

Glucosamine and Glucosamine-6-phosphate Derivatives: Catalytic Cofactor

Analogs for the *glmS* Ribozyme

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Supporting Information

General Experimental Details. Unless otherwise noted, flash chromatography was performed using a Biotage Isolera™ system and Silicycle Siliasep™ HP silica cartridges. TLC plates were visualized by dipping in a solution of 4-methoxybenzaldehyde, sulfuric acid and ethanol (1:1:10) and subsequently heating. Anion exchange chromatography was performed on TSKgel DEAE-5PW on an analytical size (7.5 mm ID x 7.5cm L, 10 μm) at 1 mL/min or a preparative size (21.5 mm ID x 15 Cm, 13μm) at 6 mL/min using ÄKTA Purifier 10. Semipreparative reversed phase HPLC was carried out using a Supelco Discovery C18 (10 mm i.d. x 25cm; 5 μm, 180 Å) or an Agilent ZORBAX Eclipse XDB C18 (9.4 mm i.d. x 25cm; 5 μm, 80 Å) columns at 3.5 and 4 mL/min, respectively. For compounds with weak or no chromophores, semi-preparative HPLC and anion exchange chromatography eluate fractions were monitored with a combination of UV₂₂₀ and MS analyses. HPLC and HRMS analyses were performed by ESI-TOF. NMR experiments were performed at the following frequencies: ¹H 500 MHz or 600

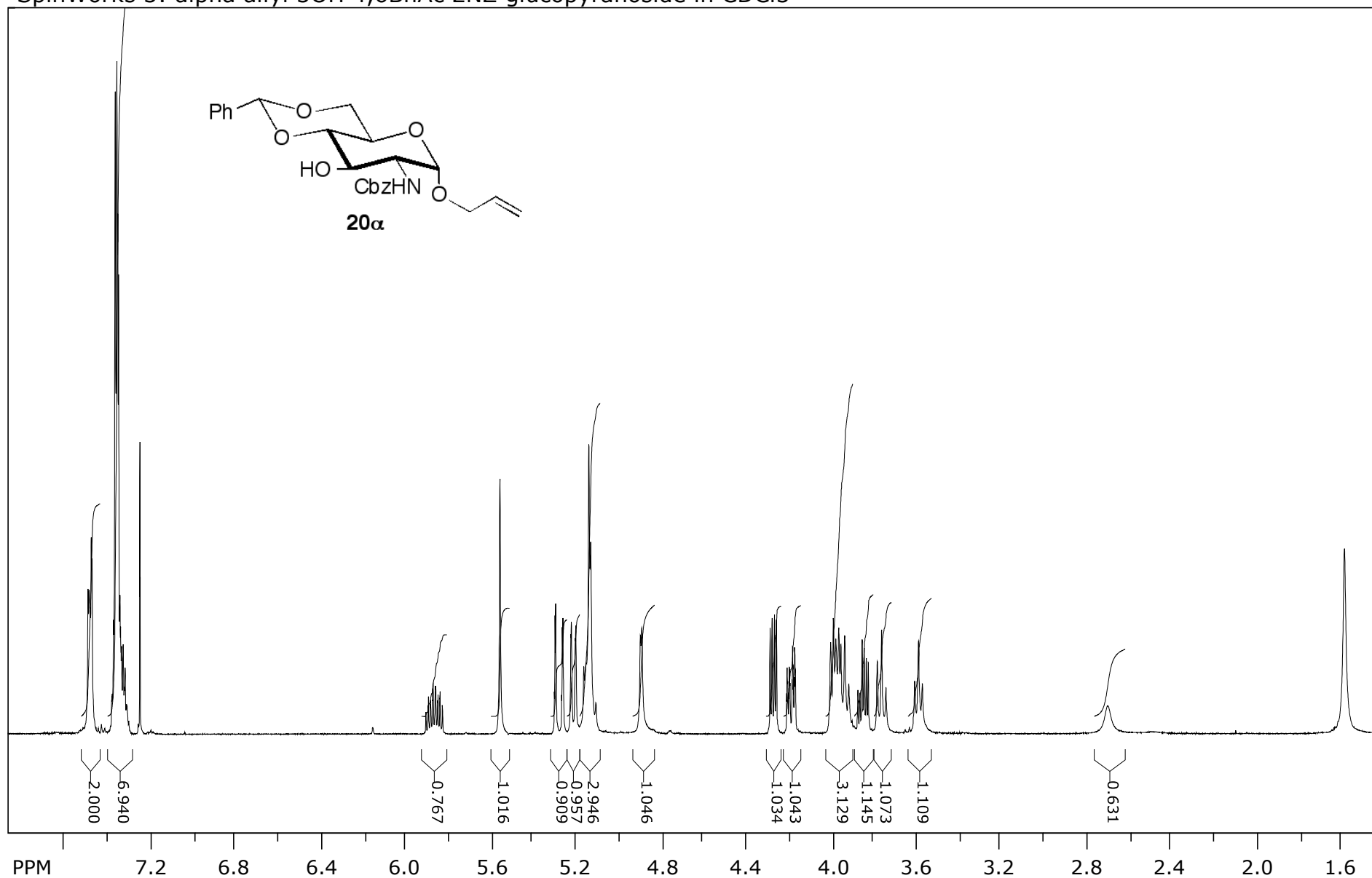
MHz; ^{13}C 125 MHz or 150 MHz; COSY 600 MHz; HMBC and HMQC (^1H at 600 MHz, ^{13}C at 150 MHz).

Table of Contents for Characterization Data

Each compound's characterization data includes ^1H , ^{13}C , and COSY NMR, and MS/HRMS unless otherwise indicated. Additional characterization information is shown in parentheses.

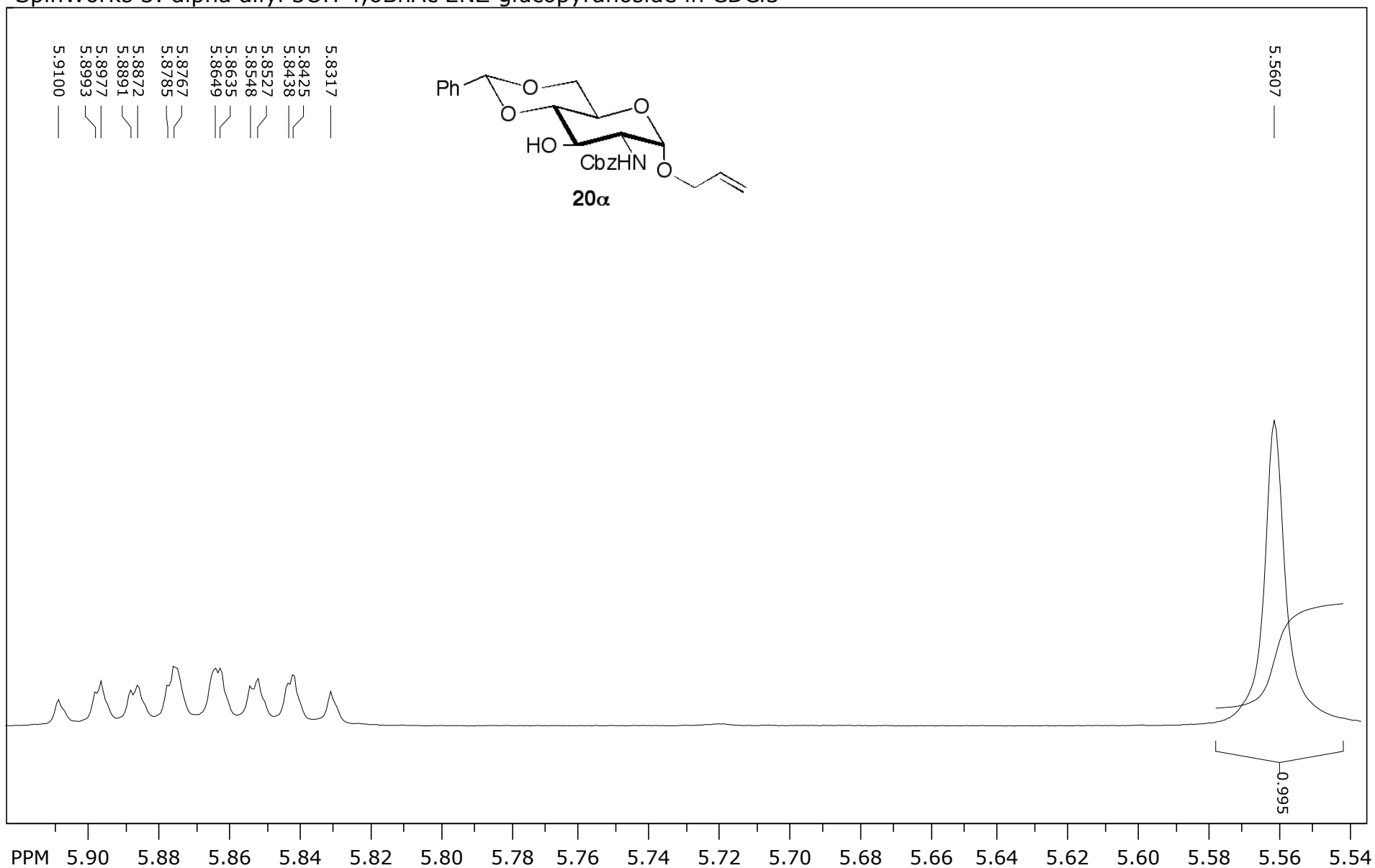
20α (HPLC; no COSY data)	S-4
20β (HPLC)	S-12
20β-mesylate	S-21
21	S-30
22	S-39
23	S-52
23-mesylate (HPLC)	S-60
24 (HPLC).....	S-69
25	S-77
26	S-85
27a (HPLC).....	S-94
27b (HPLC)	S-107
28a	S-119
28b (HPLC)	S-128
28c	S-138
29a (HPLC).....	S-147
29b (HPLC)	S-157
30a (HPLC).....	S-166
30b	S-175
31	S-184
33	S-190
34	S-198
35 (HMBC, HMQC NMR).....	S-206
36	S-216
37	S-223

38	S-232
39 (no COSY data).....	S-238
40 (no COSY data).....	S-248
41	S-260
42	S-271
43	S-280
47	S-289
48	S-300
49 (analysis of NMR spectra and proposed structures)	S-316
25-6-phosphate preparation (no ¹³C data)	S-327



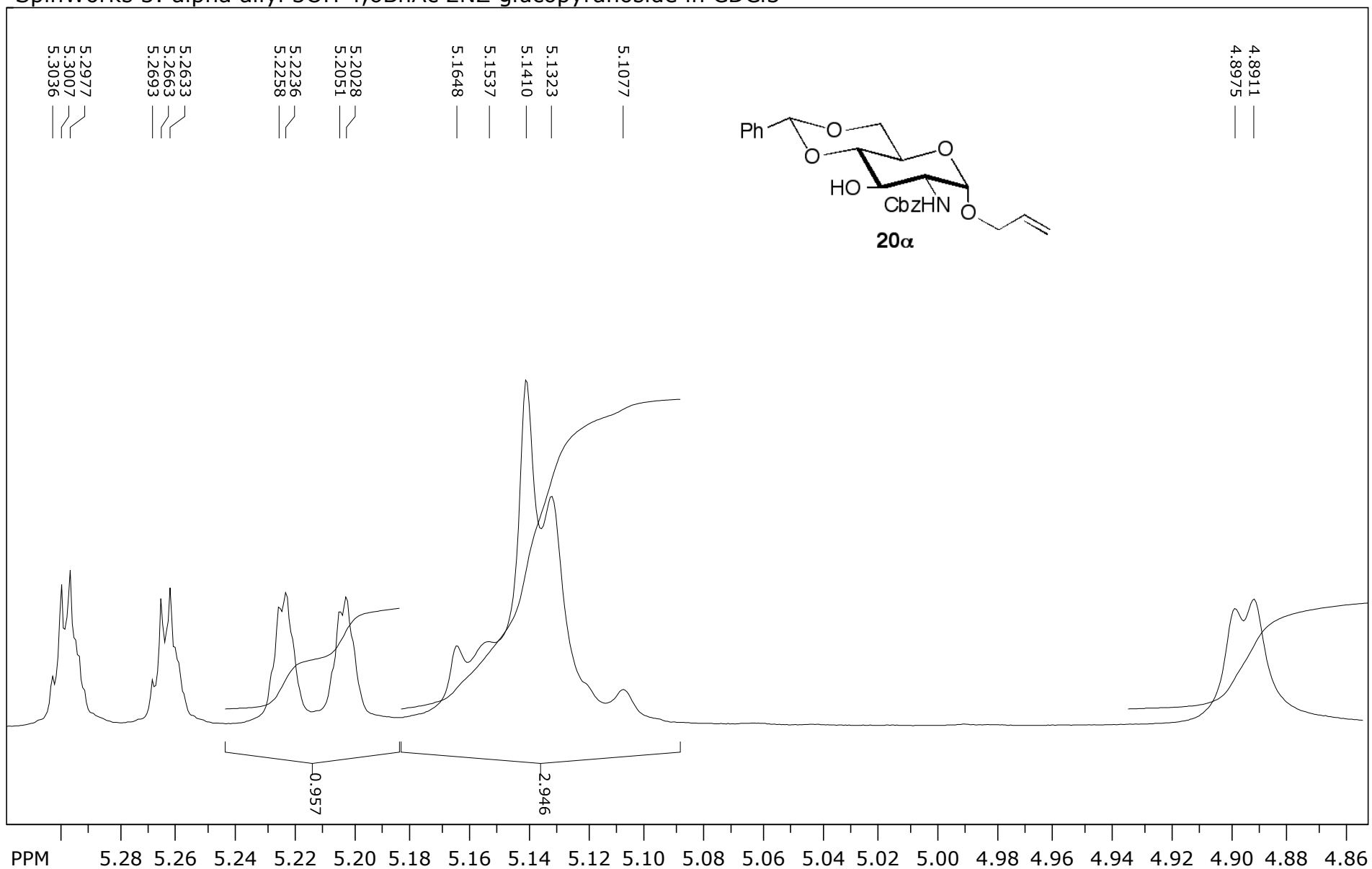
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number of scans: 64

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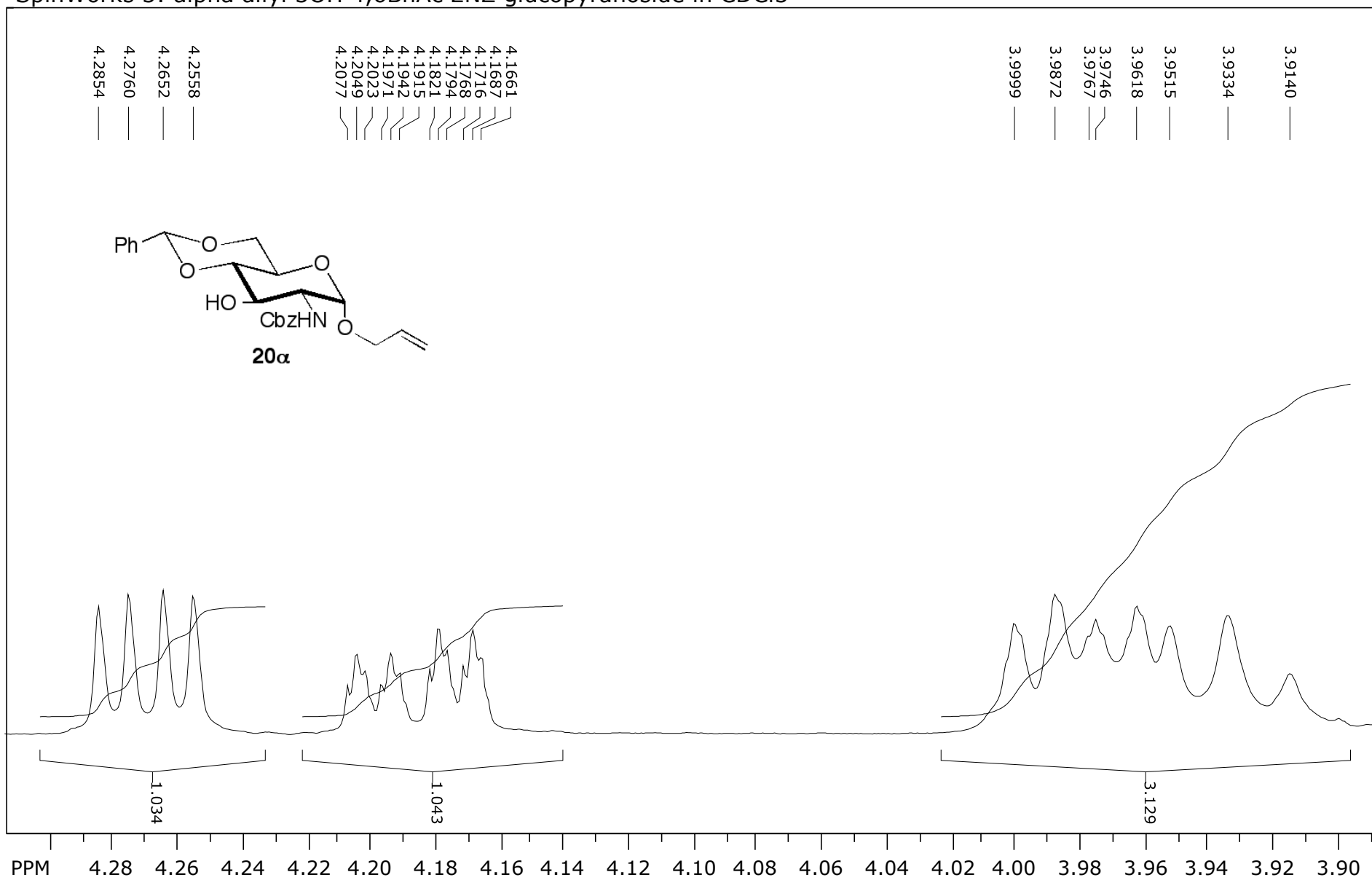
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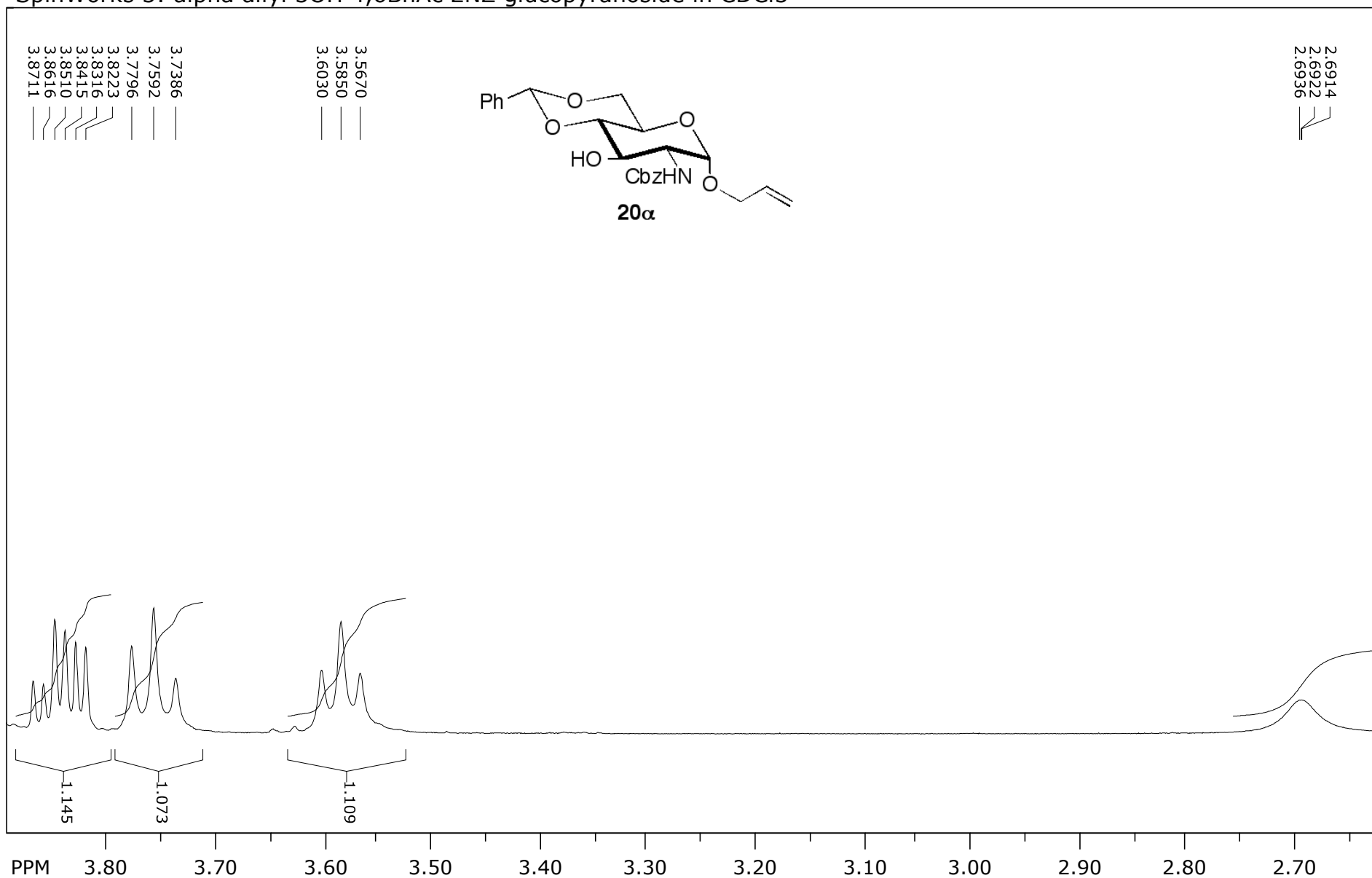
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number of scans: 64

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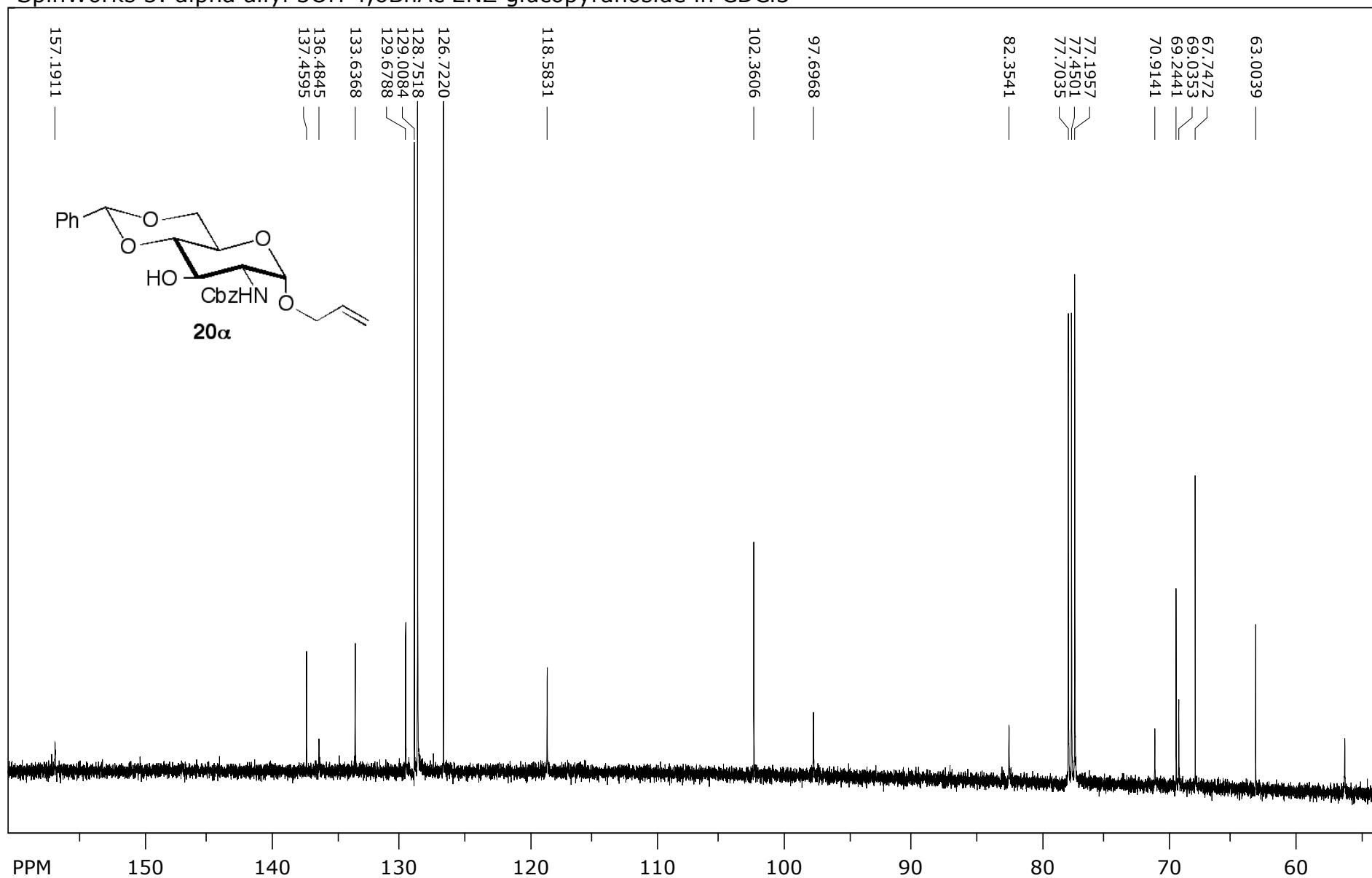
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 number of scans: 64

freq. of 0 ppm: 499.850012 MHz
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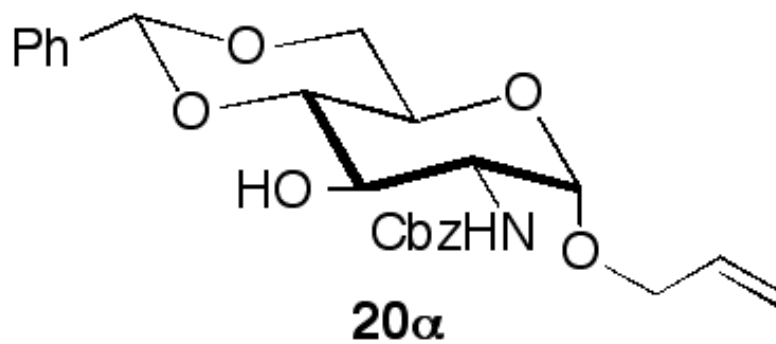
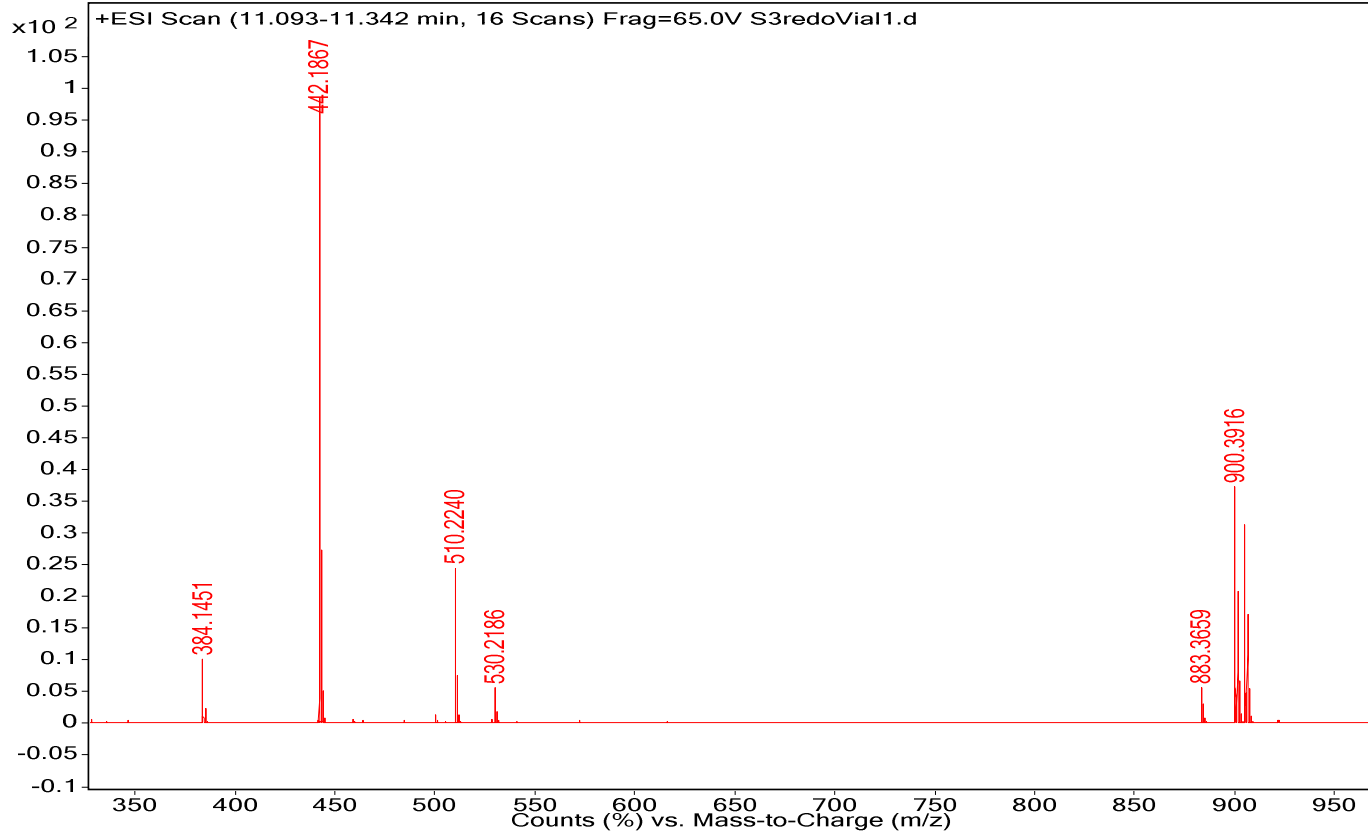
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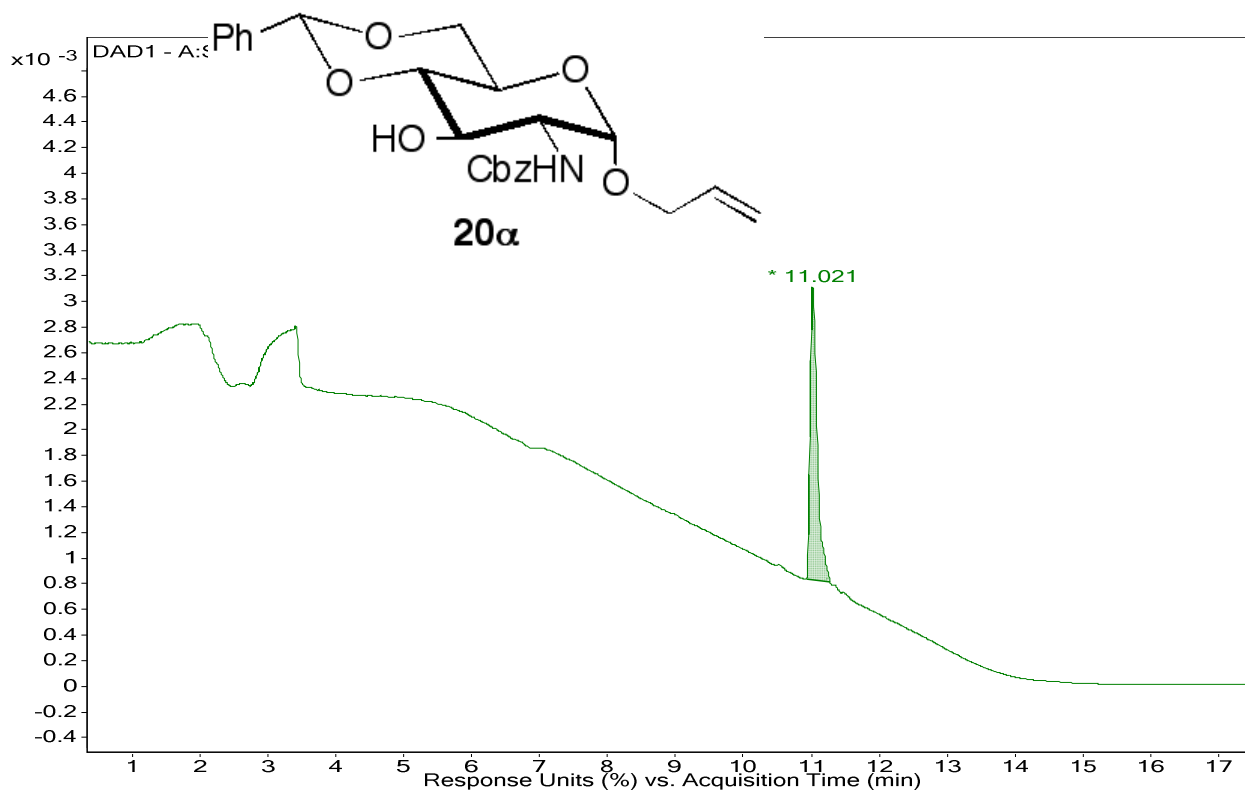


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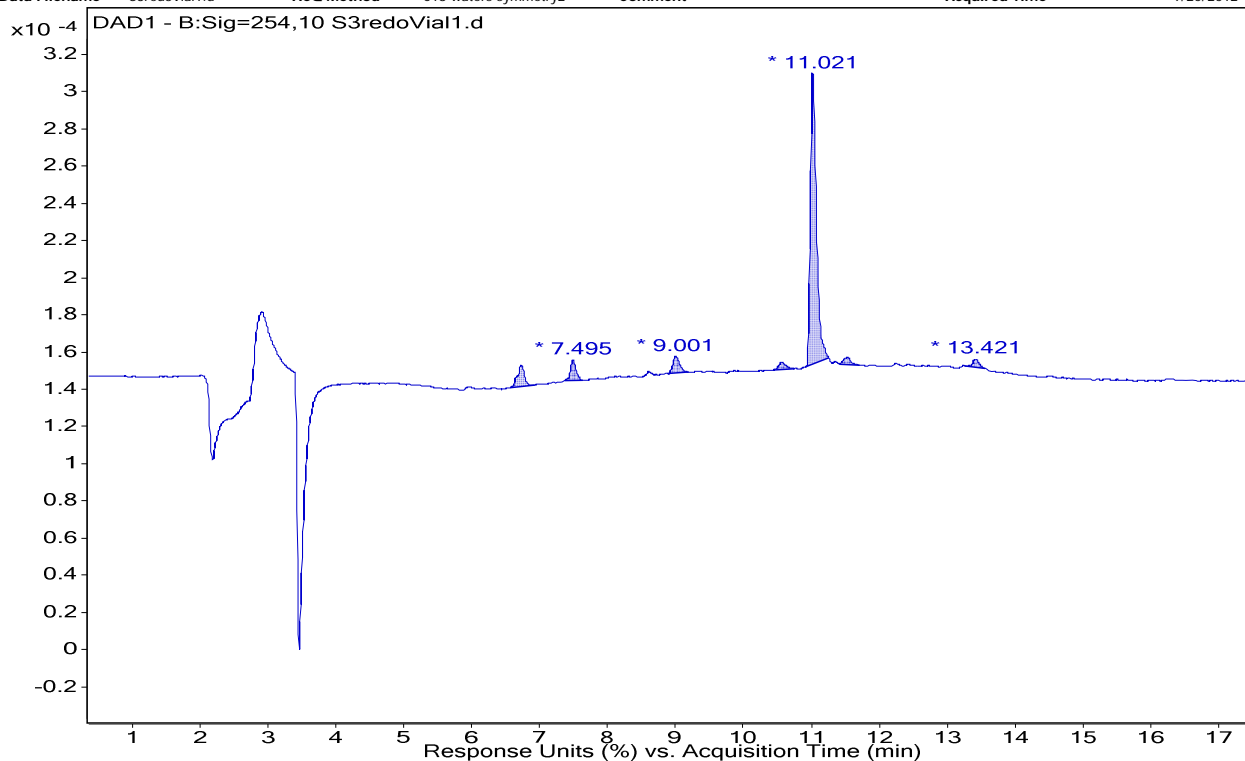
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Inj Vol	3	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	S3redoVial1.d	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/20/2012 11:51:30 PM



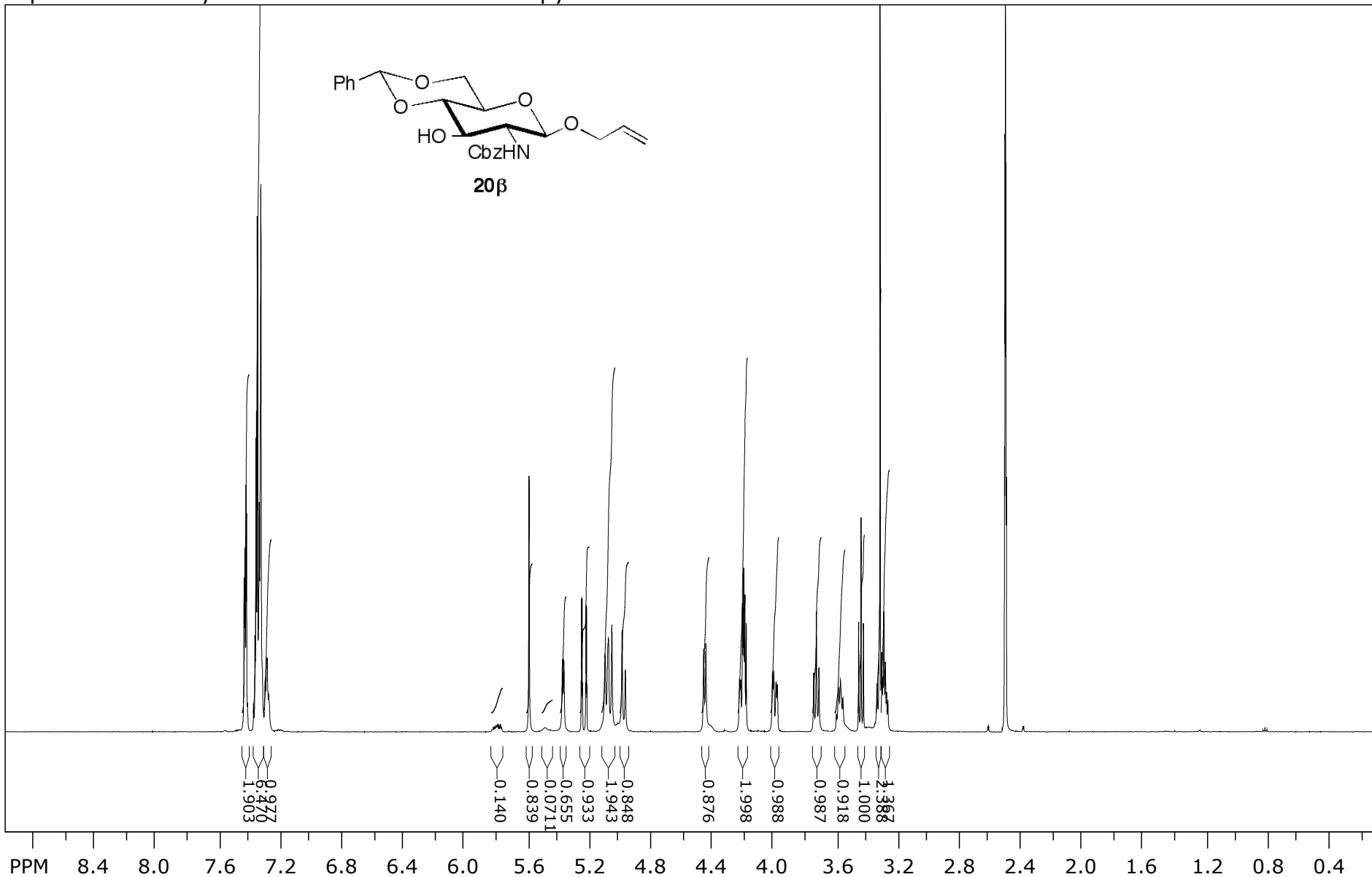
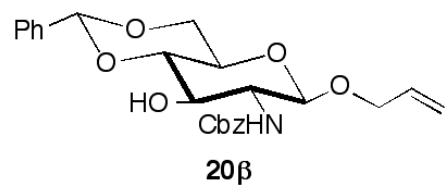


Sample Name	Samp3 vial1	Position	Vial 21	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	3	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	S3redoVial1.d	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/20/2012 11:51:30 PM



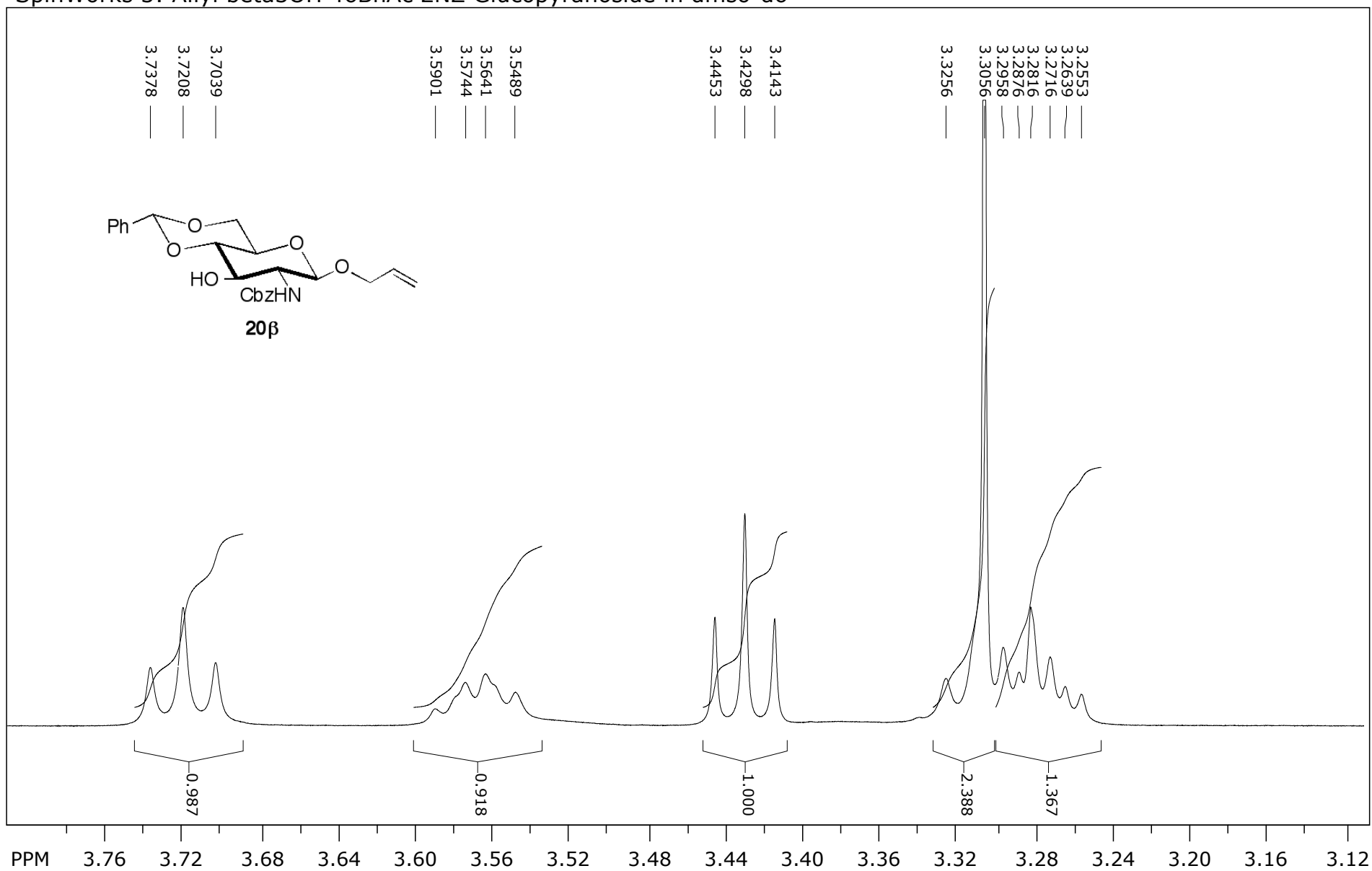
Analysis on a Waters SymmetryShield™ C18 (4.6 mm X 15 cm (i.d. x l.), 3.5 μ m) at 0.5 mL/min. Solvent A: 50 mM NH₄OAc (aq); B: CH₃CN

Time (min)	% B
0	20
1	20
10	100
20	100



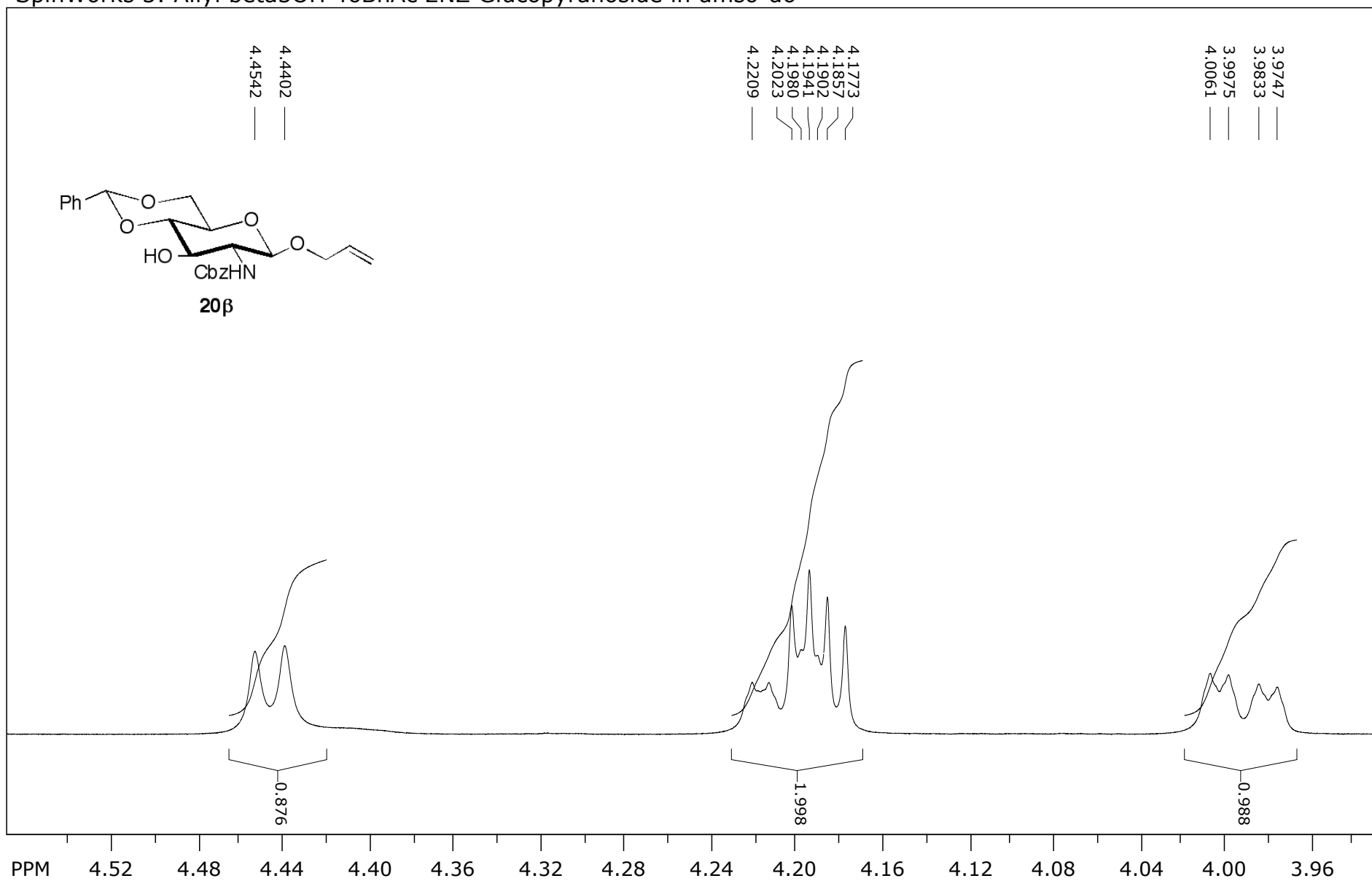
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width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

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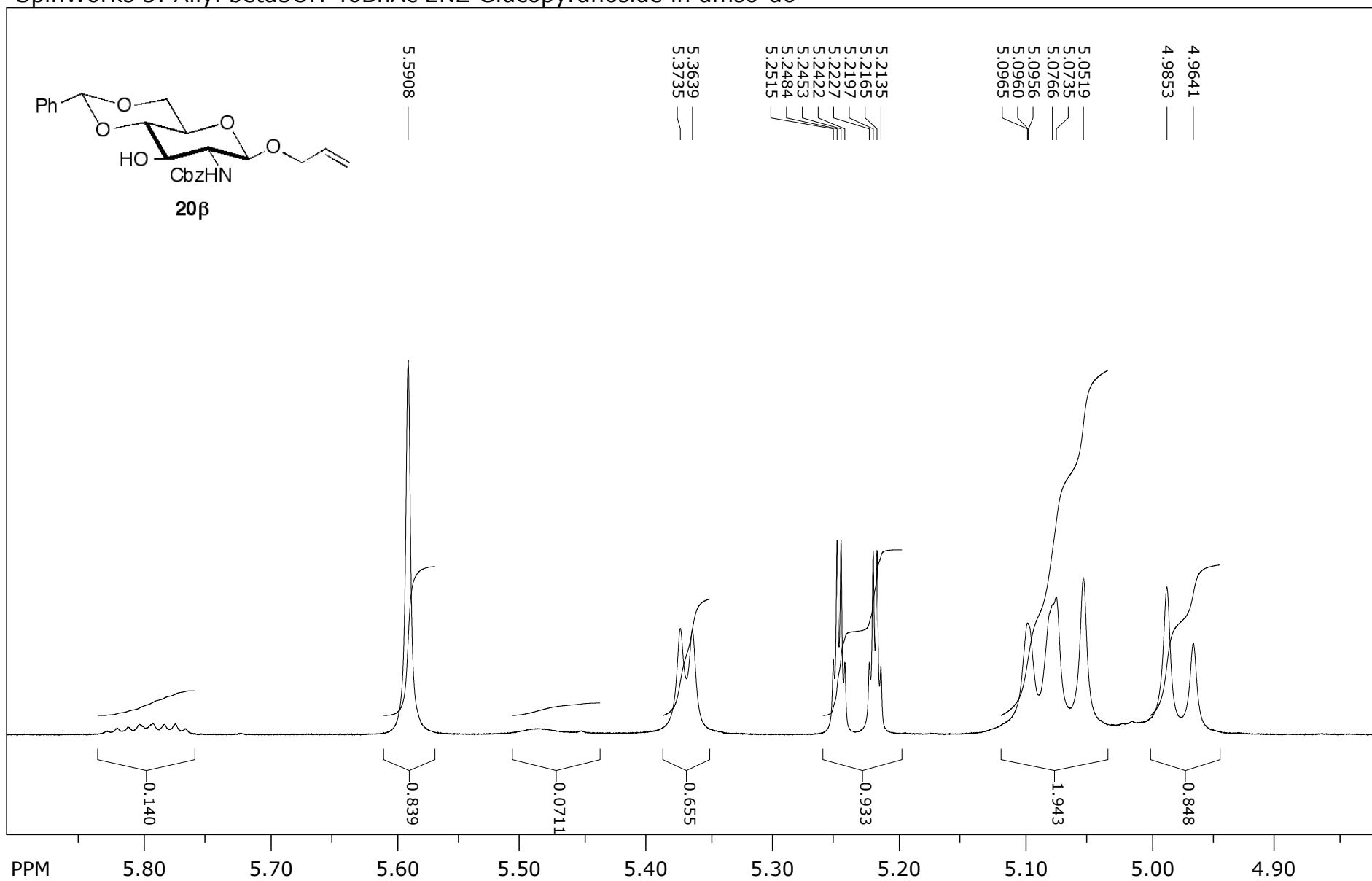
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 number of scans: 32

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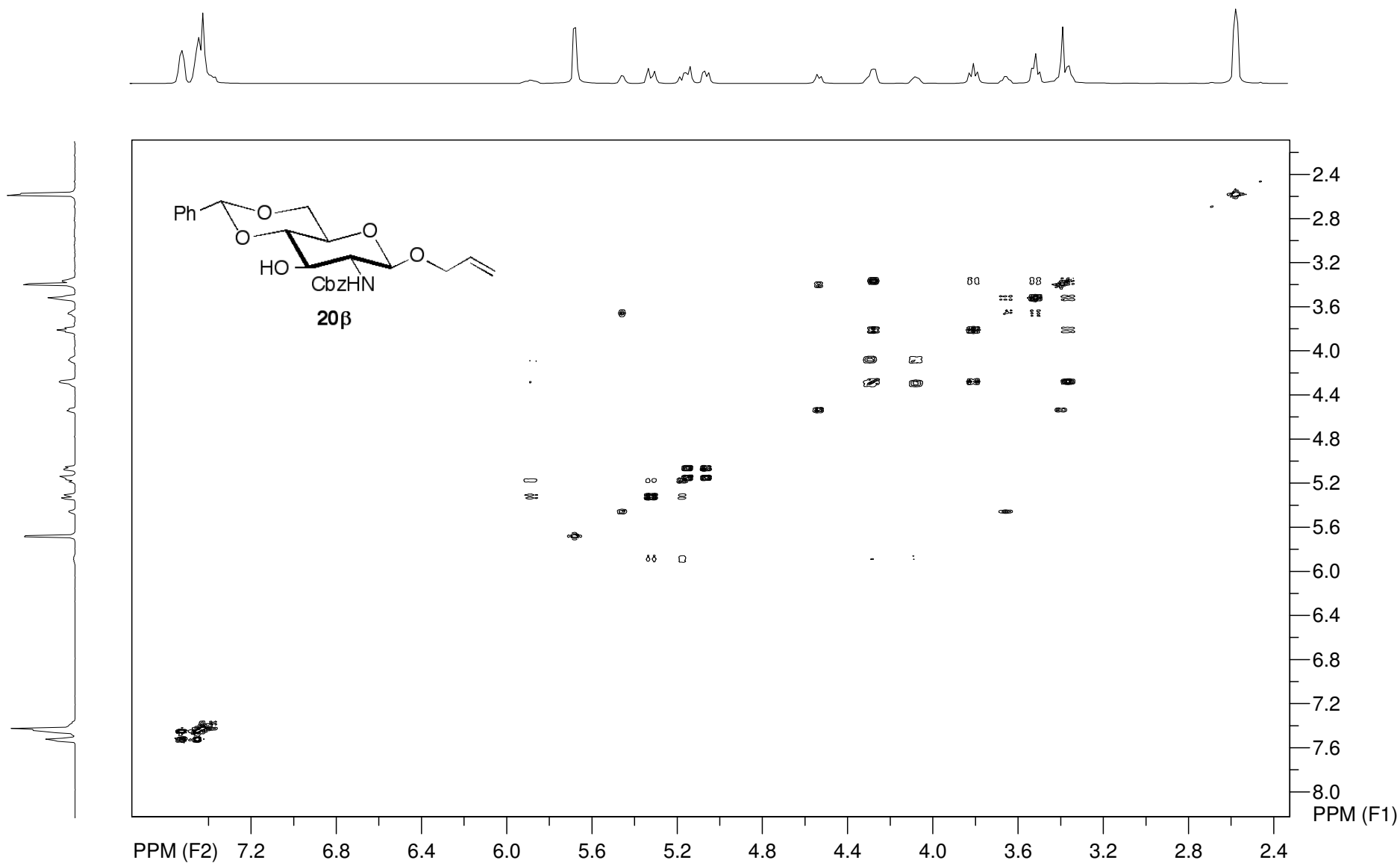
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time domain size: 65536 points
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number of scans: 32

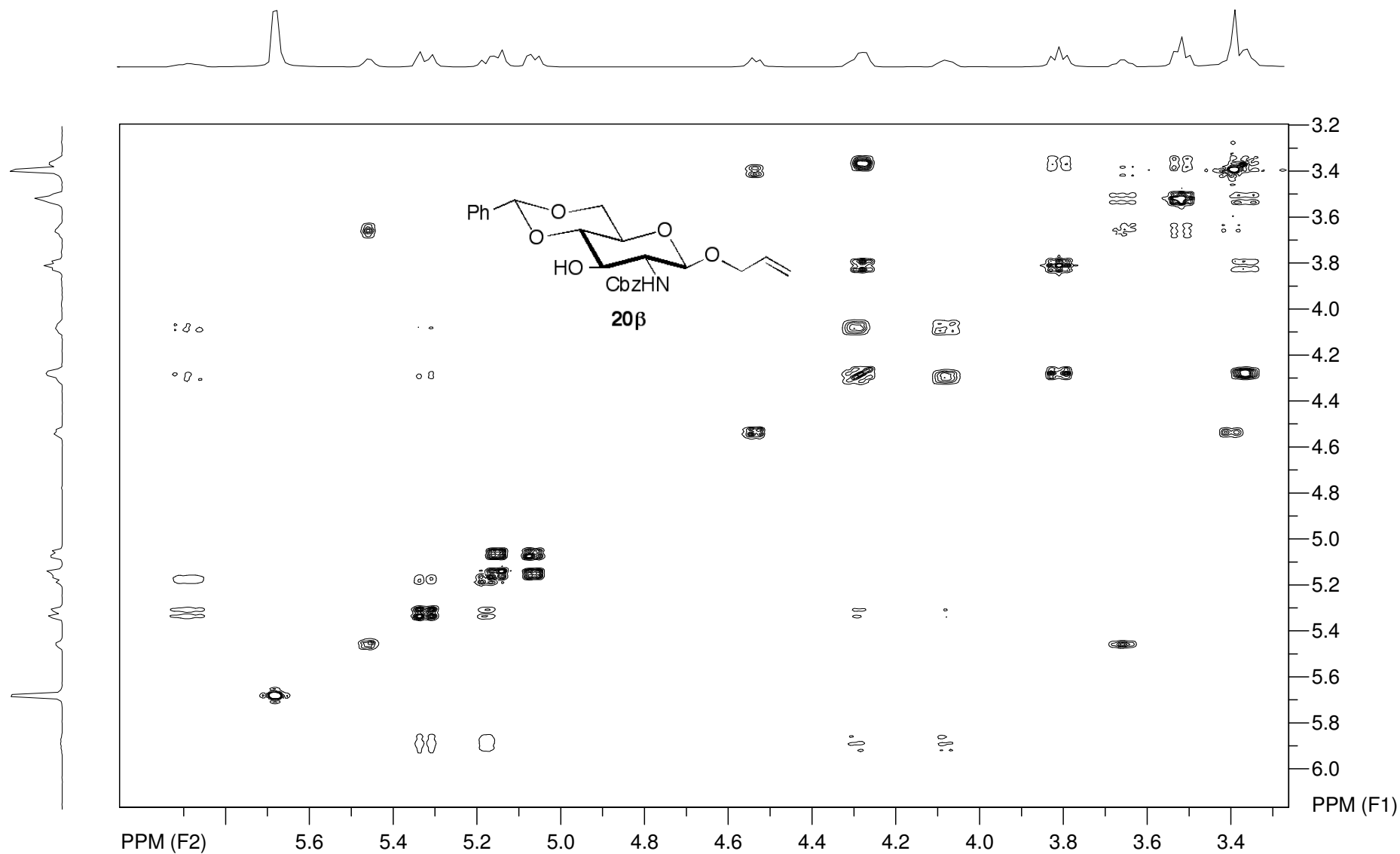
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transmitter freq.: 600.552832 MHz
time domain size: 2048 by 1024 points
width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
number of scans: 2

processed size: 1024 complex points
window function: Sine
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Hz/cm: 159.213 ppm/cm: 0.26511

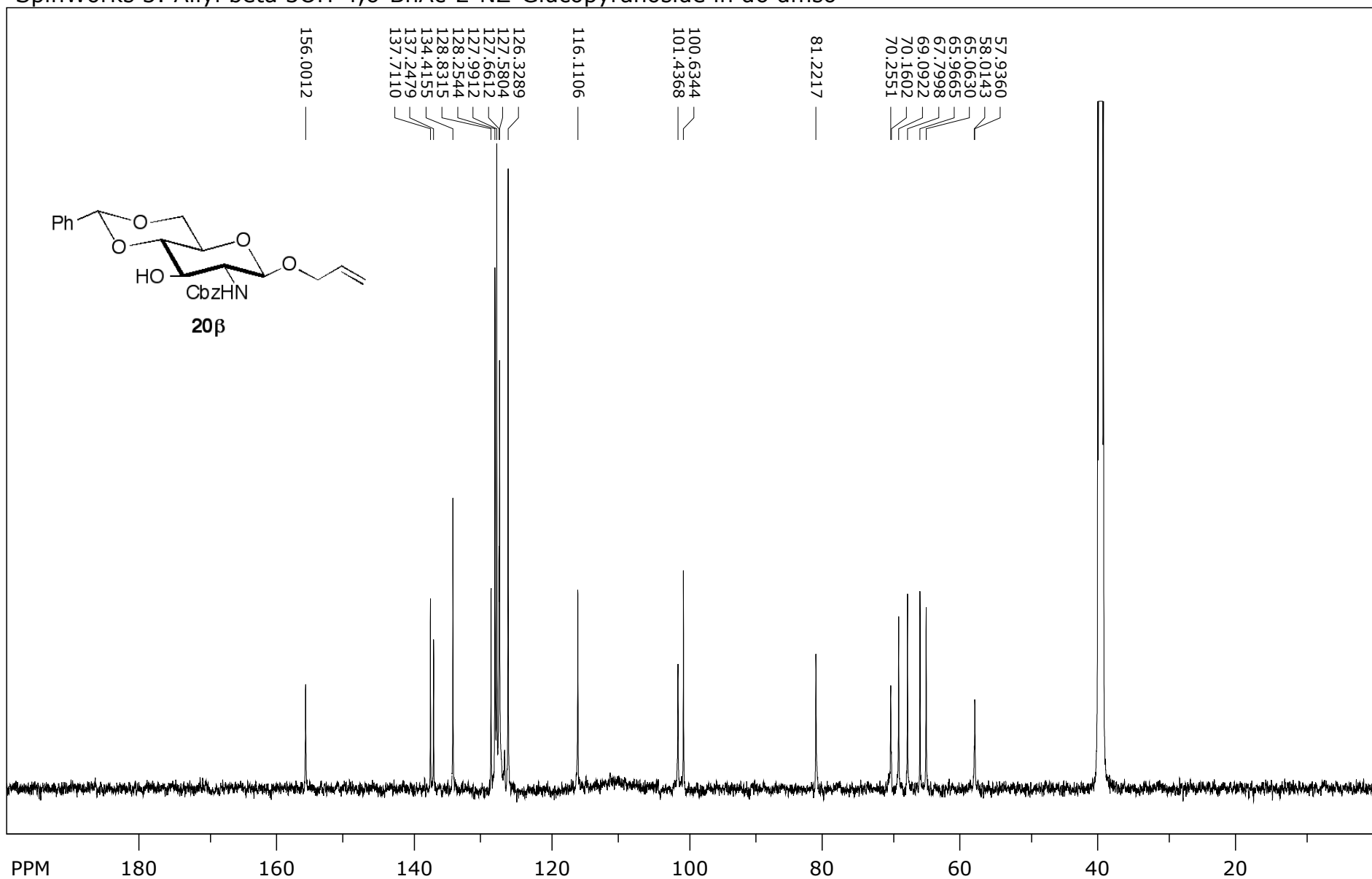
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Hz/cm: 307.245 ppm/cm: 0.51160



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\Allyl_beta3OHGluBnAcdrF2: freq. of 0 ppm: 600.549962 MHz
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time domain size: 2048 by 1024 points
width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
number of scans: 2

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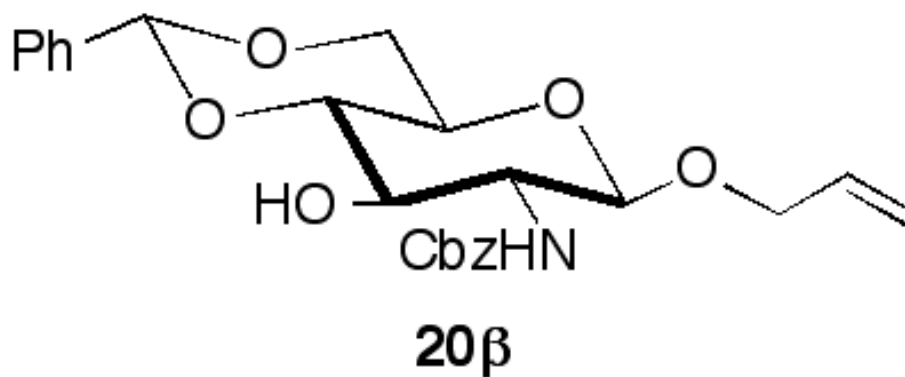
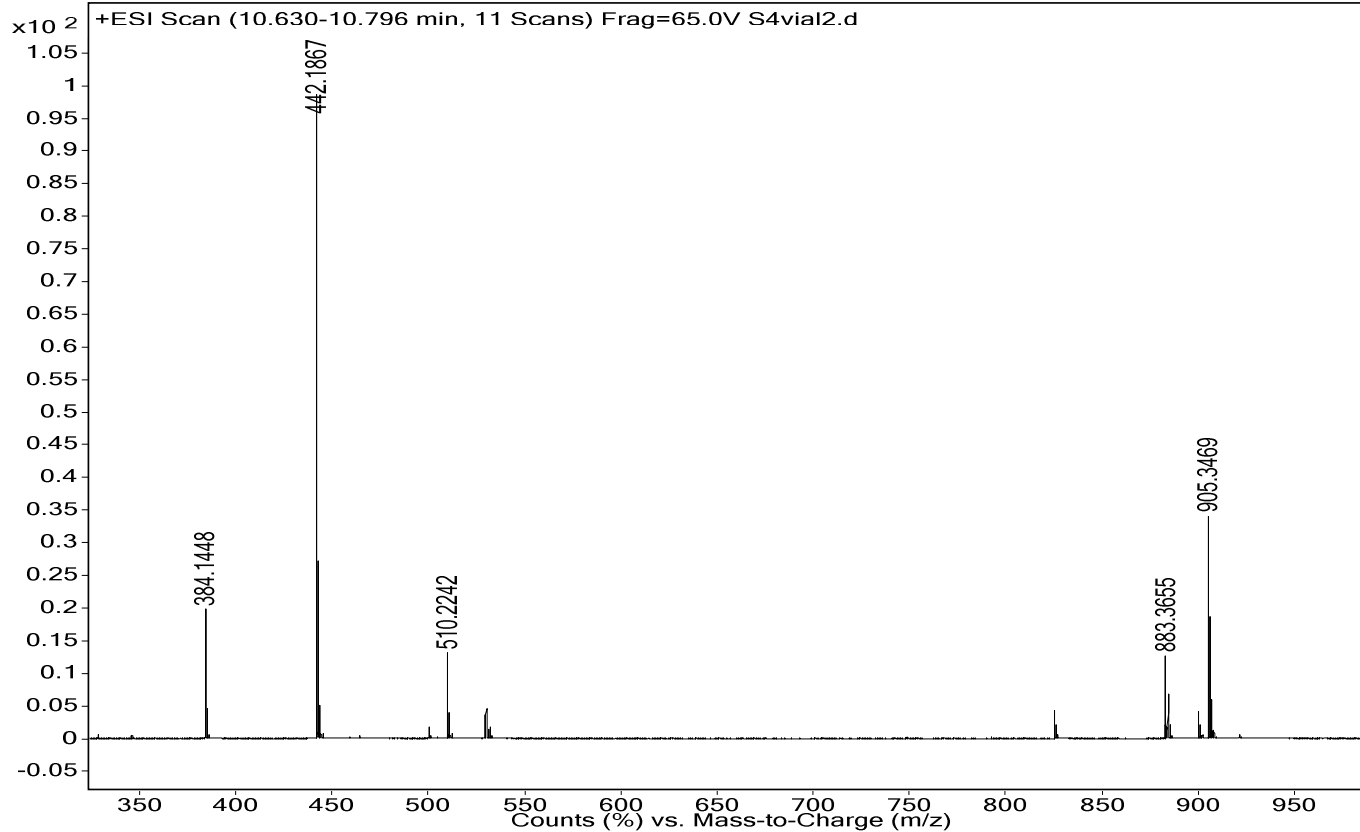
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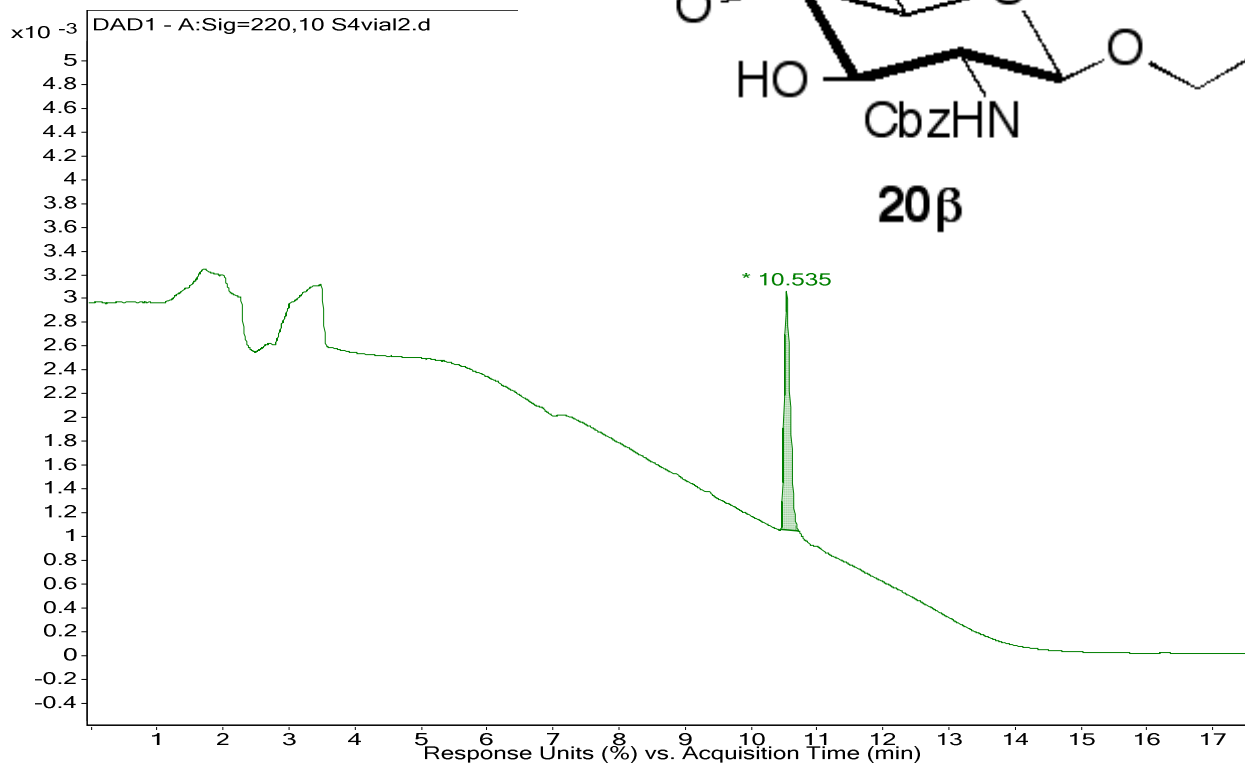
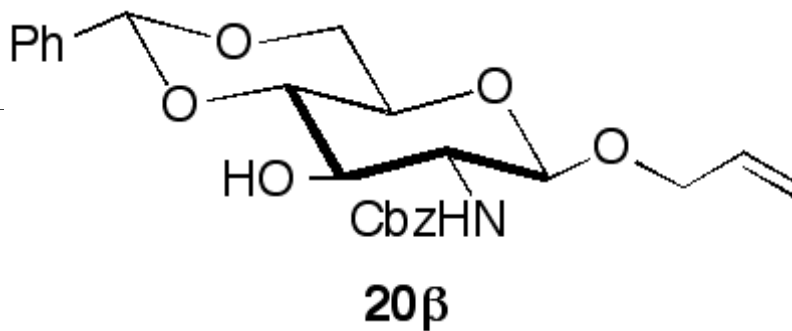


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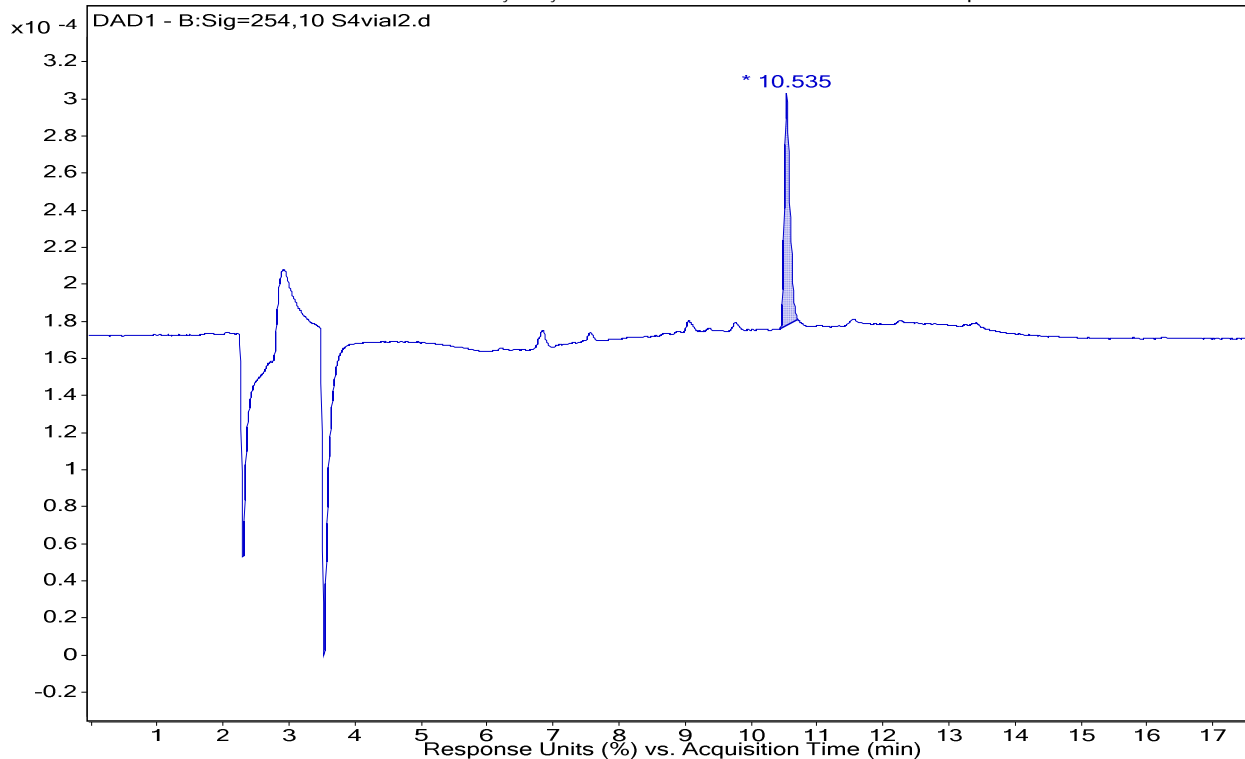
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Sample Name	columnprep	Position	Vial 24	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	3	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	S4vial2.d	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/21/2012 2:32:27 AM



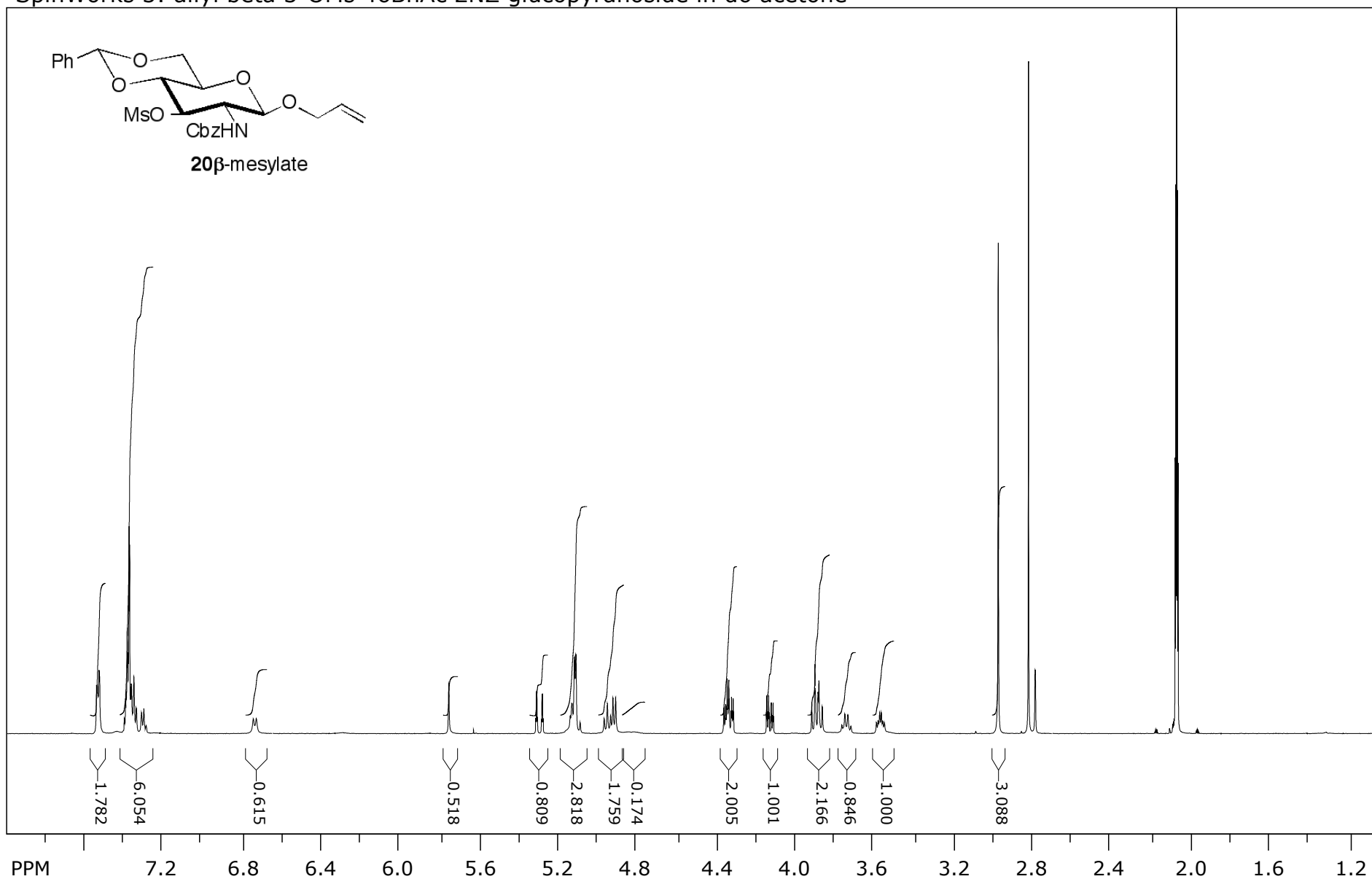


Sample Name	columnprep	Position	Vial 24	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	3	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	S4vial2.d	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/21/2012 2:32:27 AM



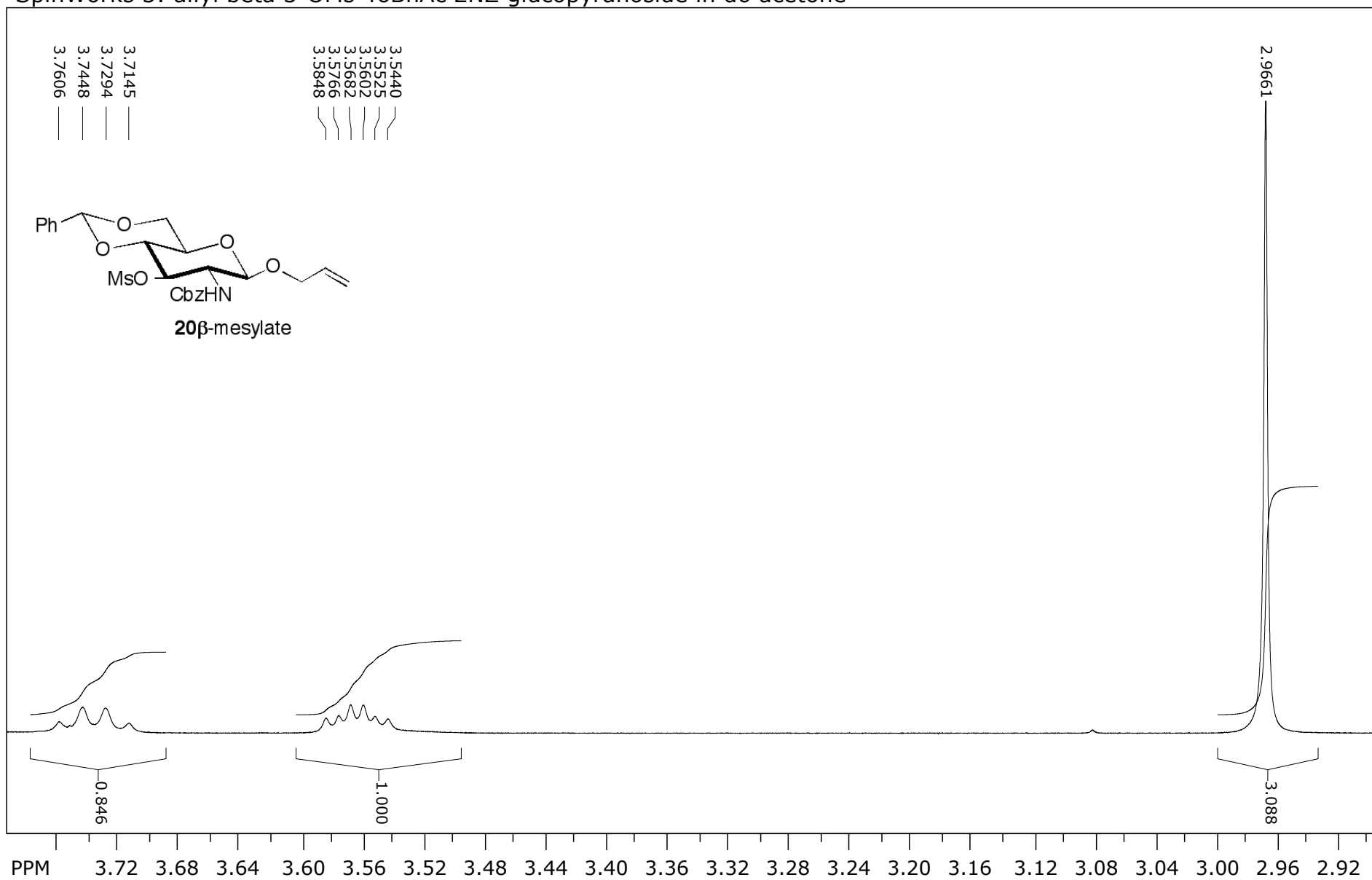
Analysis on a Waters SymmetryShield™ C18 (4.6 mm X 15 cm (i.d. x l.), 3.5 μ m) at 0.5 mL/min. Solvent A: 50 mM NH₄OAc (aq); B: CH₃CN

Time (min)	% B
0	20
1	20
10	100
20	100



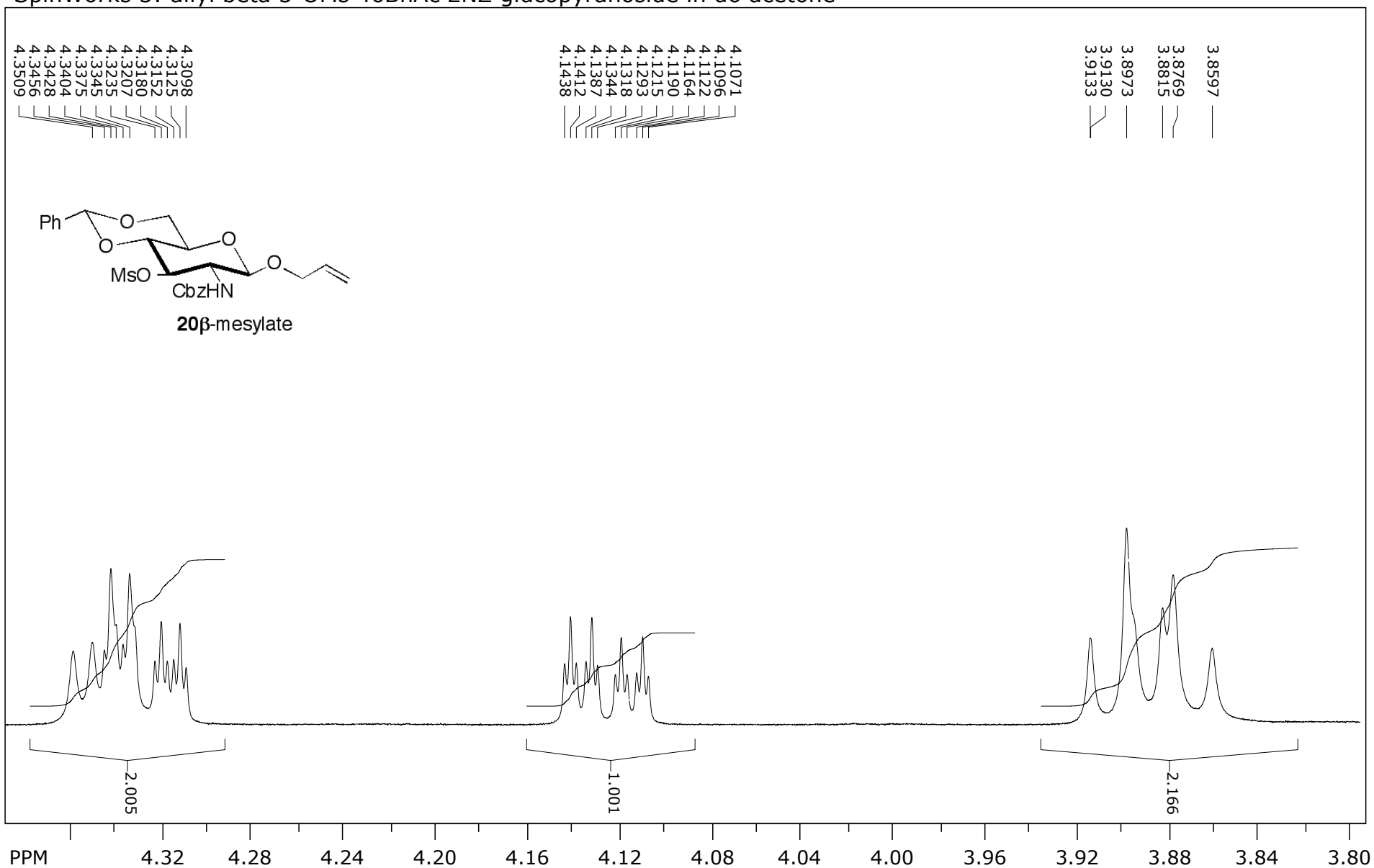
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time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

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processed size: 262144 complex points
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Hz/cm: 167.411 ppm/cm: 0.27876



