Supplementary Material

Microwave-promoted Heck and Suzuki coupling reactions of new 3-(5-bromobenzofuranyl)pyrazole in aqueous media

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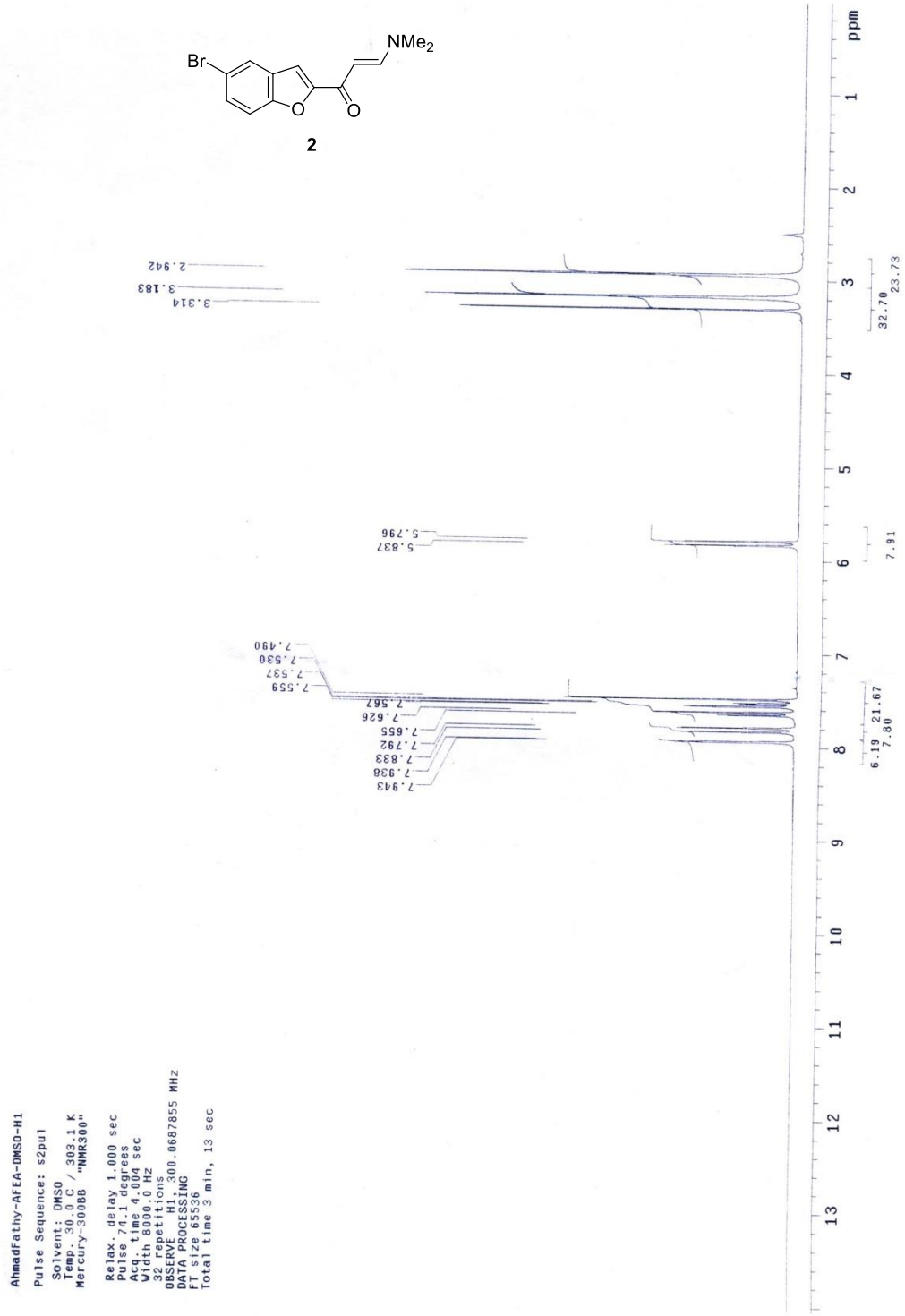

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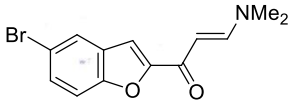

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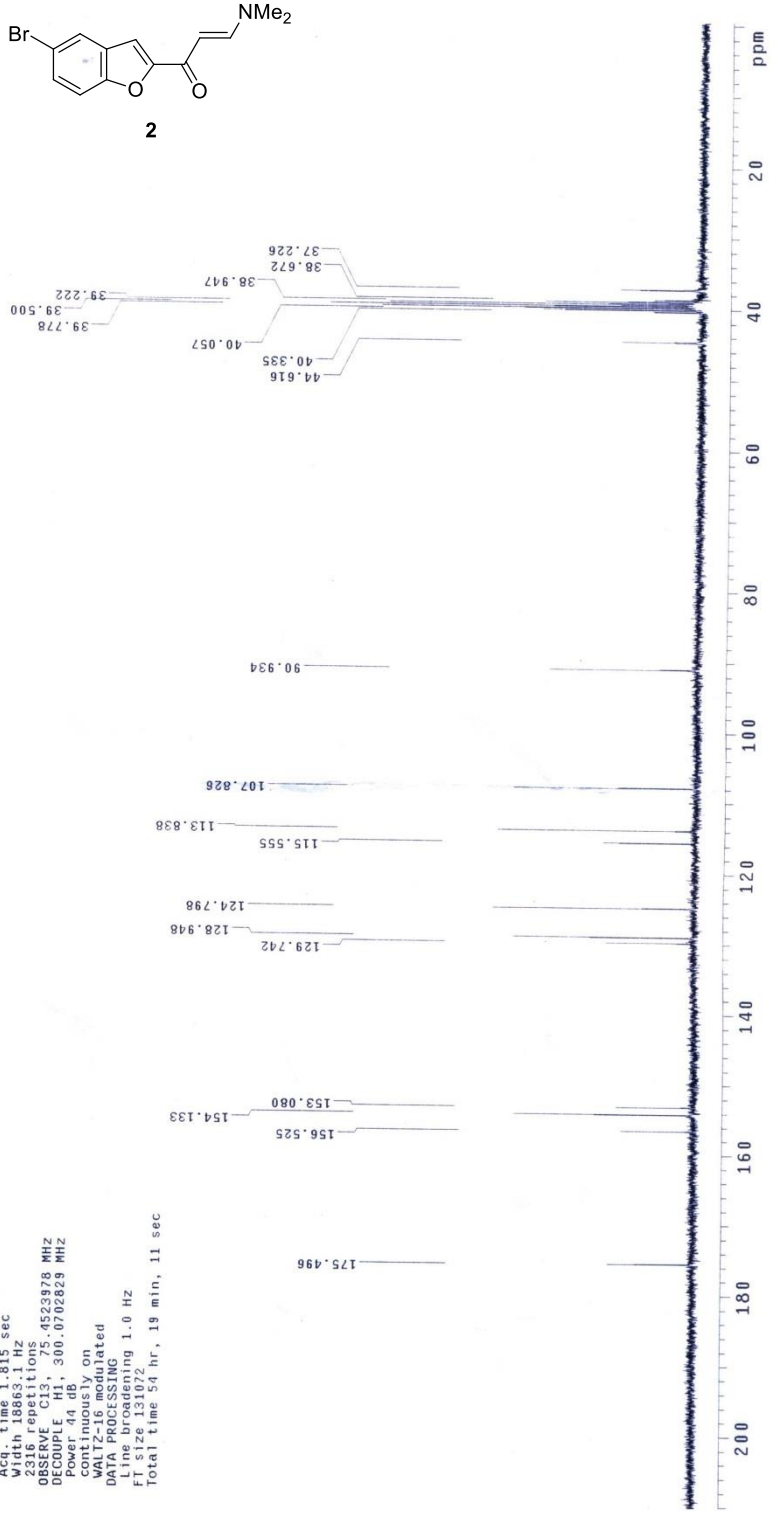

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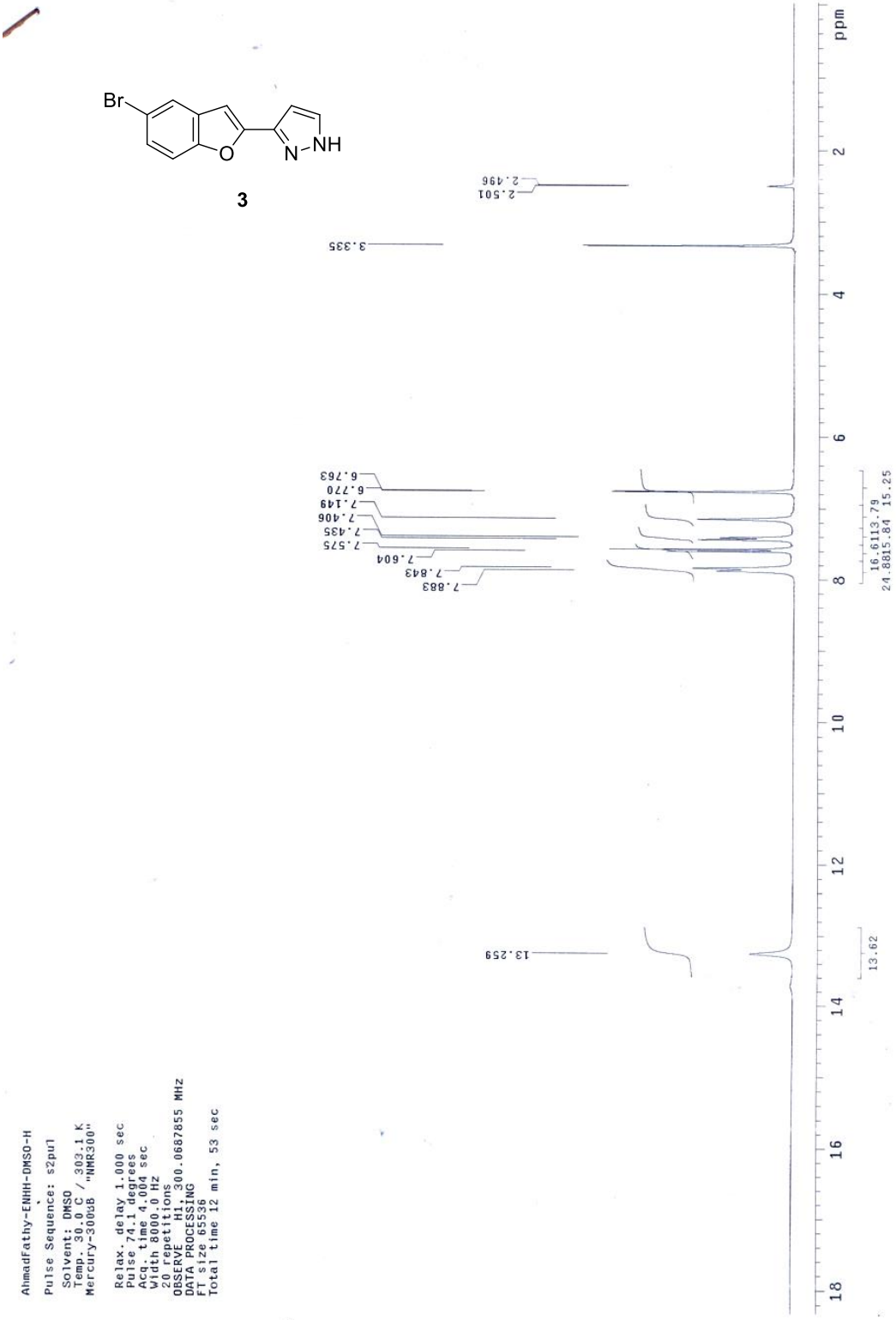

