Supporting Information

Synthesis of Novel Polyhydroxylated Pyrrolidine-Triazole/-Isoxazole Hybrid Molecules

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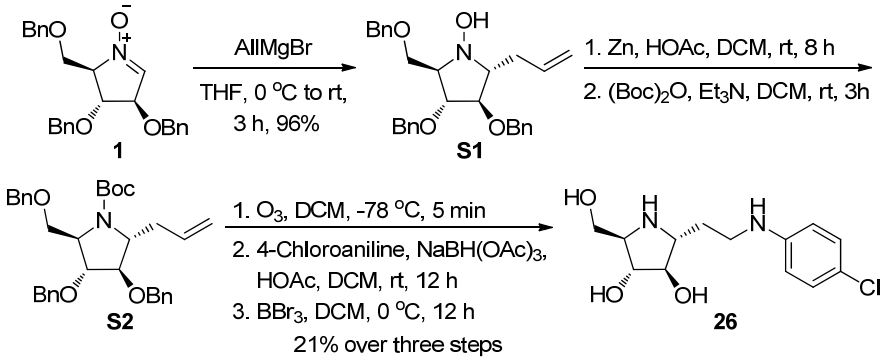
Section A. Experimental

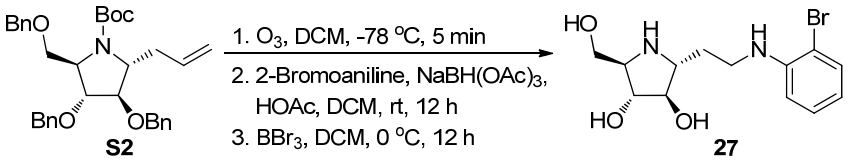


Compound S1. AllylMgBr (1.7M in THF, 4.6 mL, 3 equiv) was slowly added to a solution of compound 1 (1.1 g, 2.63 mmol) in dry THF (10 mL) at 0 °C under argon atmosphere. The reaction was allowed to warm up to room temperature and stirred for 3 h. The reaction was quenched by sat. $NH_4Cl_{(aq)}$ and extracted with CH_2Cl_2. The combined organic layers were dried over anh. $MgSO_4$, concentrated and purified by column chromatography to give compound **S1** as colorless oil (1.16 g, 96 %); TLC (Hexanes/EtOAc = 3/1, v/v) R_f = 0.3.

Compound S2. A suspension of compound **S1** (1.16 g, 2.52 mmol), zinc dust (1.65 g, 10 equiv) and HOAc (2.5 mL) in CH_2Cl_2 (3.9 mL) was stirred at room temperature for 8 h. The excess of zinc dust was filtrated through a pad of Celite. The filtrate was neutralized with $NaHCO_{3(aq)}$ and extracted with CH_2Cl_2. The combined organic layers were dried over anh. $MgSO_4$ and concentrated to give the pyrrolidine. TLC (Hexanes/EtOAc = 1/1, v/v) R_f = 0.6. The pyrrolidine in dry CH_2Cl_2 (10 mL) was treated with $(Boc)_2O$ (720 µL, 1.25 equiv) and triethylamine (770 µL, 2 equiv). The reaction was stirred at room temperature for 3 h. The reaction was concentrated and purified by column chromatography to give compound **S2** (1.02 g, 75 %) as colorless oil. TLC (Hexanes/EtOAc = 5/1, v/v) R_f = 0.4.

Compound 26. Compound **S2** (100 mg, 0.18 mmol) in CH_2Cl_2 (3 mL) at –78 °C was formed to aldehyde by ozonolysis. To a solution of the crude aldehyde and 4-chloroaniline (23 mg, 1 equiv) in CH_2Cl_2 (3 mL) was added acetic acid (32 µl, 0.56 mmol) and $NaBH(OAc)_3$ (117 mg, 3 equiv). The reaction mixture was stirred at room temperature for 12 h, and the reaction was quenched by sat. $NaHCO_{3(aq)}$ and extracted with CH_2Cl_2. The combined organic layers were dried over anh. $MgSO_4$, concentrated and purified by column chromatography to give the protected pyrrolidine as colorless oil (57 mg, 47 %); TLC (Hexane/EtOAc = 5/1, v/v) R_f = 0.5. To a solution of the protected pyrrolidine (57 mg, 0.085 mmol) in dry CH_2Cl_2 (5 mL) at 0 °C was added BBr_3 (1M in dichloromethane, 852 µl, 10 equiv). The reaction was warm up to room temperature and kept

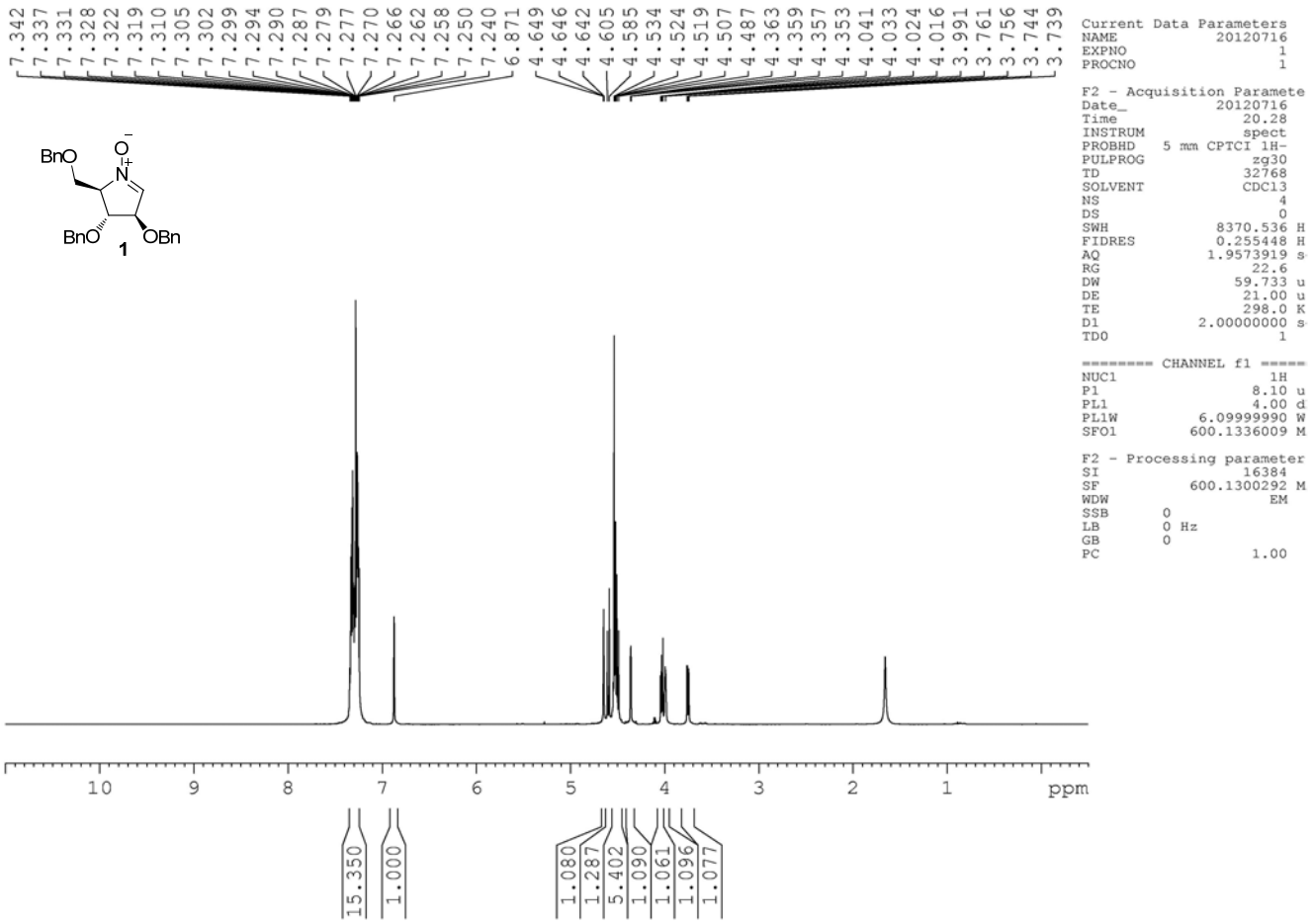
stirring for 12 h. After the reaction was complete, the reaction mixture was quenched with MeOH, concentrated and purified by column chromatography to give compound **26** as white solid (11 mg, 44 %); TLC (MeOH/CH_2Cl_2 = 1/4, v/v) R_f = 0.1. $[\alpha]_D^{20}$ +28.86 (*c* 0.2 in MOH); ^{1}H NMR (600 MHz, D_2O) δ 7.25 (d, *J* = 8.8 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 3.88 (t, *J* = 7.0 Hz, 1H), 3.78 (t, *J* = 7.4 Hz, 1H), 3.74 (dd, *J* = 11.8, 4.3 Hz, 1H), 3.68 (dd, *J* = 11.8, 6.2 Hz, 1H), 3.25–3.09 (m, 4H), 2.03–1.98 (m, 1H), 1.83–1.78 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 146.7, 129.0, 123.0, 115.9, 80.7, 76.9, 61.7, 61.2, 58.4, 41.3, 31.8; HRMS (ESI-TOF) calcd for $C_{13}H_{19}ClN_2O_3$+H^+ [M+H^+] 287.1157, found: 287.1160.



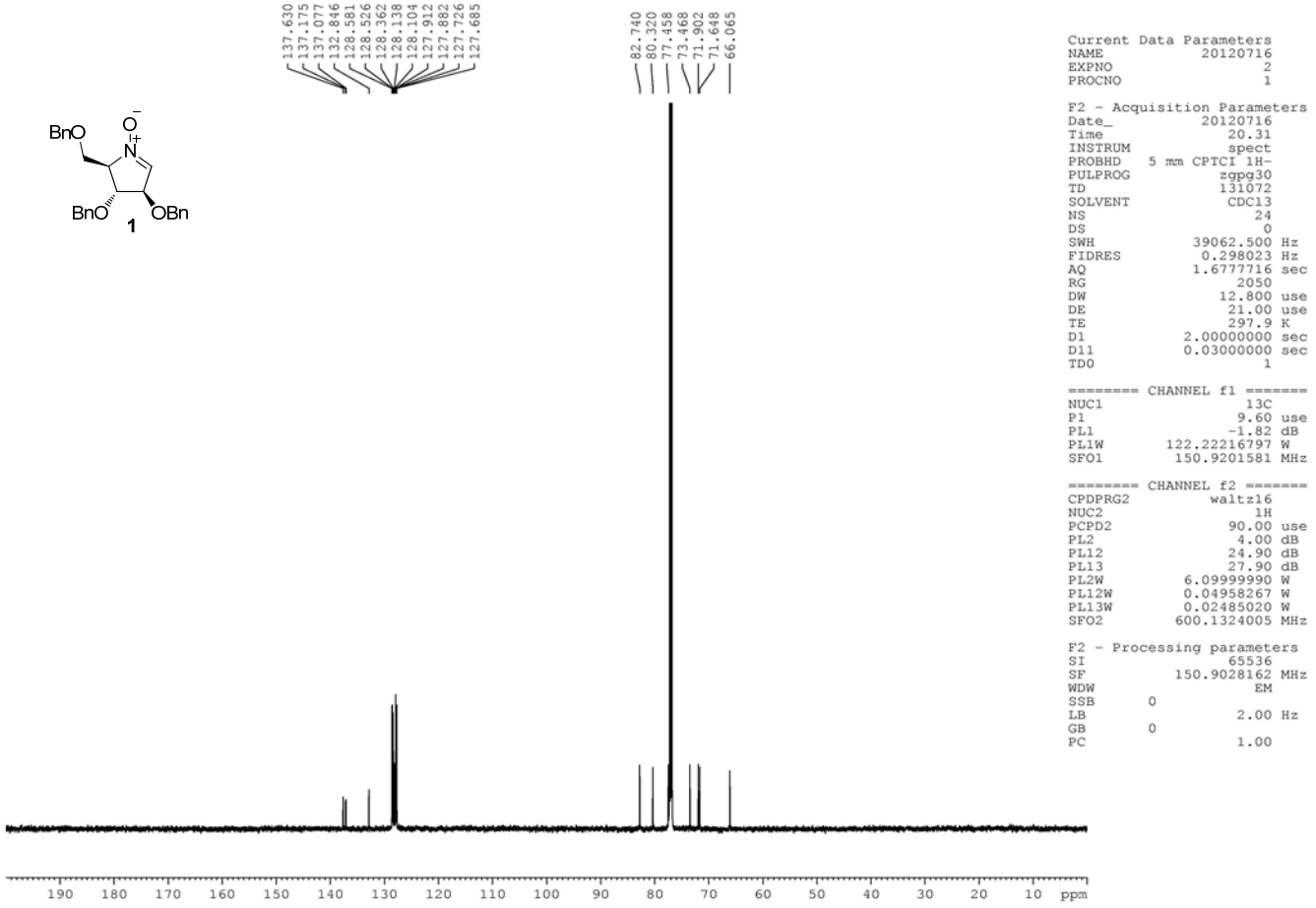
Compound 27. The title compound **27** was synthesized by the procedure as described for the preparation of compound **26** except for using 2-bromoaniline in the step of reductive amination as write solid. $[\alpha]_D^{20}$ +27.16 (*c* 0.16 in MOH); ^{1}H NMR (600 MHz, D_2O) δ 7.54 (d, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 7.5 Hz, 1H), 6.74 (d, *J* = 7.5 Hz, 1H), 3.83 (t, *J* = 7.0 Hz, 1H), 3.73 (t, *J* = 7.4 Hz, 1H), 3.69 (dd, *J* = 11.5, 4.3 Hz, 1H), 3.64 (dd, *J* = 11.5, 6.4 Hz, 1H), 3.35–3.24 (m, 2H), 3.05–2.98 (m, 2H), 2.01–1.99 (m, 1H), 1.78–1.75 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.7, 132.7, 119.5, 113.4, 110.4, 81.4, 77.7, 62.0, 61.5, 58.1, 41.1, 32.2; HRMS (ESI-TOF) calcd for $C_{13}H_{19}BrN_2O_3$+H^+ [M+H^+] 331.0652, found: 331.0652.

Section B

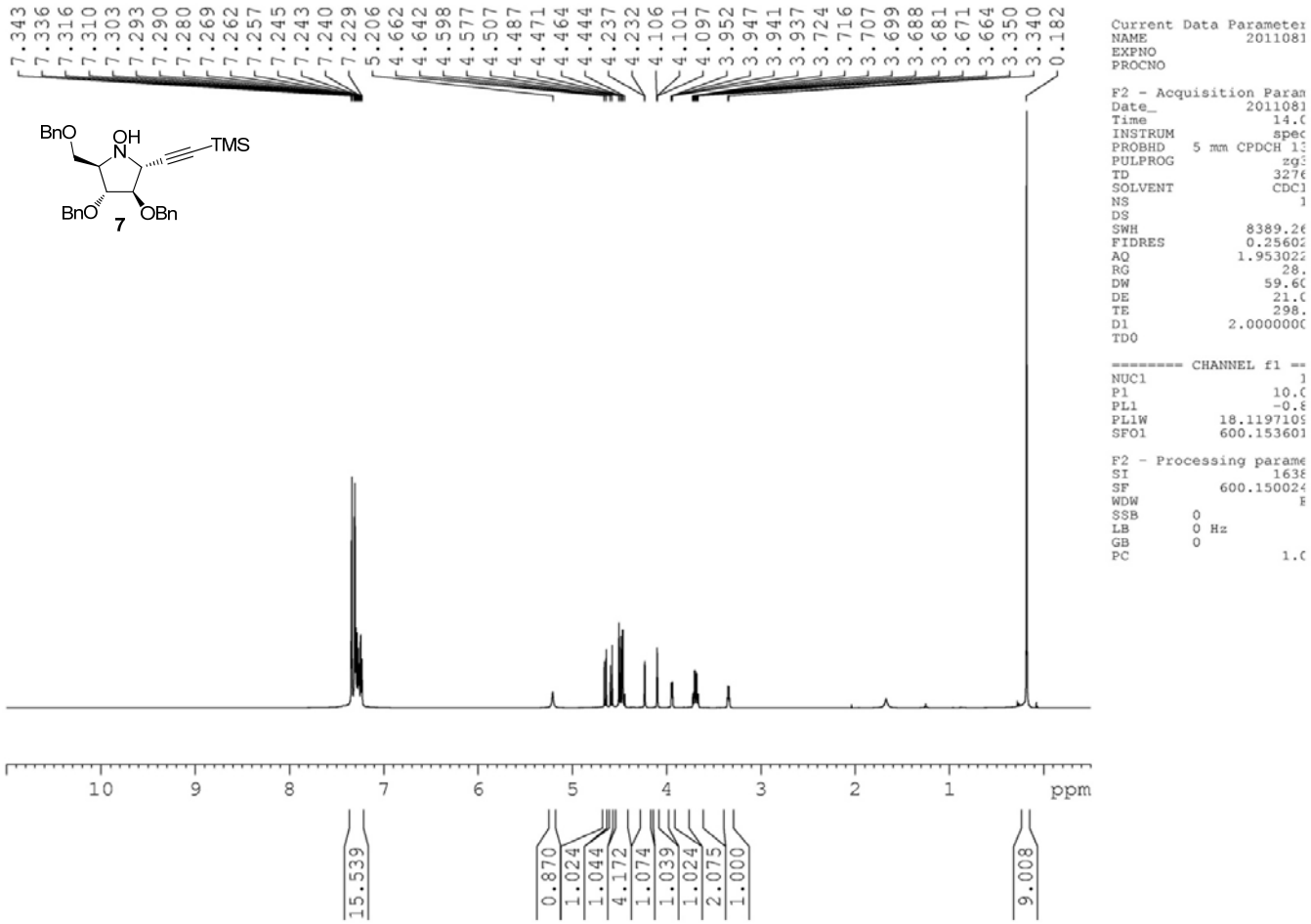
^{1}H NMR spectrum of compound **1** (600 MHz, $CDCl_3$).



