Supporting Information

A new type of ferrocene-based phosphine-tert-butylsulfinamide ligands: synthesis and application in asymmetric catalysis

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General Information

All commercially obtained reagents and solvents were used without further purification. Compounds **6, 7** were prepared according to published procedures. [1] NMR spectra were recorded on Bruker 400 spectrometer. ^{1}H NMR, ^{13}C NMR spectra were measured at 400 MHz and 100 MHz in $CDCl_3$. Data for ^{1}H NMR spectra are reported as follows: chemical shift (ppm, referenced to TMS; s = singlet, d = doublet, t = triplet, dd = doublet of doublets, dt = doublet of triplets, m = multiplet), coupling constant (Hz), and integration. Data for ^{13}C NMR are reported in terms of chemical shift (ppm) relative to residual solvent peak ($CDCl_3$: 77.0 ppm) with complete proton decoupling. ^{31}P NMR shifts are referenced to 85% H_3PO_4 as an external standard. Coupling constants are reported in Hz. High-Resolution Mass Spectroscopy (HRMS) was carried out on a VARIA FT-ICR MS. High performance liquid chromatography (HPLC) was performed on an Agilent 1260 series using Daicel Chiralcel chiral column. Optical rotations were obtained on a Perkin-Elmer 343 polarimeter.

General procedure for synthesis of chiral ligands 4a-g

To a solution of amine **7** (1 g, 2.4 mmol) in dry THF (5 mL) was added *n*-BuLi (1 mL, 2.4 mmol, 2.4 M) at -30 °C under an N_2 atmosphere, and the mixture was stirred for 10 min. A solution of enantiopure *tert*-butanethiosulfinate (0.47 g, 2.4 mmol) in 1 mL of dry THF was added slowly to the lithium amine solution. Then the mixture was stirred for 2 h at -30 °C, and then ice water were carefully added. The volatile material was removed, and the residue was extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried (Na_2SO_4), concentrated and purified by flash chromatography (petroleum ether/ethyl acetate 4:1) to afford the chiral sulfinamide-phosphine **4a-g** .

(R_C,S_{Fc},R_S)-4a: Yellow amorphous solid, 45% yield. $[\alpha]_D^{25}$ = -356.9 (*c* 0.54, CH_2Cl_2); m.p. 185-187 °C； ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49-7.45 (m, 2H), 7.42-7.37 (m, 3H), 7.35-7.22 (m, 5H), 4.60 (q, 1H), 4.45 (s, 1H), 4.31 (dd, *J* = 4.0, 4.3 Hz, 1H), 4.10 (s, 5H), 3.89 (s, 1H), 3.71 (s, 1H), 1.34 (d, *J* = 4.0 Hz, 3H), 1.06 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ139.28 (d, $^{1}J_{C-P}$ = 10.9 Hz, PPh_2, Ph-*ipso*), 137.16 (d, $^{1}J_{C-P}$

= 10.6 Hz, PPh_2, Ph-*ipso*), 134.84 (d, $^2J_{C\text{-}P}$ = 21.3 Hz, PPh_2, Ph-*ortho*), 133.06 (d, $^2J_{C\text{-}P}$ = 19.1 Hz, PPh_2, Ph-*ortho*), 129.06 (s, PPh_2, Ph-*para*), 128.37 (s, PPh_2, Ph-*para*), 128.34 (d, $^3J_{C\text{-}P}$ = 6.7 Hz, PPh_2, Ph-*meta*), 128.09 (d, $^3J_{C\text{-}P}$ = 7.6 Hz, PPh_2, Ph-*meta*), 96.44 (d, $^1J_{C\text{-}P}$ = 22.0 Hz, Fc, C-1), 74.38 (d, $^2J_{C\text{-}P}$ = 12.3 Hz, Fc, C-5), 71.98 (d, $^2J_{C\text{-}P}$ = 4.0 Hz, Fc, C-2), 70.75 (d, $^3J_{C\text{-}P}$ = 4.1 Hz, Fc, C-4), 69.88 (s, Fc, Cp'), 69.36 (s, Fc, C-3), 55.18 (s, $\underline{C}(CH_3)_3$), 48.65 (d, J = 3.9 Hz, $\underline{C}HN$), 22.45 (d, J = 1.1 Hz, $C(\underline{C}H_3)_3$), 21.57 (s, $NCH\underline{C}H_3$); ^{31}P NMR (162 MHz, $CDCl_3$): δ -24.57; HRMS *m/z* calcd for $C_{28}H_{32}FeNOPS$ $[M+H]^+$ 518.1364, found 518.1365.

(R_C,S_{Fc},R_S)-4b: Yellow amorphous solid, 66% yield. $[\alpha]_D^{25}$ = -343.0 (*c* 0.64, CH_2Cl_2); m.p. 161-163 °C; ^1H NMR (400 MHz, $CDCl_3$): δ 7.70-7.60 (m, 2H), 7.37-7.34 (m, 5H), 7.26-7.23 (m, 3H), 4.52 (s, 1H), 4.45-4.36 (m, 1H), 4.34 (s, 1H), 4.04 (s, 1H), 3.94 (s, 5H), 2.37 (s, 3H), 1.83 (d, *J* = 7.0 Hz, 3H), 0.77 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ139.05 (d, $^1J_{C\text{-}P}$ = 8.6 Hz, PPh_2, Ph-*ipso*), 137.52 (d, $^1J_{C\text{-}P}$ = 7.8 Hz, PPh_2, Ph-*ipso*), 135.04 (d, $^2J_{C\text{-}P}$ = 22.0 Hz, PPh_2, Ph-*ortho*), 133.13 (d, $^2J_{C\text{-}P}$ = 19.8 Hz, PPh_2, Ph-*ortho*), 129.14 (s, PPh_2, Ph-*para*), 128.18 (d, $^3J_{C\text{-}P}$ = 6.5 Hz, PPh_2, Ph-*meta*), 128.06 (s, PPh_2, Ph-*para*), 127.98 (d, $^3J_{C\text{-}P}$ = 6.9 Hz, PPh_2, Ph-*meta*), 97.09(d, $^1J_{C\text{-}P}$ = 26.7 Hz, Fc, C-1), 74.57 (d, $^2J_{C\text{-}P}$ = 9.3 Hz, Fc, C-5), 71.44 (d, $^2J_{C\text{-}P}$ = 4.6 Hz, Fc, C-2), 69.85(overlapped, Fc, C-4), 69.78 (s, Fc, Cp'), 69.27 (s, Fc, C-4), 57.85 (d, *J* = 11.6 Hz, $\underline{C}HN$), 57.51 (s, $\underline{C}(CH_3)_3$), 30.33 (s, $N\underline{C}H_3$), 23.50 (s, $C(\underline{C}H_3)_3$), 18.42 (d, J = 1.9 Hz, $NCH\underline{C}H_3$); ^{31}P NMR (162 MHz, $CDCl_3$): δ -25.36; HRMS *m/z* calcd for $C_{29}H_{34}FeNOPS$ $[M+H]^+$ 532.1521, found 532.1520

(R_C,S_{Fc},R_S)-4c: Yellow amorphous solid, 12% yield. $[\alpha]_D^{25}$ = -294.5 (*c* 0.56, CH_2Cl_2); m.p. 172-174 °C; ^1H NMR (400 MHz, $CDCl_3$): δ 7.10-6.80 (m, 6H), 4.59 (d, *J* = 6.4 Hz, 1H), 4.42 (s, 1H), 4.28 (s, 1H), 4.09 (s, 4H), 3.95 (s, 1H), 3.70 (s, 1H), 2.31 (s, 6H), 2.20 (s, 6H), 1.34 (d, *J* = 6.5 Hz, 3H), 1.05 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.86 (d, $^1J_{C\text{-}P}$ = 10.1 Hz, PAr_2, Ar-*ipso*), 137.51 (d, $^3J_{C\text{-}P}$ = 6.9 Hz, PAr_2, Ar-*meta*), 137.37 (d, $^3J_{C\text{-}P}$ = 7.9 Hz, PAr_2, Ar-*meta*), 136.95 (d, $^1J_{C\text{-}P}$ = 10.2 Hz, PAr_2, Ar-*ipso*), 132.55 (d, $^2J_{C\text{-}P}$ = 21.2 Hz, PAr_2, Ar-*ortho*), 130.83 (d, $^2J_{C\text{-}P}$ = 19.0 Hz, PAr_2, Ar-*ortho*), 130.74 (s, PAr_2, Ar-*para*), 130.11 (s, PAr_2, Ar-*para*), 96.35 (d, $^1J_{C\text{-}P}$ = 21.8 Hz, Fc, C-1), 74.93 (d, $^2J_{C\text{-}P}$ = 12.6 Hz, Fc, C-5), 72.06 (d, $^2J_{C\text{-}P}$ = 3.8 Hz, Fc, C-2), 70.47

(d, $^{3}J_{C\text{-}P}$ = 4.1 Hz, Fc, C-4), 69.83 (s, Fc, Cp'), 69.09 (s, Fc, C-3), 55.11 (s, $\underline{C}(CH_3)_3$), 48.71 (d, J = 3.8 Hz, $\underline{C}HN$), 22.45 (s, $C(\underline{C}H_3)_3$), 21.37 (s, $NCH\underline{C}H_3$), 21.30 (s, PAr_2, *meta*-CH_3); ^{31}P NMR (162 MHz, $CDCl_3$): δ -24.27; HRMS *m/z* calcd for $C_{32}H_{40}FeNOPS$ $[M+H]^+$ 574.1990, found 574.1993.

(R_C,S_{Fc},R_S)-4d: Yellow amorphous solid, 48% yield. $[\alpha]_D^{25}$ = -208.2 (*c* 0.54, CH_2Cl_2); m.p. 91-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ7.37-7.10 (m, 6H), 4.60 (d, J = 6.4 Hz, 1H), 4.40 (s, 1H), 4.26 (s, 1H), 4.10 (s, 5H), 3.99 (s, 1H), 3.64 (s, 1H), 1.27 (s, 18H), 1.20 (s, 18H), 1.03 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ150.19 (d, $^{3}J_{C\text{-}P}$ = 6.6 Hz, PAr_2, Ar-*meta*), 149.98 (d, $^{3}J_{C\text{-}P}$ = 7.3 Hz, PAr_2, Ar-*meta*), 137.84 (d, $^{1}J_{C\text{-}P}$ = 8.8 Hz, PAr_2, Ar-*ipso*), 136.01 (d, $^{1}J_{C\text{-}P}$ = 9.5 Hz, PAr_2, Ar-*ipso*), 129.03 (d, $^{2}J_{C\text{-}P}$ = 21.5 Hz, PAr_2, Ar-*ortho*), 127.75(d, $^{2}J_{C\text{-}P}$ = 19.9 Hz, PAr_2, Ar-*ortho*), 122.73 (s, PAr_2, Ar-*para*), 122.36(s, PAr_2, Ar-*para*), 95.84 (d, $^{1}J_{C\text{-}P}$ = 20.8 Hz, Fc, C-1), 76.21 (d, $^{2}J_{C\text{-}P}$ = 12.8 Hz, Fc, C-5), 71.81 (d, $^{2}J_{C\text{-}P}$ = 4.0 Hz, Fc, C-2), 70.45 (d, $^{3}J_{C\text{-}P}$ = 3.8 Hz, Fc, C-4), 69.73 (s, Fc, Cp'), 68.90 (s, Fc, C-3), 55.03 (s, $S\underline{C}(CH_3)_3$), 48.67 (d, *J* = 3.8 Hz, $\underline{C}HN$), 34.86 (s, PAr_2, $\underline{C}(CH_3)_3$), 34.79(s, PAr_2, $\underline{C}(CH_3)_3$), 31.46 (s, PAr_2, $C(\underline{C}H_3)_3$), 31.40 (s, PAr_2, *meta*-$C(\underline{C}H_3)_3$), 22.52 (s, $SC(\underline{C}H_3)_3$), 21.23 (s, $NCH\underline{C}H_3$); ^{31}P NMR (162 MHz, $CDCl_3$) δ -23.82; HRMS *m/z* calcd for $C_{44}H_{64}FeNOPS$ $[M+H]^+$ 742.3868, found 742.3882.

(R_C,S_{Fc},R_S)-4e: Yellow oil, 48% yield. $[\alpha]_D^{25}$ = -204.3 (*c* 0.8 CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.54 (q, *J* = 6.4 Hz, 1H), 4.33 (s, 1H), 4.27 (s, 1H), 4.18 (s, 5H), 4.12 (s, 1H), 1.80-1.76 (m, 2H), 1.63-1.48 (m, 9H), 1.25-1.21 (m, 13H), 0.99 (t, *J* = 6.8 Hz, 3H), 0.82 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 96.06 (d, $^{1}J_{C\text{-}P}$ = 19.1 Hz, Fc, C-1), 76.08 (d, $^{2}J_{C\text{-}P}$ = 18.1 Hz, Fc, C-5), 70.70 (d, $^{2}J_{C\text{-}P}$ = 19.8 Hz, Fc, C-2), 69.73 (s, Fc, Cp'), 69.56 (d, $^{3}J_{C\text{-}P}$ = 3.1 Hz, Fc, C-4), 68.75 (s, Fc, C-3), 55.43 (s, $S\underline{C}(CH_3)_3$), 49.25 (s, $\underline{C}HN$), 29.10 (d, *J* = 19.1 Hz, $P\underline{C}H_2CH_2CH_2CH_3$), 28.85 (d, *J* = 13.5 Hz, $P\underline{C}H_2CH_2CH_2CH_3$), 27.40 (d, *J* = 6.9 Hz, $PCH_2CH_2\underline{C}H_2CH_3$), 25.22 (d, *J* = 10.0 Hz, $PCH_2\underline{C}H_2CH_2CH_3$), 24.58 (d, *J* = 13.3 Hz, $PCH_2\underline{C}H_2CH_2CH_3$), 24.41 (d, *J* = 8.3 Hz, $PCH_2CH_2\underline{C}H_2CH_3$), 23.68 (s, $NCH\underline{C}H_3$), 22.71 (d, *J* = 1.6 Hz, $SC(\underline{C}H_3)_3$), 13.98 (s, $PCH_2CH_2CH_2\underline{C}H_3$),13.80 (s, $PCH_2CH_2CH_2\underline{C}H_3$); ^{31}P NMR (162 MHz, $CDCl_3$): δ -39.65; HRMS *m/z* calcd for $C_{24}H_{40}FeNOPS$ $[M+H]^+$ 478.1990, found

478.1980

(R_C,S_{Fc},S_S)-4f: Yellow amorphous solid, 50% yield. $[\alpha]_D^{25}$ = -304.0 (*c* 0.58, CH_2Cl_2); m.p. 147-148 °C； ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57-7.53 (m, 2H), 7.38-7.37 (m, 3H), 7.20 (q, *J* = 5.6 Hz, 3H), 7.15-7.11 (m, 2H), 4.69-4.63 (m, 1H), 4.51 (s, 1H), 4.36 (t, *J* = 2.3 Hz, 1H), 3.94 (s, 5H), 3.01 (d, *J* = 8.4 Hz, 1H), 1.77 (d, *J* = 6.7 Hz, 3H), 0.82 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.37 (d, $^1J_{C\text{-}P}$ = 8.2 Hz, PPh_2, Ph-*ipso*), 137.72 (d, $^1J_{C\text{-}P}$ = 8.2 Hz, PPh_2, Ph-*ipso*), 135.32 (d, $^2J_{C\text{-}P}$ = 21.7 Hz, PPh_2, Ph-*ortho*), 132.44 (d, $^2J_{C\text{-}P}$ = 17.5 Hz, PPh_2, Ph-*ortho*), 129.27 (s, PPh_2, Ph-*para*), 128.16 (d, $^3J_{C\text{-}P}$ = 4.2 Hz, PPh_2, Ph-*meta*), 128.09 (d, $^3J_{C\text{-}P}$ = 6.5 Hz, PPh_2, Ph-*meta*), 127.78 (s, PPh_2, Ph-*para*), 96.90(d, $^1J_{C\text{-}P}$ = 25.7 Hz, Fc, C-1), 74.74 (d, $^2J_{C\text{-}P}$ = 9.9 Hz, Fc, C-5), 71.89 (d, $^2J_{C\text{-}P}$ = 4.6 Hz, Fc, C-2), 69.73 (s, Fc, Cp'), 69.71 (s, Fc, C-3), 69.15 (d, $^3J_{C\text{-}P}$ = 4.5 Hz, Fc, C-4), 55.58 (s, S<u>C</u>$(CH_3)_3$), 51.69 (d, *J* = 8.3 Hz, <u>C</u>HN), 23.01 (s, NCH<u>C</u>H_3), 22.13 (s, SC(<u>C</u>$H_3)_3$); ^{31}P NMR (162 MHz, $CDCl_3$): δ -25.19; HRMS *m/z* calcd for $C_{28}H_{32}FeNOPS$ $[M+H]^+$ 518.1364, found 518.1352.

(R_C,S_{Fc},S_S)-4g: Yellow amorphous solid, 68% yield. $[\alpha]_D^{25}$ = -360.5 (*c* 0.53 CH_2Cl_2); m.p. 67-69°C； ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, *J* = 22.1 Hz, 2H), 7.38 (s, 3H), 7.17 (s, 3H), 7.02 (s, 2H), 4.82 (d, *J* = 4.5 Hz, 1H), 4.53 (s, 1H), 4.40 (s, 1H), 4.09 (s, 1H), 4.00 (s, 1H), 3.90 (s, 4H), 2.08 (s, 3H), 1.70 (d, *J* = 6.6 Hz, 3H), 0.81 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.19 (d, $^1J_{C\text{-}P}$ = 8.1 Hz, PPh_2, Ph-*ipso*), 138.33 (d, $^1J_{C\text{-}P}$ = 8.4 Hz, PPh_2, Ph-*ipso*), 135.67 (d, $^2J_{C\text{-}P}$ = 22.1 Hz, PPh_2, Ph-*ortho*), 132.05 (d, $^2J_{C\text{-}P}$ = 16.5 Hz, PPh_2, Ph-*ortho*), 129.26 (s, PPh_2, Ph-*para*), 128.02 (d, *J* = 8.3 Hz, PPh_2, Ph-*meta*), 127.75 (d, *J* = 5.6 Hz, PPh_2, Ph-*meta*), 127.38 (s, PPh_2, Ph-*para*), 94.40 (d, $^1J_{C\text{-}P}$ = 27.3 Hz, Fc, C-1), 75.21 (d, $^2J_{C\text{-}P}$ = 10.3 Hz, Fc, C-5), 72.20 (d, $^2J_{C\text{-}P}$ = 4.9 Hz, Fc, C-2), 71.01 (d, $^3J_{C\text{-}P}$ = 4.6 Hz, Fc, C-4), 70.54 (s, Fc, C-3), 69.85 (s, Fc, Cp'), 58.69 (d, *J* = 7.6 Hz, <u>C</u>HN), 57.79 (s, S<u>C</u>$(CH_3)_3$), 23.94 (s, N<u>C</u>H_3), 23.45 (d, *J* = 2.5 Hz, SC(<u>C</u>$H_3)_3$), 16.58 (s, NCH<u>C</u>H_3); ^{31}P NMR (162 MHz, $CDCl_3$): δ -24.90; HRMS *m/z* calcd for $C_{29}H_{34}FeNOPS$ $[M+H]^+$ 532.1521, found 532.1515.

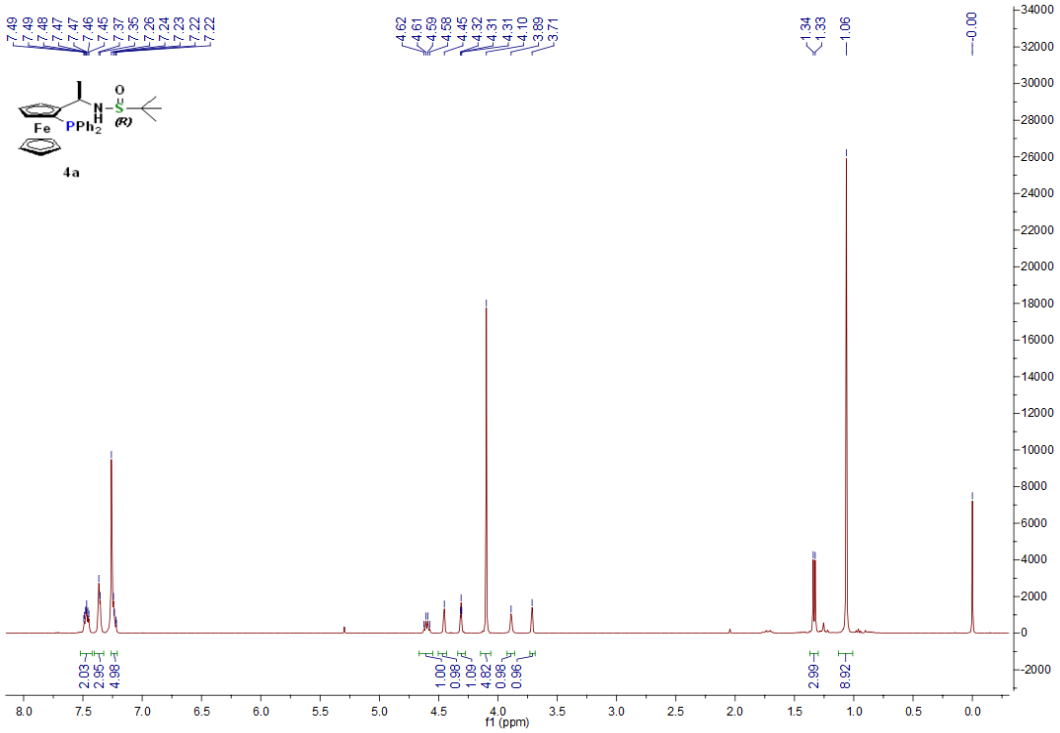
General procedure for the palladium-catalyzed asymmetric allylic alkylation

To a stirring solution of $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (2.9 mg, 0.008 mmol) in THF(1mL) was added ligand **4a** (12.4mg, 0.024 mmol) under an argon atmosphere. After 1 h, substrate **8** (0.396 mmol) was added and the solution was stirred for 15 min. nucleophile **9** (1.19mmol) was added to the mixture followed by BSA (0.29 mL, 1.19 mmol). After 24 h, the reaction was diluted with Et_2O, washed with saturated NH_4Cl(aq), saturated $NaHCO_3$(aq), and brine. The combined aqueous solutions were extracted with CH_2Cl_2. The combined organic solutions were dried over Na_2SO_4, filtered, concentrated in *vacuo*, and purified by flash chromatography (petroleum ether/ethyl acetate 10:1) to afford the desired products.

