Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Enantioselective Nickel-Catalyzed Alkylative Alkyne-Aldehyde Cross-Couplings

Ming Nie, Wenzhen Fu, Ziping Cao, Wenjun Tang*

State Key Laboratory of Bio-Organic and Natural Products Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Ling Ling Road, Shanghai 200032, China

E-mail: tangwenjun@sioc.ac.cn

Table of contents

1. General Information and Materials

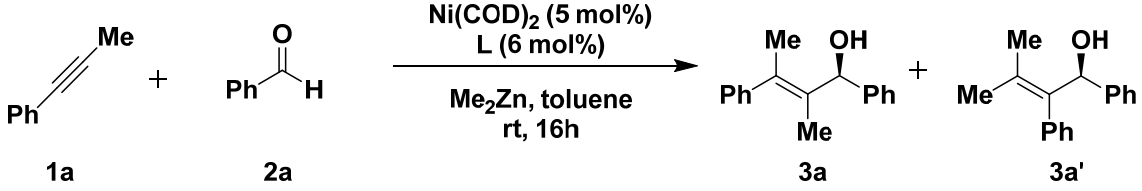
All reactions were carried out under nitrogen atmosphere unless otherwise specified. Unless otherwise noted, commercialized reagents were used without further purifications. All solvents were purified and dried according to standard methods prior to use.

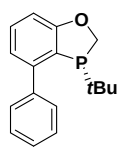
^{1}H NMR, ^{31}P NMR, ^{19}F NMR and ^{13}C NMR data were recorded on a Bruker-Ultrashield PLUS400 NMR or a 500 MHz Agilent spectrometer with $CDCl_3$ or $(CD_3)_2CO$ as the solvent. ^{1}H chemical shifts were referenced to $CDCl_3$ at 7.26 ppm. ^{13}C chemical shifts were referenced to $CDCl_3$ at 77 ppm and obtained with ^{1}H decoupling. ^{31}P chemical shifts were referenced to 85% H_3PO_4 in D_2O at 0.0 ppm as external standard and obtained with ^{1}H decoupling. Multiplicities are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), doublet-doublet (dd), quintet (quint), sextet (sextet), septet (septet), multiplet (m), and broad (br). MS was measured on Agilent 5973N (EI) or Agilent 1100 Series LC/MSD (ESI) or Shimadzu LCMS-2010EV or BRUKERDALTONICS APEX III (HR-ESI) or Waters GCT CA 176 (HR-EI) mass spectrometers. Column chromatography was performed with silica gel (200-300 mesh).

2. General procedures for Asymmetric Alkylative Coupling Reaction

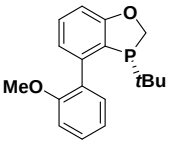
In a glove box, $Ni(COD)_2$ (2.8 mg, 0.01 mmol, 5 mol%) and **L3** (4.0 mg, 0.012 mmol, 6 mol%) were placed into a 10 mL oven-dried Schlenk tube and then sealed with a rubber septum. Toluene (1.4 mL) and $ZnMe_2$ (0.6 mL, 0.6 mmol, 1.0 M in toluene) were added via syringe. The solution was stirred for 5 minutes and aldehyde (0.40 mmol) and alkyne (0.20 mmol) were added respectively. The resulting solution was stirred at ambient temperature for 16 h and quenched with saturated aqueous NH_4Cl solution. The product was extracted with ethyl acetate (3 × 5 mL), and the extract was washed with brine, dried over anhydrous Na_2SO_4, and concentrated in vacuum. The residue was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:20, v/v) to afford the product. Its enantiomeric excess was determined by chiral HPLC.

3. Comparison of Other Ligands

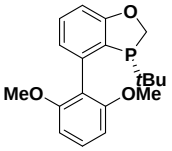




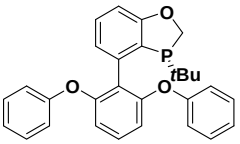
L1
yield 67%, ee 50%



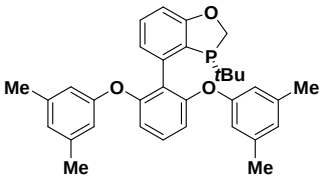
L2
yield 90%, ee 80%



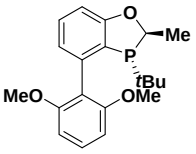
L3
yield 95%, ee 90%



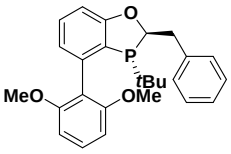
L4
yield 12%, ee 74%



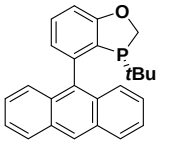
L5
yield < 5%



L6
yield 36%, ee 76%

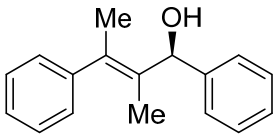


L7
yield < 5%



L8
yield 46%, ee 42%

4. Analytical Data of Chiral Allylic Alcohols



3a

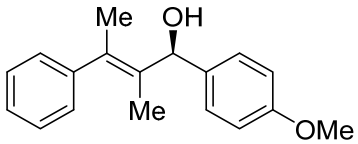
Colorless oil, 90% ee, $[\alpha]_D^{25.5}$ -35.5 (c 0.35, $CHCl_3$) ; $[\alpha]_D^{27.2}$ -24.4 (c 0.53, CH_2Cl_2). The absolute configuration was determined by comparison of its optical rotation to reported data (Y. Yun, S.-F. Zhu, C.-Y. Zhou, Q.-L. Zhou, *J. Am. Chem. Soc*. **2008**, 130, 14052. $[\alpha]_D^{20}$ +21.9 (c 0.5, CH_2Cl_2)).

HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 98:2, 1.0 mL/min, 254 nm UV detector, tR = 12.961 min (*R*) and tR = 21.126min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.41 (m, 2H), 7.39 – 7.34 (m, 2H), 7.34 – 7.30 (m, 2H), 7.29 – 7.25 (m, 1H), 7.24 – 7.20 (m, 1H), 7.17 – 7.13 (m, 2H), 5.97 (d, *J* = 3.8 Hz, 1H), 2.17 (d, *J* = 1.5 Hz, 3H), 1.98 (d, *J* = 4.2 Hz, 1H), 1.43 (d, *J* = 1.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.7, 142.9, 134.2, 132.7, 128.4, 128.3, 128.2, 127.1, 126.5, 125.7, 72.4, 21.0, 14.0.

EI-MS: *m/z* 238.1.



3b

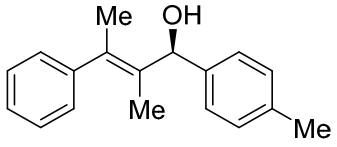
Colorless oil, 93% ee, $[\alpha]_D^{24.6}$ -33.4 (c 0.24, $CHCl_3$). The absolute configuration was determined by comparison of its optical rotation to reported data (Y. Yun, S.-F. Zhu, C.-Y. Zhou, Q.-L. Zhou, *J. Am. Chem. Soc*. **2008**, 130, 14052. $[\alpha]_D^{20}$ +15.0 (c 0.5, CH_2Cl_2)).

HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 6.750 min (*S*) and tR = 7.637 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.32 (m, 4H), 7.25 – 7.21(m, 1H), 7.18 – 7.13 (m, 2H), 6.95 – 6.90 (m, 2H), 5.93 (s, 1H), 3.83 (s, 3H), 2.15 (d, *J* = 1.4 Hz, 3H), 1.91 (d, *J* = 3.2 Hz, 1H), 1.46 (d, *J* = 1.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.8, 144.8, 135.0, 133.9, 132.9, 128.3, 128.2, 126.9, 126.4, 113.9, 72.1, 55.4, 20.9, 14.0.

EI-MS: *m/z* 268.1.



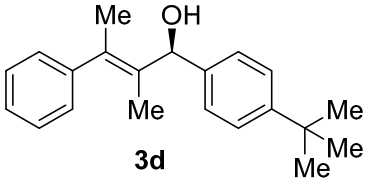
3c

Colorless oil, 94% ee, $[\alpha]_D^{25.4}$ -31.3 (c 0.33, $CHCl_3$). The absolute configuration was determined by comparison of its optical rotation to reported data (Y. Yun, S.-F. Zhu, C.-Y. Zhou, Q.-L. Zhou, *J. Am. Chem. Soc*. **2008**, 130, 14052. $[\alpha]_D^{20}$ +19.7 (c 0.5, CH_2Cl_2)). HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 6.091 min (*S*) and tR = 6.576 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.28(m, 4H), 7.24 – 7.20 (m, 1H), 7.19 – 7.12 (m, 4H), 5.93 (d, *J* = 3.6 Hz, 1H), 2.35 (s, 3H), 2.15 (d, *J* = 1.4 Hz, 3H), 1.94 (d, *J* = 4.2 Hz, 1H), 1.44 (d, *J* = 1.4 Hz, 3H).

^{13}C NMR (126 MHz, CDCl3) δ 144.7, 139.9, 136.7, 133.9, 132.8, 129.1, 128.3, 128.2, 126.4, 125.7, 72.3, 21.2, 20.9, 13.97.

EI-MS: *m/z* 252.2.



3d

Colorless oil, 91% ee, $[\alpha]_D^{25.3}$ -36.1 (c 1.48, $CHCl_3$). The absolute configuration was assigned by analogy.

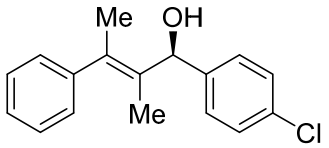
HPLC condition: Chiralcel IC-H column, n-hexane/2-propanol = 98:2, 1.0 mL/min, 230 nm UV detector, tR = 7.352 min (*S*) and tR = 9.542 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.38 (m, 4H), 7.38 – 7.33 (m, 2H), 7.27 – 7.24 (m, 1H), 7.22 – 7.15 (m, 2H), 5.97 (s, 1H), 2.18 (d, *J* = 0.9 Hz, 3H), 2.01 (s, 1H), 1.49 (s, 3H), 1.37 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.0, 144.8, 139.8, 133.9, 132.8, 128.3, 128.2, 126.4, 125.5, 125.4, 72.3, 34.6, 31.5, 20.9, 14.0.

EI-MS: *m/z* 294.

HRMS (EI) Calcd for $C_{21}H_{26}O$: 294.1984; Found 294.1983.



3e

Colorless oil, 86% ee, $[\alpha]_D^{25.6}$ -20.8 (c 0.27, $CHCl_3$). The absolute configuration was assigned by analogy.

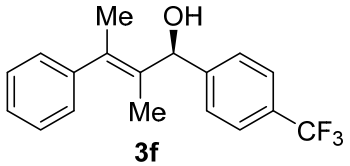
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR =10.520 min (*S*) and tR = 11.542 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.36 (m, 2H), 7.35 – 7.31 (m, 4H), 7.25 – 7.22 (m, 1H), 7.16 – 7.11 (m, 2H), 5.94 (d, *J* = 3.2 Hz, 1H), 2.17 (d, *J* = 1.5 Hz, 3H), 1.93 (d, *J* = 3.9 Hz, 1H), 1.40 (d, *J* = 1.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.4, 141.3, 134.6, 132.8, 132.4, 128.6, 128.4, 128.1, 127.1, 126.6, 71.8, 21.0, 13.9.

EI-MS: *m/z* 272.1

HRMS (EI) Calcd for $C_{17}H_{17}ClO$: 272.0968; Found 272.0973.



3f

Colorless oil, 83% ee, $[\alpha]_D^{24.5}$ -35.9 (c 1.18, $CHCl_3$). The absolute configuration was determined by comparison of its optical rotation to reported data (Y. Yun, S.-F. Zhu, C.-Y. Zhou, Q.-L. Zhou, *J. Am. Chem. Soc*. **2008**, 130, 14052. $[\alpha]_D^{20}$ +20.5 (c 0.5, CH_2Cl_2)).

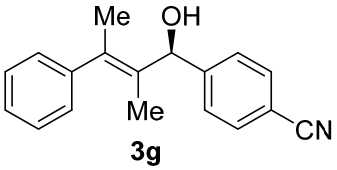
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 98:2, 1.0 mL/min, 254 nm UV detector, tR =11.358 min (*S*) and tR = 12.447 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 – 7.52 (m, 4H), 7.38 – 7.33 (m, 2H), 7.28 – 7.24 (m, 1H), 7.20 – 7.10 (m, 2H), 6.03 (s, 1H), 2.21 (d, *J* = 1.4 Hz, 3H), 2.07 (s, 1H), 1.41 (d, *J* = 1.0 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.9, 144.2, 135.1, 132.2, 130.4, 129.4 (d, *J* = 32.8Hz), 128.2 (d, *J* = 47.9 Hz), 127.2 (d, *J* = 240.7 Hz), 126.7, 126.0, 125.4 (q, *J* = 3.8 Hz), 71.9, 21.0, 13.9.

EI-MS: *m/z* 306.

HRMS (EI) Calcd for $C_{18}H_{17}F_3O$: 306.1232; Found 306.1229.



3g

Colorless oil, 90% ee, $[\alpha]_D^{27.1}$ -28.2 (c 0.44, $CHCl_3$). The absolute configuration was assigned by analogy.

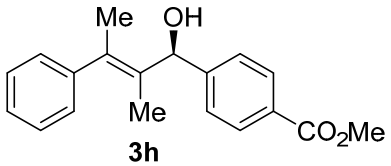
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 98:2, 1.0 mL/min, 254 nm UV detector, tR =30.747 min (*S*) and tR = 33.648 min (*R*).

^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.79 – 7.73 (m, 2H), 7.72 – 7.67 (m, 2H), 7.37 – 7.31 (m, 2H), 7.26 – 7.20 (m, 1H), 7.19 – 7.14 (m, 2H), 6.06 (d, *J* = 3.8 Hz, 1H), 4.79 (d, *J* = 3.9 Hz, 1H), 2.21 (d, *J* = 1.5 Hz, 3H), 1.33 (d, *J* = 1.5 Hz, 3H).

^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 150.9, 145.6, 134.6, 133.8, 132.8, 129.2, 128.9, 127.6, 127.3, 119.7, 111.1, 71.6, 21.2, 14.2.

EI-MS: *m/z* 263.

HRMS (EI) Calcd for $C_{18}H_{17}N O$: 263.1310; Found 263.1313.



3h

Bright yellow oil, 83% ee, $[\alpha]_D^{27.1}$ -19.5 (c 0.62, $CHCl_3$). The absolute configuration was assigned by analogy.

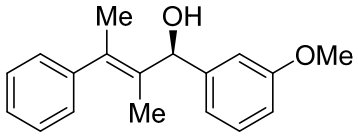
HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 97:3, 1.0 mL/min, 254 nm UV detector, tR =25.385 min (*S*) and tR = 28.238 min (*R*).

^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 8.05 – 7.97 (m, 2H), 7.67 – 7.59 (m, 2H), 7.37 – 7.31 (m, 2H), 7.26 – 7.20 (m, 1H), 7.19 – 7.13 (m, 2H), 6.05 (d, *J* = 3.8 Hz, 1H), 4.68 (d, *J* = 3.9 Hz, 1H), 3.88 (s, 3H), 2.21 (d, *J* = 1.4 Hz, 3H), 1.35 (d, *J* = 1.4 Hz, 3H).

^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 167.3, 150.7, 145.7, 134.2, 134.1, 130.1, 129.5, 129.1, 128.9, 127.2, 126.7, 71.7, 52.3, 21.2, 14.3.

EI-MS: *m/z* 296.

HRMS (EI) Calcd for $C_{19}H_{20}O_3$: 296.1412; Found 296.1409.



3i

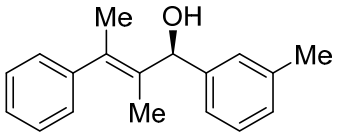
Colorless oil, 96% ee, $[\alpha]_D^{25.5}$ -36.2 (c 0.34, $CHCl_3$). The absolute configuration was determined by comparison of its optical rotation to reported data (Y. Yun, S.-F. Zhu, C.-Y. Zhou, Q.-L. Zhou, *J. Am. Chem. Soc*. **2008**, 130, 14052. $[\alpha]_D^{20}$ +19.1 (c 0.5, CH_2Cl_2)).

HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 254 nm UV detector, tR = 13.322 min (*R*) and tR = 14.553 min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.30 (m, 2H), 7.30 – 7.26 (m, 1H), 7.25 – 7.20 (m, 1H), 7.17 – 7.12 (m, 2H), 7.05 – 7.00 (m, 2H), 6.81 (dd, *J* = 8.1, 2.4 Hz, 1H), 5.94 (s, 1H), 3.83 (s, 3H), 2.16 (d, *J* = 1.4 Hz, 3H), 1.99 (s, 1H), 1.43 (d, *J* = 1.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 144.7, 144.6, 134.2, 132.6, 129.5, 128.3, 128.2, 126.5, 118.1, 112.4, 111.5, 72.3, 55.3, 21.0, 14.0.

EI-MS: *m/z* 268.1.



3j

Colorless oil, 93% ee, $[\alpha]_D^{25.4}$ -34.8 (c 0.32, $CHCl_3$). The absolute configuration was assigned by analogy.

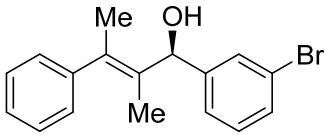
HPLC condition: Chiralcel OD column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 4.903 min (*R*) and tR = 6.017 min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.30 (m, 2H), 7.27 (s, 1H), 7.26 – 7.20 (m, 3H), 7.18 – 7.13 (m, 2H), 7.11 – 7.06 (m, 1H), 5.94 (s, 1H), 2.38 (s, 3H), 2.17(d, *J* = 1.2 Hz, 3H), 1.93 (d, *J* = 3.3 Hz, 1H), 1.44 (d, *J* = 1.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.7, 142.8, 138.1, 134.1, 132.8, 128.34, 128.30, 128.2, 127.9, 126.43, 126.38, 122.8, 72.4, 21.8, 21.0, 14.0.

EI-MS: *m/z* 252.1.

HRMS (EI) Calcd for $C_{18}H_{20}O$: 252.1514; Found 252.1512.



3k

Colorless oil, 90% ee, $[\alpha]_D^{24.9}$ -31.6 (c 0.44, $CHCl_3$). The absolute configuration was assigned by analogy.

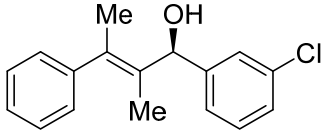
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 5.020 min (*R*) and tR = 8.161 min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 – 7.59 (m, 1H), 7.41 – 7.38 (m, 1H), 7.36 – 7.31 (m, 3H), 7.25 – 7.21 (m, 2H), 7.16 – 7.12 (m, 2H), 5.93 (s, 1H), 2.17(d, *J* = 1.5 Hz, 3H), 2.03 (s, 1H), 1.40 (d, *J* = 1.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.3, 144.3, 134.9, 132.2, 130.2, 130.0, 128.9, 128.4, 128.1, 126.6, 124.3, 122.8, 71.7, 21.0, 13.9.

EI-MS: *m/z* 361.1.

HRMS (EI) Calcd for $C_{17}H_{17}BrO$: 316.0463; Found 316.0462.



3l

Colorless oil, 78% ee, $[\alpha]_D^{24.5}$ -33.5 (c 0.42, $CHCl_3$). The absolute configuration was assigned by analogy.

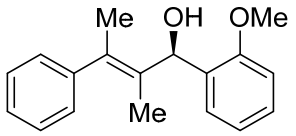
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 4.900 min (*R*) and tR = 7.457 min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.43 (m, 1H), 7.35 – 7.30 (m, 2H), 7.30 – 7.29 (m, 1H), 7.27 – 7.17 (m, 3H), 7.16 – 7.12 (m, 2H), 5.93 (s, 1H), 2.17(d, *J* = 1.5 Hz, 3H), 2.05 (s, 1H), 1.40 (d, *J* = 1.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.0, 144.3, 134.8, 134.5, 132.2, 129.7, 128.4, 128.1, 127.3, 126.6, 126.0, 123.9, 71.8, 21.0, 13.9.

EI-MS: *m/z* 272.0.

HRMS (EI) Calcd for $C_{17}H_{17}ClO$: 272.0968; Found 272.0967.



3m

Colorless oil, 93% ee, $[\alpha]_D^{25.2}$ +3.40 (c 0.67, $CHCl_3$). The absolute configuration was assigned by analogy.

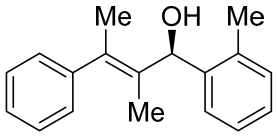
HPLC condition: Chiralcel IC-H column, n-hexane/2-propanol = 99.2:0.8, 1.0 mL/min, 254 nm UV detector, tR = 19.486 min (*R*) and tR = 20.442 min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.5 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.28 – 7.24 (m, 1H), 7.23 – 7.20 (m, 1H), 7.18 – 7.13 (m, 2H), 7.00 – 6.95 (m, 1H), 6.92 – 6.88 (m, 1H), 6.11 (s, 1H), 3,87 (s, 3H), 2.82 (s, 1H), 2.07 (s, 3H), 1.53 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.2, 145.1, 134.2, 131.1, 130.8, 128.4, 128.23, 128.19, 127.2, 126.2, 120.7, 110.5, 69.2, 55.5, 20.8, 14.7.

EI-MS: *m/z* 268.

HRMS (EI) Calcd for $C_{18}H_{20}O_2$: 268.1463; Found 268.1457.



3n

Light yellow oil, 93% ee, $[\alpha]_D^{24.9}$ +37.0 (c 0.32, $CHCl_3$). The absolute configuration was assigned by analogy.

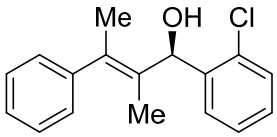
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 5.900 min (*S*) and tR = 7.620 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.7 Hz, 1H), 7.34 – 7.28 (m, 2H), 7.27 – 7.21 (m, 2H), 7.20 – 7.16 (m, 1H), 7.16 – 7.09 (m, 3H), 5.93 (s, 1H), 2.30 (s, 3H), 2.18 (d, *J* = 1.5 Hz, 3H), 1.88 (s, 1H), 1.32 (d, *J* = 1.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.7, 140.9, 135.4, 134.9, 131.3, 130.3, 128.3, 128.0, 127.1, 126.5, 126.0, 125.8, 70.4, 20.7, 19.3, 15.0.

EI-MS: *m/z* 252.1.

HRMS (EI) Calcd for $C_{18}H_{20}O$: 252.1514; Found 252.1513.



3o

Colorless oil, 90% ee, $[\alpha]_D^{24.4}$ +39.6 (c 0.33, $CHCl_3$). The absolute configuration was assigned by analogy.

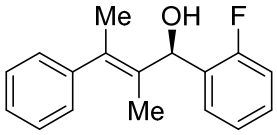
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 5.300 min (*S*) and tR = 5.787 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.2 Hz, 1H), 7.40 – 7.35 (m, 1H), 7.35 – 7.30 (m, 3H), 7.26 – 7.21 (m, 2H), 7.17 – 7.13 (m, 2H), 6.11 (s, 1H), 2.22 (d, *J* = 1.1 Hz, 3H), 1.99 (s, 1H), 1.34 (d, *J* = 1.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.7, 140.3, 136.4, 132.2, 130.1, 129.5, 128.4, 128.3, 128.1, 128.0, 126.8, 126.5, 70.4, 21.1, 14.7.

EI-MS: *m/z* 272.0.

HRMS (EI) Calcd for $C_{17}H_{17}ClO$: 272.0968; Found 272.0969.



3p

Colorless oil, 83% ee, $[\alpha]_D^{25.8}$ -26.8 (c 2.40, $CHCl_3$). The absolute configuration was assigned by analogy.

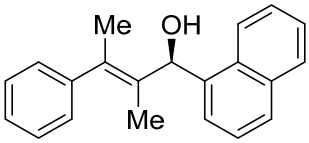
HPLC condition: Chiralcel IC-H column, n-hexane/2-propanol = 99.2:0.8, 1.0 mL/min, 254 nm UV detector, tR = 6.413 (*R*) and tR = 7.219 min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 – 7.60 (m, 1H), 7.35 – 7.31 (m, 2H), 7.30 – 7.26 (m, 1H), 7.25 – 7.21 (m, 1H), 7.20 – 7.17 (m, 1H), 7.16 – 7.12 (m, 2H), 7.08 – 7.03 (m, 1H), 6.21 (s, 1H), 2.18 (s, 3H), 2.08 (s, 1H), 1.46 (d, *J* = 1.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.1 (d, *J* = 246.6 Hz), 144.8, 135.0, 130.7, 129.9 (d, *J* = 13.1 Hz), 128.7 (d, *J* = 8.2Hz), 128.2, 128.1, 127.7 (d, *J* = 4.2 Hz), 126.4, 124.0 (d, *J* = 41.2Hz), 115.2 (d, *J* = 21.6Hz), 67.6, 20.7, 14.0.

EI-MS: *m/z* 256.

HRMS (EI) Calcd for $C_{17}H_{17}OF$: 255.1263; Found 256.1257.



3q

Colorless oil, 92% ee, $[\alpha]_D^{25.0}$ +119.2 (c 0.39, $CHCl_3$). The absolute configuration was assigned by analogy.

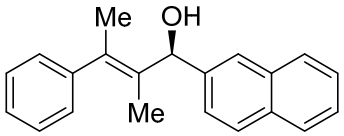
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 93:7, 1.0 mL/min, 254 nm UV detector, tR = 17.322 min (*S*) and tR = 33.342 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 – 8.00 (m, 1H), 7.90 – 7.85 (m, 1H), 7.82 – 7.76 (m, 2H), 7.52 – 7.47 (m, 3H), 7.32 – 7.27 (m, 2H), 7.23 – 7.18 (m, 1H), 7.17 – 7.10 (m, 2H), 6.46 (s, 1H), 2.30 (d, *J* = 1.5 Hz, 3H), 2.02 (s, 1H), 1.32 (d, *J* = 1.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.5, 138.3, 135.3, 133.8, 132.7, 130.8, 129.0, 128.3, 128.1, 128.0, 126.6, 126.1, 125.6, 125.5, 123.5, 123.2, 70.4, 20.9, 15.4.

EI-MS: *m/z* 288.1.

HRMS (EI) Calcd for $C_{21}H_{20}O$: 288.1514; Found 288.1516



3r

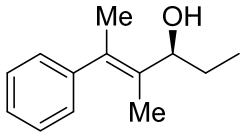
Colorless oil, 93% ee, $[\alpha]_D^{25.6}$-56.5 (c 0.50, $CHCl_3$). The absolute configuration was determined by comparison of its optical rotation to reported data (Y. Yun, S.-F. Zhu, C.-Y. Zhou, Q.-L. Zhou, *J. Am. Chem. Soc*. **2008**, 130, 14052. $[\alpha]_D^{20}$ +35.0 (c 0.5, CH_2Cl_2)).

HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 8.018 min (*S*) and tR = 9.271 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 – 7.93 (m, 1H), 7.87 – 7.78 (m, 3H), 7.50 – 7.43 (m, 3H), 7.34 – 7.29 (m, 2H), 7.24 – 7.19 (m, 1H), 7.19 – 7.14 (m, 2H), 6.11 (s, 1H), 2.22 (d, *J* = 1.5 Hz, 3H), 2.13 (s, 1H), 1.44 (d, *J* = 1.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.6, 140.4, 134.5, 133.5, 132.8, 132.6, 128.3, 128.17, 128.15, 128.12, 127.7, 126.5, 126.2, 125.8, 124.2, 124.1, 72.5, 21.1, 14.0.

EI-MS: *m/z* 288.1.



3s

Colorless oil, 88% ee, $[\alpha]_D^{24.9}$ +49.2 (c 0.49, $CHCl_3$). The absolute configuration was assigned by analogy.

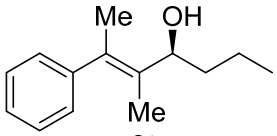
HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 94:6, 1.0 mL/min, 254 nm UV detector, tR = 5.375 min (*R*) and tR = 6.92 min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (t, *J* = 7.6 Hz, 2H), 7.25 – 7.18 (m, 1H), 7.12 (d, *J* = 7.1 Hz, 2H), 4.71 (t, *J* = 7.2 Hz, 1H), 2.01 (d, *J* = 1.2 Hz, 3H), 1.78 – 1.69 (m, 1H), 1.66 – 1.56 (m, 2H), 1.53 (d, *J* = 1.3 Hz, 3H), 0.97 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.2, 133.5, 132.6, 128.3, 128.1, 126.3, 72.7, 28.3, 20.5, 13.2, 10.4.

EI-MS: *m/z* 190.

HRMS (EI) Calcd for $C_{13}H_{18}O$:190.1358; Found 190.1361.



3t

Colorless oil, 85% ee, $[\alpha]_D^{25.6}$ +33.6 (c 1.51, $CHCl_3$). The absolute configuration was determined by comparison of its optical rotation to reported data (Y. Yun, S.-F. Zhu, C.-Y. Zhou, Q.-L. Zhou, *J. Am. Chem. Soc*. **2008**, 130, 14052. $[\alpha]_D^{20}$ -18.0 (c 0.5, CH_2Cl_2)).

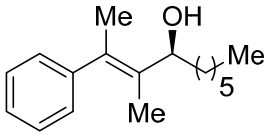
HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 99.2:0.8, 1.0 mL/min, 210 nm UV detector, tR = 13.805 min (*R*) and tR = 18.357 min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (t, *J* = 7.5 Hz, 2H), 7.25 – 7.20 (m, 1H), 7.11 (d, *J* = 7.4 Hz, 2H), 4.80 (t, *J* = 7.0 Hz, 1H), 2.00 (s, 3H), 1.73 – 1.66 (m, 1H), 1.57 – 1.53 (m, 4H), 1.50 – 1.43 (m, 1H), 1.41 – 1.34 (m, 1H), 1.27 (s, 1H), 1.00 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.2, 133.1, 133.0, 128.3, 128.2, 126.3, 71.0, 37.6, 20.5, 19.3, 14.3, 13.3.

EI-MS: *m/z* 204.

HRMS (EI) Calcd for $C_{14}H_{20}O$:204.1514; Found 204.1513.



3u

Light yellow oil, 84% ee, $[\alpha]_D^{25.7}$ +22.1(c 2.23, $CHCl_3$). The absolute configuration was assigned by analogy.

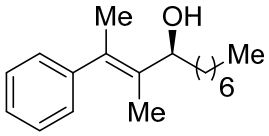
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 99.2:0.8, 1.0 mL/min, 254 nm UV detector, tR = 9.399 min (*S*) and tR = 10.369 min (*R*).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.29 (m, 2H), 7.25 – 7.19 (m, 1H), 7.11 (d, *J* = 7.0 Hz, 2H), 4.78 (t, *J* = 7.0 Hz, 1H), 2.00 (d, *J* = 1.2 Hz, 3H), 1.73 – 1.67 (m, 1H), 1.65 – 1.56 (m, 2H), 1.53 (d, *J* = 1.2 Hz, 3H), 1.37 – 1.29 (m, 8H), 0.93 – 0.89 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.2, 133.1, 133.0, 128.3, 128.1, 126.3, 71.2, 35.4, 32.0, 29.5, 26.0, 22.8, 20.5, 14.2, 13.3.

EI-MS: *m/z* 246.

HRMS (EI) Calcd for $C_{17}H_{26}O$:246.1984; Found 246.1981.



3v

Colorless oil, 87% ee, $[\alpha]_D^{25.7}$ +23.4 (c 2.75, $CHCl_3$). The absolute configuration was assigned by analogy.

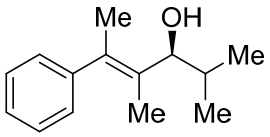
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 99.2:0.8, 1.0 mL/min, 210 nm UV detector, tR = 8.824 min (*S*) and tR = 9.696 min (*R*).

^{1}H NMR (500 MHz, $(CD_3)_2CO$) δ 7.37 – 7.30 (m, 2H), 7.25 – 7.19 (m, 1H), 7.12 (d, *J* = 8.0 Hz, 2H), 4.78 – 4.71 (m, 1H), 3.63 (d, *J* = 4.0 Hz, 1H), 1.98 (s, 3H), 1.72 – 1.64 (m, 1H), 1.55 – 1.50 (m, 4H), 1.43 – 1.26 (m, 10H), 0.94 – 0.88 (m, 3H).

^{13}C NMR (126 MHz, $(CD_3)_2CO$) δ 146.6, 135.4, 132.0, 129.14, 129.06, 127.0, 70.9, 36.5, 32.8, 30.7, 30.3, 26.9, 23.5, 20.7, 14.6, 14.0.

EI-MS: *m/z* 260.

HRMS (EI) Calcd for $C_{18}H_{28}O$:260.2140; Found 260.2144.



3w

Colorless oil, 95% ee, $[\alpha]_D^{26.0}$ +84.0 (c 1.24, $CHCl_3$). The absolute configuration was assigned by analogy.

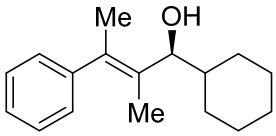
HPLC condition: Chiralcel IC-H column, n-hexane/2-propanol = 99.2:0.8, 1.0 mL/min, 210 nm UV detector, tR = 7.556 min (*R*) and tR = 8.022 min (*S*).

^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.36 – 7.29 (m, 2H), 7.24 – 7.18 (m, 1H), 7.15 – 7.07 (m, 2H), 4.29 (d, *J* = 9.2 Hz, 1H), 3.68 (s, 1H), 1.97 (d, *J* = 1.4 Hz, 3H), 1.86 – 1.75 (m, 1H), 1.49 (d, *J* = 1.4 Hz, 3H), 1.09 (d, *J* = 6.5 Hz, 3H), 0.87 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 146.7, 134.5, 133.1, 129.1, 128.9, 127.0, 76.6, 33.3, 21.0, 20.3, 19.3, 14.2.

EI-MS: *m/z* 204.

HRMS (EI) Calcd for $C_{14}H_{20}O$:204.1514; Found 204.1518.



3x

Colorless oil, 93% ee, $[\alpha]_D^{24.9}$ +68.0 (c 0.54, $CHCl_3$). The absolute configuration was assigned by analogy.

HPLC condition: Chiralcel IC-H column, n-hexane/2-propanol = 99.2:0.8, 1.0 mL/min, 250 nm UV detector, tR = 9.195 min (*S*) and tR = 10.520 min (*R*).

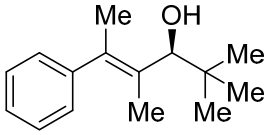
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.29 (m, 2H), 7.25 – 7.19 (m, 1H), 7.15 – 7.08 (m, 2H), 4.40 (d, *J* = 9.4 Hz, 1H), 2.17 (d, *J* = 12.8 Hz, 1H), 1.99 (d, *J* = 1.5 Hz, 3H), 1.84 –

1.68 (m, 3H), 1.64 – 1.59 (m, 1H), 1.54 – 1.52 (m, 1H), 1.51 (d, *J* = 1.5 Hz, 3H), 1.37 – 1.10 (m, 4H), 1.10 – 1.01 (m, 1H), 0.98 – 0.90 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.3, 134.3, 131.9, 128.3, 128.1, 126.3, 75.8, 41.9, 30.3, 29.1, 26.7, 26.4, 26.1, 20.8, 13.7.

EI-MS: *m/z* 244.

HRMS (EI) Calcd for $C_{17}H_{24}O$:244.1827; Found 244.1830.



3y

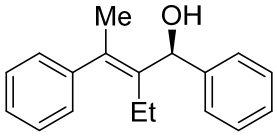
Light yellow oil, 95% ee, $[\alpha]_D^{26.5}$ +67.1 (c 0.76, $CHCl_3$). The absolute configuration was assigned by analogy.

HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 99.2:0.8, 1.0 mL/min, 210 nm UV detector, tR = 10.238 min (*R*) and tR = 13.711 min (*S*).

^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.37 – 7.29 (m, 2H), 7.24 – 7.18 (m, 1H), 7.16 – 7.08 (m, 2H), 4.51 (d, *J* = 4.4 Hz, 1H), 3.73 (d, *J* = 4.4 Hz, 1H), 1.95 (d, *J* = 1.4 Hz, 3H), 1.53 (d, *J* = 1.4 Hz, 3H), 1.02 (s, 9H).

^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 147.1, 134.5, 134.0, 129.3, 128.9, 126.9, 77.3, 38.0, 27.7, 22.3, 16.4.

EI-MS: *m/z* 218.



3z

Colorless oil, 90% ee, $[\alpha]_D^{25.5}$-32.5 (c 0.37, $CHCl_3$). The absolute configuration was assigned by analogy.

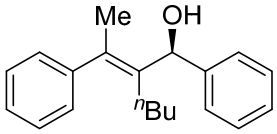
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 5.113 min (*R*) and tR = 7.524 min (*S*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 – 7.44 (m, 2H), 7.39 – 7.30 (m, 4H), 7.28 – 7.22 (m, 2H), 7.19 – 7.15 (m, 2H), 5.95 (s, 1H), 2.10 (s, 3H), 2.02 – 1.93 (m, 2H), 1.88 – 1.80 (m, 1H), 0.67 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.9, 143.3, 138.7, 135.6, 128.4, 128.1, 127.9, 127.0, 126.4, 125.8, 72.9, 22.2, 21.7, 15.2.

EI-MS: *m/z* 252.0.

HRMS (EI) Calcd for $C_{18}H_{20}O$:252.1514; Found 252.1511.



3aa

Colorless oil, 90% ee, $[\alpha]_D^{25.5}$-28.3 (c 0.17, $CHCl_3$). The absolute configuration was assigned by analogy.

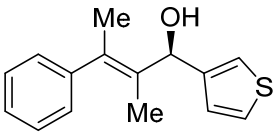
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 90:10, 1.0 mL/min, 254 nm UV detector, tR = 10.520 min (*S*) and tR = 11.542 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 – 7.46 (m, 2H), 7.41 – 7.37 (m, 2H), 7.37 – 7.33 (m, 2H), 7.31 – 7.23 (m, 2H), 7.20 – 7.15 (m, 2H), 5.96 (s, 1H), 2.13 (s, 3H), 1.99 – 1.89 (m, 2H), 1.82 – 1.76 (m, 1H), 1.39 – 1.09 (m, 2H), 0.96 – 0.92 (m, 2H), 0.58 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.9, 143.3, 137.7, 135.8, 128.4, 128.3, 127.9, 127.0, 126.4, 125.8, 73.0, 32.7, 29.1, 23.1, 21.8, 13.6.

EI-MS: *m/z* 280.3.

HRMS (EI) Calcd for $C_{20}H_{24}O$:280.1827; Found 280.1829.



3ab

Light yellow oil, 90 % ee, $[\alpha]_D^{25.9}$ -61.8 (c 1.38, $CHCl_3$). The absolute configuration was assigned by analogy.

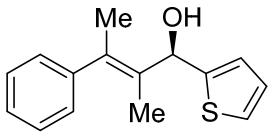
HPLC condition: Chiralcel OD-H column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 254 nm UV detector, tR = 9.299 (*S*) and tR = 12.682 min (*R*).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 3H), 7.28 – 7.23 (m, 2H), 7.20 – 7.15 (m, 2H), 7.09 – 7.05 (m, 1H), 5.98 (s, 1H), 2.14 (s, 3H), 2.06 (s, 1H), 1.51 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.6, 144.5, 133.7, 132.5, 128.3, 128.1, 126.5, 126.1, 126.0, 120.6, 70.5, 20.7, 14.0.

EI-MS: *m/z* 244.

HRMS (EI) Calcd for $C_{15}H_{16}OS$: 244.0922; Found 244.0927.



3ac

Bright yellow oil, 93 % ee, $[\alpha]_D^{26.2}$ -53.2 (c 1.52, $CHCl_3$). The absolute configuration was determined by comparison of its optical rotation to reported data (Y. Yun, S.-F. Zhu, C.-Y. Zhou, Q.-L. Zhou, *J. Am. Chem. Soc*. **2008**, 130, 14052. $[\alpha]_D^{20}$ +15.7 (c 0.5, CH_2Cl_2)).

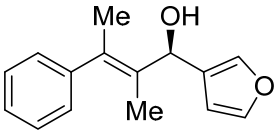
HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 95:5, 1.0 mL/min, 210 nm UV detector, tR = 9.622 (*S*) and tR = 10.702 min (*R*).

^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.37 – 7.31 (m, 3H), 7.26 – 7.21 (m, 1H), 7.20 – 7.15 (m, 2H), 7.03 – 6.96 (m, 2H), 6.12 (d, *J* = 4.6 Hz, 1H), 4.81 (d, *J* = 4.6 Hz, 1H), 2.10 (d, *J* = 1.4 Hz, 3H), 1.55 (d, *J* = 1.4 Hz, 3H).

^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 149.5, 145.6, 134.6, 133.0, 129.0, 128.8, 127.4, 127.1, 124.7, 123.7, 69.7, 20.7, 14.3.

EI-MS: *m/z* 244.

HRMS (EI) Calcd for $C_{15}H_{16}OS$: 244.0922; Found 244.0927.



3ad

Bright yellow oil, 84% ee, $[\alpha]_D^{26.0}$ -40.1 (c 0.68, $CHCl_3$). The absolute configuration was assigned by analogy.

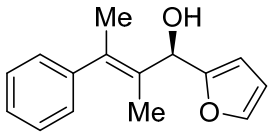
l = 95:5, 1.0 mL/min, 210 nm UV detector, tR = 9.622 (*S*) and tR = 10.702 min (*R*).

^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.49 – 7.38 (m, 2H), 7.30 – 7.24 (m, 2H), 7.19 – 7.13 (m, 1H), 7.13 – 7.05 (m, 2H), 6.37 (s, 1H), 5.79 (d, *J* = 3.2 Hz, 1H), 4.26 (d, *J* = 3.8 Hz, 1H), 2.00 (s, 3H), 1.44 (s, 3H).

^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 145.8, 143.8, 140.1, 134.3, 132.4, 129.6, 129.0, 128.9, 127.0, 110.1, 66.9, 20.6, 14.3.

EI-MS: *m/z* 228.

HRMS (EI) Calcd for $C_{15}H_{16}O_2$: 228.1150; Found 228.1152.



3ae

Yellow oil, 79% ee, $[\alpha]_D^{24.1}$ -22.3 (c 0.29, $CHCl_3$). The absolute configuration was assigned by analogy.

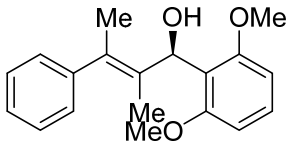
HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 99.2:0.8, 1.0 mL/min, 250 nm UV detector, tR = 33.258 (*S*) and tR = 42.687 min (*R*).

^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.49 – 7.46 (m, 1H), 7.37 – 7.32 (m, 2H), 7.25 – 7.20 (m, 1H), 7.17 – 7.13 (m, 2H), 6.40 – 6.36 (m, 1H), 6.34 – 6.28 (m, 1H), 5.85 (d, *J* = 4.0 Hz, 1H), 4.56 (d, *J* = 4.5 Hz, 1H), 2.05 (d, *J* = 1.4 Hz, 3H), 1.57 (d, *J* = 1.4 Hz, 3H).

^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 157.8, 145.7, 142.4, 133.7, 132.6, 129.0, 128.8, 127.1, 110.9, 106.4, 67.9, 20.6, 14.8.

EI-MS: *m/z* 228.

HRMS (EI) Calcd for $C_{15}H_{16}O_2$: 228.1150; Found 228.1155.



3af

Colorless oil, 98% ee, $[\alpha]_D^{27.1}$ -4.1 (c 0.62, $CHCl_3$). The absolute configuration was assigned by analogy.

HPLC condition: Chiralcel AD-H column, n-hexane/2-propanol = 97:3, 1.0 mL/min, 254 nm UV detector, tR = 15.933 (*S*) and tR = 20.016 min (*R*).

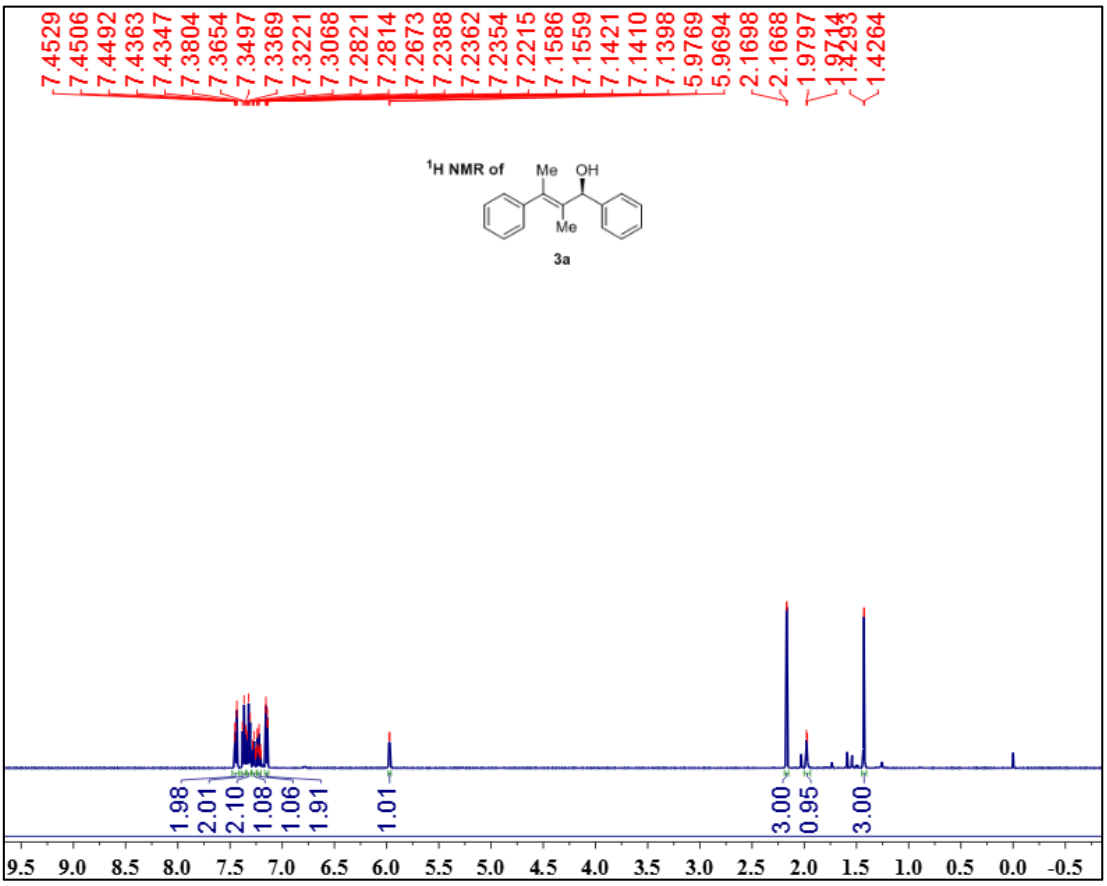
^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.33 – 7.27 (m, 2H), 7.26 – 7.15 (m, 2H), 7.11 – 7.05 (m, 2H), 6.70 (d, *J* = 8.4 Hz, 2H), 6.20 – 6.13 (m, 1H), 4.57 – 4.47 (m, 1H), 3.88 (s, 6H), 2.03 (s, 3H), 1.57 (s, 3H).