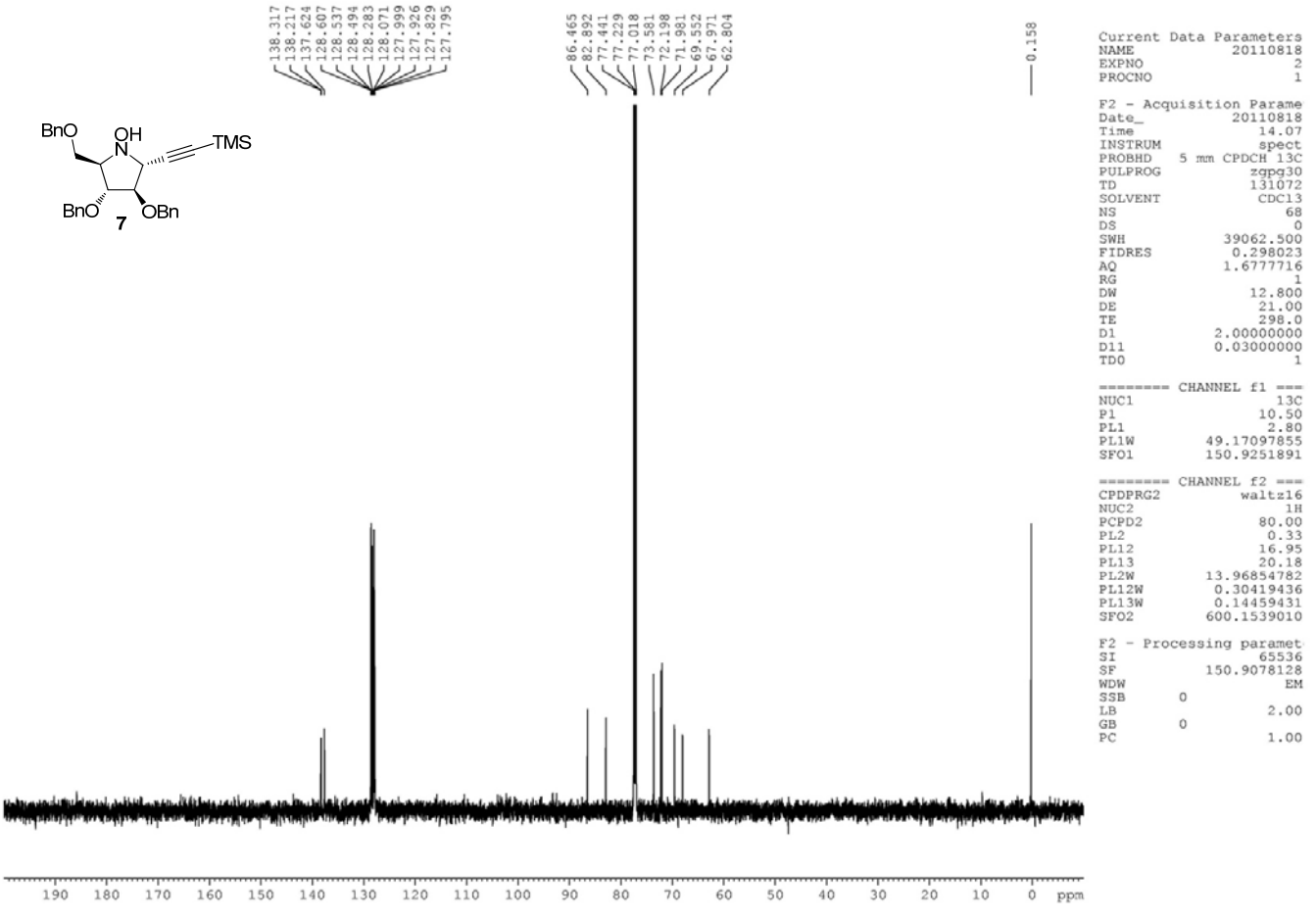
^{13}C NMR spectrum of compound **1** (150 MHz, $CDCl_3$).



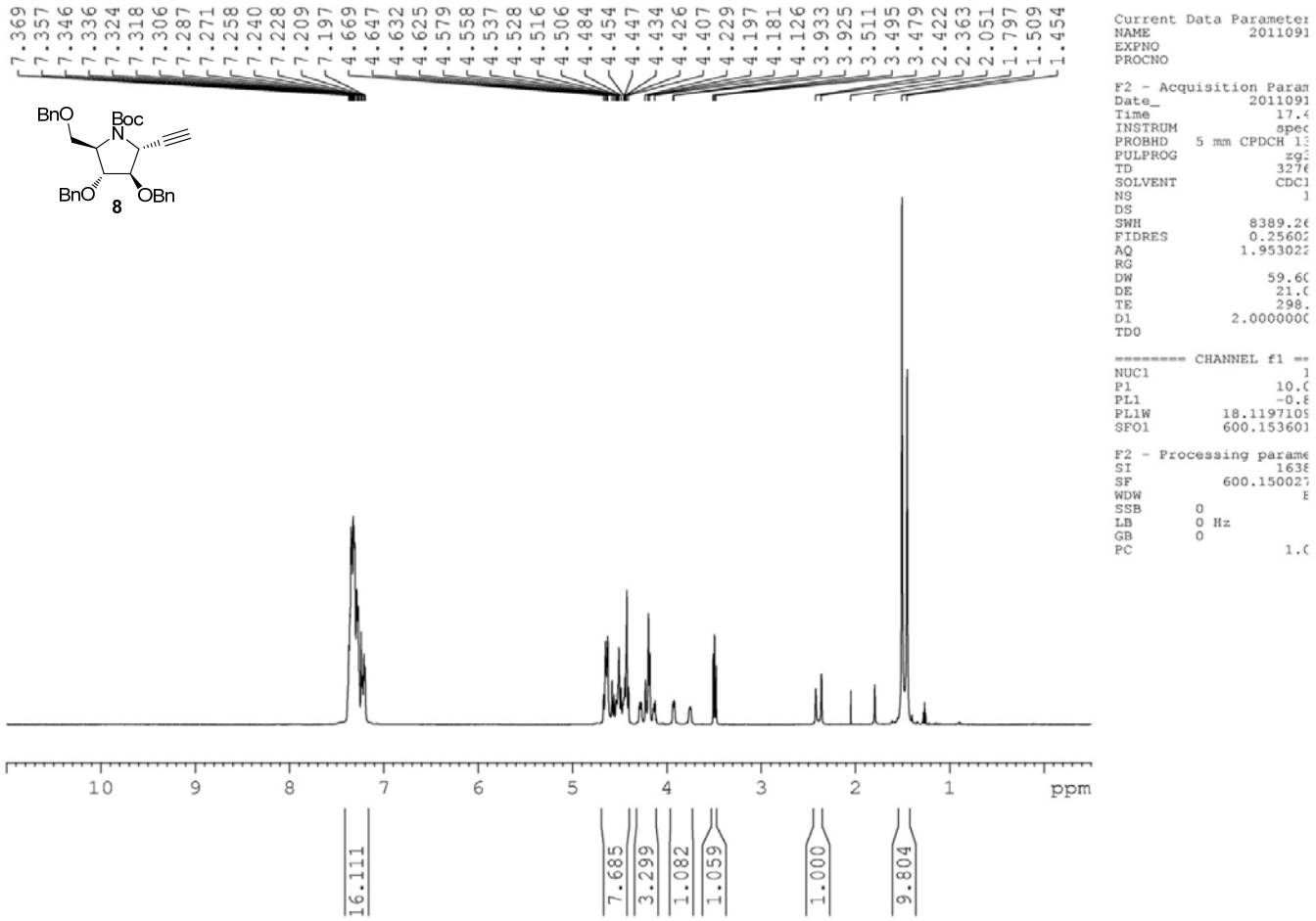
^{1}H NMR spectrum of compound **7** (600 MHz, $CDCl_3$).



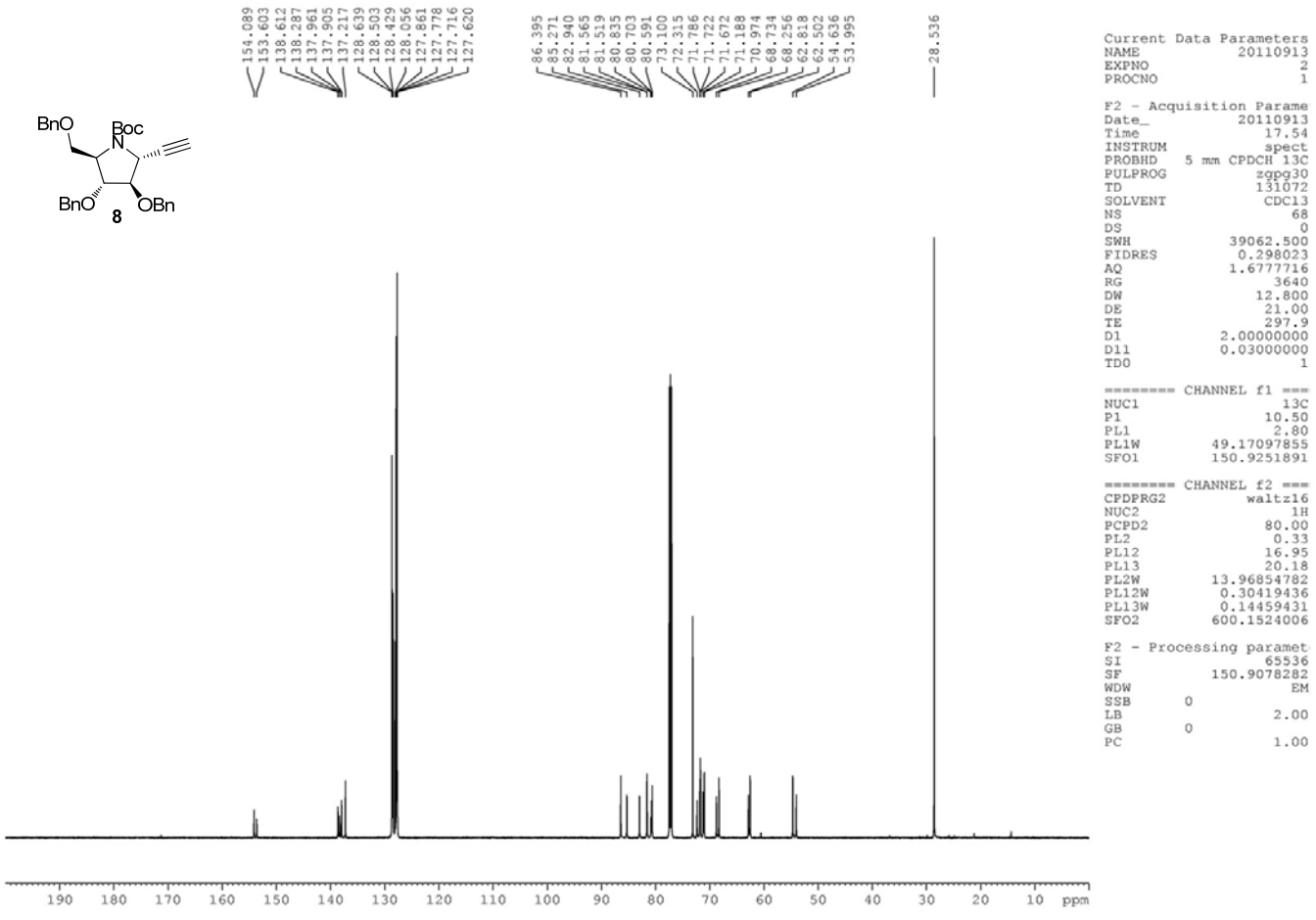
^{13}C NMR spectrum of compound **7** (150 MHz, $CDCl_3$).



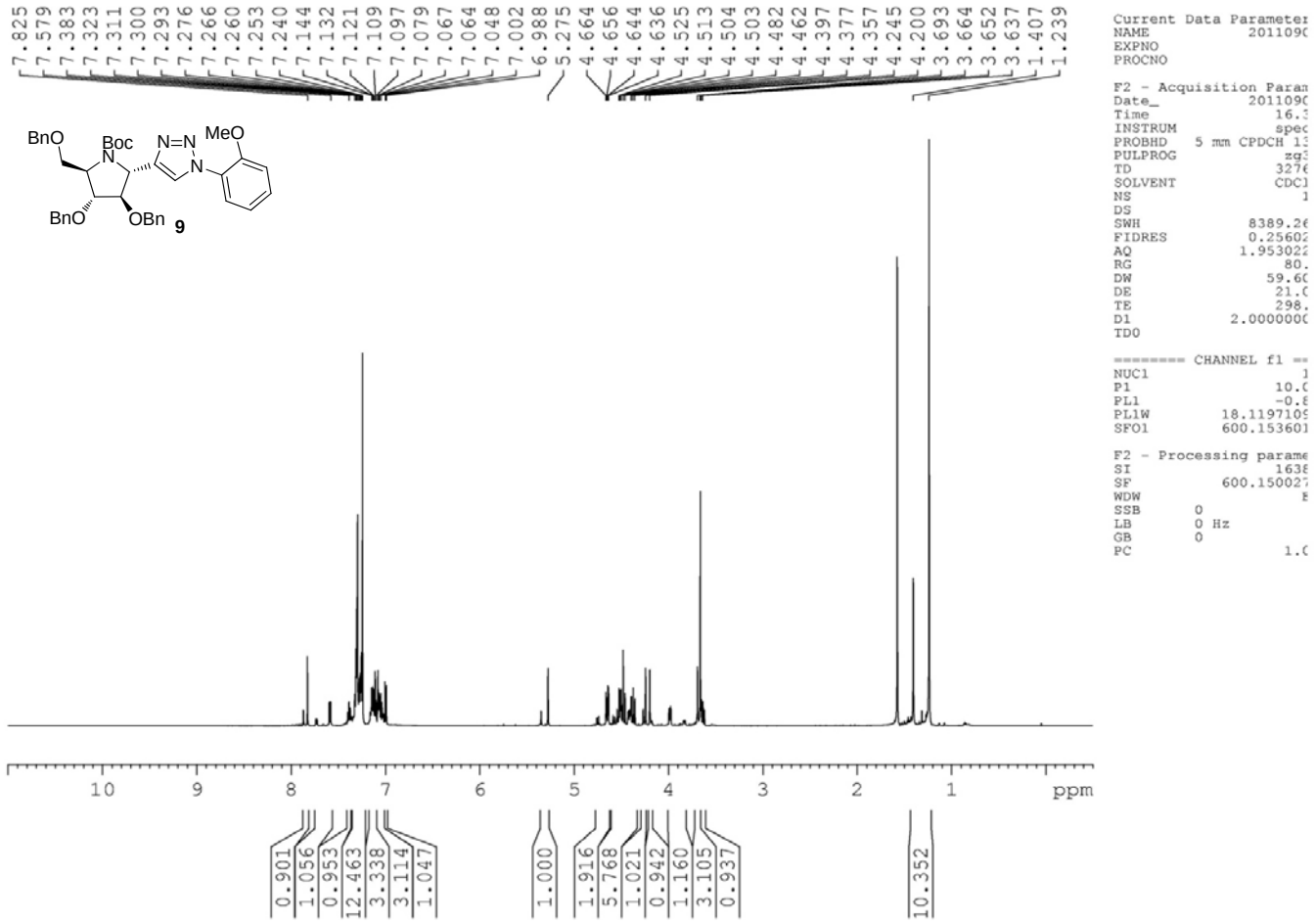
^{1}H NMR spectrum of compound **8** (600 MHz, $CDCl_3$).



