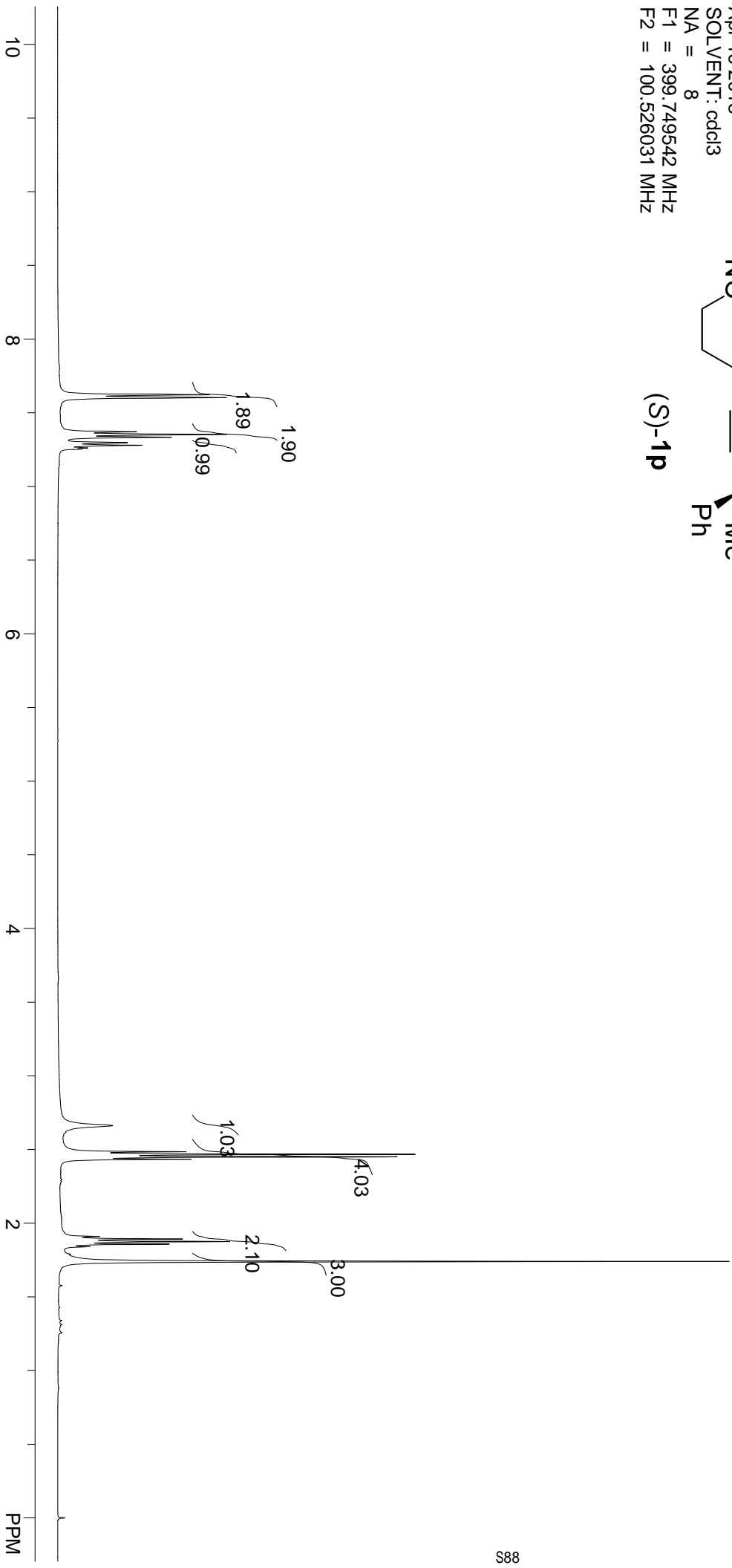
峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		12.642	494191.656	10208660.000	49.7952
2		16.425	367504.719	10292623.000	50.2048
总计			861696.375	20501283.000	100.0000

zwf-3-043-1H
Apr 16 2018
SOLVENT: cdcl3
NA = 8
F1 = 399.749542 MHz
F2 = 100.526031 MHz

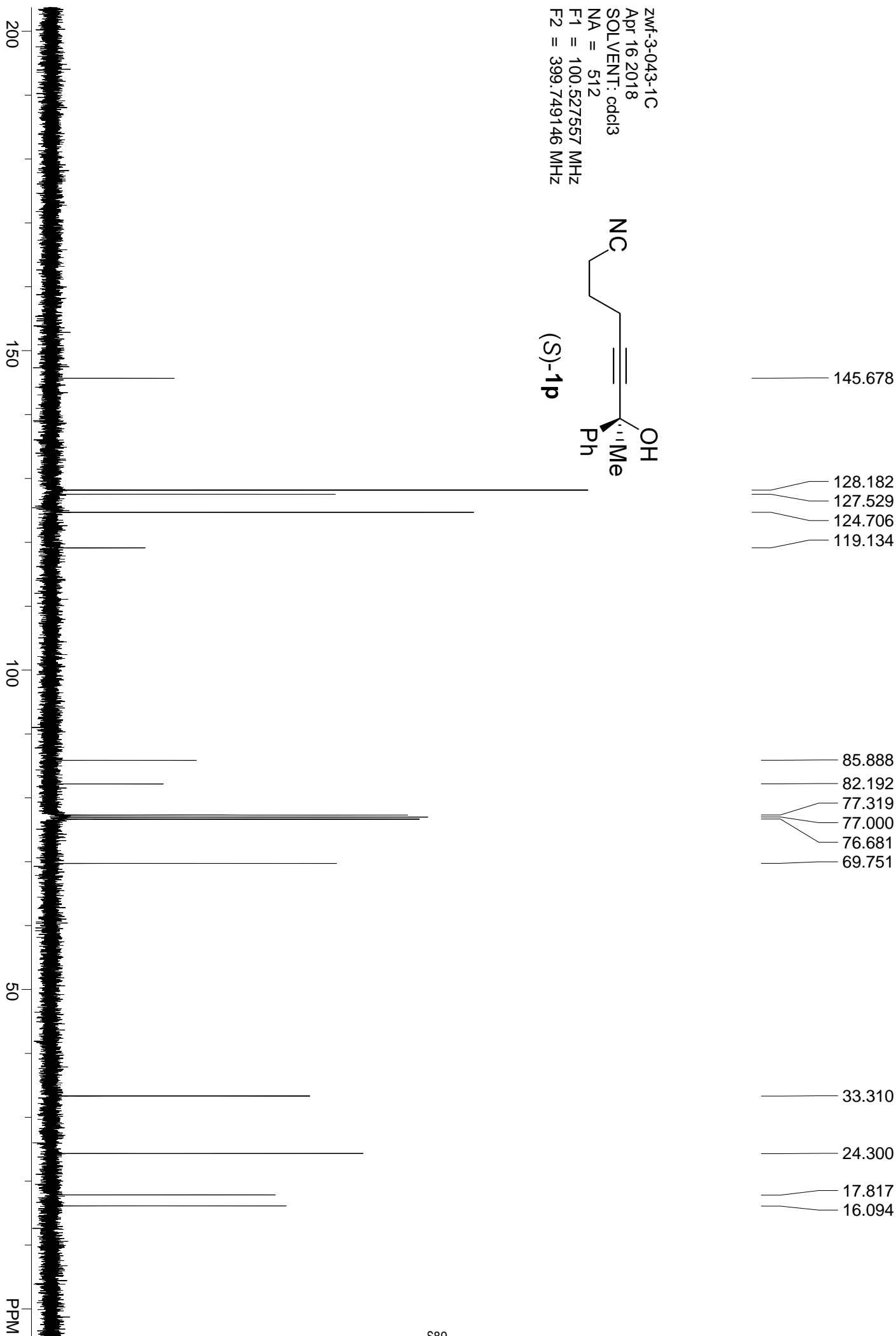
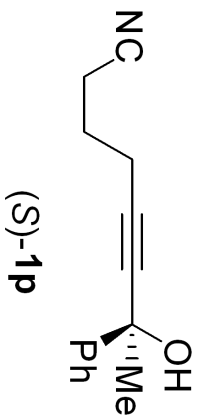


- 7.622
- 7.602
- 7.371
- 7.353
- 7.333
- 7.297
- 7.279
- 7.261
- 7.254

- 2.662
- 2.485
- 2.468
- 2.451
- 2.434
- 1.910
- 1.893
- 1.875
- 1.858
- 1.840
- 1.740



zwf-3-043-1C
Apr 16 2018
SOLVENT: cdcl3
NA = 512
F1 = 100.527557 MHz
F2 = 399.749146 MHz

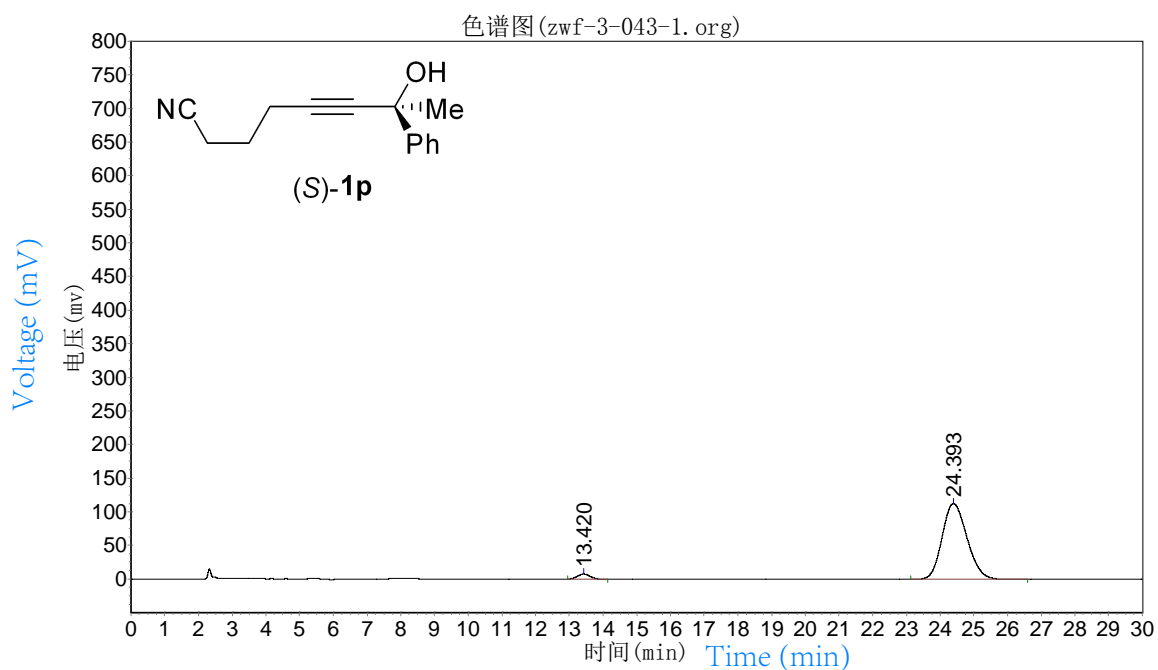


zwf-3-043-1-AS-H-90-10-1.3-214

实验时间: 2018-04-16, 14:30:05
谱图文件: E:\data\zwf\zwf-3-043-1.org
方法文件: E:\data\yaoyuan\0414.mtd

报告时间: 2018-04-16, 15:03:00

实验内容简介:



分析结果表

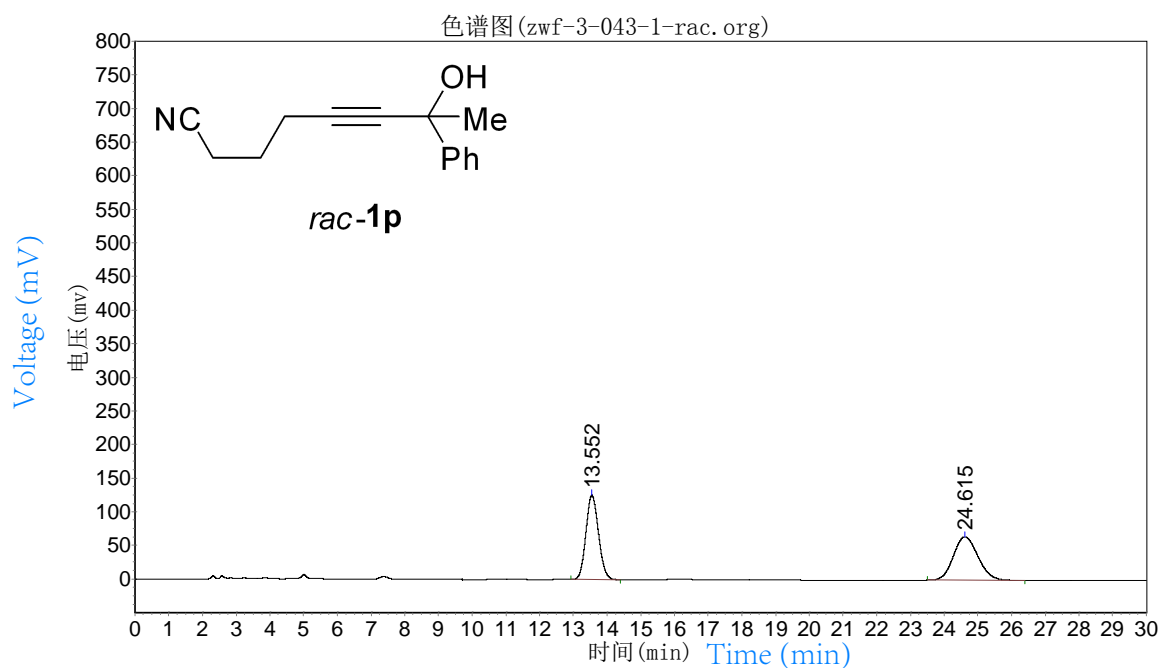
峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		13.420	7437.636	187279.047	3.1397
2		24.393	112726.828	5777681.000	96.8603
总计			120164.464	5964960.047	100.0000

zwf-3-043-1-rac-AS-H-90-10-1.3-214

实验时间: 2018-04-16, 13:58:15
谱图文件: E:\data\zwf\zwf-3-043-1-rac.org
方法文件: E:\data\yaoyuan\0414.mtd

报告时间: 2018-04-16, 14:33:01

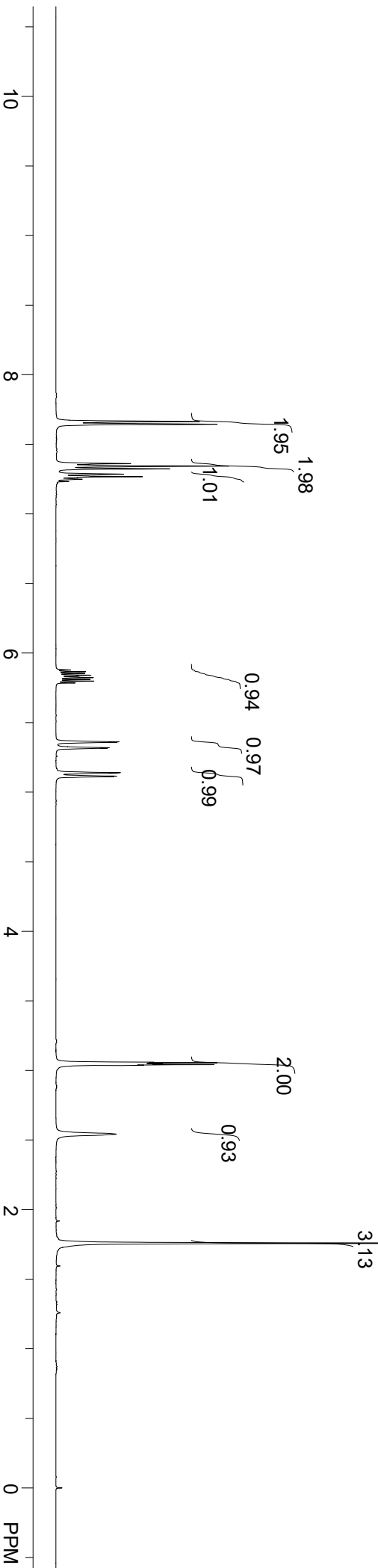
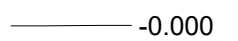
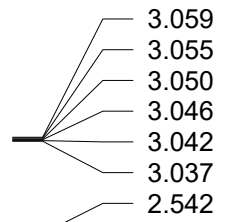
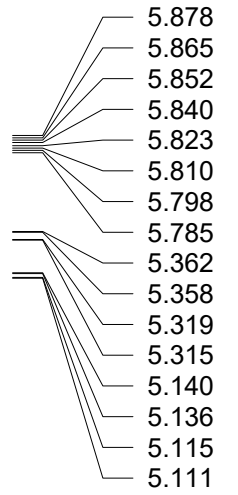
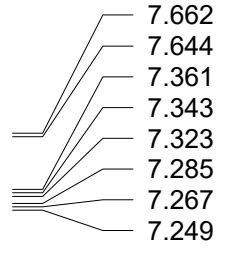
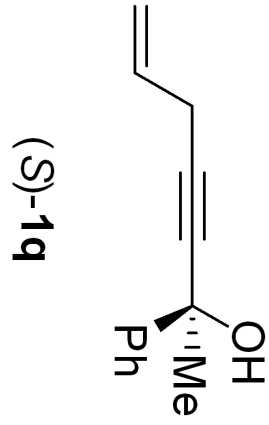
实验内容简介:



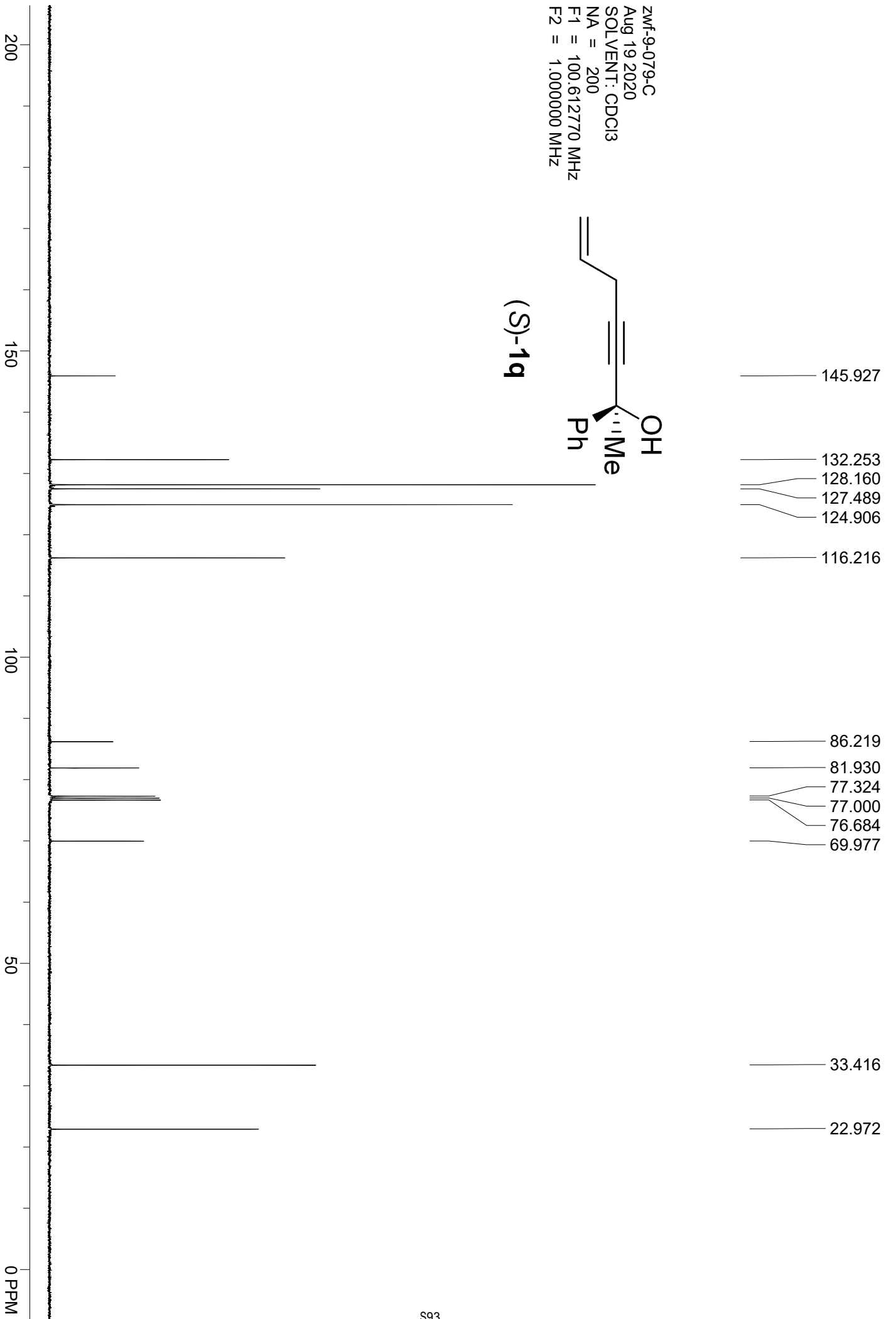
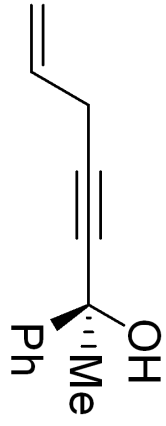
分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		13.552	125189.141	3246437.750	49.9017
2		24.615	64463.164	3259226.750	50.0983
总计			189652.305	6505664.500	100.0000

ZWF-9-079-H
Aug 19 2020
SOLVENT: CDCl3
NA = 4
F1 = 400.130035 MHz
F2 = 1.000000 MHz



ZWf-9-079-C
Aug 19 2020
SOLVENT: CDCl3
NA = 200
F1 = 100.612770 MHz
F2 = 1.000000 MHz



Area Percent Report

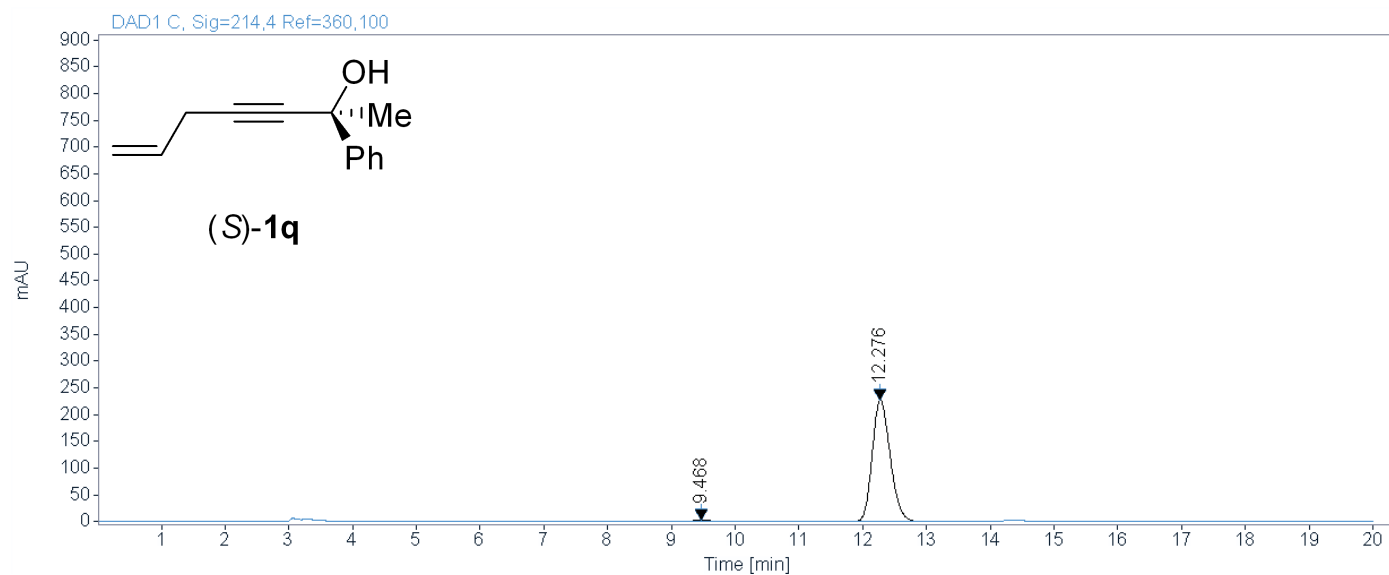


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sample zwf-9-079-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\YuanYuan 2020-08-17 15-30-05\132-P2-C5-zwf-9-079-1.D

Acquisition Data:



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
9.468	0.2761	3.6310	66.0091	1.4600
12.276	0.3041	227.8208	4455.1304	98.5400
	Sum		4521.1394	100.0000

Area Percent Report

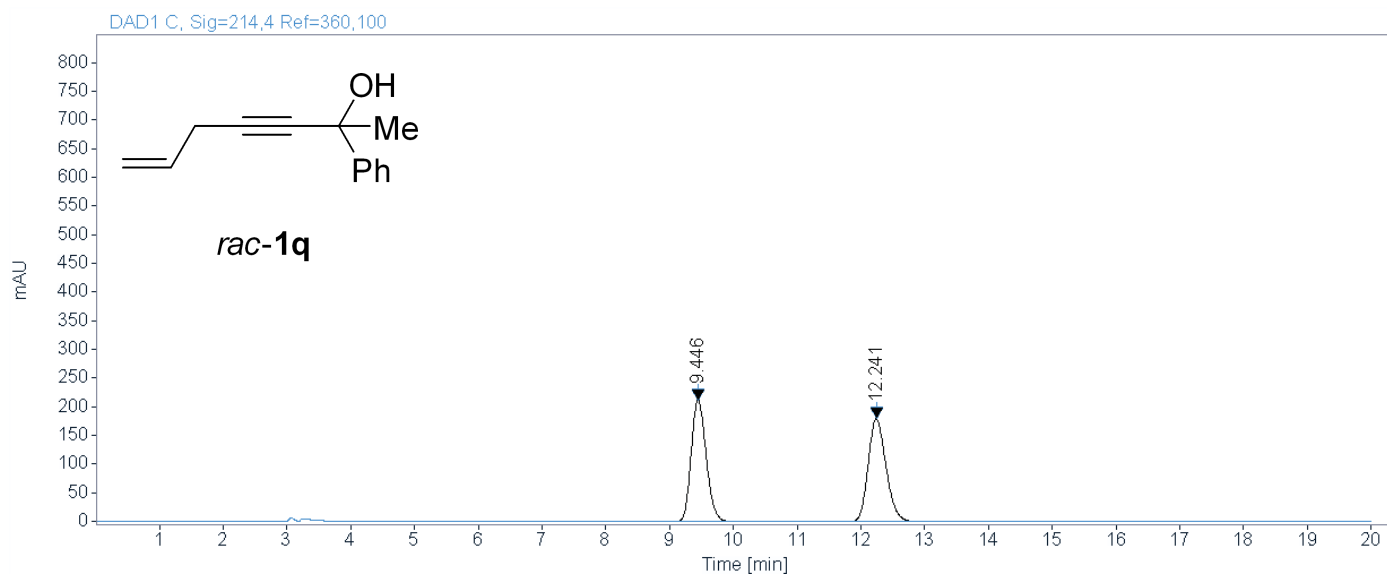


Agilent Technologies

sample zwf-9-079-rac-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\YuanYuan 2020-08-17 15-30-05\133-P2-C6-zwf-9-079-1-rac.D

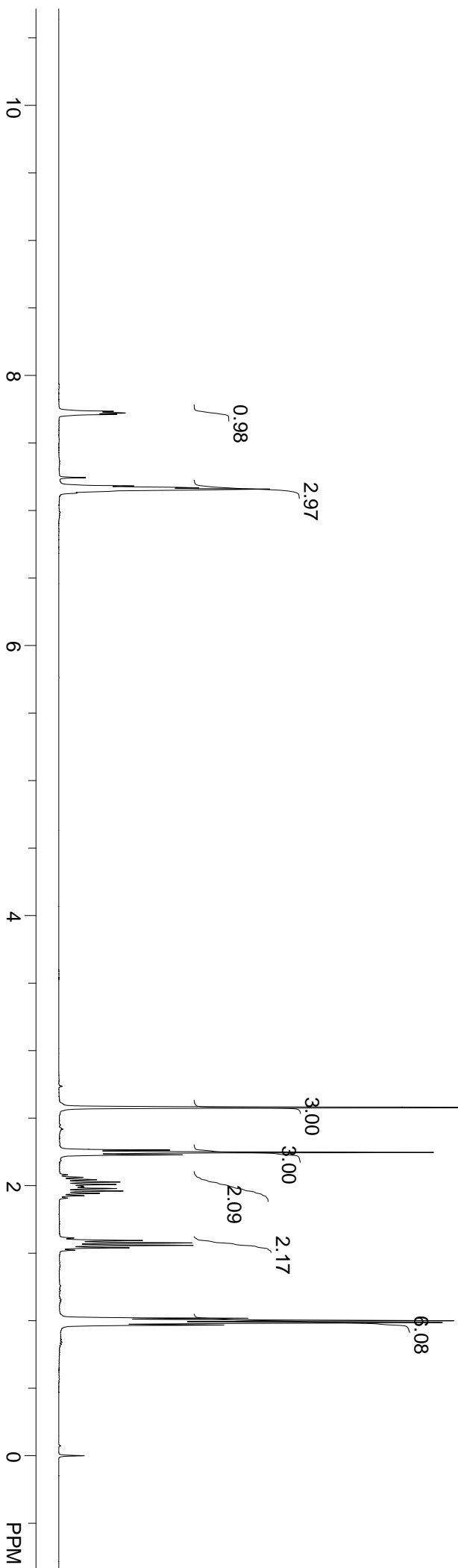
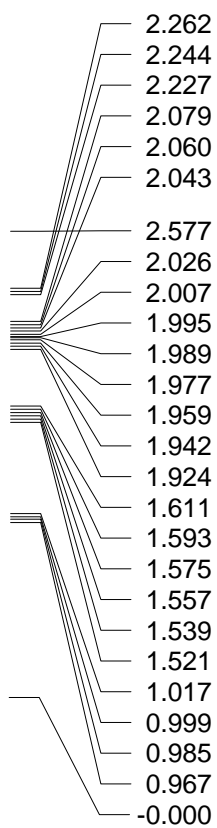
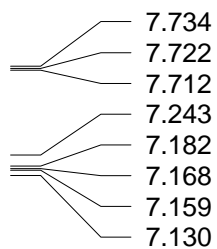
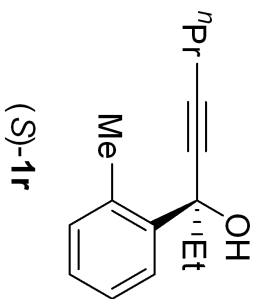
Acquisition Data:



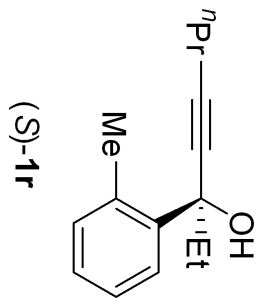
Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
9.446	0.2577	212.5906	3492.5410	49.9381
12.241	0.3037	179.4059	3501.1985	50.0619
Sum			6993.7395	100.0000

ZWF-4-137-1
Nov 10 2018
SOLVENT: CDCl3
NA = 4
F1 = 400.130005 MHz
F2 = 1.000000 MHz



Zwf-4-137-1
Nov 10 2018
SOLVENT: CDCl3
NA = 200
F1 = 100.612770 MHz
F2 = 1.000000 MHz