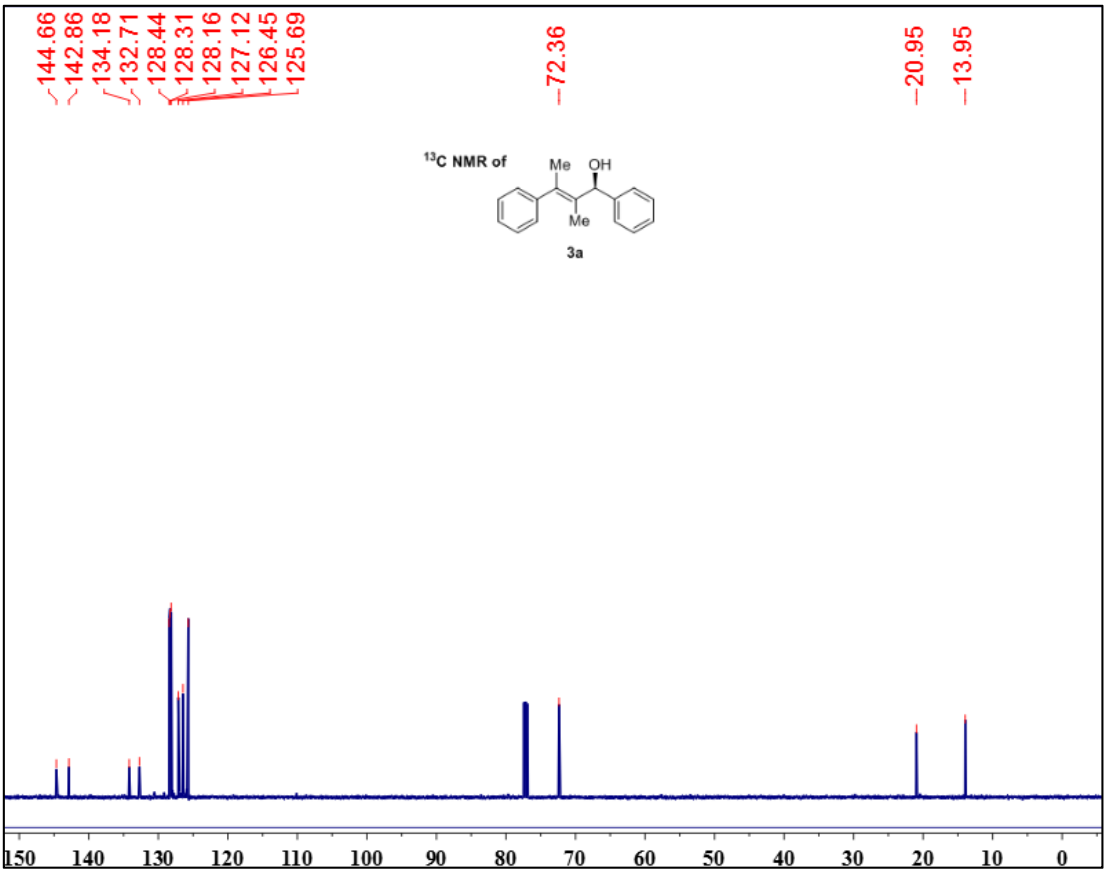
^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 159.1, 146.8, 135.1, 132.3, 129.2, 128.94, 128.86, 126.6, 120.3, 105.5, 68.3, 56.2, 21.0, 15.5.

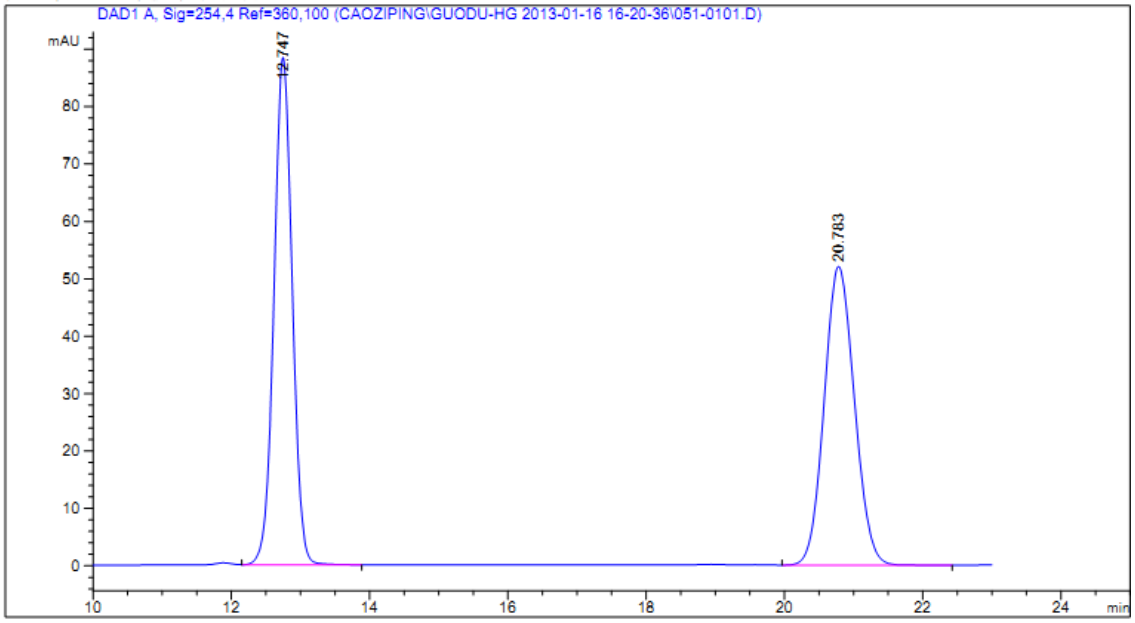
EI-MS: *m/z* 298.

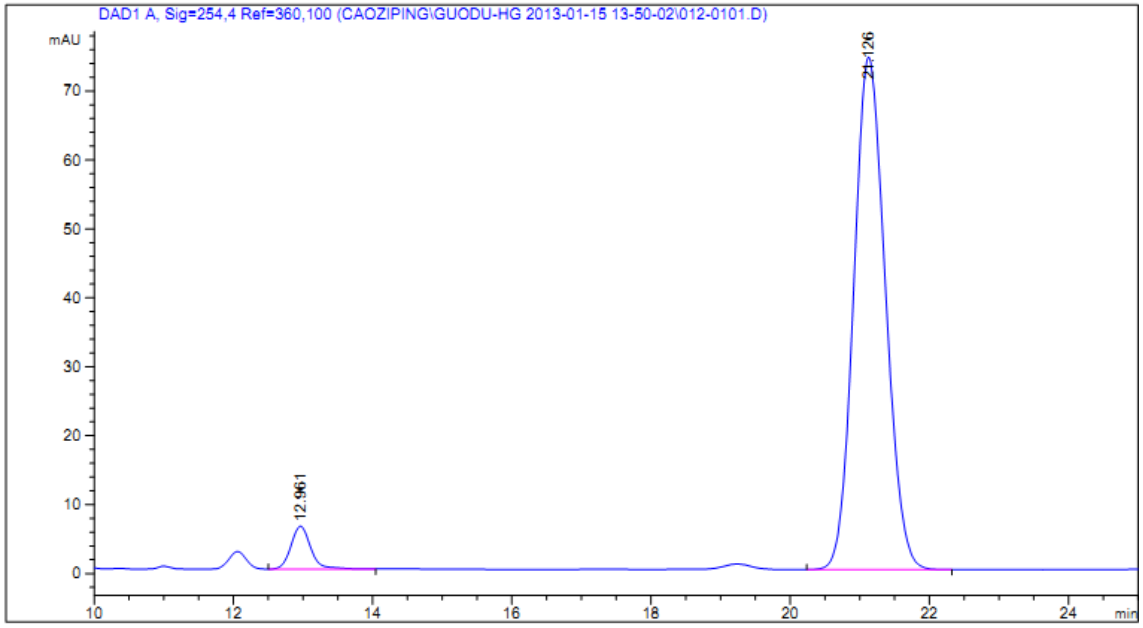
HRMS (EI) Calcd for $C_{19}H_{22}O_3$: 298.1569; Found 298.1570.

5. NMR Spectra and HPLC Charts for the Chiral Allylic Alcohols

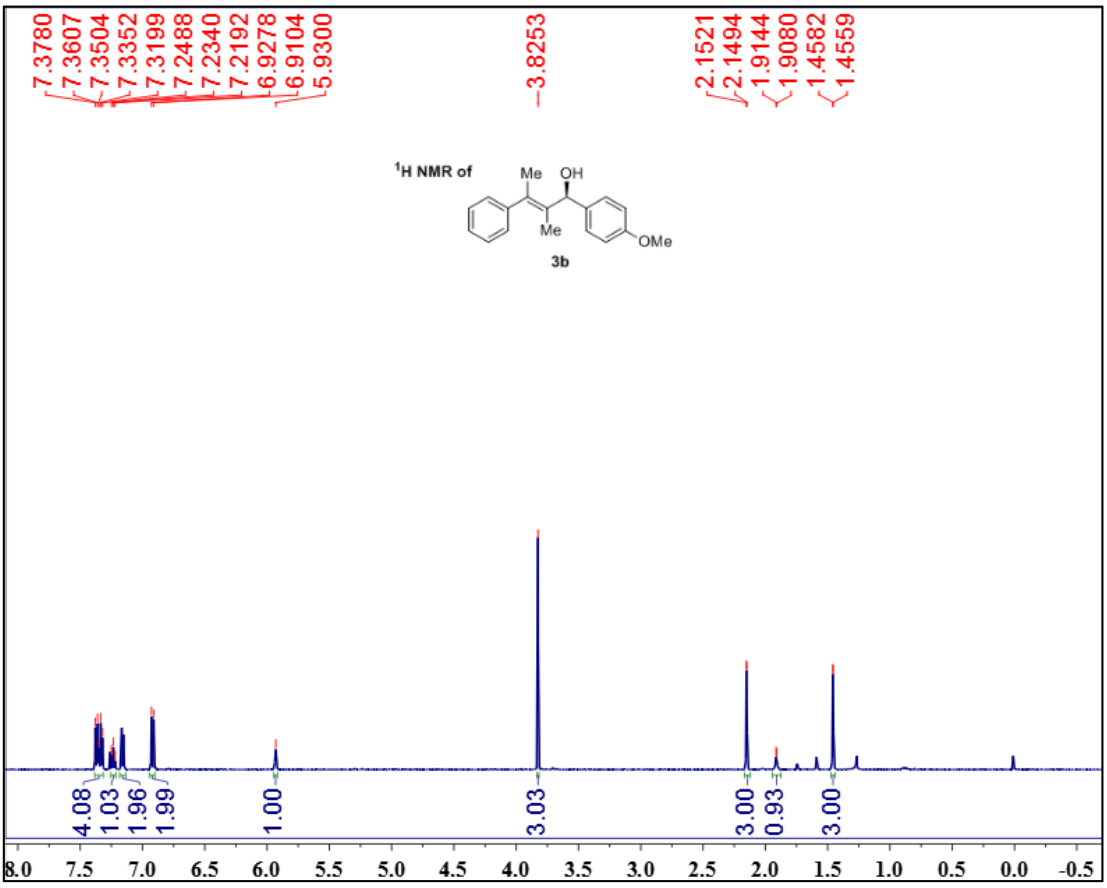

7.4529
7.4506
7.4492
7.4363
7.4347
7.3804
7.3654
7.3497
7.3369
7.3221
7.3068
7.2821
7.2814
7.2673
7.2388
7.2362
7.2354
7.2215
7.1586
7.1559
7.1421
7.1410
7.1398
5.9769
5.9694
2.1698
2.1668
1.9797
1.4293
1.4264
1H NMR of
Me
OH
Me
3a
1.98
2.01
2.10
1.08
1.06
1.91
1.01
3.00
0.95
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

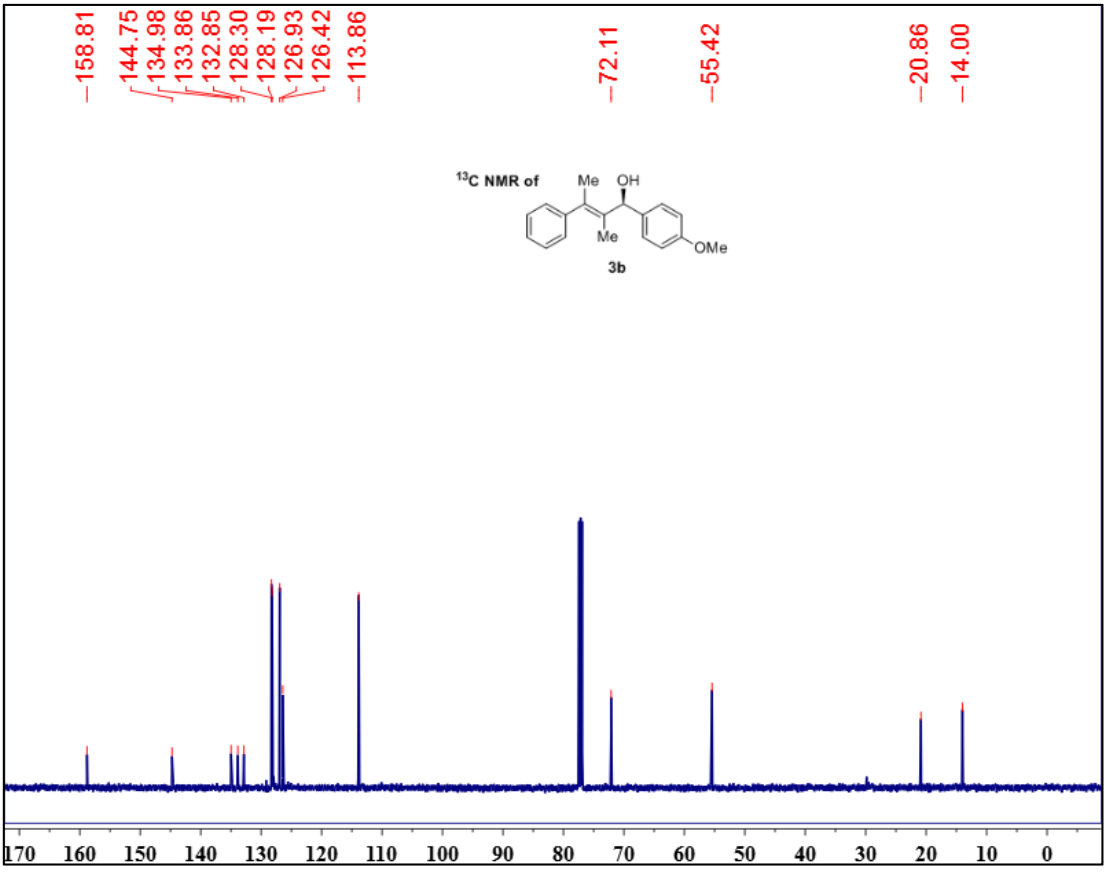

144.66
142.86
134.18
132.71
128.44
128.31
128.16
127.12
126.45
125.69
72.36
20.95
13.95
13C NMR of
Me
OH
Me
3a
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

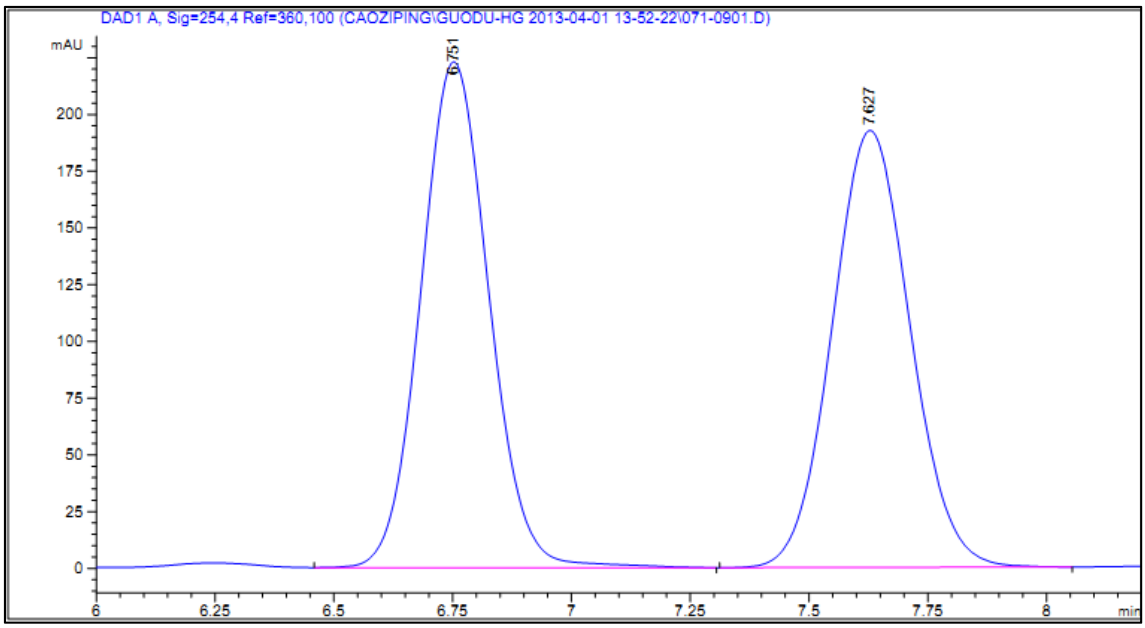


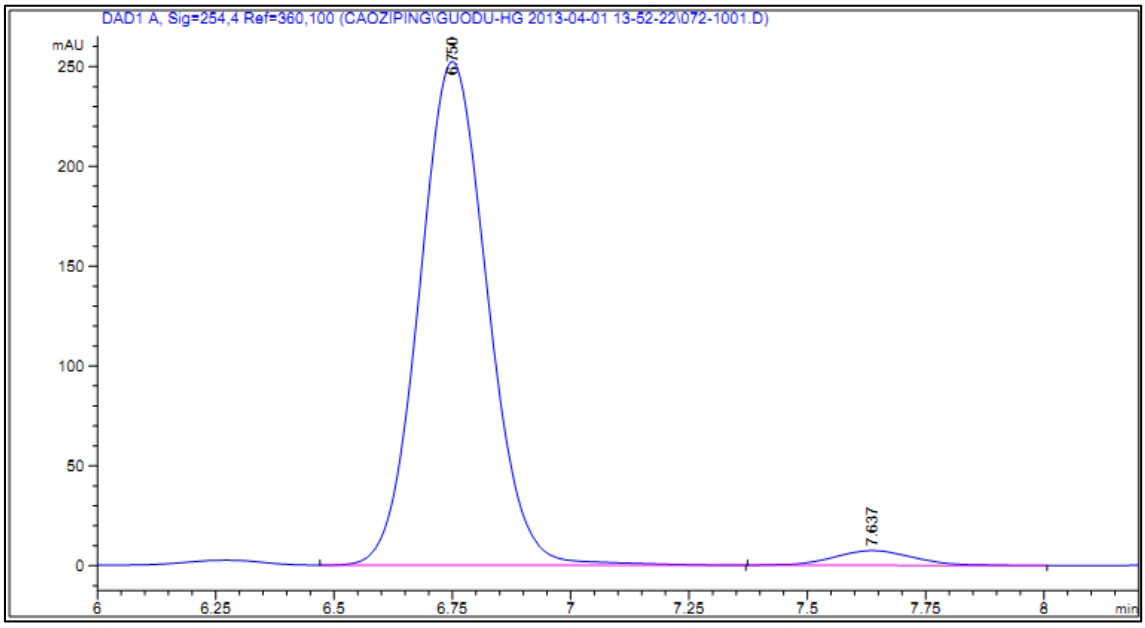


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.961	BB	0.3035	123.81458	6.24003	5.0211
2	21.126	BB	0.4895	2342.09277	74.36173	94.9789
总量：				2465.90736	80.60176	

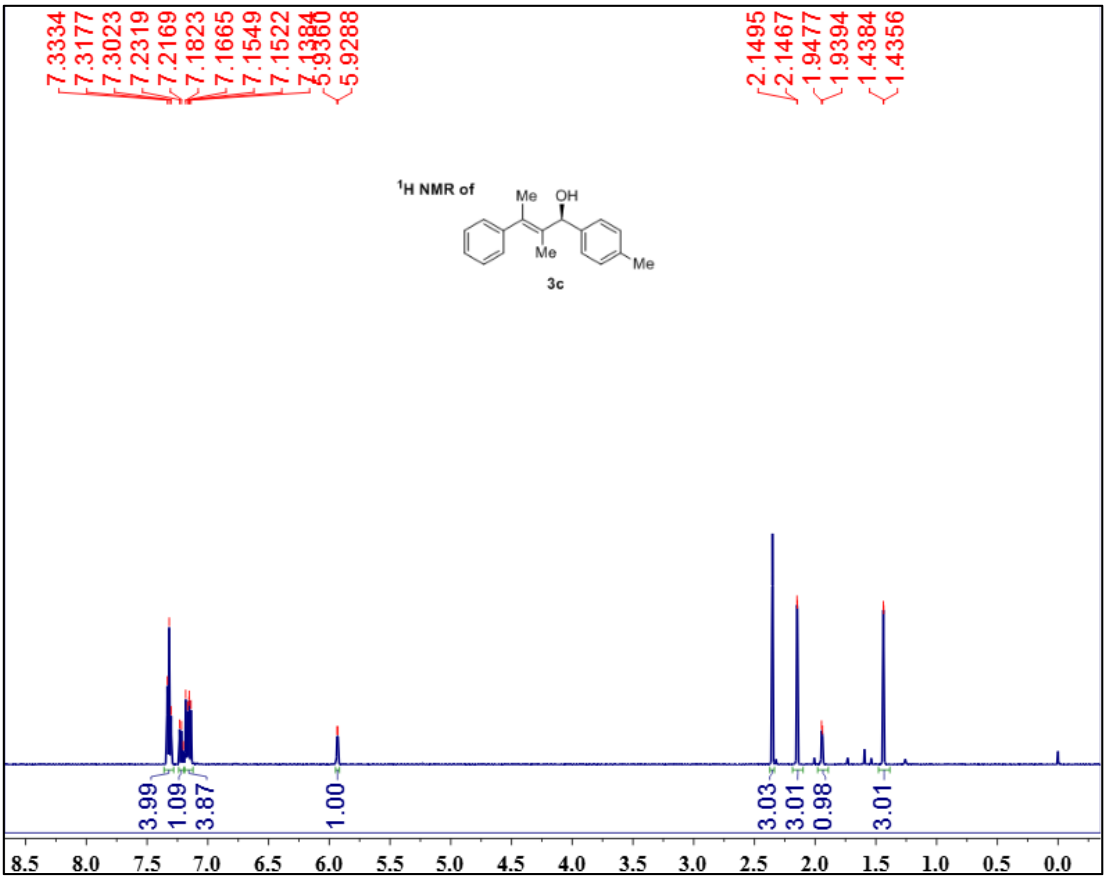

7.3780
7.3607
7.3504
7.3352
7.3199
7.2488
7.2340
7.2192
6.9278
6.9104
5.9300
3.8253
2.1521
2.1494
1.9144
1.9080
1.4582
1.4559
^{1}H NMR of
Me
OH
Me
OMe
3b
4.08
1.03
1.96
1.99
1.00
3.03
3.00
0.93
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

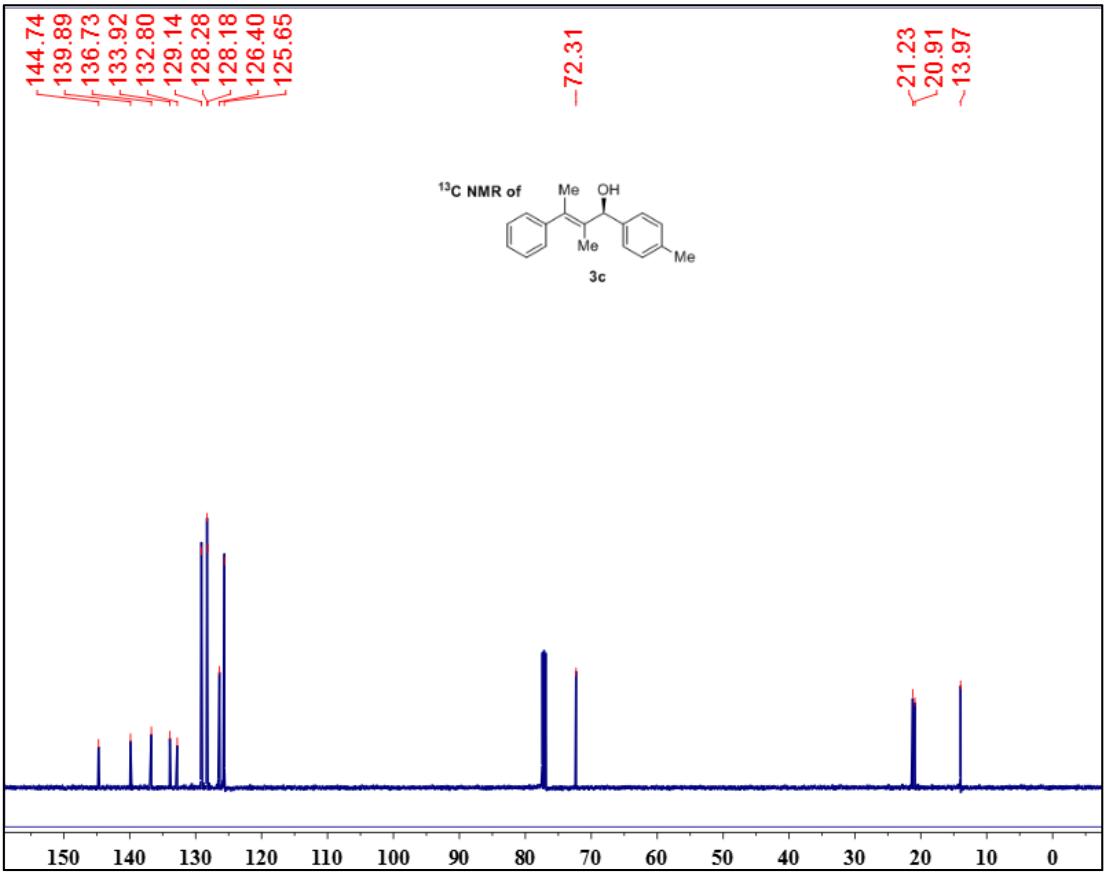

158.81
144.75
134.98
133.86
132.85
128.30
128.19
126.93
126.42
113.86
72.11
55.42
20.86
14.00
^{13}C NMR of
Me
OH
Me
OMe
3b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

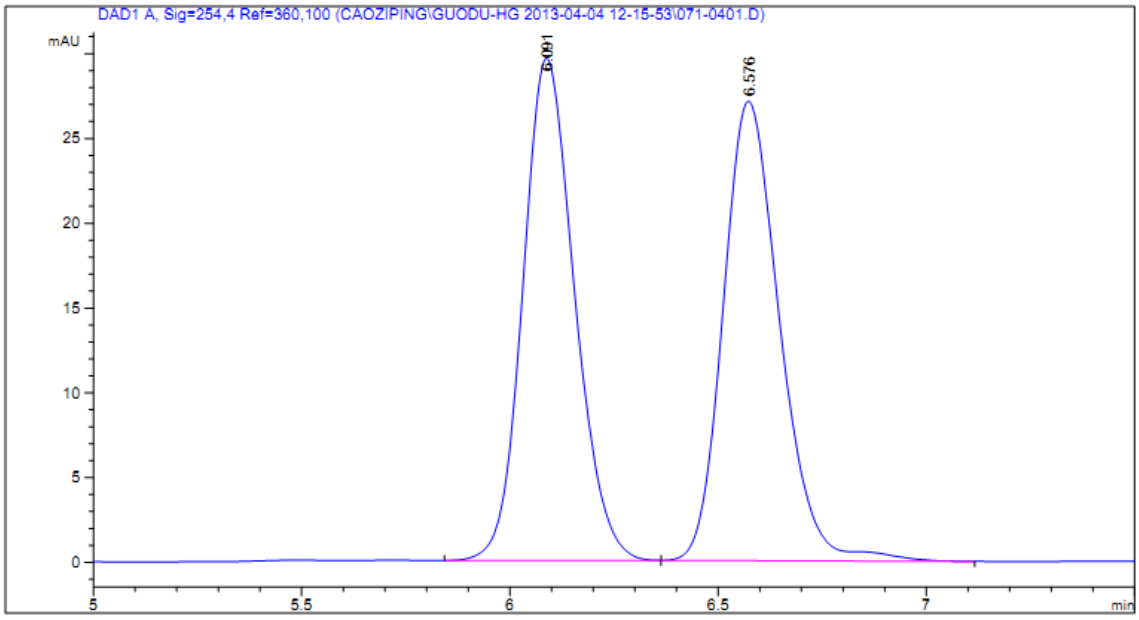


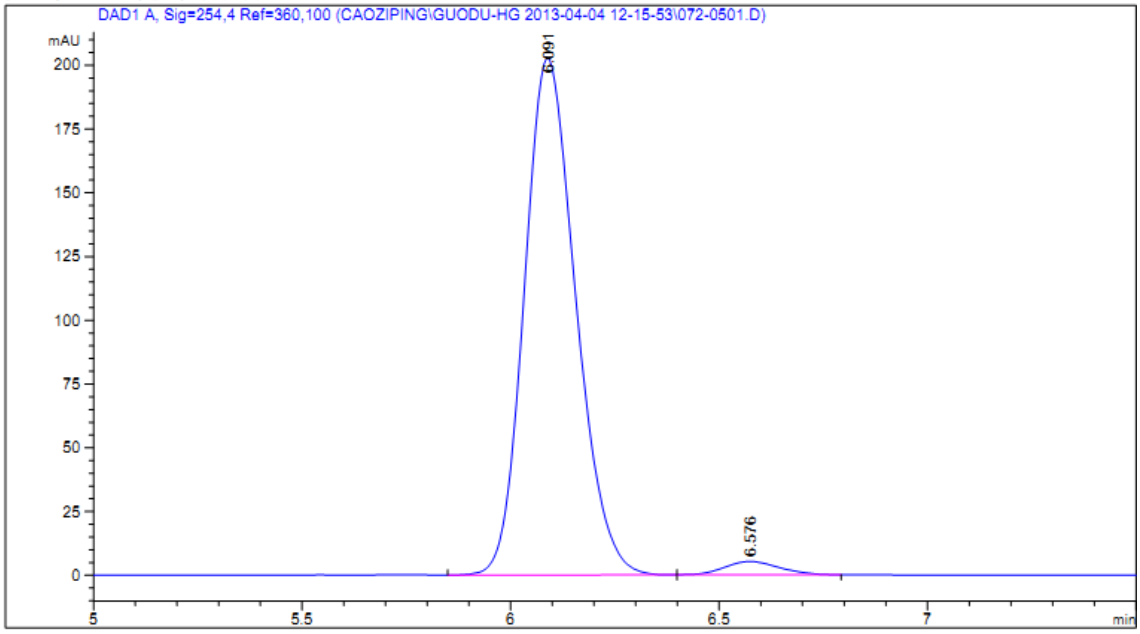


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.750	VB	0.1561	2512.85889	252.51463	96.7255
2	7.637	BB	0.1784	85.06966	7.38704	3.2745
总量：				2597.92854	259.90167	

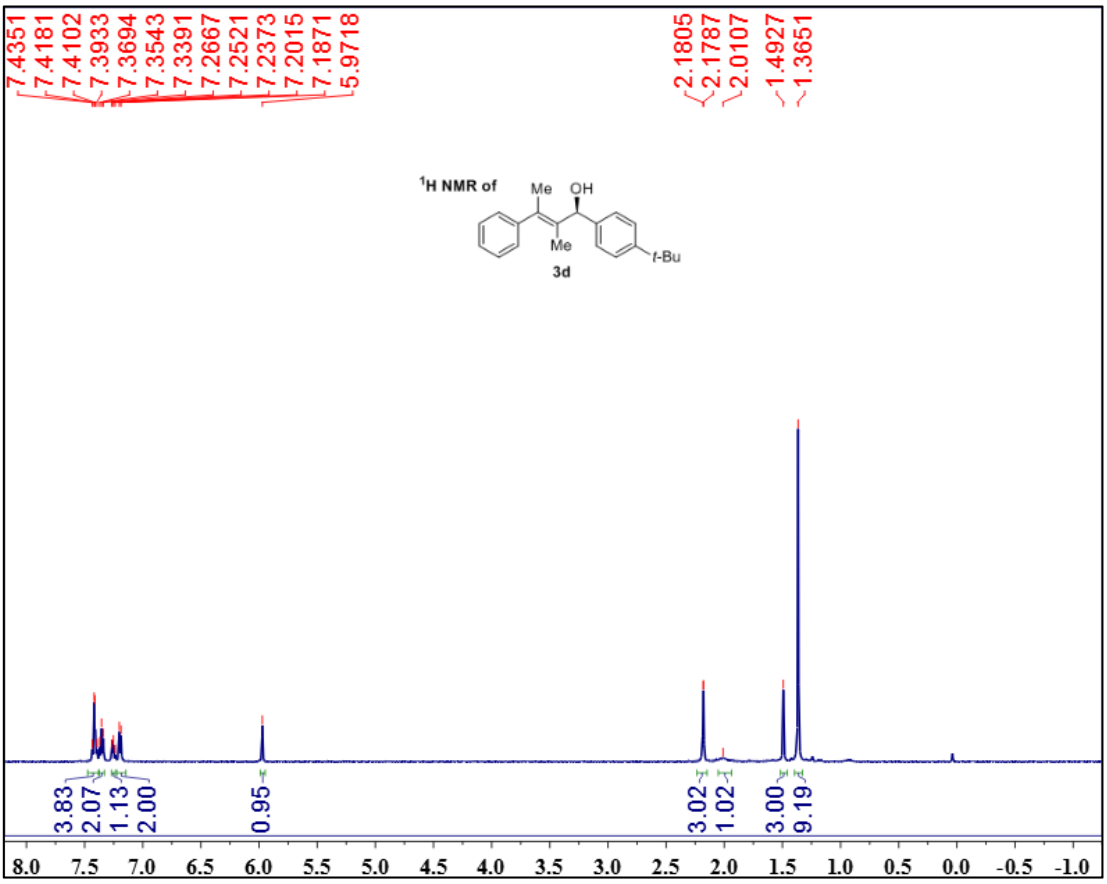

7.3334
7.3177
7.3023
7.2319
7.2169
7.1823
7.1665
7.1549
7.1522
7.1384
5.9360
5.9288
2.1495
2.1467
1.9477
1.9394
1.4384
1.4356
1H NMR of
Me
OH
Me
Me
3c
3.99
1.09
3.87
1.00
3.03
3.01
0.98
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

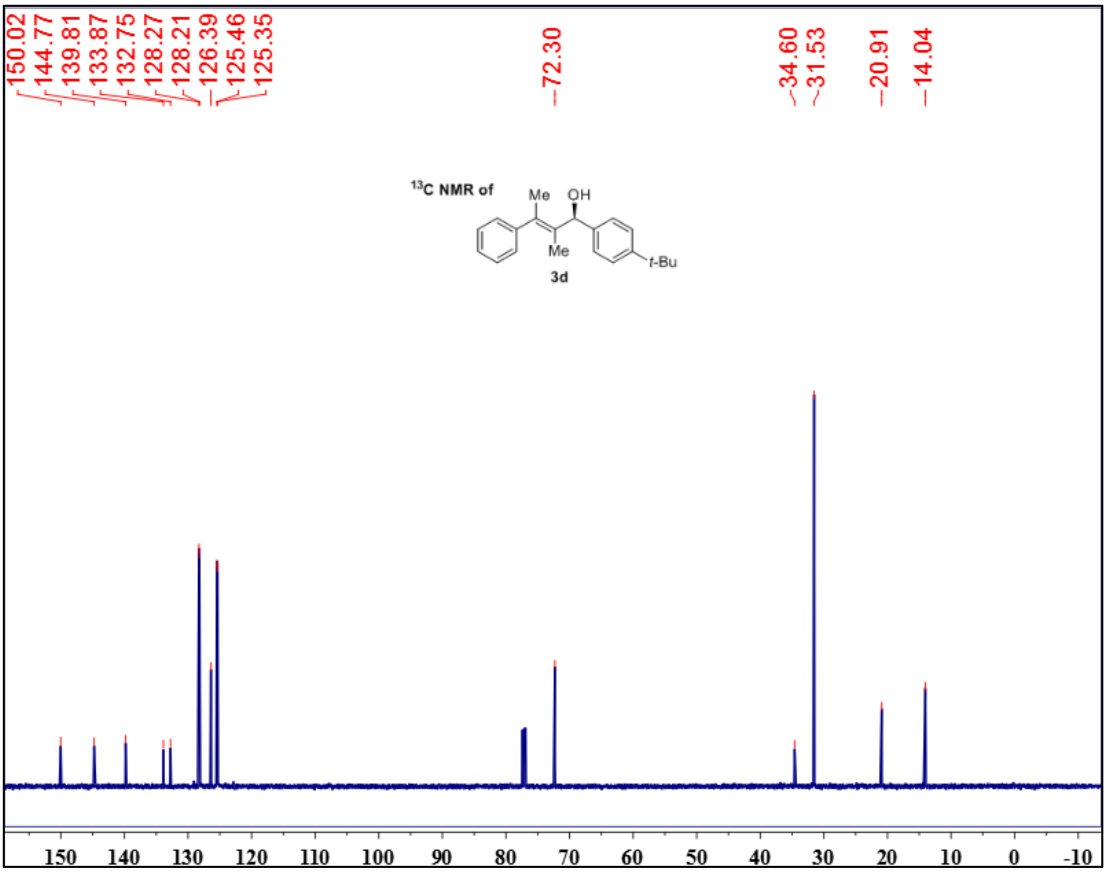

144.74
139.89
136.73
133.92
132.80
129.14
128.28
128.18
126.40
125.65
72.31
21.23
20.91
13.97
13C NMR of
Me
OH
Me
Me
3c
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

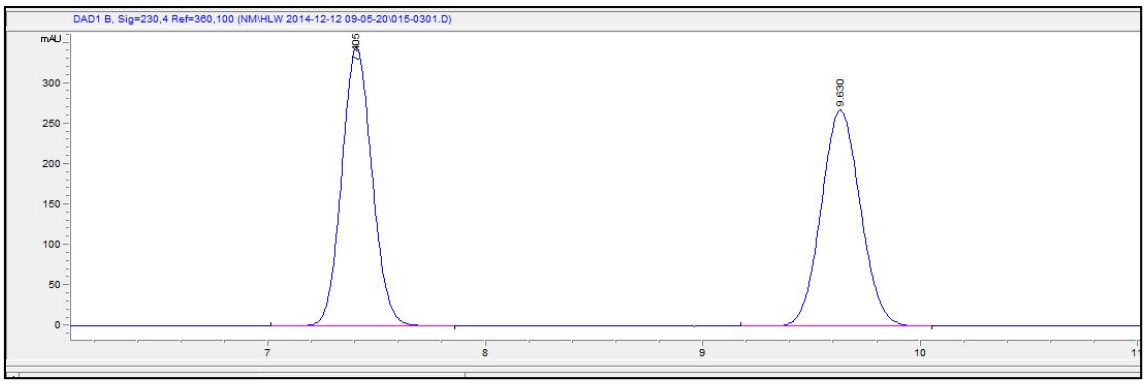


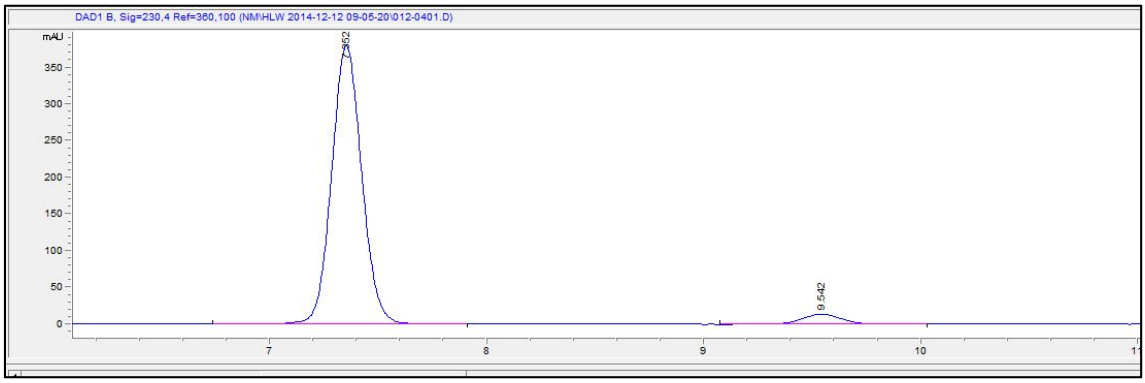


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.091	BV	0.1315	1729.50781	202.86763	97.3402
2	6.576	VB	0.1390	47.25809	5.24906	2.6598
总量：				1776.76591	208.11669	

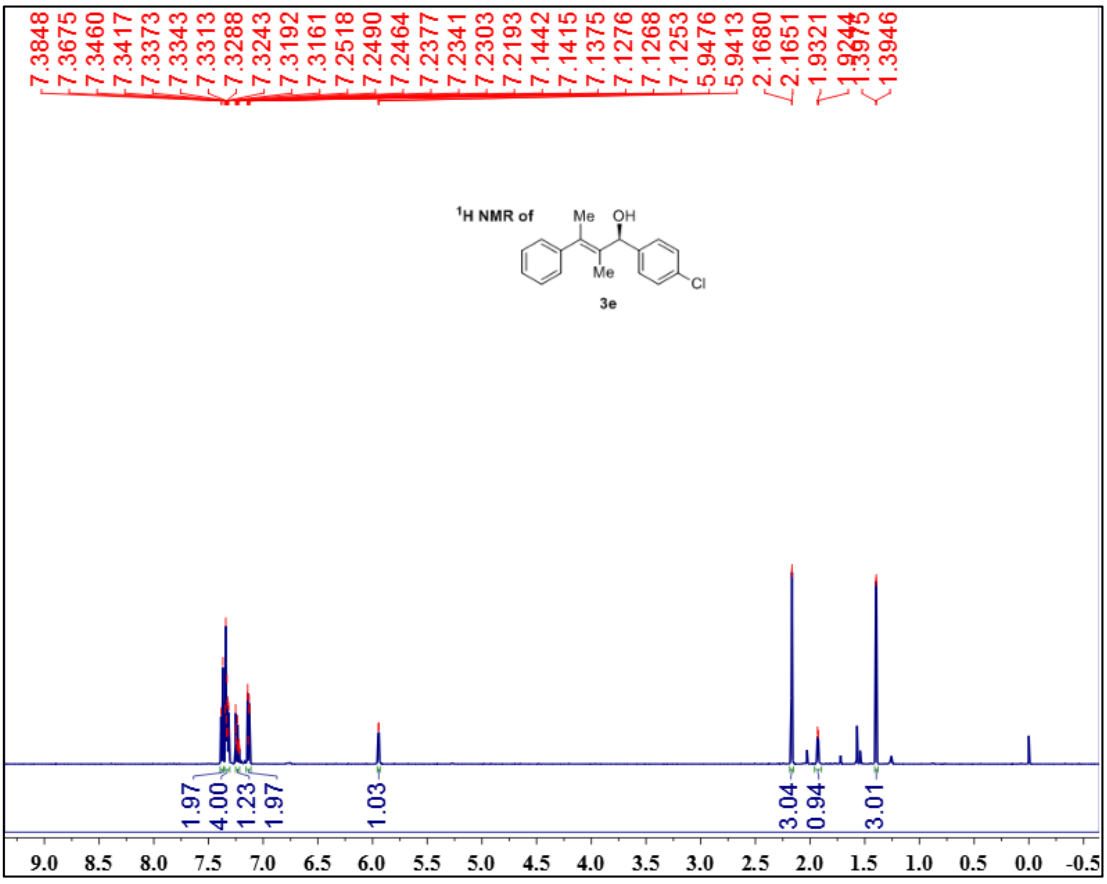

7.4351
7.4181
7.4102
7.3933
7.3694
7.3543
7.3391
7.2667
7.2521
7.2373
7.2015
7.1871
5.9718
2.1805
2.1787
2.0107
1.4927
1.3651
^{1}H NMR of
Me
OH
Me
t-Bu
3d
3.83
2.07
1.13
2.00
0.95
3.02
1.02
3.00
9.19
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

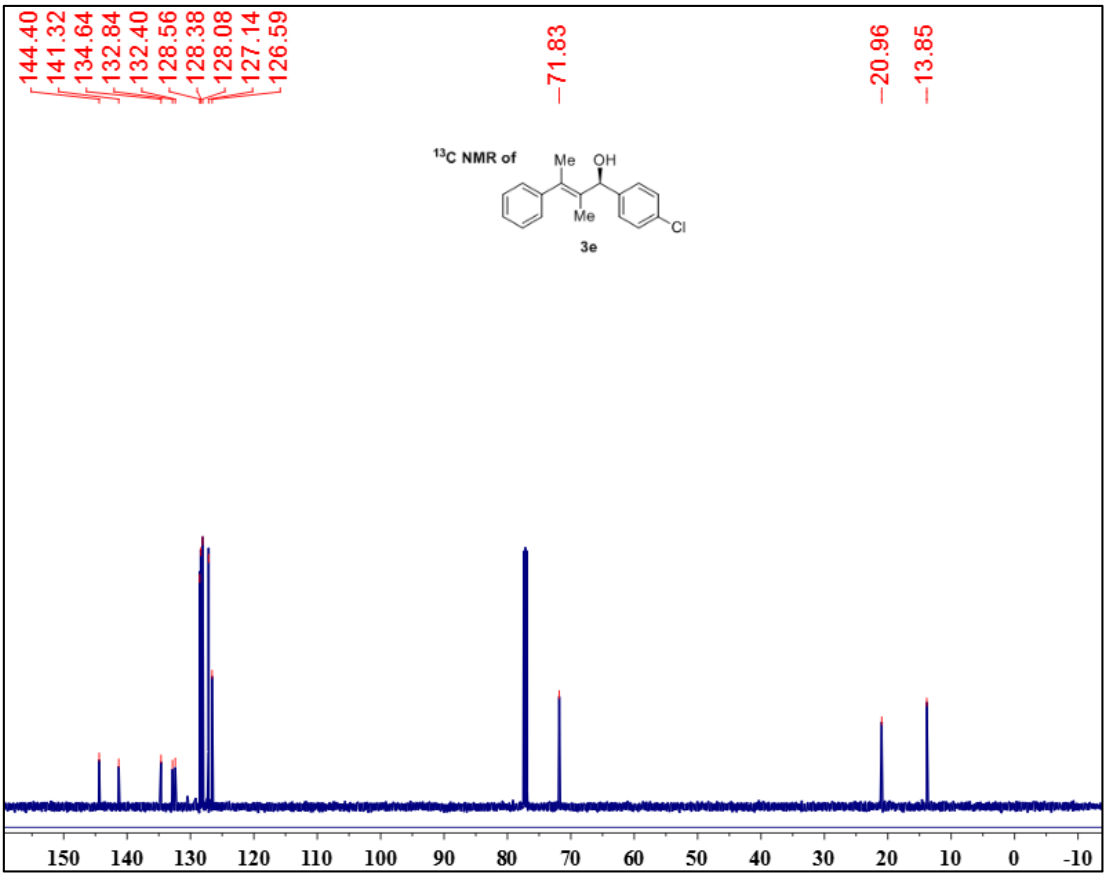

150.02
144.77
139.81
133.87
132.75
128.27
128.21
126.39
125.46
125.35
72.30
34.60
31.53
20.91
14.04
^{13}C NMR of
Me
OH
Me
t-Bu
3d
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

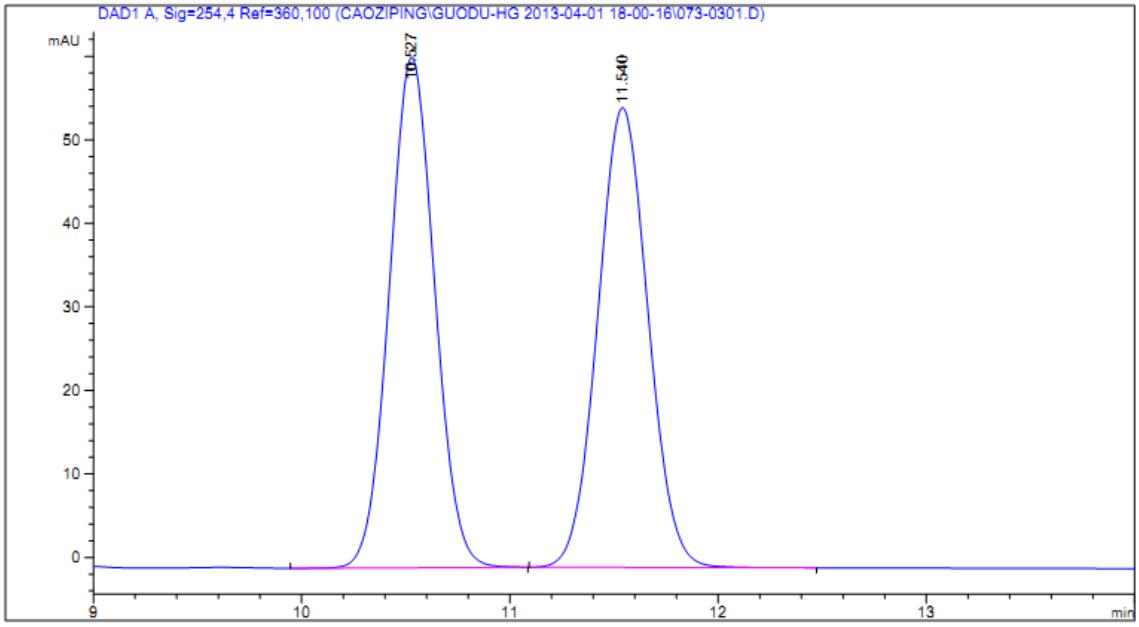


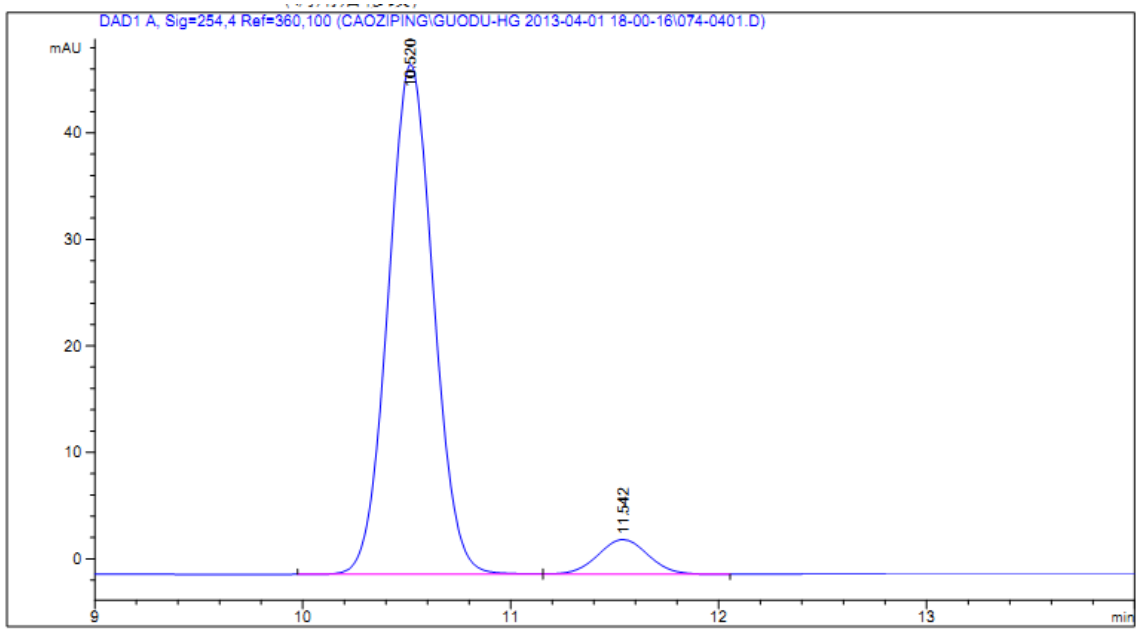


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.352	BB	0.1504	3662.13330	380.26617	95.5167
2	9.542	BB	0.1947	171.89128	13.67206	4.4833
总量：				3834.02458	393.93823	