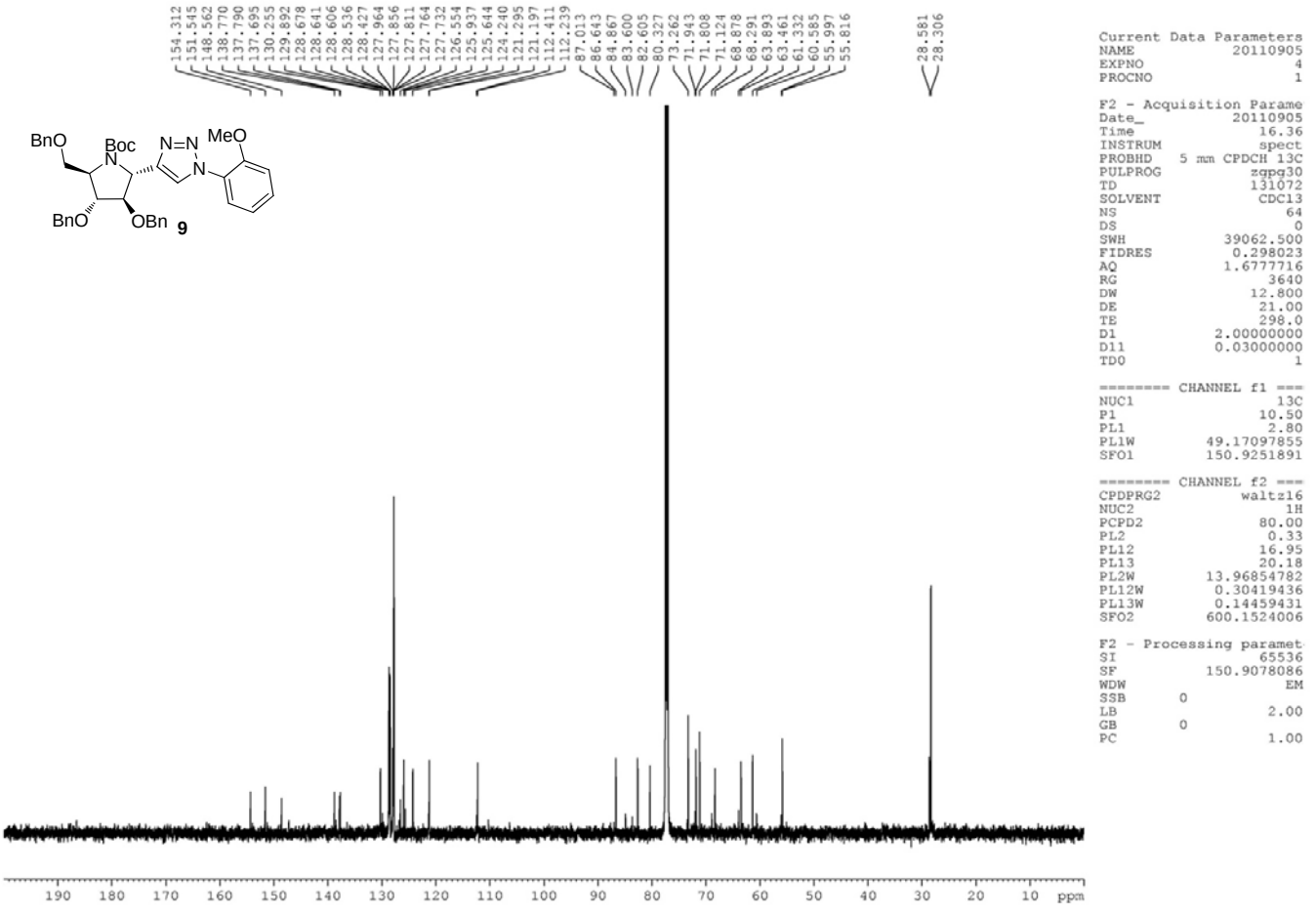
^{13}C NMR spectrum of compound **8** (150 MHz, $CDCl_3$).



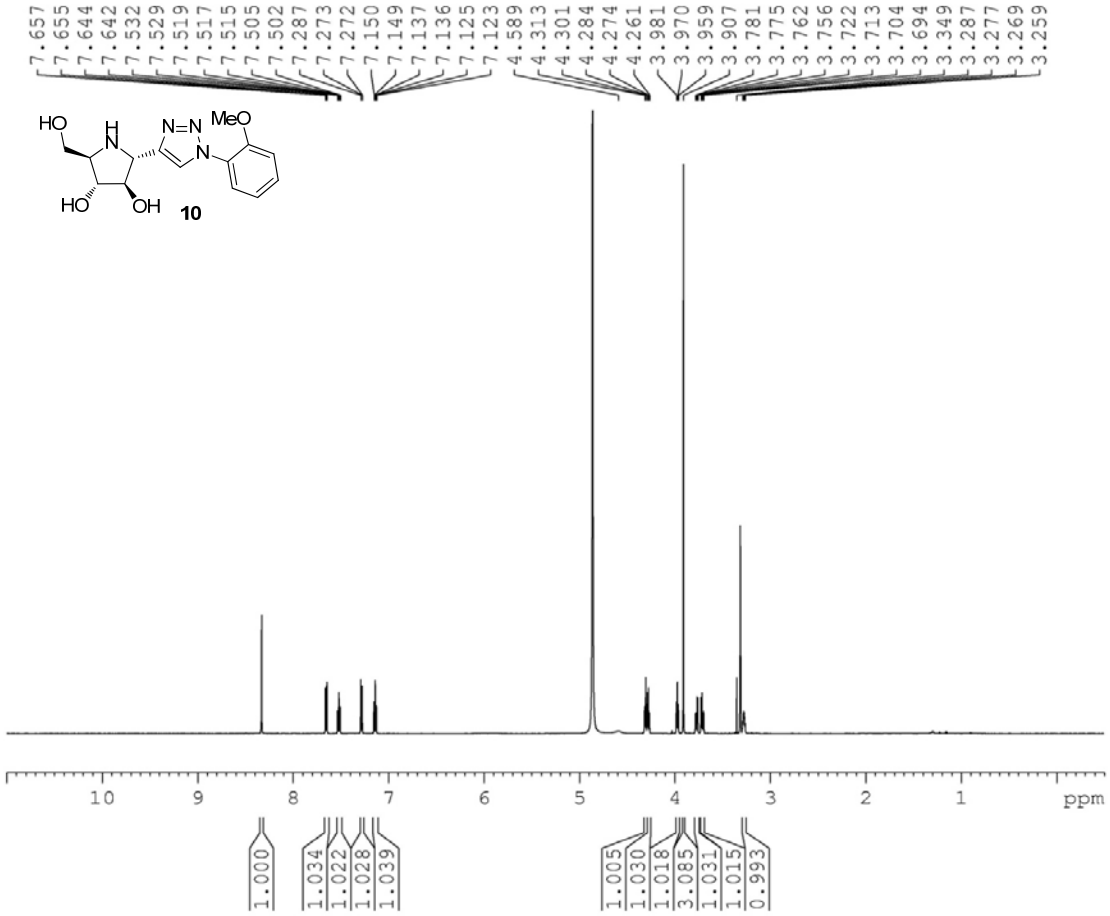
^{1}H NMR spectrum of compound **9** (600 MHz, $CDCl_3$).



^{13}C NMR spectrum of compound **9** (150 MHz, $CDCl_3$).



^{1}H NMR spectrum of compound **10** (600 MHz, CD_3OD).

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PROCNO

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SOLVENT                MeC
NS                       1
DS
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FIDRES              0.2554
AQ                  1.957391
RG
DW                     59.7
DE                     21.
TE                     298.
D1                  2.000000
TD0

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P1                       7.
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F2 - Processing parame
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PC                       1.
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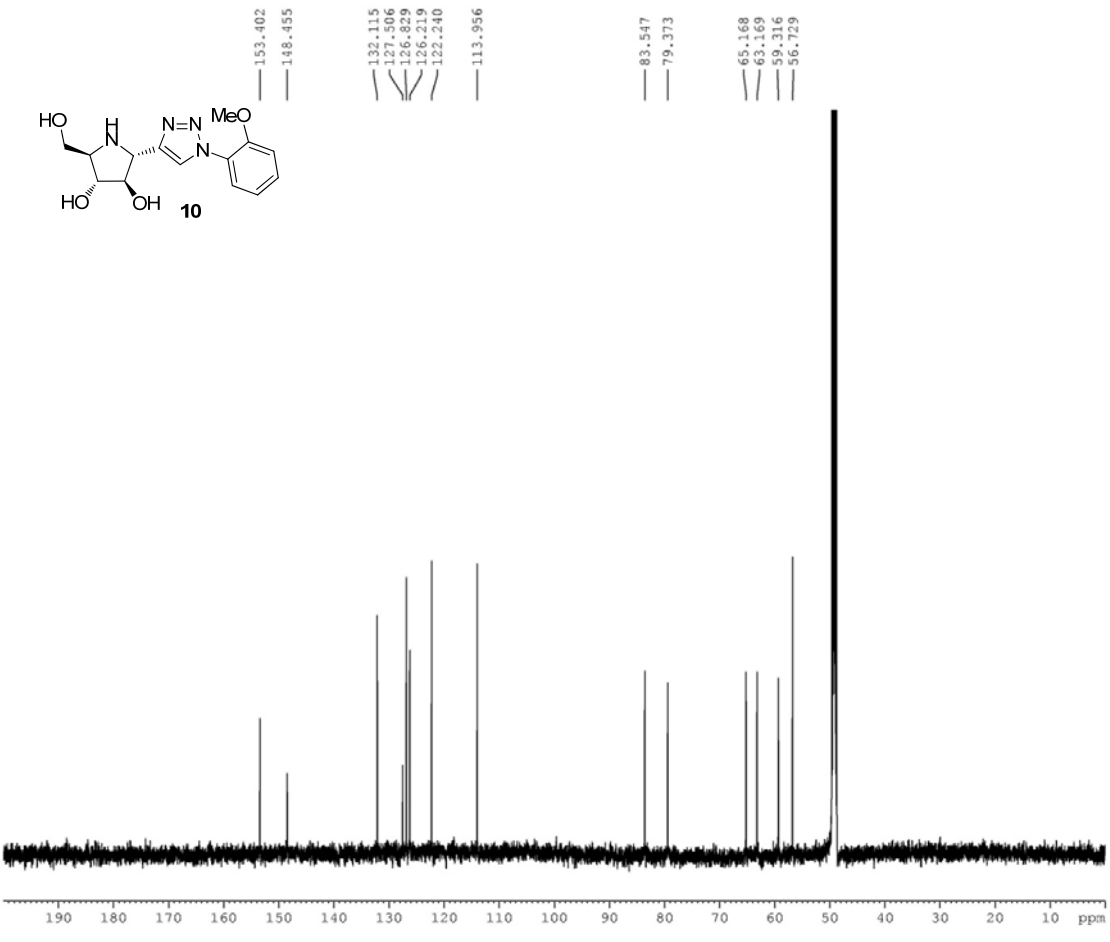
^{13}C NMR spectrum of compound **10** (150 MHz, CD_3OD).

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FIDRES             0.298023
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PL1                     -1.82
PL1W          122.22216797
SFO1           150.9201586

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NUC2                       1H
PCPD2                   90.00
PL2                      4.00
PL12                    25.13
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PL2W           6.09999990
PL12W          0.04702512
PL13W          0.02356839
SFO2           600.1324005

F2 - Processing paramet
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SF                150.9025758
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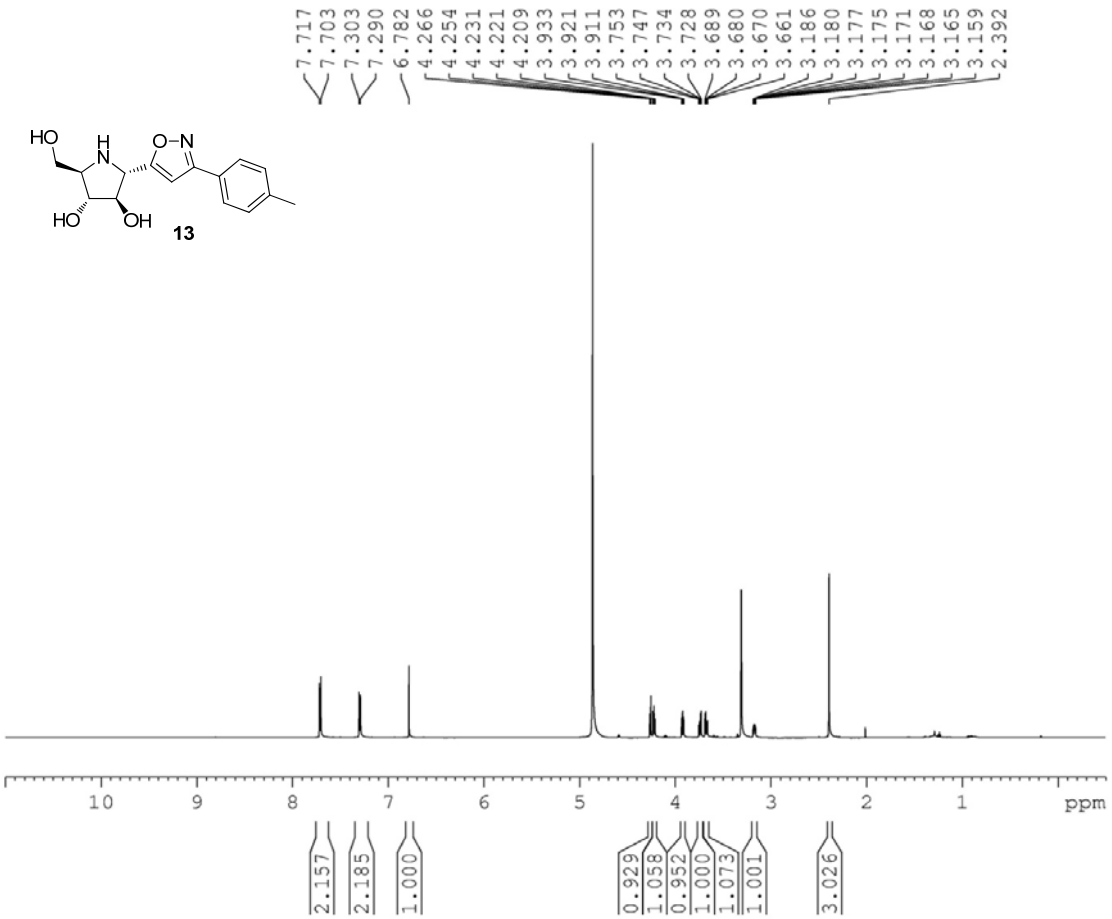
^{1}H NMR spectrum of compound **13** (600 MHz, CD_3OD).

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EXPNO
PROCNO

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SOLVENT                MeC
NS
DS
SWH                 8389.26
FIDRES              0.25602
AQ                  1.95302
RG                     50.
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DE                     21.(
TE                     298.
D1                2.0000000
TD0

======== CHANNEL f1 ==
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P1                     10.(
PL1                    -0.6
PL1W             18.1197105
SFO1             600.153601

F2 - Processing parame
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PC                     1.(
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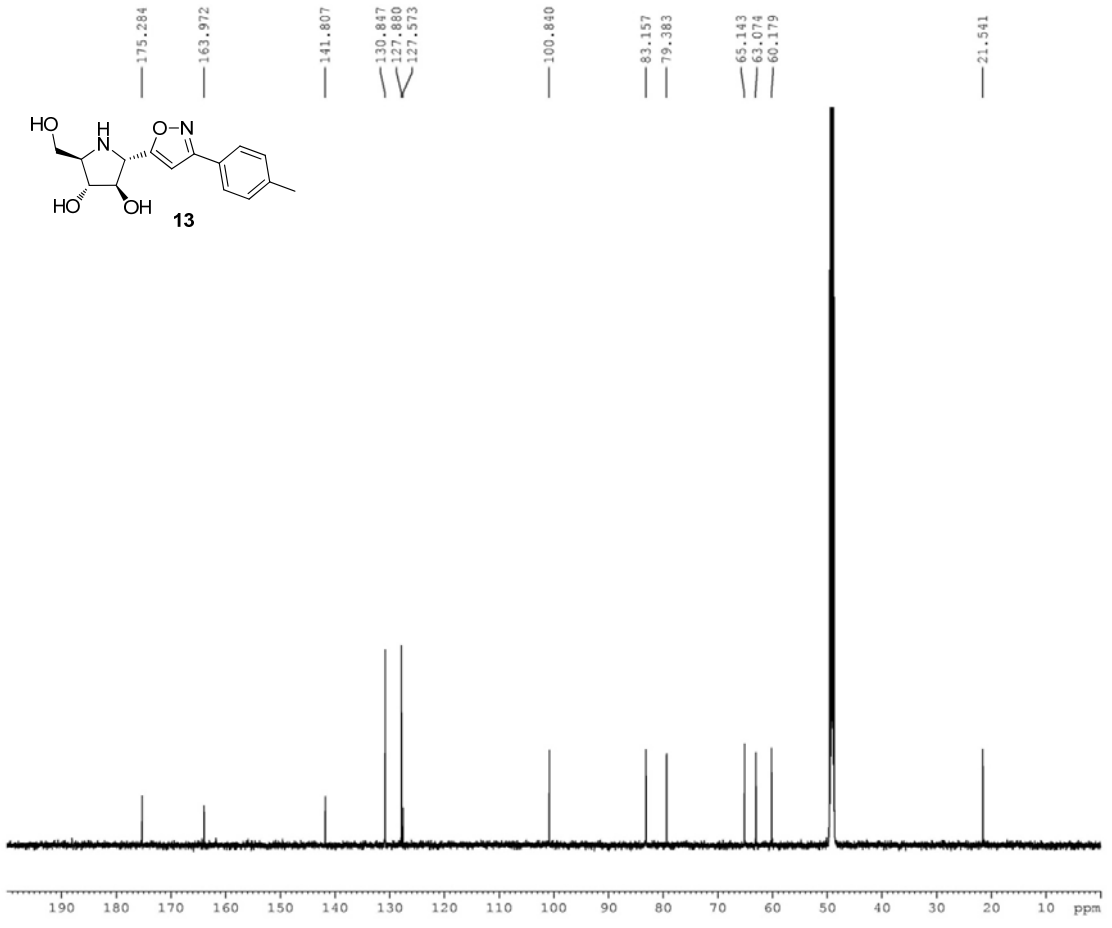
^{13}C NMR spectrum of compound **13** (150 MHz, CD_3OD).

