# SUPPLEMENTAL INFORMATION

## Additives Promote Noyori Type Reductions of a β-Keto-γ-Lactam: Asymmetric Syntheses of Serotonin Norepinephrine Reuptake Inhibitors

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Dedicated to Professor Philip D. Magnus, F.R.S., The University of Texas at Austin, on the occasion of his 70th birthday

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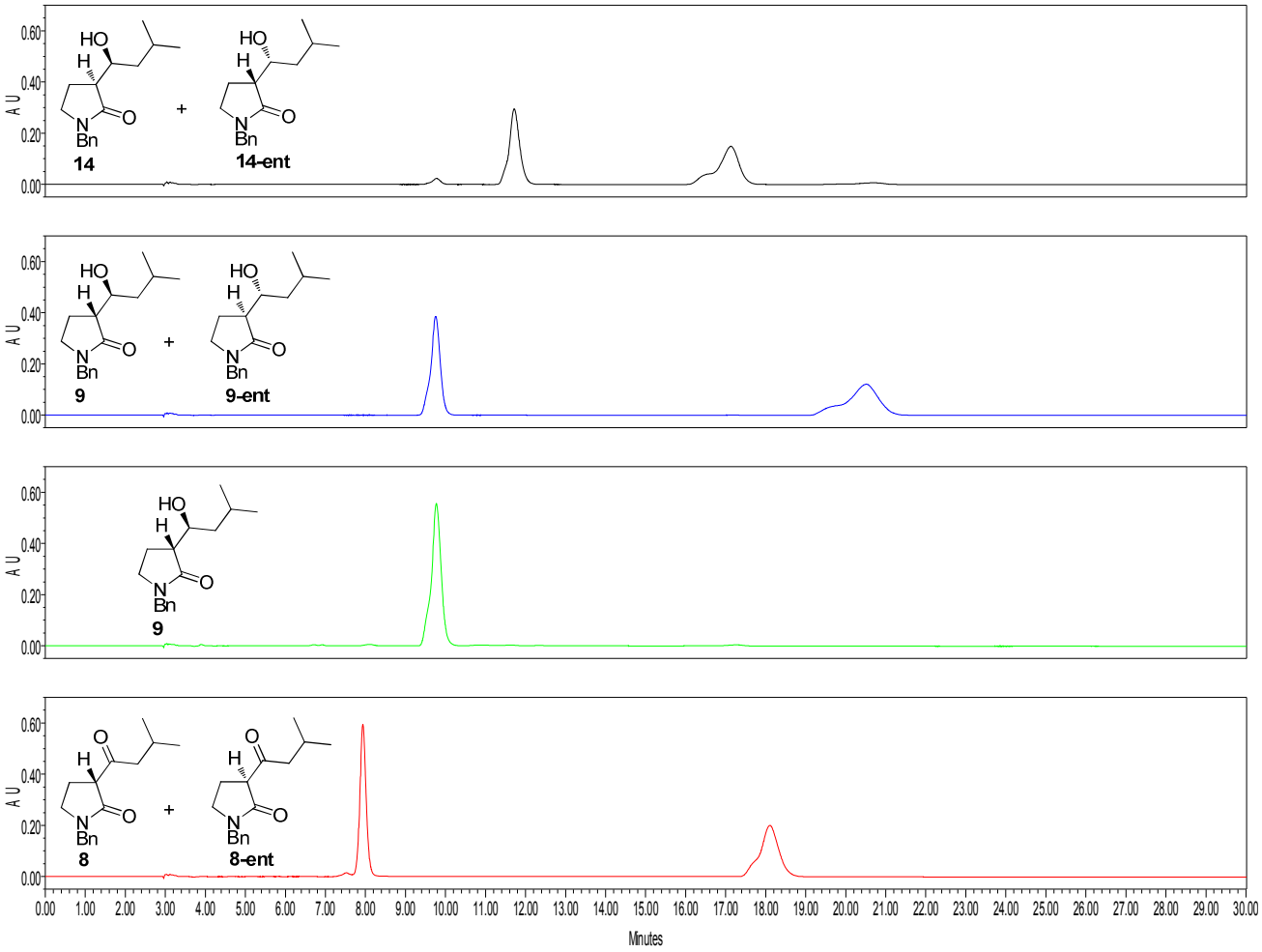
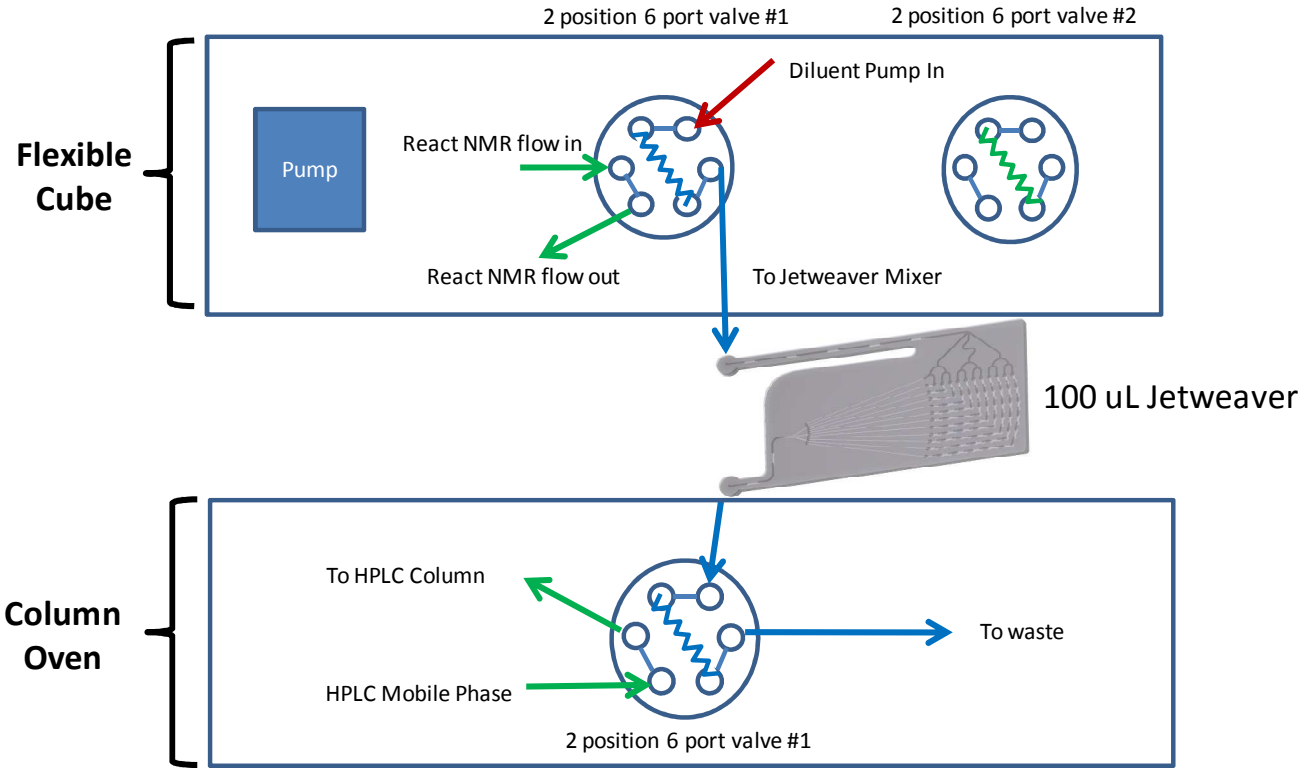
Chiral HPLC method used for all analyses: Column: Chiralpak IA-3, 4.6 x 250 mm 3 µm particle. Mobile Phase: 90/10 Heptane/Ethanol. Sample Prep: 1 mg/mL (v/v) in Ethanol. Flow Rate: 1 mL/min.. Injection Volume: 10 µL. Column Temperature: 25 C. Detection Wavelength: 220 nm.

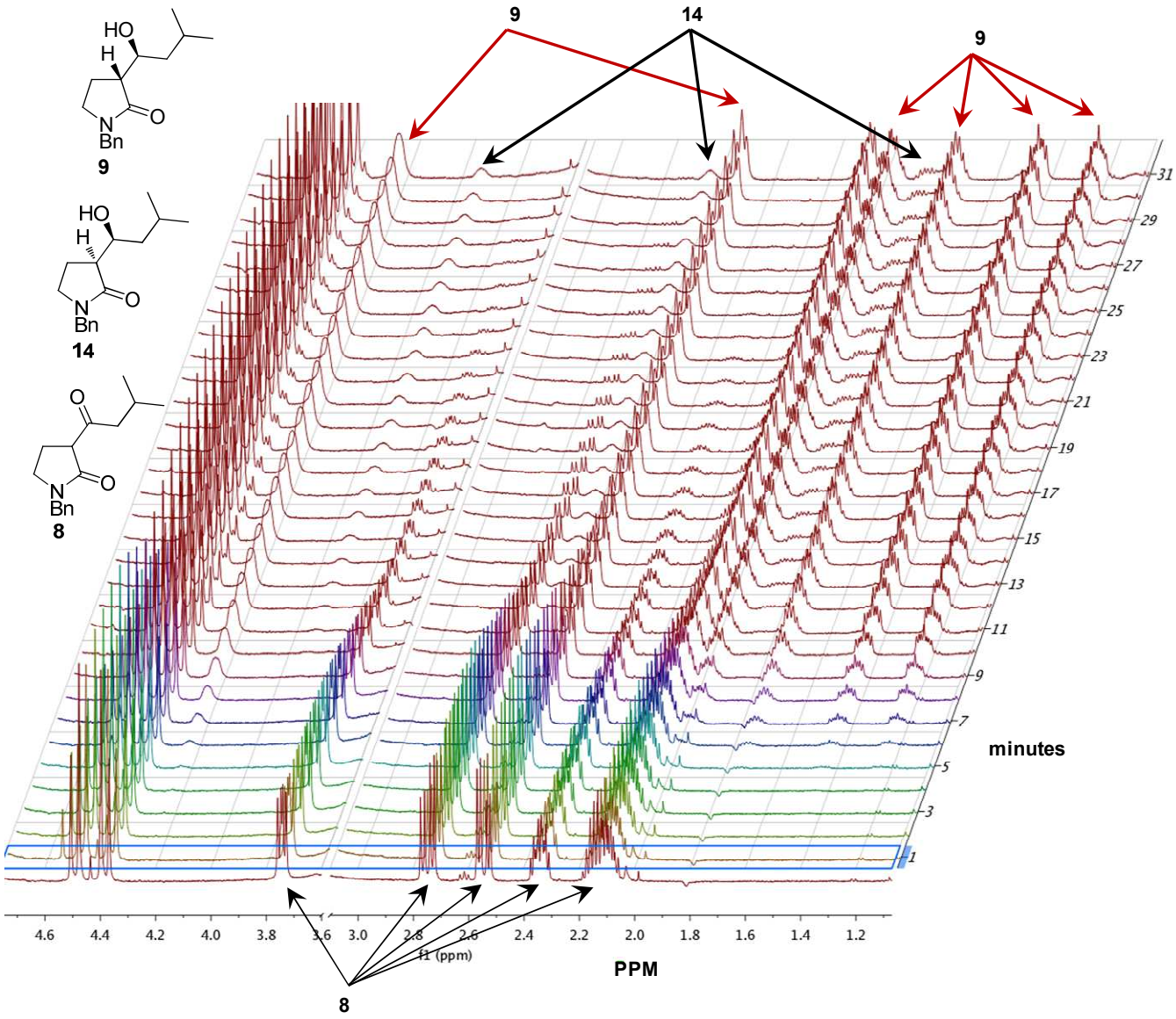



The on-line NMR/HPLC experiments were conducted in a 100-mL Parr reactor. Reaction solution was continuously circulated through both a custom-designed NMR flow cell and a HPLC injection valve module that were in a flow path outside the reactor. The NMR spectrometer was equipped with a broad-band SmartProbe™ was used for continuous $^{1}$HNMR spectral acquisition.

On-line chromatographic analysis of the dynamic kinetic resolution reaction was performed using an HPLC equipped with a Flex Cube module and a second HPLC pump. The Flex Cube module has a 2 position 6 port valve that is plumbed with a 2 µL loop to enable the reaction to flow through the valve. When the valve is actuated the loop is switched from the reaction flow path into the flow path of a

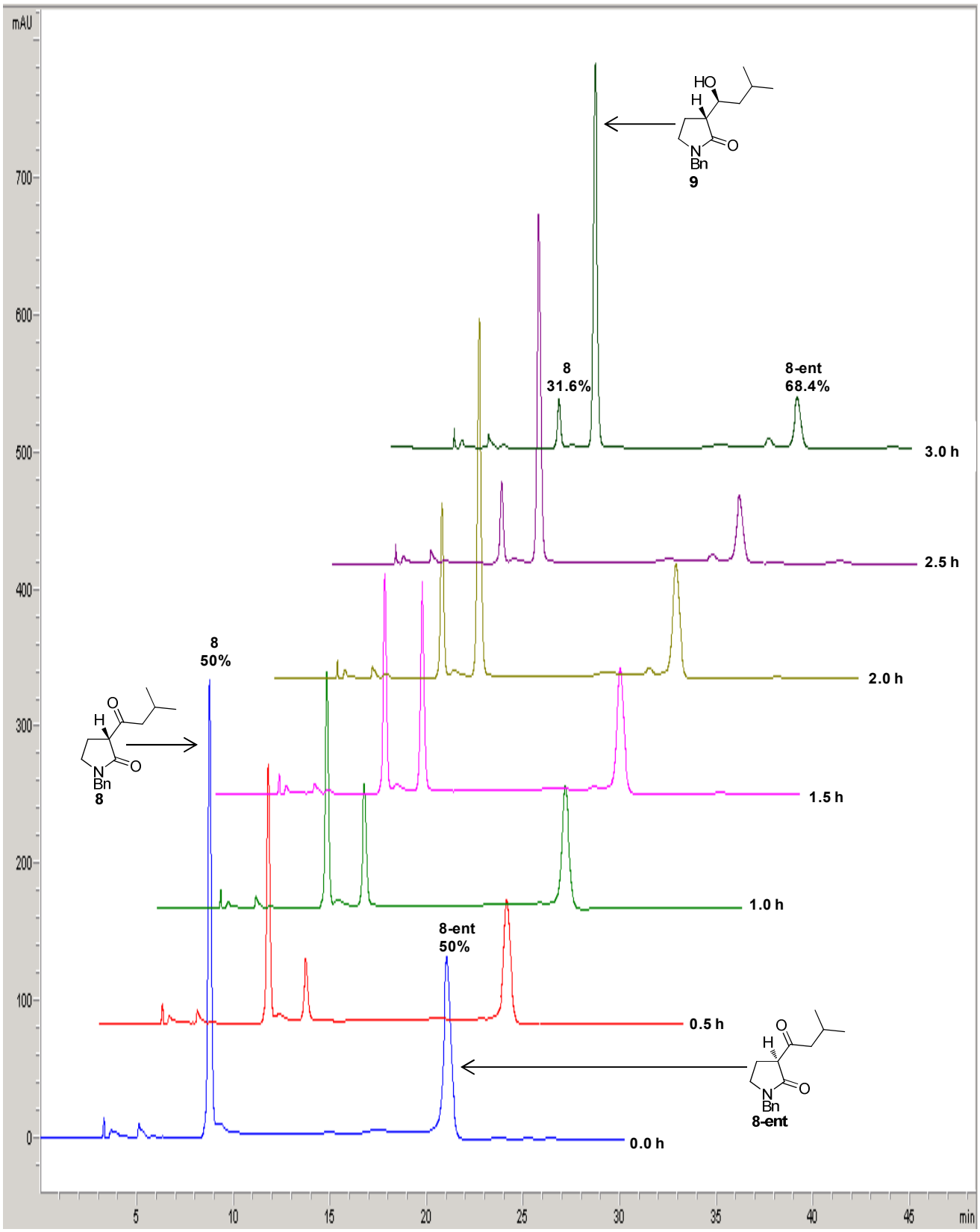
second HPLC pump. The loop is swept into a microfluidic mixer (100 µL volume) where the 2 µL process sample is diluted. The diluted process sample is swept to a second 2 position 6 port valve contained within the column thermostat compartment. This valve is plumbed with a 10 µL loop and it serves as the injector valve for the HPLC. When the second valve is actuated the 10 µL loop is in the flow path of the first HPLC pump and the contents are swept onto the HPLC column.






**DKR-hydrogenation analyzed by on-line $^{1}$HNMR**

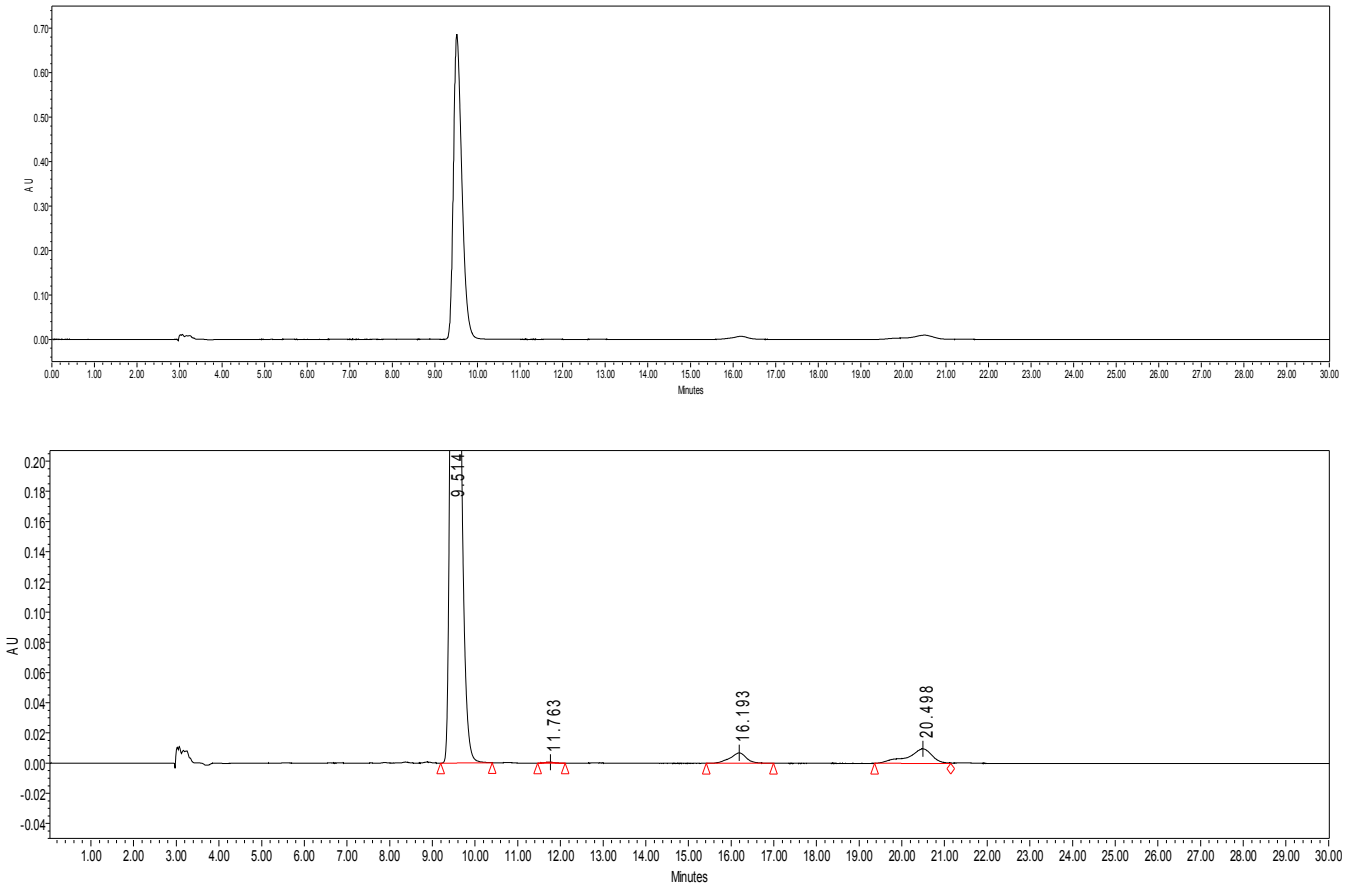
**8**/MeOH/HCl (3 mol%)/ $Ru(OAc)_2$[(*S*)-BINAP)] (170 S/C)/$H_2$ (70 psi)/65 °C.




## DKR-hydrogenation analyzed by on-line chiral HPLC

**8**/MeOH/HCl (3 mol%)/ $Ru(OAc)_2$[(*S*)-BINAP)] (170 S/C)/$H_2$ (70 psi)/40 °C.

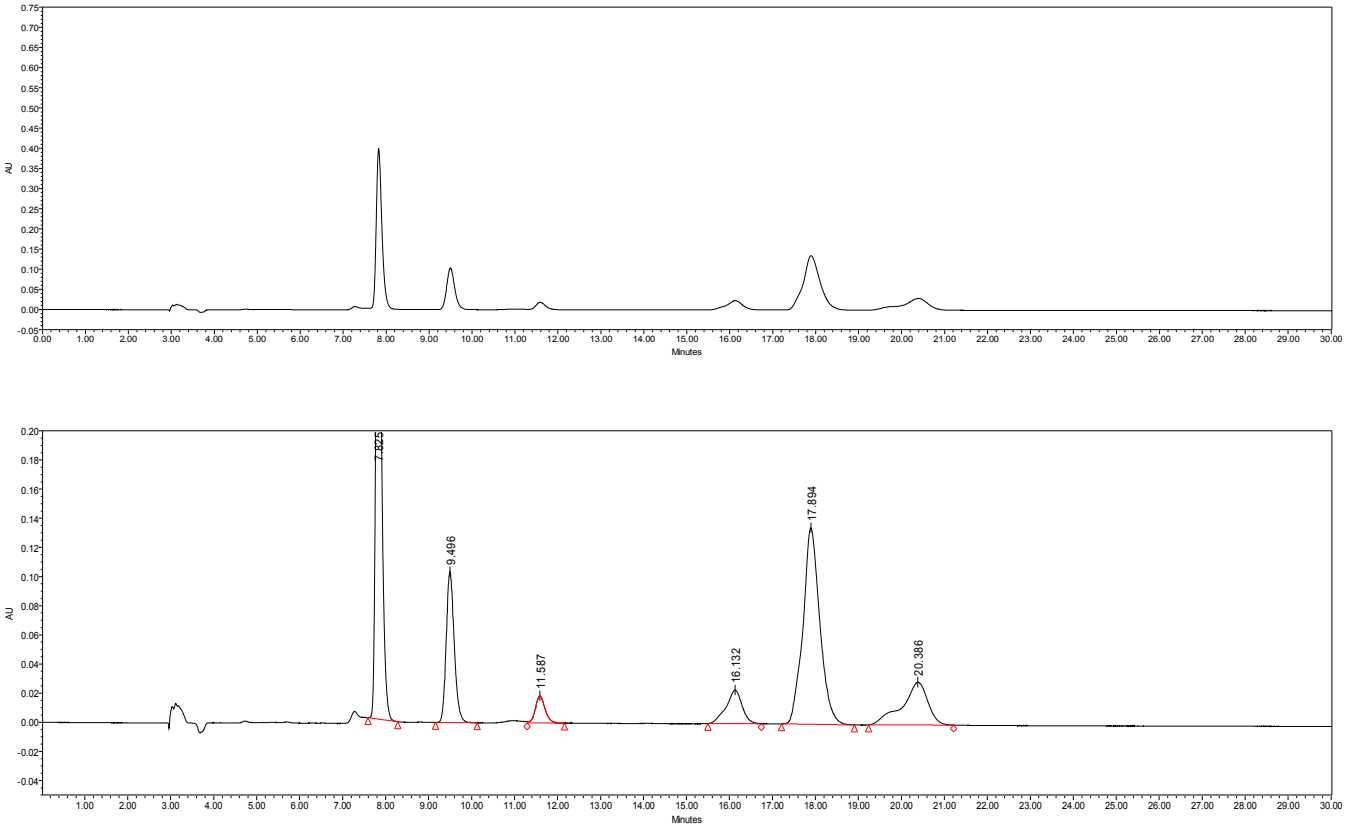
Chiral HPLC chromatogram for 10.00 g scale DKR-hydrogenation of **8** to produce **9** (reaction details in the Experimenal Section).




**8** = ND **9** = 95.4A% **9-ent** = 1.75A% **14** + **14-ent** = 2.85A%

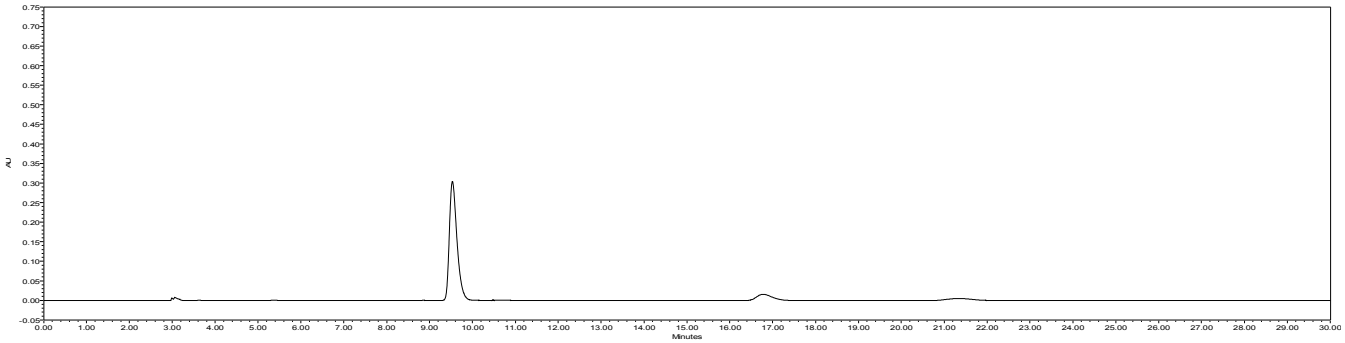
**Table 1 Chiral HPLC chromatograms**:

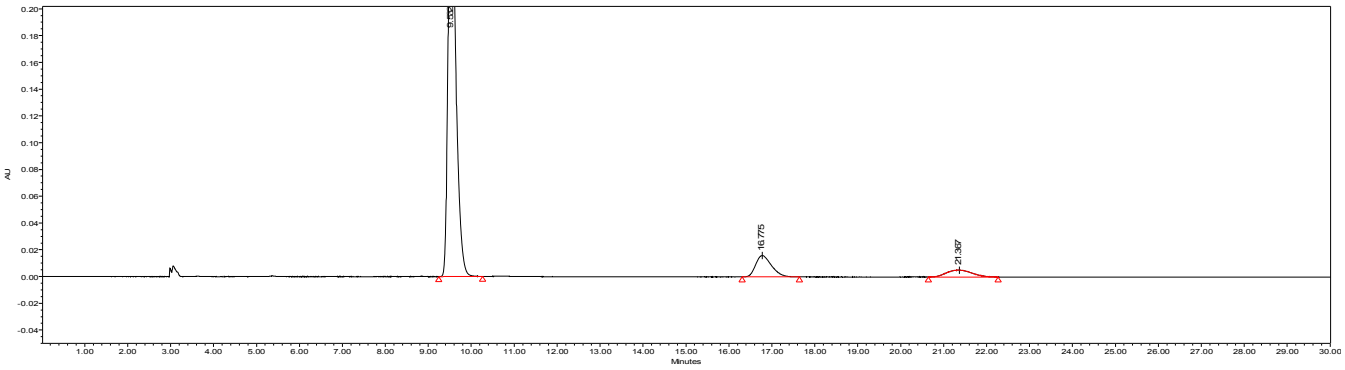
Entry 1: **8** (400 mg; 1.54 mmol); MeOH (5.0 mL); $Ru(OAc)_2$[(*S*)-BINAP] (5.0 mg, 0.0059 mmol).




**8** = 67.30A%  **9** = 13.50A%  **9-ent** = 11.10A%  **14** + **14-ent** = 8.09A%

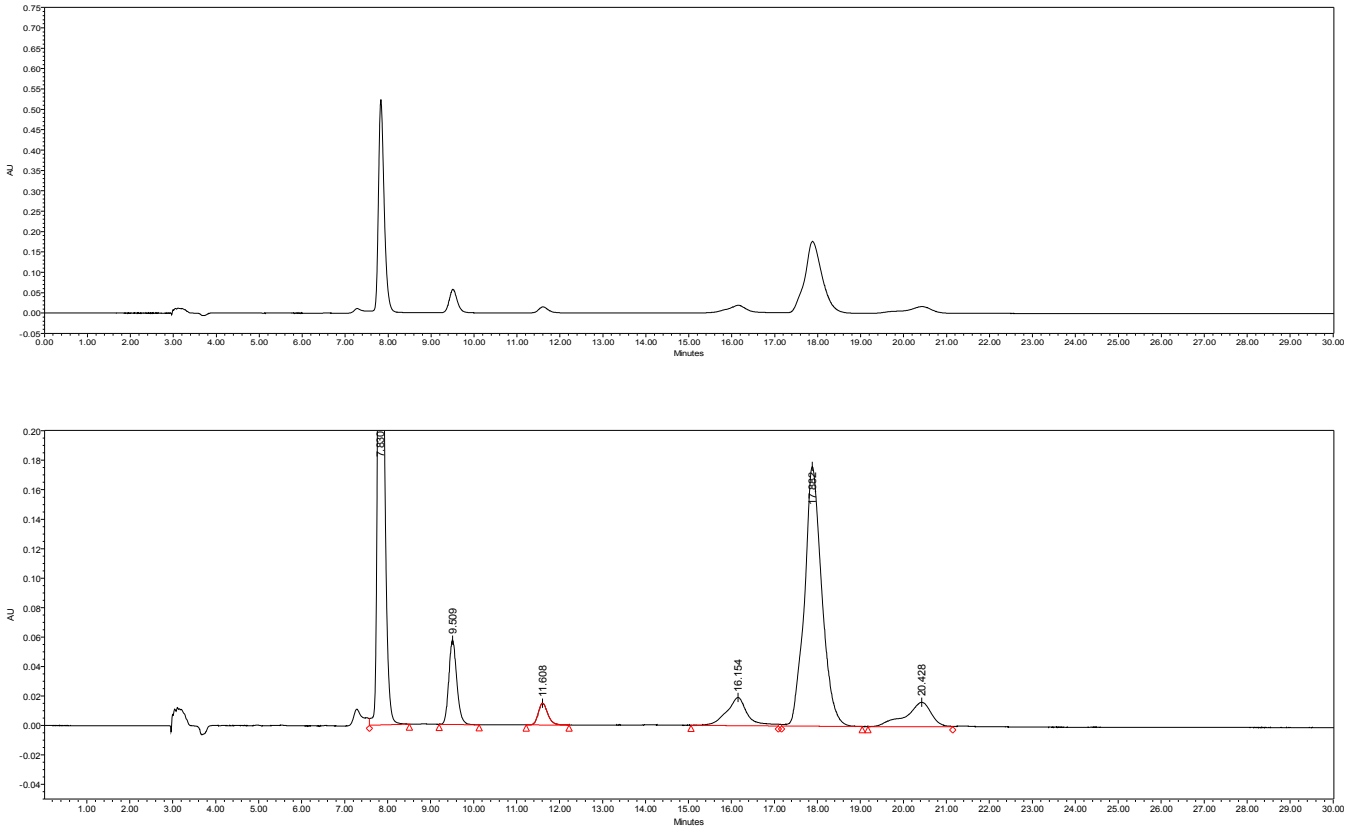
Entry 2: **8** (400 mg; 1.54 mmol); MeOH (4.92 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in MeOH); $Ru(OAc)_2$[(*S*)-BINAP] (5.0 mg, 0.0059 mmol).





