Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Asymmetric Synthesis of Multifunctional Aryl Allyl Ethers by Nucleophilic Catalysis

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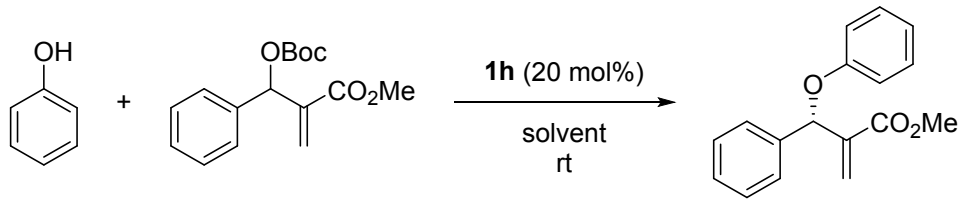
Contents

1. General information

All glassware was thoroughly oven-dried. Chemicals and solvents were either purchased from commercial suppliers or purified by standard techniques. Thin-layer chromatography plates were visualized by exposure to ultraviolet light and/or staining with phosphomolybdic acid followed by heating on a hot plate. Flash chromatography was carried out using silica gel (160-200 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded using Bruker AV-300 / AV-400 spectrometers. Chemical shifts are given in δ relative to tetramethylsilane (TMS), Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet), integration, coupling constant (Hz) and assignment. The spectra were recorded in $CDCl_3$ as the solvent at room temperature, TMS served as internal standard (δ = 0 ppm) for ^{1}H NMR and $CDCl_3$ used as an internal standard (δ = 77.00 ppm) for ^{13}C NMR. Optical rotations were measured on an Autopol IV (d = 589 nm, Hg lamp, 50mmcell) instrument (Rudolph, NJ, USA). High resolution mass spectra were acquired on Thermo Orbitrap Elite, instrument (Agilent, Palo Alto, CA, USA). Enantiomeric excess values were determined by HPLC with Chiralcel OD-H, IC, ID, IB columns on Agilent LC-1260 eluting with *i*-PrOH and n-hexane.

2. Optimization of the solvent of the asymmetric allylic substitution reaction



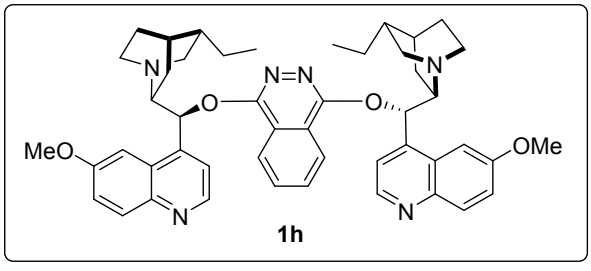
2a **3a** **4a**

Entry[a]	Solvent	t (h)	Yield[b] (%)	Ee[c] (%)
1	DCM	84	92	77
2	PhMe	120	93	85
3	EA	72	92	87

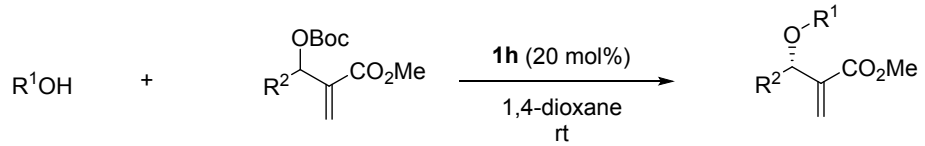
4	1,4-dioxane	96	95	95
5	THF	72	92	91
6	Et_2O	86	57	91
7[d]	THF	76	90	75
8[e]	THF	72	-	-
9[f]	Et_2O	72	-	-

[a] Unless otherwise noted, the reaction was carried out with **2a** (0.1 mmol), **3a** (0.3 mmol) and **1** (20 mol%) in 2mL specified solvent at room temperature. [b] The isolated yield. [c] Determined by HPLC. [d] The reaction was carried out at 0 °C. [e] The reaction was carried out at -40 °C.

3. General procedure of the asymmetric allylic substitution reactions and analytical data of the products



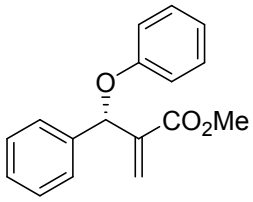
1h



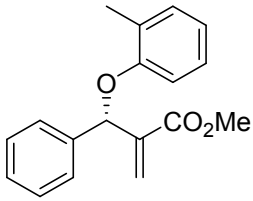
2 **3** **4**

A solution of phenol **2** (0.1 mmol), MBH carbonate **3** (0.3 mmol) and catalysts **1h** (0.02 mmol) in 1, 4-dioxane (2 mL) was stirred at room temperature. The reaction was

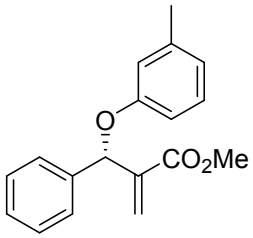
monitored by TLC spectroscopy. After the reaction time given, the reaction mixture was directly purified by flash column chromatograph (eluted with EtOAc/petroleum ether: 10:1) to afford the product **4**.



Methyl (*S*)-2-(phenoxy(phenyl)methyl)acrylate (4a) Colorless oil; 95% yield; 95% ee; [α]28 D = 128.0 (*c* 0.550, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 11.1 min, $t_{R(major)}$ = 13.5 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.46 (d, *J* = 1.8 Hz, 2H), 7.44-7.20 (m, 5H), 6.94-6.89 (m, 3H), 6.39 (s, 1H), 6.16 (s, 1H), 5.97 (t, *J* = 1.2 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.0, 157.5, 140.1, 138.8, 129.4, 128.5, 128.1, 127.4, 126.3, 121.2, 115.9, 77.2, 52.0. HRMS(ESI) for $C_{17}H_{16}NaO_3$ $[M+Na]^+$calcd 291.0992, found 291.0992.

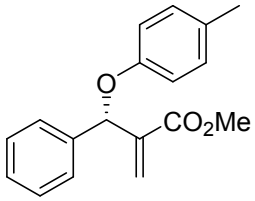


Methyl (*S*)-2-(phenyl(o-tolyloxy)methyl)acrylate (4b) Colorless oil; 95% yield; 91% ee; [α]28 D = 82.8 (*c* 1.000, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 11.2 min, $t_{R(major)}$ = 14.7 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.48-7.45 (m, 2H), 7.36-7.25 (m, 3H), 7.12 (dd, *J* = 0.6, 7.2 Hz, 1H), 7.05 (d, *J* = 1.5 Hz, 1H), 6.84 (dd, *J* = 0.9, 7.5 Hz, 1H), 6.76 (d, *J* = 8.1 Hz, 1H), 6.36 (s, 1H), 6.16 (s, 1H), 6.01 (t, *J* = 1.1 Hz, 1H), 3.74 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.1, 155.5, 140.7, 139.4, 130.8, 128.5, 128.0, 127.2, 126.7, 125.7, 120.8, 112.8, 76.9, 52.0, 16.6. HRMS(ESI) for $C_{18}H_{18}NaO_3$ $[M+Na]^+$calcd 305.1148, found 305.1147.

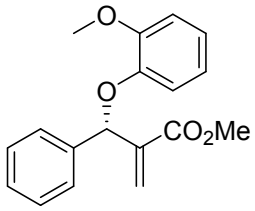


Methyl (*S*)-2-(phenyl(m-tolyloxy)methyl)acrylate (4c) Colorless oil; 94% yield; 90% ee; [α]28 D = 120.3 (*c* 1.185, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 11.1 min, $t_{R(major)}$ = 12.9 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.45-7.43 (m, 2H), 7.37-7.28 (m, 3H), 7.10 (t, *J* = 7.8 Hz, 1H), 6.75-6.69 (m, 3H), 6.38 (s, 1H), 6.14 (s, 1H), 5.98 (t, *J* = 1.1 Hz, 1H), 3.74 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.1, 157.5, 140.2, 139.4, 138.9, 129.1, 128.5, 128.1, 127.4, 126.2, 122.0, 116.8, 112.6, 77.1, 52.0, 21.5. HRMS(ESI) for $C_{18}H_{18}NaO_3$ $[M+Na]^+$calcd 305.1148, found

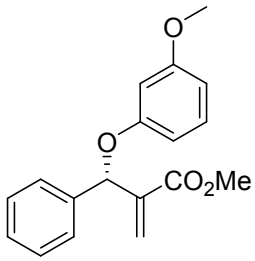
305.1147.



Methyl (*S*)-2-(phenyl(p-tolyloxy)methyl)acrylate (4d) Colorless oil; 93% yield; 91% ee; [α]28 D = 110.0 (*c* 1.200, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 11.2 min, $t_{R(major)}$ = 10.1 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.46-7.42 (m, 2H), 7.37-7.25 (m, 3H), 7.02 (d, *J* = 8.1 Hz, 2H), 6.82 (dd, *J* = 2.1, 6.6 Hz, 2H), 6.38 (s, 1H), 6.11 (s, 1H), 5.97 (t, *J* = 1.1 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.2, 155.5, 140.3, 139.0, 130.5, 129.9, 128.5, 128.1, 127.5, 126.3, 115.8, 77.4, 52.0, 20.5. HRMS(ESI) for $C_{18}H_{18}NaO_3$ $[M+Na]^+$calcd 305.1148, found 305.1149.

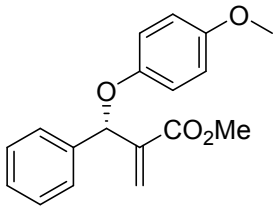


Methyl (*S*)-2-((2-methoxyphenoxy)(phenyl)methyl)acrylate (4e). Colorless oil; 54% yield; 87% ee; [α]25 D = 70.4 (*c* 0.6, $CHCl_3$); The enantiomeric excess was determined by HPLC analysis with an OD-H column. (*n*-hexane:*i*PrOH = 97:3), 0.5 mL/min, λ = 270 nm, t_R (major) = 16.5 min, t_R (minor) = 22.4 min. ^{1}H NMR (400 MHz, $CDCl_3$): 7.52-7.50 (m, 2H), 7.38-7.29 (m, 3H), 6.95-6.83 (m, 4H), 6.45 (s, 1H), 6.19 (s, 1H), 6.18 (s, 1H), 3.87 (s, 3H), 3.76 (s, 3H); ^{13}C NMR(100 MHz, $CDCl_3$): 166.1, 150.3, 147.1, 140.3, 139.1, 128.4, 128.1, 127.5, 126.3, 122.1, 120.8, 116.5, 112.4, 78.5, 56.1, 52.0. HRMS (ESI) For $C_{18}H_{18}NaO_4$ $[M+Na]^+$calcd 321.1097, found 321.1098.

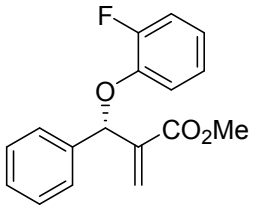


Methyl (*S*)-2-((3-methoxyphenoxy)(phenyl)methyl)acrylate (4f). Colorless oil; 69% yield; 92% ee; [α]25 D = 104.0 (*c* 1.0, $CHCl_3$); The enantiomeric excess was determined by HPLC analysis with an OD-H column. (*n*-hexane:*i*PrOH = 97:3), 0.5 mL/min, λ = 270 nm, t_R (major) = 16.4 min, t_R (minor) = 18.3 min. ^{1}H NMR (400 MHz, $CDCl_3$): 7.45-7.43 (m, 2H), 7.36-7.25 (m, 3H), 7.14-7.10 (m, 1H), 6.53-6.47 (m,

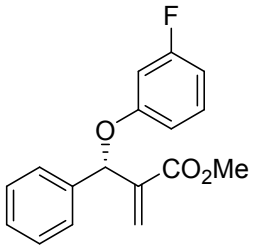
3H), 6.39 (s, 1H), 6.14 (s, 1H), 5.97 (s, 1H), 3.74 (s, 6H); ^{13}C NMR(100 MHz, $CDCl_3$): 166.1, 160.7, 158.8, 140.1, 138.8, 129.8, 128.6, 128.2, 127.5, 126.4, 108.0, 106.9, 102.4, 77.3, 55.3, 52.1. HRMS (ESI) For $C_{18}H_{18}NaO_4$ $[M+Na]^+$calcd 321.1097, found 321.1098.



Methyl (*S*)-2-((4-methoxyphenoxy)(phenyl)methyl)acrylate (4g) Colorless oil; 89% yield; 93% ee; [α]27 D= 86.6 (*c* 1.0, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 11.2 min, $t_{R(major)}$ = 12.4 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.45-7.42 (m, 2H), 7.37-7.25 (m, 3H), 6.89-6.83 (m, 2H), 6.79-6.74 (m, 2H), 6.39 (s, 1H), 6.04 (s, 1H), 5.97 (t, J = 1.2 Hz, 1H), 3.74 (s, 3H), 3.73 (s, 3H); ^{13}C NMR (75 MHz, CDCl3): 166.1, 154.1, 151.7, 140.3, 139.0, 128.5, 128.1, 127.4, 126.2, 117.1, 114.5, 78.2, 55.6, 52.0. HRMS (ESI) for $C_{18}H_{19}O_4$ $[M+H]^+$ calcd 299.1278, found 299.1274.

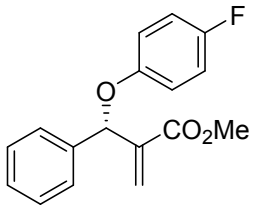


Methyl (*S*)-2-((2-fluorophenoxy)(phenyl)methyl)acrylate (4h) Colorless oil; 58% yield; 95% ee; [α]28 D = 107.7 (*c* 0.665, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 97:3), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 12.8 min, $t_{R(major)}$ = 13.8 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.46 (dd, *J* = 1.2, 8.1 Hz, 2H), 7.37-7.26 (m, 3H), 7.08-7.01 (m, 1H), 6.96-6.86 (m, 3H), 6.42 (s, 1H), 6.17 (s, 1H), 6.09 (t, *J* = 1.1 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.9, 154.8, 151.5, 145.5, 145.4, 140.0, 138.4, 128.5, 128.3, 127.4, 126.4, 124.2, 124.1, 121.9, 121.8, 117.2, 116.5, 116.2, 78.6, 52.0. HRMS(ESI) for $C_{17}H_{15}FNaO_3$ $[M+Na]^+$calcd 309.0897, found 309.0897.

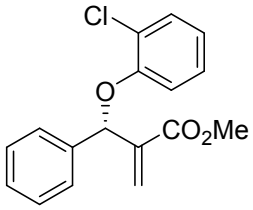


Methyl (*S*)-2-((3-fluorophenoxy)(phenyl)methyl)acrylate (4i) Colorless oil; 76% yield; 95% ee; [α]28 D = 106.6 (*c* 0.910, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 97:3), 0.5 mL/min, λ

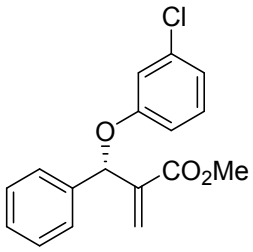
= 270 nm, $t_{R(minor)}$ = 13.1 min, $t_{R(major)}$ = 12.0 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.43 (dd, *J* = 1.7, 8.0 Hz, 2H), 7.38-7.30 (m, 3H), 7.20-7.12 (m, 1H), 6.72-6.60 (m, 3H), 6.40 (s, 1H), 6.13 (s, 1H), 5.93 (t, *J* = 1.1 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.9, 165.1, 161.8, 158.9, 158.8, 139.9, 138.3, 130.2, 130.1, 128.6, 128.3, 127.3, 126.5, 111.6, 111.5, 108.2, 107.9, 103.9, 103.5, 77.6, 52.1. HRMS(ESI) for $C_{17}H_{15}FNaO_3$ $[M+Na]^+$calcd 309.0897, found 309.0894.



Methyl (*S*)-2-((4-fluorophenoxy)(phenyl)methyl)acrylate (4j) Colorless oil; 70% yield; 93% ee; [α]28 D = 106.5 (*c* 0.550, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 97:3), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 11.5 min, $t_{R(major)}$ = 10.1 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.44-7.41 (m, 2H), 7.38-7.29 (m, 3H), 6.94-6.84 (m, 2H), 6.39 (t, *J* = 0.8 Hz, 1H), 6.06 (s, 1H), 5.94 (t, *J* = 1.1 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.0, 159.1, 155.9, 153.7, 140.1, 138.6, 128.6, 128.2, 127.4, 126.4, 117.2, 117.1, 115.9, 115.6, 78.2, 52.1. HRMS(ESI) for $C_{17}H_{15}FNaO_3$ $[M+Na]^+$calcd 309.0897, found 309.0896.

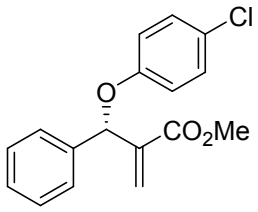


Methyl (*S*)-2-((2-chlorophenoxy)(phenyl)methyl)acrylate (4k) Colorless oil; 79% yield; 93% ee; [α]28 D = 82.3 (*c* 0.700, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 12.3 min, $t_{R(major)}$ = 14.9 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.51-7.48 (m, 2H), 7.37-7.27 (m, 4H), 7.12-7.06 (m, 1H), 6.89-6.82 (m, 2H), 6.39 (s, 1H), 6.22 (s, 1H), 6.16 (d, *J* = 0.9 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.9, 152.8, 140.1, 138.5, 130.3, 128.5, 128.2, 127.5, 127.2, 126.2, 123.6, 121.8, 115.2, 77.7, 52.0. HRMS(ESI) for $C_{17}H_{15}ClNaO_3$ $[M+Na]^+$calcd 325.0602, found 325.0600.

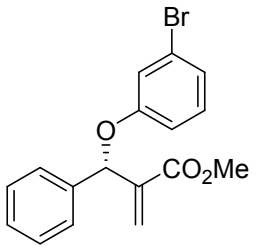


Methyl (*S*)-2-((3-chlorophenoxy)(phenyl)methyl)acrylate (4l) Colorless oil; 93% yield; 92% ee; [α]28 D = 96.0 (*c* 0.950, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ

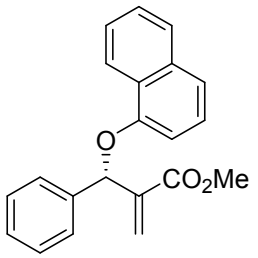
= 270 nm, $t_{R(minor)}$ = 12.2 min, $t_{R(major)}$ = 11.1 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.44-7.41 (m, 2H), 7.38-7.30 (m, 3H), 7.14 (t, *J* = 8.3 Hz, 1H), 6.94-6.89 (m, 2H), 6.82-6.78 (m, 1H), 6.40 (s, 1H), 6.12 (s, 1H), 5.92 (t, *J* = 1.1 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.9, 158.3, 139.8, 138.2, 134.8, 130.2, 128.6, 128.3, 127.3, 126.5, 121.5, 116.5, 114.1, 77.5, 52.1. HRMS(ESI) for $C_{17}H_{15}ClNaO_3$ $[M+Na]^+$calcd 325.0602, found 325.0596.



Methyl (*S*)-2-((4-chlorophenoxy)(phenyl)methyl)acrylate (4m) Colorless oil; 73% yield; 94% ee; [α]28 D = 107.8 (*c* 0.850, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 12.2 min, $t_{R(major)}$ = 10.4 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.44-7.41 (m, 2H), 7.38-7.29 (m, 3H), 7.17 (d, *J* = 9.0 Hz, 2H), 6.84 (d, *J* = 9.3 Hz, 2H), 6.39 (s, 1H), 6.10 (s, 1H), 5.92 (t, *J* = 1.1 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.0, 156.1, 139.9, 138.3, 129.3, 128.6, 128.3, 127.3, 126.4, 126.1, 117.2, 77.6, 52.1. HRMS(ESI) for $C_{17}H_{15}ClNaO_3$ $[M+Na]^+$calcd 325.0602, found 325.0591.

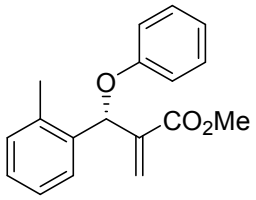


Methyl (*S*)-2-((3-bromophenoxy)(phenyl)methyl)acrylate (4n) Colorless oil; 93% yield; 89% ee; [α]28 D = 93.1 (*c* 1.057, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 13.3 min, $t_{R(major)}$ = 11.7 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.42 (dd, *J* = 1.5, 8.1 Hz, 2H), 7.38-7.29 (m, 3H), 7.11-7.06 (m, 3H), 6.86-6.82 (m, 1H), 6.39 (s, 1H), 6.12 (s, 1H), 5.92 (t, *J* = 1.1 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.9, 158.3, 139.8, 138.2, 130.5, 128.6, 128.3, 127.3, 126.5, 124.4, 122.7, 119.5, 114.5, 77.5, 52.1. HRMS(ESI) for $C_{17}H_{14}BrO_3$ $[M-H]^-$calcd 345.0132, found 345.0128.

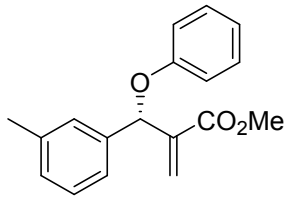


Methyl (*S*)-2-((naphthalen-1-yloxy)(phenyl)methyl)acrylate (4o) Colorless oil; 94%

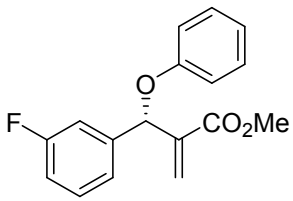
yield; 86% ee; [α]28 D = 24.9 (*c* 0.907, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 16.1 min, $t_{R(major)}$ = 12.8 min. ^{1}H NMR (300 MHz, $CDCl_3$): 8.35-8.31 (m, 1H), 7.78-7.75 (m, 1H), 7.56-7.52 (m, 2H), 7.48-7.20 (m, 7H), 6.78 (d, *J* = 7.5 Hz, 1H), 6.39 (d, *J* = 5.1 Hz, 2H), 6.07 (t, *J* = 1.1 Hz, 2H), 3.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.1, 152.9, 140.2, 139.0, 134.5, 128.5, 128.1, 127.5, 127.2, 126.3, 125.9, 125.9, 125.7, 125.2, 122.0, 120.7, 106.8, 77.2, 52.0. HRMS(ESI) for $C_{21}H_{18}NaO_3$ $[M+Na]^+$calcd 341.1148, found 341.1144.



Methyl (*S*)-2-(phenoxy(o-tolyl)methyl)acrylate (4p) Colorless oil; 73% yield; 95% ee; [α]28 D = 65.4 (*c* 0.700, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 13.3 min, $t_{R(major)}$ = 15.2 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.41-7.37 (m, 1H), 7.25-7.19 (m, 5H), 6.94-6.88 (m, 3H), 6.44 (s, 1H), 6.34 (s, 1H), 5.74 (t, *J* = 1.2 Hz, 1H), 3.75 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.3, 157.9, 139.1, 136.3, 136.2, 130.6, 129.4, 128.2, 127.6, 127.1, 126.2, 121.1, 115.6, 74.5, 52.1, 19.2. HRMS(ESI) for $C_{18}H_{18}NaO_3$ $[M+Na]^+$calcd 305.1148, found 305.1151.

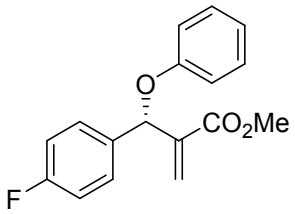


Methyl (*S*)-2-(phenoxy(o-tolyl)methyl)acrylate (4q) Colorless oil; 94% yield; 94% ee; [α]28 D = 128.6 (*c* 1.325, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 10.1 min, $t_{R(major)}$ = 17.4 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.25-7.20 (m, 5H), 7.12-7.09 (m, 1H), 6.94-6.89 (m, 3H), 6.38 (t, *J* = 0.8 Hz, 1H), 6.12 (s, 1H), 5.96 (t, *J* = 1.2 Hz, 1H), 3.74 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.1, 157.6, 140.0, 138.7, 138.2, 129.3, 129.0, 128.4, 128.0, 126.3, 124.5, 121.1, 115.8, 77.2, 52.0, 21.4. HRMS(ESI) for $C_{18}H_{18}NaO_3$ $[M+Na]^+$calcd 305.1148, found 305.1152.

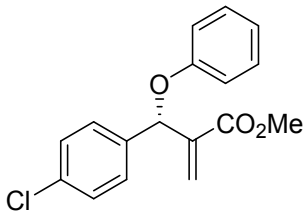


Methyl (*S*)-2-((3-fluorophenyl)(phenoxy)methyl)acrylate (4r) Colorless oil; 93% yield; 95% ee; [α]28 D = 106.1 (*c* 0.867, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 97:3), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 10.3 min, $t_{R(major)}$ = 21.9 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.33-7.15 (m, 5H), 7.00-6.89 (m, 4H), 6.40 (s, 1H), 6.15 (s, 1H), 5.99 (t, *J* = 1.1 Hz, 1H),

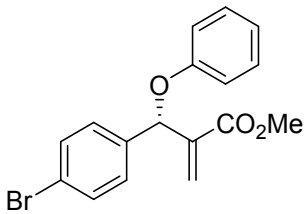
3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.8, 164.4, 161.2, 157.2, 141.6, 141.5, 139.7, 130.1, 130.0, 129.4, 126.6, 123.0, 123.0, 121.4, 115.8, 115.2, 114.9, 114.4, 114.1, 76.5, 76.4, 52.1. HRMS(ESI) for $C_{18}H_{17}FNaO_3$ $[M+Na]^+$calcd 309.0897, found 309.0898.



Methyl (*S*)-2-((4-fluorophenyl)(phenoxy)methyl)acrylate (4s) Colorless oil; 95% yield; 95% ee; [α]28 D = 132.5 (*c* 1.135, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 97:3), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 10.0 min, $t_{R(major)}$ = 17.6 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.42 (dd, *J* = 5.4, 8.7 Hz, 2H), 7.26-7.21 (m, 2H), 7.02 (t, *J* = 8.7 Hz, 2H), 6.95-6.89 (m, 3H), 6.39 (s, 1H), 6.13 (s, 1H), 5.99 (t, *J* = 1.1 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.9, 164.1, 160.8, 157.3, 139.9, 134.7, 134.6, 129.4, 129.2, 129.1, 126.1, 121.3, 115.9, 115.6, 115.3, 76.6, 52.1. HRMS(ESI) for $C_{18}H_{17}FNaO_3$ $[M+Na]^+$calcd 309.0897, found 309.0896.

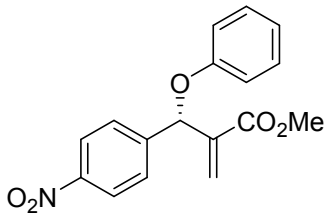


Methyl (*S*)-2-((4-chlorophenyl)(phenoxy)methyl)acrylate (4t) Colorless oil; 92% yield; 91% ee; [α]28 D = 119.1 (*c* 0.833, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an IA column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 18.8 min, $t_{R(major)}$ = 17.0 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.40-7.37 (m, 2H), 7.33-7.29 (m, 2H), 7.24-7.21 (m, 2H), 6.96-6.88 (m, 3H), 6.39 (s, 1H), 6.11 (s, 1H), 6.00 (t, *J* = 1.1 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.8, 157.2, 139.7, 137.4, 133.9, 129.4, 128.8, 128.7, 126.3, 121.4, 115.8, 76.5, 52.1. HRMS(ESI) for $C_{17}H_{15}ClNaO_3$ $[M+Na]^+$calcd 325.0602, found 325.0604.

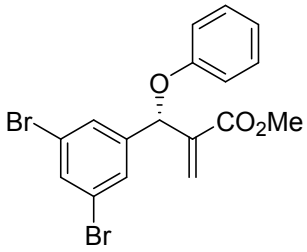


Methyl (*S*)-2-((4-bromophenyl)(phenoxy)methyl)acrylate (4u) Colorless oil; 79% yield; 91% ee; [α]28 D = 117.7 (*c* 1.025, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 97:3), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 9.8 min, $t_{R(major)}$ = 17.5 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.46 (dd, *J* = 2.0, 6.8 Hz, 2H), 7.33 (dd, *J* = 1.8, 6.6 Hz, 2H), 7.23-7.20 (m, 2H), 6.95-6.88 (m,

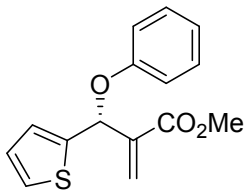
3H), 6.39 (s, 1H), 6.10 (s, 1H), 5.99 (t, J = 1.1 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.8, 157.2, 139.7, 138.0, 131.6, 129.4, 129.1, 126.4, 122.1, 121.4, 115.8, 76.5, 52.0. HRMS(ESI) for $C_{17}H_{15}BrNaO_3$ $[M+Na]^+$calcd 369.0097, found 369.0100.



Methyl (*S*)-2-((4-nitrophenyl)(phenoxy)methyl)acrylate (4v) Colorless oil; 77% yield; 93% ee; [α]28 D = 150.9 (*c* 0.790, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 97:3), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 25.0 min, $t_{R(major)}$ = 46.8 min. ^{1}H NMR (300 MHz, $CDCl_3$): 8.20 (dd, J = 1.8, 6.9 Hz, 2H), 7.66 (d, J = 8.7 Hz, 2H), 7.25 (dd, J = 7.5, 8.7 Hz, 2H), 6.99-6.89 (m, 3H), 6.45 (s, 1H), 6.23 (s, 1H), 6.10 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.6, 156.8, 147.6, 146.3, 139.2, 129.6, 128.1, 127.1, 123.7, 121.8, 115.8, 76.2, 52.2. HRMS(ESI) for $C_{17}H_{15}NNaO_5$ $[M+Na]^+$calcd 336.0842, found 336.0847.



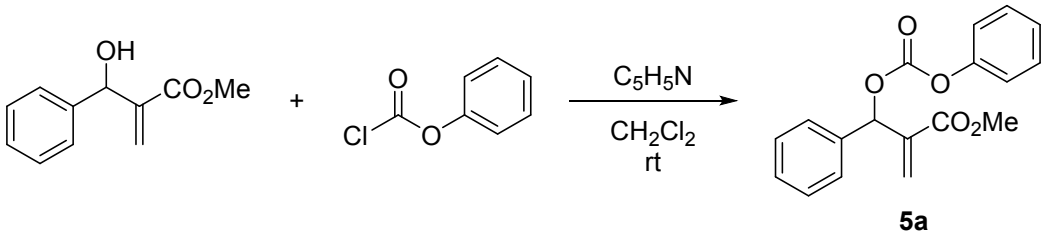
Methyl (*S*)-2-((3,5-dibromophenyl)(phenoxy)methyl)acrylate (4w) Colorless oil; 96% yield; 91% ee; [α]28 D = 90.1 (*c* 1.083, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 8.7 min, $t_{R(major)}$ = 27.9 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.59-7.54 (m, 3H), 7.28-7.22 (m, 2H), 6.98-6.88 (m, 3H), 6.43 (s, 1H), 6.05 (s, 1H), 6.04 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.5, 156.9, 143.0, 139.0, 133.7, 129.5, 129.1, 127.0, 123.0, 121.7, 115.8, 75.8, 52.2. HRMS(ESI) for $C_{17}H_{14}Br_2NaO_3$ $[M+Na]^+$calcd 448.9181, found 448.9181.



Methyl (*R*)-2-(phenoxy(thiophen-2-yl)methyl)acrylate (4x) Colorless oil; 93% yield; 92% ee; [α]28 D = 145.3 (*c* 0.950, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an OD-H column. (*n*-hexane:*i*PrOH = 95:5), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 12.9 min, $t_{R(major)}$ = 14.6 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.59 (t, J = 1.7 Hz, 1H), 7.54 (d, J = 1.8 Hz, 1H), 7.28-7.23 (m, 2H), 6.99-6.88 (m, 3H), 6.43 (s, 1H), 6.05-6.04 (m, 2H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.5, 156.9,

143.0, 139.1, 133.8, 129.6, 129.2, 127.1, 123.0, 121.8, 115.8, 75.9, 52.2. HRMS(ESI) for $C_{15}H_{14}SNaO_3$ $[M+Na]^+$calcd 297.0556, found 297.0563.

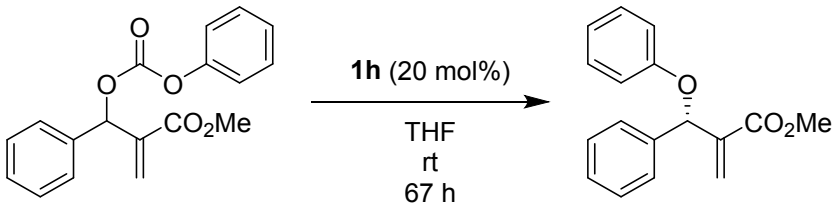
4. Synthesis and characterization of MBH carbonate 5a



5a

To a solution of racemic MBH alcohol (10 mmol) and pyridine (1 mL) in CH_2Cl_2 (20 mL) was added Phenyl chloroformate (12 mmol) at room temperature. The reaction was monitored by TLC spectroscopy. After completion of the reaction, the reaction mixture was directly purified by flash column chromatograph to afford the product **5a**. **Methyl 2-(((phenoxycarbonyl)oxy)(phenyl)methyl)acrylate (5a)** Colorless solid; 70% yield. ^{1}H NMR (300 MHz, $CDCl_3$): 7.47-7.44 (m, 2H), 7.41-7.32 (m, 5H), 7.24-7.13 (m, 3H), 6.63 (s, 1H), 6.48 (s, 1H), 6.02-6.01 (m, 1H), 3.72 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): 165.1, 152.5, 151.0, 138.9, 136.7, 129.4, 128.8, 128.6, 127.7, 126.4, 126.0, 120.9, 77.5, 52.1.

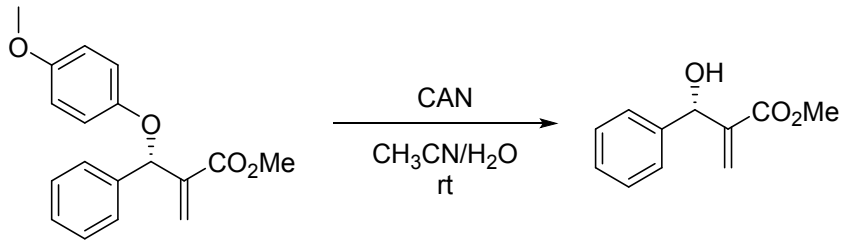
5. General procedure of asymmetric allylic substitution reaction of 5a



5a **4a**

A solution of MBH carbonate **5a** (0.2 mmol) and catalyst **1h** (0.04 mmol) in THF (4 mL) was stirred at room temperature. The reaction was monitored by TLC spectroscopy. After the reaction time given, the reaction mixture was directly purified by flash column chromatograph (eluted with EtOAc/petroleum ether: 10:1) to afford the product **4a**.

6. Synthesis and characterization of chiral MBH alcohol 6

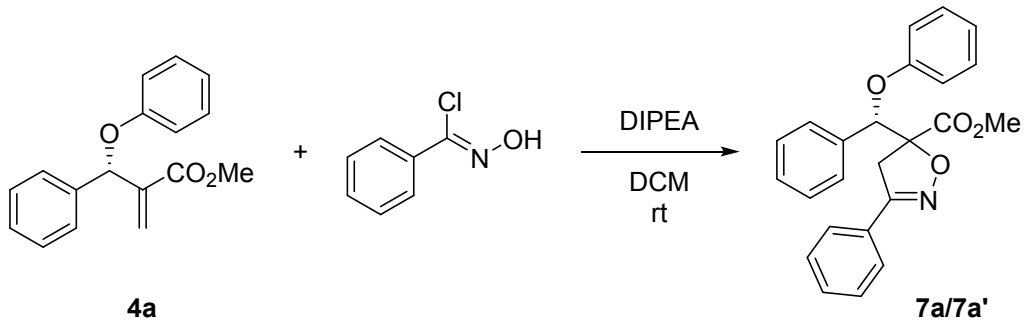


4g **6**

To a solution of **4g** (0.1 mmol) in CH_3CN:H_2O (4:1, 2.5mL) was added ceric ammonium nitrate (CAN, 0.3 mmol) at room temperature. After stirring for 5 minutes at room temperature, all the solvents were removed and the residue was purified by flash column chromatograph to afford the product **6**.

Methyl (*S*)-2-(hydroxy(phenyl)methyl)acrylate (6) Colorless oil; 71% yield; 92% ee; [α]28 D = 70.0 (*c* = 0.100, MeOH); The enantiomeric excess was determined by HPLC with an IC column. (*n*-hexane : *i*PrOH = 95:5), 0.5 mL/min, λ = 254 nm, $t_{R(minor)}$ = 15.2 min, $t_{R(major)}$ = 23.8 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.39-7.26 (m, 5H), 6.34 (t, *J* = 0.9 Hz, 1H), 5.84 (t, *J* = 1.2 Hz, 1H), 5.56 (d, *J* = 5.7 Hz, 1H), 3.72 (s, 3H), 3.08 (d, *J* = 5.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): 166.7, 141.9, 141.2, 128.4, 127.8, 126.5, 126.1, 73.2, 51.9. HRMS(ESI) for $C_{11}H_{12}NaO_3$ $[M+Na]^+$ calcd 215.0679, found 215.0682.

7. General procedure of 1, 3-dipolar cycloaddition reaction of aryl allyl ether 4a



4a **7a/7a'**

To a solution of **4a** (0.1 mmol) and hydroximoyl chloride (0.12 mmol) in DCM (1mL) was added DIPEA (0.1 mmol) at room temperature. The reaction was monitored by TLC spectroscopy. After the reaction was complete, the reaction mixture was directly purified by flash column chromatograph to afford the products **7a** and **7a'**.

