Electronic Supplementary Material (ESI) for ChemComm.
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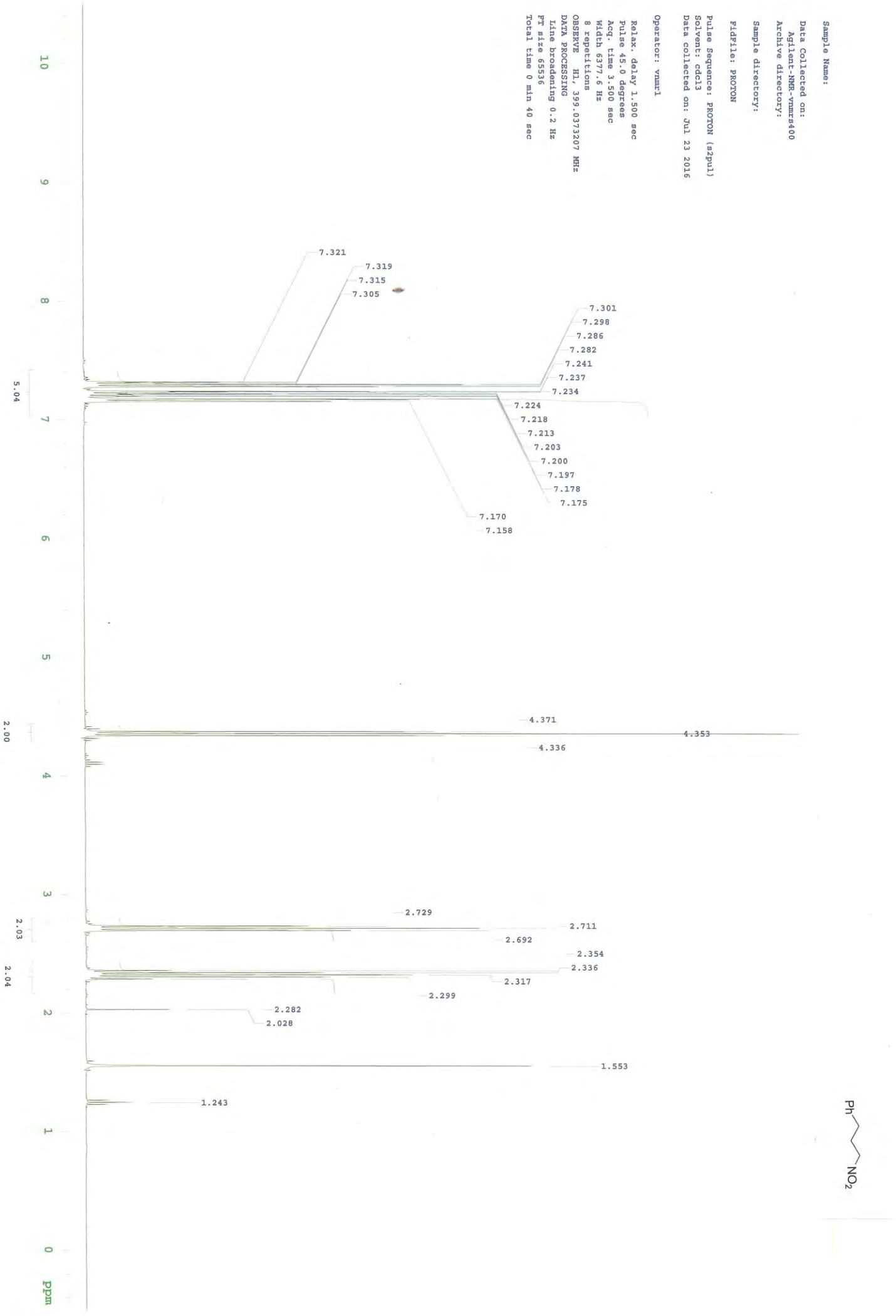


Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

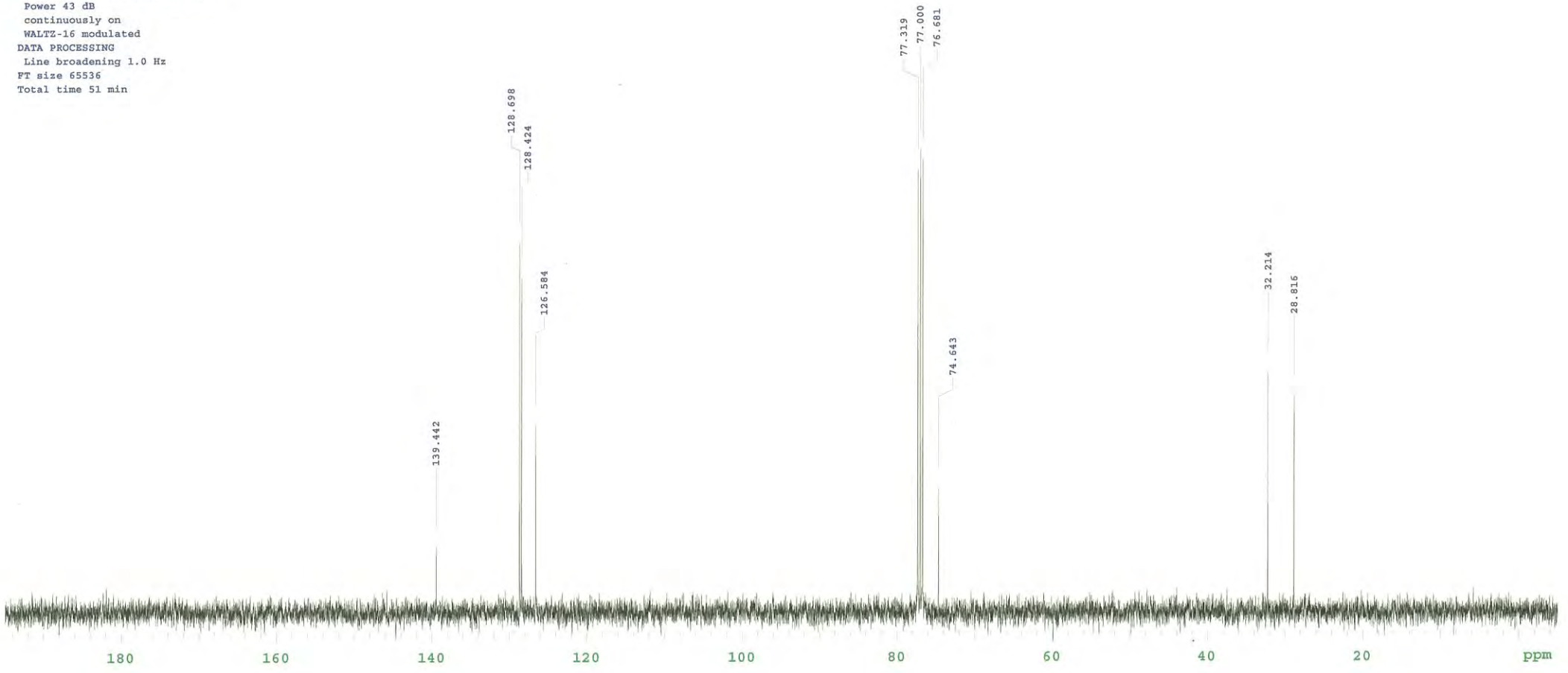
Sample directory:

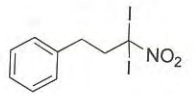
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 23 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

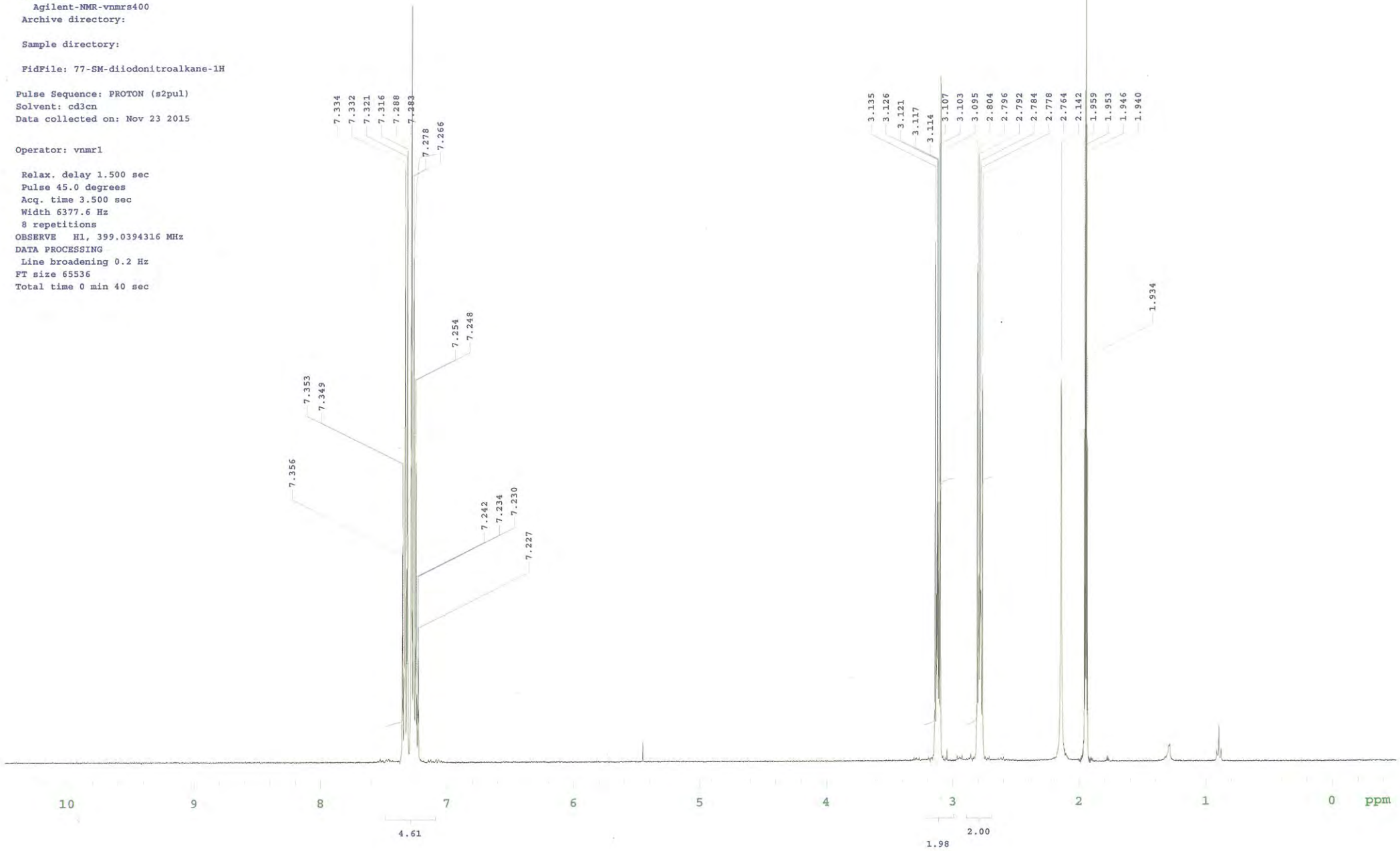
Sample directory:

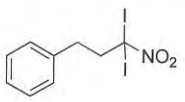
FidFile: 77-SM-diiodonitroalkane-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: Nov 23 2015

Operator: vnmrl

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0394316 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

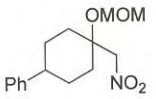
Sample directory:

FidFile: 77-SM-diiodonitroalkane-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 23 2015

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
832 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min



STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

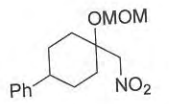
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 24 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

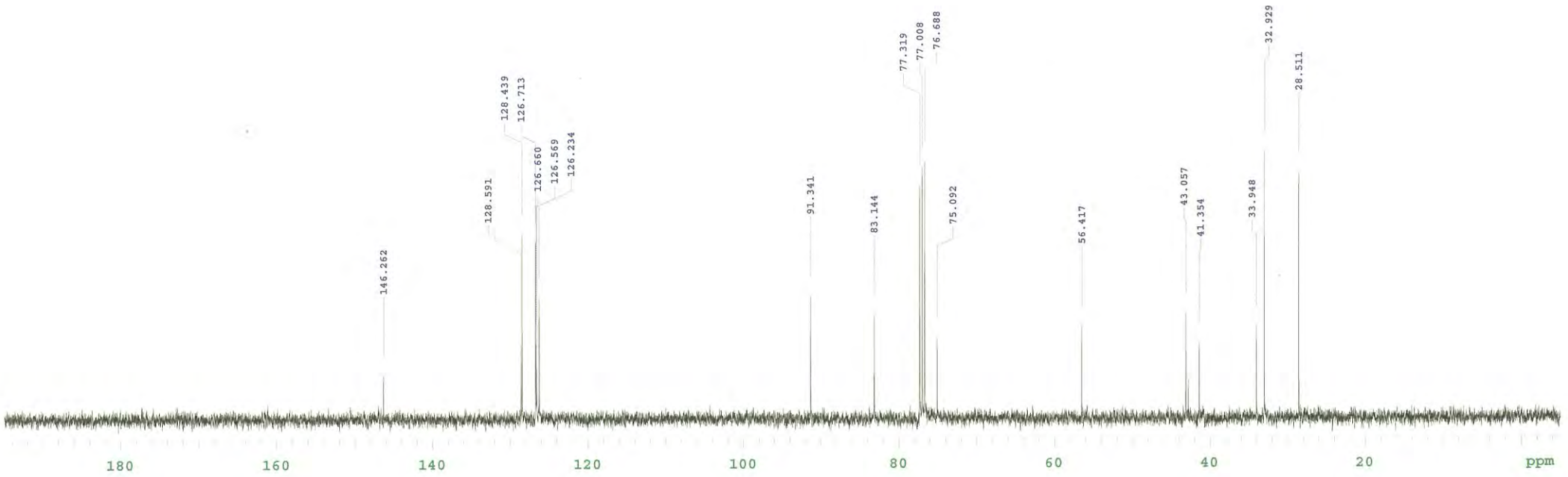
Sample directory:

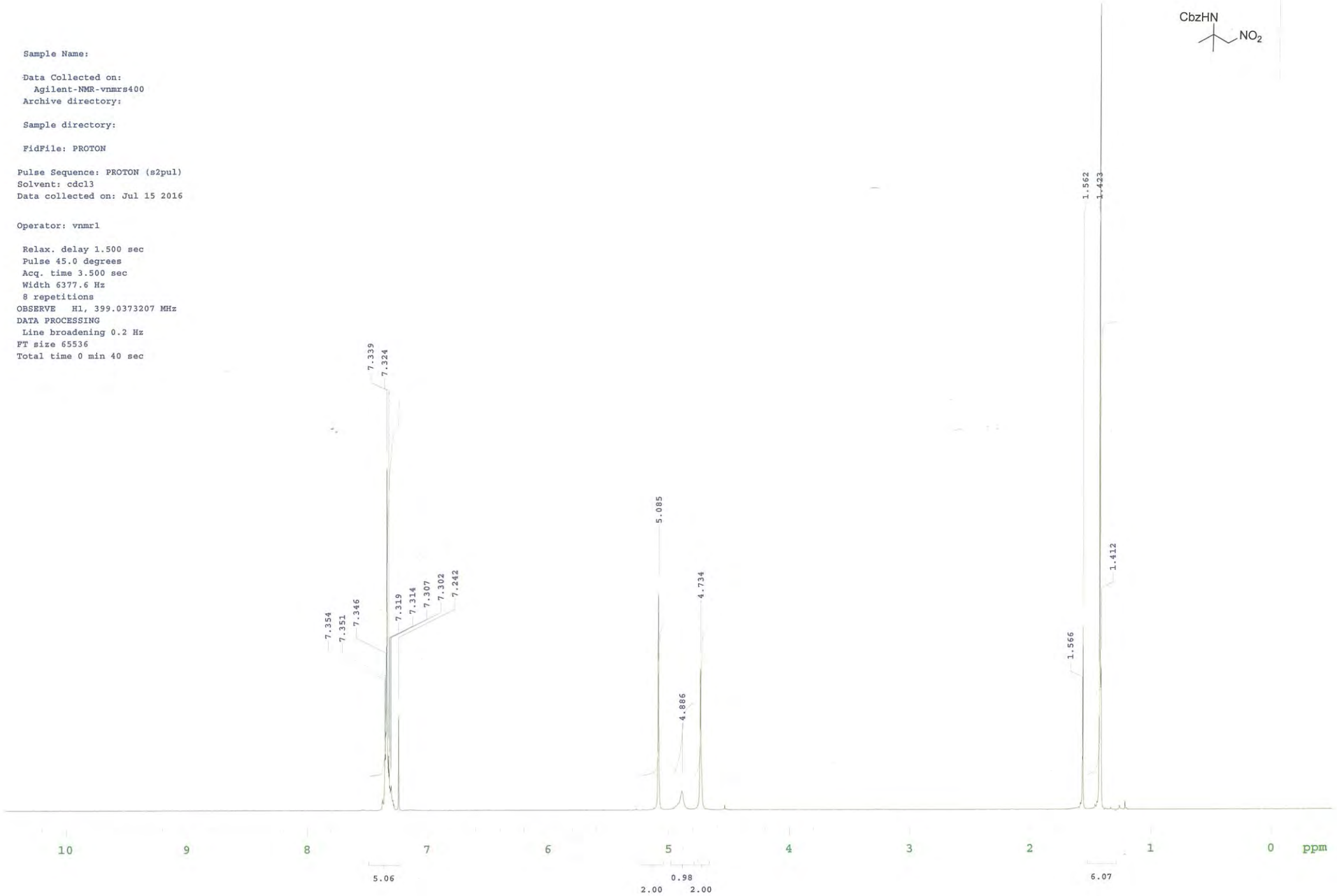
FidFile: CARBON

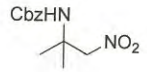
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 24 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min




CbzHN
NO2
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 15 2016
Operator: vnmr1
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec
7.339
7.324
7.354
7.351
7.346
7.319
7.314
7.307
7.302
7.242
5.085
4.734
4.886
1.562
1.423
1.412
1.566
10
9
8
7
6
5
4
3
2
1
0
ppm
5.06
0.98
2.00
2.00
6.07



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

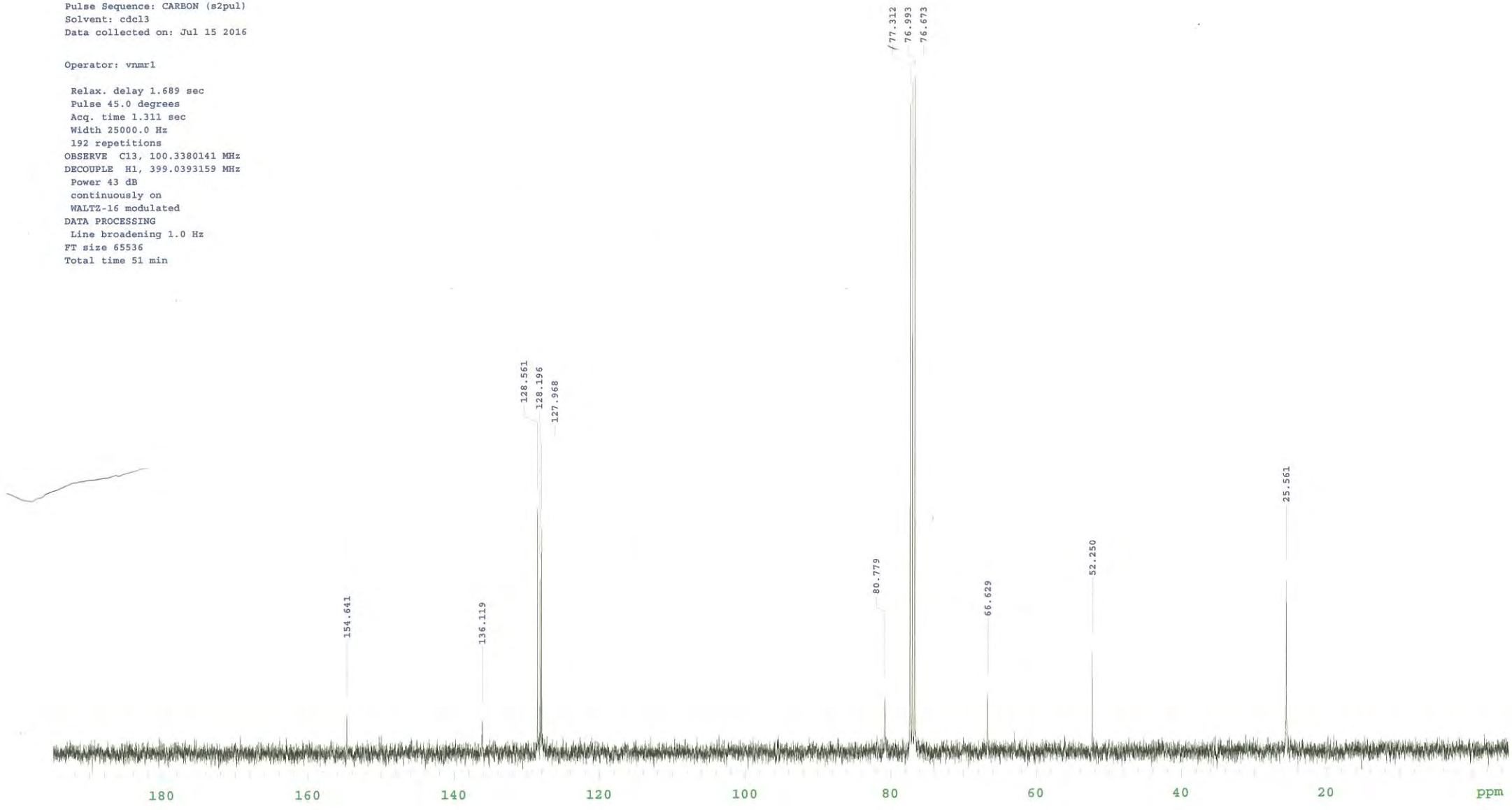
Sample directory:

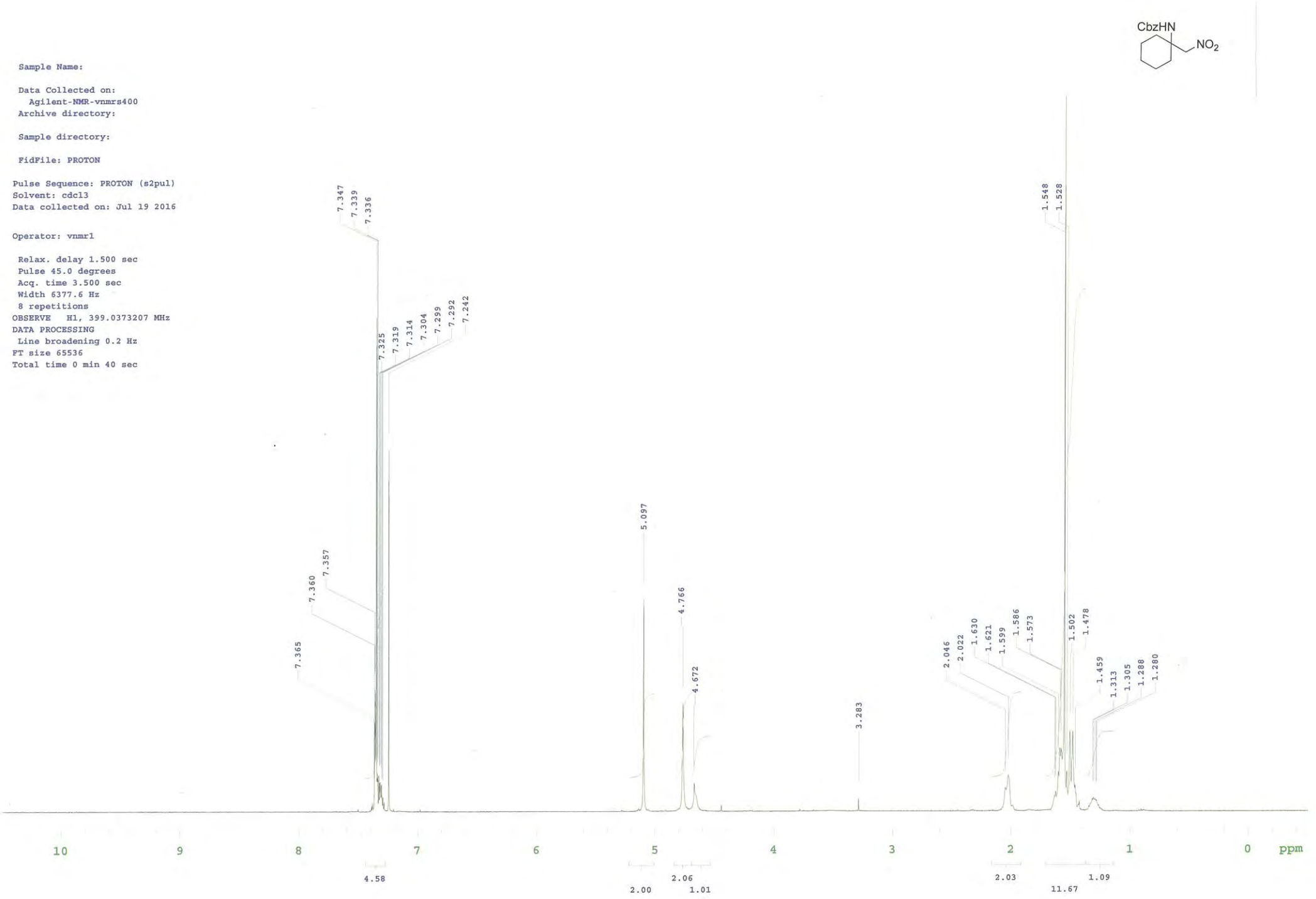
FidFile: CARBON

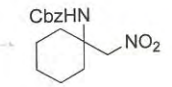
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 15 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
192 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min




CbzHN
NO2
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 19 2016
Operator: vnmr1
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec
7.347
7.339
7.336
7.325
7.319
7.314
7.304
7.299
7.292
7.242
7.365
7.360
7.357
5.097
4.766
4.672
3.283
2.046
2.022
1.630
1.621
1.599
1.586
1.573
1.548
1.528
1.502
1.478
1.459
1.313
1.305
1.288
1.280
10
9
8
7
6
5
4
3
2
1
0
ppm
4.58
2.00
2.06
1.01
2.03
1.09
11.67



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

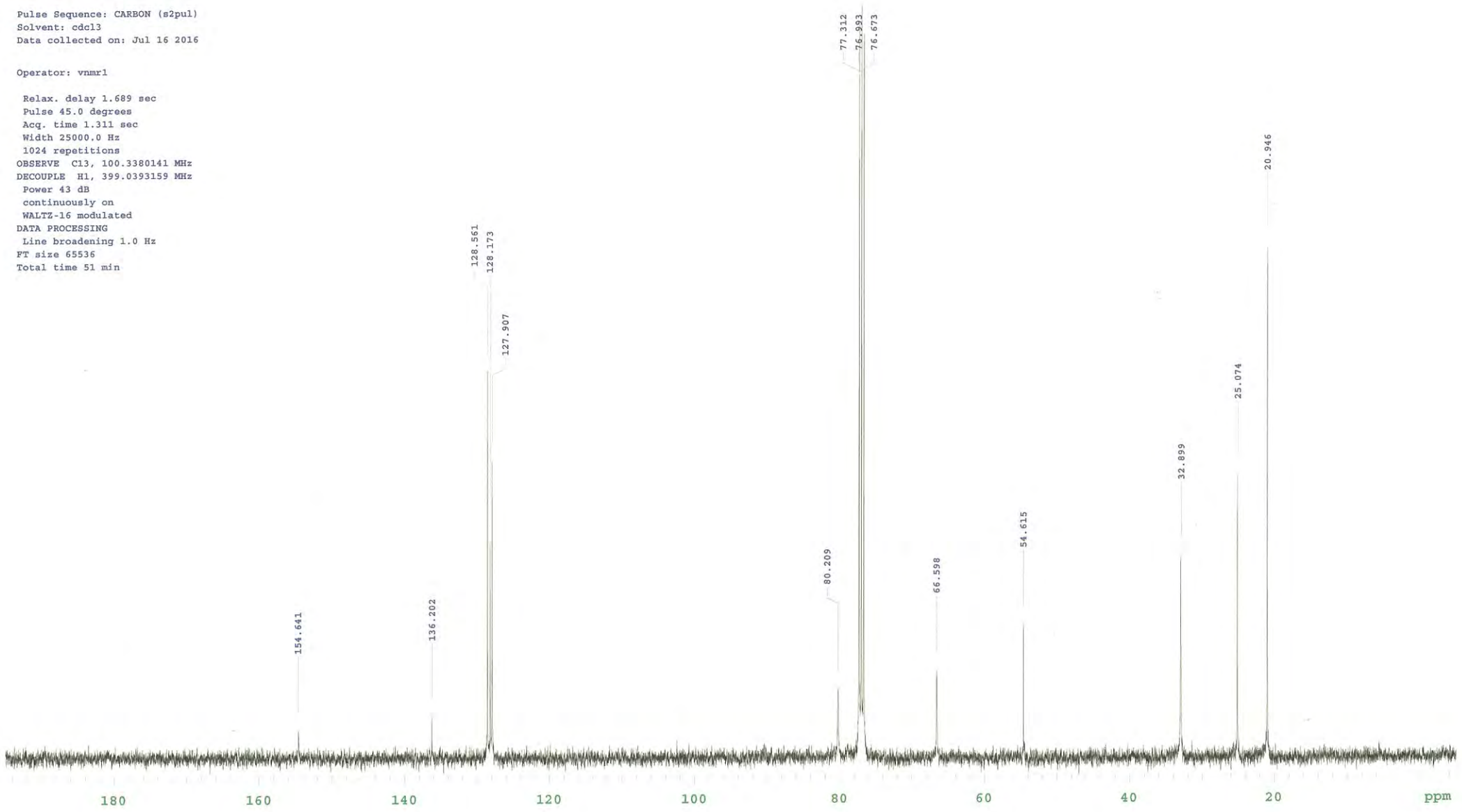
Sample directory:

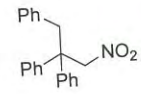
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 16 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1024 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

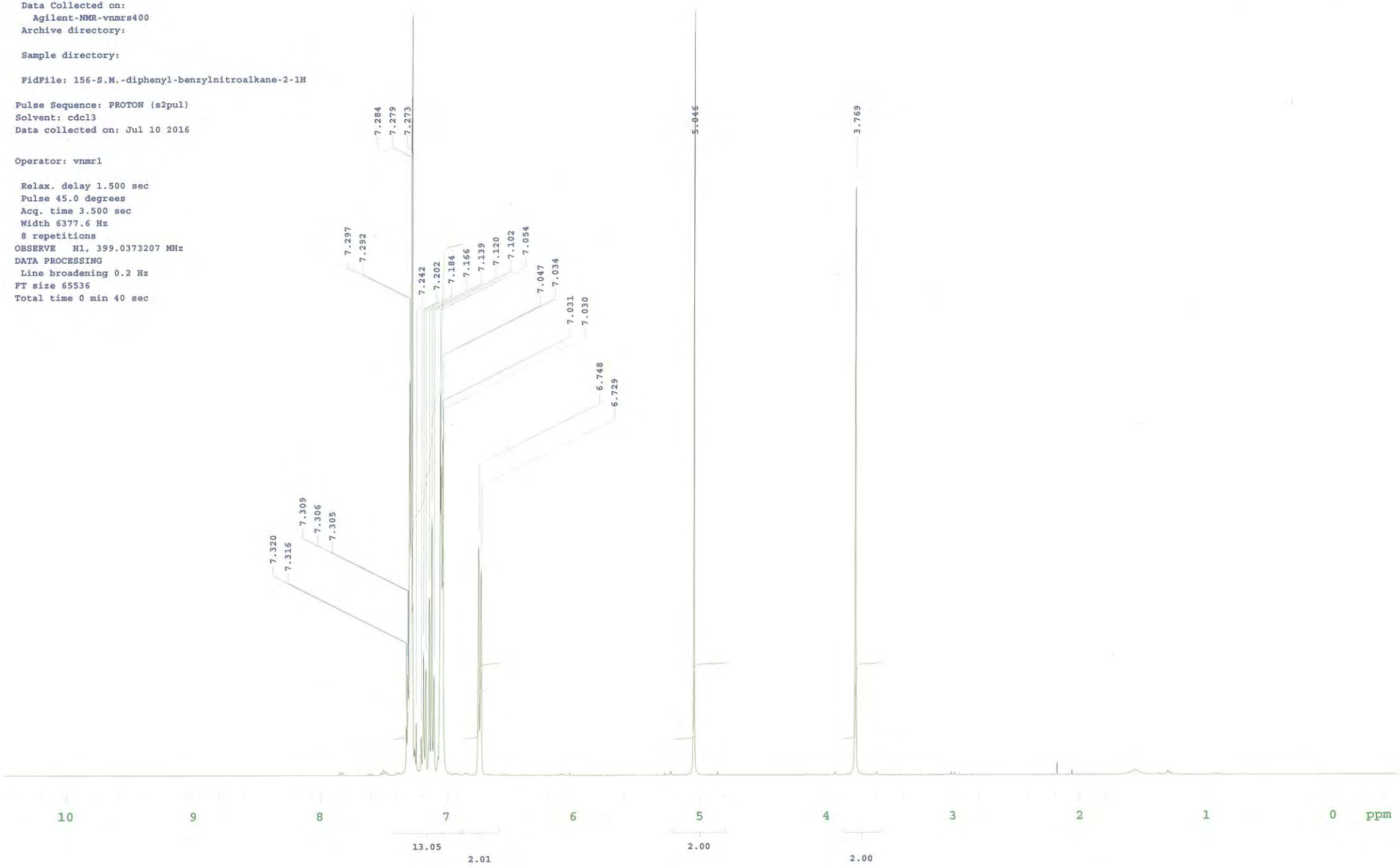
Sample directory:

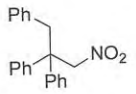
FidFile: 156-S.M.-diphenyl-benzylnitroalkane-2-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 10 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

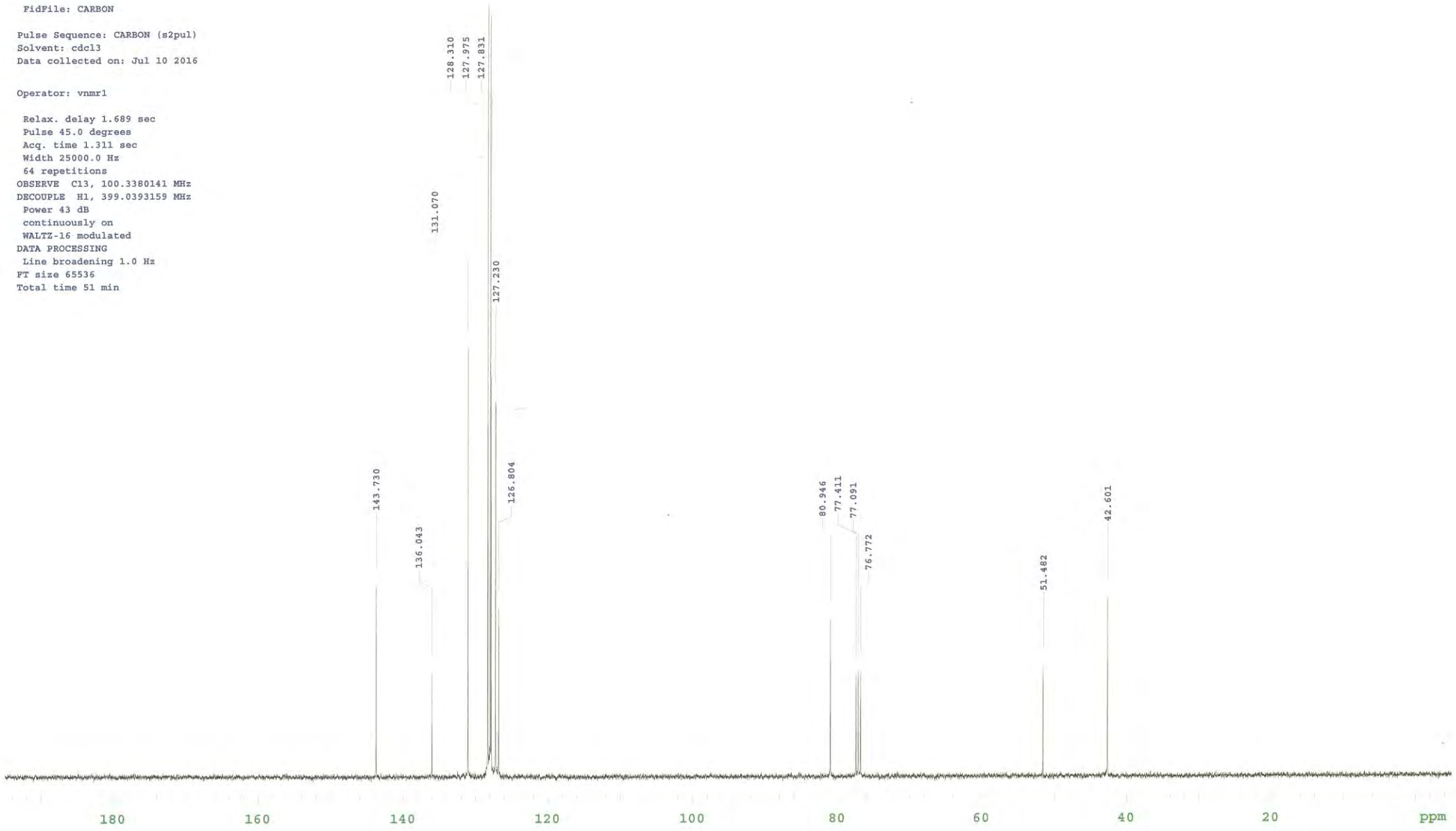
Sample directory:

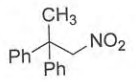
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 10 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

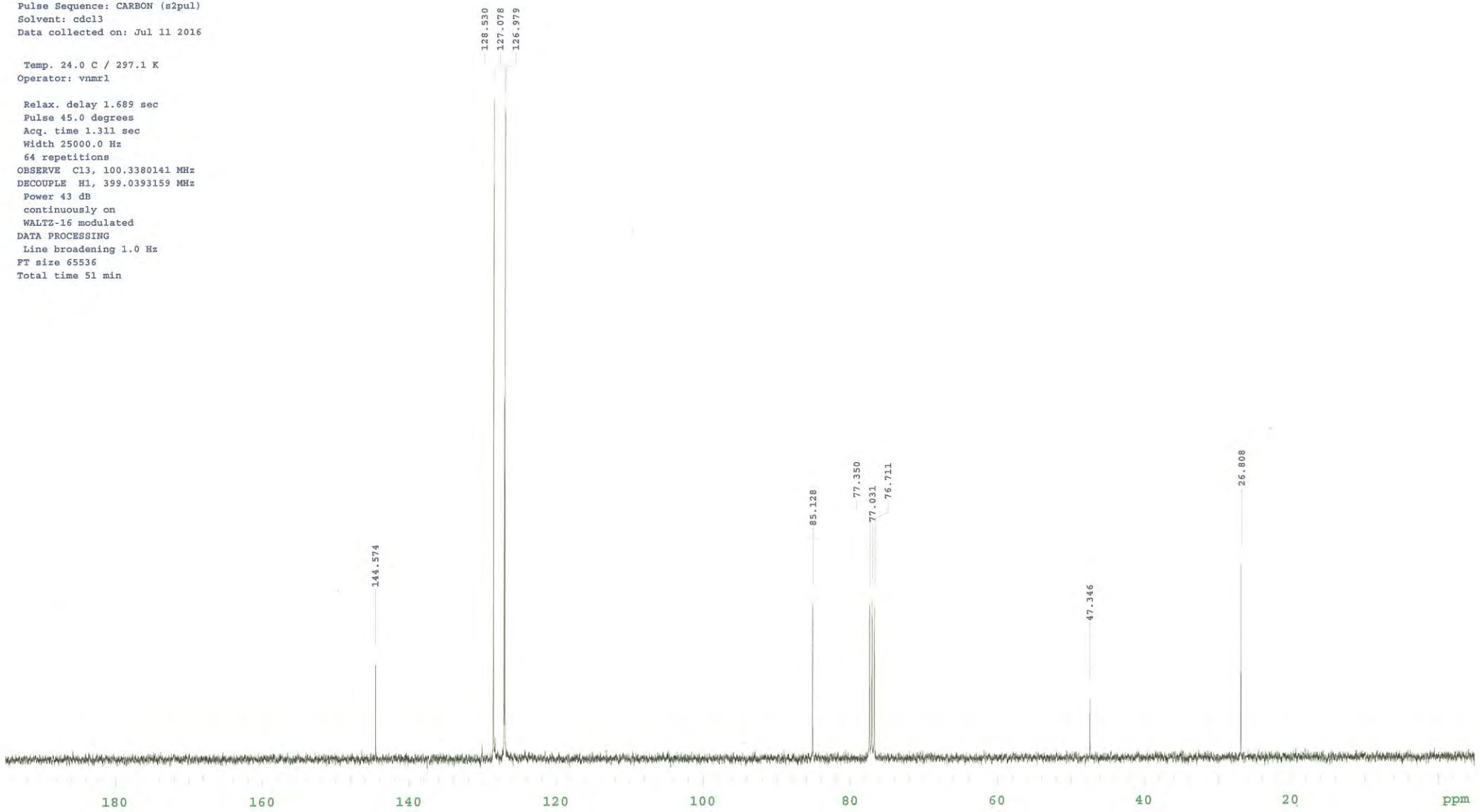
Sample directory:

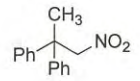
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 11 2016