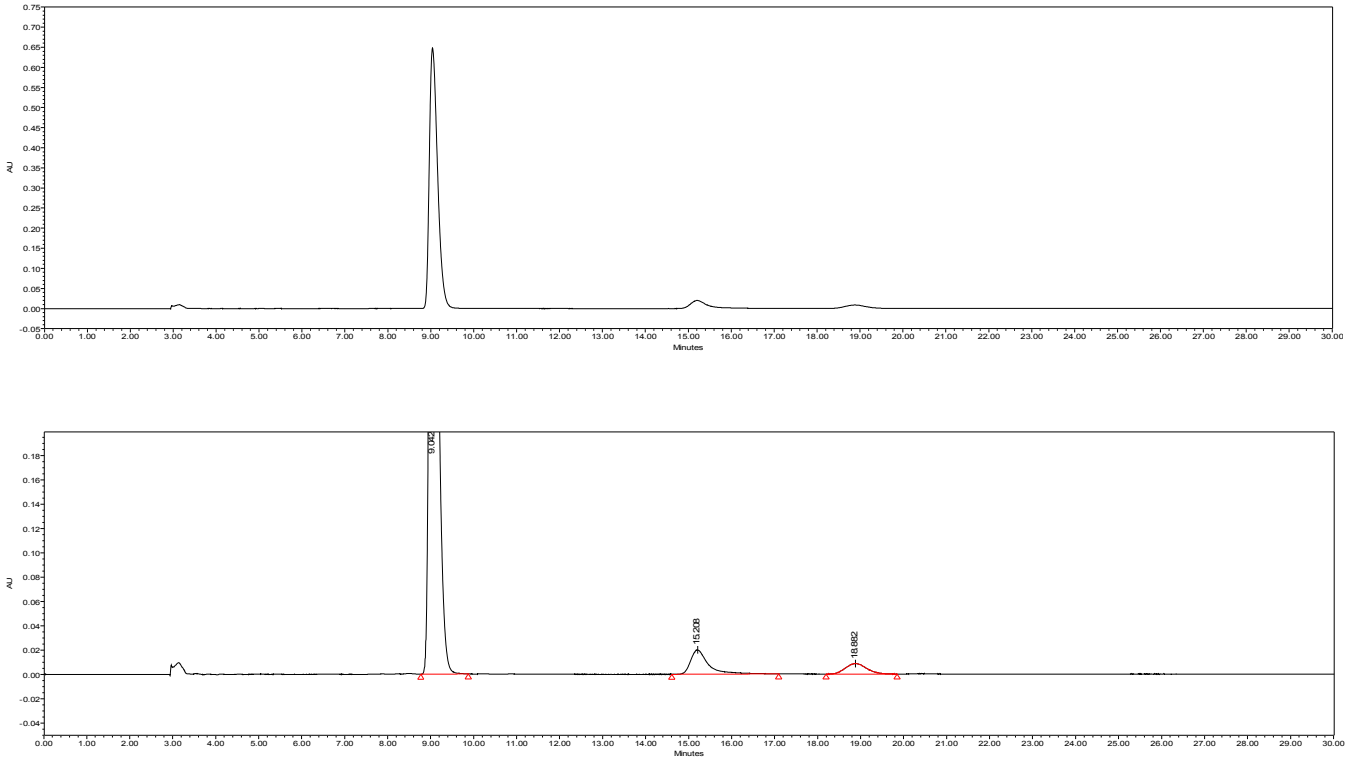

**8** = ND (non-detect) **9** = 85.90A% **9-ent** = 4.82A% **14** + **14-ent** = 9.32A%

Entry 3: **8** (400 mg; 1.54 mmol); MeOH (5.0 mL); $Ru(OAc)_2$[(*S*)-tol-BINAP)] (5.0 mg, 0.0055 mmol).



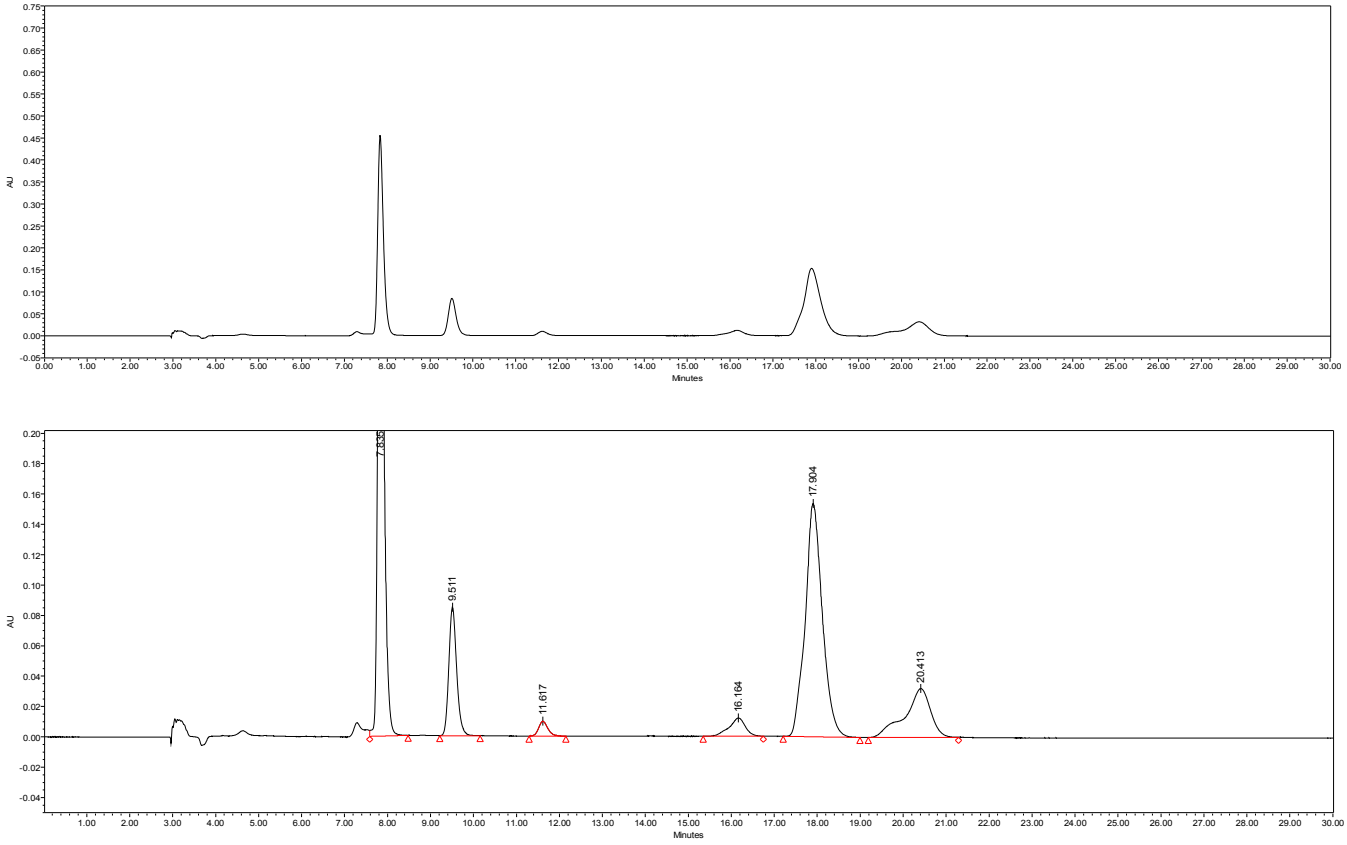

**8** = 80.00A% **9** = 7.41A% **9-ent** = 5.57A% **14** + **14-ent** = 7.01A%

Entry 4: **8** (400 mg; 1.54 mmol); MeOH (4.92 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in MeOH); $Ru(OAc)_2$[(*S*)-tol-BINAP)] (5.0 mg, 0.0055 mmol).



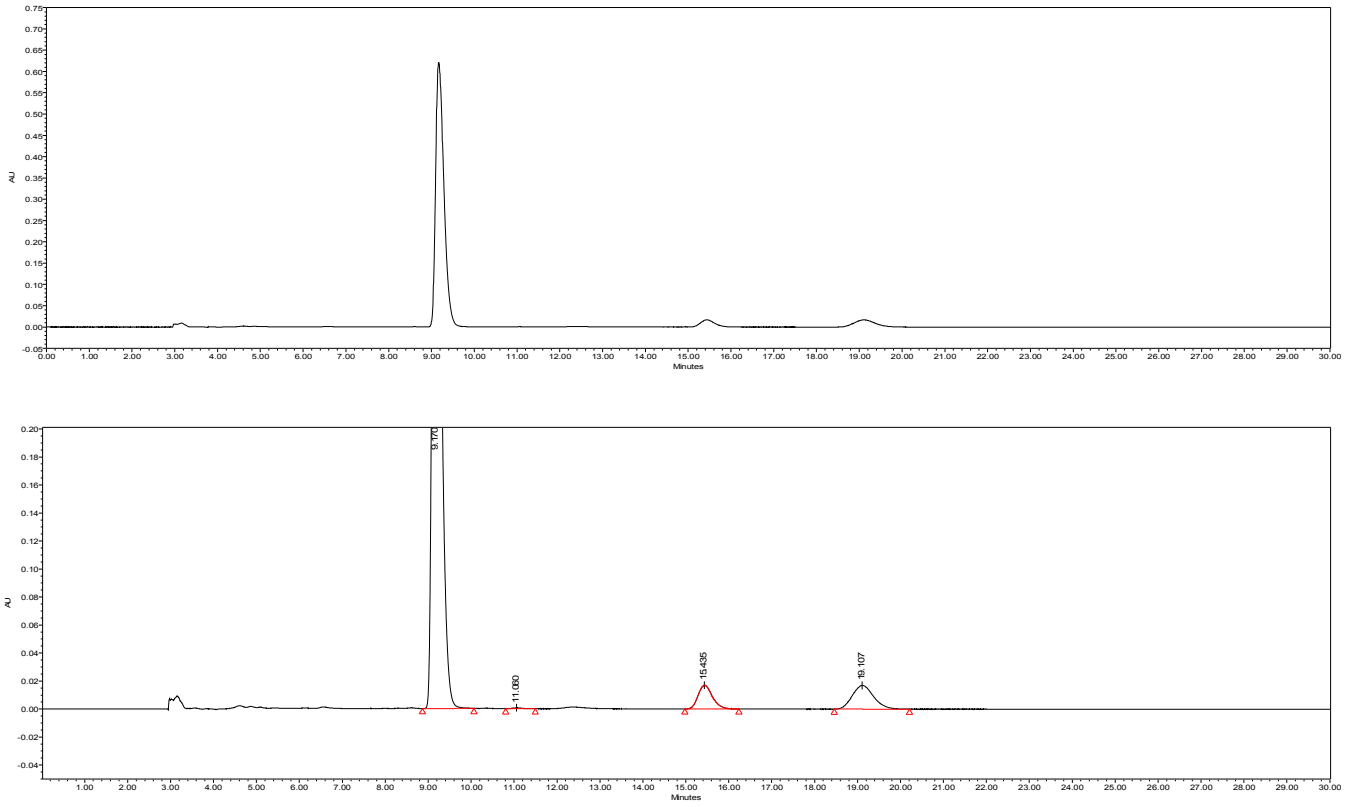

**8** = ND **9** = 90.90A% **9-ent** = 3.10A% **14** + **14-ent** = 5.96A%

Entry 5: **8** (400 mg; 1.54 mmol); MeOH (5.0 mL); $Ru(OAc)_2$[(*S*)-xyl-BINAP)] (5.0 mg, 0.0052 mmol).



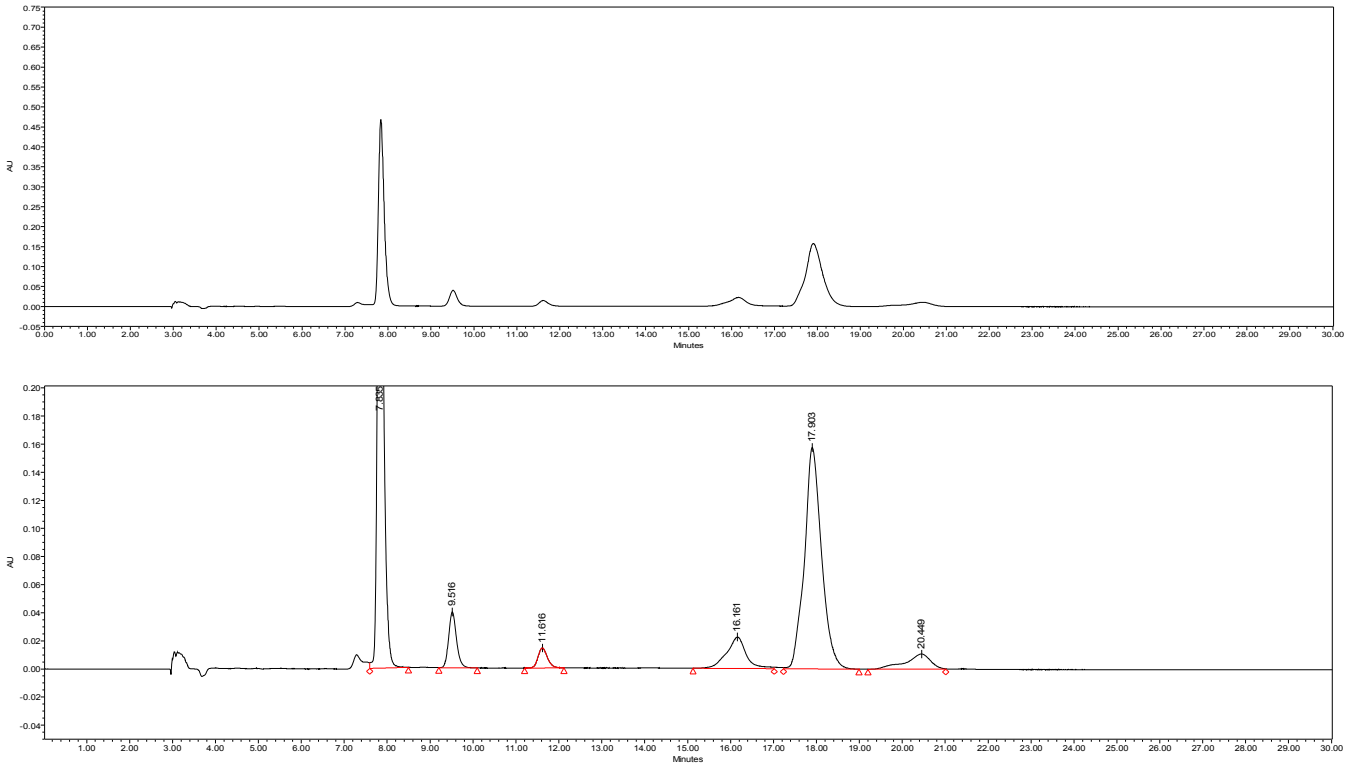

**8** = 73.80A%  **9** = 10.60A%  **9-ent** = 11.60A%  **14** + **14-ent** = 4.00A%

Entry 6: **8** (400 mg; 1.54 mmol); MeOH (4.92 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in MeOH); $Ru(OAc)_2$[(*S*)-xyl-BINAP)] (5.0 mg, 0.0052 mmol).



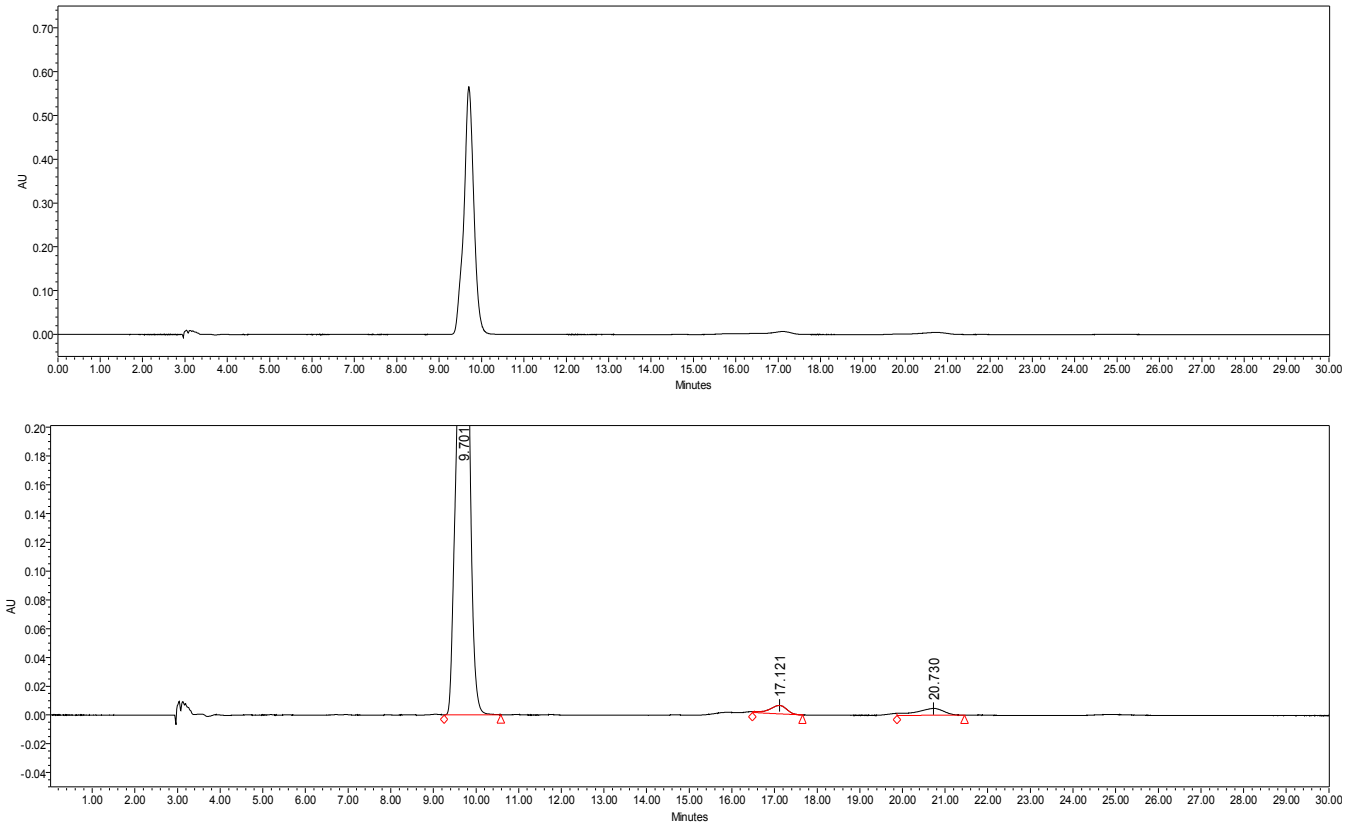

**8** = ND **9** = 88.80A% **9-ent** = 6.18A% **14** + **14-ent** = 4.66A%

Entry 7: **8** (400 mg; 1.54 mmol); EtOH (5.0 mL); $Ru(OAc)_2$[(*S*)-tol-BINAP)] (5.0 mg, 0.0055 mmol).



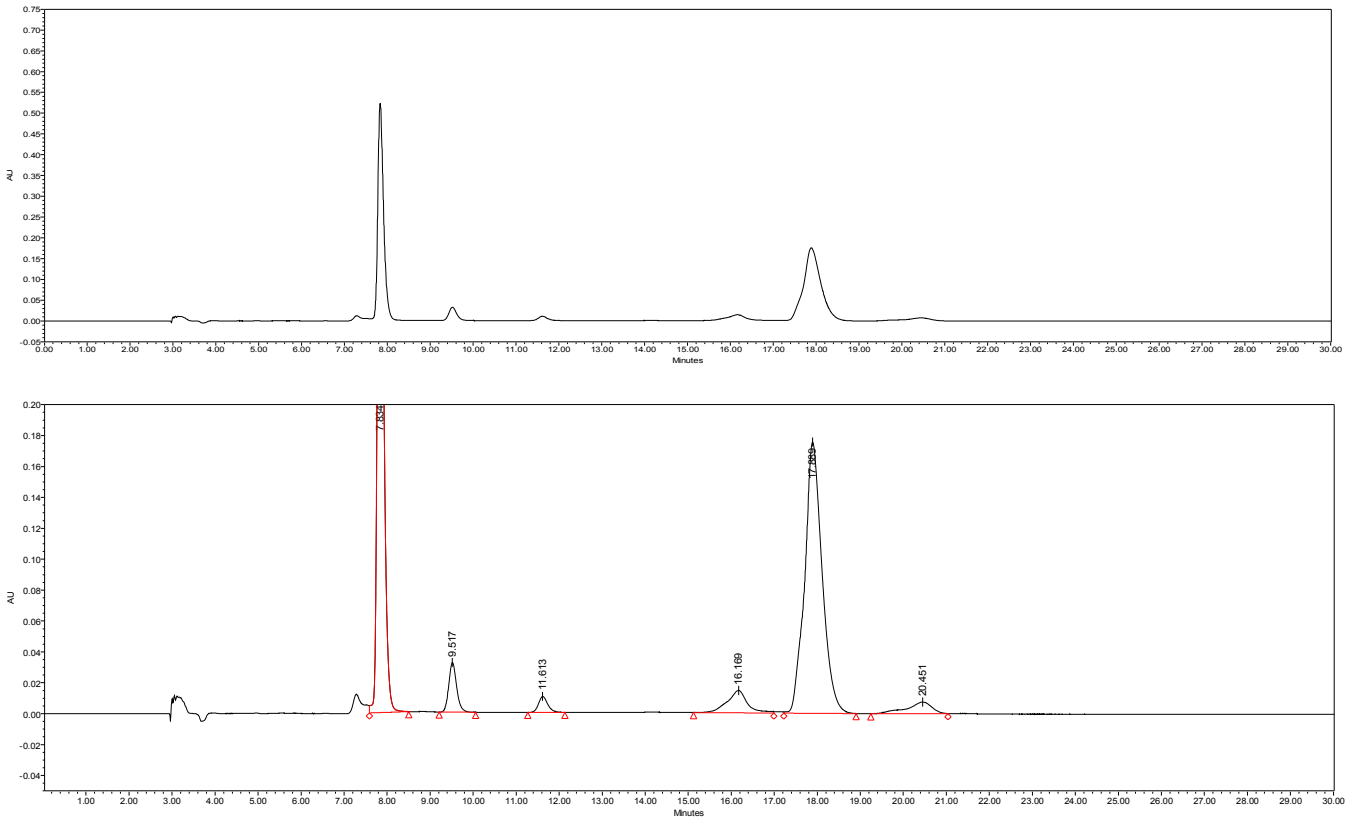

**8** = 81.2A%  **9** = 6.13A%  **9-ent** = 4.10A%  **14** + **14-ent** = 8.58A%

Entry 8: **8** (400 mg; 1.54 mmol); EtOH (4.92 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in EtOH); $Ru(OAc)_2$[(*S*)-tol-BINAP)] (5.0 mg, 0.0055 mmol).



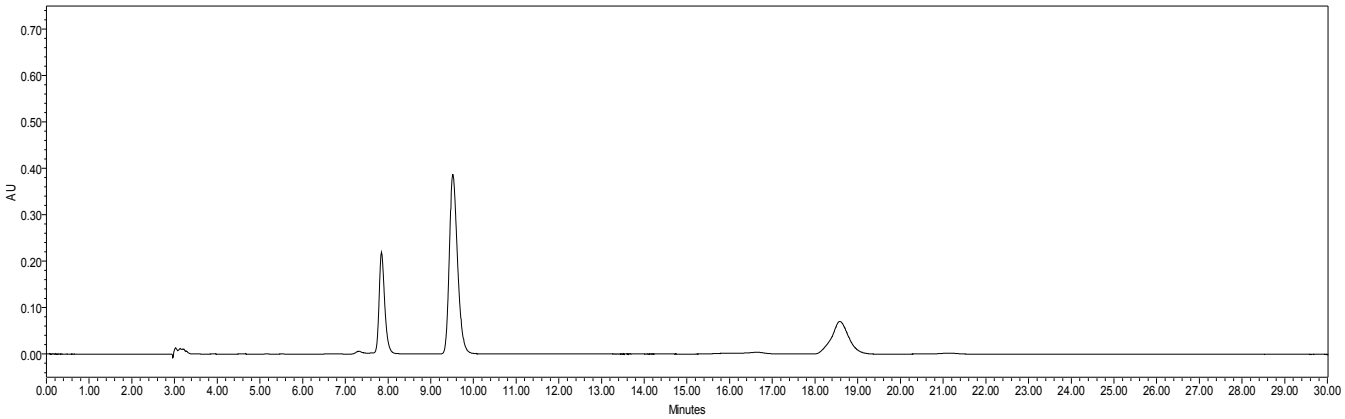

**8** = ND **9** = 94.10A% **9-ent** = 2.50A% **14** + **14-ent** = 3.45A%

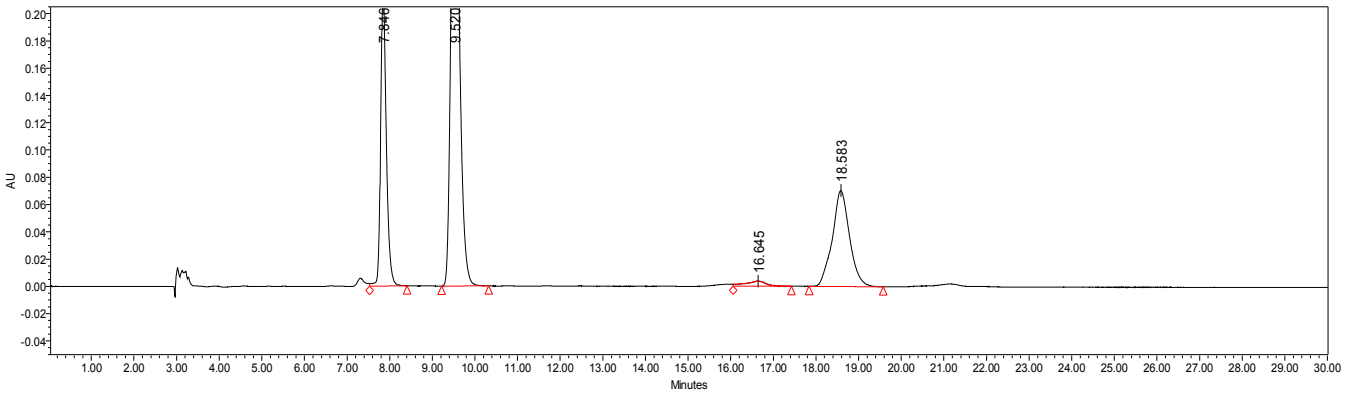
Entry 9: **8** (400 mg; 1.54 mmol); IPA (5.0 mL); $Ru(OAc)_2$[(*S*)-tol-BINAP)] (5.0 mg, 0.0055 mmol).




**8** = 86.5A%  **9** = 5.18A%  **9-ent** = 2.72A%  **14** + **14-ent** = 5.61A%

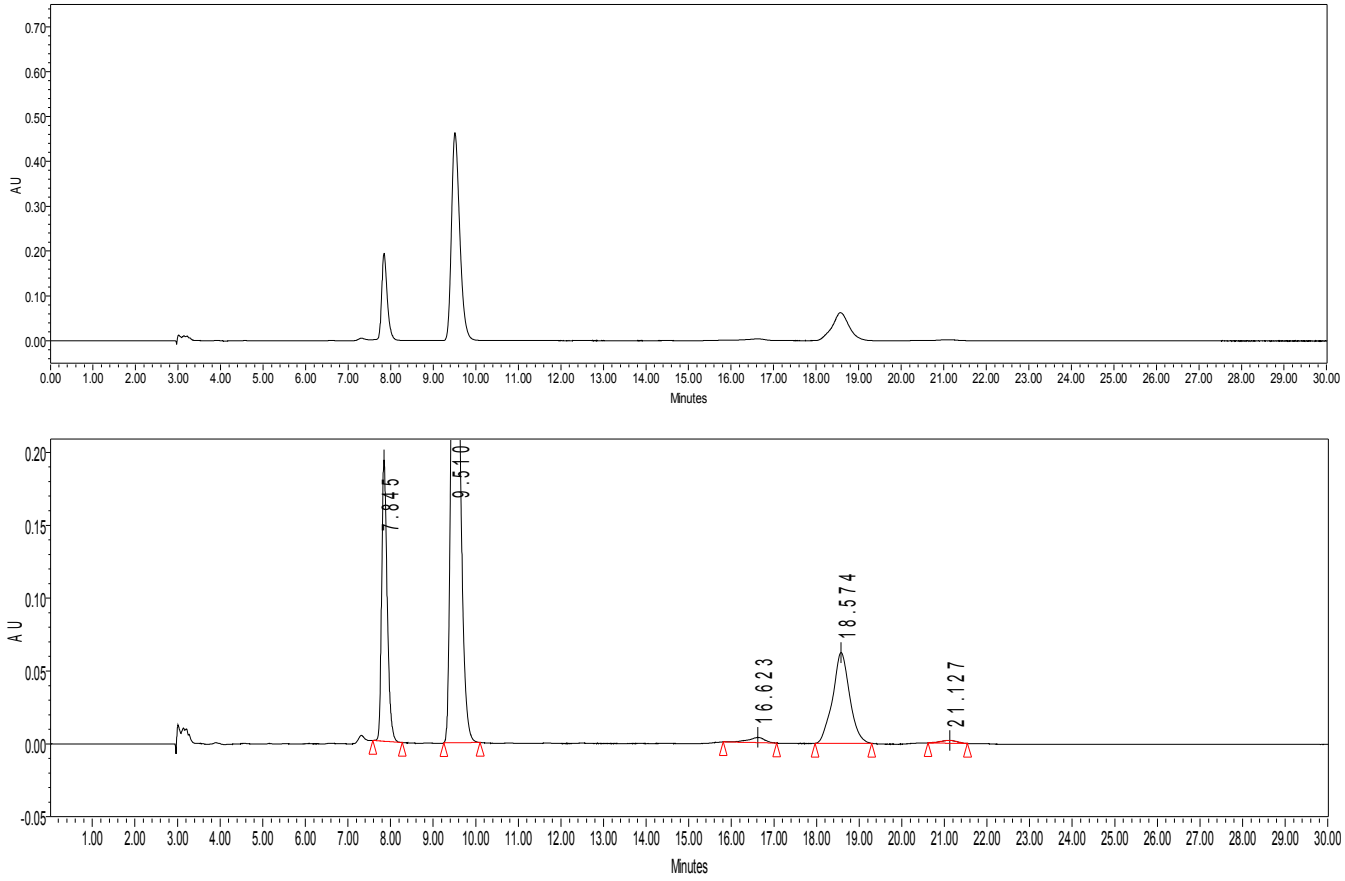
Entry 10: **8** (400 mg; 1.54 mmol); IPA (4.92 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in IPA); $Ru(OAc)_2$[(*S*)-tol-BINAP)] (5.0 mg, 0.0055 mmol).