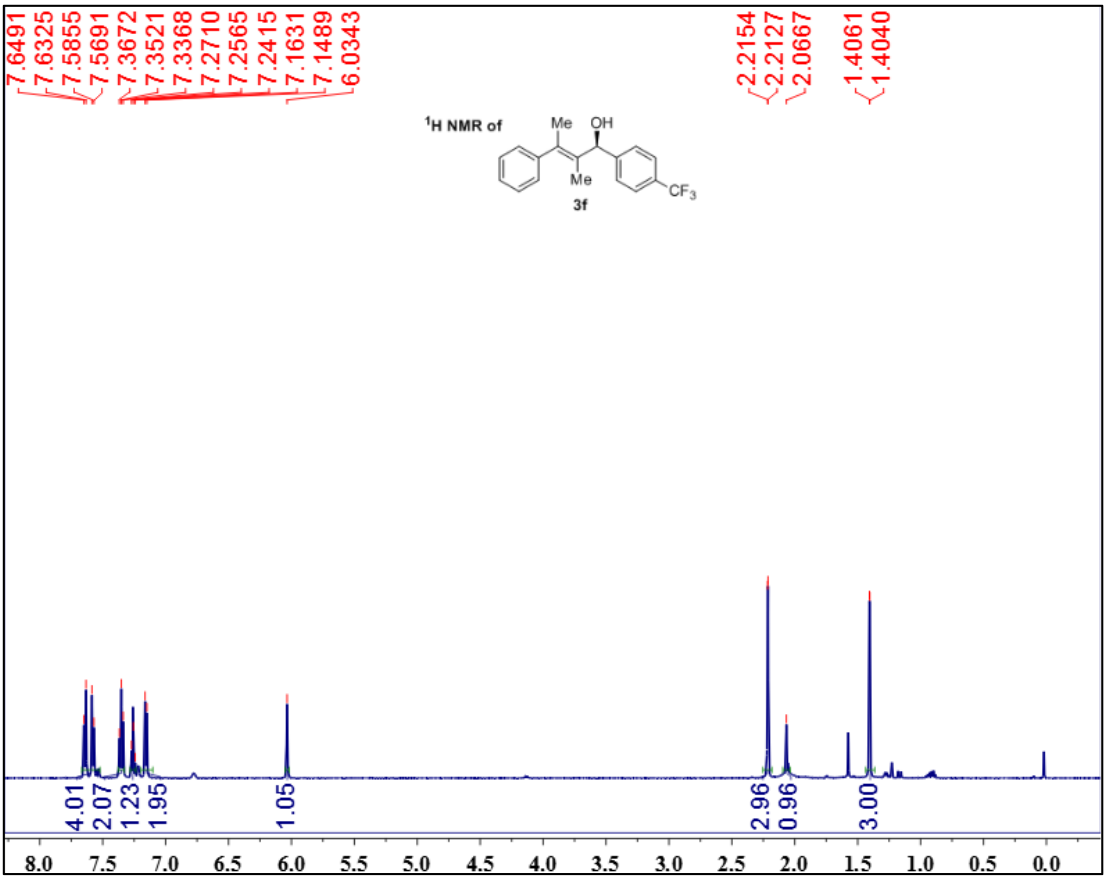

7.3848
7.3675
7.3460
7.3417
7.3373
7.3343
7.3313
7.3288
7.3243
7.3192
7.3161
7.2518
7.2490
7.2464
7.2377
7.2341
7.2303
7.2193
7.1442
7.1415
7.1375
7.1276
7.1268
7.1253
5.9476
5.9413
2.1680
2.1651
1.9321
1.3975
1.3946
1H NMR of
Me
OH
Me
Cl
3e
1.97
4.00
1.23
1.97
1.03
3.04
0.94
3.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

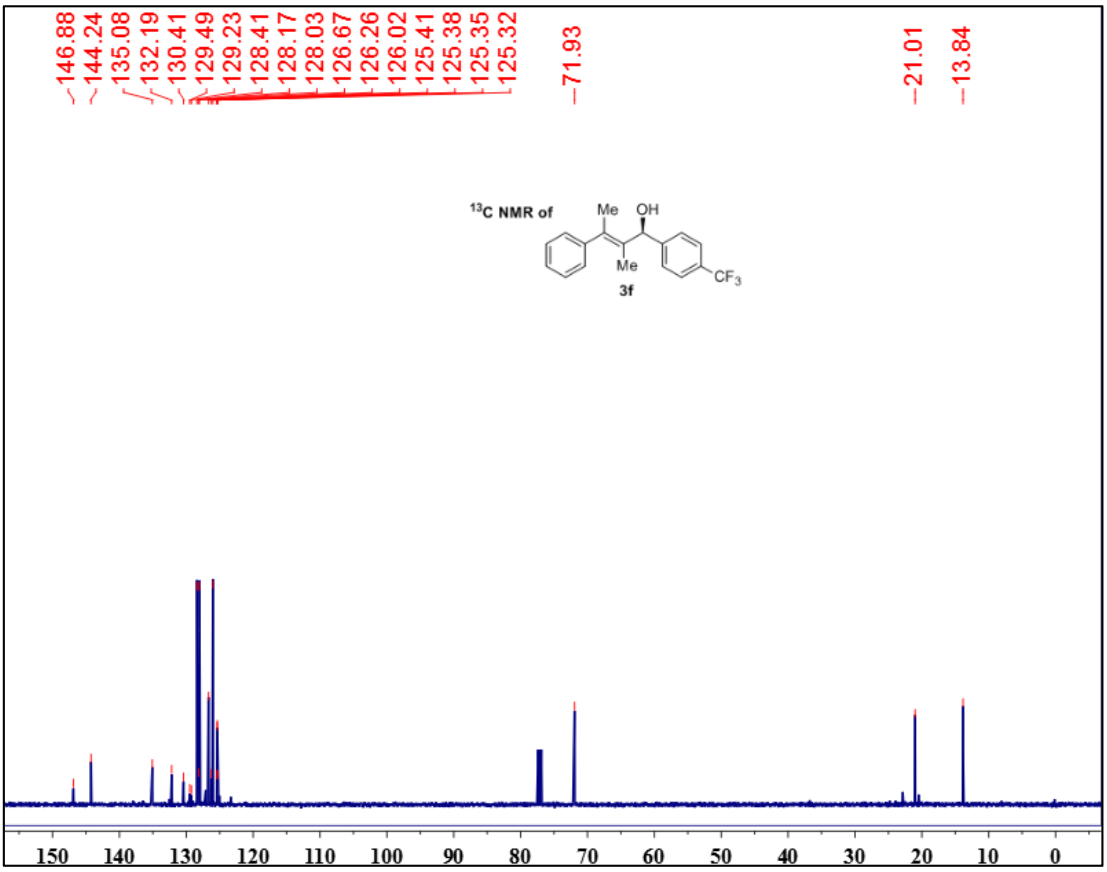

144.40
141.32
134.64
132.84
132.40
128.56
128.38
128.08
127.14
126.59
71.83
20.96
13.85
13C NMR of
Me
OH
Me
Cl
3e
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

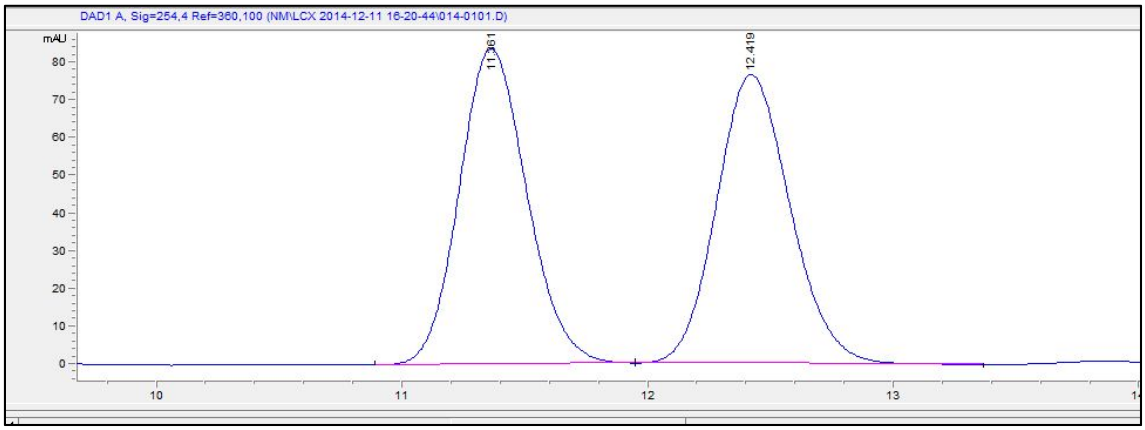


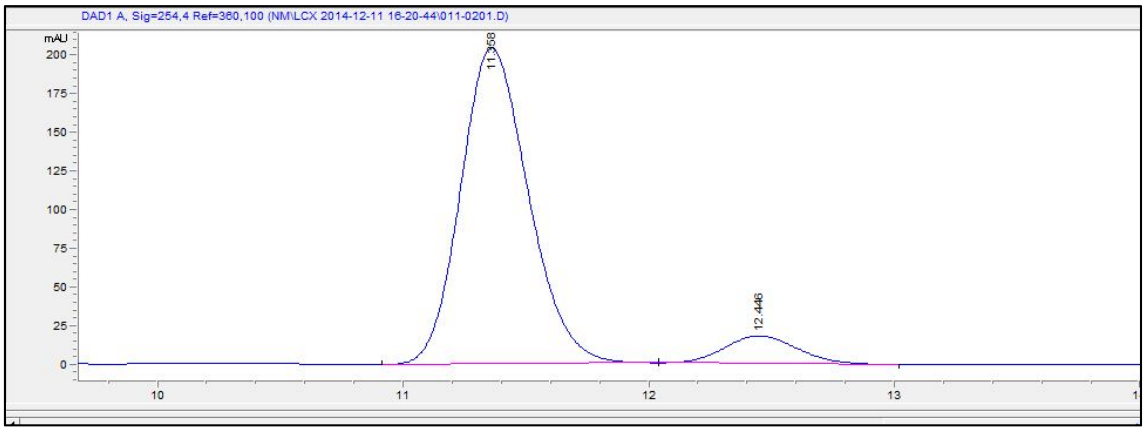


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.520	BB	0.2362	723.25513	47.87633	92.9966
2	11.542	BB	0.2629	54.46720	3.26112	7.0034
总量：				777.72233	51.13744	

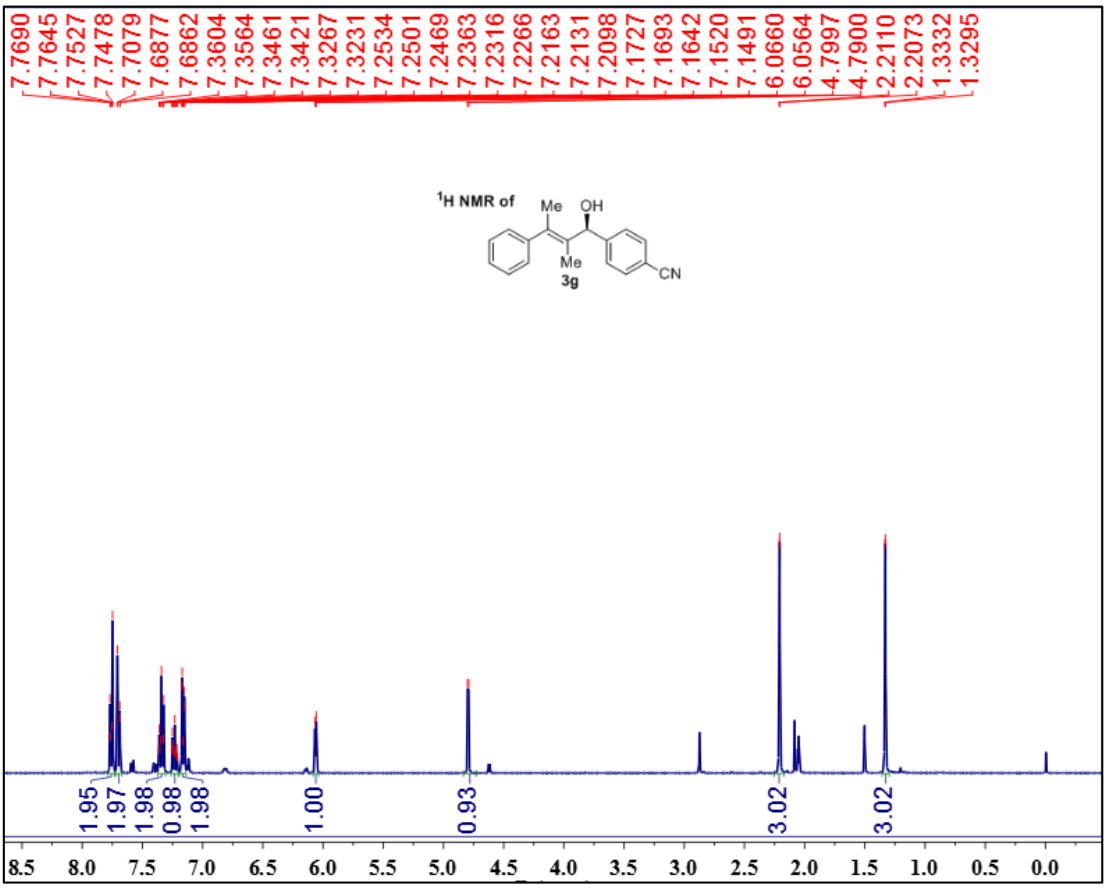

7.6491
7.6325
7.5855
7.5691
7.3672
7.3521
7.3368
7.2710
7.2565
7.2415
7.1631
7.1489
6.0343
2.2154
2.2127
2.0667
1.4061
1.4040
^{1}H NMR of
Me
OH
Me
CF$_3$
3f
4.01
2.07
1.23
1.95
1.05
2.96
0.96
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

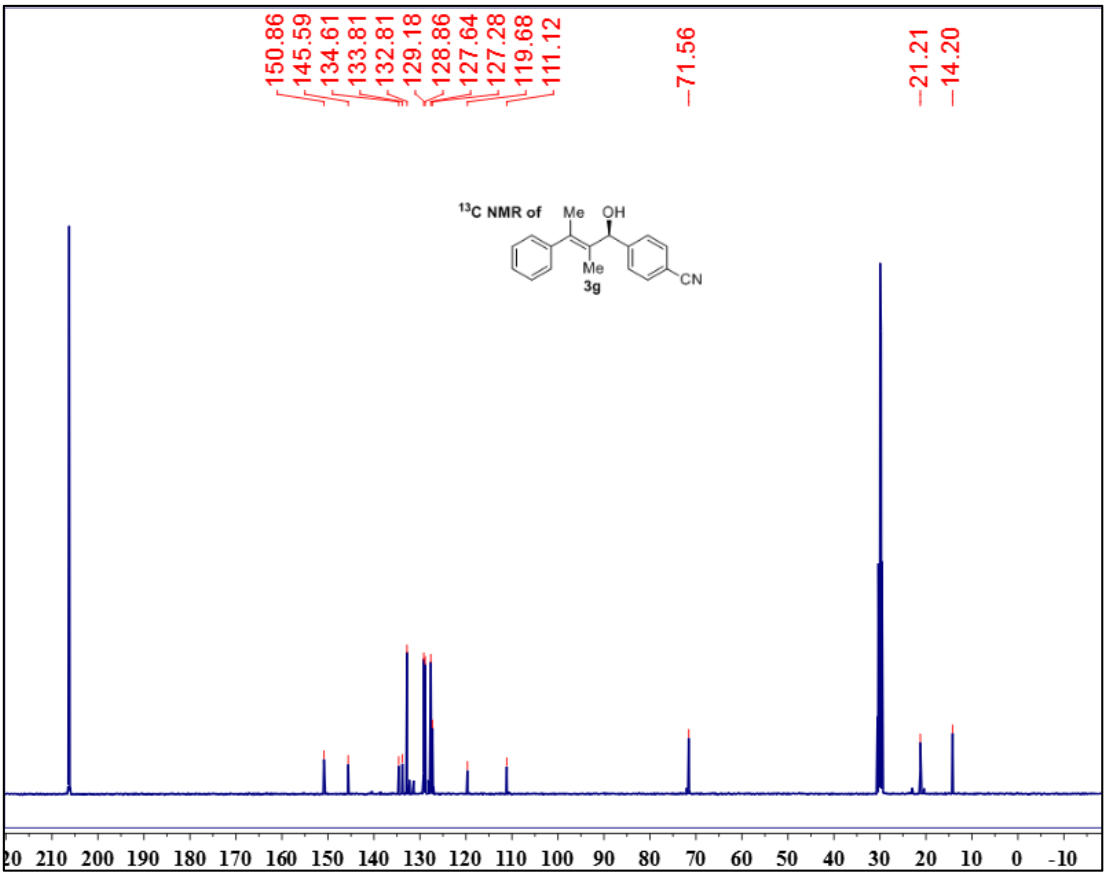

146.88
144.24
135.08
132.19
130.41
129.49
129.23
128.41
128.17
128.03
126.67
126.26
126.02
125.41
125.38
125.35
125.32
71.93
21.01
13.84
^{13}C NMR of
Me
OH
Me
CF$_3$
3f
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

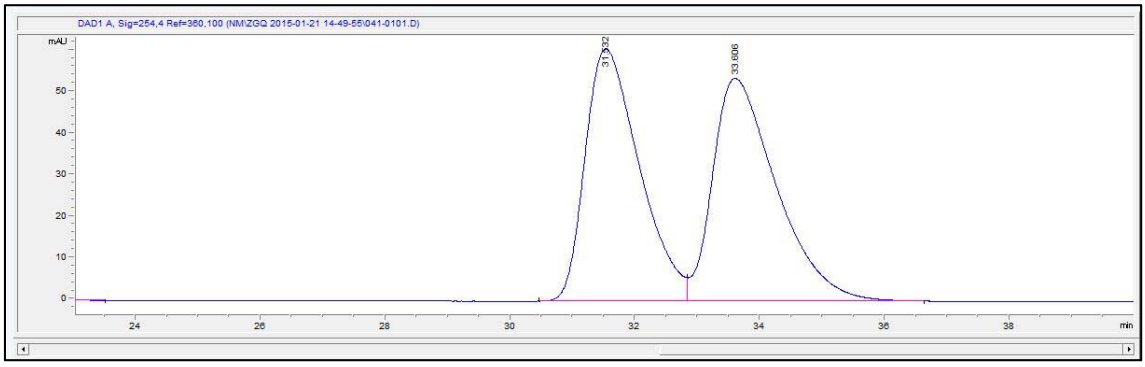


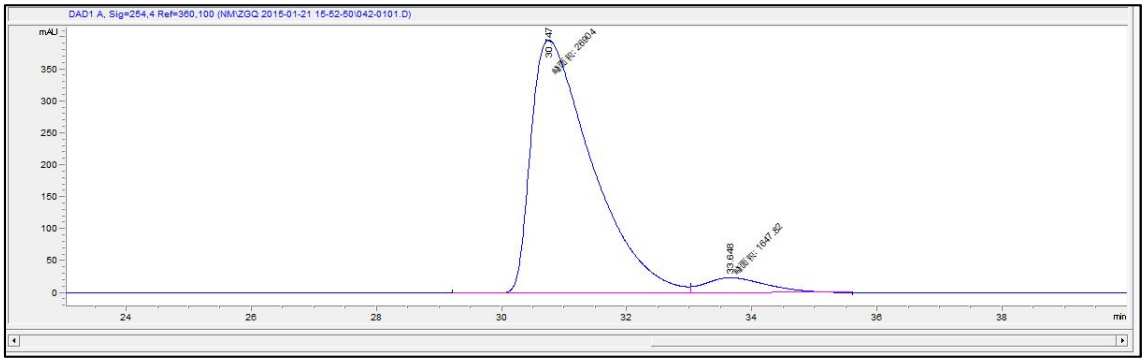


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.358	BB	0.2977	3914.55273	204.18329	91.4276
2	12.446	BB	0.3174	367.03644	17.88885	8.5724
总量：				4281.58917	222.07214	

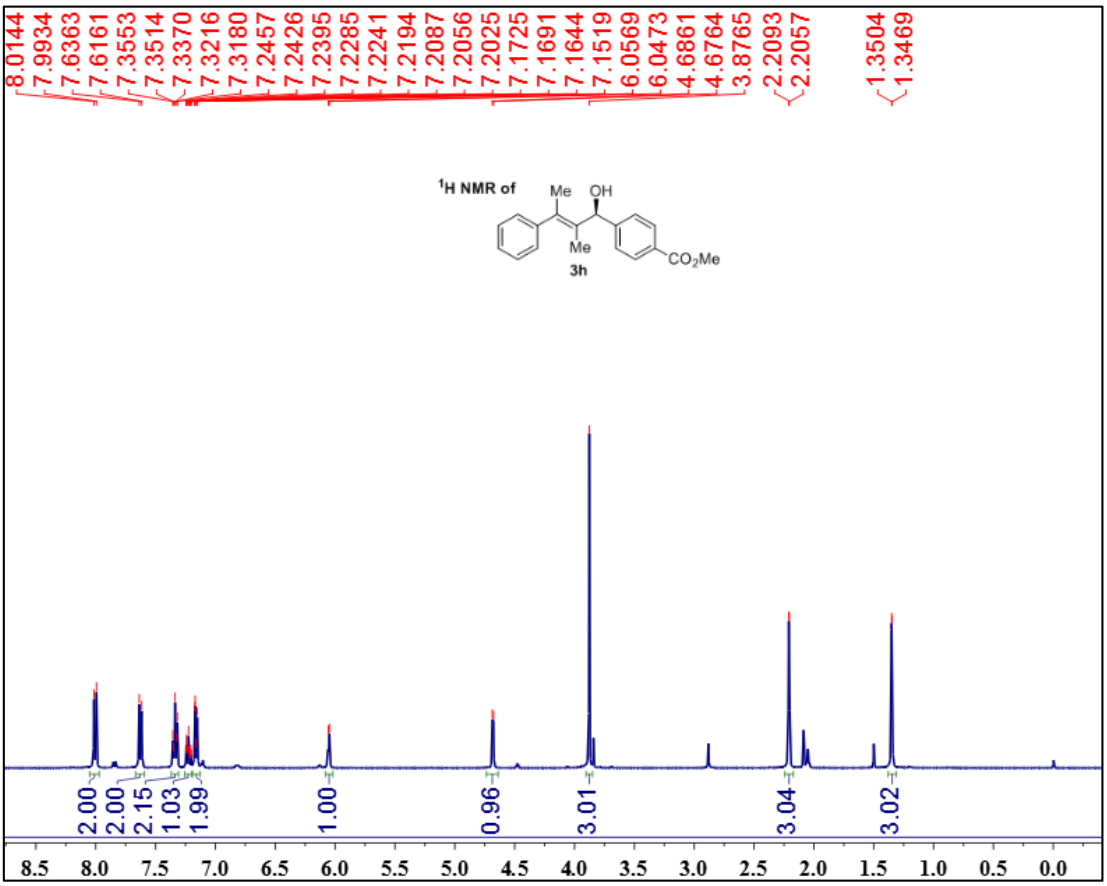

7.7690
7.7645
7.7527
7.7478
7.7079
7.6877
7.6862
7.3604
7.3564
7.3461
7.3421
7.3267
7.3231
7.2534
7.2501
7.2469
7.2363
7.2316
7.2266
7.2163
7.2131
7.2098
7.1727
7.1693
7.1642
7.1520
7.1491
6.0660
6.0564
4.7997
4.7900
2.2110
2.2073
1.3332
1.3295
1H NMR of
Me
OH
Me
CN
3g
1.95
1.97
1.98
0.98
1.98
1.00
0.93
3.02
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

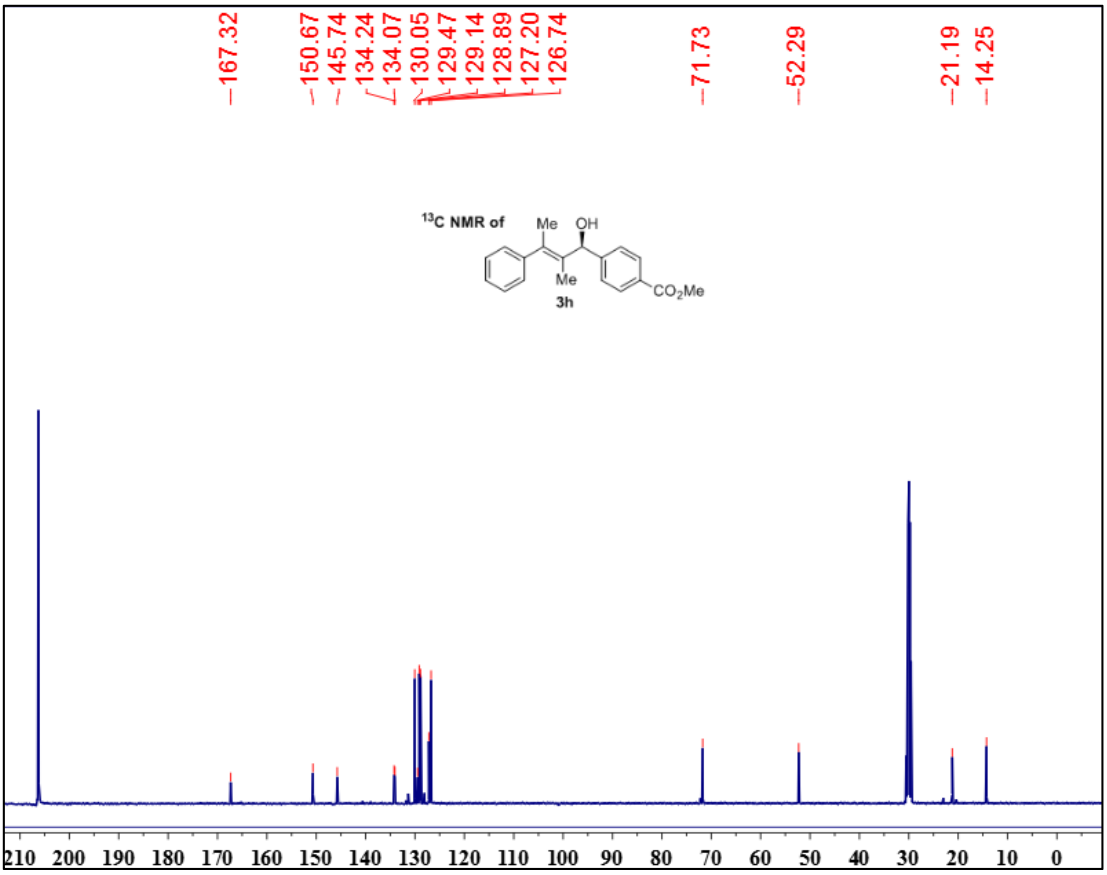

150.86
145.59
134.61
133.81
132.81
129.18
128.86
127.64
127.28
119.68
111.12
71.56
21.21
14.20
13C NMR of
Me
OH
Me
CN
3g
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

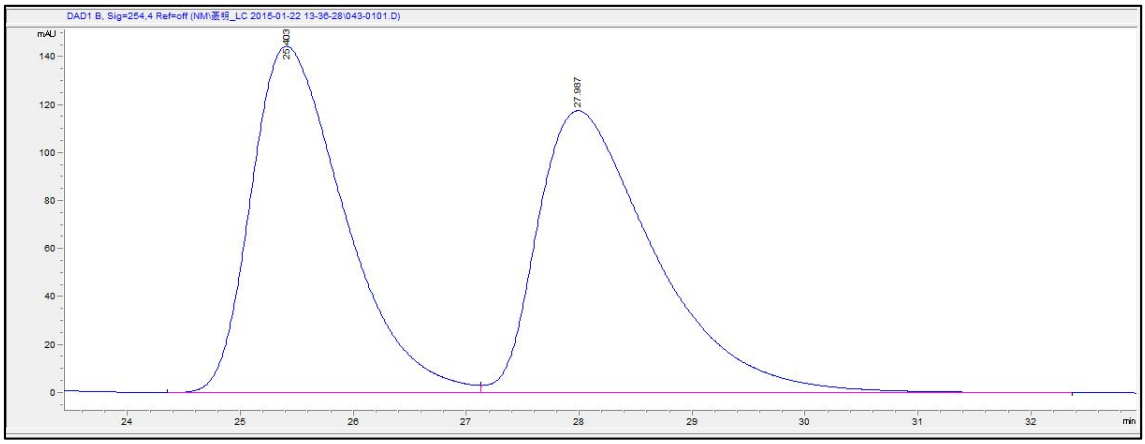


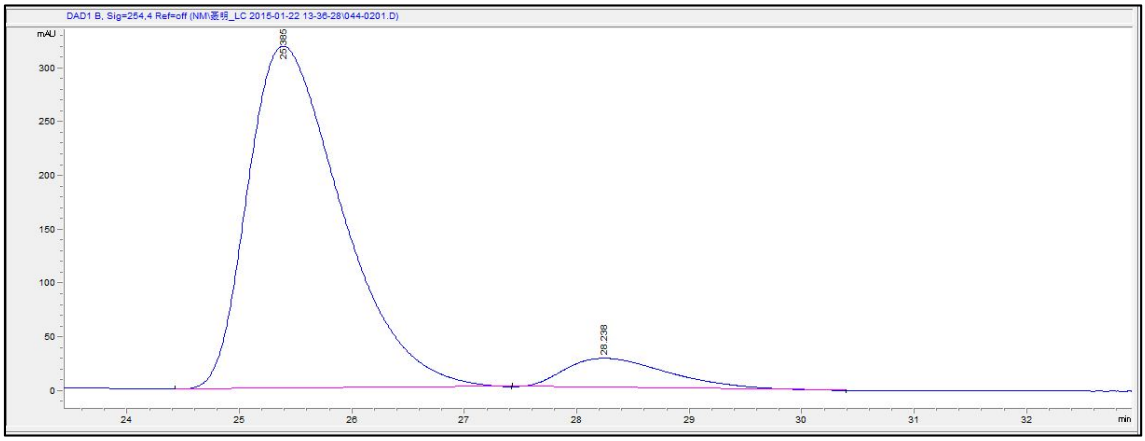


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	30.747	MF	1.1311	2.69040e4	396.41791	94.2287
2	33.648	FM	1.1570	1647.82446	23.73645	5.7713
总量：				2.85519e4	420.15435	

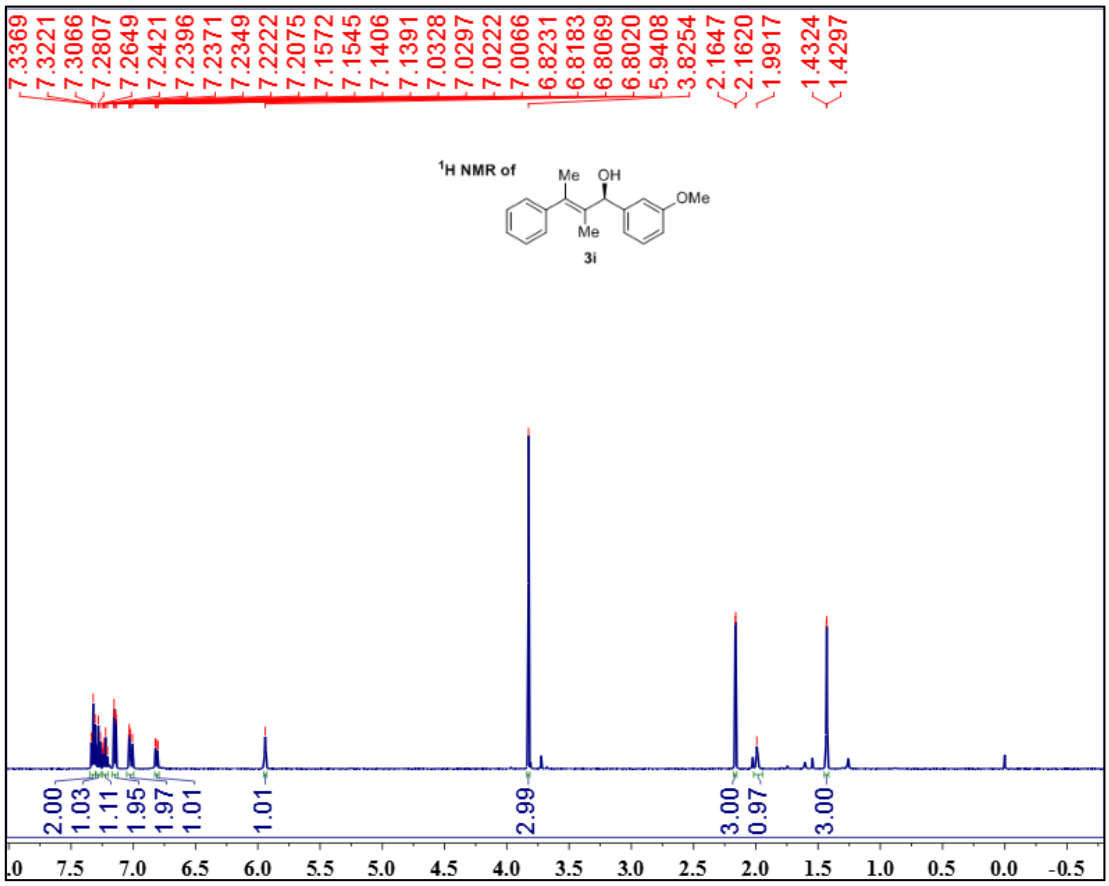

8.0144
7.9934
7.6363
7.6161
7.3553
7.3514
7.3370
7.3216
7.3180
7.2457
7.2426
7.2395
7.2285
7.2241
7.2194
7.2087
7.2056
7.2025
7.1725
7.1691
7.1644
7.1519
6.0569
6.0473
4.6861
4.6764
3.8765
2.2093
2.2057
1.3504
1.3469
^{1}H NMR of
Me
OH
Me
CO$_2$Me
3h
2.00
2.00
2.15
1.03
1.99
1.00
0.96
3.01
3.04
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

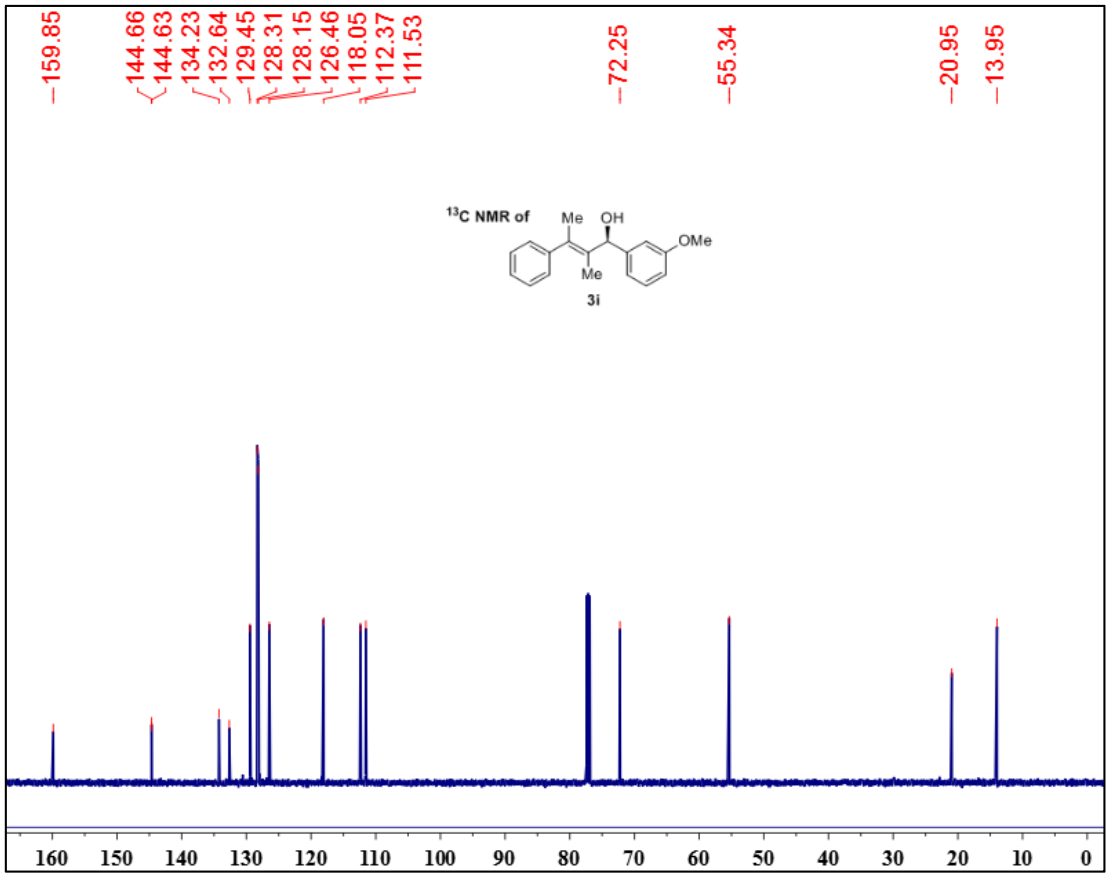

167.32
150.67
145.74
134.24
134.07
130.05
129.47
129.14
128.89
127.20
126.74
71.73
52.29
21.19
14.25
^{13}C NMR of
Me
OH
Me
CO$_2$Me
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

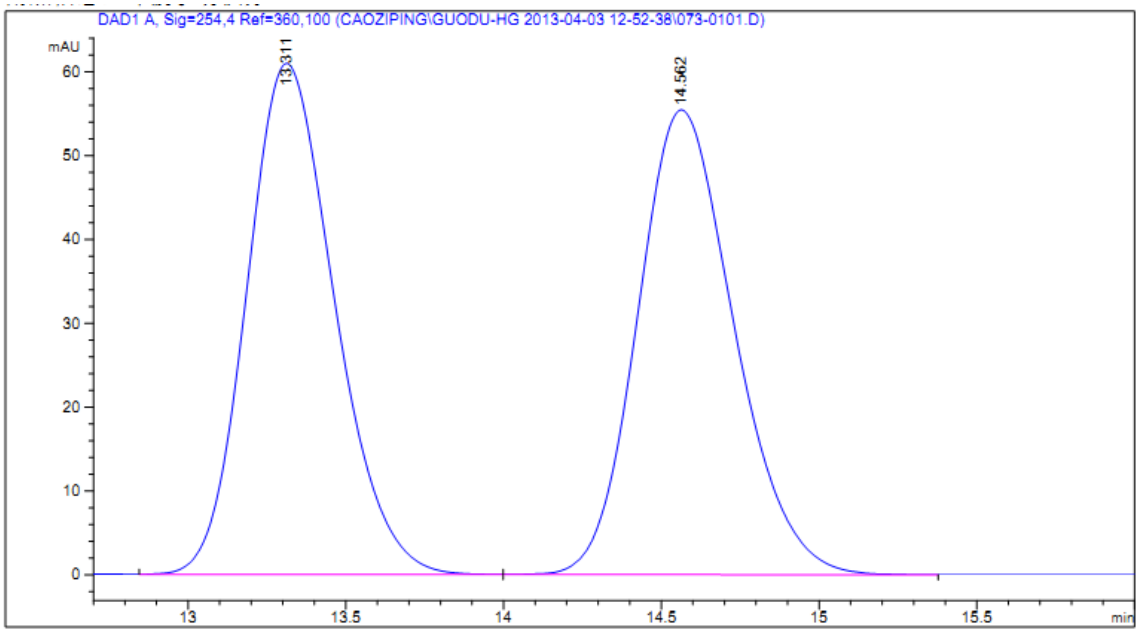


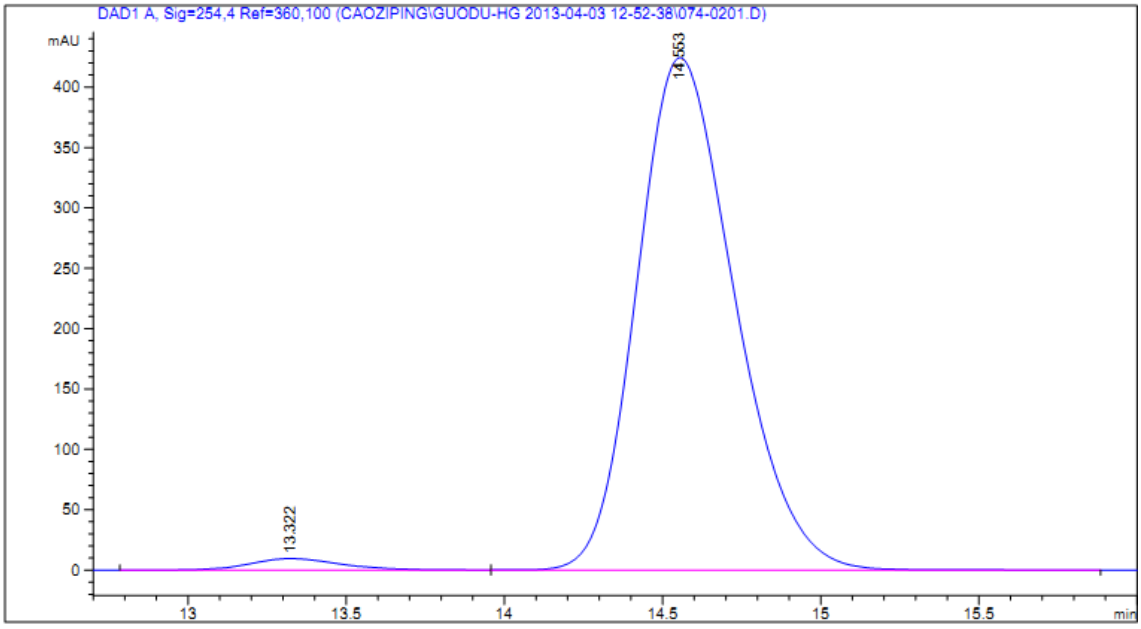


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	25.385	BB	0.8906	1.84481e4	318.08975	91.2007
2	28.238	BB	0.9833	1779.92236	27.34866	8.7993
总量：				2.02280e4	345.43841	

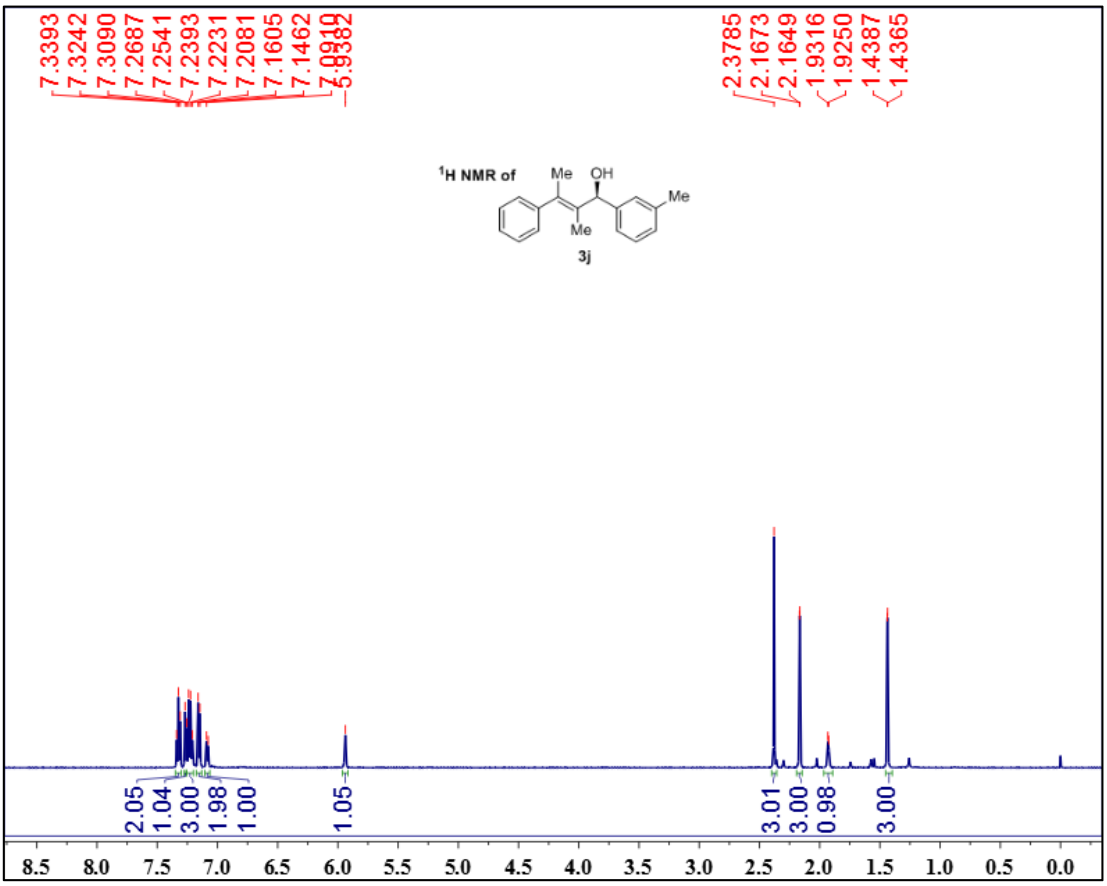

7.3369
7.3221
7.3066
7.2807
7.2649
7.2421
7.2396
7.2371
7.2349
7.2222
7.2075
7.1572
7.1545
7.1406
7.1391
7.0328
7.0297
7.0222
7.0066
6.8231
6.8183
6.8069
6.8020
5.9408
3.8254
2.1647
2.1620
1.9917
1.4324
1.4297
1H NMR of
Me
OH
OMe
Me
3i
2.00
1.03
1.11
1.95
1.97
1.01
1.01
2.99
3.00
0.97
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

