Supplementary Materials

Synthesis and evaluation of (1,4-disubstituted)-1,2,3-triazoles as estrogen receptor beta agonists

Edward A. Wetzel, Grace C. Corriero, Sandra Brown-Ford, Daniel S. Sem, and William A. Donaldson

Figure S1. ERβ TR-FRET displacement assay data
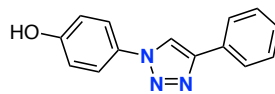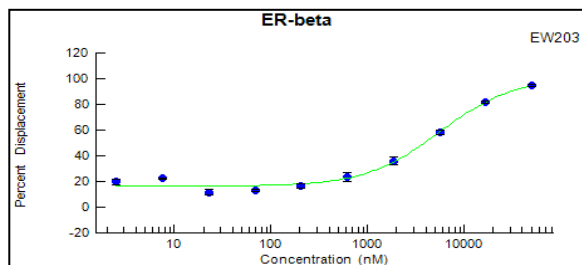
5   EC_{50} = 5.53 μM
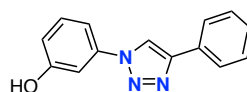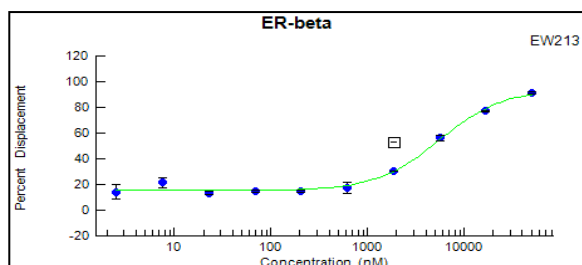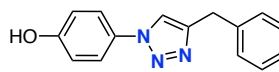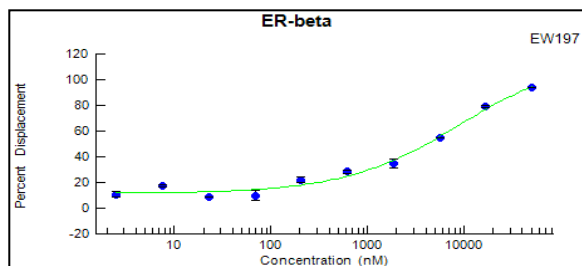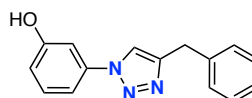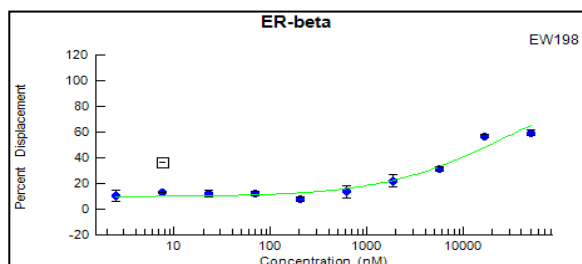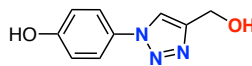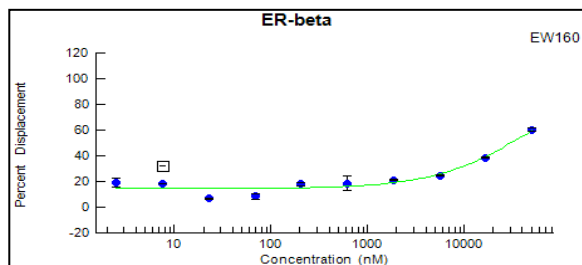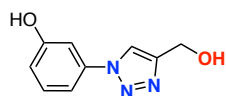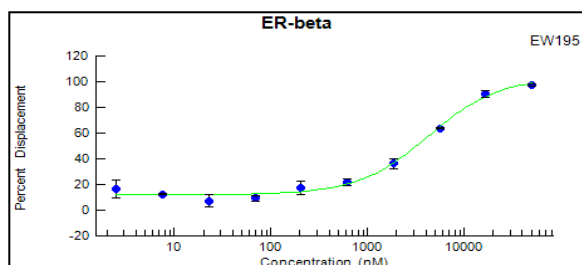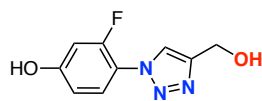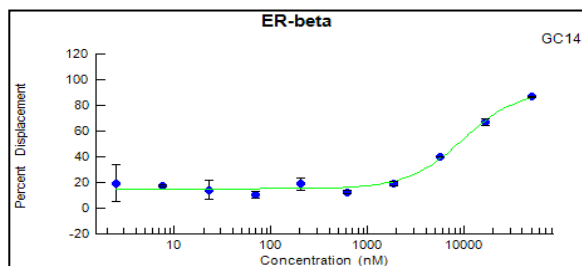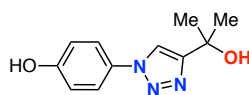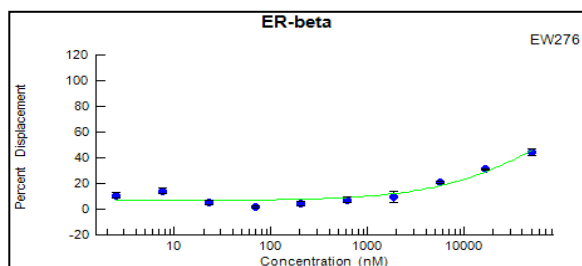
6   EC_{50} = 5.51 μM

7   EC_{50} = 9.04 μM

8   EC_{50} = 25.8 μM

9   EC_{50} = 44.6 μM

10 EC$_{50}$ = 4.28 μM

11 EC$_{50}$ = 9.69 μM

12 EC$_{50}$ = >50 μM

13 EC$_{50}$ = 9.15 μM

14 EC$_{50}$ = 48.1 μM

16 EC$_{50}$ = 18.2 μM

17 EC_{50} = >50 μM

18 EC_{50} = 18.2 μM

19 EC_{50} = >50 μM

(±)-**20** EC_{50} = 13.6 μM

(±)-**21** EC_{50} = 1.59 μM

SpinWorks 4: SC

¹H NMR
(400 MHz, CD₃OD)

5

2.039

1.008
2.101

2.082

2.071

1.000

PPM 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4
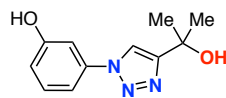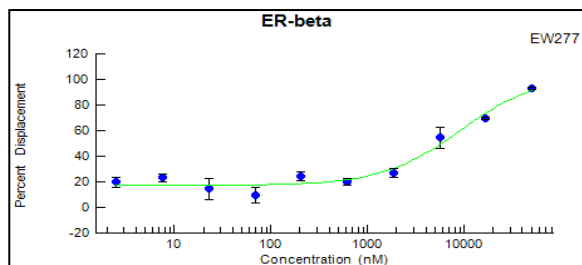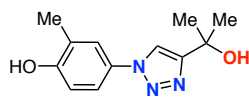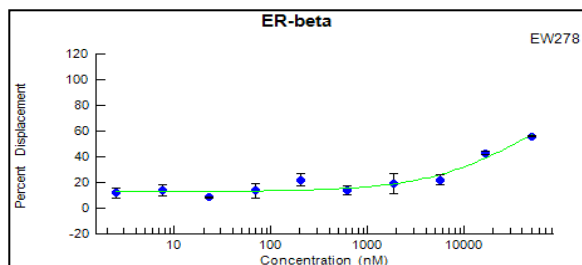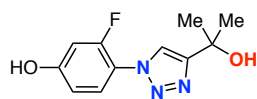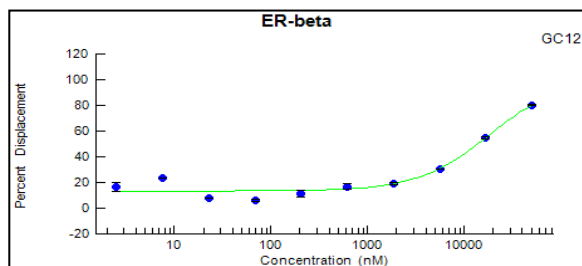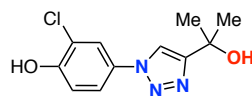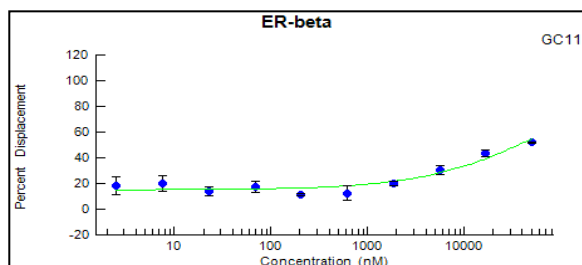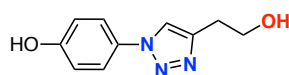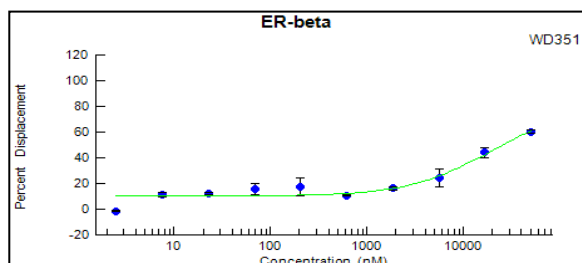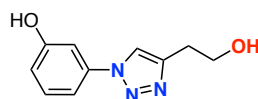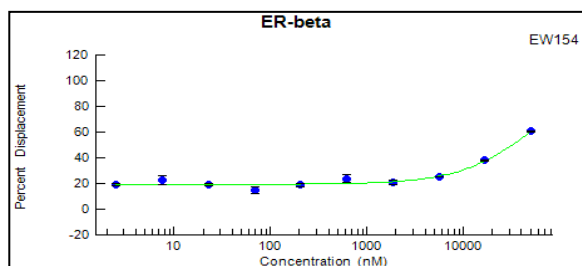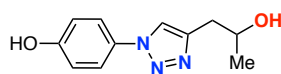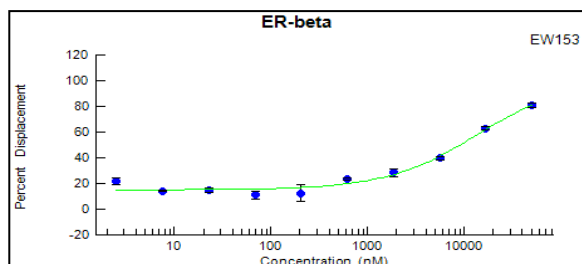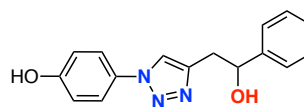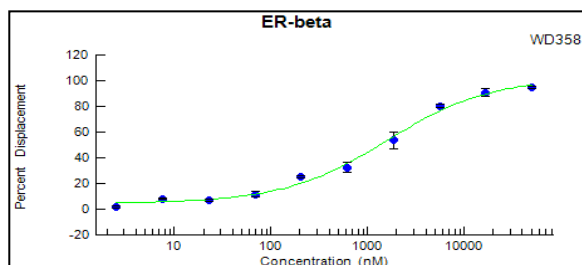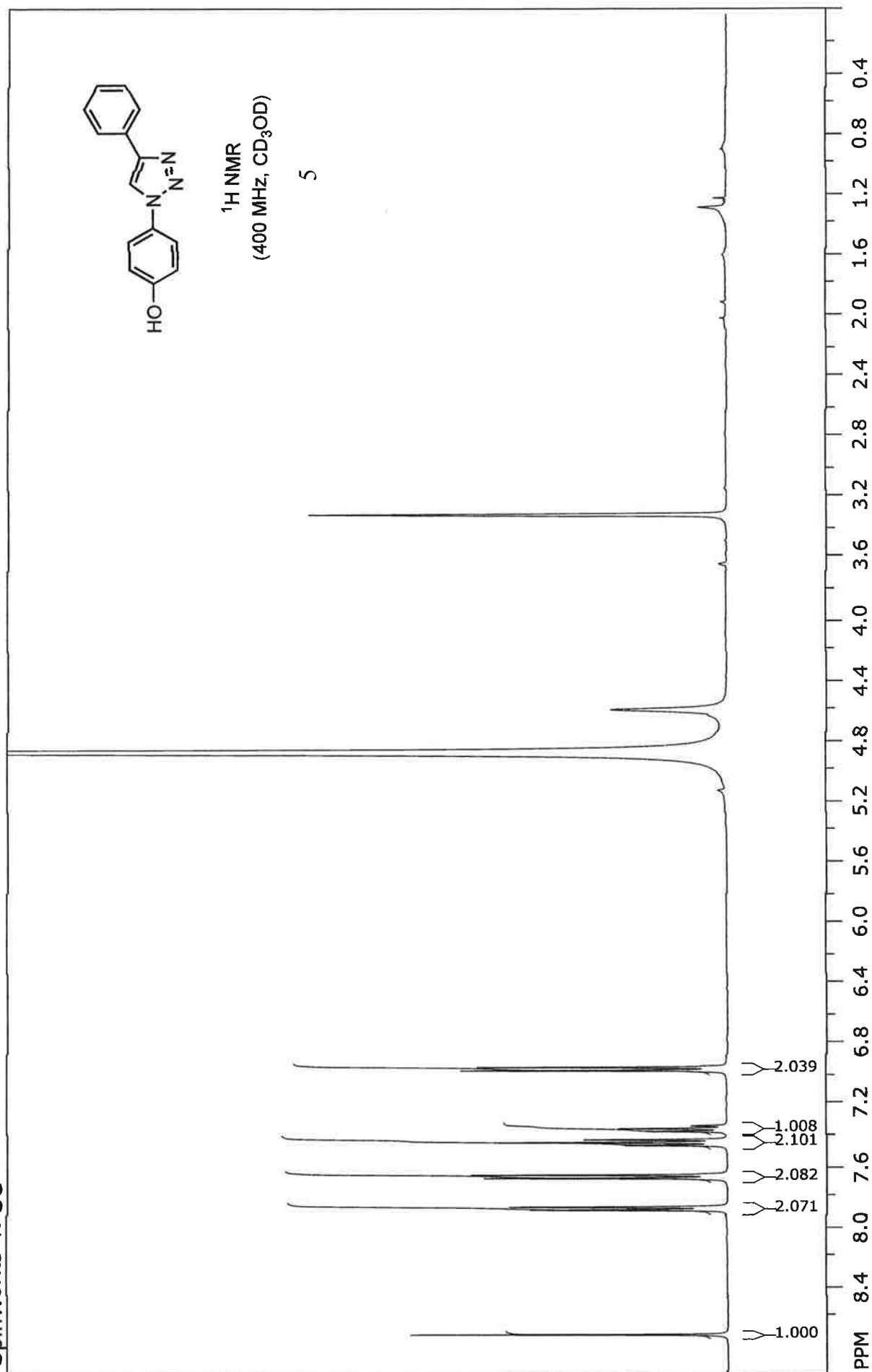
file: ...\Desktop\EAW-203-H-MeOH-d4.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.731815 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729414 MHz
processed size: 32768 complex points
LB: 0.500   GF: 0.0000
Hz/cm: 143.875   ppm/cm: 0.35993

SpinWorks 4: asdf1
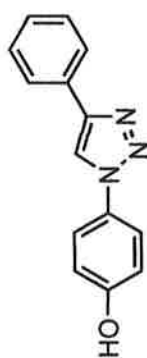
¹H NMR

(400 MHz, d₆-acetone)

5

2.002
1.000
1.998
2.002
2.028
0.981
0.809

PPM   9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

SpinWorks 4: adsf2

13C NMR

(100 MHz, d6-acetone)

5

116.991
119.580
122.890
126.338
128.844
129.681
130.764
131.910

148.447

158.684

PPM 185 175 165 155 145 135 125 115 105 95 85 75 65 55 45 35 25 15 5

file: ...nds\1_14_18_FirstNMRCARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.524207 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6963 ppm = 0.381470 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.513061 MHz
processed size: 65536 complex points
LB: 1.500 GF: 0.0000
Hz/cm: 803.371 ppm/cm: 7.99181

SpinWorks 4: STANDARD 1H OBSERVE - profile

¹H NMR
(400 MHz, CD₃OD)

6

0.933
4.026
1.999
1.951
0.925

PPM 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

file: ...riazole Compounds\EAW204-H.fid\fid block# 1 expt: "s2pul"

transmitter freq.: 399.731815 MHz

time domain size: 32768 points

width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt

number of scans: 8

freq. of 0 ppm: 399.729414 MHz

processed size: 32768 complex points

LB: 0.561   GF: 0.0000

Hz/cm: 151.852   ppm/cm: 0.37988

SpinWorks 4: 13C OBSERVE

^{13}C NMR

(75 MHz, d$_6$-DMSO)

6

107.040 ——
110.465 ——

115.760 ——

119.607 —

125.426
128.300
129.050
130.325
130.879

137.703 ——

147.294 ——

158.582 ——

PPM   160   150   140   130   120   110   100   90   80   70   60   50   40   30   20   10

file: ...unds\12_7_18_EAW418_Carbon.fid\fid block# 1   expt: "s2pul"
transmitter freq.: 75.476694 MHz
time domain size: 68492 points
width: 18867.92 Hz = 249.9835 ppm = 0.275476 Hz/pt
number of scans: 256

freq. of 0 ppm: 75.468438 MHz
processed size: 131072 complex points
LB: 1.500   GF: 0.0000
Hz/cm: 543.396   ppm/cm: 7.19952

SpinWorks 4: ghkj1111

^{1}H NMR
(400 MHz, d$_6$-acetone)

7

2.000
1.001
4.025
2.175
0.944
1.914

PPM 9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

file: ..._15_18_Naphthalenecompound.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.736224 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0362 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.733819 MHz
processed size: 32768 complex points
LB: 1.500   GF: 0.0000
Hz/cm: 159.829   ppm/cm: 0.39984

SpinWorks 4: asdfqwer

^{13}C NMR
(75 MHz, d$_6$-acetone)

7

32.435

116.893
121.060
122.703
127.056
129.203
129.260
129.454
130.755
140.417
158.500

PPM   160   150   140   130   120   110   100   90   80   70   60   50   40   30   20   10

file: ..._NaphthalenecompoundCARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.524207 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6963 ppm = 0.381470 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.513066 MHz
processed size: 65536 complex points
LB: 1.550   GF: 0.0000
Hz/cm: 723.889   ppm/cm: 7.20114

SpinWorks 4: SC

'H NMR

(400 MHz, d$_6$-DMSO)

8

2.024

1.033

8.054

1.000

file: ...naldsonw\Desktop\EAW-198-H.fid\fid block# 1 expt: "s2pul"

transmitter freq.: 399.732139 MHz

time domain size: 32768 points

width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt

number of scans: 8

freq. of 0 ppm: 399.729735 MHz

processed size: 32768 complex points

LB: 0.500   GF: 0.0000

Hz/cm: 143.875   ppm/cm: 0.35993

PPM 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

SpinWorks 4: STANDARD 1H OBSERVE

^{1}H NMR
(300 MHz, CD$_3$OD)
8

1.999

0.950

8.544

0.838

PPM   0.4 0.8 1.2 1.6 2.0 2.4 2.8 3.2 3.6 4.0 4.4 4.8 5.2 5.6 6.0 6.4 6.8 7.2 7.6

file: ...azole Compounds\1_18_18_2W.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 300.134191 MHz
time domain size: 19192 points
width: 4803.07 Hz = 16.0031 ppm = 0.250264 Hz/pt
number of scans: 8

freq. of 0 ppm: 300.132388 MHz
processed size: 32768 complex points
LB: 1.500   GF: 0.0000
Hz/cm: 102.039   ppm/cm: 0.33998

SpinWorks 4: SC

^{13}C NMR
(100 MHz, d$_6$-DMSO

8

31.220

106.842
110.273

115.429

120.712

126.254
128.469
128.560
130.711

137.746
139.329

147.036

158.467

PPM 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160

file: ...dsonw\Desktop\EAW-198-C-II.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523180 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6989 ppm = 0.381470 Hz/pt
number of scans: 10000

freq. of 0 ppm: 100.512165 MHz
processed size: 65536 complex points
LB: 1.500   GF: 0.0000
Hz/cm: 723.889   ppm/cm: 7.20121

SpinWorks 4: 11_2_18_BlackCap

^{1}H NMR

(400 MHz, CD$_3$OD)

