Supporting Information

A novel thiourea type organocatalyst possessing a single NH functionality

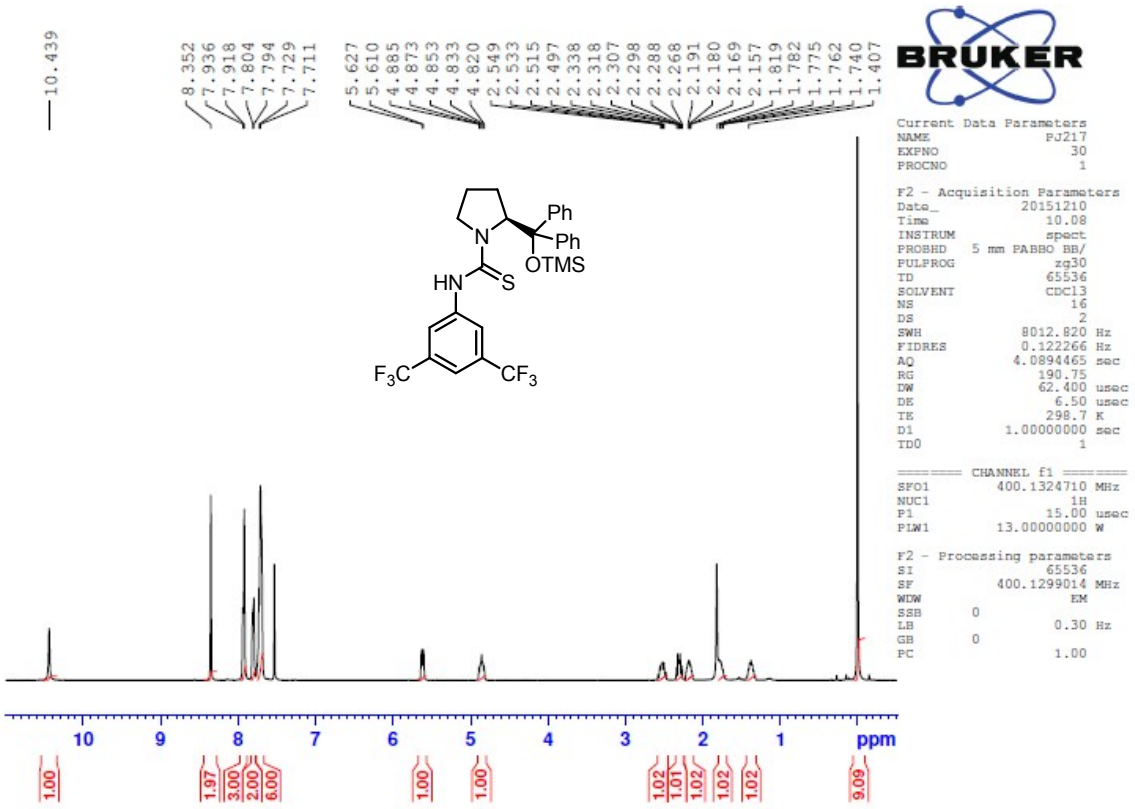
Predrag Jovanovic,[a] Milos Petkovic,[a] Milena Simic,[a] Branka Ivkovic[b] and Vladimir Savic[a]*

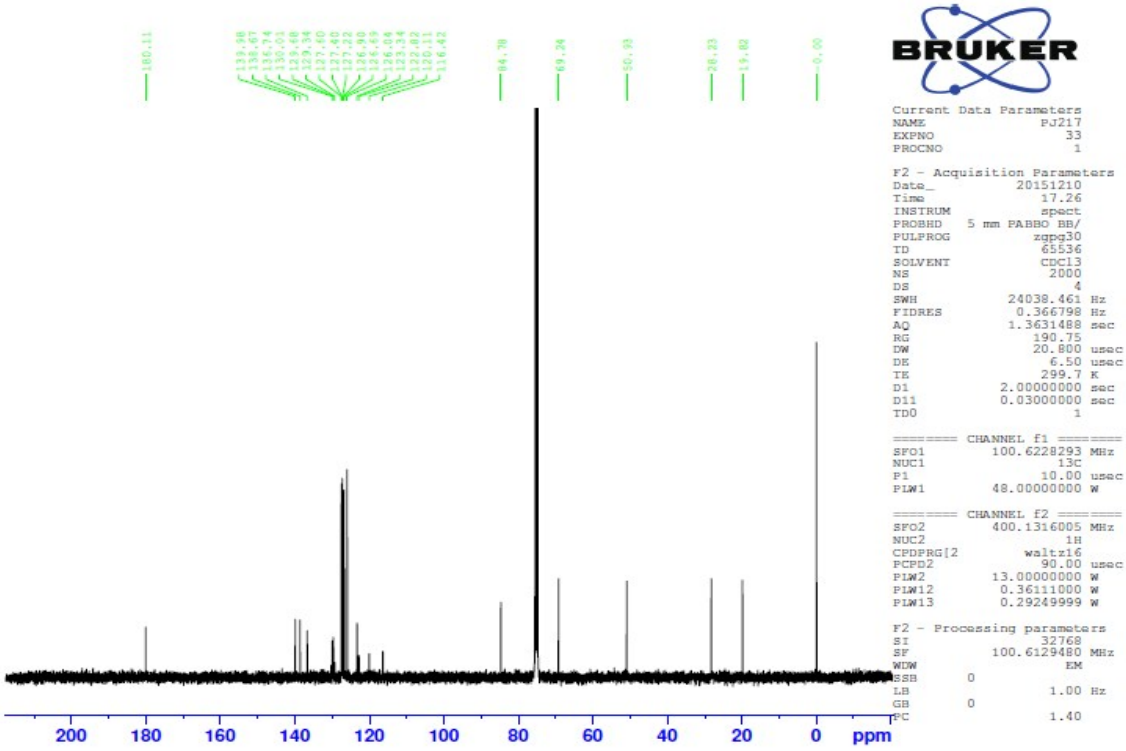
[a] *University of Belgarde, Faculty of Pharmacy, Department of Organic Chemistry, Vojvode Stepe 450, Belgrade, Serbia*

[b] *University of Belgarde, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Vojvode Stepe 450, Belgrade, Serbia*

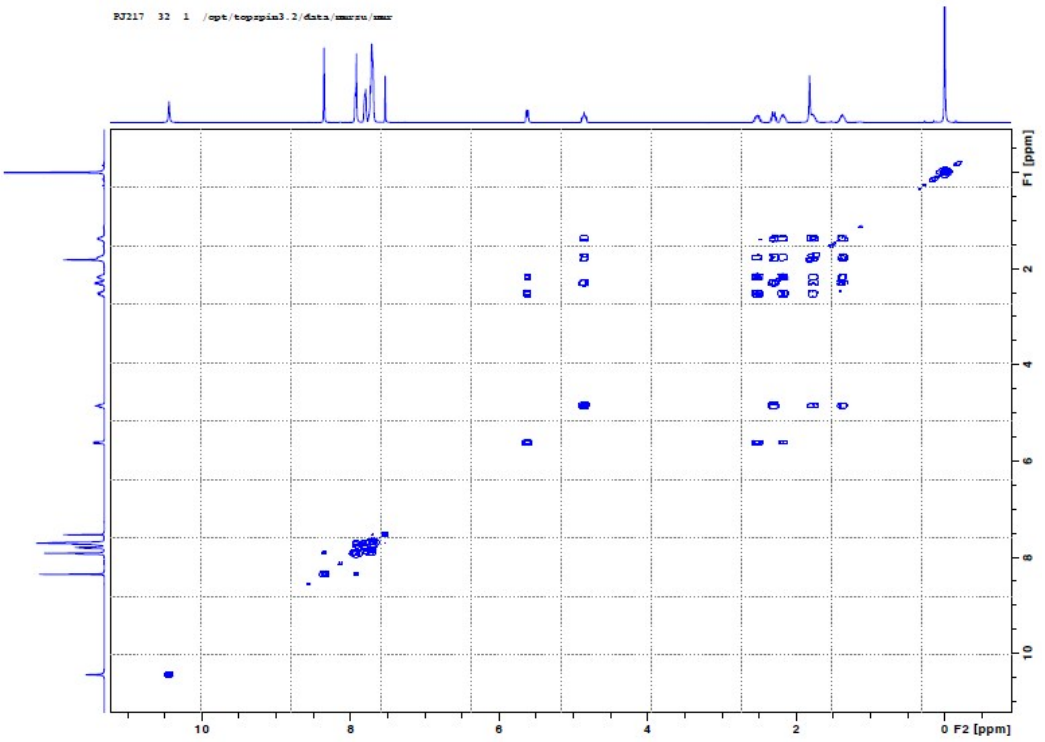
Contents

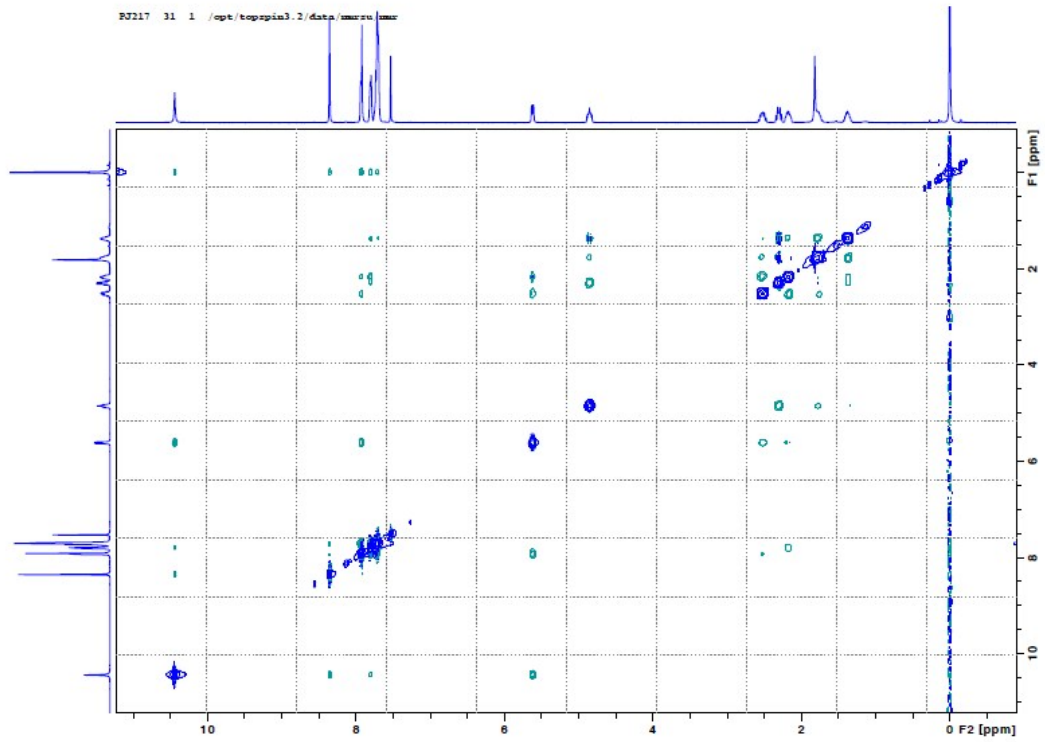
^{1}H and ^{13}C spectra of compound 1



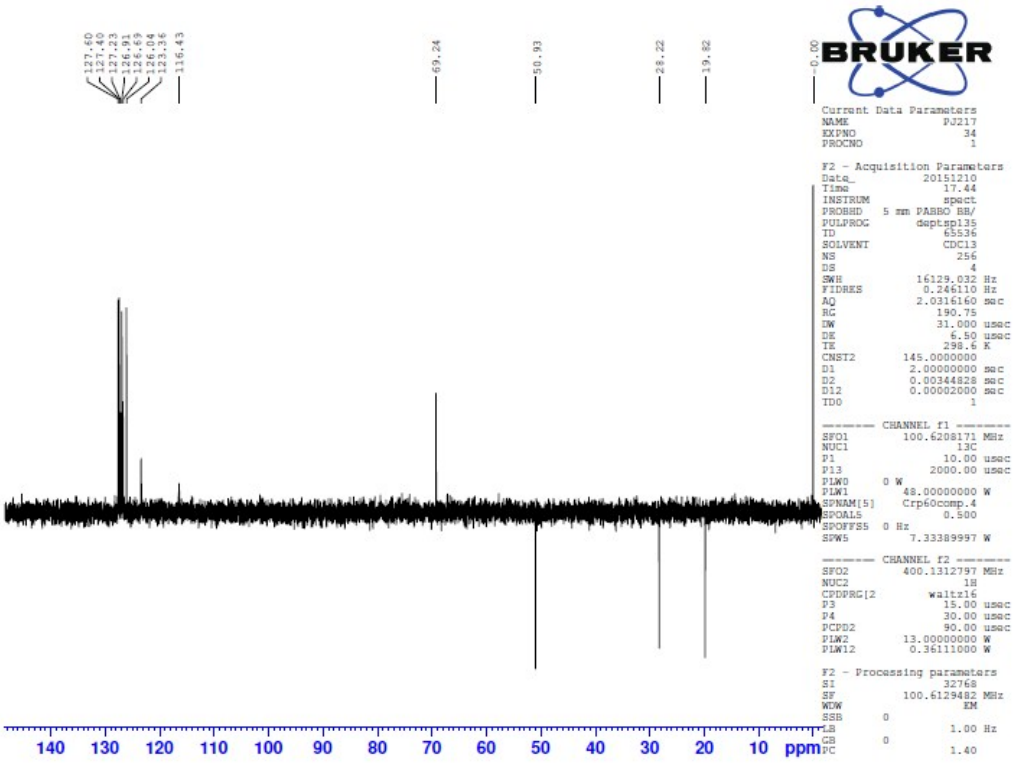


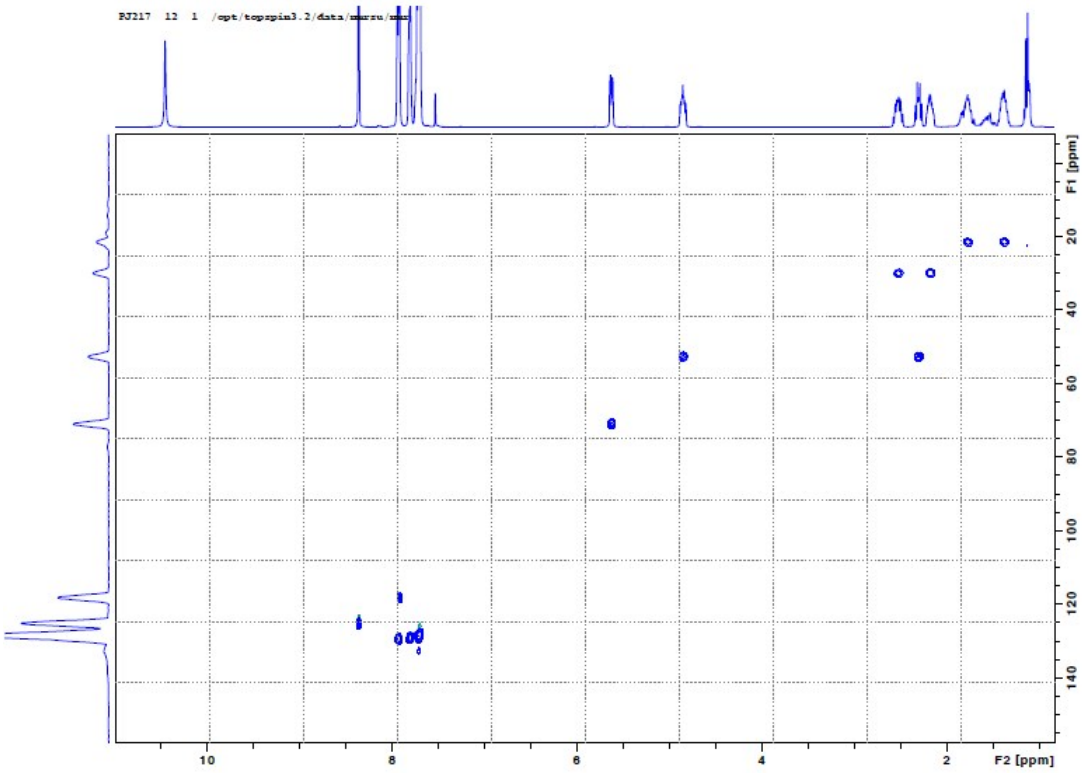
COSY and NOESY spectra of compound 1



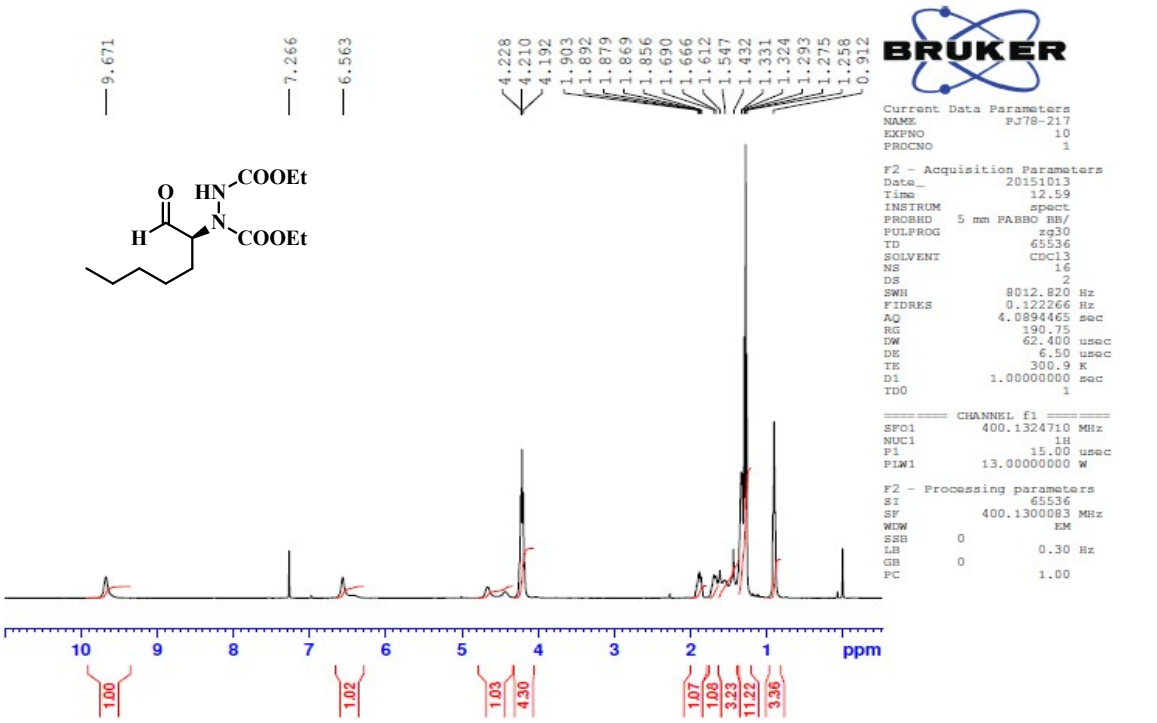


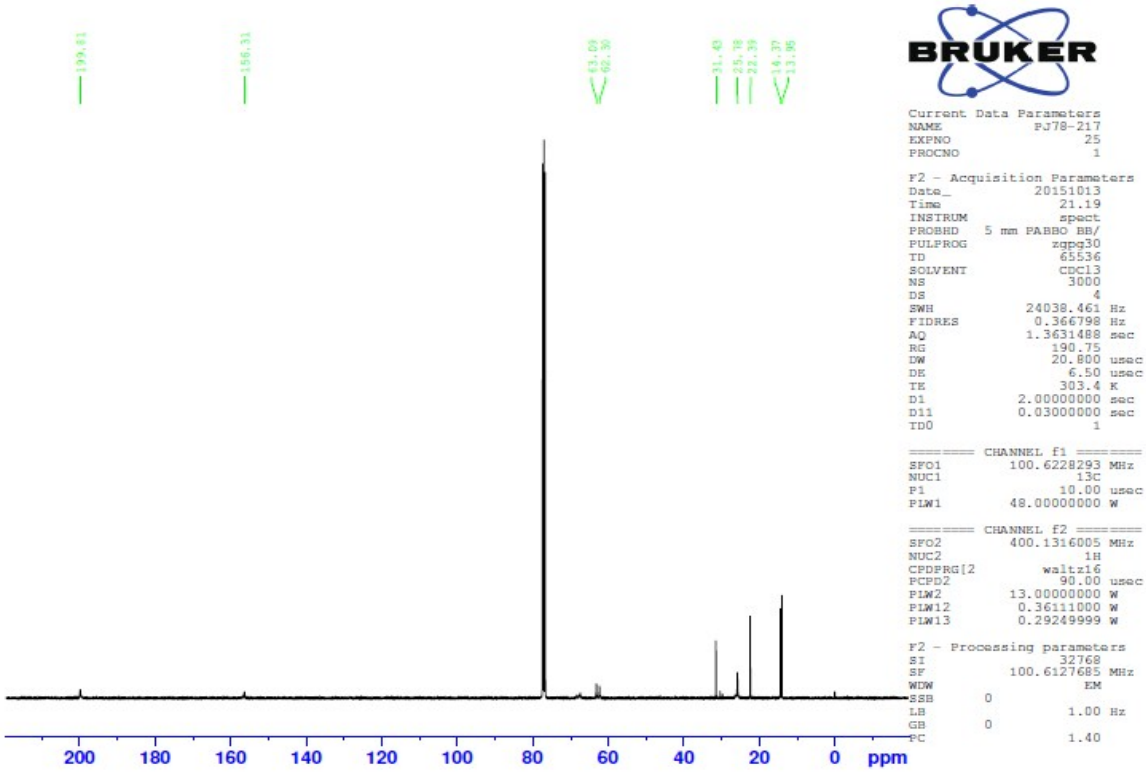
DEPT and HSQC spectra of compound 1





^{1}H and ^{13}C spectra of compound 4



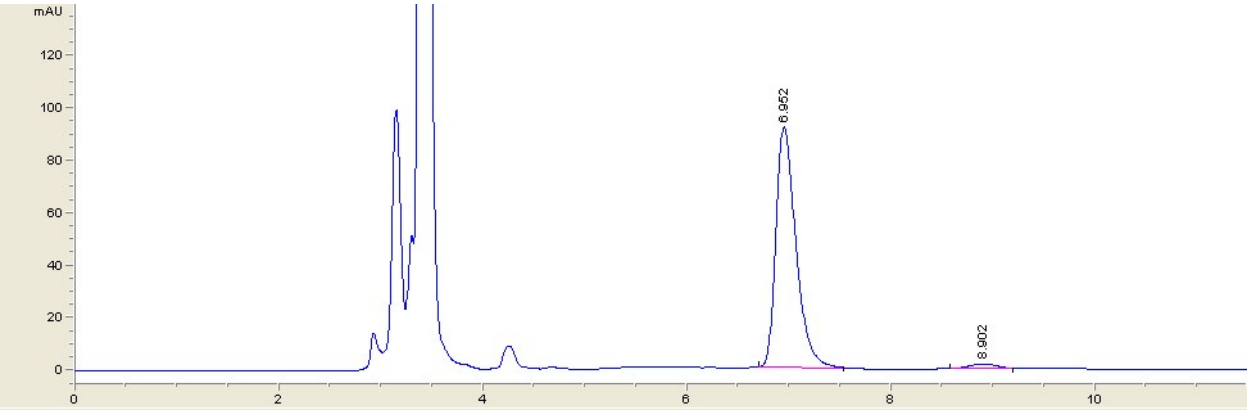


Chiral HPLC analysis of **4**:

Enantiomerically enriched

Peak Table

	RT	Area	% Area
1	6.953	1264.75110	97.1196
2	8.903	37.51013	2.8804



Racemic

Peak table

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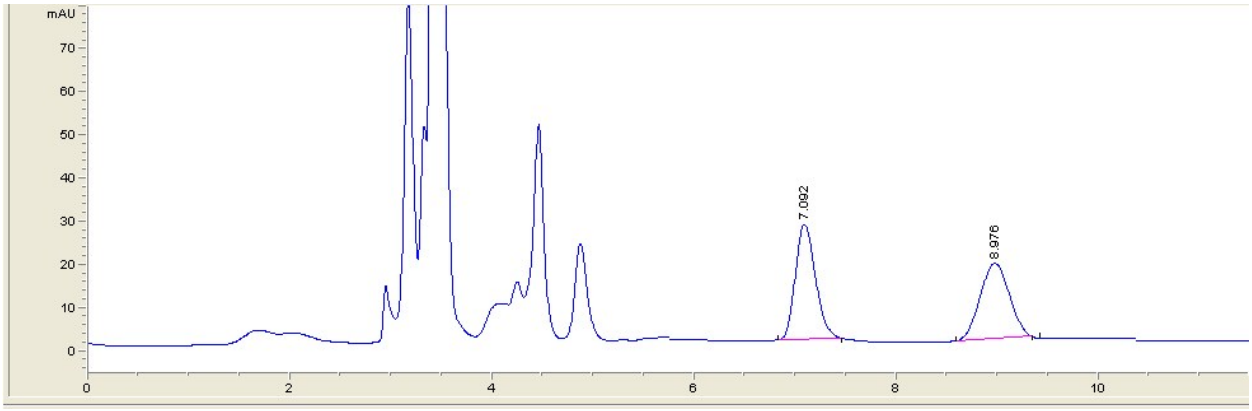
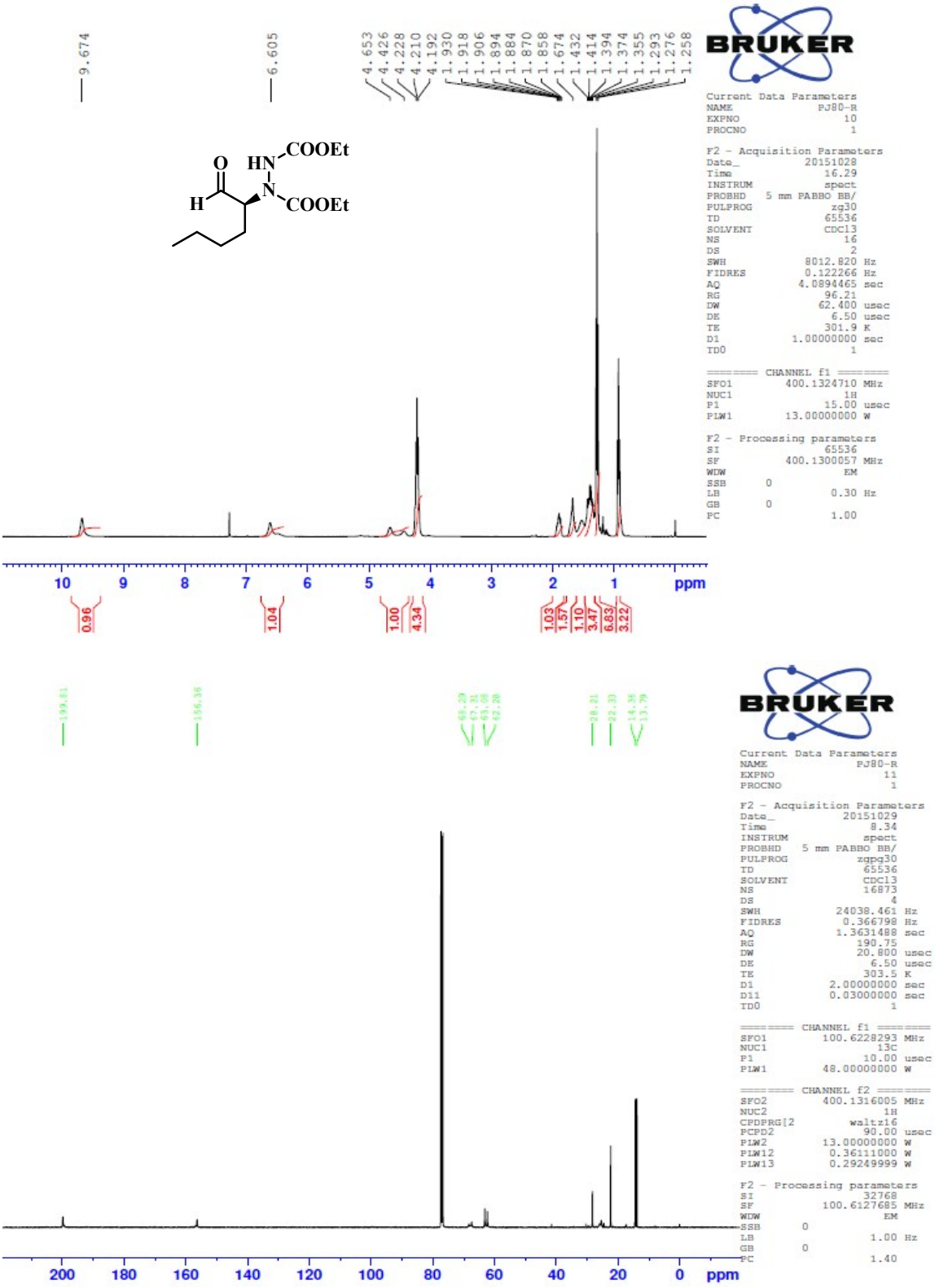


^{1}H and ^{13}C spectra of compound 5a

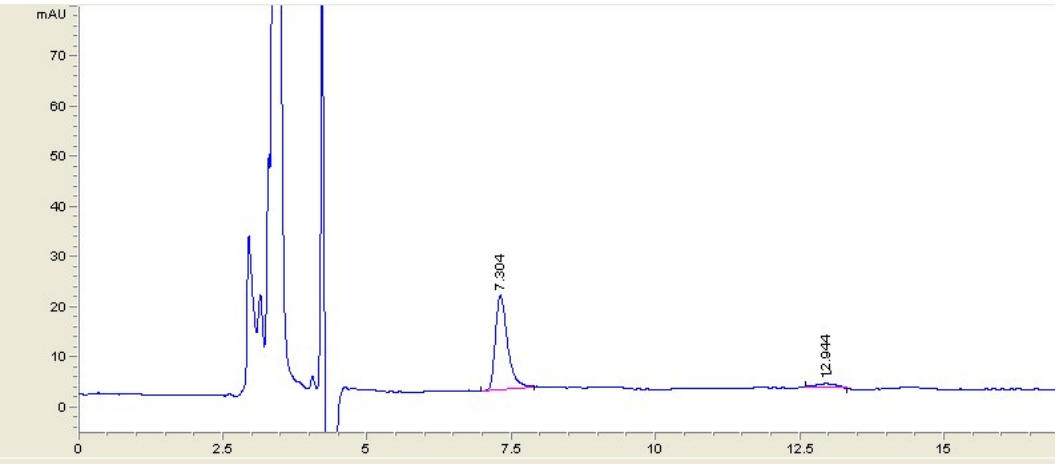


Chiral HPLC analysis of **5a**:

Enantiomerically enriched

Peak Table

	RT	Area	% Area
1	7.304	262.99173	96.8681
2	12.949	8.50289	3.1319



Racemic

Peak table

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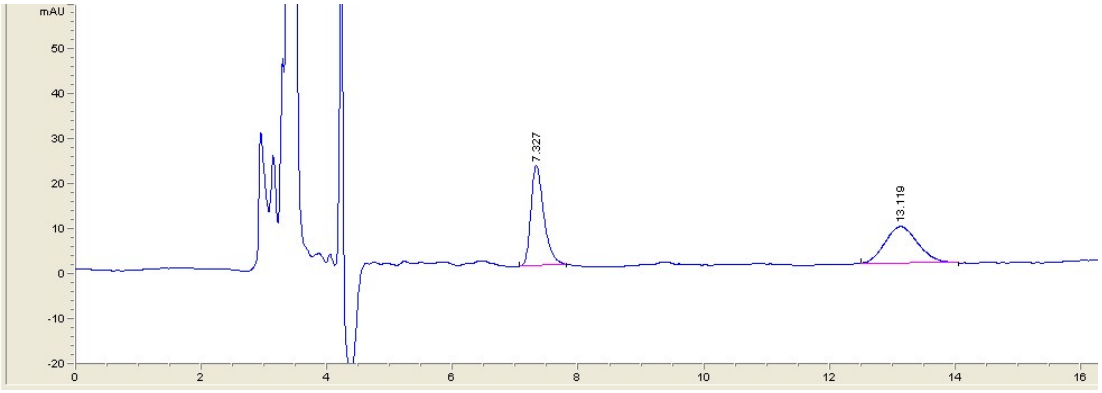
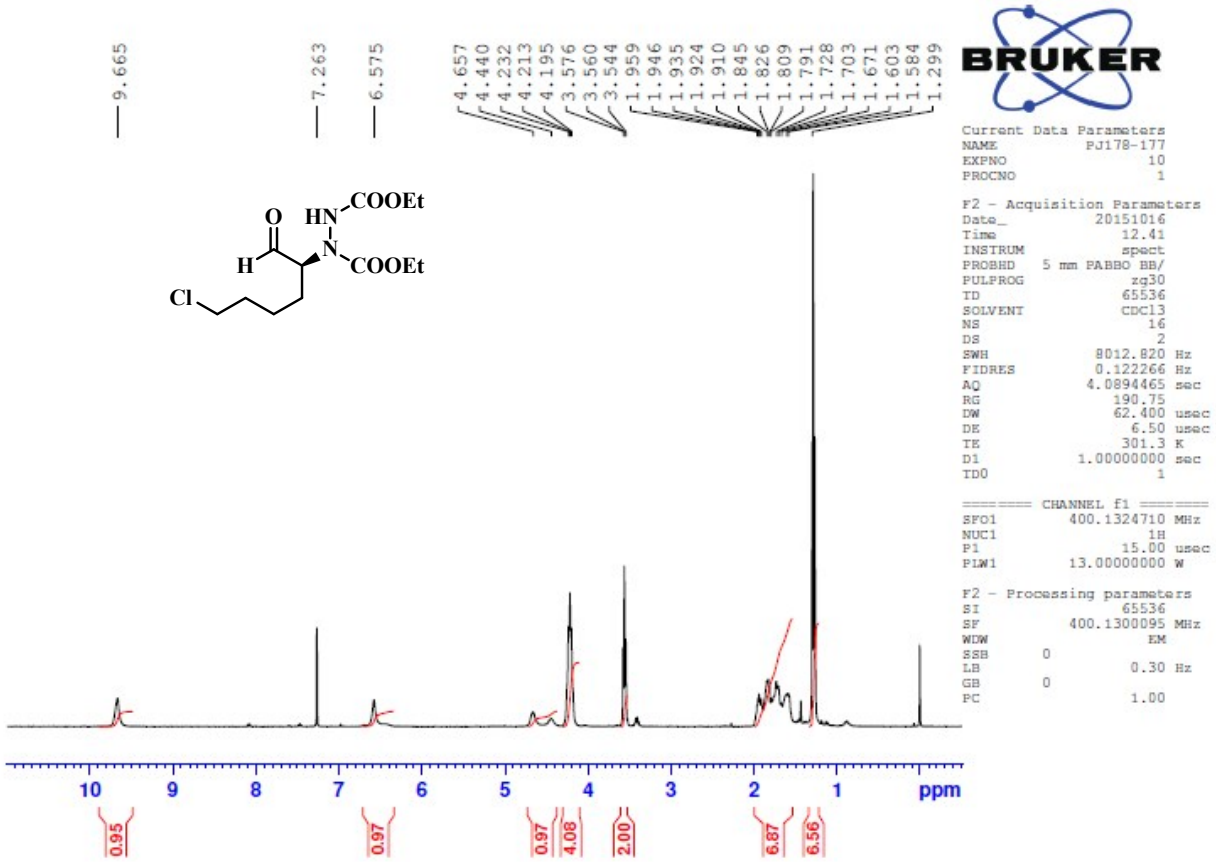
2	13.119	294.52484	48.1010



^{1}H and ^{13}C spectra of compound 5b

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PROCNO                        1

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INSTRUM                   spect
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PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           16
DS                            2
SWH                    8012.820 Hz
FIDRES                 0.122266 Hz
AQ                     4.0894465 sec
RG                        190.75
DW                        62.400 usec
DE                         6.50 usec
TE                        301.3 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                400.1324710 MHz
NUC1                        1H
P1                        15.00 usec
PLW1                13.00000000 W

F2 - Processing parameters
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GB                   0
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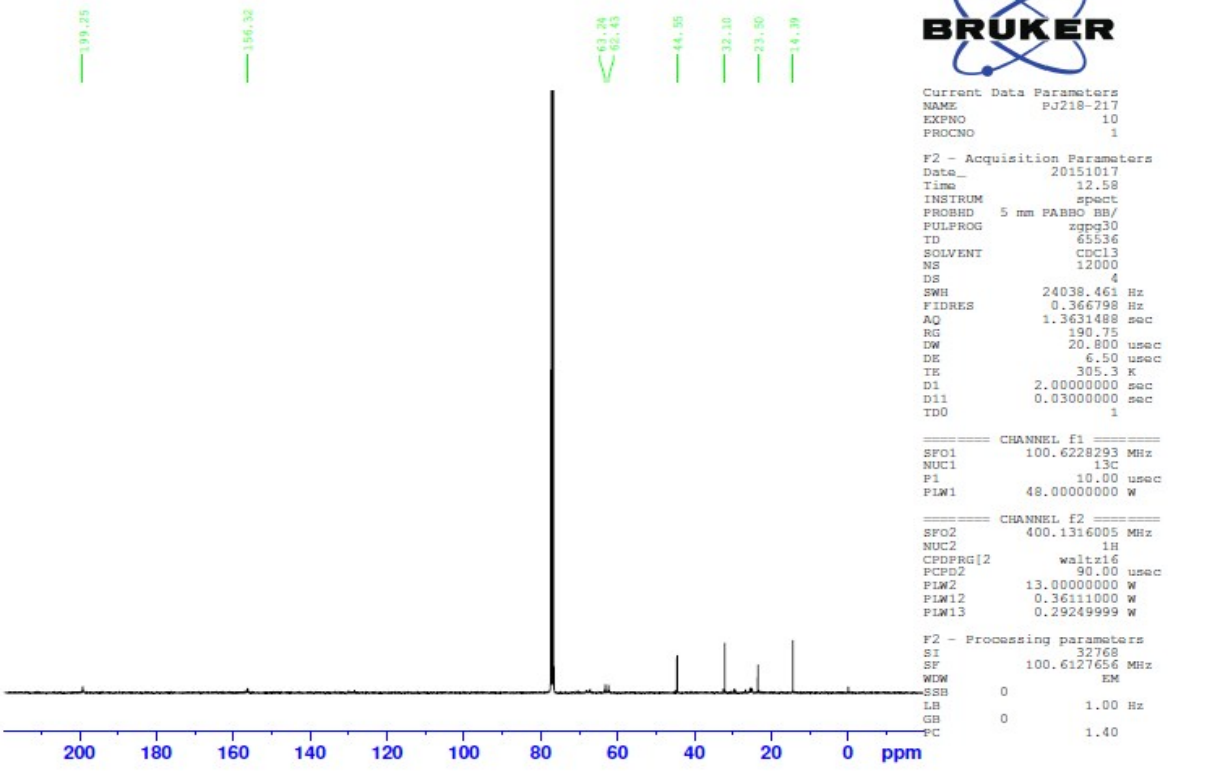


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PROCNO                        1

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INSTRUM                   spect
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PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                       12000
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.366798 Hz
AQ                     1.3631488 sec
RG                        190.75
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TE                        305.3 K
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D11                   0.03000000 sec
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NUC1                        13C
P1                        10.00 usec
PLW1                48.00000000 W

======== CHANNEL f2 ========
SFO2                400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2                13.00000000 W
PLW12                0.36111000 W
PLW13                0.29249999 W

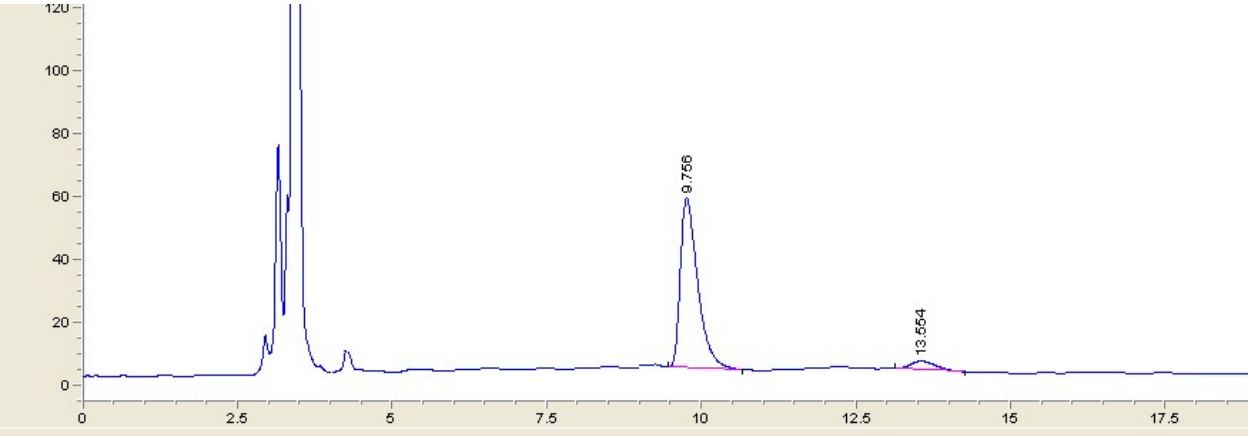
F2 - Processing parameters
SI                       32768
SF                  100.6127656 MHz
WDW                         EM
SSB                  0
LB                        1.00 Hz
GB                   0
PC                        1.40
```

Chiral HPLC analysis of **5b**:

Enantiomerically enriched

Peak Table

	RT	Area	% Area
1	9.756	1081.62793	94.6389
2	13.554	61.27143	5.3611



Racemic

Peak table

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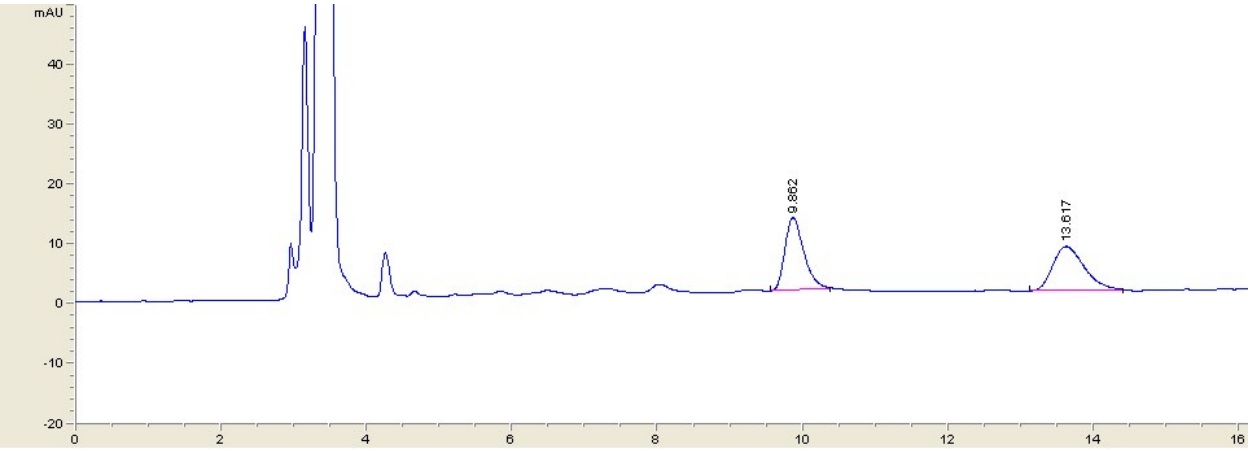
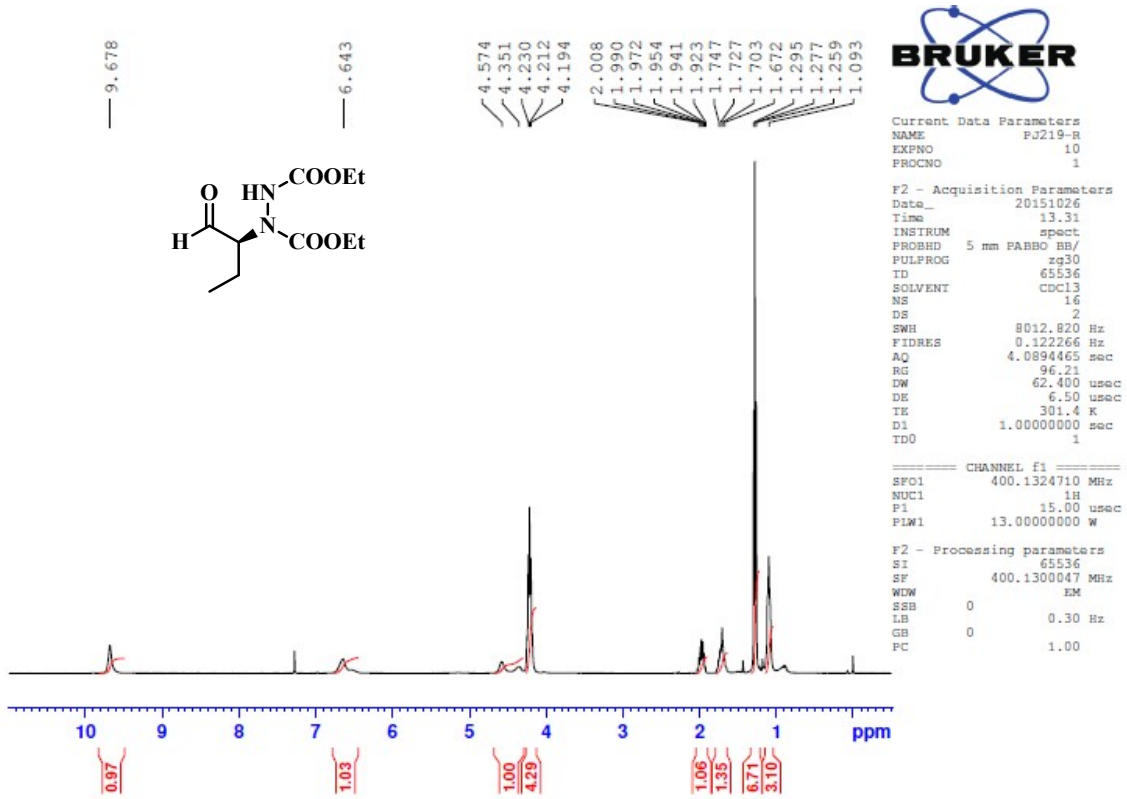
1	9.862	221.28650	49.4329
2	13.617	226.36339	50.5671



^{1}H and ^{13}C spectra of compound 5c



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EXPNO                      10
PROCNO                      1

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Date_               20151026
Time                   13.31
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                     96.21
DW                    62.400 usec
DE                     6.50 usec
TE                    301.4 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                     1H
P1                    15.00 usec
PLW1          13.00000000 W

F2 - Processing parameters
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WDW                      EM
SSB                   0
LB                     0.30 Hz
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PC                     1.00
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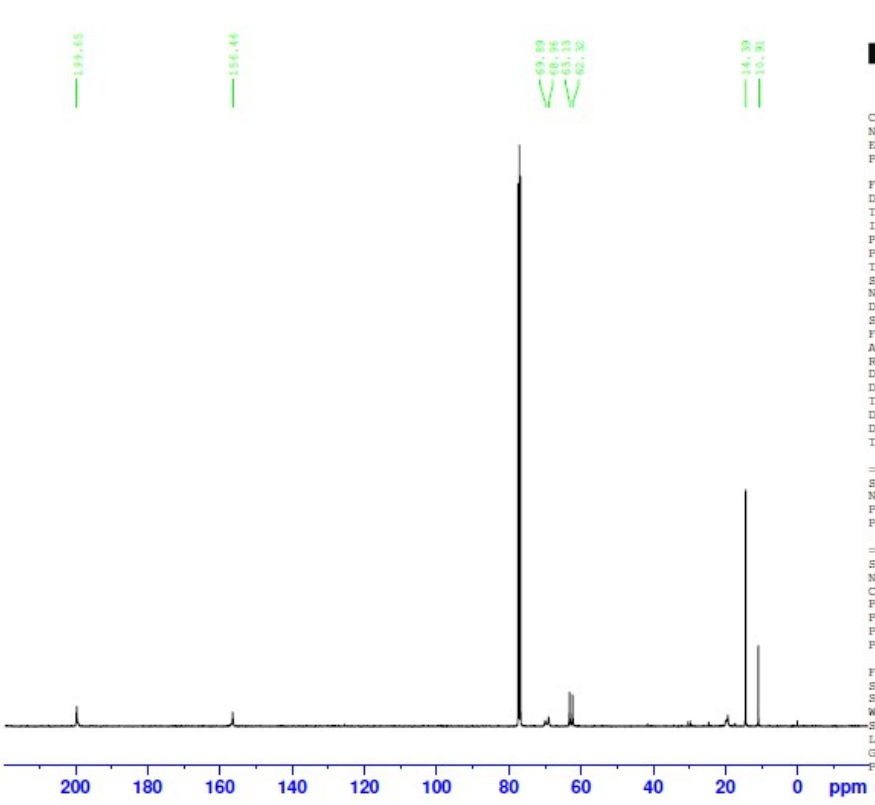

BRUKER

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EXPNO                      10
PROCNO                      1

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INSTRUM                spect
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PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       16000
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    190.75
DW                    20.800 usec
DE                     6.50 usec
TE                    303.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                    13C
P1                    10.00 usec
PLW1          48.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2          13.00000000 W
PLW12          0.36111000 W
PLW13          0.29249999 W

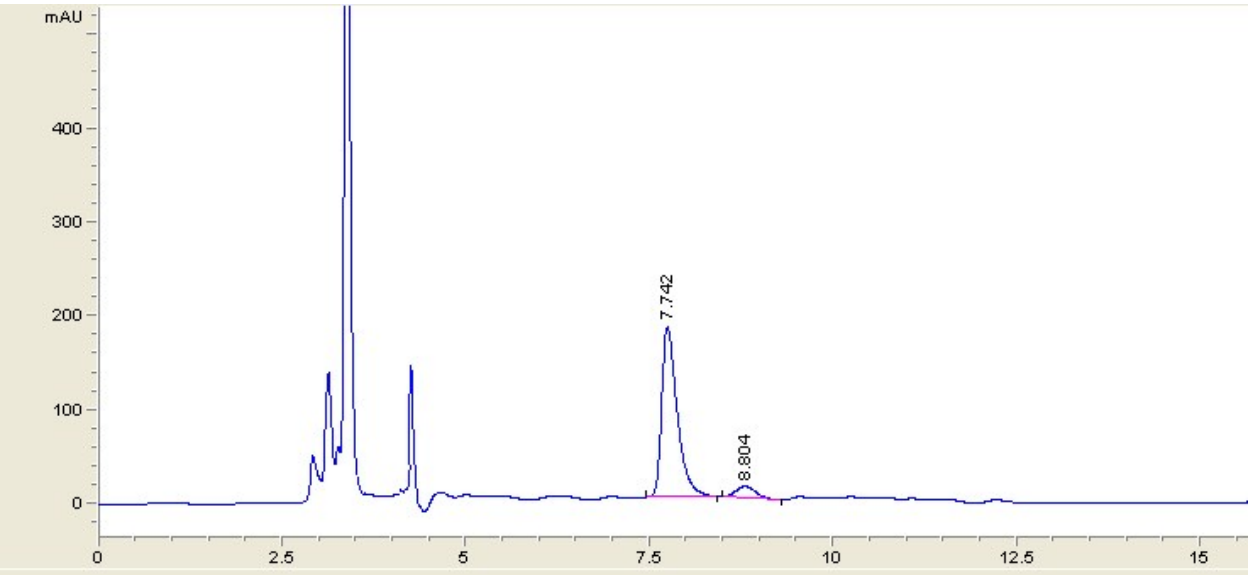
F2 - Processing parameters
SI                    32768
SF               100.6127644 MHz
WDW                      EM
SSB                   0
LB                     1.00 Hz
GB                    0
PC                     1.40
```