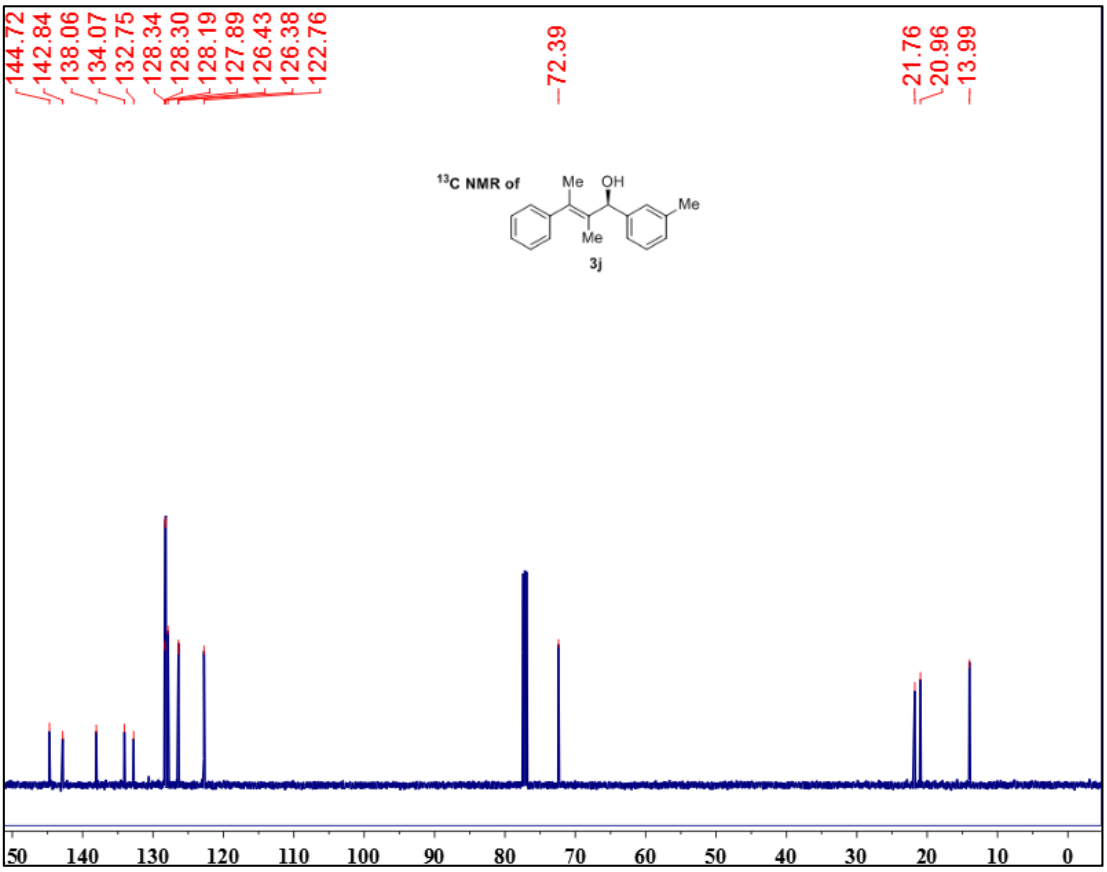

159.85
144.66
144.63
134.23
132.64
129.45
128.31
128.15
126.46
118.05
112.37
111.53
72.25
55.34
20.95
13.95
13C NMR of
Me
OH
OMe
Me
3i
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

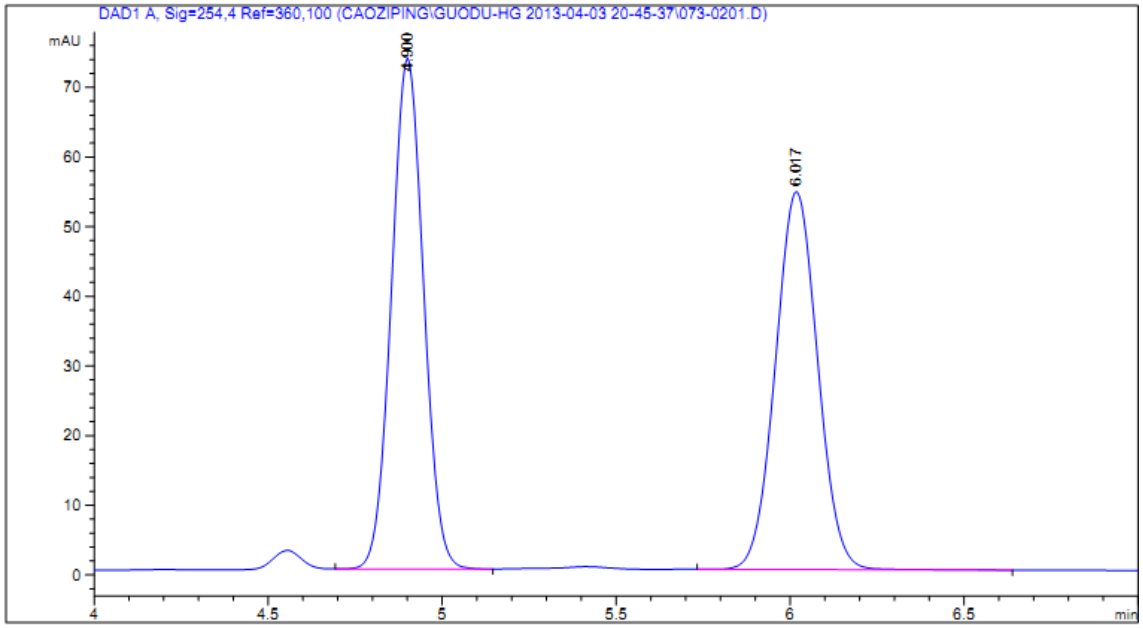


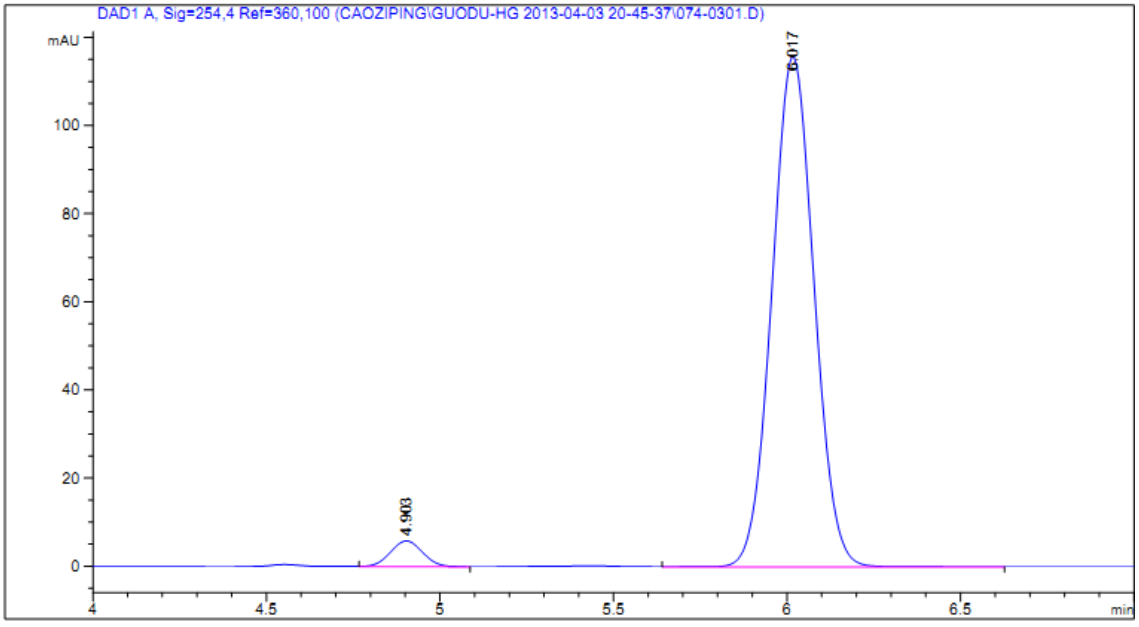


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.322	BB	0.2979	185.43396	9.57837	1.9982
2	14.553	BB	0.3300	9094.81250	424.37741	98.0018
总量：				9280.24646	433.95578	

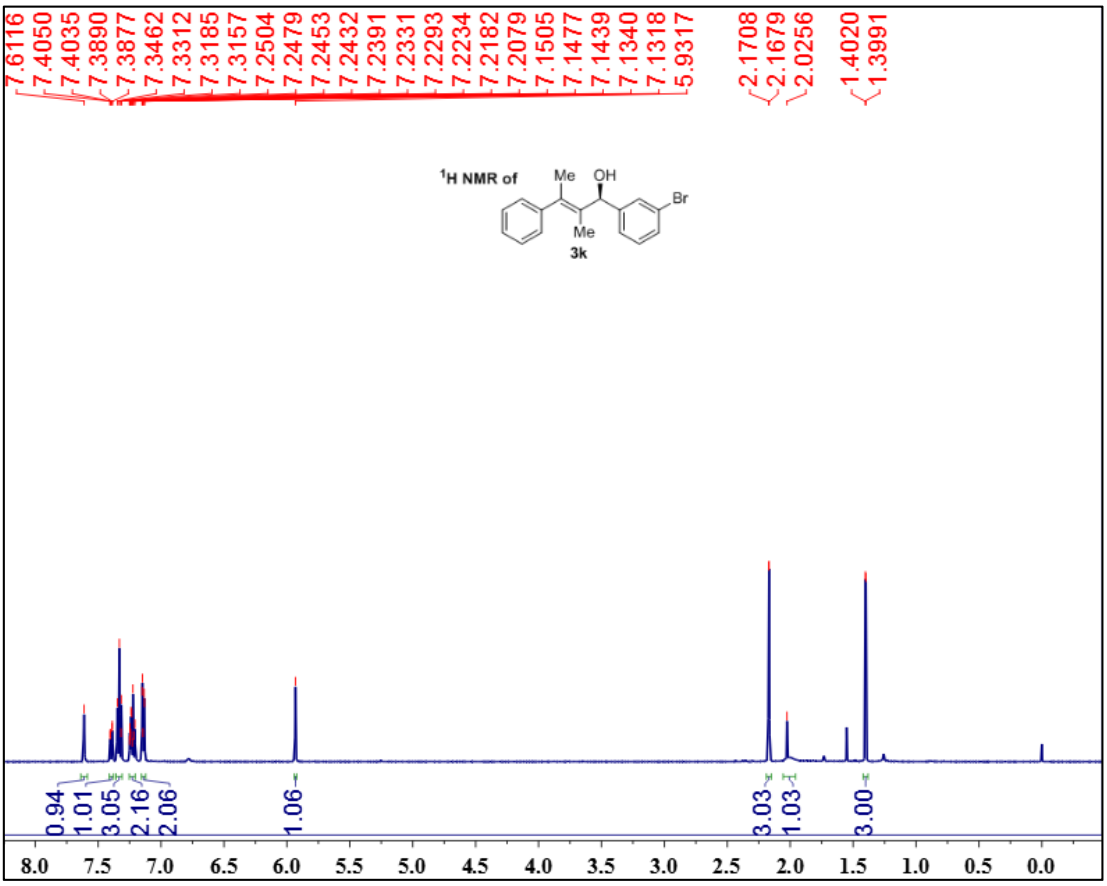

7.3393
7.3242
7.3090
7.2687
7.2541
7.2393
7.2231
7.2081
7.1605
7.1462
7.0910
5.9382
2.3785
2.1673
2.1649
1.9316
1.9250
1.4387
1.4365
1H NMR of
Me
OH
Me
Me
3j
2.05
1.04
3.00
1.98
1.00
1.05
3.01
3.00
0.98
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

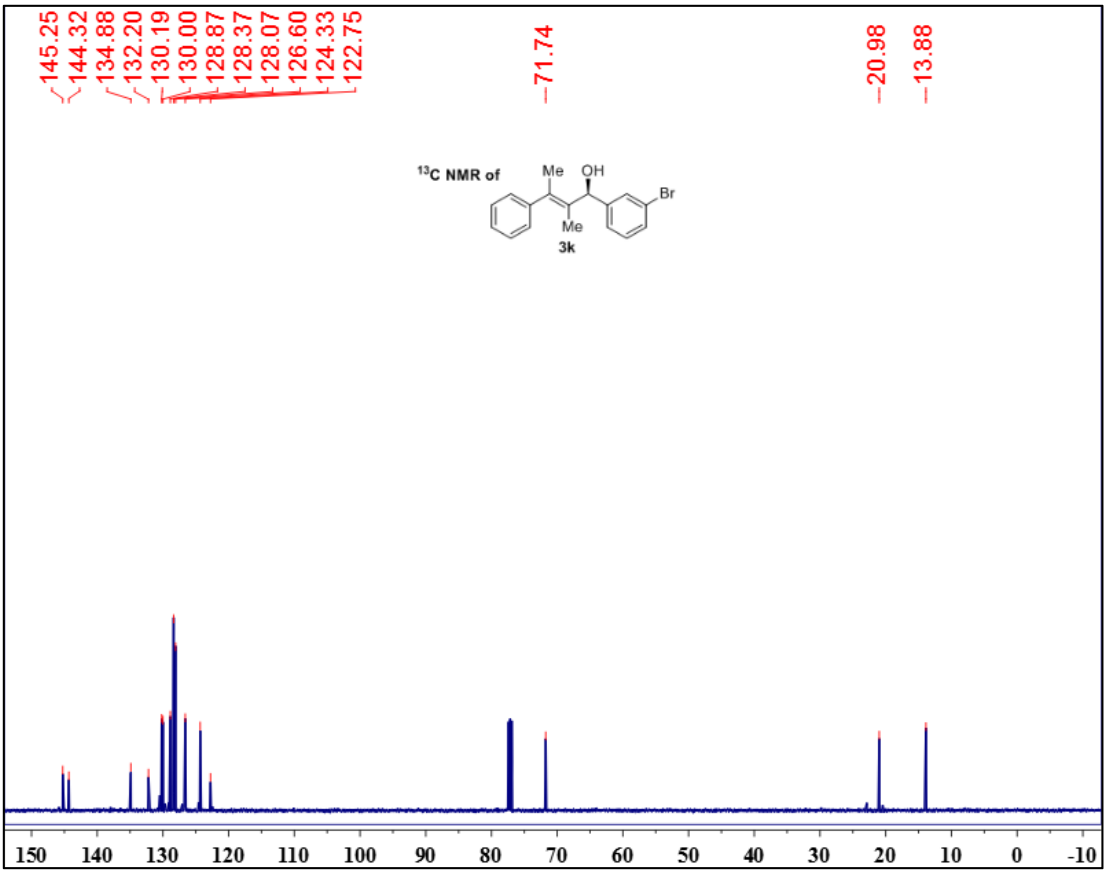

144.72
142.84
138.06
134.07
132.75
128.34
128.30
128.19
127.89
126.43
126.38
122.76
72.39
21.76
20.96
13.99
13C NMR of
Me
OH
Me
Me
3j
50
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

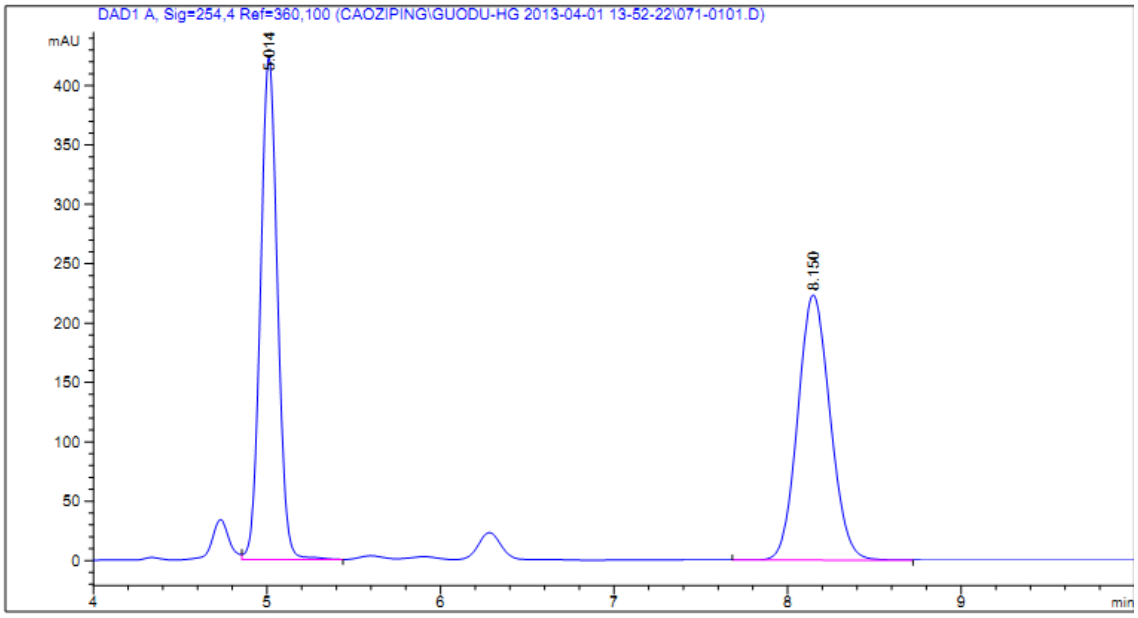


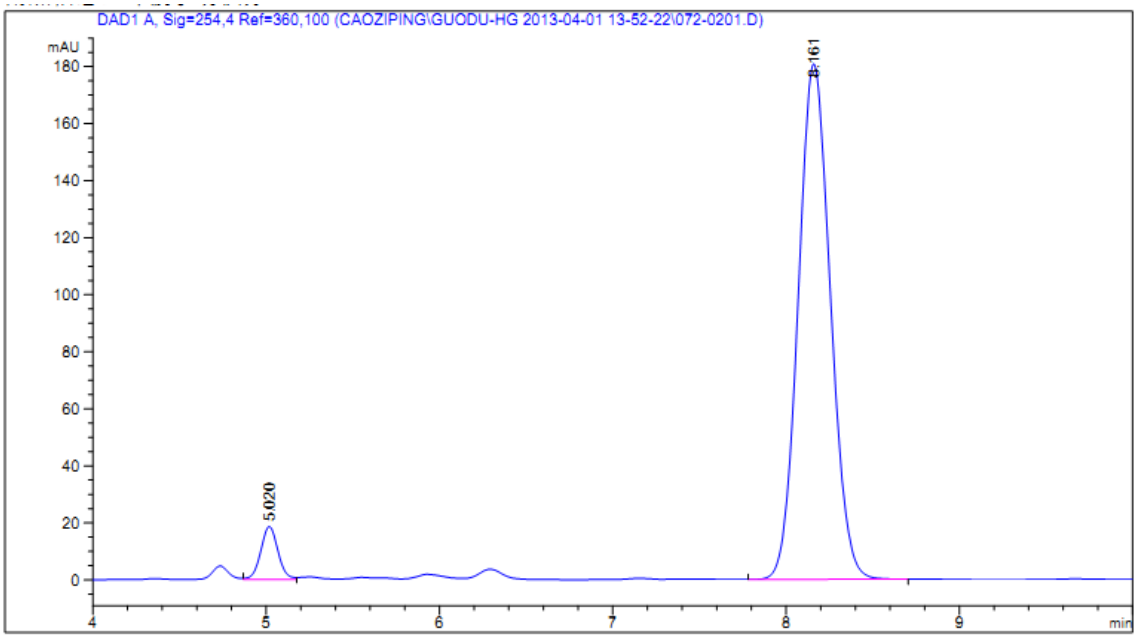


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	4.903	BB	0.0983	37.27598	5.85029	3.6839
2	6.017	BB	0.1301	974.57495	115.89968	96.3161
总量：				1011.85093	121.74997	

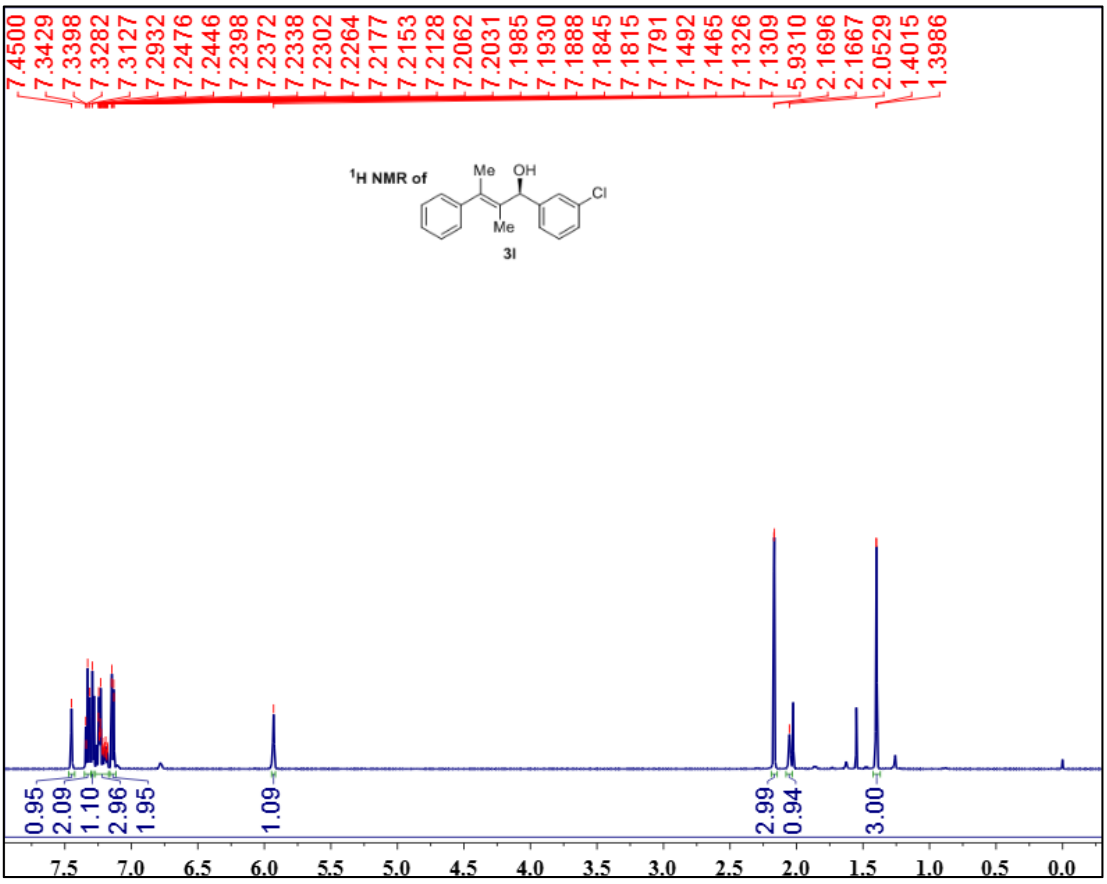

7.6116
7.4050
7.4035
7.3890
7.3877
7.3462
7.3312
7.3185
7.3157
7.2504
7.2479
7.2453
7.2432
7.2391
7.2331
7.2293
7.2234
7.2182
7.2079
7.1505
7.1477
7.1439
7.1340
7.1318
5.9317
2.1708
2.1679
2.0256
1.4020
1.3991
^{1}H NMR of
Me
OH
Br
Me
3k
0.94
1.01
3.05
2.16
2.06
1.06
3.03
1.03
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

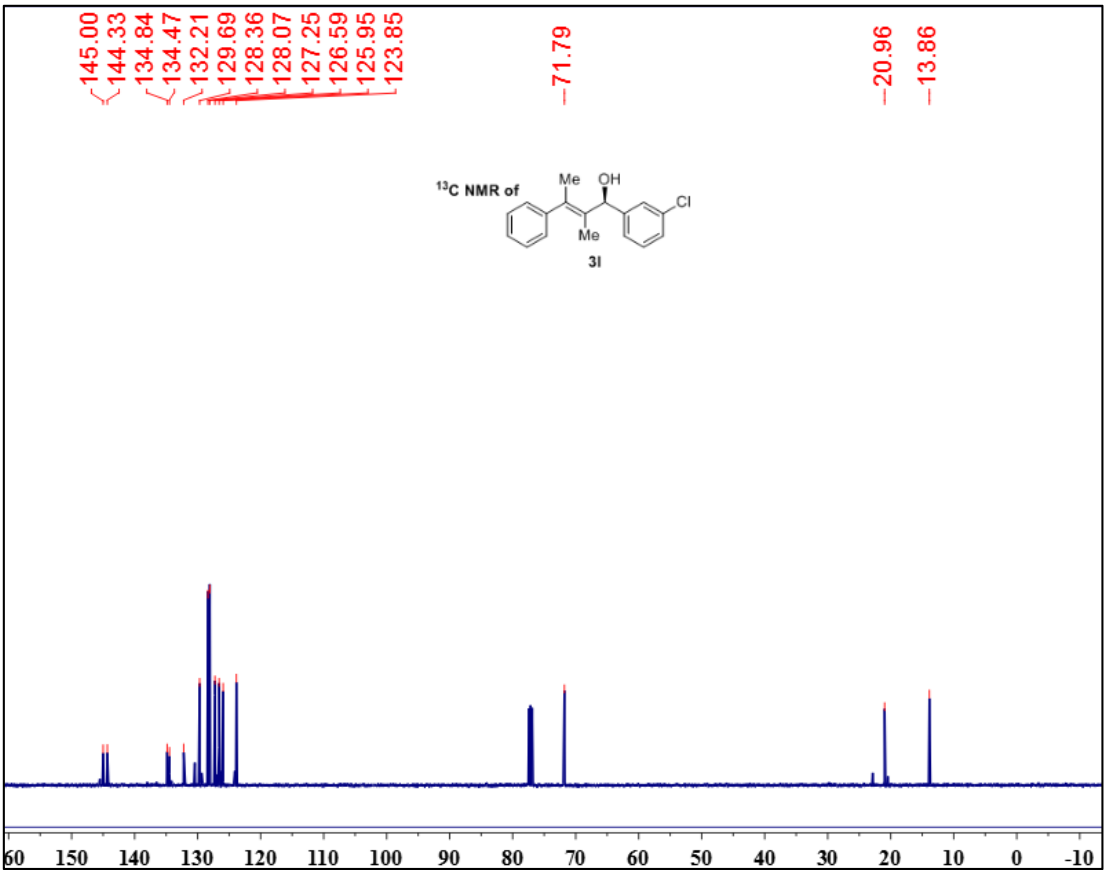

145.25
144.32
134.88
132.20
130.19
130.00
128.87
128.37
128.07
126.60
124.33
122.75
71.74
20.98
13.88
^{13}C NMR of
Me
OH
Br
Me
3k
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

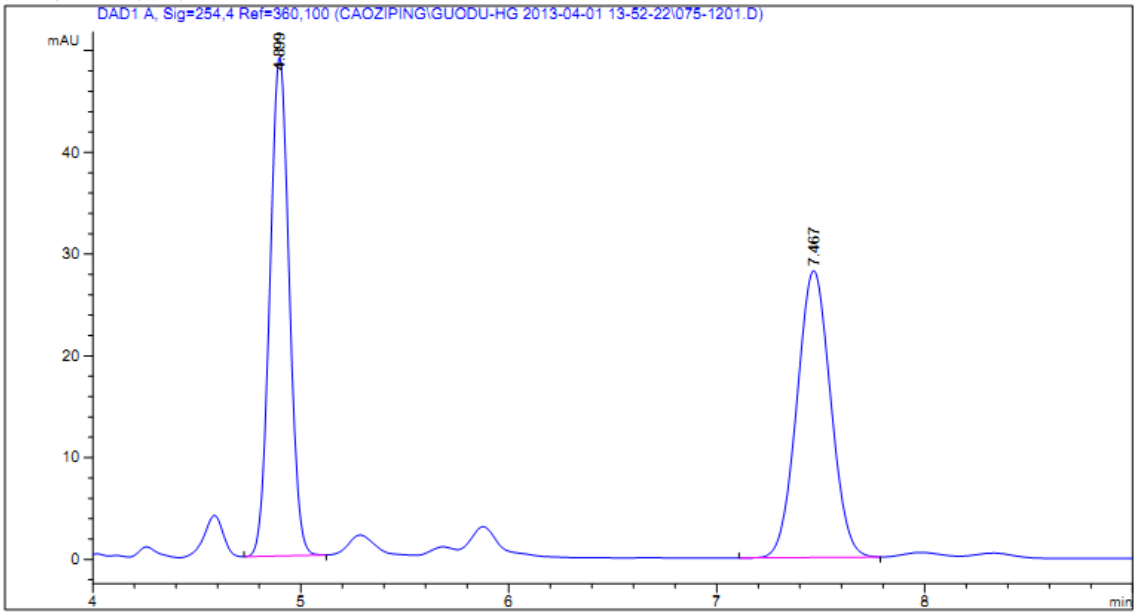


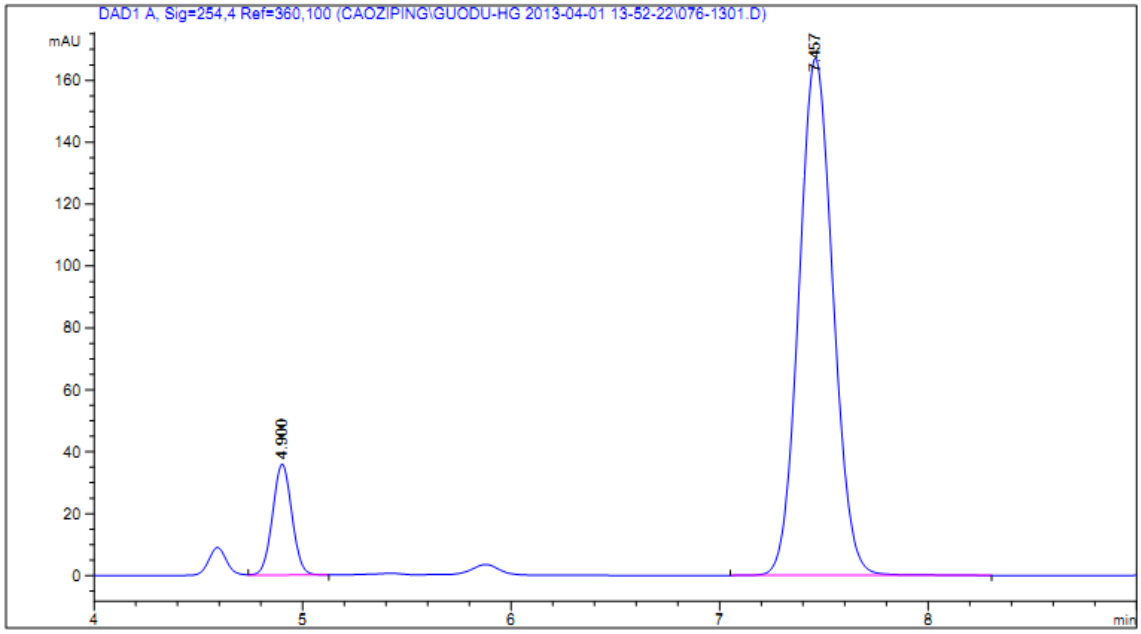


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.020	VV	0.1058	126.61292	18.50983	5.1636
2	8.161	BB	0.2001	2325.40234	180.78058	94.8364
总量：				2452.01526	199.29041	

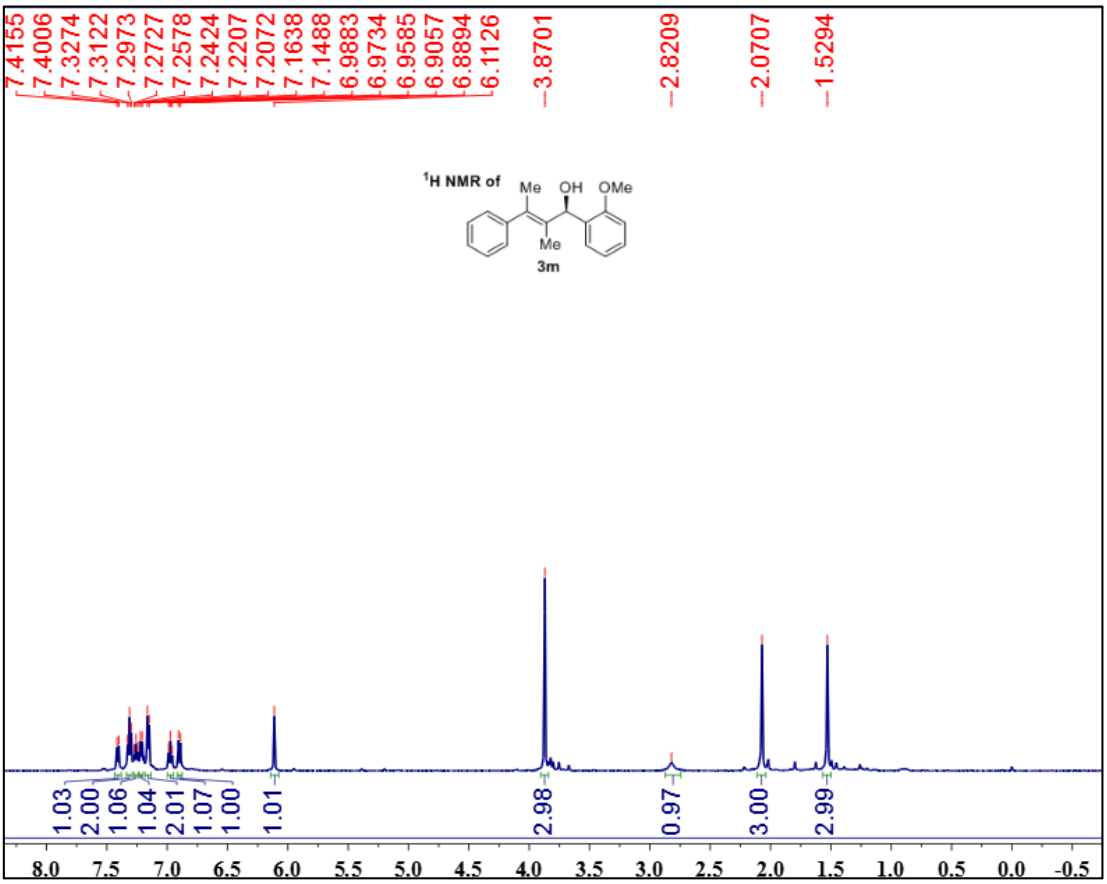

7.4500
7.3429
7.3398
7.3282
7.3127
7.2932
7.2476
7.2446
7.2398
7.2372
7.2338
7.2302
7.2264
7.2177
7.2153
7.2128
7.2062
7.2031
7.1985
7.1930
7.1888
7.1845
7.1815
7.1791
7.1492
7.1465
7.1326
7.1309
5.9310
2.1696
2.1667
2.0529
1.4015
1.3986
1H NMR of
Me
OH
Cl
Me
3l
0.95
2.09
1.10
2.96
1.95
1.09
2.99
0.94
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

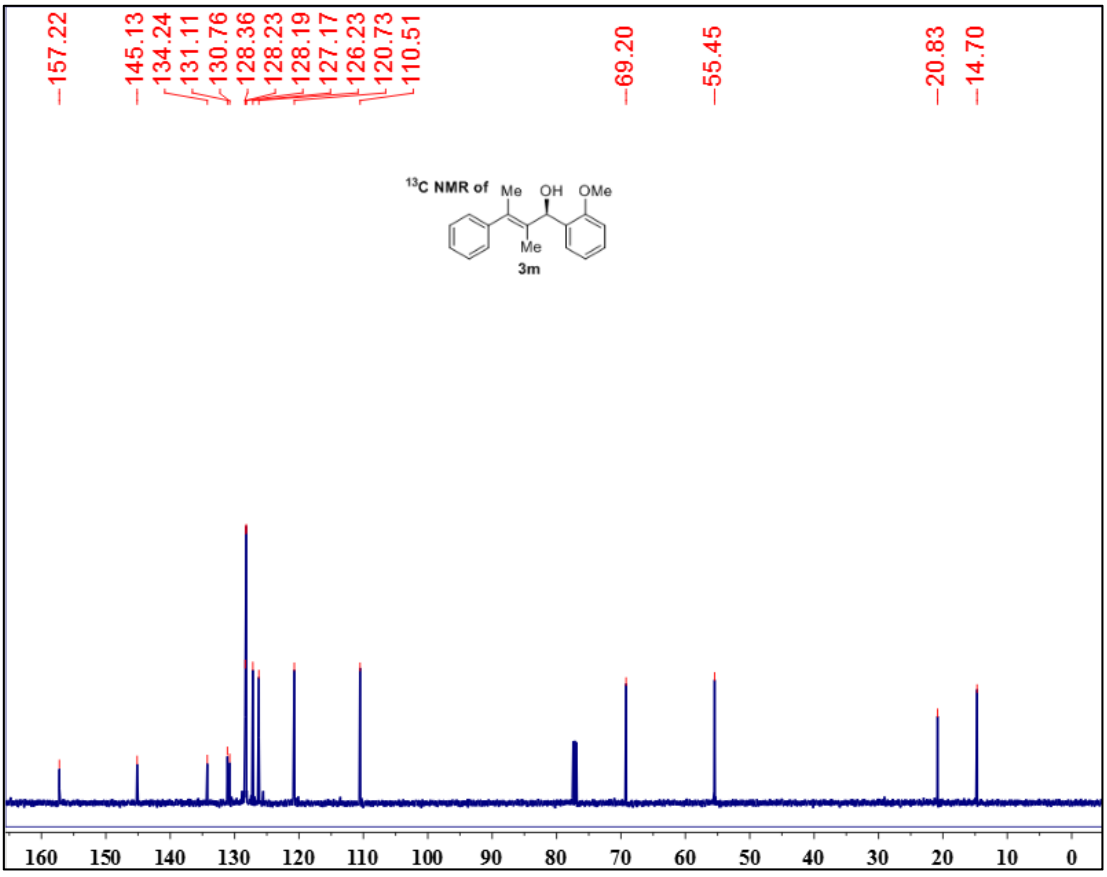

145.00
144.33
134.84
134.47
132.21
129.69
128.36
128.07
127.25
126.59
125.95
123.85
71.79
20.96
13.86
13C NMR of
Me
OH
Cl
Me
3l
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

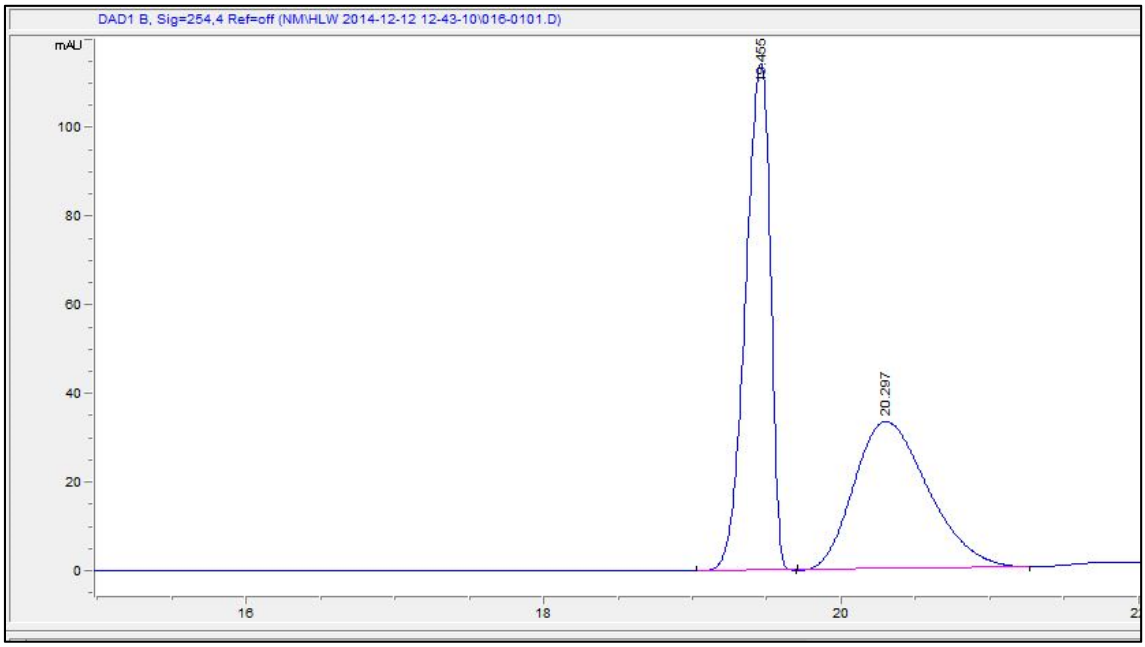


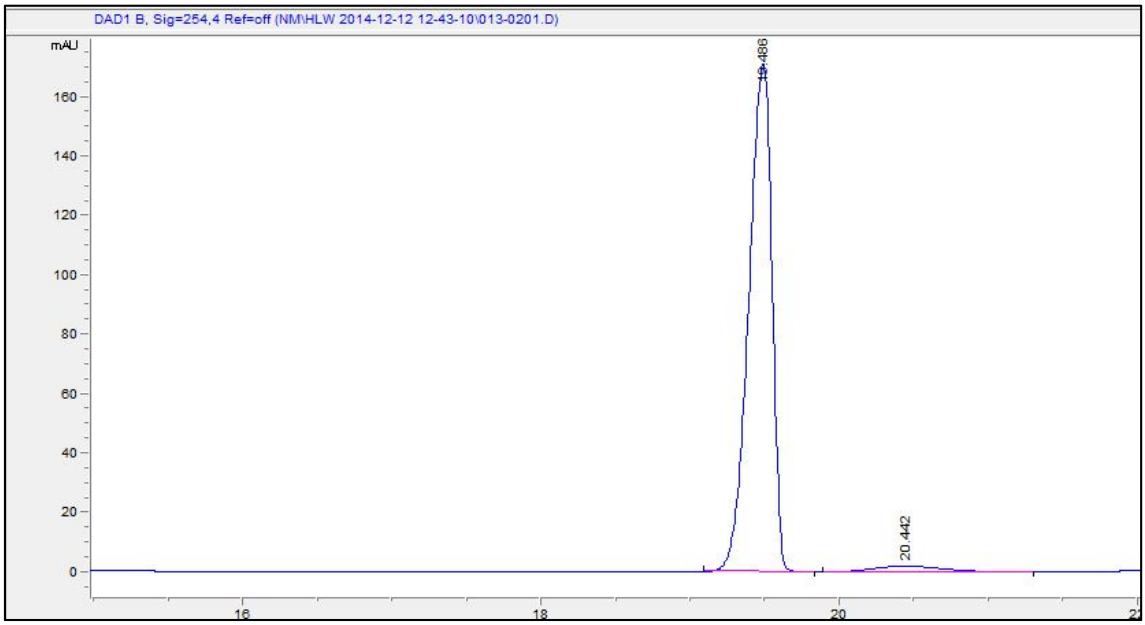


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	4.900	VB	0.1011	230.75443	35.86571	10.8492
2	7.457	BB	0.1784	1896.17529	167.10973	89.1508
总量 :				2126.92972	202.97544	

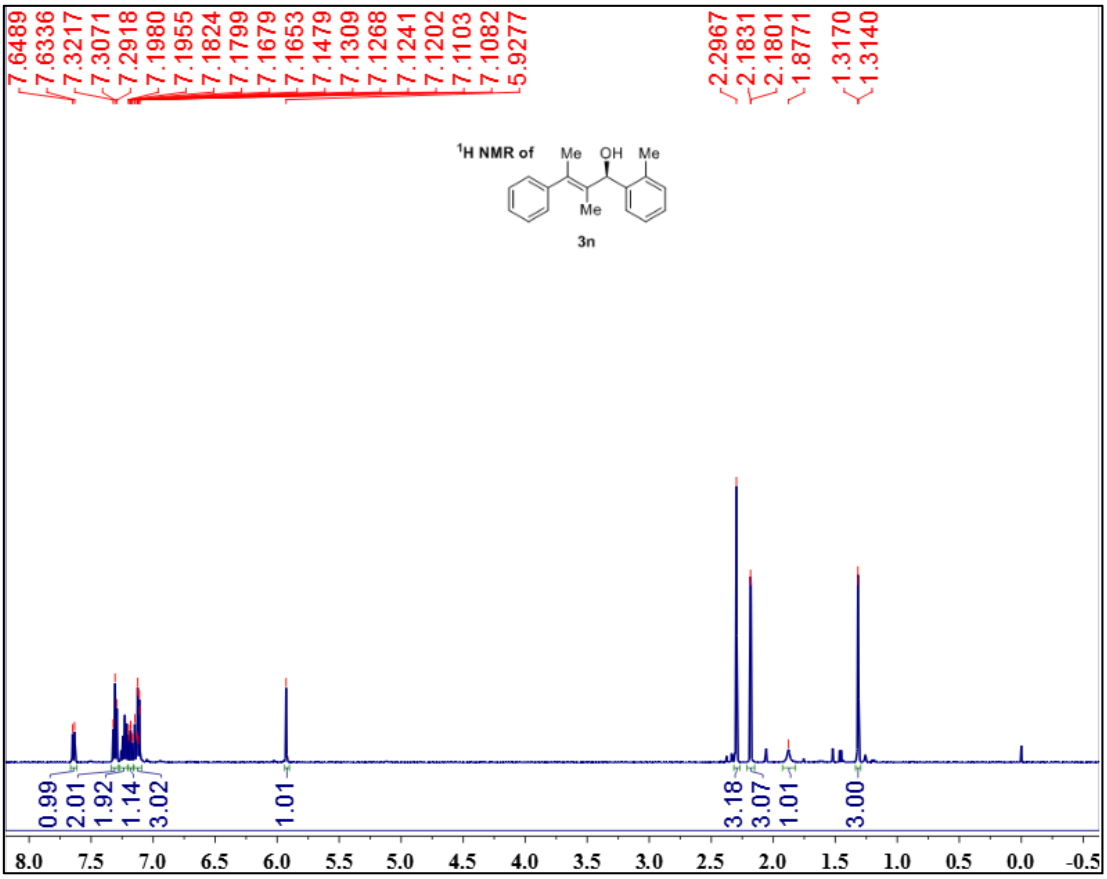

7.4155
7.4006
7.3274
7.3122
7.2973
7.2727
7.2578
7.2424
7.2207
7.2072
7.1638
7.1488
6.9883
6.9734
6.9585
6.9057
6.8894
6.1126
3.8701
2.8209
2.0707
1.5294
1H NMR of
Me
OH
OMe
Me
3m
1.03
2.00
1.06
1.04
2.01
1.07
1.00
1.01
2.98
0.97
3.00
2.99
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

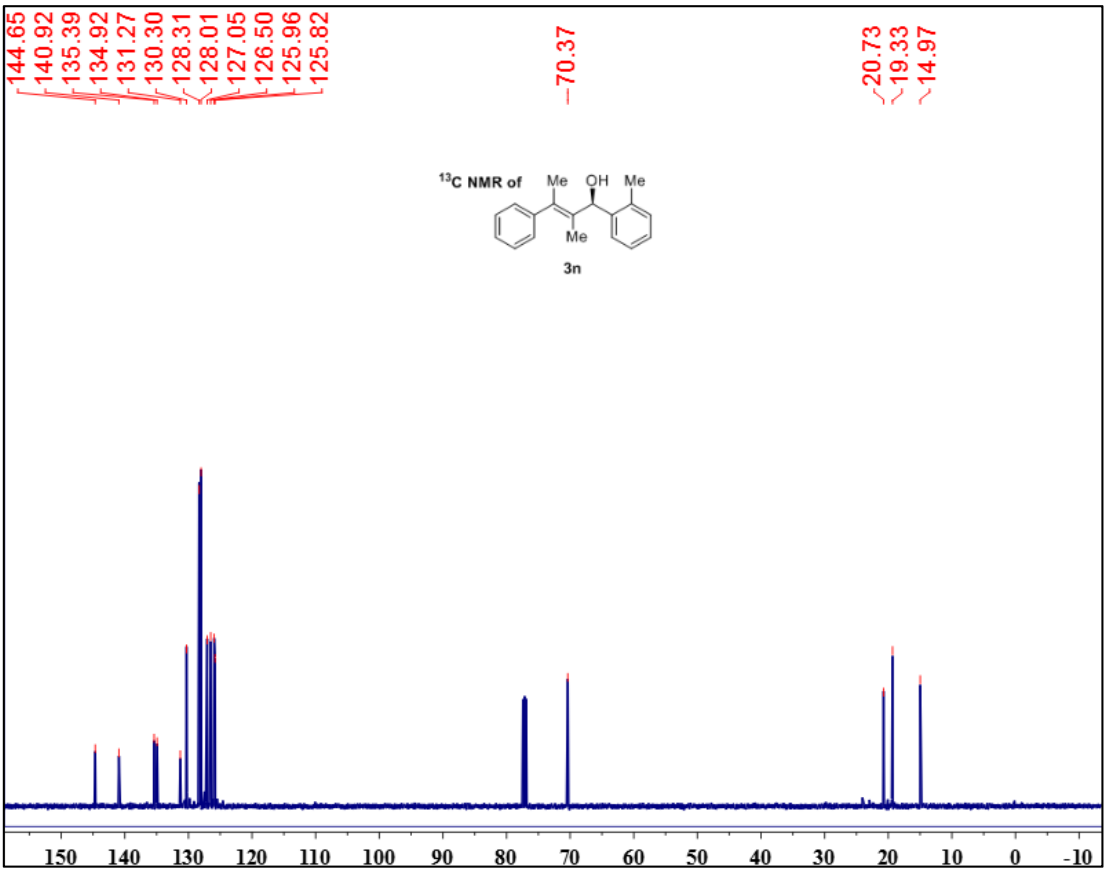

157.22
145.13
134.24
131.11
130.76
128.36
128.23
128.19
127.17
126.23
120.73
110.51
69.20
55.45
20.83
14.70
13C NMR of
Me
OH
OMe
Me
3m
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