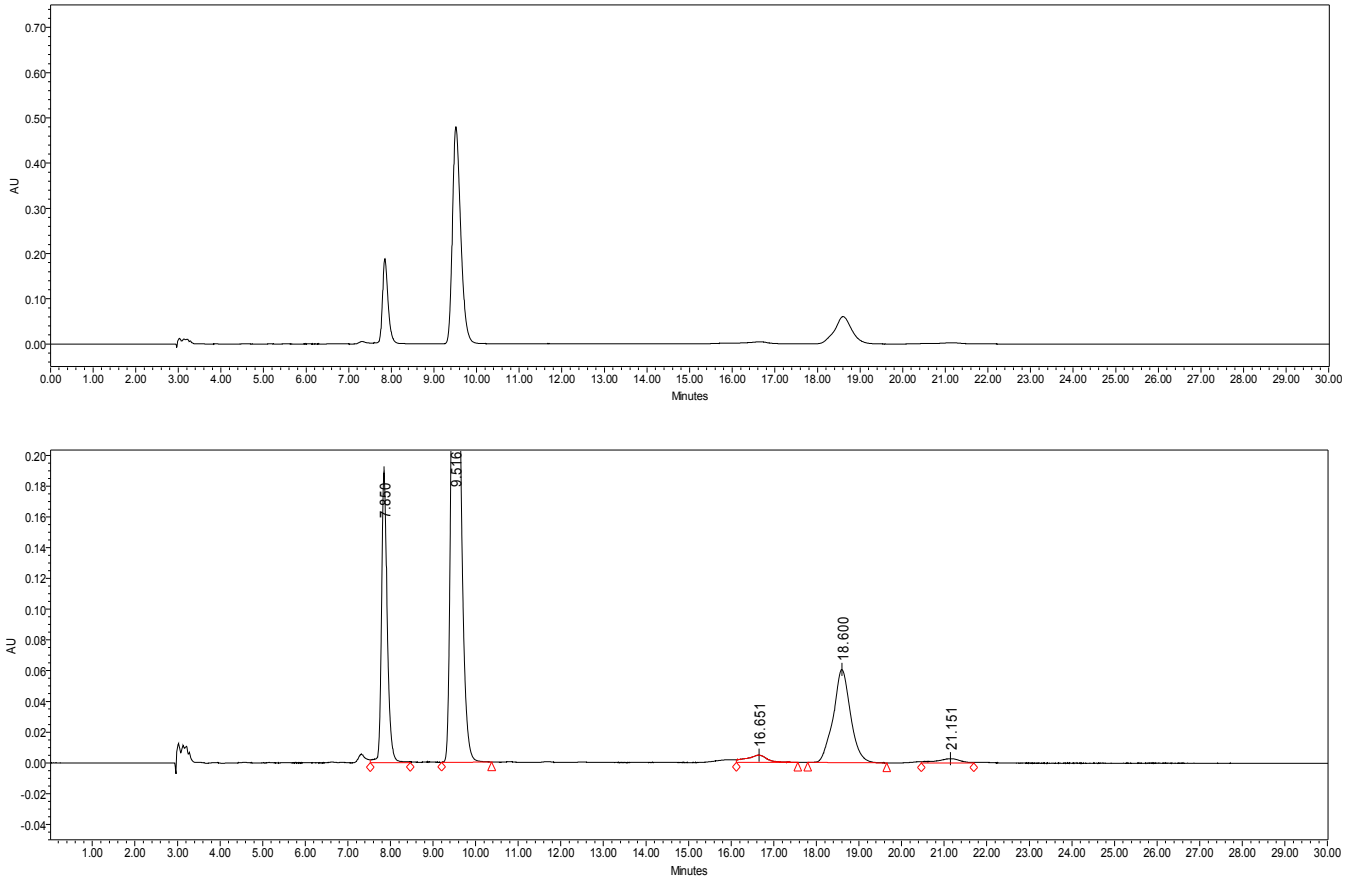

**8** = 42.2A%  **9** = 55.50A%  **9-ent** = 0.51A%  **14** + **14-ent** = 1.84A%

Entry 11: **8** (400 mg; 1.54 mmol); IPA (4.77 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in IPA); LiCl 0.001M in IPA (150 uL = 0.0065 mg, 0.00015 mmol); $Ru(OAc)_2$[(S)-tol- BINAP] (5.0 mg, 0.0055 mmol).



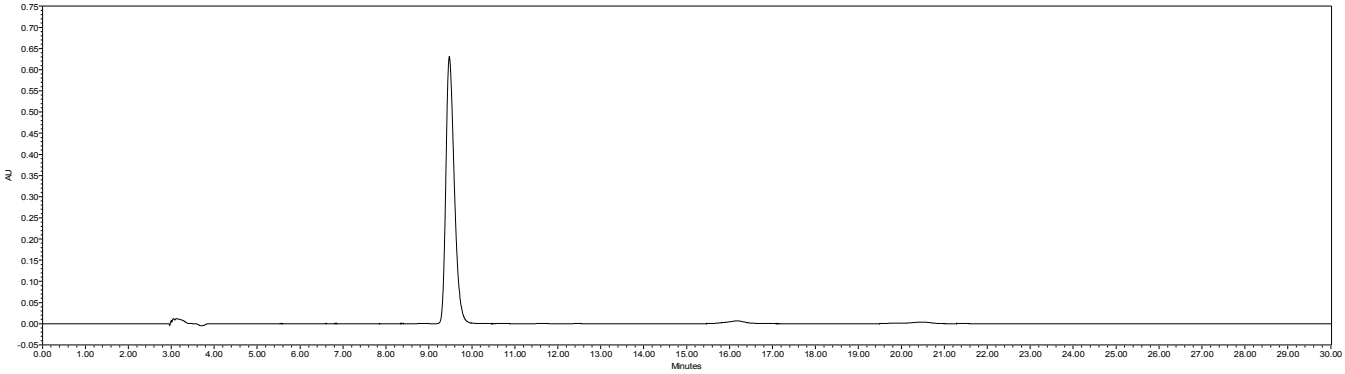

**8** = 35.10A% **9** = 62.10A% **9-ent** = 1.03A% **14** + **14-ent** = 1.73A%

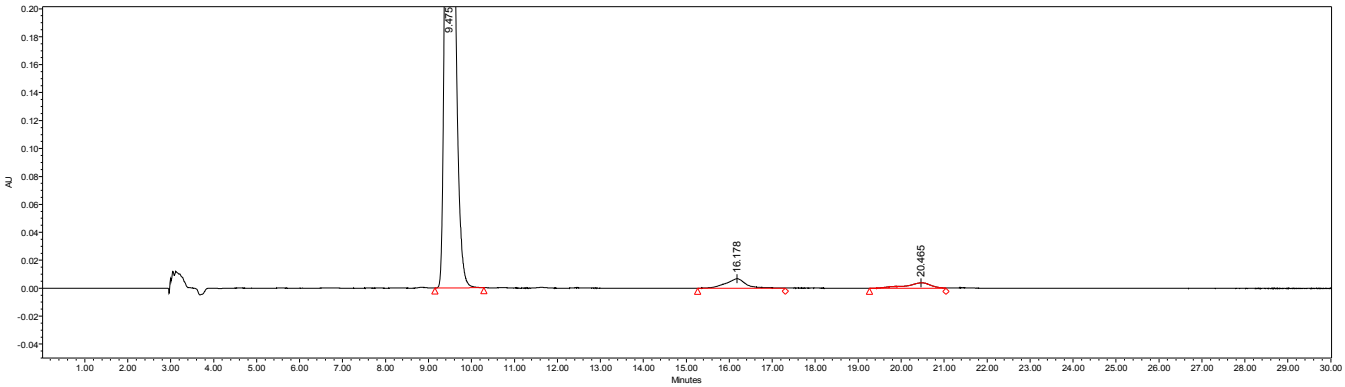
Entry 12: **8** (400 mg; 1.54 mmol); IPA (4.77 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in IPA); LiCl 0.01M in IPA (150 uL =0.065 mg, 0.0015 mmol); $Ru(OAc)_2$[(S)-tol- BINAP] (5.0 mg, 0.0055 mmol).




**8** = 33.30A% **9** = 63.50A% **9-ent** = 1.20A% **14** + **14-ent** = 2.04A%

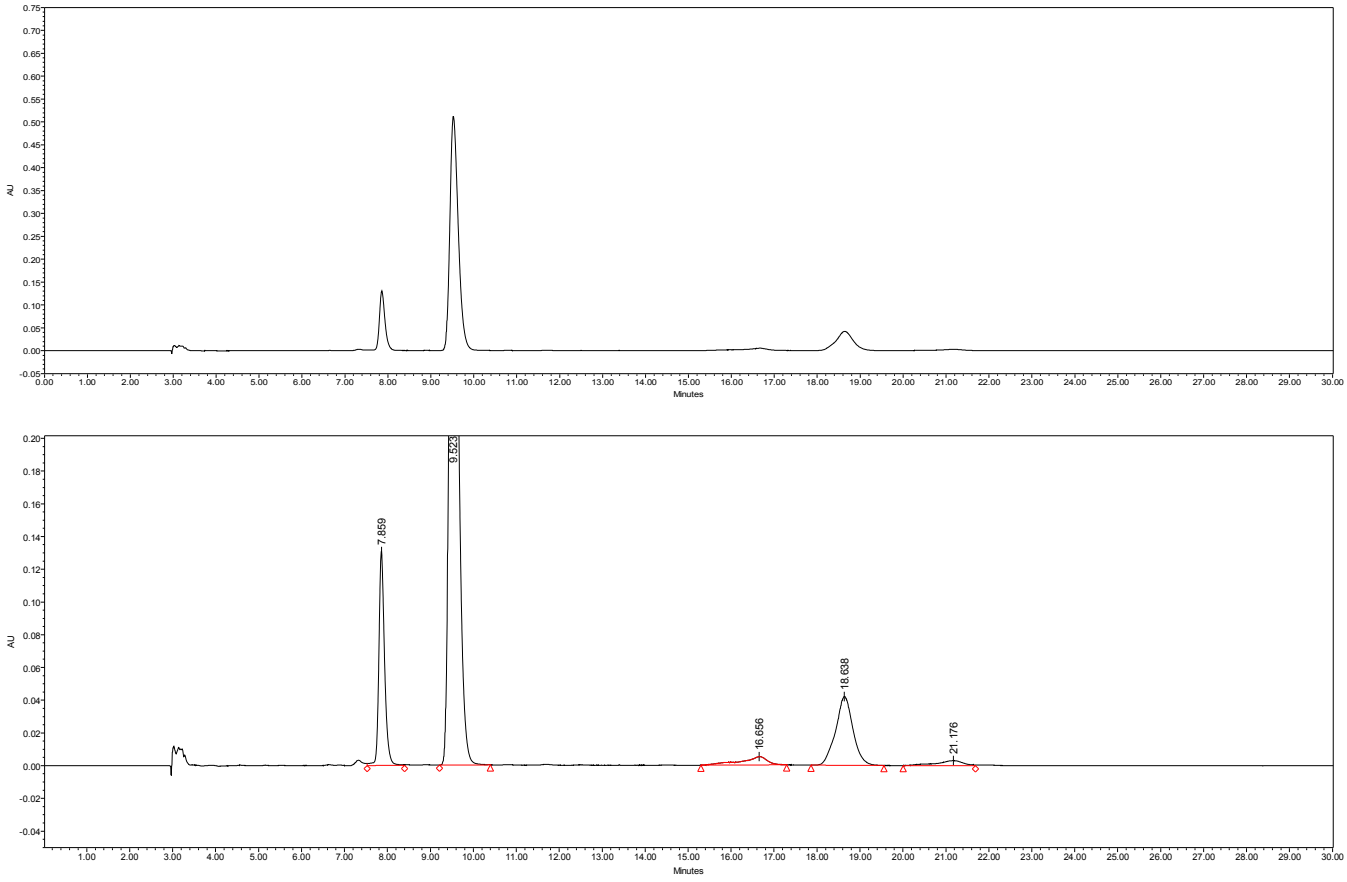
Entry 13: **8** (400 mg; 1.54 mmol); IPA (4.77 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in IPA); LiCl 0.1M in IPA (150 uL = 0.65 mg; 0.015 mmol); $Ru(OAc)_2$[(S)-tol- BINAP] (5.0 mg, 0.0055 mmol).



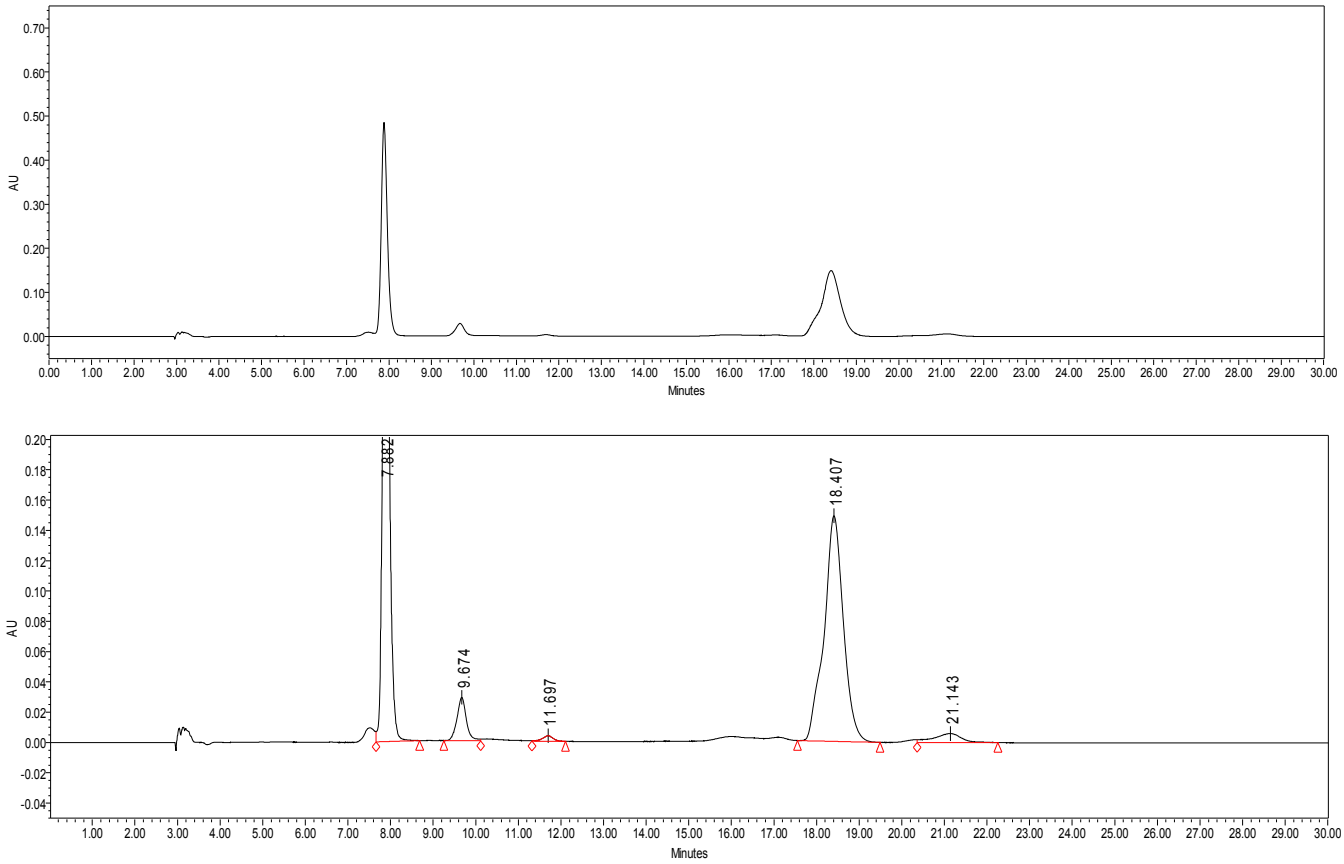

**8** = ND **9** = 95.80A% **9-ent** = 1.82A% **14** + **14-ent** = 2.37A%

Entry 14: **8** (400 mg; 1.54 mmol); IPA (4.77 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in IPA); LiCl 1.0M in IPA (150 uL = 6.5 mg; 0.15 mmol); $Ru(OAc)_2$[(S)-tol- BINAP] (5.0 mg, 0.0055 mmol).



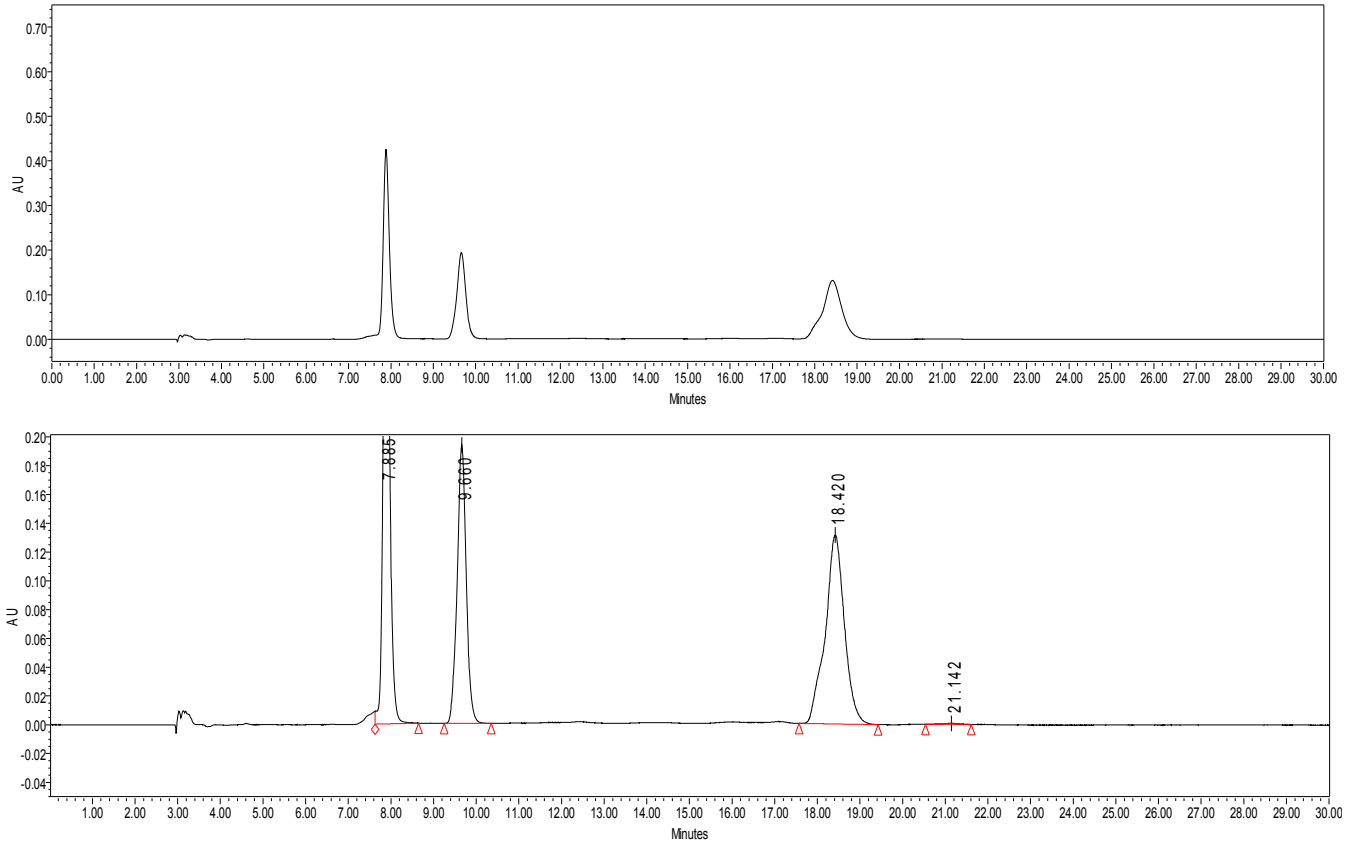

**8** = 24.30A%  **9** = 71.90A%  **9-ent** = 1.37A%  **14** + **14-ent** = 2.41A%

Entry 15: **8** (400 mg; 1.54 mmol); IPA (4.85 mL); LiCl 0.1M in IPA (150 uL = 0.65 mg; 0.015 mmol); $Ru(OAc)_2$[(S)-tol- BINAP] (5.0 mg, 0.0055 mmol).



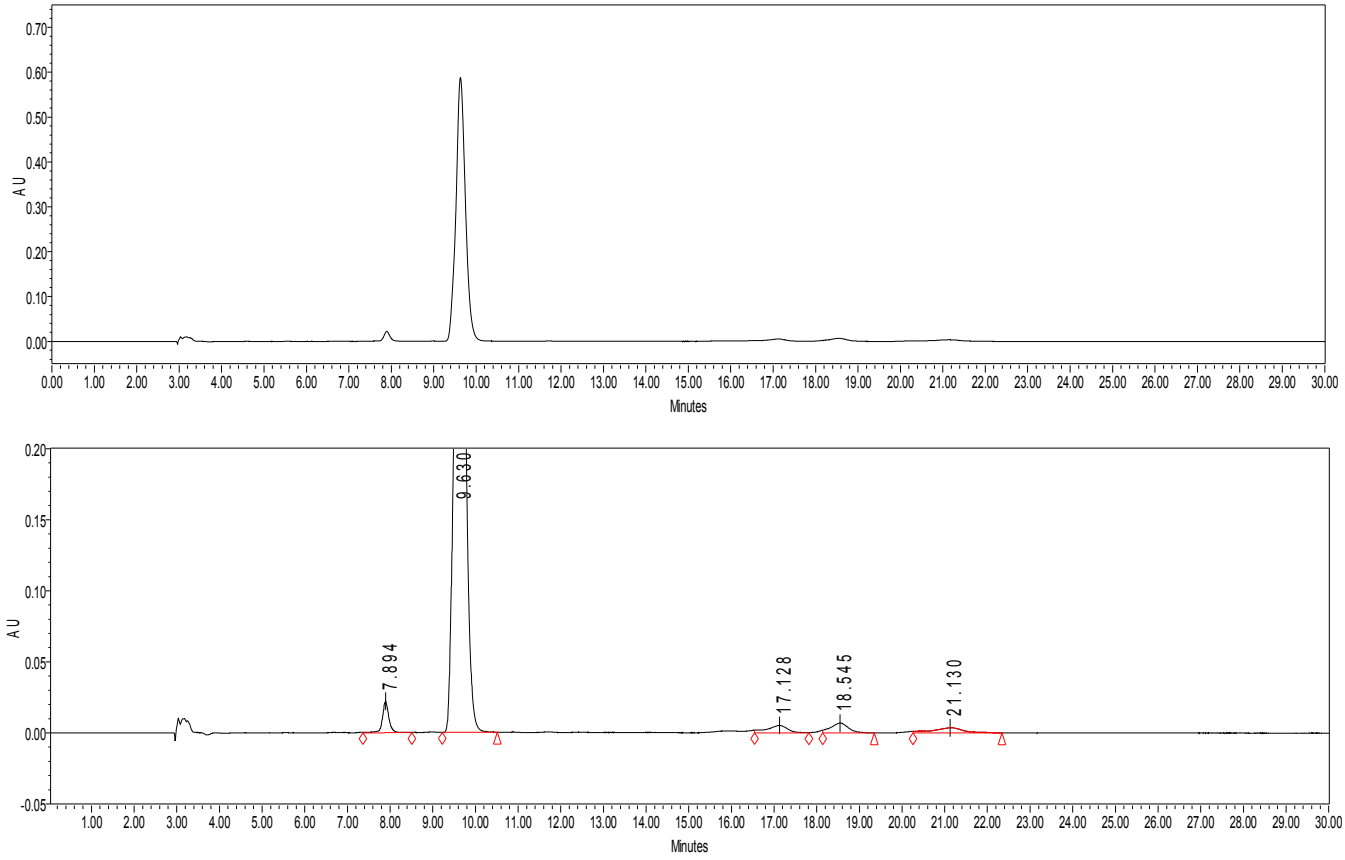

**8** = 88.00A% **9** = 4.00A% **9-ent** = 2.46A% **14** + **14-ent** = 0.95A%

Entry 16: **8** (400 mg; 1.54 mmol); IPA (4.82 mL); 35% HCl (requires 2.7 uL; 0.031 mmol; therefore: charged 27 uL of 10% stock solution of 35% HCl in IPA); LiCl 0.1M in IPA (150 uL = 0.65 mg; 0.015 mmol); $Ru(OAc)_2$[(S)-tol- BINAP] (5.0 mg, 0.0055 mmol).



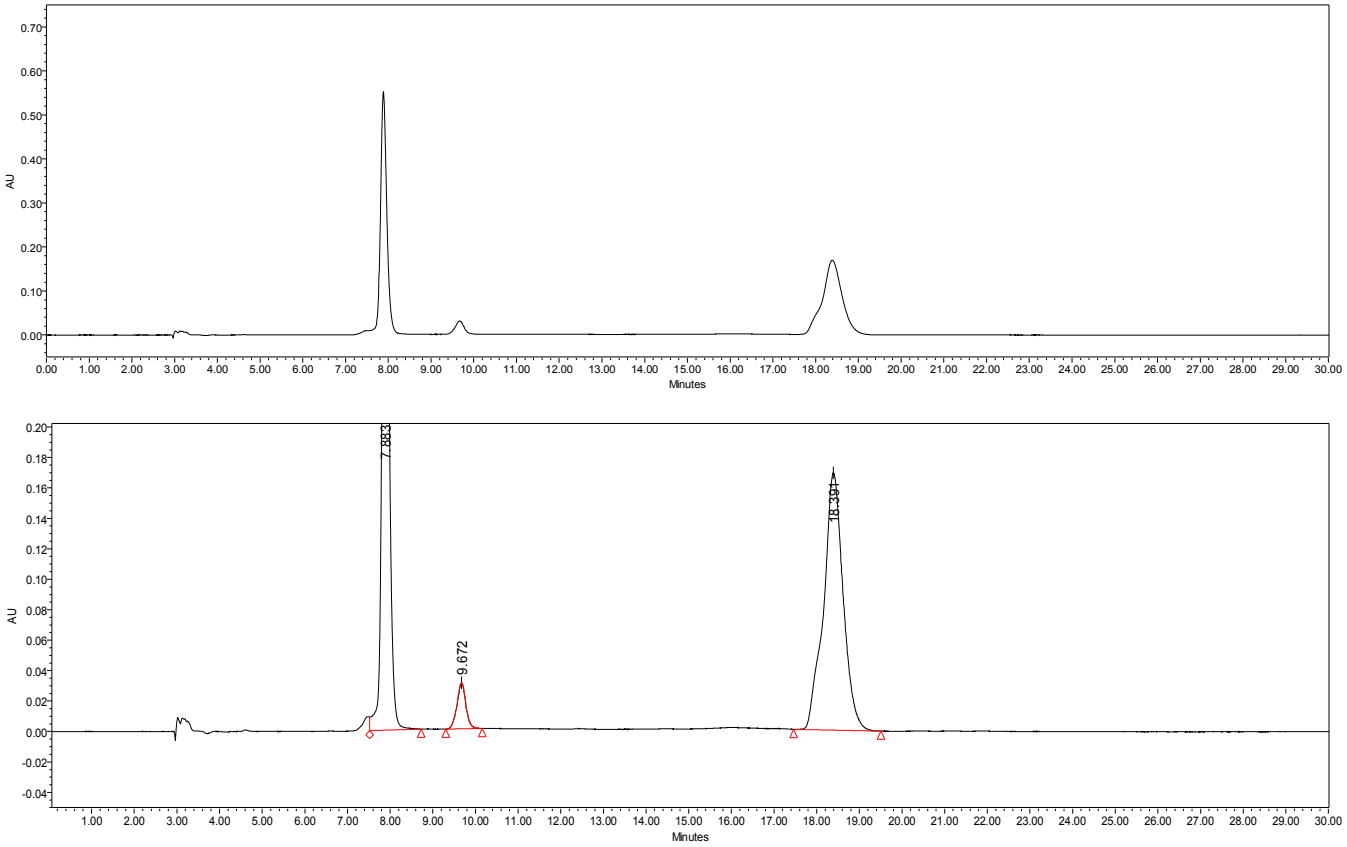

**8** = 73.10A%  **9** = 24.90A%  **9-ent** = 0.20A%  **14** + **14-ent** = 0.20A%

Entry 17: **8** (400 mg; 1.54 mmol); IPA (4.82 mL); 35% HCl (requires 13.33 uL; 0.153 mmol; therefore: charged 133 uL of 10% stock solution of 35% HCl in IPA); LiCl 0.1M in IPA (150 uL = 0.65 mg; 0.015 mmol); $Ru(OAc)_2$[(S)-tol- BINAP] (5.0 mg, 0.0055 mmol).