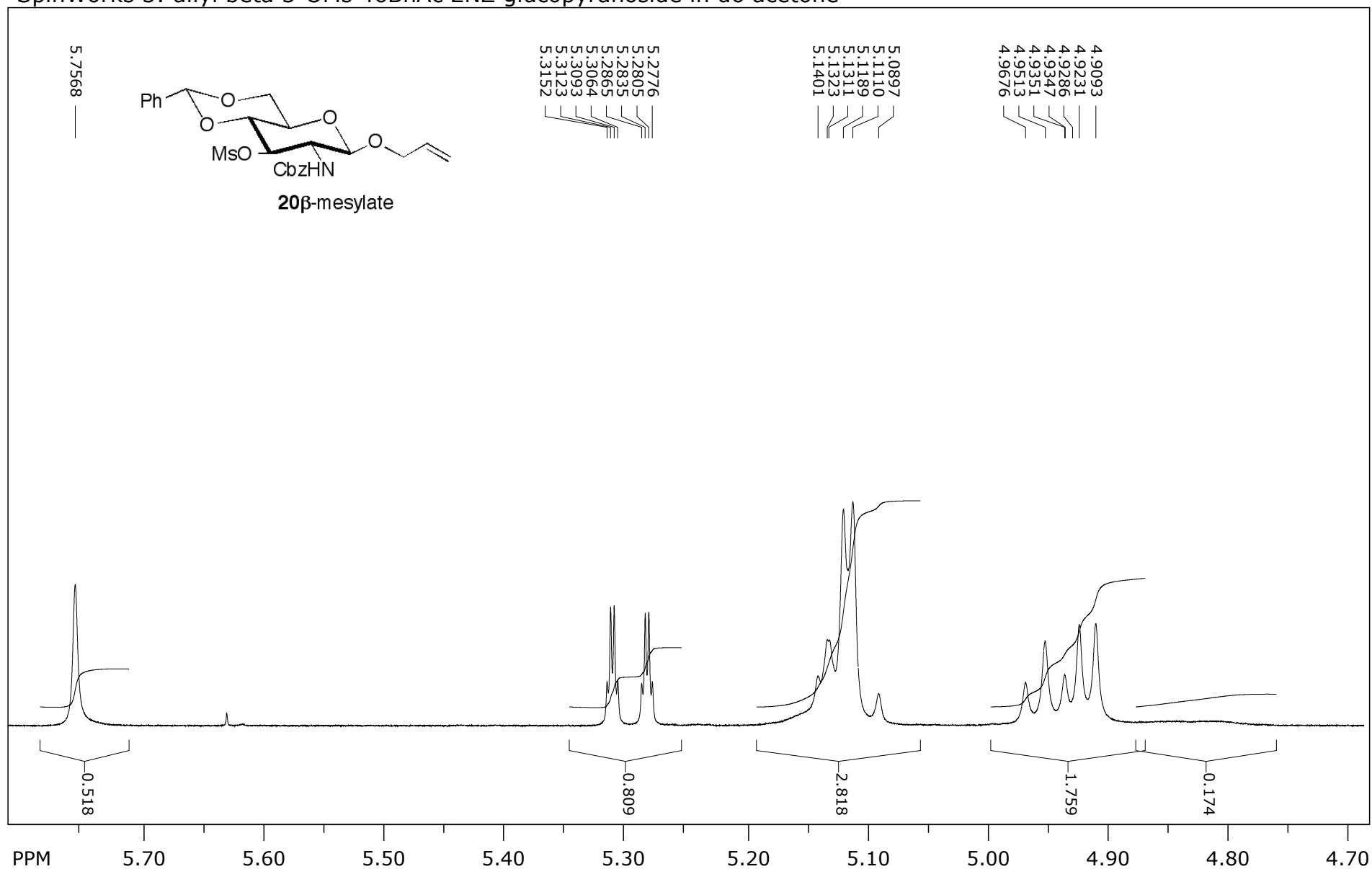
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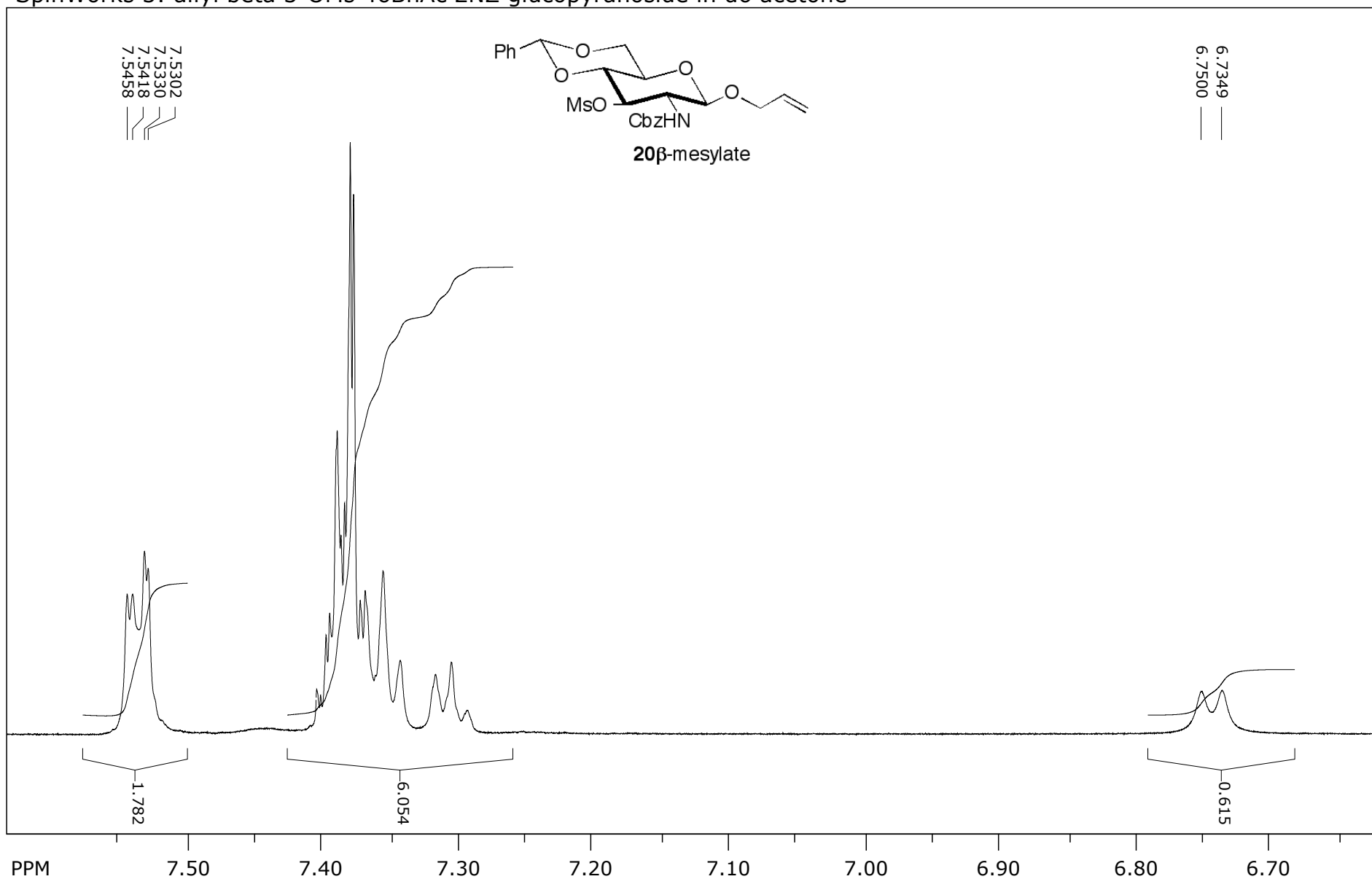
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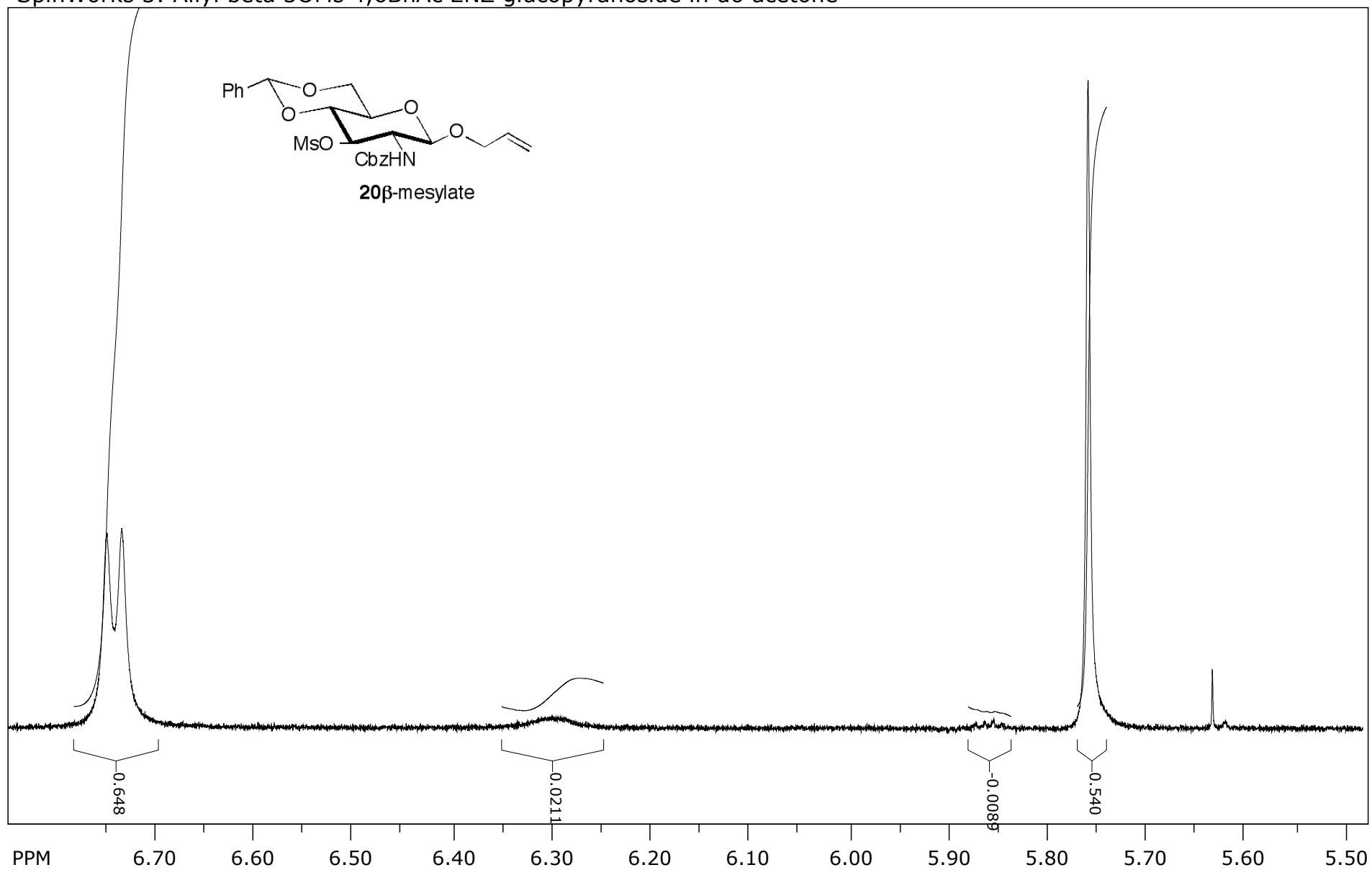
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time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
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Hz/cm: 27.056 ppm/cm: 0.04505



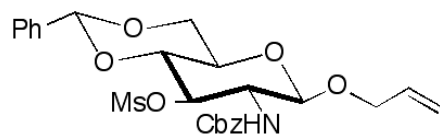
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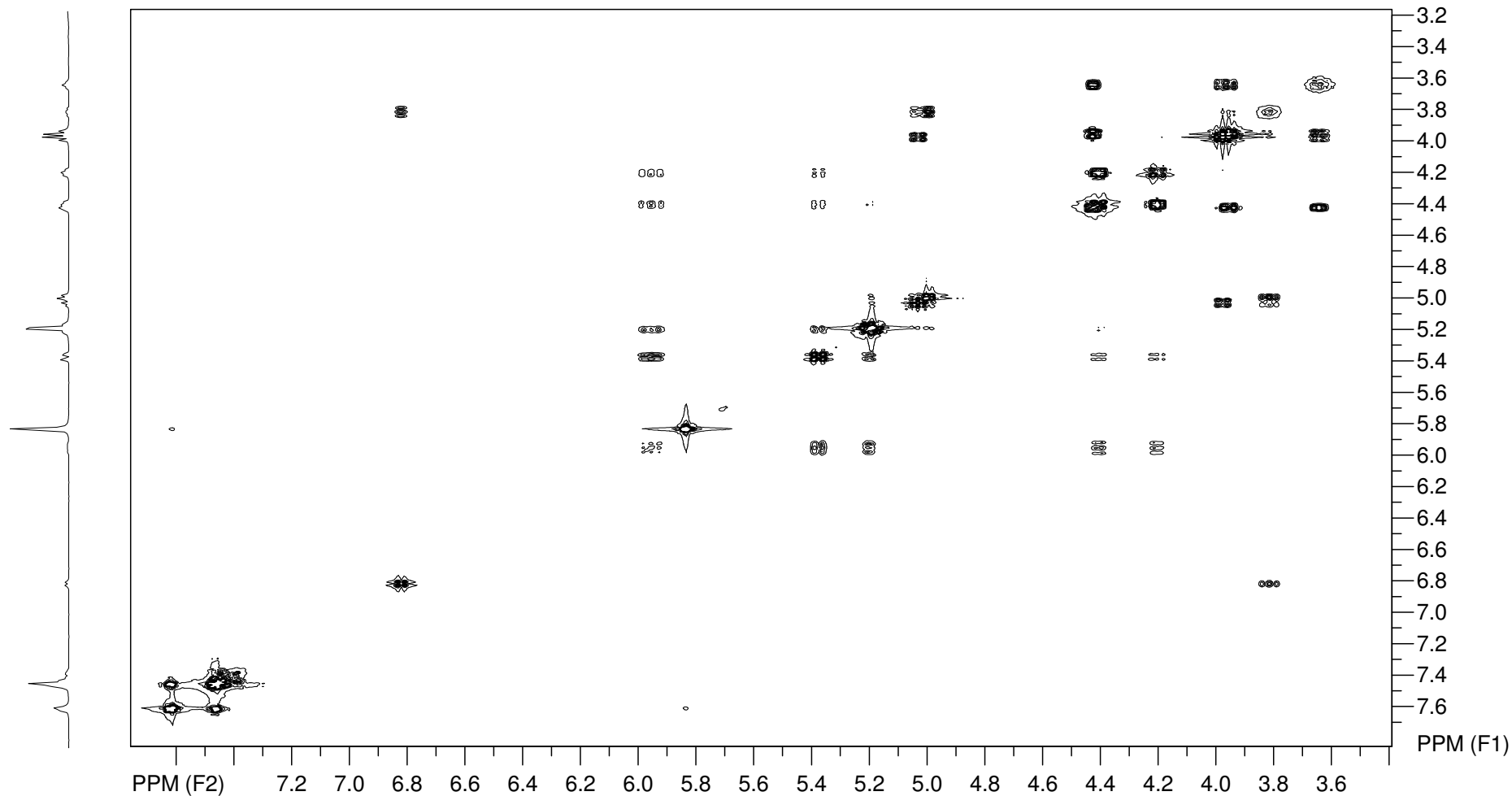


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time domain size: 65536 points
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number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 32.925 ppm/cm: 0.05482

in Acetone-*d*₆

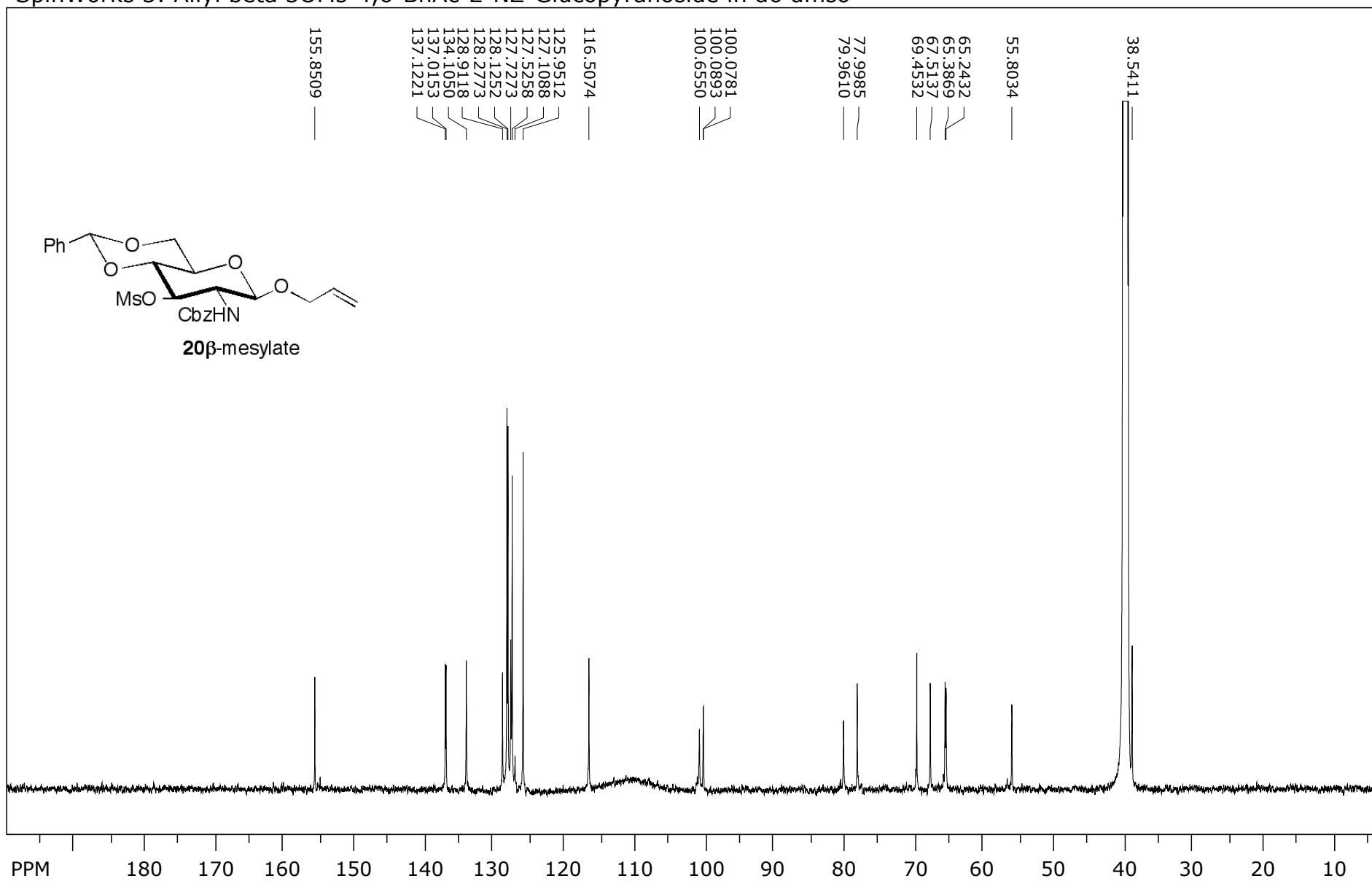
20β-mesylate



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\BetaGlu3OMsd6AcetCOSF2:\freq. of 0 ppm: 600.549962 MHz
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
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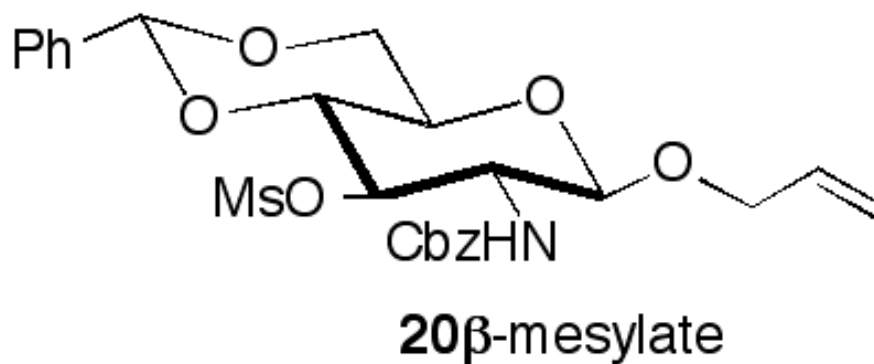
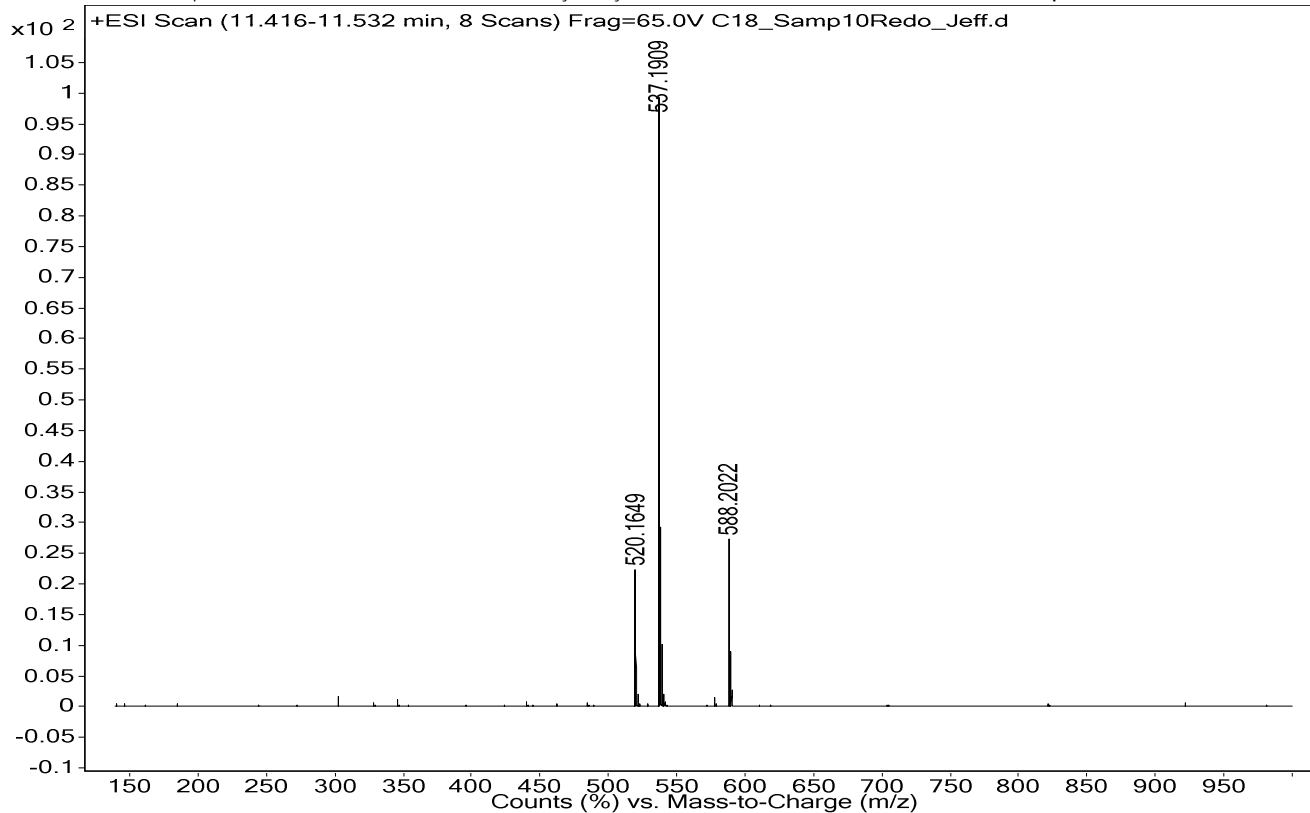
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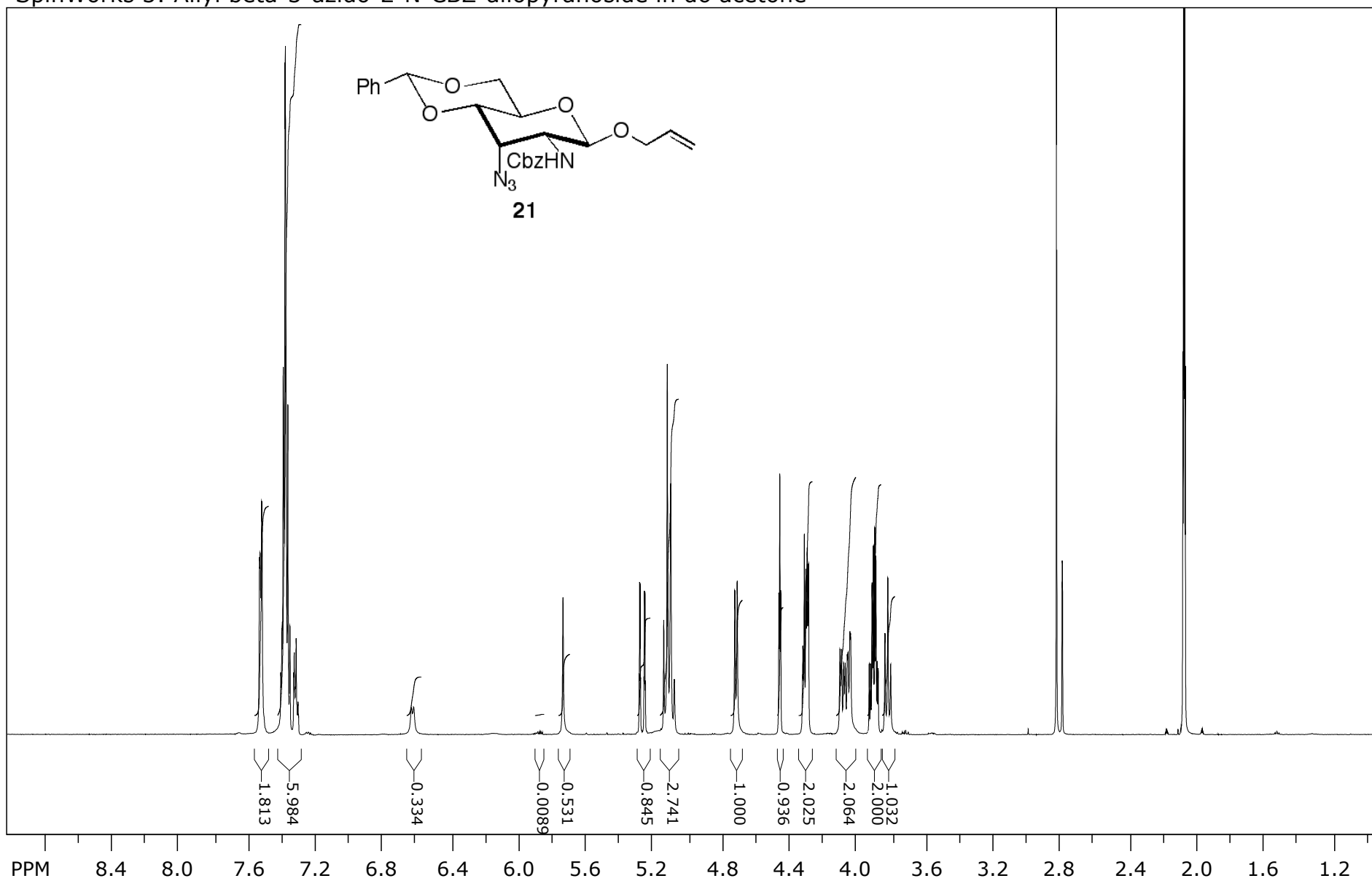


file: ...process\BetaGlu3OMsd6dms013C\1\fid expt: <zpgg30>
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time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 28672

freq. of 0 ppm: 151.008493 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 1189.582 ppm/cm: 7.87680

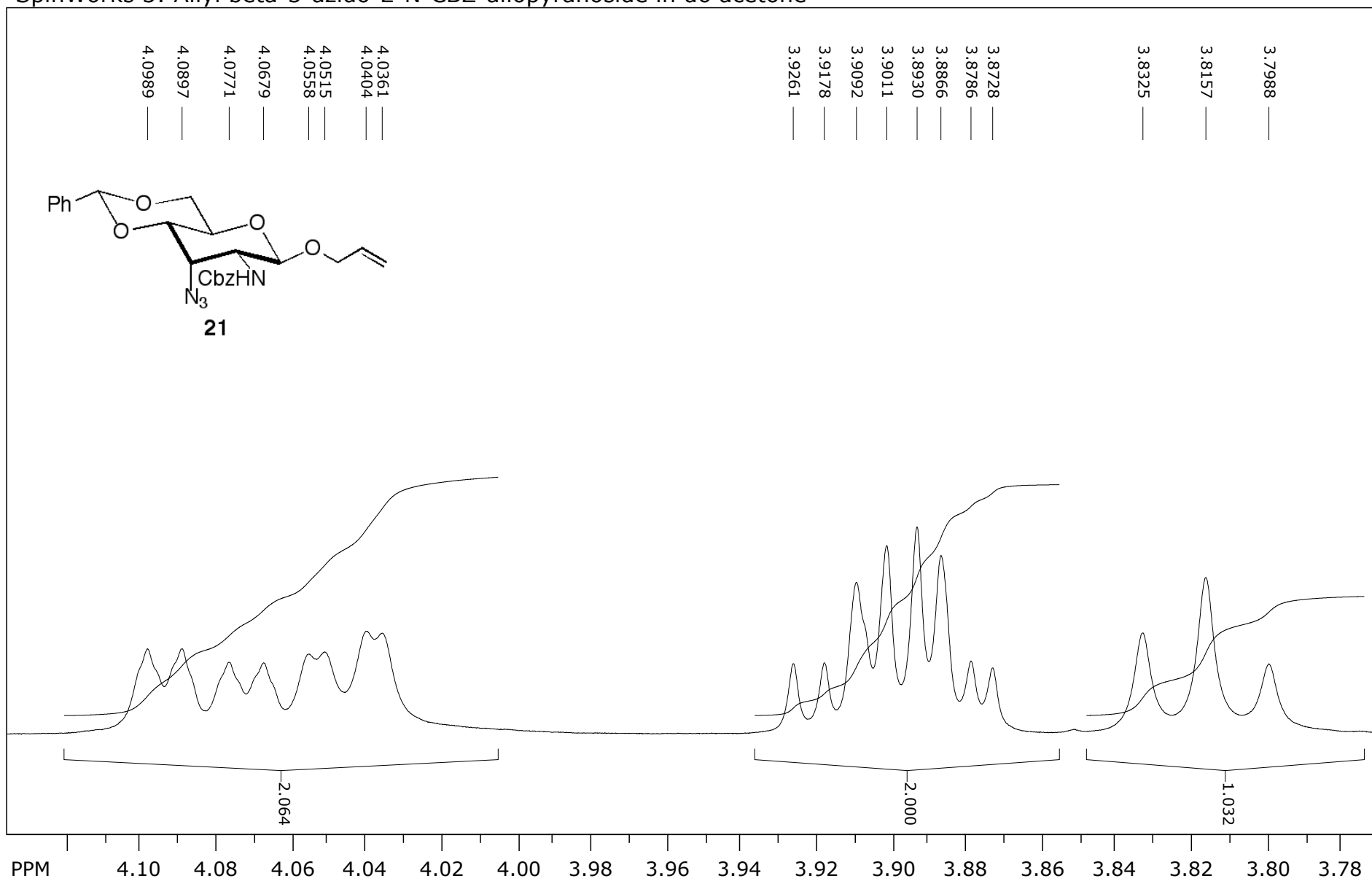
Sample Name	Sample10 redo	Position	Vial 5	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	3	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
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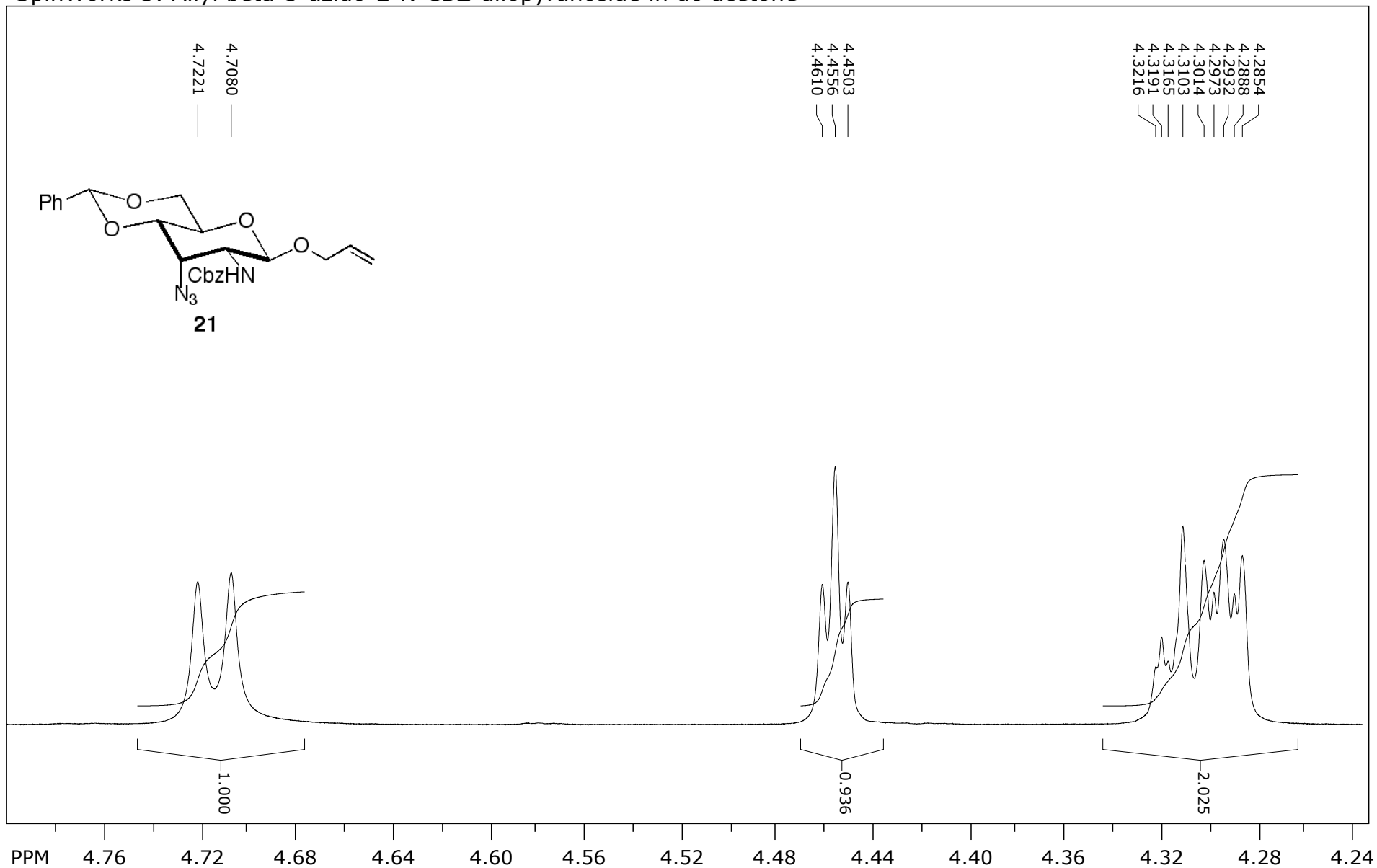
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transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

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Hz/cm: 195.275 ppm/cm: 0.32516



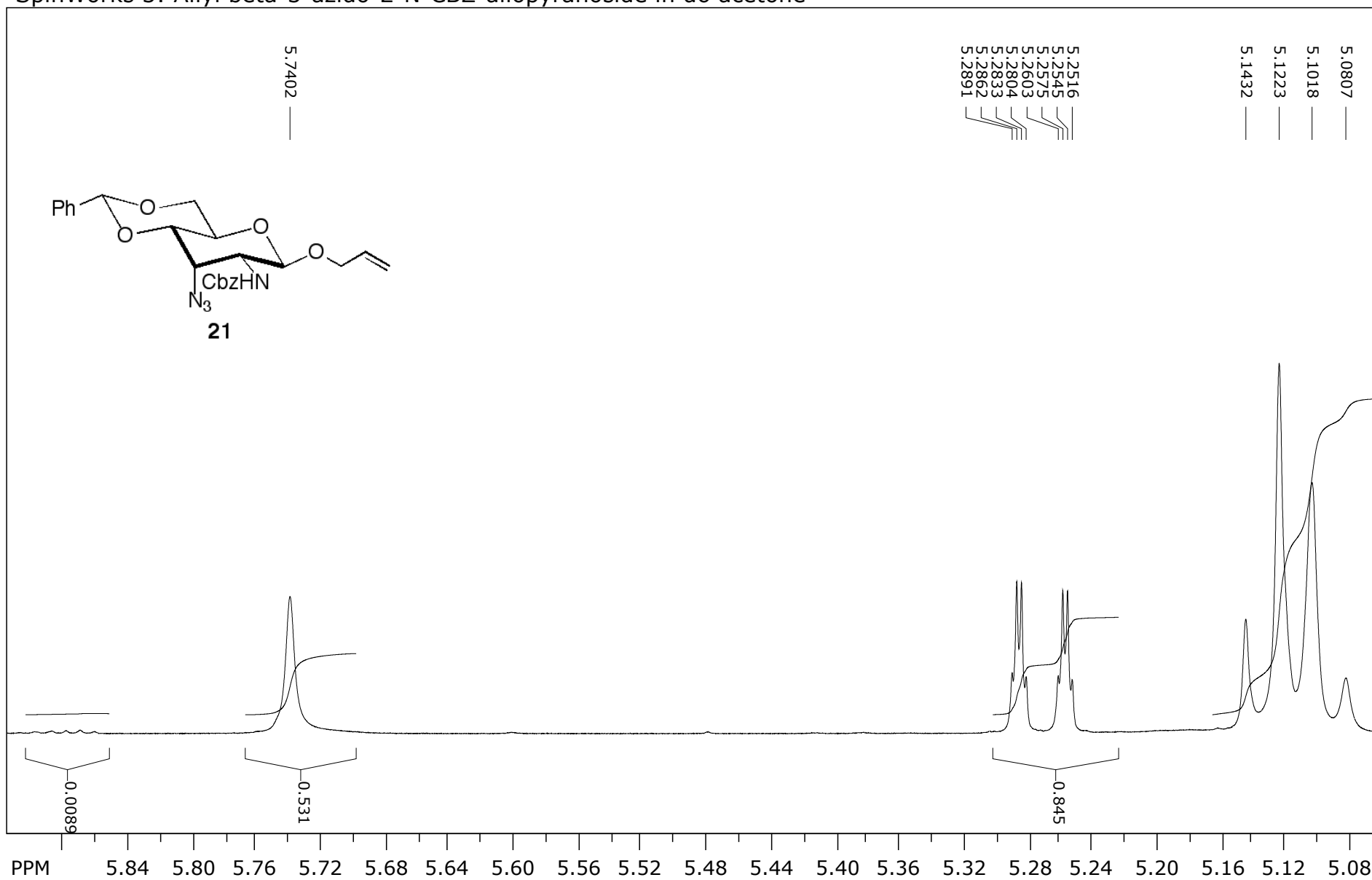
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time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

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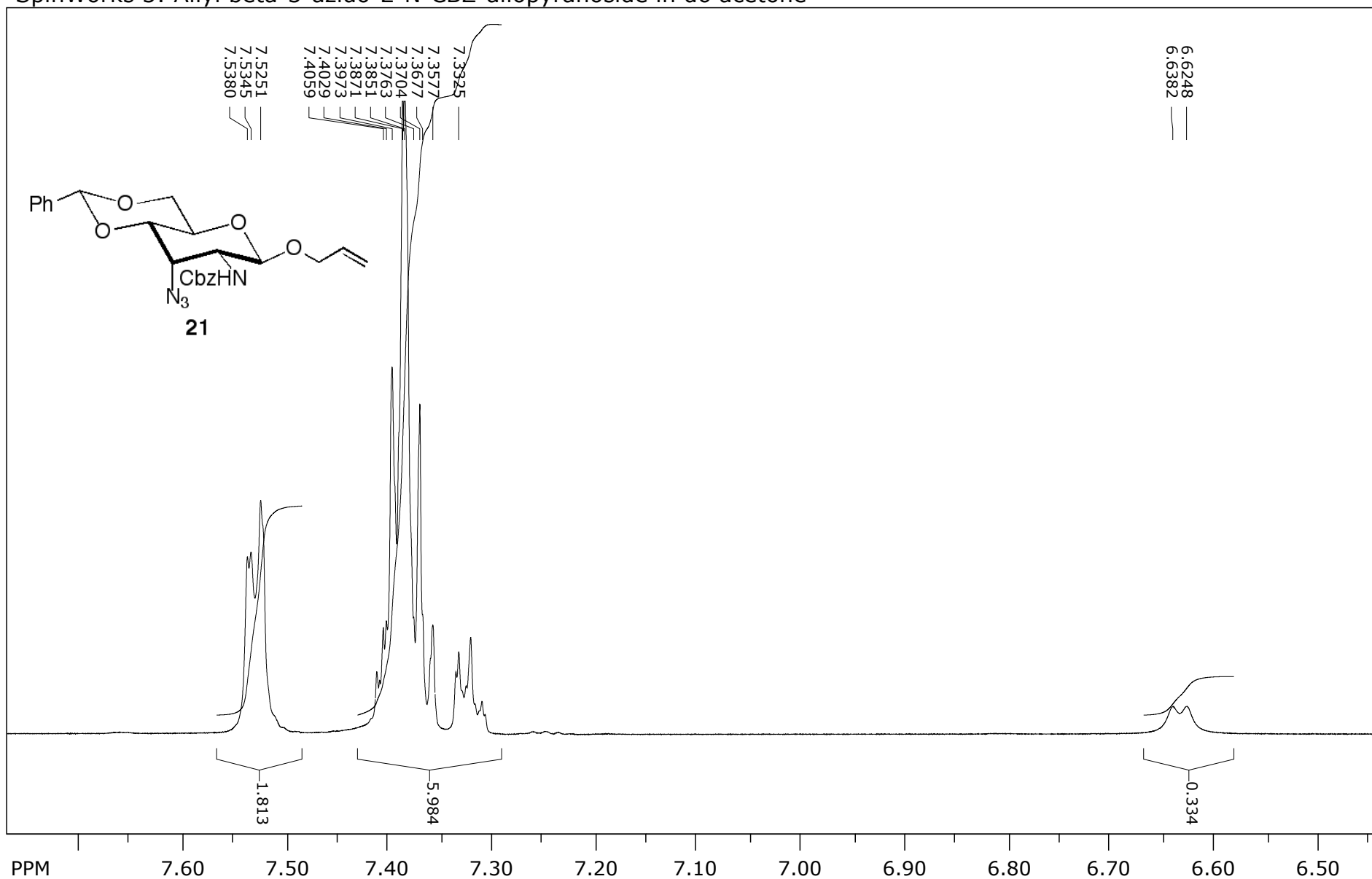
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time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 13.625 ppm/cm: 0.02269



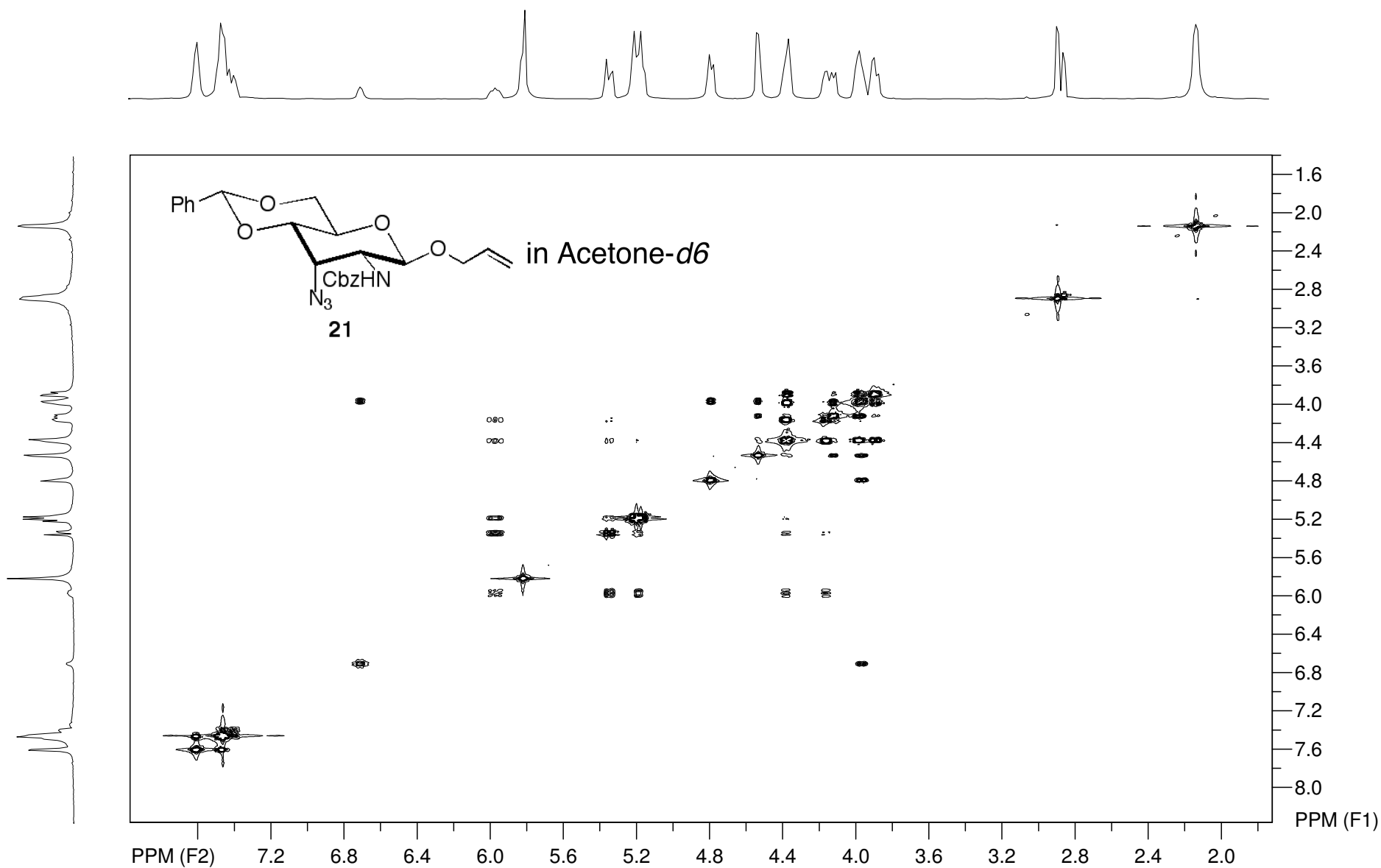
file: ...Data\b_allo3N3BnAc_d6acetone\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 20.565 ppm/cm: 0.03424



file: ...Data\b_allo3N3BnAc_d6acetone\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

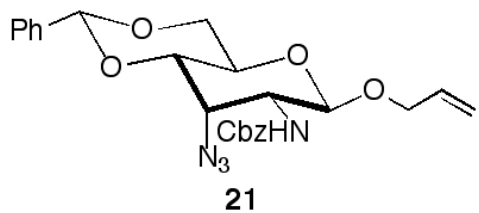
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 32.049 ppm/cm: 0.05337



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\b_allo3N3BnAc_COSY\1\ser
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 7211.50 Hz = 12.008167 ppm = 3.521242 Hz/pt
 number of scans: 2

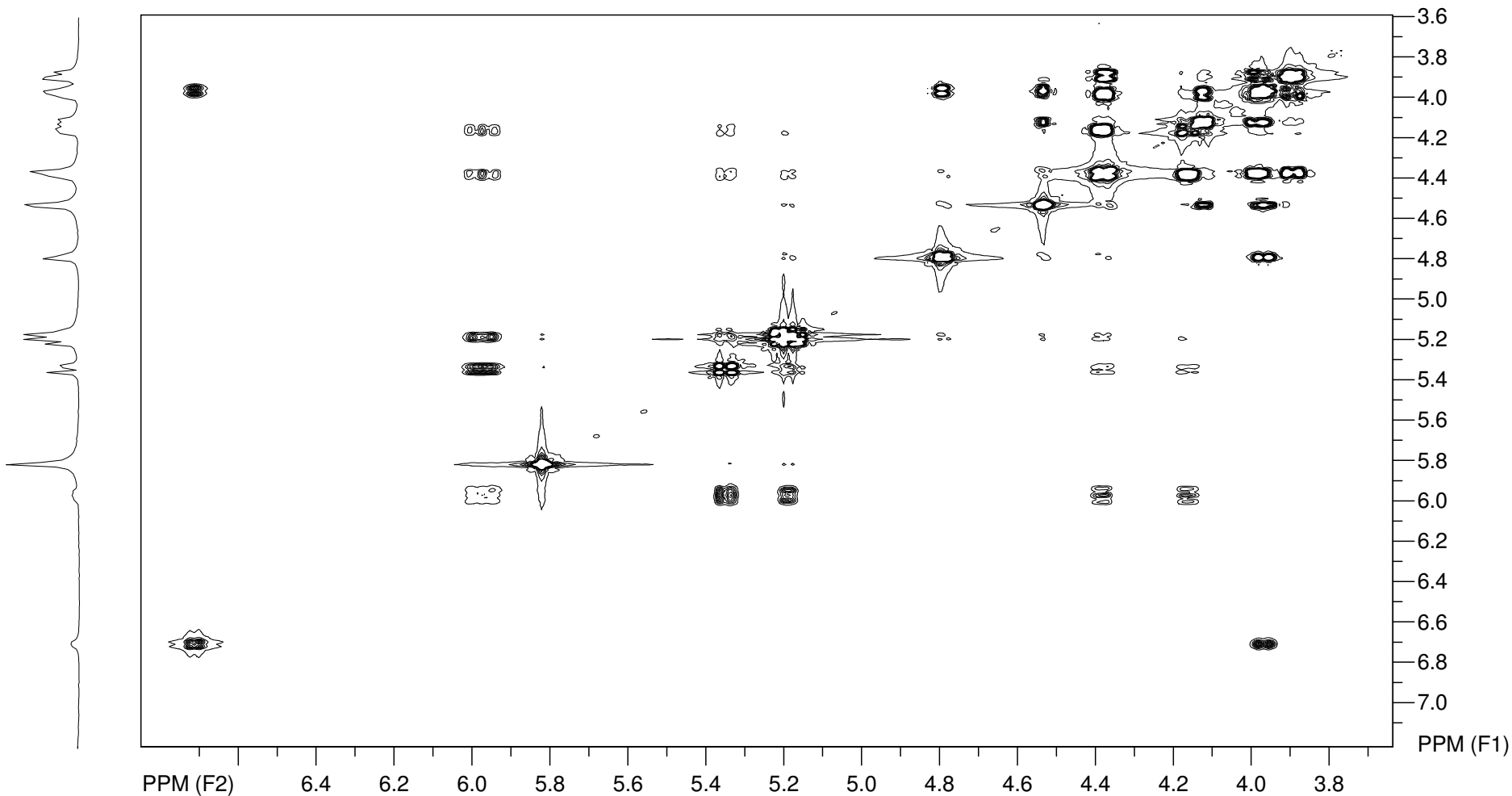
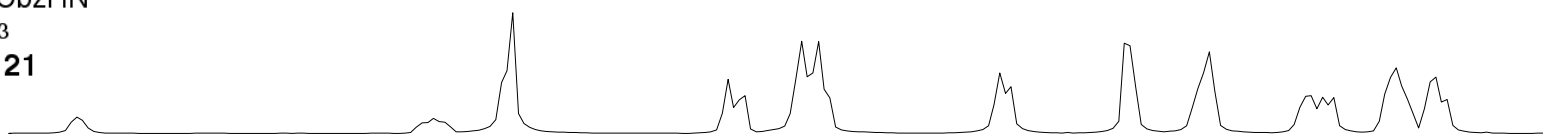
expt: <cosygpqf>F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 183.086 ppm/cm: 0.30486

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 348.739 ppm/cm: 0.58070



in Acetone-*d*6

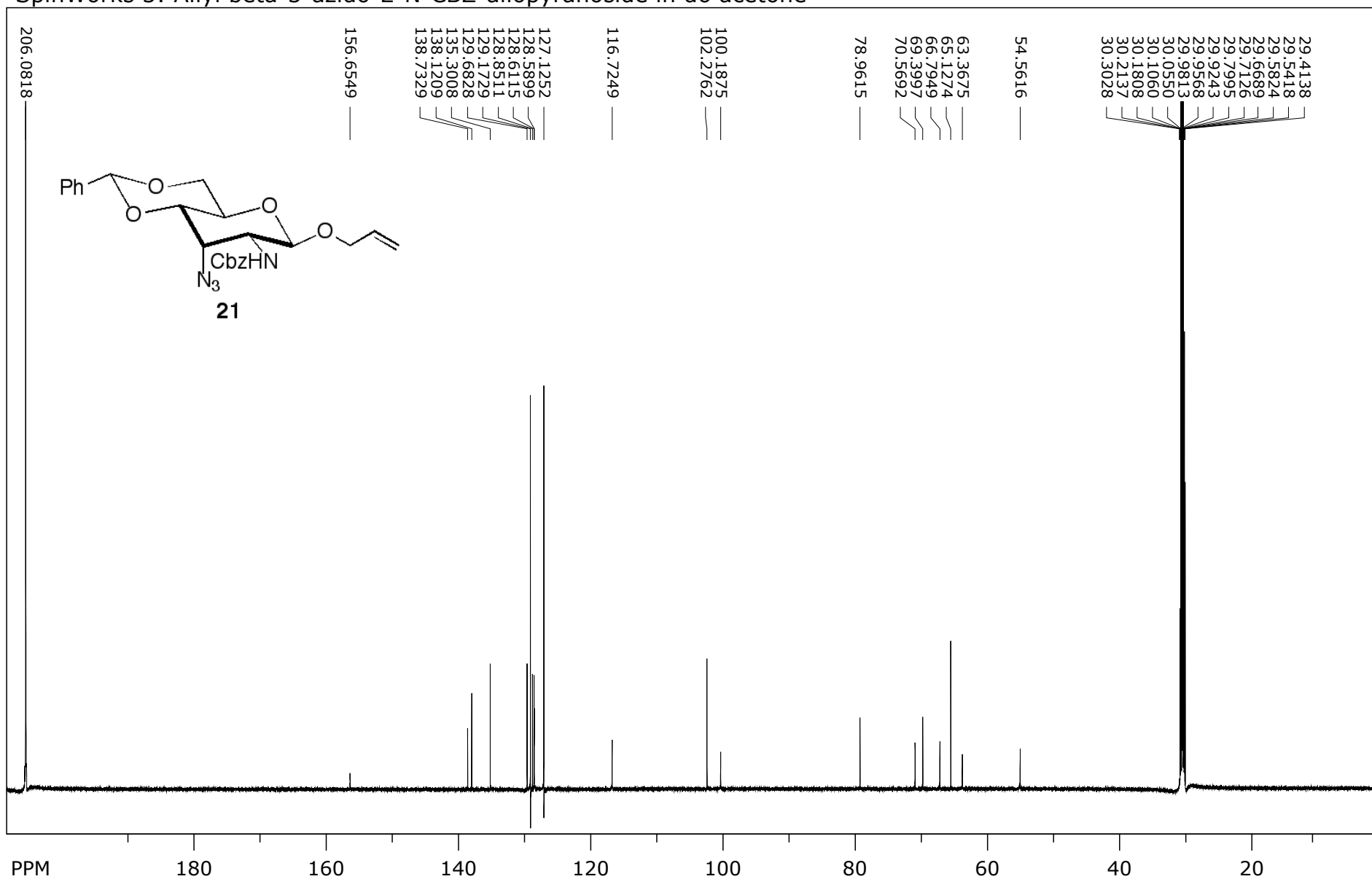
S-36



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\b_allo3N3BnAc_COSY\1\ser
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 7211.50 Hz = 12.008167 ppm = 3.521242 Hz/pt
 number of scans: 2

expt: <cosygpqf>F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 94.136 ppm/cm: 0.15675

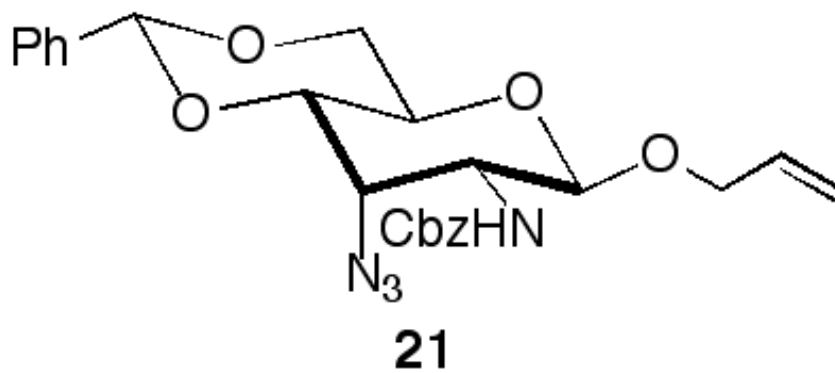
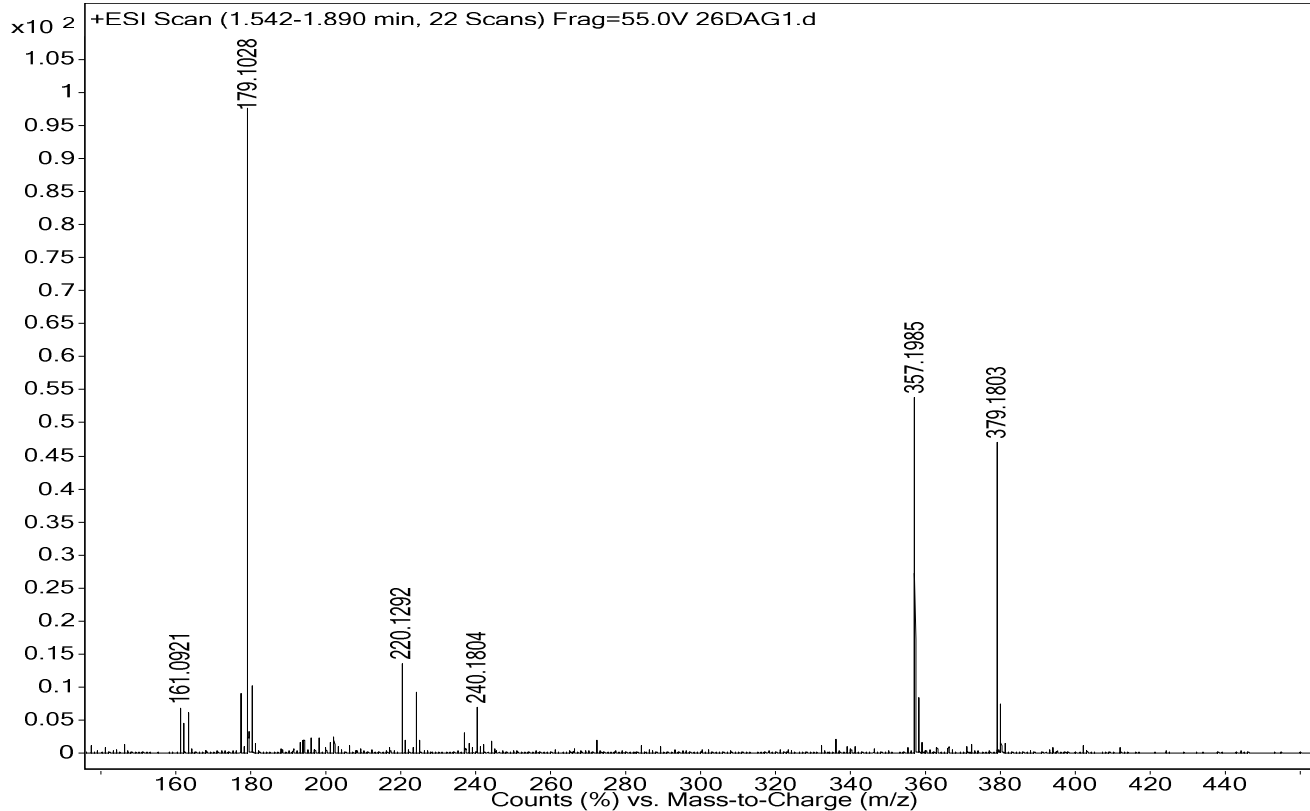
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 181.543 ppm/cm: 0.30229

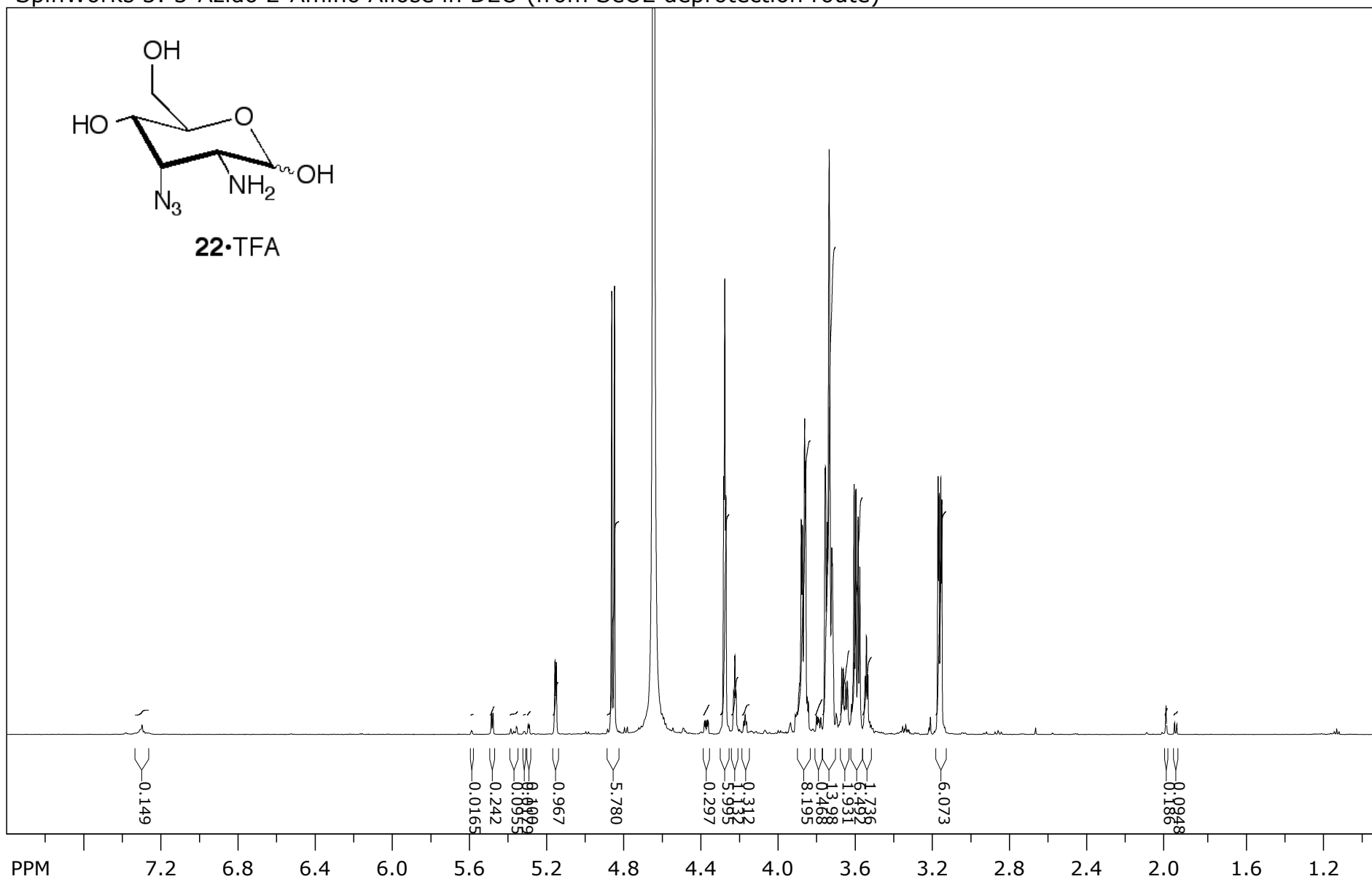


file: ...a\b-alloN3BnAc_13C_d6Acetone\1\fid exp: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 8192

freq. of 0 ppm: 151.008291 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1262.718 ppm/cm: 8.36107

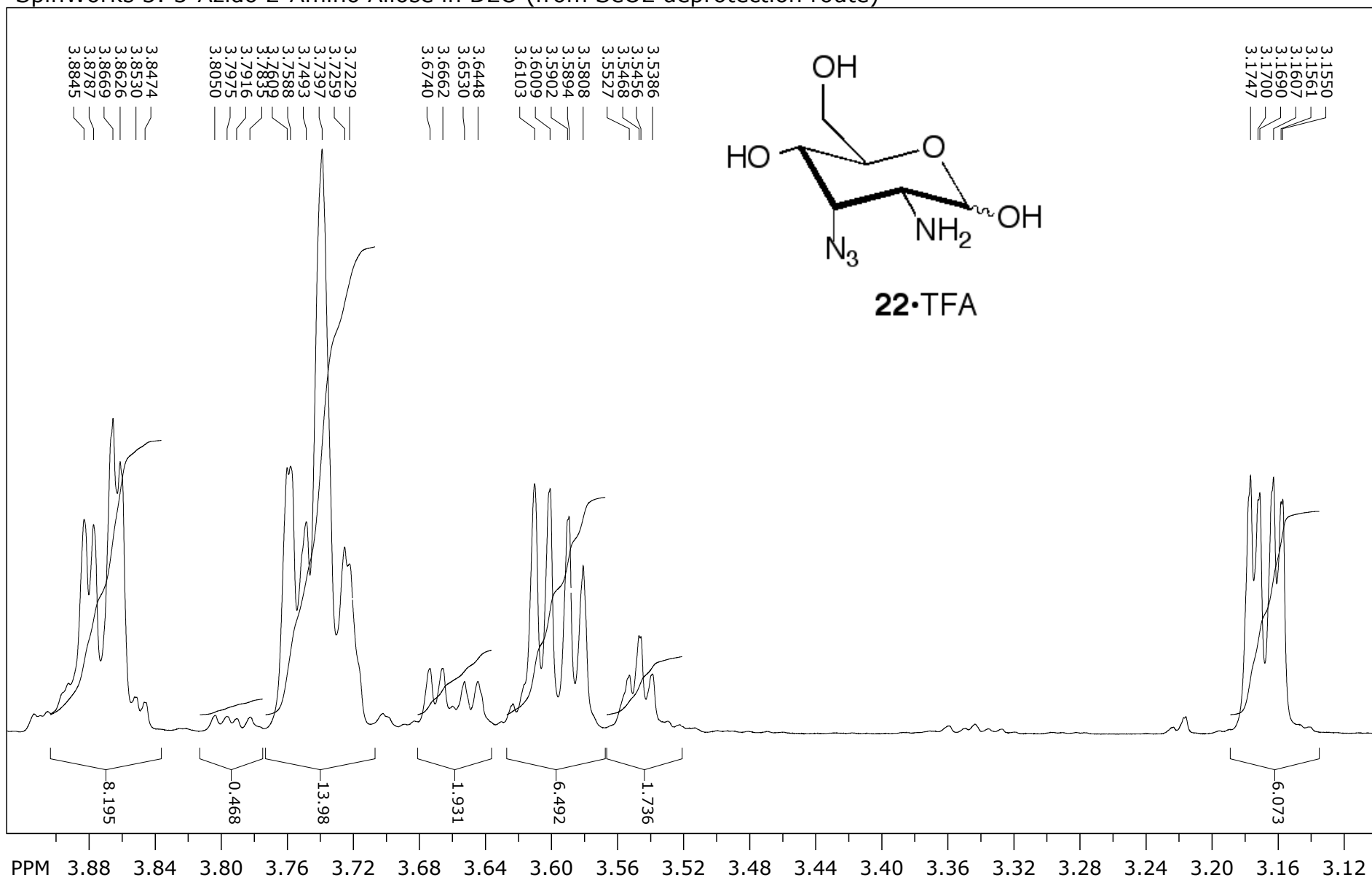
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	26DAG1.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable





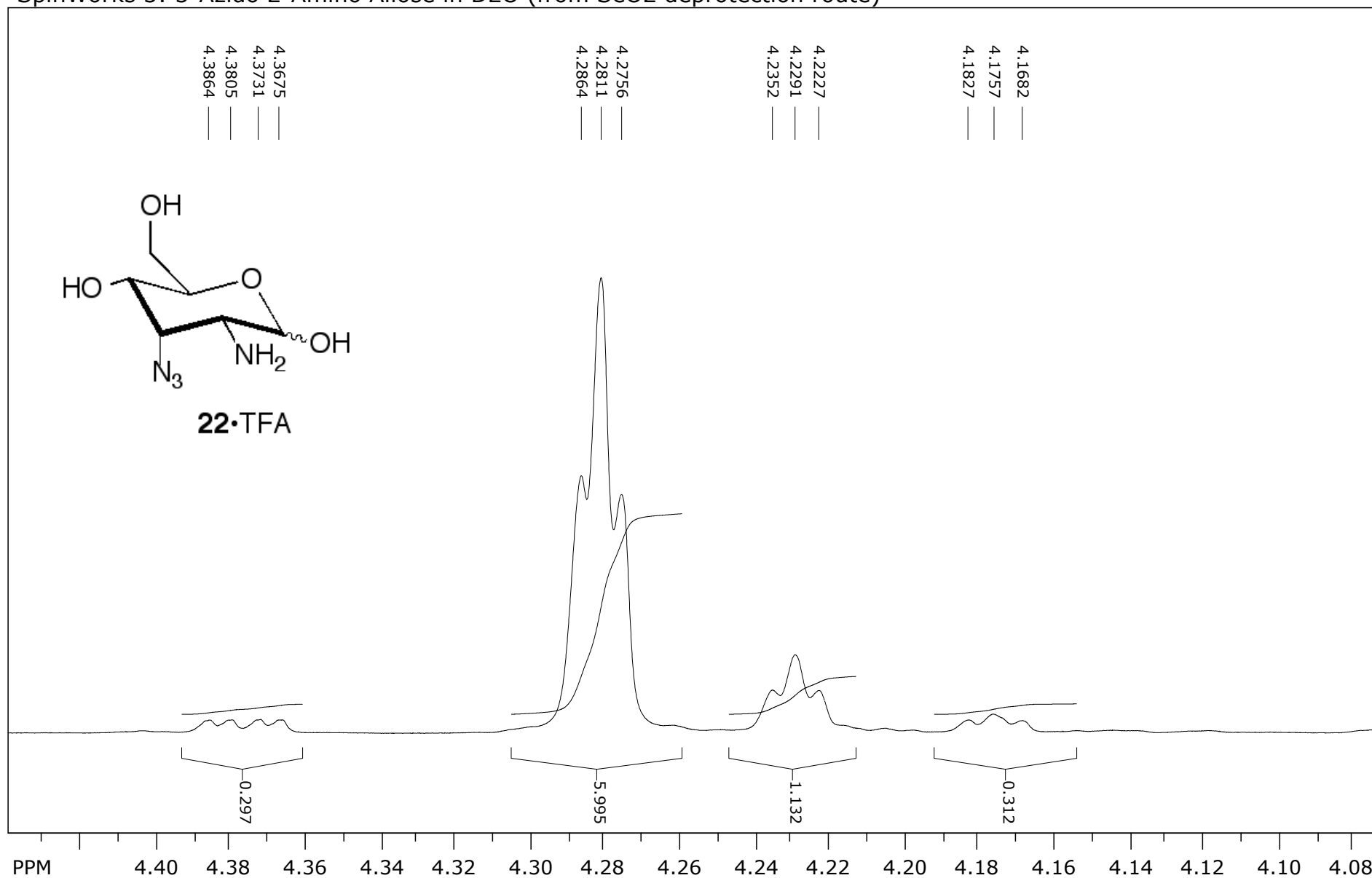
file: ...ocess\3azido2aminoAllose_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550036 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 170.981 ppm/cm: 0.28471



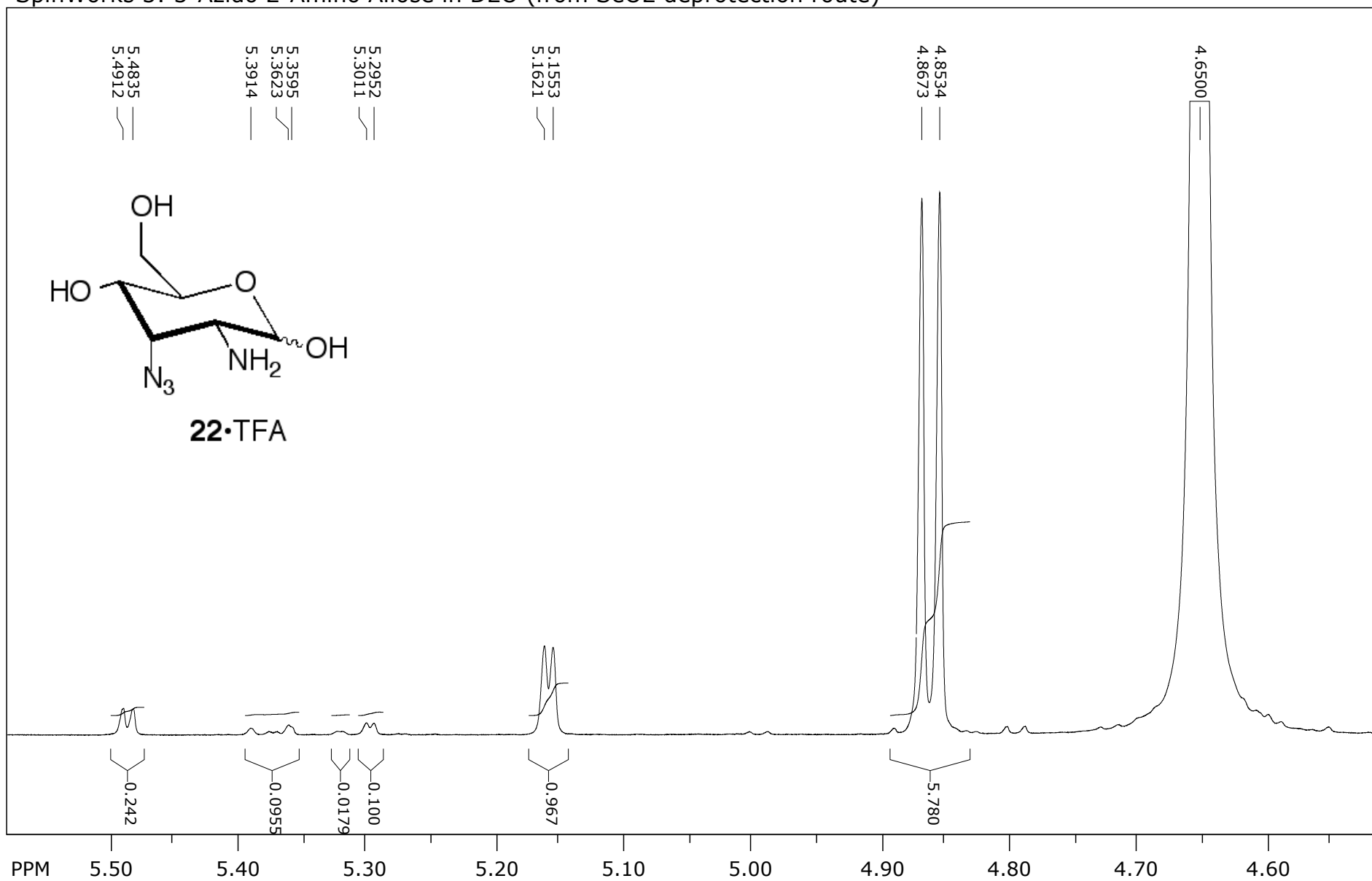
file: ...ocess\3azido2aminoAllose_D2O\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550036 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 20.037 ppm/cm: 0.03336



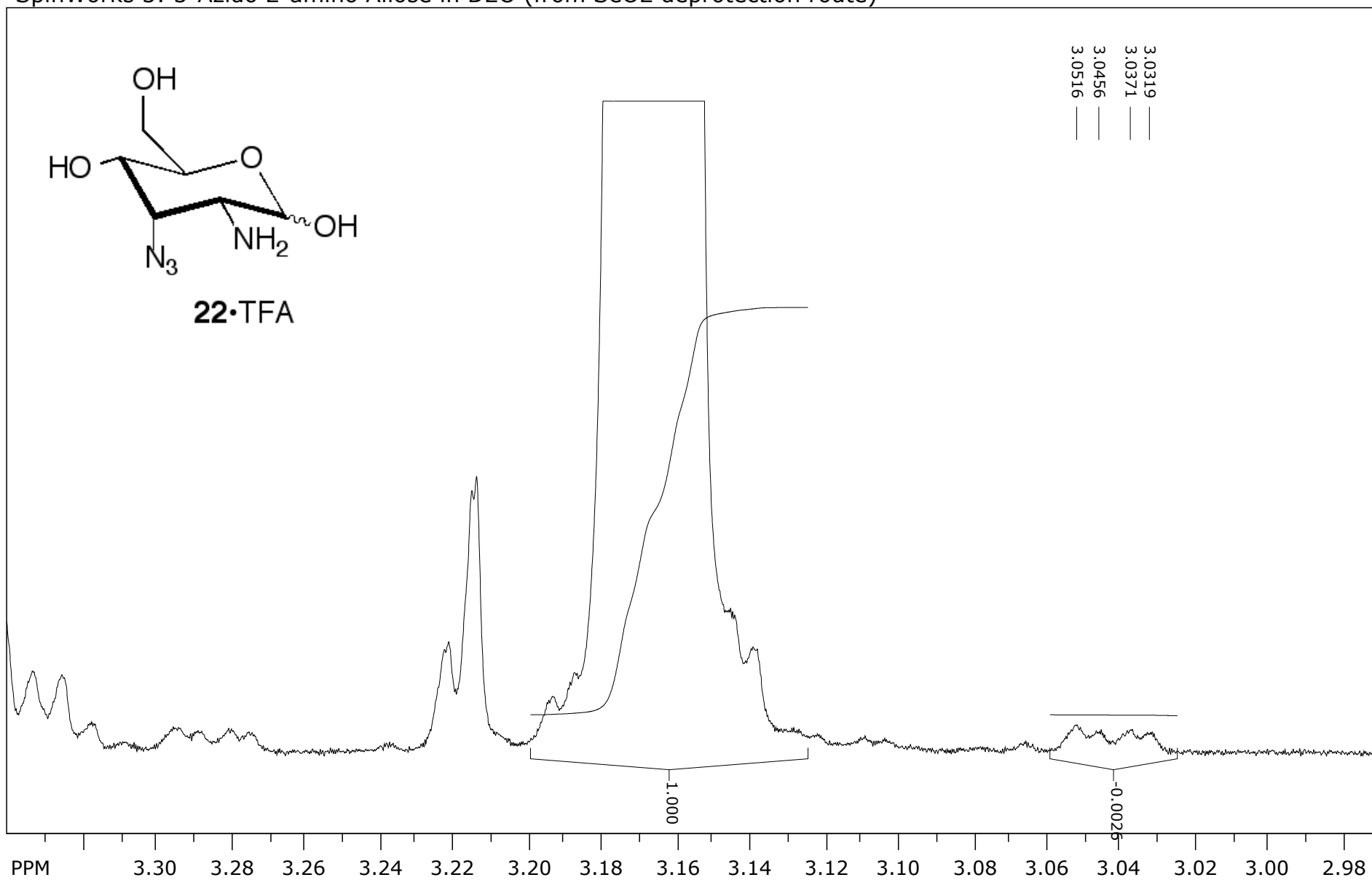
file: ...ocess\3azido2aminoAllose_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550036 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 8.831 ppm/cm: 0.01470



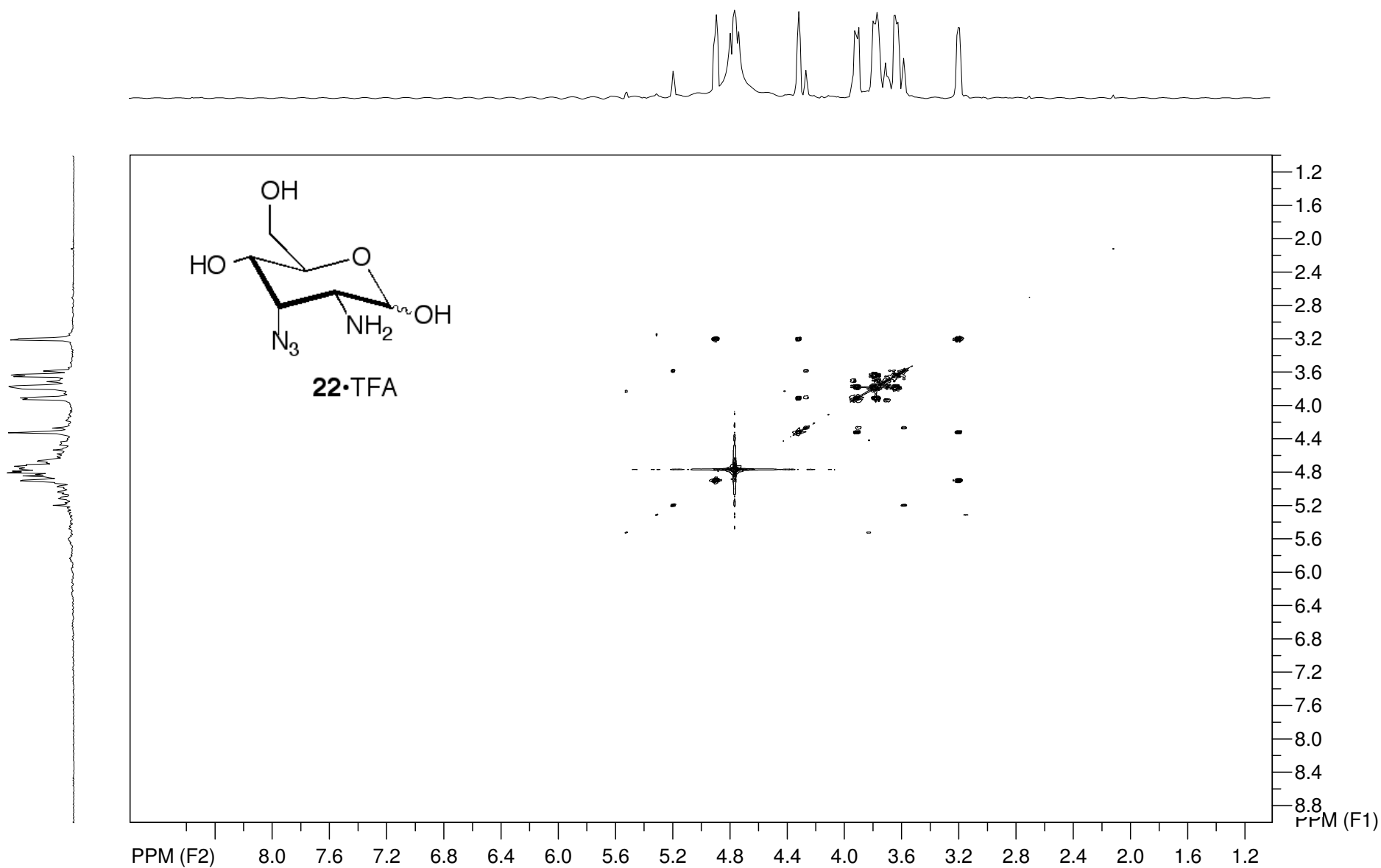
file: ...ocess\3azido2aminoAllose_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550036 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 25.741 ppm/cm: 0.04286



file: ...o2aminoAllose_D2O SeO2 route\1\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550036 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 8.913 ppm/cm: 0.01484

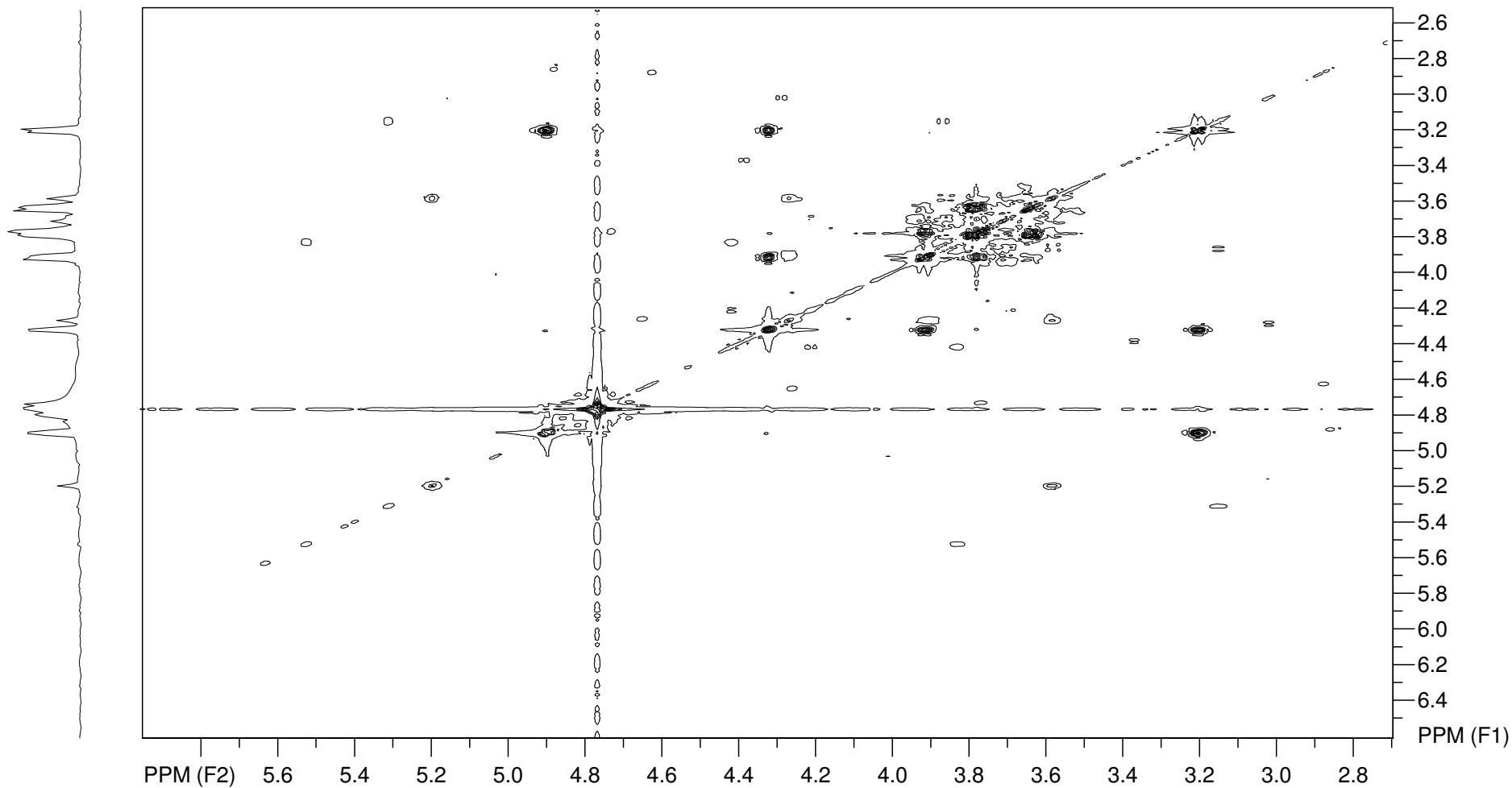
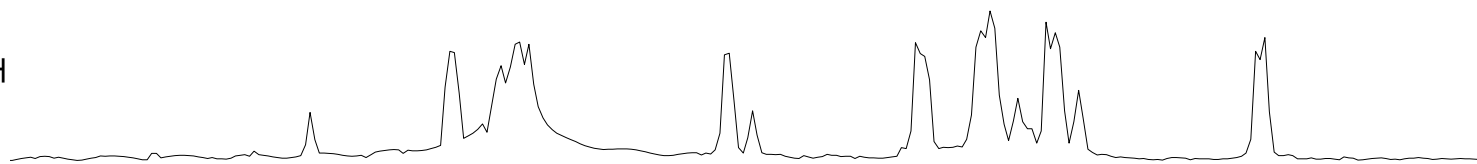
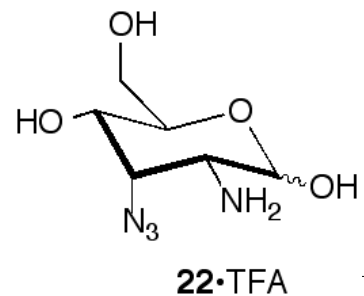


file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\3Azido2Aminoallose_Dpr\F2.freq. of 0 ppm: 600.549962 MHz
transmitter freq.: 600.552832 MHz
time domain size: 2048 by 2048 points
width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
number of scans: 2

processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 233.931 ppm/cm: 0.38953

F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 400.685 ppm/cm: 0.66719

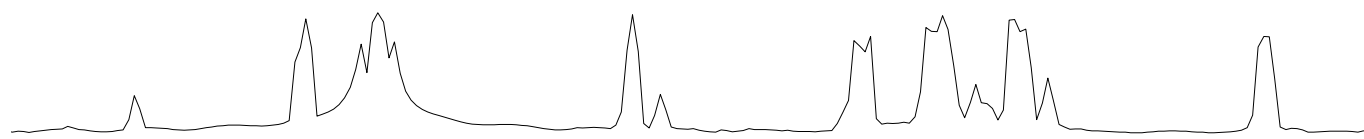
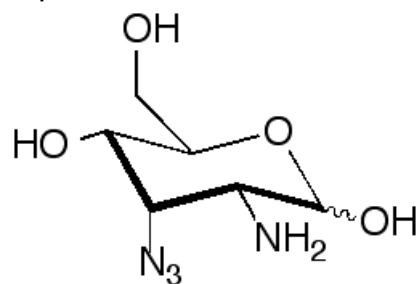
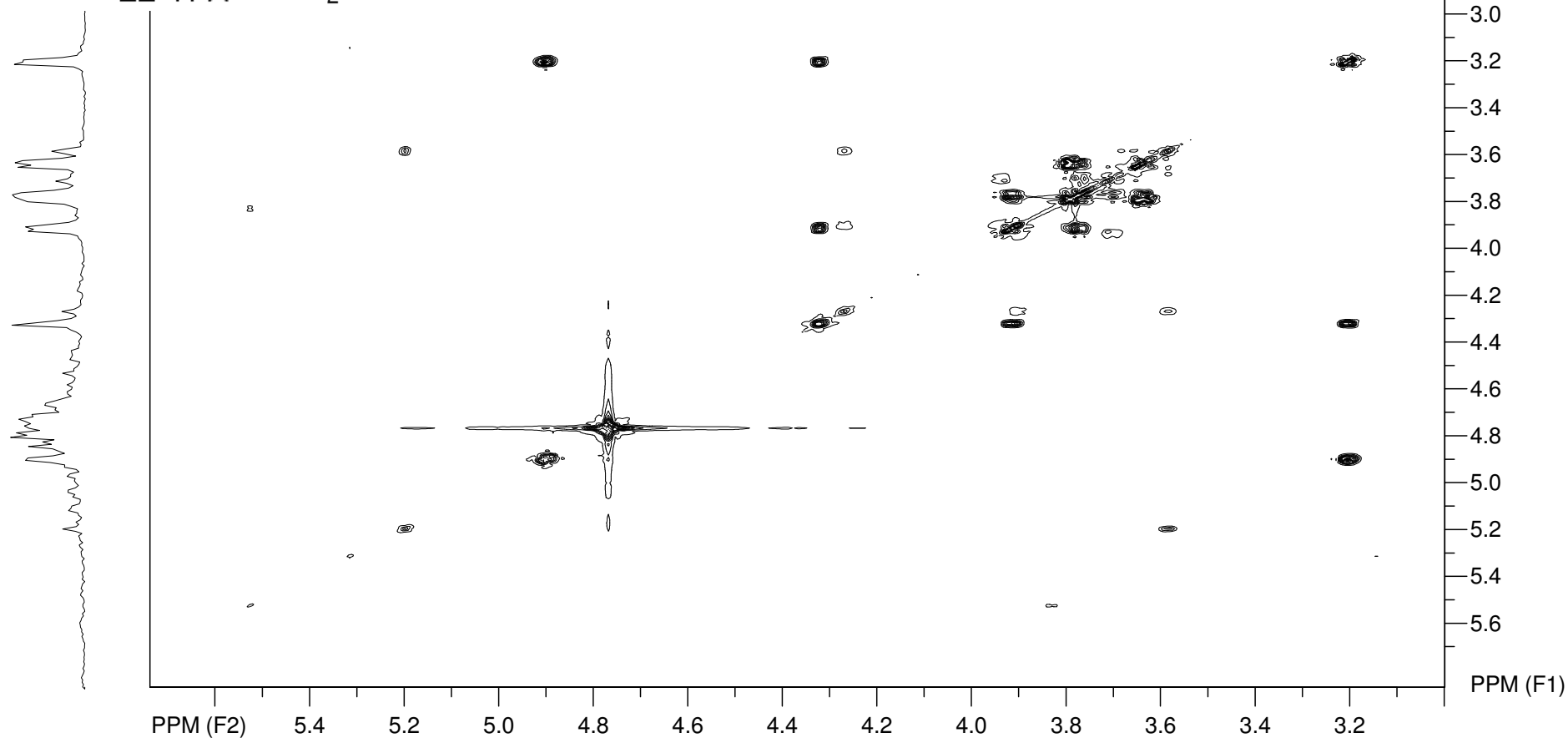
3N3 2-aminoallose. TFA salt



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\3Azido2Aminoallose_Dprotd_COSY\1\ser
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

exp1F2::freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 95.380 ppm/cm: 0.15882

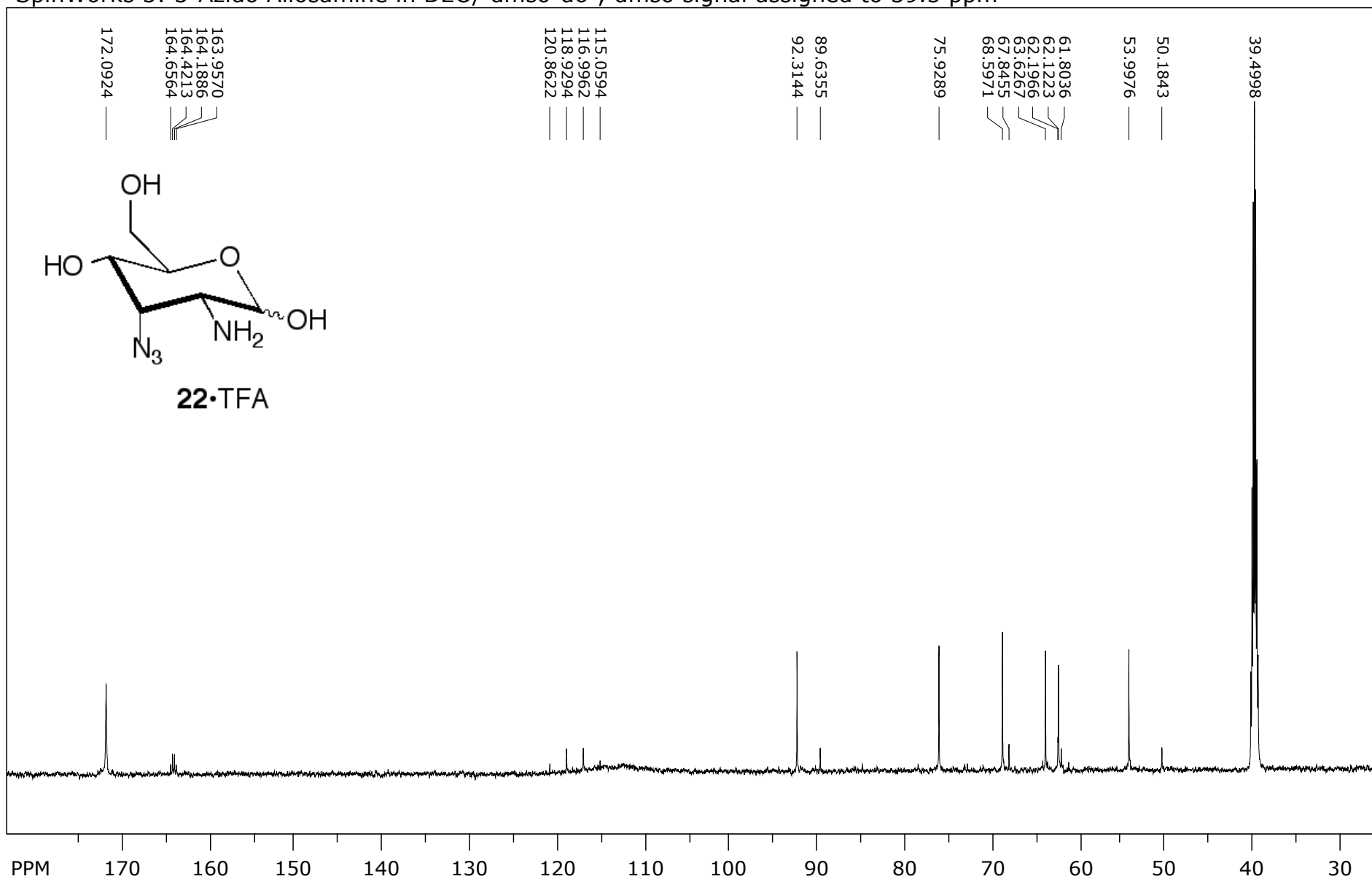
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 205.094 ppm/cm: 0.34151