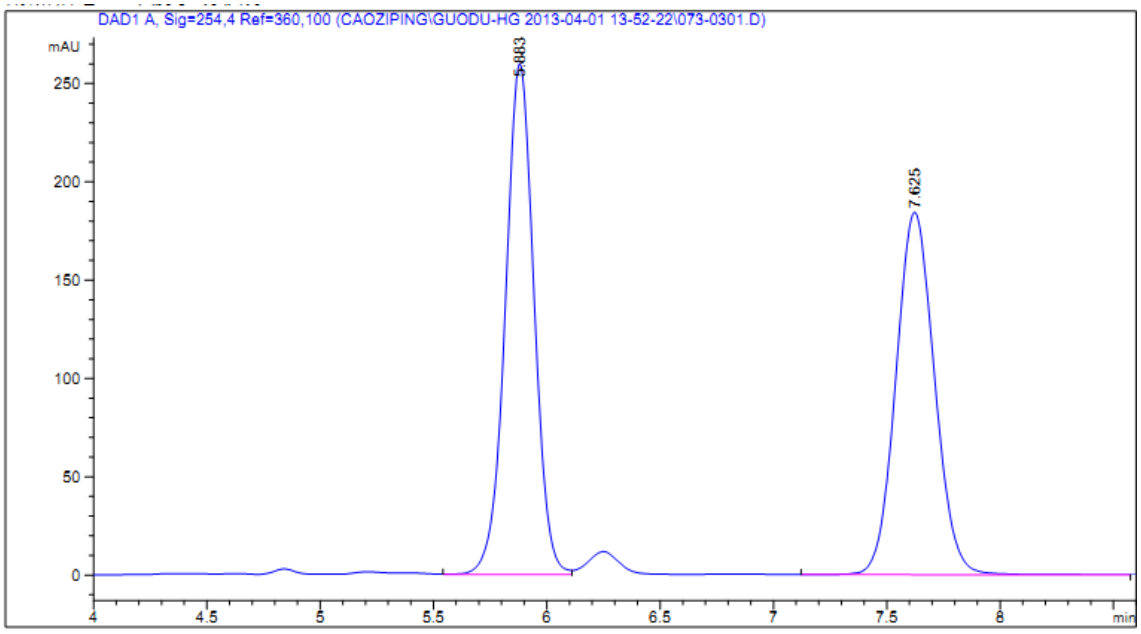


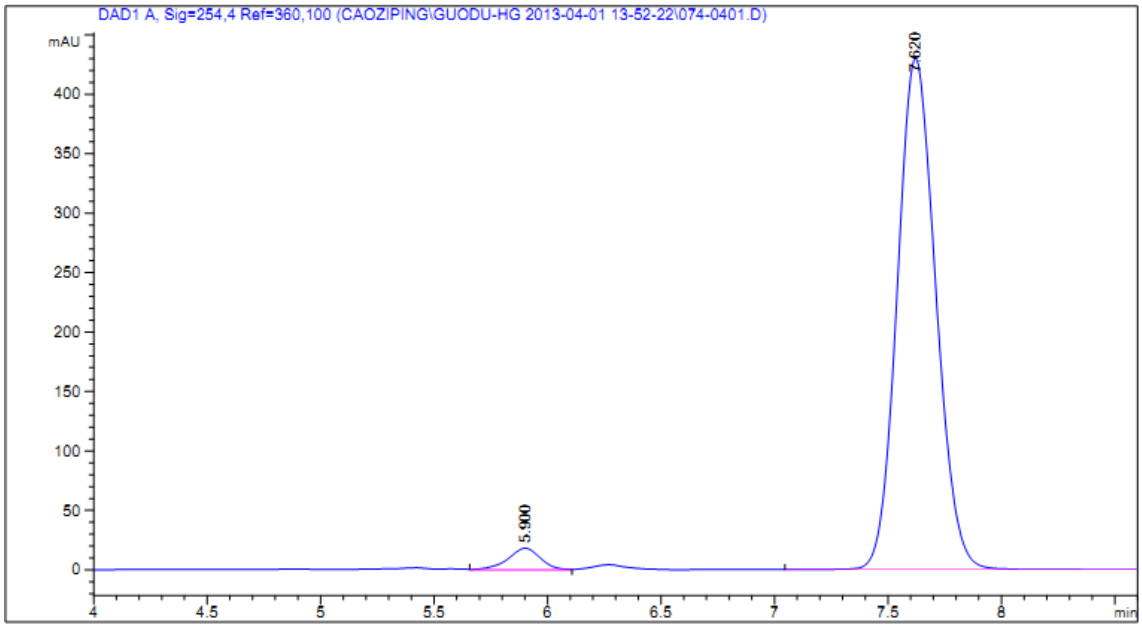


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	19.486	BB	0.1703	1853.55164	171.25873	96.3668
2	20.442	BB	0.4431	69.88297	2.06354	3.6332
总量：				1923.43460	173.32226	

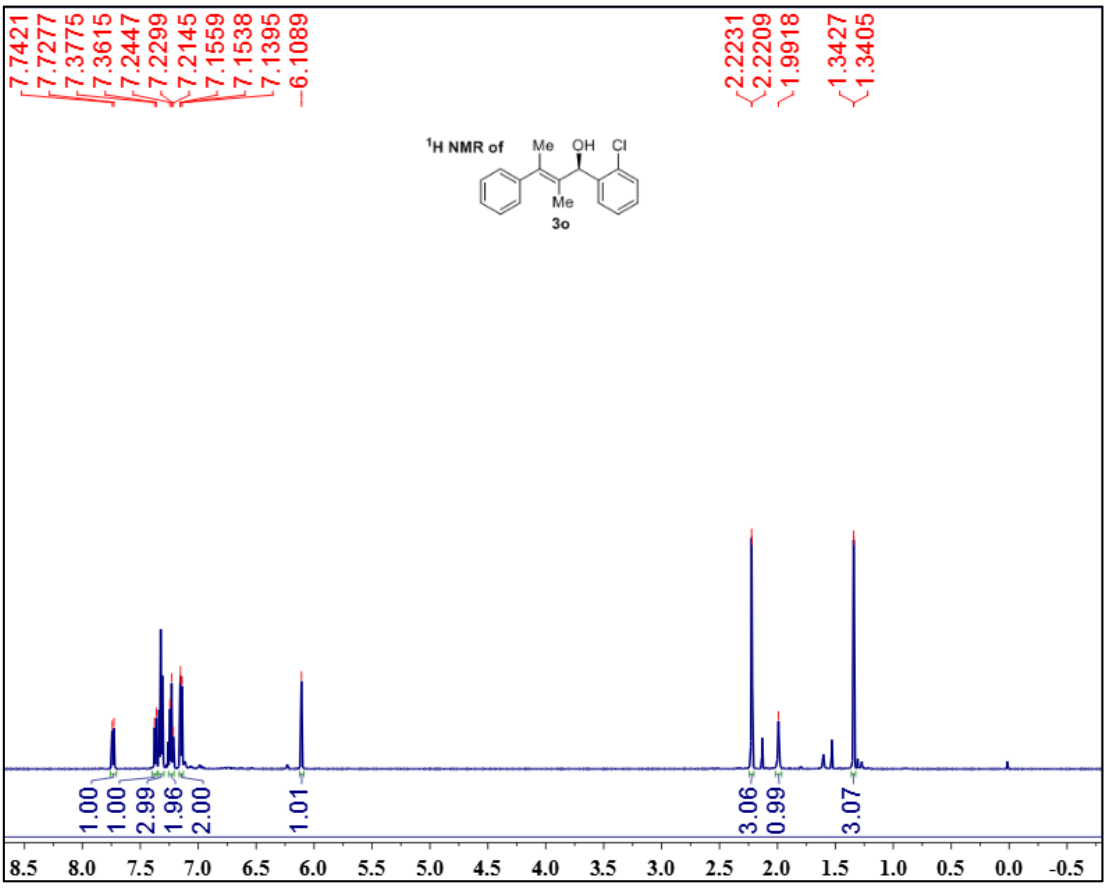

7.6489
7.6336
7.3217
7.3071
7.2918
7.1980
7.1955
7.1824
7.1799
7.1679
7.1653
7.1479
7.1309
7.1268
7.1241
7.1202
7.1103
7.1082
5.9277
2.2967
2.1831
2.1801
1.8771
1.3170
1.3140
1H NMR of
Me
OH
Me
Me
3n
0.99
2.01
1.92
1.14
3.02
1.01
3.18
3.07
1.01
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

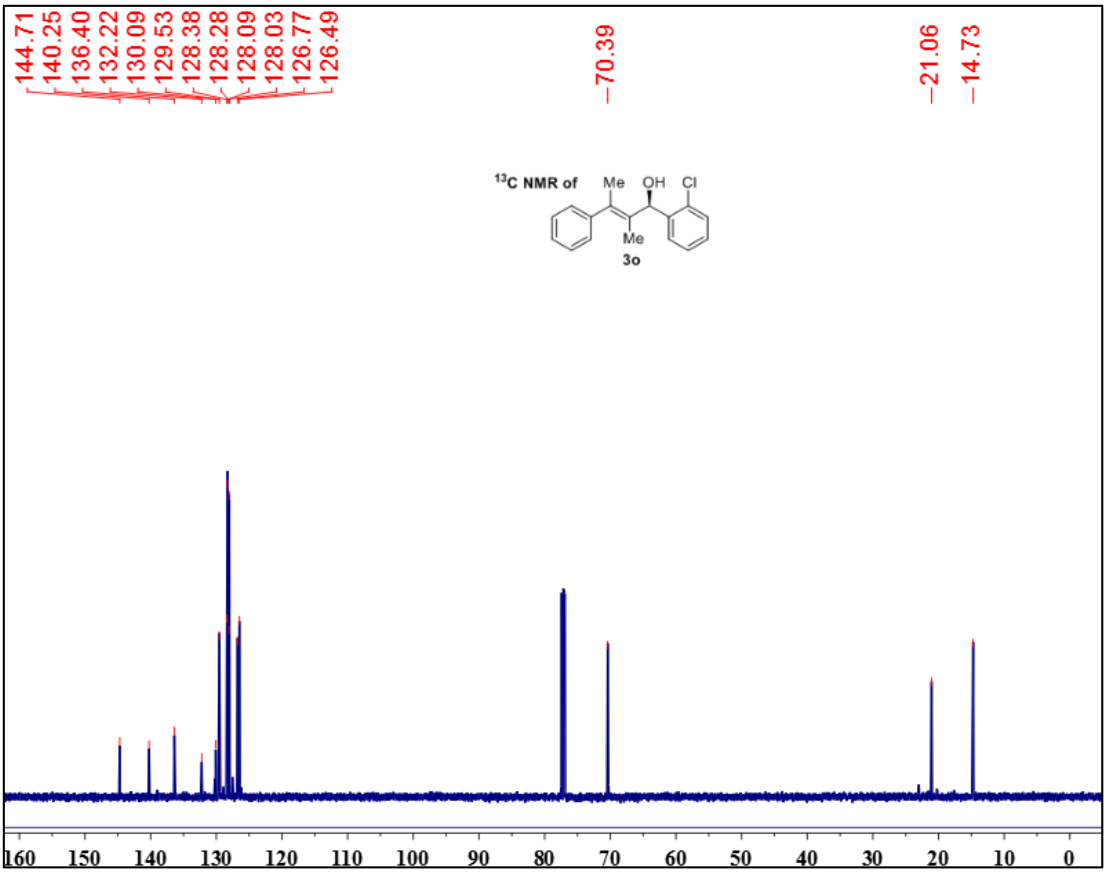

144.65
140.92
135.39
134.92
131.27
130.30
128.31
128.01
127.05
126.50
125.96
125.82
70.37
20.73
19.33
14.97
13C NMR of
Me
OH
Me
Me
3n
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

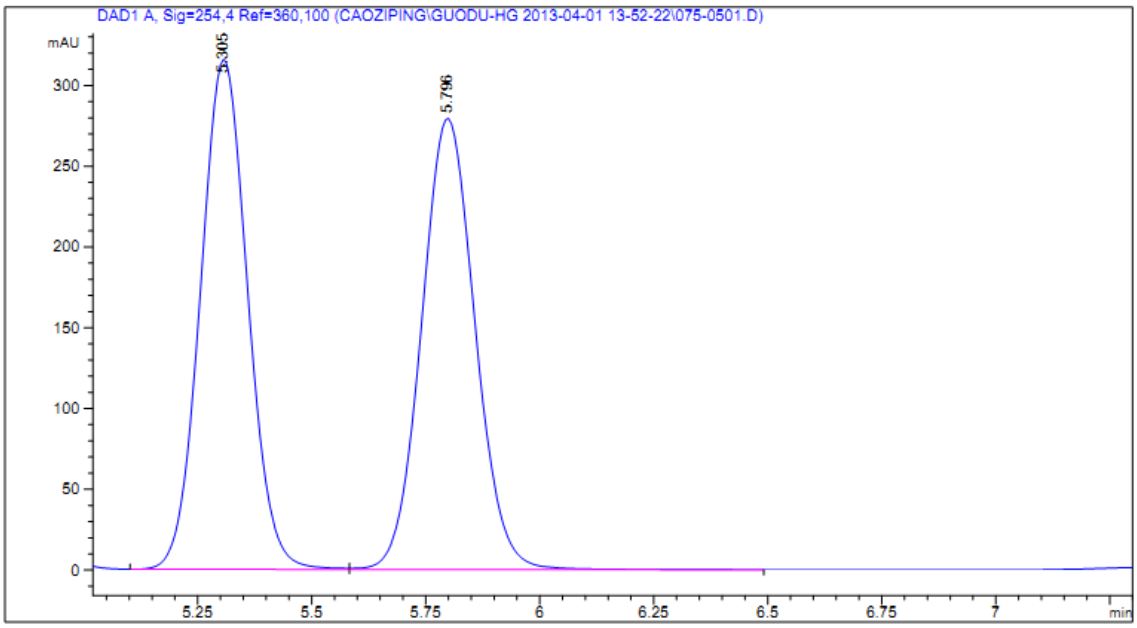


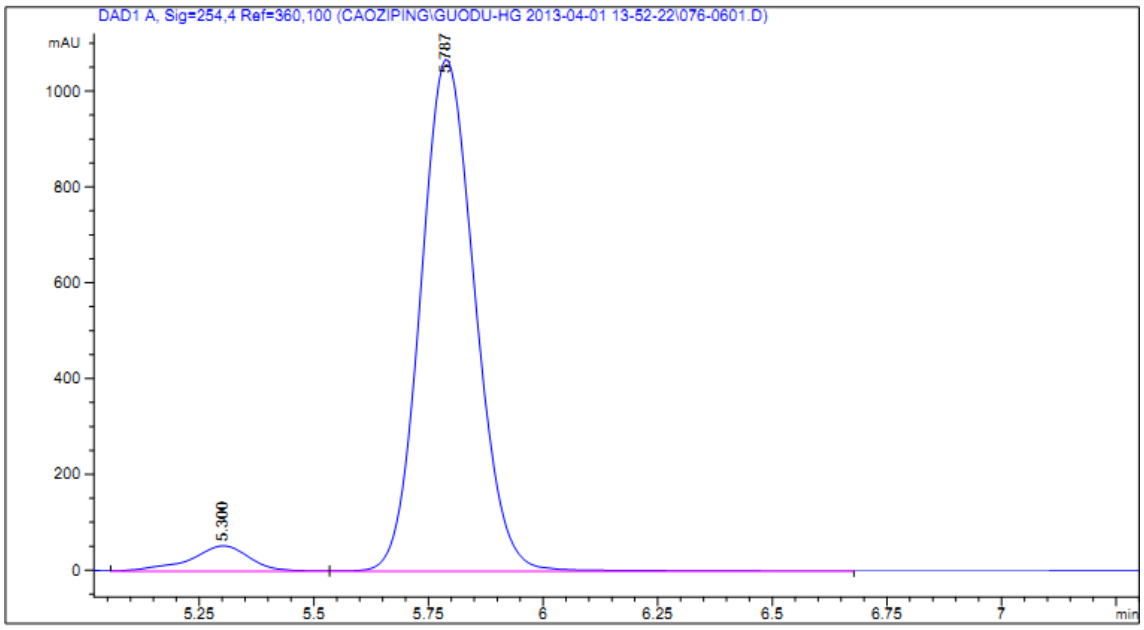


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.900	VV	0.1513	178.68979	18.08621	3.3993
2	7.620	BB	0.1837	5078.01221	430.26016	96.6007
总量：				5256.70200	448.34637	

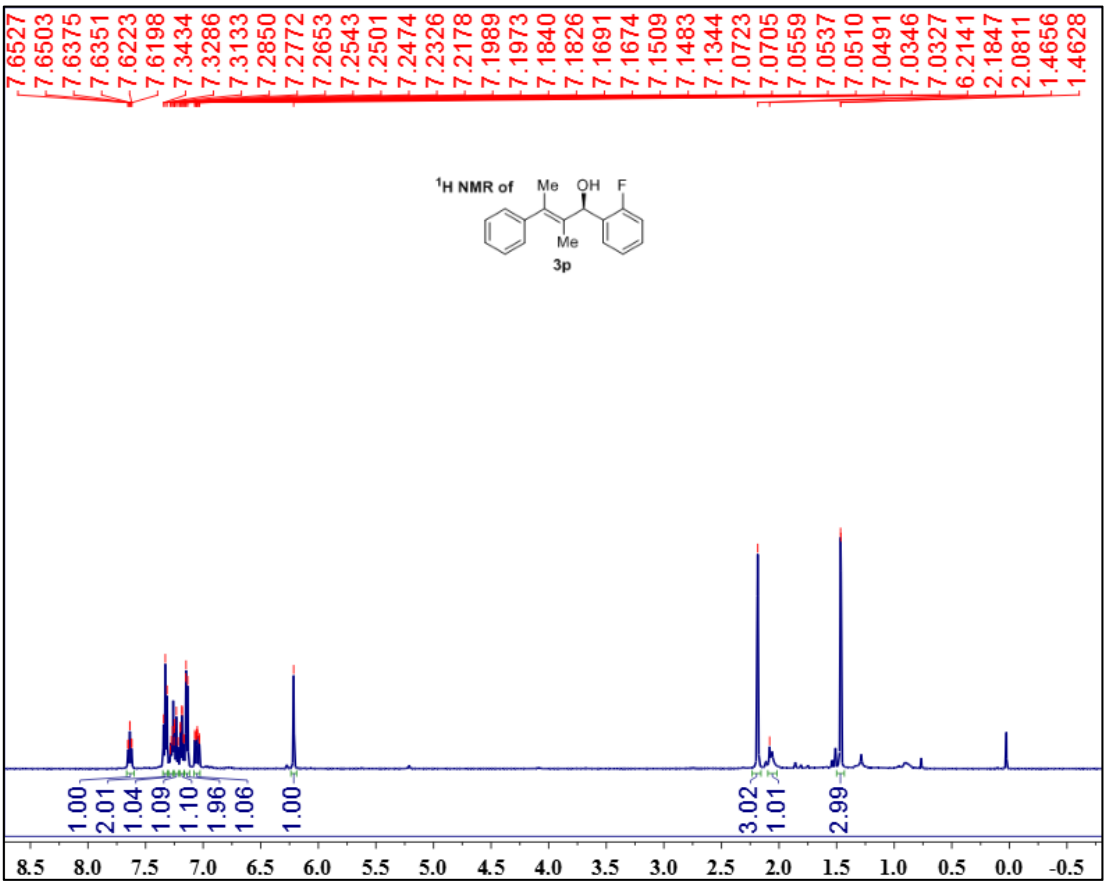

7.7421
7.7277
7.3775
7.3615
7.2447
7.2299
7.2145
7.1559
7.1538
7.1395
6.1089
2.2231
2.2209
1.9918
1.3427
1.3405
1H NMR of
Me
OH
Cl
Me
3o
1.00
1.00
2.99
1.96
2.00
1.01
3.06
0.99
3.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

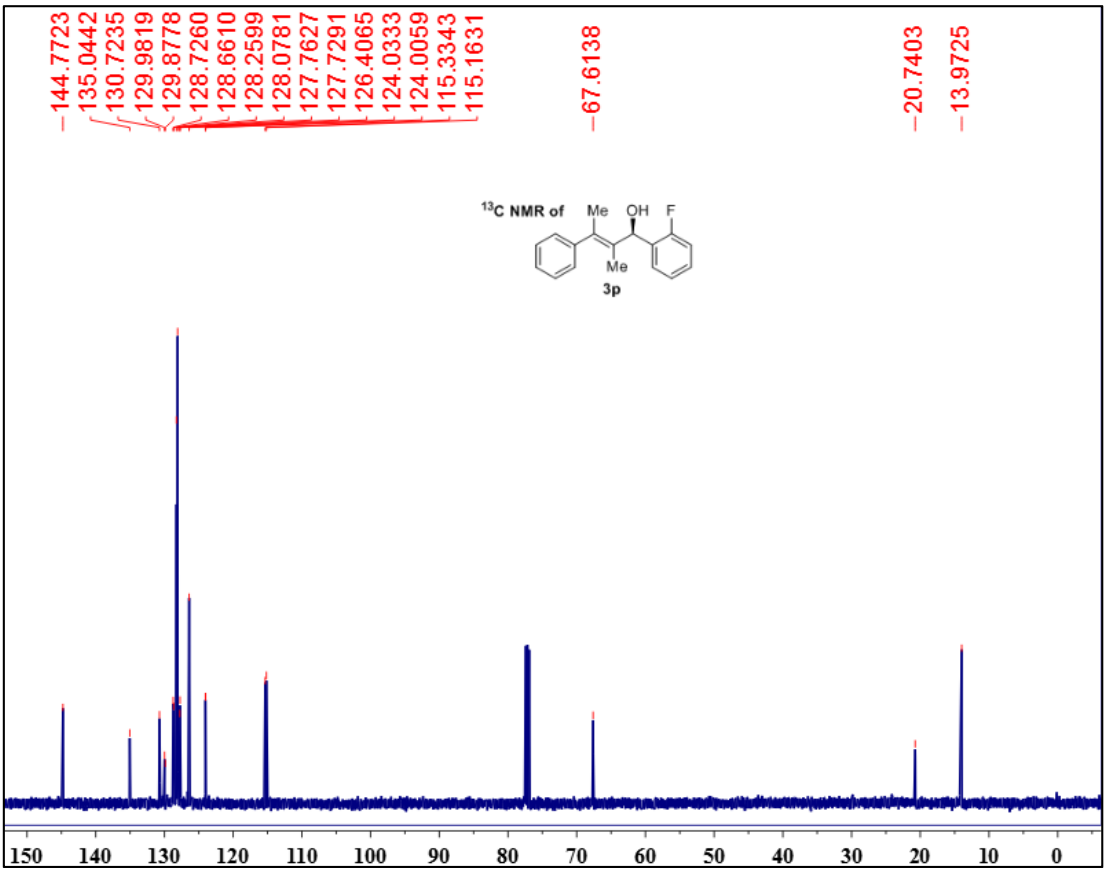

144.71
140.25
136.40
132.22
130.09
129.53
128.38
128.28
128.09
128.03
126.77
126.49
70.39
21.06
14.73
13C NMR of
Me
OH
Cl
Me
3o
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

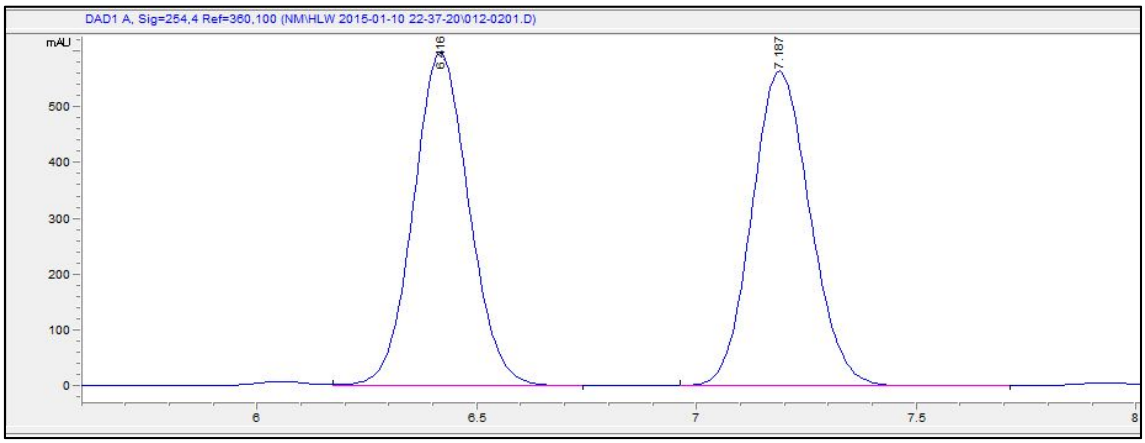


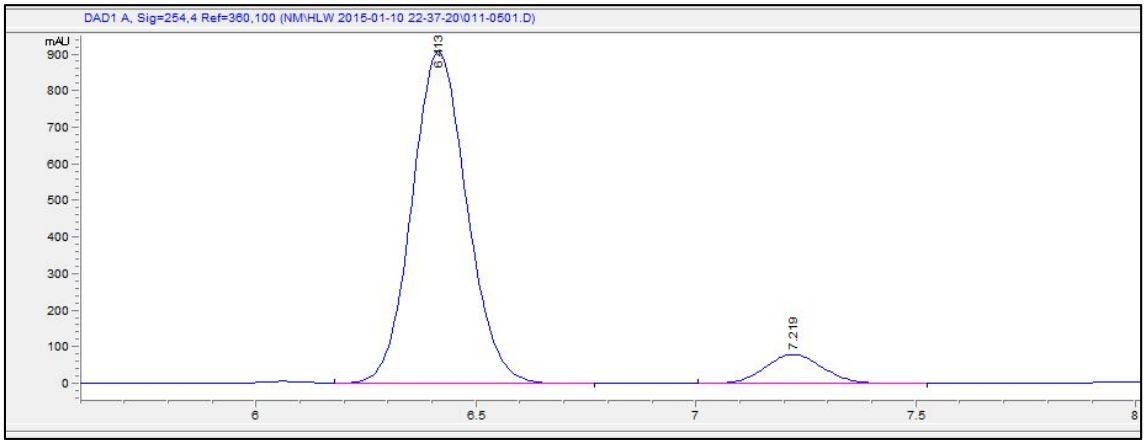


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.300	VV	0.1339	481.46420	53.05452	5.2126
2	5.787	VB	0.1275	8755.03711	1069.39294	94.7874
总量：				9236.50131	1122.44746	

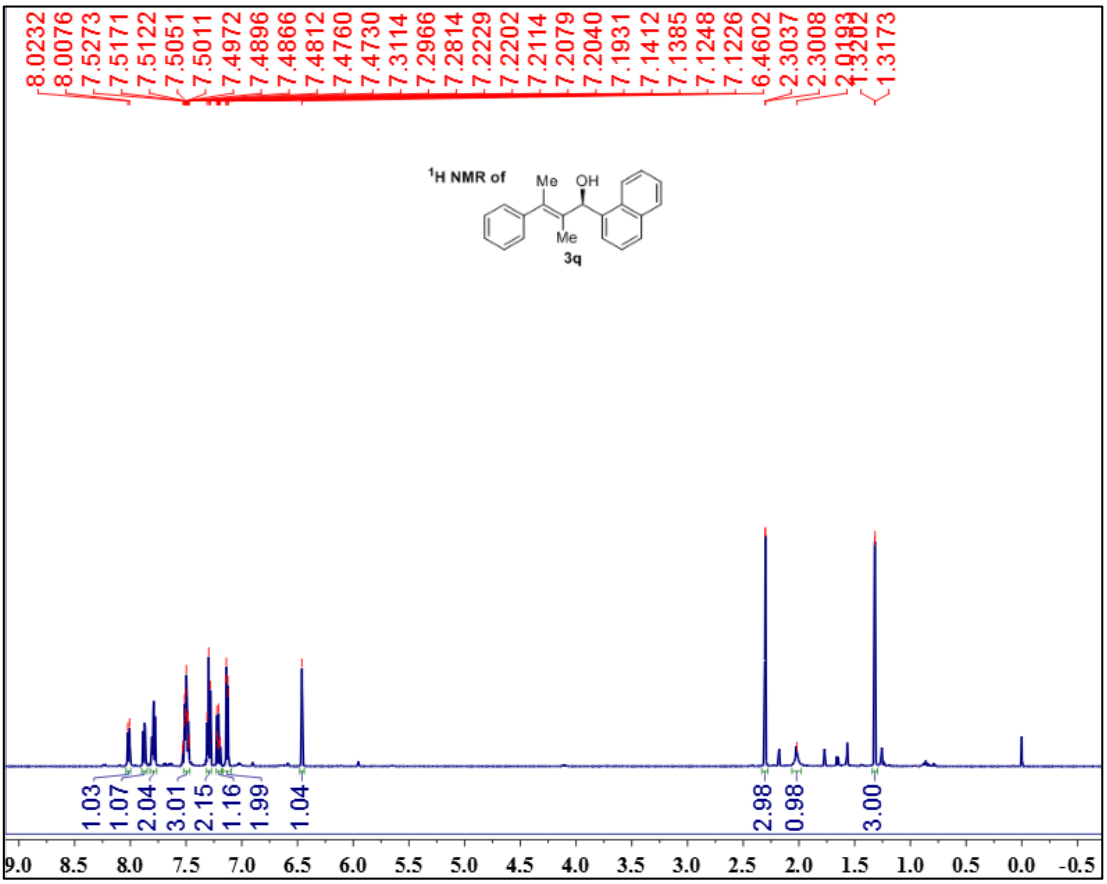

7.6527
7.6503
7.6375
7.6351
7.6223
7.6198
7.3434
7.3286
7.3133
7.2850
7.2772
7.2653
7.2543
7.2501
7.2474
7.2326
7.2178
7.1989
7.1973
7.1840
7.1826
7.1691
7.1674
7.1509
7.1483
7.1344
7.0723
7.0705
7.0559
7.0537
7.0510
7.0491
7.0346
7.0327
6.2141
2.1847
2.0811
1.4656
1.4628
1H NMR of
Me
OH
F
Me
3p
1.00
2.01
1.04
1.09
1.10
1.96
1.06
1.00
3.02
1.01
2.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

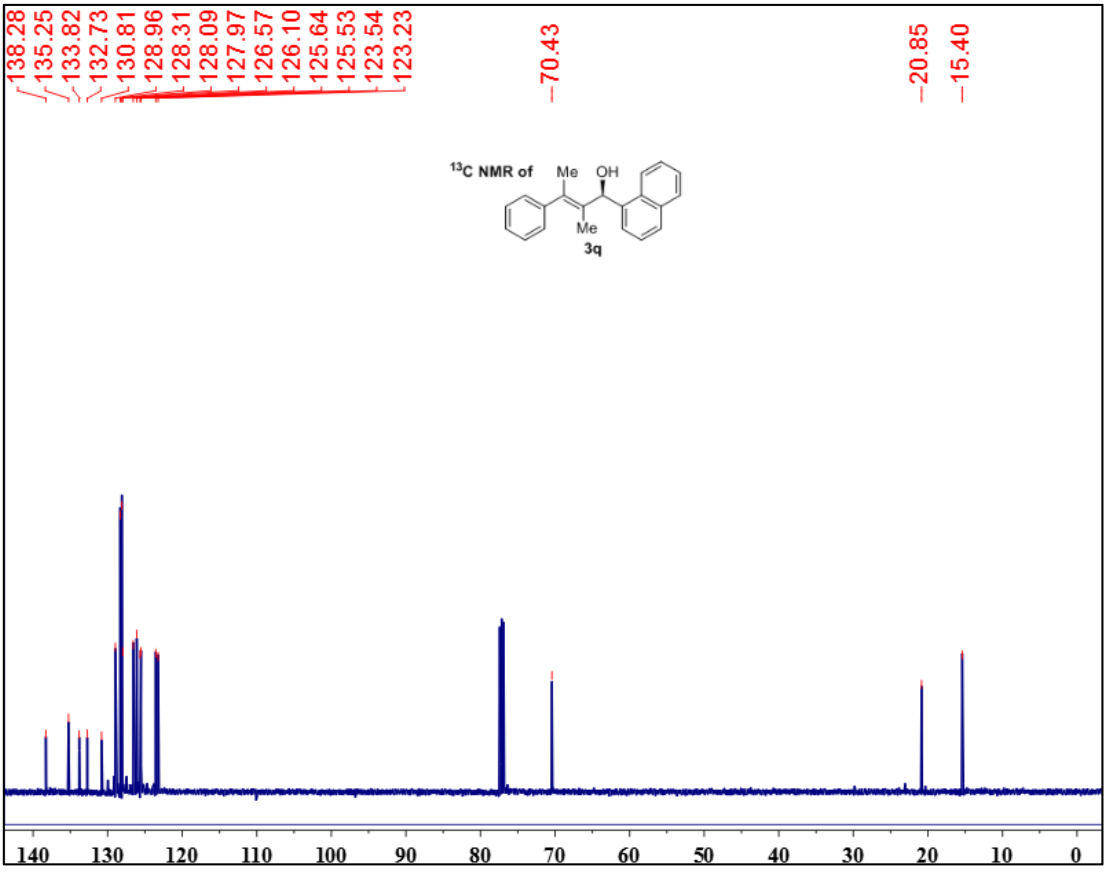

144.7723
135.0442
130.7235
129.9819
129.8778
128.7260
128.6610
128.2599
128.0781
127.7627
127.7291
126.4065
124.0333
124.0059
115.3343
115.1631
67.6138
20.7403
13.9725
13C NMR of
Me
OH
F
Me
3p
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

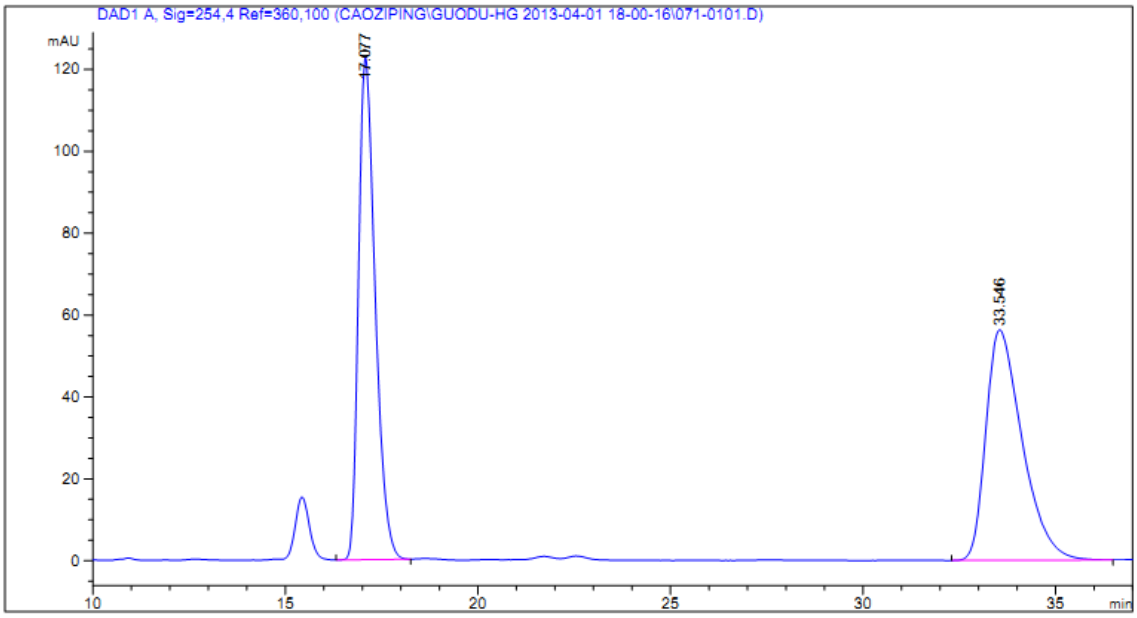


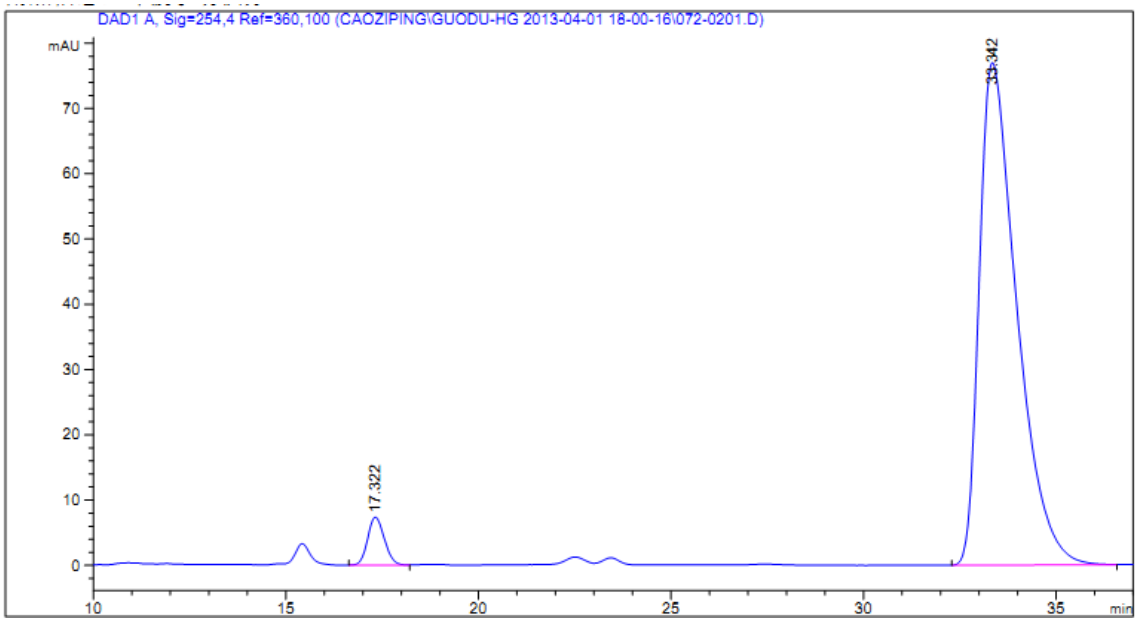


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.413	VV	0.1354	7892.38184	908.04321	91.5404
2	7.219	VB	0.1426	729.36237	79.83598	8.4596
总量：				8621.74420	987.87919	

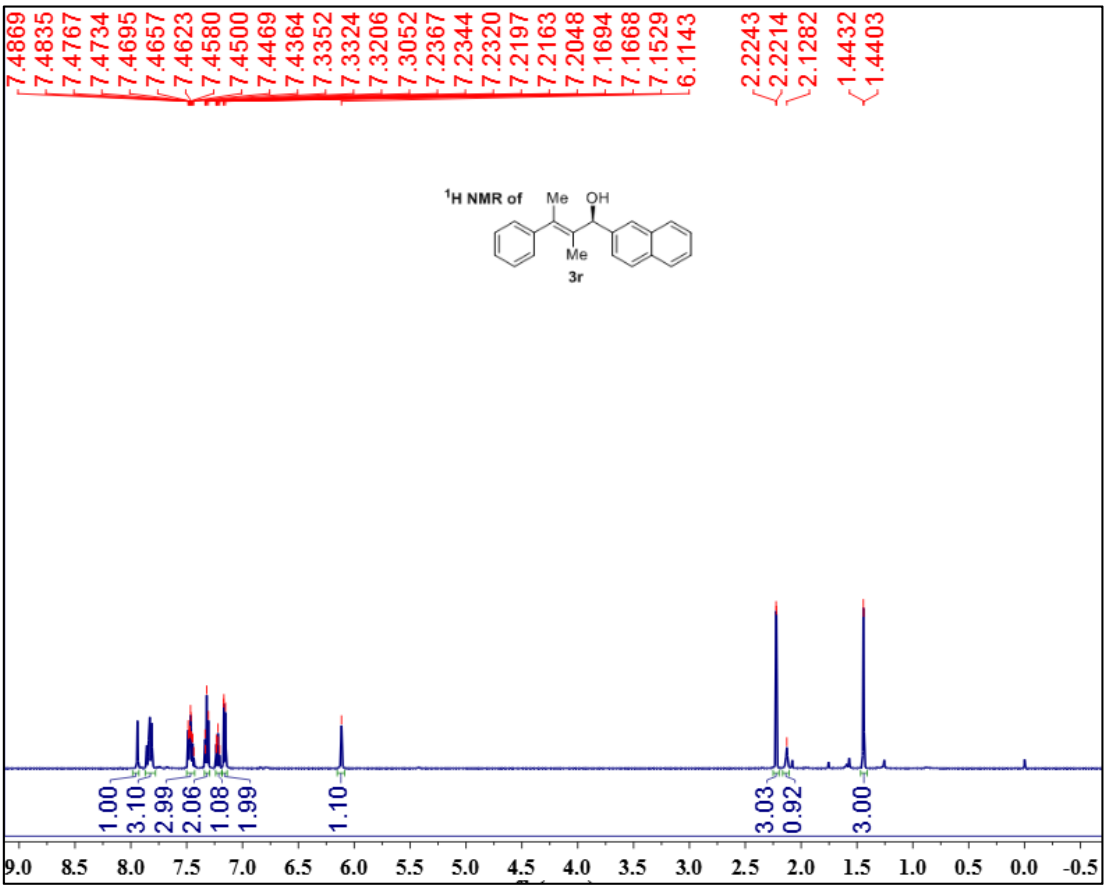

8.0232
8.0076
7.5273
7.5171
7.5122
7.5051
7.5011
7.4972
7.4896
7.4866
7.4812
7.4760
7.4730
7.3114
7.2966
7.2814
7.2229
7.2202
7.2114
7.2079
7.2040
7.1931
7.1412
7.1385
7.1248
7.1226
6.4602
2.3037
2.3008
1.3202
1.3173
1H NMR of
Me
OH
Me
3q
1.03
1.07
2.04
3.01
2.15
1.16
1.99
1.04
2.98
0.98
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

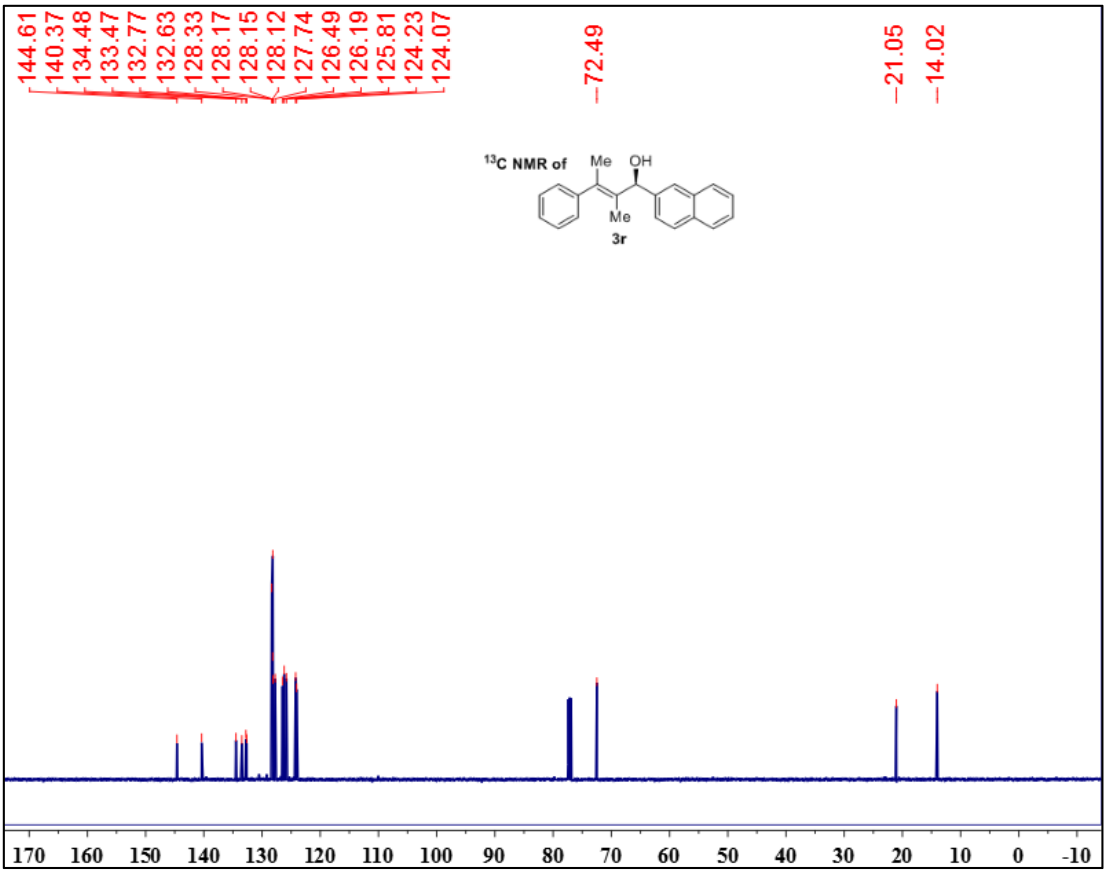

138.28
135.25
133.82
132.73
130.81
128.96
128.31
128.09
127.97
126.57
126.10
125.64
125.53
123.54
123.23
70.43
20.85
15.40
13C NMR of
Me
OH
Me
3q
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

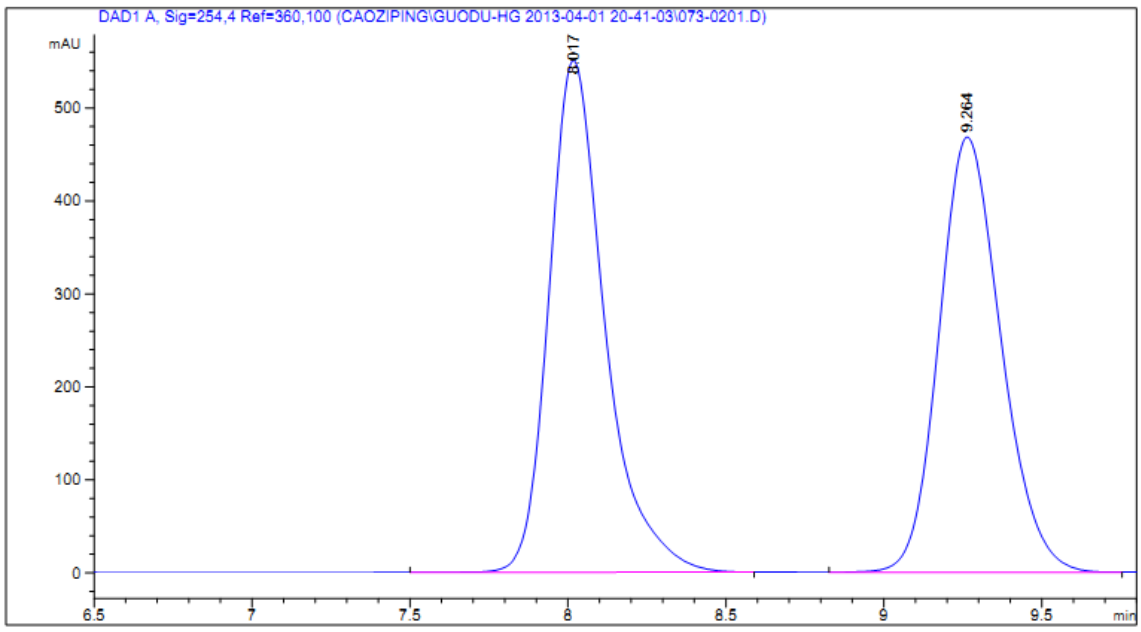


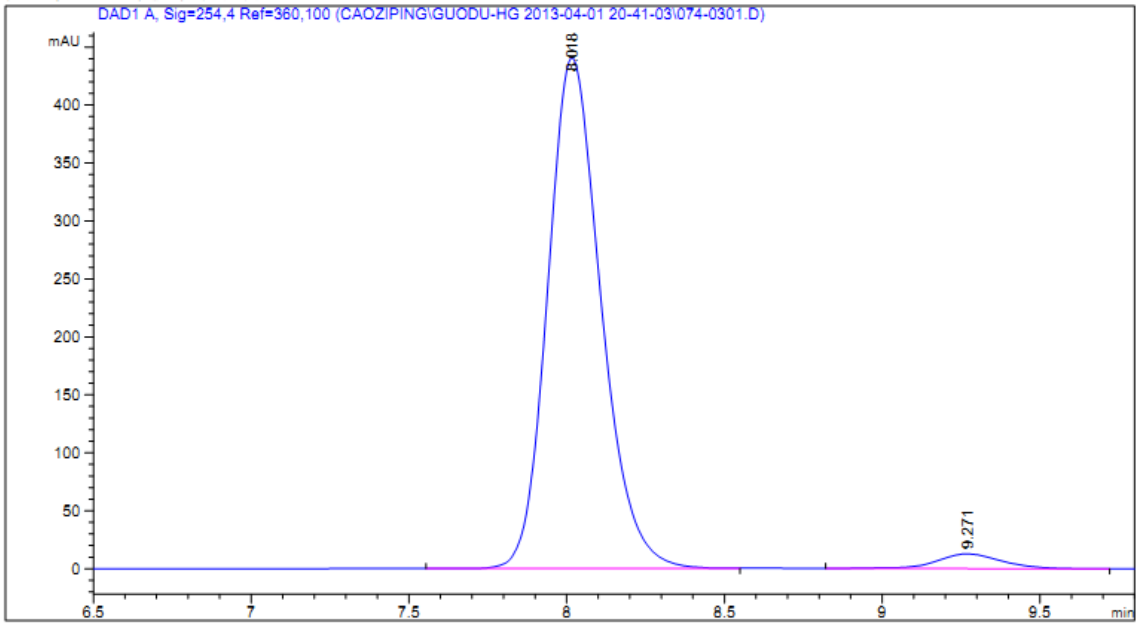


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.322	BB	0.4569	219.97202	7.35476	4.0598
2	33.342	BB	0.9995	5198.32813	77.01524	95.9402
总量：				5418.30014	84.37001	

