

Supporting Information

Highly Enantioselective [4+2] Annulation *via* Organocatalytic Mannich-reductive Cyclization: One-pot Synthesis of Functionalized Piperidines

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General Experimental Methods:

All reactions under standard conditions were monitored by thin-layer chromatography (TLC) on SiO₂ gel F-254 plates. The normal column chromatography was performed on silica gel (100-200 mesh) and Flash column chromatography was performed on silica gel (230-400 meshes) using the mixture of Hexane-EtOAc as eluting solvent. All reagents were of analytical grade and used without further purification. ¹H and ¹³C NMR spectra were recorded in CDCl₃ solution and spectral data were reported in ppm relative to tetramethylsilane (TMS) as internal standard. High resolution mass spectra were recorded using quadrupole electrospray ionization (ESI) technique. HPLC was performed on Water-2998 Instrument using CHIRALPAK-IA and IB columns and *i*-PrOH/Hexane as solvent system.

General procedure for the organocatalytic Mannich-intramolecular reductive cyclization cascade as [4+2] annulation reaction:

Glutaraldehyde solution **5** (25% in water, 0.30 mL, 0.9 mmol) was added to a mixture of preformed *N*-PMP aldimine **6** (0.3 mmol) and L-proline (6.9 mg, 0.06 mmol) in DMSO (3.0 mL) at 10 °C. The reaction mixture was further stirred at the same temperature until the imine was consumed as monitored by TLC. Once the imine is over, reaction was taken to 0 °C and cold water (2.0 mL), CH₃CO₂H (100 mol%, 18 μL) was added. To this reaction mixture NaBH₄ was added cautiously at 0 °C, further stirred for 3 h and allows it come to room temperature. The reaction was subsequently quenched with NaHCO₃ solution (20 % sol, 10 mL). The aqueous solution was extracted with ethyl acetate (2 x 10 mL) and combined organic extracts were washed with brine once, dried over anhydrous Na₂SO₄ and concentrated in vacuum after filtration. The residue was purified by column chromatography on silica gel (Hexane: EtOAc) to afford *trans*-2,3-disubstituted piperidine **7** with 57-90% yields.

The enantiomeric excess (*ee*) of the products were determined by HPLC analysis using CHIRALPAK-IA and IB columns. The relative and absolute configuration was established through the comparison of optical rotation with known compound as well as by the single crystal X-ray of **7t**. The ORTP-diagram of X-ray structure chosen for refinement has C2-(*S*), and C3-(*S*) stereochemistry, as expected through the well documented *syn*-selective direct Mannich reaction catalyzed by L-proline.

Procedure for the preparation of functionalized anabasine 8:

Compounds **7s** (0.045 g, 0.15 mmol) solution in CH₃CN (2 mL) was added slowly to the stirred solution of Ceric Ammonium Nitrate (CAN, 0.208 g, 0.38 mmol) in distilled water (2.0 mL) at 0 °C. The total reaction mixture was further stirred at same temperature for about 3 h, till the reaction complete by TLC. The reaction was quenched by adding the NaHCO₃ solution to bring the pH 10 and extracted with EtOAc (5 x 4 mL). The combined organic layer was washed with brine solution, dried over Na₂SO₄ and evaporated under reduced pressure. The crude material was passed through a small pad of column by eluting Hexane/acetone (70:30 to 40:60 ratio), to gave 0.023 g, 82% yield.

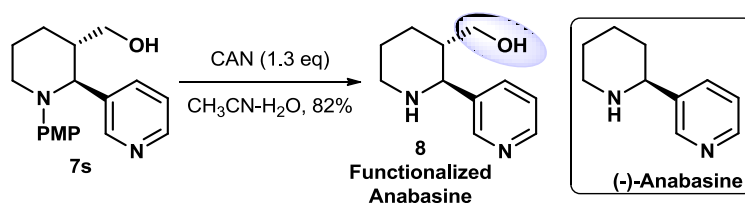
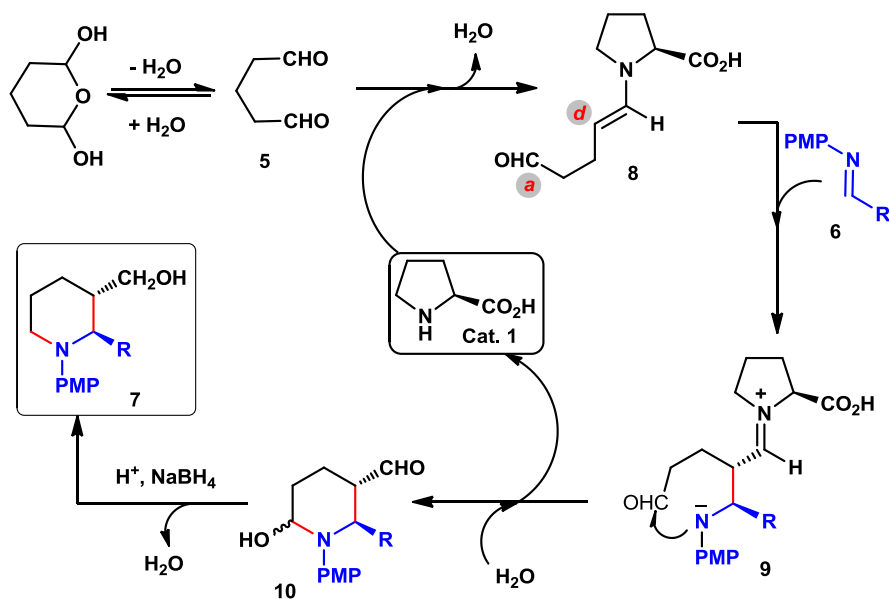
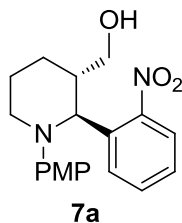


Figure 1: Plausible mechanism of the cascade [4+2] annulation reaction



((2*S*,3*S*)-1-(4-Methoxyphenyl)-2-(2-nitrophenyl)piperidin-3-yl)methanol (7a):

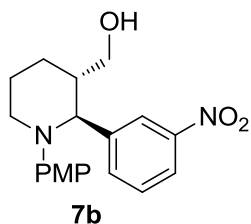


7a: ^1H NMR (400 MHz, CDCl_3) δ 1.58-1.64 (m, 1H), 1.86-1.94 (m, 3H), 2.01-2.04 (m, 1H), 2.78 (dt, $J = 3.5$ Hz, 11.6 Hz, 1H), 3.20 (d, $J = 11.7$ Hz, 1H), 3.34-3.42 (m, 2H), 3.65 (s, 3H), 4.46 (d, $J = 9.6$ Hz, 1H), 6.60 (d, $J = 8.9$ Hz, 2H), 6.90 (d, $J = 8.9$ Hz, 2H), 7.17 (t, $J = 7.2$ Hz, 1H), 7.41 (t, $J = 8.1$ Hz, 1H), 7.49 (d, $J = 8.1$ Hz, 1H) 7.81 (d, $J = 8.0$ Hz, 1H); ^{13}C -NMR (CDCl_3) δ 25.81, 27.50, 47.22, 55.16, 57.85, 60.92, 64.43, 113.91 (2C), 123.26, 125.92 (2C), 127.46, 130.52, 132.49, 137.11, 145.56, 150.82, 156.15; HRMS (ESI): Calcd. for $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}_4$ (MH^+) 343.1658, Found 343.1649.

$[\alpha]_{\text{D}}^{25} = +41.2$ (c 0.5, CHCl_3 , >99% ee),

Enantiomeric excess was determined by HPLC with a Chiralpak-IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 18.108$ min, major enantiomer $t_{\text{R}} = 19.477$ min.

((2*S*, 3*S*)-1-(4-Methoxyphenyl)-2-(3-nitrophenyl)piperidin-3-yl)methanol (7b):



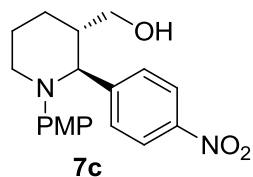
7b: ^1H NMR (400 MHz, CDCl_3) δ 1.53-1.60 (m, 2H), 1.87-1.91 (m, 2H), 1.97-2.02 (m, 1H), 2.84 (dt, $J = 3.6$ Hz, 11.2 Hz, 1H), 3.27 (dd, $J = 5.0$ Hz, 10.7 Hz, 2H), 3.42 (dd, $J = 3.5$ Hz, 10.7 Hz, 1H), 3.65 (s, 3H), 4.04 (d, $J = 9.1$ Hz, 1H), 6.62 (d, $J = 8.6$ Hz, 2H), 6.91 (d, $J = 8.5$ Hz, 2H), 7.29 (t, $J = 8.0$ Hz, 1H), 7.58 (d, $J = 7.5$ Hz, 1H), 7.92 (d, $J = 8.2$ Hz, 1H), 8.15 (s, 1H); ^{13}C -NMR (CDCl_3) δ 25.48, 27.23, 45.86, 55.17, 56.94, 64.39, 66.11, 113.91 (2C), 121.83, 123.35, 125.57 (2C), 128.72, 134.78, 144.83, 145.39, 148.06, 155.68;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}_4$ (MH^+) 343.1658, Found 343.1657.

$[\alpha]_{\text{D}}^{25} = +8.7$ (c 1.0, CHCl_3 , >99% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 20.376$ min, major enantiomer $t_{\text{R}} = 21.716$ min.

((2*S*, 3*S*)-1-(4-Methoxyphenyl)-2-(4-nitrophenyl)piperidin-3-yl)methanol (7c):

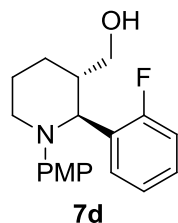


7c: ^1H NMR (400 MHz, CDCl_3) δ 1.43-1.50 (m, 1H), 1.77-1.83 (m, 3H), 1.87-1.91 (m, 1H), 2.75 (dt, $J = 3.5$ Hz, 11.6 Hz, 1H), 3.13-3.19 (m, 2H), 3.30 (dd, $J = 3.5$ Hz, 10.7 Hz, 1H), 3.56 (s, 3H), 3.96 (d, $J = 9.1$ Hz, 1H), 6.53 (d, $J = 8.9$ Hz, 2H), 6.81 (d, $J = 8.9$ Hz, 2H), 7.36 (d, $J = 8.7$ Hz, 2H), 7.89 (d, $J = 8.7$ Hz, 2H); ^{13}C -NMR (CDCl_3) δ 25.38, 27.10, 45.79, 55.11, 56.79, 64.17, 66.08, 113.86 (2C), 123.08 (2C), 125.24 (2C), 129.26 (2C), 145.39, 146.51, 150.51, 155.58;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}_4$ (MH^+) 343.1659, Found 343.1659.

$[\alpha]_{\text{D}}^{25} = +18.2$ (c 0.5, CHCl_3 , 98% ee); Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 25.343$ min, major enantiomer $t_{\text{R}} = 35.604$ min.

((2S, 3S)-2-(2-fluorophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7d):



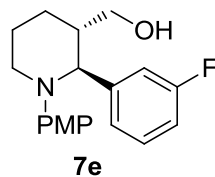
7d: ^1H NMR (400 MHz, CDCl_3) δ 1.48-1.55 (m, 1H), 1.84-1.95 (m, 3H), 2.03-2.07 (m, 1H), 2.78 (dt, $J = 3.3$ Hz, 11.6 Hz, 1H), 3.29-3.42 (m, 3H), 3.65 (s, 3H), 4.18 (d, $J = 9.7$ Hz, 1H), 6.63 (d, $J = 9.0$ Hz, 2H), 6.84 (t, $J = 8.6$ Hz, 1H), 6.92 (m, 1H), 6.94 (d, $J = 9.0$ Hz, 2H), 7.00-7.06 (m, 1H), 7.42 (dt, 1.7 Hz, 7.5 Hz, 1H); ^{13}C -NMR (CDCl_3) δ 25.78, 27.64, 46.23, 55.11, 58.10, 58.39, 64.85, 113.68 (2C), 114.38, 114.57, 124.23, 125.17 (2C), 128.02, 129.43, 130.84, 148.99, 155.60;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{FNO}_2$ (MH^+) 316.1714, Found 316.1715.

$[\alpha]_{\text{D}}^{25} = +33.20$ (c 0.5, CHCl_3 , 92% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IB column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 16.282$ min, major enantiomer $t_{\text{R}} = 17.811$ min.

((2S, 3S)-2-(3-fluorophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7e):



7e: ^1H NMR (400 MHz, CDCl_3) δ 1.45 (m, 1H), 1.52 (bs, -OH, 1H), 1.83-1.87 (m, 3H), 1.94-1.99 (m, 1H), 2.83 (dt, $J = 3.8$ Hz, 11.6 Hz, 1H), 3.22-3.30 (m, 2H), 3.42 (dd, $J = 4.2$ Hz, 10.8 Hz, 1H), 3.66 (s,

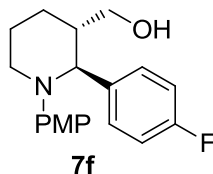
3H), 3.87 (d, $J = 8.9$ Hz, 1H), 6.63 (d, $J = 8.9$ Hz, 2H), 6.73-6.77 (m, 1H), 6.90 (d, $J = 8.9$ Hz, 2H), 6.99 (m, 2H), 7.01-7.11 (m, 1H); ^{13}C NMR (CDCl_3); ^{13}C -NMR (75 MHz, CDCl_3) δ 25.42, 27.22, 45.81, 55.22, 56.60, 65.81, 66.56, 113.51, 113.77 (2C), 115.07, 115.28, 124.25, 125.11 (2C), 129.24, 129.32, 145.82, 155.36;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{FNO}_2$ (MH^+) 316.1714, Found 316.1710.

$[\alpha]_{\text{D}}^{25} = +11.10$ (c 1.0, CHCl_3 , 91% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 14.376$ min, major enantiomer $t_{\text{R}} = 16.556$ min.

((2S, 3S)-2-(4-fluorophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7f):



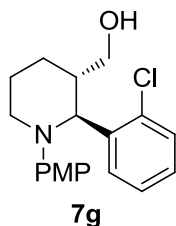
7f: ^1H NMR (300 MHz, CDCl_3) δ 1.48-1.53 (m, 1H), 1.82-1.91 (m, 3H), 1.96-2.01 (m, 1H), 2.83 (dt, $J = 3.7$ Hz, 11.5 Hz, 1H), 3.22-3.28 (m, 2H), 3.40 (dd, $J = 4.1$ Hz, 10.8 Hz, 1H), 3.66 (s, 4H), 3.81 (d, $J = 9.1$ Hz, 1H), 6.62 (d, $J = 8.9$ Hz, 2H), 6.82 (t, $J = 8.7$ Hz, 2H), 6.88 (d, $J = 8.8$ Hz, 2H), 7.19 (dd, $J = 5.7$ Hz, 8.6 Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 25.50, 27.38, 45.88, 55.14, 56.80, 64.84, 66.58, 113.64 (2C), 114.66, 114.83, 125.39 (2C), 129.80, 129.86, 137.81, 145.81, 155.36, 160.37;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{FNO}_2$ (MH^+) 316.1714, Found 316.1721.

$[\alpha]_{\text{D}}^{25} = +9.1$ (c 1.0, CHCl_3 , 75% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 94:06), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 21.161$ min, major enantiomer $t_{\text{R}} = 26.494$ min.

((2S, 3S)-2-(2-chlorophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7g):



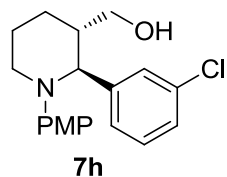
7g: ^1H NMR (400 MHz, CDCl_3) δ 1.49-1.56 (m, 1H), 1.80-1.95 (m, 3H), 2.04-2.08 (m, 1H), 2.78 (dt, $J = 3.3$ Hz, 11.6 Hz, 1H), 3.29-3.41 (m, 3H), 3.65 (s, 3H), 4.32 (d, $J = 9.7$ Hz, 1H), 6.63 (d, $J = 8.9$ Hz, 2H), 6.94-6.99 (m, 3H), 7.07 (t, $J = 7.8$ Hz, 1H), 7.15 (d, $J = 7.9$ Hz, 1H), 7.54 (dd, $J = 1.6$ Hz, 7.8 Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 25.88, 27.67, 47.47, 55.13, 58.28, 61.92, 64.55, 113.67 (2C), 125.40 (2C), 127.05, 127.74, 128.60, 129.96, 133.74, 140.19, 145.96, 155.65;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{ClNO}_2$ (MH^+) 332.1417, Found: 332.1419.

$[\alpha]_{\text{D}}^{25} = +74.00$ (c 0.5, CHCl_3 , 96% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IB column (*n*-Hexane: *i*-PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_R = 13.442$ min, major enantiomer $t_R = 16.753$ min.

((2*S*, 3*S*)-2-(3-chlorophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7h):



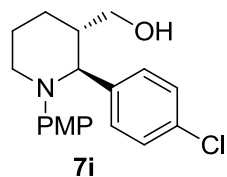
7h: $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 1.42-1.48 (m, 1H), 1.81-1.86 (m, 3H), 1.93-1.98 (m, 1H), 2.83 (dt, $J = 4.0$ Hz, 11.7 Hz, 1H), 3.20-3.28 (m, 2H), 3.38 (dd, $J = 4.0$ Hz, 10.8 Hz, 1H), 3.63 (s, 3H), 3.85 (d, $J = 8.8$ Hz, 1H), 6.62 (d, $J = 8.9$ Hz, 2H), 6.88 (d, $J = 9.0$ Hz, 2H), 7.01-7.05 (m, 2H), 7.08-7.10 (m, 1H), 7.26 (s, 1H); $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 25.29, 27.08, 45.63, 55.10, 56.40, 64.56, 66.29, 113.74 (2C), 125.00 (2C), 126.72, 126.78, 128.34, 129.07, 133.78, 144.47, 145.66, 155.28;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{ClNO}_2$ (MH^+) 332.1417, Found: 332.1415.

$[\alpha]_D^{25} = +6.0$ (c 1.0, CHCl_3 , 89% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (*n*-Hexane: *i*-PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_R = 14.141$ min, major enantiomer $t_R = 15.436$ min.

((2*S*, 3*S*)-2-(4-chlorophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7i):



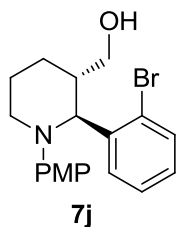
7i: $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 1.41-1.49 (m, 1H), 1.79-1.87 (m, 3H), 1.94-1.98 (m, 1H), 2.82 (dt, $J = 3.4$ Hz, 10.4 Hz, 1H), 3.21-3.25 (m, 2H), 3.37 (dd, $J = 4.0$ Hz, 10.7 Hz, 1H), 3.64 (s, 3H), 3.83 (d, $J = 9.0$ Hz, 1H), 6.62 (d, $J = 9.0$ Hz, 2H), 6.87 (d, $J = 8.9$ Hz, 2H), 7.09 (d, $J = 8.5$ Hz, 2H), 7.16 (d, $J = 8.4$ Hz, 2H); $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 25.36, 27.19, 45.66, 55.05, 56.68, 64.56, 66.29, 113.67 (2C), 125.13 (2C), 128.02 (2C), 129.71 (2C), 131.97, 140.68, 145.64, 155.30;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{ClNO}_2$ (MH^+) 332.1417, Found: 332.1416.

$[\alpha]_D^{25} = +10.4$ (c 0.5, CHCl_3 , 88% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (*n*-Hexane: *i*-PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_R = 15.440$ min, major enantiomer $t_R = 19.712$ min.

((2*S*, 3*S*)-2-(2-bromophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7j):



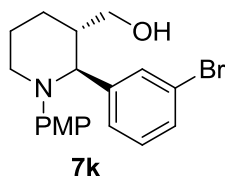
7j: ^1H NMR (400 MHz, CDCl_3) δ 1.50-1.57 (m, 1H), 1.81-1.93 (m, 3H), 2.04-2.07 (m, 1H), 2.79 (dt, $J = 3.3$ Hz, 11.7 Hz, 1H), 3.29 (d, $J = 11.7$ Hz, 1H), 3.39 (d, $J = 5.4$ Hz, 1H), 3.66 (s, 3H), 4.26 (d, $J = 9.6$ Hz, 1H), 6.63 (d, $J = 8.9$ Hz, 2H), 6.90 (dt, $J = 1.7$ Hz, 7.5 Hz, 1H), 6.97 (d, $J = 8.8$ Hz, 2H), 7.12 (t, $J = 7.1$ Hz, 1H), 7.33 (dd, $J = 1.1$ Hz, 8.0 Hz, 1H), 7.53 (dd, $J = 1.7$ Hz, 7.9 Hz, 1H); ^{13}C -NMR (75 MHz, CDCl_3) δ 25.89, 27.62, 47.73, 55.15, 58.17, 64.53, 64.75, 113.66 (2C), 124.81, 125.70 (2C), 127.63, 128.14, 130.43, 131.94, 141.78, 148.90, 155.73;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{BrNO}_2$ (MH^+) 376.0912, Found 376.0914.

$[\alpha]_{\text{D}}^{25} = +61.0$ (c 0.5, CHCl_3 , 96% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IB column (n -Hexane: i -PrOH = 84:16), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 16.358$ min, major enantiomer $t_{\text{R}} = 21.195$ min.

((2S, 3S)-2-(3-bromophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7k):



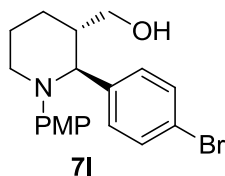
7k: ^1H NMR (400 MHz, CDCl_3) δ 1.45-1.52 (m, 1H), 1.82-1.89 (m, 3H), 1.95-2.00 (m, 1H), 2.81-2.87 (dt, $J = 3.3$ Hz, 11.6 Hz, 1H), 3.22-3.31 (m, 2H), 3.43 (dd, $J = 4.0$ Hz, 10.8 Hz, 1H), 3.67 (s, 3H), 3.85 (d, $J = 8.9$ Hz, 1H), 6.64 (d, $J = 8.9$ Hz, 2H), 6.90 (d, $J = 9.0$ Hz, 2H), 6.99 (t, $J = 7.8$ Hz, 1H), 7.15 (d, $J = 7.7$ Hz, 1H), 7.16-7.20 (m, 1H), 7.43 (t, $J = 1.7$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 25.35, 27.14, 45.74, 55.21, 56.46, 64.74, 66.35, 113.82 (2C), 122.18, 125.07 (2C), 127.23, 129.45, 129.77, 131.31, 144.81, 145.71, 155.38;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{BrNO}_2$ (MH^+) 376.0912, Found 376.0910.

$[\alpha]_{\text{D}}^{25} = -10.0$ (c 0.5, CHCl_3 , 97% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 14.346$ min, major enantiomer $t_{\text{R}} = 15.340$ min.

((2S, 3S)-2-(4-bromophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7l):



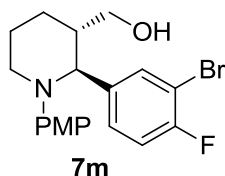
7l: ^1H NMR (400 MHz, CDCl_3) δ 1.47-1.54 (m, 1H), 1.83-1.89 (m, 3H), 1.98-2.02 (m, 1H), 2.85 (dt, $J = 4.0$ Hz, 10.4 Hz, 1H), 3.24-3.30 (m, 2H), 3.42 (dd, $J = 4.0$ Hz, 10.8 Hz, 1H), 3.69 (s, 3H), 3.85 (d, $J = 9.1$ Hz, 1H), 6.66 (d, $J = 8.9$ Hz, 2H), 6.91 (d, $J = 8.9$ Hz, 2H), 7.14 (d, $J = 8.4$ Hz, 2H) 7.28 (d, $J = 8.4$ Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 25.43, 27.25, 40.79, 55.18, 56.69, 64.76, 66.41, 113.78 (2C), 125.18 (2C), 128.52, 130.16 (2C), 131.06 (2C), 141.32, 145.75, 155.39;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{22}\text{BrNO}_2$ (MH^+) 376.0913, Found 376.0909.

$[\alpha]_{\text{D}}^{25} = -6.4$ (c 1.0, CHCl_3 , 90% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 16.002$ min, major enantiomer $t_{\text{R}} = 21.944$ min.

((2S, 3S)-2-(3-bromo-4-fluorophenyl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7m):



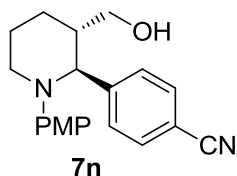
7m: ^1H NMR (400 MHz, CDCl_3) δ 1.79-1.88 (m, 4H), 1.95-1.99 (m, 1H), 2.83 (dt, $J = 4.1$ Hz, 11.6 Hz, 1H), 3.20-3.27 (m, 2H), 3.40 (dd, $J = 3.8$ Hz, 10.7 Hz, 1H), 3.67 (s, 3H), 3.84 (d, $J = 9.1$ Hz, 1H), 6.64 (d, $J = 8.9$ Hz, 2H), 6.85 (m, 1H), 6.89 (d, $J = 9.0$ Hz, 2H), 7.11-7.14 (m, 1H), 7.47 (dd, $J = 2.1$ Hz, 6.7 Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 25.37, 27.15, 45.78, 55.17, 56.63, 64.46, 65.71, 113.85 (2C), 115.58, 115.80, 125.27 (2C), 128.90, 133.10, 139.82, 145.54, 155.53, 158.70;

HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{21}\text{BrFNO}_2$ (MH^+) 394.0818, Found 394.0821.

$[\alpha]_{\text{D}}^{25} = -6.2$ (c 1.0, CHCl_3 , 92% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 14.096$ min, major enantiomer $t_{\text{R}} = 15.592$ min.

4-((2S, 3S)-3-(hydroxymethyl)-1-(4-methoxyphenyl)piperidin-2-yl)benzotrile (7n):



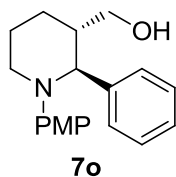
7n: ^1H NMR (400 MHz, CDCl_3) δ 1.49- 1.56 (m, 1H), 1.80-1.86 (m, 3H), 1.94-1.98 (m, 1H), 2.82 (dt, $J = 4.2$ Hz, 10.4 Hz, 1H), 3.19-3.25 (m, 2H), 3.35 (dd, $J = 3.7$ Hz, 10.7 Hz, 1H), 3.64 (s, 3H), 3.97 (d, $J = 9.1$ Hz, 1H), 6.61 (d, $J = 9.0$ Hz, 2H), 6.87 (d, $J = 9.0$, 2H), 7.38 (q, $J = 8.6$ Hz, 12.2 Hz, 4H); ^{13}C NMR (75 MHz, CDCl_3) δ 25.31, 27.03, 45.61, 55.12, 56.59, 64.16, 66.27, 110.12, 113.81 (2C), 118.82, 125.11 (2C), 129.22 (2C), 131.66 (2C), 145.40, 148.27, 155.48;

HRMS (ESI): Calcd for $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_2$ (MH^+) 323.1759, Found 323.1763.

$[\alpha]_{\text{D}}^{25} = +8.8$ (c 1.0, CHCl_3 , 97% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (*n*-Hexane: *i*-PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_R = 24.835$ min, major enantiomer $t_R = 34.001$ min.

((2*S*, 3*S*)-1-(4-methoxyphenyl)-2-phenylpiperidin-3-yl)methanol (7o):



7o: ^1H NMR (400 MHz, CDCl_3) δ 1.85-1.89 (m, 2H), 1.94-2.06 (m, 3H), 2.85 (dt, $J = 3.5$ Hz, 11.7 Hz, 1H), 3.24-3.32 (m, 2H), 3.45 (dd, $J = 4.4$ Hz, 11.0 Hz, 1H), 3.66 (s, 3H), 3.84 (d, $J = 8.6$ Hz, 1H), 6.62 (d, $J = 9.0$ Hz, 2H), 6.91 (d, $J = 9.4$ Hz, 2H), 7.08 (d, $J = 7.2$ Hz, 1H), 7.15 (t, $J = 7.2$ Hz, 2H), 7.24 (d, $J = 7.1$ Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 25.51, 27.42, 45.96, 55.18, 56.60, 65.27, 67.46, 113.66 (2C), 125.11 (2C), 126.72, 128.02 (2C), 128.47 (2C), 142.13, 146.05, 155.21;

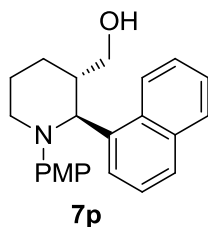
HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{23}\text{NO}_2$ (MH^+) 298.1807, Found: 298.1811.

$[\alpha]_D^{25} = +2.6$ (c 0.5, CHCl_3 , 73% ee); Lit: $[\alpha]_D^{25} +3.5$ (c 0.2, CHCl_3).^{Ref.}

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (*n*-Hexane: *i*-PrOH = 90:10), 1.0 mL/min; minor enantiomer $t_R = 29.181$ min, major enantiomer $t_R = 23.841$ min.

Ref.: R. M. de Figueiredo, R. Fröhlich, and M. Christmann, *J. Org. Chem.* 2006, **71**, 4147.

((2*S*, 3*S*)-1-(4-methoxyphenyl)-2-(naphthalen-1-yl)piperidin-3-yl)methanol (7p):



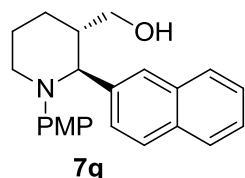
7p: ^1H NMR (400 MHz, CDCl_3) δ 1.45-1.56 (m, 1H), 1.84-1.90 (m, 1H), 1.95-2.07 (m, 2H), 2.18-2.27 (m, 1H), 2.85-2.94 (m, 1H), 3.13 (dd, $J = 5.4$ Hz, 5.6 Hz, 1H), 3.23 (dd, 4.3 Hz, 4.3 Hz, 1H), 3.38 (d, $J = 12.7$ Hz, 1H), 3.51 (s, 3H), 4.50 (d, $J = 9.2$ Hz, 1H), 6.45 (d, $J = 9.0$ Hz, 2H), 6.90 (d, $J = 8.9$ Hz, 2H), 7.23 (d, $J = 7.7$ Hz, 1H), 7.37-7.51 (m, 4H), 7.55 (d, $J = 8.2$ Hz, 1H), 7.72 (d, $J = 8.2$ Hz, 1H); ^{13}C -NMR (75 MHz, CDCl_3) δ 25.78, 27.82, 45.70, 55.00, 57.98, 63.53, 65.15, 113.47 (2C), 124.40, 124.97, 125.08, 125.16, 125.40, 126.96, 127.34, 128.70, 129.49, 131.81, 133.68, 138.10, 146.03, 155.19;

HRMS (ESI): Calcd for $\text{C}_{23}\text{H}_{25}\text{NO}_2$ (MH^+): 348.1963, Found 348.1967.

$[\alpha]_D^{25} = +34.4$ (c 0.5, CHCl_3 , 81% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (*n*-Hexane: *i*-PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_R = 16.925$ min, major enantiomer $t_R = 18.265$ min.

((2S, 3S)-1-(4-methoxyphenyl)-2-(naphthalen-2-yl)piperidin-3-yl)methanol (7q):



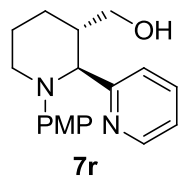
7q: $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 1.50-1.57 (m, 1H), 1.86-1.94 (m, 2H), 2.00-2.08 (m, 2H), 2.93 (dt, $J = 3.4$ Hz, 11.6 Hz, 1H), 3.28-3.35 (m, 2H), 3.40 (dd, $J = 4.1$ Hz, 10.9 Hz, 1H), 3.59 (s, 3H), 4.04 (d, $J = 8.7$ Hz, 1H), 6.60 (d, $J = 9.0$ Hz, 2H), 6.99 (d, $J = 9.0$ Hz, 2H), 7.38-7.43 (m, 2H), 7.51 (dd, $J = 6.9$ Hz, 8.4 Hz, 1H), 7.65-7.74 (m, 4H); $^{13}\text{C-NMR}$ (75 MHz, CDCl_3) δ 25.47, 27.32, 45.63, 55.03, 56.70, 64.96, 67.22, 113.67 (2C), 125.06, 125.11, 125.31, 125.60, 126.37, 127.34, 127.44, 127.64, 127.69, 132.51, 133.03, 139.76, 145.94, 155.16;

HRMS (ESI): Calcd for $\text{C}_{23}\text{H}_{25}\text{NO}_2$ (MH^+): 348.1963, Found 348.1959.

$[\alpha]_{\text{D}}^{25} = +9.5$ (c 1.0, CHCl_3 , 94% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 18.405$ min, major enantiomer $t_{\text{R}} = 23.997$ min.

((2S, 3S)-1-(4-methoxyphenyl)-2-(pyridin-2-yl)piperidin-3-yl)methanol (7r):

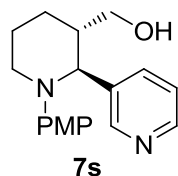


7r: $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 1.66-1.73 (m, 1H), 1.84-1.87 (m, 4H), 2.81-2.87 (m, 1H), 3.27 (dd, $J = 4.4$ Hz, 11.6 Hz, 1H), 3.34-3.42 (m, 2H), 3.65 (s, 3H), 4.24 (d, $J = 8.8$ Hz, 1H), 6.63 (d, $J = 9.0$ Hz, 2H), 6.91 (d, $J = 8.9$ Hz, 2H), 6.97-7.01 (m, 1H), 7.28 (d, $J = 7.9$ Hz, 1H), 7.44 (dt, $J = 1.6$ Hz, 7.7 Hz, 1H), 8.38 (d, $J = 4.8$ Hz, 1H); $^{13}\text{C-NMR}$ (75 MHz, CDCl_3) δ 25.40, 27.32, 45.74, 55.21, 56.40, 64.66, 67.30, 113.87 (2C), 121.68, 122.61, 123.91 (2C), 136.60, 146.04, 147.97, 154.88, 162.55;

HRMS (ESI): Calcd for $\text{C}_{18}\text{H}_{22}\text{N}_2\text{O}_2$ (MH^+) 299.1759, Found: 299.1757.

$[\alpha]_{\text{D}}^{25} = +32.4$ (c 0.5, CHCl_3 , 80% ee); Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 85:15), 0.5 mL/min; major enantiomer $t_{\text{R}} = 42.928$ min, minor enantiomer $t_{\text{R}} = 48.704$ min.

((2S, 3S)-1-(4-methoxyphenyl)-2-(pyridin-3-yl)piperidin-3-yl)methanol (7s):

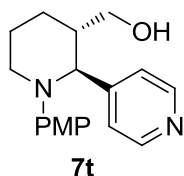


7s: ^1H NMR (400 MHz, CDCl_3) δ 1.54-1.60 (m, 2H), 1.81-1.89 (m, 3H), 2.82 (dt, $J = 4.0$ Hz, 10.4 Hz, 1H), 3.21-3.25 (m, 2H), 3.38 (dd, $J = 3.6$ Hz, 11.7 Hz, 1H), 3.64 (s, 3H), 3.94 (d, $J = 9.2$ Hz, 1H), 6.60 (d, $J = 9.0$ Hz, 2H), 6.88 (d, $J = 8.9$ Hz, 2H), 7.06 (dd, $J = 4.8$ Hz, 11.8 Hz, 1H), 7.60 (d, $J = 7.9$ Hz, 1H), 8.23 (dd, $J = 1.6$ Hz, 4.7 Hz, 1H) 8.39 (s, 1H); ^{13}C -NMR (75 MHz, CDCl_3) δ 25.54, 27.31, 40.80, 45.75, 55.18, 62.53, 64.33, 113.89 (2C), 123.26, 123.49, 125.53 (2C), 145.51, 148.26, 148.46, 149.82, 155.62; HRMS (ESI): Calcd for $\text{C}_{18}\text{H}_{22}\text{N}_2\text{O}_2$ (MH^+) 299.1759, Found: 299.1764.

$[\alpha]_{\text{D}}^{25} = +11.1$ (c 1.0, MeOH, 81% ee);

Enantiomeric excess was determined by HPLC with a Chiral pak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; major enantiomer $t_{\text{R}} = 46.112$ min, minor enantiomer $t_{\text{R}} = 52.412$ min.

((2S, 3S)-1-(4-methoxyphenyl)-2-(pyridin-4-yl)piperidin-3-yl)methanol (7t):

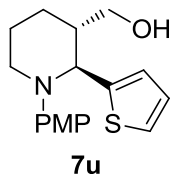


7t: ^1H NMR (400 MHz, CDCl_3) δ 1.52-1.58 (m, 2H), 1.81-1.86 (m, 3H), 2.84-2.90 (m, 1H), 3.21-3.25 (m, 2H), 3.40 (dd, $J = 3.9$ Hz, 10.7 Hz, 1H), 3.65 (s, 3H), 4.03 (d, $J = 8.6$ Hz, 1H), 6.63 (d, $J = 9.0$ Hz, 2H), 6.88 (d, $J = 9.0$ Hz, 2H), 7.22 (d, $J = 6.0$ Hz, 2H), 8.29 (d, $J = 6.0$ Hz, 2H); ^{13}C -NMR (75 MHz, CDCl_3) δ 24.82, 26.42, 40.37, 44.89, 55.61, 61.88, 64.76, 113.68 (2C), 123.80 (2C), 124.23 (2C), 145.29, 148.46 (2C), 152.30, 154.98;

HRMS (ESI): Calcd for $\text{C}_{18}\text{H}_{22}\text{N}_2\text{O}_2$ (MH^+) 299.1759, Found: 299.1762.

$[\alpha]_{\text{D}}^{25} = +12.4$ (c 1.0, CHCl_3 , 90% ee); Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 85:15), 0.5 mL/min; minor enantiomer $t_{\text{R}} = 16.558$ min, major enantiomer $t_{\text{R}} = 18.641$ min.

((2S, 3S)-1-(4-methoxyphenyl)-2-(thiophen-2-yl)piperidin-3-yl)methanol (7u):

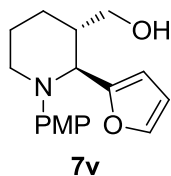


7u: ^1H NMR (300 MHz, CDCl_3) δ 1.54-1.59 (m, 1H), 1.76-1.84 (m, 3H), 1.97-2.03 (m, 1H), 2.07-2.12 (m, 1H), 2.97-3.07 (m, 1H), 3.19-3.25 (m, 1H), 3.58 (dd, $J = 5.2$ Hz, 10.6 Hz, 1H), 3.72 (s, 3H), 4.56 (d, $J = 6.5$ Hz, 1H), 6.72 (d, $J = 8.9$ Hz, 2H), 6.75 (d, $J = 3.7$ Hz, 1H), 6.78 (dd, 3.5 Hz, 5.0 Hz, 1H), 6.95 (d, $J = 8.9$ Hz, 2H), 7.09 (dd, 1.1 Hz, $J = 5.0$ Hz, 1H); ^{13}C -NMR (75 MHz, CDCl_3) δ 25.42, 28.91, 44.97, 51.93, 55.33, 61.44, 65.23, 113.96 (2C), 122.81 (2C), 124.20, 125.64, 125.83, 130.86, 145.57, 154.72;

HRMS (ESI): Calcd for $\text{C}_{17}\text{H}_{21}\text{NO}_2\text{S}$ (MH^+) 304.1371, Found. 304.1375.