22·TFA In D₂O

file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\3Azido2Aminoallose_Dpr\F2.freq. of 0 ppm: 600.549962 MHz
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

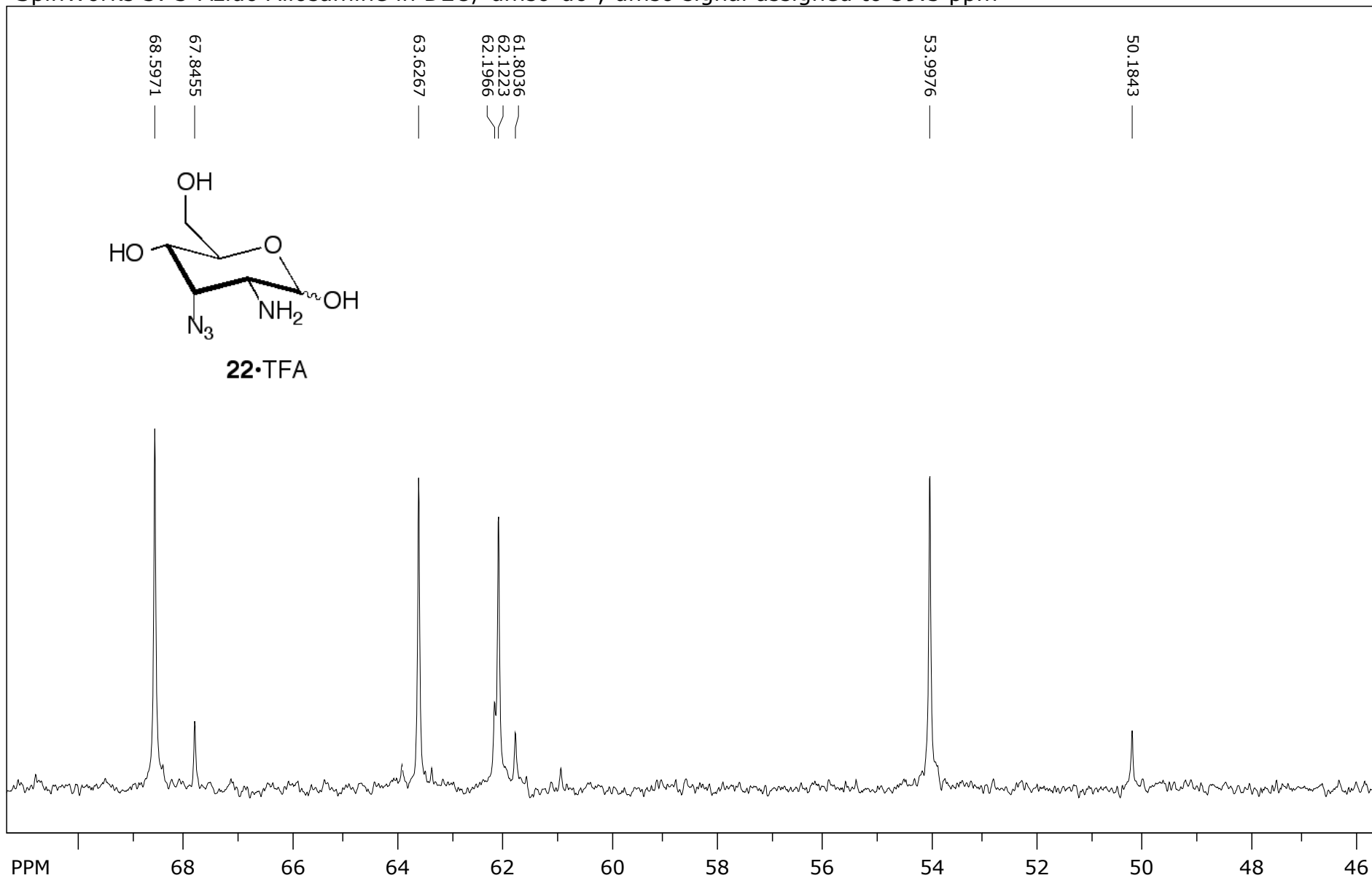
processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 80.234 ppm/cm: 0.13360

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 161.669 ppm/cm: 0.26920



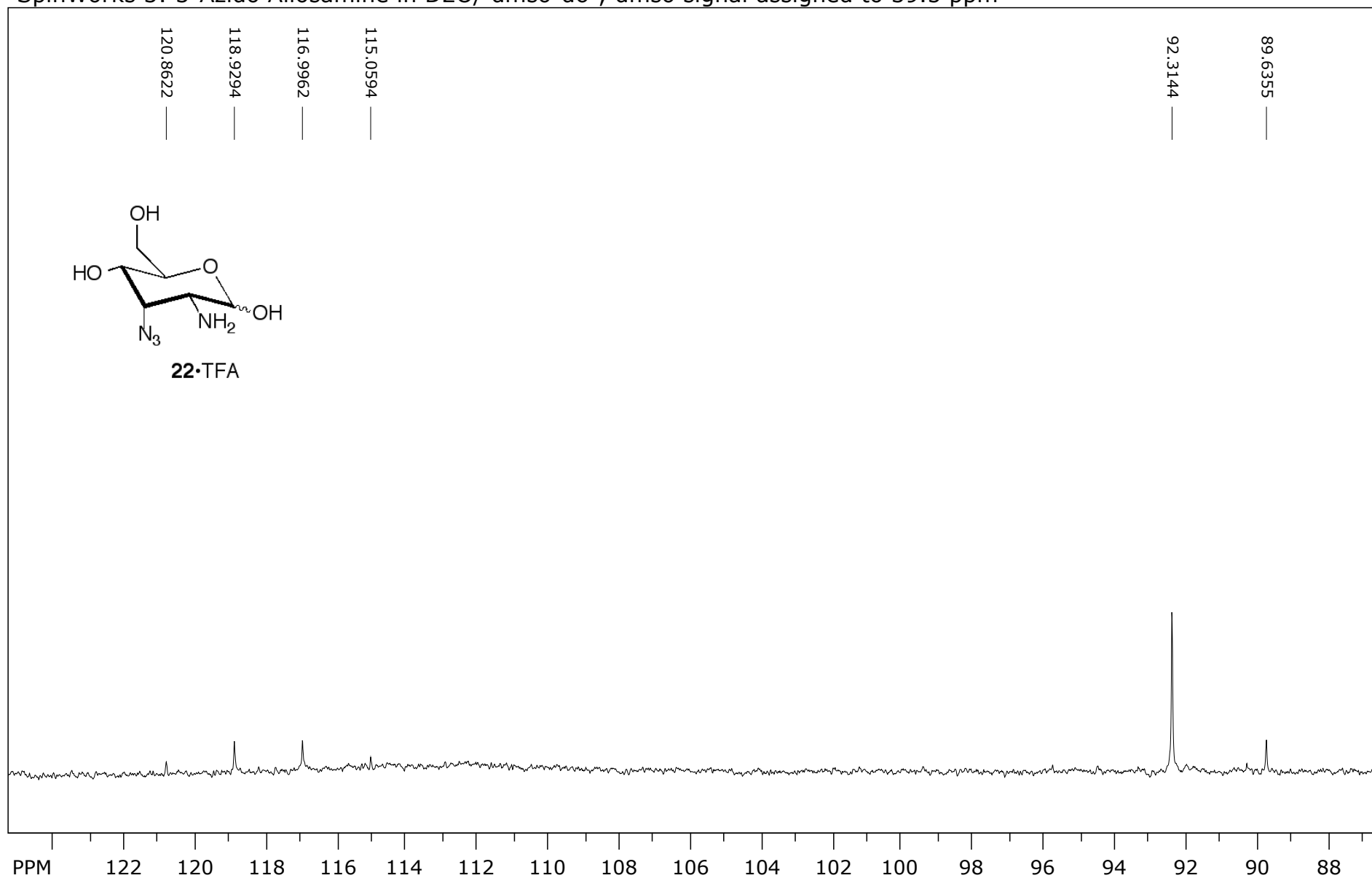
file: ...minoallose_DprotD_D2Odmso13C\1\fid expt: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 30720

freq. of 0 ppm: 151.008169 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 956.978 ppm/cm: 6.33661



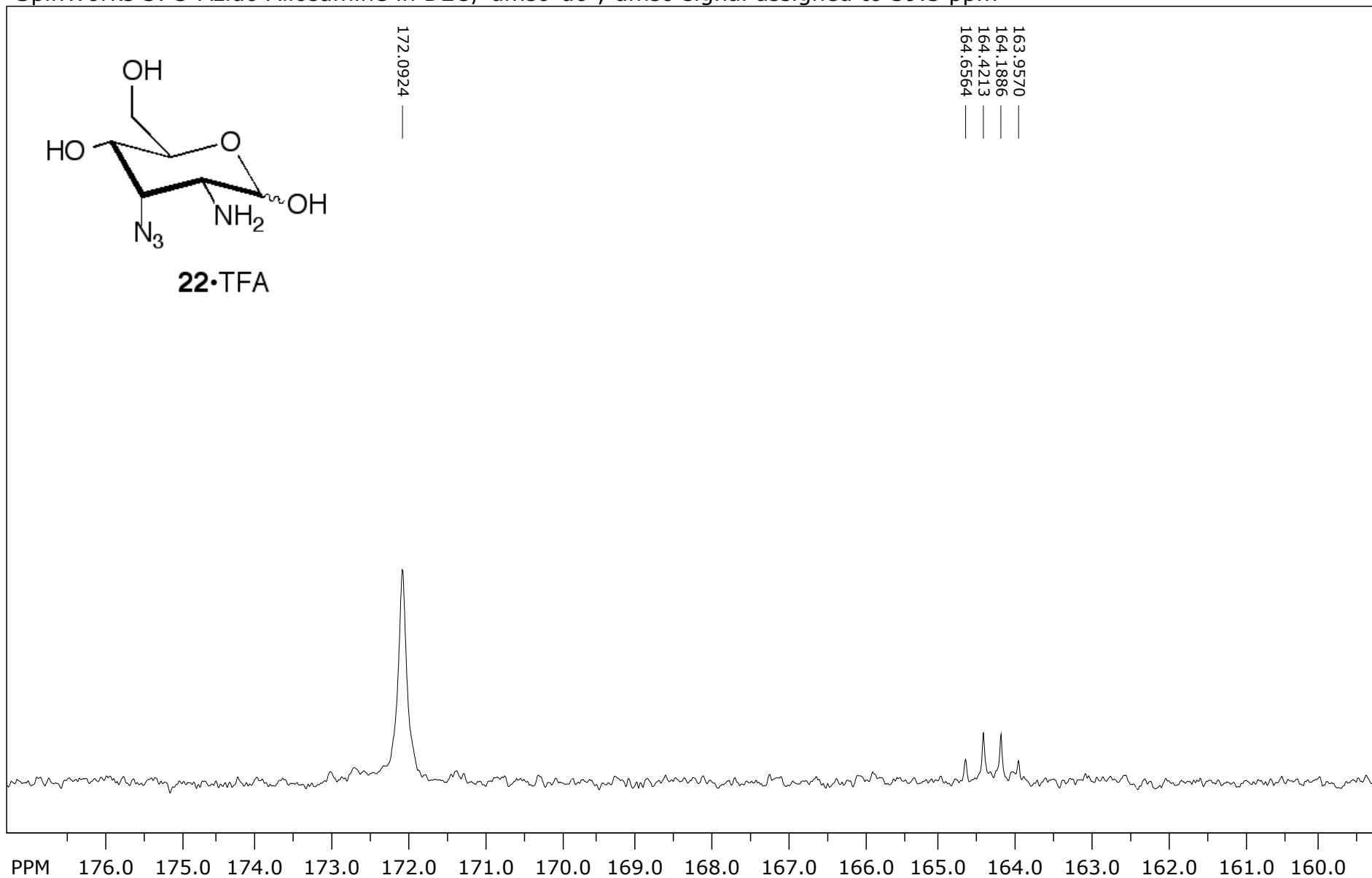
file: ...minoallose_Dprotd_D2OdmsO13C\1\fid expt: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 30720

freq. of 0 ppm: 151.008169 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 156.143 ppm/cm: 1.03390



file: ...minoallose_DprotD_D2Odmso13C\1\fid expt: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 30720

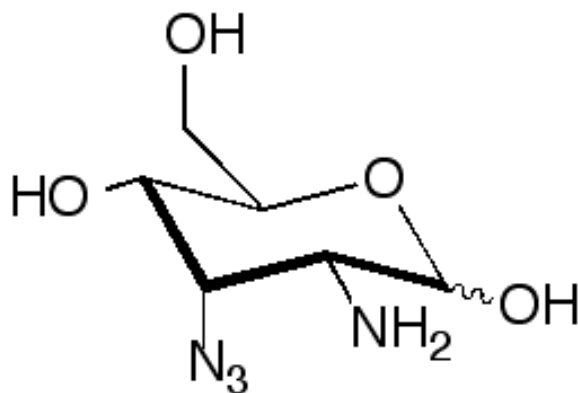
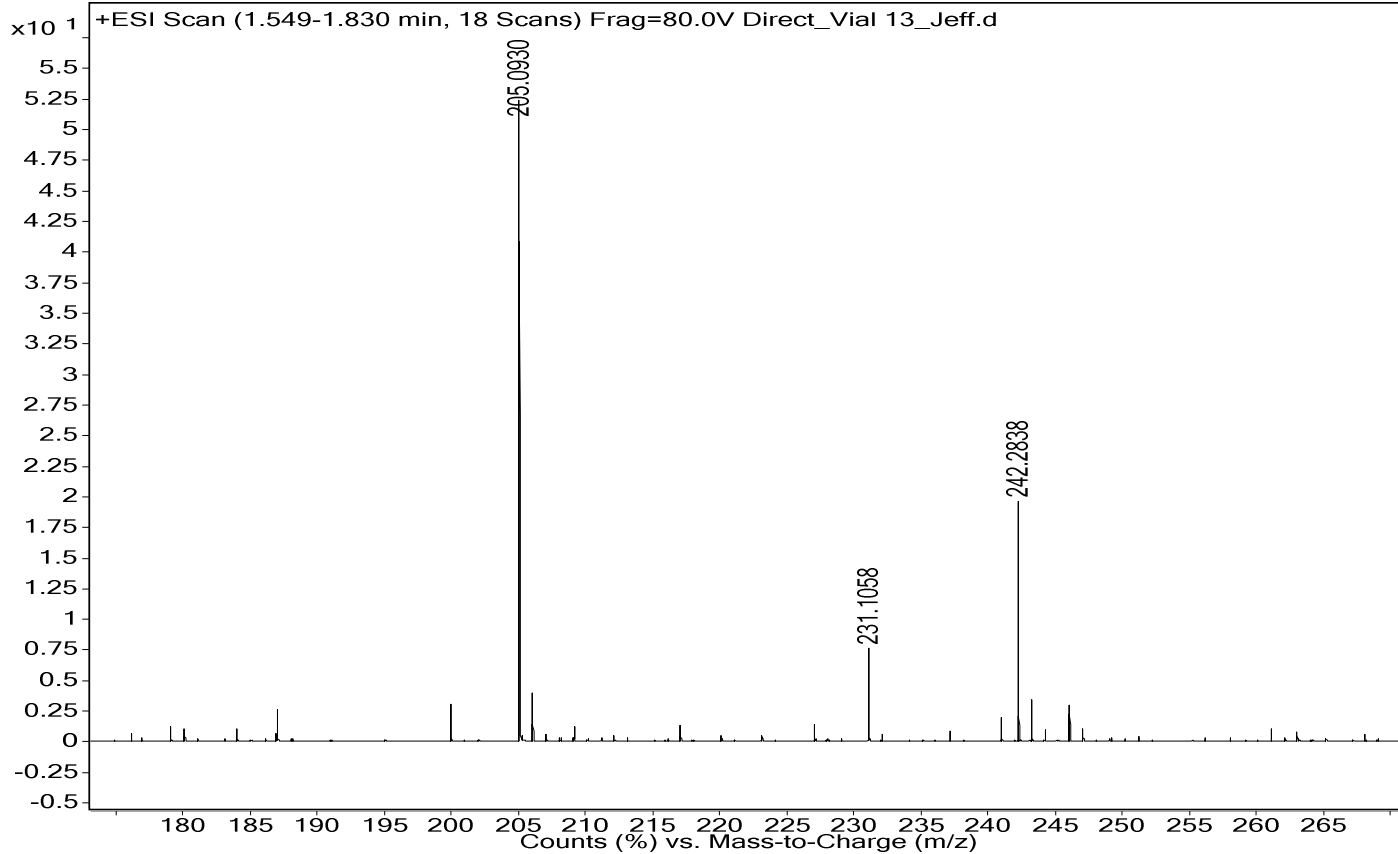
freq. of 0 ppm: 151.008169 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 235.019 ppm/cm: 1.55617

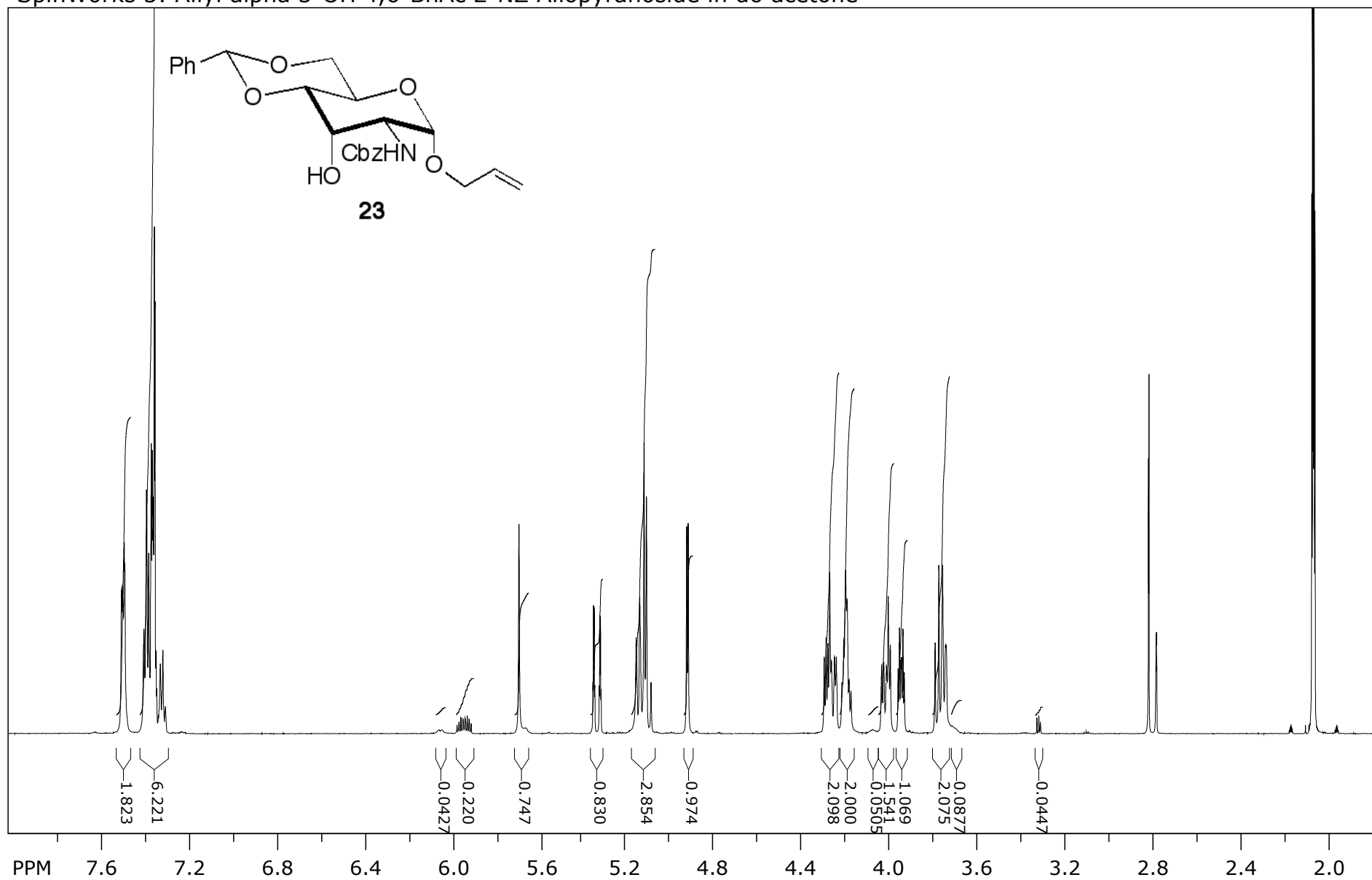


file: ...minoallose_DprotD_D2Odmso13C\1\fid expt: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 30720

freq. of 0 ppm: 151.008169 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 109.461 ppm/cm: 0.72479

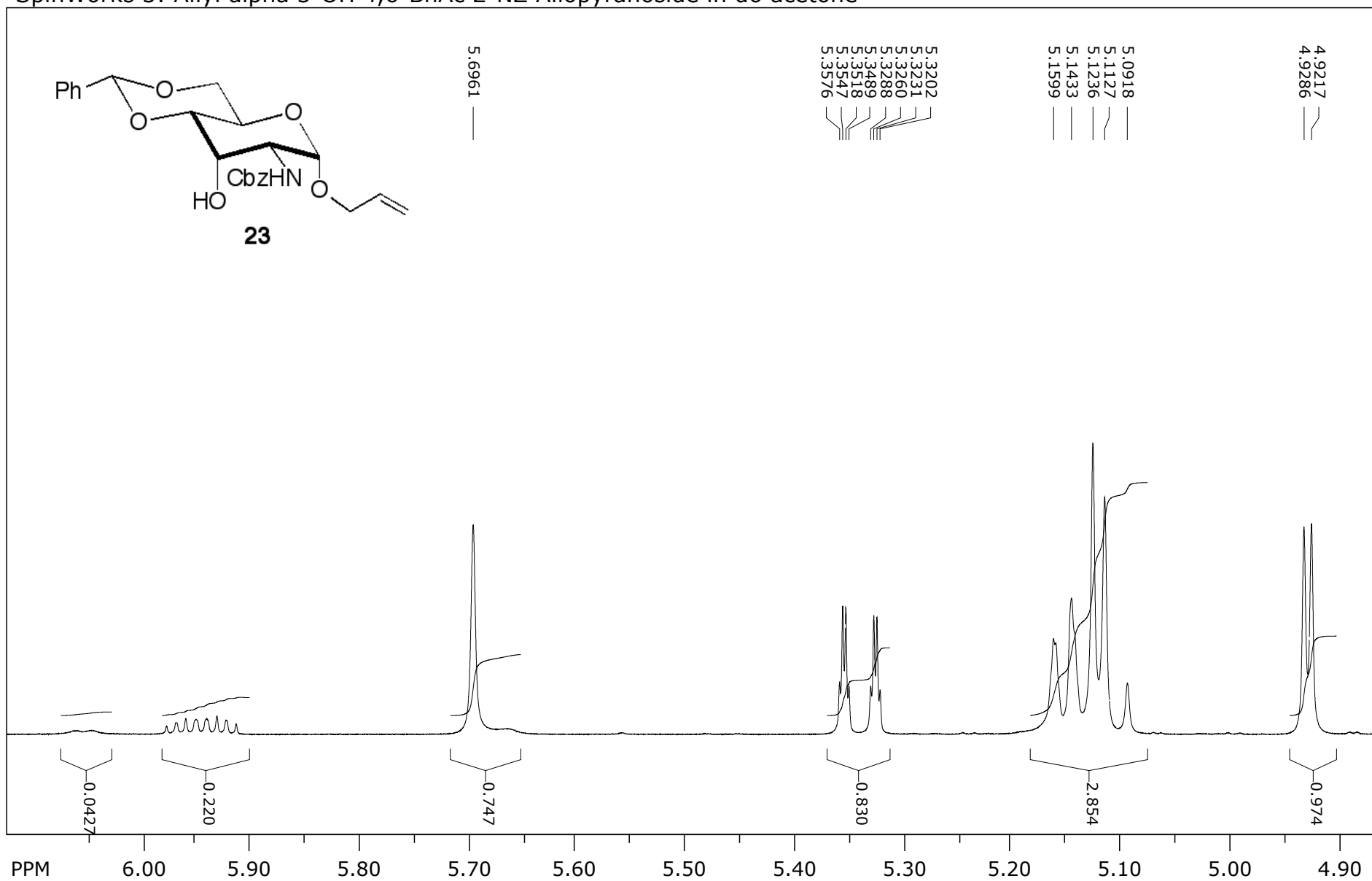
Sample Name	Jeff 13	Position	Vial 13	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 13_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 11:36:28 AM

**22-TFA**



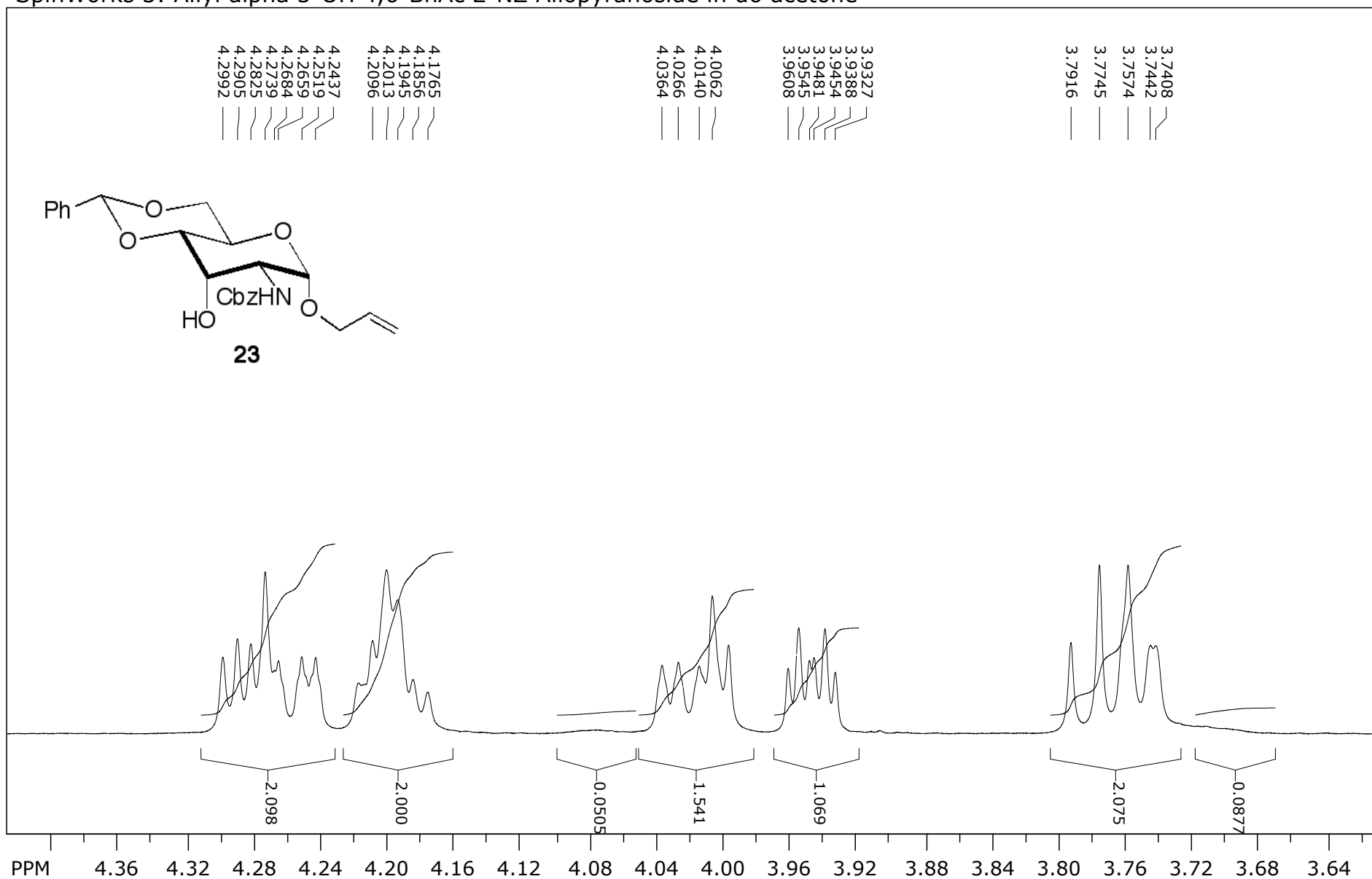
file: ...alphaBnAc_d6acetone_MeOHrext\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 150.688 ppm/cm: 0.25092



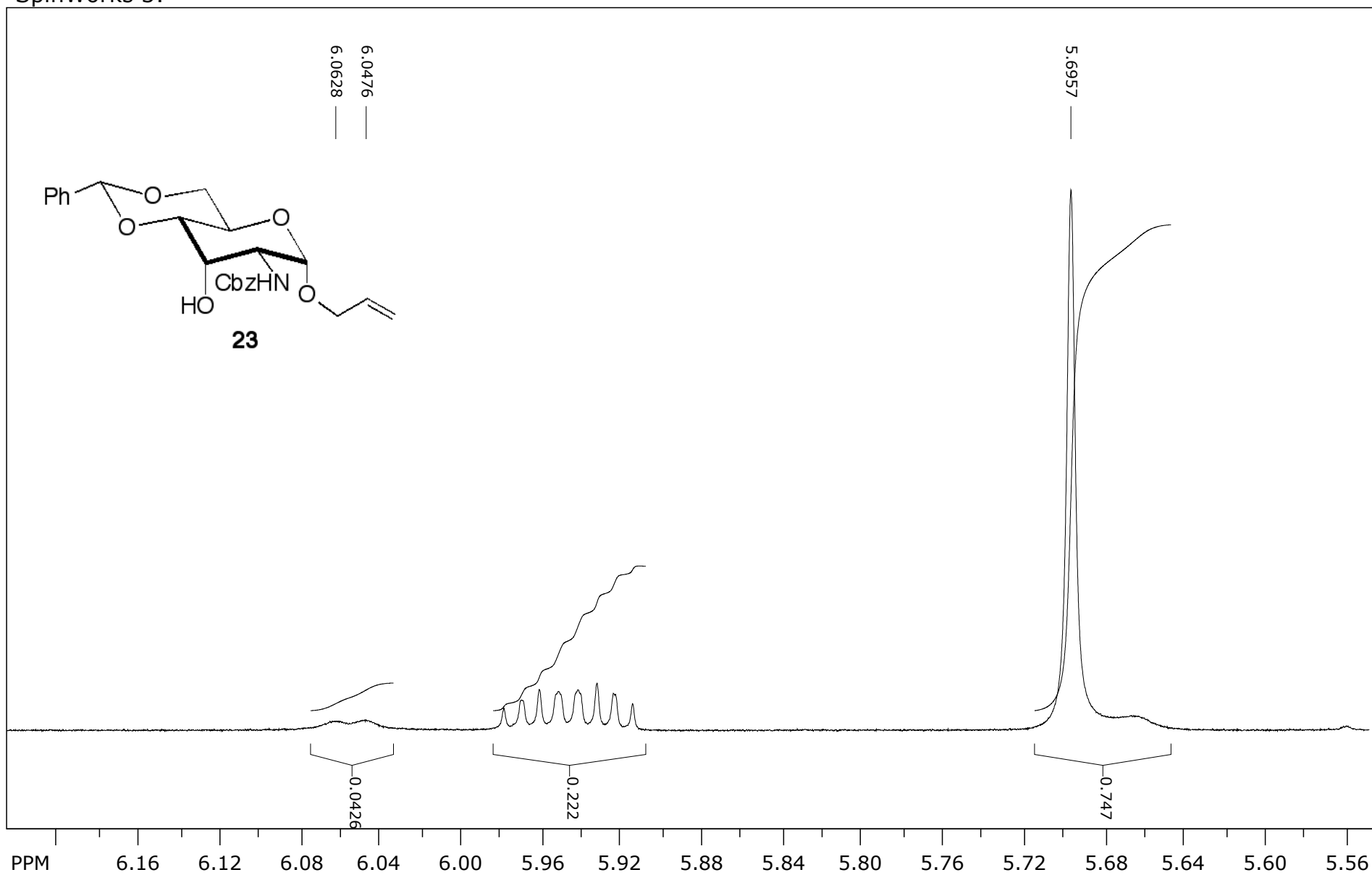
file: ...alphaBnAc_d6acetone_MeOHrect\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 30.448 ppm/cm: 0.05070



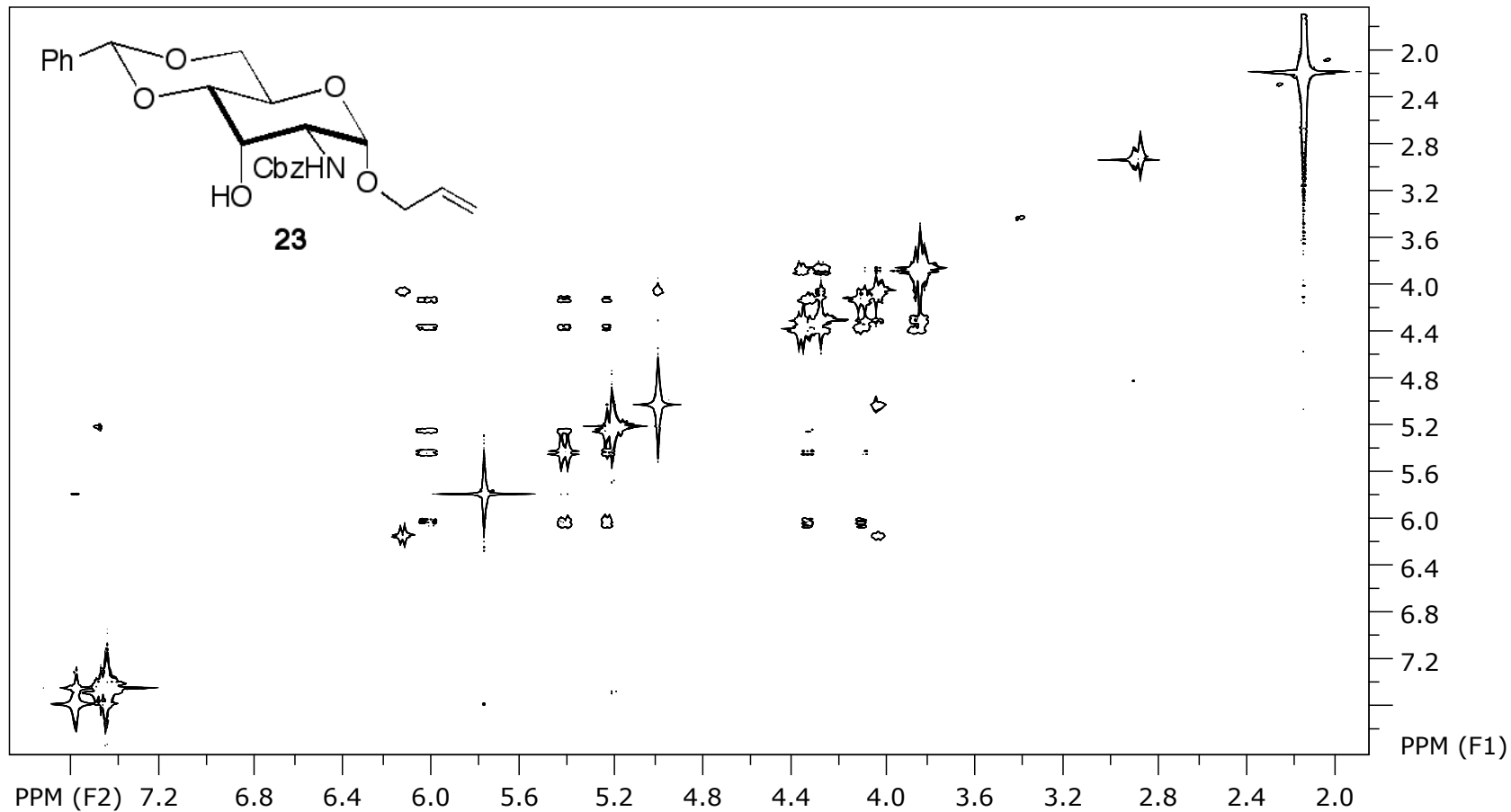
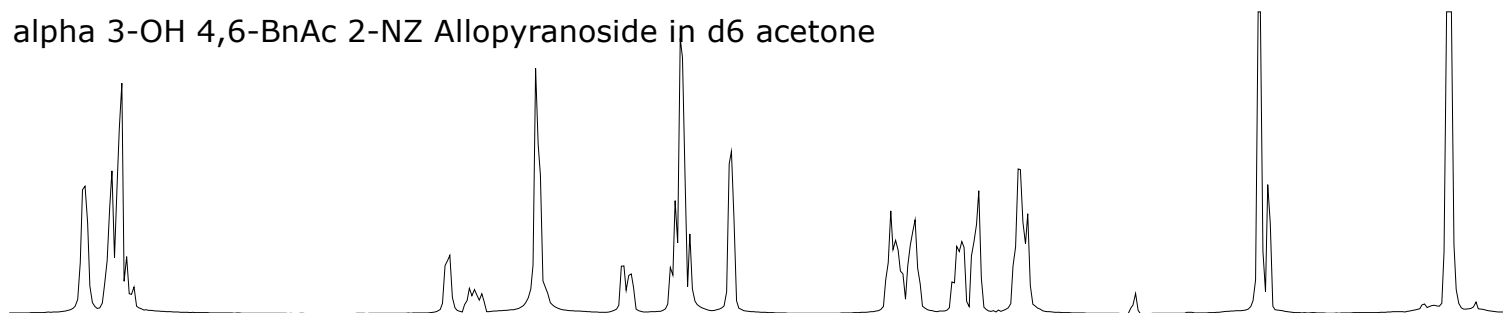
file: ...alphaBnAc_d6acetone_MeOHrext\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 19.729 ppm/cm: 0.03285



file: ...alphaBnAc_d6acetone_MeOHrext\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

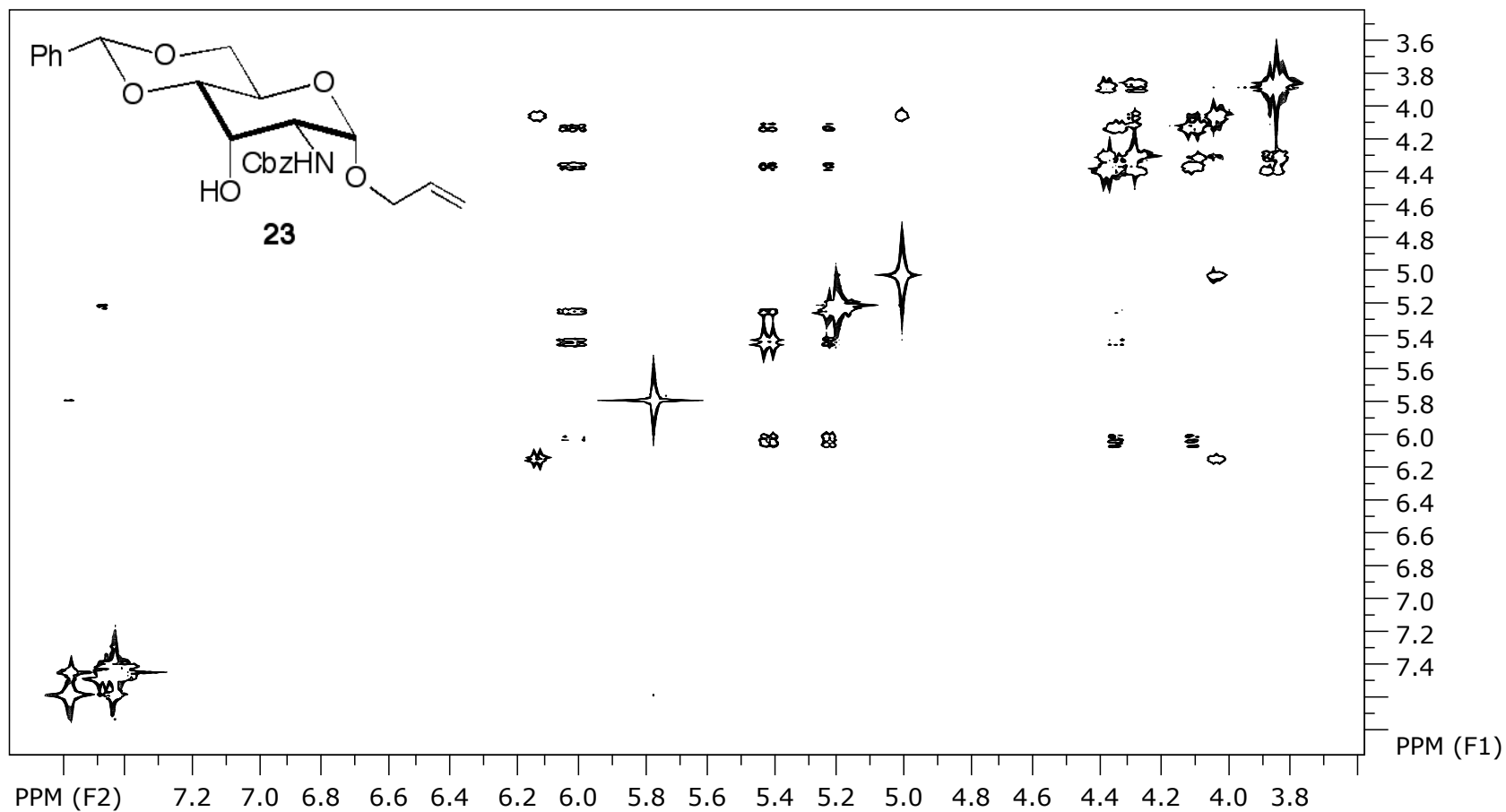
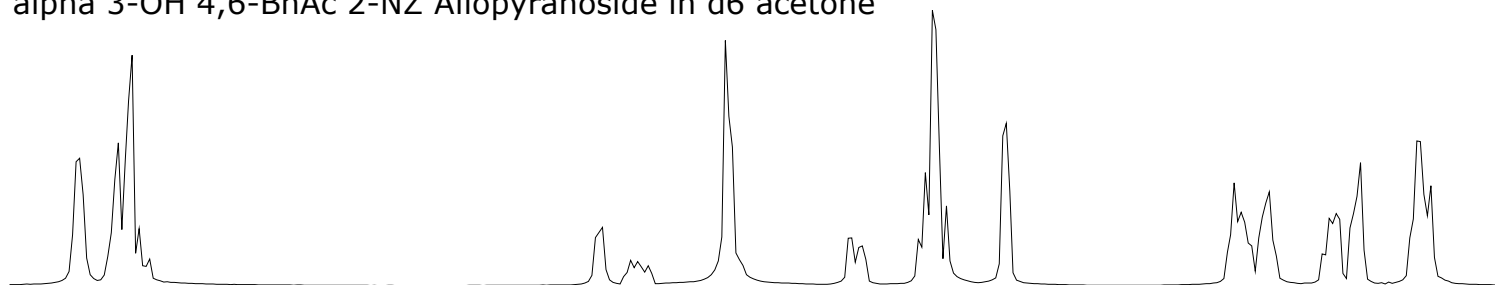
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 16.347 ppm/cm: 0.02722



file: ...alphaBnAc6acet_MeOHrextCOSY\1\ser
expt: <cosygpqf>
transmitter freq: 600.552832 MHz
time domain size: 2048 by 2048 points
width (F2): 6009.62 Hz = 10.0068 ppm = 2.9344 Hz/pt
number of scans: 8

F2: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 180.252 ppm/cm: 0.30014

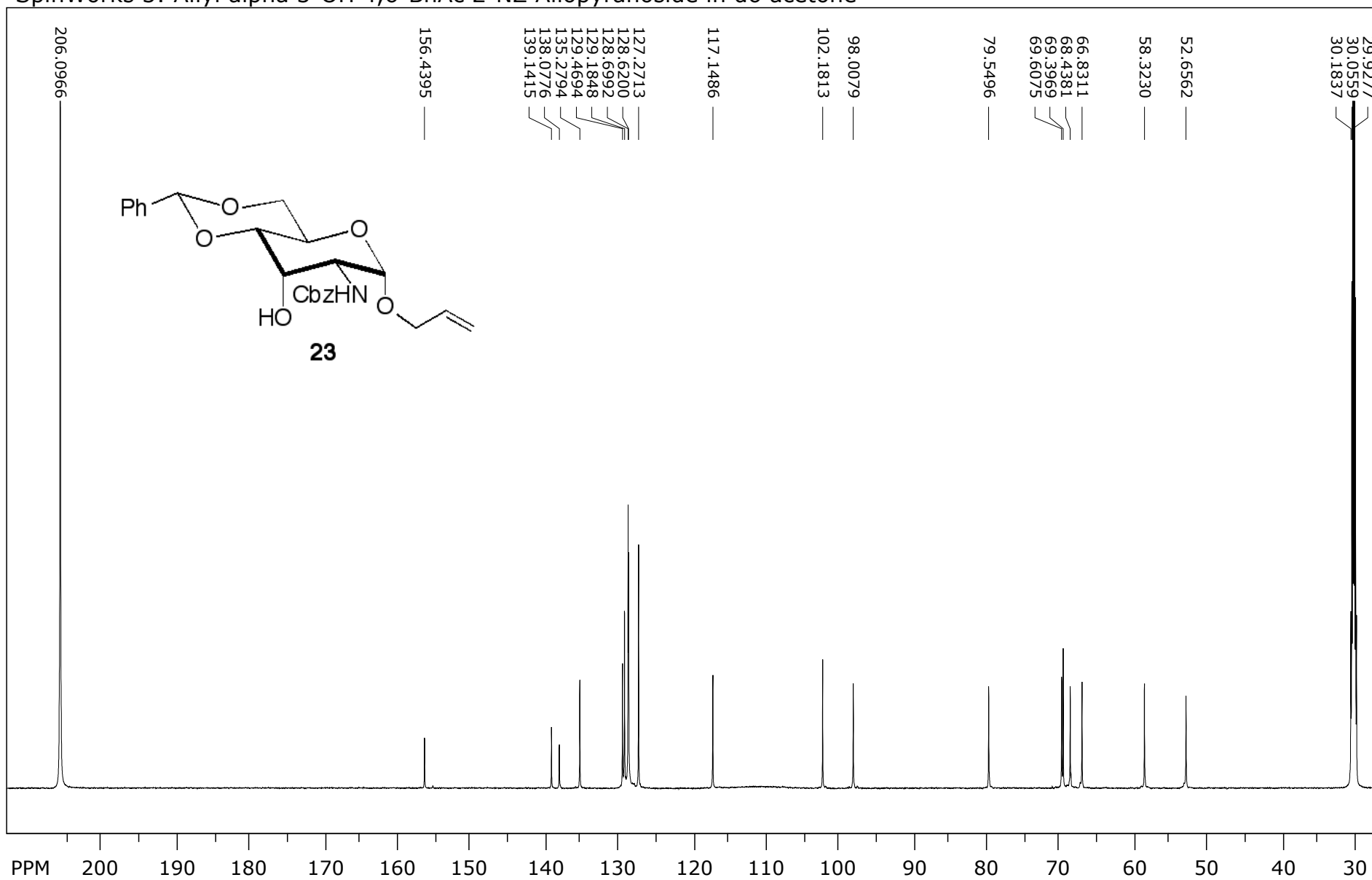
F1: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 348.787 ppm/cm: 0.58078



file: ...alphaBnAc6acet_MeOHrextCOSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.62 Hz = 10.0068 ppm = 2.9344 Hz/pt
 number of scans: 8

F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 125.763 ppm/cm: 0.20941

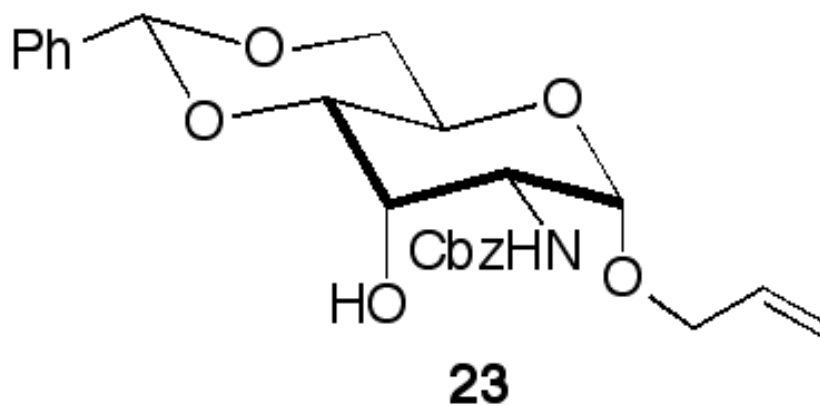
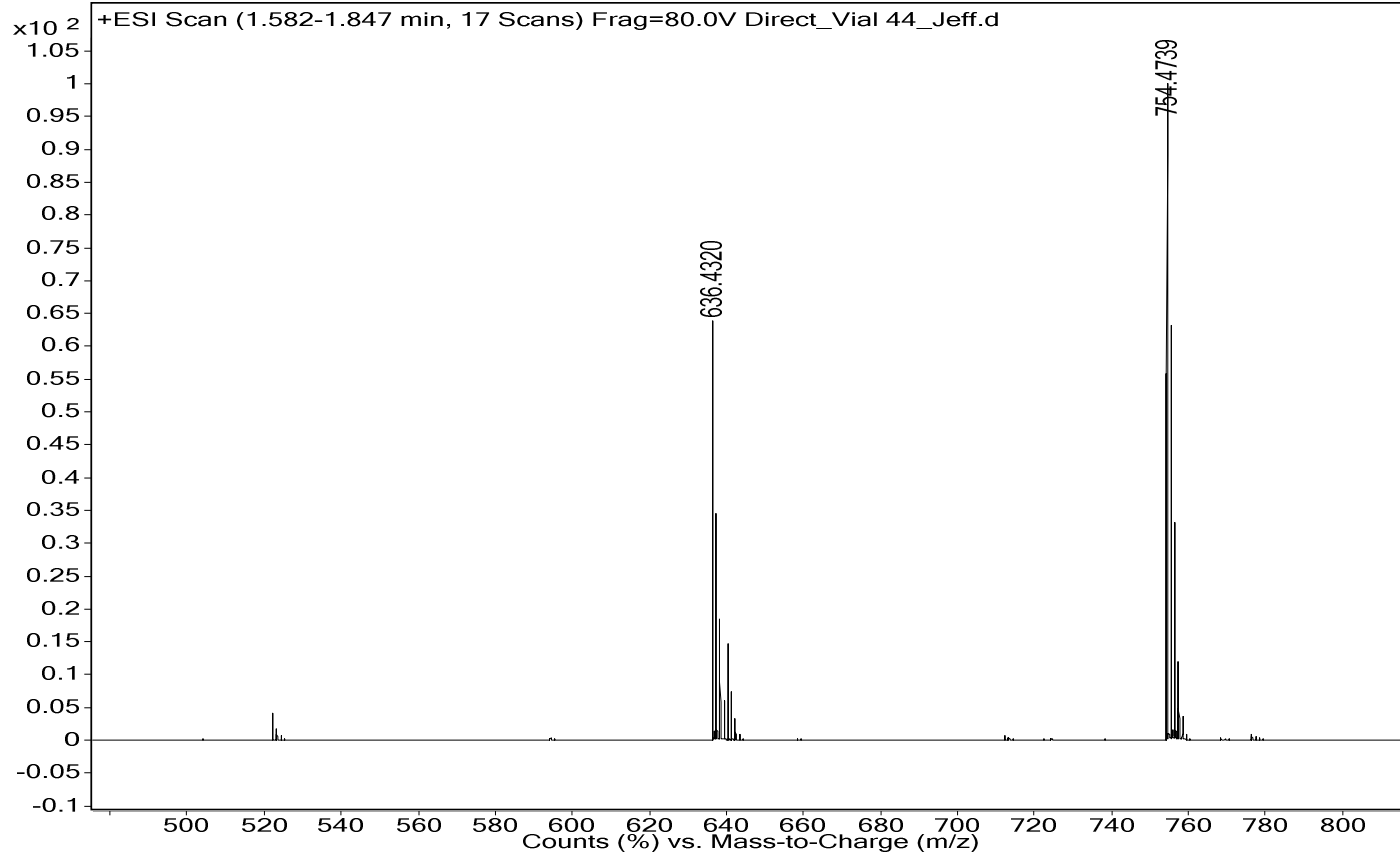
F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 247.836 ppm/cm: 0.41268

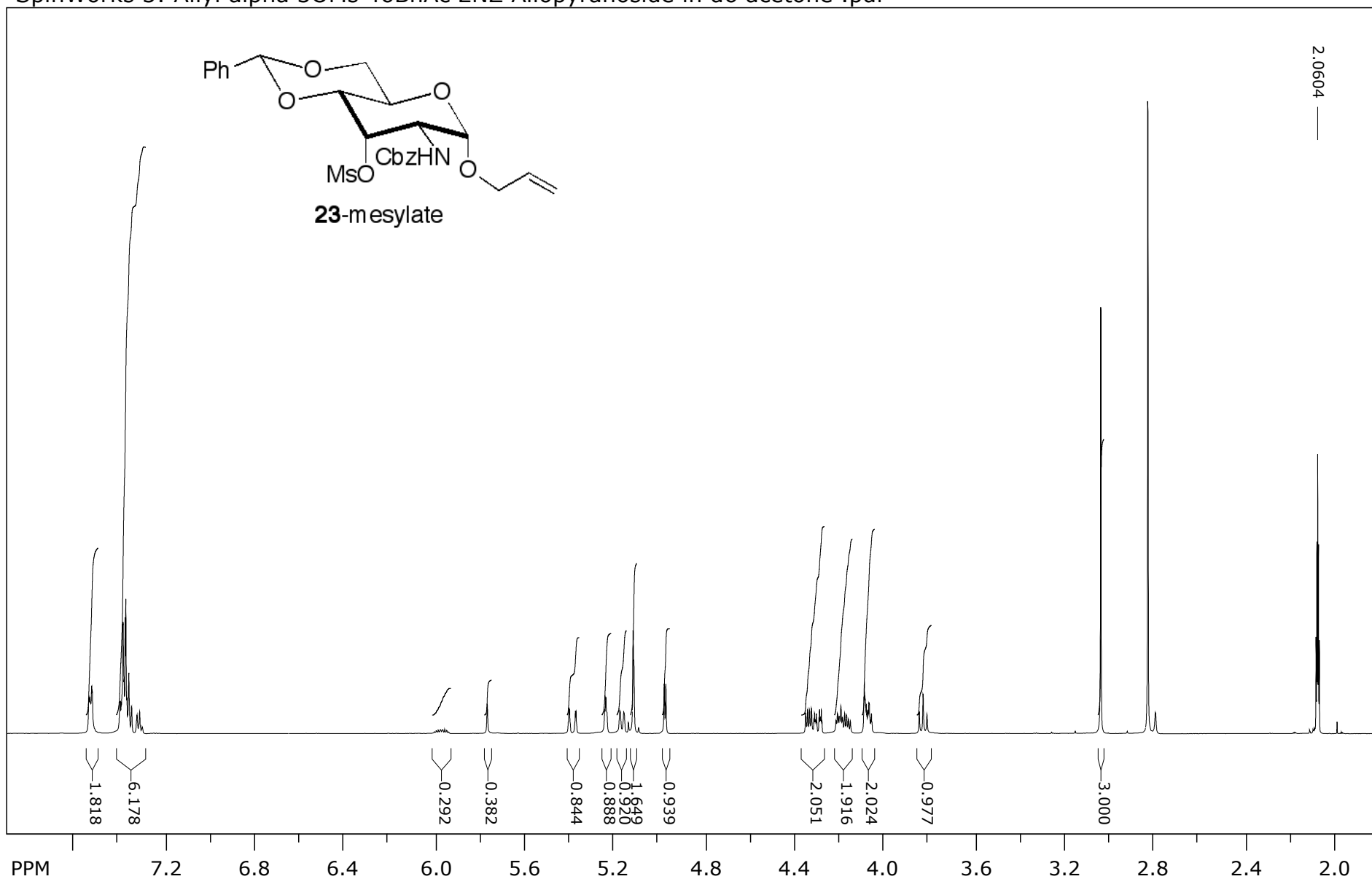


file: ...alphaBnAc6acet_MeOHrxt_C13\1\fid expt: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 34816

freq. of 0 ppm: 151.008293 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 1128.413 ppm/cm: 7.47177

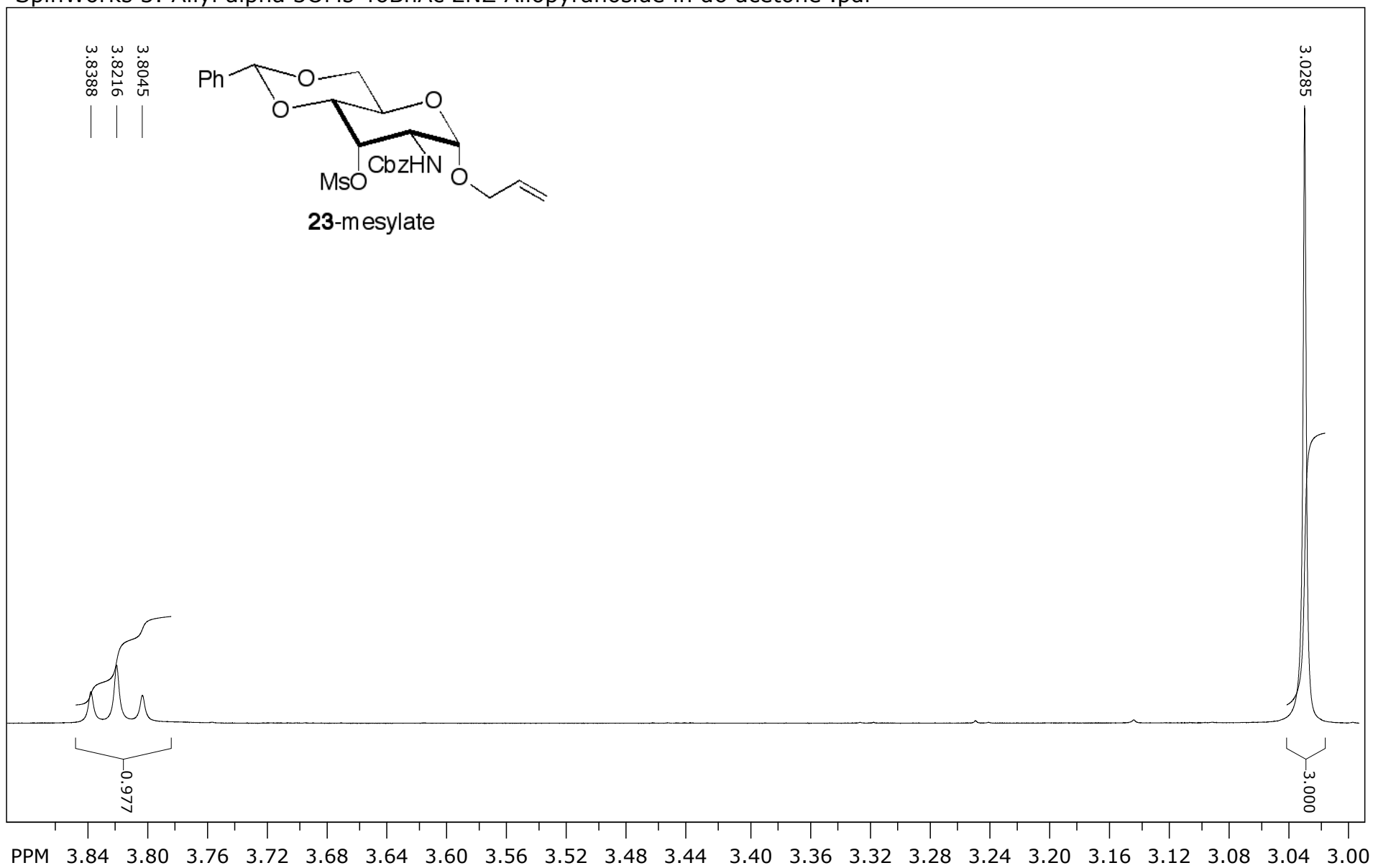
Sample Name	Jeff 44	Position	Vial 44	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 44_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 2:01:09 PM





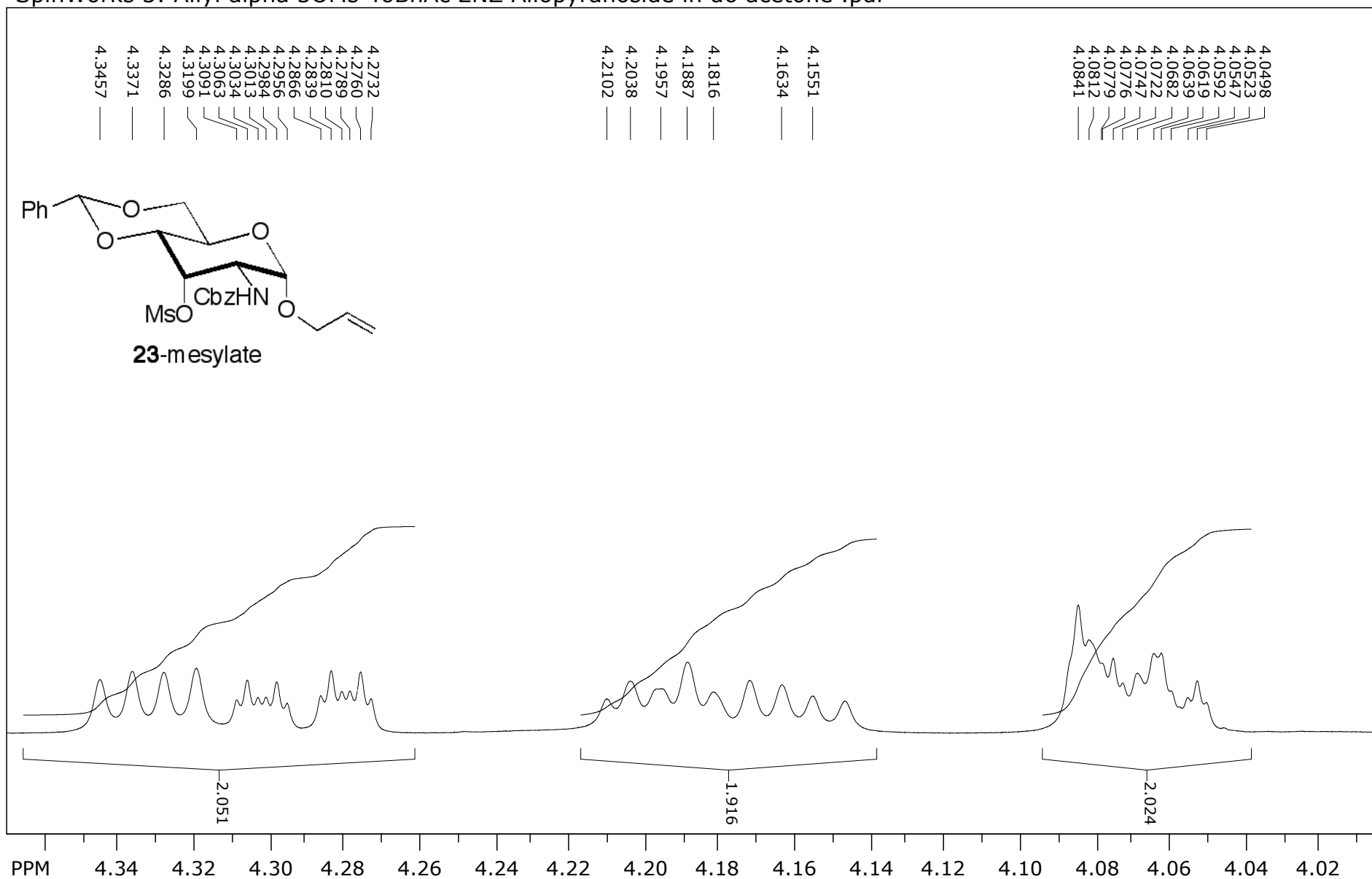
file: ...AllylAlpha3OMsBnAc_d6acetone\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 147.128 ppm/cm: 0.24499



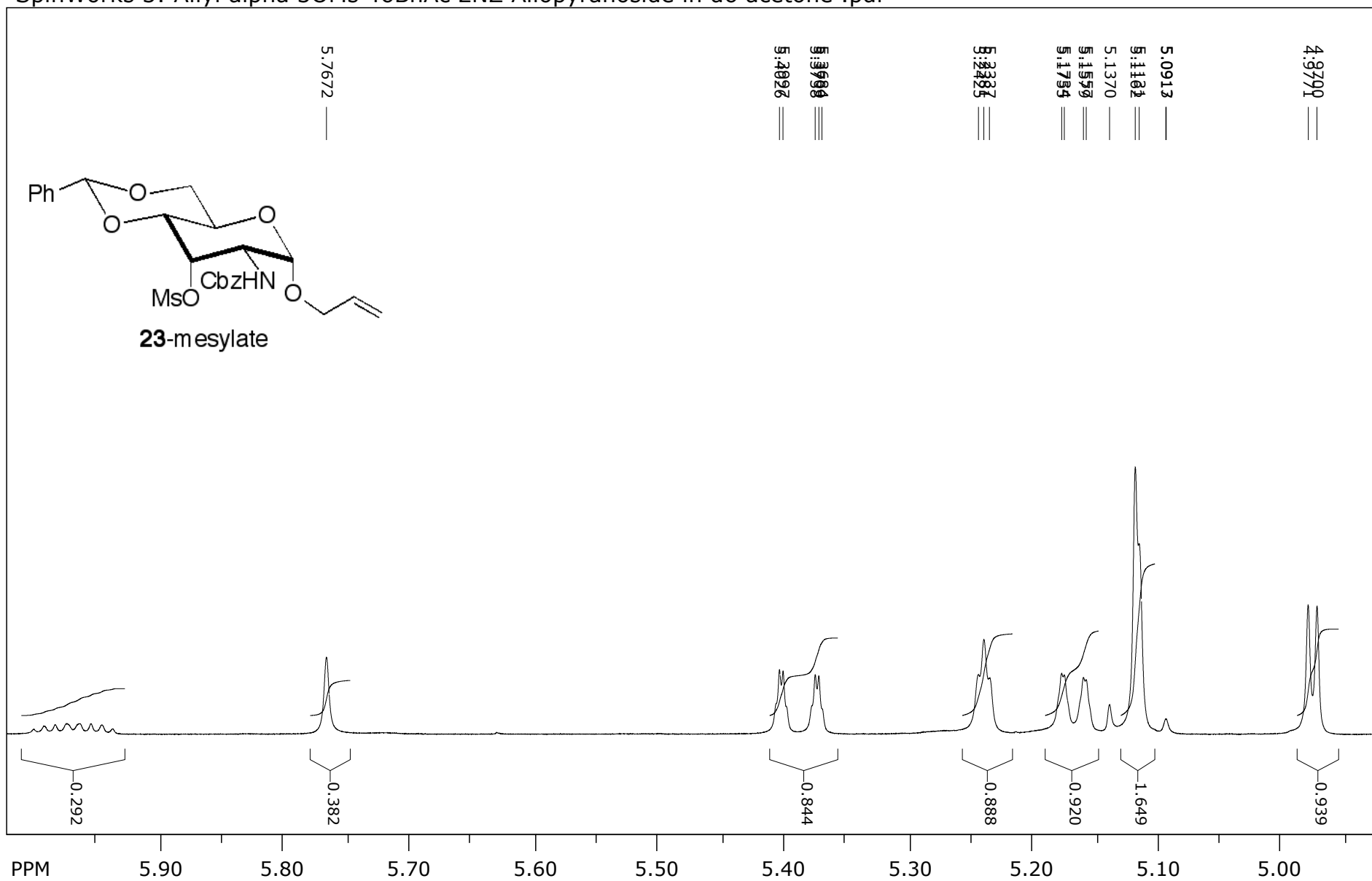
file: ...AllylAlpha3OMsBnAc_d6acetone\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 21.699 ppm/cm: 0.03613



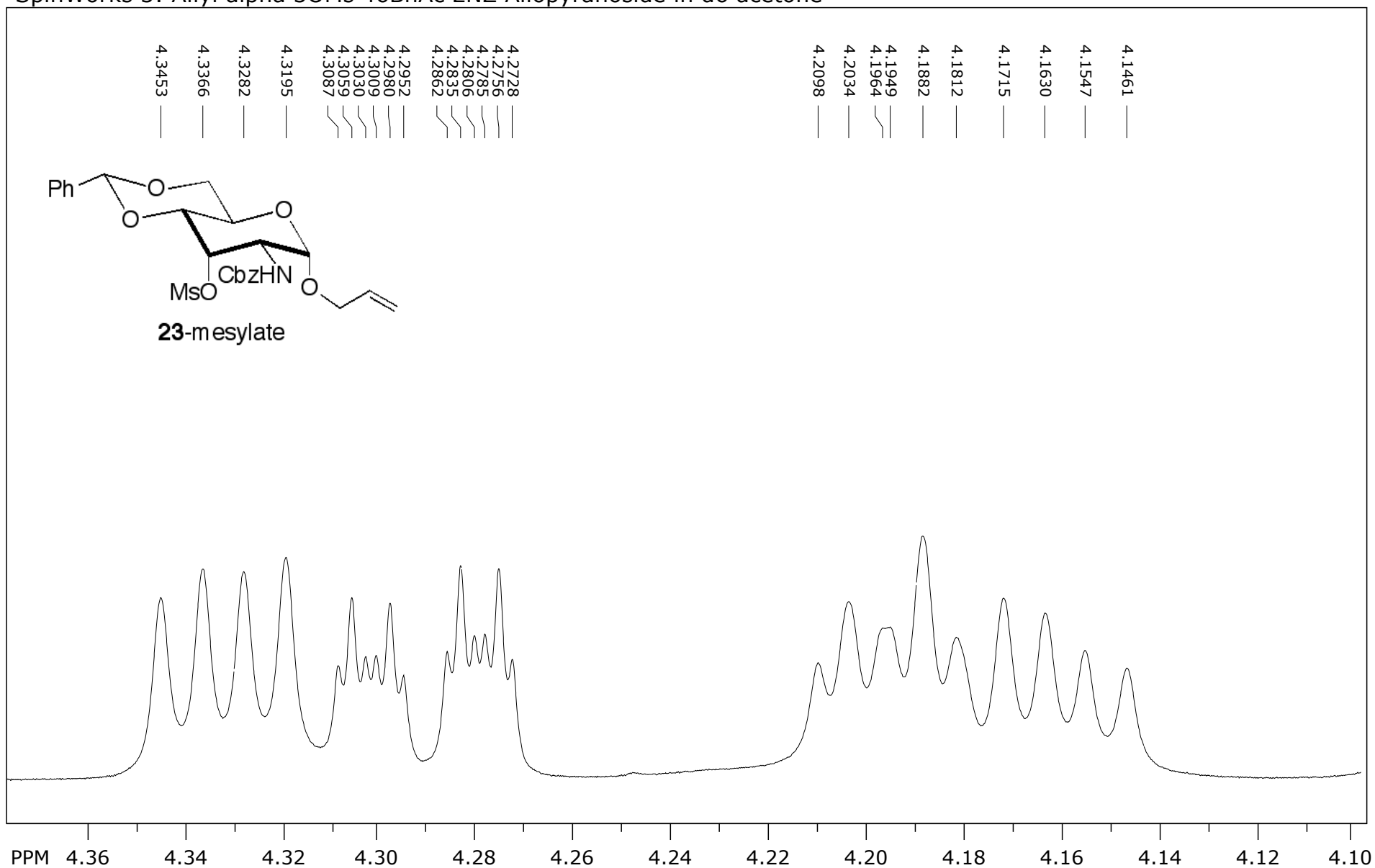
file: ...AllylAlpha3OMsBnAc_d6acetone\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 8.814 ppm/cm: 0.01468



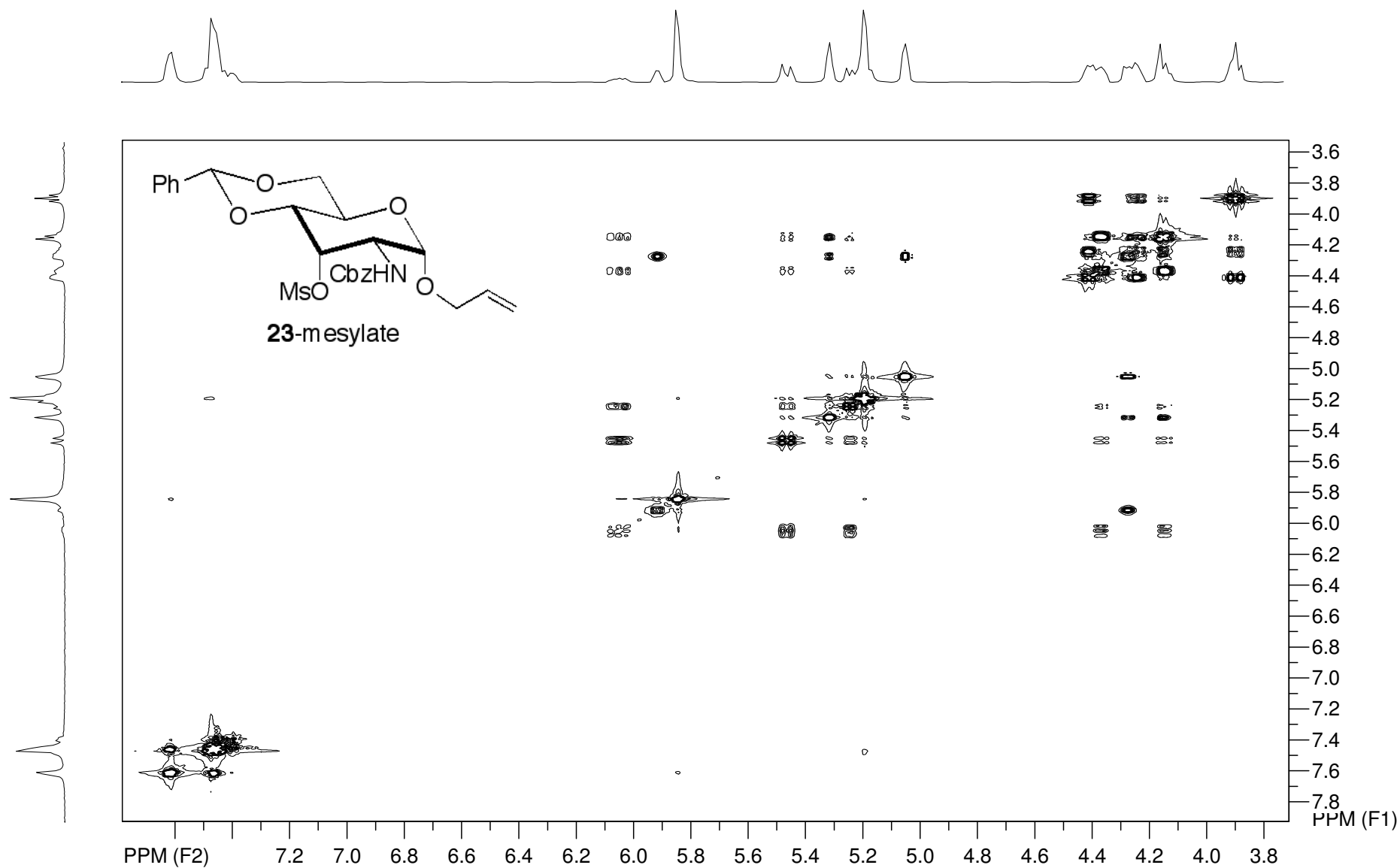
file: ...AllylAlpha3OMsBnAc_d6acetone\1\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 26.526 ppm/cm: 0.04417



file: ...AllylAlpha3OMsBnAc_d6acetone\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

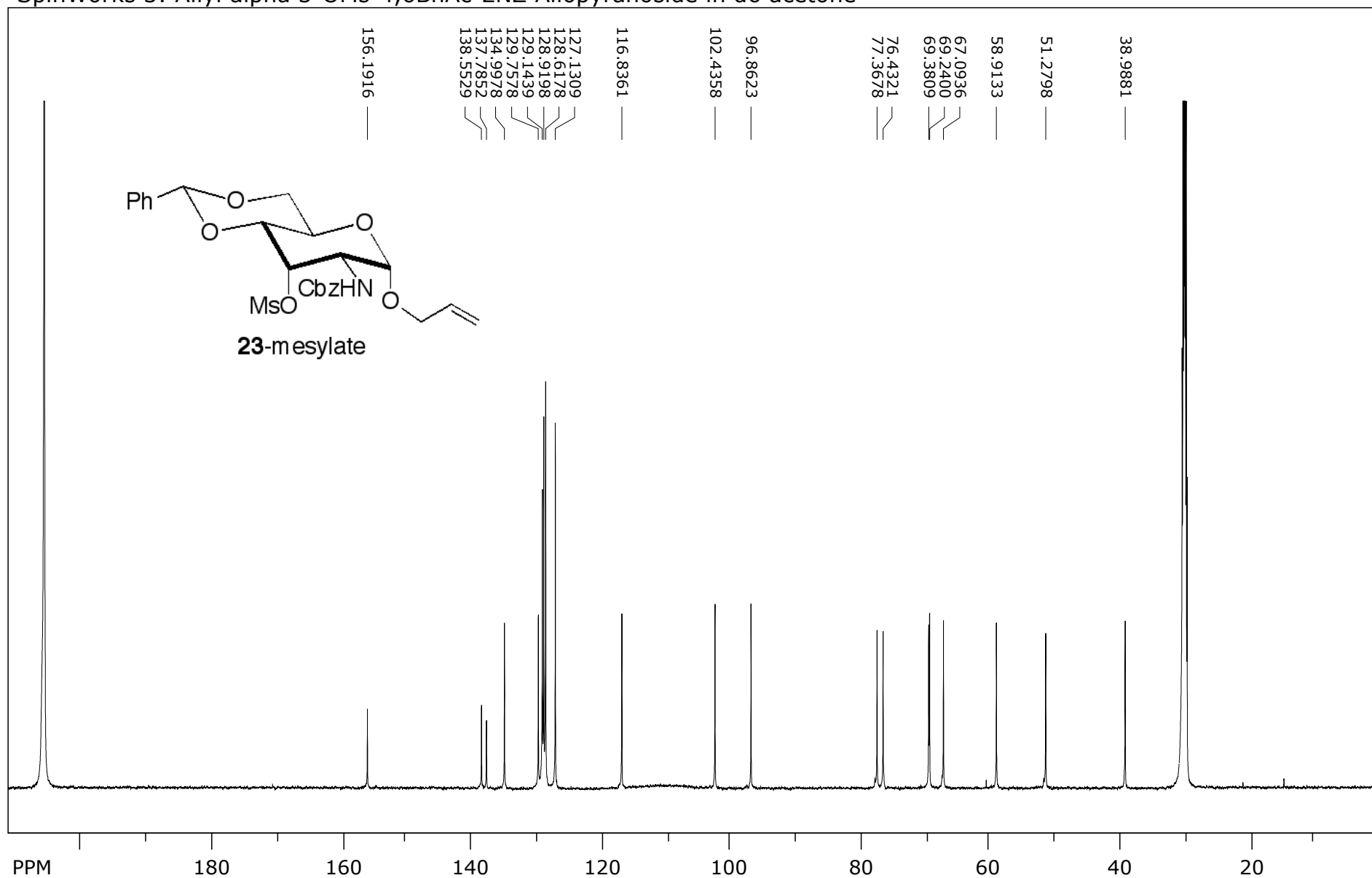
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 6.712 ppm/cm: 0.01118



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\Allyl\Alpha3OMsBnAc_Ace\F2:\freq. of 0 ppm: 600.549962 MHz
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 119.263 ppm/cm: 0.19859

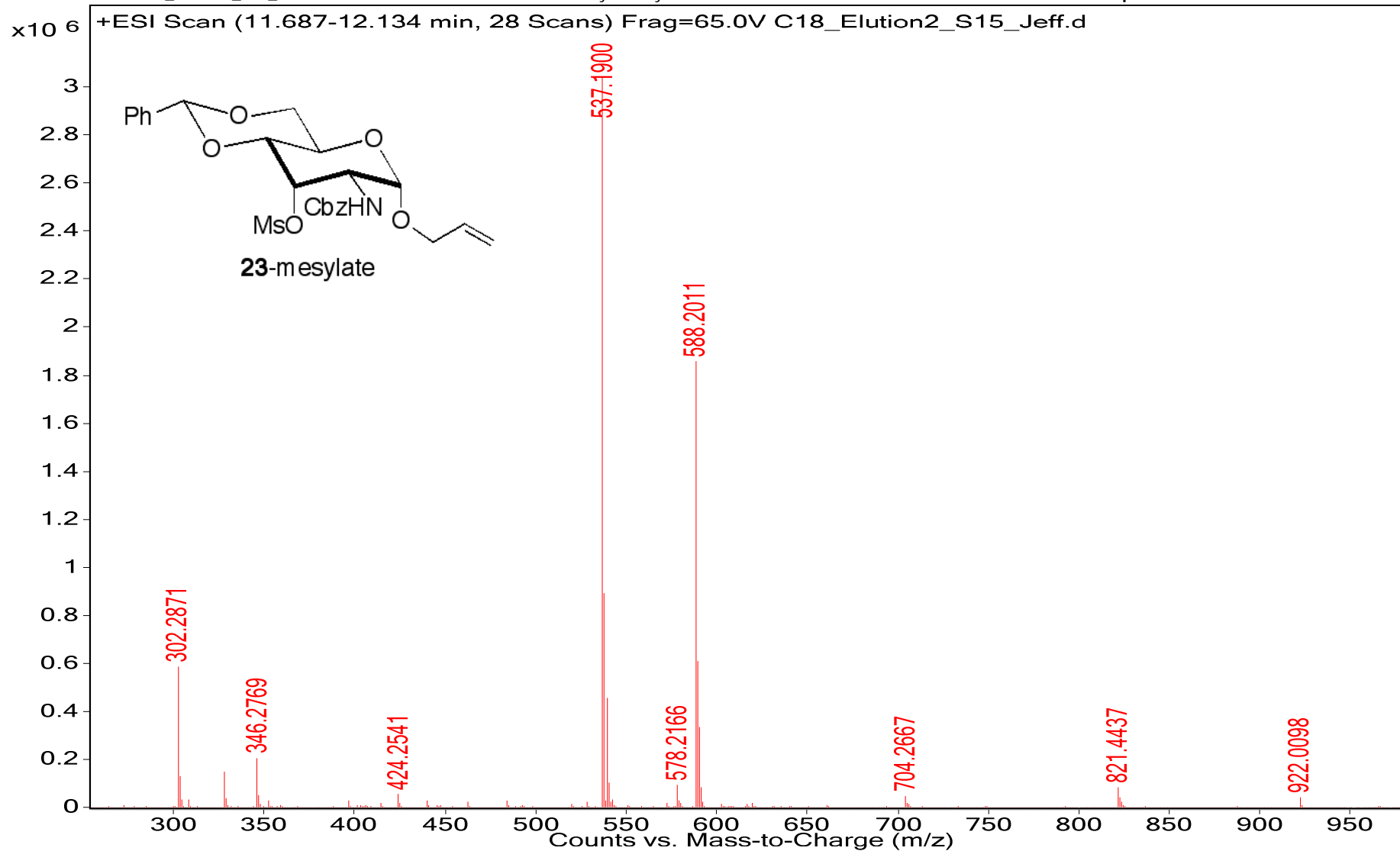
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 220.458 ppm/cm: 0.36709

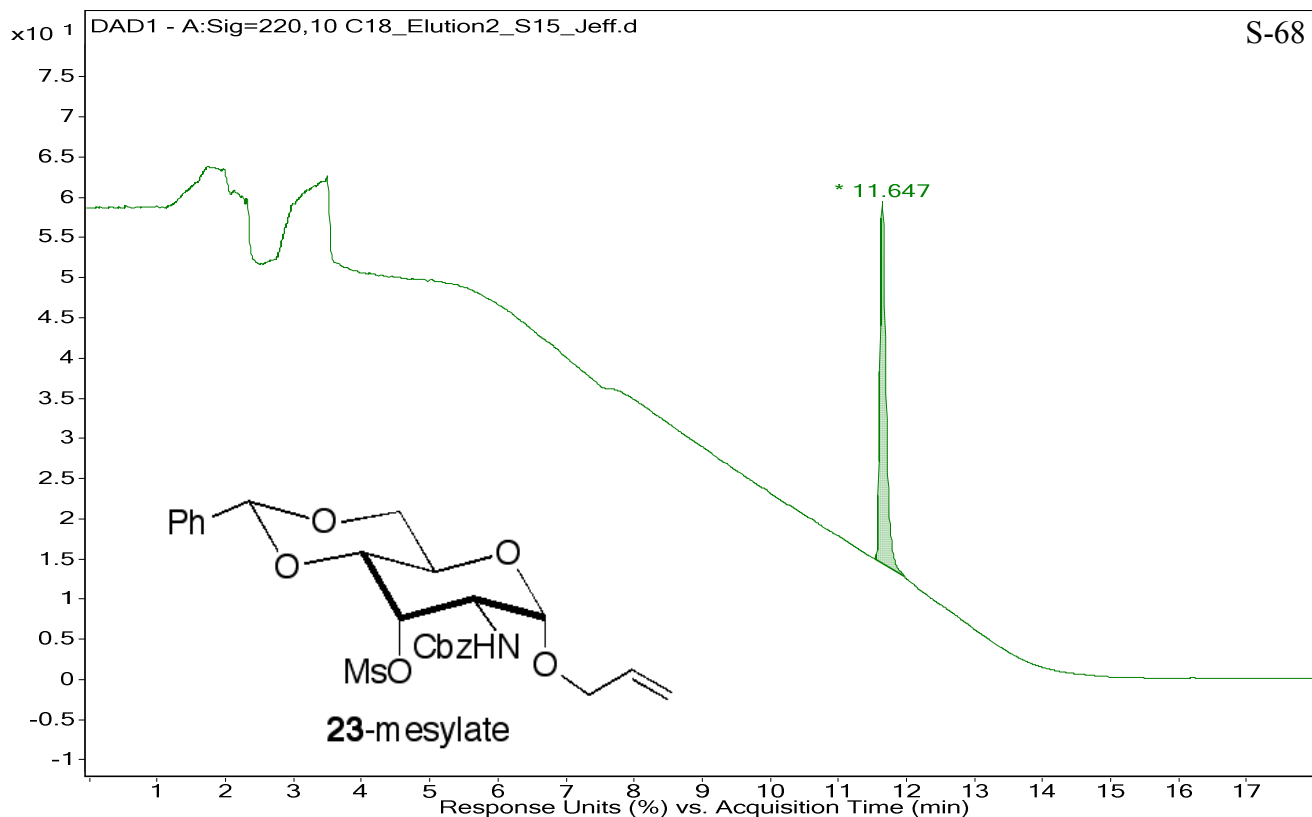


file: ...allylAlpha3OMsBnAc_d6acet13C\1\fid expt: <zgpg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 28672

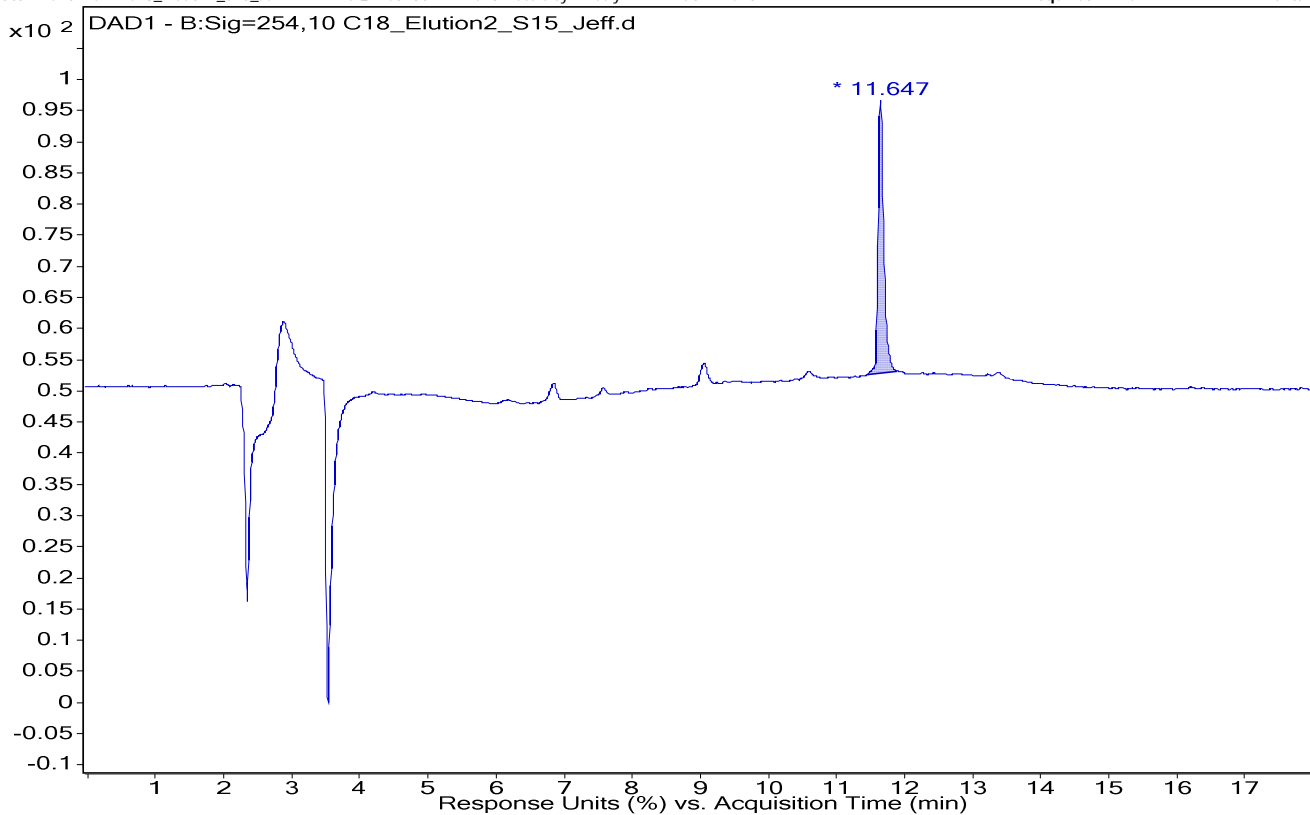
freq. of 0 ppm: 151.008298 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 1280.531 ppm/cm: 8.47902

Sample Name	Jeff-15	Position	Vial 14	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution2_S15_Jef	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/15/2012 5:39:14 /