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SOLVENT                MeOD
NS                         54
DS                          0
SWH                39062.500
FIDRES              0.298023
AQ                  1.6777716
RG                      3640
DW                     12.800
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======== CHANNEL f1 ===
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P1                     10.50
PL1                     2.80
PL1W             49.17097855
SFO1             150.9251891

======== CHANNEL f2 ===
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PCPD2                  80.00
PL2                     0.33
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PL13                   20.18
PL2W             13.96854782
PL12W             0.28850359
PL13W             0.14459431
SFO2             600.1524006

F2 - Processing paramet
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SF               150.9076079
WDW                       EM
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PC                      1.00
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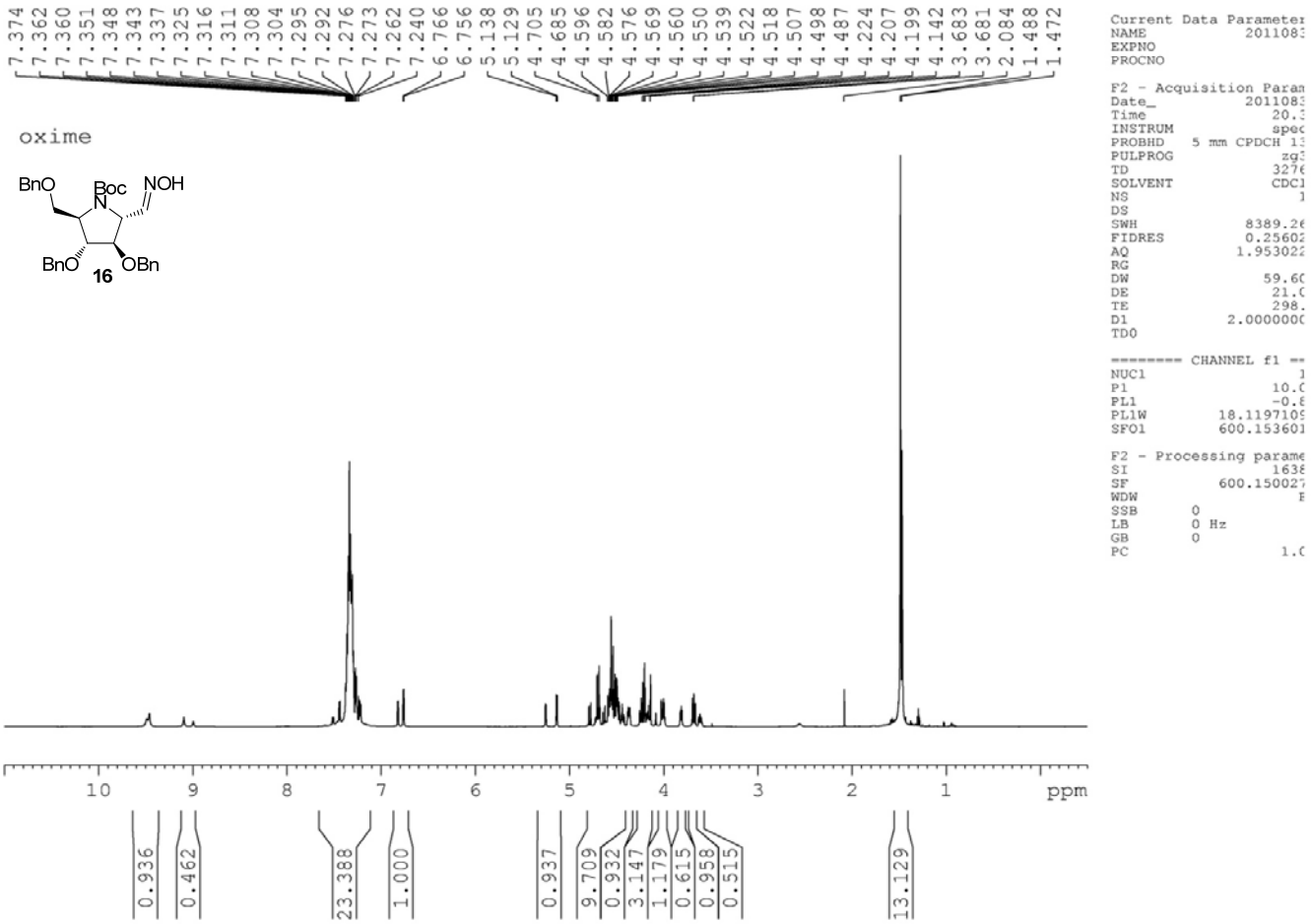
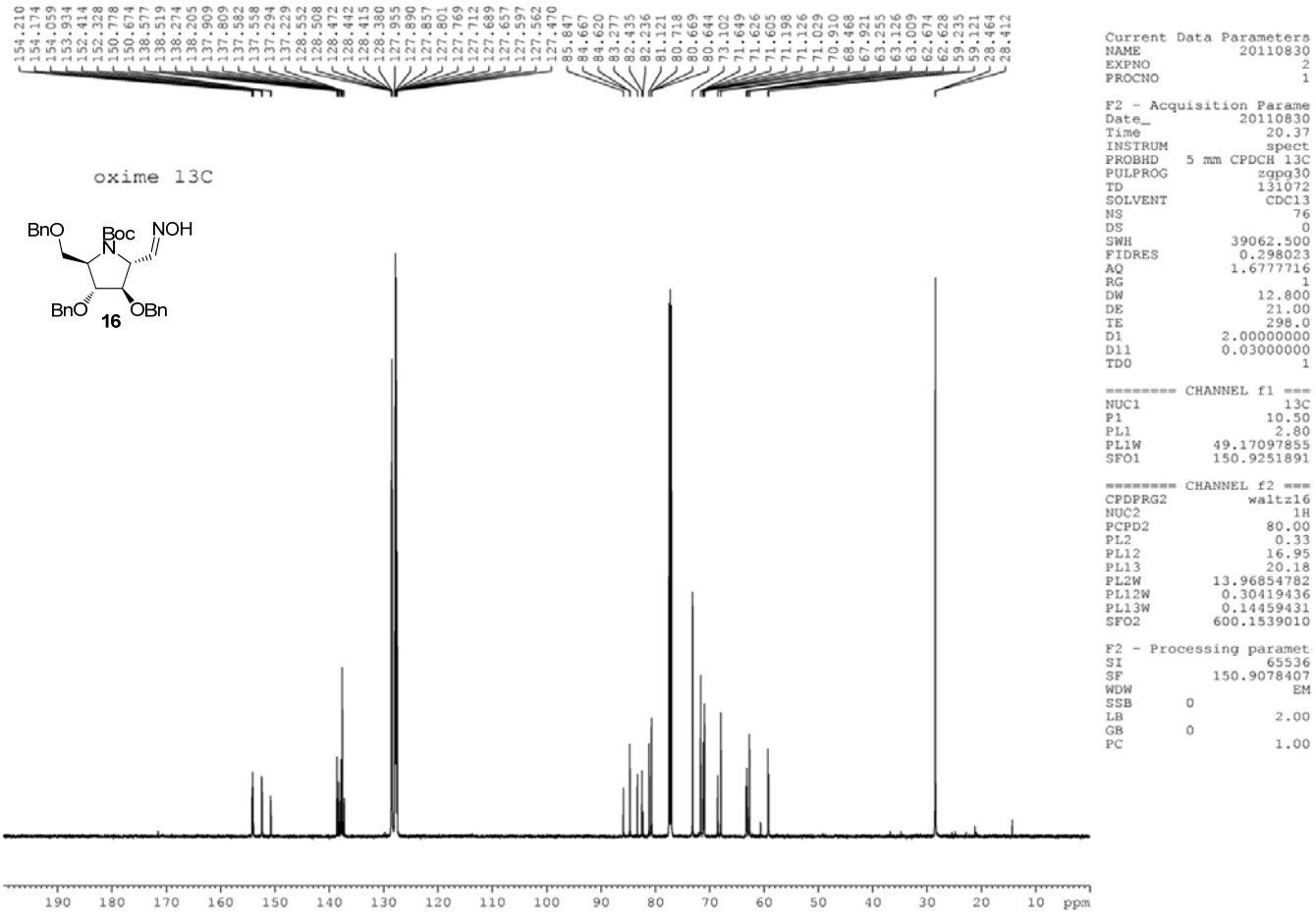
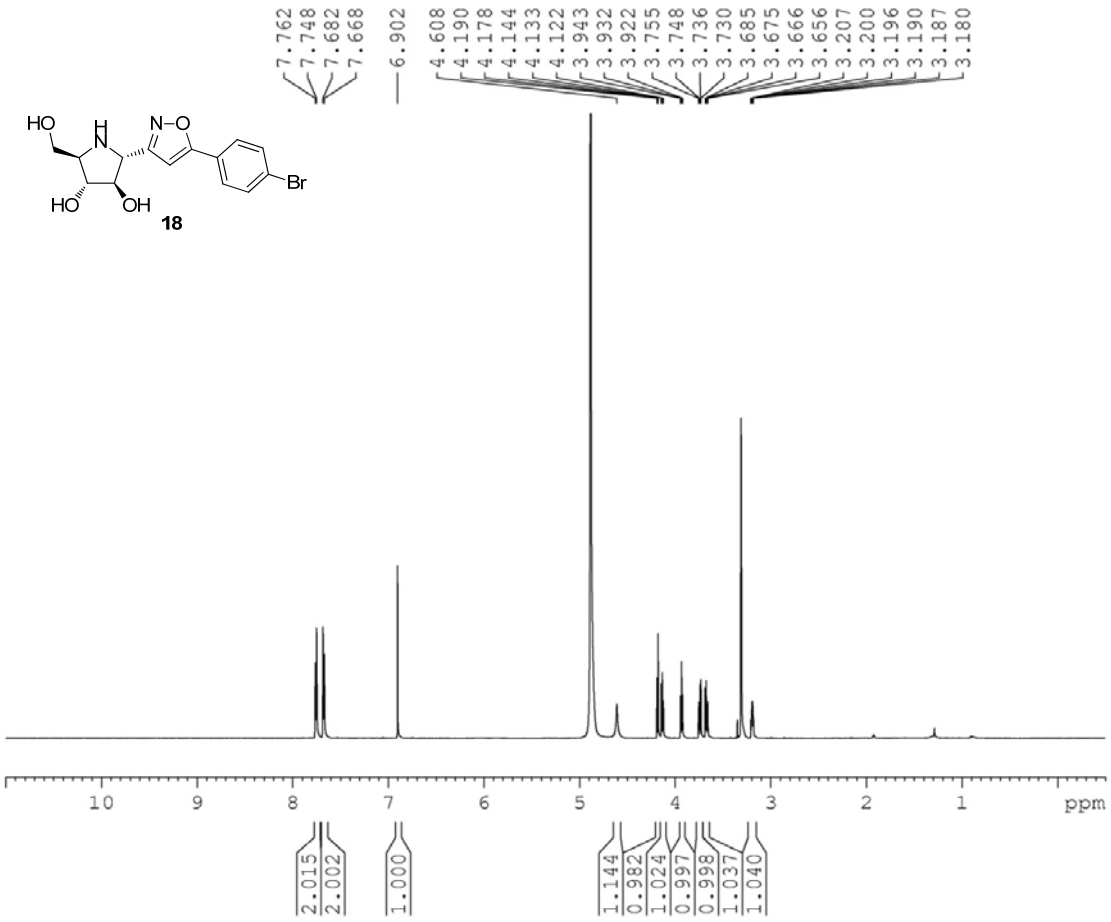
^{1}H NMR spectrum of compound **16** (600 MHz, $CDCl_3$).



^{13}C NMR spectrum of compound **16** (150 MHz, $CDCl_3$).



^{1}H NMR spectrum of compound **18** (600 MHz, CD_3OD).

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EXPNO
PROCNO

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TD                      3276
SOLVENT                  MeC
NS
DS
SWH                  8389.26
FIDRES               0.25602
AQ                1.9530222
RG                         6
DW                     59.60
DE                     21.0
TE                     298.
D1                2.0000000
TD0

======== CHANNEL f1 ==
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PL1                    -0.6
PL1W            18.11971095
SFO1            600.1536013

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SF                600.1500311
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GB           0
PC                     1.0
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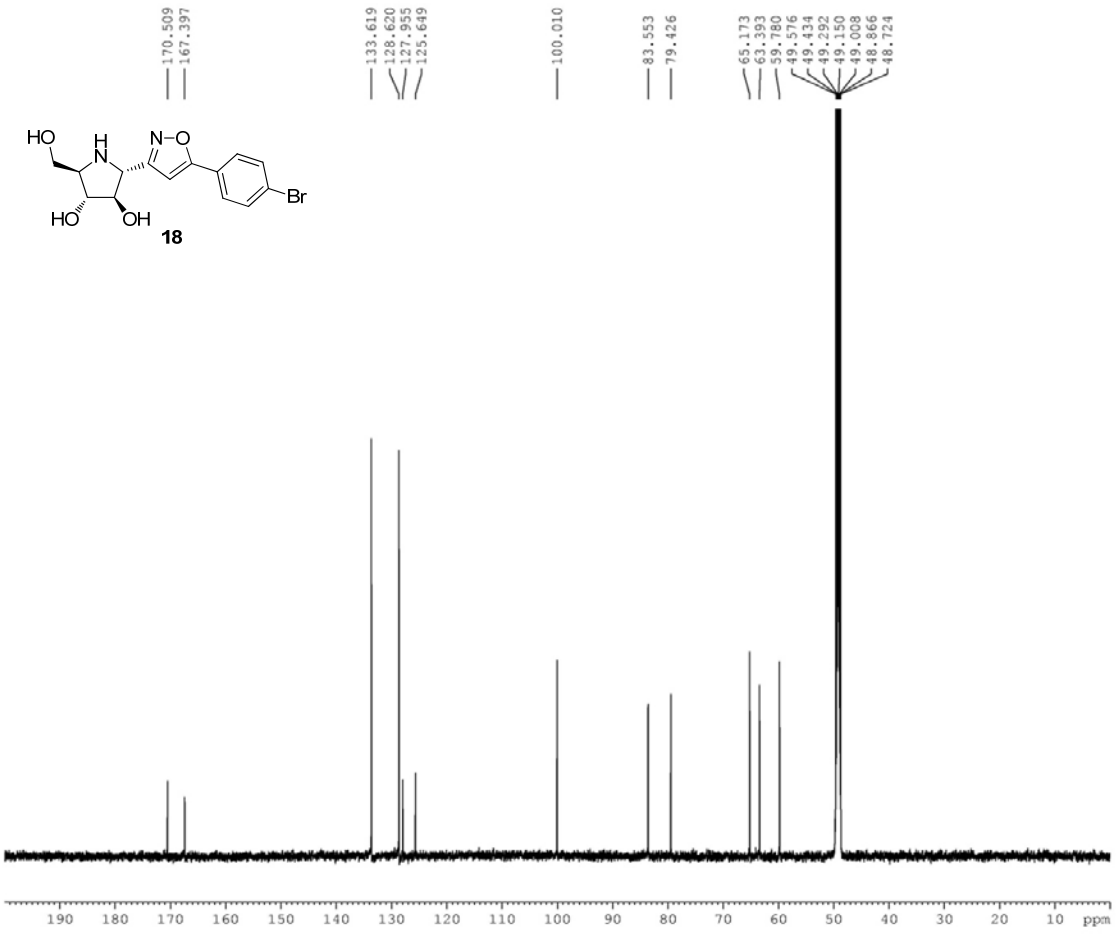
^{13}C NMR spectrum of compound **18** (150 MHz, CD_3OD).