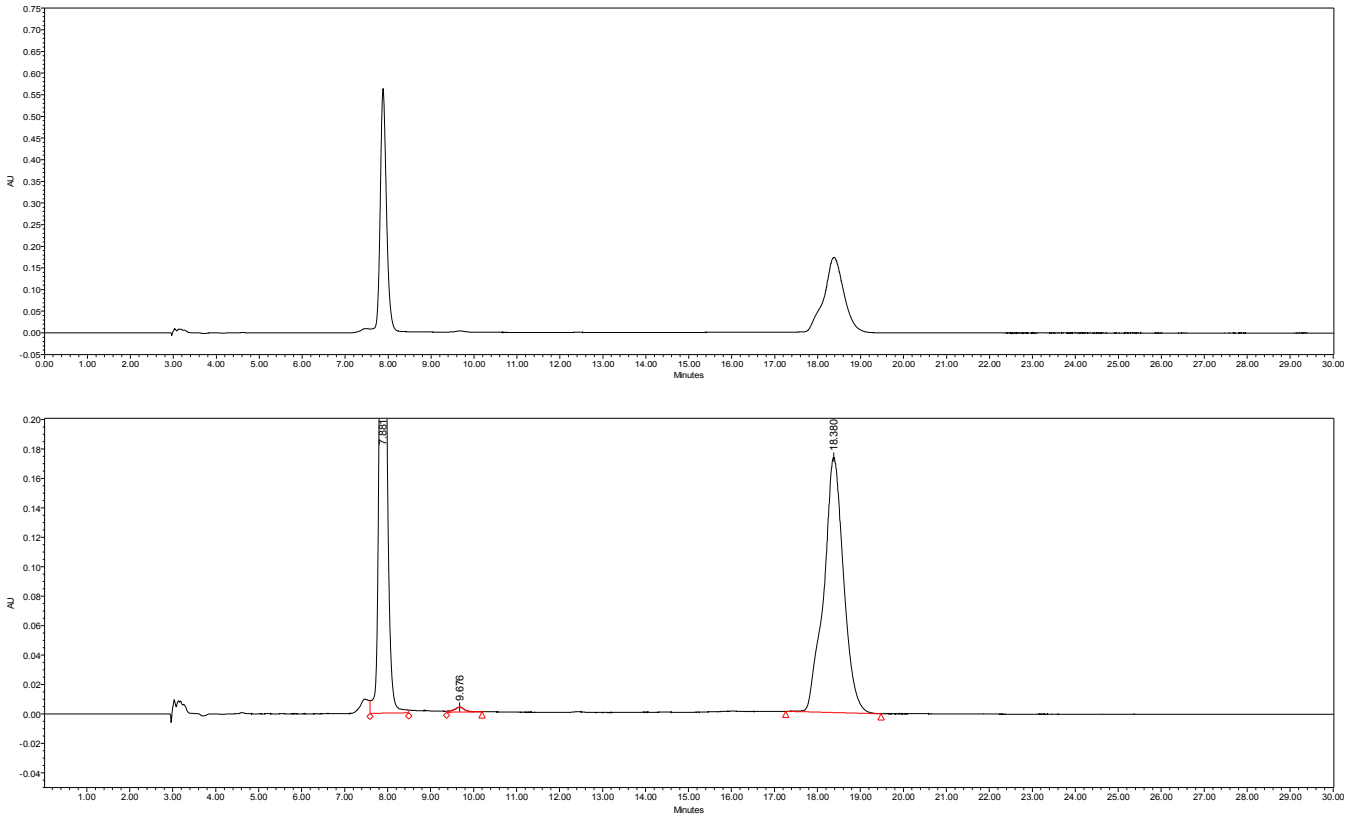

**8** = 2.50A%  **9** = 91.00A%  **9-ent** = 1.81A%  **14** + **14-ent** = 1.73A%

Entry 18: **8** (400 mg; 1.54 mmol); IPA (4.77 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in IPA); LiCl 0.1M in IPA (150 uL = 0.65 mg; 0.015 mmol); $Ru(OAc)_2$[(S)-tol- BINAP] (3.0 mg, 0.0033 mmol).



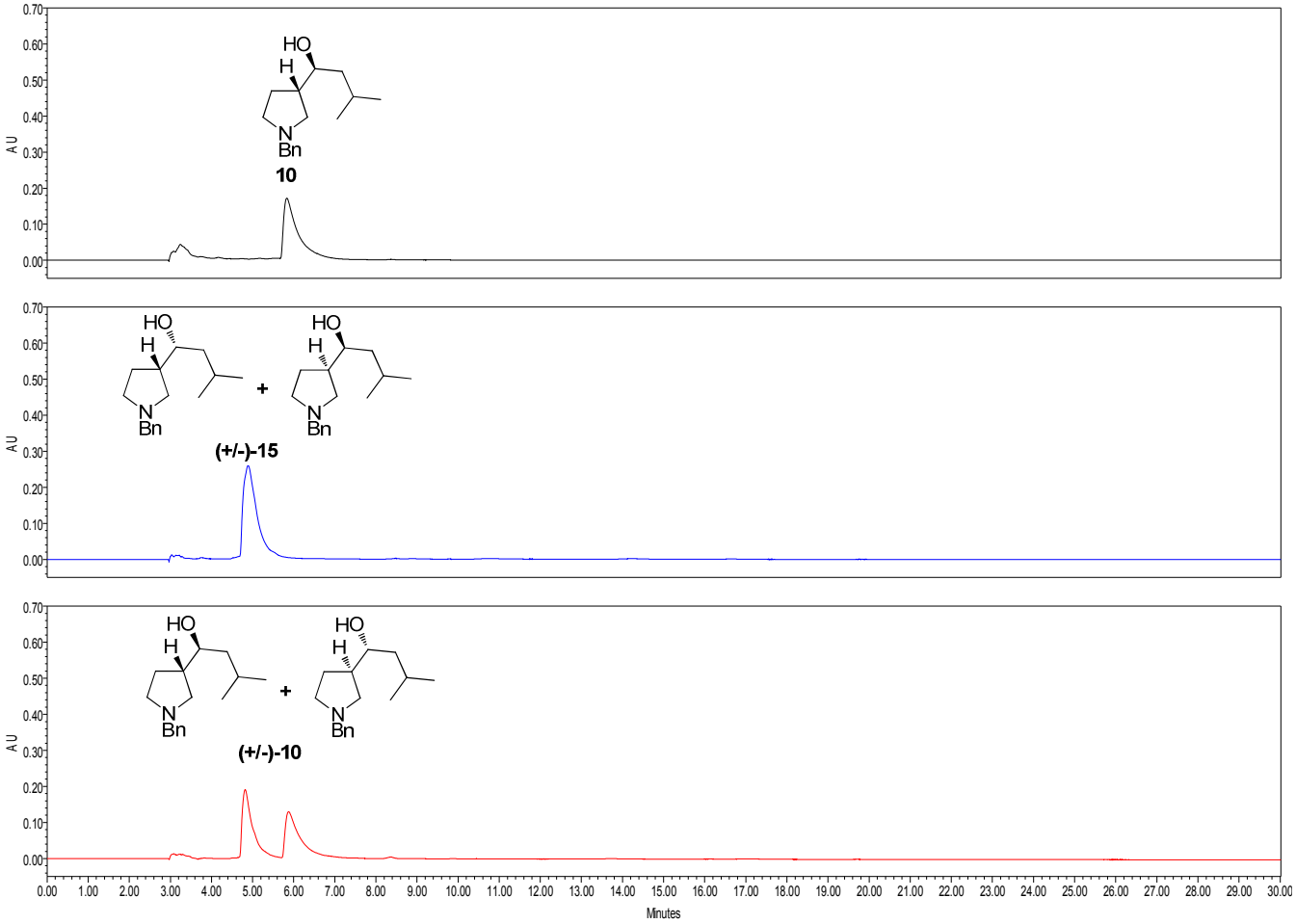

**8** = 95.10A% **9** = 4.90A% **9-ent** = ND **14** + **14-ent** = ND

Entry 19: **8** (400 mg; 1.54 mmol); IPA (4.77 mL); 35% HCl (requires 8 uL; 0.092 mmol; therefore: charged 80 uL of a 10% stock solution of 35% HCl in IPA); LiCl 0.1M in IPA (150 uL = 0.65 mg; 0.015 mmol); $Ru(OAc)_2$[(S)-tol- BINAP] (1.0 mg, 0.0011 mmol).



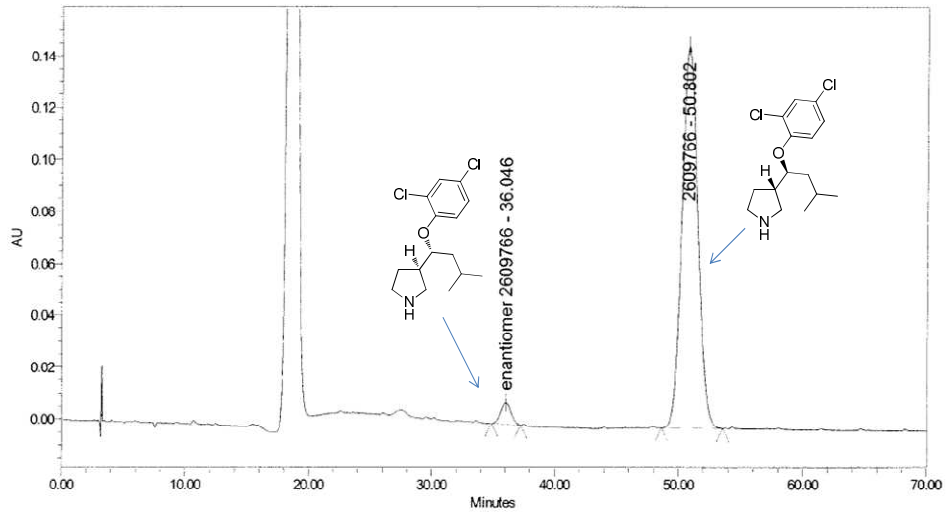

**8** = 98.00A% **9** = 2.00A% **9-ent** = ND **14** + **14-ent** = ND

Chiral HPLC chromatograms for **10** (100% ee and de) freebased from L-DBTA salt **16,** and racemic standards of the diastereomers (**(+/-)-15**) and enantiomers (**(+/-)-10**). Method: Column: Chiralpak IA-3 (4.6 x 250mm). Eluent: 90:10 heptane:EtOH. Flow rate: 1mL/min (10µL injection of 1 mg/mL solutions). Wave length: 220nm.



Chiral HPLC for (*S*)-3-((*S*)-1-(2,4-Dichlorophenoxy)-3-methylbutyl)pyrrolidine di-*p*-toluoyl-L-tartrate (**13**). Method: Column: Chiralpak IC (250 x 4.6 mm, 5 micron particles). Flow rate: Isocratic flow 1.0 mL/min., 25 °C, UV detection: 230nm. Eluent: 80:10:5 hexane:IPA:EtOH with 0.1% MSA. Run time: 70 min..

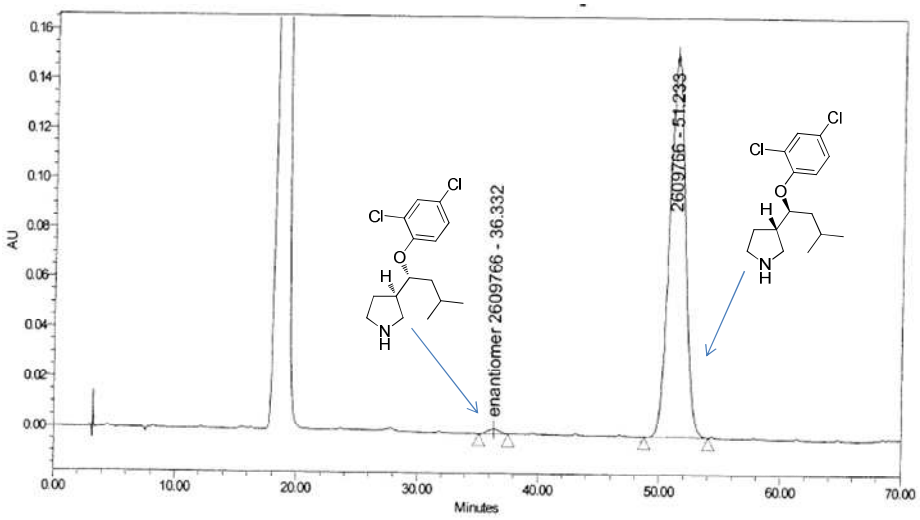
Chromatogram of the crystallized **13**:




**Processed Channel□A1100 AU 230 nm**

| | Peak Name | Processed Channel | Retention Time (min) | Area | % Area | Height |
|---|---|---|---|---|---|---|
| 1 | enantiomer 2609766 | A1100 AU 230 nm | 36.046 | 491175 | 3.60 | 8371 |
| 2 | diastereomer 2609766 | A1100 AU 230 nm | 41.710 | | | |
| 3 | 2609766 | A1100 AU 230 nm | 50.802 | 13155080 | 96.40 | 147628 |

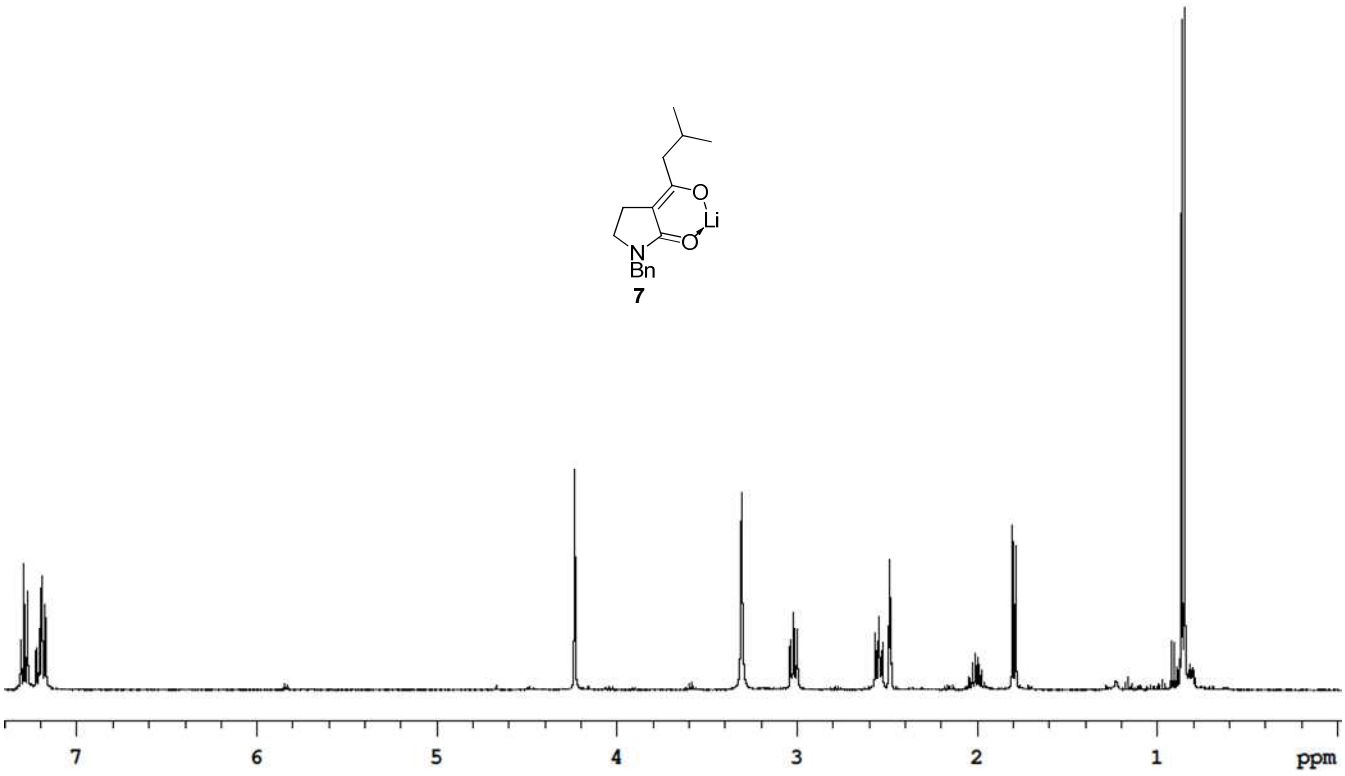
Chromatogram of re-crystallized **13**:

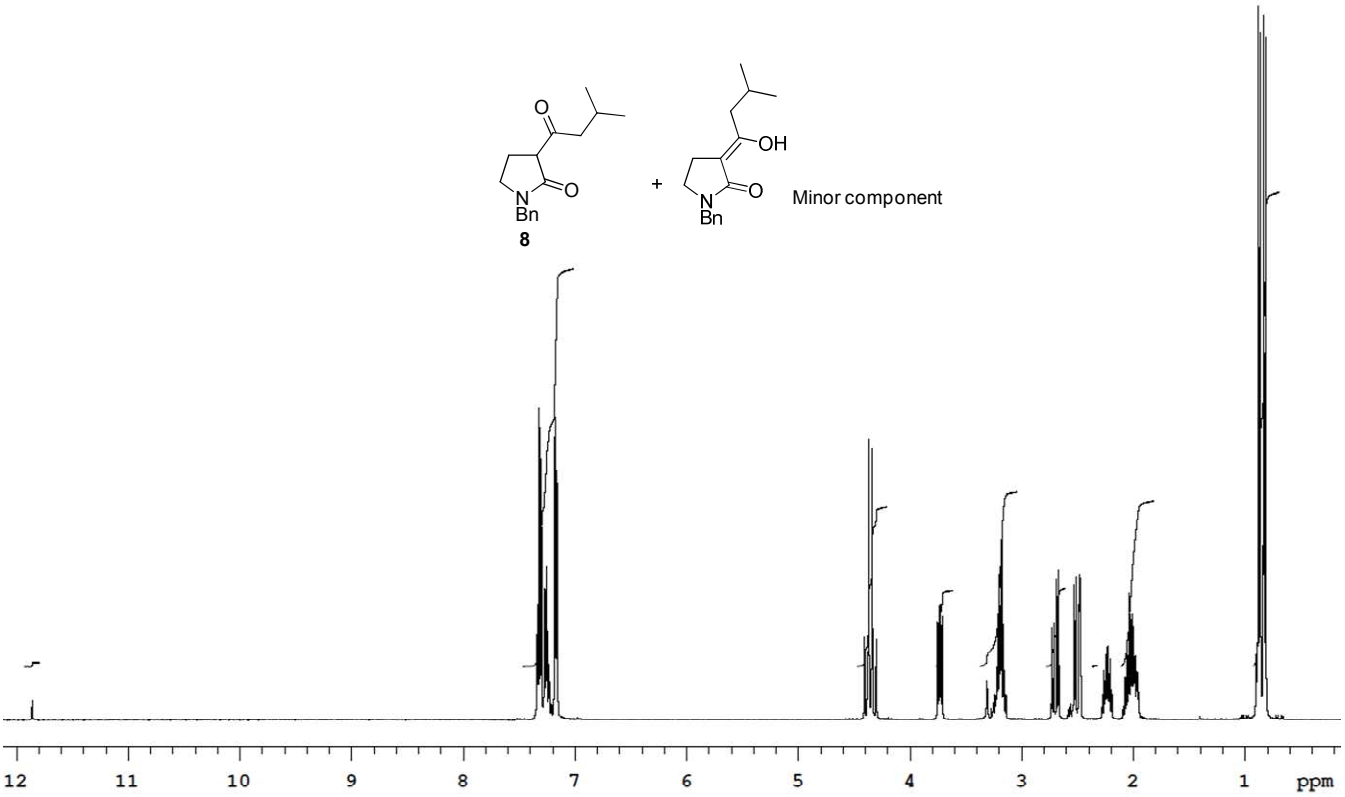


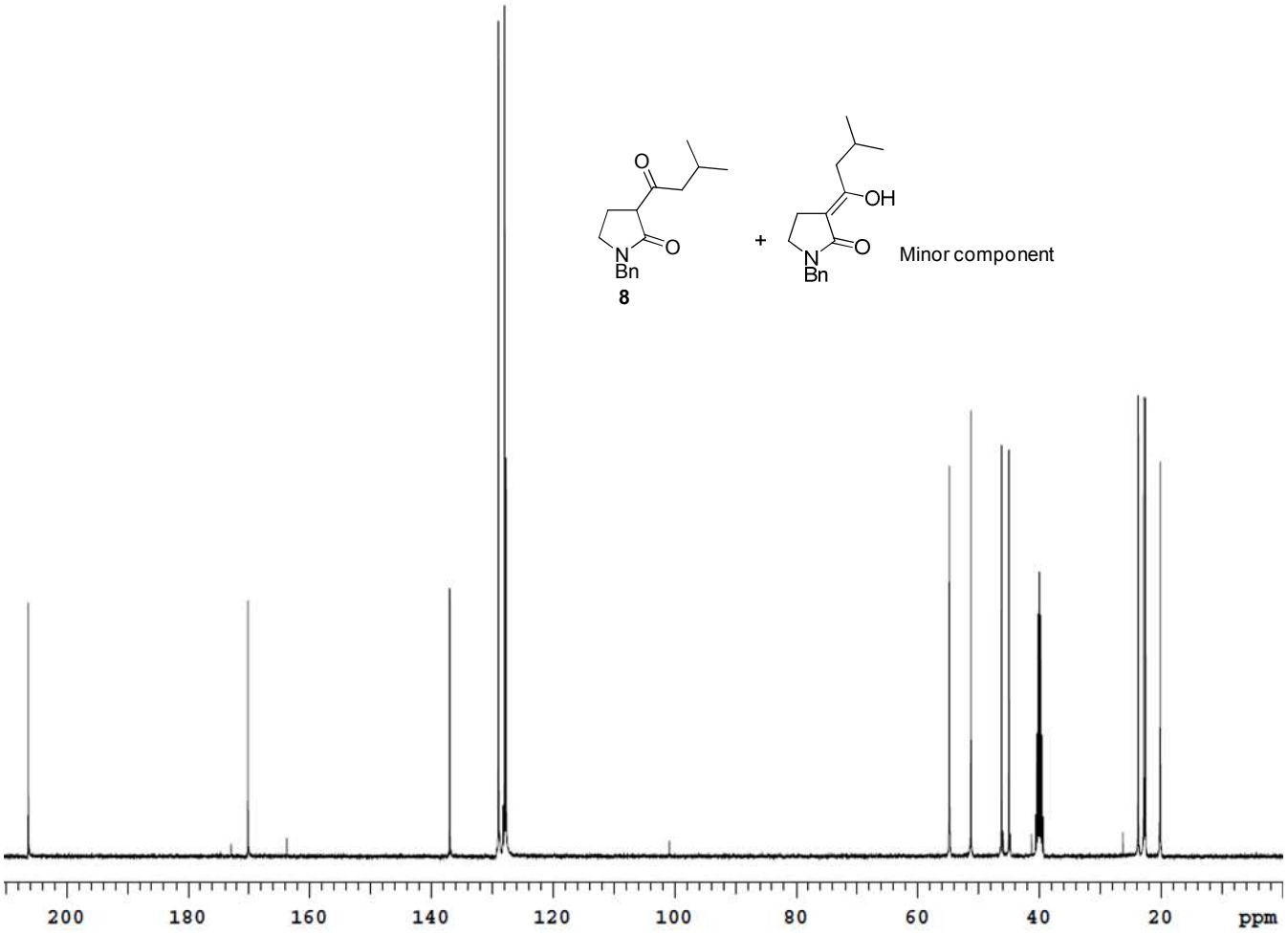

**Processed Channel: A1100 AU 230 nm**

| | Peak Name | Processed Channel | Retention Time (min) | Area | % Area | Height |
|---|---|---|---|---|---|---|
| 1 | enantiomer 2609766 | A1100 AU 230 nm | 36.332 | 125216 | 0.90 | 1939 |
| 2 | diastereomer 2609766 | A1100 AU 230 nm | 41.710 | | | |
| 3 | 2609766 | A1100 AU 230 nm | 51.233 | 13759937 | 99.10 | 153337 |

NMR Spectra


O
Li
O
N
Bn
7
7
6
5
4
3
2
1
ppm


O
O
N
Bn
8
+
OH
O
N
Bn
Minor component
12
11
10
9
8
7
6
5
4
3
2
1
ppm


O
O
N
Bn
8
+
OH
O
N
Bn
Minor component
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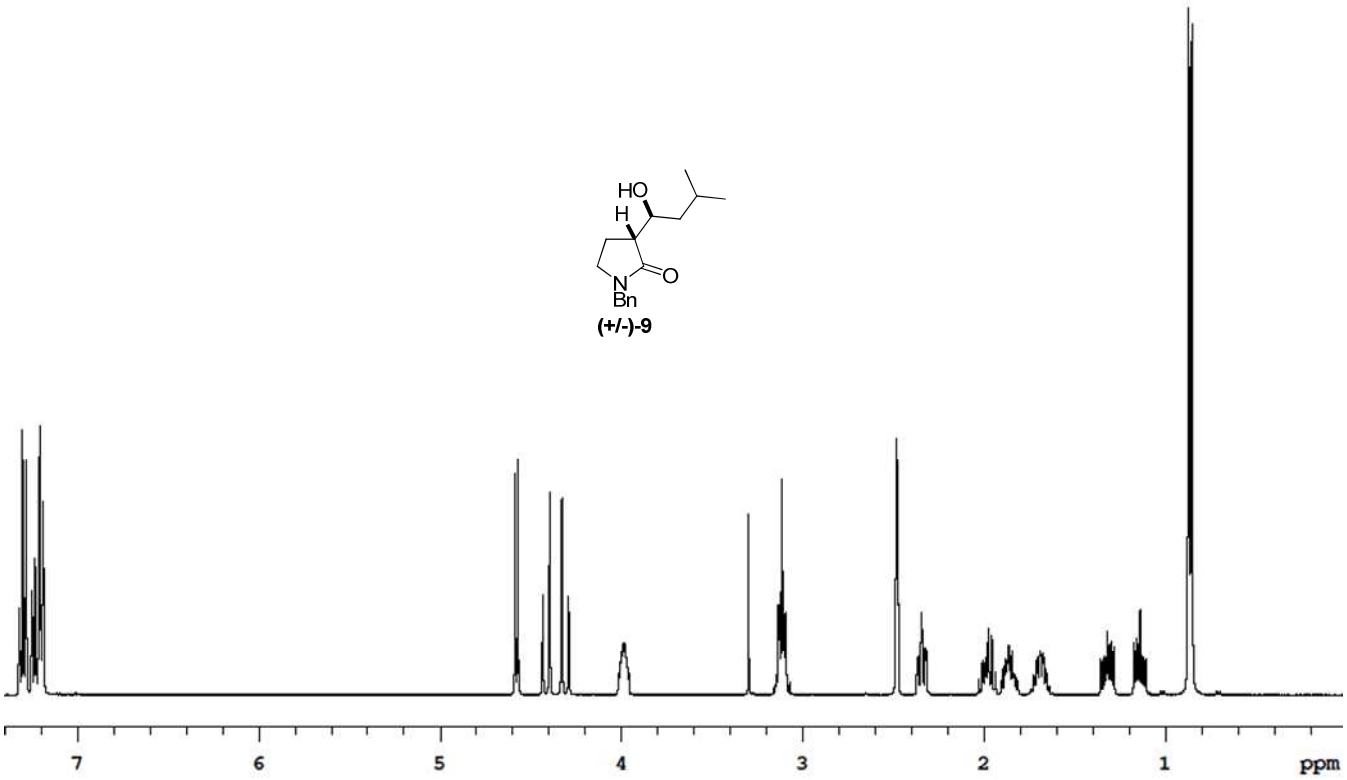
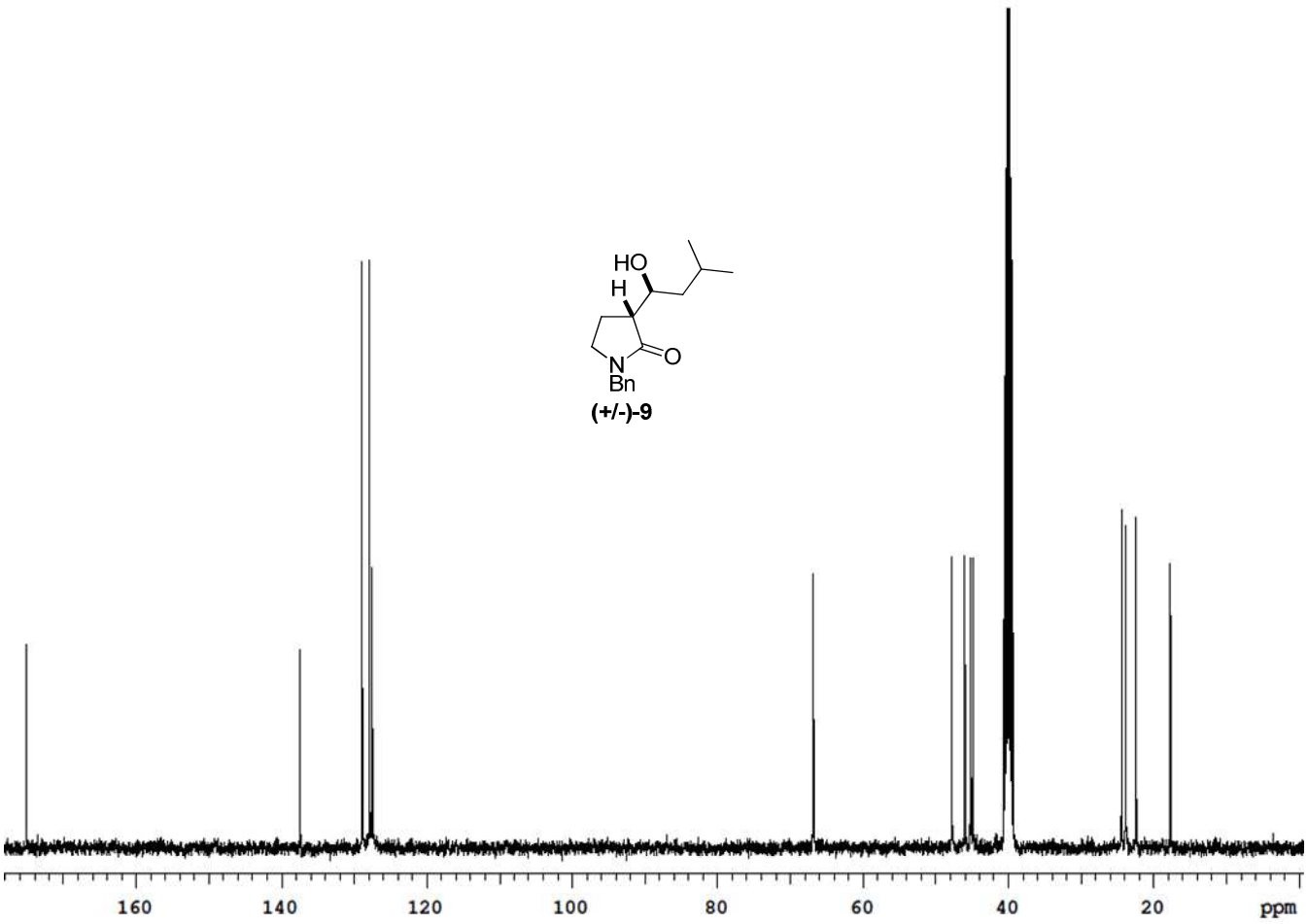
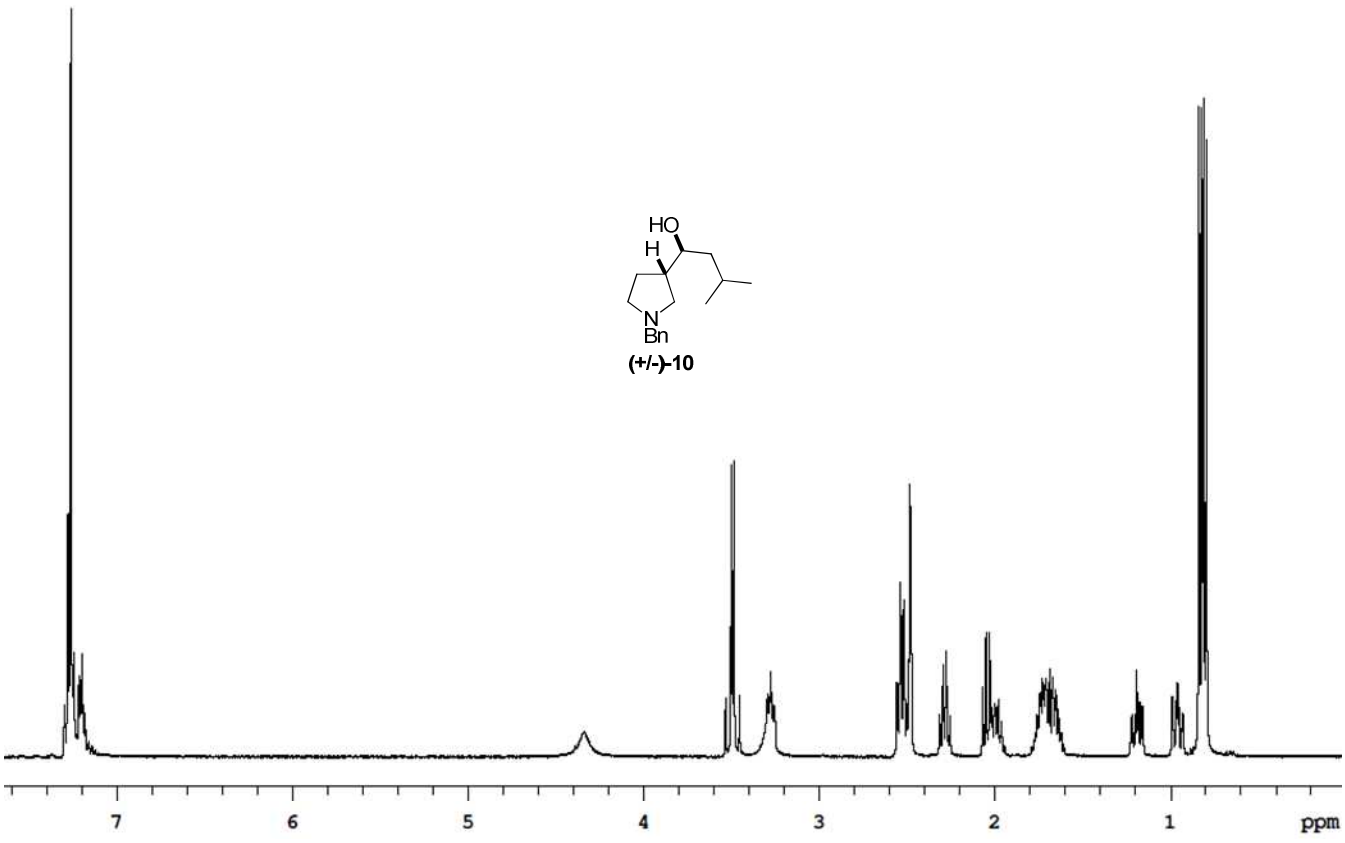
180
160
140
120
100
80
60
40
20
ppm