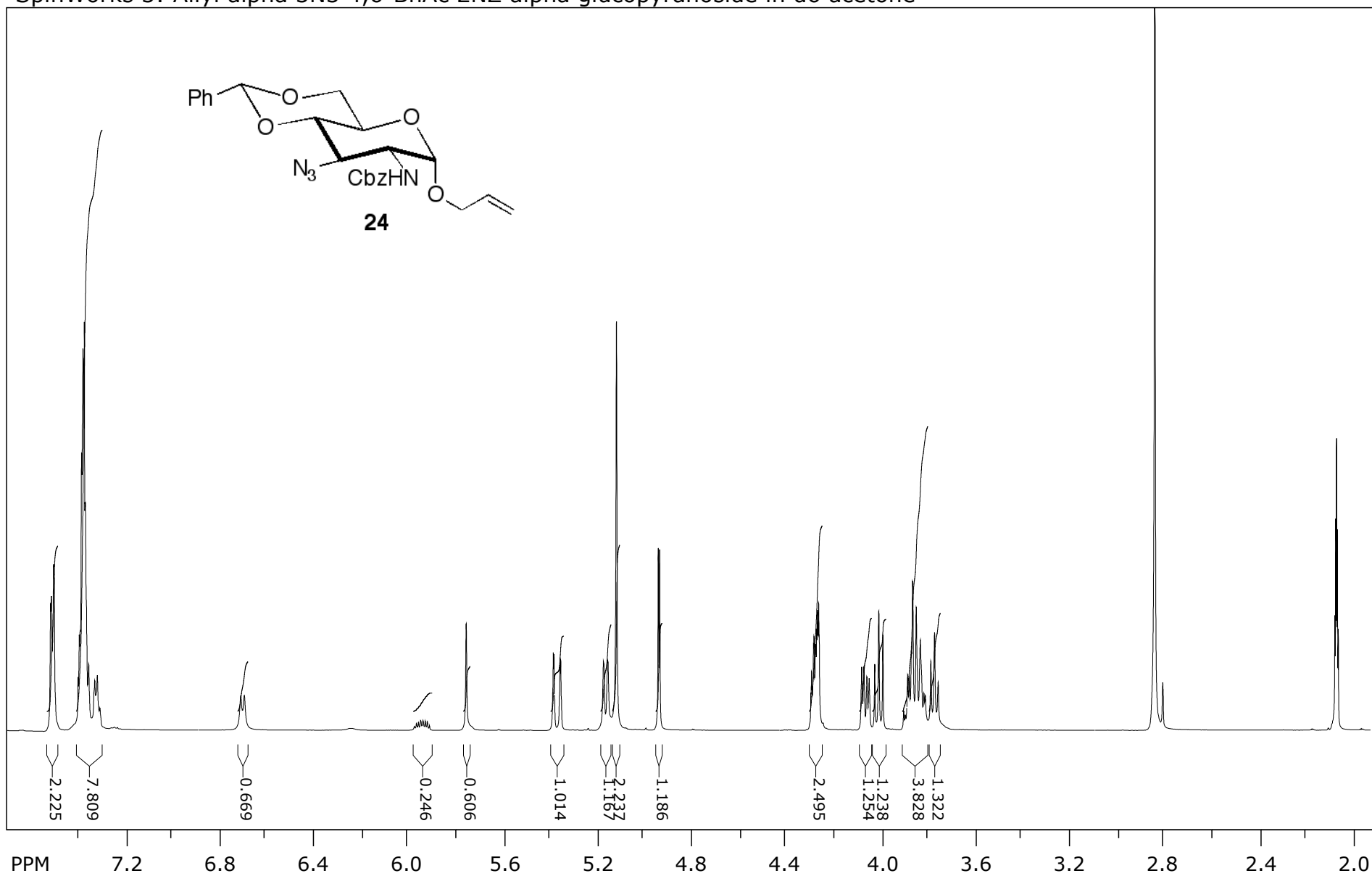


Sample Name	Jeff-15	Position	Vial 14	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution2_S15_Jef	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/15/2012 5:39:14 AM



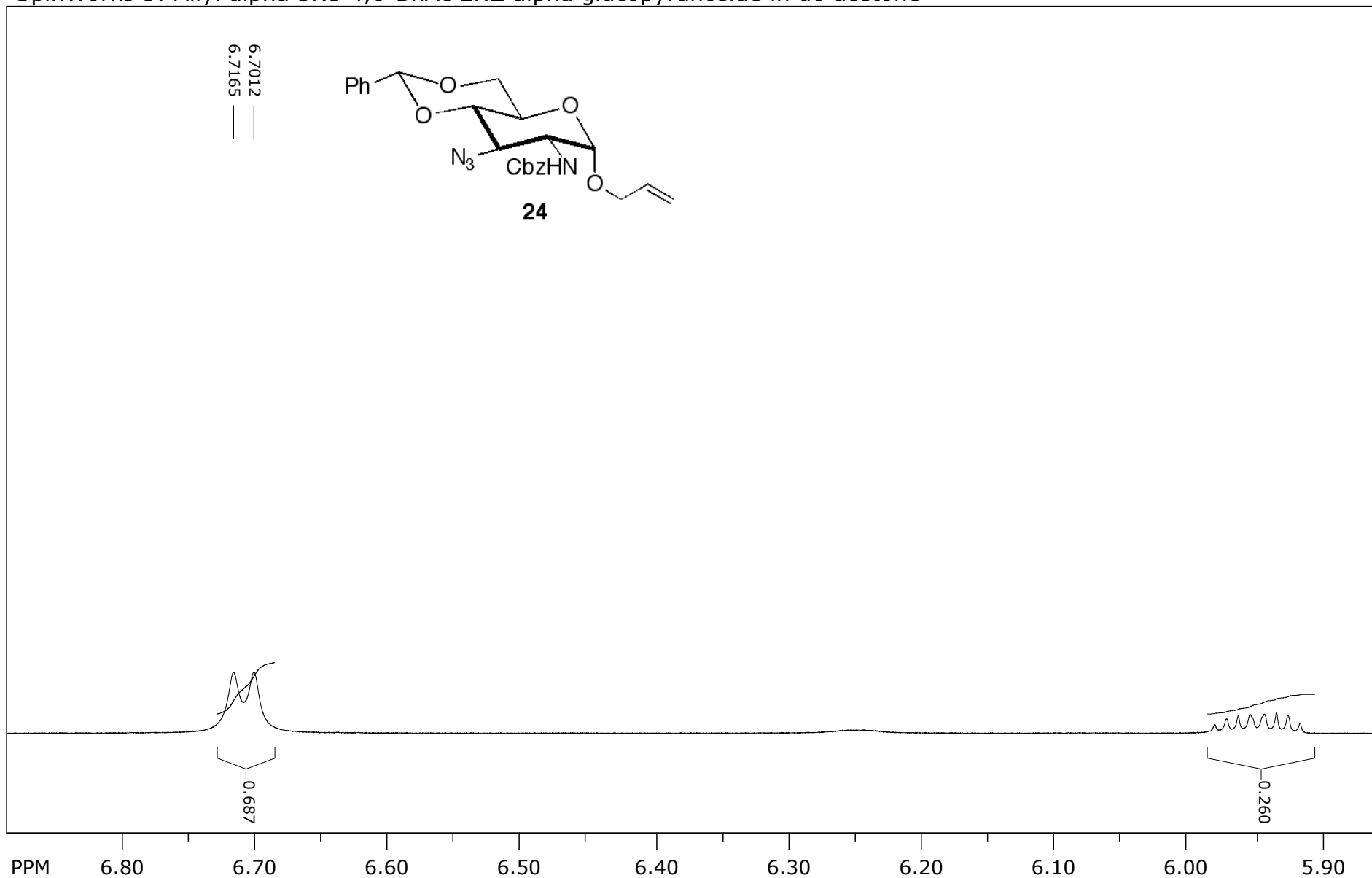
Analysis on a Waters SymmetryShield™ C18 (4.6 mm X 15 cm (i.d. x l.), 3.5 μm) at 0.5 mL/min. Solvent A: 50 mM NH₄OAc (aq); B: CH₃CN

Time (min)	% B
0	20
1	20
10	100
20	100



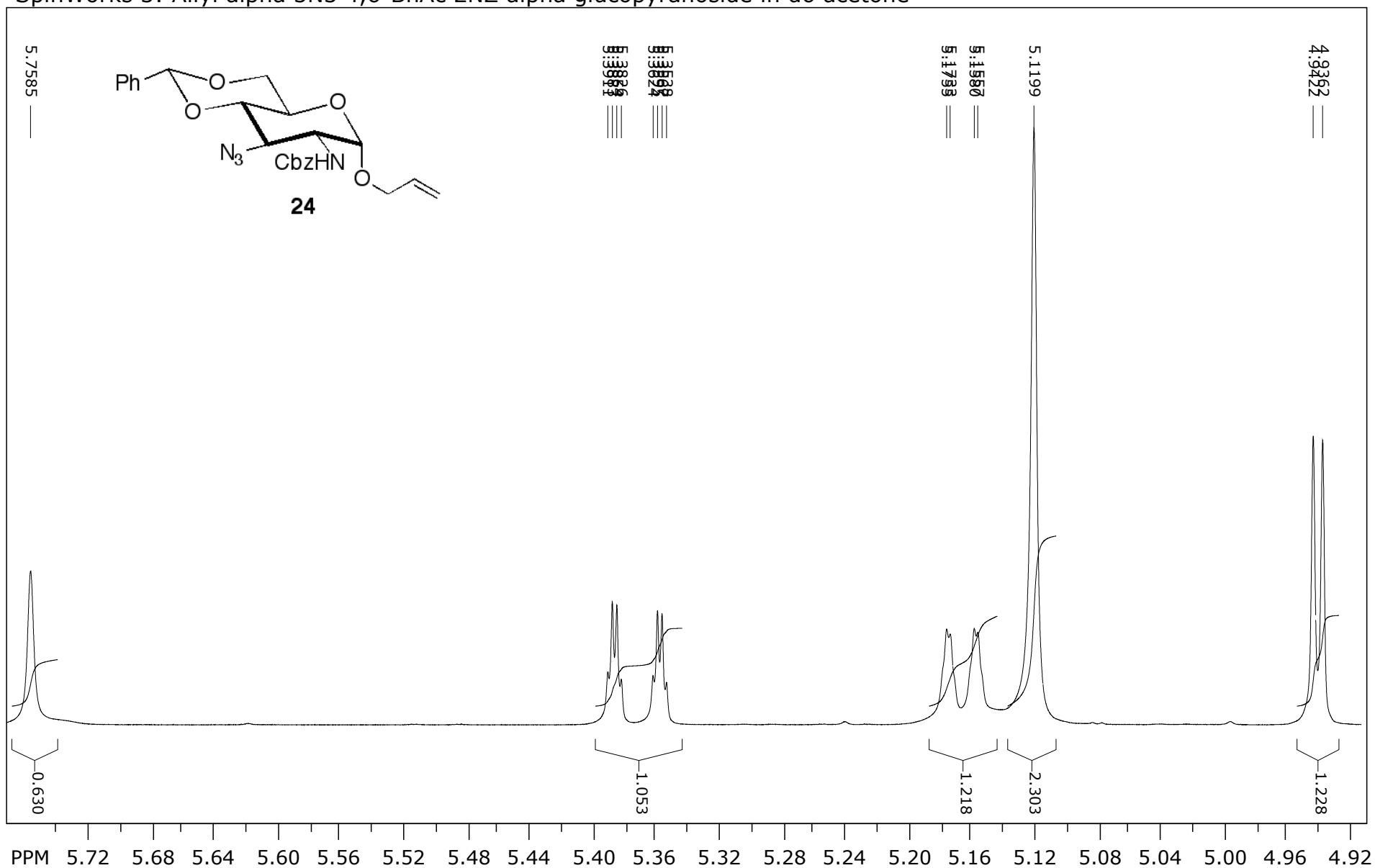
file: ...pha3N3GluBnAc2NZ1OAllyl_acet\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 139.241 ppm/cm: 0.23185



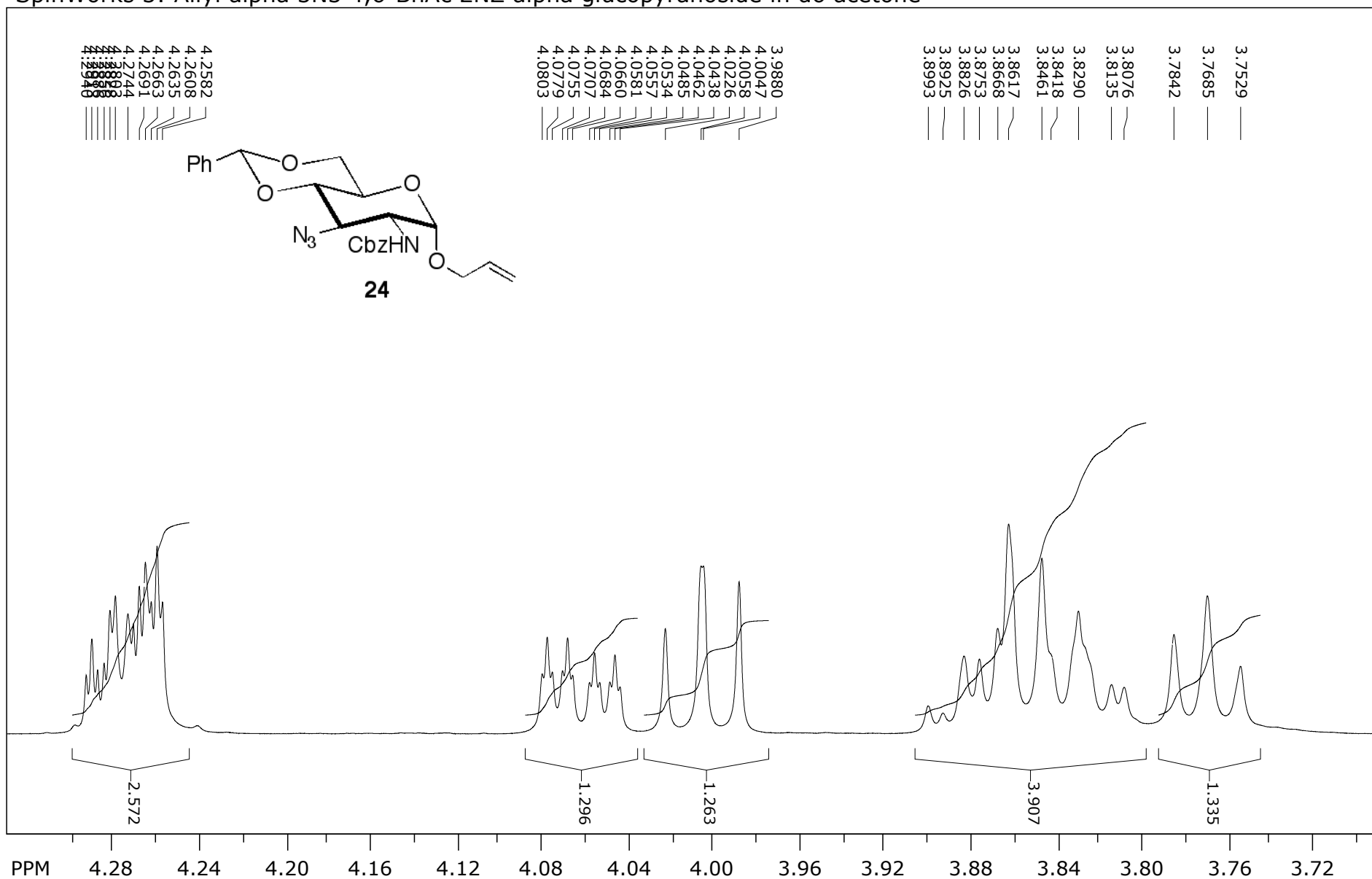
file: ...pha3N3GluBnAc2NZ1OAllyl_acet\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 24.790 ppm/cm: 0.04128



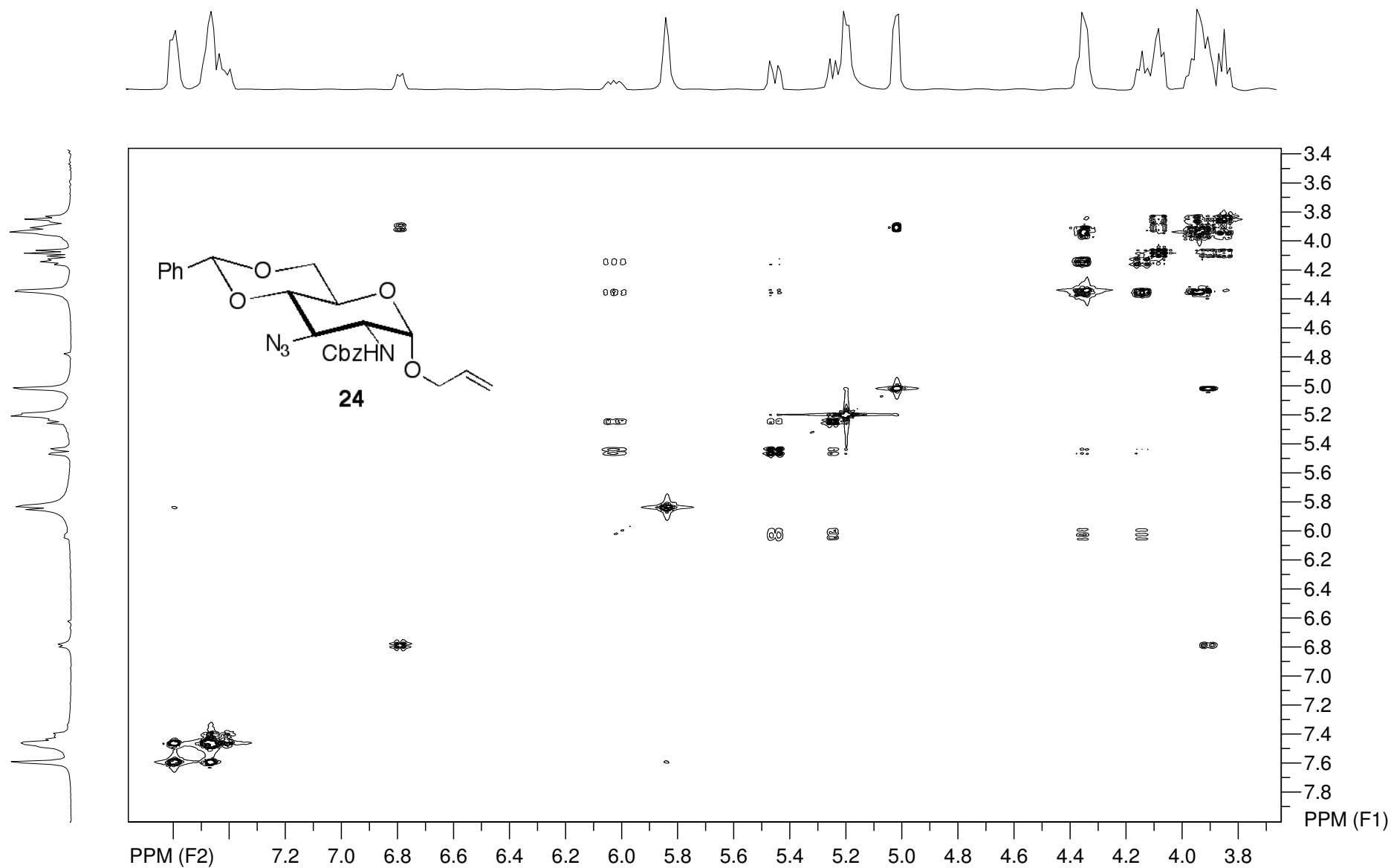
file: ...pha3N3GluBnAc2NZ1OAllyl_acet\1\fid expt: <zgr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 20.713 ppm/cm: 0.03449



file: ...pha3N3GluBnAc2NZ1OAllyl_acet\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

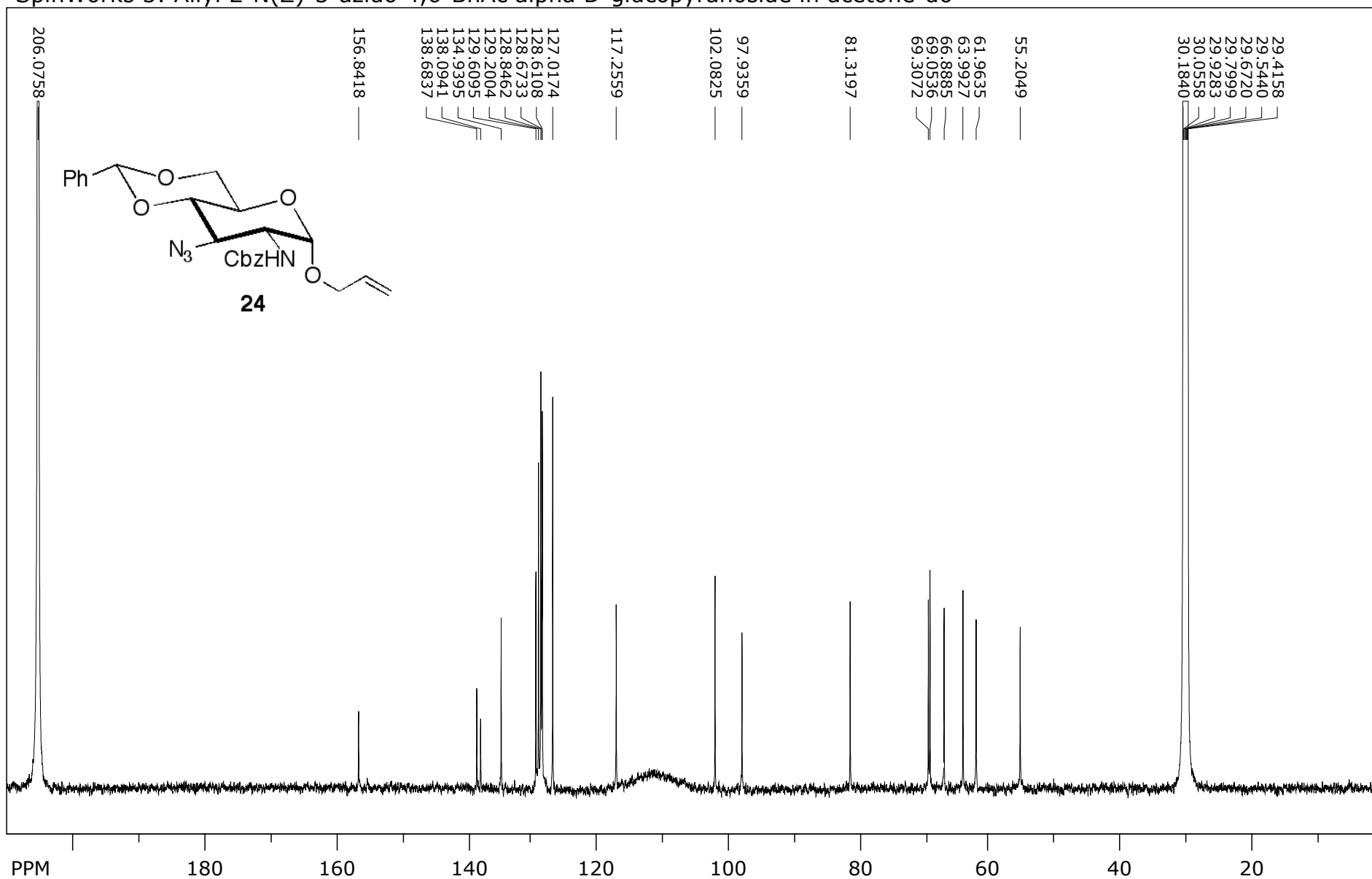
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.500 GF: 0.0000
Hz/cm: 15.447 ppm/cm: 0.02572



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\alpha3N3GluBnAc2NZ1OF2:1freq. of 0 ppm: 600.549962 MHz
transmitter freq.: 600.552832 MHz
time domain size: 2048 by 2048 points
width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
number of scans: 2

processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 120.521 ppm/cm: 0.20068

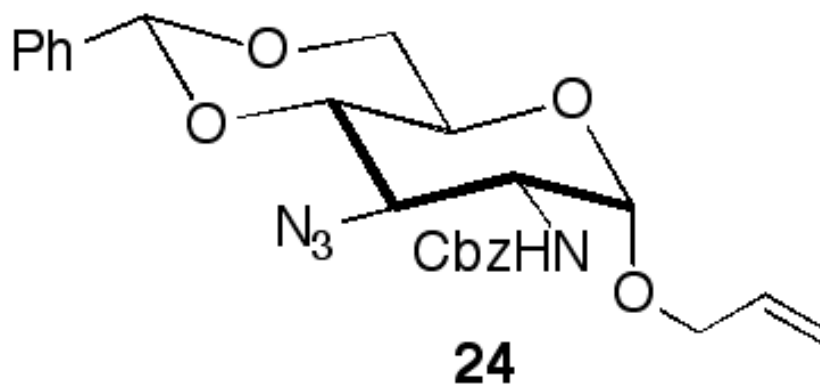
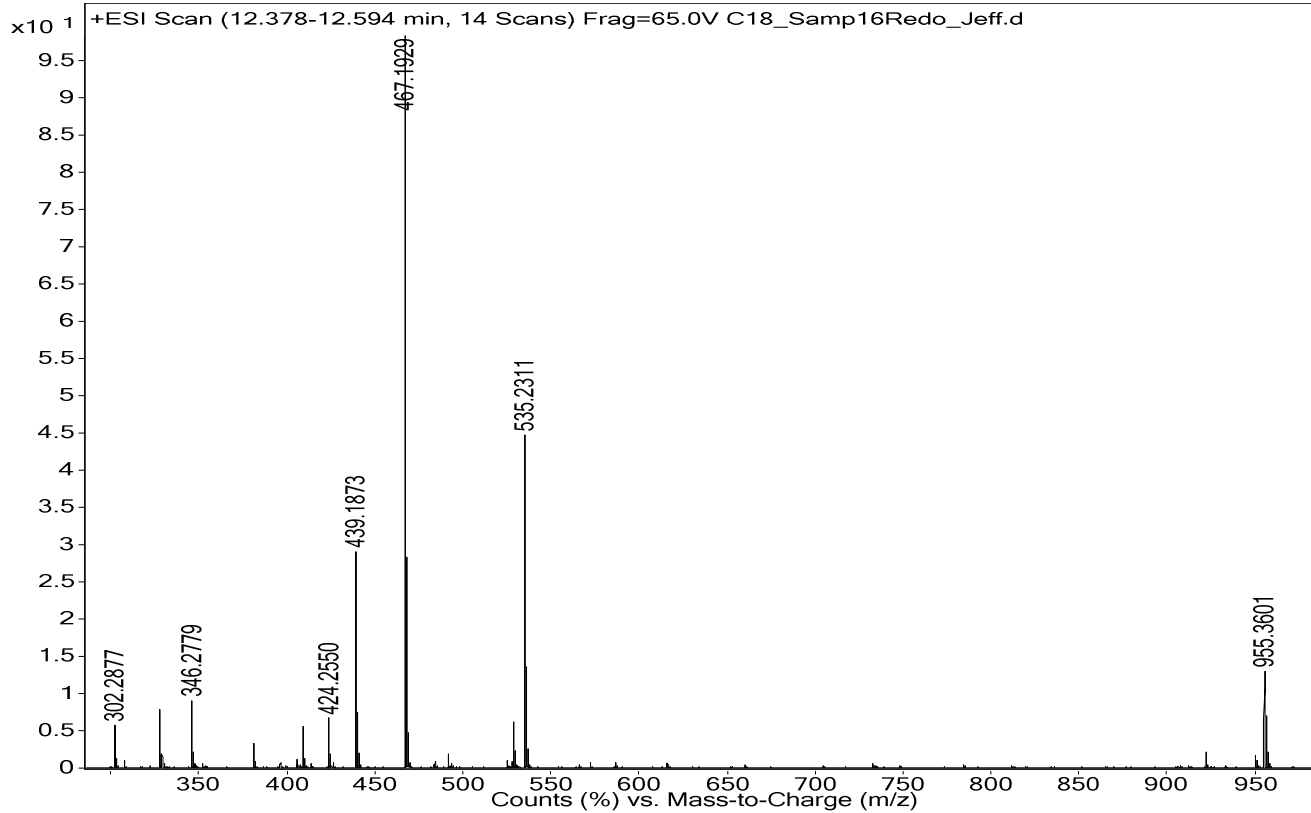
F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 232.549 ppm/cm: 0.38722

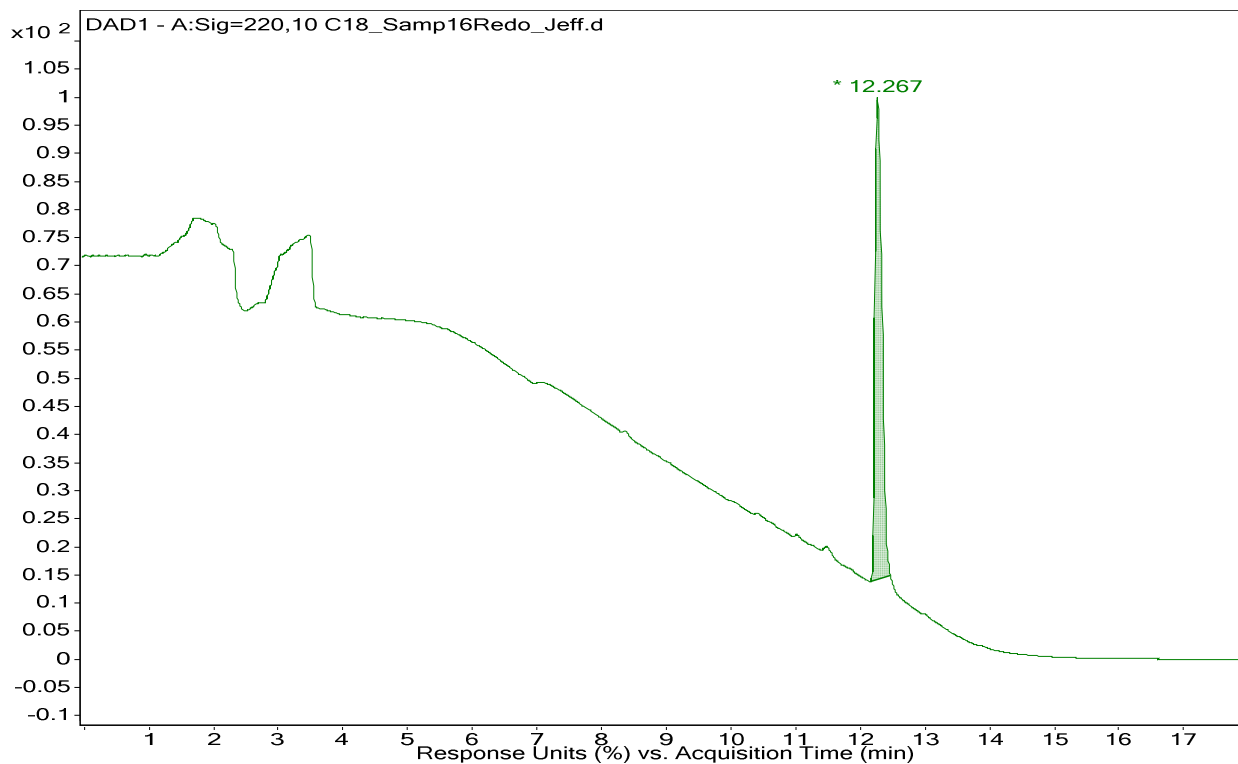


file: ...Allyl_alpha3N3Glu_Acetd6_13C\1\fid expt: <zgpg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 36864

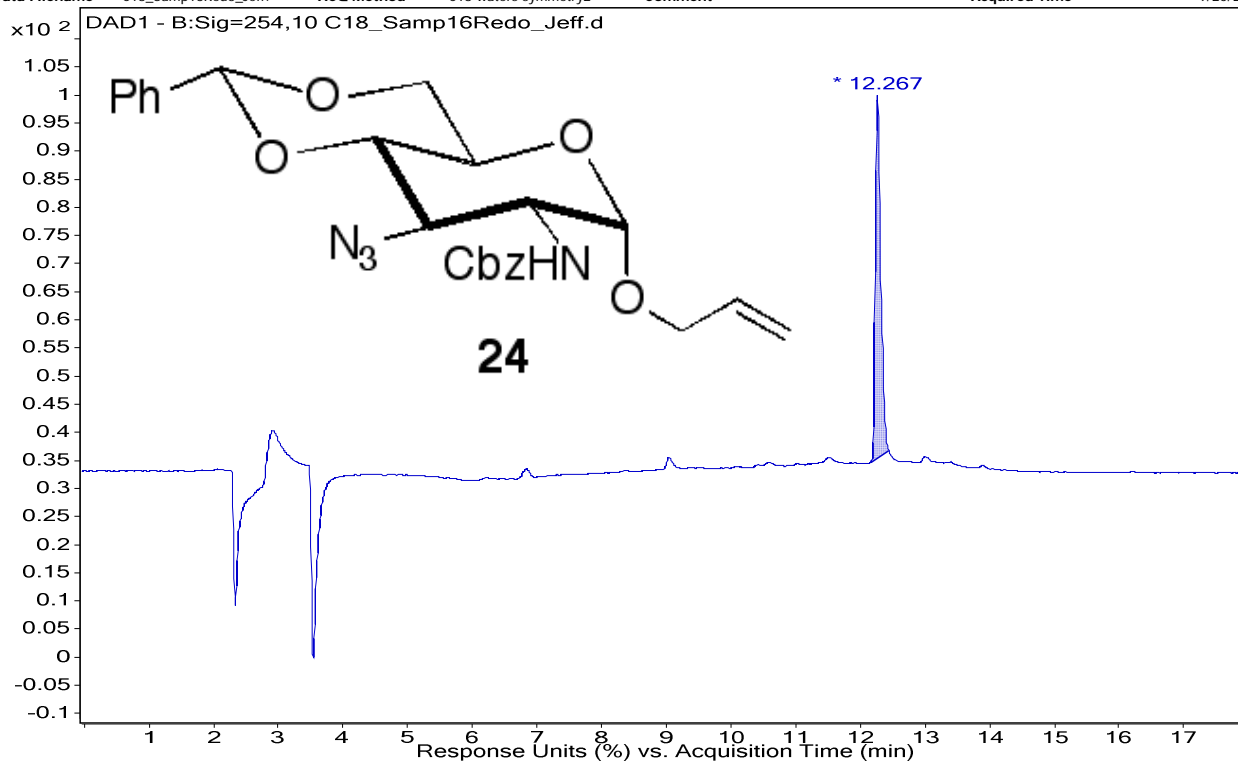
freq. of 0 ppm: 151.008287 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 1273.287 ppm/cm: 8.43105

Sample Name	Sample16 redo	Position	Vial 7	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	3	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Samp16Redo_Jeff.	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/20/2012 6:06:54 AM



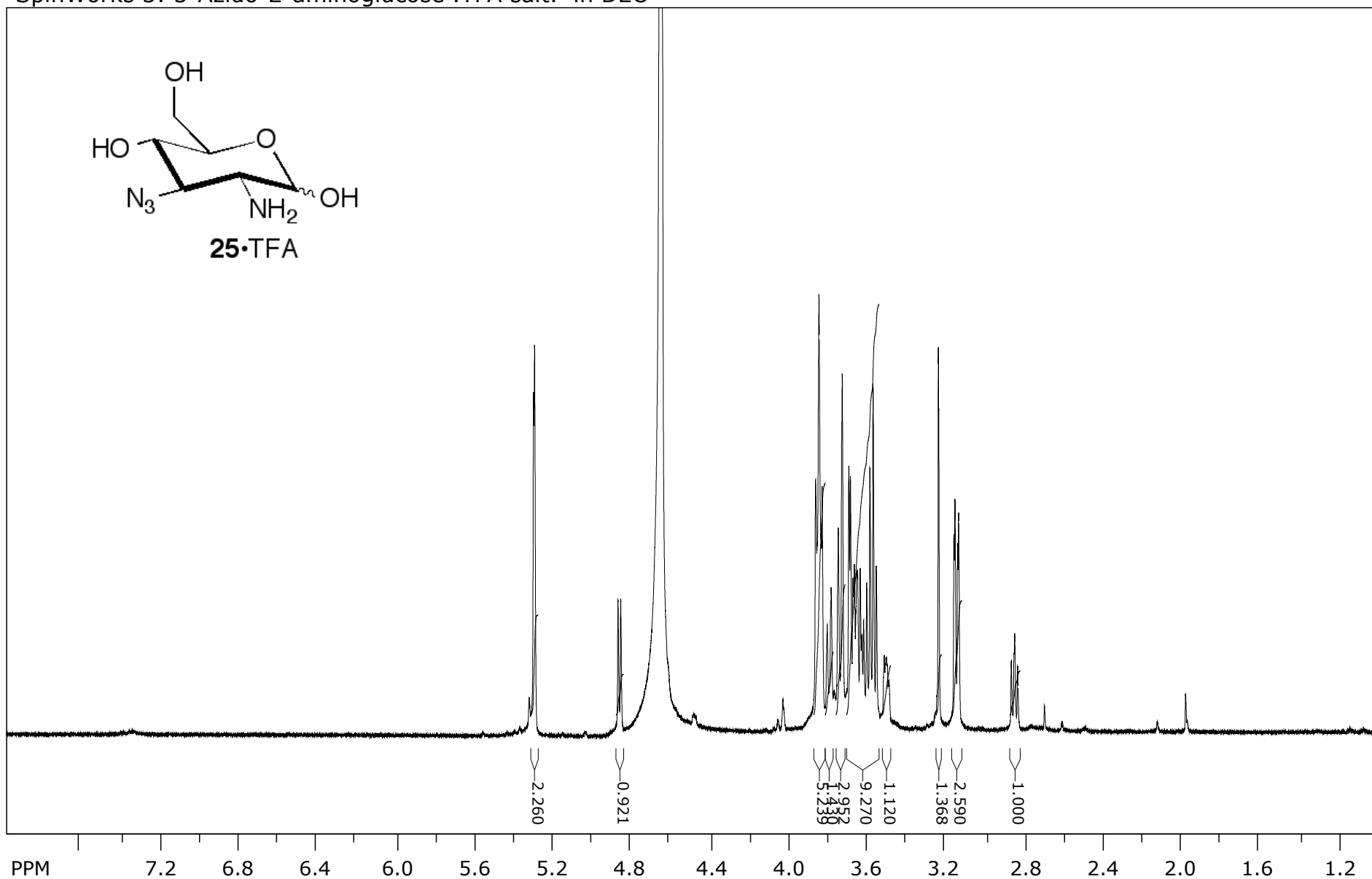


Sample Name	Sample16 redo	Position	Vial 7	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	3	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Samp16Redo_Jeff.	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/20/2012 6:06:54 AM



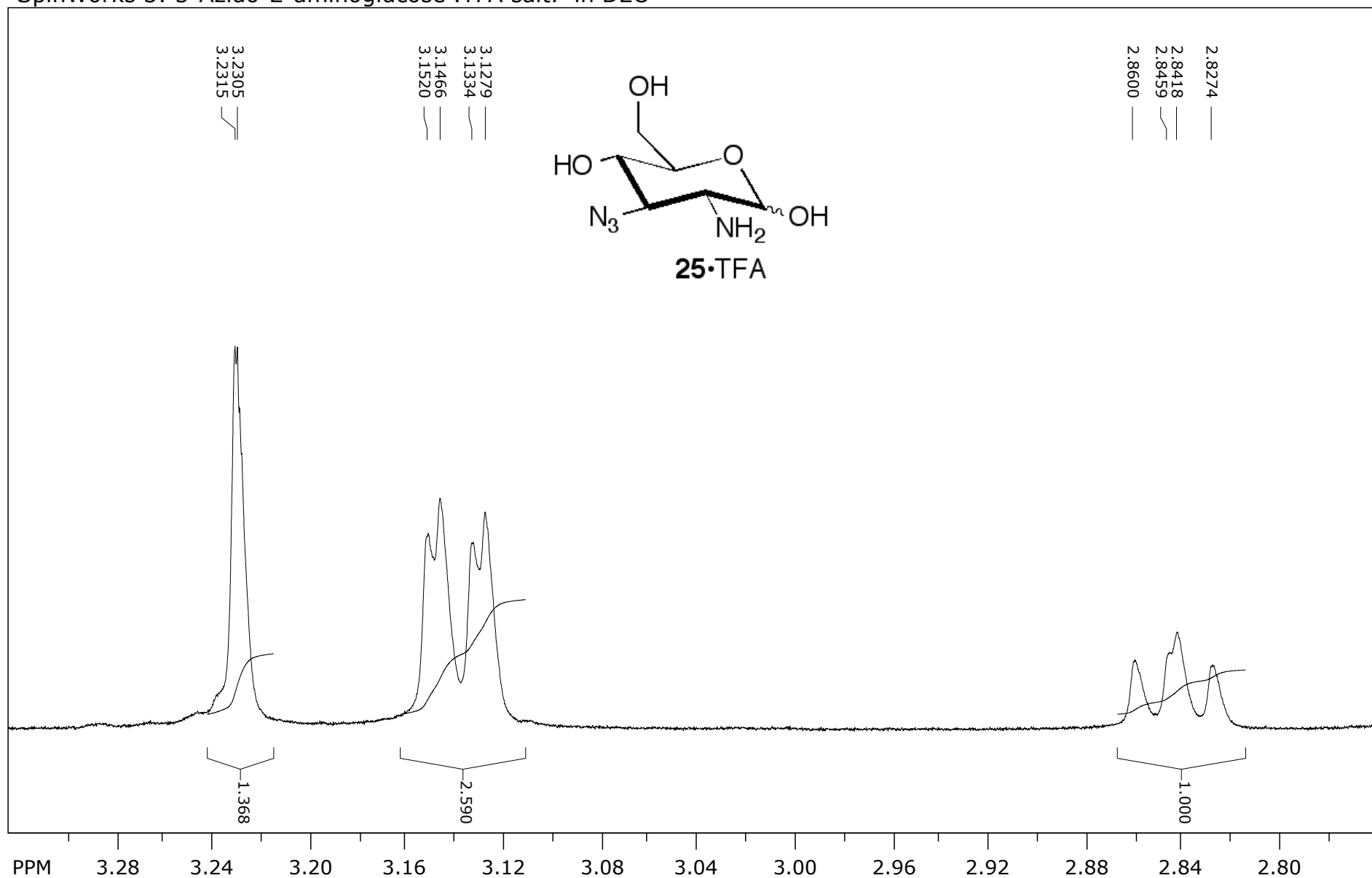
Analysis on a Waters SymmetryShield™ C18 (4.6 mm X 15 cm (i.d. x l.), 3.5 μm) at 0.5 mL/min. Solvent A: 50 mM NH₄OAc (aq); B: CH₃CN

Time (min)	% B
0	20
1	20
10	100
20	100



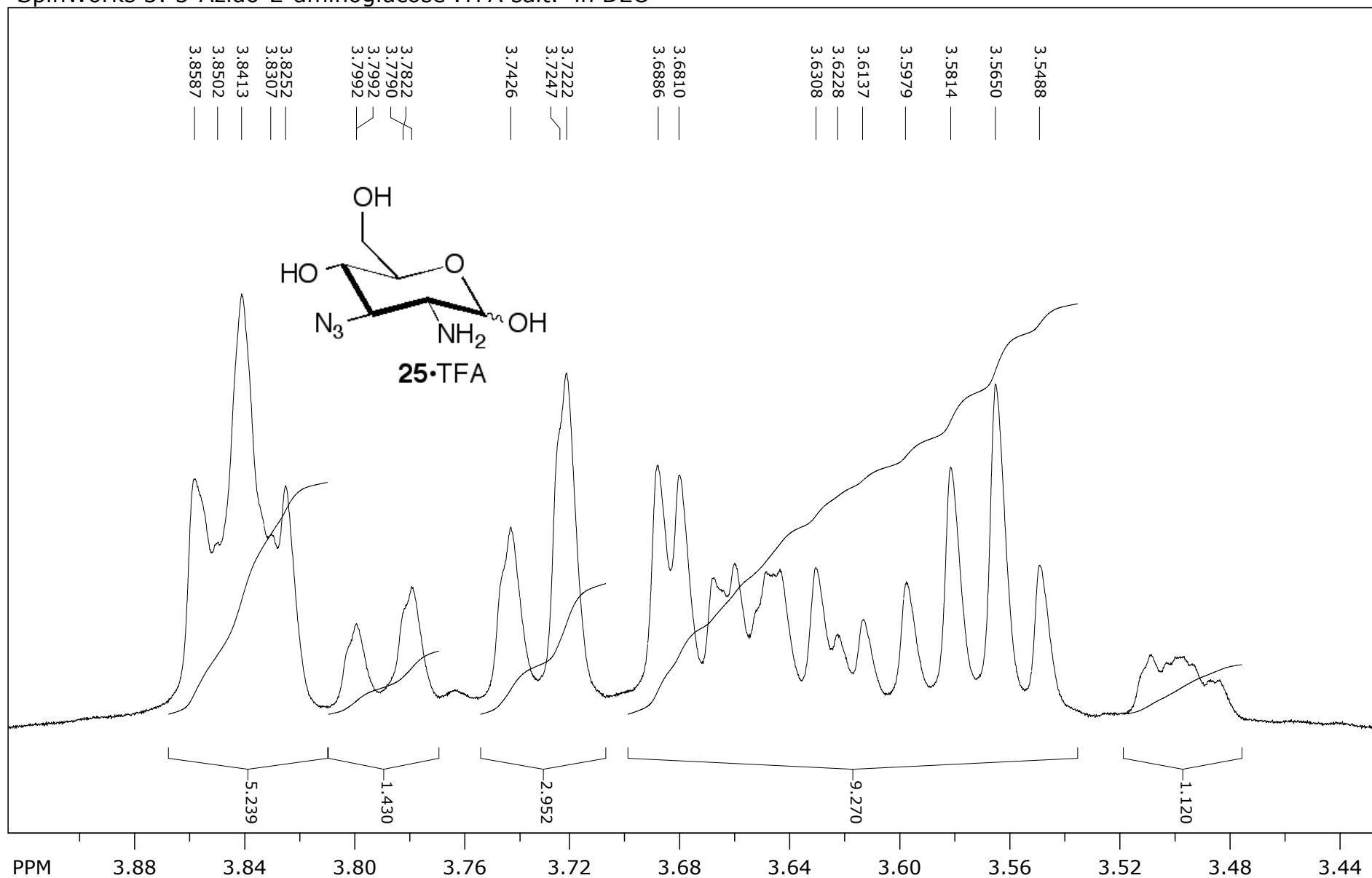
file: ... Data\Aug 2012\3N3GlcNH2_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550037 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 168.378 ppm/cm: 0.28037



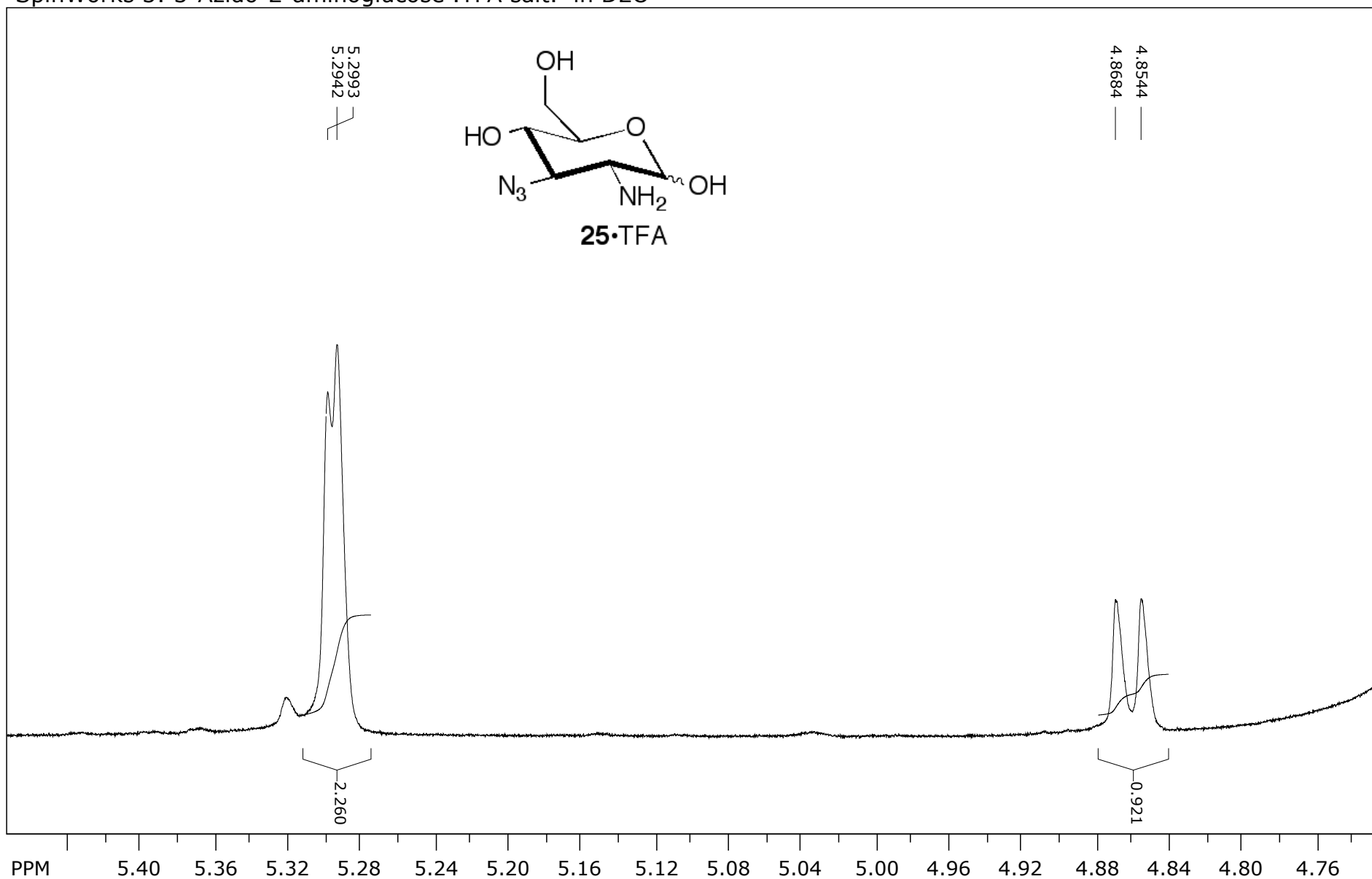
file: ... Data\Aug 2012\3N3GlcNH2_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550037 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 13.628 ppm/cm: 0.02269



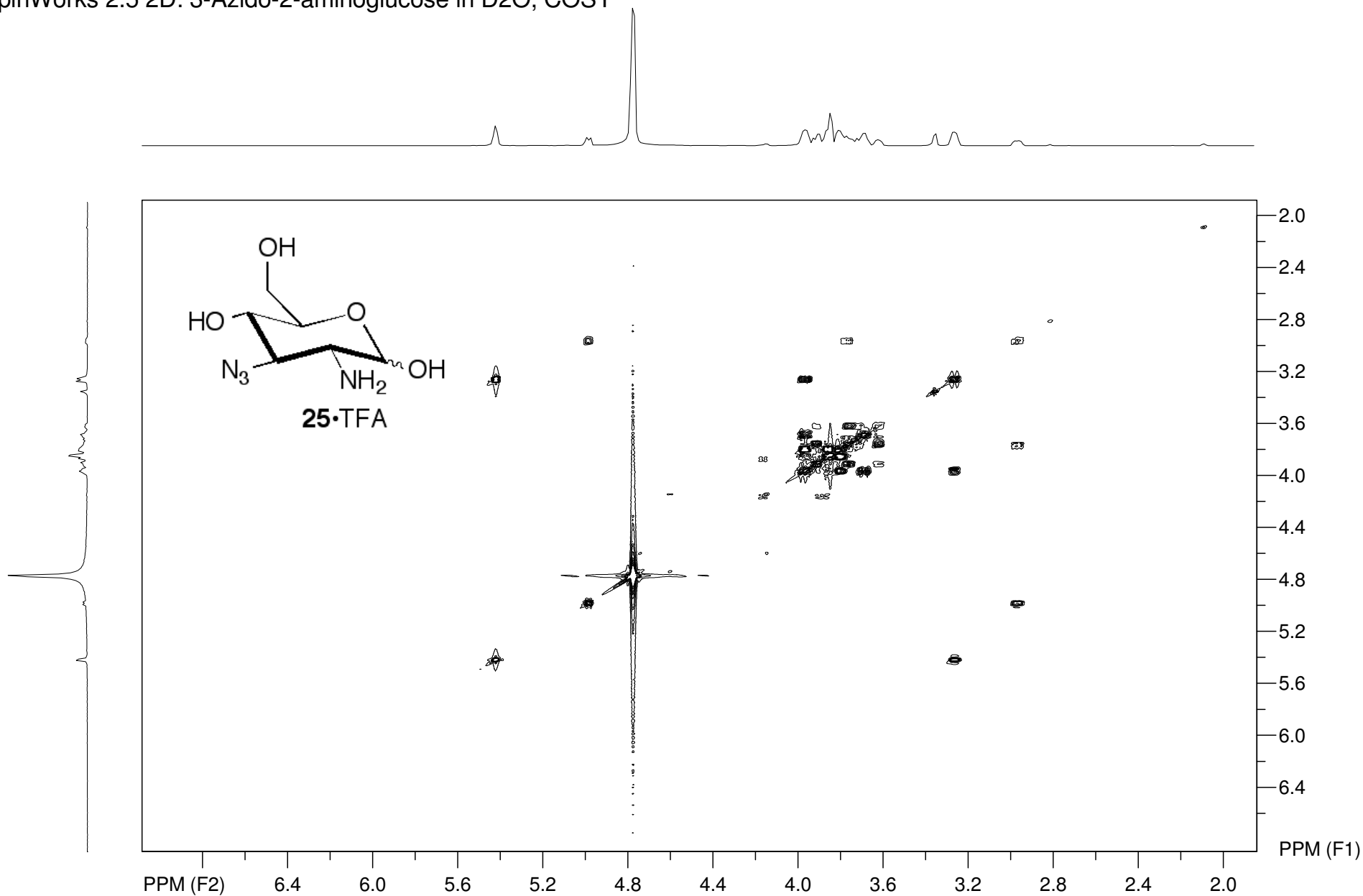
file: ... Data\Aug 2012\3N3GlcNH2_D2O\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550037 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 12.073 ppm/cm: 0.02010



file: ... Data\Aug 2012\3N3GlcNH2_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

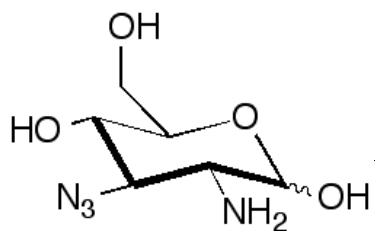
freq. of 0 ppm: 600.550037 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 18.029 ppm/cm: 0.03002



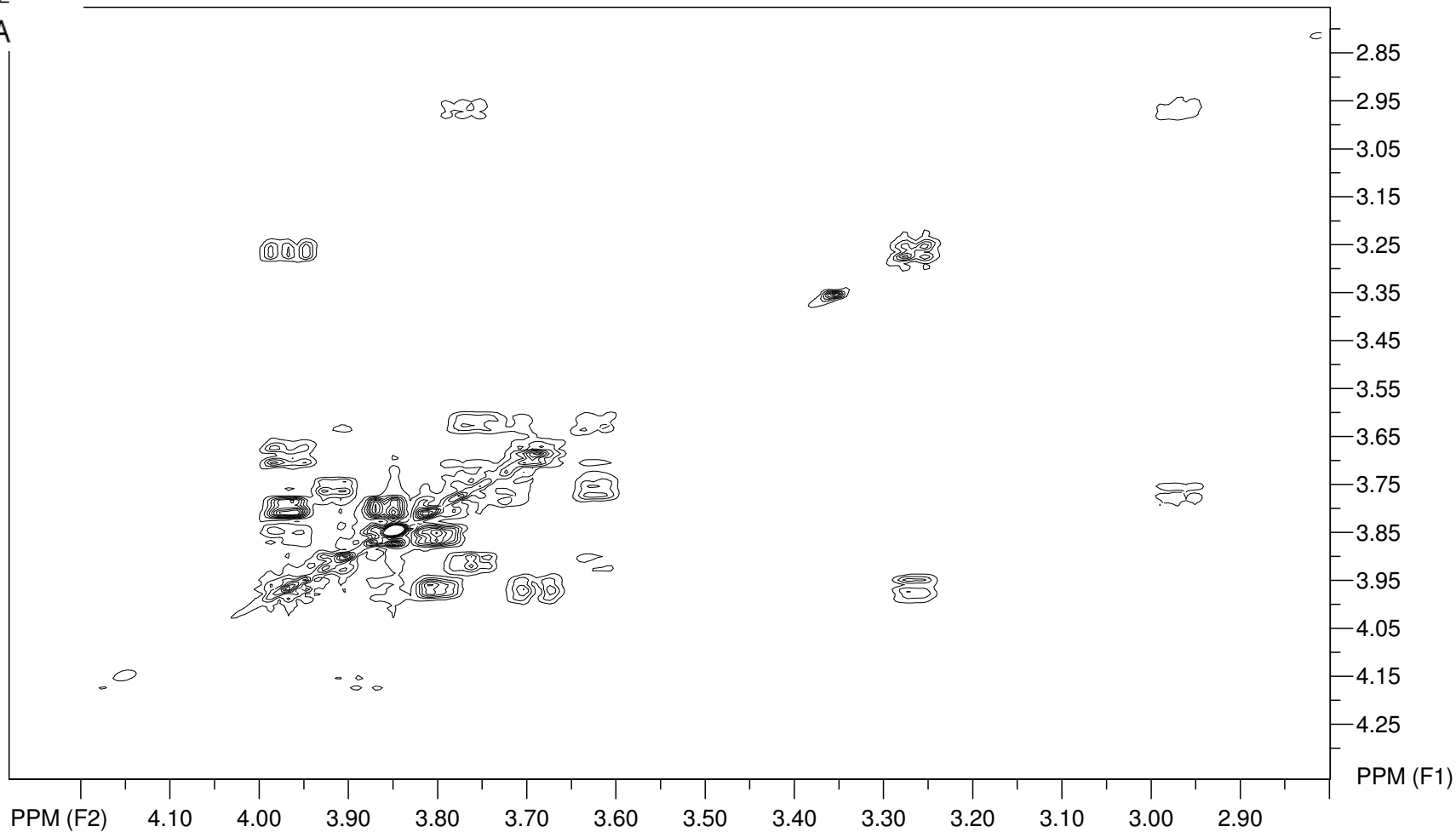
file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\Aug 2012\3N3GlcNH2_D2O_COSY\2\ser
transmitter freq.: 600.553566 MHz
time domain size: 2048 by 2048 points
width (F2): 6009.58 Hz = 10.006793 ppm = 2.934365 Hz/pt
number of scans: 2

exptF2::freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 153.572 ppm/cm: 0.25572

F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 250.871 ppm/cm: 0.41773



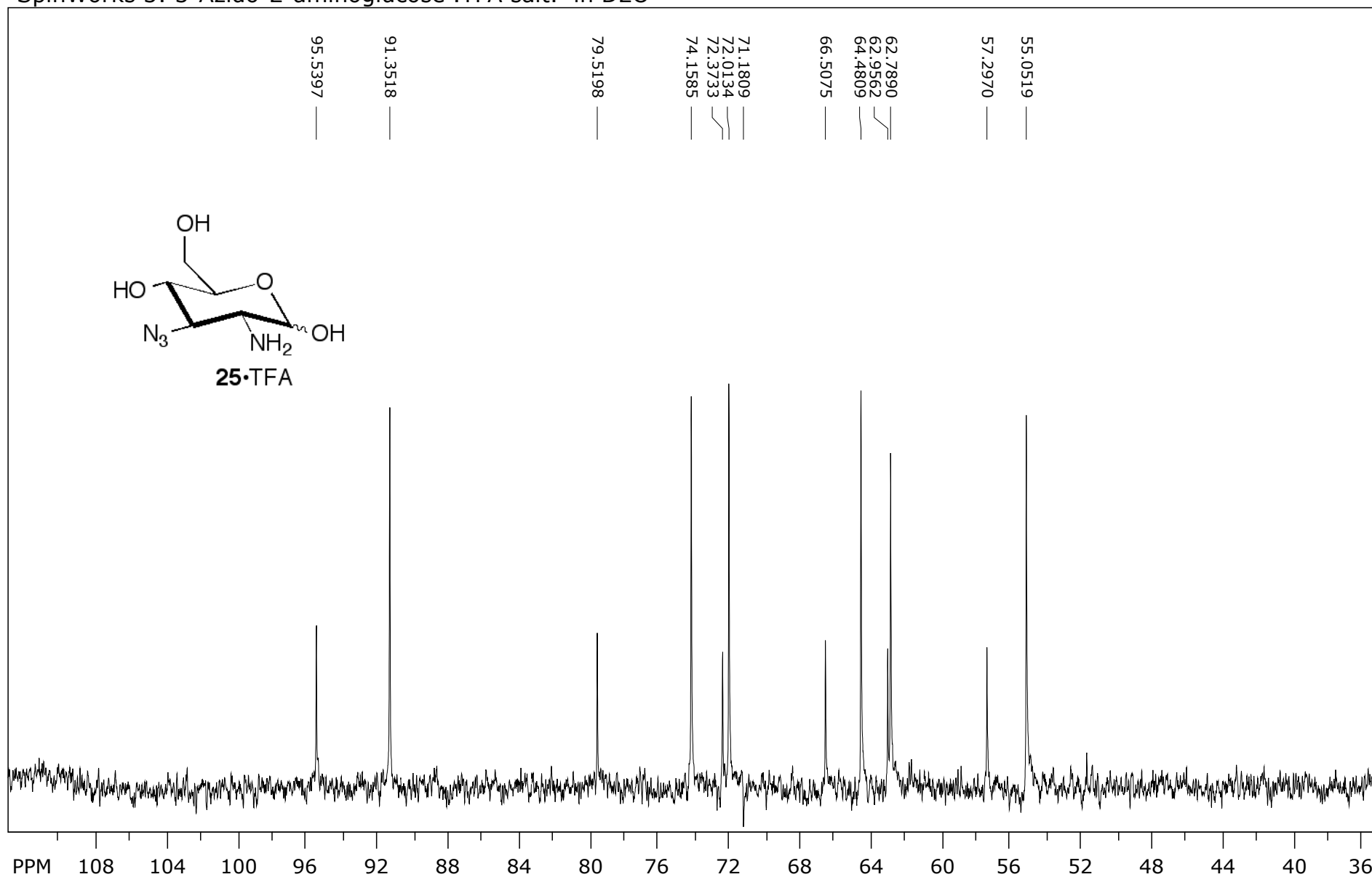
25·TFA



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\Aug 2012\3N3GlcNH2_D2O_COSY\2\ser
transmitter freq.: 600.553566 MHz
time domain size: 2048 by 2048 points
width (F2): 6009.58 Hz = 10.006793 ppm = 2.934365 Hz/pt
number of scans: 2

exptF2: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 43.394 ppm/cm: 0.07226

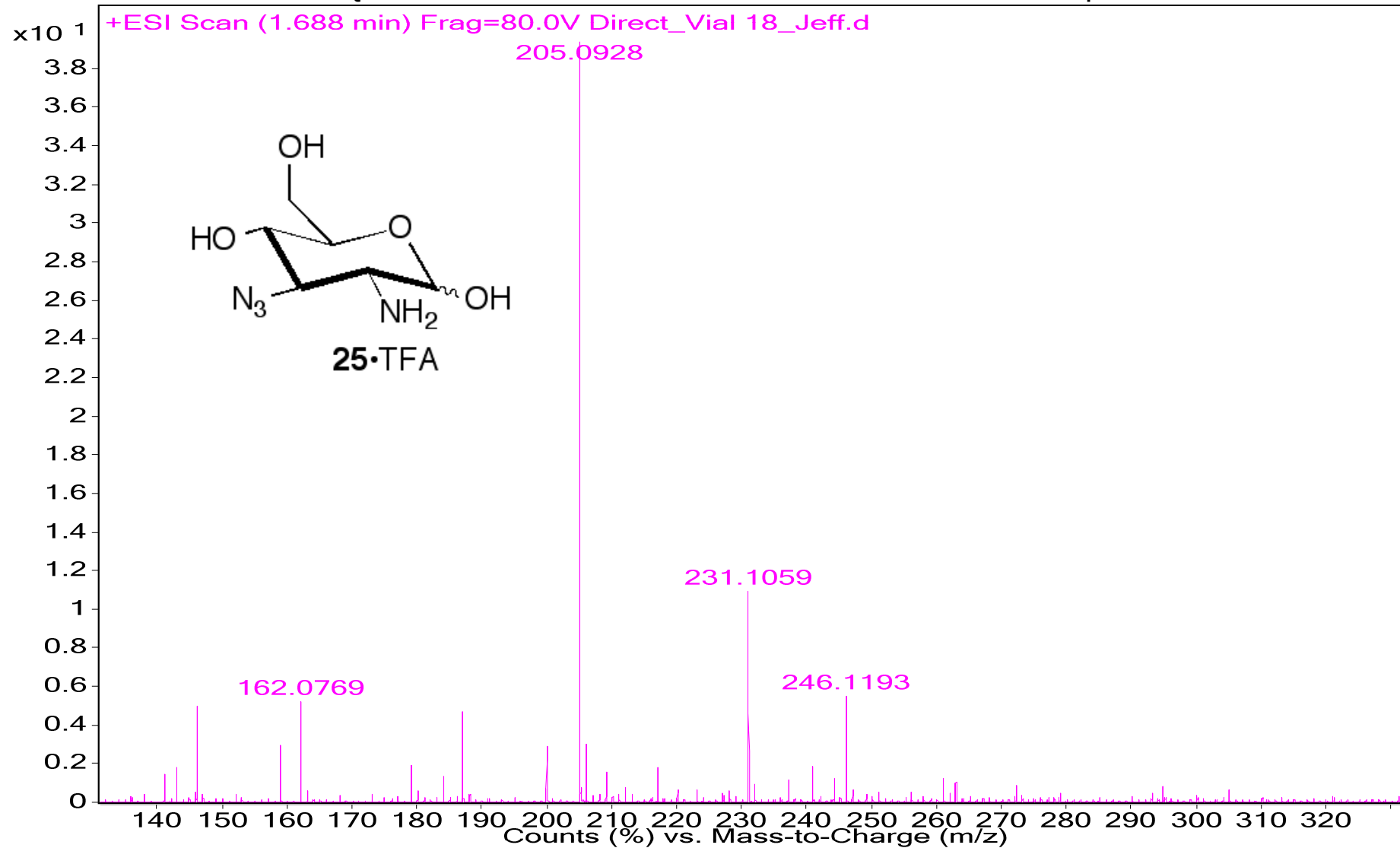
F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 80.580 ppm/cm: 0.13418

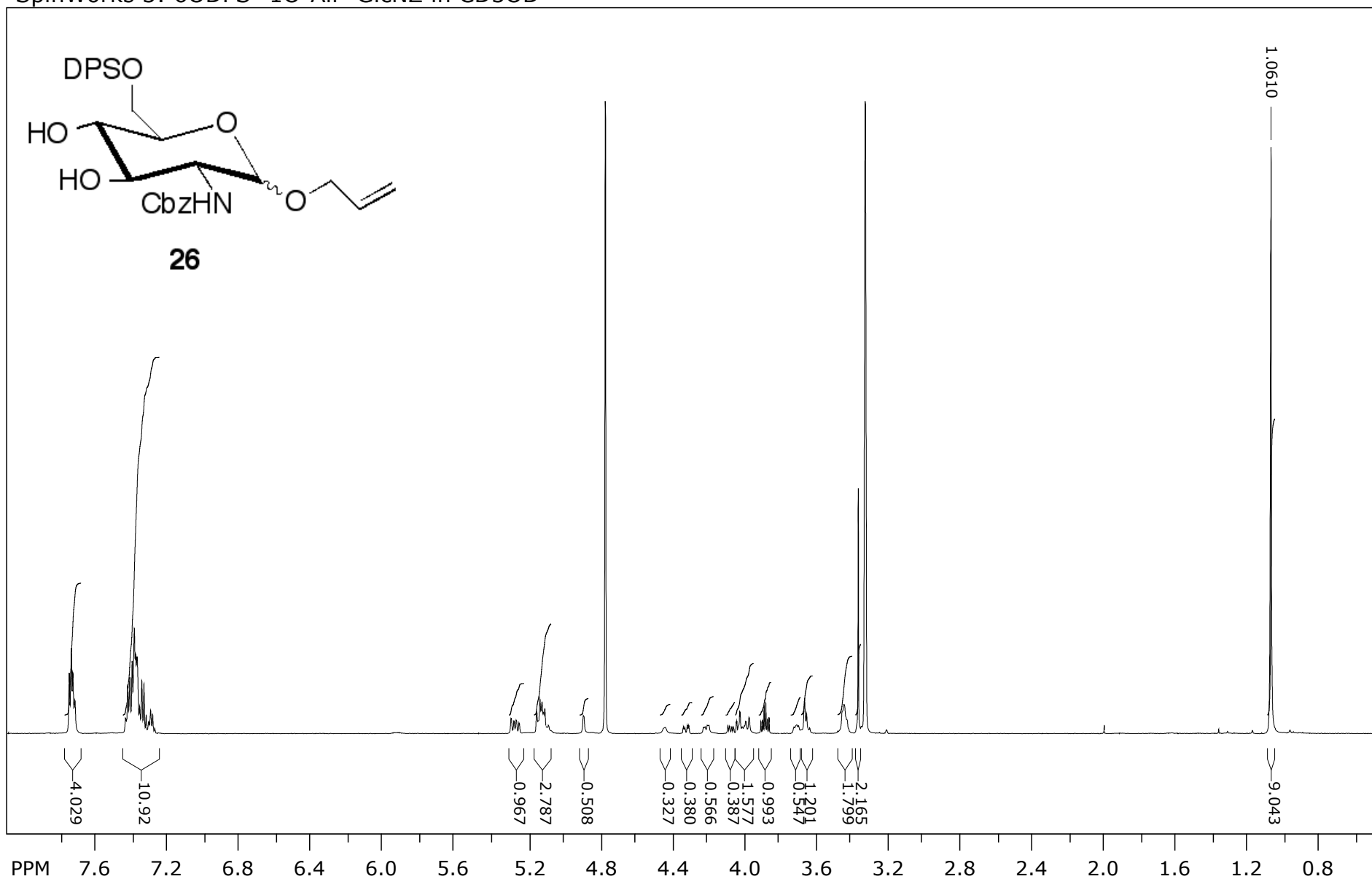


file: ...a\Aug 2012\3N3GlcNH2_D2O_13C\1\fid expt: <zgpg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 30720

freq. of 0 ppm: 151.008006 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 471.647 ppm/cm: 3.12301

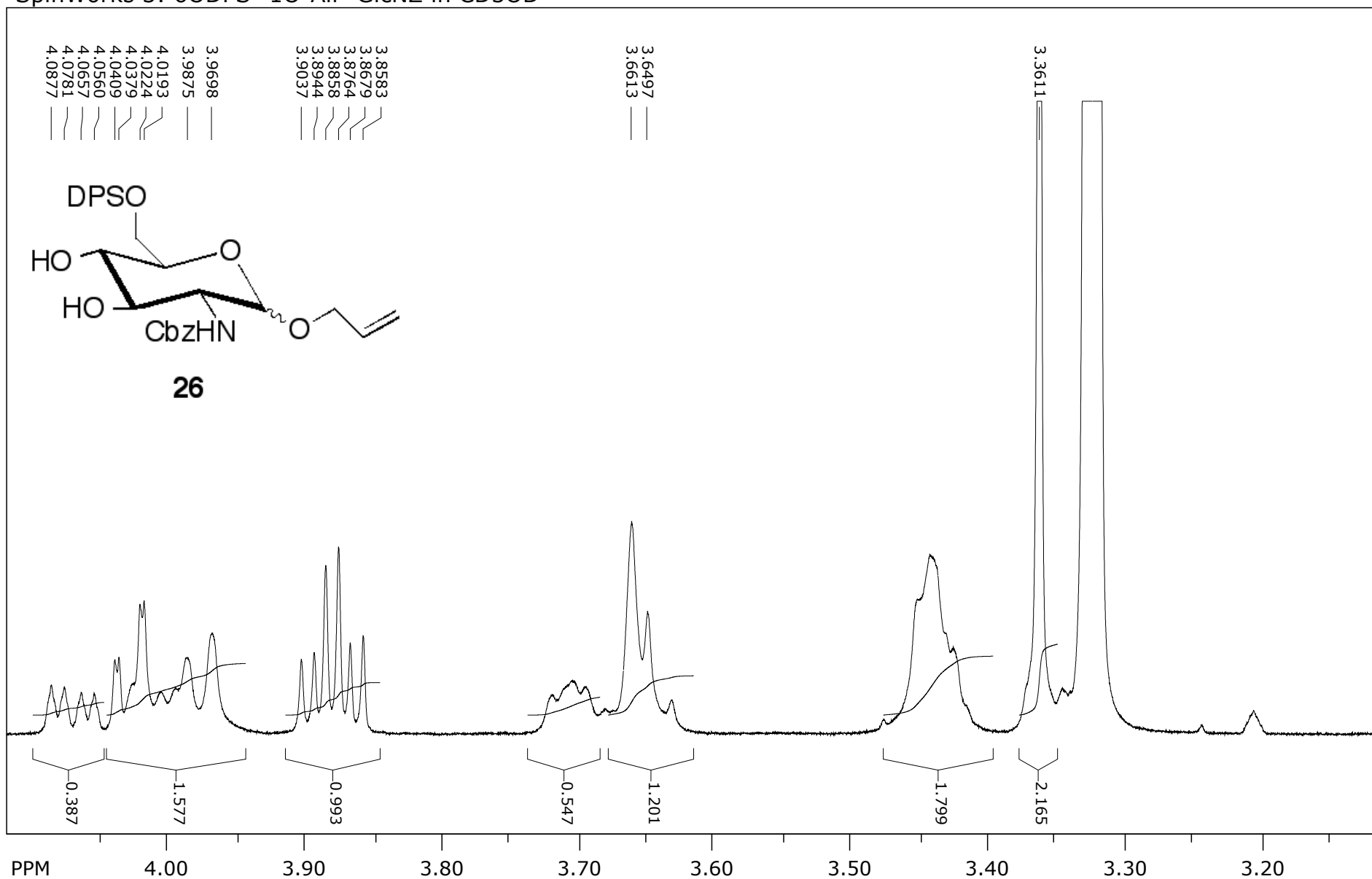
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time





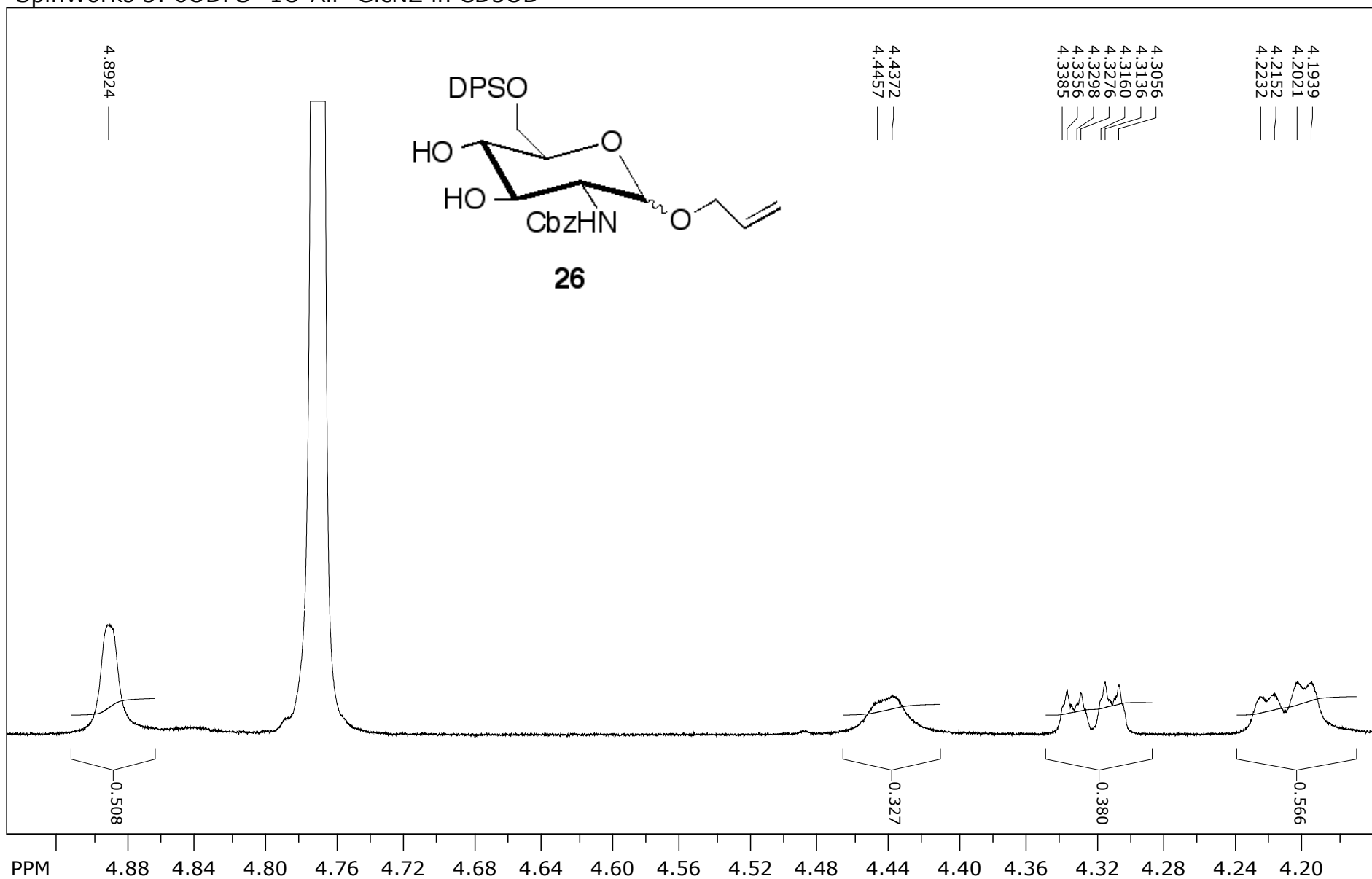
file: ...der\NMR Data\6DPS34OH2_CD3OD\1\fid exp: <zgr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 183.669 ppm/cm: 0.30583



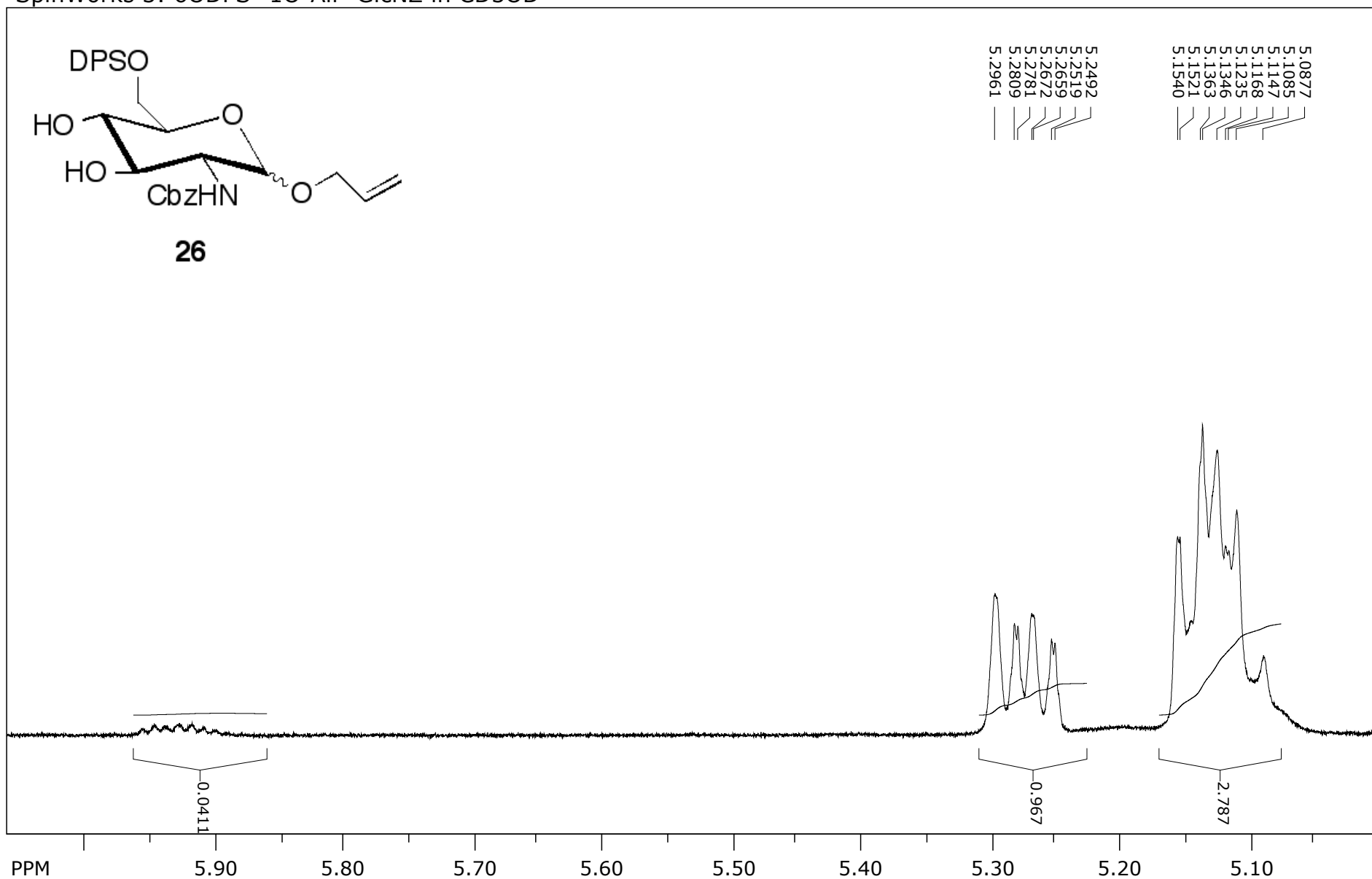
file: ...der\NMR Data\6DPS34OH2_CD3OD\1\fid expt: <zgr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 24.234 ppm/cm: 0.04035



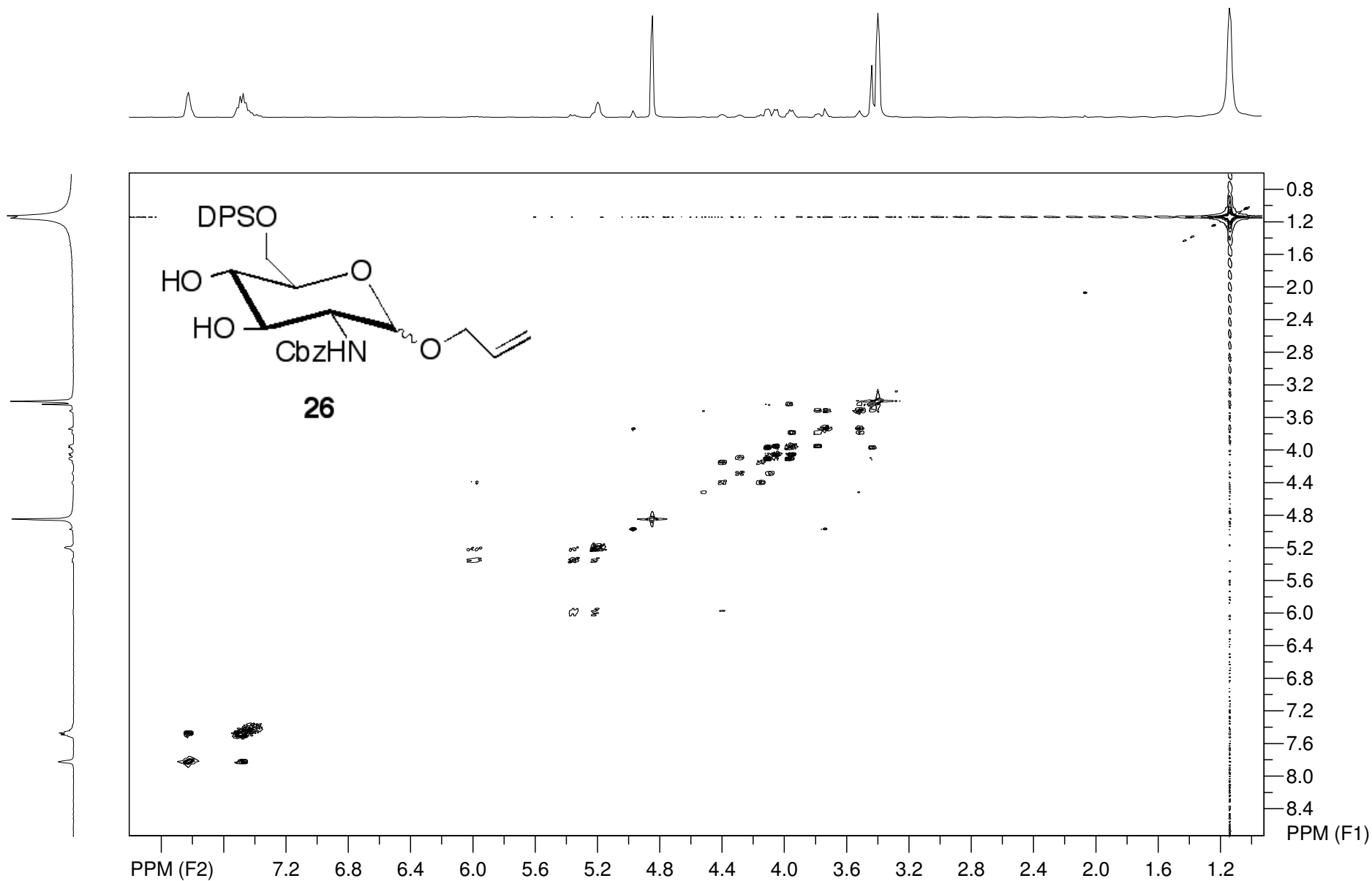
file: ...der\NMR Data\6DPS34OH2_CD3OD\1\fid exp: <zgr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 19.144 ppm/cm: 0.03188



file: ...der\NMR Data\6DPS34OH2_CD3OD\1\fid exp: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 25.595 ppm/cm: 0.04262

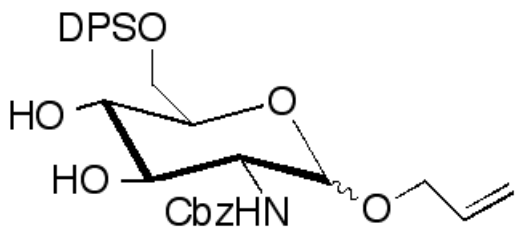


file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\6DPS34OH2_CD3OD_COSY\1\ser
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

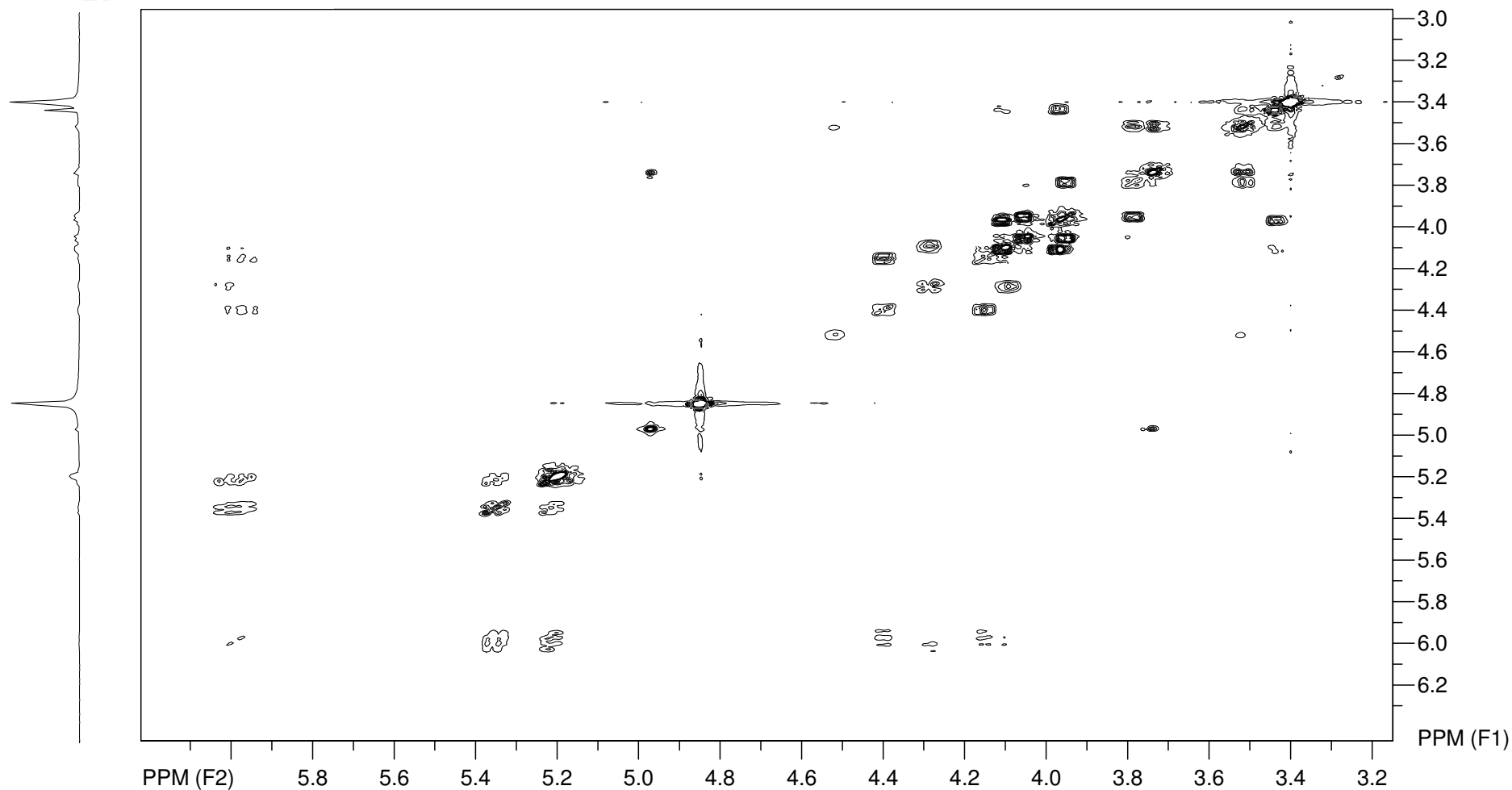
expt: <cosF2>xfreq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 213.453 ppm/cm: 0.35543