Chiral HPLC analysis of **5c**:

Enantiomerically enriched

Peak Table

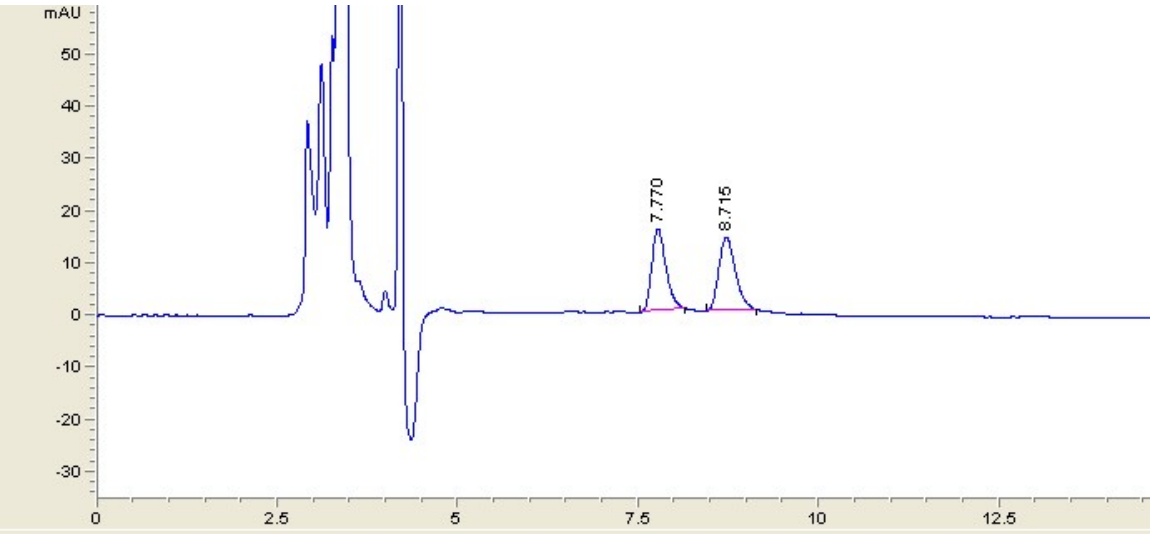
	RT	Area	% Area
1	7.742	2673.51245	92.0407
2	8.804	231.19392	7.9593



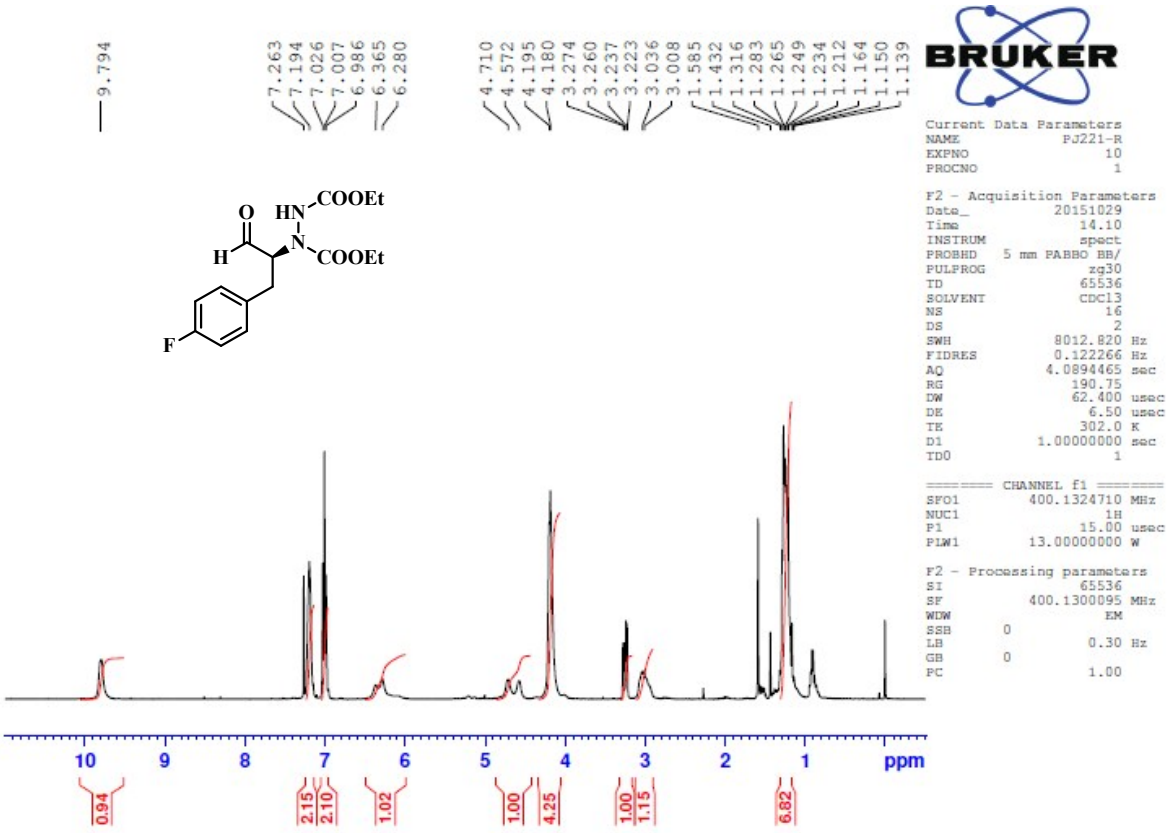
Racemic

Peak table

	RT	Area	% Area
1	7.770	224.94884	49.1507
2	8.715	232.72292	50.8493



^{1}H and ^{13}C spectra of compound 5d

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PROCNO                      1

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Time                   14.10
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                    190.75
DW                    62.400 usec
DE                     6.50 usec
TE                    302.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      15.00 usec
PLW1            13.00000000 W

F2 - Processing parameters
SI                        65536
SF               400.1300095 MHz
WDW                         EM
SSB                  0
LB                      0.30 Hz
GB                   0
PC                      1.00
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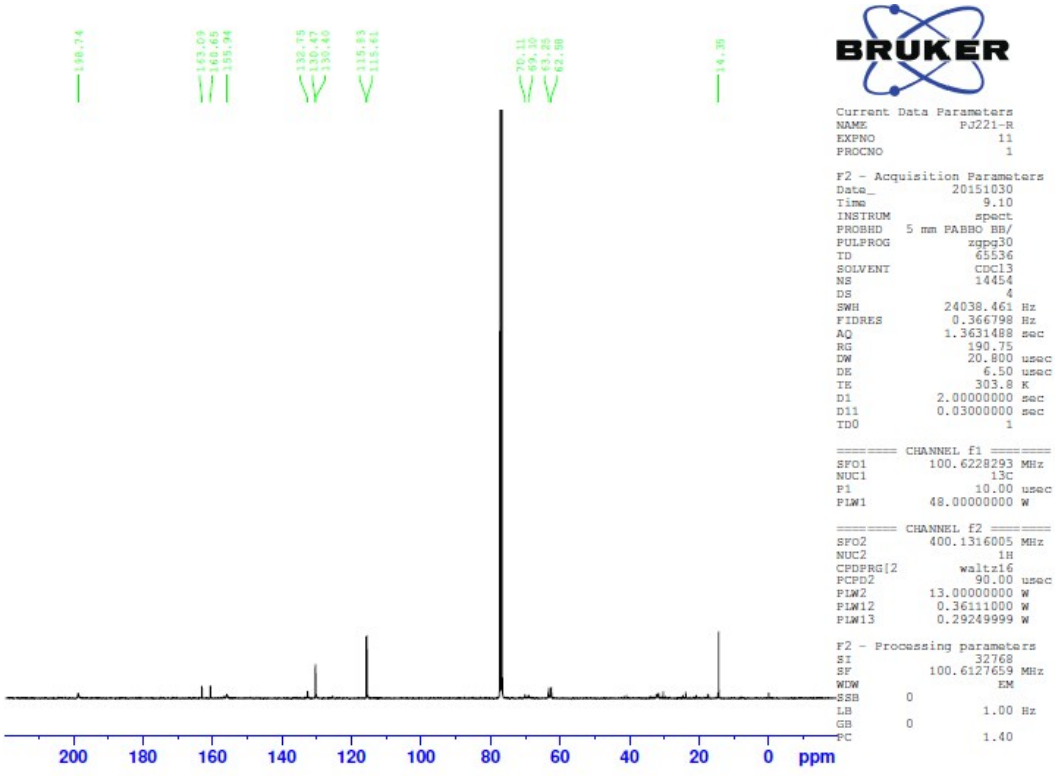


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Current Data Parameters
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EXPNO                      11
PROCNO                      1

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Time                    9.10
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                    14454
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    190.75
DW                    20.800 usec
DE                     6.50 usec
TE                    303.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             100.6228293 MHz
NUC1                      13C
P1                      10.00 usec
PLW1            48.00000000 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2            13.00000000 W
PLW12            0.36111000 W
PLW13            0.29249999 W