General procedure for the palladium-catalyzed asymmetric allylic amination

To a stirring solution of $[Pd_2(dba)_3]\cdot CHCl_3$ (8.3mg, 0.008 mmol) in THF(1 mL) was added ligand **4a** (12.4mg, 0.024 mmol) under an argon atmosphere. After 1 h, rac-(*E*)-1,3-diphenyl-2-propenyl acetate **8a** (100 mg, 0.396 mmol) was added and the solution was stirred for 15 min. Nucleophile **17** (1.19mmol) was added to the mixture followed by BSA, (0.29 mL, 1.19 mmol) and sodium acetate (4.8mg, 0.059mmol). After 24 h, the reaction was diluted with Et_2O, washed with saturated NH_4Cl(aq), saturated $NaHCO_3$(aq), and brine. The combined aqueous solutions were extracted with CH_2Cl_2. The combined organic solutions were dried over Na_2SO_4, filtered, concentrated in vacuo, and purified by flash chromatography (petroleum ether/ethyl acetate 10:1) to a yellow oil.

NMR and HRMS spectra for chiral ligands 4a-g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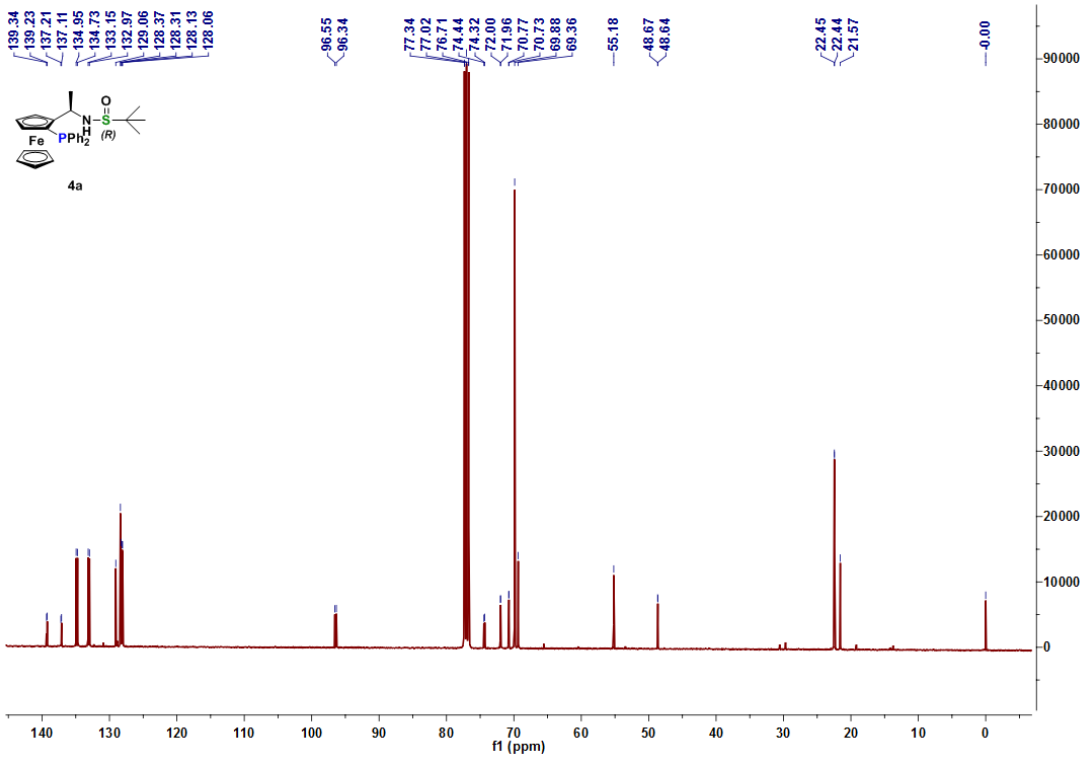
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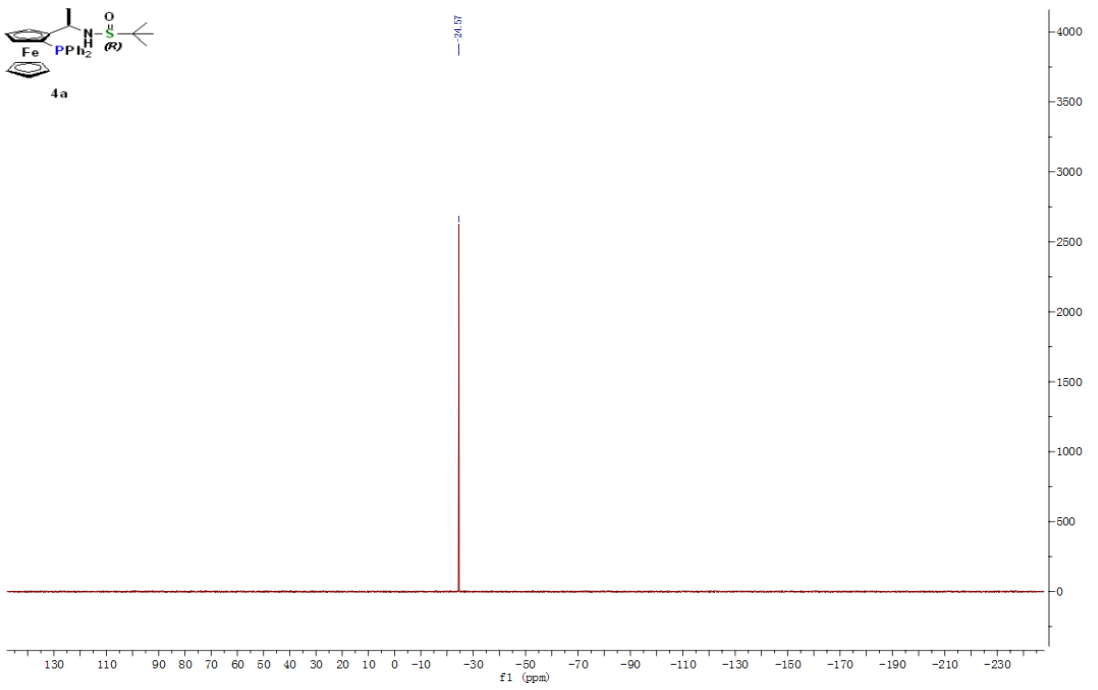
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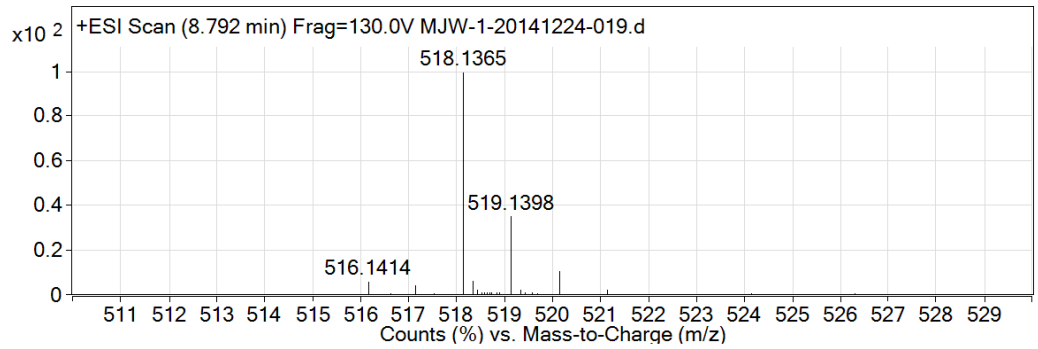
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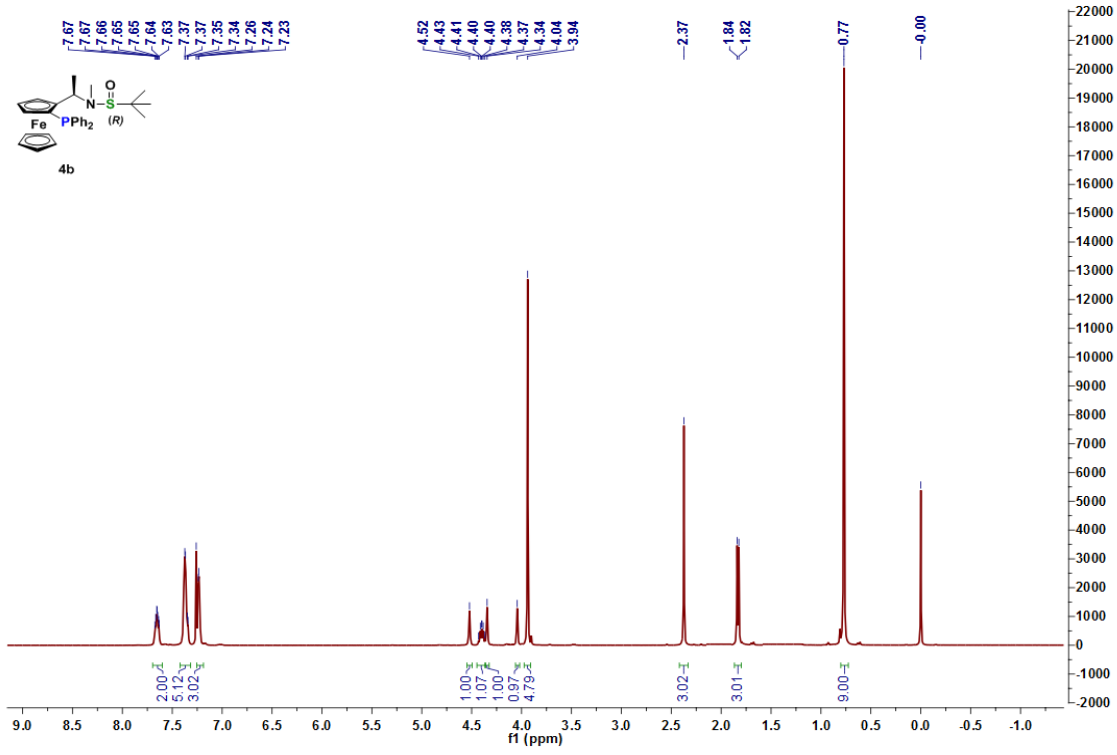
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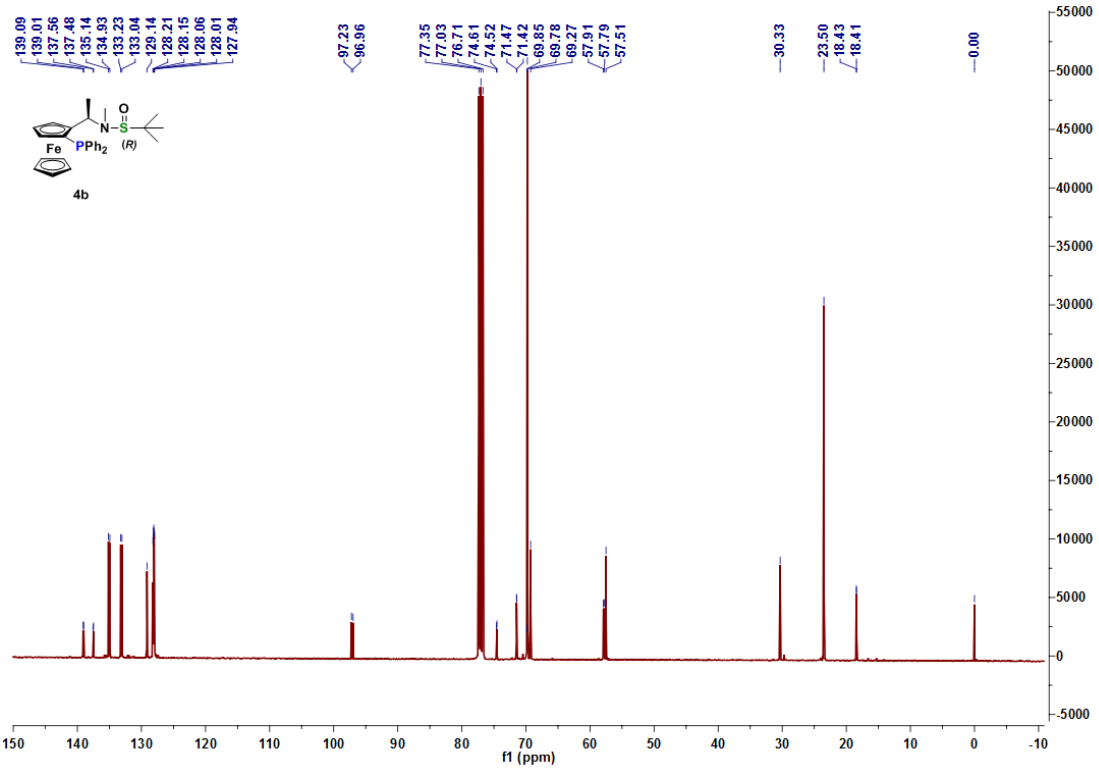
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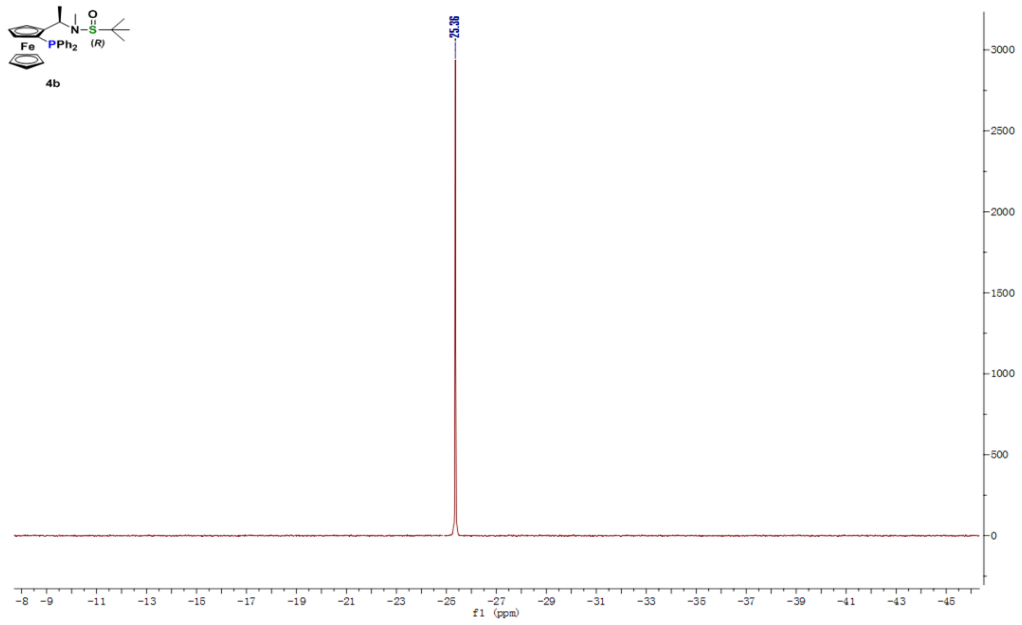
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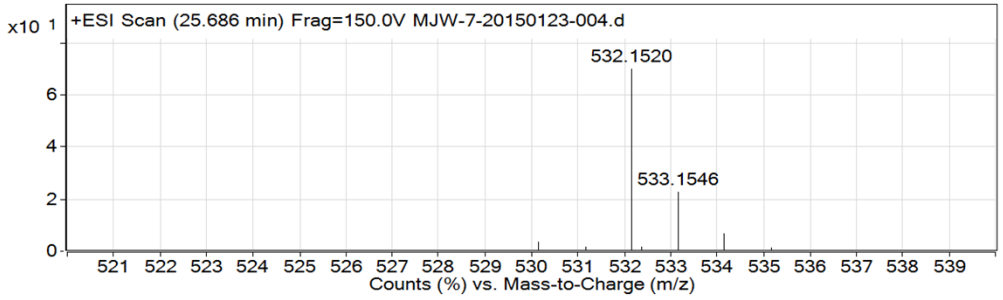
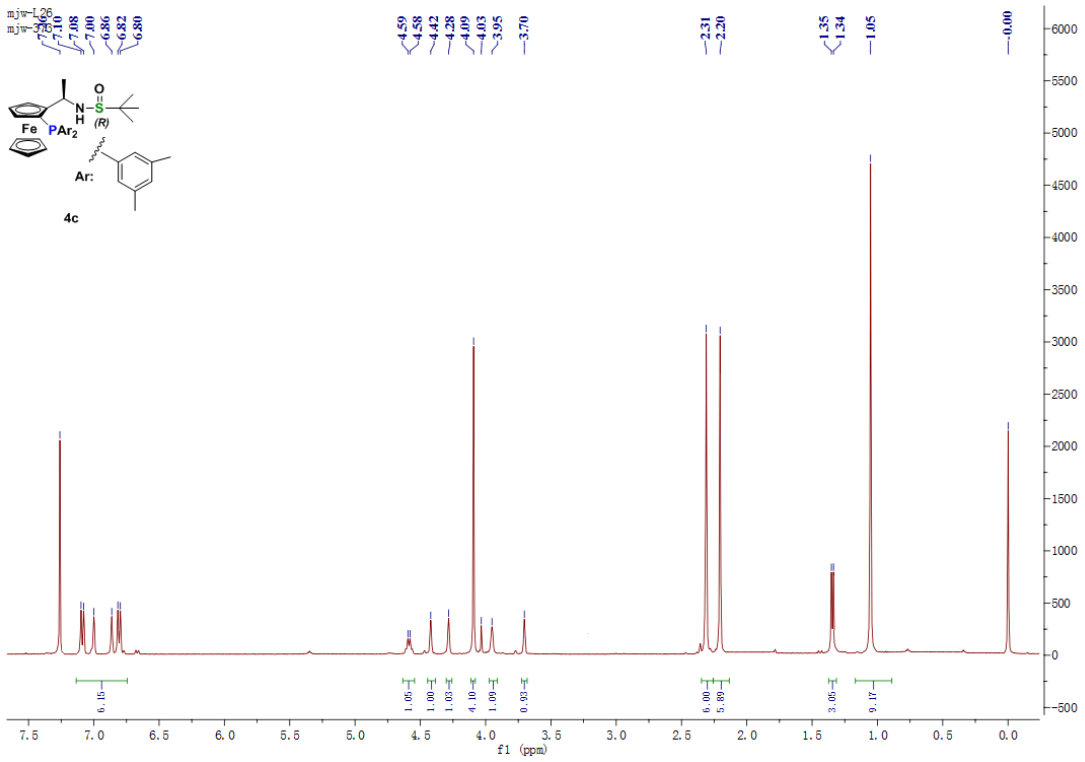
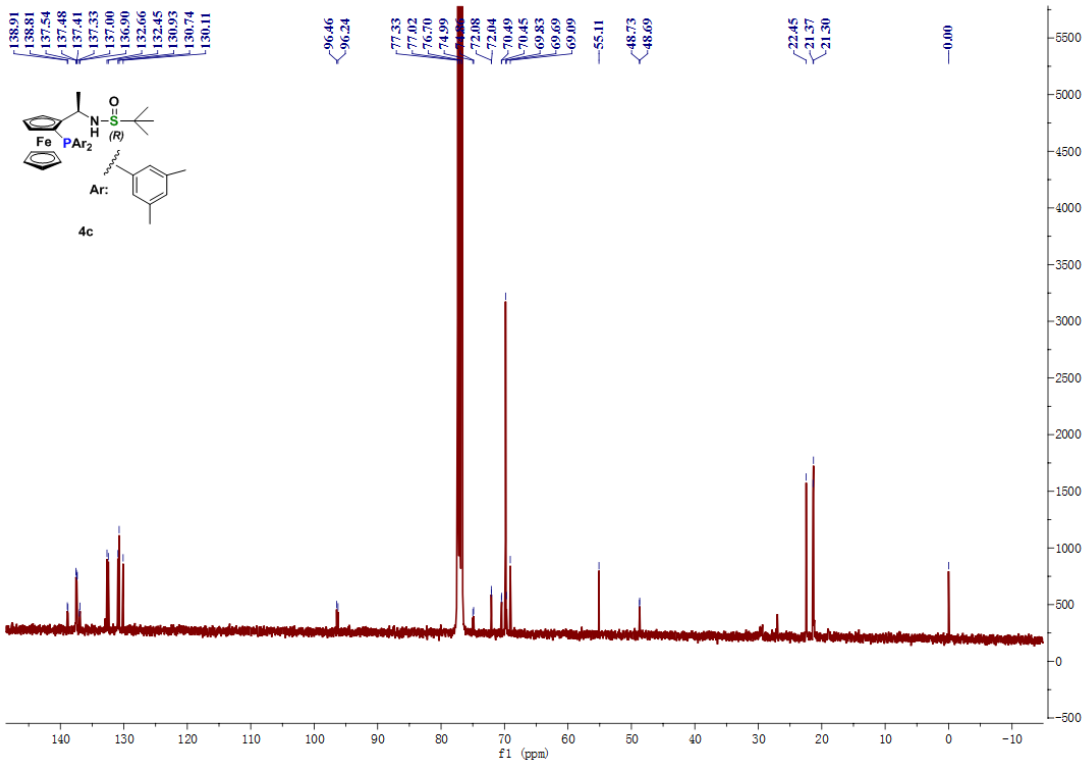
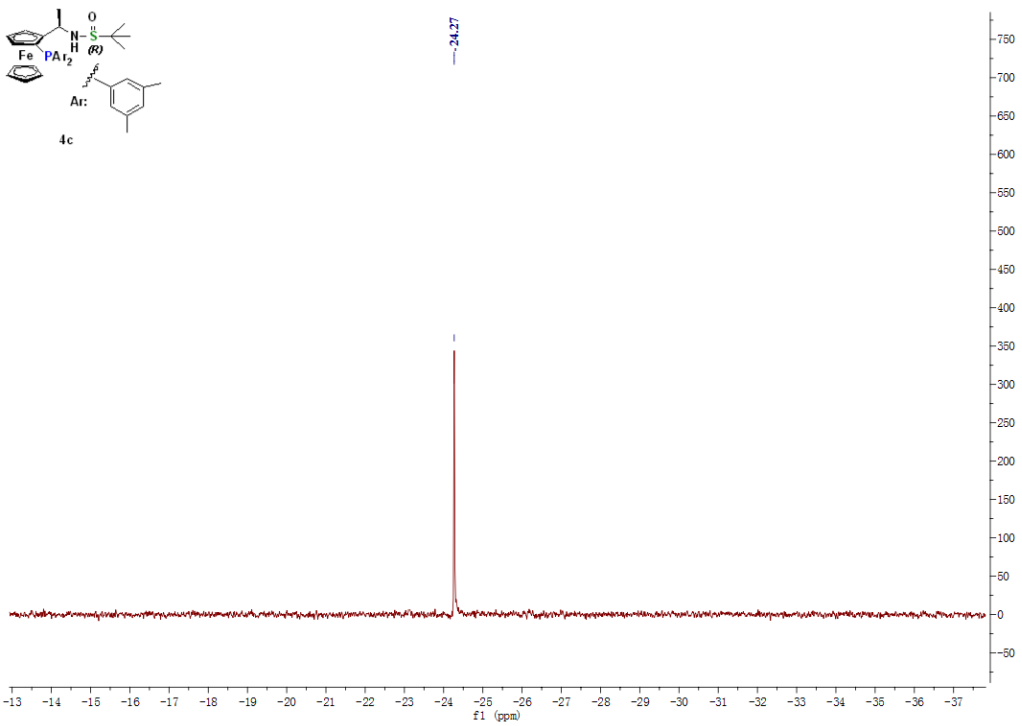
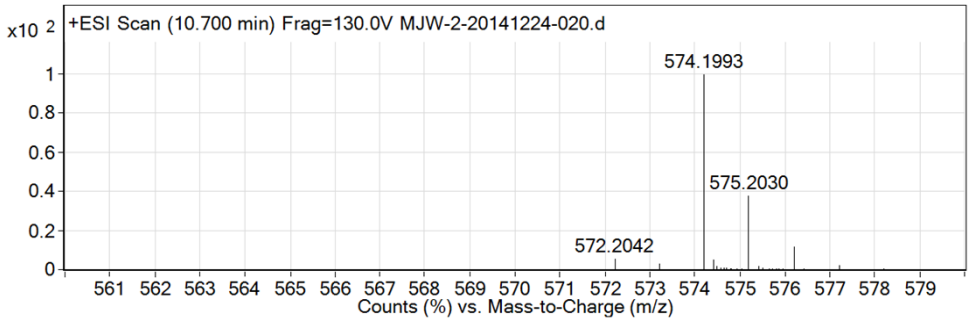
4b
f1 (ppm)