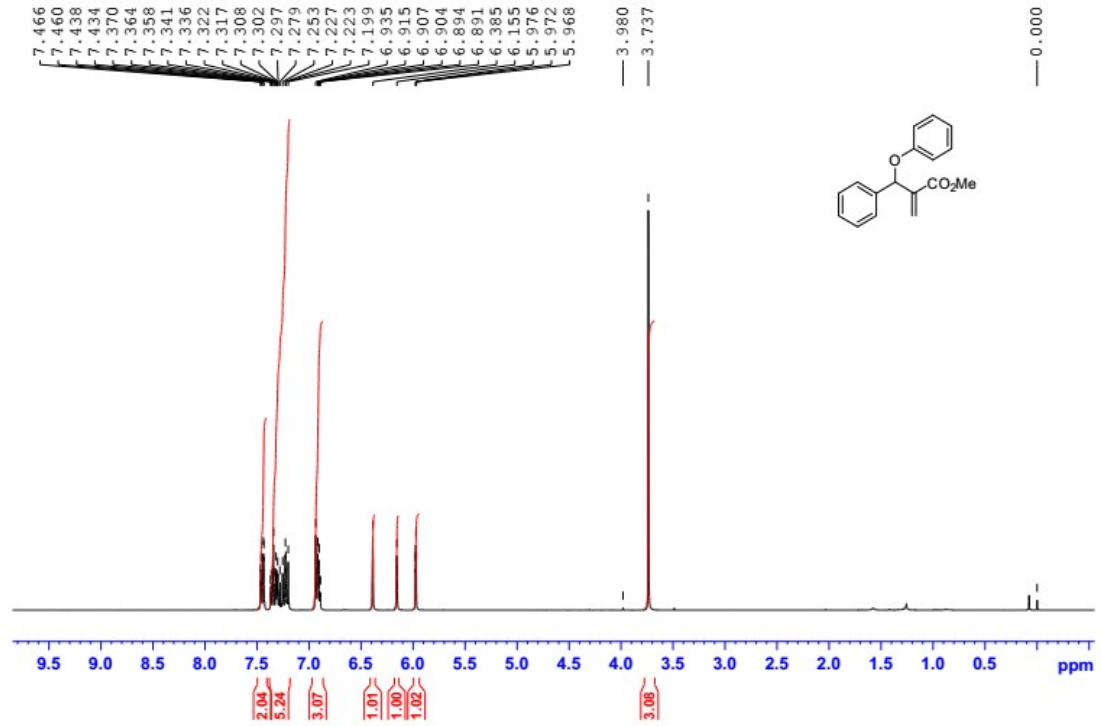
Methyl 5-((*S*)-phenoxy(phenyl)methyl)-3-phenyl-4,5-dihydroisoxazole-5-carboxylate (7a) one of the two diastereomers Colorless oil; 40% yield; 90% ee; [α]27 D = -69.9 (*c* = 0.77, CH_2Cl_2); The enantiomeric excess was determined by HPLC

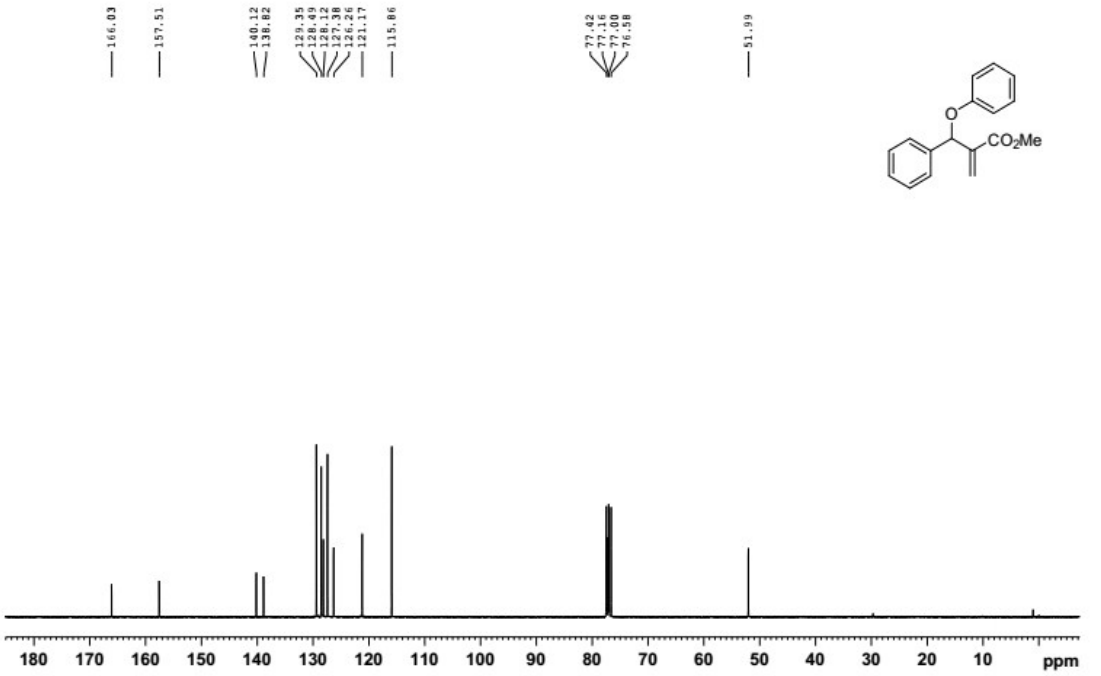
with an OD column. (*n*-hexane : *i*PrOH = 90:10), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 21.3 min, $t_{R(major)}$ = 28.2 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.52-7.46 (m, 5H), 7.36-7.28 (m, 3H), 7.25-7.16 (m, 4H), 6.91 (t, *J* = 7.5 Hz, 1H), 6.84-6.81 (m, 2H), 5.86 (s, 1H), 4.05 (d, *J* = 17.4 Hz, 1H), 3.76 (s, 3H), 3.56 (d, *J* = 17.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): 170.0, 157.2, 156.9, 134.6, 130.3, 129.4, 128.6, 128.6, 128.4, 128.4, 127.5, 126.7, 121.7, 115.8, 90.8, 79.2, 53.2, 38.6. HRMS(ESI) for $C_{24}H_{21}KNO_4$ $[M+K]^+$ calcd 426.1102, found 426.1106.

Methyl 5-((*S*)-phenoxy(phenyl)methyl)-3-phenyl-4,5-dihydroisoxazole-5-carboxylate (7a') another of the two diastereomers Colorless oil; 40% yield; 90% ee; [α]27 D = -24.6 (*c* = 0.78, CH_2Cl_2); The enantiomeric excess was determined by HPLC with an IA column. (*n*-hexane:*i*PrOH = 90:10), 0.5 mL/min, λ = 270 nm, $t_{R(minor)}$ = 18.5 min, $t_{R(major)}$ = 23.7 min. ^{1}H NMR (300 MHz, $CDCl_3$): 7.62 (dd, *J* = 1.5, 5.7 Hz, 2H), 7.47 (d, *J* = 5.1 Hz, 2H), 7.39-7.30 (m, 6H), 7.16 (t, *J* = 6Hz, 2H), 6.87 (d, *J* = 5.7 Hz, 3H), 5.69 (s, 1H), 3.78 (s, 5H); ^{13}C NMR (75 MHz, $CDCl_3$): 170.4, 157.6, 156.1, 135.0, 130.3, 129.3, 129.0, 128.7, 128.7, 127.7, 126.8, 121.8, 116.6, 92.2, 81.4, 53.0, 39.0. HRMS(ESI) for $C_{24}H_{21}KNO_4$ $[M+K]^+$ calcd 426.1102, found 426.1106.

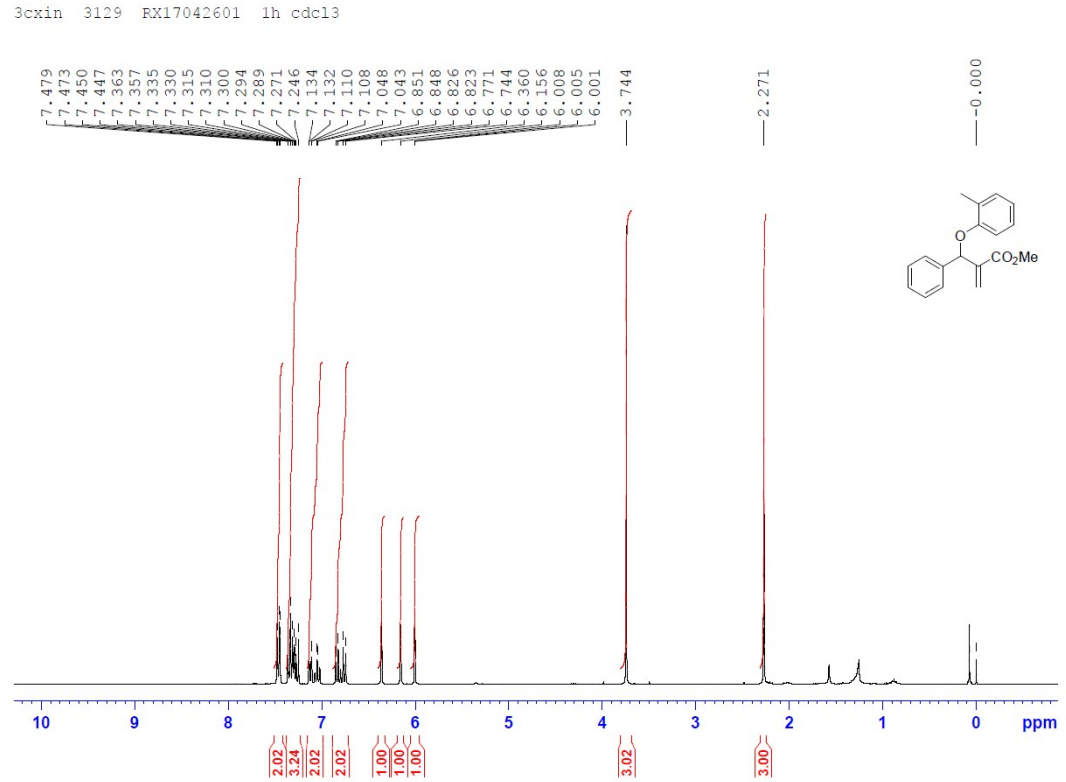
8. ^{1}H NMR and ^{13}C NMR spectra of 4, 5, 6, 7

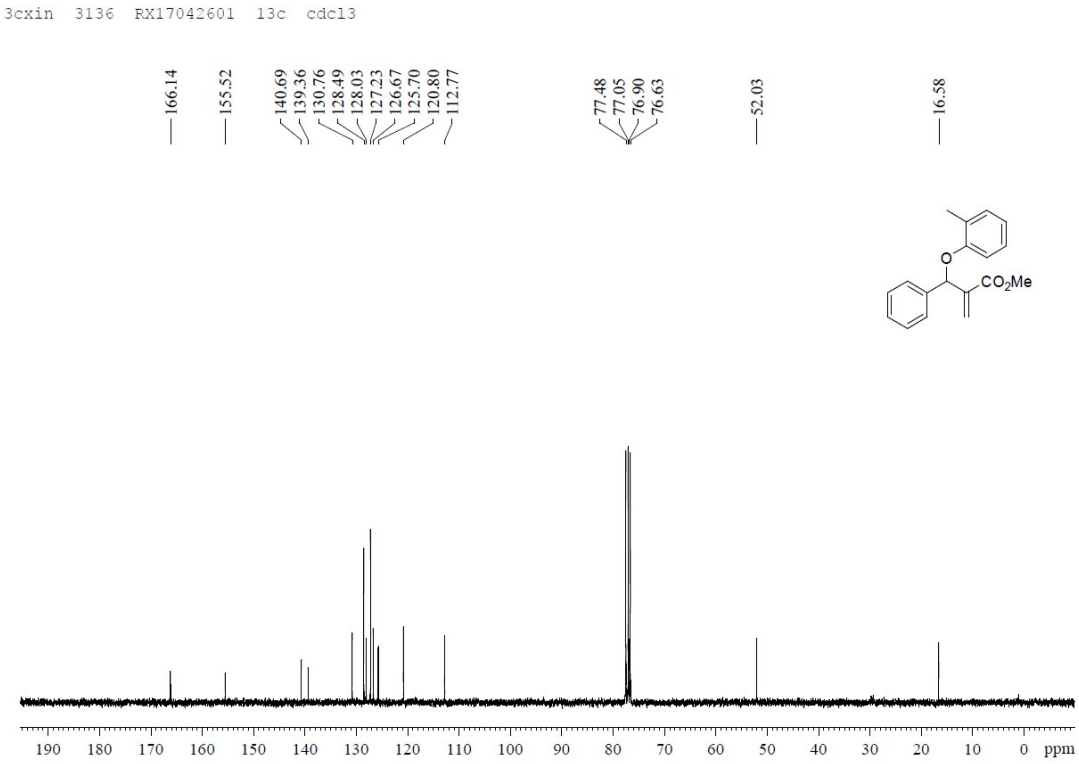
4a



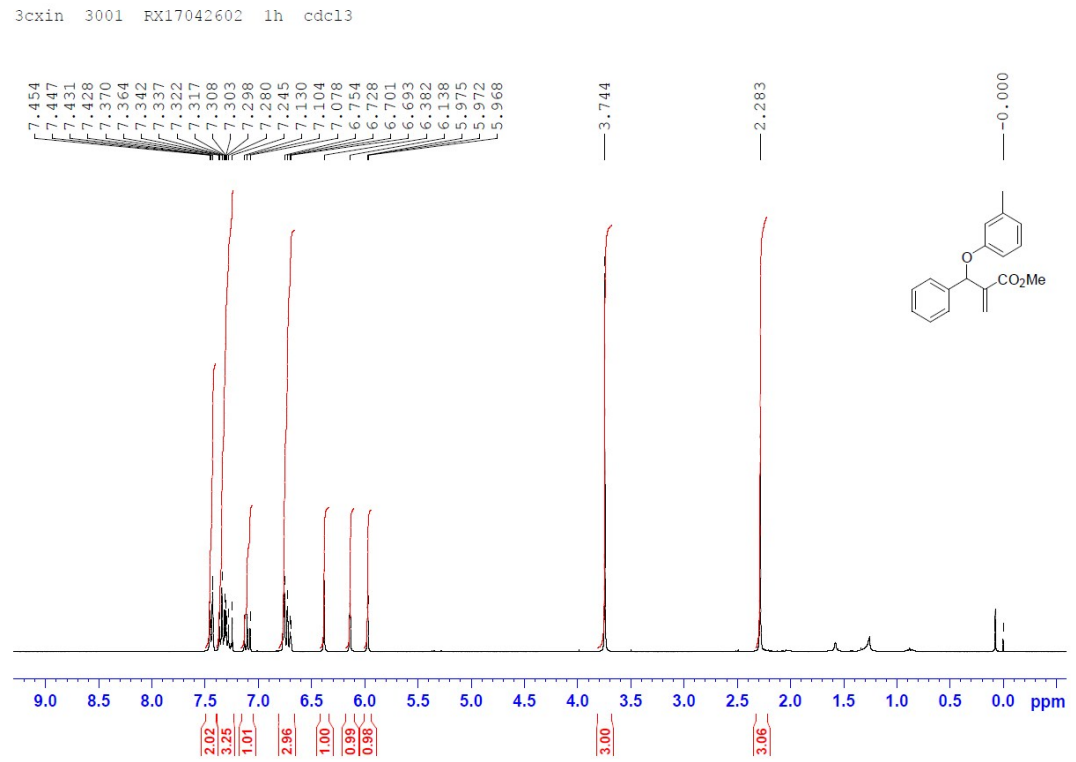


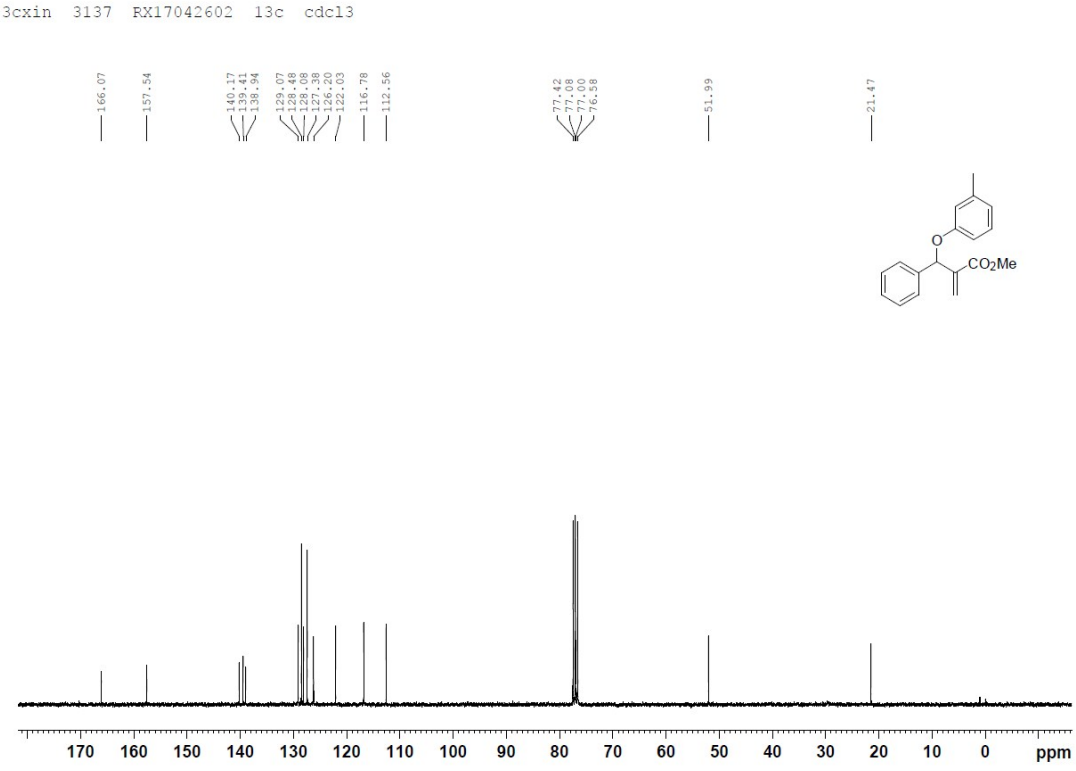
4b


3cxin 3129 RX17042601 1h cdcl3
7.479
7.473
7.450
7.447
7.363
7.357
7.335
7.330
7.315
7.310
7.300
7.294
7.289
7.271
7.246
7.134
7.132
7.110
7.108
7.048
7.043
6.851
6.848
6.826
6.823
6.771
6.744
6.360
6.156
6.008
6.005
6.001
3.744
2.271
0.000
CO2Me
10 9 8 7 6 5 4 3 2 1 0 ppm
2.02
3.24
2.02
2.02
1.00
1.00
1.00
3.02
3.00

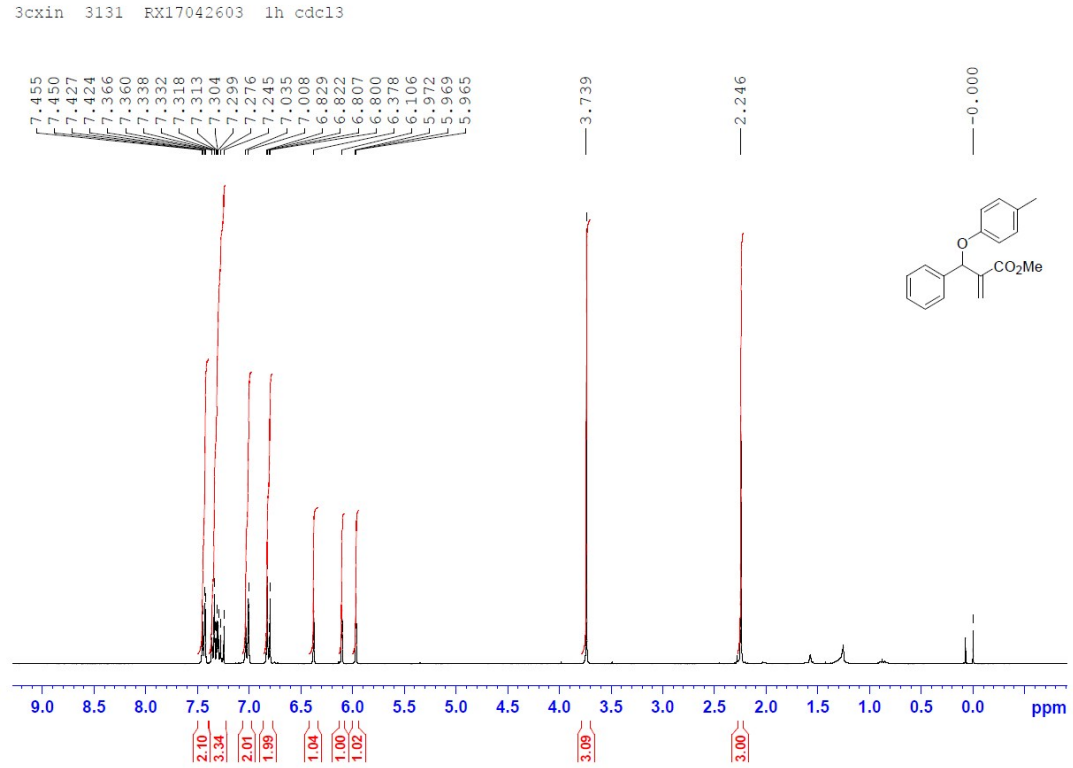

3cxin 3136 RX17042601 13c cdcl3
166.14
155.52
140.69
139.36
130.76
128.49
128.03
127.23
126.67
125.70
120.80
112.77
77.48
77.05
76.90
76.63
52.03
16.58
CO2Me
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

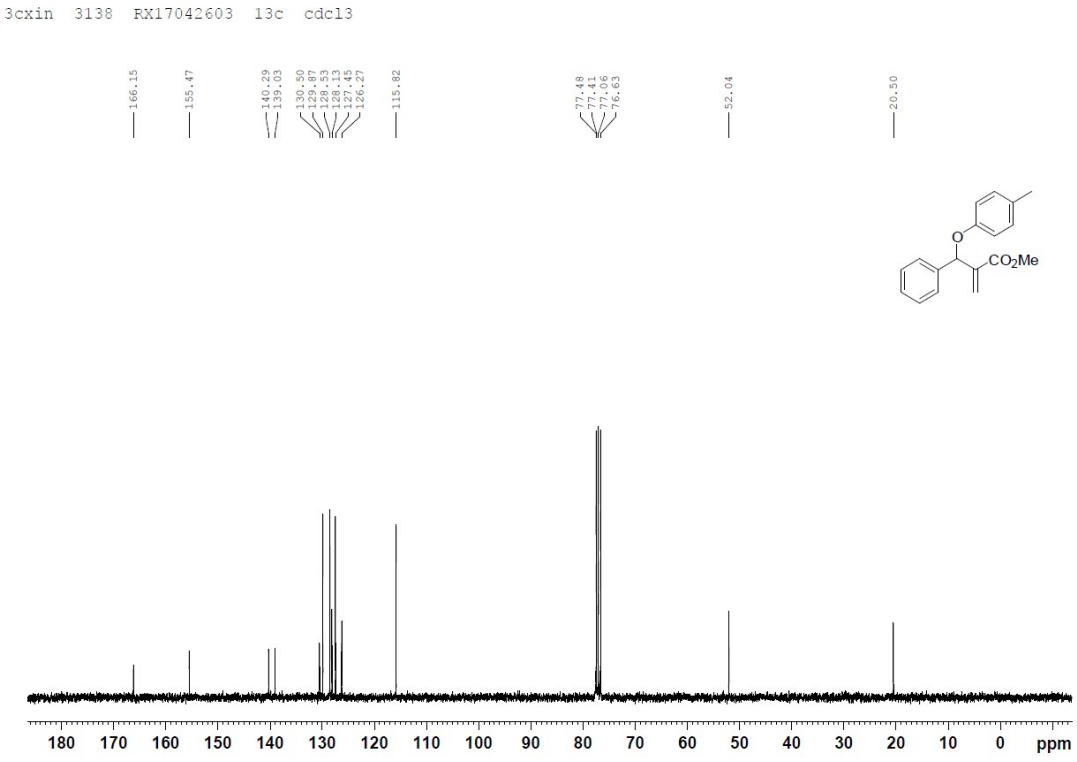
4c


3cxin 3001 RX17042602 1h cdcl3
7.454
7.447
7.431
7.428
7.370
7.364
7.342
7.337
7.322
7.317
7.308
7.303
7.298
7.280
7.245
7.130
7.104
7.078
6.754
6.728
6.701
6.693
6.382
6.138
5.975
5.972
5.968
3.744
2.283
0.000
CO2Me
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 ppm
2.02
3.25
1.01
2.96
1.00
0.99
0.98
3.00
3.06

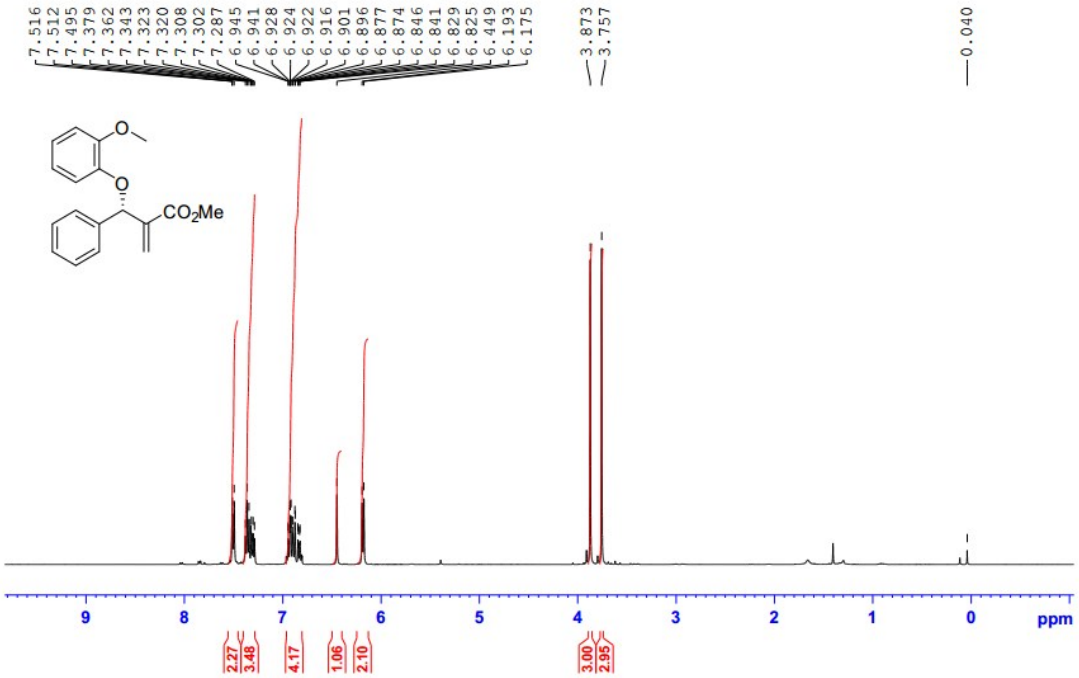

3cxin 3137 RX17042602 13c cdcl3
166.07
157.54
140.17
139.41
138.94
129.07
128.48
128.08
127.38
126.20
122.03
116.78
112.56
77.42
77.08
77.00
76.58
51.99
21.47
CO2Me
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

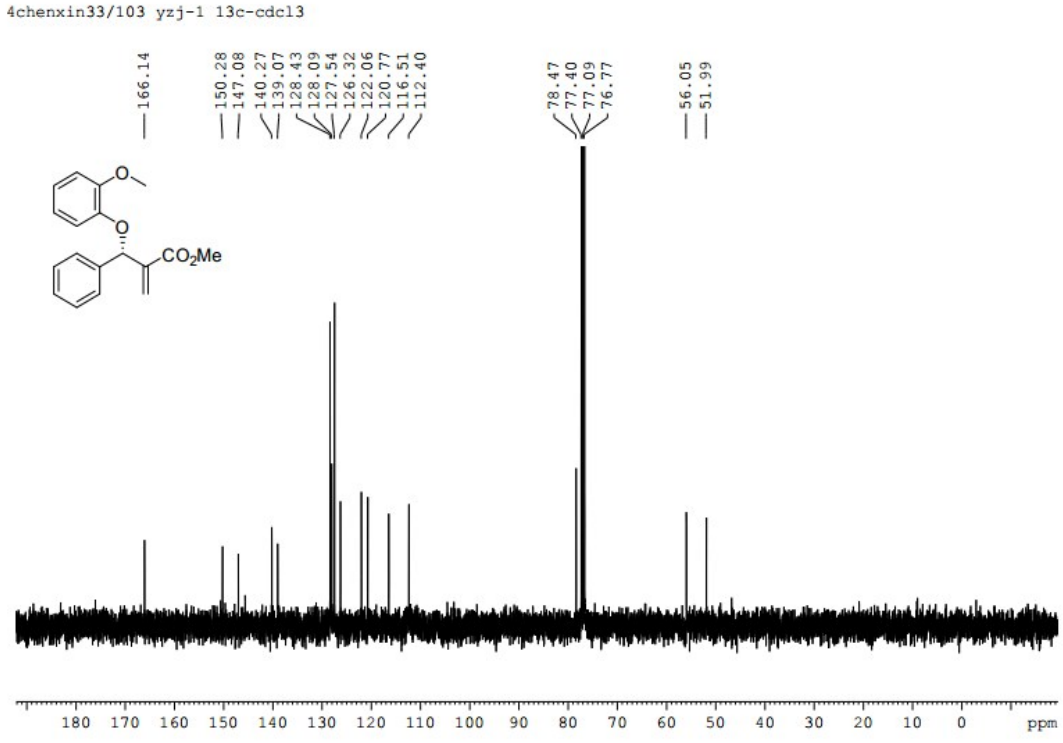
4d


3cxin 3131 RX17042603 1h cdcl3
7.455
7.450
7.427
7.424
7.366
7.360
7.338
7.332
7.318
7.313
7.304
7.299
7.276
7.245
7.035
7.008
6.829
6.822
6.807
6.800
6.378
6.106
5.972
5.969
5.965
3.739
2.246
0.000
O
CO2Me
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 ppm
2.10
3.34
2.01
1.99
1.04
1.00
1.02
3.09
3.00

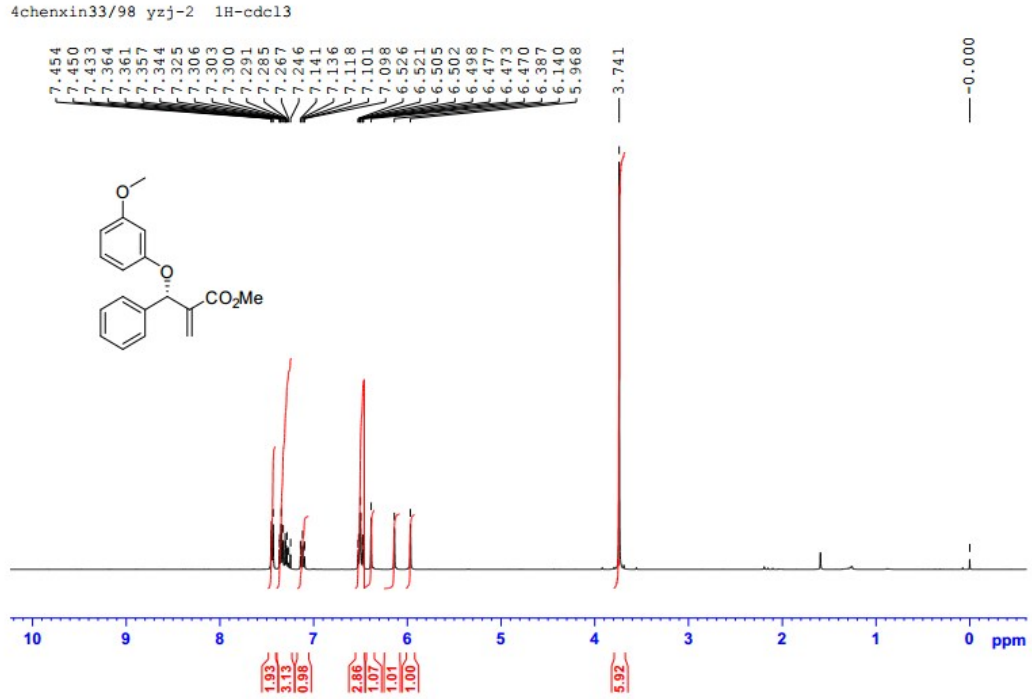

3cxin 3138 RX17042603 13c cdcl3
166.15
155.47
140.29
139.03
130.50
129.87
128.53
128.13
127.45
126.27
115.82
77.48
77.41
77.06
76.63
52.04
20.50
O
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

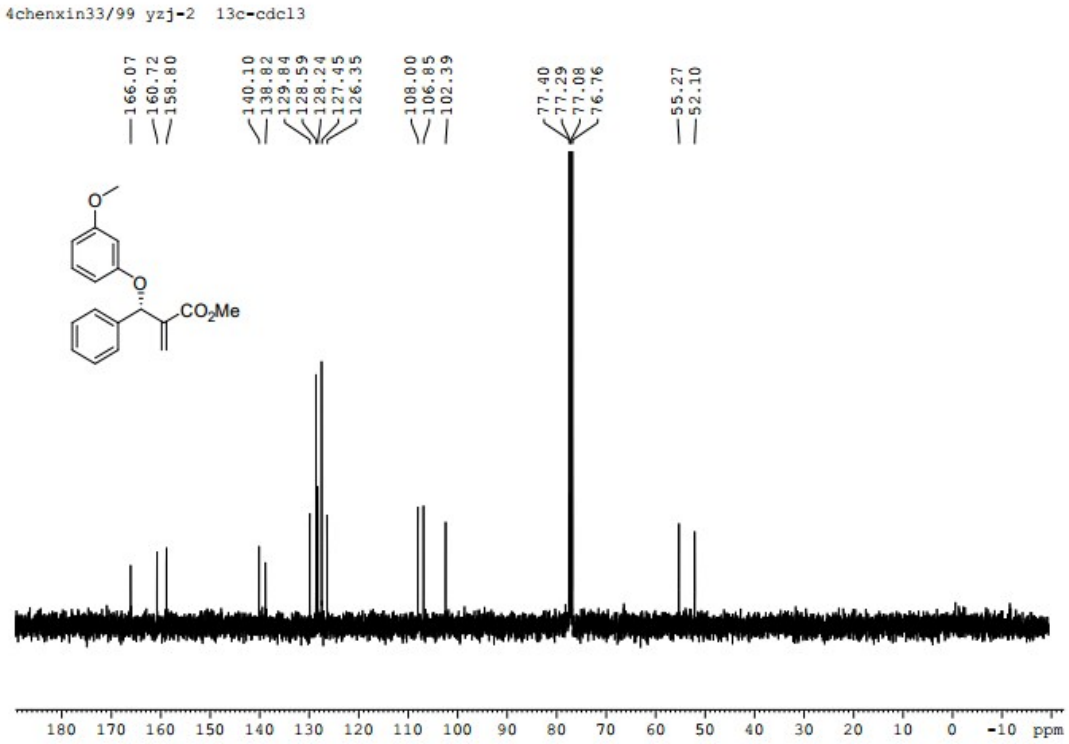
4e


7.516
7.512
7.495
7.379
7.362
7.343
7.323
7.320
7.308
7.302
7.287
6.945
6.941
6.928
6.924
6.922
6.916
6.901
6.896
6.877
6.874
6.846
6.841
6.829
6.825
6.449
6.193
6.175
3.873
3.757
0.040
CO2Me
9
8
7
6
5
4
3
2
1
0
ppm
2.27
3.48
4.17
1.06
2.10
3.00
2.95

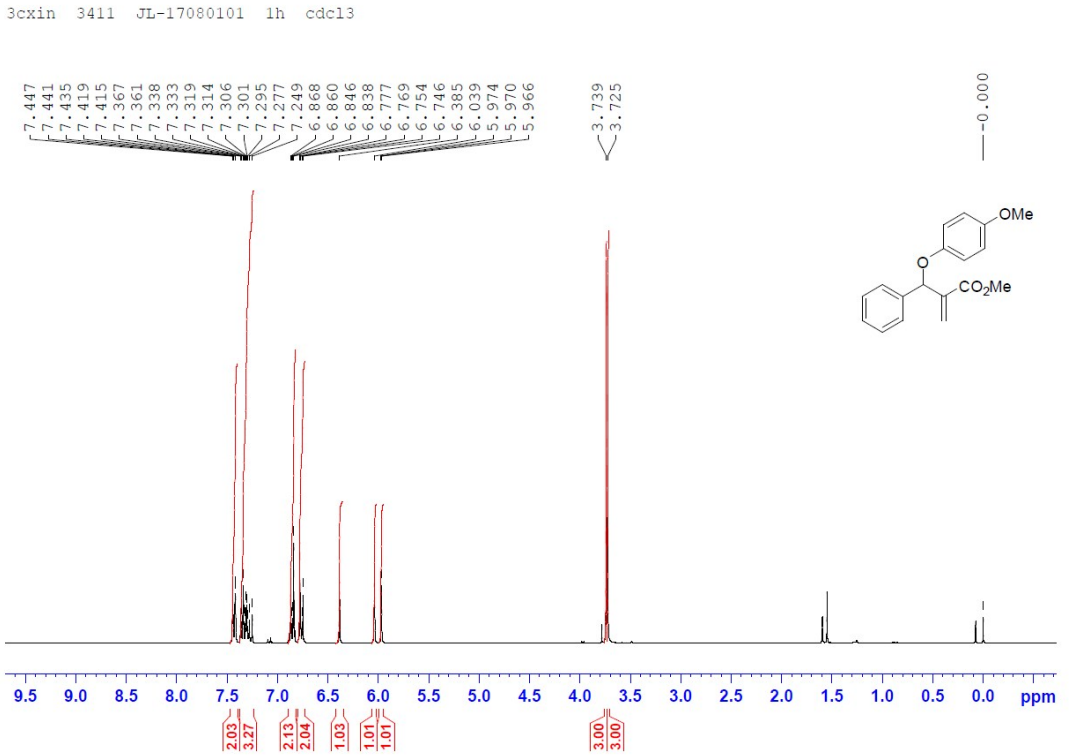

4chenxin33/103 yzj-1 13c-cdcl3
166.14
150.28
147.08
140.27
139.07
128.43
128.09
127.54
126.32
122.06
120.77
116.51
112.40
78.47
77.40
77.09
76.77
56.05
51.99
CO2Me
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

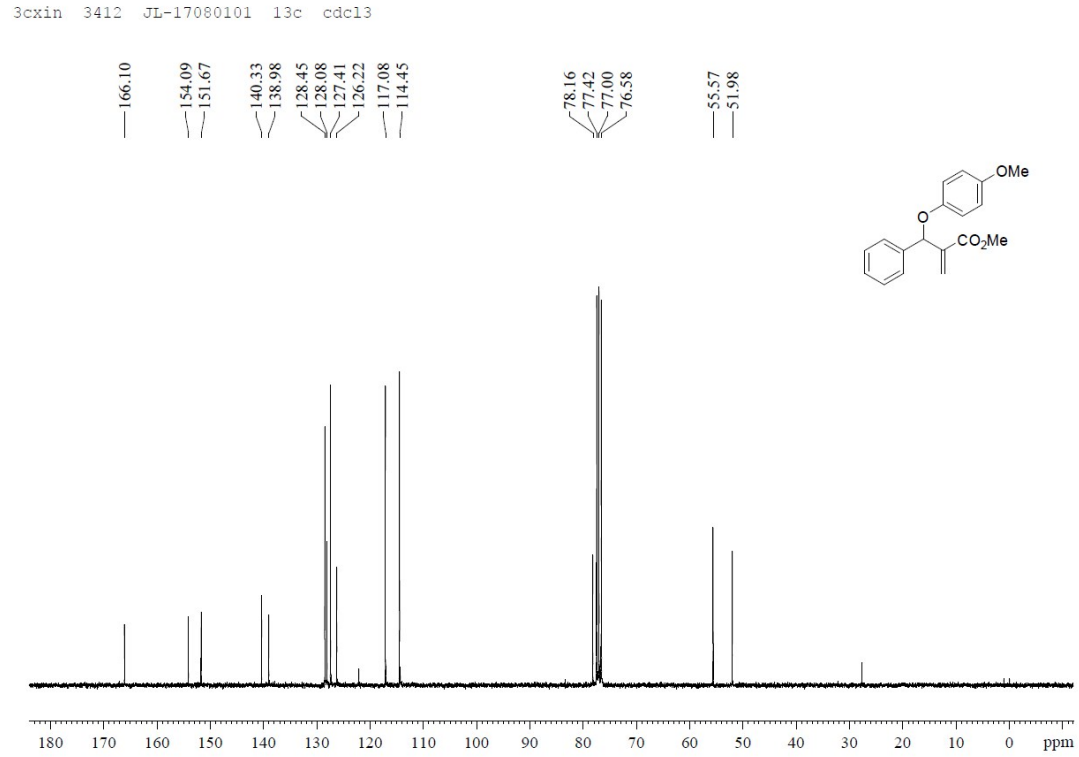
4f


4chenxin33/98 yzj-2 1H-cdcl3
7.454
7.450
7.433
7.364
7.361
7.357
7.344
7.325
7.306
7.303
7.300
7.291
7.285
7.267
7.246
7.141
7.136
7.118
7.101
7.098
6.526
6.521
6.505
6.502
6.498
6.477
6.473
6.470
6.387
6.140
5.968
3.741
-0.000
CO2Me
10 9 8 7 6 5 4 3 2 1 0 ppm
1.93
3.13
0.98
2.86
1.07
1.01
1.00
5.92

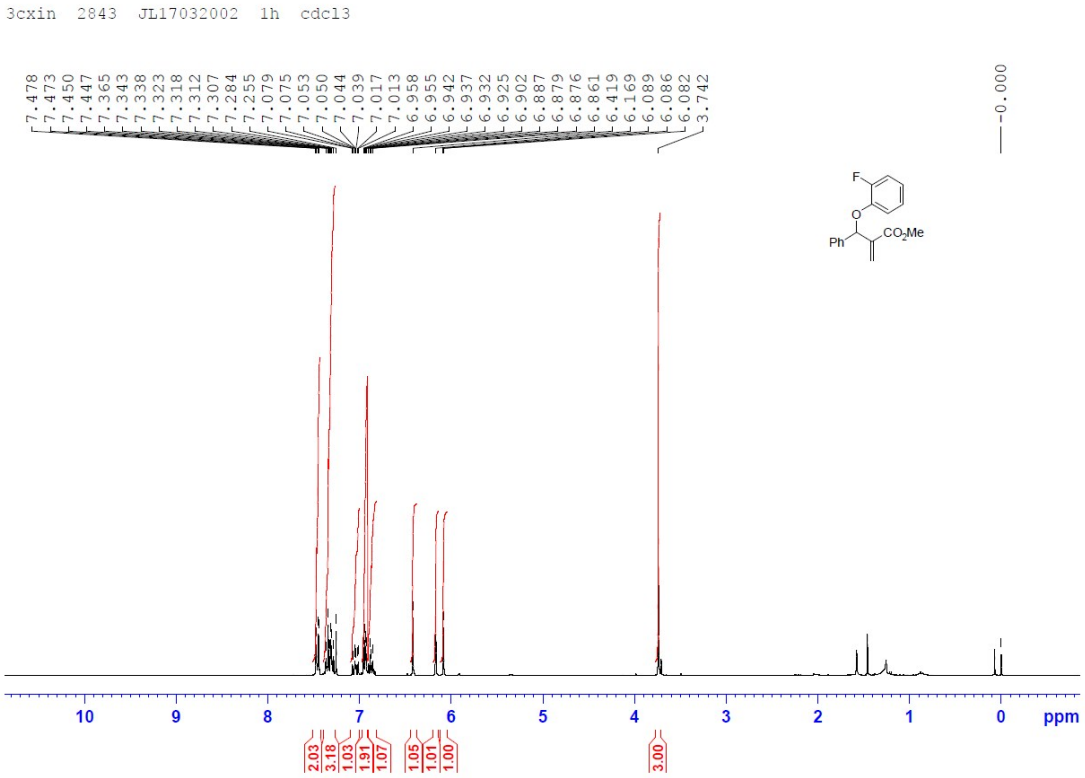

4chenxin33/99 yzj-2 13c-cdcl3
166.07
160.72
158.80
140.10
138.82
129.84
128.59
128.24
127.45
126.35
108.00
106.85
102.39
77.40
77.29
77.08
76.76
55.27
52.10
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