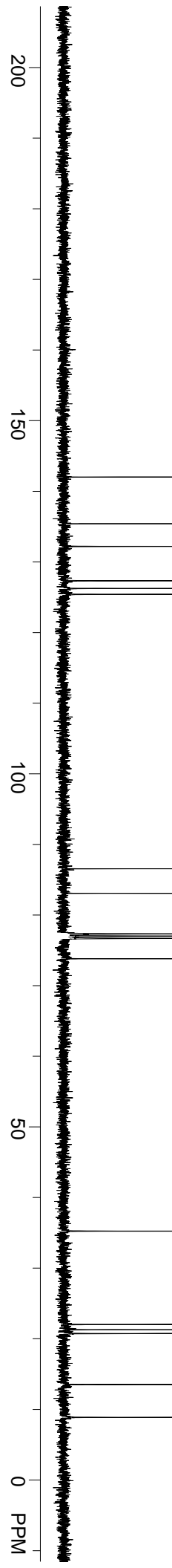
- 142.009
- 135.405
- 132.189
- 127.323
- 126.241
- 125.403

- 86.535
- 83.059
- 77.316
- 77.000
- 76.684
- 73.793

- 35.256

- 22.048
- 21.305
- 20.768
- 13.555

- 8.910



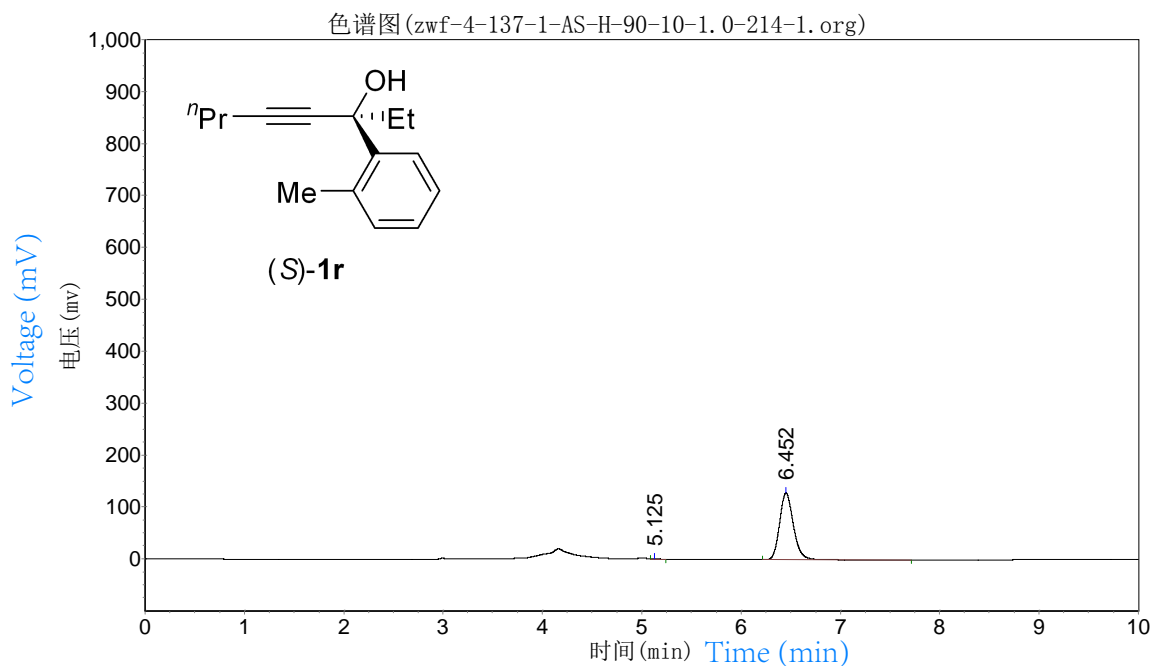
zwf-4-137-1-AS-H-98-2-1.0-214

实验时间: 2018-11-09, 21:07:30

报告时间: 2018-11-09, 21:46:33

谱图文件: E:\data\zwf\zwf-4-137-1-AS-H-90-10-1.0-214-1.org

实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		5.125	959.209	5468.495	0.4388
2		6.452	128742.766	1240850.125	99.5612
总计			129701.974	1246318.620	100.0000

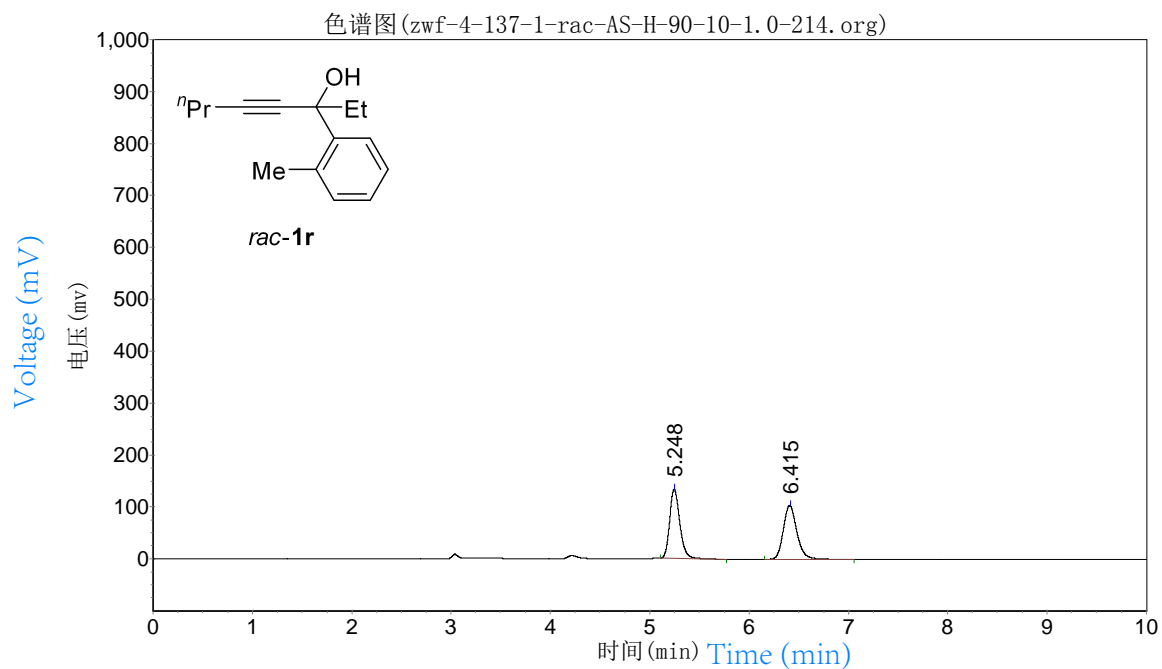
zwf-4-137-1-rac-AS-H-98-2-1.0-214

实验时间: 2018-11-09, 21:31:33

报告时间: 2018-11-09, 21:47:12

谱图文件: E:\data\zwf\zwf-4-137-1-rac-AS-H-90-10-1.0-214.org

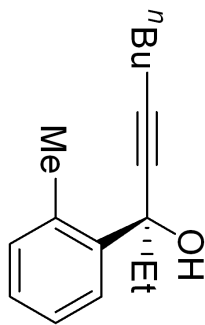
实验内容简介:



分析结果表

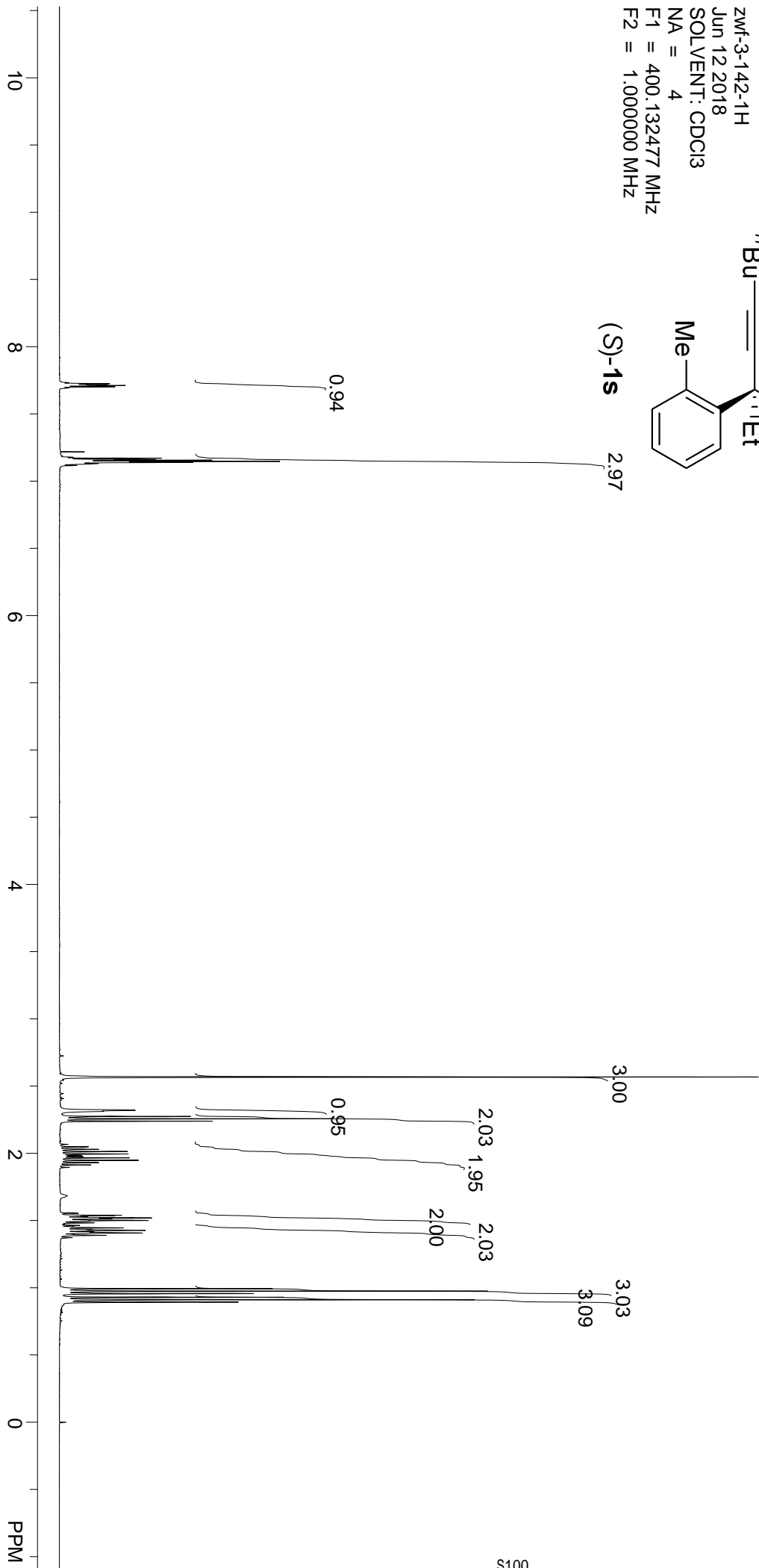
峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		5.248	134365.906	975821.063	50.1024
2		6.415	103029.656	971831.688	49.8976
总计			237395.563	1947652.750	100.0000

ZWF-3-142-1H
Jun 12 2018
SOLVENT: CDCl3
NA = 4
F1 = 400.132477 MHz
F2 = 1.000000 MHz

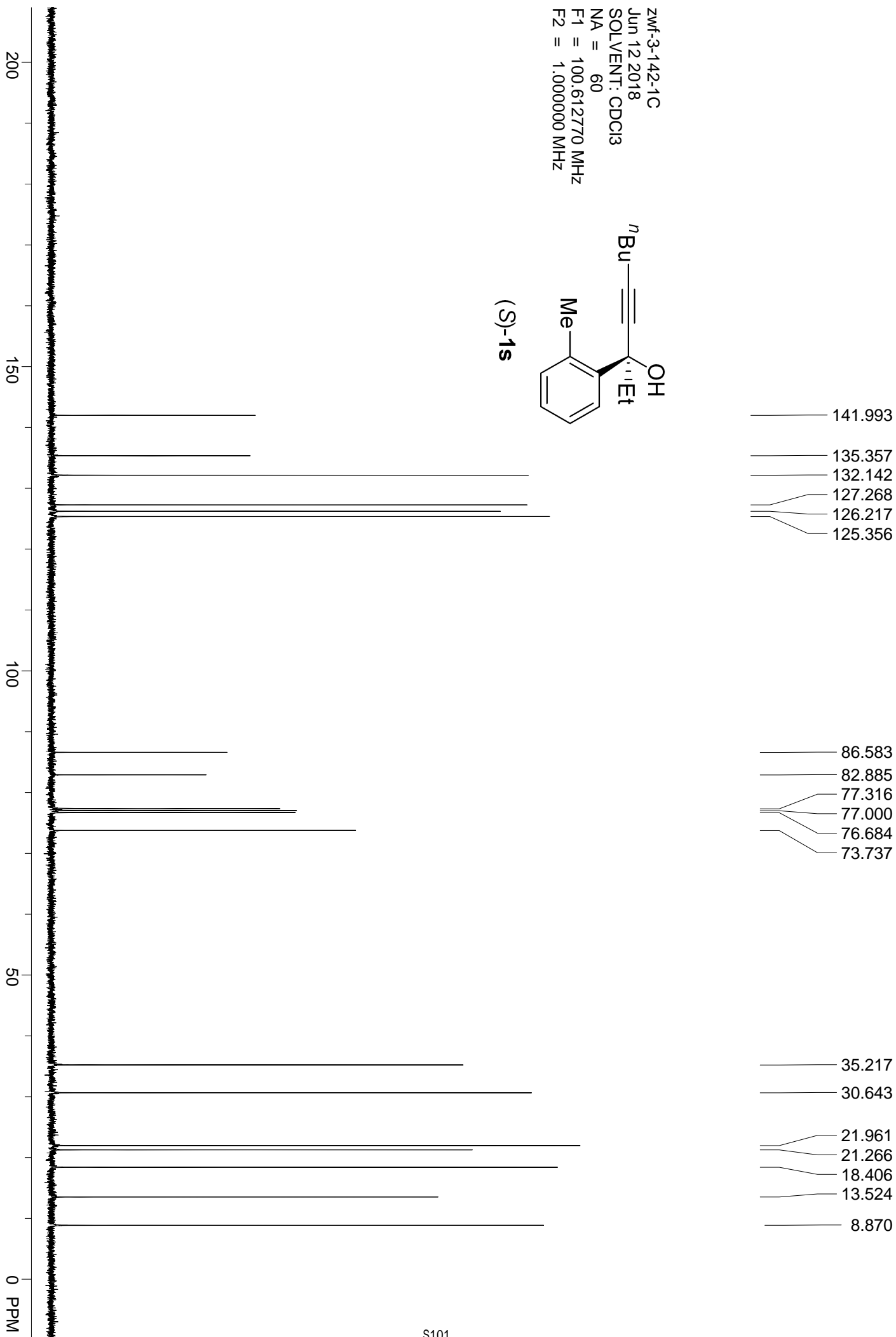
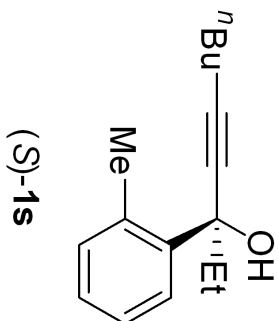


- 7.733
- 7.724
- 7.711
- 7.702
- 7.694
- 7.218
- 7.178
- 7.170
- 7.160
- 7.156
- 7.147
- 7.139
- 7.131
- 7.117

- 2.319
- 2.274
- 2.257
- 2.239
- 2.066
- 2.048
- 2.030
- 2.013
- 1.995
- 1.984
- 2.567
- 1.976
- 1.966
- 1.948
- 1.929
- 1.913
- 1.895
- 1.556
- 1.539
- 1.519
- 1.501
- 1.483
- 1.463
- 1.445
- 1.426
- 1.407
- 1.389
- 1.372
- 0.993
- 0.975
- 0.956
- 0.929
- 0.911
- 0.893