9

2.179

2.079

2.071

1.000

PPM   8.4   8.0   7.6   7.2   6.8   6.4   6.0   5.6   5.2   4.8   4.4   4.0   3.6   3.2   2.8   2.4   2.0   1.6   1.2   0.8   0.4
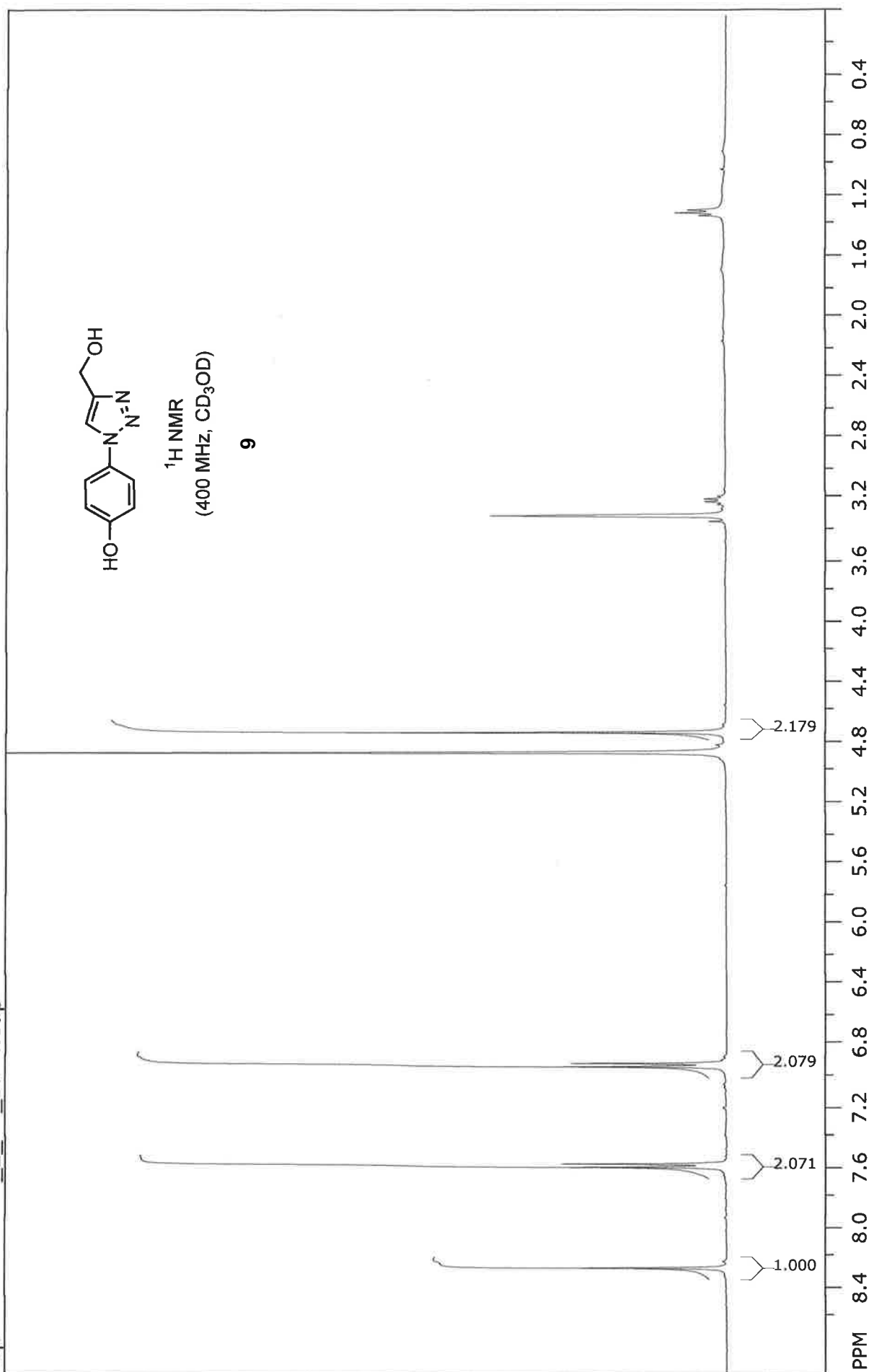
file: ...Compounds\11_2_18_blackCap.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.735724 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0362 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.733317 MHz
processed size: 32768 complex points
LB: 1.500   GF: 0.0000
Hz/cm: 143.875   ppm/cm: 0.35992

SpinWorks 4: 12_18_17_4-azidophenol_propargylalcoholCARBON

56.081

^{13}C NMR
(100 MHz, d$_6$-acetone)

9

116.782
121.448
122.751
130.282
158.683

PPM   10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160

file: ...nol_propargylalcoholCARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.524163 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6964 ppm = 0.381470 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.513072 MHz
processed size: 65536 complex points
LB: 2.500   GF: 0.0000
Hz/cm: 723.333   ppm/cm: 7.19562

SpinWorks 4: SC

^{1}H NMR
(400 MHz, CD$_3$OD)

10

2.088

1.075

2.095
1.144

0.999

PPM   8.4   8.0   7.6   7.2   6.8   6.4   6.0   5.6   5.2   4.8   4.4   4.0   3.6   3.2   2.8   2.4   2.0   1.6   1.2   0.8   0.4

file: ...naldsonw\Desktop\EAW-195-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.731815 MHz
time domain size: 32768 points
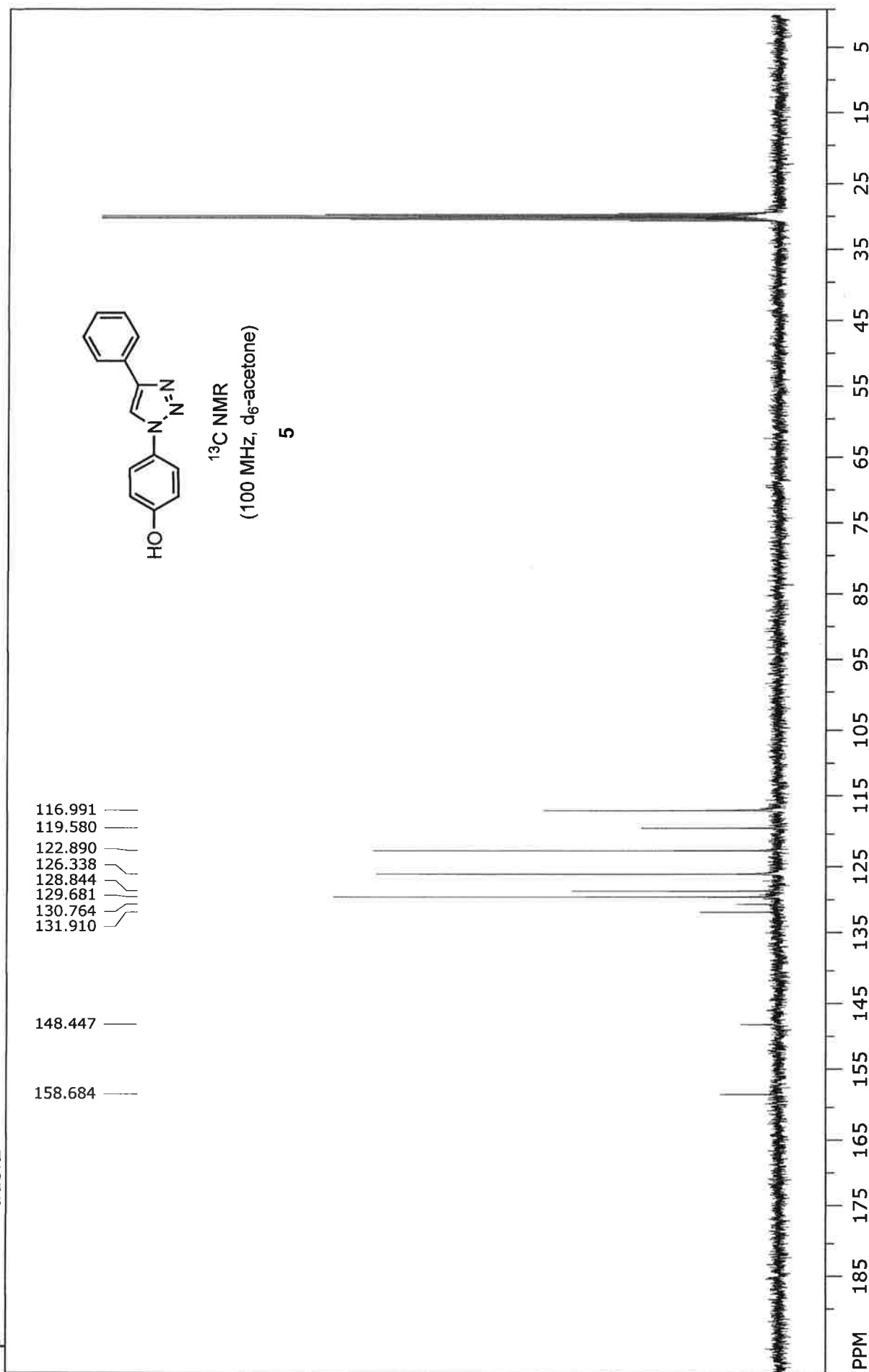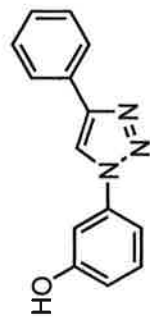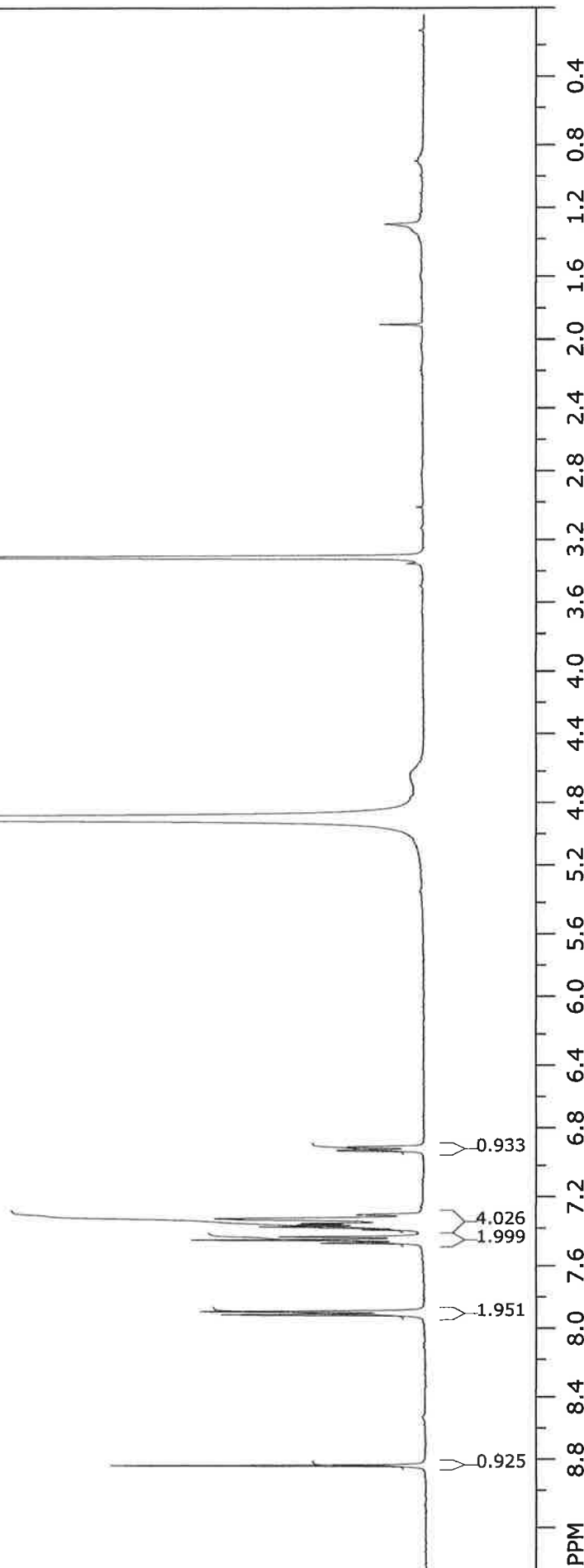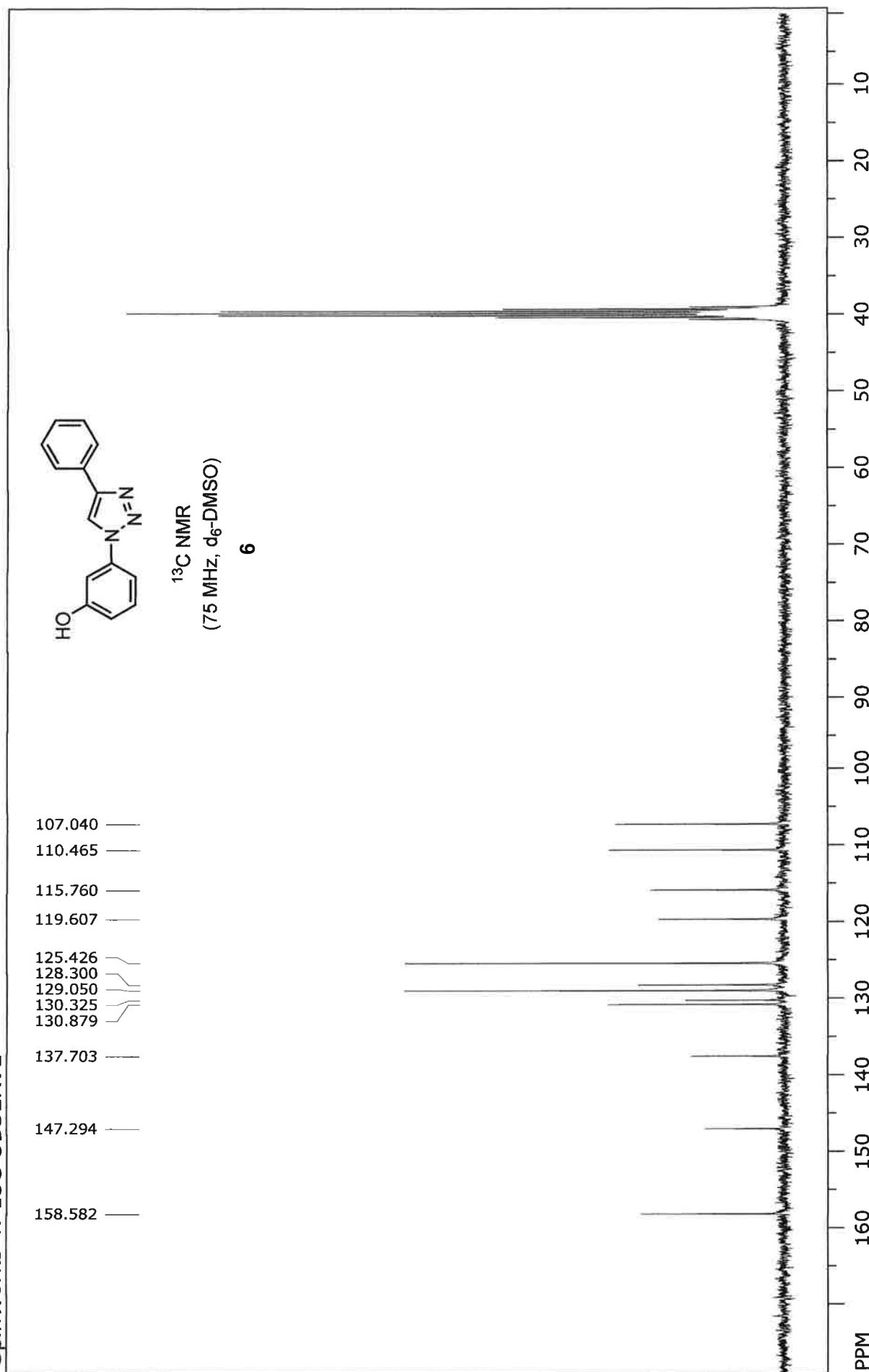width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729415 MHz
processed size: 32768 complex points
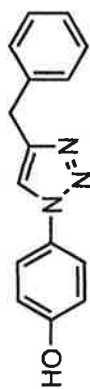LB: 0.500   GF: 0.0000
Hz/cm: 143.875   ppm/cm: 0.35993

SpinWorks 4: 13C OBSERVE

^{13}C NMR

(75 MHz, d$_6$-DMSO)

10

158.517 ——
149.029 ——
137.818 ——
130.848 ——
121.043 ——
115.552 ——
110.448 ——
106.980 ——

54.986 ——

PPM   160   150   140   130   120   110   100   90   80   70   60   50   40   30   20   10

file: ...unds\12_7_18_EAW416_Carbon.fid\fid   block# 1   expt: "s2pul"
transmitter freq.: 75.476694 MHz
time domain size: 68492 points
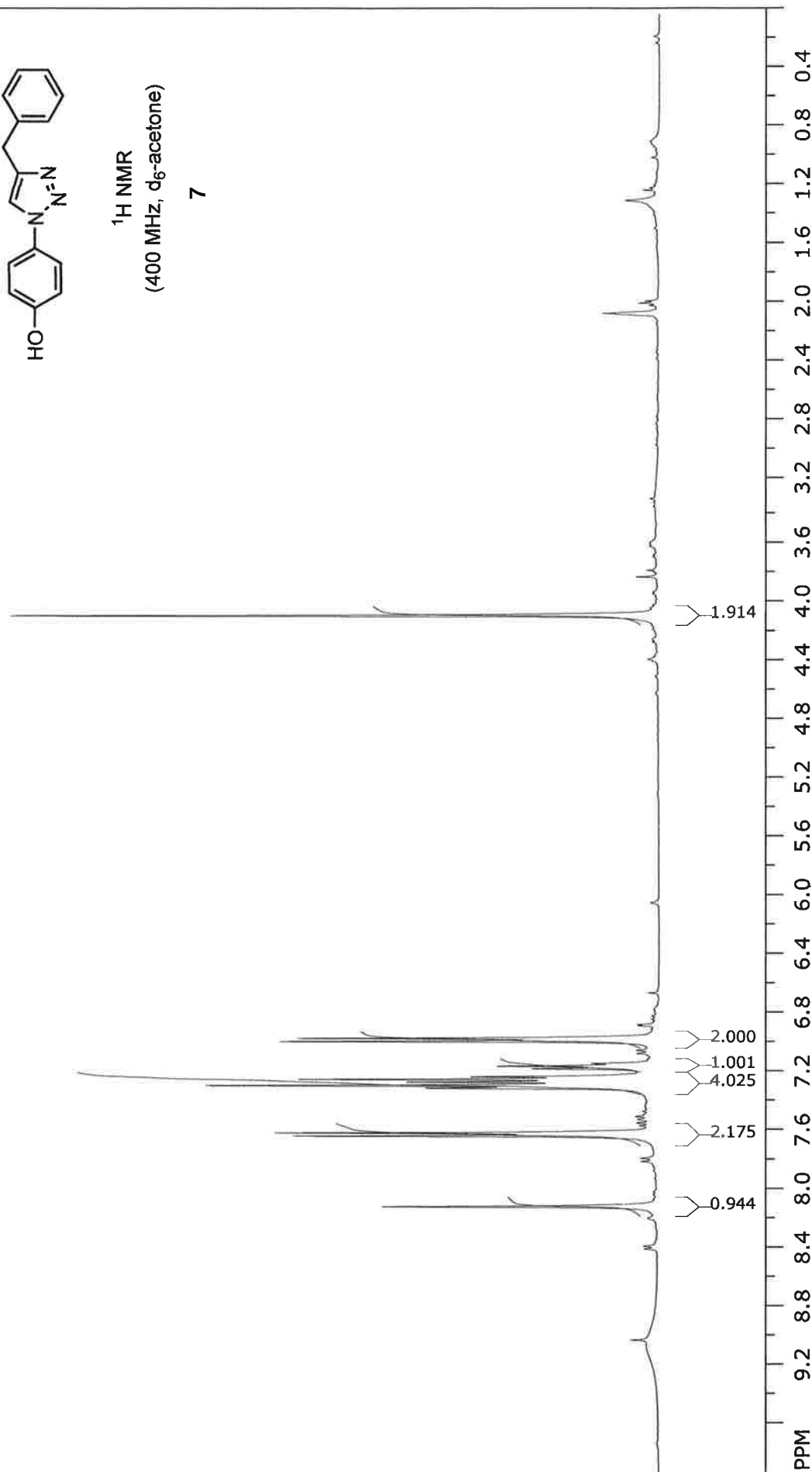width: 18867.92 Hz = 249.9835 ppm = 0.275476 Hz/pt
number of scans: 256