$[\alpha]_D^{25} = -5.2$ (c 1.0, CHCl_3 , 80% ee); Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; major enantiomer $t_R = 19.560$ min, minor enantiomer $t_R = 23.400$ min.

((2S, 3S)-2-(fuyan-2-yl)-1-(4-methoxyphenyl)piperidin-3-yl)methanol (7v):

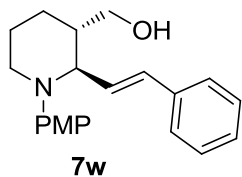


7v: ^1H NMR (300 MHz, CDCl_3) δ 1.52-1.60 (m, 1H), 1.71-1.79 (m, 1H), 1.81-1.86 (m, 1H), 1.91-1.98 (m, 1H), 2.23-2.30 (m, 1H), 3.02-3.08 (m, 1H), 3.15-3.20 (m, 1H), 3.60 (dd, $J = 5.3$ Hz, 10.7 Hz, 1H), 3.73 (s, 3H), 3.75 (dd, $J = 6$ Hz, 10.7 Hz, 1H,), 4.38 (d, $J = 6.8$ Hz, 1H), 5.91 (d, $J = 3.2$ Hz, 1H), 6.17 (dd, $J = 1.8$ Hz, 3.2 Hz, 1H), 6.74 (d, $J = 9.0$ Hz, 2H) 6.90 (d, $J = 9.0$ Hz, 2H), 7.27 (dd, $J = 0.9$ Hz, 1.9 Hz, 1H); ^{13}C -NMR (75 MHz, CDCl_3) δ 23.59, 24.83, 41.33, 50.17, 55.38, 59.55, 65.17, 107.99, 109.87, 114.00 (2C), 121.70 (2C), 141.00, 145.68, 154.26, 154.55;

HRMS (ESI): Calcd for $\text{C}_{17}\text{H}_{21}\text{NO}_3$ (MH^+): 288.1599, Found. 288.1595.

$[\alpha]_D^{25} = -41.6$ (c 0.5, CHCl_3 , 68% ee); Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; major enantiomer $t_R = 18.401$ min, minor enantiomer $t_R = 22.956$ min.

((2R, 3S)-1-(4-methoxyphenyl)-2-((E)-styryl)piperidin-3-yl)methanol (7w):



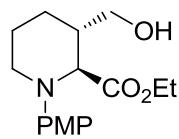
7w: ^1H NMR (400 MHz, CDCl_3) δ 1.54-1.65 (m, 1H), 1.81-1.88 (m, 2H), 1.92-2.01 (m, 2H), 3.00-3.08 (m, 1H), 3.19-3.24 (m, 1H), 3.76 (s, 3H), 3.80 (dd, $J = 5.3$ Hz, 10.7 Hz, 1H), 3.93 (dd, $J = 5.5$ Hz, 10.7 Hz, 1H) 3.97 (dd, $J = 5.3$ Hz, 7.3 Hz, 1H), 6.21 (dd, $J = 7.3$ Hz, 16.2 Hz, 1H), 6.34 (d, $J = 16.3$ Hz, 1H), 6.81 (d, $J = 9.0$ Hz, 2H), 7.00 (d, $J = 9.0$ Hz, 2H), 7.18-7.23 (m, 1H), 7.25-7.29 (m, 4H); ^{13}C -NMR (75 MHz, CDCl_3) δ 23.64, 24.37, 41.95, 49.58, 55.40, 63.55, 65.62, 114.12 (2C), 122.29 (2C), 126.16 (2C), 127.25, 128.39 (2C), 129.46, 132.13, 136.99, 145.55, 154.54;

HRMS (ESI): Calcd for $\text{C}_{21}\text{H}_{25}\text{NO}_2$ (MH^+) 324.1963, Found 324.1967.

$[\alpha]_D^{25} = -28.0$ (c 0.5, CHCl_3 , 68% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; major enantiomer $t_R = 23.015$ min, minor enantiomer $t_R = 28.844$ min.

((2S, 3S)-ethyl 3-(hydroxymethyl)-1-(4-methoxyphenyl)piperidine-2-carboxylate (7x):



7x

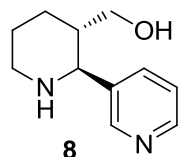
7w: ^1H NMR (500 MHz, CDCl_3) δ 1.11 (t, $J = 71$. Hz, 1H), 1.54-1.59 (m, 1H), 1.64-1.73 (m, 2H), 2.26-2.30 (m, 1H), 3.07-3.12 (m, 1H), 3.33-3.39 (m, 1H), 3.71 (dd, $J = 5.3$ Hz, 10.6 Hz, 1H), 3.73 (s, 3H), 3.88 (dd, $J = 7.8$ Hz, 10.6 Hz, 1H), 4.04 (dq, $J = 2.8$ Hz, 7.2 Hz, 14.1 Hz, 2H), 4.22 (d, $J = 6.1$ Hz, 1H), 6.78 (d, $J = 9.1$ Hz, 2H), 6.92 (d, $J = 9.0$ Hz, 2H); ^{13}C -NMR (75 MHz, CDCl_3) δ 14.06, 21.98, 23.36, 39.26, 47.90, 55.36, 60.40, 62.59, 63.88, 114.15 (2C), 119.82 (2C), 145.57, 153.86, 172.97;

HRMS (ESI): Calcd for $\text{C}_{16}\text{H}_{23}\text{NO}_4$ (MH^+) 294.1705, Found 294.1701.

$[\alpha]_{\text{D}}^{25} = +27.4$ (c 0.5, CHCl_3 , 99% ee);

Enantiomeric excess was determined by HPLC with a Chiralpak IA column (n -Hexane: i -PrOH = 90:10), 0.5 mL/min; major enantiomer $t_{\text{R}} = 20.197$ min, major enantiomer $t_{\text{R}} = 23.325$ min.

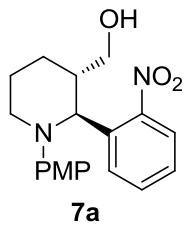
((2S, 3S)-(pyridin-3-yl)piperidin-3-yl)methanol (8):



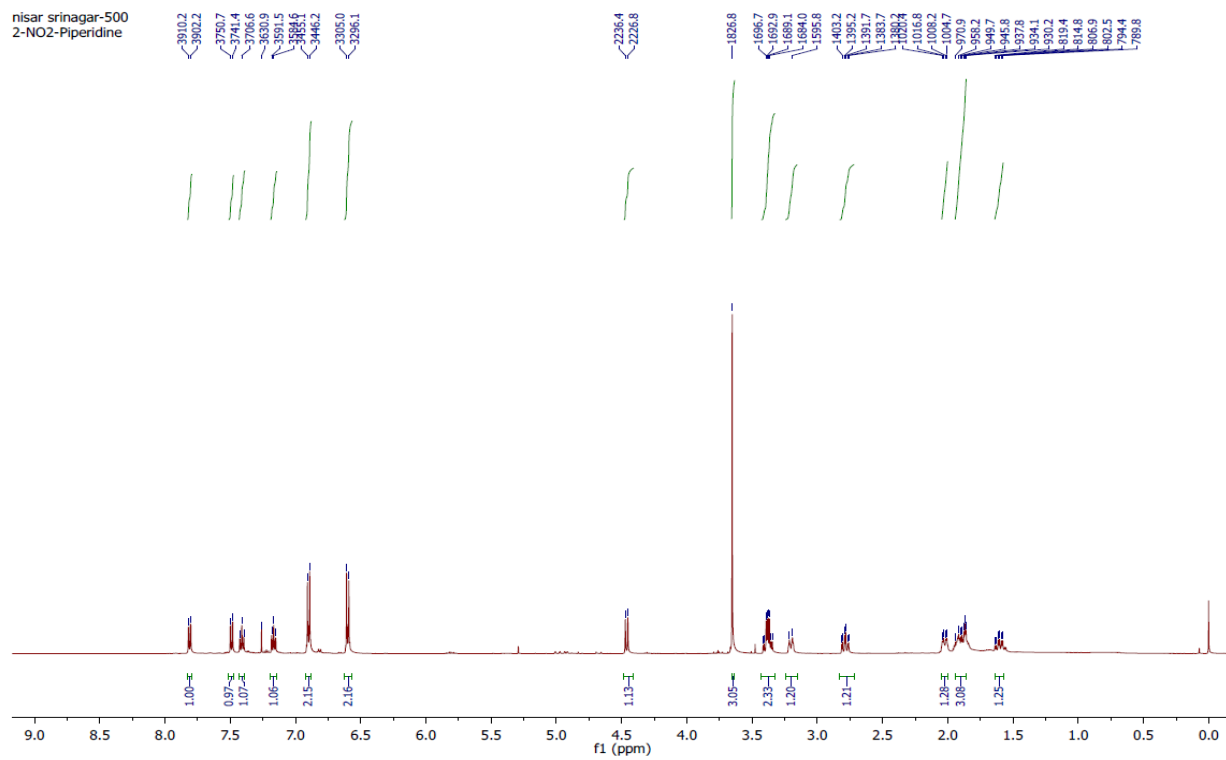
8: ^1H NMR (400 MHz, CDCl_3) δ 1.5-1.68 (m, 5H), 2.18 (s, 1H, NH), 2.35-2.39 (m, 2H), 3.37-3.40 (m, 2H), 3.77 (s, 1H, OH), 4.08 (d, $J = 8.7$ Hz, 1H), 7.30 (dd, $J = 4.9$ Hz, 11.8 Hz, 1H), 7.74 (d, $J = 7.9$ Hz, 1H), 8.52 (d, $J = 3.6$ Hz, 1H) 8.59 (s, 1H); ^{13}C -NMR (75 MHz, CDCl_3) δ 25.72, 27.64, 42.87, 46.06, 64.98, 67.62, 136.92, 146.36 148.29, 153.65, 155.20;

HRMS (ESI): Calcd. for $\text{C}_{11}\text{H}_{16}\text{N}_2\text{O}$ (MH^+) 193.1341, Found: 193.1345.

$[\alpha]_{\text{D}}^{25} = +9.2$ (c 1.0, MeOH).



nisar srinagar-500
 2-NO₂-Piperidine



156.15
 150.82
 145.56

137.11
 132.49
 130.52
 127.46
 125.92
 123.26

113.91

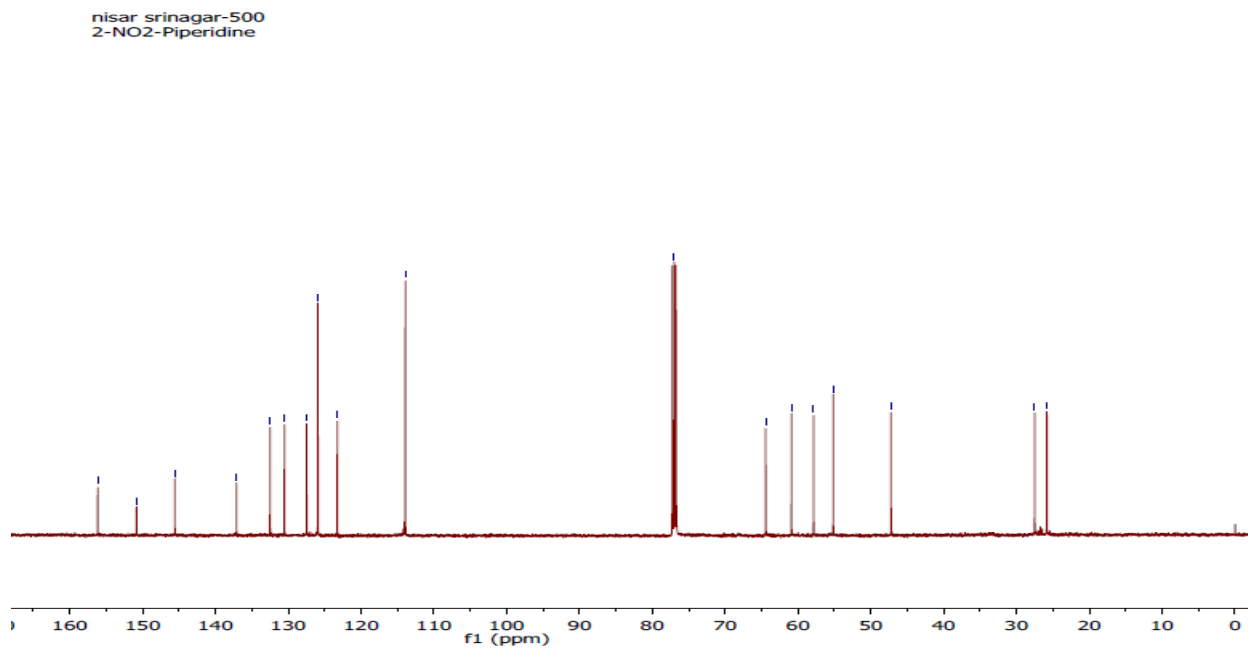
77.00

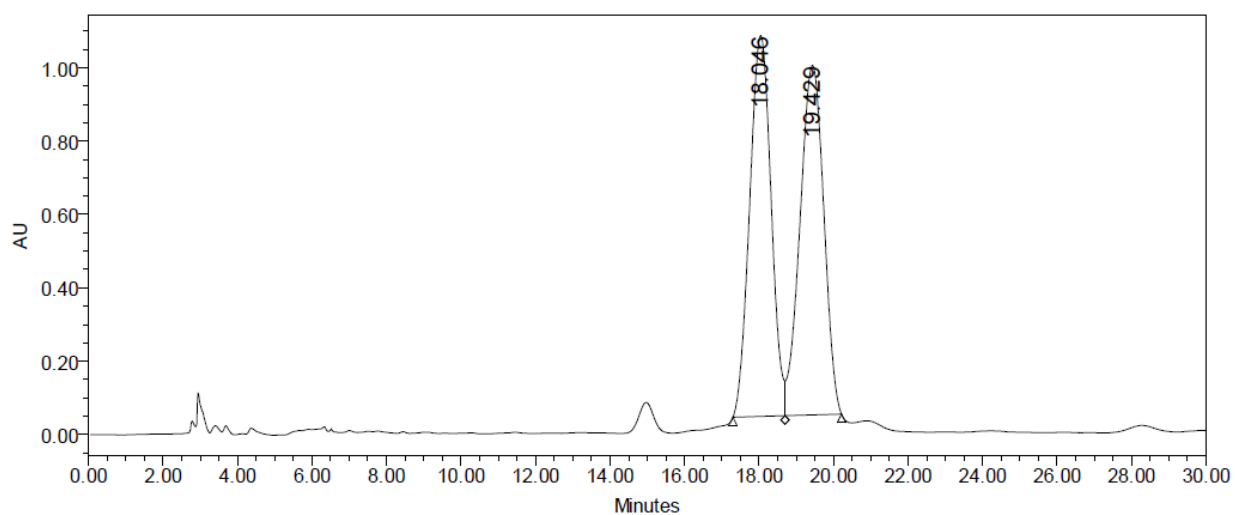
64.43
 60.89
 57.85
 55.16

47.22

27.50
 25.81

nisar srinagar-500
 2-NO₂-Piperidine

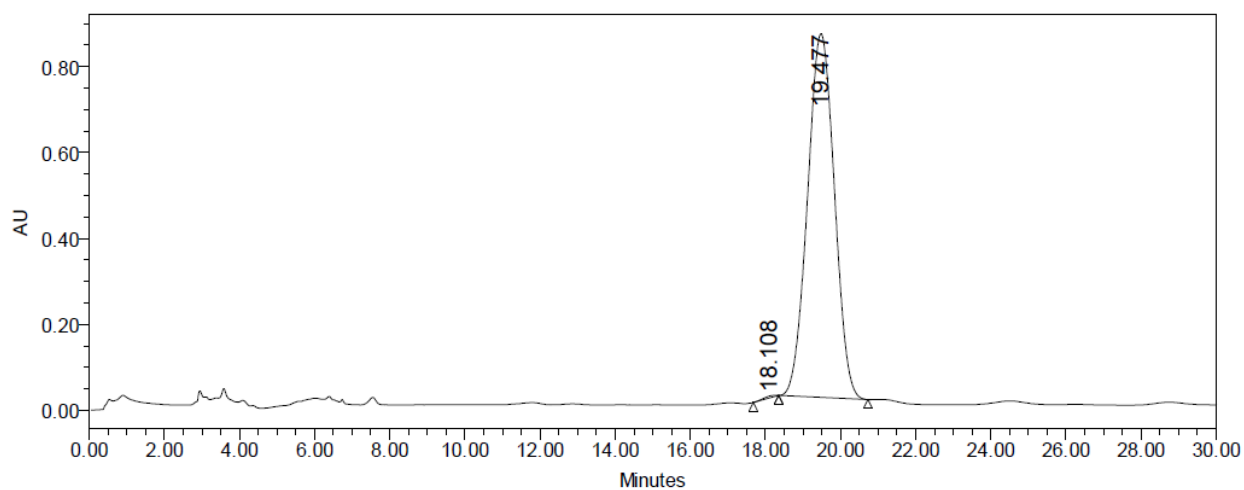




Channel: 2998; Processed Channel: PDA 210.0 nm; Result Id: 1064; Processing Method: 2Nitro recenic1

Processed Channel Descr.: PDA 210.0 nm

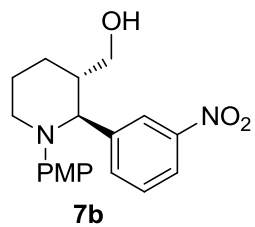
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	18.046	41469079	49.51	1038473
2	PDA 210.0 nm	19.429	42284147	50.49	953468



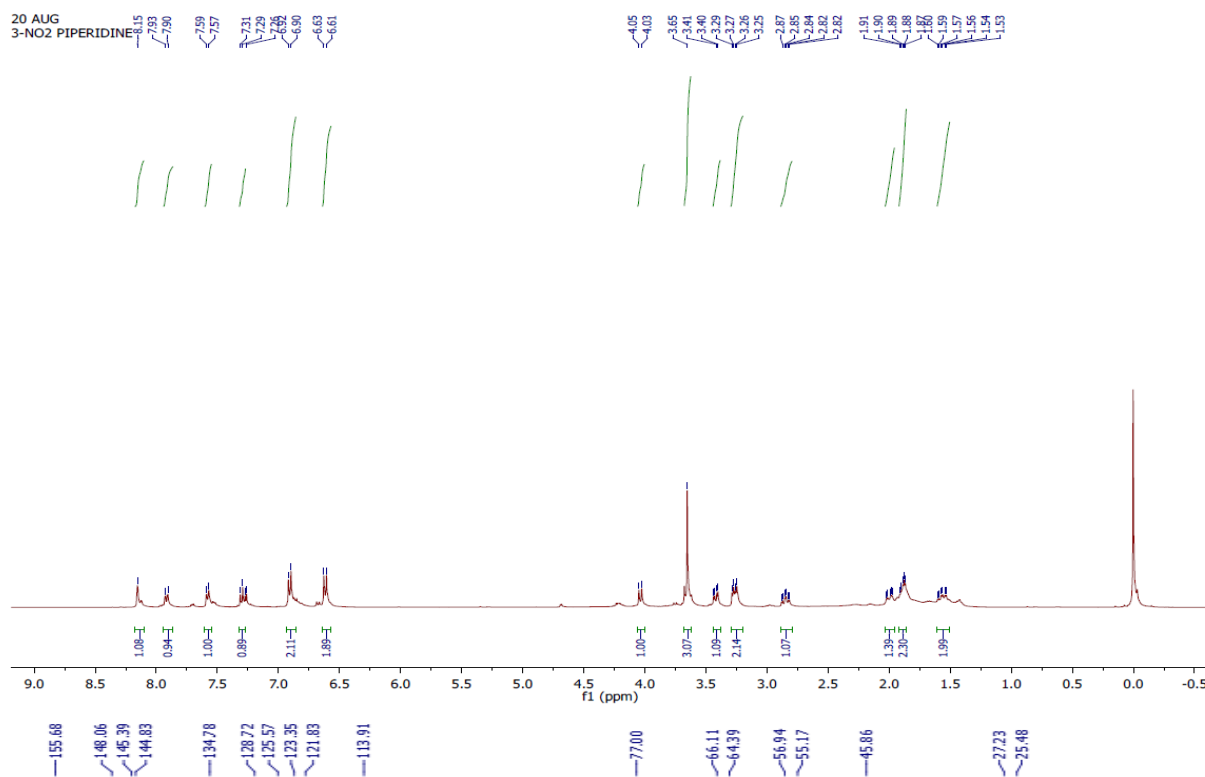
Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1985; Processing Method: 2 Nitro piperidine chiral

Processed Channel Descr.: PDA 250.0 nm

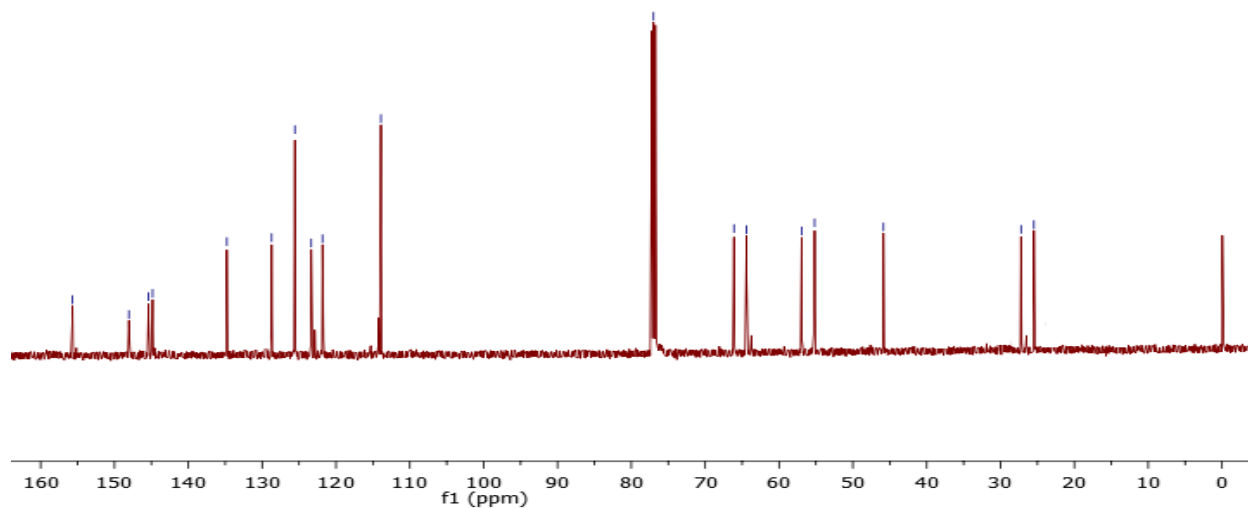
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	18.108	91731	0.22	4343
2	PDA 250.0 nm	19.477	42051291	99.78	845952

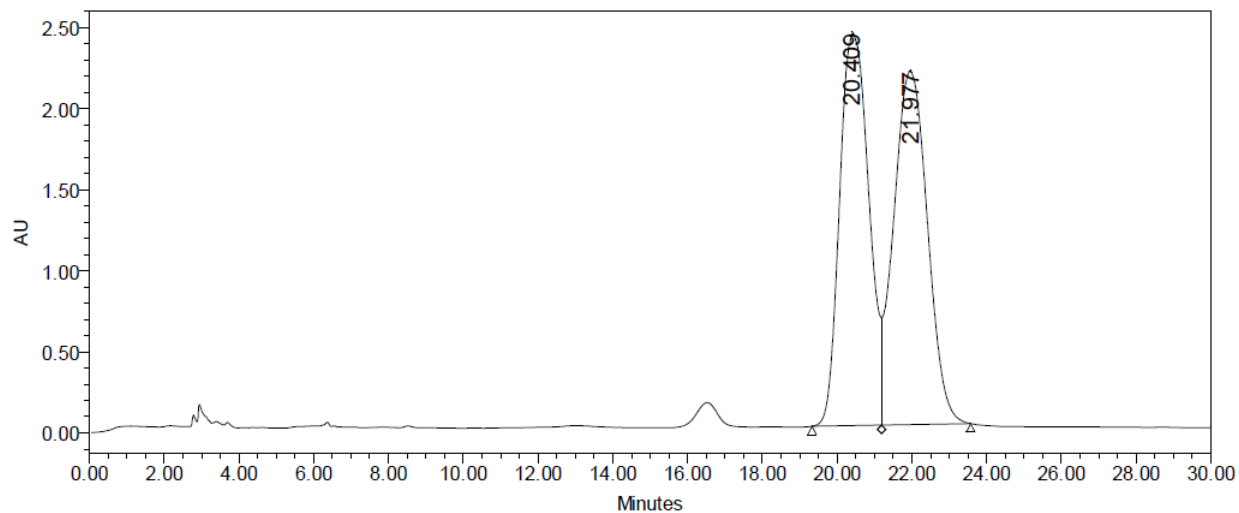


20 AUG
3-NO₂ PIPERIDINE



Aug21-2012
3-NO₂ Piperidine

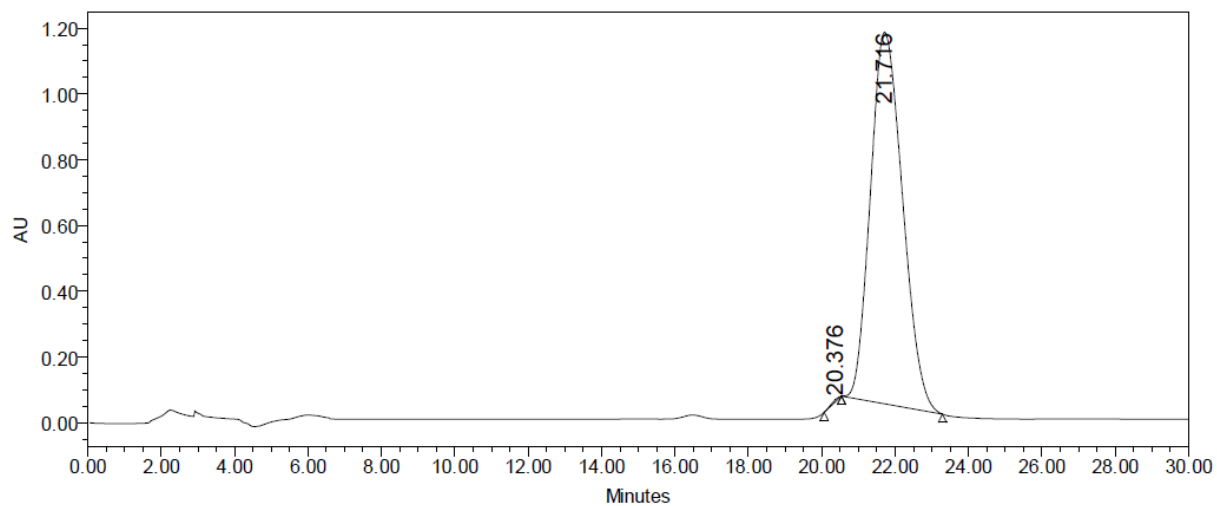




Channel: 2998; Processed Channel: PDA 210.0 nm; Result Id: 1066; Processing Method: 3Nitro recemic

Processed Channel Descr.: PDA 210.0 nm

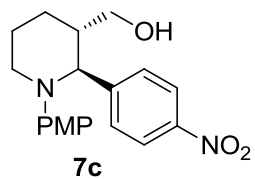
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	20.409	130810325	48.75	2430254
2	PDA 210.0 nm	21.977	137531423	51.25	2184559



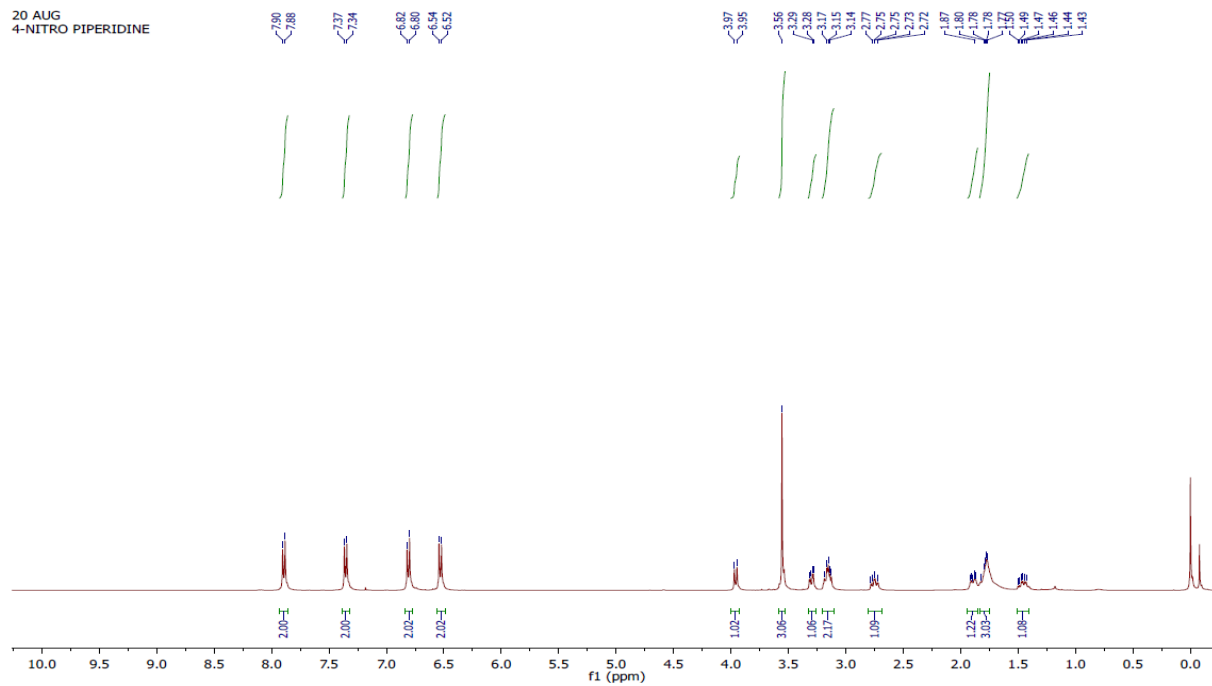
Channel: 2998; Processed Channel: PDA 290.0 nm; Result Id: 1077; Processing Method: 3Nitro chirall

Processed Channel Descr.: PDA 290.0 nm

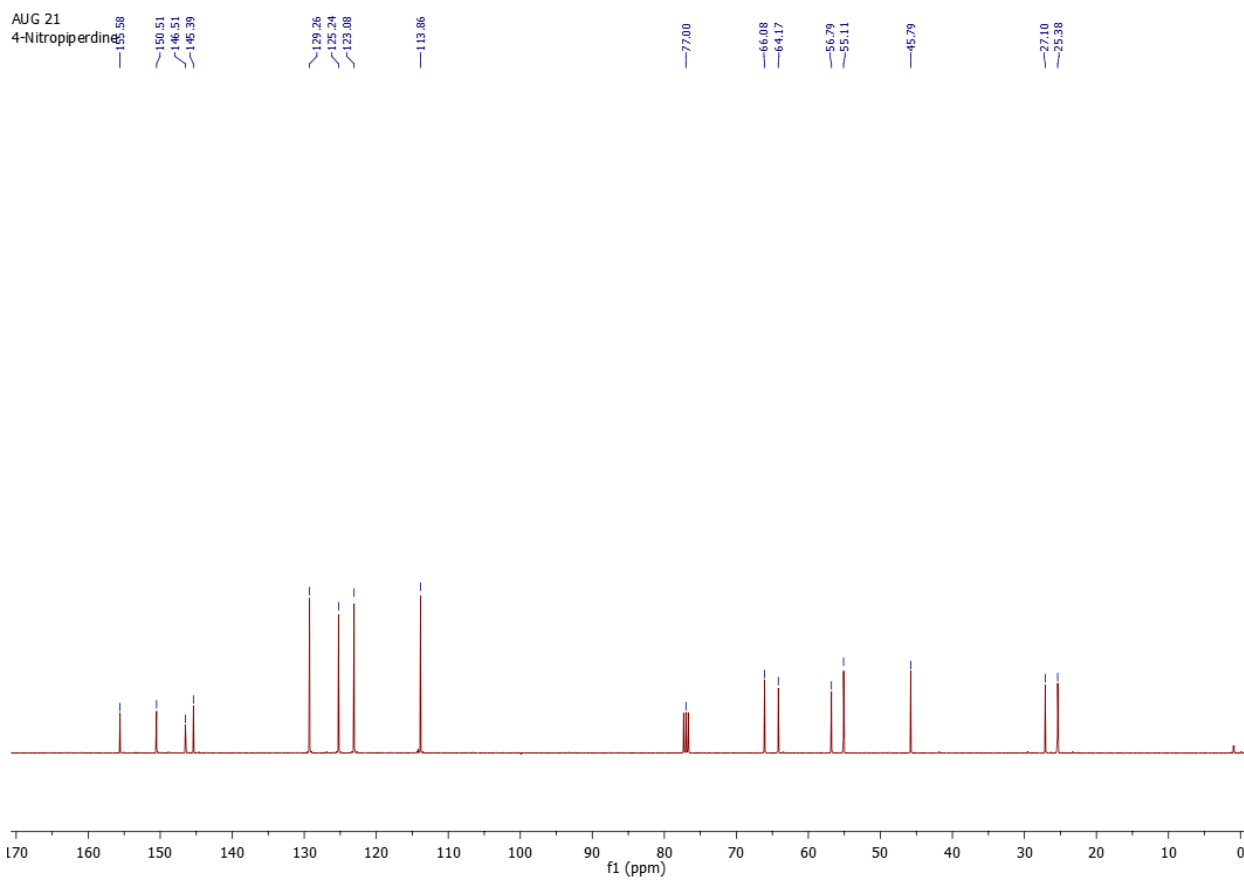
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 290.0 nm	20.376	102301	0.15	6605
2	PDA 290.0 nm	21.716	68820586	99.85	1129483

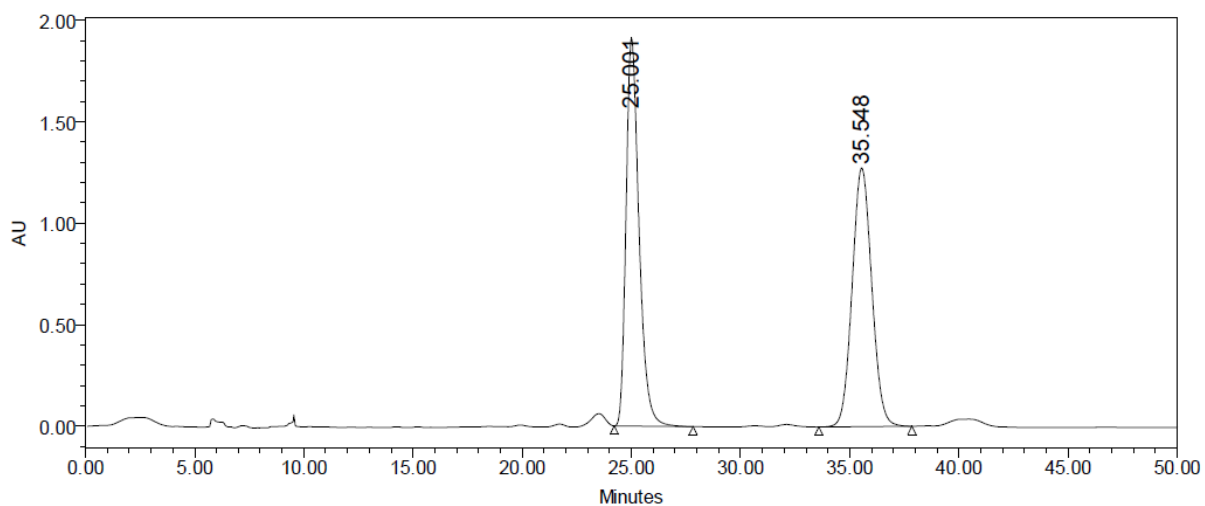


20 AUG
4-NITRO PIPERIDINE



AUG 21
4-Nitropiperidine

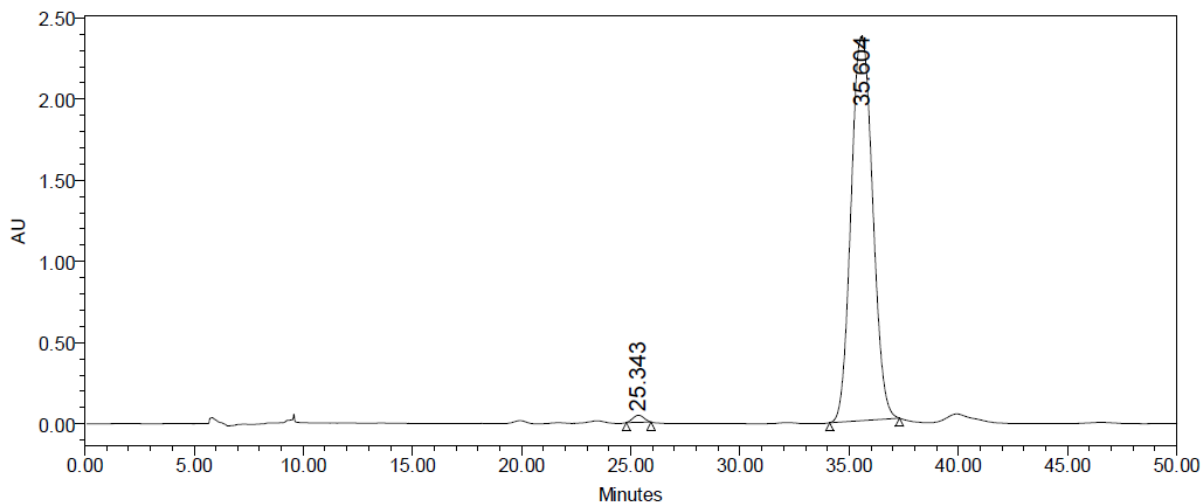




Channel: 2998; Processed Channel: PDA 210.0 nm; Result Id: 1137; Processing Method: 4Nitro recimic