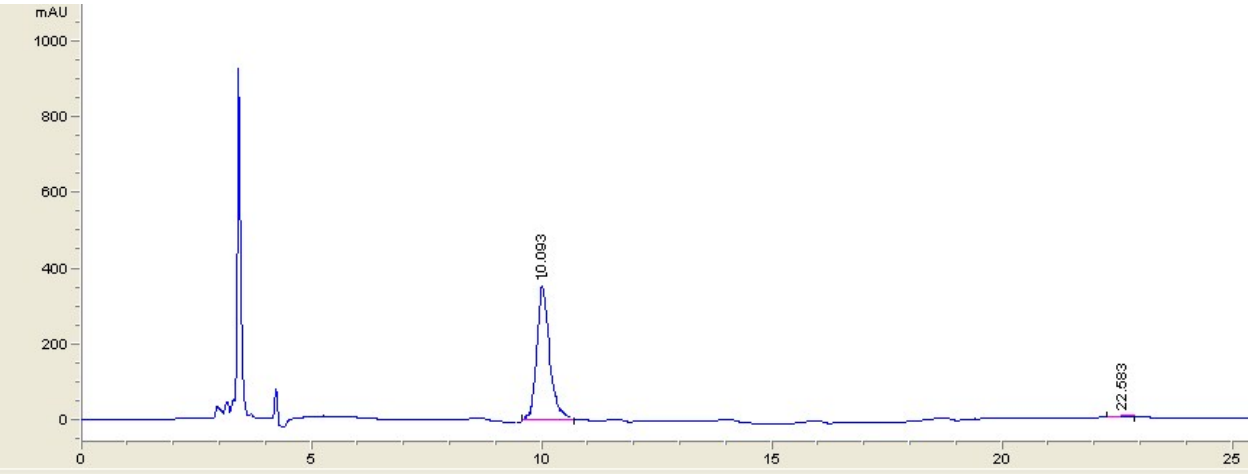
F2 - Processing parameters
SI                        32768
SF               100.6127659 MHz
WDW                         EM
SSB                  0
LB                      1.00 Hz
GB                   0
PC                      1.40
```

Chiral HPLC analysis of **5d**:

Enantiomerically enriched

Peak Table

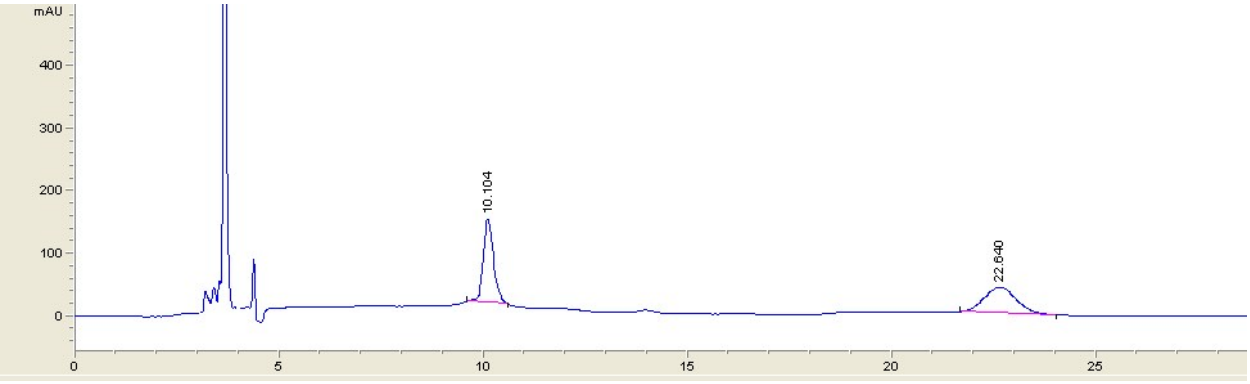
	RT	Area	% Area
1	10.093	5859,03711	100.0000
2	22.640	/	/



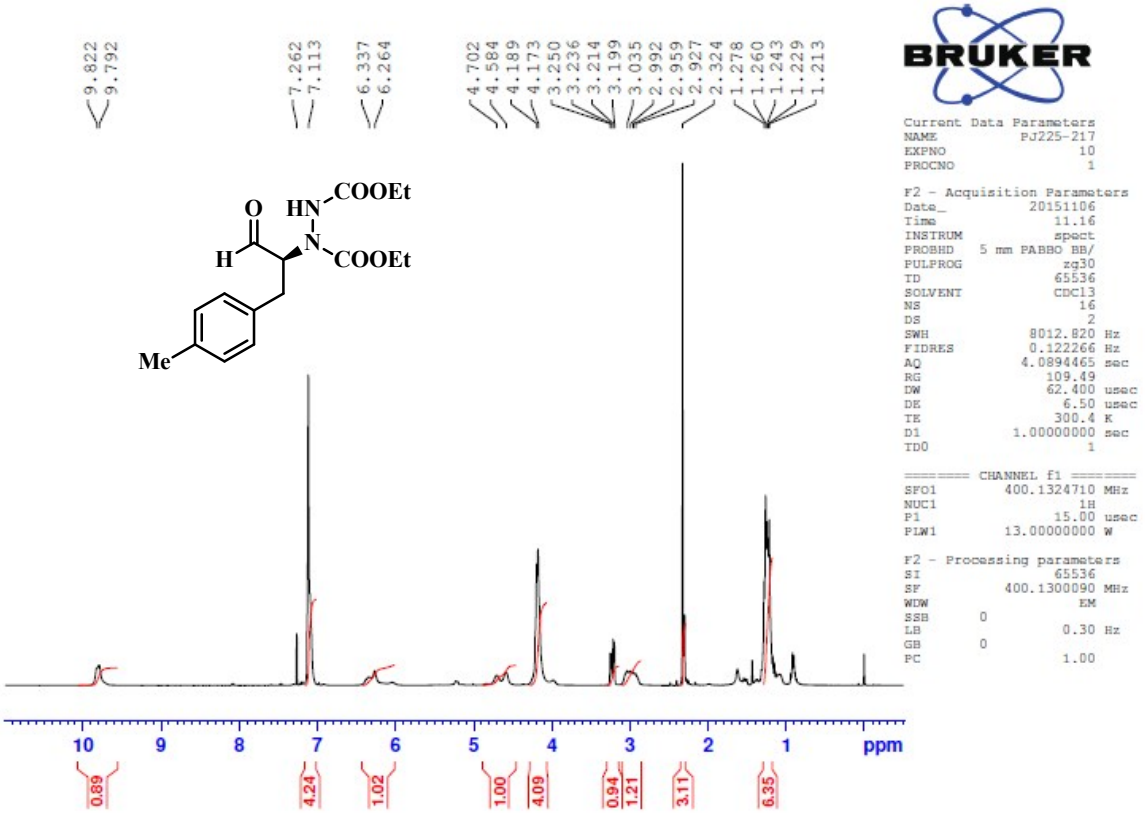
Racemic

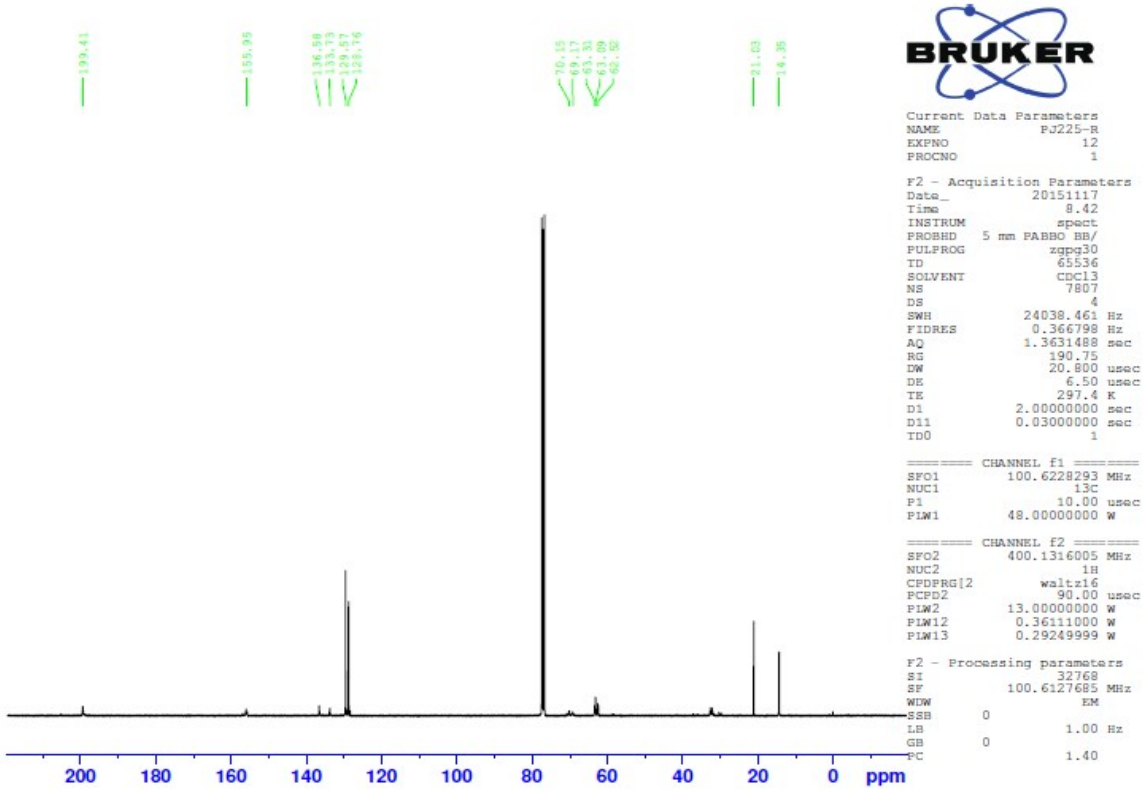
Peak table

	RT	Area	% Area
1	10.104	2390.98022	50.8621
2	22.640	2309.92578	49.1379



^{1}H and ^{13}C spectra of compound 5e



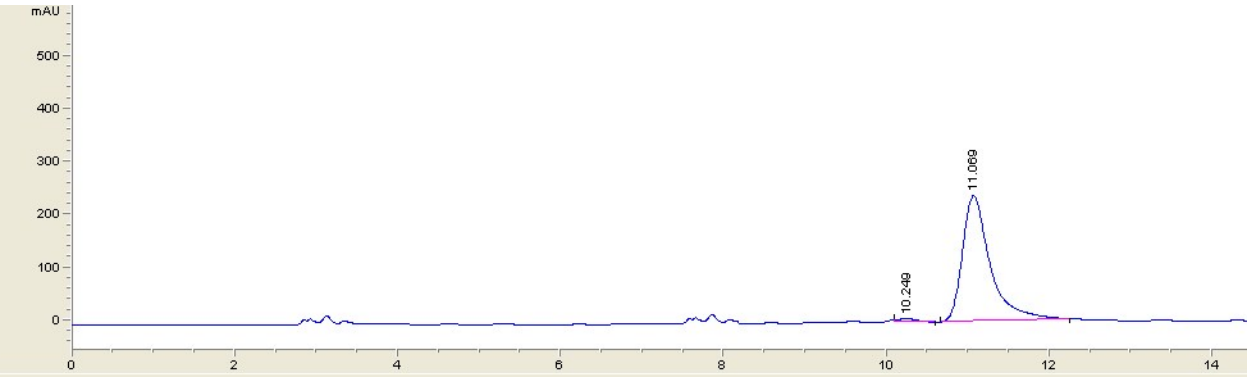


Chiral HPLC analysis of **5e**:

Enantiomerically enriched

Peak Table

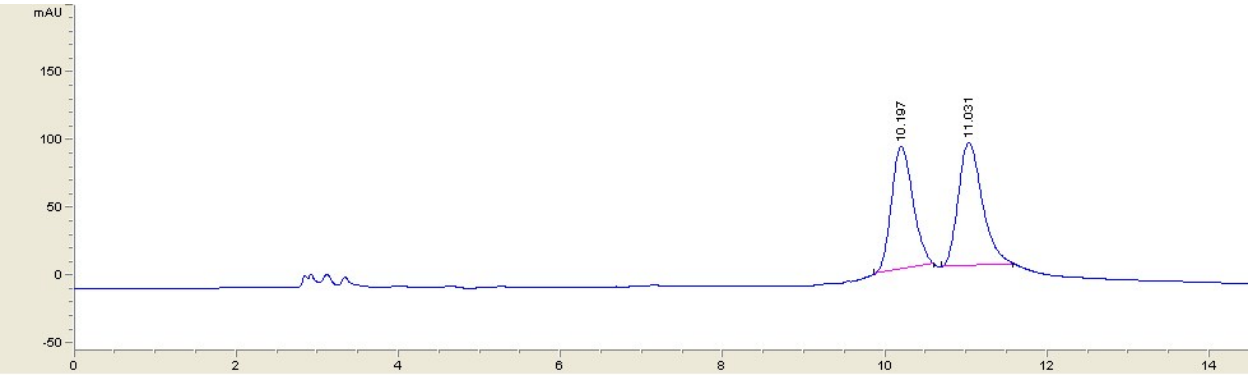
	RT	Area	% Area
1	10.269	133.14925	0.6948
2	11.069	19029.0000	99.3052



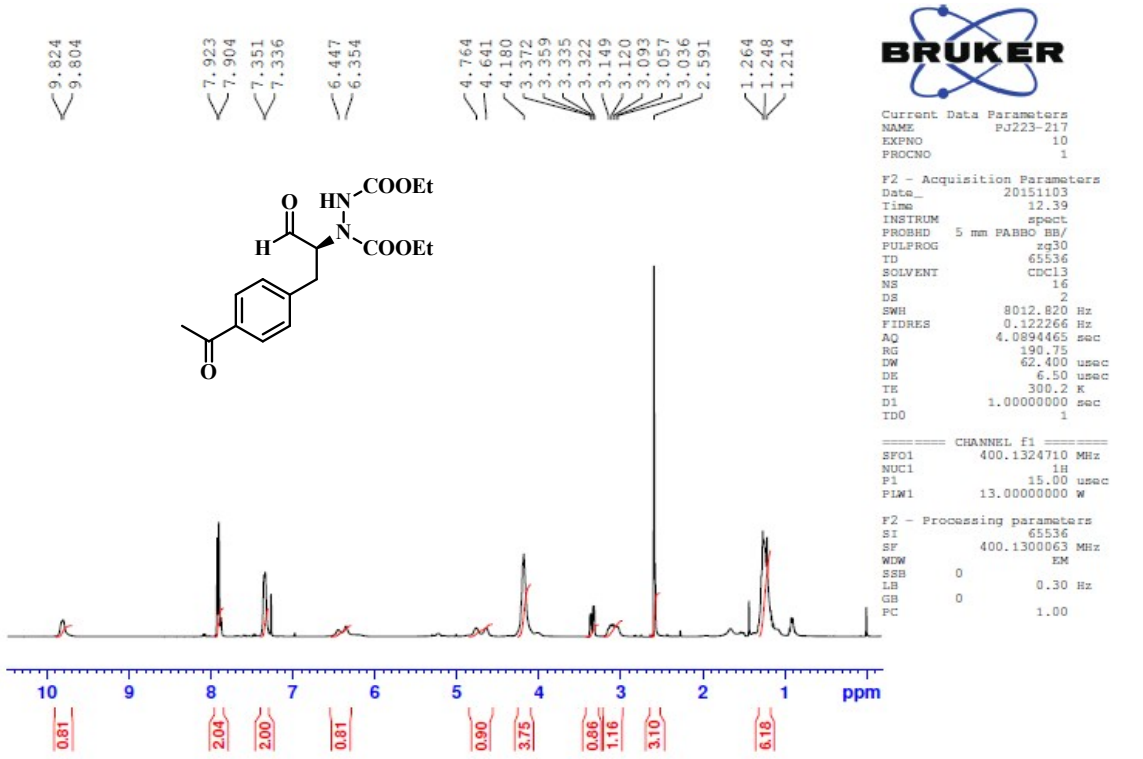
Racemic

Peak table

	RT	Area	% Area
1	10.198	5661.67871	49.1709
2	11.031	5852.59863	50.8291



^{1}H and ^{13}C spectra of compound 5f



BRUKER

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NAME                  PJ223-217
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PROCNO                        1

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Time                      12.39
INSTRUM                   spect
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PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                       190.75
DW                       62.400 usec
DE                        6.50 usec
TE                       300.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                400.1324710 MHz
NUC1                        1H
P1                       15.00 usec
PLW1                13.00000000 W

F2 - Processing parameters
SI                       65536
SF                  400.1300063 MHz
WDW                         EM
SSB                  0
LB                        0.30 Hz
GB                   0
PC                        1.00
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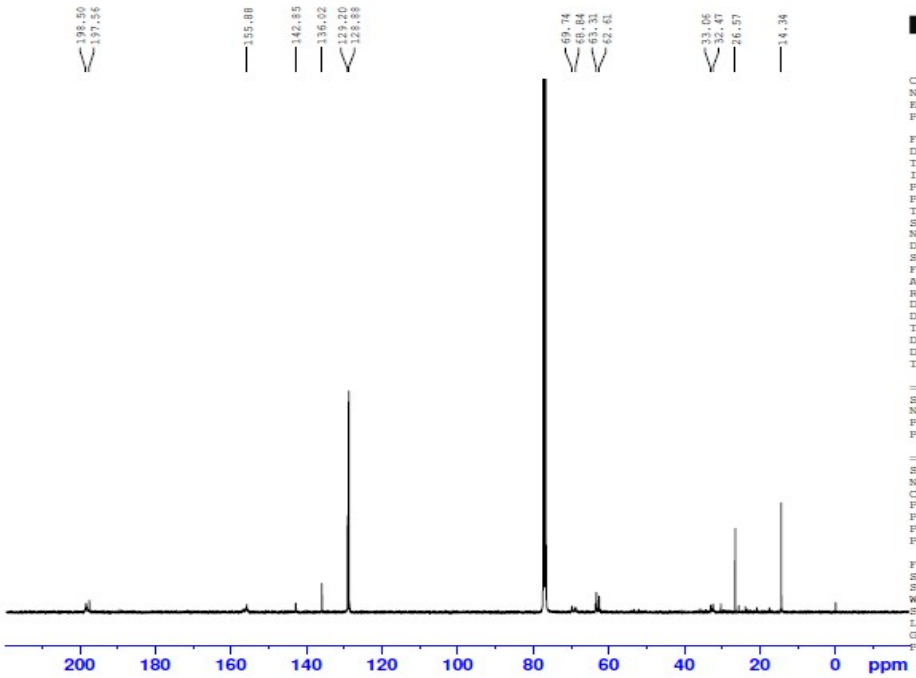

BRUKER

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Current Data Parameters
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PROCNO                      1

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INSTRUM                   spect
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PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                       30000
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631488 sec
RG                       190.75
DW                       20.800 usec
DE                        6.50 usec
TE                       302.5 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                100.6228293 MHz
NUC1                        13C
P1                       10.00 usec
PLW1                48.00000000 W

======== CHANNEL f2 ========
SFO2                400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                13.00000000 W
PLW12                0.36111000 W
PLW13                0.29249999 W

F2 - Processing parameters
SI                       32768
SF                  100.6127664 MHz
WDW                         EM
SSB                  0
LB                        1.00 Hz
GB                   0
PC                        1.40
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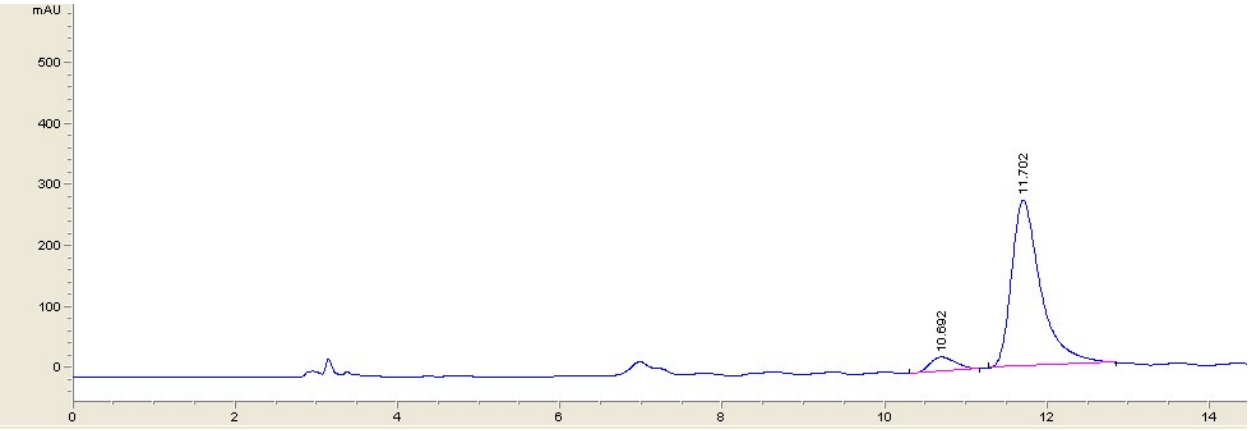
Chiral HPLC analysis of **5f**:

Enantiomerically enriched

Peak Table

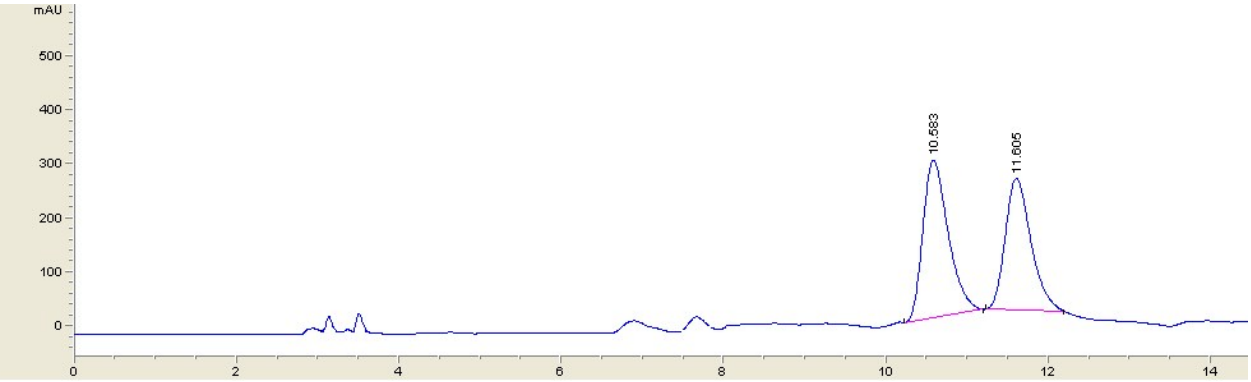
	RT	Area	% Area
1	10.690	1639.39624	7.2345
2	11.702	21021.4000	92.7655



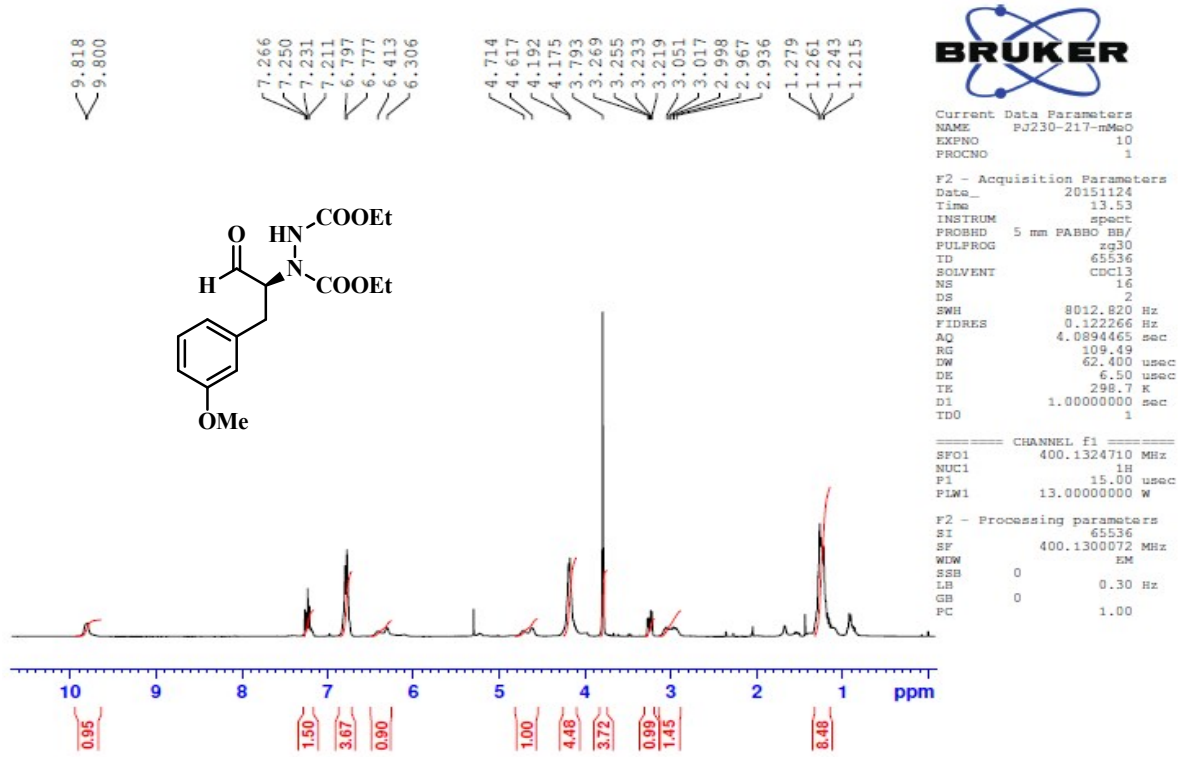
Racemic

Peak table

	RT	Area	% Area
1	10.583	18447.8000	51.4608
2	11.605	17400.4000	48.5392



^{1}H and ^{13}C spectra of compound 5g




```
Current Data Parameters
NAME      PJ230-217-mMeO
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151124
Time               13.53
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                109.49
DW                62.400 usec
DE                 6.50 usec
TE                298.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  15.00 usec
PLW1        13.00000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300072 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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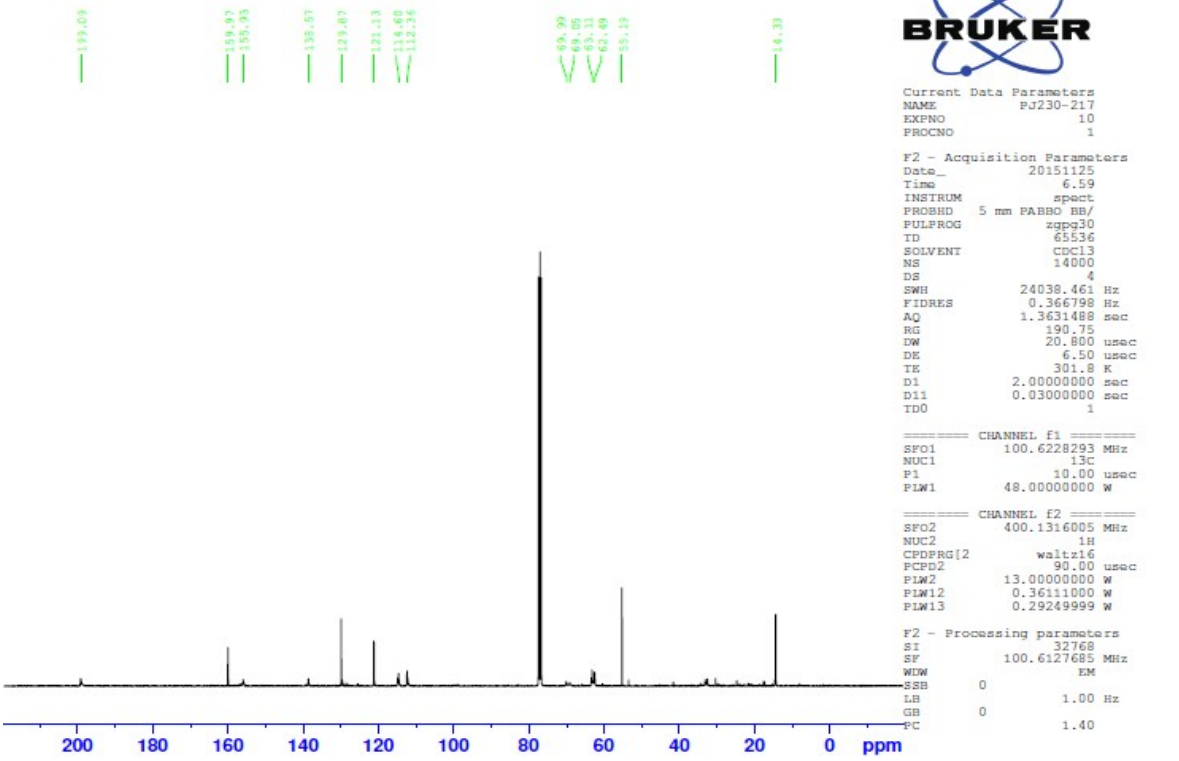


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Current Data Parameters
NAME            PJ230-217
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151125
Time               6.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                14000
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                190.75
DW                20.800 usec
DE                 6.50 usec
TE                301.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                  13C
P1                  10.00 usec
PLW1        48.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2        13.00000000 W
PLW12        0.36111000 W
PLW13        0.29249999 W

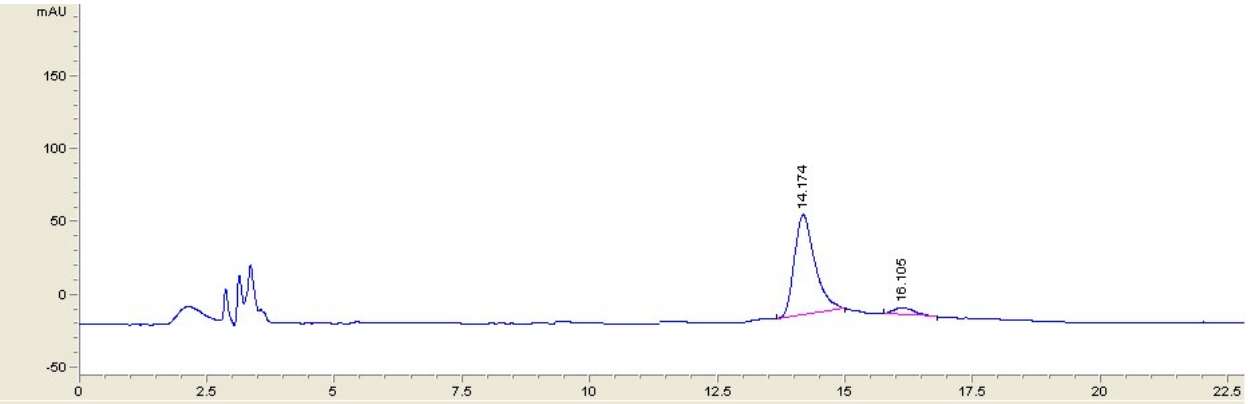
F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Chiral HPLC analysis of **5g**:

Enantiomerically enriched

Peak Table

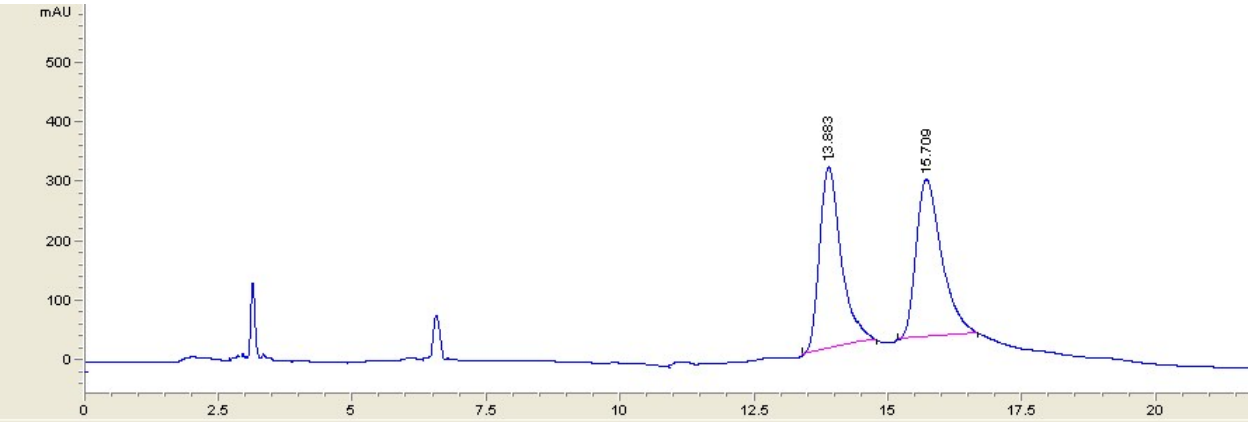
	RT	Area	% Area
1	14.174	2112.60571	95.5351
2	16.105	98.73514	4.4649