freq. of 0 ppm: 75.468436 MHz
processed size: 131072 complex points
LB: 1.500   GF: 0.0000
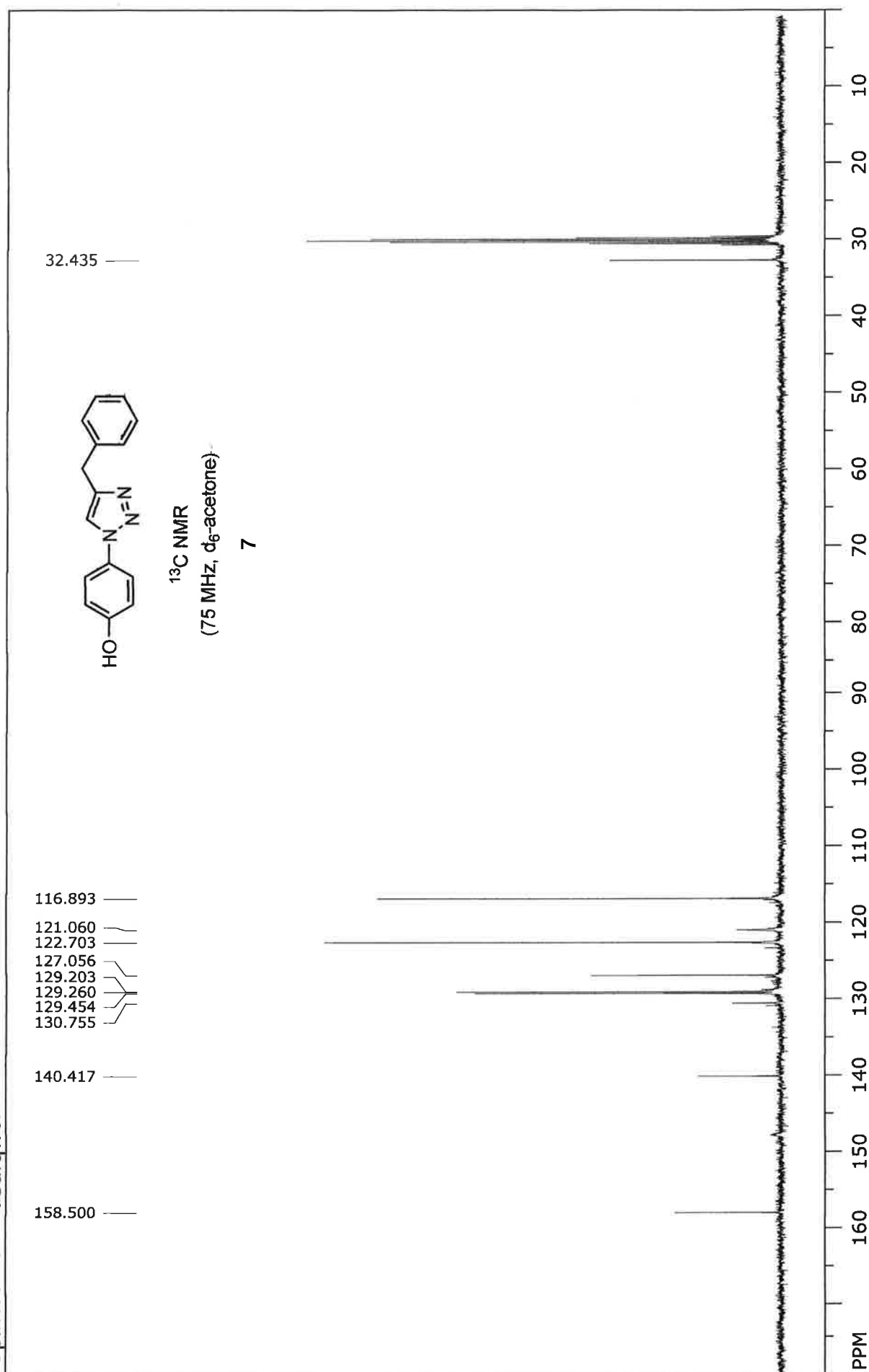Hz/cm: 543.396   ppm/cm: 7.19952
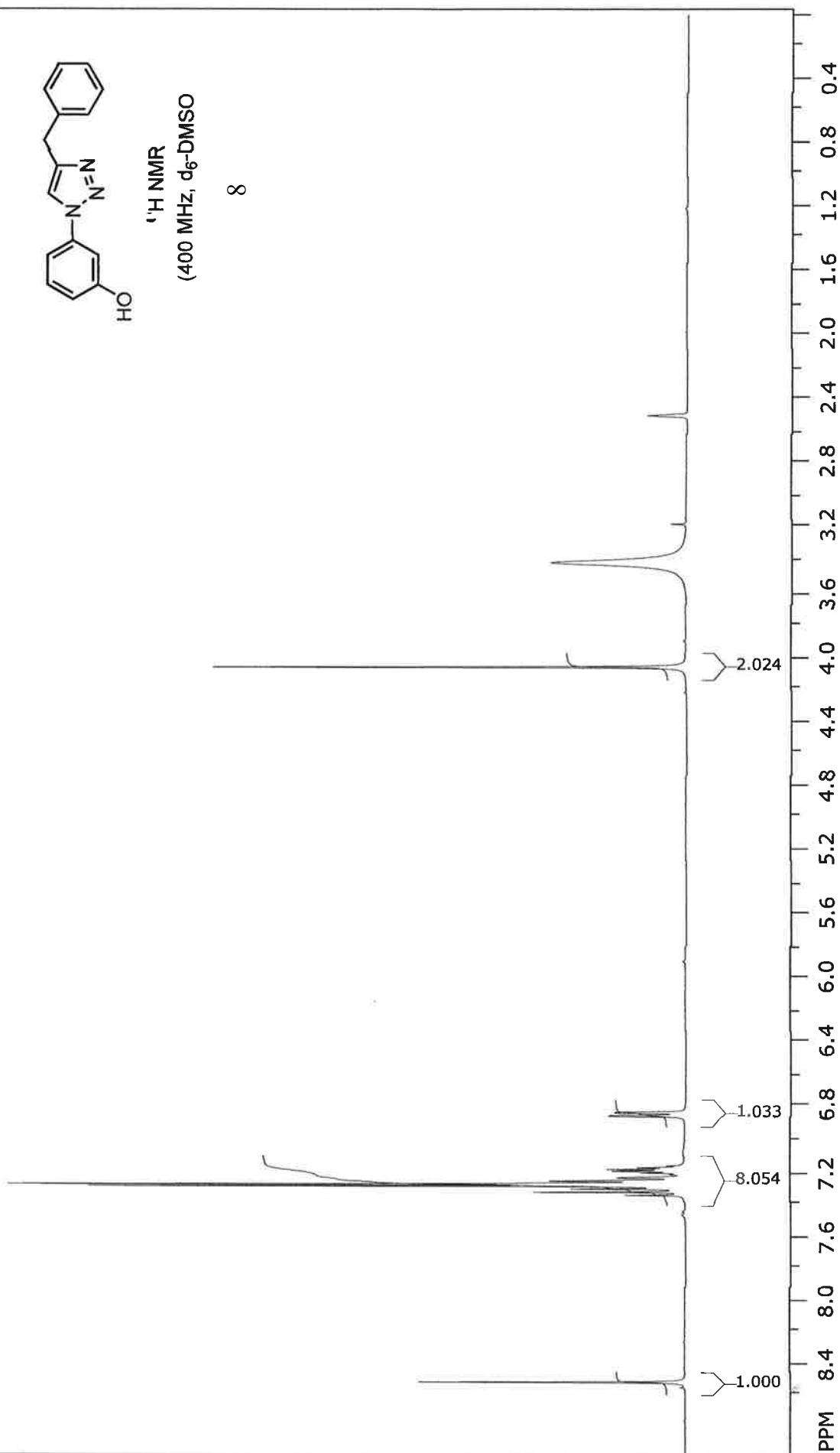
SpinWorks 4: 4_16_18_GCC13

^{1}H NMR
(400 MHz, CD$_3$OD)

11

2.284

2.114

1.072

1.000

PPM

0.4 0.8 1.2 1.6 2.0 2.4 2.8 3.2 3.6 4.0 4.4 4.8 5.2 5.6 6.0 6.4 7.2 7.6

file: ...le Compounds\4_16_18_GCC13.fid\fid block# 1 expt: "s2pul"
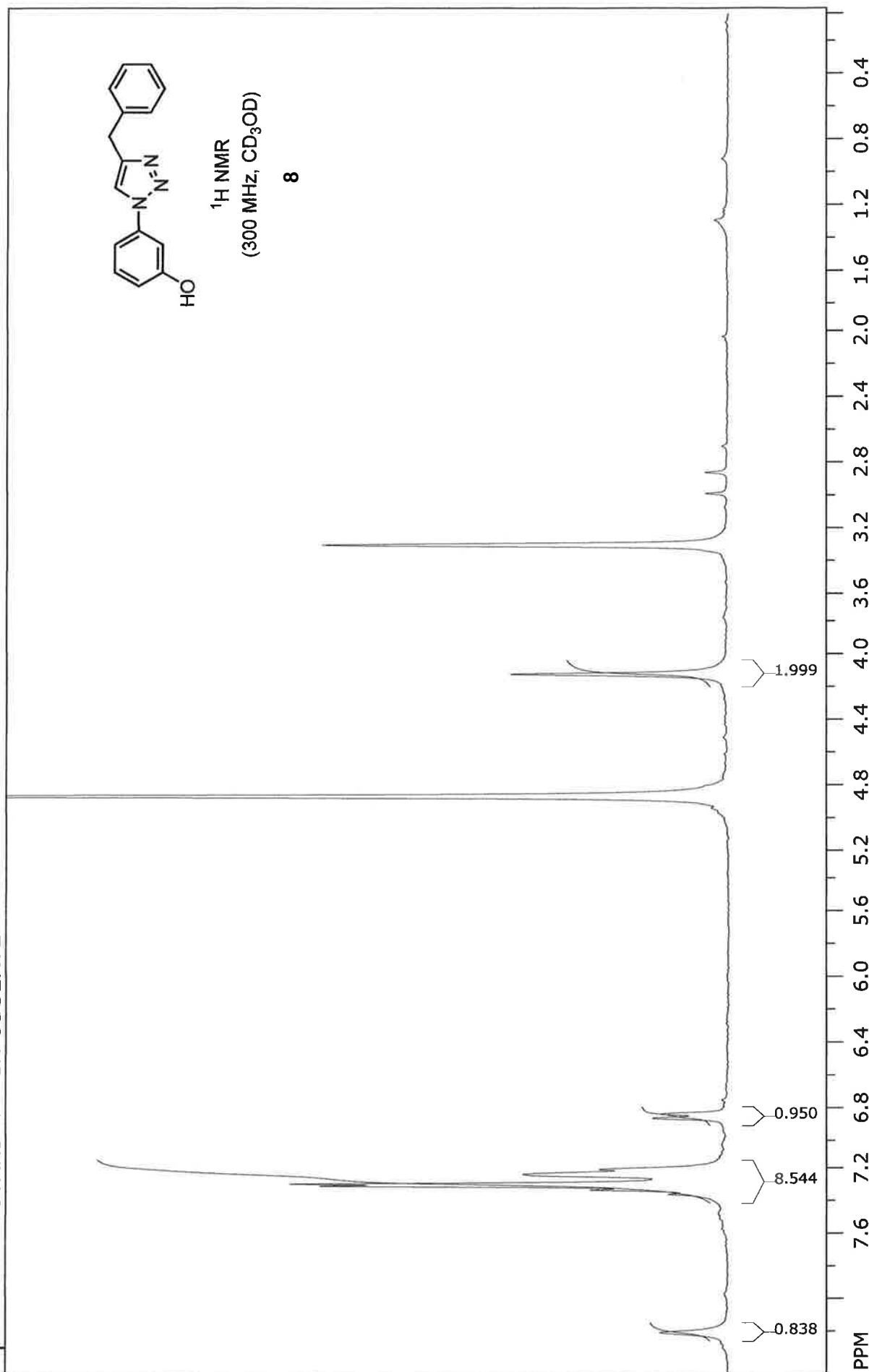transmitter freq.: 399.735724 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0362 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.733315 MHz
processed size: 32768 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 135.897 ppm/cm: 0.33997

SpinWorks 4: 4_16_18_Gcc13CARBON

^{13}C NMR

(100 MHz, CD$_3$OD)

11

56.317

104.451
104.671

113.040
113.067

118.040
118.156

125.494
125.536
127.584

149.051

155.341
157.824

161.276
161.387

PPM 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

file: ...pounds\4_16_18_GCC13CARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.524081 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6966 ppm = 0.381470 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.512889 MHz
processed size: 65536 complex points
LB: 1.500   GF: 0.0000
Hz/cm: 723.889   ppm/cm: 7.20115

SpinWorks 4: SC

^{19}F NMR
(376 MHz, CD$_3$OD)

11

-125.354

PPM -88 -92 -96 -100 -104 -108 -112 -116 -120 -124 -128 -132 -136 -140 -144 -148 -152 -156

file: ...naldsonw\Desktop\Gcc-014-F.fid\fid\fid block# 1 expt: "s2pul"
transmitter freq.: 376.089471 MHz
time domain size: 131072 points
width: 89285.71 Hz = 237.4055 ppm = 0.681196 Hz/pt
number of scans: 16

freq. of 0 ppm: 376.121730 MHz
processed size: 131072 complex points
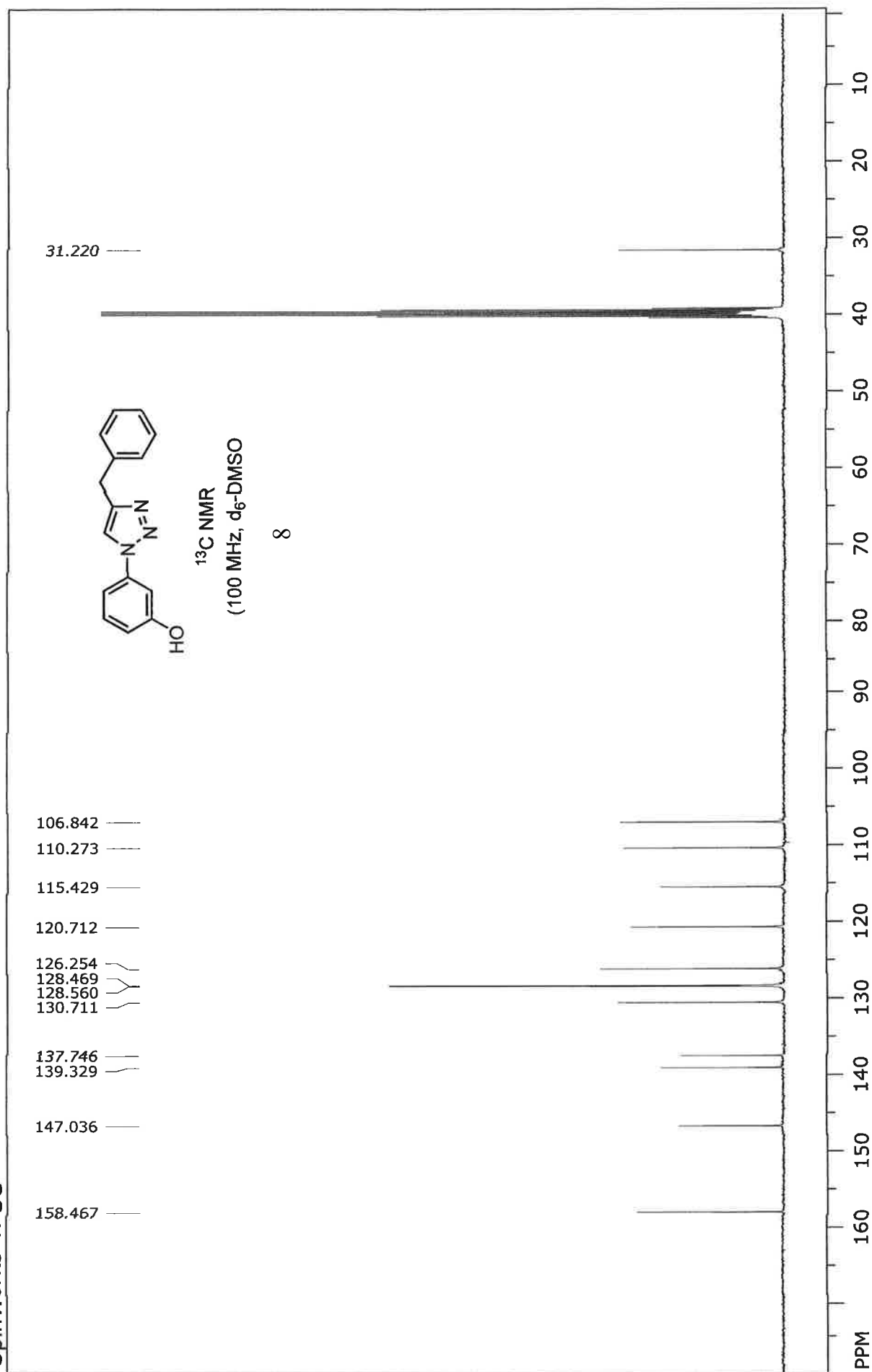LB: 3.000   GF: 0.0000
Hz/cm: 1204.365   ppm/cm: 3.20234

SpinWorks 4: 3_26_18_clickether

Me Me
OH

^{1}H NMR
(400 MHz, CD$_3$OD)

