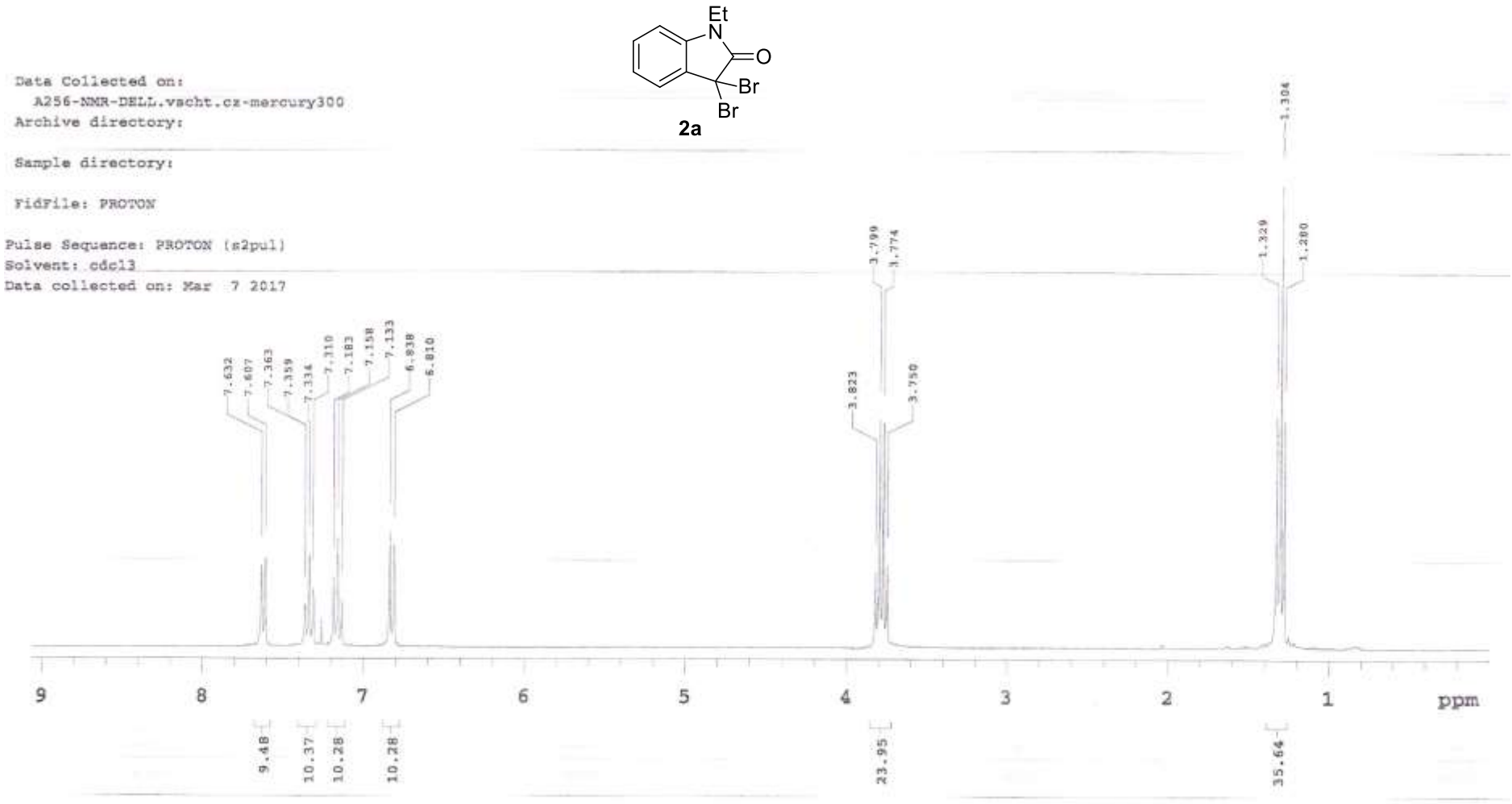
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

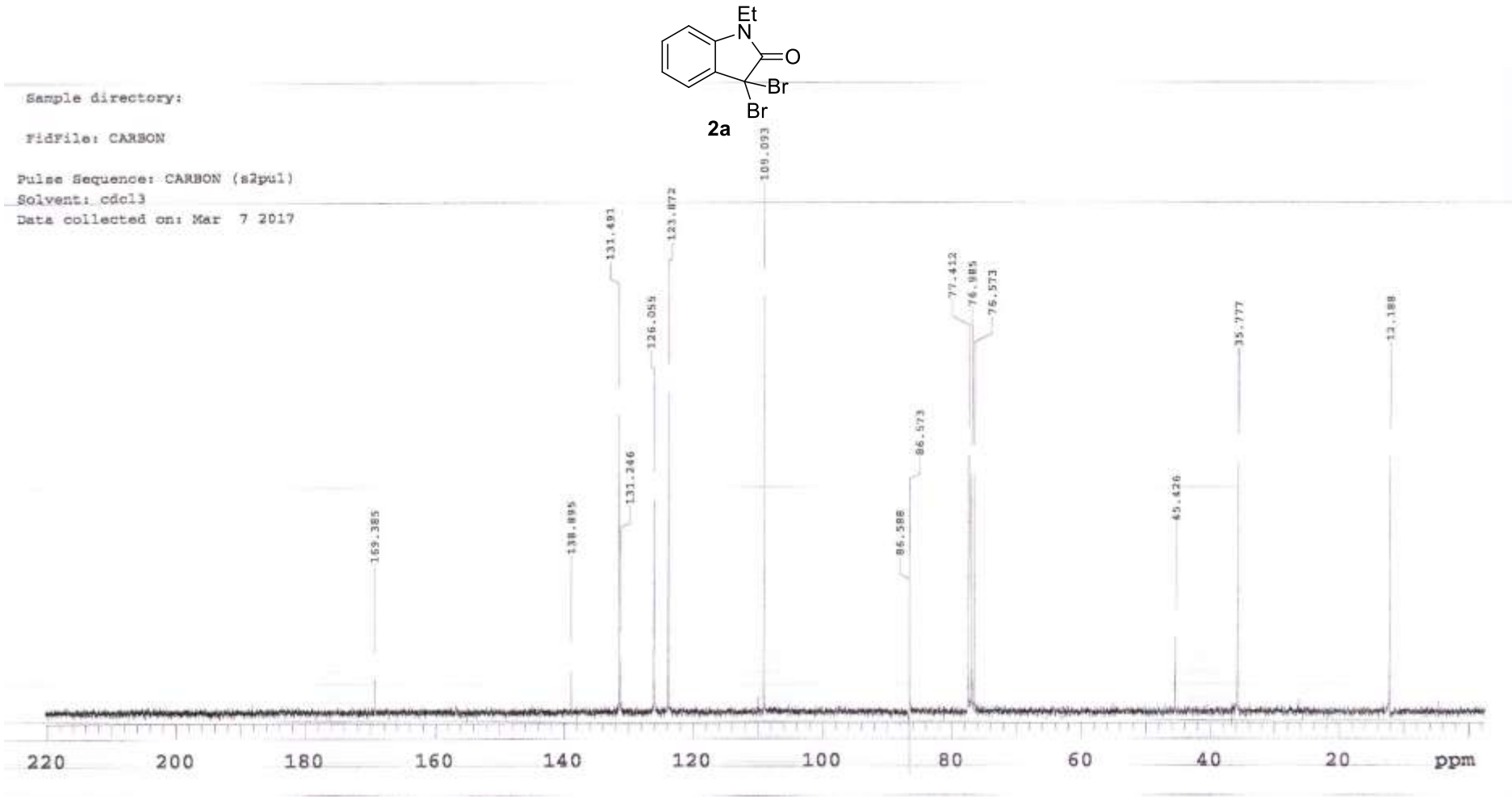
The Synthesis of Polysubstituted Indoles from 3-Bromo-2-indolyl Phosphates

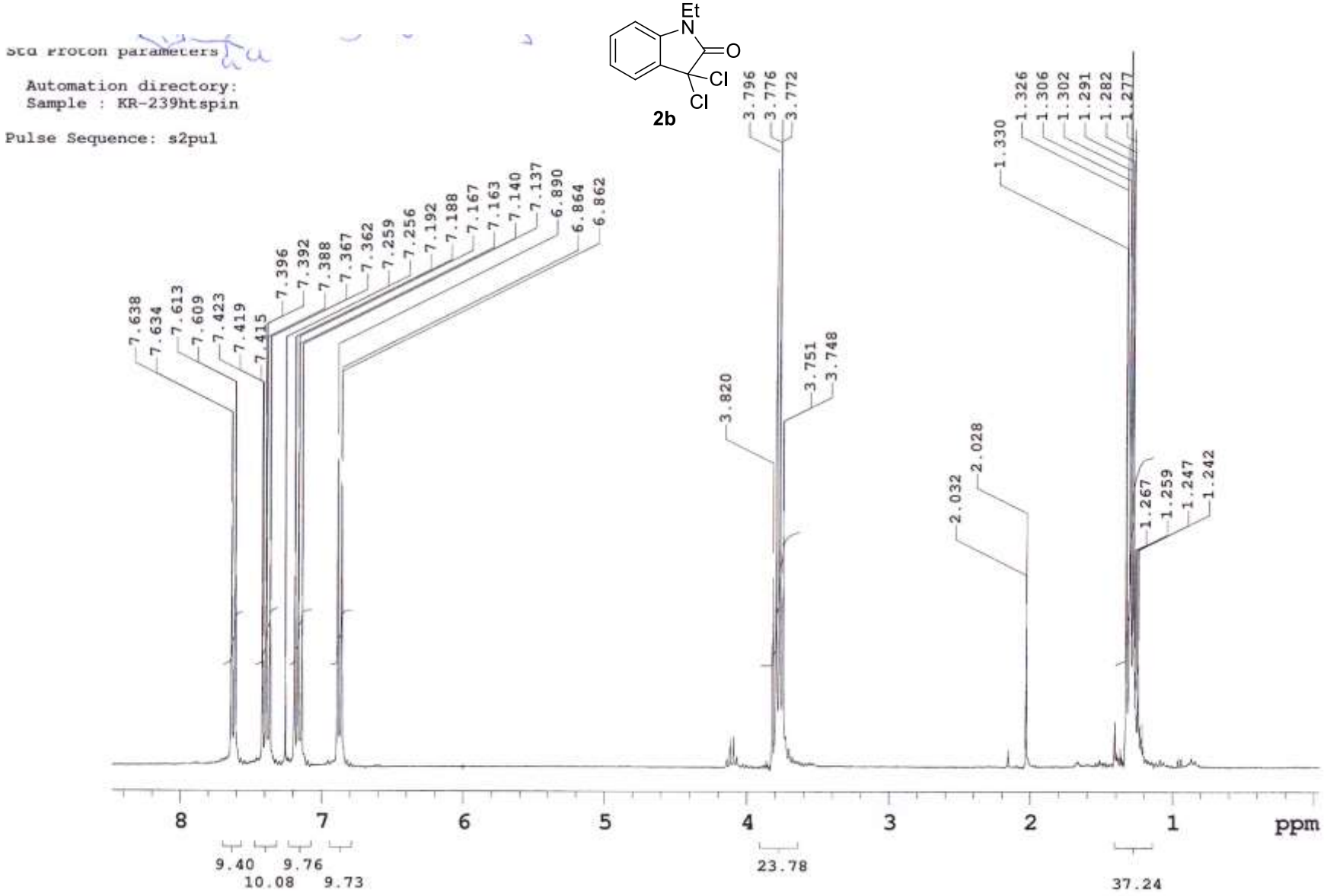
Peter Polák,[a] Tomáš Tobrman*[a]

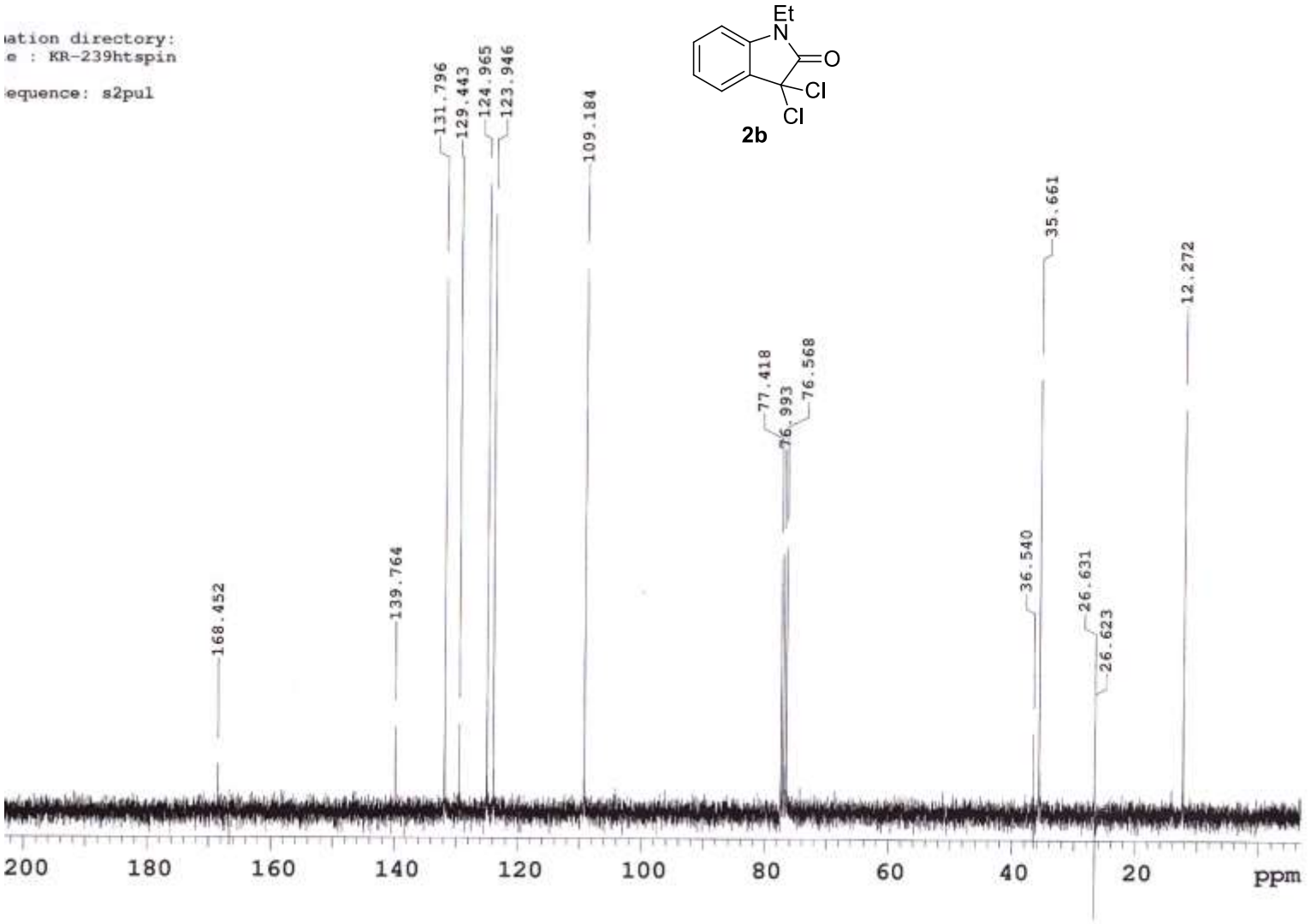
[a] *Department of Organic Chemistry, University of Chemistry and Technology, Prague, Technická 5, 166 28 Prague 6, Czech Republic. E-mail: tobrmant@vscht.cz*

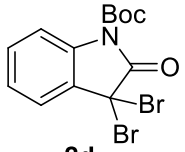
Copies of ^{1}H and ^{13}C NMR spectra


Et
N
O
Br
Br
2a
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 7 2017
7.632
7.607
7.363
7.359
7.334
7.310
7.183
7.158
7.133
6.838
6.810
3.823
3.799
3.774
3.750
1.329
1.304
1.280
9
8
7
6
5
4
3
2
1
ppm
9.48
10.37
10.28
10.28
23.95
35.64


Et
N
O
Br
Br
2a
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 7 2017
169.385
138.895
131.491
131.246
126.055
123.872
109.093
86.588
86.573
77.412
76.985
76.573
45.426
35.777
13.188
220
200
180
160
140
120
100
80
60
40
20
ppm


Std Proton parameters
Automation directory:
Sample : KR-239htspin
Pulse Sequence: s2pul
Et
N
O
Cl
Cl
2b
7.638
7.634
7.613
7.609
7.423
7.419
7.415
7.396
7.392
7.388
7.367
7.362
7.259
7.256
7.192
7.188
7.167
7.163
7.140
7.137
6.890
6.864
6.862
3.796
3.776
3.772
3.820
3.751
3.748
2.032
2.028
1.330
1.326
1.306
1.302
1.291
1.282
1.277
1.267
1.259
1.247
1.242
8
7
6
5
4
3
2
1
ppm
9.40
10.08
9.76
9.73
23.78
37.24


ation directory:
e : KR-239htspin
equence: s2pul
Et
N
O
Cl
Cl
2b
131.796
129.443
124.965
123.946
109.184
77.418
76.993
76.568
168.452
139.764
36.540
35.661
26.631
26.623
12.272
200
180
160
140
120
100
80
60
40
20
ppm



2d

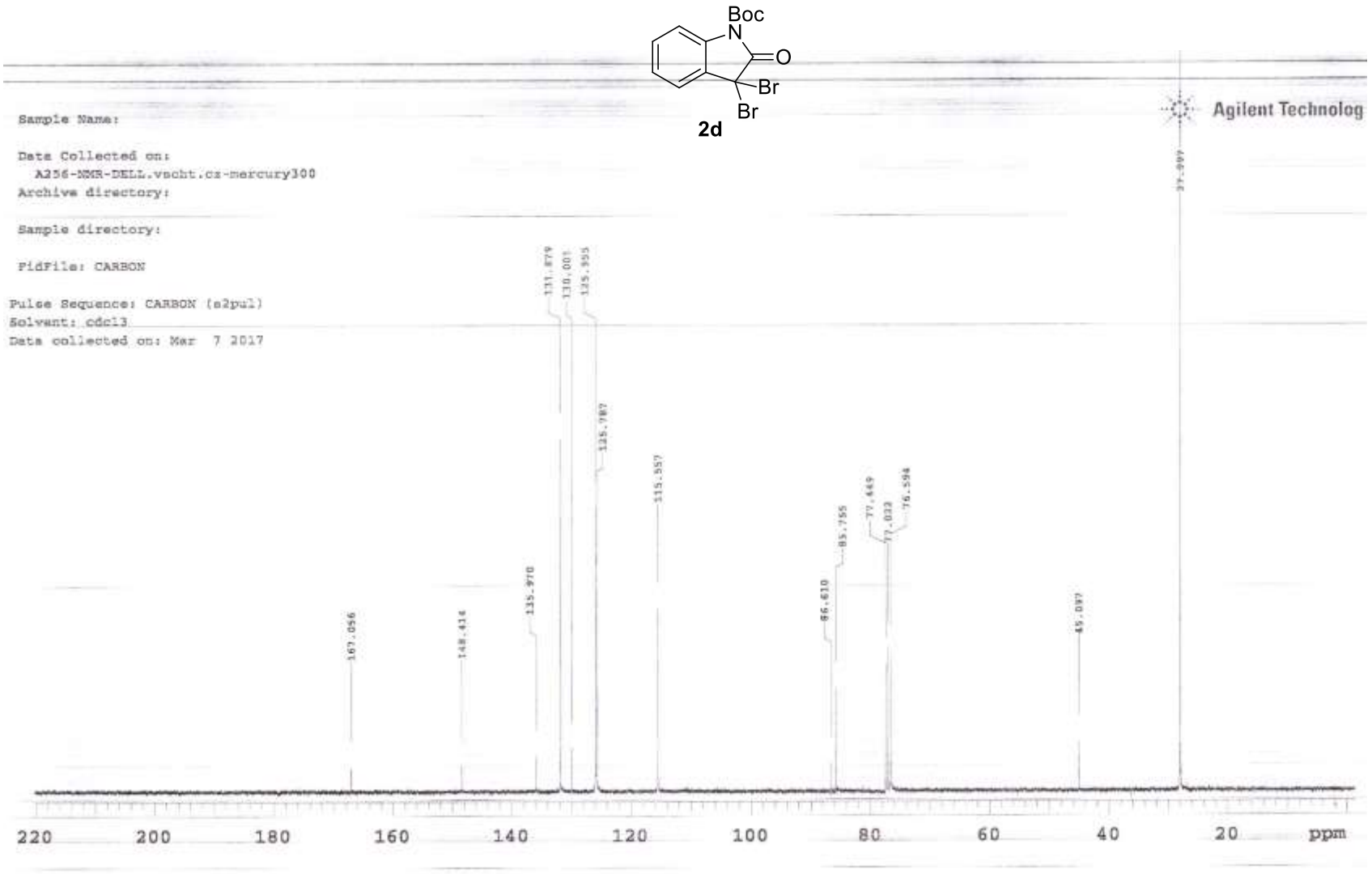
Sample Name:

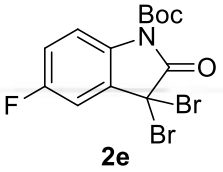
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:

Sample directory:

FidFile: PROTON

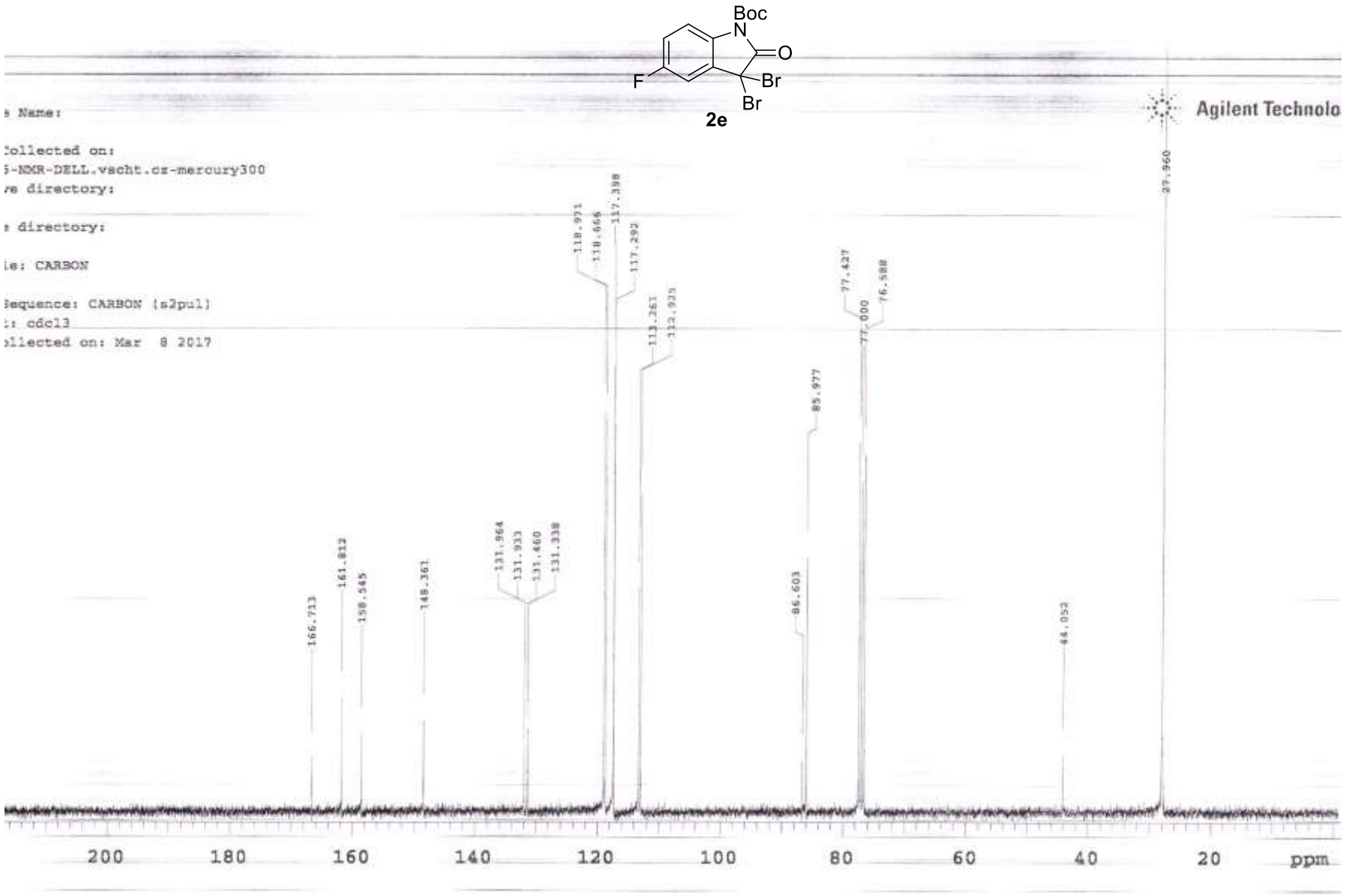
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 7 2016

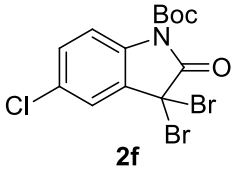

Boc
N
O
Br
Br
2d
Agilent Technolog
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 7 2017
167.056
148.414
135.970
131.679
130.001
125.955
125.787
115.557
86.610
85.755
77.449
77.032
76.594
45.097
37.969
220
200
180
160
140
120
100
80
60
40
20
ppm


Boc
N
O
F
Br
Br

2e

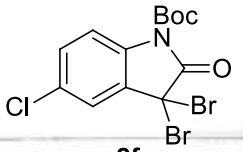
mple Name:
ta Collected on:
A256-NMR-DELL.vscht.cz-mercury300
chive directory:
mple directory:
dFile: PROTON
se Sequence: PROTON (s2pul)
vent: cdcl3
a collected on: Oct 21 2016
Agilent T
7.892
7.877
7.861
7.847
7.396
7.386
7.371
7.363
7.259
7.117
7.097
7.088
7.066
1.649
1.673
1.632
8
7
6
5
4
3
2
1
7.67
7.22
7.80
77.30


Boc
N
O
F
Br
Br
2e
Agilent Technolo
Name:
Collected on:
NMR-DELL.vscht.cz-mercury300
ve directory:
directory:
le: CARBON
Sequence: CARBON (s2pul)
: cdcl3
ollected on: Mar 8 2017
166.713
161.812
158.545
148.361
131.964
131.933
131.460
131.338
118.991
118.666
117.398
117.292
113.361
113.035
86.603
85.977
77.427
77.000
76.588
44.052
27.960
200
180
160
140
120
100
80
60
40
20
ppm

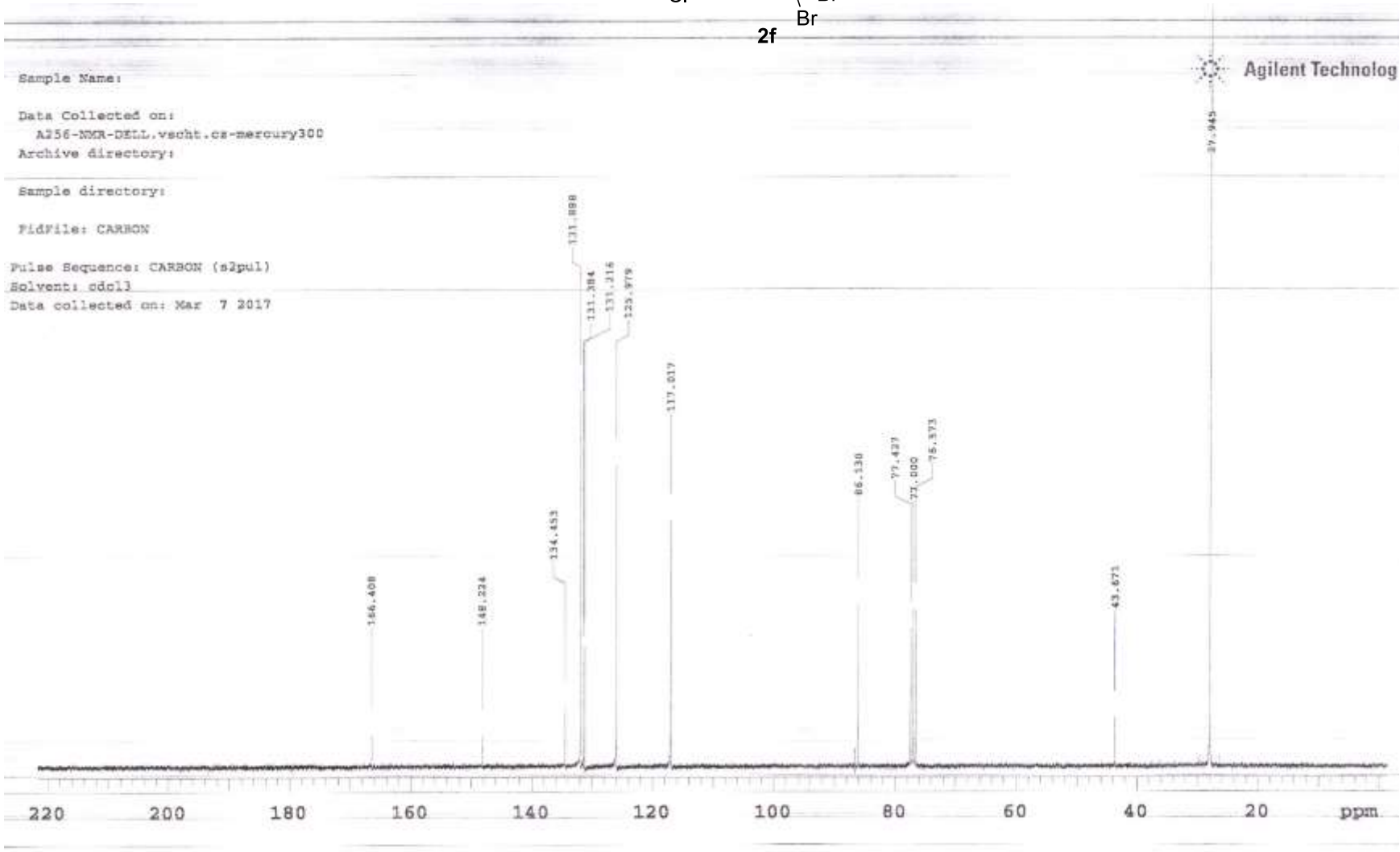

Boc
N
O
Cl
Br
Br

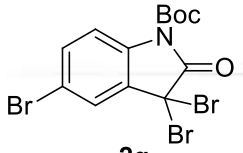
2f

le Name:
Collected on:
56-NMR-DELL.vscht.cz-mercury300
ive directory:
le directory:
ile: D441-H-CDCl3
Sequence: PROTON (s2pul)
nt: cdcl3
collected on: Oct 10 2016
7.843
7.814
7.646
7.640
7.365
7.357
7.336
7.328
7.259
1.647
1.632
8
7
6
5
4
3
2
1
ppm
7.95
6.19
8.16
77.70


Boc
N
O
Cl
Br
Br

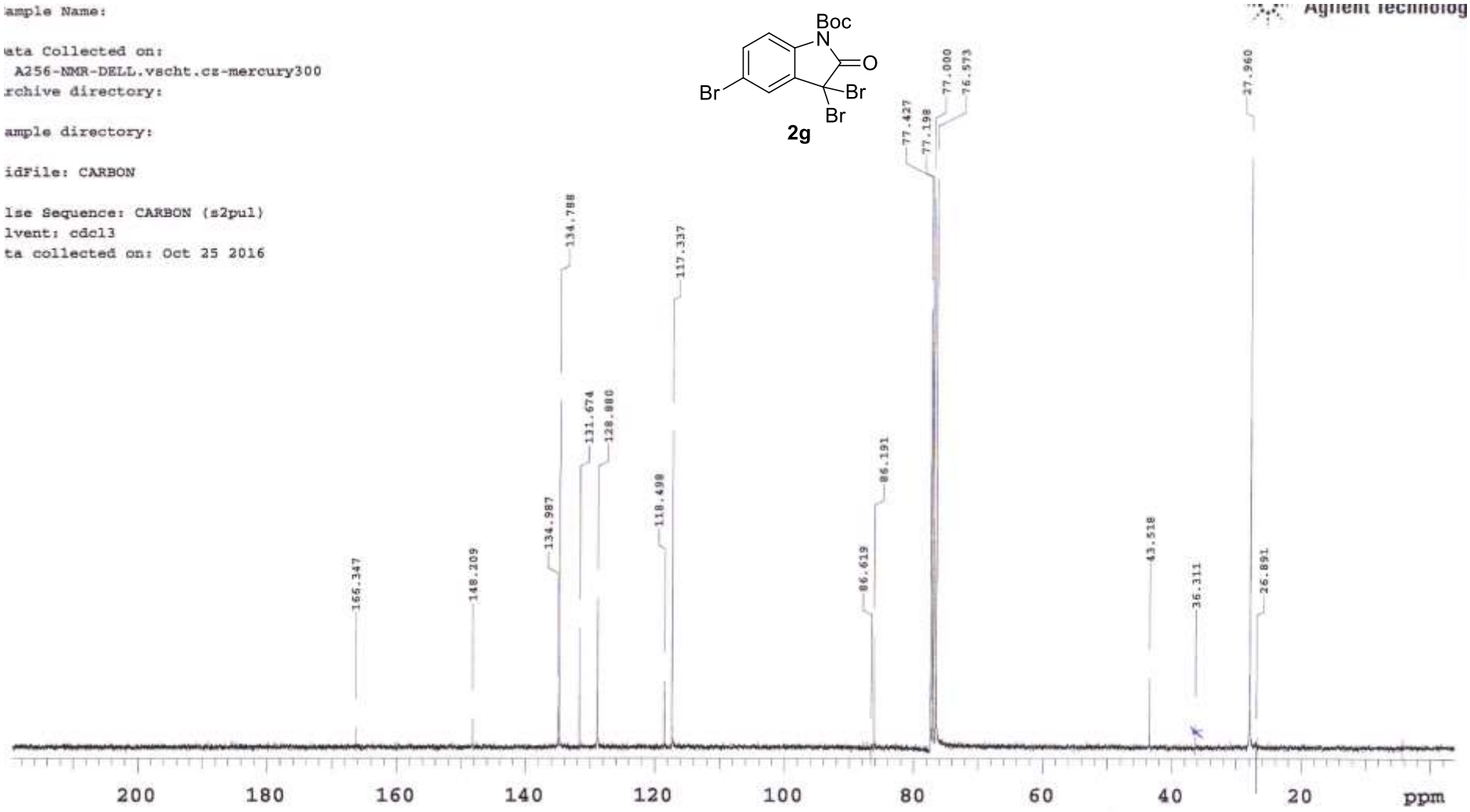
2f

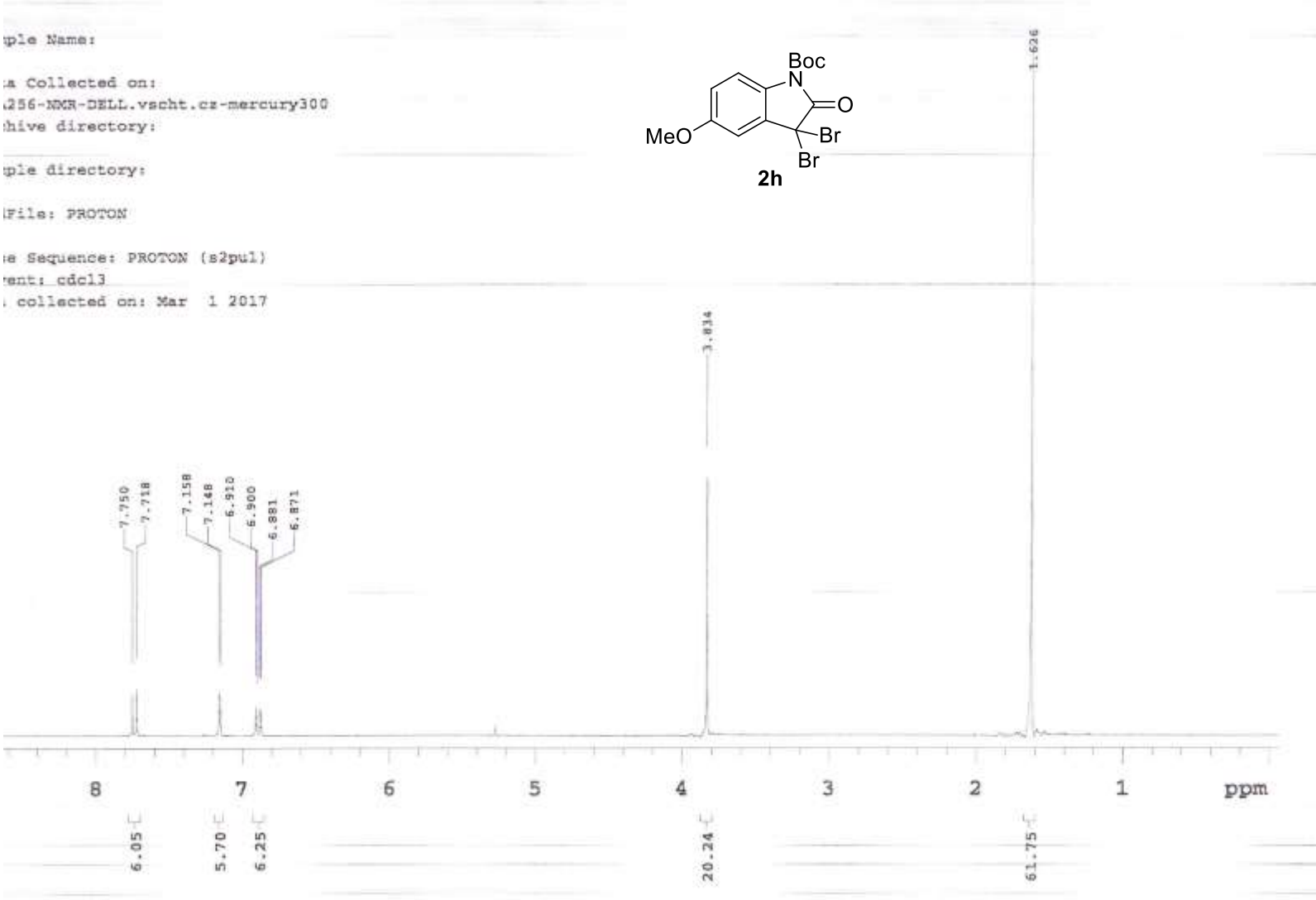

Agilent Technolog
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cs-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 7 2017
166.408
148.234
134.453
131.888
131.384
131.316
129.979
117.017
86.130
77.427
77.000
75.573
43.671
27.945
220
200
180
160
140
120
100
80
60
40
20
ppm

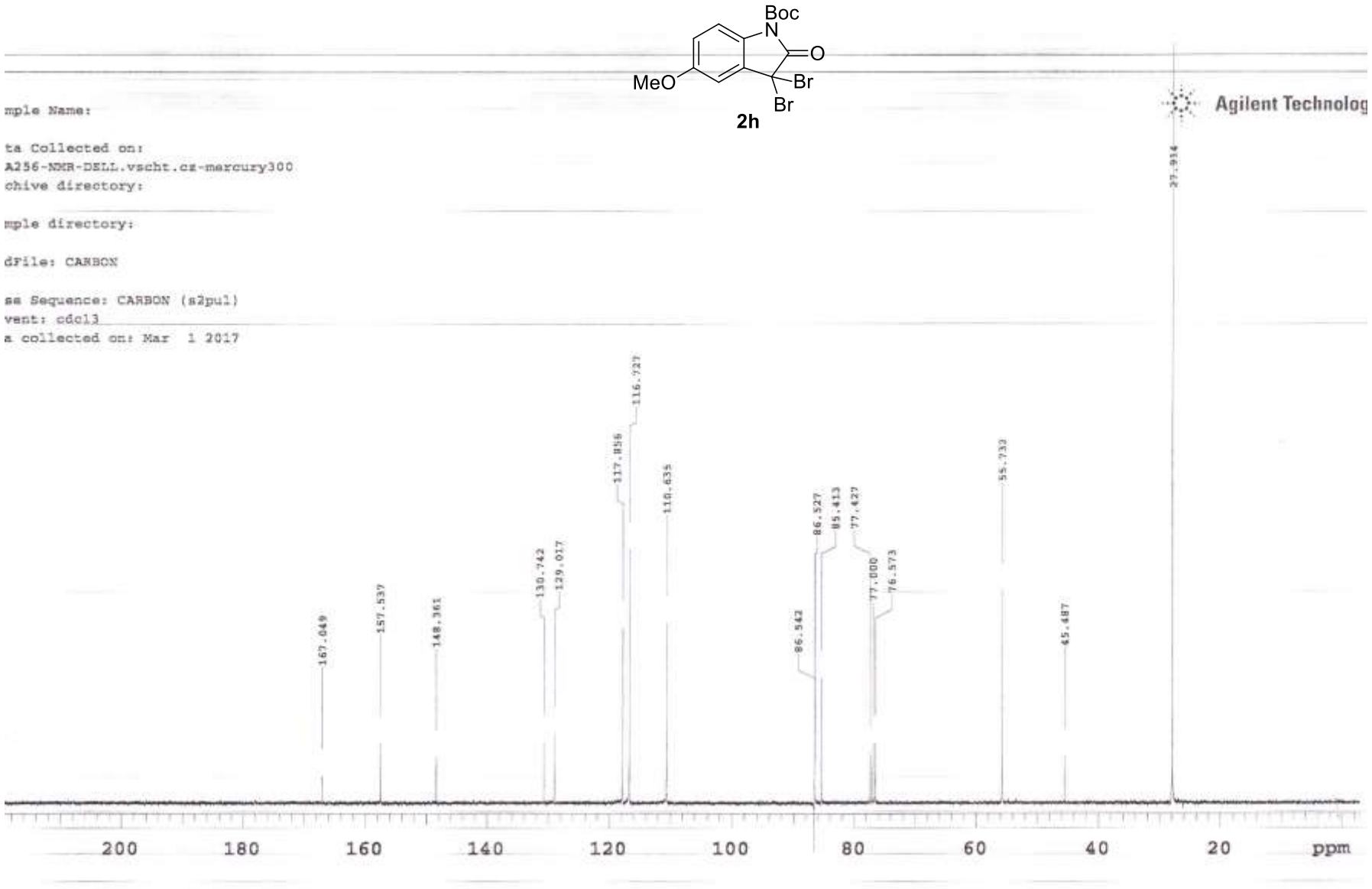

Boc
N
O
Br
Br
Br

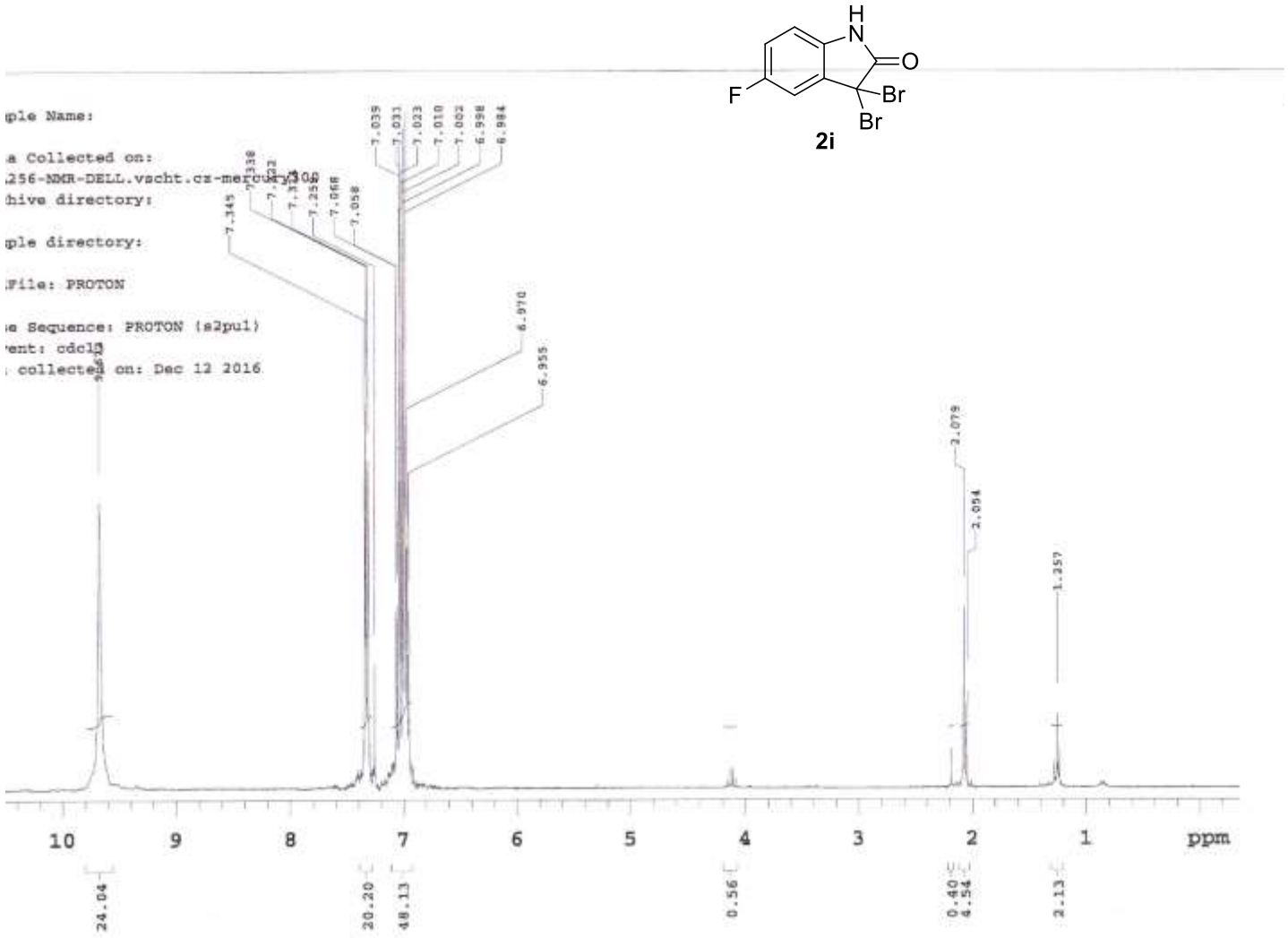
2g

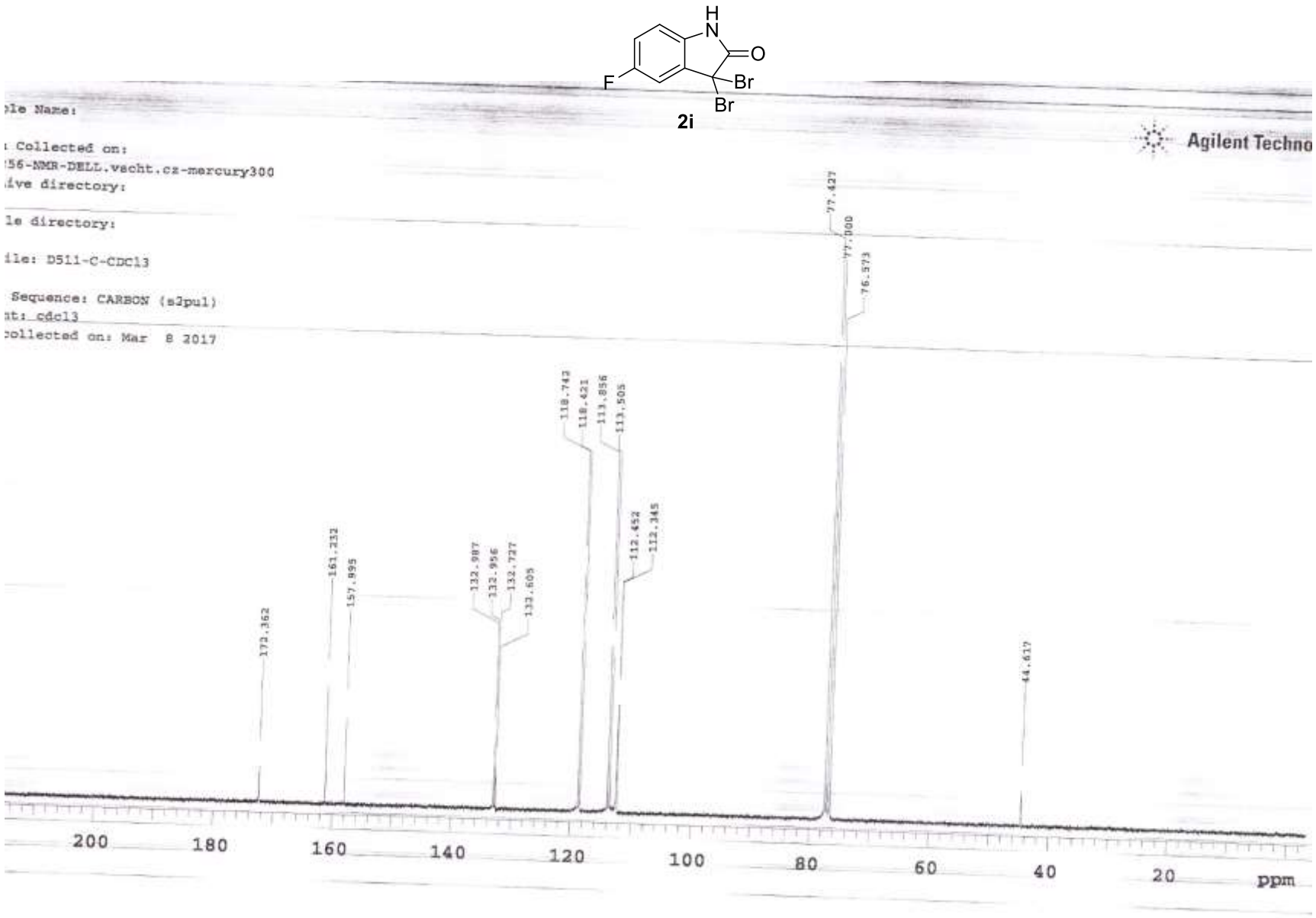
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 25 2016
Agilent Technolo
7.791
7.783
7.755
7.517
7.509
7.480
7.259
1.649
9
8
7
6
5
4
3
2
1
ppm
15.17
8.13
76.70

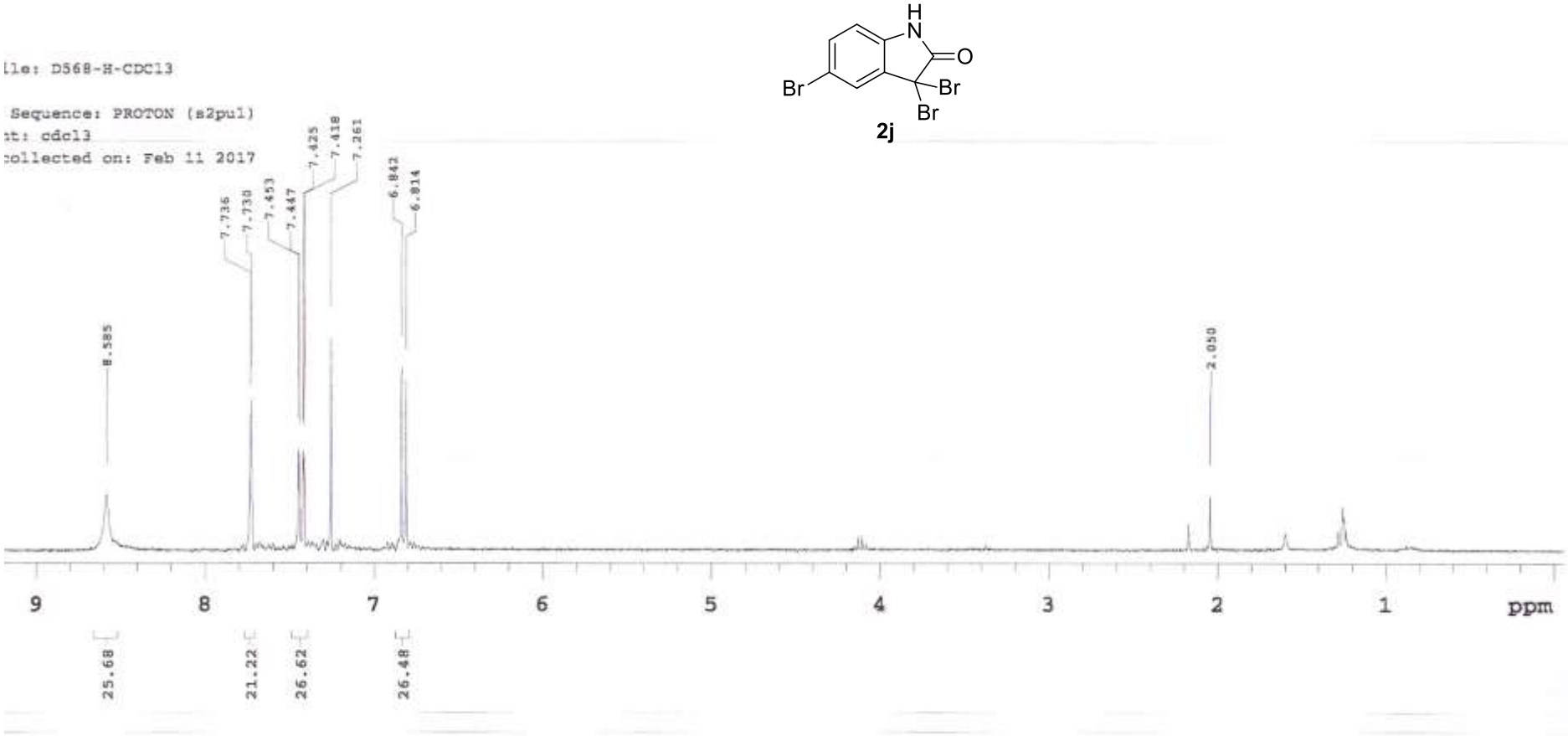

ample Name:
ata Collected on:
A256-NMR-DELL.vscht.cz-mercury300
rchive directory:
ample directory:
idFile: CARBON
lse Sequence: CARBON (s2pul)
lvent: cdcl3
ta collected on: Oct 25 2016
Boc
N
O
Br
Br
Br
2g
Agilent Technolog
166.347
148.209
134.987
134.788
131.674
128.880
118.498
117.337
86.619
86.191
77.427
77.198
77.000
76.573
43.518
36.311
27.960
26.891
200
180
160
140
120
100
80
60
40
20
ppm

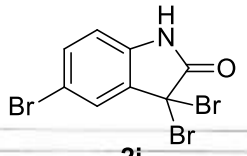

ple Name:
a Collected on:
256-NMR-DELL.vscht.cz-mercury300
hive directory:
ple directory:
File: PROTON
e Sequence: PROTON (s2pul)
ent: cdcl3
collected on: Mar 1 2017
Boc
N
O
MeO
Br
Br
2h
1.626
3.834
7.750
7.718
7.158
7.148
6.910
6.900
6.881
6.871
8
7
6
5
4
3
2
1
ppm
6.05
5.70
6.25
20.24
61.75


Boc
N
O
MeO
Br
Br
2h
mple Name:
ta Collected on:
A256-NMR-DELL.vscht.cz-mercury300
chive directory:
mple directory:
dFile: CARBON
se Sequence: CARBON (s2pul)
vent: cdcl3
a collected on: Mar 1 2017
Agilent Technolog
167.049
157.539
148.361
130.742
129.017
117.856
116.727
110.635
86.542
86.527
85.413
77.427
77.000
76.573
55.733
45.487
27.934
200
180
160
140
120
100
80
60
40
20
ppm

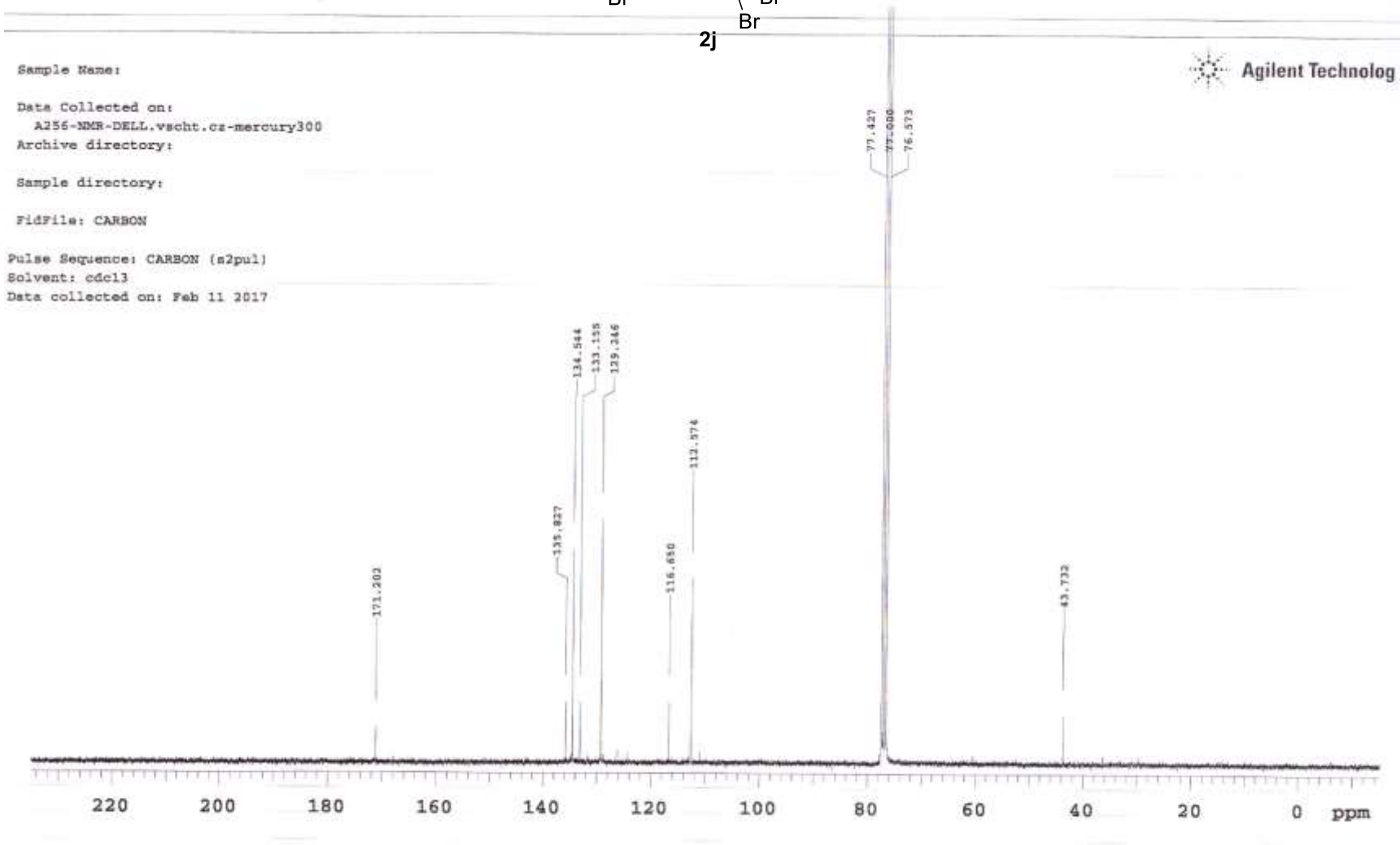

H
N
O
F
Br
Br
2i
ple Name:
a Collected on:
.256-NMR-DELL.vscht.cz-mercury
hive directory:
ple directory:
File: PROTON
e Sequence: PROTON (s2pul)
ent: cdcl3
collected on: Dec 12 2016
7.345
7.338
7.322
7.314
7.310
7.255
7.068
7.058
7.039
7.033
7.023
7.010
7.002
6.958
6.984
6.970
6.955
2.079
2.054
1.357
10
9
8
7
6
5
4
3
2
1
ppm
24.04
20.20
48.13
0.56
0.40
4.54
2.13

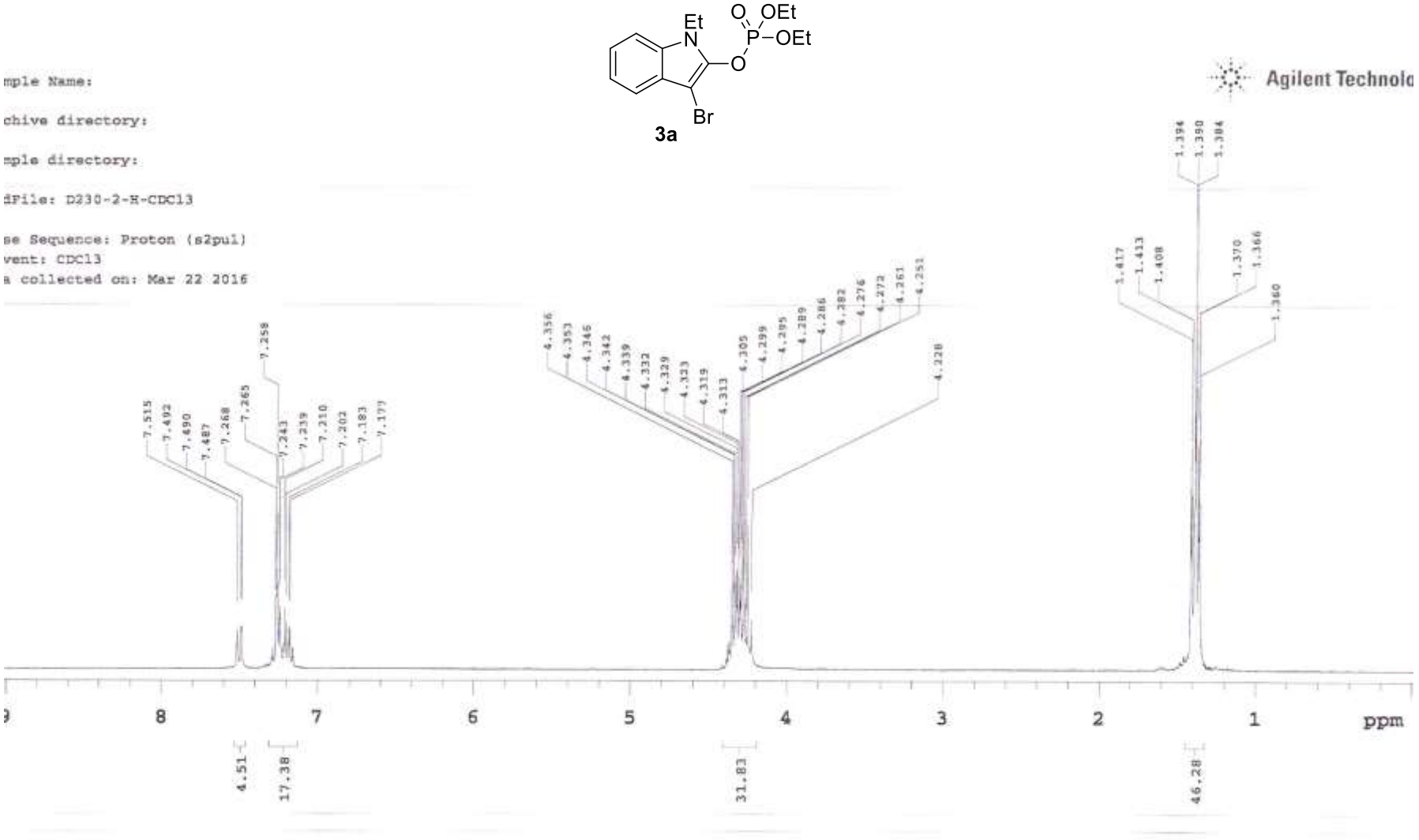

H
N
O
F
Br
Br
2i
Agilent Techno
77.427
77.000
76.573
118.743
118.431
113.856
113.505
112.452
112.345
172.362
161.232
157.995
132.987
132.956
132.727
132.605
44.617
200
180
160
140
120
100
80
60
40
20
ppm

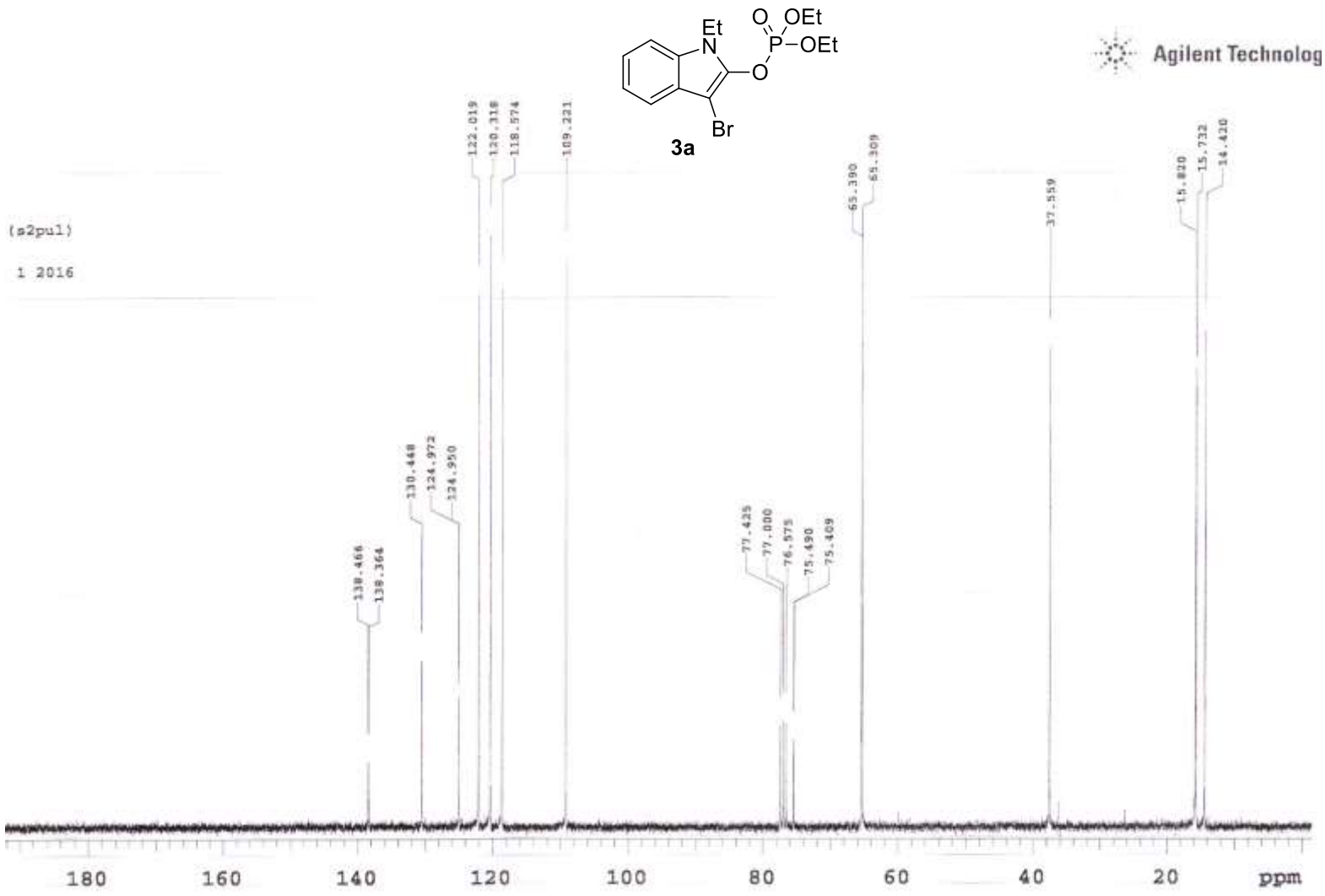

H
N
O
Br
Br
Br
2j
ile: D568-H-CDCl3
Sequence: PROTON (s2pul)
st: cdcl3
collected on: Feb 11 2017
8.585
7.736
7.730
7.453
7.447
7.425
7.418
7.261
6.842
6.814
2.050
9
8
7
6
5
4
3
2
1
ppm
25.68
21.22
26.62
26.48

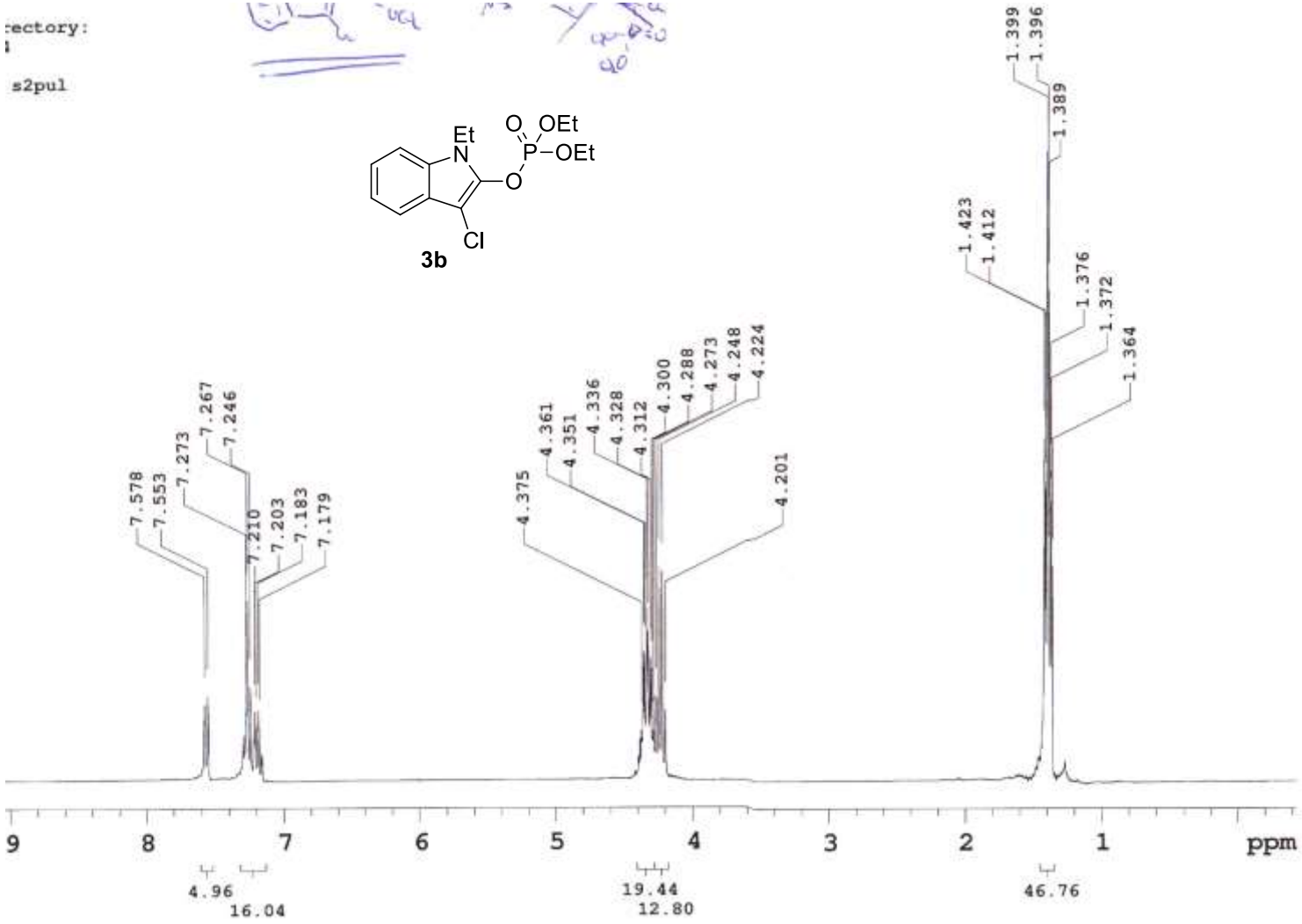

H
N
O
Br
Br
Br

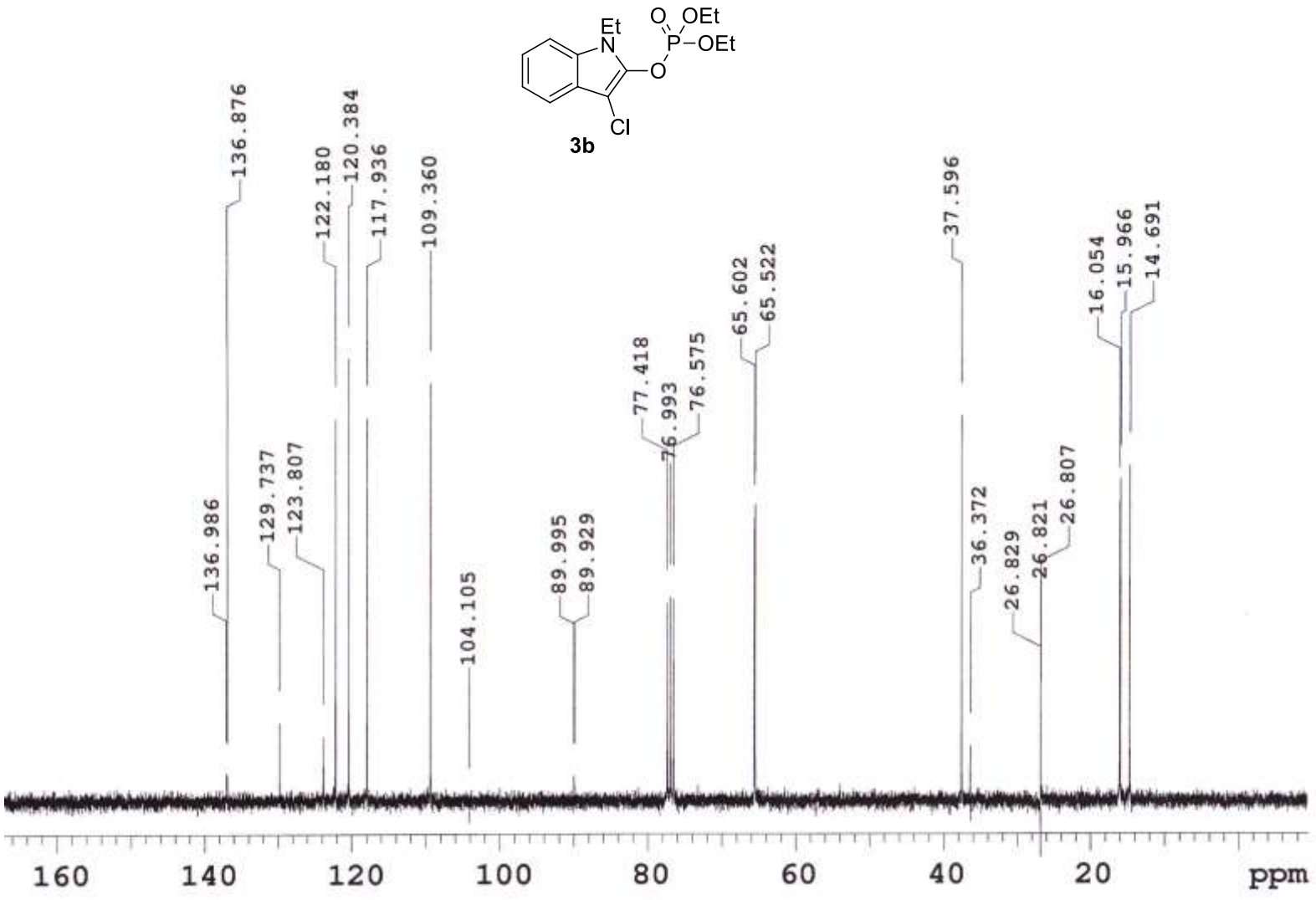
2j

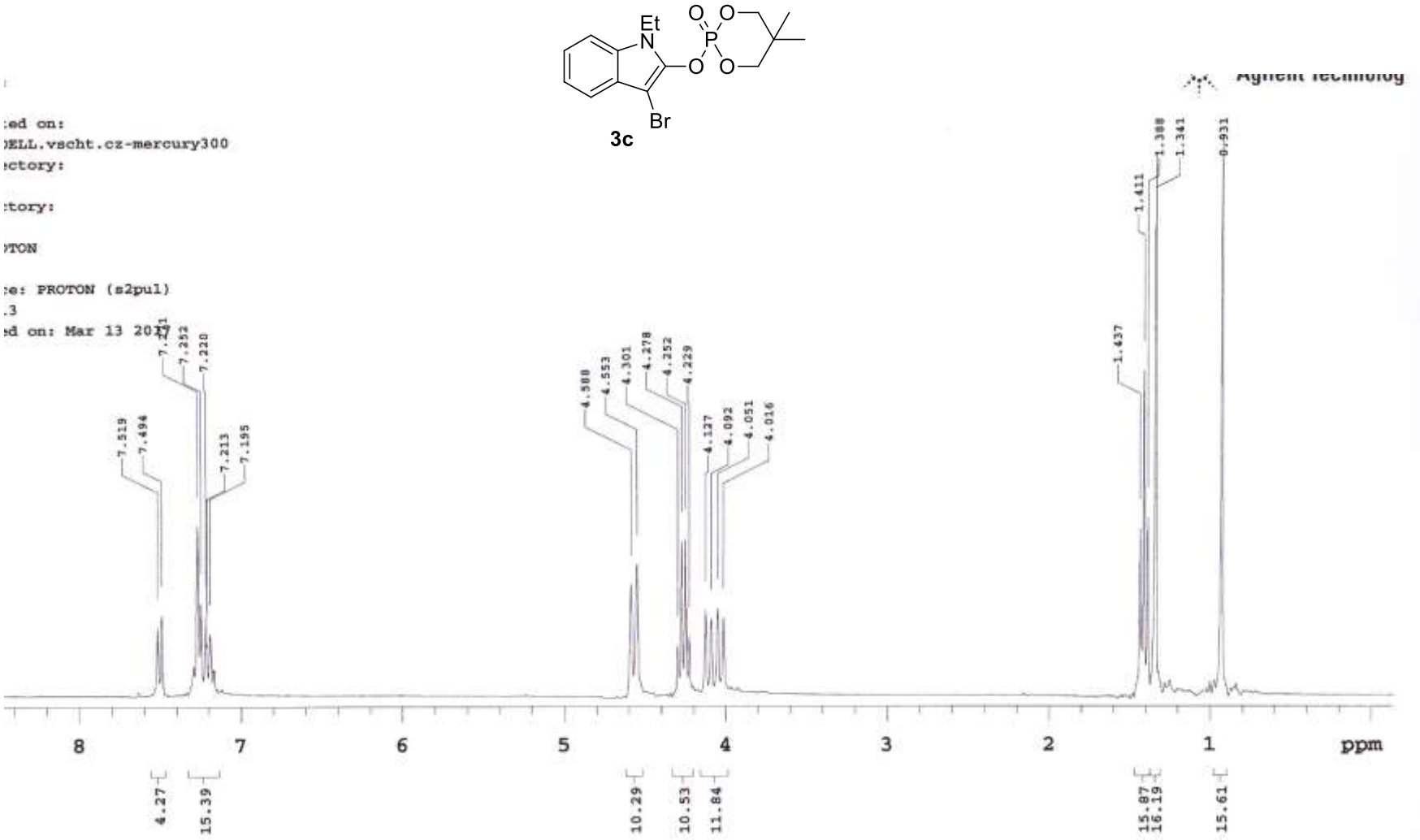

Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 11 2017
Agilent Technolog
77.427
77.000
76.573
134.544
133.155
129.246
135.827
112.574
116.650
171.202
43.732
220
200
180
160
140
120
100
80
60
40
20
0
ppm

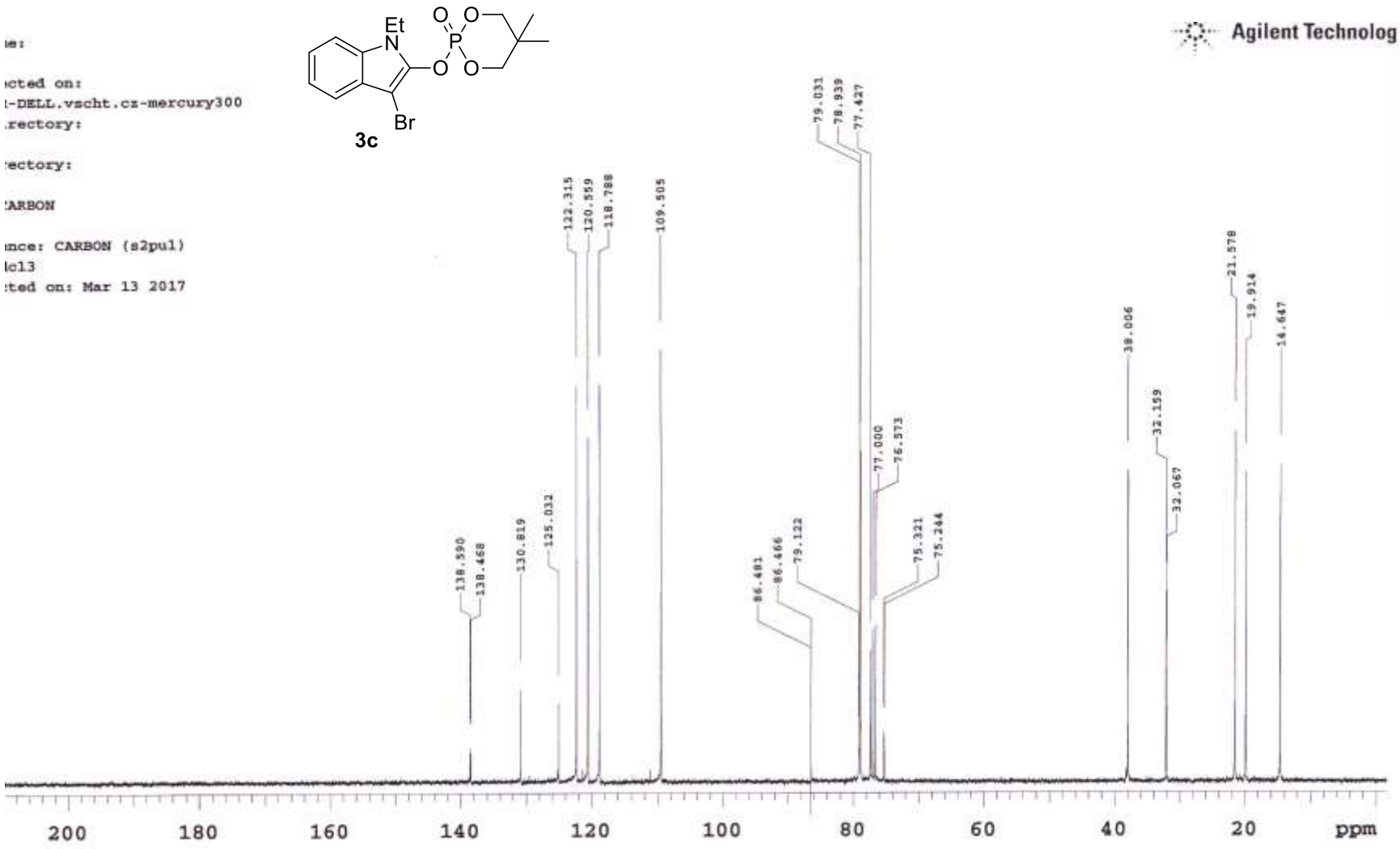

Et
N
O
OEt
P
OEt
O
Br
3a
mple Name:
chive directory:
mple directory:
dFile: D230-2-H-CDCl3
se Sequence: Proton (s2pul)
vent: CDCl3
a collected on: Mar 22 2016
Agilent Technolo
7.515
7.492
7.490
7.487
7.268
7.265
7.258
7.243
7.239
7.210
7.202
7.183
7.177
4.356
4.353
4.346
4.342
4.339
4.332
4.329
4.323
4.319
4.313
4.305
4.299
4.295
4.289
4.286
4.282
4.276
4.272
4.261
4.251
4.228
1.417
1.413
1.408
1.394
1.390
1.384
1.370
1.366
1.360
8
7
6
5
4
3
2
1
ppm
4.51
17.38
31.83
46.28

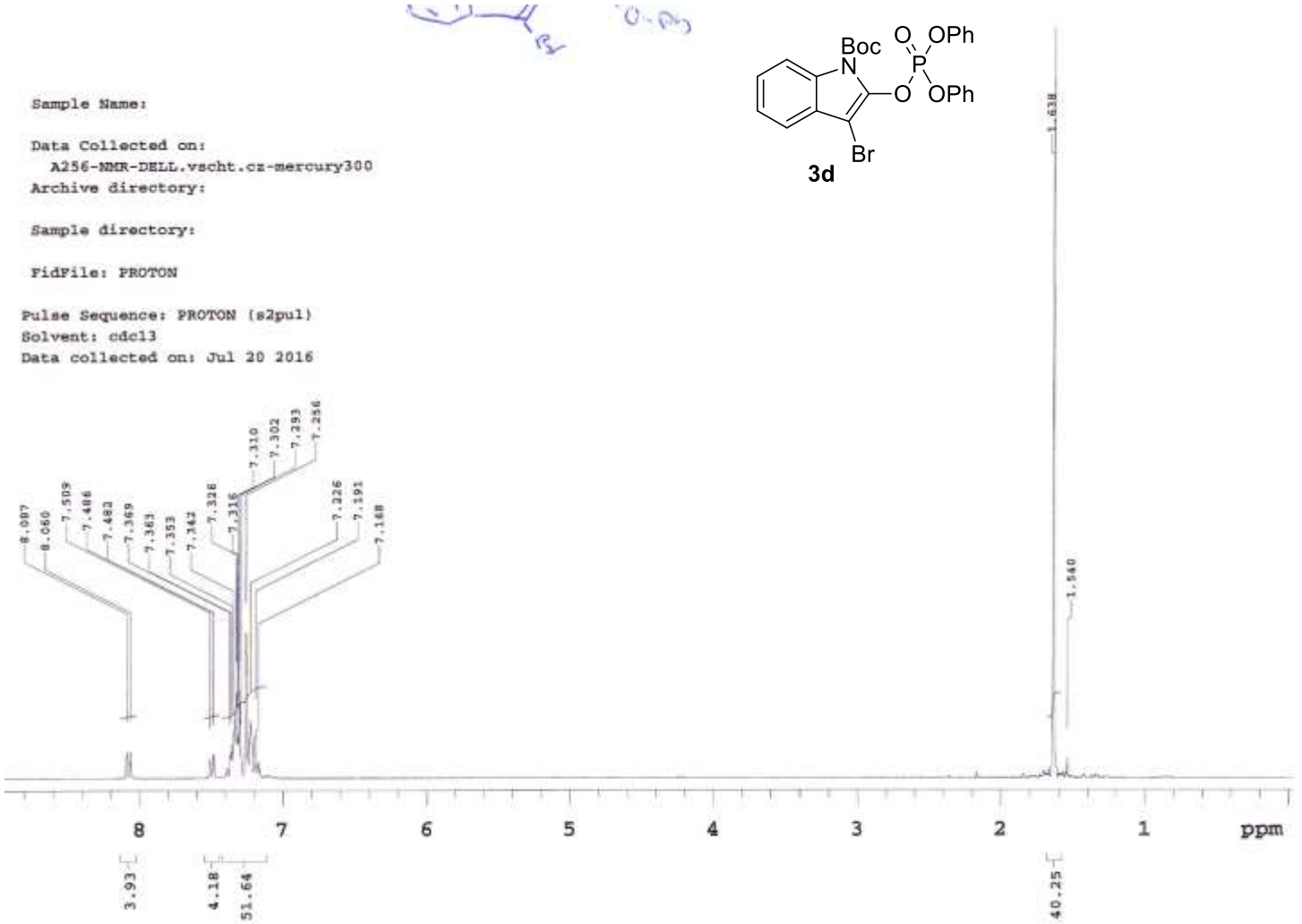

Et
N
O
O
OEt
P
OEt
O
Br
3a
Agilent Technolog
(s2pul)
1 2016
122.019
120.318
118.574
109.221
65.390
65.309
37.559
15.820
15.732
14.420
138.466
138.364
130.448
124.972
124.950
77.425
77.000
76.575
75.490
75.409
180
160
140
120
100
80
60
40
20
ppm

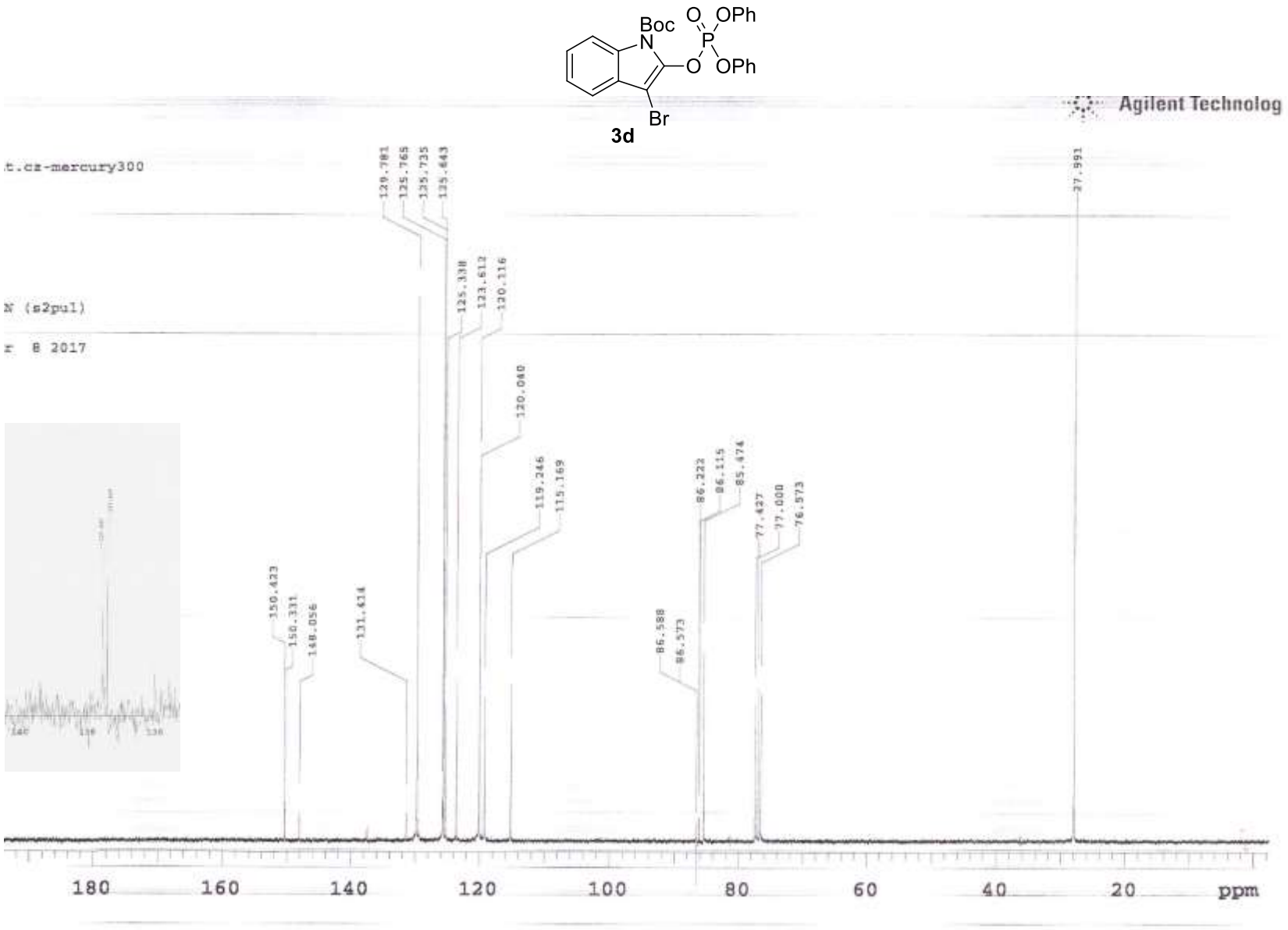

ectory:
s2pul
Et
N
O
OEt
P
OEt
O
Cl
3b
7.578
7.553
7.273
7.267
7.246
7.210
7.203
7.183
7.179
4.375
4.361
4.351
4.336
4.328
4.312
4.300
4.288
4.273
4.248
4.224
4.201
1.423
1.412
1.399
1.396
1.389
1.376
1.372
1.364
9
8
7
6
5
4
3
2
1
ppm
4.96
16.04
19.44
12.80
46.76

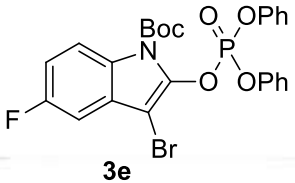

Et
N
O
O
OEt
P
OEt
Cl
3b
136.876
122.180
120.384
117.936
109.360
104.105
89.995
89.929
77.418
76.993
76.575
65.602
65.522
37.596
36.372
26.829
26.821
26.807
16.054
15.966
14.691
136.986
129.737
123.807
160
140
120
100
80
60
40
20
ppm


Et
N
O
O
P
O
O
Br
3c
:ed on:
)ELL.vscht.cz-mercury300
:ctory:
:tory:
)TON
:e: PROTON (s2pul)
.3
:d on: Mar 13 20
7.519
7.494
7.271
7.252
7.220
7.213
7.195
4.588
4.553
4.301
4.278
4.252
4.229
4.127
4.092
4.051
4.016
1.437
1.411
1.388
1.341
0.931
8
7
6
5
4
3
2
1
ppm
4.27
15.39
10.29
10.53
11.84
15.87
16.19
15.61

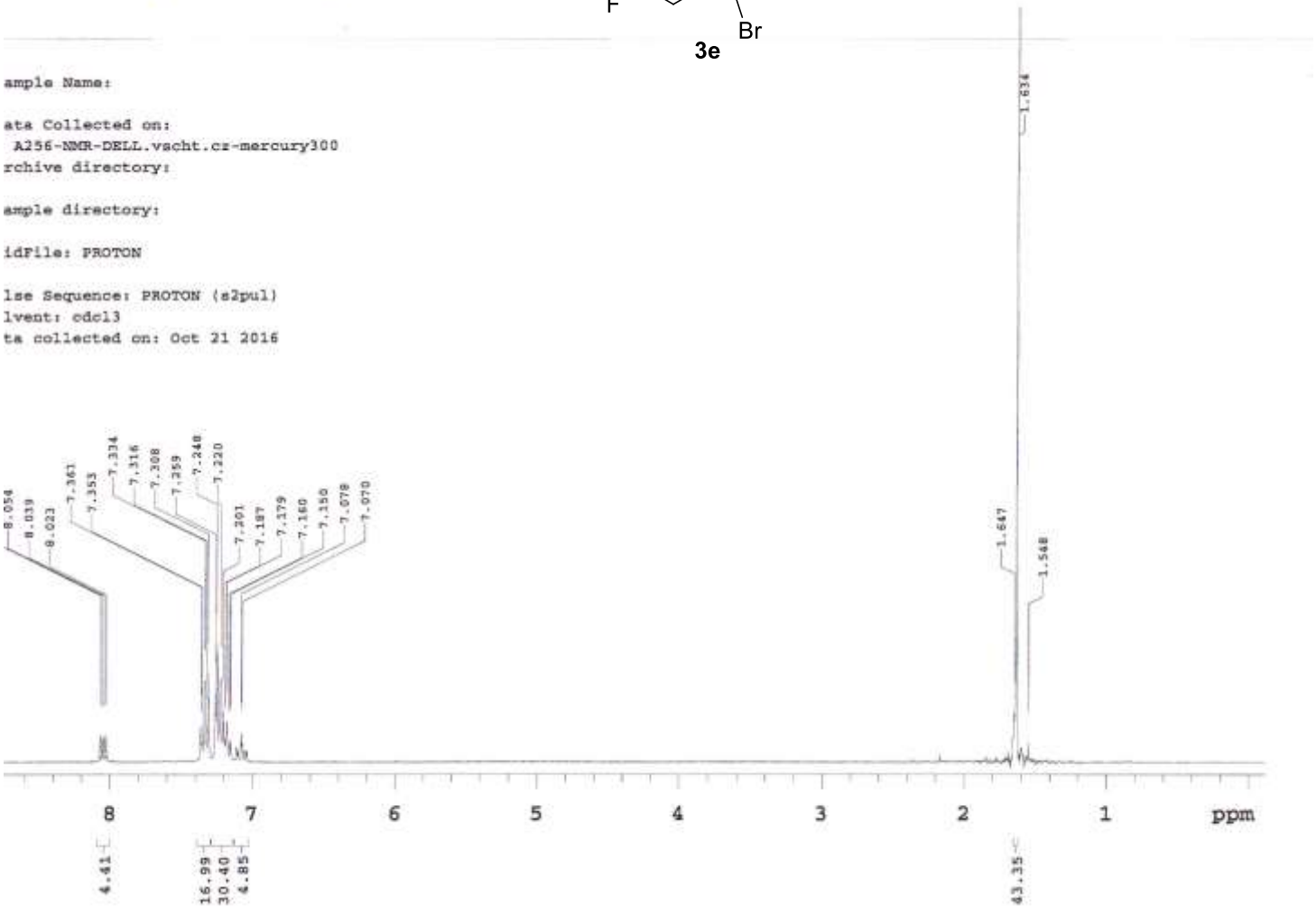

Et
N
O
O
P
O
O
Br
3c
Agilent Technolog
cted on:
-DELL.vscht.cz-mercury300
rectory:
ectory:
ARBON
nce: CARBON (s2pul)
lcl3
ted on: Mar 13 2017
138.590
138.468
130.819
125.032
122.315
120.559
118.788
109.505
86.481
86.466
79.122
79.031
78.939
77.427
77.000
76.573
75.321
75.244
38.006
32.159
32.067
21.578
19.914
14.647
200
180
160
140
120
100
80
60
40
20
ppm

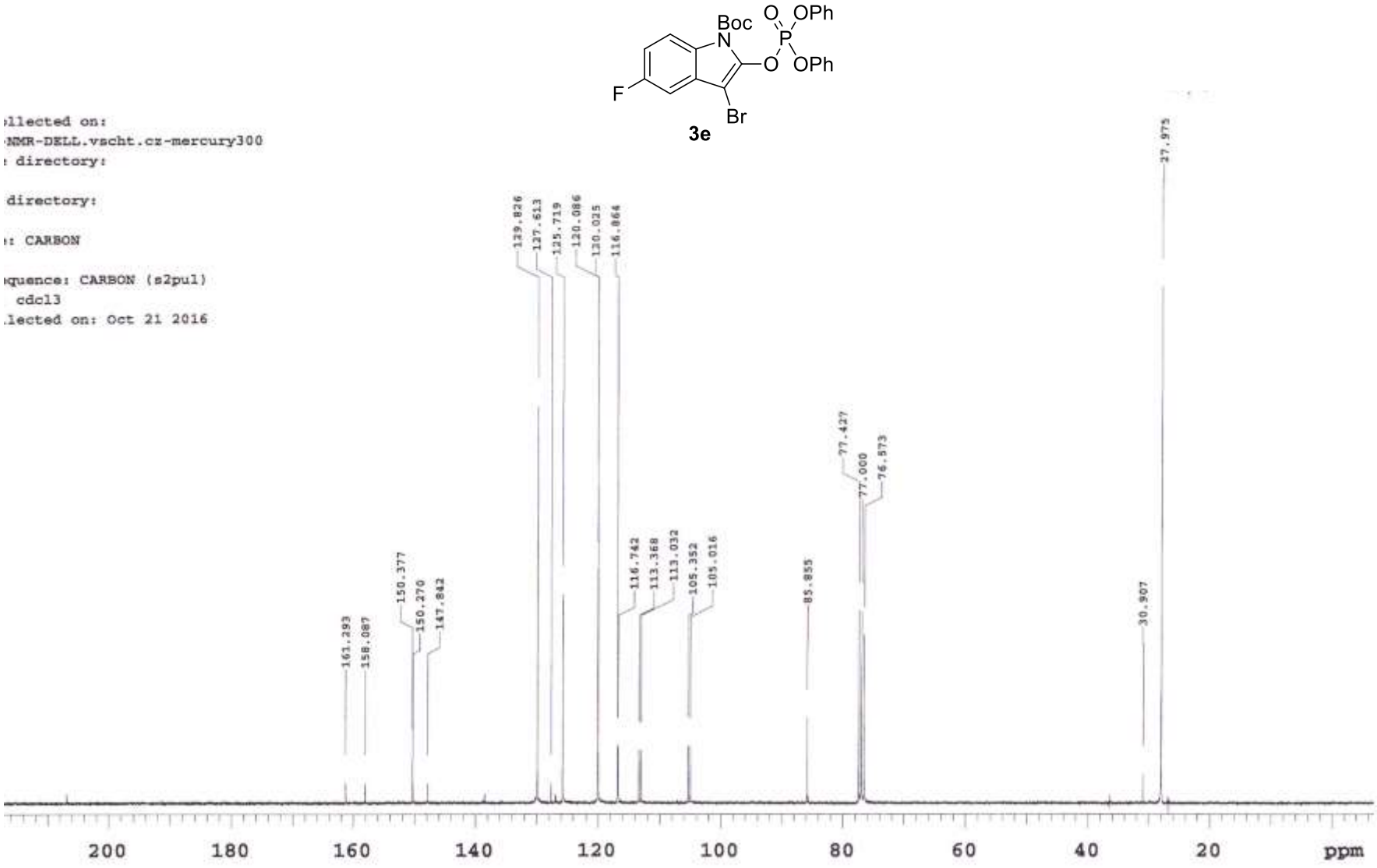

Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2016
Boc
N
O
OPh
P
O
OPh
Br
3d
8.087
8.060
7.509
7.486
7.482
7.369
7.363
7.353
7.343
7.328
7.316
7.310
7.302
7.293
7.256
7.226
7.191
7.168
1.638
1.540
8
7
6
5
4
3
2
1
ppm
3.93
4.18
51.64
40.25

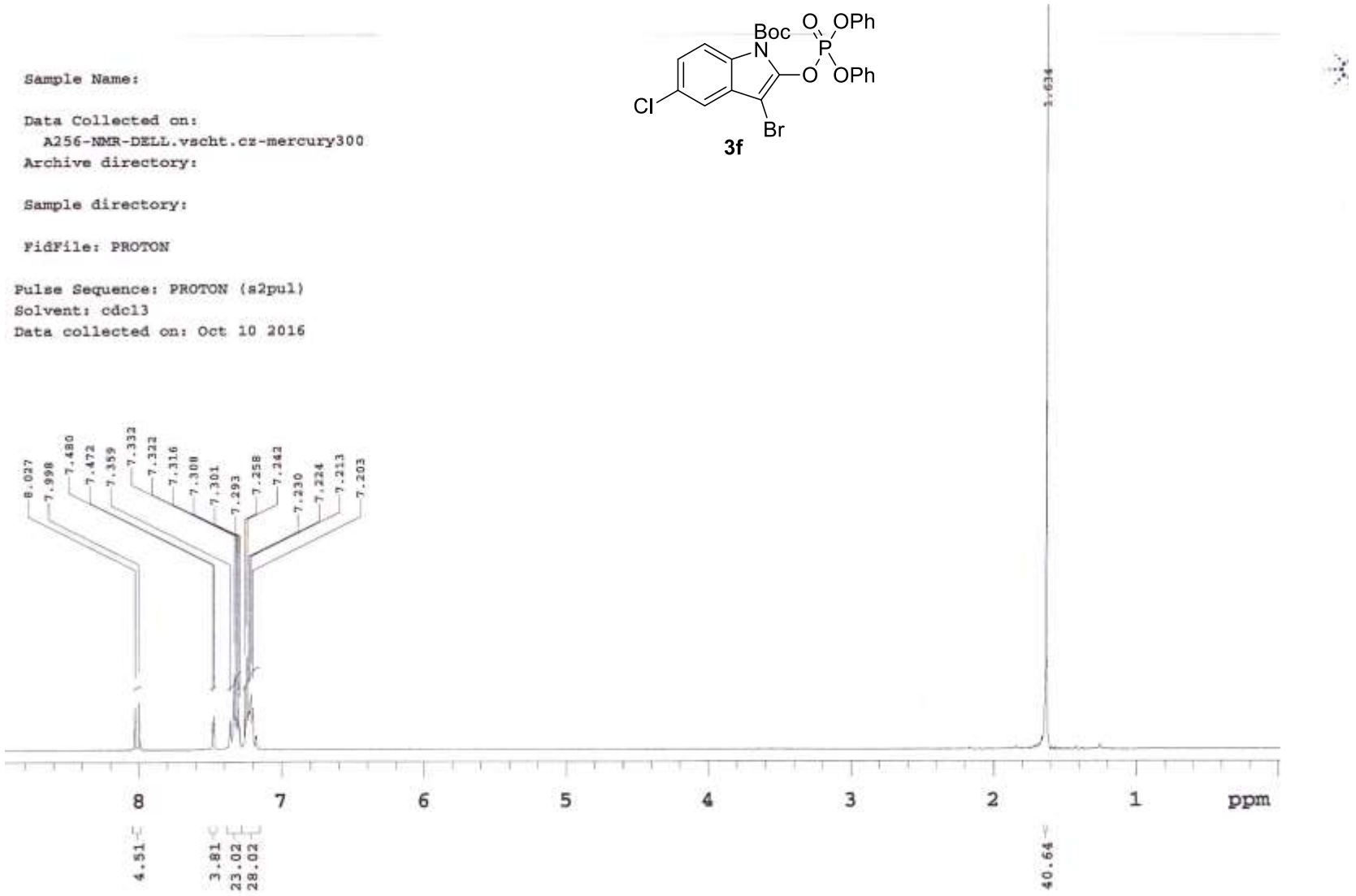

Boc
O
OPh
N
P
O
OPh
Br
3d
Agilent Technolog
t.cz-mercury300
N (s2pul)
B 2017
129.781
125.765
125.735
125.443
125.338
123.612
120.116
120.040
119.246
115.169
86.588
86.573
86.222
86.115
85.474
77.427
77.000
76.573
150.423
150.331
148.056
131.414
37.991
180
160
140
120
100
80
60
40
20
ppm

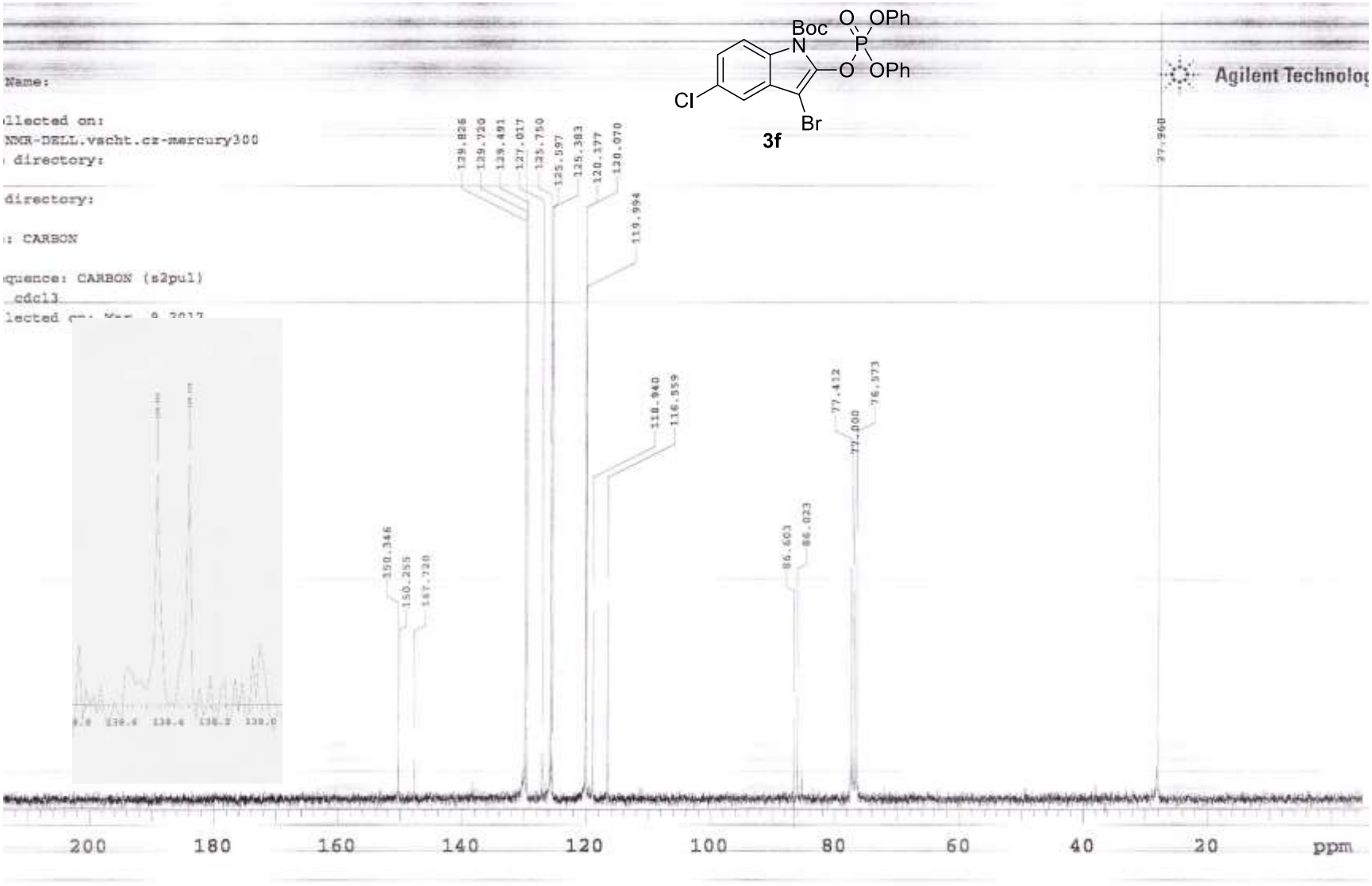

Boc
N
O
OPh
P
O
OPh
F
Br

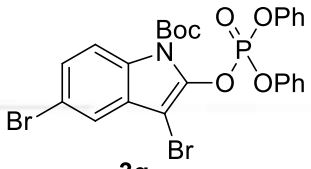
3e


ample Name:
ata Collected on:
A256-NMR-DELL.vscht.cz-mercury300
rchive directory:
ample directory:
idFile: PROTON
lse Sequence: PROTON (s2pul)
lvent: cdcl3
ta collected on: Oct 21 2016
8.054
8.039
8.023
7.361
7.353
7.334
7.316
7.308
7.259
7.248
7.220
7.201
7.187
7.179
7.160
7.150
7.078
7.070
1.634
1.647
1.548
8
7
6
5
4
3
2
1
ppm
4.41
16.99
30.40
4.85
43.35


Boc
N
O
OPh
P
O
OPh
F
Br
3e
llected on:
NMR-DELL.vscht.cz-mercury300
directory:
directory:
: CARBON
quence: CARBON (s2pul)
cdcl3
lected on: Oct 21 2016
161.293
158.087
150.377
150.270
147.842
139.826
127.613
125.719
120.086
120.035
116.864
116.742
113.368
113.032
105.352
105.016
85.855
77.427
77.000
76.573
30.907
27.975
200
180
160
140
120
100
80
60
40
20
ppm


Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 10 2016
Boc
N
O
OPh
P
O
OPh
Cl
Br
3f
8.027
7.998
7.480
7.472
7.359
7.332
7.322
7.316
7.308
7.301
7.293
7.258
7.242
7.230
7.224
7.213
7.203
1.634
8
7
6
5
4
3
2
1
ppm
4.51
3.81
23.02
28.02
40.64


Boc
O
OPh
N
P
O
OPh
Cl
Br
3f
Agilent Technolog
Name:
llected on:
NMR-DELL.vscht.cz-mercury300
directory:
directory:
: CARBON
quence: CARBON (s2pul)
cdcl3
139.826
139.720
139.491
127.017
125.750
125.597
125.383
120.377
120.070
119.994
118.940
116.559
77.412
77.000
76.573
86.603
86.023
150.346
150.255
147.720
77.960
200
180
160
140
120
100
80
60
40
20
ppm



3g

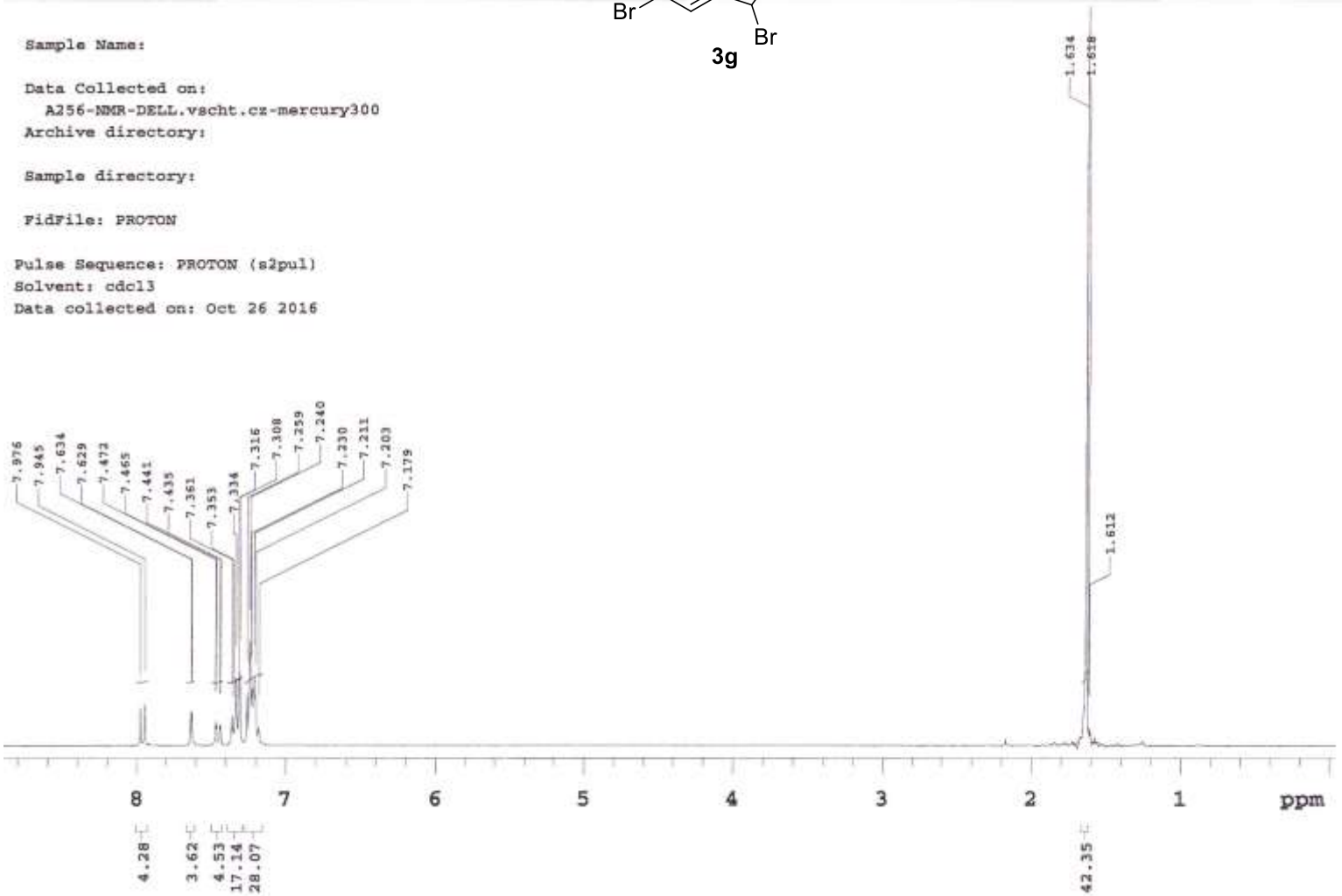
Sample Name:

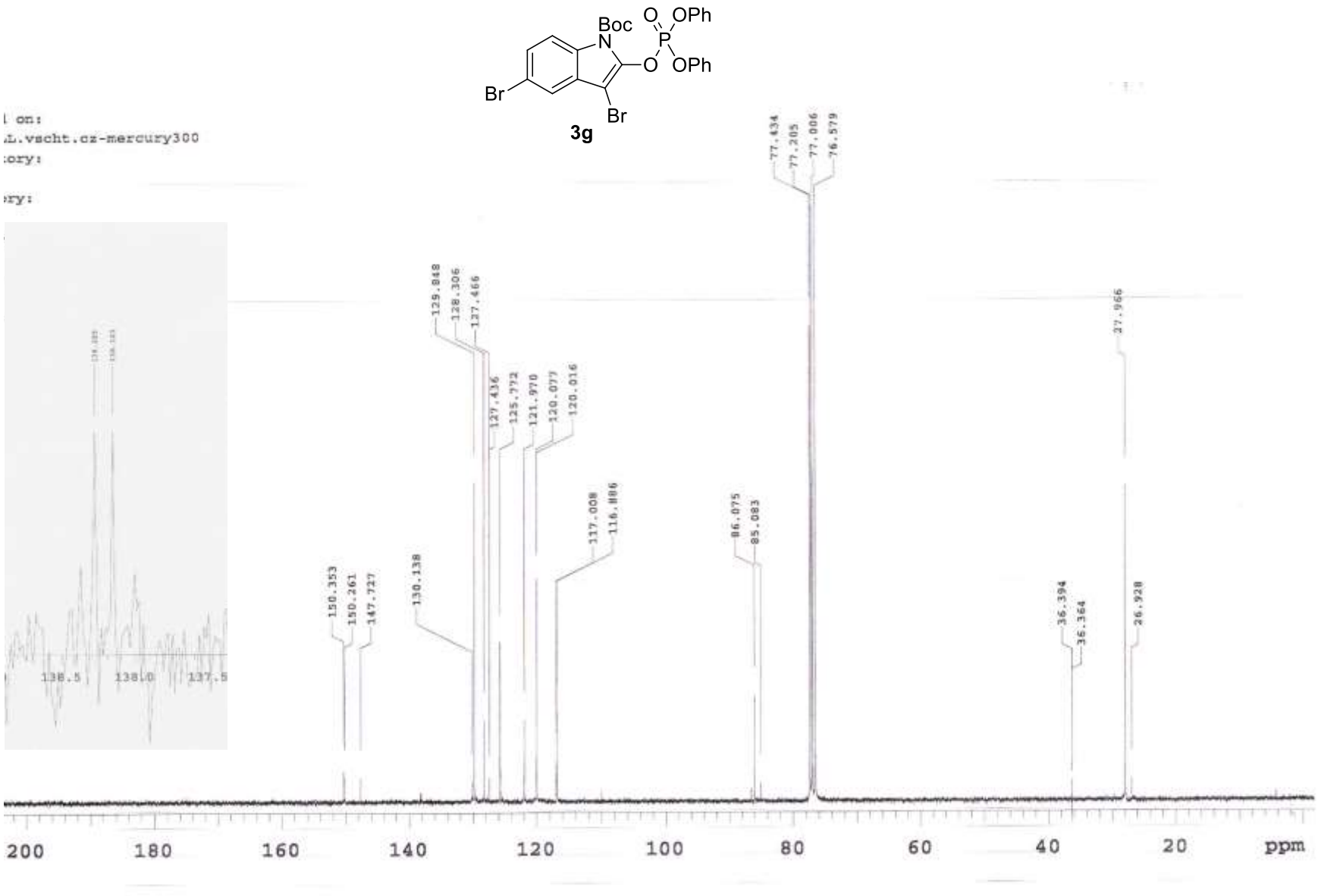
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:

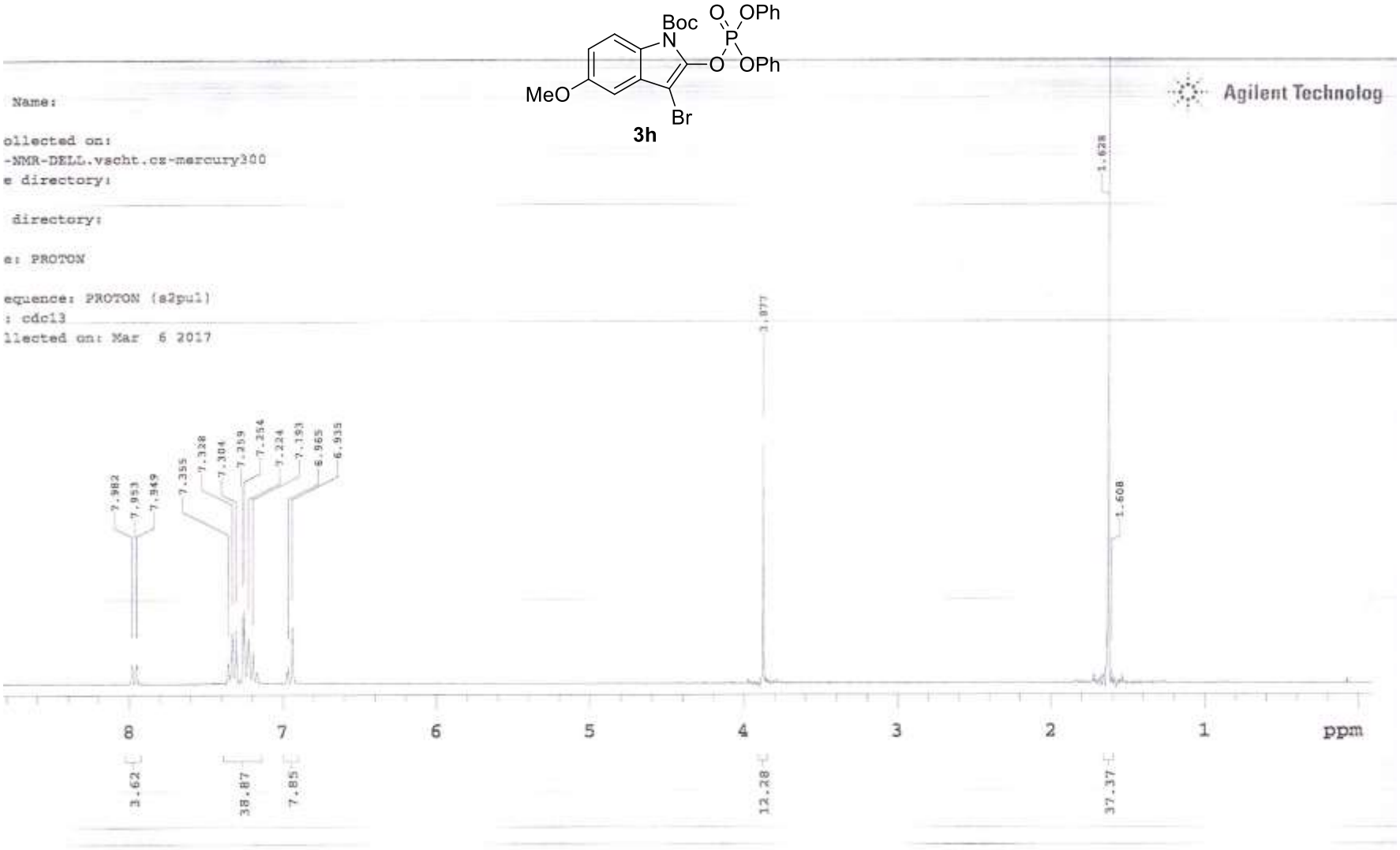
Sample directory:

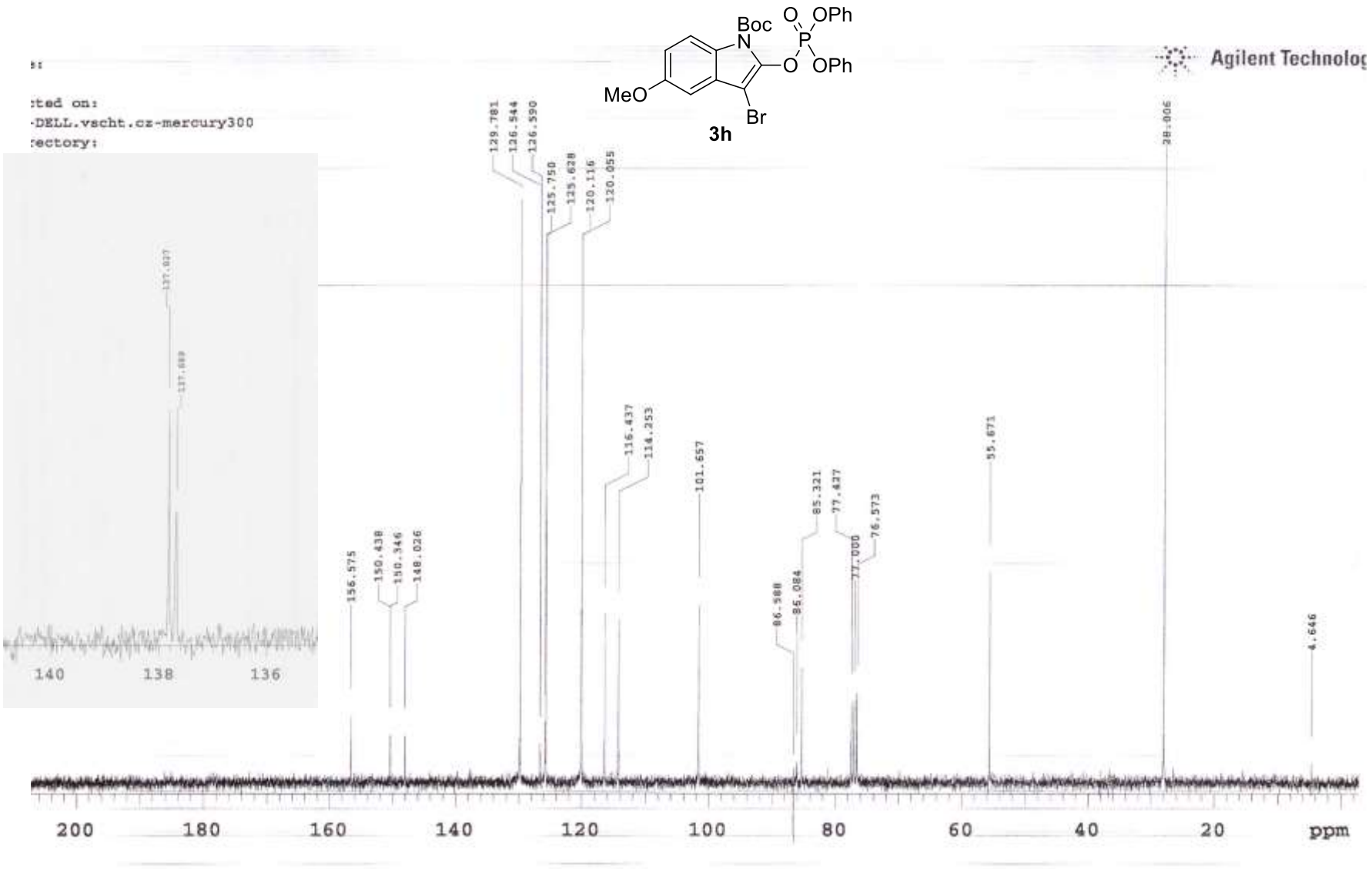
FidFile: PROTON

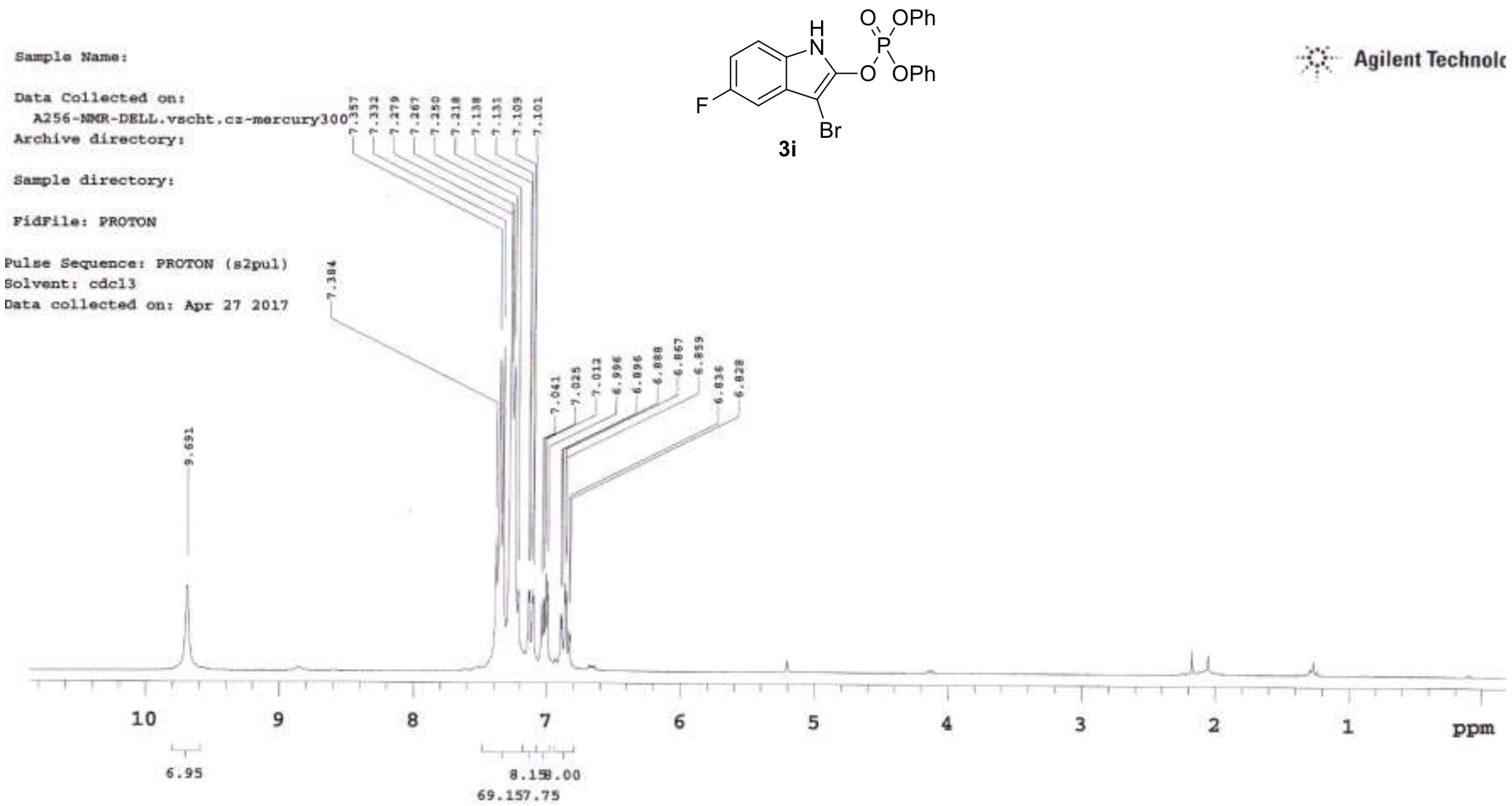
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 26 2016

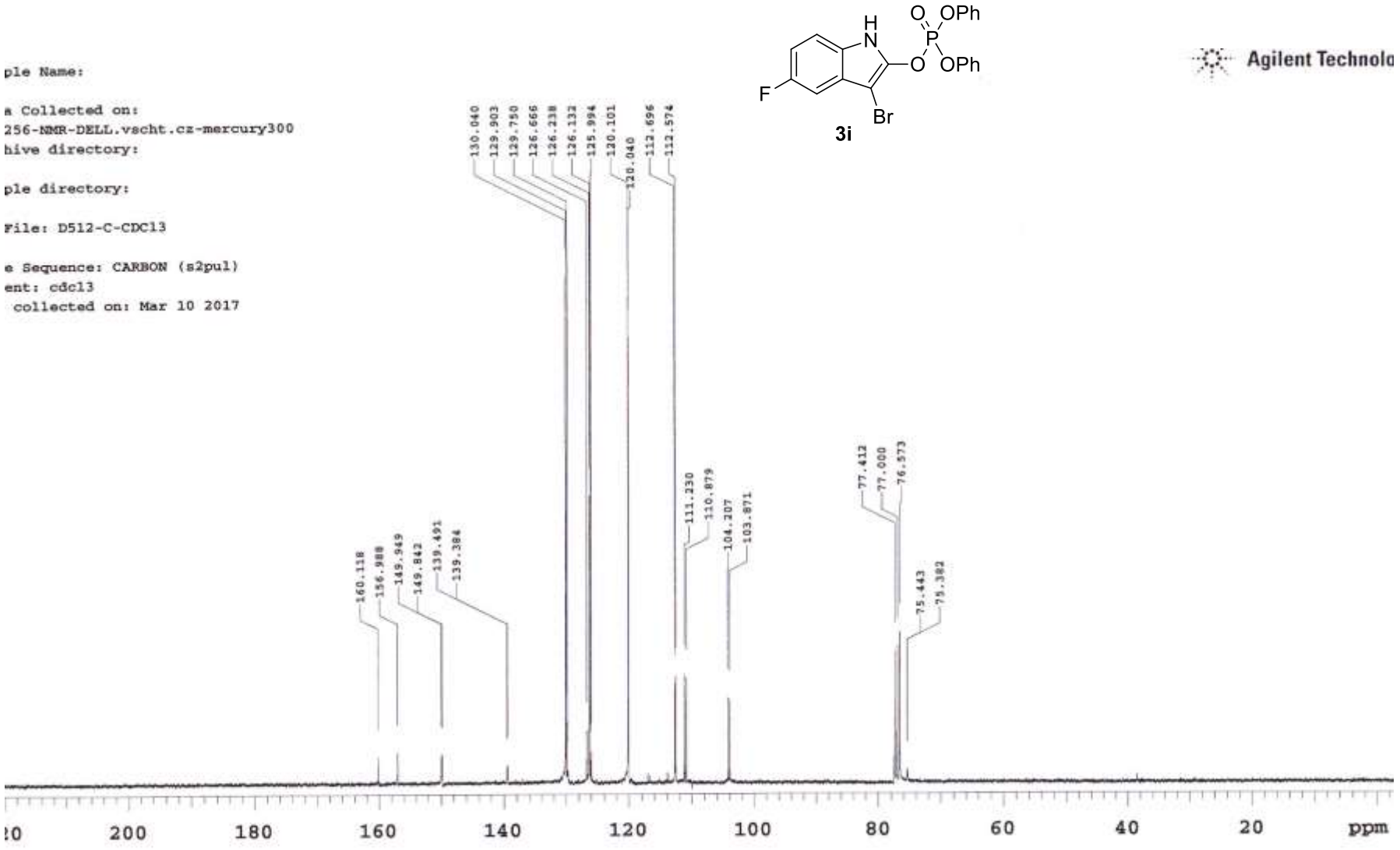


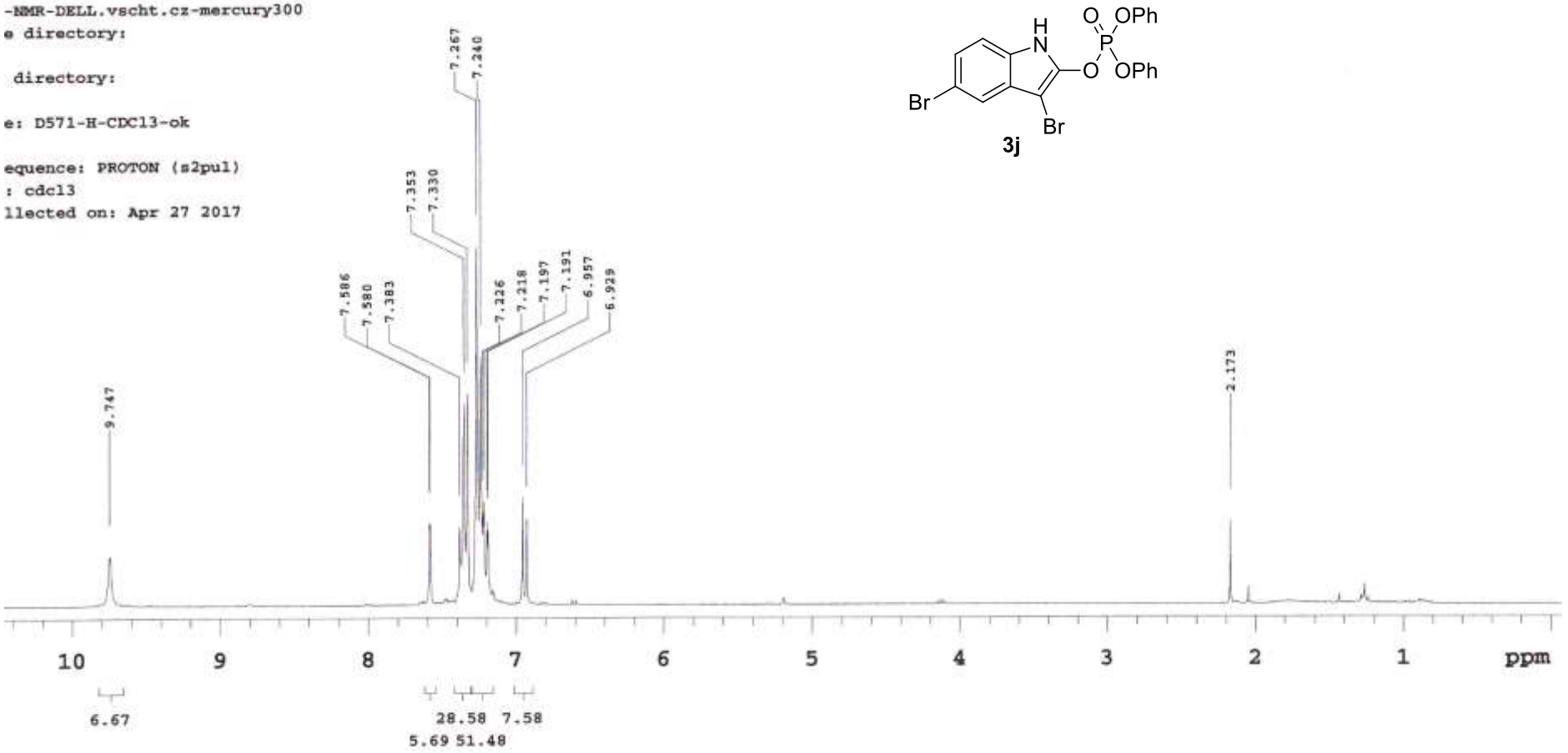

Boc
N
O
OPh
P
O
OPh
Br
Br
3g
77.434
77.205
77.006
76.579
129.848
128.306
127.466
127.436
125.772
121.970
120.077
120.016
117.008
116.886
86.075
85.083
37.966
36.394
36.364
26.928
150.353
150.261
147.727
130.138
138.5
138.0
137.5
200
180
160
140
120
100
80
60
40
20
ppm


Boc
N
O
P
OPh
O
OPh
MeO
Br
3h
Agilent Technolog
Name:
ollected on:
-NMR-DELL.vscht.cz-mercury300
e directory:
directory:
e: PROTON
equence: PROTON (s2pul)
: cdcl3
llected on: Mar 6 2017
7.982
7.953
7.949
7.355
7.328
7.304
7.259
7.254
7.224
7.193
6.965
6.935
3.877
1.628
1.608
8
7
6
5
4
3
2
1
ppm
3.62
38.87
7.85
12.28
37.37


Boc
N
O
P
OPh
O
OPh
MeO
Br
3h
Agilent Technolog
ted on:
DELL.vscht.cz-mercury300
rectory:
129.781
126.544
126.590
125.750
125.628
120.116
120.055
38.006
116.437
114.253
101.657
85.321
77.437
77.000
76.573
55.671
156.575
150.438
150.346
148.026
86.988
86.084
4.646
137.627
137.489
140
138
136
200
180
160
140
120
100
80
60
40
20
ppm

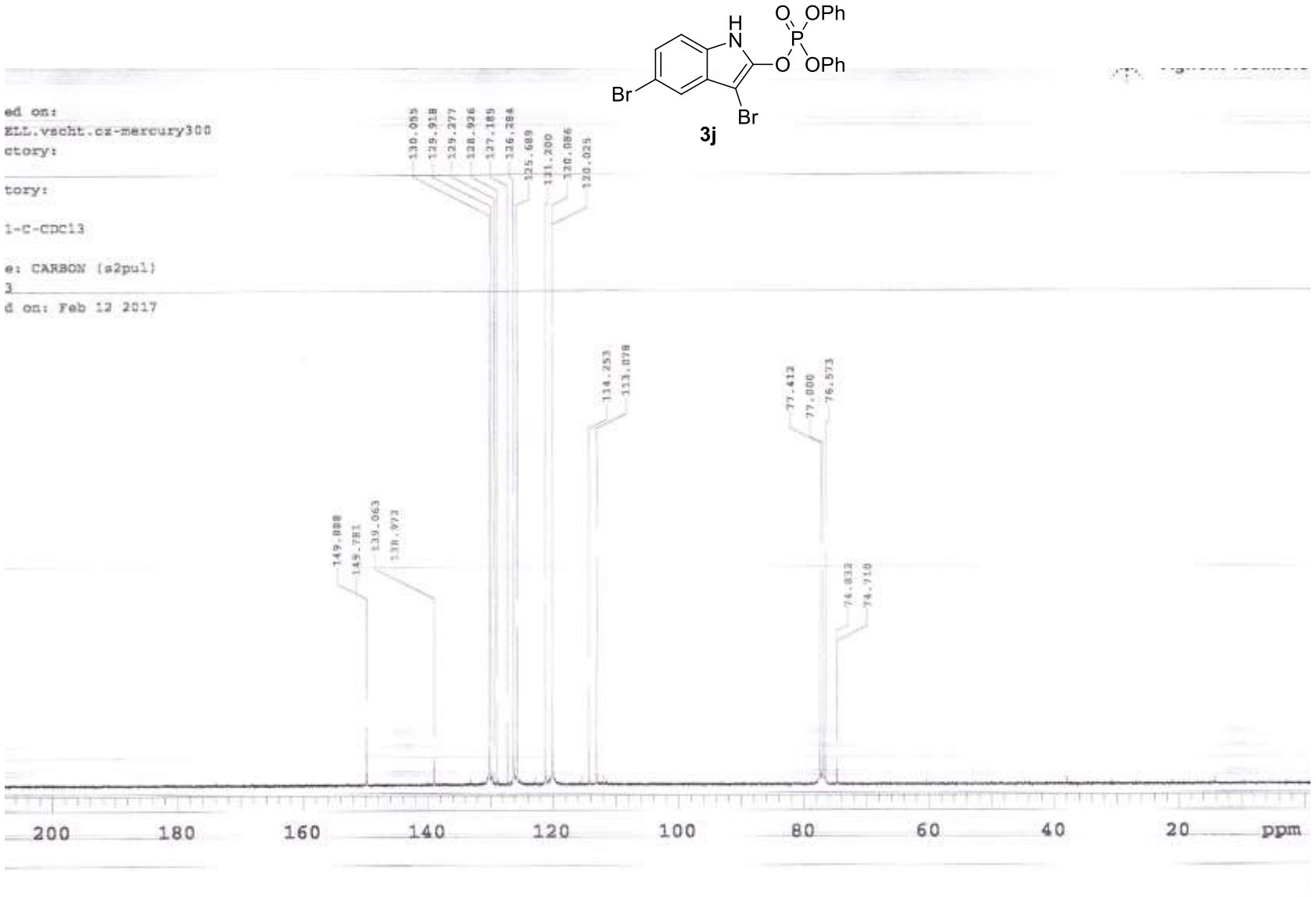

Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 27 2017
7.357
7.332
7.279
7.267
7.250
7.218
7.138
7.131
7.109
7.101
7.384
9.691
7.041
7.025
7.012
6.996
6.896
6.888
6.867
6.859
6.836
6.828
10
9
8
7
6
5
4
3
2
1
ppm
6.95
8.15
8.00
69.15
7.75
H
N
O
OPh
P
O
OPh
F
Br
3i
Agilent Technolc


ple Name:
a Collected on:
256-NMR-DELL.vscht.cz-mercury300
hive directory:
ple directory:
File: D512-C-CDCl3
e Sequence: CARBON (s2pul)
ent: cdcl3
collected on: Mar 10 2017
3i
Agilent Technolo
160.118
156.988
149.949
149.842
139.491
139.384
130.040
129.903
129.750
126.666
126.238
126.132
125.994
120.101
120.040
112.696
112.574
111.230
110.879
104.207
103.871
77.412
77.000
76.573
75.443
75.382
200
180
160
140
120
100
80
60
40
20
ppm

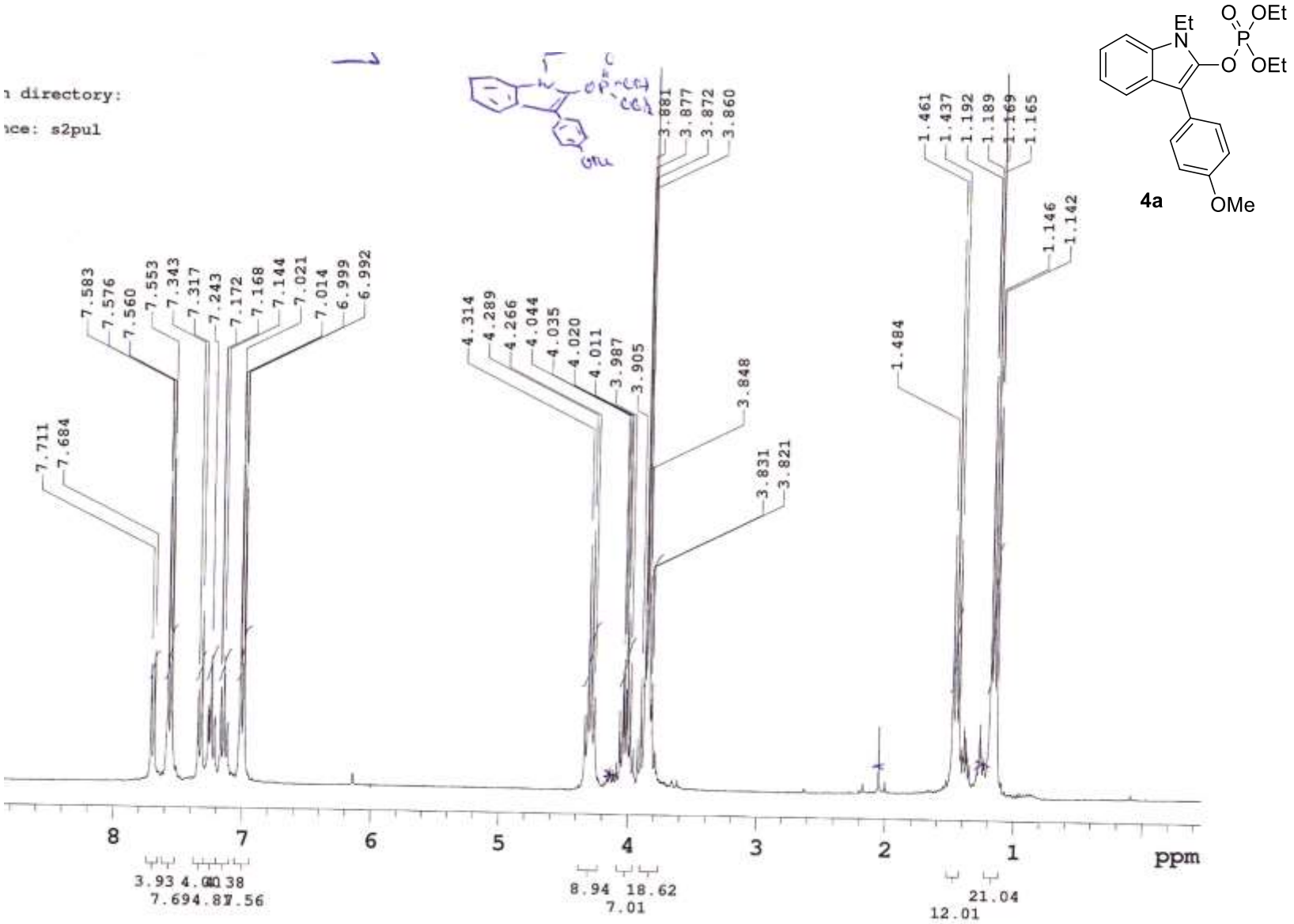

-NMR-DELL.vscht.cz-mercury300
e directory:
directory:
e: D571-H-CDCl3-ok
equence: PROTON (s2pul)
: cdcl3
llected on: Apr 27 2017
7.267
7.240
7.353
7.330
7.586
7.580
7.383
7.226
7.218
7.197
7.191
6.957
6.929
9.747
2.173
10
9
8
7
6
5
4
3
2
1
ppm
6.67
28.58
7.58
5.69
51.48

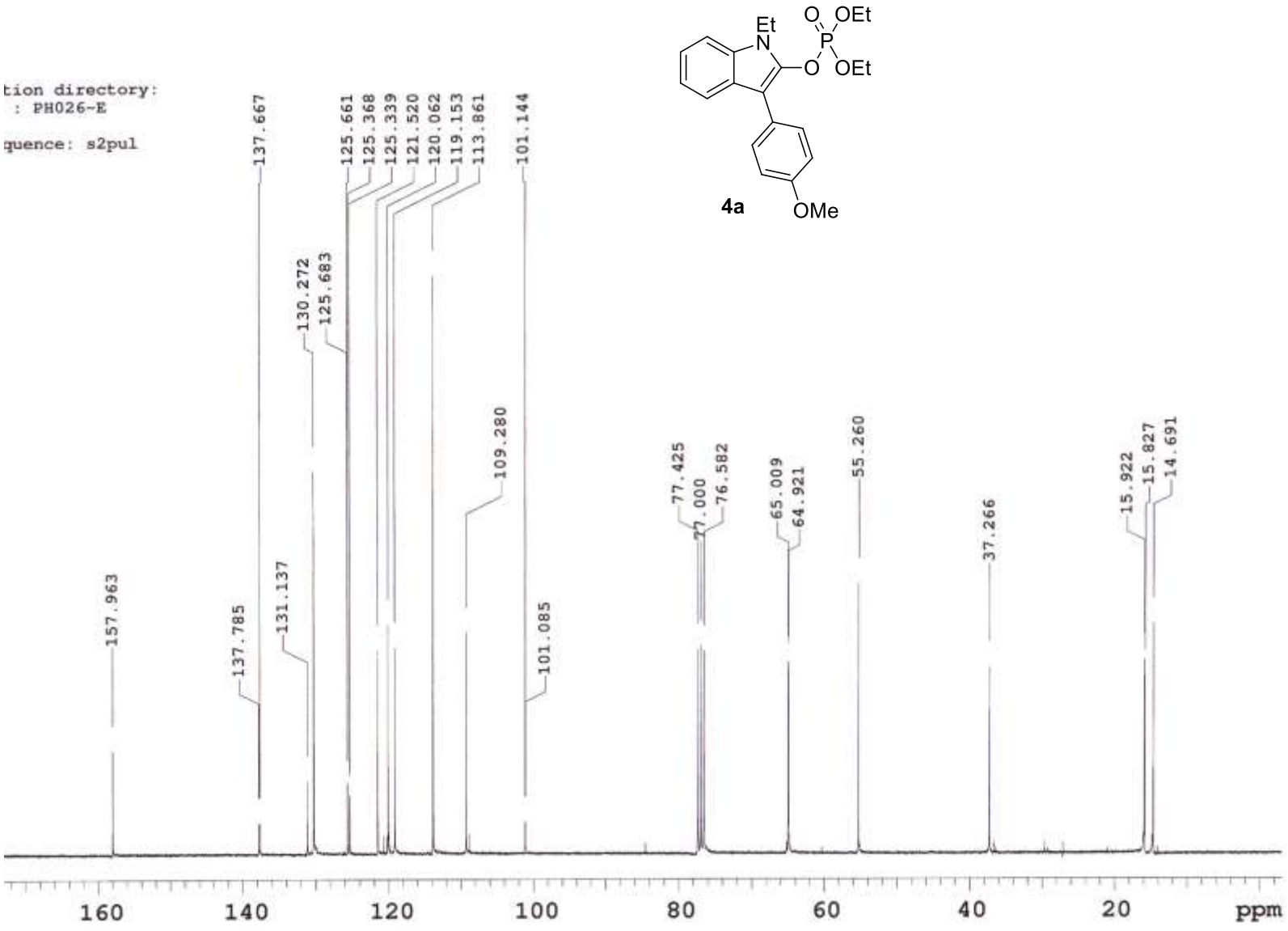
H
N
O
OPh
P
O
OPh
Br
Br

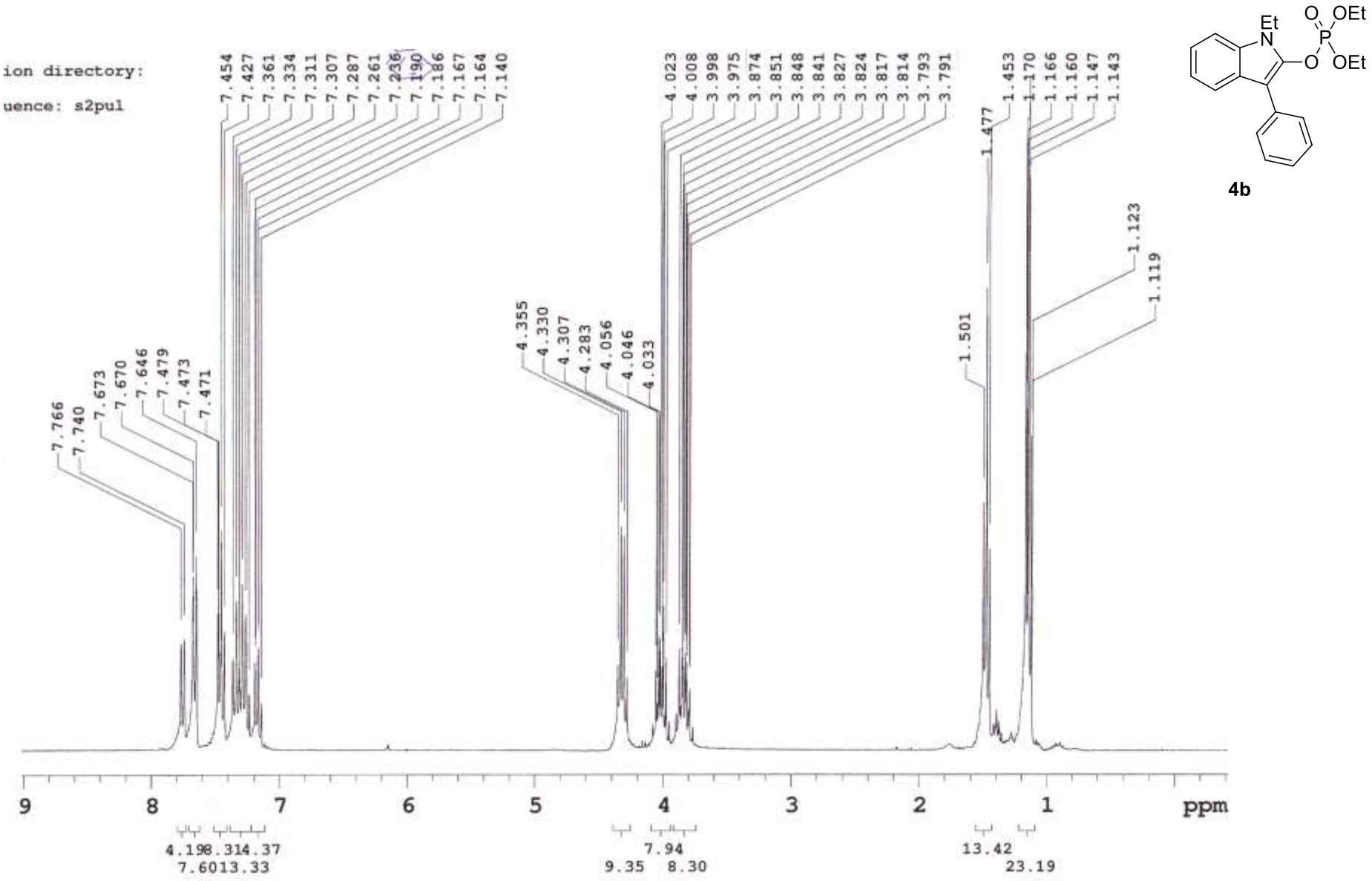
3j


ed on:
ZLL.vscht.cz-mercury300
ctory:
tory:
1-C-CDCl3
e: CARBON (s2pul)
3
d on: Feb 12 2017
130.055
129.918
129.277
128.926
127.185
126.284
125.689
121.300
120.086
120.025
134.253
113.078
77.412
77.000
76.573
74.832
74.710
149.088
149.781
139.063
138.973
200
180
160
140
120
100
80
60
40
20
ppm

3j

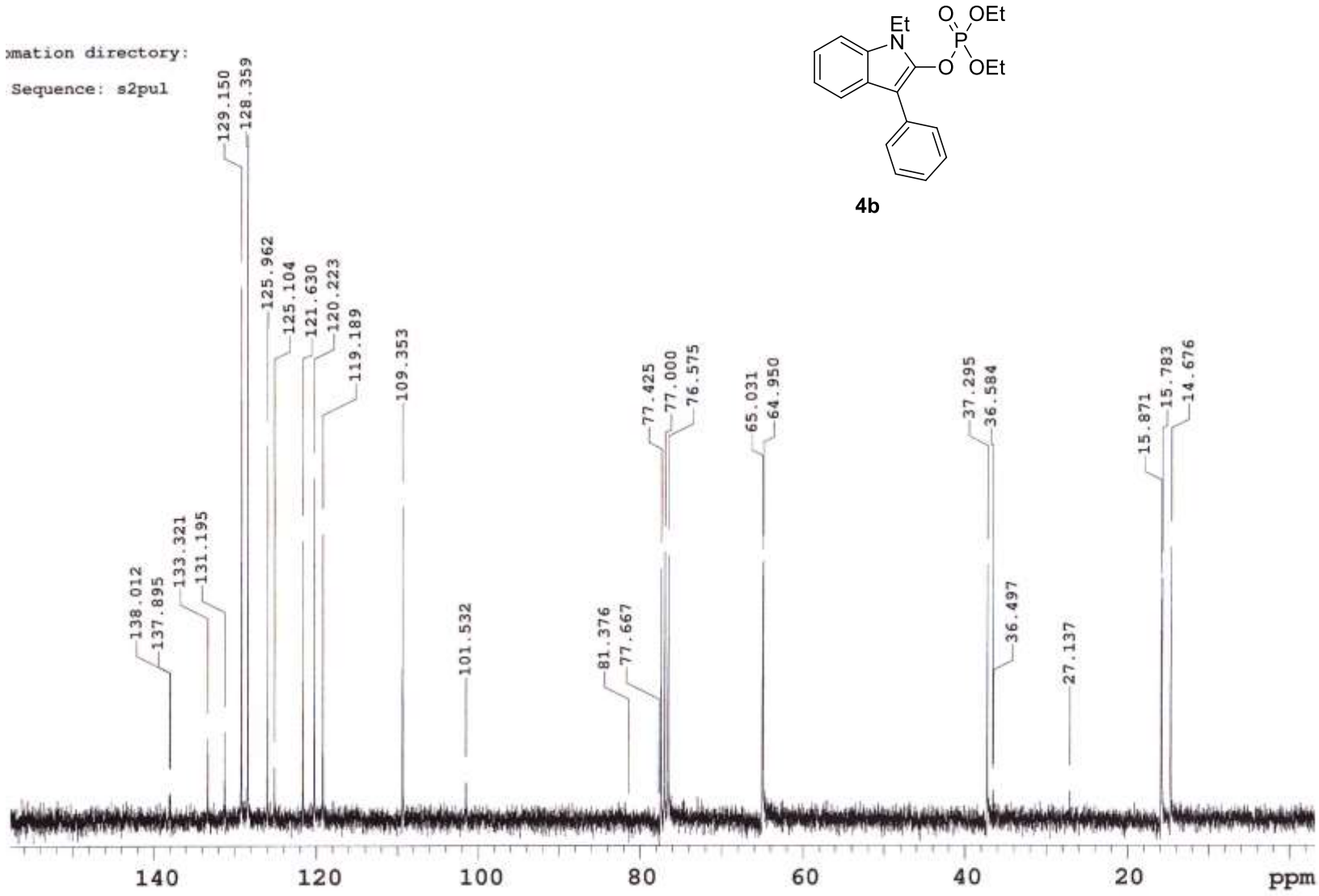

directory:
ce: s2pul
Et
N
O
OEt
P
O
OEt
4a
OMe
7.711
7.684
7.583
7.576
7.560
7.553
7.343
7.317
7.243
7.172
7.168
7.144
7.021
7.014
6.999
6.992
4.314
4.289
4.266
4.044
4.035
4.020
4.011
3.987
3.905
3.881
3.877
3.872
3.860
3.848
3.831
3.821
1.484
1.461
1.437
1.192
1.189
1.169
1.165
1.146
1.142
8
7
6
5
4
3
2
1
ppm
3.93 4.0 1.38
7.69 4.87 7.56
8.94 18.62
7.01
21.04
12.01


tion directory:
: PH026-E
quence: s2pul
137.667
125.661
125.368
125.339
121.520
120.062
119.153
113.861
101.144
130.272
125.683
109.280
157.963
137.785
131.137
101.085
77.425
77.000
76.582
65.009
64.921
55.260
37.266
15.922
15.827
14.691
Et
N
O
OEt
P
O
OEt
4a
OMe
160
140
120
100
80
60
40
20
ppm


ion directory:
uence: s2pul
7.766
7.740
7.673
7.670
7.646
7.479
7.473
7.471
7.454
7.427
7.361
7.334
7.311
7.307
7.287
7.261
7.236
7.190
7.186
7.167
7.164
7.140
4.355
4.330
4.307
4.283
4.056
4.046
4.033
4.023
4.008
3.998
3.975
3.874
3.851
3.848
3.841
3.827
3.824
3.817
3.814
3.793
3.791
1.501
1.477
1.453
1.170
1.166
1.160
1.147
1.143
1.123
1.119
9
8
7
6
5
4
3
2
1
ppm
4.19 8.31 4.37
7.60 13.33
7.94
9.35 8.30
13.42
23.19

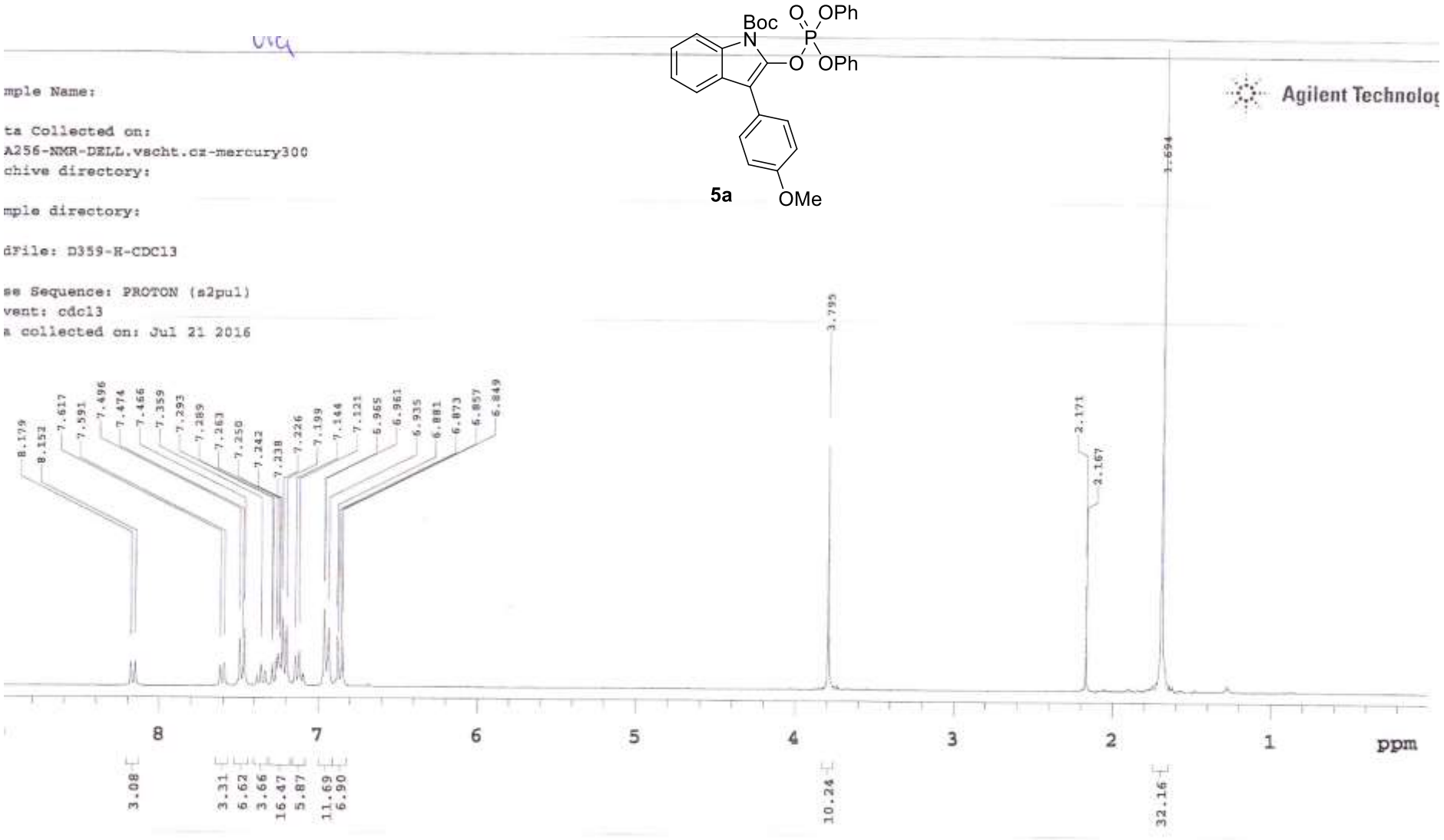
Et
N
O
P
O
OEt
O
OEt

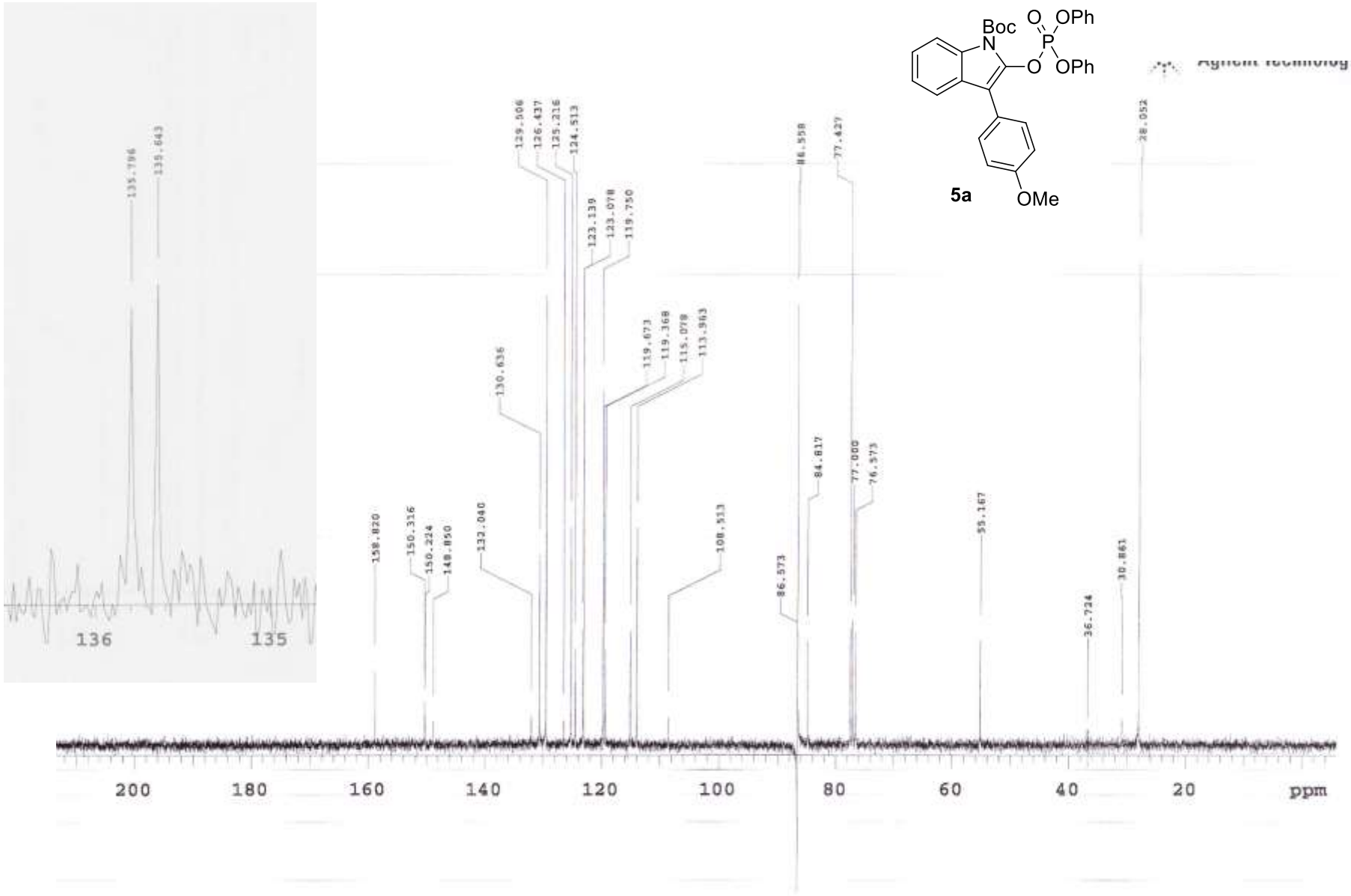
4b

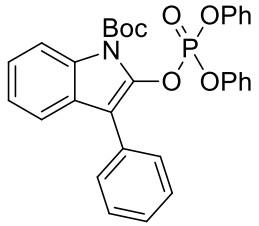

ɔmation directory:
Sequence: s2pul
129.150
128.359
125.962
125.104
121.630
120.223
119.189
109.353
101.532
81.376
77.667
77.425
77.000
76.575
65.031
64.950
37.295
36.584
36.497
27.137
15.871
15.783
14.676
138.012
137.895
133.321
131.195
140
120
100
80
60
40
20
ppm

Et
N
O
OEt
P
O
OEt

4b

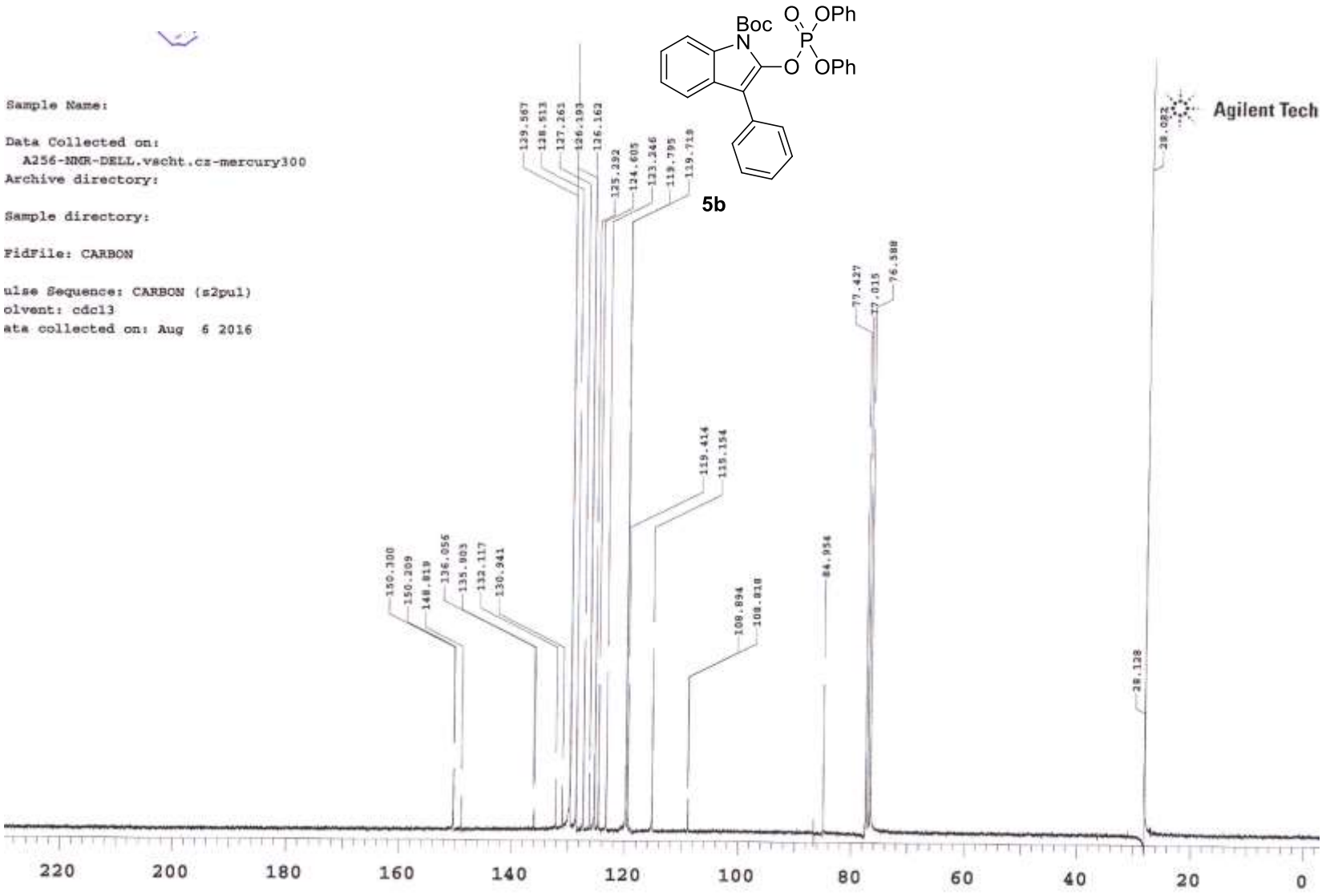

Boc
N
O
OPh
P
O
OPh
OMe
5a
Agilent Technolo
mple Name:
ta Collected on:
A256-NMR-DELL.vscht.cz-mercury300
chive directory:
mple directory:
dFile: D359-H-CDCl3
se Sequence: PROTON (s2pul)
vent: cdcl3
a collected on: Jul 21 2016
8.179
8.152
7.617
7.591
7.496
7.474
7.466
7.359
7.293
7.289
7.263
7.250
7.242
7.238
7.226
7.199
7.144
7.121
6.965
6.961
6.935
6.881
6.873
6.857
6.849
3.795
2.171
2.167
1.694
8
7
6
5
4
3
2
1
ppm
3.08
3.31
6.62
3.66
16.47
5.87
11.69
6.90
10.24
32.16

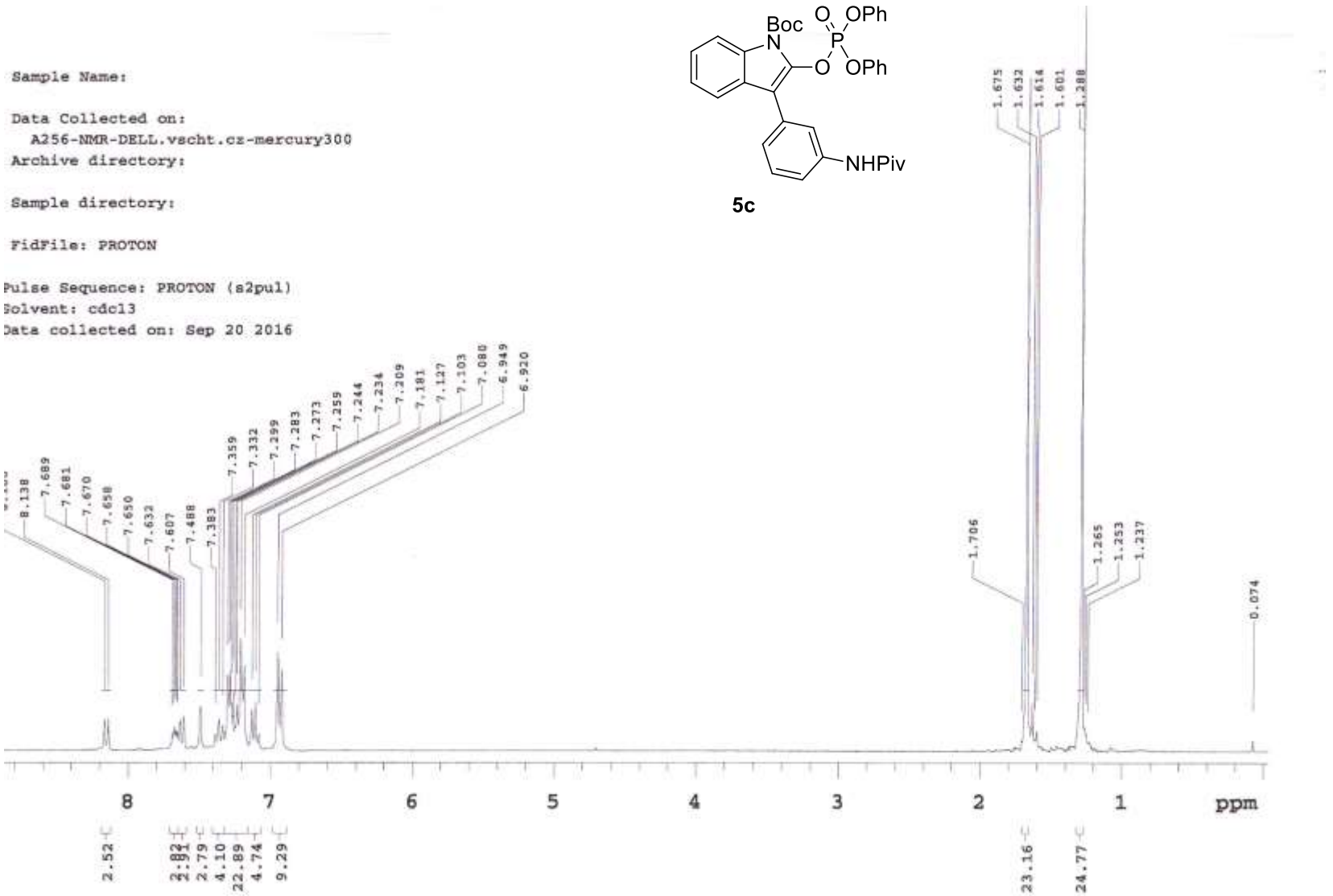

Boc
N
O
P
O
OPh
OPh
OMe
5a
Agilent Technology
135.796
135.643
136
135
129.506
126.437
125.216
124.513
123.139
123.078
119.750
119.673
119.368
115.078
113.963
130.636
158.820
150.316
150.224
148.850
132.040
108.513
86.573
86.558
84.817
77.427
77.000
76.573
55.167
36.724
30.861
28.052
200
180
160
140
120
100
80
60
40
20
ppm

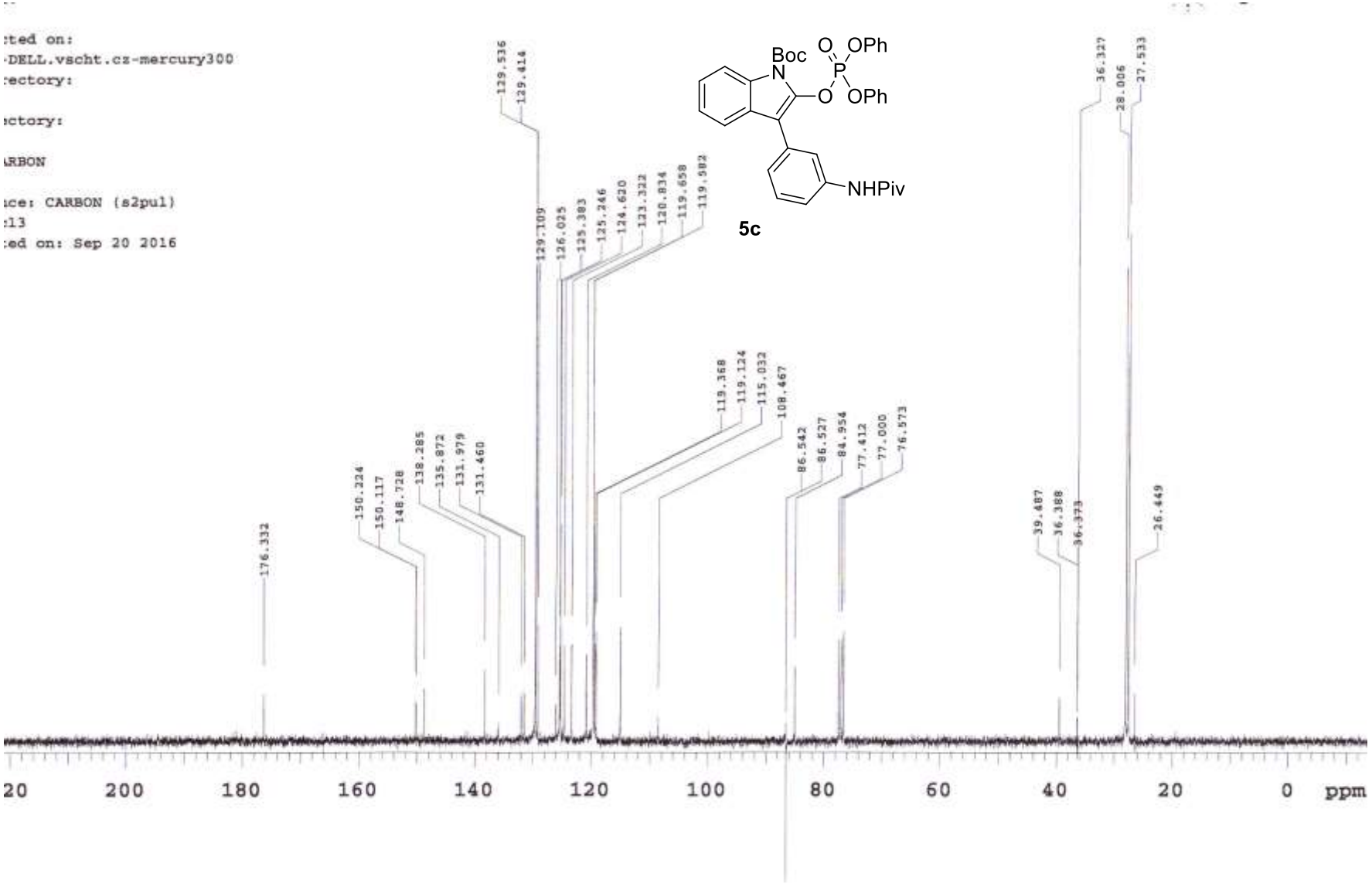

Boc
N
O
P
OPh
O
OPh

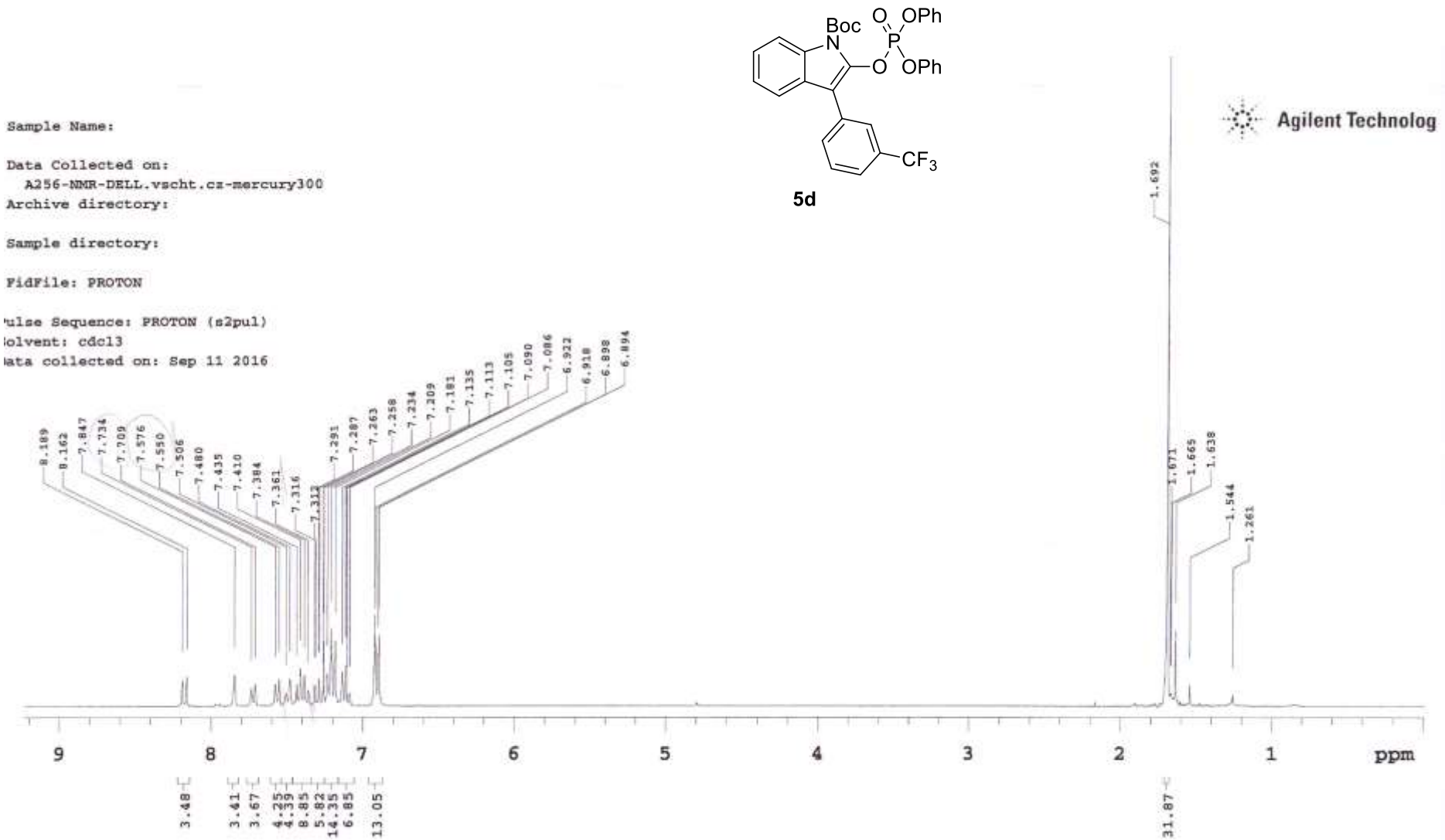
5b

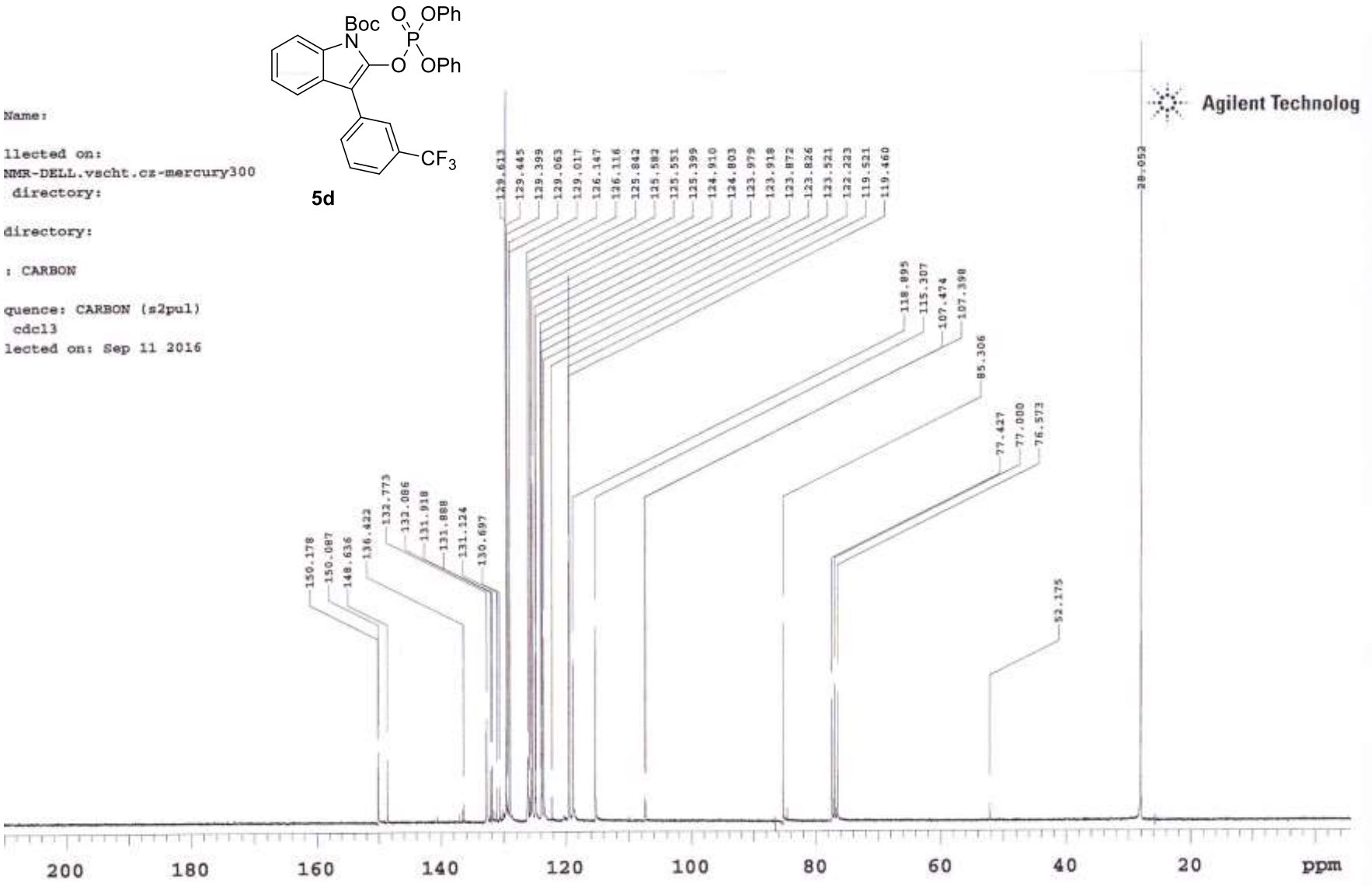
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 6 2016
8.175
8.148
7.646
7.621
7.586
7.582
7.574
7.558
7.554
7.388
7.377
7.371
7.365
7.349
7.343
7.324
7.303
7.295
7.283
7.273
7.269
7.265
7.258
7.240
7.215
7.187
7.138
7.113
7.090
6.916
6.912
6.904
6.887
1.690
1.667
1.610
1.573
1.435
9
8
7
6
5
4
3
2
1
ppm
3.10
3.55
6.78
39.44
12.85
34.27

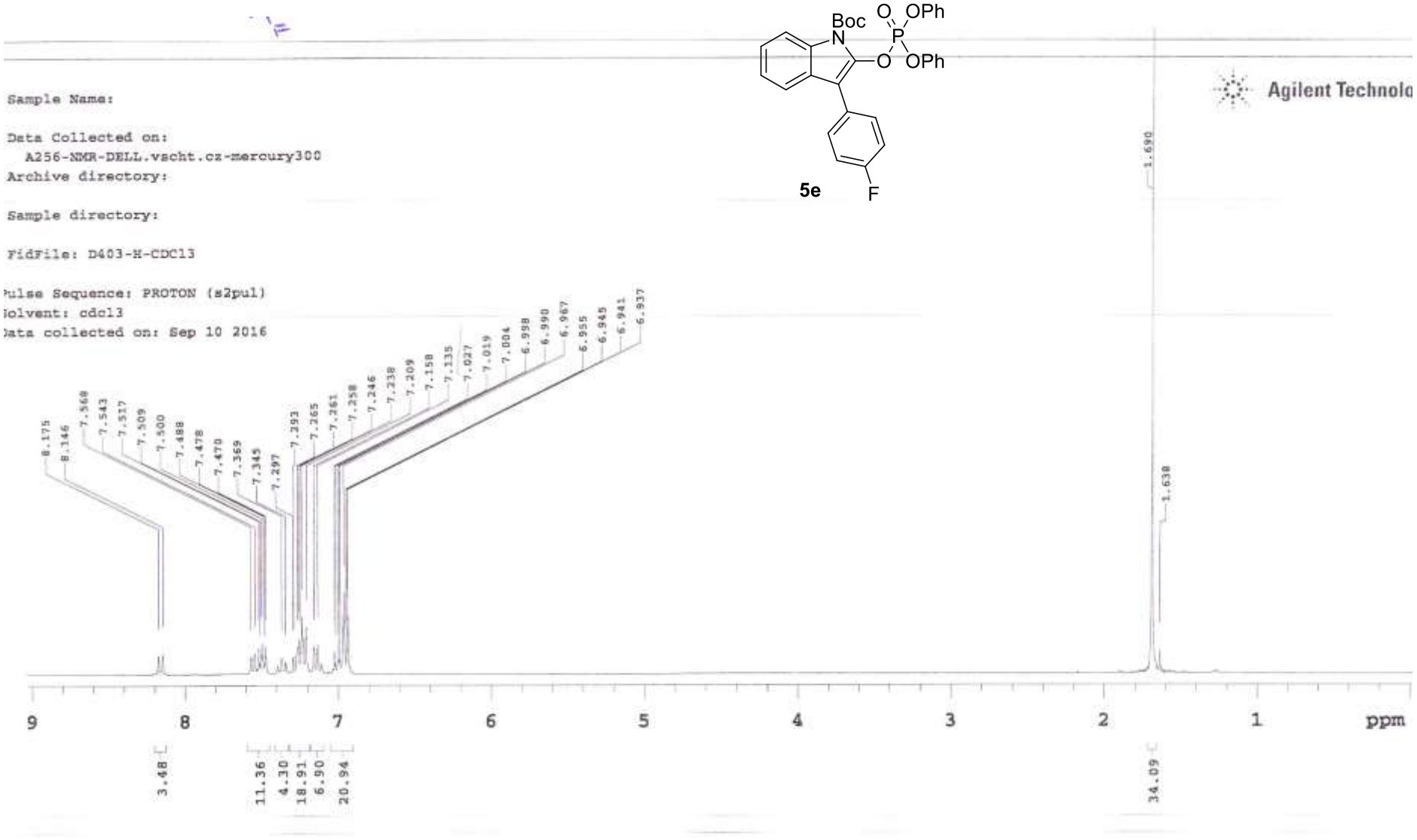

Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
ulse Sequence: CARBON (s2pul)
olvent: cdcl3
ata collected on: Aug 6 2016
Boc
N
O
P
O
OPh
O
OPh
5b
Agilent Tech
139.567
138.513
137.261
136.193
136.162
135.292
124.605
123.346
119.795
119.719
119.414
115.154
108.894
108.818
84.954
77.427
77.015
76.588
38.082
28.128
150.300
150.209
148.819
136.056
135.903
132.117
130.941
220
200
180
160
140
120
100
80
60
40
20
0

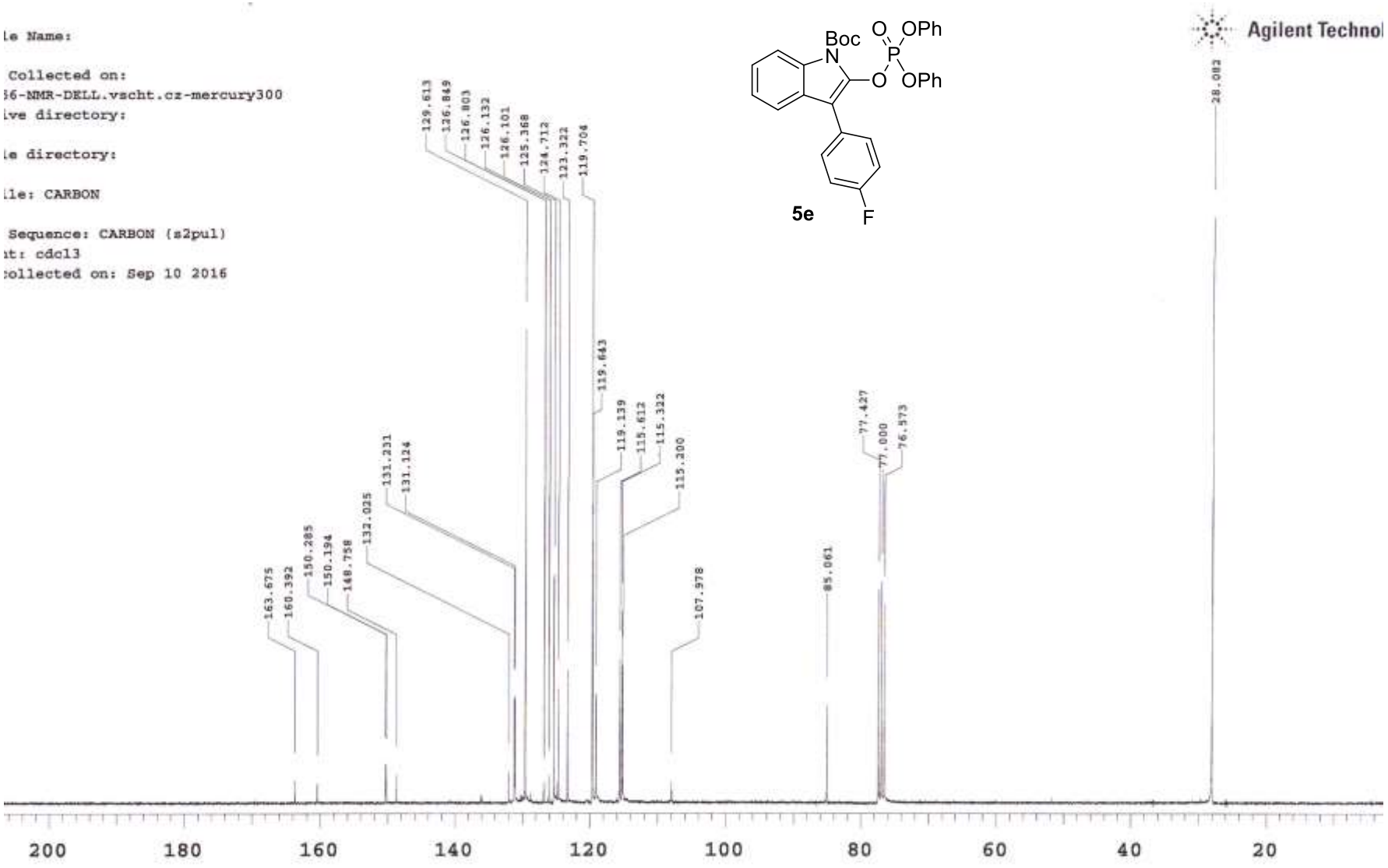

Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 20 2016
Boc
N
O
P
OPh
OPh
NHPiv
5c
8.138
7.689
7.681
7.670
7.658
7.650
7.632
7.607
7.488
7.383
7.359
7.332
7.299
7.283
7.273
7.259
7.244
7.234
7.209
7.181
7.127
7.103
7.080
6.949
6.920
1.706
1.675
1.632
1.614
1.601
1.288
1.265
1.253
1.237
0.074
8
7
6
5
4
3
2
1
ppm
2.52
2.82
2.91
2.79
4.10
22.89
4.74
9.29
23.16
24.77

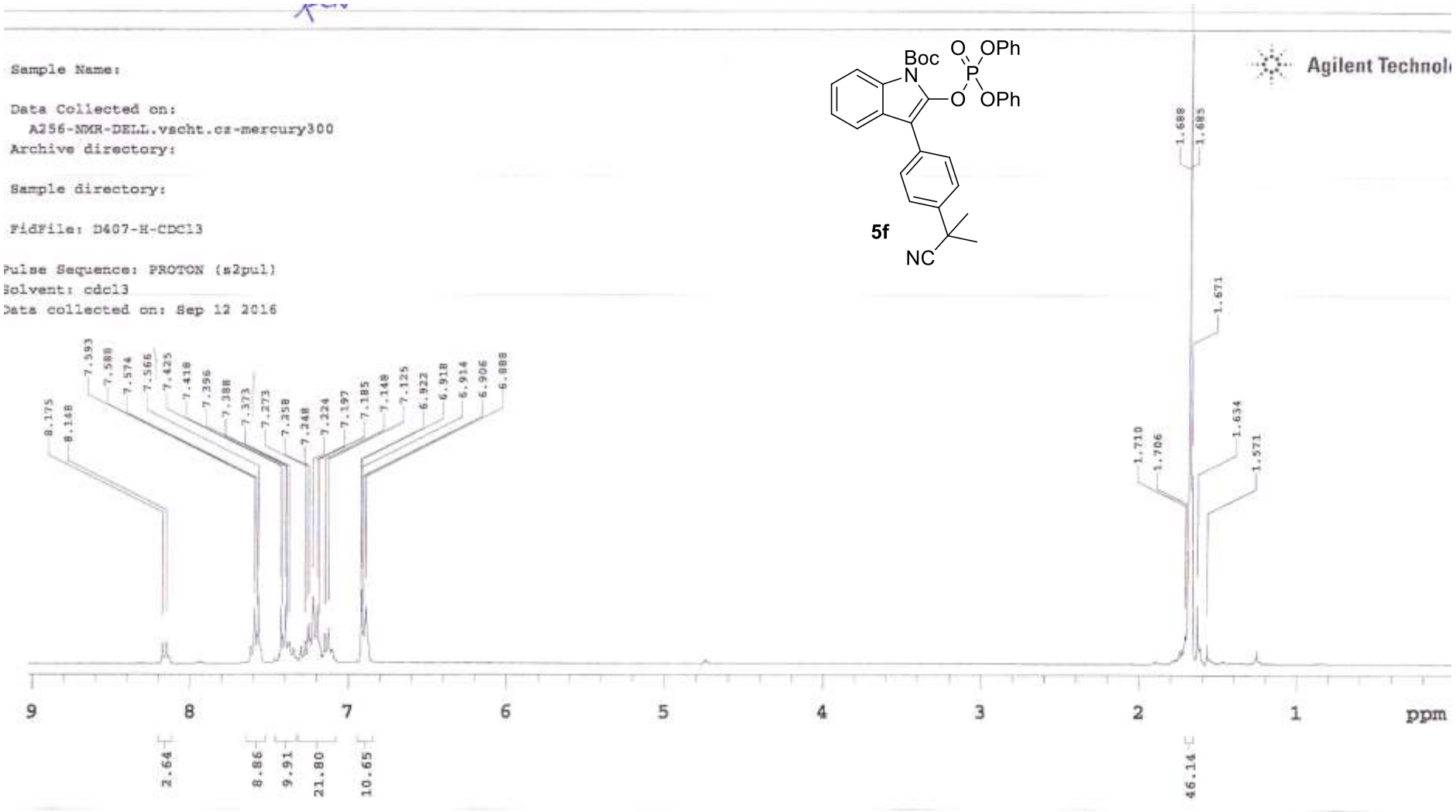

:ted on:
·DELL.vscht.cz-mercury300
:ectory:
:ctory:
ARBON
ice: CARBON (s2pul)
:13
:ed on: Sep 20 2016
Boc
N
O
P
O
OPh
O
OPh
NHPiv
5c
139.536
129.414
129.109
126.025
125.383
125.246
124.620
123.322
120.834
119.658
119.582
119.368
119.124
115.032
108.467
86.542
86.527
84.954
77.412
77.000
76.573
176.332
150.224
150.117
148.728
138.285
135.872
131.979
131.460
39.487
36.388
36.373
36.327
28.006
27.533
26.449
220
200
180
160
140
120
100
80
60
40
20
0
ppm

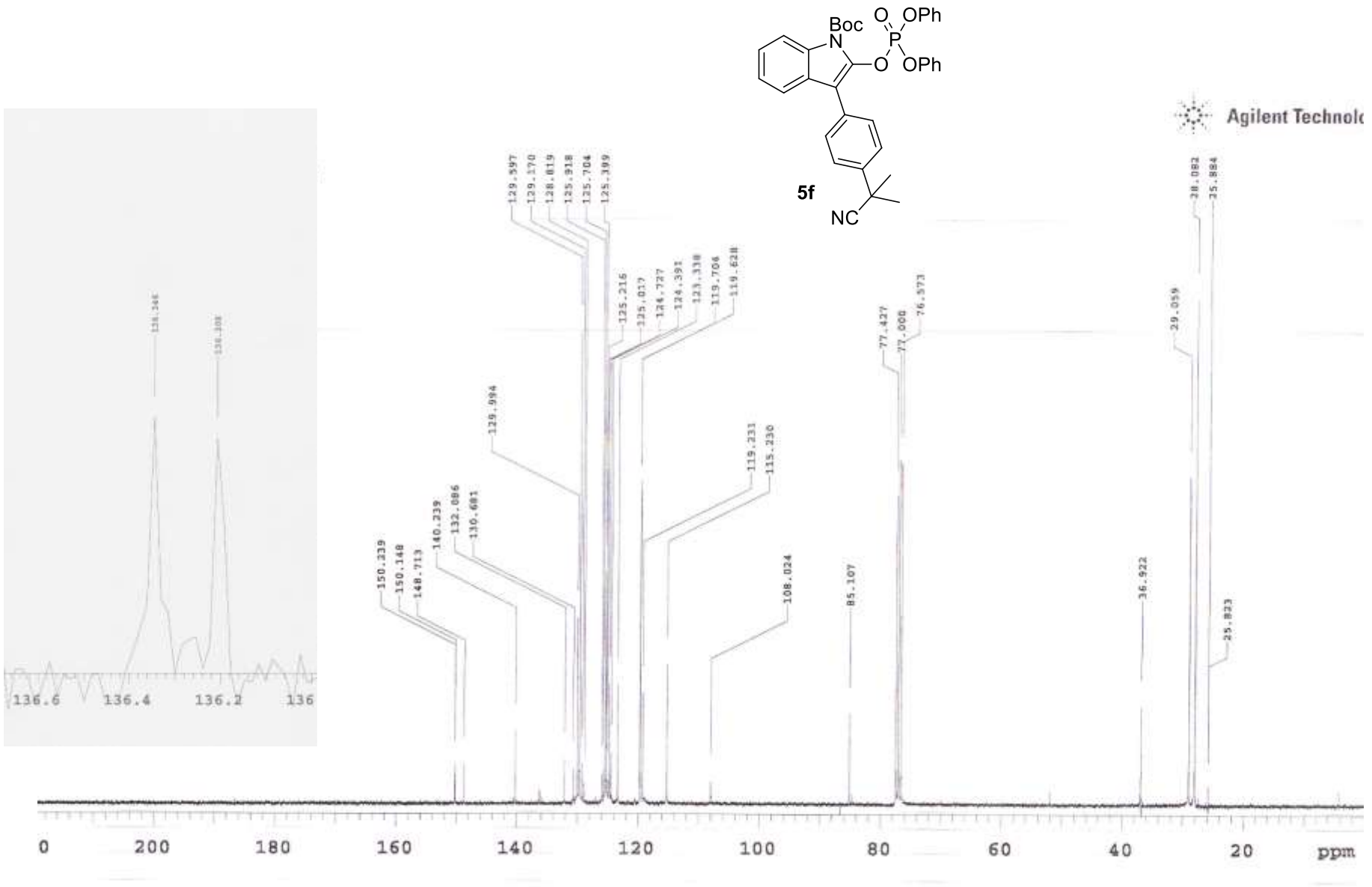

Boc
N
O
P
O
OPh
O
OPh
CF3
5d
Agilent Technolog
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: PROTON
ulse Sequence: PROTON (s2pul)
olvent: cdcl3
ata collected on: Sep 11 2016
8.189
8.162
7.847
7.734
7.709
7.576
7.550
7.506
7.480
7.435
7.410
7.384
7.361
7.316
7.312
7.291
7.287
7.263
7.258
7.234
7.209
7.181
7.135
7.113
7.105
7.090
7.086
6.922
6.918
6.898
6.894
1.692
1.671
1.665
1.638
1.544
1.261
9
8
7
6
5
4
3
2
1
ppm
3.48
3.41
3.67
4.25
4.39
8.85
5.82
14.35
6.85
13.05
31.87

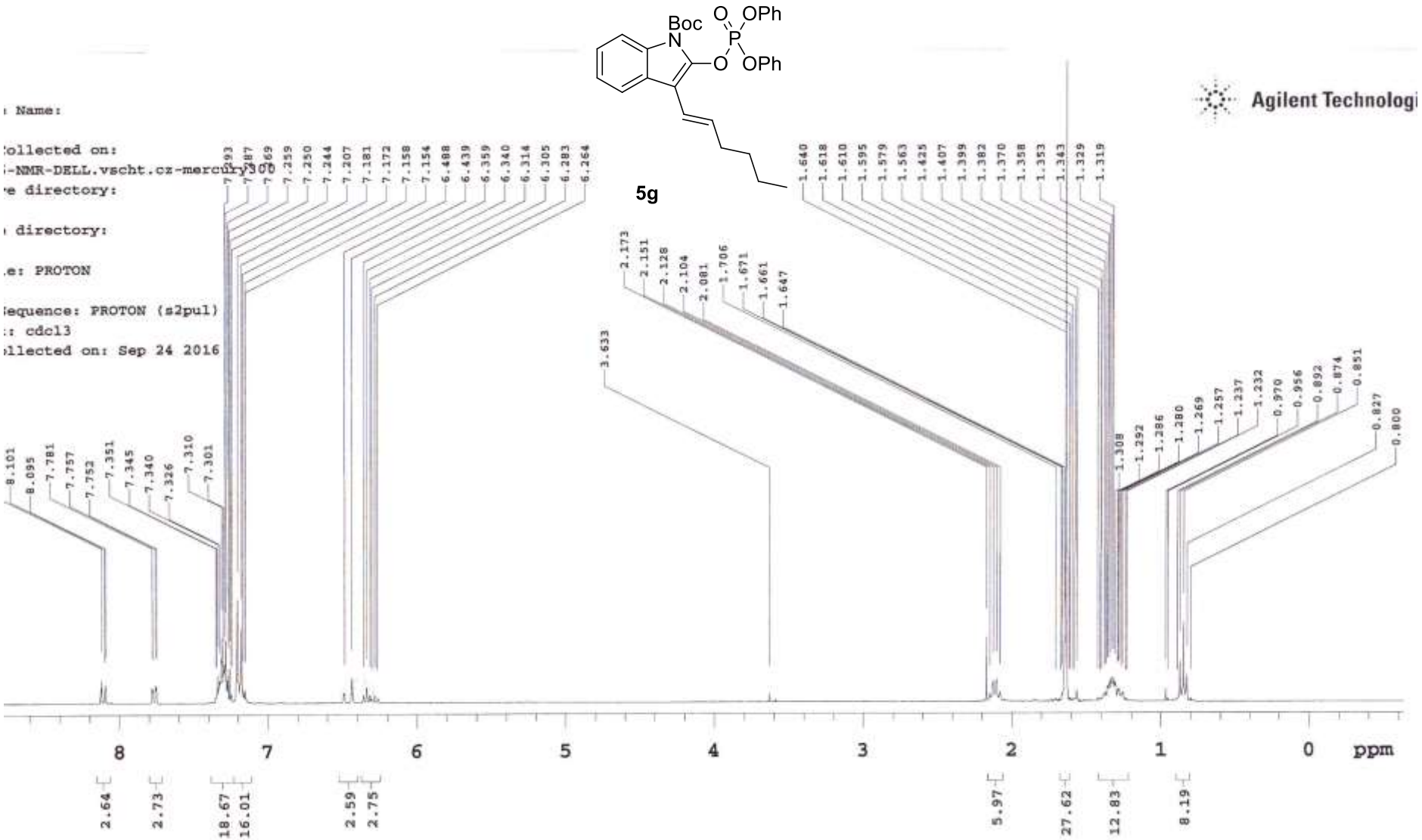

Boc
N
O
P
O
OPh
OPh
CF3
5d
Name:
llected on:
NMR-DELL.vscht.cz-mercury300
directory:
directory:
: CARBON
quence: CARBON (s2pul)
cdcl3
lected on: Sep 11 2016
Agilent Technolog
139.613
139.445
139.399
139.063
139.017
136.147
136.116
135.842
135.582
135.551
135.399
134.910
134.803
133.979
133.918
133.872
133.826
133.521
132.233
119.521
119.460
118.895
115.307
107.474
107.398
85.306
77.427
77.000
76.573
52.175
150.178
150.087
148.636
136.422
132.773
132.086
131.918
131.888
131.124
130.697
30.052
200
180
160
140
120
100
80
60
40
20
ppm

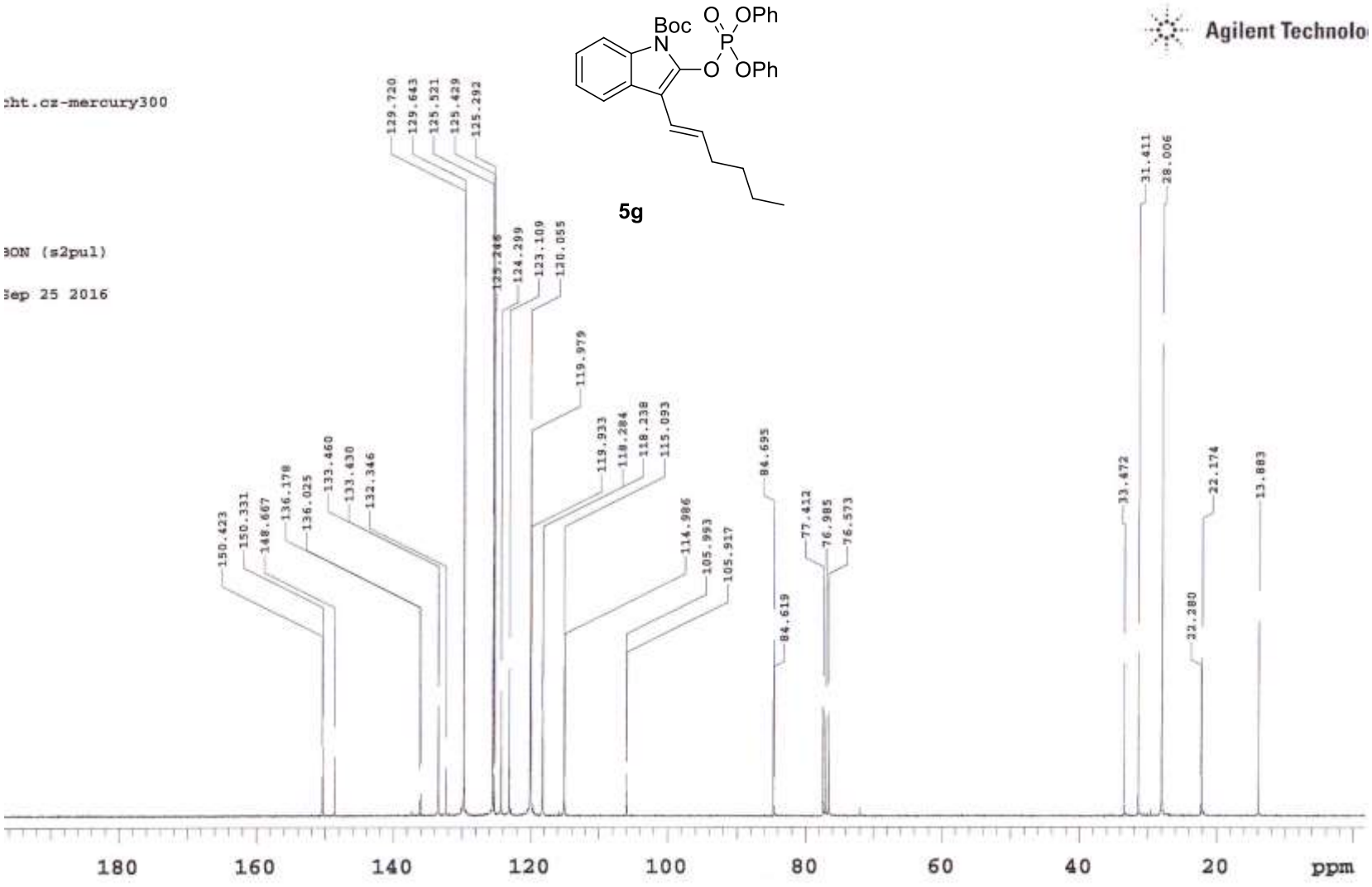

Boc
N
O
P
OPh
OPh
O
F
5e
Agilent Technolo
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: D403-H-CDCl3
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 10 2016
8.175
8.146
7.568
7.543
7.517
7.509
7.500
7.488
7.478
7.470
7.369
7.345
7.297
7.293
7.265
7.261
7.258
7.246
7.238
7.209
7.158
7.135
7.027
7.019
7.004
6.998
6.990
6.967
6.955
6.945
6.941
6.937
1.690
1.638
9
8
7
6
5
4
3
2
1
ppm
3.48
11.36
4.30
18.91
6.90
20.94
34.09

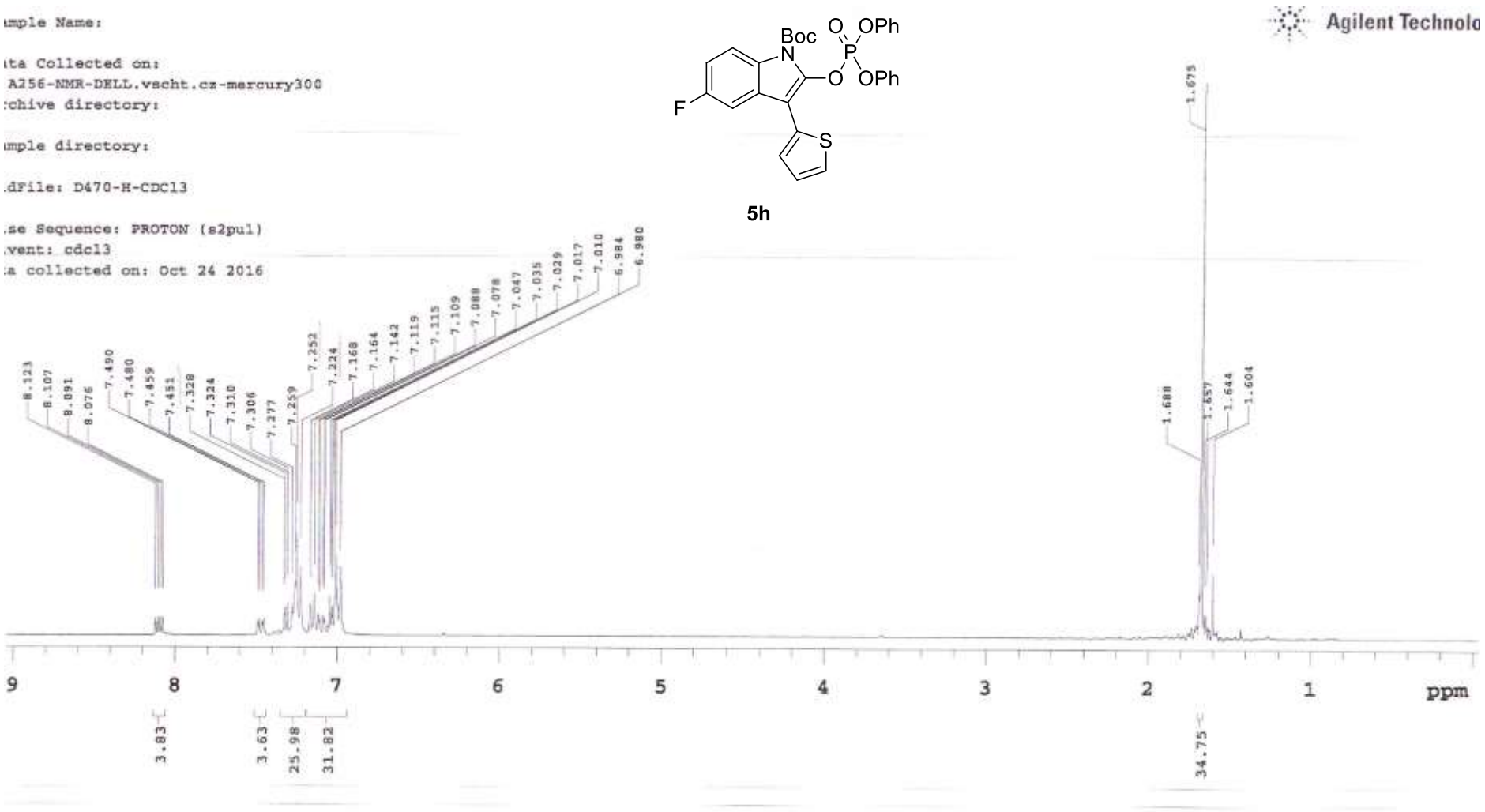

le Name:
Collected on:
36-NMR-DELL.vscht.cz-mercury300
ive directory:
le directory:
ile: CARBON
Sequence: CARBON (s2pul)
nt: cdcl3
collected on: Sep 10 2016
Boc
N
O
P
OPh
OPh
O
F
5e
Agilent Technol
129.613
126.849
126.803
126.132
126.101
125.368
124.712
123.322
119.704
119.643
119.139
115.612
115.332
115.300
131.231
131.124
132.025
163.675
160.392
150.285
150.194
148.758
107.978
85.061
77.427
77.000
76.573
28.082
200
180
160
140
120
100
80
60
40
20

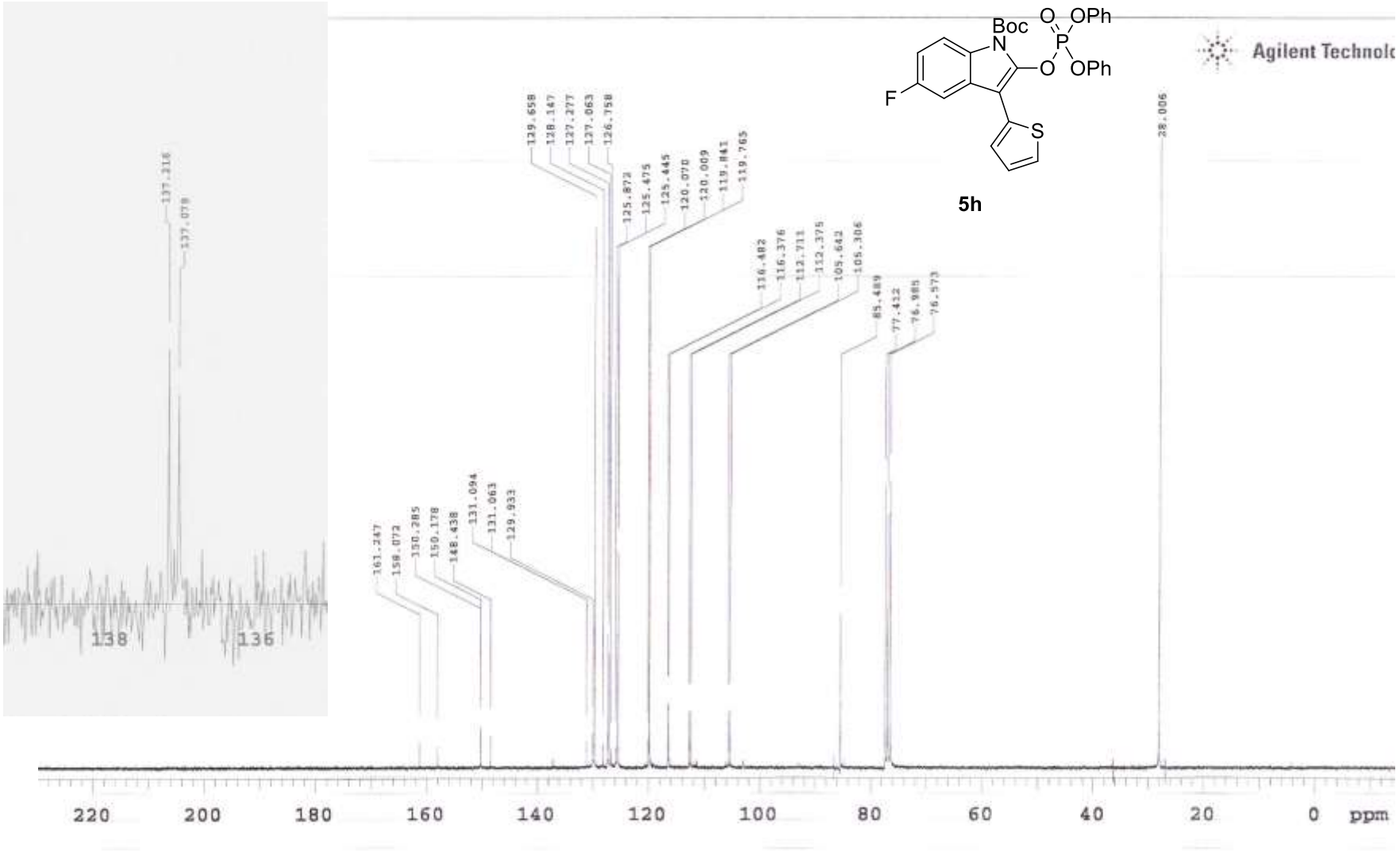

Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: D407-H-CDCl3
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 12 2016
Boc
N
O
OPh
P
O
OPh
5f
NC
Agilent Technol
8.175
8.148
7.593
7.588
7.574
7.566
7.425
7.418
7.396
7.388
7.373
7.273
7.258
7.248
7.224
7.197
7.185
7.148
7.125
6.922
6.918
6.914
6.906
6.888
1.688
1.685
1.671
1.710
1.706
1.634
1.571
9
8
7
6
5
4
3
2
1
ppm
2.64
8.86
9.91
21.80
10.65
46.14

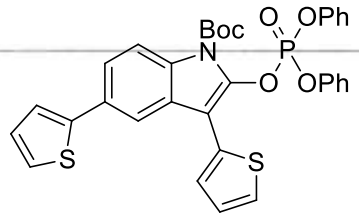

Boc
N
O
P
O
OPh
OPh
5f
NC
Agilent Technol
129.597
129.170
128.819
125.918
125.704
125.399
125.216
125.017
124.727
124.391
123.338
119.704
119.628
129.984
119.231
115.230
150.239
150.148
148.713
140.239
132.086
130.681
108.024
85.107
77.427
77.000
76.573
29.059
28.082
25.884
36.922
25.823
136.6
136.4
136.2
136
0
200
180
160
140
120
100
80
60
40
20
ppm


Boc
N
O
P
O
OPh
OPh
5g
Agilent Technologi
Name:
collected on:
-NMR-DELL.vscht.cz-mercury300
e directory:
directory:
e: PROTON
equence: PROTON (s2pul)
: cdcl3
llected on: Sep 24 2016
8.101
8.095
7.781
7.757
7.752
7.351
7.345
7.340
7.326
7.310
7.301
7.293
7.287
7.269
7.259
7.250
7.244
7.207
7.181
7.172
7.158
7.154
6.408
6.439
6.359
6.340
6.314
6.305
6.283
6.264
3.633
2.173
2.151
2.128
2.104
2.081
1.706
1.671
1.661
1.647
1.640
1.618
1.610
1.595
1.579
1.563
1.425
1.407
1.399
1.382
1.370
1.358
1.353
1.343
1.329
1.319
1.308
1.292
1.286
1.280
1.269
1.257
1.237
1.232
0.970
0.956
0.892
0.874
0.851
0.827
0.800
8
7
6
5
4
3
2
1
0
ppm
2.64
2.73
18.67
16.01
2.59
2.75
5.97
27.62
12.83
8.19

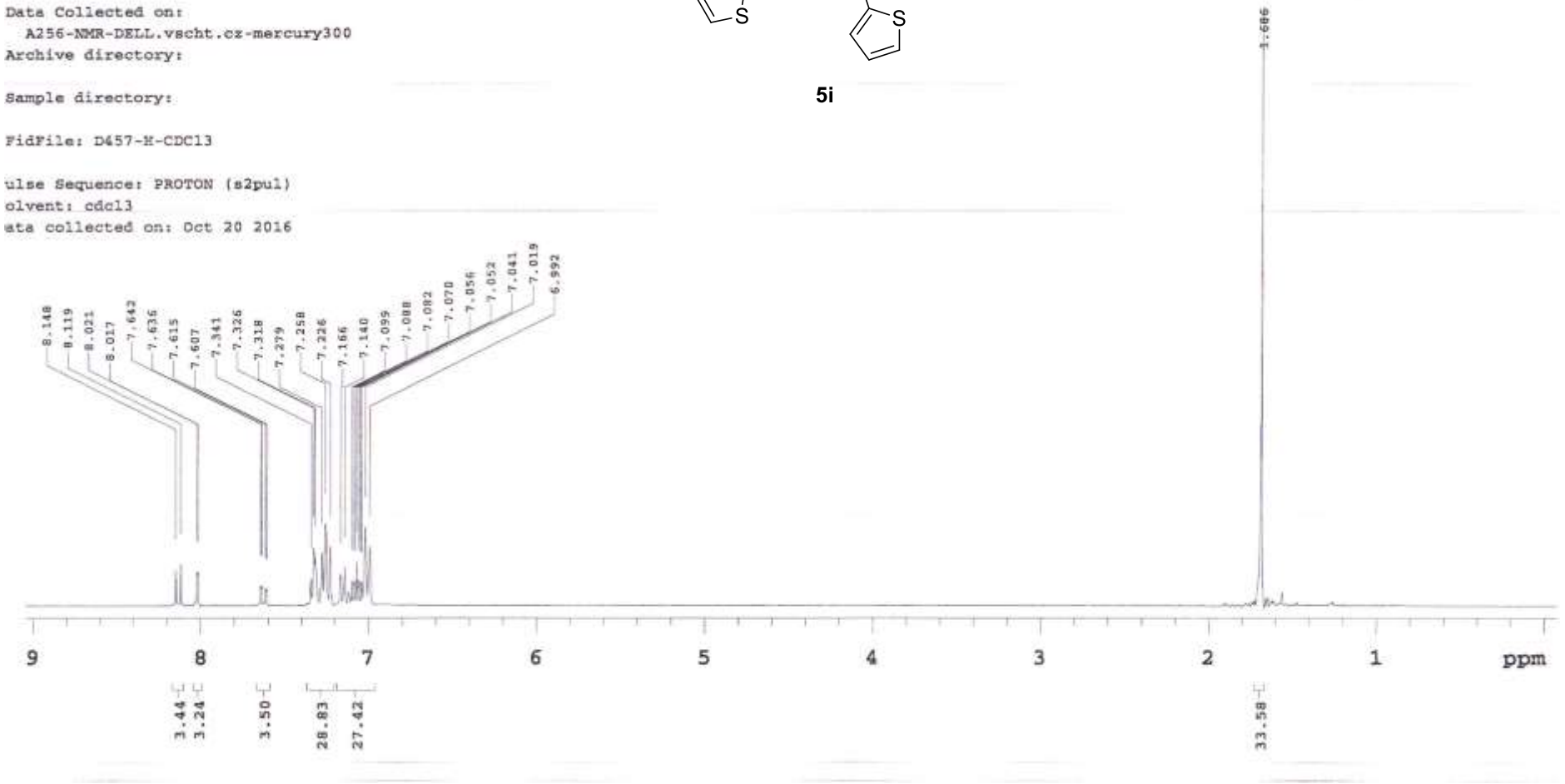

Boc
N
O
OPh
P
O
OPh
5g
Agilent Technolo
cht.cz-mercury300
3ON (s2pul)
Sep 25 2016
129.720
129.643
125.521
125.429
125.292
125.246
124.299
123.109
120.055
119.979
119.933
118.284
118.238
115.093
114.986
105.993
105.917
84.695
84.619
77.412
76.985
76.573
150.423
150.331
148.667
136.178
136.025
133.460
133.430
132.346
31.411
28.006
33.472
22.280
22.174
13.883
180
160
140
120
100
80
60
40
20
ppm

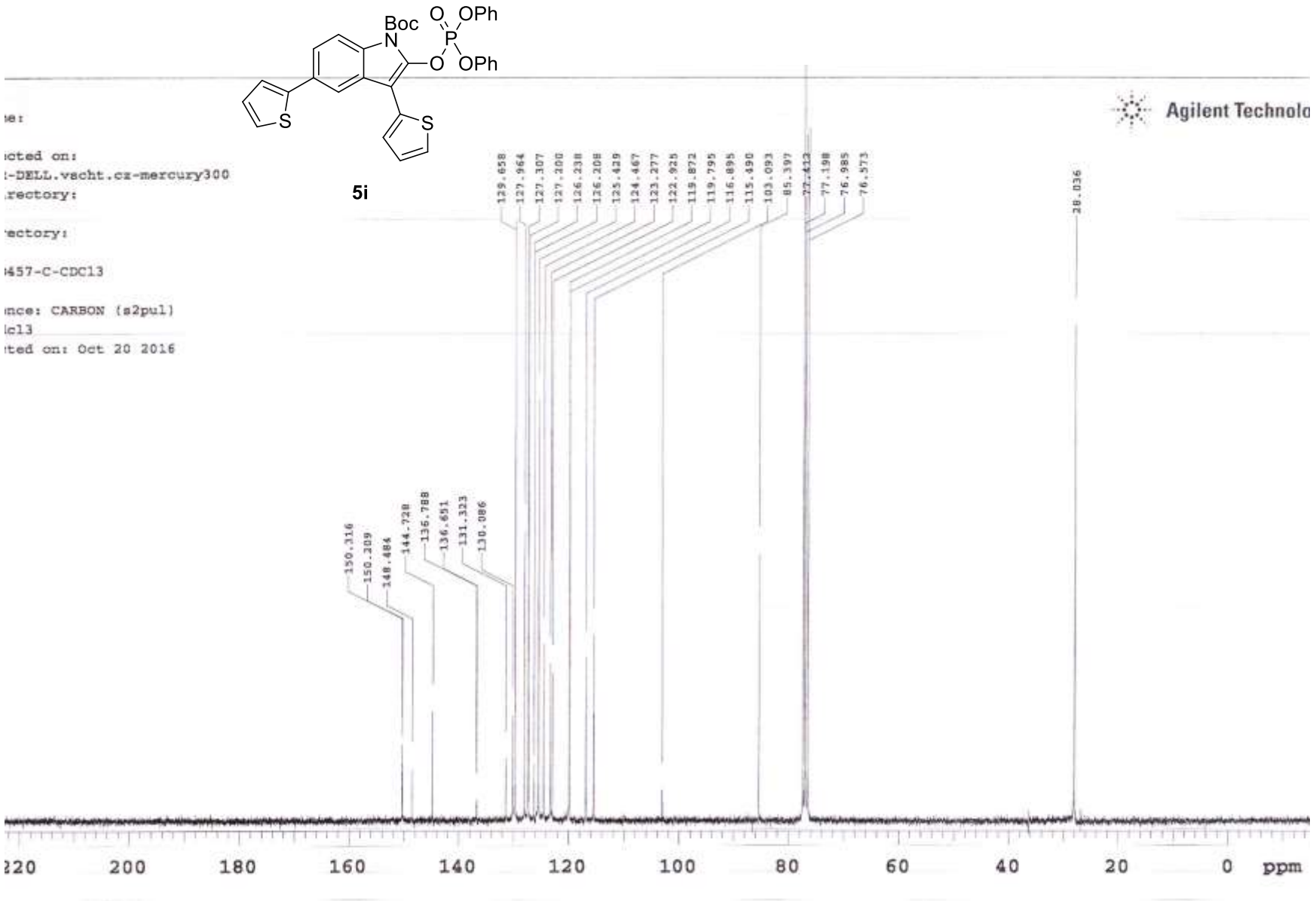

mple Name:
ta Collected on:
A256-NMR-DELL.vscht.cz-mercury300
chive directory:
mple directory:
dFile: D470-H-CDCl3
se Sequence: PROTON (s2pul)
vent: cdcl3
a collected on: Oct 24 2016
Agilent Technolo
Boc
N
O
OPh
P
O
OPh
F
S
5h
8.123
8.107
8.091
8.076
7.490
7.480
7.459
7.451
7.328
7.324
7.310
7.306
7.277
7.259
7.252
7.224
7.168
7.164
7.142
7.119
7.115
7.109
7.088
7.078
7.047
7.035
7.029
7.017
7.010
6.984
6.980
1.675
1.688
1.657
1.644
1.604
9
8
7
6
5
4
3
2
1
ppm
3.83
3.63
25.98
31.82
34.75

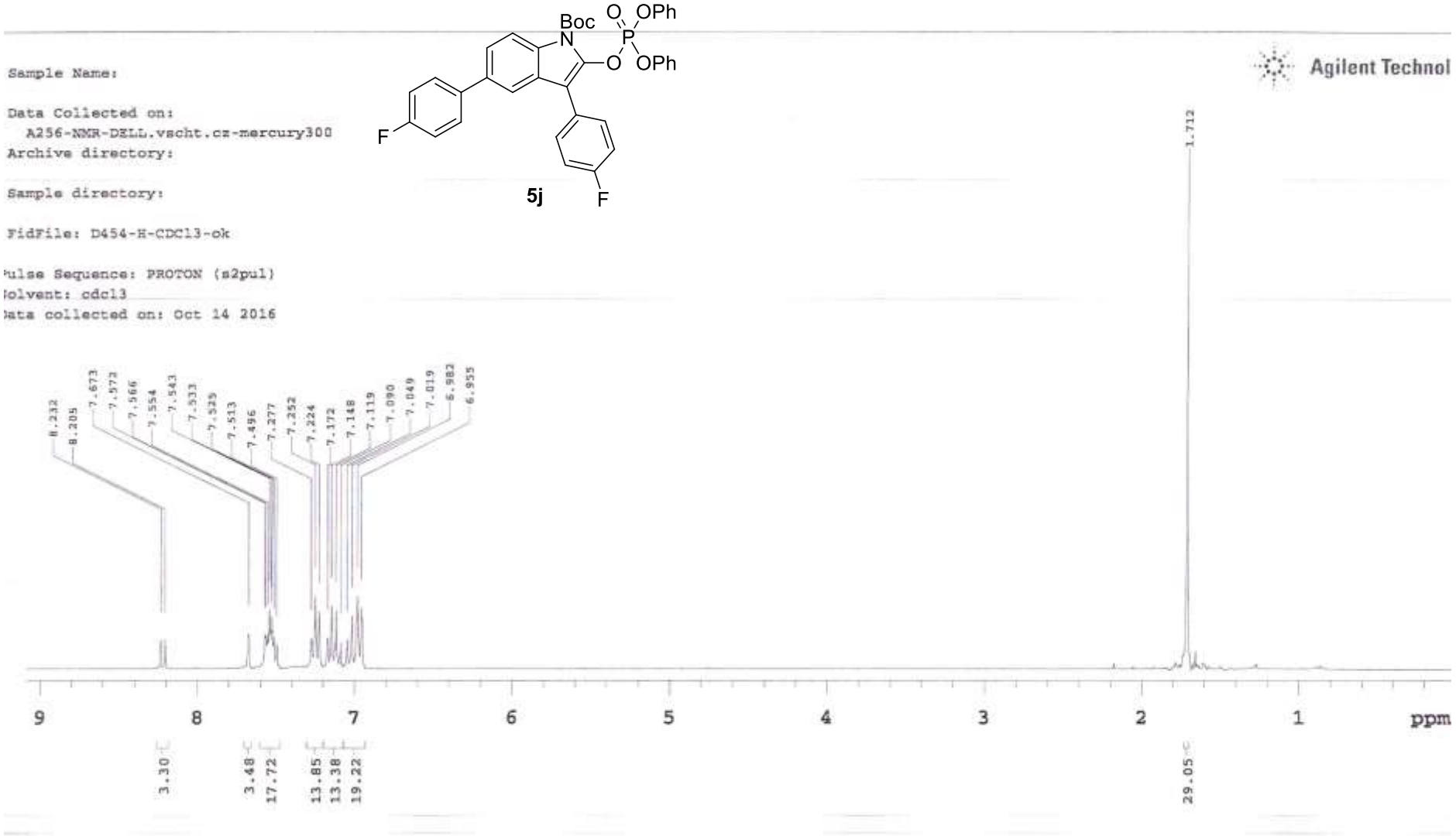

Boc
N
O
OPh
P
O
OPh
F
S
5h
Agilent Technol
139.658
138.147
137.277
137.063
136.758
125.872
125.475
125.445
120.078
120.009
119.841
119.765
116.482
116.376
112.711
112.375
105.642
105.306
85.489
77.412
76.985
76.573
28.006
161.247
158.072
150.285
150.178
148.438
131.094
131.063
129.933
137.216
137.078
138
136
220
200
180
160
140
120
100
80
60
40
20
0
ppm

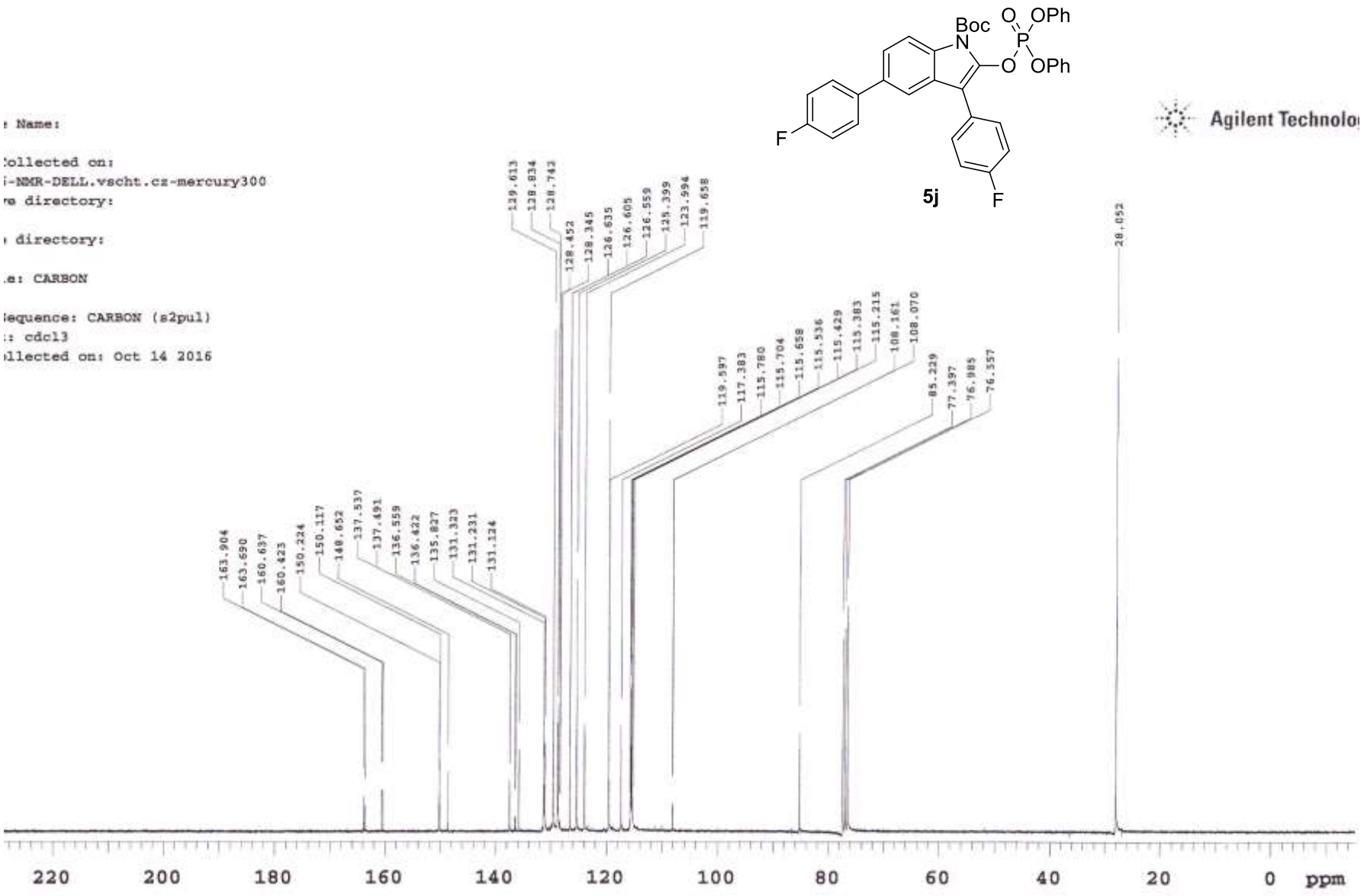

Boc
N
O
P
O
OPh
O
OPh
S
S

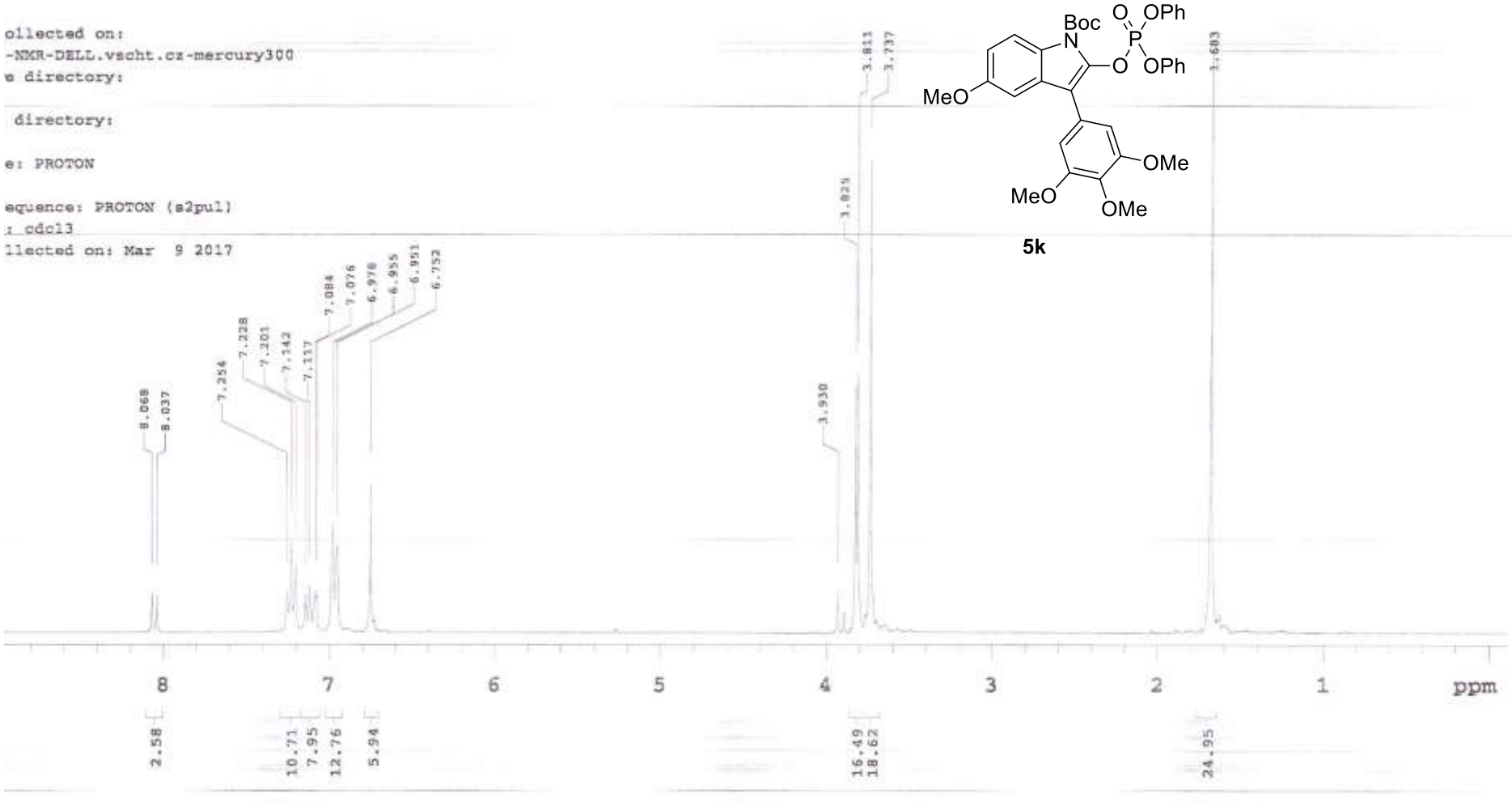
5i


Agilent Technolo
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: D457-H-CDCl3
ulse Sequence: PROTON (s2pul)
olvent: cdcl3
ata collected on: Oct 20 2016
8.148
8.119
8.021
8.017
7.643
7.636
7.615
7.607
7.341
7.326
7.318
7.279
7.258
7.226
7.166
7.140
7.099
7.088
7.082
7.070
7.056
7.052
7.041
7.019
6.992
1.686
9
8
7
6
5
4
3
2
1
ppm
3.44
3.24
3.50
28.83
27.42
33.58


Boc
N
O
P
O
OPh
O
OPh
S
S
5i
Agilent Technolo
ıcted on:
:-DELL.vacht.cz-mercury300
:rectory:
'ectory:
:457-C-CDC13
ınce: CARBON (s2pul)
lc13
ted on: Oct 20 2016
129.658
127.964
127.307
127.200
126.238
126.208
125.429
124.467
123.277
122.925
119.872
119.795
116.895
115.490
103.093
85.397
77.412
77.198
76.985
76.573
28.036
150.316
150.209
148.484
144.728
136.788
136.651
131.323
130.086
220
200
180
160
140
120
100
80
60
40
20
0
ppm

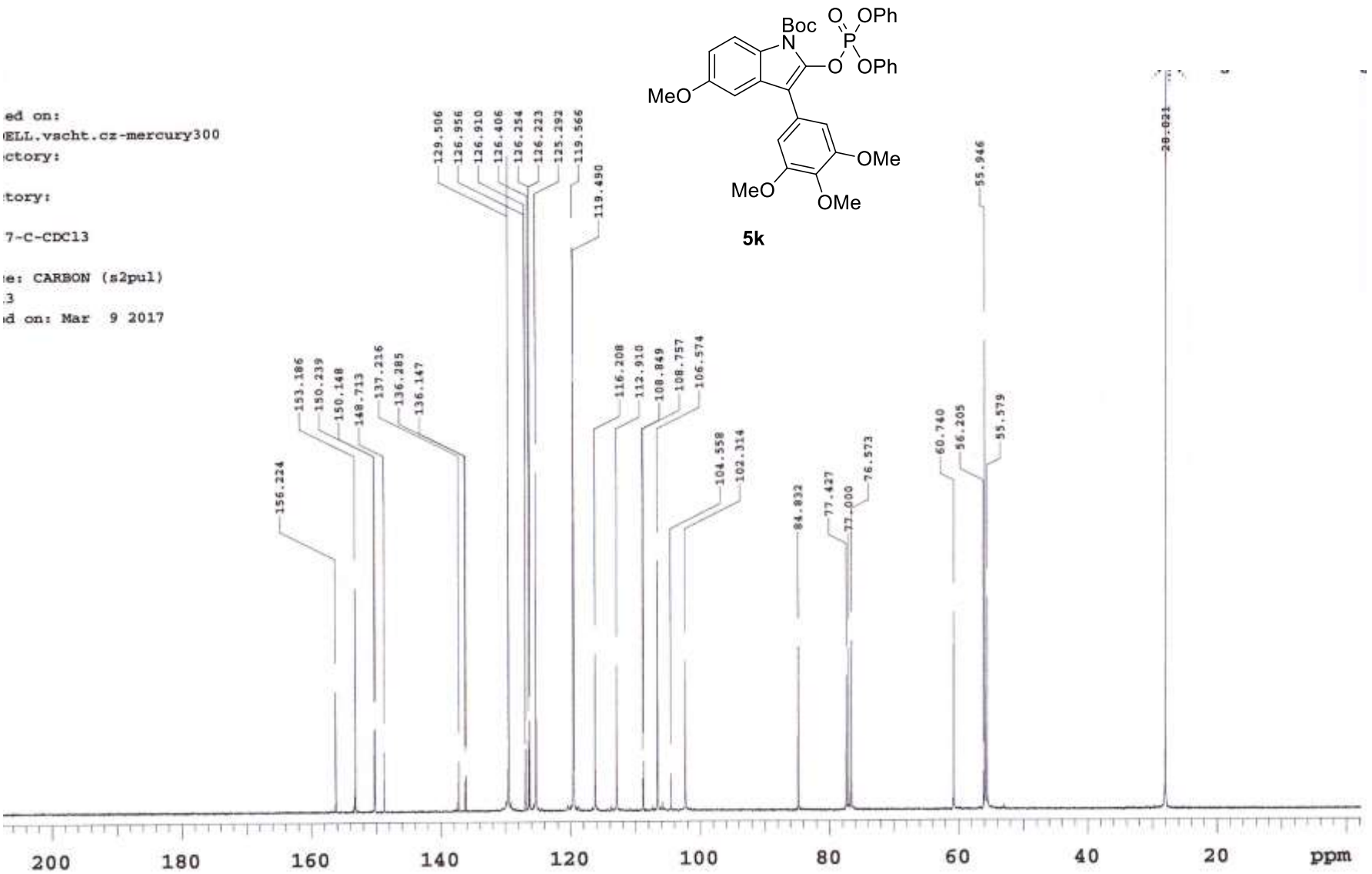

Boc
O
OPh
N
P
O
OPh
F
F
5j
Agilent Technol
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: D454-H-CDCl3-ok
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 14 2016
8.232
8.205
7.673
7.573
7.566
7.554
7.543
7.533
7.525
7.513
7.496
7.277
7.252
7.224
7.172
7.148
7.119
7.090
7.049
7.019
6.982
6.955
1.712
9
8
7
6
5
4
3
2
1
ppm
3.30
3.48
17.72
13.85
13.38
19.22
29.05

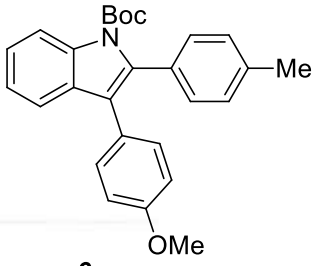

Name:
collected on:
i-NMR-DELL.vscht.cz-mercury300
e directory:
directory:
e: CARBON
equence: CARBON (s2pul)
: cdcl3
llected on: Oct 14 2016
Boc
N
O
P
O
OPh
OPh
F
F
5j
Agilent Technolo
139.613
138.834
138.743
138.452
138.345
126.635
126.605
126.559
125.399
123.994
119.658
119.597
117.383
115.780
115.704
115.658
115.536
115.429
115.383
115.215
108.161
108.070
85.229
77.397
76.985
76.557
28.052
163.904
163.690
160.637
160.423
150.224
150.117
140.652
137.537
137.491
136.559
136.422
135.827
131.323
131.231
131.124
220
200
180
160
140
120
100
80
60
40
20
0
ppm


ollected on:
-NMR-DELL.vscht.cz-mercury300
e directory:
directory:
e: PROTON
equence: PROTON (s2pul)
: cdcl3
llected on: Mar 9 2017
8.068
8.037
7.354
7.228
7.201
7.143
7.117
7.084
7.076
6.978
6.955
6.951
6.752
3.930
3.829
3.811
3.737
1.683
8
7
6
5
4
3
2
1
ppm
2.58
10.71
7.95
12.76
5.94
16.49
18.62
24.95

Boc
N
O
OPh
P
O
OPh
MeO
OMe
MeO
OMe

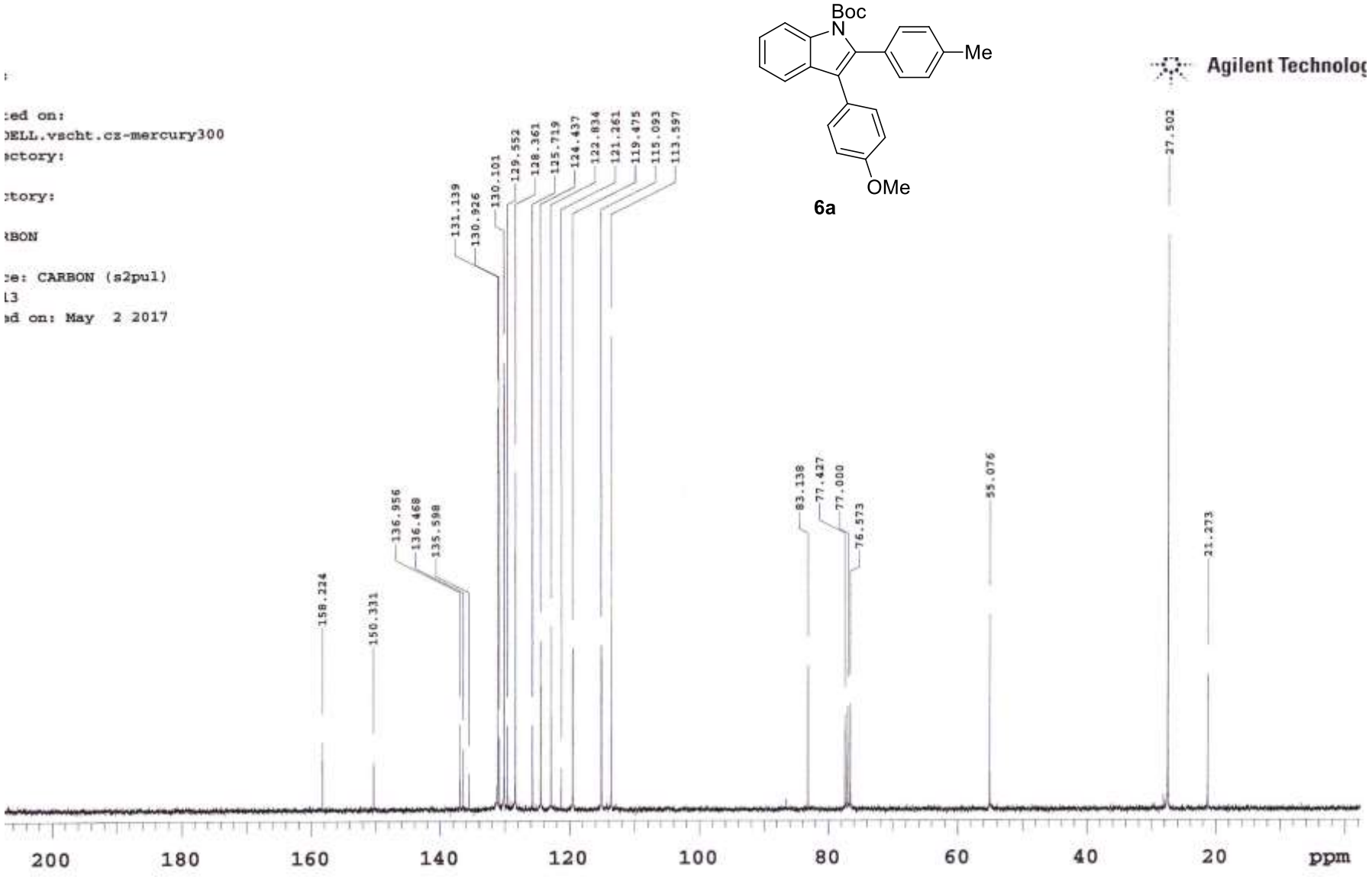
5k

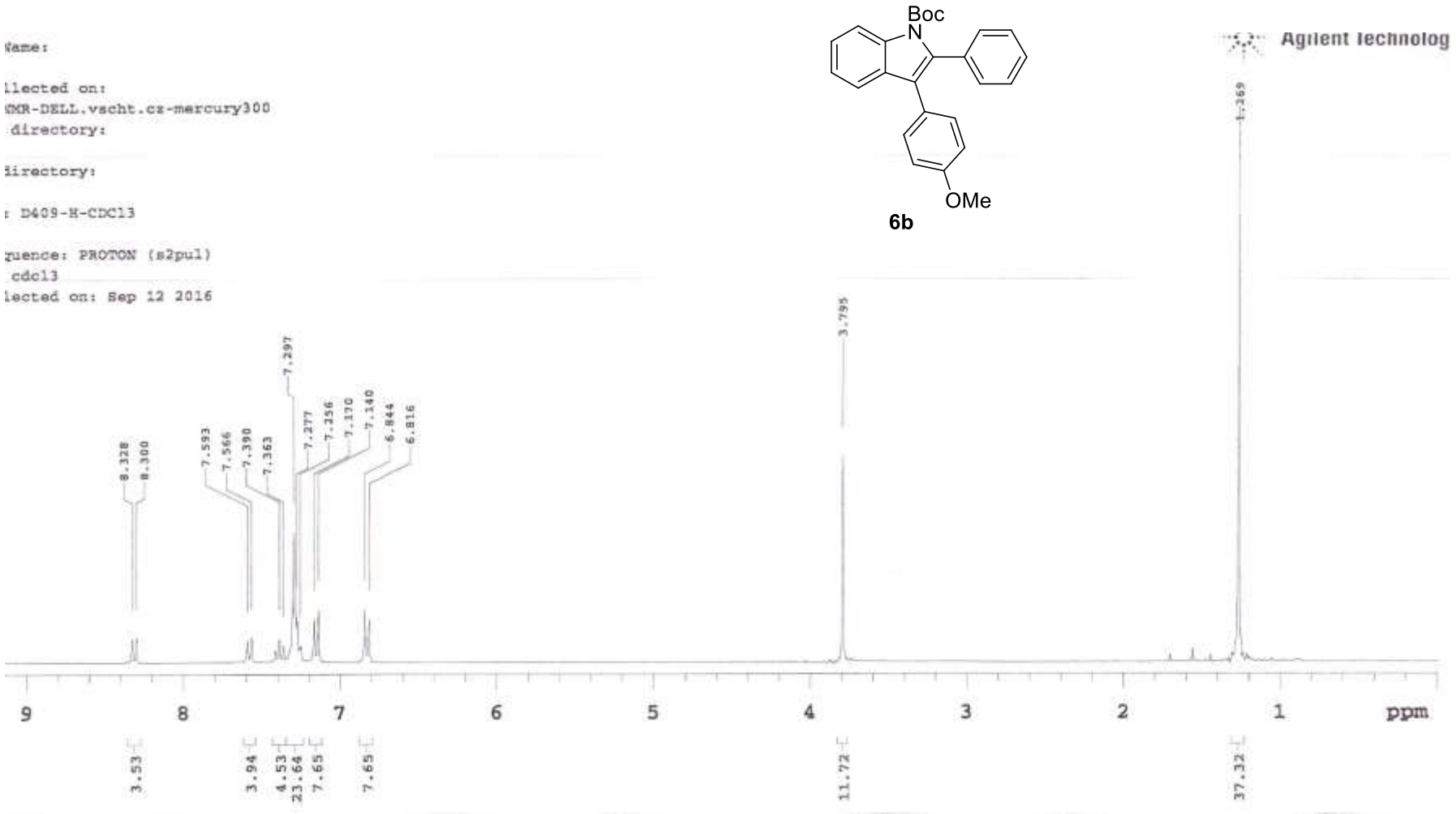

ed on:
ELL.vscht.cz-mercury300
ctory:
tory:
7-C-CDCl3
e: CARBON (s2pul)
3
d on: Mar 9 2017
Boc
N
O
OPh
P
O
OPh
MeO
OMe
MeO
OMe
5k
129.506
126.956
126.910
126.406
126.254
126.223
125.292
119.565
119.490
156.224
153.186
150.239
150.148
148.713
137.216
136.285
136.147
116.208
112.910
108.849
108.757
106.574
104.558
102.314
84.032
77.427
77.000
76.573
60.740
56.205
55.946
55.579
28.021
200
180
160
140
120
100
80
60
40
20
ppm

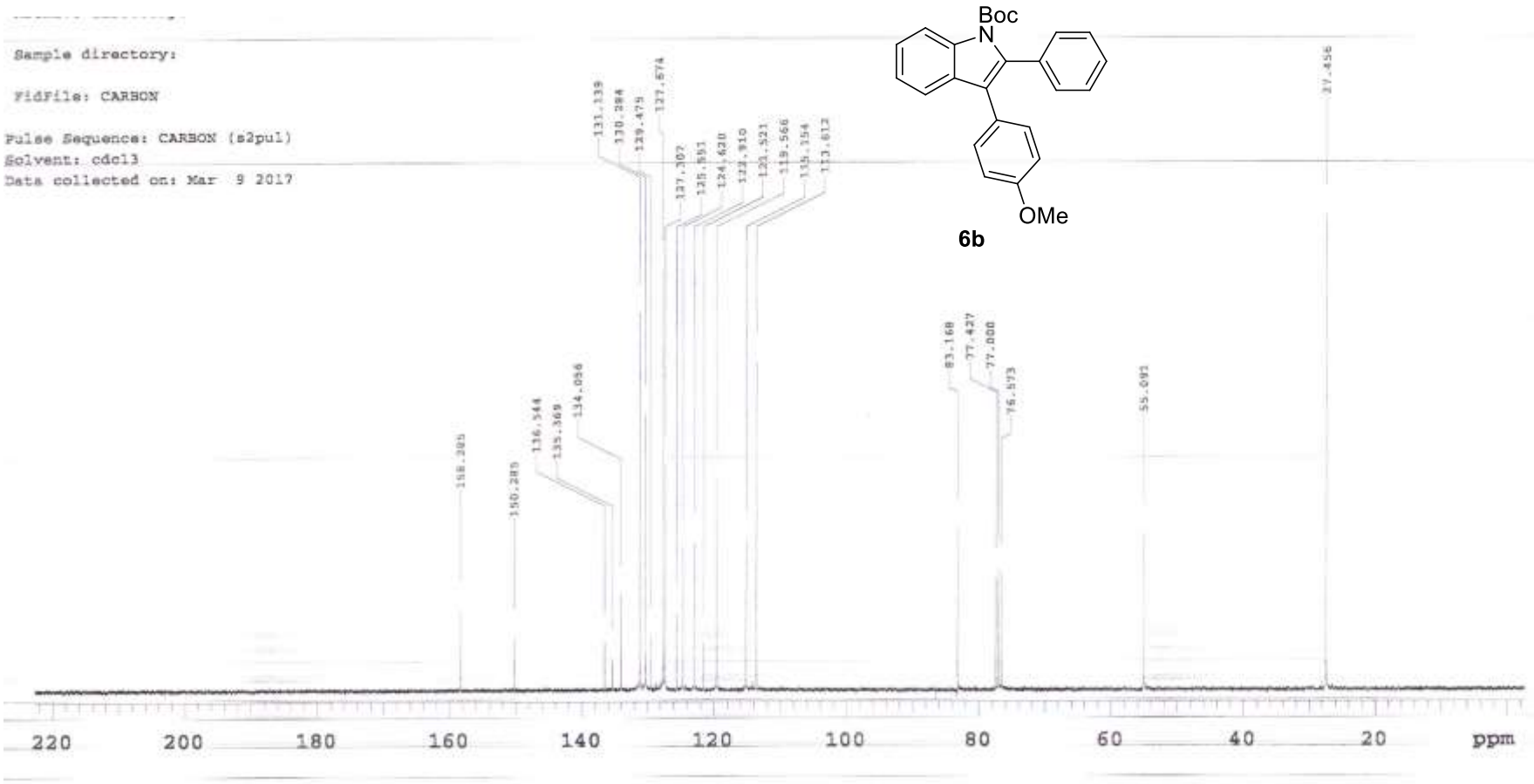

Boc
N
Me
OMe

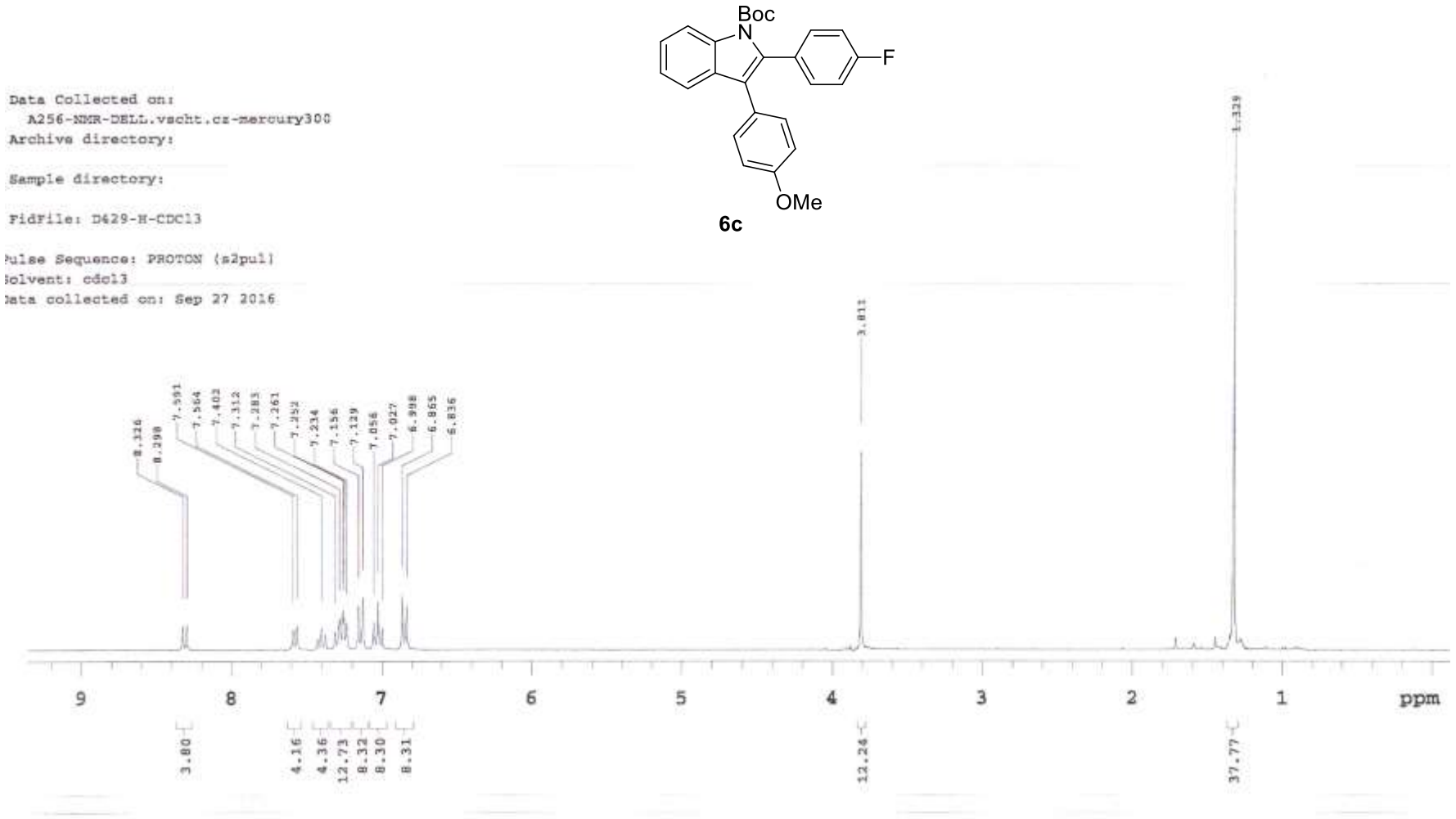
6a

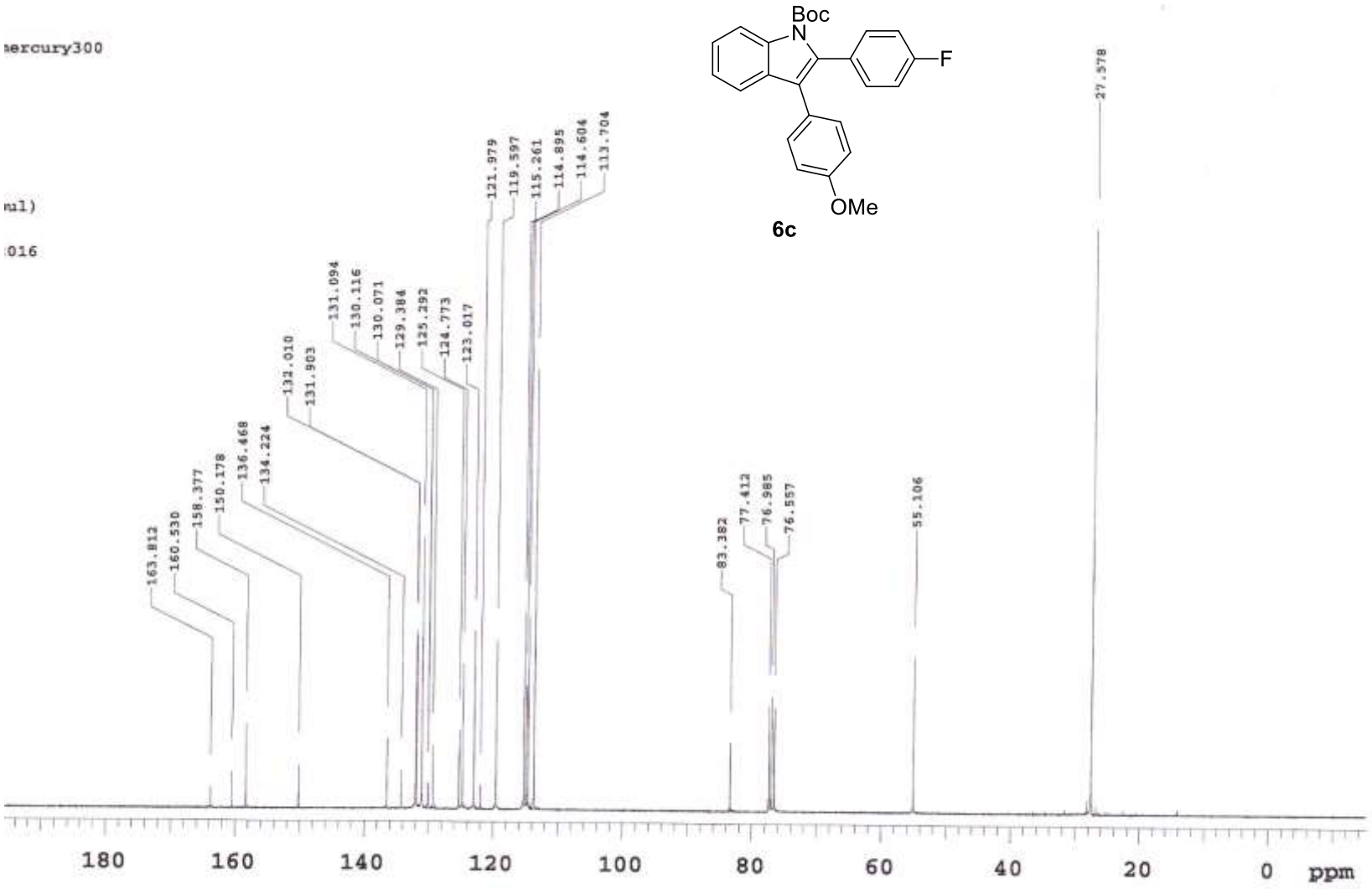
Agilent Technolog
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: D399a-H-CDCl3
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 7 2016
8.283
8.255
7.568
7.545
7.365
7.342
7.283
7.258
7.170
7.140
7.117
7.090
6.844
6.838
6.822
6.814
3.797
2.360
1.554
1.290
1.259
9
8
7
6
5
4
3
2
1
ppm
3.07
3.18
3.58
4.68
21.23
7.56
11.08
11.06
34.56

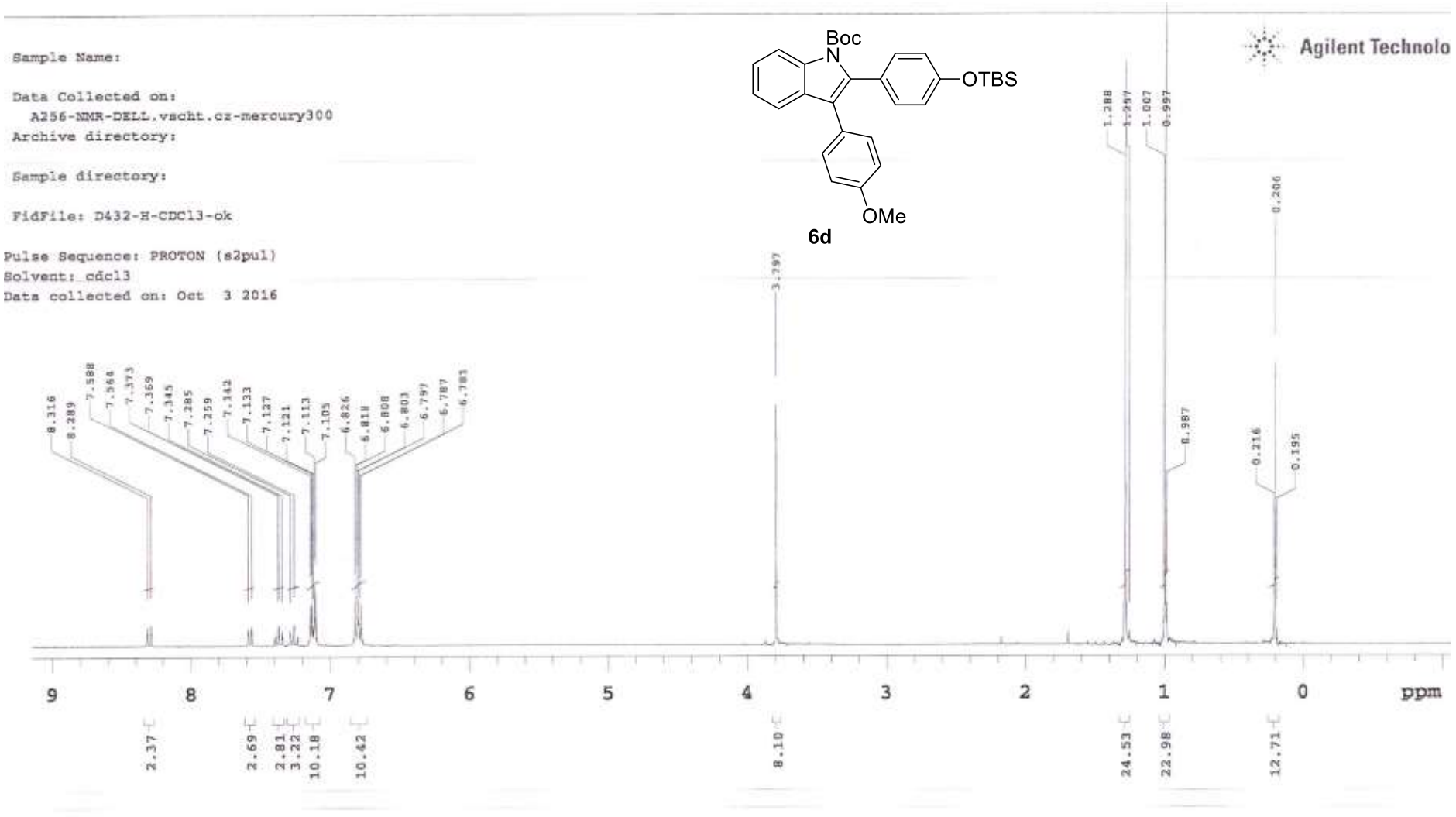

Boc
N
Me
OMe
6a
Agilent Technolog
ced on:
DELL.vscht.cz-mercury300
ectory:
tory:
RBON
ce: CARBON (s2pul)
13
ed on: May 2 2017
158.224
150.331
136.956
136.468
135.598
131.139
130.926
130.101
129.552
128.361
125.719
124.437
122.834
121.261
119.475
115.093
113.597
83.138
77.427
77.000
76.573
55.076
27.502
21.273
200
180
160
140
120
100
80
60
40
20
ppm

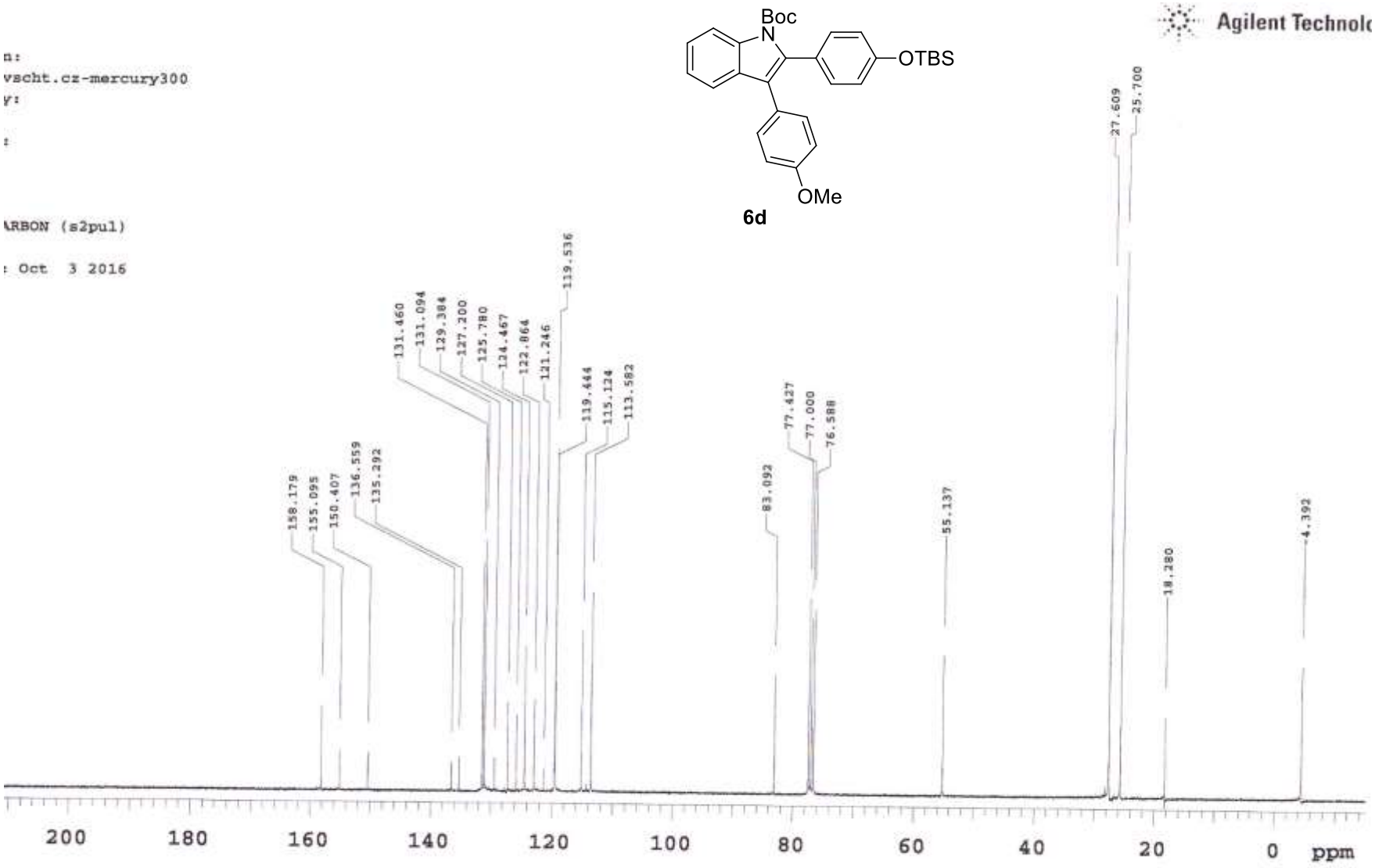

Boc
N
OMe
6b
Agilent Technolog
Name:
llected on:
MR-DELL.vscht.cz-mercury300
directory:
irectory:
: D409-H-CDCl3
quence: PROTON (s2pul)
cdcl3
lected on: Sep 12 2016
8.328
8.300
7.593
7.566
7.390
7.363
7.297
7.277
7.256
7.170
7.140
6.844
6.816
3.795
1.269
9
8
7
6
5
4
3
2
1
ppm
3.53
3.94
4.53
23.64
7.65
7.65
11.72
37.32

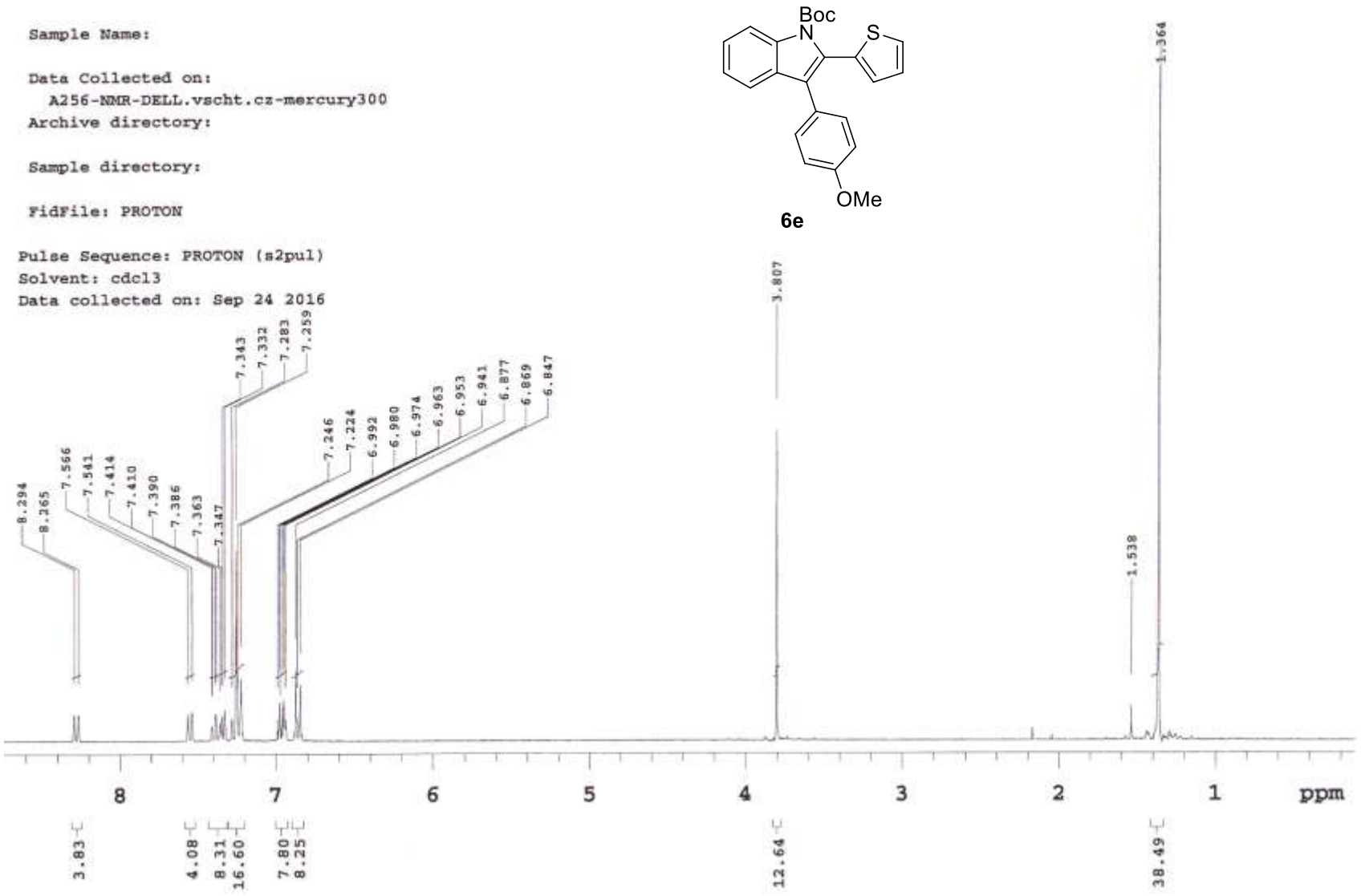

Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 9 2017
Boc
N
OMe
6b
158.285
150.285
136.544
135.369
134.056
131.139
130.284
129.479
127.674
127.307
125.551
124.620
123.930
121.521
119.566
115.154
113.612
83.168
77.427
77.000
76.573
55.691
27.456
220
200
180
160
140
120
100
80
60
40
20
ppm

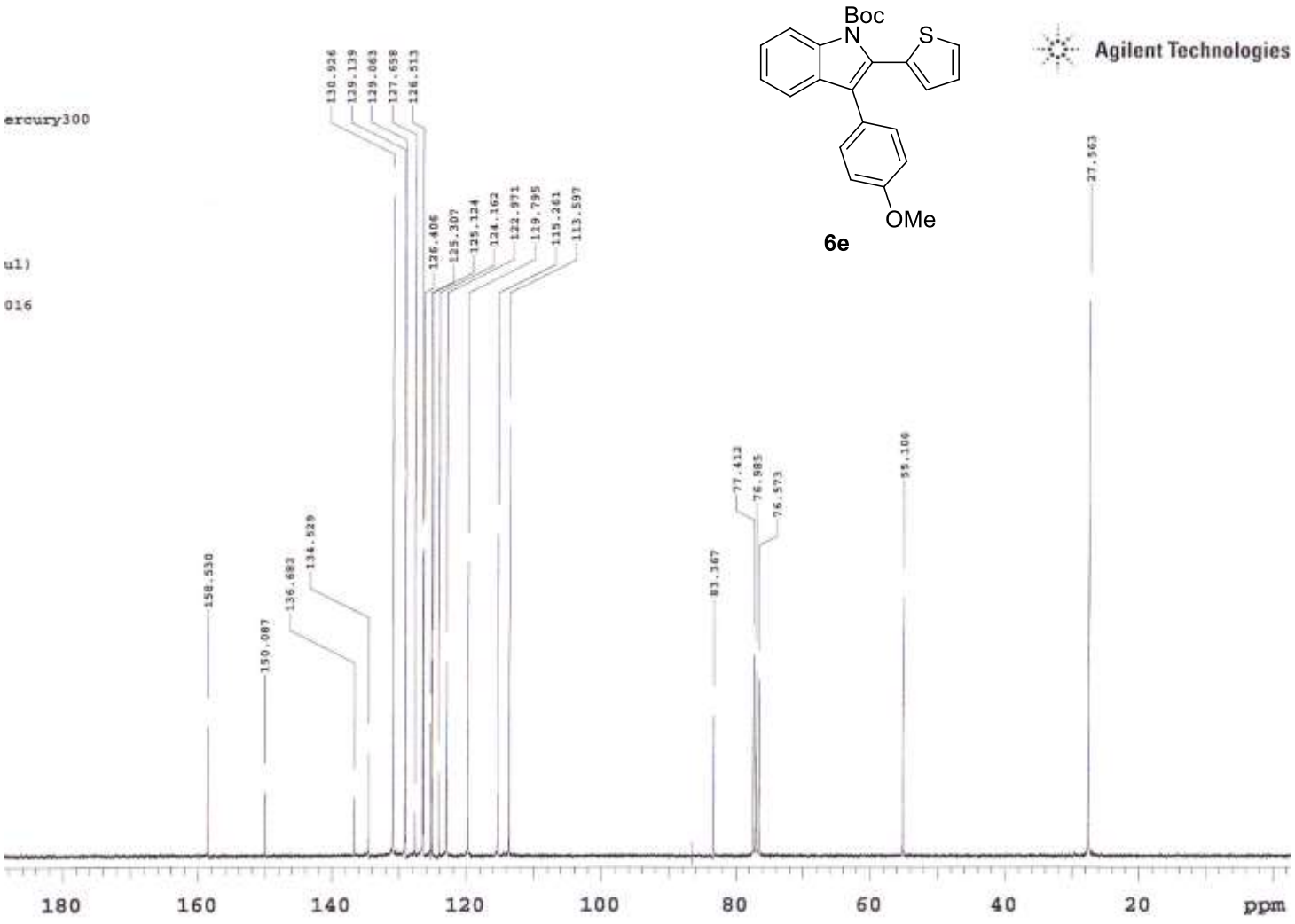

Boc
N
F
OMe
6c
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: D429-H-CDCl3
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 27 2016
8.326
8.298
7.591
7.564
7.402
7.312
7.283
7.261
7.252
7.234
7.156
7.139
7.056
7.027
6.998
6.865
6.836
3.811
1.329
9
8
7
6
5
4
3
2
1
ppm
3.80
4.16
4.36
12.73
8.32
8.30
8.31
12.24
37.77

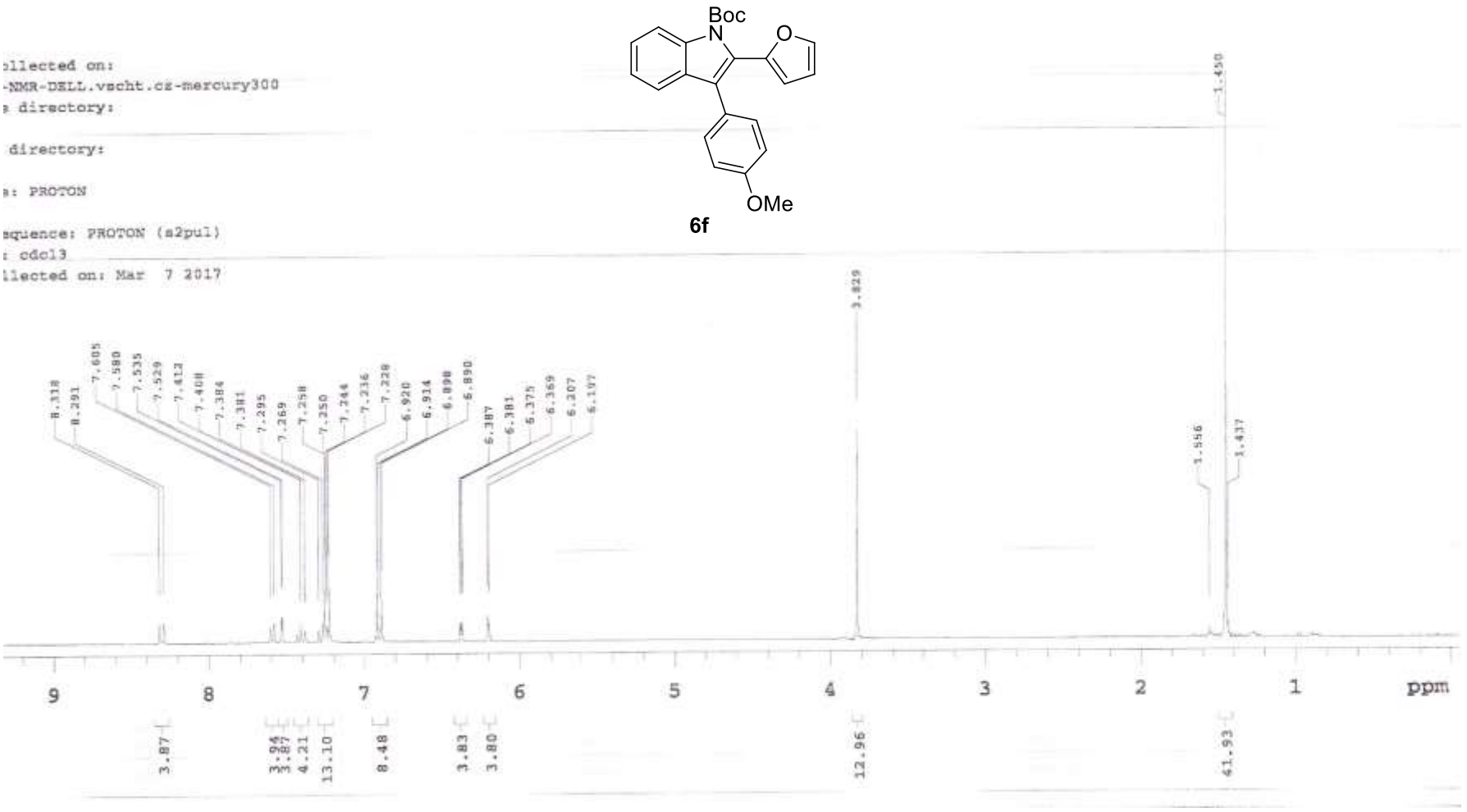

ercury300
ul)
016
Boc
N
F
OMe
6c
163.812
160.530
158.377
150.178
136.468
134.224
132.010
131.903
131.094
130.116
130.071
129.384
125.292
124.773
123.017
121.979
119.597
115.261
114.895
114.604
113.704
83.382
77.412
76.985
76.557
55.106
27.578
180
160
140
120
100
80
60
40
20
0
ppm

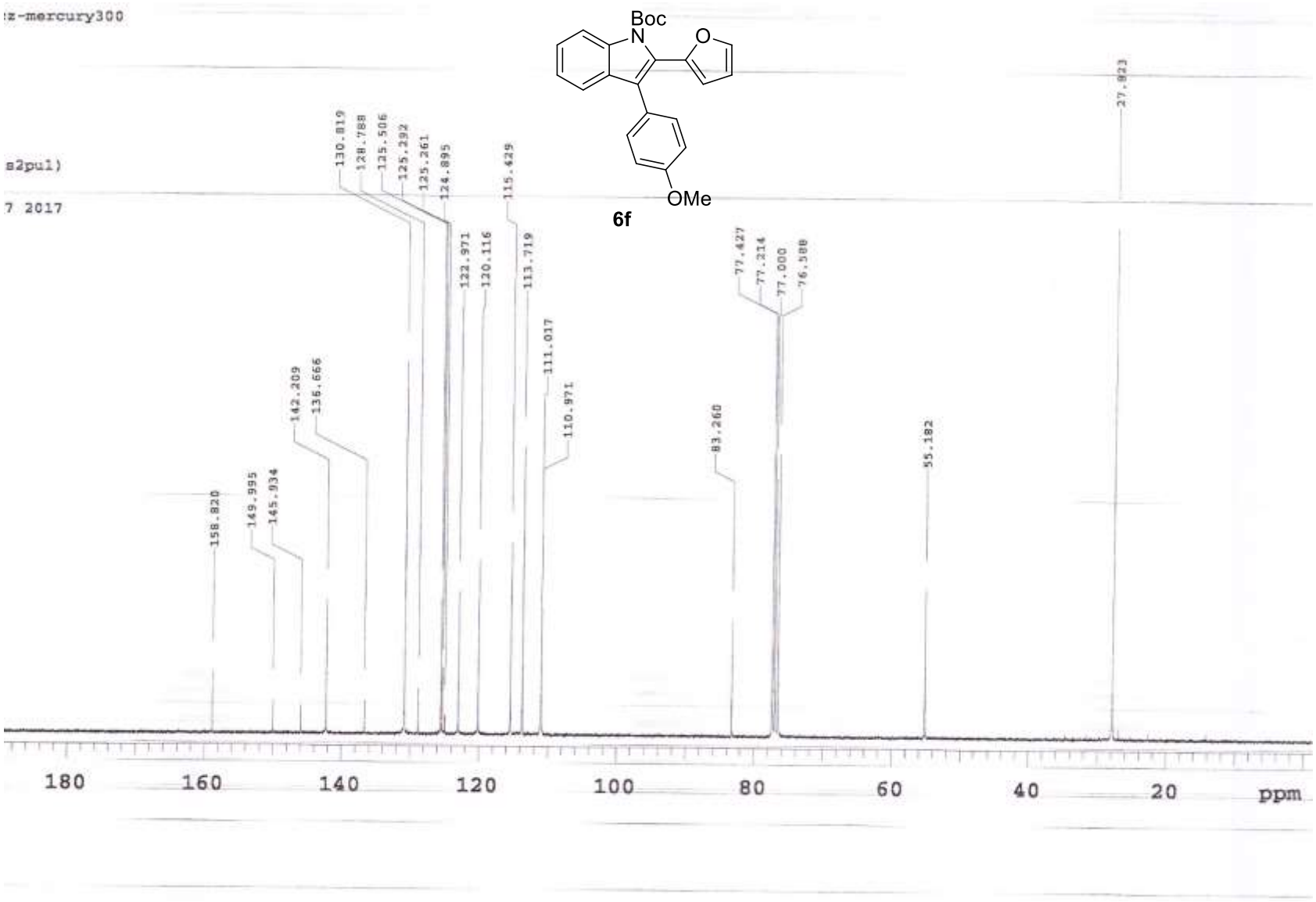

Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: D432-H-CDCl3-ok
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 3 2016
Boc
N
OTBS
OMe
6d
Agilent Technolo
8.316
8.289
7.588
7.564
7.373
7.369
7.345
7.285
7.259
7.142
7.133
7.127
7.121
7.113
7.105
6.826
6.818
6.808
6.803
6.797
6.787
6.781
3.797
1.288
1.257
1.007
0.997
0.987
0.316
0.206
0.195
9
8
7
6
5
4
3
2
1
0
ppm
2.37
2.69
2.81
3.22
10.18
10.42
8.10
24.53
22.98
12.71

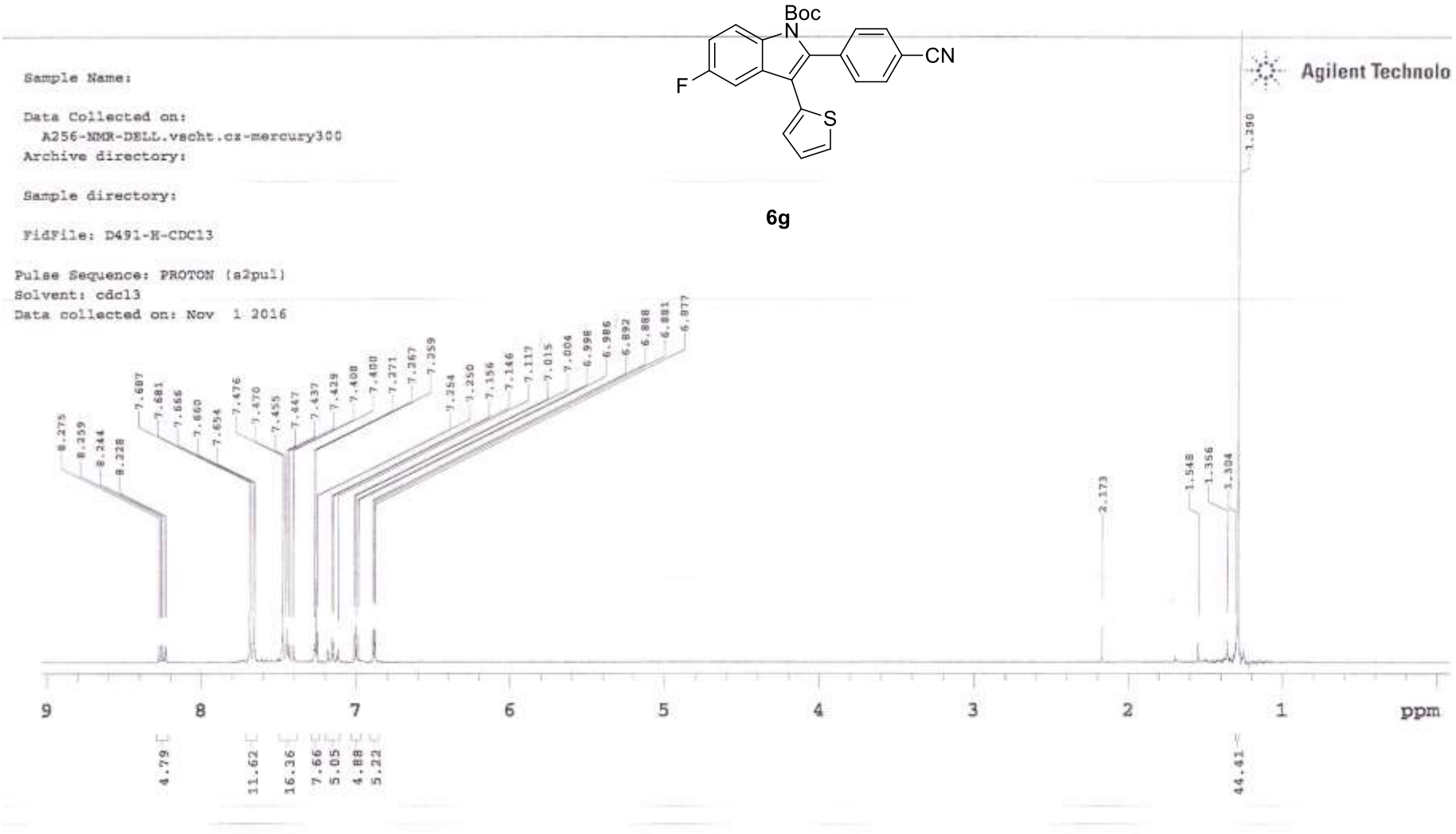

Boc
N
OTBS
OMe
6d
Agilent Technol
vscht.cz-mercury300
ARBON (s2pul)
Oct 3 2016
158.179
155.095
150.407
136.559
135.292
131.460
131.094
129.384
127.200
125.780
124.467
122.864
121.246
119.536
119.444
115.124
113.582
83.092
77.427
77.000
76.588
55.137
27.609
25.700
18.280
-4.392
200
180
160
140
120
100
80
60
40
20
0
ppm

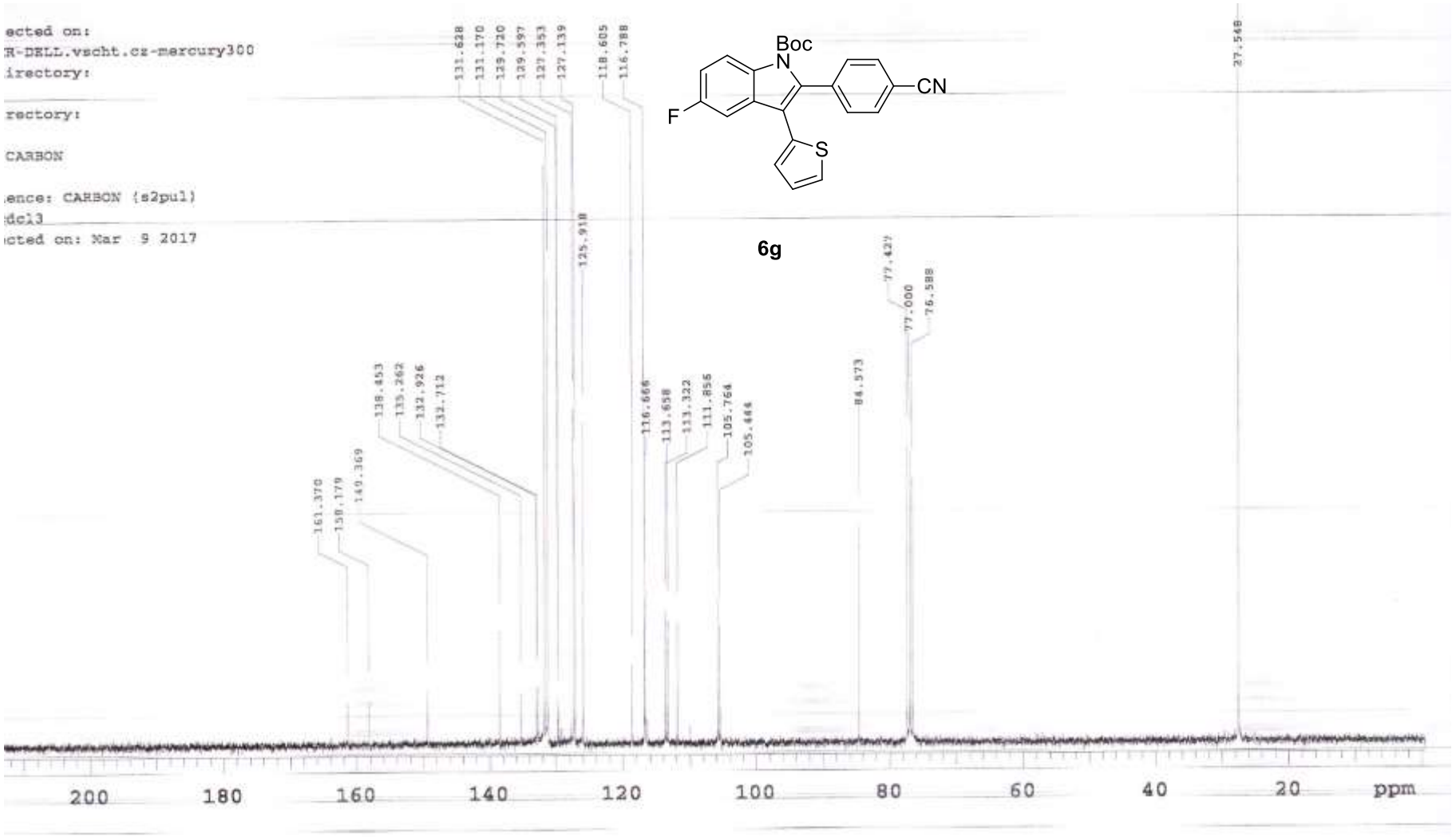

Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 24 2016
Boc
N
S
OMe
6e
8.294
8.265
7.566
7.541
7.414
7.410
7.390
7.386
7.363
7.347
7.343
7.332
7.283
7.259
7.246
7.224
6.992
6.980
6.974
6.963
6.953
6.941
6.877
6.869
6.847
3.807
1.538
1.364
8
7
6
5
4
3
2
1
ppm
3.83
4.08
8.31
16.60
7.80
8.25
12.64
38.49

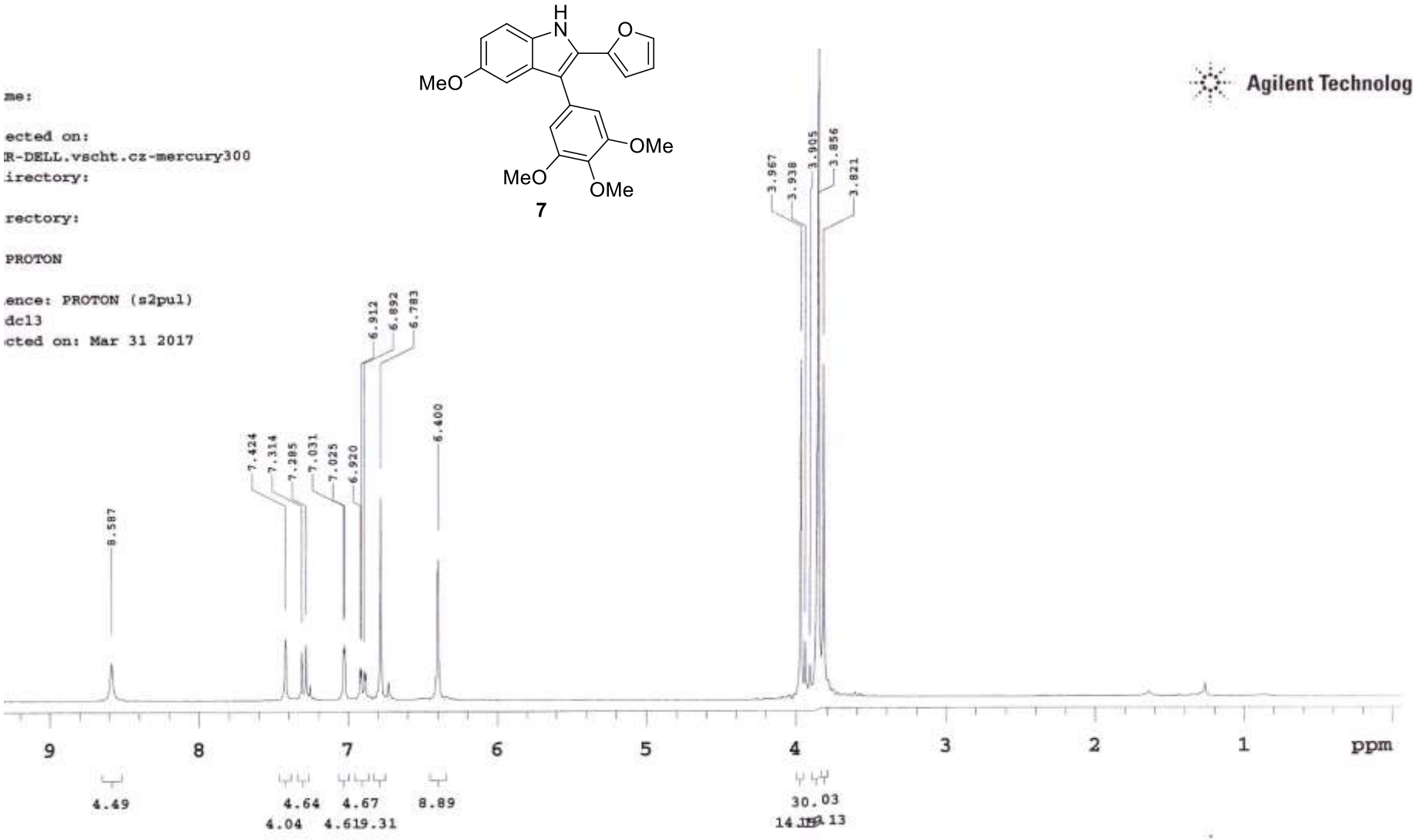

Boc
N
S
OMe
6e
Agilent Technologies
ercury300
u1)
016
130.926
129.139
129.063
127.658
126.513
126.406
125.307
125.124
124.162
122.971
119.795
115.261
113.597
158.530
150.087
136.682
134.529
83.367
77.413
76.985
76.573
55.306
27.563
180
160
140
120
100
80
60
40
20
ppm

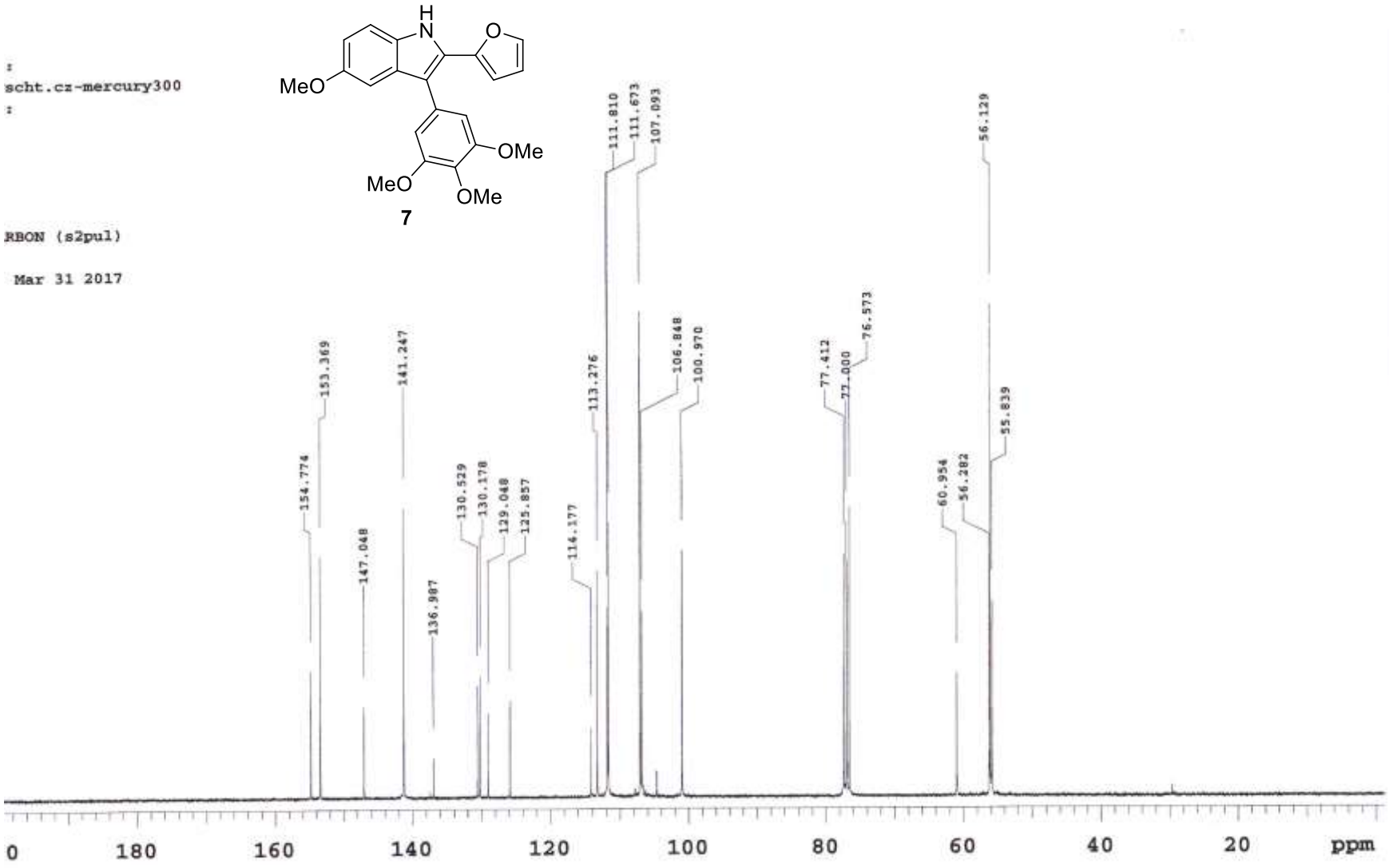

Boc
N
O
OMe
6f
llected on:
-NMR-DELL.vscht.cz-mercury300
directory:
directory:
: PROTON
equence: PROTON (s2pul)
: cdcl3
llected on: Mar 7 2017
8.318
8.291
7.605
7.580
7.535
7.529
7.413
7.408
7.384
7.381
7.295
7.269
7.258
7.250
7.244
7.236
7.228
6.920
6.914
6.898
6.890
6.387
6.381
6.375
6.369
6.207
6.197
3.829
3.556
1.450
1.437
9
8
7
6
5
4
3
2
1
ppm
3.87
3.94
3.87
4.21
13.10
8.48
3.83
3.80
12.96
41.93


z-mercury300
s2pul)
7 2017
Boc
N
O
OMe
6f
158.820
149.995
145.934
142.209
136.666
130.819
128.788
125.506
125.392
125.261
124.895
122.971
120.116
115.429
113.719
111.017
110.971
83.260
77.427
77.214
77.000
76.588
55.182
27.823
180
160
140
120
100
80
60
40
20
ppm


Boc
N
CN
F
S
6g
Sample Name:
Data Collected on:
A256-NMR-DELL.vscht.cz-mercury300
Archive directory:
Sample directory:
FidFile: D491-H-CDCl3
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 1 2016
Agilent Technolo
8.275
8.259
8.244
8.228
7.687
7.681
7.656
7.660
7.654
7.476
7.470
7.455
7.447
7.437
7.429
7.408
7.400
7.271
7.267
7.259
7.254
7.250
7.156
7.146
7.117
7.015
7.004
6.998
6.986
6.892
6.888
6.881
6.877
2.173
1.548
1.356
1.304
1.290
9
8
7
6
5
4
3
2
1
ppm
4.79
11.62
16.36
7.66
5.05
4.88
5.22
44.41


ected on:
R-DELL.vscht.cz-mercury300
irectory:
rectory:
CARBON
ence: CARBON (s2pul)
dcl3
cted on: Mar 9 2017
131.628
131.170
129.730
129.597
127.353
127.139
125.918
118.605
116.788
27.548
Boc
N
CN
F
S
6g
77.421
77.000
76.588
161.370
158.179
149.369
138.453
135.262
132.926
132.712
116.666
113.658
113.322
111.855
105.764
105.444
84.573
200
180
160
140
120
100
80
60
40
20
ppm


me:
ected on:
R-DELL.vscht.cz-mercury300
irectory:
rectory:
PROTON
ence: PROTON (s2pul)
dcl3
cted on: Mar 31 2017
MeO
OMe
MeO
OMe
7
Agilent Technolog
8.587
7.424
7.314
7.285
7.031
7.025
6.920
6.912
6.892
6.783
6.400
3.967
3.938
3.905
3.856
3.821
9
8
7
6
5
4
3
2
1
ppm
4.49
4.64
4.04
4.67
4.61
9.31
8.89
30.03
14.13


:
scht.cz-mercury300
:
RBON (s2pul)
Mar 31 2017
MeO
H
N
O
OMe
MeO
OMe
7
154.774
153.369
147.048
141.247
136.987
130.529
130.178
129.048
125.857
114.177
113.276
111.810
111.673
107.093
106.848
100.970
77.412
77.000
76.573
60.954
56.282
56.129
55.839
0
180
160
140
120
100
80
60
40
20
ppm