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 407.020 ppm/cm: 0.67774

S-2NZ-glucopyranoside in CD3OD



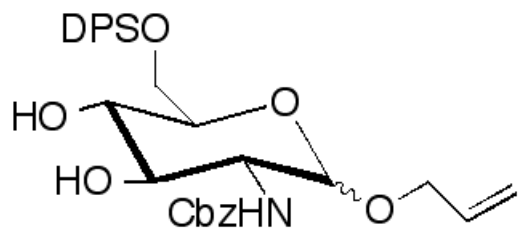
26



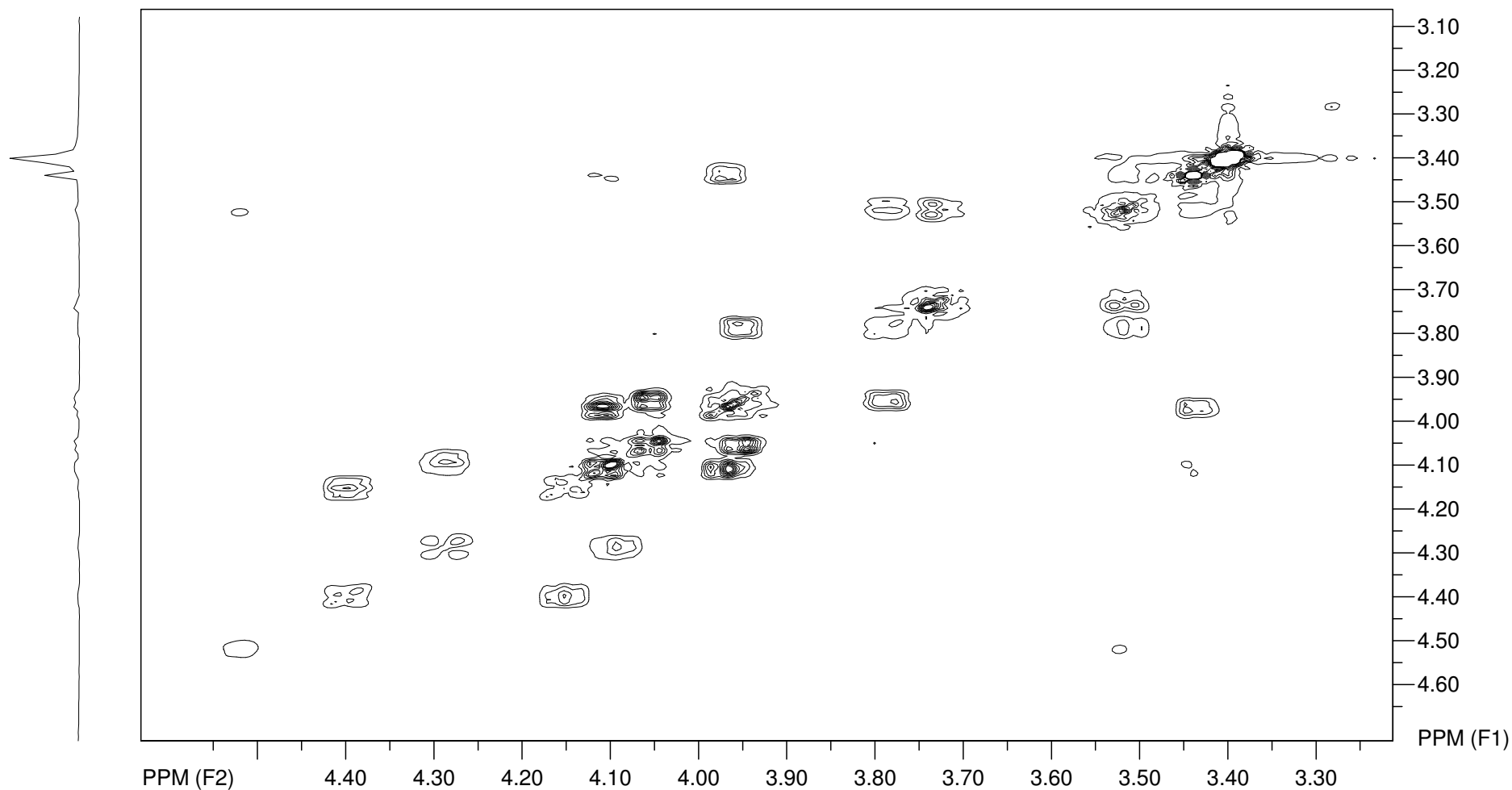
file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\6DPS34OH2_CD3OD_COSY\1\ser
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

expt: <cosF2>:freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 90.002 ppm/cm: 0.14987

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 175.817 ppm/cm: 0.29276

α -2NZ-glucopyranoside in CD3OD

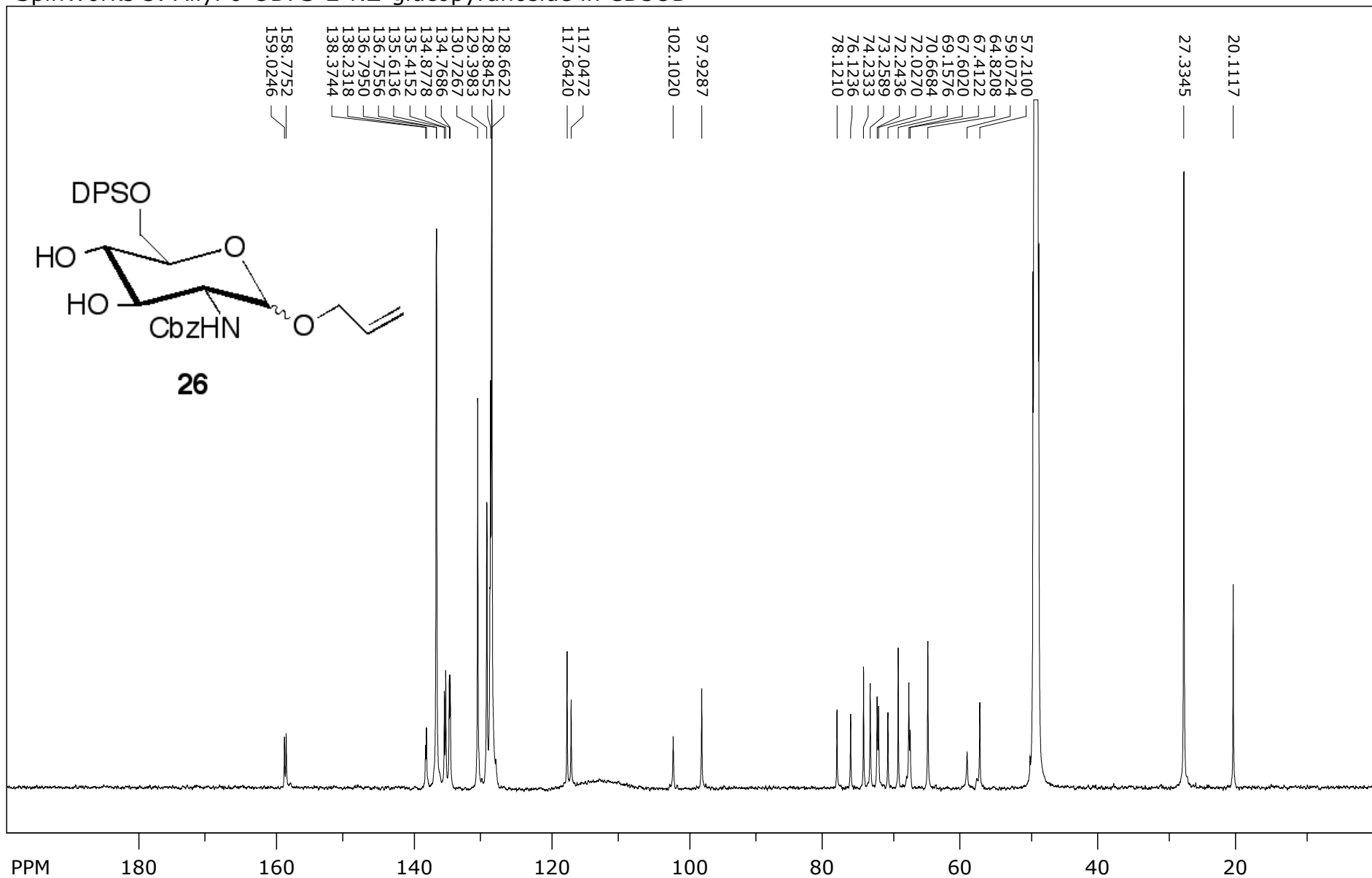
26



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\6DPS34OH2_CD3OD_COSY\1\ser exp: <cosF2>:freq. of 0 ppm: 600.549962 MHz
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 41.574 ppm/cm: 0.06923

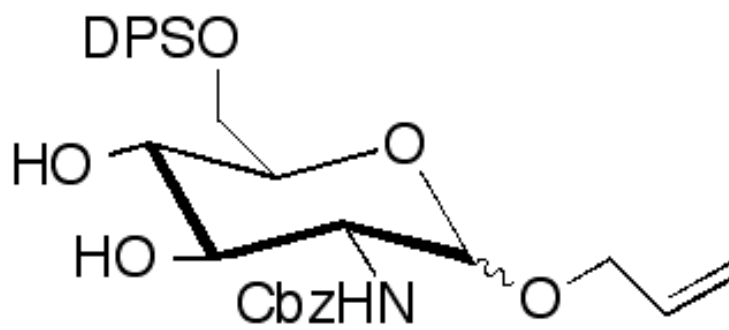
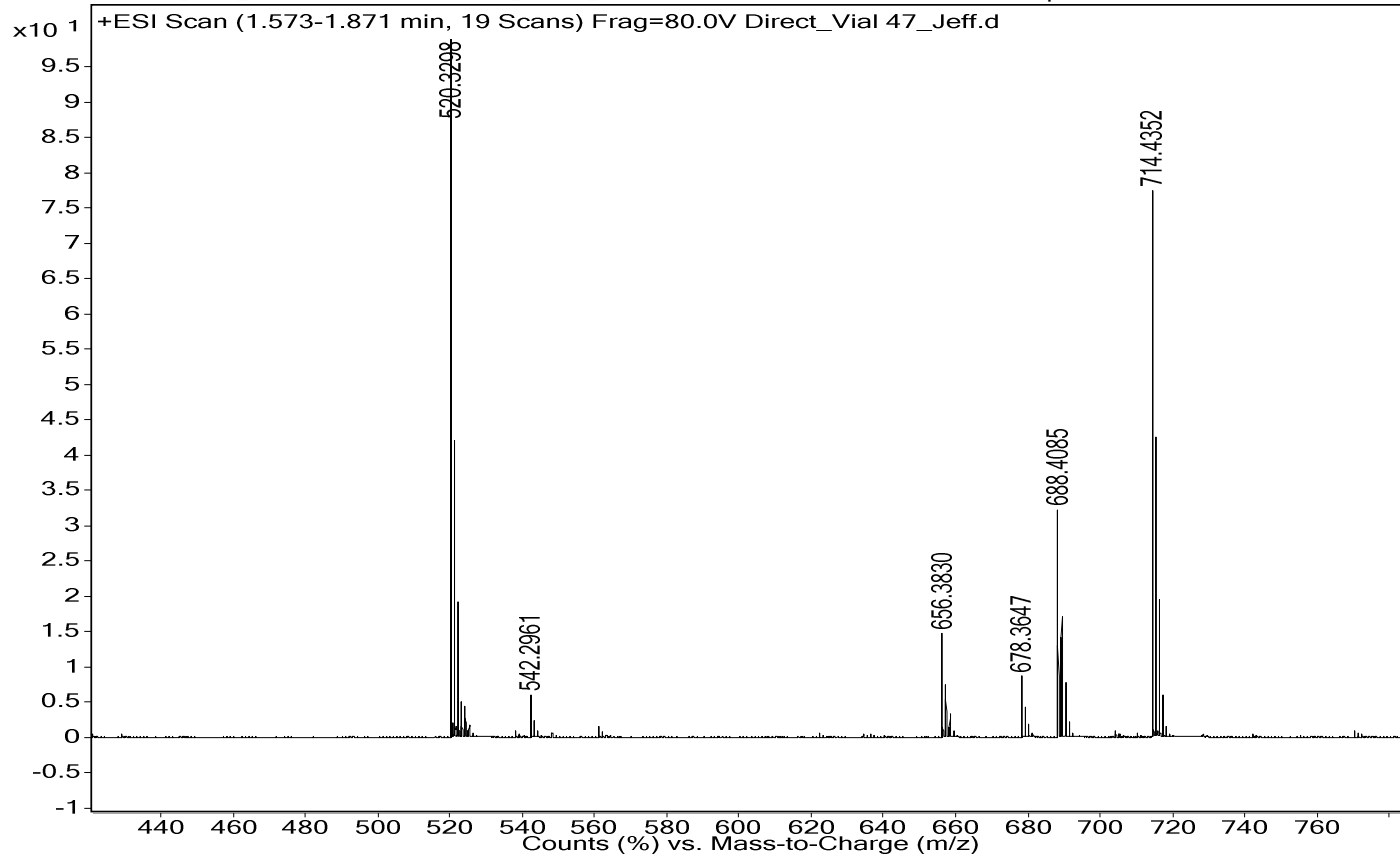
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 83.458 ppm/cm: 0.13897



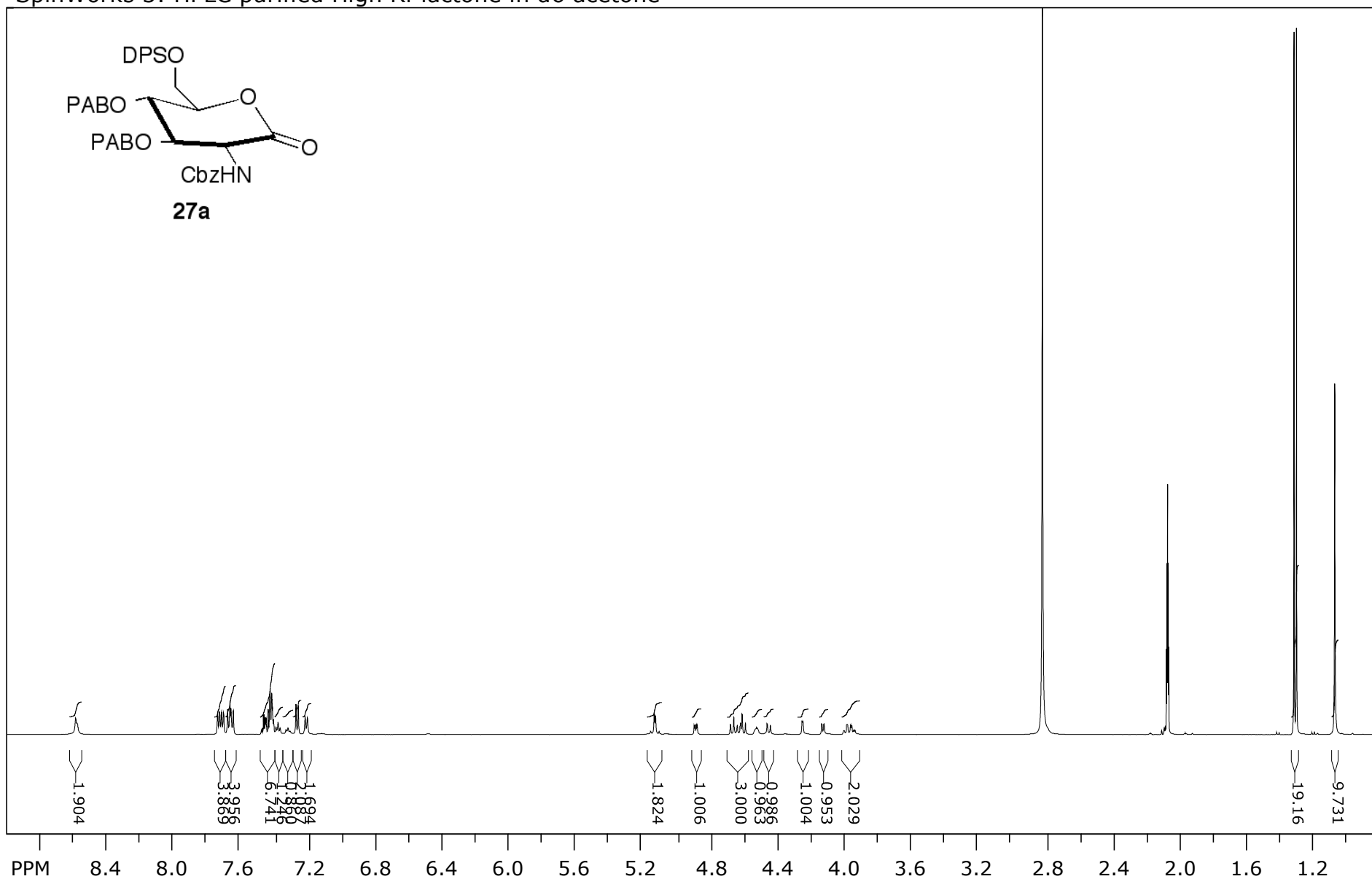
file: ...ta\6DPS2NZ1All_CD3ODrepur13C\1\fid expt: <zgpg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 20480

freq. of 0 ppm: 151.008215 MHz
processed size: 32768 complex points
LB: 10.000 GF: 0.0000
Hz/cm: 1213.511 ppm/cm: 8.03525

Sample Name	Jeff 47	Position	Vial 47	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial_47_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 2:15:15 PM

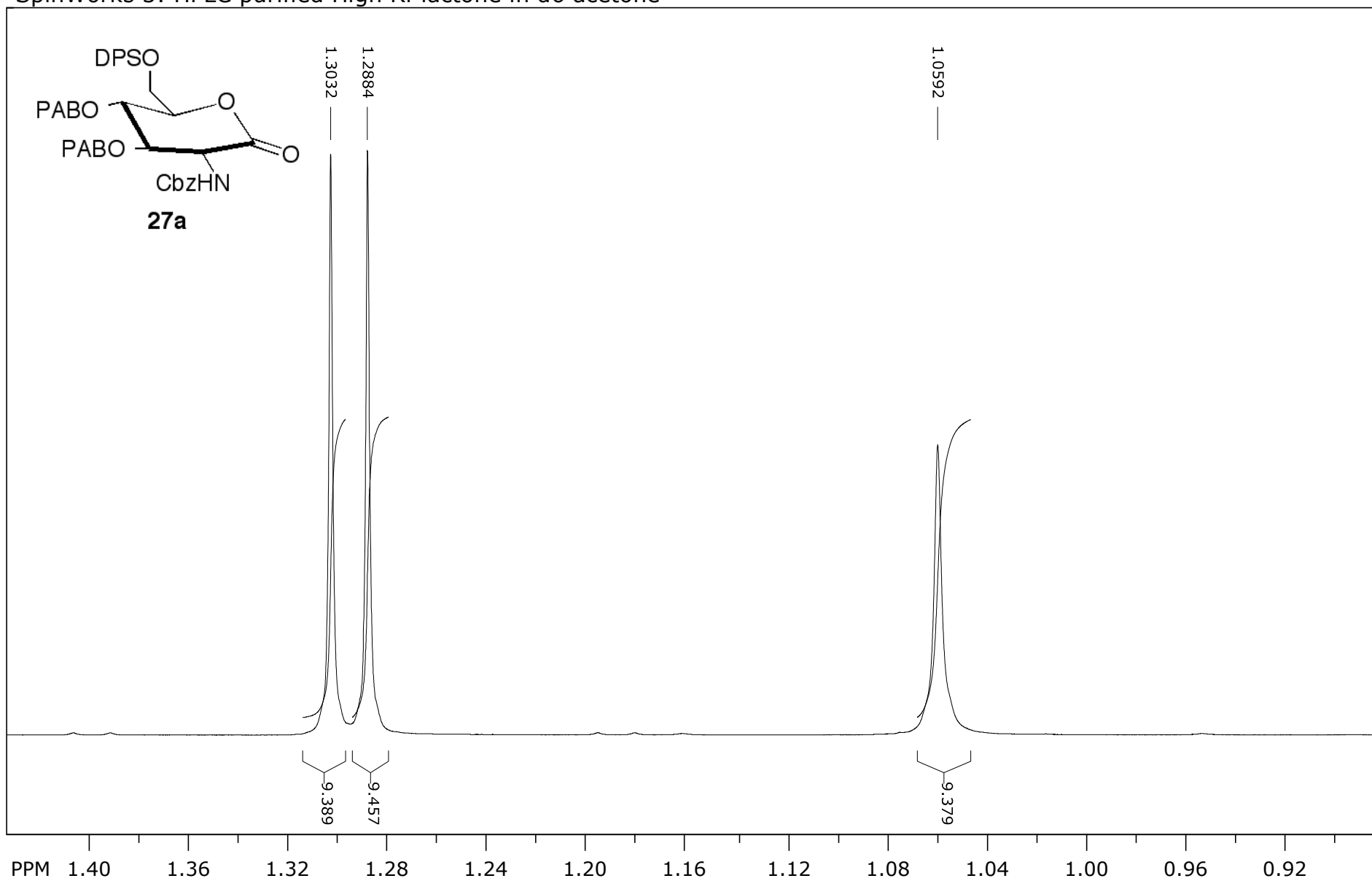


26



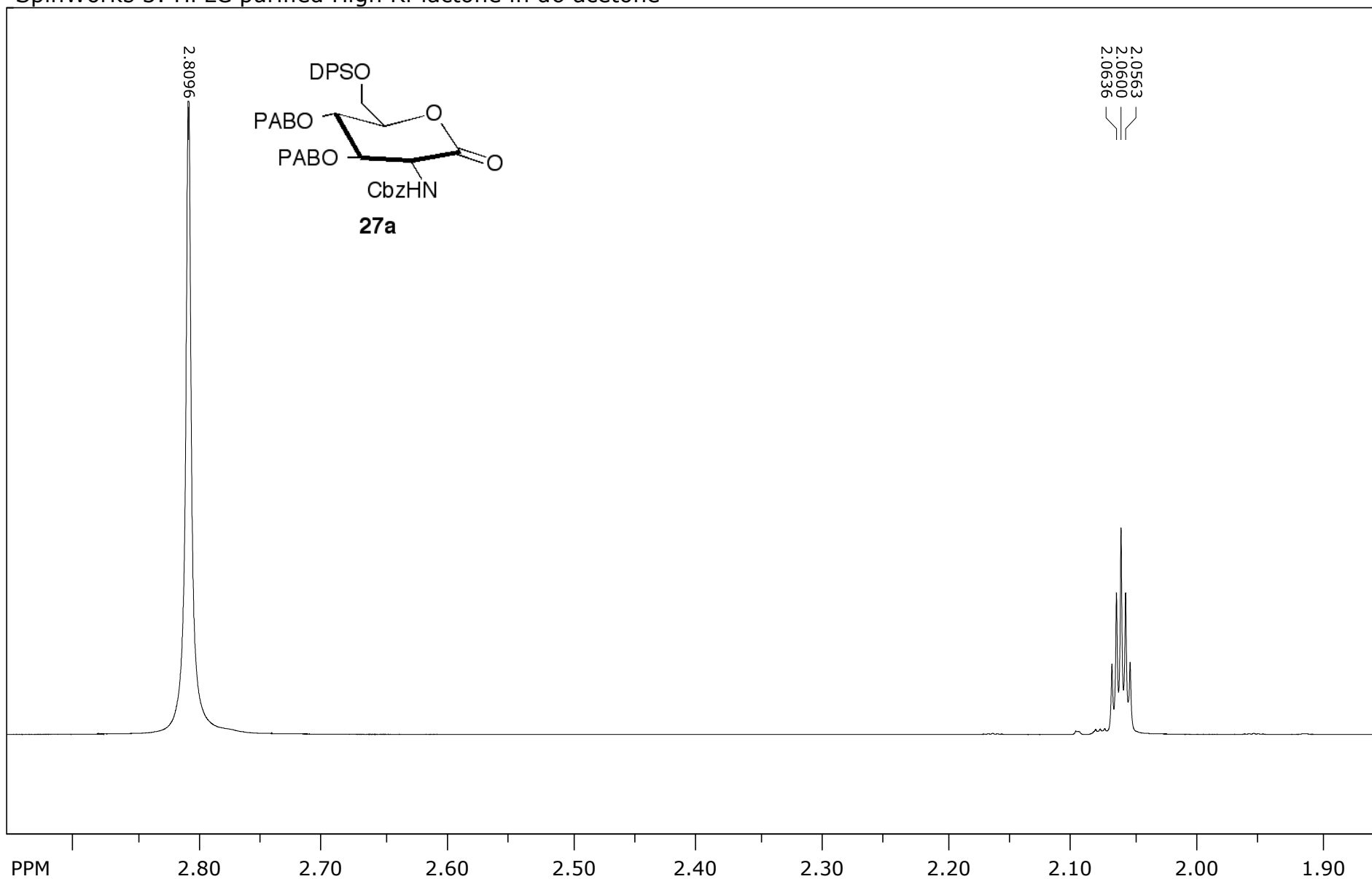
file: ...MR Data\HiRfLactone\HPLCPur_1H\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 197.351 ppm/cm: 0.32861



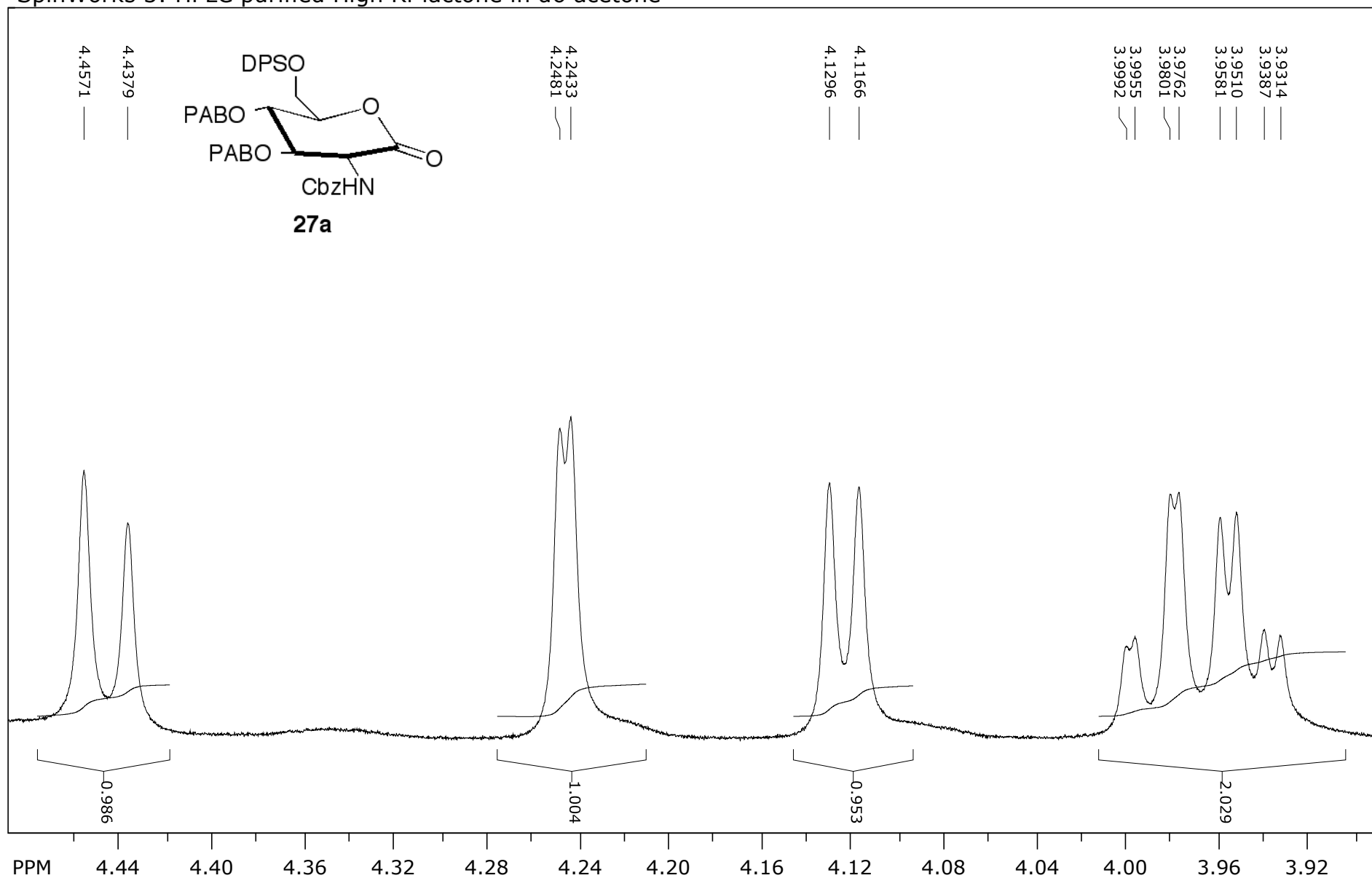
file: ...MR Data\HiRfLactone\HPLCPur_1H\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 13.251 ppm/cm: 0.02206



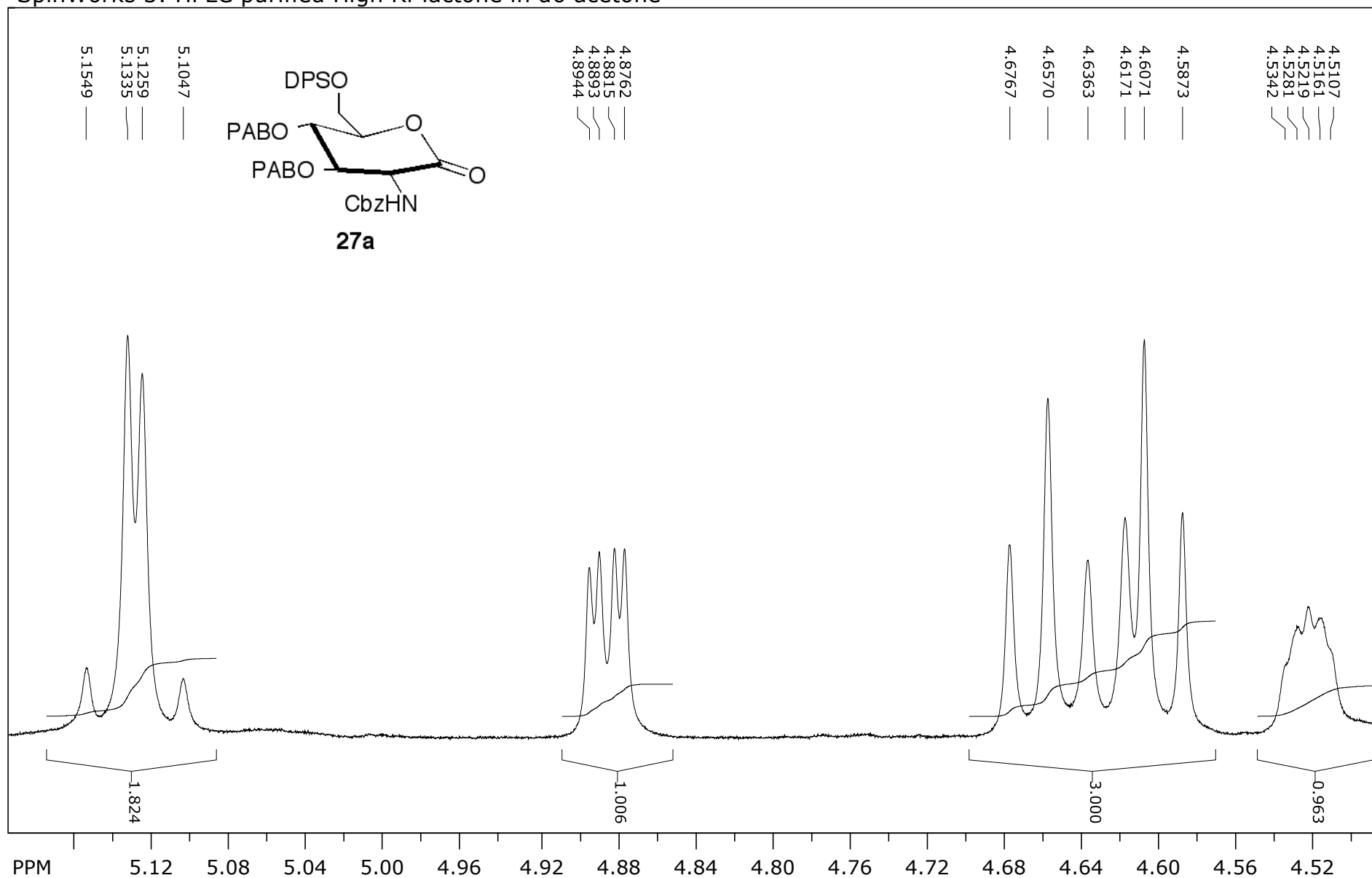
file: ...MR Data\HiRfLactone\HPLCPur_1H\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 26.499 ppm/cm: 0.04412



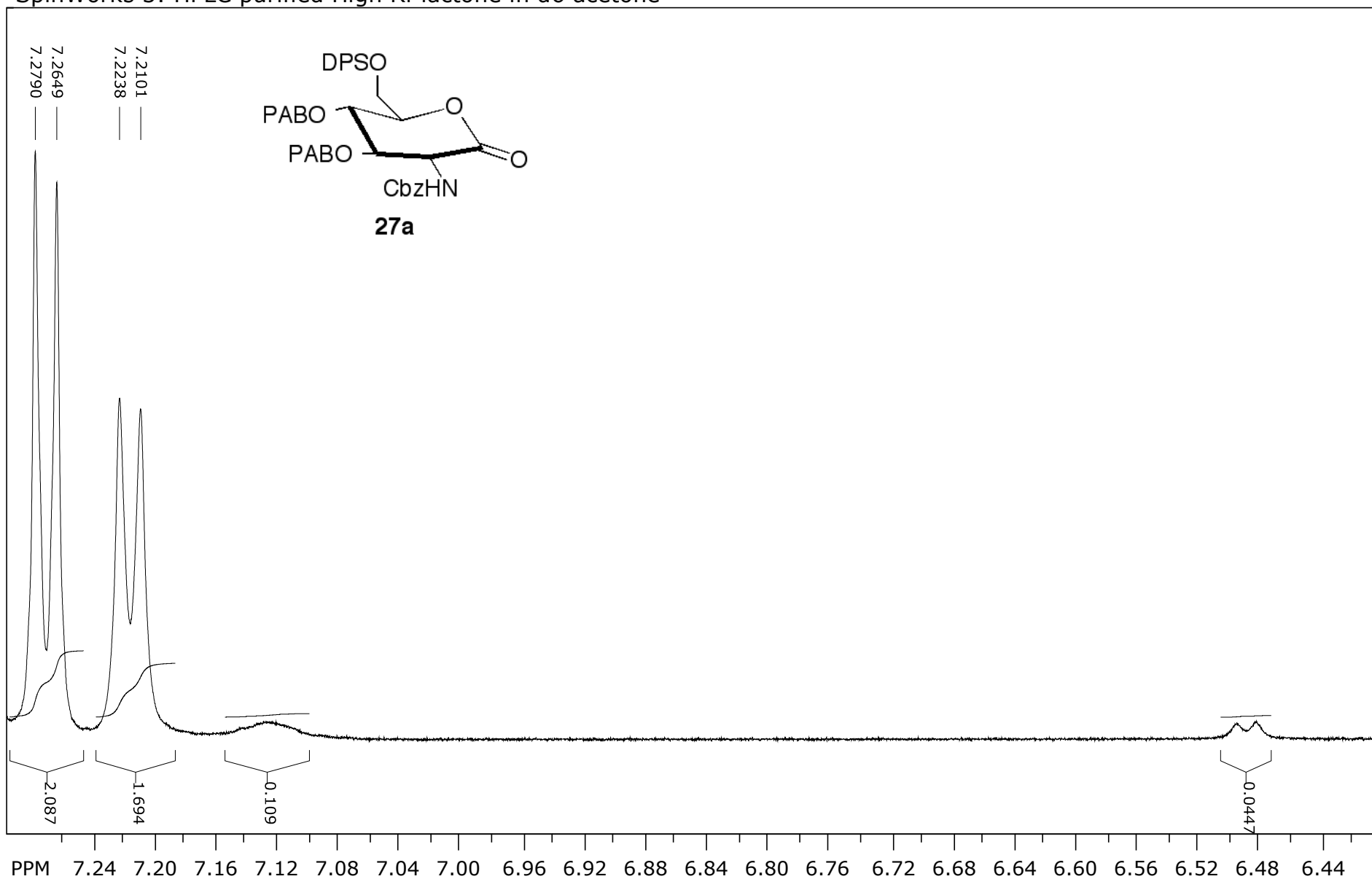
file: ...MR Data\HiRfLactone\HPLCPur_1H\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 14.460 ppm/cm: 0.02408



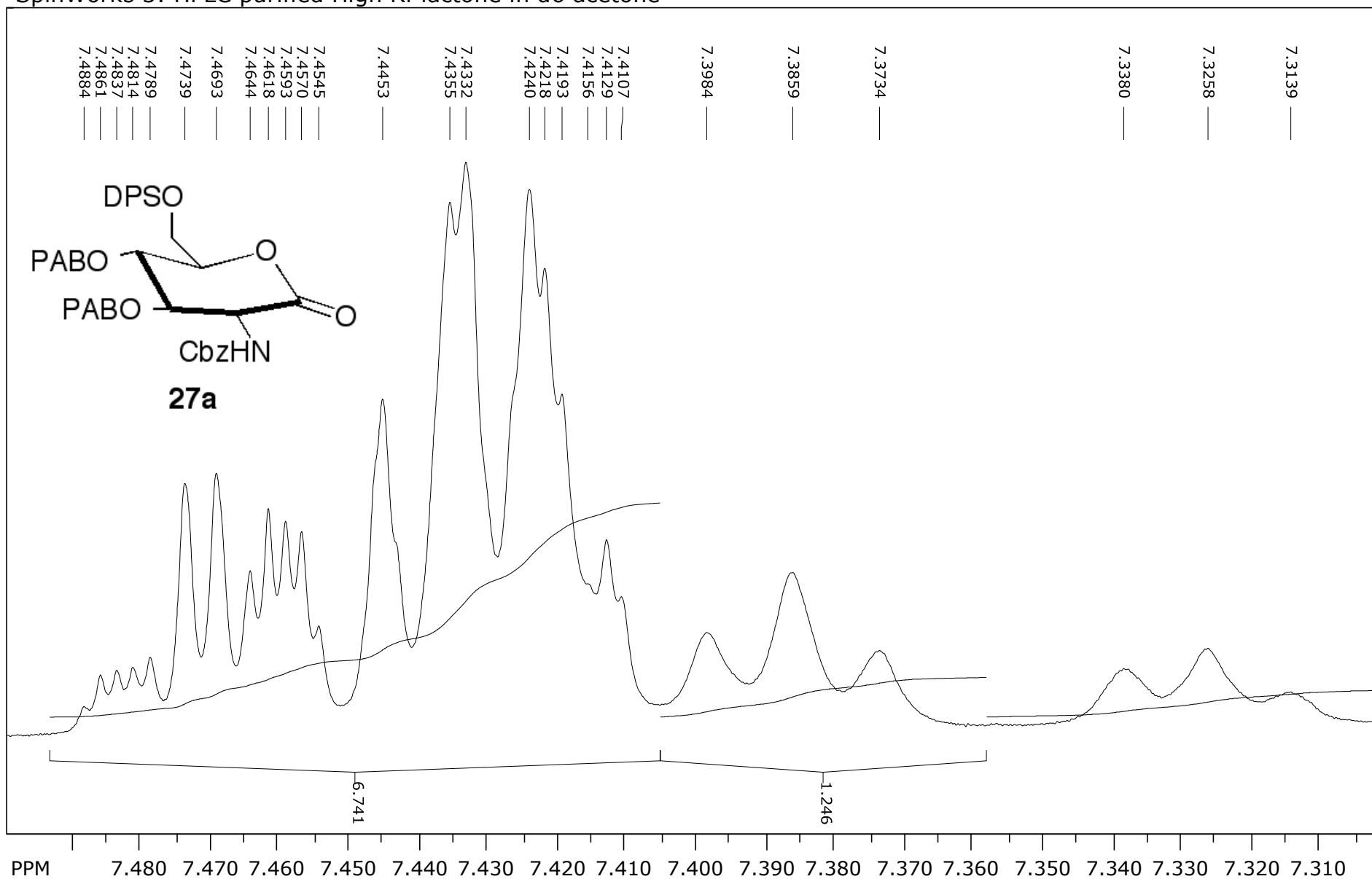
file: ...MR Data\HiRfLactone\HPLCPur_1H\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 17.047 ppm/cm: 0.02839



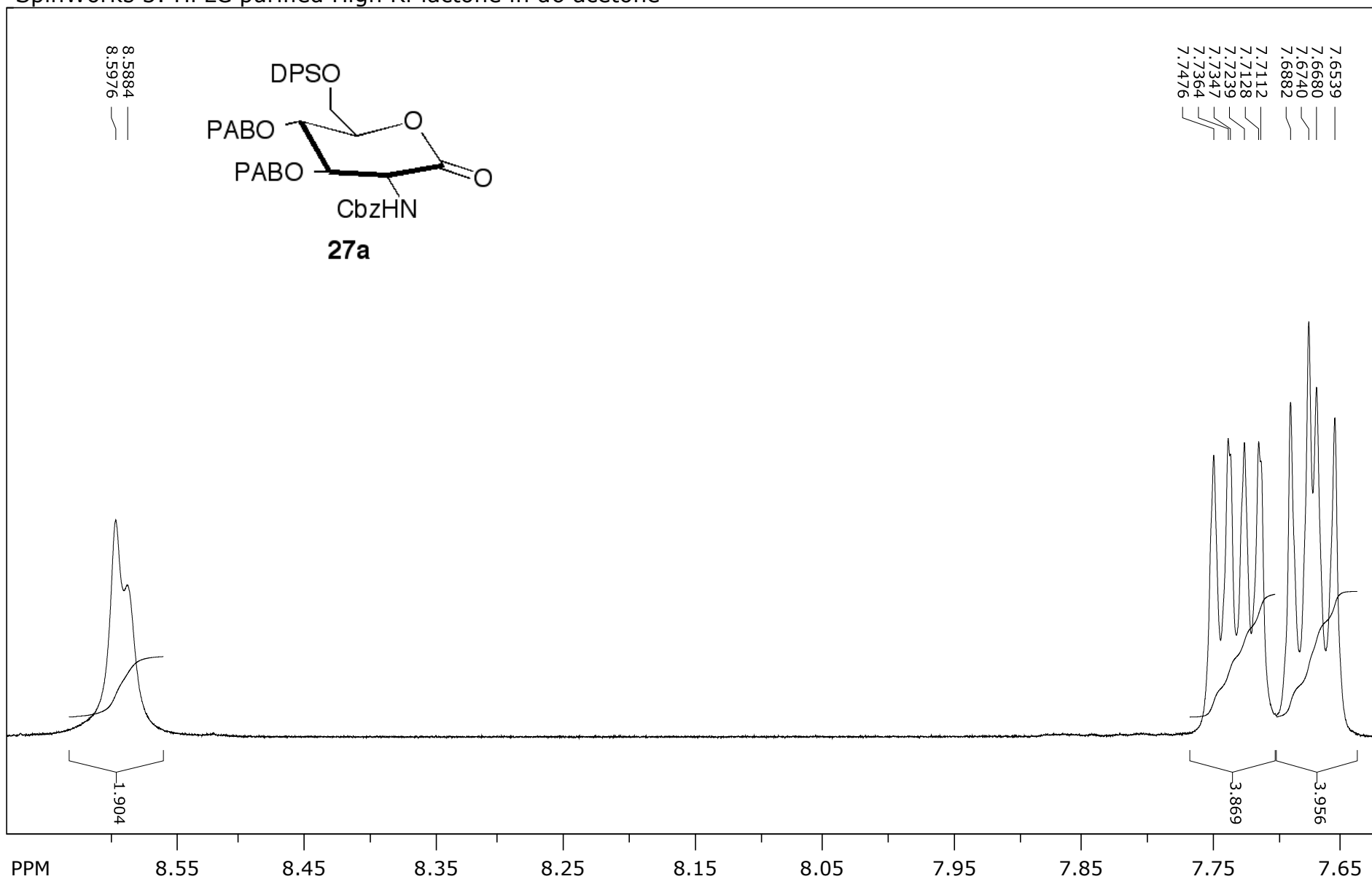
file: ...MR Data\HiRfLactone\HPLCPur_1H\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 21.548 ppm/cm: 0.03588



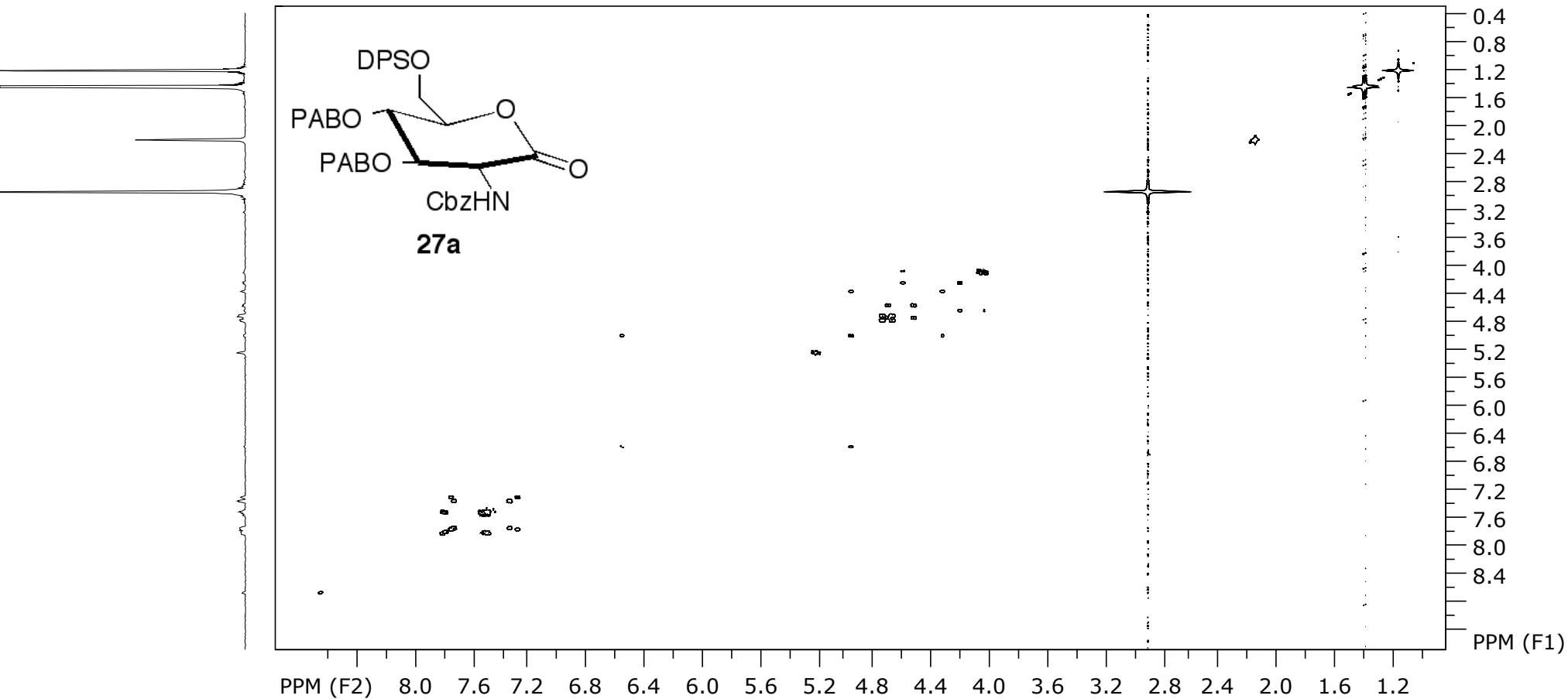
file: ...MR Data\HiRfLactone\HPLCPur_1H\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 4.768 ppm/cm: 0.00794



file: ...MR Data\HiRfLactone\HPLCPur_1H\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

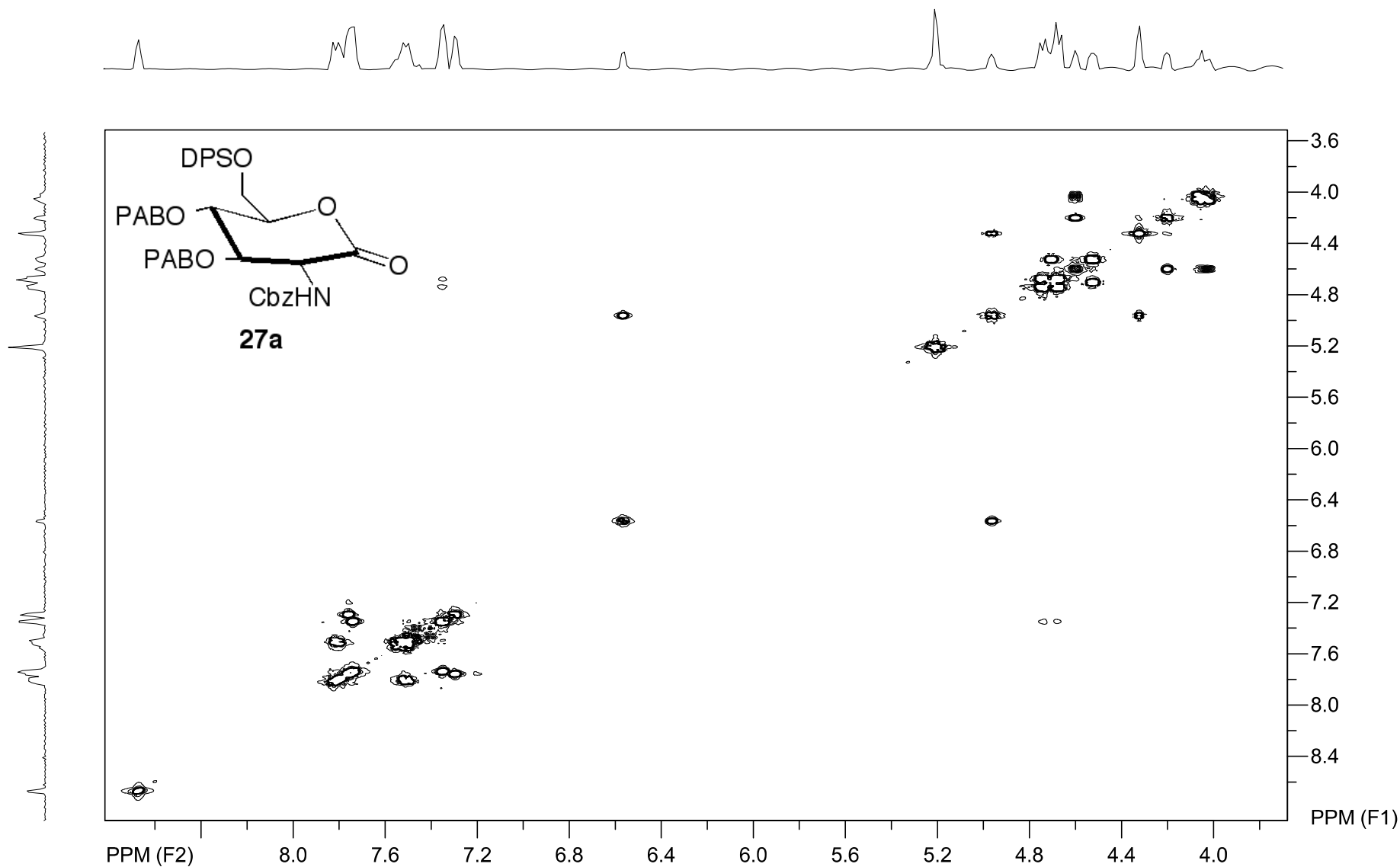
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 25.518 ppm/cm: 0.04249



file: ... Data\HiRfLactone\HPLCPur_COSY\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 4096 by 1024 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 1.7606 Hz/pt
 number of scans: 2

F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 2048 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 244.532 ppm/cm: 0.40718

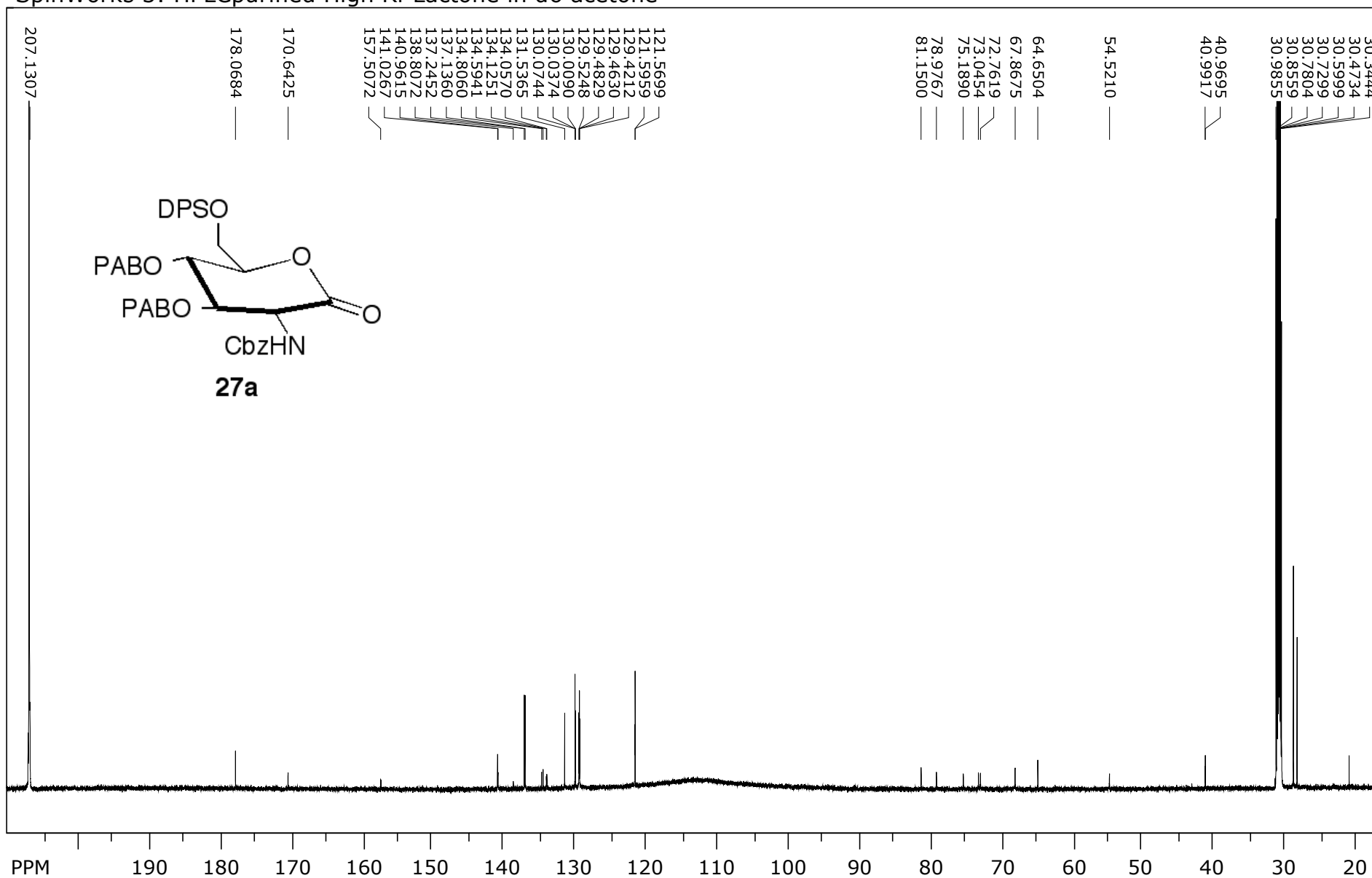
F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 2048 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 502.313 ppm/cm: 0.83642



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\HiRfLactone\HPLCPur_COSY\ser
 transmitter freq.: 600.552832 MHz
 time domain size: 4096 by 1024 points
 width (F2): 7211.50 Hz = 12.008167 ppm = 1.760621 Hz/pt
 number of scans: 2

expt: <cosyF2:ffreq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 150.550 ppm/cm: 0.25069

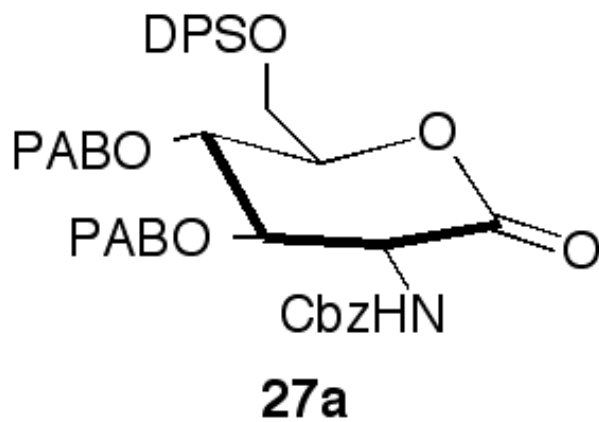
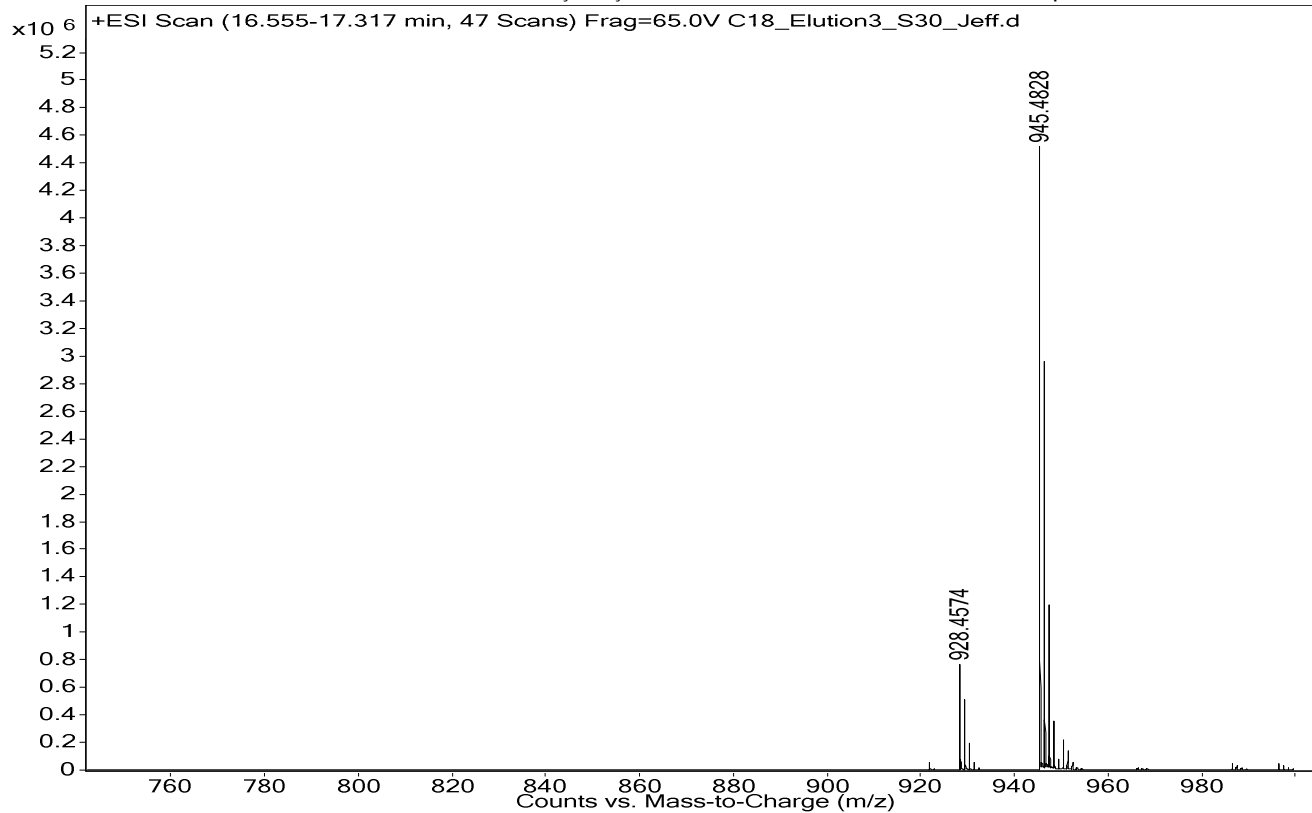
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 269.562 ppm/cm: 0.44886

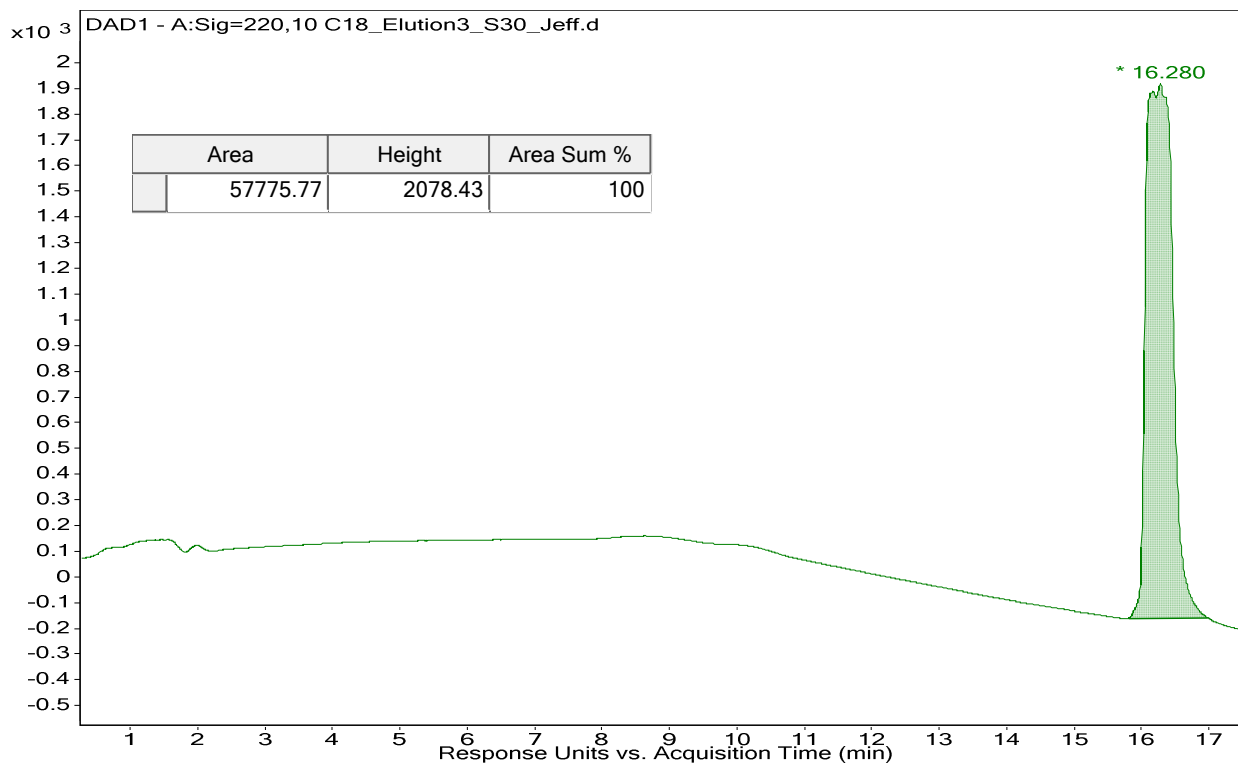


file: ...R Data\HiRfLactone\HPLCPur_13C\fid expt: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 10240

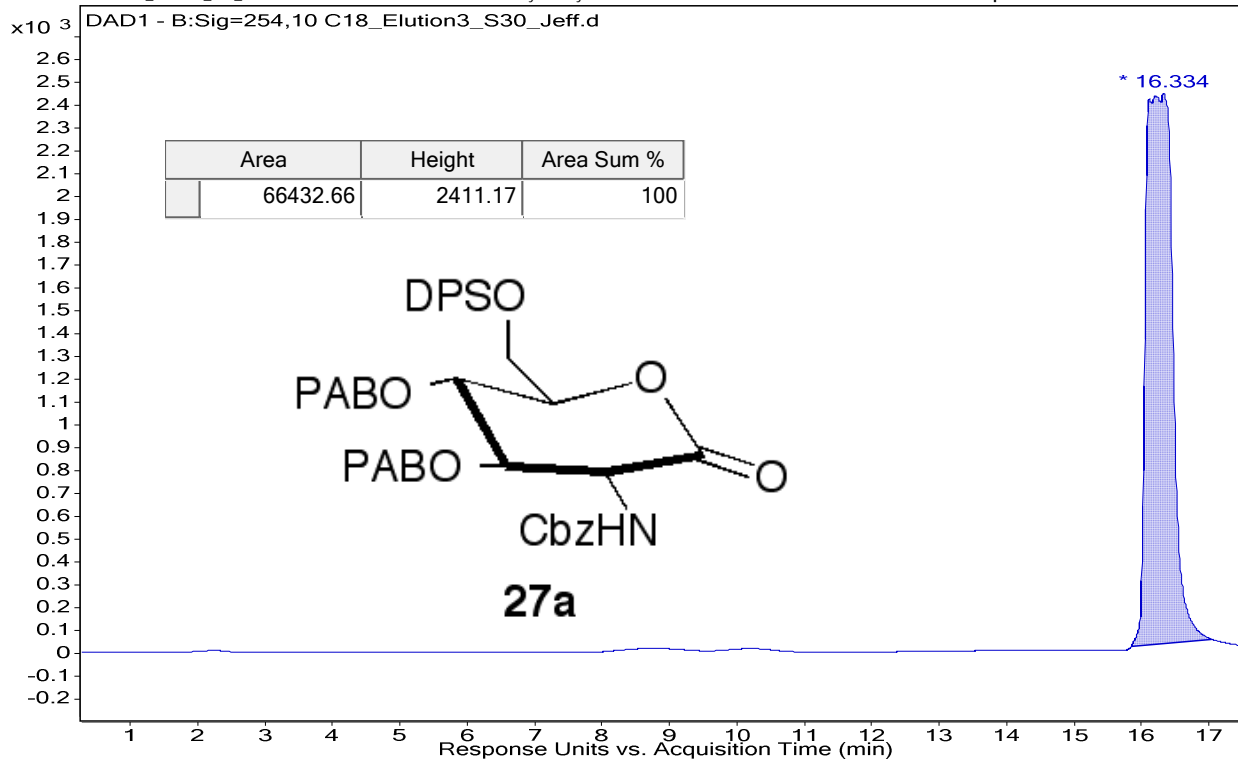
freq. of 0 ppm: 151.008166 MHz
processed size: 32768 complex points
LB: 0.700 GF: 0.0000
Hz/cm: 1170.356 ppm/cm: 7.74949

Sample Name	Jeff-30	Position	Vial 31	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution3_S30_Jef	ACQ Method	C18 waters symmetry3	Comment		Acquired Time	9/16/2012 3:21:24 AM



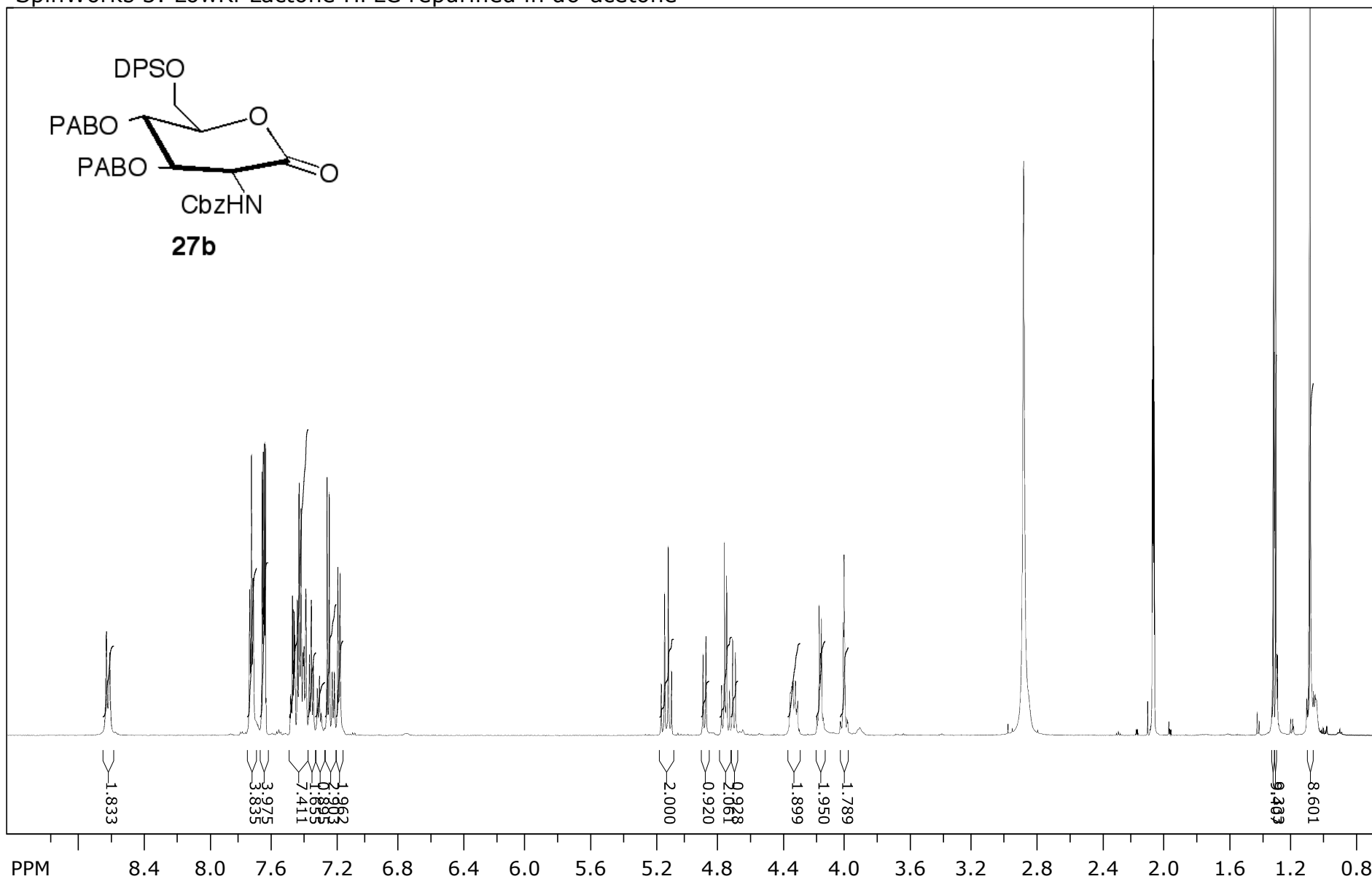


Sample Name	Jeff-30	Position	Vial 31	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution3_S30_Jef	ACQ Method	C18 waters symmetry3	Comment		Acquired Time	9/16/2012 3:21:24 AM



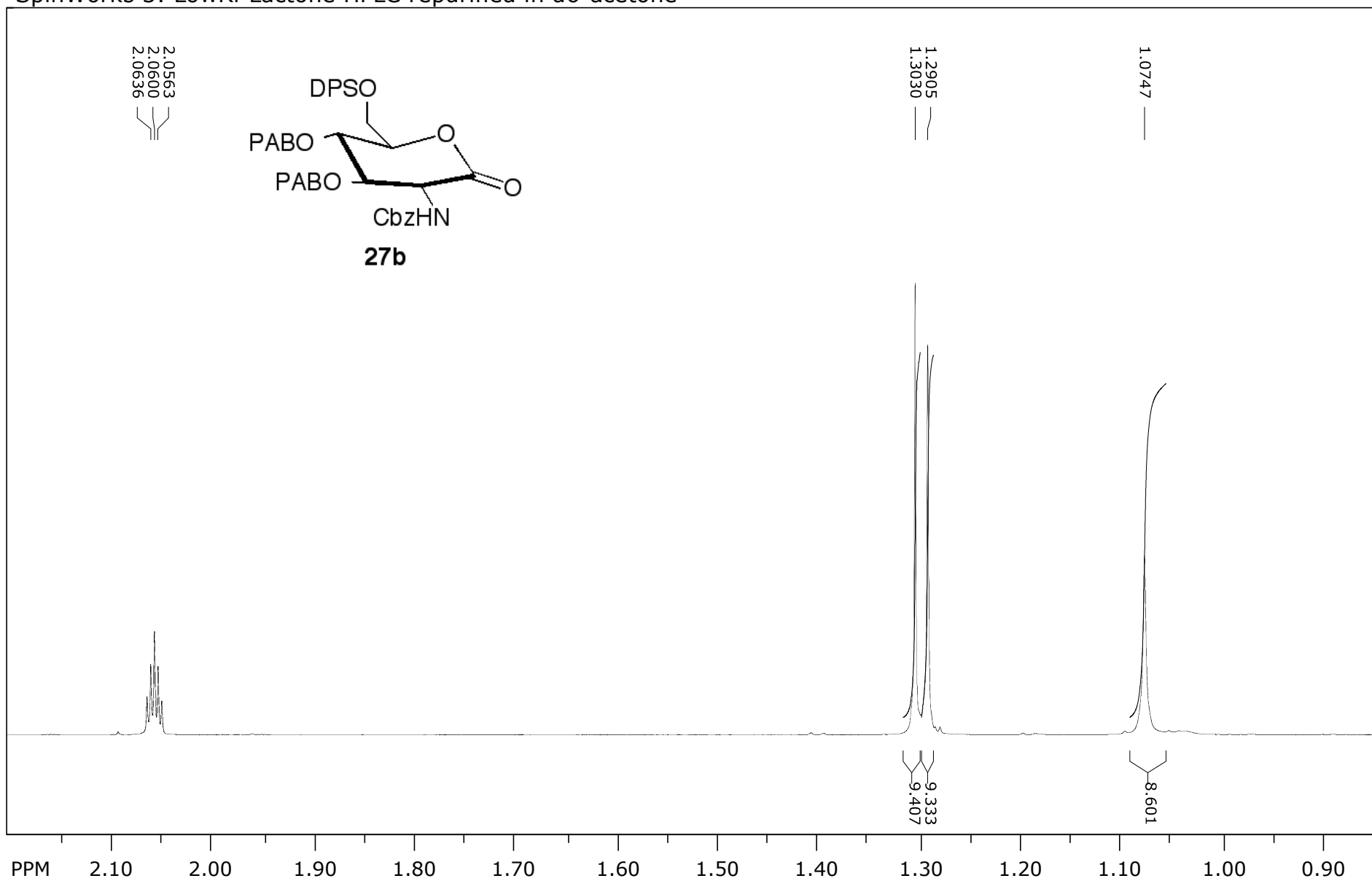
Analysis on a Waters SymmetryShield™ C18 (4.6 mm X 15 cm (i.d. x l.), 3.5 μm) at 0.5 mL/min. Solvent A: 50 mM NH₄OAc (aq); B: CH₃CN

Time (min)	% B
0	50
1	50
10	100
20	100



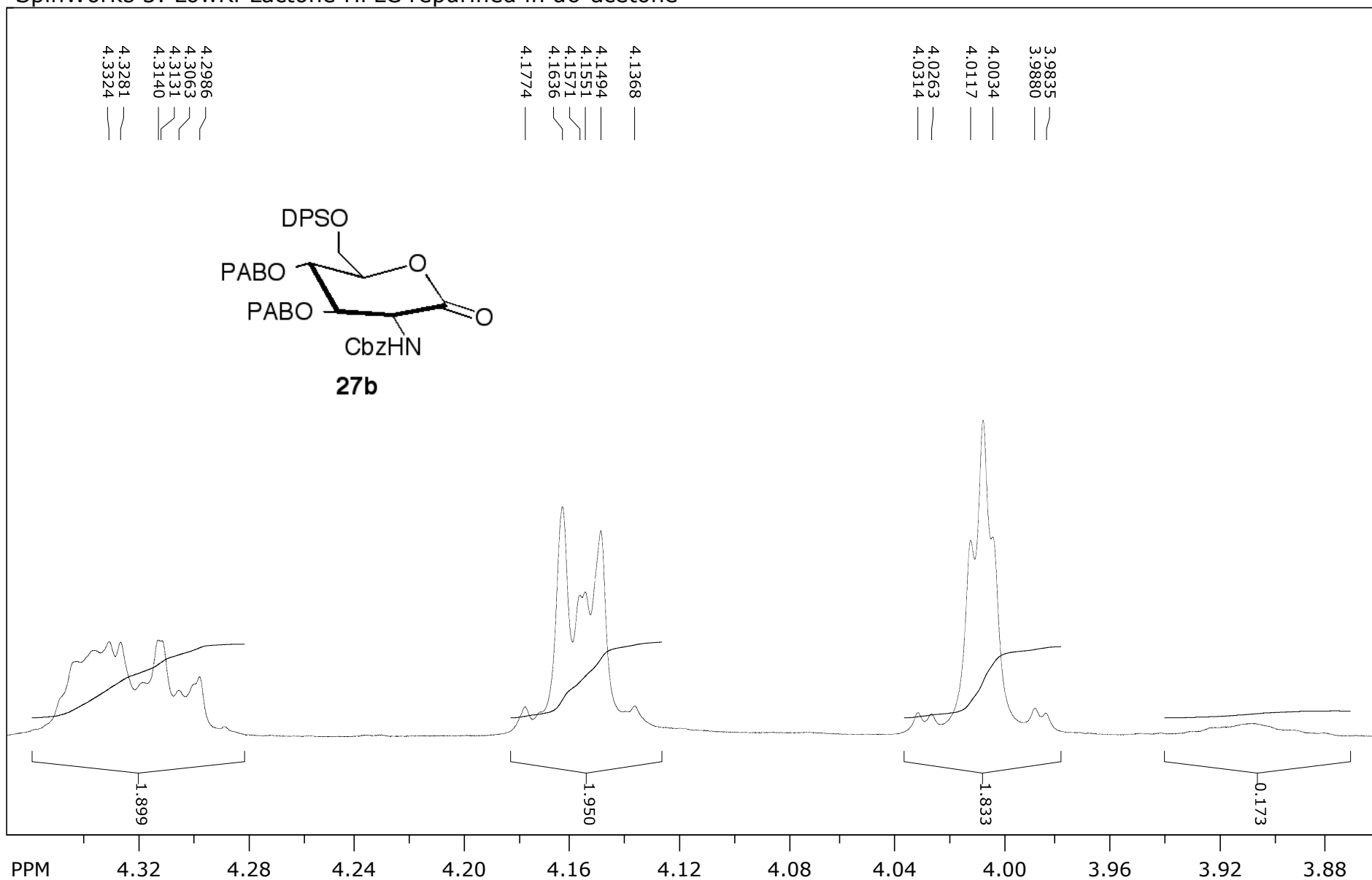
file: ...R Data\lowRfLactoned6acet_1H\1\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 207.542 ppm/cm: 0.34559



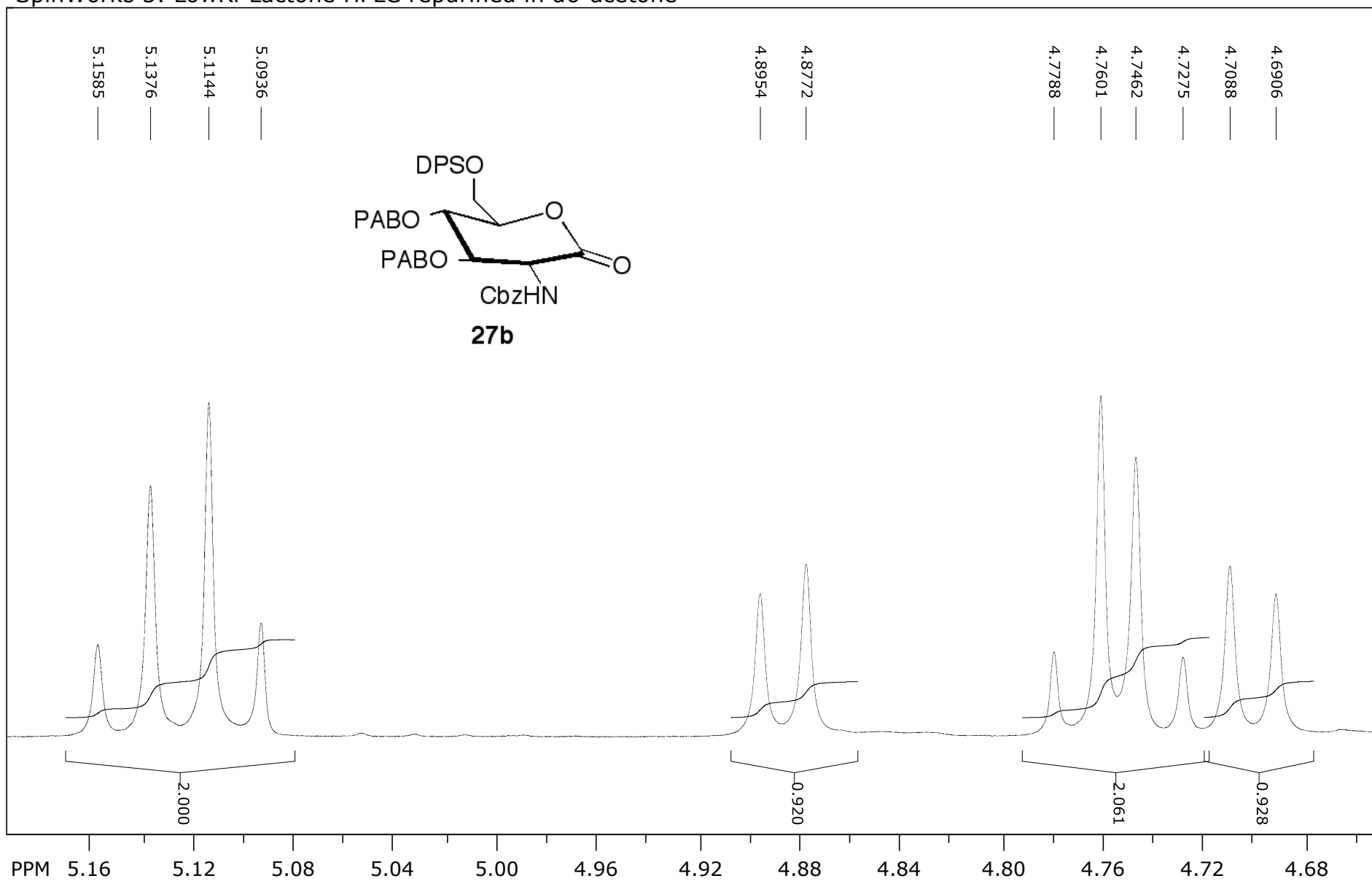
file: ...R Data\lowRfLactoned6acet_1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 32.799 ppm/cm: 0.05461



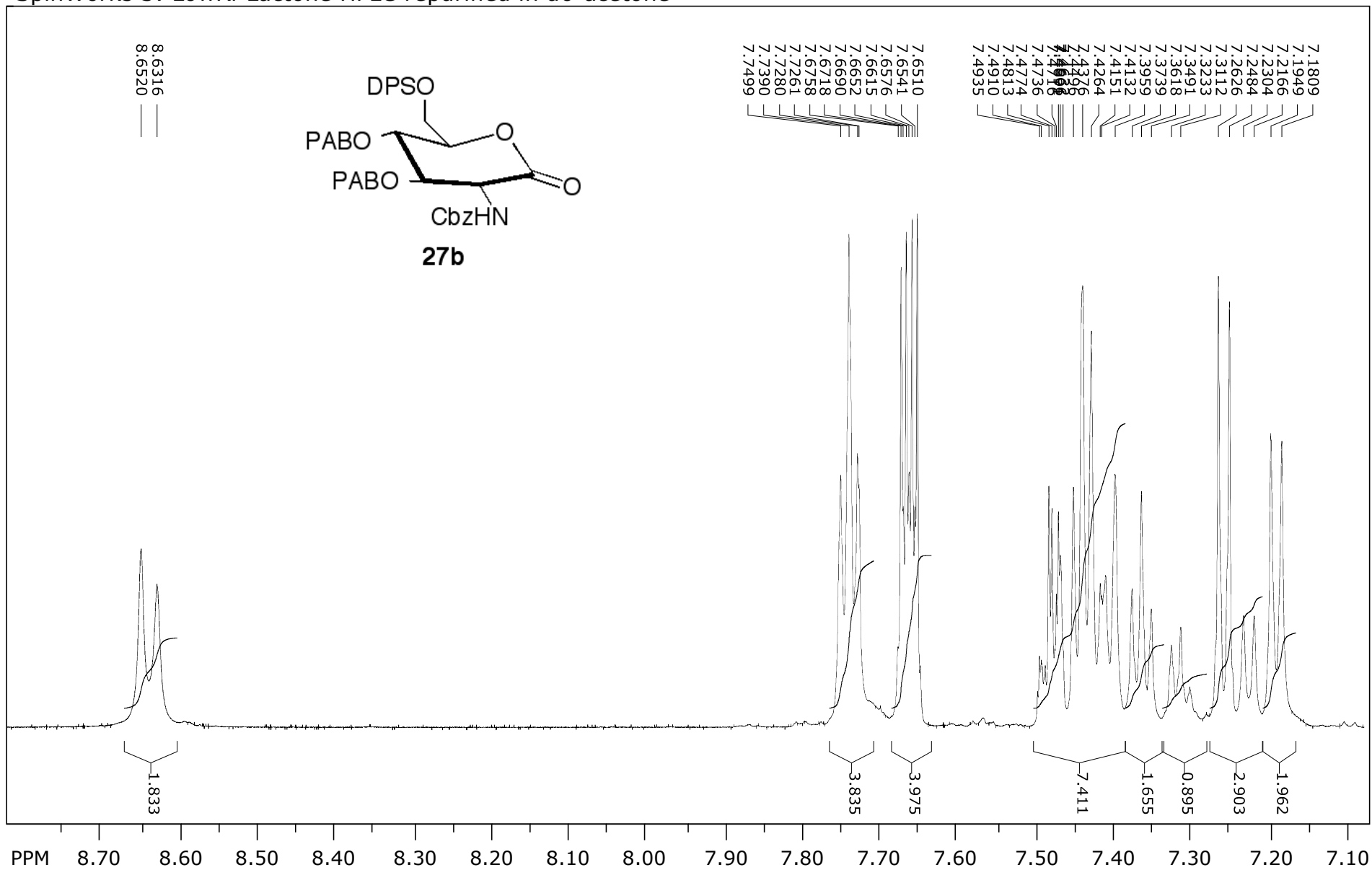
file: ...R Data\lowRfLactoned6acet_1H\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 12.279 ppm/cm: 0.02045



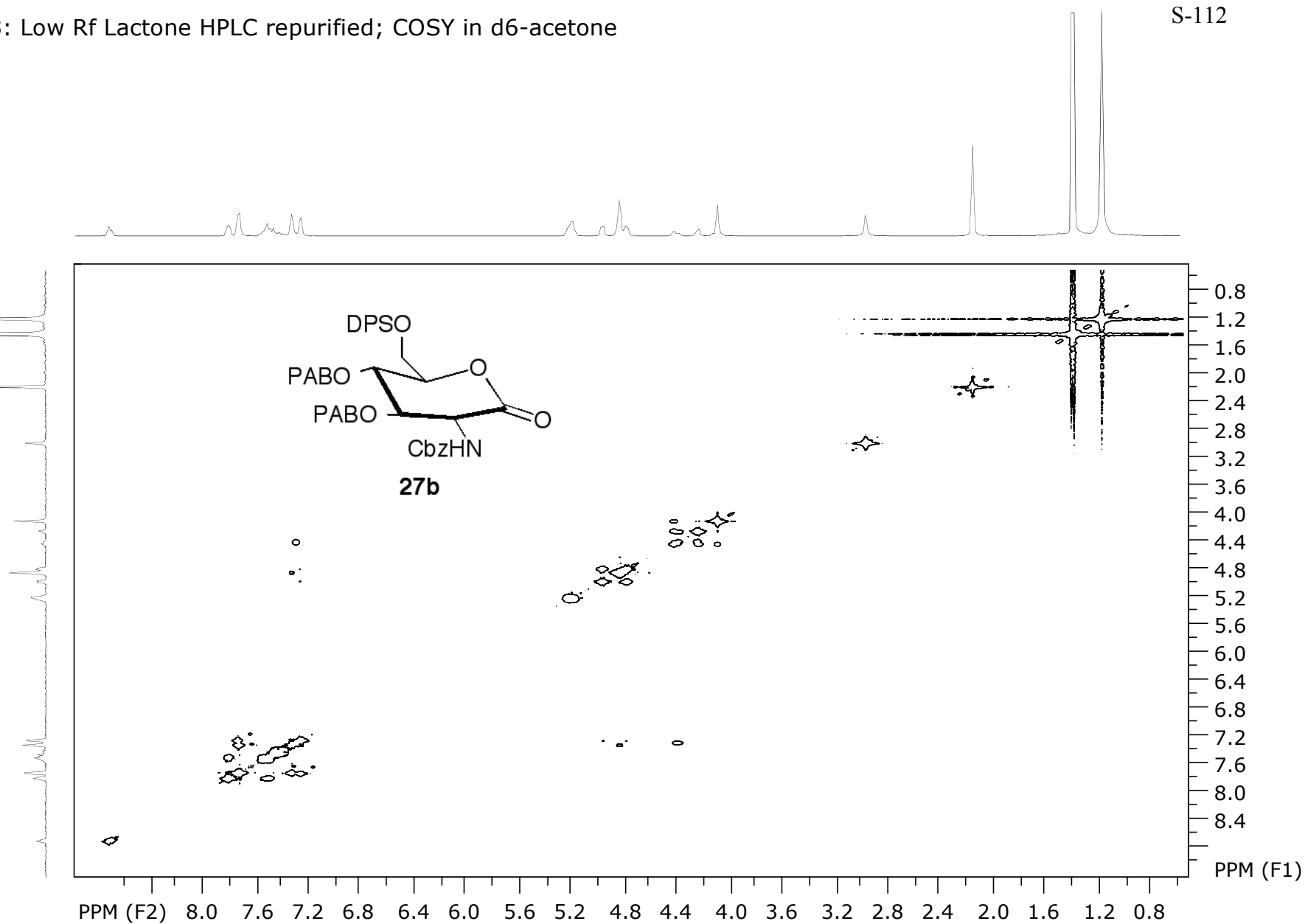
file: ...R Data\lowRfLactoned6acet_1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 13.090 ppm/cm: 0.02180



file: ...R Data\lowRfLactoned6acet_1H\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

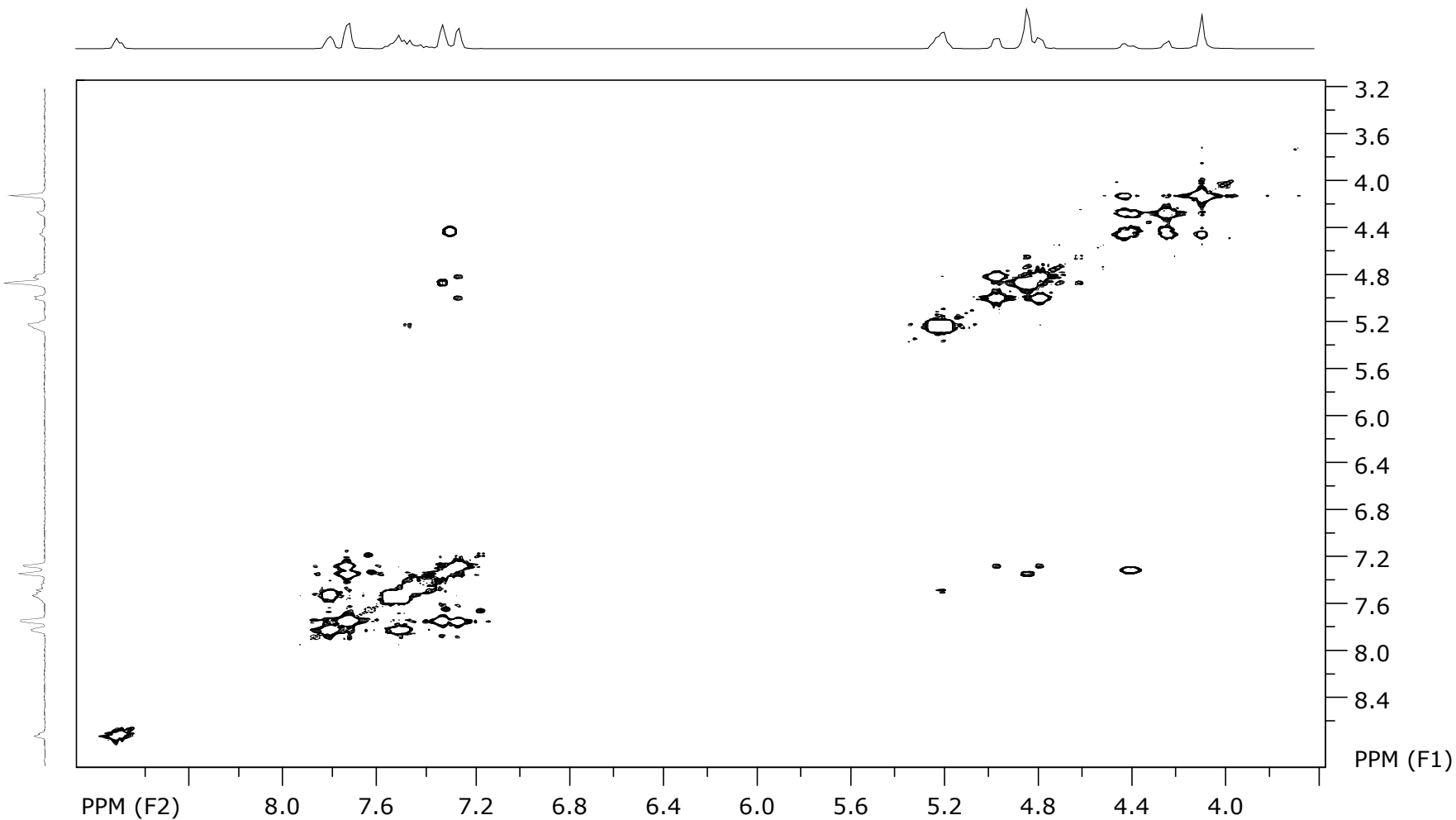
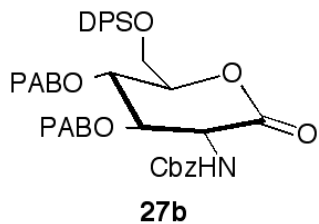
freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 42.064 ppm/cm: 0.07004



file: ...Data\lowRfLactone_d6acetCOSY\1\ser
expt: <cosygpqf>
transmitter freq: 600.552832 MHz
time domain size: 2048 by 1024 points
width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
number of scans: 2