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PROCNO                      1

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INSTRUM                 spect
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SOLVENT                 MeOD
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DS                         0
SWH                39062.500
FIDRES              0.298023
AQ                1.6777716
RG                      2050
DW                     12.800
DE                     21.00
TE                     298.0
D1                2.00000000
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======== CHANNEL f1 ===
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P1                     10.50
PL1                     2.80
PL1W           49.17097855
SFO1           150.9251891

======== CHANNEL f2 ===
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NUC2                     1H
PCPD2                  80.00
PL2                     0.33
PL12                   16.95
PL13                   20.18
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PL12W           0.30419436
PL13W           0.14459431
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F2 - Processing paramet
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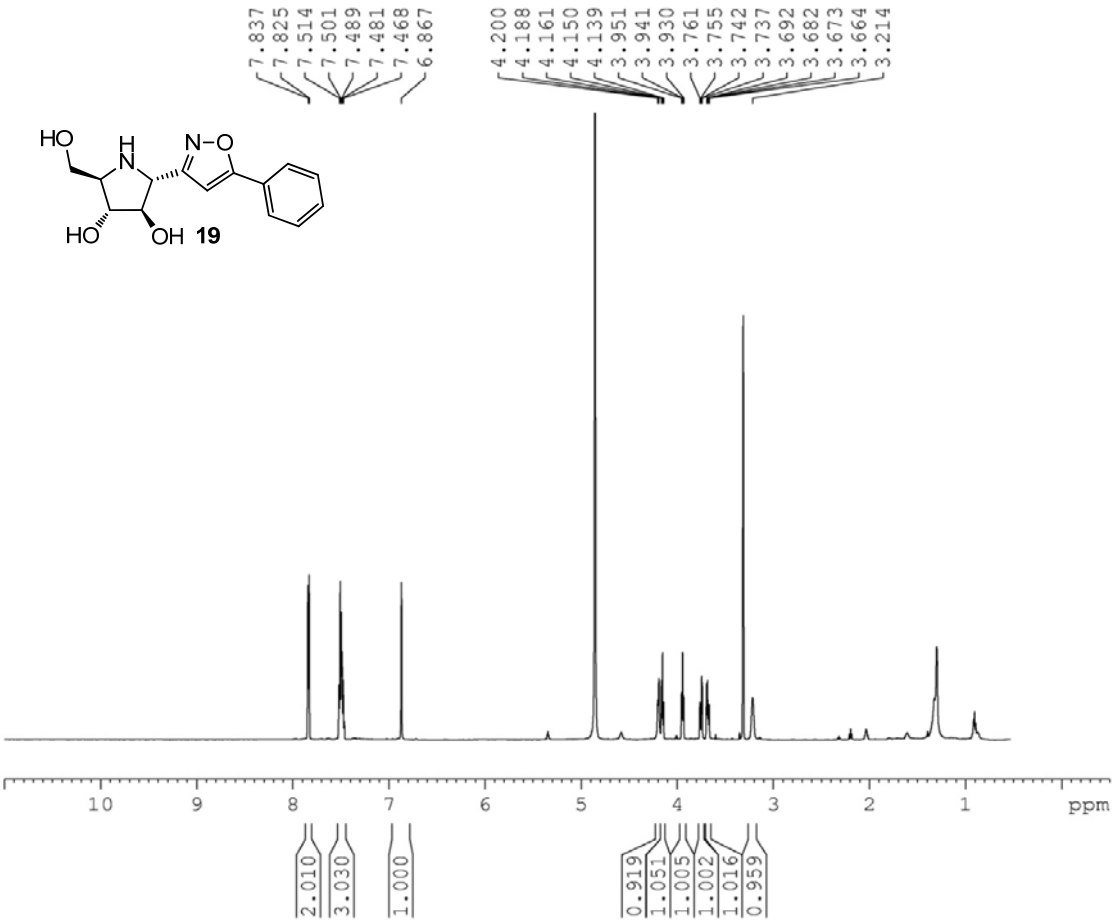
^{1}H NMR spectrum of compound **19** (600 MHz, CD_3OD).

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Current Data Parameter
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EXPNO
PROCNO

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PULPROG               zg3
TD                    327(
SOLVENT               MeC
NS
DS
SWH                8370.51
FIDRES             0.25544
AQ                 1.957391
RG                      5
DW                   59.73
DE                    21.(
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D1                 2.000000(
TD0

======== CHANNEL f1 ==
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P1                    7.9
PL1                   4.(
PL1W           6.0999995
SFO1           600.13360(

F2 - Processing parame
SI                    163(
SF             600.129095
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SSB         0
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GB          0
PC                    1.(
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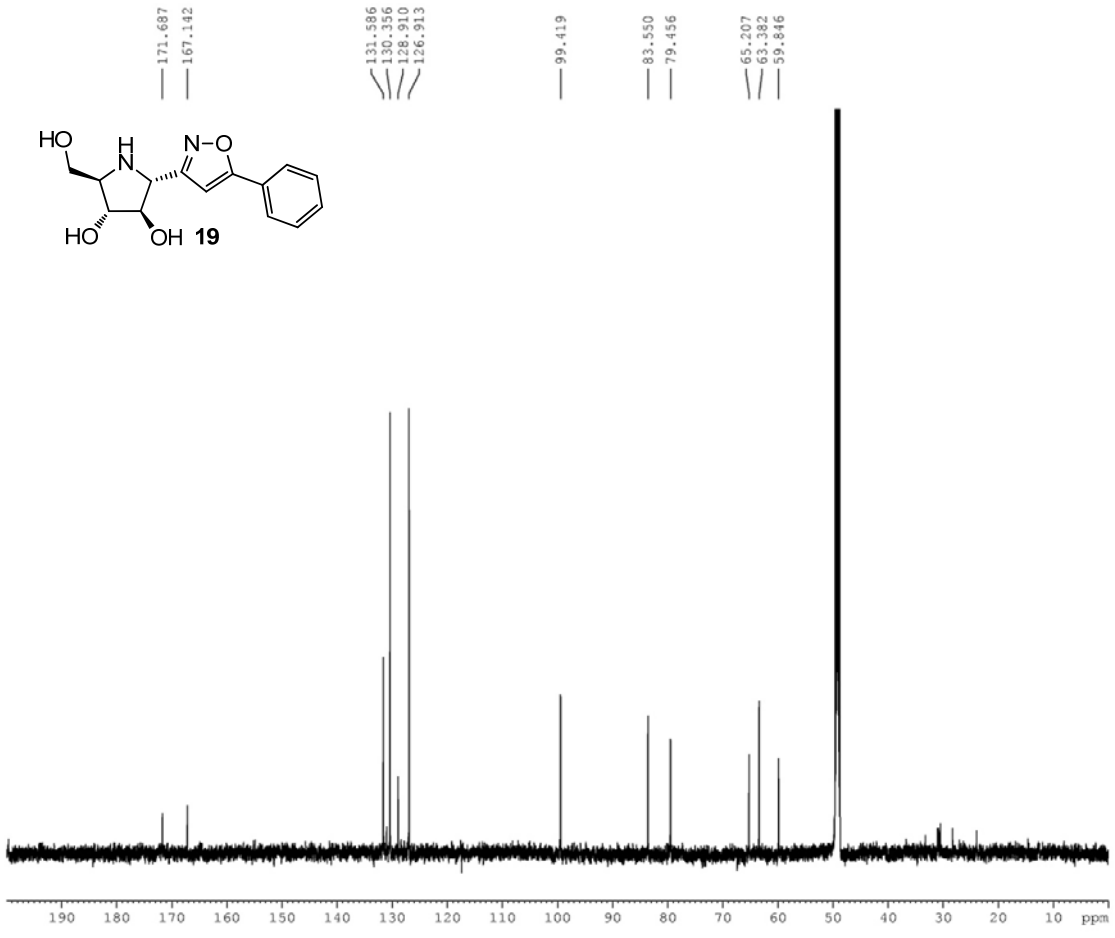
^{13}C NMR spectrum of compound **19** (150 MHz, CD_3OD).

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TD                   131072
SOLVENT                MeOD
NS                       64
DS                        0
SWH                39062.500
FIDRES             0.298023
AQ                 1.6777716
RG                      2050
DW                    12.800
DE                    21.00
TE                    298.0
D1                 2.00000000
D11                0.03000000
TD0                        1

======== CHANNEL f1 ===
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P1                      9.60
PL1                    -1.82
PL1W          122.22216797
SFO1           150.9201581

======== CHANNEL f2 ===
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NUC2                     1H
PCPD2                 90.00
PL2                    4.00
PL12                  24.90
PL13                  27.90
PL2W           6.09999990
PL12W          0.04958267
PL13W          0.02485020
SFO2           600.1324005

F2 - Processing paramet
SI                     65536
SF             150.9023459
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SSB         0
LB                     2.00
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PC                     1.00
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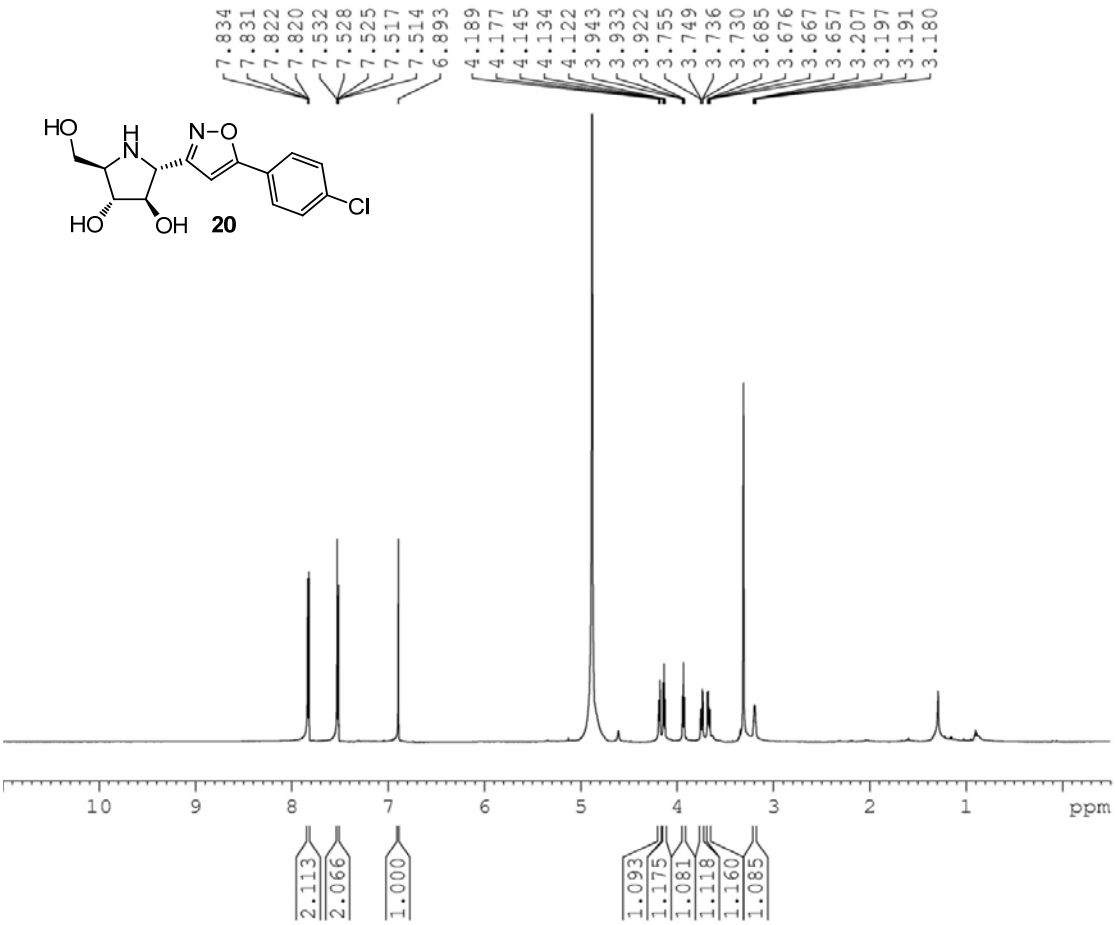
^{1}H NMR spectrum of compound **20** (600 MHz, CD_3OD).



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PROCNO

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INSTRUM spec
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SOLVENT MeC
NS 1
DS
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FIDRES 0.2560
AQ 1.9530
RG 80.
DW 59.6
DE 21.
TE 298.
D1 2.000000
TD0

======== CHANNEL f1 ==
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P1 10.
PL1 -0.
PL1W 18.1197109
SFO1 600.153601

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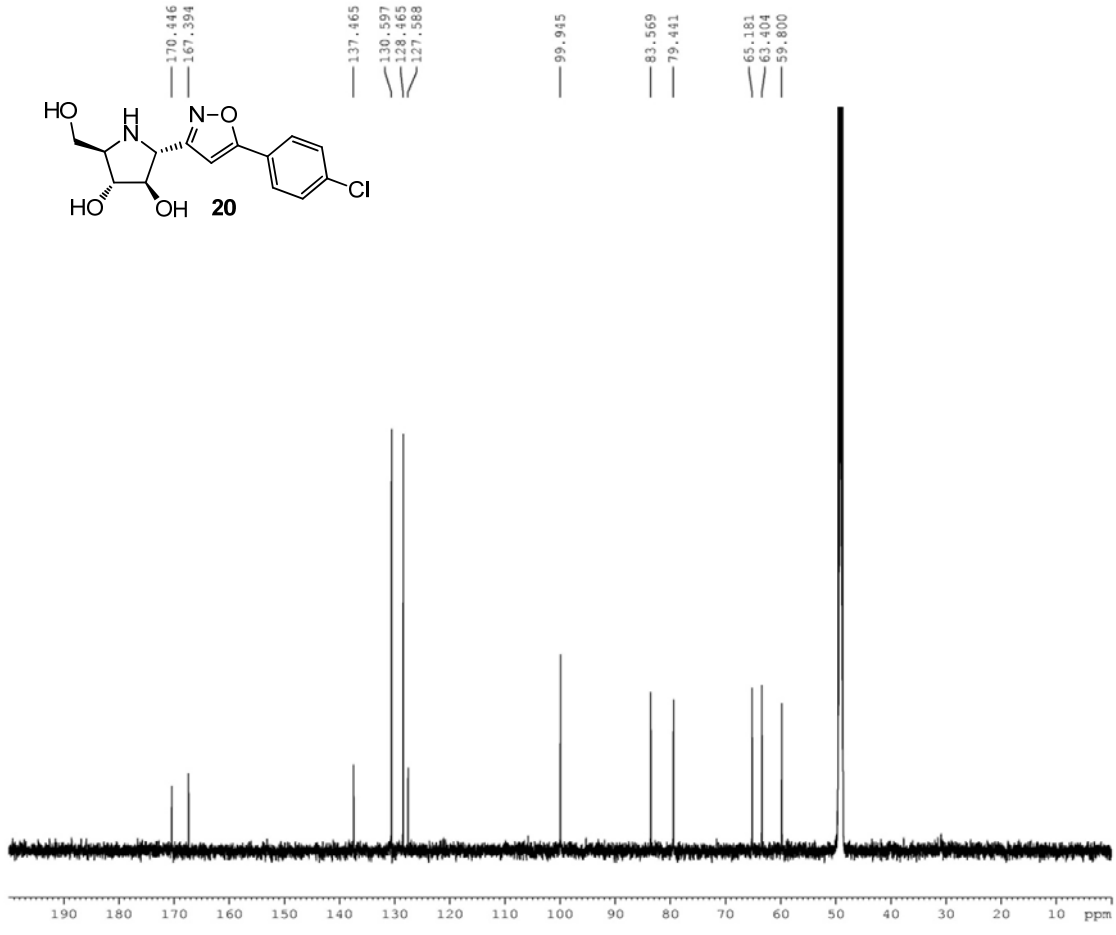
^{13}C NMR spectrum of compound **20** (150 MHz, CD_3OD).



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DS 0
SWH 39062.500
FIDRES 0.298023
AQ 1.6777716
RG 1
DW 12.800
DE 21.00
TE 298.0
D1 2.00000000
D11 0.03000000
TD0 1

======== CHANNEL f1 ===
NUC1 13C
P1 10.50
PL1 2.80
PL1W 49.17097855
SFO1 150.9251891

======== CHANNEL f2 ===
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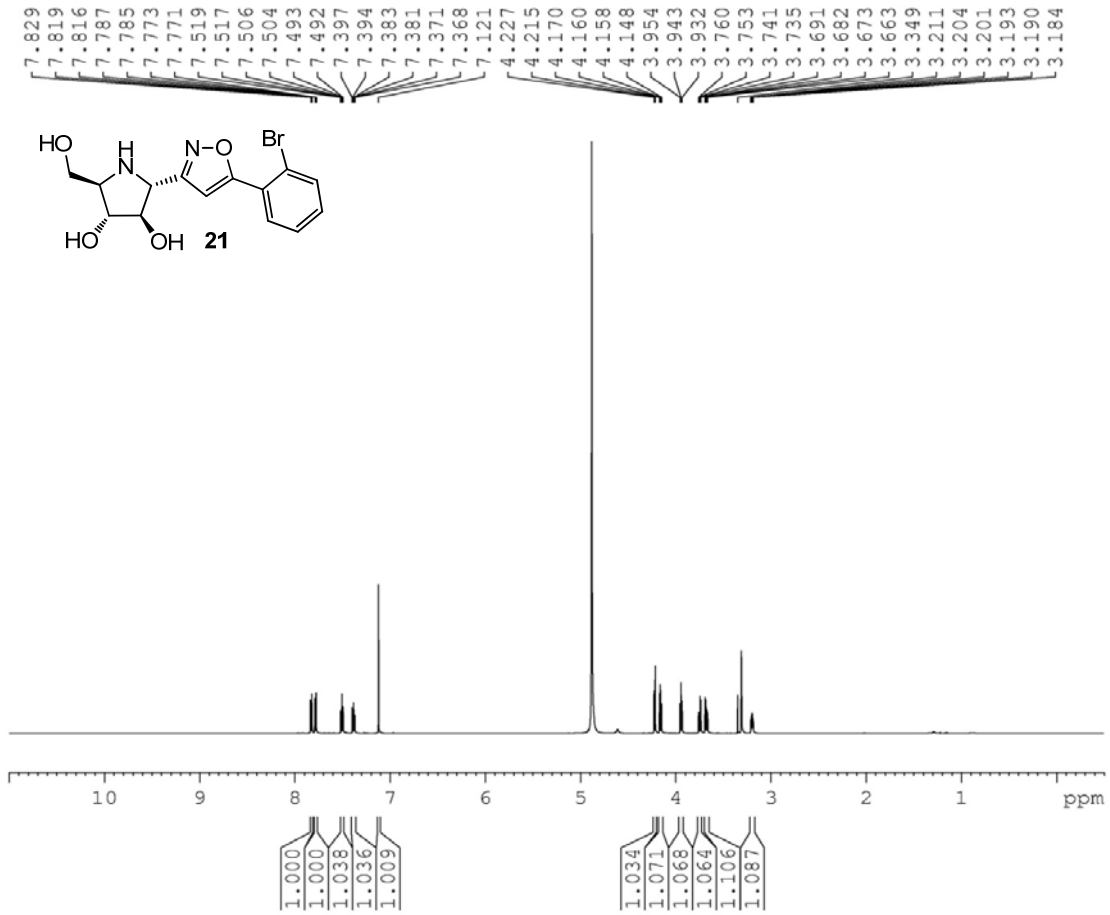
NUC2 1H
PCPD2 80.00
PL2 0.33
PL12 16.95
PL13 20.18
PL2W 13.96854782
PL12W 0.30419436
PL13W 0.14459431
SFO2 600.1539010