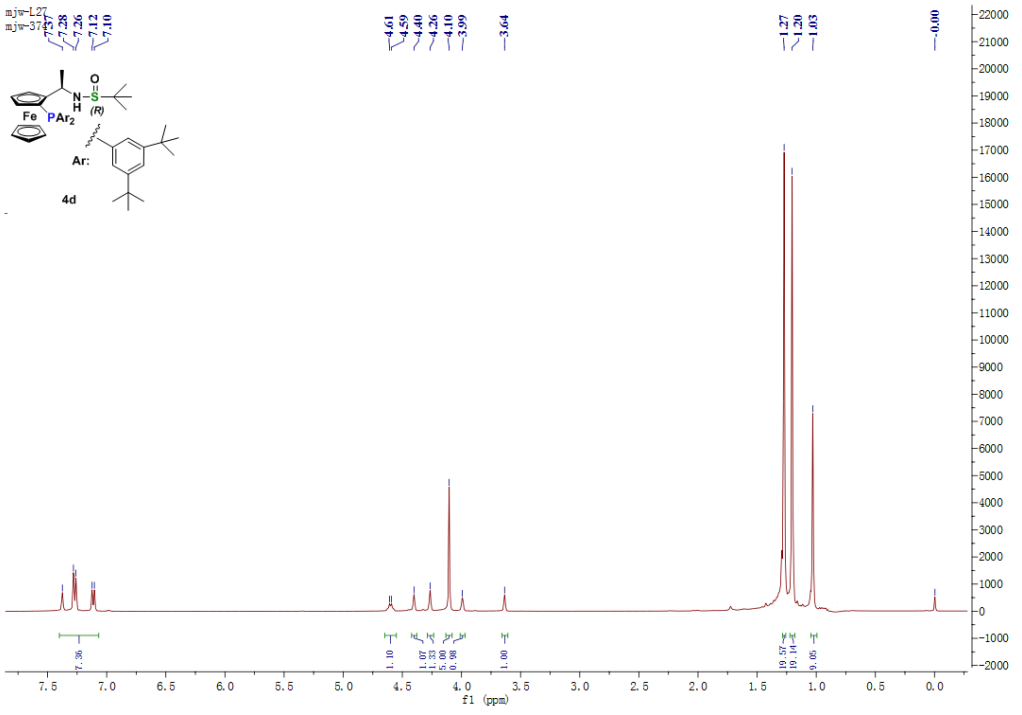

+ESI Scan (25.686 min) Frag=150.0V MJW-7-20150123-004.d
x10 1
532.1520
533.1546
Counts (%) vs. Mass-to-Charge (m/z)

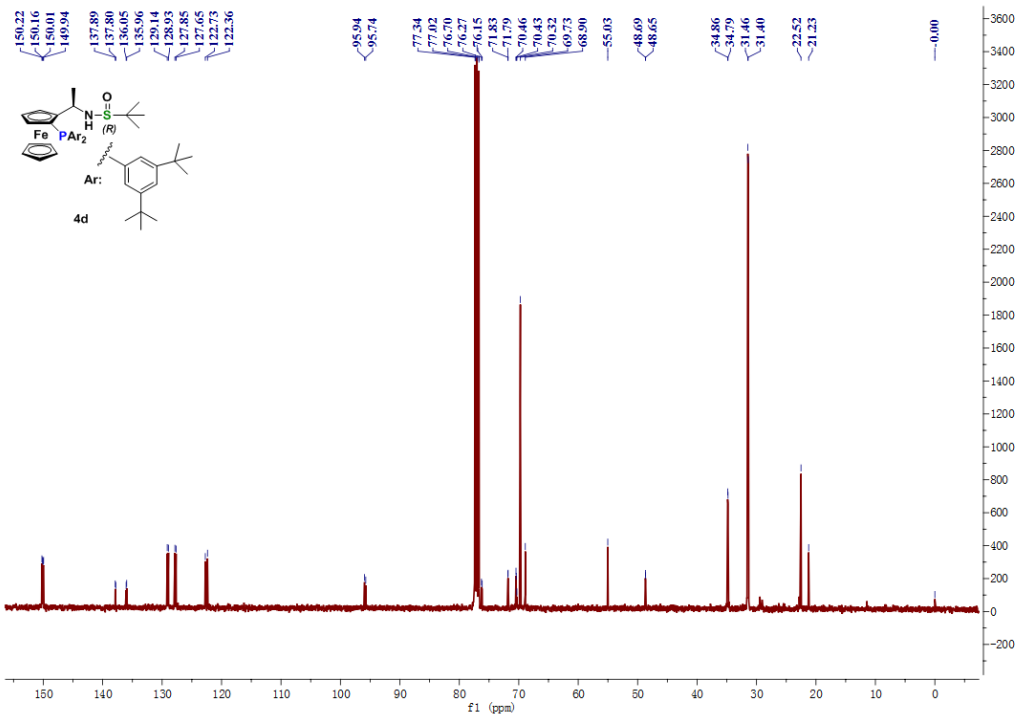

mjw-1-26
7.26
7.10
7.08
7.00
6.86
6.82
6.80
4.59
4.58
4.42
4.28
4.09
4.03
3.95
3.70
2.31
2.20
1.35
1.34
1.05
0.00
Fe
PAr2
(R)
Ar:
4c
f1 (ppm)

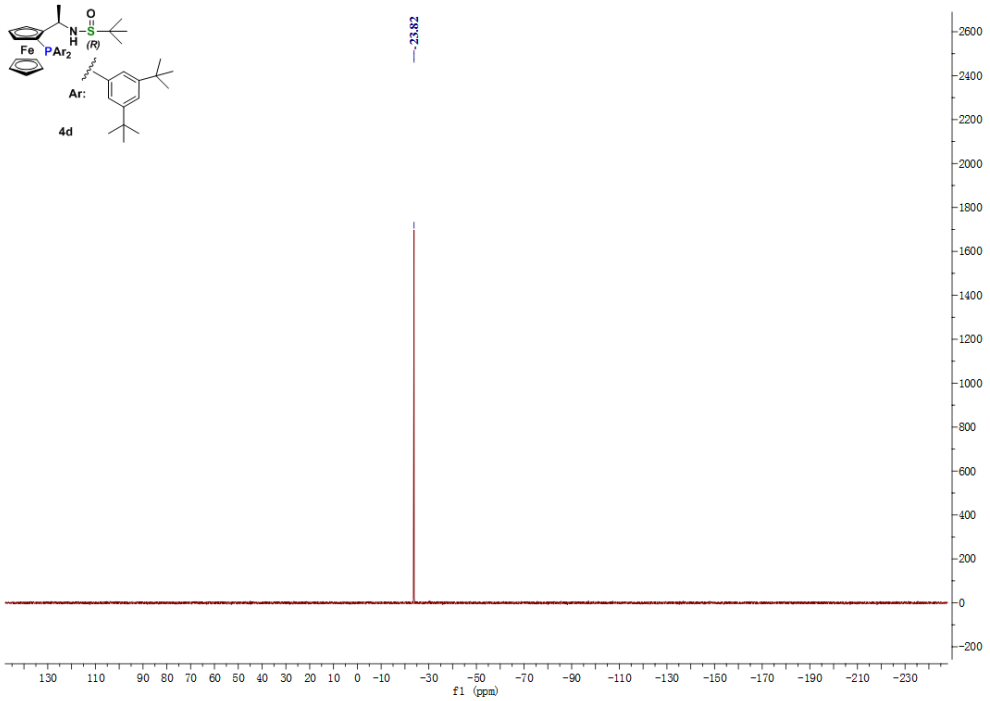

138.91
138.81
137.54
137.48
137.41
137.33
137.00
136.90
132.66
132.45
130.93
130.74
130.11
96.46
96.24
77.33
77.02
76.70
74.99
72.08
72.04
70.49
70.45
69.83
69.69
69.09
55.11
48.73
48.69
22.45
21.37
21.30
0.00
Fe
PAr2
(R)
Ar:
4c
f1 (ppm)

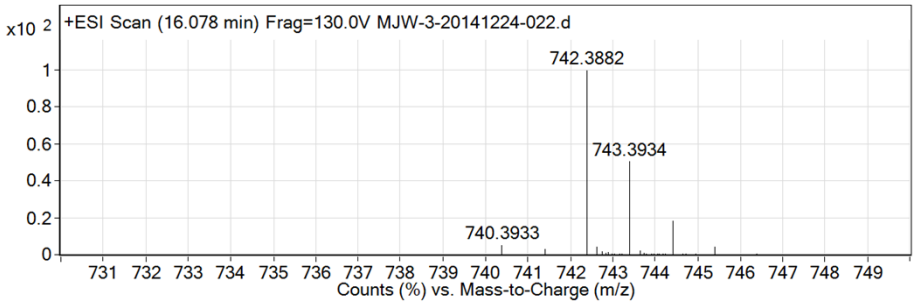

Fe
PAr2
N
H
O
S
(R)
Ar:
4c
24.27
f1 (ppm)

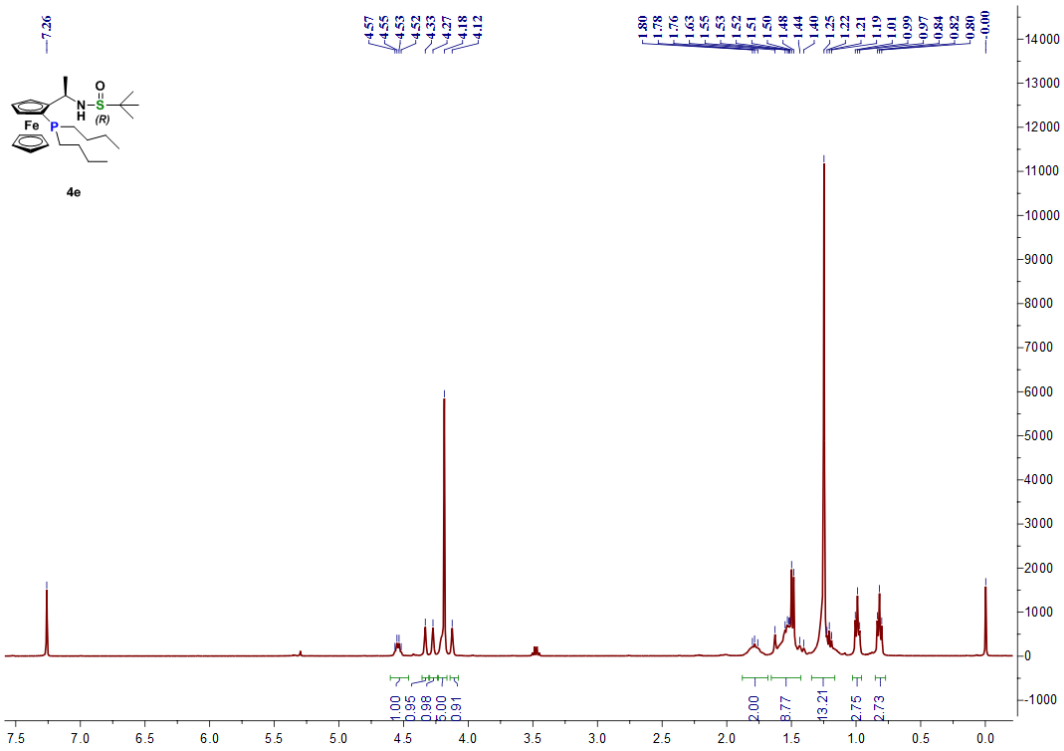

x10 2
+ESI Scan (10.700 min) Frag=130.0V MJW-2-20141224-020.d
574.1993
575.2030
572.2042
Counts (%) vs. Mass-to-Charge (m/z)

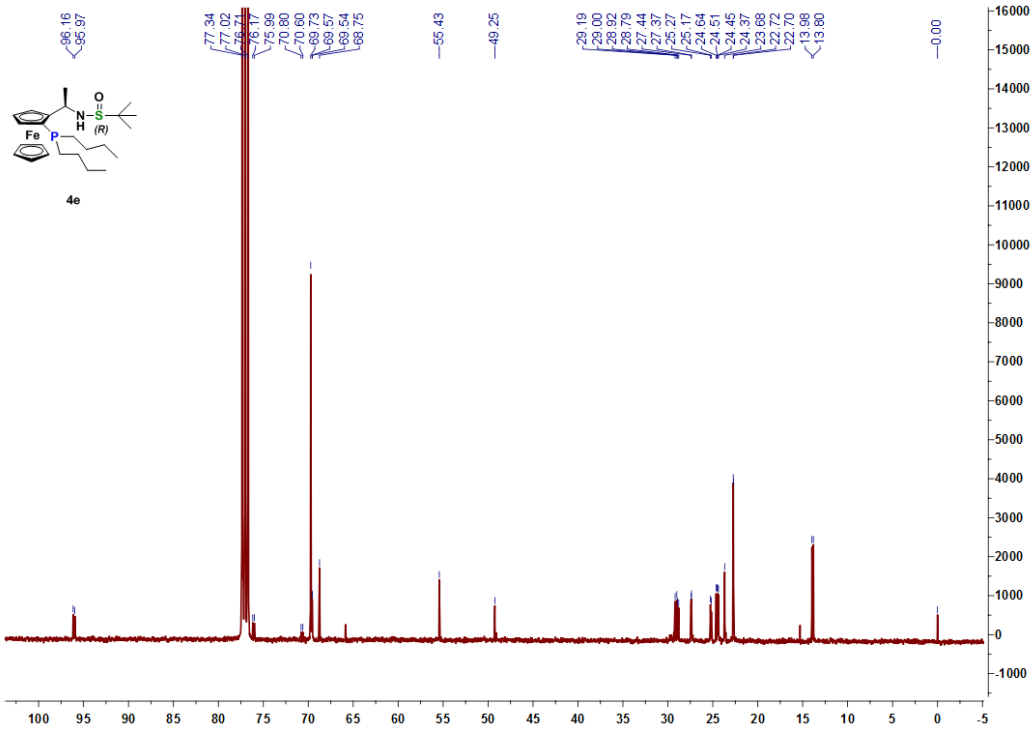

mjw-L27
mjw-3747
7.38
7.26
7.12
7.10
4.61
4.59
4.40
4.26
4.10
3.99
3.64
1.27
1.20
1.03
0.00
Fe
PAr2
N
H
O
S
(R)
Ar:
4d
f1 (ppm)

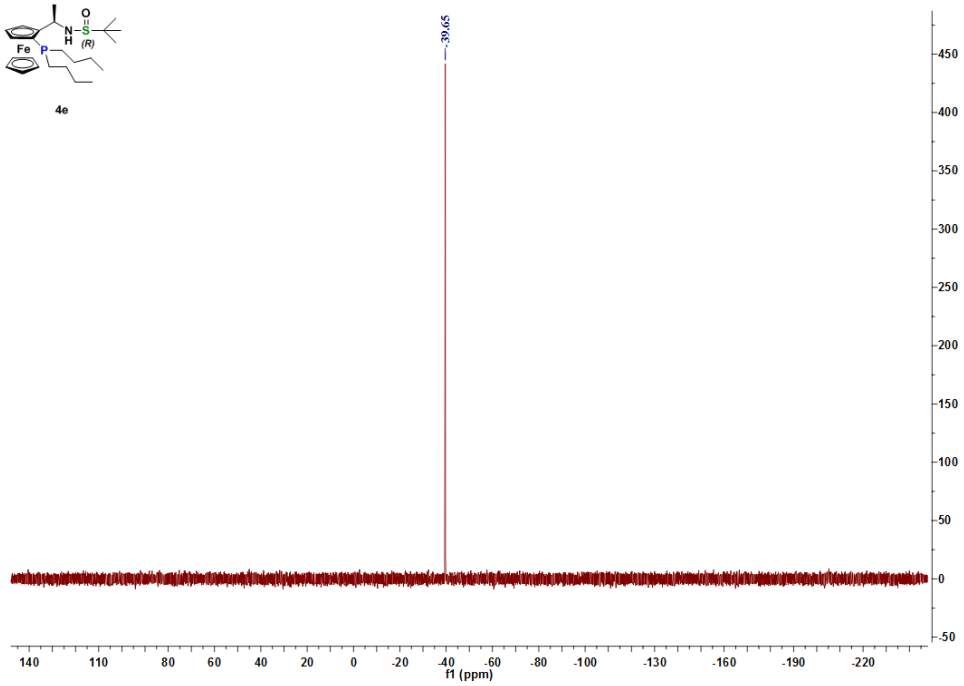

150.22
150.16
150.01
149.94
137.89
137.80
136.05
135.96
129.14
128.93
127.85
127.65
122.73
122.36
95.94
95.74
77.34
77.02
76.70
76.27
76.15
71.83
71.79
70.46
70.43
70.32
69.73
68.90
55.03
48.69
48.65
34.86
34.79
31.46
31.40
22.52
21.23
0.00
Fe
PAr2
N
H
O
S
(R)
Ar:
4d
f1 (ppm)