F2: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 254.103 ppm/cm: 0.42311

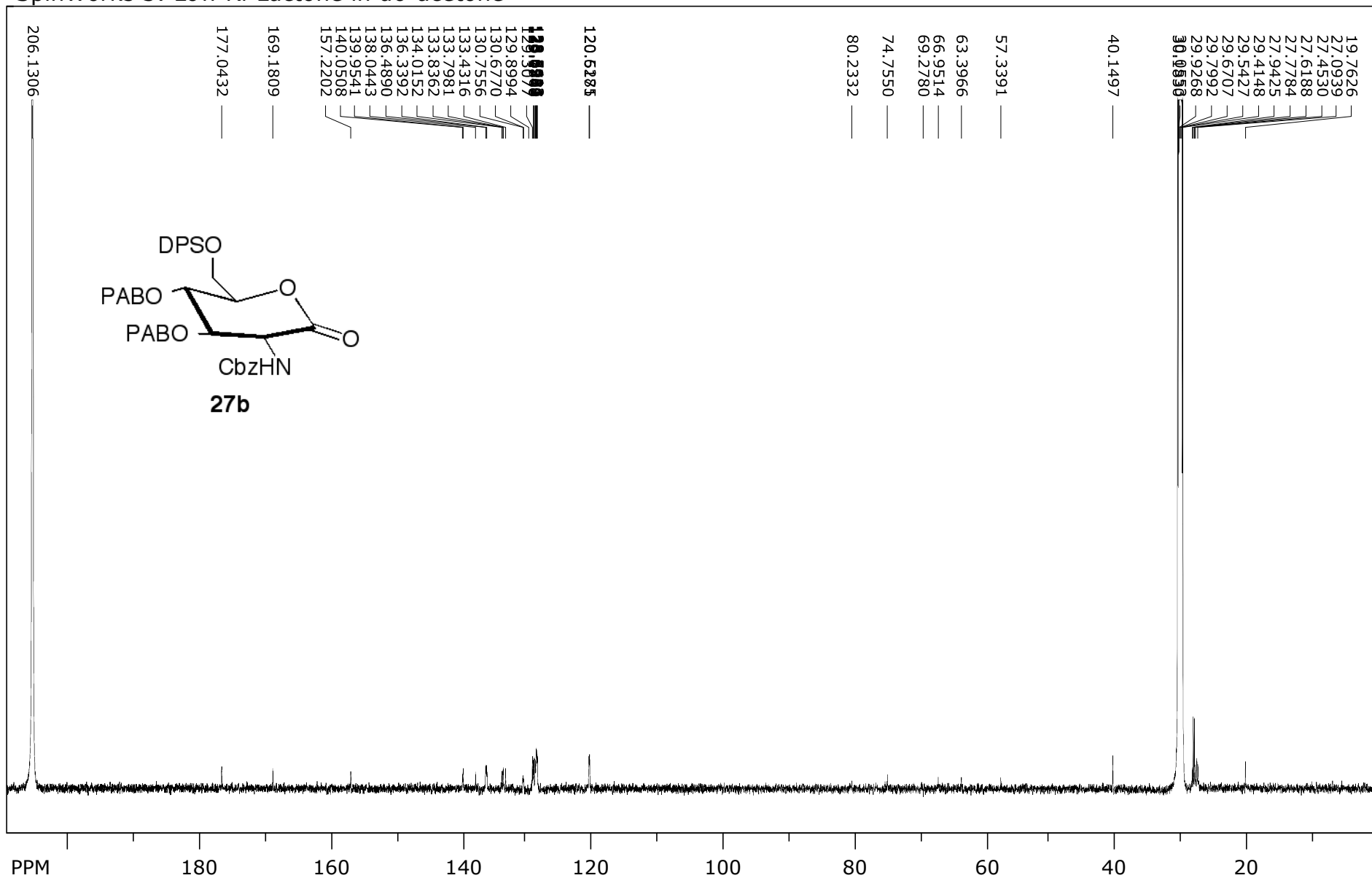
F1: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 480.897 ppm/cm: 0.80076



file: ...Data\lowRfLactone_d6acetCOSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
 number of scans: 2

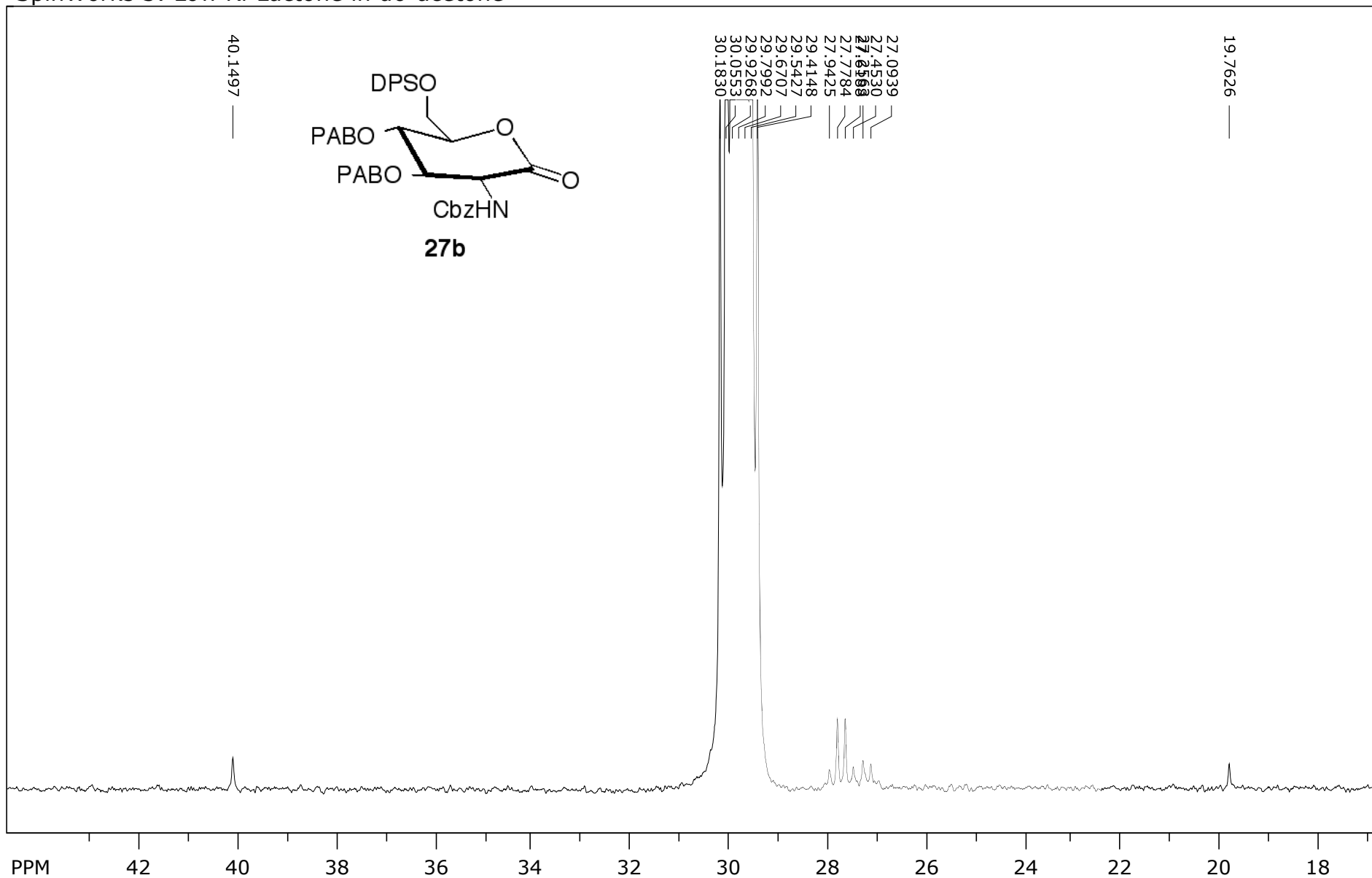
F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 159.678 ppm/cm: 0.26589

F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 319.407 ppm/cm: 0.53185



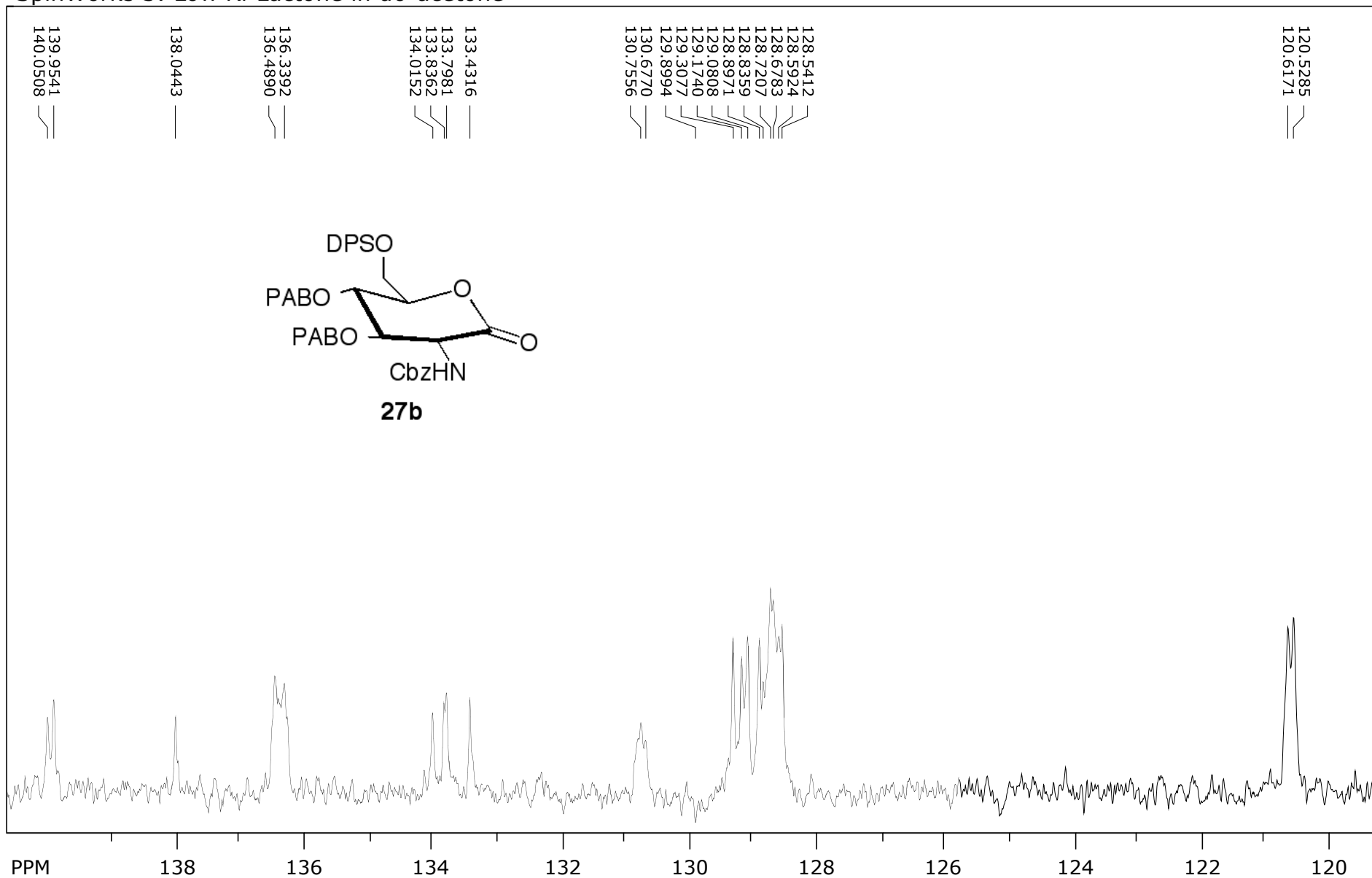
file: ... Data\loRflactone_13C_d6acet\1\fid expt: <zpgg30>
 transmitter freq.: 151.023519 MHz
 time domain size: 65536 points
 width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
 number of scans: 22528

freq. of 0 ppm: 151.008292 MHz
 processed size: 32768 complex points
 LB: 4.000 GF: 0.0000
 Hz/cm: 1273.231 ppm/cm: 8.43068



file: ... Data\loRflactone_13C_d6acet\1\fid expt: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 22528

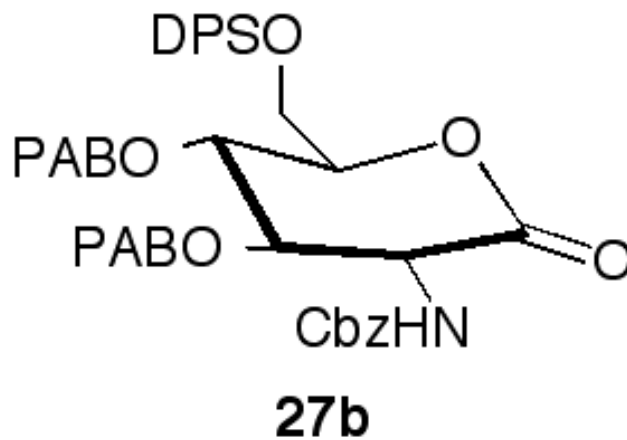
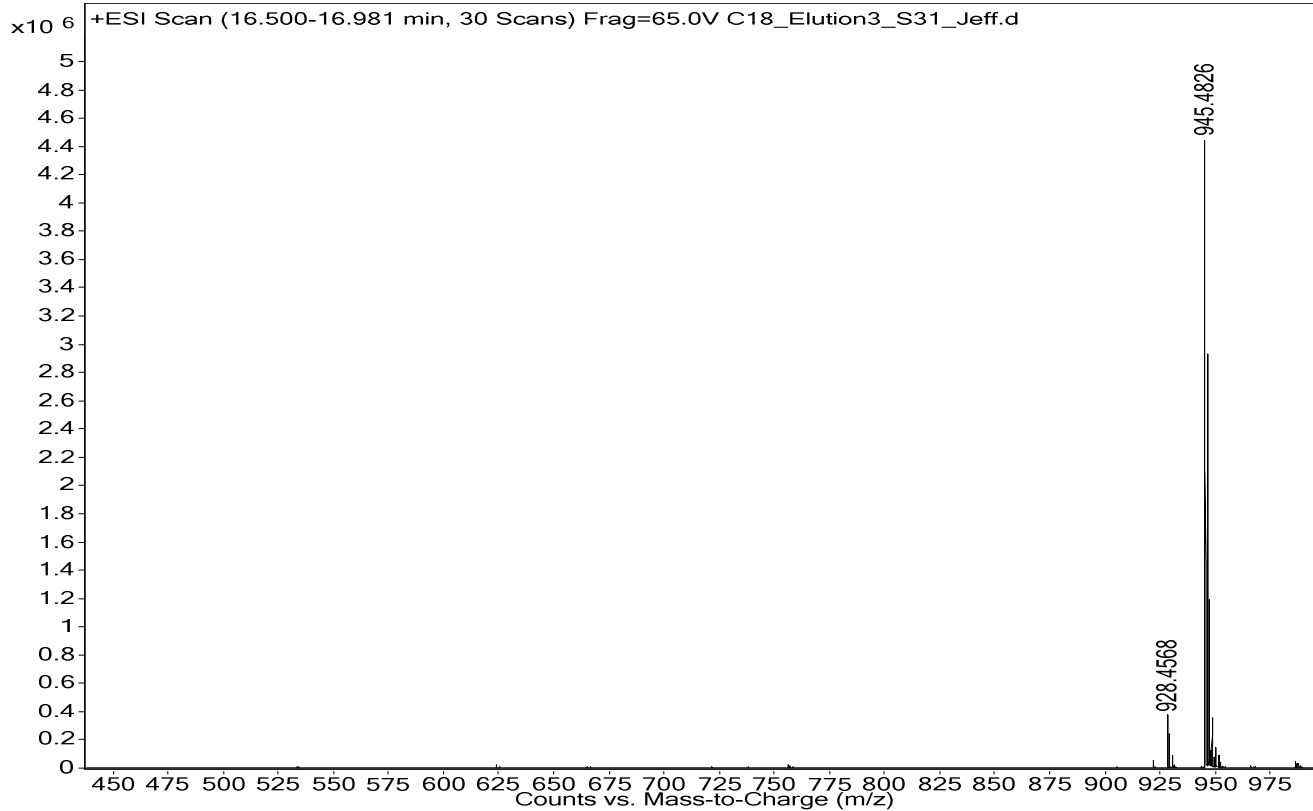
freq. of 0 ppm: 151.008292 MHz
processed size: 32768 complex points
LB: 4.000 GF: 0.0000
Hz/cm: 169.577 ppm/cm: 1.12285

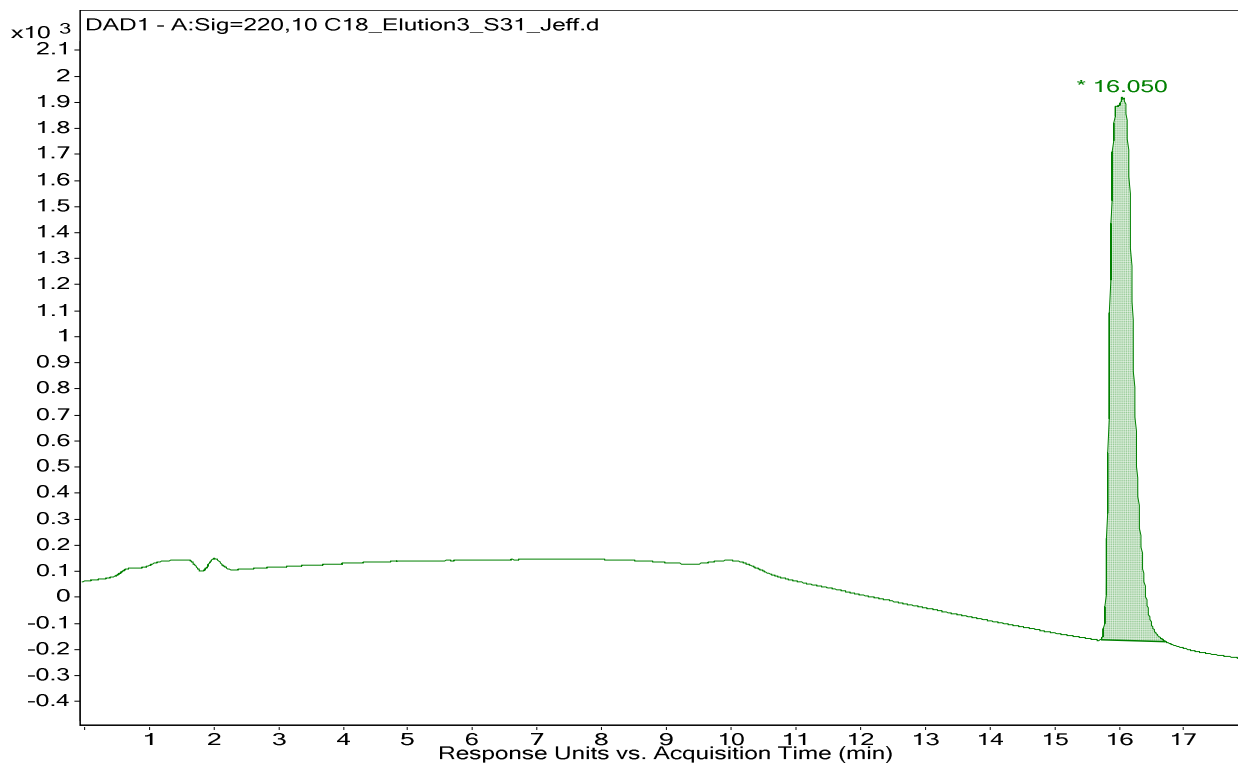


file: ... Data\loRflactone_13C_d6acet\1\fid exp: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 22528

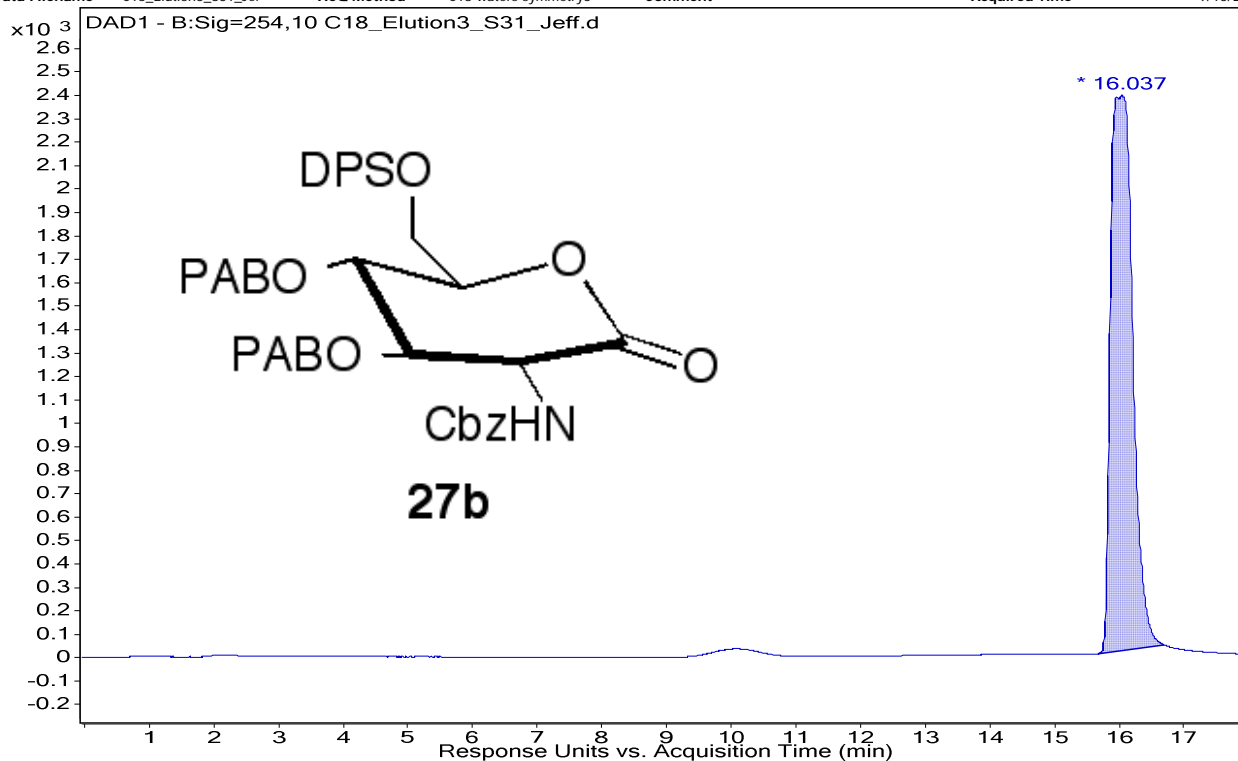
freq. of 0 ppm: 151.008292 MHz
processed size: 32768 complex points
LB: 4.000 GF: 0.0000
Hz/cm: 129.862 ppm/cm: 0.85988

Sample Name	Jeff-31	Position	Vial 32	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution3_S31_Jef	ACQ Method	C18 waters symmetry3	Comment		Acquired Time	9/16/2012 3:48:07 AM





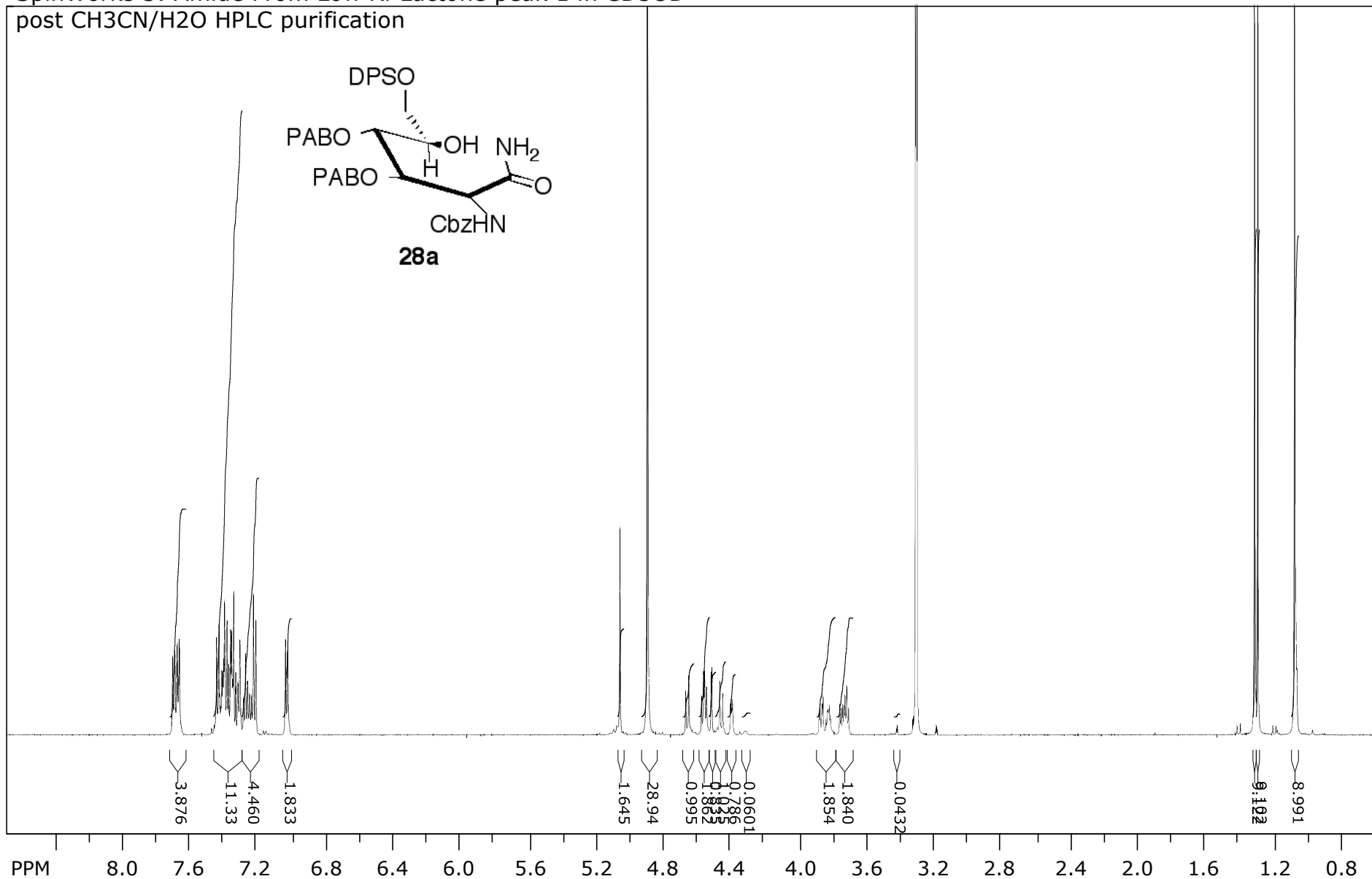
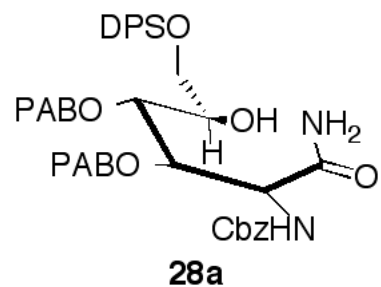
Sample Name	Jeff-31	Position	Vial 32	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution3_S31_Jef	ACQ Method	C18 waters symmetry3	Comment		Acquired Time	9/16/2012 3:48:07 AM



Analysis on a Waters SymmetryShield™ C18 (4.6 mm X 15 cm (i.d. x l.), 3.5 μm) at 0.5 mL/min. Solvent A: 50 mM NH₄OAc (aq); B: CH₃CN

Time (min)	% B
0	50
1	50
10	100
20	100

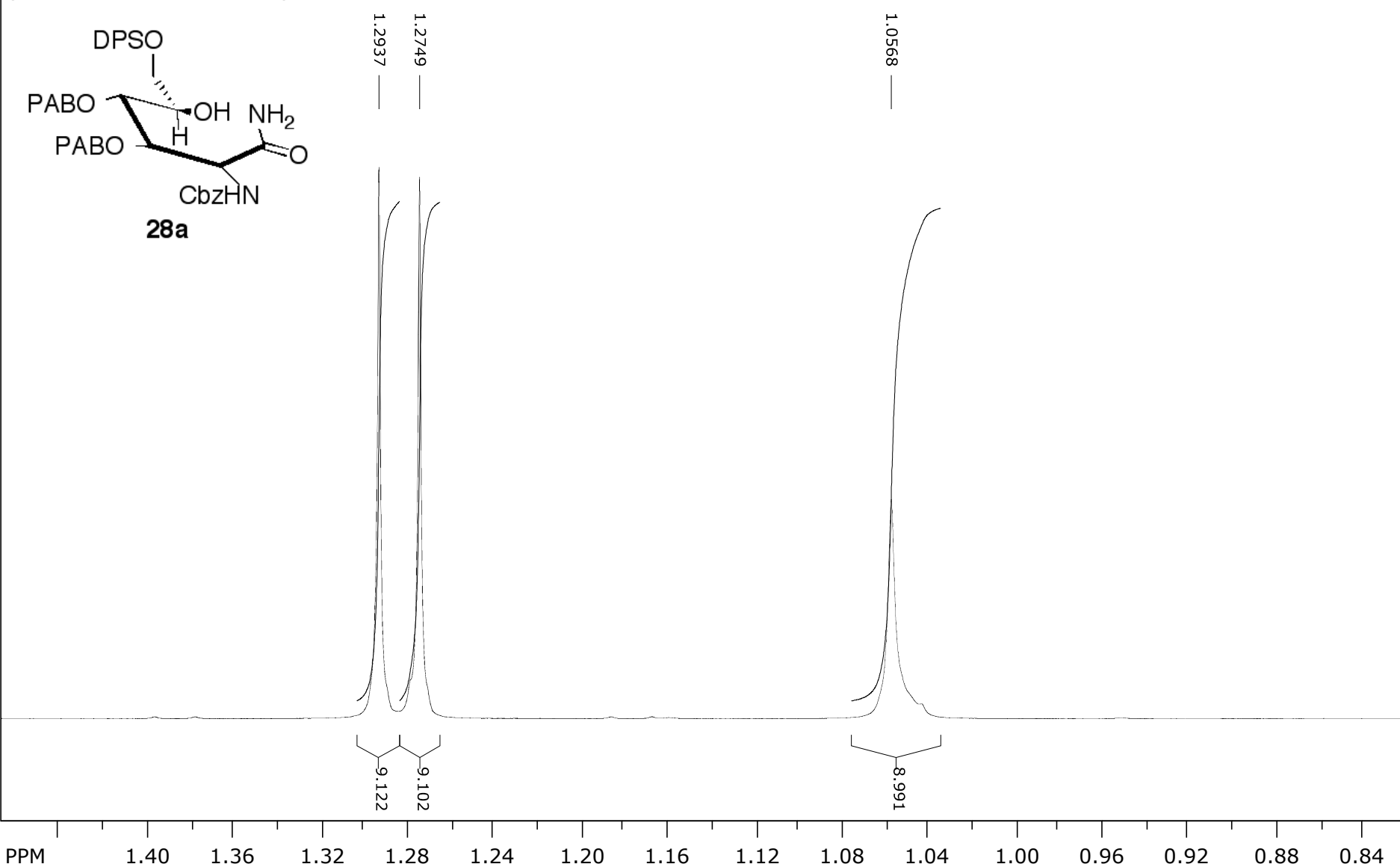
post CH3CN/H2O HPLC purification



file: ...der\NMR Data\AmFrLoPk1_CD3OD\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 195.683 ppm/cm: 0.32584

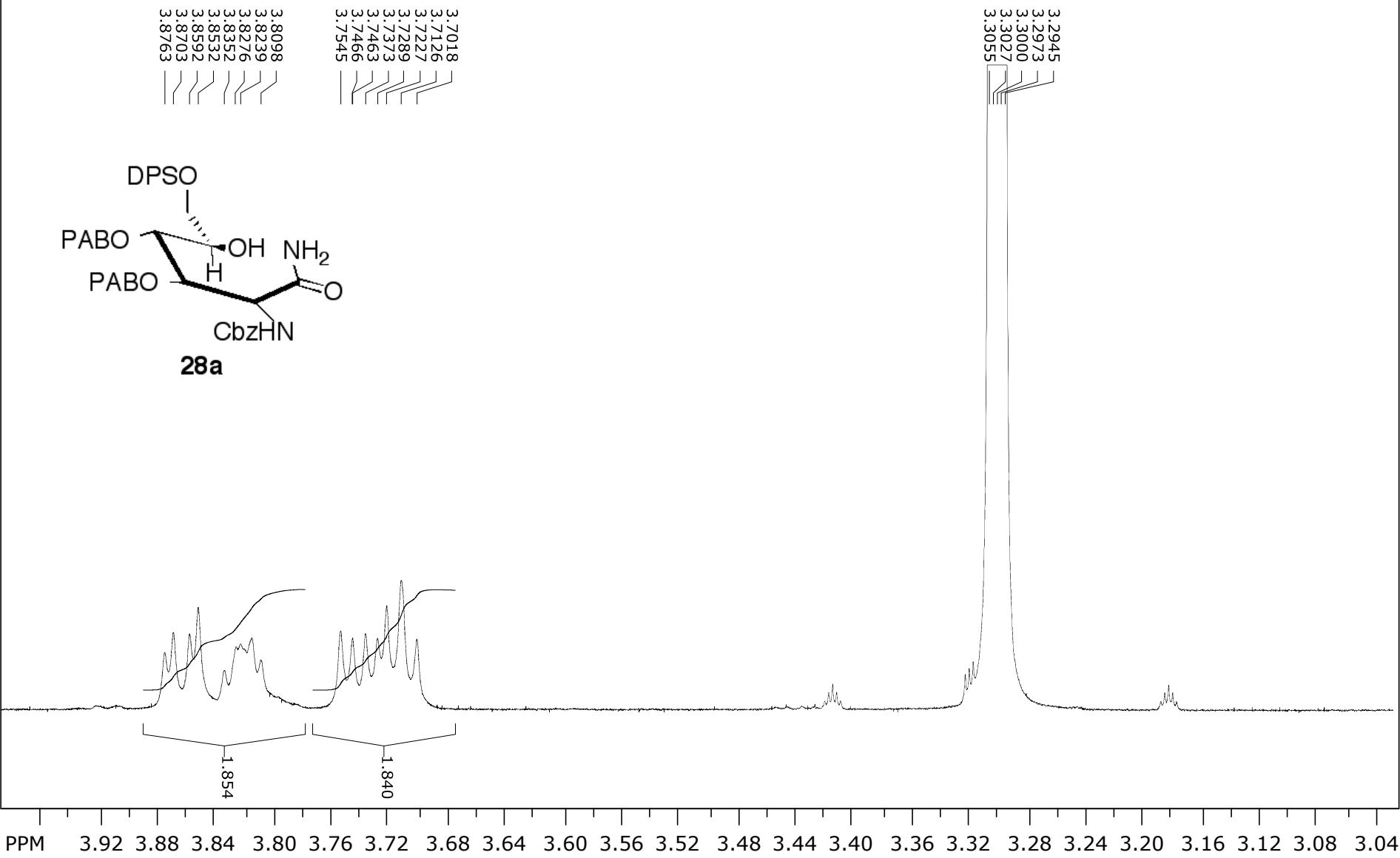
post CH3CN/H2O HPLC purification



file: ...der\NMR Data\AmFrLoPk1_CD3OD\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

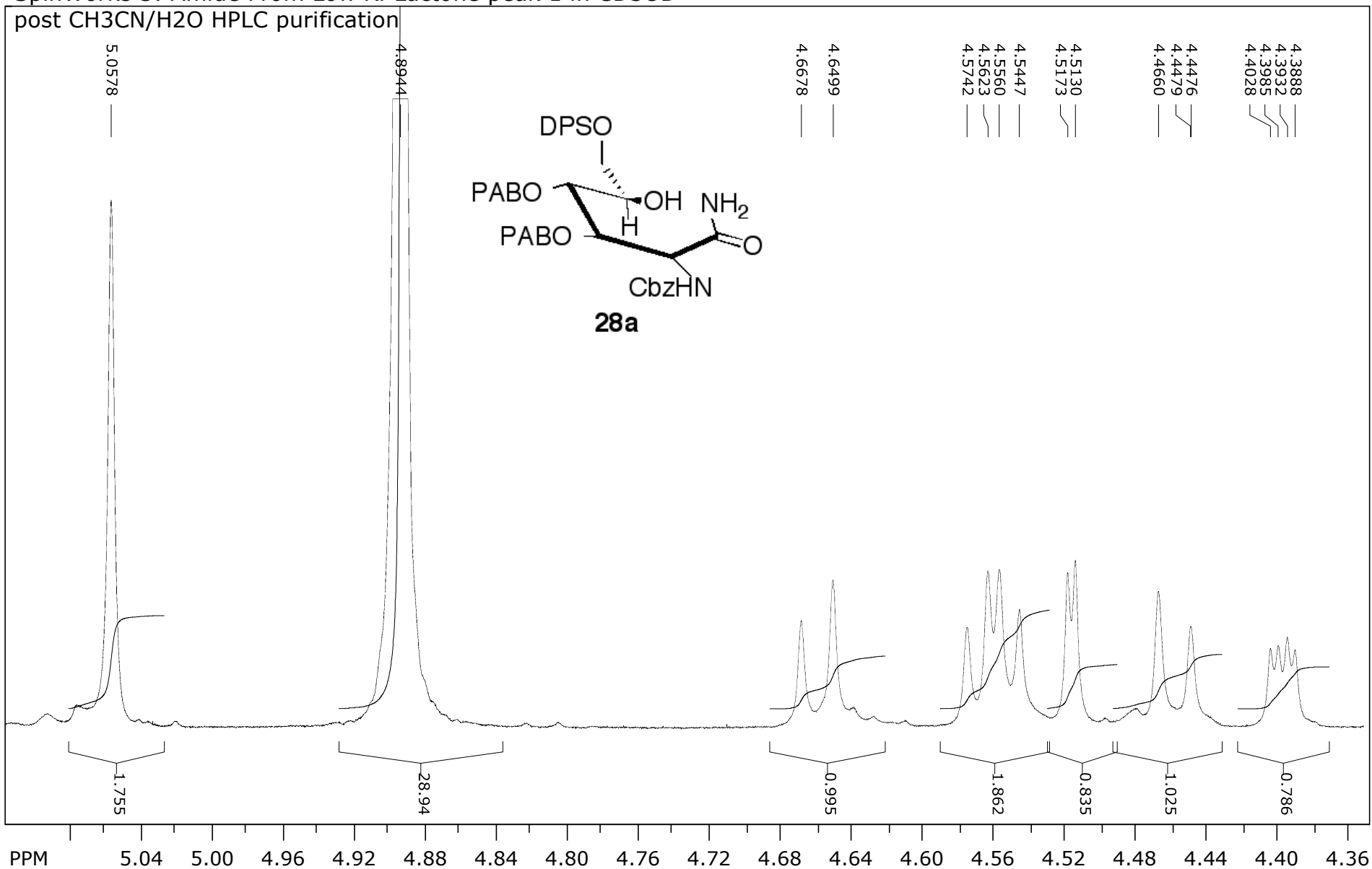
freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 15.616 ppm/cm: 0.02600

post CH3CN/H2O HPLC purification



file: ...der\NMR Data\AmFrLoPk1_CD3OD\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

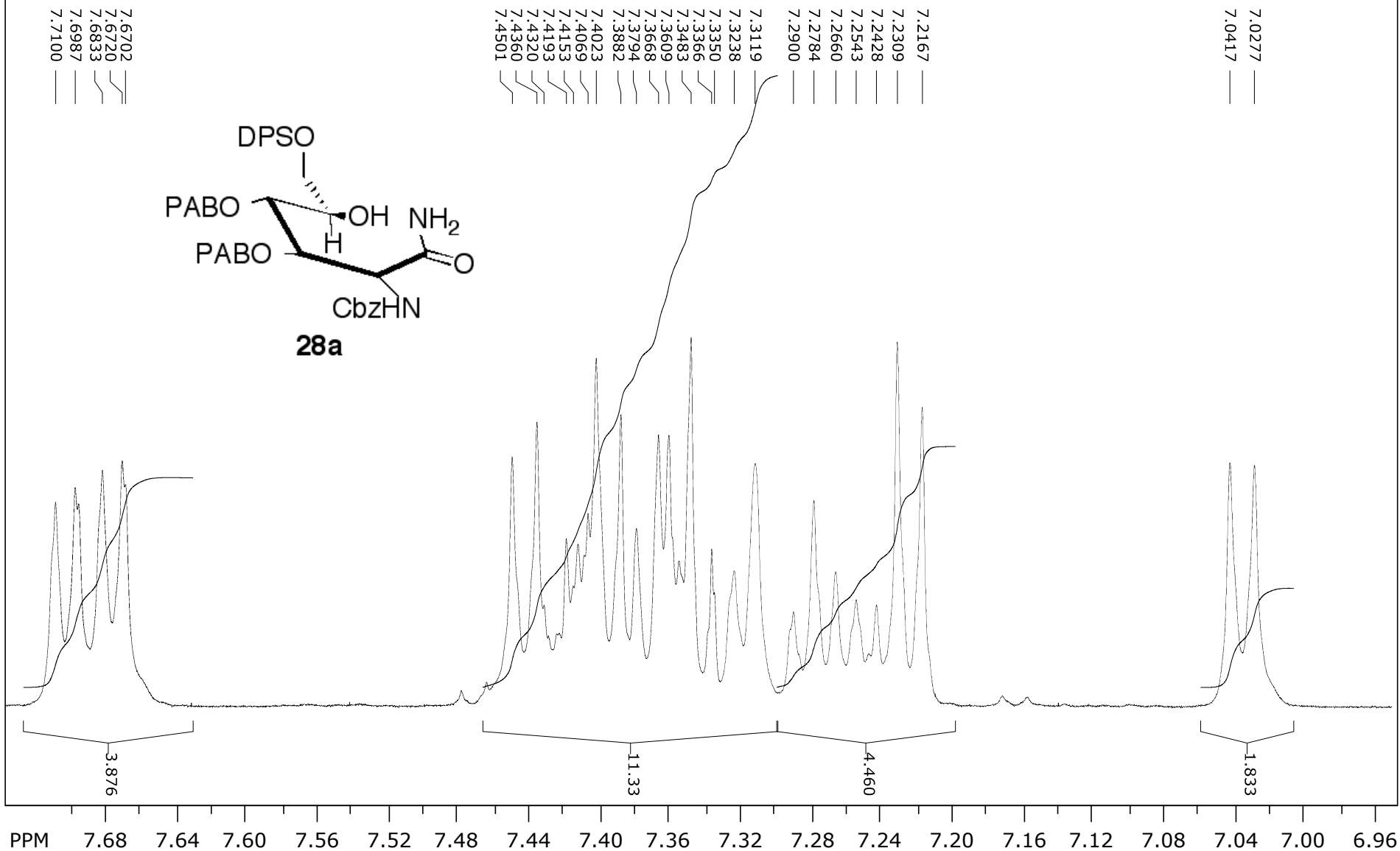
freq. of 0 ppm: 600.550023 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 23.163 ppm/cm: 0.03857



file: ...der\NMR Data\AmFrLoPk1_CD3OD\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

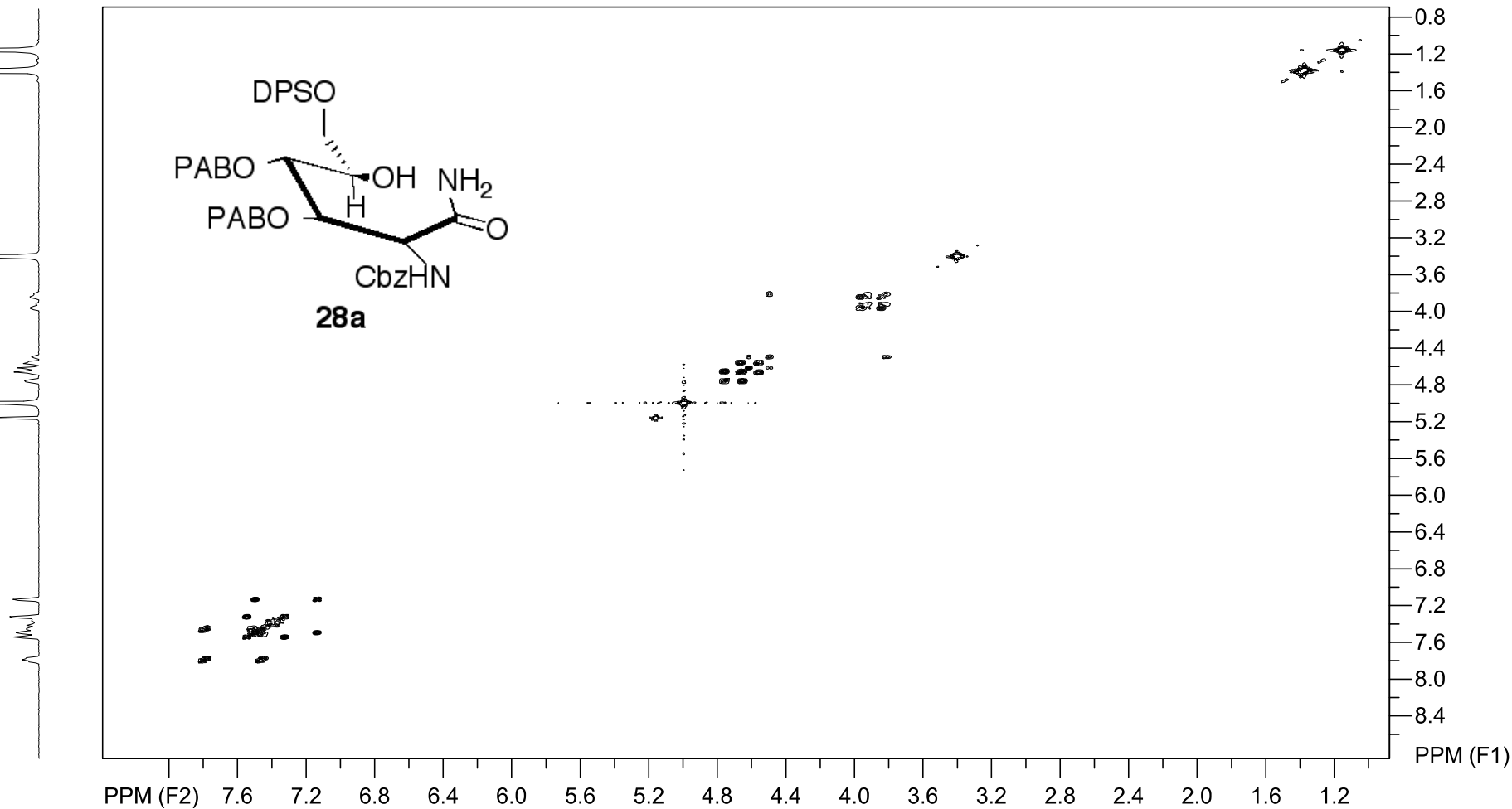
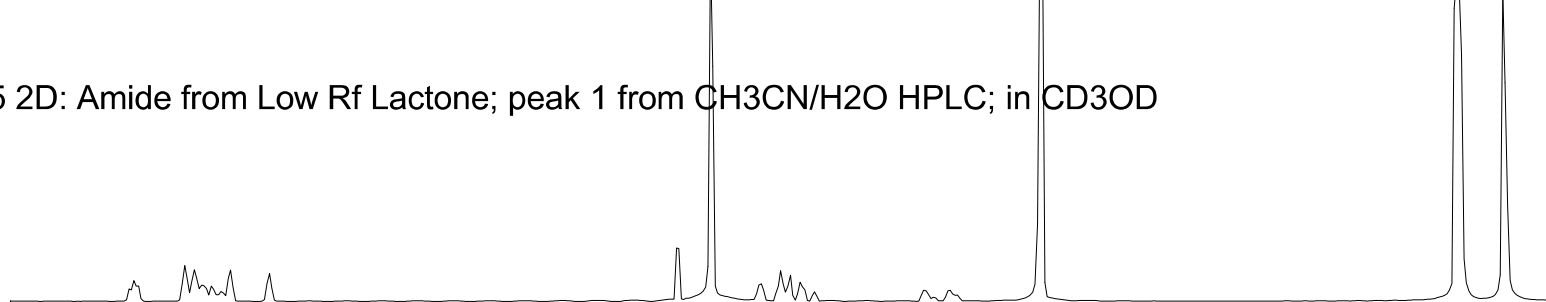
freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 18.448 ppm/cm: 0.03072

post CH3CN/H2O HPLC purification



file: ...der\NMR Data\AmFrLoPk1_CD3OD\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

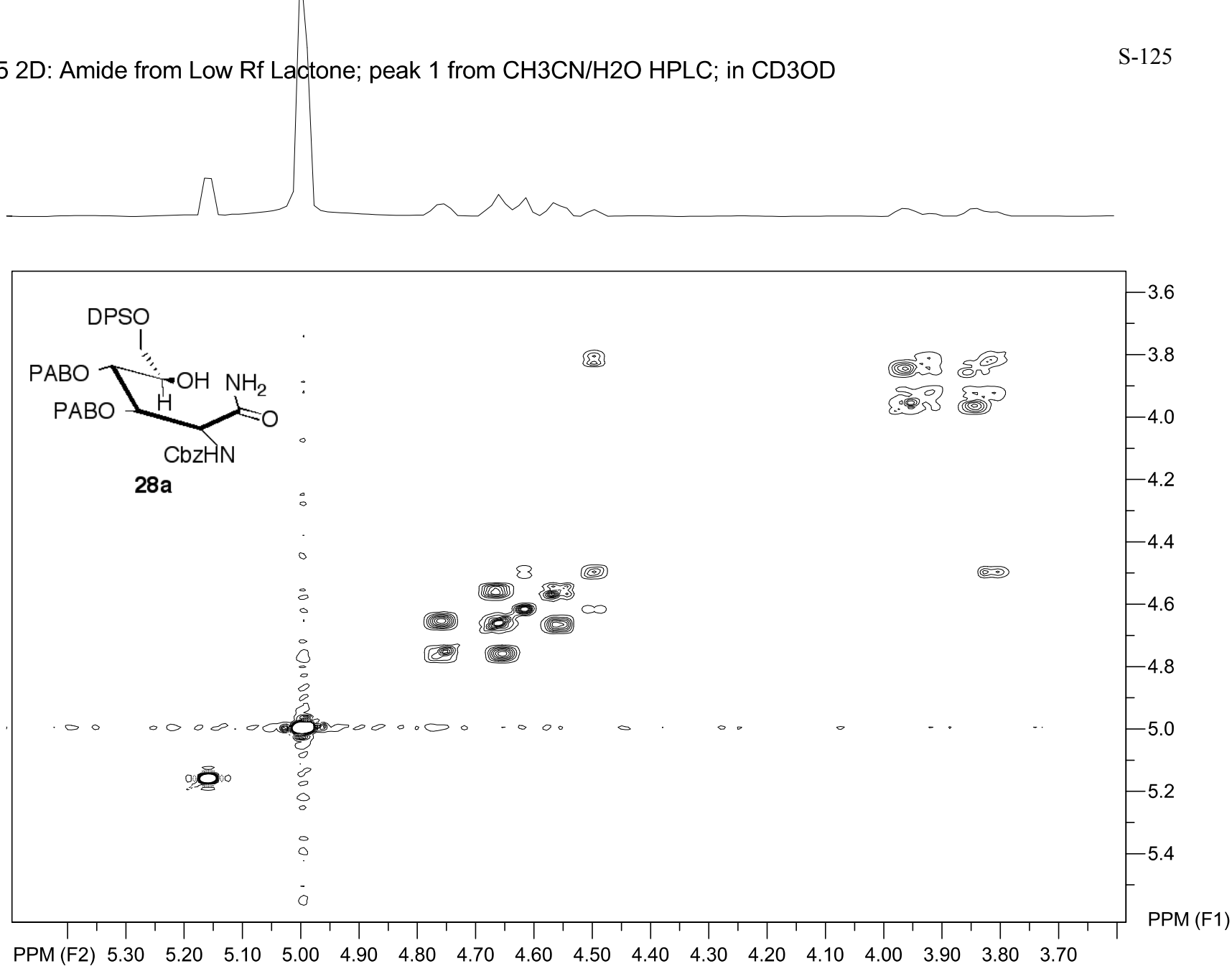
freq. of 0 ppm: 600.550023 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 18.958 ppm/cm: 0.03157



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\AmFrLoPk1COSY\1\ser exp: <cosygpqf>
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.50 Hz = 12.008167 ppm = 3.521242 Hz/pt
 number of scans: 2

F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 220.000 ppm/cm: 0.36633

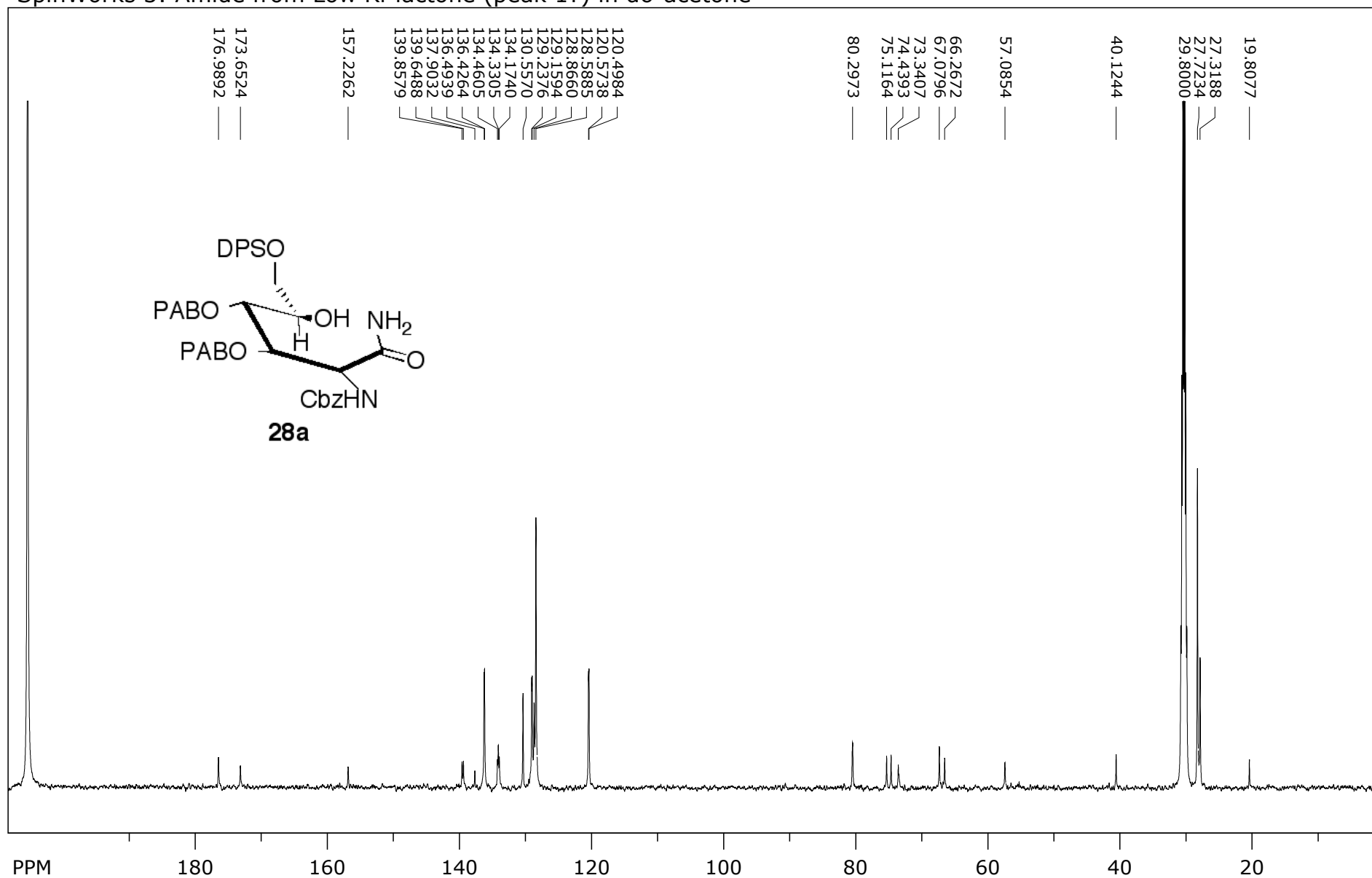
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 409.149 ppm/cm: 0.68129



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\AmFrLoPk1COSY\1\ser exp: <cosygpqf>
transmitter freq.: 600.552832 MHz
time domain size: 2048 by 1024 points
width (F2): 7211.50 Hz = 12.008167 ppm = 3.521242 Hz/pt
number of scans: 2

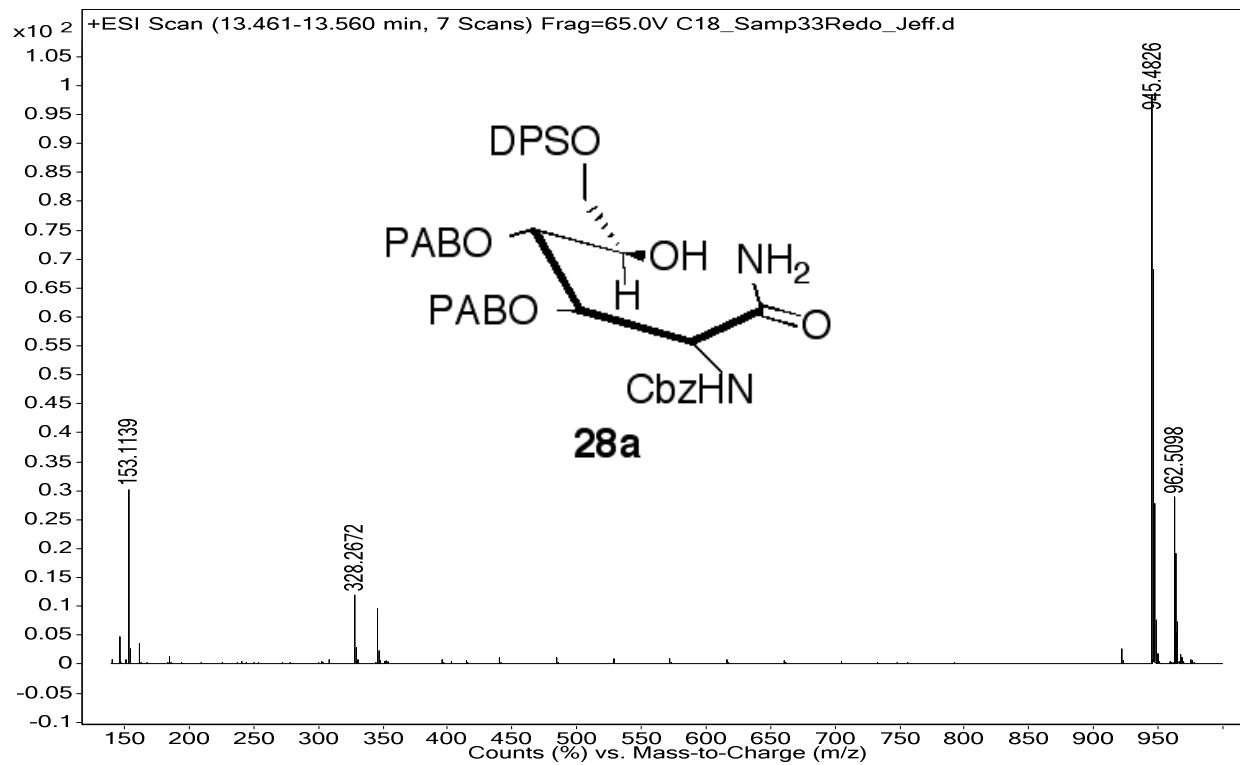
F2: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 55.980 ppm/cm: 0.09321

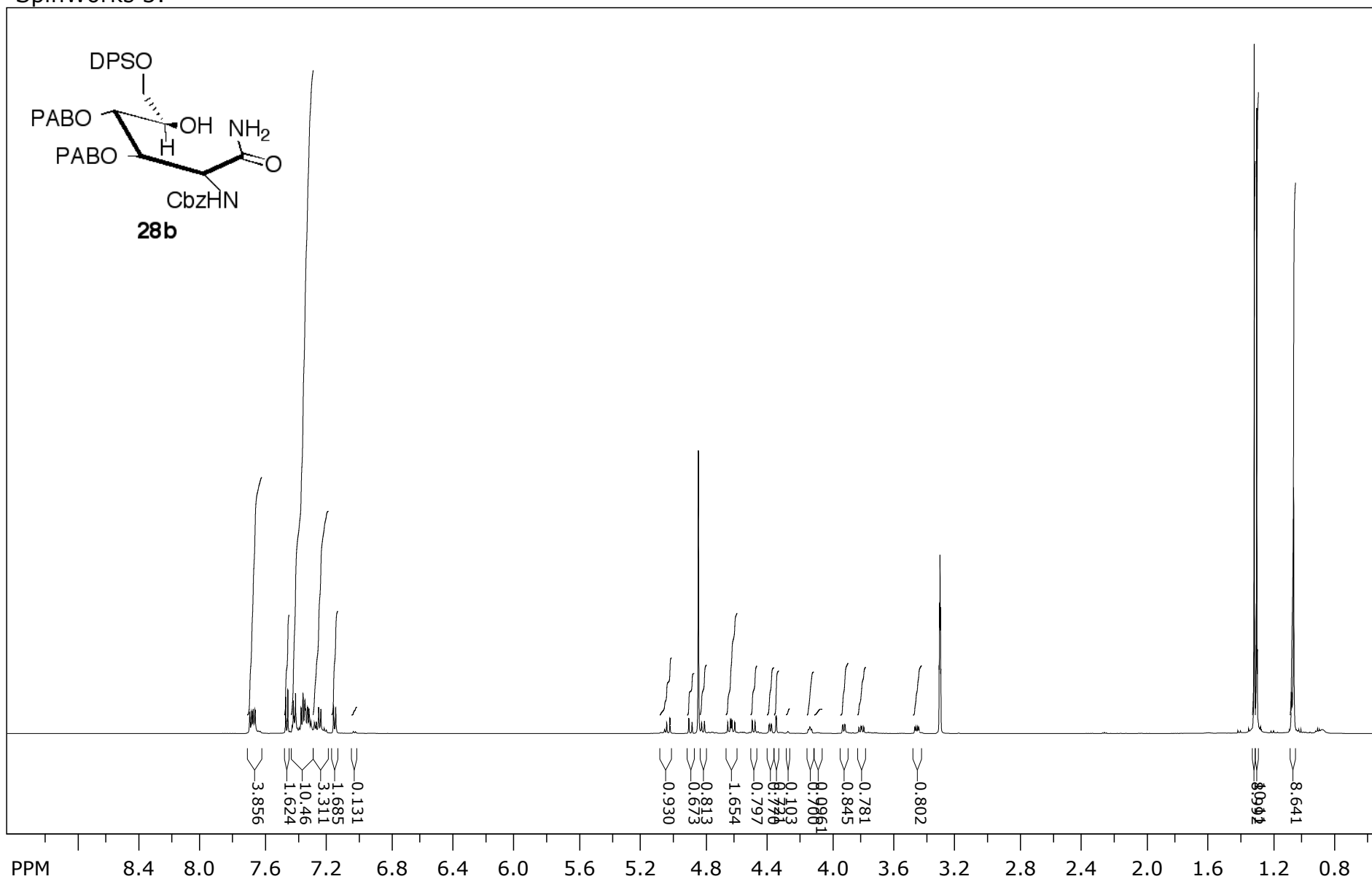
F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 104.482 ppm/cm: 0.17398



file: ...m lowRf lactone in d6acetone\2\fid expt: <zgpg>
transmitter freq.: 125.699901 MHz
time domain size: 65536 points
width: 27777.78 Hz = 220.9849 ppm = 0.423855 Hz/pt
number of scans: 2800

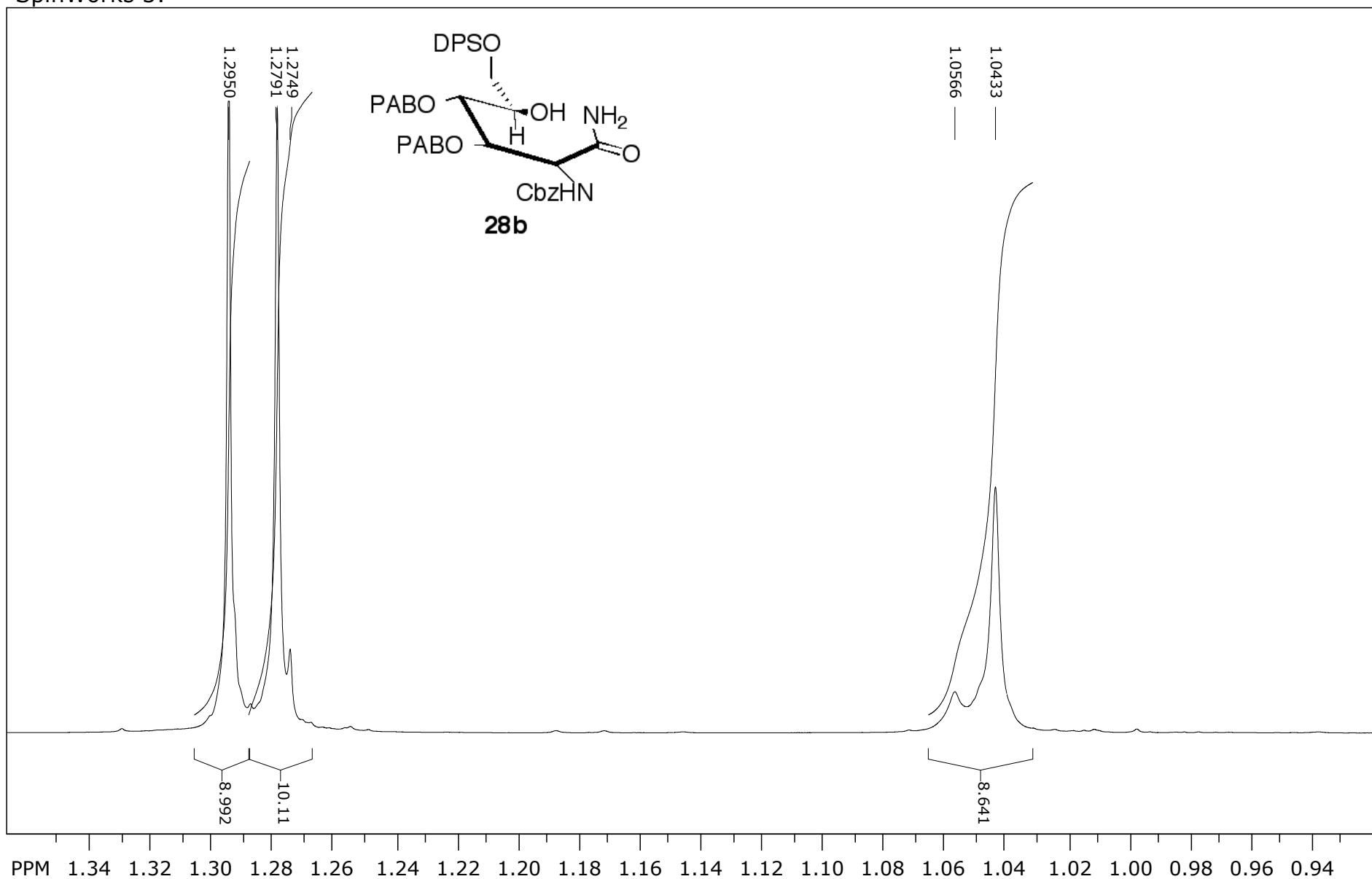
freq. of 0 ppm: 125.687276 MHz
processed size: 32768 complex points
LB: 10.000 GF: 0.0000
Hz/cm: 1050.698 ppm/cm: 8.35878





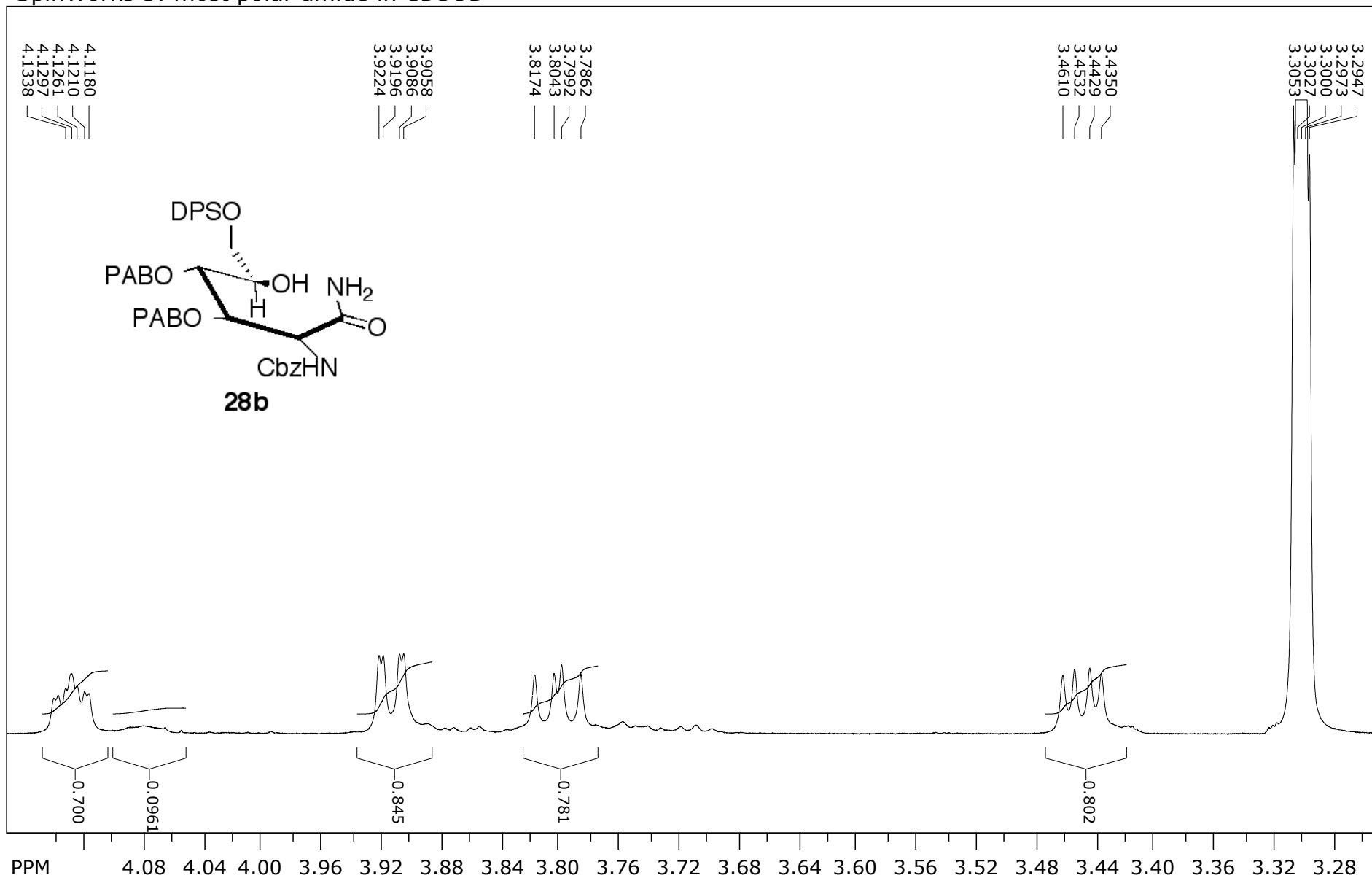
file: ...\\NMR Data\\mostPolAmide_CD3OD\\1\\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 210.335 ppm/cm: 0.35023



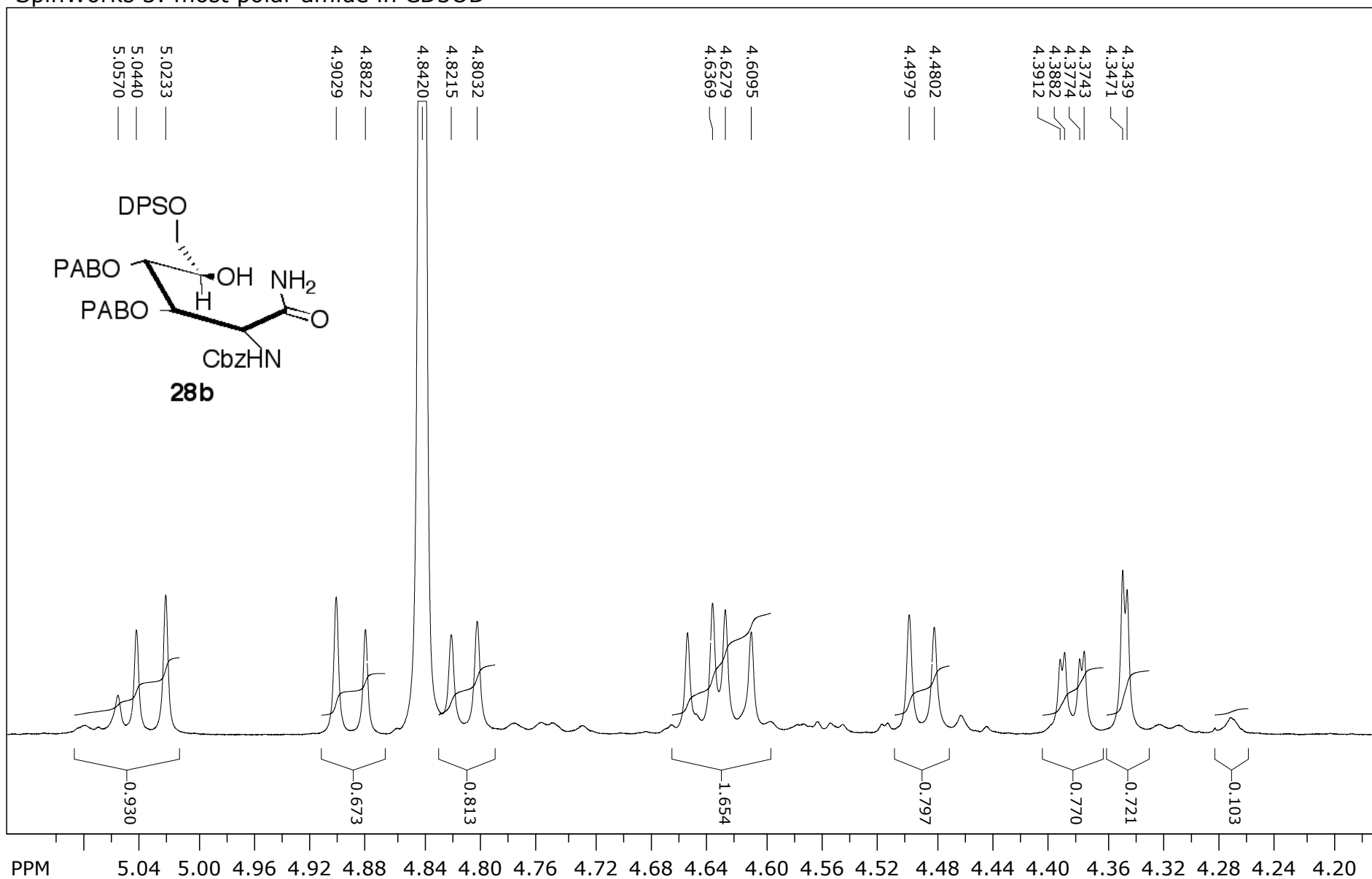
file: ...\\NMR Data\\mostPolAmide_CD3OD\\1\\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 10.825 ppm/cm: 0.01803



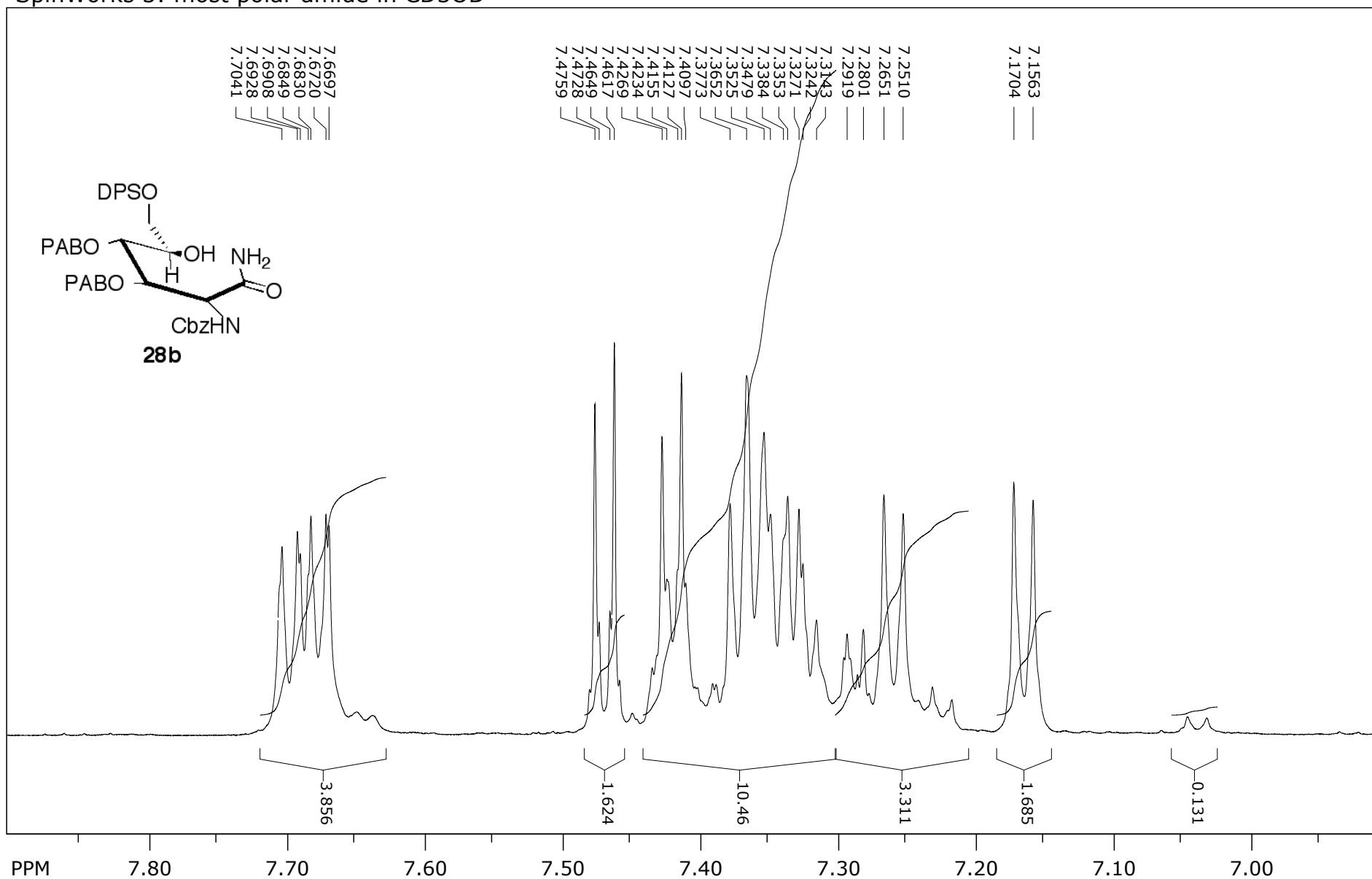
file: ...\\NMR Data\\mostPolAmide_CD3OD\\1\\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 22.236 ppm/cm: 0.03703



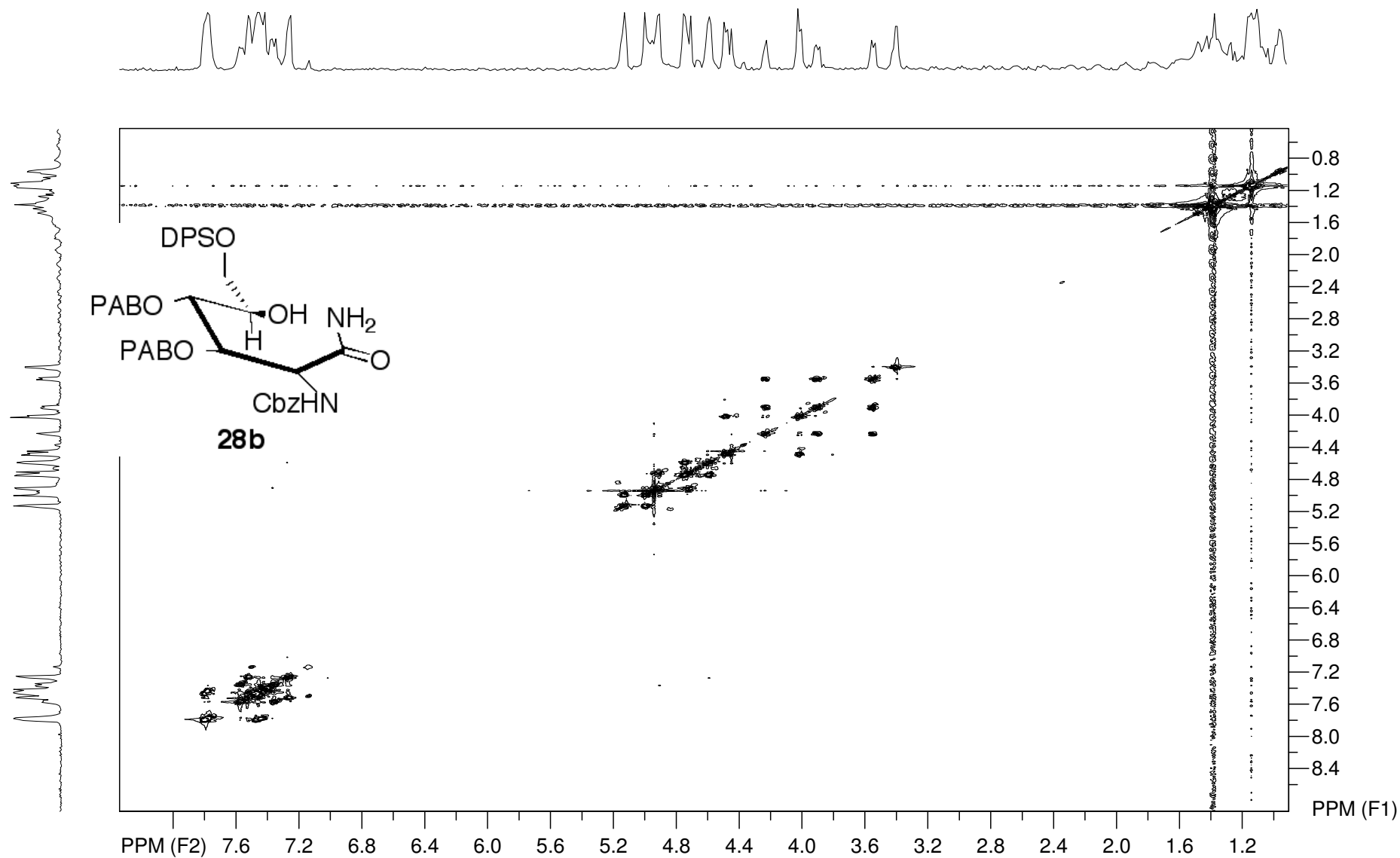
file: ...\\NMR Data\\mostPolAmide_CD3OD\\1\\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 23.291 ppm/cm: 0.03878



file: ...\\NMR Data\\mostPolAmide_CD3OD\\1\\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

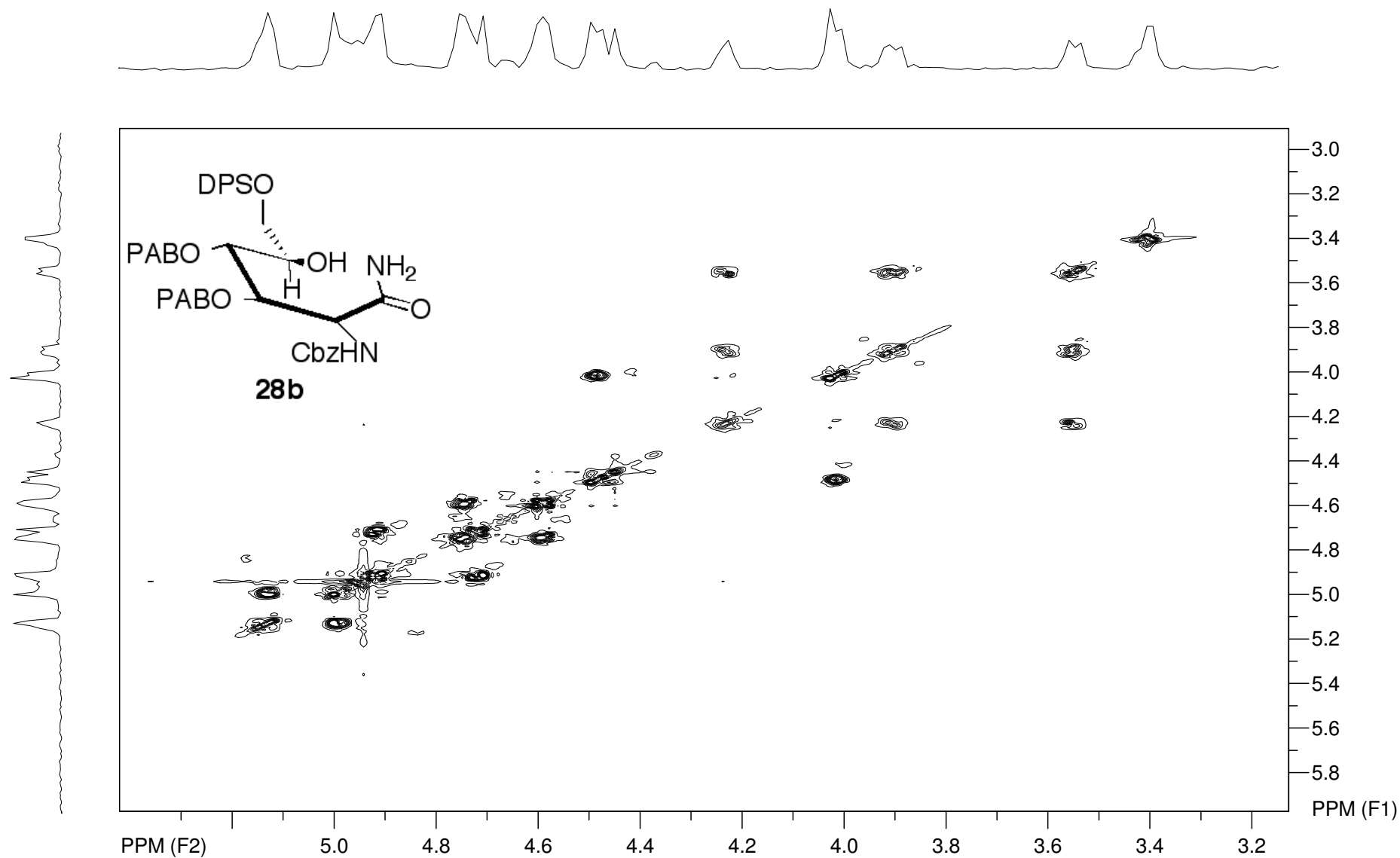
freq. of 0 ppm: 600.550023 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 24.037 ppm/cm: 0.04002



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\mostPolAmide_COSY\1\sF2: freq. of 0 ppm: 600.549962 MHz
transmitter freq.: 600.552832 MHz
time domain size: 2048 by 2048 points
width (F2): 7211.50 Hz = 12.008167 ppm = 3.521242 Hz/pt
number of scans: 2

processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 217.844 ppm/cm: 0.36274

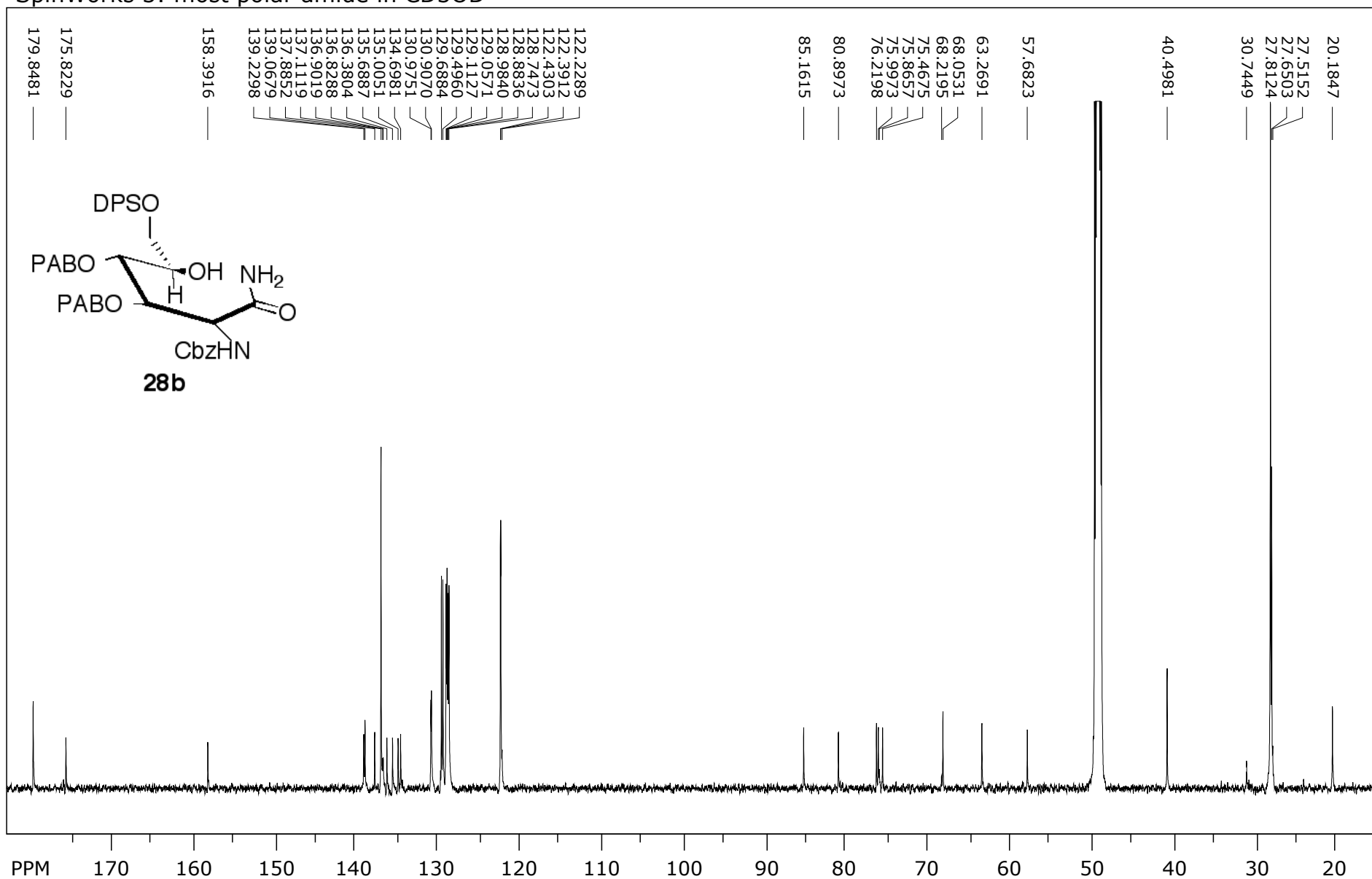
F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 425.708 ppm/cm: 0.70886