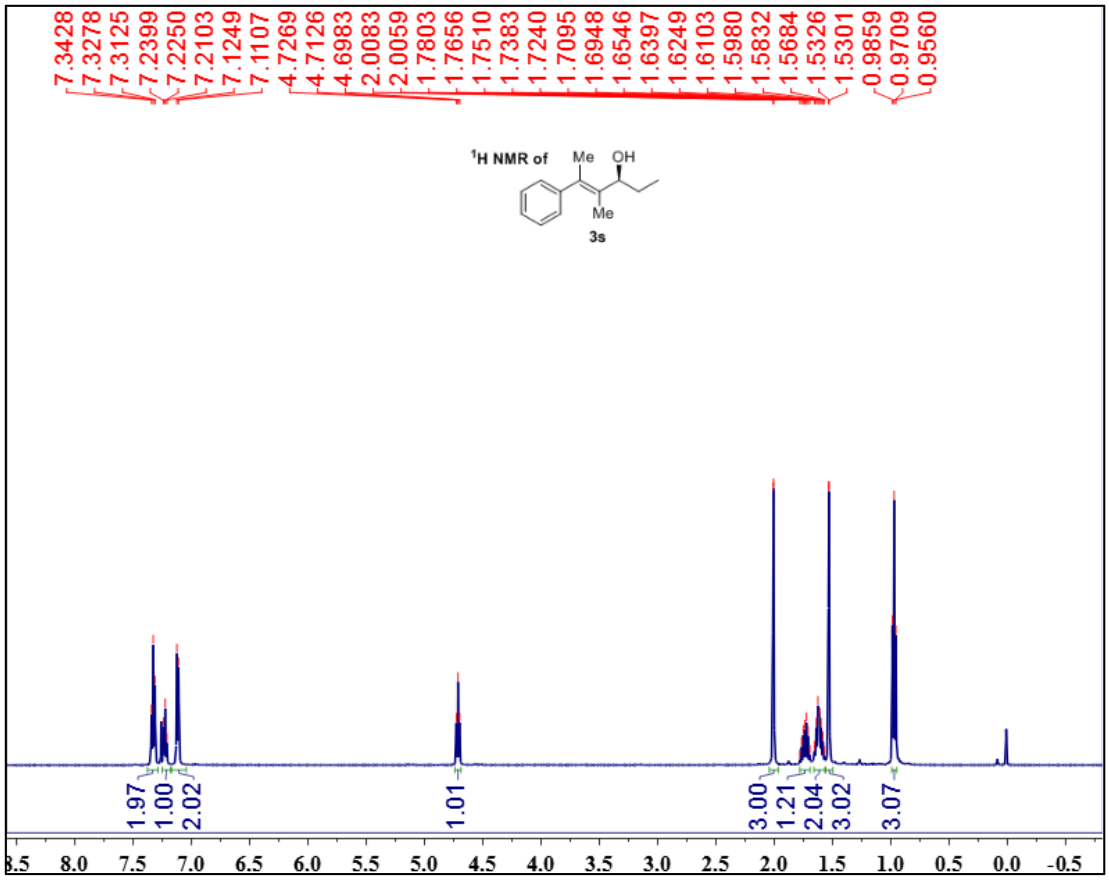

7.4869
7.4835
7.4767
7.4734
7.4695
7.4657
7.4623
7.4580
7.4500
7.4469
7.4364
7.3352
7.3324
7.3206
7.3052
7.2367
7.2344
7.2320
7.2197
7.2163
7.2048
7.1694
7.1668
7.1529
6.1143
2.2243
2.2214
2.1282
1.4432
1.4403
1H NMR of
Me
OH
Me
3r
1.00
3.10
2.99
2.06
1.08
1.99
1.10
3.03
0.92
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

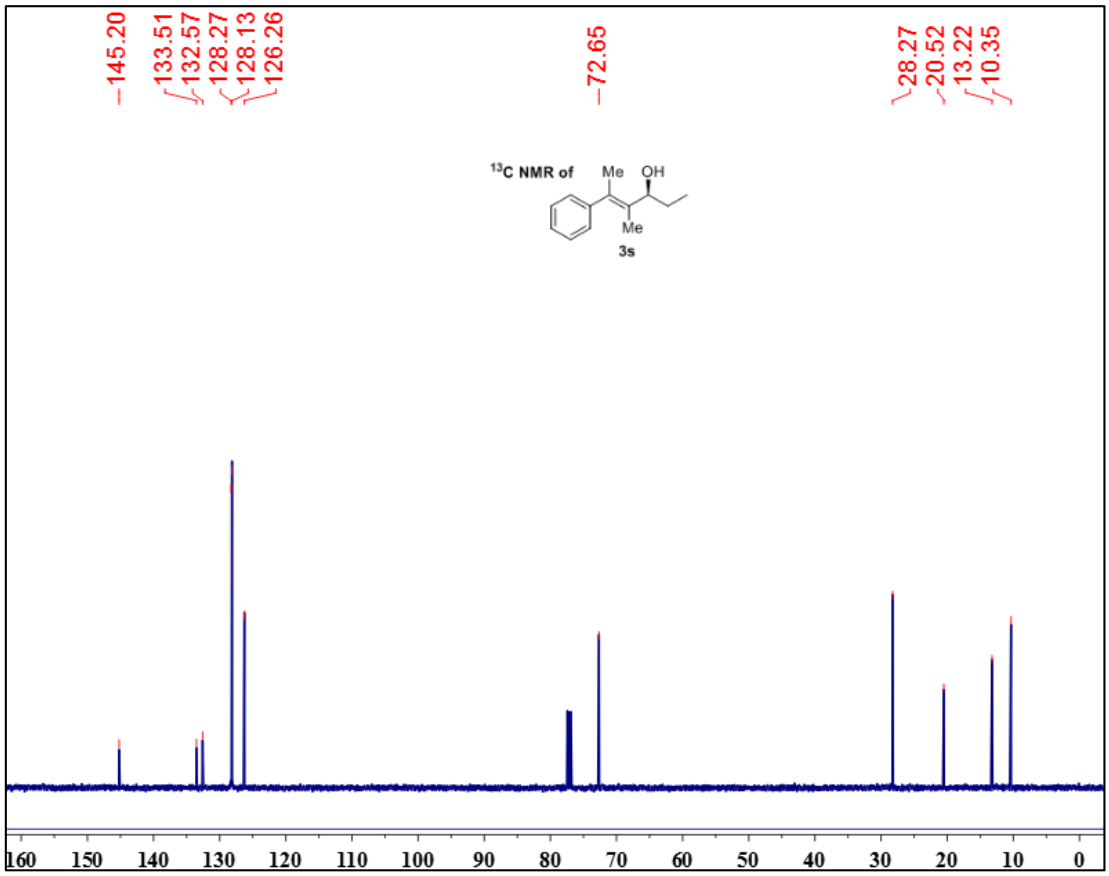

144.61
140.37
134.48
133.47
132.77
132.63
128.33
128.17
128.15
128.12
127.74
126.49
126.19
125.81
124.23
124.07
72.49
21.05
14.02
13C NMR of
Me
OH
Me
3r
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

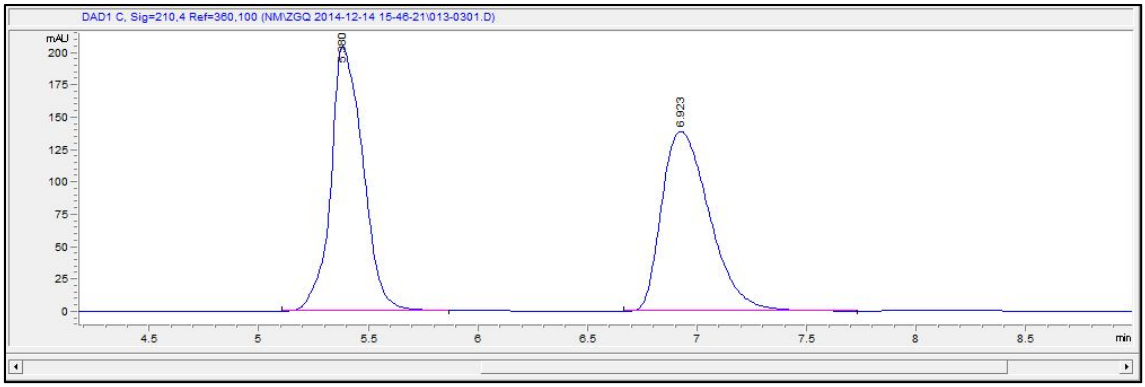


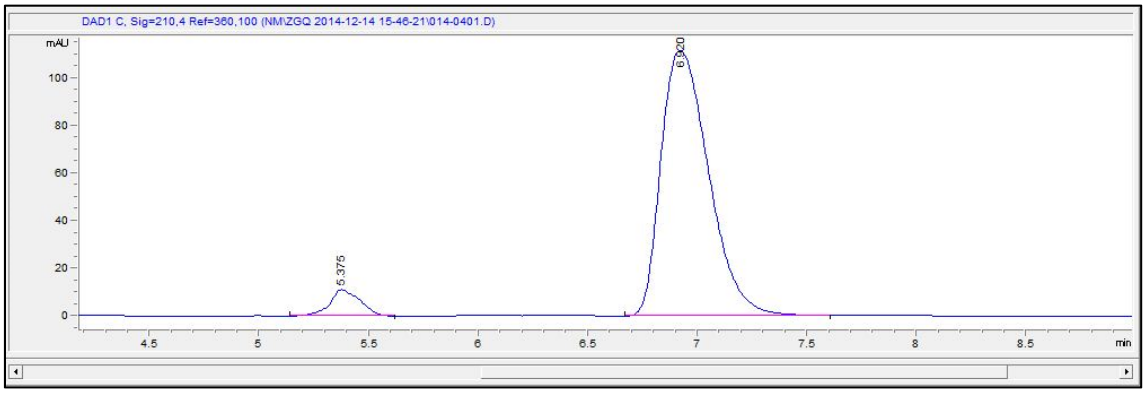


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.018	BB	0.1808	5170.54980	440.89322	96.6429
2	9.271	BB	0.2142	179.61140	12.76469	3.3571
总量：				5350.16121	453.65791	

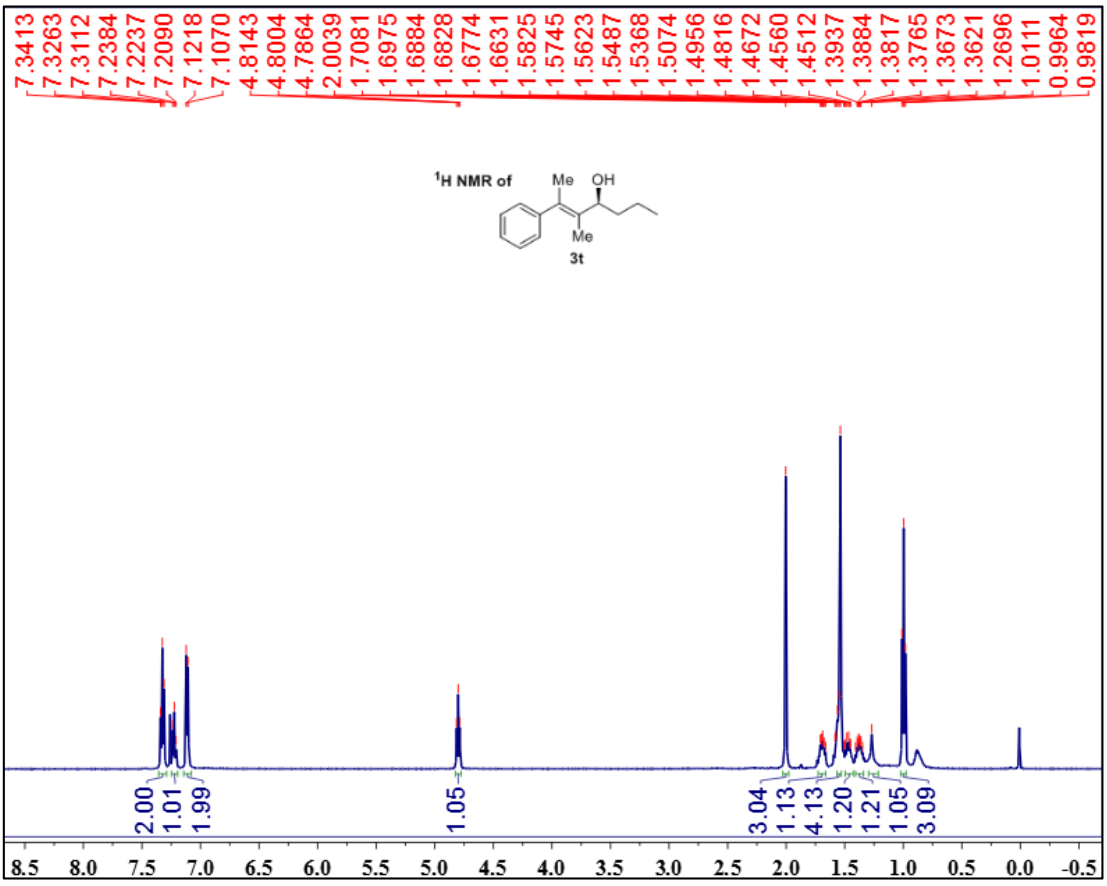

7.3428
7.3278
7.3125
7.2399
7.2250
7.2103
7.1249
7.1107
4.7269
4.7126
4.6983
2.0083
2.0059
1.7803
1.7656
1.7510
1.7383
1.7240
1.7095
1.6948
1.6546
1.6397
1.6249
1.6103
1.5980
1.5832
1.5684
1.5326
1.5301
0.9859
0.9709
0.9560
1H NMR of
Me
OH
Me
3s
1.97
1.00
2.02
1.01
3.00
1.21
2.04
3.02
3.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

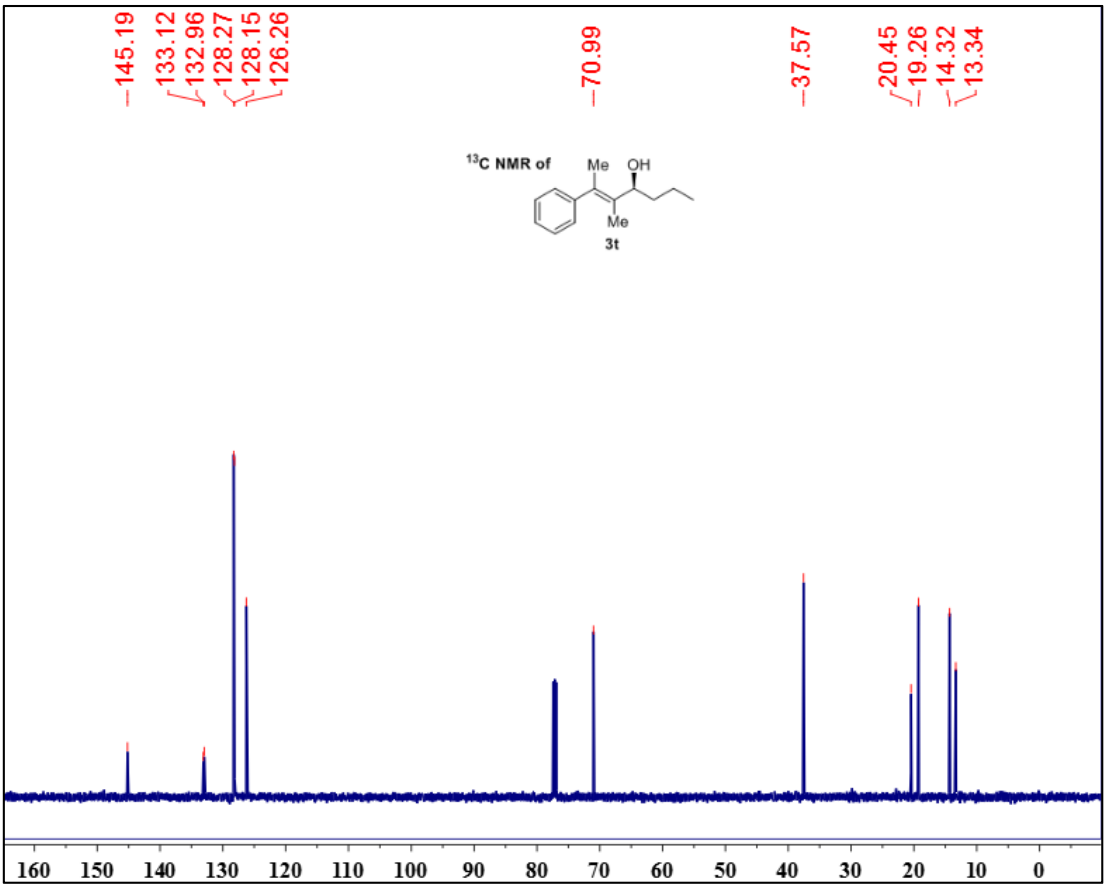

145.20
133.51
132.57
128.27
128.13
126.26
72.65
28.27
20.52
13.22
10.35
13C NMR of
Me
OH
Me
3s
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

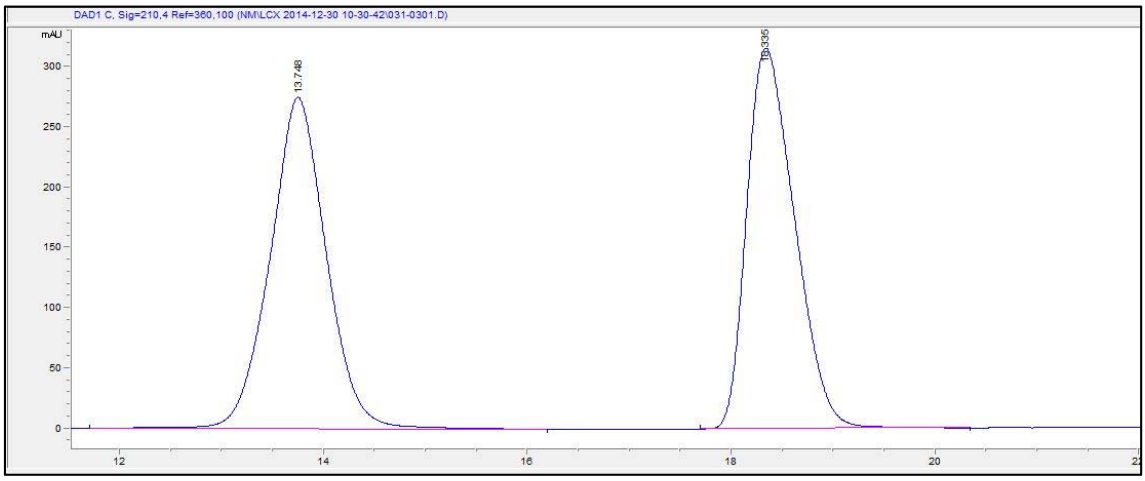


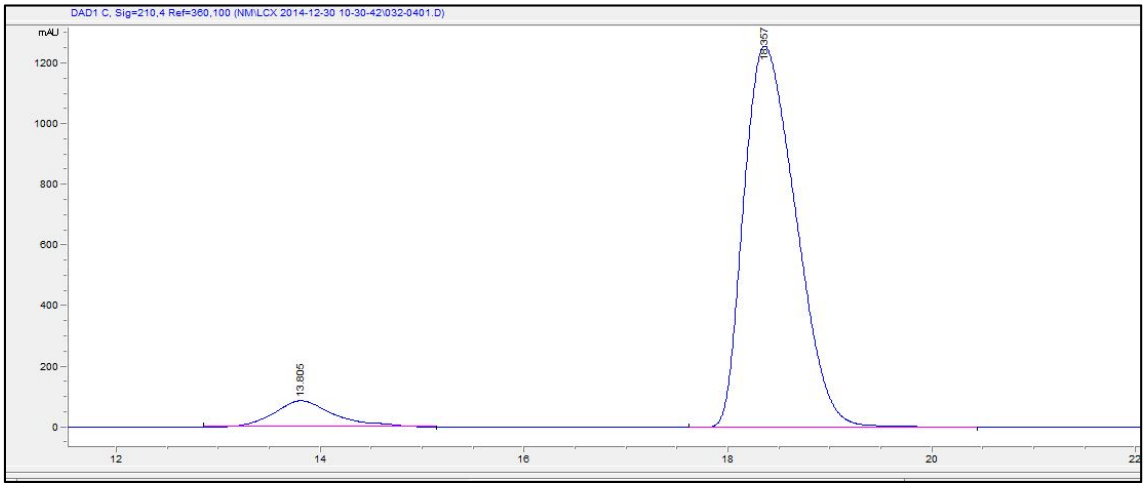


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.375	BB	0.1300	105.97630	11.03949	5.9030
2	6.920	BB	0.2385	1689.31042	111.67589	94.0970
总量：				1795.28672	122.71538	


7.3413
7.3263
7.3112
7.2384
7.2237
7.2090
7.1218
7.1070
4.8143
4.8004
4.7864
2.0039
1.7081
1.6975
1.6884
1.6828
1.6774
1.6631
1.5825
1.5745
1.5623
1.5487
1.5368
1.5074
1.4956
1.4816
1.4672
1.4560
1.4512
1.3937
1.3884
1.3817
1.3765
1.3673
1.3621
1.2696
1.0111
0.9964
0.9819
1H NMR of
Me
OH
Me
3t
2.00
1.01
1.99
1.05
3.04
1.13
4.13
1.20
1.21
1.05
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

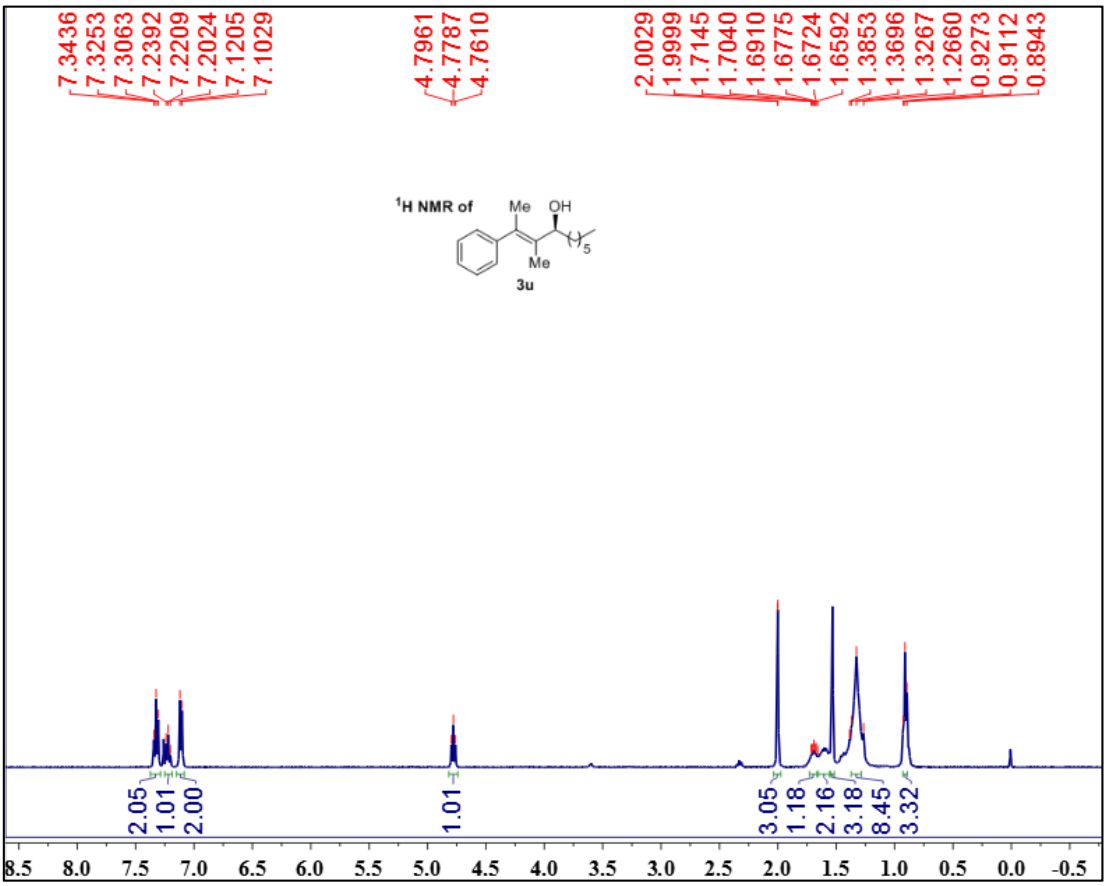

145.19
133.12
132.96
128.27
128.15
126.26
70.99
37.57
20.45
19.26
14.32
13.34
13C NMR of
Me
OH
Me
3t
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

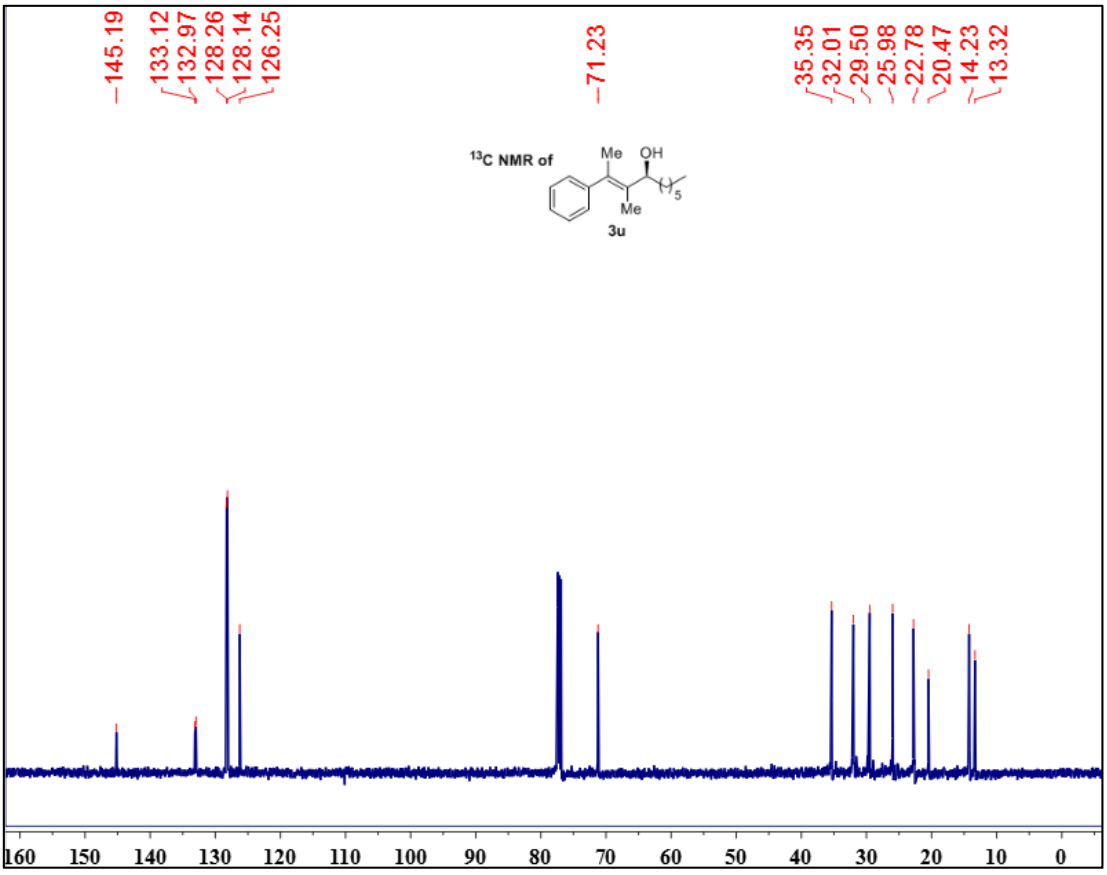


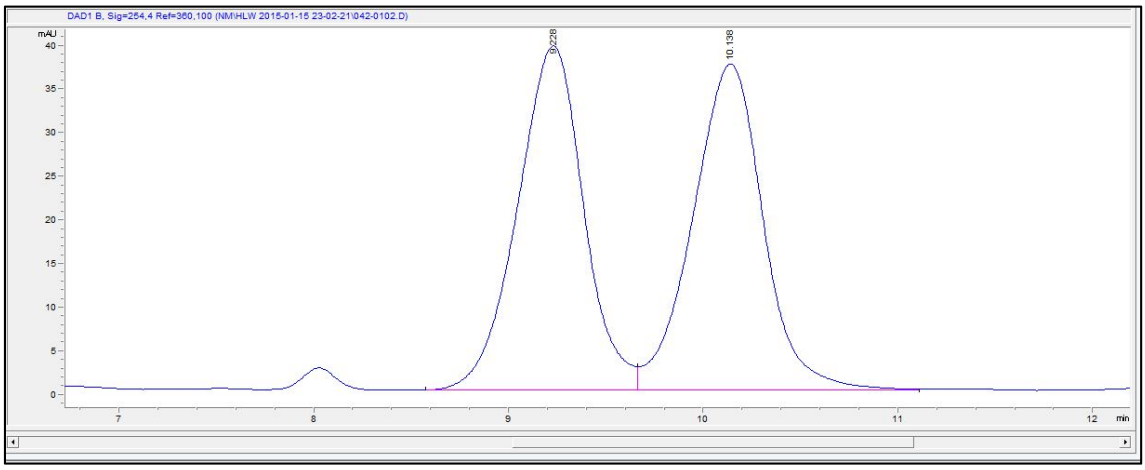


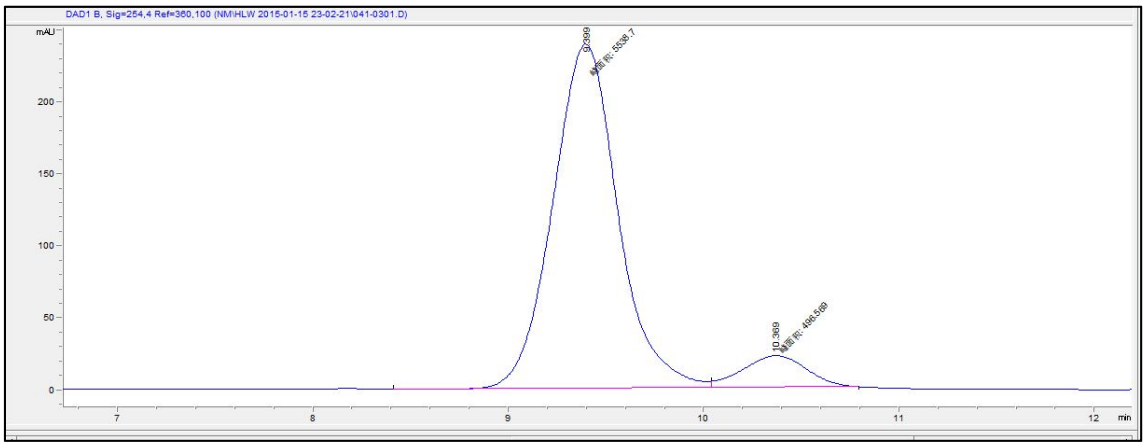
信号 1: DAD1 C, Sig=210,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.805	BB	0.6034	3615.93823	86.55200	7.5334
2	18.357	BB	0.5758	4.43828e4	1257.35510	92.4666
总量：				4.79987e4	1343.90710	

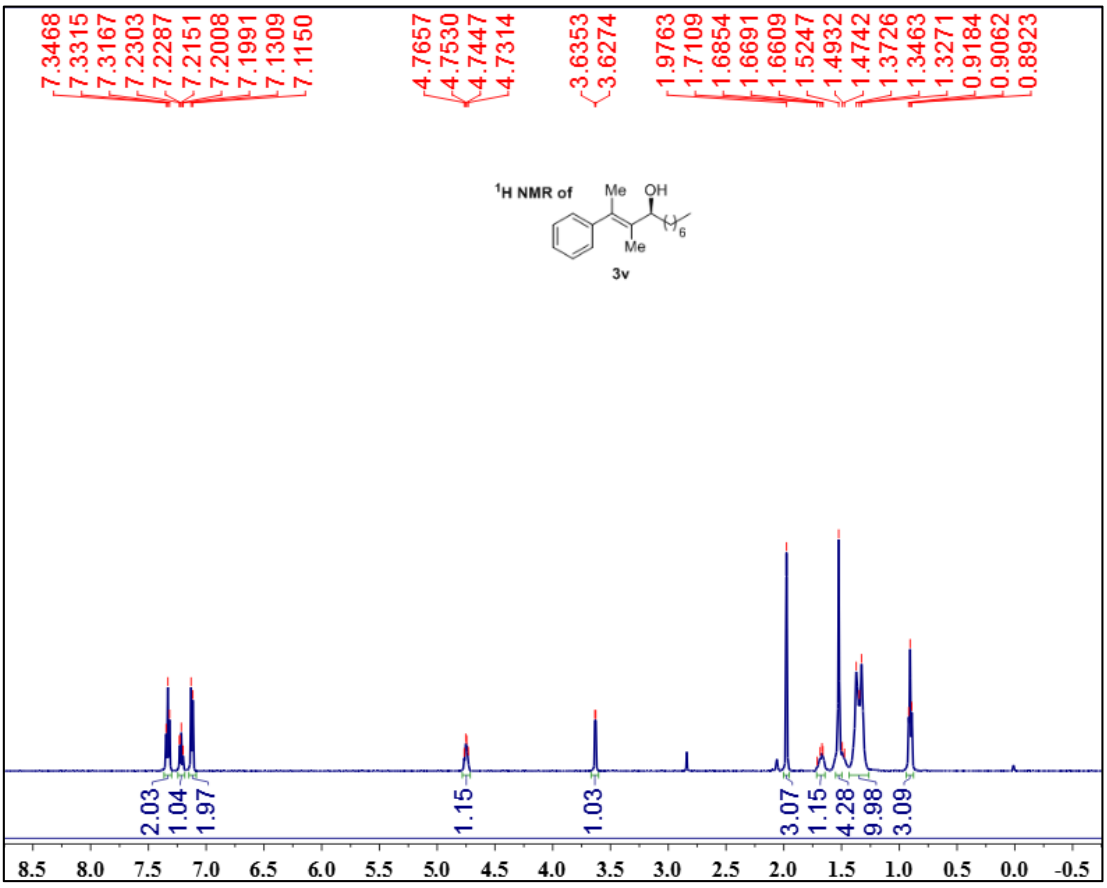

7.3436
7.3253
7.3063
7.2392
7.2209
7.2024
7.1205
7.1029
4.7961
4.7787
4.7610
2.0029
1.9999
1.7145
1.7040
1.6910
1.6775
1.6724
1.6592
1.3853
1.3696
1.3267
1.2660
0.9273
0.9112
0.8943
1H NMR of
Me
OH
Me
5
3u
2.05
1.01
2.00
1.01
3.05
1.18
2.16
3.18
8.45
3.32
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

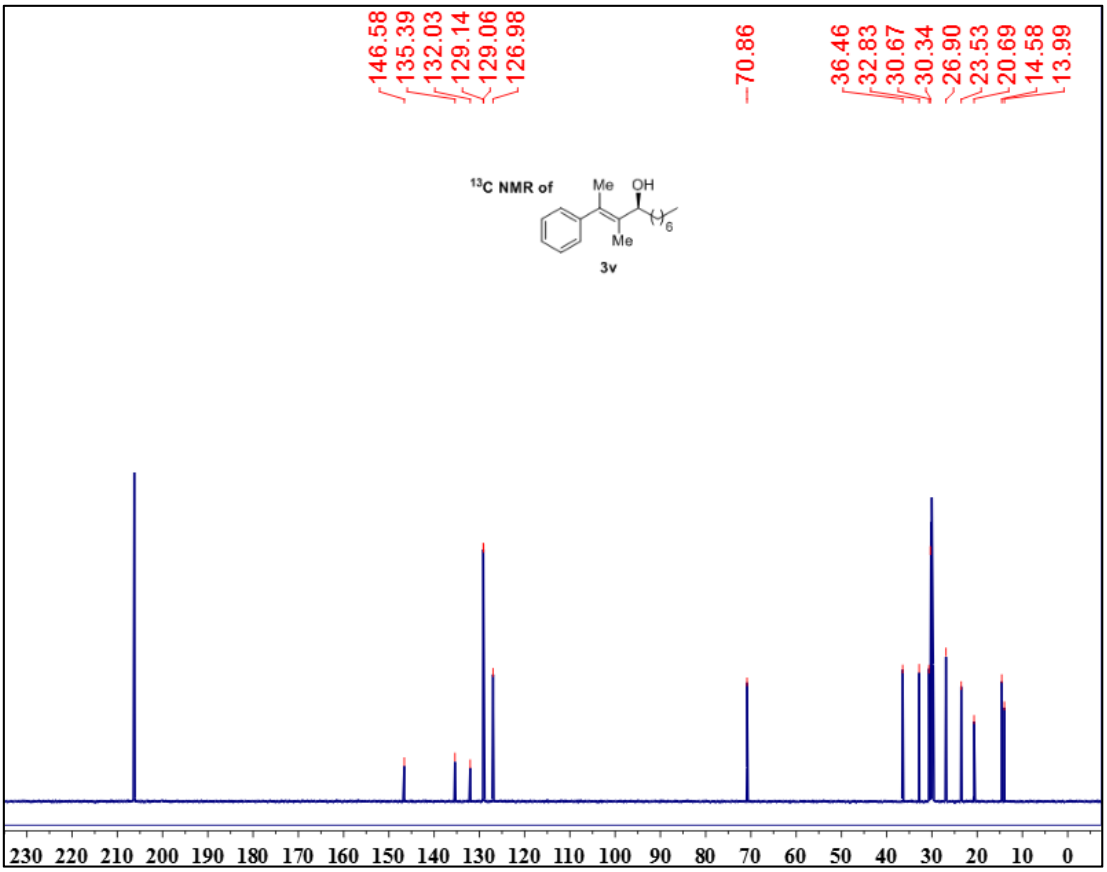

145.19
133.12
132.97
128.26
128.14
126.25
71.23
35.35
32.01
29.50
25.98
22.78
20.47
14.23
13.32
13C NMR of
Me
OH
Me
5
3u
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

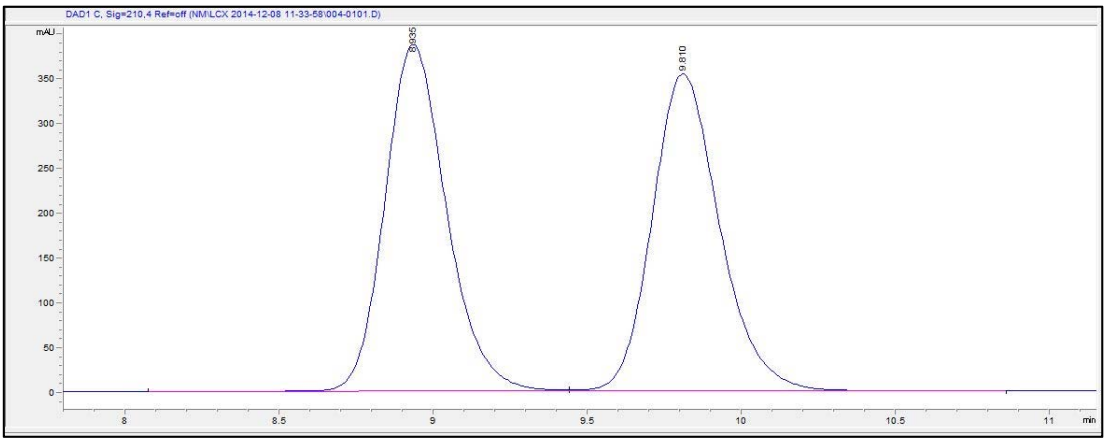


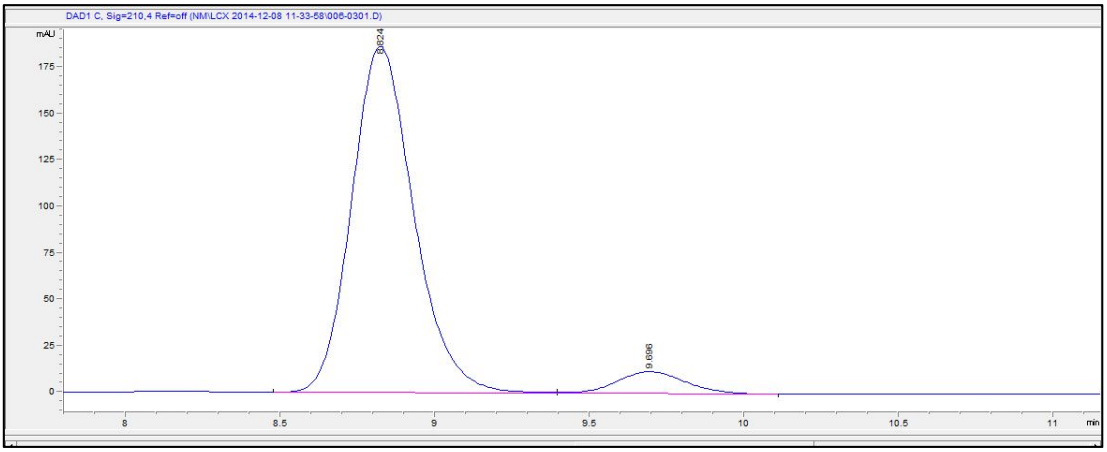


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.399	MF T	0.6029	5538.69922	238.84984	91.7722
2	10.369	FM T	0.3778	496.56891	21.90356	8.2278
总量：				6035.26813	260.75340	

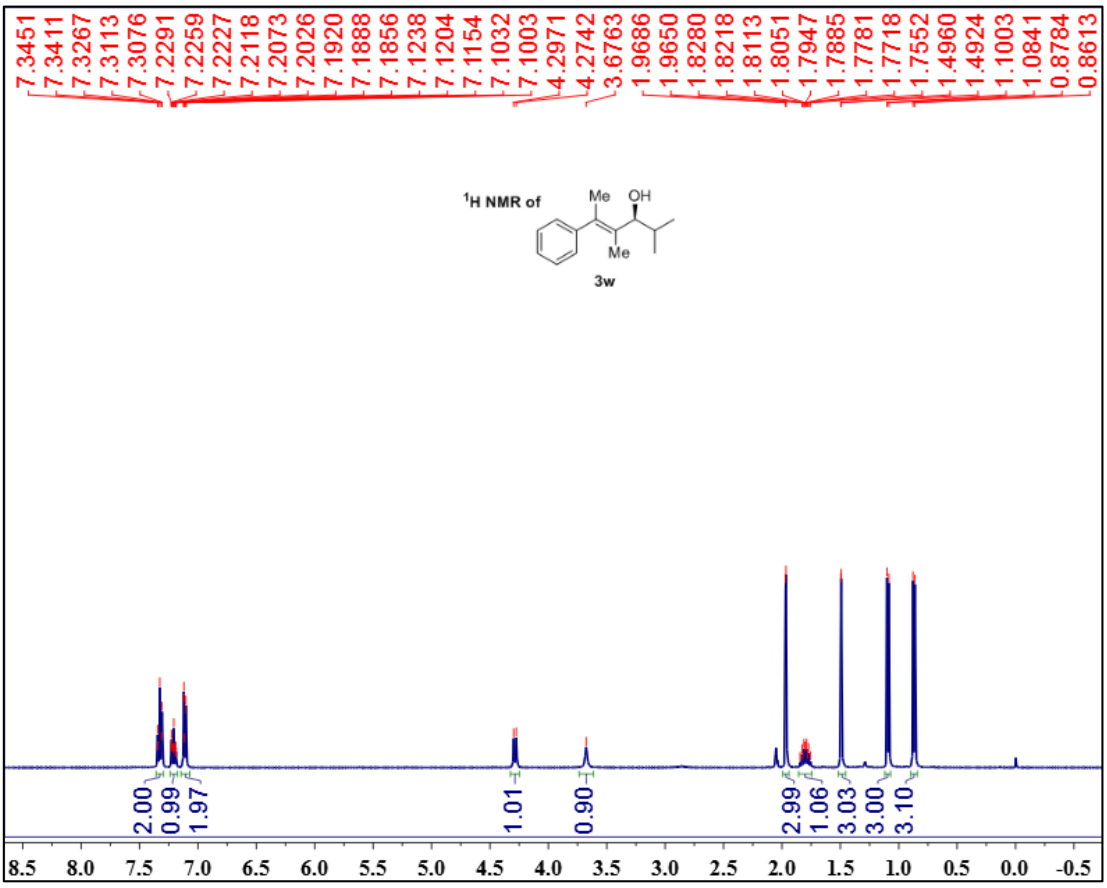

7.3468
7.3315
7.3167
7.2303
7.2287
7.2151
7.2008
7.1991
7.1309
7.1150
4.7657
4.7530
4.7447
4.7314
3.6353
3.6274
1.9763
1.7109
1.6854
1.6691
1.6609
1.5247
1.4932
1.4742
1.3726
1.3463
1.3271
0.9184
0.9062
0.8923
1H NMR of
Me
OH
Me
6
3v
2.03
1.04
1.97
1.15
1.03
3.07
1.15
4.28
9.98
3.09
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

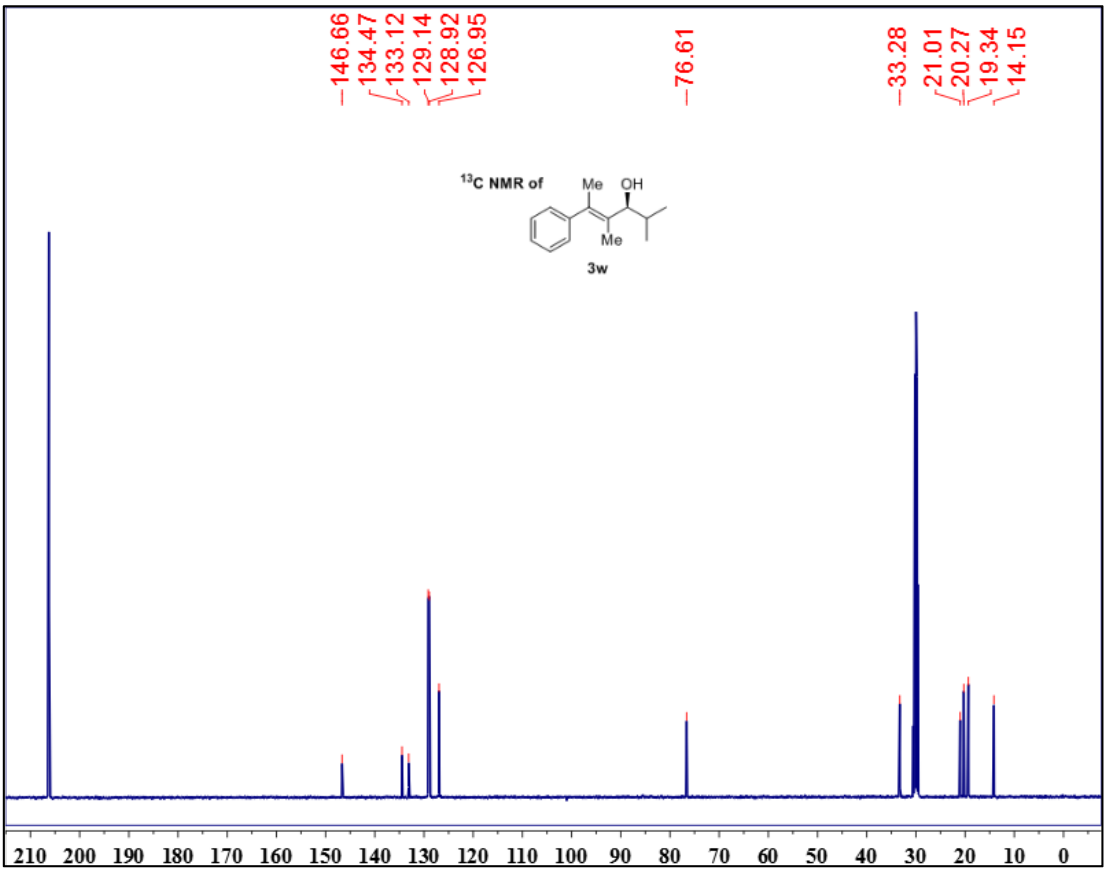

146.58
135.39
132.03
129.14
129.06
126.98
70.86
36.46
32.83
30.67
30.34
26.90
23.53
20.69
14.58
13.99
13C NMR of
Me
OH
Me
6
3v
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