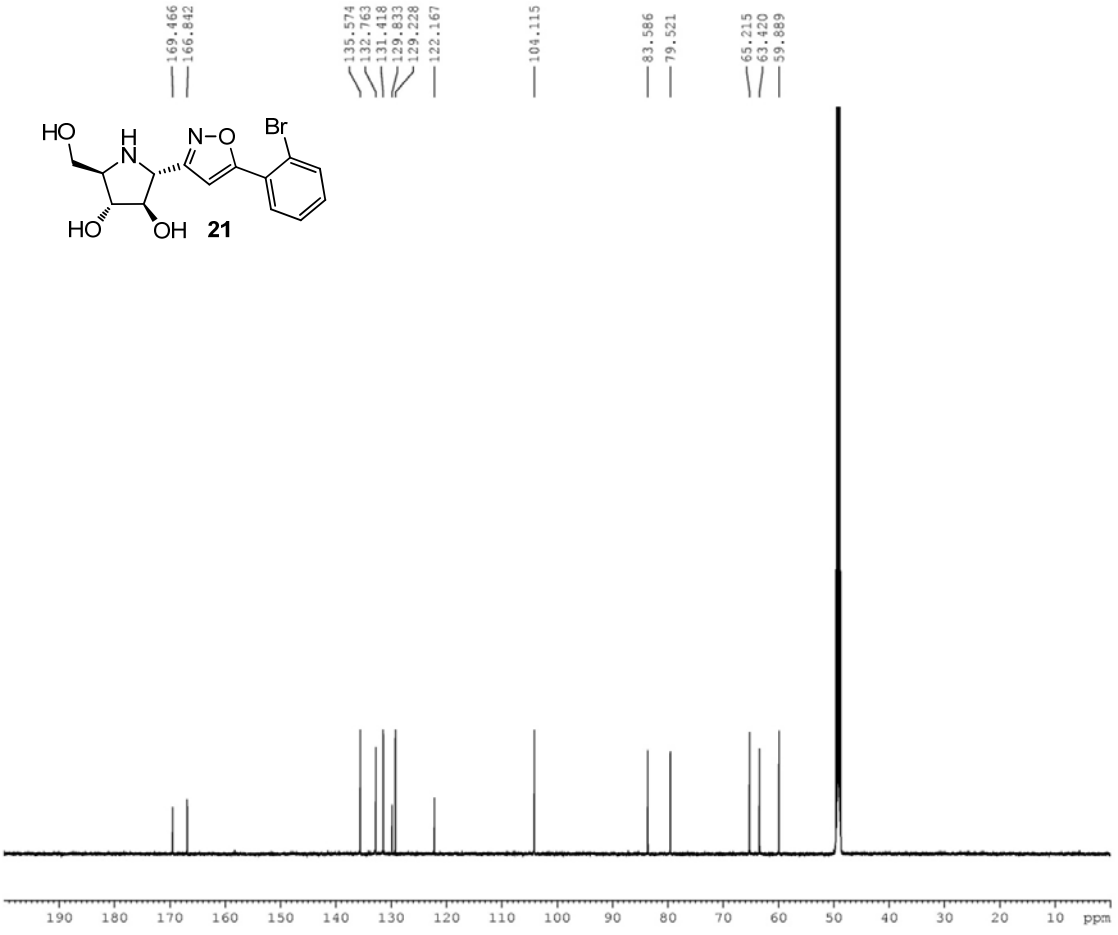
F2 - Processing paramet
SI 65536
SF 150.9076085
WDW EM
SSB 0
LB 2.00
GB 0
PC 1.00

^{1}H NMR spectrum of compound **21** (600 MHz, CD_3OD).



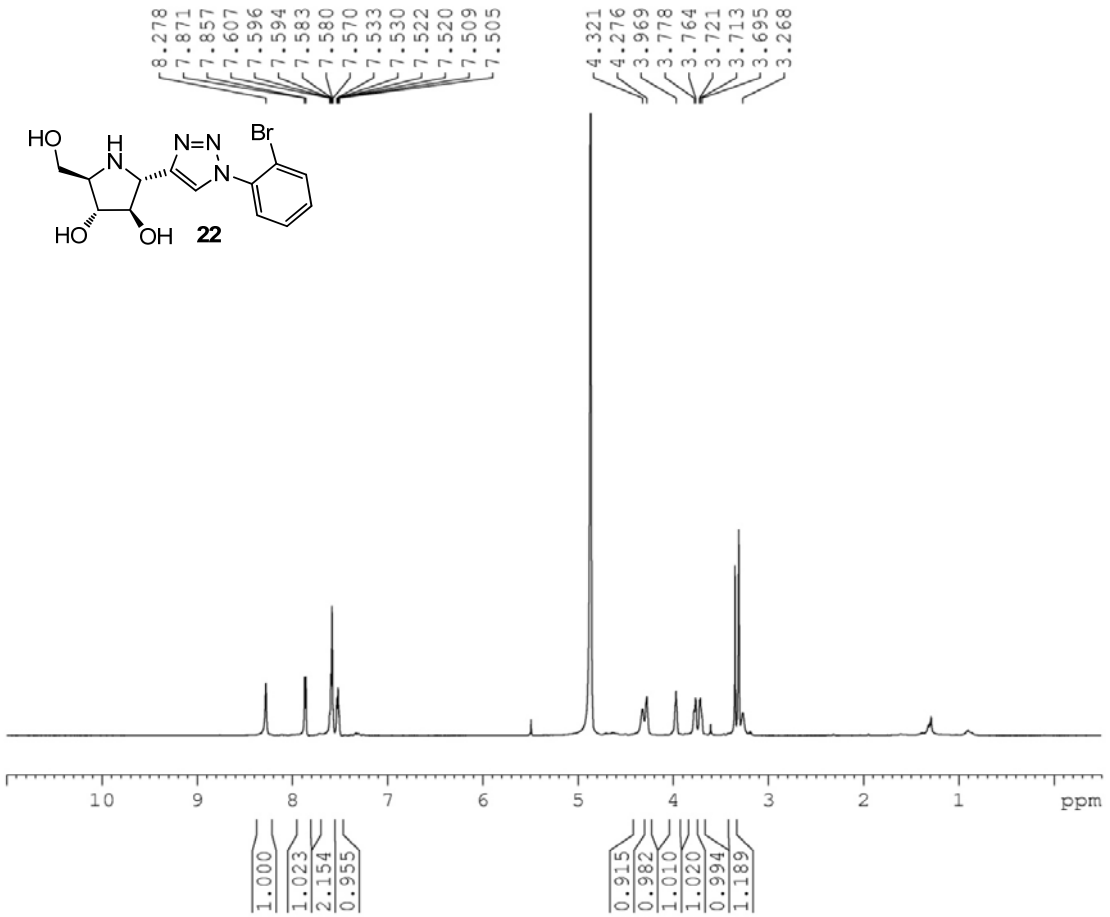

```
Current Data Parameter
NAME                 201109
EXPNO
PROCNO

F2 - Acquisition Param
Date_                201109
Time                   14.
INSTRUM                spe
PROBHD    5 mm CPDCH 1
PULPROG                zg
TD                    327
SOLVENT                Me
NS                      
DS                      
SWH                8389.2
FIDRES             0.2560
AQ                 1.9530
RG                      
DW                   59.6
DE                   21.
TE                   298.
D1                 2.0000000
TD0

======== CHANNEL f1 ==
NUC1                    
P1                   10.
PL1                  -0.
PL1W            18.1197109
SFO1            600.1536019

F2 - Processing parame
SI                    163
SF              600.1500319
WDW                     E
SSB         0
LB          0 Hz
GB          0
PC                    1.
```

^{13}C NMR spectrum of compound **21** (150 MHz, CD_3OD).



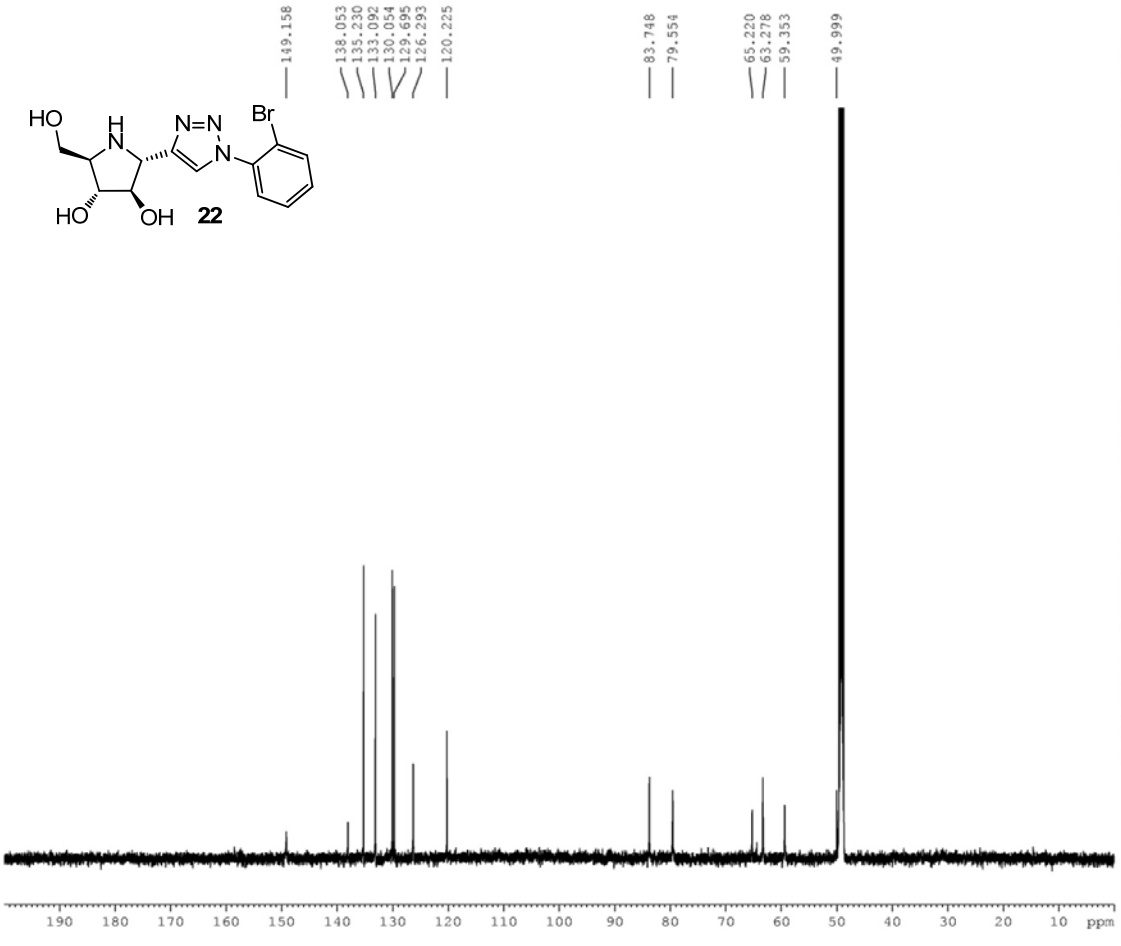

```
Current Data Parameters
NAME                 20110923
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parame
Date_                20110923
Time                    14.17
INSTRUM                 spect
PROBHD    5 mm CPDCH 13C
PULPROG              zgpg30
TD                   131072
SOLVENT                MeOD
NS                        64
DS                         0
SWH                39062.500
FIDRES             0.298023
AQ                 1.6777716
RG                      3640
DW                    12.800
DE                    21.00
TE                    298.0
D1                 2.00000000
D11                0.03000000
TD0                         1

======== CHANNEL f1 ===
NUC1                      13C
P1                      10.38
PL1                      2.80
PL1W            49.17097855
SFO1            150.9251891

======== CHANNEL f2 ===
CPDPRG2               waltz16
NUC2                       1H
PCPD2                   80.00
PL2                      0.33
PL12                    17.18
PL13                    20.18
PL2W            13.96854782
PL12W            0.28850359
PL13W            0.14459431
SFO2            600.1524006

F2 - Processing paramet
SI                      65536
SF              150.9076097
WDW                        EM
SSB         0
LB                      2.00
GB          0
PC                      1.00
```

^{1}H NMR spectrum of compound **22** (600 MHz, CD_3OD).



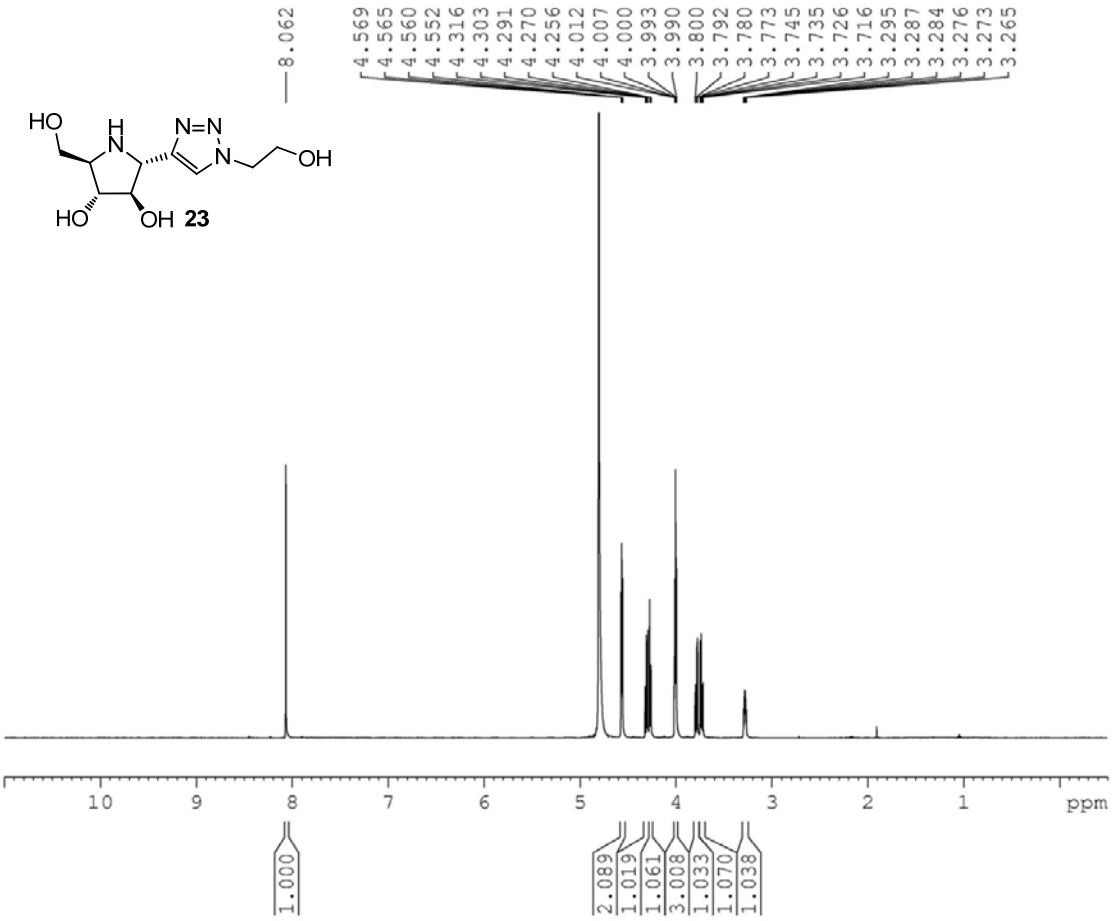

```
Current Data Parameter
NAME                 2012031
EXPNO
PROCNO

F2 - Acquisition Paran
Date_                2012031
Time                    12.5
INSTRUM                 spec
PROBHD    5 mm CPDCH 13
PULPROG                 zg3
TD                      327
SOLVENT                 MeC
NS
DS
SWH                  8389.26
FIDRES               0.25602
AQ                1.9530222
RG                      45.
DW                    59.6(
DE                      21.(
TE                      298.
D1                2.0000000(
TD0

======== CHANNEL f1 ==
NUC1                     1
P1                    10.(
PL1                   -0.6
PL1W             18.1197105
SFO1             600.153601

F2 - Processing parame
SI                      163
SF               600.150031
WDW                      E
SSB          0
LB           0 Hz
GB           0
PC                    1.(
```

^{13}C NMR spectrum of compound **22** (150 MHz, CD_3OD).