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\mostPolAmide_COSY\1\F2: freq. of 0 ppm: 600.549962 MHz
transmitter freq.: 600.552832 MHz
time domain size: 2048 by 2048 points
width (F2): 7211.50 Hz = 12.008167 ppm = 3.521242 Hz/pt
number of scans: 2

processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 67.177 ppm/cm: 0.11186

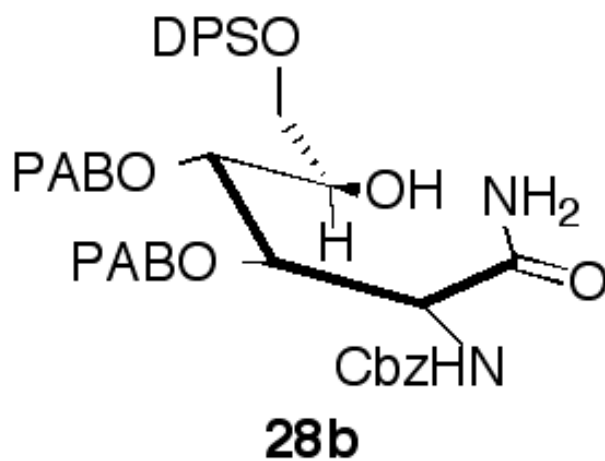
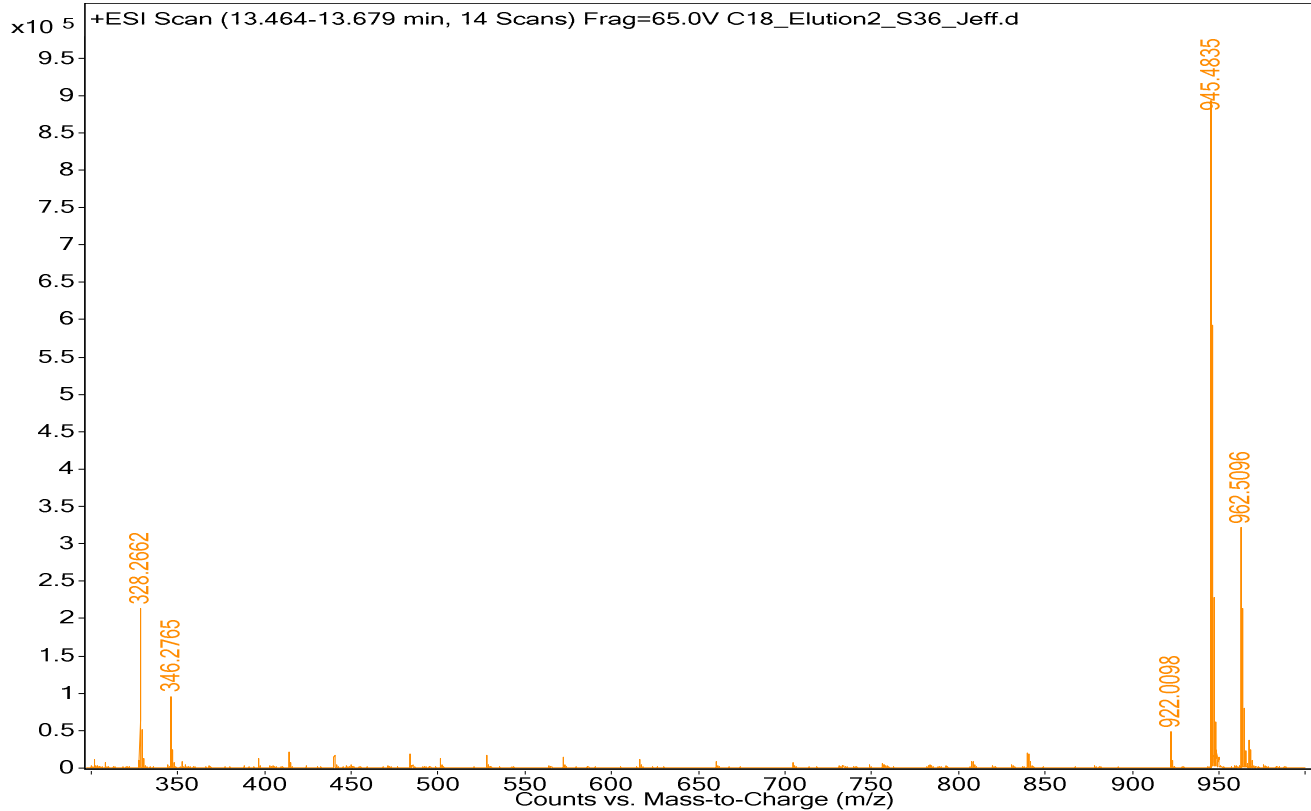
F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 153.578 ppm/cm: 0.25573

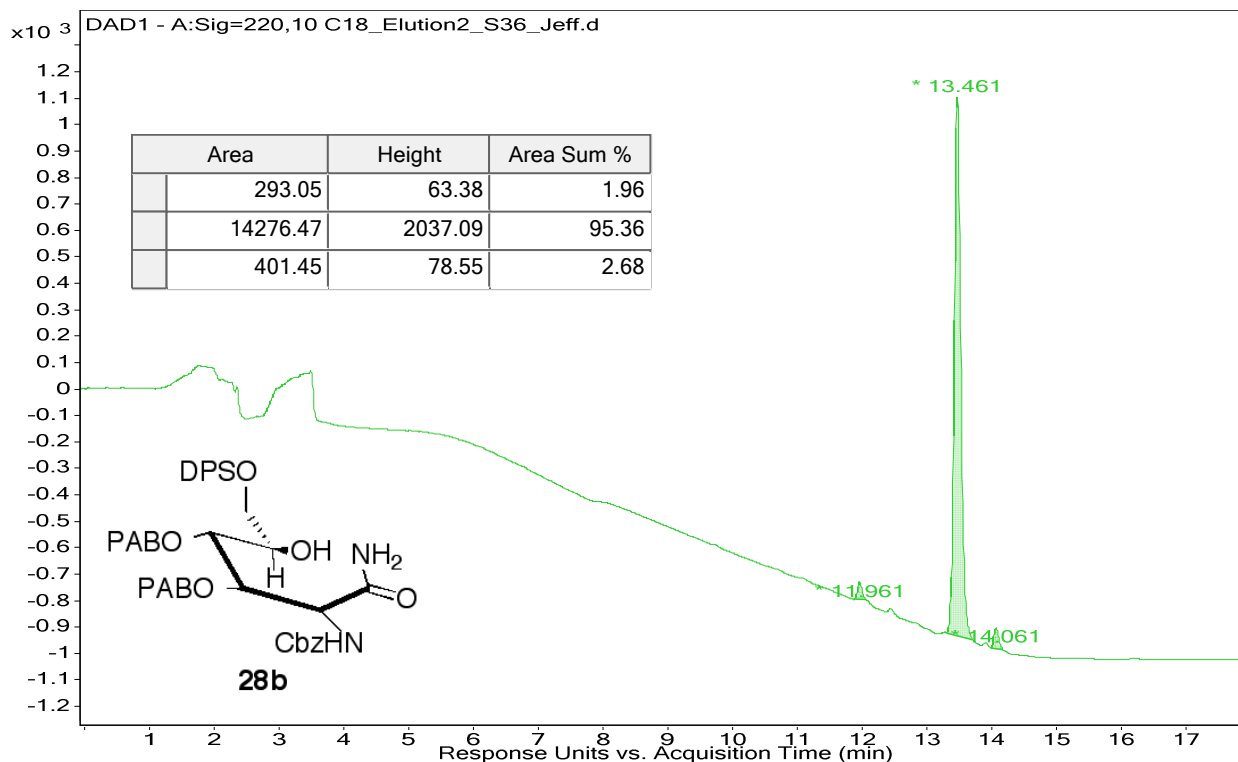


file: ...R Data\mostPolAmide_13CCD3OD\1\fid expt: <zpgg30>
 transmitter freq.: 151.023519 MHz
 time domain size: 65536 points
 width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
 number of scans: 22528

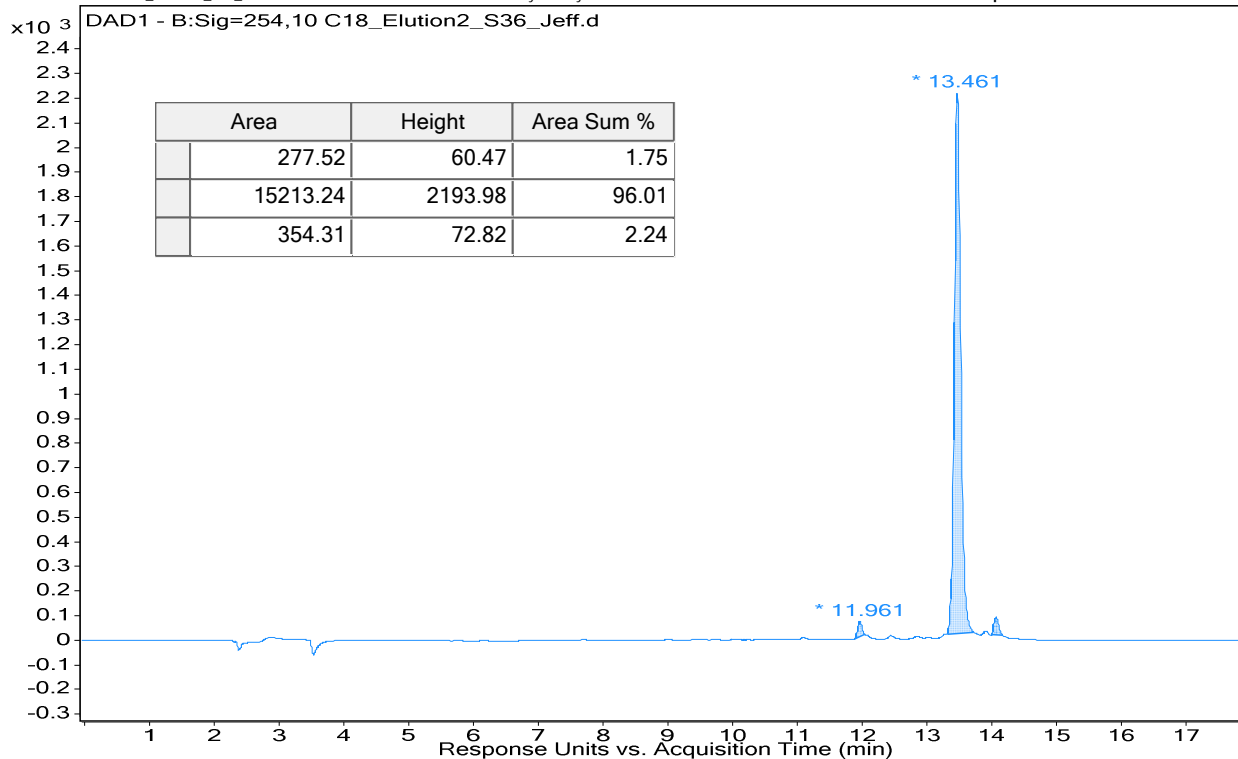
freq. of 0 ppm: 151.008207 MHz
 processed size: 32768 complex points
 LB: 5.000 GF: 0.0000
 Hz/cm: 1018.475 ppm/cm: 6.74382

Sample Name	Jeff-36	Position	Vial 22	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution2_S36_Jef	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/15/2012 9:39:15 AM



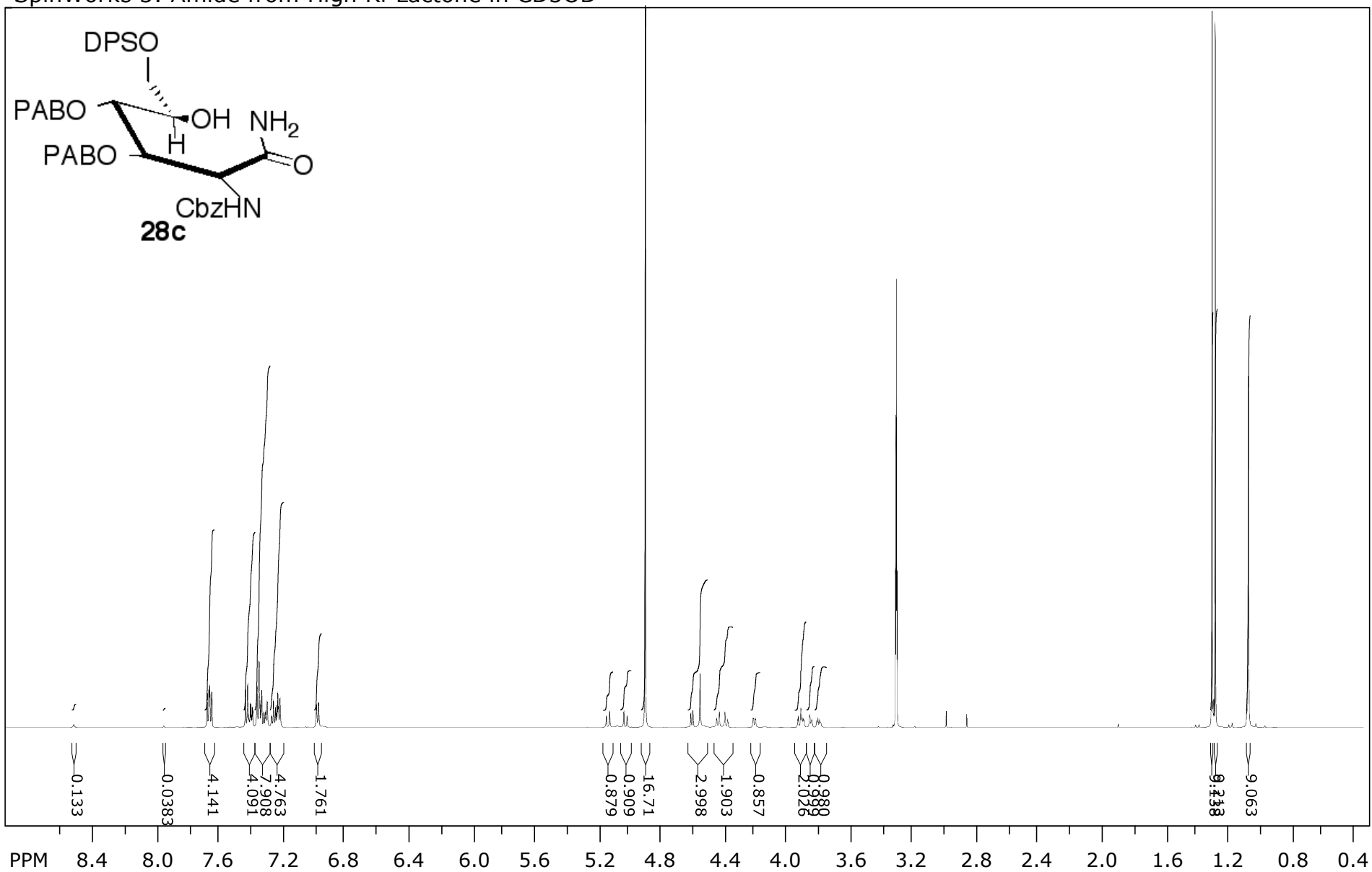


Sample Name	Jeff-36	Position	Vial 22	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution2_S36_Jef	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/15/2012 9:39:15 AM



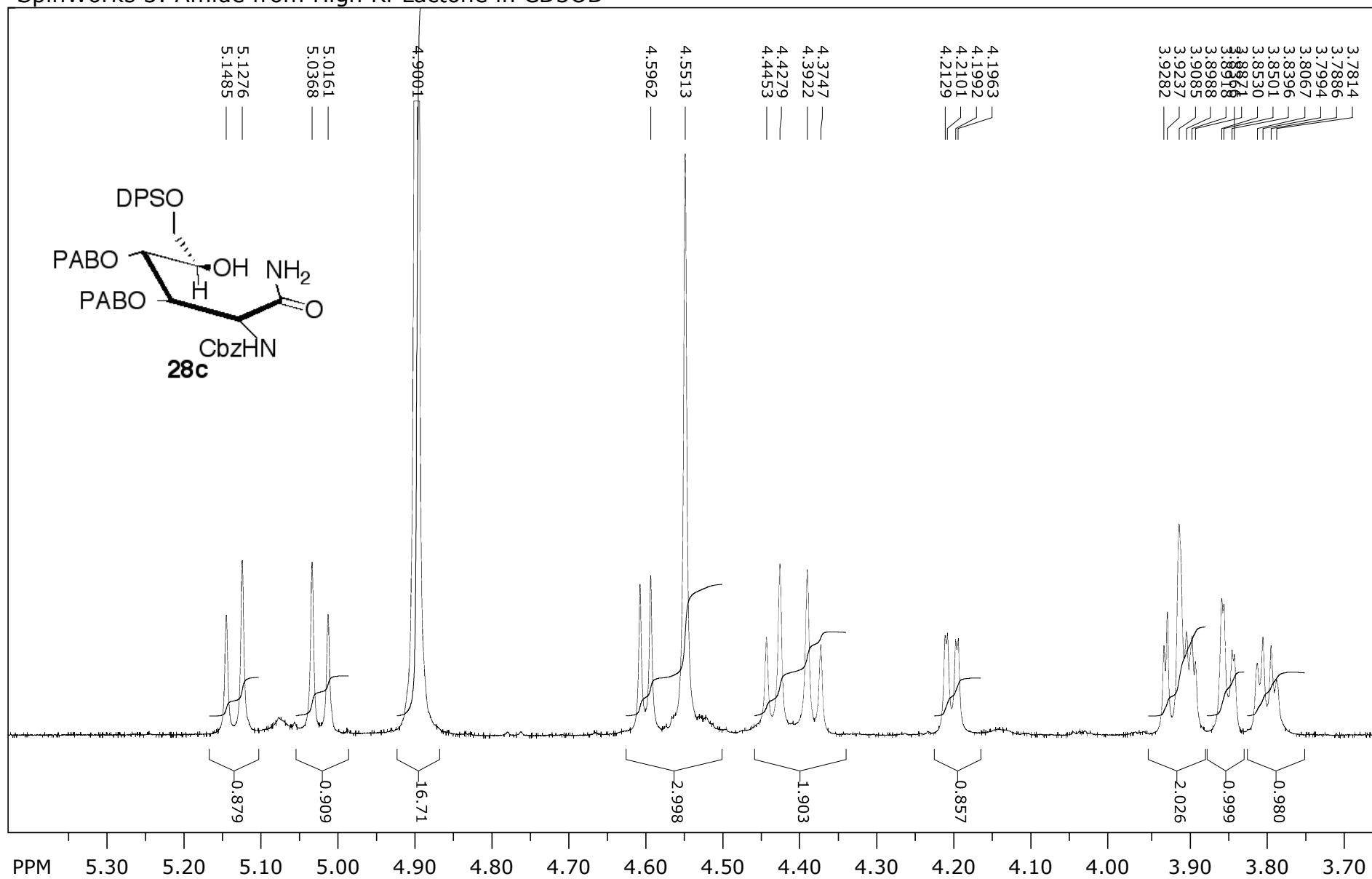
Analysis on a Waters SymmetryShield™ C18 (4.6 mm X 15 cm (i.d. x l.), 3.5 μm) at 0.5 mL/min. Solvent A: 50 mM NH₄OAc (aq); B: CH₃CN

Time (min)	% B
0	20
1	20
10	100
20	100



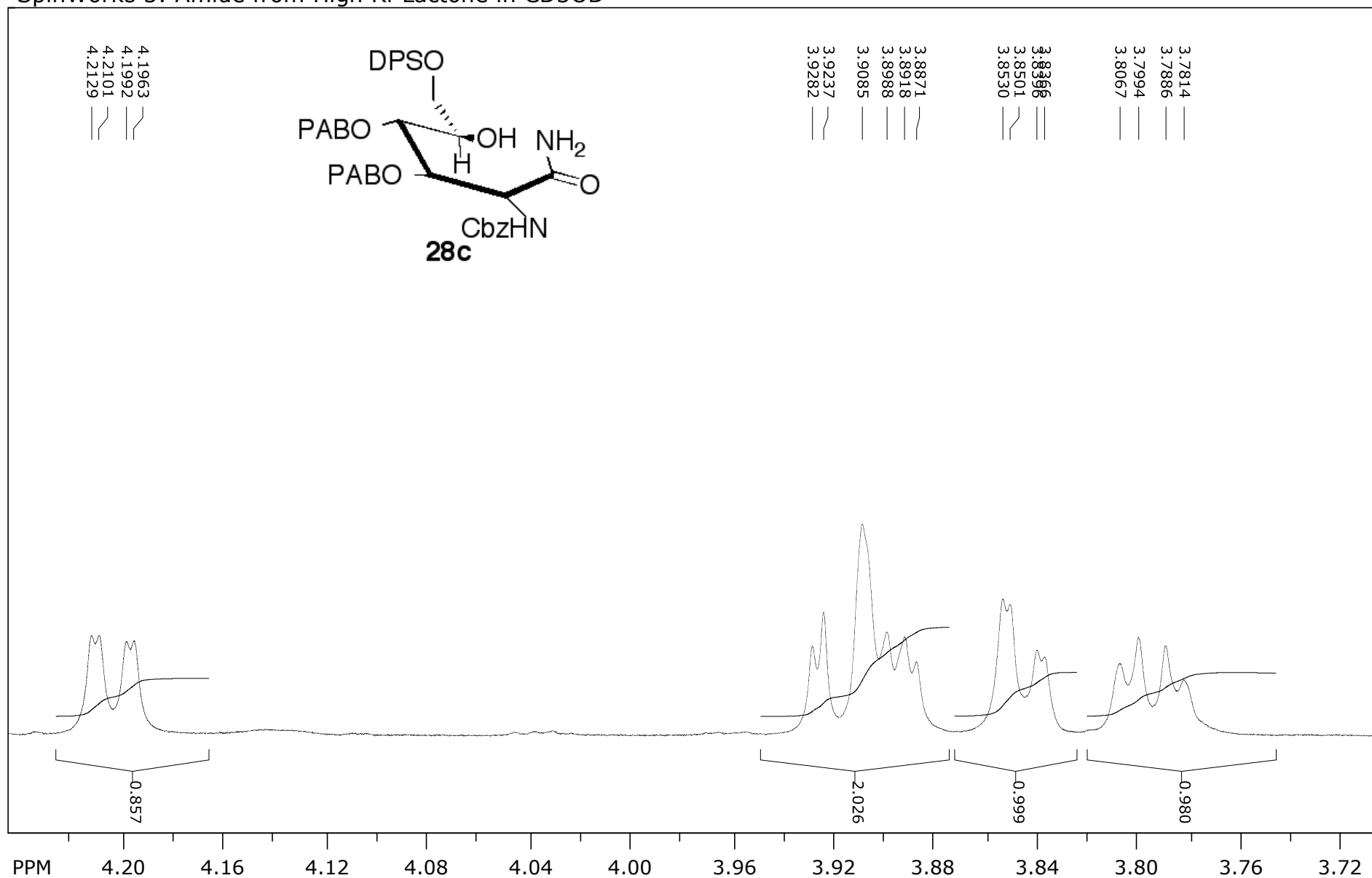
file: ...er\NMR Data\AmFrHi_pk1_CD3OD\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 208.098 ppm/cm: 0.34651



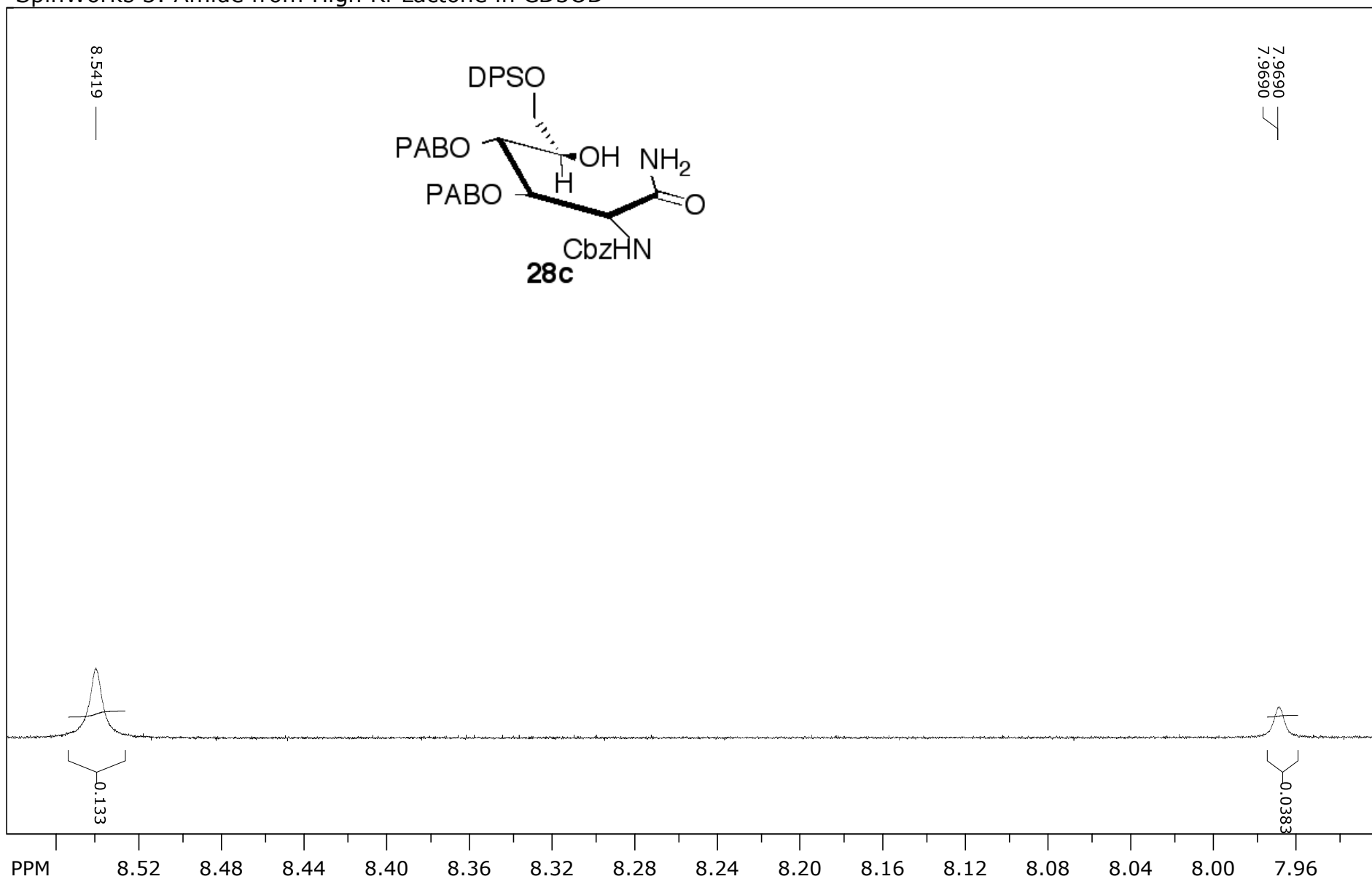
file: ...er\NMR Data\AmFrHi_pk1_CD3OD\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550023 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 42.806 ppm/cm: 0.07128



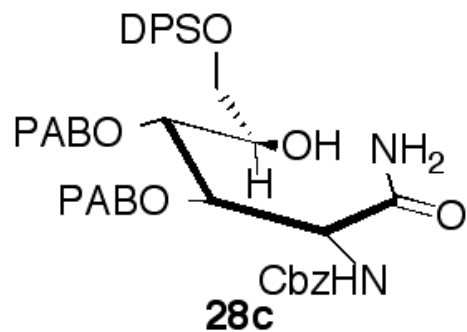
file: ...er\NMR Data\AmFrHi_pk1_CD3OD\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550023 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 13.004 ppm/cm: 0.02165

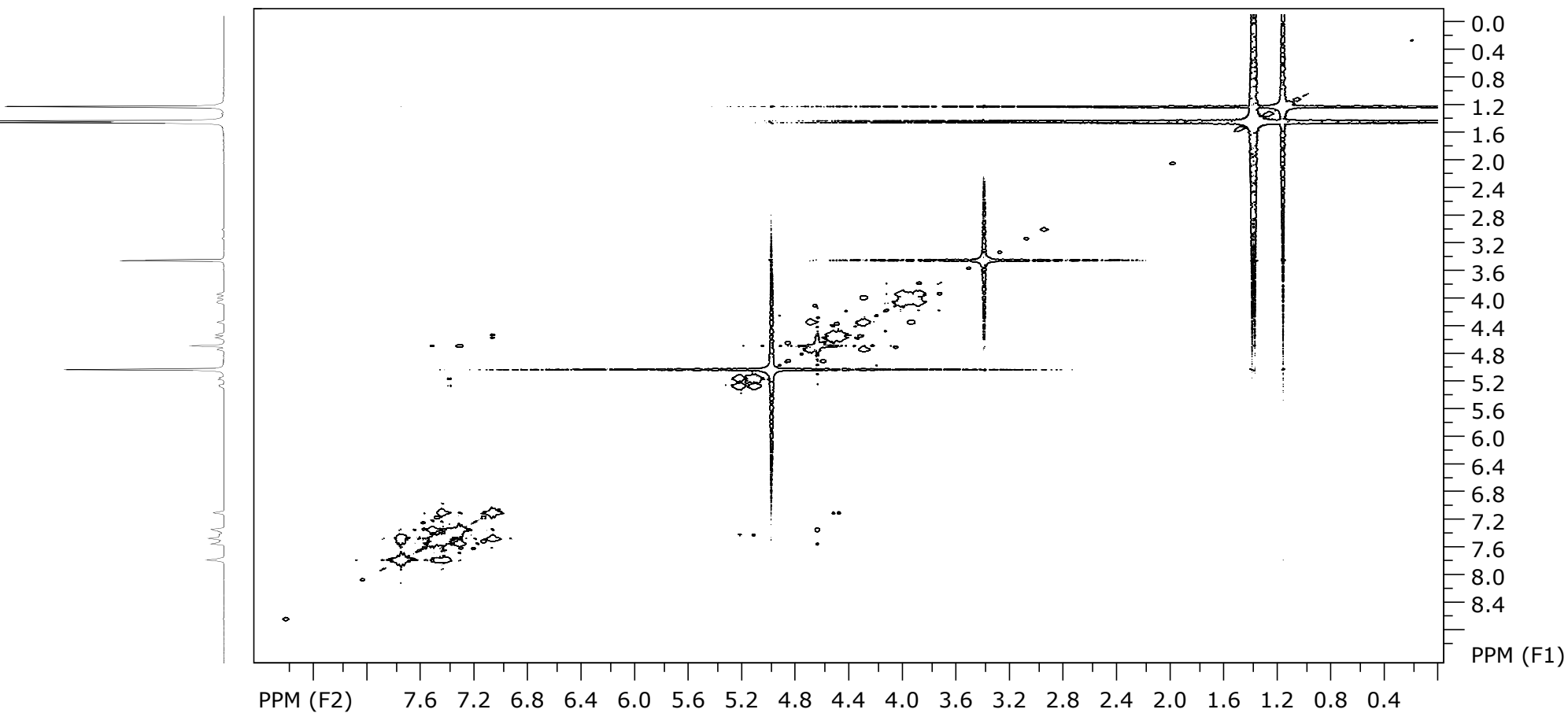
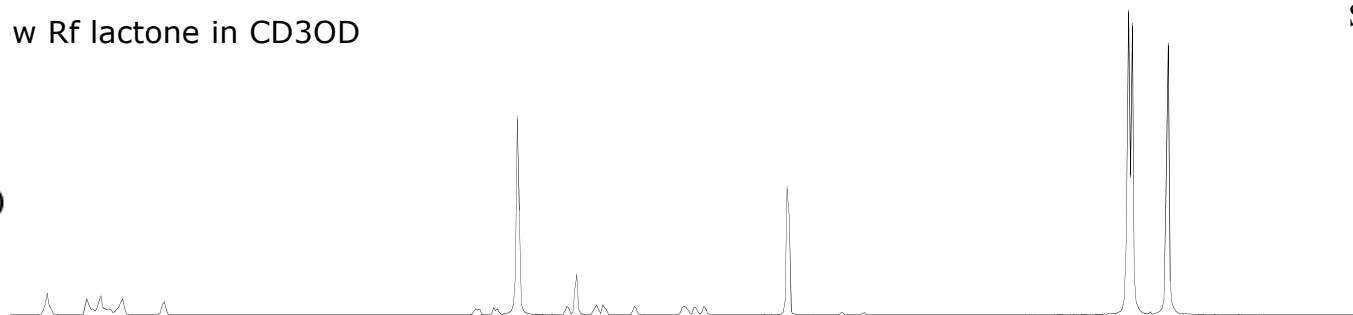


file: ...er\NMR Data\AmFrHi_pk1_CD3OD\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 15.977 ppm/cm: 0.02660



w Rf lactone in CD3OD

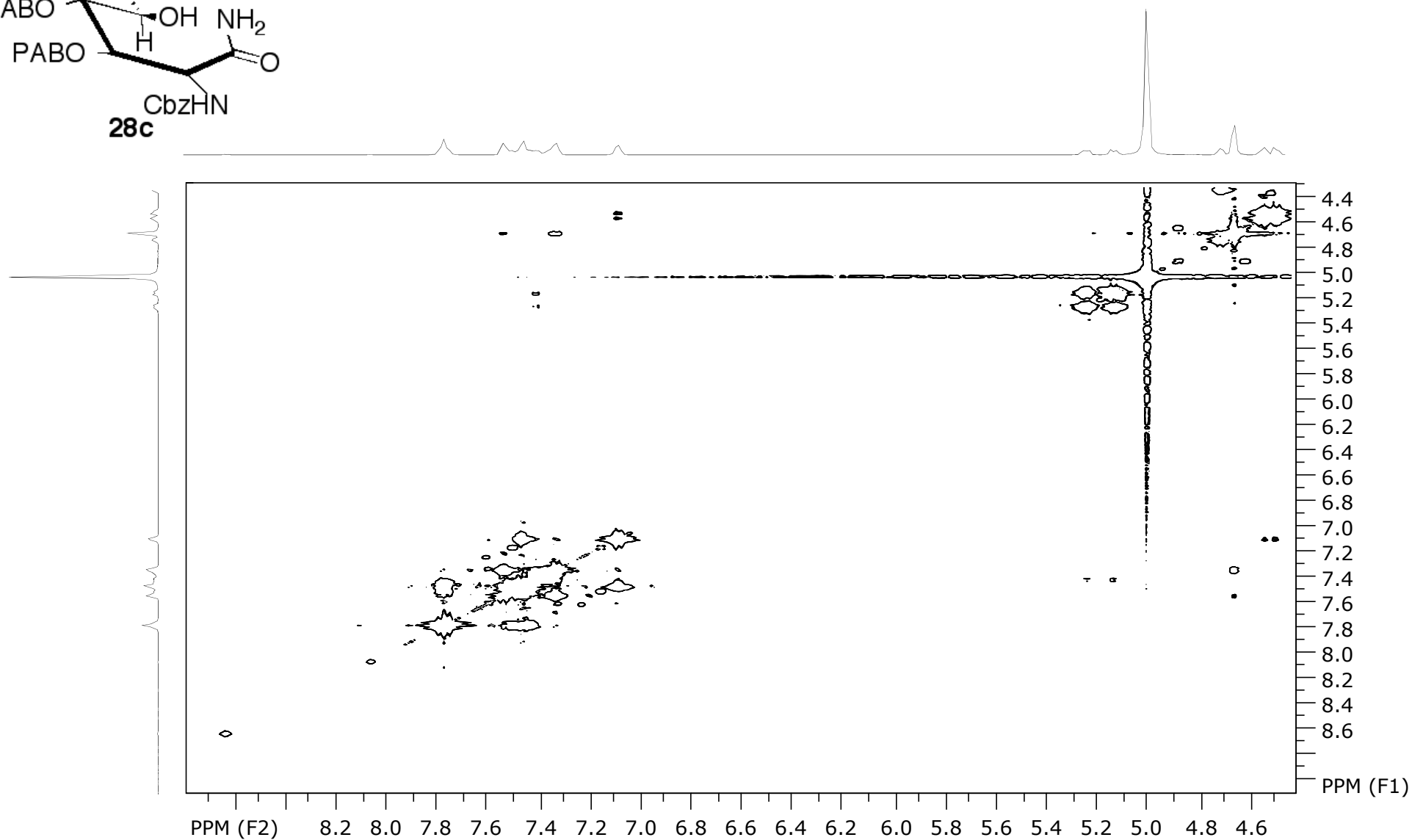
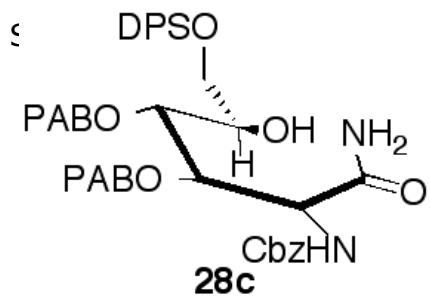


file: ...lder\NMR Data\AmFrHi_pk1COSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
 number of scans: 2

F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 267.023 ppm/cm: 0.44463

F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 516.915 ppm/cm: 0.86073

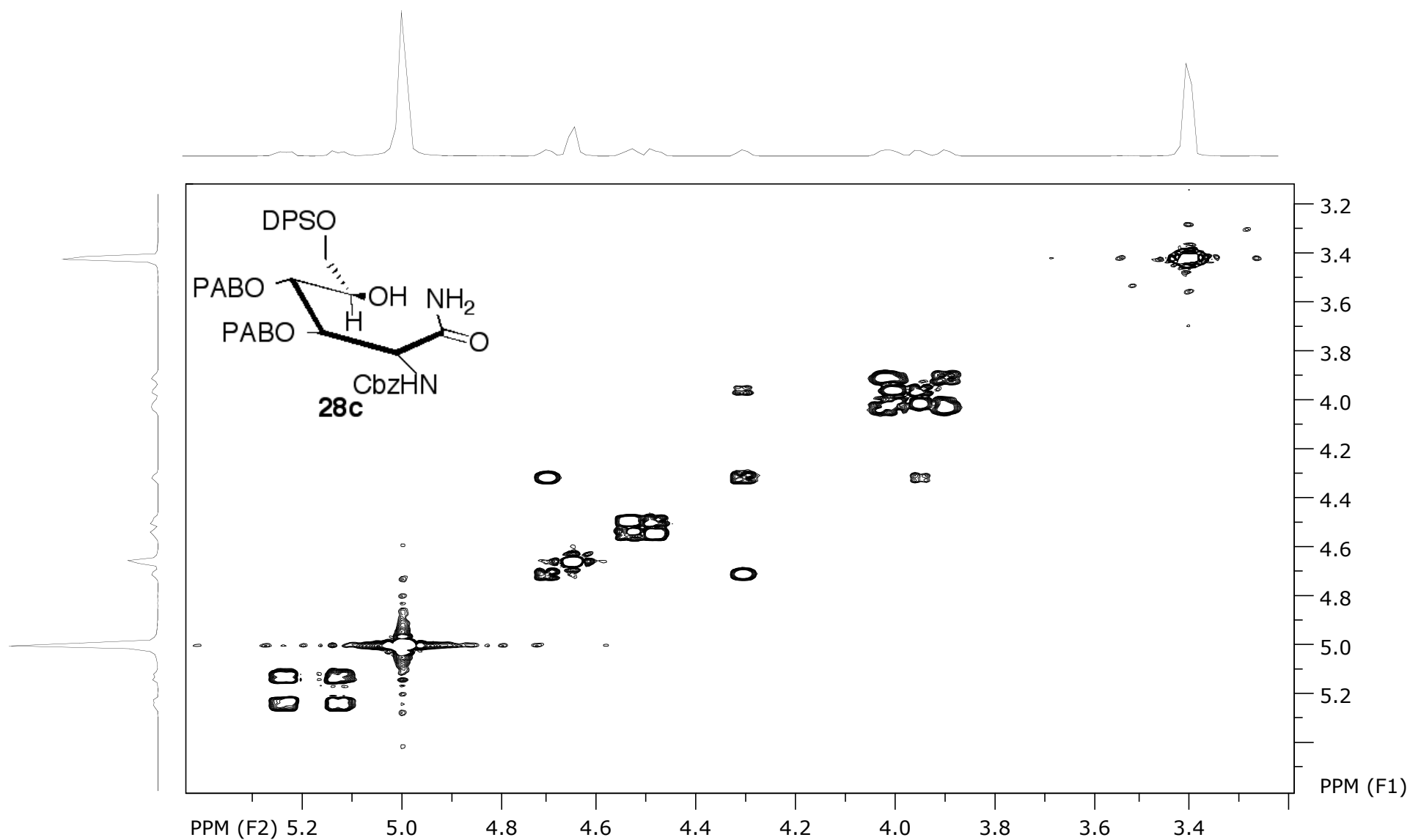
low Rf lactone in CD3OD



file: ...lder\NMR Data\AmFrHi_pk1COSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
 number of scans: 2

F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 131.274 ppm/cm: 0.21859

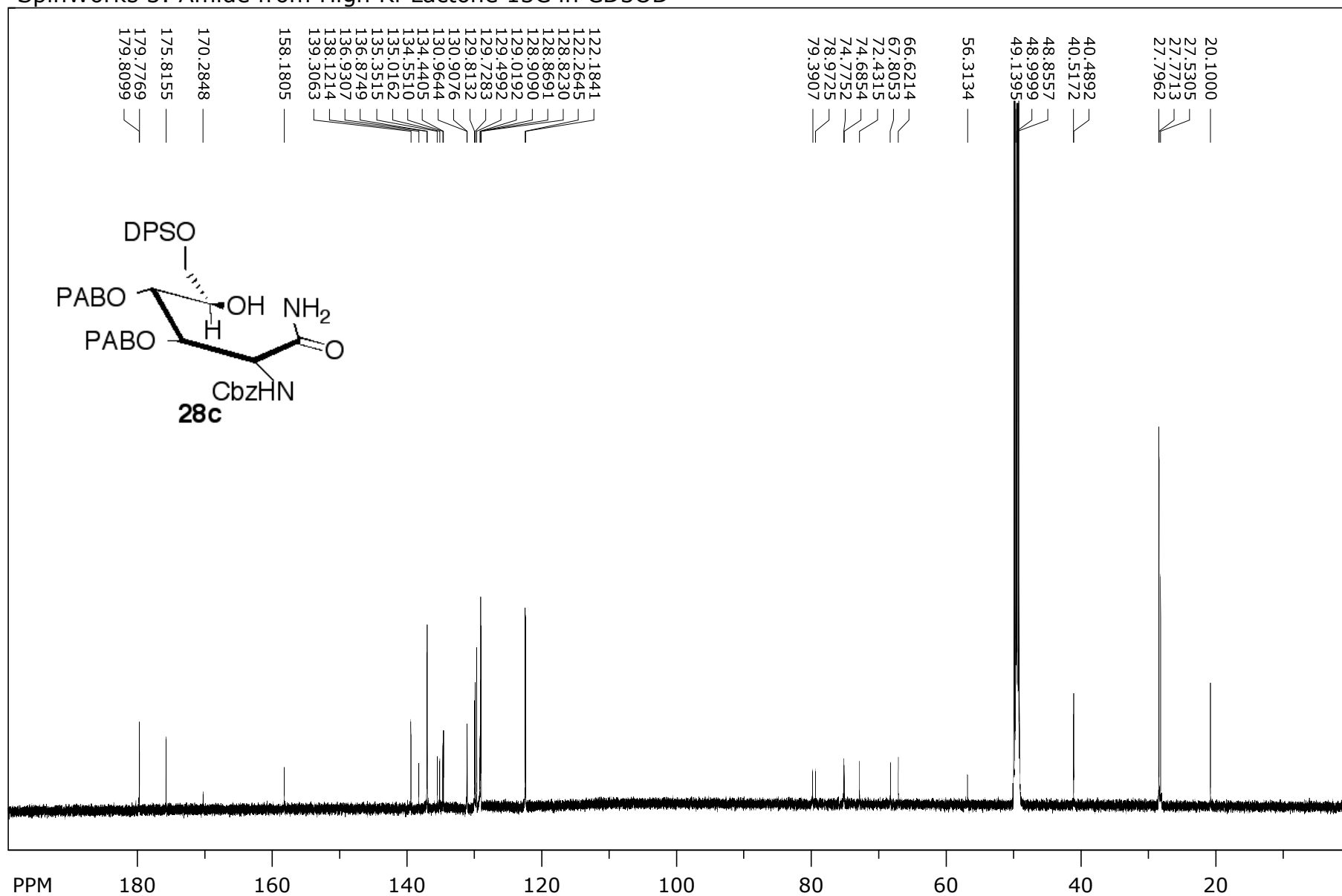
F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 263.394 ppm/cm: 0.43859



file: ...lder\NMR Data\AmFrHi_pk1COSY\1\ser
expt: <cosygpqf>
transmitter freq: 600.552832 MHz
time domain size: 2048 by 1024 points
width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
number of scans: 2

F2: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 67.332 ppm/cm: 0.11212

F1: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 135.949 ppm/cm: 0.22637

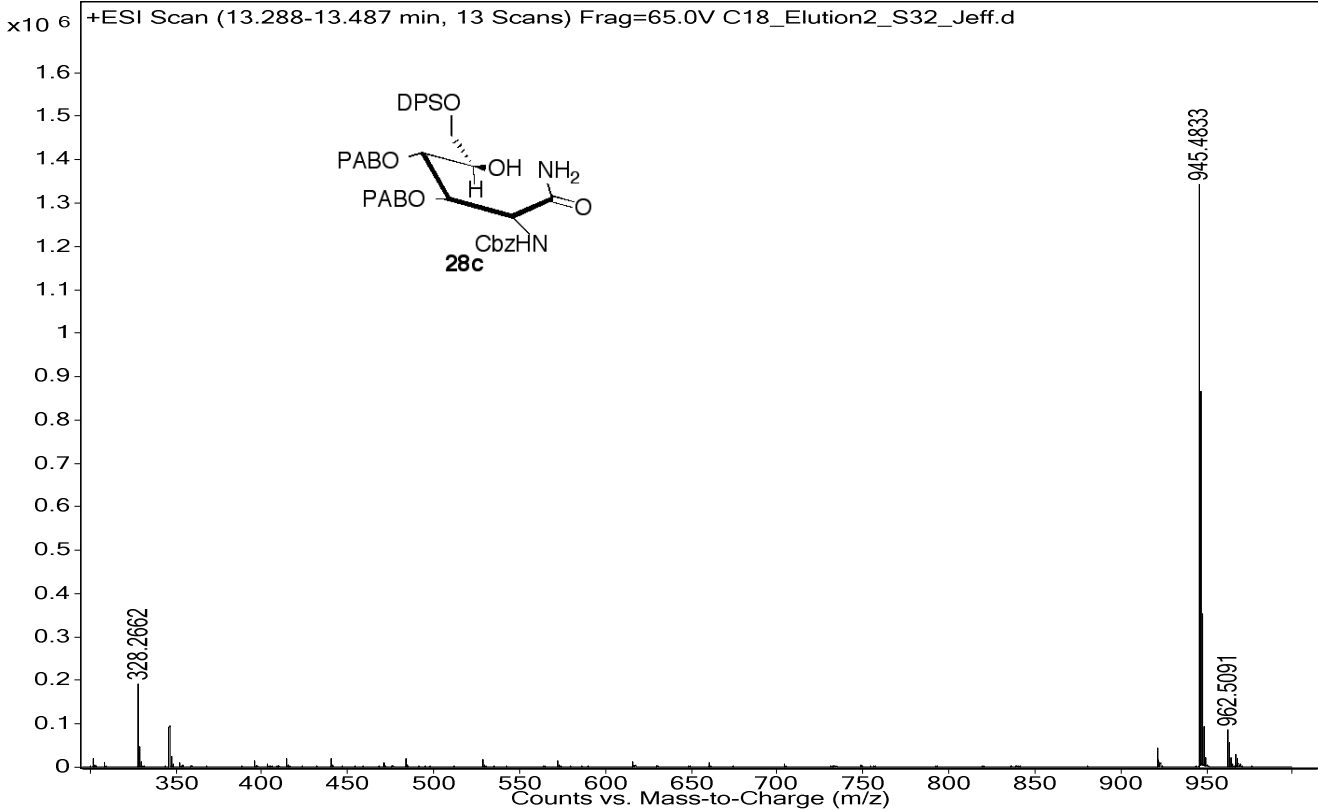


file: ...NMR Data\AmFrHi_pk1_13CCD3OD\2\fid exp: <zggp30>
 transmitter freq.: 151.023518 MHz
 time domain size: 65536 points
 width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
 number of scans: 15360

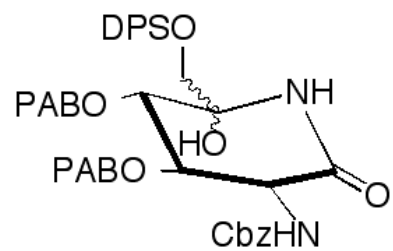
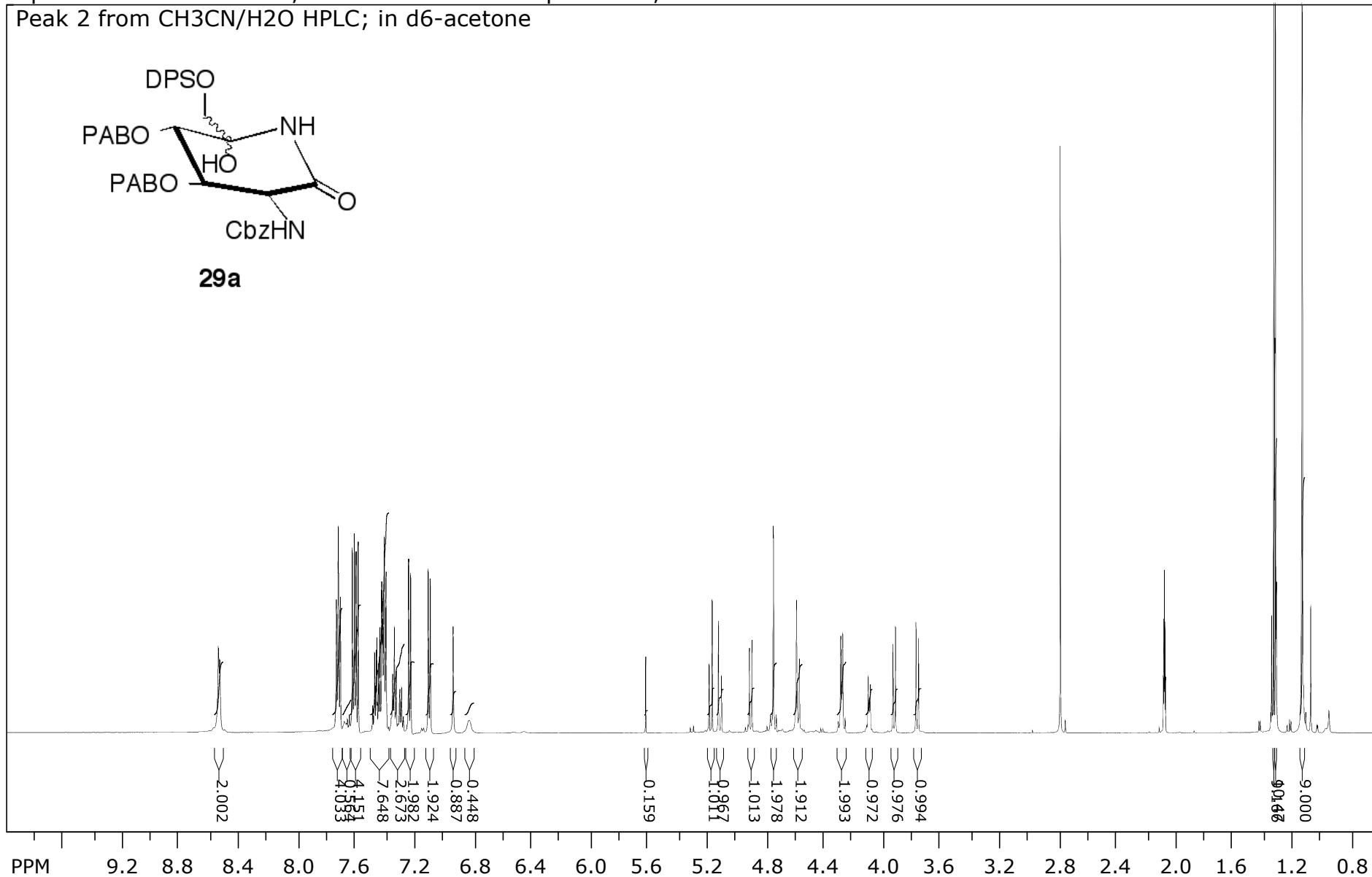
freq. of 0 ppm: 151.008207 MHz
 processed size: 32768 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 1259.307 ppm/cm: 8.33848

Sample Name	Jeff-32	Position	Vial 18	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution2_S32_Jef	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/15/2012 7:25:59 AM

9-146



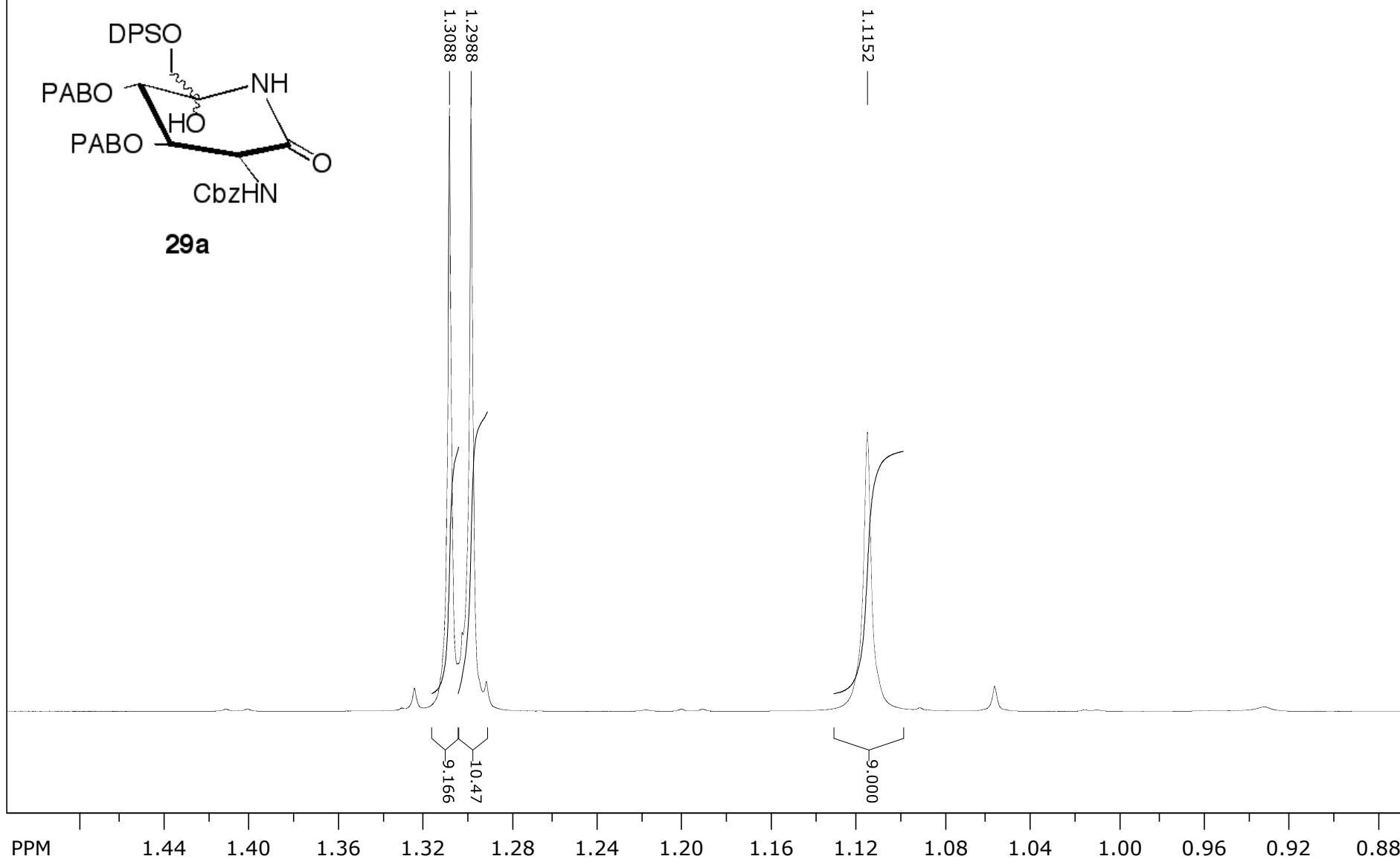
Peak 2 from CH3CN/H2O HPLC; in d6-acetone

**29a**

file: ...\\NMR Data\\OxAm055_pk2_d6Acet\\1\\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 226.443 ppm/cm: 0.37706

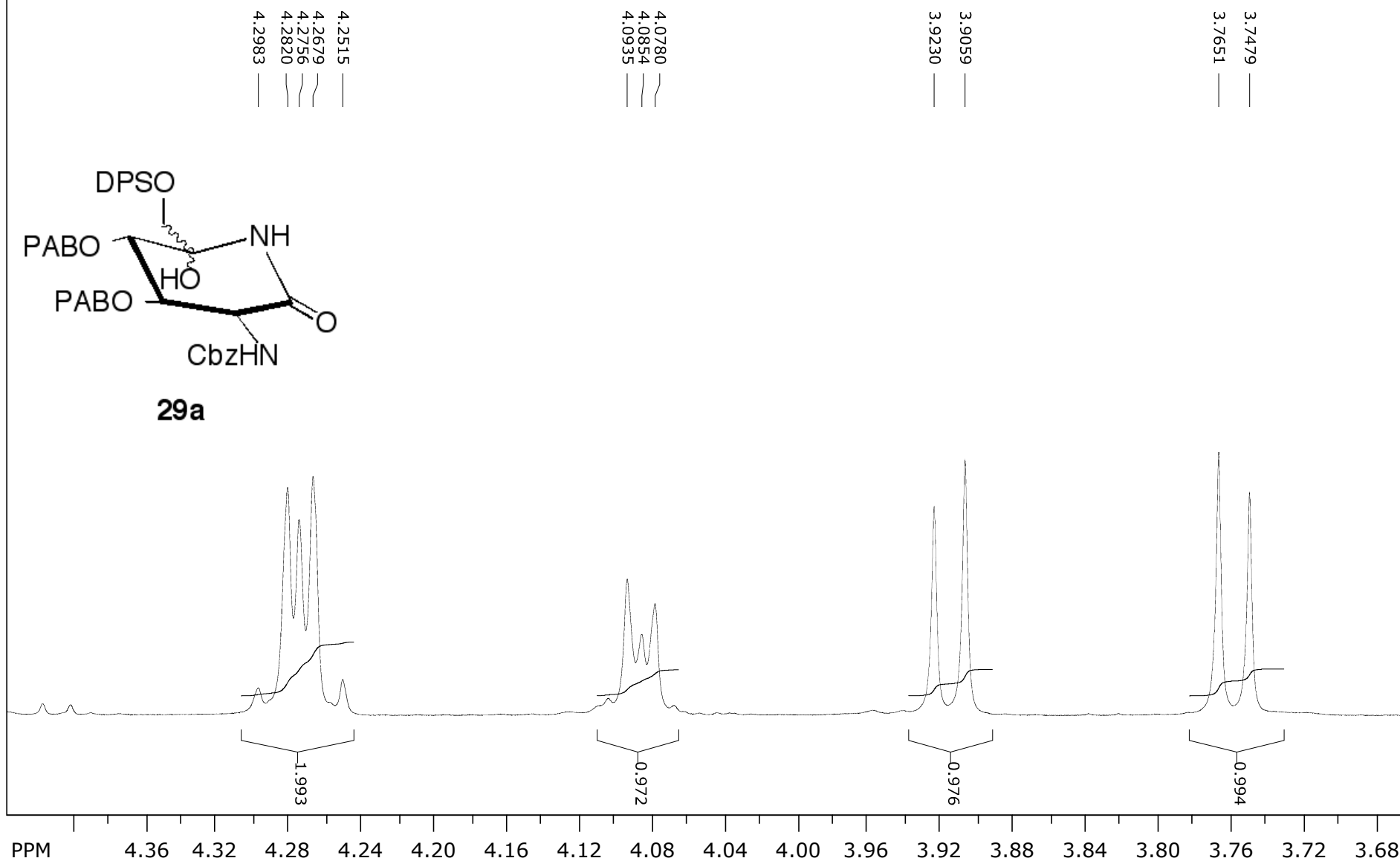
Peak 2 from CH3CN/H2O HPLC; in d6-acetone



file: ...\\NMR Data\\OxAm055_pk2_d6Acet\\1\\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 15.578 ppm/cm: 0.02594

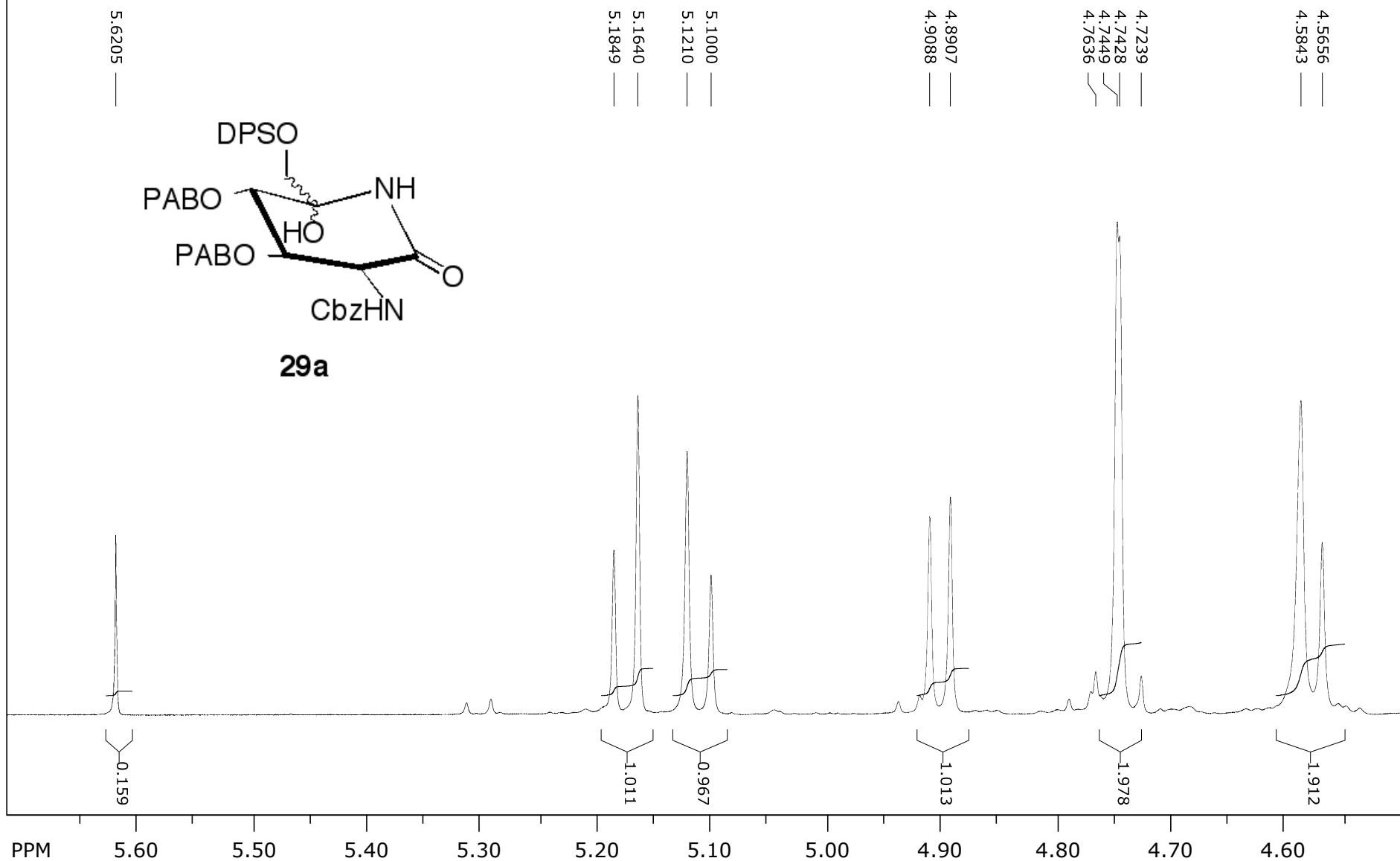
Peak 2 from CH3CN/H2O HPLC; in d6-acetone



file: ...\\NMR Data\\OxAm055_pk2_d6Acet\\1\\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 18.653 ppm/cm: 0.03106

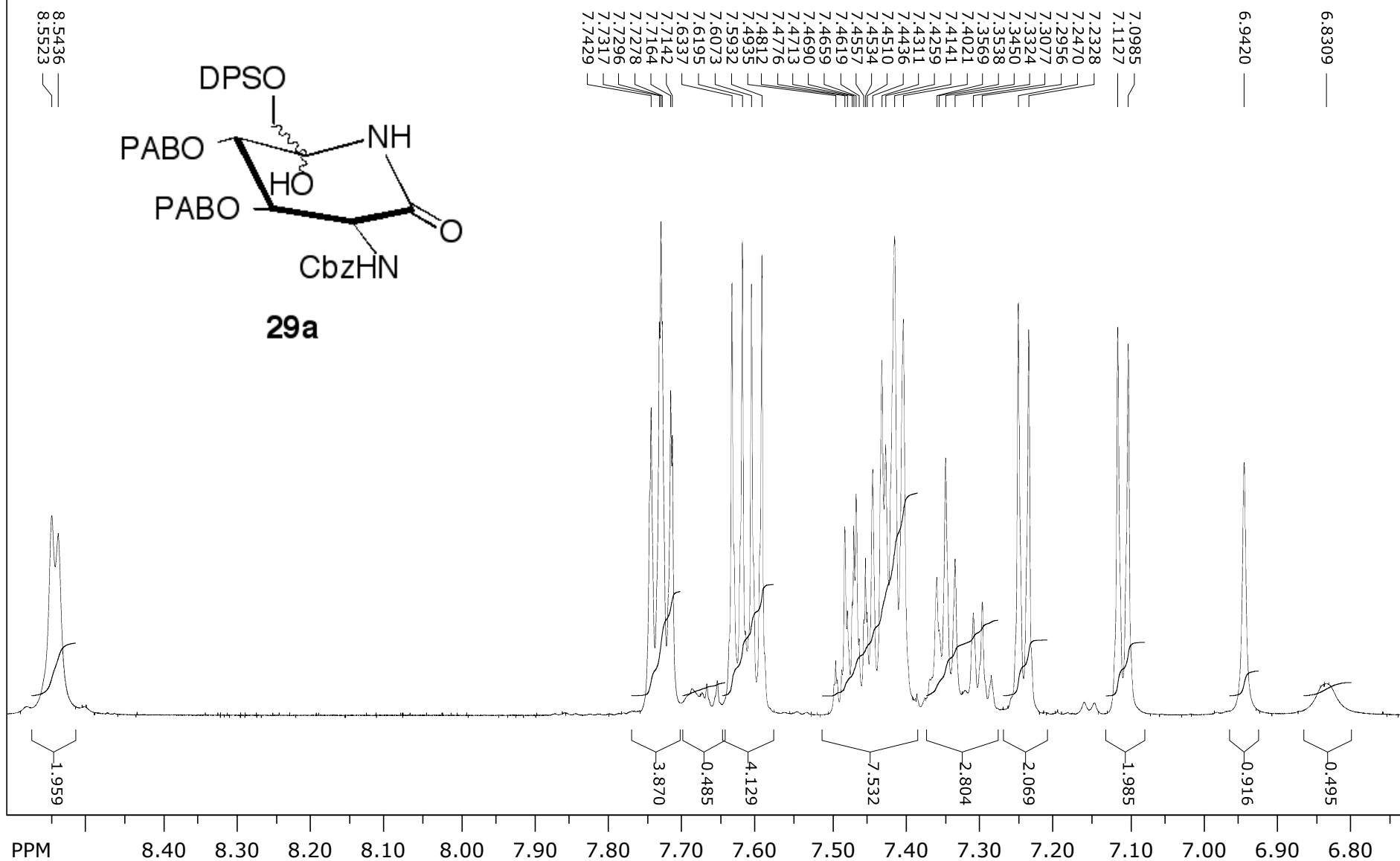
Peak 2 from CH3CN/H2O HPLC; in d6-acetone



file: ...\\NMR Data\\OxAm055_pk2_d6Acet\\1\\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

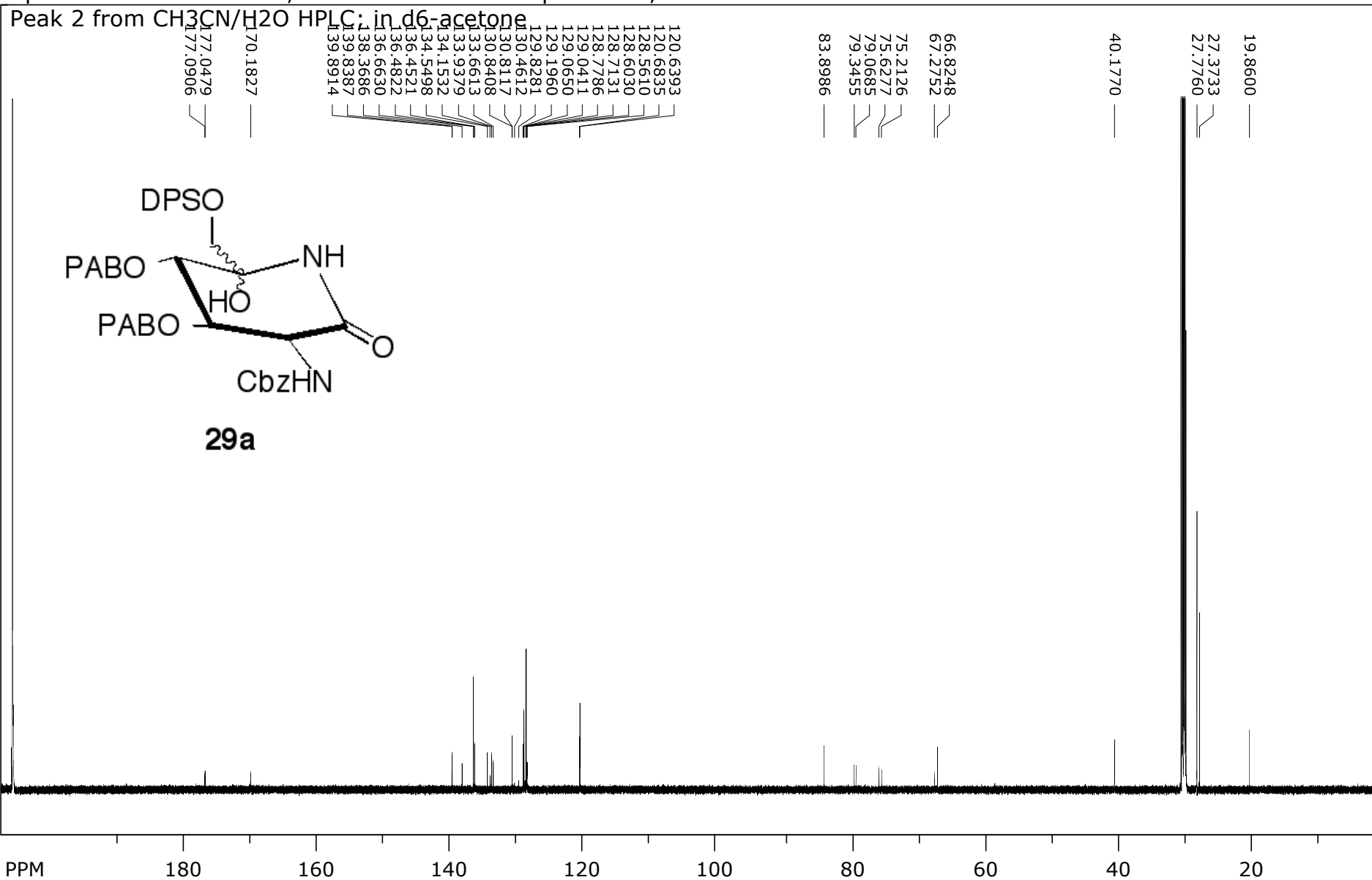
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 29.406 ppm/cm: 0.04897

Peak 2 from CH3CN/H2O HPLC; in d6-acetone



file: ...\\NMR Data\\OxAm055_pk2_d6Acet\\1\\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

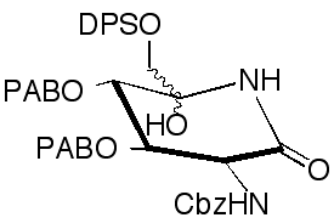
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 45.419 ppm/cm: 0.07563



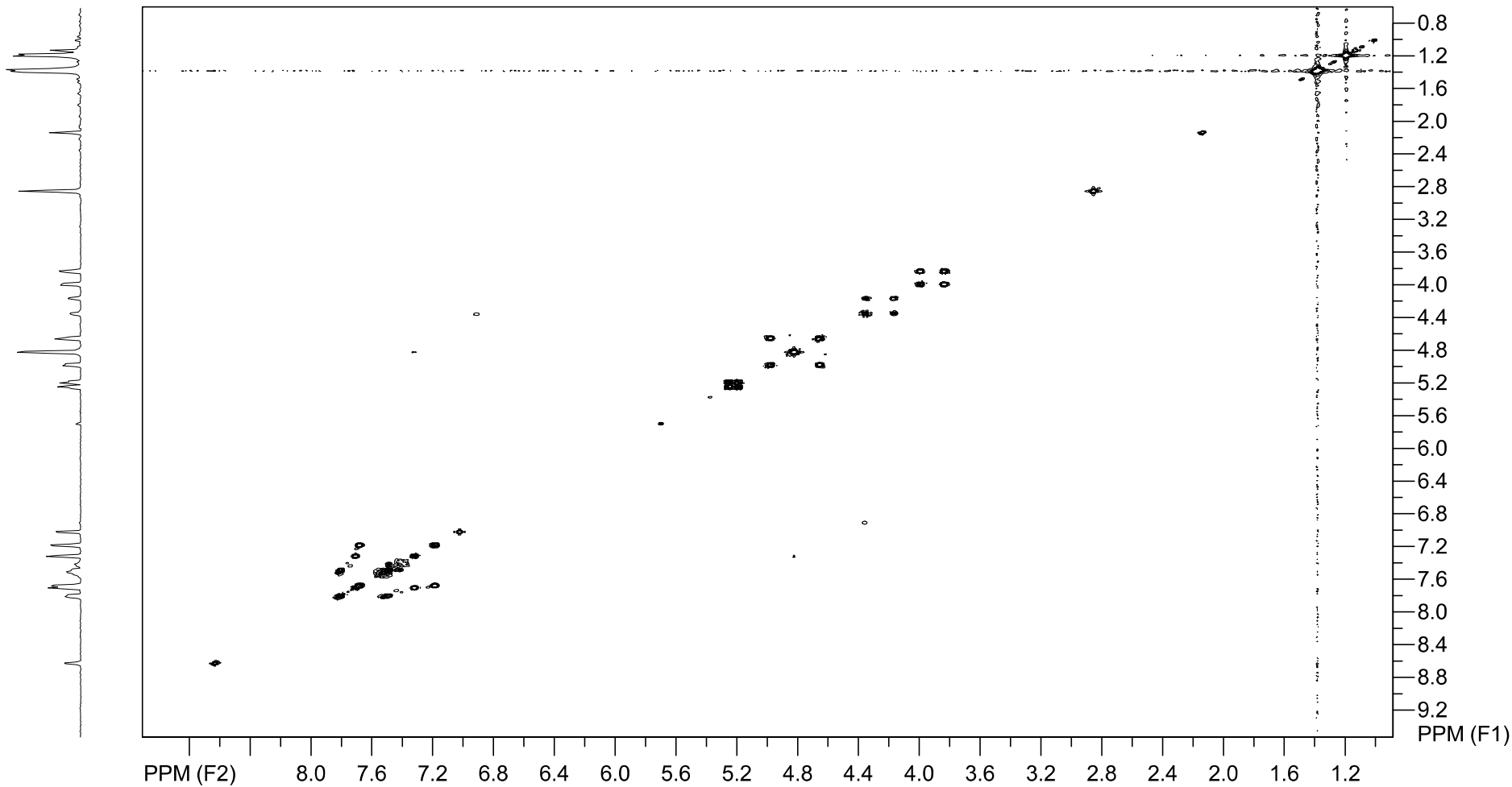
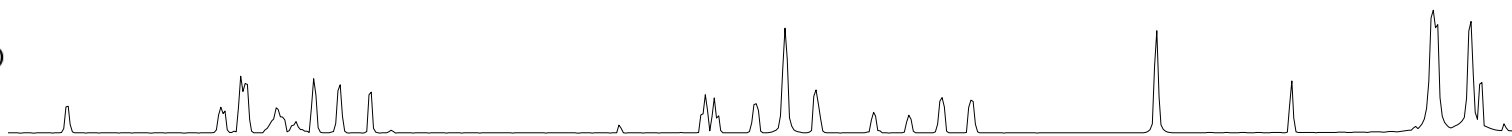
file: ...R Data\OxAm055_pk2_13Cd6Acet\1\fid expt: <zgpg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 28672

freq. of 0 ppm: 151.008282 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1252.593 ppm/cm: 8.29403

2: 6-tBDPS-3,4-PAB2-5-oxo lactam precursor; Rf 0.55 ; Peak 2 ACN/H2O HPLC d6 aceton



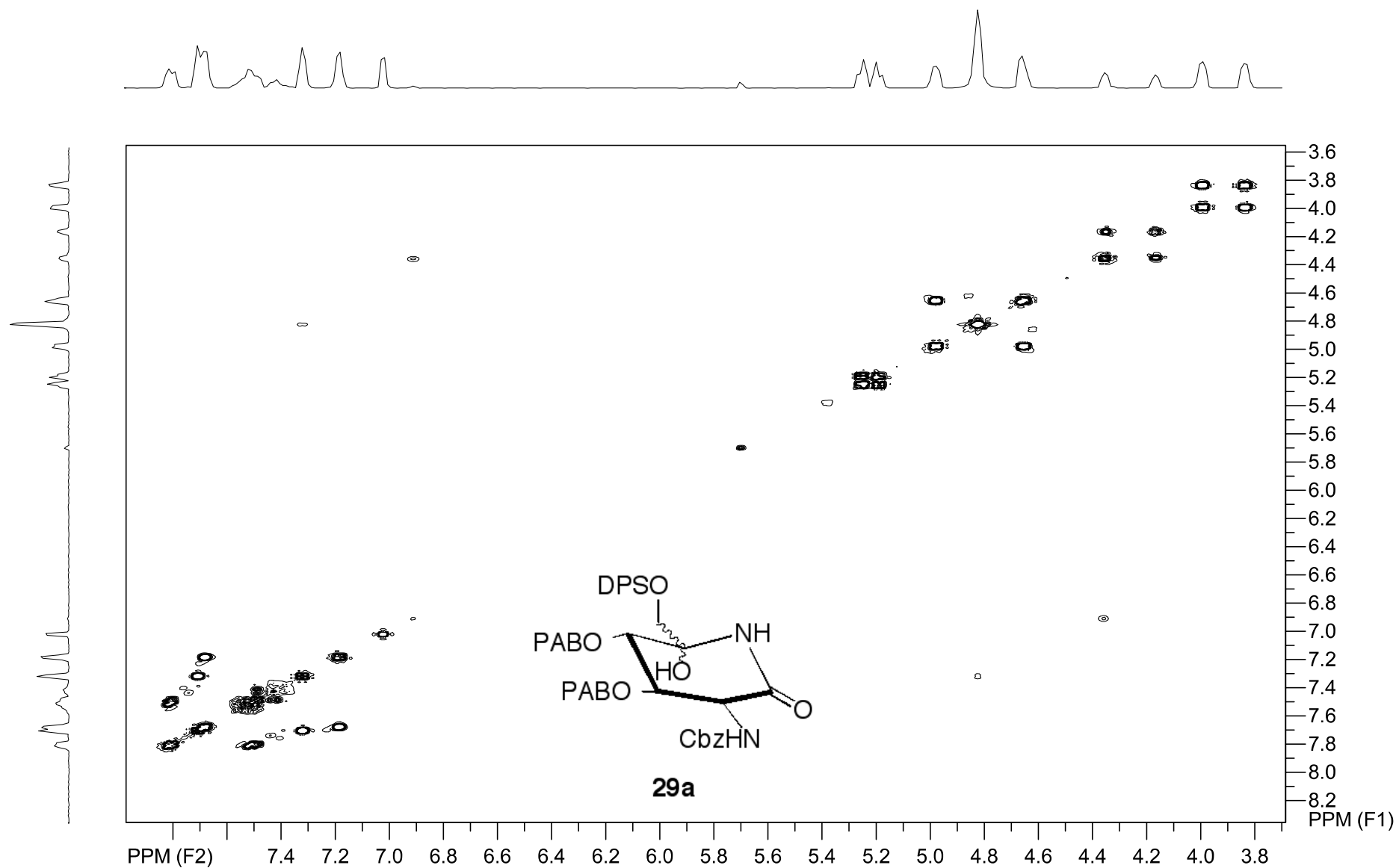
29a



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\OxAm055pk2_COSY\1\ser exp: <cosygpqf>
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.50 Hz = 12.008167 ppm = 3.521242 Hz/pt
 number of scans: 2

F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 240.911 ppm/cm: 0.40115

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 446.903 ppm/cm: 0.74415

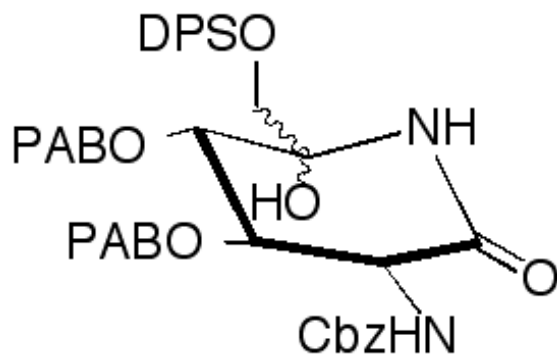
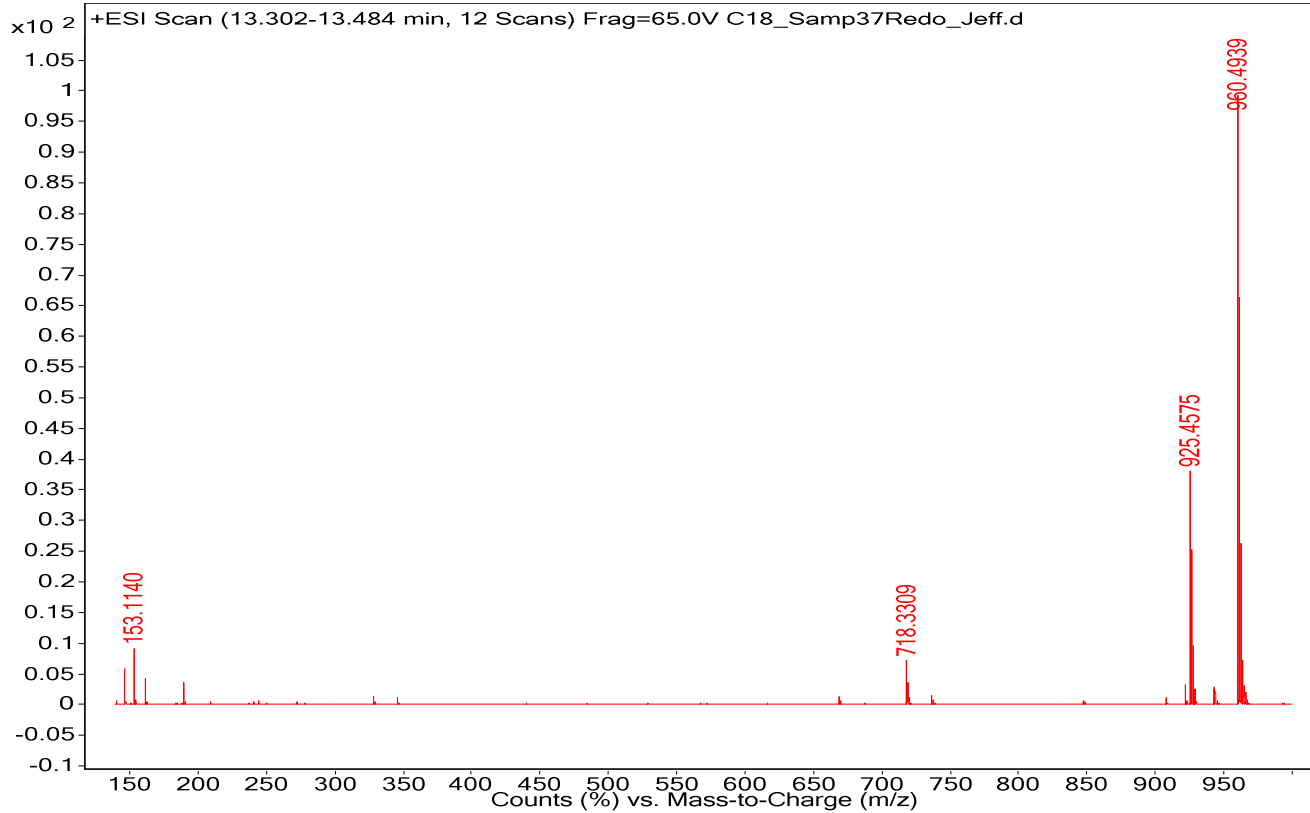


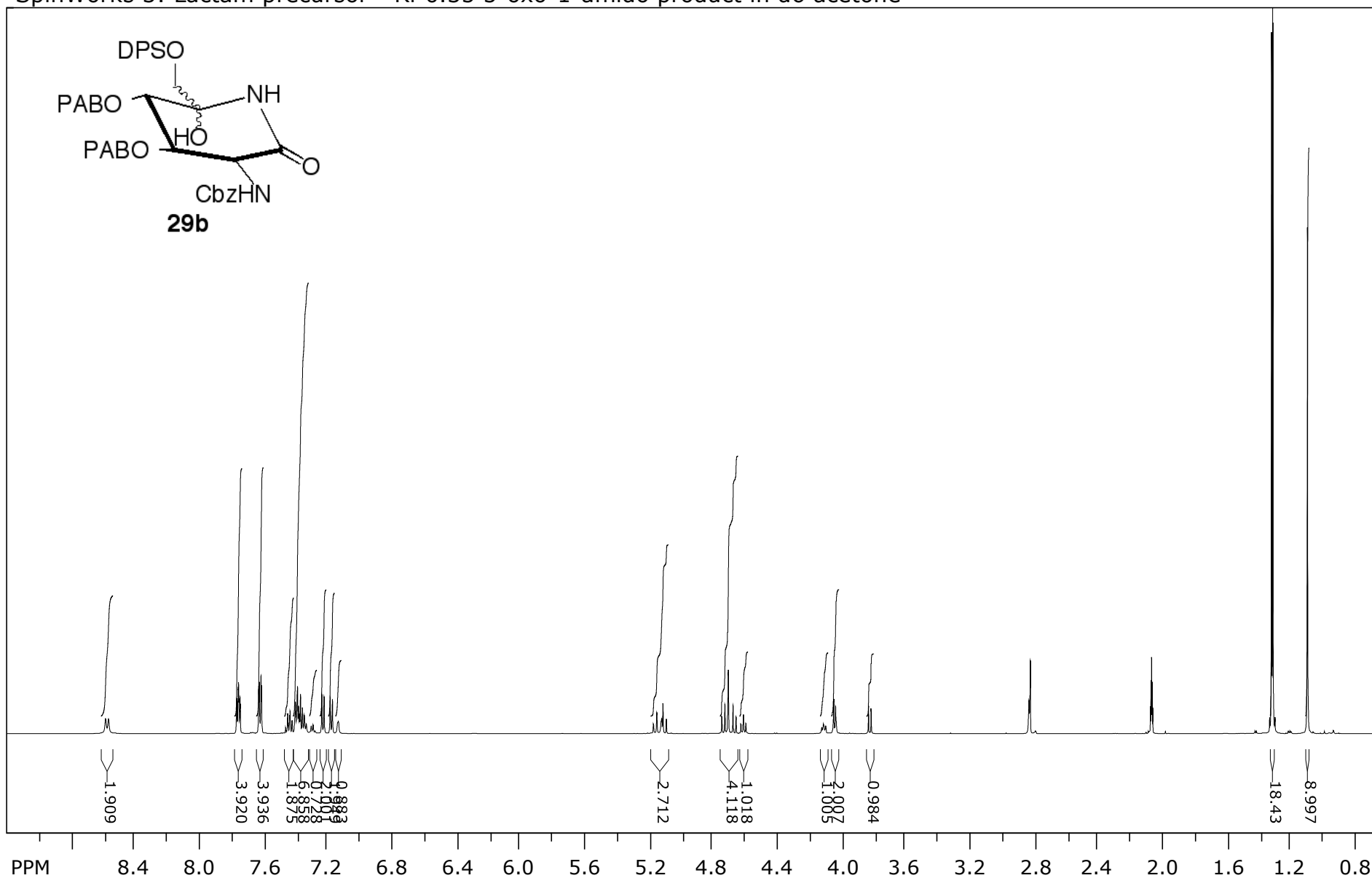
file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\OxAm055pk2_COSY\1\ser exp: <cosygpqf>
transmitter freq.: 600.552832 MHz
time domain size: 2048 by 1024 points
width (F2): 7211.50 Hz = 12.008167 ppm = 3.521242 Hz/pt
number of scans: 2