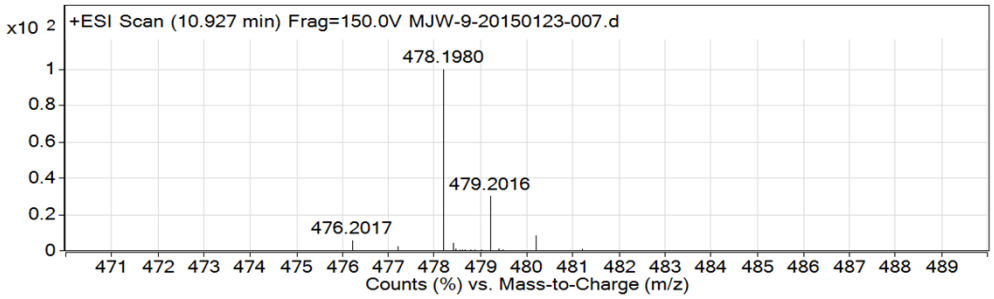

23.82
Fe
PAr2
N
H
O
S
(R)
Ar:
4d
f1 (ppm)

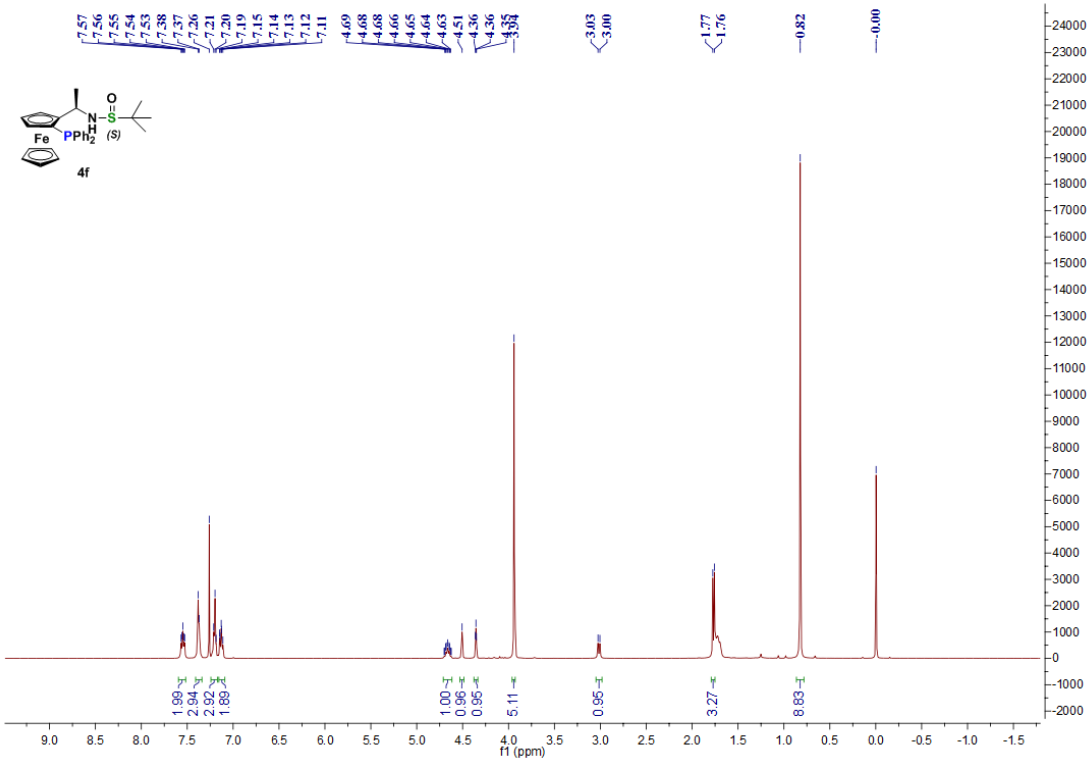

x10 2
+ESI Scan (16.078 min) Frag=130.0V MJW-3-20141224-022.d
742.3882
743.3934
740.3933
Counts (%) vs. Mass-to-Charge (m/z)

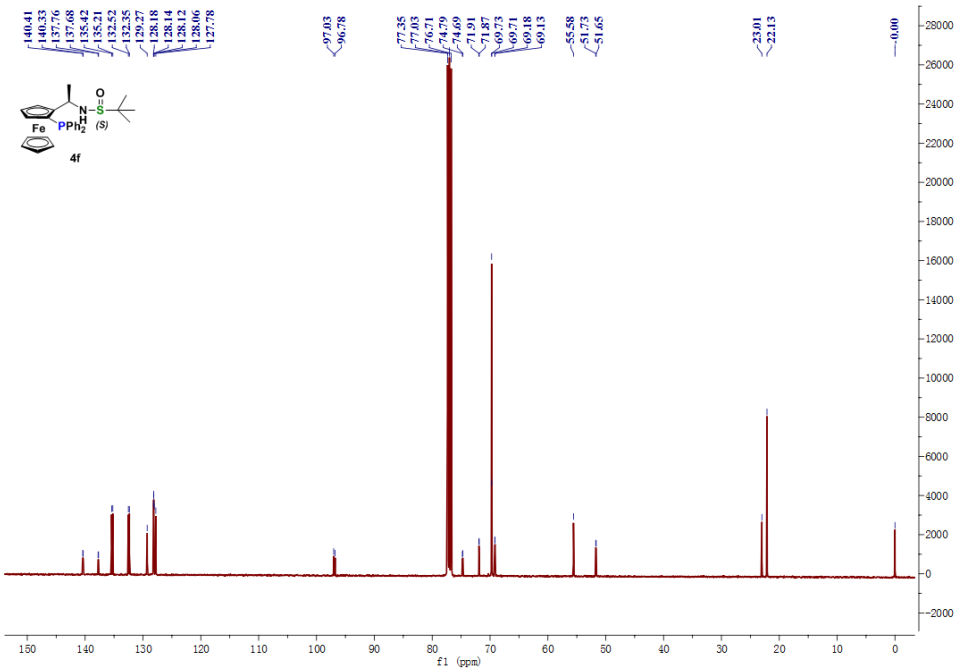

7.26
4.57
4.55
4.53
4.52
4.33
4.27
4.18
4.12
1.80
1.78
1.76
1.63
1.55
1.53
1.52
1.51
1.50
1.48
1.44
1.40
1.25
1.22
1.21
1.19
1.01
0.99
0.97
0.84
0.82
0.80
0.00
1.00
0.95
0.98
5.00
0.91
2.00
8.77
13.21
2.75
2.73
4e

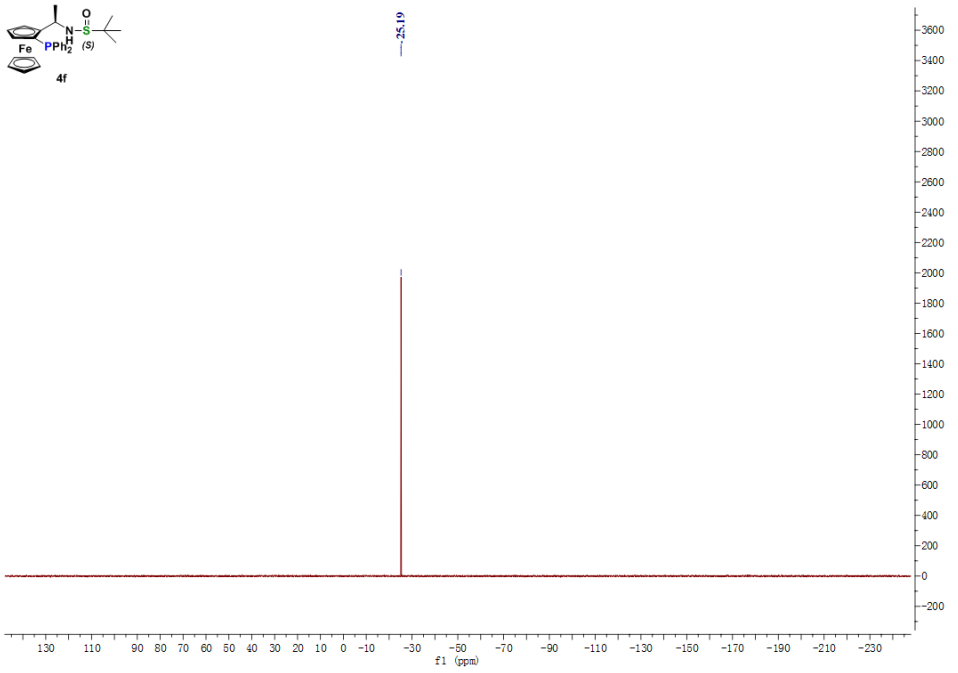

96.16
95.97
77.34
77.02
76.71
76.17
75.99
70.80
70.60
69.73
69.57
69.54
68.75
55.43
49.25
29.19
29.00
28.92
28.79
27.44
27.37
25.27
25.17
24.64
24.51
24.45
24.37
23.68
22.72
22.70
13.98
13.80
0.00
4e

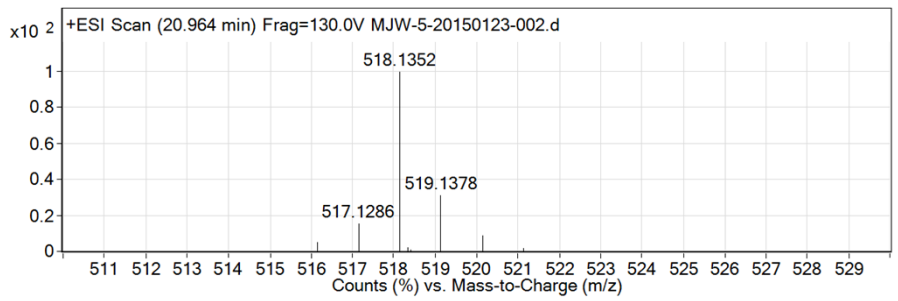

4e
39.65
f1 (ppm)

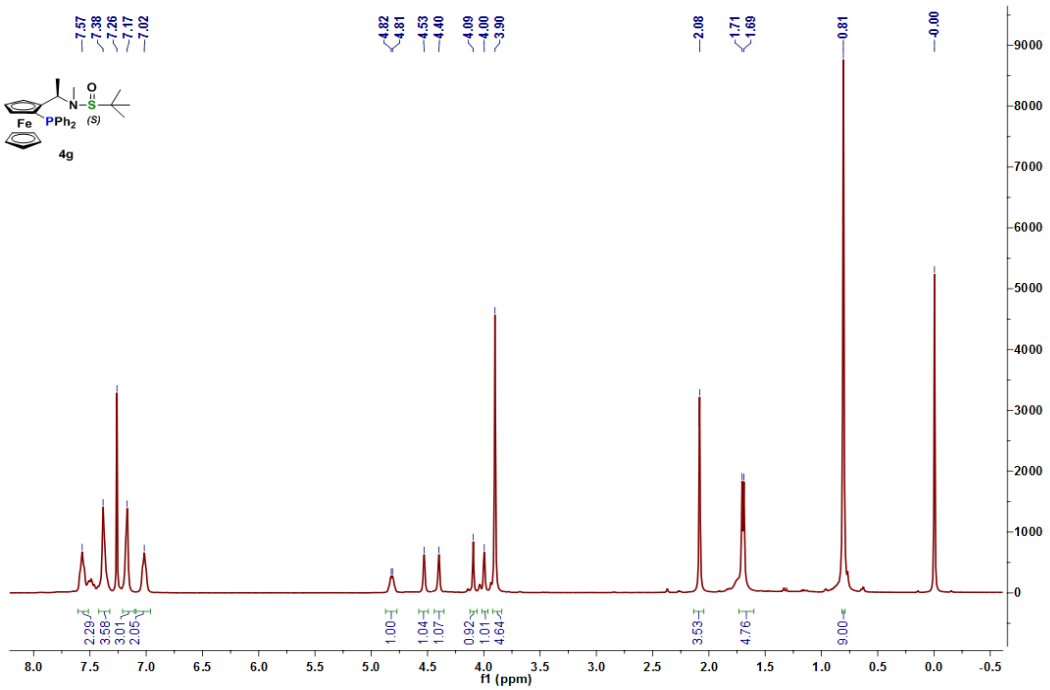

+ESI Scan (10.927 min) Frag=150.0V MJW-9-20150123-007.d
x10 2
478.1980
479.2016
476.2017
Counts (%) vs. Mass-to-Charge (m/z)

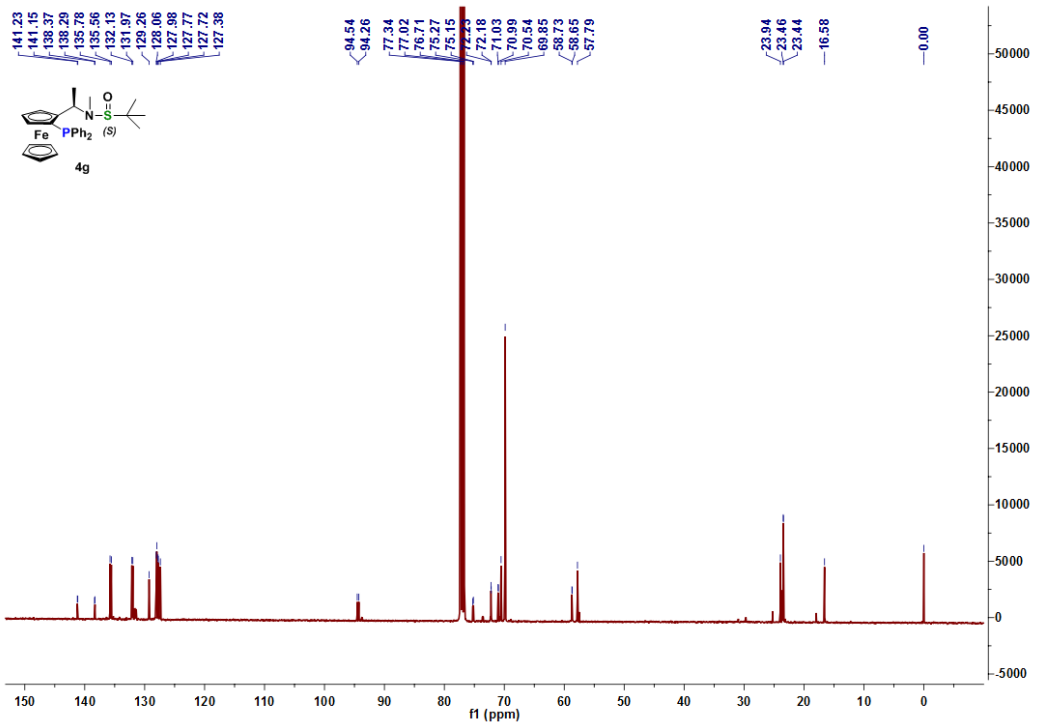

4f
f1 (ppm)

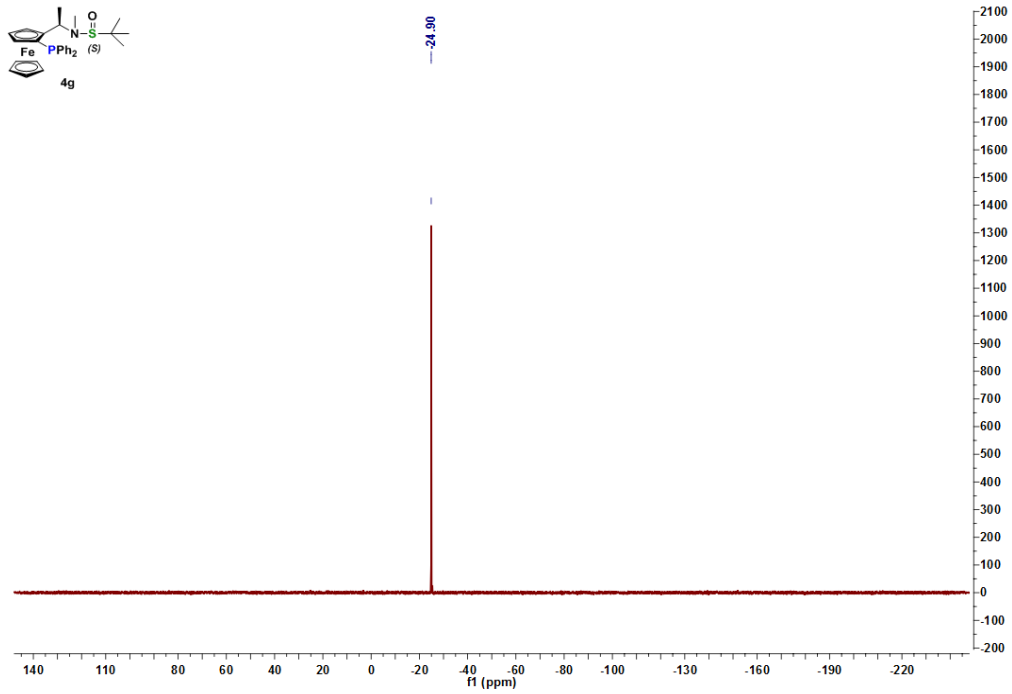

140.41
140.33
137.76
137.68
135.42
135.21
132.52
132.35
129.27
128.18
128.14
128.12
128.06
127.78
97.03
96.78
77.35
77.03
76.71
74.79
74.69
71.91
71.87
69.73
69.71
69.18
69.13
55.58
51.73
51.65
23.01
22.13
0.00
Fe
PPh2
(S)
4f
f1 (ppm)

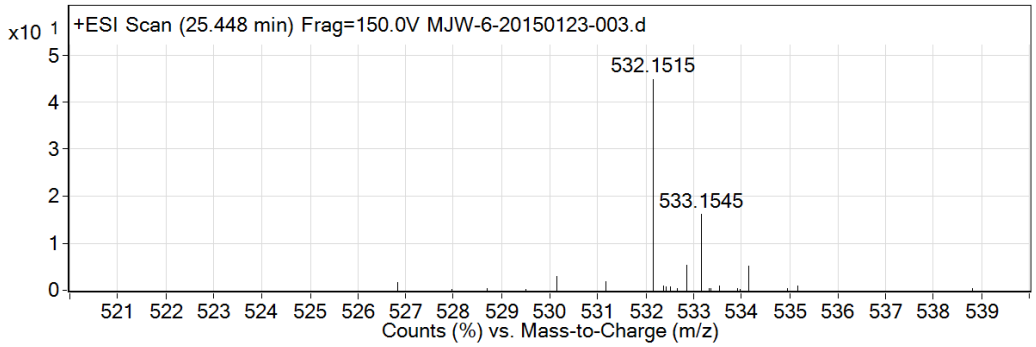

25.19
Fe
PPh2
(S)
4f
f1 (ppm)


+ESI Scan (20.964 min) Frag=130.0V MJW-5-20150123-002.d
x10 2
518.1352
519.1378
517.1286
Counts (%) vs. Mass-to-Charge (m/z)


7.57
7.38
7.26
7.17
7.02
4.82
4.81
4.53
4.40
4.09
4.00
3.90
2.08
1.71
1.69
0.81
0.00
Fe
PPh2
(S)
4g
2.29
3.58
3.01
2.05
1.00
1.04
1.07
0.92
1.01
4.64
3.53
4.76
9.00
f1 (ppm)


141.23
141.15
138.37
138.29
135.78
135.56
132.13
131.97
129.26
128.06
127.98
127.77
127.72
127.38
94.54
94.26
77.34
77.02
76.71
75.27
75.15
72.23
72.18
71.03
70.99
70.54
69.85
58.73
58.65
57.79
23.94
23.46
23.44
16.58
0.00
Fe
PPh2
(S)
4g
f1 (ppm)

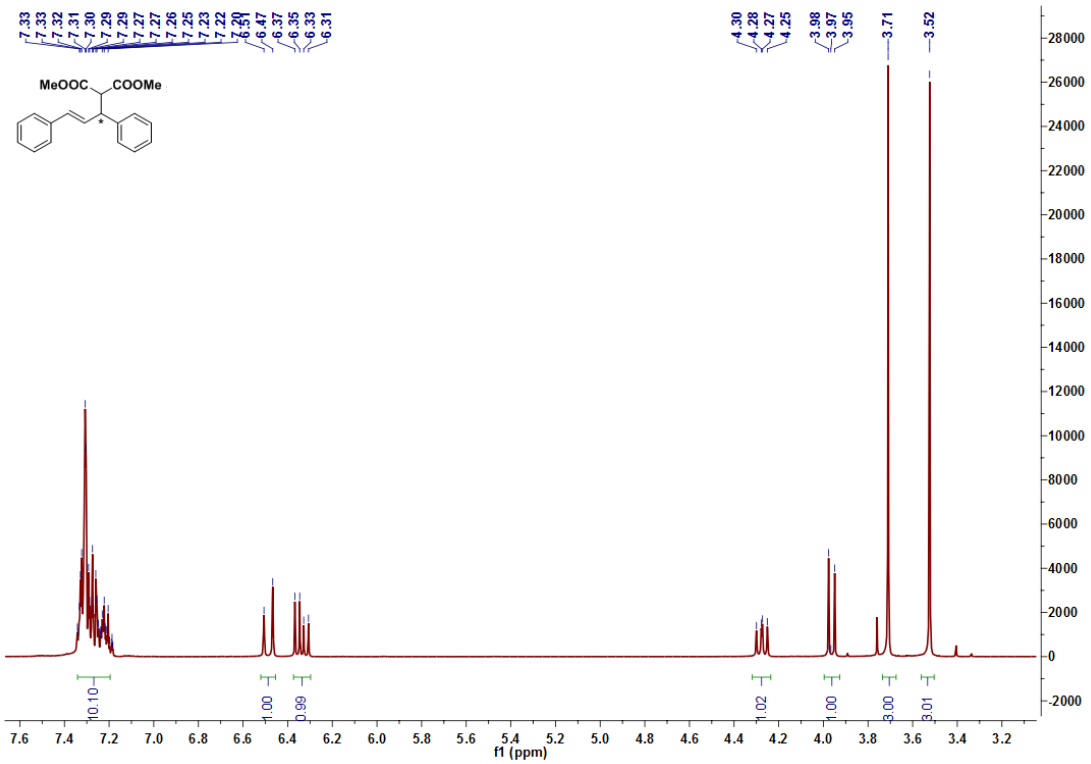


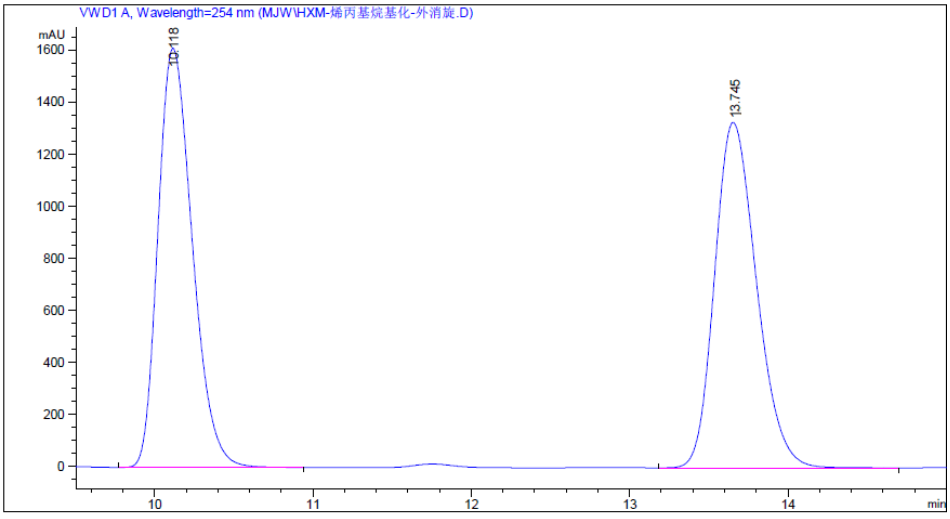


NMR spectra and HPLC analysis of products

(R,E)-dimethyl 2-(1,3-diphenylallyl)malonate (10a)

White solid; yield: 62%; ee: 89%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.20 (m, 10H), 6.51-6.47 (m, 1H), 6.37-6.31 (m, 1H), 4.30-4.25 (m, 1H), 3.98-3.95 (m, 1H), 3.71 (s, 3H),3.52 (s, 3H); HPLC (Chiralpak AD-H column, 254 nm, 80:20 hexane/isopropanol, flow =0.8mL/min) t_R = 10.1min, 13.7 min.