ZWF-3-142-1C
Jun 12 2018
SOLVENT: CDCl3
NA = 60
F1 = 100.612770 MHz
F2 = 1.000000 MHz



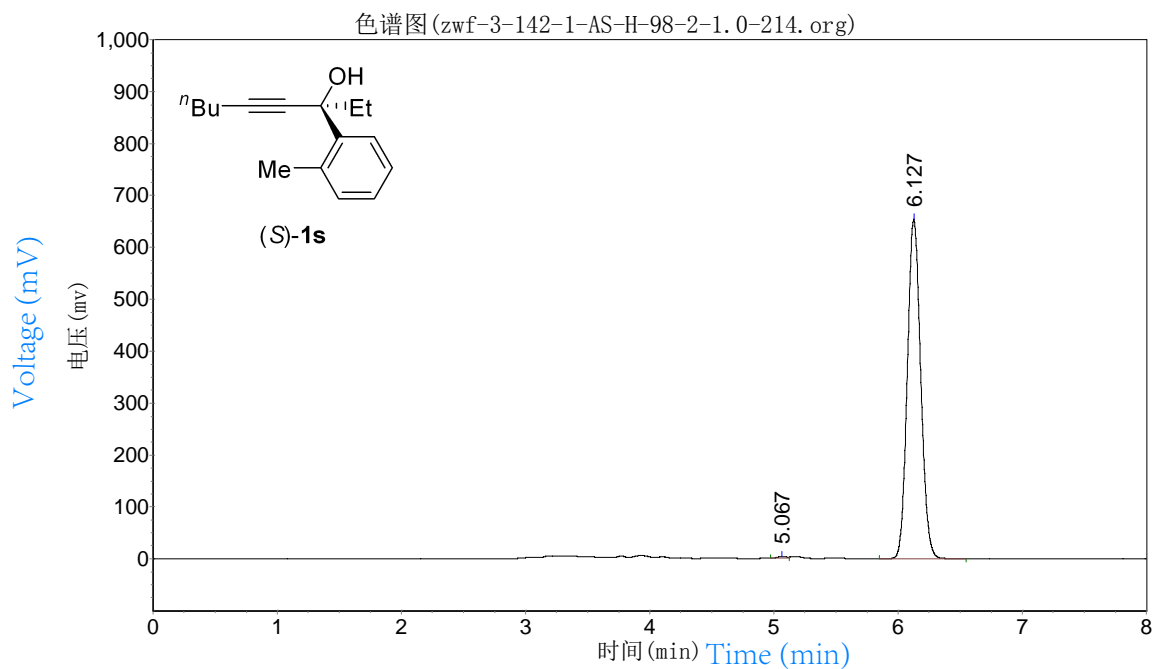
zwf-3-142-1-AS-H-98-2-1.0-214

实验时间: 2018-06-12, 17:08:01

报告时间: 2018-06-12, 17:32:44

谱图文件: E:\data\zwf\zwf-3-142-1-AS-H-98-2-1.0-214.org

实验内容简介:



分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		5.067	3182.304	18142.625	0.3693
2		6.127	653425.688	4894885.500	99.6307
总计			656607.991	4913028.125	100.0000

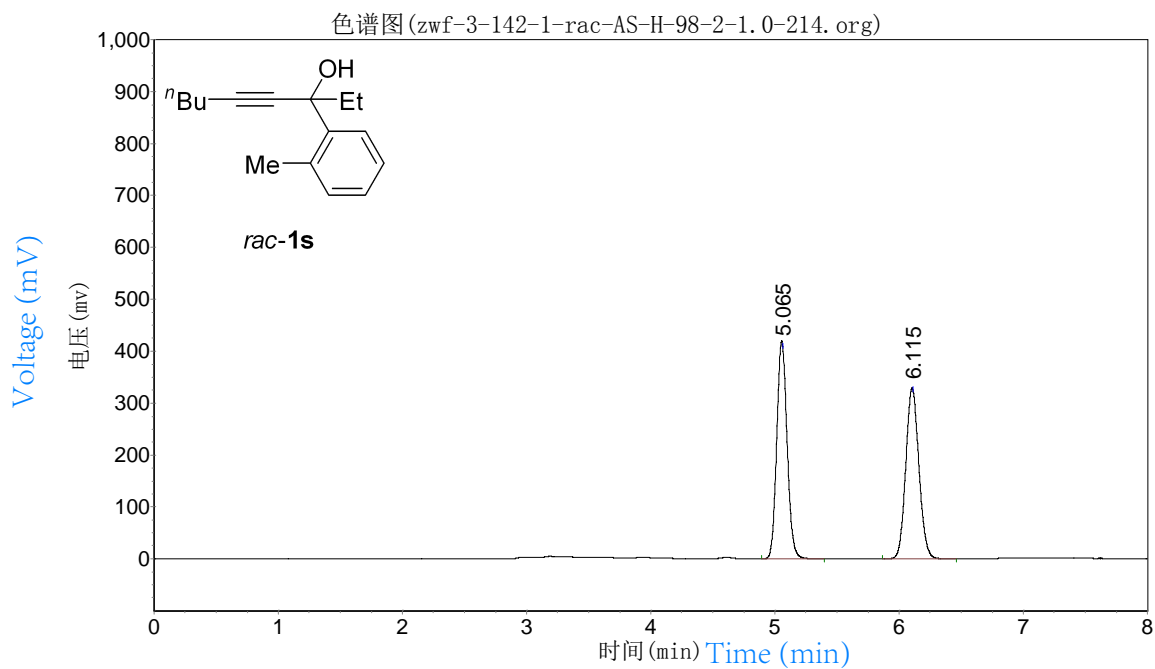
zwf-3-142-1-rac-AS-H-98-2-1.0-214

实验时间: 2018-06-12, 17:20:41

报告时间: 2018-06-12, 17:31:56

谱图文件: E:\data\zwf\zwf-3-142-1-rac-AS-H-98-2-1.0-214.org

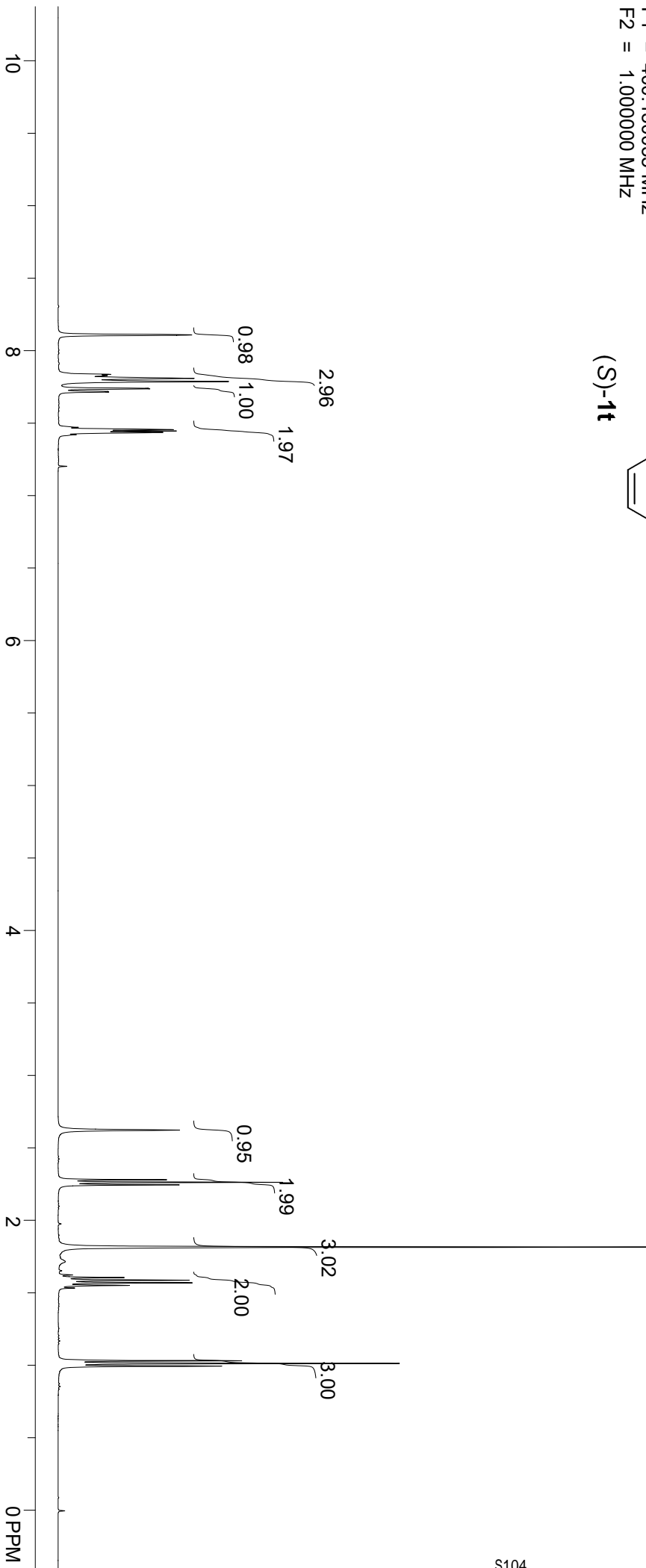
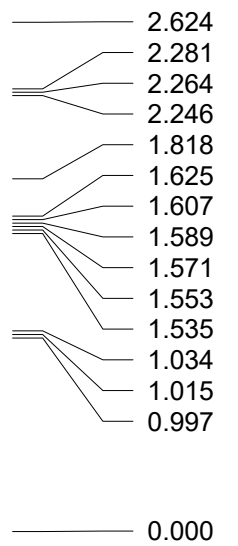
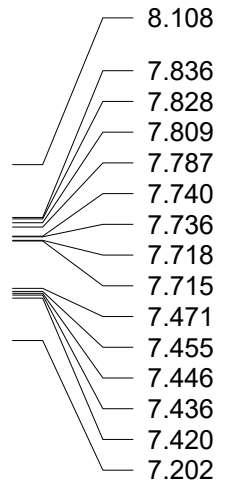
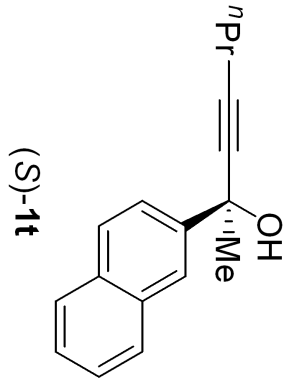
实验内容简介:



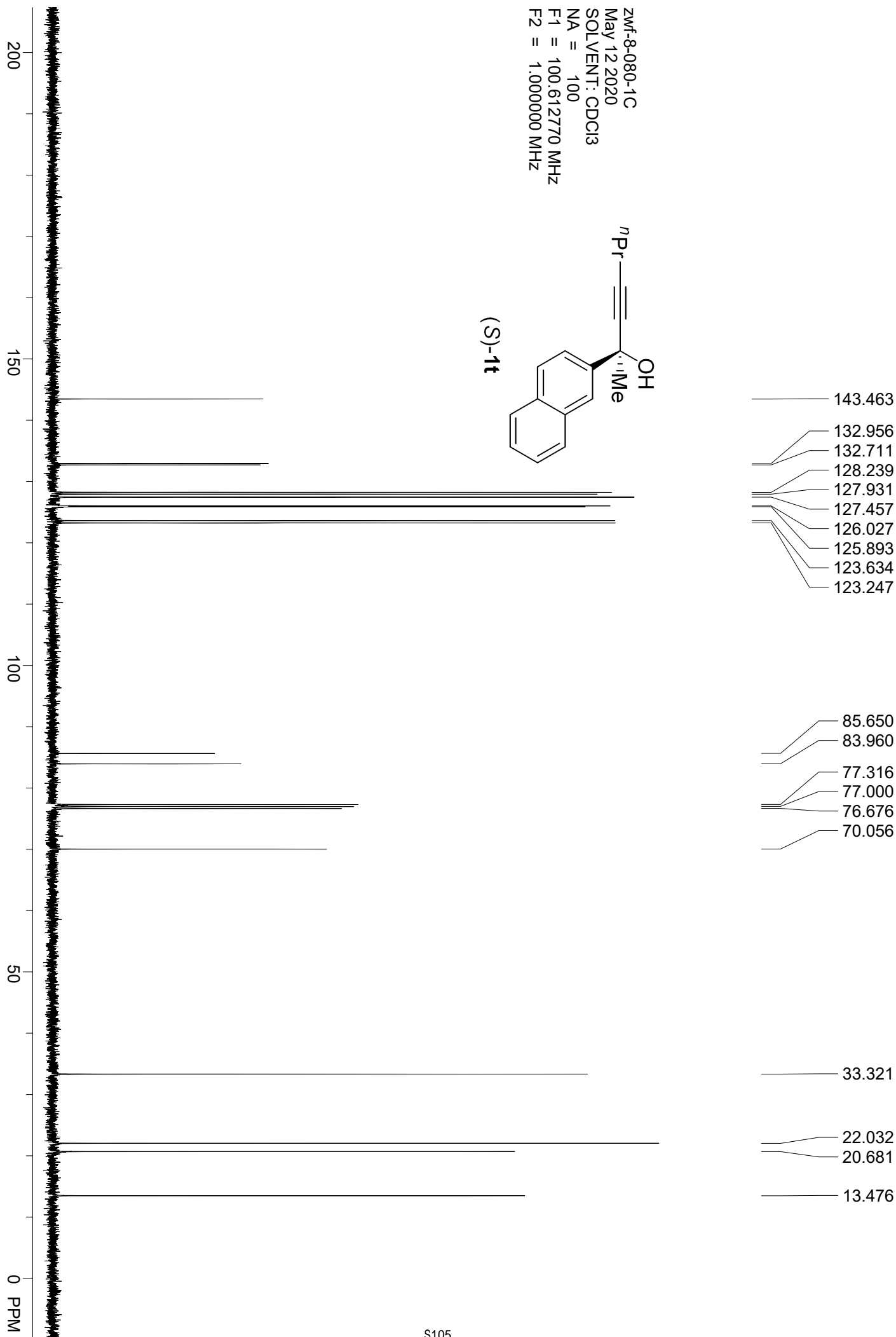
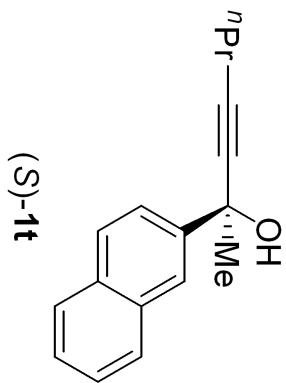
分析结果表

峰号	峰名	保留时间 RT [min]	峰高 Height	峰面积 Area	含量 Area %
1		5.065	415529.375	2439057.500	50.1080
2		6.115	327165.250	2428547.750	49.8920
总计			742694.625	4867605.250	100.0000

zwf-8-080-1
May 12 2020
SOLVENT: CDCl3
NA = 4
F1 = 400.130035 MHz
F2 = 1.000000 MHz



zwf-8-080-1C
May 12 2020
SOLVENT: CDCl3
NA = 100
F1 = 100.612770 MHz
F2 = 1.000000 MHz