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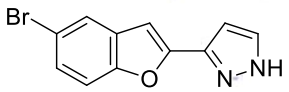
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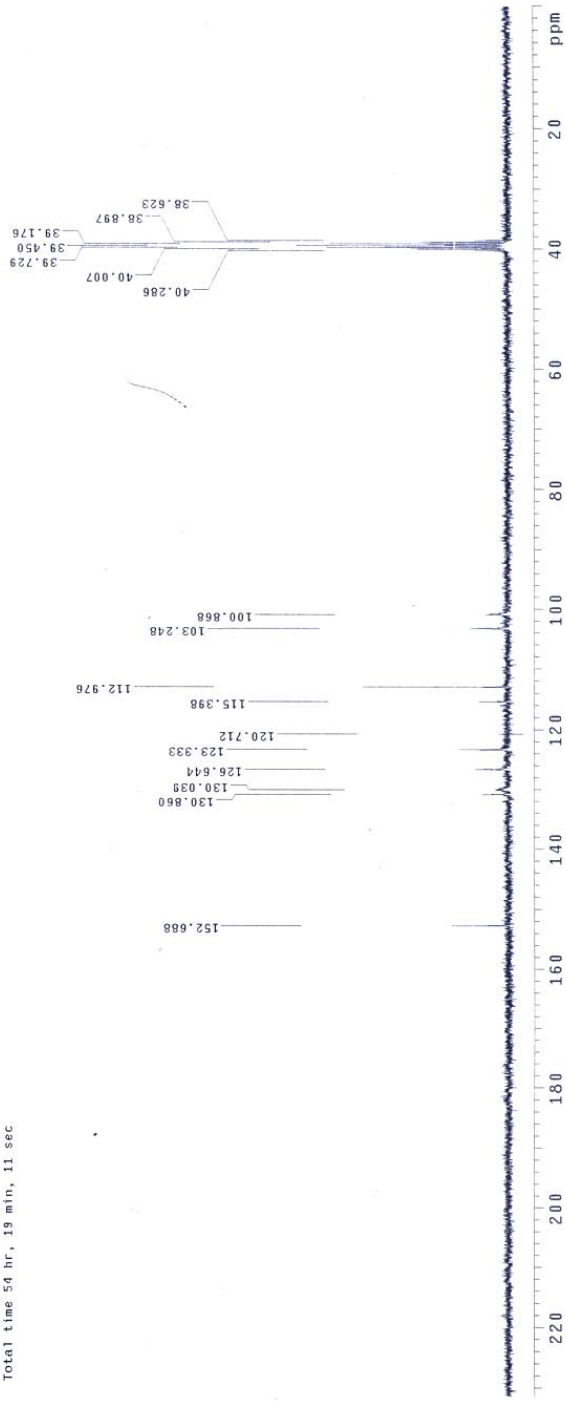
O
N
NH

3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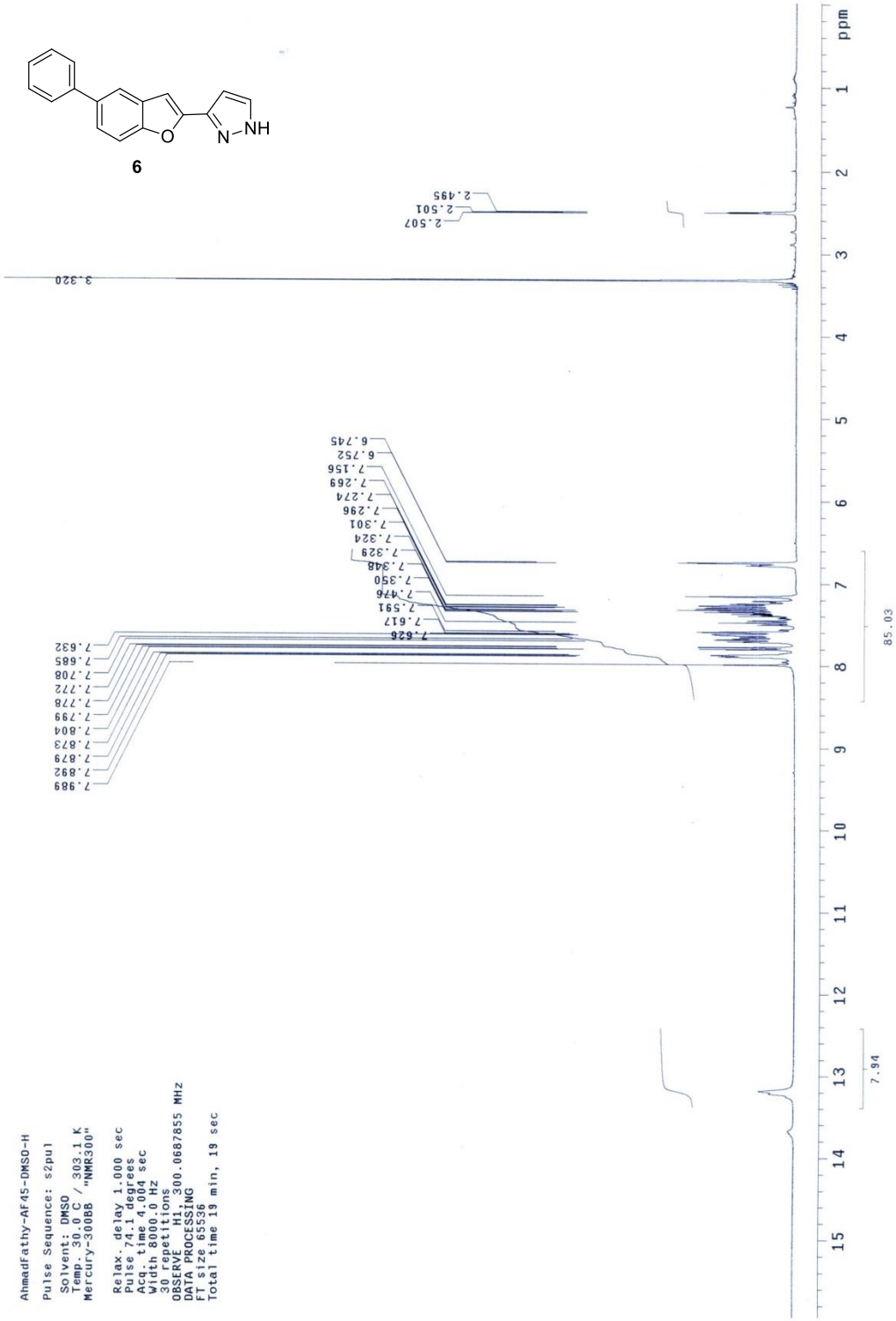
Solvent: DMSO
Temp. 30.0 C / 303.1 K
File: Ahmadfathy-ENHH-DMSO-C13
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18863.1 Hz
648 repetitions
OBSERVE C13, 75.4523858 MHz
DECOUPLE H1, 300.0702829 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 54 hr, 19 min, 11 sec
ppm
20
40
60
80
100
120
140
160
180
200
220
38.623
38.897
39.176
39.450
39.729
40.007
40.286
100.868
103.248
112.976
115.398
120.712
123.333
126.644
130.039
130.860
152.688

6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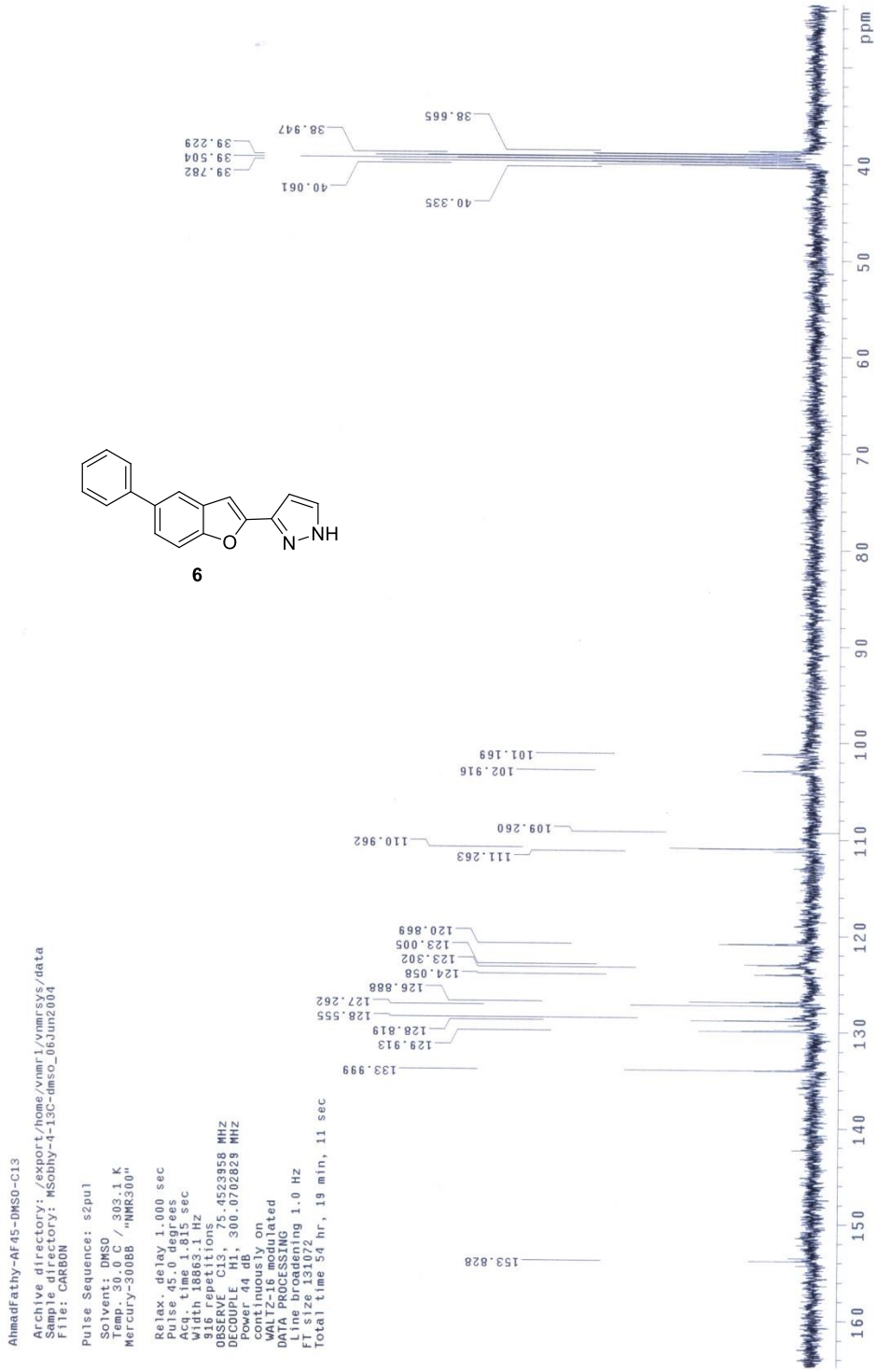
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 74.1 degrees
Acq. time 4.004 sec
Width 8000.0 Hz
30 repetitions
OBSERVE H1, 300.0687855 MHz
DATA PROCESSING
FT size 65536
Total time 19 min, 19 sec
7.989
7.892
7.879
7.873
7.804
7.799
7.778
7.772
7.708
7.685
7.632
7.626
7.617
7.591
7.476
7.350
7.348
7.329
7.324
7.301
7.296
7.274
7.269
7.156
6.752
6.745
3.320
2.507
2.501
2.495
85.03
7.94
ppm

6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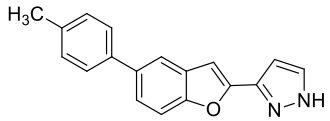
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: MSobhy-4-13C-dmso_06Jun2004
File: CARBON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18863.1 Hz
916 repetitions
OBSERVE C13, 75.4523958 MHz
DECOUPLE H1, 300.0702829 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 54 hr, 19 min, 11 sec
153.828
133.999
129.913
128.819
128.555
127.262
126.888
124.058
123.302
123.005
120.869
111.263
110.962
109.260
102.916
101.169
40.335
40.061
39.782
39.504
39.229
38.947
38.665
ppm