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面积百分比报告

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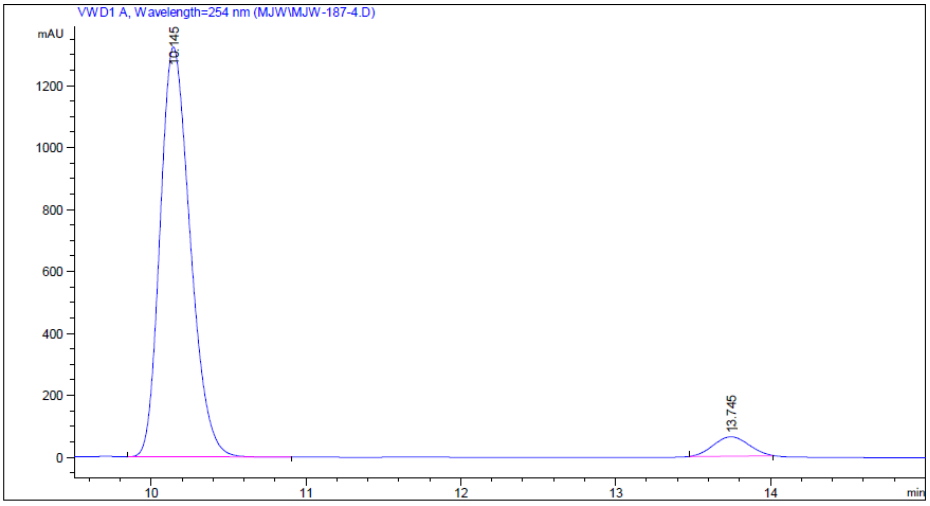
排序 : 保留时间
乘积因子 : 1.0000
稀释因子 : 1.0000
内标中不使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	信号	类型	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.118	1	BV	2.42826e4	1610.23438	49.8899
2	13.745	1	VV	2.43898e4	1326.31616	50.1101
总量 :				4.86725e4	2936.55054	



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面积百分比报告

==========

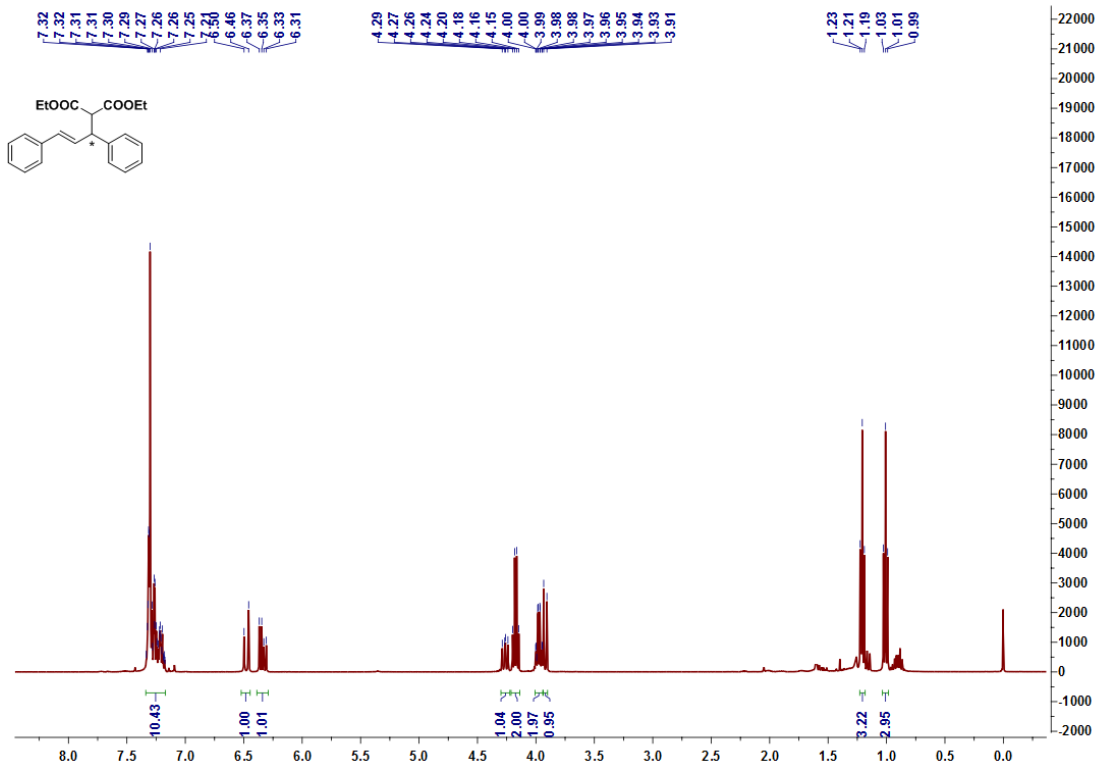
排序 : 保留时间
乘积因子 : 1.0000
稀释因子 : 1.0000
内标中不使用乘积因子和稀释因子

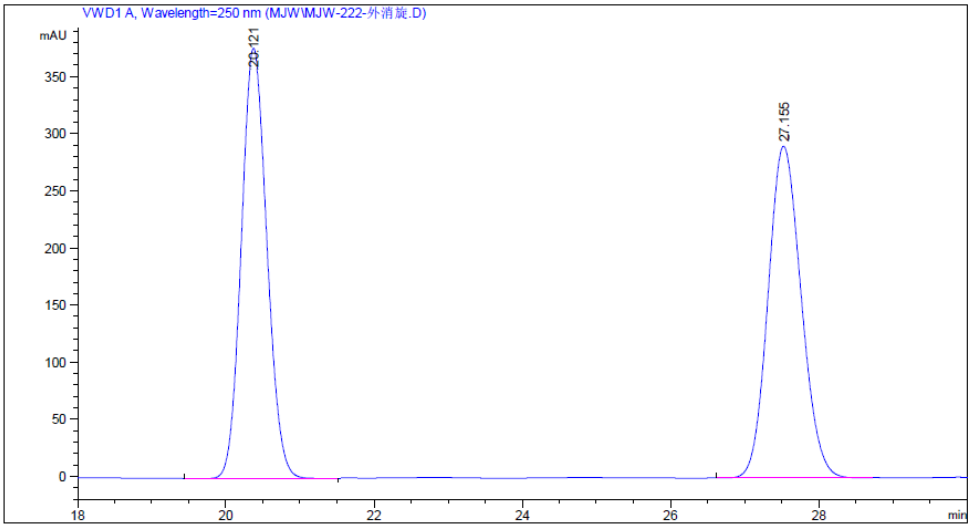
信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	信号	类型	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.145	1	BB	1.78631e4	1323.28235	94.6948
2	13.745	1	MM	1000.76367	62.90810	5.3052
总量 :				1.88638e4	1386.19045	

(*R*,*E*)-diethyl 2-(1,3-diphenylallyl)malonate (10b)

Colorless oil; yield: 65%; ee: 88%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.21 (m, 10H), 6.46 (d, *J* = 15.8 Hz, 1H), 6.33 (dd, *J* = 15.7, 8.6 Hz, 1H), 4.27 (t, *J* = 9.6 Hz, 1H), 4.20-4.15 (m, 2H), 3.95 (m, 3H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.01 (t, *J*= 7.1 Hz, 3H); HPLC (Chiralpak AD-H column, 250 nm, 93:7 hexane/isopropanol, flow =1mL/min) t_R = 20.1 min, 27.1 min.





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面积百分比报告

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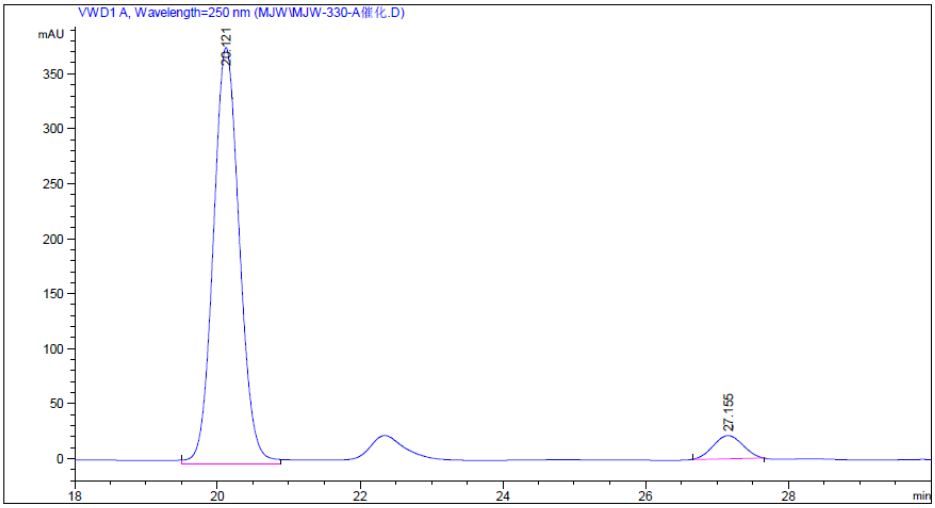
排序 : 保留时间
乘积因子 : 1.0000
稀释因子 : 1.0000
内标中不使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=250 nm

峰 #	保留时间 [min]	信号	类型	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.121	1	BV	1.64238e4	631.17773	49.9619
2	27.155	1	BBA	1.64488e4	489.20831	50.0381

总量 : 1.01759e4 399.59596



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面积百分比报告

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排序 : 保留时间
乘积因子 : 1.0000
稀释因子 : 1.0000
内标中不使用乘积因子和稀释因子

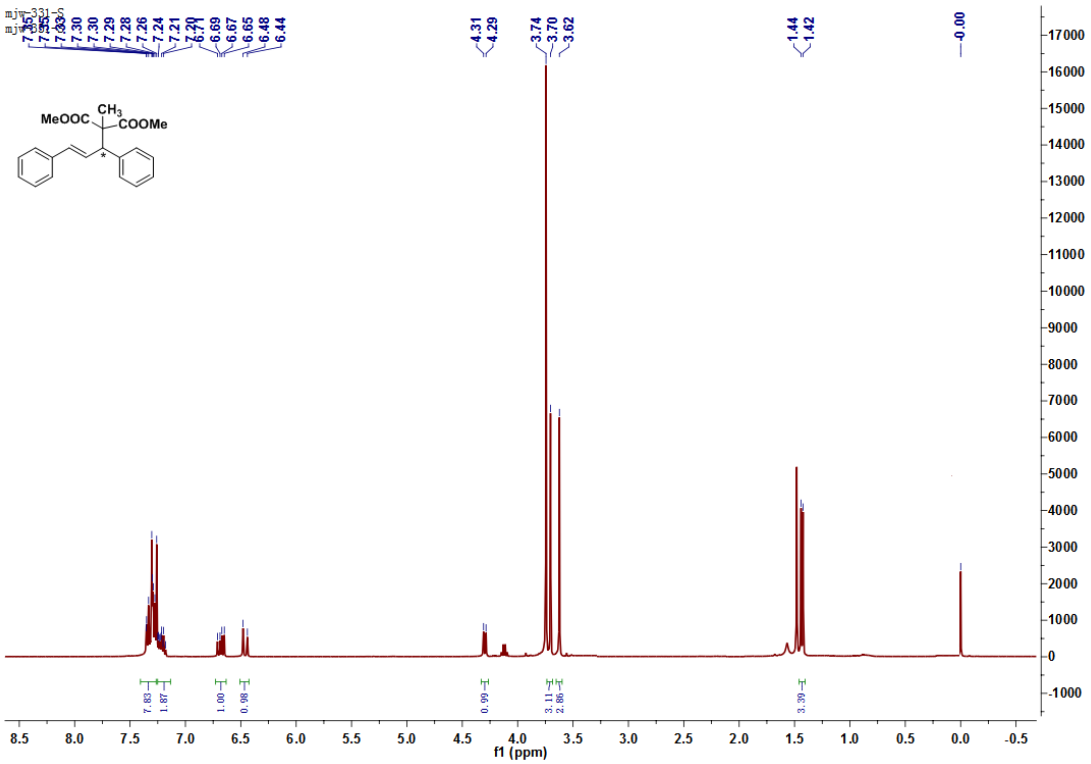
信号 1: VWD1 A, Wavelength=250 nm

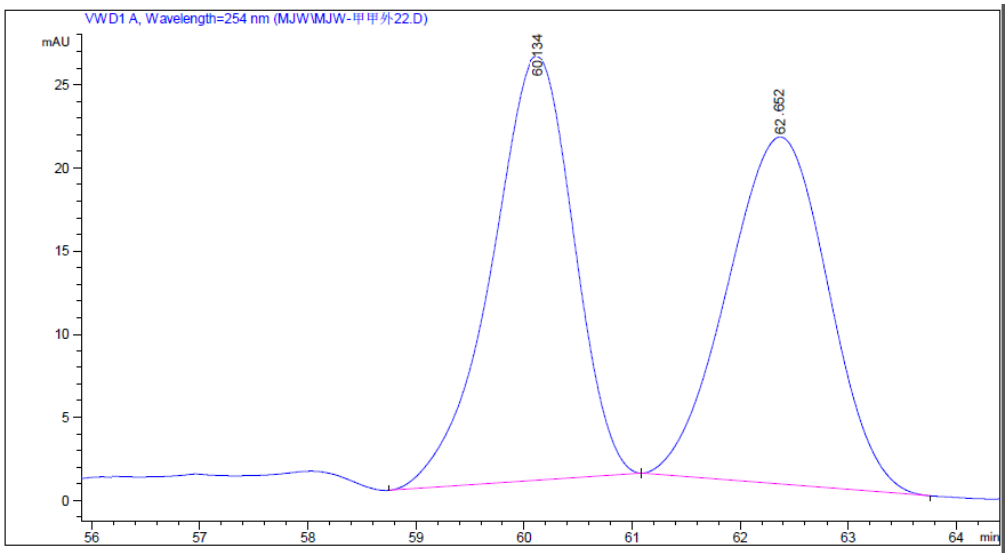
峰 #	保留时间 [min]	信号	类型	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.121	1	MM	9570.53320	378.46024	94.0508
2	27.155	1	MM	605.39026	21.13572	5.9492

总量 : 1.01759e4 399.59596

(*R*,*E*)-dimethyl 2-(1,3-diphenylallyl) -2-methyl-malonate (10c)

Colorless oil; yield: 55%; ee: 76%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.28 (m, 8H), 7.24-7.20 (m, 2H), 6.68 (dd, *J* = 15.7, 9.0 Hz, 1H), 6.46 (d, *J* = 15.7 Hz, 1H), 4.30 (d, *J* = 9.0 Hz, 1H), 3.74 (s, 3H), 3.62 (s, 3H), 1.43 (d, J = 7.3 Hz, 3H); HPLC (Chiralpak AD-H + AD-H column, 254 nm, 99:1 hexane/isopropanol, flow =0.5 mL/min) t_R = 60.1min, 62.7 min.





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面积百分比报告

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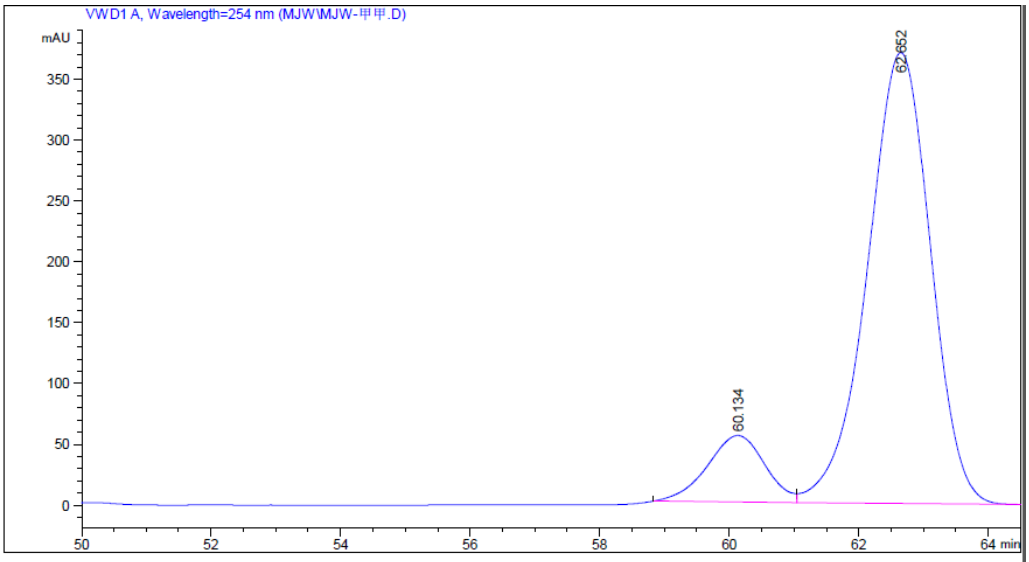
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	60.134	BB	0.9400	1575.77173	25.49616	49.8155
2	62.652	BB	1.1835	1587.44519	20.86811	50.1845



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面积百分比报告

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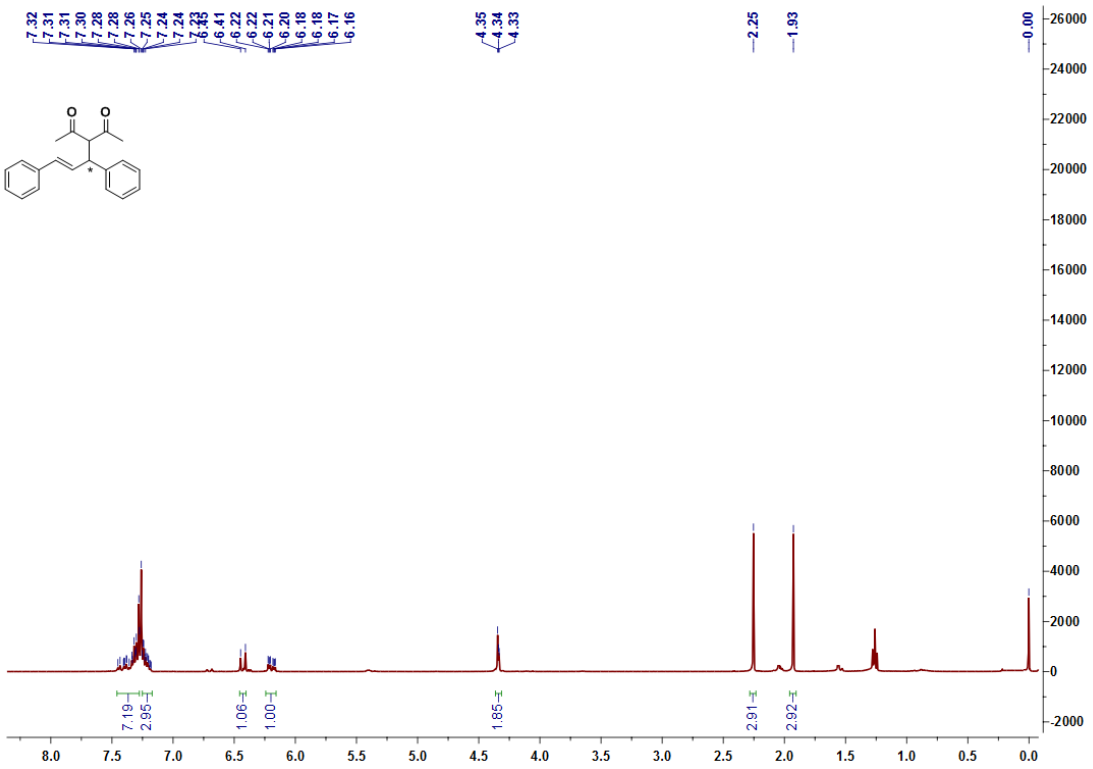
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

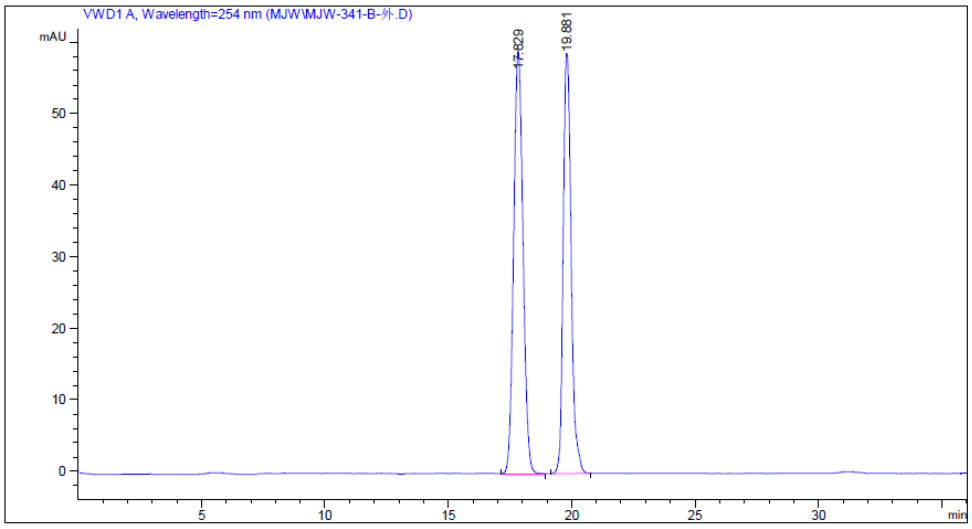
信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	60.134	BV	0.9169	3368.10791	54.50529	11.8504
2	62.652	VBA	1.0503	2.50538e4	370.34085	88.1496

(*R*,*E*)-3-(1,3-diphenylallyl)pentane-2,4-dione (10d)

Colorless oil; yield: 41%; ee: 29%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.23 (m, 10H), 6.44 (d, *J* = 16 Hz, 1H), 6.19 (ddd, *J* = 15.8, 5.1, 2.9 Hz, 1H), 4.35-4.33 (m, 2H), 2.25 (s, 3H), 1.93 (s, 3H); HPLC (Chiralpak AD-H column, 254 nm, 99:1 hexane/isopropanol, flow =0.5 mL/min) t_R = 17.8min, 19.9 min.