Temp. 24.0 C / 297.1 K
Operator: vnmrl

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

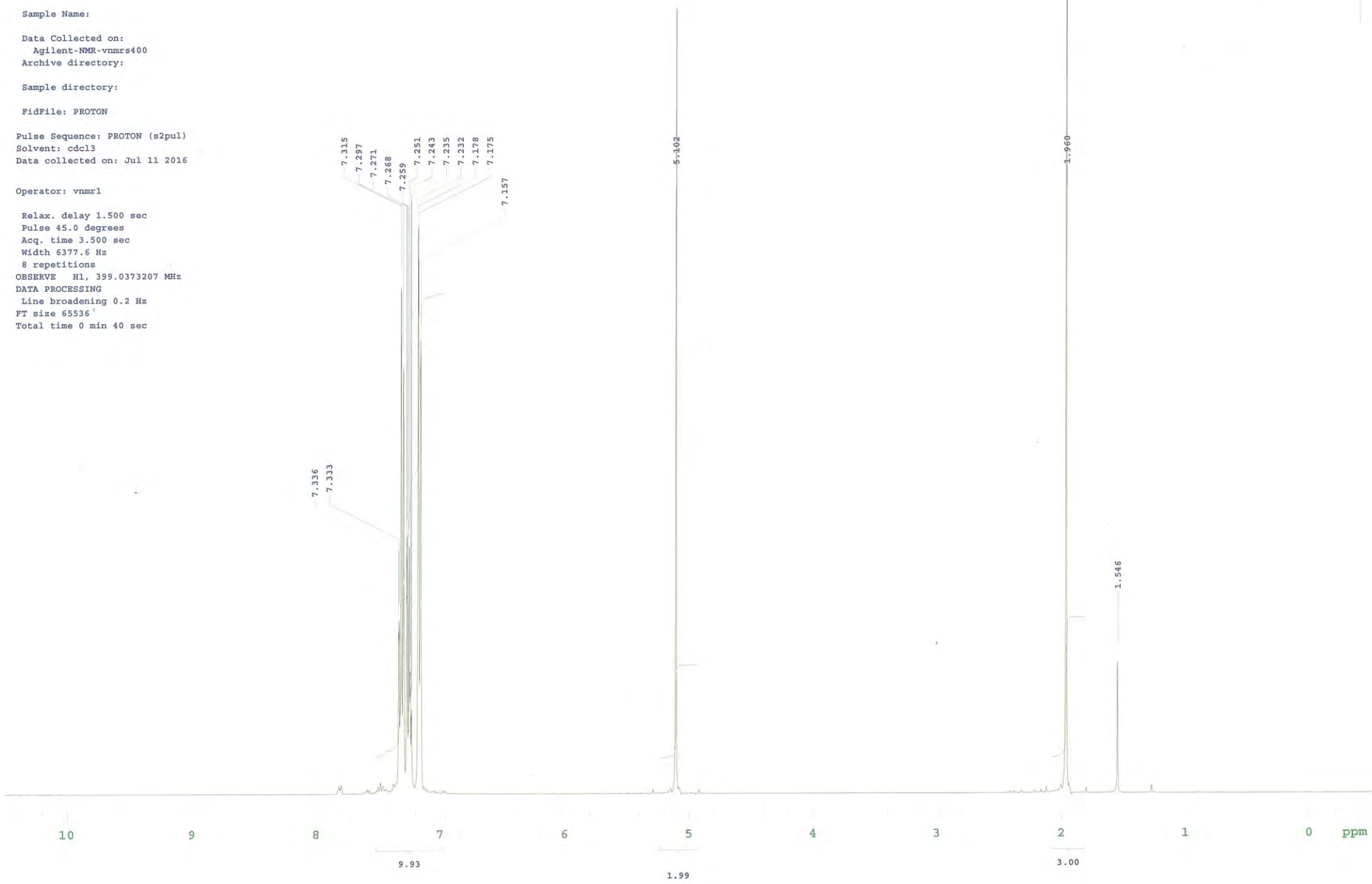
Sample directory:

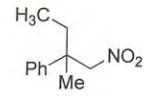
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 11 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

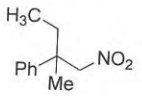
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

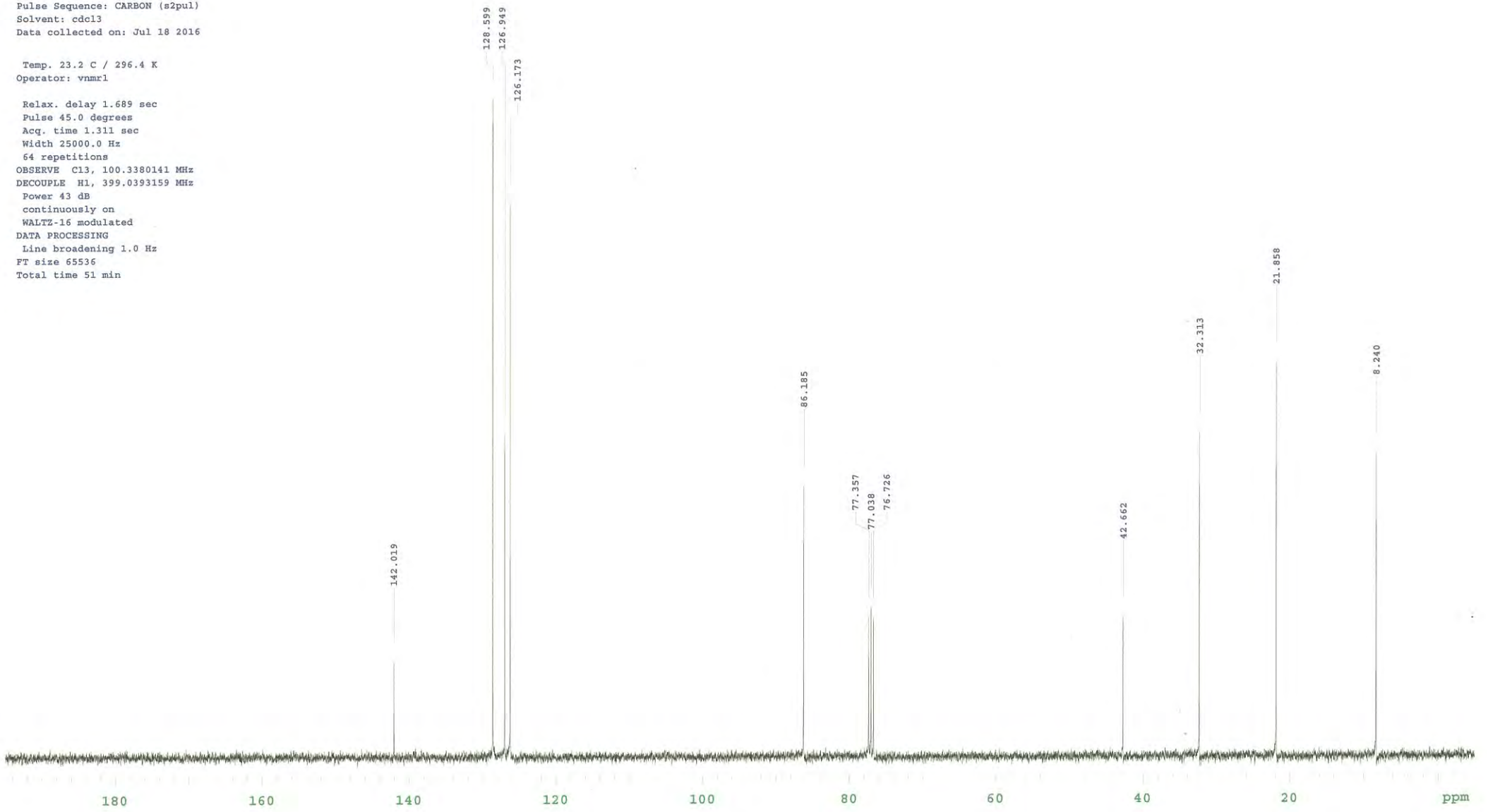
Sample directory:

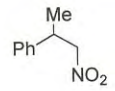
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2016

Temp. 23.2 C / 296.4 K
Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

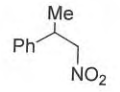
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 23 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

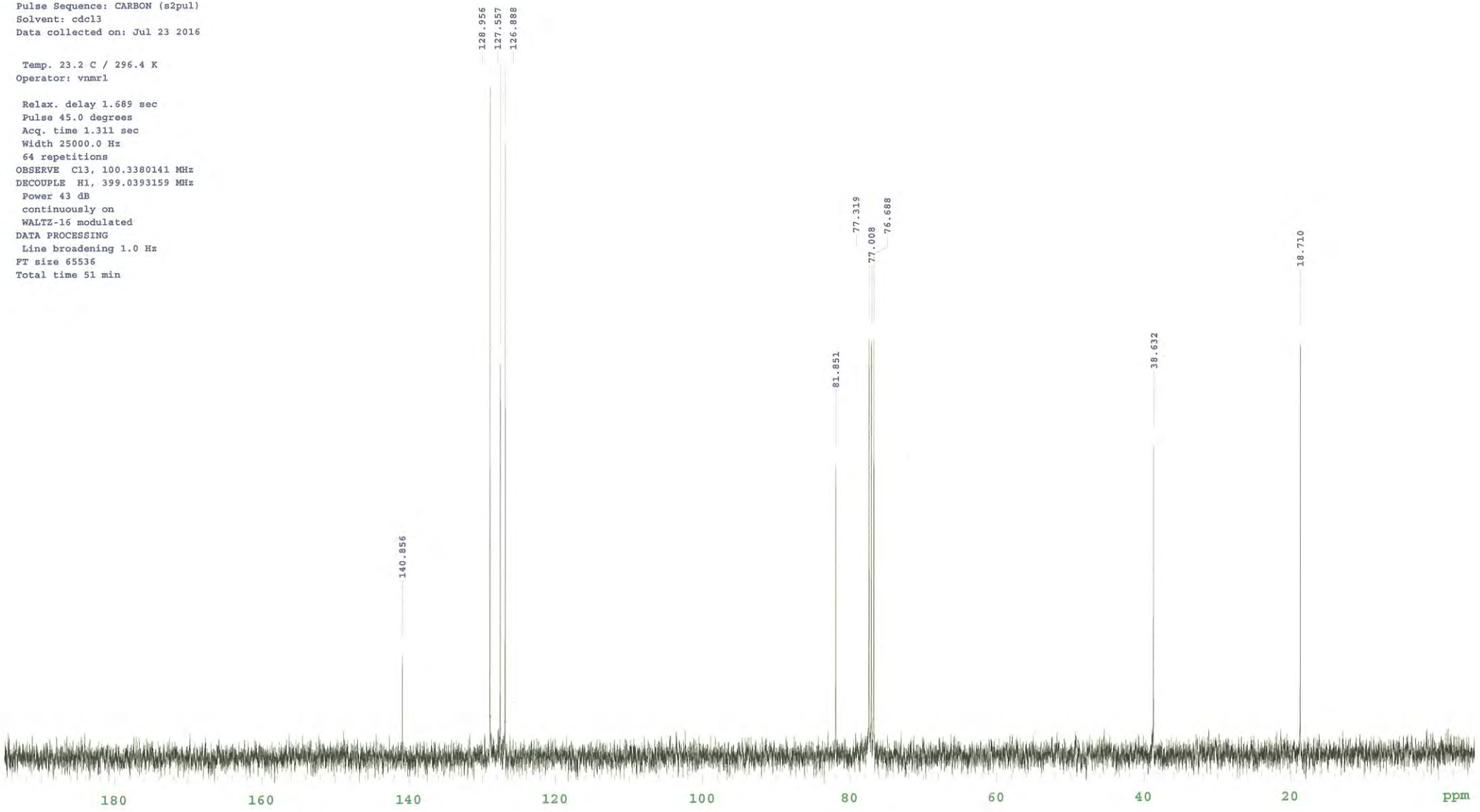
Sample directory:

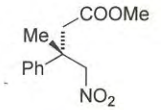
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 23 2016

Temp. 23.2 C / 296.4 K
Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

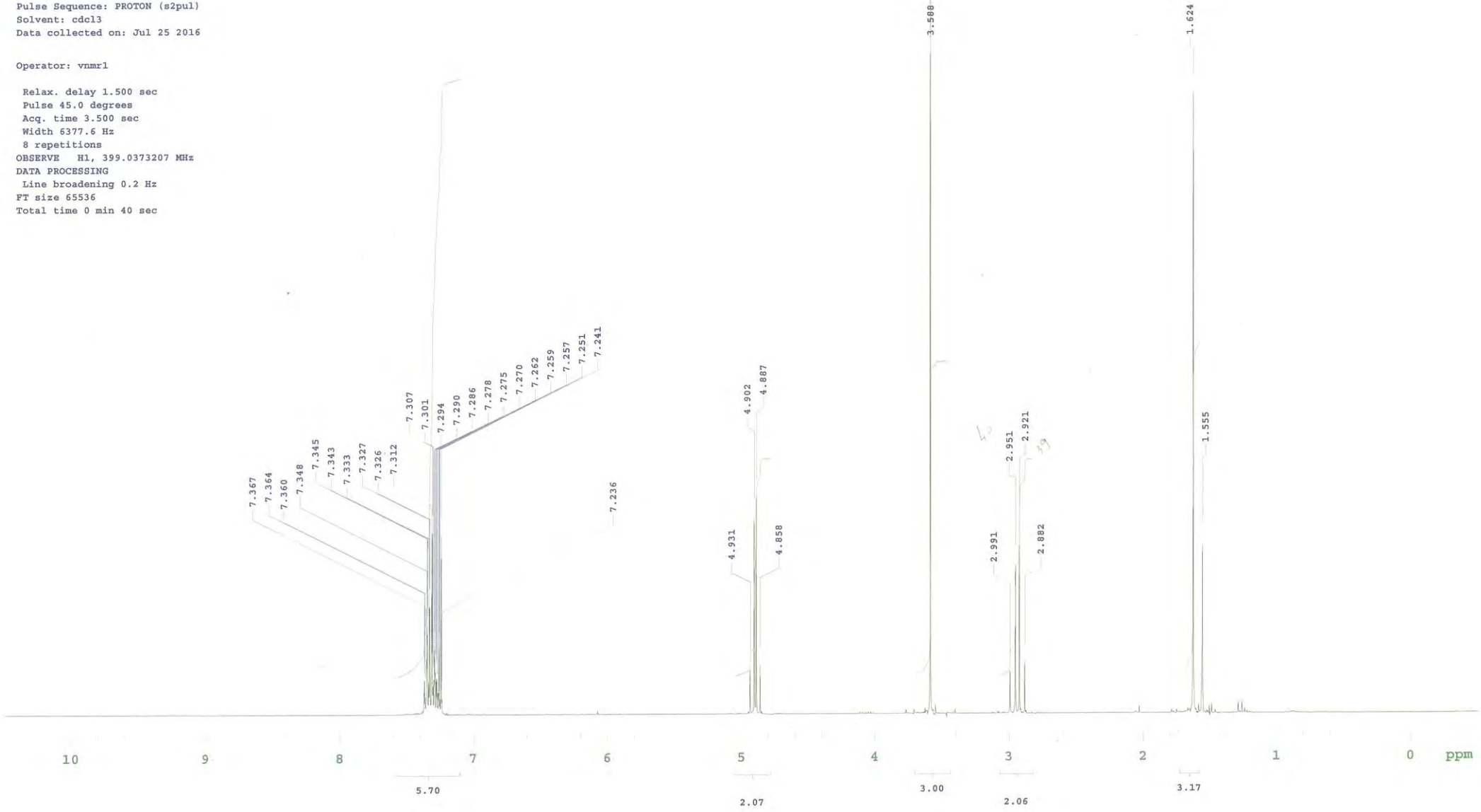
Sample directory:

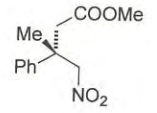
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 25 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

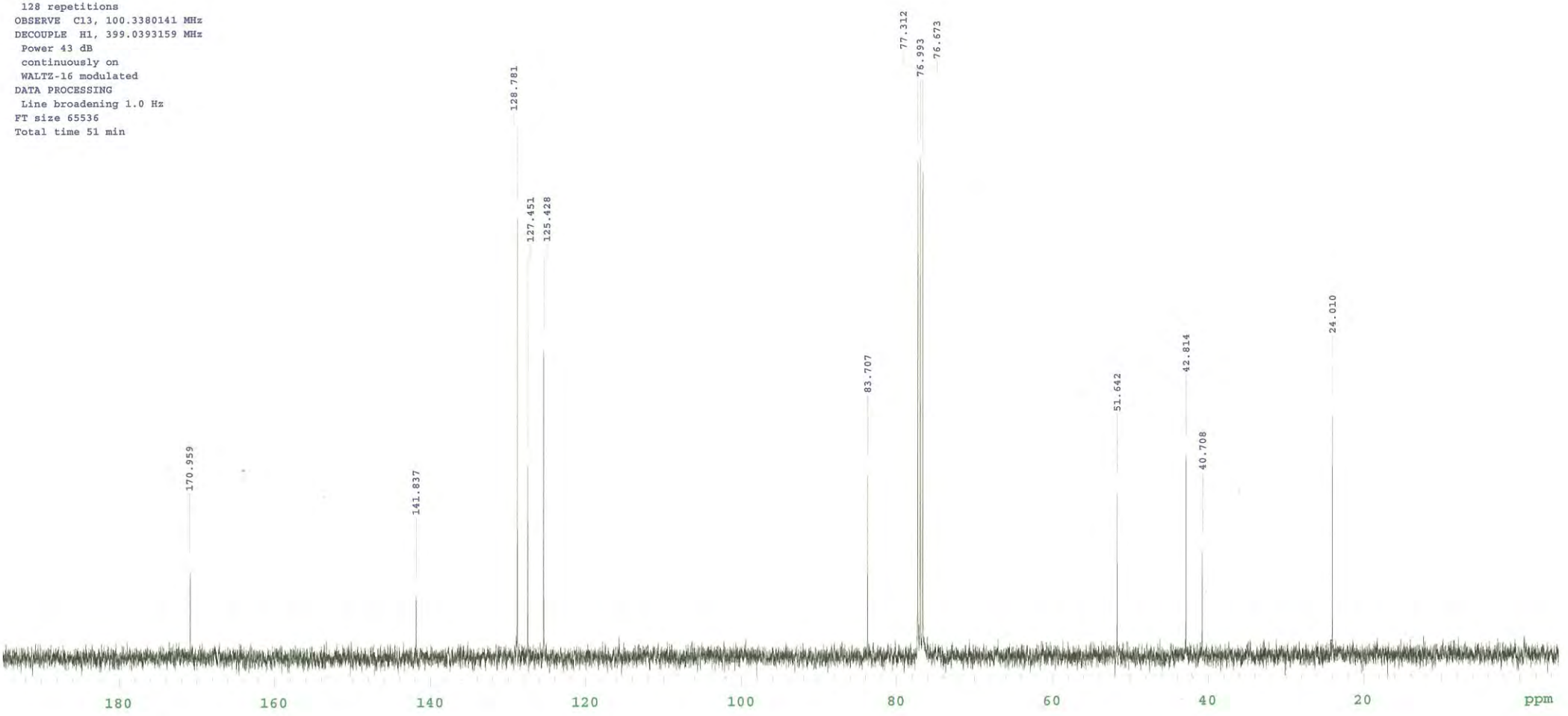
Sample directory:

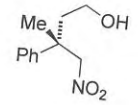
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 25 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
128 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

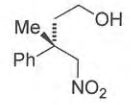
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 25 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

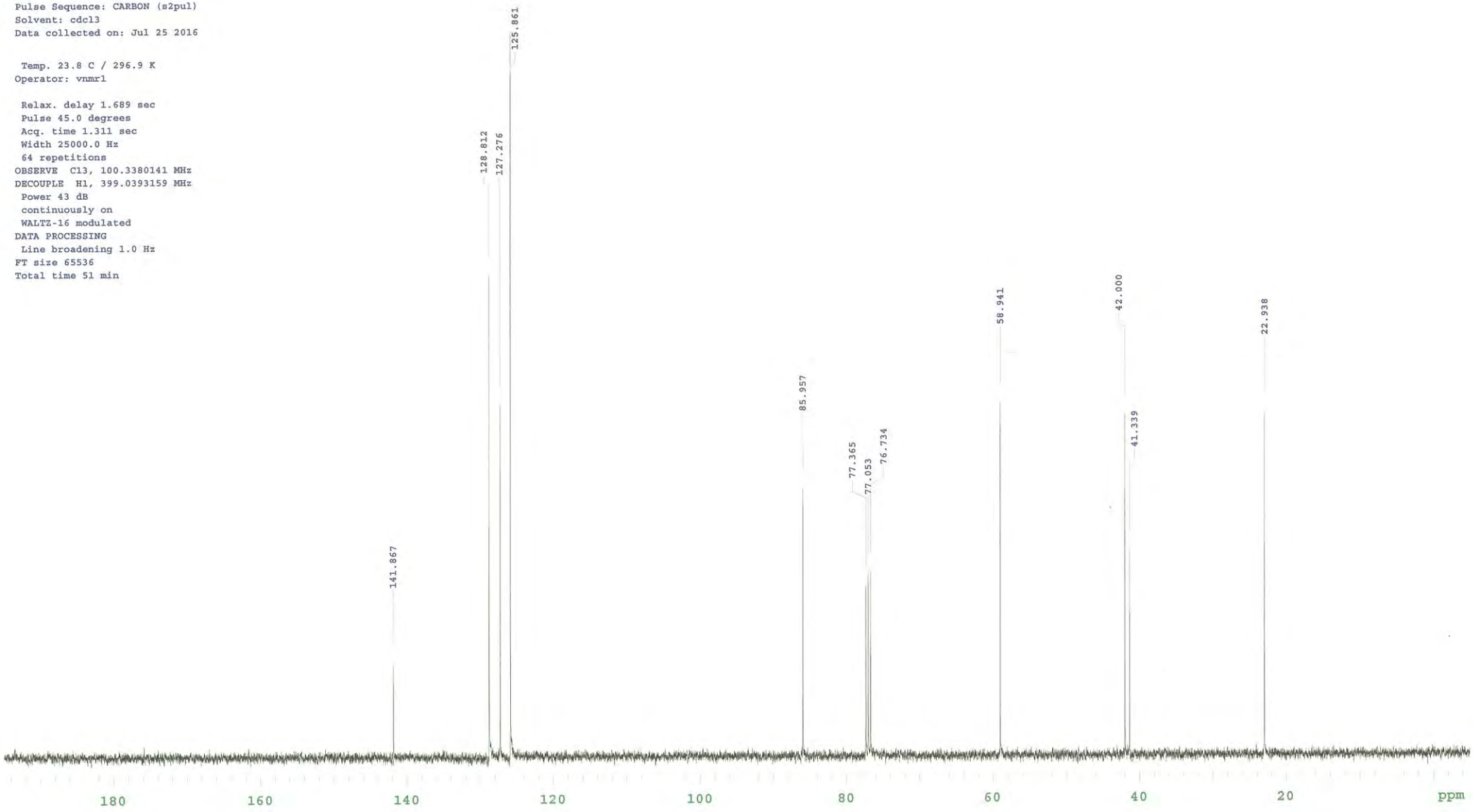
Sample directory:

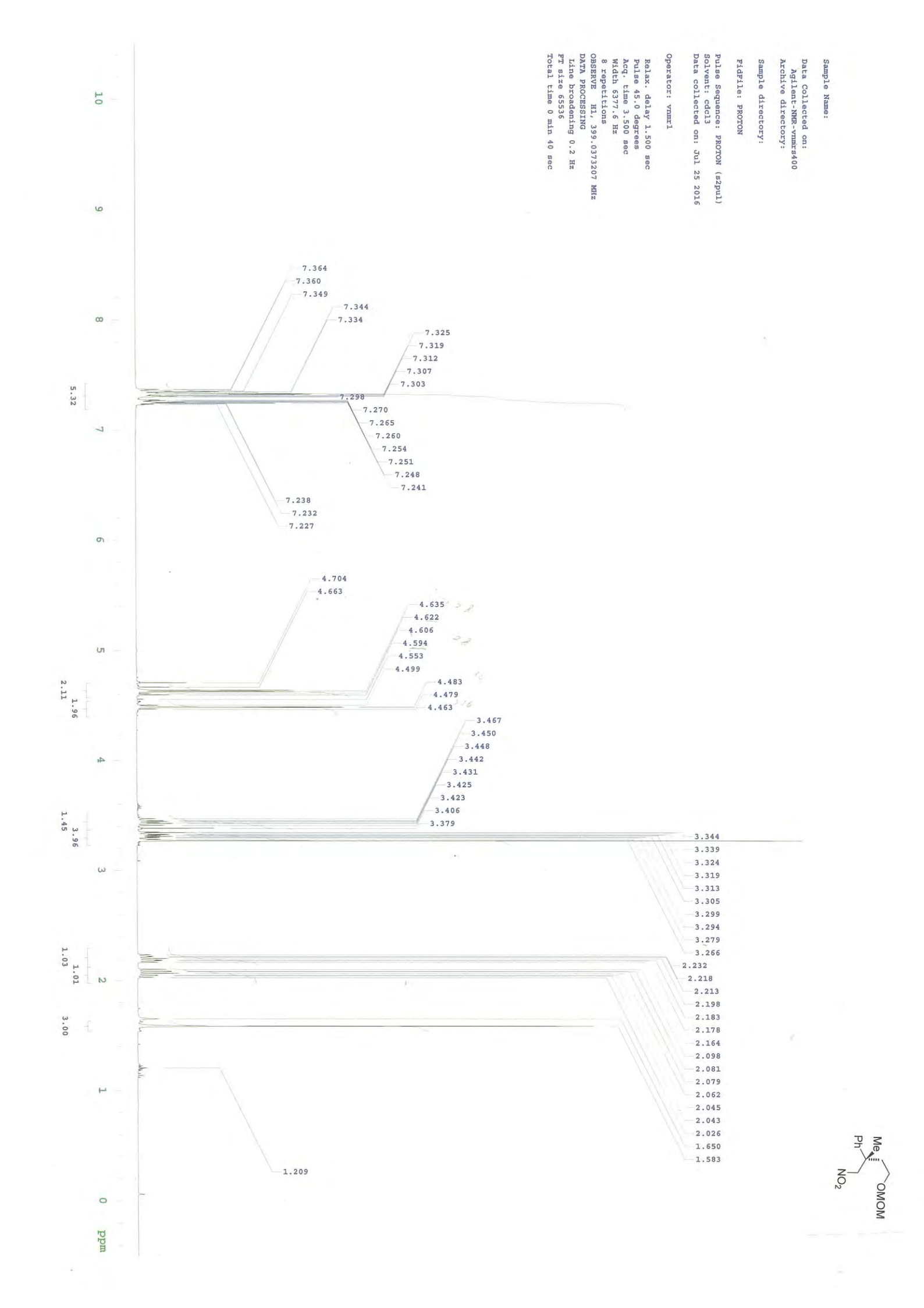
FidFile: CARBON

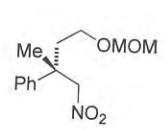
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 25 2016

Temp. 23.8 C / 296.9 K
Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min




Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 25 2016
Operator: vnmr1
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec
7.364
7.360
7.349
7.344
7.334
7.325
7.319
7.312
7.307
7.303
7.298
7.270
7.265
7.260
7.254
7.251
7.248
7.241
7.238
7.232
7.227
4.704
4.663
4.635
4.622
4.606
4.594
4.553
4.499
4.483
4.479
4.463
3.467
3.450
3.448
3.442
3.431
3.425
3.423
3.406
3.379
3.344
3.339
3.324
3.319
3.313
3.305
3.299
3.294
3.279
3.266
2.232
2.218
2.213
2.198
2.183
2.178
2.164
2.098
2.081
2.079
2.062
2.045
2.043
2.026
1.650
1.583
1.209
5.32
2.11
1.96
1.45
3.96
1.03
1.01
3.00
10
9
8
7
6
5
4
3
2
1
0
ppm
Me
Ph
OMOM
NO2



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

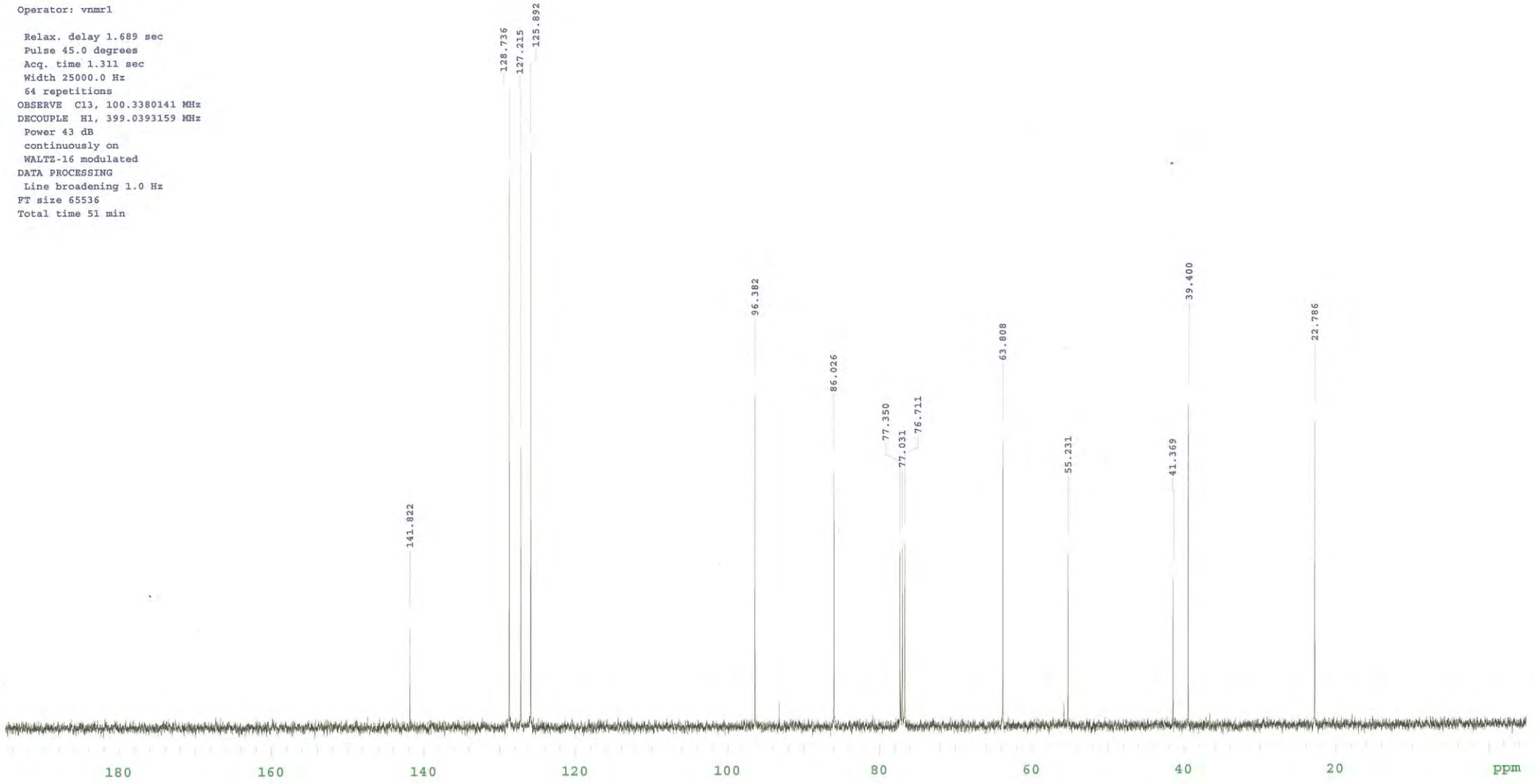
Sample directory:

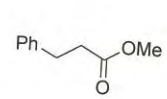
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 25 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Selective band center: 3.92 (ppm); width: 47.9 (Hz)

Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

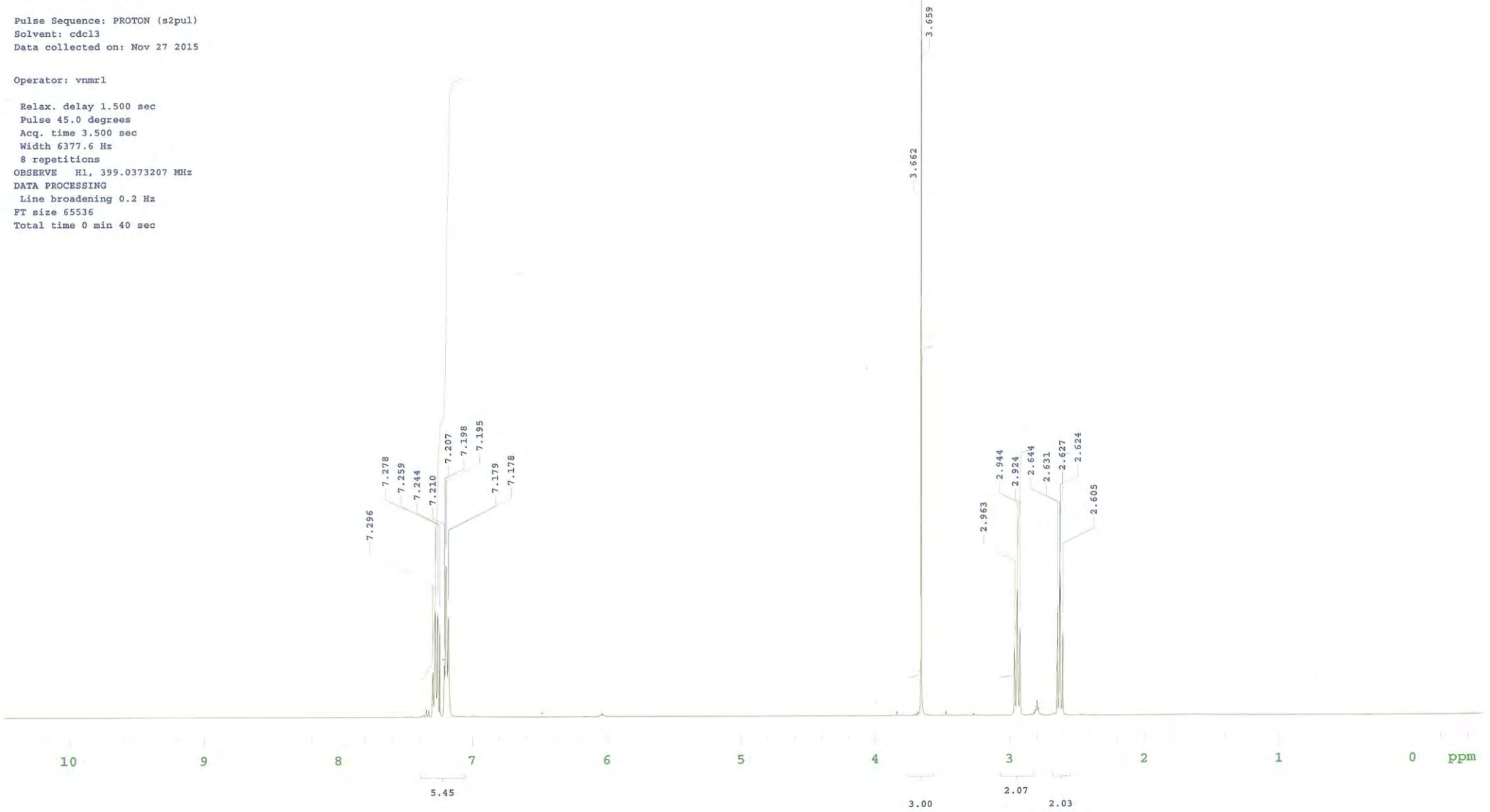
Sample directory:

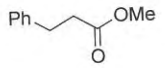
FidFile: 78-Pure-ester-13C

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 27 2015

Operator: vnmrl

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec





Selective band center: 3.92 (ppm); width: 47.9 (Hz)

Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

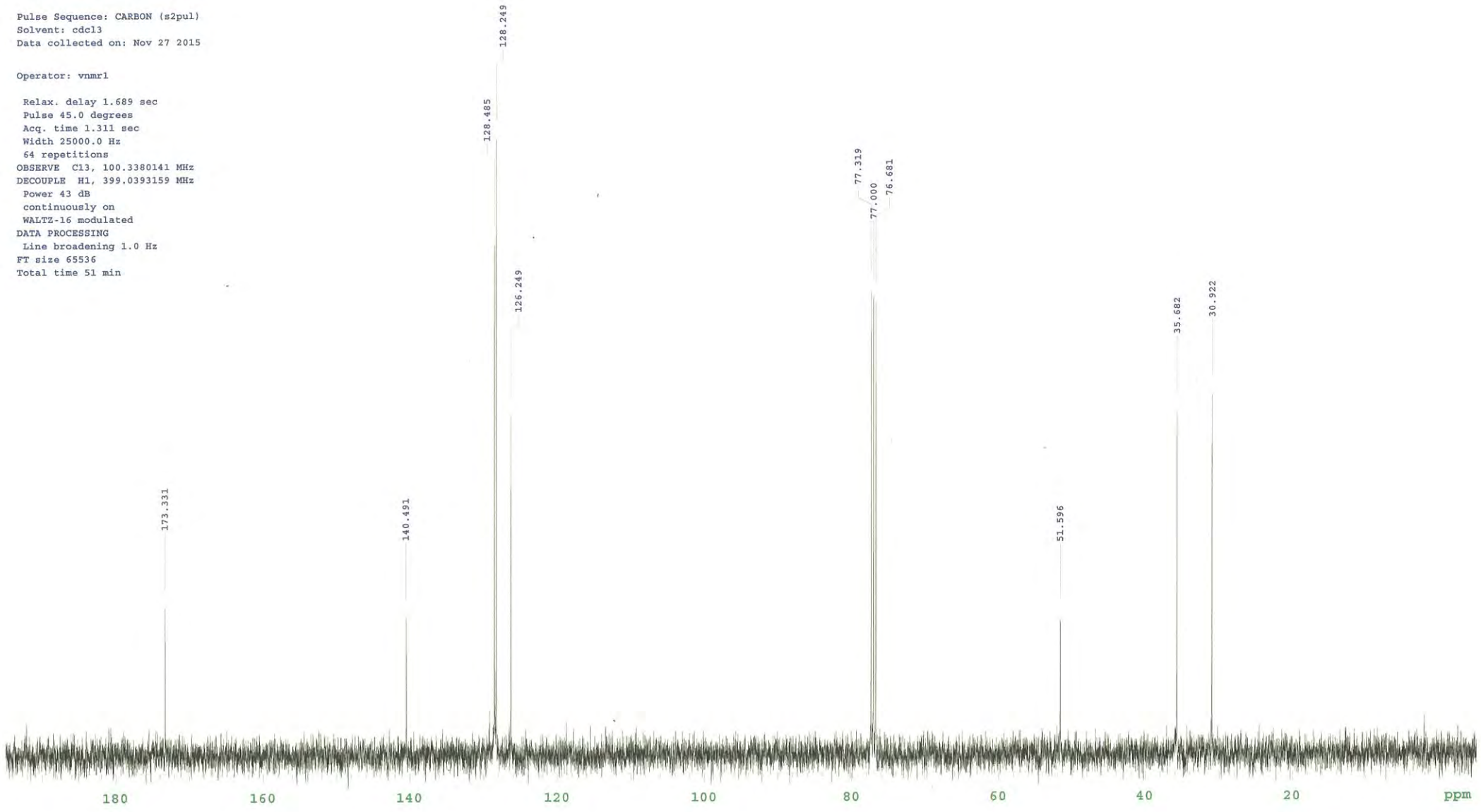
Sample directory:

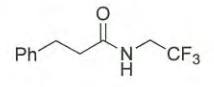
FidFile: 78-Pure-ester-13-2C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 27 2015

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

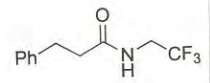
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2016

Operator: vnmrl

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

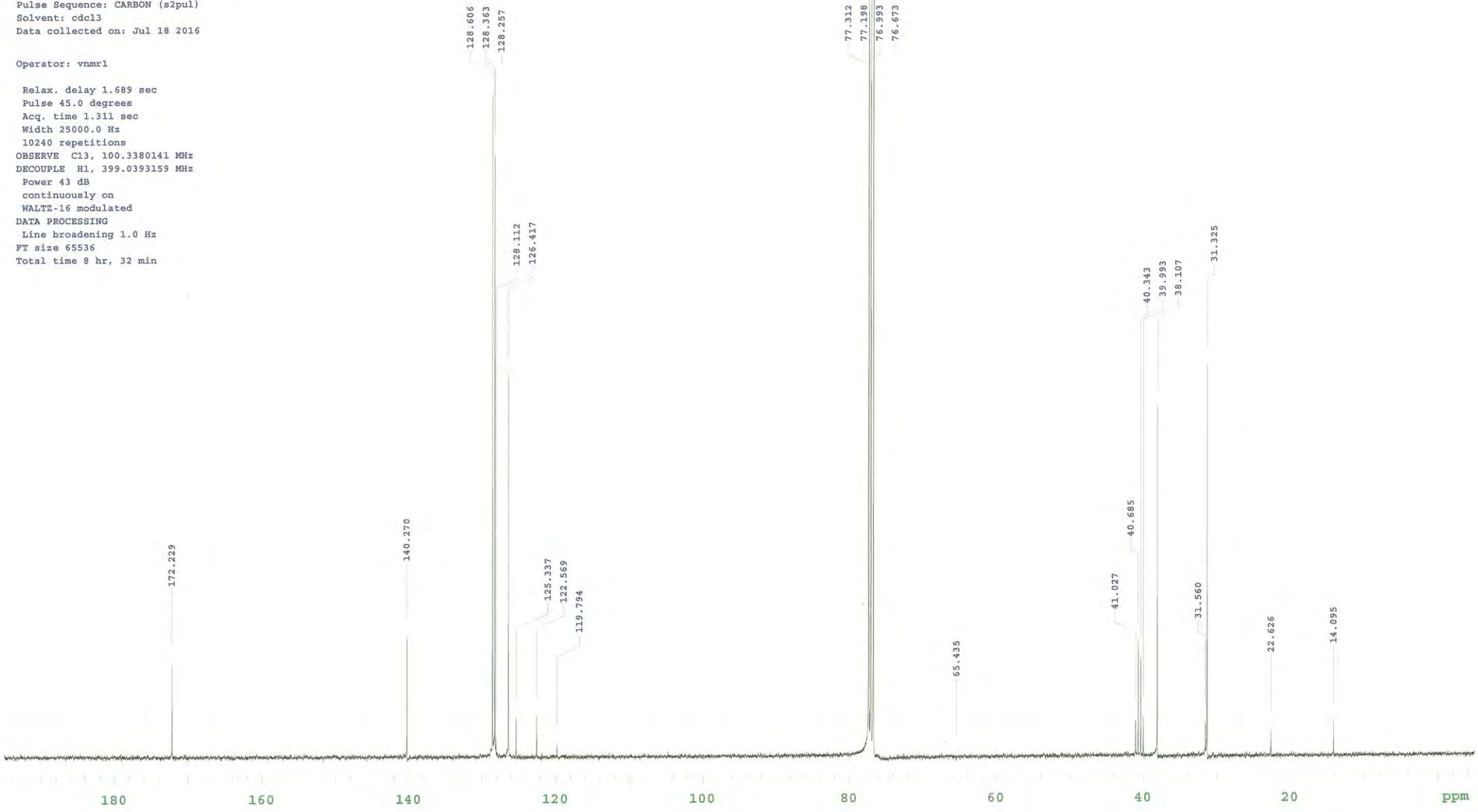
Sample directory:

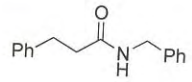
FidFile: 157-trifluroethylamine-13C-2

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
10240 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 8 hr, 32 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

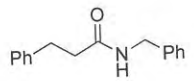
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