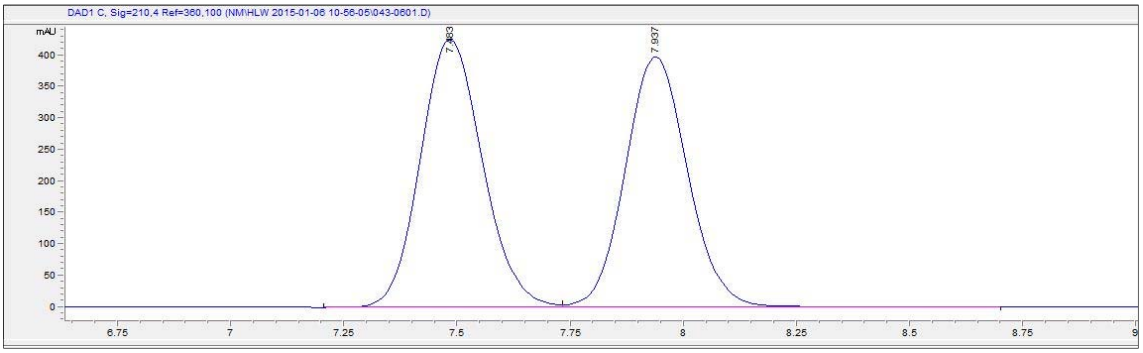


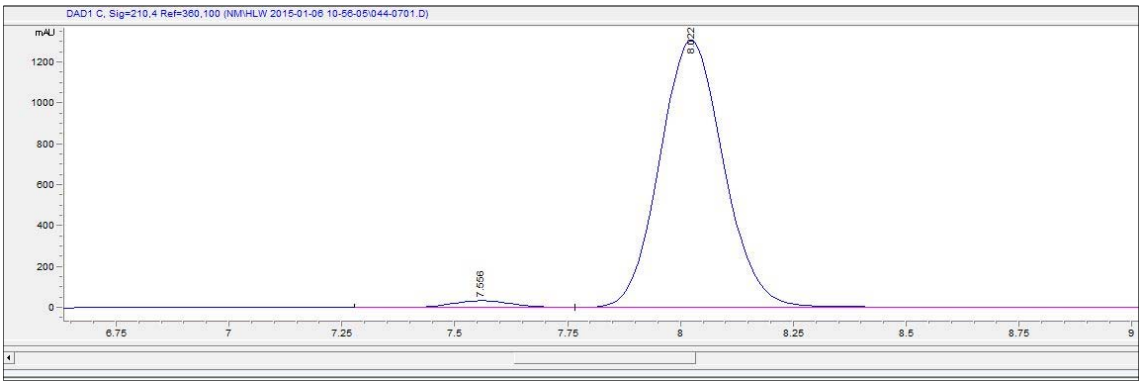


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.824	BV	0.2151	2607.63745	186.52142	93.4595
2	9.696	VB	0.2358	182.48689	11.83908	6.5405
总量：				2790.12434	198.36050	

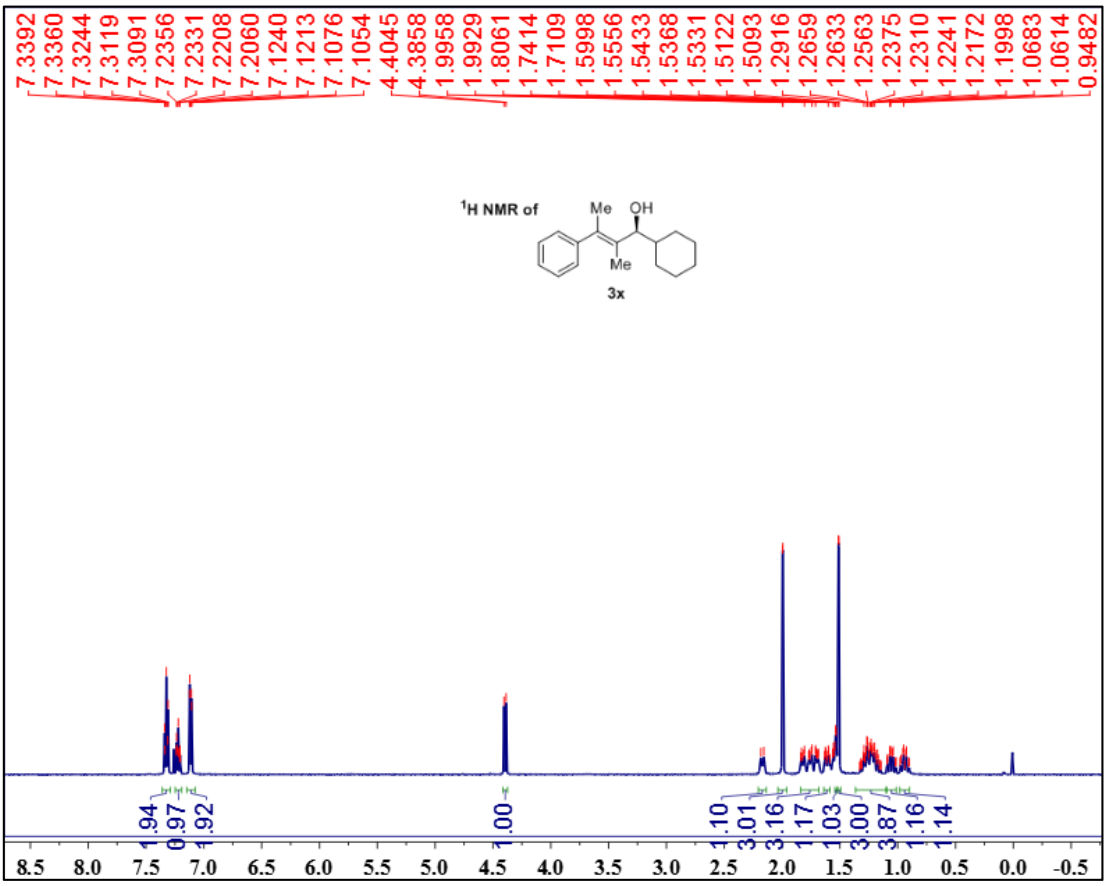

7.3451
7.3411
7.3267
7.3113
7.3076
7.2291
7.2259
7.2227
7.2118
7.2073
7.2026
7.1920
7.1888
7.1856
7.1238
7.1204
7.1154
7.1032
7.1003
4.2971
4.2742
3.6763
1.9686
1.9650
1.8280
1.8218
1.8113
1.8051
1.7947
1.7885
1.7781
1.7718
1.7552
1.4960
1.4924
1.1003
1.0841
0.8784
0.8613
1H NMR of
Me
OH
Me
3w
2.00
0.99
1.97
1.01
0.90
2.99
1.06
3.03
3.00
3.10
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

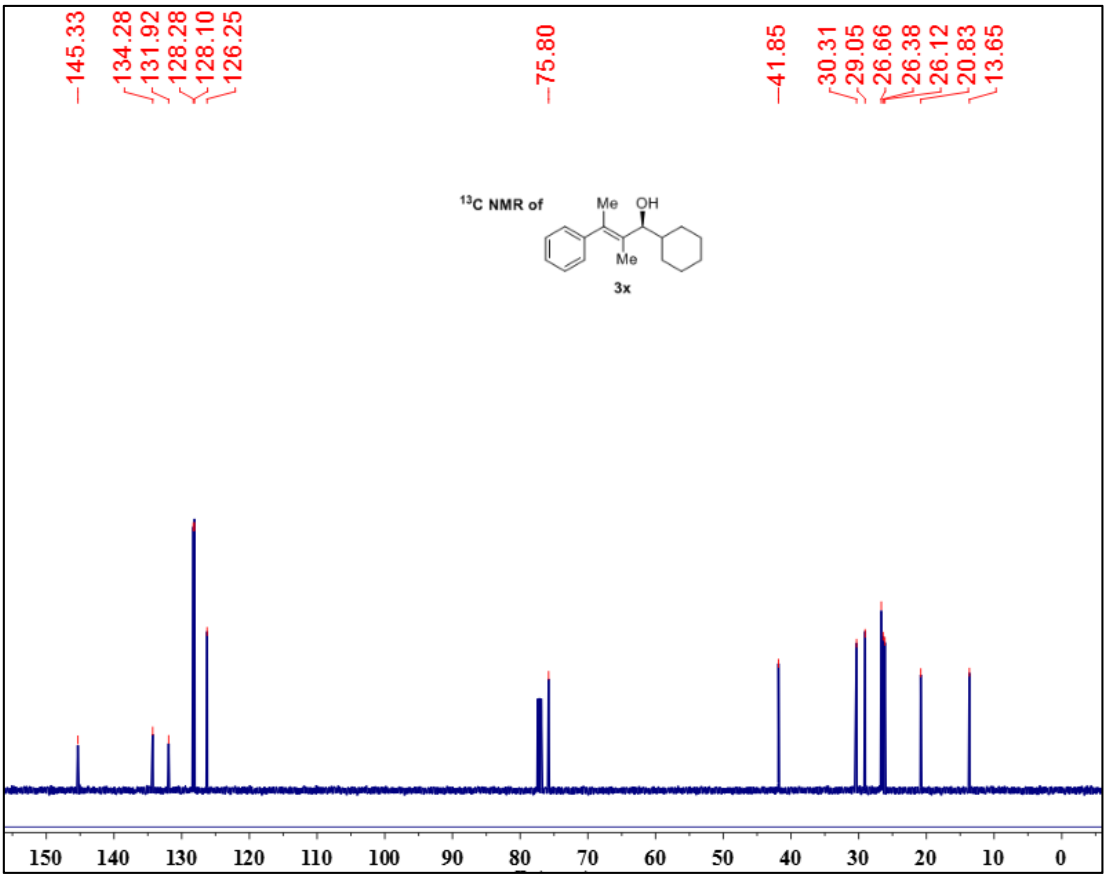

146.66
134.47
133.12
129.14
128.92
126.95
76.61
33.28
21.01
20.27
19.34
14.15
13C NMR of
Me
OH
Me
3w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

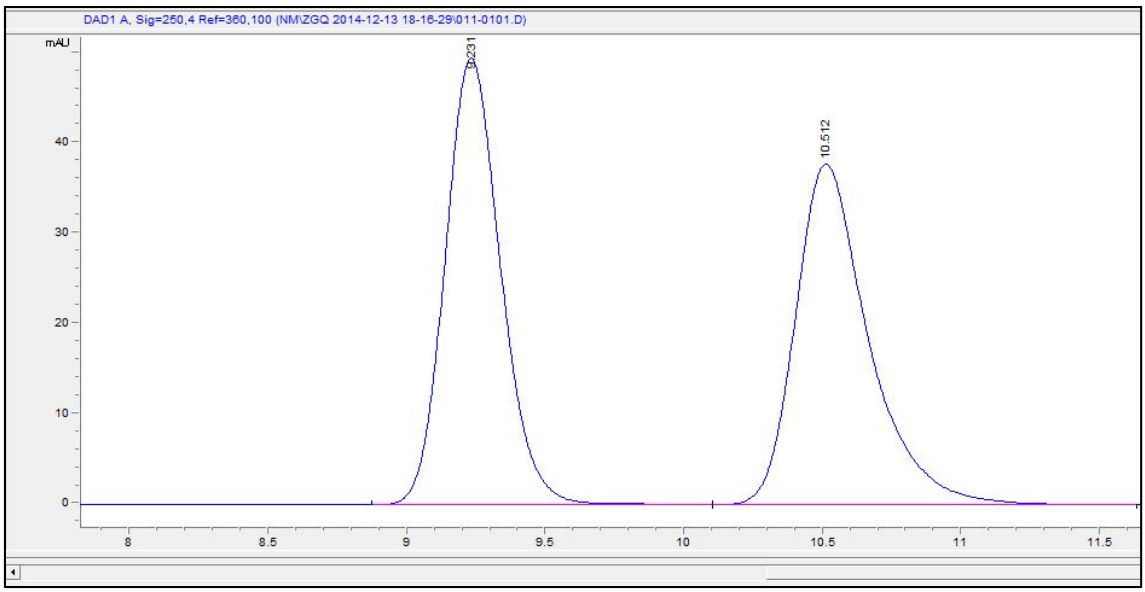


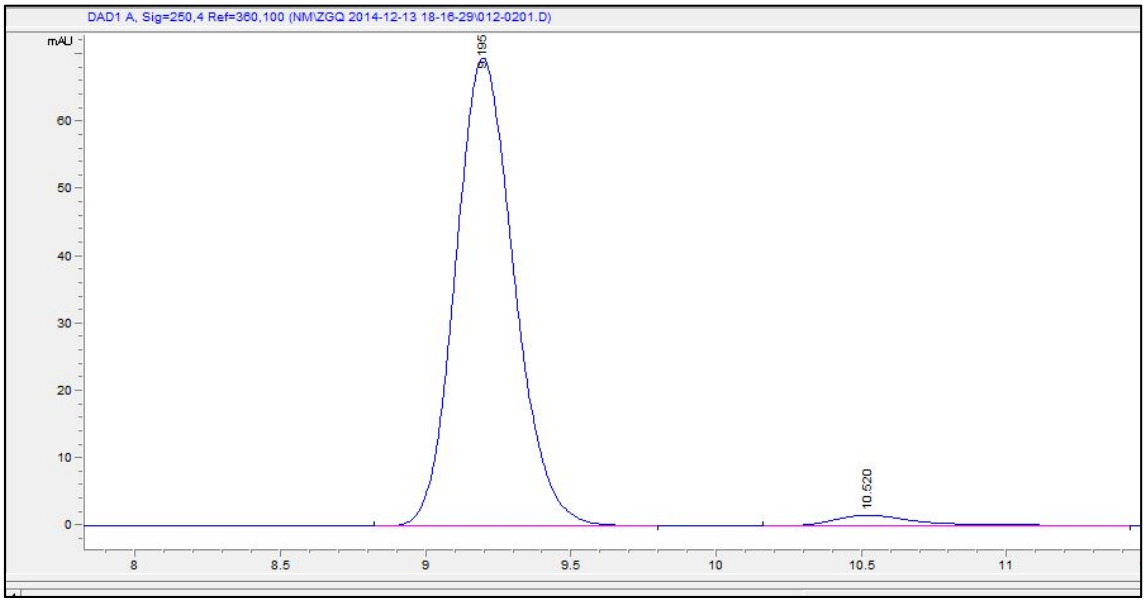


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.556	BV	0.1466	320.47900	33.80932	2.4241
2	8.022	VB	0.1531	1.29002e4	1308.11169	97.5759
总量：				1.32207e4	1341.92101	

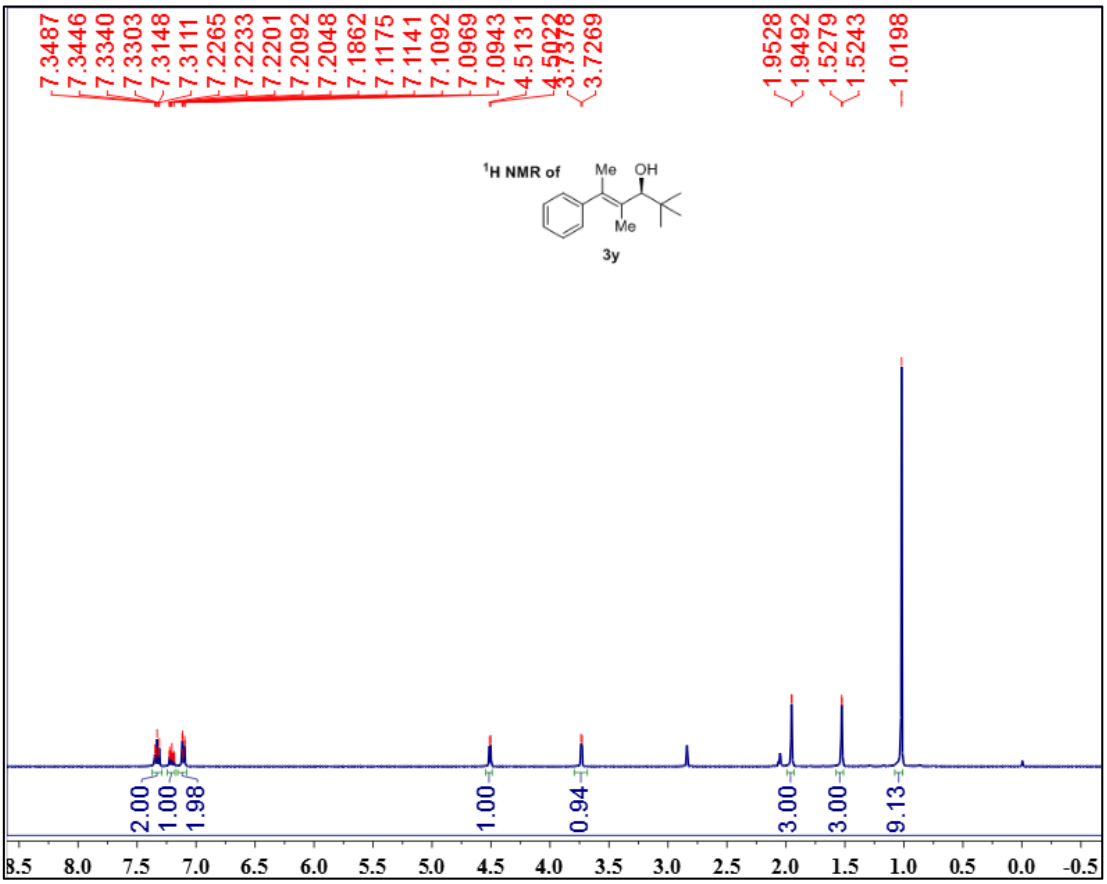

7.3392
7.3360
7.3244
7.3119
7.3091
7.2356
7.2331
7.2208
7.2060
7.1240
7.1213
7.1076
7.1054
4.4045
4.3858
1.9958
1.9929
1.8061
1.7414
1.7109
1.5998
1.5556
1.5433
1.5368
1.5331
1.5122
1.5093
1.2916
1.2659
1.2633
1.2563
1.2375
1.2310
1.2241
1.2172
1.1998
1.0683
1.0614
0.9482
1H NMR of
Me
OH
Me
3x
1.94
0.97
1.92
1.00
1.10
3.01
3.16
1.17
1.03
3.00
3.87
1.16
1.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

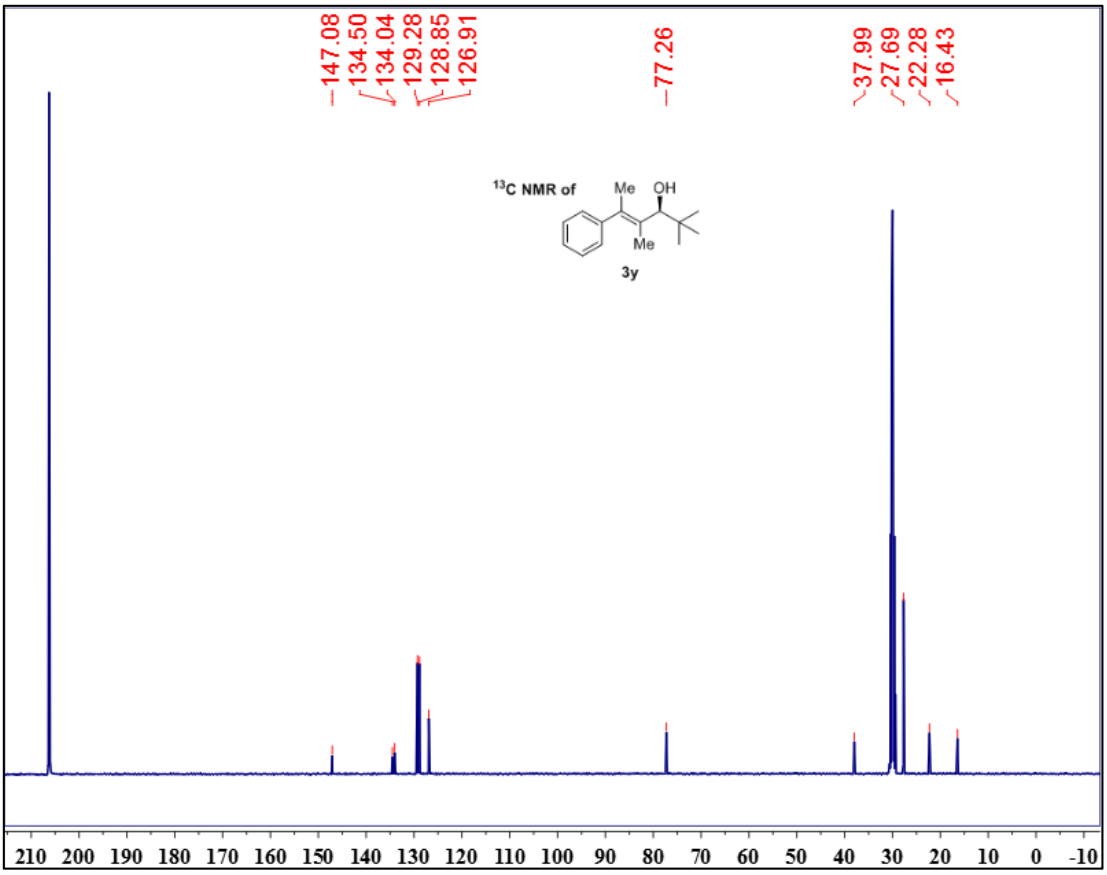

145.33
134.28
131.92
128.28
128.10
126.25
75.80
41.85
30.31
29.05
26.66
26.38
26.12
20.83
13.65
13C NMR of
Me
OH
Me
3x
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

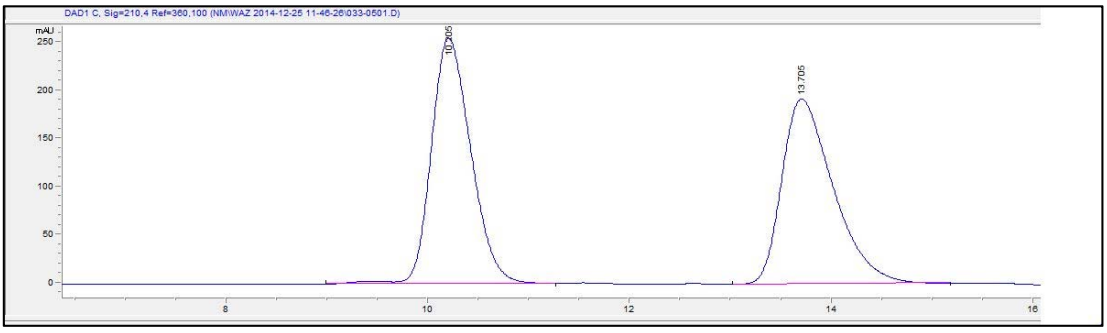


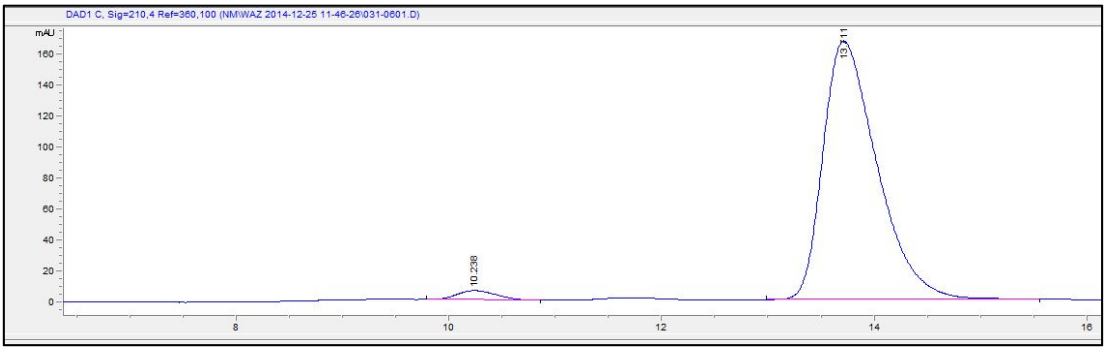


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.195	BB	0.2175	974.11078	69.50636	96.5739
2	10.520	BB	0.3039	34.55757	1.62614	3.4261
总量：				1008.66835	71.13250	


7.3487
7.3446
7.3340
7.3303
7.3148
7.3111
7.2265
7.2233
7.2201
7.2092
7.2048
7.1862
7.1175
7.1141
7.1092
7.0969
7.0943
4.5131
3.7269
1.9528
1.9492
1.5279
1.5243
1.0198
1H NMR of
Me
OH
Me
3y
2.00
1.00
1.98
1.00
0.94
3.00
3.00
9.13
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

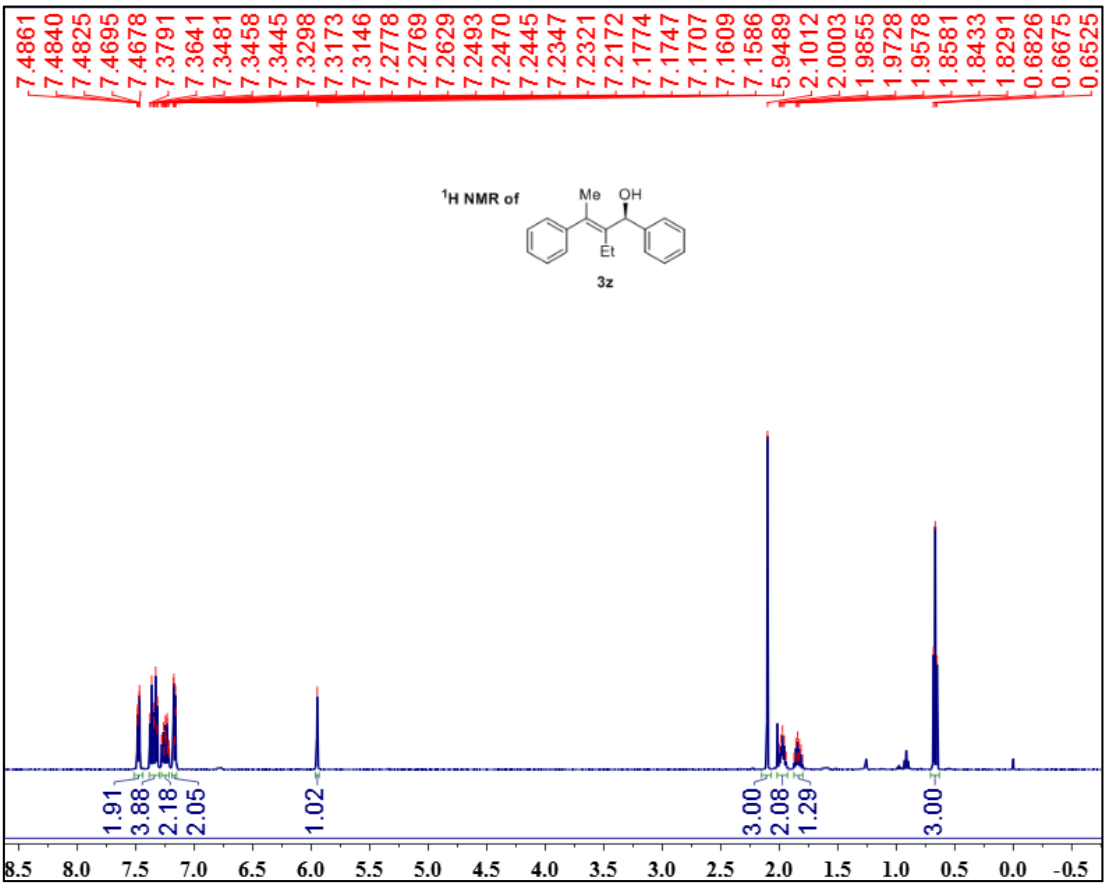

147.08
134.50
134.04
129.28
128.85
126.91
77.26
37.99
27.69
22.28
16.43
13C NMR of
Me
OH
Me
3y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

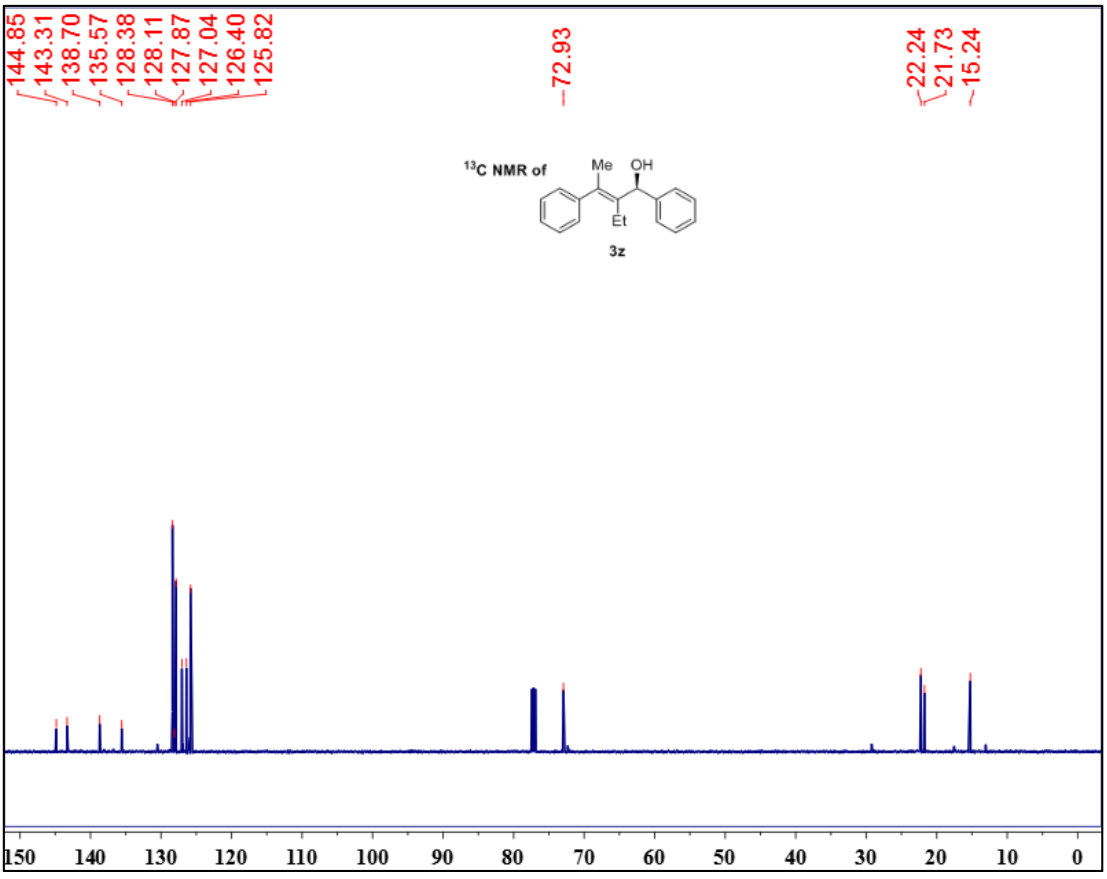


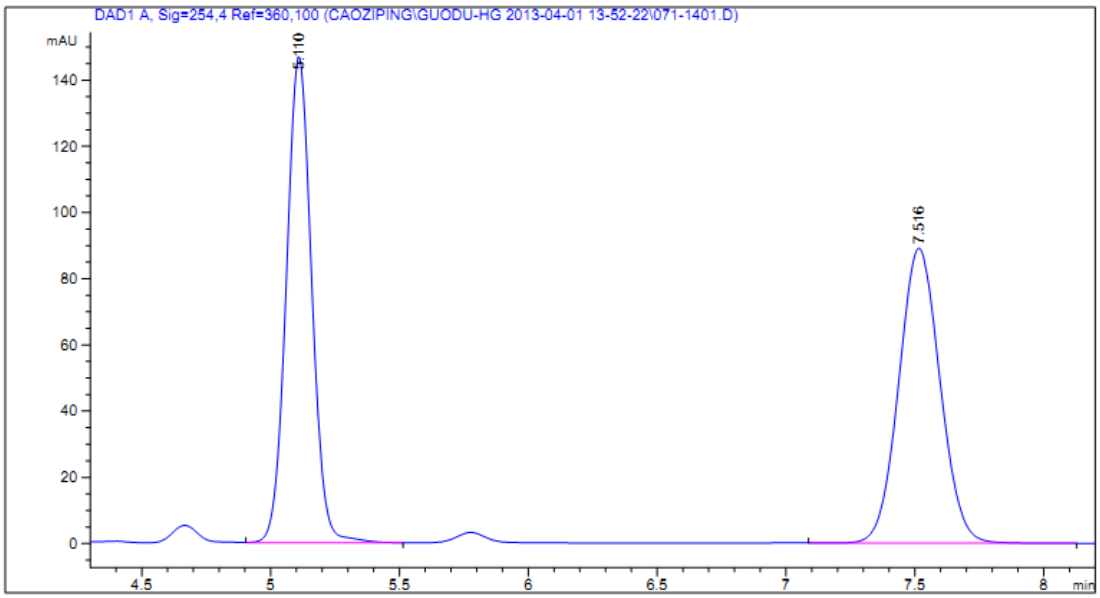


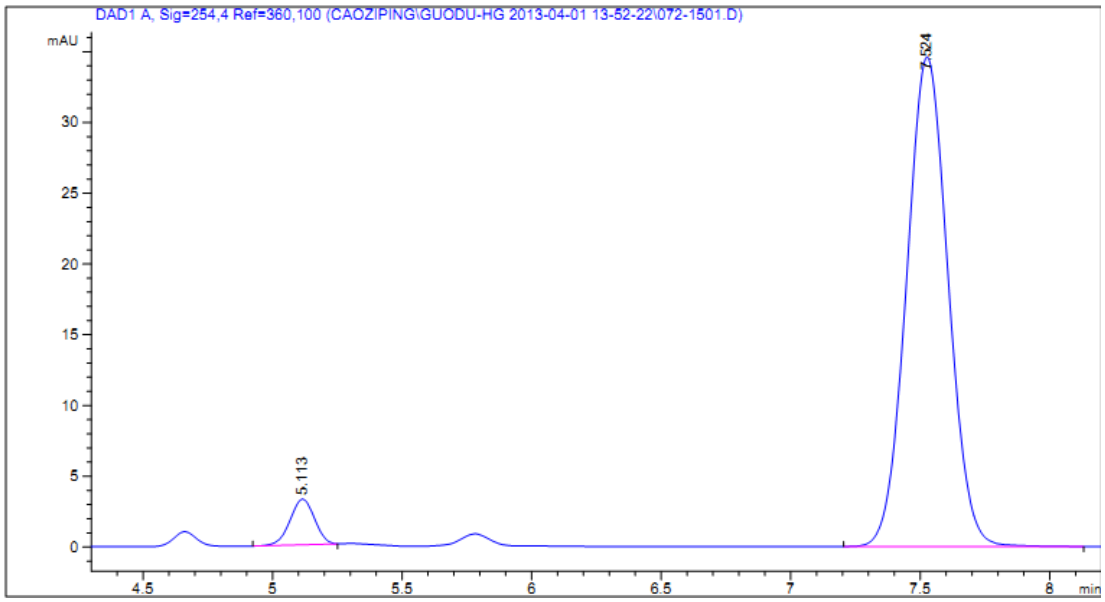
信号 1: DAD1 C, Sig=210,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.238	BB	0.3926	152.03572	5.94006	2.5122
2	13.711	BB	0.5361	5899.83252	167.01645	97.4878
总量：				6051.86824	172.95651	

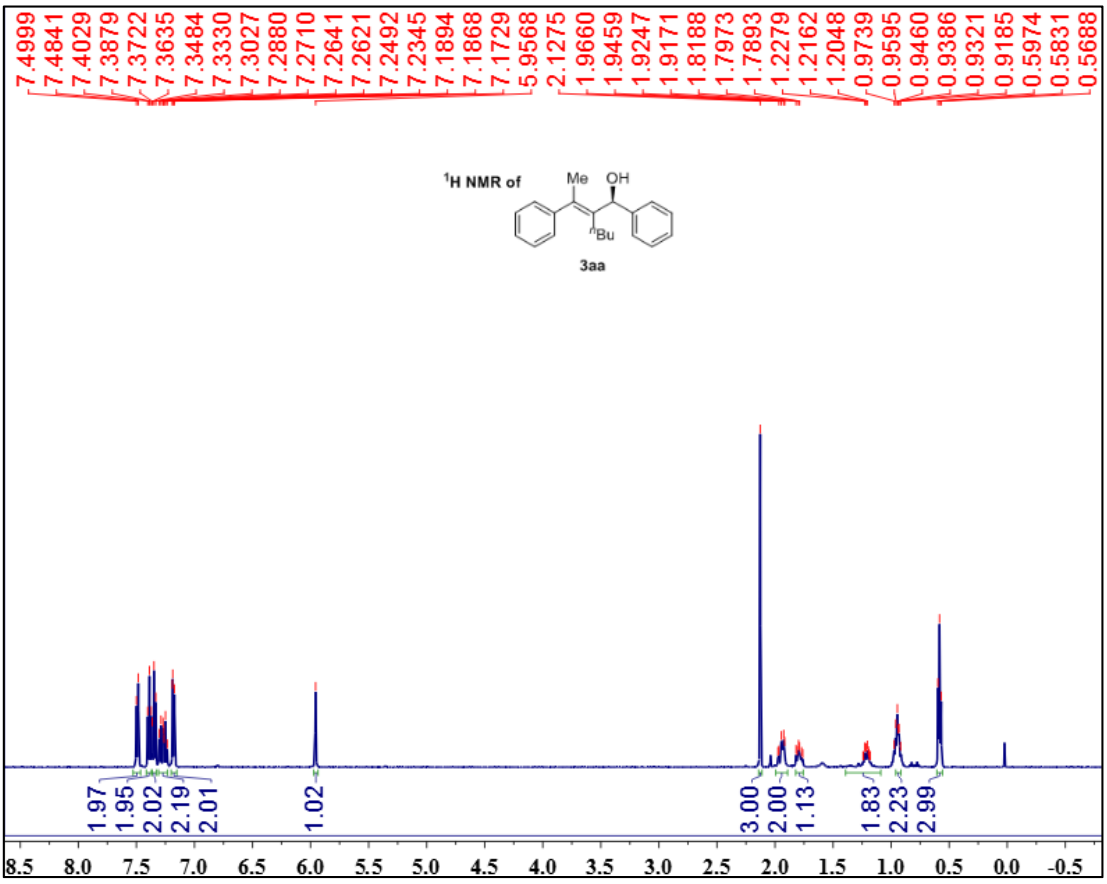

7.4861
7.4840
7.4825
7.4695
7.4678
7.3791
7.3641
7.3481
7.3458
7.3445
7.3298
7.3173
7.3146
7.2778
7.2769
7.2629
7.2493
7.2470
7.2445
7.2347
7.2321
7.2172
7.1774
7.1747
7.1707
7.1609
7.1586
5.9489
2.1012
2.0003
1.9855
1.9728
1.9578
1.8581
1.8433
1.8291
0.6826
0.6675
0.6525
1H NMR of
Me
OH
Et
3z
1.91
3.88
2.18
2.05
1.02
3.00
2.08
1.29
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

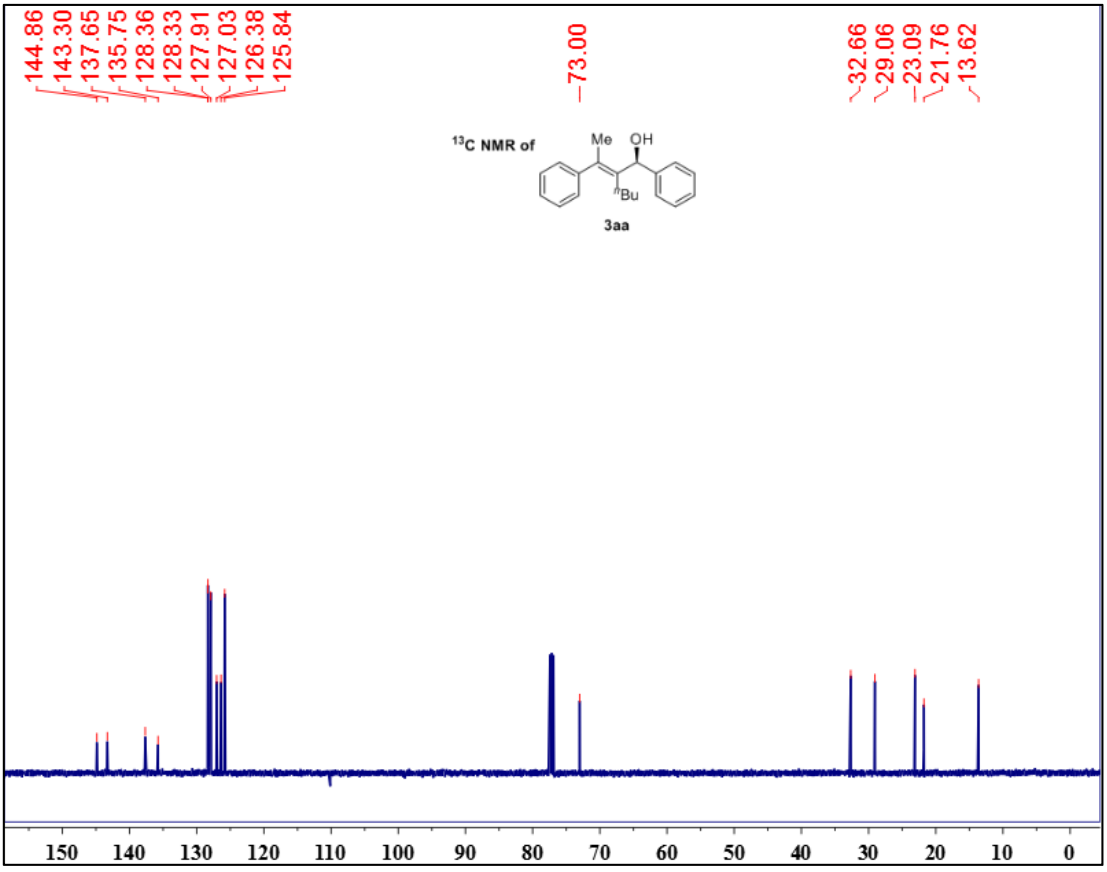

144.85
143.31
138.70
135.57
128.38
128.11
127.87
127.04
126.40
125.82
72.93
22.24
21.73
15.24
13C NMR of
Me
OH
Et
3z
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

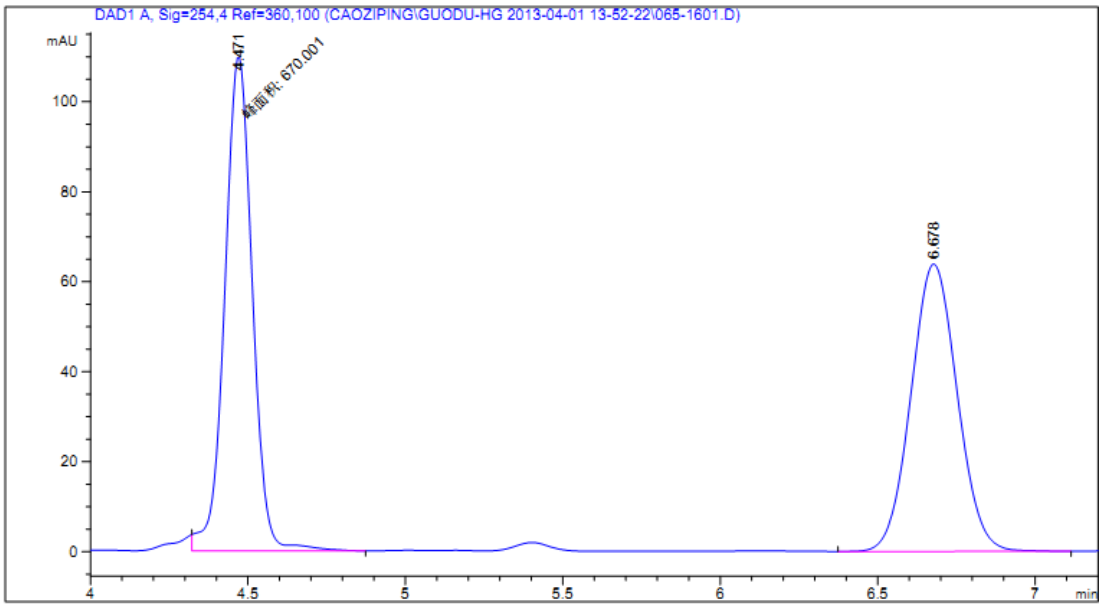


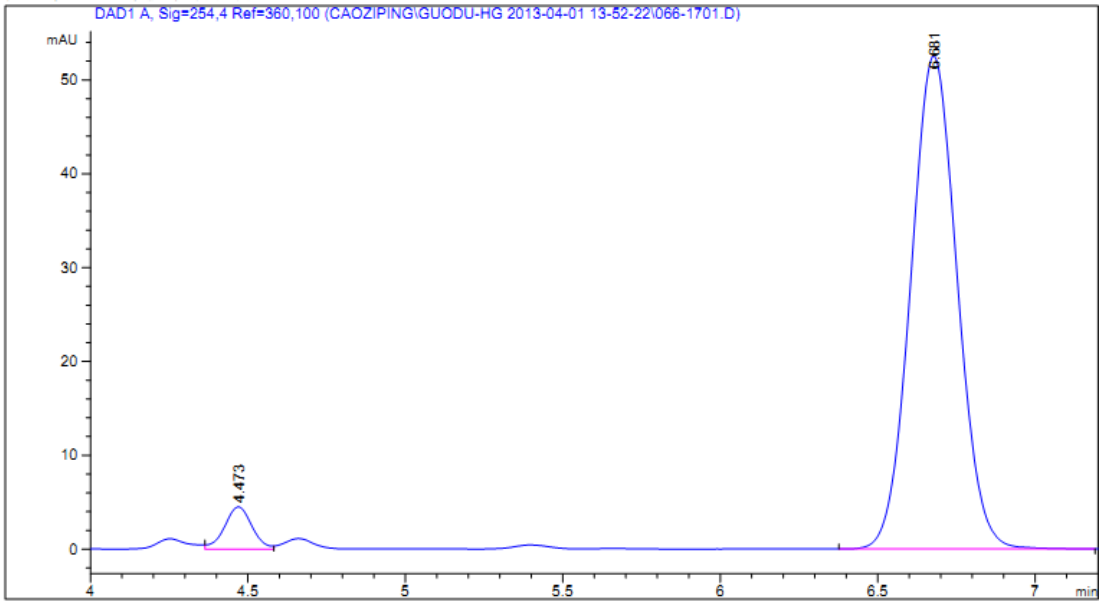


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.113	BB	0.1046	21.19274	3.22771	5.2152
2	7.524	BB	0.1718	385.16882	34.61226	94.7848
总量：				406.36156	37.83996	