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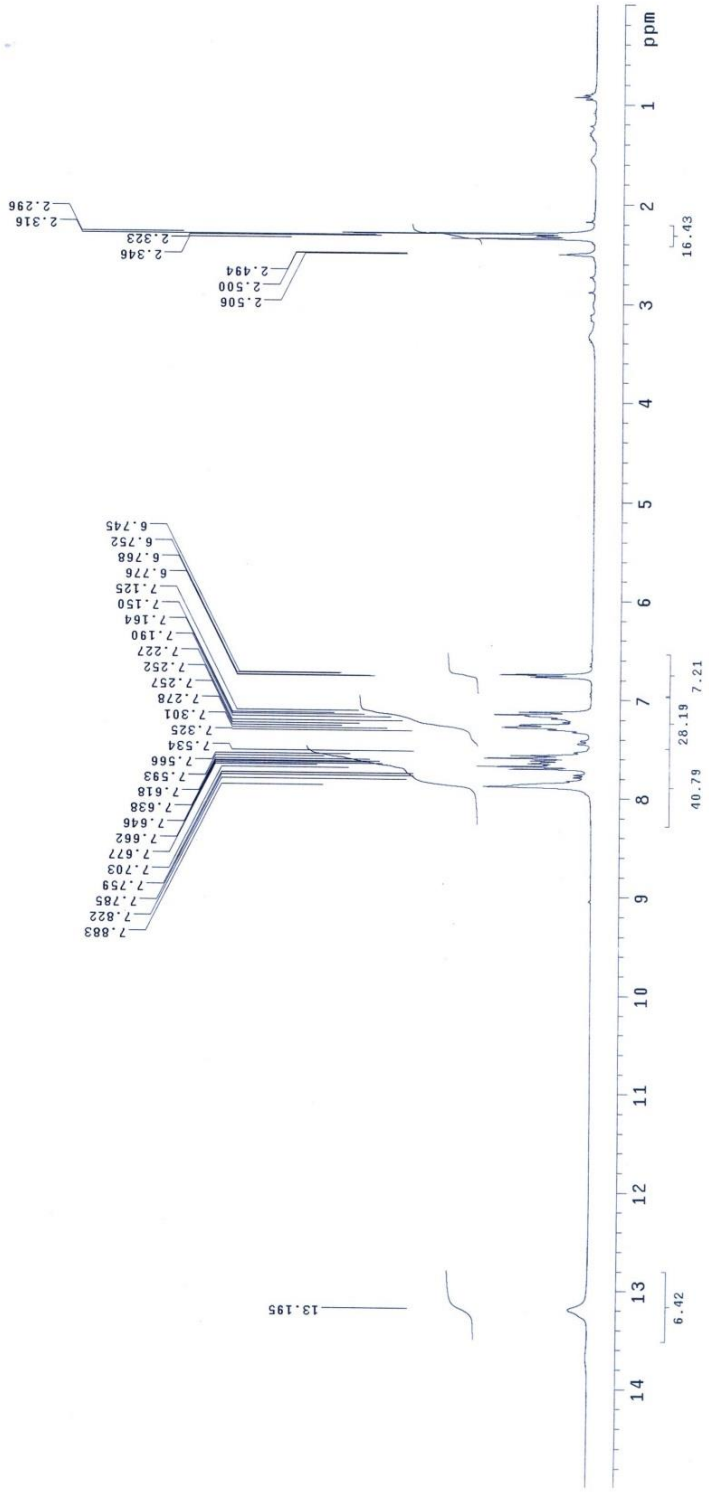

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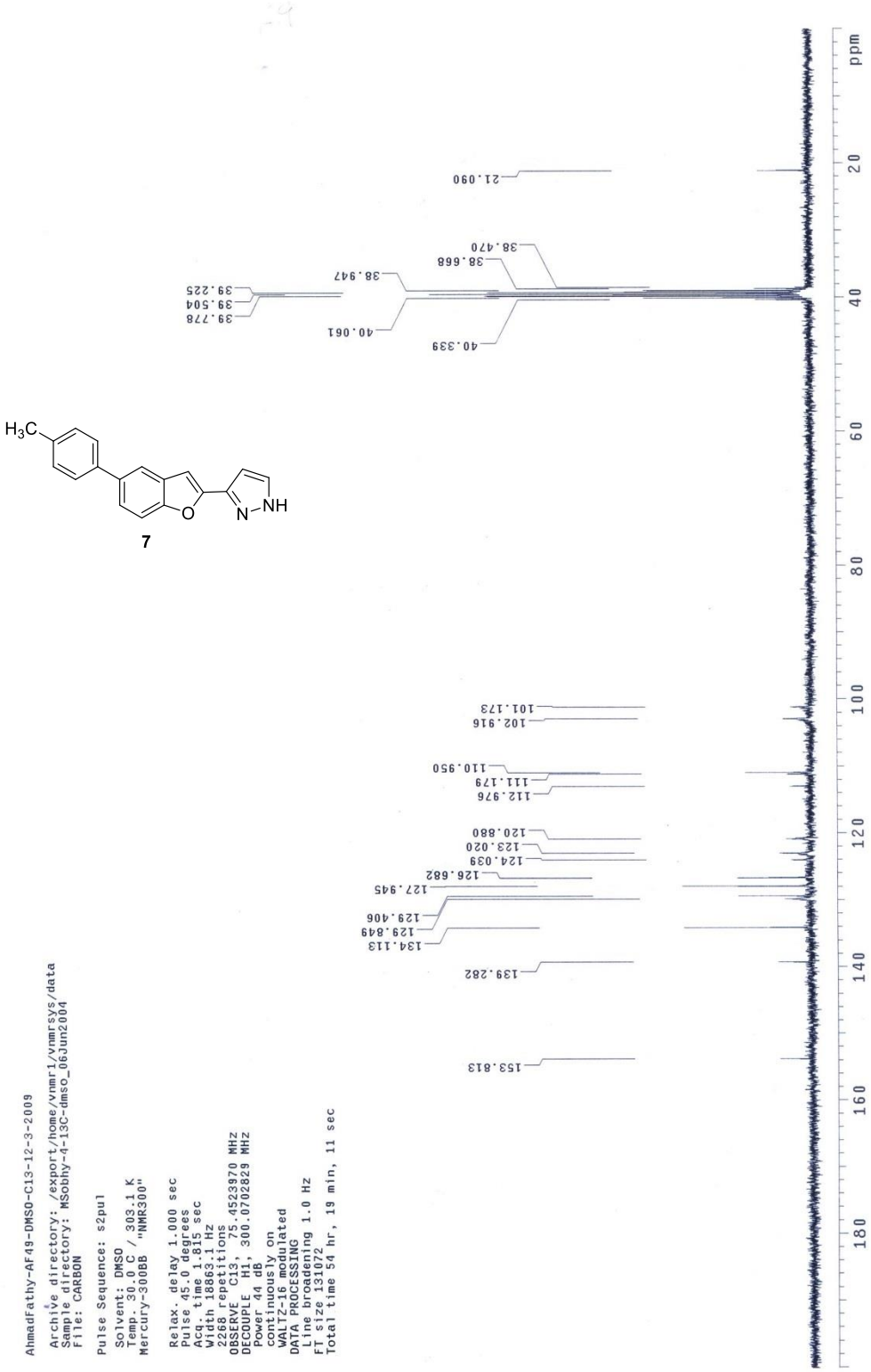
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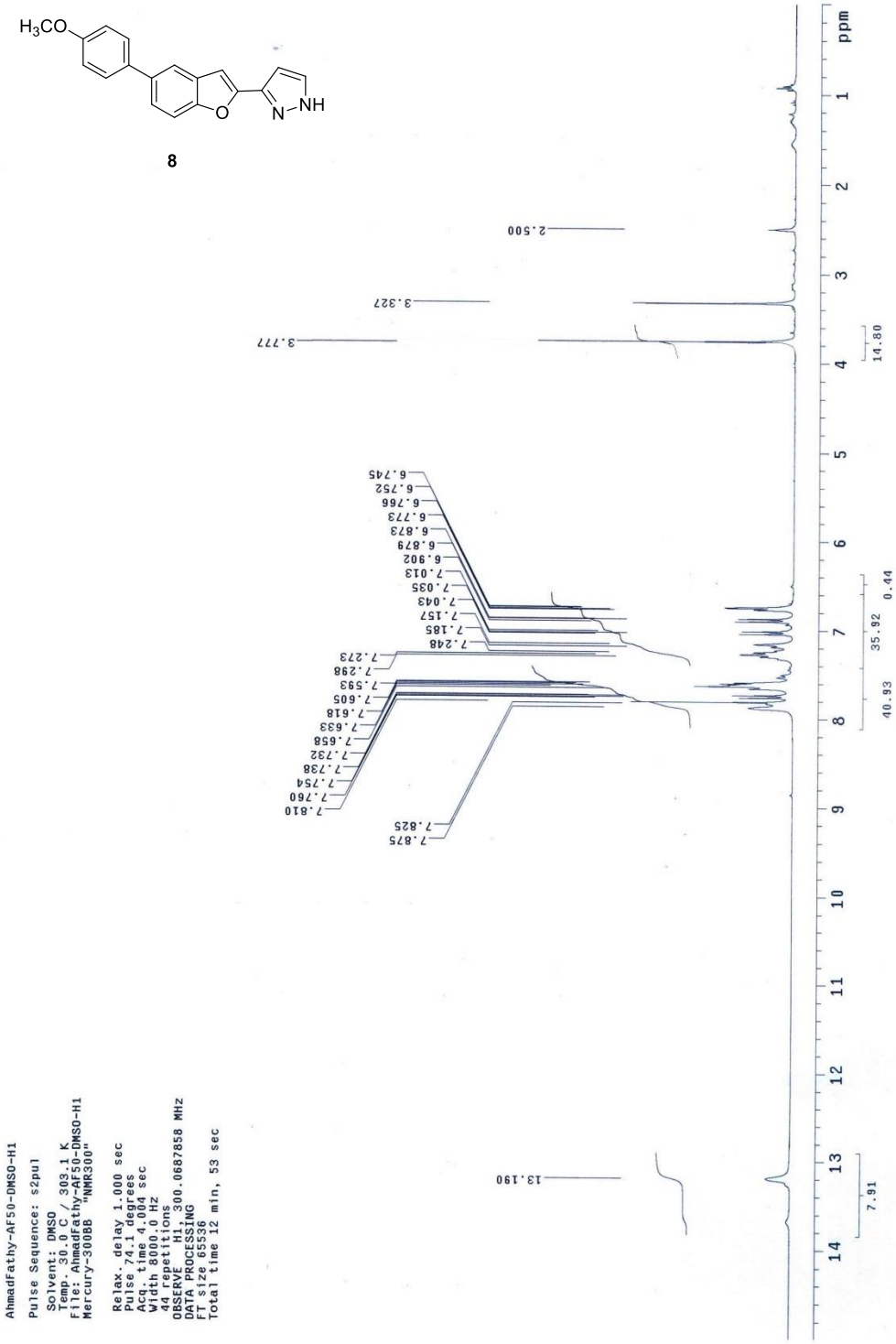
File: CARBON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18863.1 Hz
2268 repetitions
OBSERVE C13, 75.4523970 MHz
DECOUPLE H1, 300.0702829 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 54 hr, 19 min, 11 sec
153.813
139.282
134.113
129.849
129.406
127.945
126.682
124.039
123.020
120.880
112.976
111.179
110.950
102.916
101.173
40.339
40.061
39.778
39.504
39.225
38.947
38.668
38.470
21.090
ppm
20
40
60
80
100
120
140
160
180
H3C
O
N
NH
7