HO
H
O
N
Bn
(+/-)-9
7
6
5
4
3
2
1
ppm


HO
H
N
Bn
O
(+/-)-9
160
140
120
100
80
60
40
20
ppm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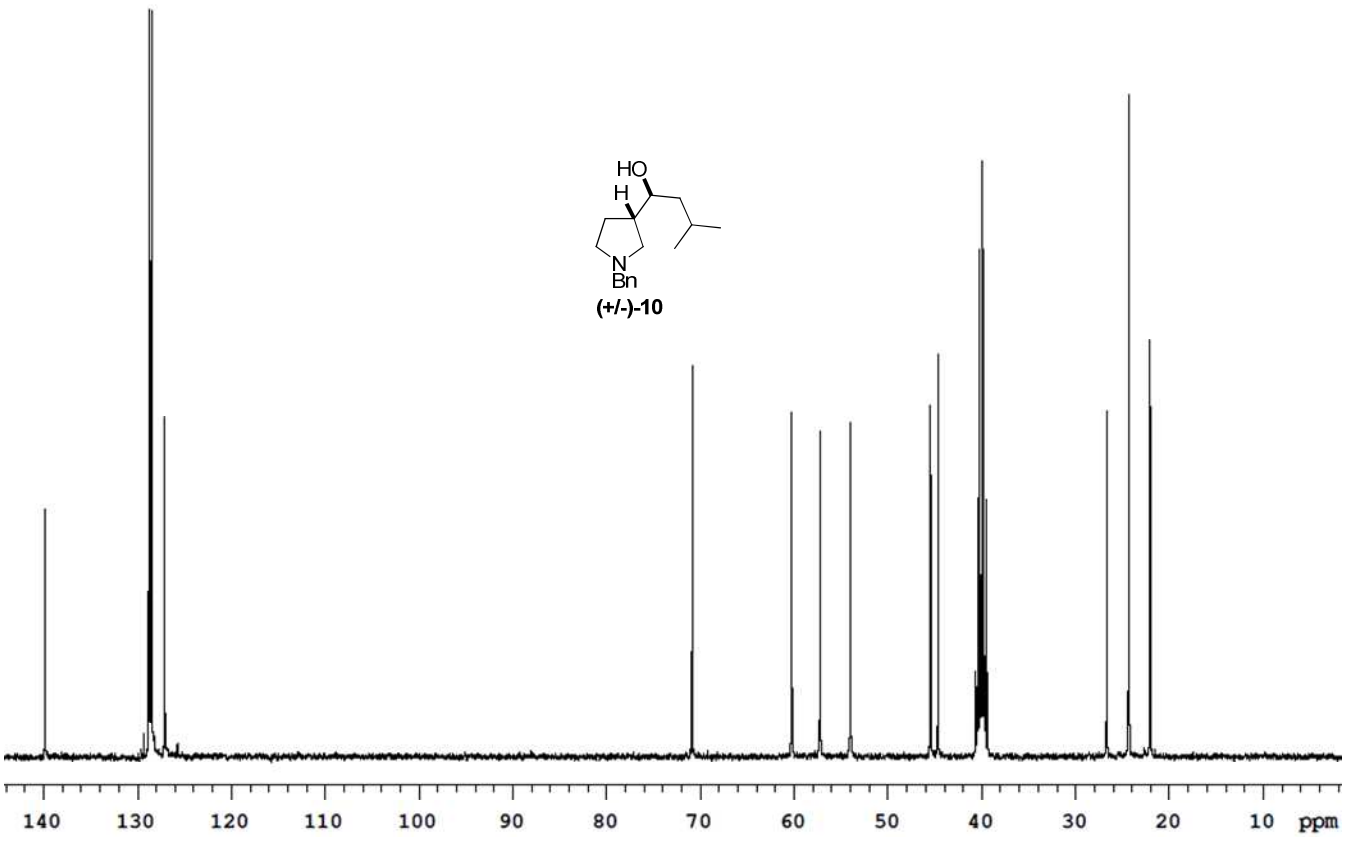
H
N
Bn
(+/-)-10
7
6
5
4
3
2
1
ppm


HO
H
N
Bn
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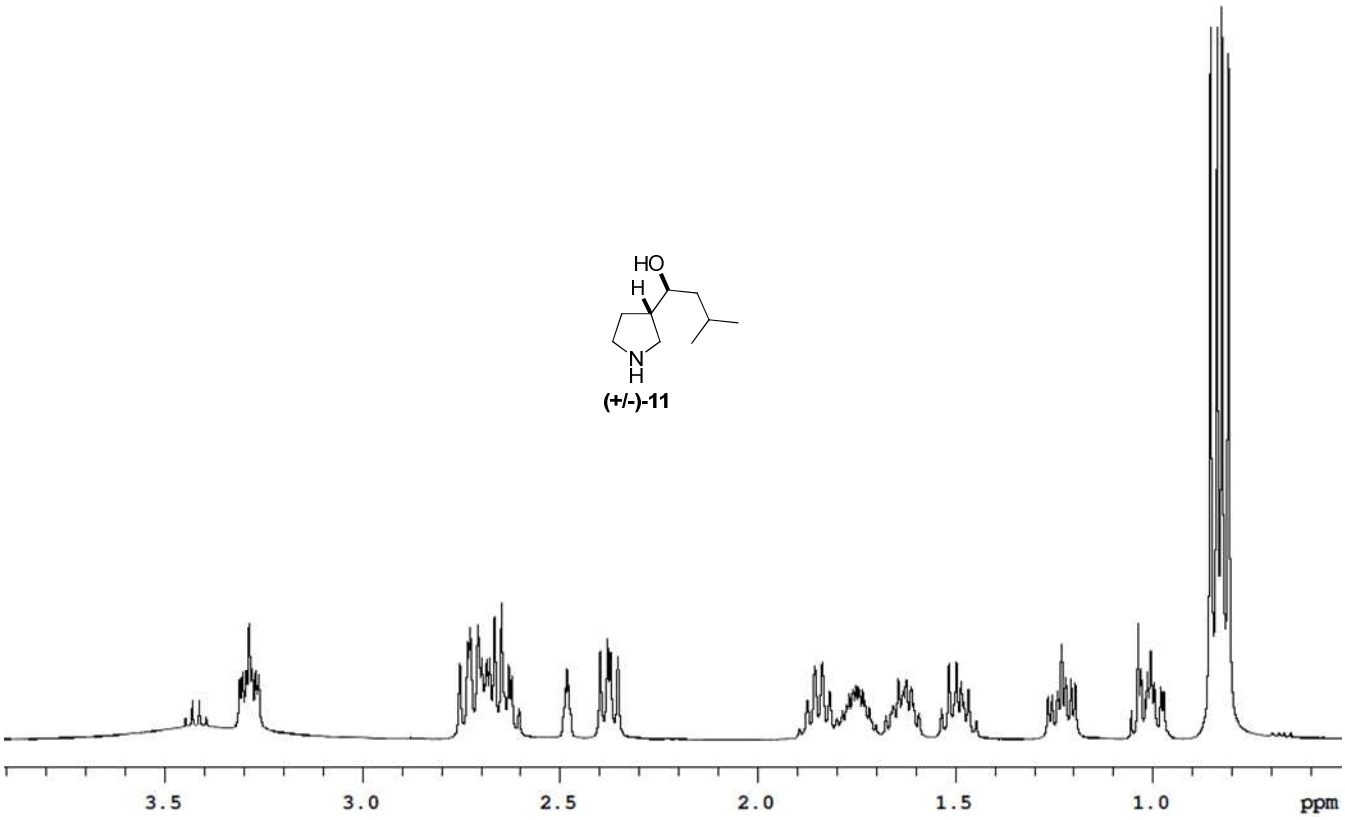
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

**(+/-)-10**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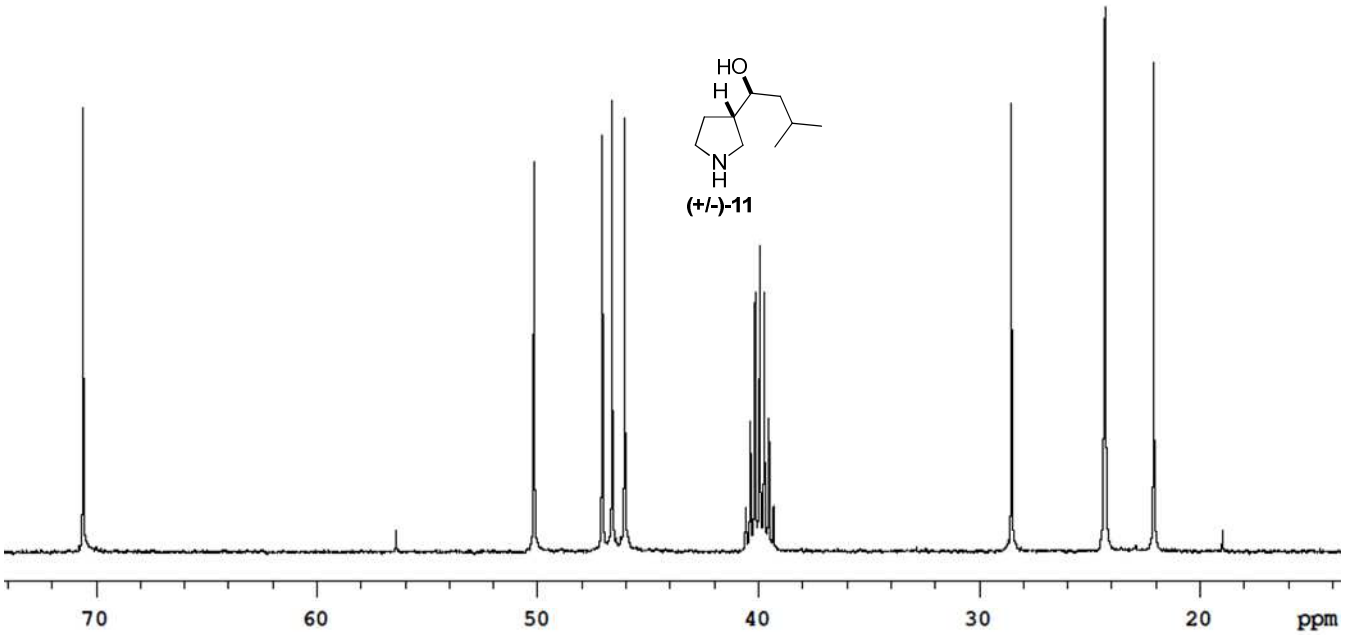
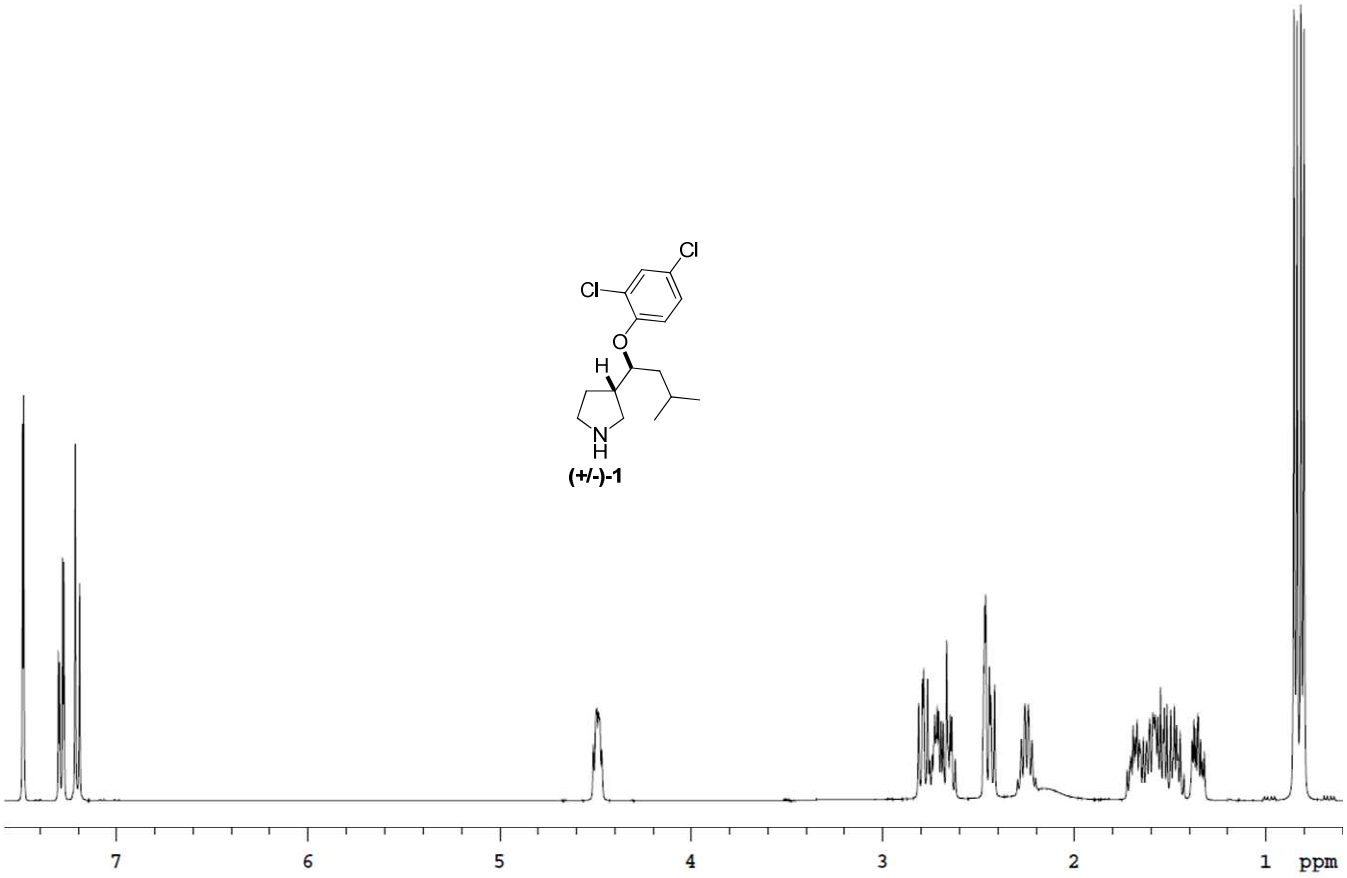
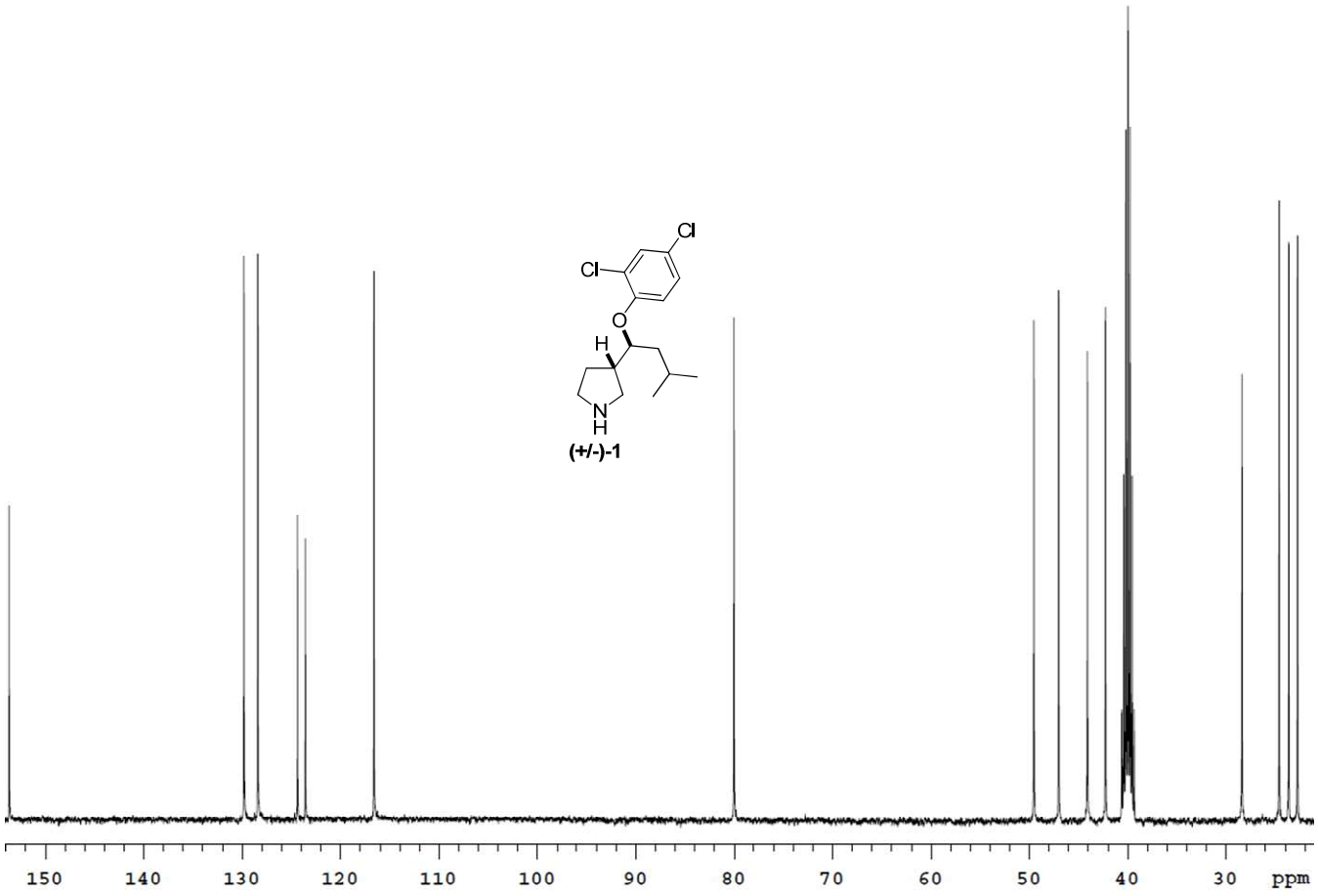
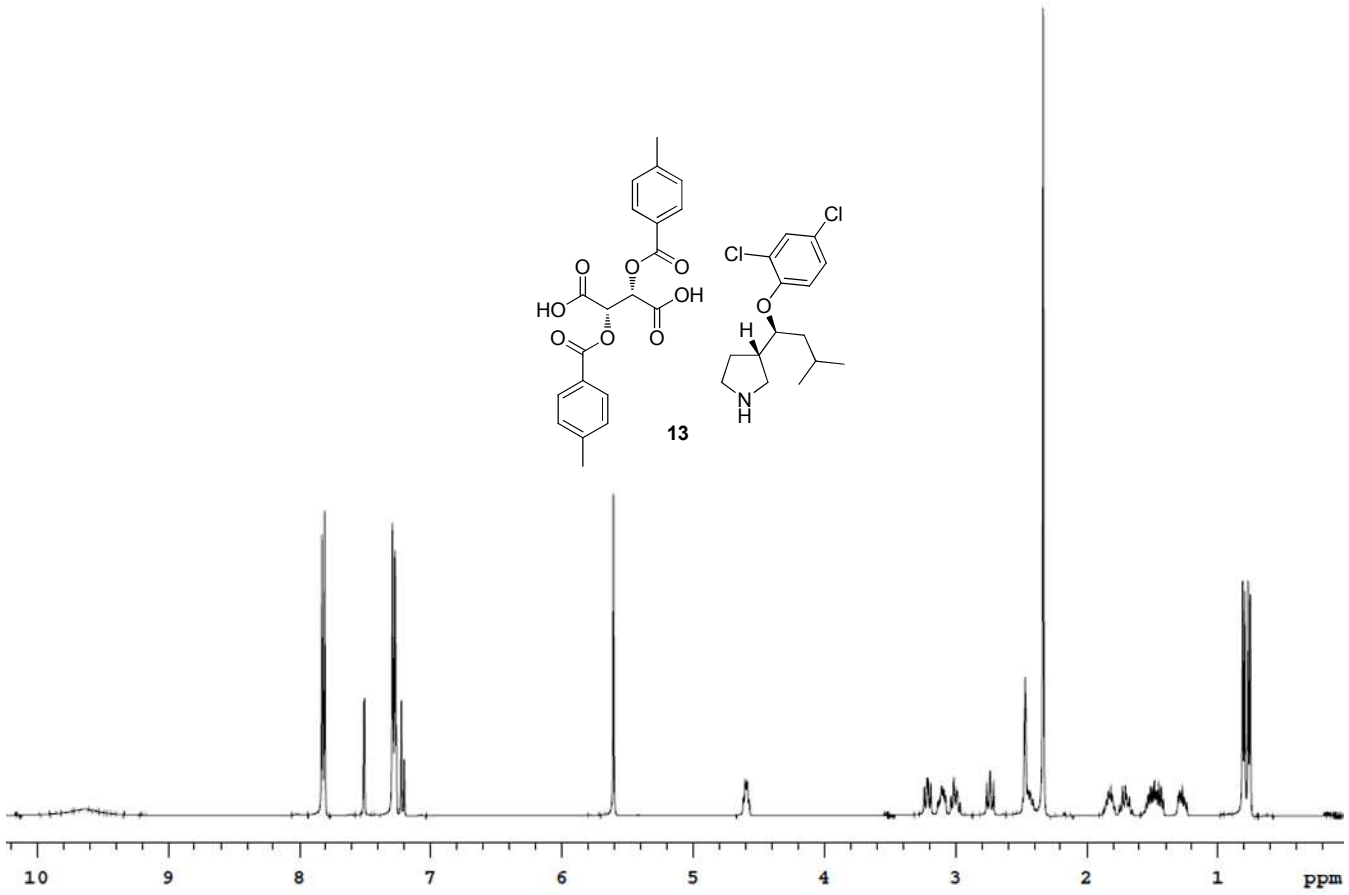
H
N
H
3.5
3.0
2.5
2.0
1.5
1.0
ppm