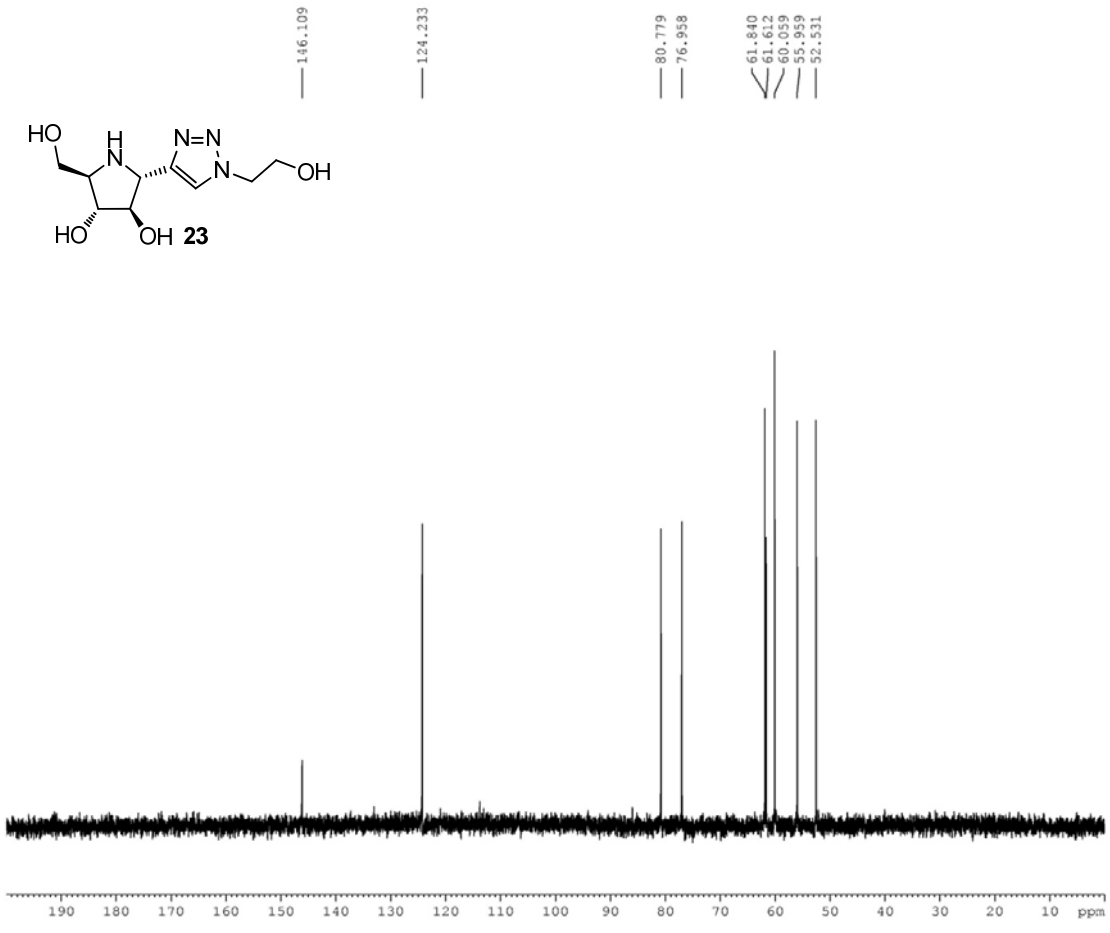

```
Current Data Parameters
NAME                 20120311
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parame
Date_                20120312
Time                    13.04
INSTRUM                 spect
PROBHD    5 mm CPDCH 13C
PULPROG              zgpg30
TD                      131072
SOLVENT                 MeOD
NS                         64
DS                          0
SWH                  39062.500
FIDRES               0.298023
AQ                1.6777716
RG                       3640
DW                     12.800
DE                      21.00
TE                      298.0
D1                2.00000000
D11               0.03000000
TD0                         1

======== CHANNEL f1 ===
NUC1                     13C
P1                     10.50
PL1                     2.80
PL1W             49.17097855
SFO1             150.9251886

======== CHANNEL f2 ===
CPDPRG2              waltz16
NUC2                     1H
PCPD2                  80.00
PL2                     0.33
PL12                   17.18
PL13                   20.18
PL2W             13.96854782
PL12W             0.28850359
PL13W             0.14459431
SFO2             600.1524006

F2 - Processing paramet
SI                      65536
SF               150.9076109
WDW                        EM
SSB          0
LB                      2.00
GB           0
PC                      1.00
```

^{1}H NMR spectrum of compound **23** (600 MHz, D_2O).



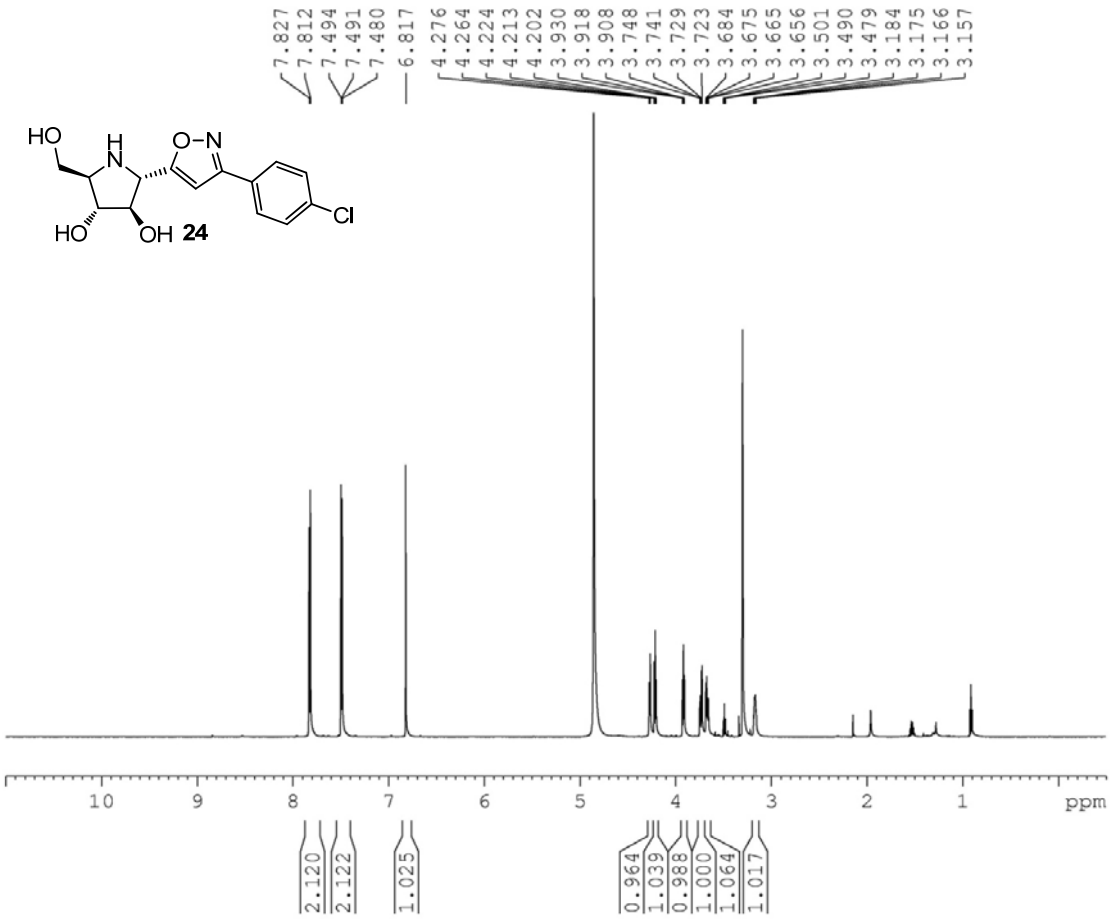

```
Current Data Parameter
NAME                 2011111
EXPNO
PROCNO

F2 - Acquisition Param
Date_                2011111
Time                    12.(
INSTRUM                 spec
PROBHD    5 mm CPDCH 13
PULPROG                 zg3
TD                      3276
SOLVENT                   D2
NS                         1
DS
SWH                  8389.26
FIDRES               0.25602
AQ                1.9530222
RG                      71.
DW                    59.60
DE                    21.0
TE                    298.
D1                 2.0000000
TD0

======== CHANNEL f1 ==
NUC1                       1
P1                      10.0
PL1                     -0.8
PL1W             18.11971095
SFO1             600.1536010

F2 - Processing parame
SI                      1638
SF               600.1499411
WDW                        E
SSB          0
LB           0 Hz
GB           0
PC                      1.0
```

^{13}C NMR spectrum of compound **23** (150 MHz, D_2O).



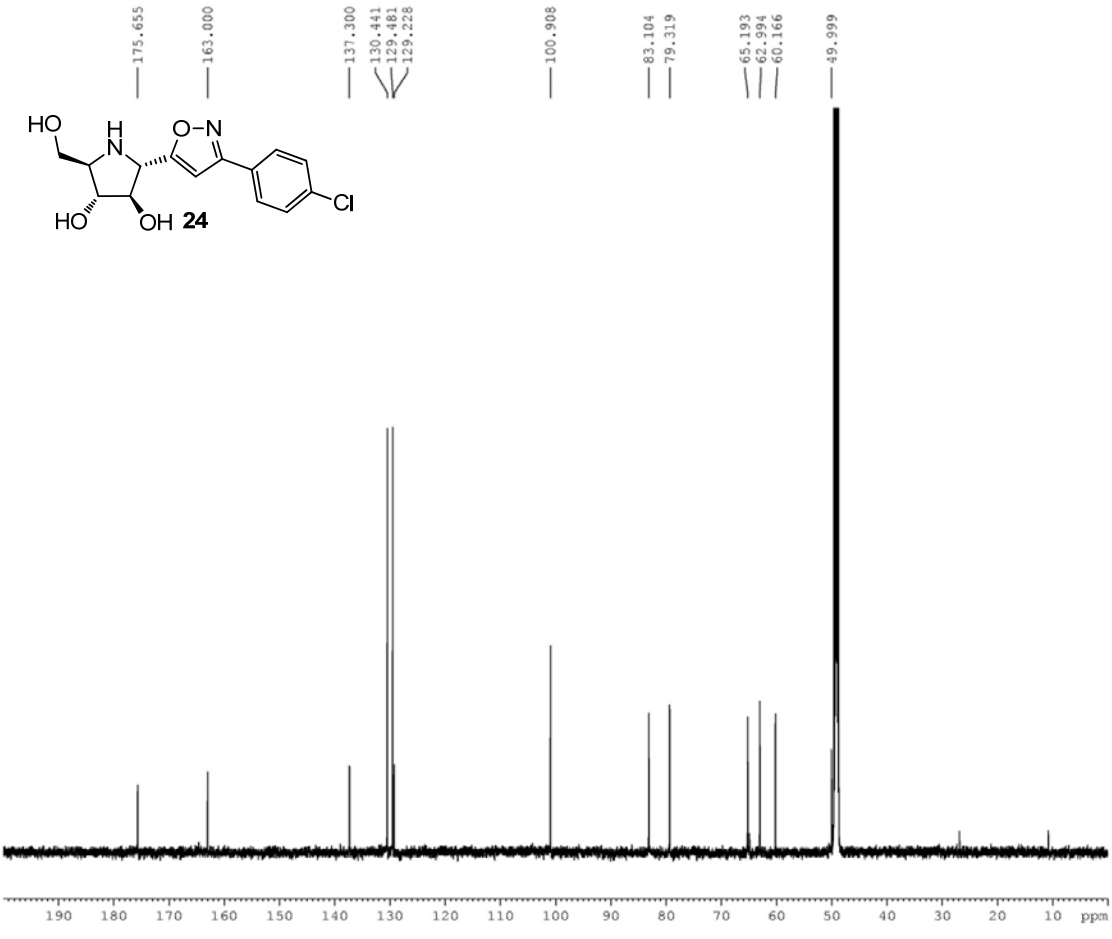

```
Current Data Parameters
NAME                 20111118
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parame
Date_                20111118
Time                    12.11
INSTRUM                 spect
PROBHD    5 mm CPDCH 13C
PULPROG                zgpg30
TD                     131072
SOLVENT                   D2O
NS                         156
DS                           0
SWH                  39062.500
FIDRES               0.298023
AQ                1.6777716
RG                      3640
DW                    12.800
DE                    21.00
TE                    298.0
D1                 2.00000000
D11                0.03000000
TD0                         1

======== CHANNEL f1 ===
NUC1                       13C
P1                      10.38
PL1                      2.80
PL1W             49.17097855
SFO1             150.9251891

======== CHANNEL f2 ===
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00
PL2                      0.33
PL12                    17.18
PL13                    20.18
PL2W             13.96854782
PL12W             0.28850359
PL13W             0.14459431
SFO2             600.1524006

F2 - Processing paramet
SI                      65536
SF               150.9078380
WDW                        EM
SSB          0
LB                       2.00
GB           0
PC                      1.00
```

^{1}H NMR spectrum of compound **24** (600 MHz, CD_3OD).



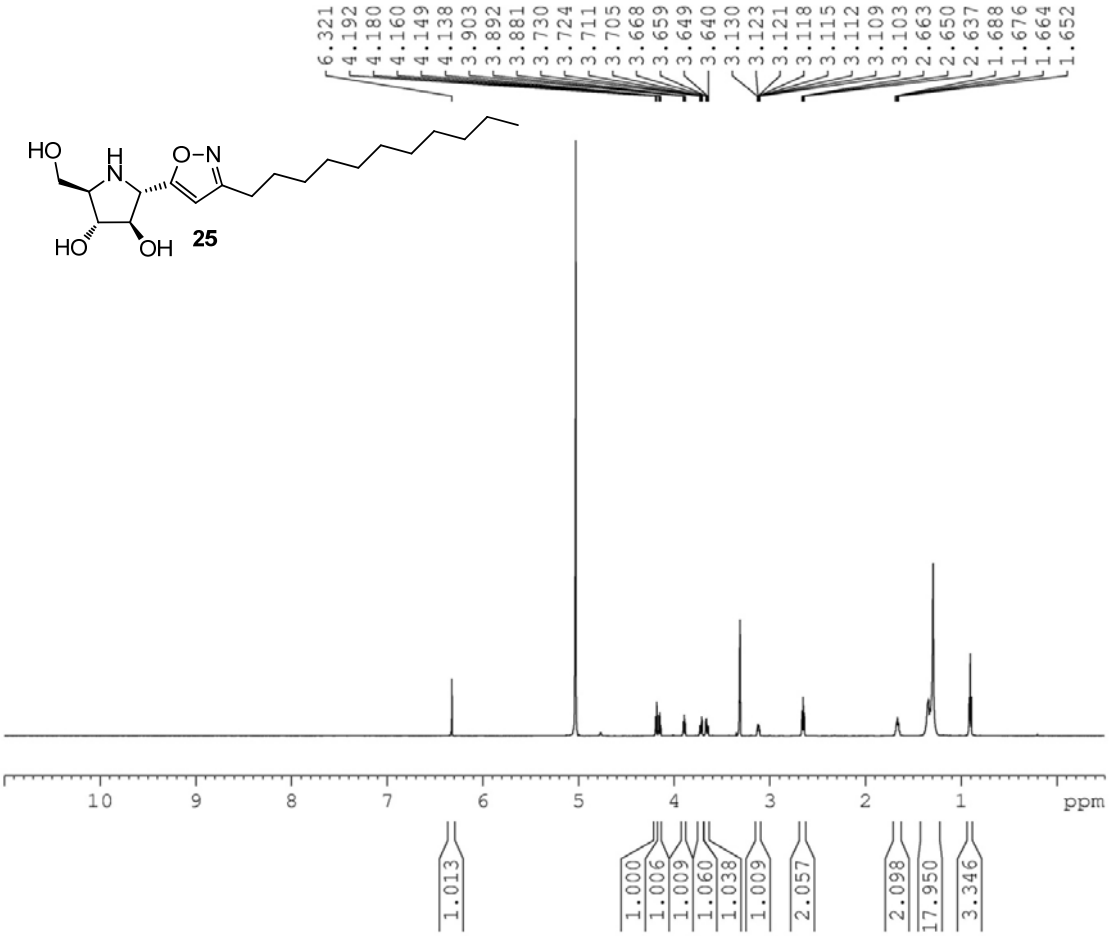

```
Current Data Parameter
NAME                 2012011
EXPNO
PROCNO

F2 - Acquisition Paran
Date_                2012011
Time                    19.3
INSTRUM                 spec
PROBHD    5 mm CPDCH 13
PULPROG                  zg3
TD                      3276
SOLVENT                  MeC
NS                          1
DS
SWH                  8389.26
FIDRES               0.25602
AQ                1.9530227
RG                         12
DW                      59.60
DE                      21.0
TE                      298.
D1                2.0000000
TDO

======== CHANNEL f1 ==
NUC1                        1
P1                        7.7
PL1                       4.2
PL1W              5.7299556
SFO1            600.1536013

F2 - Processing parame
SI                       1638
SF              600.1500036
WDW                         E
SSB          0
LB           0 Hz
GB           0
PC                        1.0
```

^{13}C NMR spectrum of compound **24** (150 MHz, CD_3OD).




```
Current Data Parameters
NAME                 20120112
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parame
Date_                20120112
Time                    19.42
INSTRUM                 spect
PROBHD    5 mm CPDCH 13C
PULPROG              zgpg30
TD                     131072
SOLVENT                 MeOD
NS                         64
DS                          0
SWH                39062.500
FIDRES             0.298023
AQ                1.6777716
RG                      3640
DW                    12.800
DE                     21.00
TE                     298.0
D1                2.00000000
D11               0.03000000
TDO                         1

======== CHANNEL f1 ===
NUC1                      13C
P1                      10.50
PL1                      2.80
PL1W             49.17097855
SFO1            150.9251891

======== CHANNEL f2 ===
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00
PL2                      0.33
PL12                    17.18
PL13                    20.18
PL2W             13.96854782
PL12W             0.28850359
PL13W             0.14459431
SFO2            600.1524006

F2 - Processing paramet
SI                      65536
SF              150.9076084
WDW                        EM
SSB          0
LB                      2.00
GB           0
PC                      1.00
```

^{1}H NMR spectrum of compound **25** (600 MHz, CD_3OD).