Processed Channel Descr.: PDA 210.0 nm

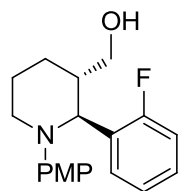
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	25.001	78936708	49.78	1912322
2	PDA 210.0 nm	35.548	79635847	50.22	1274748



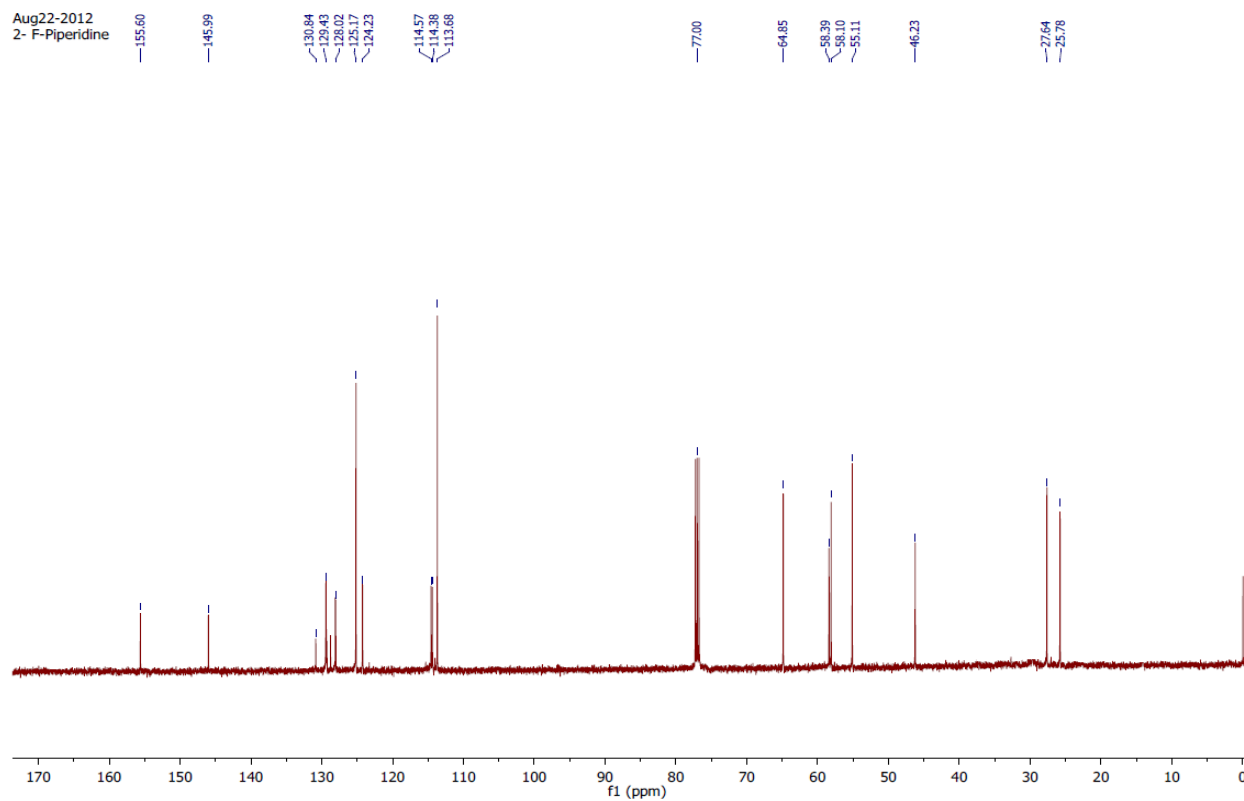
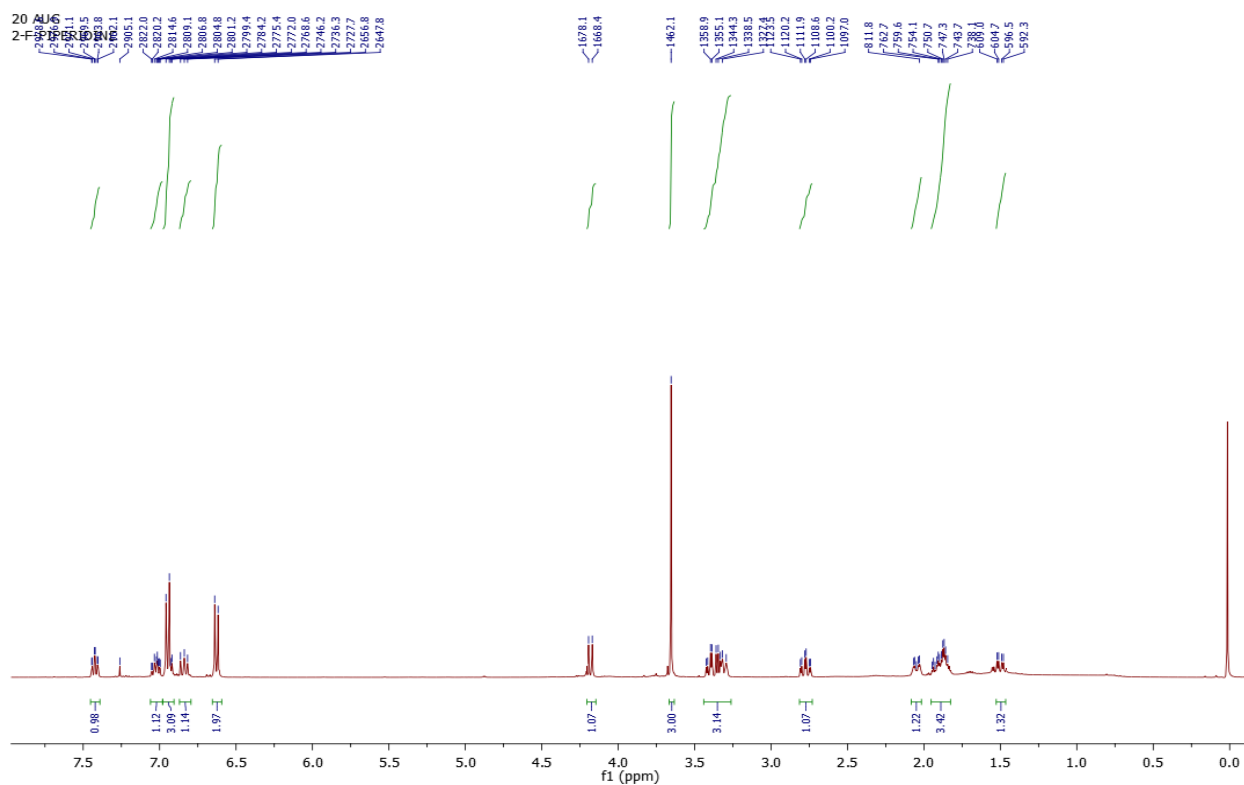
Channel: 2998; Processed Channel: PDA 210.0 nm; Result Id: 1140; Processing Method: 4Nitro chiral

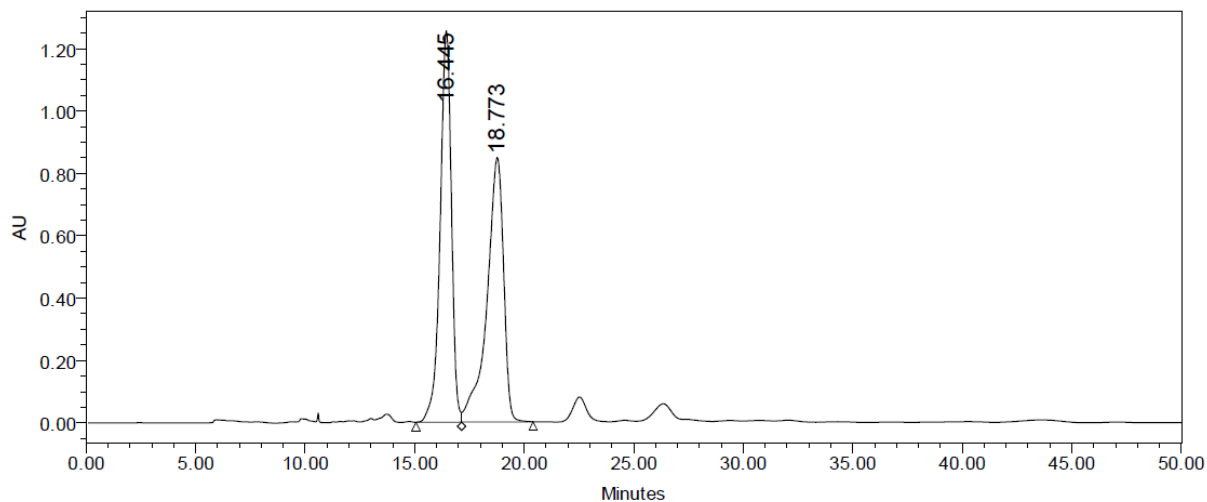
Processed Channel Descr.: PDA 210.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	25.343	1544346	0.94	44023
2	PDA 210.0 nm	35.604	162803331	99.06	2370119



7d

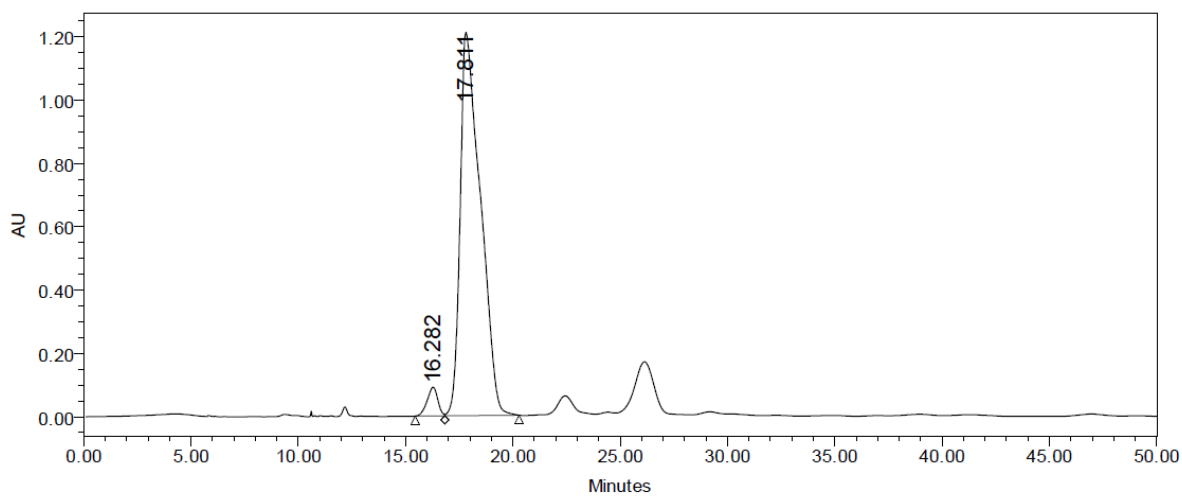




Channel: 2998; Processed Channel: PDA 270.0 nm; Result Id: 1752; Processing Method: 2F recenic

Processed Channel Descr.: PDA 270.0 nm

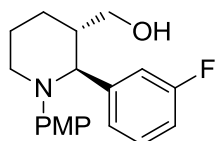
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 270.0 nm	16.445	44890220	49.97	1254449
2	PDA 270.0 nm	18.773	44946439	50.03	847666



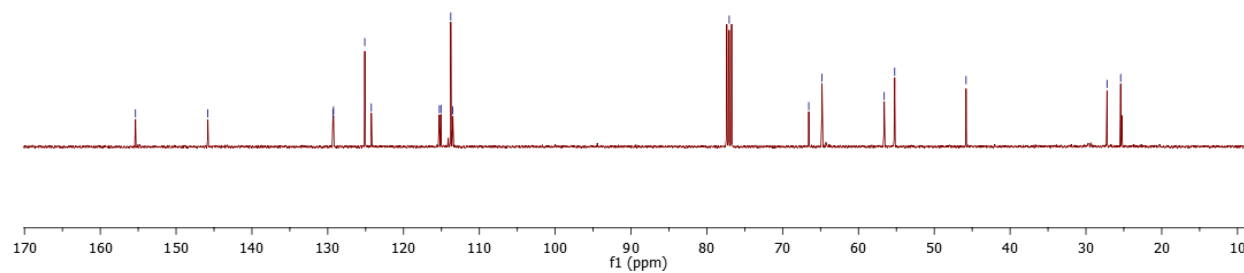
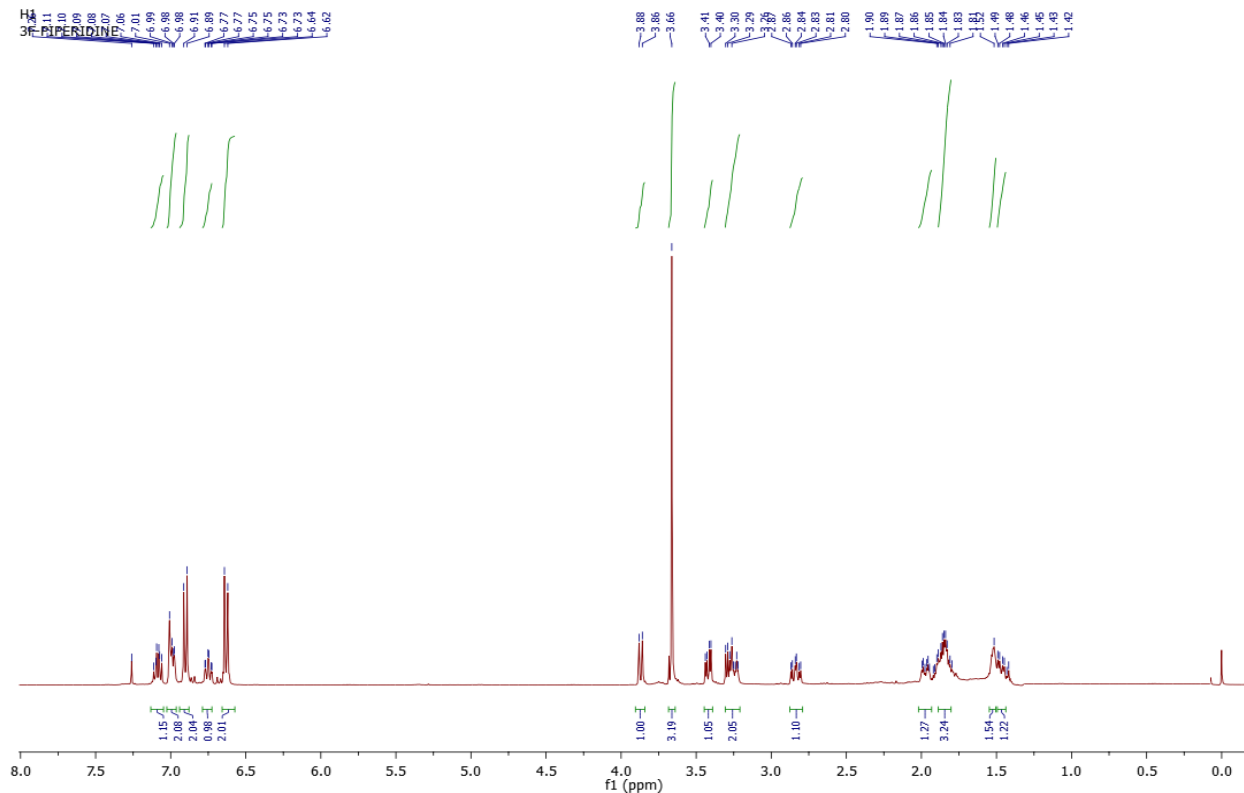
Channel: 2998; Processed Channel: PDA 330.0 nm; Result Id: 1754; Processing Method: 2F chiral

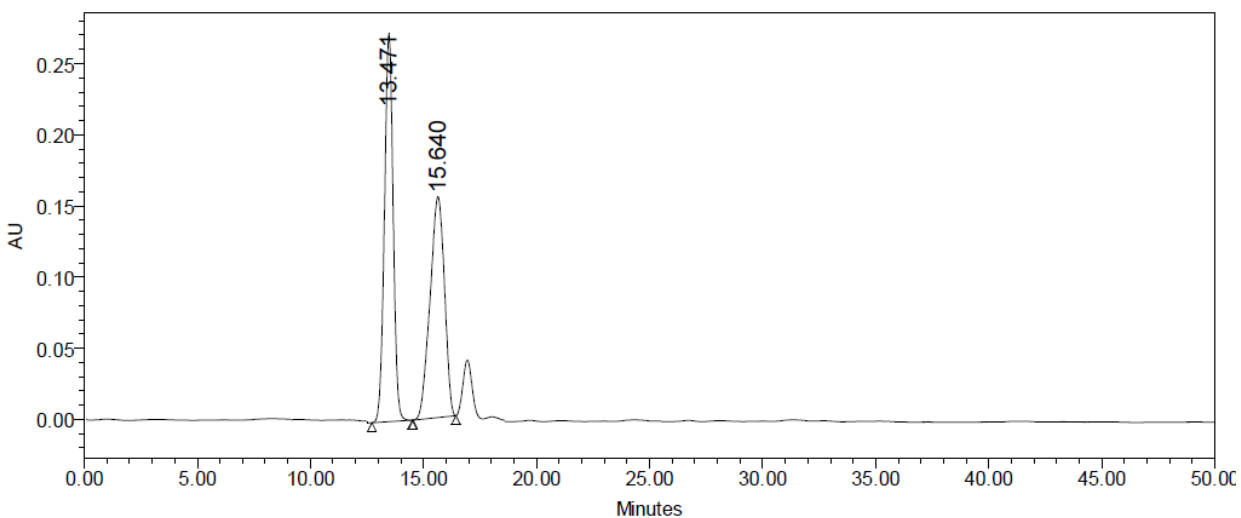
Processed Channel Descr.: PDA 330.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 330.0 nm	16.282	3112409	3.77	90847
2	PDA 330.0 nm	17.811	79373988	96.23	1209574



7e

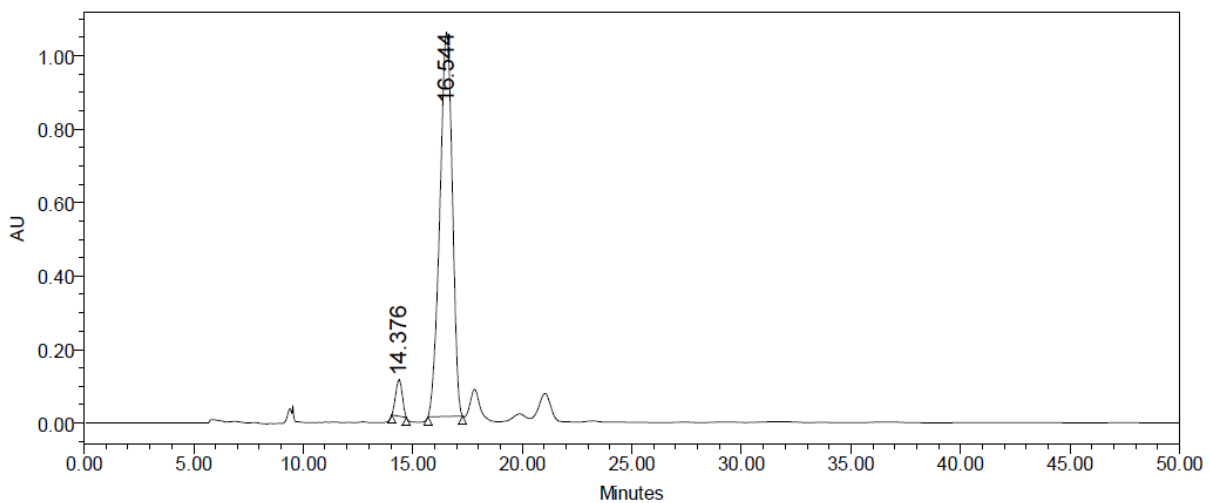




Channel: 2998; Processed Channel: PDA 240.0 nm; Result Id: 1471; Processing Method: 3F recemic

Processed Channel Descr.: PDA 240.0 nm

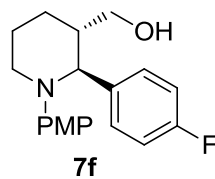
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 240.0 nm	13.471	7288927	51.43	272804
2	PDA 240.0 nm	15.640	6884027	48.57	155233



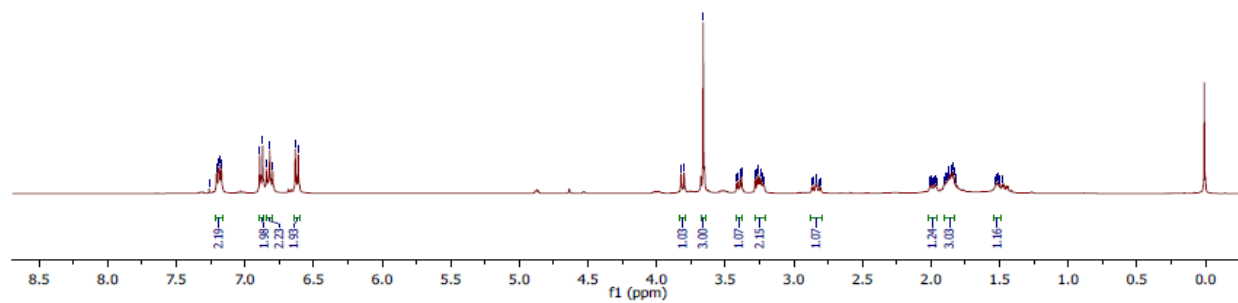
Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1479; Processing Method: 3F chiral

Processed Channel Descr.: PDA 250.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	14.376	2073031	4.77	98996
2	PDA 250.0 nm	16.544	41431402	95.23	1045288

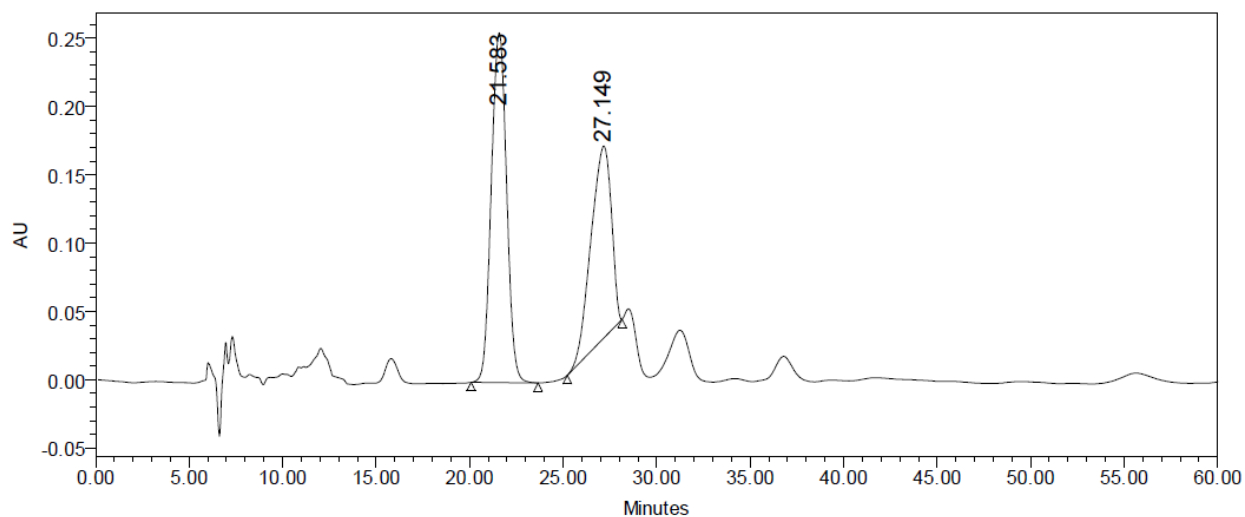


20 AUG
4-F-PIPERIDINE



21 AUG
4-F-Piperidine

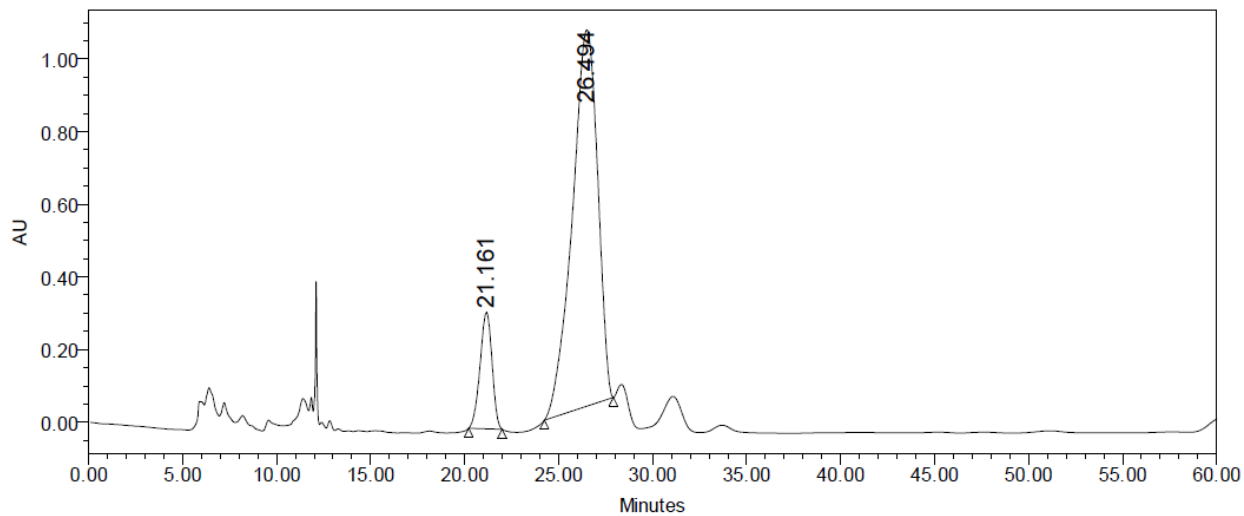




Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1057; Processing Method: 4F pip racemic

Processed Channel Descr.: PDA 250.0 nm

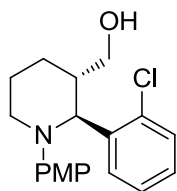
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	21.583	14578306	57.65	255984
2	PDA 250.0 nm	27.149	10707781	42.35	140594



Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1054; Processing Method: 4F pip chiral new

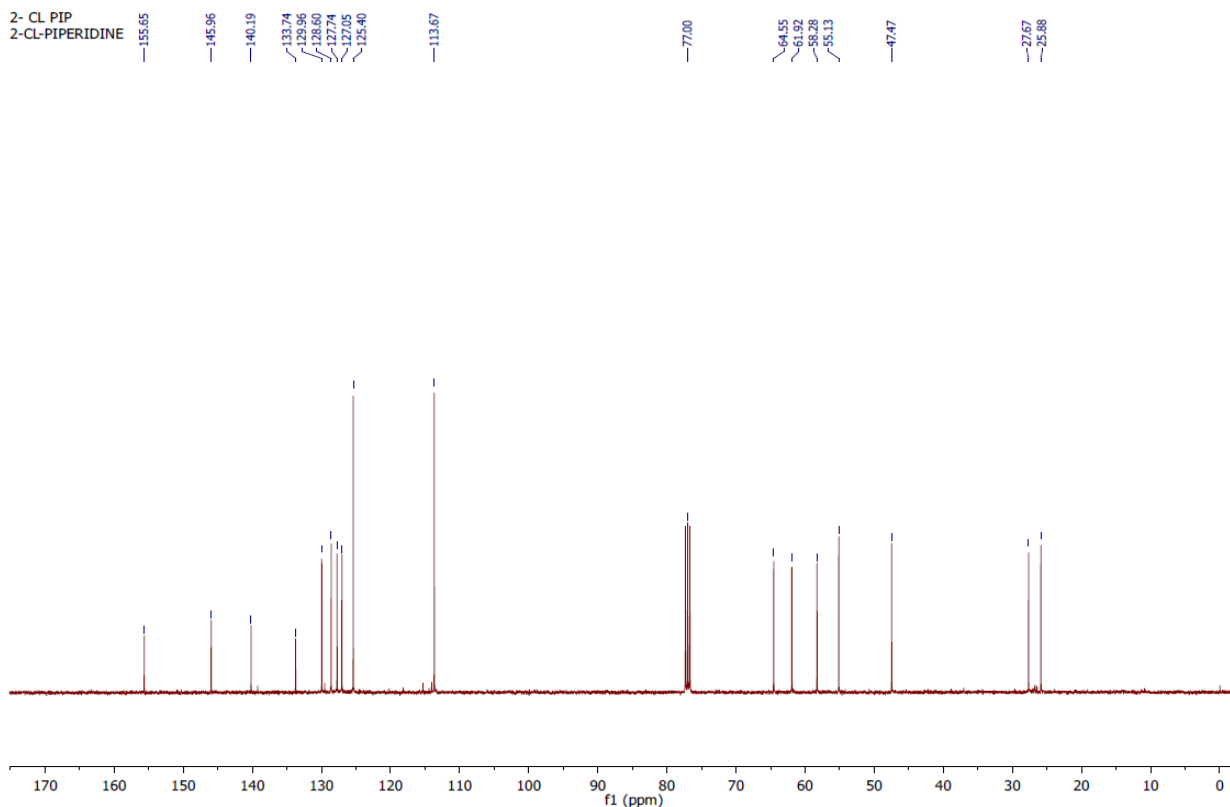
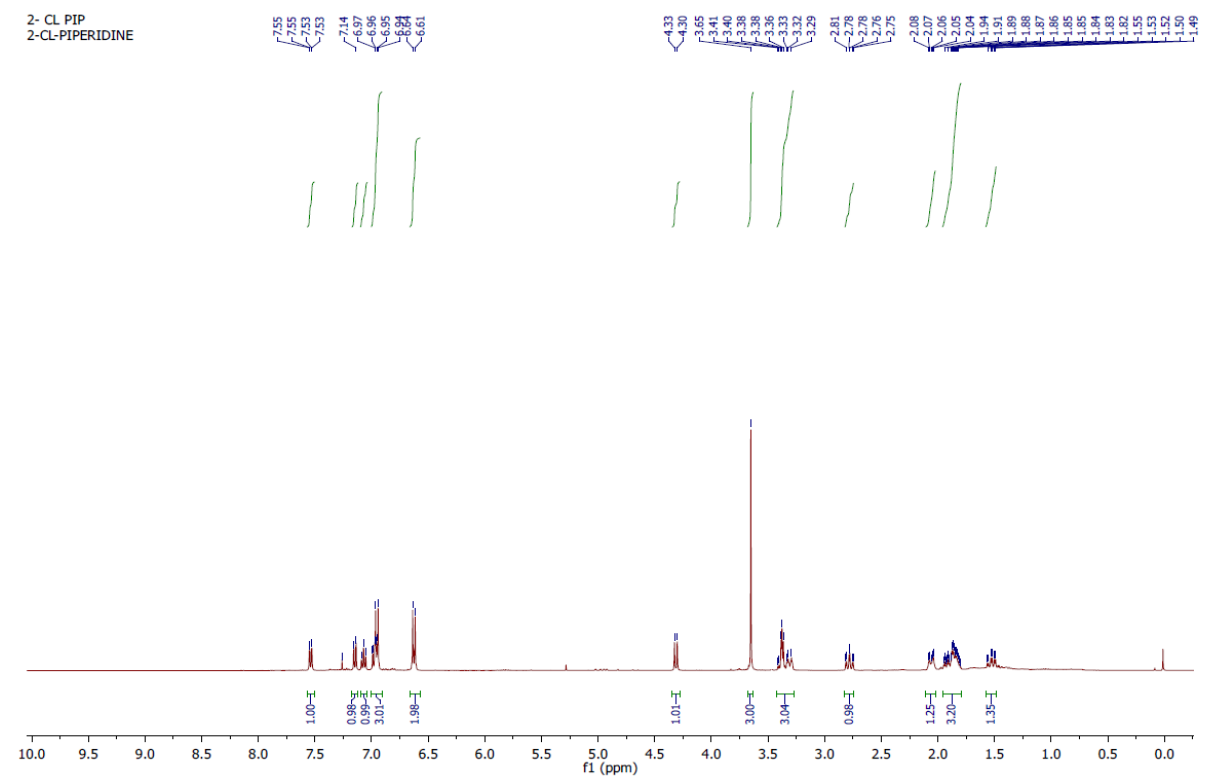
Processed Channel Descr.: PDA 250.0 nm

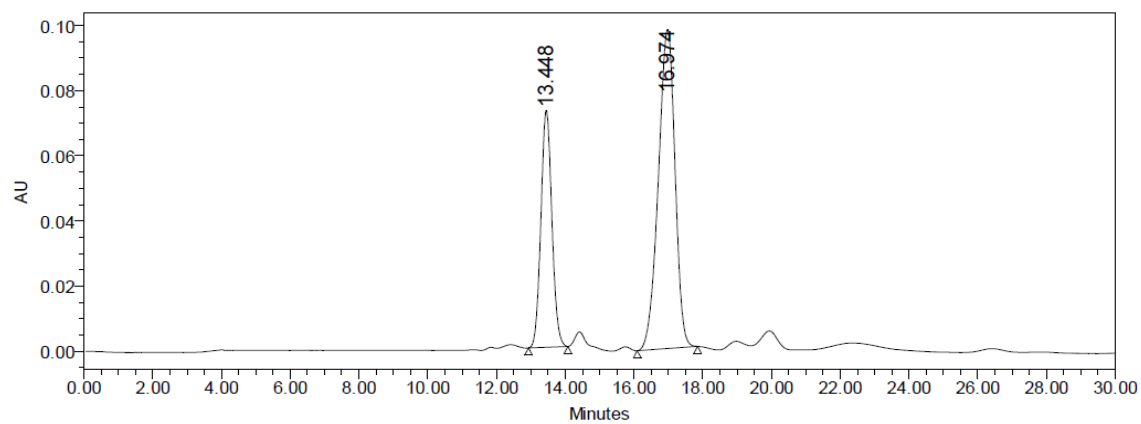
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	21.161	14194207	12.75	319965
2	PDA 250.0 nm	26.494	97114795	87.25	1036415



7g

2- CL PIP
2-CL-PIPERIDINE

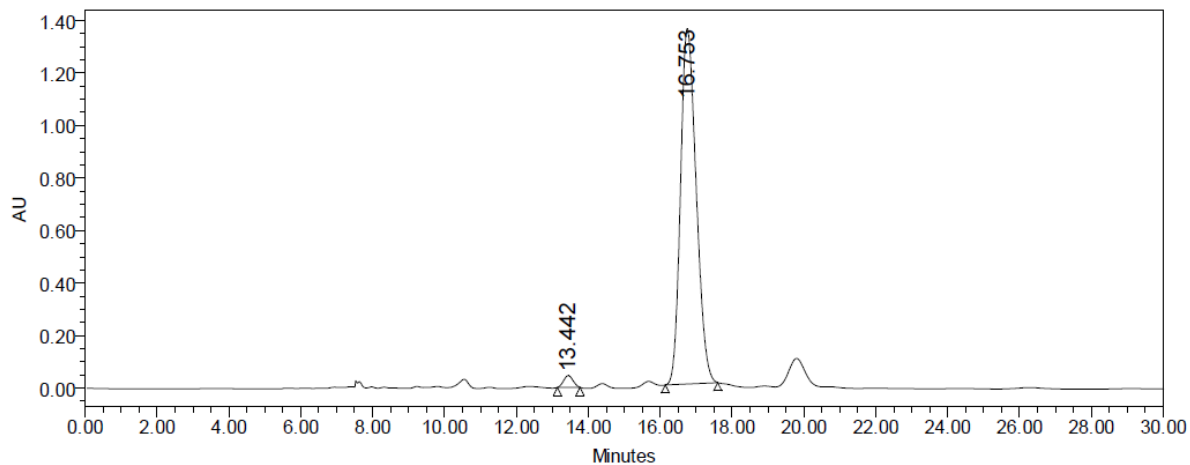




Channel: 2998; Processed Channel: PDA 300.0 nm; Result Id: 1767; Processing Method: 2Cl piperidine reneric

Processed Channel Descr.: PDA 300.0 nm

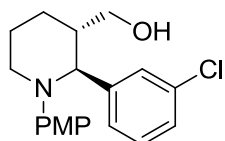
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 300.0 nm	13.448	1613647	32.86	72813
2	PDA 300.0 nm	16.974	3297467	67.14	97936



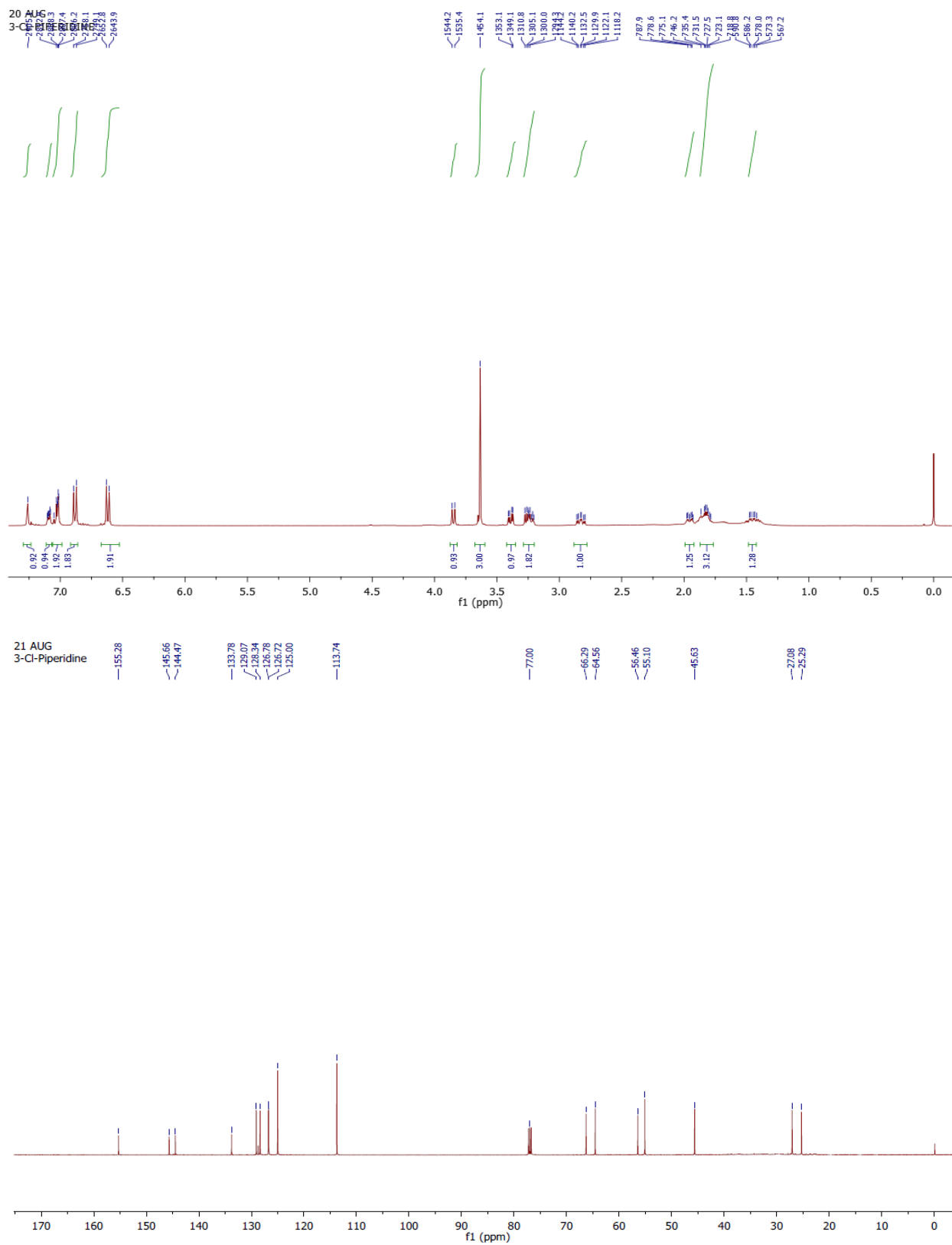
Channel: 2998; Processed Channel: PDA 300.0 nm; Result Id: 1772; Processing Method: 2Cl piperidine chiral