12

6.254

1.961

2.000

0.946

PPM   0.4 0.8 1.2 1.6 2.0 2.4 2.8 3.2 3.6 4.0 4.4 4.8 5.2 5.6 6.0 6.4 6.8 7.2 7.6

file: ...mpounds\3_26_18_clickether.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.735724 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0362 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.733316 MHz
processed size: 32768 complex points
LB: 1.500   GF: 0.0000
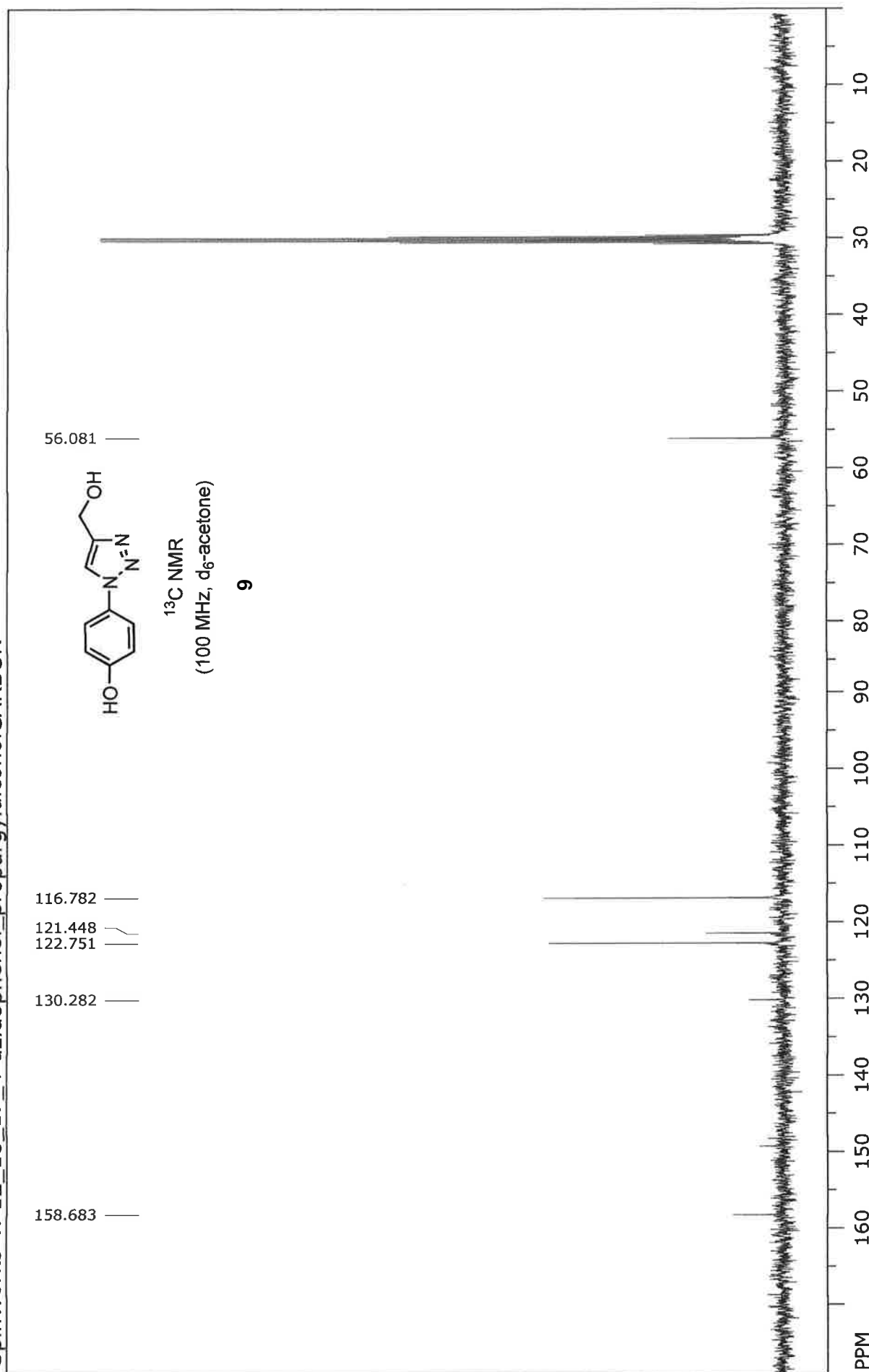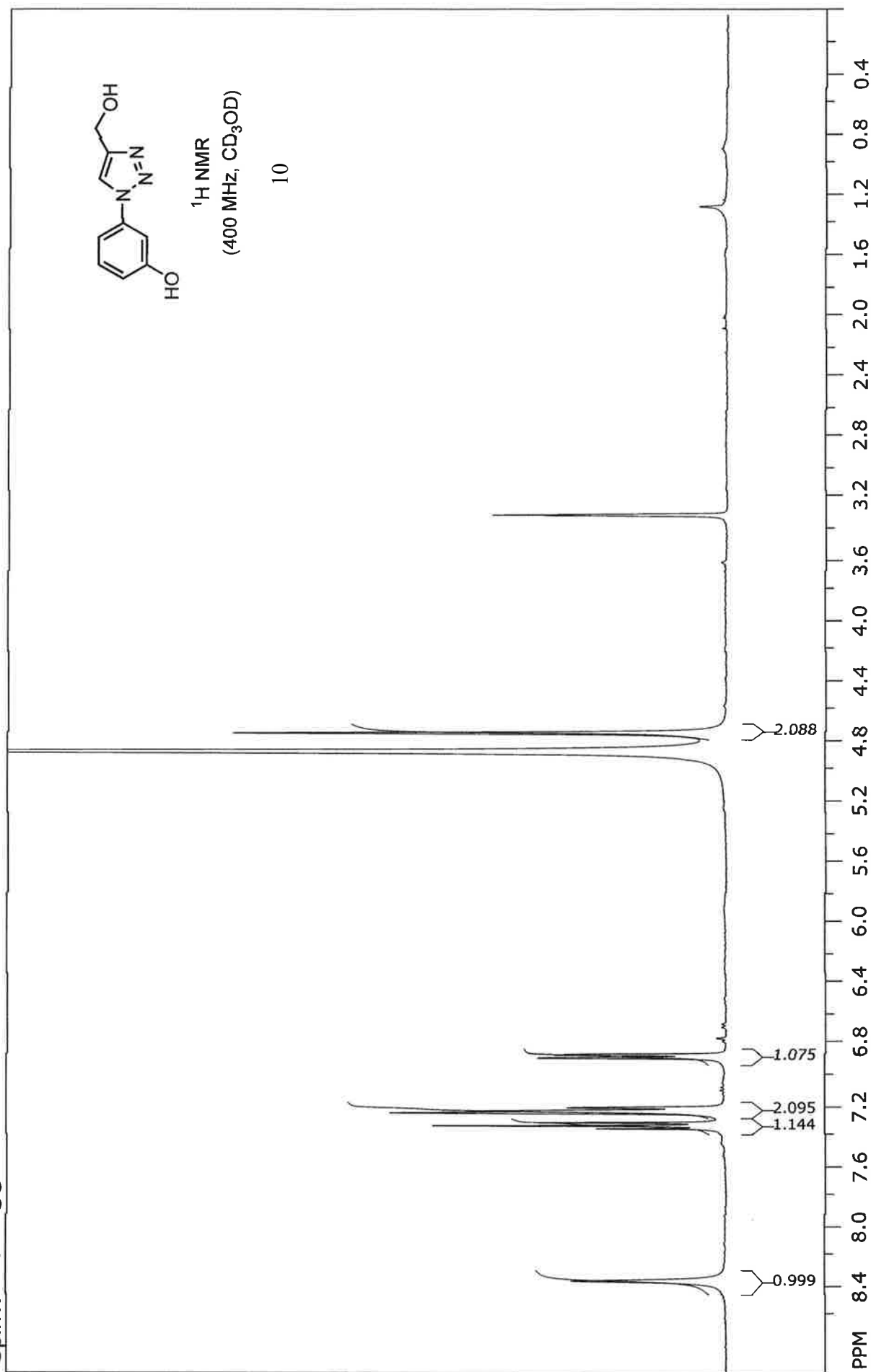Hz/cm: 135.897   ppm/cm: 0.33997

SpinWorks 4: 3_26_18_clicketherCARBON

30.620 ——

69.060 ——

117.104 ——
120.184 ——
123.363 ——

130.755 ——

157.539 ——
159.468 ——

^{13}C NMR
(100 MHz, CD$_3$OD)

12

PPM   10   20   30   40   50   60   70   80   90   100   110   120   130   140   150   160

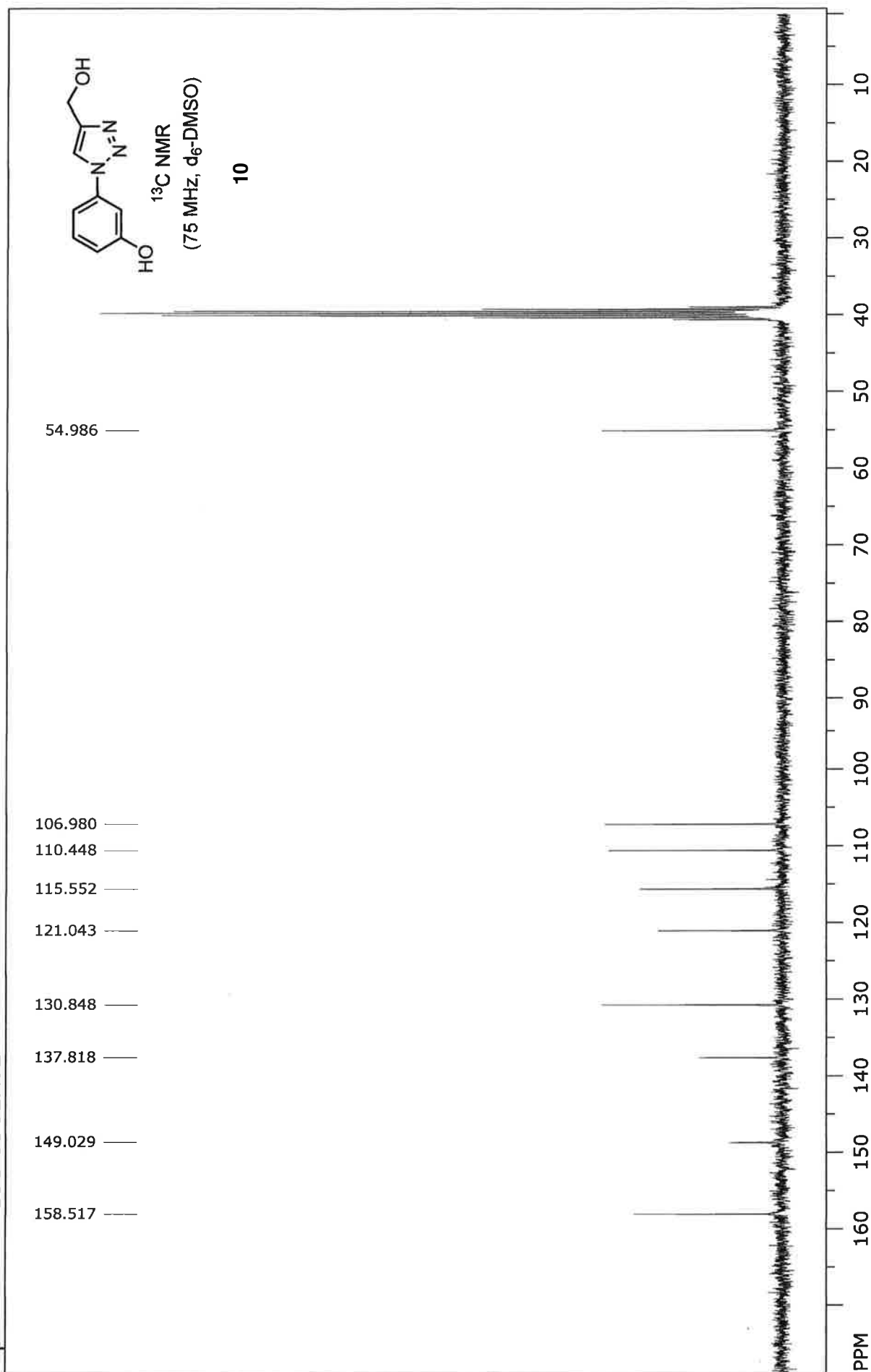file: ...s\3_26_18_clicketherCARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.524081 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6966 ppm = 0.381470 Hz/pt
number of scans: 256

freq. of 0 ppm: 100.512882 MHz
processed size: 65536 complex points
LB: 2.500   GF: 0.0000
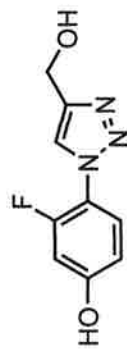Hz/cm: 723.333   ppm/cm: 7.19562

SpinWorks 4: STANDARD 1H OBSERVE

^{1}H NMR

(300 MHz, CD$_3$OD)

13

6.358

0.979

1.000

0.953

0.975

PPM 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

file: ...e Compounds\4_5_18_Sample1.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 300.134191 MHz
time domain size: 19192 points
width: 4803.07 Hz = 16.0031 ppm = 0.250264 Hz/pt
number of scans: 8

freq. of 0 ppm: 300.132388 MHz
processed size: 32768 complex points
LB: 1.500   GF: 0.0000
Hz/cm: 108.123   ppm/cm: 0.36025
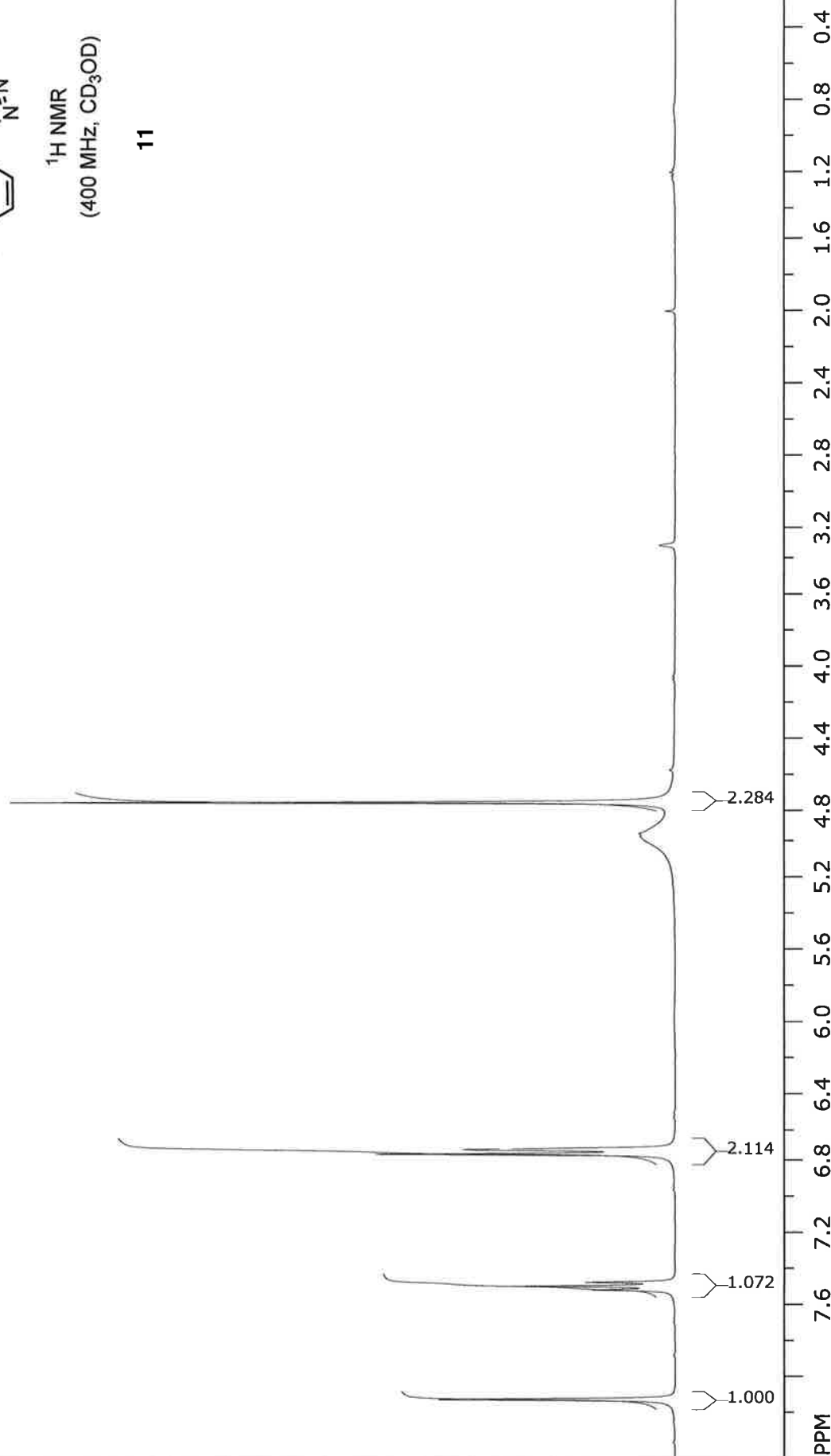
SpinWorks 4: 13C OBSERVE

30.570
31.115

69.021

118.037
120.059
120.155
121.429
122.485
123.498

131.038

155.115
157.653
157.686
157.728

^{13}C NMR
(75 MHz, CD$_3$OD)

13

Me Me
OH

HO

PPM   10   20   30   40   50   60   70   80   90   100   110   120   130   140   150   160
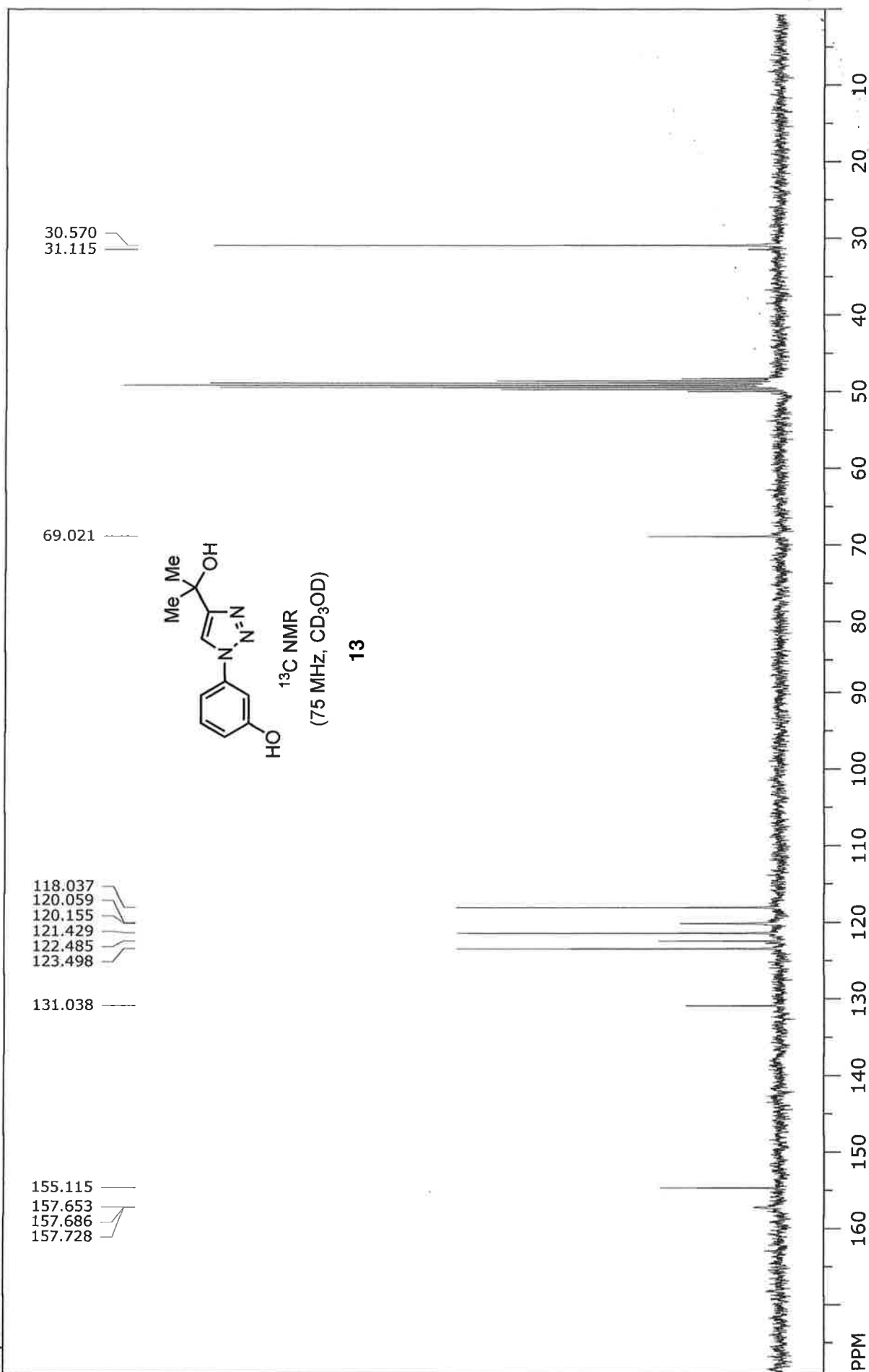
file: ...ounds\4_5_18_sample1CARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 75.476633 MHz
time domain size: 68492 points
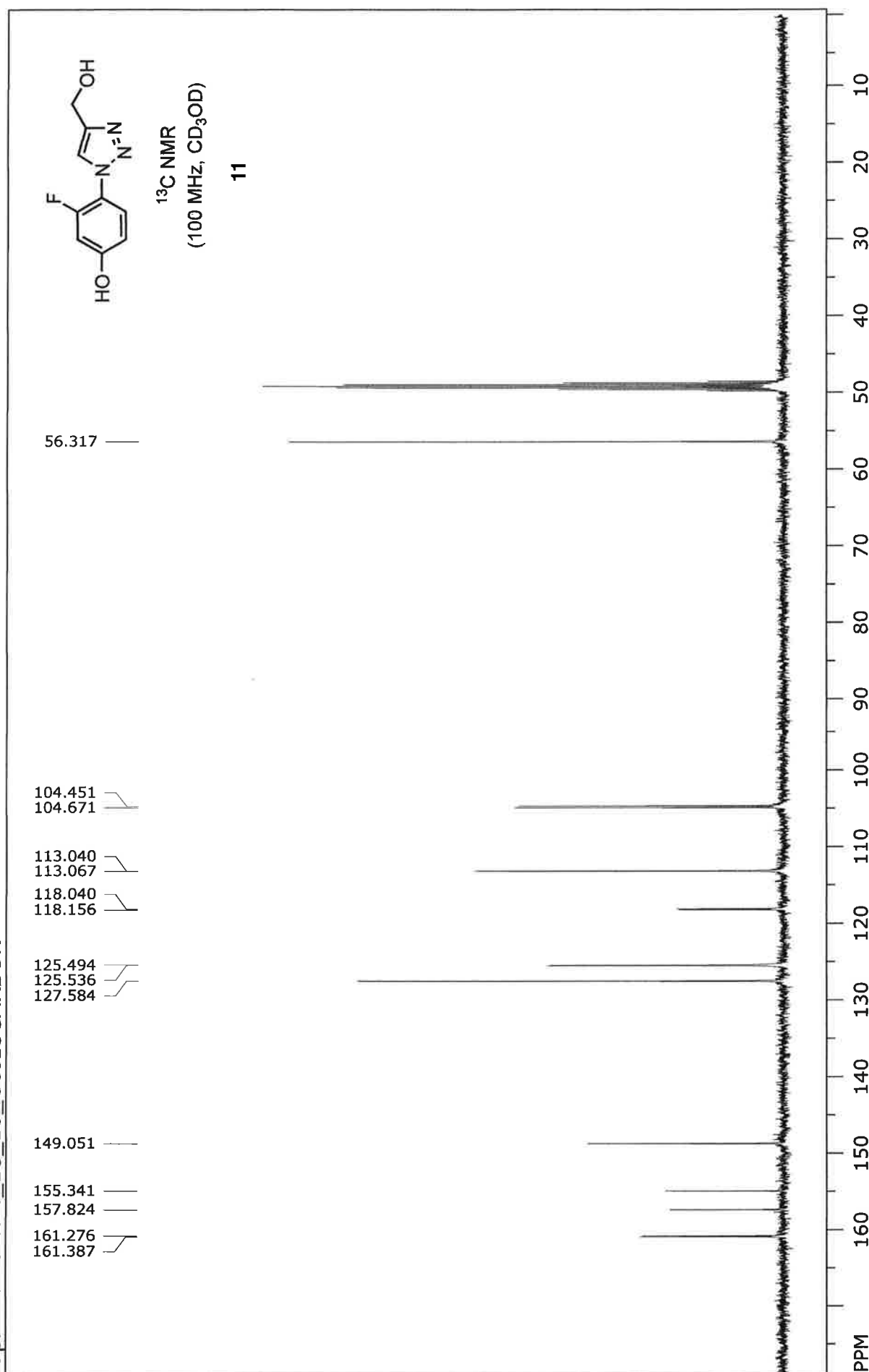width: 18867.92 Hz = 249.9837 ppm = 0.275476 Hz/pt
number of scans: 64

freq. of 0 ppm: 75.468245 MHz
processed size: 131072 complex points
LB: 2.000   GF: 0.0000
Hz/cm: 543.396   ppm/cm: 7.19953