8



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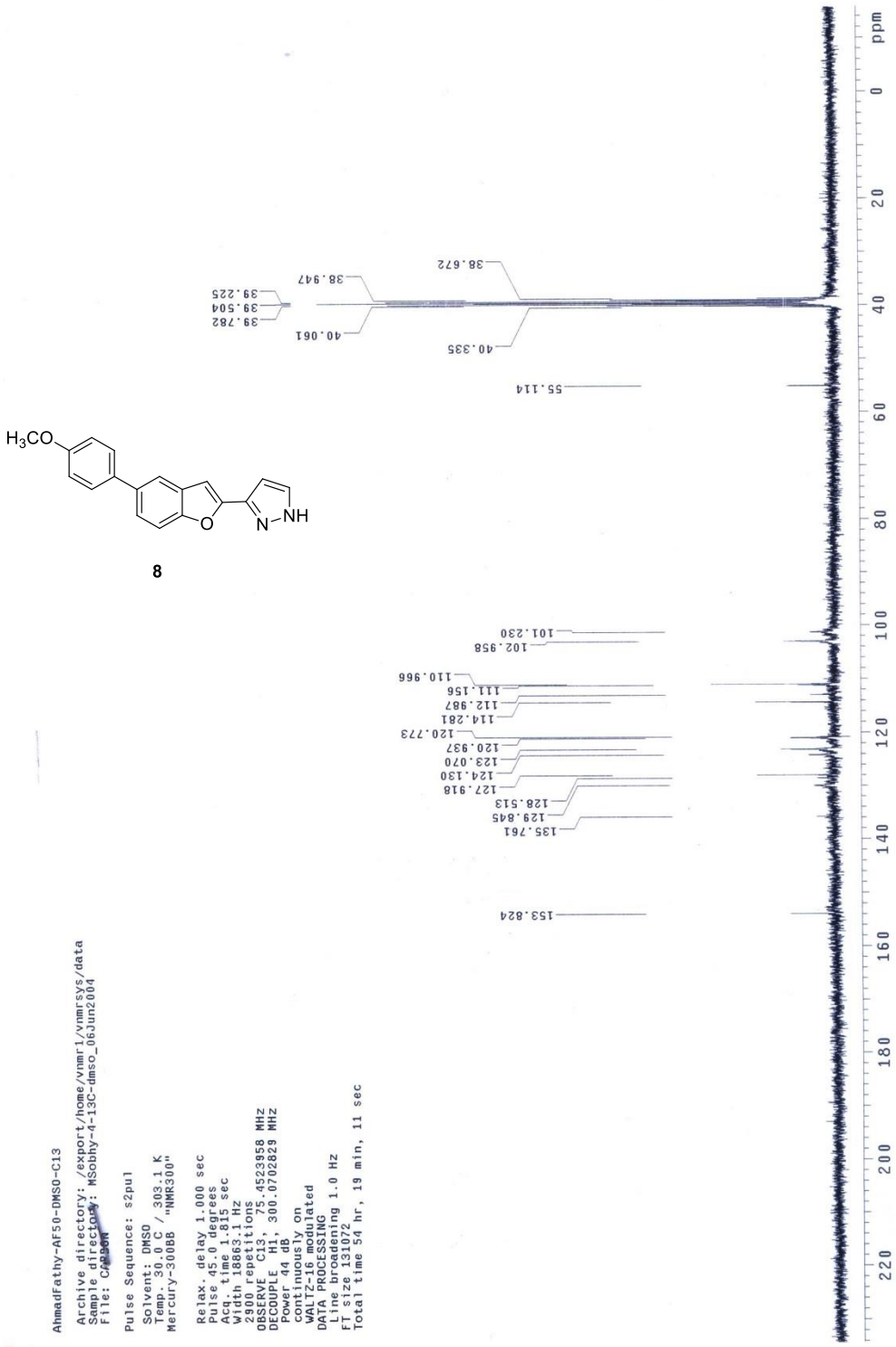
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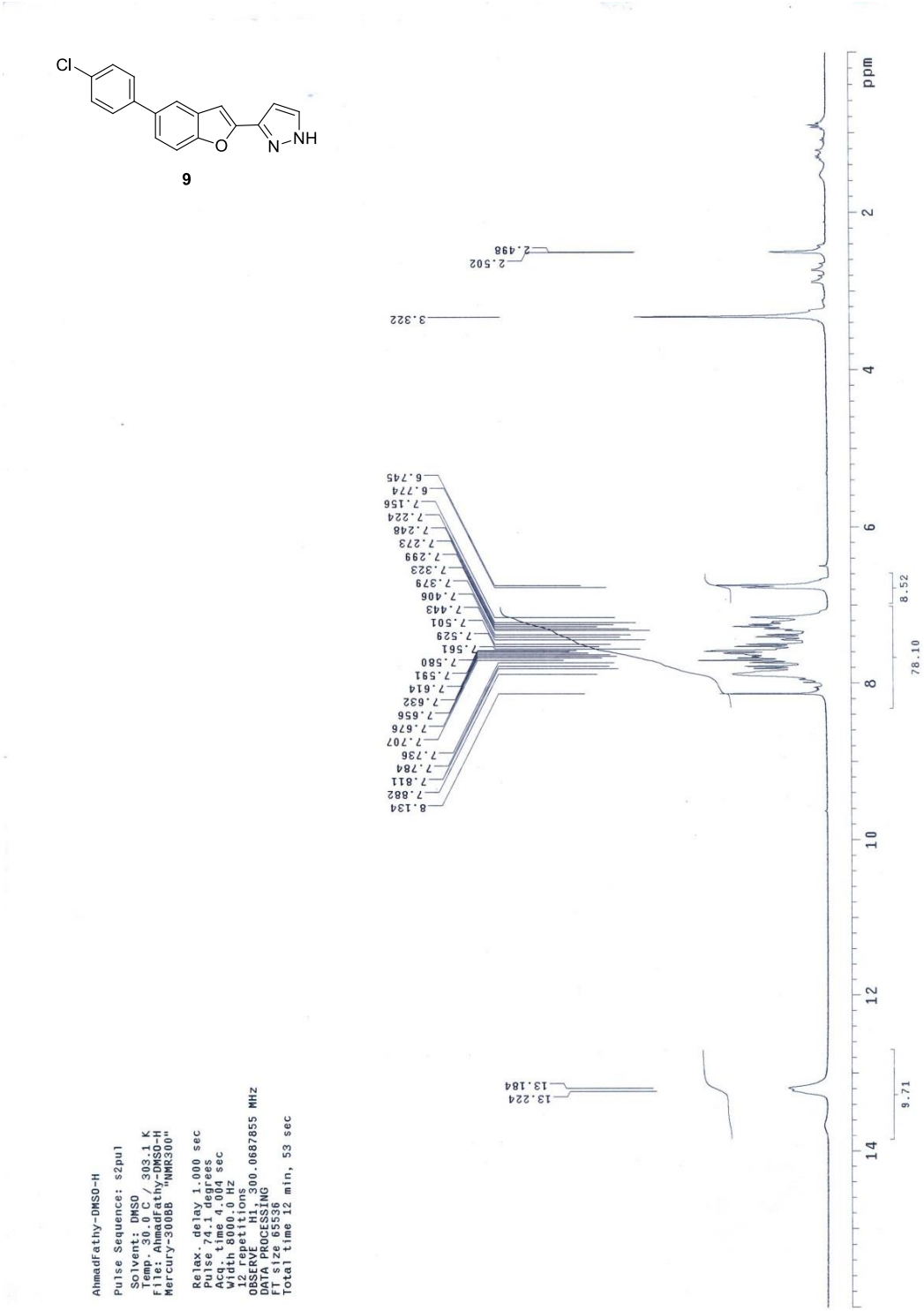
Sample directory: MSobhy-4-13C-dmso_06Jun2004
File: CARBON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18863.1 Hz
2800 repetitions
OBSERVE C13, 75.4523958 MHz
DECOUPLE H1, 300.0702829 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 54 hr, 19 min, 11 sec
153.824
135.761
129.845
128.513
127.918
124.130
123.070
120.937
120.773
114.281
112.987
111.156
110.966
102.958
101.230
55.114
40.335
40.061
39.782
39.504
39.225
38.947
38.672
ppm
0
20
40
60
80
100
120
140
160
180
200
220

H_3CO

8

9


AhmadFathy-DMSO-H
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
File: AhmadFathy-DMSO-H
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 74.1 degrees
Acq. time 4.004 sec
Width 8000.0 Hz
1 repetitions
OBSERVE H1, 300.0687855 MHz
DATA PROCESSING
FT size 65536
Total time 12 min, 53 sec
ppm
2
4
6
8
10
12
14
13.224
13.184
8.134
7.882
7.811
7.784
7.736
7.707
7.676
7.656
7.632
7.614
7.591
7.580
7.561
7.529
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7.323
7.299
7.273
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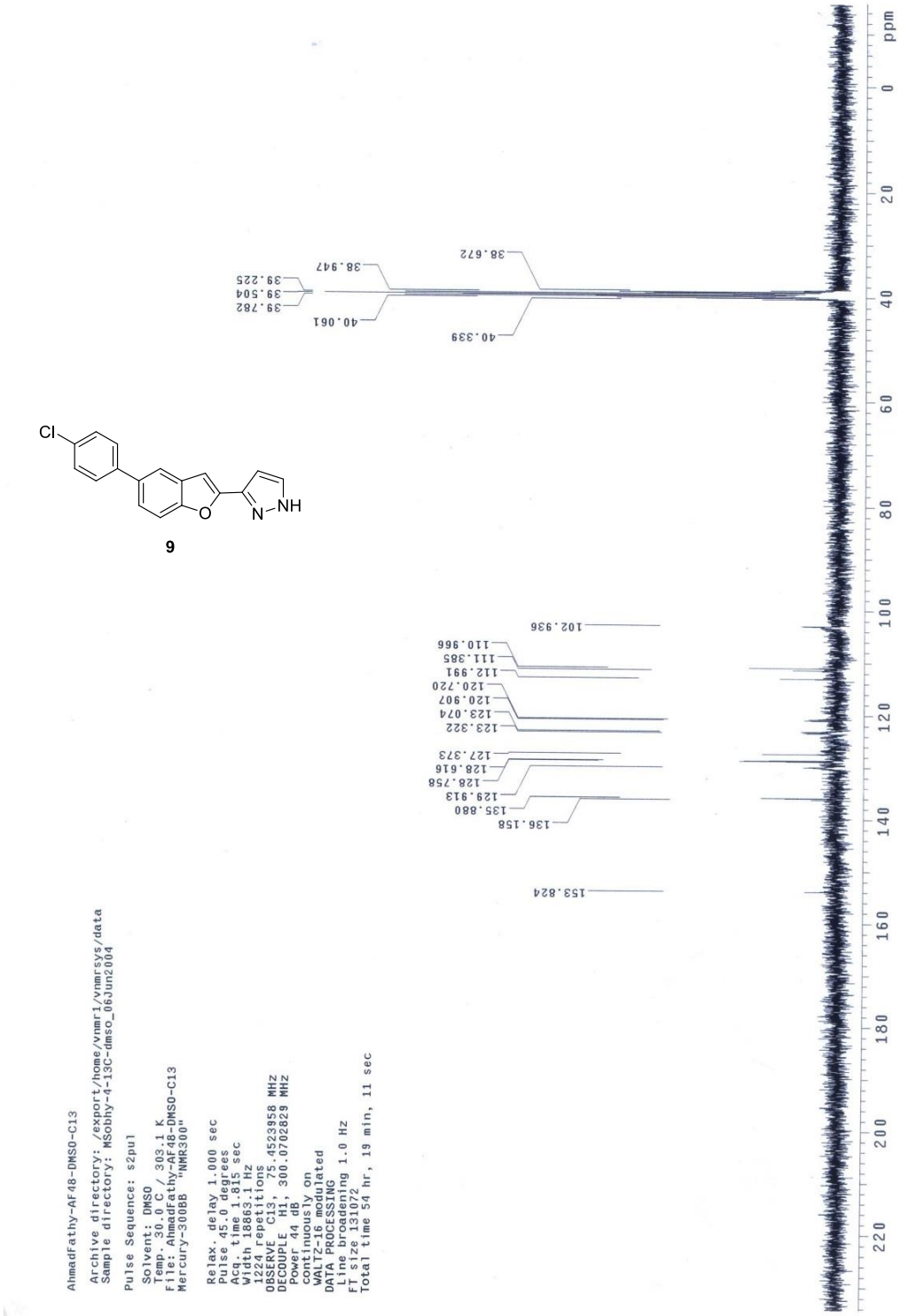
6.745
3.322
2.502
2.498
8.52
78.10
9.71

9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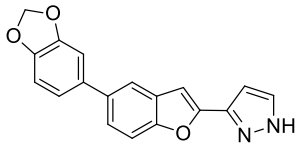
Sample directory: NSobhy-4-13C-dmso_06Jun2004
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
File: AhmadFathy-AF48-DMSO-C13
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18863.1 Hz
1224 repetitions
OBSERVE C13, 75.4523958 MHz
DECOUPLE H1, 300.0702829 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 54 hr, 19 min, 11 sec
153.824
136.158
135.880
129.913
128.758
128.616
127.373
123.322
123.074
120.907
120.720
112.991
111.385
110.966
102.936
40.339
40.061
39.782
39.504
39.225
38.947
38.672
ppm