Area Percent Report

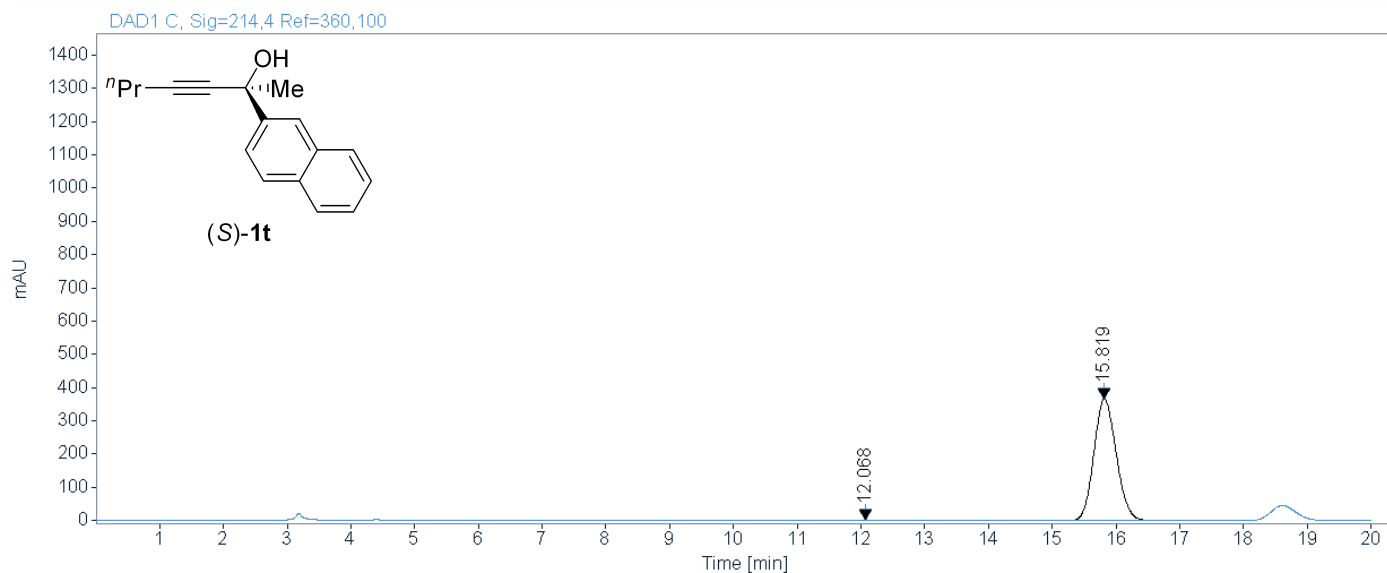


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sample zwf-8-080-1-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\linj 2020-05-12 10-02-00\011-P1-C1-zwf-8-080-1.D

Acquisition Data:



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
12.068	0.2859	2.3332	43.1758	0.4808
15.819	0.3806	366.2718	8935.9346	99.5192
		Sum	8979.1104	100.0000

Area Percent Report

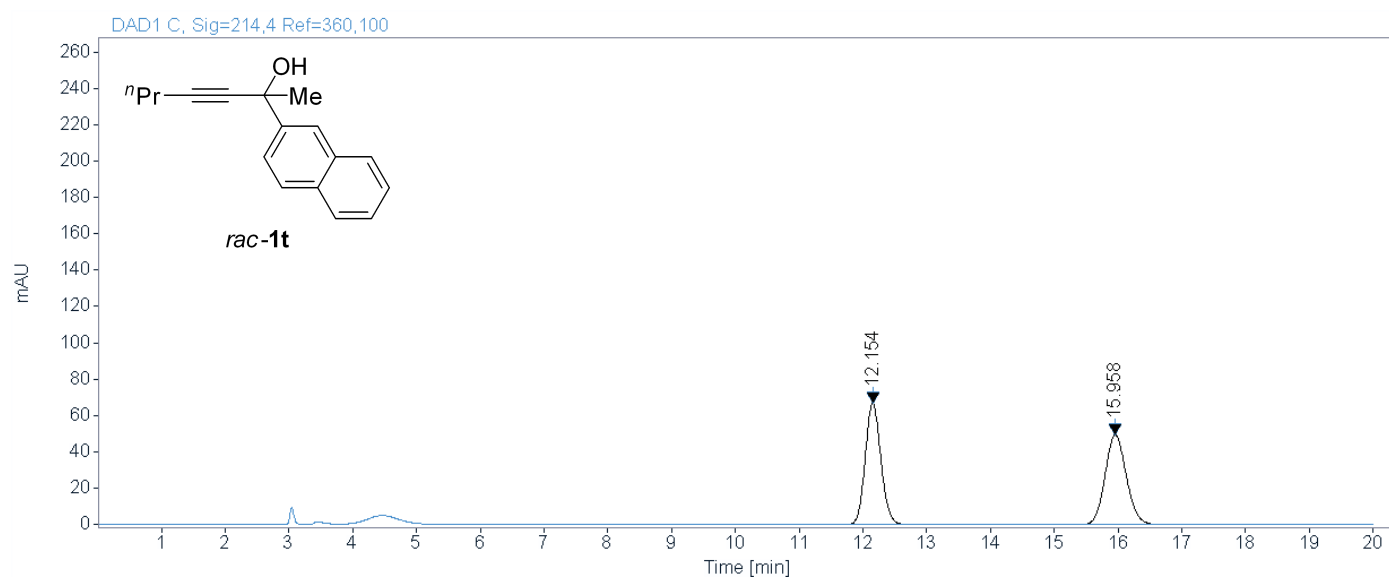


Agilent Technologies

sample zwf-8-080-1-rac-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\linj 2020-05-12 10-02-00\010-P1-C2-zwf-8-080-1-rac.D

Acquisition Data:



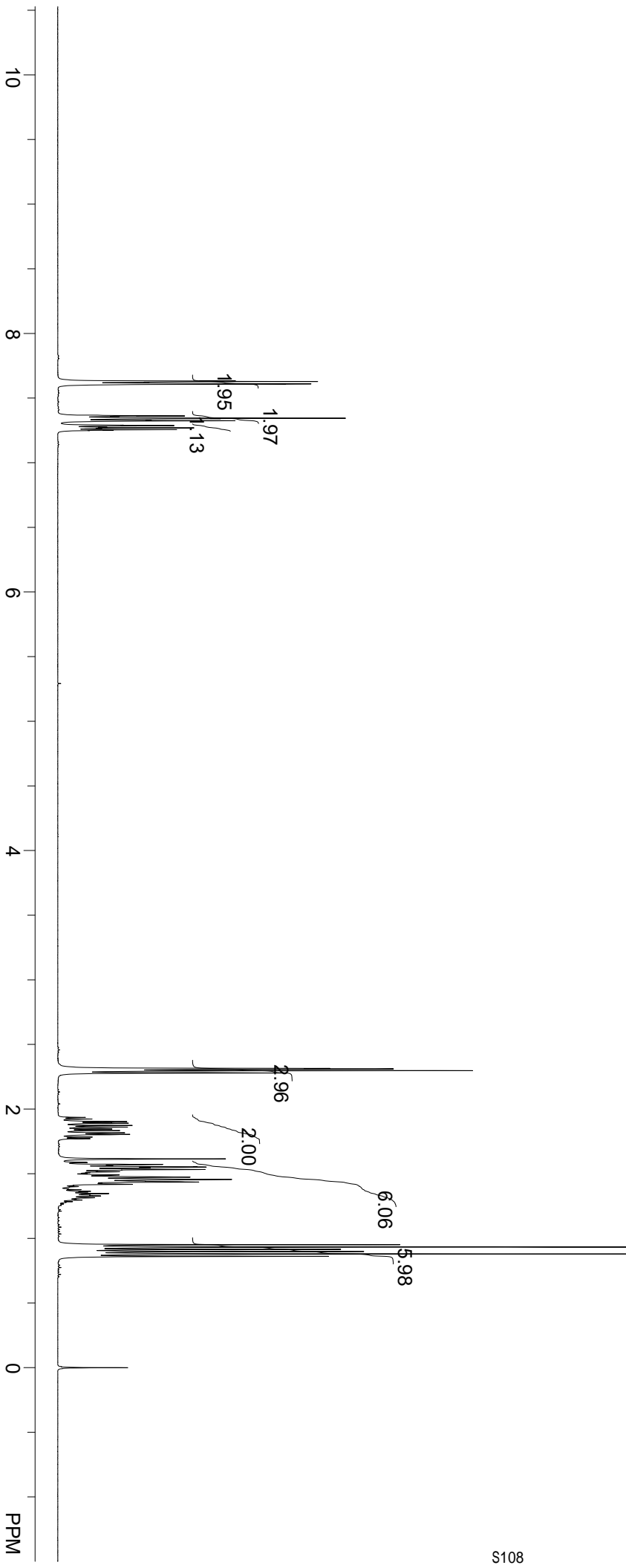
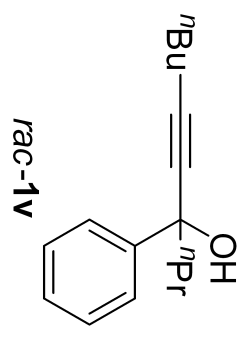
Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
12.154	0.2625	67.0573	1140.9266	49.9645
15.958	0.3597	49.4305	1142.5488	50.0355
	Sum		2283.4755	100.0000

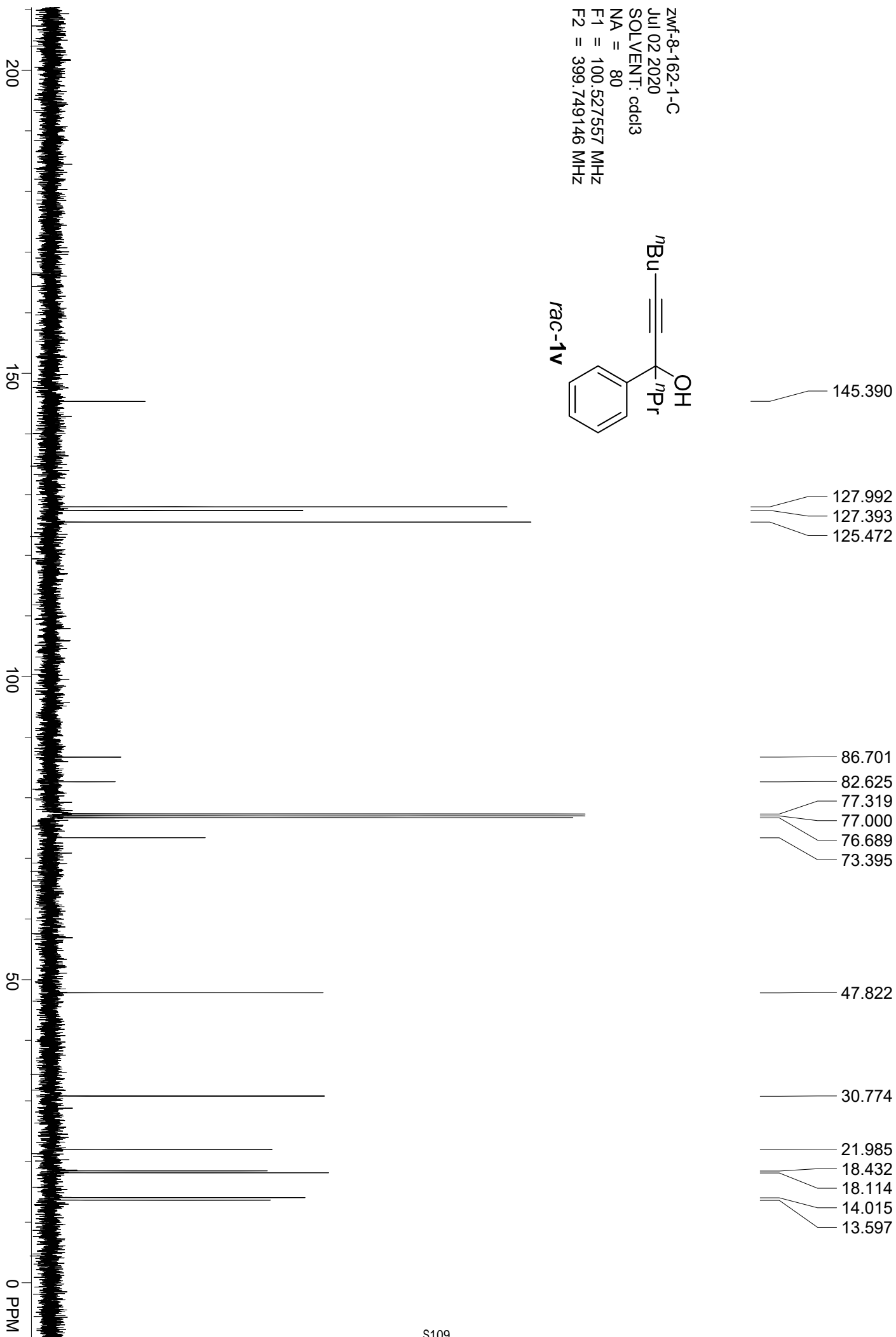
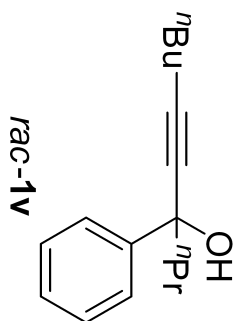
7.628
7.610
7.362
7.344
7.324
7.287
7.270
7.256

2.315
2.311
2.297
2.280
1.936
1.903
1.873
1.861
1.846
1.817
1.805
1.783
1.589
1.572
1.551
1.534
1.474
1.456
1.436
1.417
1.364
1.347
1.328
1.315
1.296
0.951
0.933
0.915
0.899
0.880
0.861
-0.000

Zwf-8-162-1-H
Jul 02 2020
SOLVENT: cdcl3
NA = 4
F1 = 399.749542 MHz
F2 = 100.526031 MHz



ZWF-8-162-1-C
Jul 02 2020
SOLVENT: cdcl3
NA = 80
F1 = 100.527557 MHz
F2 = 399.749146 MHz



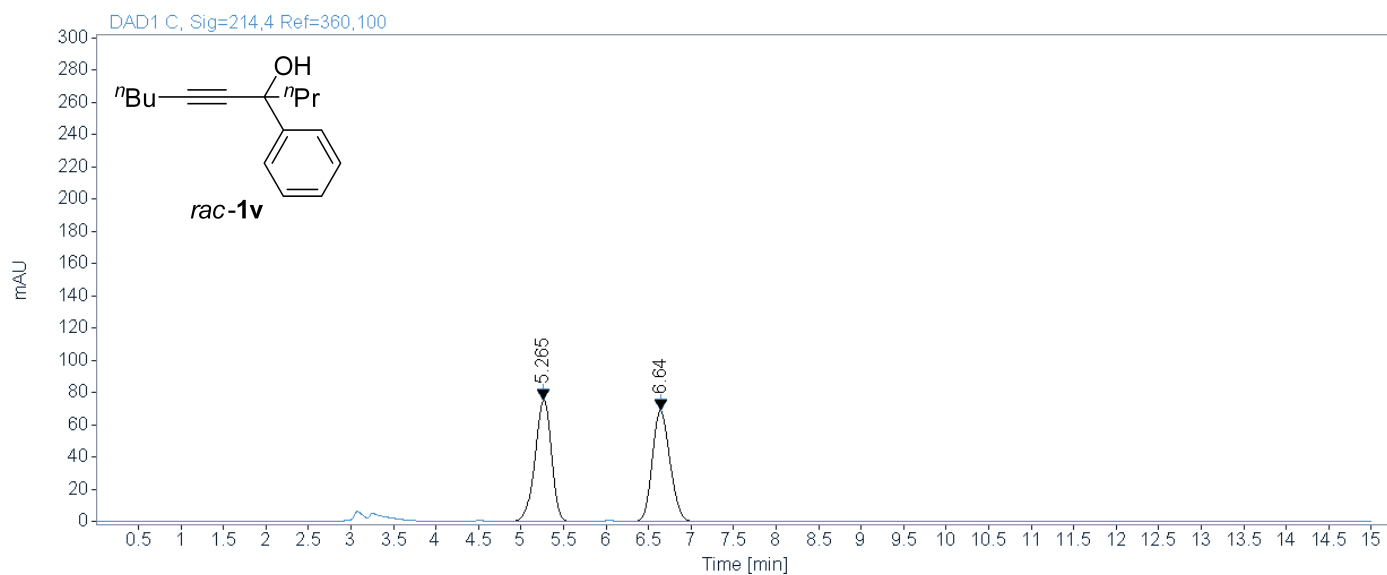
Area Percent Report



sample zwf-8-162-1-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\wgl 2020-07-01 08-16-22\039-P1-C1-zwf-8-162-1.D