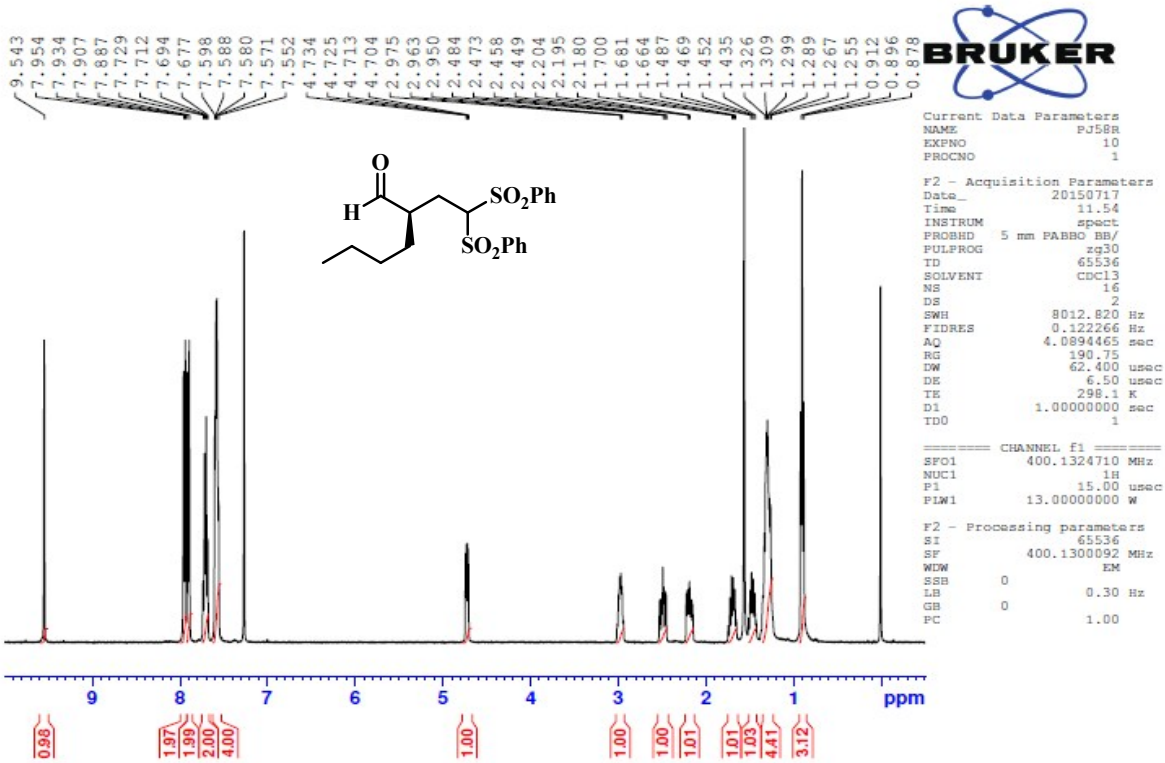
Racemic

Peak table

	RT	Area	% Area
1	13.883	8808.53125	50.2336
2	15.709	8726.59570	49.7664



^{1}H and ^{13}C spectra of compound 8a



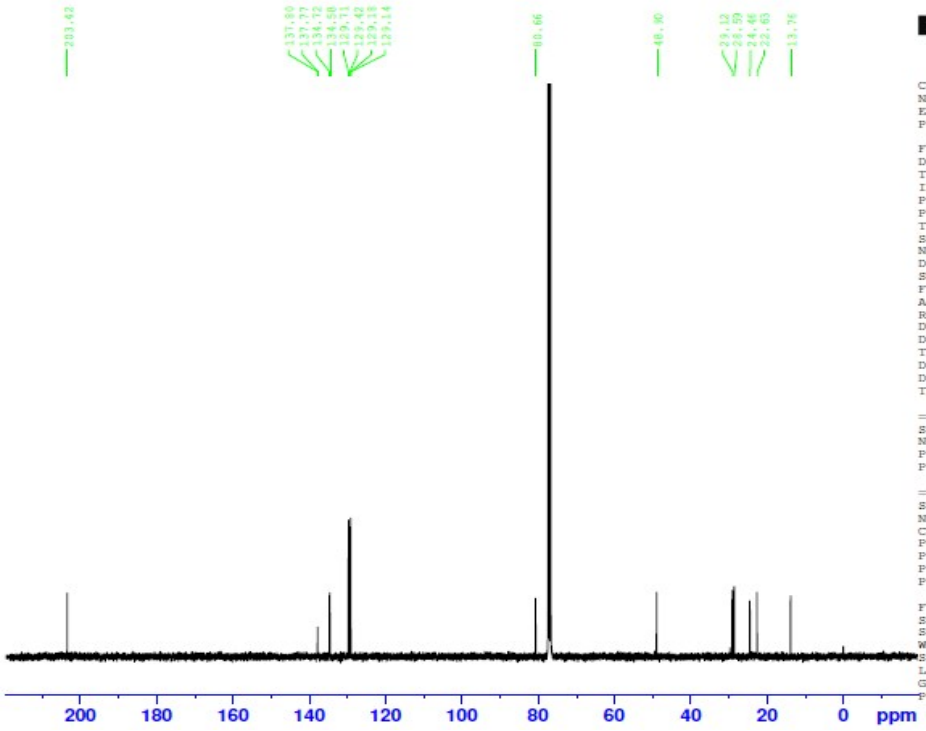
BRUKER

```
Current Data Parameters
NAME                  PJ58R
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150717
Time                  11.54
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894465 sec
RG                    190.75
DW                    62.400 usec
DE                     6.50 usec
TE                    298.1 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                      1H
P1                     15.00 usec
PLW1            13.00000000 W

F2 - Processing parameters
SI                        65536
SF               400.1300092 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



BRUKER

```
Current Data Parameters
NAME                  PJ58R
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150717
Time                  13.41
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1829
DS                        4
SWH               24038.461 Hz
FIDRES                0.366798 Hz
AQ                 1.3631488 sec
RG                    190.75
DW                    20.800 usec
DE                     6.50 usec
TE                    300.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             100.6228293 MHz
NUC1                      13C
P1                     10.00 usec
PLW1            48.00000000 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2            13.00000000 W
PLW12            0.36111000 W
PLW13            0.29249999 W

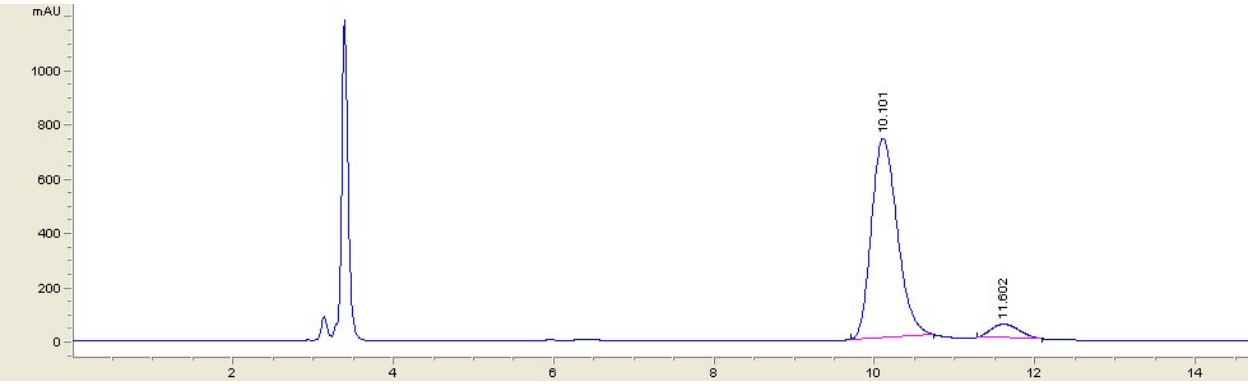
F2 - Processing parameters
SI                        32768
SF               100.6127685 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

Chiral HPLC analysis of **8a**:

Enantiomerically enriched

Peak Table

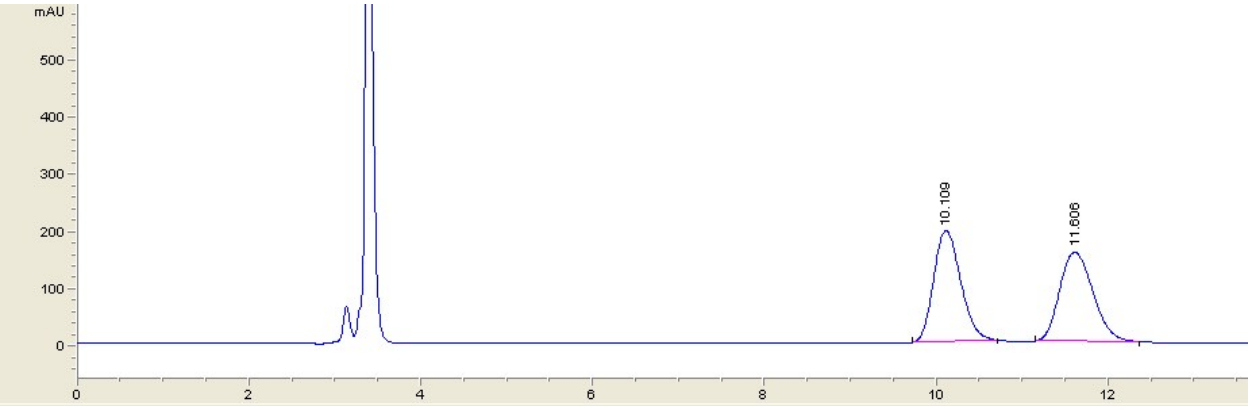
	RT	Area	% Area
1	10.101	17073.9000	93.0391
2	11.602	1277.41418	6.9609



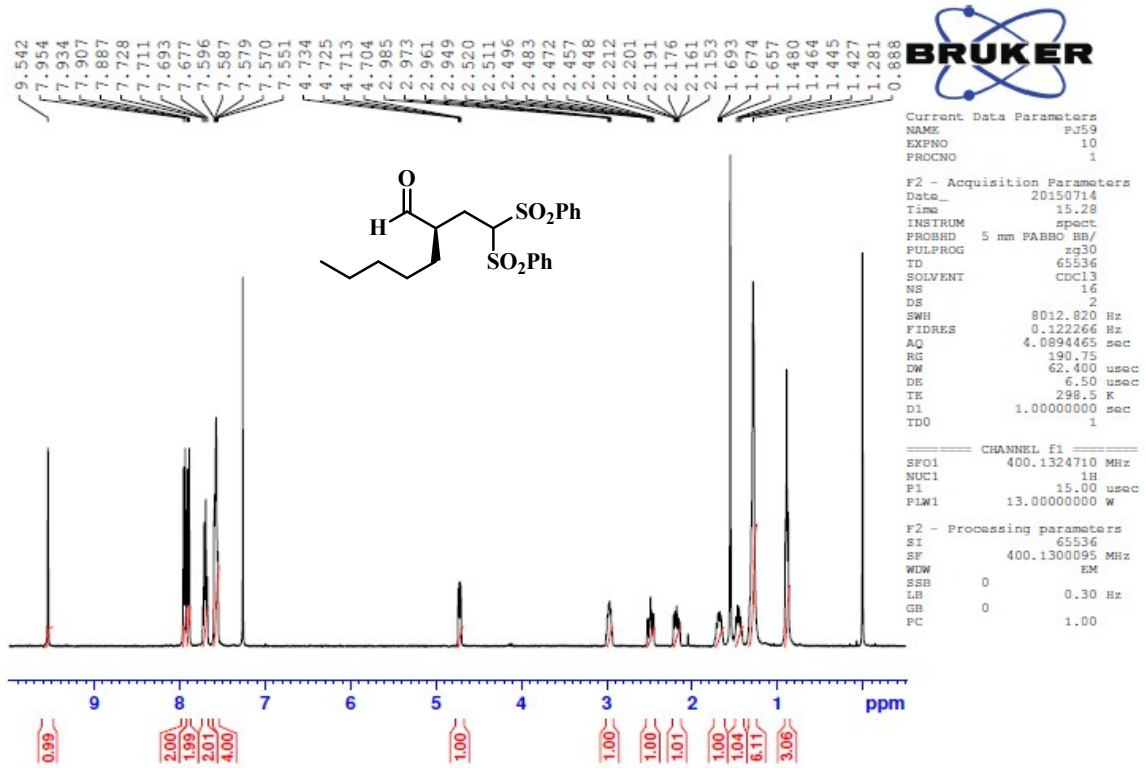
Racemic

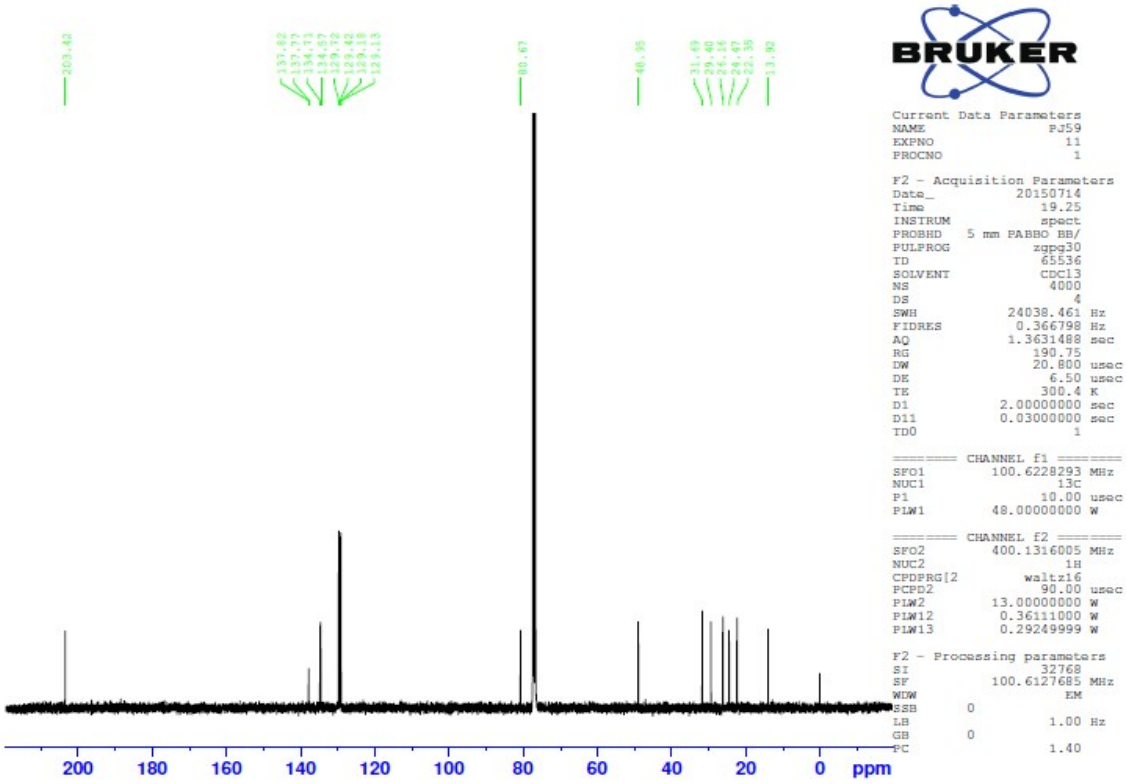
Peak table

	RT	Area	% Area
1	10.109	4337.27881	50.5718
2	11.606	4239.19189	49.4282



^{1}H and ^{13}C spectra of compound 8b



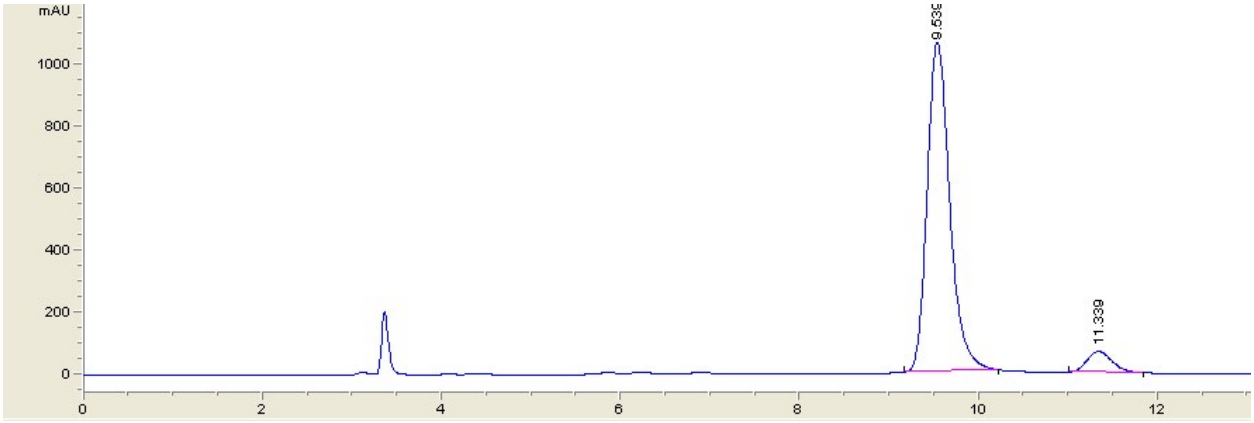


Chiral HPLC analysis of **8b**:

Enantiomerically enriched

Peak Table

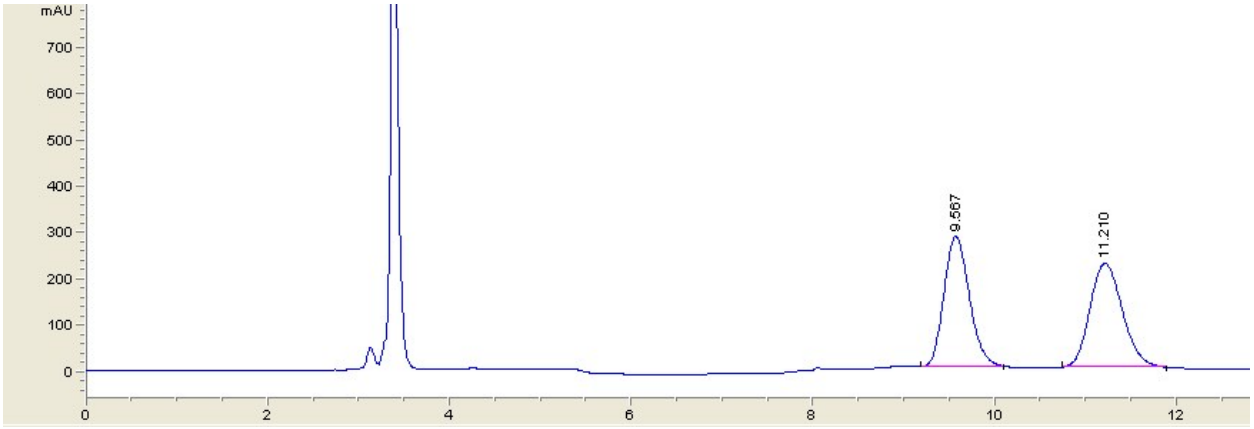
	RT	Area	% Area
1	9.676	13235.6000	93.5158
2	11.374	917.73486	6.4842



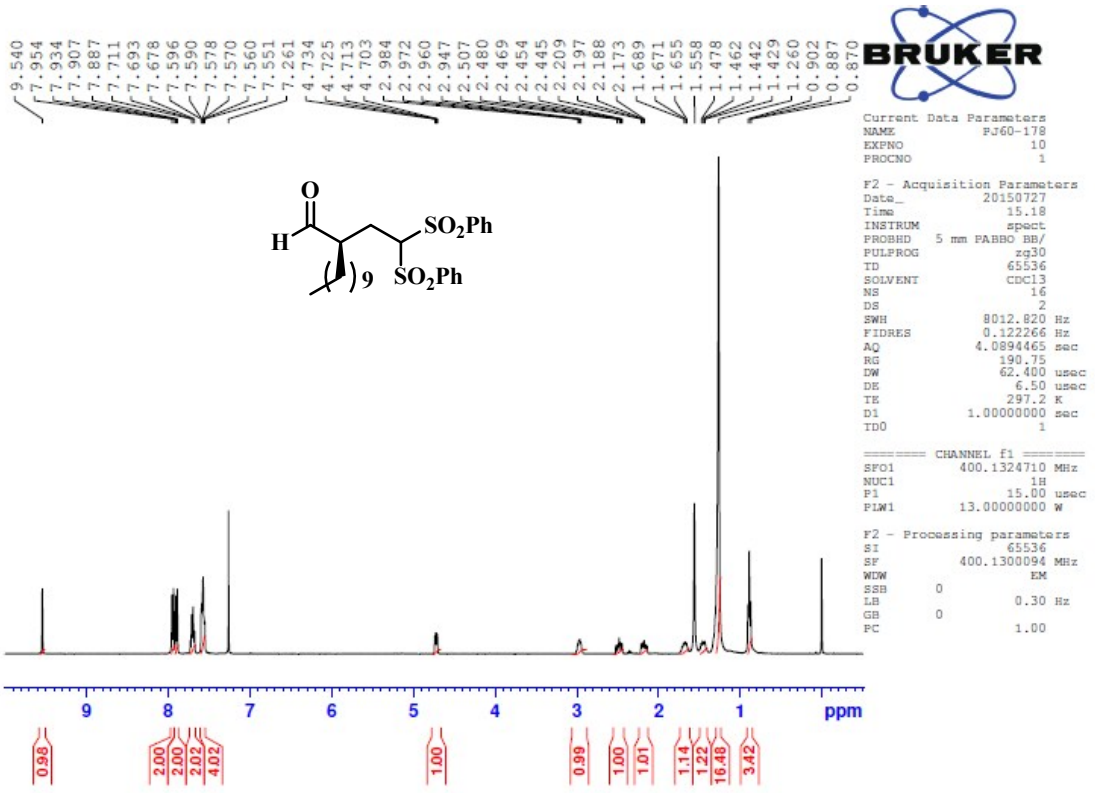
Racemic

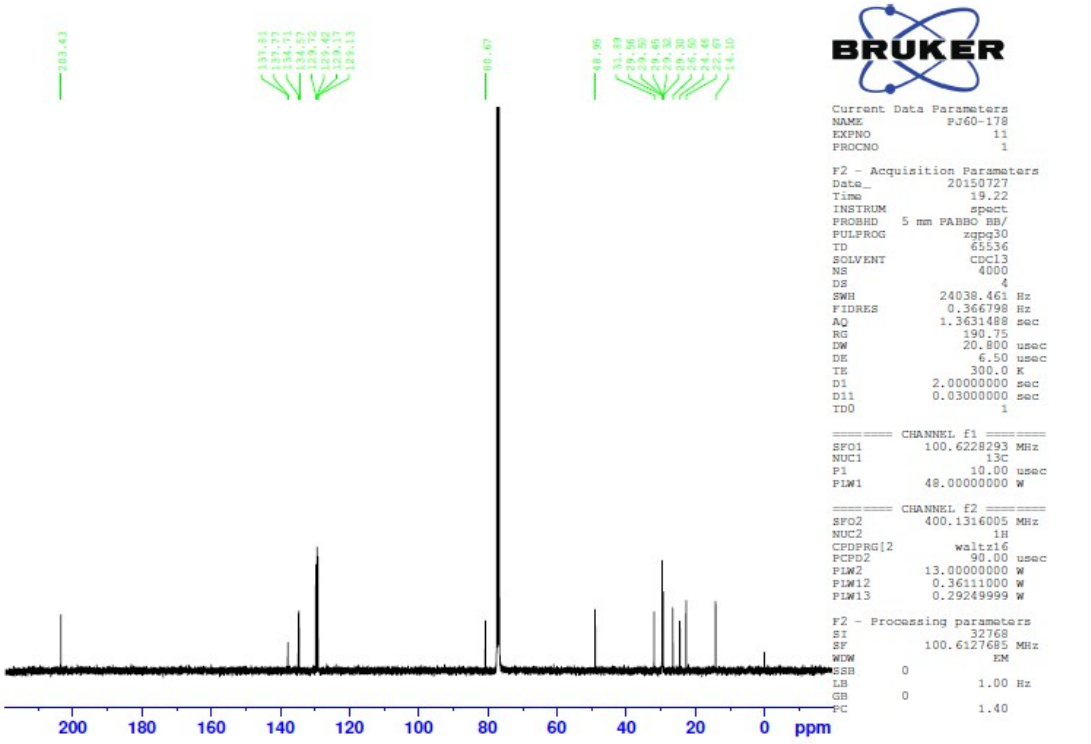
Peak table

	RT	Area	% Area
1	9.567	5462.17334	49.5093
2	11.210	5570.43652	50.4907



^{1}H and ^{13}C spectra of compound 8c



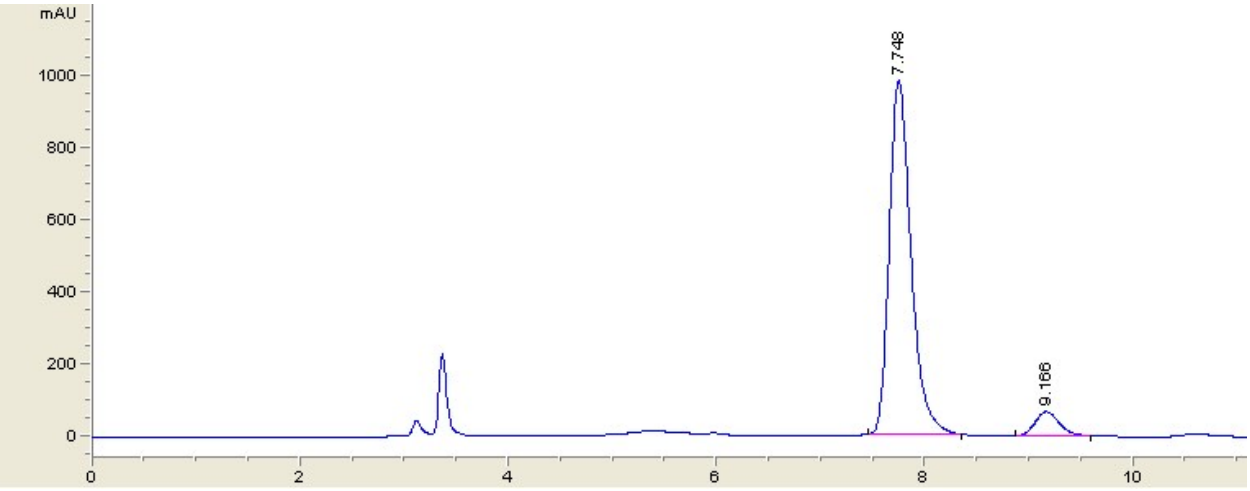


Chiral HPLC analysis of **8c**:

Enantiomerically enriched

Peak Table

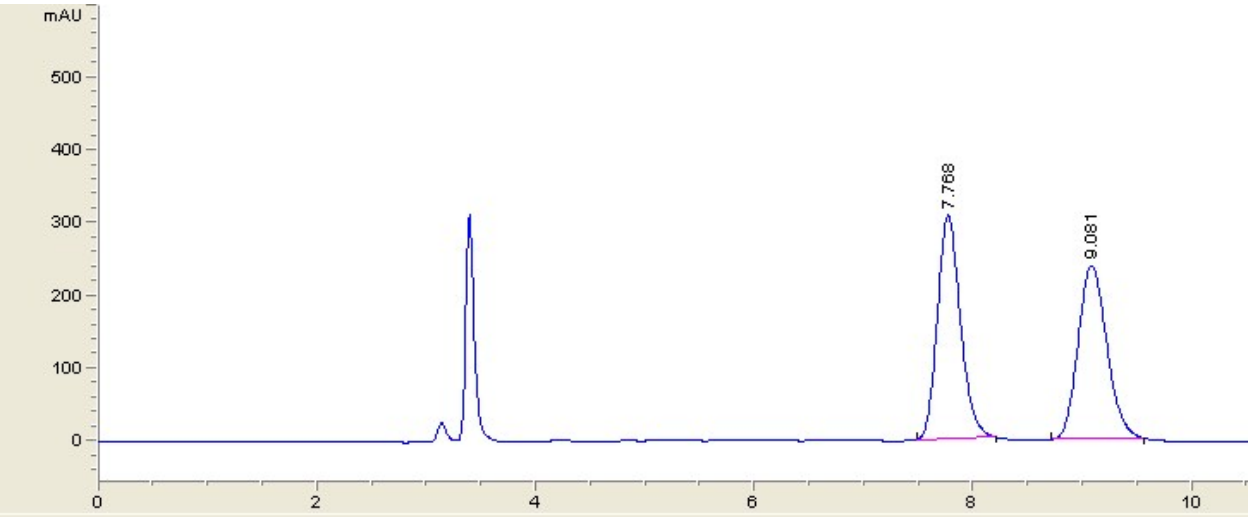
	RT	Area	% Area
1	7.748	21203.3000	92.8763
2	9.166	1633.97327	7.1237



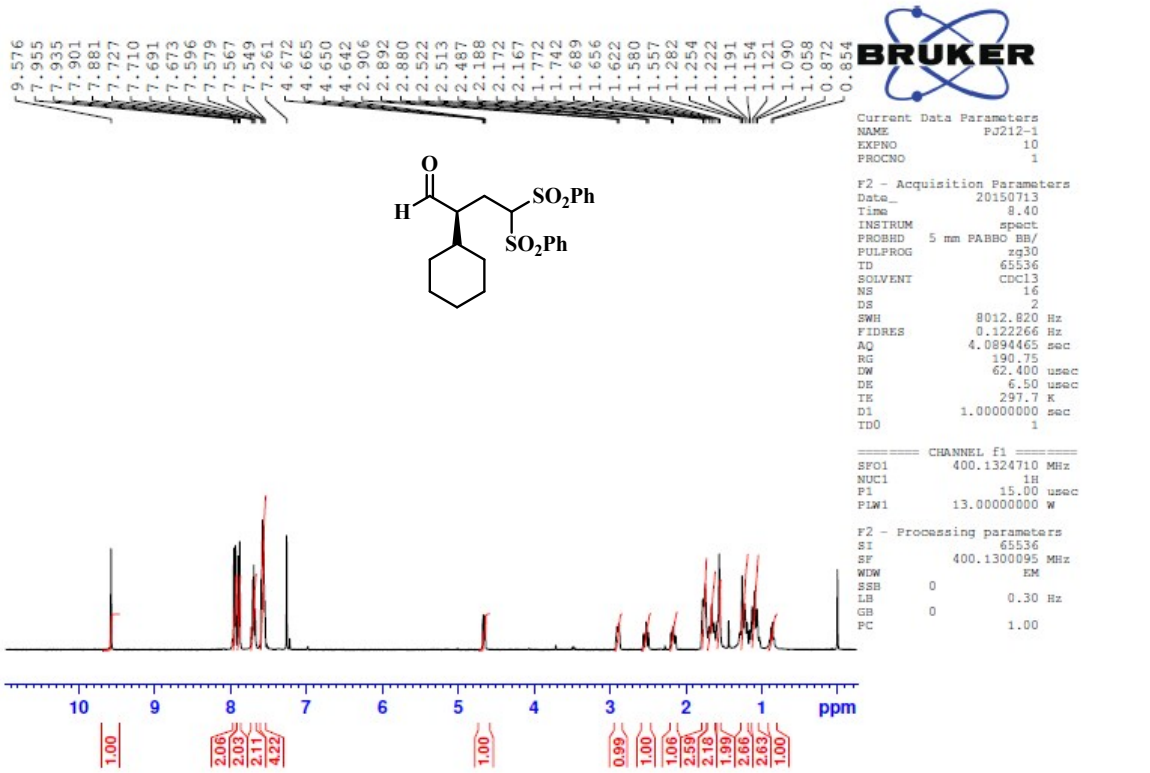
Racemic

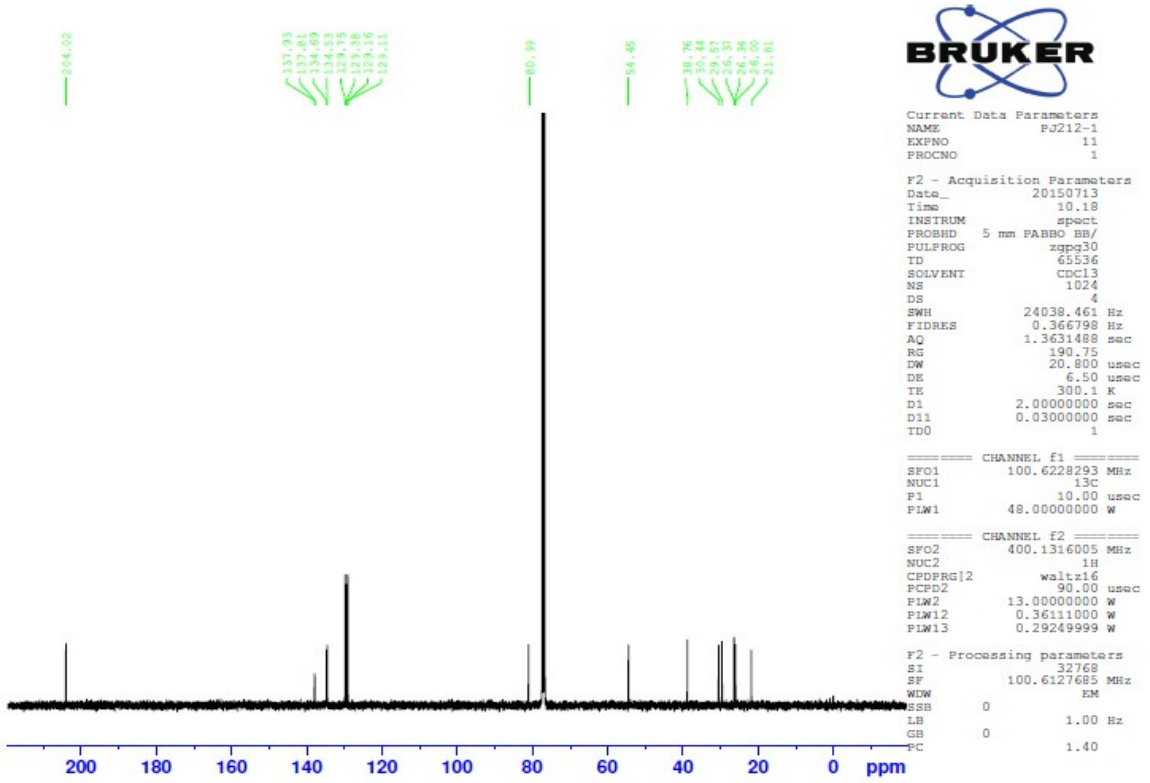
Peak table

	RT	Area	% Area
1	7.768	6459.96094	50.8195
2	9.081	6251.62012	49.1805



^{1}H and ^{13}C spectra of compound 8d



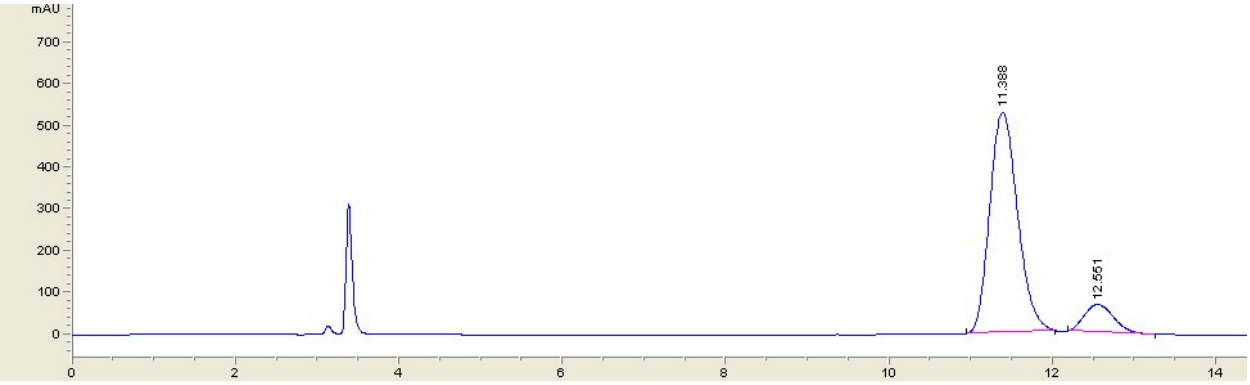


Chiral HPLC analysis of **8d**:

Enantiomerically enriched

Peak Table

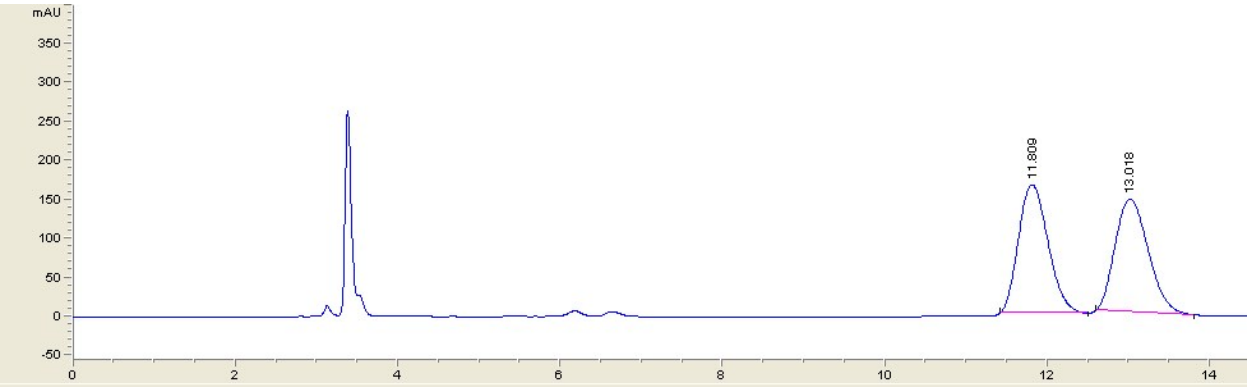
	RT	Area	% Area
1	11.388	17910.5000	88.6741
2	12.551	2287.62573	11.3259



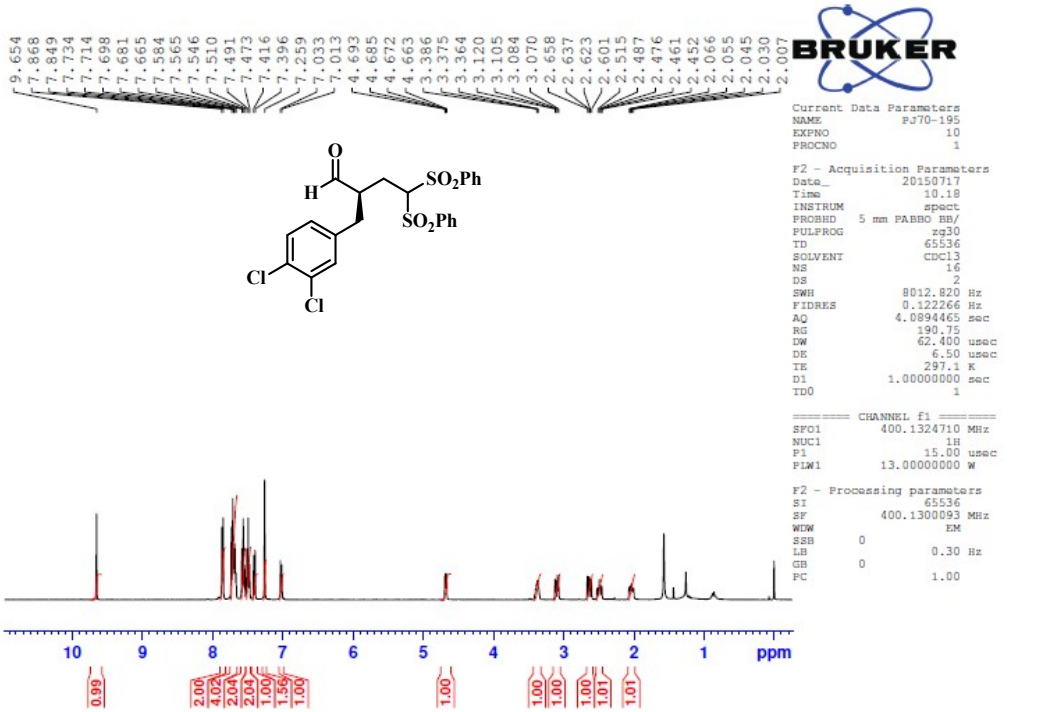
Racemic

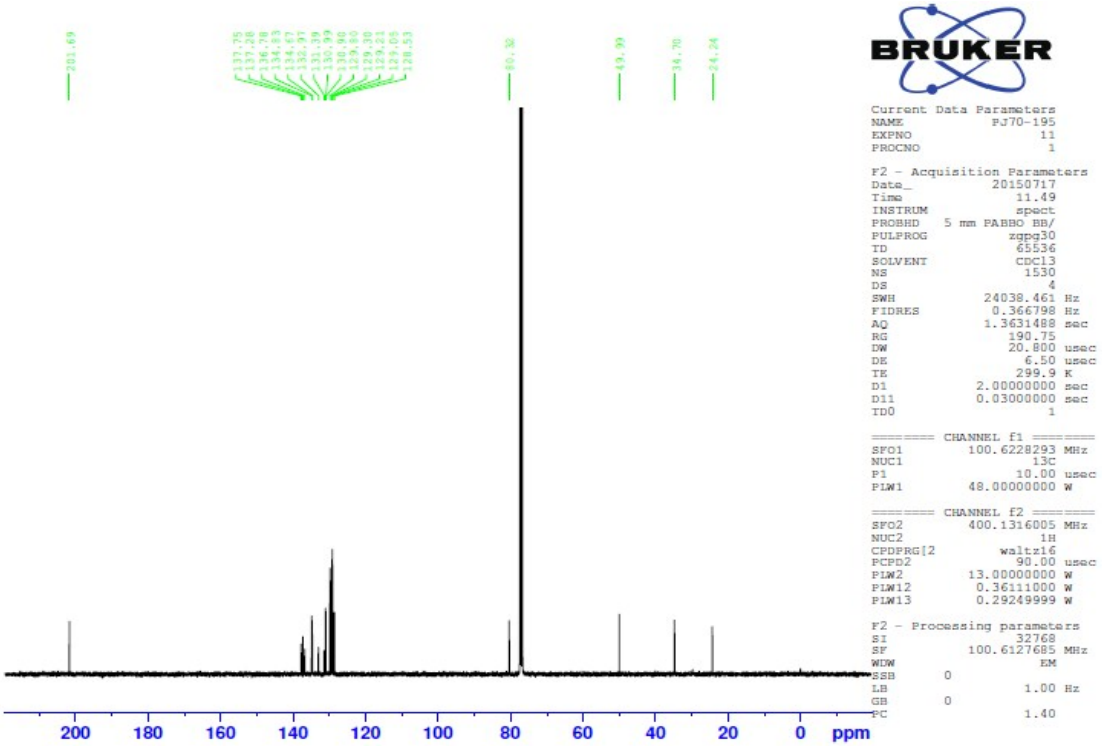
Peak table

	RT	Area	% Area
1	11.809	6063.60107	50.2594
2	13.018	6001.01416	49.7406



^{1}H and ^{13}C spectra of compound 8e



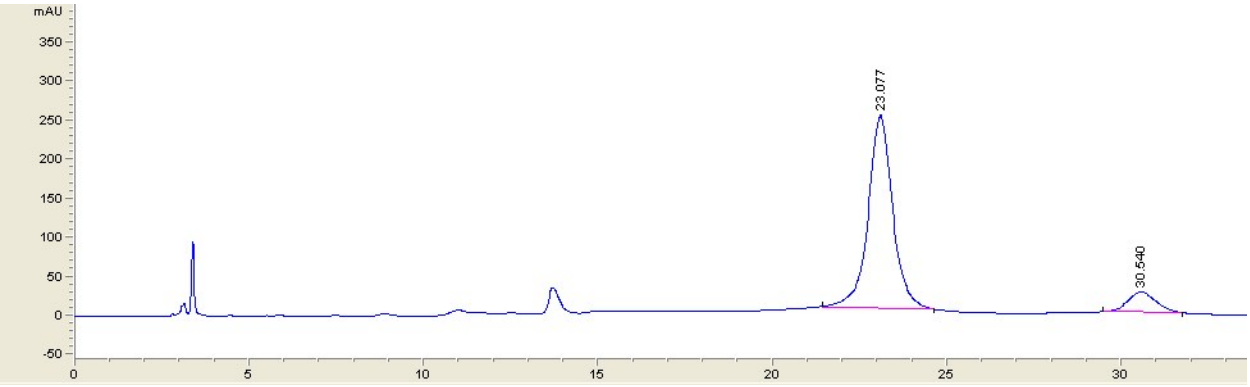


Chiral HPLC analysis of **8e**:

Enantiomerically enriched

Peak Table

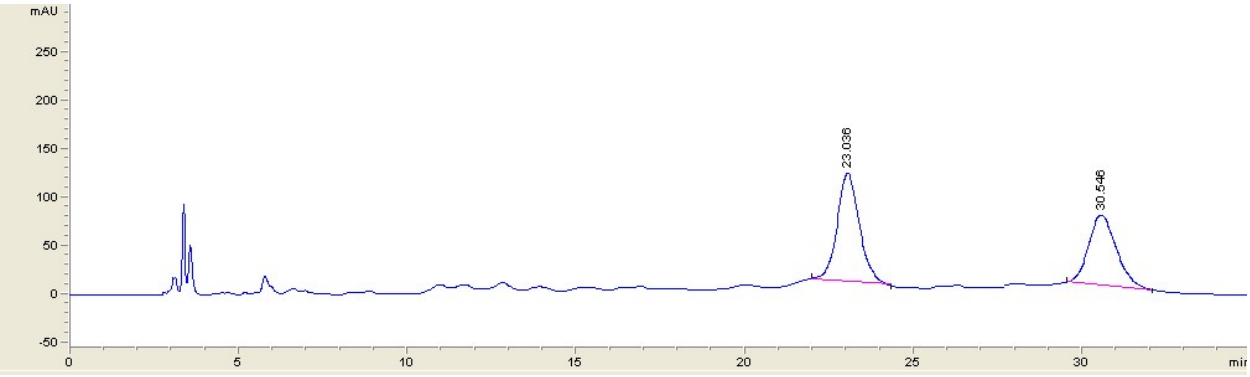
	RT	Area	% Area
1	23.077	25343.6000	90.9546
2	30.541	2520.40820	9.0454