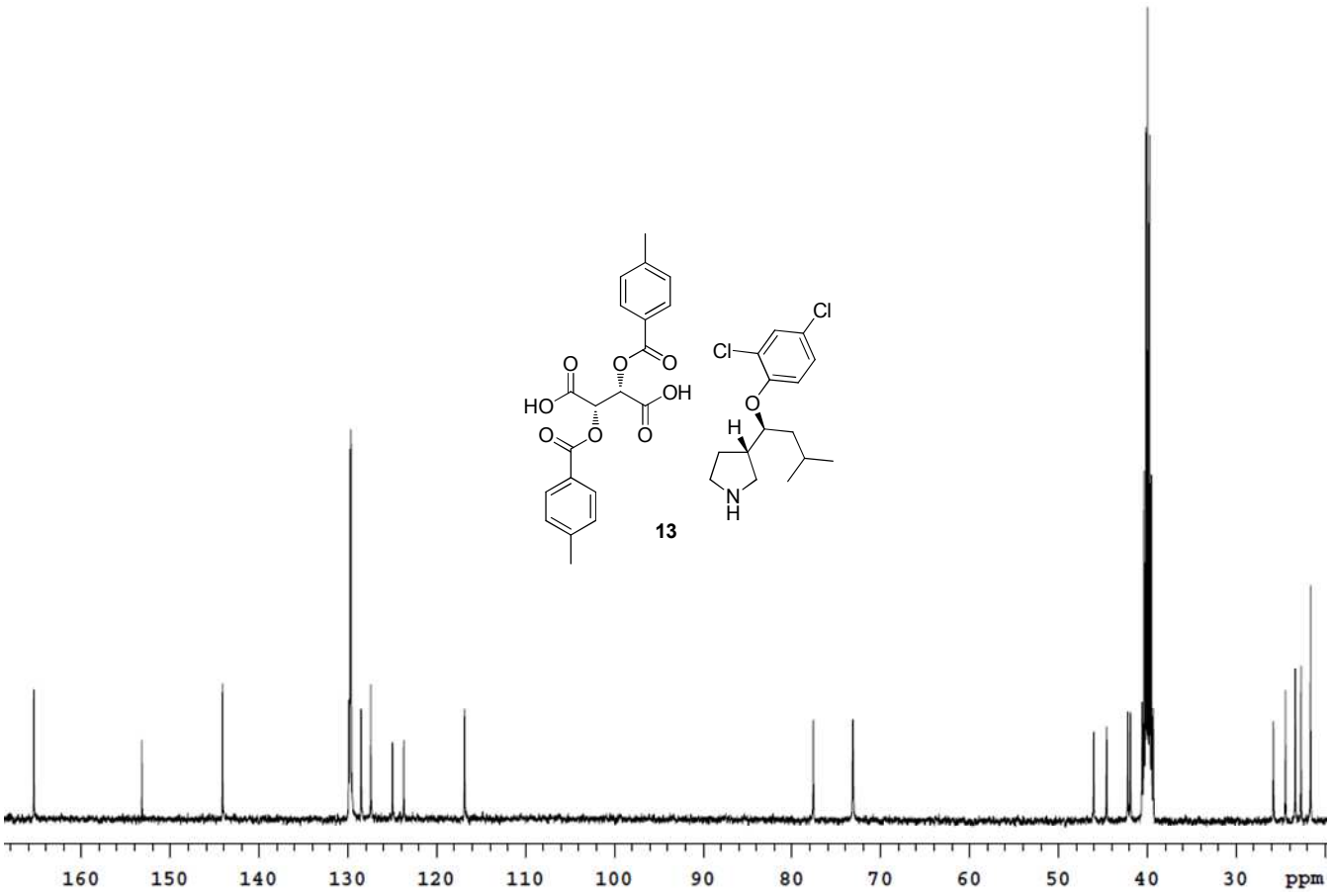
**(+/-)-11**


HO
H
N
H
(+/-)-11
70
60
50
40
30
20
ppm


Cl
Cl
O
H
N
H
(+/-)-1
7
6
5
4
3
2
1
ppm


Cl
Cl
O
H
N
H
(+/-)-1
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm


HO
O
O
O
O
O
O
OH
13
Cl
Cl
O
H
N
H
10
9
8
7
6
5
4
3
2
1
ppm


13
160
150
140
130
120
110
100
90
80
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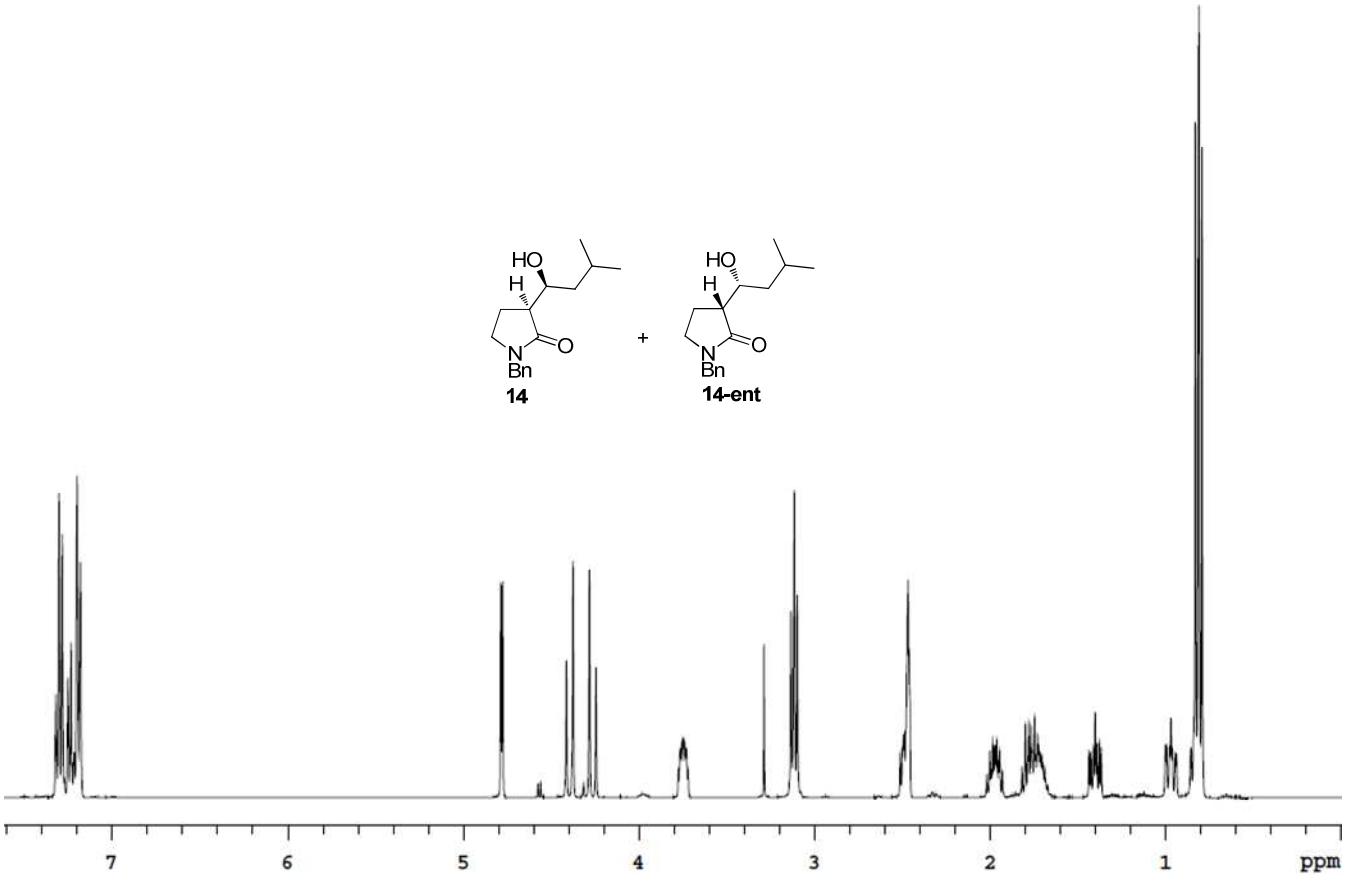
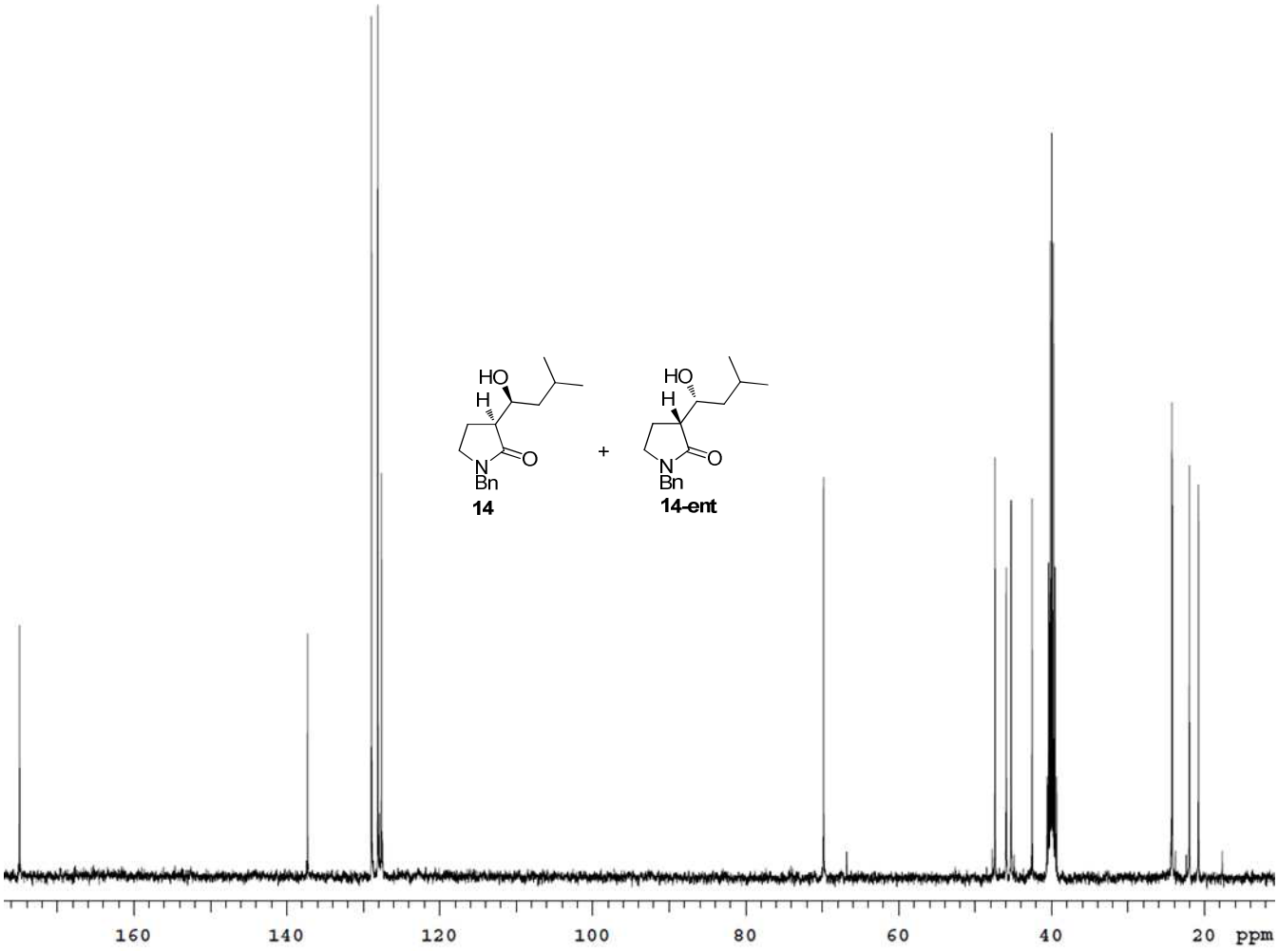
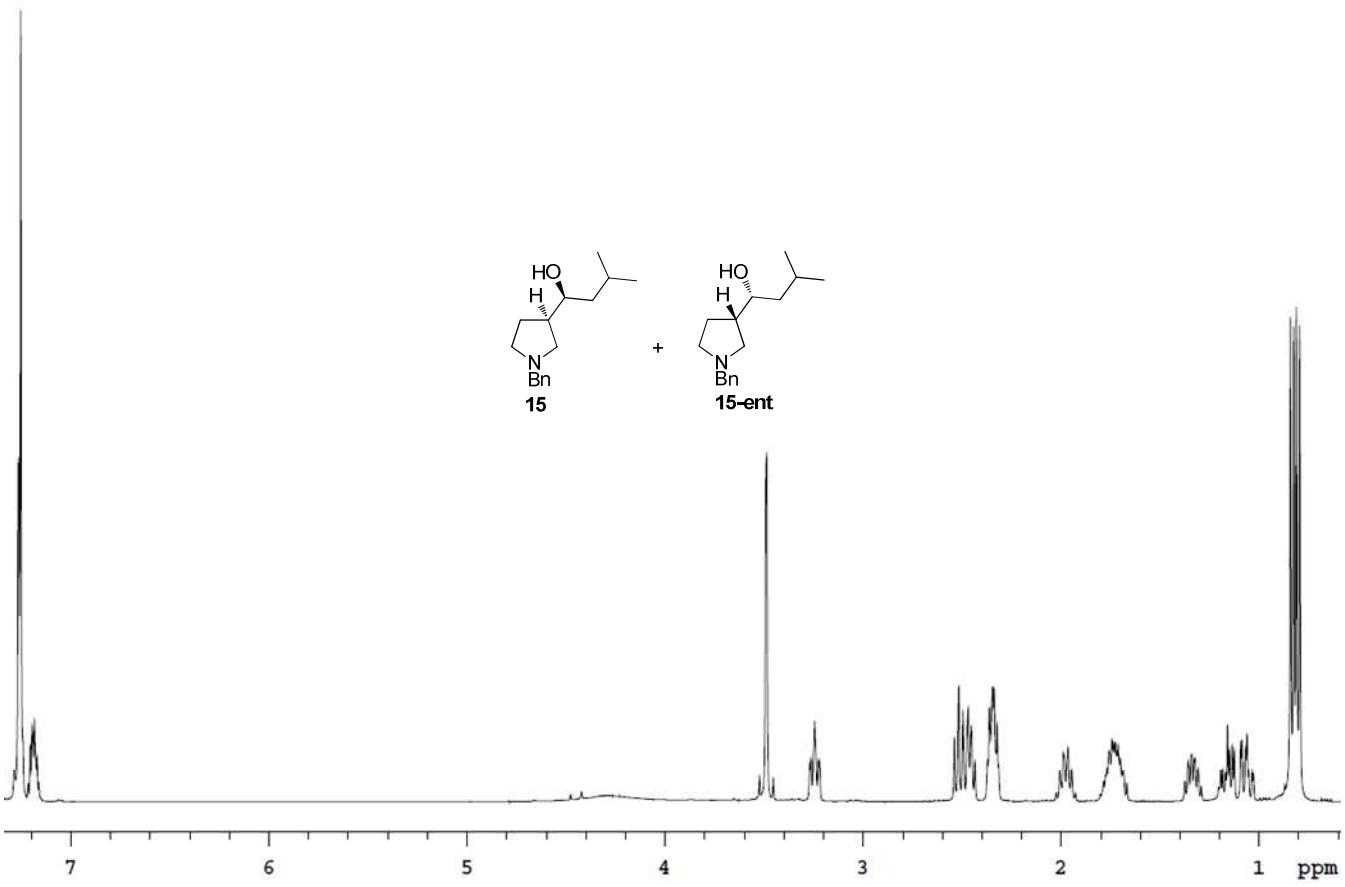
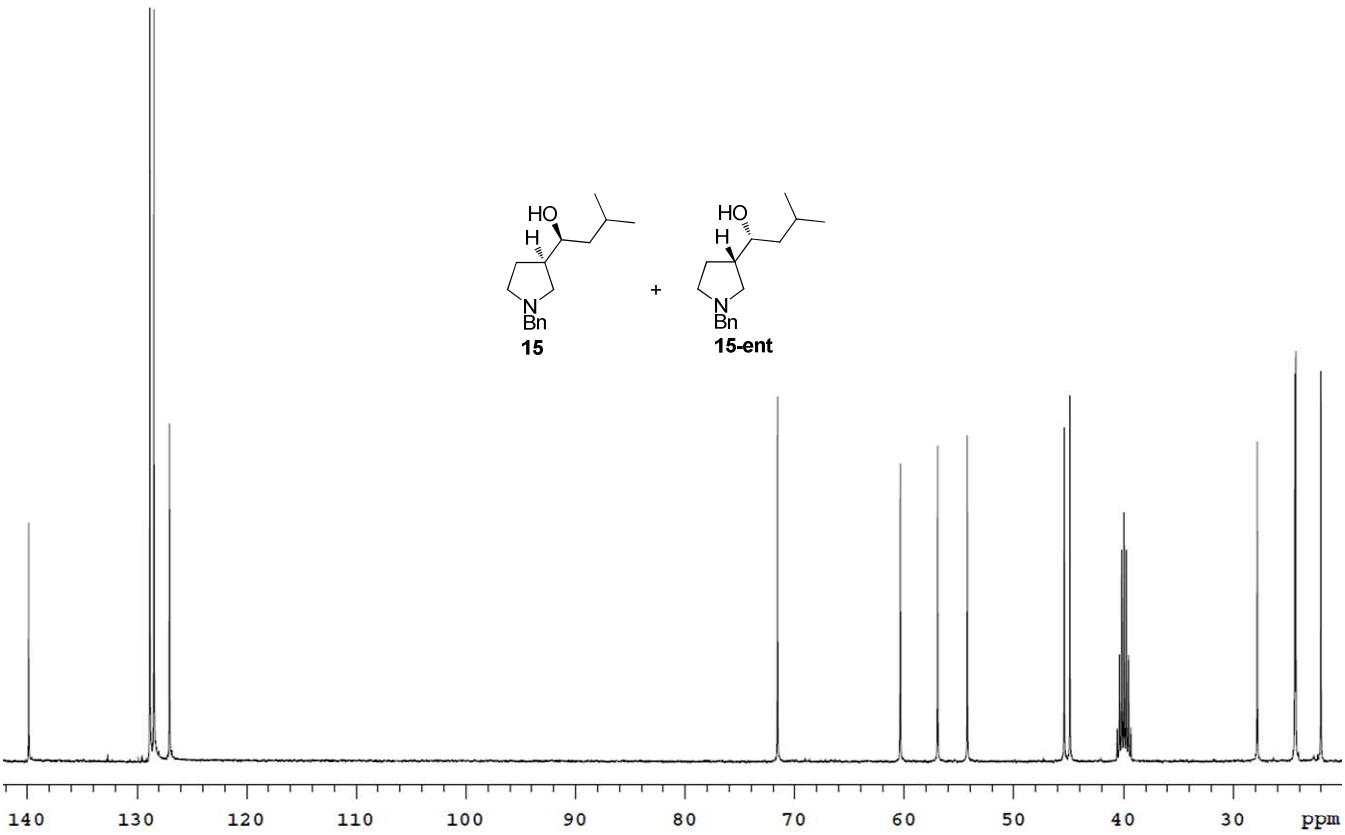
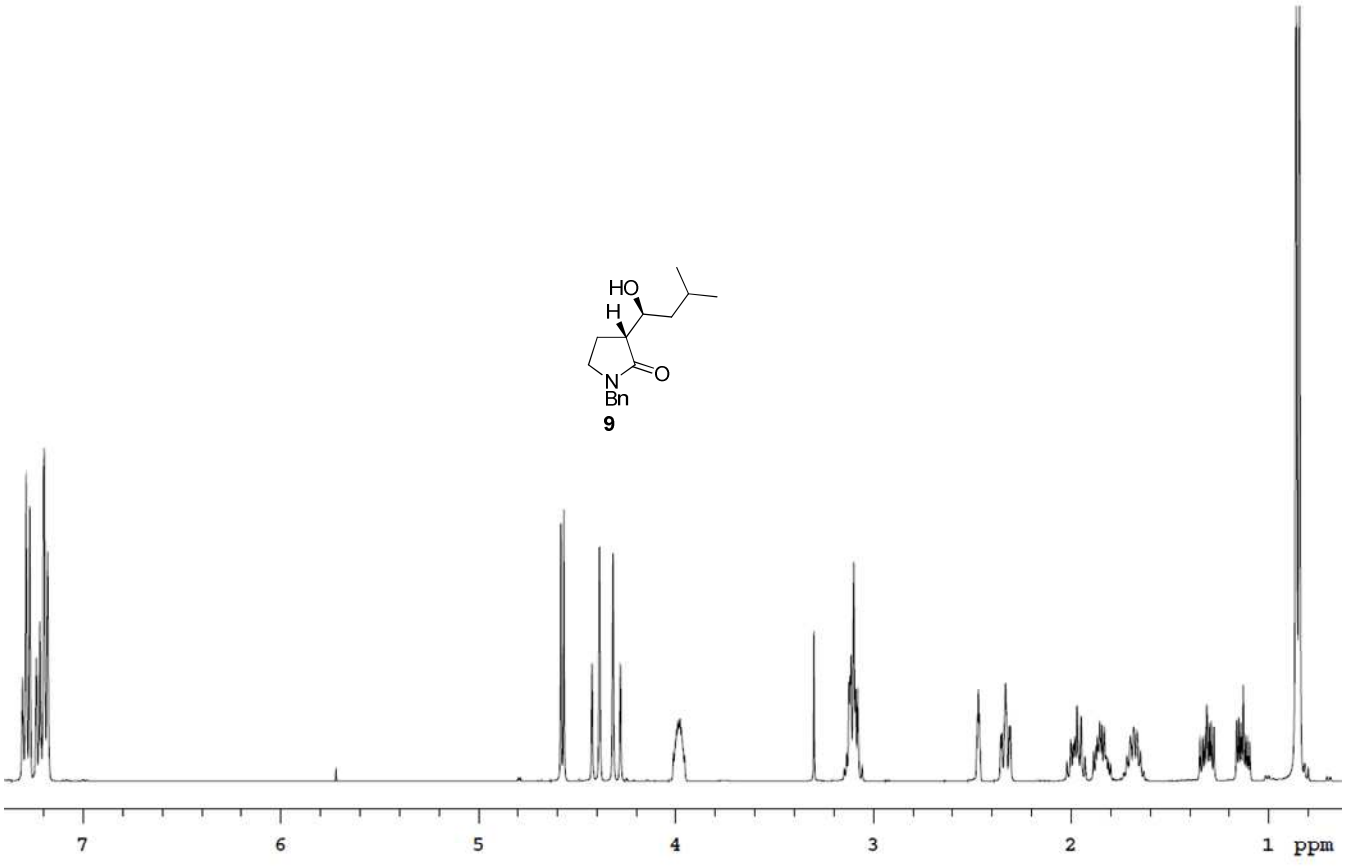
60
50
40
30
ppm