Acquisition Data:



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
5.265	0.2082	75.4529	1010.2364	50.3166
6.640	0.2248	68.9570	997.5244	49.6834
	Sum		2007.7608	100.0000

Area Percent Report

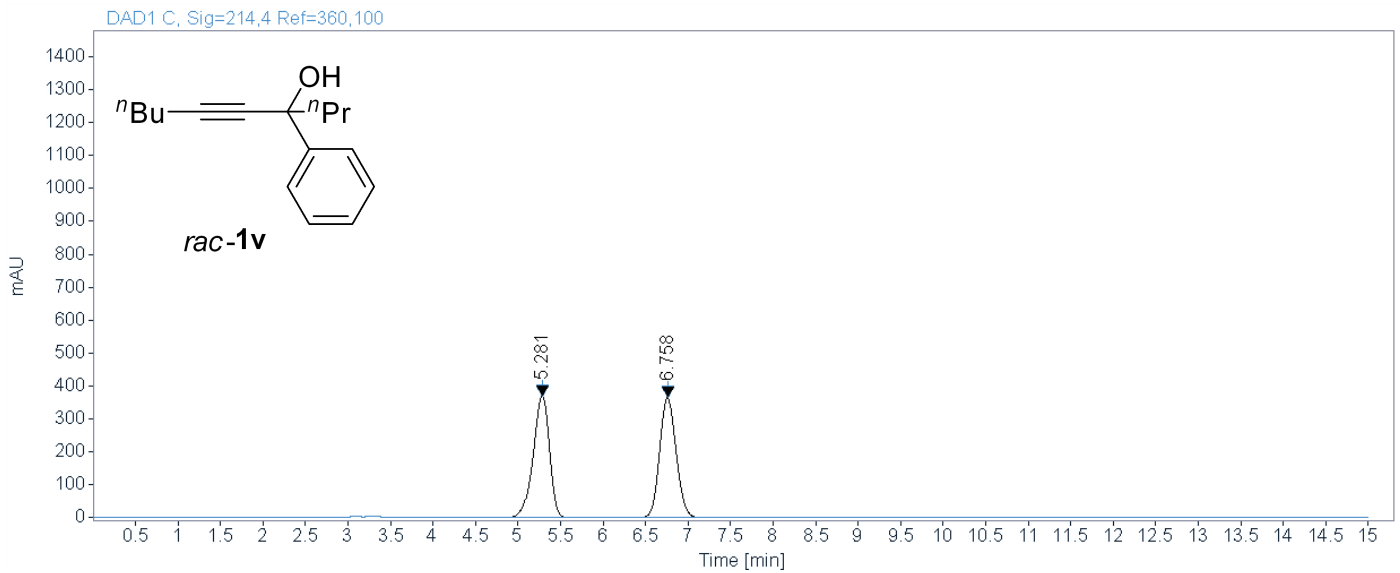


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sample zwf-8-162-1-rac-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\wgl 2020-07-01 08-16-22\040-P1-C2-zwf-8-162-1-rac.D

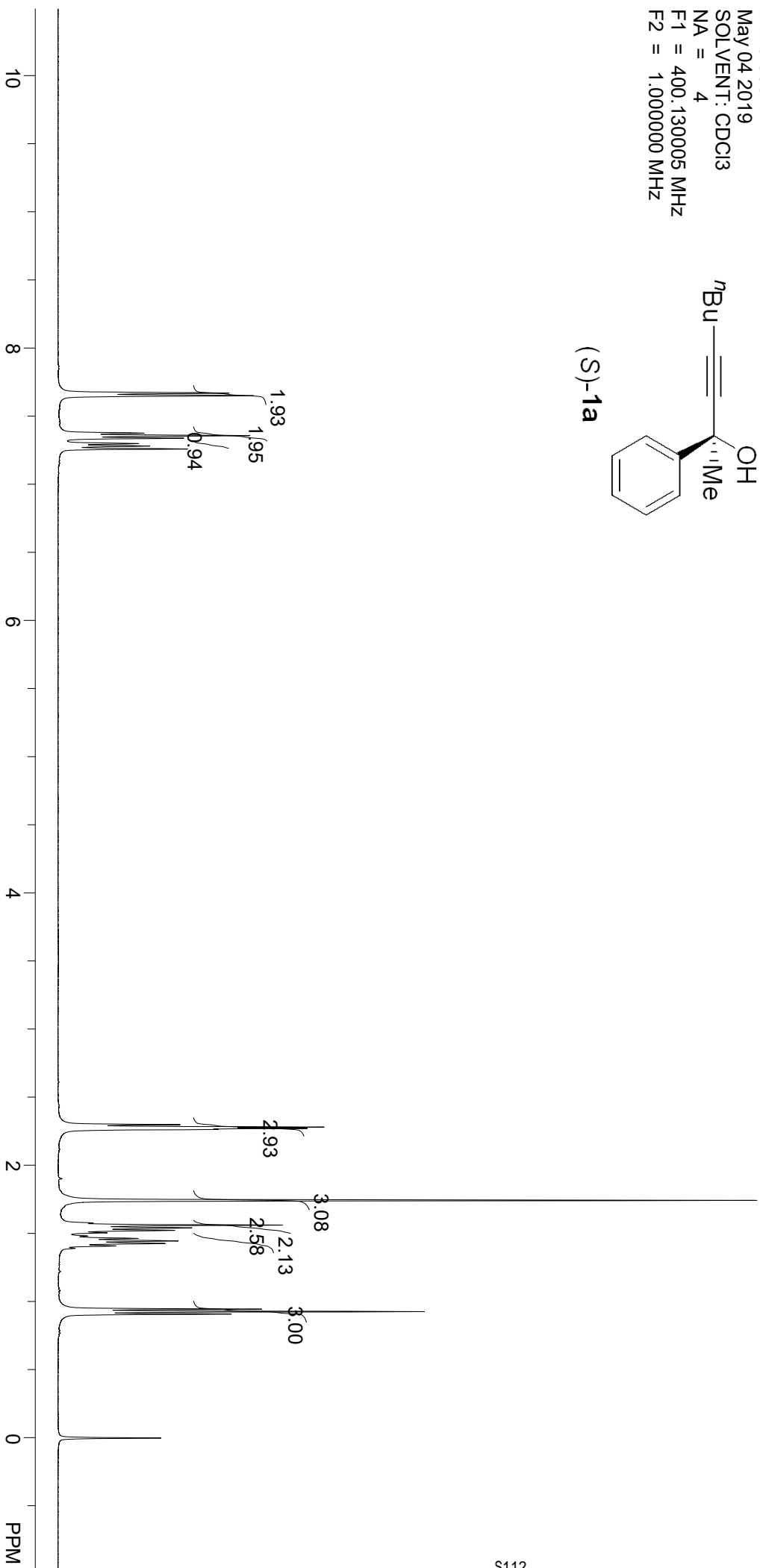
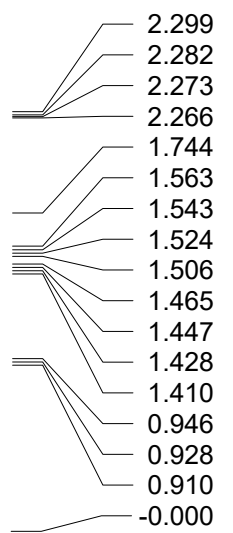
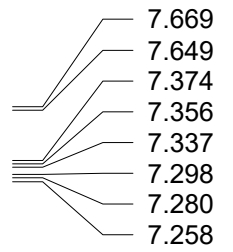
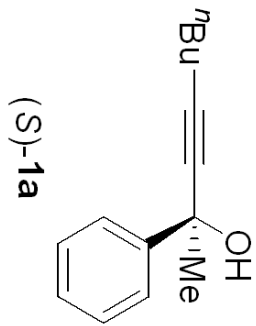
Acquisition Data:



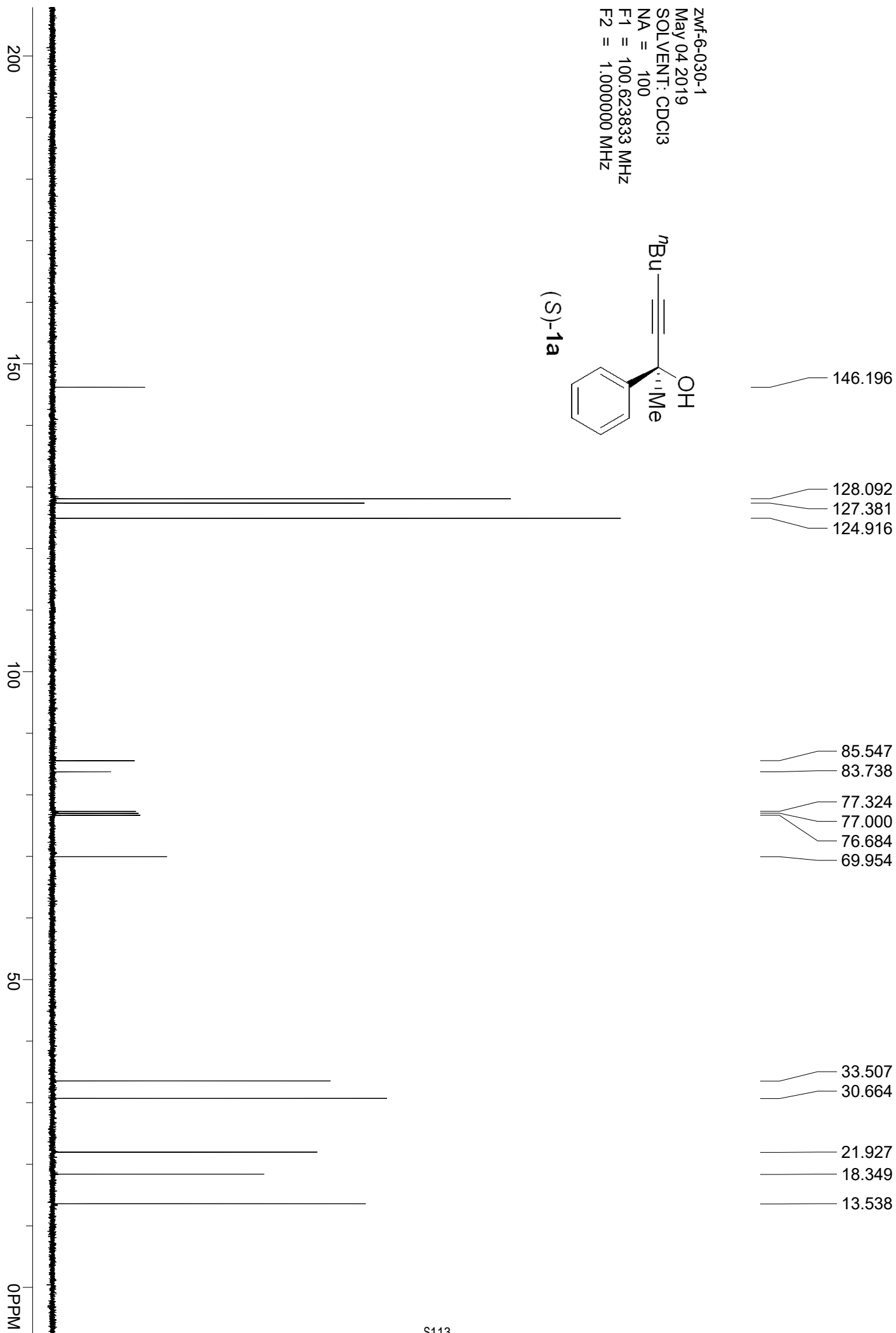
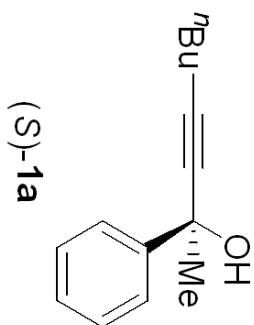
Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
5.281	0.2050	369.4388	4906.7617	49.9637
6.758	0.2118	363.2932	4913.8936	50.0363
		Sum	9820.6553	100.0000

ZWF-6-030-1
May 04 2019
SOLVENT: CDCl3
NA = 4
F1 = 400.130005 MHz
F2 = 1.000000 MHz



Zwf-6-030-1
May 04 2019
SOLVENT: CDCl3
NA = 100
F1 = 100.623833 MHz
F2 = 1.000000 MHz



Area Percent Report

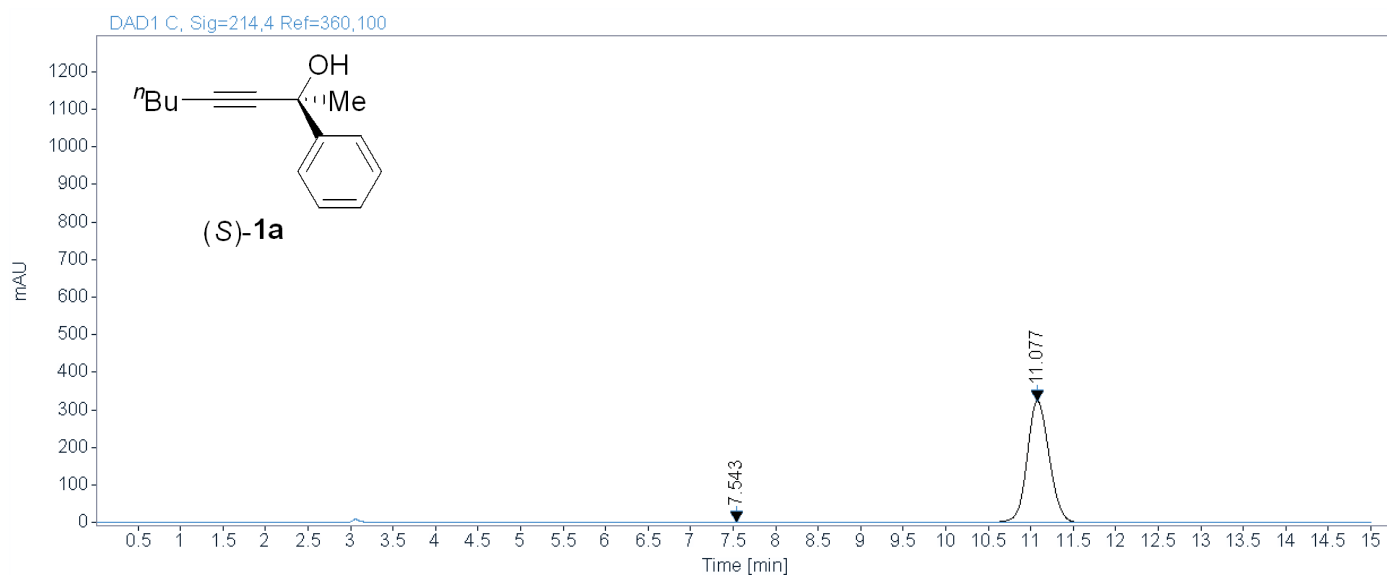


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sample zwf-6-030-1-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\zwf-allenioc acid_LC 2019-05-05 08-23-41\004-P1-C1-zwf-6-030-1.D

Acquisition Data: 5/5/2019 9:12:35 AM



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
7.543	0.2203	0.4801	6.3457	0.1084
11.077	0.2805	324.1383	5847.9878	99.8916
		Sum	5854.3335	100.0000