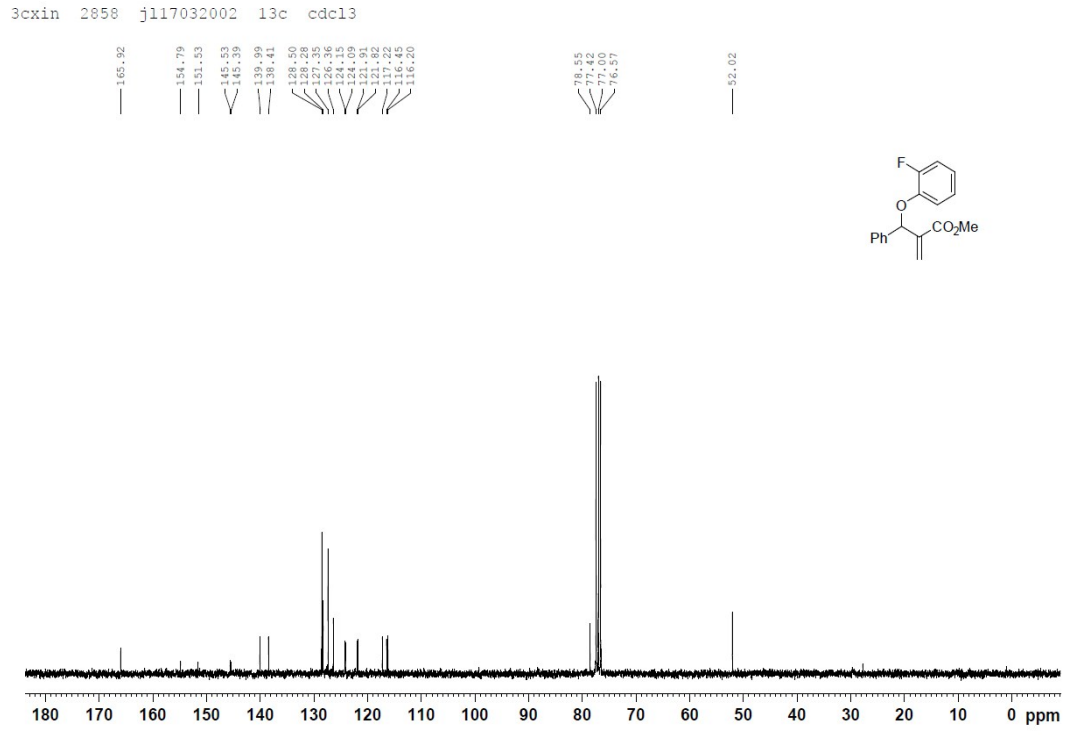
4g


3cxin 3411 JL-17080101 1h cdcl3
7.447
7.441
7.435
7.419
7.415
7.367
7.361
7.338
7.333
7.319
7.314
7.306
7.301
7.295
7.277
7.249
6.868
6.860
6.846
6.838
6.777
6.769
6.754
6.746
6.385
6.039
5.974
5.970
5.966
3.739
3.725
0.000
OMe
O
CO2Me
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 ppm
2.03
3.27
2.13
2.04
1.03
1.01
1.01
3.00
3.00

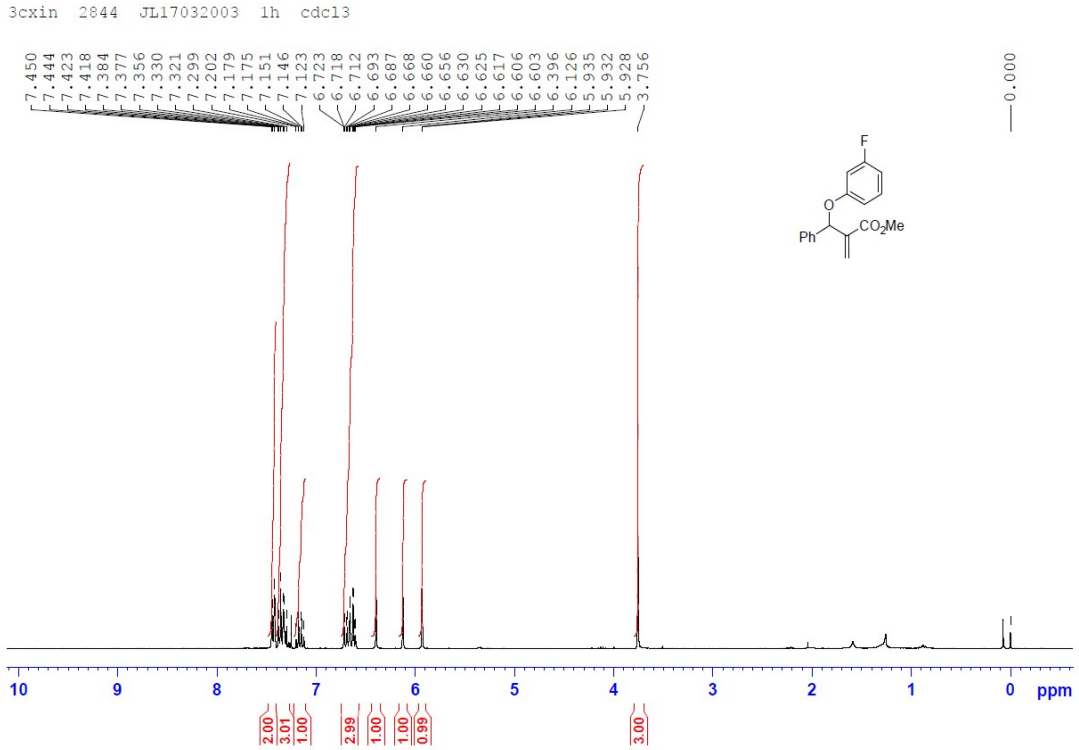

3cxin 3412 JL-17080101 13c cdcl3
166.10
154.09
151.67
140.33
138.98
128.45
128.08
127.41
126.22
117.08
114.45
78.16
77.42
77.00
76.58
55.57
51.98
OMe
O
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

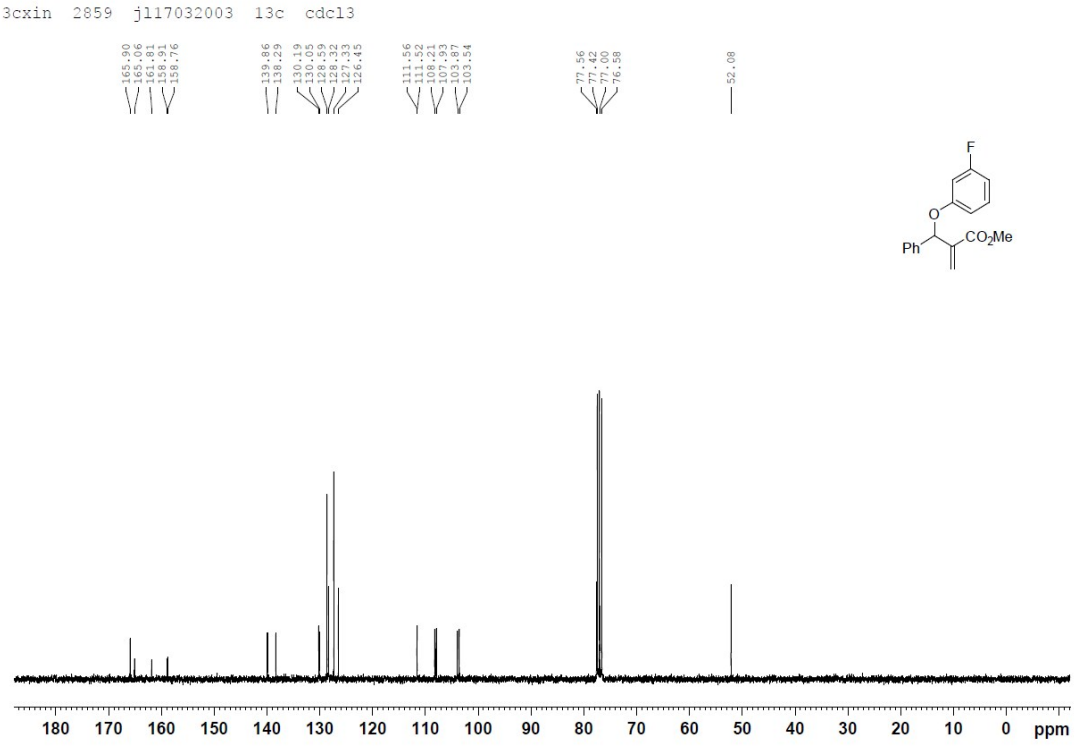
4h


3cxin 2843 JL17032002 1h cdcl3
7.478
7.473
7.450
7.447
7.365
7.343
7.338
7.323
7.318
7.312
7.307
7.284
7.255
7.079
7.075
7.053
7.050
7.044
7.039
7.017
7.013
6.958
6.955
6.942
6.937
6.932
6.925
6.902
6.887
6.879
6.876
6.861
6.419
6.169
6.089
6.086
6.082
3.742
0.000
F
O
Ph
CO2Me
10 9 8 7 6 5 4 3 2 1 0 ppm
2.03
3.18
1.03
1.91
1.07
1.05
1.01
1.00
3.00

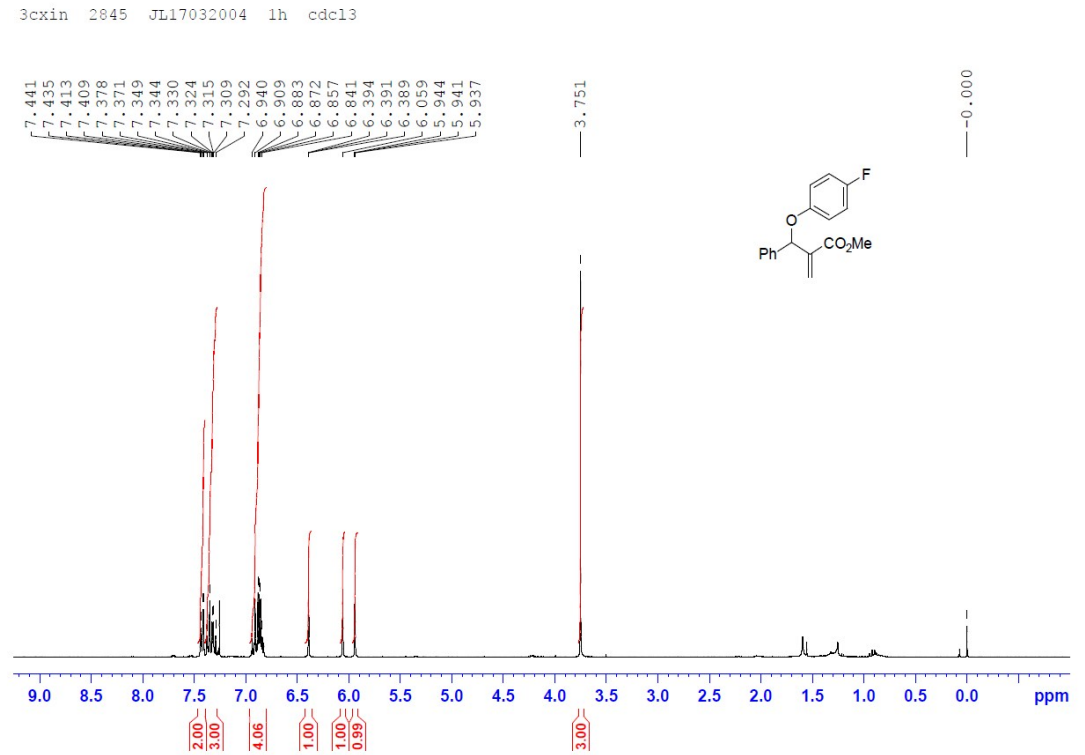

3cxin 2858 jl17032002 13c cdcl3
165.92
154.79
151.53
145.53
145.39
139.99
138.41
128.50
128.28
128.15
126.36
124.15
124.09
121.91
121.82
117.22
116.45
116.20
78.55
77.42
77.00
76.57
52.02
F
O
Ph
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

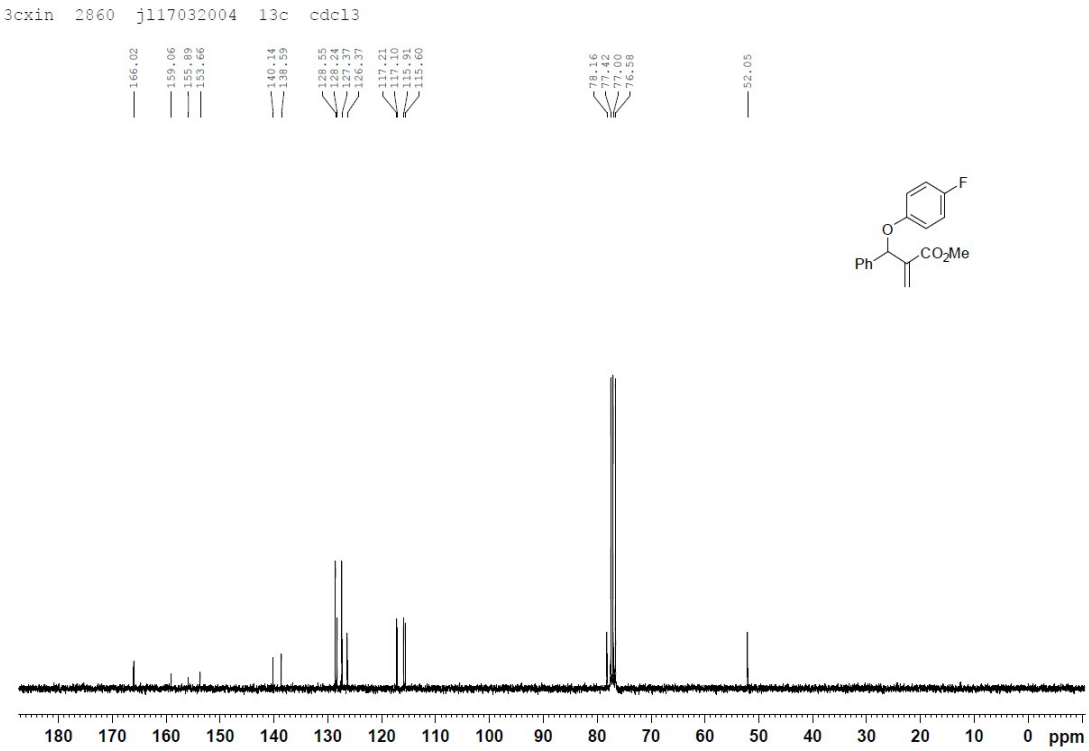
4i


3cxin 2844 JL17032003 1h cdcl3
7.450
7.444
7.423
7.418
7.384
7.377
7.356
7.330
7.321
7.299
7.202
7.179
7.175
7.151
7.146
7.123
6.723
6.718
6.712
6.693
6.687
6.668
6.660
6.656
6.630
6.625
6.617
6.606
6.603
6.396
6.126
5.935
5.932
5.928
3.756
0.000
F
O
Ph
CO2Me
10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
3.01
1.00
2.99
1.00
1.00
0.99
3.00

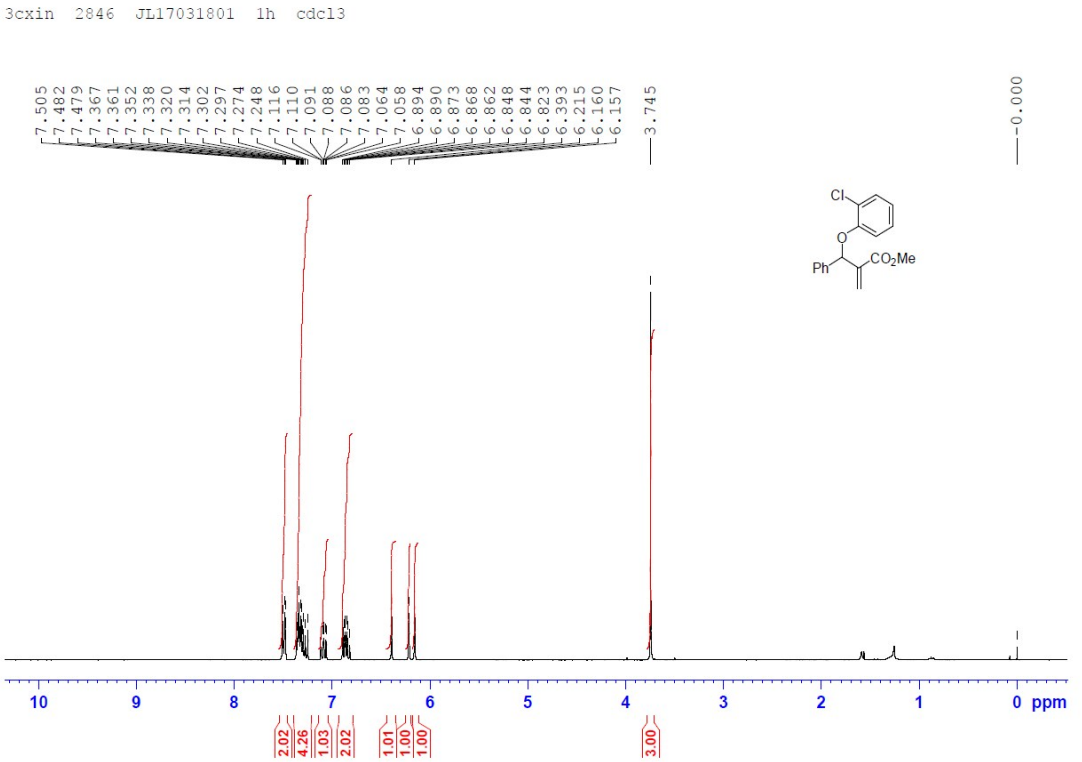

3cxin 2859 jl17032003 13c cdcl3
165.90
165.06
161.81
158.91
158.76
139.86
138.29
130.19
130.05
128.59
128.32
127.33
126.45
111.56
111.52
108.21
107.93
103.87
103.54
77.56
77.42
77.00
76.58
52.08
F
O
Ph
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

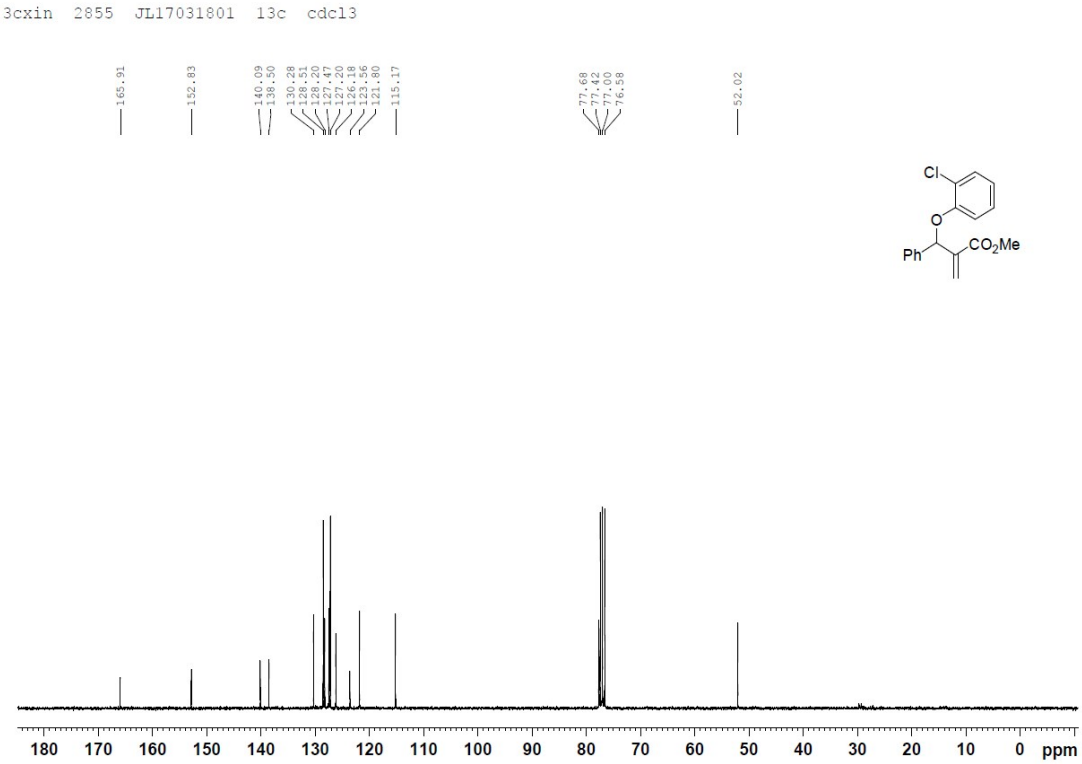
4j


3cxin 2845 JL17032004 1h cdcl3
7.441
7.435
7.413
7.409
7.378
7.371
7.349
7.344
7.330
7.324
7.315
7.309
7.292
6.940
6.909
6.883
6.872
6.857
6.841
6.394
6.391
6.389
6.059
5.944
5.941
5.937
3.751
-0.000
F
O
Ph
CO2Me
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 ppm
2.00
3.00
4.06
1.00
1.00
0.99
3.00

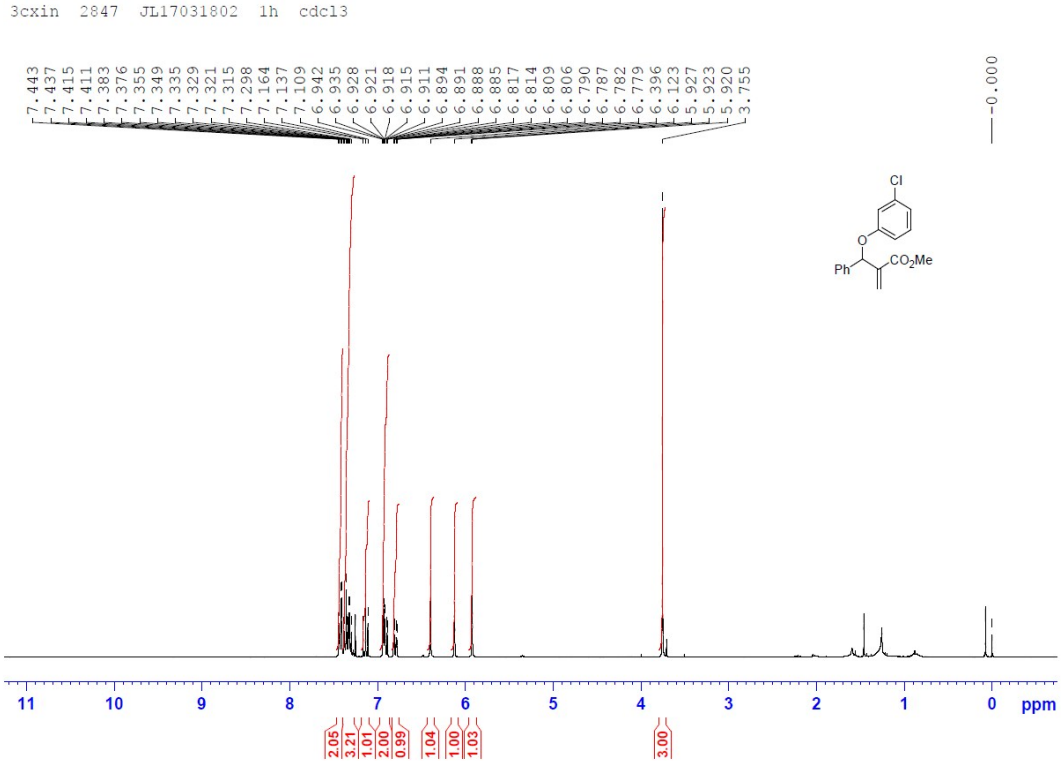

3cxin 2860 jl17032004 13c cdcl3
166.02
159.06
155.89
153.66
140.14
138.59
128.55
128.24
127.37
126.37
117.21
117.10
115.91
115.60
78.16
77.42
77.00
76.58
52.05
F
O
Ph
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

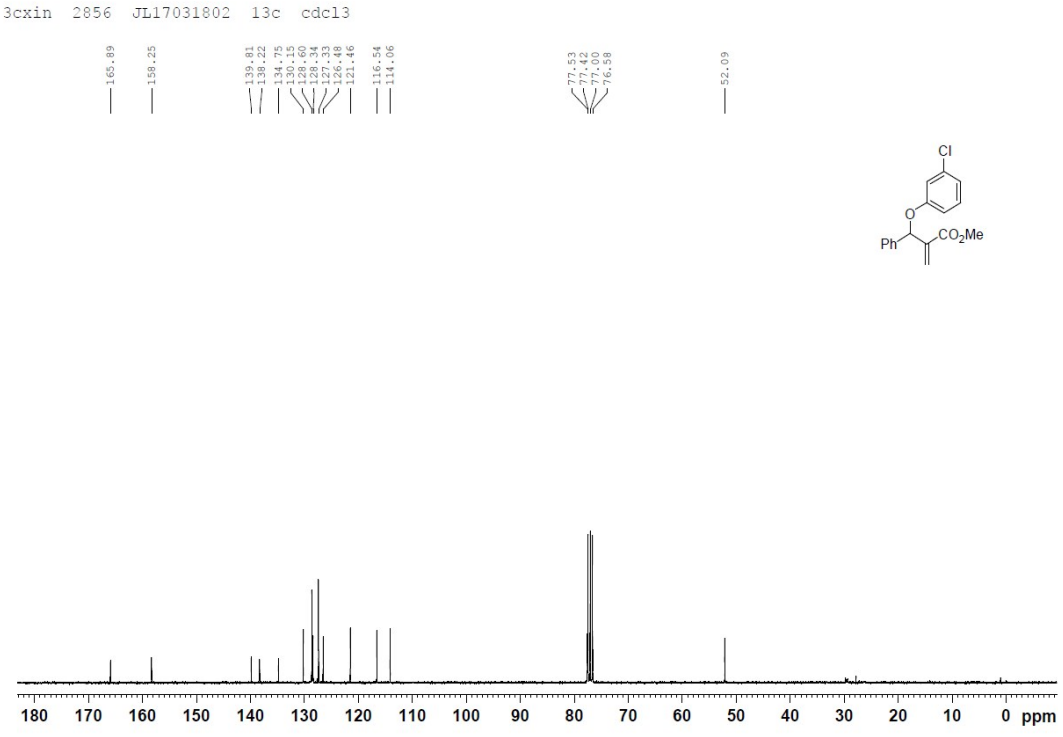
4k


3cxin 2846 JL17031801 1h cdcl3
7.505
7.482
7.479
7.367
7.361
7.352
7.338
7.320
7.314
7.302
7.297
7.274
7.248
7.116
7.110
7.091
7.088
7.086
7.083
7.064
7.058
6.894
6.890
6.873
6.868
6.862
6.848
6.844
6.823
6.393
6.215
6.160
6.157
3.745
0.000
Cl
O
Ph
CO2Me
10 9 8 7 6 5 4 3 2 1 0 ppm
2.02
4.26
1.03
2.02
1.01
1.00
1.00
3.00

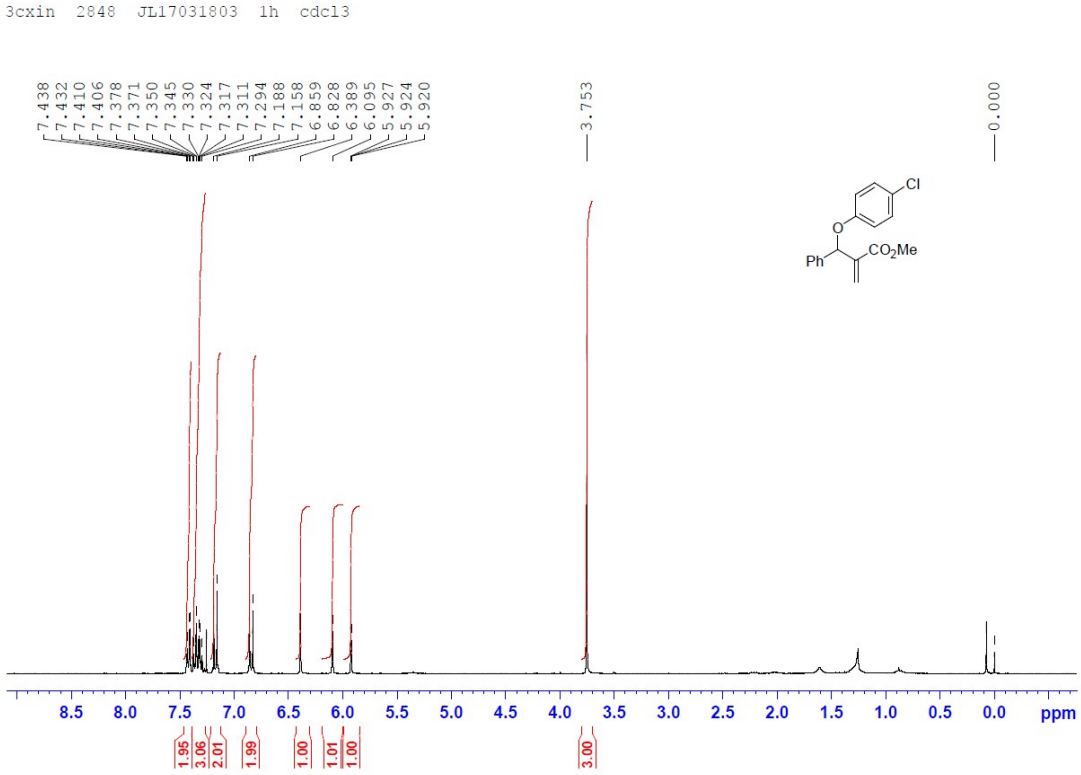

3cxin 2855 JL17031801 13c cdcl3
165.91
152.83
140.09
138.50
130.28
128.51
128.20
127.47
127.20
126.18
123.56
121.80
115.17
77.68
77.42
77.00
76.58
52.02
Cl
O
Ph
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

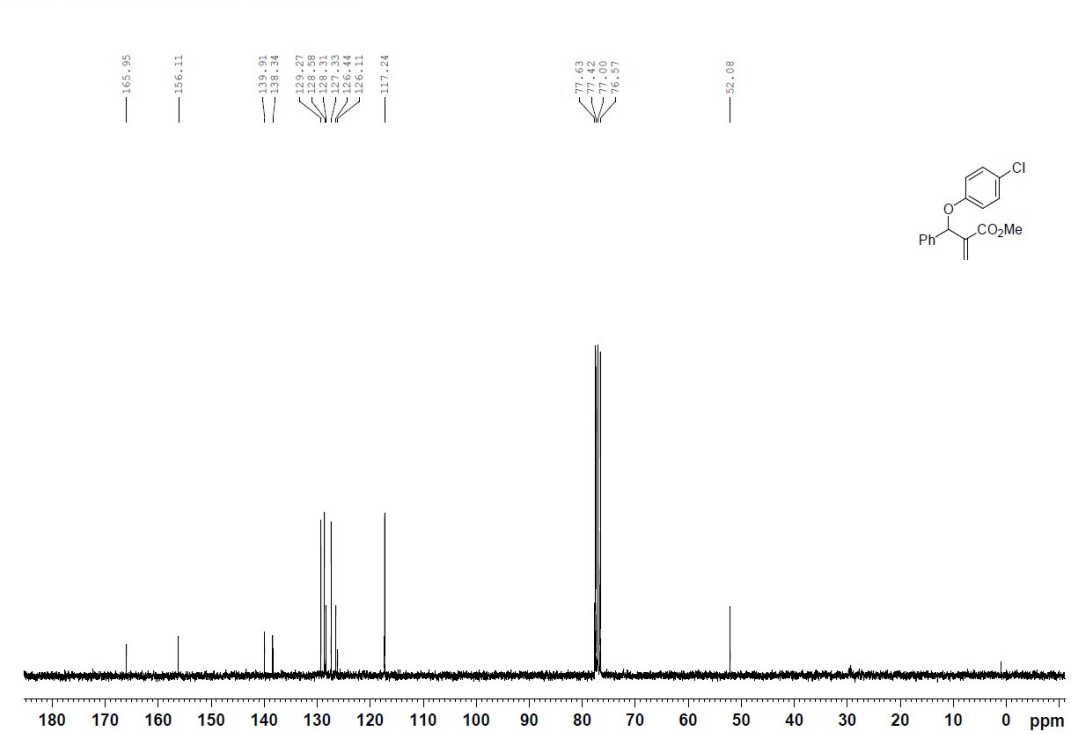
4l


3cxin 2847 JL17031802 1h cdcl3
7.443
7.437
7.415
7.411
7.383
7.376
7.355
7.349
7.335
7.329
7.321
7.315
7.298
7.164
7.137
7.109
6.942
6.935
6.928
6.921
6.918
6.915
6.911
6.894
6.891
6.888
6.885
6.817
6.814
6.809
6.806
6.790
6.787
6.782
6.779
6.396
6.123
5.927
5.923
5.920
3.755
-0.000
Cl
O
Ph
CO2Me
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.05
3.21
1.01
2.00
0.99
1.04
1.00
1.03
3.00

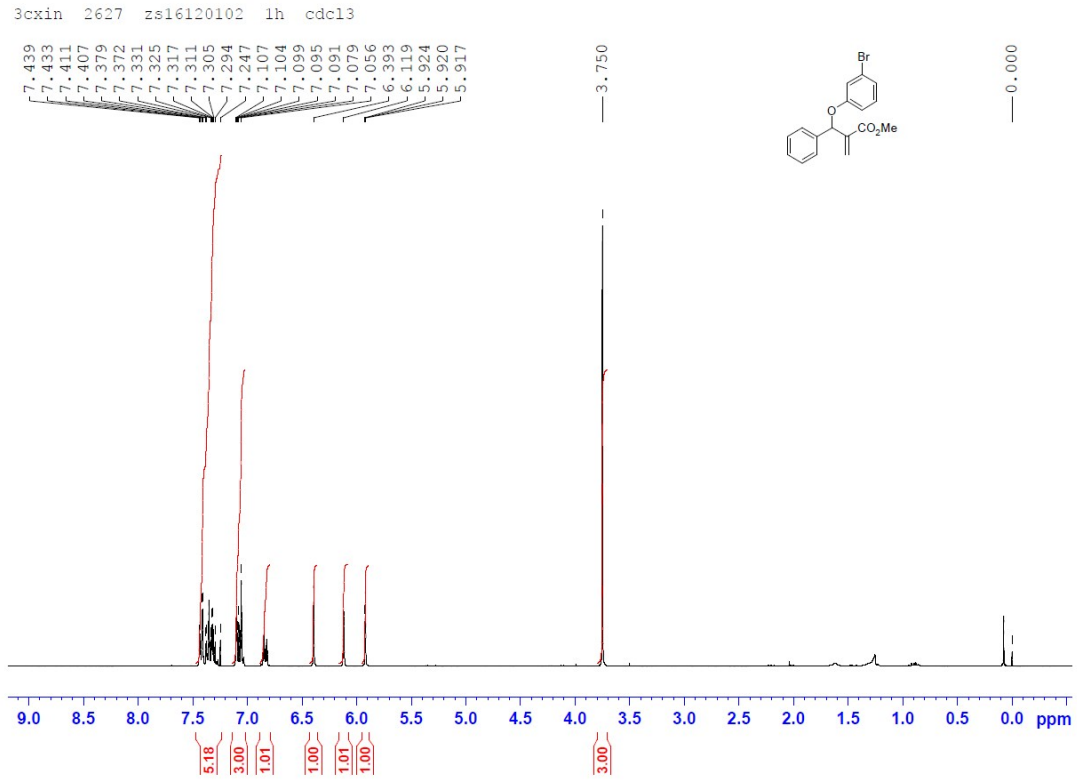

3cxin 2856 JL17031802 13c cdcl3
165.89
158.25
139.81
138.22
134.75
130.15
128.60
128.34
127.33
126.48
121.46
116.54
114.06
77.53
77.42
77.00
76.58
52.09
Cl
O
Ph
CO2Me
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

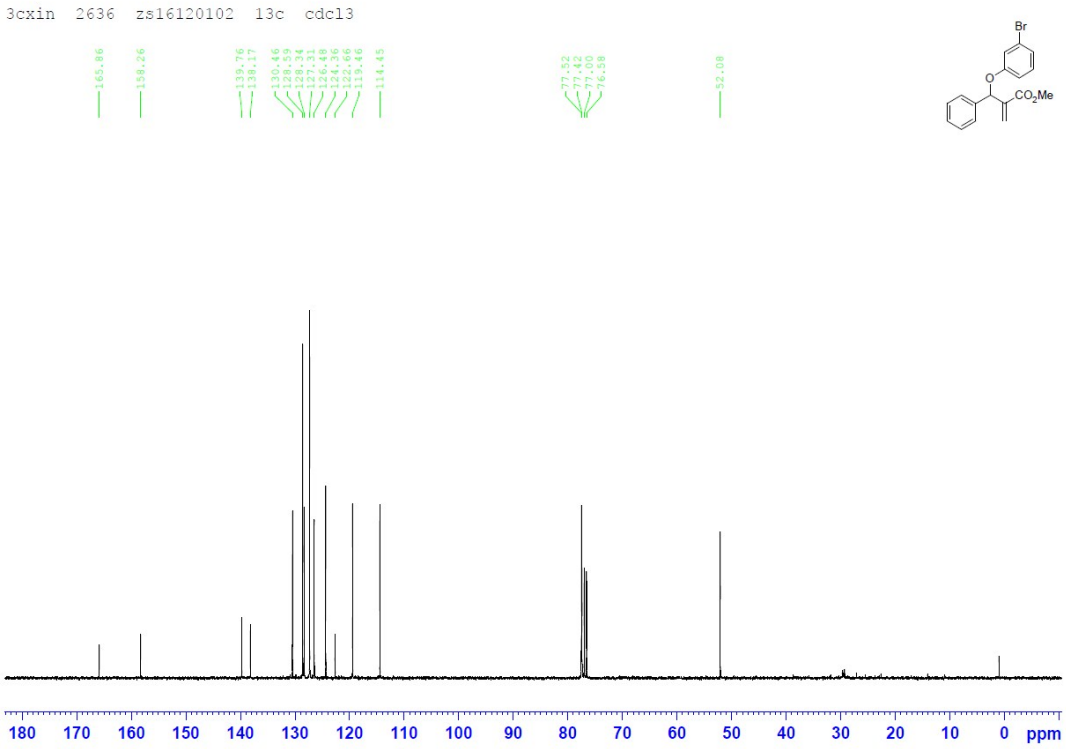
4m


3cxin 2848 JL17031803 1h cdcl3
7.438
7.432
7.410
7.406
7.378
7.371
7.350
7.345
7.330
7.324
7.317
7.311
7.294
7.188
7.158
6.859
6.828
6.389
6.095
5.927
5.924
5.920
3.753
0.000
Cl
O
Ph
CO2Me
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 ppm
1.95
3.06
2.01
1.99
1.00
1.01
1.00
3.00