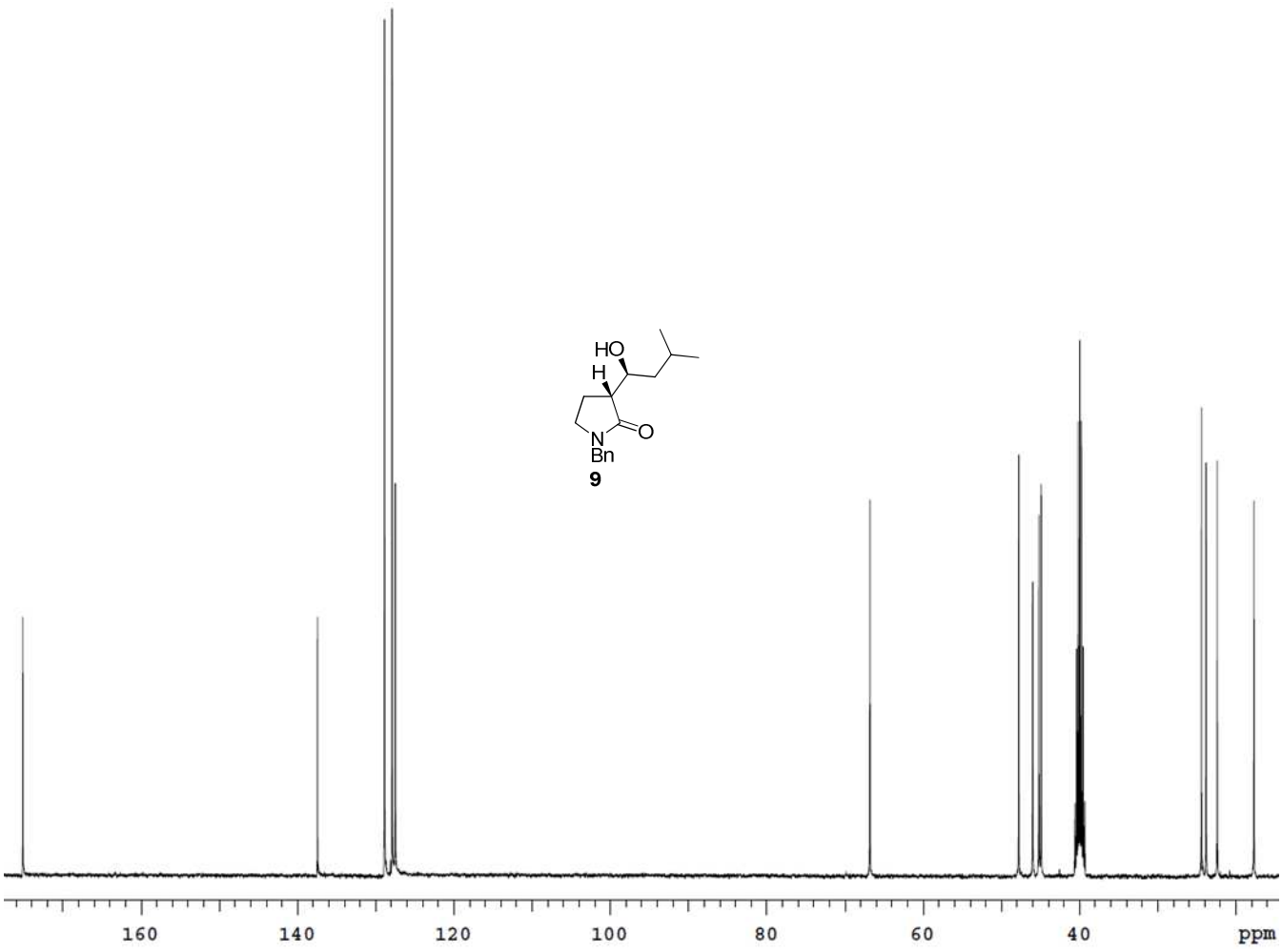

14
14-ent
7
6
5
4
3
2
1
ppm


HO
H
N
Bn
O
14
+
HO
H
N
Bn
O
14-ent
160
140
120
100
80
60
40
20
ppm

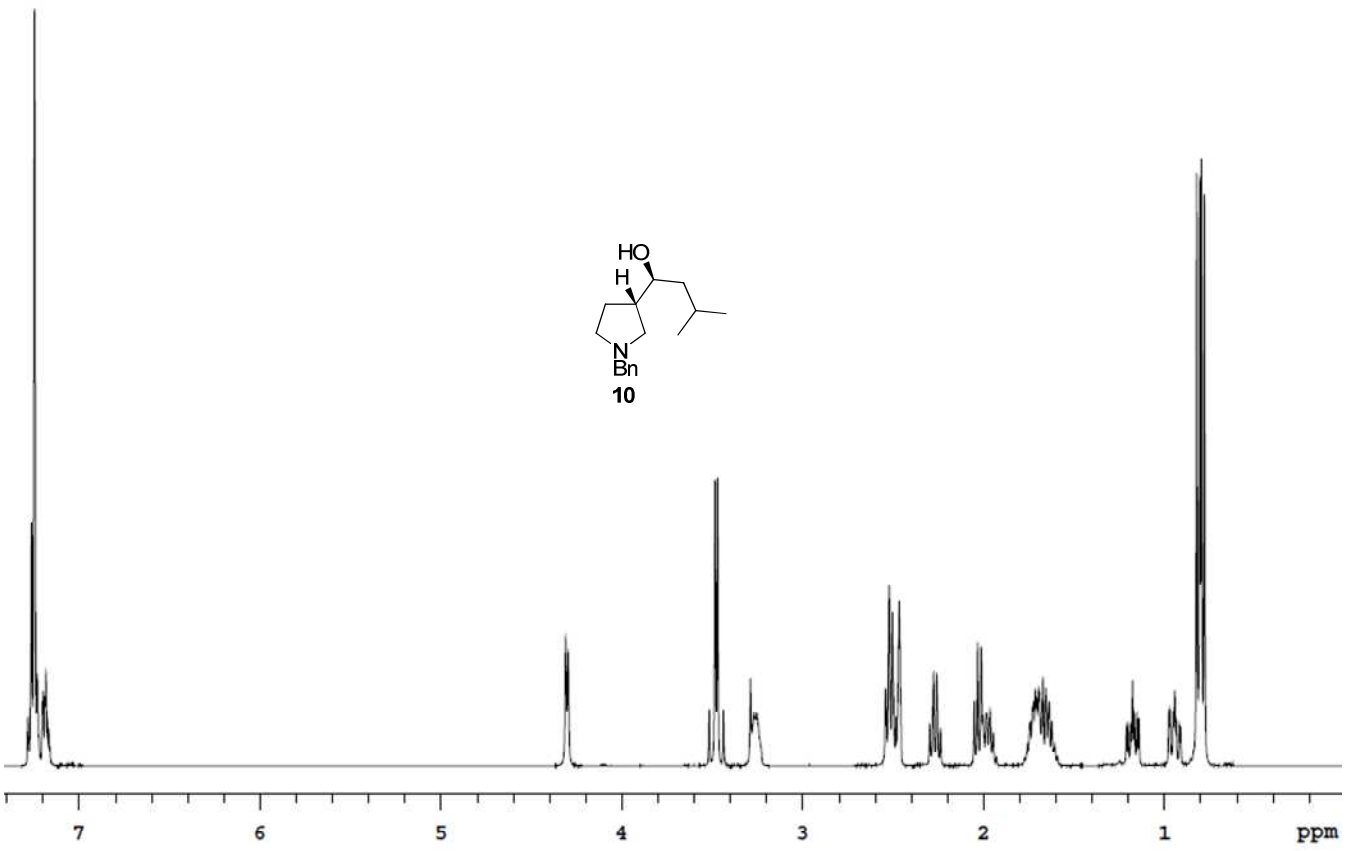

HO
H
N
Bn
15
+
HO
H
N
Bn
15-ent
7
6
5
4
3
2
1
ppm

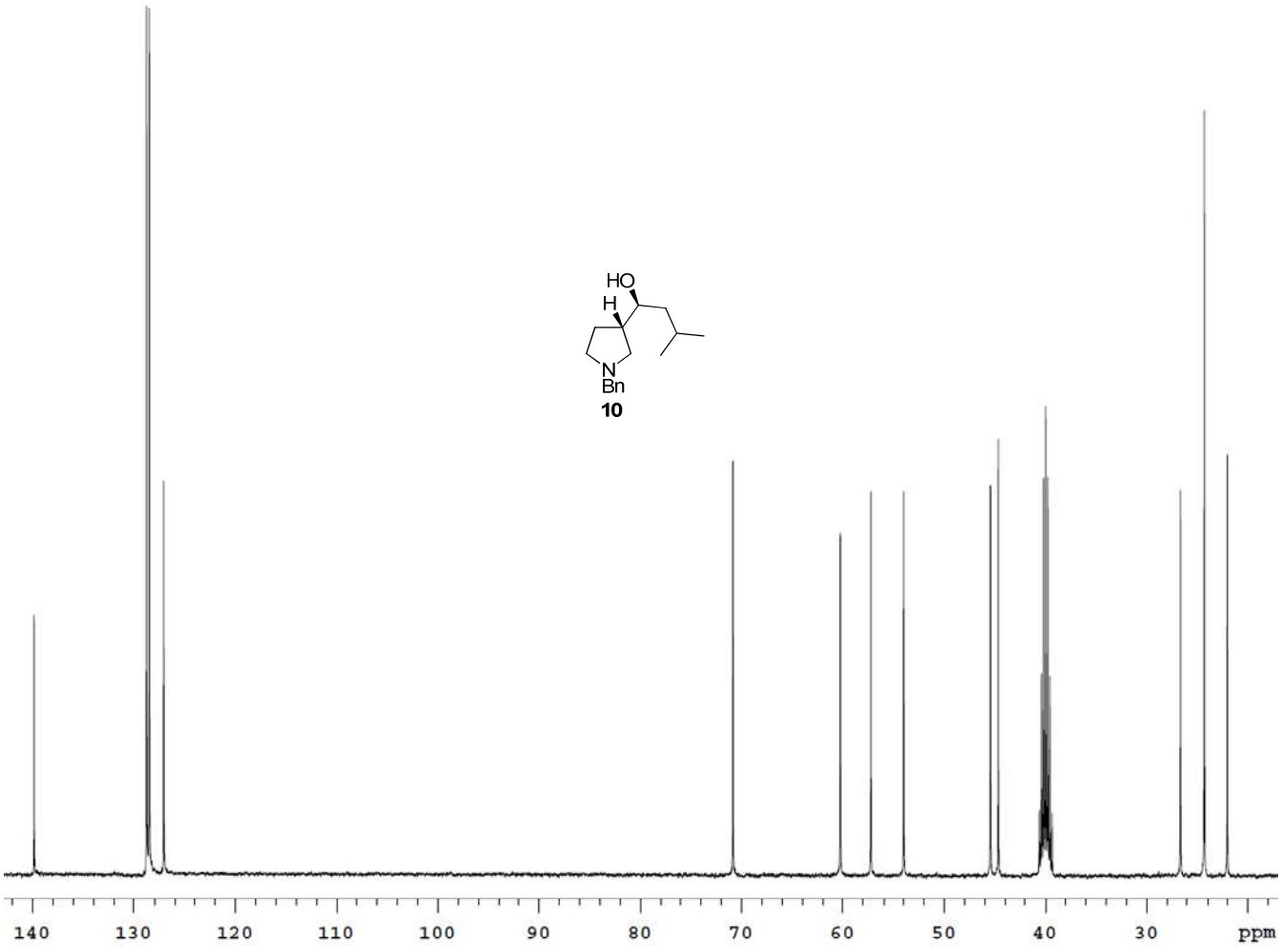

HO
H
N
Bn
15
+
HO
H
N
Bn
15-ent
140
130
120
110
100
90
80
70
60
50
40
30
ppm

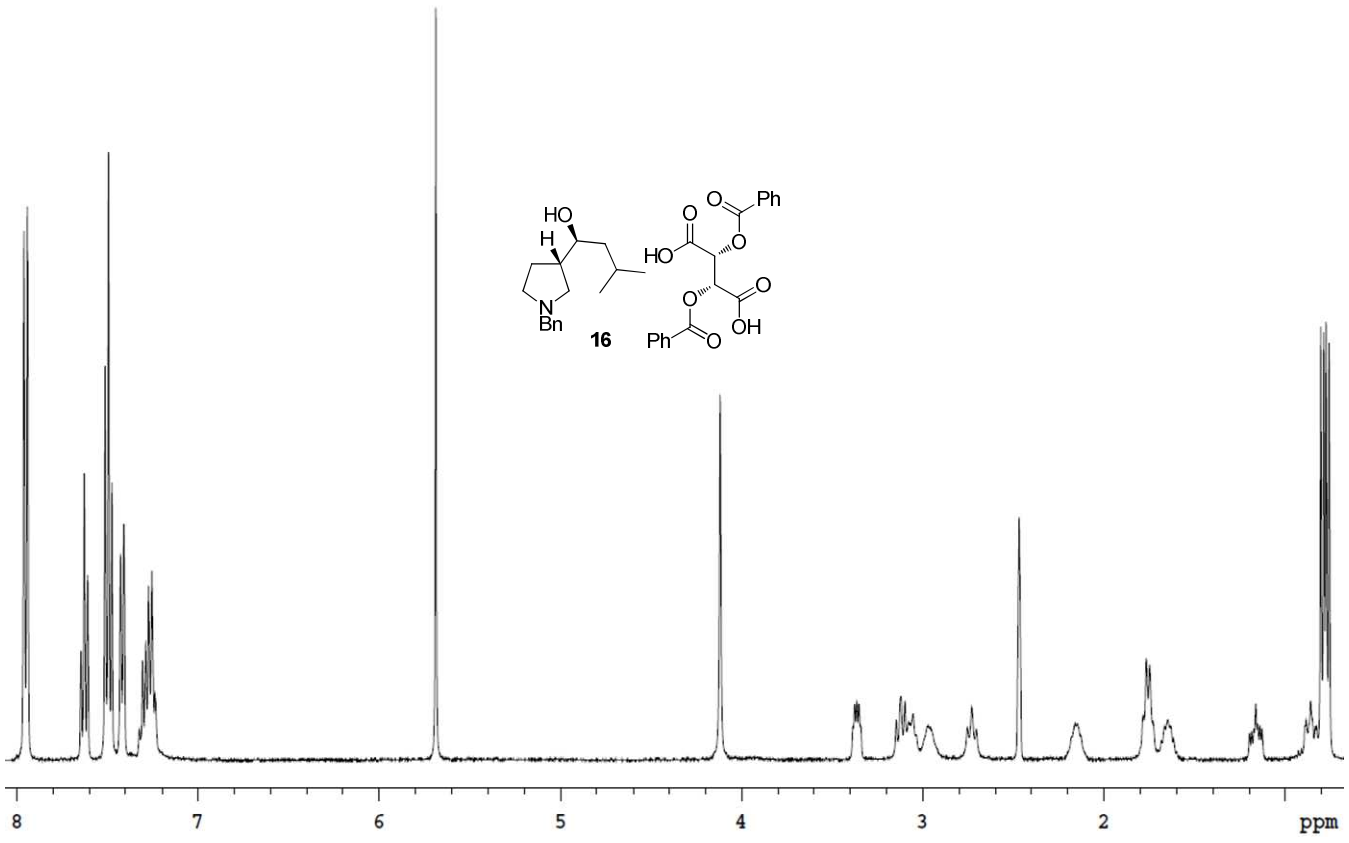

HO
H
O
N
Bn
9
7
6
5
4
3
2
1
ppm

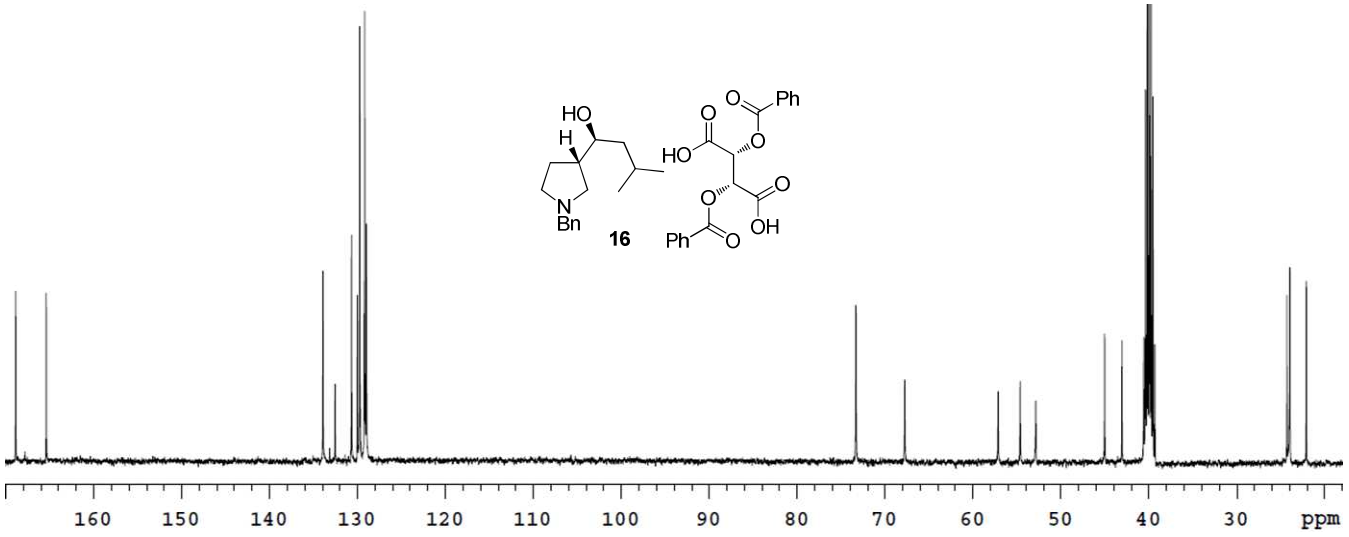


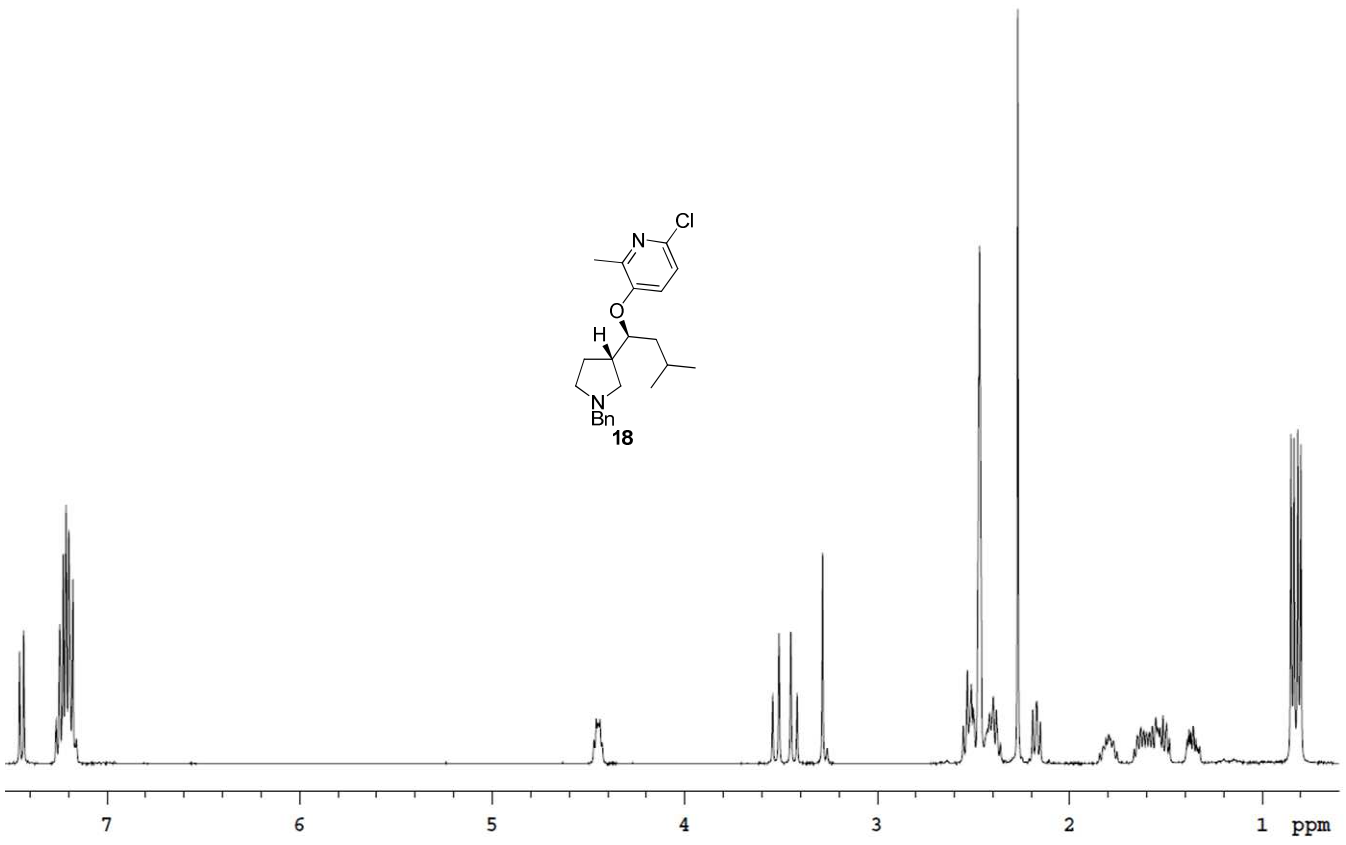

**9**

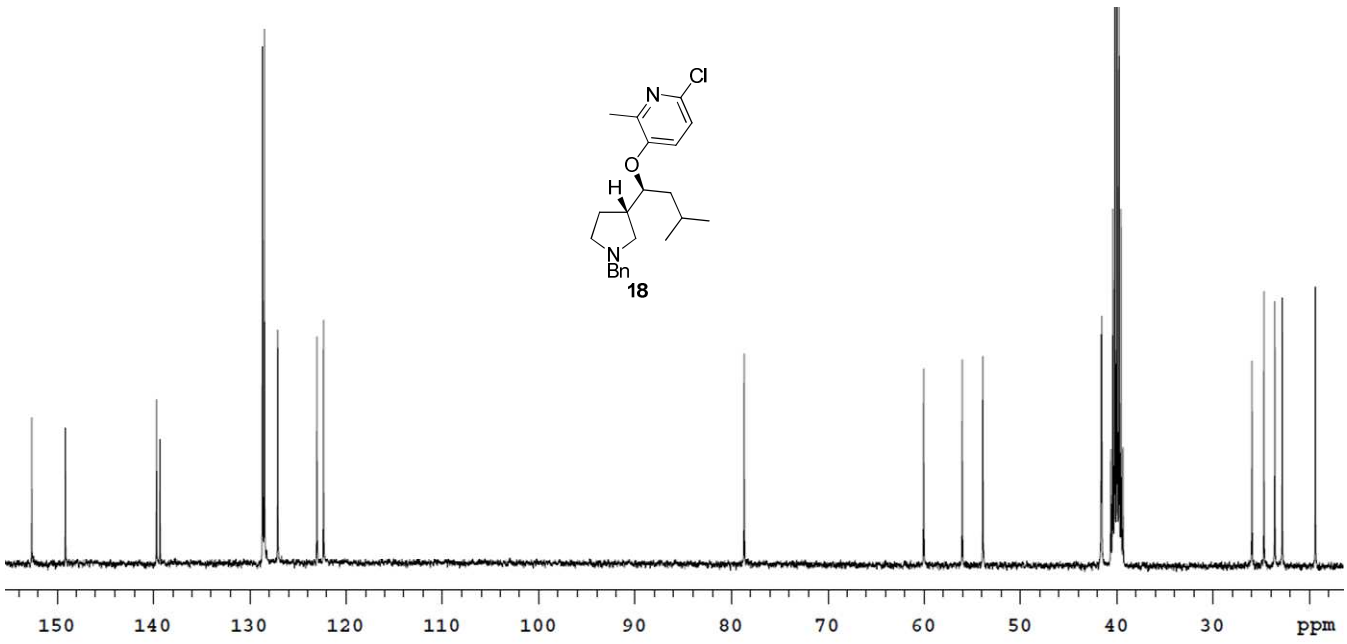

HO
H
N
Bn
10
7
6
5
4
3
2
1
ppm

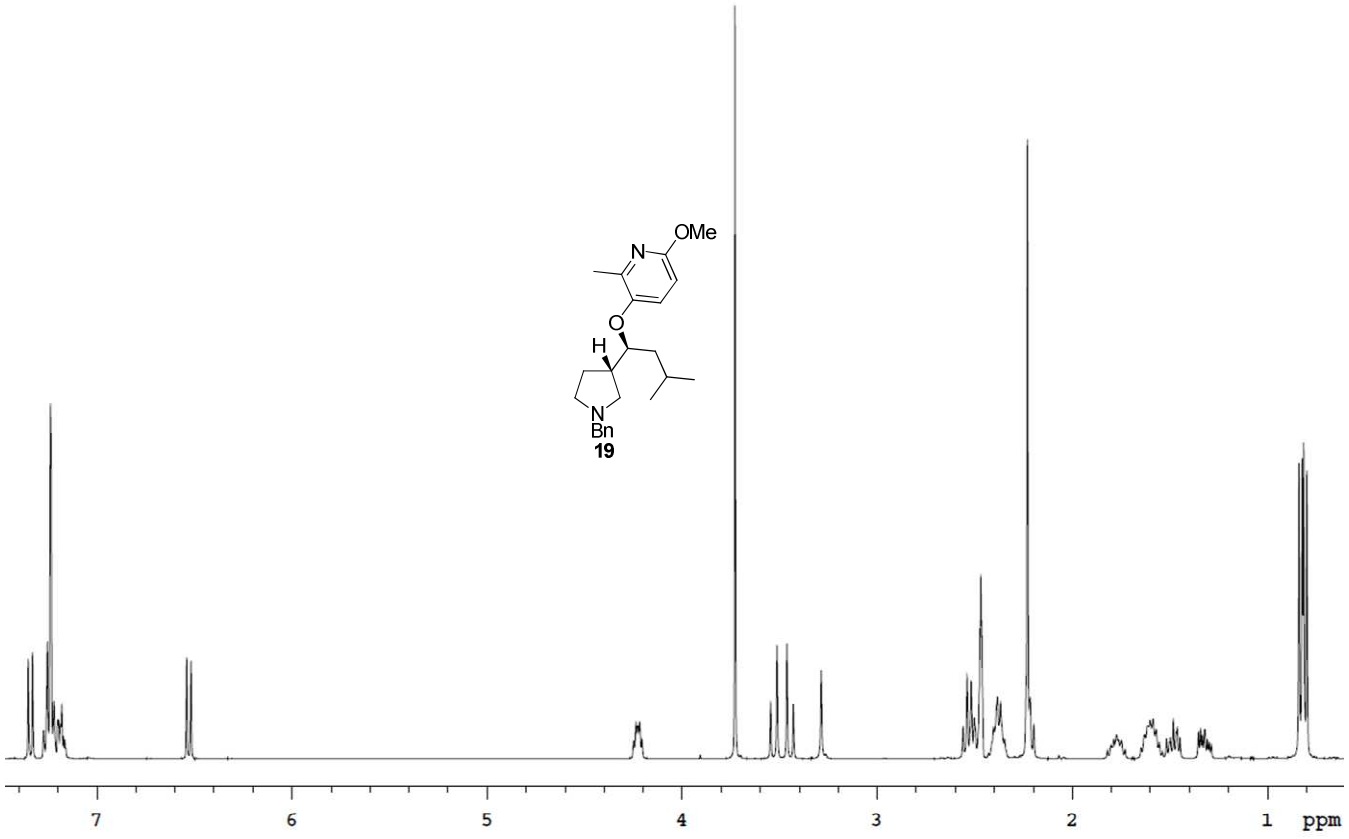

HO
H
N
Bn
10
140
130
120
110
100
90
80
70
60
50
40
30
ppm

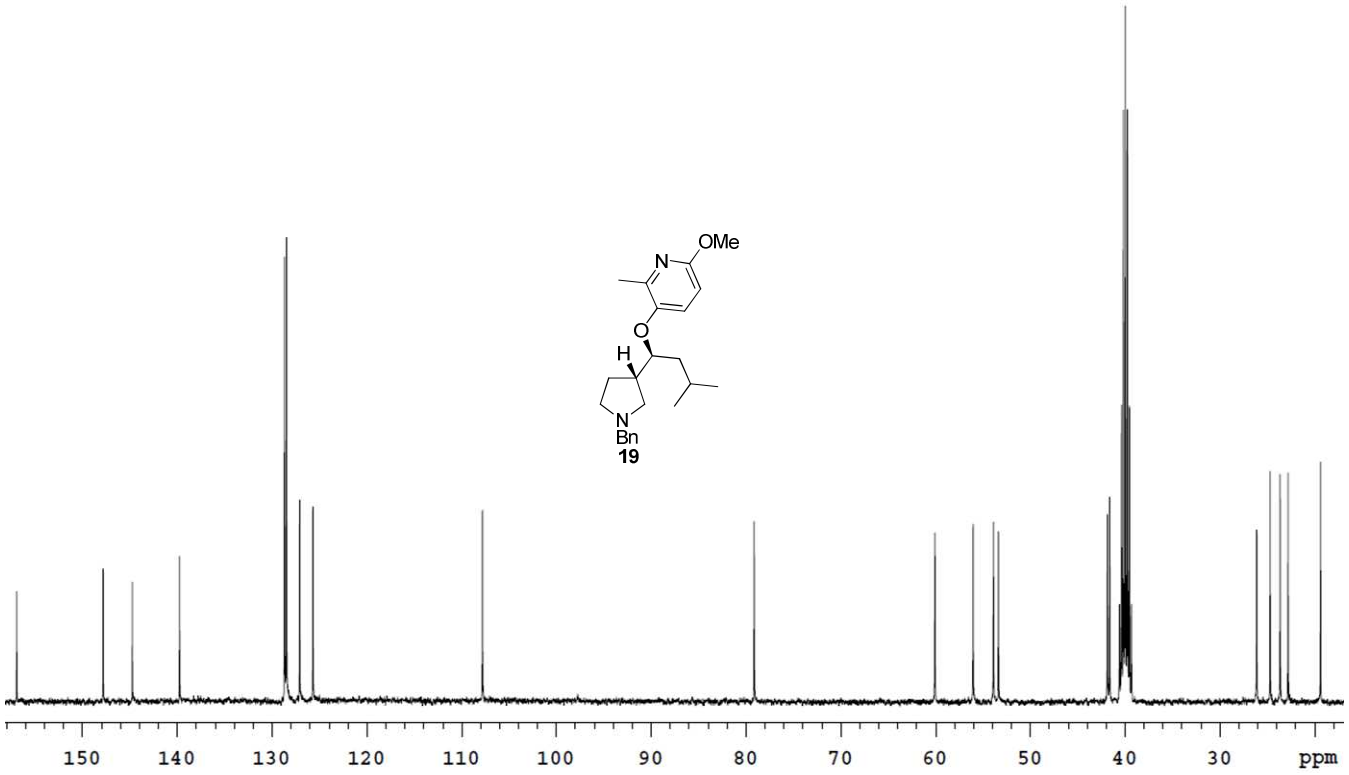

HO
H
N
Bn
HO
O
O
Ph
O
O
O
OH
Ph
O
16
8
7
6
5
4
3
2
ppm

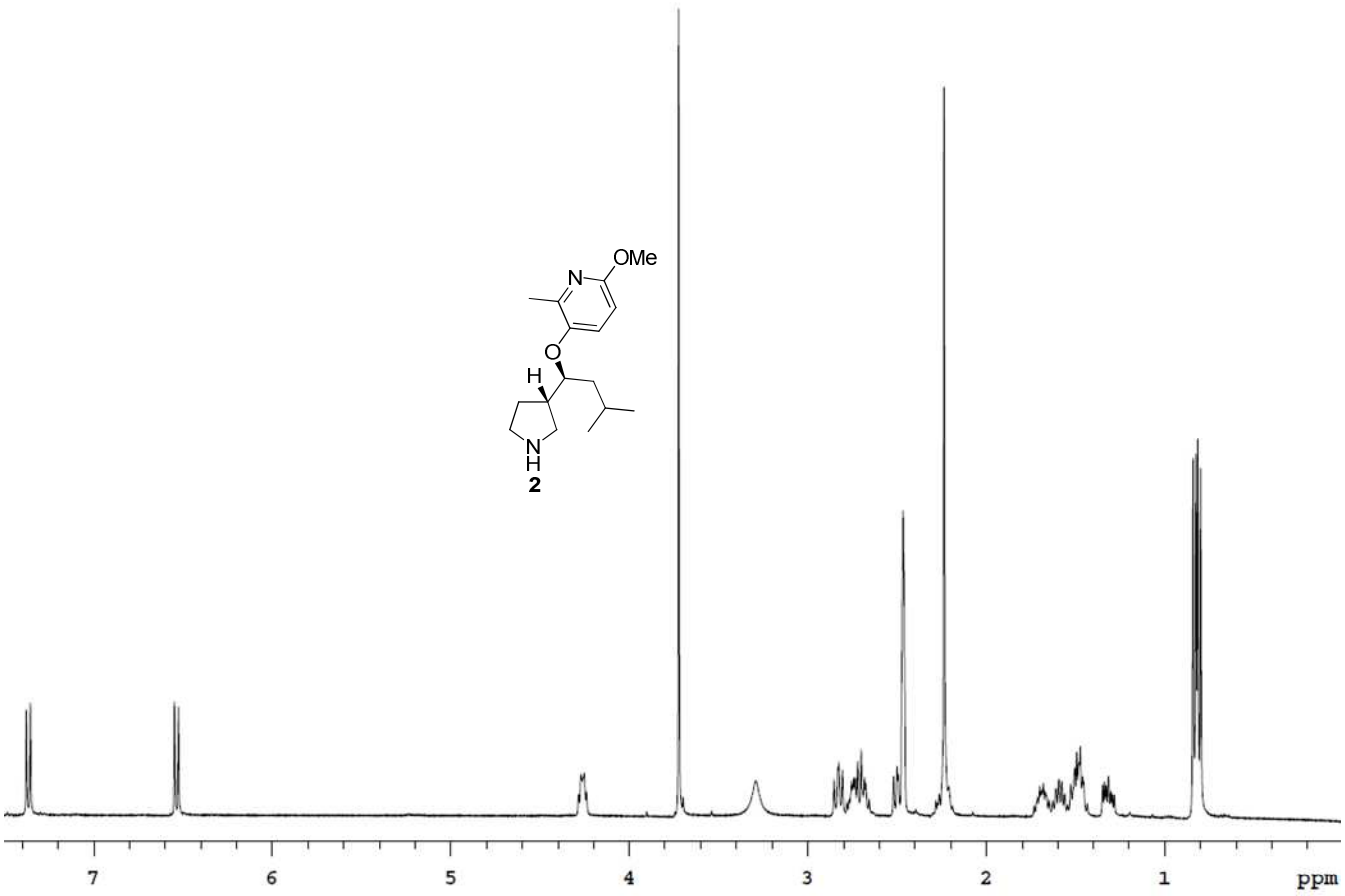

HO
H
N
Bn
HO
O
O
Ph
O
O
O
OH
Ph
O
16
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

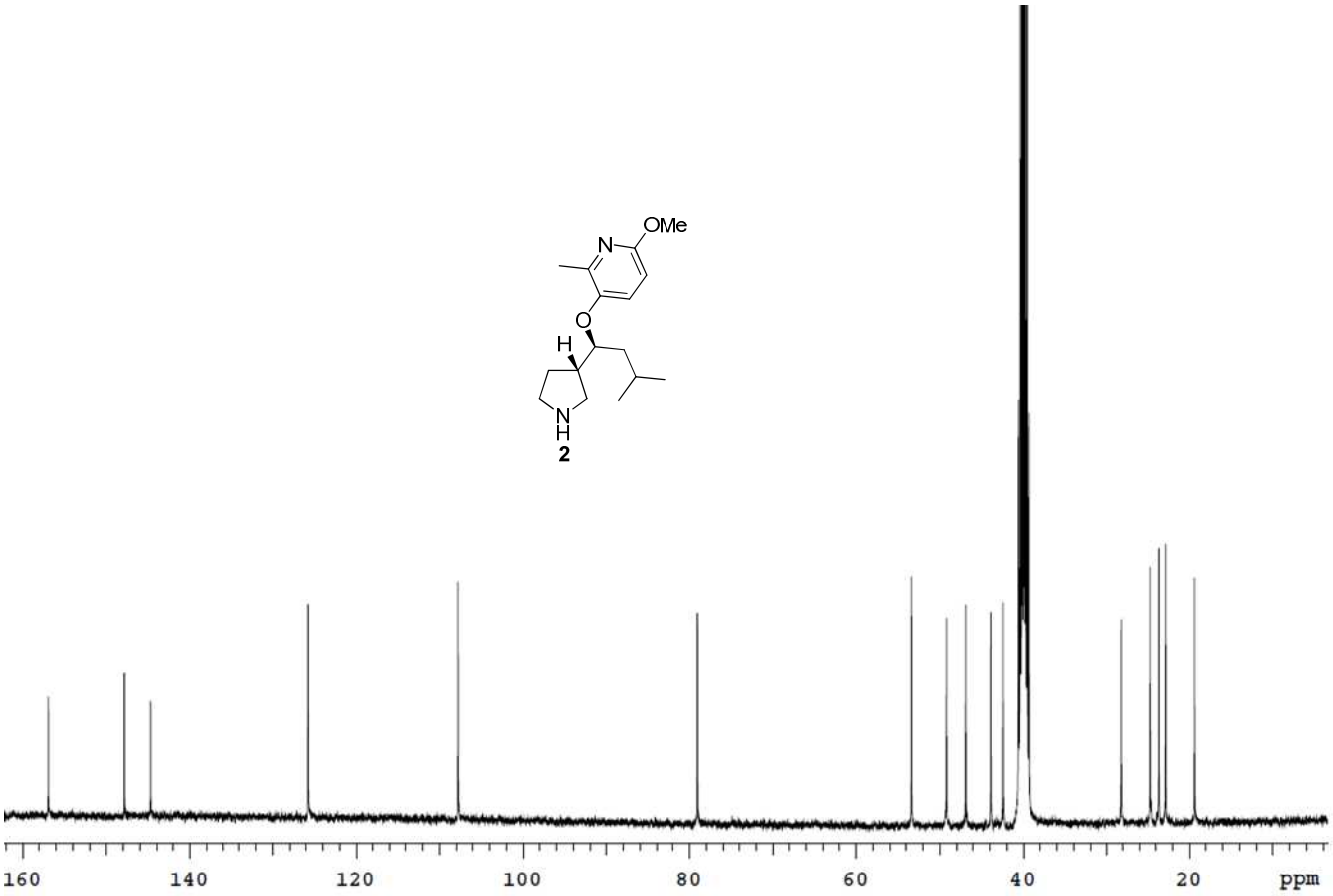

Cl
N
O
H
N
Bn
18
7
6
5
4
3
2
1
ppm


Cl
N
O
H
N
Bn
18
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

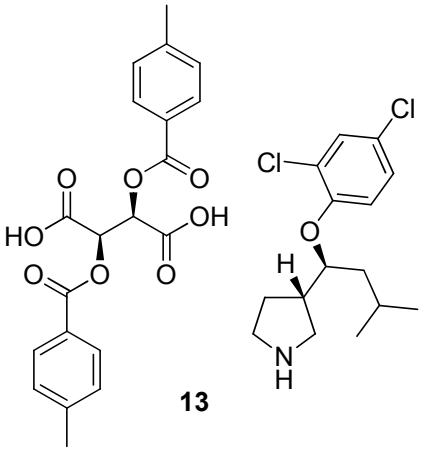

OMe
N
O
H
N
Bn
19
7
6
5
4
3
2
1
ppm


OMe
N
O
H
N
Bn
19
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

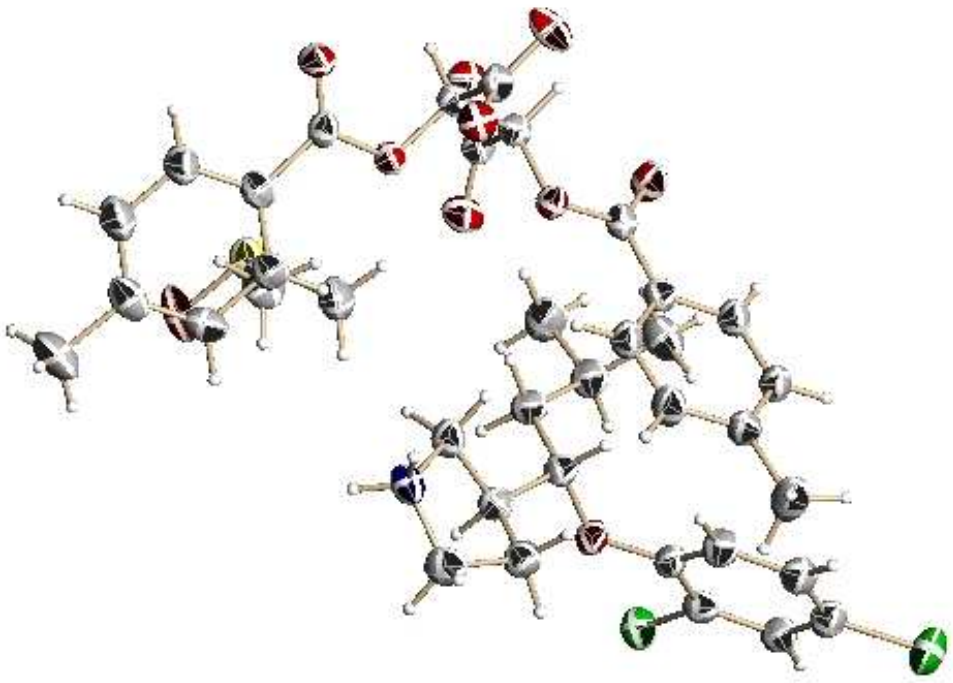

OMe
N
O
H
N
H
2
7
6
5
4
3
2
1
ppm


OMe
N
O
H
N
H
2
160
140
120
100
80
60
40
20
ppm

X-Ray structure data for (*S*)-3-((*S*)-1-(2,4-dichlorophenoxy)-3-methylbutyl)pyrrolidine di-*p*-toluoyl-L-tartrate (**13**) as a DMSO solvate to confirm the absolute configuration of (*S*)-3-(( *S*)-1-(2,4-dichlorophenoxy)-3-methylbutyl)pyrrolidine **1**.