Area Percent Report

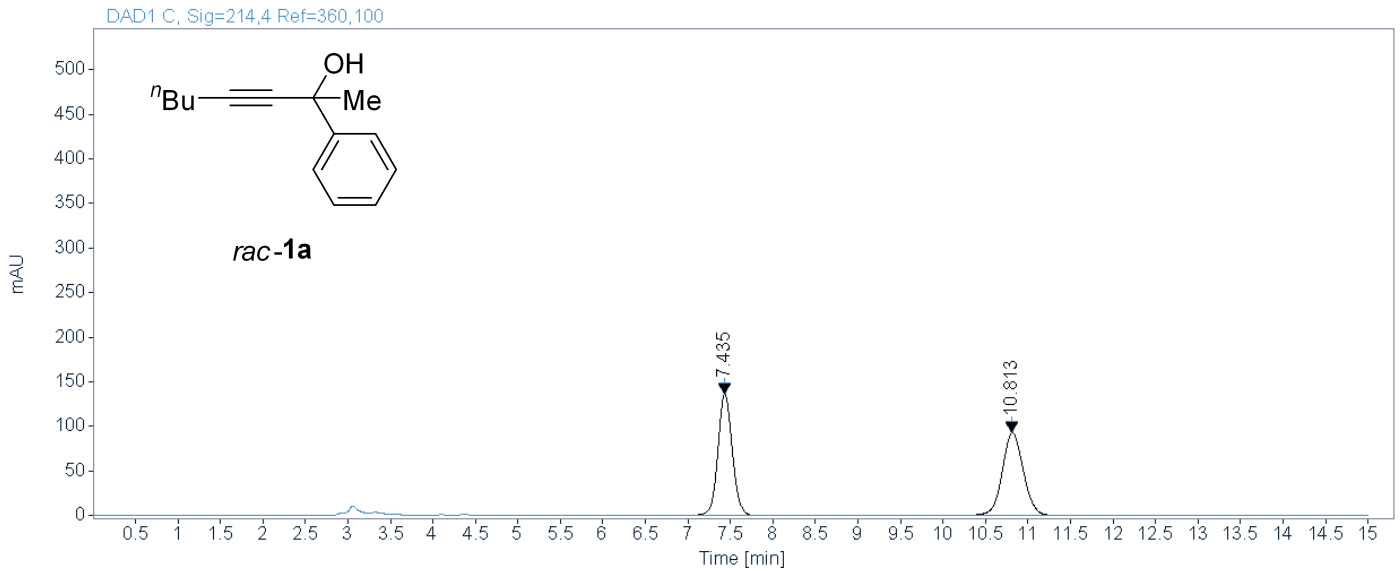


Agilent Technologies

sample zwf-6-030-1-rac-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\zwf-allenioc acid_LC 2019-05-05 08-23-41\005-P1-C2-zwf-6-030-1-rac.D

Acquisition Data: 5/5/2019 9:28:33 AM



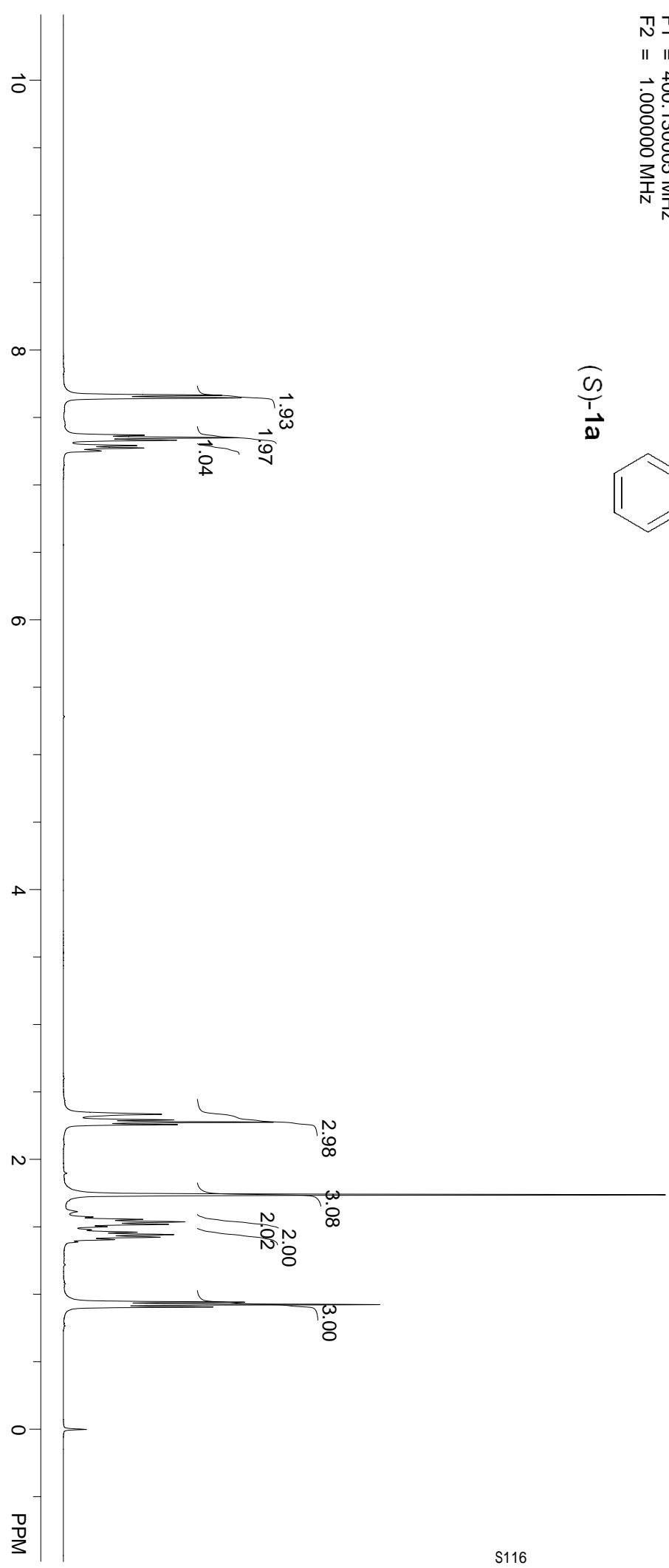
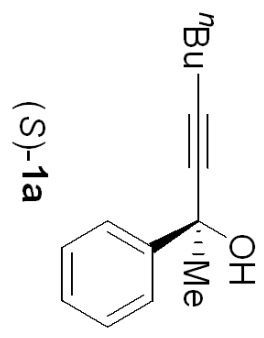
Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
7.435	0.1807	136.3681	1598.3152	49.9177
10.813	0.2677	92.7393	1603.5850	50.0823
		Sum	3201.9001	100.0000

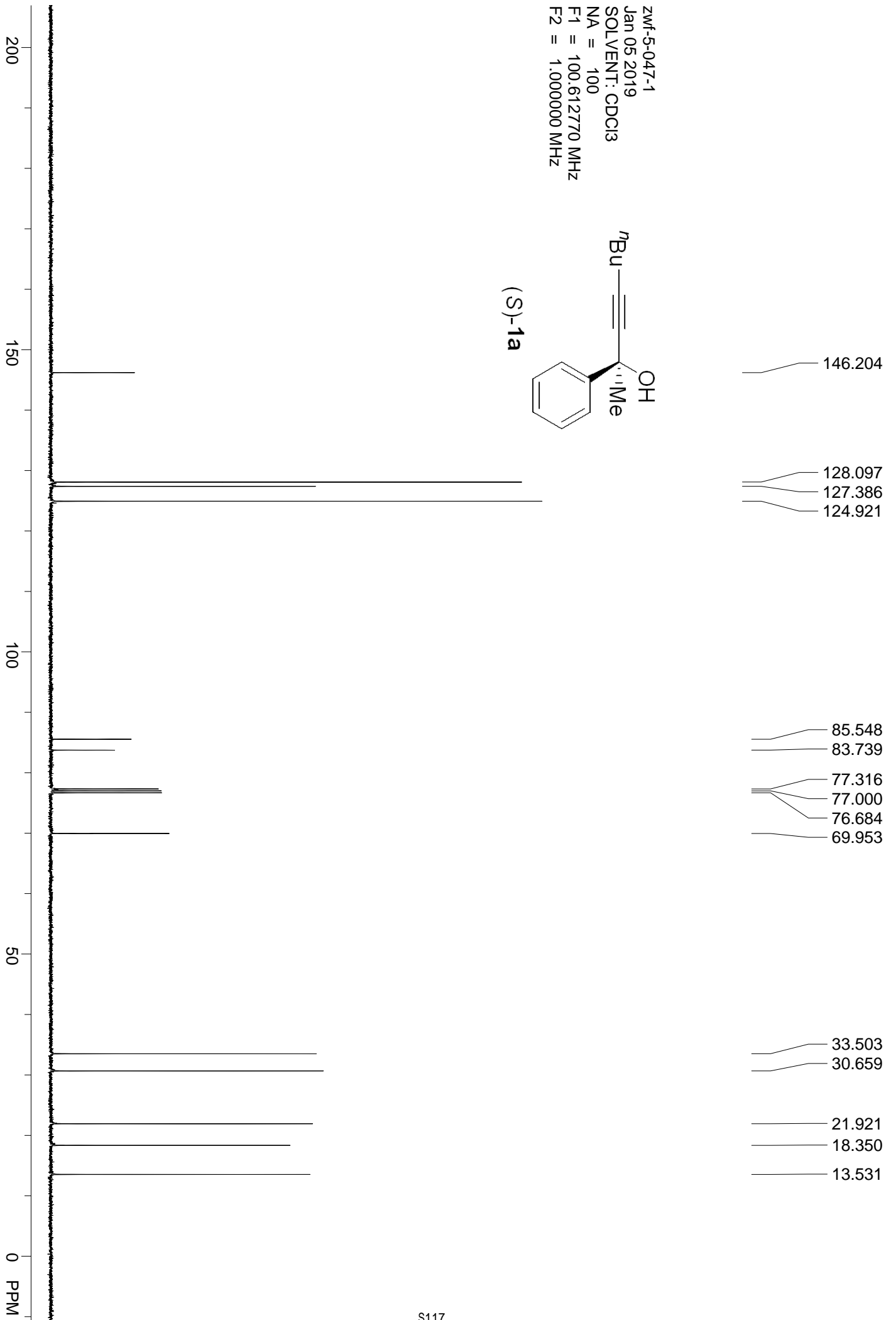
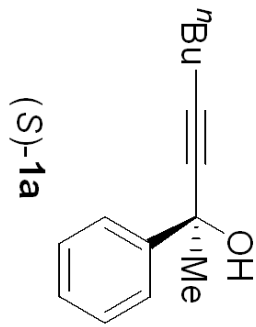
7.664
7.645
7.368
7.350
7.331
7.291
7.274
7.252

2.336
2.294
2.277
2.259
1.739
1.574
1.557
1.539
1.520
1.502
1.480
1.462
1.444
1.425
1.407
1.389
0.943
0.925
0.907
-0.000

zmf-5-047-1
Jan 05 2019
SOLVENT: CDCl3
NA = 4
F1 = 400.130005 MHz
F2 = 1.000000 MHz



zwf-5-047-1
Jan 05 2019
SOLVENT: CDCl3
NA = 100
F1 = 100.612770 MHz
F2 = 1.000000 MHz

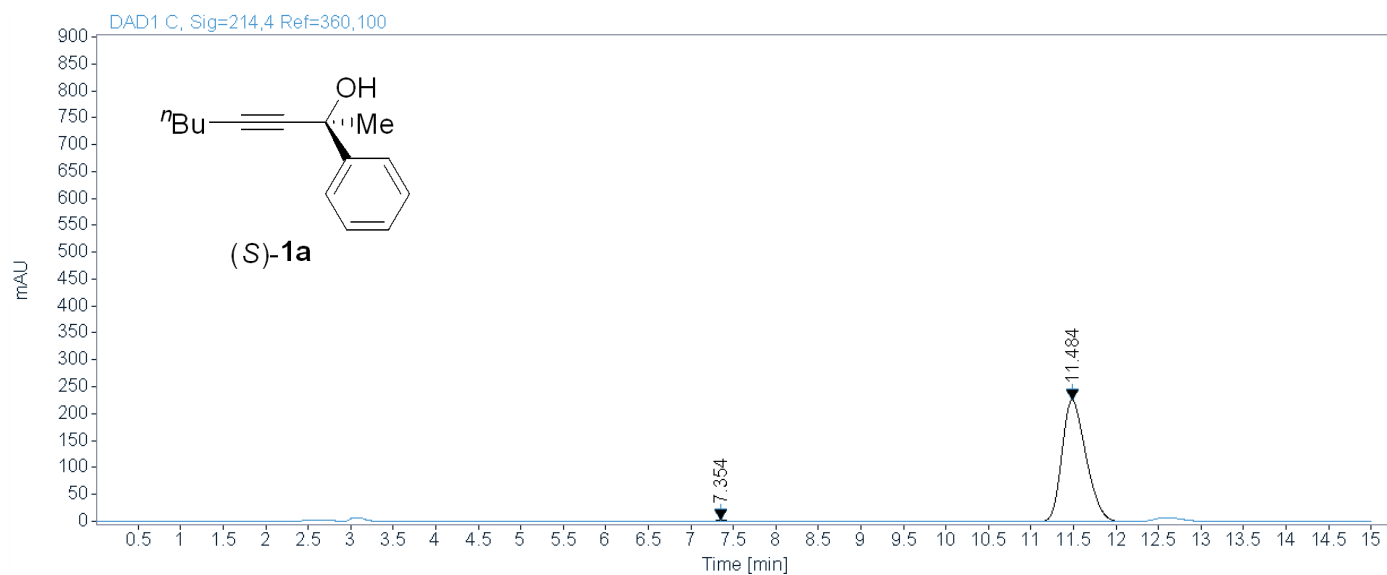


Area Percent Report



Sample name: zwf-5-047-1-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\zwf-allenioc acid_LC 2019-01-06 09-25-17\003-P1-C1-zwf-5-047-1.D



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
7.354	0.1741	2.0668	23.7616	0.5286
11.484	0.3066	226.2634	4471.8086	99.4714
Sum			4495.5702	100.0000