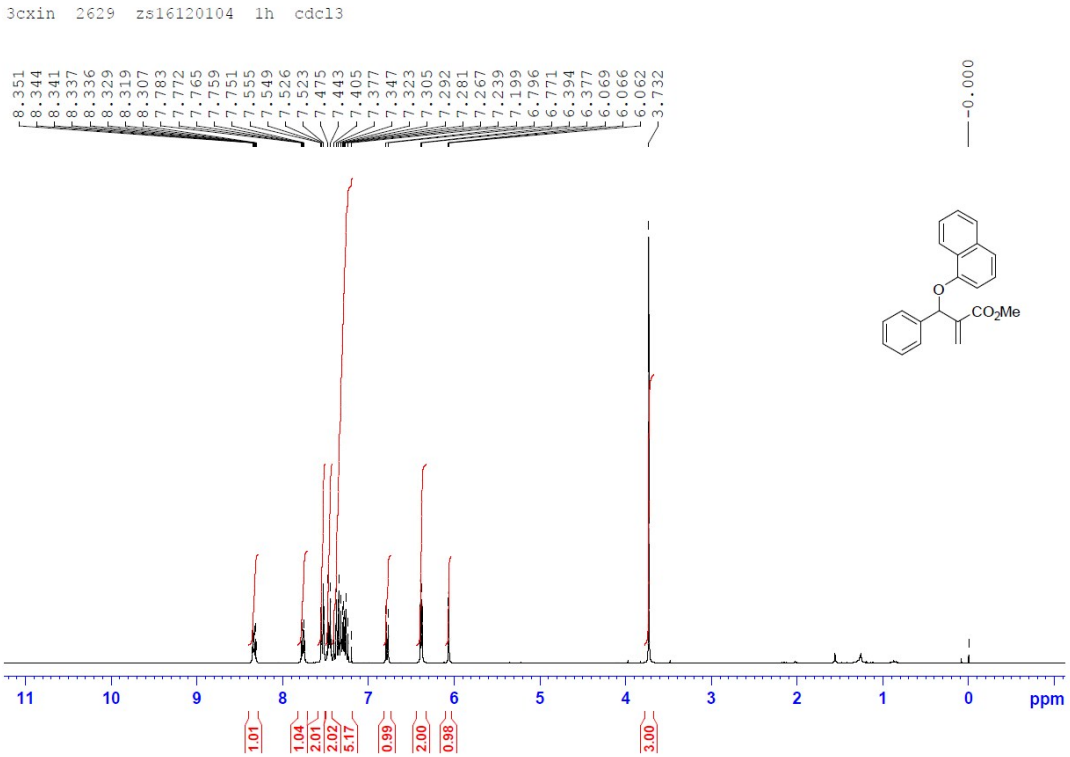

3cxin 2857 JL17031803 13c cdcl3
165.95
156.11
139.91
138.34
129.27
128.58
128.31
127.33
126.44
126.11
117.24
77.63
77.42
77.00
76.57
52.08
Cl
O
Ph
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

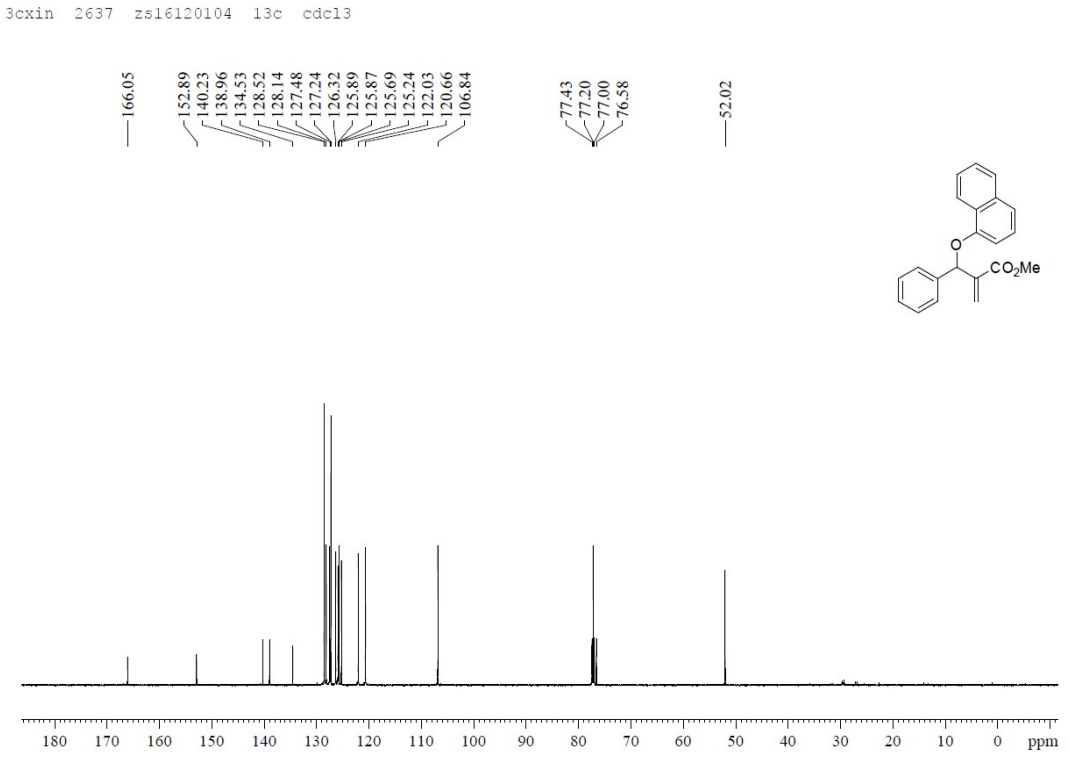
4n


3cxin 2627 zs16120102 1h cdcl3
7.439
7.433
7.411
7.407
7.379
7.372
7.331
7.325
7.317
7.311
7.305
7.294
7.247
7.107
7.104
7.099
7.095
7.091
7.079
7.056
6.393
6.119
5.924
5.920
5.917
3.750
0.000
Br
O
CO2Me
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 ppm
5.18
3.00
1.01
1.00
1.01
1.00
3.00

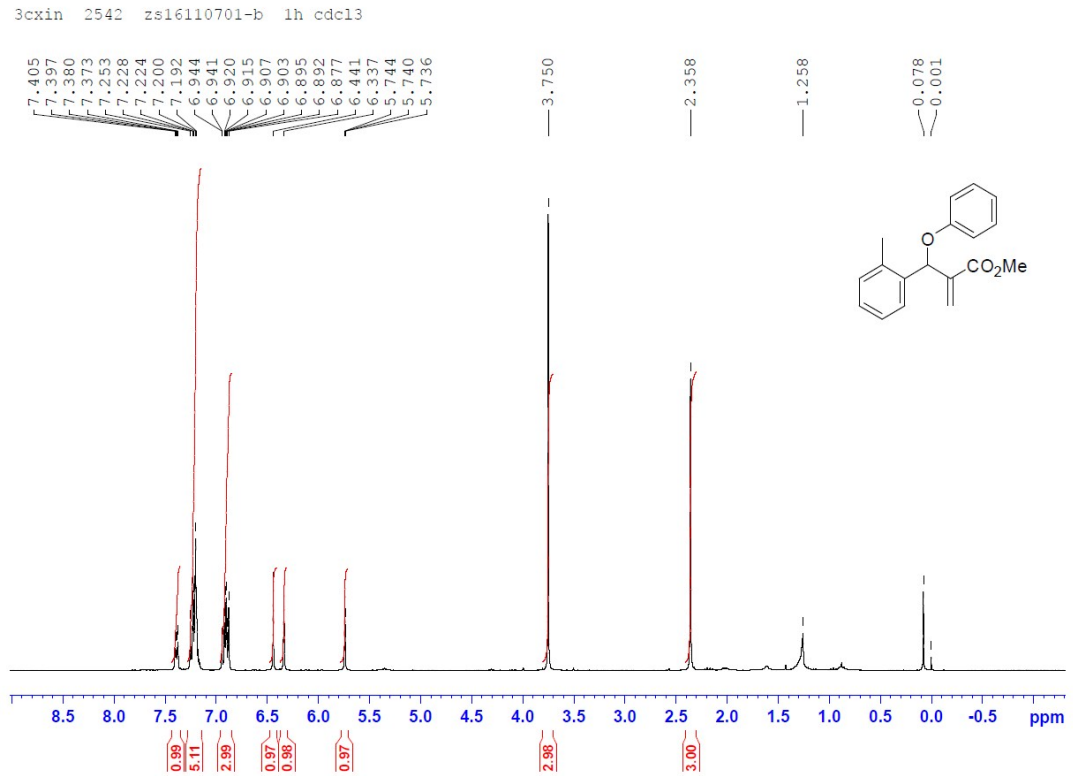

3cxin 2636 zs16120102 13c cdcl3
165.86
158.26
139.76
139.17
130.46
128.59
128.34
127.31
126.48
124.36
123.66
119.46
114.45
77.52
77.42
77.00
76.58
52.08
Br
O
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

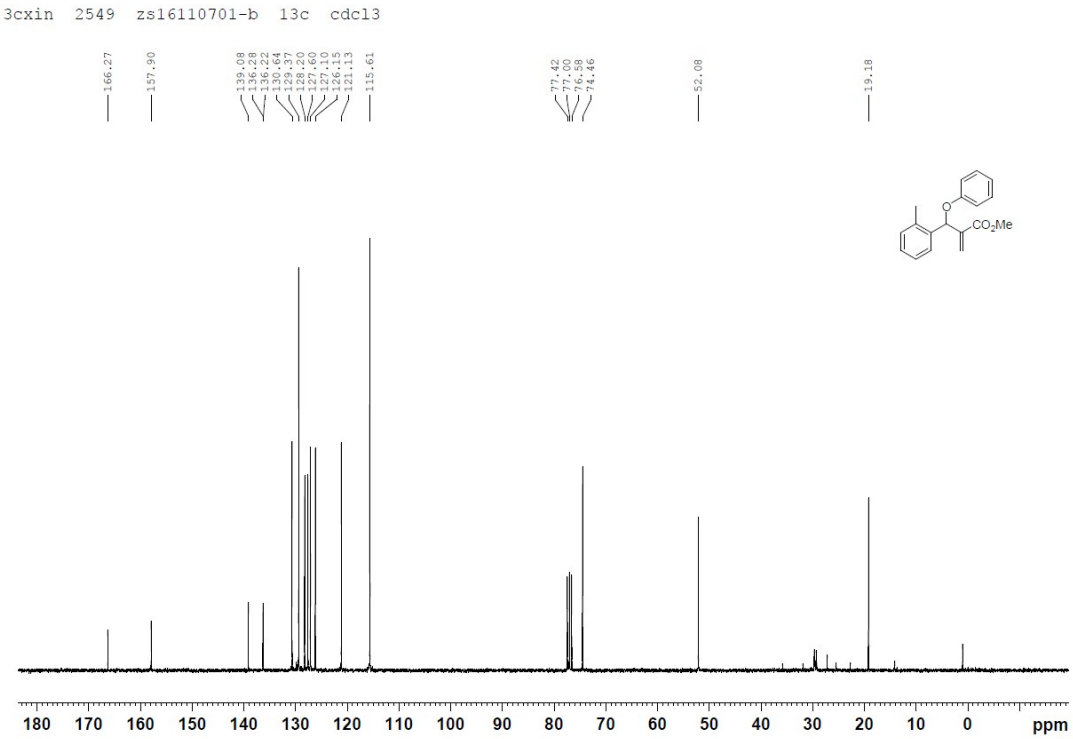
4o


3cxin 2629 zs16120104 1h cdcl3
8.351
8.344
8.341
8.337
8.336
8.329
8.319
8.307
7.783
7.772
7.765
7.759
7.751
7.555
7.549
7.526
7.523
7.475
7.443
7.405
7.377
7.347
7.323
7.305
7.292
7.281
7.267
7.239
7.199
6.796
6.771
6.394
6.377
6.069
6.066
6.062
3.732
0.000
CO2Me
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.01
1.04
2.01
2.02
5.17
0.99
2.00
0.98
3.00

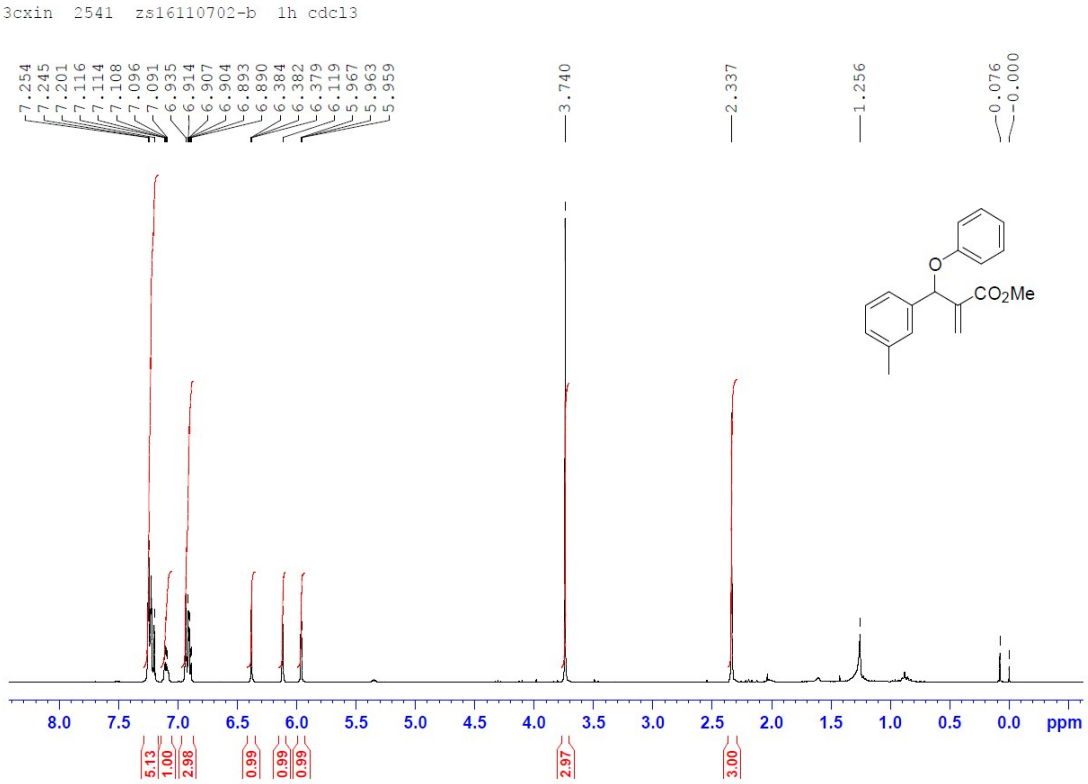

3cxin 2637 zs16120104 13c cdcl3
166.05
152.89
140.23
138.96
134.53
128.52
128.14
127.48
127.24
126.32
125.89
125.87
125.69
125.24
122.03
120.66
106.84
77.43
77.20
77.00
76.58
52.02
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

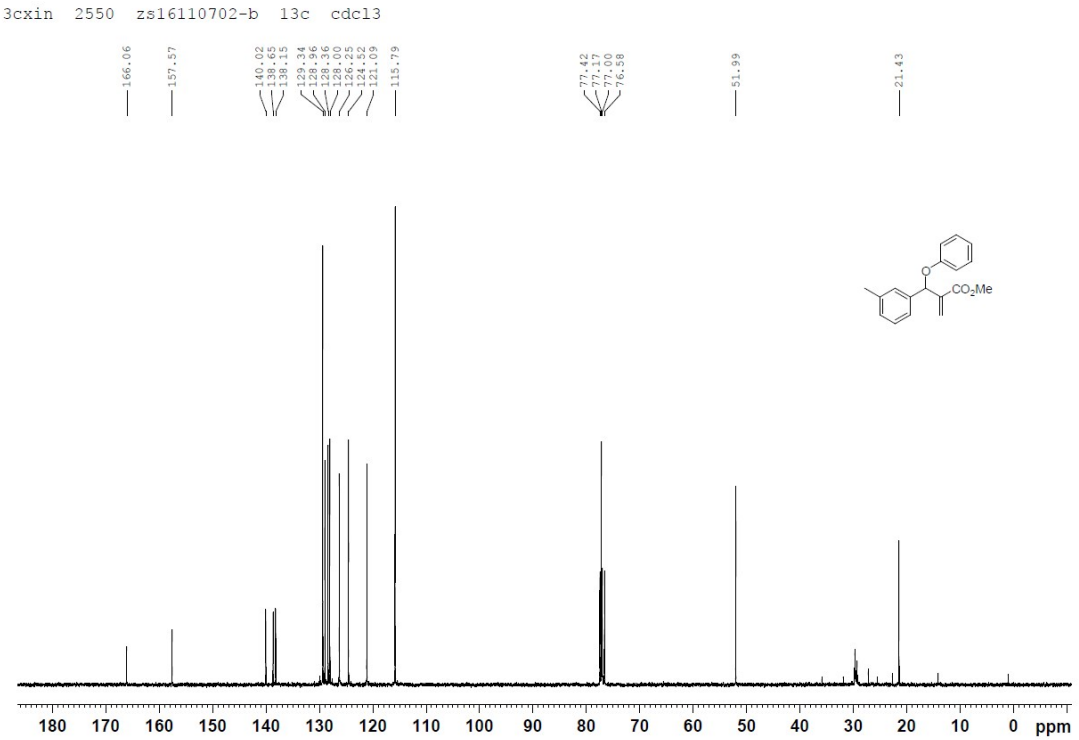
4p


3cxin 2542 zs16110701-b 1h cdcl3
7.405
7.397
7.380
7.373
7.253
7.228
7.224
7.200
7.192
6.944
6.941
6.920
6.915
6.907
6.903
6.895
6.892
6.877
6.441
6.337
5.744
5.740
5.736
3.750
2.358
1.258
0.078
0.001
CO2Me
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 ppm
0.99
5.11
2.99
0.97
0.98
0.97
2.98
3.00

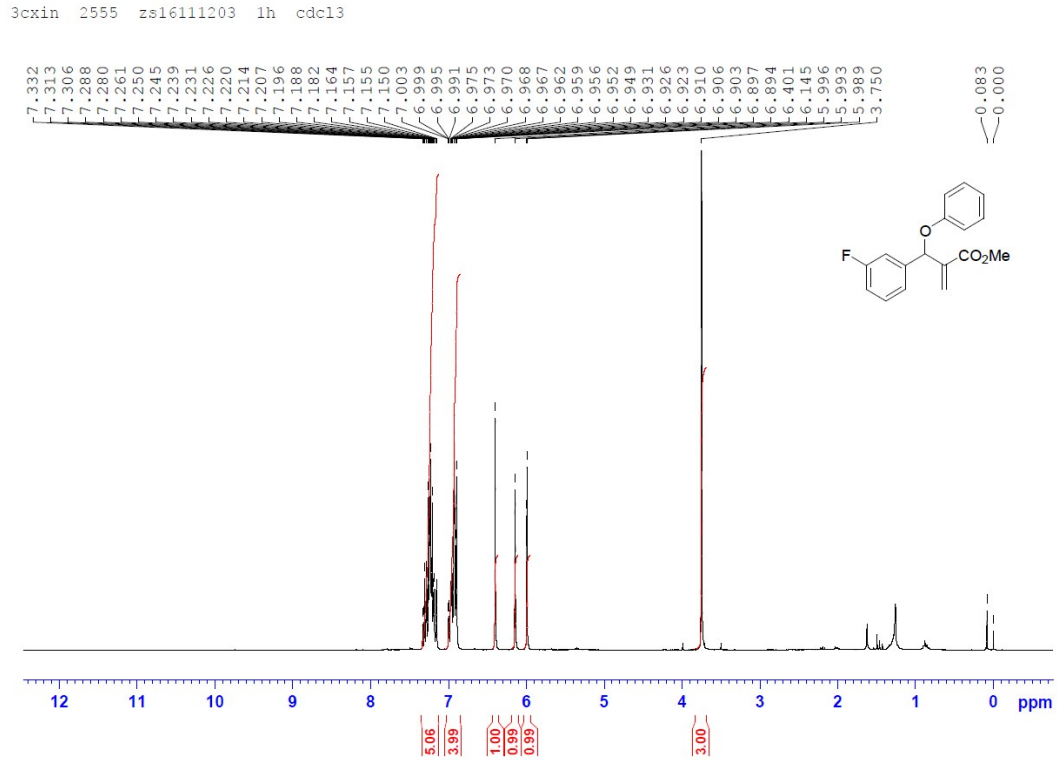

3cxin 2549 zs16110701-b 13c cdcl3
166.27
157.90
139.08
136.28
136.22
130.64
129.37
128.20
127.60
127.10
126.15
121.13
115.61
77.42
77.00
76.58
74.46
52.08
19.18
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

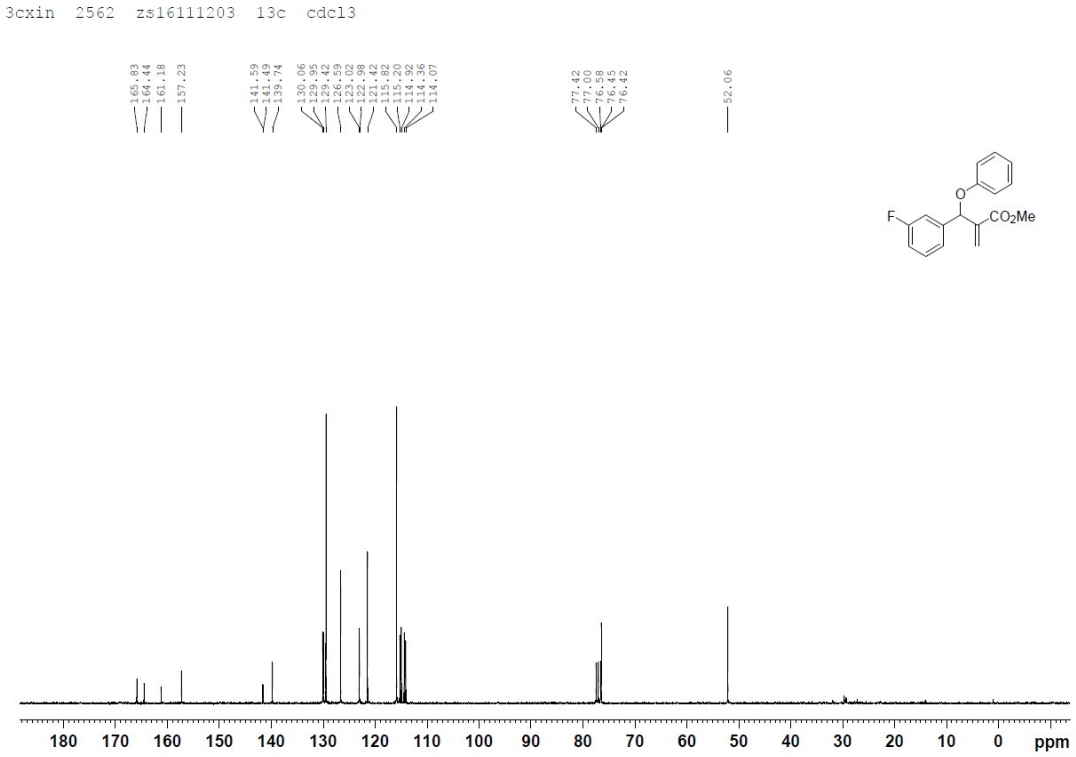
4q


3cxin 2541 zs16110702-b 1h cdcl3
7.254
7.245
7.201
7.116
7.114
7.108
7.096
7.091
6.935
6.914
6.907
6.904
6.893
6.890
6.384
6.382
6.379
6.119
5.967
5.963
5.959
3.740
2.337
1.256
0.076
0.000
CO2Me
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 ppm
5.13
1.00
2.98
0.99
0.99
0.99
2.97
3.00

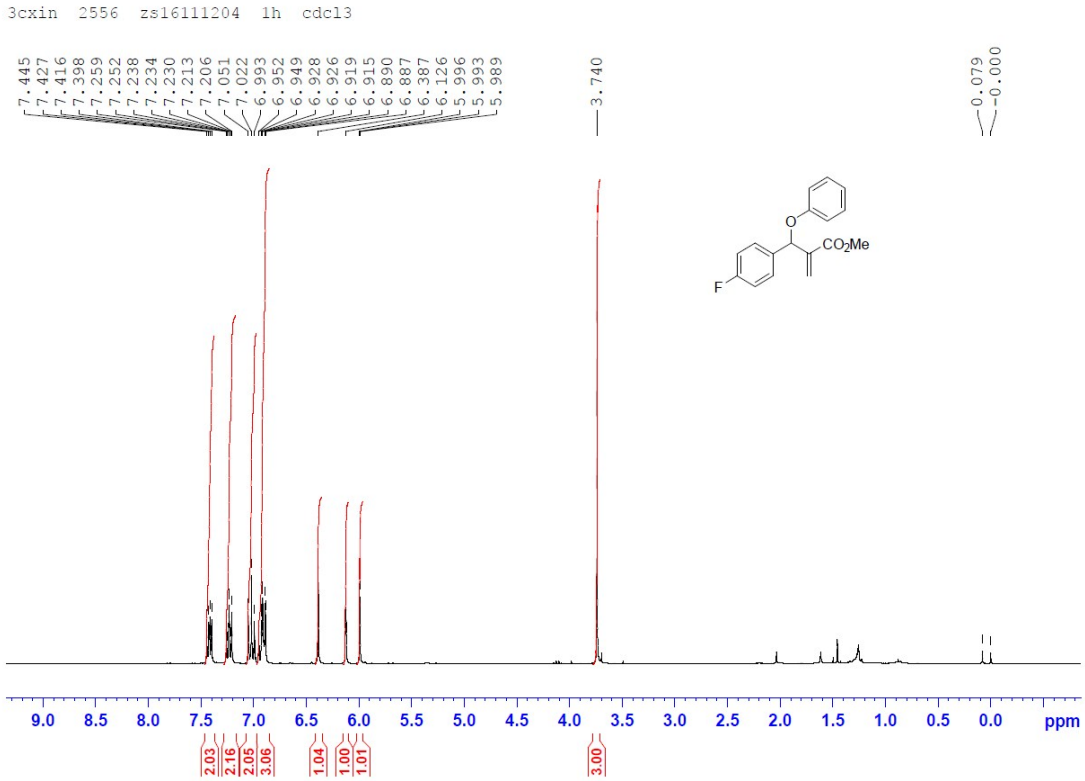

3cxin 2550 zs16110702-b 13c cdcl3
166.06
157.57
140.02
138.65
138.15
129.34
128.96
128.36
128.00
126.55
124.52
121.09
115.79
77.42
77.17
77.00
76.58
51.99
21.43
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

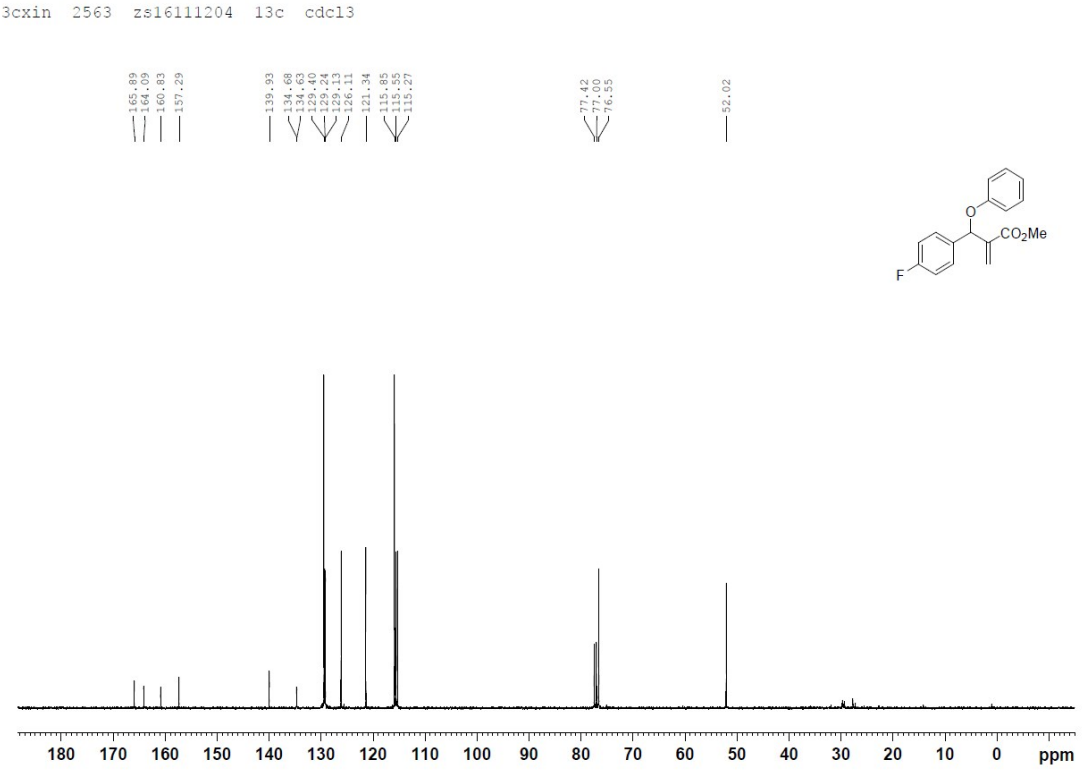
4r


3cxin 2555 zs16111203 1h cdcl3
7.332
7.313
7.306
7.288
7.280
7.261
7.250
7.245
7.239
7.231
7.226
7.220
7.214
7.207
7.196
7.188
7.182
7.164
7.157
7.155
7.150
7.003
6.999
6.995
6.991
6.975
6.973
6.970
6.968
6.967
6.962
6.959
6.956
6.952
6.949
6.931
6.926
6.923
6.910
6.906
6.903
6.897
6.894
6.401
6.145
5.996
5.993
5.989
3.750
0.083
0.000
F
O
CO2Me
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
5.06
3.99
1.00
0.99
0.99
3.00

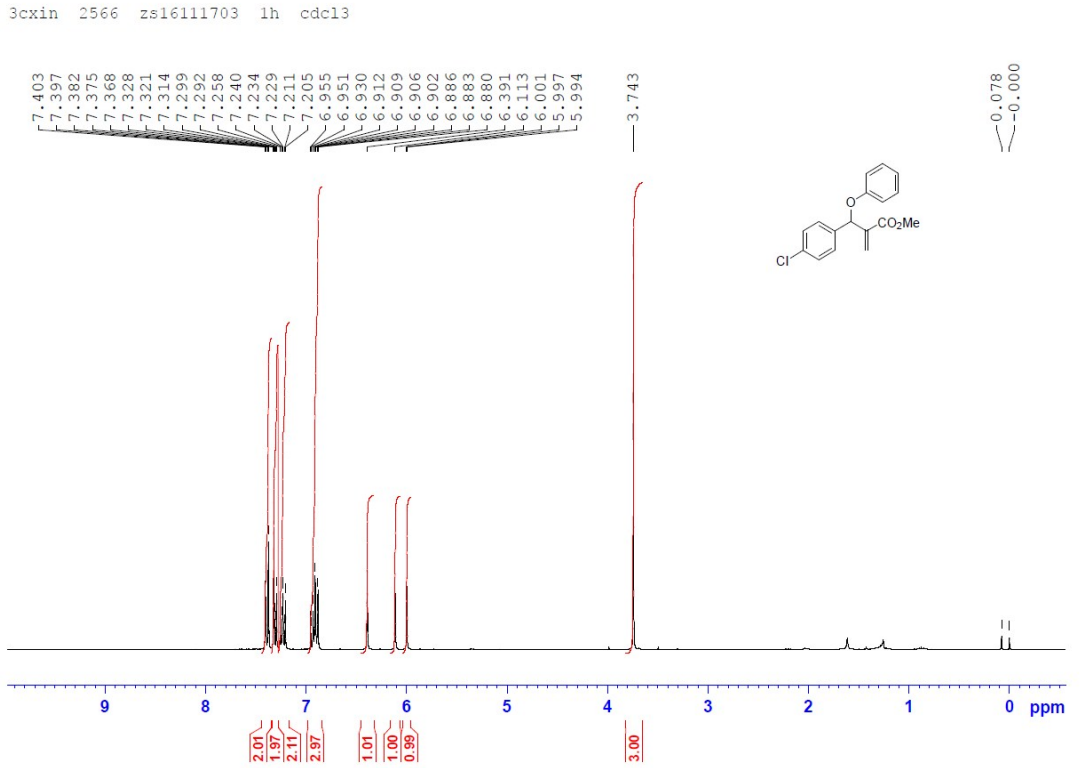

3cxin 2562 zs16111203 13c cdcl3
165.83
164.44
161.18
157.23
141.59
141.49
139.74
130.06
129.95
129.42
126.59
123.02
122.88
122.42
115.82
115.20
114.92
114.36
114.07
77.42
77.00
76.58
76.45
76.42
52.06
F
O
CO2Me
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

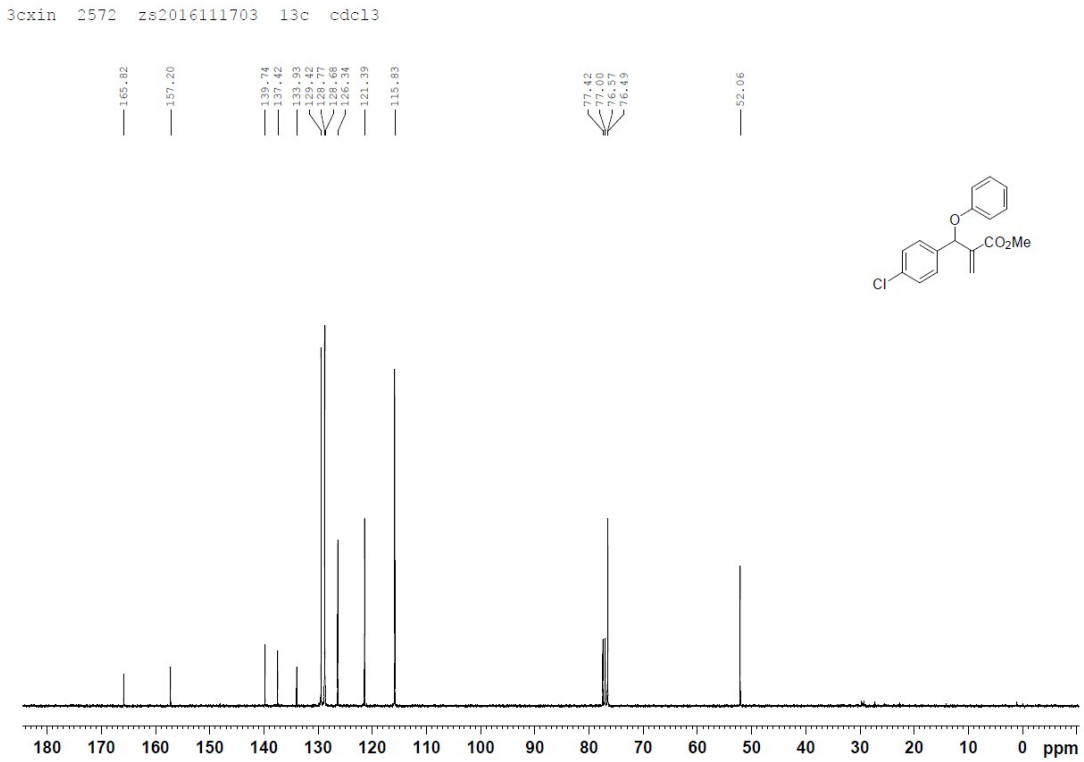
4s


3cxin 2556 zs16111204 1h cdcl3
7.445
7.427
7.416
7.398
7.259
7.252
7.238
7.234
7.230
7.213
7.206
7.051
7.022
6.993
6.952
6.949
6.928
6.926
6.919
6.915
6.890
6.887
6.387
6.126
5.996
5.993
5.989
3.740
0.079
-0.000
O
CO2Me
F
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 ppm
2.03
2.16
2.05
3.06
1.04
1.00
1.01
3.00


3cxin 2563 zs16111204 13c cdcl3
165.89
164.09
160.83
157.29
139.93
134.68
134.63
129.40
129.24
129.13
126.11
121.34
115.85
115.55
115.27
77.42
77.00
76.55
52.02
O
CO2Me
F
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

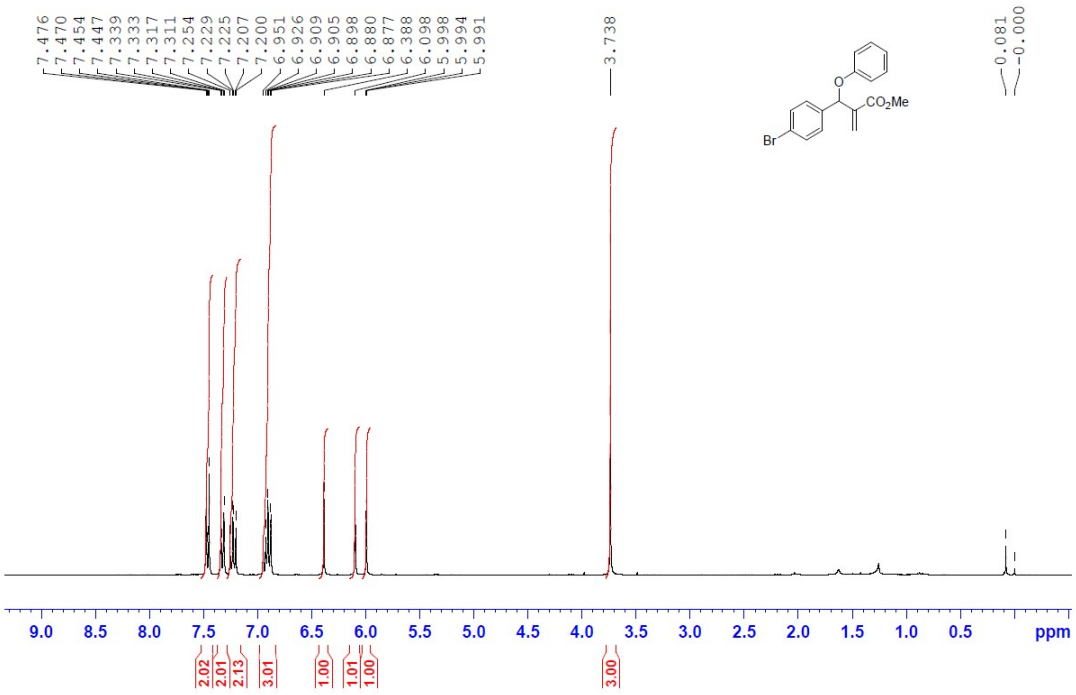
4t


3cxin 2566 zs16111703 1h cdcl3
7.403
7.397
7.382
7.375
7.368
7.328
7.321
7.314
7.299
7.292
7.258
7.240
7.234
7.229
7.211
7.205
6.955
6.951
6.930
6.912
6.909
6.906
6.902
6.886
6.883
6.880
6.391
6.113
6.001
5.997
5.994
3.743
0.078
-0.000
CO2Me
Cl
9
8
7
6
5
4
3
2
1
0 ppm
2.01
1.97
2.11
2.97
1.01
1.00
0.99
3.00

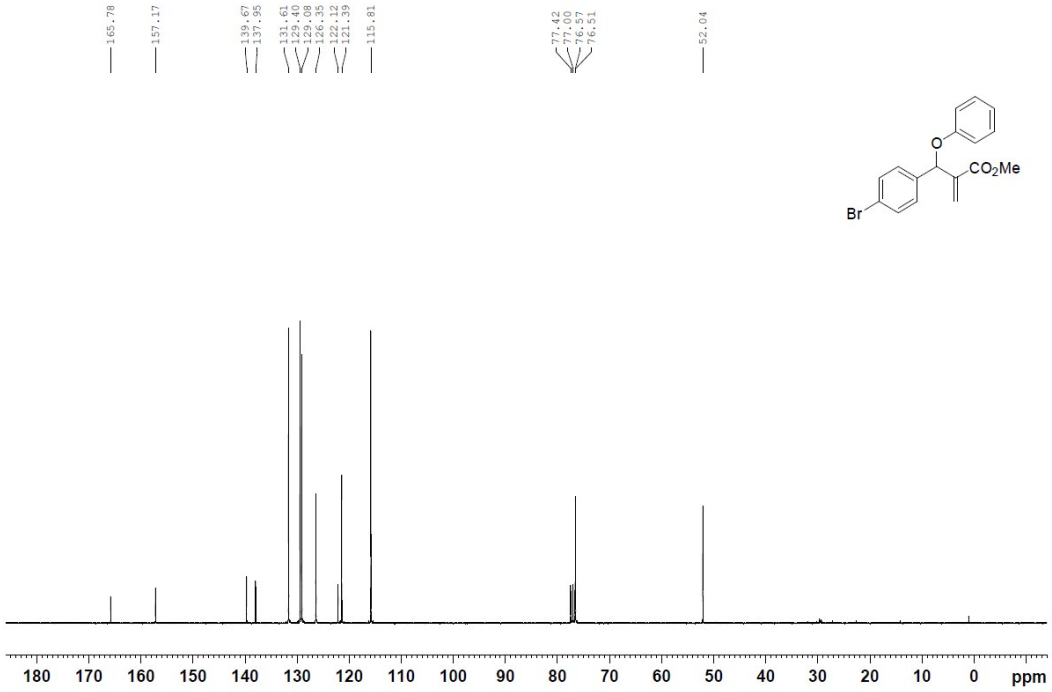

3cxin 2572 zs2016111703 13c cdcl3
165.82
157.20
139.74
137.42
133.93
129.42
128.77
128.68
126.34
121.39
115.83
77.42
77.00
76.57
76.49
52.06
CO2Me
Cl
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