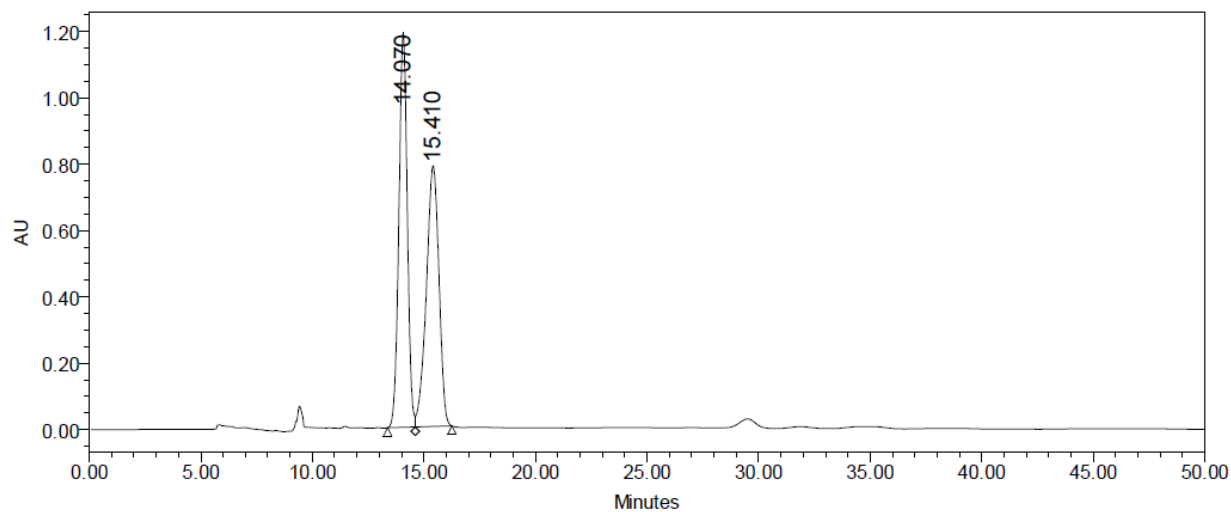
Processed Channel Descr.: PDA 300.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 300.0 nm	13.442	823932	1.97	45031
2	PDA 300.0 nm	16.753	41026803	98.03	1353690



7h

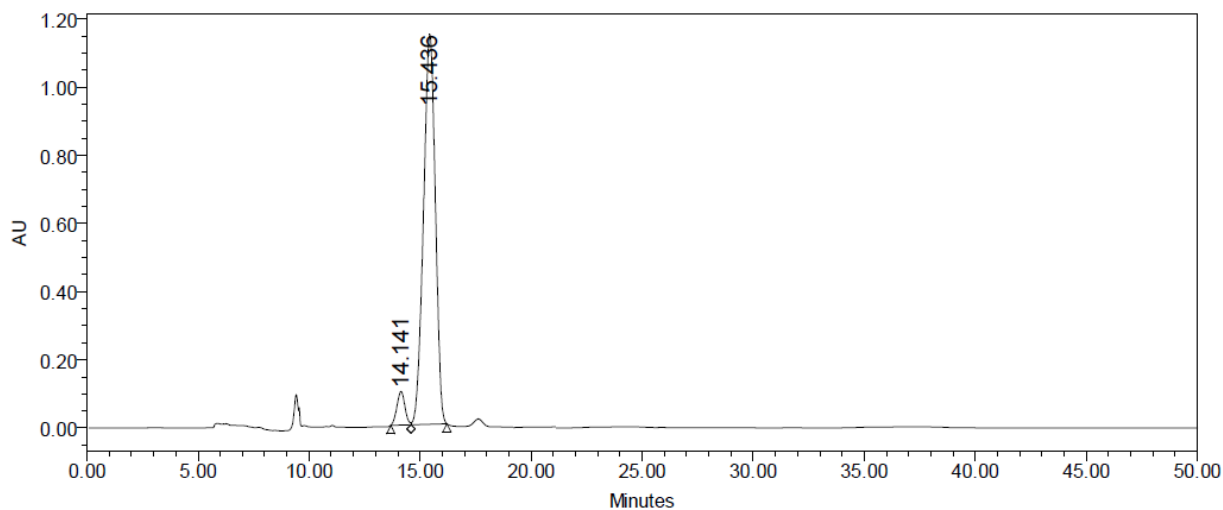




Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1306; Processing Method: 3Cl recemic

Processed Channel Descr.: PDA 250.0 nm

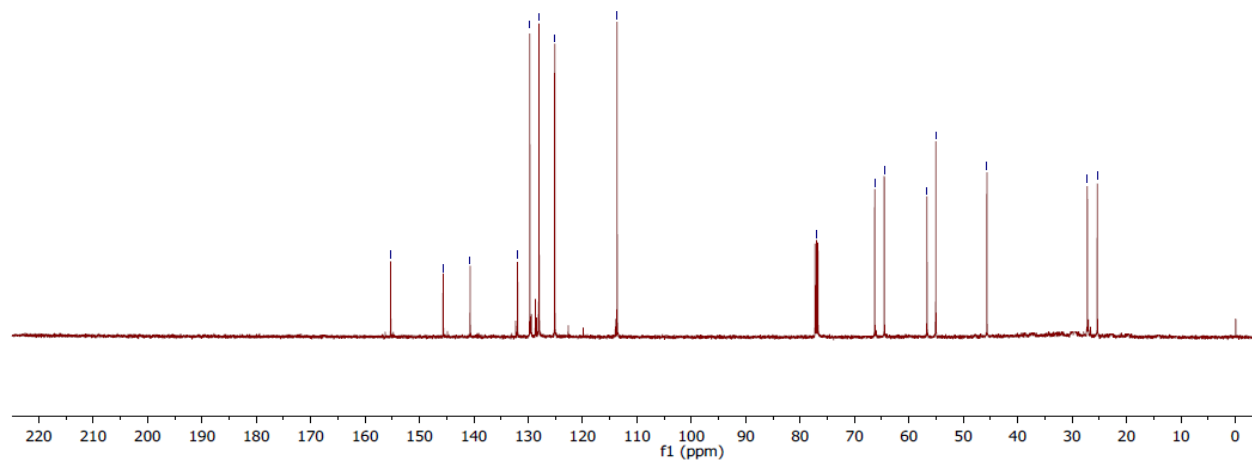
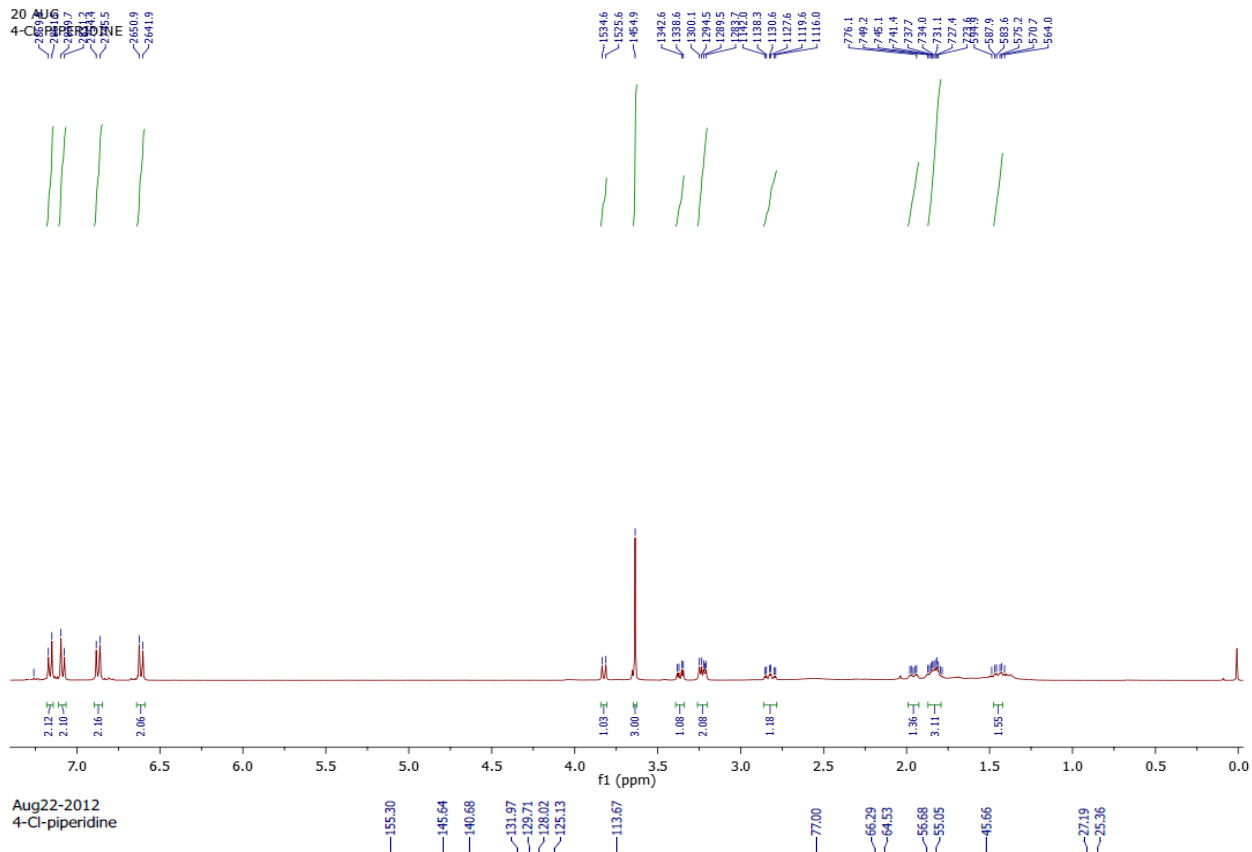
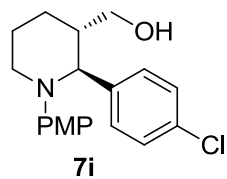
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	14.070	31139180	50.21	1189865
2	PDA 250.0 nm	15.410	30874380	49.79	785864

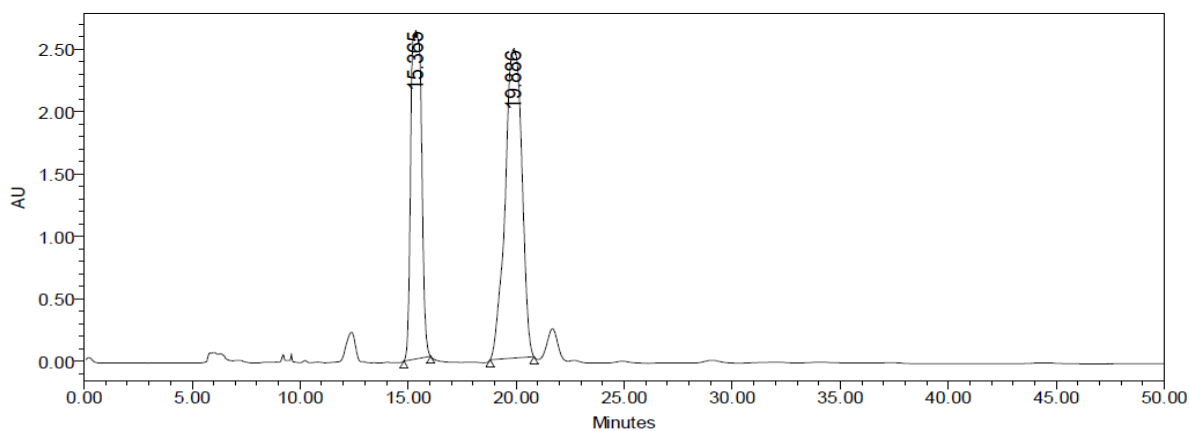


Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1308; Processing Method: 3Cl chiral

Processed Channel Descr.: PDA 250.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	14.141	2464969	5.50	98920
2	PDA 250.0 nm	15.436	42313747	94.50	1144466

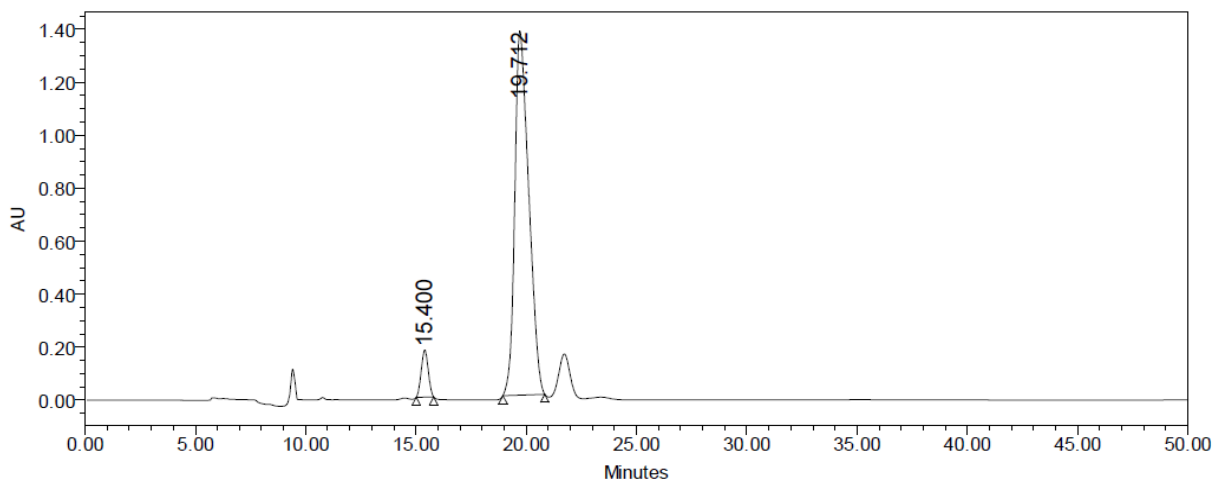




Channel: 2998; Processed Channel: PDA 210.0 nm; Result Id: 1287; Processing Method: 4Cl recemic

Processed Channel Descr.: PDA 210.0 nm

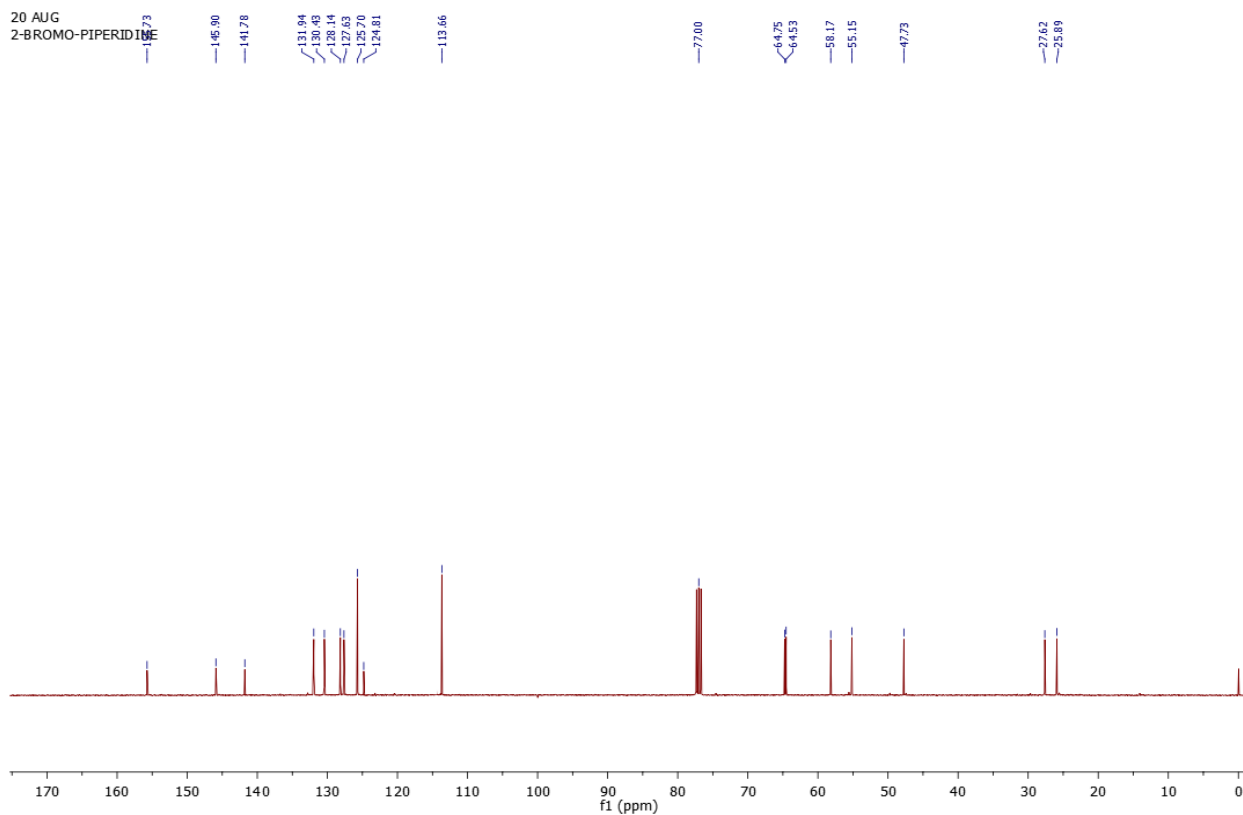
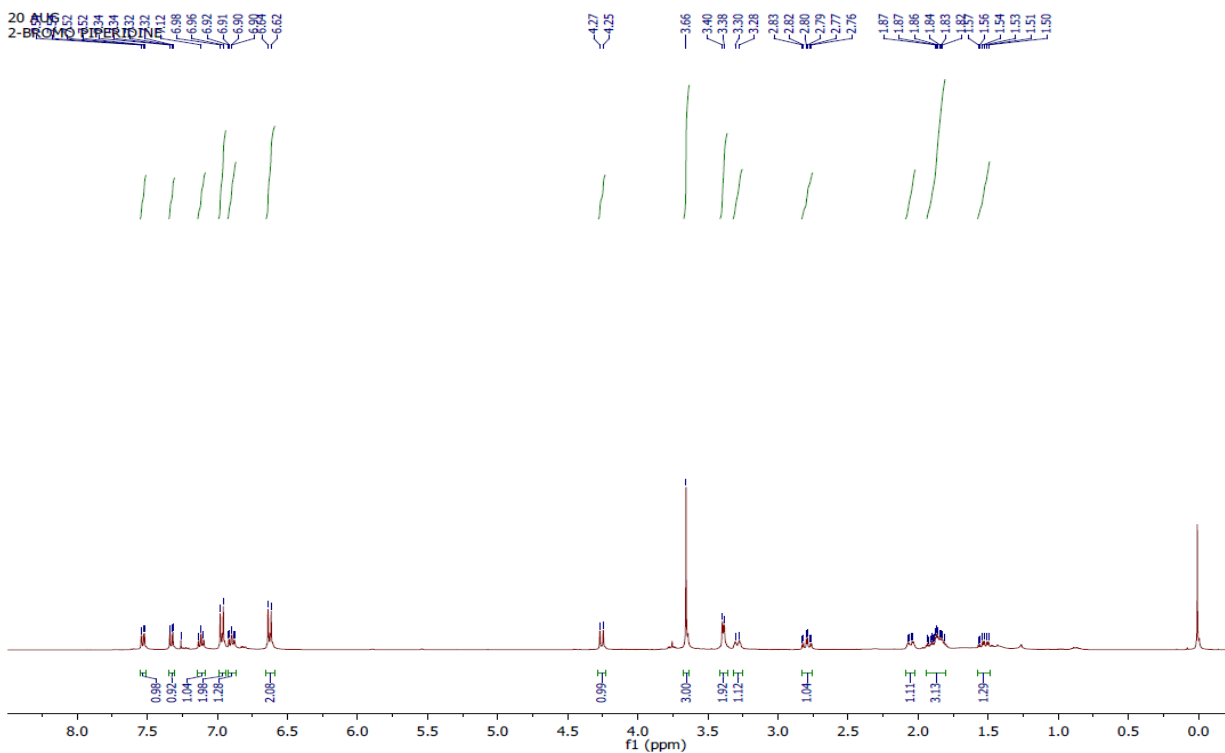
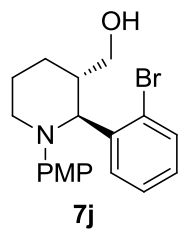
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	15.365	91272006	40.51	2629622
2	PDA 210.0 nm	19.886	134056490	59.49	2478964

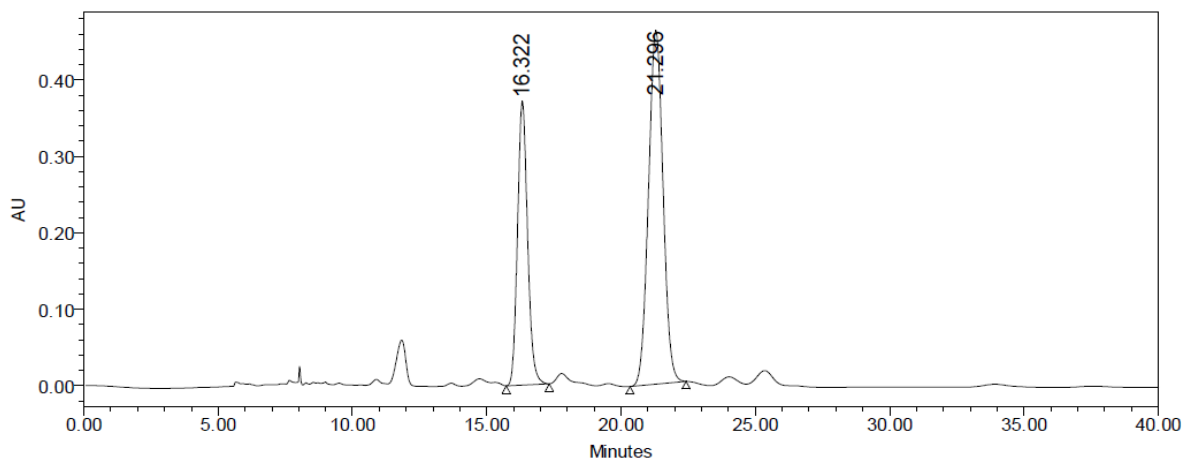


Channel: 2998; Processed Channel: PDA 282.7 nm; Result Id: 1293; Processing Method: 4Cl chiral

Processed Channel Descr.: PDA 282.7 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 282.7 nm	15.400	3887100	6.05	177507
2	PDA 282.7 nm	19.712	60404025	93.95	1373424

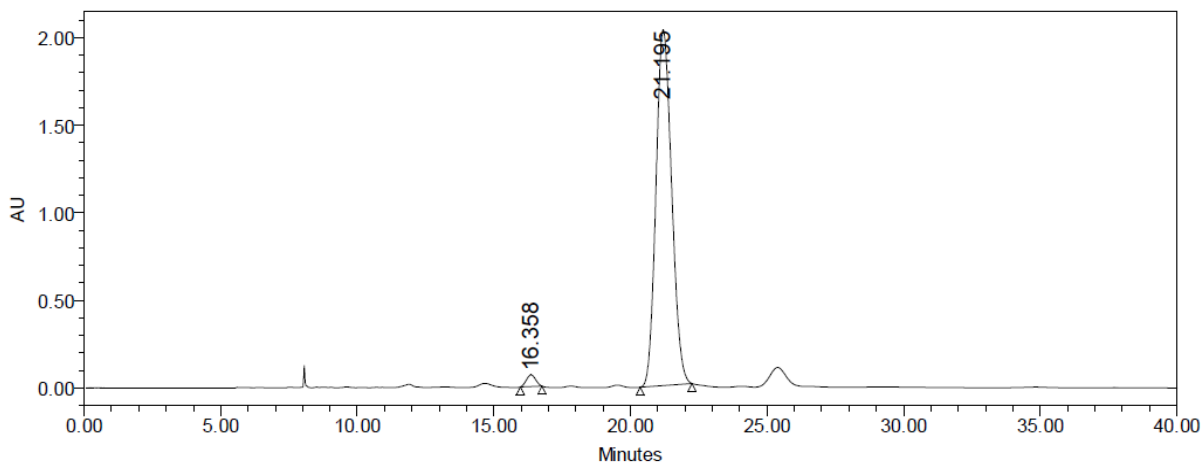




Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1813; Processing Method: 2Br Recenic

Processed Channel Descr.: PDA 250.0 nm

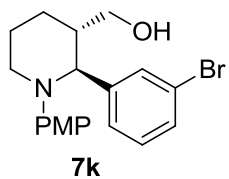
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	16.322	9679938	35.69	371809
2	PDA 250.0 nm	21.296	17441934	64.31	463158



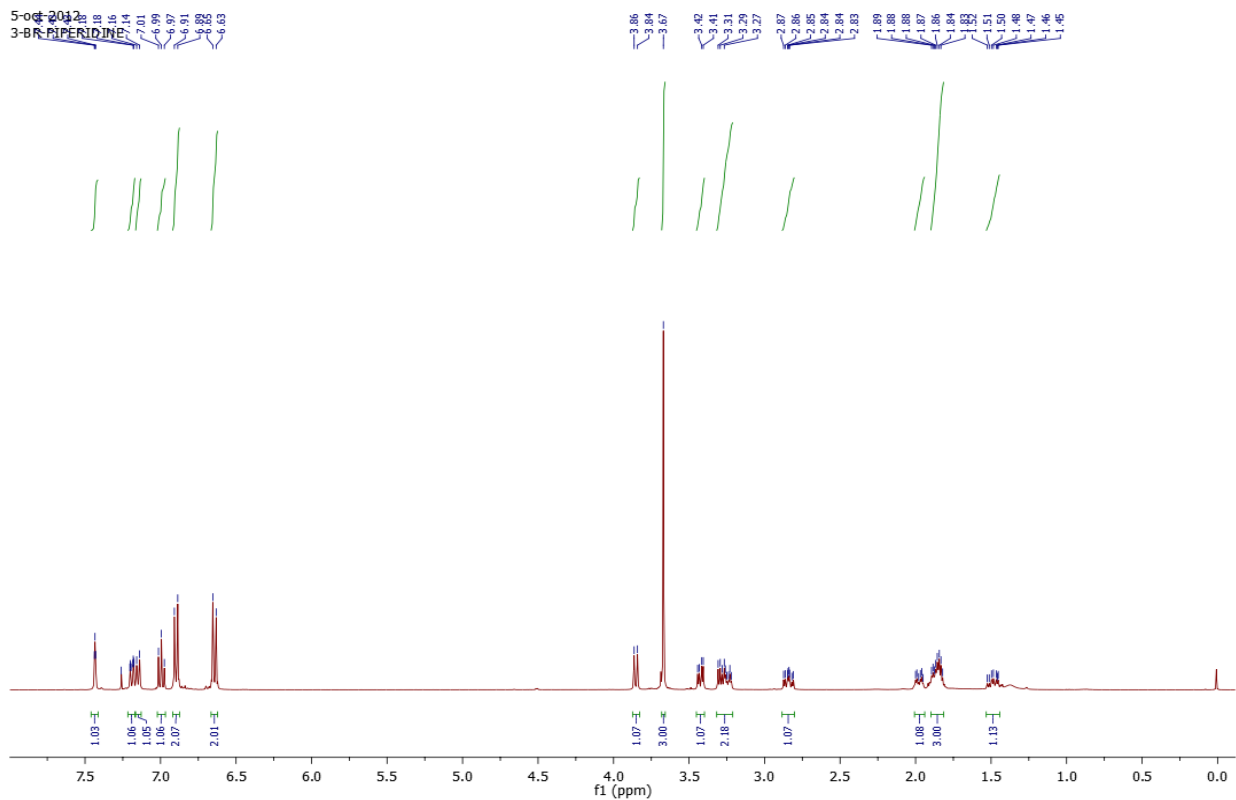
Channel: 2998; Processed Channel: PDA 270.0 nm; Result Id: 1816; Processing Method: 2Br piperidine chiral

Processed Channel Descr.: PDA 270.0 nm

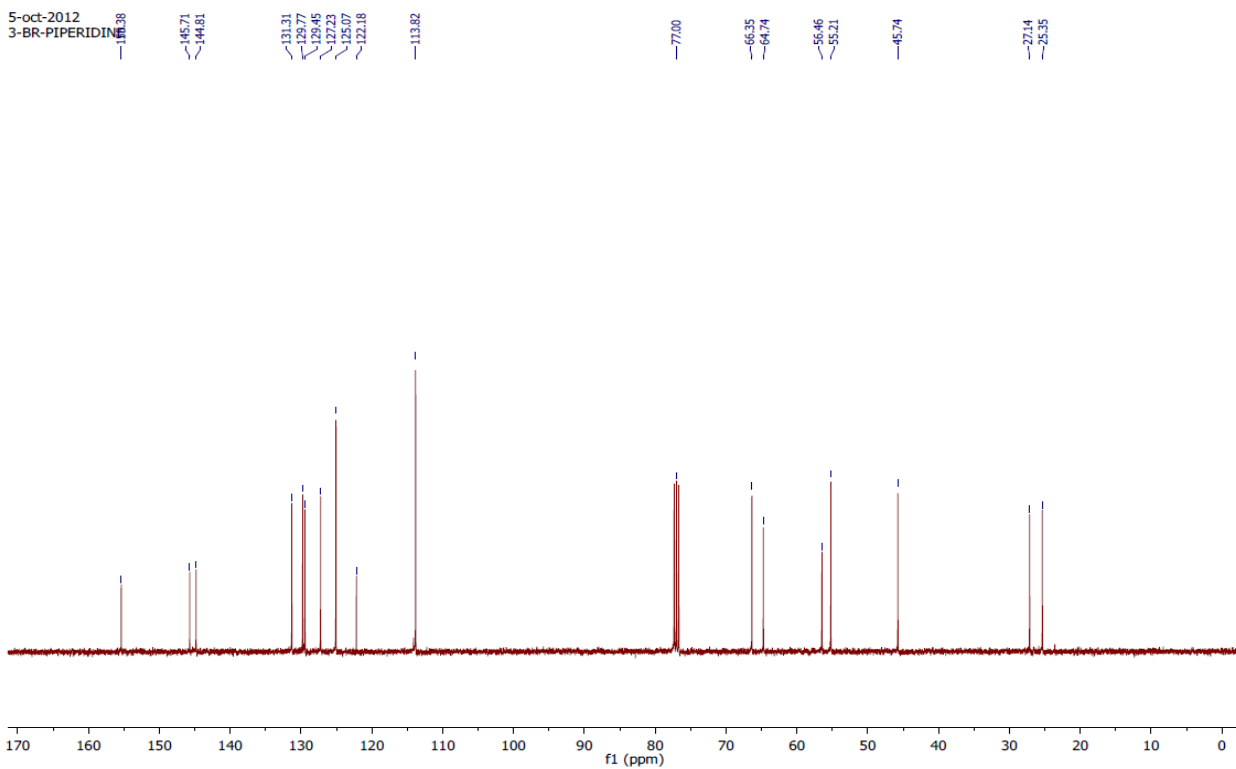
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 270.0 nm	16.358	1558627	1.89	66994
2	PDA 270.0 nm	21.195	81101716	98.11	2031551

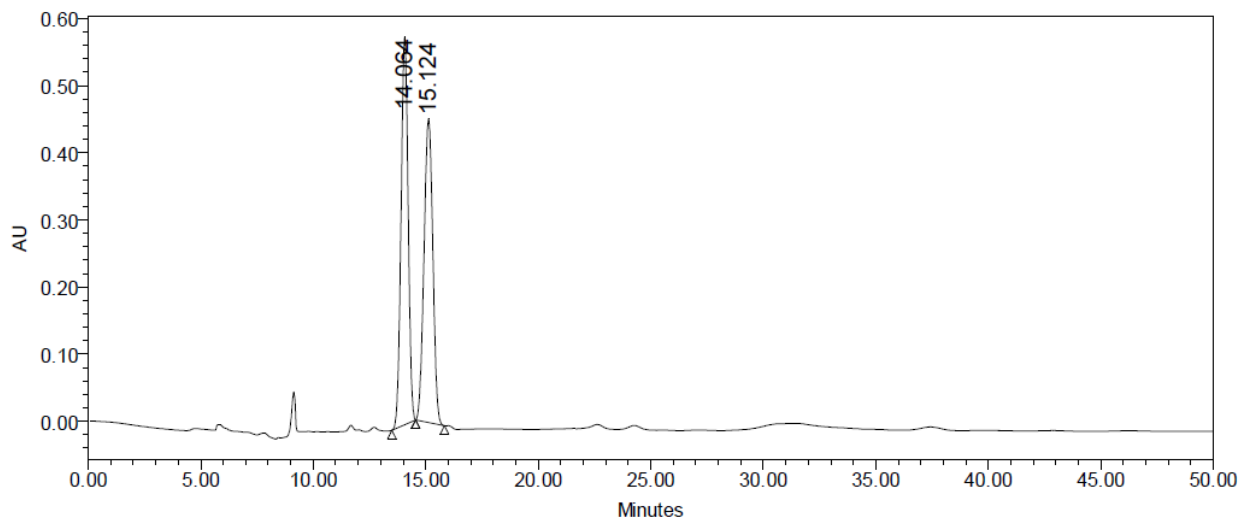


5-oct-2012
3-BR-PIPERIDINE



5-oct-2012
3-BR-PIPERIDINE

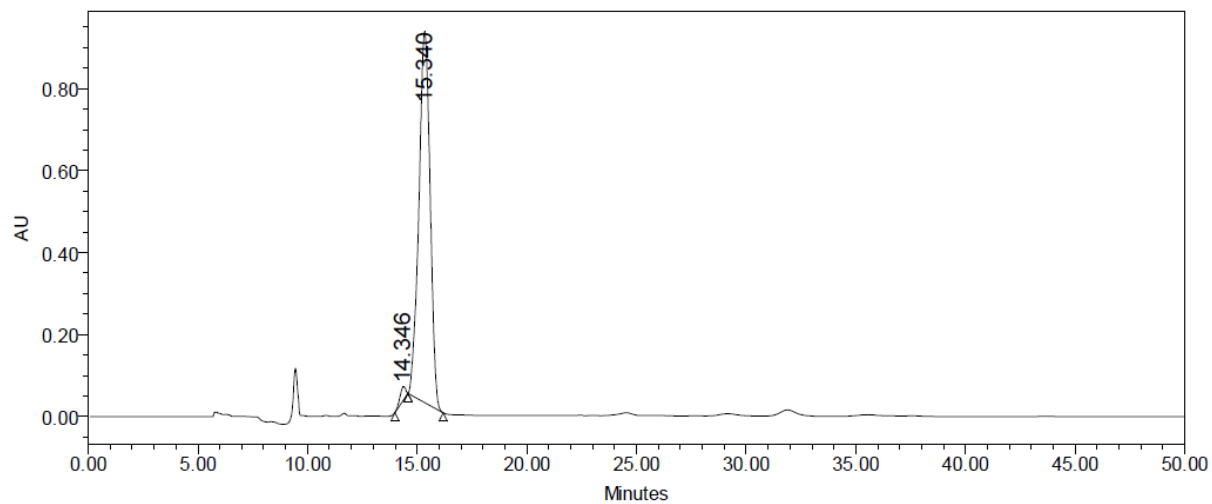




Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1176; Processing Method: 3Br recinic

Processed Channel Descr.: PDA 250.0 nm

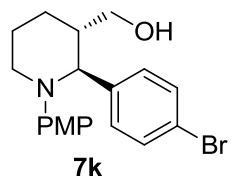
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	14.064	12623688	50.62	578041
2	PDA 250.0 nm	15.124	12313694	49.38	452875