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面积百分比报告

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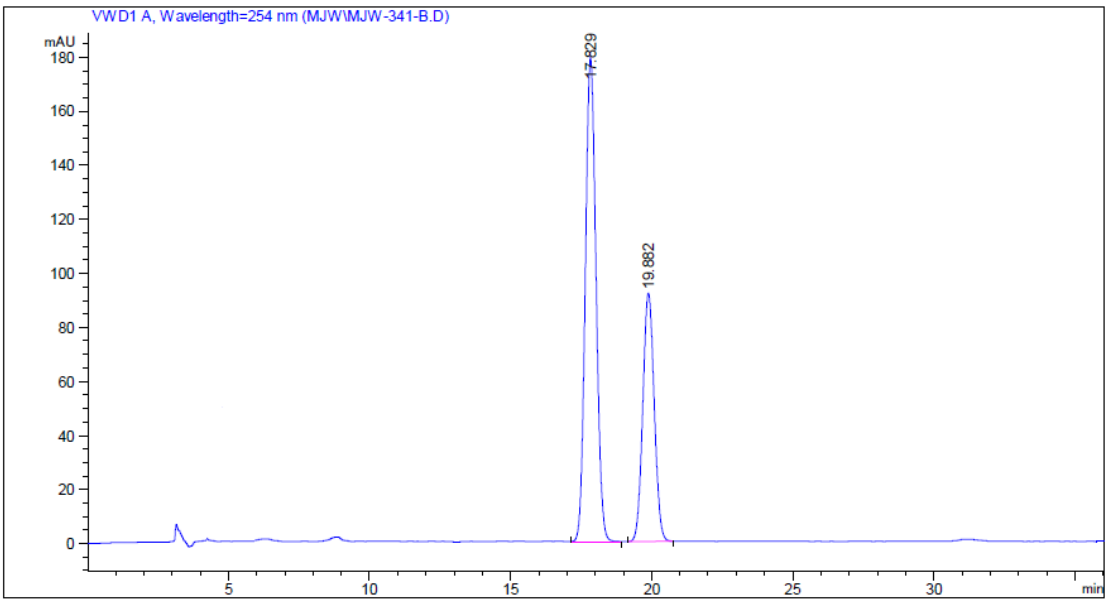
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.829	BB	0.4118	4997.05322	59.53874	50.0110
2	19.881	BB	0.4105	4994.86475	58.97426	49.9890



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面积百分比报告

==========

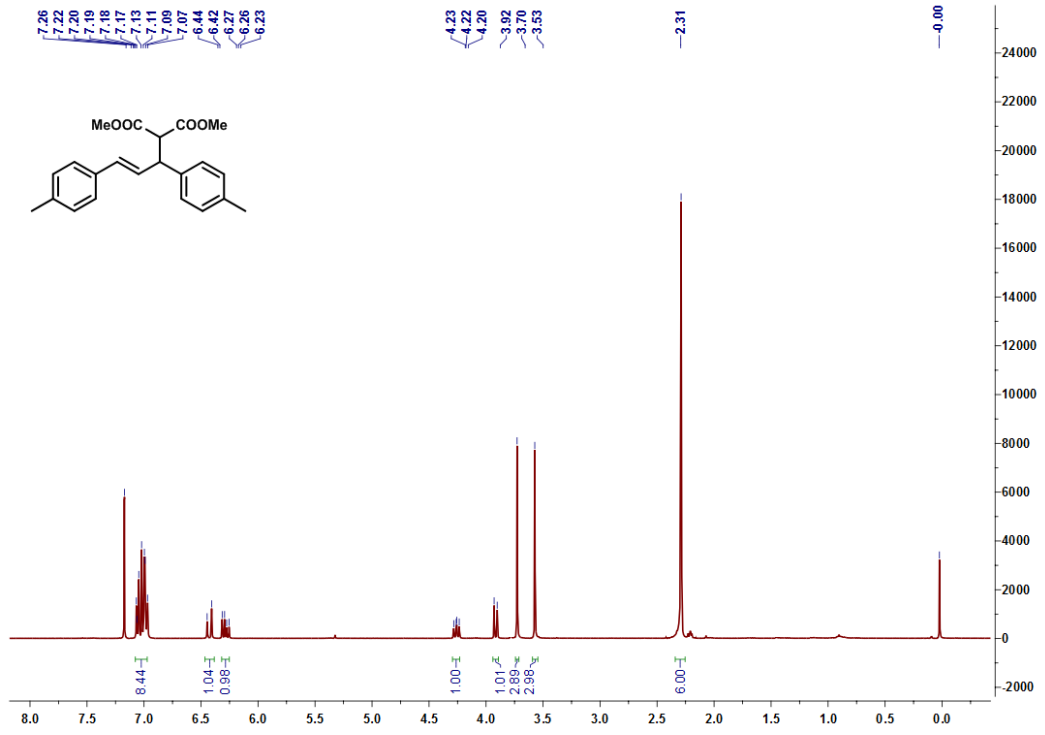
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

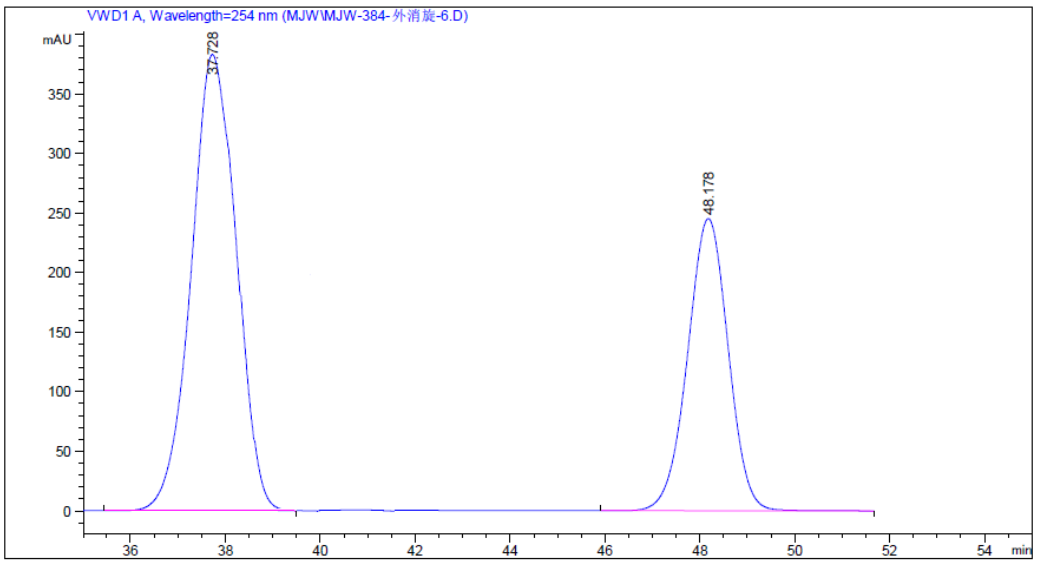
信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.829	BB	0.4118	4711.36035	179.13857	64.5788
2	19.882	BB	0.4390	2584.16284	91.91933	35.4212

(*R*,*E*)-dimethyl 2-(1,3-dip-tolylallyl)malonate (10e)

Colorless oil; yield: 55%; ee: 62%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.07 (m, 8H), 6.42 (d, *J* = 15.7 Hz, 1H), 6.25 (dd, *J* = 15.7, 8.7 Hz, 1H), 4.22 (dd, *J* = 10.7, 8.8 Hz, 1H), 3.92 (d, *J* = 10.9 Hz, 1H), 3.70 (s, 3H), 3.53 (s, 3H), 2.31 (s, 6H); HPLC (Chiralpak AD-H column, 254 nm, 94:6 hexane/isopropanol, flow =0.5 mL/min) t_R = 37.8min, 48.4min.





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面积百分比报告

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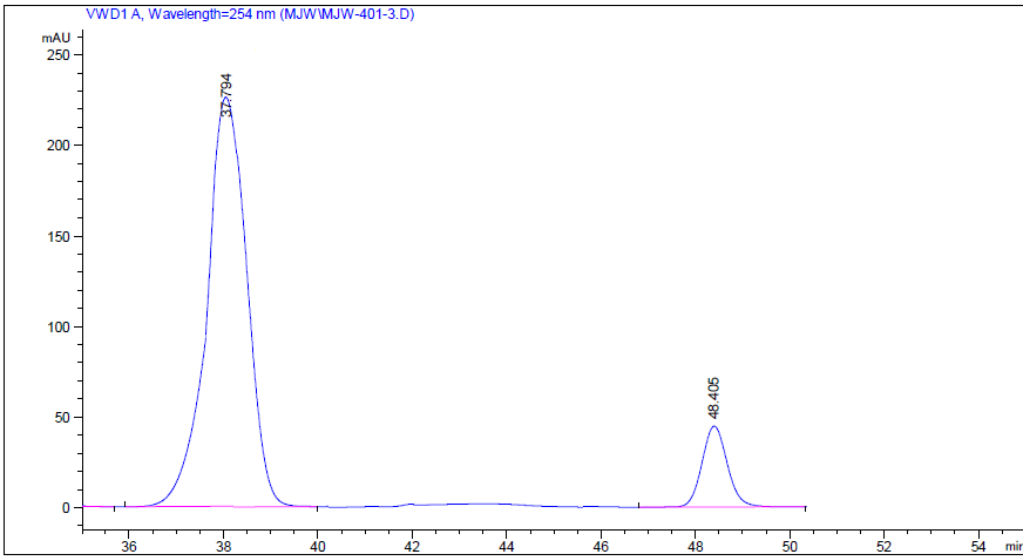
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	37.728	BV	0.8409	1.48487e4	382.93793	50.4286
2	48.178	BBA	0.9184	1.45963e4	245.23520	49.5714



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面积百分比报告

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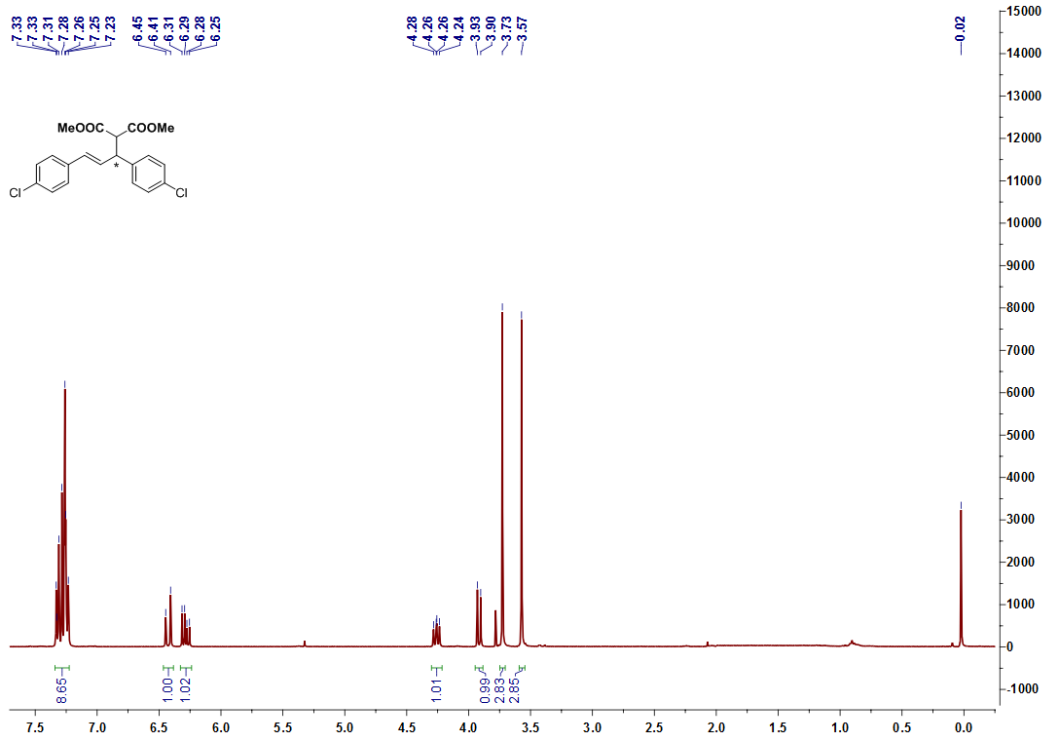
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

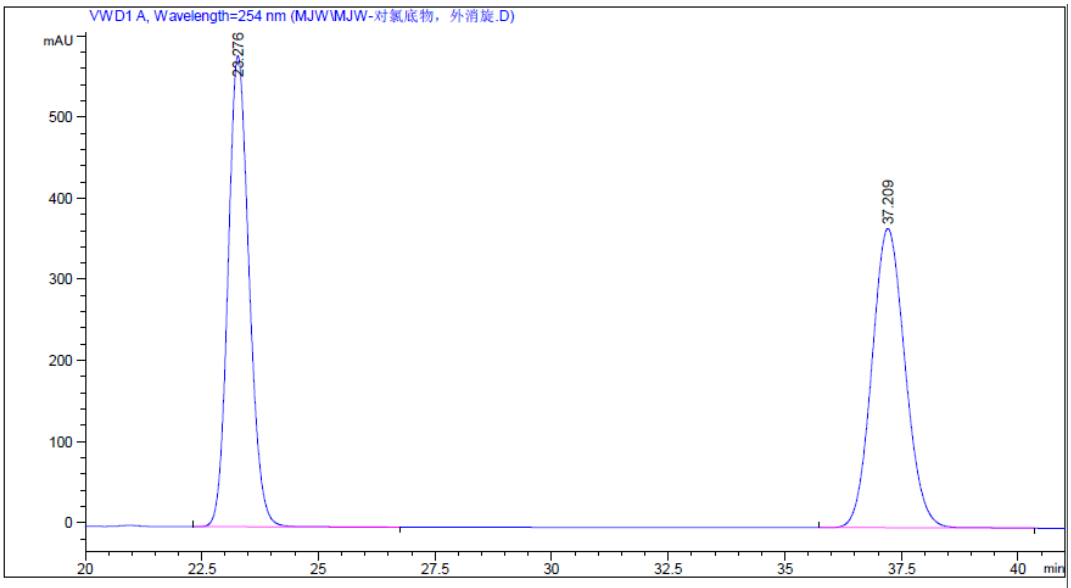
信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	37.794	BV	0.8509	5981.40030	237.23520	81.0049
2	48.405	BBA	0.7746	1402.59953	73.18202	18.9951

(*R*,*E*)-dimethyl 2-(1,3-bis(4-chlorophenyl)allyl)malonate (10f)

Colorless oil; yield =59%; ee = 78%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.23 (m,8H), 6.43 (d, *J* = 15.8 Hz, 1H), 6.28 (dd, *J* = 15.7, 8.5 Hz, 1H), 4.26 (dd, *J* = 10.7, 8.6 Hz, 1H), 3.92 (d, *J* = 10.8 Hz, 1H), 3.73 (s, 3H), 3.57 (s, 3H). (Chiralpak AD-H column, 254 nm, 85:15 hexane/isopropanol, flow =0.8 mL/min) t_R = 23.1min, 37.0 min.





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面积百分比报告

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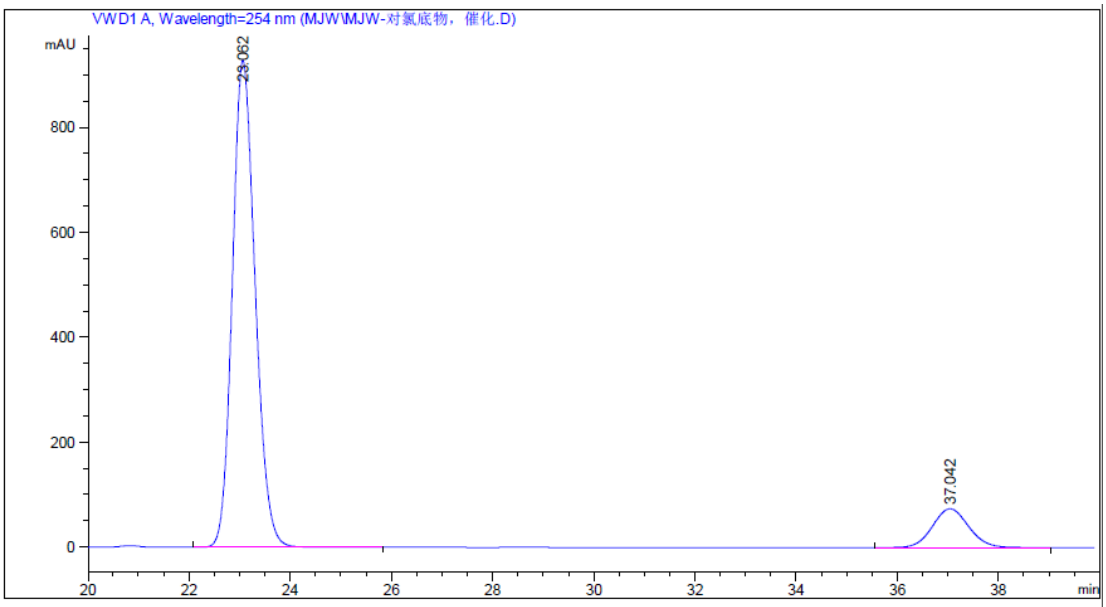
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.276	BB	0.4852	1.82190e4	580.44214	50.0461
2	37.209	BB	0.7662	1.81854e4	368.83459	49.9539



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面积百分比报告

==========

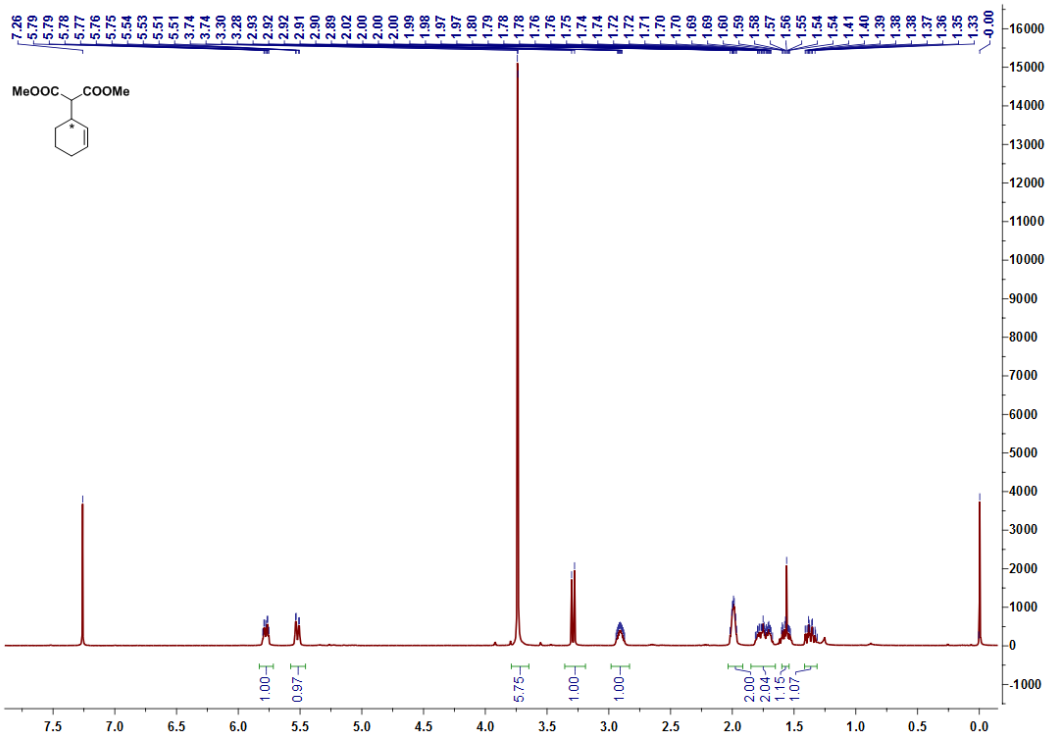
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

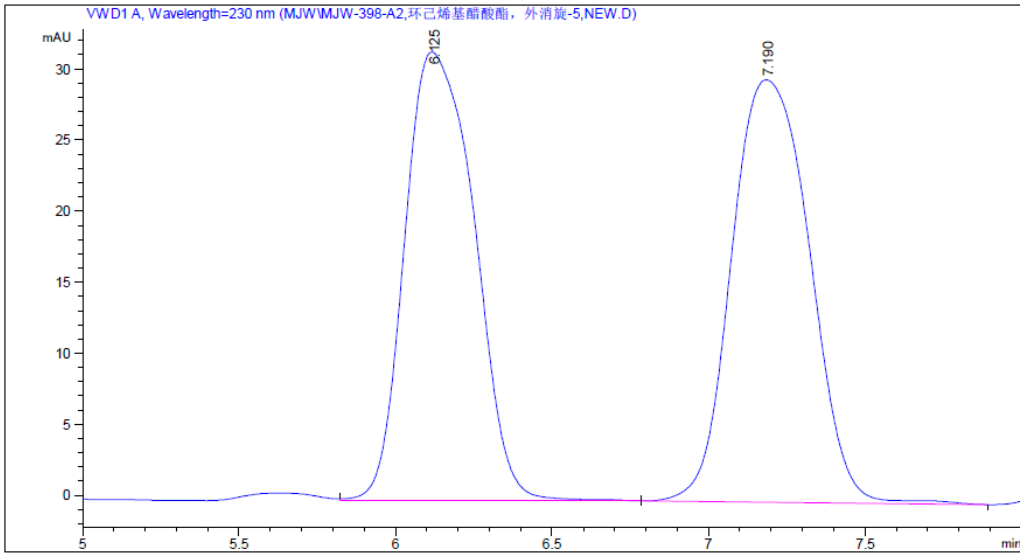
信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.062	BB	0.4827	2.90311e4	928.73175	88.8806
2	37.042	BB	0.7682	3631.92163	73.53185	11.1194

(*R*)-dimethyl 2-(cyclohex-2-en-1-yl)malonate (12)

Colorless oil; yield =51%; ee = 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.78 (ddd, *J* = 9.7, 5.9, 3.6 Hz, 1H), 5.52 (dd, *J* = 10.2, 2.0 Hz, 1H), 3.74 (d, *J* = 1.6 Hz, 6H), 3.29 (d, *J* = 9.5 Hz, 1H), 2.98-2.83 (m, 1H), 1.99 (qd, *J* = 7.3, 4.2 Hz, 2H), 1.85-1.65 (m, 2H), 1.60-1.54 (m, 1H), 1.41-1.33 (m, 1H); (Chiralpak AS-H column, 230 nm,95:5 hexane/isopropanol, flow =1.0 mL/min) t_R = 6.1min, 7.1 min.