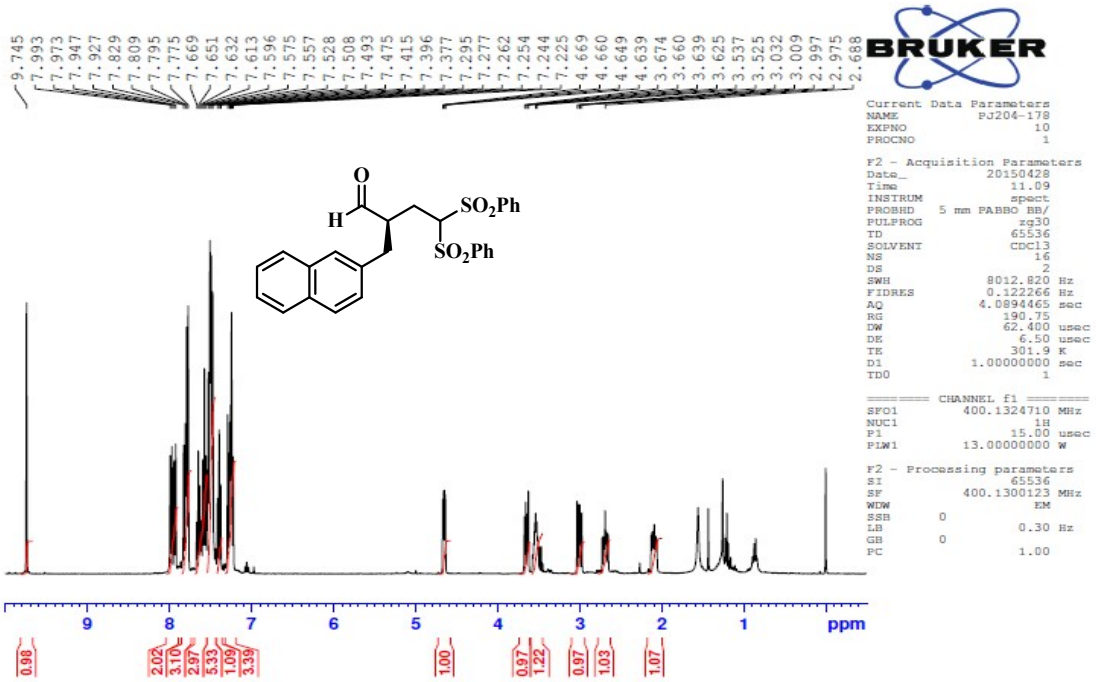
Racemic

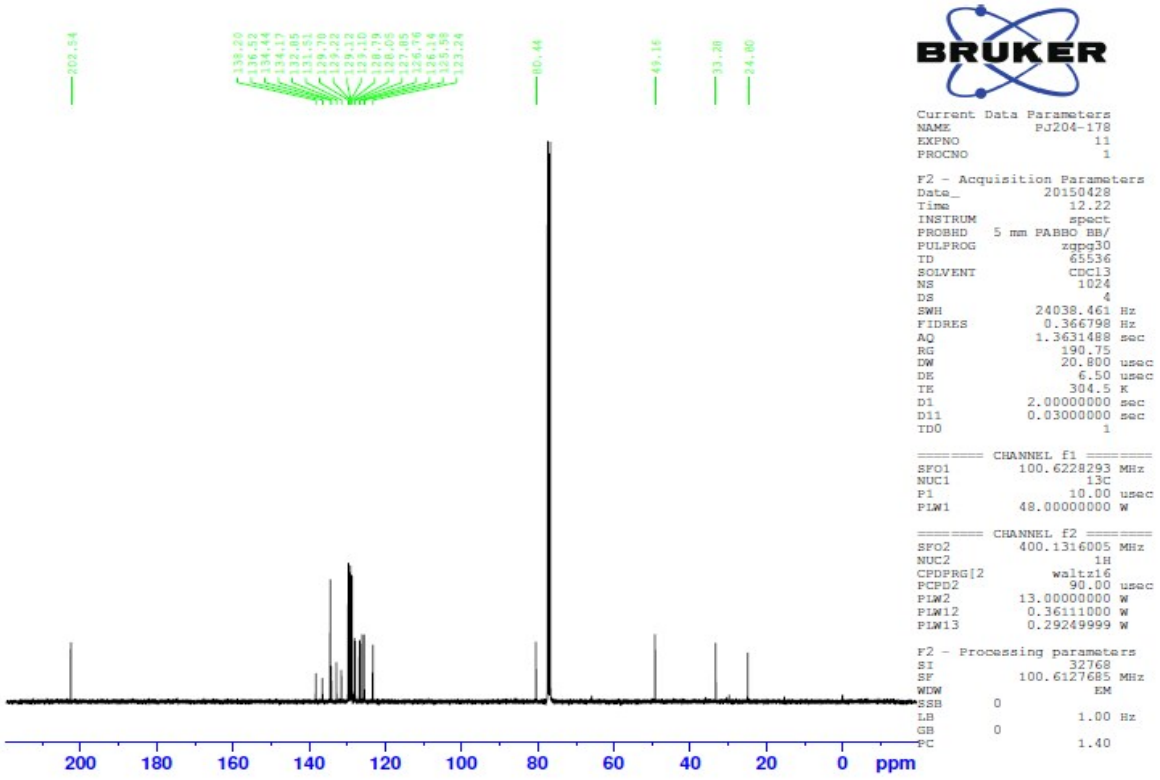
Peak table

	RT	Area	% Area
1	23.035	9890.13184	52.9970
2	30.546	8771.56543	47.0030



^{1}H and ^{13}C spectra of compound 8f



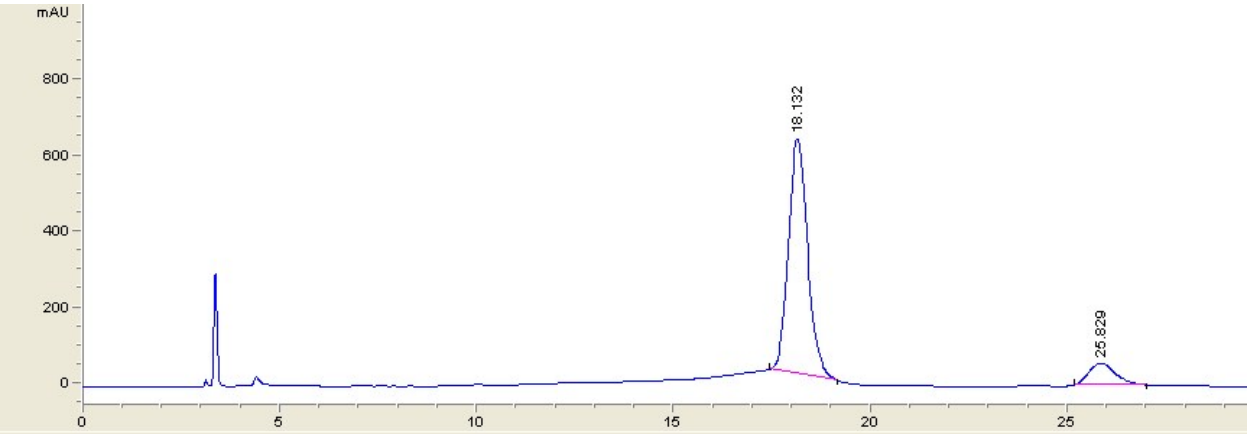


Chiral HPLC analysis of **8f**:

Enantiomerically enriched

Peak Table

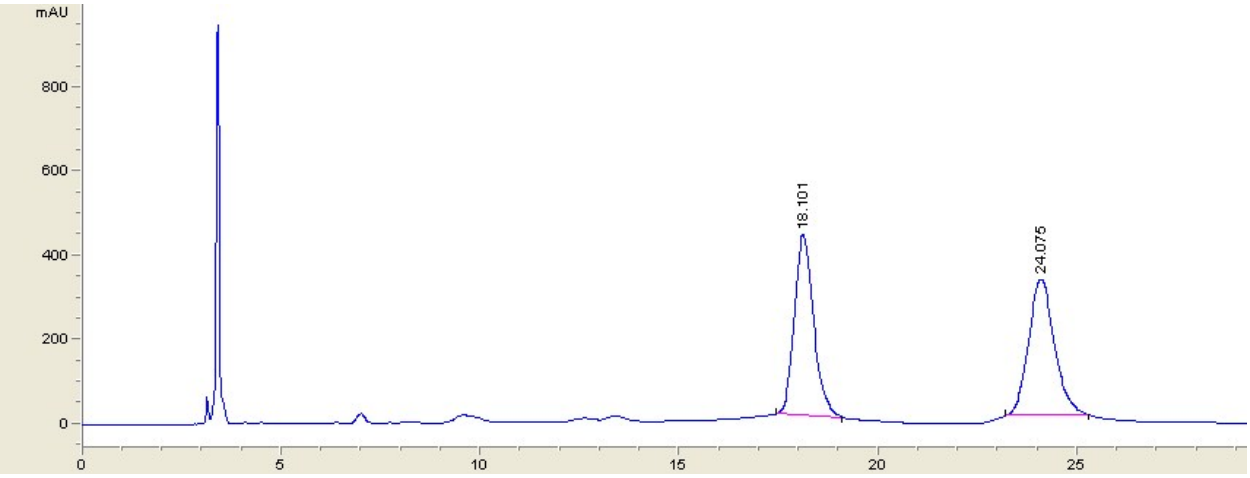
	RT	Area	% Area
1	18.132	21518.8000	89.1567
2	25.828	2617.13672	10.8433



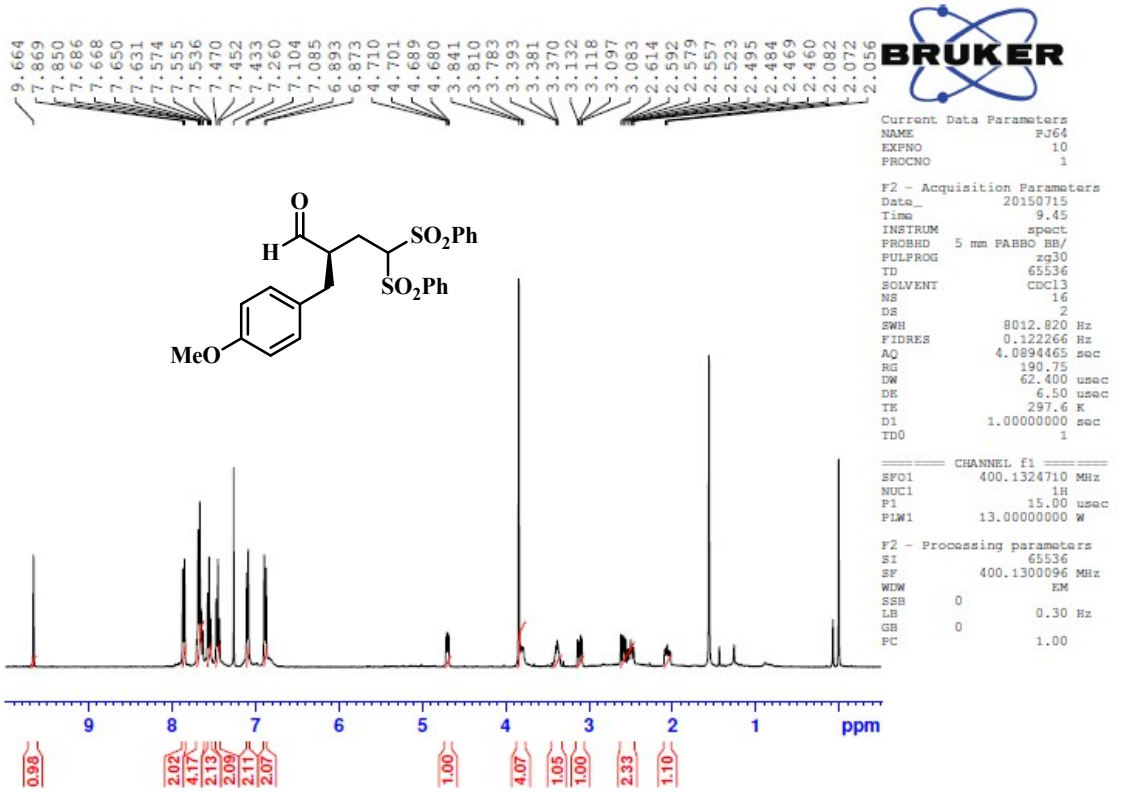
Racemic

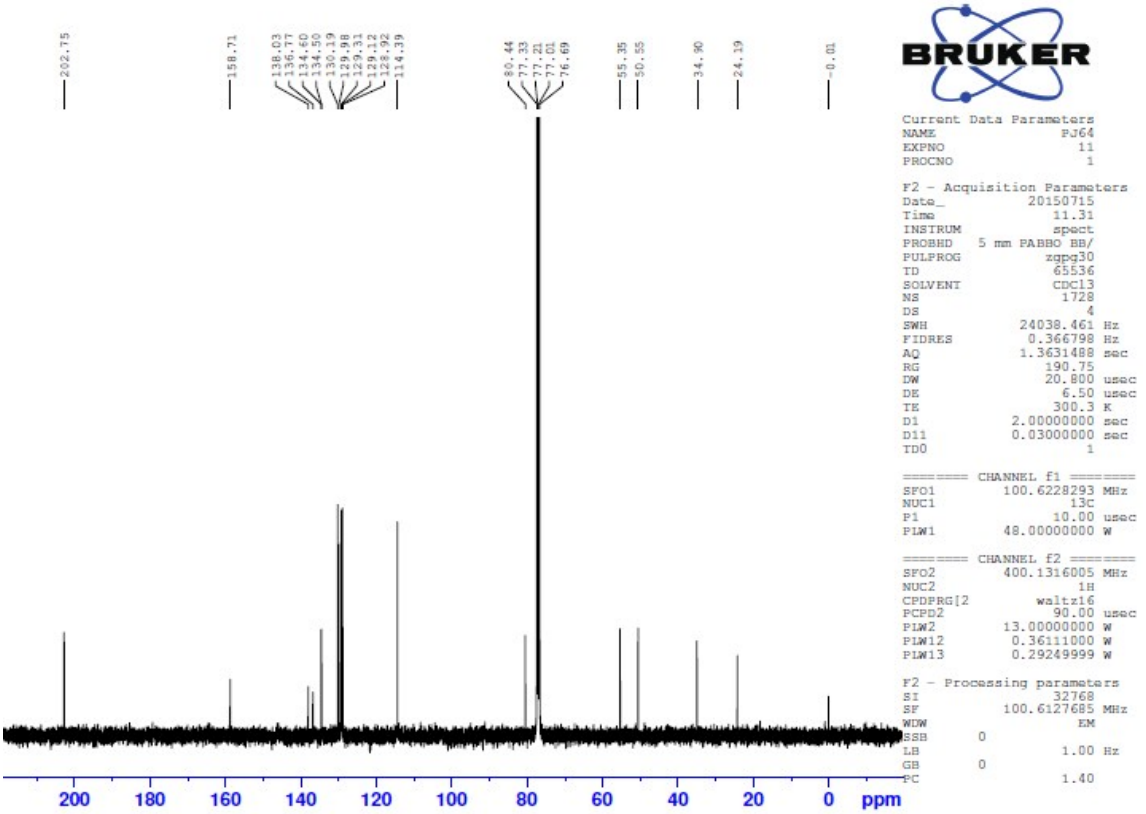
Peak table

	RT	Area	% Area
1	18.101	1.46087e4	49.4061
2	24.075	1.49599e4	50.5939



^{1}H and ^{13}C spectra of compound 8g



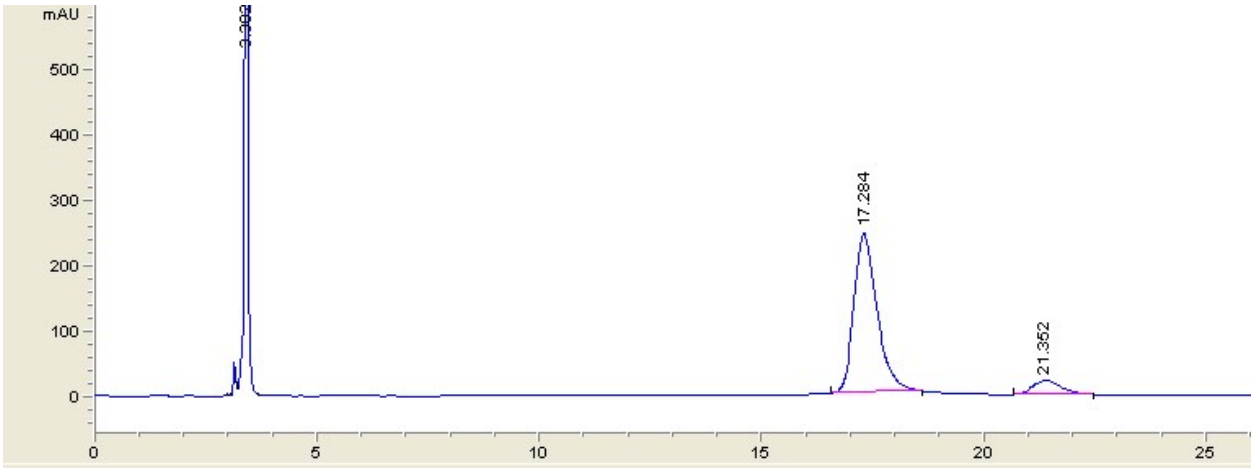


Chiral HPLC analysis of **8g**:

Enantiomerically enriched

Peak Table

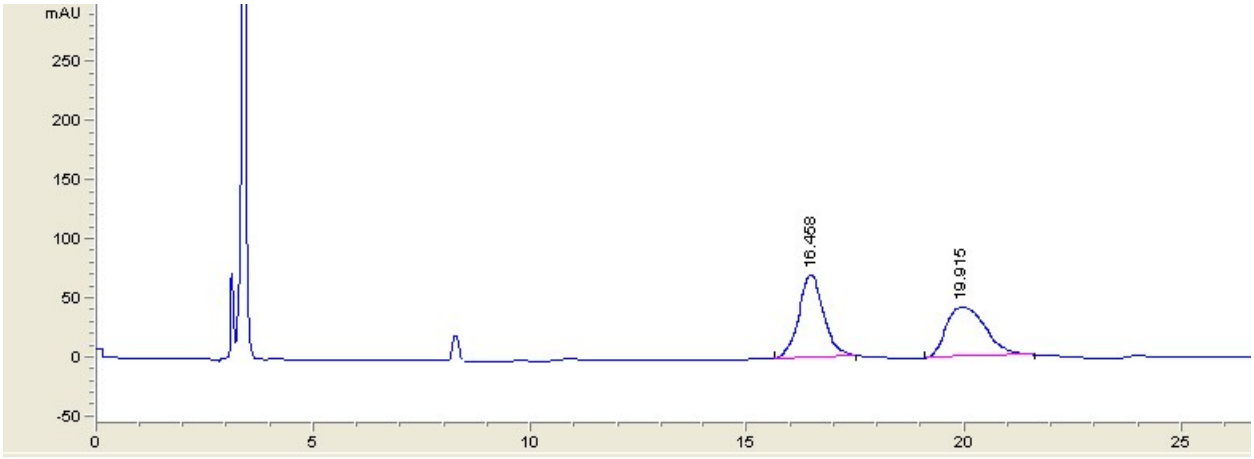
	RT	Area	% Area
1	17.284	8914.90527	91.8198
2	21.352	794.22742	8.1802



Racemic

Peak table

	RT	Area	% Area
1	16.458	2774.25854	52.9488
2	19.910	2465.24902	47.0512



Computational study of ligand 1

The structures **1a** - **1d** and the additional conformation **1b'**, in which the H-bond was formed, were prepared manually and then optimized using DFT with the B3LYP hybrid functional and Ahlrichs def2-SVP basis set[1] for all atoms with Weigend J auxiliary basis set[2] and Resolution of Identity approximation for Coulomb integrals (J) and COSX numerical integration for HF exchange (RIJCOSX)[3], in vacuum.[1,4-6] Vibrational frequencies were calculated for all structures, and no significant imaginary frequencies were found (structure **1d** had 1 imaginary frequency of -9 cm^{-1}). The calculations were repeated in dichloromethane using the COSMO solvation model.[7]Coordinates and energies of all compounds are available in the Supporting Information. ORCA software was used for all calculations. The exact setup for optimizations in vacuum was "! B3LYP/G def2-SVP def2-SVP/J RIJCOSX TightSCF Grid4 NoFinalGrid Opt NumFreq".

1. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.
2. F. Weigend, *Phys. Chem. Chem. Phys*., 2006,**8**, 1057-1065
3. F. Neese, F. Wennmohs, A. Hansen, and U. Becker. *Chem. Phys.*, 2009, **356**, 98–109.
4. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648–5652.
5. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785–789.
6. S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200–1211.
7. A. Klamt and G. Schüürmann *J. Chem. Soc., Perkin Trans.* 2, 1993, 799-805.