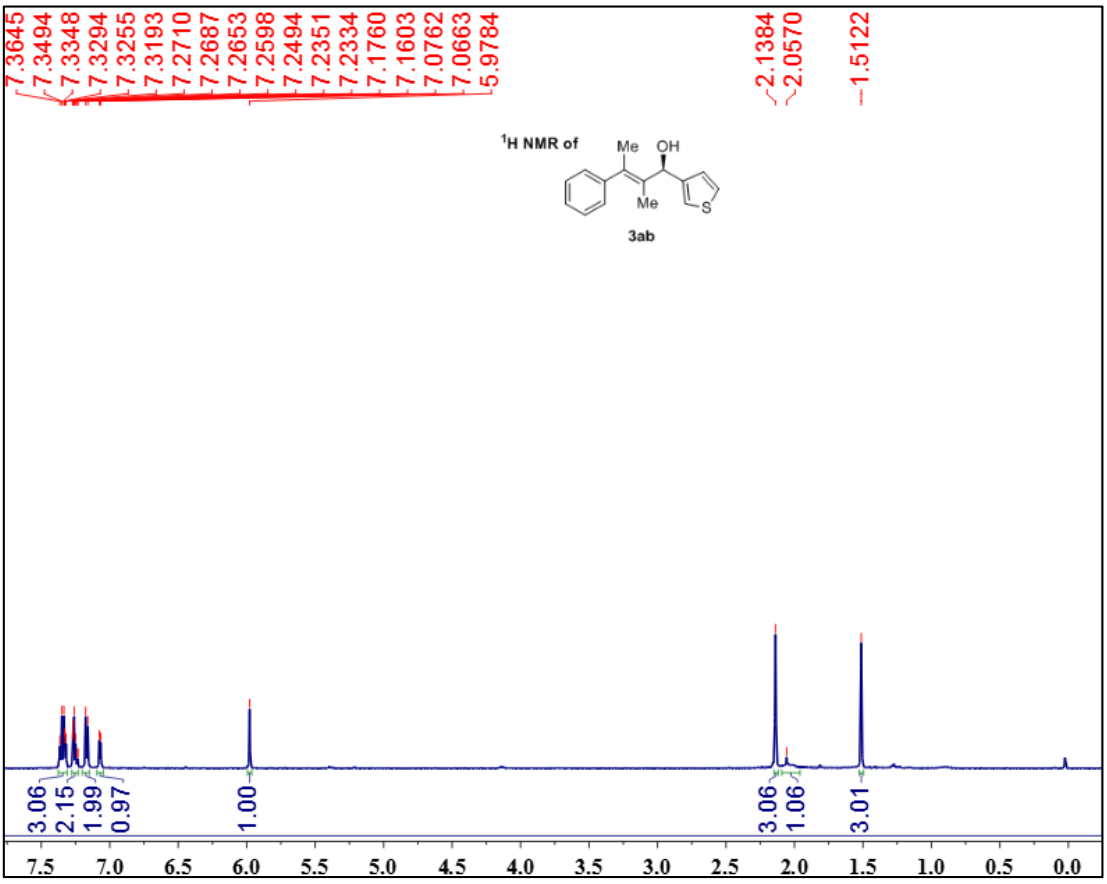

7.4999
7.4841
7.4029
7.3879
7.3722
7.3635
7.3484
7.3330
7.3027
7.2880
7.2710
7.2641
7.2621
7.2492
7.2345
7.1894
7.1868
7.1729
5.9568
2.1275
1.9660
1.9459
1.9247
1.9171
1.8188
1.7973
1.7893
1.2279
1.2162
1.2048
0.9739
0.9595
0.9460
0.9386
0.9321
0.9185
0.5974
0.5831
0.5688
1H NMR of
Me
OH
nBu
3aa
1.97
1.95
2.02
2.19
2.01
1.02
3.00
2.00
1.13
1.83
2.23
2.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

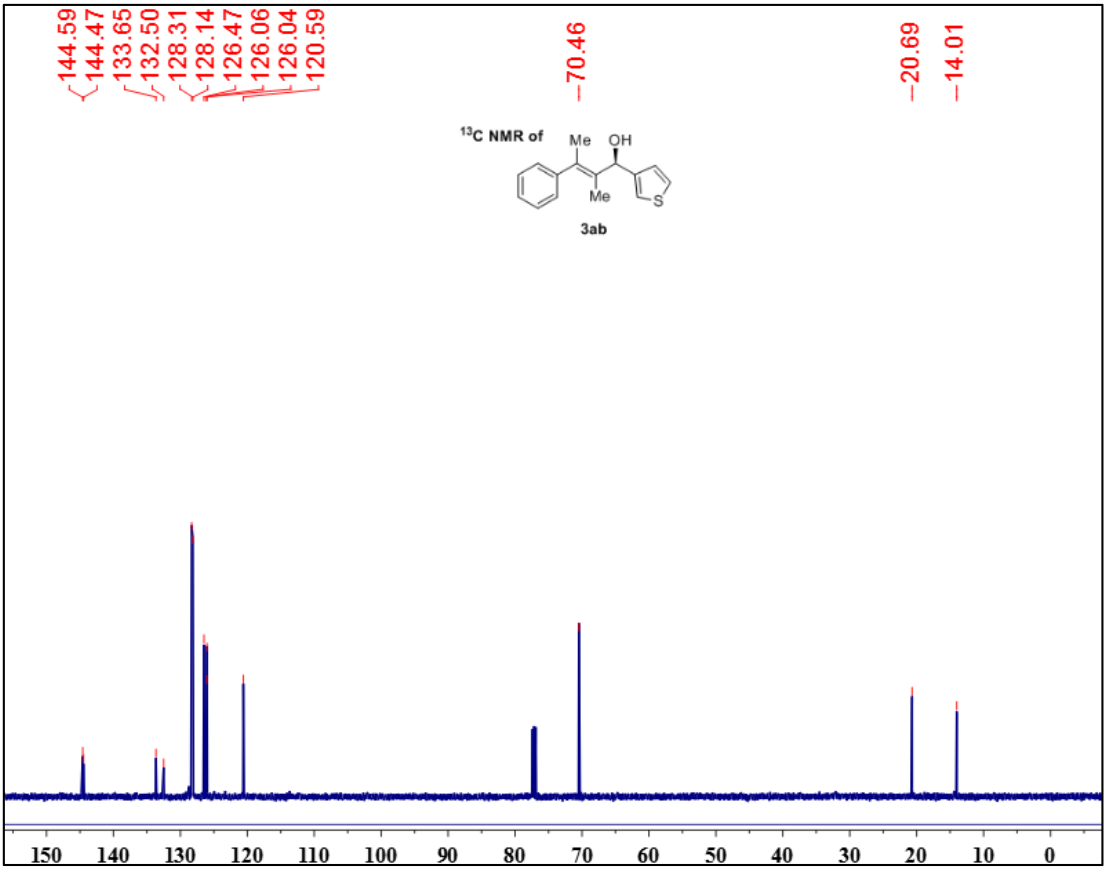

144.86
143.30
137.65
135.75
128.36
128.33
127.91
127.03
126.38
125.84
73.00
32.66
29.06
23.09
21.76
13.62
13C NMR of
Me
OH
nBu
3aa
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

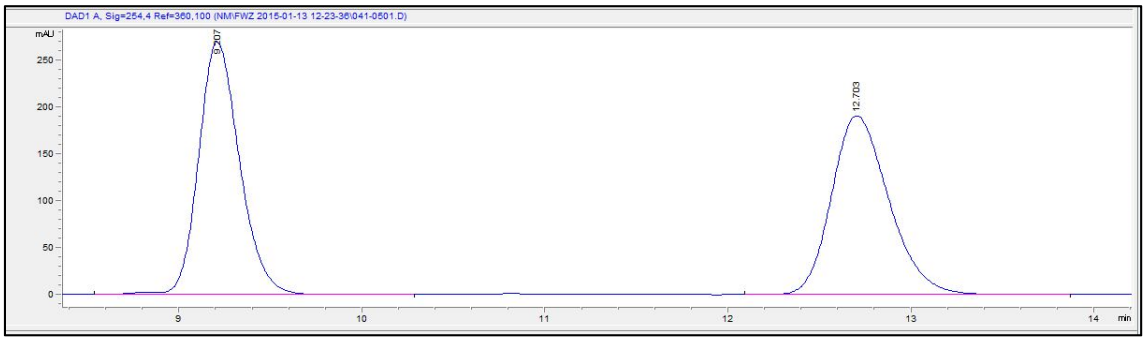


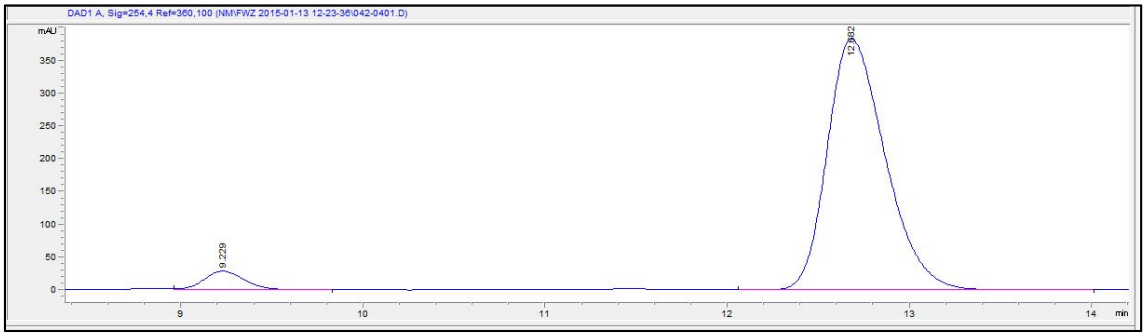


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	4.473	VV	0.0943	27.13688	4.50365	4.8072
2	6.681	BB	0.1593	537.36963	52.56710	95.1928
总量：				564.50651	57.07074	

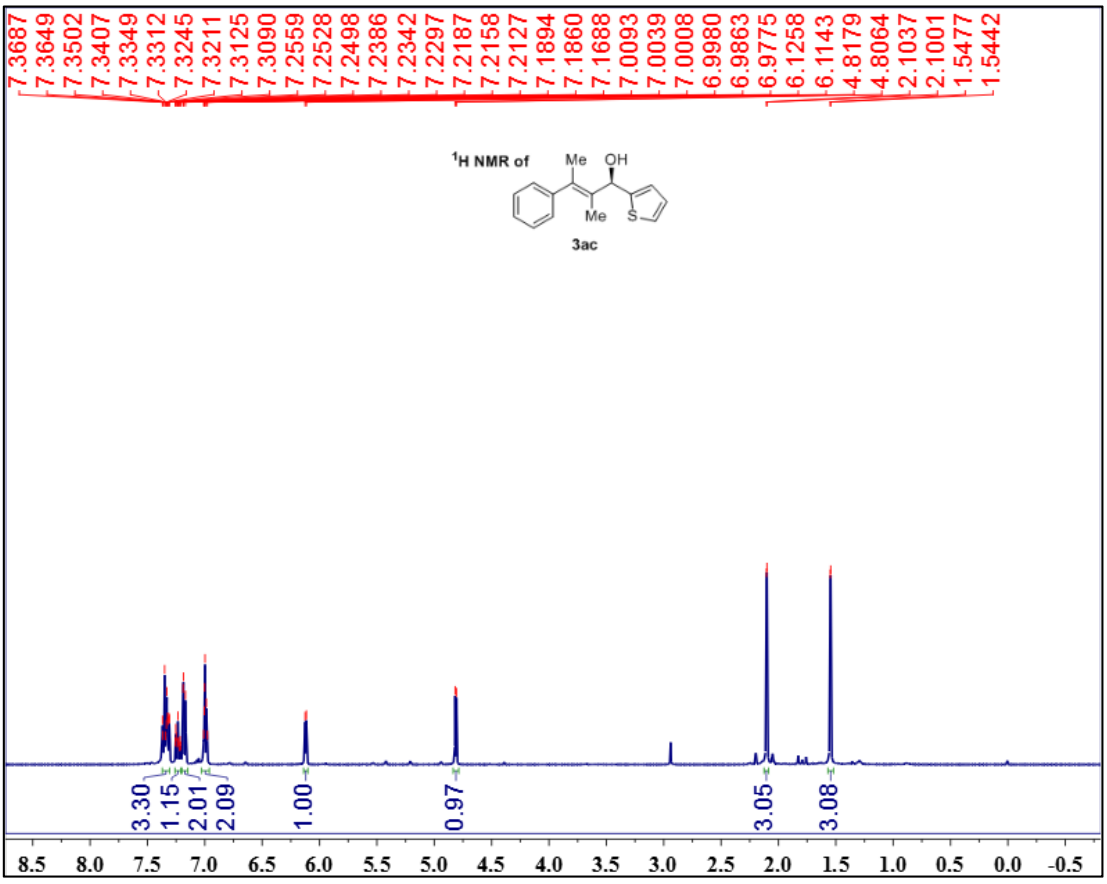

7.3645
7.3494
7.3348
7.3294
7.3255
7.3193
7.2710
7.2687
7.2653
7.2598
7.2494
7.2351
7.2334
7.1760
7.1603
7.0762
7.0663
5.9784
2.1384
2.0570
1.5122
1H NMR of
Me
OH
Me
S
3ab
3.06
2.15
1.99
0.97
1.00
3.06
1.06
3.01
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

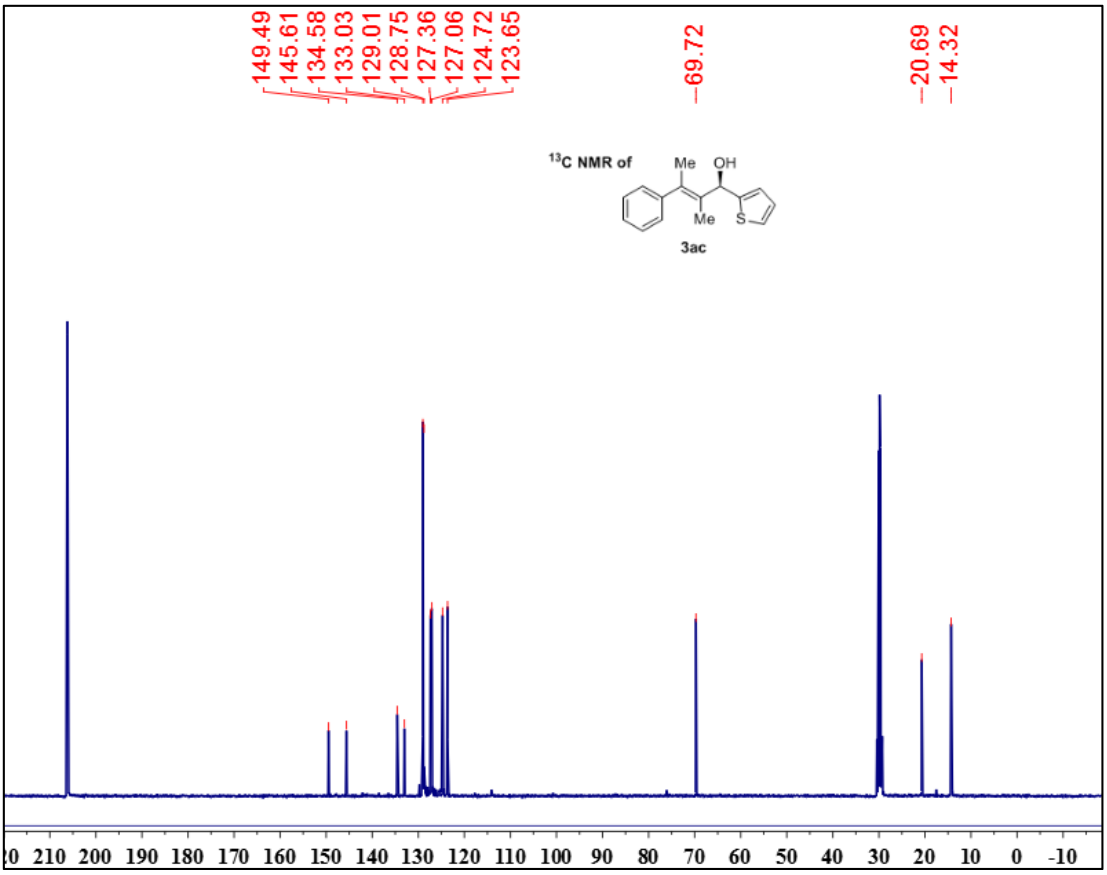

144.59
144.47
133.65
132.50
128.31
128.14
126.47
126.06
126.04
120.59
70.46
20.69
14.01
13C NMR of
Me
OH
Me
S
3ab
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

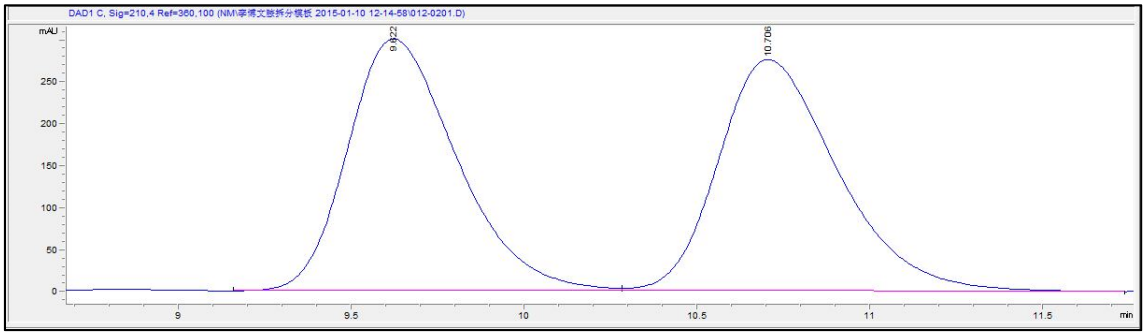


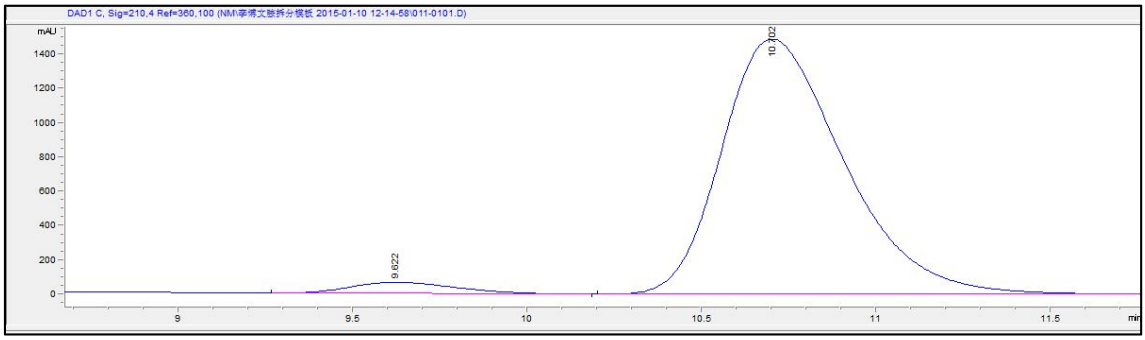


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.229	VB	0.2391	443.75223	28.58714	4.9784
2	12.682	BB	0.3417	8469.88770	383.51706	95.0216
总量：				8913.63992	412.10420	

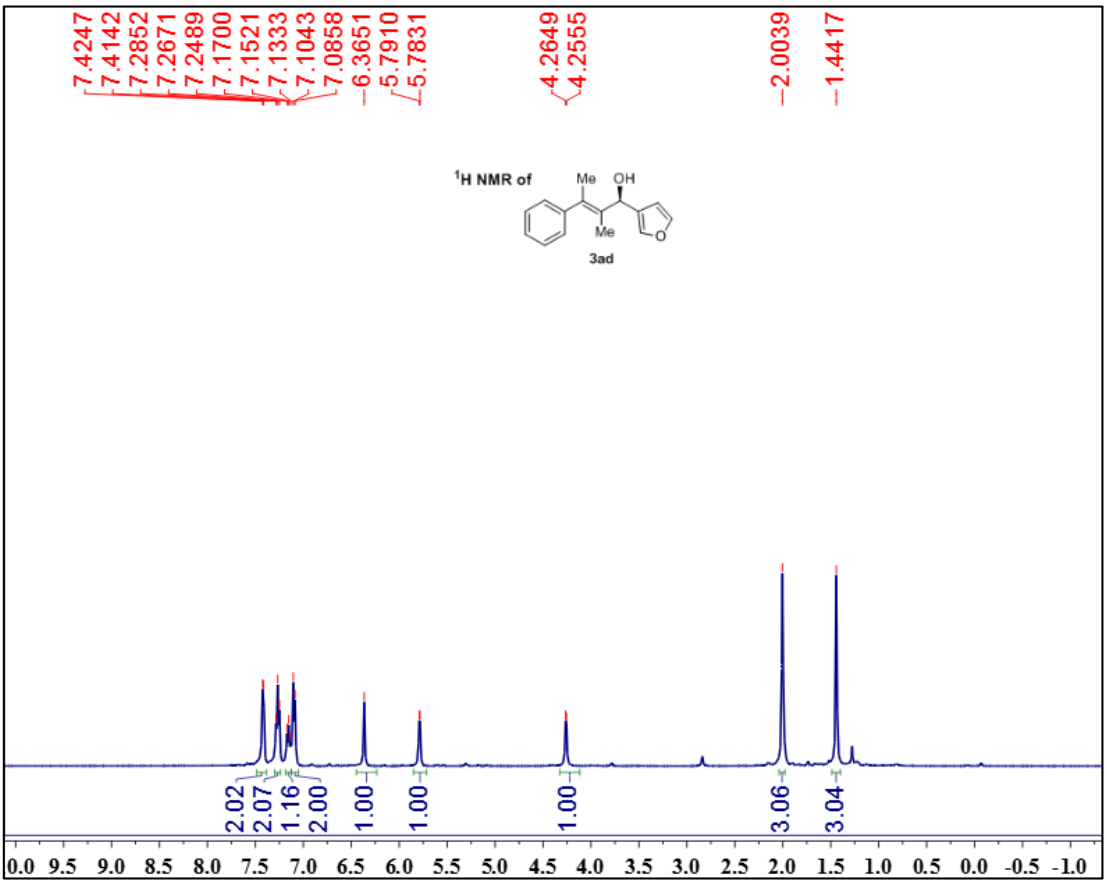

7.3687
7.3649
7.3502
7.3407
7.3349
7.3312
7.3245
7.3211
7.3125
7.3090
7.2559
7.2528
7.2498
7.2386
7.2342
7.2297
7.2187
7.2158
7.2127
7.1894
7.1860
7.1688
7.0093
7.0039
7.0008
6.9980
6.9863
6.9775
6.1258
6.1143
4.8179
4.8064
2.1037
2.1001
1.5477
1.5442
1H NMR of
Me
OH
Me
S
3ac
3.30
1.15
2.01
2.09
1.00
0.97
3.05
3.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

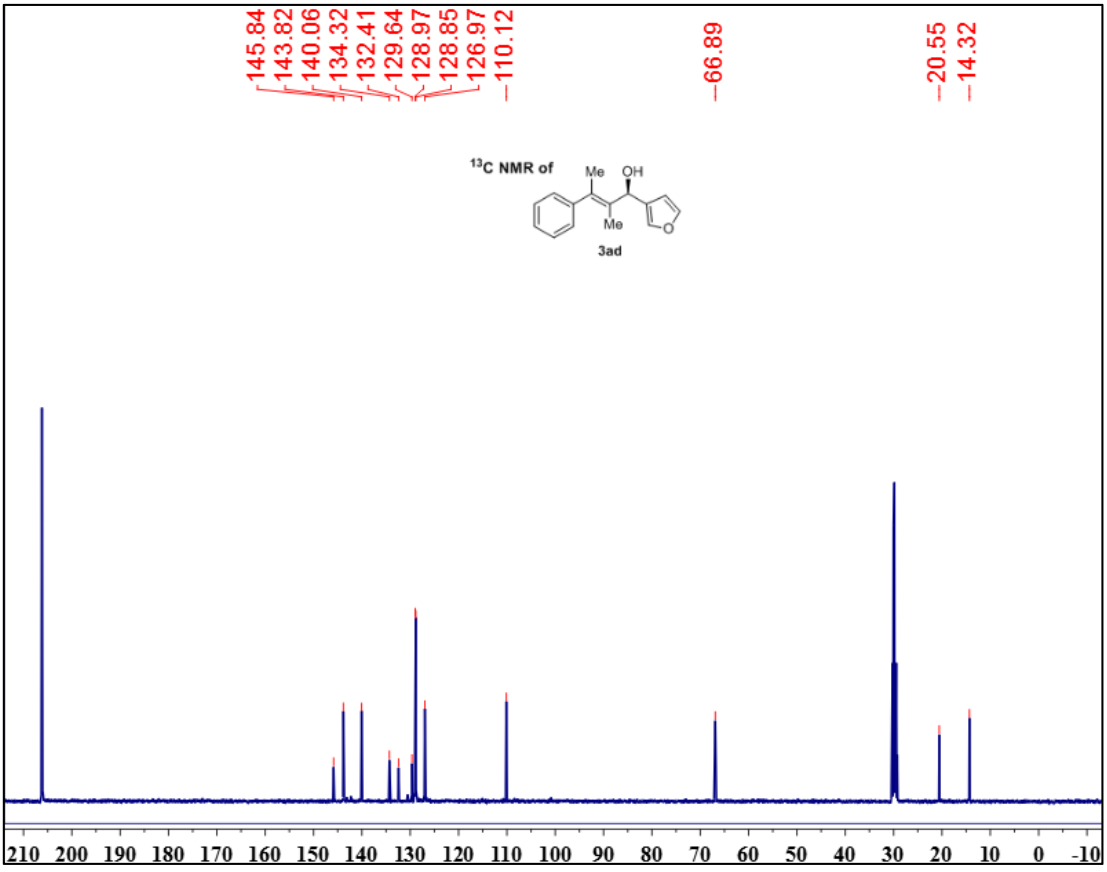

149.49
145.61
134.58
133.03
129.01
128.75
127.36
127.06
124.72
123.65
69.72
20.69
14.32
13C NMR of
Me
OH
Me
S
3ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

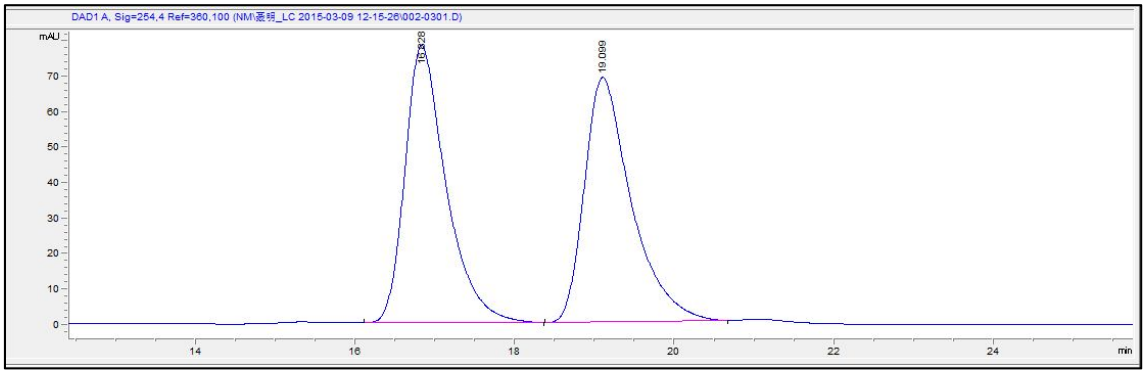


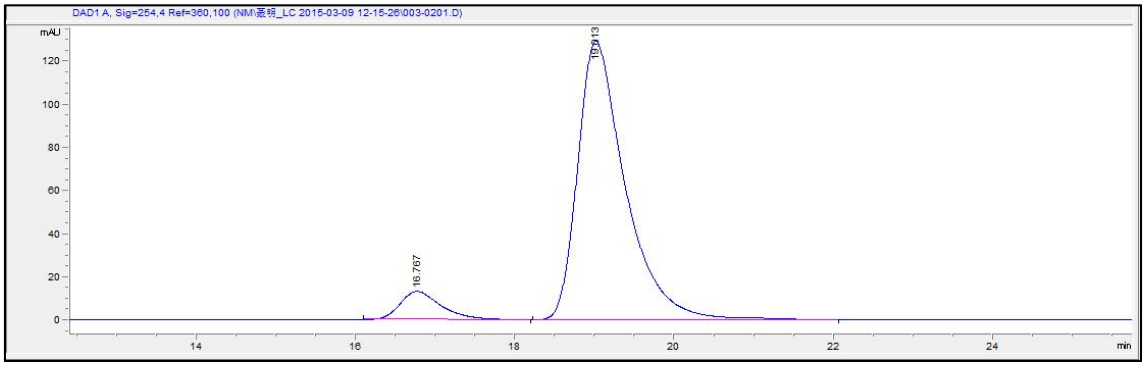


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.622	BB	0.3272	1373.84631	65.35693	3.6387
2	10.702	BV	0.3752	3.63830e4	1488.36145	96.3613
总量：				3.77568e4	1553.71838	

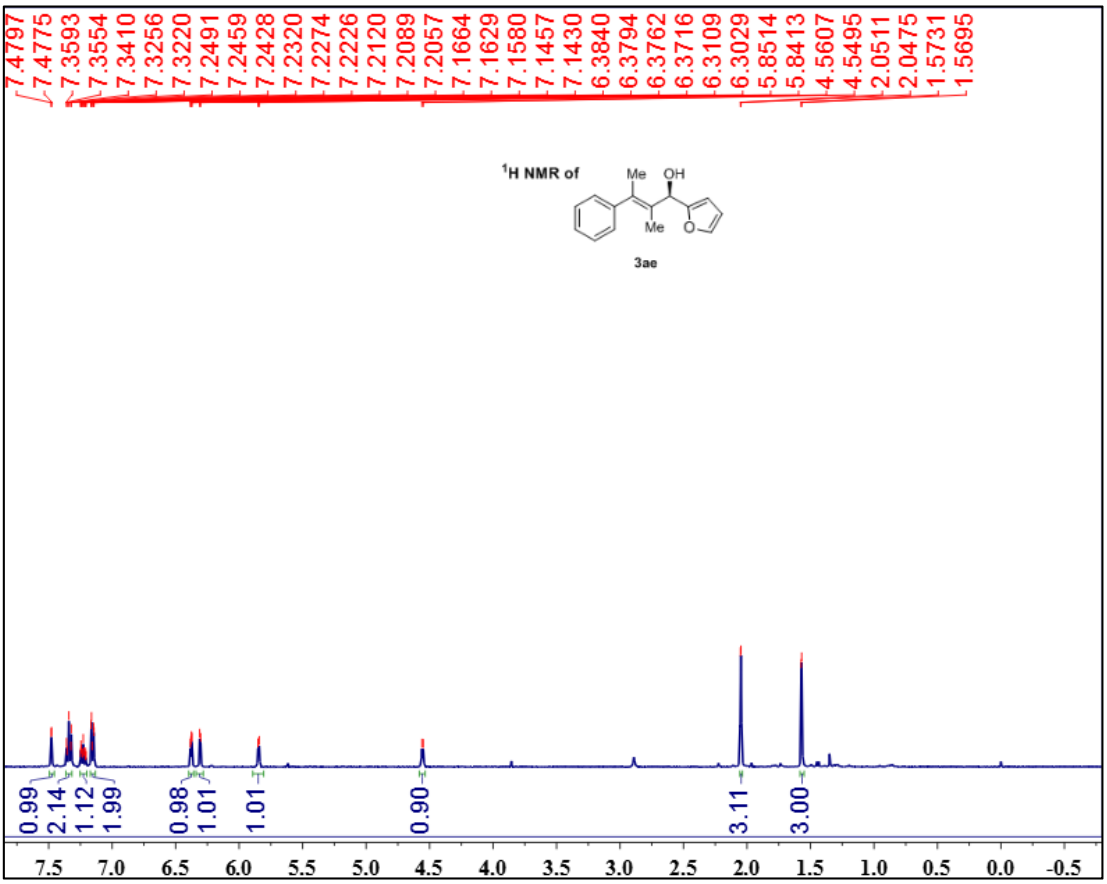

7.4247
7.4142
7.2852
7.2671
7.2489
7.1700
7.1521
7.1333
7.1043
7.0858
6.3651
5.7910
5.7831
4.2649
4.2555
2.0039
1.4417
1H NMR of
Me
OH
Me
3ad
2.02
2.07
1.16
2.00
1.00
1.00
1.00
3.06
3.04
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0

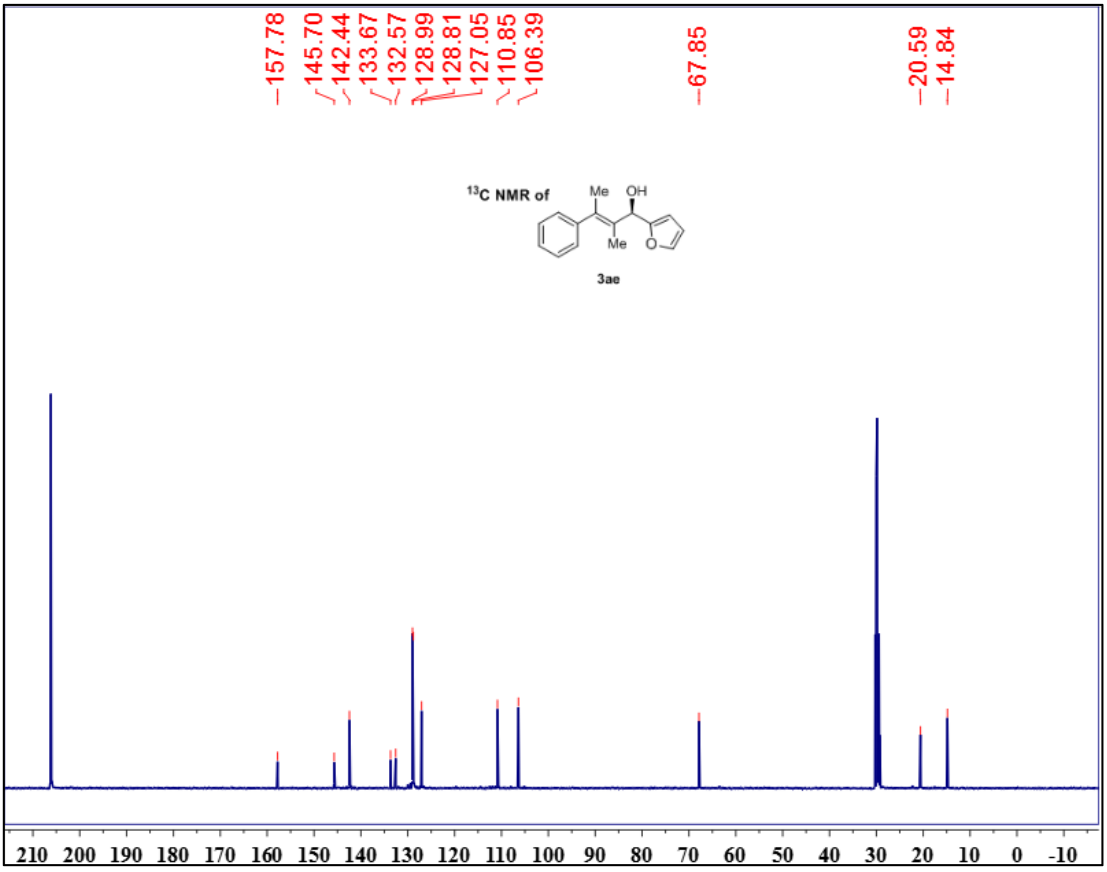

145.84
143.82
140.06
134.32
132.41
129.64
128.97
128.85
126.97
110.12
66.89
20.55
14.32
13C NMR of
Me
OH
Me
3ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

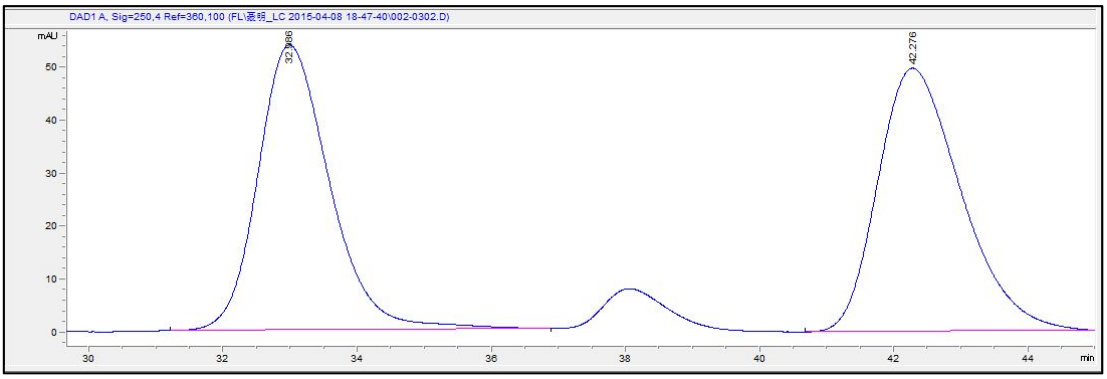


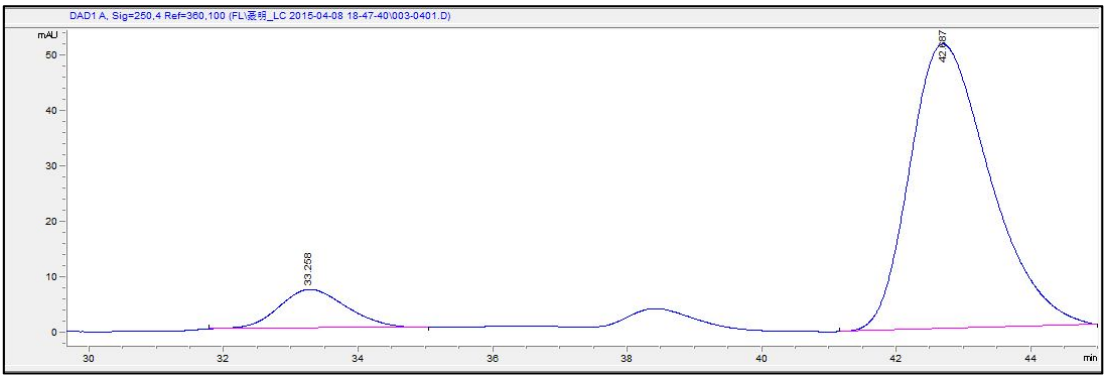


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.767	BB	0.5286	466.59814	13.06537	7.9977
2	19.013	BB	0.6142	5367.56396	129.32825	92.0023
总量：				5834.16211	142.39362	


7.4797
7.4775
7.3593
7.3554
7.3410
7.3256
7.3220
7.2491
7.2459
7.2428
7.2320
7.2274
7.2226
7.2120
7.2089
7.2057
7.1664
7.1629
7.1580
7.1457
7.1430
6.3840
6.3794
6.3762
6.3716
6.3109
6.3029
5.8514
5.8413
4.5607
4.5495
2.0511
2.0475
1.5731
1.5695
1H NMR of
Me
OH
Me
O
3ae
0.99
2.14
1.12
1.99
0.98
1.01
1.01
0.90
3.11
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

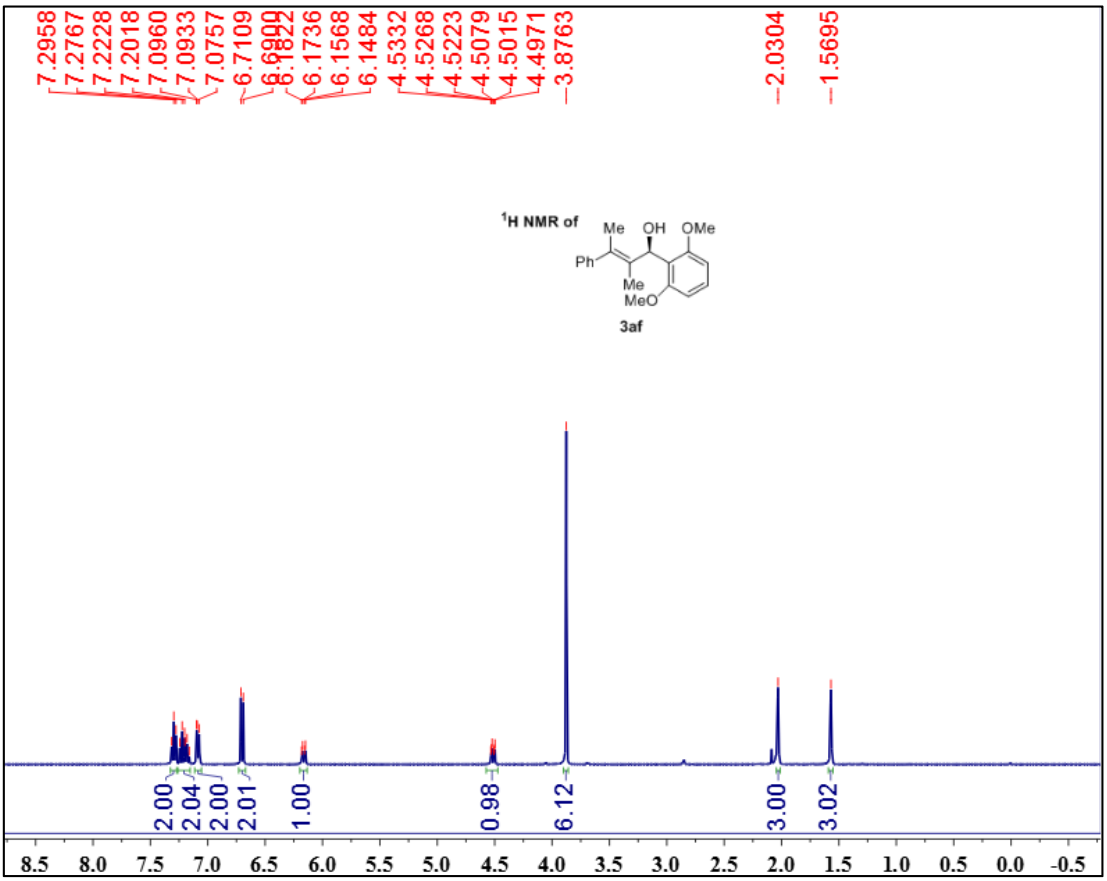

157.78
145.70
142.44
133.67
132.57
128.99
128.81
127.05
110.85
106.39
67.85
20.59
14.84
13C NMR of
Me
OH
Me
O
3ae
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

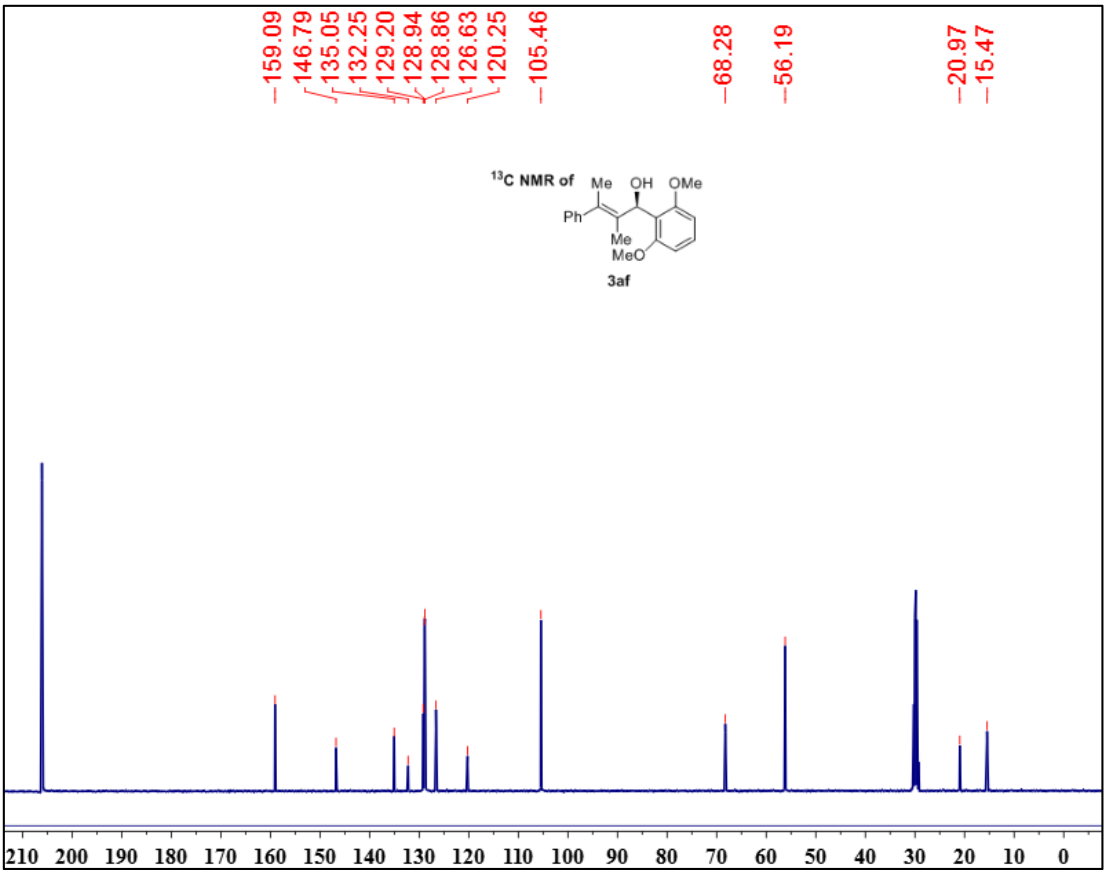


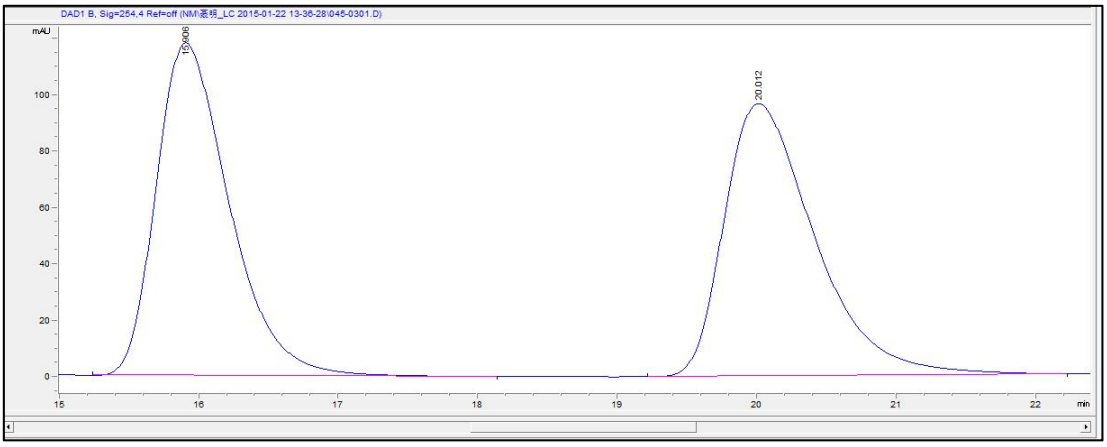


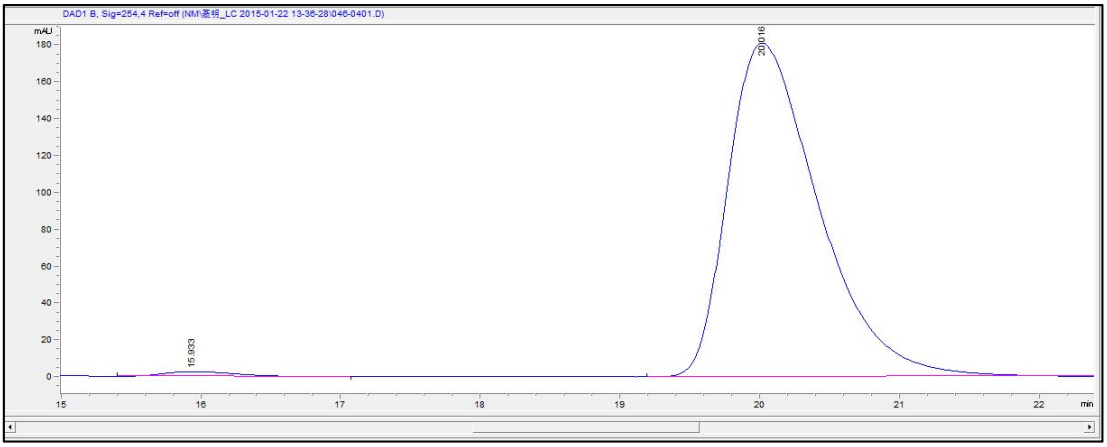
信号 1: DAD1 A, Sig=250,4 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	33.258	BB	0.8371	492.48947	6.99777	10.3587
2	42.687	BBA	1.2045	4261.87061	51.44579	89.6413
总量：				4754.36008	58.44356	


7.2958
7.2767
7.2228
7.2018
7.0960
7.0933
7.0757
6.7109
6.1736
6.1568
6.1484
4.5332
4.5268
4.5223
4.5079
4.5015
4.4971
3.8763
2.0304
1.5695
1H NMR of
Me
OH
OMe
Ph
Me
MeO
3af
2.00
2.04
2.00
2.01
1.00
0.98
6.12
3.00
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


159.09
146.79
135.05
132.25
129.20
128.94
128.86
126.63
120.25
105.46
68.28
56.19
20.97
15.47
13C NMR of
Me
OH
OMe
Ph
Me
MeO
3af
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0





峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.933	BB	0.5009	94.94915	2.66970	1.1491
2	20.016	BB	0.6944	8168.21777	181.03474	98.8509
总量：				8263.16692	183.70444	