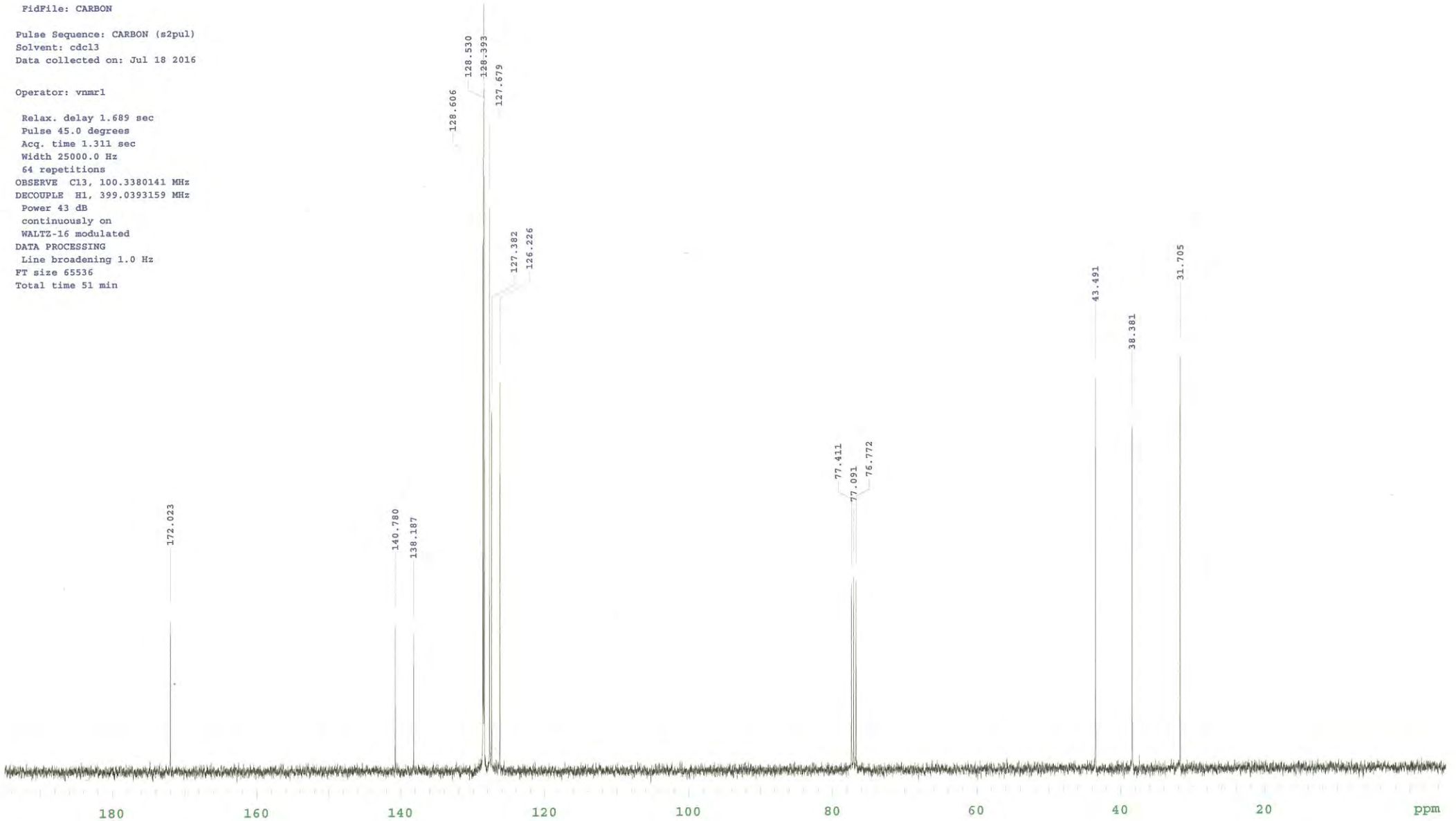
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2016

Operator: vnmrl

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

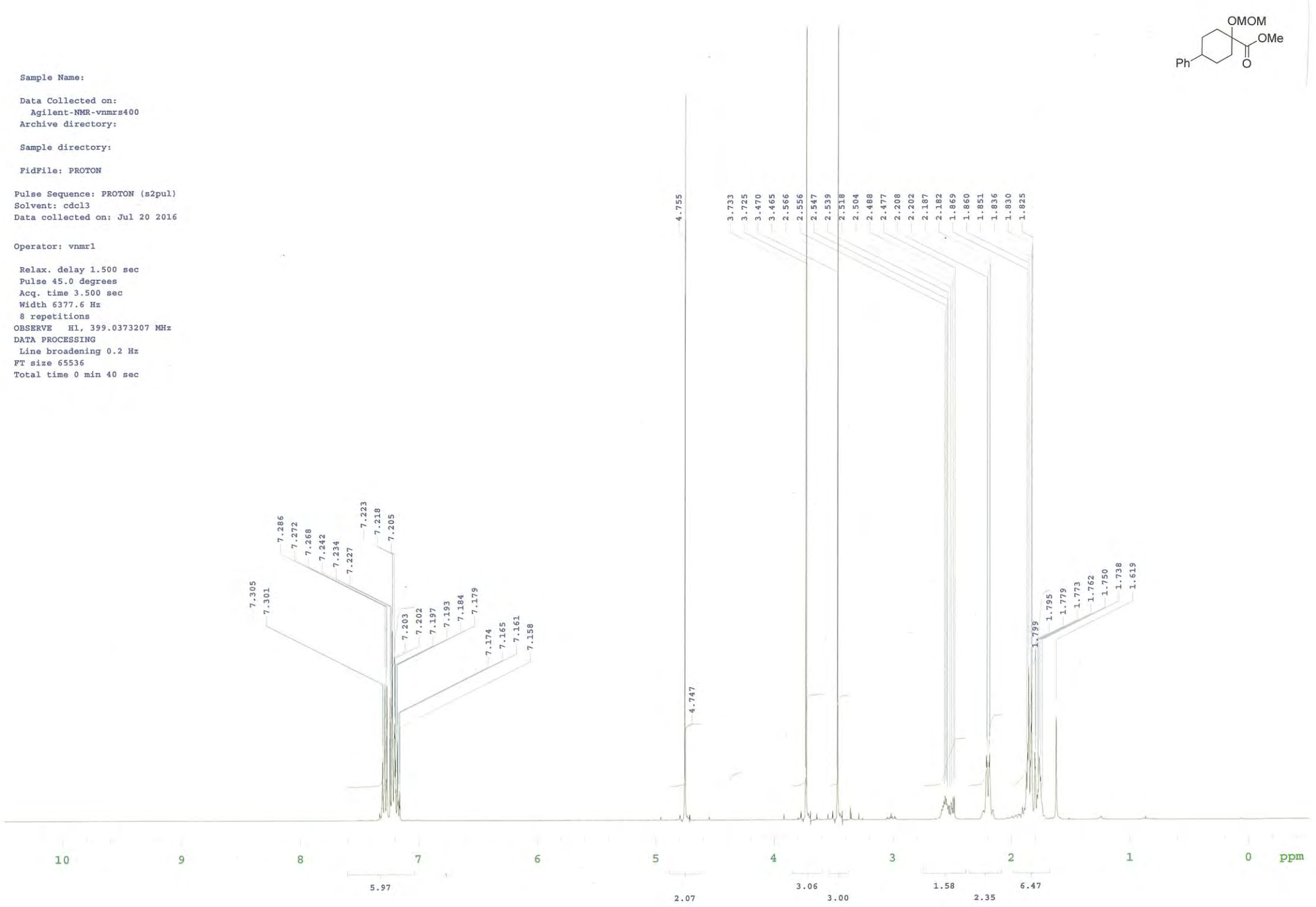
Sample directory:

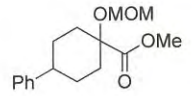
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

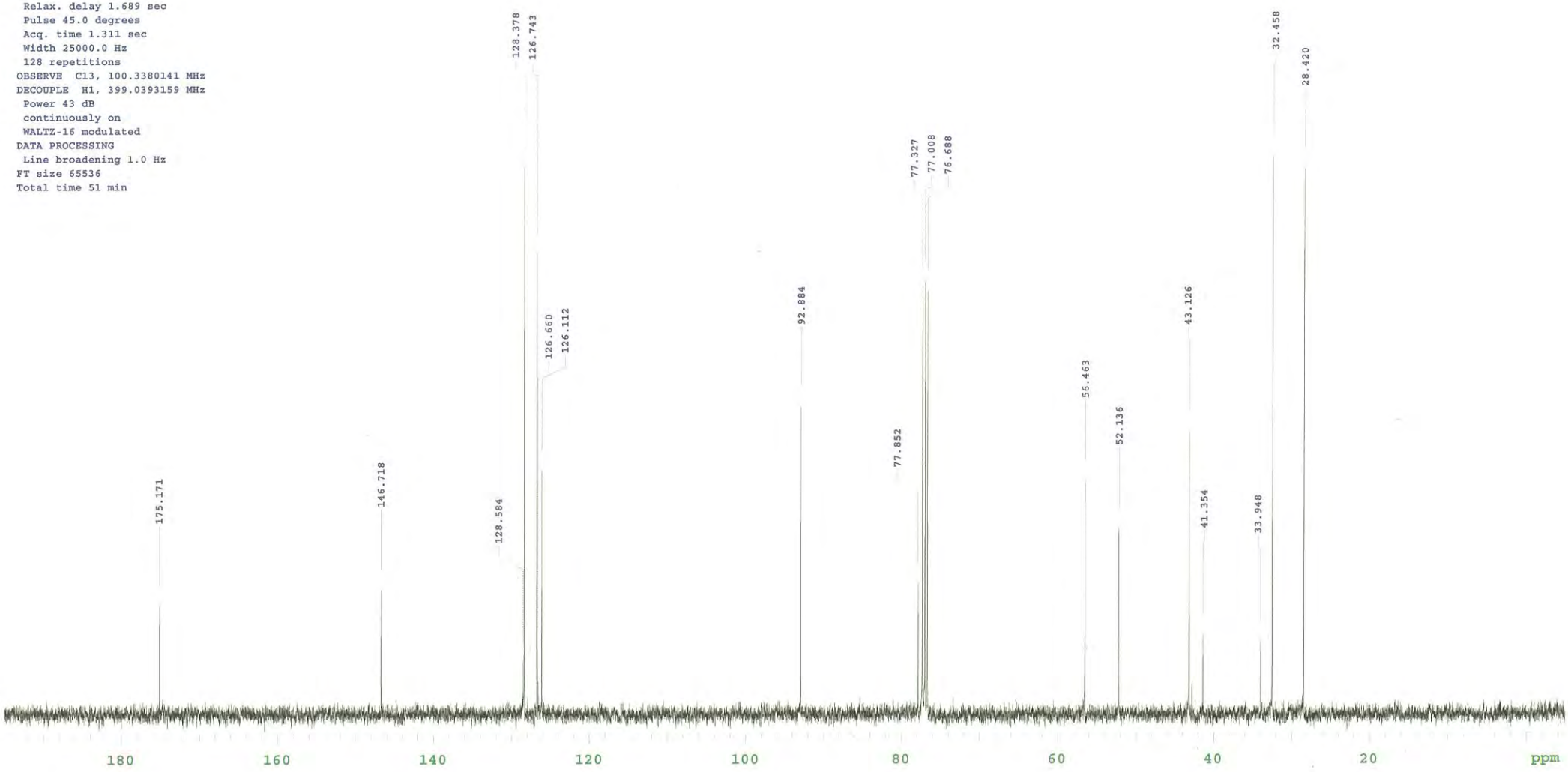
Sample directory:

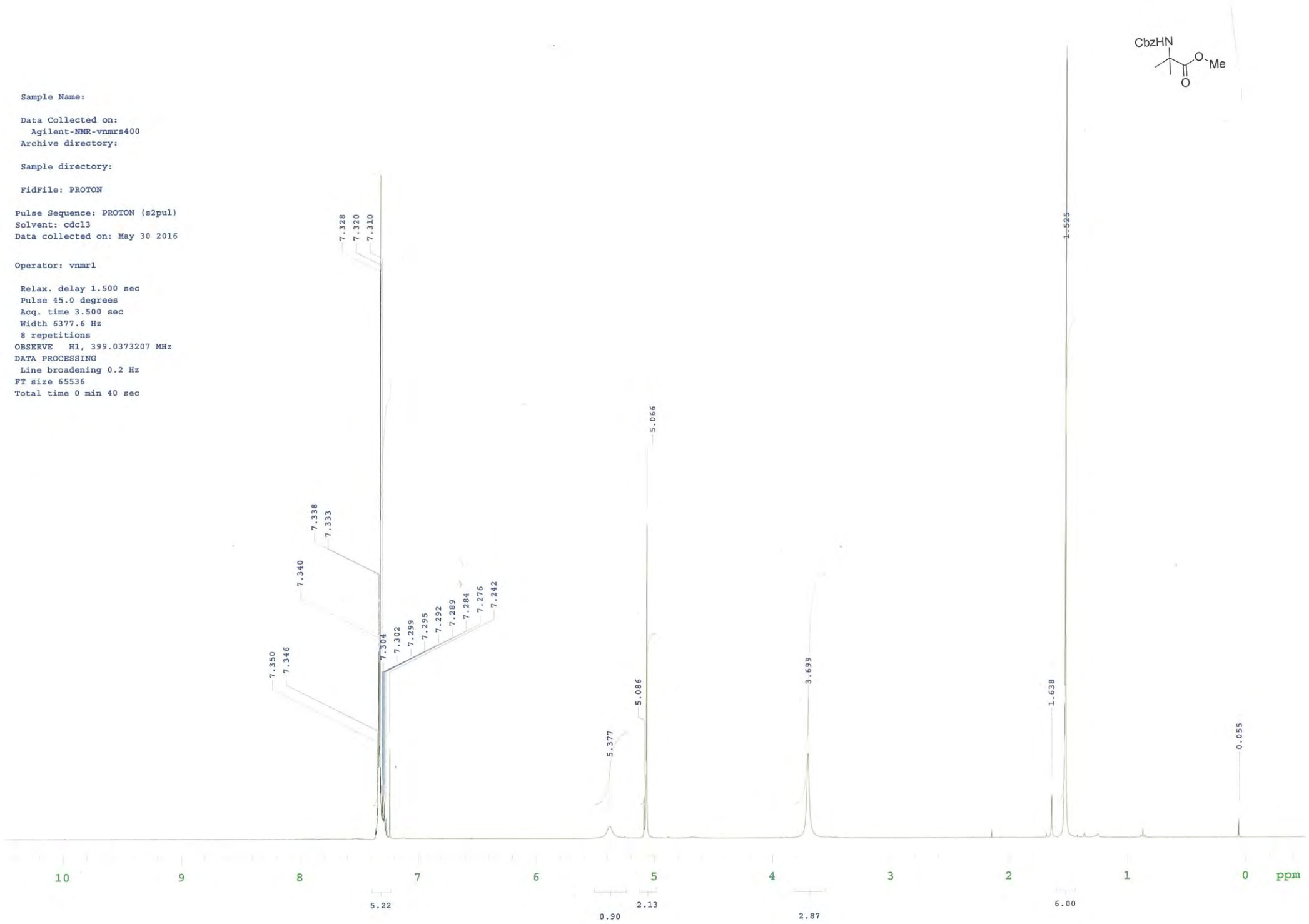
FidFile: CARBON

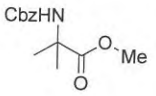
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
128 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min




CbzHN
O
Me
O
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 30 2016
Operator: vnmr1
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec
7.328
7.320
7.310
7.338
7.333
7.340
7.350
7.346
7.304
7.302
7.299
7.295
7.292
7.289
7.284
7.276
7.242
5.377
5.086
5.066
3.699
1.638
1.525
0.055
10
9
8
7
6
5
4
3
2
1
0
ppm
5.22
0.90
2.13
2.87
6.00



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

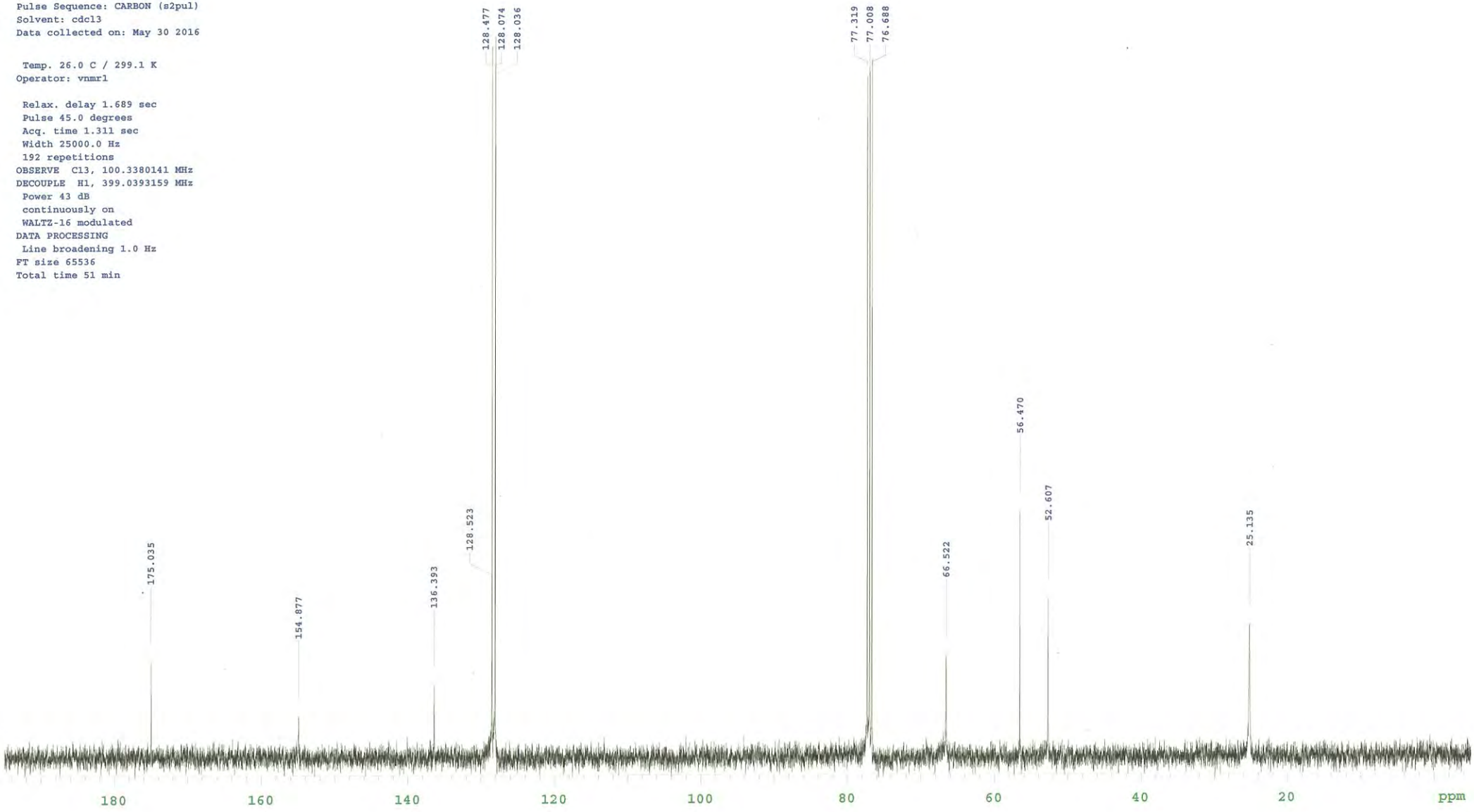
Sample directory:

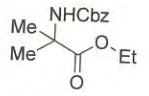
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 30 2016

Temp. 26.0 C / 299.1 K
Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
192 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

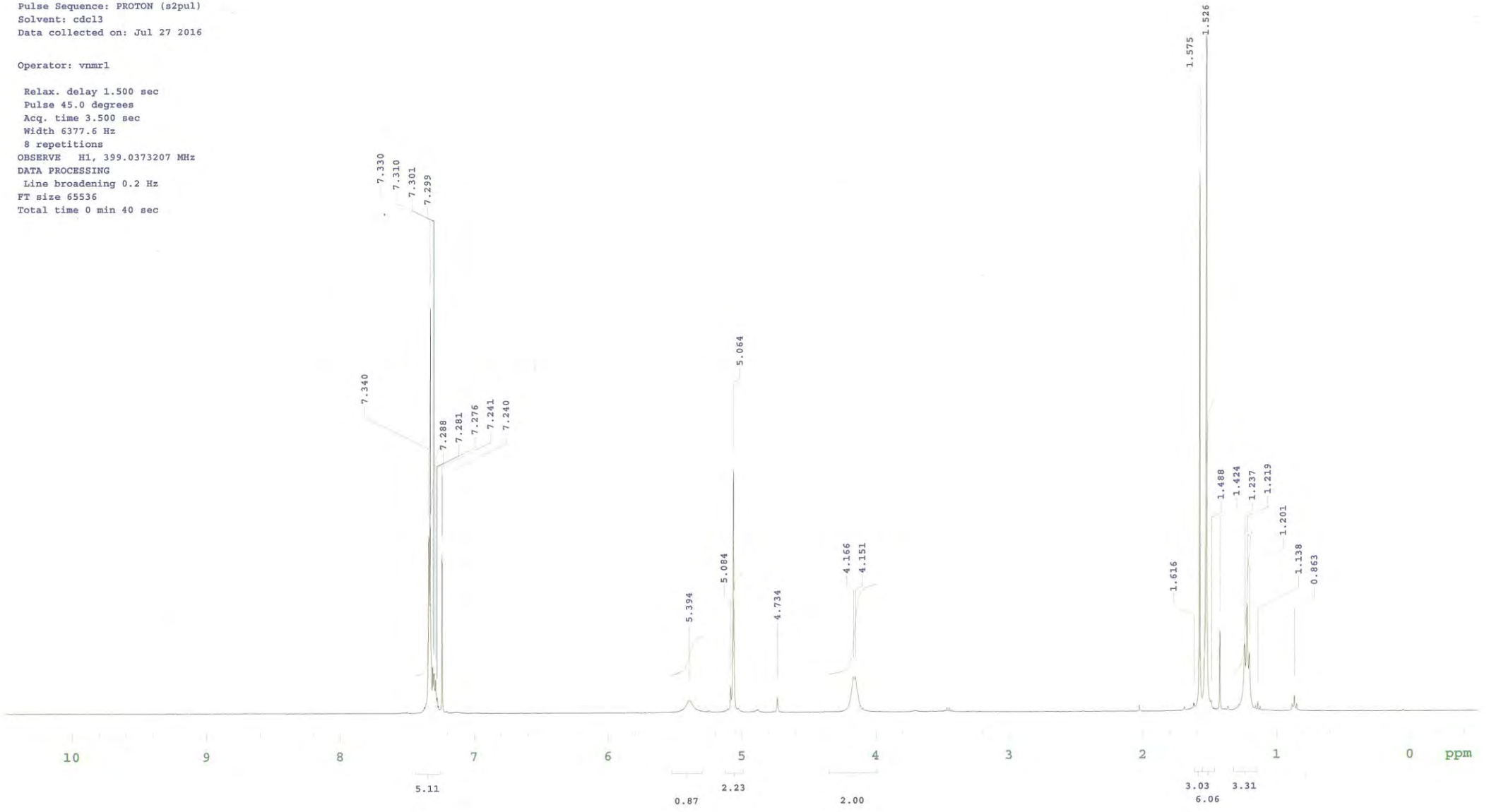
Sample directory:

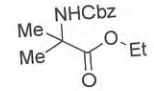
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2016