4u

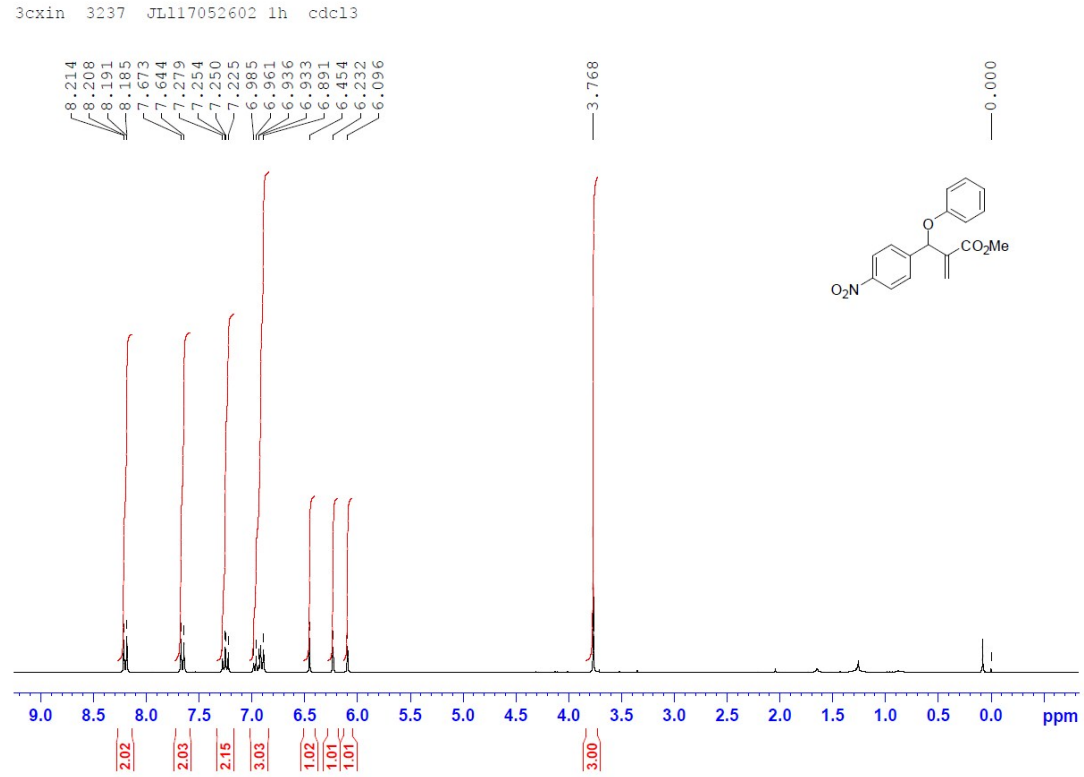
3cxin 2565 zs16111702 1h cdcl3

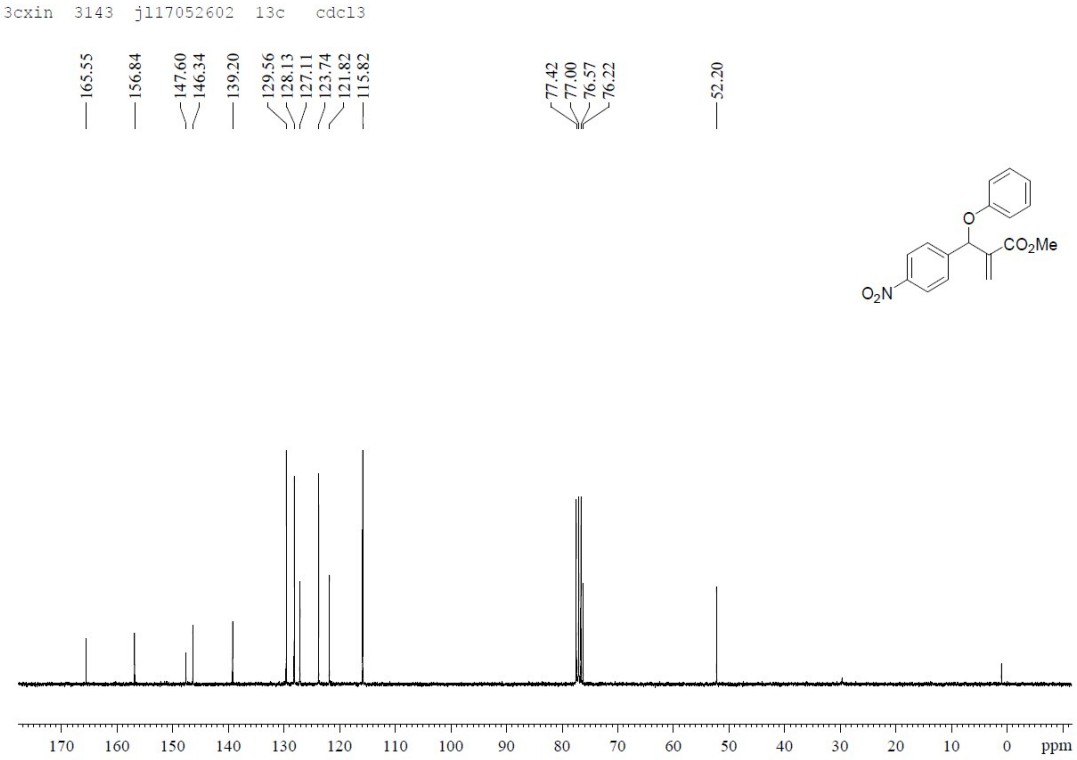


3cxin 2571 zs2016111702 13c cdcl3

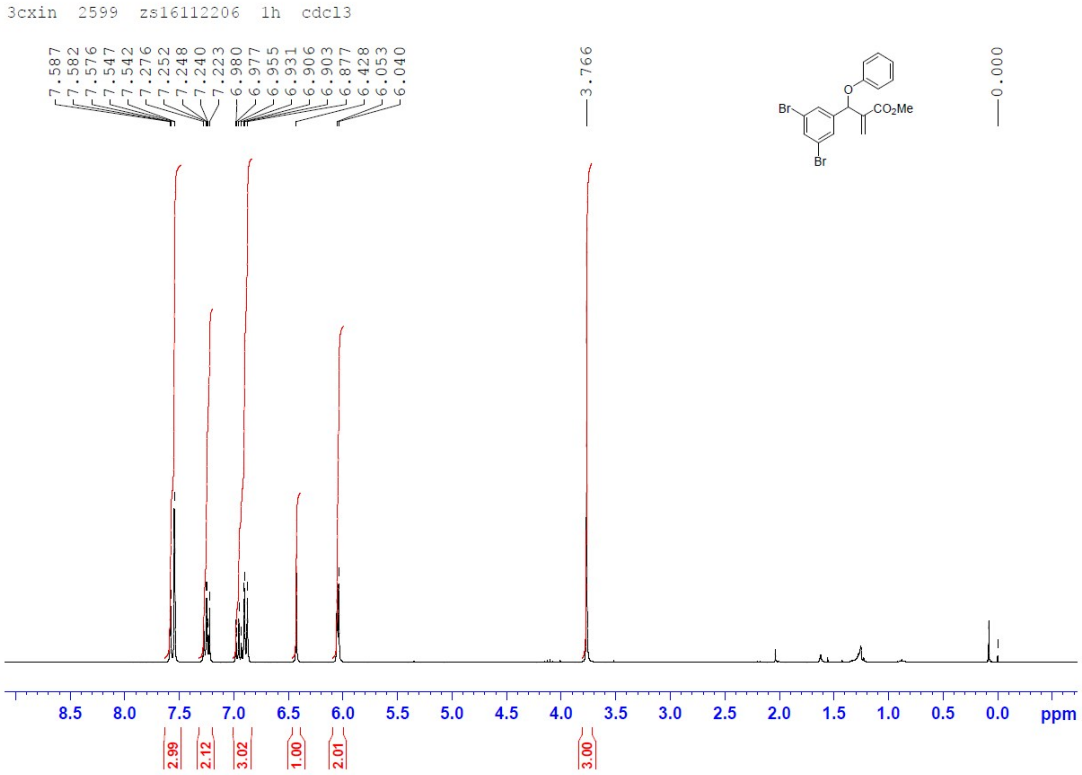


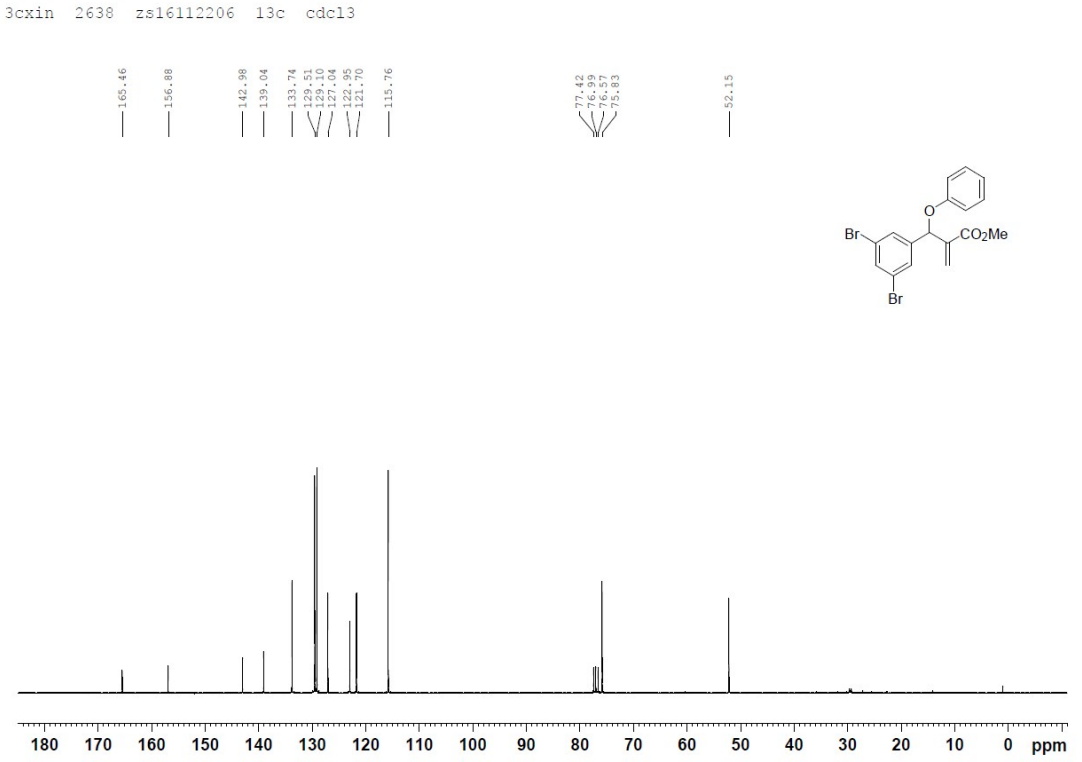
4v


3cxin 3237 JL117052602 1h cdcl3
8.214
8.208
8.191
8.185
7.673
7.644
7.279
7.254
7.250
7.225
6.985
6.961
6.936
6.933
6.891
6.454
6.232
6.096
3.768
0.000
CO2Me
O2N
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 ppm
2.02
2.03
2.15
3.03
1.02
1.01
1.01
3.00

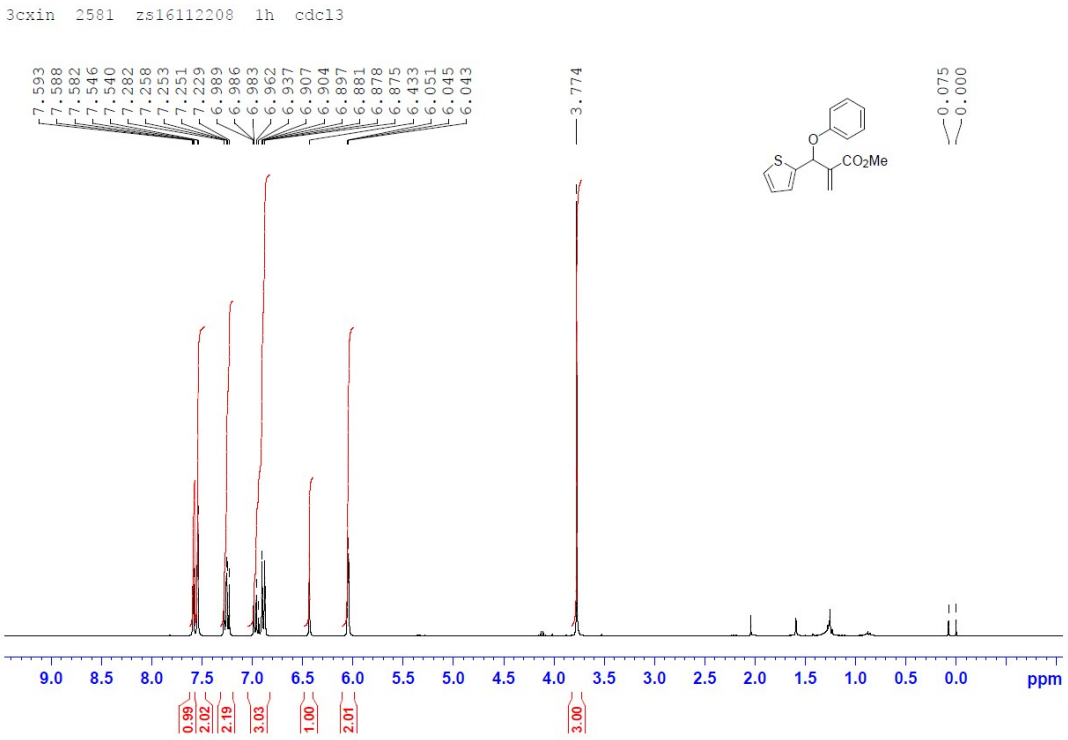

3cxin 3143 jl117052602 13c cdcl3
165.55
156.84
147.60
146.34
139.20
129.56
128.13
127.11
123.74
121.82
115.82
77.42
77.00
76.57
76.22
52.20
CO2Me
O2N
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

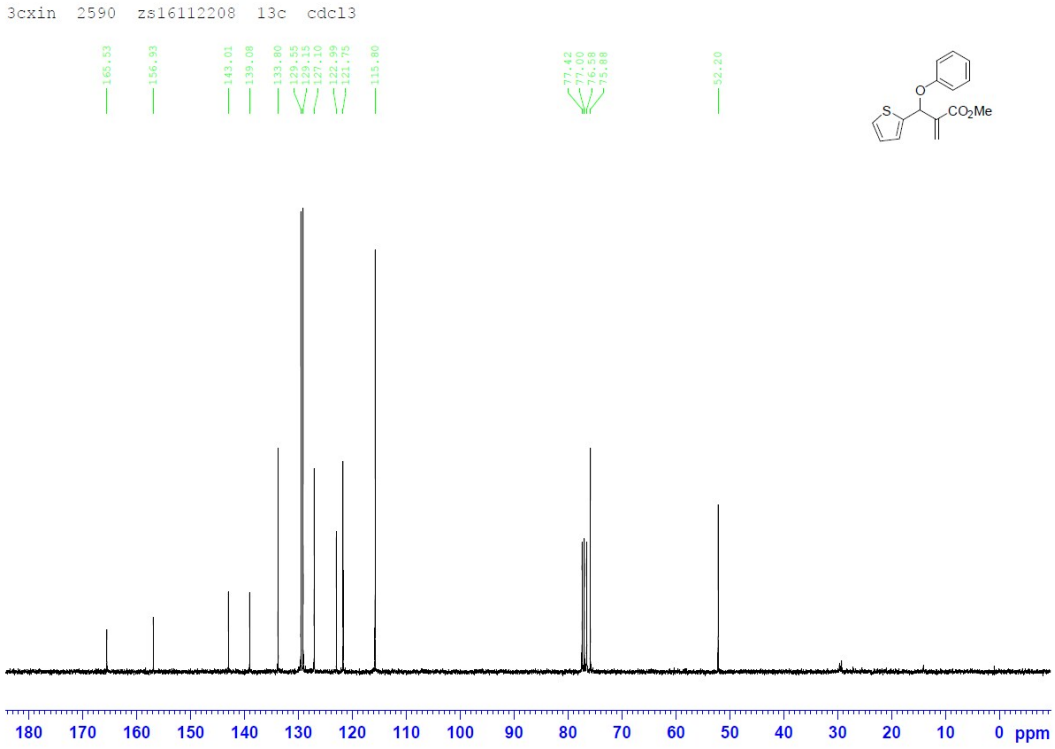
4w


3cxin 2599 zs16112206 1h cdcl3
7.587
7.582
7.576
7.547
7.542
7.276
7.252
7.248
7.240
7.223
6.980
6.977
6.955
6.931
6.906
6.903
6.877
6.428
6.053
6.040
3.766
0.000
Br
O
CO2Me
Br
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 ppm
2.99
2.12
3.02
1.00
2.01
3.00

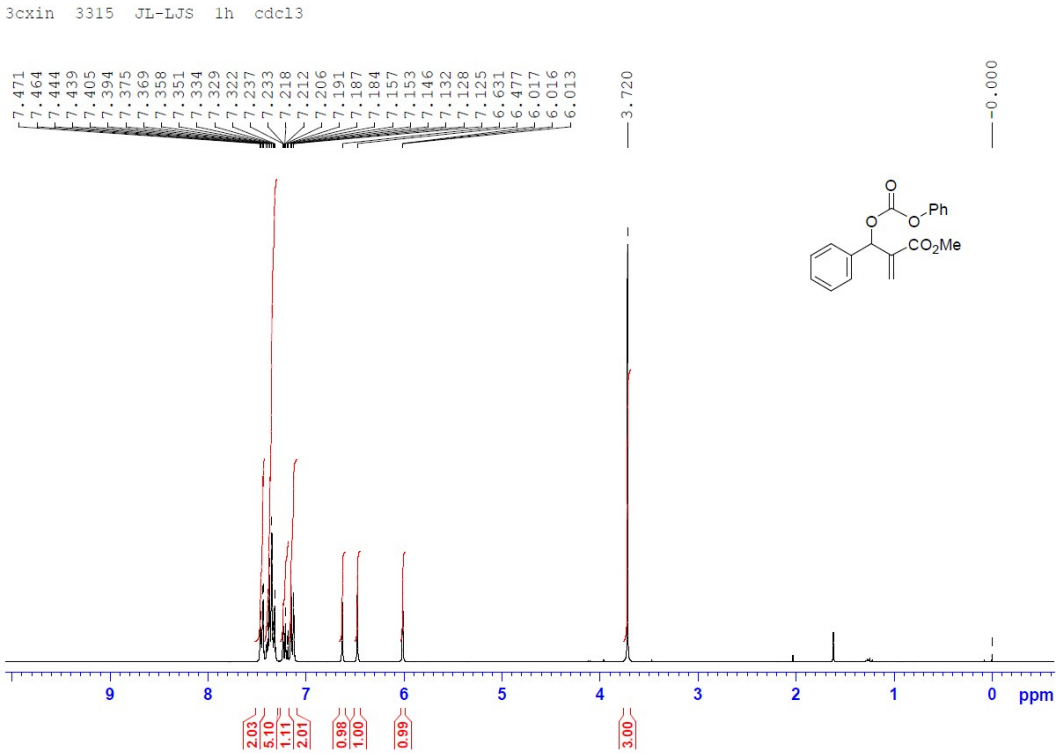

3cxin 2638 zs16112206 13c cdcl3
165.46
156.88
142.98
139.04
133.74
129.51
129.10
127.04
122.95
121.70
115.76
77.42
76.99
76.57
75.83
52.15
Br
O
CO2Me
Br
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

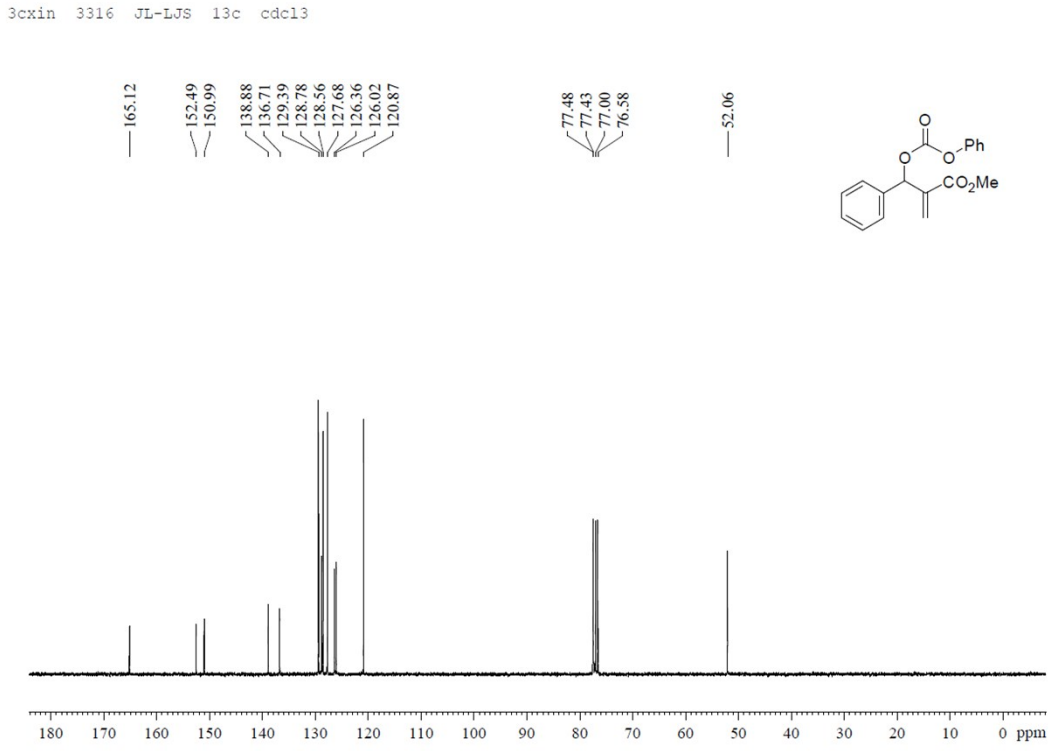
4x


3cxin 2581 zs16112208 1h cdcl3
7.593
7.588
7.582
7.546
7.540
7.282
7.258
7.253
7.251
7.229
6.989
6.986
6.983
6.962
6.937
6.907
6.904
6.897
6.881
6.878
6.875
6.433
6.051
6.045
6.043
3.774
0.075
0.000
O
S
CO2Me
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 ppm
0.99
2.02
2.19
3.03
1.00
2.01
3.00


3cxin 2590 zs16112208 13c cdcl3
165.53
156.93
143.01
139.08
133.80
129.55
129.15
127.10
122.99
121.75
115.80
77.42
77.00
76.58
75.80
52.20
O
S
CO2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

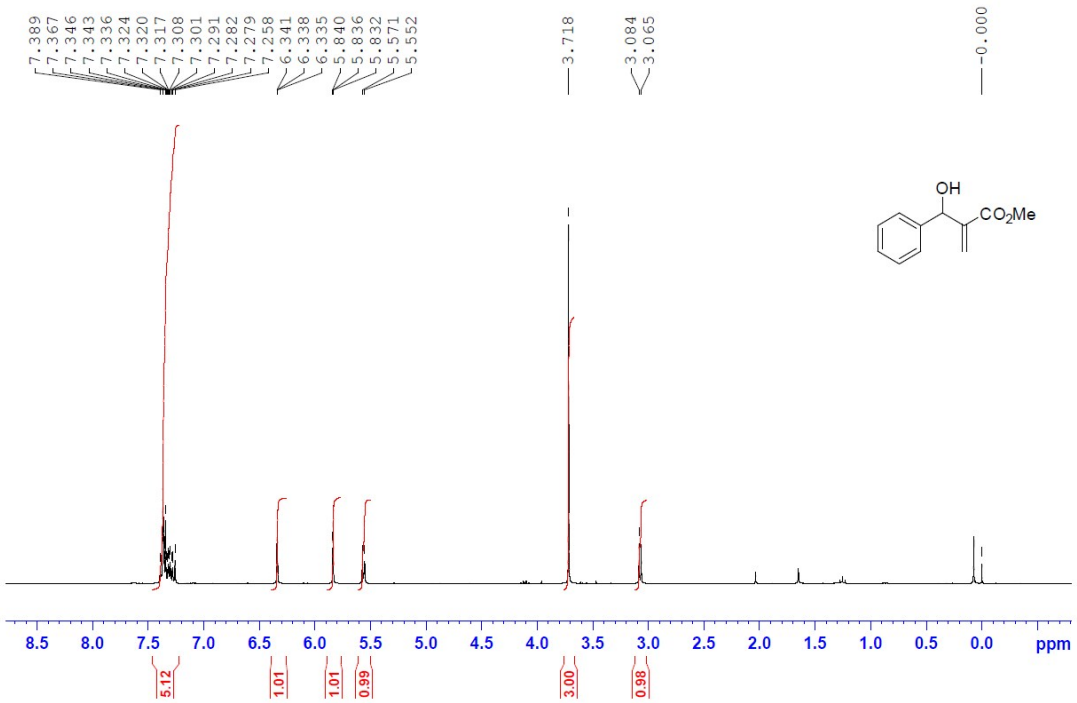
5a


3cxin 3315 JL-LJS 1h cdcl3
7.471
7.464
7.444
7.439
7.405
7.394
7.375
7.369
7.358
7.351
7.334
7.329
7.322
7.237
7.233
7.218
7.212
7.206
7.191
7.187
7.184
7.157
7.153
7.146
7.132
7.128
7.125
6.631
6.477
6.017
6.016
6.013
3.720
0.000
Ph
CO2Me
9
8
7
6
5
4
3
2
1
0
ppm
2.03
5.10
1.11
2.01
0.98
1.00
0.99
3.00

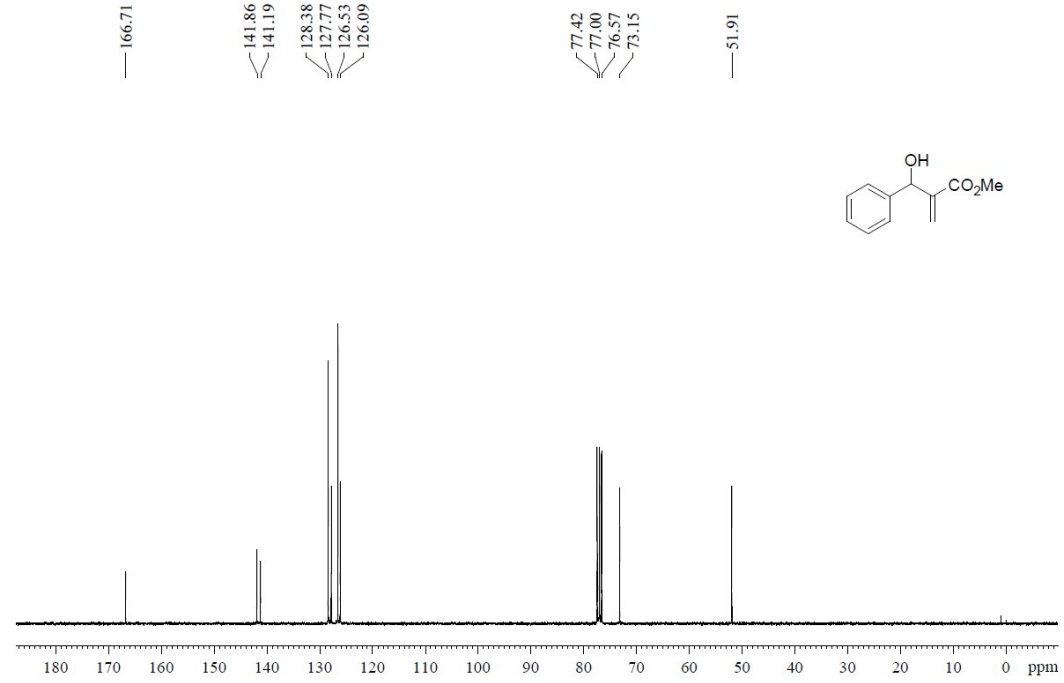

3cxin 3316 JL-LJS 13c cdcl3
165.12
152.49
150.99
138.88
136.71
129.39
128.78
128.56
127.68
126.36
126.02
120.87
77.48
77.43
77.00
76.58
52.06
Ph
CO2Me
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

6

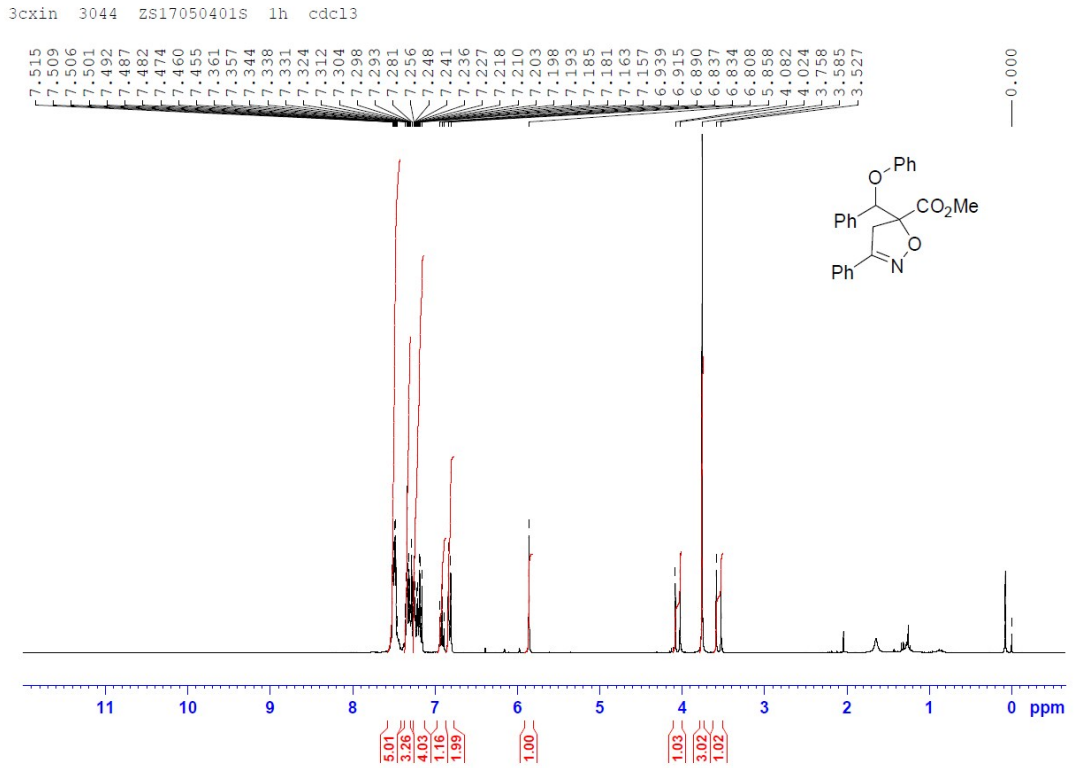
3cxin 3141 jl-oh 1h cdcl3

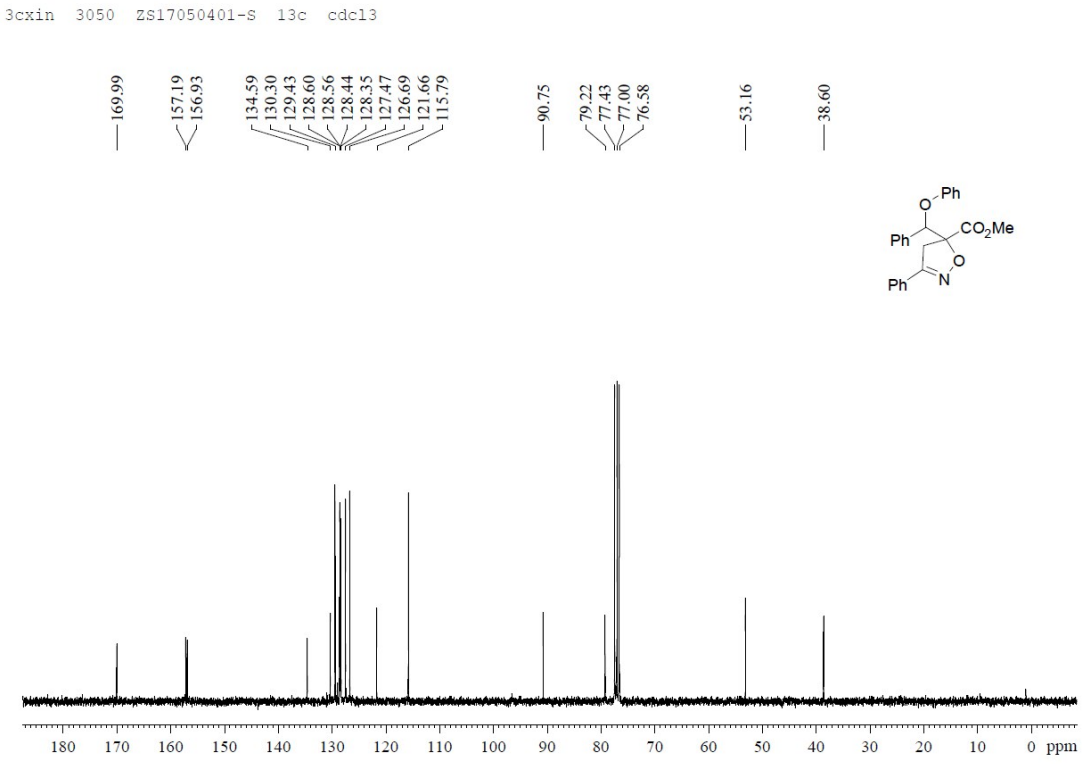


3cxin 3410 JL-OH 13c cdcl3



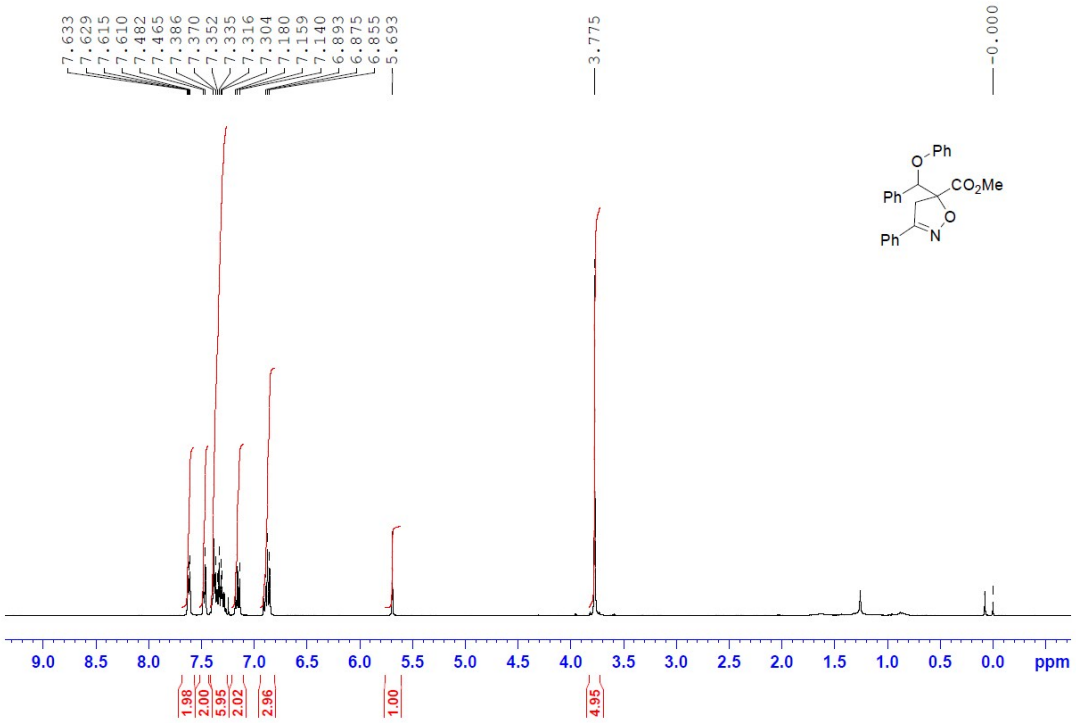
7a (one of the two diastereomers)



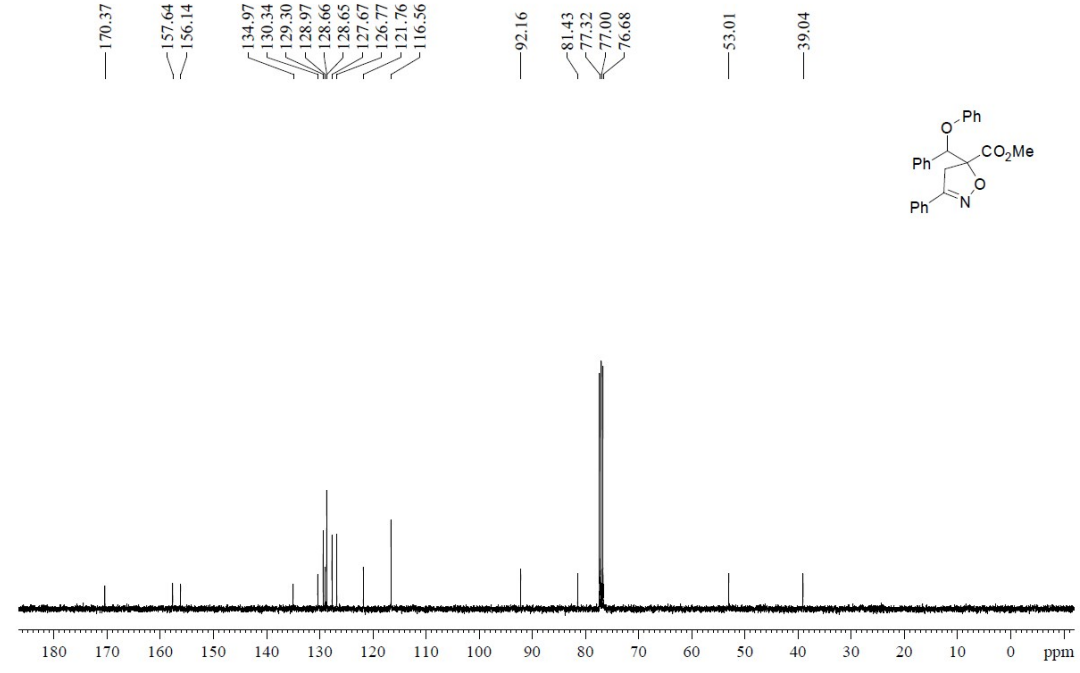


7a’ (another of the two diastereomers)