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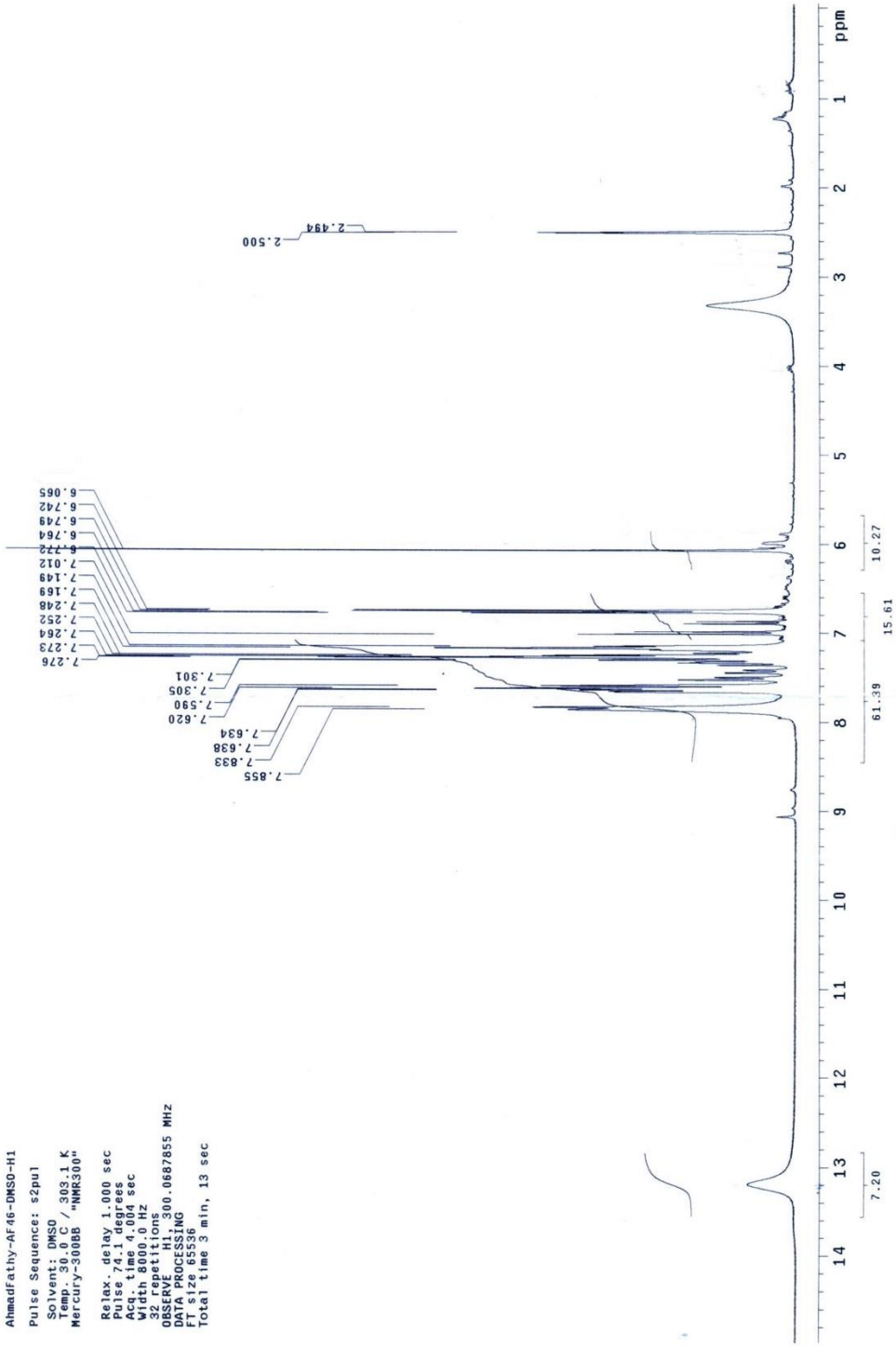
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Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 74.1 degrees
Acq. time 4.000 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 300.0687855 MHz
DATA PROCESSING
FT size 65536
Total time 3 min, 13 sec
ppm
2.500
2.494
7.855
7.833
7.638
7.634
7.620
7.590
7.305
7.301
7.276
7.273
7.264
7.252
7.246
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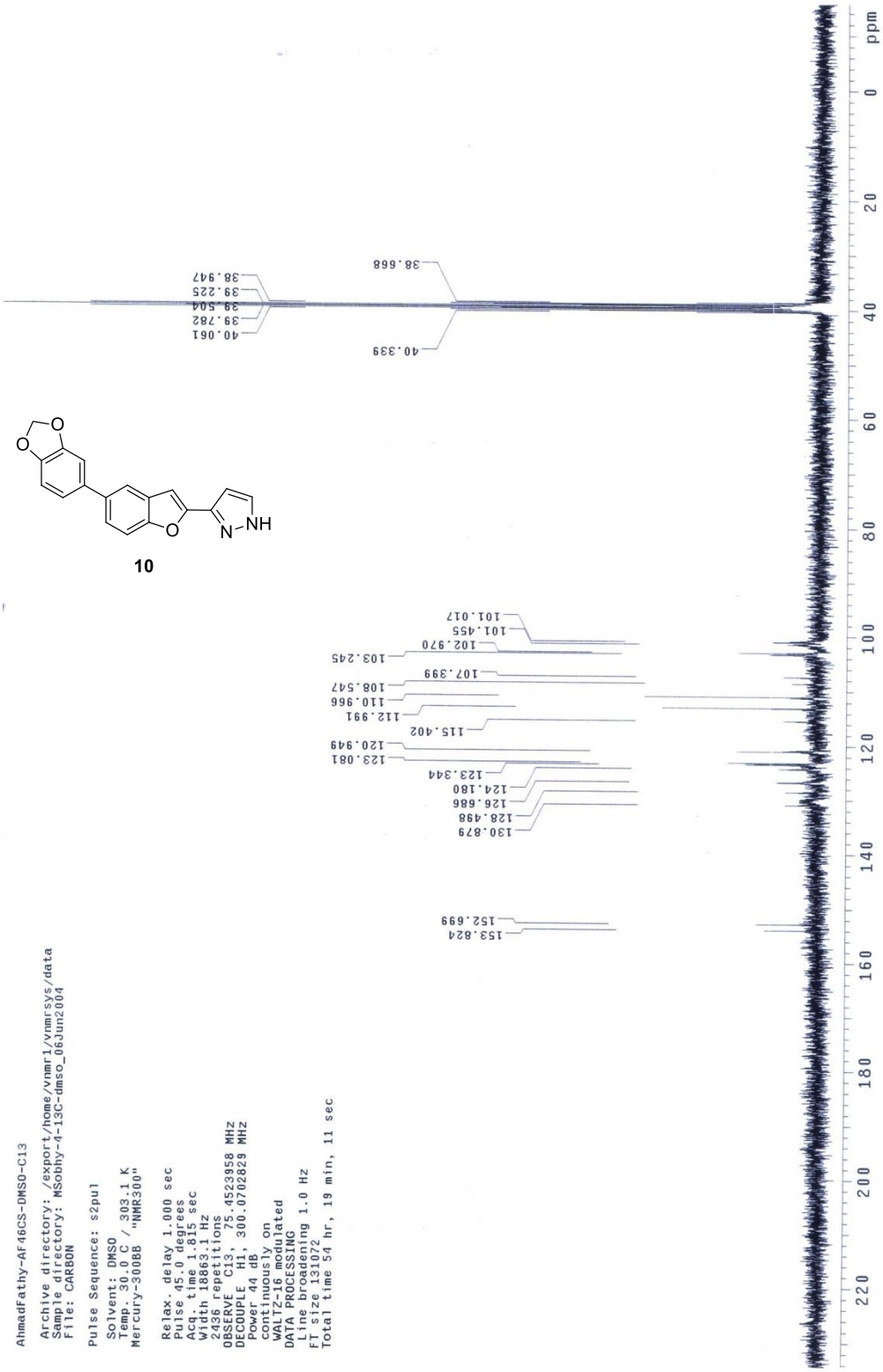

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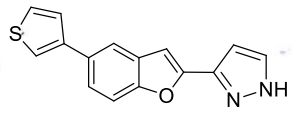

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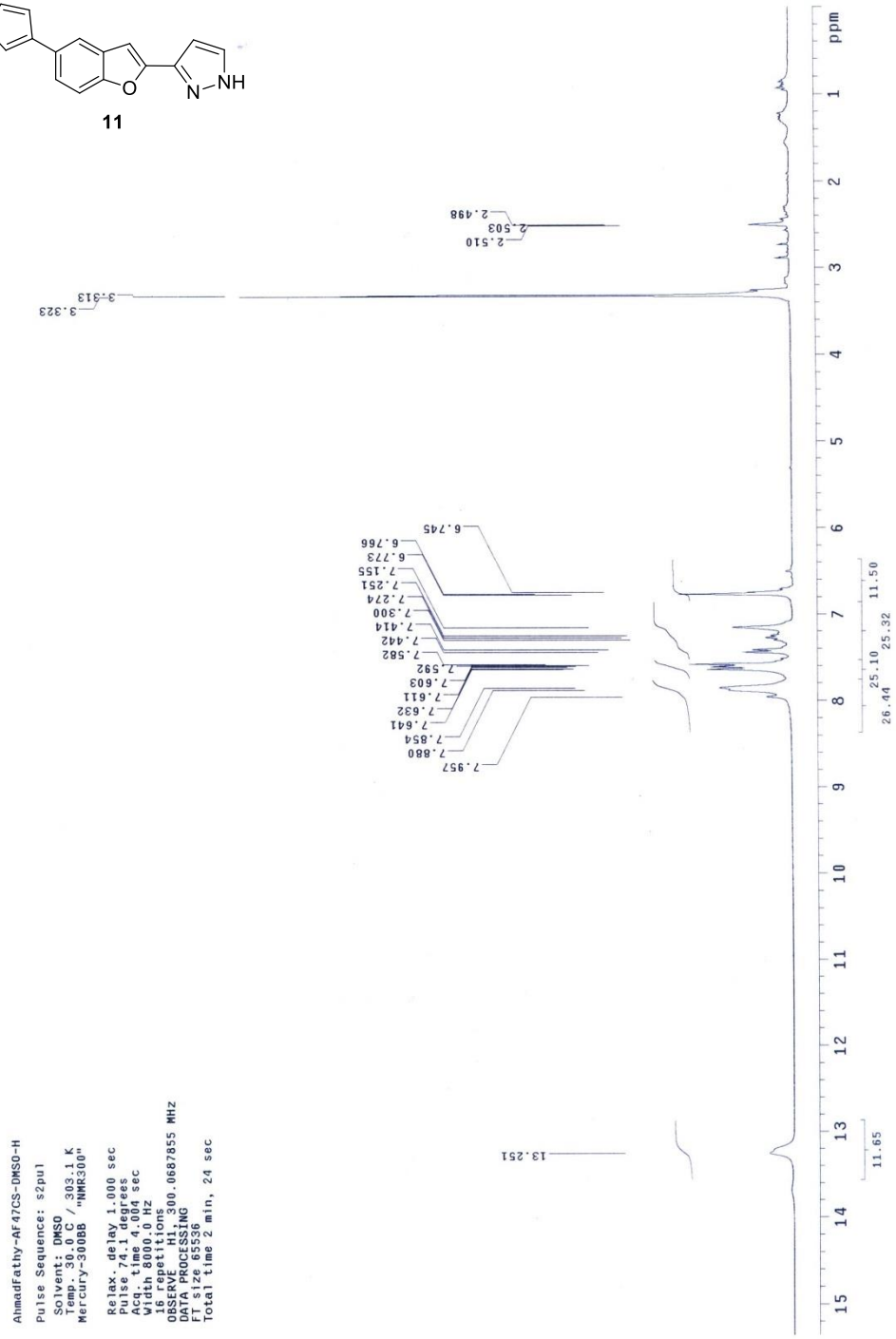

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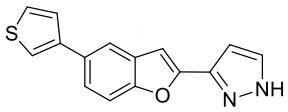

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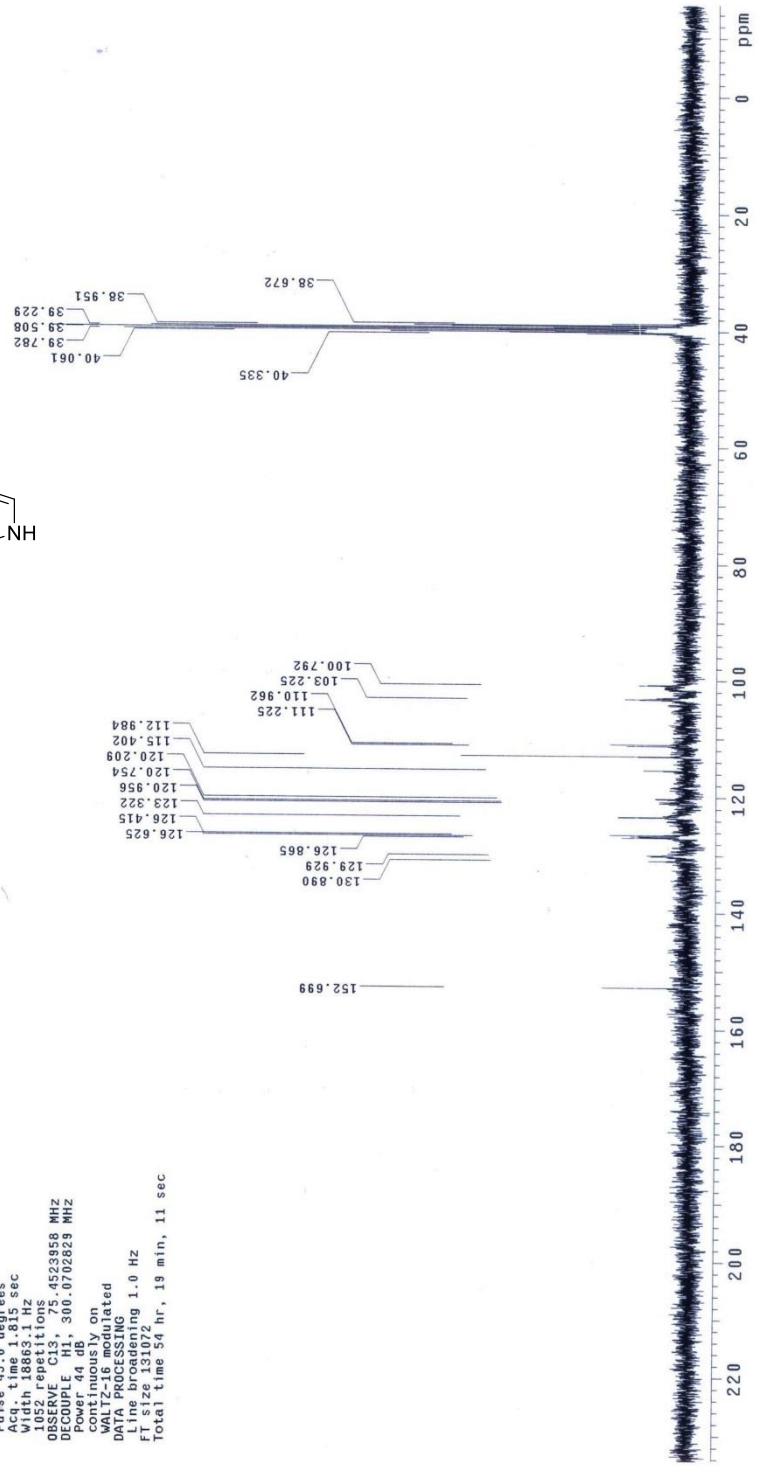
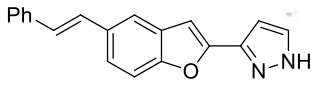

AhmadFathy-AF47-DMSO-C13
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: MSobhy-4-13C-dmso_06Jun2004
File: CARBON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.835 sec
Width 18863.1 Hz
1052 repetitions
OBSERVE C13, 75.4523958 MHz
DECOUPLE H1, 300.0702829 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 54 hr, 19 min, 11 sec
38.672
38.951
39.229
39.508
39.782
40.061
40.335
100.792
103.225
110.962
111.225
112.984
115.402
120.209
120.754
120.956
123.322
126.415
126.625
126.865
129.929
130.890
152.699
ppm



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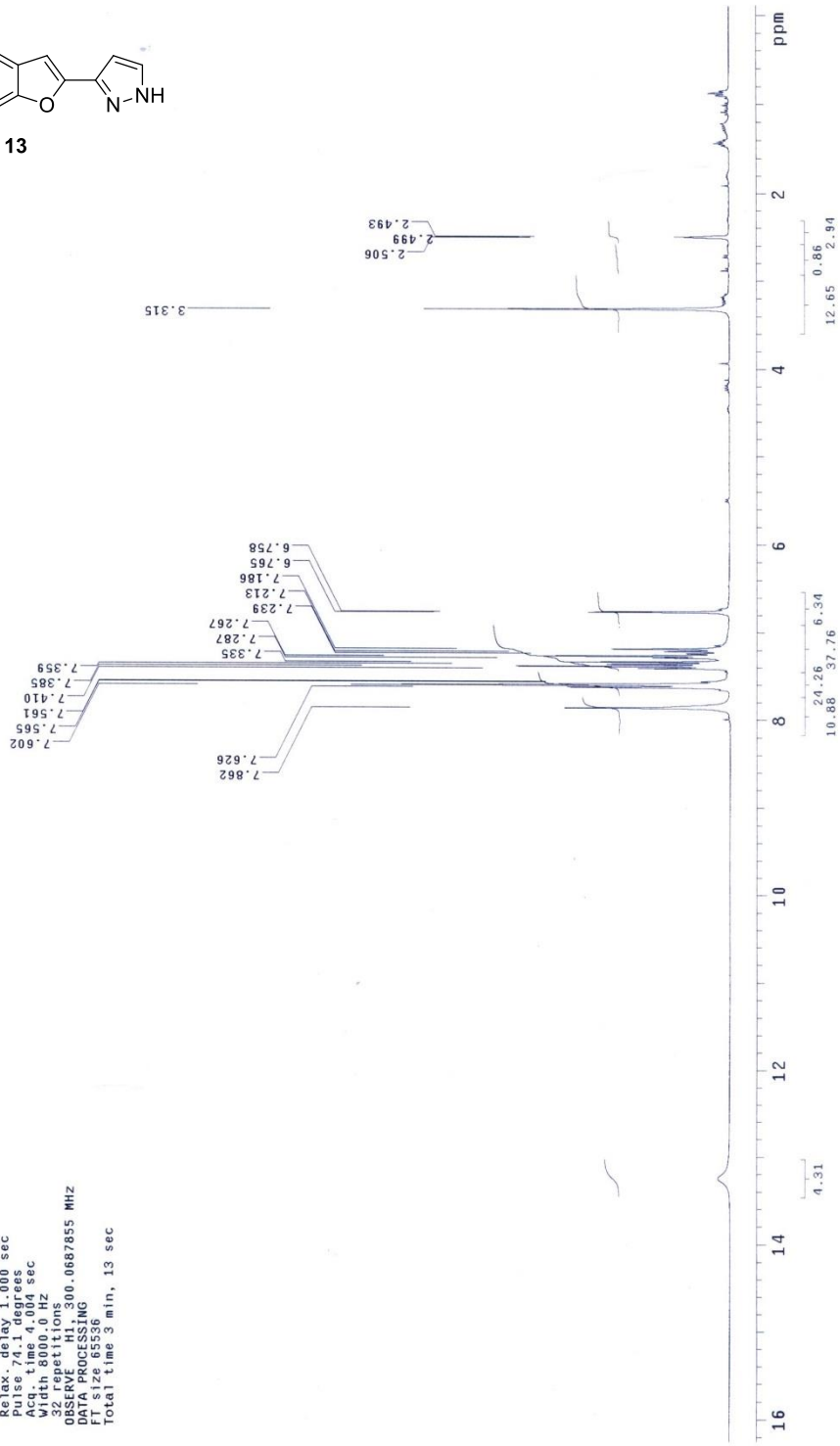

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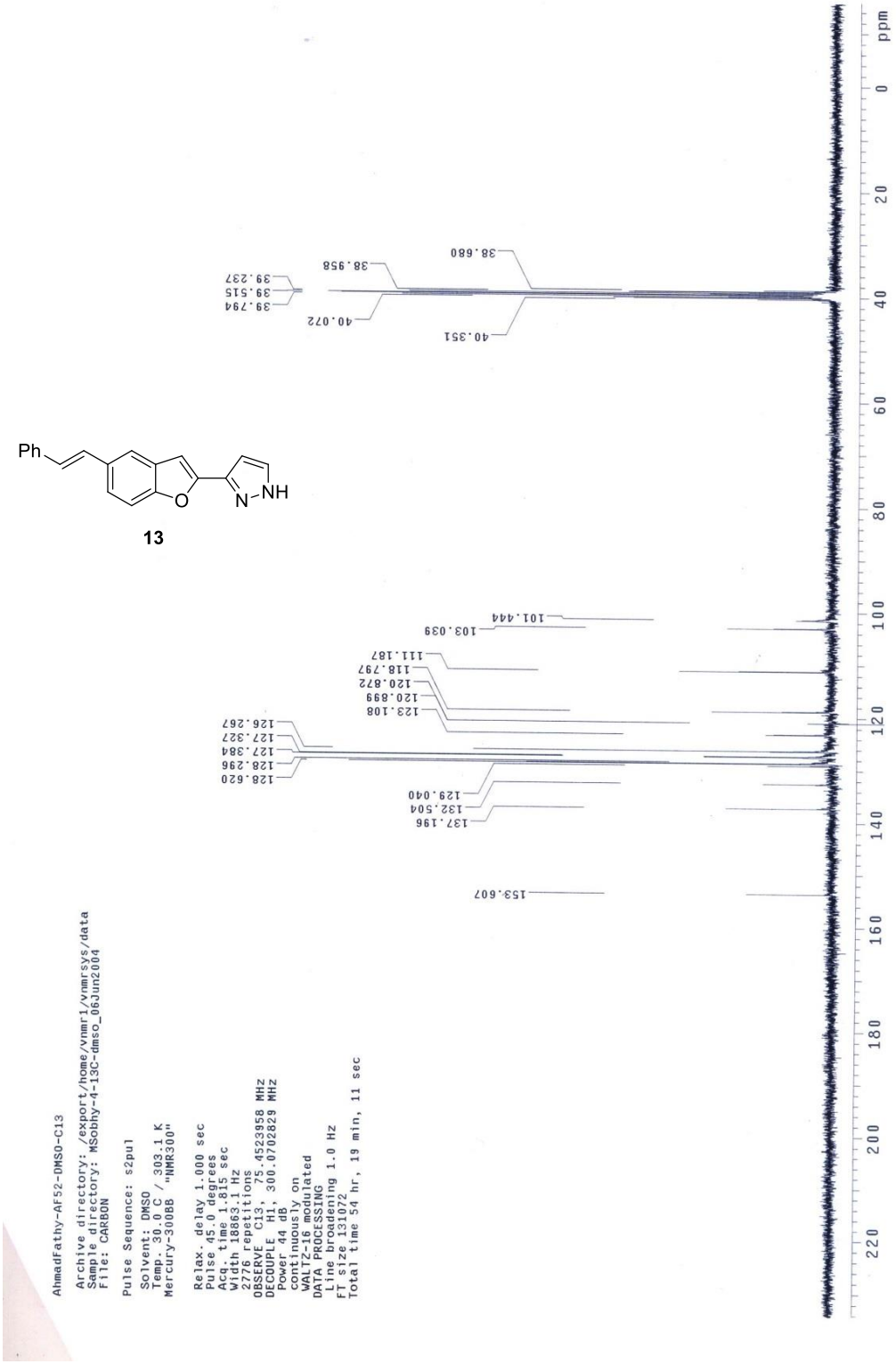
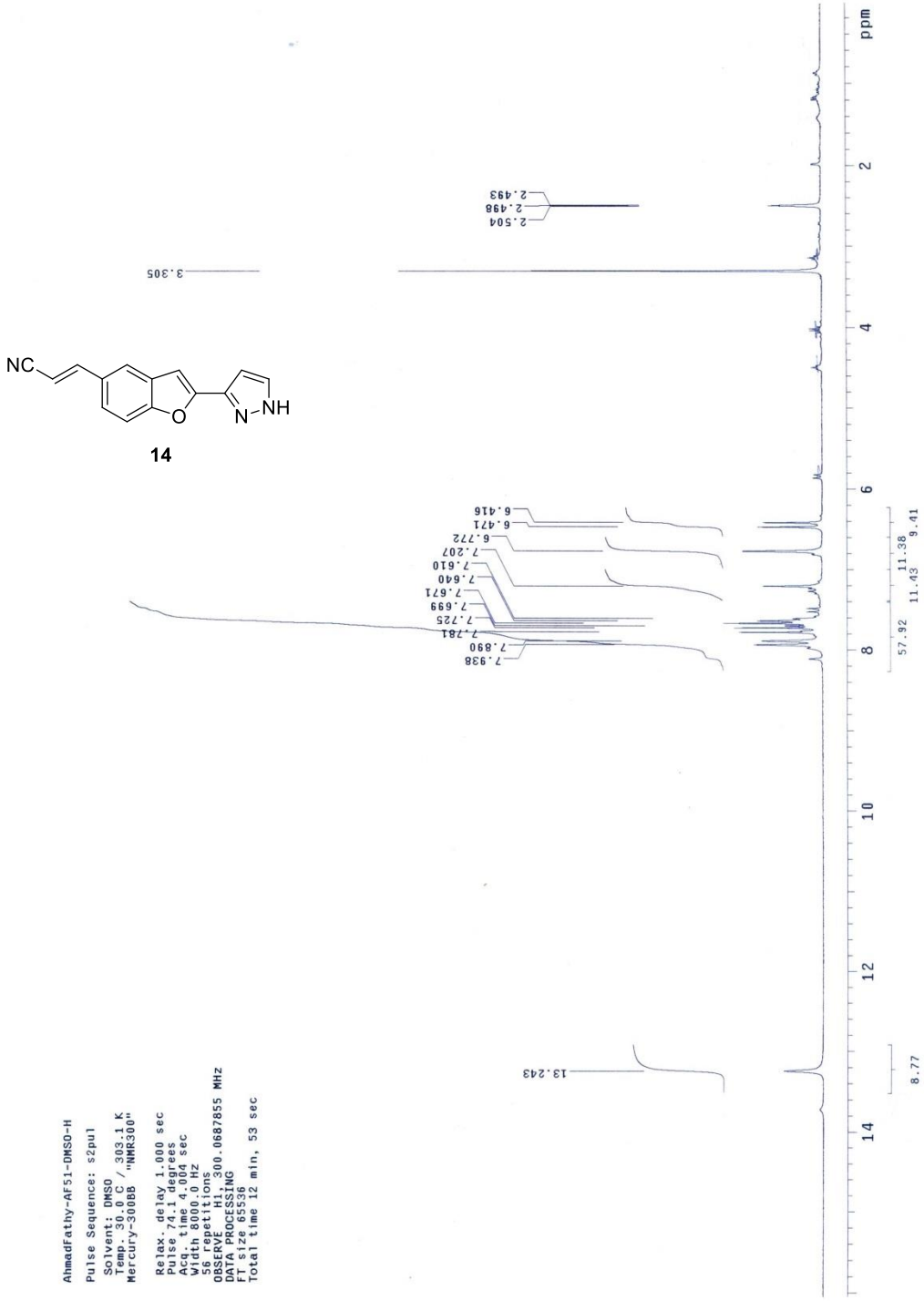
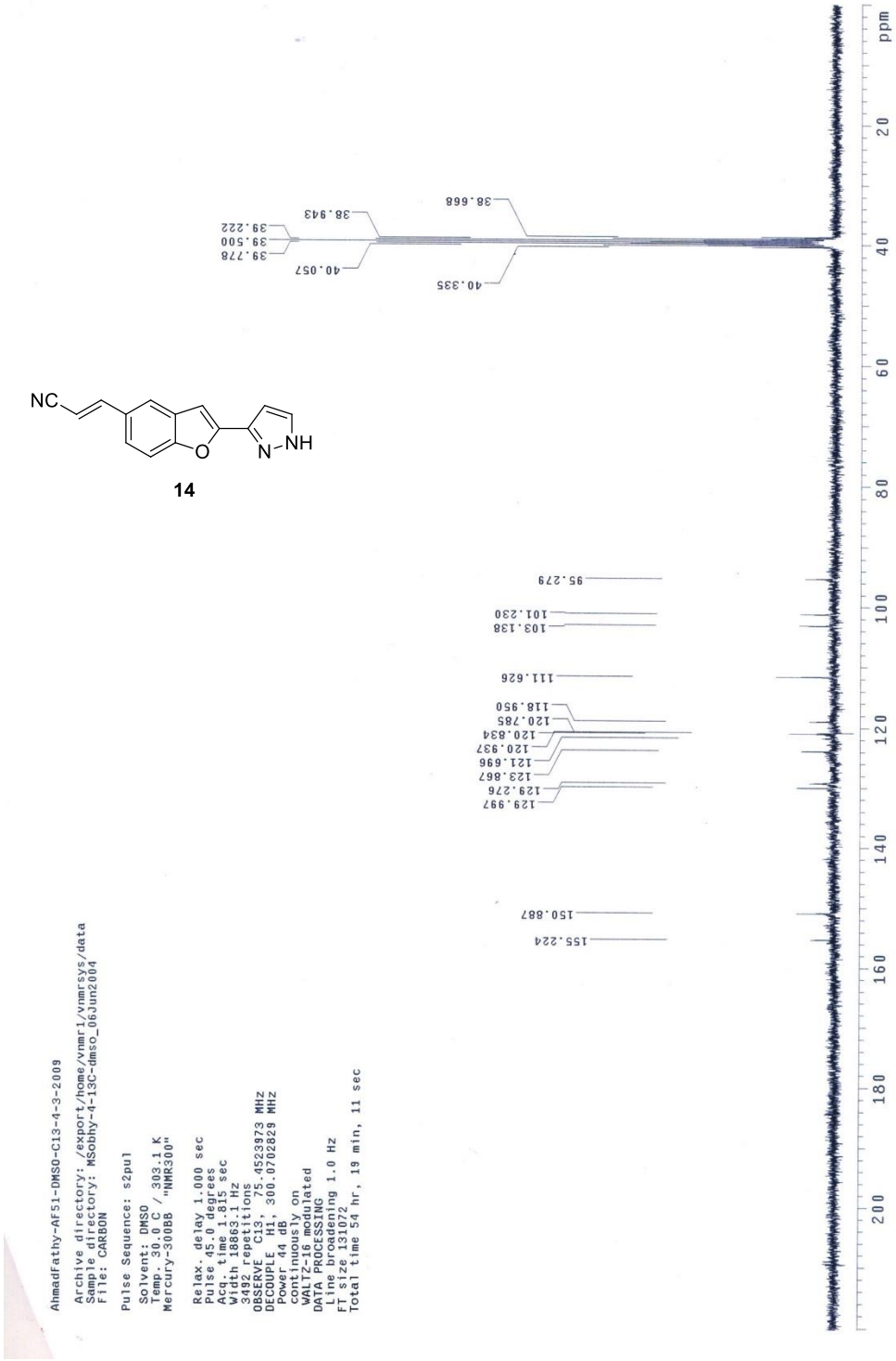
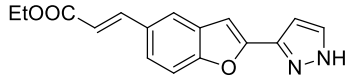

Ph
O
N
NH
13
AhmadFathy-AF52-DMSO-C13
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: MSobhy-4-13C-dmso_06Jun2004
File: CARBON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.835 sec
Width 18863.1 Hz
2776 repetitions
OBSERVE C13, 75.4523958 MHz
DECOUPLE H1, 300.0702829 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 54 hr, 19 min, 11 sec
38.680
38.958
39.237
39.515
39.794
40.072
40.351
101.444
103.039
111.187
118.797
120.872
120.899
123.108
126.267
127.327
127.384
128.296
128.620
129.040
132.504
137.196
153.607
ppm


NC
O
N
NH
14
AhmadFathy-AF51-DMSO-H
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 74.1 degrees
Acq. time 4.004 sec
Width 8000.0 Hz
56 repetitions
OBSERVE H1, 300.0687855 MHz
DATA PROCESSING
FT size 65536
Total time 12 min, 53 sec
ppm
2
4
6
8
10
12
14
13.243
7.938
7.890
7.781
7.725
7.699
7.671
7.640
7.610
7.207
6.772
6.471
6.416
3.305
2.504
2.498
2.493
57.92
11.43
11.38
9.41
8.77

NC
O
N
NH

14


AhmadFathy-AF51-DMSO-C13-4-3-2009
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: MSobhy-4-13C-dmso_06Jun2004
File: CARBON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18863.1 Hz
3492 repetitions
OBSERVE C13, 75.4523973 MHz
DECOUPLE H1, 300.0702829 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 54 hr, 19 min, 11 sec
38.668
38.943
39.222
39.500
39.778
40.057
40.335
95.279
101.230
103.138
111.626
118.950
120.785
120.834
120.937
121.696
123.867
129.276
129.997
150.887
155.224
ppm
20
40
60
80
100
120
140
160
180
200



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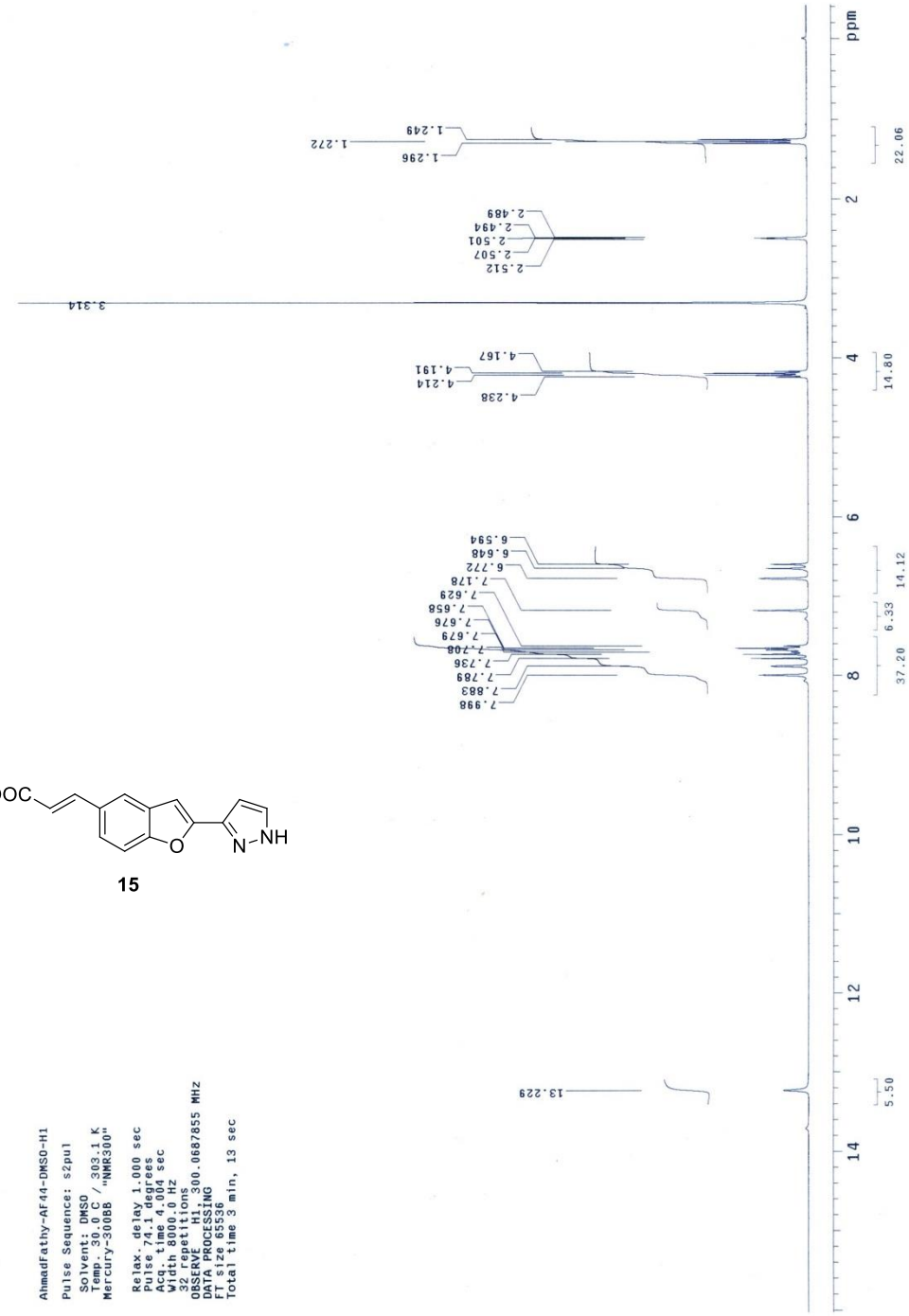

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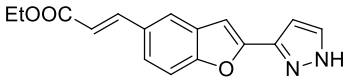

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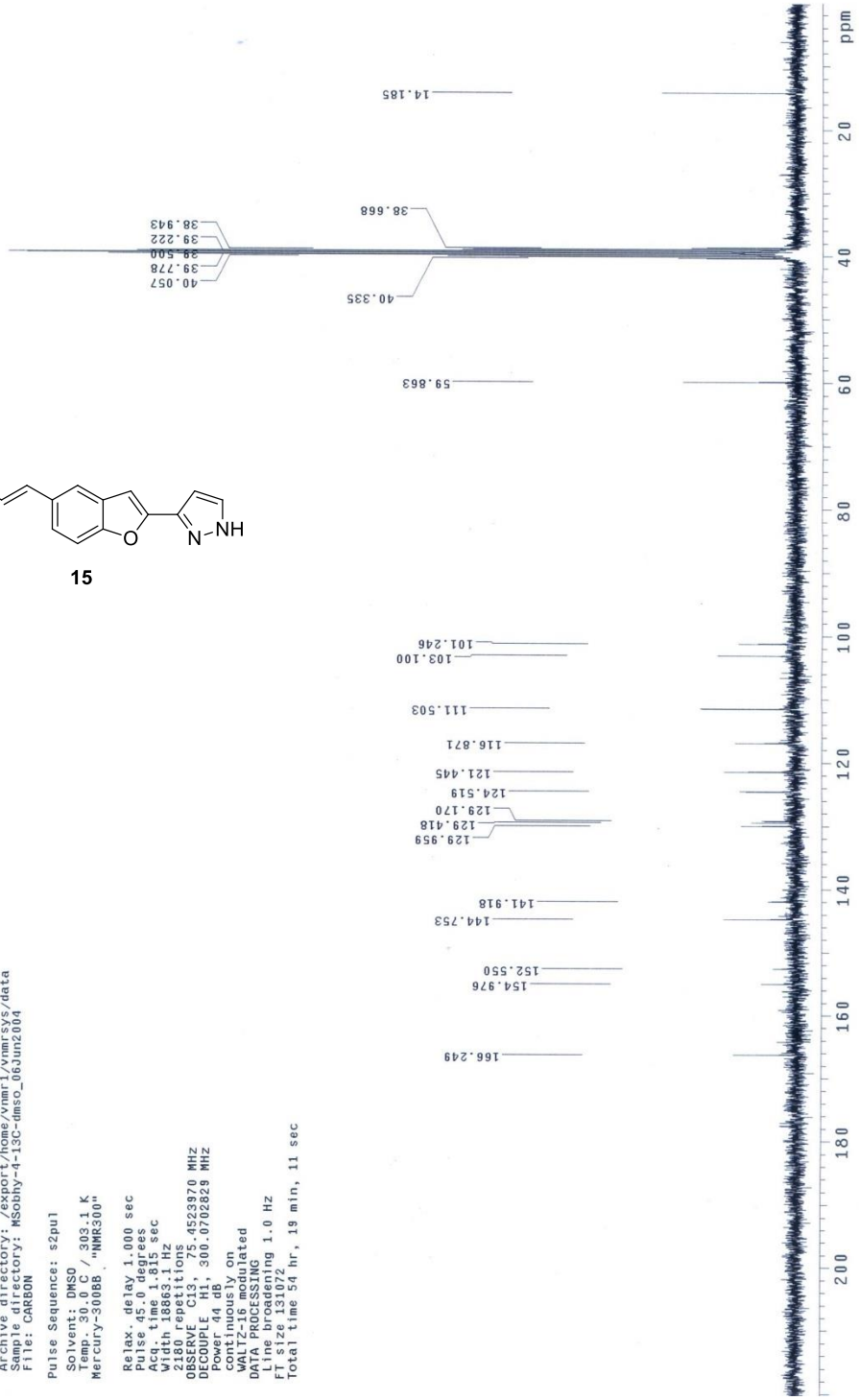


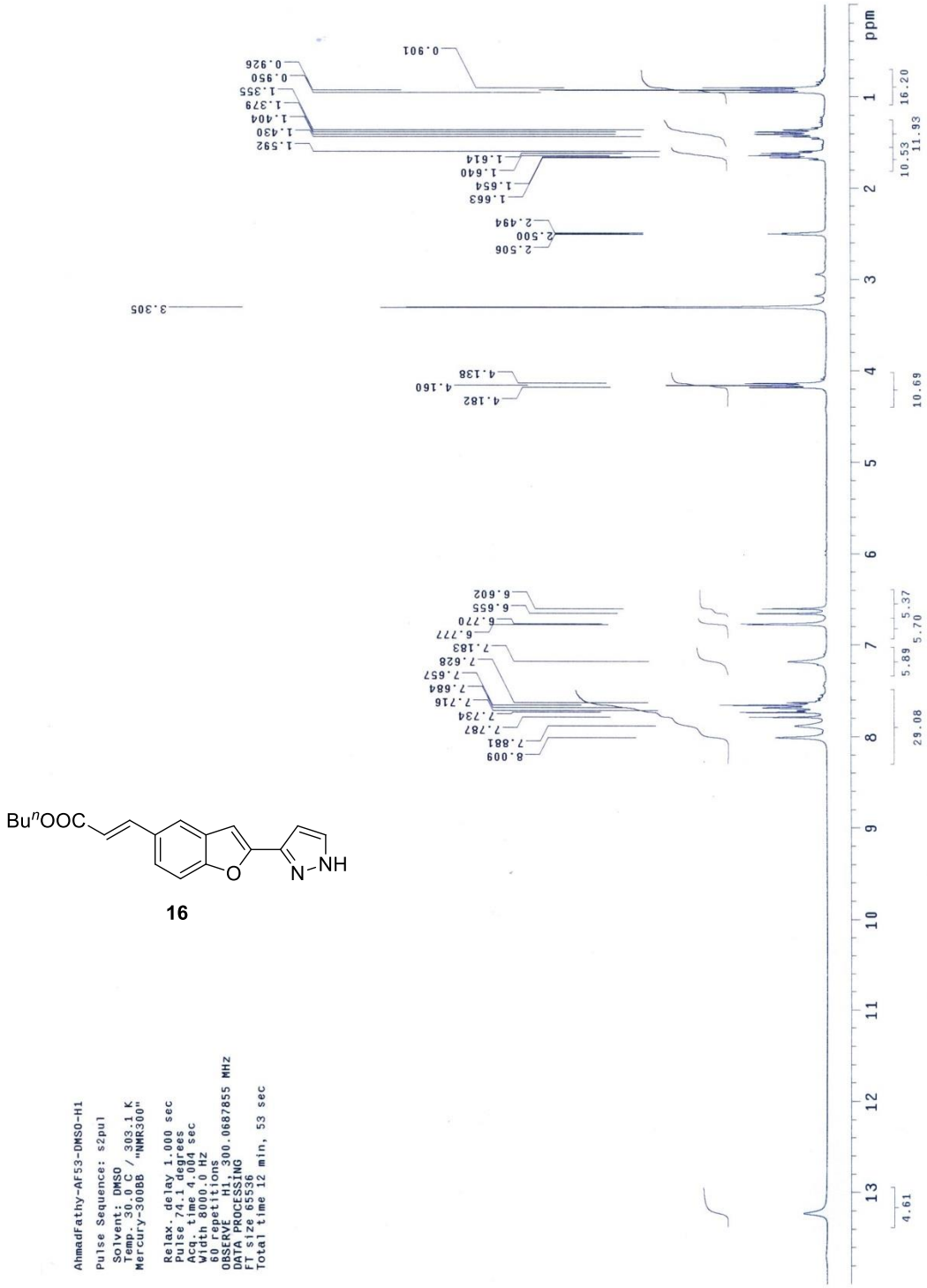
AhmadFathy-AF44-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: MSobhy-4-13C-dmso_06Jun2004
File: CARBON

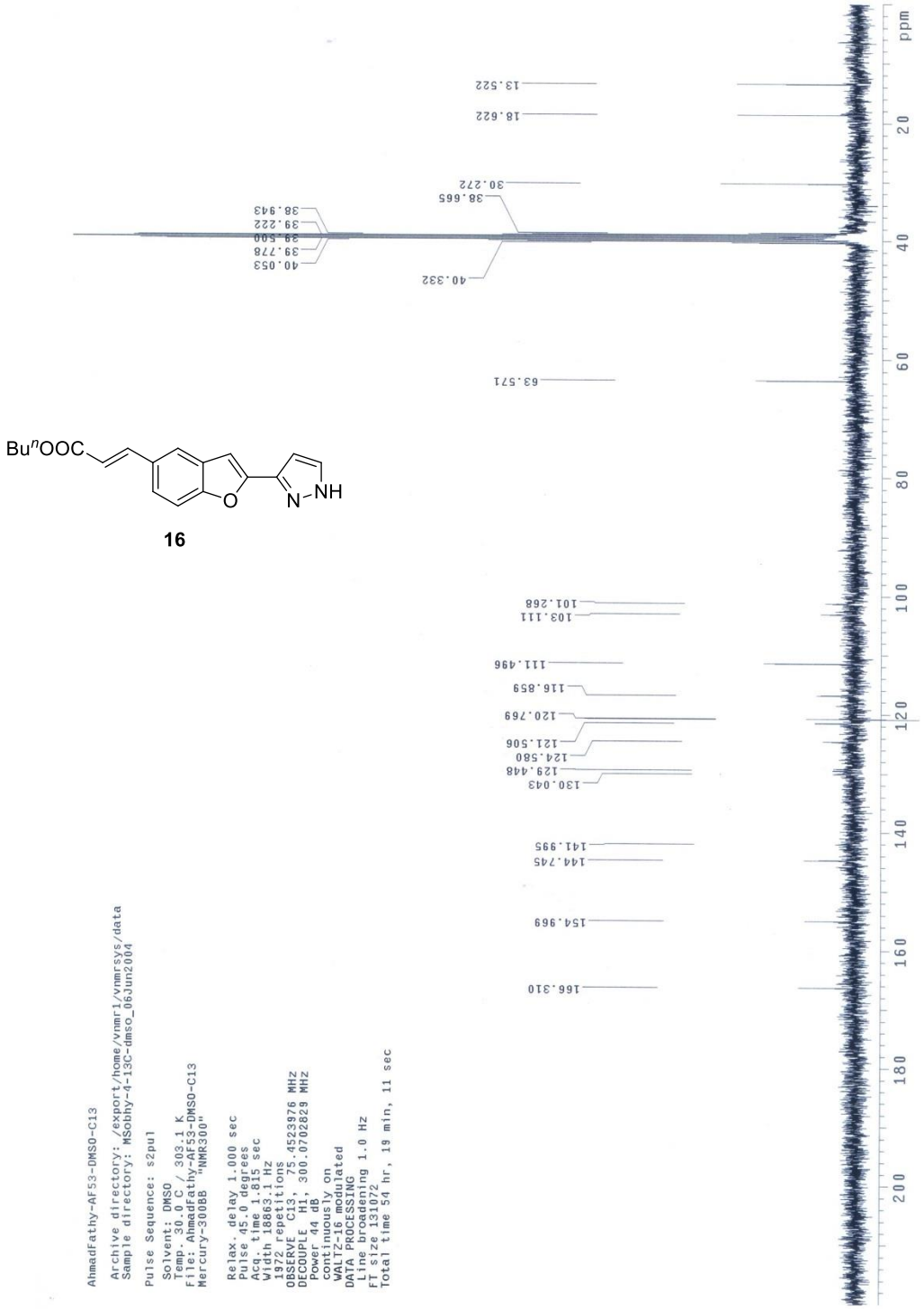
Pulse Sequence: s2pul

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18863.1 Hz
2180 repetitions
OBSERVE C13, 75.4523970 MHz
DECOUPLE H1, 300.0702829 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 54 hr, 19 min, 11 sec


AhmadFathy-AF53-DMSO-H1
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 74.1 degrees
Acq. time 4.084 sec
Width 8000.0 Hz
60 repetitions
OBSERVE H1, 300.0687855 MHz
DATA PROCESSING
FT size 65536
Total time 12 min, 53 sec
ppm
Bu^{n}OOC
O
N
NH

16



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