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面积百分比报告

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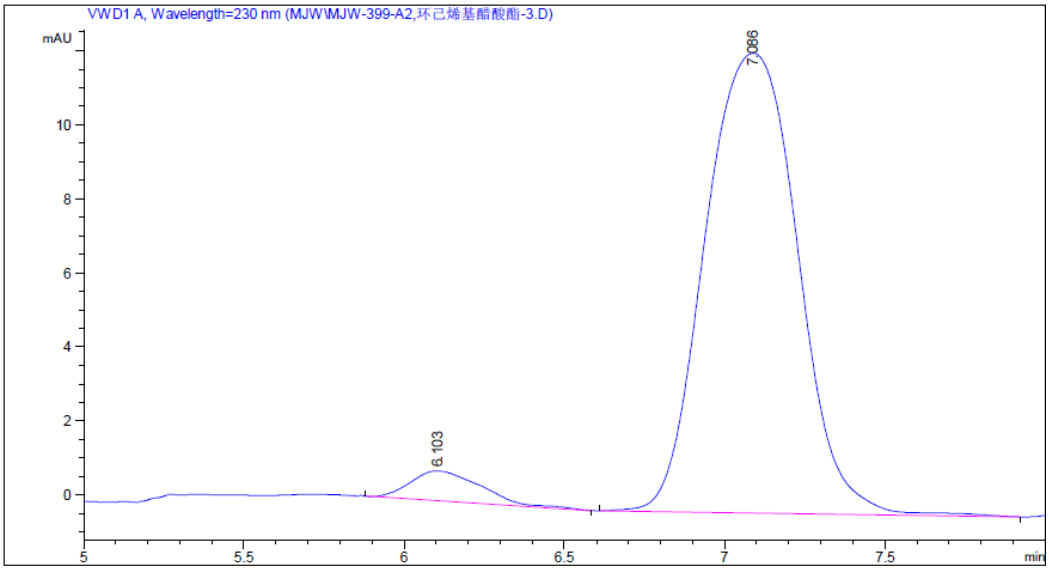
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=230 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.125	VB	0.2530	489.27914	31.53961	48.7146
2	7.190	BB	0.2823	515.10028	29.70126	51.2854



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面积百分比报告

==========

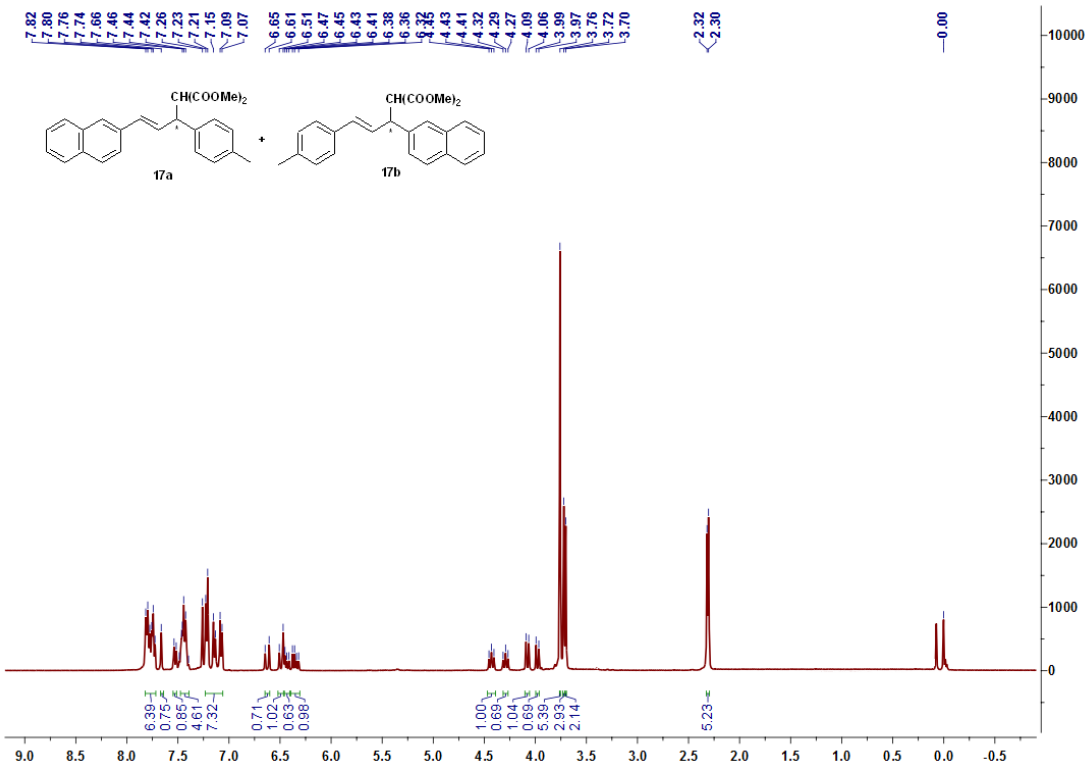
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

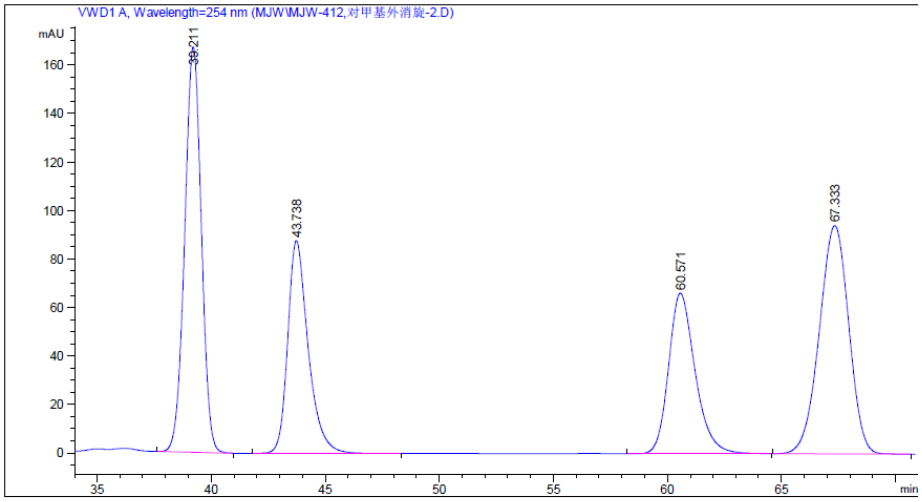
信号 1: VWD1 A, Wavelength=230 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.103	MM	0.2569	12.29001	7.97349e-1	4.7012
2	7.086	BB	0.3224	249.13376	12.40039	95.2988

(*R*,*E*)-dimethyl 2-(1-(naphthalen-2-yl)-3-(p-tolyl)allyl)malonate (14a) and (*R*,*E*)-dimethyl 2-(3-(naphthalen-2-yl)-1-(p-tolyl)allyl)malonate (14b)

Colorless oil; yield = 65%; **14a**:**14b** = 41:59 and 87%/70% ee; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.07 (m, 20H, 17a+17b), 6.63 (d, *J* = 16 Hz, 1H, 17a), 6.51-6.32 (m, 3H, 17a+17b), 4.43 (t, 1H, 17b), 4.29 (t, 1H, 17a), 4.08 (d, *J* = 12 Hz, 1H, 17b), 3.98 (d, *J* = 12 Hz, 1H, 17a), 3.76-3.70 (m, 12H, 17a+17b), 2.32-2.30 (m, 6H, 17a+17b); (Chiralpak AD-H column, 254 nm, 94:6 hexane/isopropanol, flow =0.5 mL/min) 17a: t_R = 43.7 min, 61.2 min; 17b: t_R = 39.4 min, 67.9 min.





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面积百分比报告

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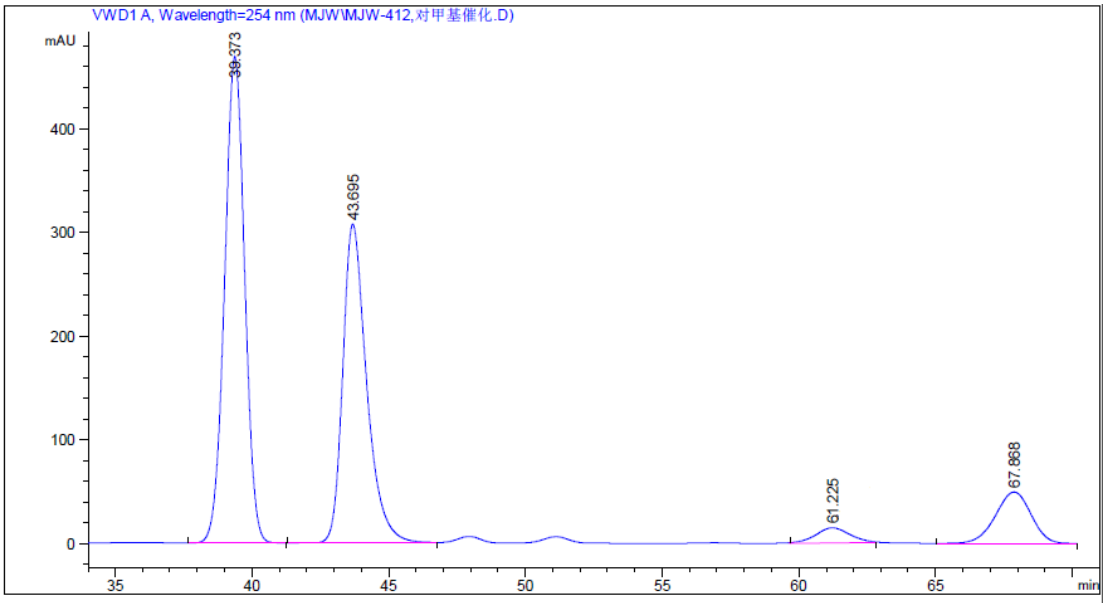
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	39.211	BB	0.8001	8469.91406	166.88069	30.5642
2	43.738	BB	0.9514	5456.64502	87.51402	19.6906
3	60.571	BB	1.2330	5360.91504	66.18493	19.3452
4	67.333	BBA	1.4133	8424.42090	94.02234	30.4000



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面积百分比报告

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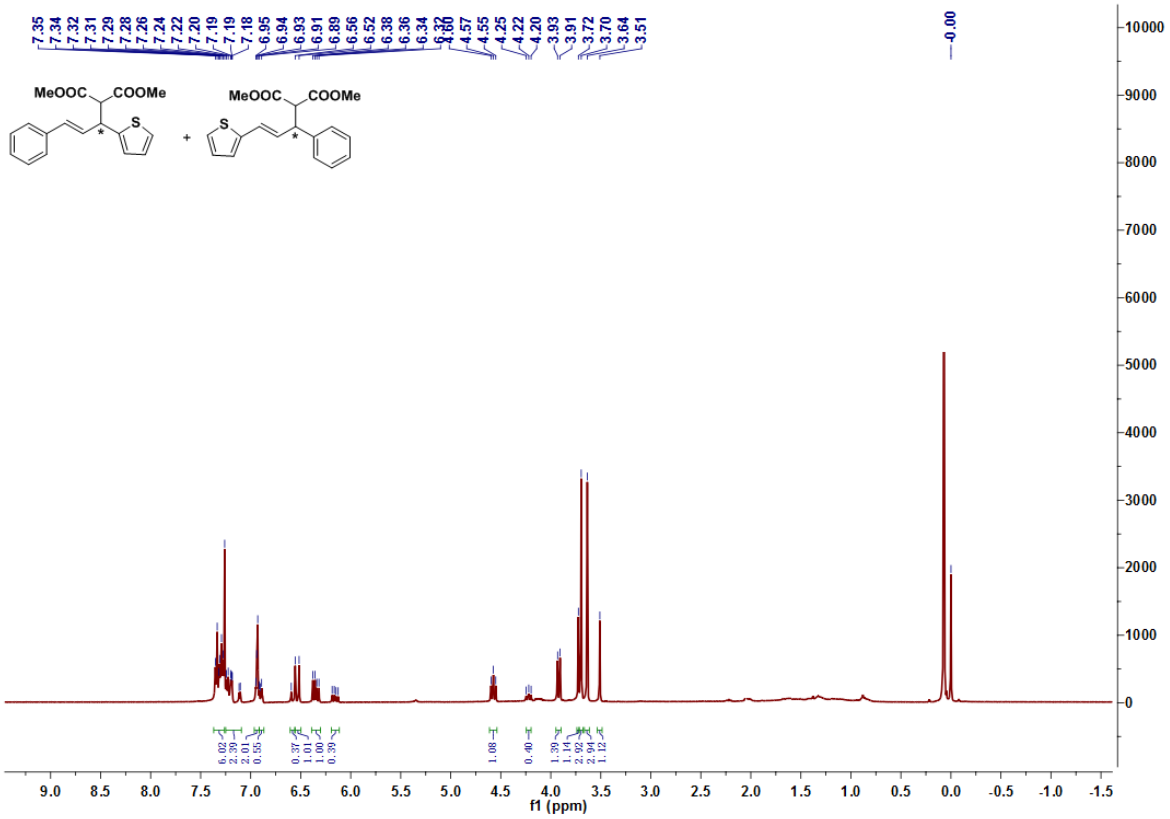
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

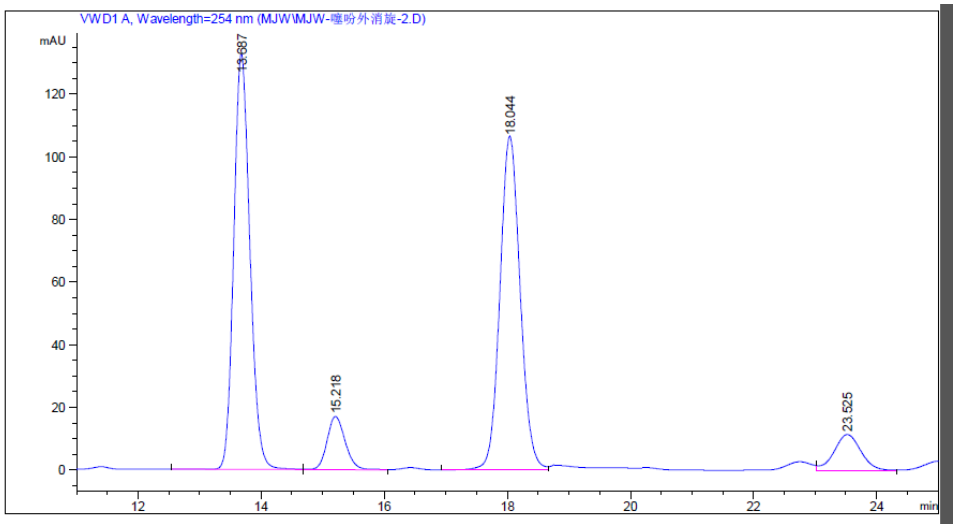
信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	39.373	BB	0.8030	2.39089e4	468.82605	49.4811
2	43.695	BV	0.9176	1.86894e4	307.26947	38.6790
3	61.225	MM	1.4390	1255.51611	14.54173	2.5984
4	67.868	VBA	1.4212	4465.45264	49.46382	9.2415

(*R*,*E*)-dimethyl 2-(1-phenyl-3-(thiophen-2-yl)allyl)malonate (16a) and (*R*,*E*)-dimethyl 2-(3-phenyl-1-(thiophen-2-yl)allyl)malonate (16b)

Colorless oil; yield = 60%; **16a**:**16b** = 28:72 and 89%/62% ee; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.18 (m, 12H, 19a+19b), 6.95 (m, 1H, 19a), 6.56 (m, 1H, 19b), 6.38 (m, 1H, 19b), 6.34 (m, 1H, 19a), 4.57 (t, 1H, 19b), 4.22 (t, 1H, 19a), 3.93 (d, J = 8 Hz, 2H, 19a+19b), 3.72-3.51 (m, 8H, 19a+19b); (Chiralpak AD-H column, 254 nm, 90:10 hexane/isopropanol, flow =0.8 mL/min) 19a: t_R = 15.1 min, 23.6 min; 19b: t_R = 13.6 min, 18.1 min.





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面积百分比报告

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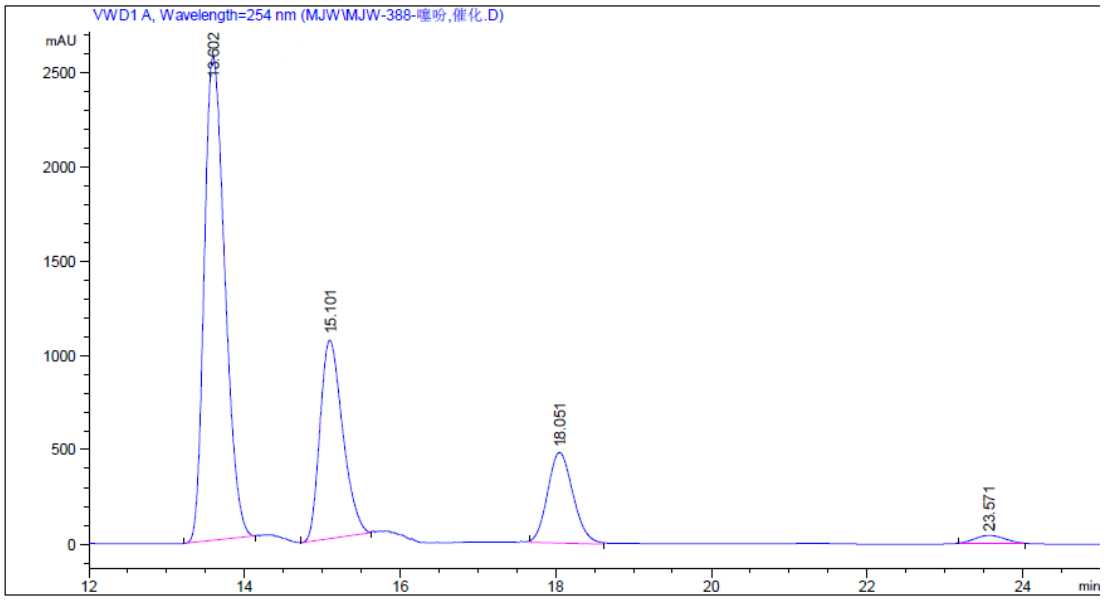
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.687	BV	0.2944	2419.82568	131.69771	43.6490
2	15.218	VV	0.3378	347.68283	16.77871	6.2715
3	18.044	BV	0.3806	2434.70313	105.77067	43.9173
4	23.525	VV	0.4798	341.62253	11.32827	6.1622



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面积百分比报告

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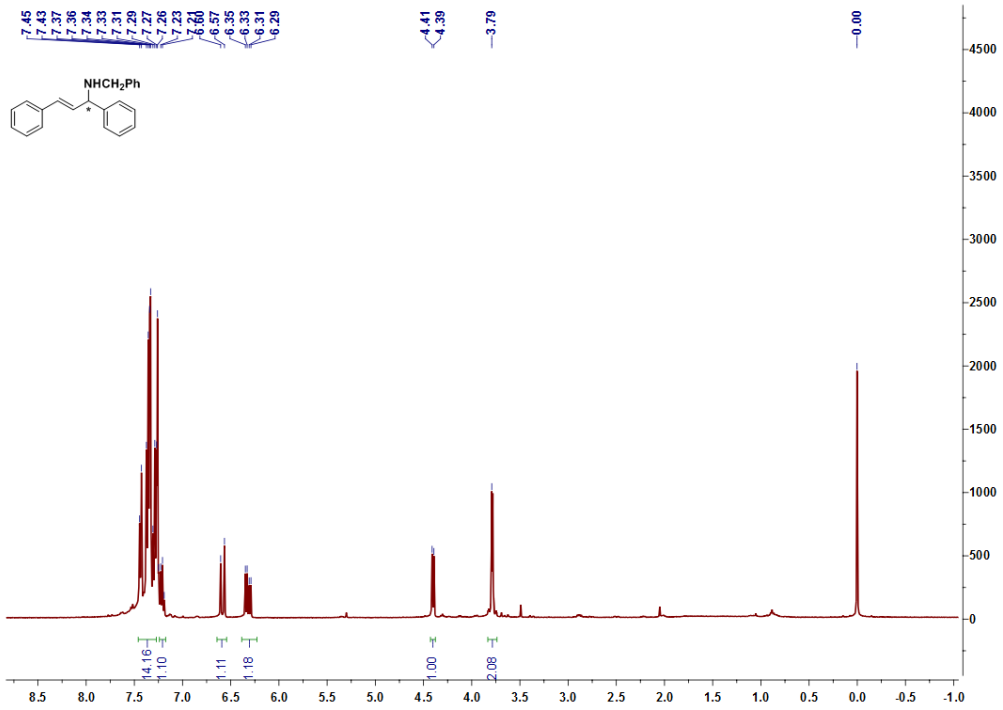
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