SpinWorks 4: 11_7_18_EAW278_Carbon

^{1}H NMR
(400 MHz, CD$_3$OD)

14

6.111

3.015

0.999

0.986
1.007

0.826

PPM   7.6   7.2   6.8   6.4   6.0   5.6   5.2   4.8   4.4   4.0   3.6   3.2   2.8   2.4   2.0   1.6   1.2   0.8   0.4
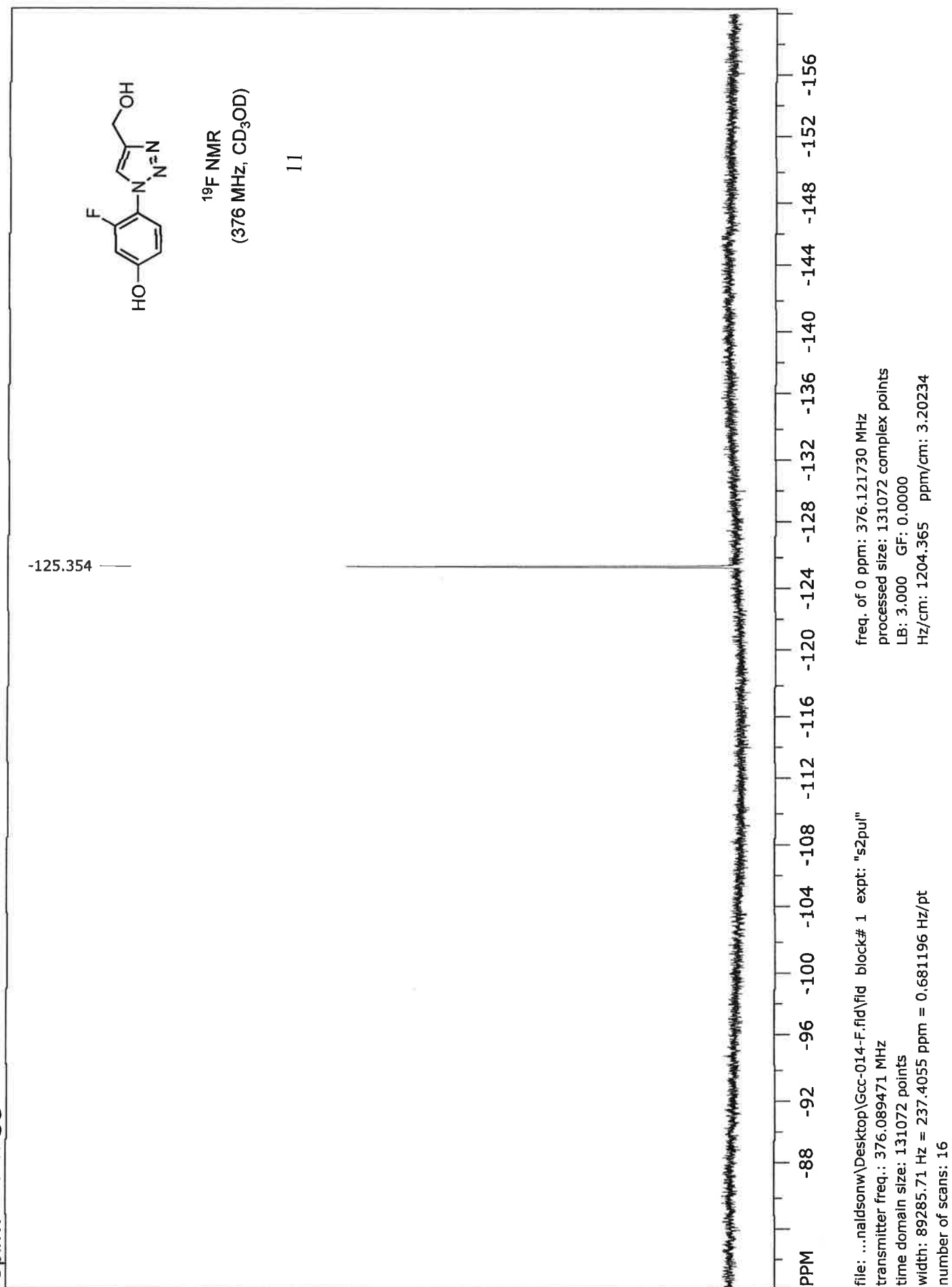
file: ...unds\10_7_18_EAW278_Proton.fid\fid block# 1 expt: "s2pul"

transmitter freq.: 399.735724 MHz

time domain size: 32768 points

width: 6410.26 Hz = 16.0362 ppm = 0.195626 Hz/pt

number of scans: 8

freq. of 0 ppm: 399.733317 MHz

processed size: 32768 complex points

LB: 1.500   GF: 0.0000
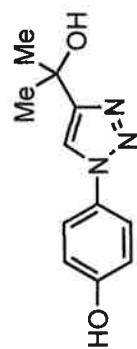
Hz/cm: 135.897   ppm/cm: 0.33997

SpinWorks 4: 11_7_18_Eaw2878Carbon

16.250 ——

30.661 ——

116.009 ——
120.493 ——
124.336 ——
127.333 ——

157.482 ——

^{13}C NMR
(100 MHz, CD$_3$OD)

14

PPM   10   20   30   40   50   60   70   80   90   100   110   120   130   140   150   160

file: ...unds\10_7_18_EAW278_Carbon.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.524081 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6966 ppm = 0.381470 Hz/pt
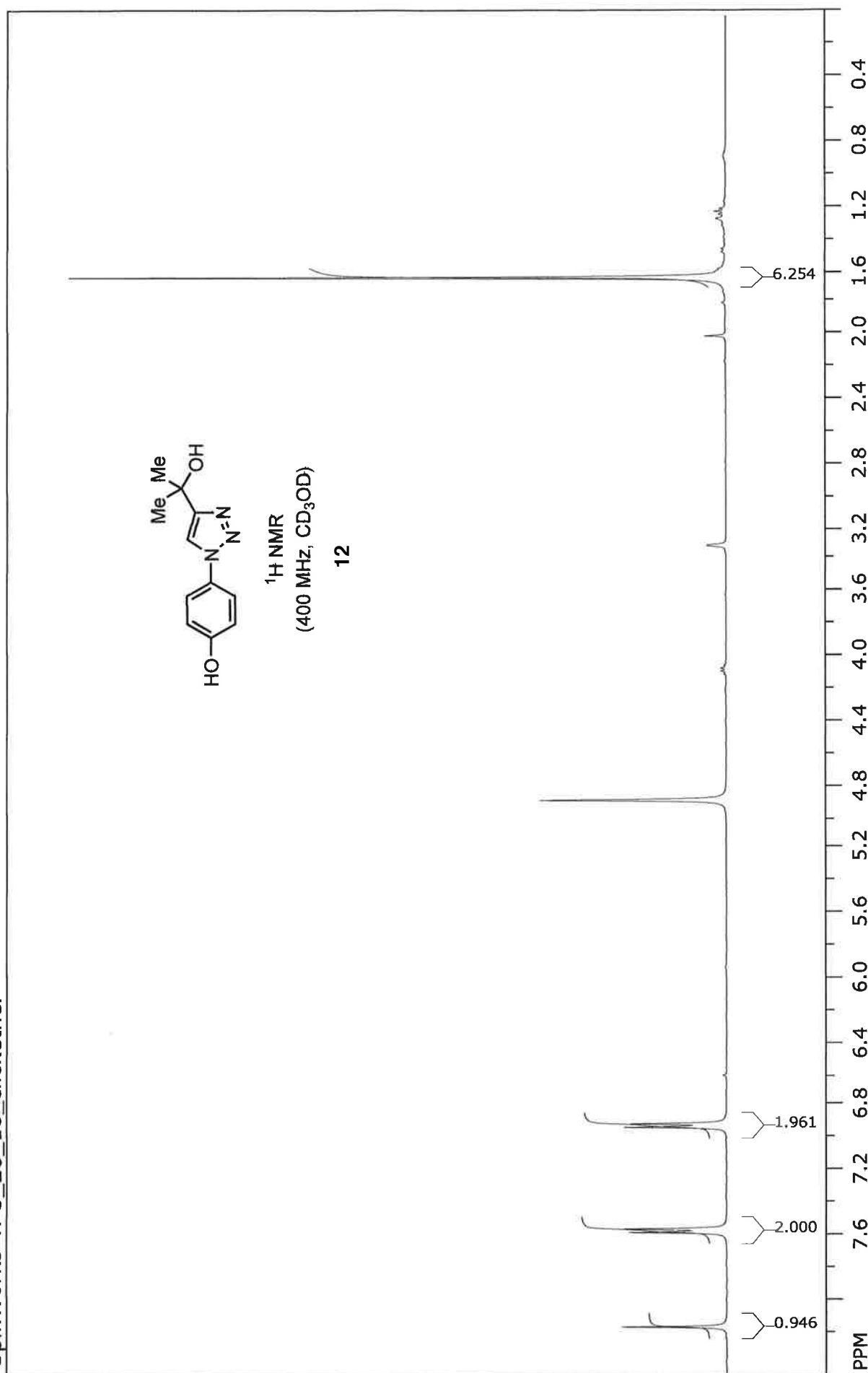number of scans: 256

freq. of 0 ppm: 100.512881 MHz
processed size: 65536 complex points
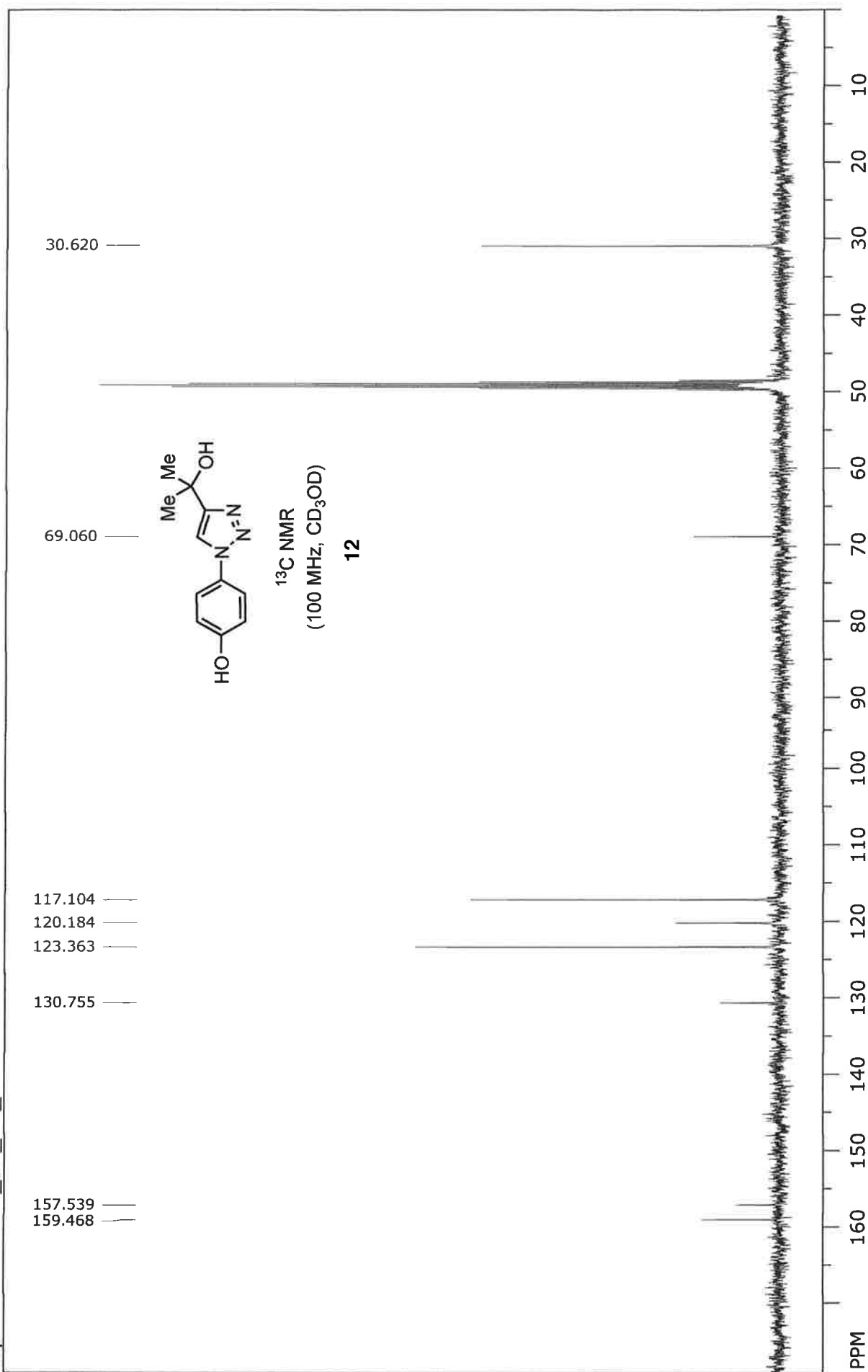LB: 1.500   GF: 0.0000
Hz/cm: 723.333   ppm/cm: 7.19562

SpinWorks 4: 3_29_18_sample1

^1H NMR
(400 MHz, CD$_3$OD)

15

6.000
3.012
1.778
0.949
0.910

PPM 9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4
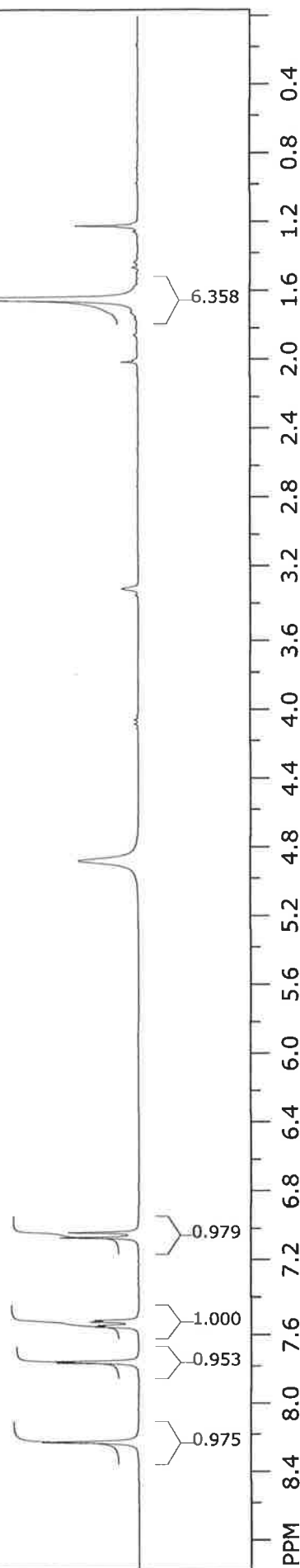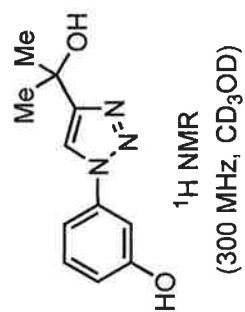
file: ... Compounds\3_29_18_sample1.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.735724 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0362 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.733316 MHz
processed size: 32768 complex points
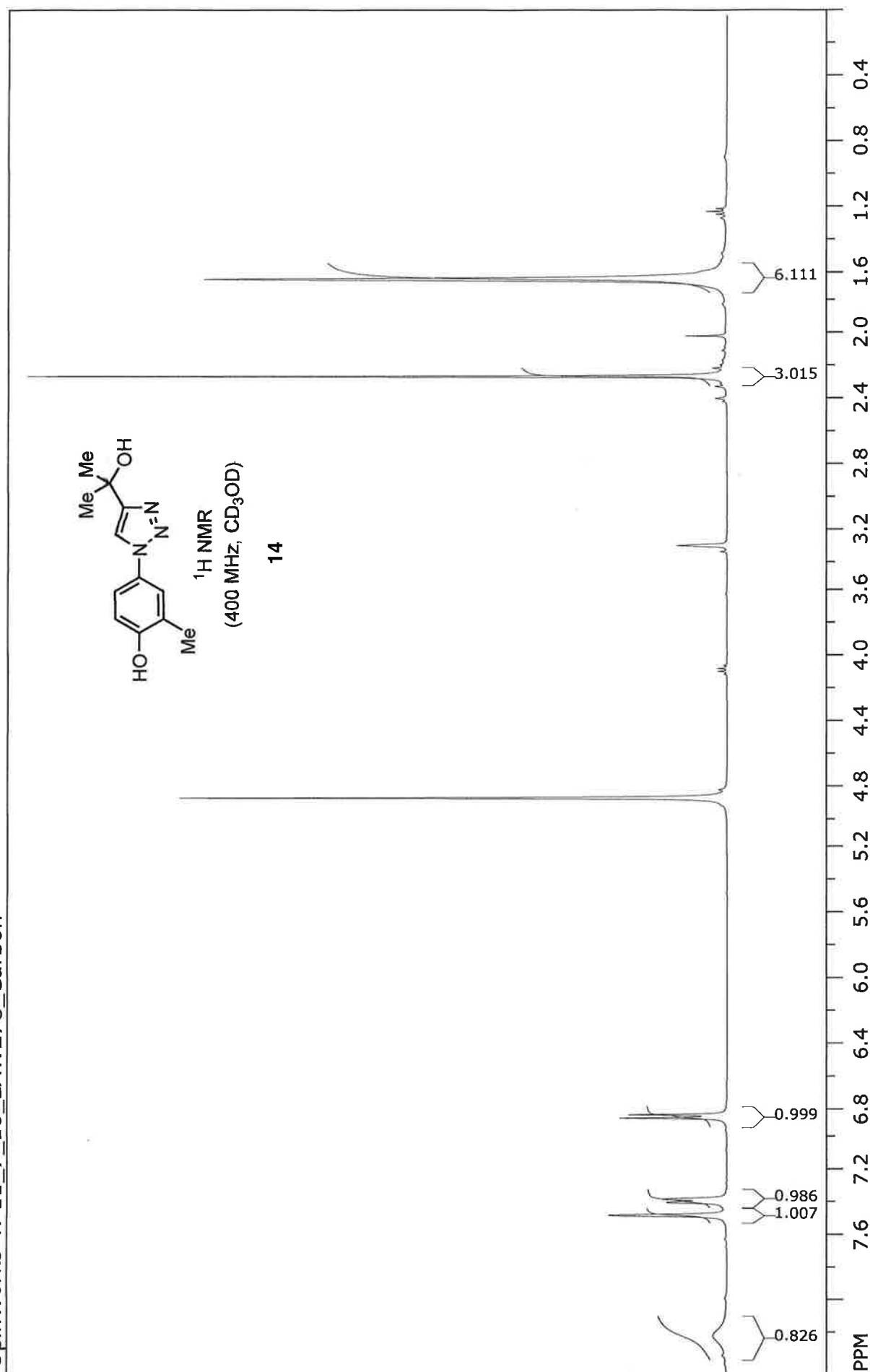LB: 1.500   GF: 0.0000
Hz/cm: 159.829   ppm/cm: 0.39984

SpinWorks 4: 13C OBSERVE

17.732 ——

30.677 ——

69.063 ——

^{13}C NMR

(75 MHz, CD$_3$OD)

15

114.433 ——
118.421 ——
123.859 ——
128.362
129.692
136.528 ——

159.956 ——

PPM   180   160   140   120   100   80   60   40   20

freq. of 0 ppm: 75.468249 MHz
processed size: 131072 complex points
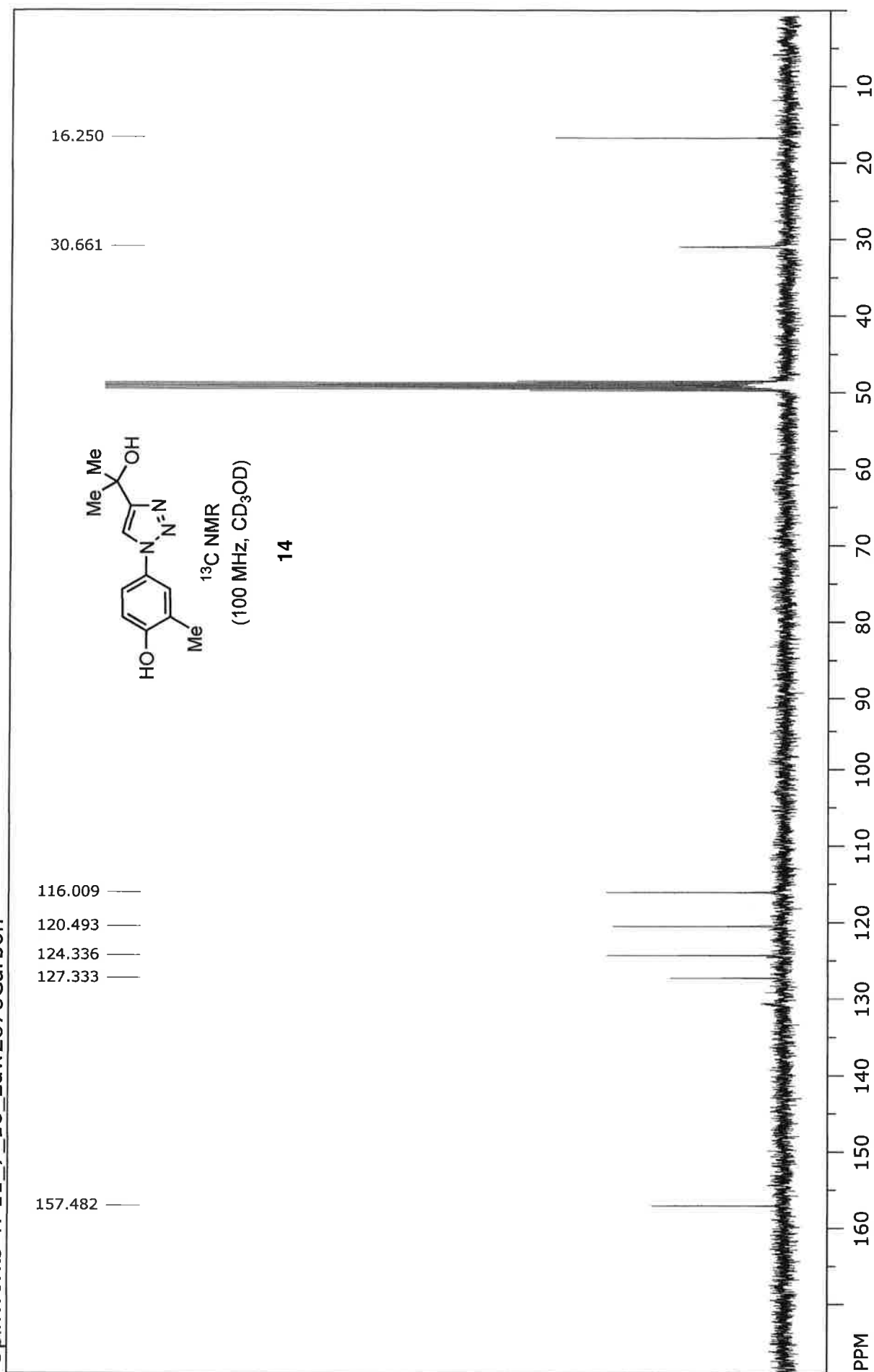LB: 1.000   GF: 0.0000
Hz/cm: 603.774   ppm/cm: 7.99948

file: ...unds\3_30_18_Sample1CARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 75.476633 MHz
time domain size: 68492 points
width: 18867.92 Hz = 249.9837 ppm = 0.275476 Hz/pt
number of scans: 128

SpinWorks 4: STANDARD 1H OBSERVE - profile

^{1}H NMR
(400 MHz, CD$_3$OD)

16

6.523

1.959

0.999

0.916

PPM   7.6   7.2   6.8   6.4   6.0   5.6   5.2   4.8   4.4   4.0   3.6   3.2   2.8   2.4   2.0   1.6   1.2   0.8   0.4
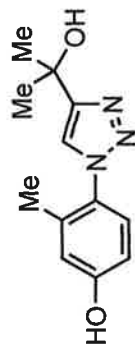
file: ...Triazole Compounds\GCC12-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.731815 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.729414 MHz
processed size: 32768 complex points
LB: 0.610   GF: 0.0000
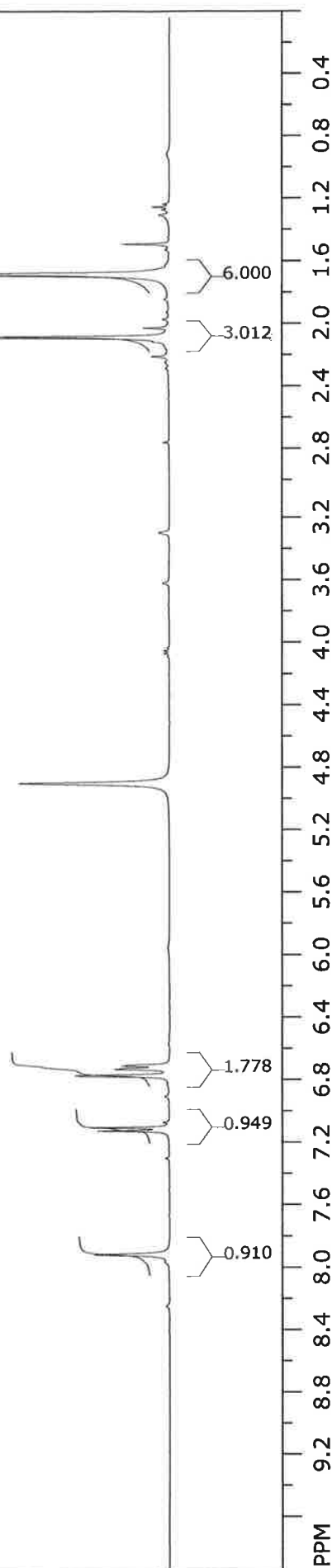Hz/cm: 135.897   ppm/cm: 0.33997

SpinWorks 4: STANDARD 1H OBSERVE - profile

30.617 ——

69.087 ——

104.475
104.695

113.101 —
118.195
118.309

123.308
123.348

127.791 —

155.557
157.200
158.040
161.453
161.564

¹³C NMR
(100 MHz, CD₃OD)

16

^{13}C NMR
(100 MHz, CD$_3$OD)

PPM   10   20   30   40   50   60   70   80   90   100   110   120   130   140   150   160

SpinWorks 4: SC

¹⁹F NMR
(376 MHz, CD₃OD)

16

-125.267

PPM -88 -92 -96 -100 -104 -108 -112 -116 -120 -124 -128 -132 -136 -140 -144 -148 -152 -156

file: ...naldsonw\Desktop\Gcc-012-F.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 376.089471 MHz
time domain size: 131072 points
width: 89285.71 Hz = 237.4055 ppm = 0.681196 Hz/pt
number of scans: 16

freq. of 0 ppm: 376.121736 MHz
processed size: 131072 complex points
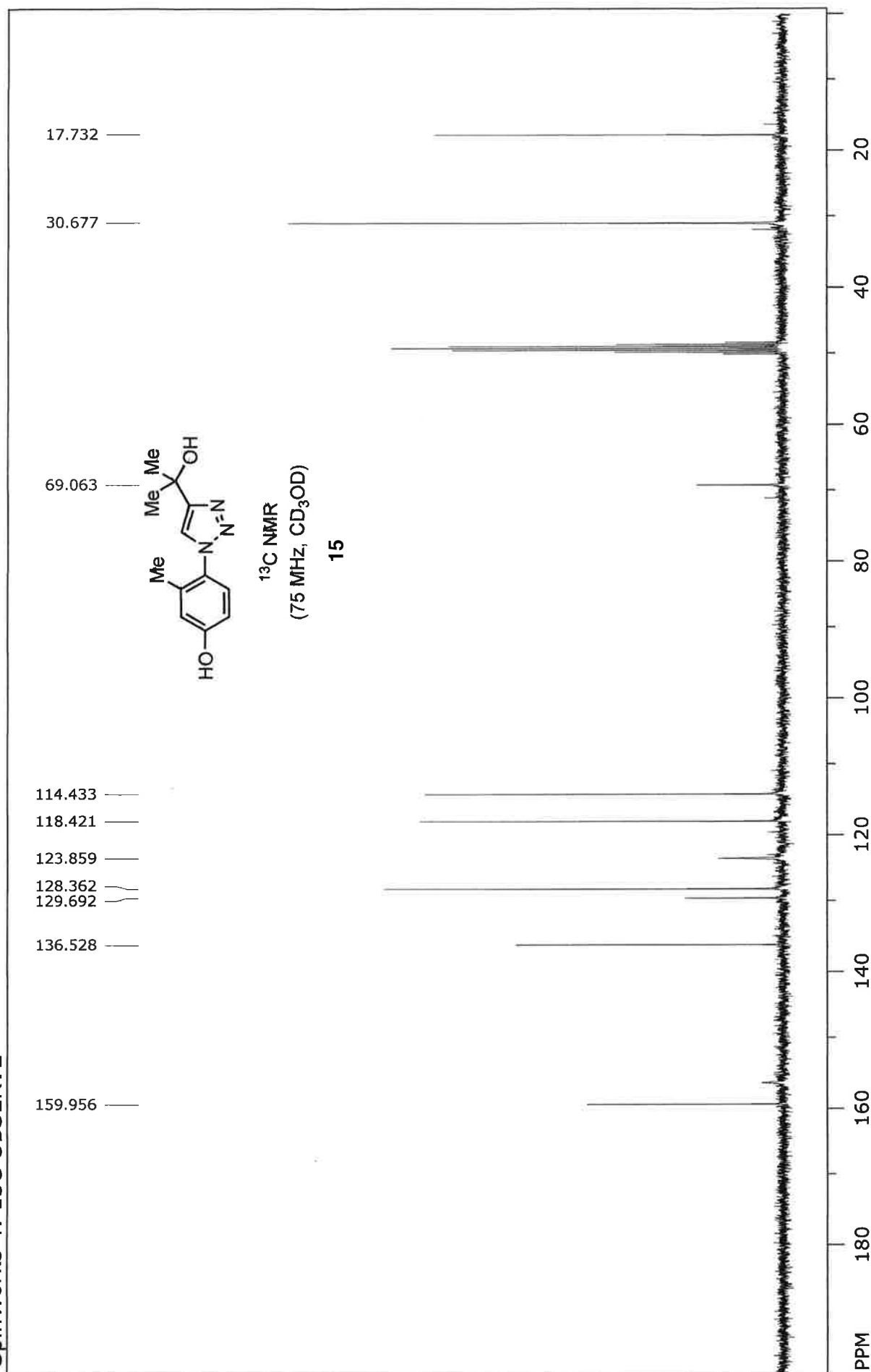LB: 1.500   GF: 0.0000
Hz/cm: 1204.365   ppm/cm: 3.20234

SpinWorks 4: GCC11

^{1}H NMR
(400 MHz, CD$_3$OD)

17

PPM   9.2   8.8   8.4   8.0   7.6   7.2   6.8   6.4   6.0   5.6   5.2   4.8   4.4   4.0   3.6   3.2   2.8   2.4   2.0   1.6   1.2   0.8   0.4

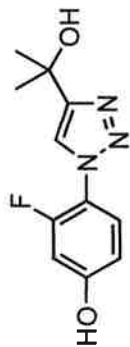0.911   0.862   0.960   0.931

1.428

5.999

file: ...le Compounds\4_16_18_GCC11.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.735724 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0362 ppm = 0.195626 Hz/pt
number of scans: 8

freq. of 0 ppm: 399.733316 MHz
processed size: 32768 complex points
LB: 1.500   GF: 0.0000
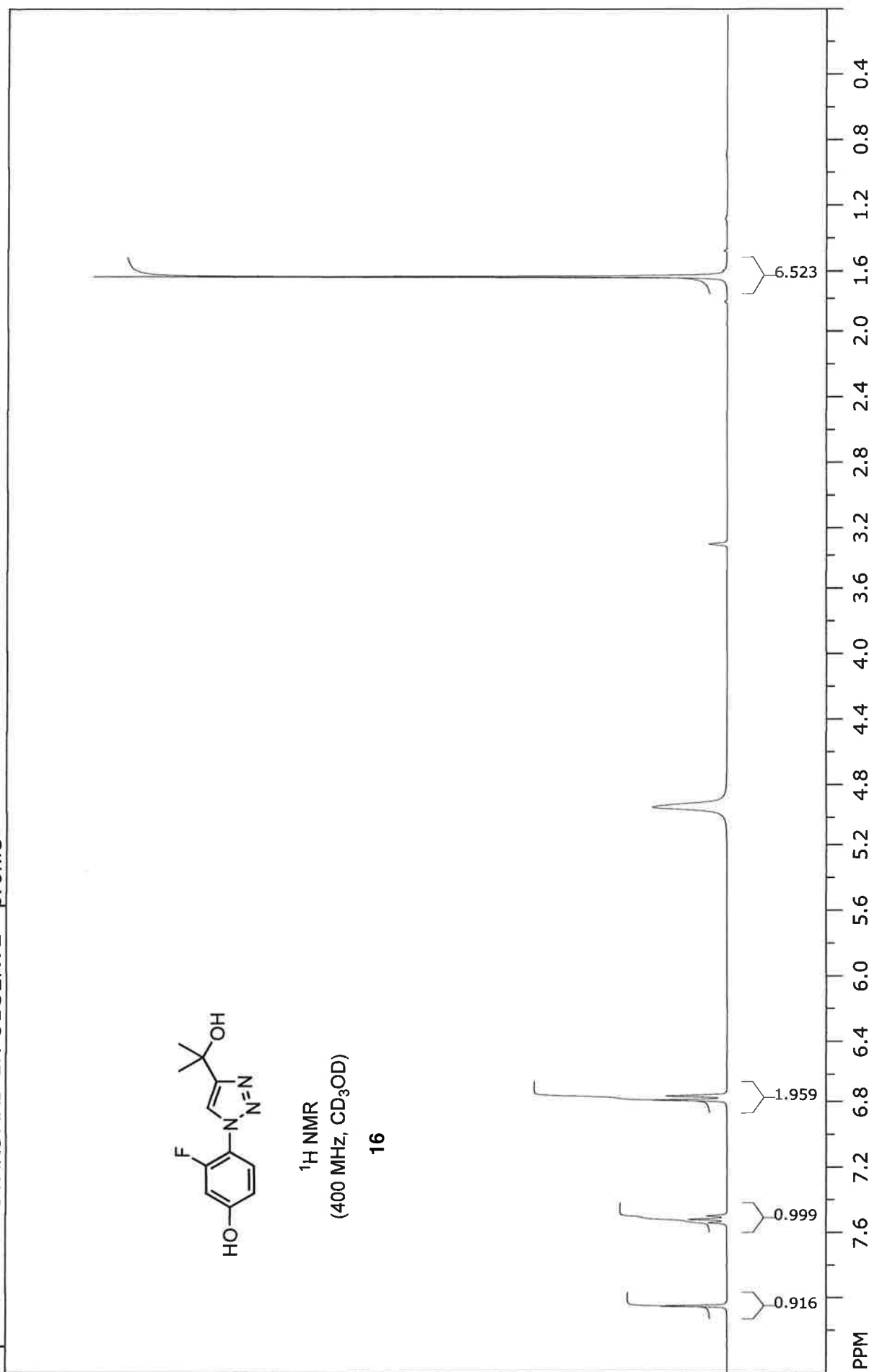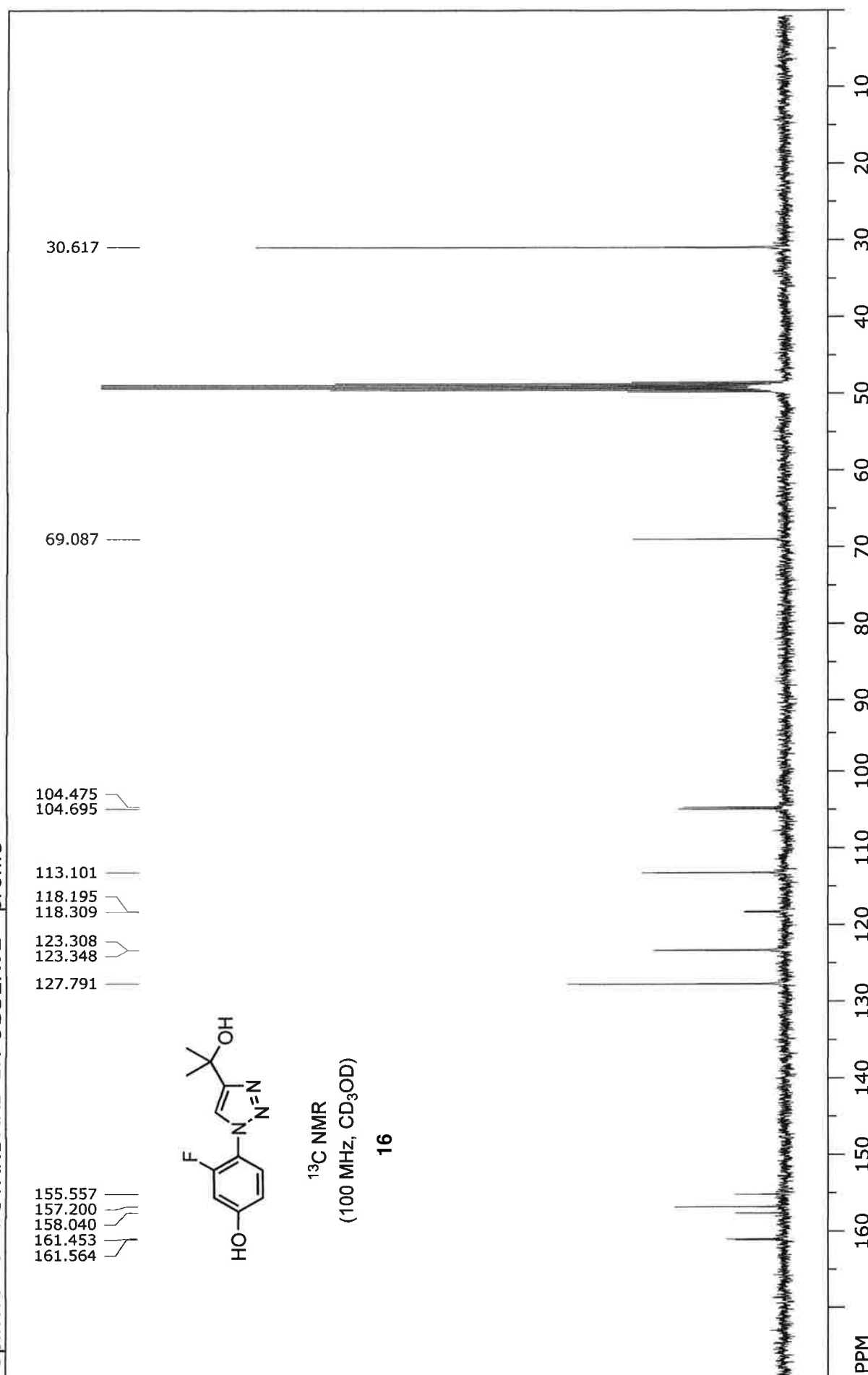Hz/cm: 159.829   ppm/cm: 0.39984