Operator: vnmrl

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

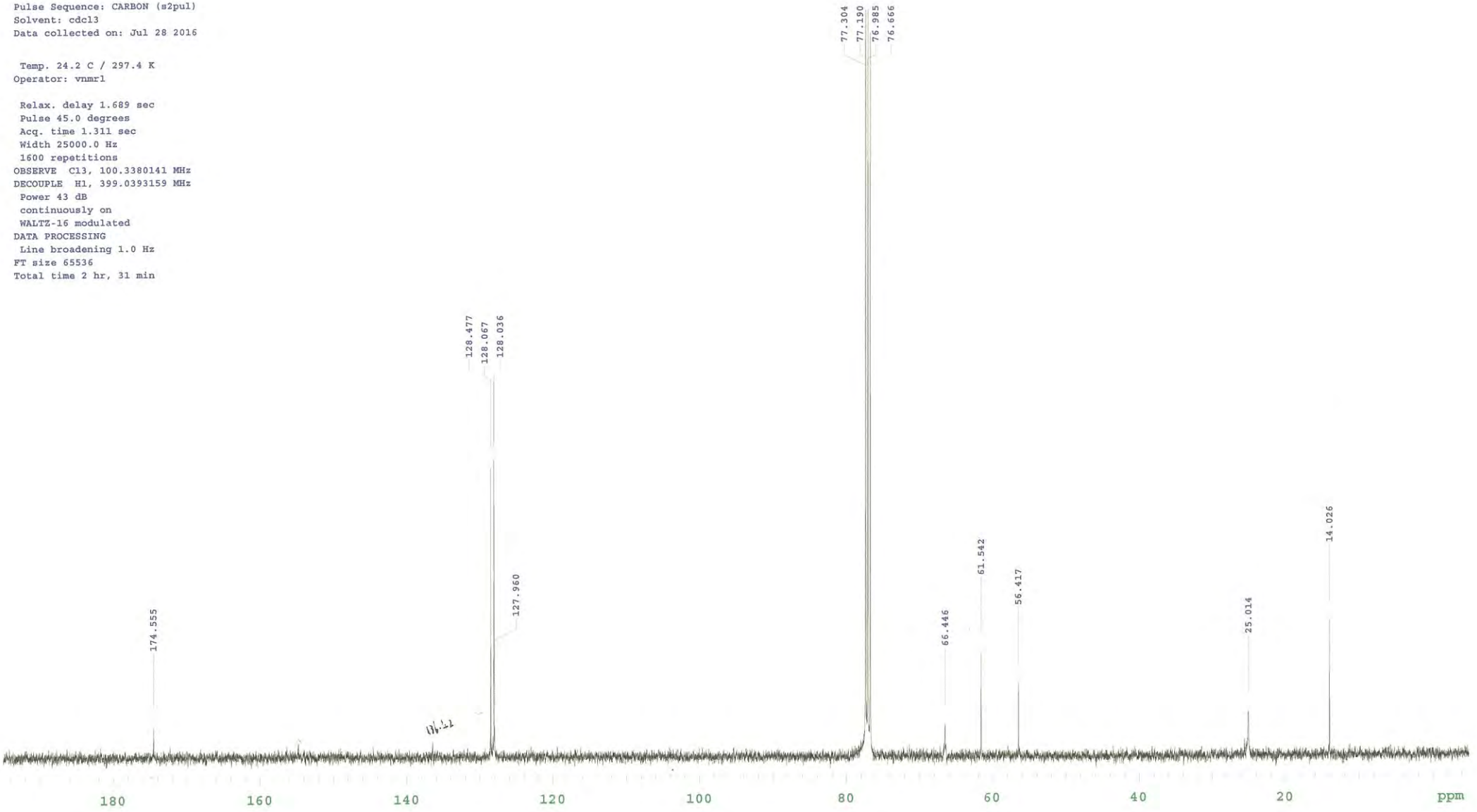
Sample directory:

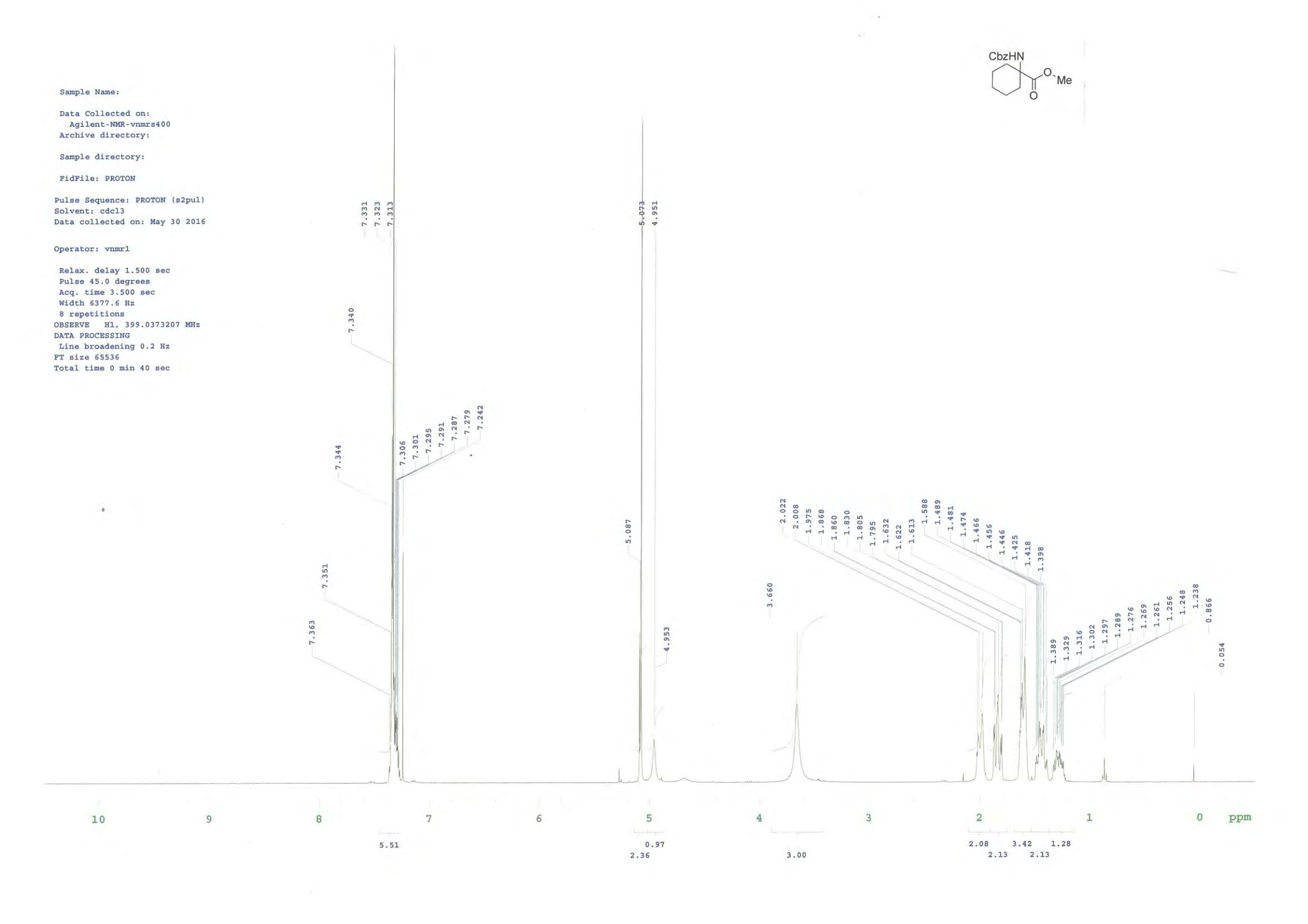
FidFile: CARBON

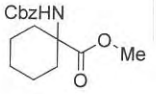
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 28 2016

Temp. 24.2 C / 297.4 K
Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1600 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2 hr, 31 min




Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 30 2016
Operator: vnmr1
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec
CbzHN
O
Me
O
7.363
7.351
7.344
7.340
7.331
7.323
7.313
7.306
7.301
7.295
7.291
7.287
7.279
7.242
5.087
4.953
5.073
4.951
3.660
2.022
2.008
1.975
1.868
1.860
1.830
1.805
1.795
1.632
1.622
1.613
1.588
1.489
1.481
1.474
1.466
1.456
1.446
1.425
1.418
1.398
1.389
1.329
1.316
1.302
1.297
1.289
1.276
1.269
1.261
1.256
1.248
1.238
0.866
0.054
10
9
8
7
6
5
4
3
2
1
0
ppm
5.51
2.36
0.97
3.00
2.08
2.13
3.42
2.13
1.28



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

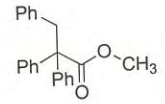
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 30 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
128 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

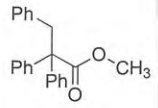
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 30 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

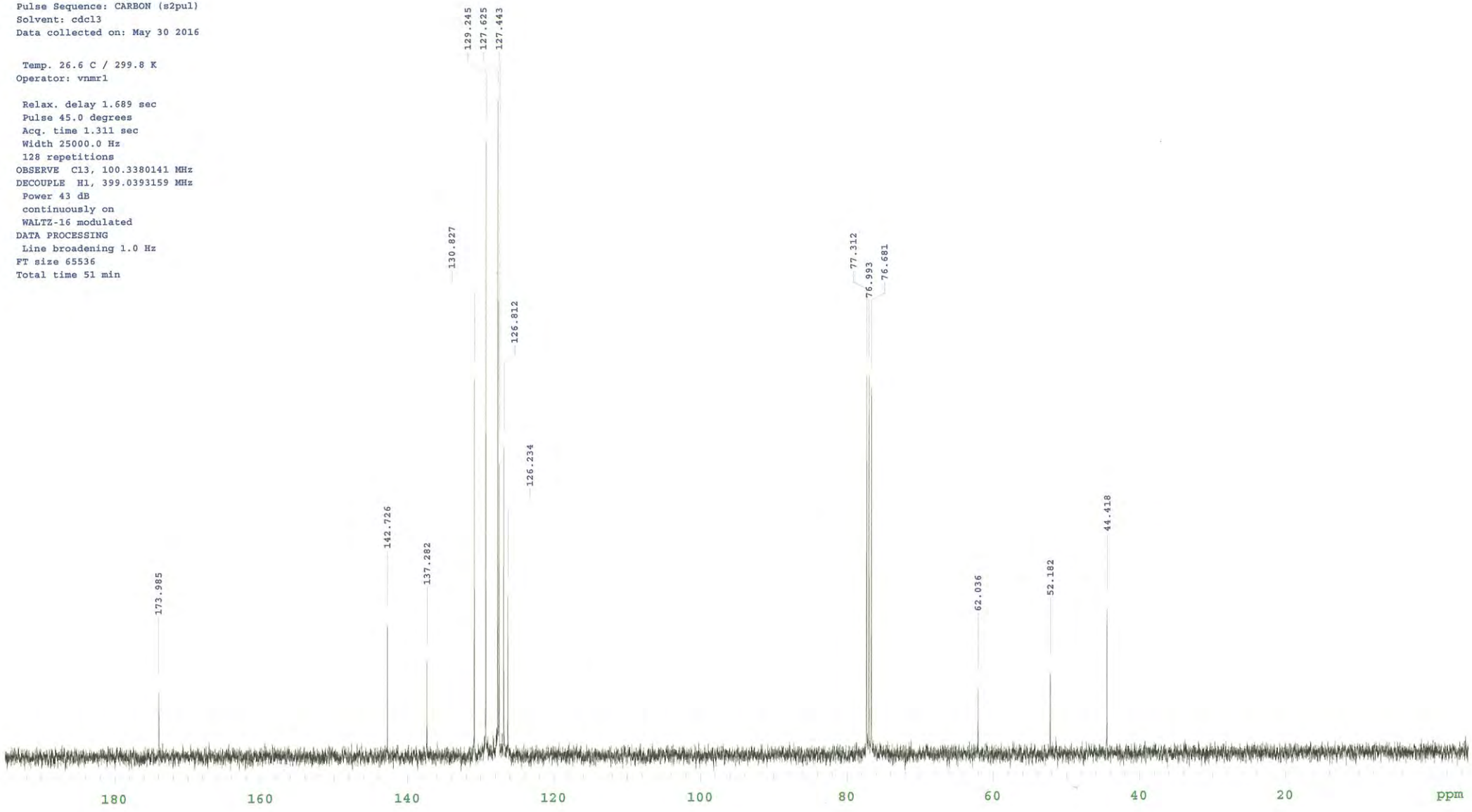
Sample directory:

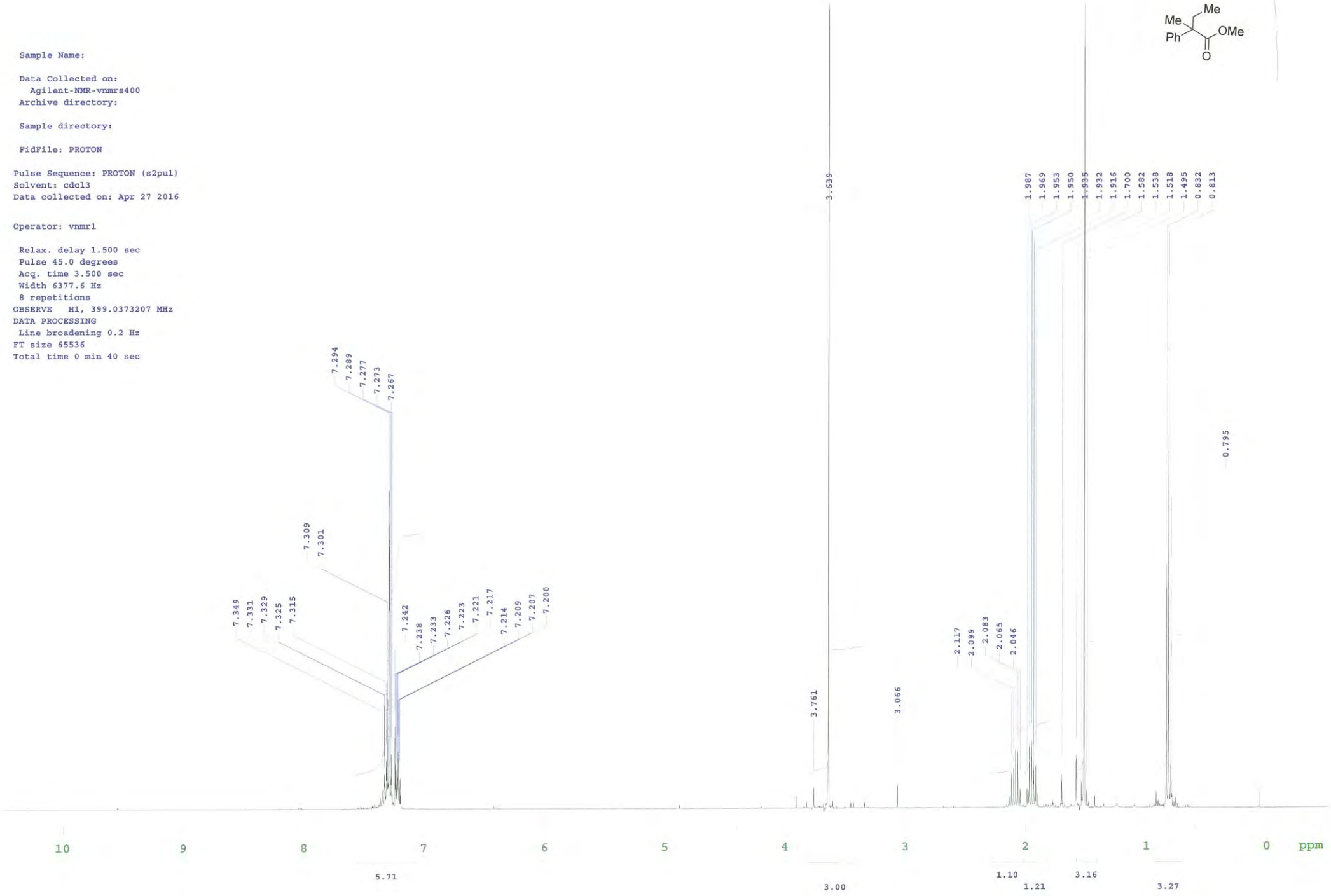
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 30 2016

Temp. 26.6 C / 299.8 K
Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
128 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min




Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 27 2016
Operator: vnmr1
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec
Me
Me
Ph
OMe
O
7.349
7.331
7.329
7.325
7.315
7.309
7.301
7.294
7.289
7.277
7.273
7.267
7.242
7.238
7.233
7.226
7.223
7.221
7.217
7.214
7.209
7.207
7.200
3.761
3.639
3.066
2.117
2.099
2.083
2.065
2.046
1.987
1.969
1.953
1.950
1.935
1.932
1.916
1.700
1.582
1.538
1.518
1.495
0.832
0.813
0.795
10
9
8
7
6
5
4
3
2
1
0
ppm
5.71
3.00
1.10
1.21
3.16
3.27

Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

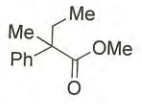
Sample directory:

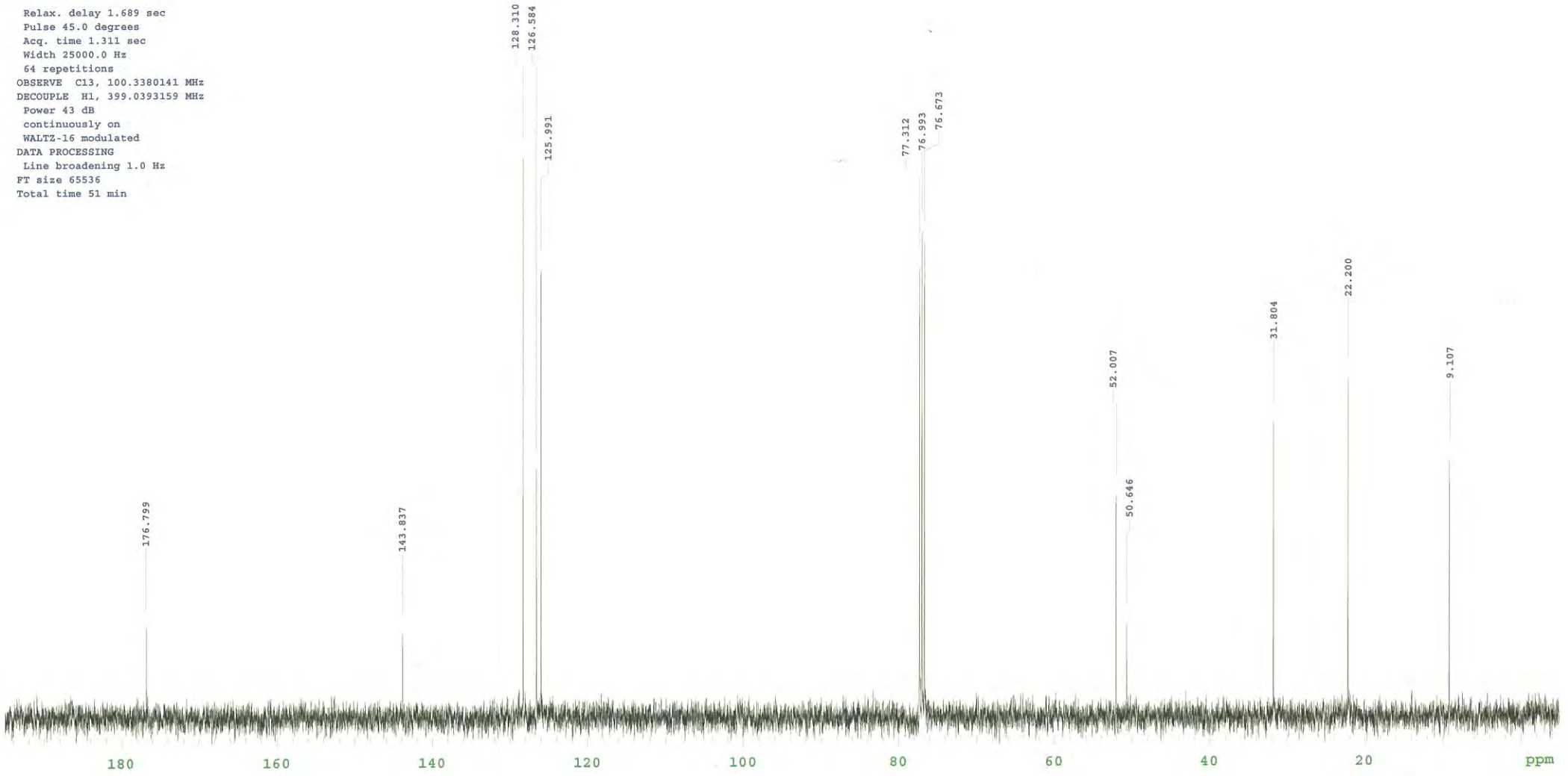
FidFile: CARBON

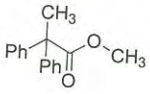
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min







Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

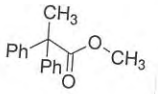
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