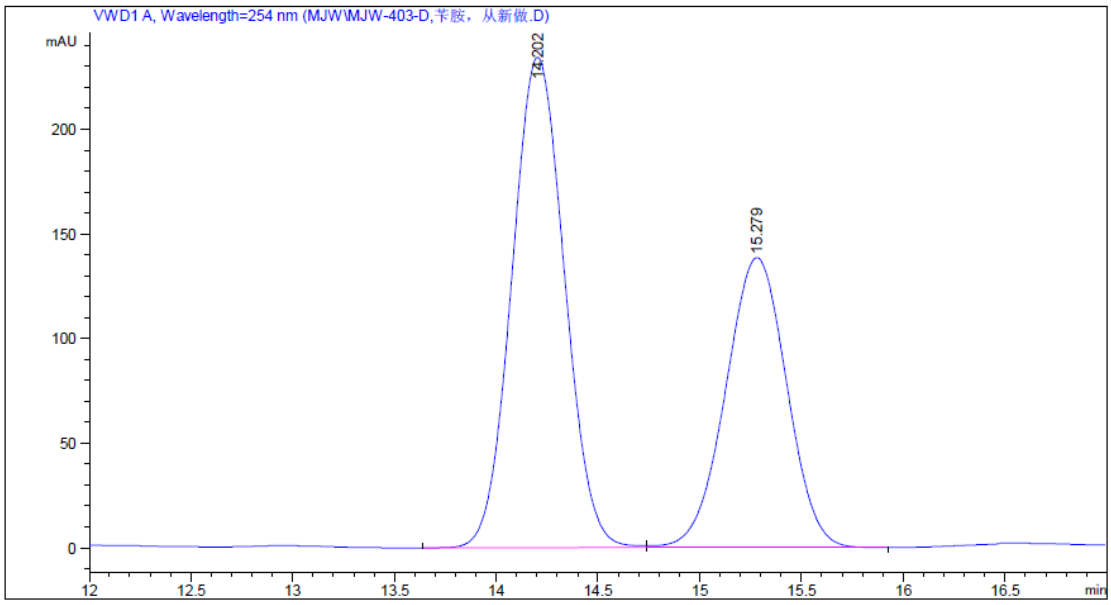
信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.602	MM	0.3047	4.71931e4	2581.50293	58.5100
2	15.101	MM	0.3352	2.13265e4	1060.42212	26.4406
3	18.051	MM	0.3775	1.09333e4	482.71359	13.5551
4	23.571	MM	0.4554	1205.33447	44.11488	1.4944

(*R*,*E*)-*N*-Benzyl-1,3-diphenylprop-2-en-1-amine (18a)

Yellow oil; yield: 45%; ee: 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45-7.21 (m, 15H), 6.58 (d, *J* = 15.9 Hz, 1H), 6.32 (dd, *J* = 15.8, 7.4 Hz, 1H), 4.40 (d, *J* = 7.4 Hz, 1H), 3.80 (s, 2H); HPLC (Chiralpak AD-H column, 254 nm, 90:10 hexane/isopropanol, flow =0.5mL/min) t_R = 14.7min, 15.8min.





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面积百分比报告

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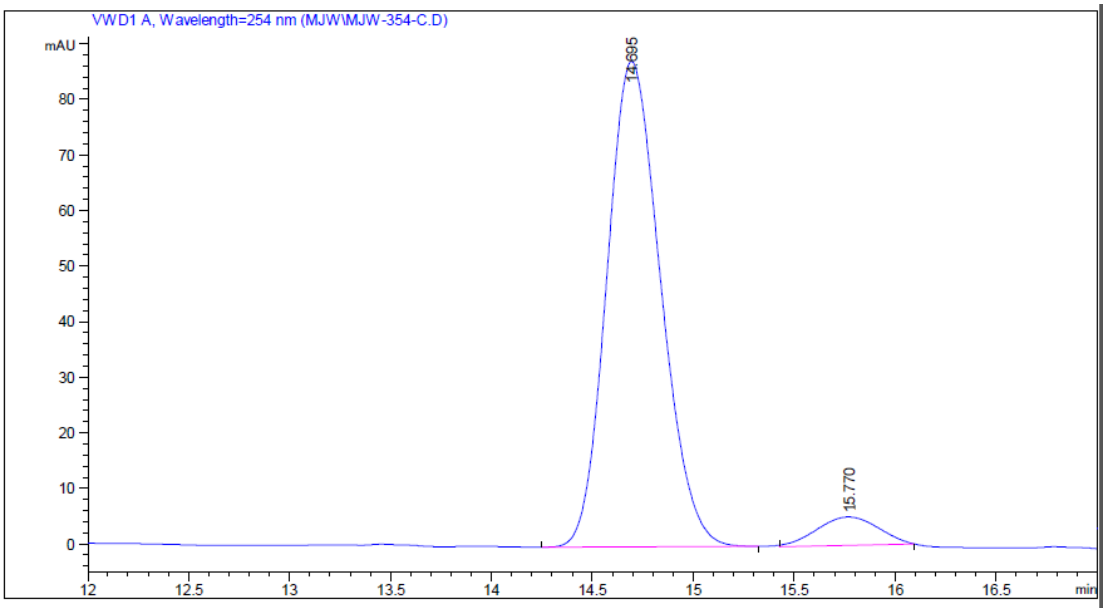
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.202	BV	0.2828	4215.23877	234.45152	59.2905
2	15.279	VB	0.3266	2894.22461	138.61351	40.7095



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面积百分比报告

==========

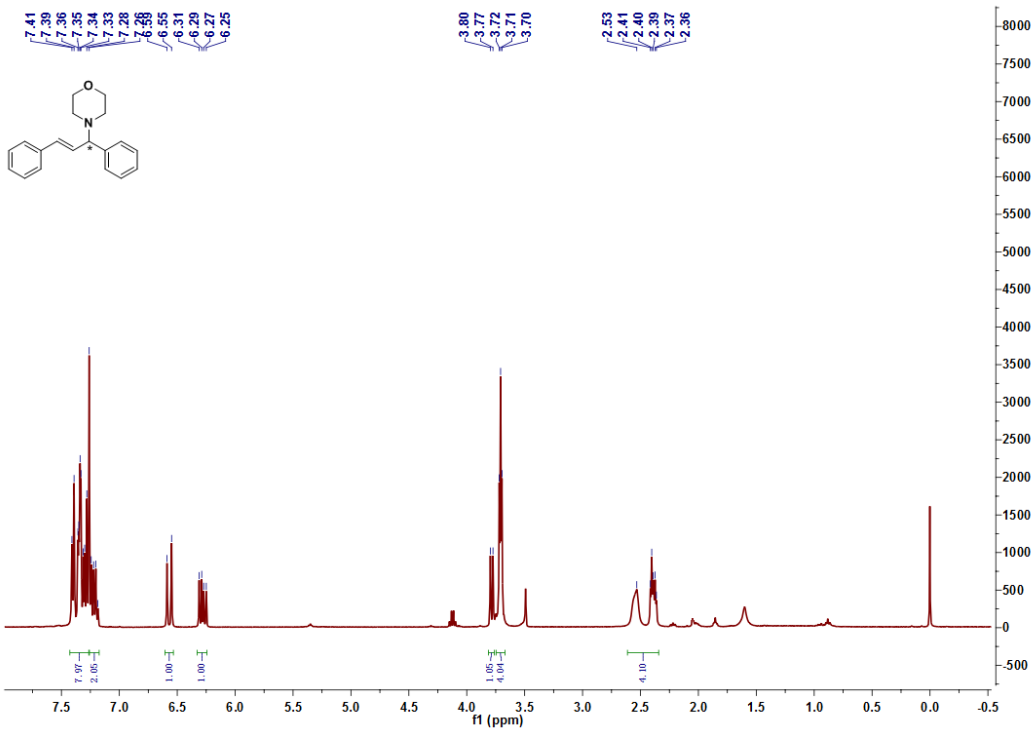
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

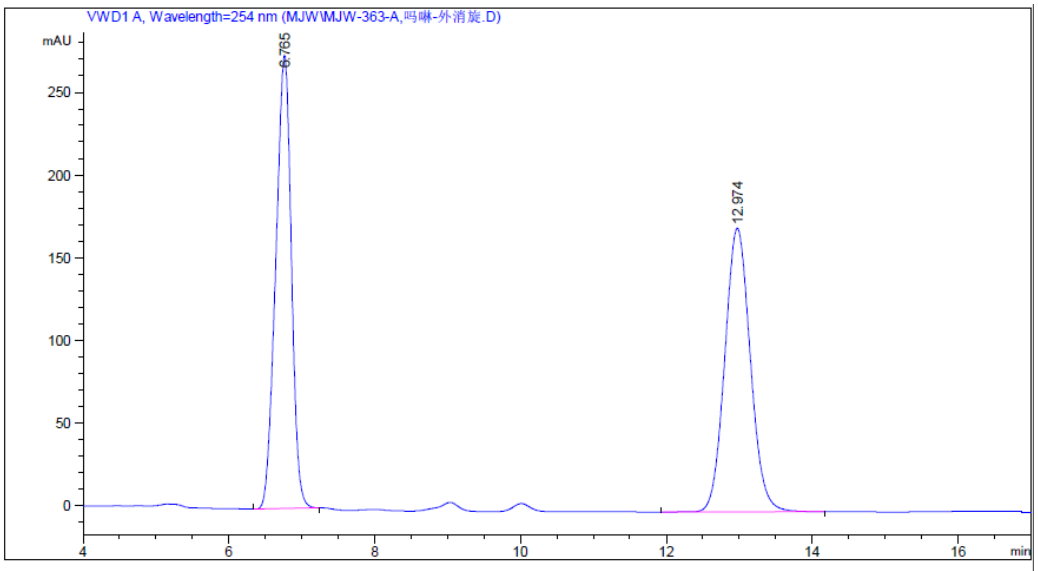
信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.695	BB	0.2875	1613.95886	87.37426	93.7341
2	15.770	MM	0.3520	107.88851	5.10767	6.2659

(*R*,*E*)- N- 1,3-Diphenylprop-2-enyl] morpholine (18b)

White solid; yield: 72%; ee: 55%; ^{1}H NMR (400 MHz, CDCl3) δ 7.41-7.26 (m, 10H), 6.57 (d, *J* = 15.8 Hz, 1H), 6.28 (dd, *J* = 15.8, 8.9 Hz, 1H), 3.78 (d, *J* = 8.9 Hz, 1H), 3.71 (t, *J* = 4.6 Hz, 4H), 2.53-2.36 (m, 4H); HPLC (Chiralpak OD-H column, 254 nm, 90:10 hexane/isopropanol, flow =1mL/min) t_R = 6.7min, 12.9min..





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面积百分比报告

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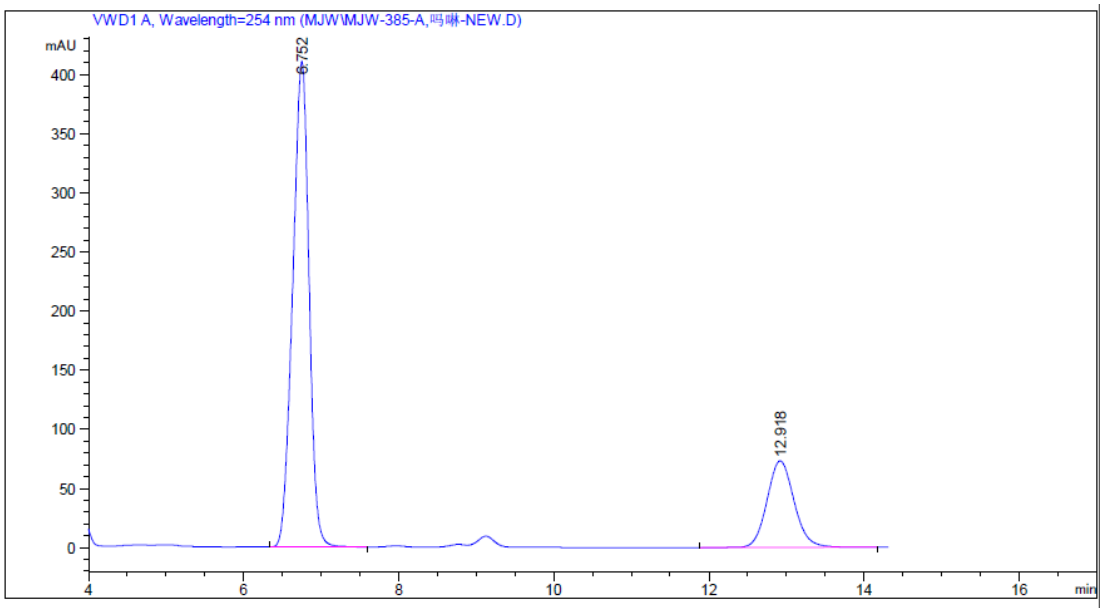
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.765	BB	0.2263	4070.60767	273.96298	49.4049
2	12.974	BB	0.3767	4168.67432	171.40359	50.5951



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面积百分比报告

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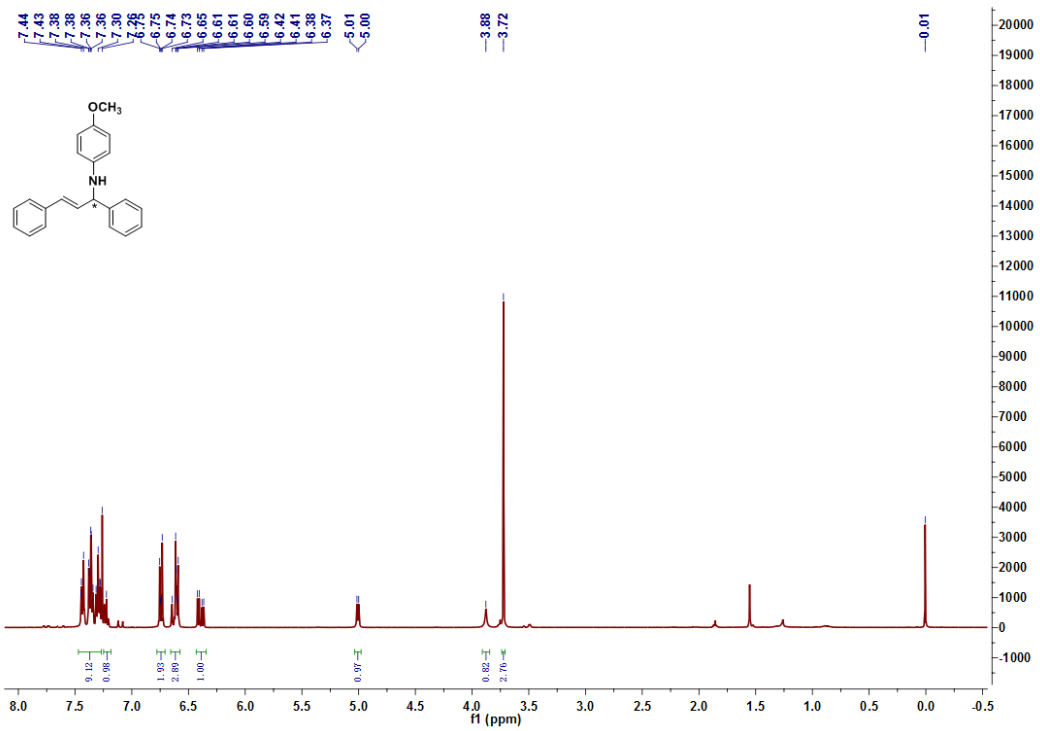
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

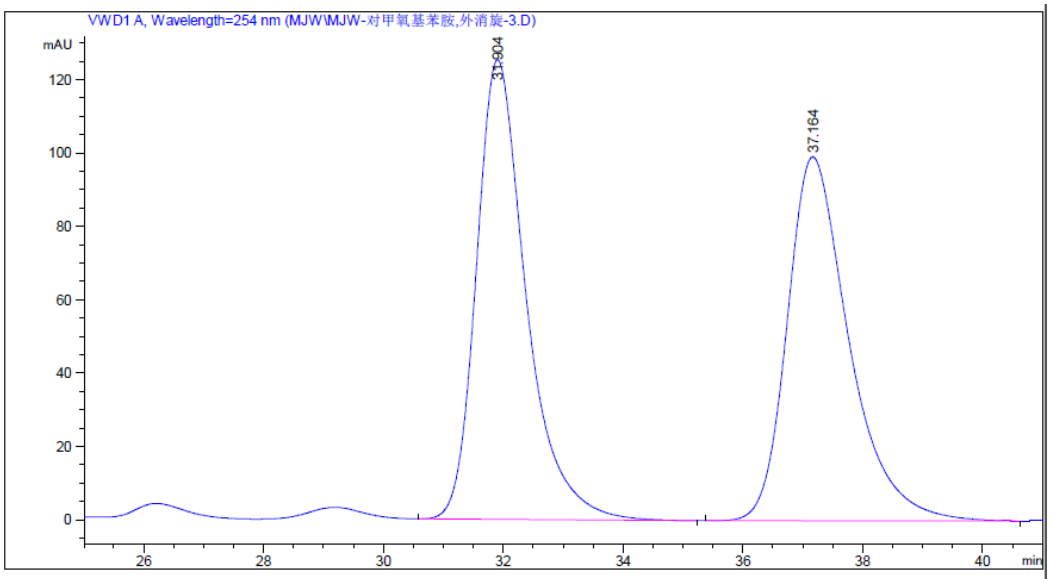
信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.752	VB	0.2222	5992.45020	410.64621	77.1689
2	12.918	BB	0.3746	1772.92358	73.18202	22.8311

(*R*,*E*)- (1,3-diphenylallyl)-(4-methoxyphenyl) amine (18c)

pale yellow solid; yield: 16%; ee: 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.26 (m, 10H), 6.75-6.73 (m, 2H), 6.65-6.59 (m, 3H), 6.39 (dd, *J* = 15.8, 6.3 Hz, 1H), 5.01 (d, *J* = 6.3 Hz, 1H), 3.88 (s, 1H), 3.72 (s, 3H). (Chiralcel OD-H, 254 nm, 90:10 hexane/isopropanol, flow = 0.5 mL/min) t_R = 32.3 min, 37.2 min.





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面积百分比报告

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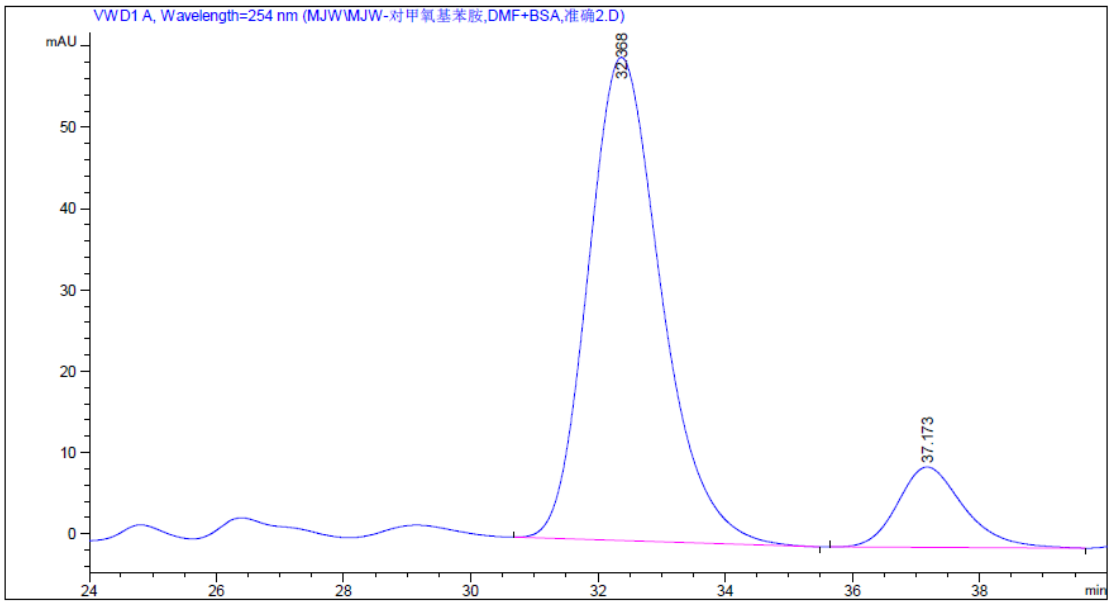
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	31.904	BB	0.8679	7229.99414	125.35849	50.4905
2	37.164	BB	1.0807	7089.52881	99.20995	49.5095



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面积百分比报告

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排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, Wavelength=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	32.368	BB	1.2151	4744.59766	59.44941	86.9361
2	37.173	BB	1.0512	712.97076	9.88814	13.0639

References

1 W. Chen, W. Mbafor, S. M. Roberts and J. Whittall, *Tetrahedron: Asymmetry*, 2006, **17**, 1161.