**13**



Crystal data and structure refinement for **13** DMSO solvate.

| | | |
|---|---|---|
| Empirical formula | C37 H45 Cl2 N O10 S | |
| Formula weight | 766.70 | |
| Temperature | 100(2) K | |
| Wavelength | 1.54178 Å | |
| Crystal system | Monoclinic | |
| Space group | P2(1) | |
| Unit cell dimensions | a = 9.9176(5) Å | α= 90°. |
| | b = 13.8269(7) Å | β= 102.099(3)°. |
| | c = 14.4534(7) Å | γ = 90°. |
| Volume | 1937.96(17) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.314 $Mg/m^3$ | |
| Absorption coefficient | 2.479 $mm^{-1}$ | |
| F(000) | 808 | |
| Crystal size | 0.20 x 0.10 x 0.05 $mm^3$ | |
| Theta range for data collection | 3.13 to 64.99°. | |
| Index ranges | -11<=h<=11, -16<=k<=16, -16<=l<=16 | |
| Reflections collected | 16499 | |
| Independent reflections | 5816 [R(int) = 0.0972] | |
| Completeness to theta = 64.99° | 99.7 % | |
| Absorption correction | Multi-scan | |
| Max. and min. transmission | 0.8861 and 0.6370 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5816 / 1 / 469 | |

| | |
|---|---|
| Goodness-of-fit on $F^2$ | 1.038 |
| Final R indices [I>2sigma(I)] | R1 = 0.0500, wR2 = 0.1317 |
| R indices (all data) | R1 = 0.0557, wR2 = 0.1406 |
| Absolute structure parameter | -0.004(16) |
| Extinction coefficient | 0.0036(5) |
| Largest diff. peak and hole | 0.383 and -0.387 e.$Å^{-3}$ |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for 08037_0m. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cl(4A) | 2711(1) | 3176(1) | -507(1) | 43(1) |
| Cl(1A) | 1659(1) | 6001(1) | -3126(1) | 55(1) |
| O(8A) | 3313(3) | 4732(2) | 833(2) | 37(1) |
| C(3A) | 2233(4) | 4663(3) | -1727(3) | 39(1) |
| C(14A) | 5683(4) | 6031(3) | 1799(3) | 43(1) |
| C(4A) | 2628(3) | 4397(3) | -790(3) | 34(1) |
| C(5A) | 2944(4) | 5088(3) | -63(2) | 35(1) |
| C(16A) | 830(4) | 4561(3) | 1608(3) | 43(1) |
| N(12A) | 6252(3) | 6220(2) | 3479(2) | 40(1) |
| C(7A) | 2542(4) | 6340(3) | -1250(3) | 43(1) |
| C(6A) | 2919(4) | 6060(3) | -320(3) | 42(1) |
| C(9A) | 3222(4) | 5320(3) | 1649(2) | 35(1) |
| C(17A) | 45(4) | 3994(4) | 2245(3) | 53(1) |
| C(10A) | 4677(4) | 5416(3) | 2224(2) | 35(1) |
| C(11A) | 4761(4) | 5914(3) | 3185(2) | 38(1) |
| C(15A) | 2274(4) | 4806(3) | 2185(3) | 39(1) |
| C(13A) | 6902(4) | 6140(3) | 2634(3) | 45(1) |
| C(2A) | 2193(4) | 5647(3) | -1954(3) | 41(1) |
| C(18A) | 28(5) | 5457(4) | 1215(4) | 56(1) |
| O(3B) | 1680(2) | 8029(2) | 3722(2) | 31(1) |

| | | | | |
|---|---|---|---|---|
| O(16B) | 2933(3) | 9733(2) | 5346(2) | 42(1) |
| O(6B) | 2973(2) | 7798(2) | 5663(2) | 33(1) |
| O(1B) | -243(3) | 7638(2) | 2661(2) | 43(1) |
| O(18B) | -321(3) | 6531(2) | 4906(2) | 38(1) |
| C(2B) | 946(4) | 7903(3) | 2827(2) | 32(1) |
| C(19B) | 1731(3) | 8142(3) | 2101(2) | 33(1) |
| C(7B) | 3558(4) | 7954(3) | 6580(2) | 33(1) |
| C(5B) | 1657(3) | 8261(2) | 5357(2) | 30(1) |
| C(15B) | 1781(4) | 9362(3) | 5231(2) | 35(1) |
| C(23B) | 3753(4) | 8700(3) | 1589(3) | 45(1) |
| C(21B) | 1711(4) | 8348(3) | 443(2) | 39(1) |
| C(9B) | 5493(5) | 7408(3) | 7830(3) | 48(1) |
| C(20B) | 1051(4) | 8084(3) | 1157(2) | 37(1) |
| C(4B) | 917(4) | 7814(3) | 4432(2) | 31(1) |
| C(8B) | 4895(4) | 7446(3) | 6878(3) | 36(1) |
| C(24B) | 3107(4) | 8452(3) | 2314(3) | 39(1) |
| C(14B) | 8642(5) | 5829(4) | 7882(4) | 67(1) |
| C(17B) | 710(4) | 6722(3) | 4493(2) | 32(1) |
| C(13B) | 5561(4) | 7002(3) | 6238(3) | 40(1) |
| C(25B) | 3768(4) | 8965(5) | -141(3) | 61(1) |
| C(22B) | 3064(4) | 8671(3) | 640(3) | 43(1) |
| C(11B) | 7345(4) | 6420(3) | 7514(3) | 48(1) |
| C(12B) | 6775(4) | 6493(3) | 6560(3) | 45(1) |
| C(10B) | 6705(5) | 6897(4) | 8149(3) | 56(1) |
| O(15B) | 620(3) | 9759(2) | 5012(2) | 49(1) |

| | | | | |
|---|---|---|---|---|
| O(17B) | 1413(3) | 6134(2) | 4188(2) | 44(1) |
| O(7B) | 3025(3) | 8434(2) | 7107(2) | 41(1) |
| S(1) | 2974(1) | 3870(1) | 5804(1) | 42(1) |
| O(1C) | 3994(3) | 3055(2) | 6079(2) | 58(1) |
| C(1C) | 2280(5) | 3735(4) | 4588(3) | 52(1) |
| C(2C) | 4032(5) | 4891(3) | 5741(4) | 55(1) |

Table 3. Bond lengths [Å] and angles [°] for 08037_0m.

| | |
|---|---|
| Cl(4A)-C(4A) | 1.735(4) |
| Cl(1A)-C(2A) | 1.735(4) |
| O(8A)-C(5A) | 1.361(4) |
| O(8A)-C(9A) | 1.452(4) |
| C(3A)-C(4A) | 1.379(5) |
| C(3A)-C(2A) | 1.397(6) |
| C(14A)-C(13A) | 1.526(6) |
| C(14A)-C(10A) | 1.533(5) |
| C(4A)-C(5A) | 1.406(5) |
| C(5A)-C(6A) | 1.393(6) |
| C(16A)-C(18A) | 1.517(7) |
| C(16A)-C(15A) | 1.537(5) |
| C(16A)-C(17A) | 1.540(6) |
| N(12A)-C(13A) | 1.500(5) |
| N(12A)-C(11A) | 1.511(5) |
| C(7A)-C(6A) | 1.374(5) |
| C(7A)-C(2A) | 1.388(6) |
| C(9A)-C(10A) | 1.513(5) |
| C(9A)-C(15A) | 1.513(5) |
| C(10A)-C(11A) | 1.537(5) |
| O(3B)-C(2B) | 1.357(4) |
| O(3B)-C(4B) | 1.429(4) |
| O(16B)-C(15B) | 1.231(5) |

| | |
|---|---|
| O(6B)-C(7B) | 1.348(4) |
| O(6B)-C(5B) | 1.438(4) |
| O(1B)-C(2B) | 1.210(4) |
| O(18B)-C(17B) | 1.315(5) |
| C(2B)-C(19B) | 1.470(5) |
| C(19B)-C(20B) | 1.391(5) |
| C(19B)-C(24B) | 1.401(5) |
| C(7B)-O(7B) | 1.212(5) |
| C(7B)-C(8B) | 1.483(5) |
| C(5B)-C(4B) | 1.515(5) |
| C(5B)-C(15B) | 1.541(5) |
| C(15B)-O(15B) | 1.255(5) |
| C(23B)-C(24B) | 1.381(5) |
| C(23B)-C(22B) | 1.398(5) |
| C(21B)-C(20B) | 1.382(5) |
| C(21B)-C(22B) | 1.386(6) |
| C(9B)-C(8B) | 1.381(6) |
| C(9B)-C(10B) | 1.387(6) |
| C(4B)-C(17B) | 1.530(5) |
| C(8B)-C(13B) | 1.387(6) |
| C(14B)-C(11B) | 1.523(6) |
| C(17B)-O(17B) | 1.213(4) |
| C(13B)-C(12B) | 1.387(6) |
| C(25B)-C(22B) | 1.502(6) |
| C(11B)-C(12B) | 1.380(6) |

| | |
|---|---|
| C(11B)-C(10B) | 1.387(7) |
| S(1)-O(1C) | 1.510(3) |
| S(1)-C(1C) | 1.758(4) |
| S(1)-C(2C) | 1.773(4) |

| | |
|---|---|
| C(5A)-O(8A)-C(9A) | 121.4(3) |
| C(4A)-C(3A)-C(2A) | 118.6(4) |
| C(13A)-C(14A)-C(10A) | 102.3(3) |
| C(3A)-C(4A)-C(5A) | 121.8(4) |
| C(3A)-C(4A)-Cl(4A) | 118.7(3) |
| C(5A)-C(4A)-Cl(4A) | 119.5(3) |
| O(8A)-C(5A)-C(6A) | 126.1(3) |
| O(8A)-C(5A)-C(4A) | 116.0(3) |
| C(6A)-C(5A)-C(4A) | 117.8(3) |
| C(18A)-C(16A)-C(15A) | 112.3(4) |
| C(18A)-C(16A)-C(17A) | 110.4(4) |
| C(15A)-C(16A)-C(17A) | 108.6(3) |
| C(13A)-N(12A)-C(11A) | 108.3(3) |
| C(6A)-C(7A)-C(2A) | 119.8(4) |
| C(7A)-C(6A)-C(5A) | 121.3(4) |
| O(8A)-C(9A)-C(10A) | 106.3(3) |
| O(8A)-C(9A)-C(15A) | 107.7(3) |
| C(10A)-C(9A)-C(15A) | 112.6(3) |
| C(9A)-C(10A)-C(14A) | 117.0(3) |
| C(9A)-C(10A)-C(11A) | 113.6(3) |

| | |
|---|---|
| C(14A)-C(10A)-C(11A) | 101.4(3) |
| N(12A)-C(11A)-C(10A) | 104.1(3) |
| C(9A)-C(15A)-C(16A) | 115.7(3) |
| N(12A)-C(13A)-C(14A) | 104.3(3) |
| C(7A)-C(2A)-C(3A) | 120.7(4) |
| C(7A)-C(2A)-Cl(1A) | 119.9(3) |
| C(3A)-C(2A)-Cl(1A) | 119.5(3) |
| C(2B)-O(3B)-C(4B) | 113.5(3) |
| C(7B)-O(6B)-C(5B) | 114.0(3) |
| O(1B)-C(2B)-O(3B) | 122.3(3) |
| O(1B)-C(2B)-C(19B) | 124.5(3) |
| O(3B)-C(2B)-C(19B) | 113.1(3) |
| C(20B)-C(19B)-C(24B) | 118.9(3) |
| C(20B)-C(19B)-C(2B) | 117.8(3) |
| C(24B)-C(19B)-C(2B) | 123.3(3) |
| O(7B)-C(7B)-O(6B) | 123.5(3) |
| O(7B)-C(7B)-C(8B) | 123.9(3) |
| O(6B)-C(7B)-C(8B) | 112.6(3) |
| O(6B)-C(5B)-C(4B) | 109.3(3) |
| O(6B)-C(5B)-C(15B) | 112.7(3) |
| C(4B)-C(5B)-C(15B) | 109.5(3) |
| O(16B)-C(15B)-O(15B) | 128.9(4) |
| O(16B)-C(15B)-C(5B) | 119.4(3) |
| O(15B)-C(15B)-C(5B) | 111.7(3) |
| C(24B)-C(23B)-C(22B) | 121.8(4) |

| | |
|---|---|
| C(20B)-C(21B)-C(22B) | 121.4(3) |
| C(8B)-C(9B)-C(10B) | 120.8(4) |
| C(21B)-C(20B)-C(19B) | 120.6(3) |
| O(3B)-C(4B)-C(5B) | 108.5(3) |
| O(3B)-C(4B)-C(17B) | 110.1(3) |
| C(5B)-C(4B)-C(17B) | 113.4(3) |
| C(9B)-C(8B)-C(13B) | 118.8(4) |
| C(9B)-C(8B)-C(7B) | 118.6(3) |
| C(13B)-C(8B)-C(7B) | 122.6(3) |
| C(23B)-C(24B)-C(19B) | 119.6(3) |
| O(17B)-C(17B)-O(18B) | 126.3(3) |
| O(17B)-C(17B)-C(4B) | 123.2(3) |
| O(18B)-C(17B)-C(4B) | 110.5(3) |
| C(8B)-C(13B)-C(12B) | 120.1(4) |
| C(21B)-C(22B)-C(23B) | 117.7(3) |
| C(21B)-C(22B)-C(25B) | 121.0(4) |
| C(23B)-C(22B)-C(25B) | 121.4(4) |
| C(12B)-C(11B)-C(10B) | 118.6(4) |
| C(12B)-C(11B)-C(14B) | 121.8(4) |
| C(10B)-C(11B)-C(14B) | 119.6(4) |
| C(11B)-C(12B)-C(13B) | 121.2(4) |
| C(11B)-C(10B)-C(9B) | 120.4(4) |
| O(1C)-S(1)-C(1C) | 106.5(2) |
| O(1C)-S(1)-C(2C) | 103.6(2) |
| C(1C)-S(1)-C(2C) | 98.3(2) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x $10^3$)for 08037_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12} ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Cl(4A) | 45(1) | 38(1) | 42(1) | -2(1) | 2(1) | -2(1) |
| Cl(1A) | 72(1) | 59(1) | 33(1) | 6(1) | 6(1) | -3(1) |
| O(8A) | 44(1) | 38(1) | 28(1) | -3(1) | 5(1) | 4(1) |
| C(3A) | 32(2) | 49(2) | 35(2) | -4(2) | 5(1) | -4(2) |
| C(14A) | 42(2) | 48(2) | 39(2) | -3(2) | 9(2) | -1(2) |
| C(4A) | 26(2) | 37(2) | 38(2) | -2(2) | 7(1) | -4(2) |
| C(5A) | 29(2) | 47(2) | 28(2) | 0(2) | 3(1) | -1(2) |
| C(16A) | 38(2) | 51(2) | 38(2) | -6(2) | 3(2) | -4(2) |
| N(12A) | 37(2) | 35(2) | 43(2) | -1(1) | -2(1) | 1(1) |
| C(7A) | 42(2) | 46(2) | 40(2) | 1(2) | 8(2) | 0(2) |
| C(6A) | 42(2) | 45(2) | 37(2) | -6(2) | 5(2) | -3(2) |
| C(9A) | 39(2) | 36(2) | 29(2) | -5(1) | 6(2) | 5(2) |
| C(17A) | 41(2) | 69(3) | 48(2) | 2(2) | 7(2) | -13(2) |
| C(10A) | 36(2) | 34(2) | 34(2) | -5(2) | 5(2) | -1(2) |
| C(11A) | 34(2) | 42(2) | 35(2) | 2(2) | 3(1) | -4(2) |
| C(15A) | 35(2) | 46(2) | 37(2) | -6(2) | 7(2) | -2(2) |
| C(13A) | 36(2) | 48(2) | 50(2) | -5(2) | 9(2) | -6(2) |
| C(2A) | 37(2) | 49(2) | 37(2) | 2(2) | 7(2) | -5(2) |
| C(18A) | 40(2) | 58(3) | 66(3) | 1(2) | 1(2) | 3(2) |
| O(3B) | 32(1) | 33(1) | 28(1) | 0(1) | 4(1) | -2(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O(16B) | 42(2) | 35(1) | 47(1) | -1(1) | 7(1) | -6(1) |
| O(6B) | 31(1) | 33(1) | 32(1) | -1(1) | 3(1) | 3(1) |
| O(1B) | 36(2) | 54(2) | 36(1) | 2(1) | 5(1) | -9(1) |
| O(18B) | 44(2) | 27(1) | 47(1) | 3(1) | 15(1) | -1(1) |
| C(2B) | 31(2) | 32(2) | 31(2) | 3(1) | 2(1) | -1(2) |
| C(19B) | 31(2) | 33(2) | 36(2) | 4(2) | 6(1) | 1(2) |
| C(7B) | 31(2) | 36(2) | 30(2) | 2(1) | 3(1) | -5(2) |
| C(5B) | 33(2) | 23(2) | 34(2) | -5(1) | 5(1) | 1(1) |
| C(15B) | 40(2) | 29(2) | 32(2) | -2(1) | 2(2) | -1(2) |
| C(23B) | 30(2) | 60(3) | 42(2) | 9(2) | 2(2) | -5(2) |
| C(21B) | 33(2) | 50(2) | 31(2) | 6(2) | 2(1) | 2(2) |
| C(9B) | 51(2) | 51(3) | 38(2) | -4(2) | 1(2) | 12(2) |
| C(20B) | 33(2) | 42(2) | 35(2) | 4(2) | 4(1) | -1(2) |
| C(4B) | 31(2) | 28(2) | 34(2) | 2(1) | 8(1) | 0(1) |
| C(8B) | 32(2) | 33(2) | 41(2) | 0(2) | 4(2) | -1(2) |
| C(24B) | 35(2) | 44(2) | 35(2) | 4(2) | 3(2) | 0(2) |
| C(14B) | 43(2) | 63(3) | 90(3) | 5(3) | 2(2) | 14(2) |
| C(17B) | 35(2) | 28(2) | 32(2) | -5(1) | 4(2) | 2(2) |
| C(13B) | 34(2) | 46(2) | 40(2) | -3(2) | 6(2) | -5(2) |
| C(25B) | 38(2) | 101(4) | 44(2) | 15(2) | 6(2) | -8(3) |
| C(22B) | 36(2) | 54(3) | 39(2) | 9(2) | 9(2) | 4(2) |
| C(11B) | 35(2) | 39(2) | 66(3) | 6(2) | 3(2) | -1(2) |
| C(12B) | 36(2) | 46(2) | 57(2) | -9(2) | 14(2) | 0(2) |
| C(10B) | 48(2) | 65(3) | 50(2) | 3(2) | -4(2) | 13(2) |
| O(15B) | 40(2) | 26(1) | 75(2) | -3(1) | 2(1) | 5(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O(17B) | 48(2) | 30(1) | 55(2) | -3(1) | 15(1) | 5(1) |
| O(7B) | 41(1) | 46(2) | 36(1) | -9(1) | 7(1) | 7(1) |
| S(1) | 41(1) | 40(1) | 43(1) | 7(1) | 5(1) | -3(1) |
| O(1C) | 44(2) | 41(2) | 78(2) | 21(2) | -13(1) | -3(1) |
| C(1C) | 50(2) | 55(3) | 48(2) | 5(2) | 3(2) | 8(2) |
| C(2C) | 57(3) | 33(2) | 74(3) | 11(2) | 10(2) | -5(2) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (Å$^2$x $10^3$) for 08037_0m.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3A) | 1994 | 4188 | -2209 | 47 |
| H(14A) | 5958 | 5695 | 1262 | 51 |
| H(14B) | 5277 | 6667 | 1583 | 51 |
| H(16A) | 933 | 4137 | 1066 | 52 |
| H(12A) | 6306 | 6847 | 3696 | 47 |
| H(12C) | 6707 | 5827 | 3958 | 47 |
| H(7A) | 2520 | 7007 | -1412 | 51 |
| H(6A) | 3167 | 6538 | 157 | 50 |
| H(9A) | 2841 | 5972 | 1440 | 42 |
| H(17A) | -19 | 4388 | 2799 | 80 |
| H(17B) | 538 | 3393 | 2454 | 80 |
| H(17C) | -885 | 3842 | 1889 | 80 |
| H(10A) | 5076 | 4752 | 2344 | 42 |
| H(11A) | 4140 | 6482 | 3123 | 45 |
| H(11B) | 4510 | 5460 | 3652 | 45 |
| H(15A) | 2169 | 5217 | 2726 | 47 |
| H(15B) | 2725 | 4198 | 2446 | 47 |
| H(13A) | 7517 | 5570 | 2688 | 54 |
| H(13B) | 7441 | 6728 | 2564 | 54 |

| | | | | |
|---|---|---|---|---|
| H(18A) | -61 | 5888 | 1737 | 84 |
| H(18B) | -892 | 5268 | 866 | 84 |
| H(18C) | 518 | 5794 | 787 | 84 |
| H(18D) | -460 | 5931 | 4899 | 57 |
| H(5B) | 1093 | 8142 | 5844 | 36 |
| H(23B) | 4692 | 8895 | 1739 | 54 |
| H(21B) | 1226 | 8308 | -197 | 47 |
| H(9B) | 5070 | 7735 | 8272 | 57 |
| H(20B) | 125 | 7861 | 1003 | 45 |
| H(4B) | -12 | 8124 | 4245 | 37 |
| H(24B) | 3593 | 8491 | 2953 | 46 |
| H(14C) | 8861 | 5441 | 7365 | 100 |
| H(14D) | 8487 | 5399 | 8389 | 100 |
| H(14E) | 9412 | 6265 | 8129 | 100 |
| H(13C) | 5186 | 7046 | 5579 | 48 |
| H(25A) | 4241 | 9584 | 20 | 92 |
| H(25B) | 3080 | 9034 | -732 | 92 |
| H(25C) | 4441 | 8470 | -220 | 92 |
| H(12B) | 7221 | 6190 | 6116 | 55 |
| H(10B) | 7100 | 6873 | 8807 | 68 |
| H(1C1) | 3028 | 3739 | 4239 | 78 |
| H(1C2) | 1645 | 4270 | 4369 | 78 |
| H(1C3) | 1780 | 3120 | 4477 | 78 |
| H(2C1) | 4450 | 5108 | 6383 | 83 |
| H(2C2) | 3472 | 5414 | 5400 | 83 |

| | | | | |
|---|---|---|---|---|
| H(2C3) | 4761 | 4715 | 5407 | 83 |

Table 6. Torsion angles [°] for 08037_0m.

| | |
|---|---|
| C(2A)-C(3A)-C(4A)-C(5A) | 2.1(5) |
| C(2A)-C(3A)-C(4A)-Cl(4A) | -178.8(3) |
| C(9A)-O(8A)-C(5A)-C(6A) | 24.0(6) |
| C(9A)-O(8A)-C(5A)-C(4A) | -159.3(3) |
| C(3A)-C(4A)-C(5A)-O(8A) | 179.7(3) |
| Cl(4A)-C(4A)-C(5A)-O(8A) | 0.6(5) |
| C(3A)-C(4A)-C(5A)-C(6A) | -3.4(5) |
| Cl(4A)-C(4A)-C(5A)-C(6A) | 177.6(3) |
| C(2A)-C(7A)-C(6A)-C(5A) | -0.8(6) |
| O(8A)-C(5A)-C(6A)-C(7A) | 179.3(4) |
| C(4A)-C(5A)-C(6A)-C(7A) | 2.7(6) |
| C(5A)-O(8A)-C(9A)-C(10A) | -117.6(4) |
| C(5A)-O(8A)-C(9A)-C(15A) | 121.5(3) |
| O(8A)-C(9A)-C(10A)-C(14A) | 69.4(4) |
| C(15A)-C(9A)-C(10A)-C(14A) | -172.8(3) |
| O(8A)-C(9A)-C(10A)-C(11A) | -172.8(3) |
| C(15A)-C(9A)-C(10A)-C(11A) | -55.1(4) |
| C(13A)-C(14A)-C(10A)-C(9A) | 168.5(3) |
| C(13A)-C(14A)-C(10A)-C(11A) | 44.4(4) |
| C(13A)-N(12A)-C(11A)-C(10A) | 13.9(4) |
| C(9A)-C(10A)-C(11A)-N(12A) | -162.3(3) |
| C(14A)-C(10A)-C(11A)-N(12A) | -35.8(4) |
| O(8A)-C(9A)-C(15A)-C(16A) | -55.4(4) |

| | |
|---|---|
| C(10A)-C(9A)-C(15A)-C(16A) | -172.3(3) |
| C(18A)-C(16A)-C(15A)-C(9A) | -60.9(5) |
| C(17A)-C(16A)-C(15A)-C(9A) | 176.8(3) |
| C(11A)-N(12A)-C(13A)-C(14A) | 13.8(4) |
| C(10A)-C(14A)-C(13A)-N(12A) | -36.1(4) |
| C(6A)-C(7A)-C(2A)-C(3A) | -0.6(6) |
| C(6A)-C(7A)-C(2A)-Cl(1A) | 177.8(3) |
| C(4A)-C(3A)-C(2A)-C(7A) | -0.1(6) |
| C(4A)-C(3A)-C(2A)-Cl(1A) | -178.5(3) |
| C(4B)-O(3B)-C(2B)-O(1B) | 0.4(5) |
| C(4B)-O(3B)-C(2B)-C(19B) | 179.0(3) |
| O(1B)-C(2B)-C(19B)-C(20B) | 1.7(6) |
| O(3B)-C(2B)-C(19B)-C(20B) | -176.8(3) |
| O(1B)-C(2B)-C(19B)-C(24B) | 179.7(4) |
| O(3B)-C(2B)-C(19B)-C(24B) | 1.1(5) |
| C(5B)-O(6B)-C(7B)-O(7B) | 0.5(5) |
| C(5B)-O(6B)-C(7B)-C(8B) | 178.5(3) |
| C(7B)-O(6B)-C(5B)-C(4B) | -163.6(3) |
| C(7B)-O(6B)-C(5B)-C(15B) | 74.3(4) |
| O(6B)-C(5B)-C(15B)-O(16B) | 3.6(4) |
| C(4B)-C(5B)-C(15B)-O(16B) | -118.3(3) |
| O(6B)-C(5B)-C(15B)-O(15B) | -176.5(3) |
| C(4B)-C(5B)-C(15B)-O(15B) | 61.6(4) |
| C(22B)-C(21B)-C(20B)-C(19B) | 0.5(7) |
| C(24B)-C(19B)-C(20B)-C(21B) | -1.5(6) |

| | |
|---|---|
| C(2B)-C(19B)-C(20B)-C(21B) | 176.6(4) |
| C(2B)-O(3B)-C(4B)-C(5B) | -163.0(3) |
| C(2B)-O(3B)-C(4B)-C(17B) | 72.3(4) |
| O(6B)-C(5B)-C(4B)-O(3B) | -65.2(3) |
| C(15B)-C(5B)-C(4B)-O(3B) | 58.7(4) |
| O(6B)-C(5B)-C(4B)-C(17B) | 57.5(4) |
| C(15B)-C(5B)-C(4B)-C(17B) | -178.6(3) |
| C(10B)-C(9B)-C(8B)-C(13B) | -3.0(7) |
| C(10B)-C(9B)-C(8B)-C(7B) | 176.5(4) |
| O(7B)-C(7B)-C(8B)-C(9B) | 8.7(6) |
| O(6B)-C(7B)-C(8B)-C(9B) | -169.2(4) |
| O(7B)-C(7B)-C(8B)-C(13B) | -171.8(4) |
| O(6B)-C(7B)-C(8B)-C(13B) | 10.2(5) |
| C(22B)-C(23B)-C(24B)-C(19B) | 1.4(7) |
| C(20B)-C(19B)-C(24B)-C(23B) | 0.6(6) |
| C(2B)-C(19B)-C(24B)-C(23B) | -177.4(4) |
| O(3B)-C(4B)-C(17B)-O(17B) | 19.2(5) |
| C(5B)-C(4B)-C(17B)-O(17B) | -102.6(4) |
| O(3B)-C(4B)-C(17B)-O(18B) | -160.2(3) |
| C(5B)-C(4B)-C(17B)-O(18B) | 78.0(4) |
| C(9B)-C(8B)-C(13B)-C(12B) | 2.8(6) |
| C(7B)-C(8B)-C(13B)-C(12B) | -176.6(4) |
| C(20B)-C(21B)-C(22B)-C(23B) | 1.4(7) |
| C(20B)-C(21B)-C(22B)-C(25B) | -179.4(5) |
| C(24B)-C(23B)-C(22B)-C(21B) | -2.3(7) |

| | |
|---|---|
| C(24B)-C(23B)-C(22B)-C(25B) | 178.5(5) |
| C(10B)-C(11B)-C(12B)-C(13B) | -2.3(7) |
| C(14B)-C(11B)-C(12B)-C(13B) | 177.3(4) |
| C(8B)-C(13B)-C(12B)-C(11B) | -0.2(6) |
| C(12B)-C(11B)-C(10B)-C(9B) | 2.1(7) |
| C(14B)-C(11B)-C(10B)-C(9B) | -177.5(5) |
| C(8B)-C(9B)-C(10B)-C(11B) | 0.5(7) |

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Symmetry transformations used to generate equivalent atoms: