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

Supporting Information

Total Synthesis of Agalloside, Isolated from *Aquilaria agallocha,* by the 5-*O*-Glycosylation of Flavan

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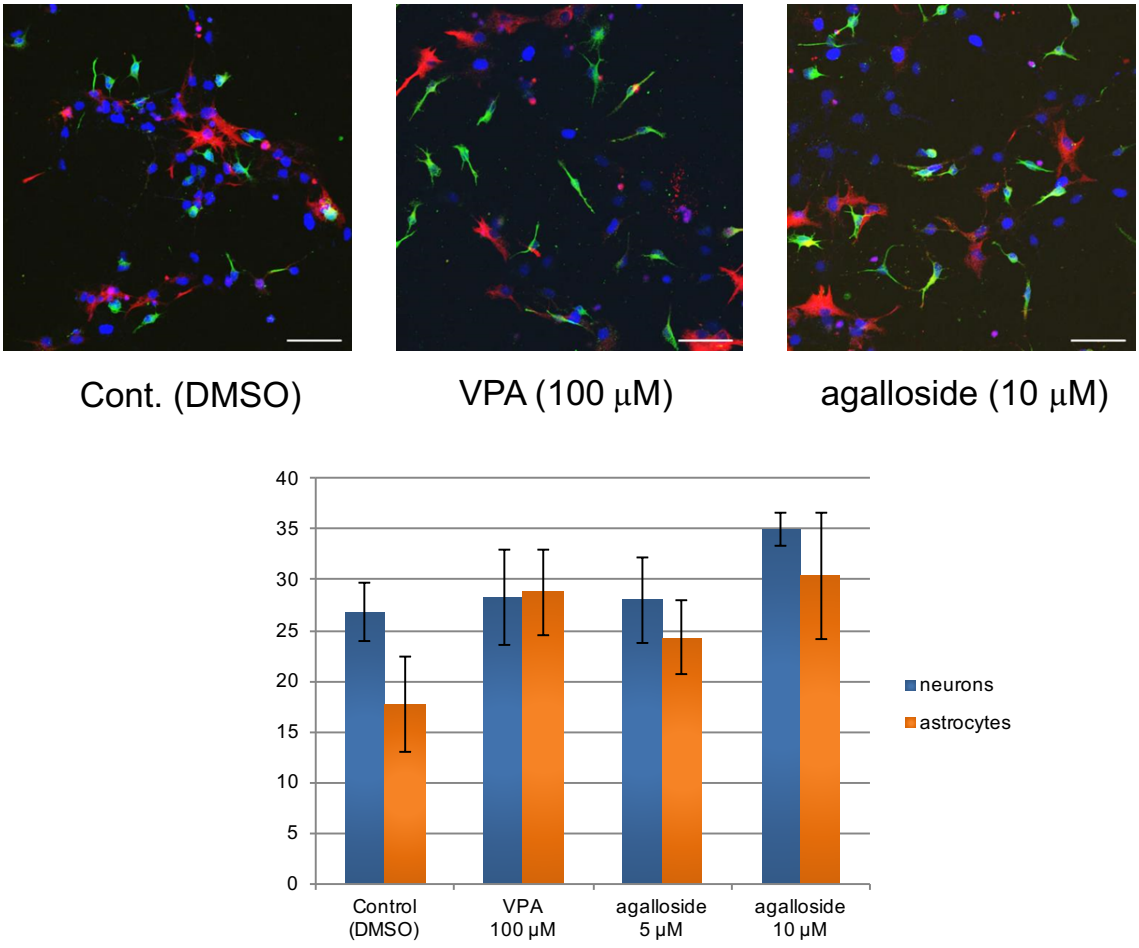
Contents

Neural stem cell differentiation assay. MEB5 cells were dissociated using the NeuroCult Chemical Dissociation Kit and seeded at a density of 2×10^4 cells/well on cover glass (MATSUNAMI GLASS) coated with poly-L-lysine and fibronectin/laminin. After incubation for 12 hrs, cells were washed with NeuroCult Basal Medium (Mouse) and treated with individual compounds in differentiation medium for 4 days.

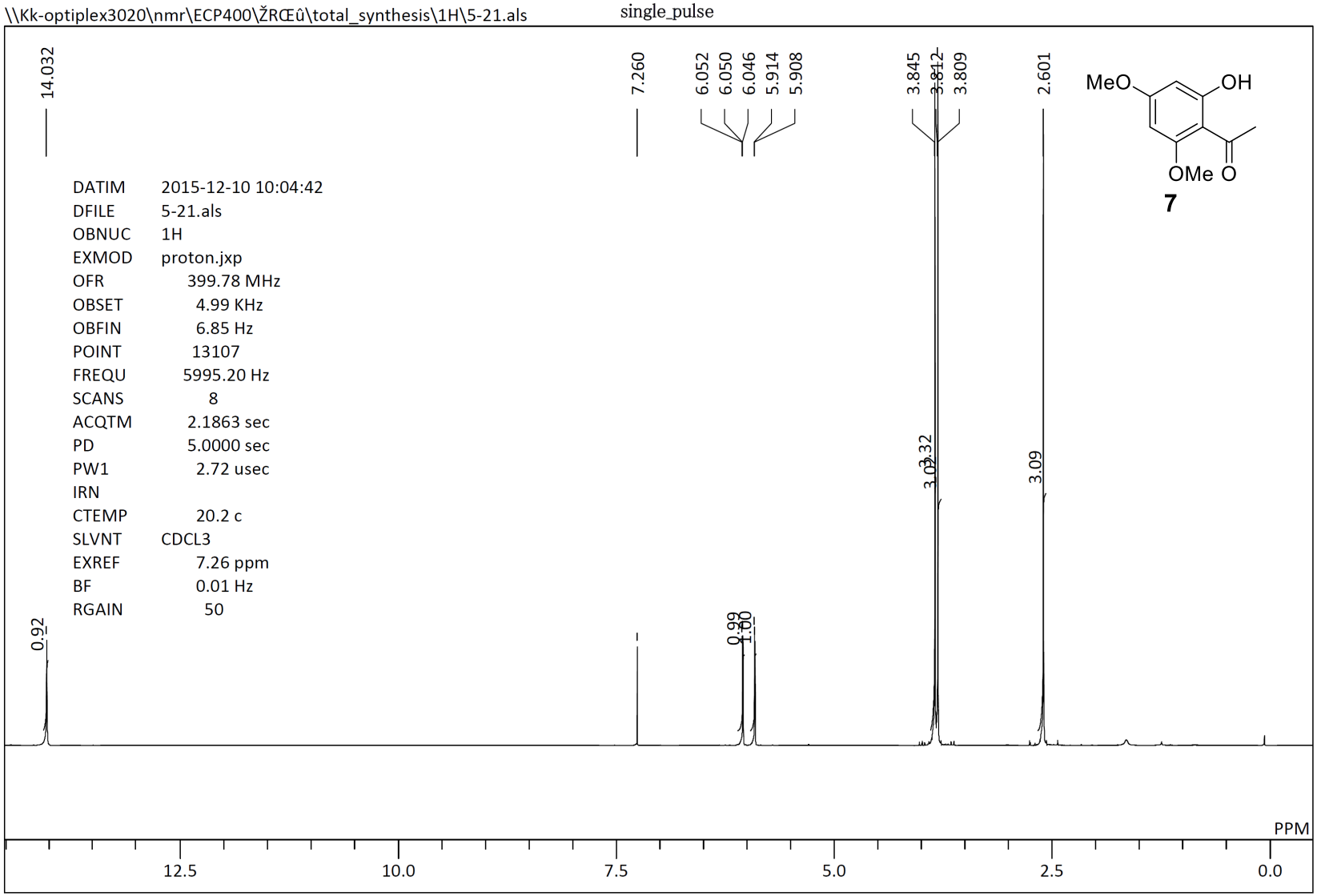
Immunofluorescence staining. After incubation for 4 days, cells were fixed with 4% paraformaldehyde in PBS for 20 min at room temperature (r.t.) and washed with 1% BSA (Merck) in PBS two times. Cells were blocked in 10% BSA in 0.3% Triton X-100 (Wako) in PBS for 45 min at r.t. and incubated with primary antibodies (0.5 mg/mL anti-βIII-Tubulin; Neuronal Class III, Mouse-Mono, 1:400, R&D Systems™; anti-GFAP, 1:400, VERITAS) for 12 hrs at 4 °C. After washing three times with 1% BSA in PBS (500 μL/well), cells were incubated with secondary antibodies (Alexa Fluor® 488 goat anti-mouse IgG (H+L), 1:400, Life Technologies; Alexa Fluor® 555 goat ant-rabbit IgG (H+L), 1:200, Life Technologies) for 1 hr at r.t. in the dark. After washing three times with 1% BSA in PBS (500 μL/well), cells were treated with 200 μg/mL RNase (Nacalai Tesque) in PBS containing 1% BSA and 0.1% Triton X-100 for 1 hr at 37 °C in the dark. After washing three times with 500 μL/well PBS, cells were incubated in 30 μM TO-PRO®-3, 1% BSA, and 0.1% Triton X-100 in PBS for 10 min at r.t. in the dark. The cover glass on which the cells were attached was transferred onto slide glass and mounted with ProLong® Gold Antifade Reagent with DAPI (Invitrogen). Slide glasses were viewed and photographed with an LSM 700 (Carl Zeiss). Four pictures were taken per well, and the assays were carried out with three individual wells per condition.



SP-Figure 1. Effect of **1** on neural stem cells (MEB5) differentiation. MEB5 cells were treated with DMSO, VPA (varproic acid, positive control, 100 μM), or synthesized agalloside (**1**) (5 or 10 μM) for 4 days. Then, cells were fixed and immunostained with Tuj-1 (green) for neurons, GFAP (red) for astrocytes, and TO-PRO-3 (blue) for nuclei.

Table 1 NMR data of synthetic and natural **1**.

position	^{1}H-NMR in DMSO-d_6		^{13}C-NMR in DMSO-d_6	
	synthetic **1** (600 MHz)	natural **1** (400 MHz)	synthetic **1** (150 MHz)	natural **1** (100 MHz)
2			161.0	160.9
3	6.80 (s)	6.80 (s)	106.5	106.5
4			177.0	176.9
5			158.2	158.2
6	6.87 (s)	6.87 (d, 2.0)	102.8	102.9
7			163.8	163.7
8	7.06 (s)	7.06 (d, 2.0)	96.6	96.7
9			158.6	158.5
10			109.2	109.2
1'			122.8	122.8
2'	8.04 (d, 8.7)	8.04 (d, 9.0)	128.2	128.1
3'	7.11 (d, 8.7)	7.09 (d, 9.0)	114.7	114.6
4'			162.2	162.1
5'	7.11 (d, 8.7)	7.09 (d, 9.0)	114.7	114.6
6'	8.04 (d, 8.7)	8.04 (d, 9.0)	128.2	128.1
OMe-7	3.89 (s)	3.89 (s)	56.2	56.2
OMe-4'	3.85 (s)	3.84 (s)	55.6	55.6
1"	4.79 (d, 7.8)	4.78 (d, 7.6)	103.5	103.7
2"	2.98 (m)	2.98 (m)	73.3	73.4
3"	3.09 (t, 8.4)	3.09 (t, 8.6)	76.4	76.6
4"		3.28 (t, 8.4)	69.5	69.5
5"		3.31 (m)	75.5	75.6
6"	3.64 (m)	3.65 (dd, 10.7, 4.6)	68.7	68.9
	3.97 (d, 10.8)	3.97 (d, 10.7)		
1"'	4.18 (d, 7.8)	4.18 (d, 7.6)	104.2	104.1
2"'		3.36 (m)	73.4	73.5
3"'	3.56 (t, 8.1)	3.56 (t, 8.0)	75.9	75.9
4"'		3.24 (m)	69.6	69.7
5"'		3.01 (m)	65.7	65.7
	3.68 (m)	3.68 (m)		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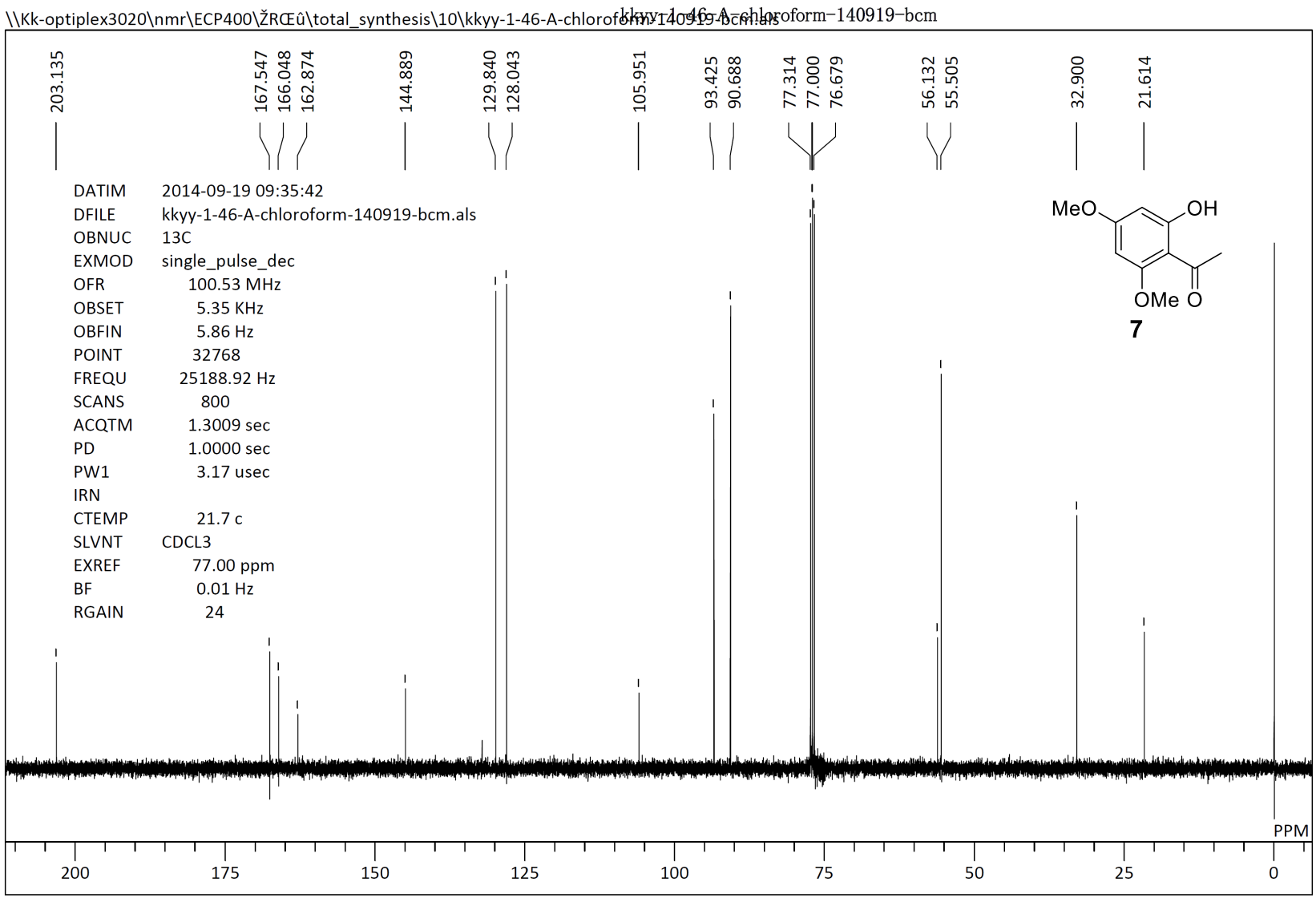
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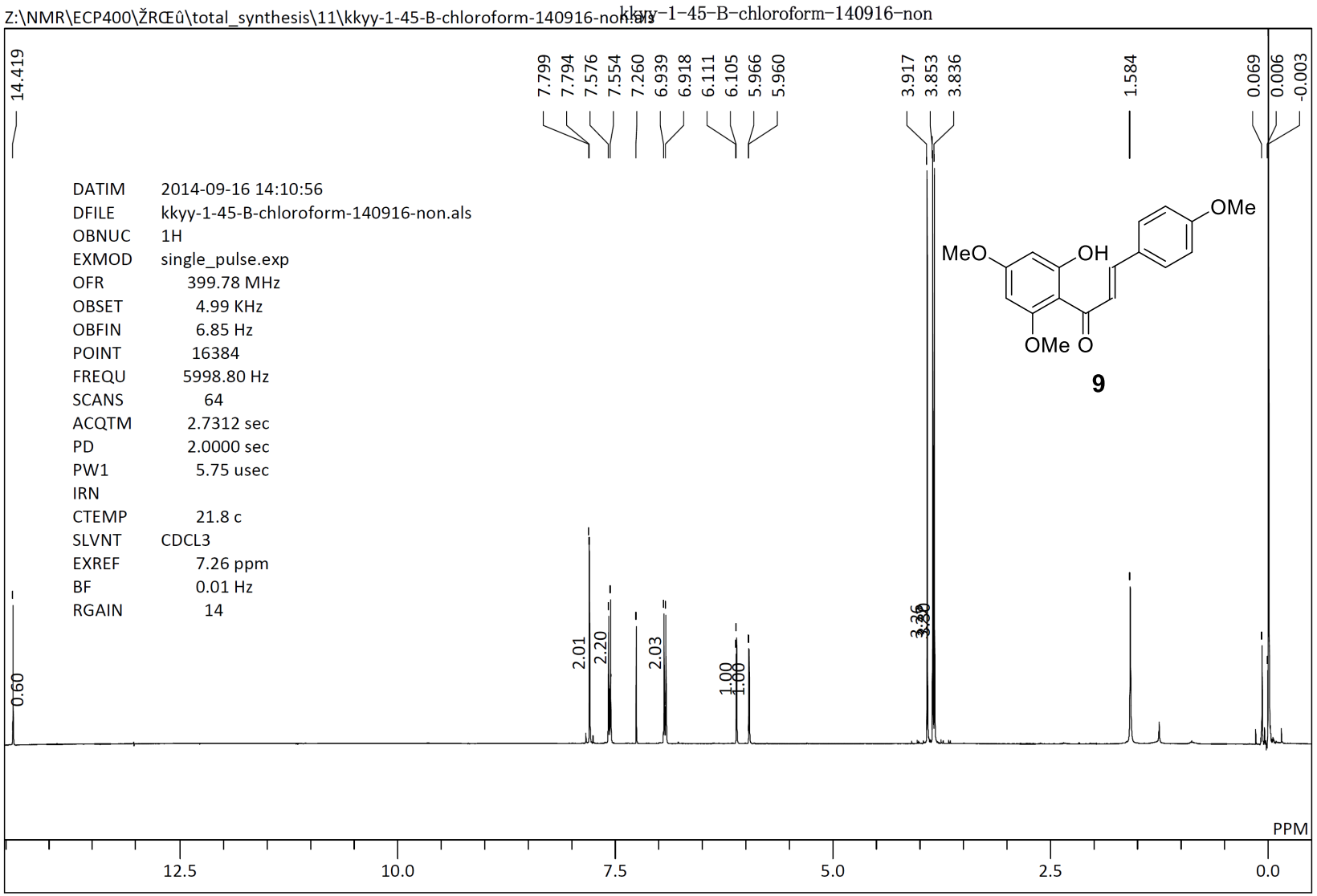
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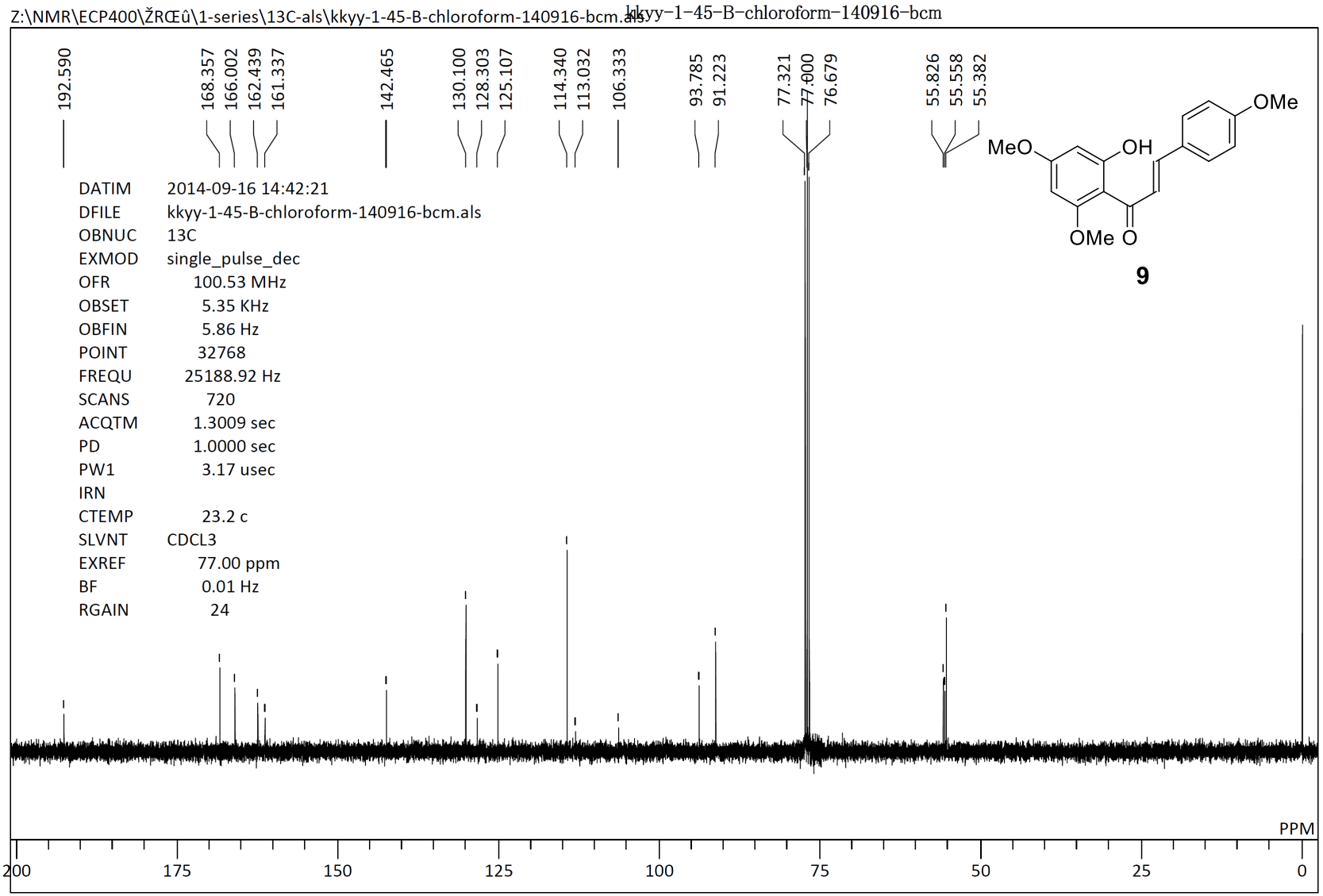
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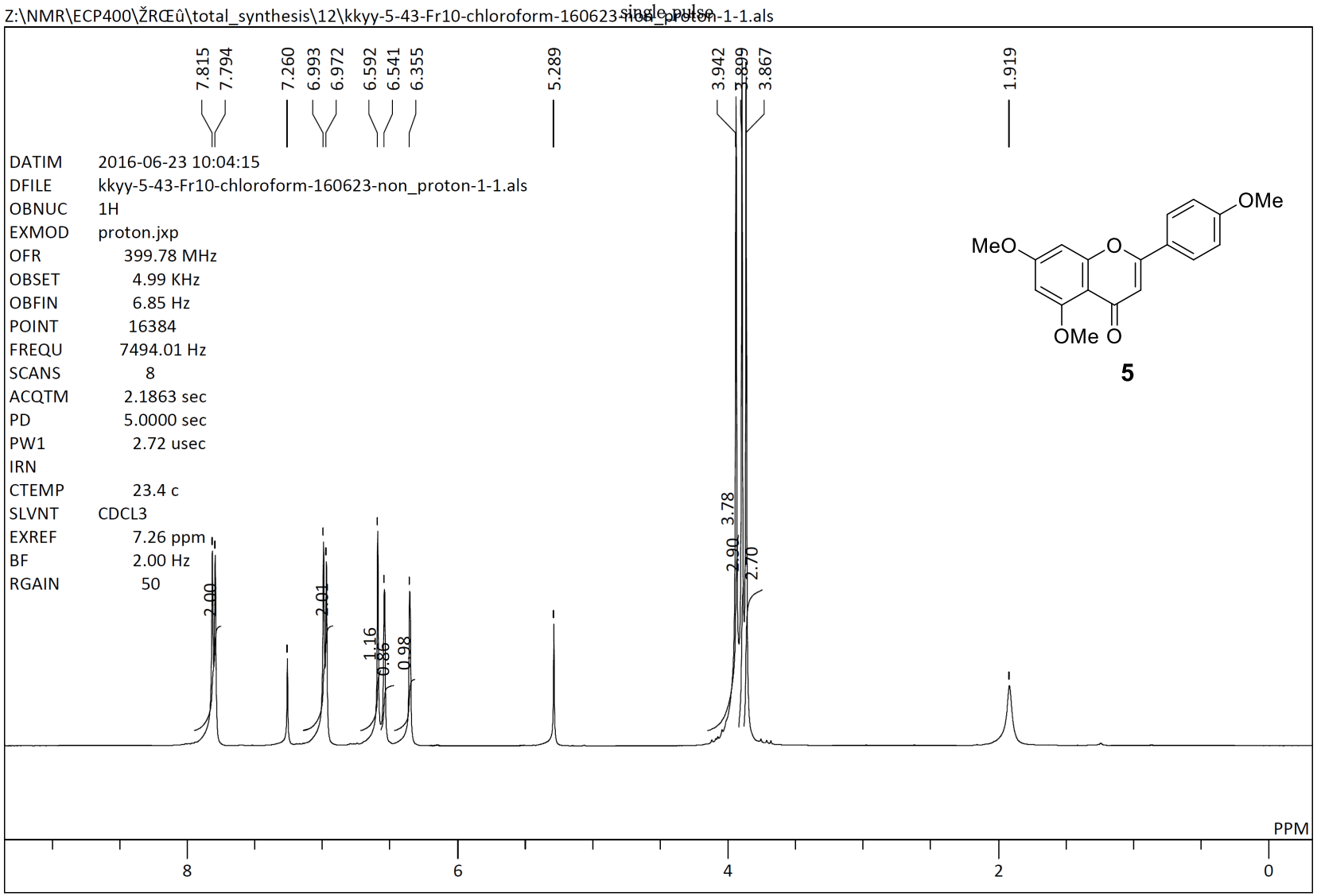
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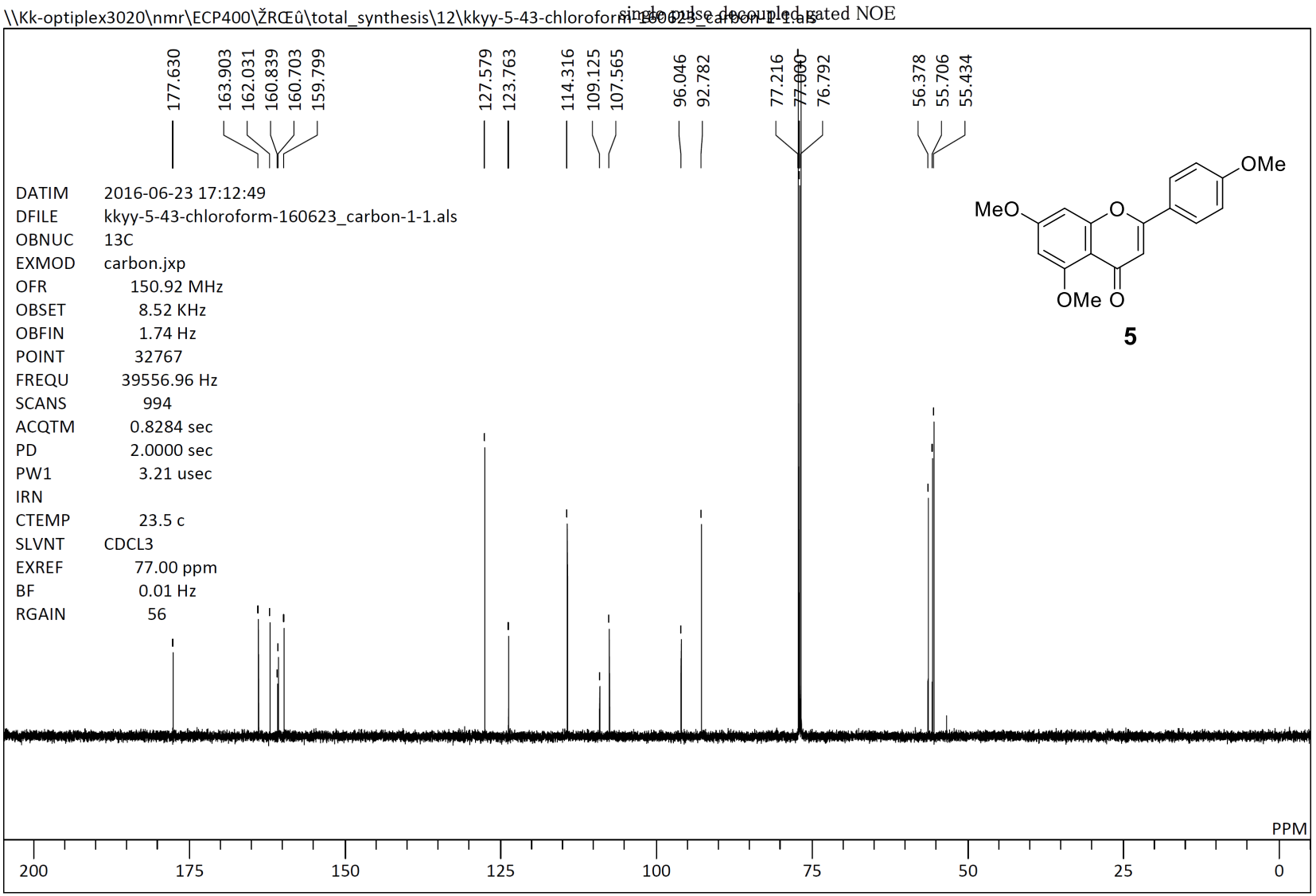
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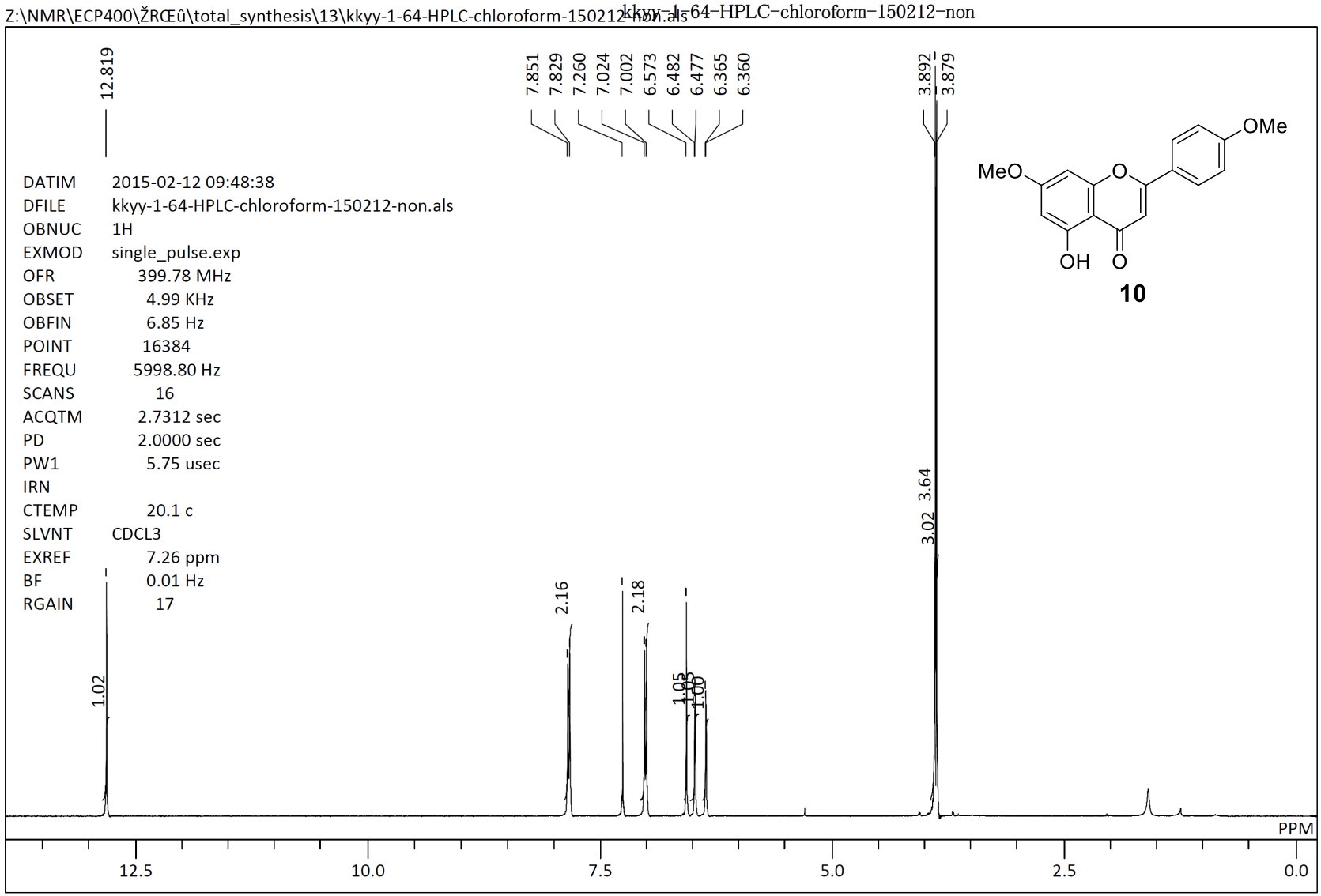
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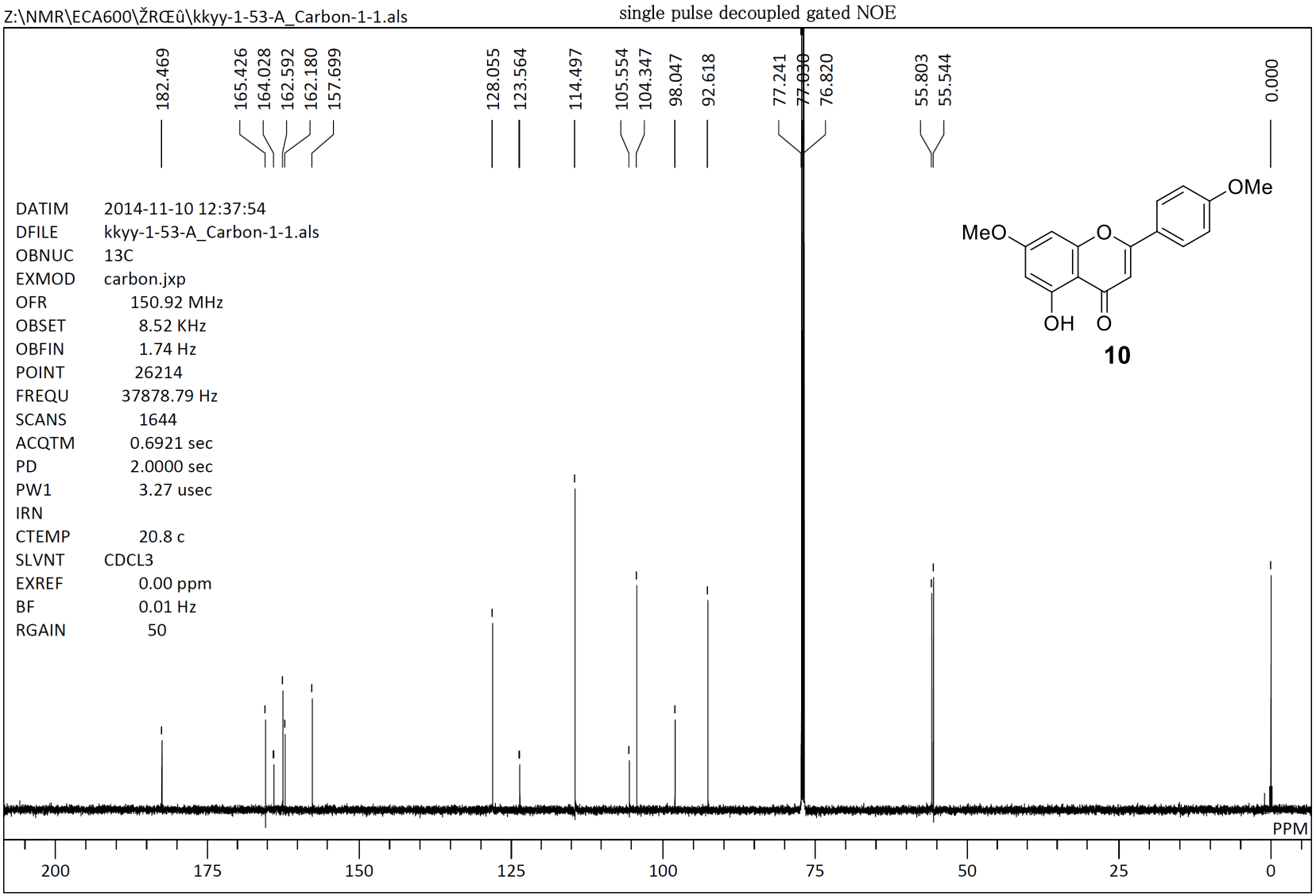
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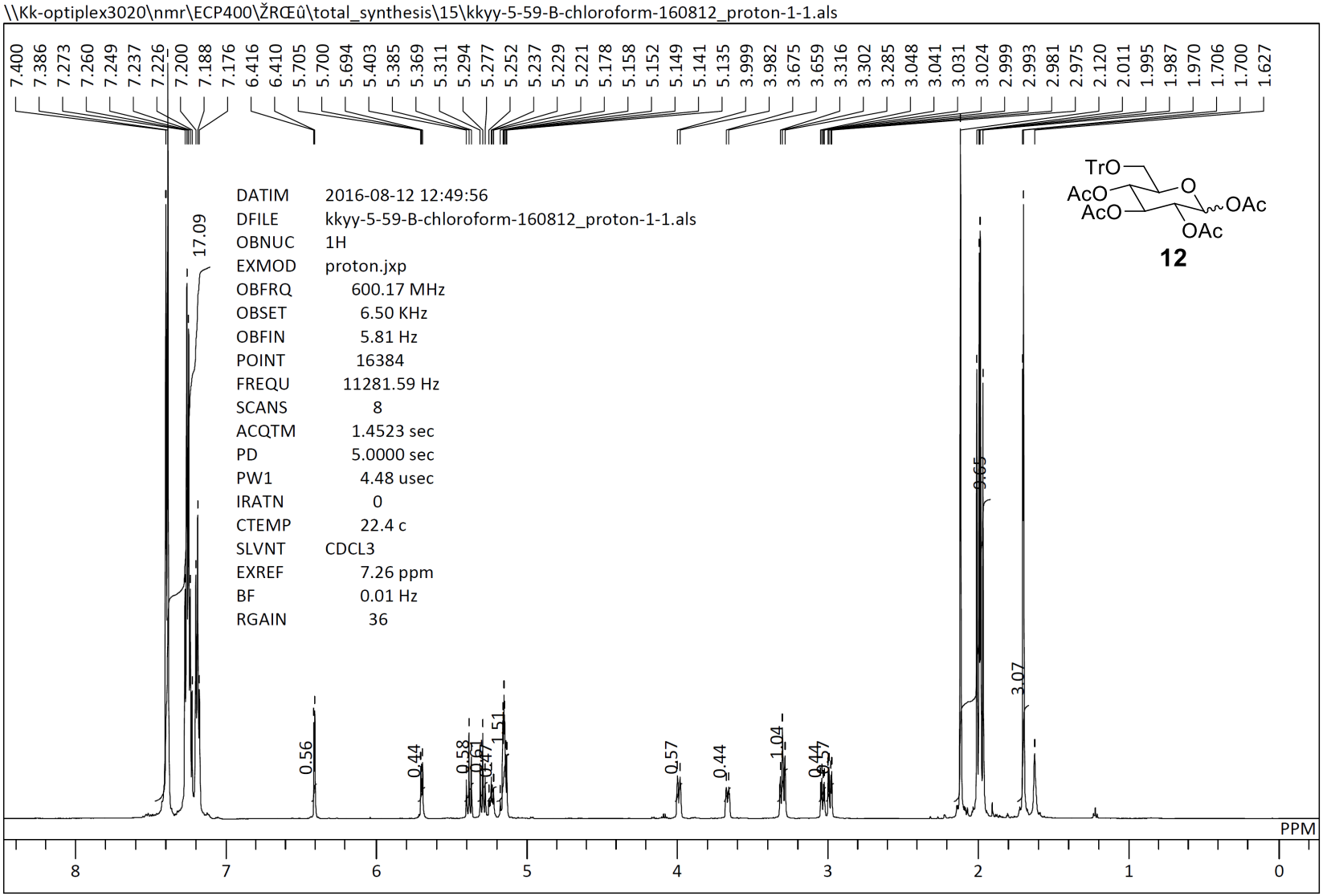
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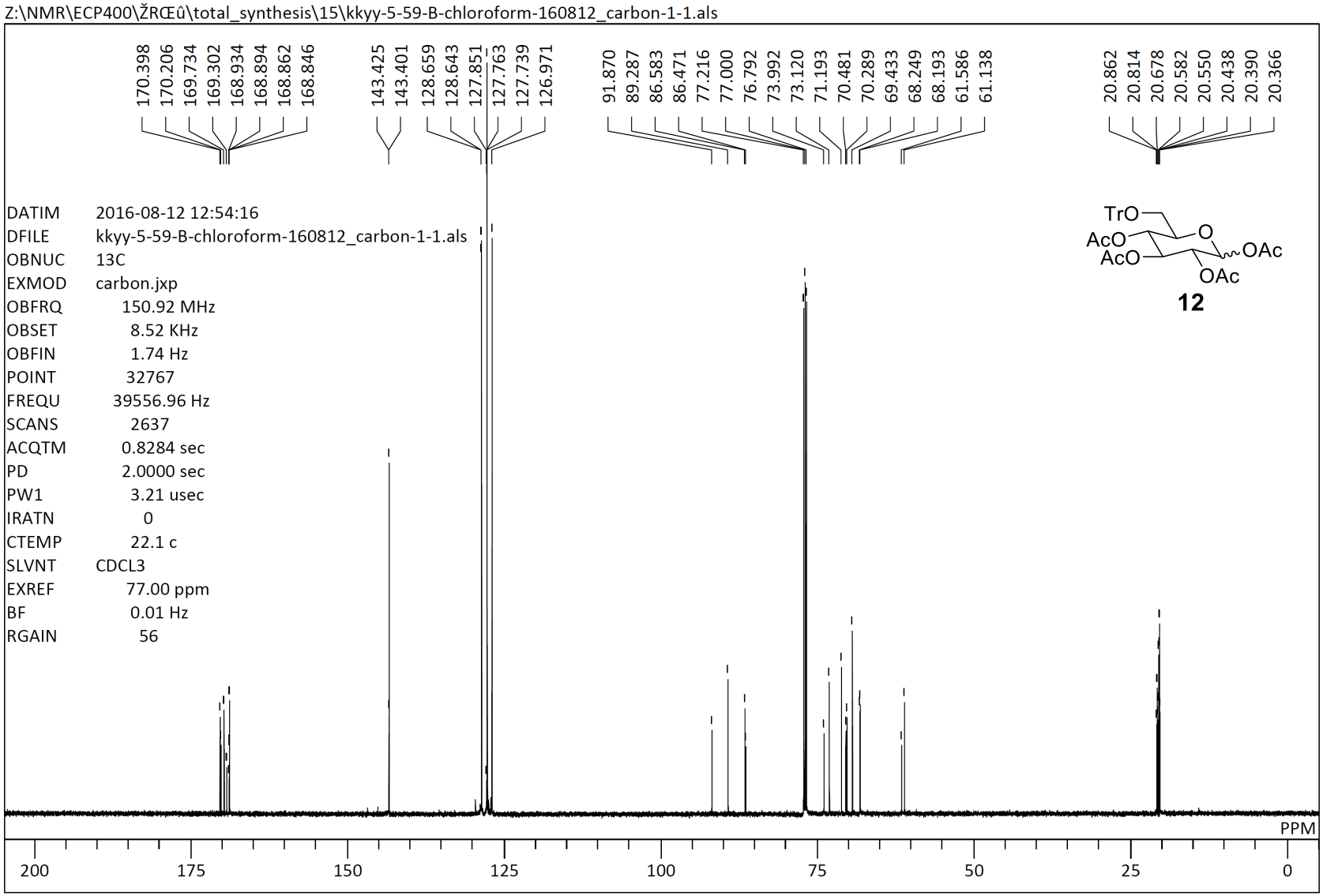
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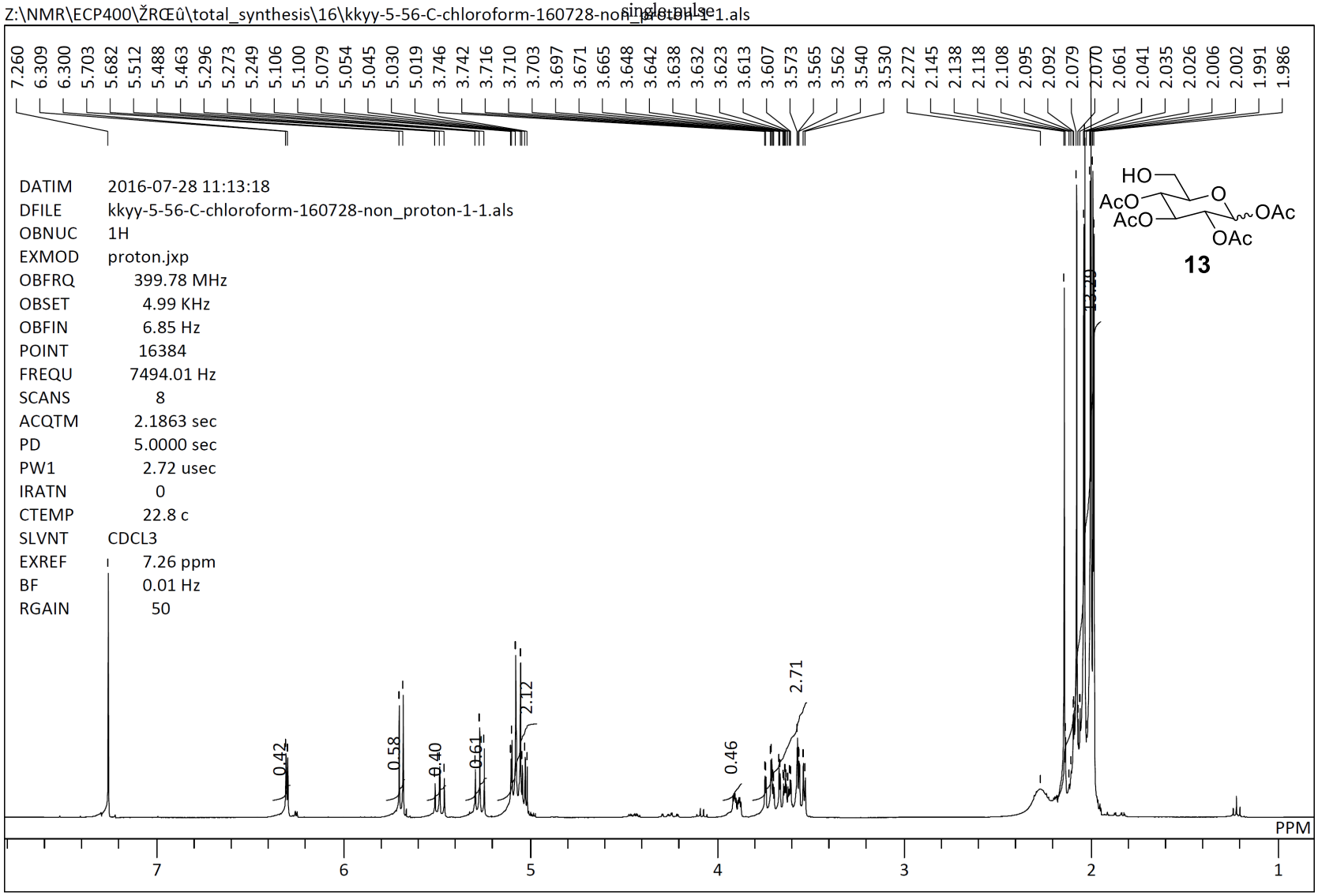
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OAc
OAc
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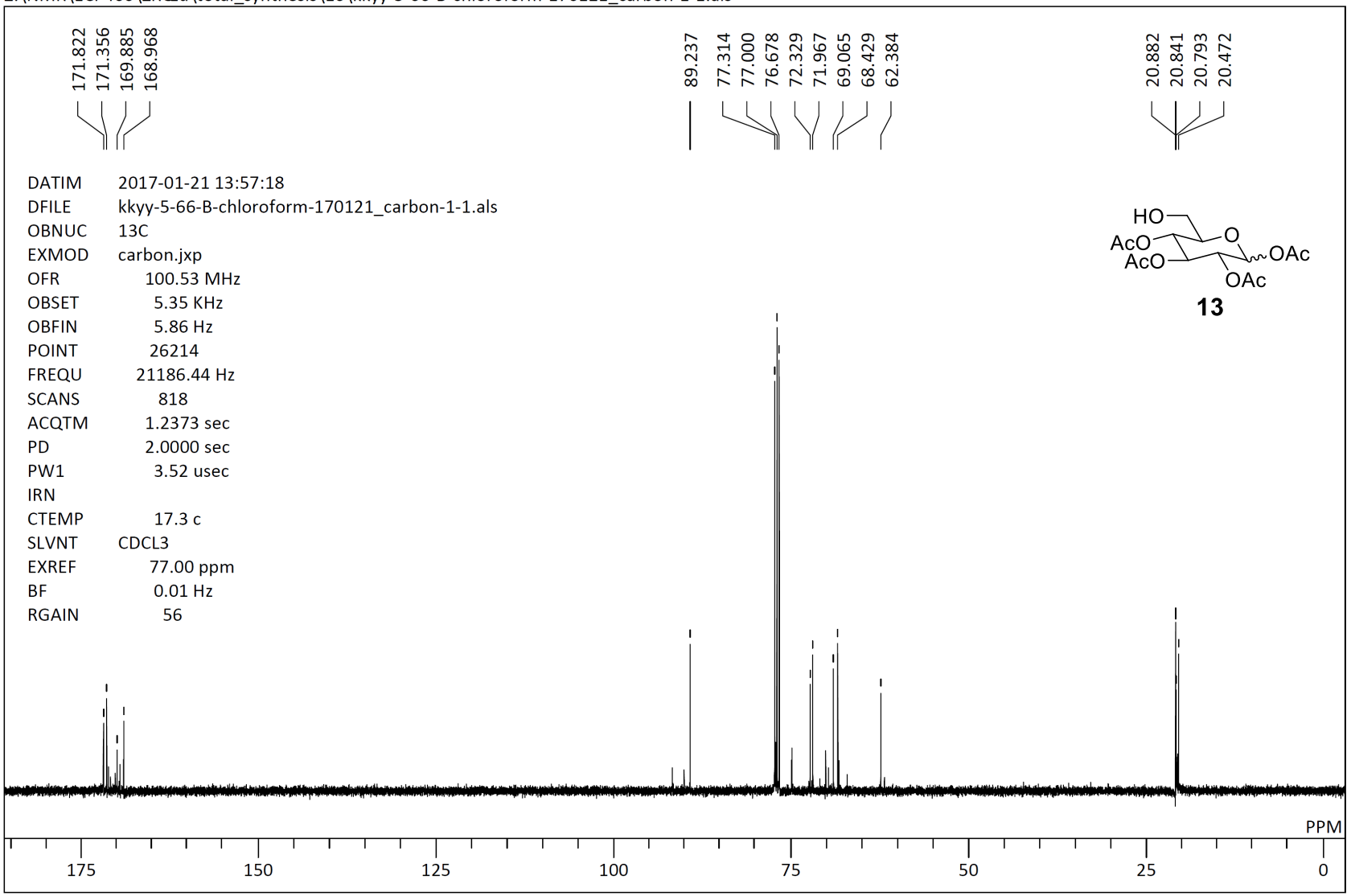

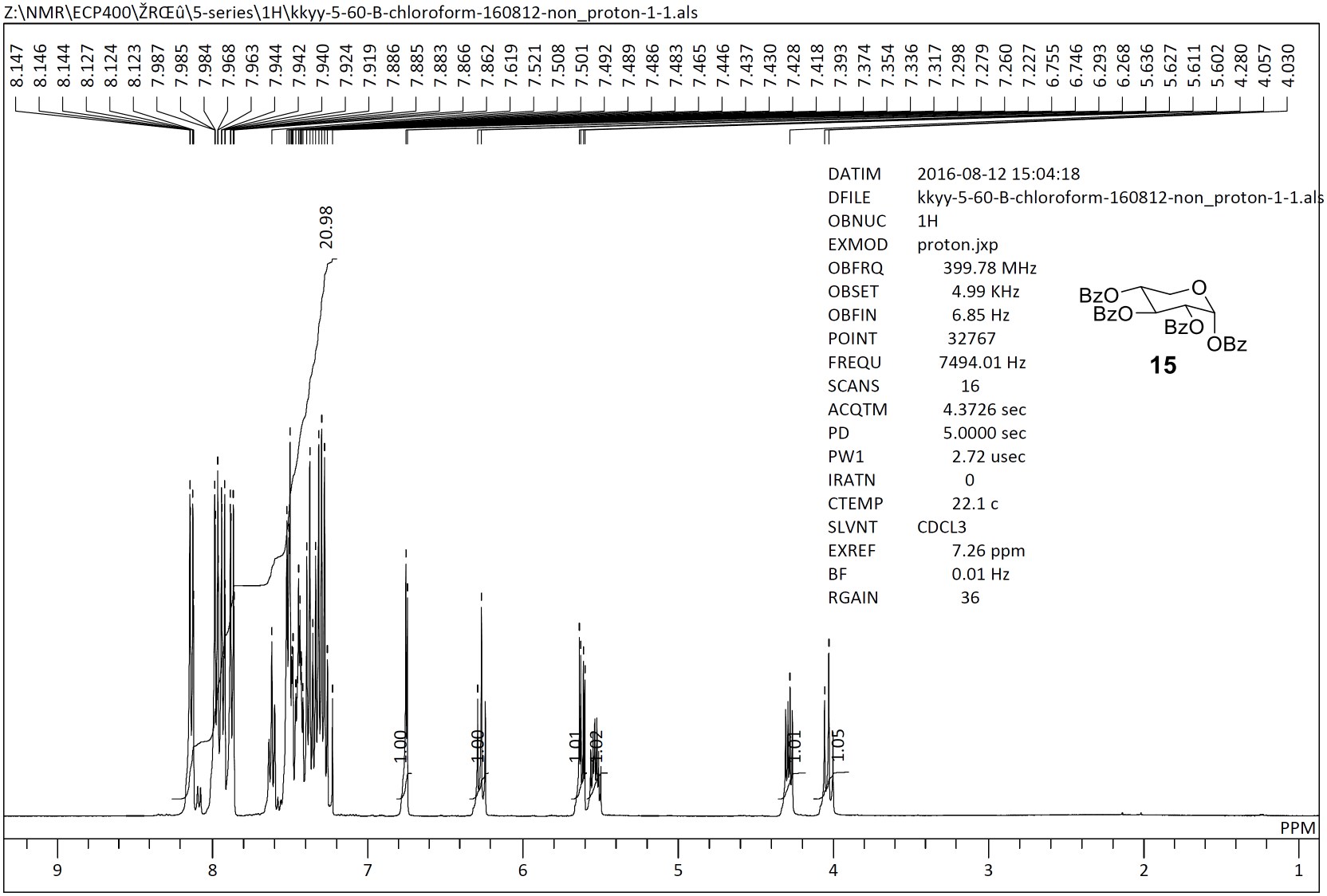
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BzO
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2
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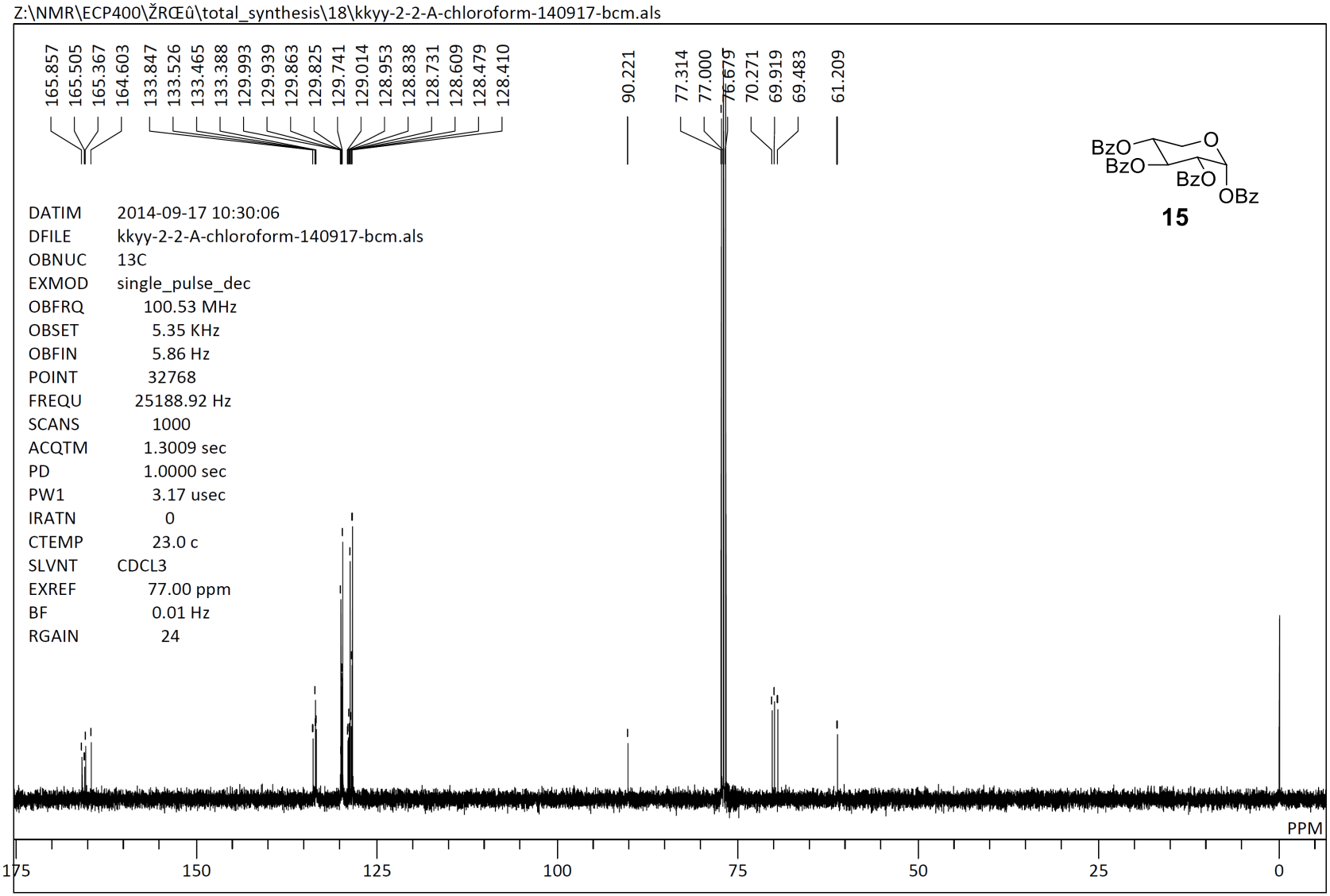
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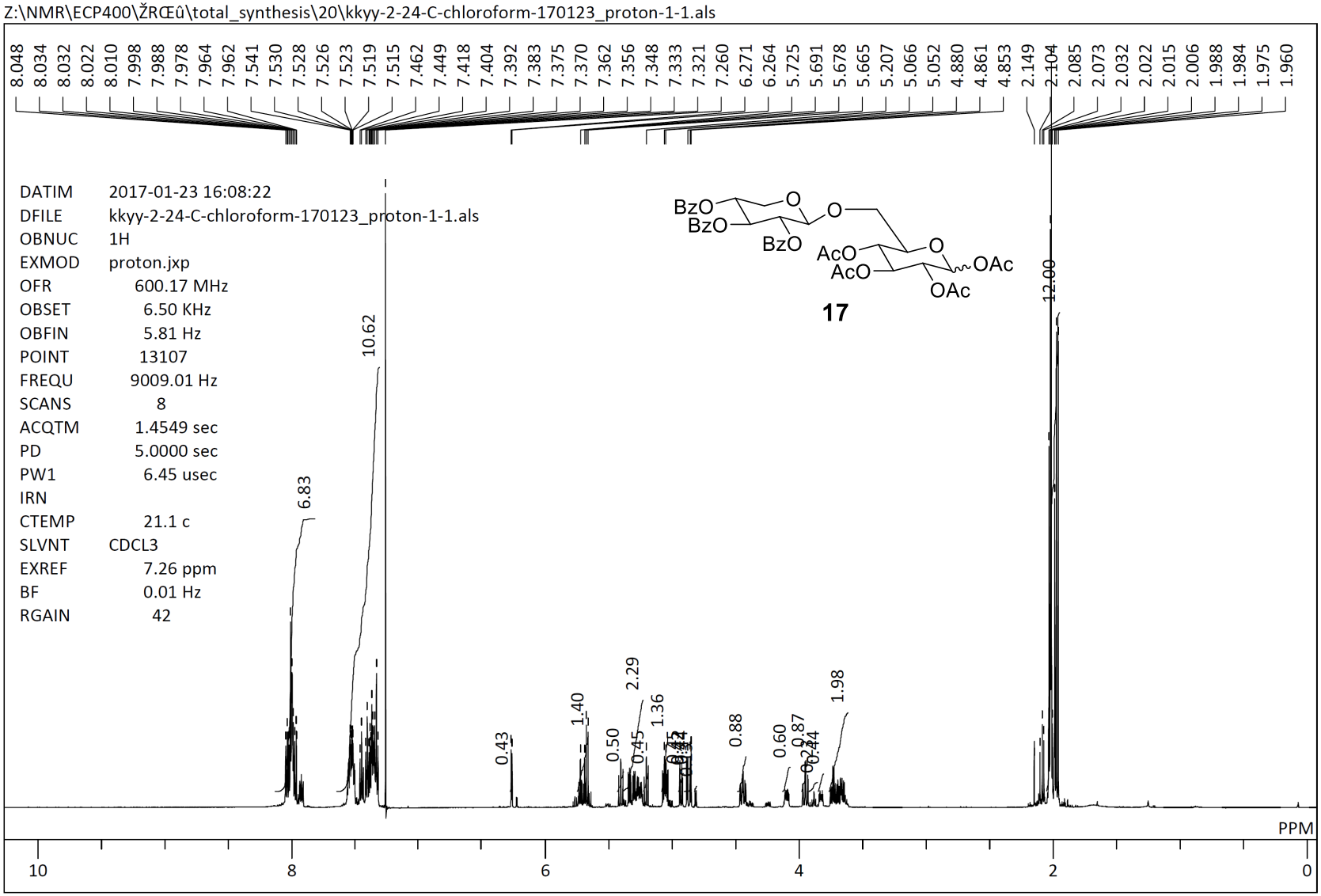
165.367
164.603
133.847
133.526
133.465
133.388
129.993
129.939
129.863
129.825
129.741
129.014
128.953
128.838
128.731
128.609
128.479
128.410
90.221
77.314
77.000
76.679
70.271
69.919
69.483
61.209
BzO
BzO
BzO
OBz
O
15
DATIM 2014-09-17 10:30:06
DFILE kkyy-2-2-A-chloroform-140917-bcm.als
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 1000
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.17 usec
IRATN 0
CTEMP 23.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.01 Hz
RGAIN 24
PPM
175
150
125
100
75
50
25
0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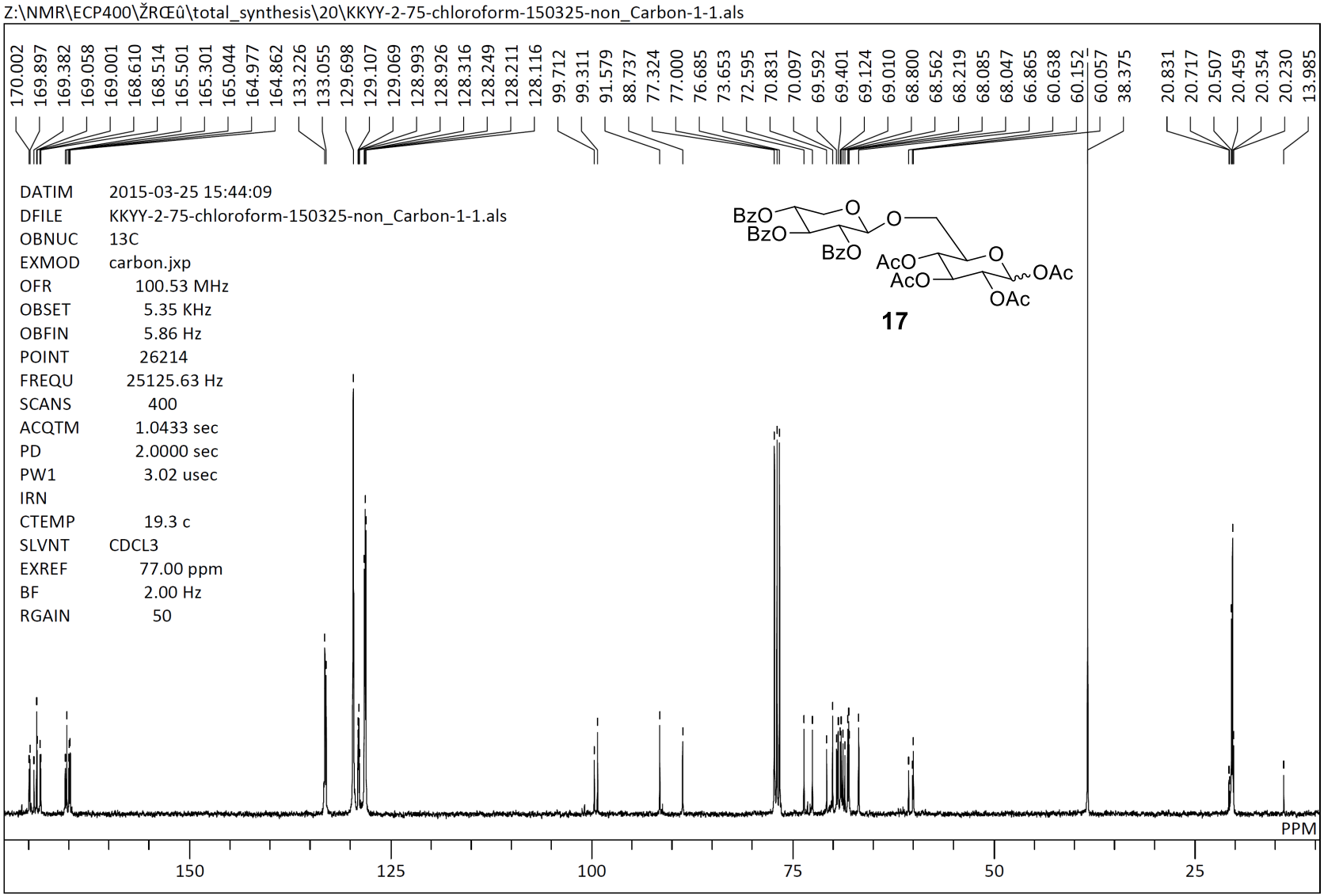
DFILE kkyy-2-24-C-chloroform-170123_proton-1-1.als
OBNUC 1H
EXMOD proton.jxp
OFR 600.17 MHz
OBSET 6.50 KHz
OBFIN 5.81 Hz
POINT 13107
FREQU 9009.01 Hz
SCANS 8
ACQTM 1.4549 sec
PD 5.0000 sec
PW1 6.45 usec
IRN
CTEMP 21.1 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.01 Hz
RGAIN 42
BzO
BzO
BzO
AcO
AcO
OAc
OAc
17
PPM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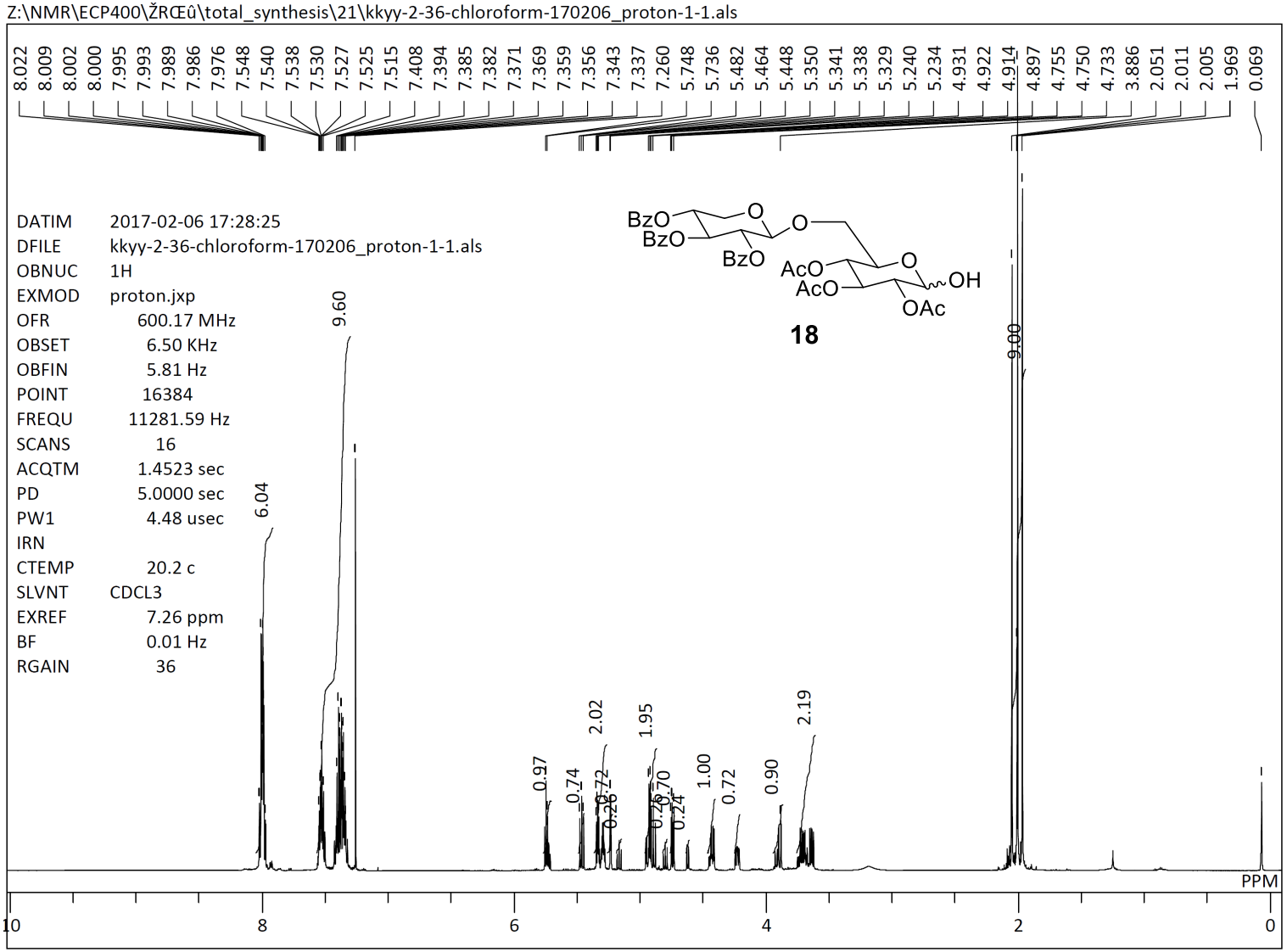
170.002 169.897 169.382 169.058 169.001 168.610 168.514 165.501 165.301 165.044 164.977 164.862 133.226 133.055 129.698 129.107 129.069 128.993 128.926 128.316 128.249 128.211 128.116 99.712 99.311 91.579 88.737 77.324 77.000 76.685 73.653 72.595 70.831 70.097 69.592 69.401 69.124 69.010 68.800 68.562 68.219 68.085 68.047 66.865 60.638 60.152 60.057 38.375 20.831 20.717 20.507 20.459 20.354 20.230 13.985
DATIM 2015-03-25 15:44:09
DFILE KKYY-2-75-chloroform-150325-non_Carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 400
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRN
CTEMP 19.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 50
BzO
BzO
BzO
O
O
AcO
AcO
O
OAc
OAc
17
PPM
150
125
100
75
50
25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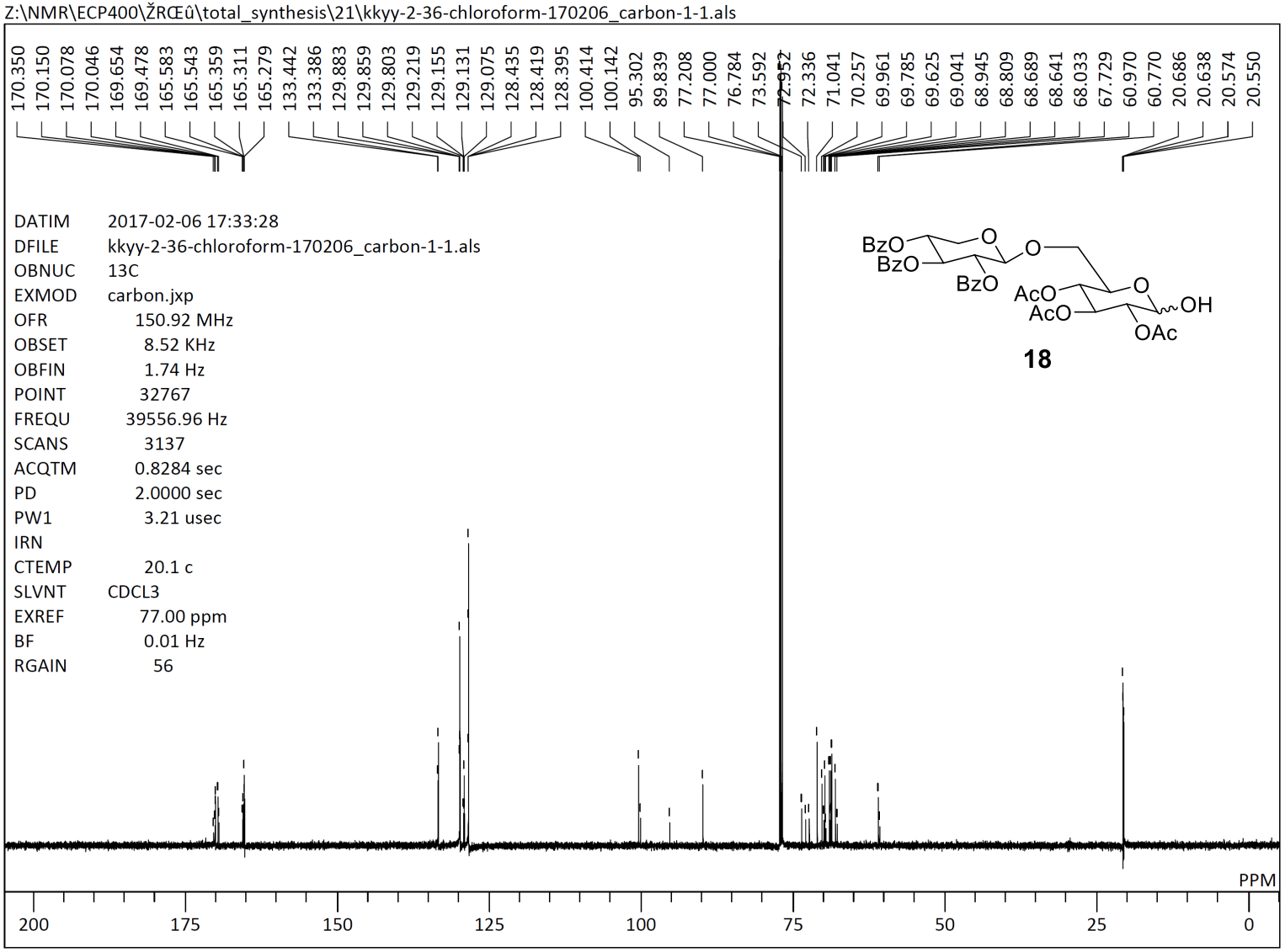
8.022 8.009 8.002 8.000 7.995 7.993 7.989 7.986 7.976 7.548 7.540 7.538 7.530 7.527 7.525 7.515 7.408 7.394 7.385 7.382 7.371 7.369 7.359 7.356 7.343 7.337 7.260 5.748 5.736 5.482 5.464 5.448 5.350 5.341 5.338 5.329 5.240 5.234 4.931 4.922 4.914 4.897 4.755 4.750 4.733 3.886 2.051 2.011 2.005 1.969 0.069
DATIM 2017-02-06 17:28:25
DFILE kkyy-2-36-chloroform-170206_proton-1-1.als
OBNUC 1H
EXMOD proton.jxp
OFR 600.17 MHz
OBSET 6.50 KHz
OBFIN 5.81 Hz
POINT 16384
FREQU 11281.59 Hz
SCANS 16
ACQTM 1.4523 sec
PD 5.0000 sec
PW1 4.48 usec
IRN
CTEMP 20.2 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.01 Hz
RGAIN 36
BzO
BzO
BzO
O
O
AcO
AcO
O
OH
OAc
18
6.04
9.60
9.00
0.97
0.74
2.02
1.95
1.00
0.72
0.90
2.19
PPM
10
8
6
4
2
0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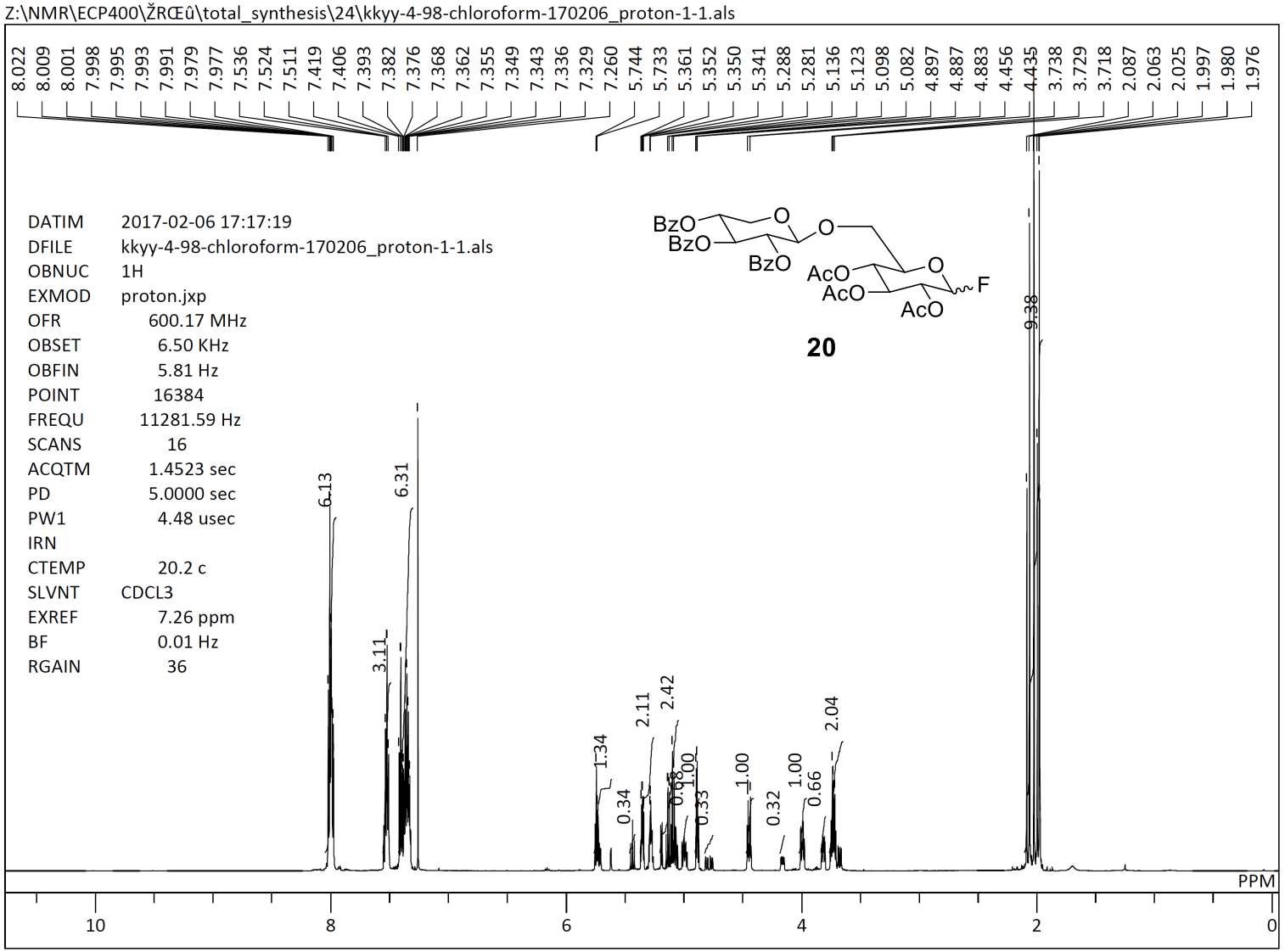
170.350 170.150 170.078 170.046 169.654 169.478 165.583 165.543 165.359 165.311 165.279 133.442 133.386 129.883 129.859 129.803 129.219 129.155 129.131 129.075 128.435 128.419 128.395 100.414 100.142 95.302 89.839 77.208 77.000 76.784 73.592 72.952 72.336 71.041 70.257 69.961 69.785 69.625 69.041 68.945 68.809 68.689 68.641 68.033 67.729 60.970 60.770 20.686 20.638 20.574 20.550
DATIM 2017-02-06 17:33:28
DFILE kkyy-2-36-chloroform-170206_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 39556.96 Hz
SCANS 3137
ACQTM 0.8284 sec
PD 2.0000 sec
PW1 3.21 usec
IRN
CTEMP 20.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.01 Hz
RGAIN 56
BzO
BzO
BzO
O
O
O
AcO
AcO
OAc
OH
18
PPM
200 175 150 125 100 75 50 25 0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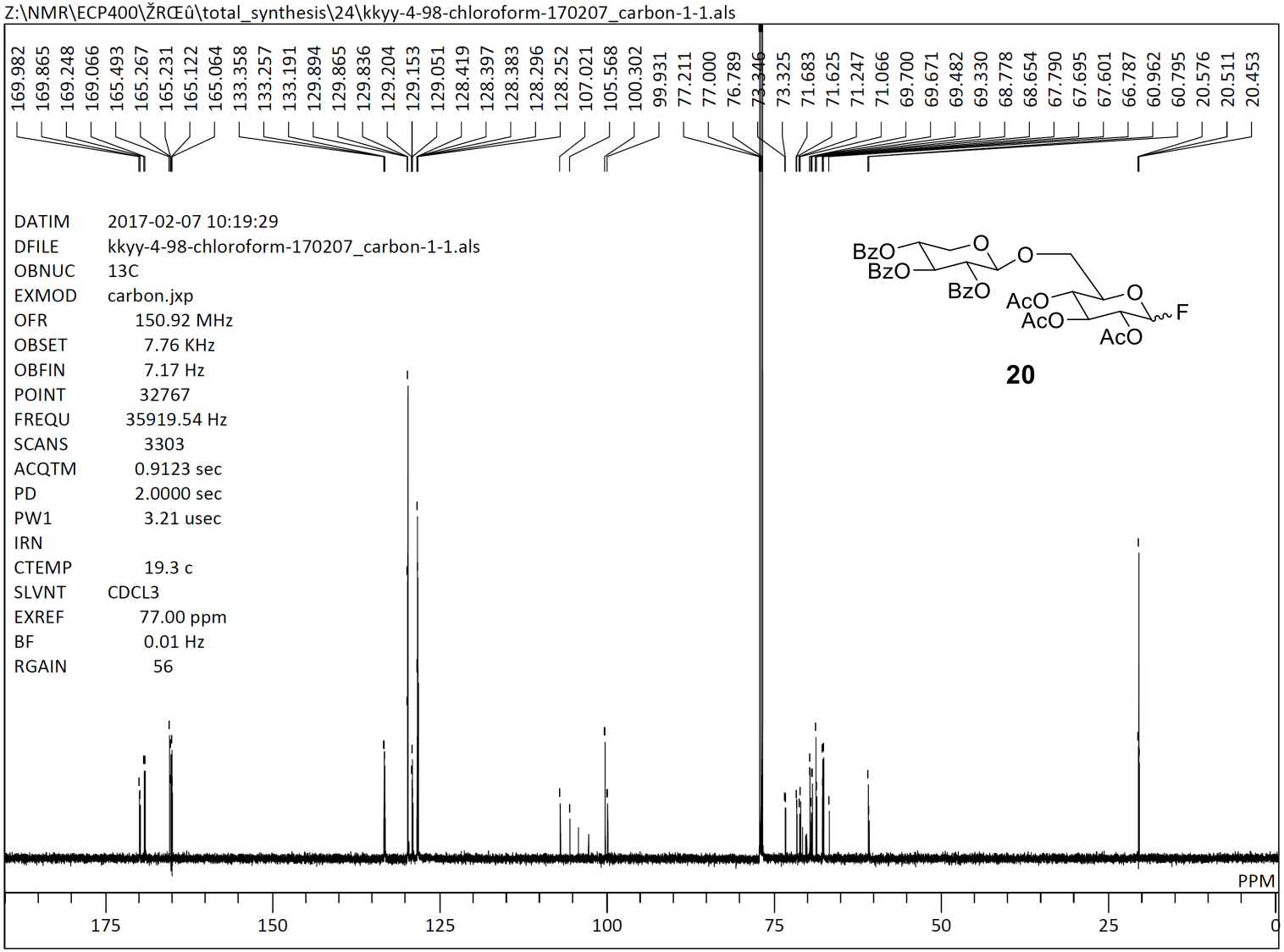
8.022 8.009 8.001 7.998 7.995 7.993 7.991 7.979 7.977 7.536 7.524 7.511 7.419 7.406 7.393 7.382 7.376 7.368 7.362 7.355 7.349 7.343 7.336 7.329 7.260 5.744 5.733 5.361 5.352 5.350 5.341 5.288 5.281 5.136 5.123 5.098 5.082 4.897 4.887 4.883 4.456 4.435 3.738 3.729 3.718 2.087 2.063 2.025 1.997 1.980 1.976
DATIM 2017-02-06 17:17:19
DFILE kkyy-4-98-chloroform-170206_proton-1-1.als
OBNUC 1H
EXMOD proton.jxp
OFR 600.17 MHz
OBSET 6.50 KHz
OBFIN 5.81 Hz
POINT 16384
FREQU 11281.59 Hz
SCANS 16
ACQTM 1.4523 sec
PD 5.0000 sec
PW1 4.48 usec
IRN
CTEMP 20.2 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.01 Hz
RGAIN 36
BzO
BzO
BzO
O
O
AcO
AcO
AcO
O
F
20
9.38
6.13
6.31
3.11
1.34
0.34
2.11
2.42
0.68
1.00
0.33
1.00
0.32
1.00
0.66
2.04
PPM
10
8
6
4
2
0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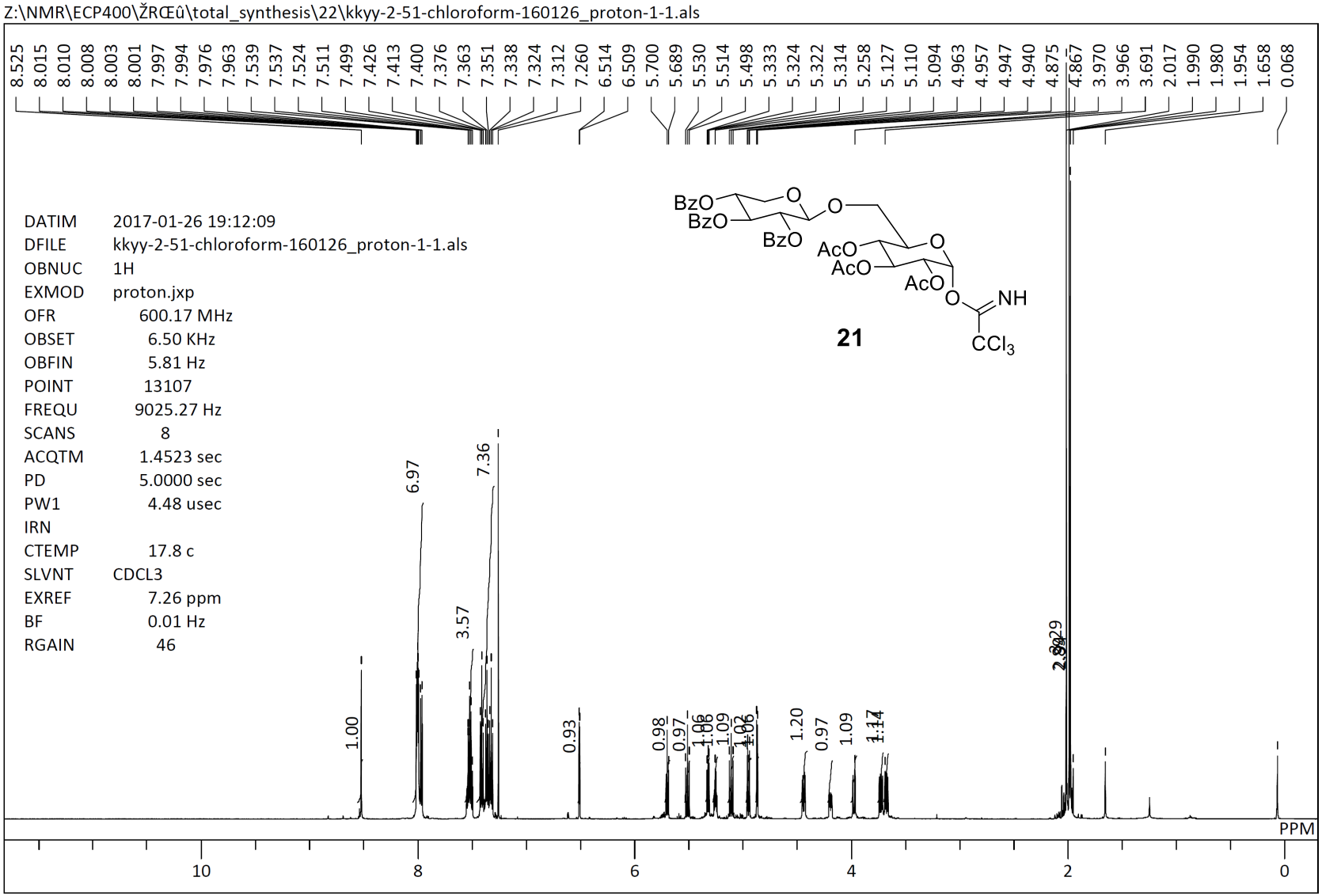
169.982 169.865 169.248 169.066 165.493 165.267 165.231 165.122 165.064 133.358 133.257 133.191 129.894 129.865 129.836 129.204 129.153 129.051 128.419 128.397 128.383 128.296 128.252 107.021 105.568 100.302 99.931 77.211 77.000 76.789 73.346 73.325 71.683 71.625 71.247 71.066 69.700 69.671 69.482 69.330 68.778 68.654 67.790 67.695 67.601 66.787 60.962 60.795 20.576 20.511 20.453
DATIM 2017-02-07 10:19:29
DFILE kkyy-4-98-chloroform-170207_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 150.92 MHz
OBSET 7.76 KHz
OBFIN 7.17 Hz
POINT 32767
FREQU 35919.54 Hz
SCANS 3303
ACQTM 0.9123 sec
PD 2.0000 sec
PW1 3.21 usec
IRN
CTEMP 19.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.01 Hz
RGAIN 56
BzO
BzO
BzO
O
O
AcO
AcO
AcO
O
F
20
PPM
175
150
125
100
75
50
25
0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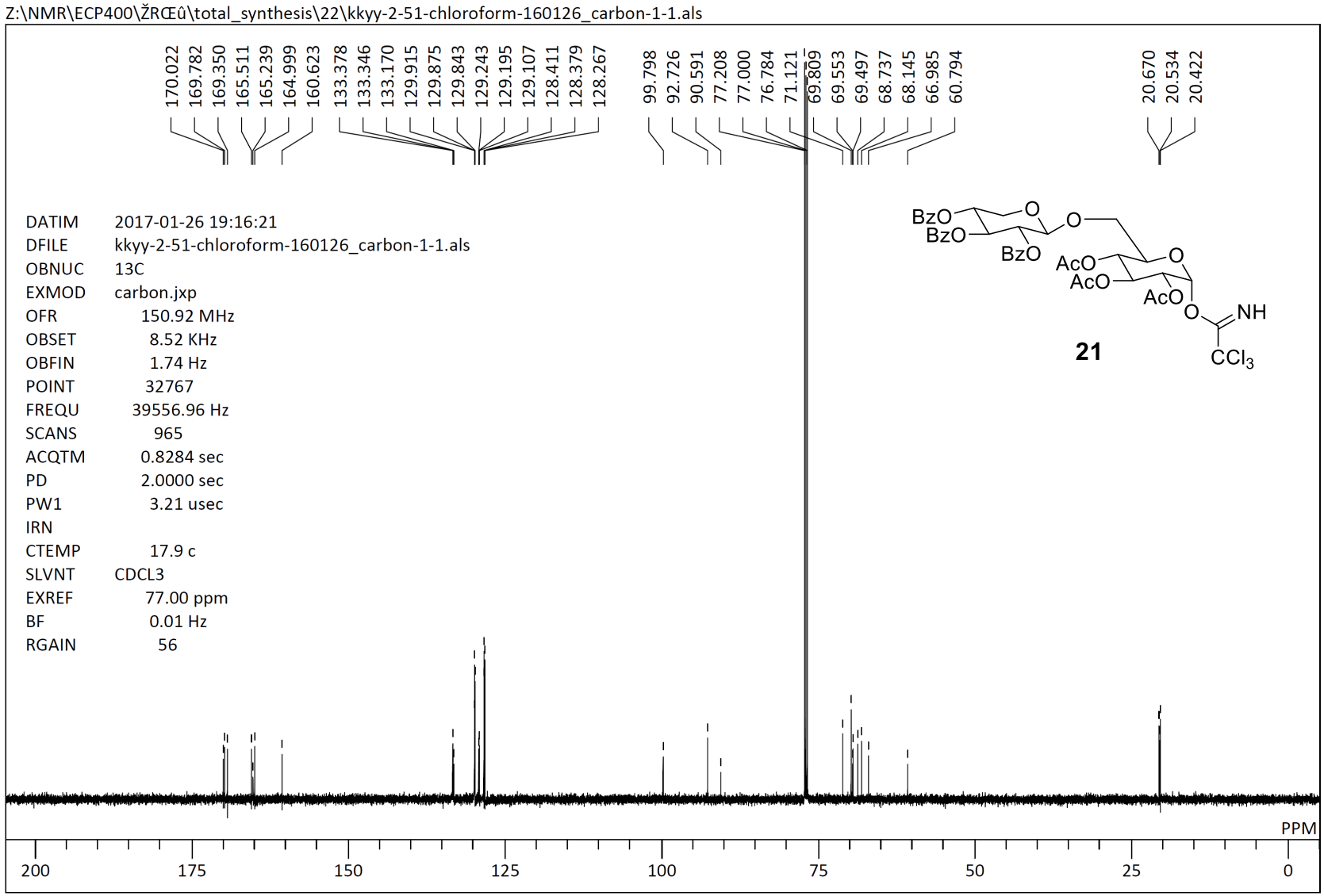
DATIM 2017-01-26 19:12:09
DFILE kkyy-2-51-chloroform-160126_proton-1-1.als
OBNUC 1H
EXMOD proton.jxp
OFR 600.17 MHz
OBSET 6.50 KHz
OBFIN 5.81 Hz
POINT 13107
FREQU 9025.27 Hz
SCANS 8
ACQTM 1.4523 sec
PD 5.0000 sec
PW1 4.48 usec
IRN
CTEMP 17.8 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.01 Hz
RGAIN 46
BzO
BzO
BzO
O
O
AcO
AcO
AcO
O
O
NH
CCl3
21
1.00
6.97
7.36
3.57
0.93
0.98
0.97
1.09
1.20
0.97
1.09
PPM
10
8
6
4
2
0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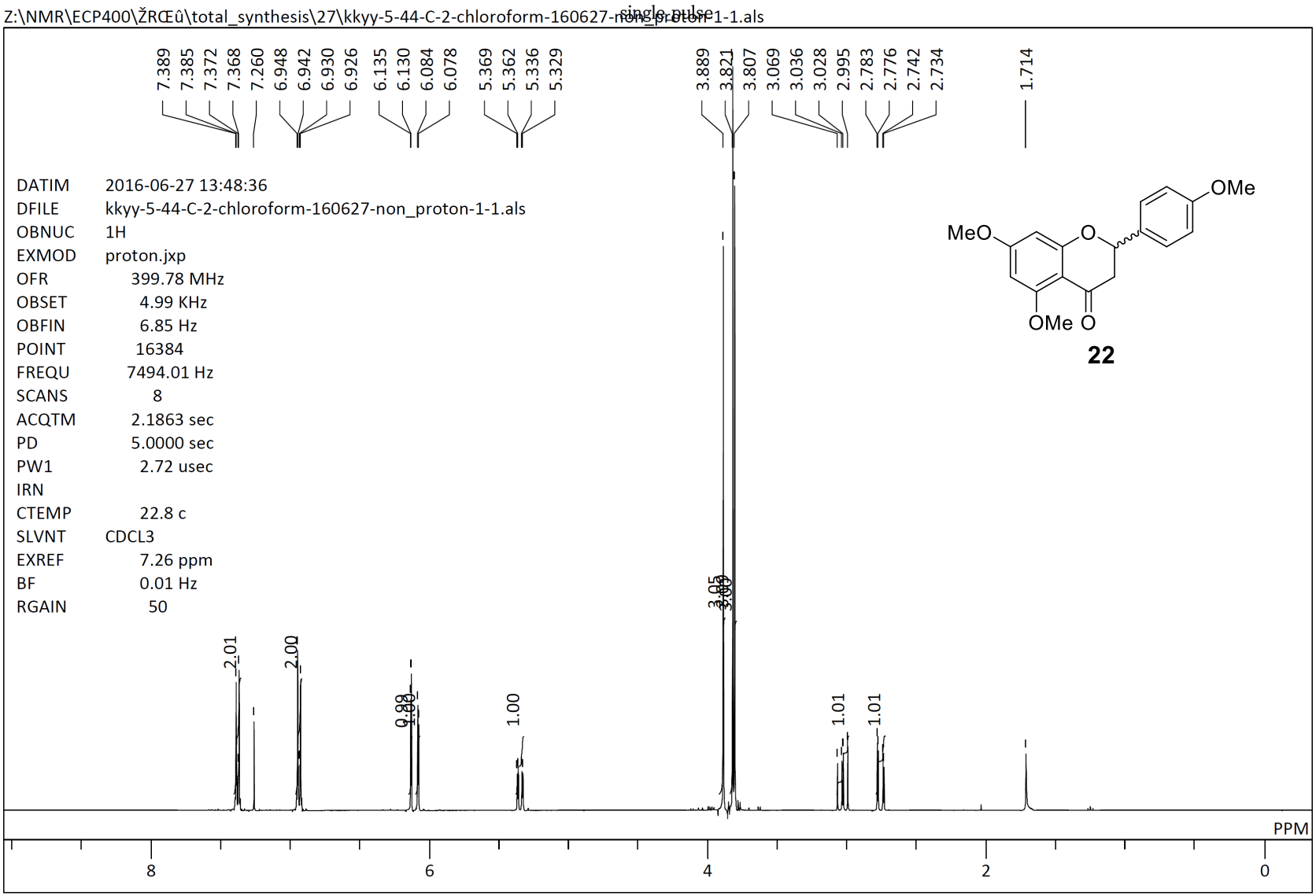
169.350
165.511
165.239
164.999
160.623
133.378
133.346
133.170
129.915
129.875
129.843
129.243
129.195
129.107
128.411
128.379
128.267
99.798
92.726
90.591
77.208
77.000
76.784
71.121
69.809
69.553
69.497
68.737
68.145
66.985
60.794
20.670
20.534
20.422
DATIM 2017-01-26 19:16:21
DFILE kkyy-2-51-chloroform-160126_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 39556.96 Hz
SCANS 965
ACQTM 0.8284 sec
PD 2.0000 sec
PW1 3.21 usec
IRN
CTEMP 17.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.01 Hz
RGAIN 56
BzO
BzO
BzO
AcO
AcO
AcO
NH
CCl3
21
PPM
200
175
150
125
100
75
50
25
0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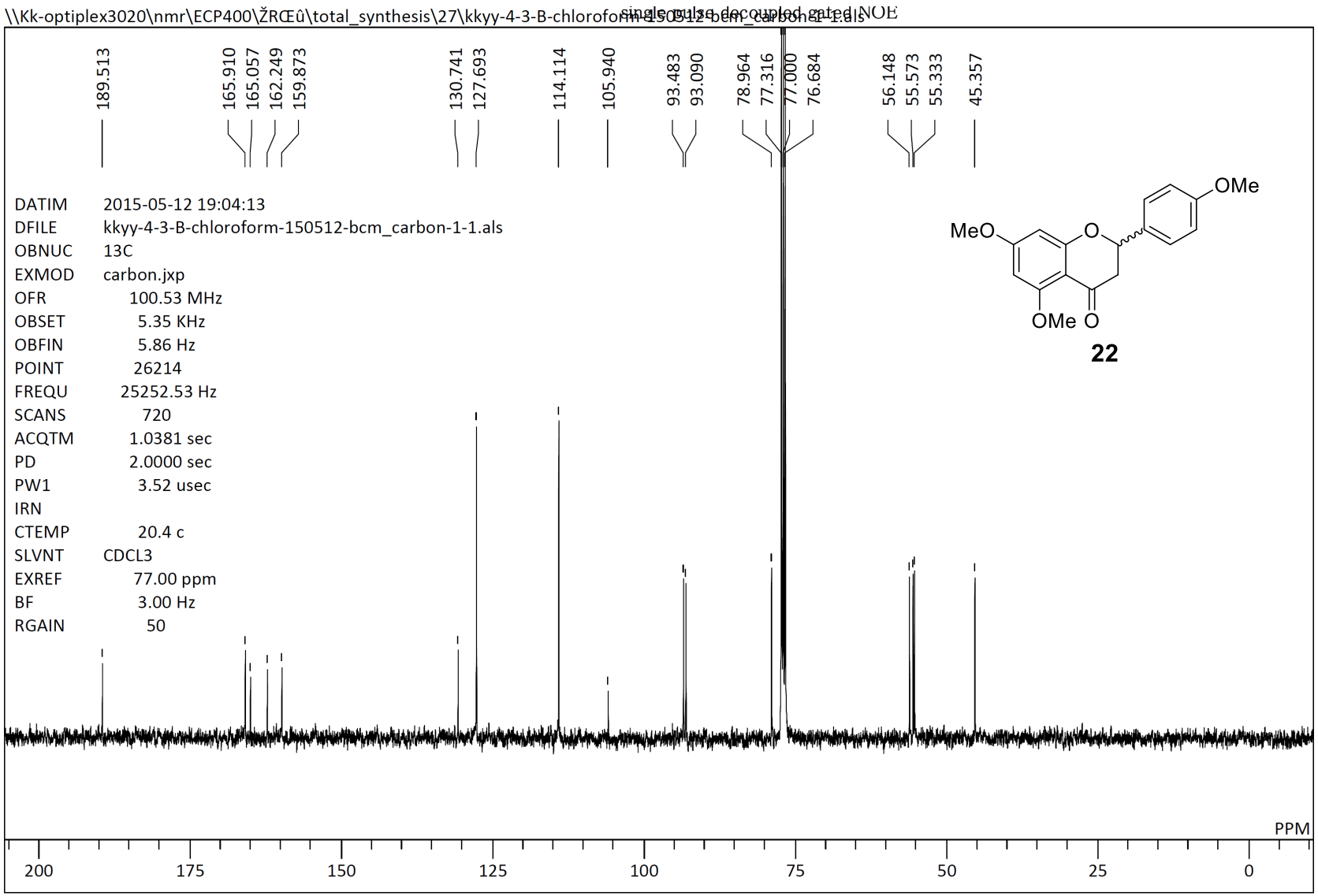
single pulse
7.389
7.385
7.372
7.368
7.260
6.948
6.942
6.930
6.926
6.135
6.130
6.084
6.078
5.369
5.362
5.336
5.329
3.889
3.821
3.807
3.069
3.036
3.028
2.995
2.783
2.776
2.742
2.734
1.714
DATIM 2016-06-27 13:48:36
DFILE kkyy-5-44-C-2-chloroform-160627-non_proton-1-1.als
OBNUC 1H
EXMOD proton.jxp
OFR 399.78 MHz
OBSET 4.99 KHz
OBFIN 6.85 Hz
POINT 16384
FREQU 7494.01 Hz
SCANS 8
ACQTM 2.1863 sec
PD 5.0000 sec
PW1 2.72 usec
IRN
CTEMP 22.8 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.01 Hz
RGAIN 50
MeO
O
OMe
OMe
O
22
2.01
2.00
1.00
3.05
1.01
1.01
PPM
8
6
4
2
0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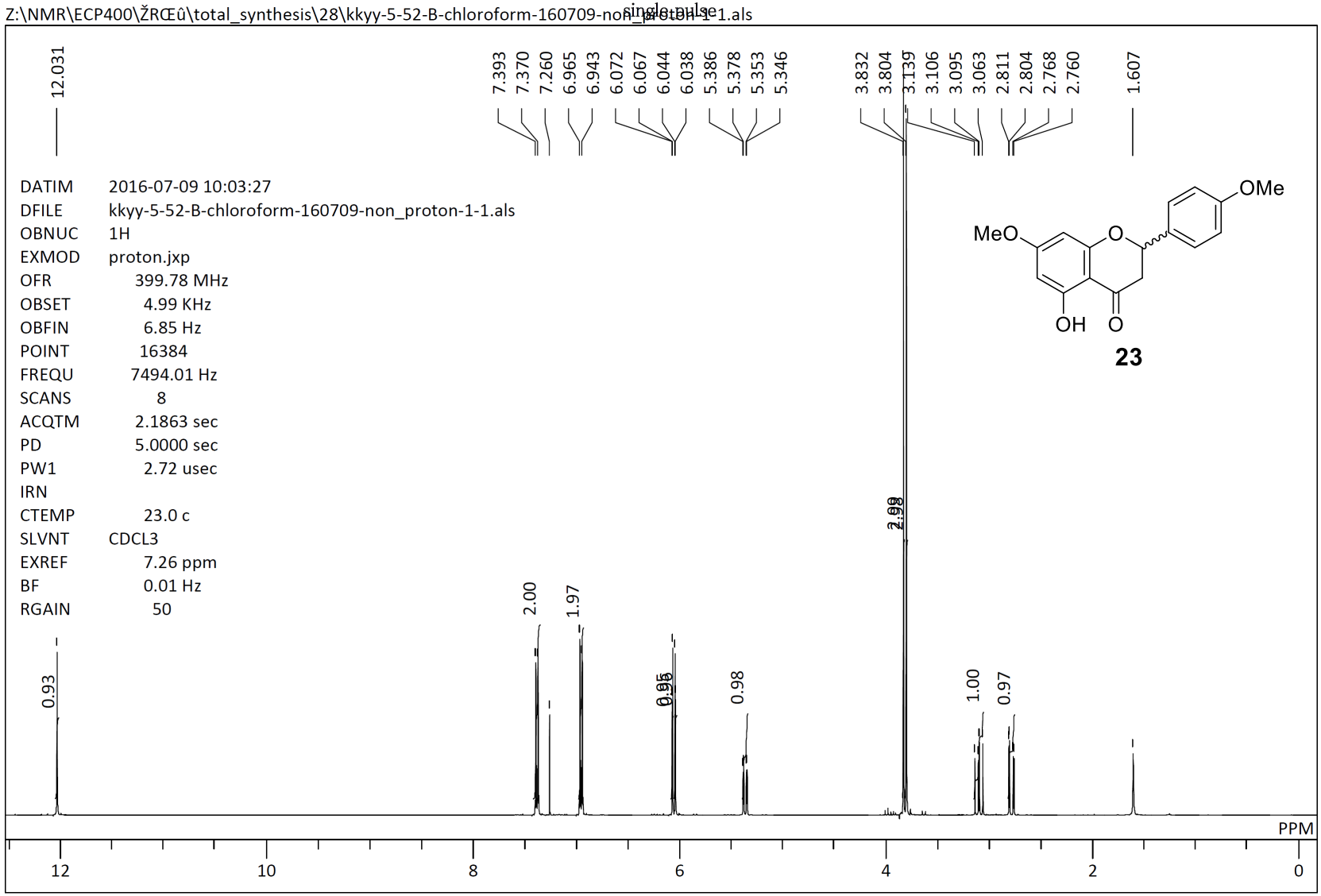
single pulse decoupled gated NOE
189.513
165.910
165.057
162.249
159.873
130.741
127.693
114.114
105.940
93.483
93.090
78.964
77.316
77.000
76.684
56.148
55.573
55.333
45.357
DATIM 2015-05-12 19:04:13
DFILE kkyy-4-3-B-chloroform-150512-bcm_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 720
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRN
CTEMP 20.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 3.00 Hz
RGAIN 50
MeO
O
OMe
OMe
O
22
PPM
200
175
150
125
100
75
50
25
0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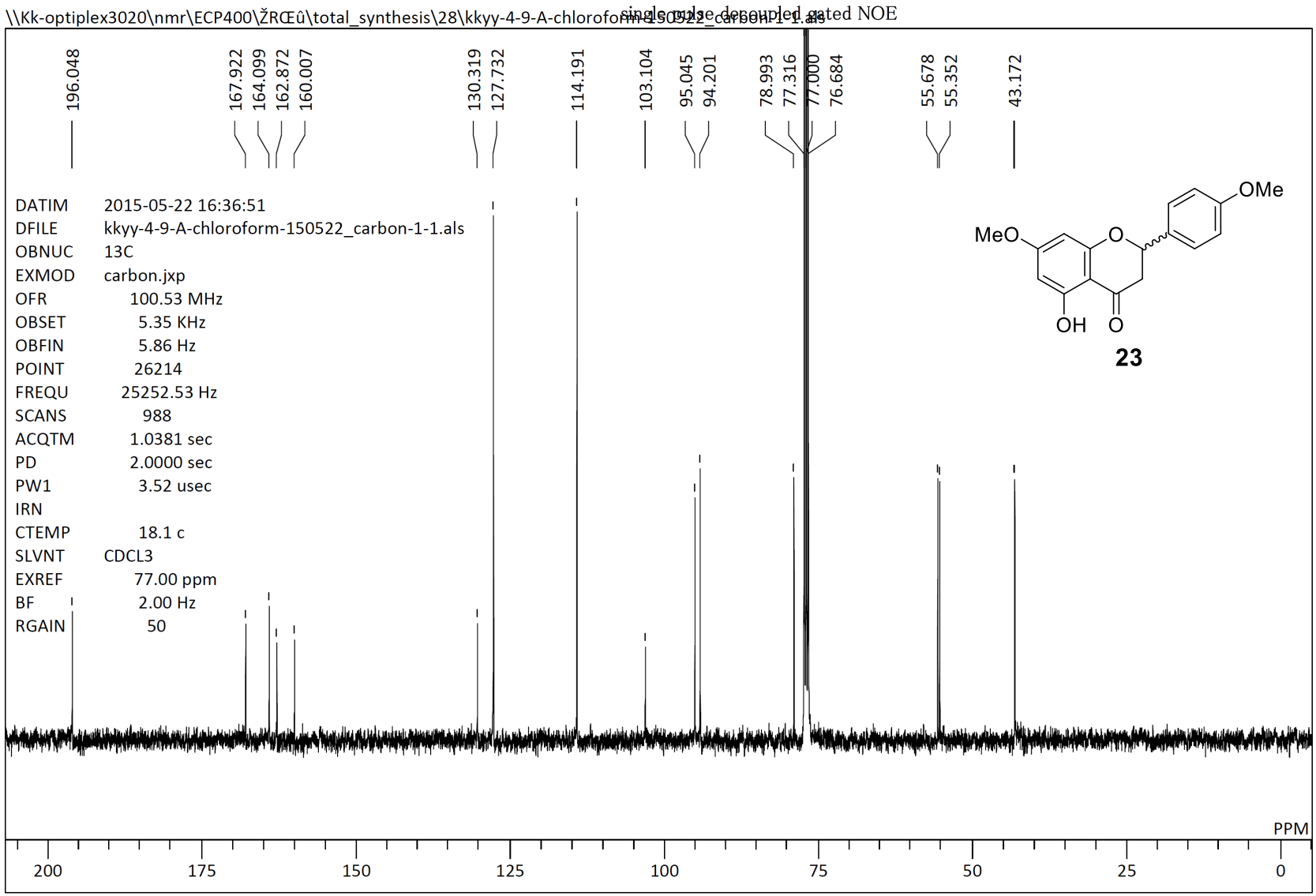
single_pulse
12.031
7.393
7.370
7.260
6.965
6.943
6.072
6.067
6.044
6.038
5.386
5.378
5.353
5.346
3.832
3.804
3.139
3.106
3.095
3.063
2.811
2.804
2.768
2.760
1.607
DATIM 2016-07-09 10:03:27
DFILE kkyy-5-52-B-chloroform-160709-non_proton-1-1.als
OBNUC 1H
EXMOD proton.jxp
OFR 399.78 MHz
OBSET 4.99 KHz
OBFIN 6.85 Hz
POINT 16384
FREQU 7494.01 Hz
SCANS 8
ACQTM 2.1863 sec
PD 5.0000 sec
PW1 2.72 usec
IRN
CTEMP 23.0 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.01 Hz
RGAIN 50
MeO
O
OMe
OH
O
23
2.00
1.97
2.99
0.93
0.98
1.00
0.97
PPM
12
10
8
6
4
2
0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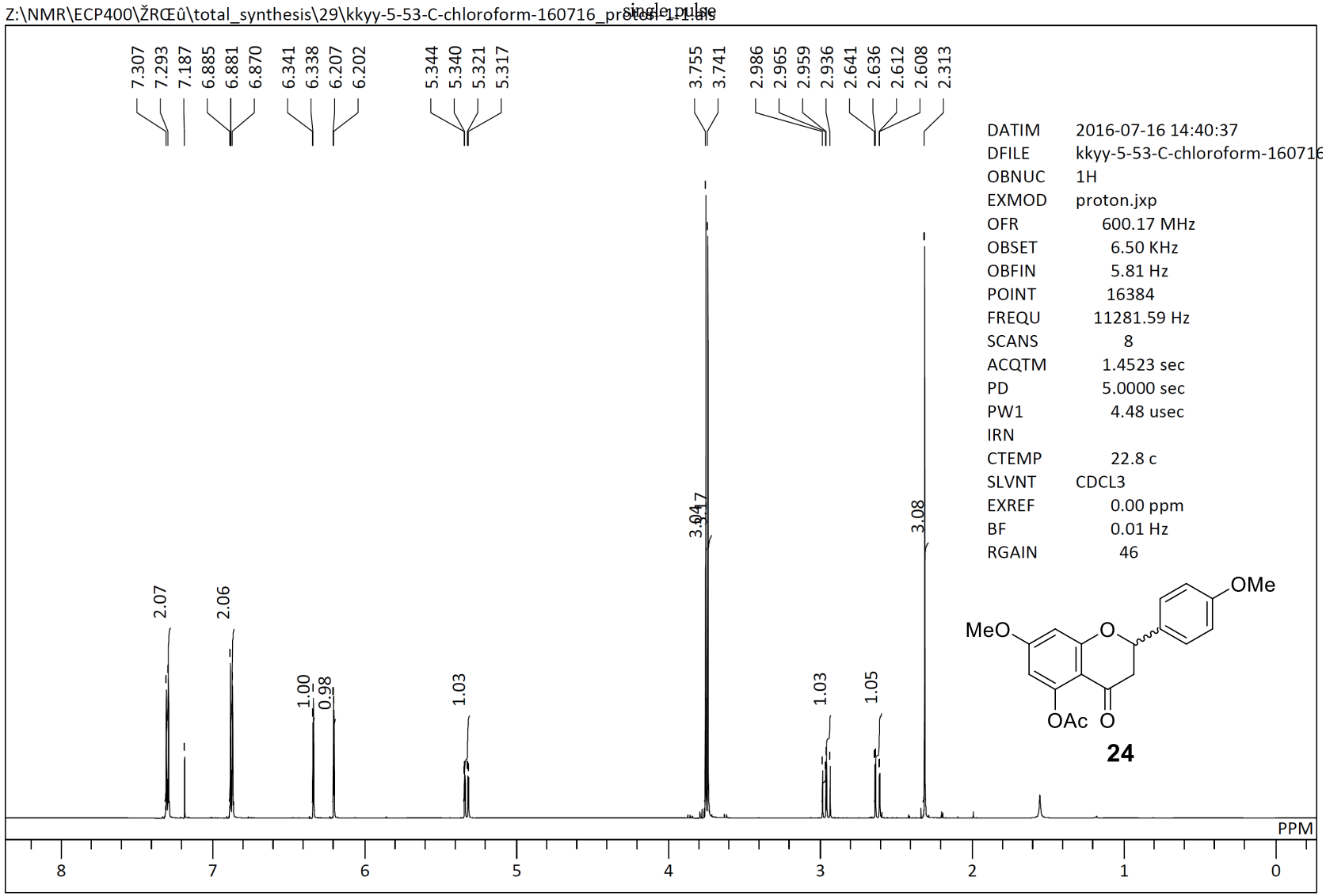
single pulse decoupled gated NOE
196.048
167.922
164.099
162.872
160.007
130.319
127.732
114.191
103.104
95.045
94.201
78.993
77.316
77.000
76.684
55.678
55.352
43.172
DATIM 2015-05-22 16:36:51
DFILE kkyy-4-9-A-chloroform-150522_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 988
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRN
CTEMP 18.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 50
MeO
O
OMe
OH
O
23
PPM
200
175
150
125
100
75
50
25
0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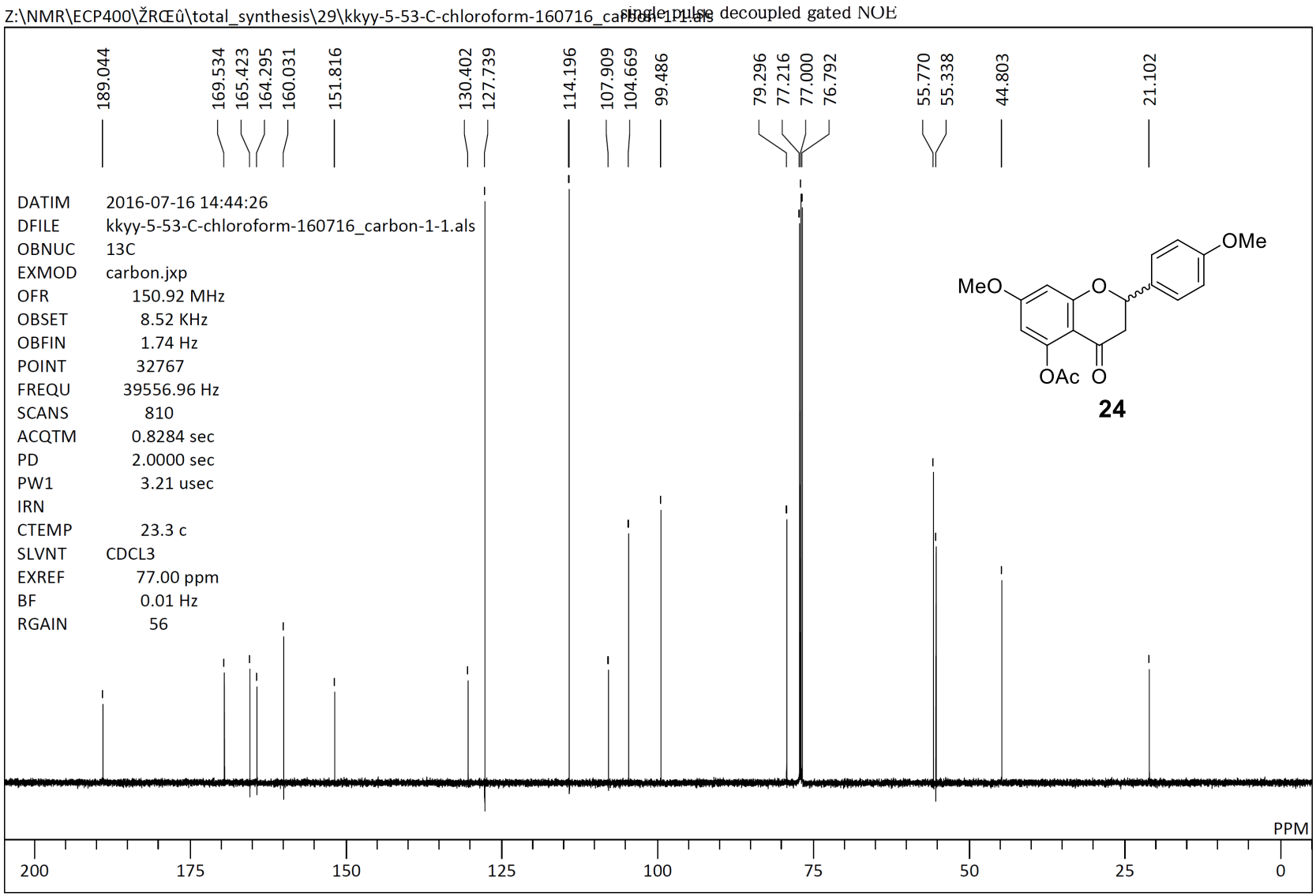
single pulse
7.307
7.293
7.187
6.885
6.881
6.870
6.341
6.338
6.207
6.202
5.344
5.340
5.321
5.317
3.755
3.741
2.986
2.965
2.959
2.936
2.641
2.636
2.612
2.608
2.313
DATIM 2016-07-16 14:40:37
DFILE kkyy-5-53-C-chloroform-160716
OBNUC 1H
EXMOD proton.jxp
OFR 600.17 MHz
OBSET 6.50 KHz
OBFIN 5.81 Hz
POINT 16384
FREQU 11281.59 Hz
SCANS 8
ACQTM 1.4523 sec
PD 5.0000 sec
PW1 4.48 usec
IRN
CTEMP 22.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.01 Hz
RGAIN 46
3.04
3.17
3.08
2.07
2.06
1.00
0.98
1.03
1.03
1.05
MeO
O
OMe
OAc
O
24
PPM
8
7
6
5
4
3
2
1
0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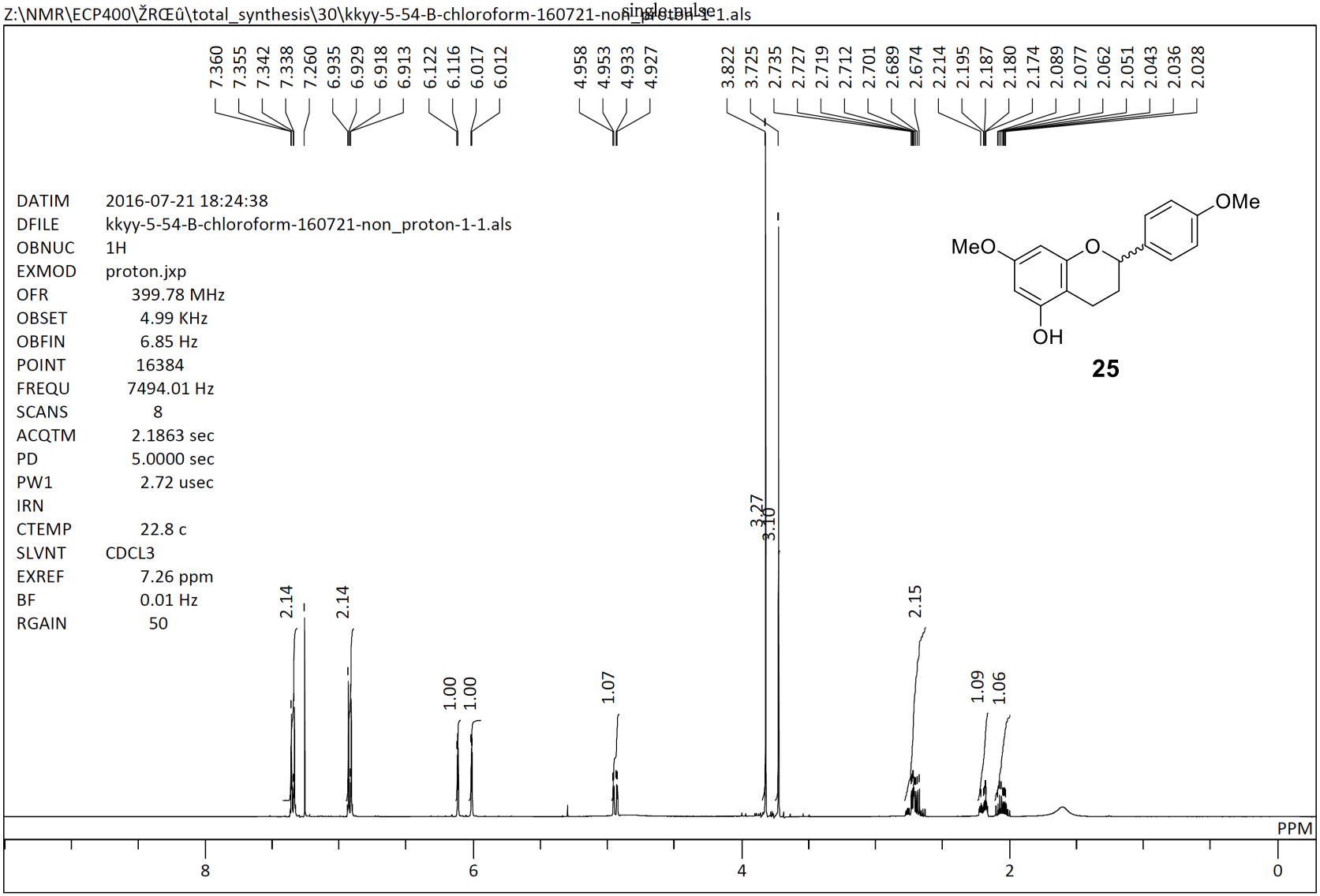
single pulse decoupled gated NOE
189.044
169.534
165.423
164.295
160.031
151.816
130.402
127.739
114.196
107.909
104.669
99.486
79.296
77.216
77.000
76.792
55.770
55.338
44.803
21.102
DATIM 2016-07-16 14:44:26
DFILE kkyy-5-53-C-chloroform-160716_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 39556.96 Hz
SCANS 810
ACQTM 0.8284 sec
PD 2.0000 sec
PW1 3.21 usec
IRN
CTEMP 23.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.01 Hz
RGAIN 56
MeO
OMe
O
OAc
O
24
PPM
200
175
150
125
100
75
50
25
0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single pulse
7.360 7.355 7.342 7.338 7.260 6.935 6.929 6.918 6.913 6.122 6.116 6.017 6.012
4.958 4.953 4.933 4.927
3.822 3.725 2.735 2.727 2.719 2.712 2.701 2.689 2.674 2.214 2.195 2.187 2.180 2.174 2.089 2.077 2.062 2.051 2.043 2.036 2.028
DATIM 2016-07-21 18:24:38
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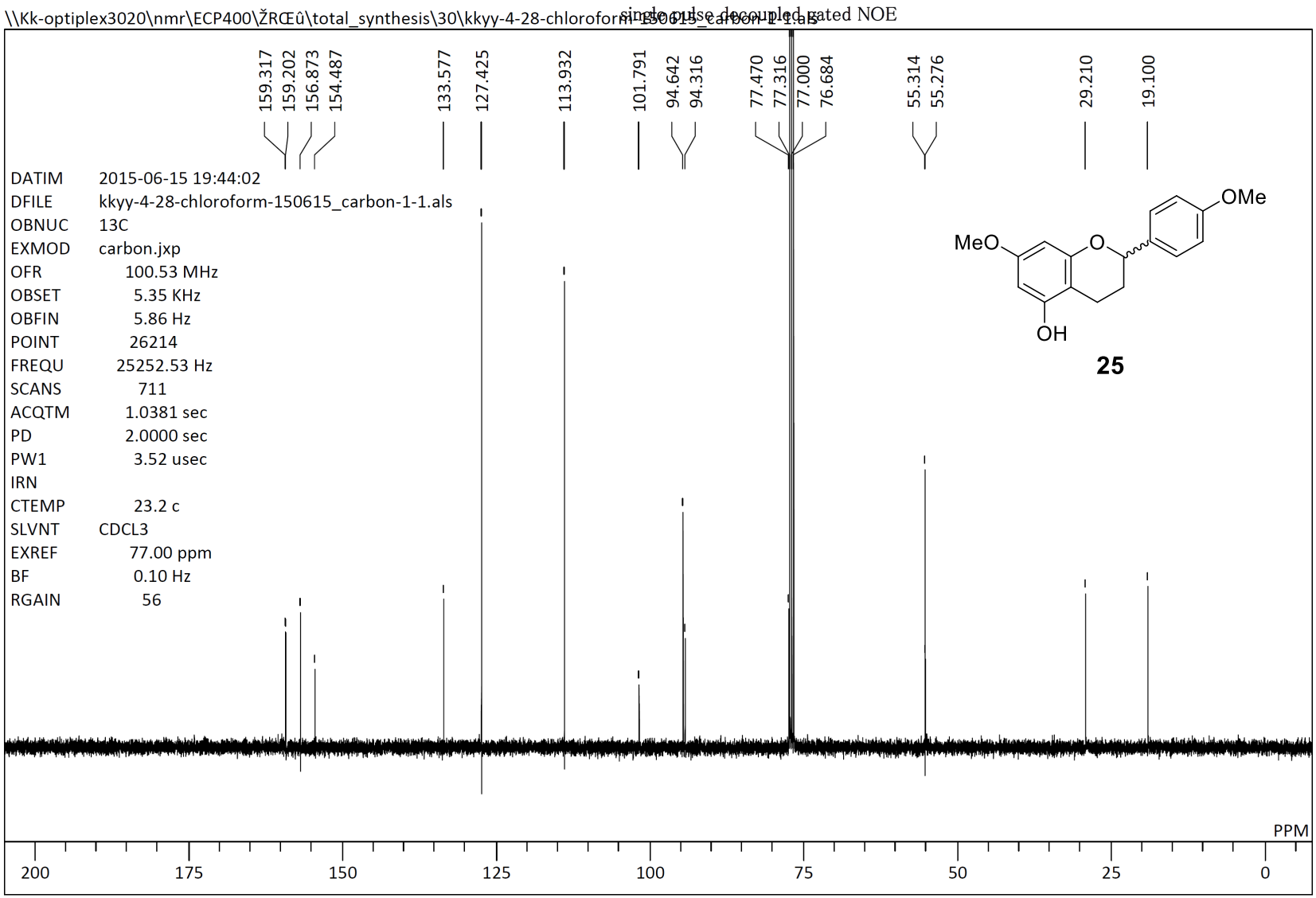
OBNUC 1H
EXMOD proton.jxp
OFR 399.78 MHz
OBSET 4.99 KHz
OBFIN 6.85 Hz
POINT 16384
FREQU 7494.01 Hz
SCANS 8
ACQTM 2.1863 sec
PD 5.0000 sec
PW1 2.72 usec
IRN
CTEMP 22.8 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.01 Hz
RGAIN 50
MeO
O
OMe
OH
25
3.27
3.10
2.14
2.14
2.15
1.00
1.00
1.07
1.09
1.06
PPM
8
6
4
2
0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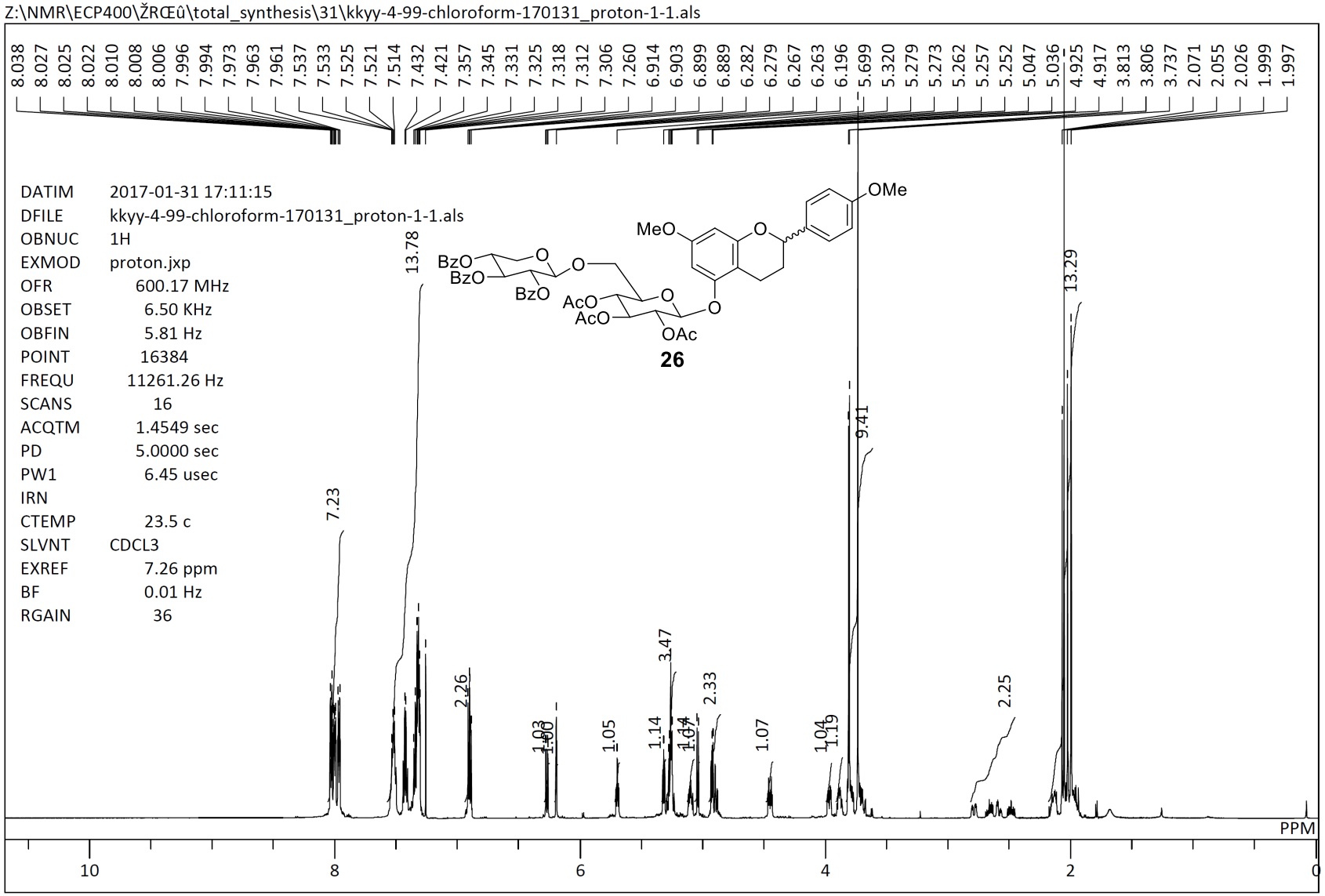
single pulse decoupled gated NOE
159.317
159.202
156.873
154.487
133.577
127.425
113.932
101.791
94.642
94.316
77.470
77.316
77.000
76.684
55.314
55.276
29.210
19.100
DATIM 2015-06-15 19:44:02
DFILE kkyy-4-28-chloroform-150615_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 711
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRN
CTEMP 23.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.10 Hz
RGAIN 56
MeO
O
OMe
OH
25
PPM
200
175
150
125
100
75
50
25
0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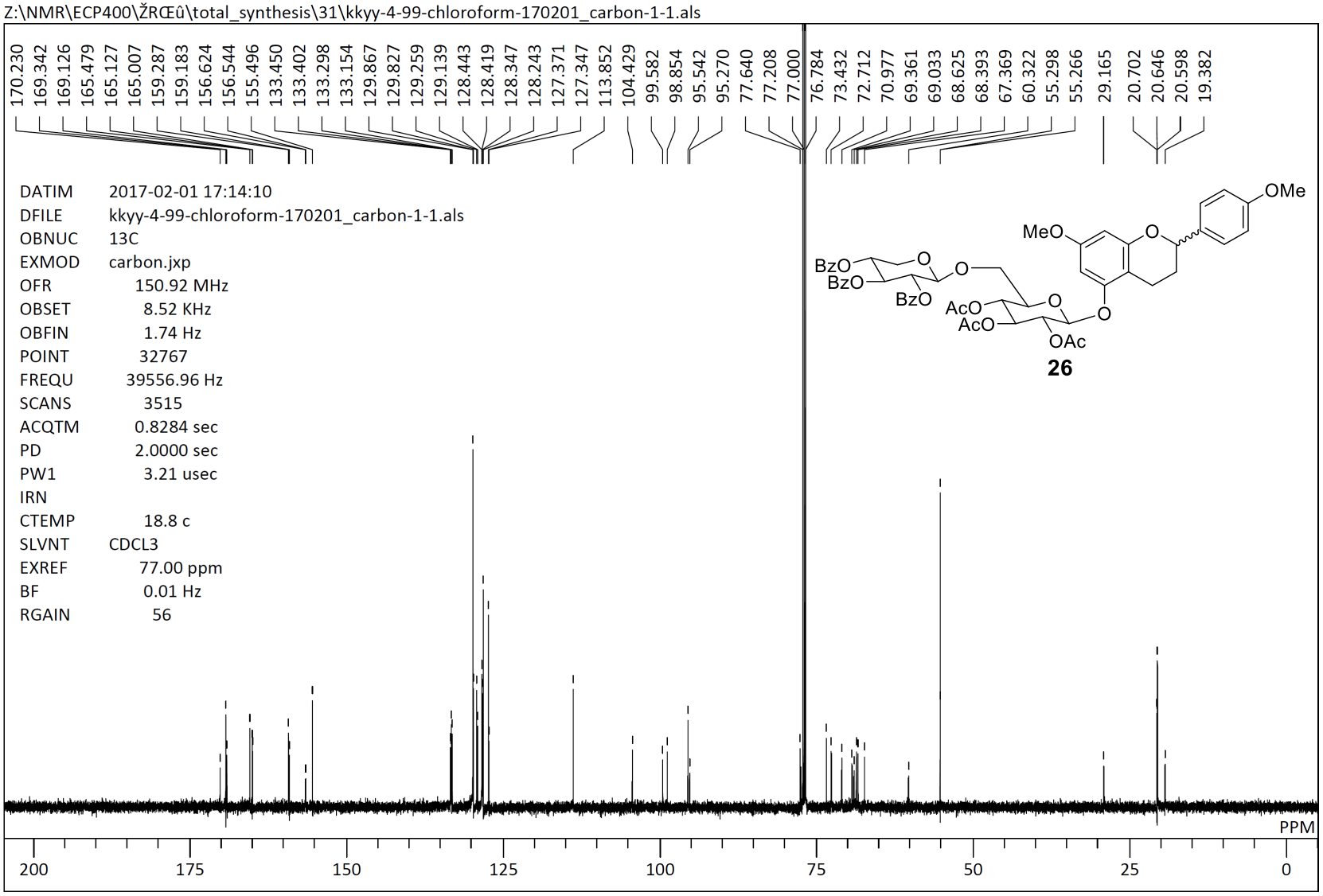
DFILE kkyy-4-99-chloroform-170131_proton-1-1.als
OBNUC 1H
EXMOD proton.jxp
OFR 600.17 MHz
OBSET 6.50 KHz
OBFIN 5.81 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 5.0000 sec
PW1 6.45 usec
IRN
CTEMP 23.5 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.01 Hz
RGAIN 36
26
PPM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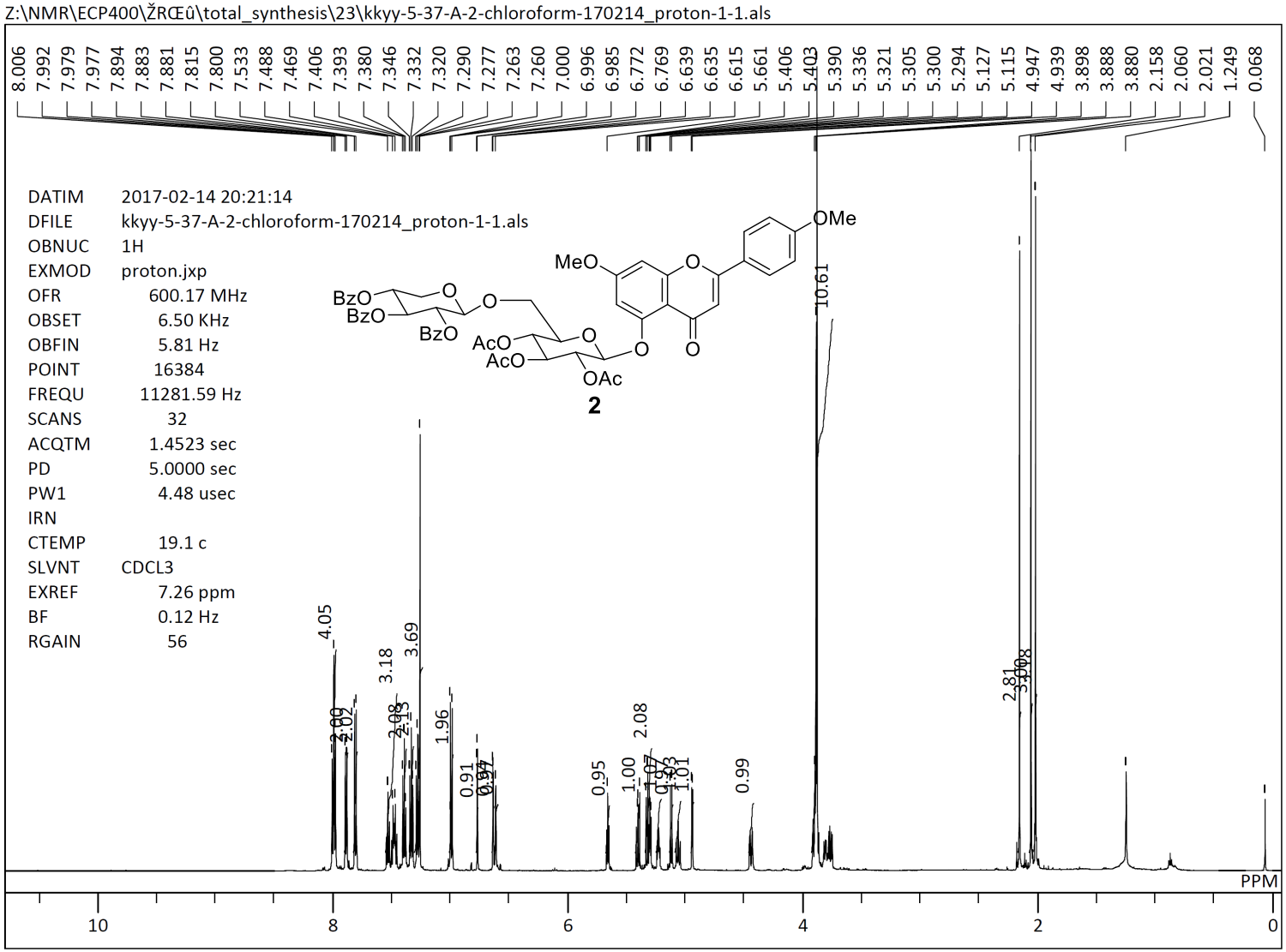
170.230 169.342 169.126 165.479 165.127 165.007 159.287 159.183 156.624 156.544 155.496 133.450 133.402 133.298 133.154 129.867 129.827 129.259 129.139 128.443 128.419 128.347 128.243 127.371 127.347 113.852 104.429 99.582 98.854 95.542 95.270 77.640 77.208 77.000 76.784 73.432 72.712 70.977 69.361 69.033 68.625 68.393 67.369 60.322 55.298 55.266 29.165 20.702 20.646 20.598 19.382
DATIM 2017-02-01 17:14:10
DFILE kkyy-4-99-chloroform-170201_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 39556.96 Hz
SCANS 3515
ACQTM 0.8284 sec
PD 2.0000 sec
PW1 3.21 usec
IRN
CTEMP 18.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.01 Hz
RGAIN 56
OMe
MeO
O
BzO
BzO
BzO
O
O
AcO
AcO
O
O
OAc
26
PPM
200 175 150 125 100 75 50 25 0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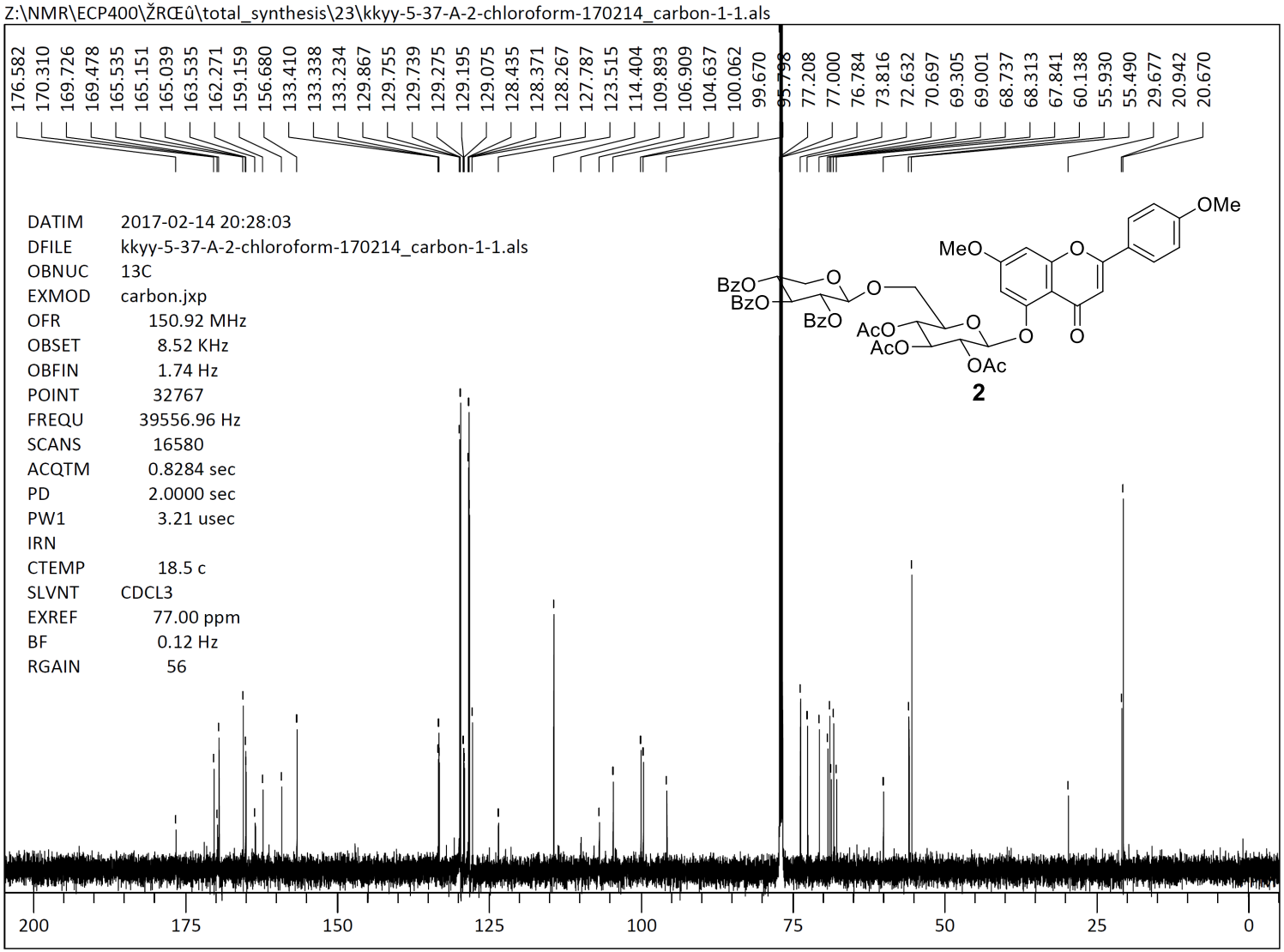
OBNUC 1H
EXMOD proton.jxp
OFR 600.17 MHz
OBSET 6.50 KHz
OBFIN 5.81 Hz
POINT 16384
FREQU 11281.59 Hz
SCANS 32
ACQTM 1.4523 sec
PD 5.0000 sec
PW1 4.48 usec
IRN
CTEMP 19.1 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.12 Hz
RGAIN 56
2
PPM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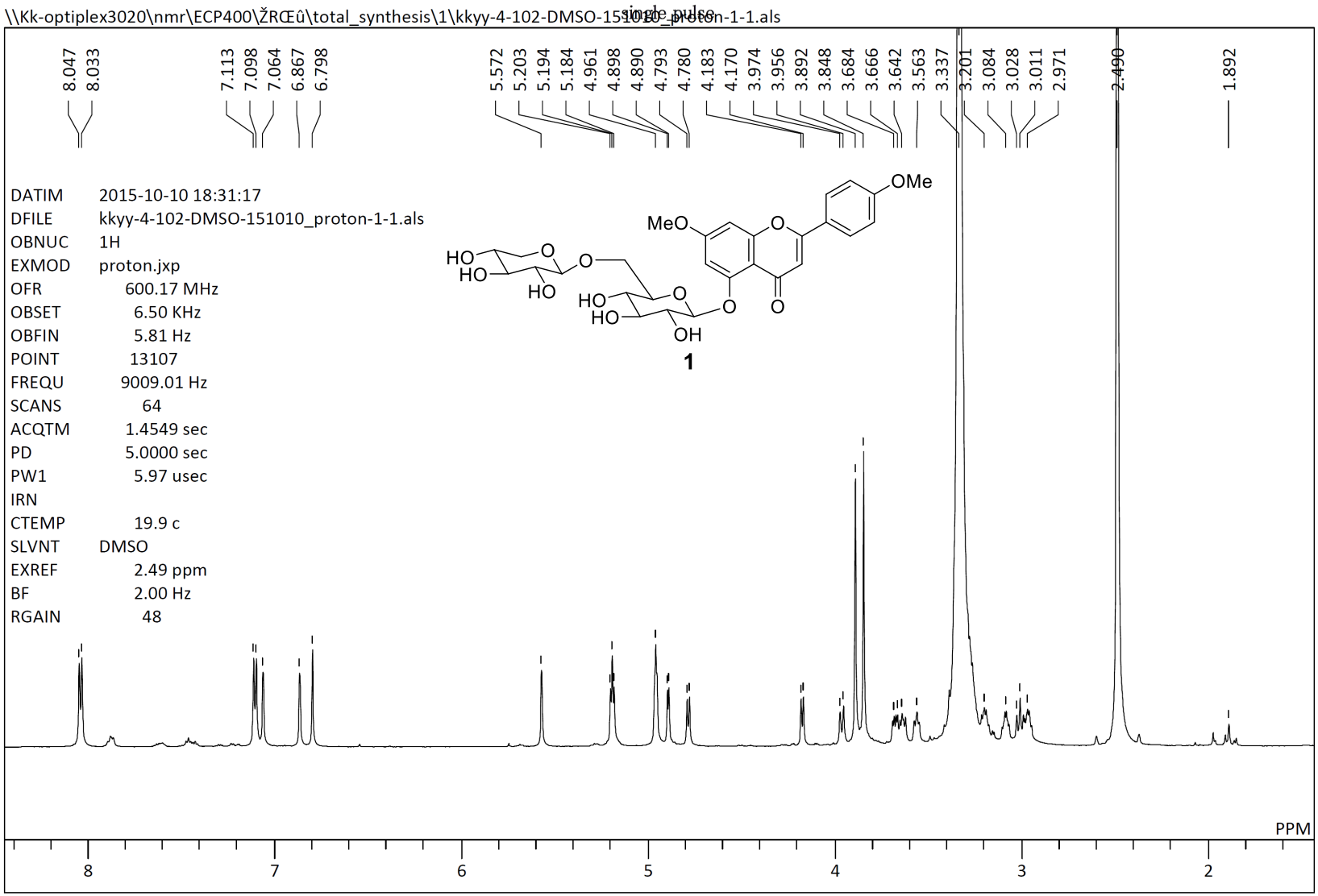
176.582
170.310
169.726
169.478
165.535
165.151
165.039
163.535
162.271
159.159
156.680
133.410
133.338
133.234
129.867
129.755
129.739
129.275
129.195
129.075
128.435
128.371
128.267
127.787
123.515
114.404
109.893
106.909
104.637
100.062
99.670
95.798
77.208
77.000
76.784
73.816
72.632
70.697
69.305
69.001
68.737
68.313
67.841
60.138
55.930
55.490
29.677
20.942
20.670
DATIM 2017-02-14 20:28:03
DFILE kkyy-5-37-A-2-chloroform-170214_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 39556.96 Hz
SCANS 16580
ACQTM 0.8284 sec
PD 2.0000 sec
PW1 3.21 usec
IRN
CTEMP 18.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 56
OMe
MeO
BzO
BzO
BzO
AcO
AcO
OAc
2
200
175
150
125
100
75
50
25
0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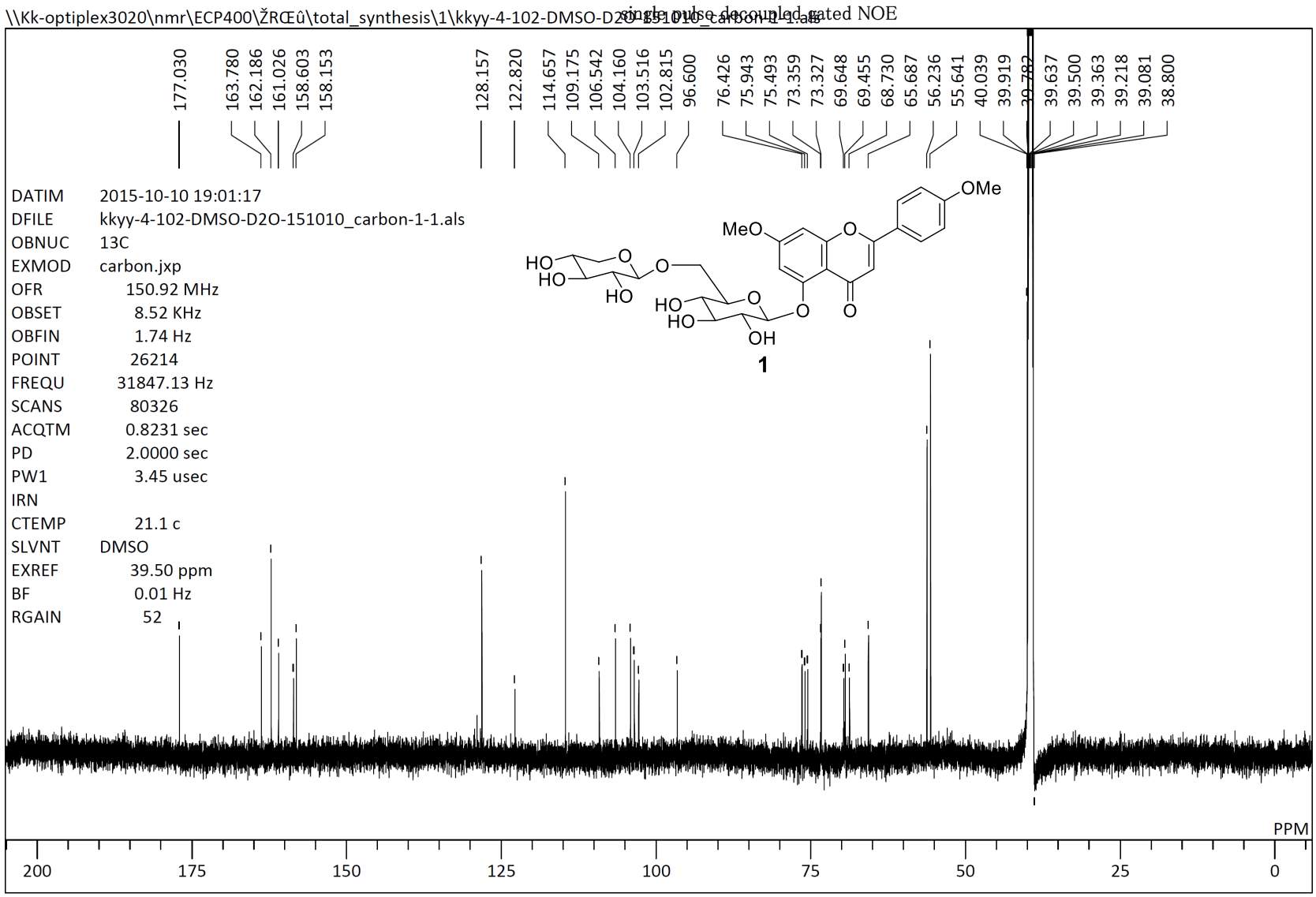
single_pulse
8.047
8.033
7.113
7.098
7.064
6.867
6.798
5.572
5.203
5.194
5.184
4.961
4.898
4.890
4.793
4.780
4.183
4.170
3.974
3.956
3.892
3.848
3.684
3.666
3.642
3.563
3.337
3.201
3.084
3.028
3.011
2.971
2.490
1.892
DATIM 2015-10-10 18:31:17
DFILE kkyy-4-102-DMSO-151010_proton-1-1.als
OBNUC 1H
EXMOD proton.jxp
OFR 600.17 MHz
OBSET 6.50 KHz
OBFIN 5.81 Hz
POINT 13107
FREQU 9009.01 Hz
SCANS 64
ACQTM 1.4549 sec
PD 5.0000 sec
PW1 5.97 usec
IRN
CTEMP 19.9 c
SLVNT DMSO
EXREF 2.49 ppm
BF 2.00 Hz
RGAIN 48
OMe
MeO
HO
HO
HO
HO
HO
OH
O
1
PPM
8
7
6
5
4
3
2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single pulse decoupled gated NOE
177.030
163.780
162.186
161.026
158.603
158.153
128.157
122.820
114.657
109.175
106.542
104.160
103.516
102.815
96.600
76.426
75.943
75.493
73.359
73.327
69.648
69.455
68.730
65.687
56.236
55.641
40.039
39.919
39.782
39.637
39.500
39.363
39.218
39.081
38.800
DATIM 2015-10-10 19:01:17
DFILE kkyy-4-102-DMSO-D2O-151010_carbon-1-1.als
OBNUC 13C
EXMOD carbon.jxp
OFR 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 26214
FREQU 31847.13 Hz
SCANS 80326
ACQTM 0.8231 sec
PD 2.0000 sec
PW1 3.45 usec
IRN
CTEMP 21.1 c
SLVNT DMSO
EXREF 39.50 ppm
BF 0.01 Hz
RGAIN 52
OMe
MeO
HO
HO
HO
HO
HO
OH
O
1
PPM
200
175
150
125
100
75
50
25
0