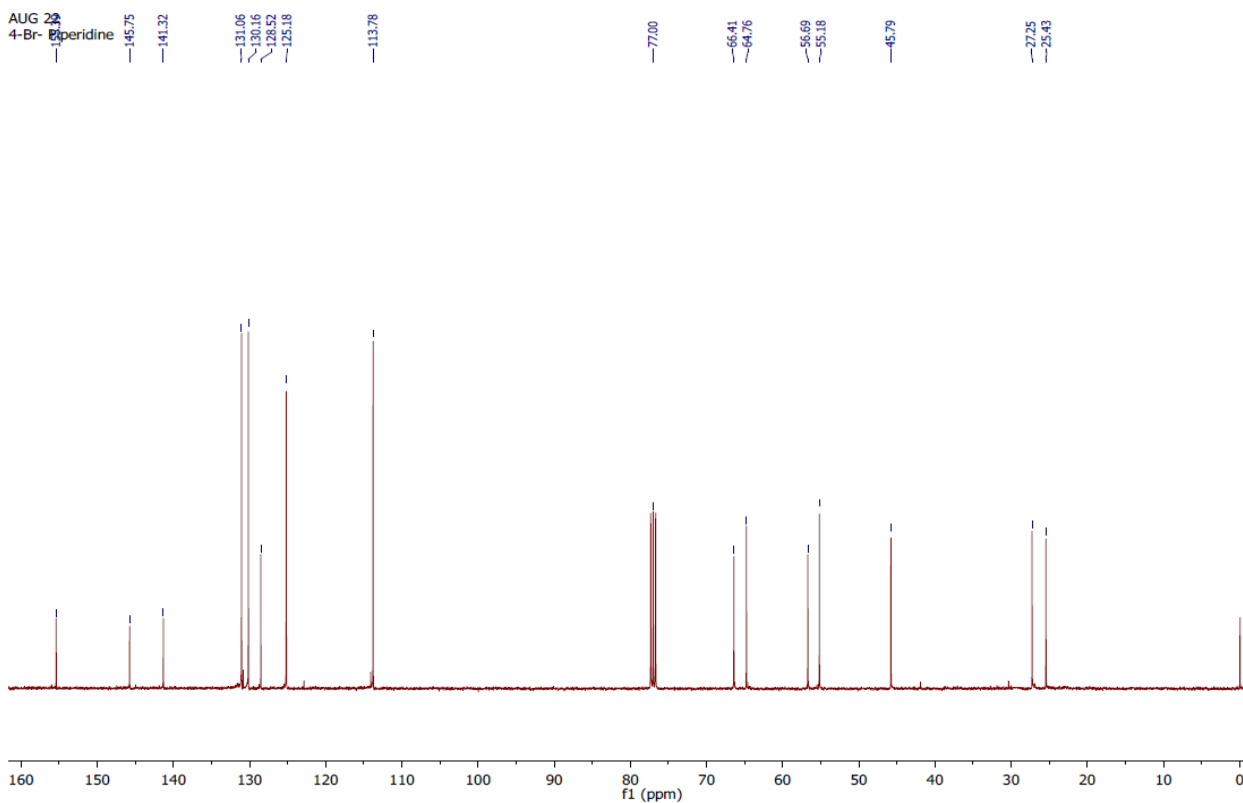
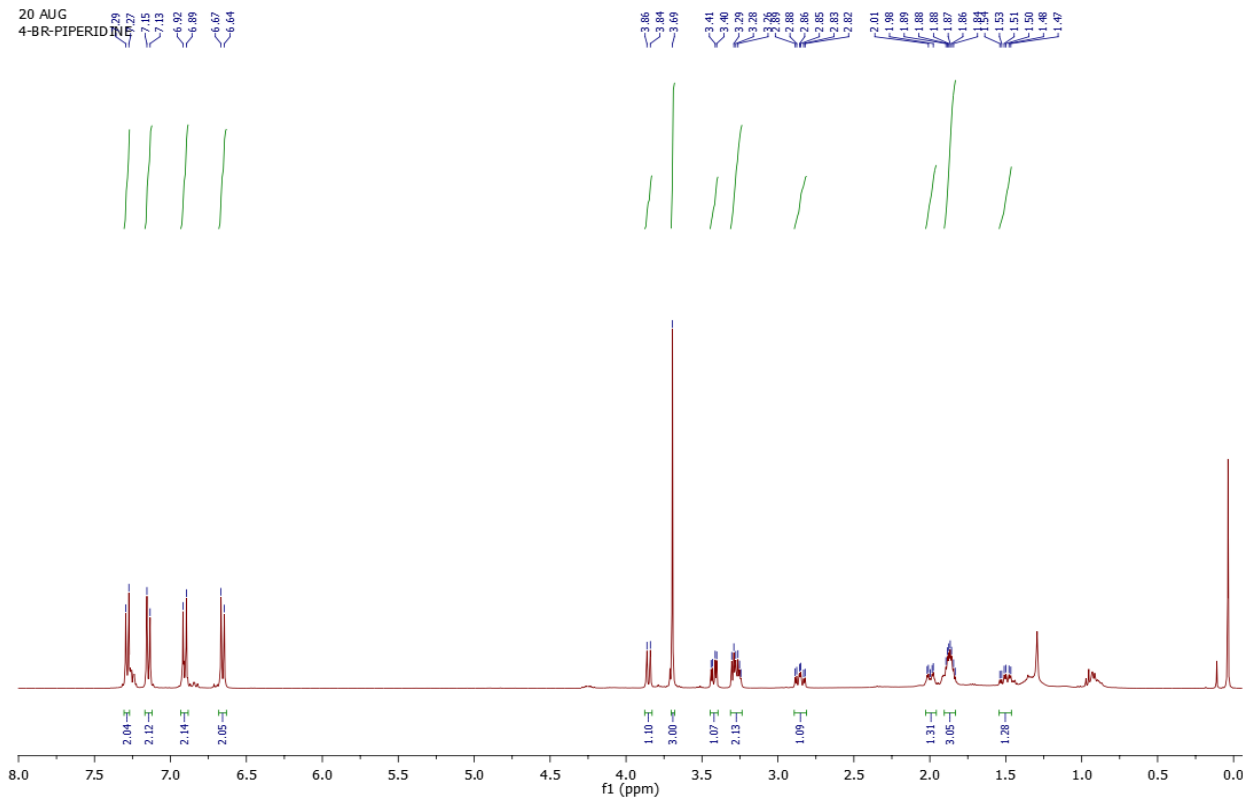
Channel: 2998; Processed Channel: PDA 260.0 nm; Result Id: 1179; Processing Method: 3Br chiral

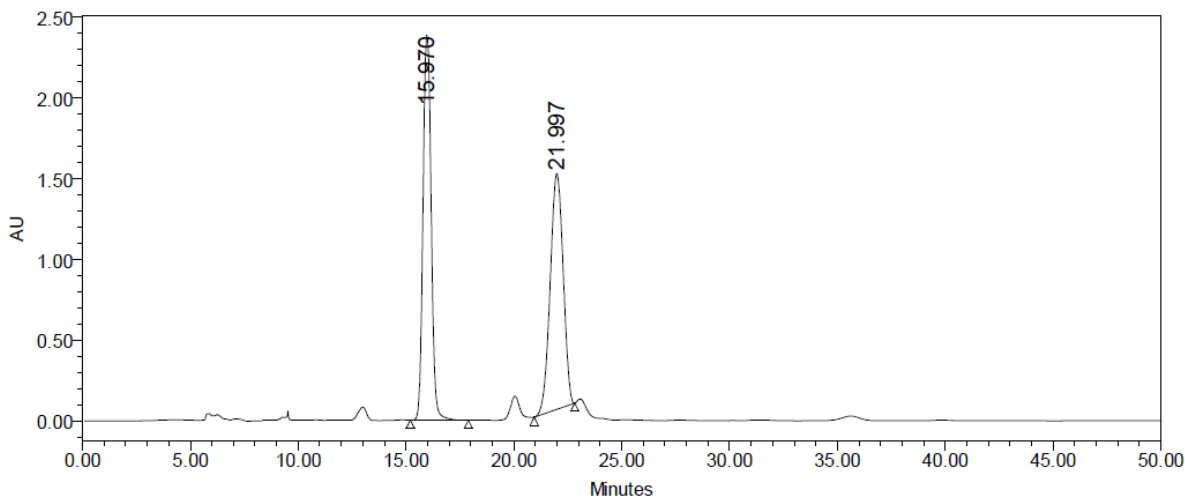
Processed Channel Descr.: PDA 260.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 260.0 nm	14.346	579088	1.76	33521
2	PDA 260.0 nm	15.340	32250417	98.24	905270



20 AUG
4-Br-PIPERIDINE

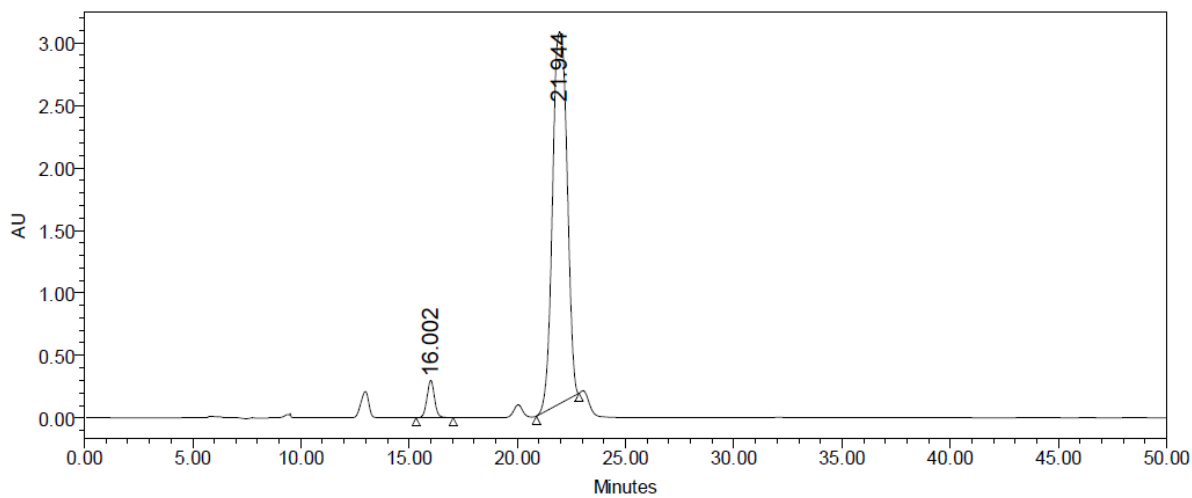




Channel: 2998; Processed Channel: PDA 210.0 nm; Result Id: 1182; Processing Method: 4Br recimic

Processed Channel Descr.: PDA 210.0 nm

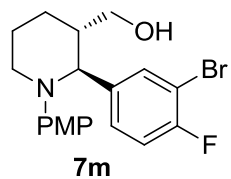
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	15.970	62919860	50.76	2382945
2	PDA 210.0 nm	21.997	61026592	49.24	1461711



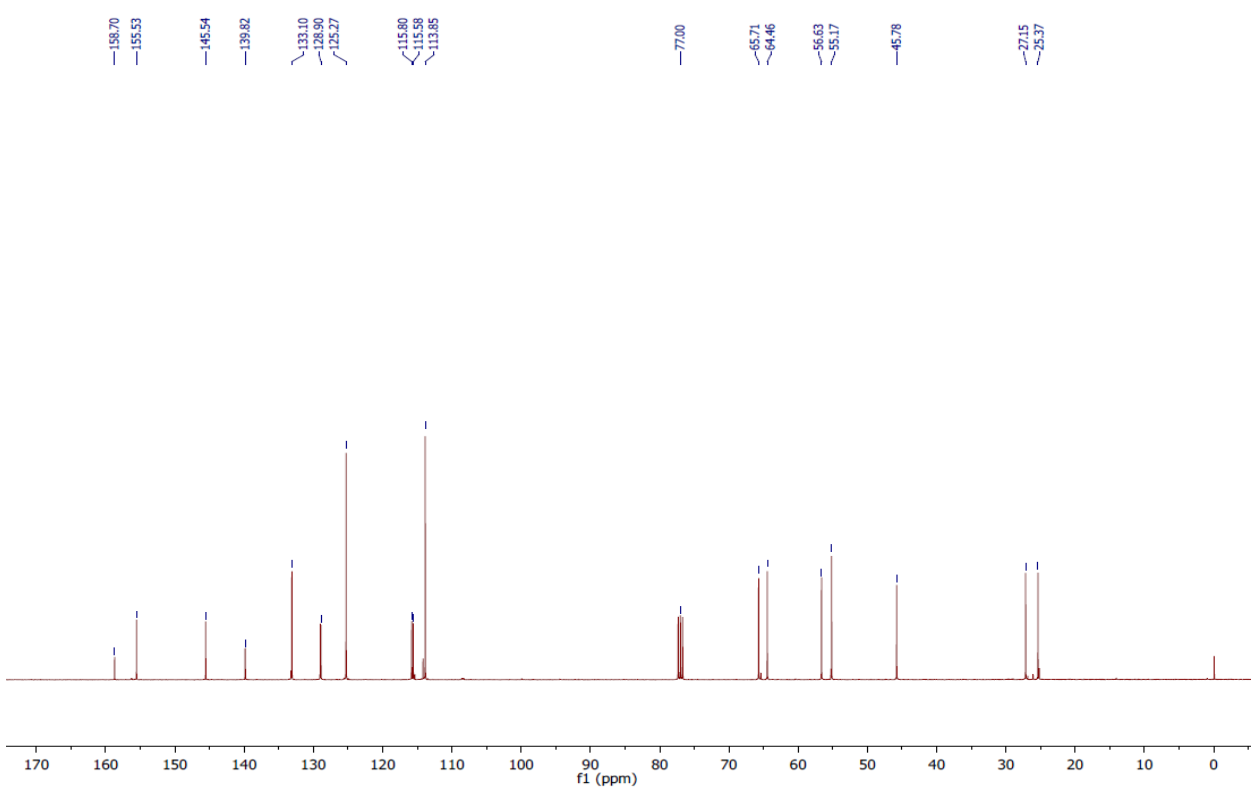
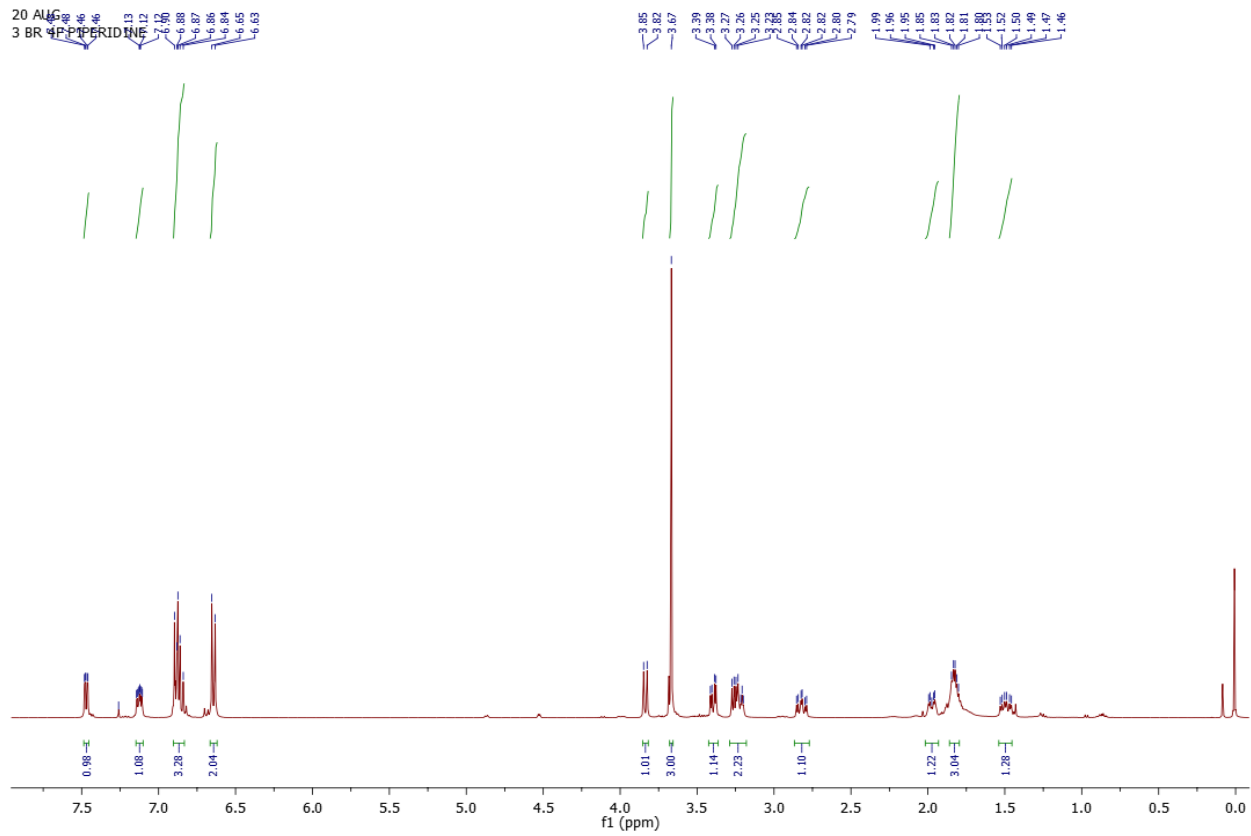
Channel: 2998; Processed Channel: PDA 230.0 nm; Result Id: 1190; Processing Method: 4Br chiral

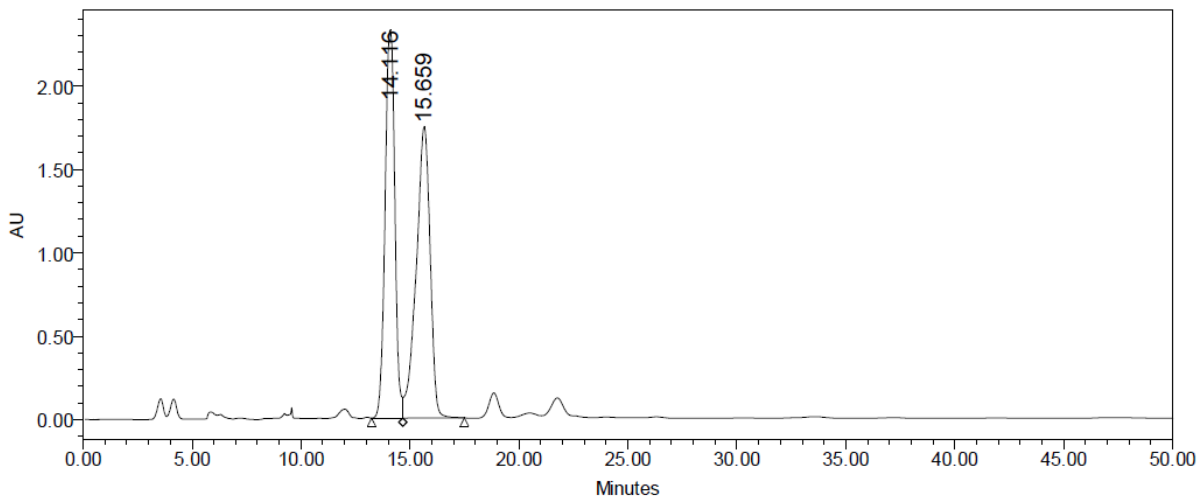
Processed Channel Descr.: PDA 230.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 230.0 nm	16.002	7184077	4.90	298653
2	PDA 230.0 nm	21.944	139363498	95.10	2975530



20 ALK
3 BR 4 F PIPERIDINE

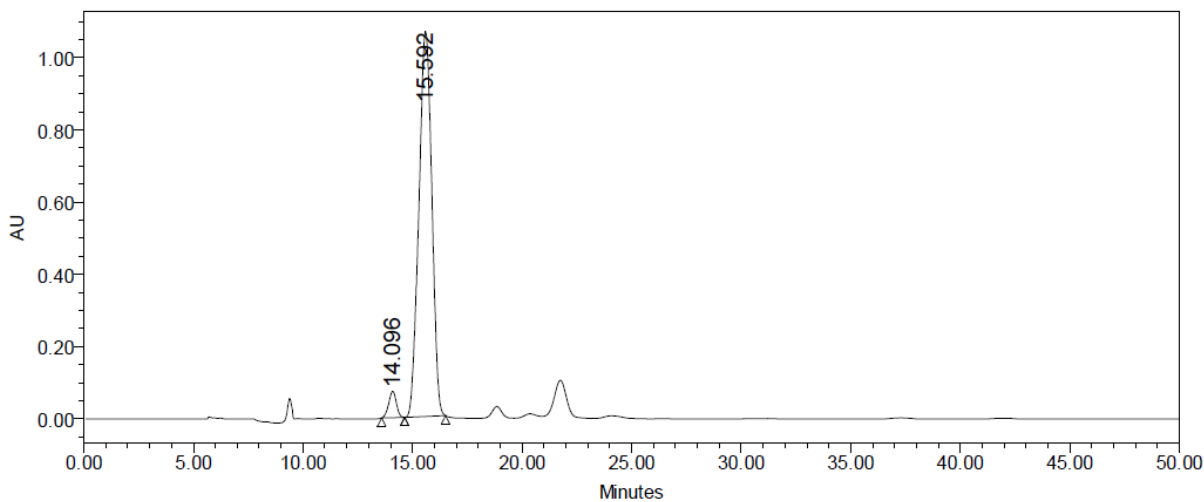




Channel: 2998; Processed Channel: PDA 210.0 nm; Result Id: 1354; Processing Method: 3Br 4F recemic

Processed Channel Descr.: PDA 210.0 nm

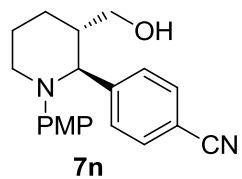
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	14.116	72261566	48.16	2326788
2	PDA 210.0 nm	15.659	77791436	51.84	1748527



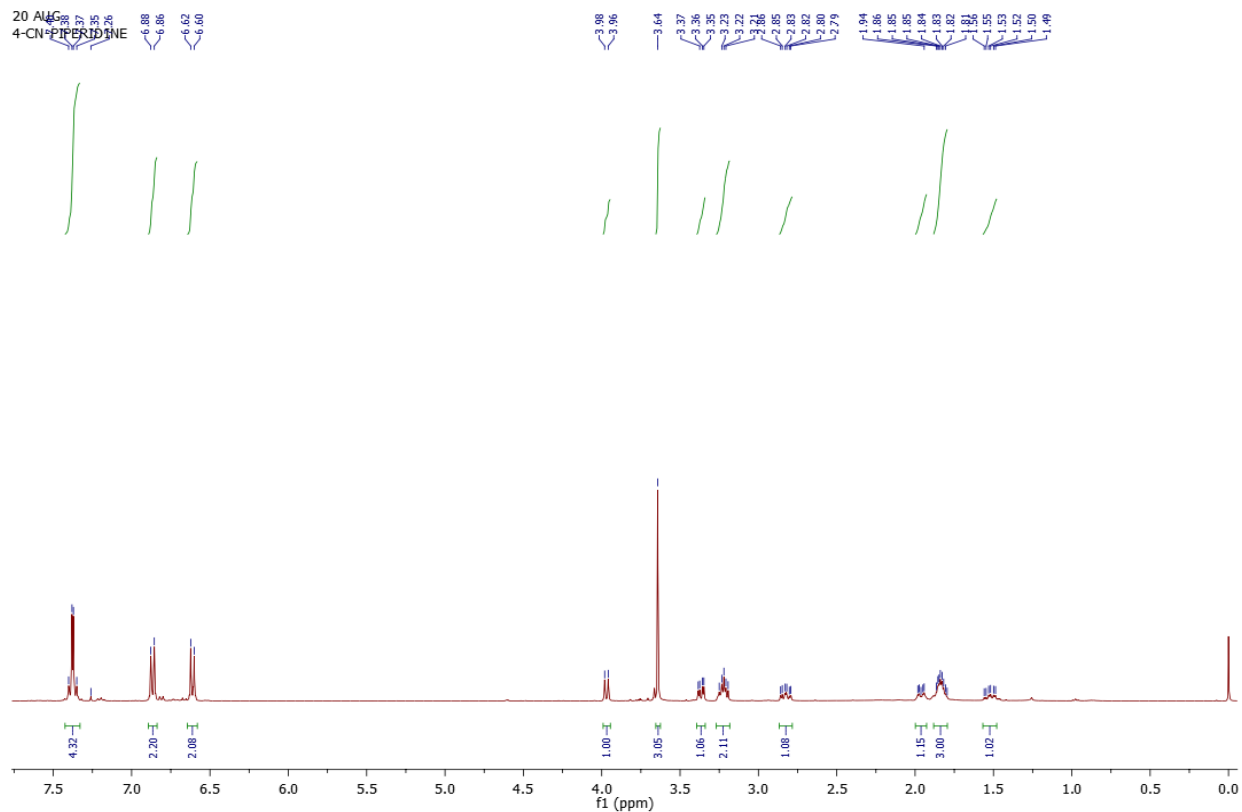
Channel: 2998; Processed Channel: PDA 300.0 nm; Result Id: 1362; Processing Method: 3Br 4F chiral

Processed Channel Descr.: PDA 300.0 nm

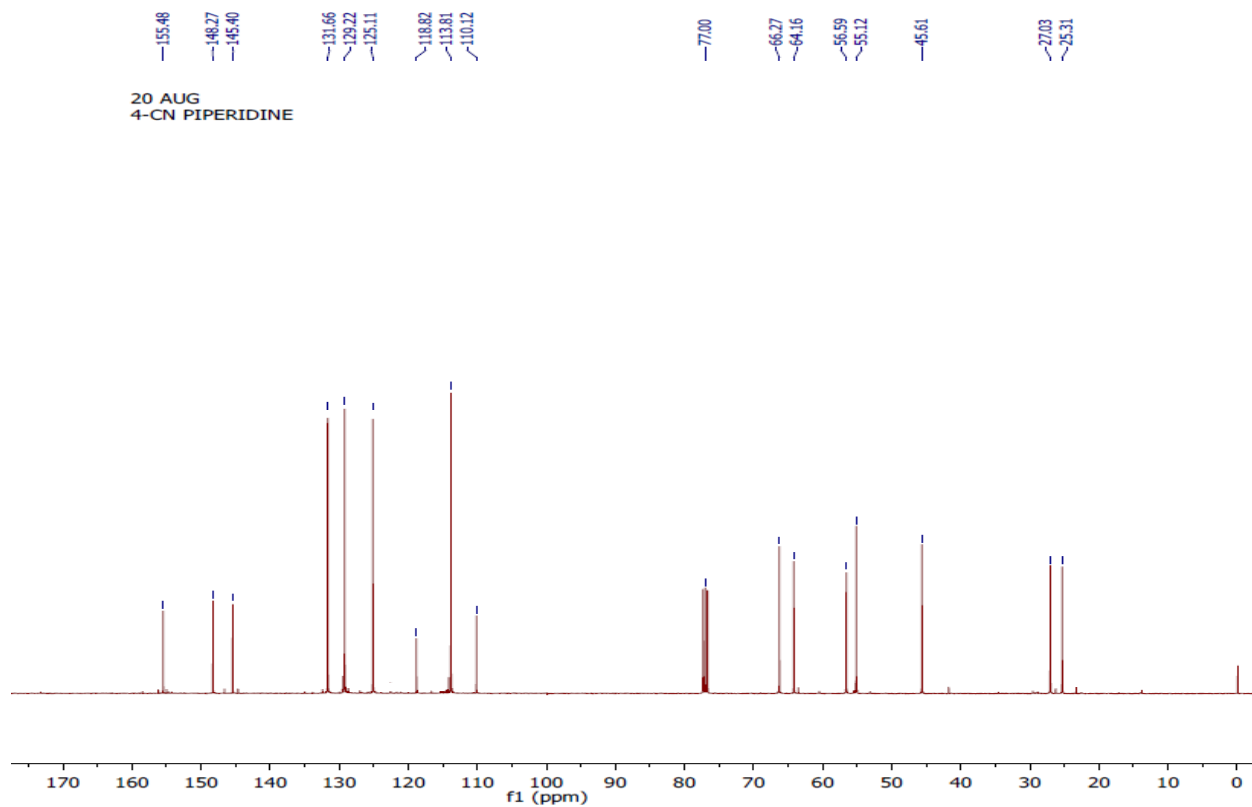
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 300.0 nm	14.096	1772320	3.89	73342
2	PDA 300.0 nm	15.592	43750015	96.11	1066251

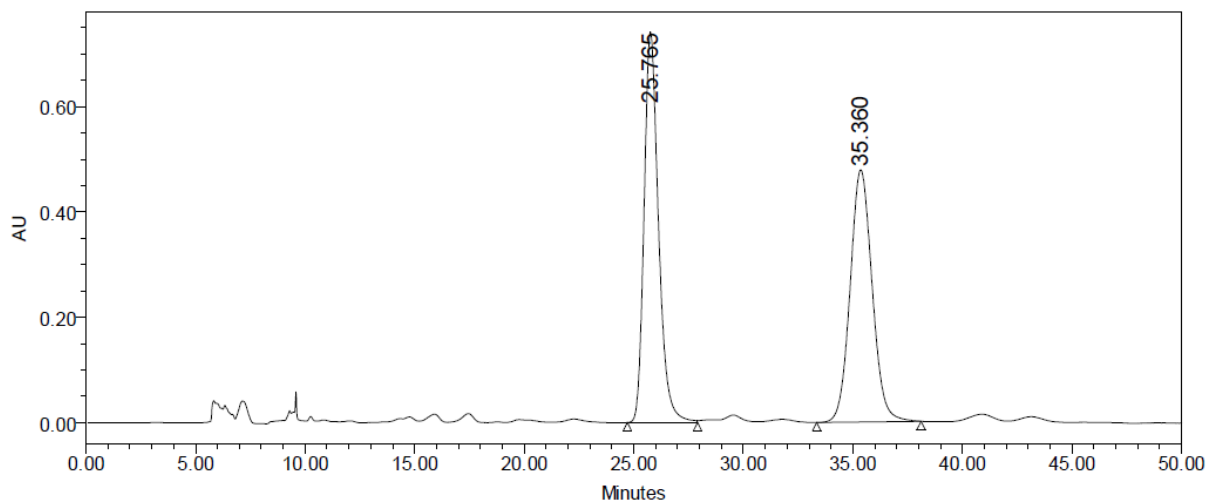


20 AUG
4-CN-PIPERIDINE



20 AUG
4-CN PIPERIDINE

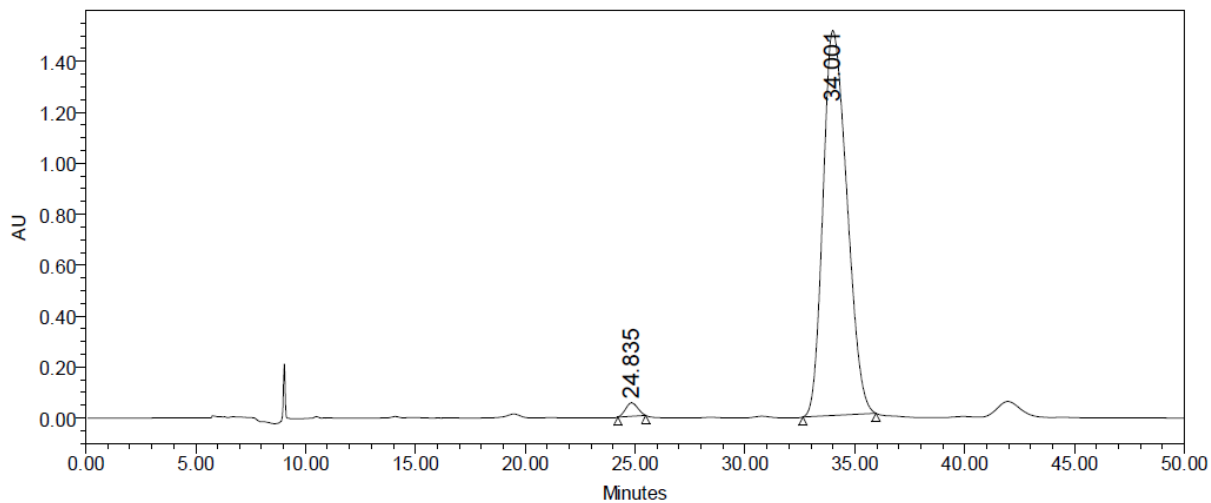




Channel: 2998; Processed Channel: PDA 210.0 nm; Result Id: 1374; Processing Method: 4CN recenic

Processed Channel Descr.: PDA 210.0 nm

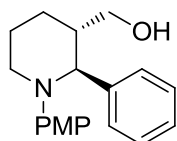
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 210.0 nm	25.765	33880253	50.36	740836
2	PDA 210.0 nm	35.360	33396864	49.64	478314



Channel: 2998; Processed Channel: PDA 280.0 nm; Result Id: 1382; Processing Method: 4CN chiral

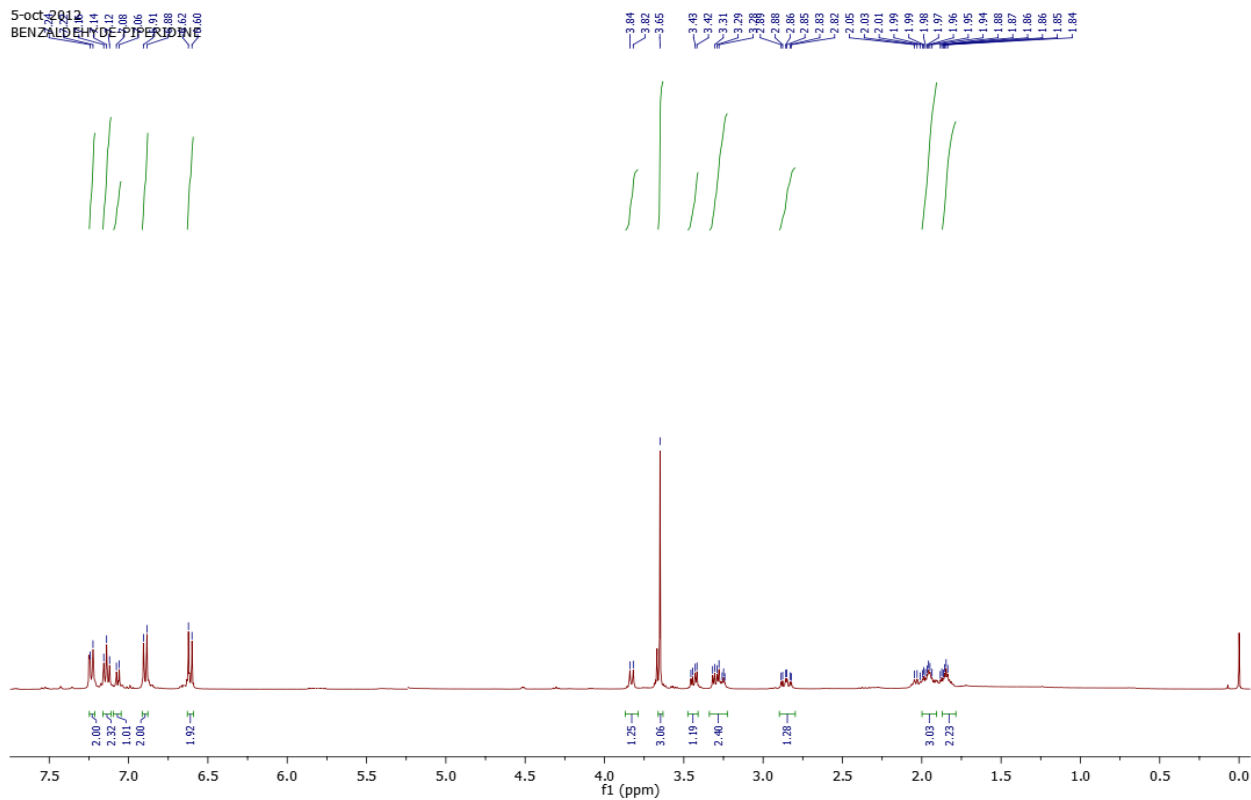
Processed Channel Descr.: PDA 280.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 280.0 nm	24.835	2000805	1.72	52418
2	PDA 280.0 nm	34.001	114332670	98.28	1510719

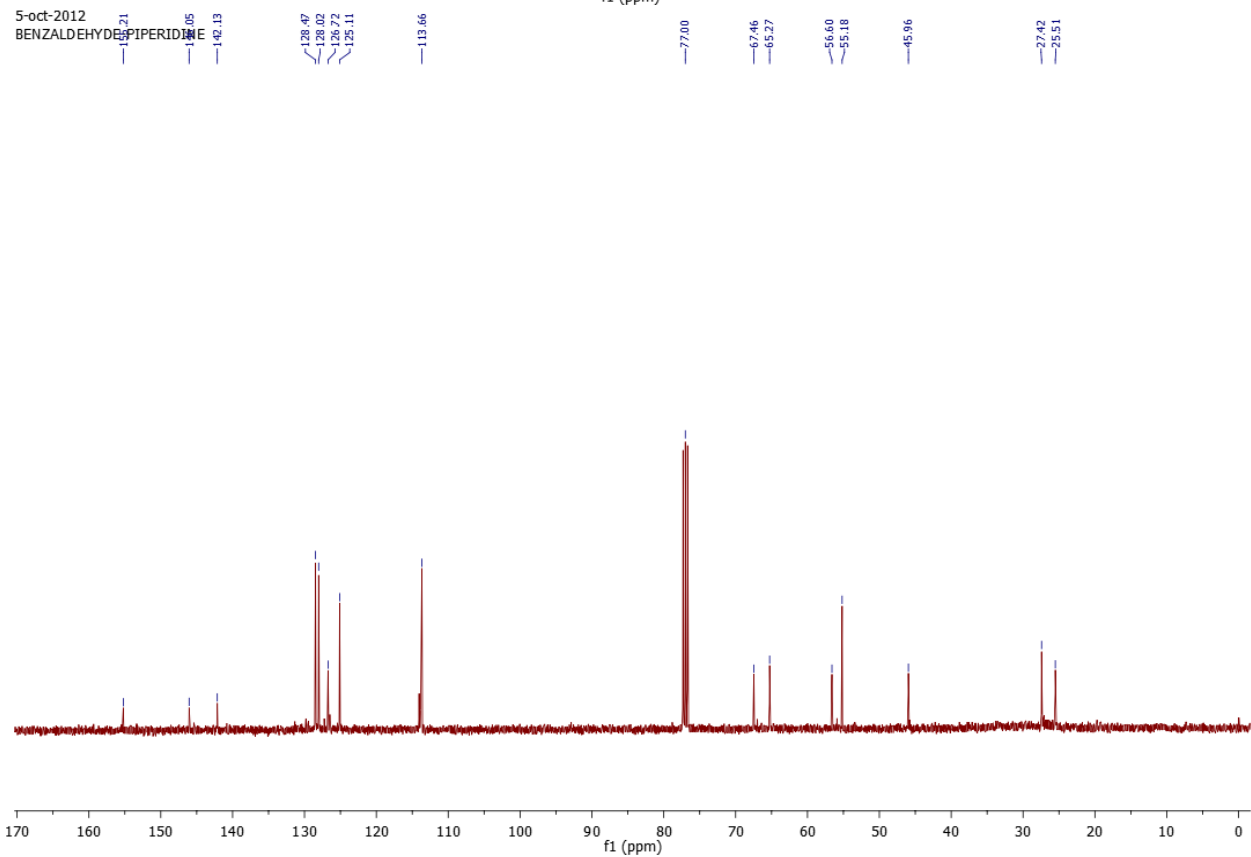


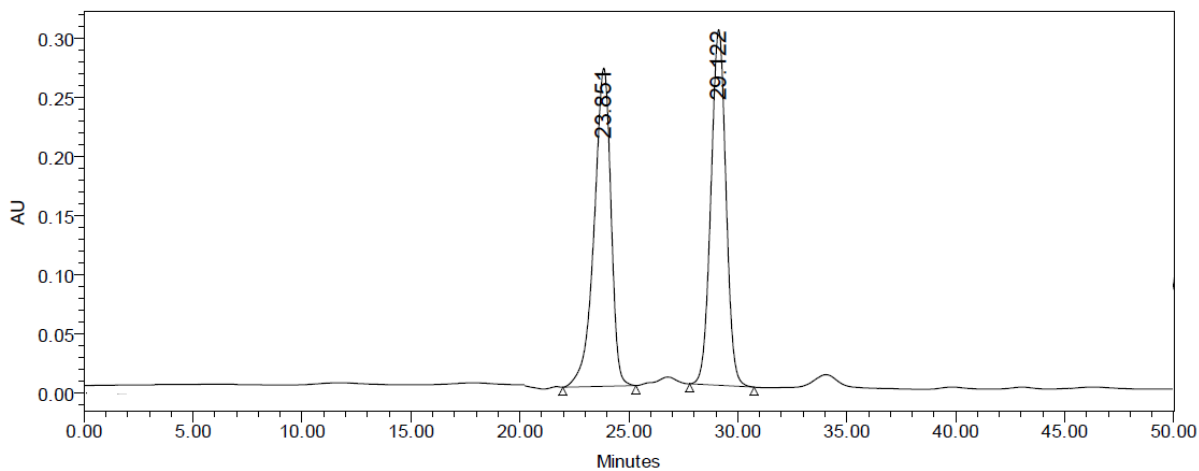
7o

5-oct-2012
BENZALDEHYDE PIPERIDINE



5-oct-2012
BENZALDEHYDE PIPERIDINE

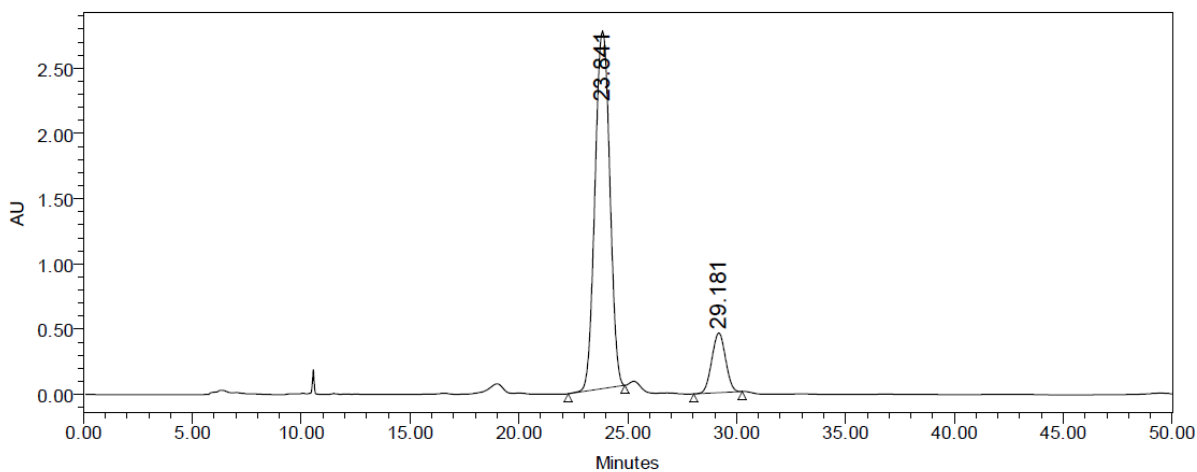




Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1832; Processing Method: benzaldehyde piperidin recemic