SpinWorks 4: 4_16_18_GCC11CARBON

30.569

69.019

118.035
120.148
121.430
122.485
123.499

131.033

155.126
157.688

¹³C NMR
(100 MHz, CD₃OD)

17

freq. of 0 ppm: 100.512883 MHz
processed size: 65536 complex points
LB: 1.500   GF: 0.0000
Hz/cm: 723.889   ppm/cm: 7.20115

file: ...pounds\4_16_18_GCC11CARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.524081 MHz
time domain size: 65536 points
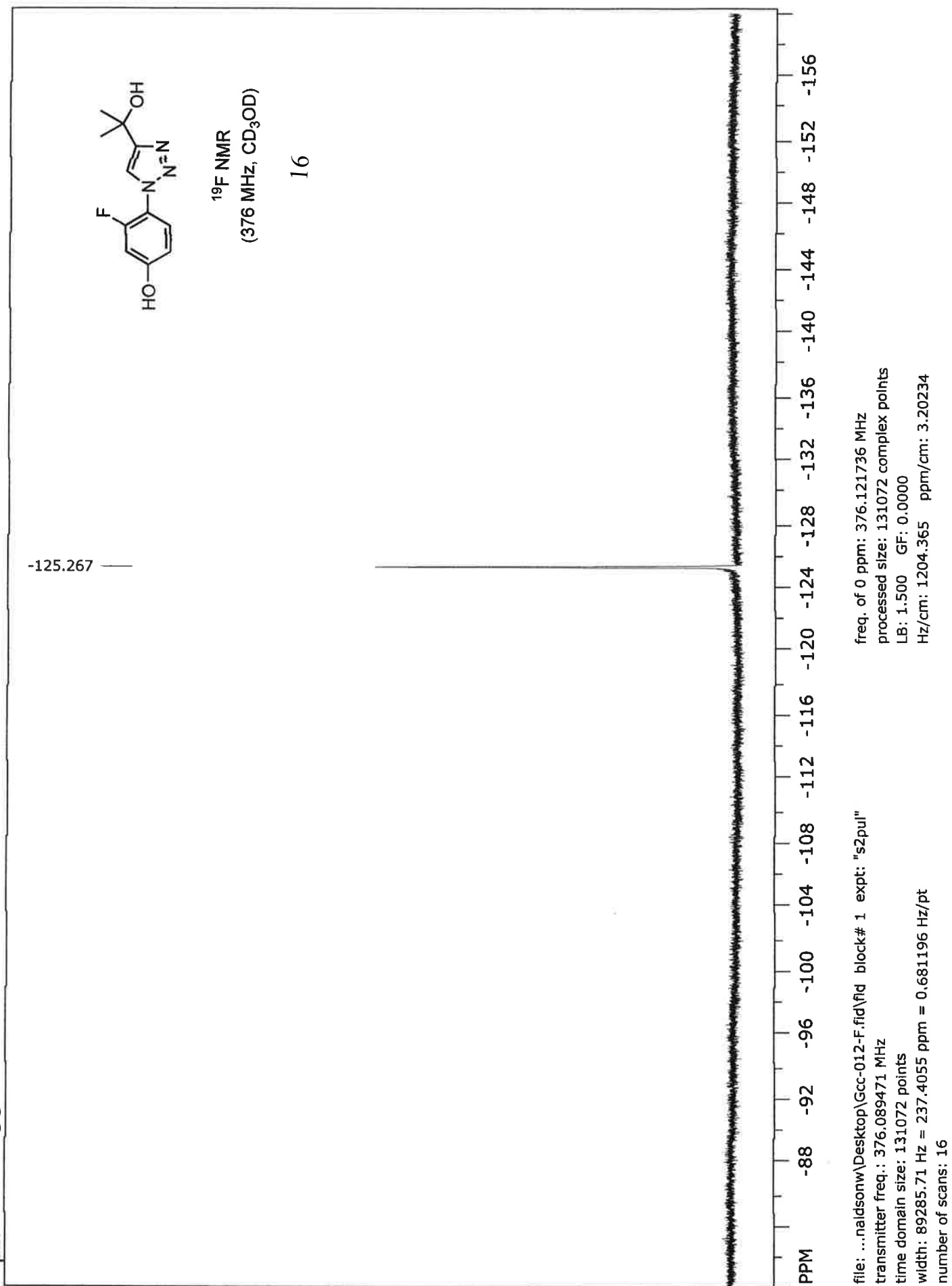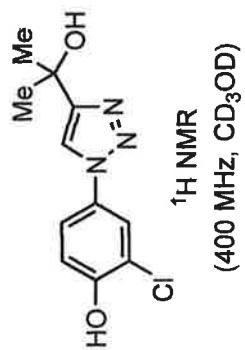width: 25000.00 Hz = 248.6966 ppm = 0.381470 Hz/pt
number of scans: 256

PPM   10   20   30   40   50   60   70   80   90   100   110   120   130   140   150   160

SpinWorks 4: STANDARD 1H OBSERVE

^{1}H NMR

(300 MHz, CD$_3$OD)

18

PPM																		

2.107
2.093
1.980
2.000
0.944
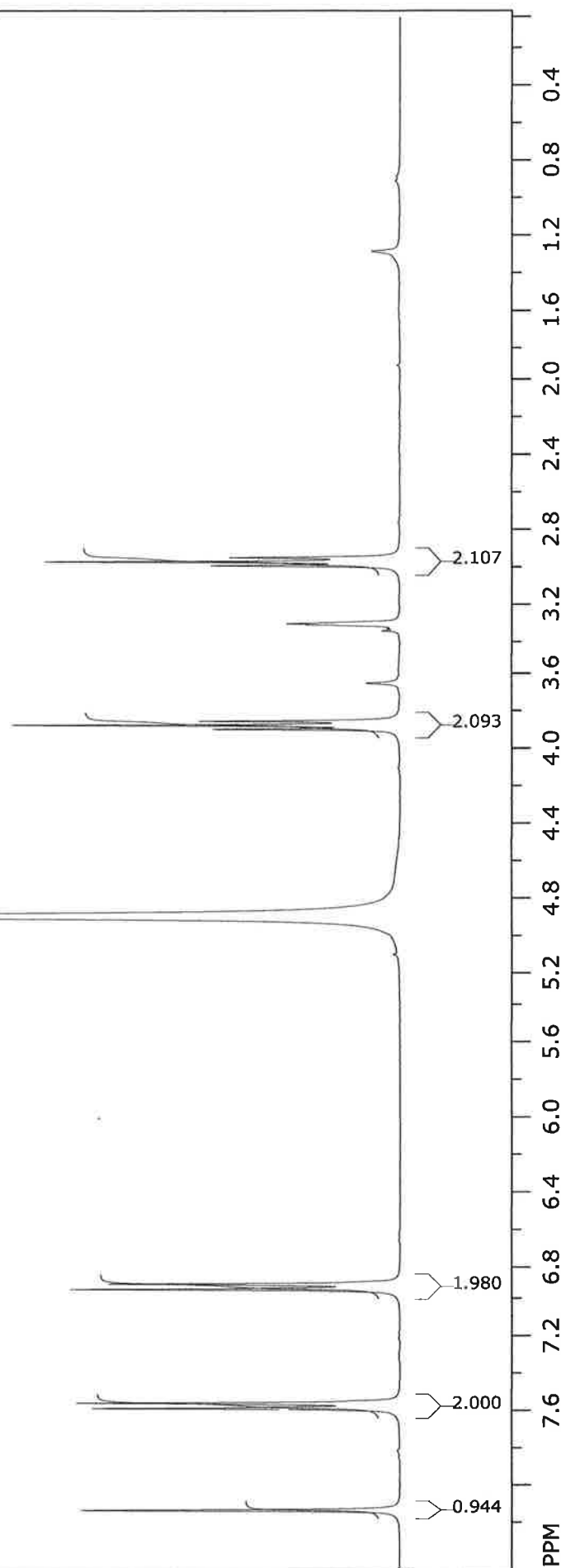
file: ...riazole Compounds\EAW152-H.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 300.134191 MHz
time domain size: 19192 points
width: 4803.07 Hz = 16.0031 ppm = 0.250264 Hz/pt
number of scans: 8

freq. of 0 ppm: 300.132388 MHz
processed size: 32768 complex points
LB: 0.500   GF: 0.0000
Hz/cm: 102.039   ppm/cm: 0.33998

SpinWorks 4: 13C OBSERVE

29.921 ——

62.030 ——

117.119 ——

122.342
123.322

130.778 ——

146.780 ——

159.519 ——

^{13}C NMR
(75 MHz, CD$_3$OD)
18

freq. of 0 ppm: 75.468242 MHz
processed size: 131072 complex points
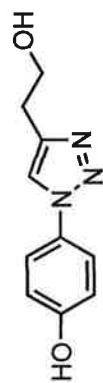LB: 2.000   GF: 0.0000
Hz/cm: 543.396   ppm/cm: 7.19953
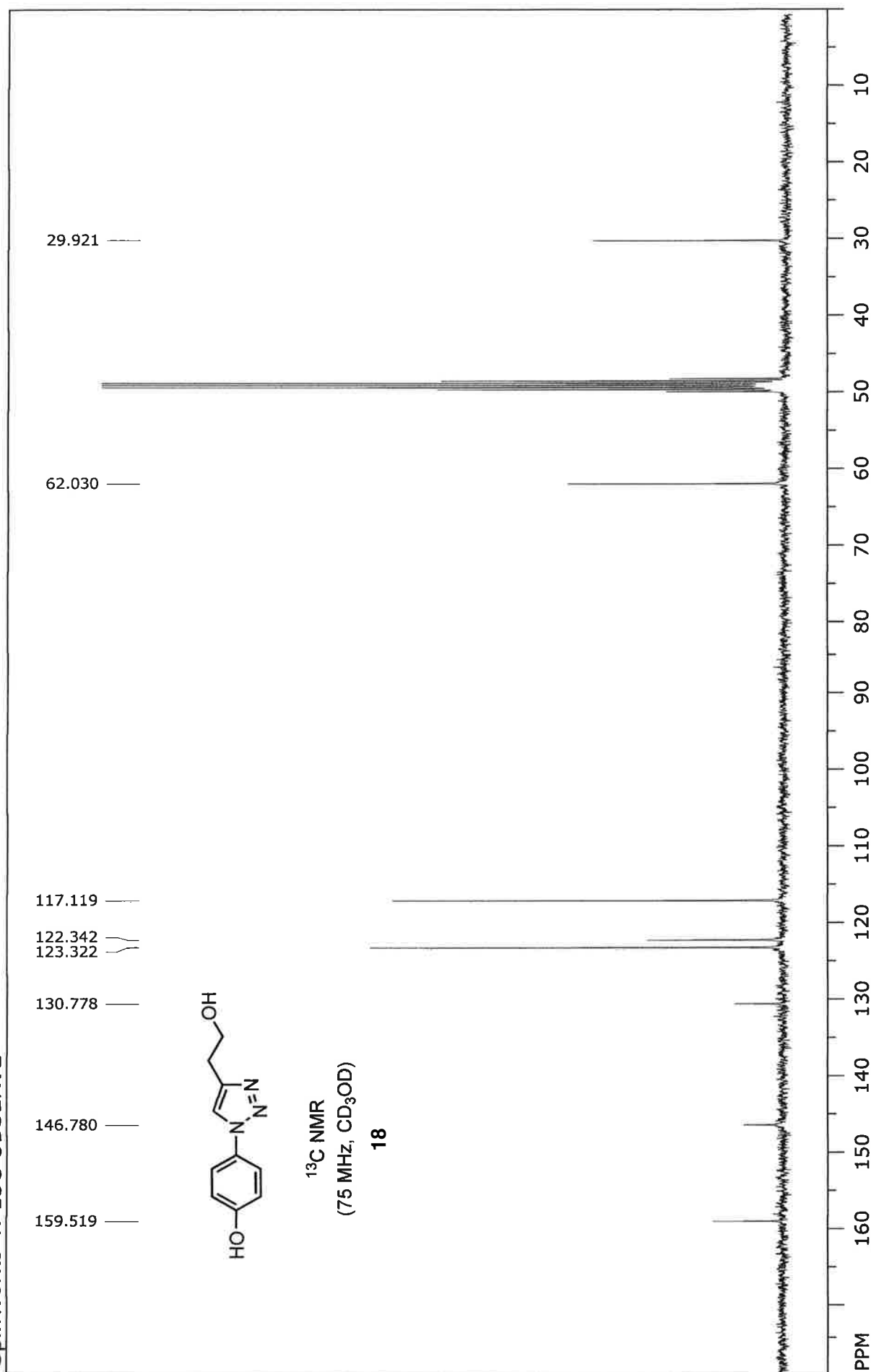
file: ...riazole Compounds\EAW152-C.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 75.476633 MHz
time domain size: 68492 points
width: 18867.92 Hz = 249.9837 ppm = 0.275476 Hz/pt
number of scans: 1024

PPM   10   20   30   40   50   60   70   80   90   100   110   120   130   140   150   160

SpinWorks 4: STANDARD 1H OBSERVE

^{1}H NMR
(300 MHz, CD$_3$OD)

19

PPM 8.0   7.6   7.2   6.8   6.4   6.0   5.6   5.2   4.8   4.4   4.0   3.6   3.2   2.8   2.4   2.0   1.6   1.2   0.8

2.103
2.101
1.051
2.104
1.051
1.000

file: ...Compounds\12_10_17_REDCAP.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 300.134191 MHz
time domain size: 19192 points
width: 4803.07 Hz = 16.0031 ppm = 0.250264 Hz/pt
number of scans: 8

freq. of 0 ppm: 300.132385 MHz
processed size: 32768 complex points
LB: 0.500   GF: 0.0000
Hz/cm: 96.061   ppm/cm: 0.32006

SpinWorks 4: 13C OBSERVE

13C NMR
(75 MHz, CD₃OD)
19

29.896 ——

61.954 ——

108.489 ——
112.071 ——
116.822 ——
122.185 ⟩
122.236 ⟩
131.714 ——
139.395 ——
159.960 ——

PPM 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

file: ...unds\12_10_17_REDCAPCARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 75.476633 MHz
time domain size: 68492 points
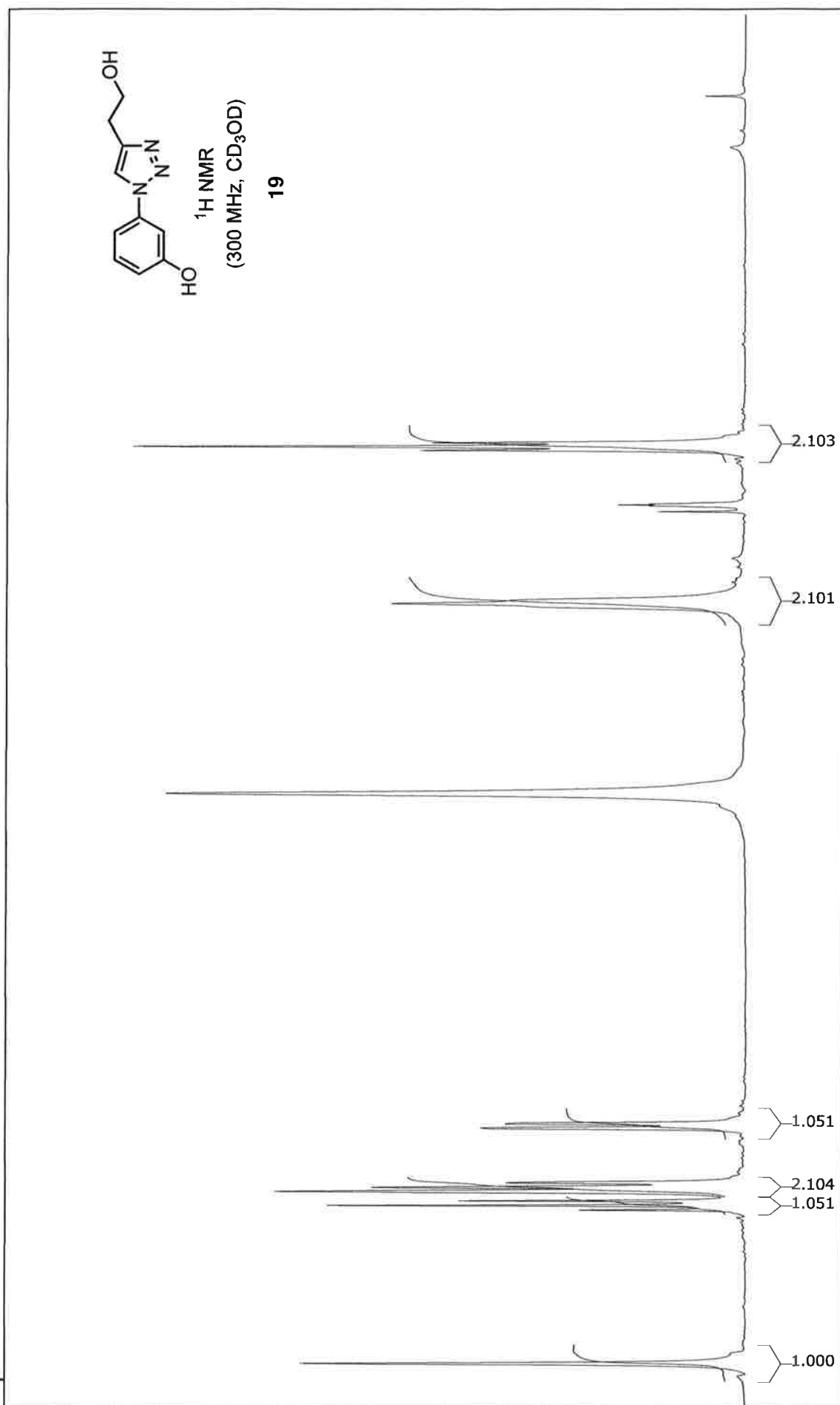width: 18867.92 Hz = 249.9837 ppm = 0.275476 Hz/pt
number of scans: 64

freq. of 0 ppm: 75.468243 MHz
processed size: 131072 complex points
LB: 1.500 GF: 0.0000
Hz/cm: 543.396 ppm/cm: 7.19953

S4

SpinWorks 4: STANDARD 1H OBSERVE

^{1}H NMR
(300 MHz, CD$_3$OD)

20

3.126

2.000

0.977

2.005

2.032

0.940
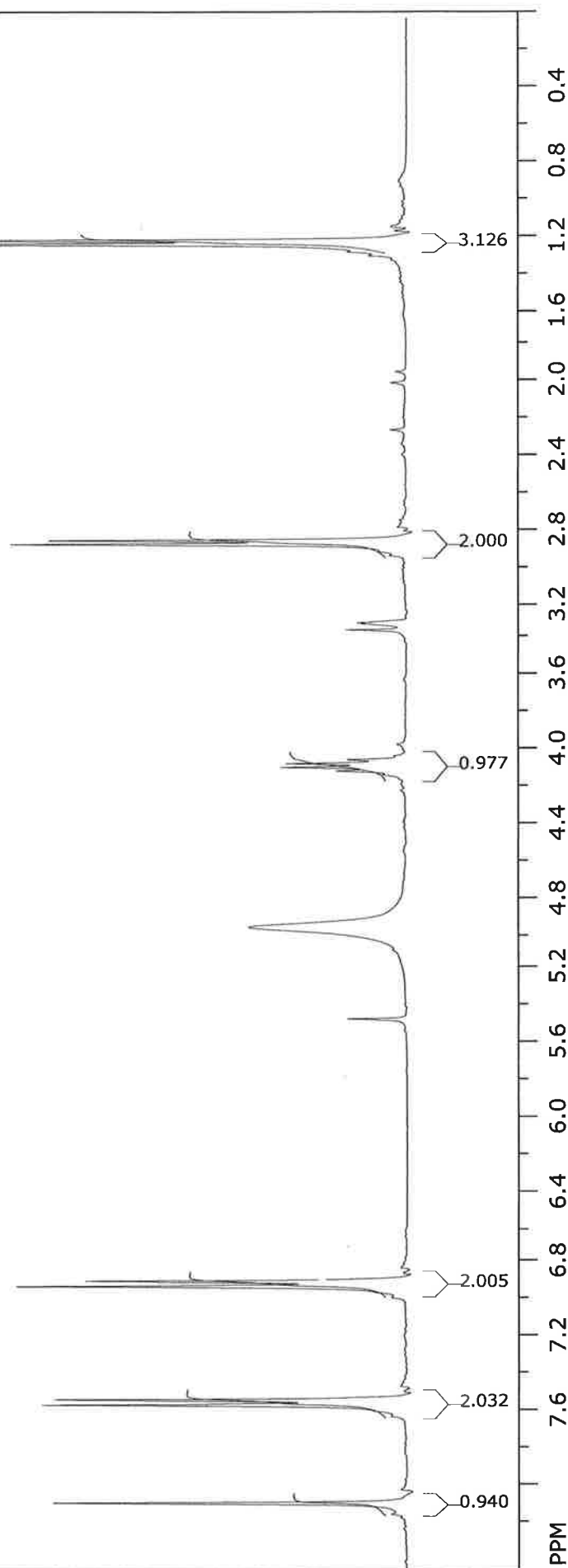
file: ..._azidophenol_4_propyn_2_ol.fid\fid block# 1 expt: "s2pul"
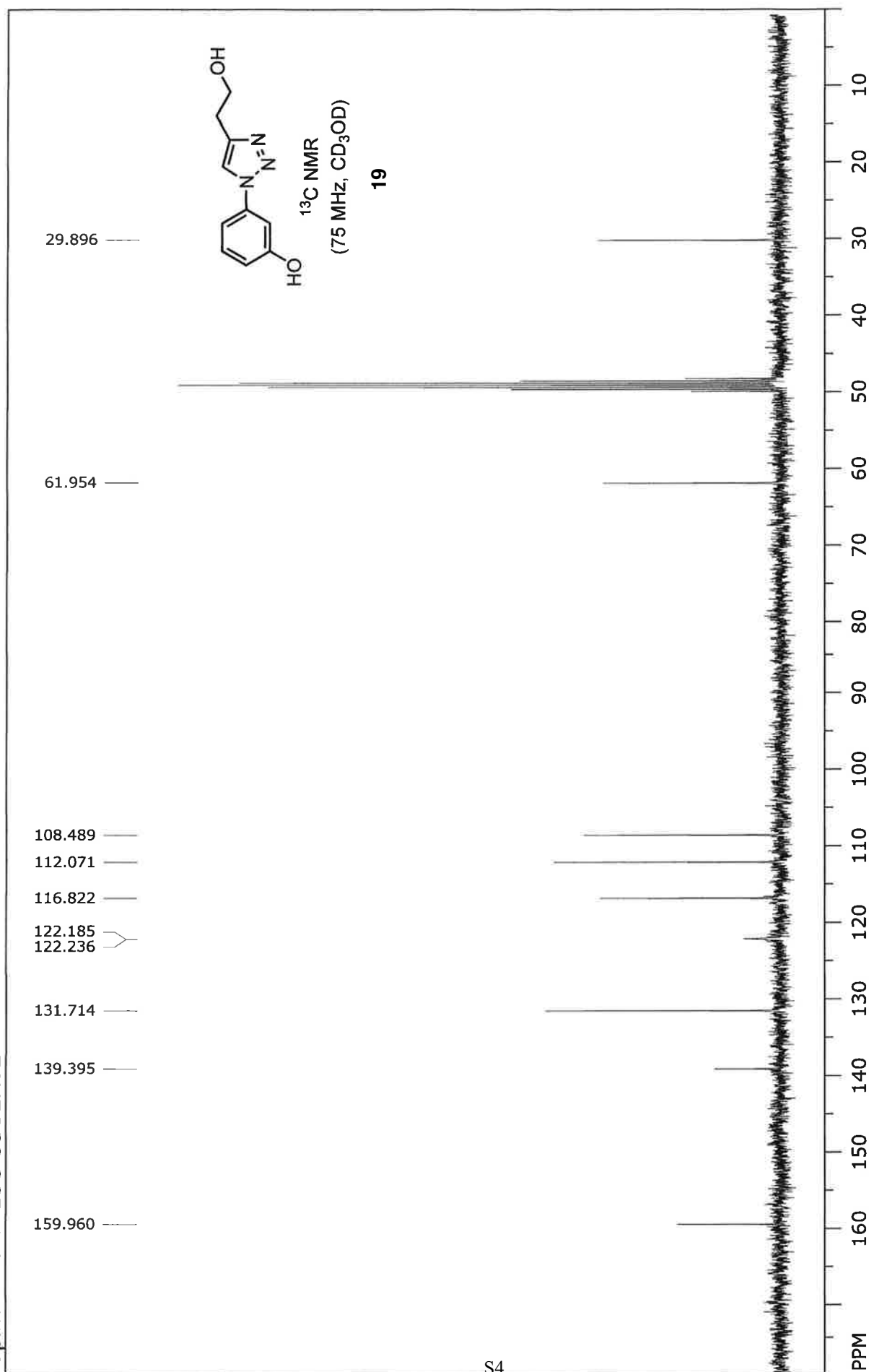transmitter freq.: 300.134191 MHz
time domain size: 19192 points.
width: 4803.07 Hz = 16.0031 ppm = 0.250264 Hz/pt
number of scans: 8

freq. of 0 ppm: 300.132382 MHz
processed size: 32768 complex points
LB: 0.500   GF: 0.0000
Hz/cm: 102.039   ppm/cm: 0.33998

PPM   0.4   0.8   1.2   1.6   2.0   2.4   2.8   3.2   3.6   4.0   4.4   4.8   5.2   5.6   6.0   6.4   6.8   7.2   7.6

SpinWorks 4: 13C OBSERVE

^{13}C NMR

(75 MHz, CD$_3$OD)

20

35.986

67.948

117.082

122.586
123.264

130.744

146.564

159.404

PPM 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

file: ...phenol_4_propyn_2_olCARBON.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 75.476633 MHz
time domain size: 68492 points
width: 18867.92 Hz = 249.9837 ppm = 0.275476 Hz/pt
number of scans: 64

freq. of 0 ppm: 75.468243 MHz
processed size: 131072 complex points
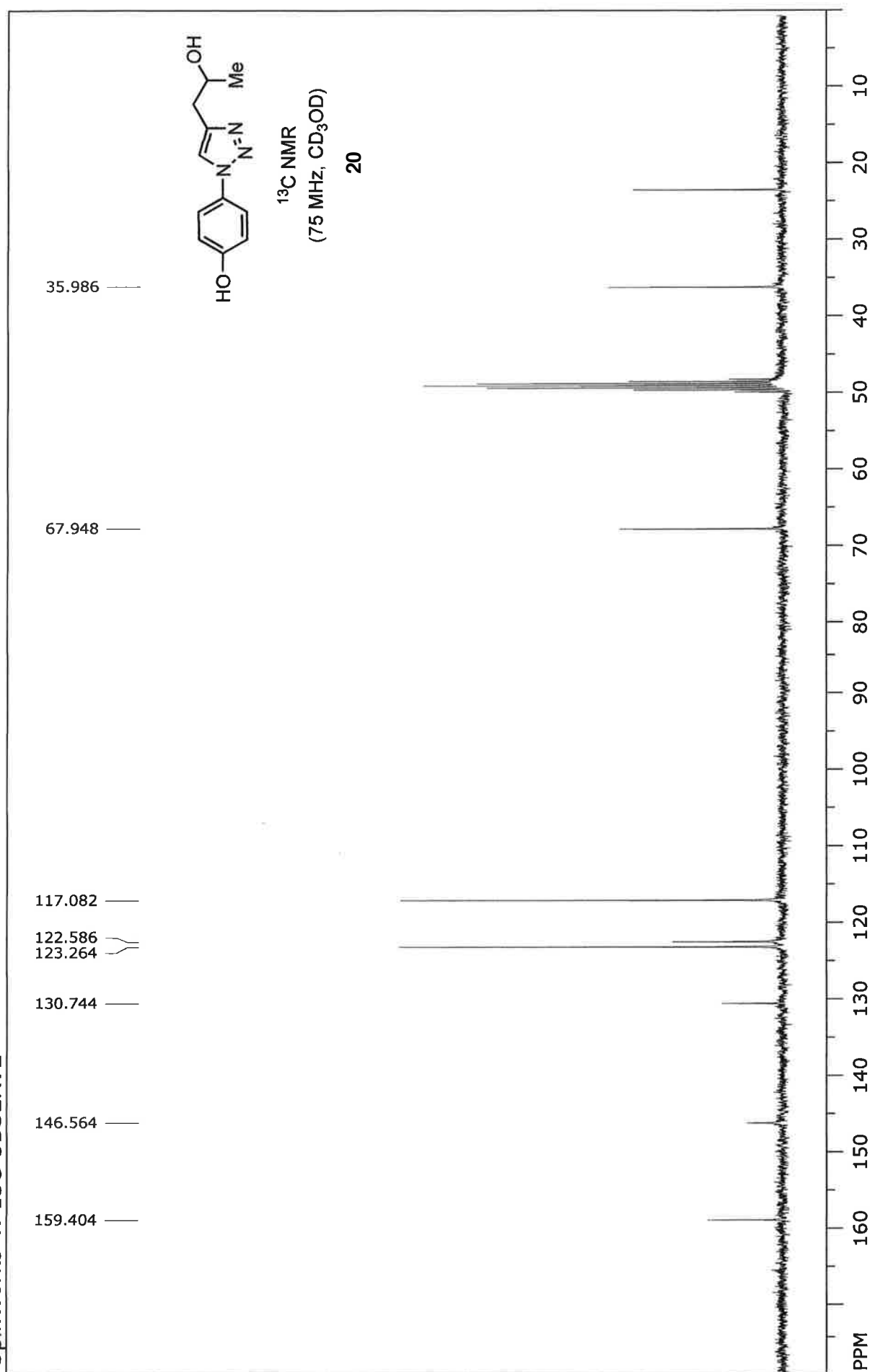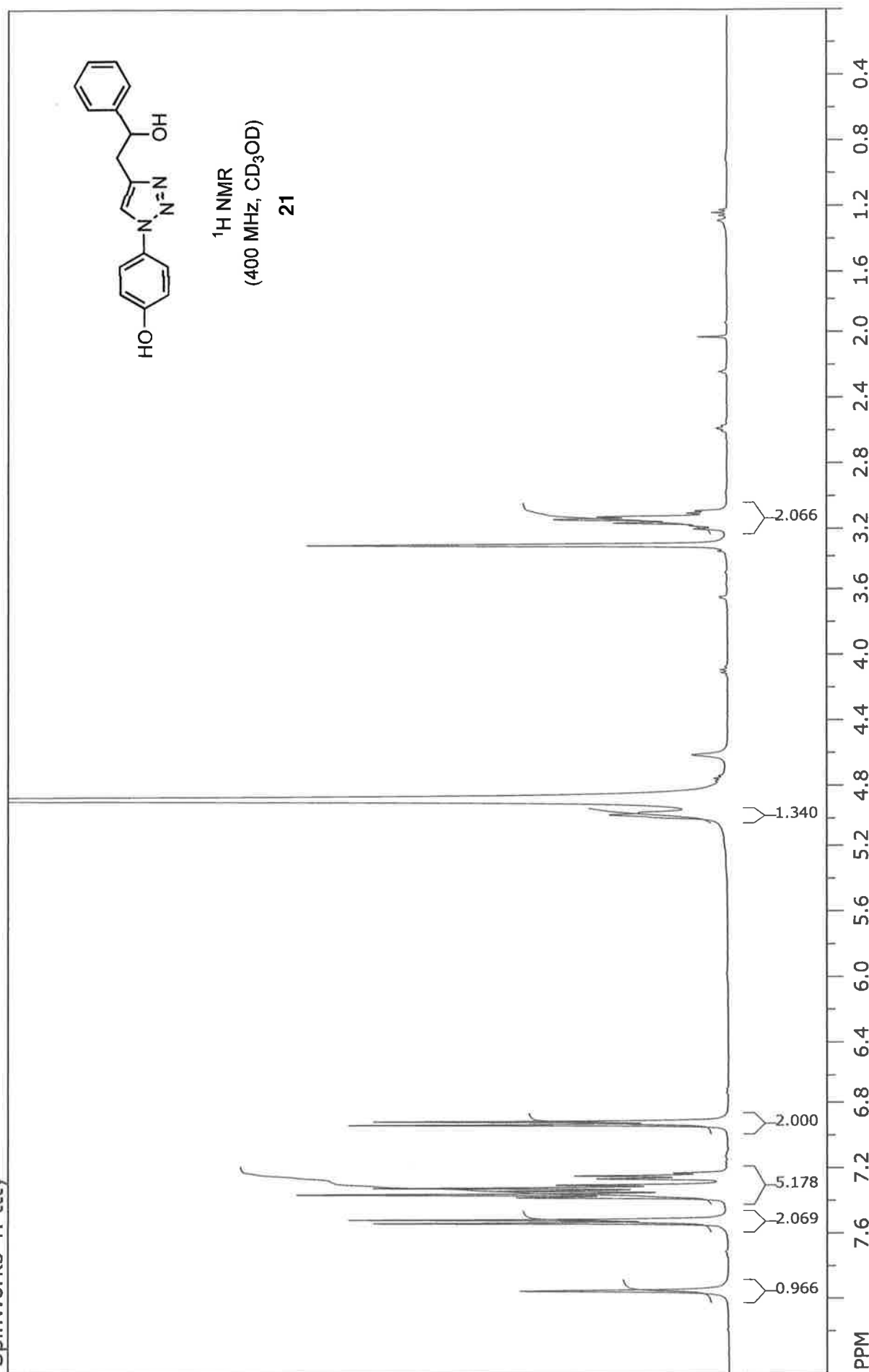LB: 1.500   GF: 0.0000
Hz/cm: 543.396   ppm/cm: 7.19953

SpinWorks 4: ttty

^{1}H NMR
(400 MHz, CD$_3$OD)
21

2.066

1.340

2.000

5.178

2.069

0.966

PPM

0.4 0.8 1.2 1.6 2.0 2.4 2.8 3.2 3.6 4.0 4.4 4.8 5.2 5.6 6.0 6.4 6.8 7.2 7.6

file: ...sonw\Desktop\WD358f1proton.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 399.731816 MHz
time domain size: 32768 points
width: 6410.26 Hz = 16.0364 ppm = 0.195626 Hz/pt
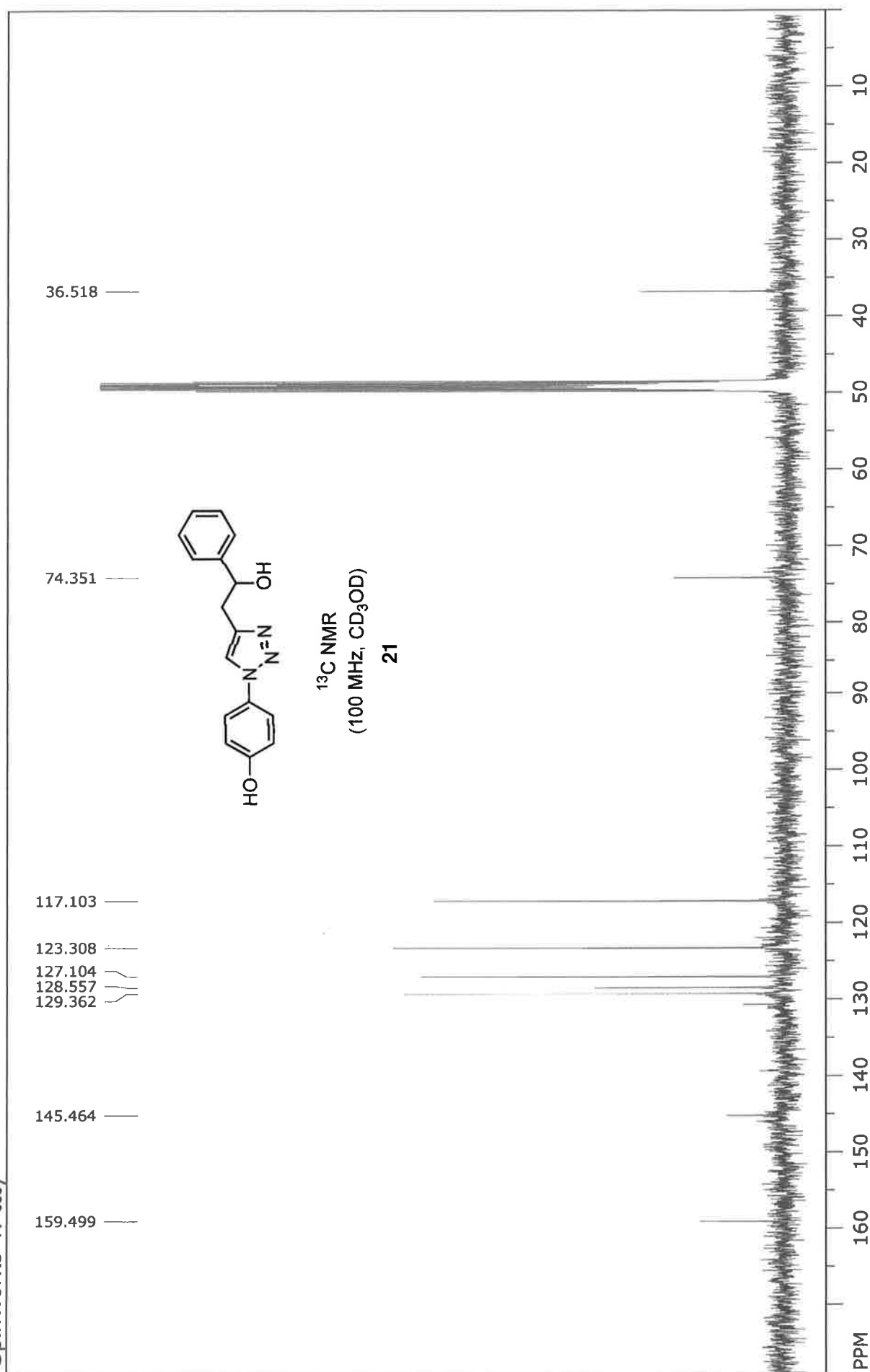number of scans: 8

freq. of 0 ppm: 399.729415 MHz
processed size: 32768 complex points
LB: 0.610   GF: 0.0000
Hz/cm: 135.897   ppm/cm: 0.33997

SpinWorks 4: ttty

36.518 ——

74.351 ——

^{13}C NMR
(100 MHz, CD$_3$OD)
21

117.103 ——

123.308 ——
127.104 ——
128.557 ——
129.362 ——

145.464 ——

159.499 ——

PPM   160   150   140   130   120   110   100   90   80   70   60   50   40   30   20   10

freq. of 0 ppm: 100.511897 MHz
processed size: 65536 complex points
LB: 2.500   GF: 0.0000
Hz/cm: 723.333   ppm/cm: 7.19569

file: ...sonw\Desktop\WD358f1carbon.fid\fid block# 1 expt: "s2pul"
transmitter freq.: 100.523098 MHz
time domain size: 65536 points
width: 25000.00 Hz = 248.6991 ppm = 0.381470 Hz/pt
number of scans: 1024