

Bicyclic guanidine-catalyzed asymmetric Michael additions of 3-benzyl-substituted oxindoles to *N*-maleimides

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1. General Information

General procedures and methods.

All experiments were monitored by analytical thin layer chromatography (TLC). TLC was performed on pre-coated plates. After elution, plate was visualized under UV illumination at 254 nm for UV active material. Further visualization was achieved by staining KMnO₄, ceric molybdate, or anisaldehyde solution. For those using the aqueous stains, the TLC plates were heated on a hot plate.

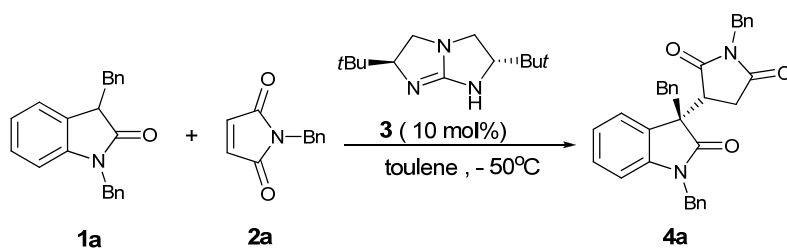
Columns for flash chromatography (FC) contained silica gel 200-300 mesh. Columns were packed as slurry of silica gel in petroleum ether and equilibrated solution using the appropriate solvent system. The elution was assisted by applying pressure of about 2 atm with an air pump.

Proton nuclear magnetic resonance (¹H NMR), carbon NMR (¹³C NMR) spectra were recorded in CDCl₃ otherwise stated. ¹H (400 MHz), ¹³C (100 MHz) with complete proton decoupling were performed on a 400 MHz spectrometer. Chemical shifts are reported in parts per million (ppm), using the residual solvent signal as an internal standard: CDCl₃ (¹H NMR: δ 7.26, singlet; ¹³C NMR: δ 77.0, triplet). Multiplicities were given as: *s* (singlet), *d* (doublet), *t* (triplet), *q* (quartet), *quintet*, *m* (multiplets), *dd* (doublet of doublets), *dt* (doublet of triplets), and *br* (broad). Coupling constants (*J*) were recorded in Hertz (Hz). The number of proton atoms (*n*) for a given resonance was indicated by *n*H. The number of carbon atoms (*n*) for a given resonance was indicated by *n*C. Low and high resolution mass spectra were obtained in EI and ESI modes. MS and HRMS were reported in units of mass of charge ratio (*m/z*).

Materials

All commercial reagents were purchased of the highest purity grade. They were used without further purification unless specified. All solvents used, mainly petroleum ether (PE) and ethyl acetate (EtOAc), were distilled. All compounds synthesized were stored in a 0 °C freezer and light-sensitive compounds were protected with aluminium foil.

2. Typical Experimental Procedure

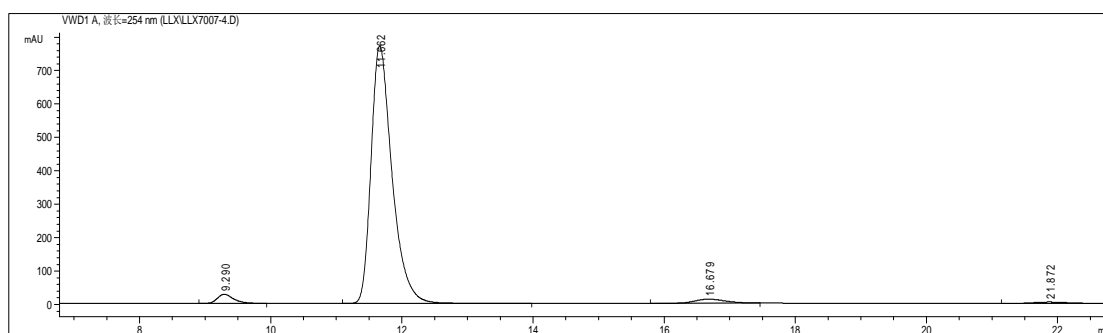
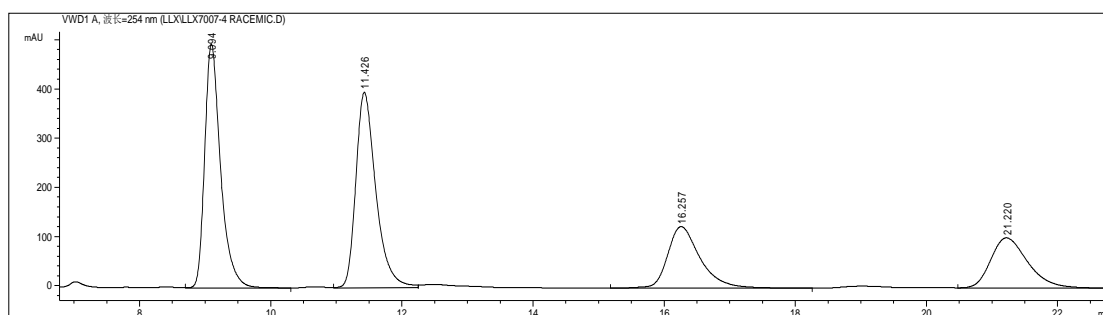


2a (22.4 mg, 0.12 mmol, 1.2 equiv.) and guanidine **3** (2.2 mg, 0.01 mmol, 0.1 equiv.) were dissolved in toluene (1.0 ml). The reaction mixtures were stirred at - 50 °C about 30 minutes. then added **1a** (31.3 mg, 0.1 mmol, 1.0 equiv.) into the solution at this temperature, the reaction mixtures were stirred about 40 hours at this temperature, and were directly loaded onto a short silica gel column, followed by gradient elution with PE/EA mixture (5/1-3/1 ratio). Removing the solvent in *vacuo*, afforded white solid **4a** (45.4 mg, 91% yield).

3. Characterization of Products

4a, white solid, M.p. 49.5 - 50.1 °C; 91% yield; 95% *ee*; $[\alpha]_{20}^D = +150.0$ (*c* 0.25, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.40 - 7.34 (m, 5H), 7.18 - 7.06 (m, 4H), 7.03 - 6.96 (m, 3H), 6.82 (d, *J* = 7.4 Hz, 1H), 6.78 (d, *J* = 7.2 Hz, 2H), 6.66 (t, *J* = 7.6 Hz, 1H), 6.60 (d, *J* = 6.8 Hz, 2H), 6.35 (d, *J* = 7.8 Hz, 1H), 4.79 (d, *J* = 15.9 Hz, 1H), 4.68 (dd, *J* = 41.7, 13.9 Hz, 2H), 4.44 (d, *J* = 15.9 Hz, 1H), 4.06 (d, *J* = 13.2 Hz, 1H), 3.56 (dd, *J* = 9.1, 5.0 Hz, 1H), 3.39 (d, *J* = 13.2 Hz, 1H), 2.73 (dd, *J* = 18.3, 9.1 Hz, 1H), 1.77 (dd, *J* = 18.3, 5.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 176.9, 176.4, 174.9, 143.4, 135.4, 135.3, 134.7, 130.1, 129.1, 129.0, 128.7, 128.6, 128.6, 127.8, 127.3, 126.6, 126.2, 124.2, 123.0, 109.5, 55.6, 44.7, 43.6, 42.6, 41.2, 31.3; LRMS (ESI) *m/z* 501.2 (M+H⁺); HRMS (ESI) *m/z* 501.2174 (M+H⁺), Calc. for C₃₃H₂₉N₂O₃ 501.2173.

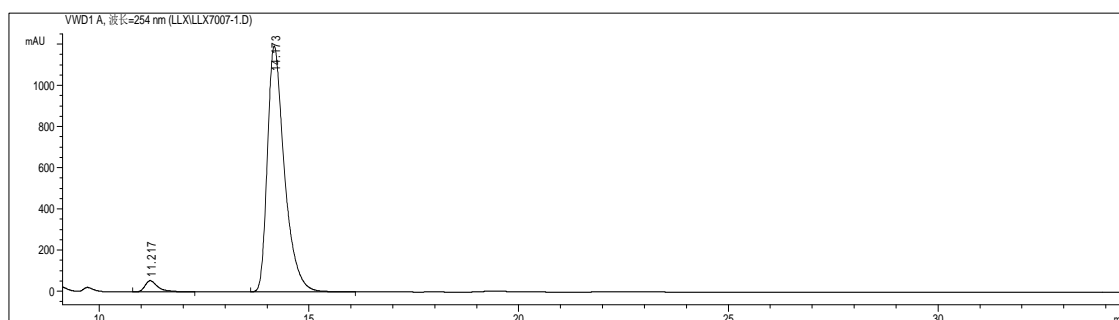
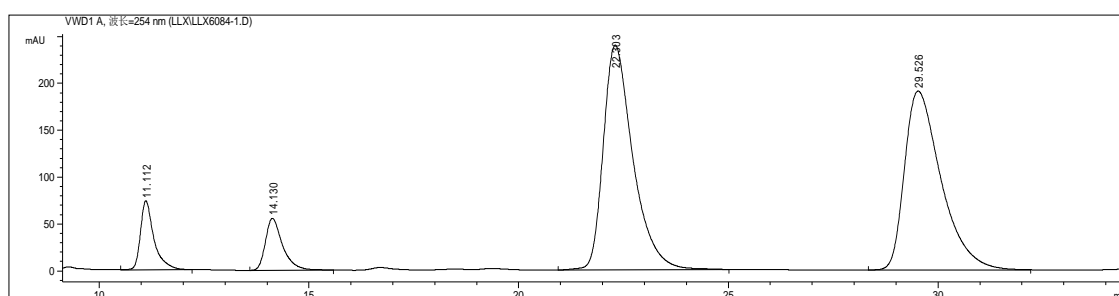
The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 9.3 min (minor) and 11.7 min (major).