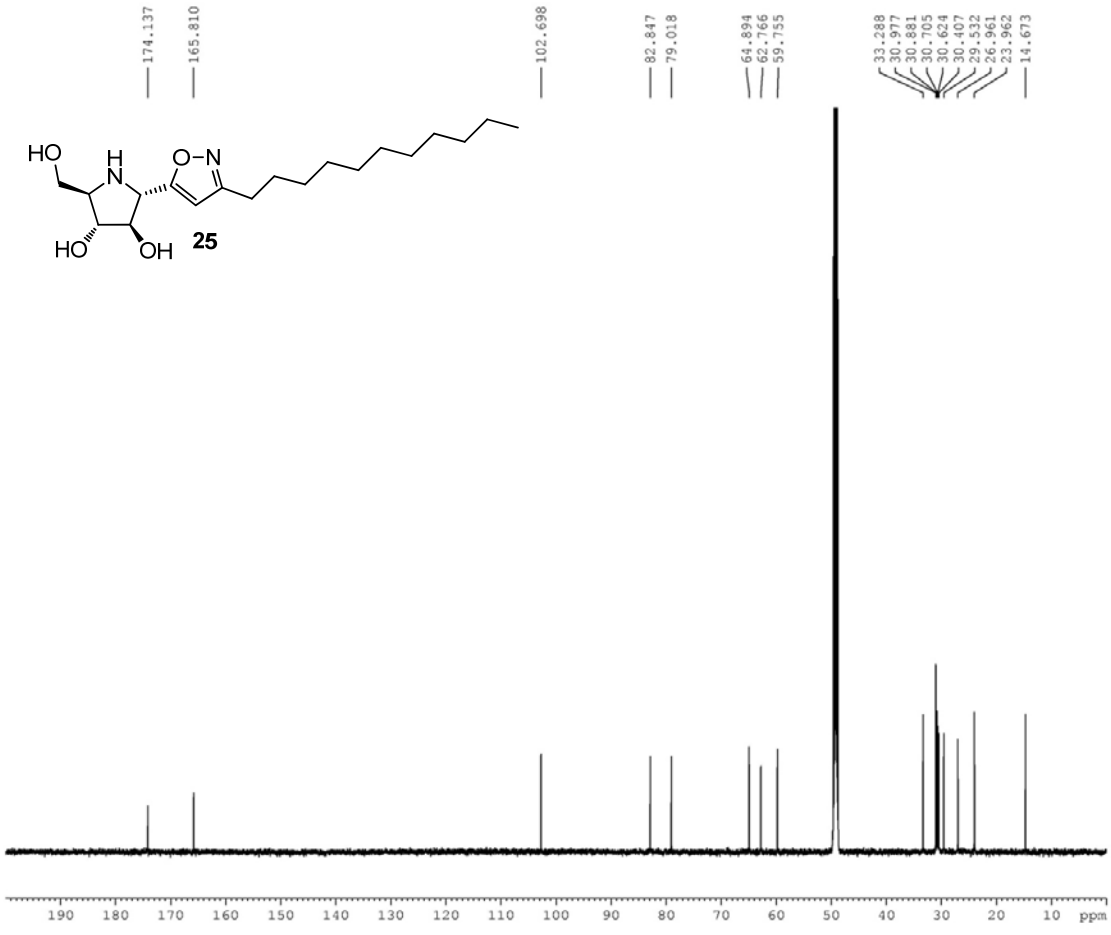
Current Data Parameter
NAME 2012021
EXPNO
PROCNO

F2 - Acquisition Paran
Date_ 2012021
Time 12.
INSTRUM spec
PROBHD 5 mm CPDCH 1
PULPROG zg
TD 327
SOLVENT MeC
NS
DS
SWH 8389.2
FIDRES 0.2560
AQ 1.9530
RG 45.
DW 59.6
DE 21.
TE 277.
D1 2.0000000
TD0

======== CHANNEL f1 ==
NUC1
P1 10.
PL1 -0.
PL1W 18.1197109
SFO1 600.1536

F2 - Processing parame
SI 163
SF 600.1500
WDW
SSB 0
LB 0 Hz
GB 0
PC 1.

^{13}C NMR spectrum of compound **25** (150 MHz, CD_3OD).



Current Data Parameters
NAME 20120210
EXPNO 2
PROCNO 1

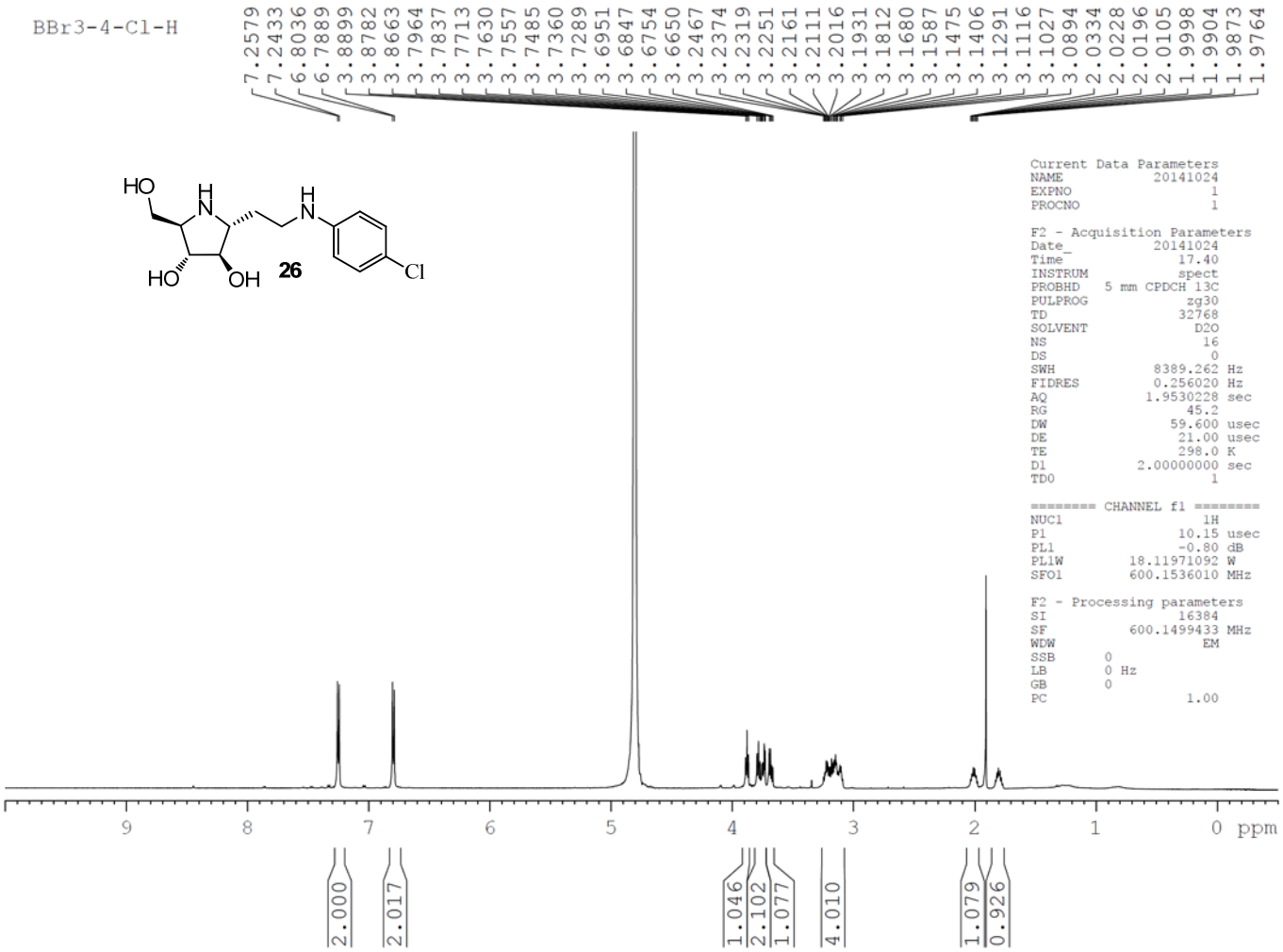
F2 - Acquisition Parame
Date_ 20120210
Time 12.56
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 131072
SOLVENT MeOD
NS 64
DS 0
SWH 39062.500
FIDRES 0.298023
AQ 1.6777716
RG 3640
DW 12.800
DE 21.00
TE 277.7
D1 2.00000000
D11 0.03000000
TD0 1

======== CHANNEL f1 ===
NUC1 13C
P1 10.50
PL1 2.80
PL1W 49.17097855
SFO1 150.9251891

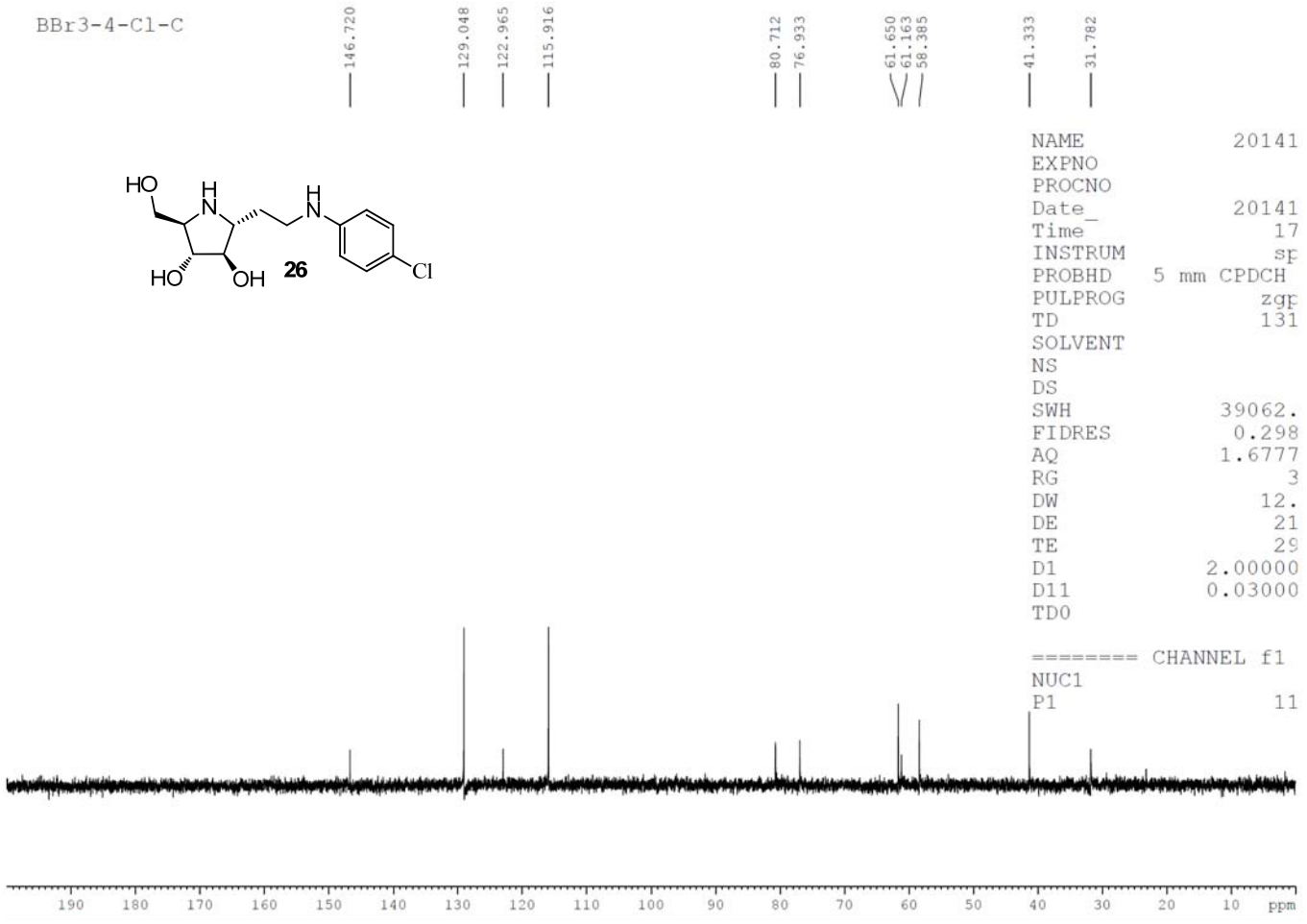
======== CHANNEL f2 ===
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00
PL2 0.33
PL12 17.18
PL13 20.18
PL2W 13.96854782
PL12W 0.28850359
PL13W 0.14459431
SFO2 600.1524006

F2 - Processing paramet
SI 65536
SF 150.9076092
WDW EM
SSB 0
LB 2.00
GB 0
PC 1.00

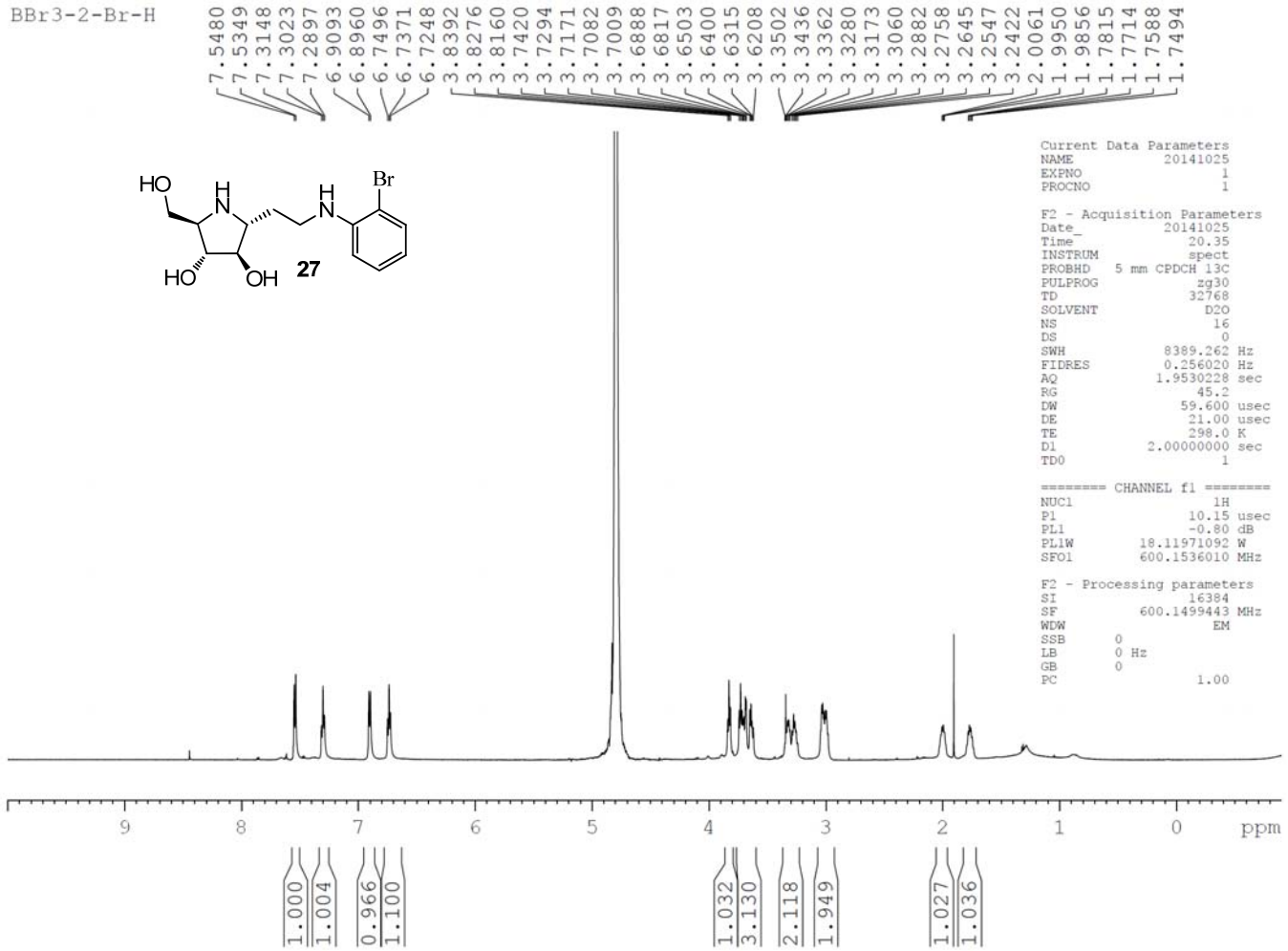
^{1}H NMR spectrum of compound **26** (600 MHz, D_2O).



^{13}C NMR spectrum of compound **26** (150 MHz, D_2O).



^{1}H NMR spectrum of compound **27** (600 MHz, D_2O).



^{13}C NMR spectrum of compound **27** (150 MHz, D_2O).