4chenxin25/29 jl17061201-x 1HCDCl3

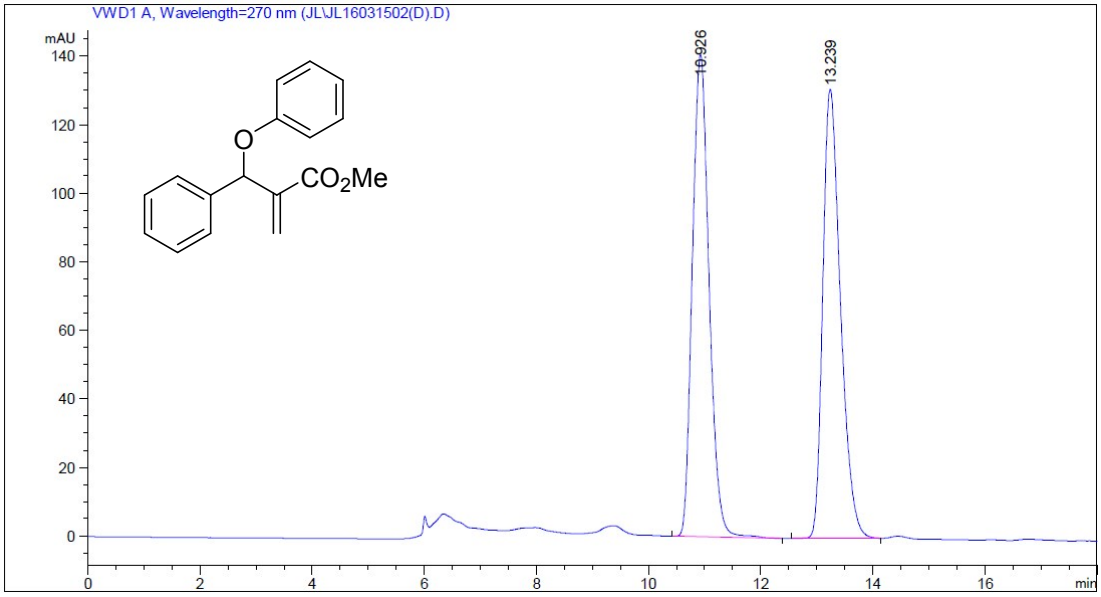


4chenxin25/30 jl17061201-x 13CCDCl3

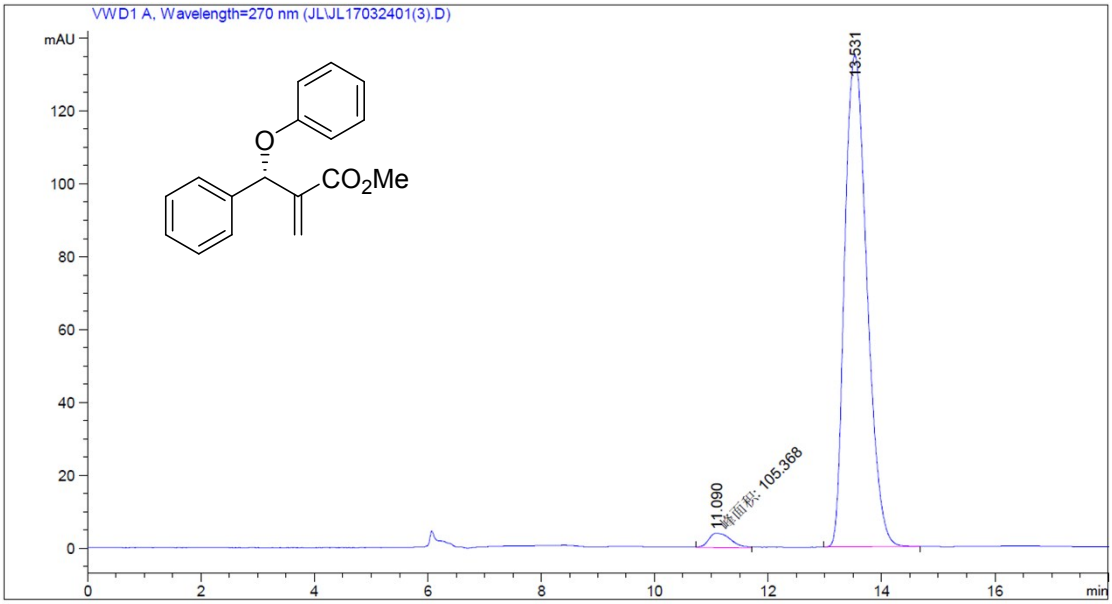


9. Chiral HPLC chromatograms of 4, 5, 6, 7

4a

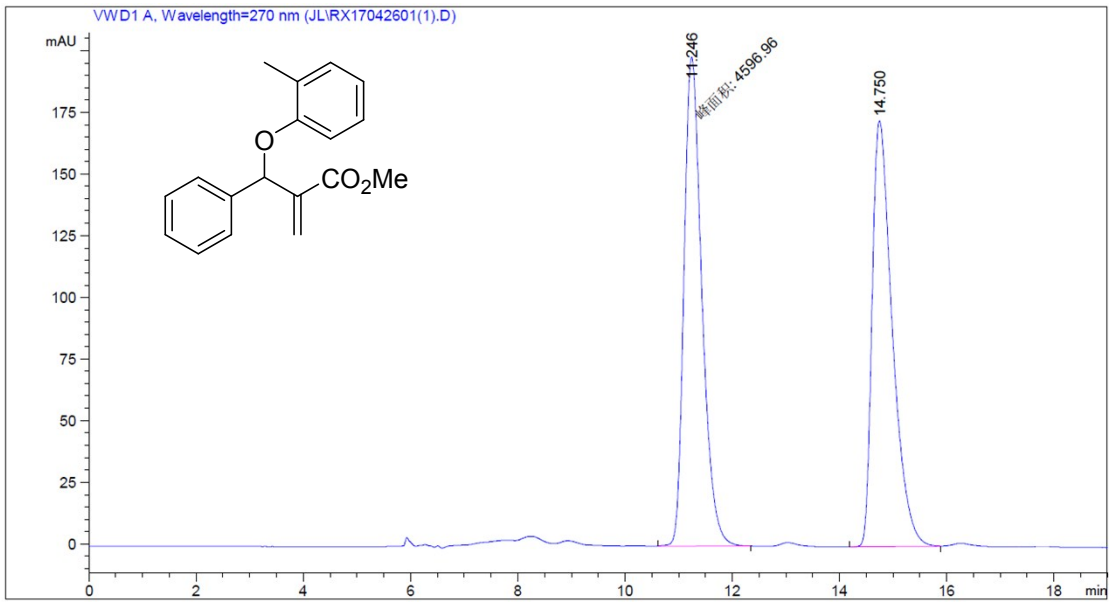


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.926	0.3270	2908.53271	140.74579	50.3021
2	13.239	0.3358	2873.59473	131.08319	49.6979

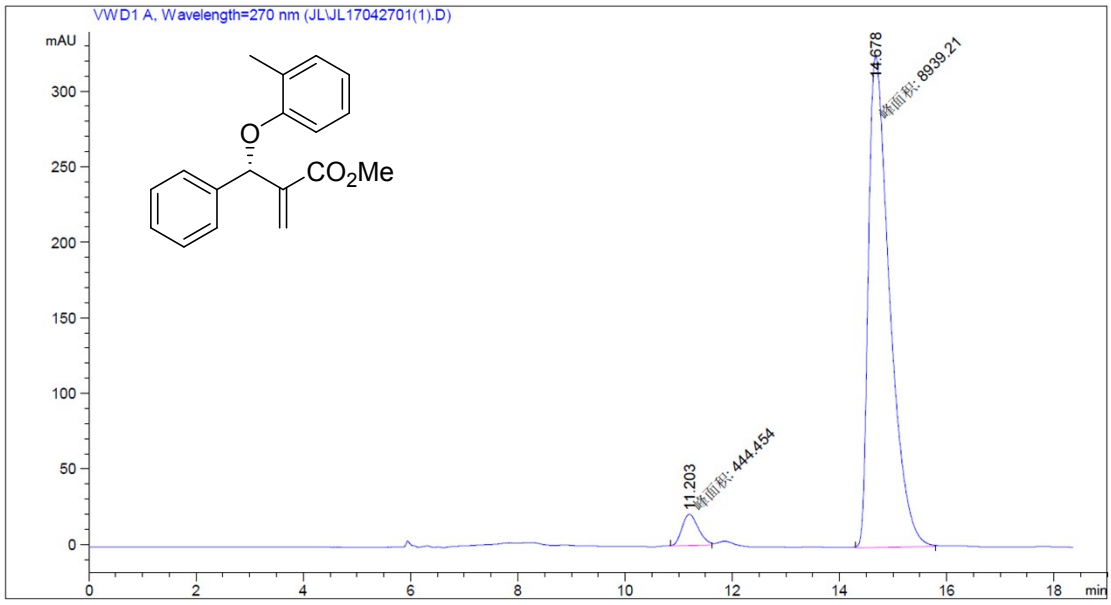


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.090	0.4481	105.36840	3.91946	2.7867
2	13.531	0.4302	3675.73633	134.82527	97.2133

4b

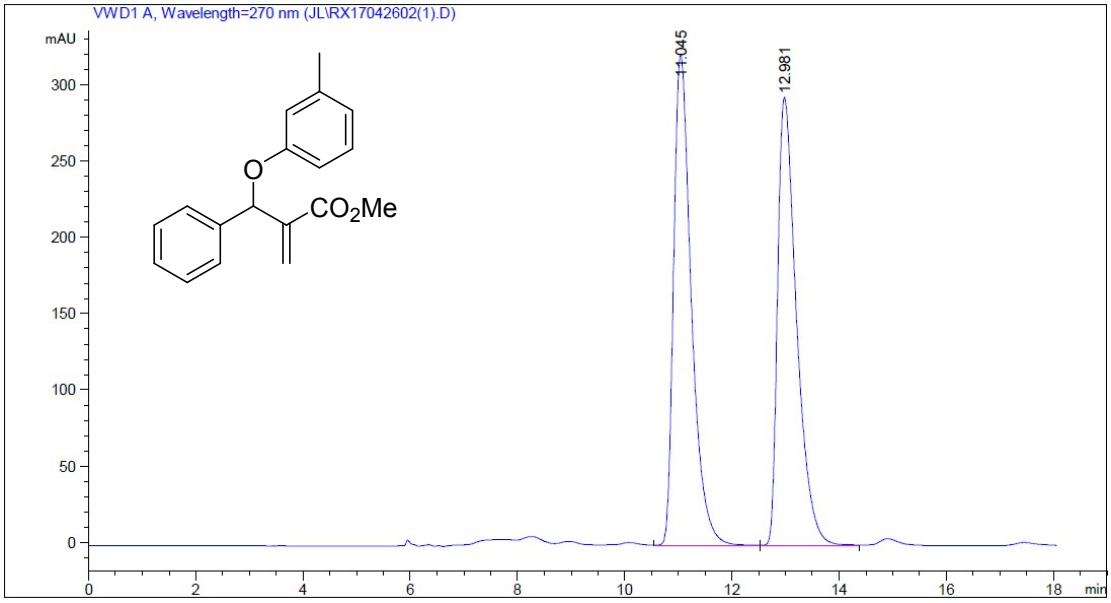


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.246	0.3864	4596.95996	198.25998	50.4570
2	14.750	0.3952	4513.67969	172.67798	49.5430

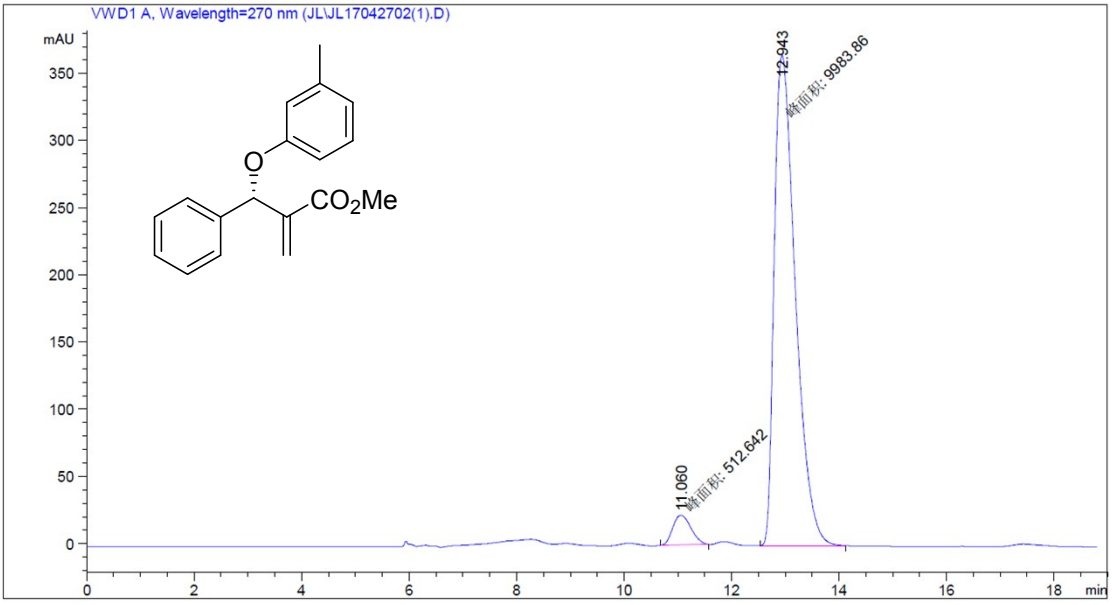


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.203	0.3563	444.45407	20.78850	4.7365
2	14.678	0.4583	8939.20508	325.06836	95.2635

4c

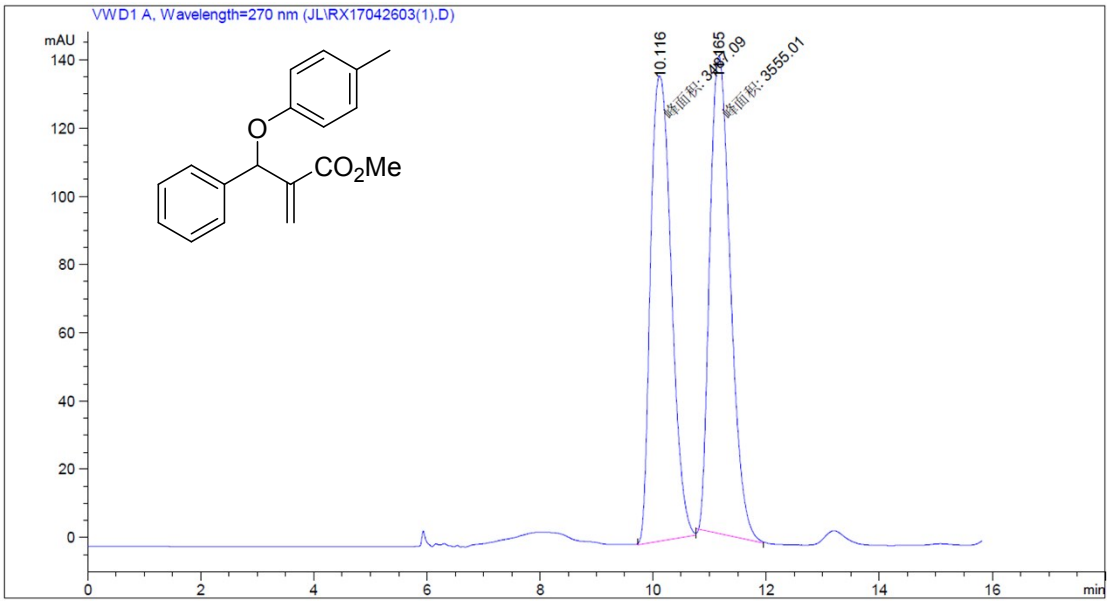


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.045	0.3507	7372.90088	321.32056	50.7051
2	12.981	0.3694	7167.83594	293.52158	49.2949

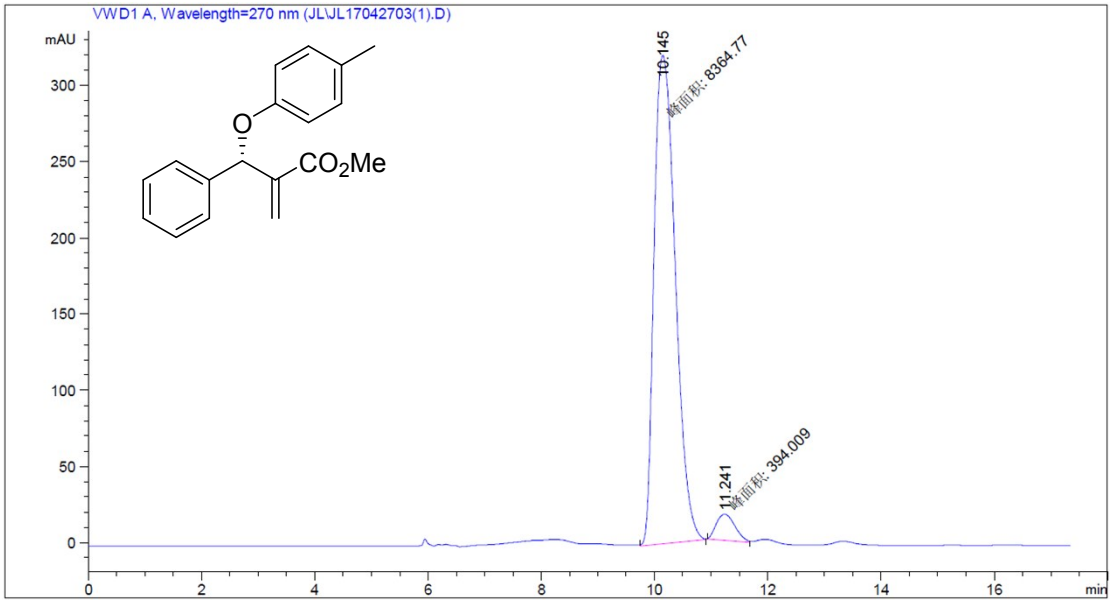


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.060	0.3897	512.64240	21.92439	4.8839
2	12.943	0.4553	9983.85742	365.43457	95.1161

4d

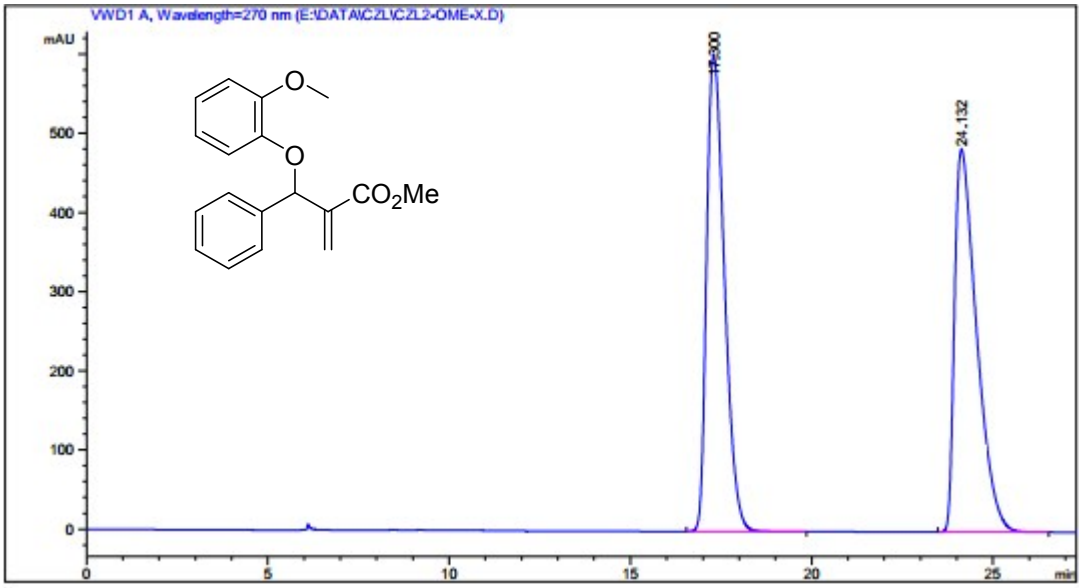


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.116	0.4265	3487.08765	136.27383	49.5177
2	11.165	0.4237	3555.01099	139.84894	50.4823

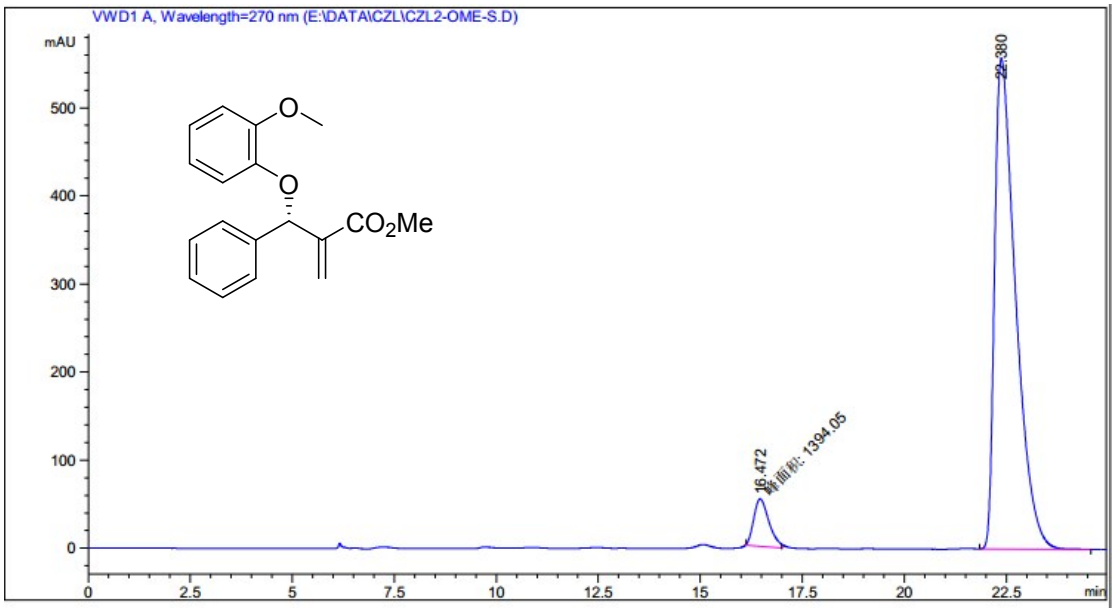


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.145	0.4348	8364.76855	320.60620	95.5015
2	11.241	0.3831	394.00943	17.14189	4.4985

4e

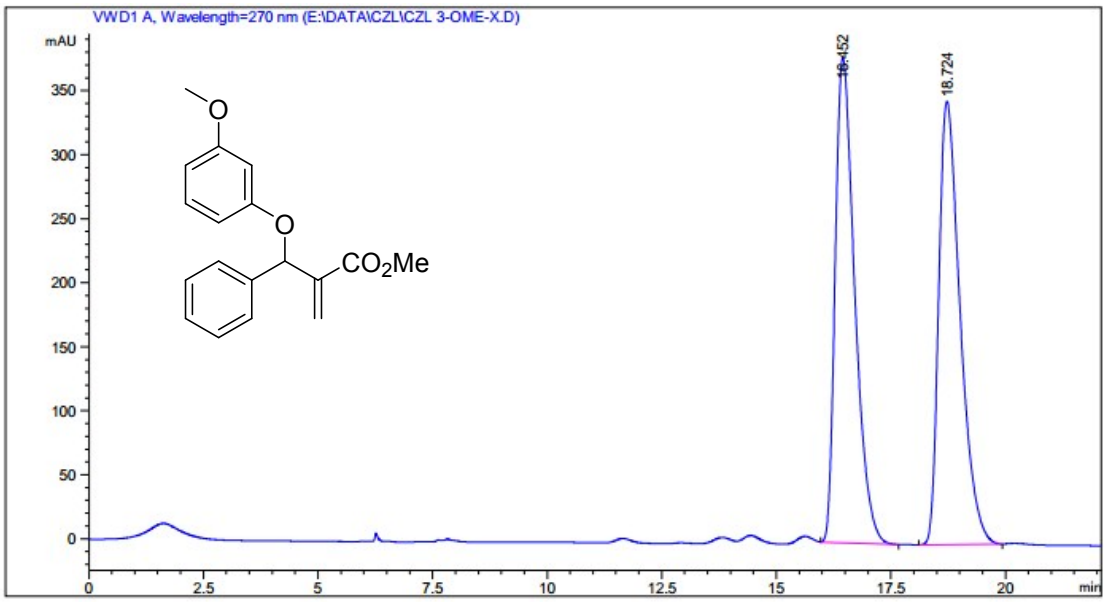


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	17.300	0.5342	2.04843e4	601.70380	50.0650
2	24.132	0.6420	2.04311e4	483.16162	49.9350

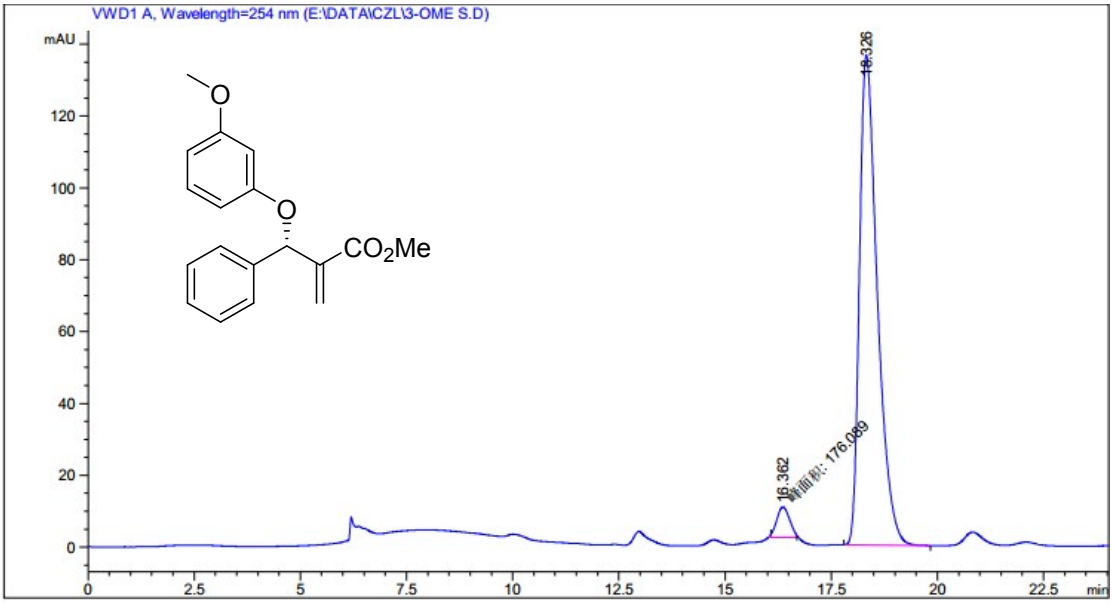


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	16.472	0.4306	1394.05212	53.95518	6.5345
2	22.380	0.5372	1.99397e4	556.91315	93.4655

4f

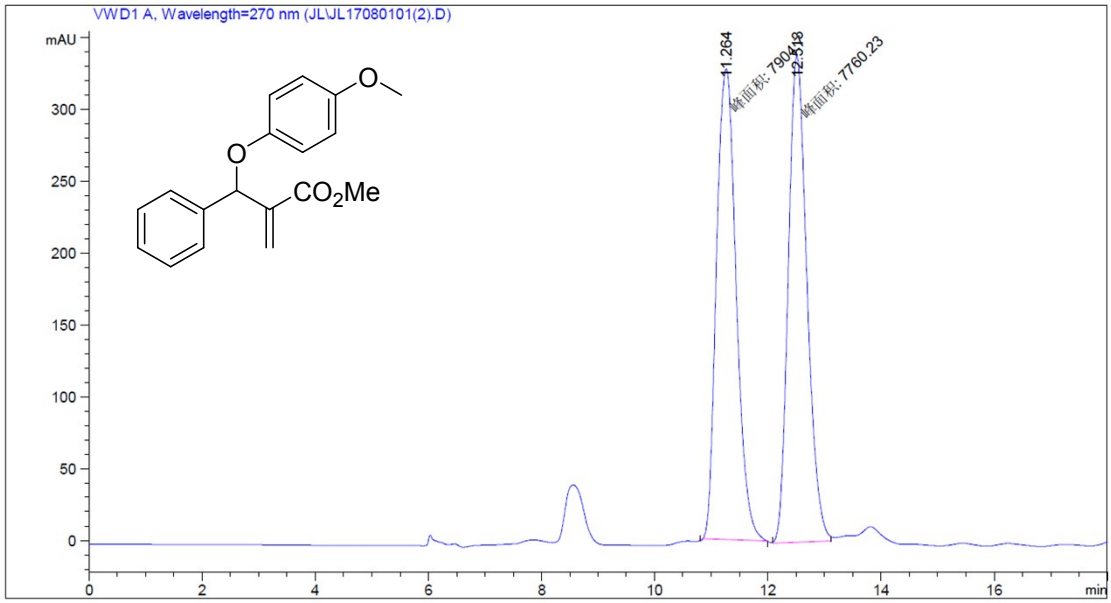


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	16.452	0.4523	1.11790e4	378.64157	49.9188
2	18.724	0.4962	346.07037	346.07037	50.0812

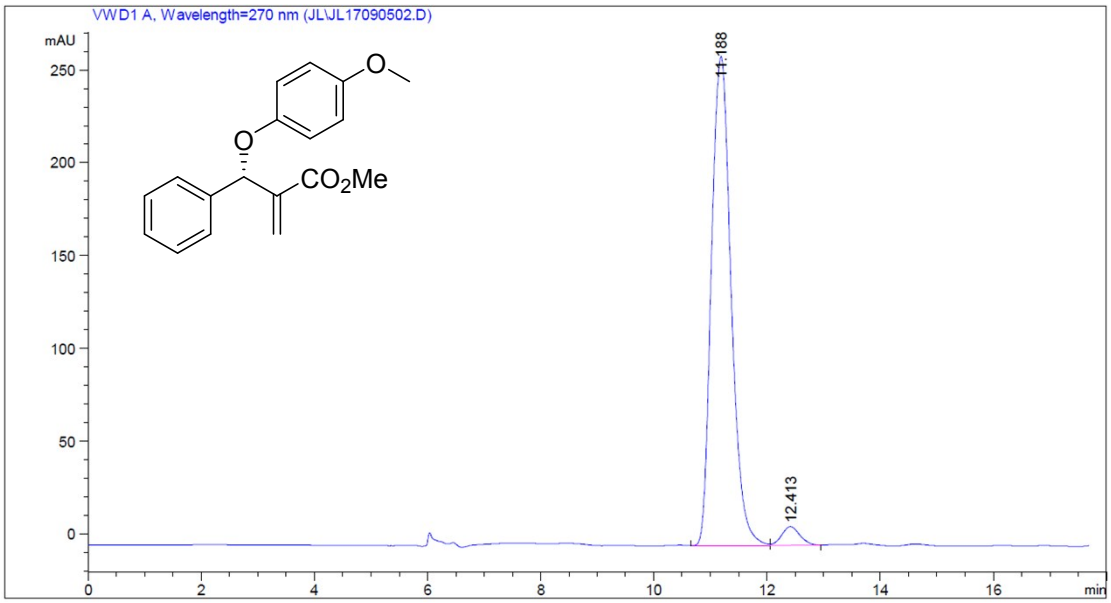


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	16.382	0.3470	176.08911	8.45808	4.2297
2	18.326	0.4431	3987.02612	136.37894	95.7703

4g

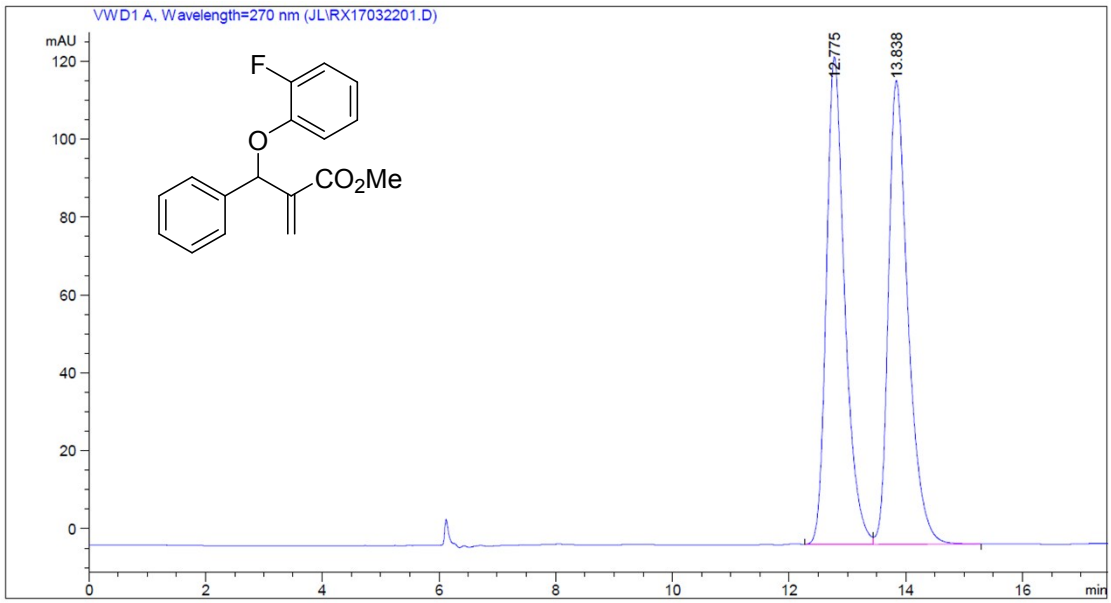


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.264	0.4022	7904.70410	327.56653	50.4611
2	12.513	0.3821	7760.23242	338.46463	49.5389

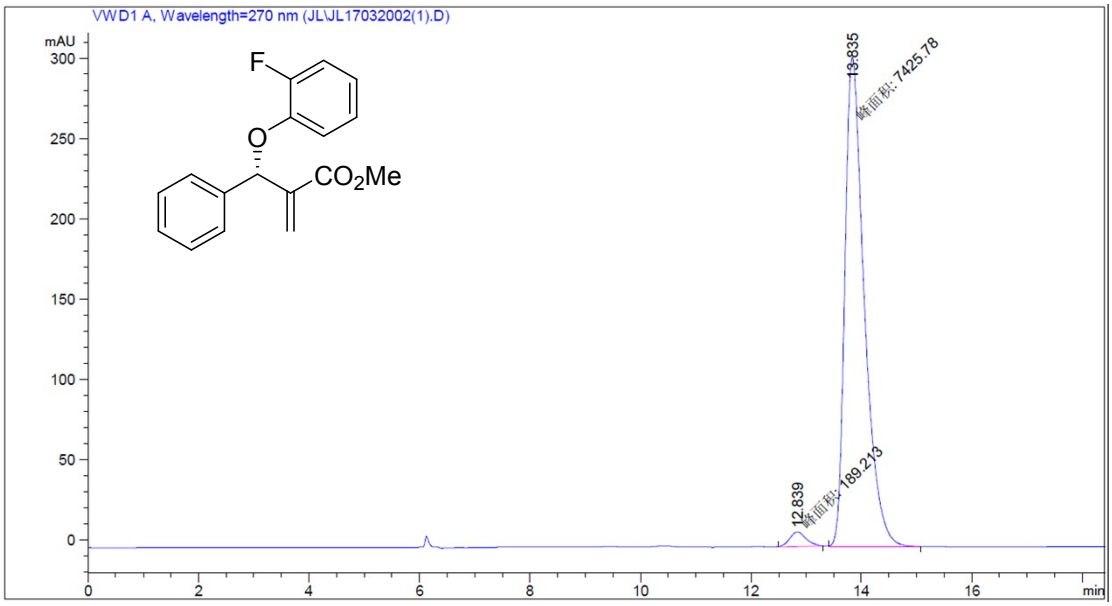


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.188	0.3802	6353.59570	263.61005	96.6040
2	12.413	0.3465	223.35489	10.05529	3.3960

4h

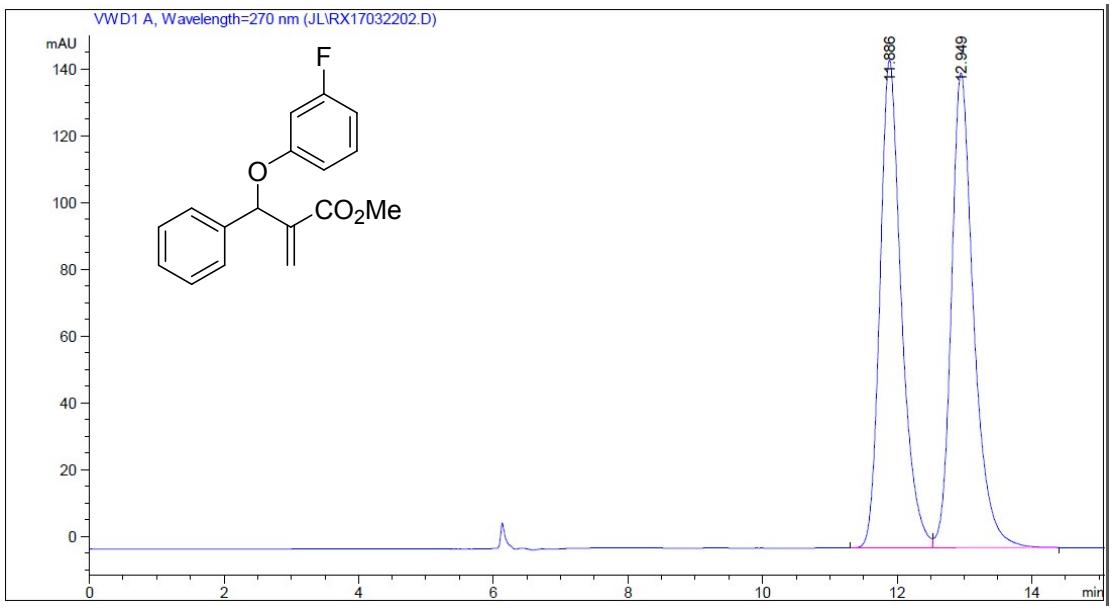


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	12.775	0.3287	2744.57227	125.12720	49.7545
2	13.838	0.3503	2771.65674	119.02826	50.2455

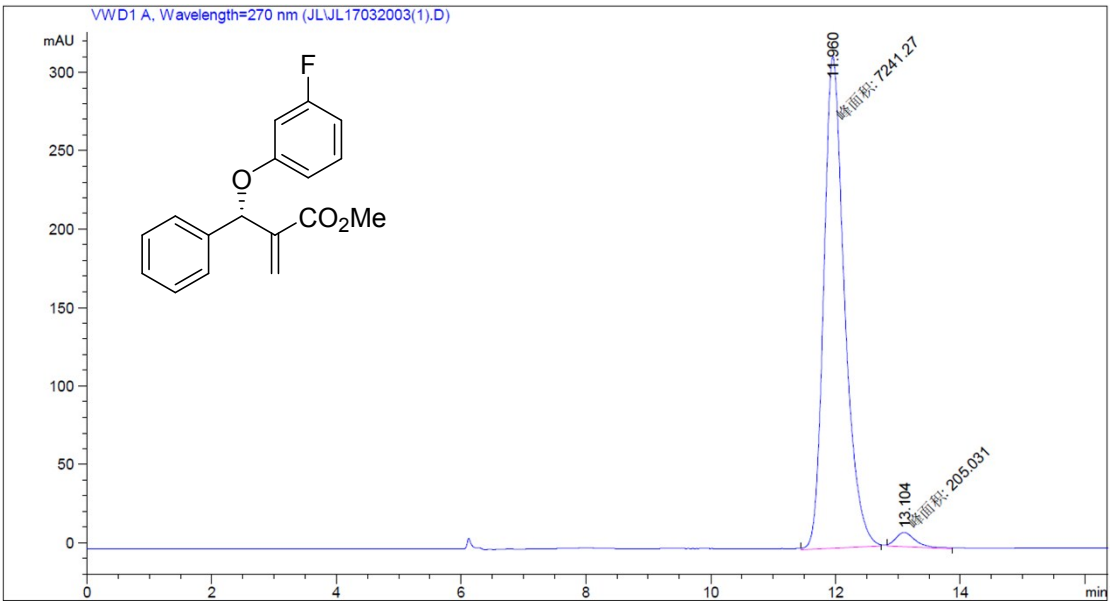


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	12.839	0.3469	189.21298	9.09151	2.4847
2	13.835	0.4062	7425.78271	304.65503	97.5153

4i

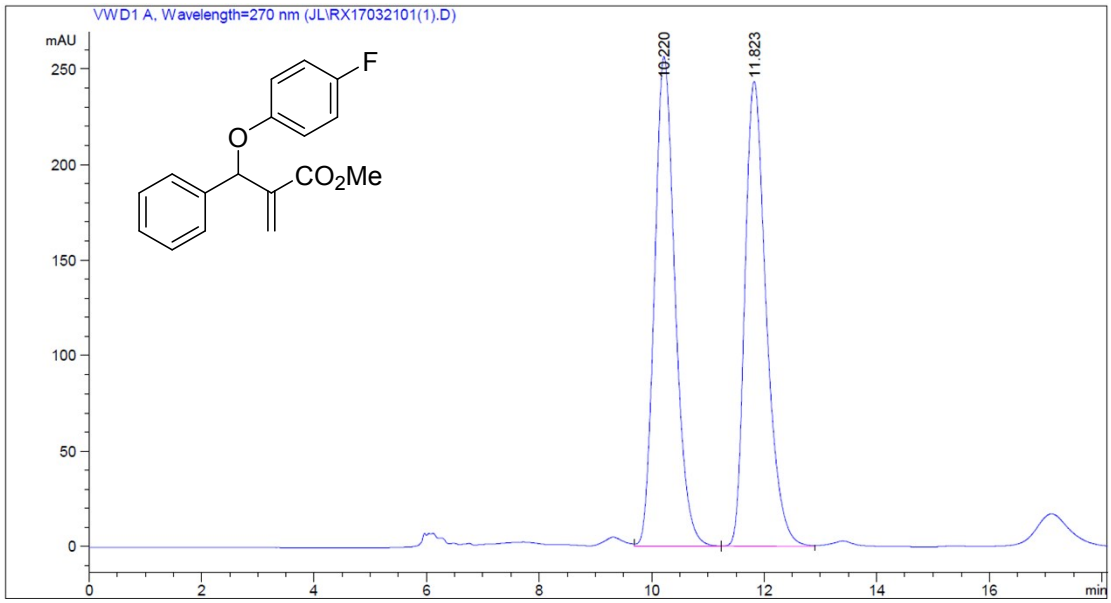


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.886	0.3305	3225.55371	146.01103	49.6637
2	12.949	0.3441	3269.23413	142.12965	50.3363

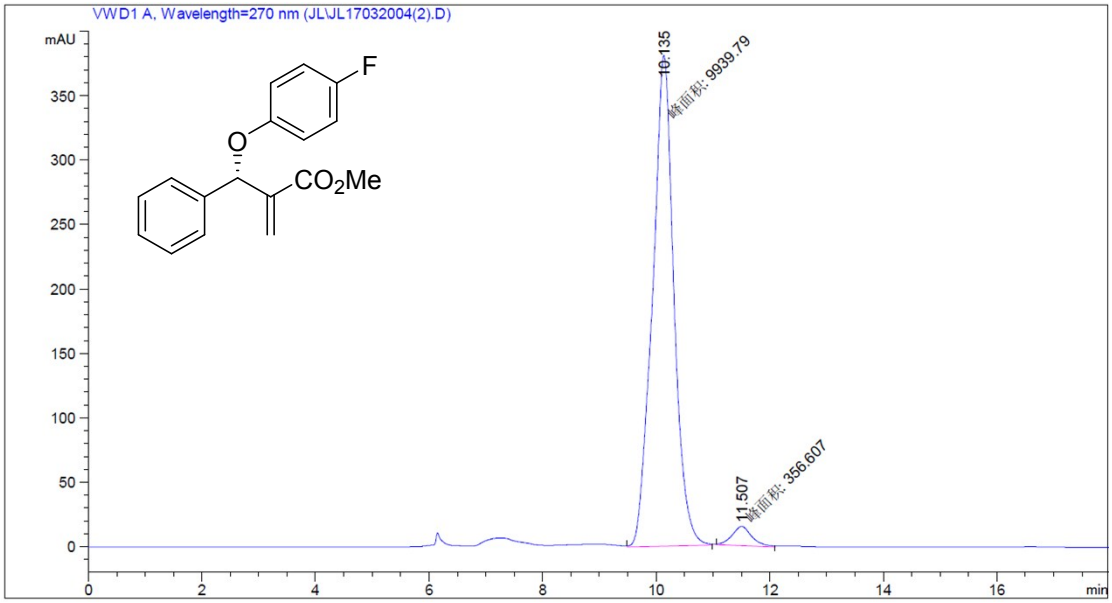


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.960	0.3851	7241.26611	313.36203	97.2465
2	13.104	0.3753	205.03076	9.10532	2.7535

4j

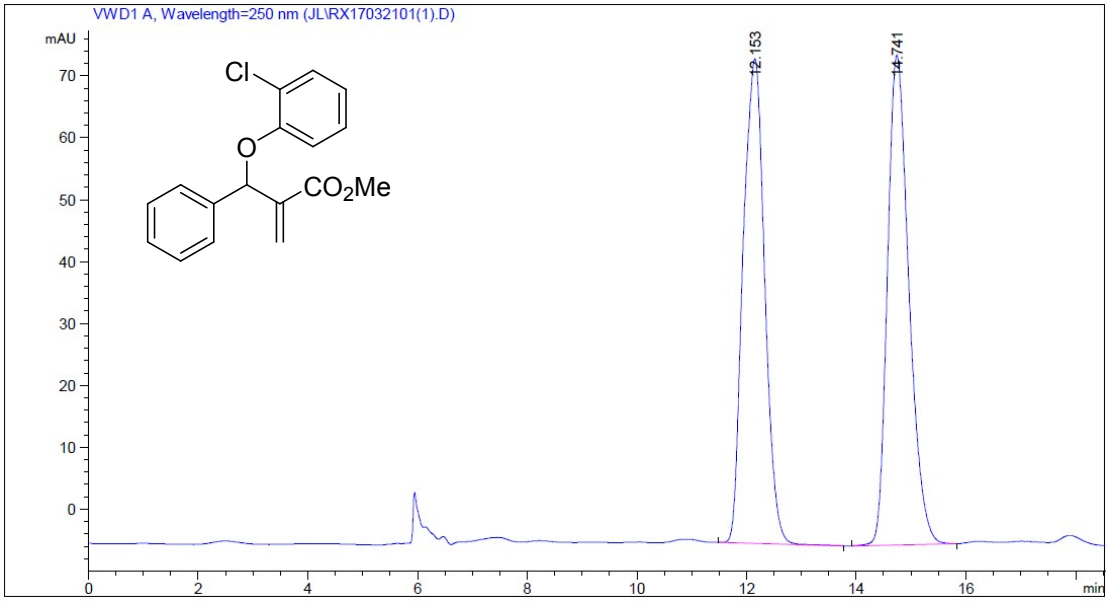


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.220	0.3842	6486.33643	256.19669	50.3183
2	11.823	0.4032	6404.28076	243.30074	49.6817

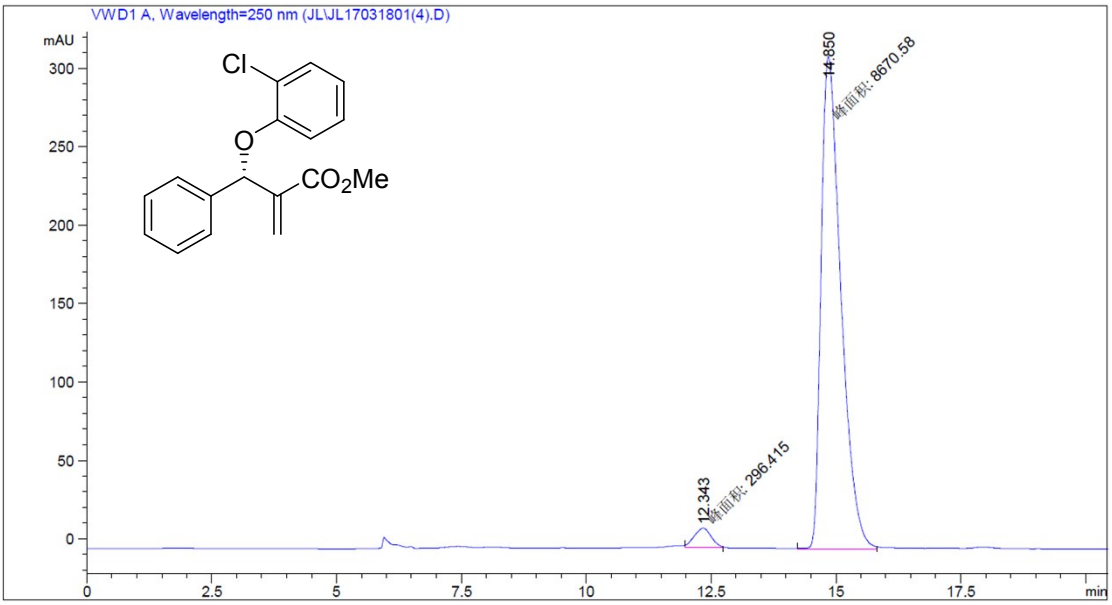


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.135	0.4351	9939.78809	380.73264	96.5366
2	11.507	0.4003	356.60742	14.84893	3.4634

4k

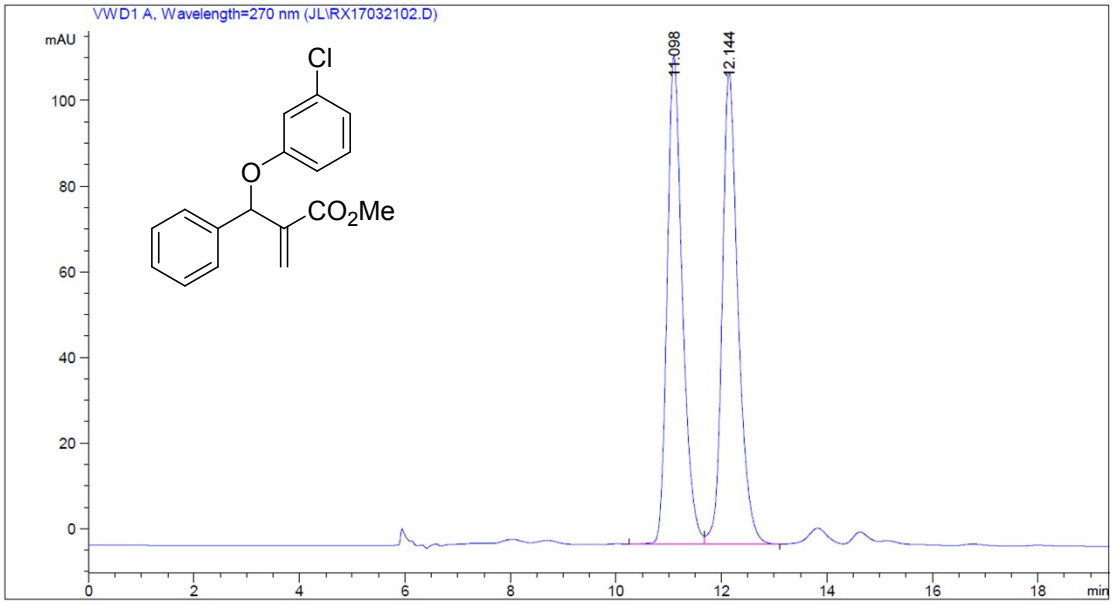


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	12.153	0.4416	2134.69653	78.35691	49.8179
2	14.741	0.4204	2150.30176	79.13994	50.1821

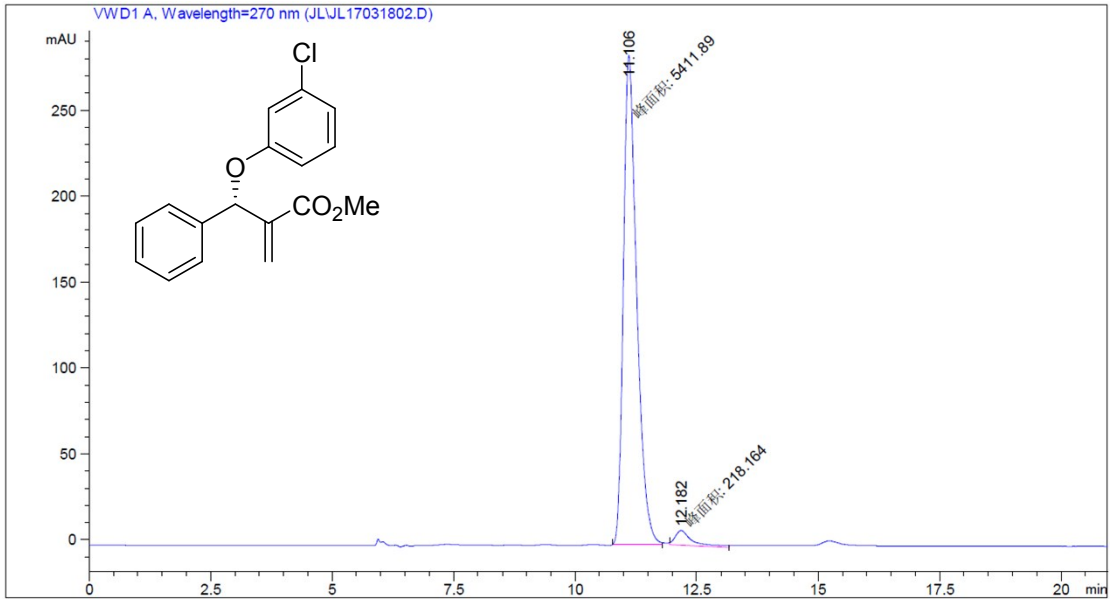


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	12.343	0.3986	296.41531	12.39357	3.3056
2	14.850	0.4599	8670.57910	314.20038	96.6944

4l

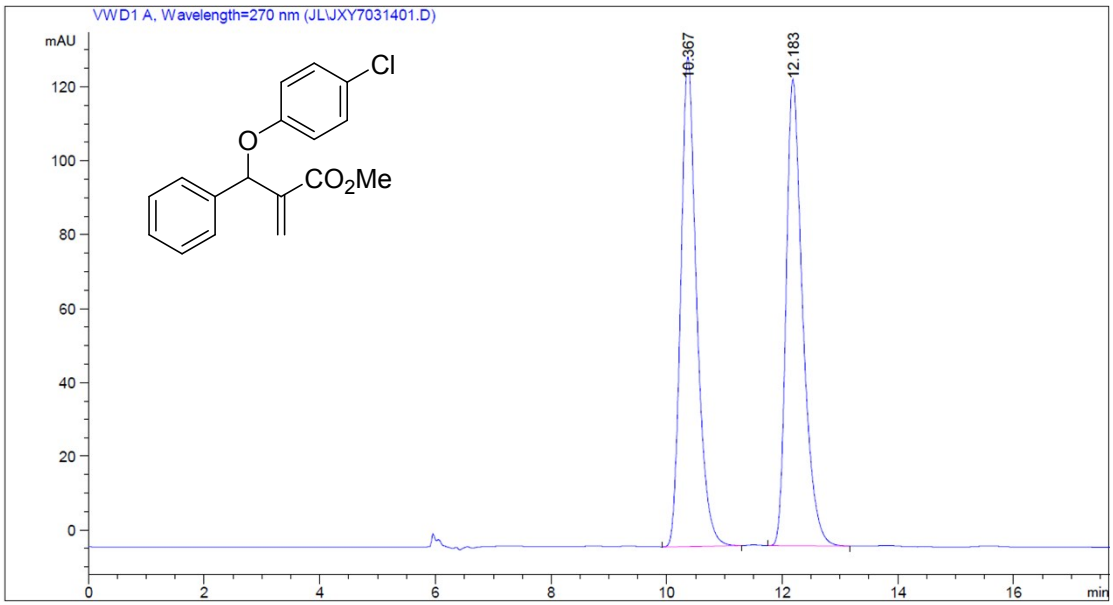


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.098	0.2986	2280.16846	114.14850	49.7457
2	12.144	0.3106	2303.47925	110.28749	50.2543

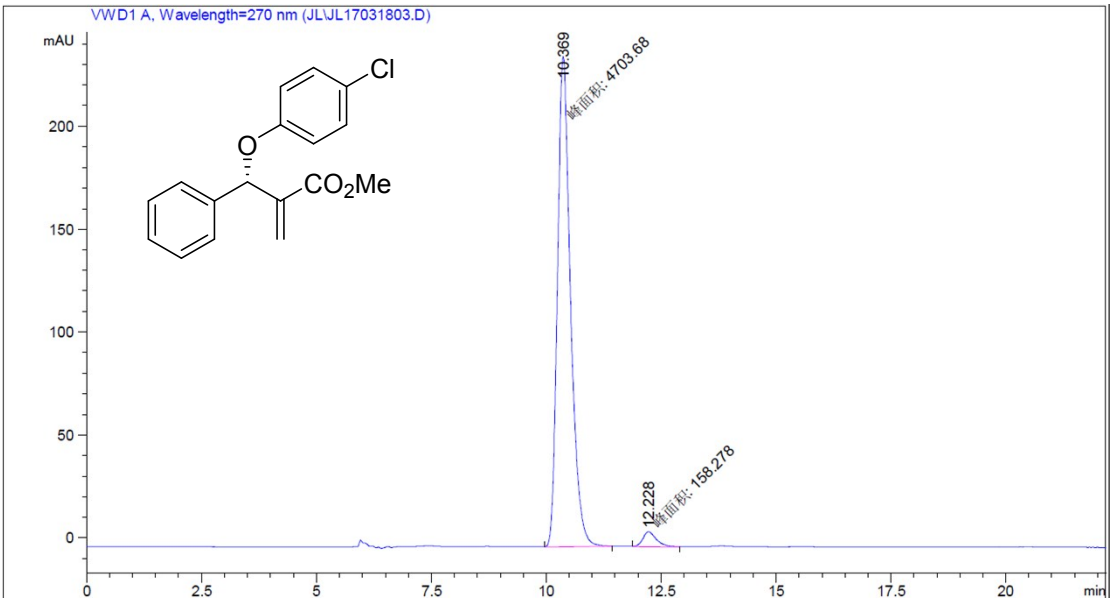


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.106	0.3167	5411.88965	284.79822	96.1250
2	12.182	0.4188	218.16431	8.68181	3.8750

4m

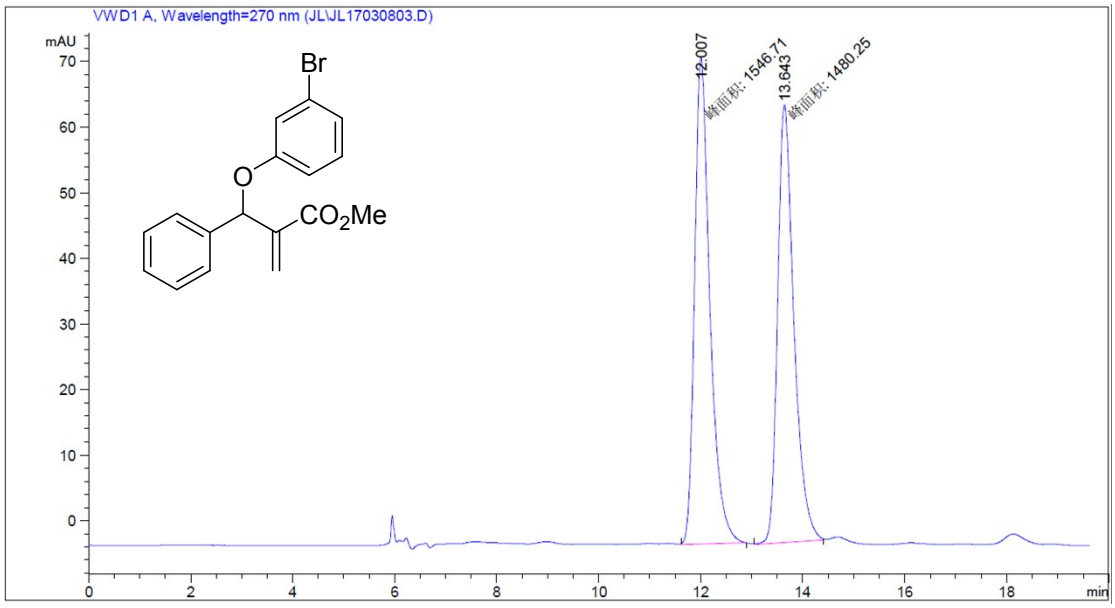


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.367	0.2838	2528.86841	132.52623	50.0958
2	12.183	0.2997	2519.19604	126.31319	49.9042

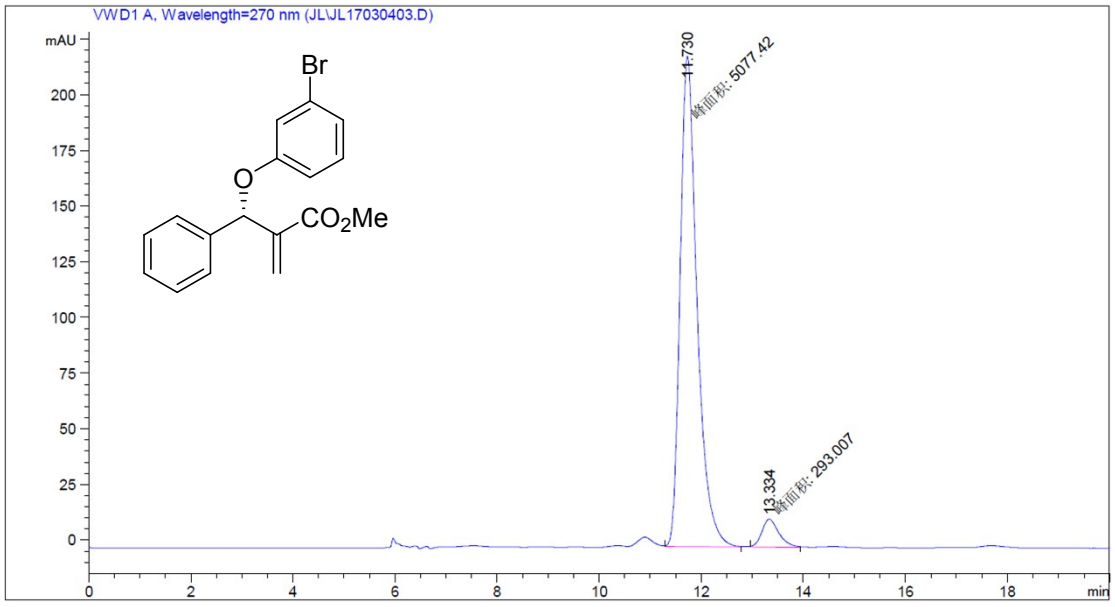


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.369	0.3292	4703.67578	238.12540	96.7446
2	12.228	0.3564	158.27824	7.40176	3.2554

4n

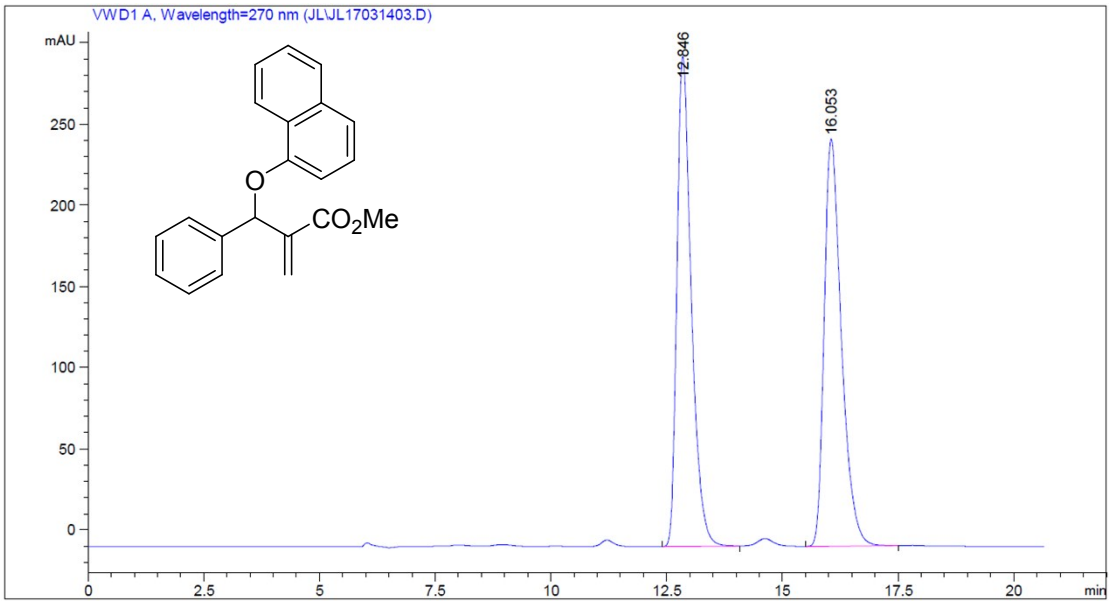


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	12.007	0.3475	1546.70667	74.18143	51.0978
2	13.643	0.3699	1480.24805	66.68851	48.9022

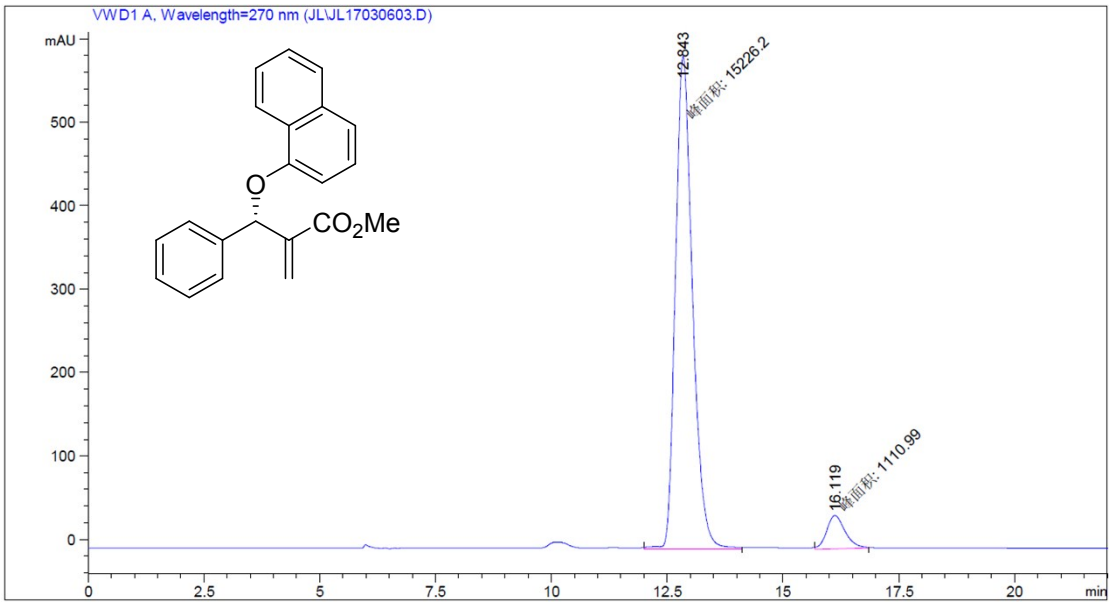


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	11.730	0.3845	5077.42383	220.09152	94.5441
2	13.334	0.3886	293.00720	12.56534	5.4559

4o

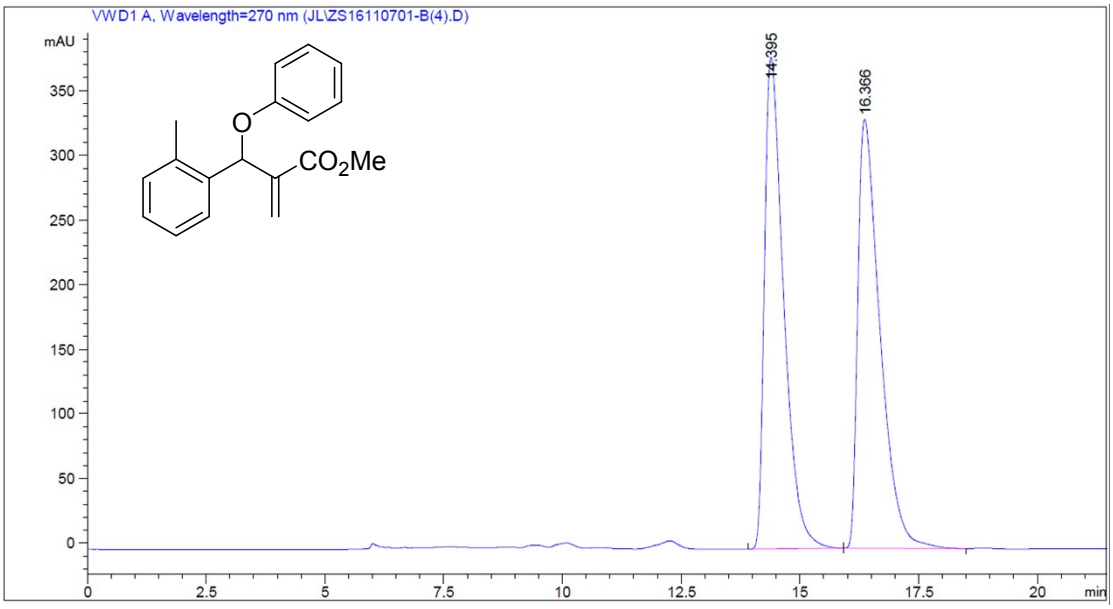


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	12.846	0.3268	6494.76025	301.73441	49.9794
2	16.053	0.3928	6500.11963	250.66284	50.0206

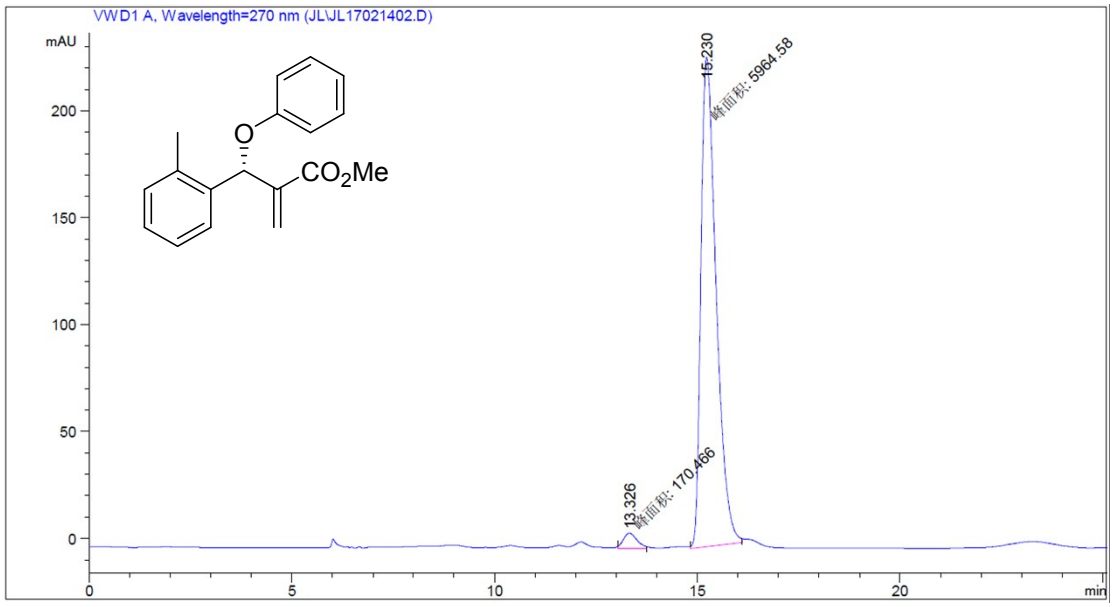


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	12.843	0.4296	1.52262e4	590.74146	93.1997
2	16.119	0.4621	1110.98511	40.07385	6.8003

4p

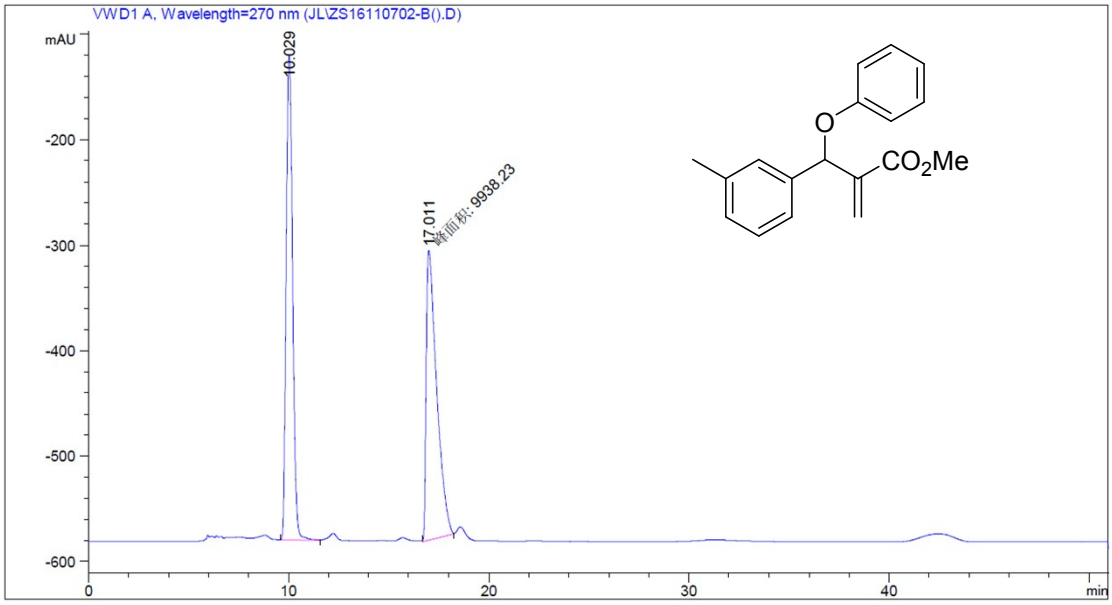


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	14.395	0.4241	1.06802e4	379.88190	49.7665
2	16.366	0.4854	1.07805e4	331.77011	50.2335

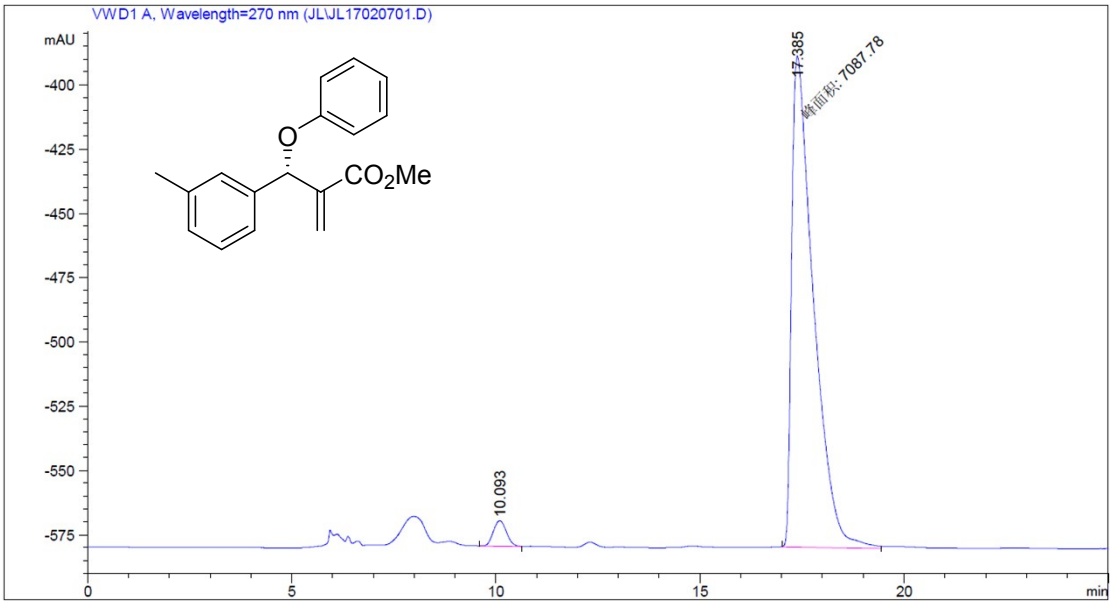


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	13.326	0.3924	170.46632	7.24092	2.7786
2	15.230	0.4345	5964.57568	228.81248	97.2214

4q

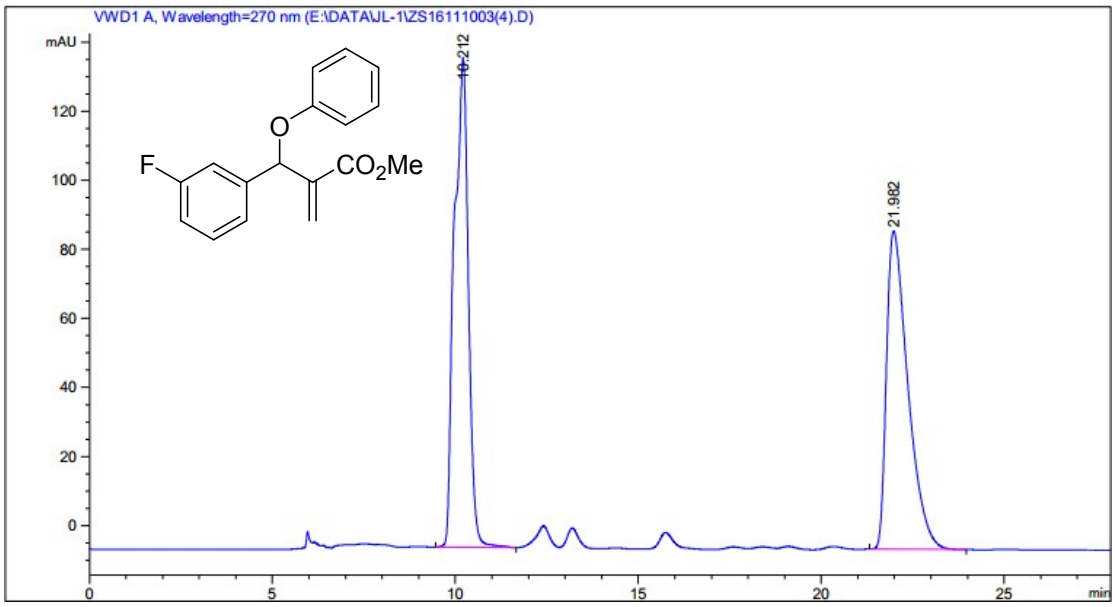


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.029	0.3585	1.02686e4	459.08438	50.8175
2	17.011	0.6015	9938.23047	275.38965	49.1825

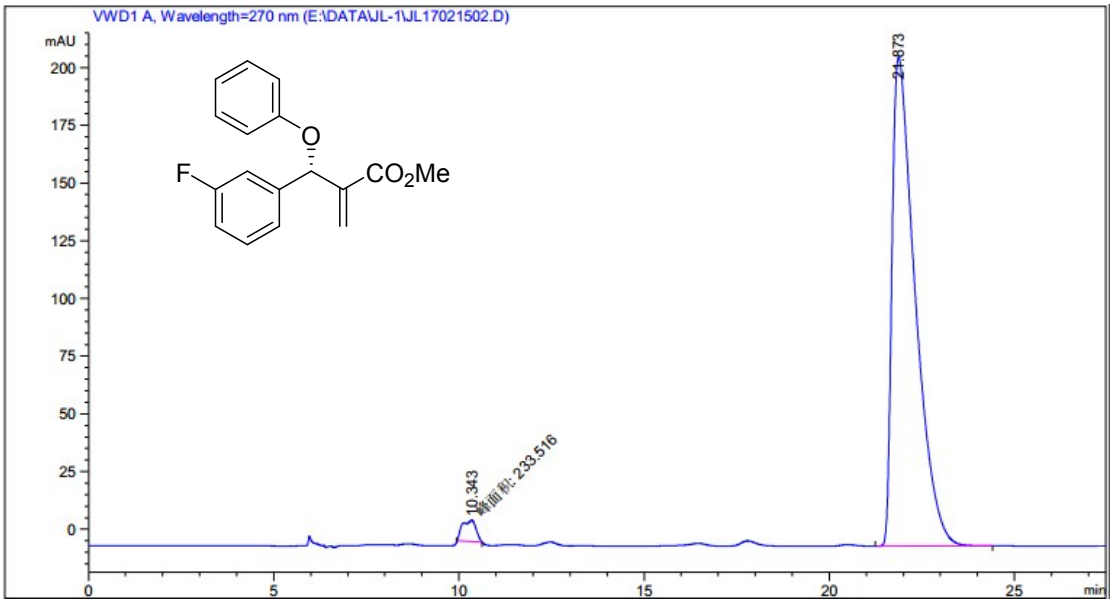


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.093	0.3545	218.29822	9.85504	2.9879
2	17.385	0.6184	7087.77588	191.03847	97.0121

4r

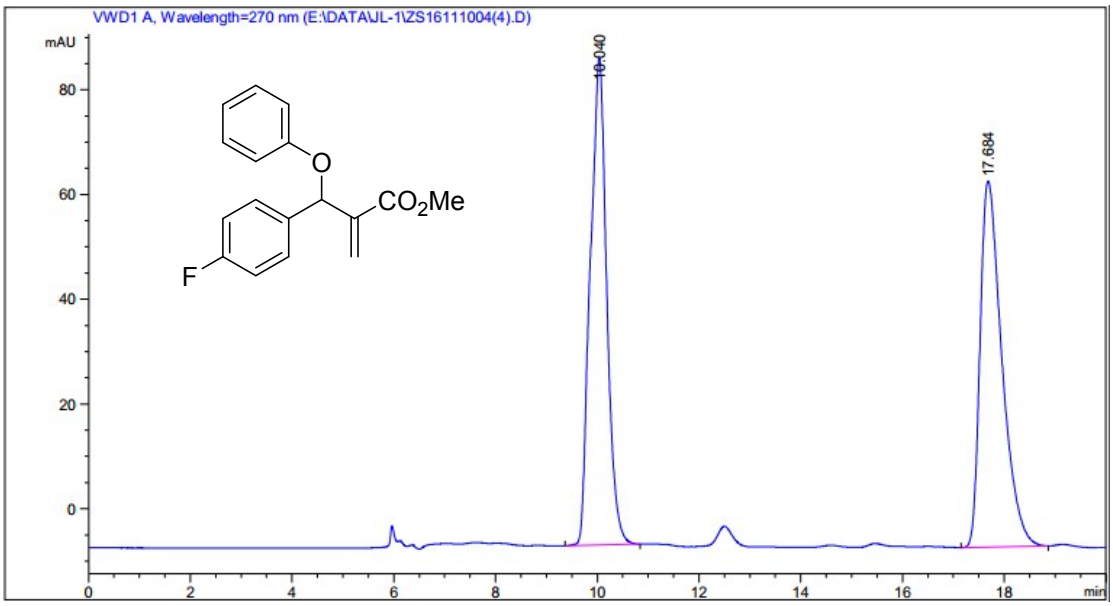


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.212	0.3671	3787.50513	141.72729	50.3130
2	21.982	0.6134	3740.38501	92.14016	49.6870

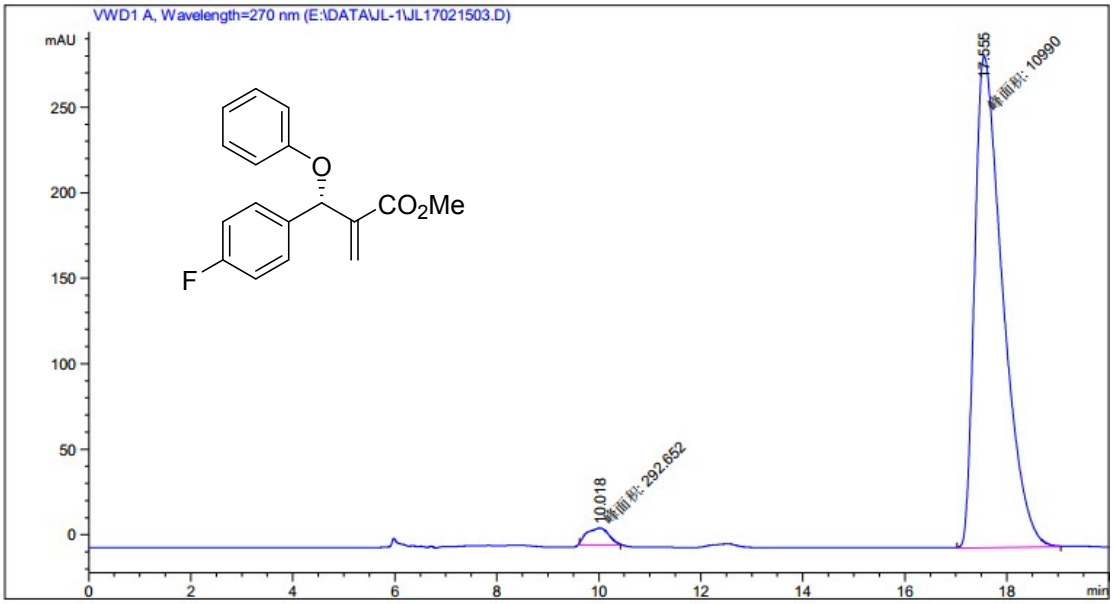


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.343	0.4226	233.51581	9.20975	2.4791
2	21.873	0.6442	9185.68164	211.85397	97.5209

4s

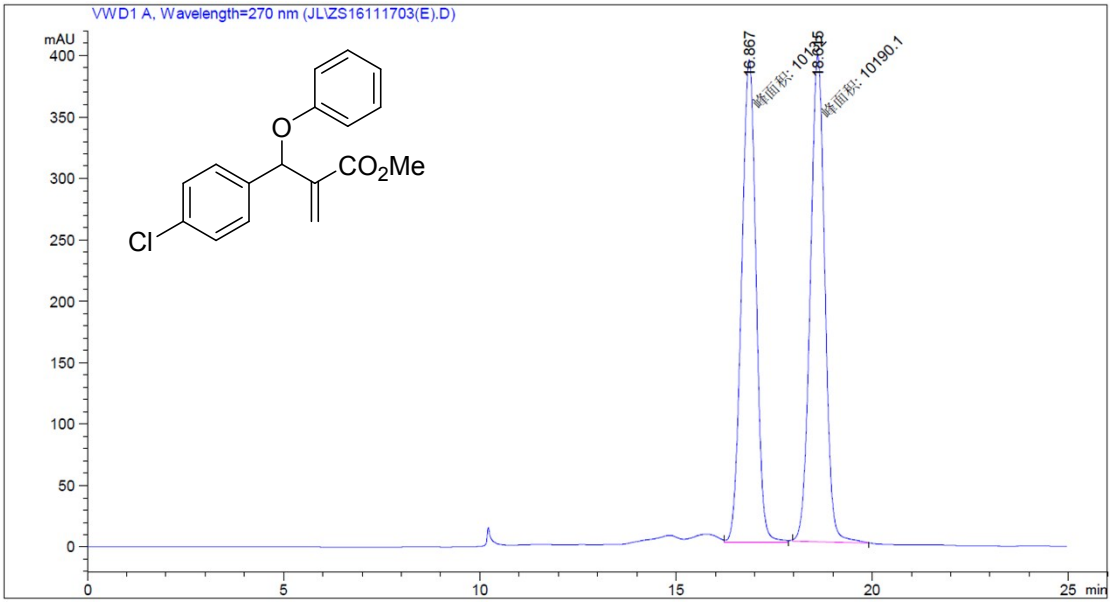


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.040	0.3167	2082.56421	92.95475	50.0886
2	17.684	0.4482	2075.19604	69.90784	49.9114

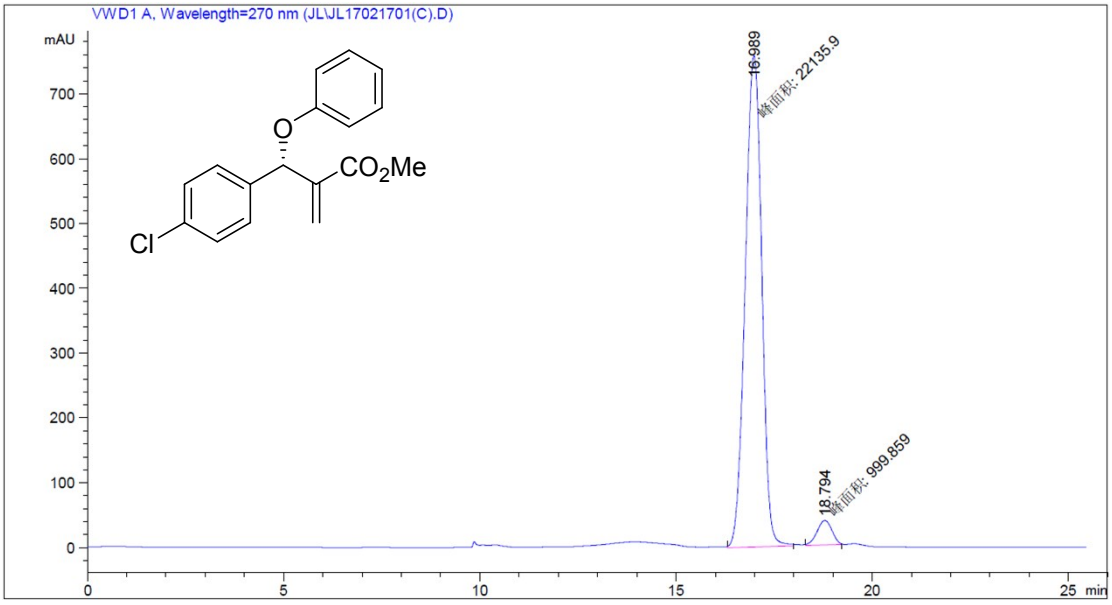


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	10.018	0.5026	292.65170	9.70524	2.5938
2	17.555	0.6372	1.09900e4	287.44113	97.4062

4t

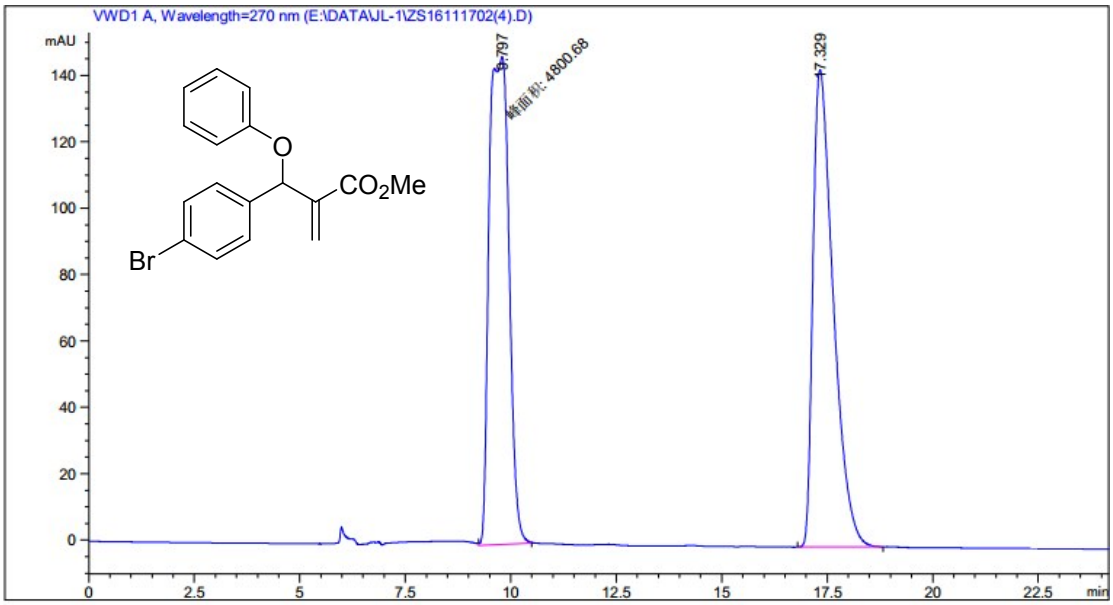


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	16.867	0.4295	1.01320e4	393.18872	49.8571
2	18.615	0.4288	1.01901e4	396.07187	50.1429

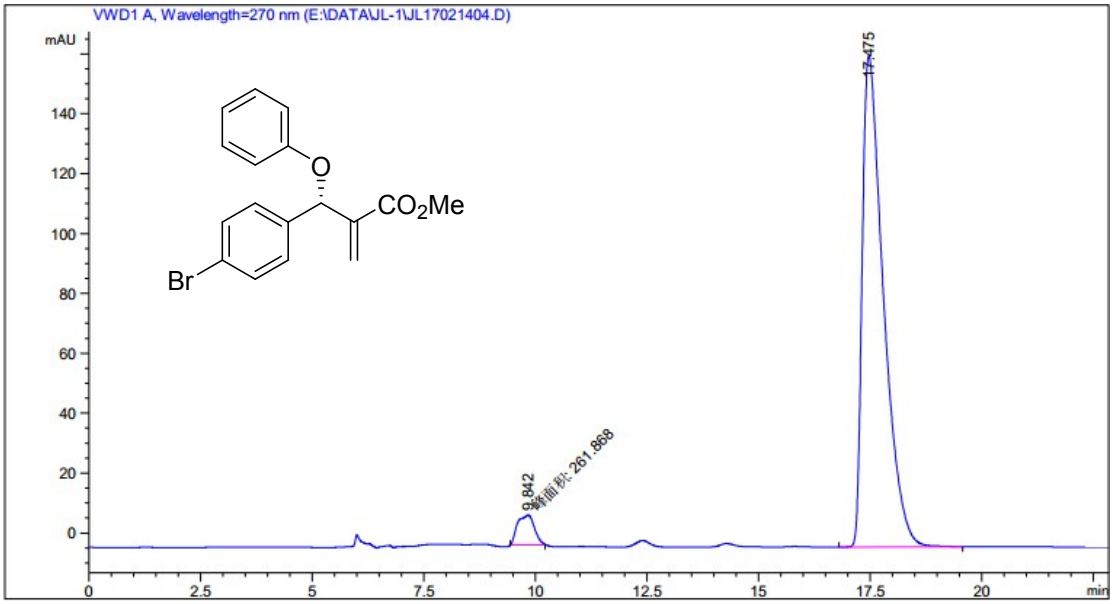


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	16.989	0.4867	2.21359e4	758.00909	95.6783
2	18.794	0.4409	999.85858	37.79251	4.3217

4u

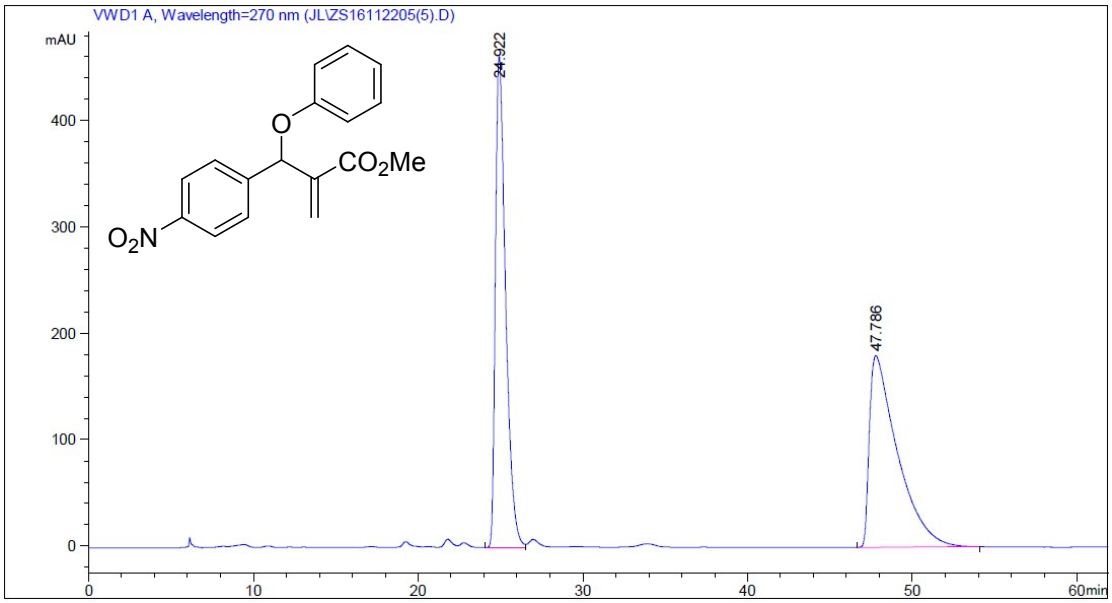


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	9.797	0.5448	4800.68457	146.85161	49.9841
2	17.329	0.5063	4803.73633	143.75893	50.0159

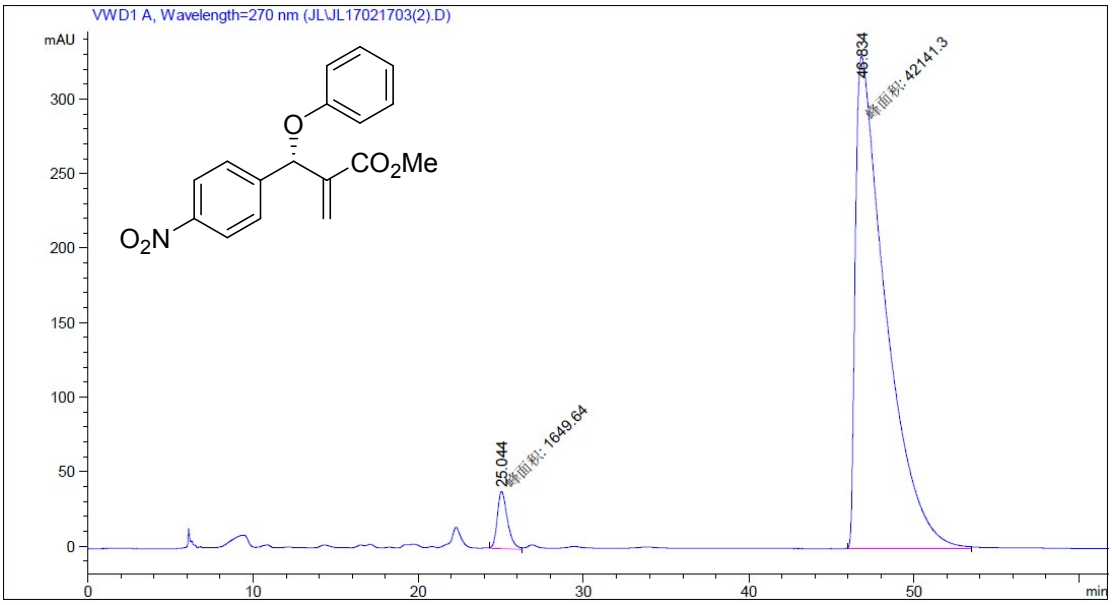


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	9.842	0.4379	262.86804	9.96642	4.6244
2	17.475	0.4949	5400.86914	163.98764	95.3756

4v

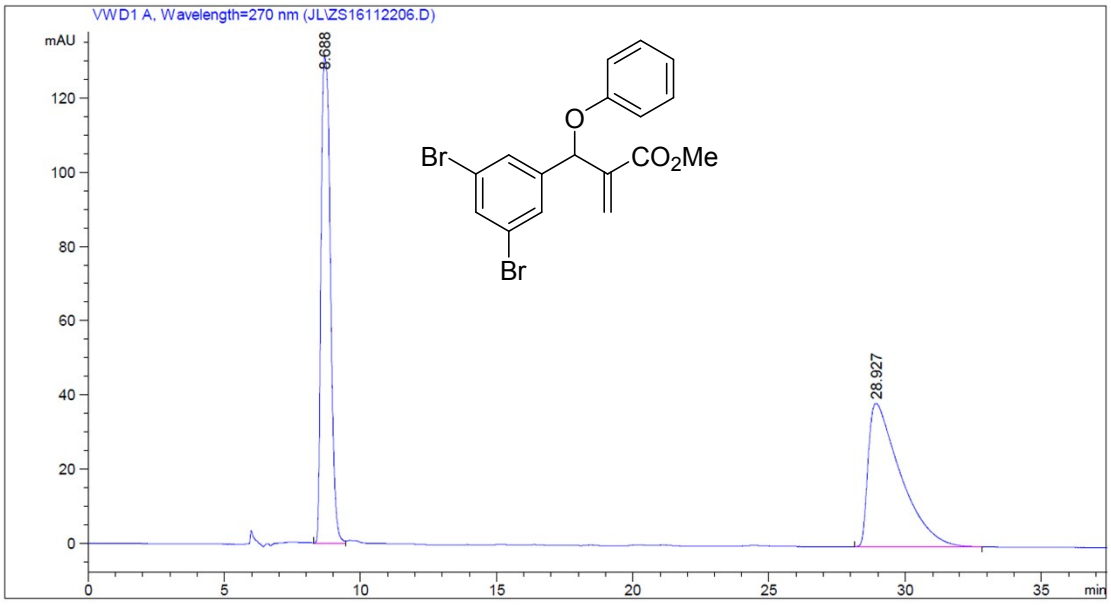


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	24.922	0.6503	1.98673e4	461.88550	48.2647
2	47.786	1.6466	2.12959e4	180.21129	51.7353

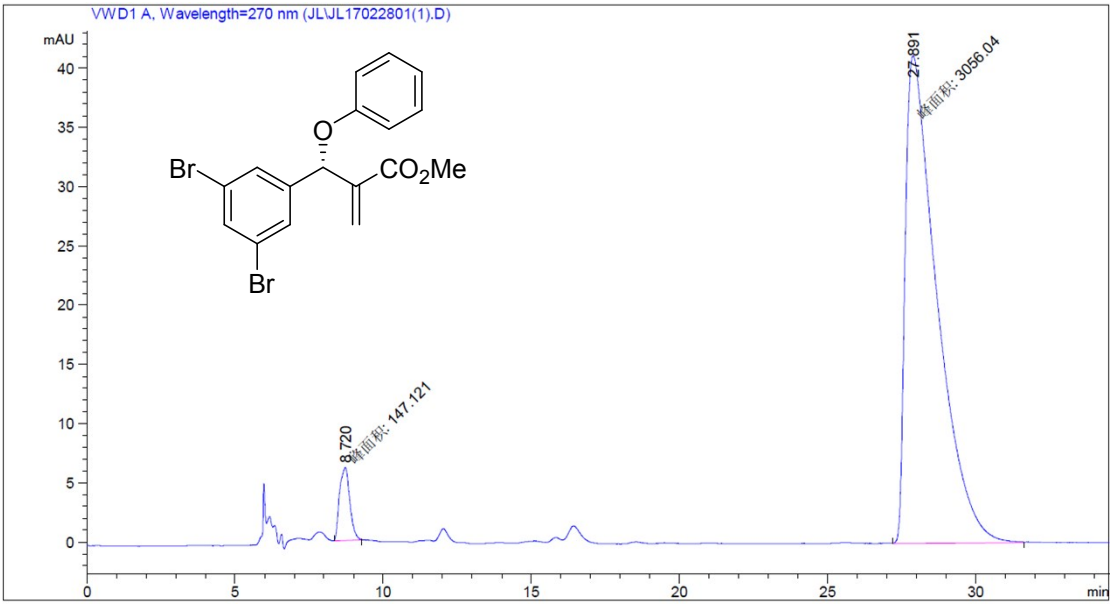


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	25.044	0.7147	1649.63867	38.47055	3.7671
2	46.834	2.1239	4.21413e4	330.69049	96.2329

4w

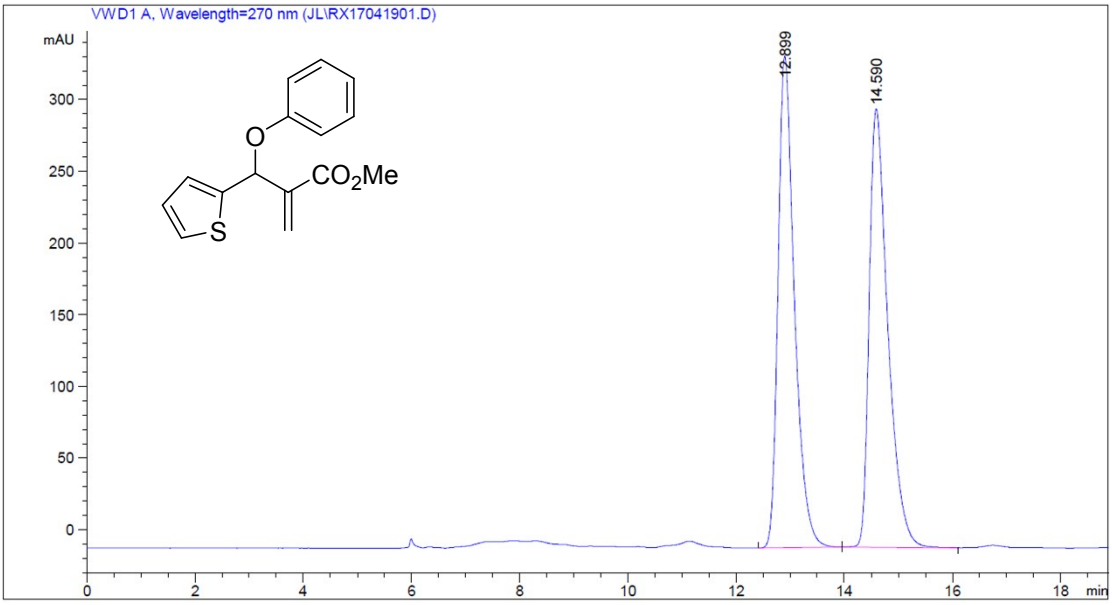


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	8.688	0.3835	3117.49341	131.21957	49.5354
2	28.927	1.1363	3175.97144	38.65076	50.4646

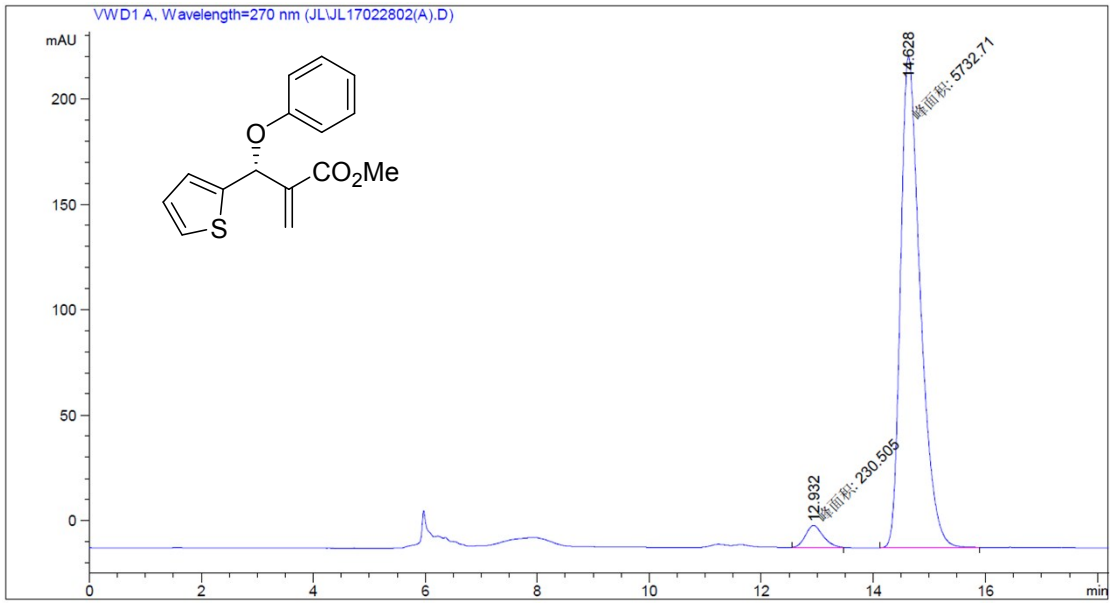


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	8.720	0.3991	147.12061	6.14407	4.5930
2	27.891	1.2367	3056.04199	41.18658	95.4070

4x

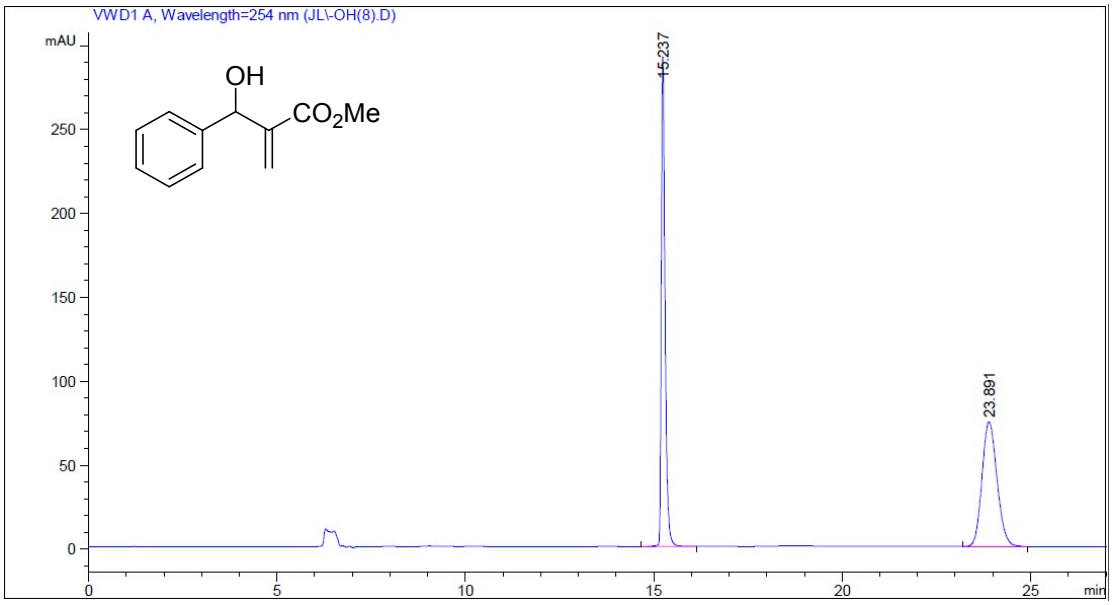


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	12.899	0.3167	7216.15723	343.13583	49.7554
2	14.590	0.3580	7287.10107	305.86911	50.2446

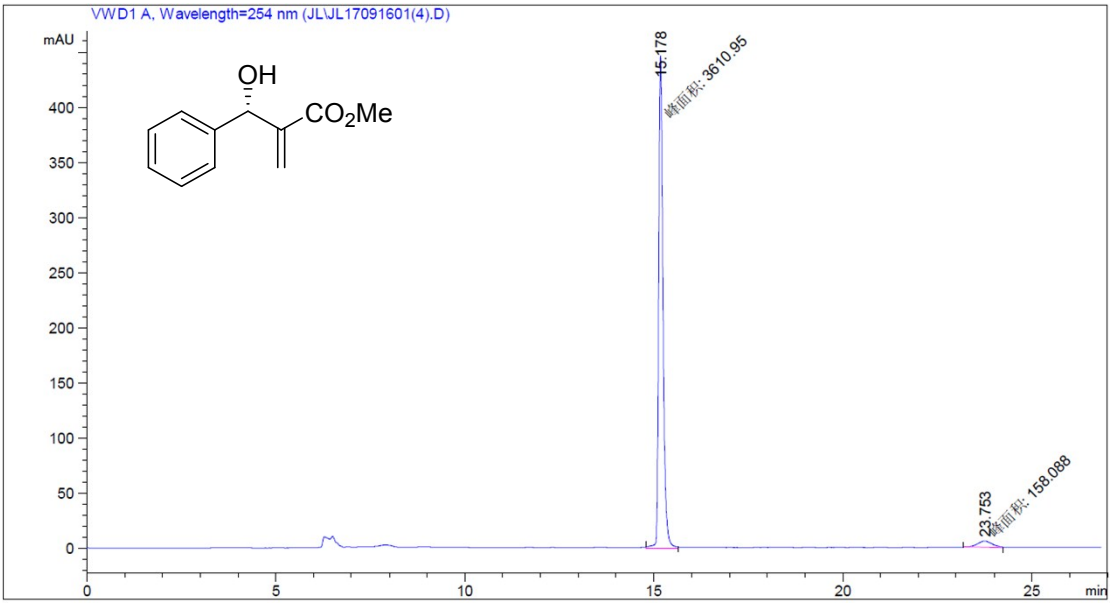


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	12.932	0.3671	230.50516	10.46448	3.8655
2	14.628	0.4099	5732.70654	233.11172	96.1345

6

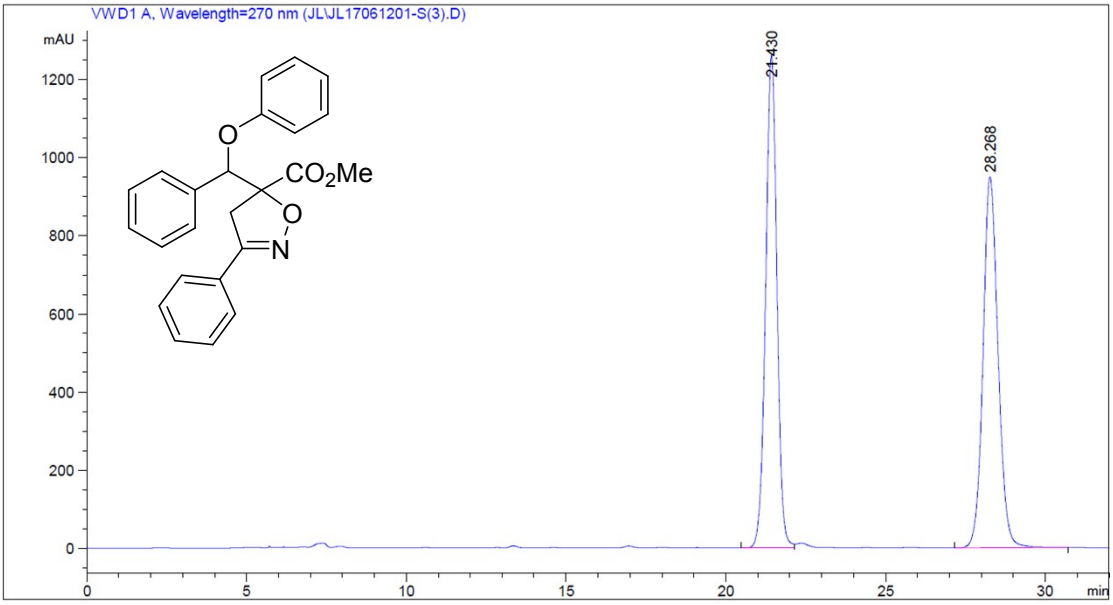


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	15.237	0.1049	2044.51758	292.38458	49.9294
2	23.891	0.4325	2050.30005	74.32244	50.0706

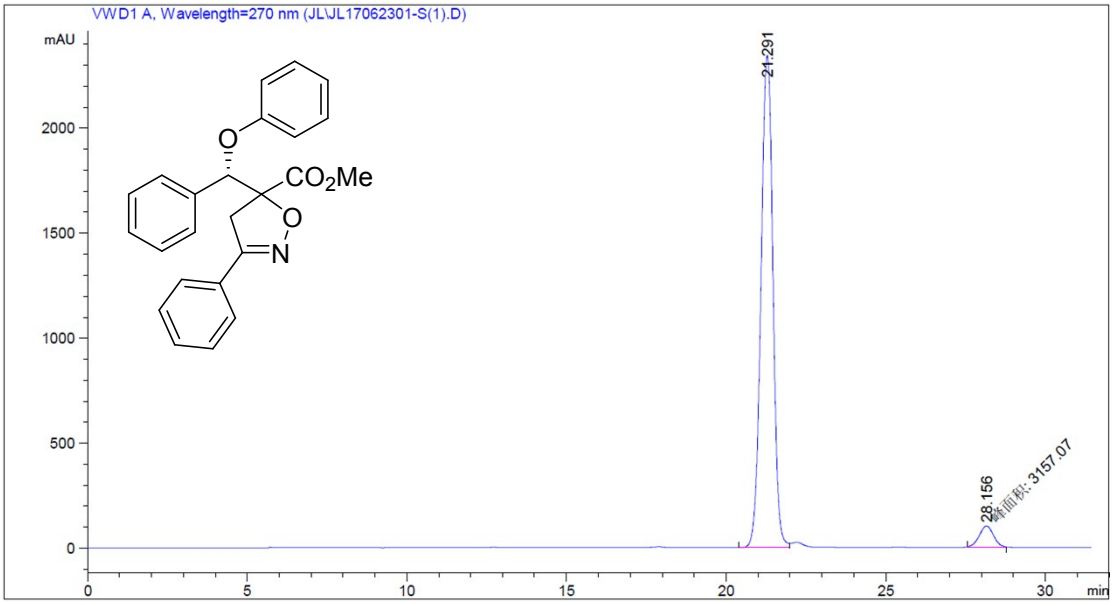


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	15.178	0.1346	3610.95264	447.27509	95.8056
2	23.753	0.4660	158.08810	5.65353	4.1944

7a (one of the two diastereomers)

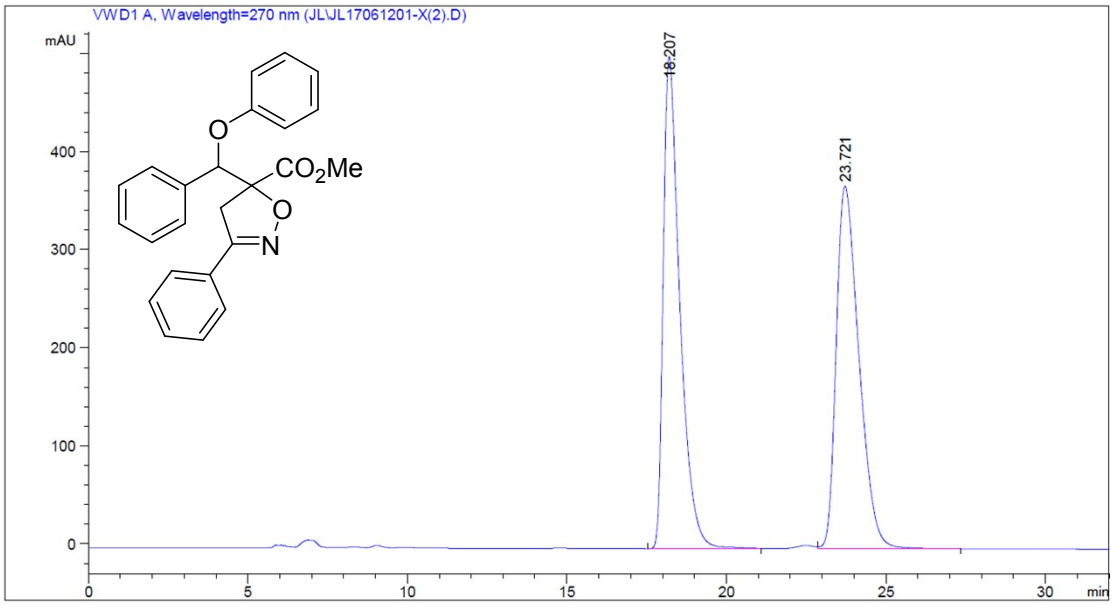


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	21.430	0.3764	3.07325e4	1259.31506	49.7615
2	28.268	0.4996	3.10271e4	948.53583	50.2385

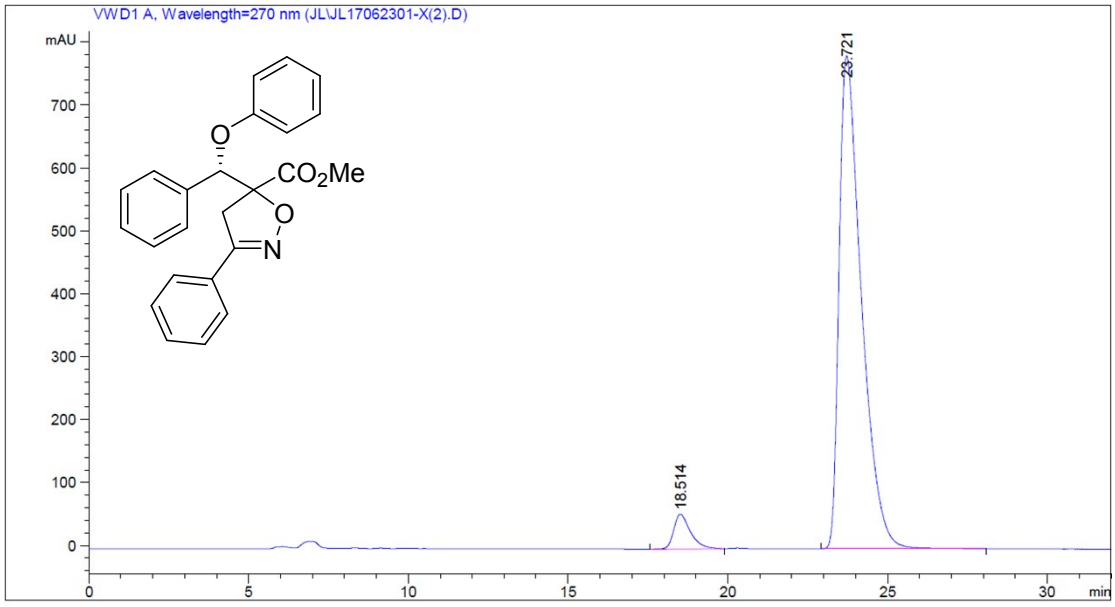


Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	21.291	0.4070	6.07554e4	2345.75171	95.0603
2	28.156	0.5208	3157.06812	101.03548	4.9397

7a' (another of the two diastereomers)



Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	18.207	0.5382	1.80674e4	501.54471	49.8384
2	23.721	0.7535	1.81846e4	369.33075	50.1616



Peak	Retention time (min)	Peak width (min)	Peak area (mAU*s)	Peak height (mAU)	Peak area (%)
1	18.514	0.5385	1983.33643	55.02317	4.9661
2	23.721	0.7240	3.79538e4	783.32397	95.0339