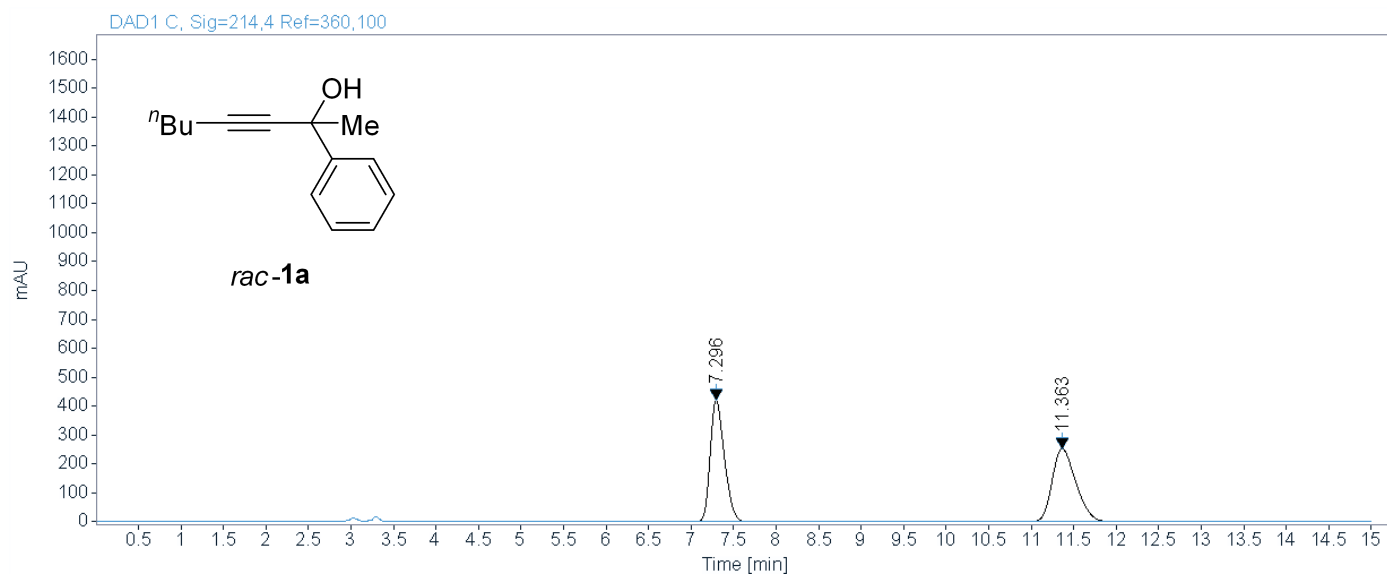
Area Percent Report



Agilent Technologies

Sample name: zwf-5-047-1-rac-AS-H-98-2-1.0-214

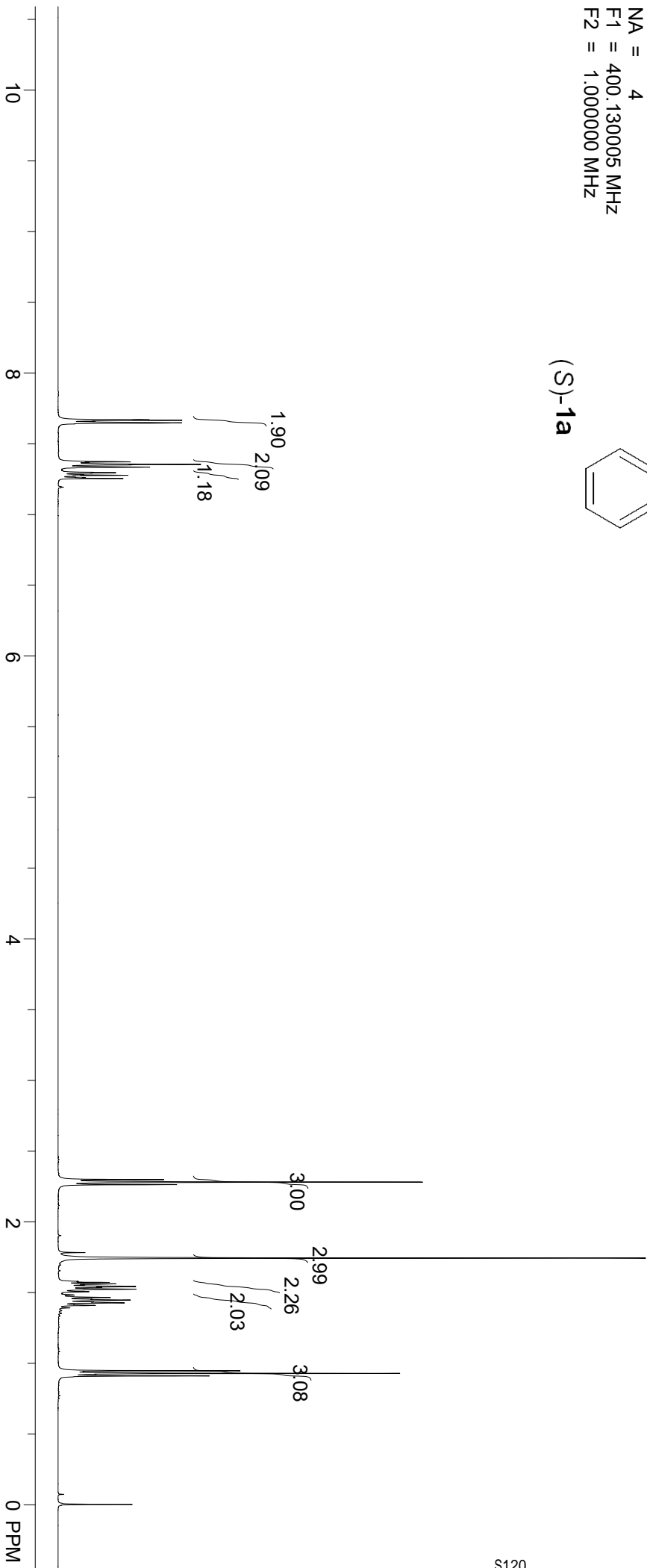
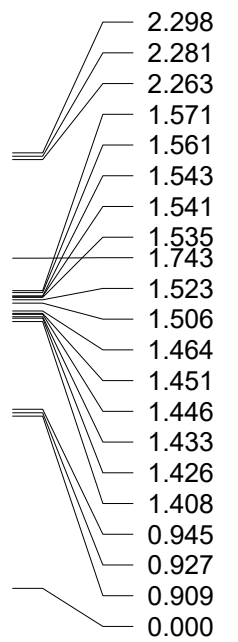
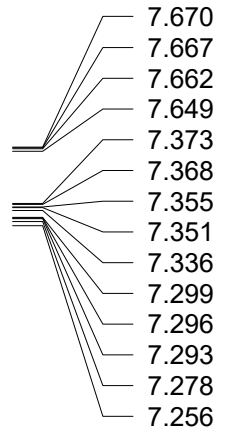
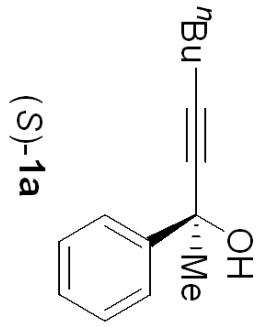
Data file: C:\Users\Public\Documents\ChemStation\1\Data\zwf-allenioc acid_LC 2019-01-06 09-25-17\004-P1-C2-zwf-5-047-1-rac.D



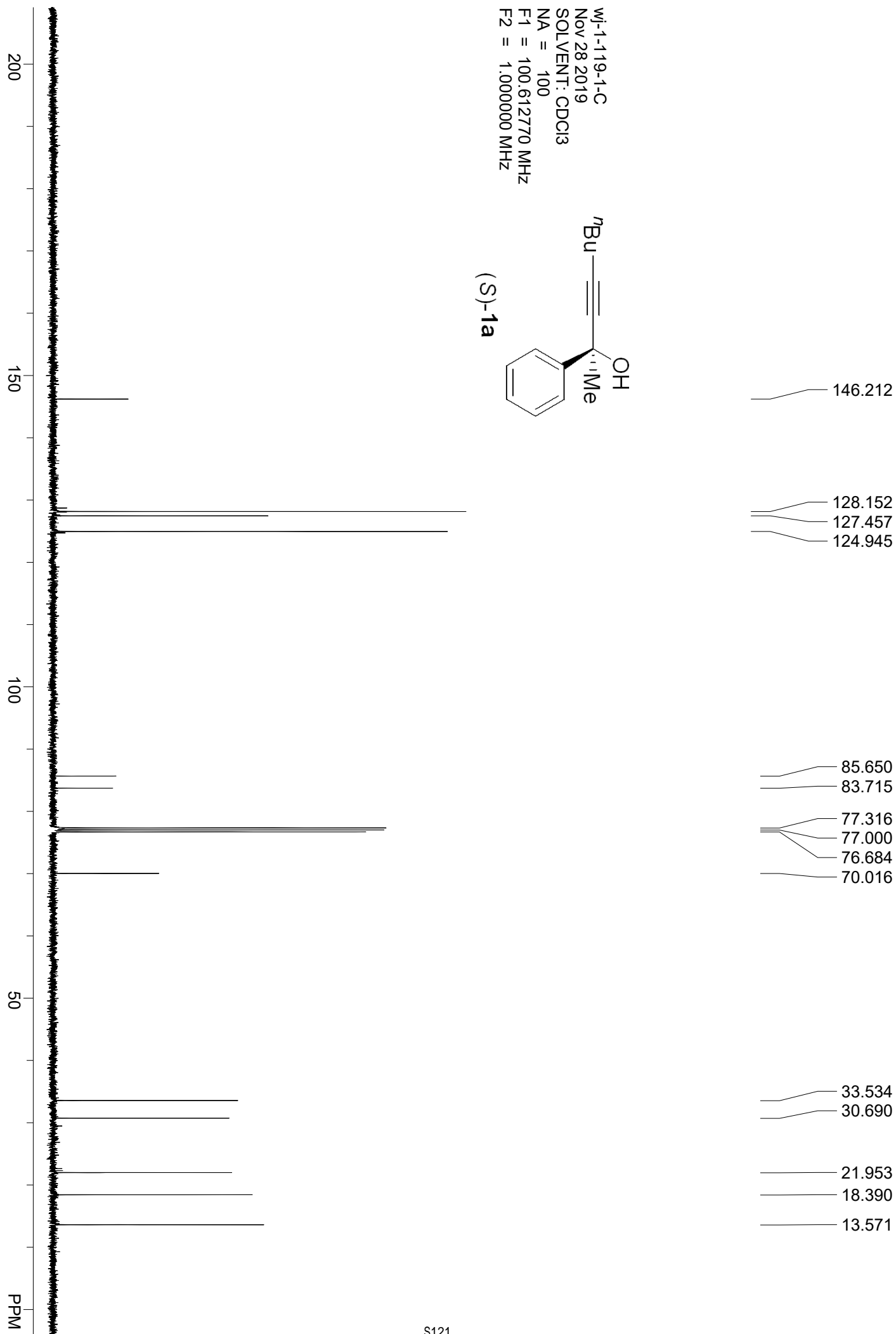
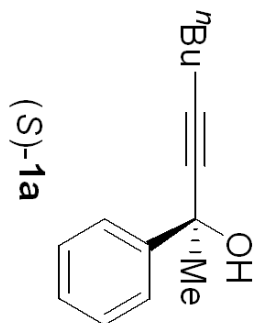
Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
7.296	0.1750	421.8644	4880.0942	49.8696
11.363	0.3006	252.5462	4905.6206	50.1304
Sum			9785.7148	100.0000

wf-1-19-1-H
Nov 28 2019
SOLVENT: CDCl3
NA = 4
F1 = 400.130005 MHz
F2 = 1.000000 MHz



wj-1-19-1-C
Nov 28 2019
SOLVENT: CDCl3
NA = 100
F1 = 100.612770 MHz
F2 = 1.000000 MHz



Area Percent Report

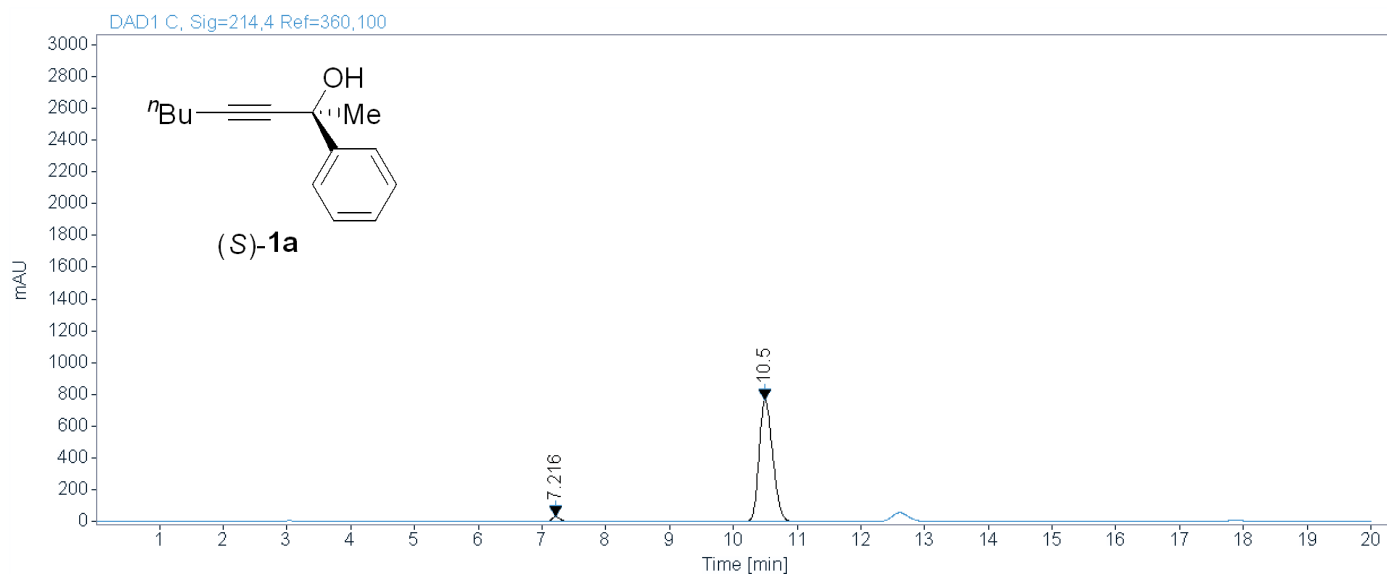


Agilent Technologies

sample wj-1-119-1-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\QAN 2019-11-28 10-39-56\017-P2-C1-wj-1-119-1.D

Acquisition Data:



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
7.216	0.1426	29.3874	268.4327	2.3094
10.500	0.2329	766.0494	11354.9678	97.6906
Sum			11623.4005	100.0000

Area Percent Report

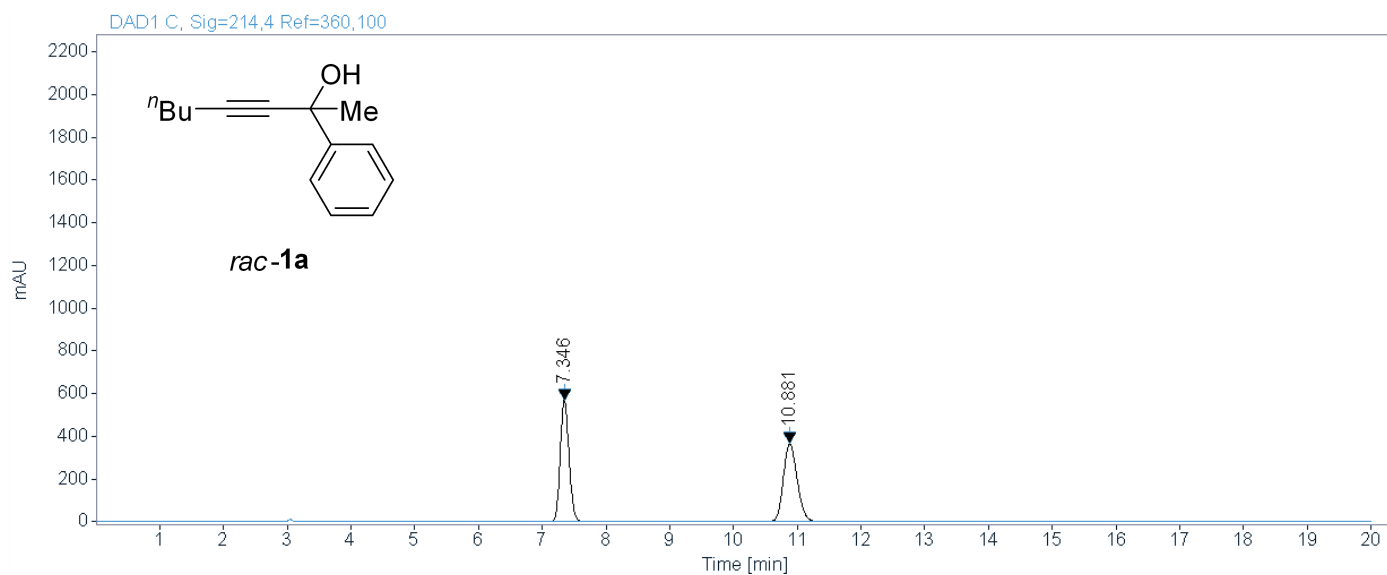


Agilent Technologies

sample wj-1-119-1-rac-AS-H-98-2-1.0-214

Data file: C:\Users\Public\Documents\ChemStation\1\Data\QAN 2019-11-28 10-39-56\018-P2-C2-wj-1-119-1-rac.D

Acquisition Data:



Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Height	Area	Area%
7.346	0.1507	571.1263	5518.2622	49.9304
10.881	0.2368	365.1378	5533.6377	50.0696
Sum			11051.8999	100.0000