Processed Channel Descr.: PDA 250.0 nm

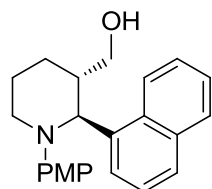
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	23.851	14442485	50.00	268633
2	PDA 250.0 nm	29.122	14444325	50.00	300286



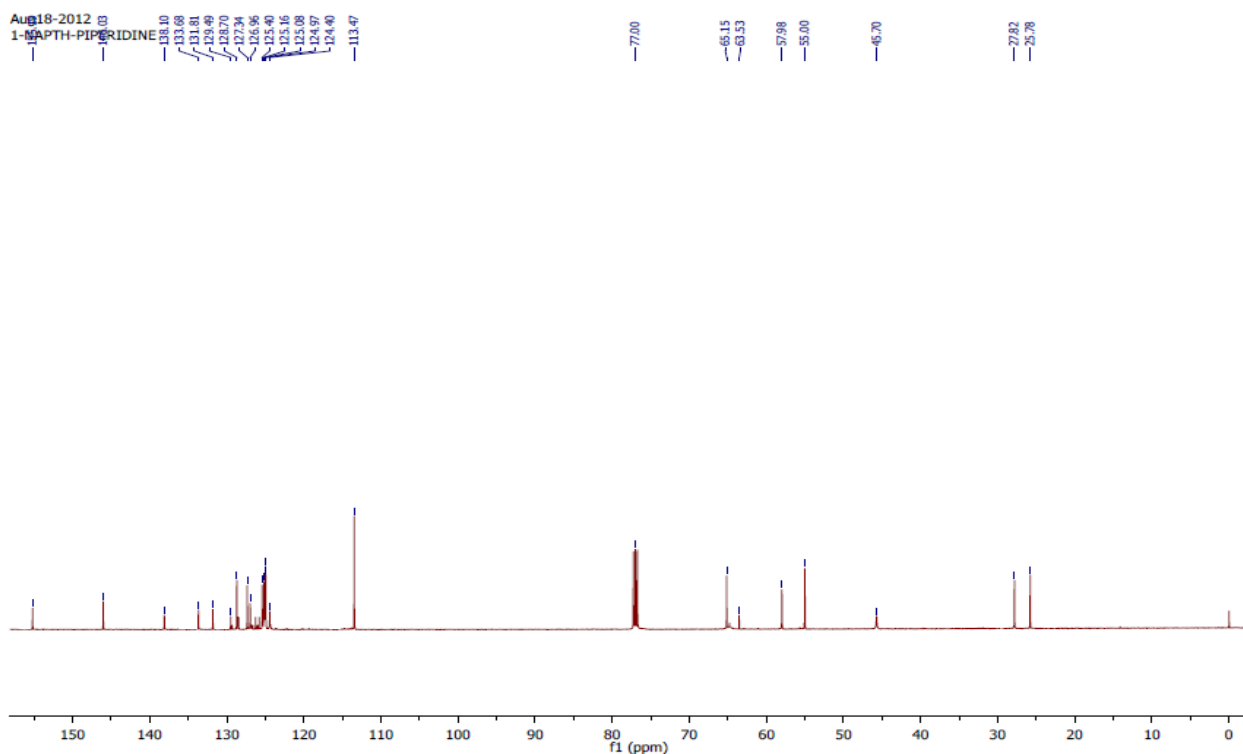
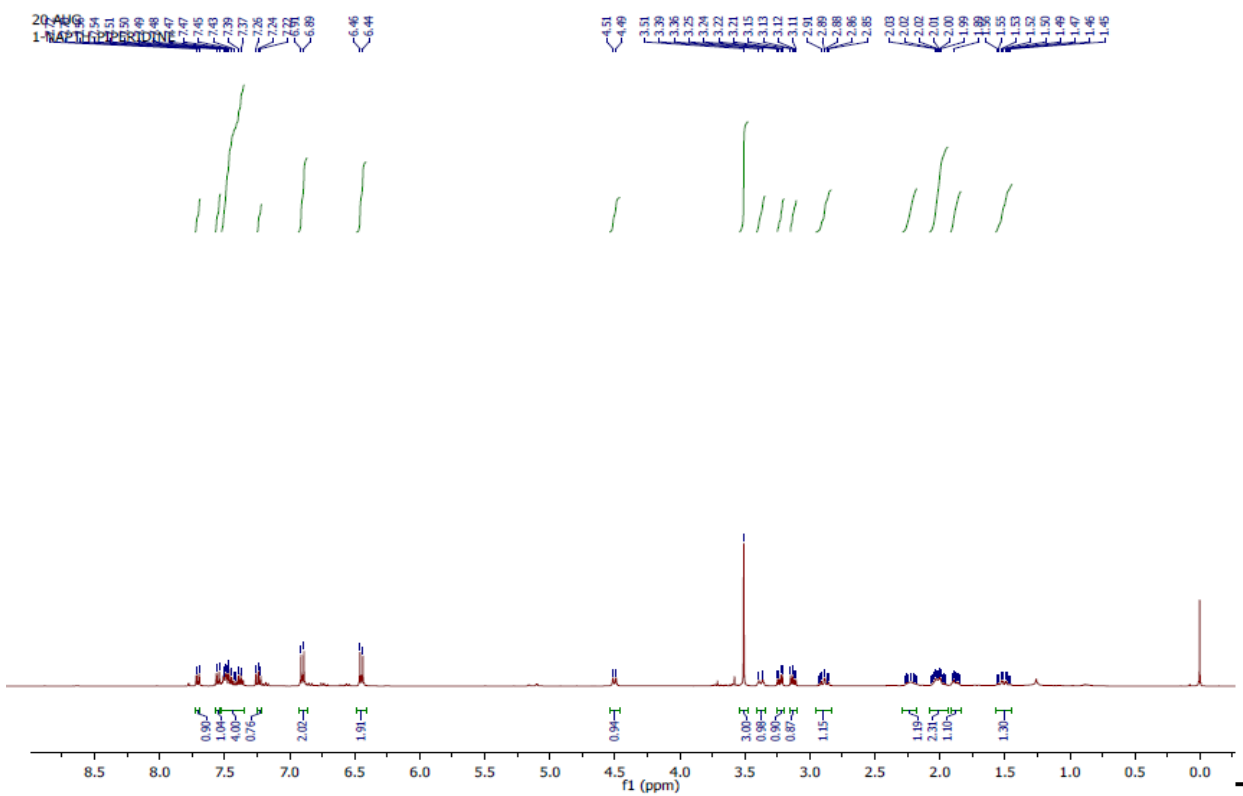
Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1835; Processing Method: benzaldehyde piperidine chiral

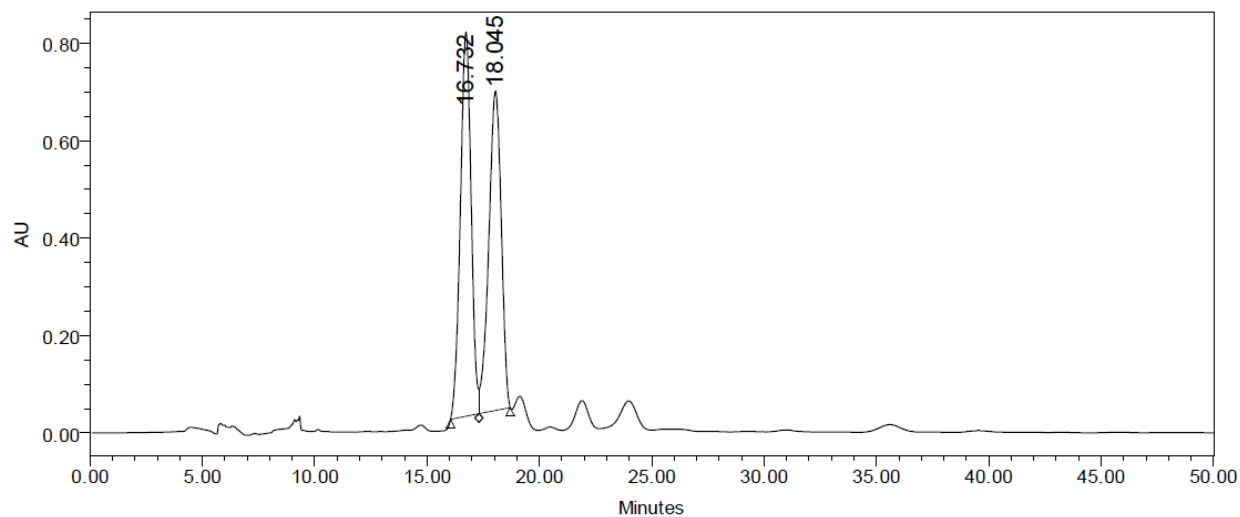
Processed Channel Descr.: PDA 250.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	23.841	129693361	86.62	2742504
2	PDA 250.0 nm	29.181	20030020	13.38	457400



7p

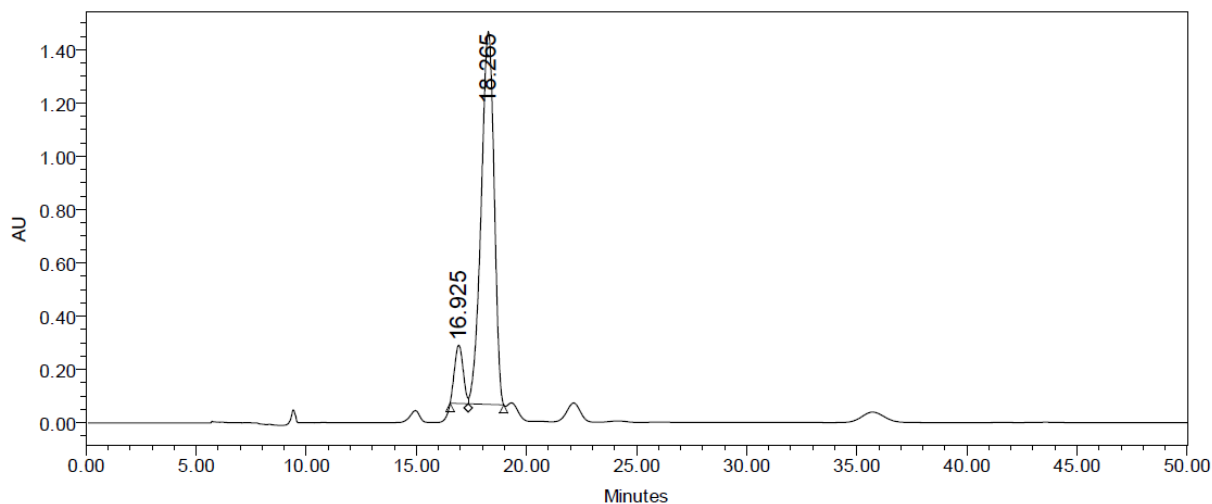




Channel: 2998; Processed Channel: PDA 230.0 nm; Result Id: 1407; Processing Method: 1 naphthyl recemic

Processed Channel Descr.: PDA 230.0 nm

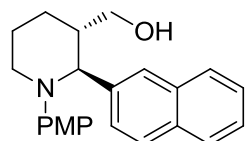
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 230.0 nm	16.732	26237147	50.86	788448
2	PDA 230.0 nm	18.045	25349306	49.14	655280



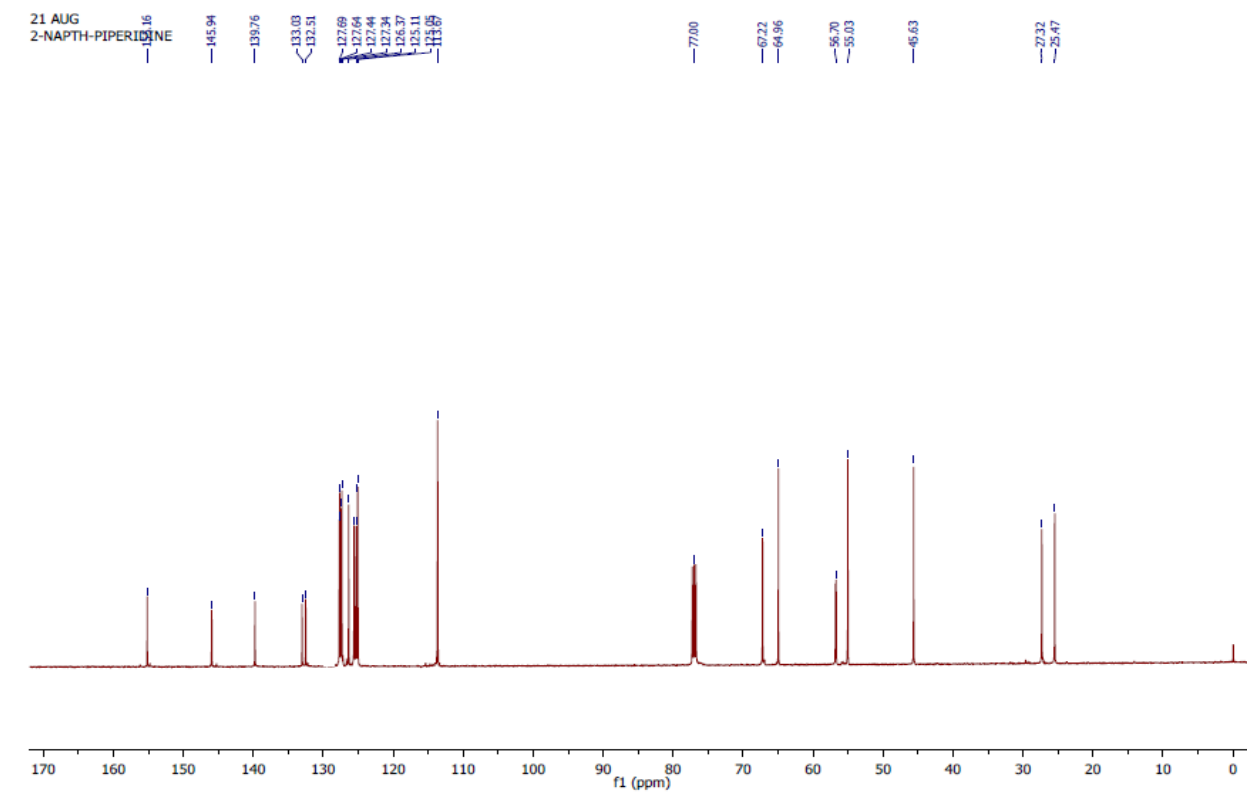
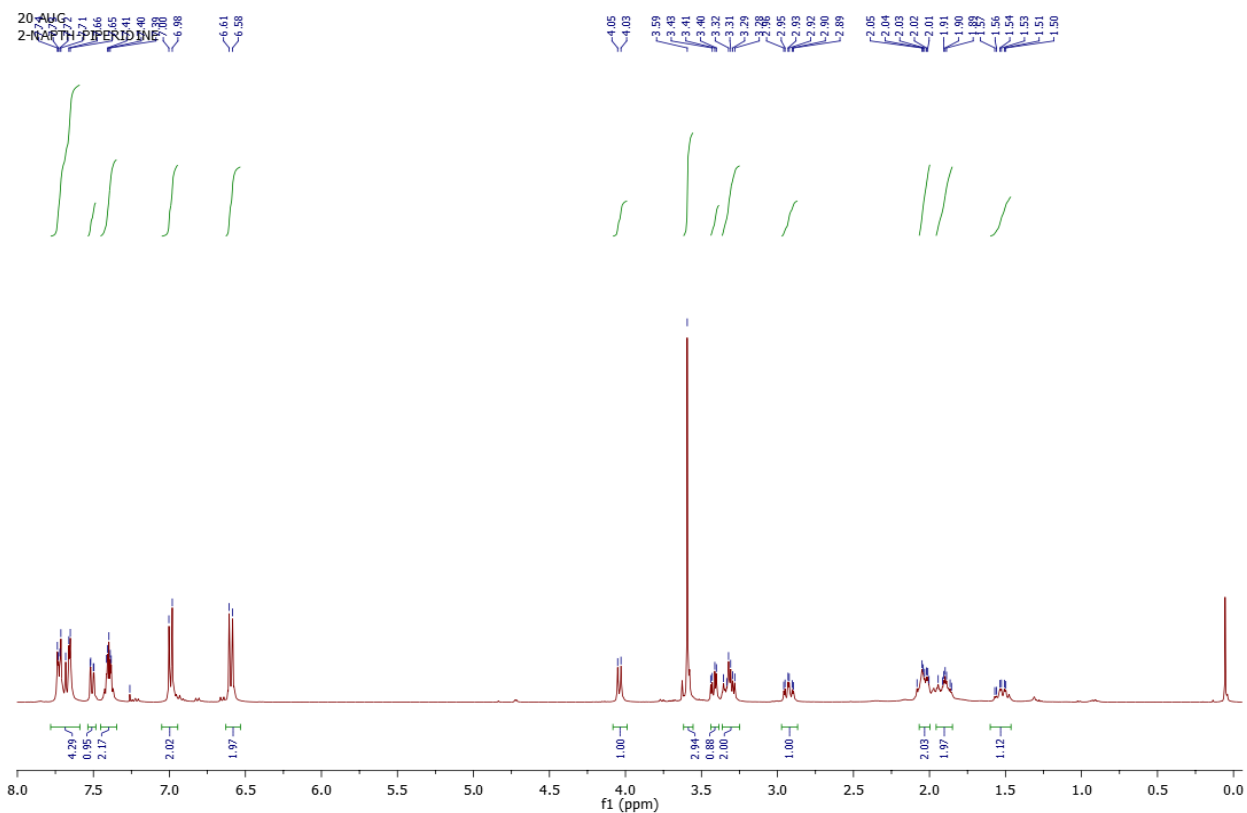
Channel: 2998; Processed Channel: PDA 290.0 nm; Result Id: 1410; Processing Method: 1naphthyl chiral

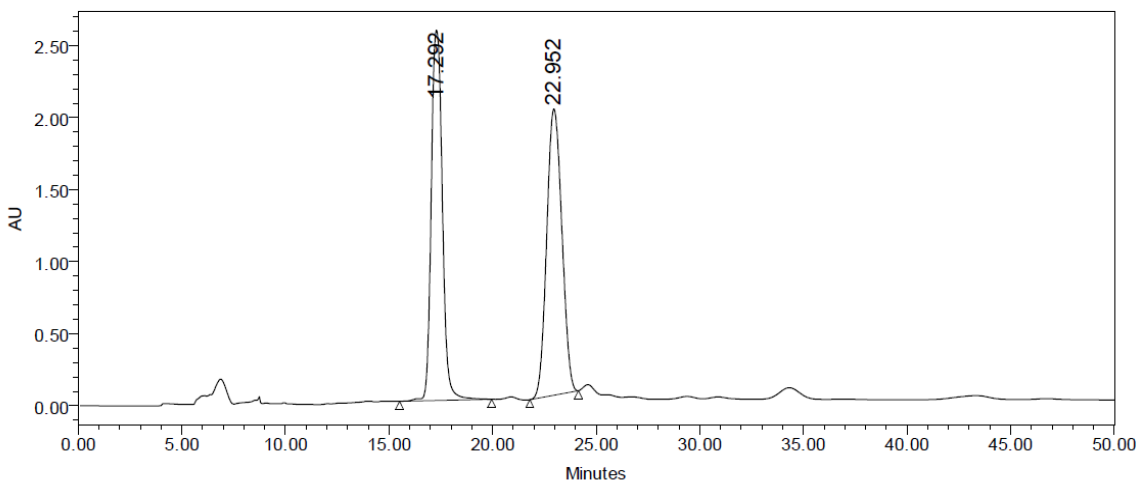
Processed Channel Descr.: PDA 290.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 290.0 nm	16.925	5896654	9.37	218962
2	PDA 290.0 nm	18.265	57024549	90.63	1398623



7q

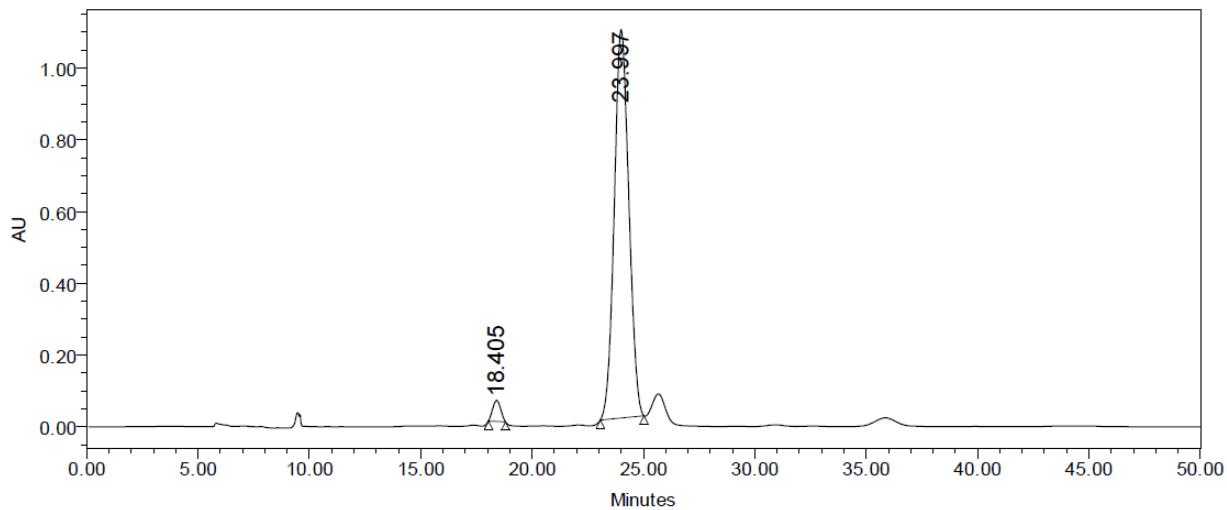




Channel: 2998; Processed Channel: PDA 230.0 nm; Result Id: 1401; Processing Method: 2Naphthyl recemic

Processed Channel Descr.: PDA 230.0 nm

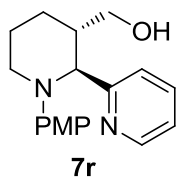
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 230.0 nm	17.292	95518095	48.59	2568272
2	PDA 230.0 nm	22.952	101065210	51.41	1985987



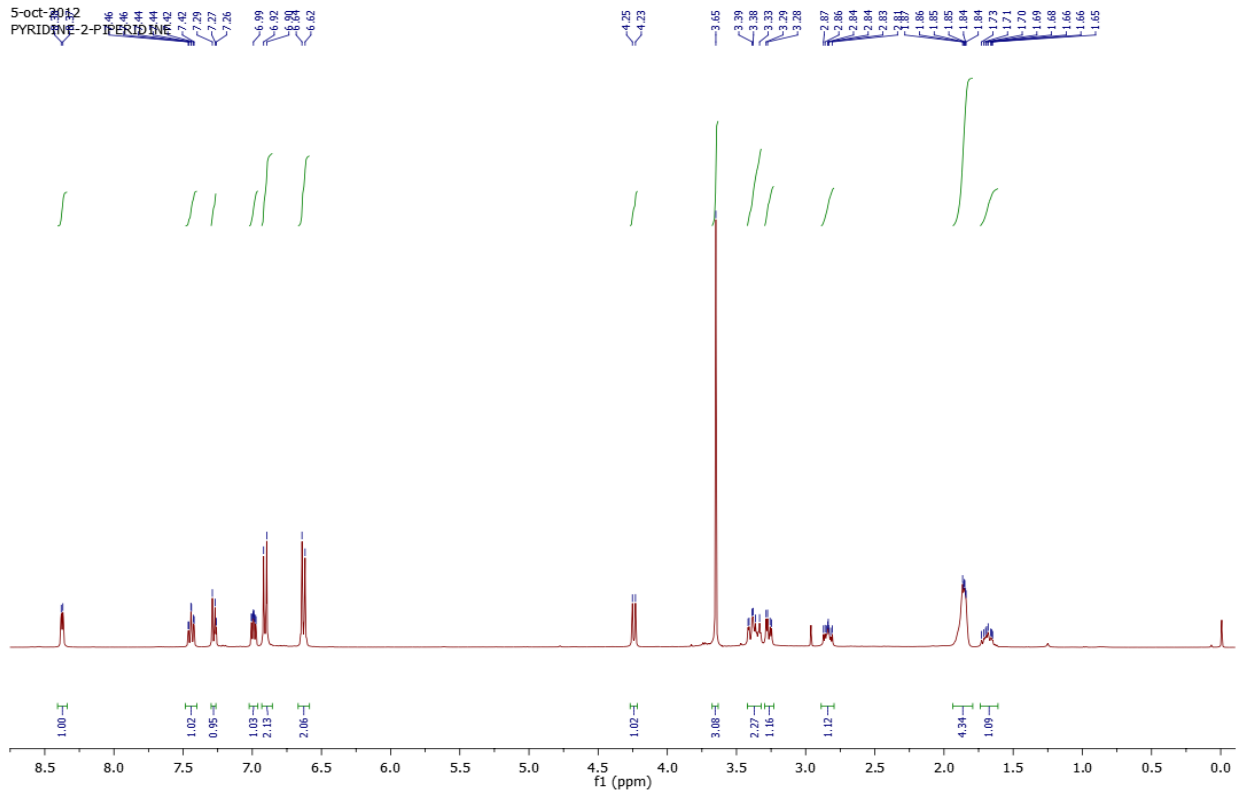
Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1404; Processing Method: 2 naphthyl chiral

Processed Channel Descr.: PDA 250.0 nm

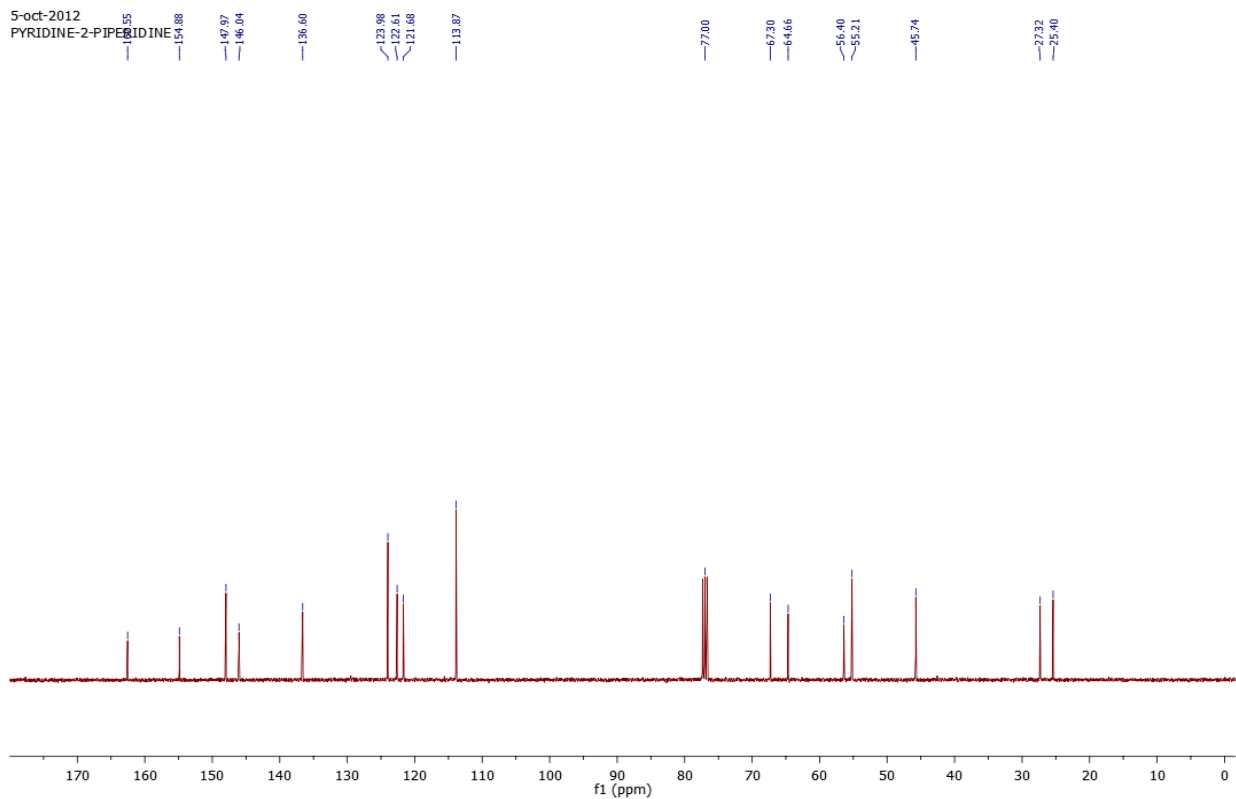
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	18.405	1444392	2.85	58190
2	PDA 250.0 nm	23.997	49201125	97.15	1082335

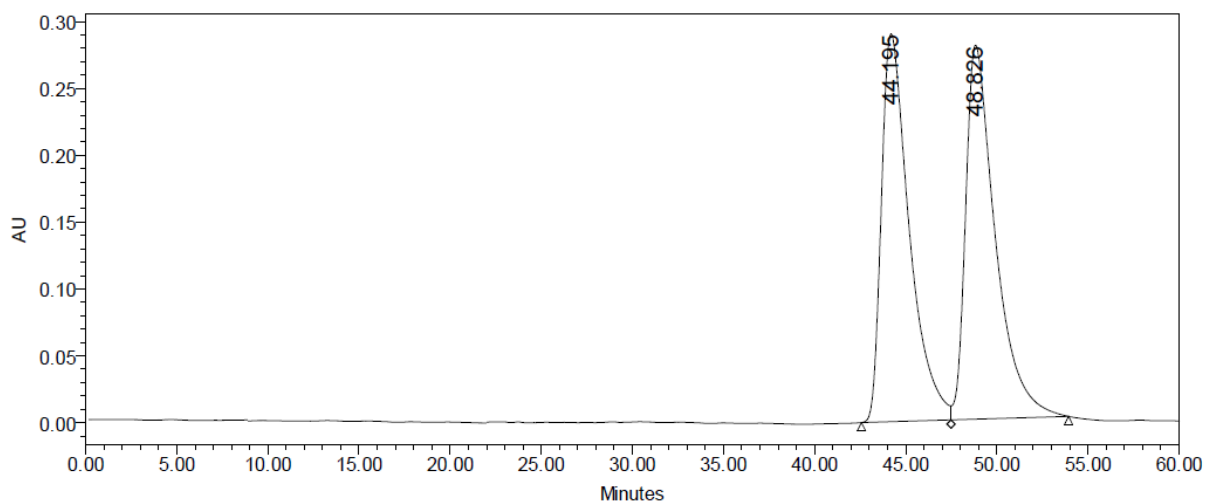


5-oct-2012
PYRIDINE-2-PIPERIDINE



5-oct-2012
PYRIDINE-2-PIPERIDINE

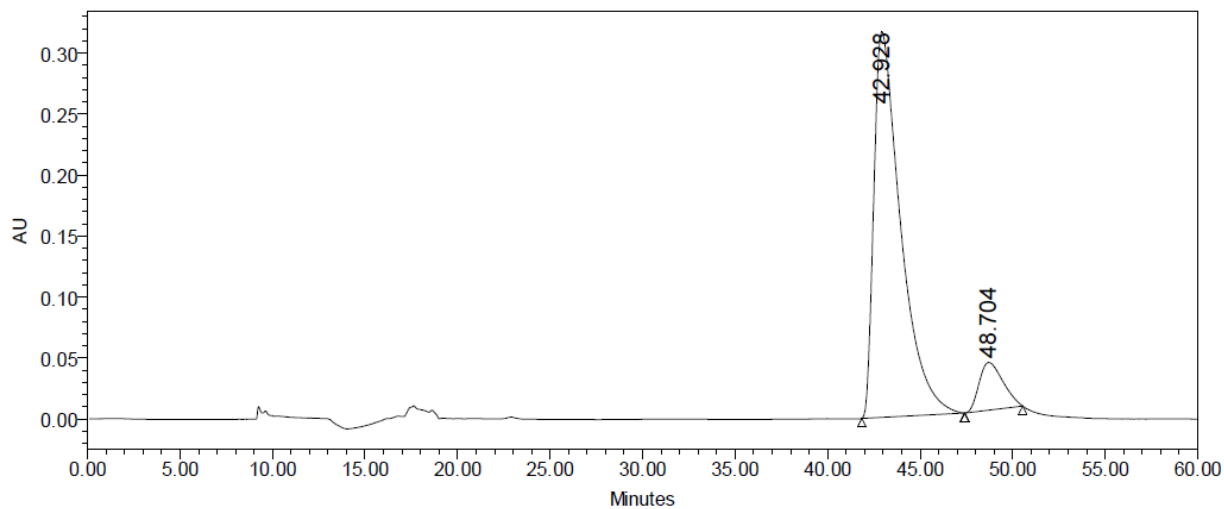




Channel: 2998; Processed Channel: PDA 260.0 nm; Result Id: 1446; Processing Method: 2py recenic