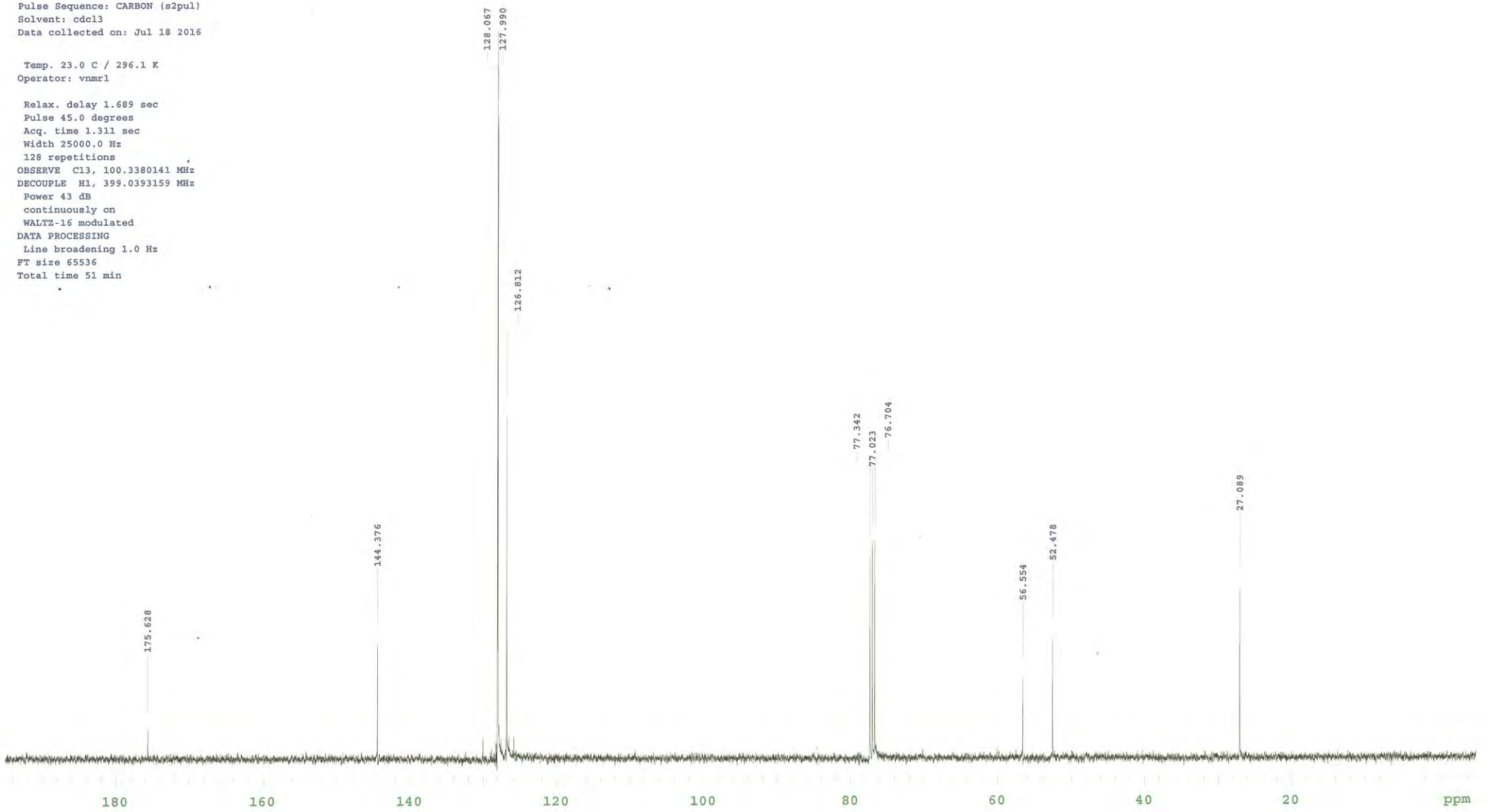
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2016

Temp. 23.0 C / 296.1 K
Operator: vnmrl

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
128 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

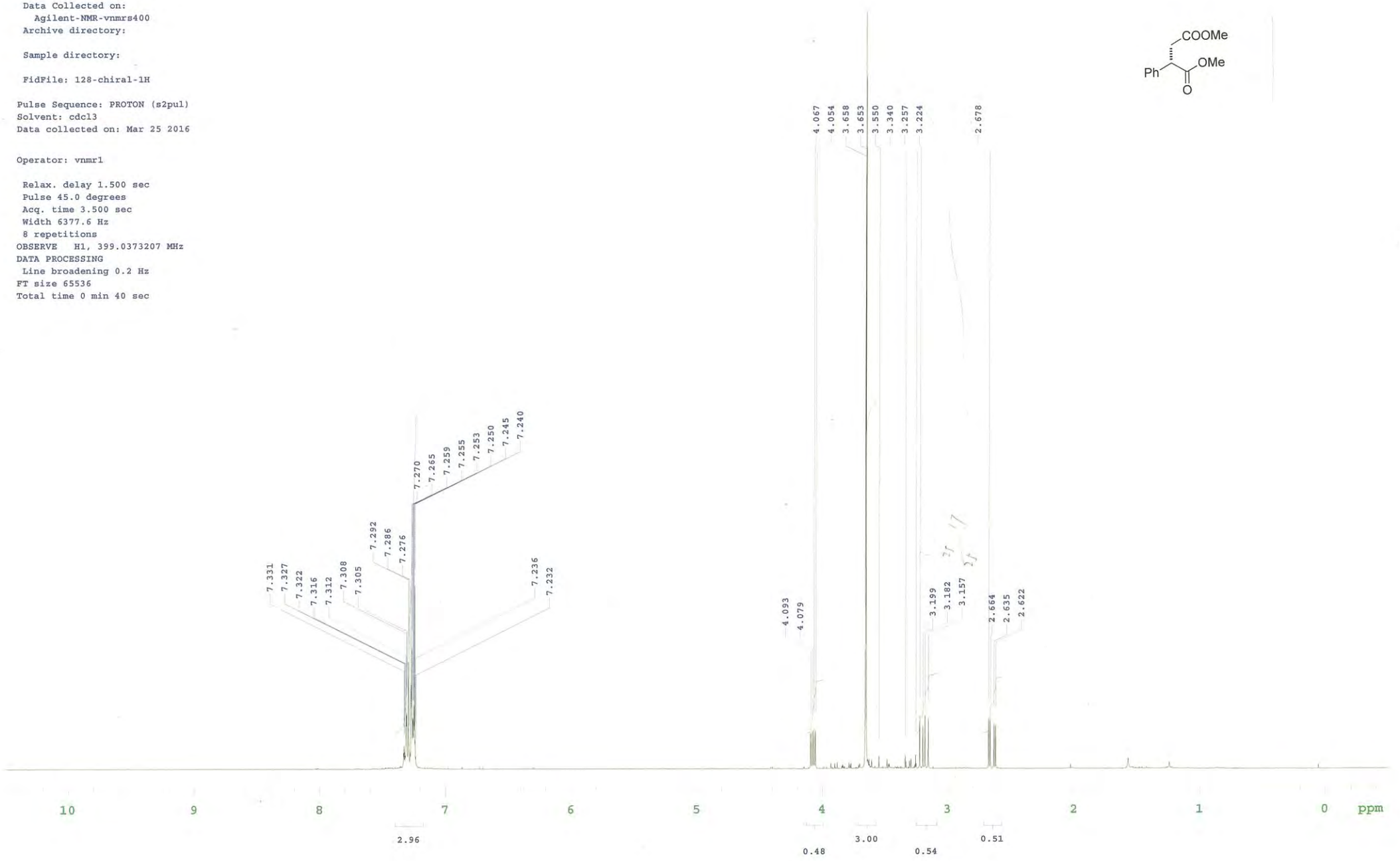
Sample directory:

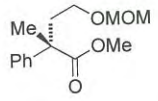
FidFile: 128-chiral-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 25 2016

Operator: vnmr1

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

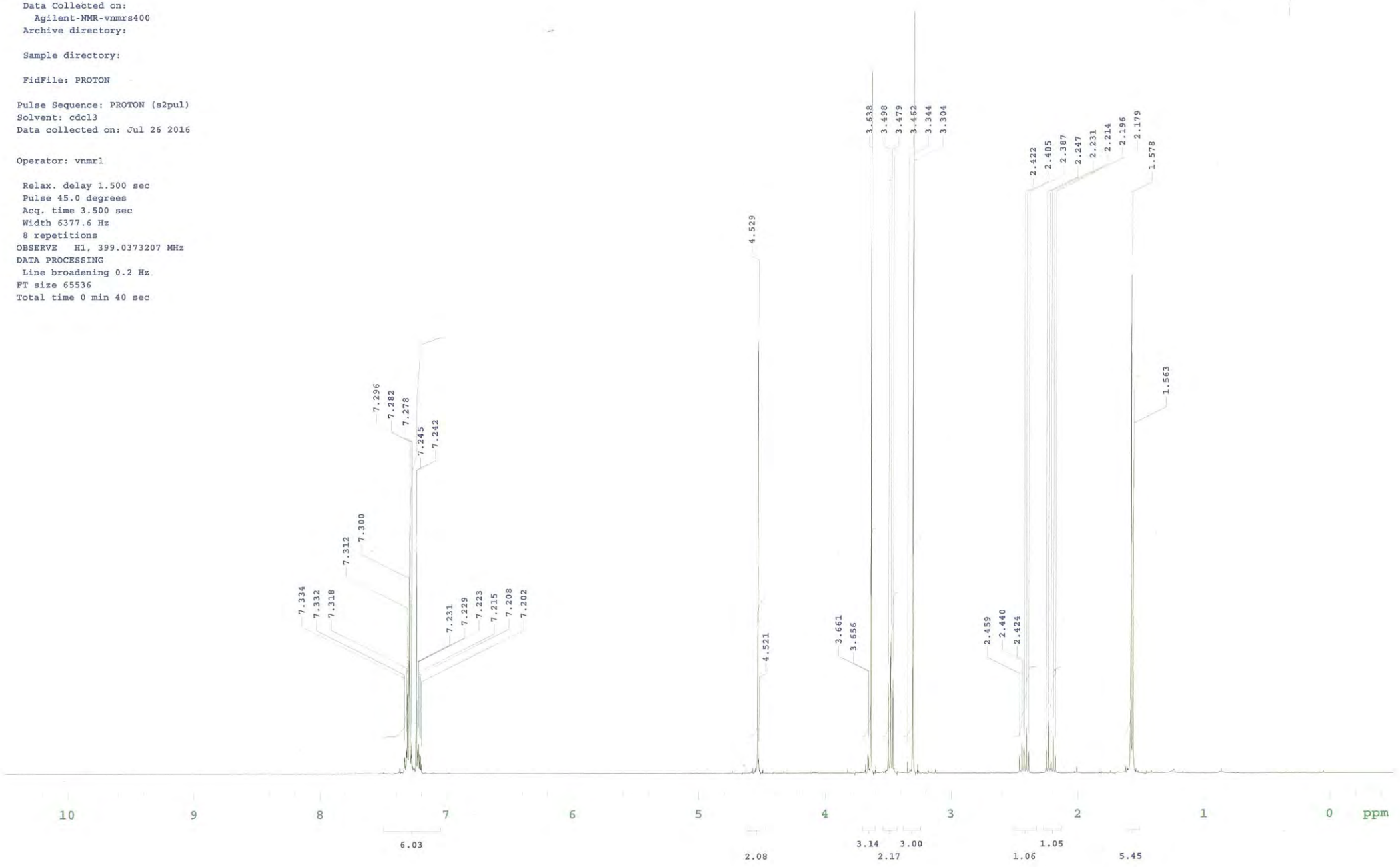
Sample directory:

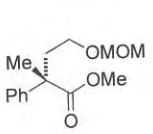
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 26 2016

Operator: vnmrl

Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

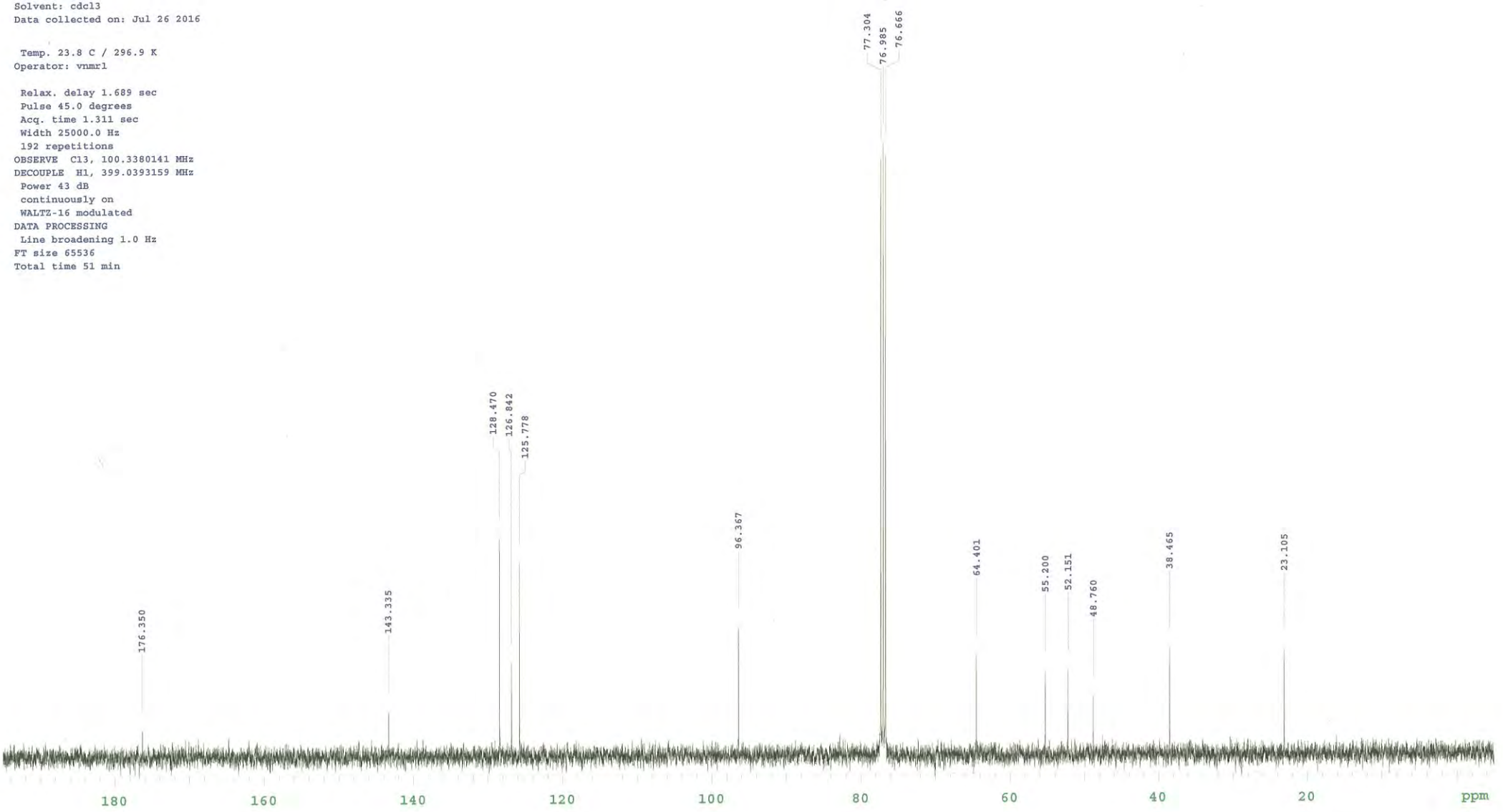
Sample directory:

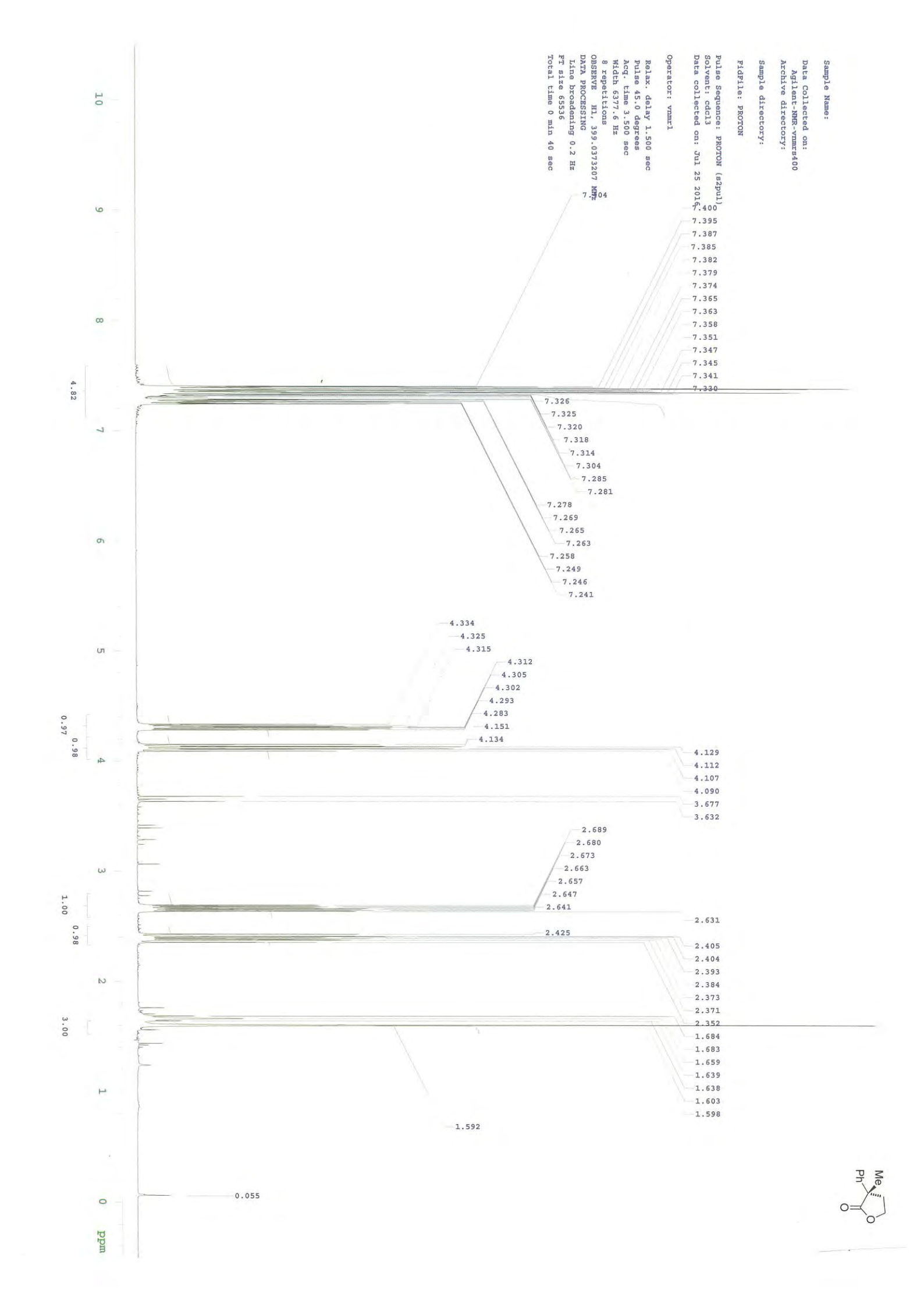
FidFile: CARBON

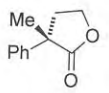
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 26 2016

Temp. 23.8 C / 296.9 K
Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
192 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min




Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 25 2016
Operator: vnmrl
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec
7.404
7.400
7.395
7.387
7.385
7.382
7.379
7.374
7.365
7.363
7.358
7.351
7.347
7.345
7.341
7.330
7.326
7.325
7.320
7.318
7.314
7.304
7.285
7.281
7.278
7.269
7.265
7.263
7.258
7.249
7.246
7.241
4.334
4.325
4.315
4.312
4.305
4.302
4.293
4.283
4.151
4.134
4.129
4.112
4.107
4.090
3.677
3.632
2.689
2.680
2.673
2.663
2.657
2.647
2.641
2.631
2.425
2.405
2.404
2.393
2.384
2.373
2.371
2.352
1.684
1.683
1.659
1.639
1.638
1.603
1.598
1.592
0.055
4.82
0.97
0.98
1.00
0.98
3.00
10
9
8
7
6
5
4
3
2
1
0
ppm
Me
Ph
O
O



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

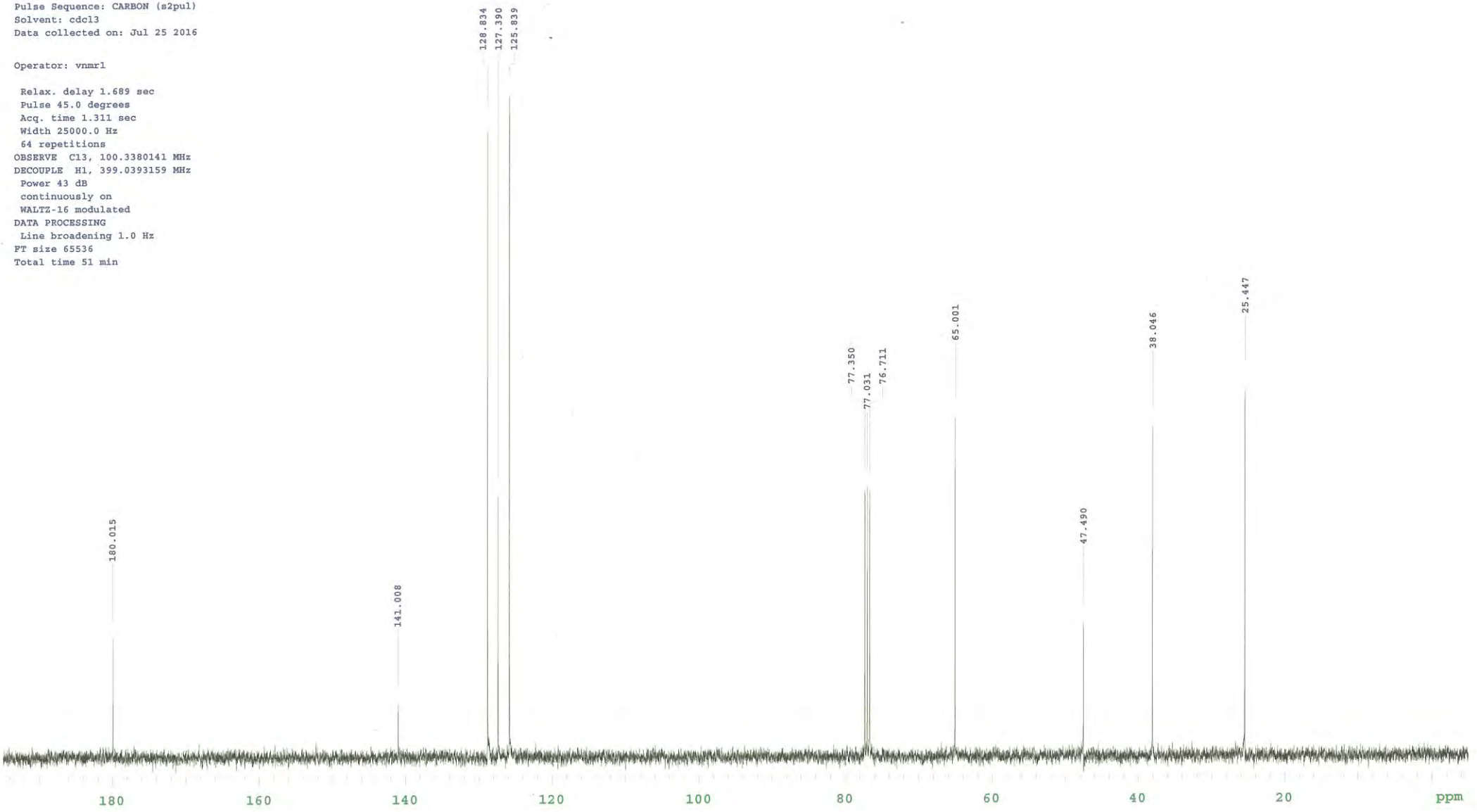
Sample directory:

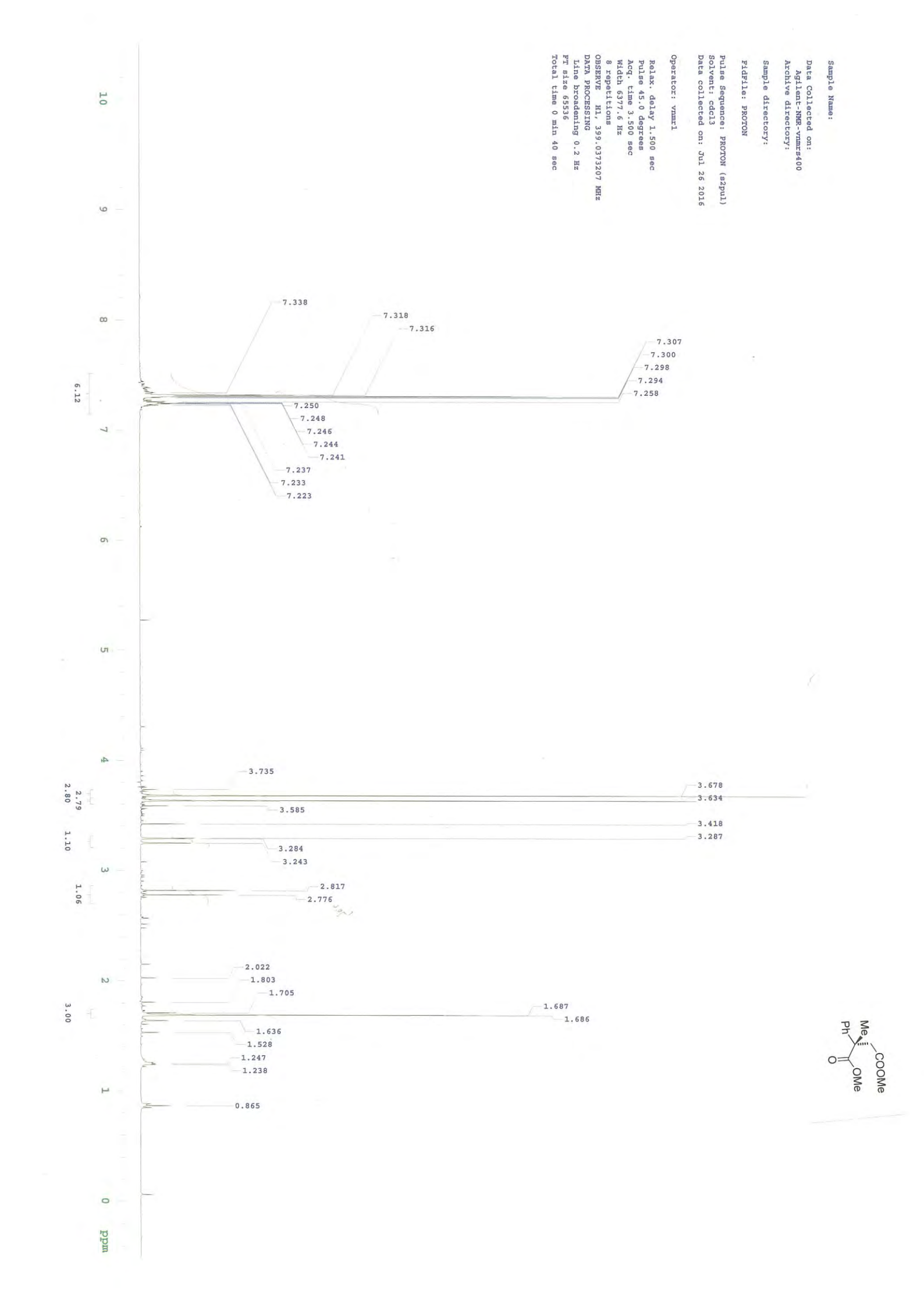
FidFile: CARBON

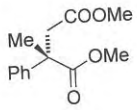
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 25 2016

Operator: vnmrl

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min




Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 26 2016
Operator: vnmrl
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec
7.338
7.318
7.316
7.307
7.300
7.298
7.294
7.258
7.250
7.248
7.246
7.244
7.241
7.237
7.233
7.223
3.735
3.678
3.634
3.585
3.418
3.287
3.284
3.243
2.817
2.776
2.022
1.803
1.705
1.687
1.686
1.636
1.528
1.247
1.238
0.865
6.12
2.79
2.80
1.10
1.06
3.00
ppm
Me
COOMe
Ph
OMe
O



Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

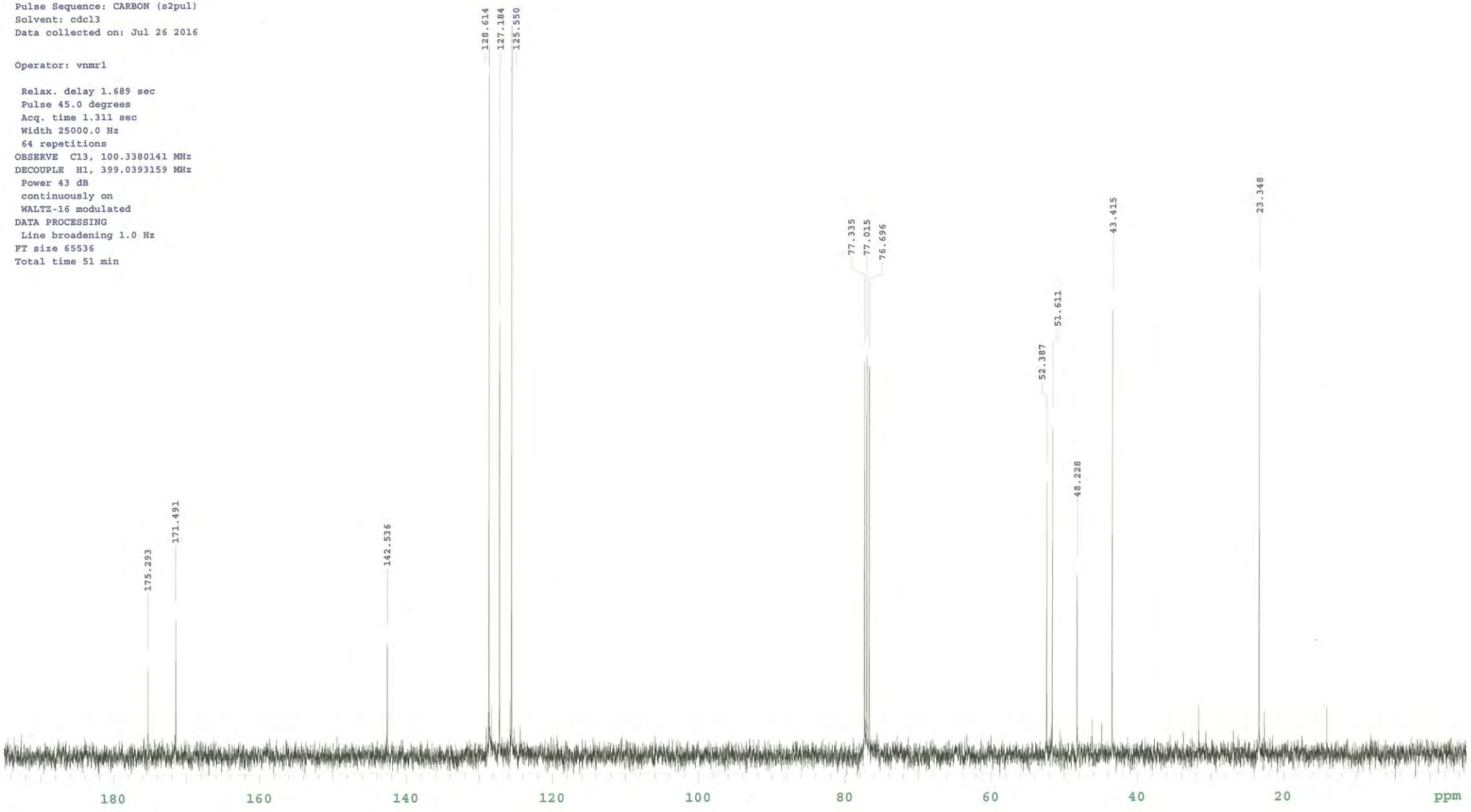
Sample directory:

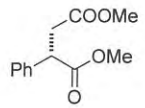
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 26 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min





Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

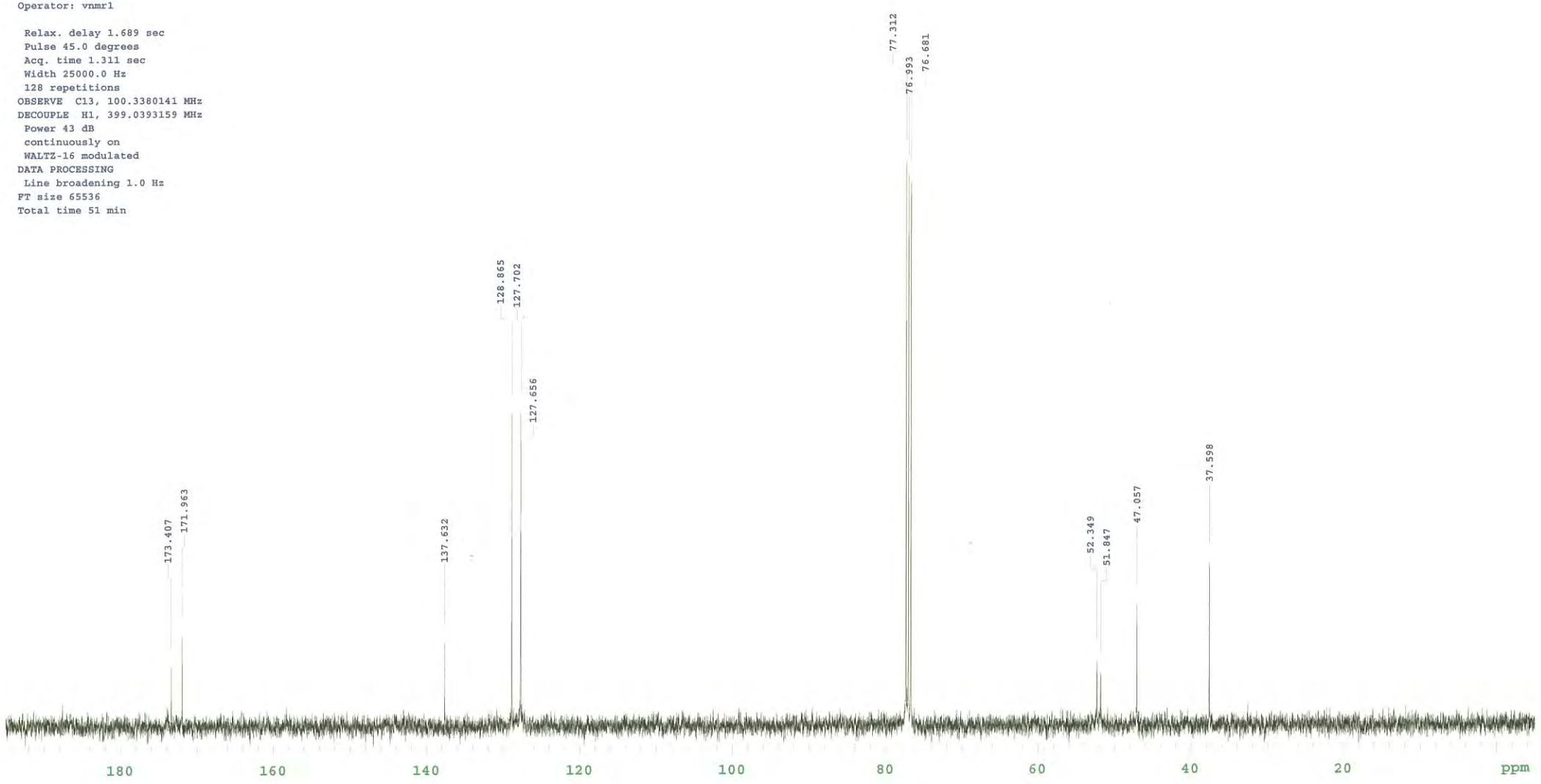
Sample directory:

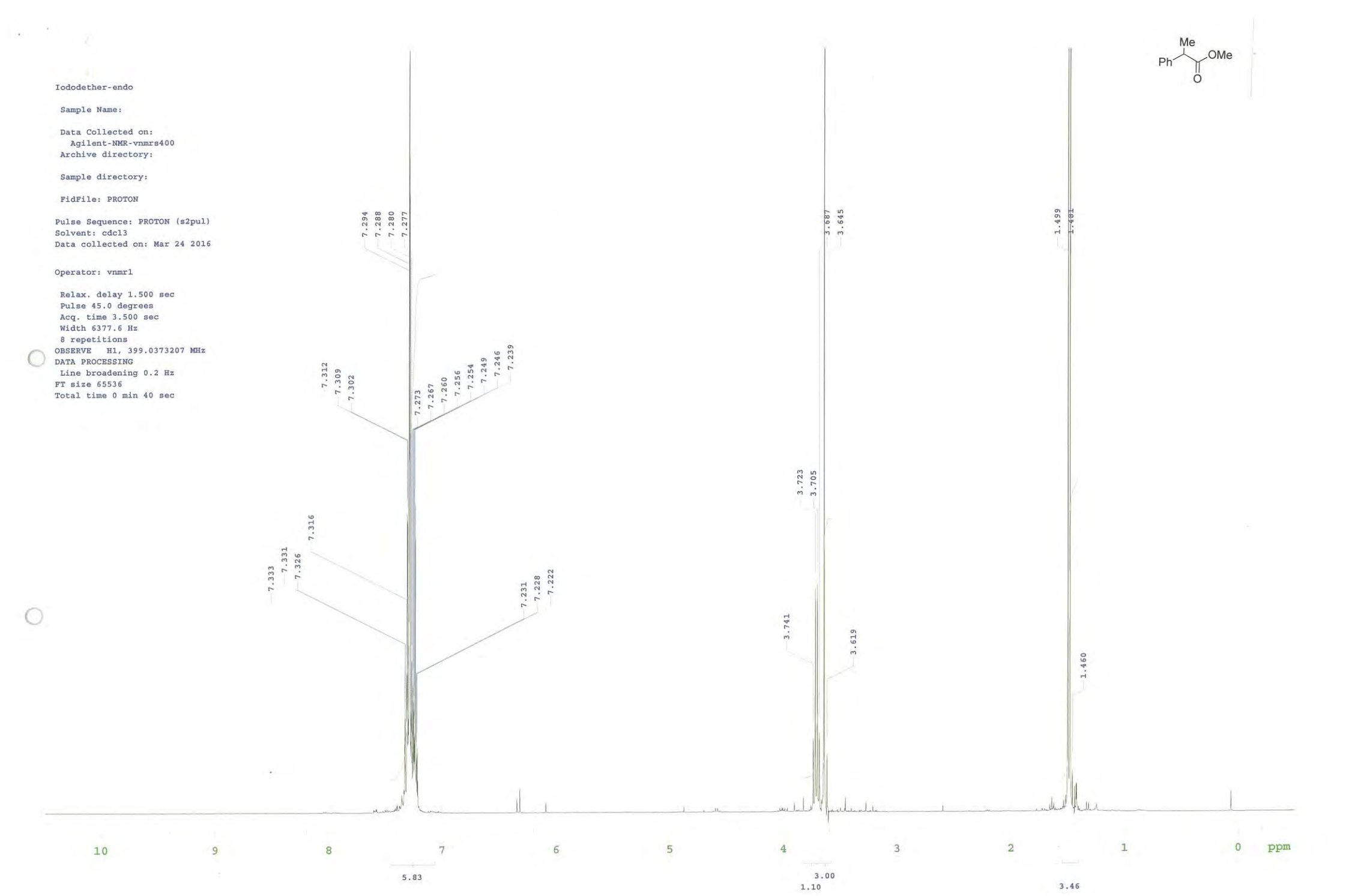
FidFile: 128-chiral-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 25 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
128 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min




Iododether-endo
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 24 2016
Operator: vnmr1
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6377.6 Hz
8 repetitions
OBSERVE H1, 399.0373207 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 40 sec
Me
Ph
OMe
O
7.333
7.331
7.326
7.316
7.312
7.309
7.302
7.294
7.288
7.280
7.277
7.273
7.267
7.260
7.256
7.254
7.249
7.246
7.239
7.231
7.228
7.222
3.741
3.723
3.705
3.687
3.645
3.619
1.499
1.481
1.460
10
9
8
7
6
5
4
3
2
1
0
ppm
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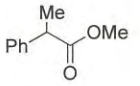
3.00
1.10
3.46



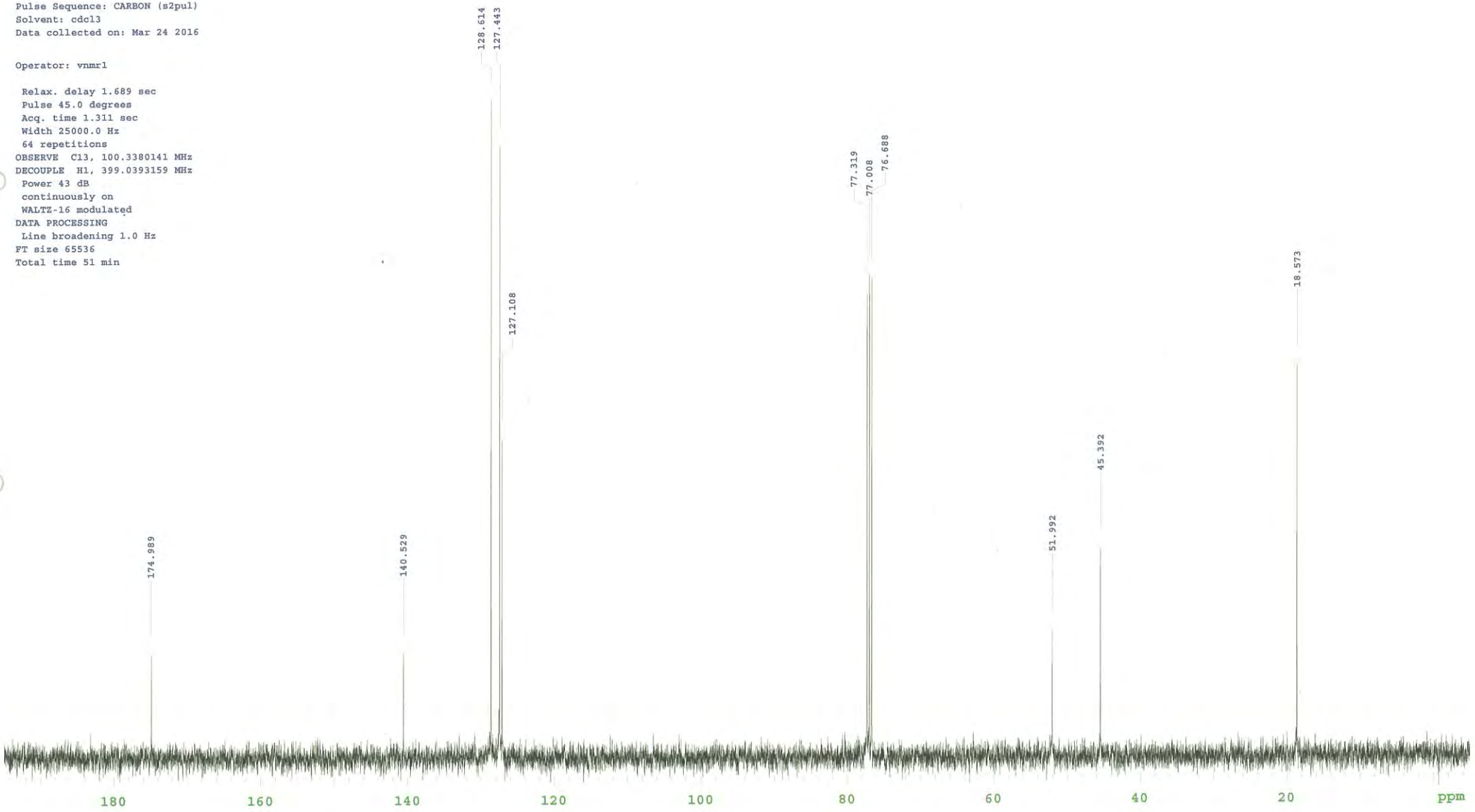
Sample Name:

Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 24 2016

Operator: vnmr1

Relax. delay 1.689 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
64 repetitions
OBSERVE C13, 100.3380141 MHz
DECOUPLE H1, 399.0393159 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 51 min