	Energies (Eh)	Energy differences (kcal/mol)	Rounded energy differences (kcal/mol)	Number of imaginary frequences
Vacuum:				
1a	-2593,14035777090	3,311996329	3,3	0
1b	-2593,14047976955	3,235442177	3,2	0
1b'	-2593,14563585266	0	0	0
1c	-2593,13714270088	5,329452767	5,3	0
1d	-2593,13316017444	7,828488108	7,8	1 (-9 cm^{-1})
COSMO (CH_2Cl_2)				
1a	-2593,15572898895	2,346448099	2,3	0
1b	-2593,15293251626	4,101234712	4,1	0
1b'	-2593,15946834847	0	0	0
1c	-2593,15032648282	5,736520695	5,7	0
1d	-2593,14546706797	8,785803514	8,8	1 (-13 cm^{-1})

@<TRIPOS>MOLECULE
Coordinates from ORCA-job 1b
70 73 1 0 0
SMALL
NO_CHARGES

@<TRIPOS>ATOM
1 C1 -4.0922 -3.8158 -2.0575 C.3 1 UNK 0.0000
2 Si1 -3.8278 -2.0236 -1.5198 Si 1 UNK 0.0000
3 C2 -5.0954 -1.6341 -0.1868 C.3 1 UNK 0.0000
4 C3 -4.0087 -0.8600 -2.9854 C.3 1 UNK 0.0000
5 O1 -2.2854 -1.9600 -0.8044 O.3 1 UNK 0.0000
6 C4 -1.0990 -1.1912 -0.8948 C.3 1 UNK 0.0000
7 C5 -0.2964 -1.5494 -2.1692 C.ar 1 UNK 0.0000
8 C6 0.9276 -0.9179 -2.4686 C.ar 1 UNK 0.0000
9 C7 1.6578 -1.2491 -3.6126 C.ar 1 UNK 0.0000
10 C8 1.1970 -2.2445 -4.4798 C.ar 1 UNK 0.0000
11 C9 0.0077 -2.9082 -4.1781 C.ar 1 UNK 0.0000
12 C10 -0.7230 -2.5650 -3.0348 C.ar 1 UNK 0.0000
13 C11 -1.4740 0.3103 -0.8080 C.ar 1 UNK 0.0000
14 C12 -1.1145 1.2771 -1.7634 C.ar 1 UNK 0.0000
15 C13 -1.4907 2.6188 -1.6141 C.ar 1 UNK 0.0000
16 C14 -2.2445 3.0229 -0.5110 C.ar 1 UNK 0.0000
17 C15 -2.6424 2.0680 0.4302 C.ar 1 UNK 0.0000
18 C16 -2.2693 0.7318 0.2777 C.ar 1 UNK 0.0000
19 C17 -0.1487 -1.6417 0.3196 C.3 1 UNK 0.0000
20 C18 -0.2173 -3.1603 0.5775 C.3 1 UNK 0.0000
21 C19 -1.2901 -3.3118 1.6639 C.3 1 UNK 0.0000
22 C20 -1.1418 -2.0445 2.5159 C.3 1 UNK 0.0000
23 N1 -0.4186 -1.0868 1.6593 N.pl3 1 UNK 0.0000
24 C21 0.2393 -0.0311 2.2363 C.2 1 UNK 0.0000
25 S1 0.1140 0.3048 3.8731 S.2 1 UNK 0.0000
26 N2 0.9779 0.7338 1.3451 N.pl3 1 UNK 0.0000
27 C22 1.9637 1.7094 1.5498 C.ar 1 UNK 0.0000
28 C23 2.7112 1.8633 2.7304 C.ar 1 UNK 0.0000
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30 C25 4.5359 2.9527 4.0611 C.3 1 UNK 0.0000
31 F1 5.2638 4.0843 4.0830 F 1 UNK 0.0000
32 F2 5.3992 1.9256 4.1751 F 1 UNK 0.0000
33 F3 3.7687 2.9462 5.1637 F 1 UNK 0.0000
34 C26 4.0163 3.6523 1.7050 C.ar 1 UNK 0.0000
35 C27 3.2808 3.4871 0.5280 C.ar 1 UNK 0.0000
36 C28 3.6598 4.2836 -0.6936 C.3 1 UNK 0.0000
37 F4 2.6439 4.3818 -1.5705 F 1 UNK 0.0000
38 F5 4.0494 5.5293 -0.3760 F 1 UNK 0.0000

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   40 C29       2.2578    2.5450    0.4536 C.ar     1 UNK    0.0000
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   42 H2       -5.1438   -3.9665   -2.3556 H        1 UNK    0.0000
   43 H3       -3.4676   -4.1132   -2.9141 H        1 UNK    0.0000
   44 H4       -4.9412   -2.2765    0.6952 H        1 UNK    0.0000
   45 H5       -5.0508   -0.5851    0.1451 H        1 UNK    0.0000
   46 H6       -6.1121   -1.8274   -0.5692 H        1 UNK    0.0000
   47 H7       -3.9269    0.1941   -2.6773 H        1 UNK    0.0000
   48 H8       -3.2499   -1.0522   -3.7597 H        1 UNK    0.0000
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   51 H11       2.5936   -0.7262   -3.8258 H        1 UNK    0.0000
   52 H12       1.7674   -2.5076   -5.3738 H        1 UNK    0.0000
   53 H13      -0.3600   -3.7023   -4.8331 H        1 UNK    0.0000
   54 H14      -1.6312   -3.1148   -2.8044 H        1 UNK    0.0000
   55 H15      -0.5462    0.9924   -2.6475 H        1 UNK    0.0000
   56 H16      -1.1890    3.3460   -2.3720 H        1 UNK    0.0000
   57 H17      -2.5325    4.0699   -0.3867 H        1 UNK    0.0000
   58 H18      -3.2447    2.3663    1.2917 H        1 UNK    0.0000
   59 H19      -2.5988    0.0020    1.0149 H        1 UNK    0.0000
   60 H20       0.8679   -1.3485    0.0322 H        1 UNK    0.0000
   61 H21      -0.4373   -3.7344   -0.3313 H        1 UNK    0.0000
   62 H22       0.7612   -3.4906    0.9630 H        1 UNK    0.0000
   63 H23      -2.2831   -3.3607    1.2012 H        1 UNK    0.0000
   64 H24      -1.1480   -4.2179    2.2712 H        1 UNK    0.0000
   65 H25      -2.1031   -1.6208    2.8509 H        1 UNK    0.0000
   66 H26      -0.5474   -2.2098    3.4273 H        1 UNK    0.0000
   67 H27       0.6341    0.7185    0.3903 H        1 UNK    0.0000
   68 H28       2.4901    1.2382    3.5927 H        1 UNK    0.0000
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SMALL
NO_CHARGES


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     3 C2         -4.9834   -0.8888    0.0553 C.3       1 UNK    0.0000
     4 C3         -3.9875   -1.3352   -2.8353 C.3       1 UNK    0.0000
     5 O1         -2.2446   -1.8174   -0.3961 O.3       1 UNK    0.0000
     6 C4         -1.0453   -1.1061   -0.7509 C.3       1 UNK    0.0000
     7 C5         -0.4033   -1.7473   -1.9932 C.ar      1 UNK    0.0000
     8 C6          0.5496   -1.0789   -2.7822 C.ar      1 UNK    0.0000
     9 C7          1.1603   -1.7109   -3.8700 C.ar      1 UNK    0.0000
    10 C8          0.8317   -3.0286   -4.1977 C.ar      1 UNK    0.0000
    11 C9         -0.1025   -3.7104   -3.4150 C.ar      1 UNK    0.0000
    12 C10        -0.7043   -3.0786   -2.3228 C.ar      1 UNK    0.0000
    13 C11        -1.4295    0.3847   -0.9087 C.ar      1 UNK    0.0000
    14 C12        -1.6131    0.9946   -2.1599 C.ar      1 UNK    0.0000
    15 C13        -2.0154    2.3308   -2.2661 C.ar      1 UNK    0.0000
    16 C14        -2.2486    3.0900   -1.1198 C.ar      1 UNK    0.0000
    17 C15        -2.0989    2.4927    0.1353 C.ar      1 UNK    0.0000
    18 C16        -1.7039    1.1583    0.2362 C.ar      1 UNK    0.0000
    19 C17        -0.0625   -1.2741    0.4992 C.3       1 UNK    0.0000
    20 C18         1.1508   -0.3139    0.5073 C.3       1 UNK    0.0000
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22	C20	2.0244	-2.5728	0.4351	C.3	1 UNK	0.0000
23	N1	0.5664	-2.6015	0.6671	N.pl3	1 UNK	0.0000
24	C21	0.0353	-3.6558	1.3746	C.2	1 UNK	0.0000
25	S1	1.0039	-4.9164	1.9176	S.2	1 UNK	0.0000
26	N2	-1.3183	-3.5508	1.5941	N.pl3	1 UNK	0.0000
27	C22	-2.1871	-4.2818	2.4154	C.ar	1 UNK	0.0000
28	C23	-1.9737	-5.5964	2.8641	C.ar	1 UNK	0.0000
29	C24	-2.9344	-6.2221	3.6634	C.ar	1 UNK	0.0000
30	C25	-2.6248	-7.5943	4.2172	C.3	1 UNK	0.0000
31	F1	-3.7428	-8.3068	4.4506	F	1 UNK	0.0000
32	F2	-1.9664	-7.4937	5.3879	F	1 UNK	0.0000
33	F3	-1.8500	-8.3180	3.3922	F	1 UNK	0.0000
34	C26	-4.1302	-5.5863	4.0093	C.ar	1 UNK	0.0000
35	C27	-4.3466	-4.2818	3.5504	C.ar	1 UNK	0.0000
36	C28	-5.5927	-3.5310	3.9524	C.3	1 UNK	0.0000
37	F4	-5.9366	-2.5920	3.0433	F	1 UNK	0.0000
38	F5	-6.6449	-4.3506	4.0925	F	1 UNK	0.0000
39	F6	-5.4273	-2.8880	5.1238	F	1 UNK	0.0000
40	C29	-3.3858	-3.6362	2.7753	C.ar	1 UNK	0.0000
41	H1	-4.1431	-4.1332	0.0634	H	1 UNK	0.0000
42	H2	-5.3461	-3.8665	-1.2214	H	1 UNK	0.0000
43	H3	-3.6829	-4.3260	-1.6461	H	1 UNK	0.0000
44	H4	-5.1254	-1.3574	1.0411	H	1 UNK	0.0000
45	H5	-4.6073	0.1354	0.2057	H	1 UNK	0.0000
46	H6	-5.9786	-0.8166	-0.4156	H	1 UNK	0.0000
47	H7	-3.9782	-0.2411	-2.9434	H	1 UNK	0.0000
48	H8	-3.1995	-1.7593	-3.4751	H	1 UNK	0.0000
49	H9	-4.9557	-1.7030	-3.2172	H	1 UNK	0.0000
50	H10	0.8251	-0.0485	-2.5544	H	1 UNK	0.0000
51	H11	1.8917	-1.1628	-4.4690	H	1 UNK	0.0000
52	H12	1.3045	-3.5212	-5.0508	H	1 UNK	0.0000
53	H13	-0.3726	-4.7423	-3.6547	H	1 UNK	0.0000
54	H14	-1.4154	-3.6324	-1.7116	H	1 UNK	0.0000
55	H15	-1.4480	0.4247	-3.0727	H	1 UNK	0.0000
56	H16	-2.1501	2.7765	-3.2551	H	1 UNK	0.0000
57	H17	-2.5613	4.1339	-1.2015	H	1 UNK	0.0000
58	H18	-2.2977	3.0668	1.0438	H	1 UNK	0.0000
59	H19	-1.6081	0.7210	1.2307	H	1 UNK	0.0000
60	H20	-0.6949	-1.0899	1.3795	H	1 UNK	0.0000
61	H21	0.9798	0.5906	-0.0893	H	1 UNK	0.0000
62	H22	1.3179	0.0206	1.5436	H	1 UNK	0.0000
63	H23	2.4665	-1.0592	-1.0688	H	1 UNK	0.0000
64	H24	3.2906	-0.7928	0.4732	H	1 UNK	0.0000
65	H25	2.3075	-3.3221	-0.3191	H	1 UNK	0.0000
66	H26	2.5325	-2.8666	1.3665	H	1 UNK	0.0000

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     69 H29       -4.8776   -6.0966    4.6172 H       1 UNK    0.0000
     70 H30       -3.5612   -2.6120    2.4424 H       1 UNK    0.0000
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@<TRIPOS>MOLECULE
Coordinates from ORCA-job 1d
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SMALL
NO_CHARGES


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4 C3	-3.7883	-2.0106	2.4409	C.3	1 UNK	0.0000
5 O1	-1.7012	-0.8385	0.9094	O.3	1 UNK	0.0000
6 C4	-1.0901	-0.3509	-0.2695	C.3	1 UNK	0.0000
7 C5	0.1810	-1.2042	-0.5412	C.ar	1 UNK	0.0000
8 C6	0.2874	-2.1095	-1.6098	C.ar	1 UNK	0.0000
9 C7	1.4222	-2.9145	-1.7705	C.ar	1 UNK	0.0000
10 C8	2.4749	-2.8458	-0.8566	C.ar	1 UNK	0.0000
11 C9	2.3732	-1.9739	0.2329	C.ar	1 UNK	0.0000
12 C10	1.2403	-1.1720	0.3870	C.ar	1 UNK	0.0000
13 C11	-2.0934	-0.3760	-1.4382	C.ar	1 UNK	0.0000
14 C12	-3.4431	-0.6844	-1.2126	C.ar	1 UNK	0.0000
15 C13	-4.3728	-0.6801	-2.2578	C.ar	1 UNK	0.0000
16 C14	-3.9719	-0.3608	-3.5564	C.ar	1 UNK	0.0000
17 C15	-2.6318	-0.0448	-3.7972	C.ar	1 UNK	0.0000
18 C16	-1.7060	-0.0537	-2.7517	C.ar	1 UNK	0.0000
19 C17	-0.6873	1.1649	0.1138	C.3	1 UNK	0.0000
20 C18	-1.7219	1.8946	0.9895	C.3	1 UNK	0.0000
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23 N1	-0.5373	2.1133	-1.0122	N.pl3	1 UNK	0.0000
24 C21	0.5099	2.2757	-1.8573	C.2	1 UNK	0.0000
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26 N2	1.7559	1.7618	-1.4731	N.pl3	1 UNK	0.0000
27 C22	2.4956	2.0409	-0.3249	C.ar	1 UNK	0.0000
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29 C24	2.8137	2.9263	1.9159	C.ar	1 UNK	0.0000
30 C25	2.1664	3.6087	3.1010	C.3	1 UNK	0.0000
31 F1	1.7982	4.8692	2.8098	F	1 UNK	0.0000
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34 C26	4.1314	2.4678	1.9530	C.ar	1 UNK	0.0000
35 C27	4.6348	1.8126	0.8163	C.ar	1 UNK	0.0000
36 C28	6.0743	1.3552	0.7489	C.3	1 UNK	0.0000
37 F4	6.8974	2.3572	0.3920	F	1 UNK	0.0000
38 F5	6.2336	0.3763	-0.1620	F	1 UNK	0.0000
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46 H6	-0.8538	-1.4579	3.8020	H	1 UNK	0.0000
47 H7	-4.0242	-2.7953	3.1790	H	1 UNK	0.0000
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     61 H21       -2.2463    1.2083    1.6614 H        1 UNK    0.0000
     62 H22       -1.1789    2.6204    1.6174 H        1 UNK    0.0000
     63 H23       -3.4823    1.9661   -0.2910 H        1 UNK    0.0000
     64 H24       -3.0816    3.5312    0.4336 H        1 UNK    0.0000
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     66 H26       -1.4554    3.9823   -1.2763 H        1 UNK    0.0000
     67 H27        2.3345    1.6205   -2.2958 H        1 UNK    0.0000
     68 H28        1.0082    3.1758    0.7700 H        1 UNK    0.0000
     69 H29        4.7491    2.6158    2.8390 H        1 UNK    0.0000
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@<TRIPOS>SUBSTRUCTURE
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@<TRIPOS>MOLECULE
Coordinates from ORCA-job 1a
70 73 1 0 0
SMALL
NO_CHARGES


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     3 C2        -0.6792   -4.2589   -4.2841 C.3      1 UNK    0.0000
     4 C3         0.8203   -4.4140   -1.6348 C.3      1 UNK    0.0000
     5 O1        -0.6508   -2.0447   -2.5103 O.3      1 UNK    0.0000
     6 C4        -1.2145   -0.9295   -1.8314 C.3      1 UNK    0.0000
     7 C5        -1.1828   -1.2149   -0.3105 C.ar     1 UNK    0.0000
     8 C6        -2.3208   -1.1996    0.5106 C.ar     1 UNK    0.0000
     9 C7        -2.2382   -1.5166    1.8709 C.ar     1 UNK    0.0000
    10 C8        -1.0140   -1.8601    2.4441 C.ar     1 UNK    0.0000
    11 C9         0.1262   -1.9073    1.6368 C.ar     1 UNK    0.0000
    12 C10        0.0380   -1.5959    0.2788 C.ar     1 UNK    0.0000
    13 C11       -2.6333   -0.6154   -2.3581 C.ar     1 UNK    0.0000
    14 C12       -3.3280    0.5126   -1.8764 C.ar     1 UNK    0.0000
    15 C13       -4.5874    0.8511   -2.3733 C.ar     1 UNK    0.0000
    16 C14       -5.1838    0.0762   -3.3736 C.ar     1 UNK    0.0000
    17 C15       -4.5035   -1.0372   -3.8678 C.ar     1 UNK    0.0000
    18 C16       -3.2392   -1.3744   -3.3671 C.ar     1 UNK    0.0000
    19 C17       -0.3608    0.3583   -2.2440 C.3      1 UNK    0.0000
    20 C18        0.1131    0.3182   -3.7070 C.3      1 UNK    0.0000
    21 C19        1.5397   -0.2523   -3.6441 C.3      1 UNK    0.0000
    22 C20        2.0736    0.1724   -2.2607 C.3      1 UNK    0.0000
    23 N1         0.8844    0.6067   -1.5067 N.pl3    1 UNK    0.0000
    24 C21        0.9402    1.4783   -0.4523 C.2      1 UNK    0.0000
    25 S1        -0.3610    2.3888    0.0833 S.2      1 UNK    0.0000
    26 N2         2.1935    1.5339    0.1432 N.pl3    1 UNK    0.0000
    27 C22        2.5826    2.2649    1.2858 C.ar     1 UNK    0.0000
    28 C23        2.2377    3.6134    1.4838 C.ar     1 UNK    0.0000
    29 C24        2.6701    4.2780    2.6346 C.ar     1 UNK    0.0000
    30 C25        2.2242    5.7038    2.8817 C.3      1 UNK    0.0000
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   34 C26       3.4657    3.6331    3.5894 C.ar    1 UNK    0.0000
   35 C27       3.8202    2.2987    3.3830 C.ar    1 UNK    0.0000
   36 C28       4.6076    1.5413    4.4279 C.3     1 UNK    0.0000
   37 F4        3.7936    0.8387    5.2412 F       1 UNK    0.0000
   38 F5        5.3383    2.3563    5.2064 F       1 UNK    0.0000
   39 F6        5.4508    0.6534    3.8678 F       1 UNK    0.0000
   40 C29       3.3828    1.6208    2.2404 C.ar    1 UNK    0.0000
   41 H1       -2.3580   -4.1139   -0.5854 H       1 UNK    0.0000
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   45 H5       -1.6076   -4.0098   -4.8231 H       1 UNK    0.0000
   46 H6        0.1522   -3.7609   -4.8081 H       1 UNK    0.0000
   47 H7        0.8061   -4.2761   -0.5431 H       1 UNK    0.0000
   48 H8        0.9224   -5.4934   -1.8396 H       1 UNK    0.0000
   49 H9        1.7176   -3.9124   -2.0342 H       1 UNK    0.0000
   50 H10      -3.2935   -0.9452    0.0930 H       1 UNK    0.0000
   51 H11      -3.1442   -1.4965    2.4819 H       1 UNK    0.0000
   52 H12      -0.9478   -2.1074    3.5066 H       1 UNK    0.0000
   53 H13       1.0871   -2.2029    2.0674 H       1 UNK    0.0000
   54 H14       0.9311   -1.6711   -0.3397 H       1 UNK    0.0000
   55 H15      -2.8773    1.1395   -1.1026 H       1 UNK    0.0000
   56 H16      -5.1029    1.7292   -1.9758 H       1 UNK    0.0000
   57 H17      -6.1650    0.3486   -3.7714 H       1 UNK    0.0000
   58 H18      -4.9518   -1.6505   -4.6538 H       1 UNK    0.0000
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   60 H20      -1.0018    1.2235   -2.0567 H       1 UNK    0.0000
   61 H21      -0.5500   -0.2771   -4.3461 H       1 UNK    0.0000
   62 H22       0.1254    1.3469   -4.1014 H       1 UNK    0.0000
   63 H23       1.5114   -1.3467   -3.7221 H       1 UNK    0.0000
   64 H24       2.1830    0.1295   -4.4506 H       1 UNK    0.0000
   65 H25       2.5982   -0.6635   -1.7601 H       1 UNK    0.0000
   66 H26       2.7855    1.0114   -2.3305 H       1 UNK    0.0000
   67 H27       2.7950    0.7399   -0.0492 H       1 UNK    0.0000
   68 H28       1.6366    4.1328    0.7413 H       1 UNK    0.0000
   69 H29       3.8143    4.1674    4.4731 H       1 UNK    0.0000
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@<TRIPOS>SUBSTRUCTURE
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Coordinates from ORCA-job 1c
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SMALL
NO_CHARGES


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     3 C2       -10.3961    2.5620   -5.2613 C.3       1 UNK    0.0000
     4 C3        -8.5746    2.7334   -2.8162 C.3       1 UNK    0.0000
     5 O1        -7.7209    3.5747   -5.4747 O.3       1 UNK    0.0000
     6 C4        -6.8446    4.4999   -6.0992 C.3       1 UNK    0.0000
     7 C5        -6.3737    5.5401   -5.0553 C.ar      1 UNK    0.0000
     8 C6        -6.2849    6.9204   -5.2856 C.ar      1 UNK    0.0000
     9 C7        -5.8307    7.7909   -4.2894 C.ar      1 UNK    0.0000
    10 C8        -5.4582    7.3048   -3.0354 C.ar      1 UNK    0.0000
    11 C9        -5.5684    5.9354   -2.7777 C.ar      1 UNK    0.0000
    12 C10       -6.0283    5.0745   -3.7750 C.ar      1 UNK    0.0000
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13	C11	-7.5039	5.1386	-7.3480	C.ar	1 UNK	0.0000
14	C12	-6.7709	5.9812	-8.2083	C.ar	1 UNK	0.0000
15	C13	-7.3553	6.5348	-9.3506	C.ar	1 UNK	0.0000
16	C14	-8.6812	6.2412	-9.6821	C.ar	1 UNK	0.0000
17	C15	-9.4076	5.3780	-8.8613	C.ar	1 UNK	0.0000
18	C16	-8.8224	4.8353	-7.7114	C.ar	1 UNK	0.0000
19	C17	-5.6278	3.6727	-6.6878	C.3	1 UNK	0.0000
20	C18	-6.0716	2.4249	-7.4710	C.3	1 UNK	0.0000
21	C19	-5.9771	1.2788	-6.4614	C.3	1 UNK	0.0000
22	C20	-4.7846	1.6595	-5.5751	C.3	1 UNK	0.0000
23	N1	-4.6361	3.1287	-5.7287	N.pl3	1 UNK	0.0000
24	C21	-3.4188	3.7360	-5.5959	C.2	1 UNK	0.0000
25	S1	-2.9194	5.1175	-6.4083	S.2	1 UNK	0.0000
26	N2	-2.4603	3.1091	-4.7948	N.pl3	1 UNK	0.0000
27	C22	-2.5237	2.4882	-3.5425	C.ar	1 UNK	0.0000
28	C23	-3.6772	2.4582	-2.7416	C.ar	1 UNK	0.0000
29	C24	-3.6586	1.8151	-1.5028	C.ar	1 UNK	0.0000
30	C25	-4.9420	1.7200	-0.7124	C.3	1 UNK	0.0000
31	F1	-5.6317	2.8804	-0.7211	F	1 UNK	0.0000
32	F2	-4.7170	1.3900	0.5664	F	1 UNK	0.0000
33	F3	-5.7646	0.7837	-1.2281	F	1 UNK	0.0000
34	C26	-2.4933	1.2237	-1.0112	C.ar	1 UNK	0.0000
35	C27	-1.3340	1.2842	-1.7896	C.ar	1 UNK	0.0000
36	C28	-0.0545	0.6413	-1.3027	C.3	1 UNK	0.0000
37	F4	0.2744	-0.4196	-2.0623	F	1 UNK	0.0000
38	F5	-0.1562	0.2109	-0.0360	F	1 UNK	0.0000
39	F6	0.9839	1.4935	-1.3570	F	1 UNK	0.0000
40	C29	-1.3452	1.9014	-3.0403	C.ar	1 UNK	0.0000
41	H1	-8.9305	5.9512	-3.5533	H	1 UNK	0.0000
42	H2	-9.9888	5.8712	-4.9848	H	1 UNK	0.0000
43	H3	-10.5761	5.2861	-3.4093	H	1 UNK	0.0000
44	H4	-11.1389	2.2232	-4.5201	H	1 UNK	0.0000
45	H5	-10.9430	3.1181	-6.0392	H	1 UNK	0.0000
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47	H7	-7.9870	3.3799	-2.1474	H	1 UNK	0.0000
48	H8	-9.4800	2.4229	-2.2678	H	1 UNK	0.0000
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54	H14	-6.1482	4.0160	-3.5516	H	1 UNK	0.0000
55	H15	-5.7269	6.2160	-7.9903	H	1 UNK	0.0000
56	H16	-6.7626	7.1917	-9.9926	H	1 UNK	0.0000
57	H17	-9.1380	6.6728	-10.5764	H	1 UNK	0.0000
58	H18	-10.4344	5.1060	-9.1214	H	1 UNK	0.0000

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     63 H23       -6.8927   1.2313  -5.8582 H       1 UNK    0.0000
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     65 H25       -4.9477   1.3676  -4.5281 H       1 UNK    0.0000
     66 H26       -3.8508   1.1755  -5.9047 H       1 UNK    0.0000
     67 H27       -1.5442   3.4873  -5.0208 H       1 UNK    0.0000
     68 H28       -4.5784   2.9589  -3.0811 H       1 UNK    0.0000
     69 H29       -2.4839   0.7330  -0.0400 H       1 UNK    0.0000
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@<TRIPOS>SUBSTRUCTURE
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