Processed Channel Descr.: PDA 260.0 nm

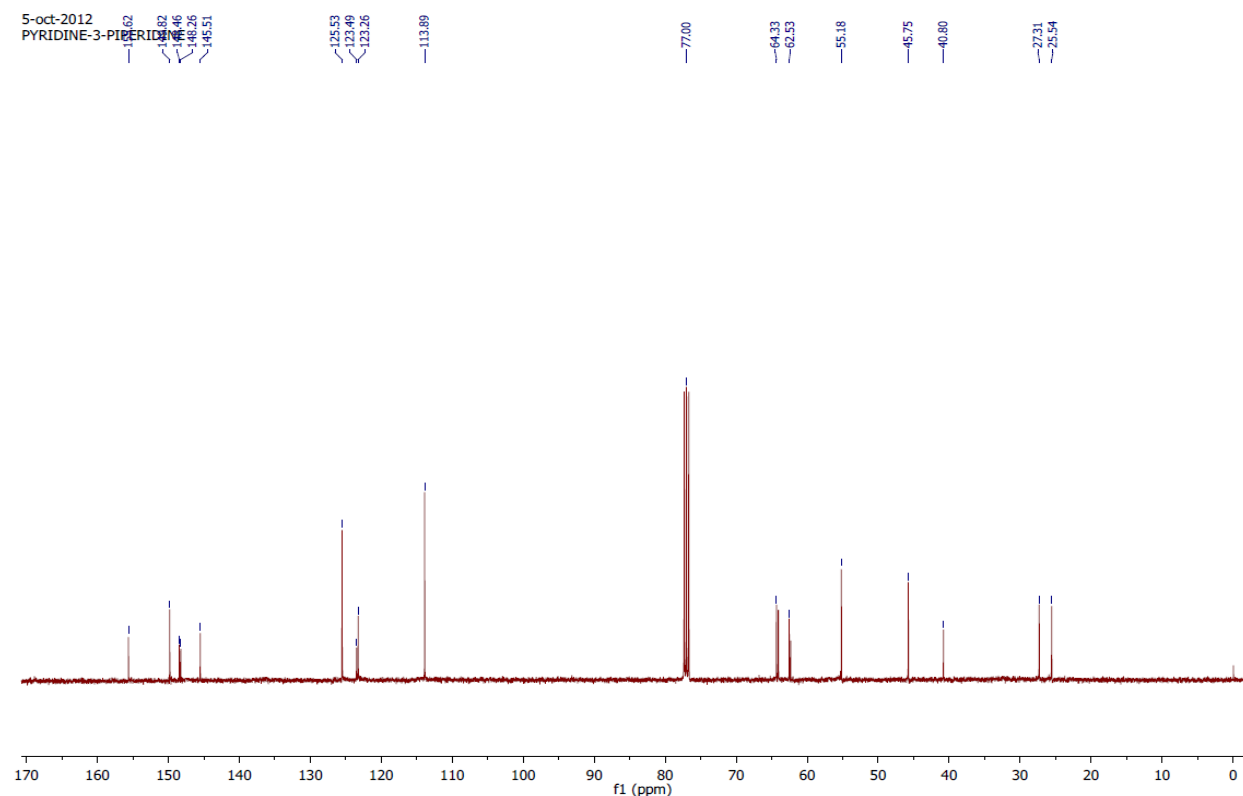
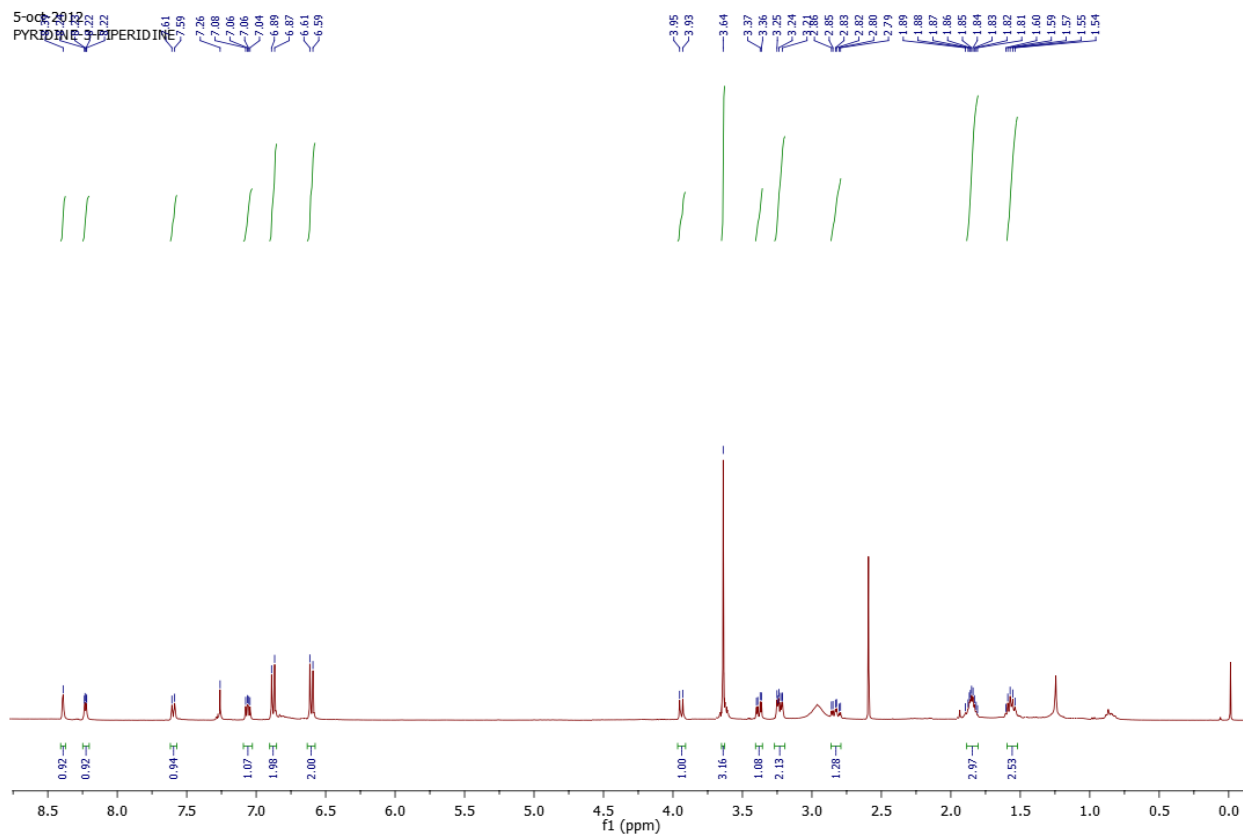
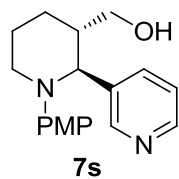
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 260.0 nm	44.195	30800114	49.32	289968
2	PDA 260.0 nm	48.826	31652637	50.68	279761

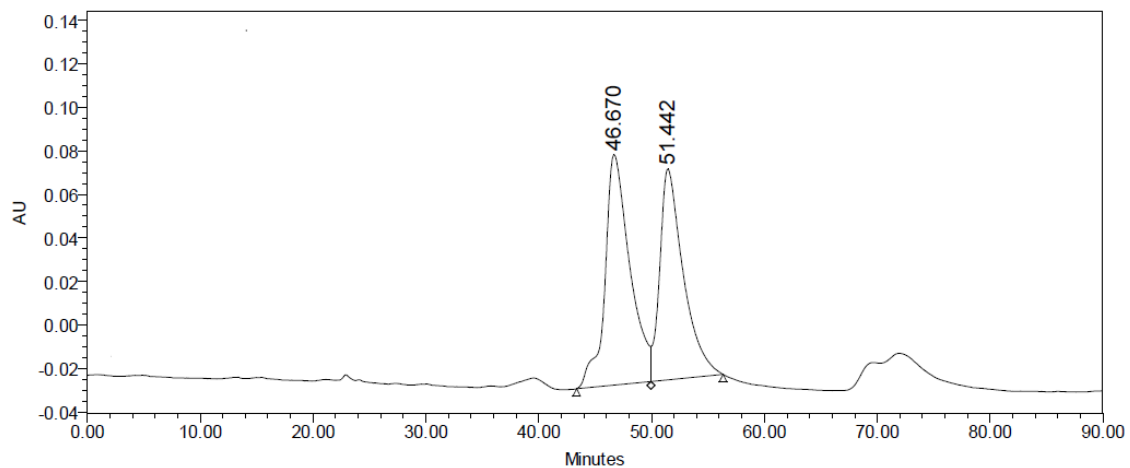


Channel: 2998; Processed Channel: PDA 290.0 nm; Result Id: 1449; Processing Method: 2py chiral

Processed Channel Descr.: PDA 290.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 290.0 nm	42.928	31851581	90.11	316302
2	PDA 290.0 nm	48.704	3497525	9.89	39140

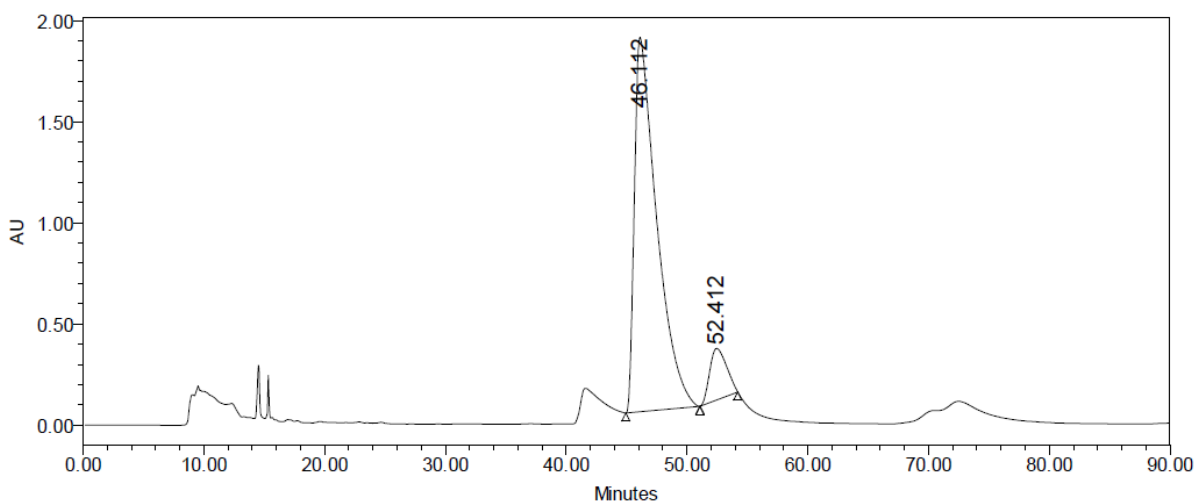




Channel: 2998; Processed Channel: PDA 260.0 nm; Result Id: 1573; Processing Method: 2py receric

Processed Channel Descr.: PDA 260.0 nm

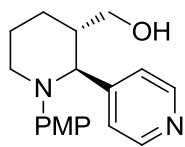
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 260.0 nm	46.670	16280969	53.64	105934
2	PDA 260.0 nm	51.442	14069615	46.36	96924



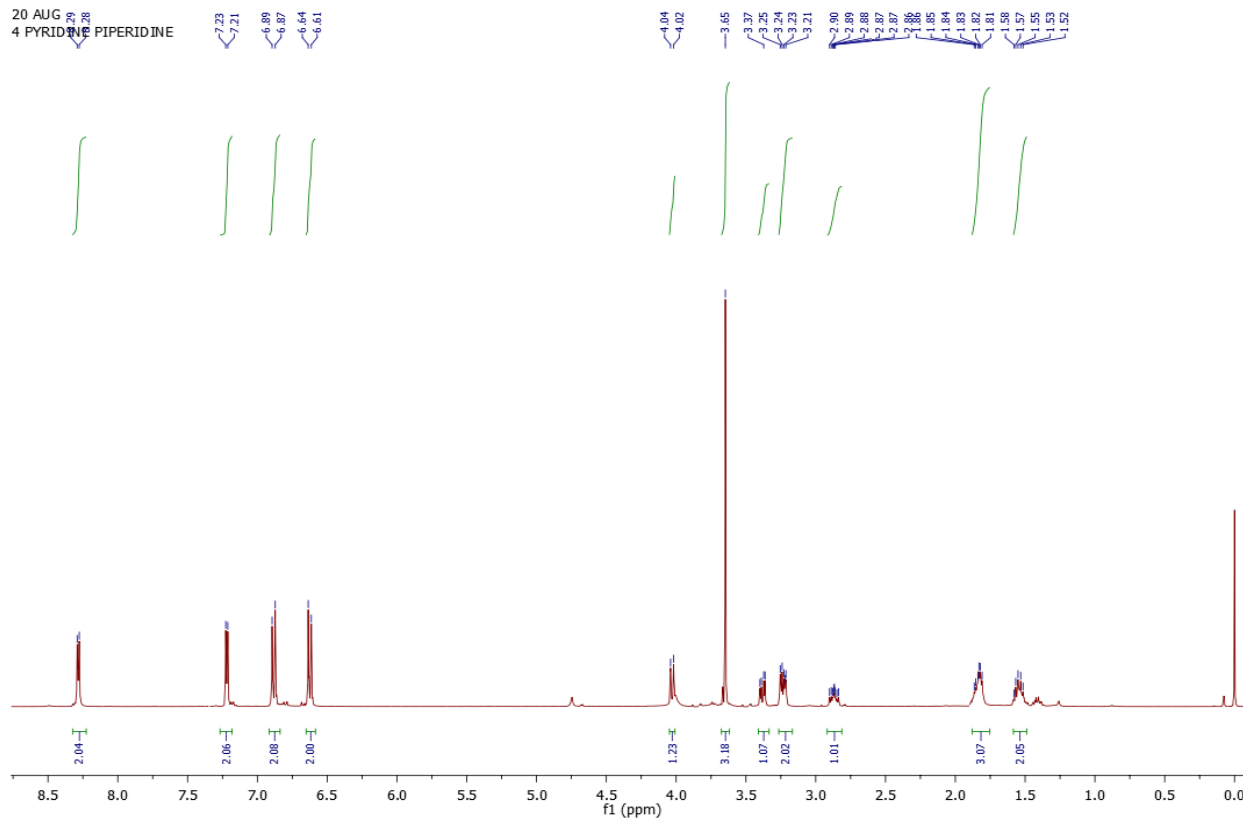
Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1577; Processing Method: 3py chiral

Processed Channel Descr.: PDA 250.0 nm

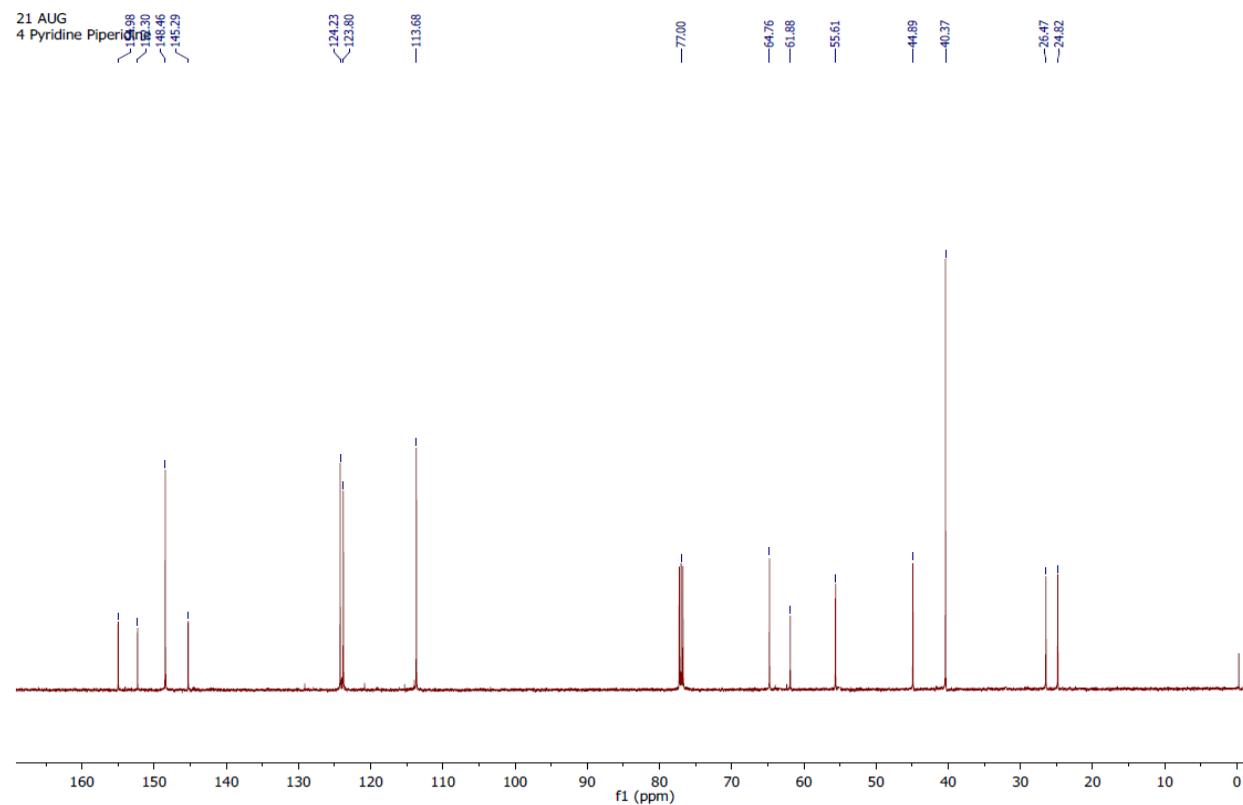
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	46.112	237643292	90.66	1849388
2	PDA 250.0 nm	52.412	24480511	9.34	255082

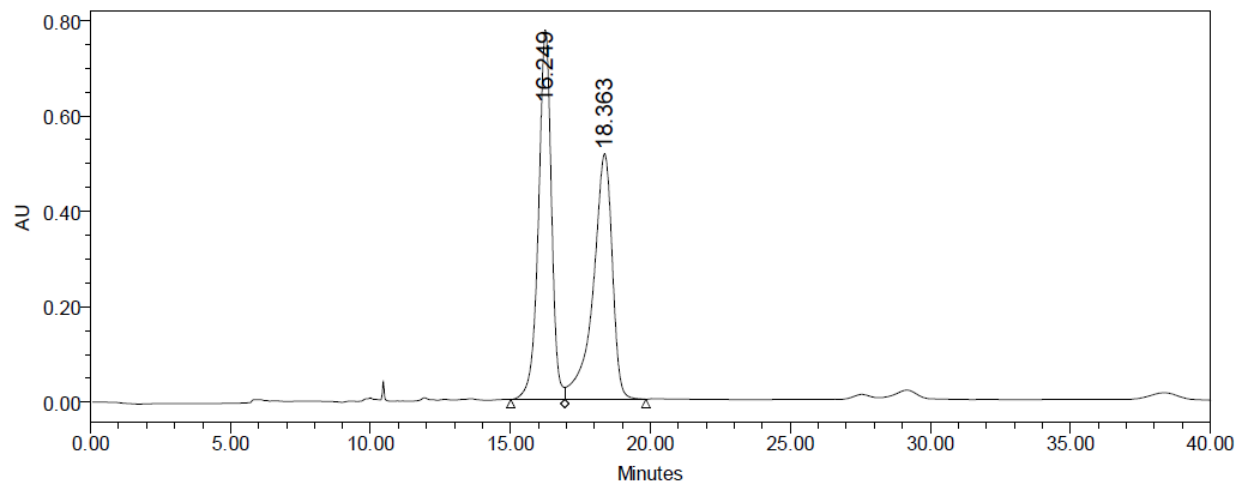


20 AUG
4 PYRIDINE PIPERIDINE



21 AUG
4 Pyridine Piperidine

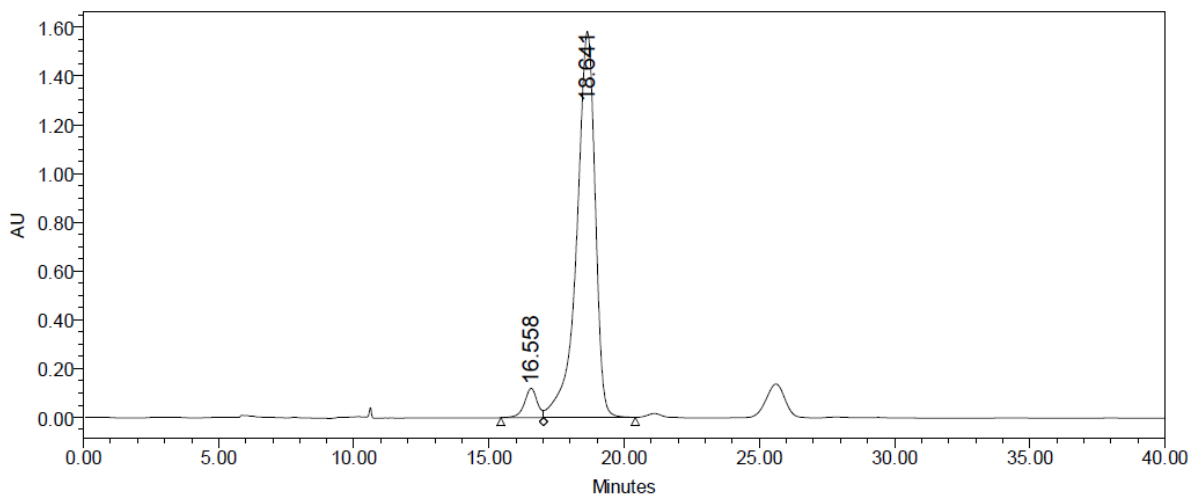




Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 2020; Processing Method: 4py piperidine recemic

Processed Channel Descr.: PDA 250.0 nm

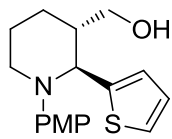
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	16.249	24850155	50.43	774140
2	PDA 250.0 nm	18.363	24425729	49.57	514434



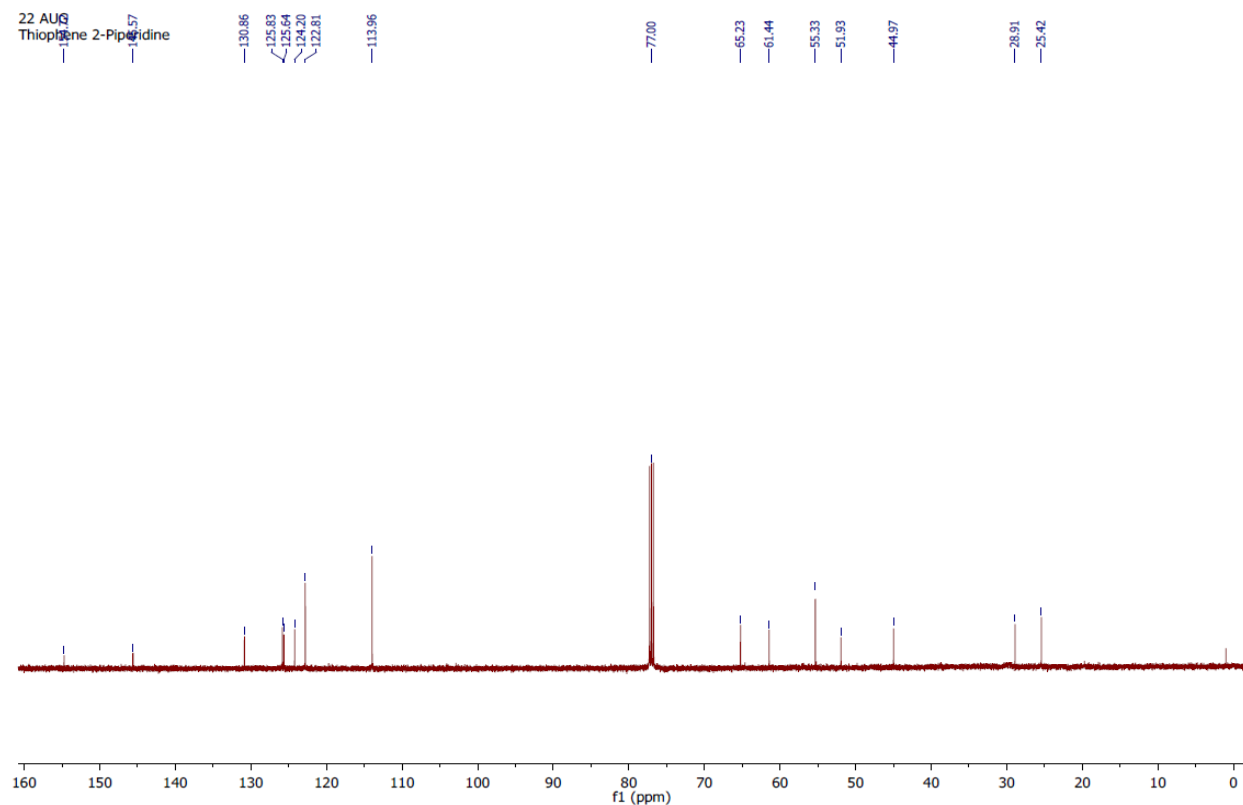
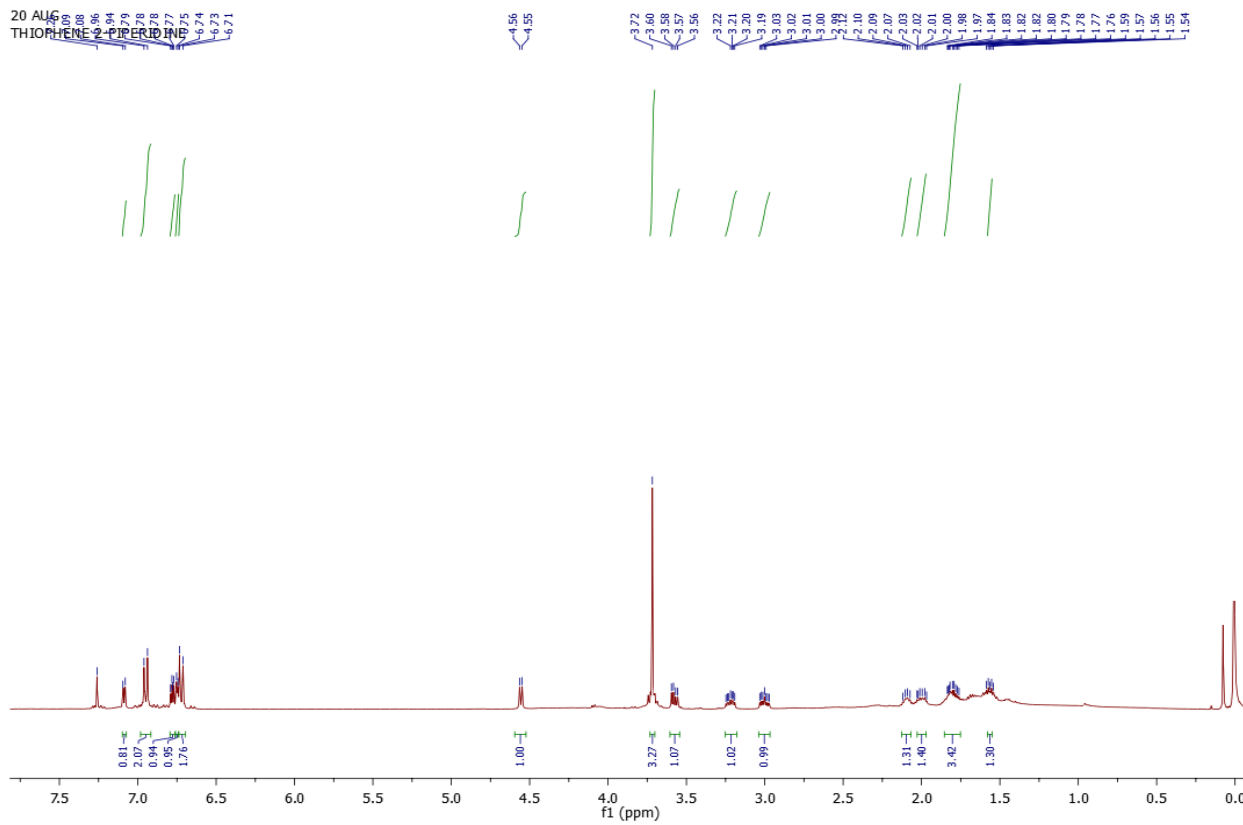
Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1988; Processing Method: 4py piperidin chiral

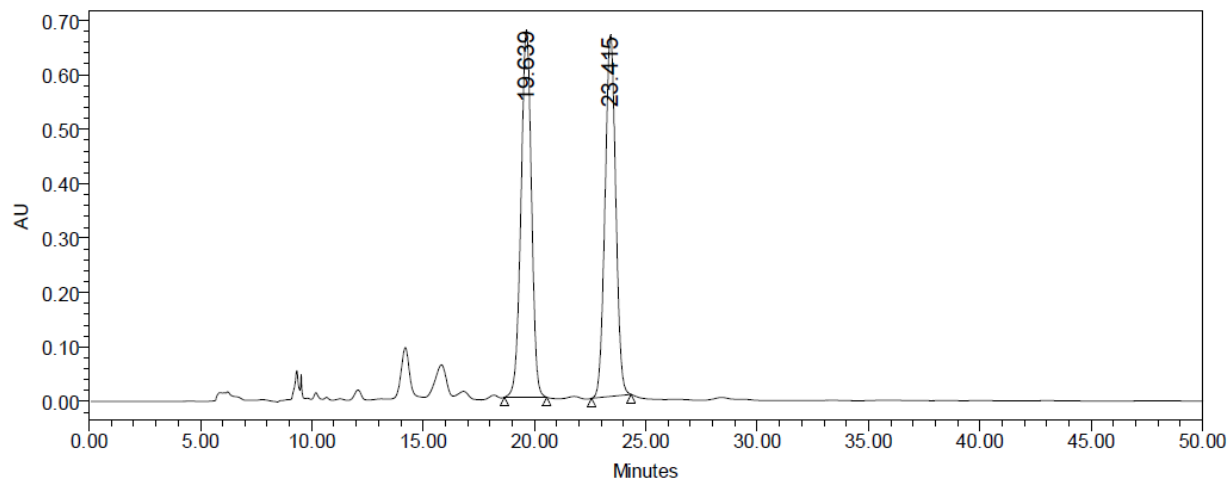
Processed Channel Descr.: PDA 250.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	16.558	3957322	5.00	120007
2	PDA 250.0 nm	18.641	75170557	95.00	1582665



7u

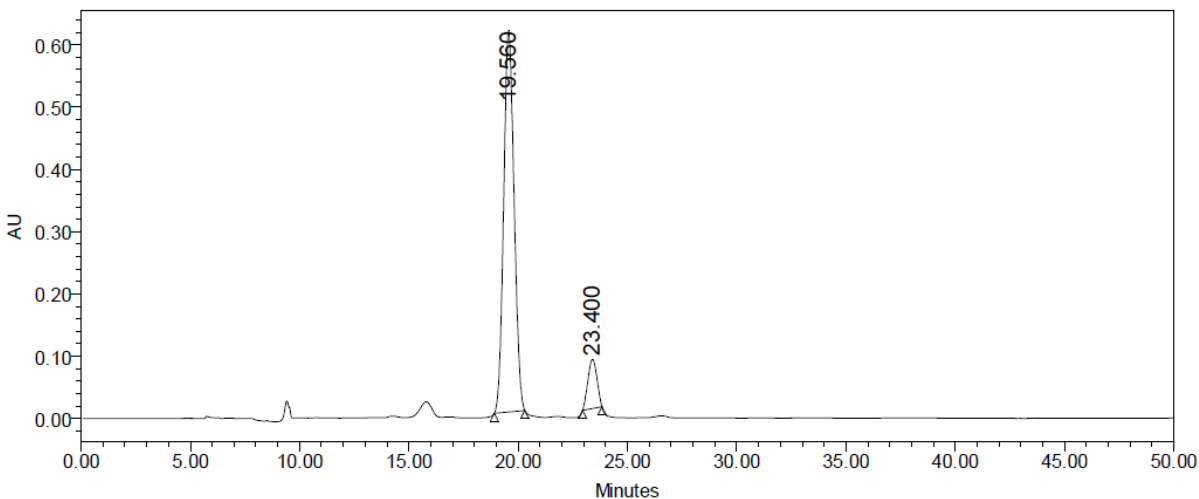




Channel: 2998; Processed Channel: PDA 240.0 nm; Result Id: 1480; Processing Method: Thiophene2 recemic

Processed Channel Descr.: PDA 240.0 nm

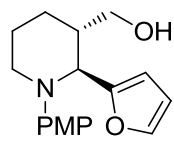
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 240.0 nm	19.639	22050362	49.89	674714
2	PDA 240.0 nm	23.415	22146167	50.11	663999



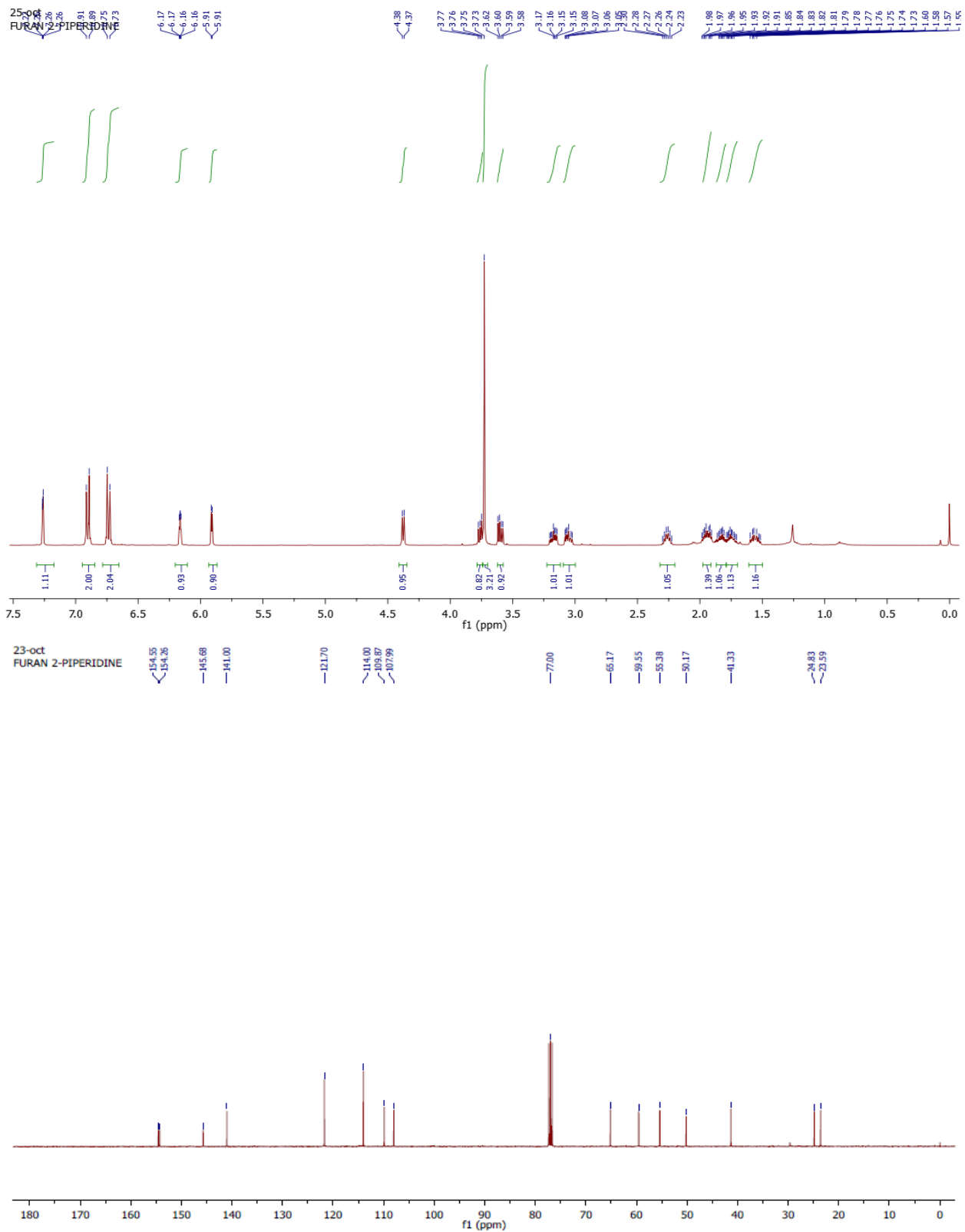
Channel: 2998; Processed Channel: PDA 300.0 nm; Result Id: 1486; Processing Method: Thiophene2 chirall

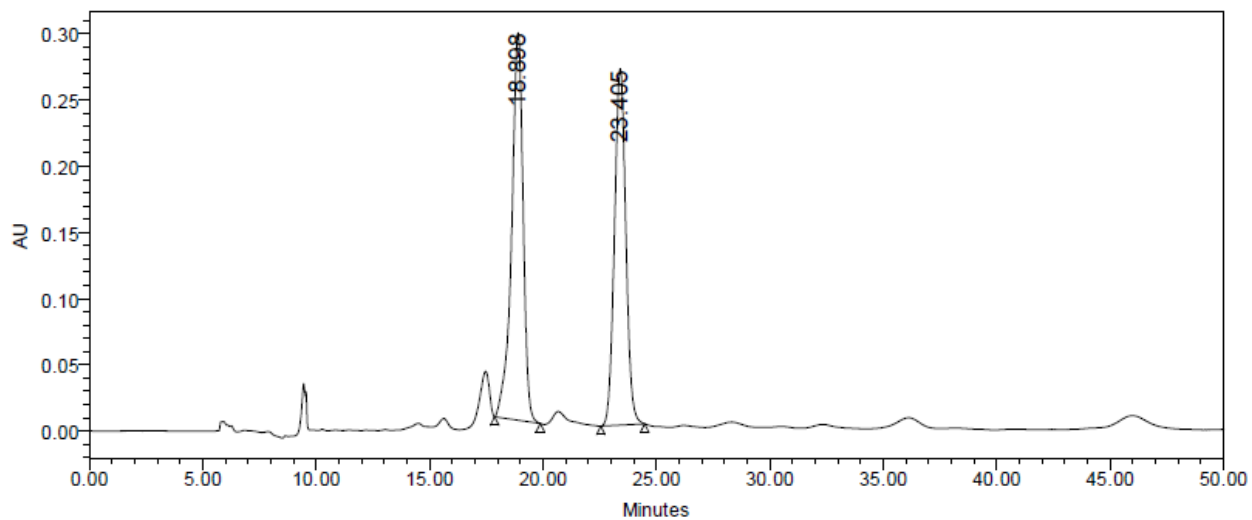
Processed Channel Descr.: PDA 300.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 300.0 nm	19.560	20244667	90.00	612321
2	PDA 300.0 nm	23.400	2249588	10.00	79085



7v

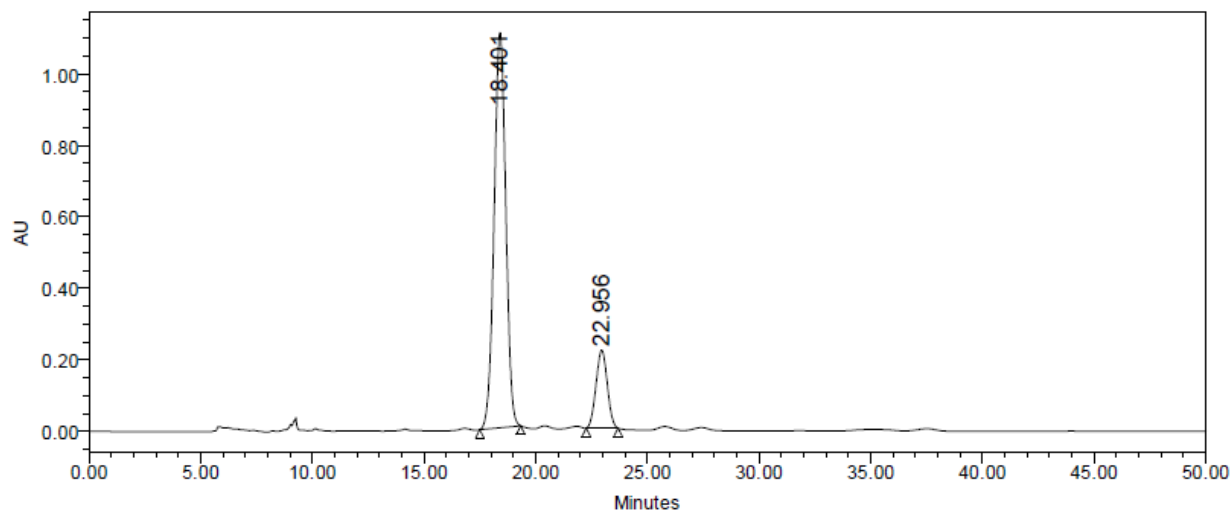




Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1413; Processing Method: furan 2 recemic

Processed Channel Descr.: PDA 250.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	18.898	10325628	52.43	292953
2	PDA 250.0 nm	23.405	9367580	47.57	269428