4b, white solid, M.p. 99.1 - 101.9 °C; 97% yield; 93% *ee*; $[\alpha]_{20}^D = +131.0$ (*c* 0.58, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.48 (d, *J* = 8.3 Hz, 2H), 7.26 (s, 1H), 7.24 (s, 1H), 7.18 - 6.96 (m, 7H), 6.78 (t, *J* = 6.9 Hz, 3H), 6.68 (t, *J* = 7.6 Hz, 1H), 6.60 (d, *J* = 6.9 Hz, 2H), 6.36 (d, *J* = 7.9 Hz, 1H), 4.79 (d, *J* = 15.9 Hz, 1H), 4.62 (dd, *J* = 43.4, 14.0 Hz, 2H), 4.44 (d, *J* = 15.9 Hz,

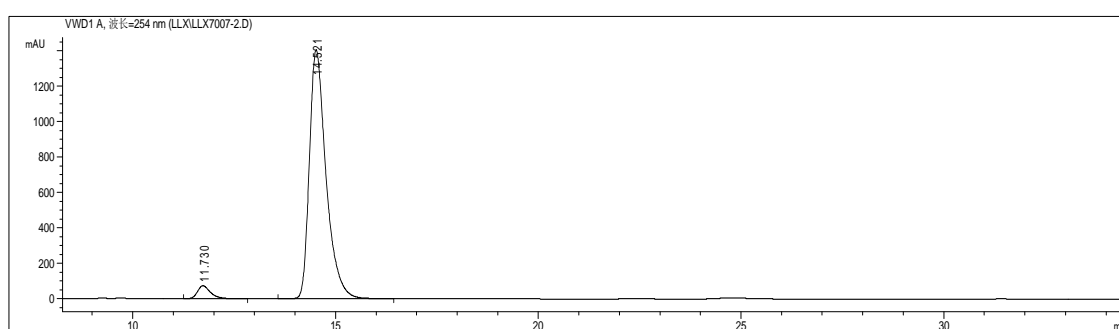
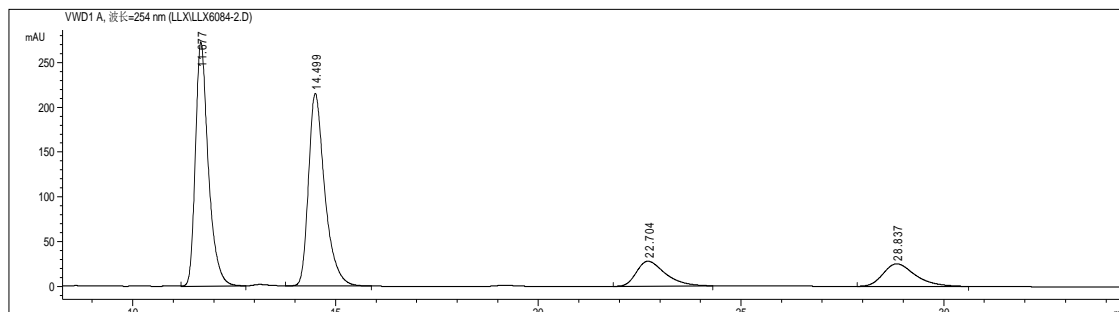
1H), 4.03 (d, $J = 13.2$ Hz, 1H), 3.56 (dd, $J = 9.1, 5.0$ Hz, 1H), 3.38 (d, $J = 13.2$ Hz, 1H), 2.74 (dd, $J = 18.3, 9.1$ Hz, 1H), 1.78 (dd, $J = 18.3, 5.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 176.8, 176.4, 174.8, 143.4, 135.2, 134.6, 134.4, 131.8, 130.9, 130.1, 129.2, 128.7, 127.8, 127.4, 126.6, 126.2, 124.0, 122.9, 122.2, 109.6, 55.6, 44.7, 43.6, 41.9, 41.2, 31.3; LRMS (ESI) m/z 579.1 ($\text{M}+\text{H}^+$); HRMS (ESI) m/z 579.1296 ($\text{M}+\text{H}^+$), Calc. for $\text{C}_{33}\text{H}_{28}\text{BrN}_2\text{O}_3$ 579.1278.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 11.2 min (minor) and 14.2 min (major).



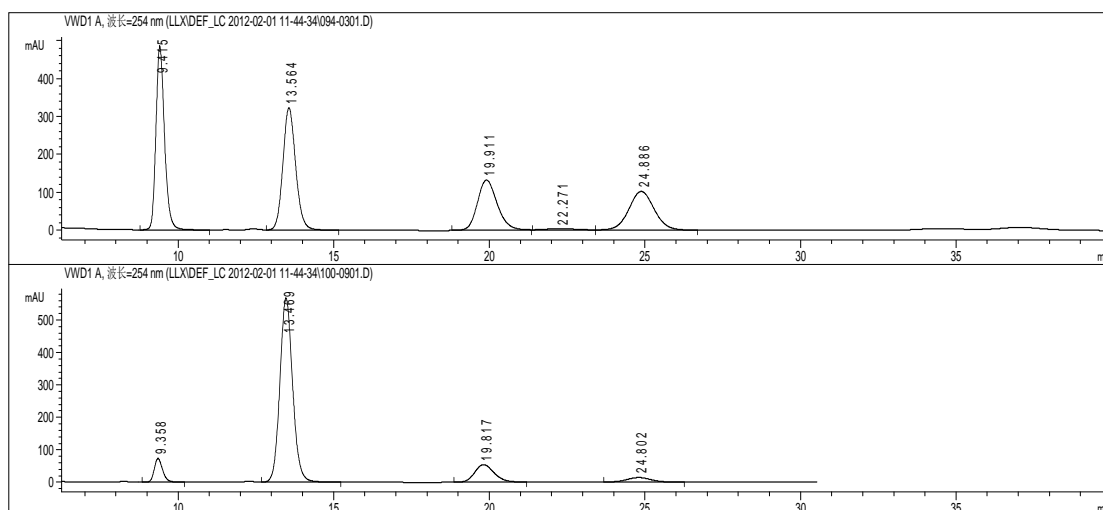
4c, white solid, M.p. 101.1 - 102.3 °C; 91% yield; 92% *ee*; $[\alpha]_{20}^{\text{D}} = +109.8$ (c 0.86, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.33 (d, $J = 8.6$ Hz, 1H), 7.17 - 7.06 (m, 2H), 7.03 - 6.96 (m, 2H), 6.87 (d, $J = 8.6$ Hz, 1H), 6.83 (d, $J = 7.3$ Hz, 1H), 6.78 (d, $J = 7.3$ Hz, 1H), 6.67 (t, $J = 7.4$ Hz, 1H), 6.59 (d, $J = 6.9$ Hz, 1H), 6.34 (d, $J = 7.8$ Hz, 1H), 4.78 (d, $J = 15.9$ Hz, 1H), 4.61 (dd, $J = 39.6, 13.8$ Hz, 1H), 4.44 (d, $J = 15.9$ Hz, 1H), 4.05 (d, $J = 13.2$ Hz, 1H), 3.83 (s, 2H), 3.54 (dd, $J = 9.1, 5.0$ Hz, 1H), 3.38 (d, $J = 13.2$ Hz, 1H), 2.71 (dd, $J = 18.3, 9.1$ Hz, 1H), 1.74 (dd, $J = 18.3, 5.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 177.0, 176.5, 175.0, 159.4, 143.3, 135.3, 134.7, 130.6, 130.1, 129.0, 128.6, 127.8, 127.3, 126.6, 126.2, 124.2, 122.9, 113.9, 109.5, 55.7, 55.3, 44.6, 43.6, 42.0, 41.2, 31.3; LRMS (ESI) m/z 553.2 ($\text{M}+\text{Na}^+$); HRMS (ESI) m/z 553.2115 ($\text{M}+\text{Na}^+$), Calc. for $\text{C}_{34}\text{H}_{30}\text{N}_2\text{NaO}_4$ 553.2098.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 11.7 min (minor) and 14.5 min (major).



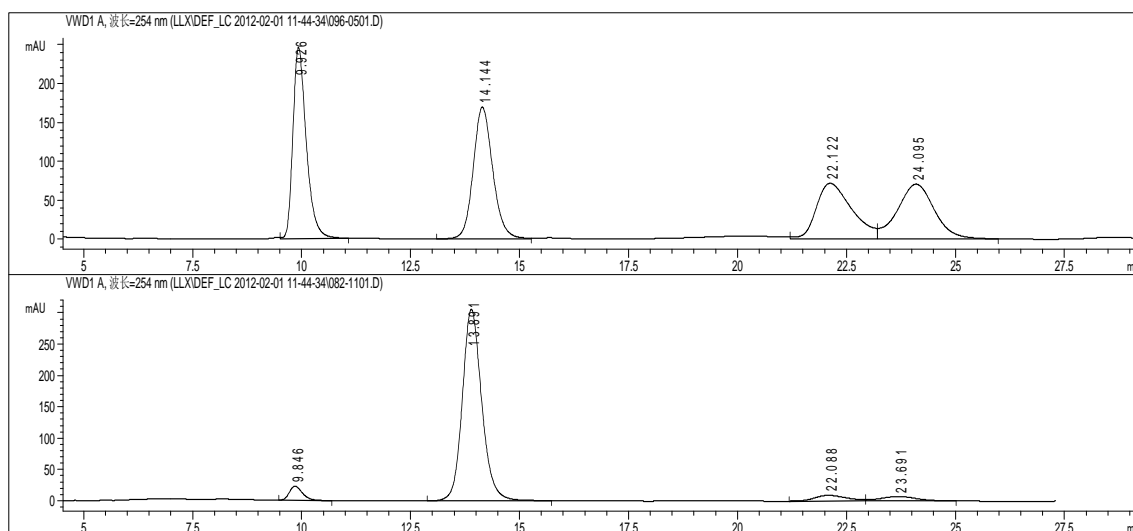
4d, white solid, M.p. 108.6 - 109.2 °C; 88% yield; 92% *ee*, $[\alpha]_{20}^D = +105.0$ (*c* 0.47, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.41 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.21 - 7.07 (m, 9H), 7.01 (t, *J* = 7.6 Hz, 2H), 6.92 (t, *J* = 7.2 Hz, 1H), 6.82 (d, *J* = 7.2 Hz, 2H), 6.61 (d, *J* = 6.8 Hz, 2H), 6.41 (d, *J* = 8.4 Hz, 1H), 4.85 (d, *J* = 16.9 Hz, 3H), 4.48 (d, *J* = 15.9 Hz, 1H), 4.11 (d, *J* = 13.2 Hz, 1H), 3.65 (dd, *J* = 9.1, 5.7 Hz, 1H), 3.42 (d, *J* = 12.0 Hz, 1H), 2.82 (dd, *J* = 18.2, 9.1 Hz, 1H), 1.93 (dd, *J* = 18.2, 5.7 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 176.8, 176.4, 174.7, 143.4, 135.2, 134.6, 133.2, 132.3, 130.1, 129.7, 129.2, 129.1, 129.0, 128.6, 127.8, 127.3, 126.8, 126.6 (two peaks), 126.4, 124.4, 123.0, 109.6, 55.4, 45.0, 43.6, 41.2, 40.1, 31.3; LRMS (EI) *m/z* 534.2; HRMS (EI) *m/z* 534.1705, Calc. for C₃₃H₂₇N₂O₃Cl 534.1710.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 9.3 min (minor) and 13.5 min (major).



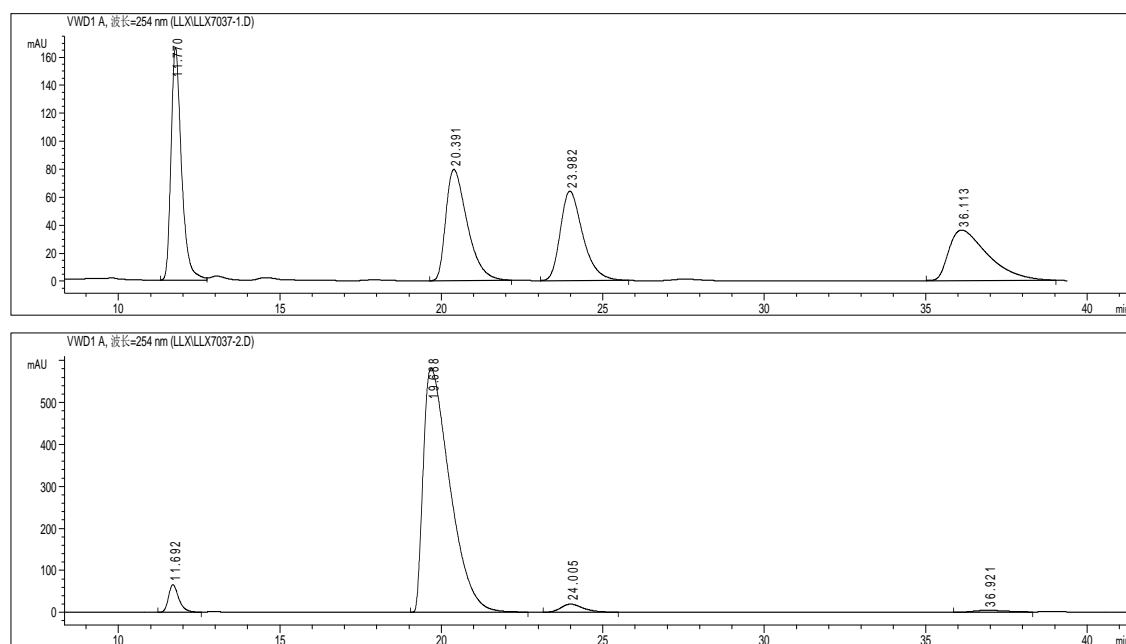
4e, white solid, M.p. 105.3 - 105.8 °C; 92% yield; 92% *ee*, $[\alpha]_{20}^D = +115.1$ (*c* 0.31, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.33 - 7.27 (m, 1H), 7.16 - 7.00 (m, 9H), 6.94 - 6.86 (m, 3H), 6.80 (d, *J* = 7.2 Hz, 2H), 6.59 (d, *J* = 6.8 Hz, 2H), 6.38 (d, *J* = 7.8 Hz, 1H), 4.85 (d, *J* = 15.9 Hz, 1H), 4.74 (q, *J* = 14.9 Hz, 2H), 4.46 (d, *J* = 15.9 Hz, 1H), 4.13 (d, *J* = 13.2 Hz, 1H), 3.79 (s, 3H), 3.59 (dd, *J* = 9.1, 5.6 Hz, 1H), 3.40 (d, *J* = 13.2 Hz, 1H), 2.77 (dd, *J* = 18.1, 9.1 Hz, 1H), 1.83 (dd, *J* = 18.1, 5.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 176.9, 176.5, 174.8, 157.1, 143.5, 135.4, 134.7, 130.2, 129.1 (two peaks), 129.0, 128.6, 127.8, 127.3, 126.6 (two peaks), 126.5, 124.5, 123.0 (two peaks), 120.3, 110.4, 109.5, 55.6, 55.3, 44.8, 43.6, 41.3, 37.9, 31.3; LRMS (EI) *m/z* 530.2; HRMS (EI) *m/z* 530.2205, Calc. for C₃₄H₃₀N₂O₄ 530.2206.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 9.8 min (minor) and 13.1 min (major).



4f, white solid, M.p. 151.6 - 152.7 °C; 92% yield; 93% *ee*; $[\alpha]_{20}^D = +132.7$ (*c* 0.075, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.53 - 7.49 (m, 2H), 7.46 - 7.38 (m, 2H), 7.26 - 7.22 (m, 2H), 7.19 - 7.08 (m, 6H), 7.03 (t, *J* = 7.5 Hz, 2H), 6.86 (d, *J* = 7.2 Hz, 2H), 6.64 (d, *J* = 6.8 Hz, 2H), 6.46 (d, *J* = 7.5 Hz, 1H), 4.90 (d, *J* = 15.9 Hz, 1H), 4.51 (d, *J* = 15.9 Hz, 1H), 4.13 (d, *J* = 13.1 Hz, 1H), 3.76 (dd, *J* = 9.2, 5.1 Hz, 1H), 3.48 (d, *J* = 13.3 Hz, 1H), 2.91 (dd, *J* = 18.4, 9.2 Hz, 1H), 2.01 (dd, *J* = 18.4, 5.1 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 176.5, 176.3, 174.2, 143.6, 135.2, 134.6, 131.6, 130.2, 129.5, 129.3, 128.9, 128.7, 127.9, 127.4, 126.7, 126.6 (two peaks), 126.4, 124.2, 123.0, 109.8, 55.8, 45.1, 43.7, 41.2, 31.5; LRMS (ESI) *m/z* 509.2 (M+Na⁺); HRMS (ESI) *m/z* 509.1832 (M+Na⁺), Calc. for C₃₂H₂₆N₂NaO₃ 509.1836.

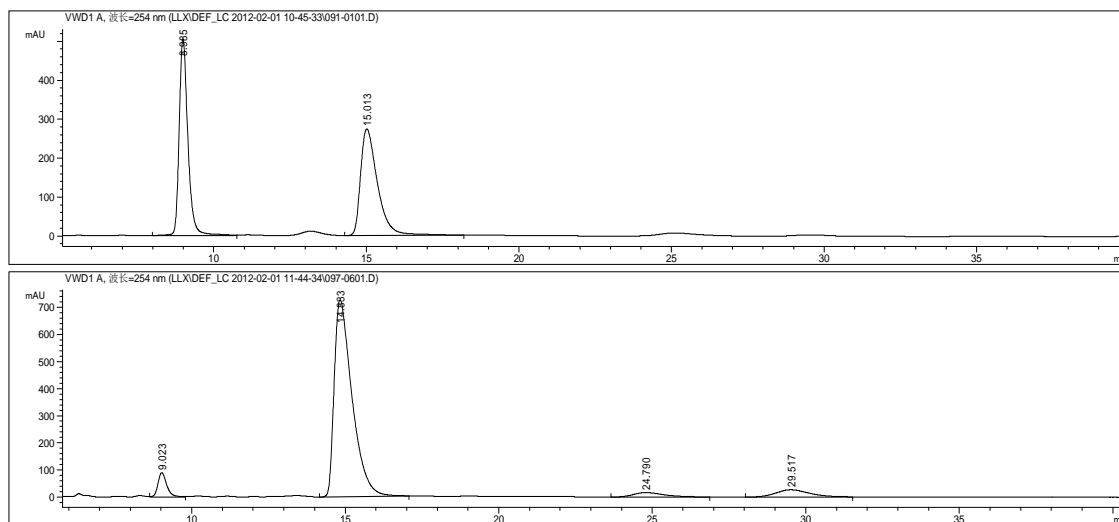
The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 11.7 min (minor) and 19.7 min (major).



4g, white solid, M.p. 150.1 - 151.2 °C; 90% yield; 90% *ee*; $[\alpha]_{20}^D = +181.3$ (*c* 0.30, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.52 (d, *J* = 8.6 Hz, 2H), 7.39 (d, *J* = 7.3 Hz, 1H), 7.20 - 7.10 (m, 8H), 7.03 (t, *J* = 7.6 Hz, 2H), 6.87 - 6.82 (m, 2H), 6.62 (d, *J* = 6.9 Hz, 2H), 6.45 (d, *J* = 7.6 Hz, 1H), 4.91 (d, *J* = 15.9 Hz, 1H), 4.50 (d, *J* = 15.9 Hz, 1H), 4.14 (d, *J* = 13.3 Hz, 1H), 3.75 (dd, *J* = 9.2, 5.0 Hz, 1H), 3.48 (d, *J* = 13.3 Hz, 1H), 2.90 (dd, *J* = 18.4, 9.2 Hz, 1H), 1.98 (dd, *J* = 18.4, 5.0 Hz, 1H), 1.35 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 176.5 (two peaks),

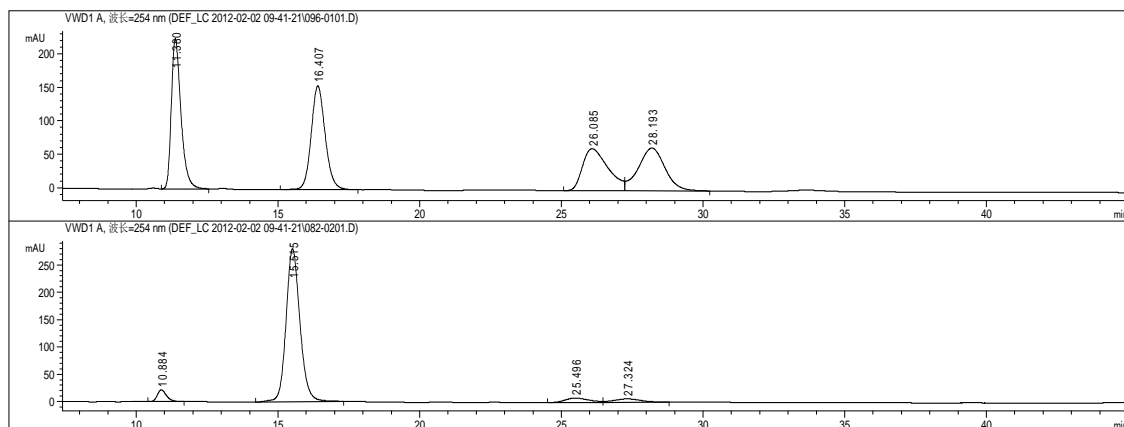
174.5, 151.9, 143.6, 135.2, 134.6, 130.2, 129.5, 128.8, 128.7, 127.9, 127.4, 126.7, 126.6, 126.4, 126.3, 126.0, 124.3, 123.0, 109.8, 55.8, 45.0, 43.6, 41.2, 34.7, 31.5, 31.2; LRMS (EI) m/z 542.3; HRMS (EI) m/z 542.2571, Calc. for $C_{36}H_{34}N_2O_3$ 542.2569.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0ml/min; 25 °C; 254 nm; retention time: 9.0 min (minor) and 11.8 min (major).



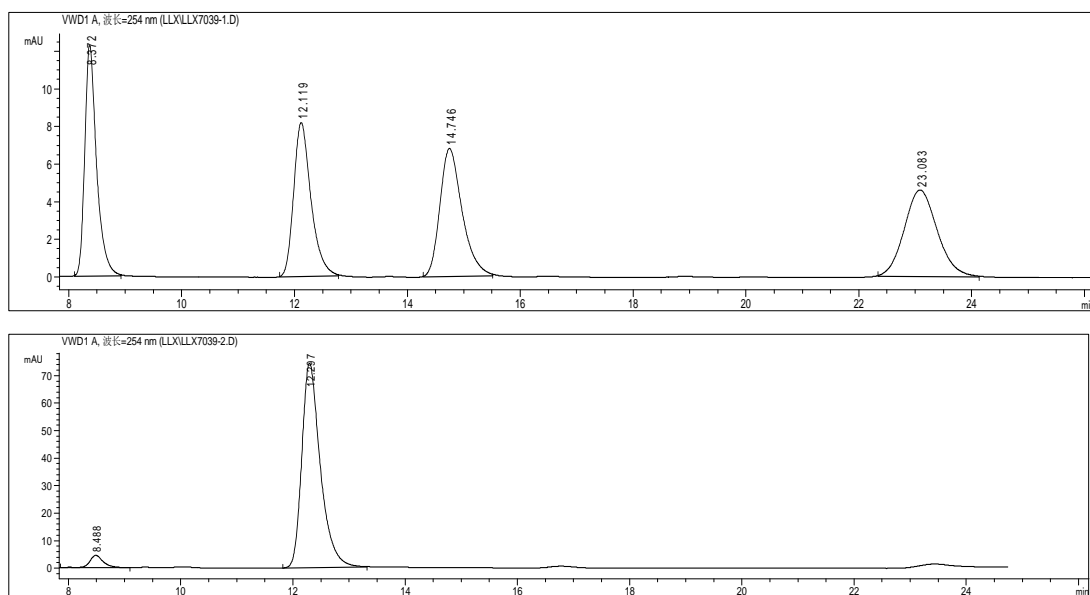
4h, white solid, M.p. 157.8 - 158.6 °C; 89% yield, 92% *ee*; $[\alpha]_{20}^D = +46.1$ (*c* 0.23, $CHCl_3$); 1H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, $J = 8.7$ Hz, 1H), 7.43 (t, $J = 1.8$ Hz, 1H), 7.37 (dd, $J = 14.7, 6.9$ Hz, 2H), 7.23 - 7.09 (m, 7H), 7.03 (t, $J = 7.6$ Hz, 2H), 6.84 (d, $J = 7.3$ Hz, 2H), 6.62 (d, $J = 7.0$ Hz, 2H), 6.46 (d, $J = 7.6$ Hz, 1H), 4.90 (d, $J = 15.9$ Hz, 1H), 4.50 (d, $J = 15.9$ Hz, 1H), 4.09 (d, $J = 13.3$ Hz, 1H), 3.75 (dd, $J = 9.2, 5.2$ Hz, 1H), 3.46 (d, $J = 13.3$ Hz, 1H), 2.91 (dd, $J = 18.4, 9.3$ Hz, 1H), 2.03 (dd, $J = 18.8, 4.8$ Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.4, 175.8, 173.8, 143.6, 135.1, 134.6, 132.7, 132.0, 130.4, 130.2, 129.7, 129.6, 128.7, 127.9, 127.4, 126.8, 126.6, 126.4, 125.2, 124.1, 123.1, 122.6, 109.9, 55.7, 45.2, 43.7, 41.2, 31.5; LRMS (EI) m/z 564.1; HRMS (EI) m/z 564.1054, Calc. for $C_{32}H_{25}N_2O_3Br$ 564.1049.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0ml/min; 25 °C; 254 nm; retention time: 10.9 min (minor) and 15.5 min (major).



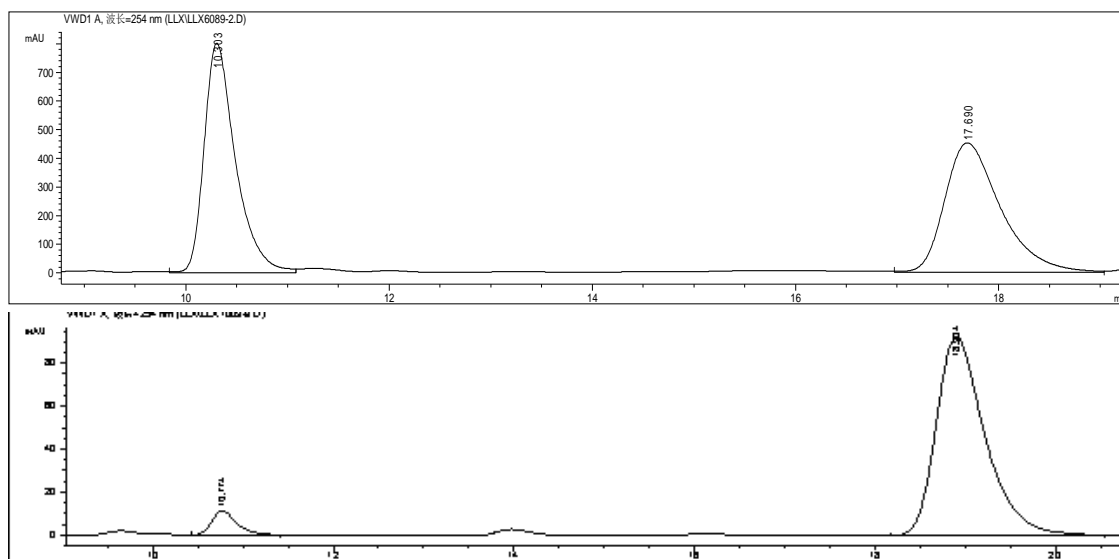
4i, white powder, M.p. 168.7 - 170.2 °C; 97% yield; 91% *ee*; $[\alpha]_{20}^D = +151.7$ (*c* 0.29, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.31 - 7.27 (m, 1H), 7.19 - 7.06 (m, 5H), 7.01 (t, *J* = 7.5 Hz, 3H), 6.83 (d, *J* = 7.2 Hz, 2H), 6.61 (d, *J* = 6.7 Hz, 2H), 6.41 (d, *J* = 7.7 Hz, 1H), 4.84 (d, *J* = 15.9 Hz, 1H), 4.47 (d, *J* = 15.9 Hz, 1H), 4.14 (d, *J* = 13.2 Hz, 1H), 3.64 - 3.50 (m, 3H), 3.42 (d, *J* = 13.3 Hz, 1H), 2.70 (dd, *J* = 18.2, 9.1 Hz, 1H), 1.77 (dd, *J* = 18.2, 5.2 Hz, 1H), 1.18 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 177.1, 176.5, 175.0, 143.5, 135.3, 134.7, 130.2, 129.3, 128.6, 127.8, 127.3, 126.6, 126.5, 124.2, 122.9, 109.6, 55.5, 44.8, 43.6, 41.2, 33.8, 31.3, 13.0; LRMS (ESI) *m/z* 461.2 (M+Na⁺); HRMS (ESI) *m/z* 461.1841 (M+Na⁺), Calc. for C₂₈H₂₆N₂NaO₃ 461.1836.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0ml/min; 25 °C; 254 nm; retention time: 8.5 min (minor) and 12.3 min (major).



4j, white solid, M.p. 77.6 - 78.4 °C; 89% yield; 90% *ee*; $[\alpha]_{20}^D = +169.1$ (*c* 0.23, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.41 - 7.32 (m, 5H), 7.23 - 7.17 (m, 3H), 7.10 (d, *J* = 8.4 Hz, 2H), 7.03 (td, *J* = 7.8, 1.1 Hz, 1H), 6.79 (d, *J* = 7.0 Hz, 1H), 6.67 - 6.59 (m, 5H), 6.41 (d, *J* = 7.9 Hz, 1H), 4.89 (d, *J* = 15.8 Hz, 1H), 4.73 (d, *J* = 13.9 Hz, 1H), 4.61 (d, *J* = 13.9 Hz, 1H), 4.41 (d, *J* = 15.8 Hz, 1H), 4.02 (d, *J* = 13.3 Hz, 1H), 3.53 (dd, *J* = 9.1, 5.0 Hz, 1H), 3.34 (d, *J* = 13.3 Hz, 1H), 2.72 (dd, *J* = 18.3, 9.1 Hz, 1H), 1.73 (dd, *J* = 18.3, 5.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 176.8, 176.1, 174.8, 143.3, 135.4, 134.5, 134.3, 131.8, 130.9, 129.3, 129.1, 128.7 (two peaks), 128.1, 127.5, 126.6, 125.7, 124.1, 123.1, 120.8, 109.6, 55.4, 44.6, 43.7, 42.6, 40.4, 31.2; LRMS (ESI) *m/z* 601.1 (M+Na⁺); HRMS (ESI) *m/z* 579.1283, Calc. for C₃₃H₂₈BrN₂O₃ 579.1278.

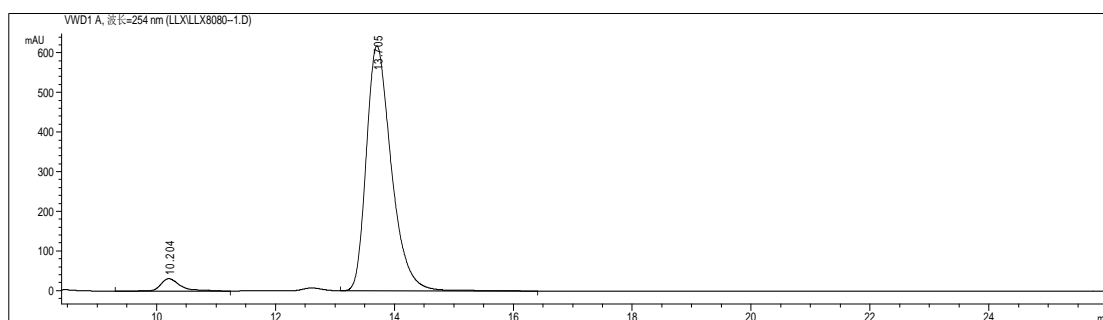
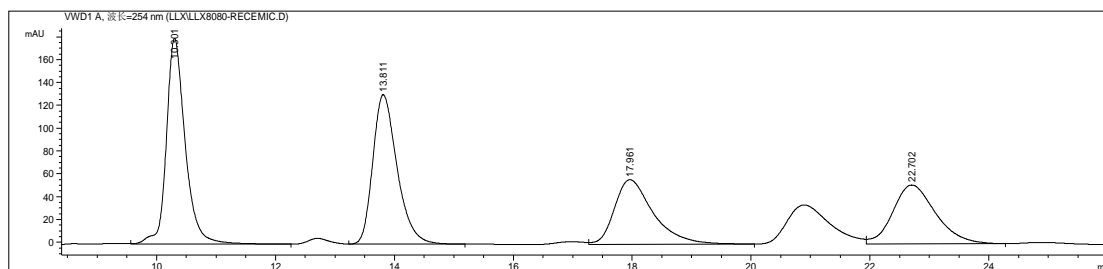
The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 10.8 min (minor) and 18.9 min (major).



4k, white solid, M.p. 80.2 - 81.8 °C; 88% yield; 92% *ee*; $[\alpha]_{20}^D = +170.5$ (*c* 0.11, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.40 - 7.33 (m, 5H), 7.23 - 7.16 (m, 4H), 7.03 (td, *J* = 7.8, 1.0 Hz, 1H), 6.93 (s, 1H), 6.83 (t, *J* = 7.8 Hz, 1H), 6.77 (d, *J* = 7.2 Hz, 1H), 6.72 - 6.67 (m, 3H), 6.65 (d, *J* = 7.5 Hz, 1H), 6.41 (d, *J* = 7.9 Hz, 1H), 4.79 (d, *J* = 15.8 Hz, 1H), 4.73 (d, *J* = 13.9 Hz, 1H), 4.65 - 4.57 (m, 1H), 4.49 (d, *J* = 15.8 Hz, 1H), 4.03 (d, *J* = 13.2 Hz, 1H), 3.53 (dd, *J* = 9.1, 5.0 Hz, 1H), 3.34 (d, *J* = 13.3 Hz, 1H), 2.73 (dd, *J* = 18.3, 9.1 Hz, 1H), 1.73 (dd, *J* = 18.3, 5.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 176.8, 176.1, 174.8, 143.3, 137.6, 135.4, 134.7,

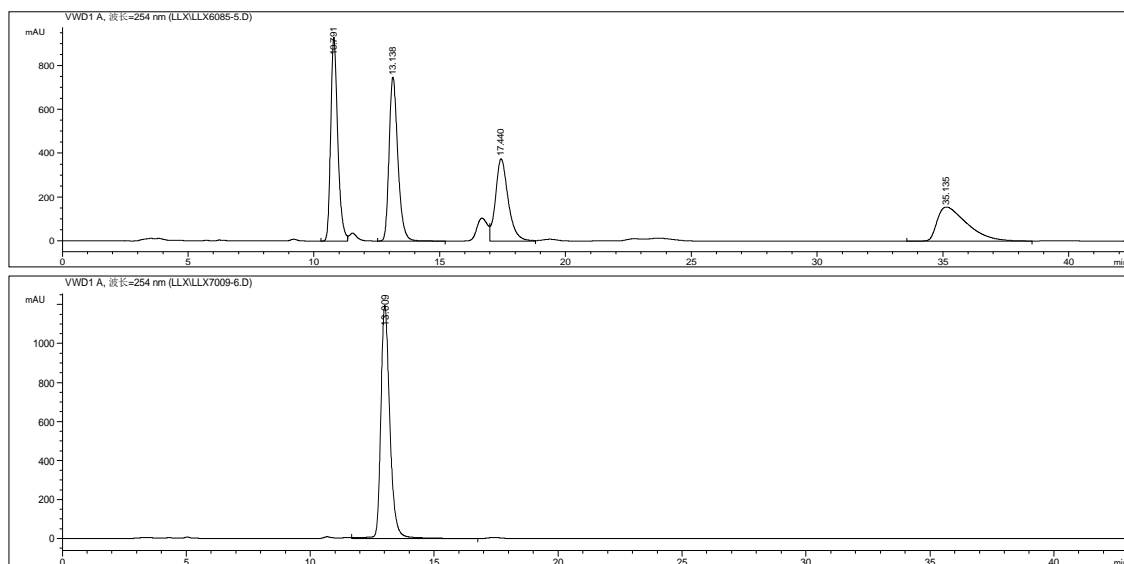
132.9, 129.8, 129.3 (two peaks), 129.1, 128.8 (two peaks), 128.7, 128.1, 127.5, 126.6, 125.7, 124.1, 123.1, 121.8, 109.6, 55.4, 44.4, 43.7, 42.6, 40.7, 31.3; LRMS (ESI) m/z 579.1 ($M+H^+$); HRMS (ESI) m/z 579.1290 ($M+H^+$), Calc. for $C_{33}H_{28}BrN_2O_3$ 579.1278.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 10.2 min (minor) and 13.7 min (major).



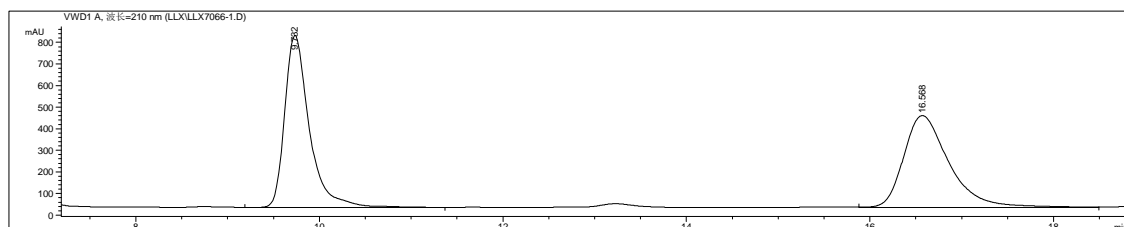
4l, white solid, M.p. 85.4 - 86.4 °C; 93% yield; 99% *ee*; $[\alpha]_{20}^D = +80.0$ (*c* 0.24, $CHCl_3$); 1H NMR (400 MHz, $CDCl_3$) δ 7.41 - 7.31 (m, 6H), 7.24 - 7.18 (m, 3H), 7.03 (t, $J = 7.4$ Hz, 1H), 6.98 - 6.86 (m, 6H), 6.62 (t, $J = 7.6$ Hz, 1H), 6.50 (d, $J = 7.8$ Hz, 1H), 4.81 - 4.62 (m, 4H), 4.32 (d, $J = 13.8$ Hz, 1H), 3.68 (d, $J = 13.9$ Hz, 1H), 3.59 (dd, $J = 9.1, 5.1$ Hz, 1H), 2.70 (dd, $J = 18.2, 9.1$ Hz, 1H), 1.74 (dd, $J = 18.2, 5.1$ Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 176.5, 174.8, 143.1, 135.4 (two peaks), 135.0, 132.9, 131.2, 129.2, 129.1, 128.7, 128.6, 128.3, 128.0, 127.6, 127.2, 126.8, 125.8, 125.7, 125.2, 122.8, 109.1, 54.8, 44.2, 44.0, 42.5, 39.2, 31.2; LRMS (ESI) m/z 601.1 ($M+Na^+$); HRMS (ESI) m/z 579.1291 ($M+H^+$), Calc. for $C_{33}H_{28}BrN_2O_3$ 579.1278.

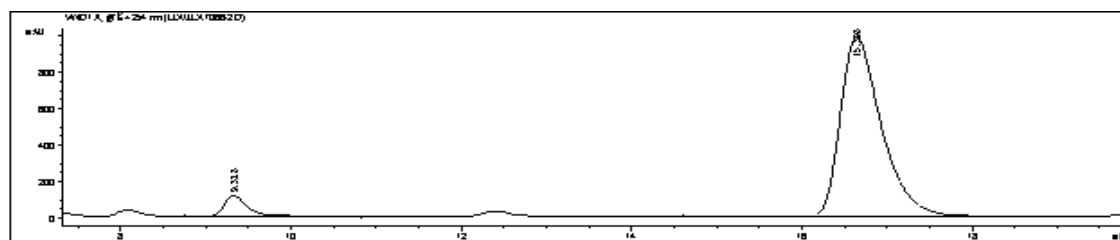
The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 13.0 min (major).



4m, white solid, M.p. 78.6 - 79.2 °C; 81% yield; 90% *ee*; $[\alpha]_{20}^D = +183.6$ (c 0.07, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.40 - 7.33 (m, 5H), 7.20 - 7.18 (m, 3H), 7.05 - 7.01 (m, 1H), 6.94 (d, $J = 8.4$ Hz, 2H), 6.79 (d, $J = 6.9$ Hz, 1H), 6.72 - 6.57 (m, 5H), 6.41 (d, $J = 7.8$ Hz, 1H), 4.88 (d, $J = 15.8$ Hz, 1H), 4.73 (d, $J = 13.9$ Hz, 1H), 4.62 (d, $J = 13.9$ Hz, 1H), 4.41 (d, $J = 15.8$ Hz, 1H), 4.04 (d, $J = 13.3$ Hz, 1H), 3.53 (dd, $J = 9.1, 5.0$ Hz, 1H), 3.35 (d, $J = 13.3$ Hz, 1H), 2.72 (dd, $J = 18.3, 9.1$ Hz, 1H), 1.73 (dd, $J = 18.3, 5.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 176.9, 176.2, 174.8, 143.3, 135.4, 134.5, 133.8, 132.6, 131.5, 129.3, 129.1, 128.7, 128.6, 128.1, 128.0, 127.5, 126.6, 125.8, 124.1, 123.1, 109.6, 55.4, 44.6, 43.7, 42.6, 40.4, 31.2; LRMS (ESI) m/z 557.2 ($\text{M}+\text{Na}^+$); HRMS (ESI) m/z 557.1607 ($\text{M}+\text{Na}^+$), Calc. for $\text{C}_{33}\text{H}_{27}\text{ClN}_2\text{NaO}_3$ 557.1602.

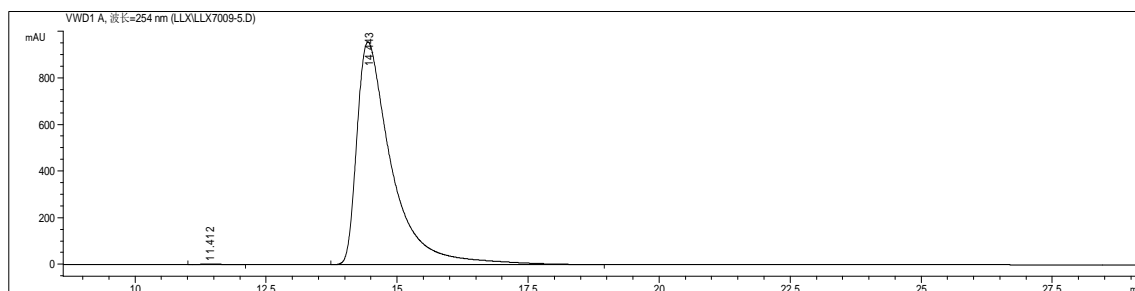
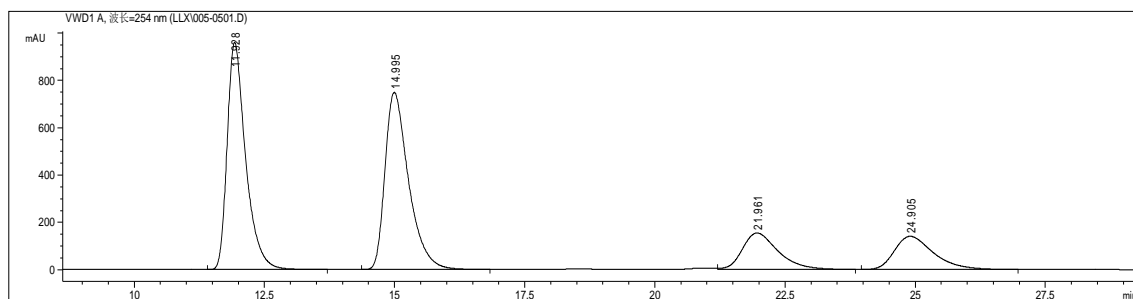
The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 9.3 min (minor) and 16.2 min (major).





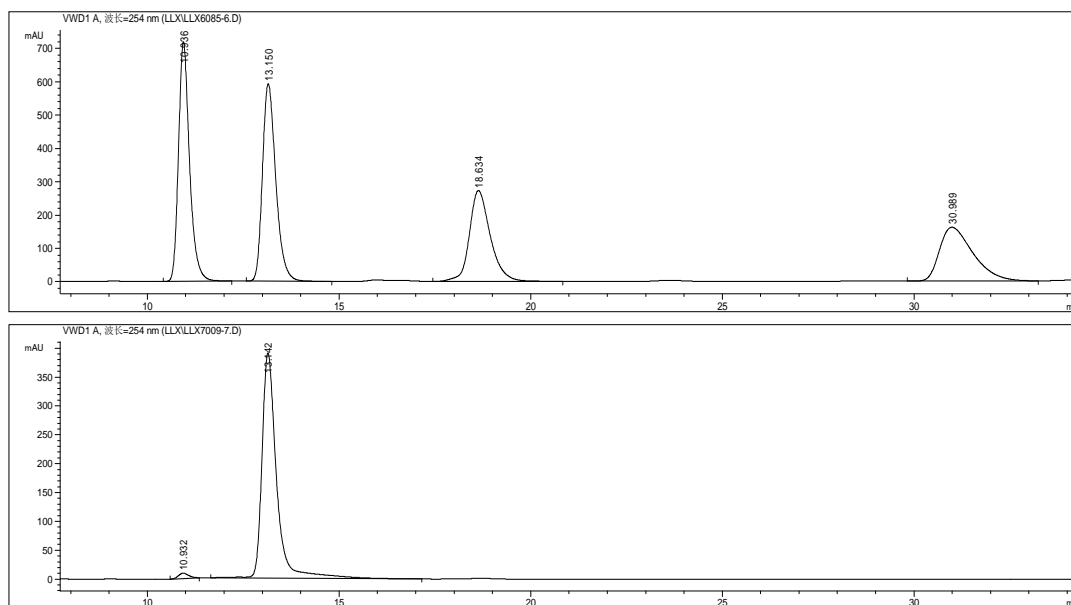
4n, white solid, M.p. 39.6 - 40.2 °C; 77% yield; 99% *ee*; $[\alpha]_{20}^D = +80.5$ (*c* 0.60, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.40 - 7.29 (m, 5H), 7.19 - 7.09 (m, 3H), 7.01 (td, *J* = 7.8, 1.1 Hz, 1H), 6.92 (t, *J* = 7.9 Hz, 1H), 6.83 (d, *J* = 6.9 Hz, 1H), 6.66 (t, *J* = 7.6 Hz, 2H), 6.60 (d, *J* = 6.6 Hz, 2H), 6.45 (d, *J* = 7.6 Hz, 1H), 6.36 (d, *J* = 7.8 Hz, 1H), 6.22 (d, *J* = 1.8 Hz, 1H), 4.84 (d, *J* = 15.9 Hz, 1H), 4.67 (dd, *J* = 43.1, 13.9 Hz, 2H), 4.43 (d, *J* = 15.9 Hz, 1H), 4.05 (d, *J* = 13.2 Hz, 1H), 3.55 (dd, *J* = 9.1, 5.0 Hz, 1H), 3.43 (s, 3H), 3.37 (d, *J* = 13.2 Hz, 1H), 2.74 (dd, *J* = 18.3, 9.1 Hz, 1H), 1.77 (dd, *J* = 18.3, 5.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 176.9, 176.4, 174.9, 158.9, 143.4, 136.7, 135.4, 134.7, 129.1, 128.8, 128.6, 128.0, 127.4, 126.5, 126.3, 124.2, 122.9, 122.6, 114.6, 113.3, 109.6, 55.6, 54.9, 44.7, 43.6, 42.6, 41.3, 31.3; LRMS (ESI) *m/z* 553.3 (M+Na⁺); HRMS (ESI) *m/z* 553.2096 (M+Na⁺), Calc. for C₃₄H₃₀N₂NaO₄ 553.2098.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 11.4 min (minor) and 14.4 min (major).



4o, white solid, M.p. 75.5 - 77.8 °C; 88% yield; 97% *ee*; $[\alpha]_{20}^D = +129.5$ (*c* 1.06, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.41 - 7.31 (m, 5H), 7.21 - 7.15 (m, 3H), 7.10 - 6.93 (m, 3H), 6.83 - 6.80 (m, 3H), 6.68 - 6.53 (m, 3H), 6.38 (d, *J* = 7.8 Hz, 1H), 4.82 (d, *J* = 15.8 Hz, 1H), 4.67 (dd, *J* = 34.2, 13.9 Hz, 2H), 4.56 (d, *J* = 15.8 Hz, 1H), 4.24 (d, *J* = 13.3 Hz, 1H), 3.56 (dd, *J* = 9.1, 5.0 Hz, 1H), 3.42 (s, 3H), 3.35 (d, *J* = 13.3 Hz, 1H), 2.70 (dd, *J* = 18.3, 9.1 Hz, 1H), 1.80 (dd, *J* = 18.3, 5.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 176.9 (two peaks), 175.1, 157.5, 143.2, 135.5, 135.2, 131.6, 129.1, 128.6 (two peaks), 128.0, 127.4, 126.9, 126.6, 125.1, 124.0, 122.2, 119.9, 110.1, 108.8, 55.1, 54.5, 44.4, 43.7, 42.5, 33.9, 31.4; LRMS (ESI) *m/z* 531.2 (M+H⁺); HRMS (ESI) *m/z* 531.2286 (M+H⁺), Calc. for C₃₄H₃₁N₂O₄ 531.2286.

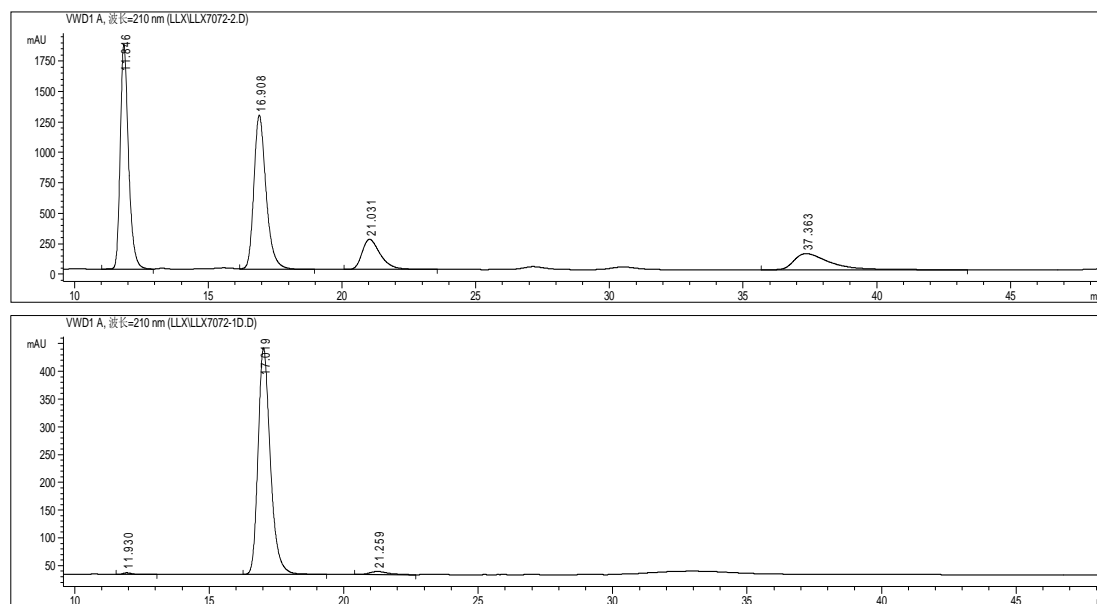
The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 10.9 min (minor) and 13.1 min (major).



4p, white solid, M.p. 51.2 - 51.7 °C; 90% yield; 99% *ee*; $[\alpha]_{20}^D = +190.0$ (*c* 0.19, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 8.18 (d, *J* = 8.5 Hz, 1H), 7.73 - 7.66 (m, 1H), 7.58 (d, *J* = 8.1 Hz, 1H), 7.46 - 7.32 (m, 7H), 7.13 (t, *J* = 7.3 Hz, 1H), 7.10 - 6.98 (m, 3H), 6.94 (d, *J* = 6.3 Hz, 1H), 6.91 - 6.83 (m, 2H), 6.57 - 6.46 (m, 3H), 6.26 (d, *J* = 7.8 Hz, 1H), 4.83 - 4.61 (m, 4H), 4.35 (d, *J* = 15.7 Hz, 1H), 3.97 (d, *J* = 14.0 Hz, 1H), 3.72 (dd, *J* = 9.1, 5.2 Hz, 1H), 2.77 (dd, *J* = 18.3, 9.1 Hz, 1H), 1.75 (dd, *J* = 18.3, 5.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 177.3, 176.9, 174.9, 143.3, 135.4, 134.7, 133.5, 132.1, 131.9, 129.1, 128.9, 128.7, 128.5, 128.2,

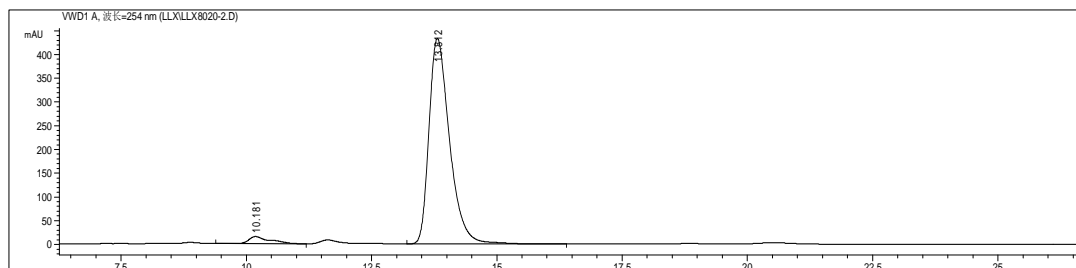
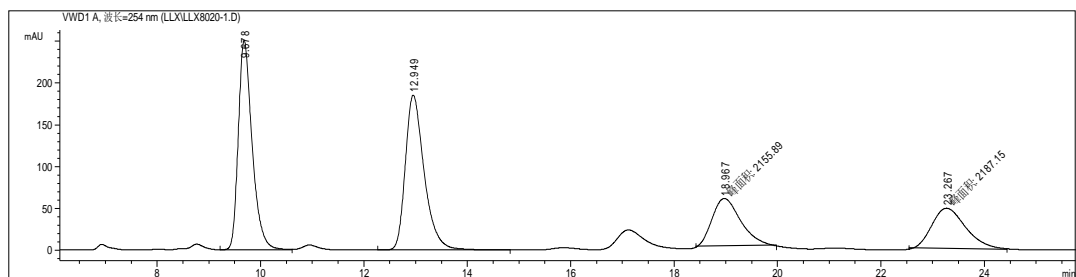
128.1, 127.4, 127.3, 126.7, 126.0, 125.3 (two peaks), 124.8, 124.7, 124.6, 122.6, 109.2, 55.6, 44.8, 43.7, 42.6, 36.1, 31.4; LRMS (ESI) m/z 573.2 ($M+Na^+$); HRMS (ESI) m/z 573.2138 ($M+Na^+$), Calc. for $C_{37}H_{30}N_2NaO_3$ 573.2149.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 11.9 min (minor) and 17.0 min (major).



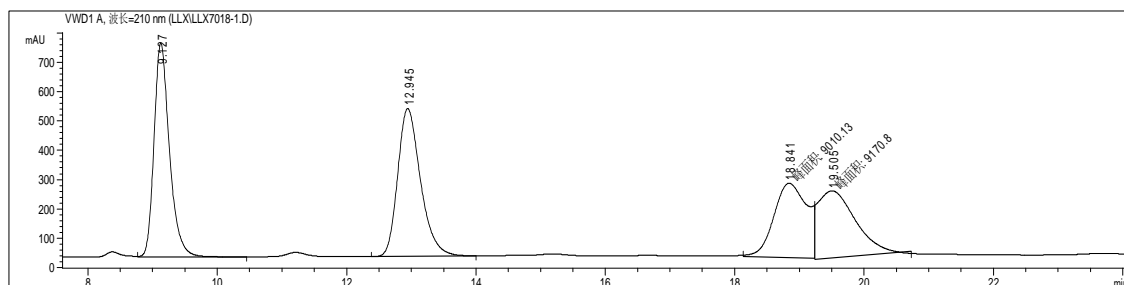
4q, white solid, M.p. 35.6 - 36.7 °C; 81% yield; 96% *ee*; $[\alpha]_{20}^D = +251.6$ (c 0.06, $CHCl_3$); 1H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.30 (m, 5H), 7.20 - 7.13 (m, 3H), 7.07 (td, $J = 7.8, 1.2$ Hz, 1H), 6.93 (dd, $J = 5.1, 0.9$ Hz, 1H), 6.80 (d, $J = 6.8$ Hz, 1H), 6.75 - 6.65 (m, 4H), 6.57 (d, $J = 3.2$ Hz, 1H), 6.46 (d, $J = 7.8$ Hz, 1H), 4.88 (d, $J = 15.8$ Hz, 1H), 4.66 (dd, $J = 41.3, 13.9$ Hz, 2H), 4.51 (d, $J = 15.8$ Hz, 1H), 4.27 (d, $J = 14.4$ Hz, 1H), 3.66 (d, $J = 14.4$ Hz, 1H), 3.52 (dd, $J = 9.1, 5.1$ Hz, 1H), 2.73 (dd, $J = 18.3, 9.1$ Hz, 1H), 1.78 (dd, $J = 18.3, 5.1$ Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 176.3, 174.8, 143.8, 136.8, 135.4, 134.8, 129.4, 129.1, 128.7 (two peaks), 128.1, 127.4, 126.7, 126.2, 124.5, 124.2, 123.2, 109.6, 55.3, 44.4, 43.8, 42.6, 35.4, 31.3; LRMS (ESI) m/z 529.1 ($M+Na^+$); HRMS (ESI) m/z 529.1563 ($M+Na^+$), Calc. for $C_{31}H_{26}N_2NaO_3S$ 529.1556.

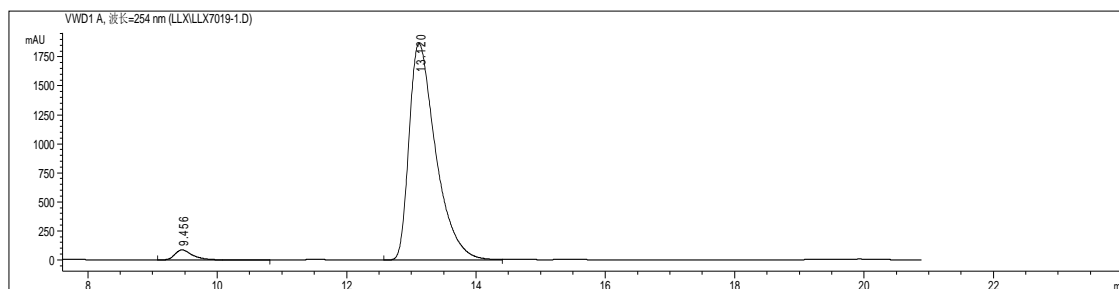
The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 10.1 min (minor) and 13.8 min (major).



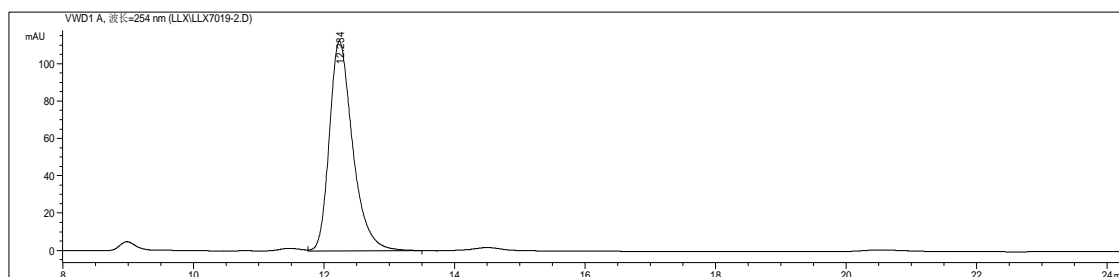
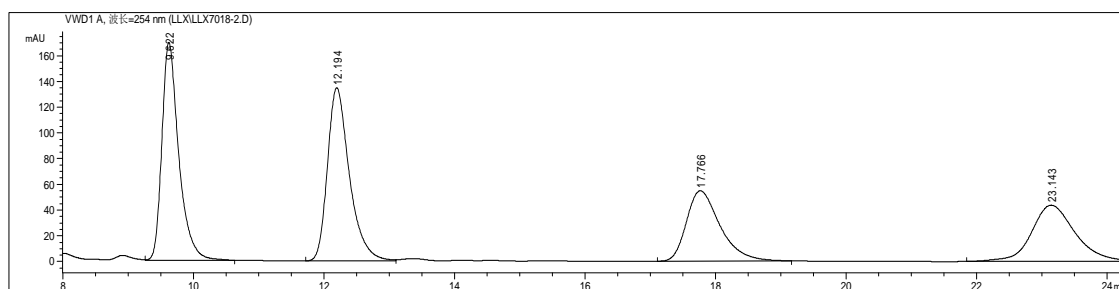
4r, white solid, M.p. 70.6 - 71.4 °C; 89% yield; 94% *ee*; $[\alpha]_{20}^D = +130.9$ (c 0.47, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.35 (d, $J = 4.4$ Hz, 4H), 7.32 - 7.28 (m, 1H), 7.20 - 7.11 (m, 5H), 7.07 - 7.02 (m, 3H), 6.84 (d, $J = 7.2$ Hz, 2H), 6.61 (d, $J = 6.9$ Hz, 2H), 6.28 (t, $J = 9.5$ Hz, 1H), 4.74 (d, $J = 15.8$ Hz, 1H), 4.69 (d, $J = 4.3$ Hz, 2H), 4.46 (d, $J = 15.9$ Hz, 1H), 4.08 (d, $J = 13.2$ Hz, 1H), 3.59 (dd, $J = 9.1, 5.9$ Hz, 1H), 3.41 (d, $J = 13.3$ Hz, 1H), 2.76 (dd, $J = 18.1, 9.1$ Hz, 1H), 1.89 (dd, $J = 18.1, 5.9$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 176.6, 176.1, 174.5, 142.0, 135.2, 134.8, 134.3, 130.1, 129.2, 128.9, 128.8, 128.6, 128.5 (two peaks), 128.1, 128.0, 127.6, 126.8, 126.6, 124.7, 110.5, 55.5, 44.9, 43.8, 42.7, 41.5, 31.3; LRMS (ESI) m/z 557.1 ($\text{M}+\text{Na}^+$); HRMS (ESI) m/z 557.1611 ($\text{M}+\text{Na}^+$), Calc. for $\text{C}_{33}\text{H}_{27}\text{ClN}_2\text{NaO}_3$ 557.1602.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 9.5 min (minor) and 13.1 min (major).





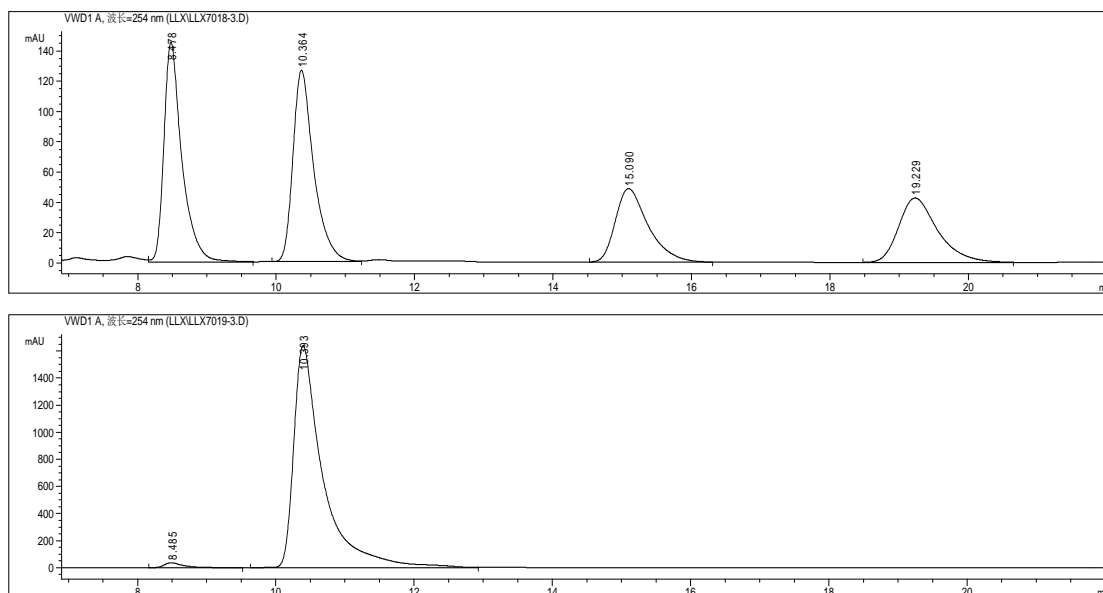
4s, white powder, M.p. 54.1 - 56.2 °C; 92% yield; 99% *ee*; $[\alpha]_{20}^D = +180.4$ (*c* 0.49, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.41 - 7.30 (m, 5H), 7.18 - 7.08 (m, 4H), 7.02 (t, *J* = 7.5 Hz, 2H), 6.87 (s, 1H), 6.83 (t, *J* = 6.9 Hz, 3H), 6.59 (d, *J* = 6.7 Hz, 2H), 6.25 (d, *J* = 7.9 Hz, 1H), 4.77 (d, *J* = 15.9 Hz, 1H), 4.68 (s, 2H), 4.44 (d, *J* = 15.9 Hz, 1H), 4.10 (d, *J* = 13.2 Hz, 1H), 3.58 (dd, *J* = 9.1, 5.6 Hz, 1H), 3.40 (d, *J* = 13.2 Hz, 1H), 2.72 (dd, *J* = 18.2, 9.1 Hz, 1H), 2.06 (s, 3H), 1.80 (dd, *J* = 18.2, 5.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 177.0, 176.3, 174.9, 141.0, 135.4 (two peaks), 134.8, 132.6, 130.1, 129.5, 128.8, 128.7, 128.5, 128.0, 127.8, 127.2, 126.6, 126.5 (two peaks), 124.7, 109.2, 55.5, 44.8, 43.6, 42.5, 41.3, 31.3, 21.0; LRMS (ESI) *m/z* 537.2 (M+Na⁺); HRMS (ESI) *m/z* 537.2153 (M+Na⁺), Calc. for C₃₄H₃₀N₂NaO₃ 537.2149. The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 12.2 min (major).



4t, white powder, M.p. 84.2 - 85.6 °C; 91% yield; 97% *ee*; $[\alpha]_{20}^D = +229.2$ (*c* 0.14, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.37 (s, 5H), 7.17 - 7.10 (m, 4H), 7.02 (t, *J* = 7.5 Hz, 2H), 6.79

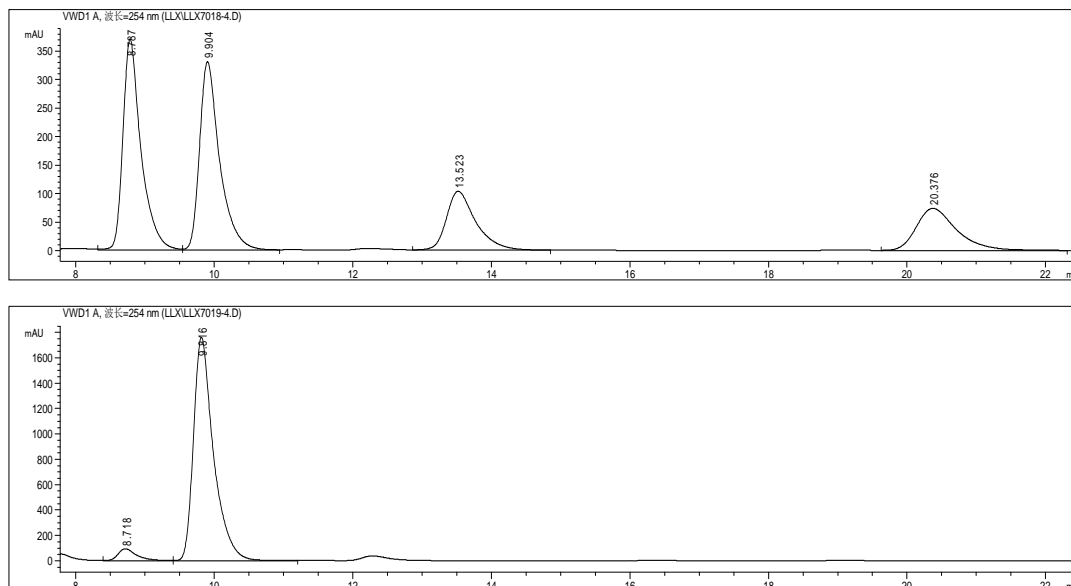
- 6.72 (m, 3H), 6.64 - 6.59 (m, 3H), 6.49 (d, $J = 1.6$ Hz, 1H), 4.75 (d, $J = 4.0$ Hz, 1H), 4.71 (s, 1H), 4.60 (d, $J = 13.9$ Hz, 1H), 4.41 (d, $J = 15.9$ Hz, 1H), 4.01 (d, $J = 13.3$ Hz, 1H), 3.54 (dd, $J = 9.1, 5.1$ Hz, 1H), 3.37 (d, $J = 13.3$ Hz, 1H), 2.74 (dd, $J = 18.3, 9.1$ Hz, 1H), 1.77 (dd, $J = 18.3, 5.1$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 176.6, 176.4, 174.6, 144.7, 135.4, 134.9, 134.2, 130.1, 129.1, 128.8, 128.7, 128.0, 128.2, 127.6, 126.8, 126.6, 125.9, 125.4, 125.3, 125.0, 122.7, 112.8, 55.4, 44.5, 43.8, 42.6, 41.2, 31.3; LRMS (ESI) m/z 601.1 ($\text{M}+\text{Na}^+$); HRMS (ESI) m/z 601.1101 ($\text{M}+\text{Na}^+$), Calc. for $\text{C}_{33}\text{H}_{27}\text{BrN}_2\text{NaO}_3$ 601.1097.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 8.5 min (minor) and 10.4 min (major).



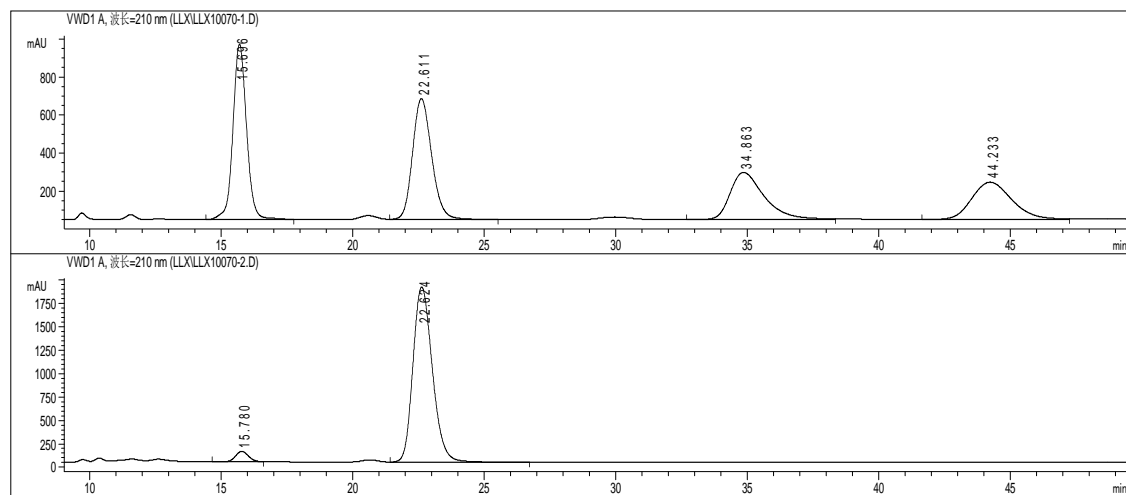
4u, white powder, M.p. 72.7 - 73.4 °C; 89% yield; 90% *ee*; $[\alpha]_{20}^{\text{D}} = +183.4$ (c 0.93, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.40 - 7.31 (m, 5H), 7.21 - 7.05 (m, 4H), 6.98 (t, $J = 7.6$ Hz, 2H), 6.84 - 6.73 (m, 5H), 6.64 - 6.55 (m, 2H), 4.80 (d, $J = 15.5$ Hz, 1H), 4.70 (dd, $J = 14.7, 8.2$ Hz, 2H), 4.61 (d, $J = 13.9$ Hz, 1H), 4.01 (d, $J = 13.3$ Hz, 1H), 3.53 (dd, $J = 9.1, 5.1$ Hz, 1H), 3.38 (d, $J = 13.3$ Hz, 1H), 2.71 (dd, $J = 18.3, 9.1$ Hz, 1H), 1.78 (dd, $J = 18.3, 5.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 176.6, 176.2, 174.6, 136.2, 135.4, 134.8, 130.0, 129.2, 128.7, 128.5, 128.1, 127.9, 127.3, 126.9, 126.8, 123.7, 123.6, 120.1, 117.4, 117.2, 55.8, 45.2, 44.7, 42.6, 41.3, 31.2; LRMS (ESI) m/z 519.1; HRMS (ESI) m/z 518.1989, Calc. for $\text{C}_{33}\text{H}_{27}\text{FN}_2\text{O}_3$ 518.1994.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 8.7 min (minor) and 9.8 min (major).

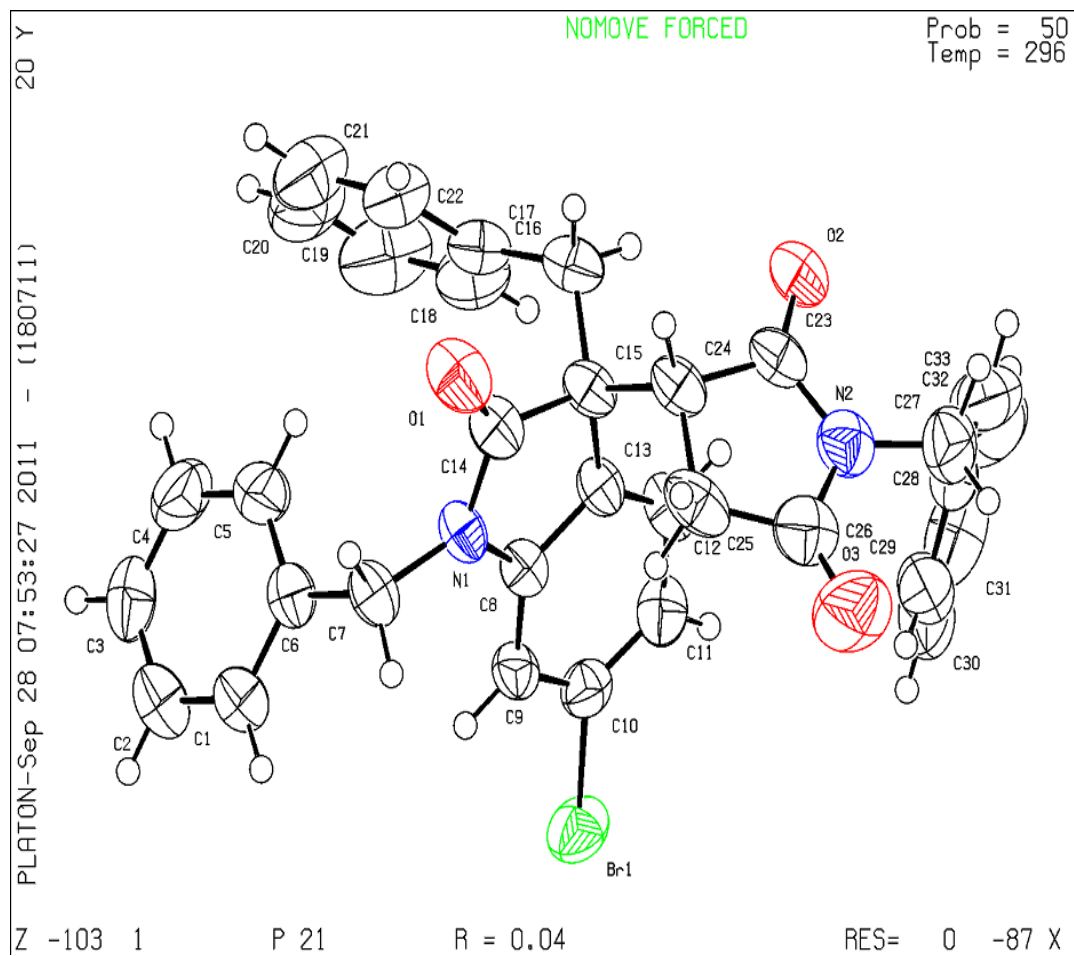


5a, white solid, M.p. 135.2 - 136.7 °C, 88% yield; 93% *ee*; $[\alpha]_{20}^D = +147.4$ (*c* 0.88, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.81 (s, 1H), 7.55 -7.41 (m, 3H), 7.33 (d, *J* = 7.5 Hz, 1H), 7.26 -7.18 (m, 3H), 7.13 - 6.98 (m, 4H), 6.86 (dd, *J* = 8.0, 1.4 Hz, 2H), 6.69 (d, *J* = 7.7 Hz, 1H), 4.03 (d, *J* = 13.3 Hz, 1H), 3.67 (dd, *J* = 9.3, 5.1 Hz, 1H), 3.42 (d, *J* = 13.3 Hz, 1H), 2.92 (dd, *J* = 18.4, 9.3 Hz, 1H), 2.11 (dd, *J* = 18.4, 5.1 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 178.3, 176.3, 174.3, 141.1, 135.0, 130.0, 129.5, 129.3, 128.9, 127.7, 126.7, 126.6, 124.6, 123.1, 110.2, 56.2, 44.4, 41.1, 31.6; LRMS (EI) *m/z* 396.2; HRMS (EI) *m/z* 396.1575, Calc. for C₂₅H₂₀N₂O₃ 396.1567.

The *ee* was determined by HPLC analysis. CHIRALCEL IA (4.6 mm i.d. x 250 mm); Hexane/2-propanol = 70/30; flow rate 1.0 ml/min; 25 °C; 254 nm; retention time: 15.8 min (minor) and 22.6 min (major).



4. X-Ray Crystal Data for Compound 4t



Datablock: 1

Bond precision: C-C = 0.0058 Å Wavelength=0.71073

Cell: a=11.654 (11) b=8.990 (8) c=14.054 (13)
 alpha=90 beta=108.273 (17) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	1398 (2)	1398 (2)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C33 H27 Br N2 O3	C33 H27 Br N2 O3
Sum formula	C33 H27 Br N2 O3	C33 H27 Br N2 O3
Mr	579.47	579.48
Dx, g cm ⁻³	1.377	1.376
Z	2	2
Mu (mm ⁻¹)	1.507	1.507
F000	596.0	596.0
F000'	595.65	
h, k, lmax	15, 11, 18	15, 11, 18
Nref	3614 [6798]	5970
Tmin, Tmax	0.566, 0.697	
Tmin'	0.480	

Correction method= Not given

Data completeness= 1.65/0.88 Theta(max)= 28.080

R(reflections)= 0.0386(3721) wR2(reflections)= 0.0798(5970)

S = 0.843 Npar= 352

5. Copies of NMR Spectra