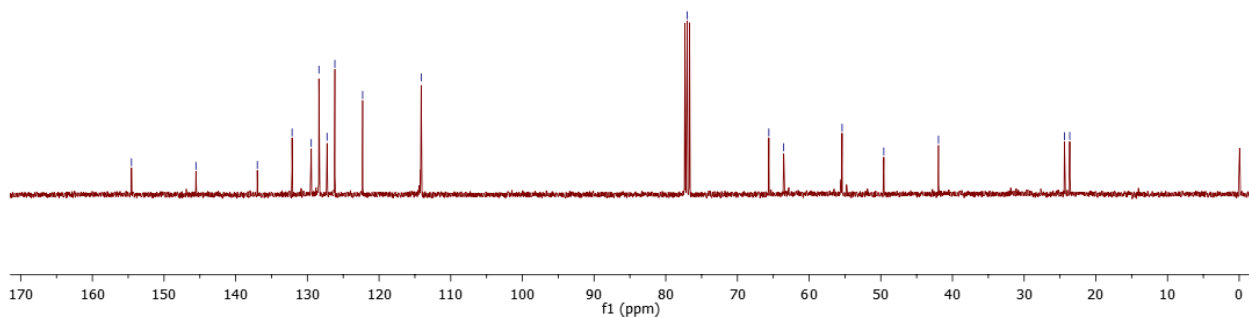
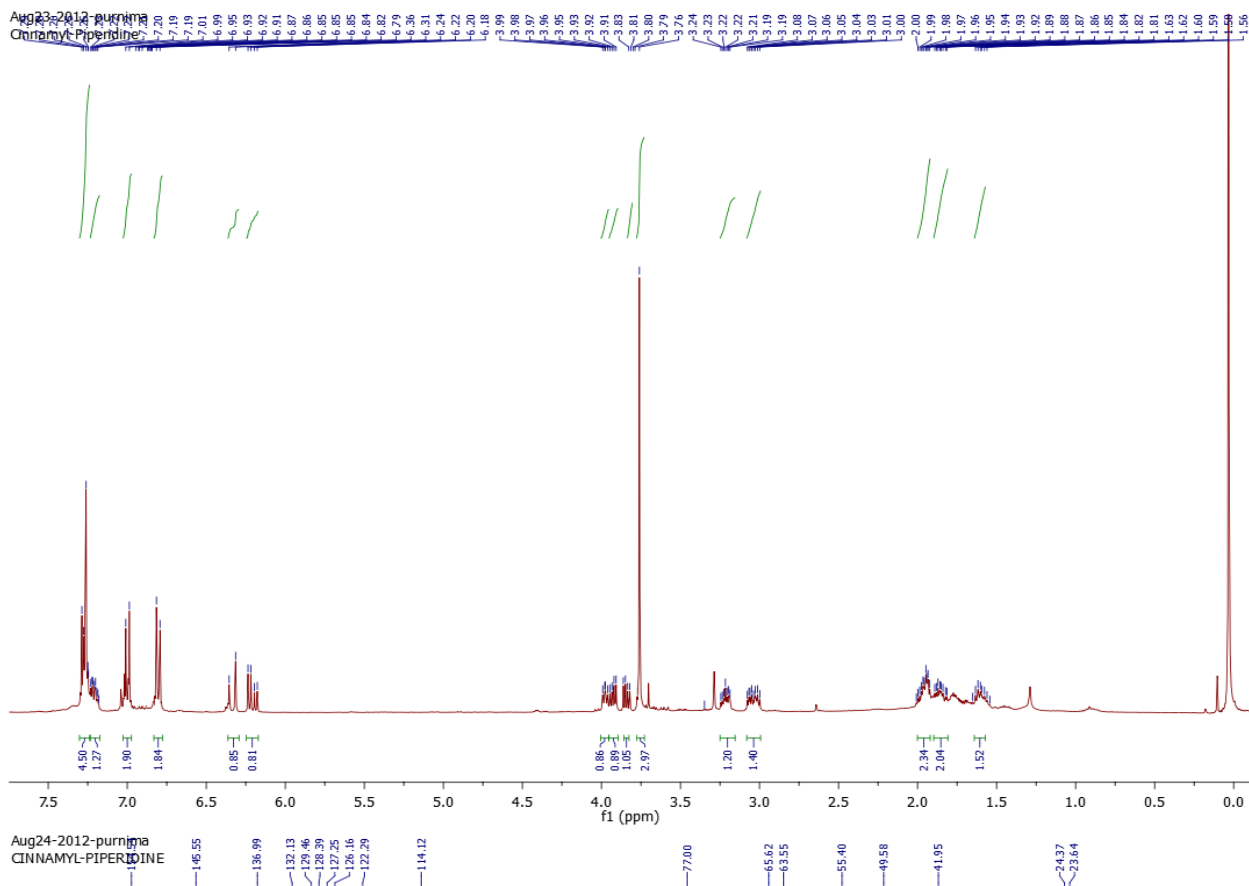
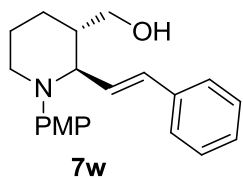


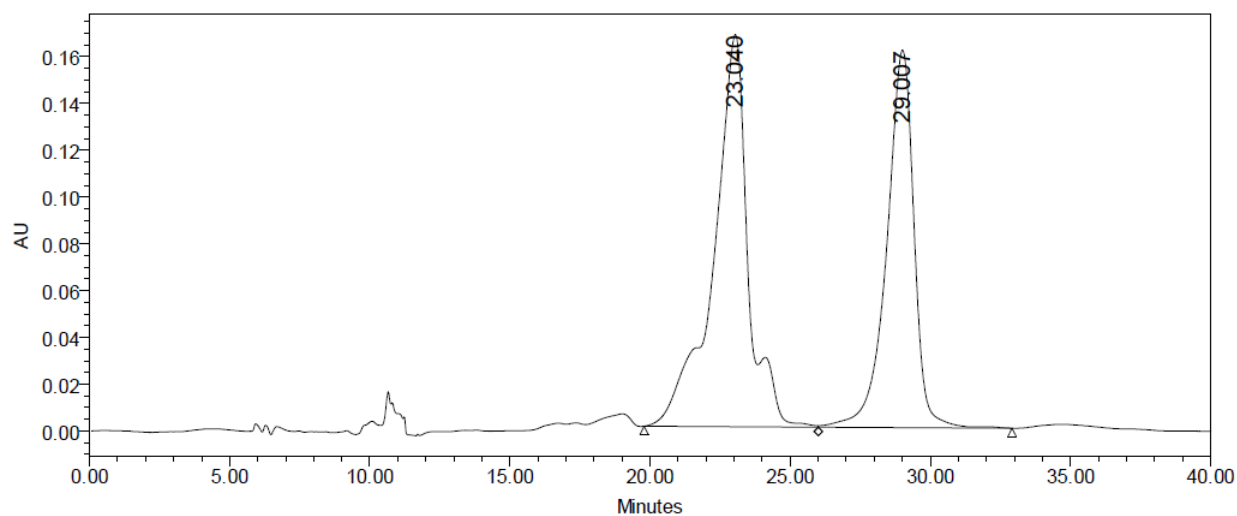
Channel: 2998; Processed Channel: PDA 240.0 nm; Result Id: 1415; Processing Method: furan2 chiral

Processed Channel Descr.: PDA 240.0 nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 240.0 nm	18.401	40034101	84.02	1104735
2	PDA 240.0 nm	22.956	7613589	15.98	217824

21.CINNAMYL PIPERIDINE:

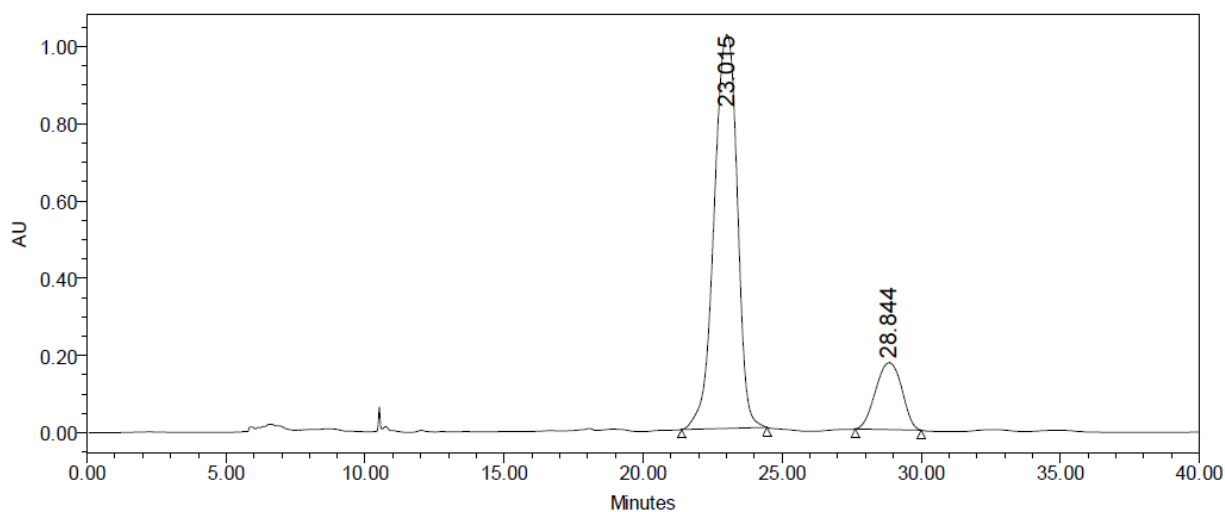




Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1838; Processing Method: cinnamyl recenic

Processed Channel Descr.: PDA 250.0 nm

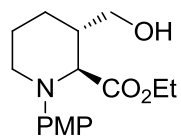
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	23.040	14372094	56.73	167533
2	PDA 250.0 nm	29.007	10961444	43.27	161324



Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1840; Processing Method: cinnamyl chiral

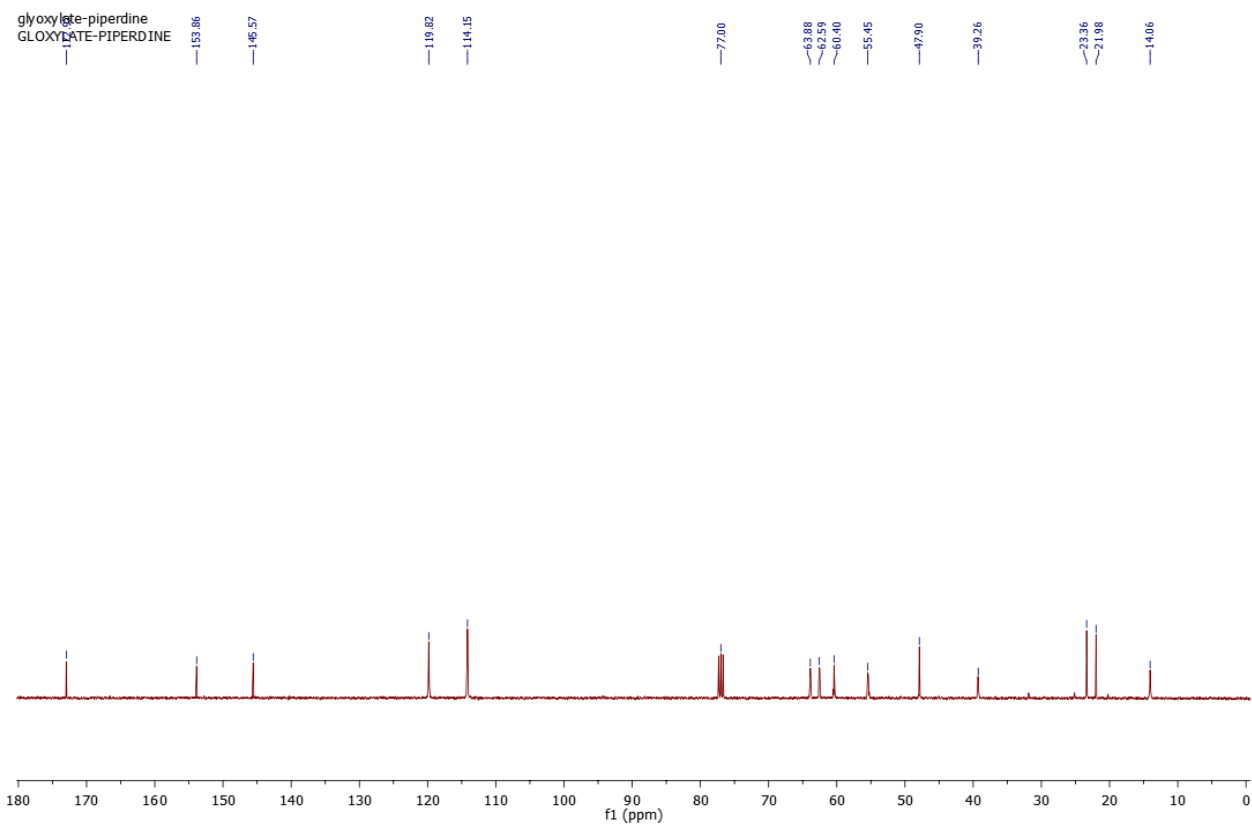
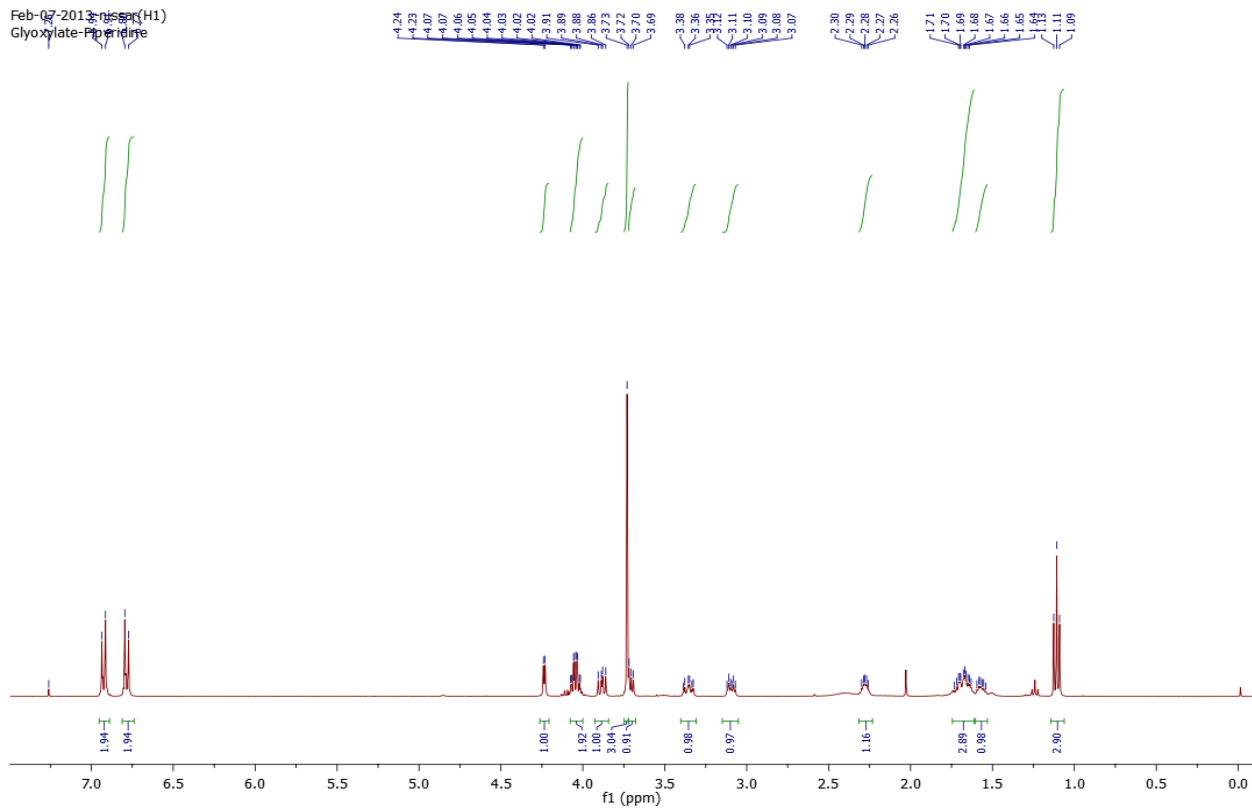
Processed Channel Descr.: PDA 250.0 nm

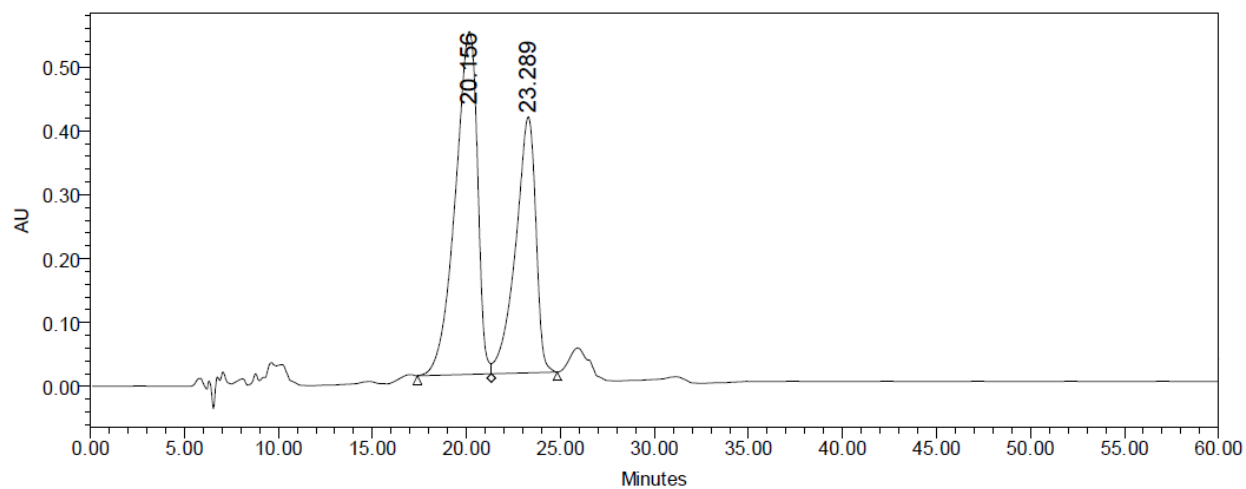
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	23.015	58908533	83.85	1018798
2	PDA 250.0 nm	28.844	11350230	16.15	172832



7x

Feb-07-2013, russan(H1)
Glyoxylate-Piperidine

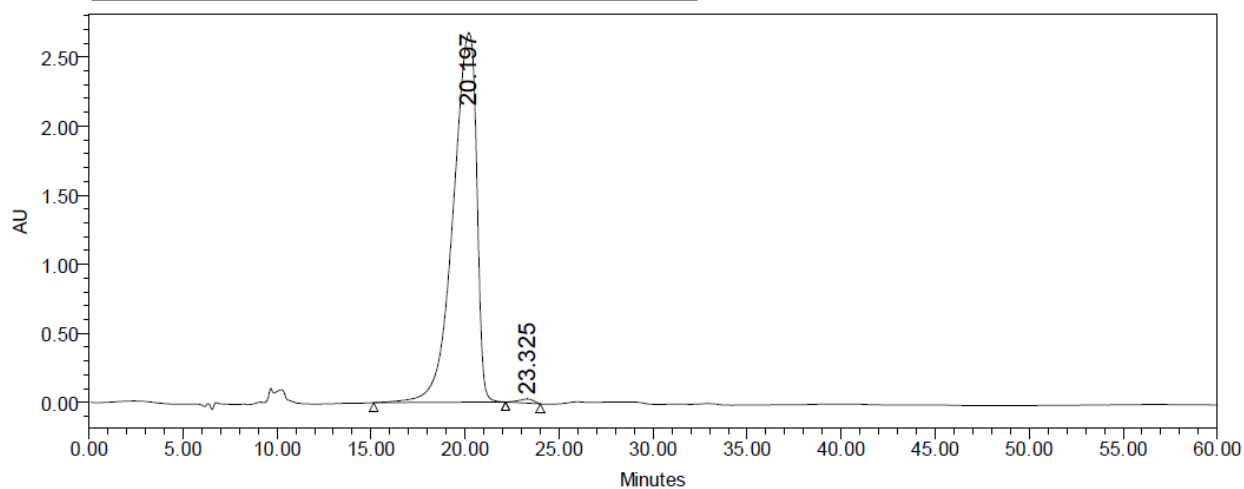




Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1084; Processing Method: glyoxylate pip racemic

Processed Channel Descr.: PDA 250.0 nm

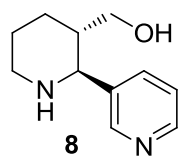
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	20.156	43965044	59.51	536709
2	PDA 250.0 nm	23.289	29917823	40.49	400721



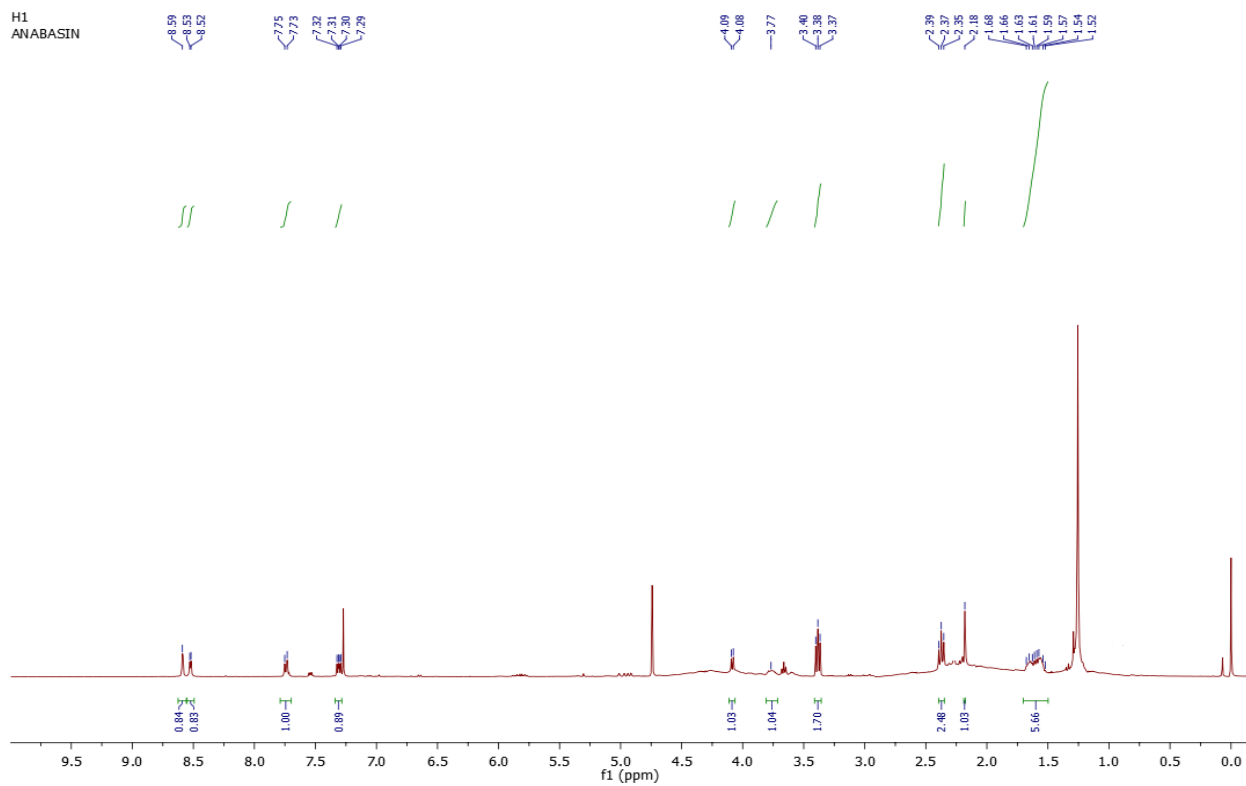
Channel: 2998; Processed Channel: PDA 250.0 nm; Result Id: 1081; Processing Method: glyoxylate pip chiral

Processed Channel Descr.: PDA 250.0 nm

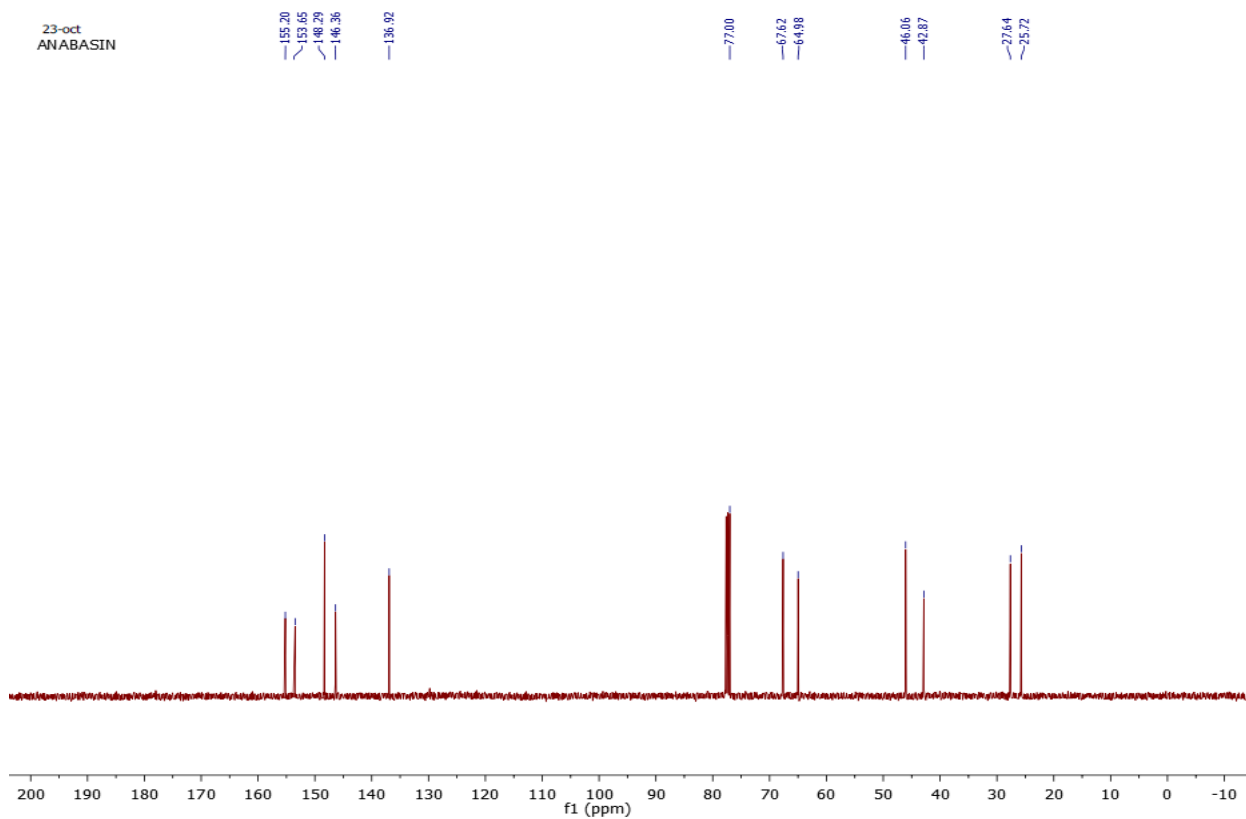
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 250.0 nm	20.197	231798737	99.32	2675270
2	PDA 250.0 nm	23.325	1577481	0.68	28828



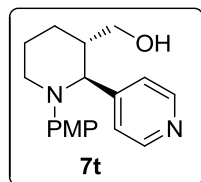
H1
ANABASIN



23-oct
ANABASIN



Crystal structure of ((2*S*, 3*S*)-1-(4-methoxyphenyl)-2-(pyridin-4-yl)piperidin-3-yl)methanol (**7t**):



[CCDC - 930264]

The title compound, ((2*S*, 3*S*)-1-(4-methoxyphenyl)-2-(pyridin-4-yl)piperidin-3-yl)methanol, C₁₈H₂₂N₂O₂, crystallizes in the monoclinic space group P2₁ with the following unit-cell parameters: *a* = 9.1775(2), *b* = 10.7628(2), *c* = 16.9499(5) Å, β = 107.577(2)°, *Z* = 4. The asymmetric unit of the title compound contains two independent molecules. In one molecule, the benzene ring and an attached methoxy group were refined as disordered over two sets of sites in a 0.612(5):0.388(5) ratio. In the same molecule, methanol group is also disordered over two sets of sites in a 0.615(11):0.385(11) ratio. The crystal structure was solved by direct methods using single-crystal X-ray diffraction data collected at room temperature and refined by full-matrix least-squares procedures to a final *R*-value of 0.0526 for 4066 observed reflections.

X-ray intensity data of 46265 reflections (of which 45604 unique) were collected on *X'calibur* CCD area-detector diffractometer equipped with graphite monochromated MoKα radiation (λ = 0.71073 Å). The crystal used for data collection was of dimensions 0.30 x 0.20 x 0.20 mm. The cell dimensions were determined by least-squares fit of angular settings of 19712 reflections in the θ range 3.43 to 29.14°. The intensities were measured by ω scan mode for θ ranges 3.44 to 25.00°. 4066 reflections were treated as observed (*I* > 2σ(*I*)). Data were corrected for Lorentz, polarization and absorption factors. The structure was solved by direct methods using SHELXS97. All non-hydrogen atoms of the molecule were located in the best E-map. Full-matrix least-squares refinement was carried out using SHELXL97. The final refinement cycles converged to an *R* = 0.0526 and *wR* (*F*²) = 0.1239 for the observed data. Residual electron densities ranged from - 0.222 to 0.190 eÅ⁻³. Atomic scattering factors were taken from International Tables for X-ray Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4). The crystallographic data are summarized in Table 1. CCDC - 930264 contains the supplementary crystallographic data for this paper.

Table 1 Crystal and experimental data

CCDC No	930264
Empirical formula	C ₁₈ H ₂₂ N ₂ O ₂

Formula weight	298.38
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2 ₁
Unit cell dimensions :	a= 9.1775(2), b= 10.7628(2), c= 16.9499(5) Å, β = 107.577(2) °
Volume	1596.07(7) Å ³
Z, Calculated density	4, 1.242 Mg/m ³
Absorption coefficient	0.081 mm ⁻¹
F(000)	640
Crystal size	0.30 x 0.20 x 0.20 mm
Theta range for data collection	3.44 to 25.00 °
Limiting indices	-10 ≤ h ≤ 10, -12 ≤ k ≤ 12, -20 ≤ l ≤ 20
Reflections collected / unique	46265 / 5604 [R(int) = 0.0621]
Completeness to theta = 25.00	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.90642
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5604 / 269 / 453
Goodness-of-fit on F ²	1.035
Final R indices [I > 2σ(I)]	R1 = 0.0526, wR2 = 0.1239
R indices (all data)	R1 = 0.0799, wR2 = 0.1359
Measurement	<i>X'calibur system – Oxford diffraction make, U.K.</i>

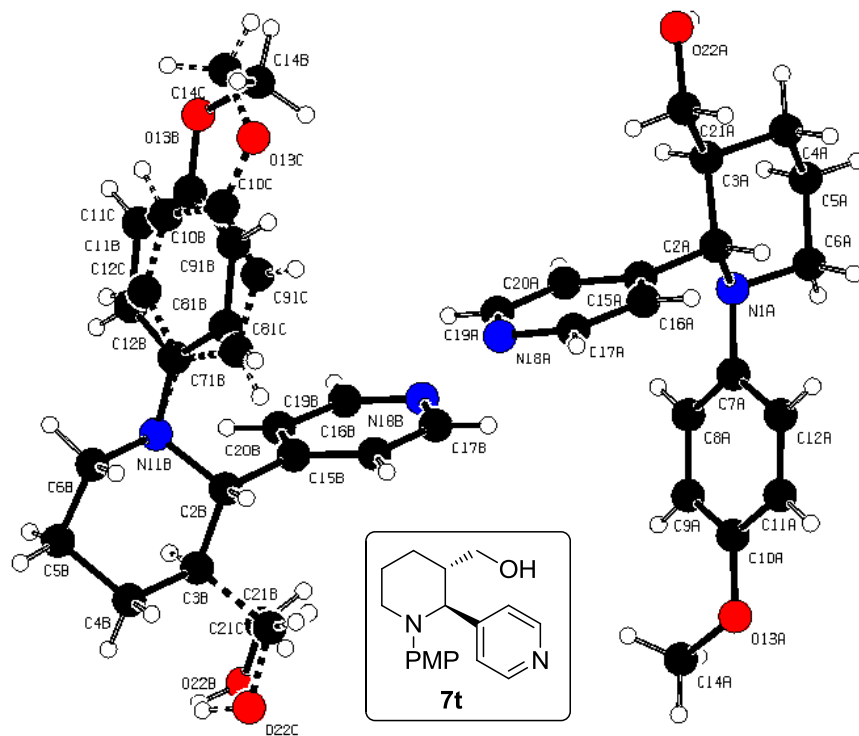


Fig. 1: ORTEP view of the molecule, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

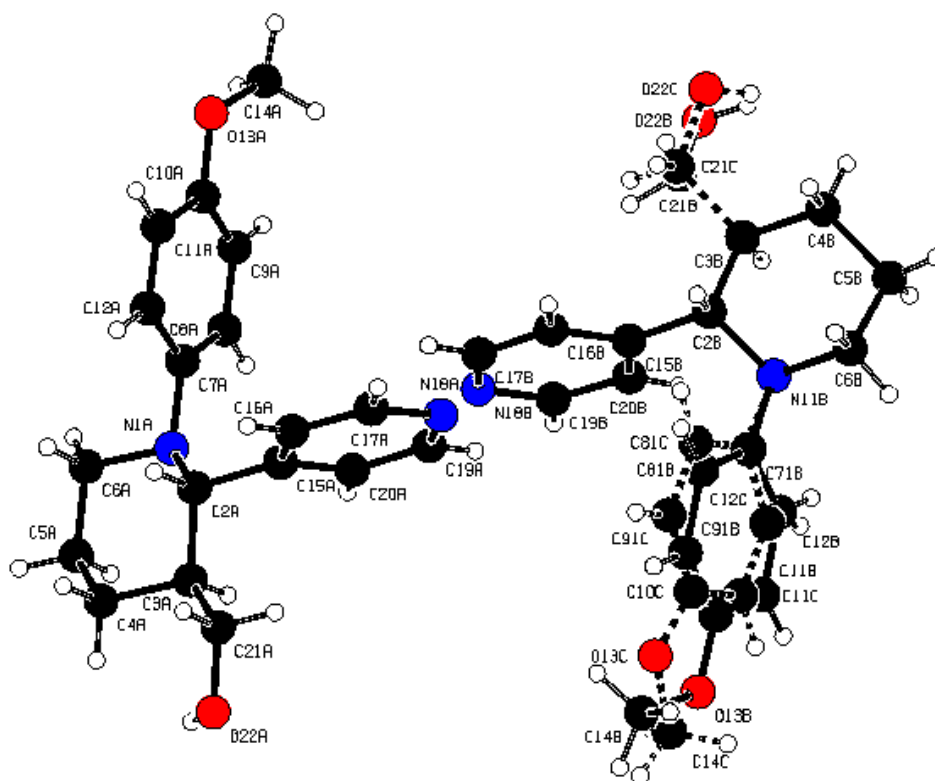


Fig. 2: A view of the molecular structure of (I), with the atomic numbering scheme.

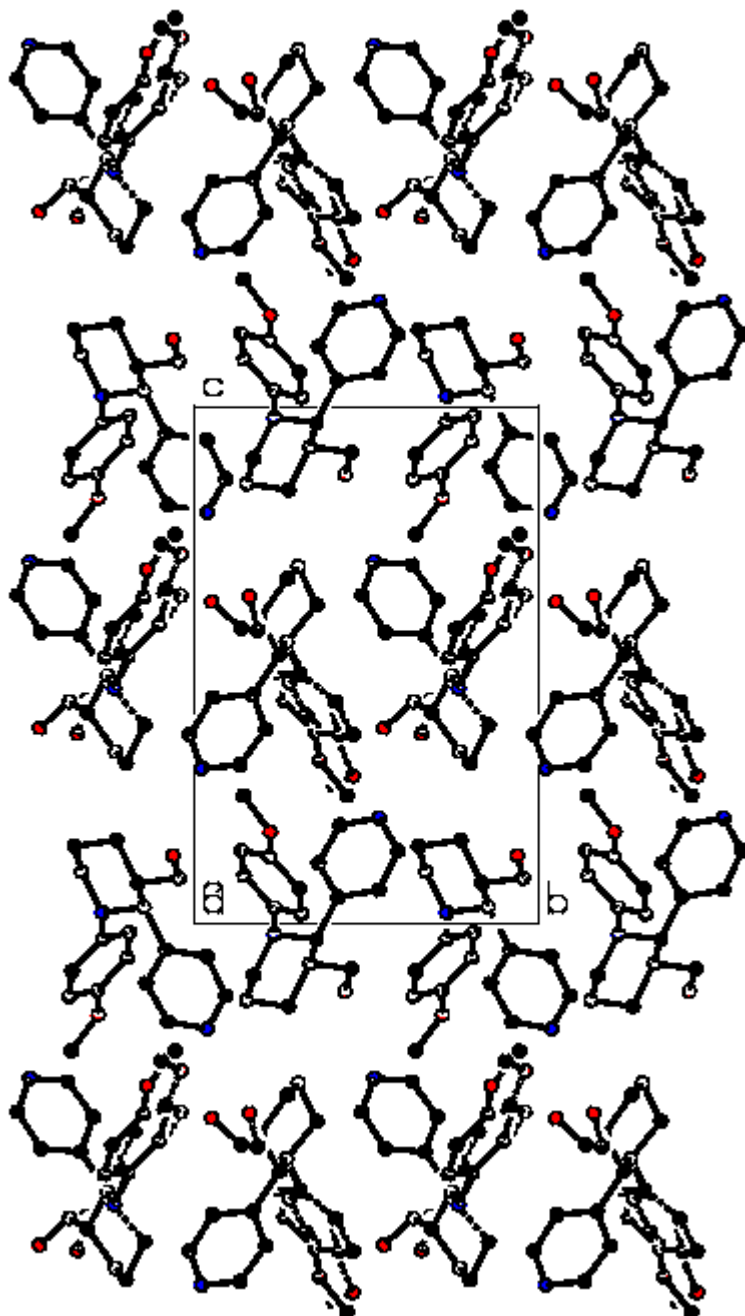


Fig. 3: The packing arrangement of molecules viewed down the a-axis.

CCDC- 930264 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.