F2: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 125.602 ppm/cm: 0.20914

F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 240.439 ppm/cm: 0.40036

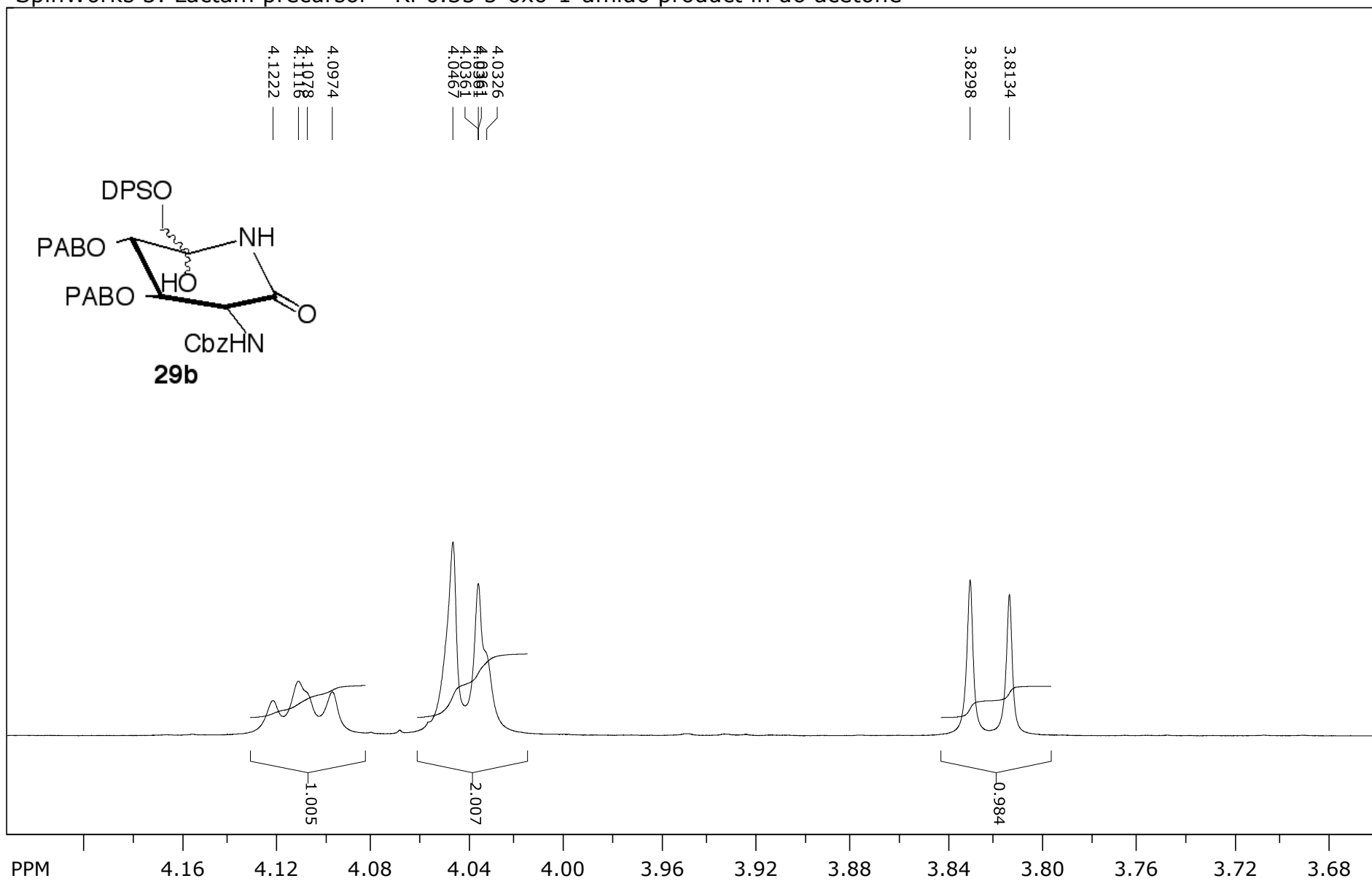
Sample Name	Sample37 redo	Position	Vial 13	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	3	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Samp37Redo_Jeff.	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/20/2012 8:13:26 AM

**29a**



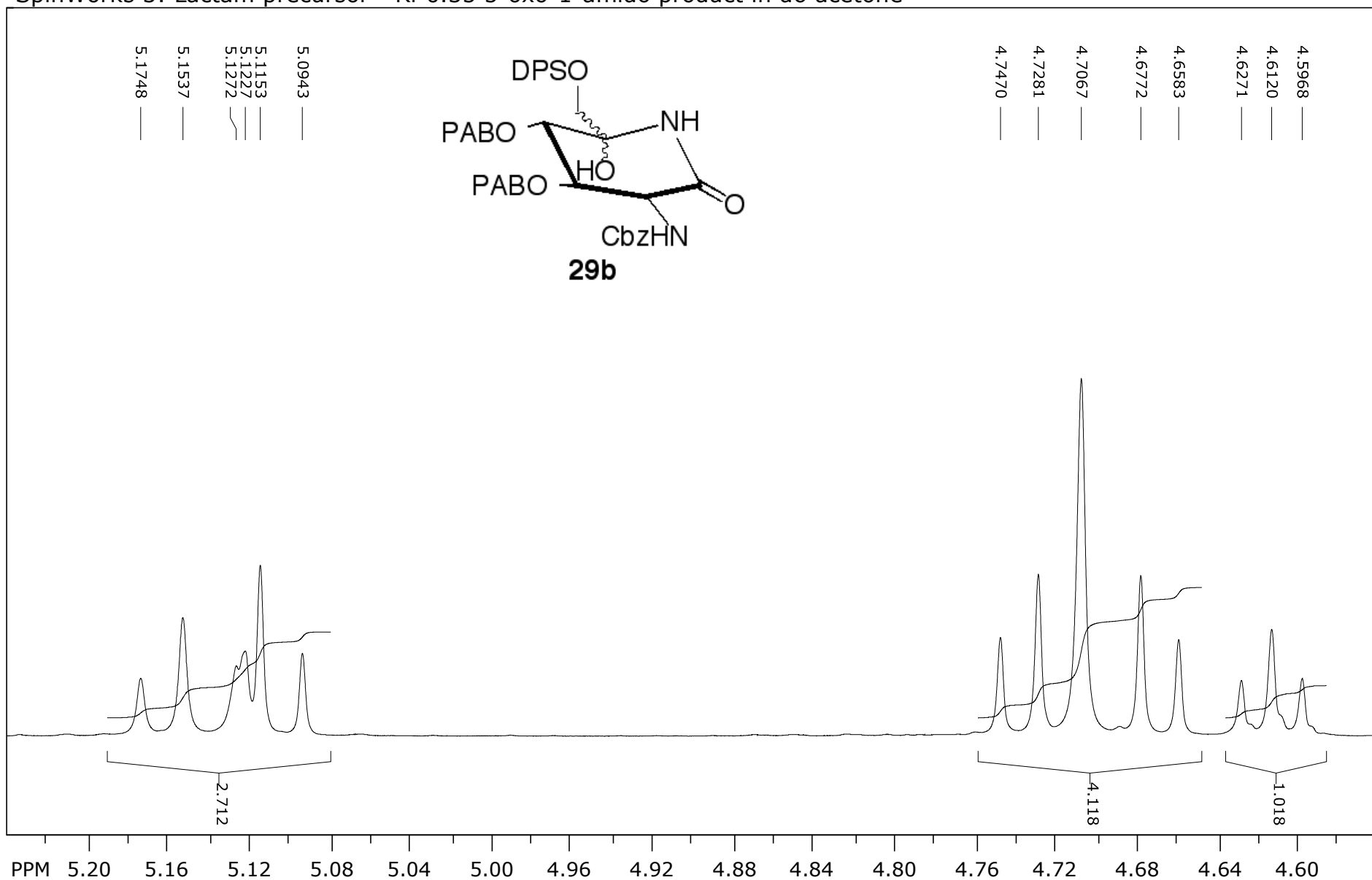
file: ...Data\OxoAmide0_35d6Acetone1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 205.875 ppm/cm: 0.34281



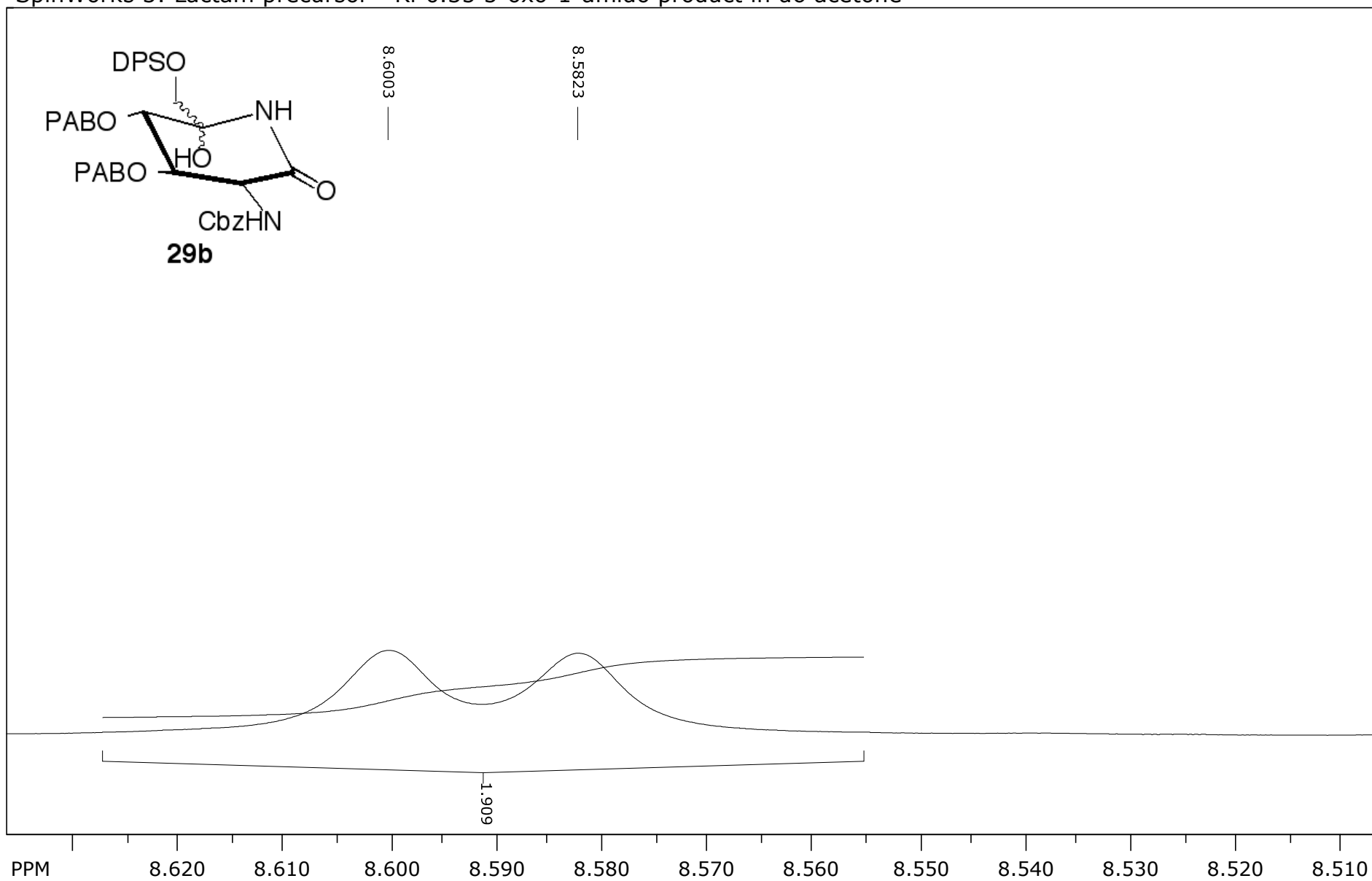
file: ...Data\OxoAmide0_35d6Acetone1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 13.823 ppm/cm: 0.02302



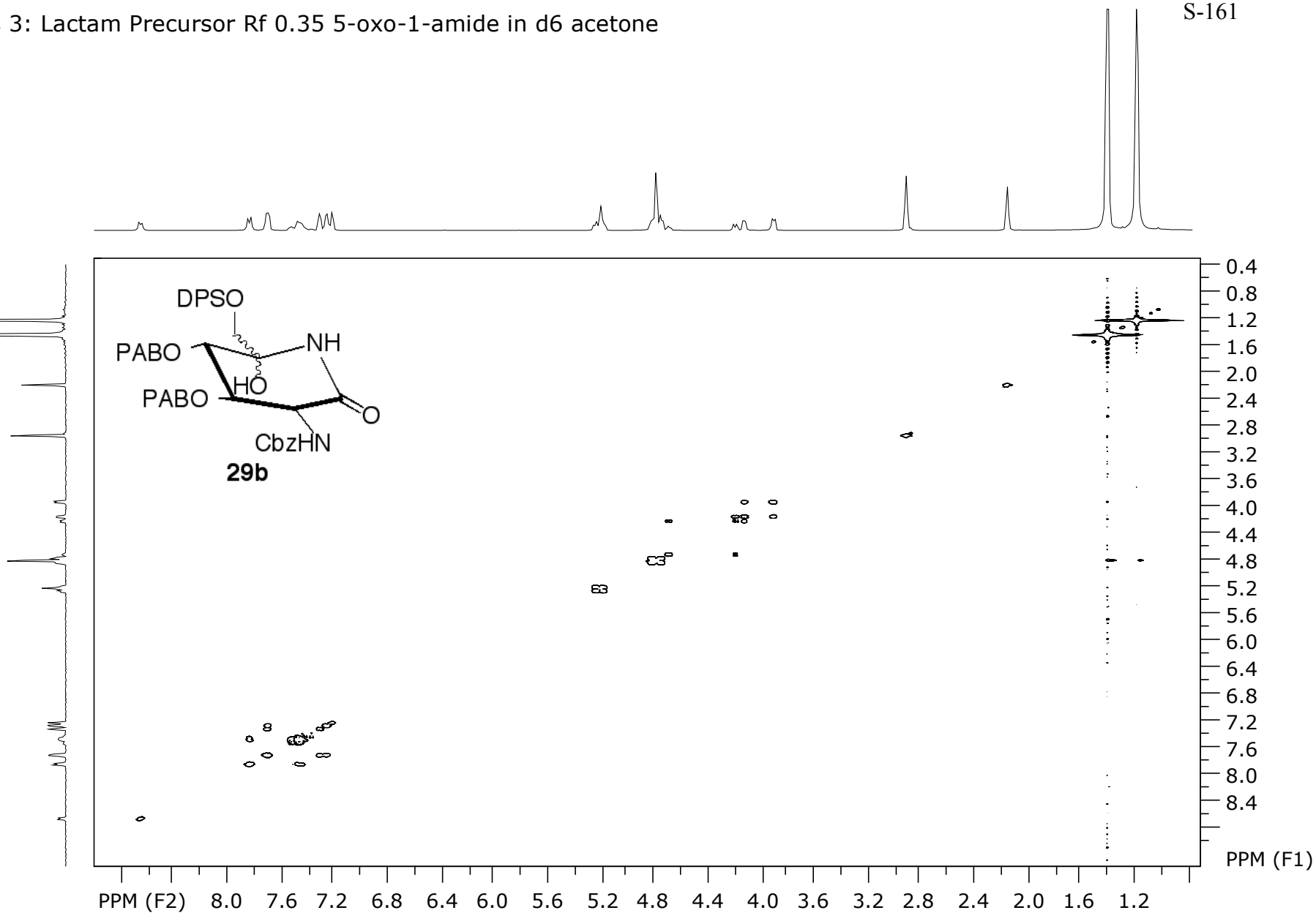
file: ...Data\OxoAmide0_35d6Acetone1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 16.417 ppm/cm: 0.02734



file: ...Data\OxoAmide0_35d6Acetone1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

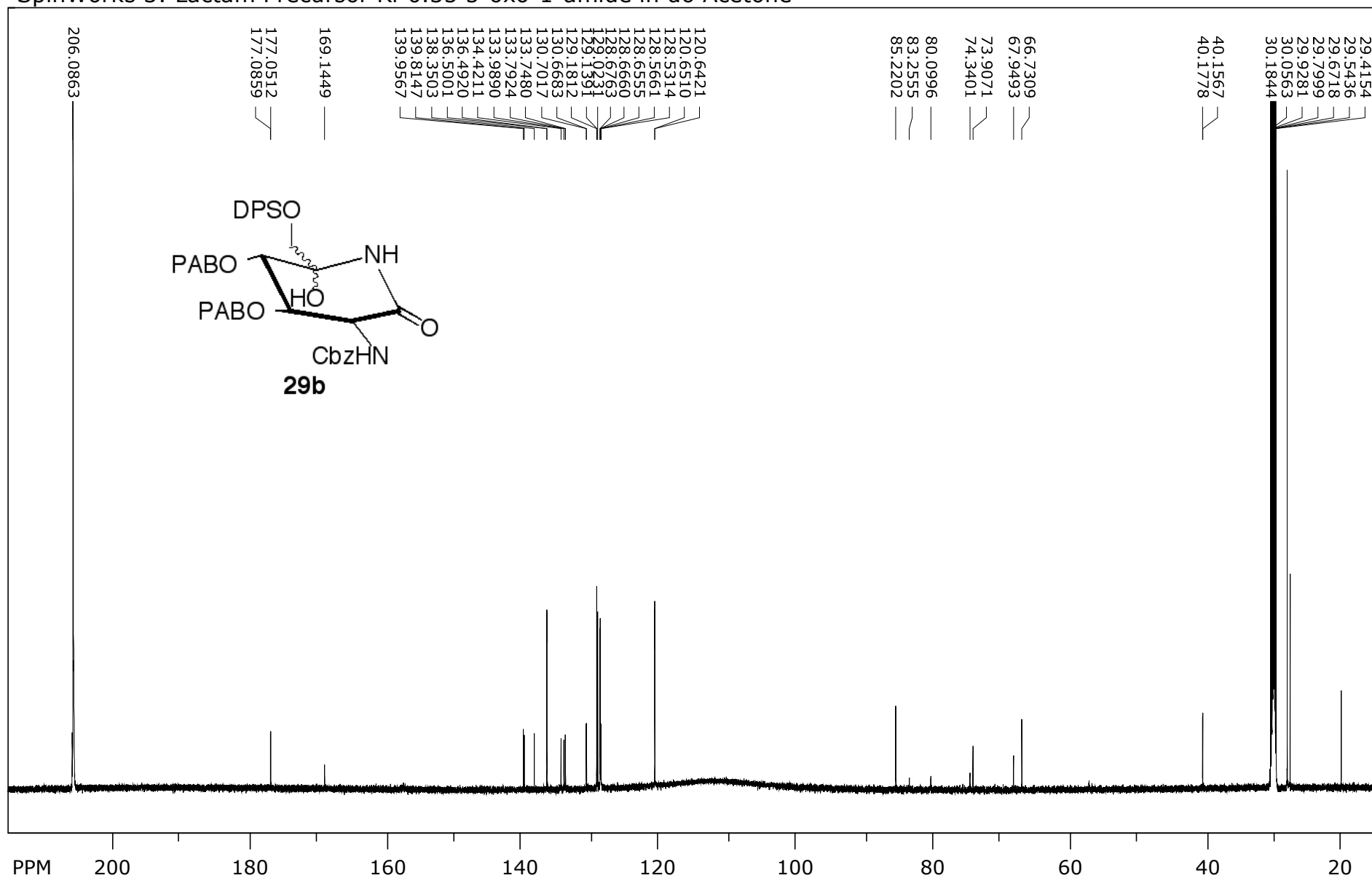
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 3.126 ppm/cm: 0.00521



file: ...ta\OxoAmide0_35d6AcetoneCOSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
 number of scans: 1

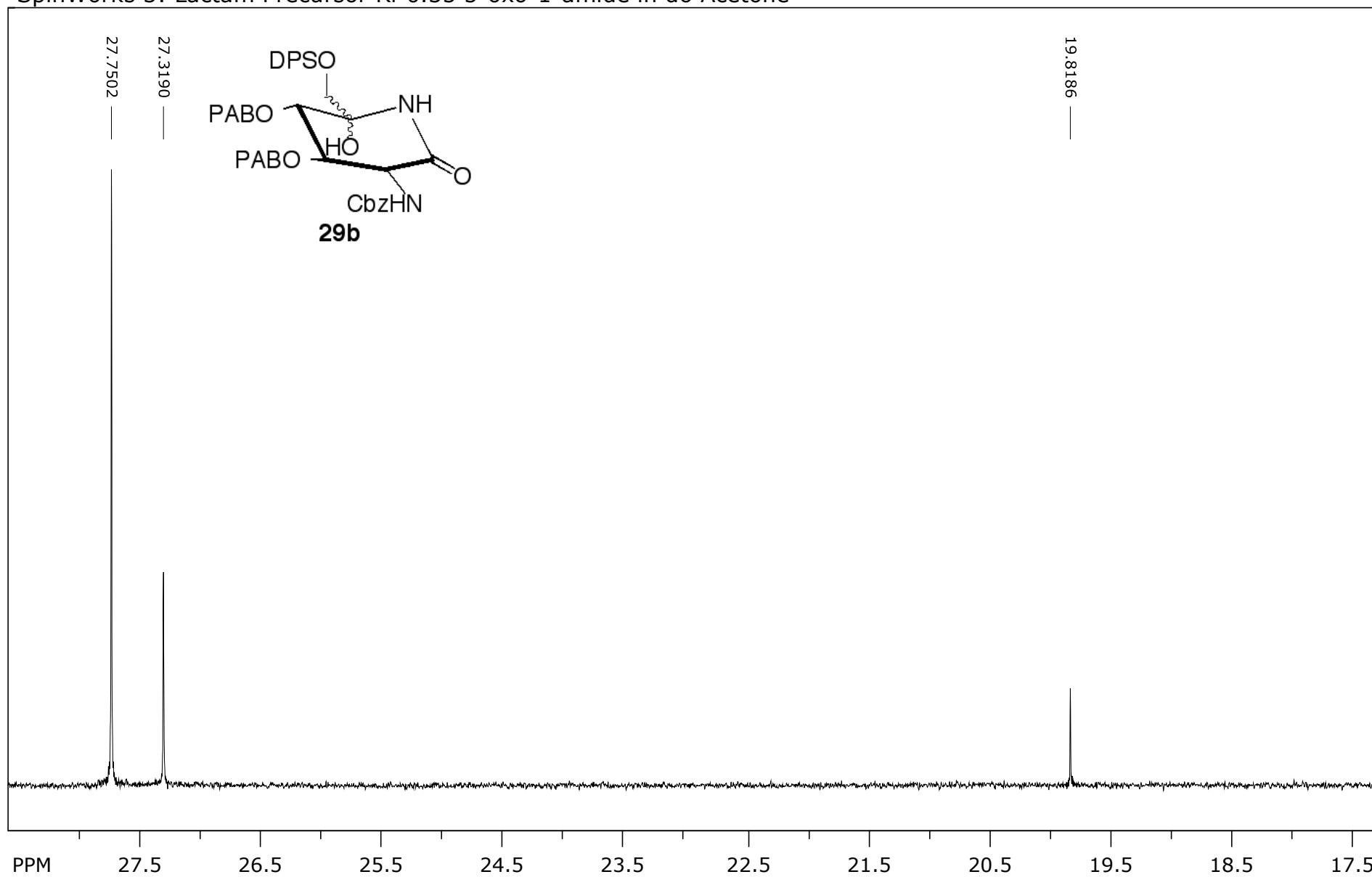
F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 249.078 ppm/cm: 0.41475

F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 495.499 ppm/cm: 0.82507



file: ...ata\OxoAmide0_35d6Acetone13C\1\fid expt: <zpgg30>
 transmitter freq.: 151.023518 MHz
 time domain size: 65536 points
 width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
 number of scans: 12288

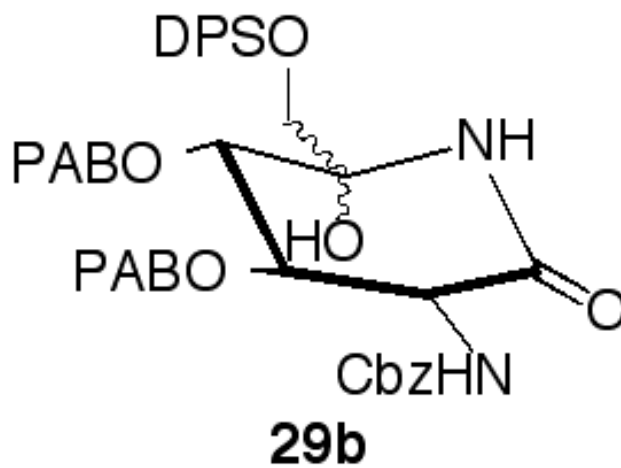
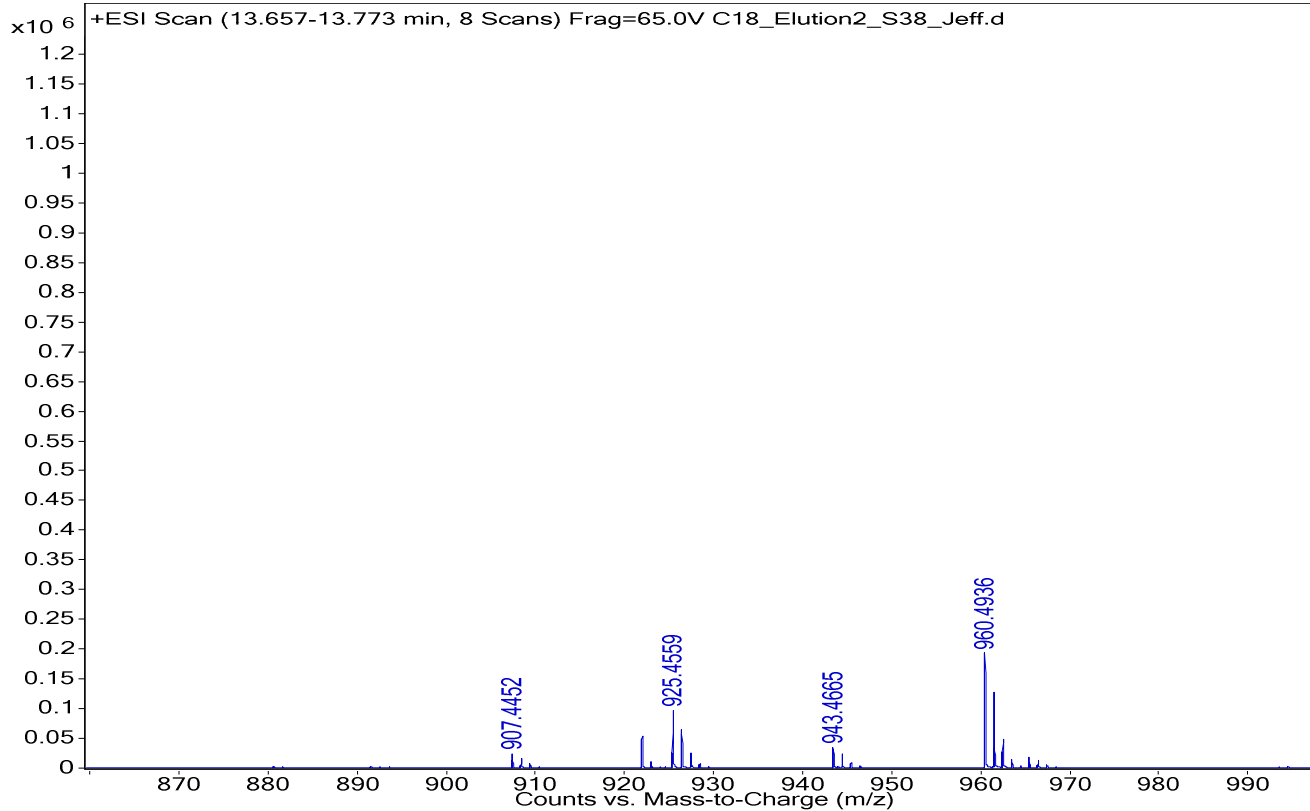
freq. of 0 ppm: 151.008288 MHz
 processed size: 131072 complex points
 LB: 0.300 GF: 0.0000
 Hz/cm: 1216.079 ppm/cm: 8.05225

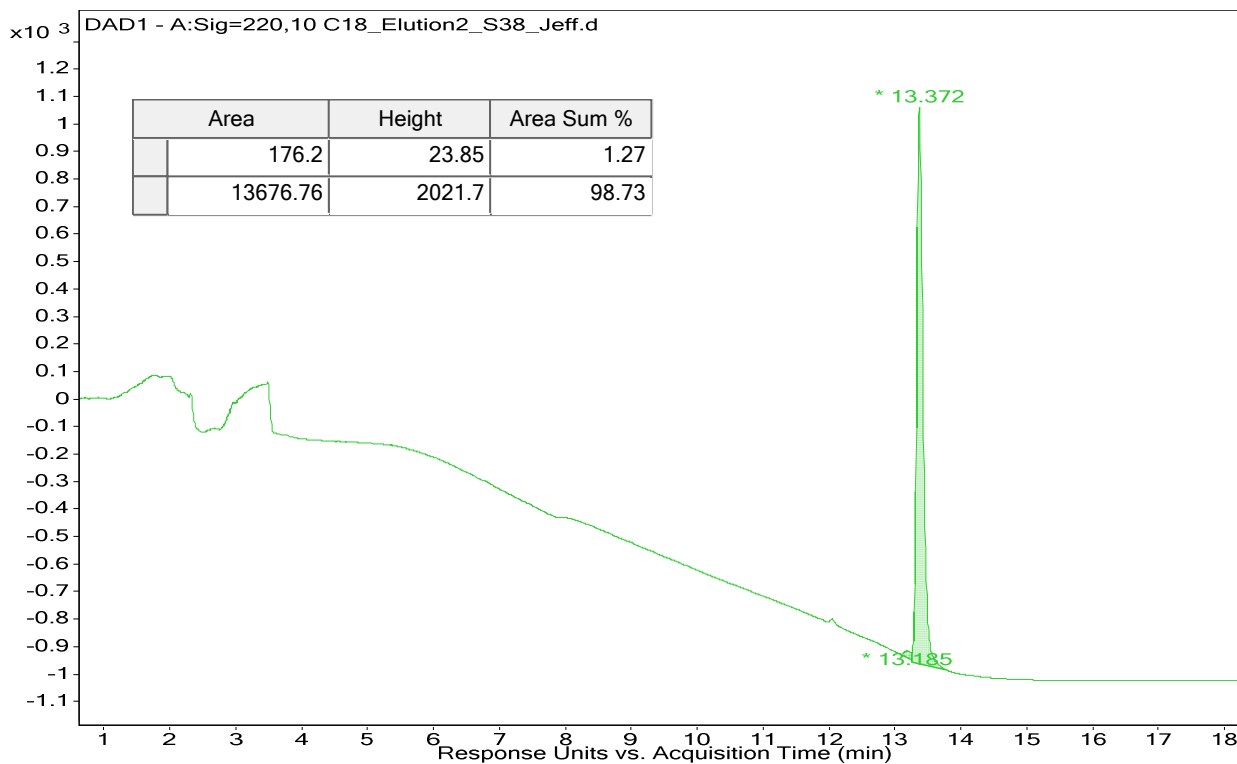


file: ...ata\OxoAmide0_35d6Acetone13C\1\fid expt: <zpgg30>
transmitter freq.: 151.023518 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 12288

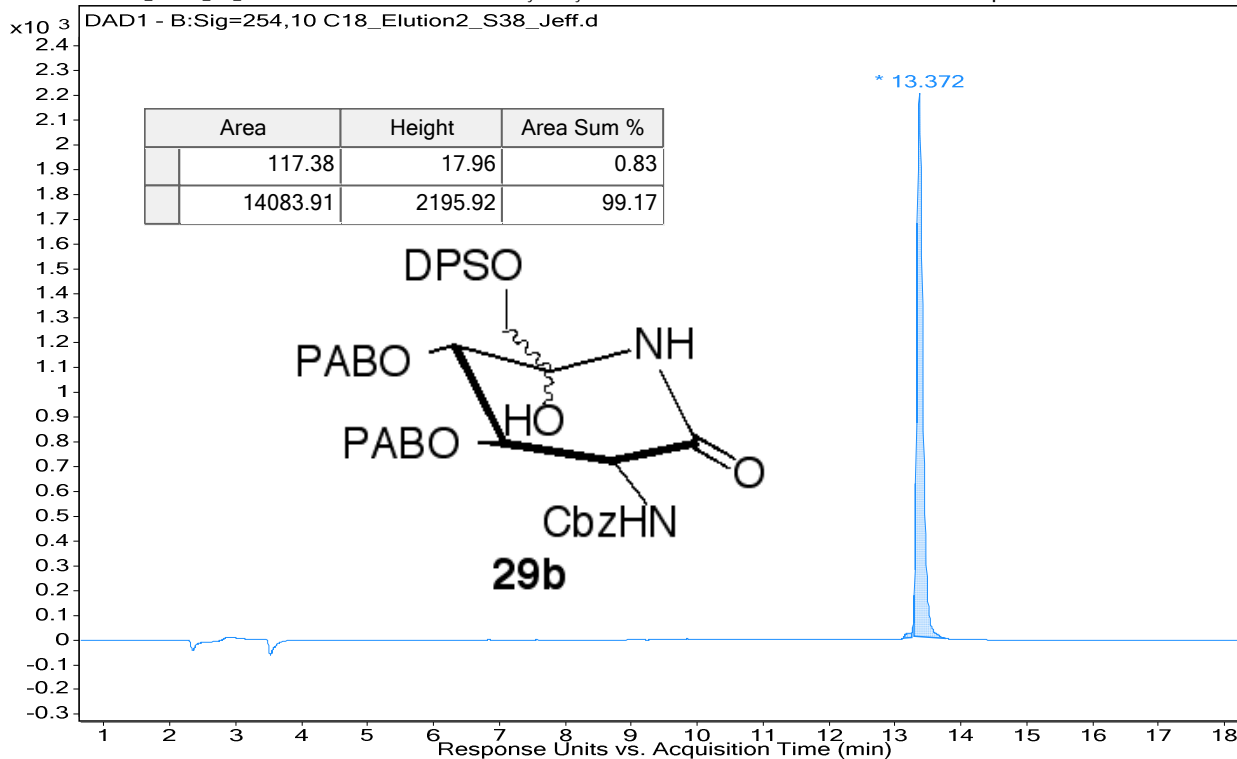
freq. of 0 ppm: 151.008288 MHz
processed size: 131072 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 68.266 ppm/cm: 0.45202

Sample Name	Jeff-38	Position	Vial 24	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution2_S38_Jef	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/15/2012 10:32:37 AM



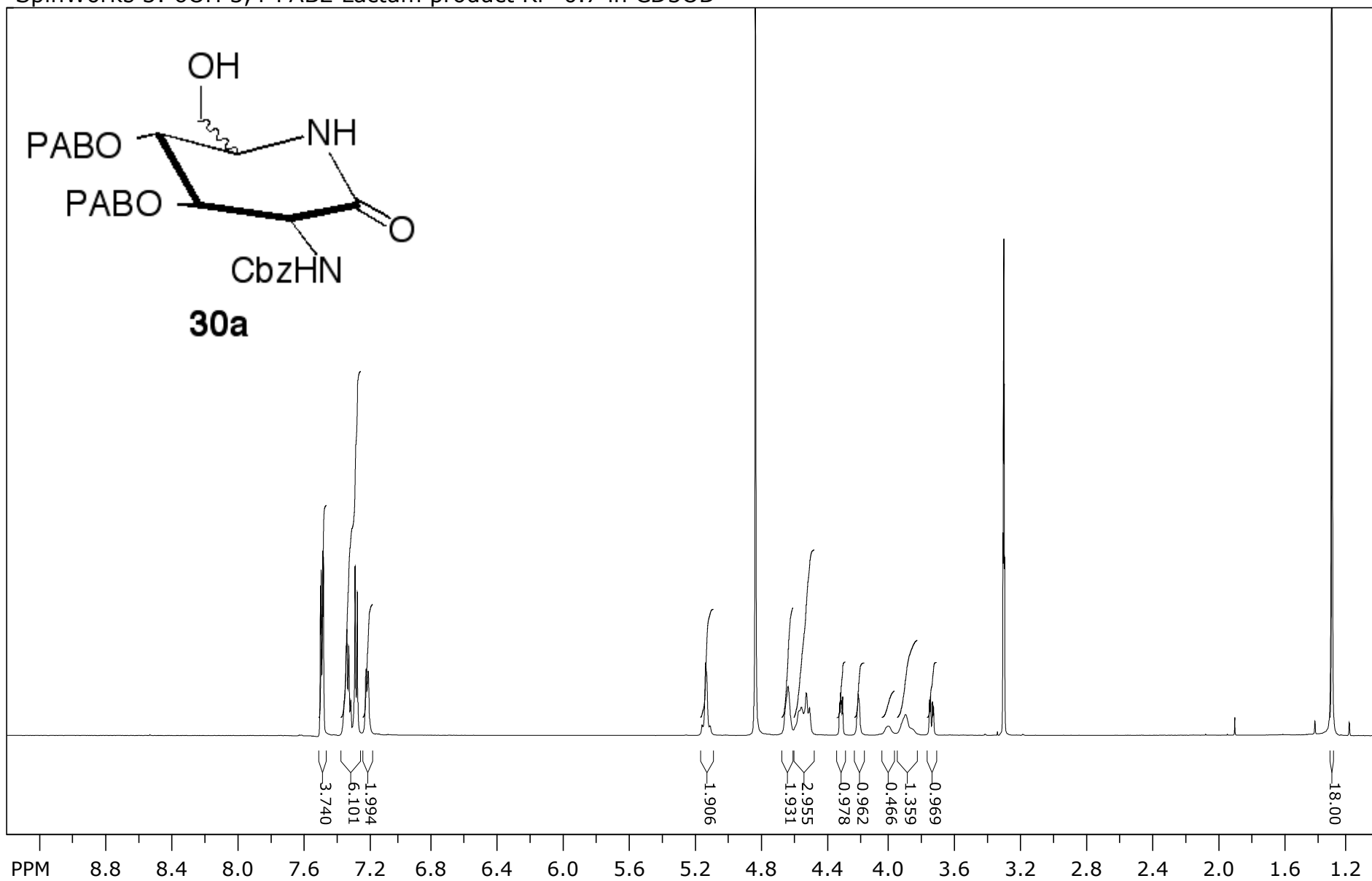


Sample Name	Jeff-38	Position	Vial 24	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution2_S38_Jef	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/15/2012 10:32:37 AM



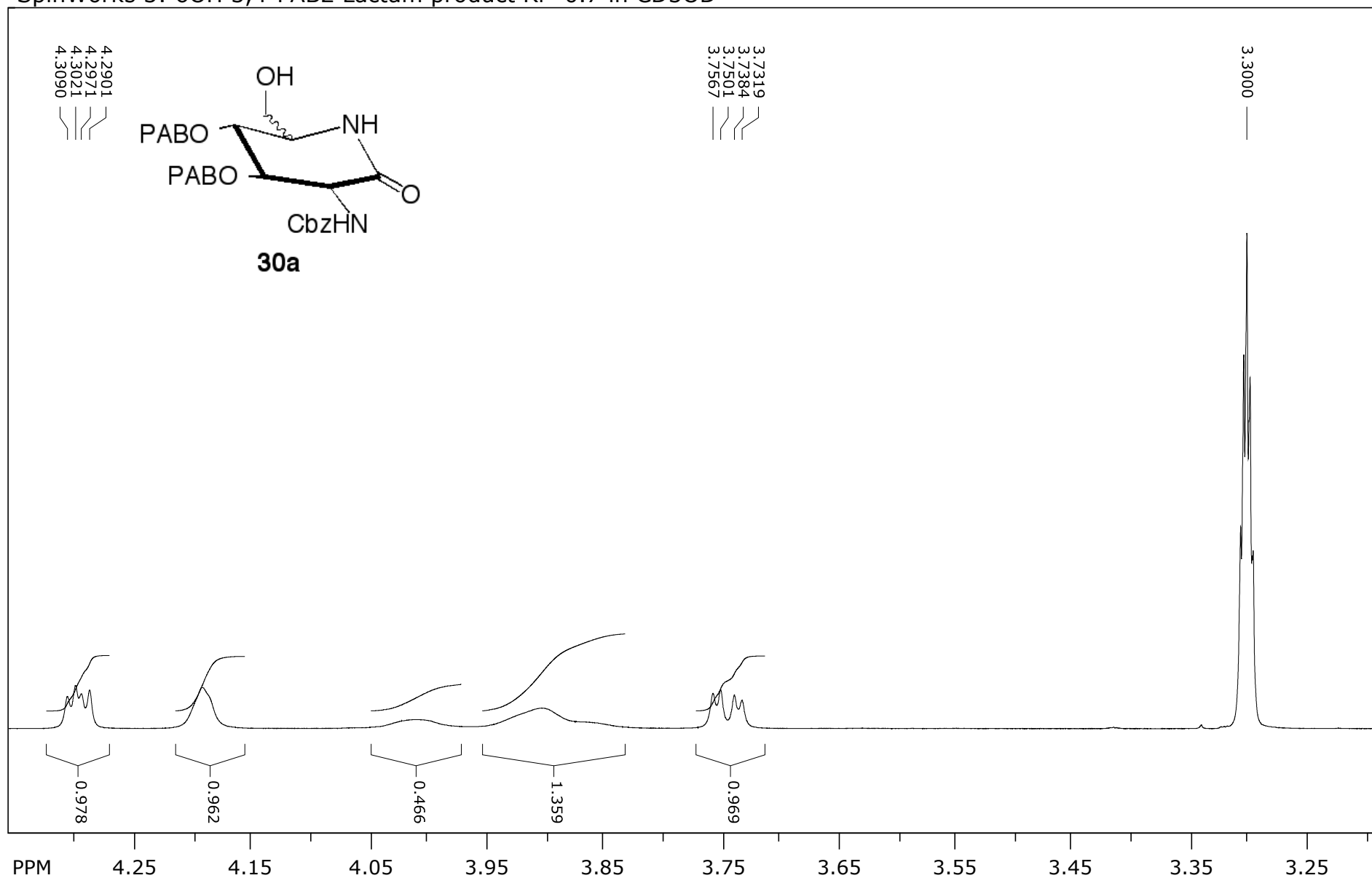
Analysis on a Waters SymmetryShield™ C18 (4.6 mm X 15 cm (i.d. x l.), 3.5 μm) at 0.5 mL/min. Solvent A: 50 mM NH₄OAc (aq); B: CH₃CN

Time (min)	% B
0	20
1	20
10	100
20	100



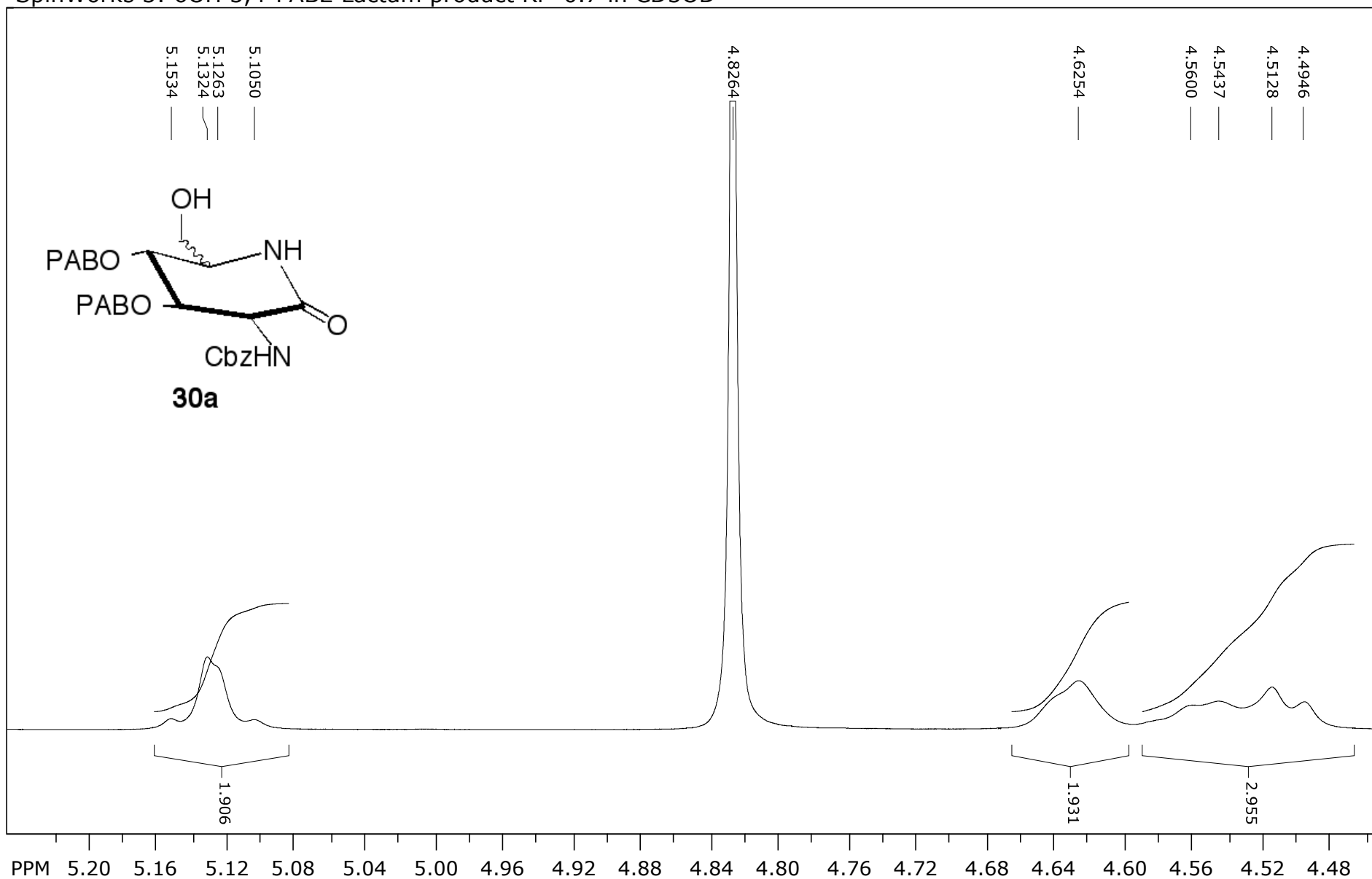
file: ...NMR Data\6OHLactam0_7CD3OD1H\1\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 202.539 ppm/cm: 0.33725



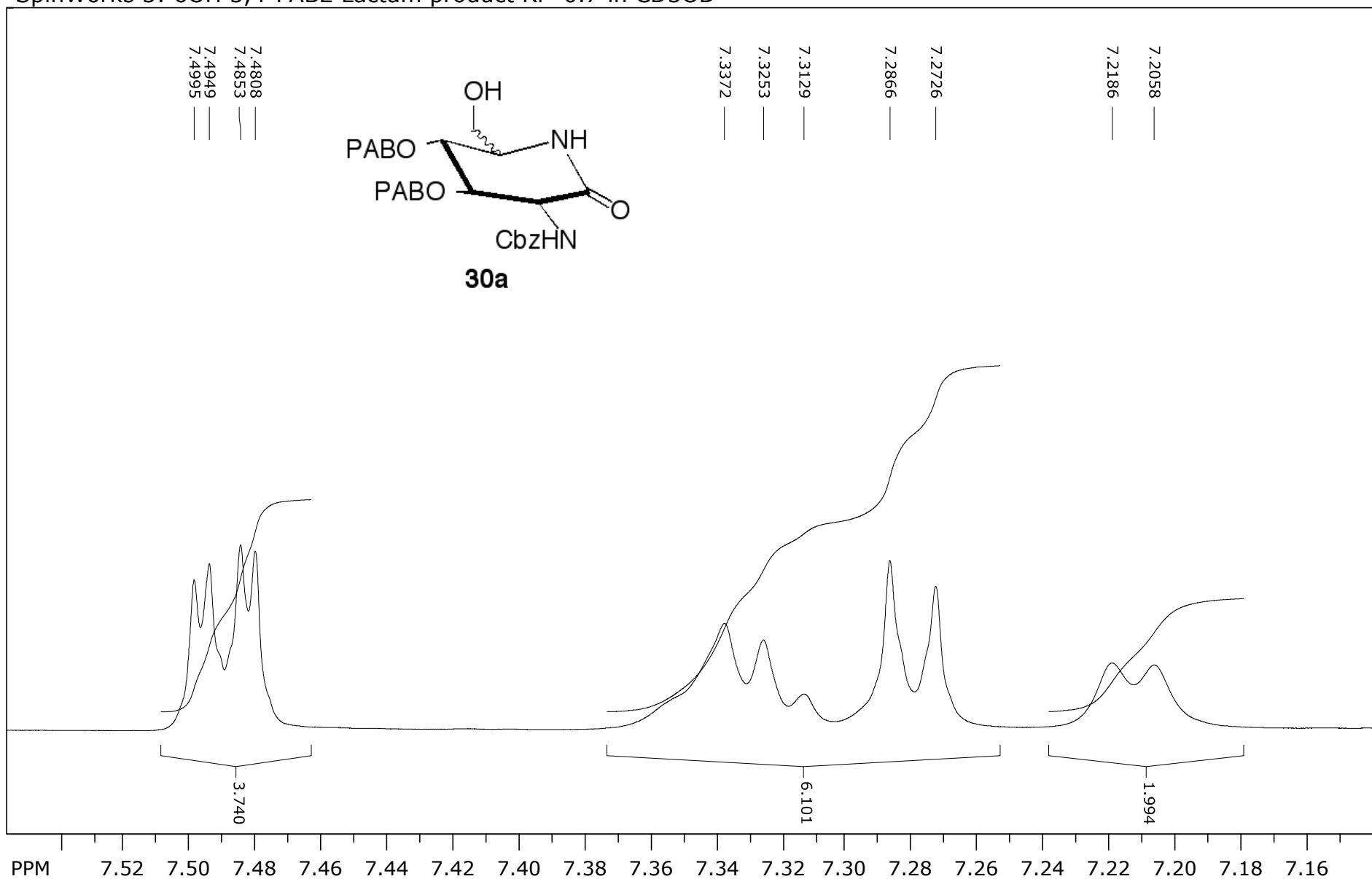
file: ...NMR Data\6OHLactam0_7CD3OD1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 28.166 ppm/cm: 0.04690



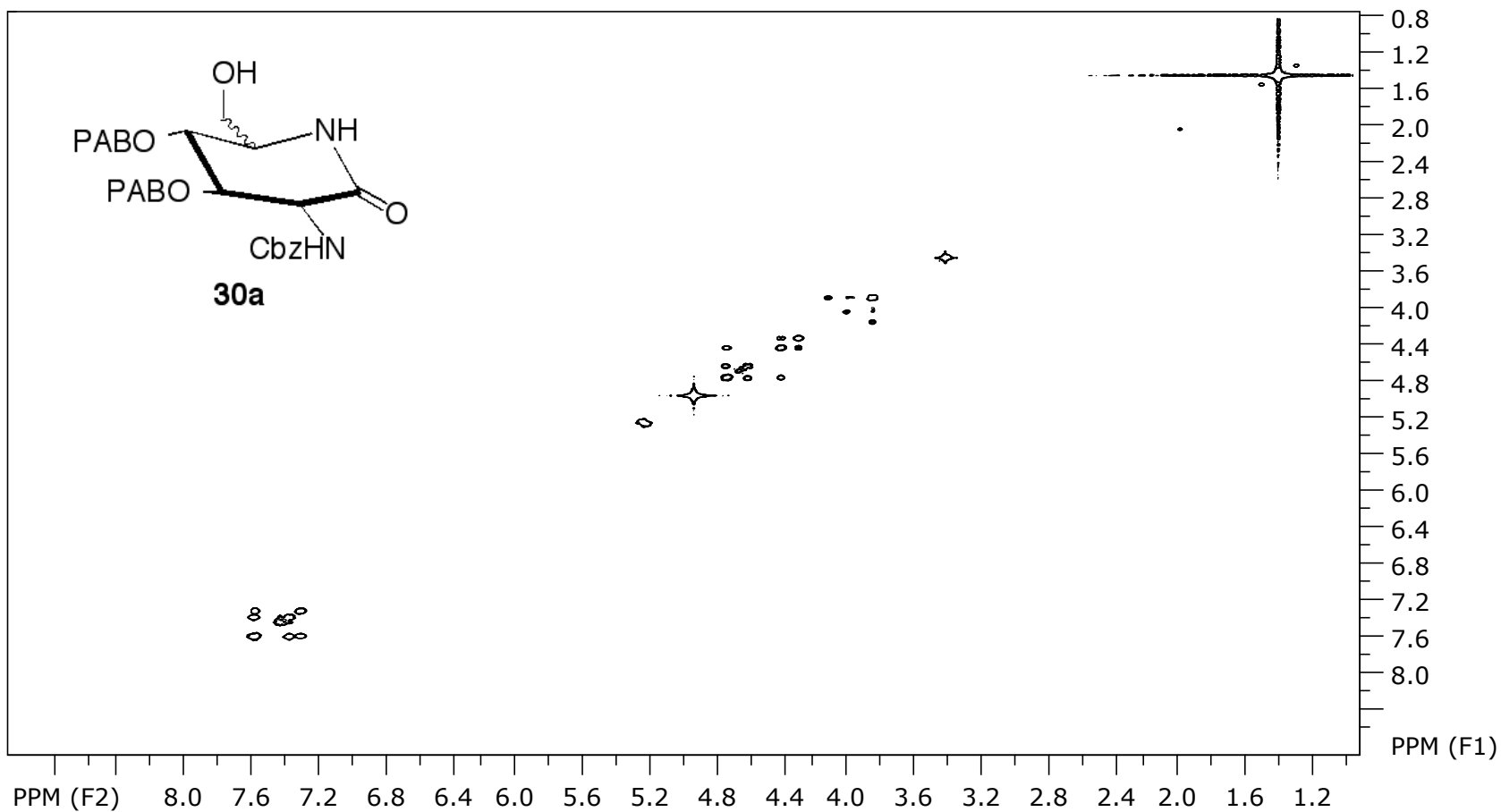
file: ...NMR Data\6OHLactam0_7CD3OD1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 19.183 ppm/cm: 0.03194



file: ...NMR Data\6OHLactam0_7CD3OD1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

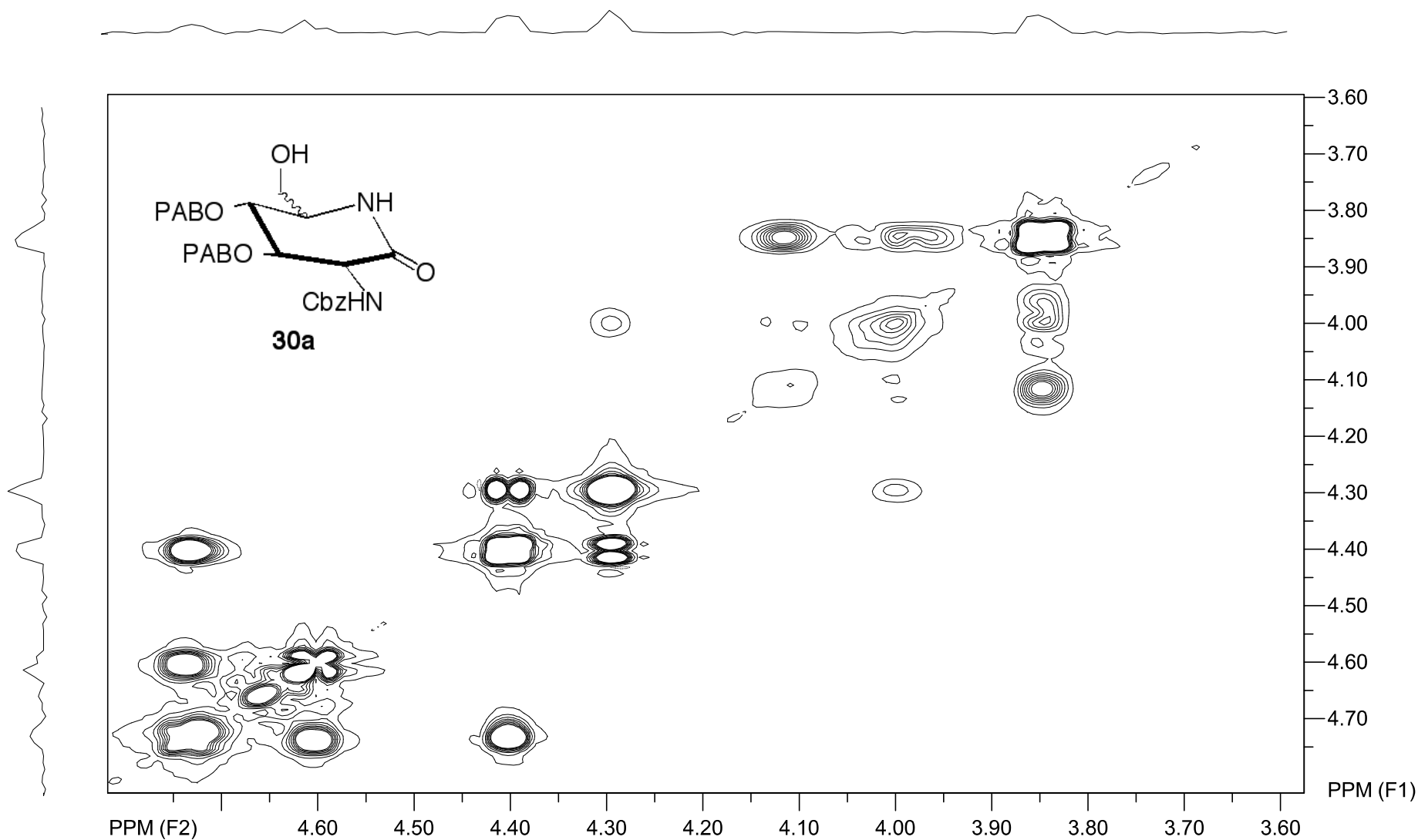
freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 10.084 ppm/cm: 0.01679



file: ...R Data\6OHLactam0_7CD3ODCOSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
 number of scans: 1

F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 245.010 ppm/cm: 0.40797

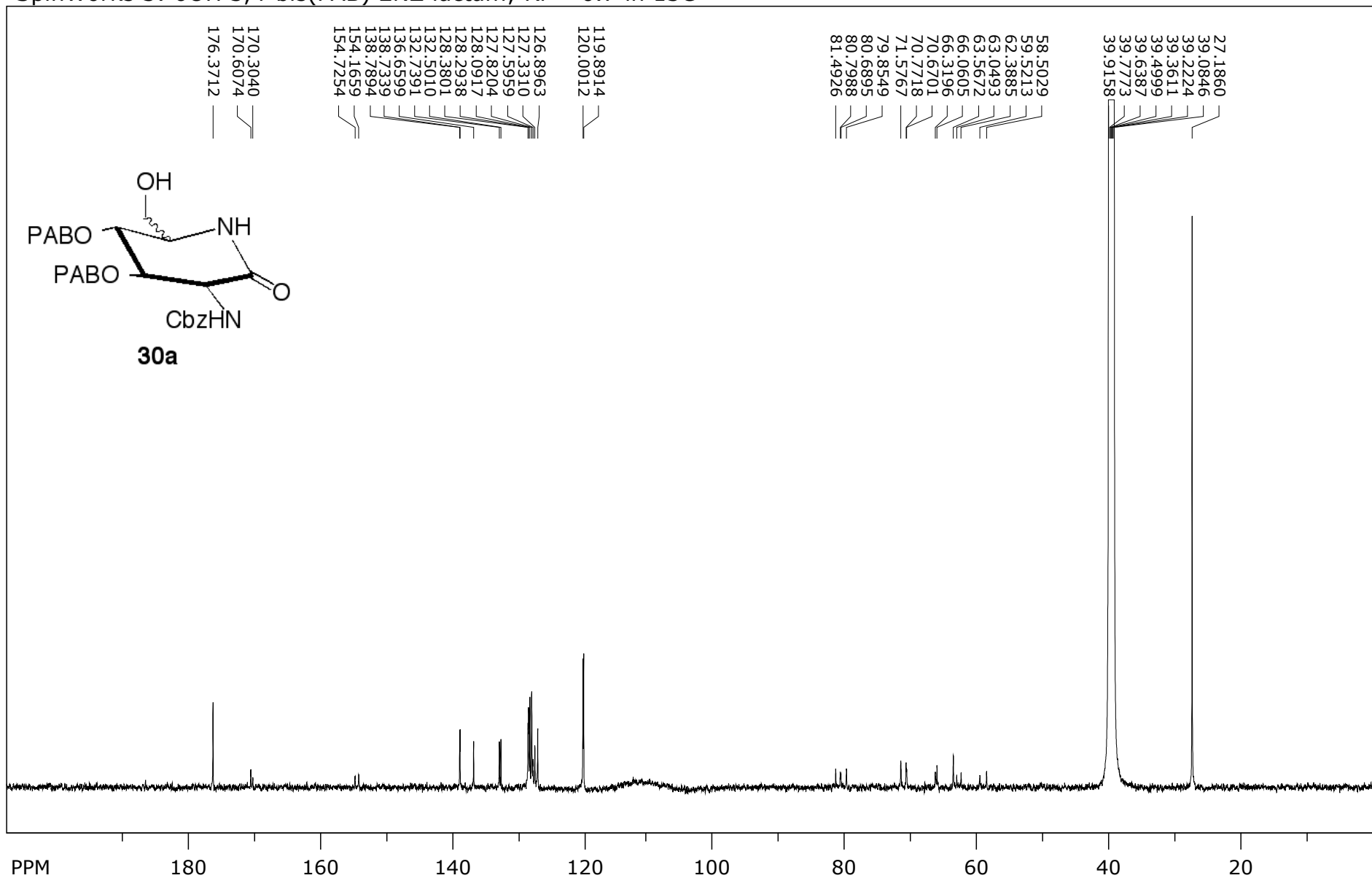
F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 444.878 ppm/cm: 0.74078



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\6OHLactam0_7CD3ODCOSY\1\ser
transmitter freq.: 600.552832 MHz
time domain size: 2048 by 1024 points
width (F2): 7211.50 Hz = 12.008167 ppm = 3.521242 Hz/pt
number of scans: 1

expt: <cosF2>:freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 36.405 ppm/cm: 0.06062

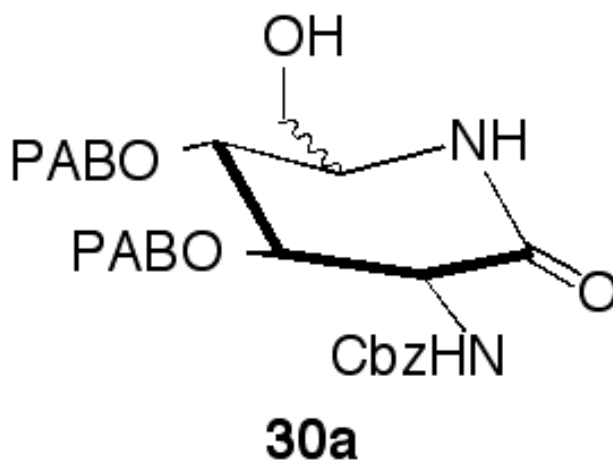
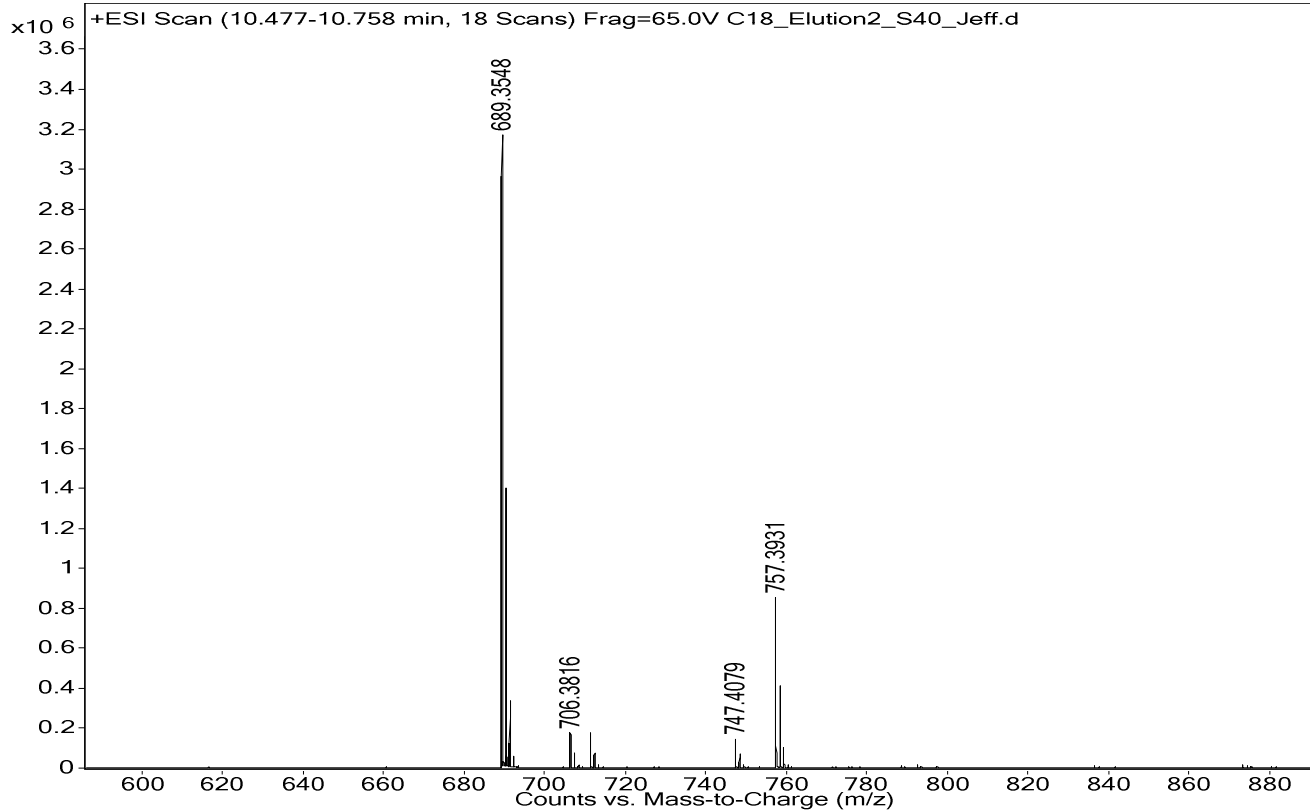
F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 61.916 ppm/cm: 0.10310

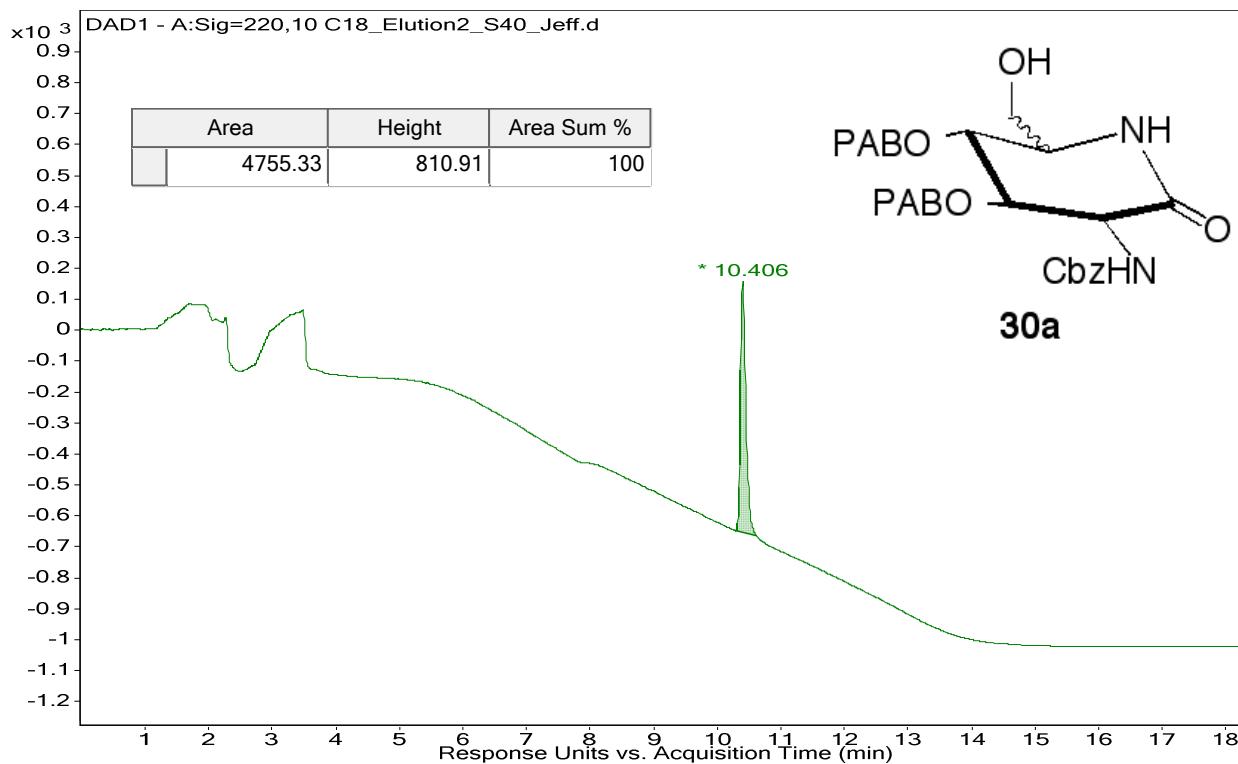


file: ...7_6OH34PAB2Lactam_13C_pl112k\1\fid expt: <zgpg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 112640

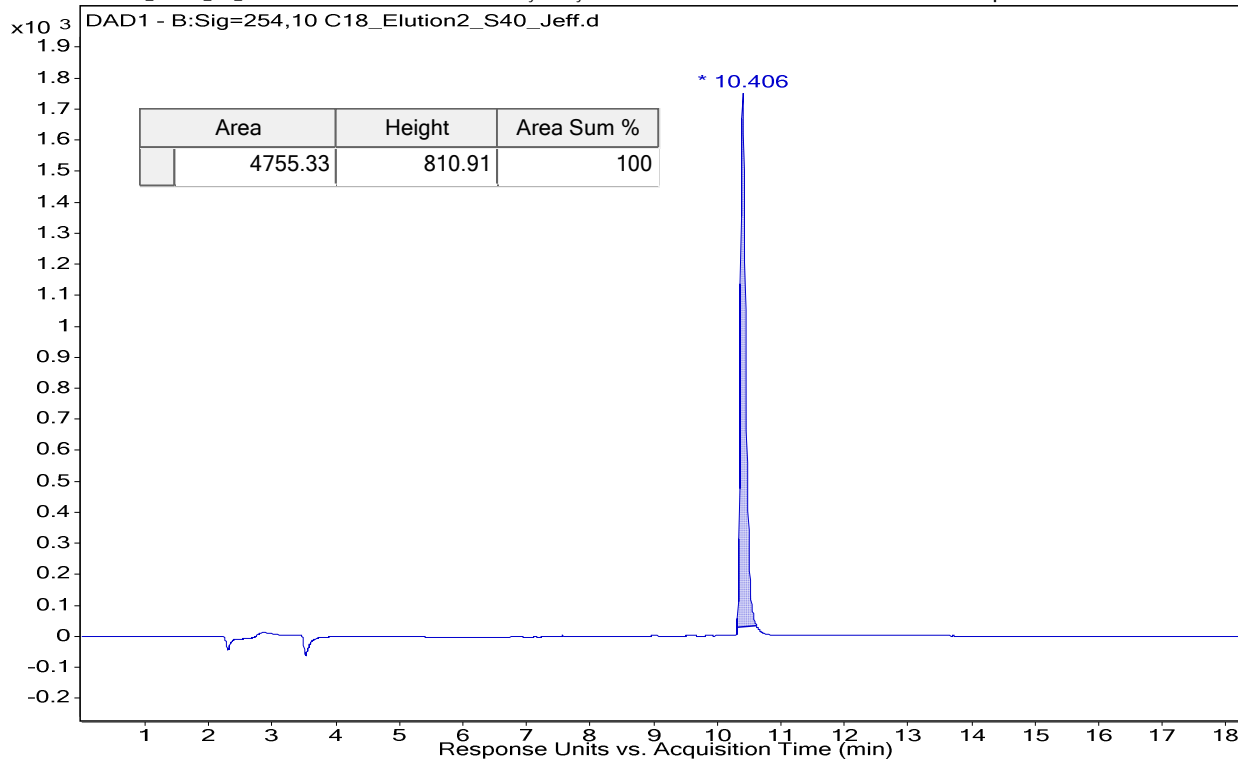
freq. of 0 ppm: 151.008493 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 1262.824 ppm/cm: 8.36177

Sample Name	Jeff-40	Position	Vial 26	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution2_S40_Jef	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/15/2012 11:26:01 AM



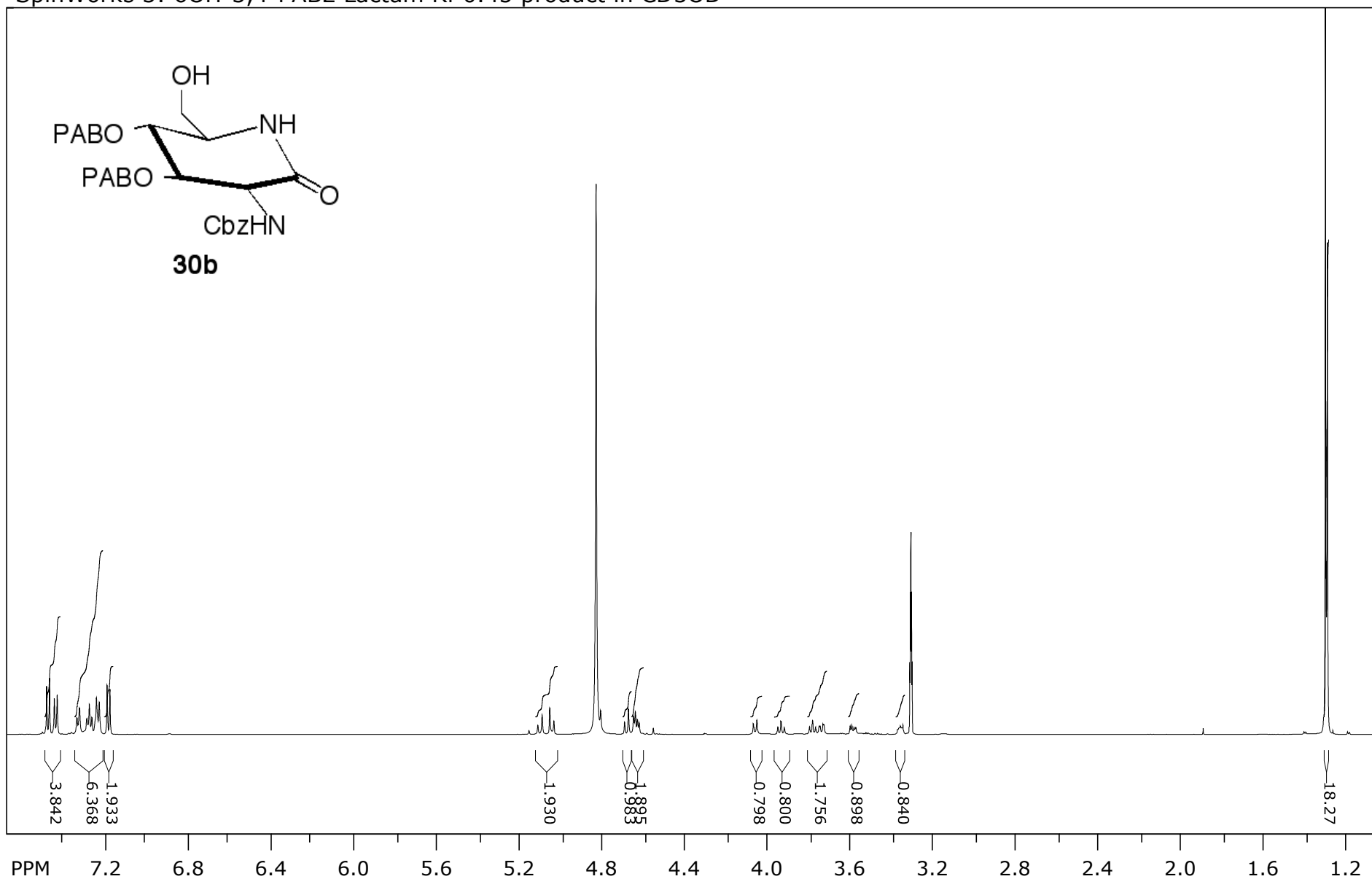


Sample Name	Jeff-40	Position	Vial 26	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	2	InjPosition		SampleType	Unknown	IRM Calibration Status	Some Ions Missed
Data Filename	C18_Elution2_S40_Jef	ACQ Method	C18 waters symmetry2	Comment		Acquired Time	9/15/2012 11:26:01 AM



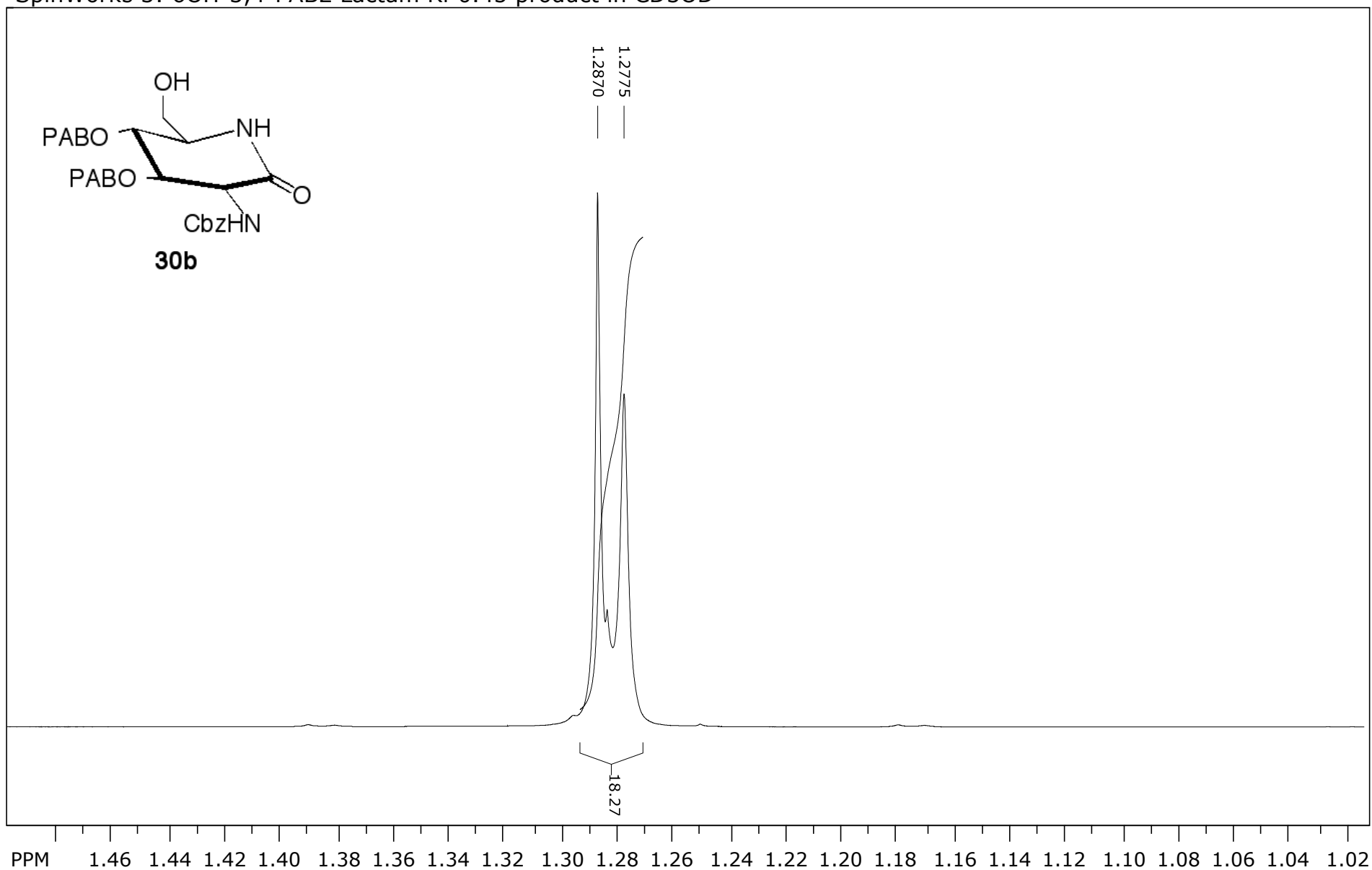
Analysis on a Waters SymmetryShield™ C18 (4.6 mm X 15 cm (i.d. x l.), 3.5 μm) at 0.5 mL/min. Solvent A: 50 mM NH₄OAc (aq); B: CH₃CN

Time [min]	% B
0	20
1	20
10	100
20	100



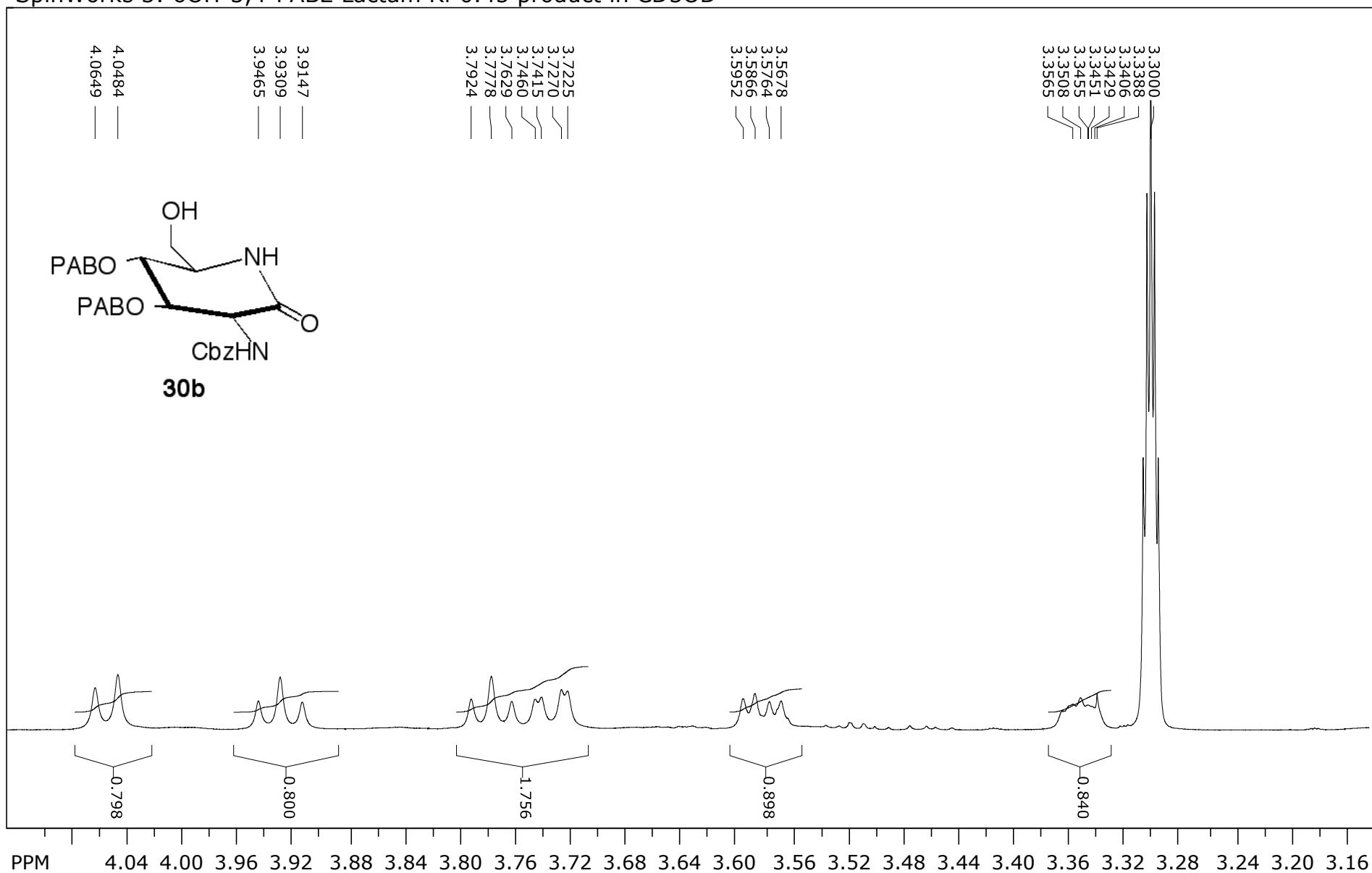
file: ...MR Data\6OHLactam0_45CD3OD1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 160.104 ppm/cm: 0.26659



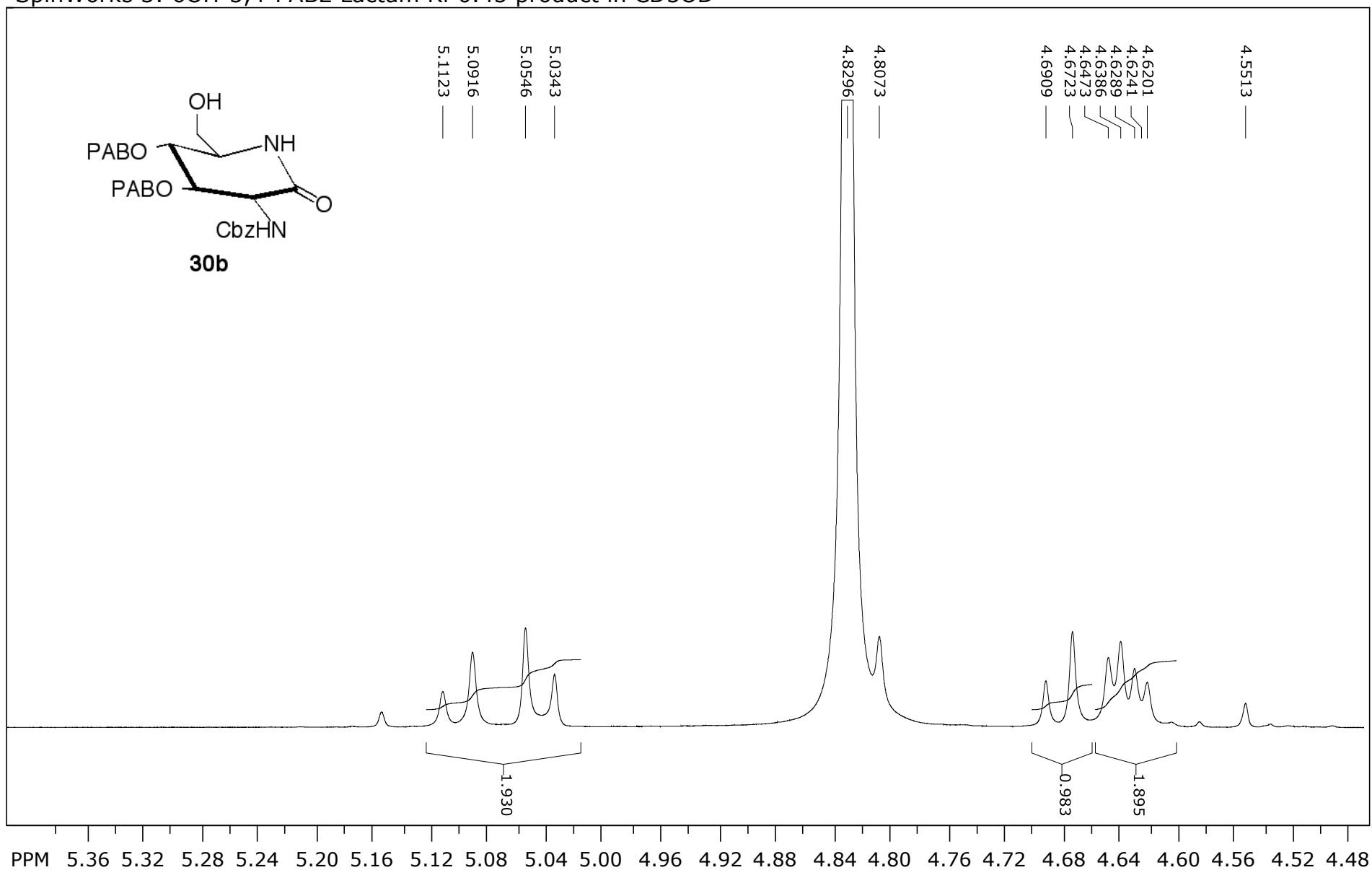
file: ...MR Data\6OHLactam0_45CD3OD1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 11.674 ppm/cm: 0.01944



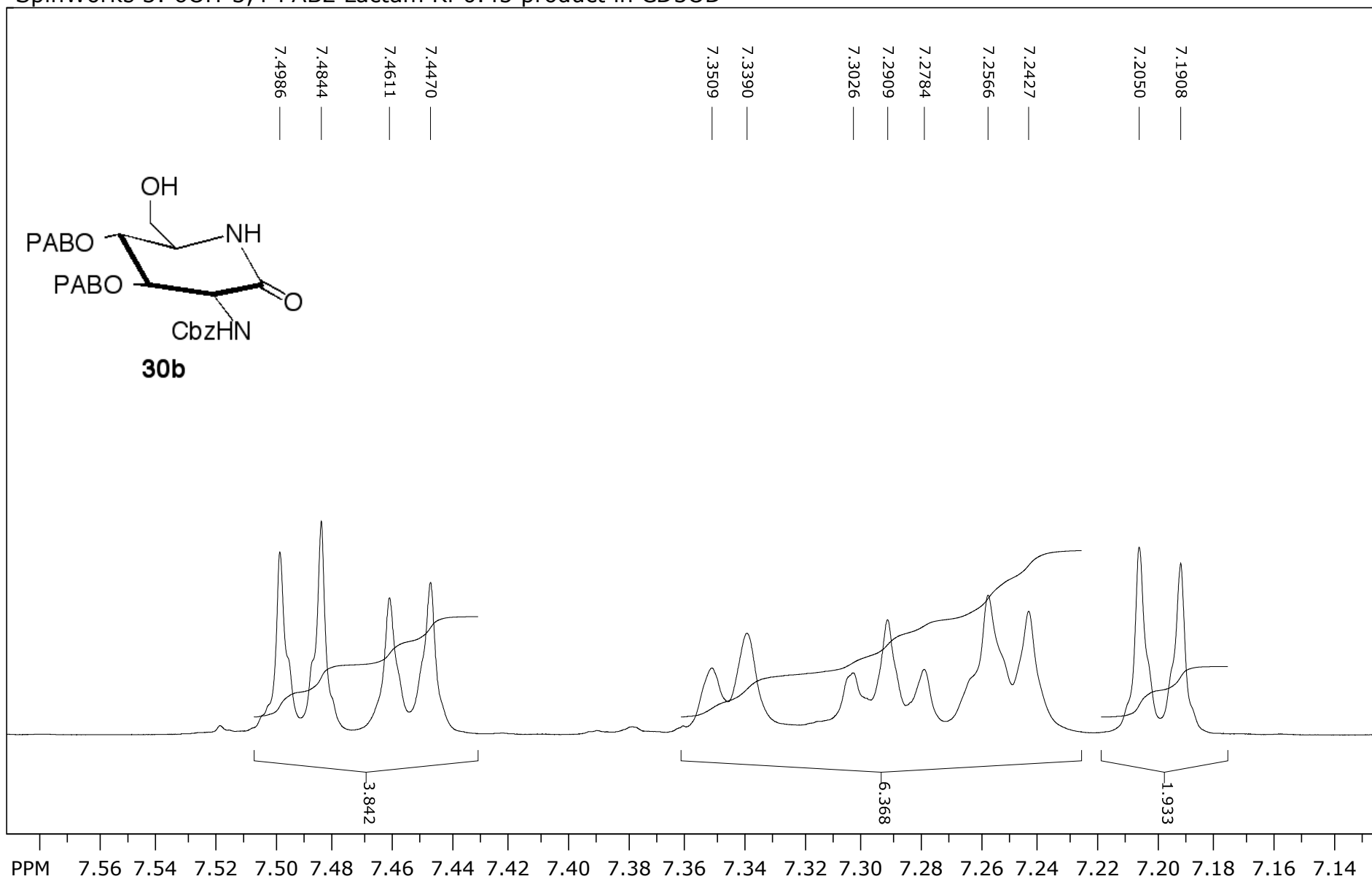
file: ...MR Data\6OHLactam0_45CD3OD1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 23.719 ppm/cm: 0.03950



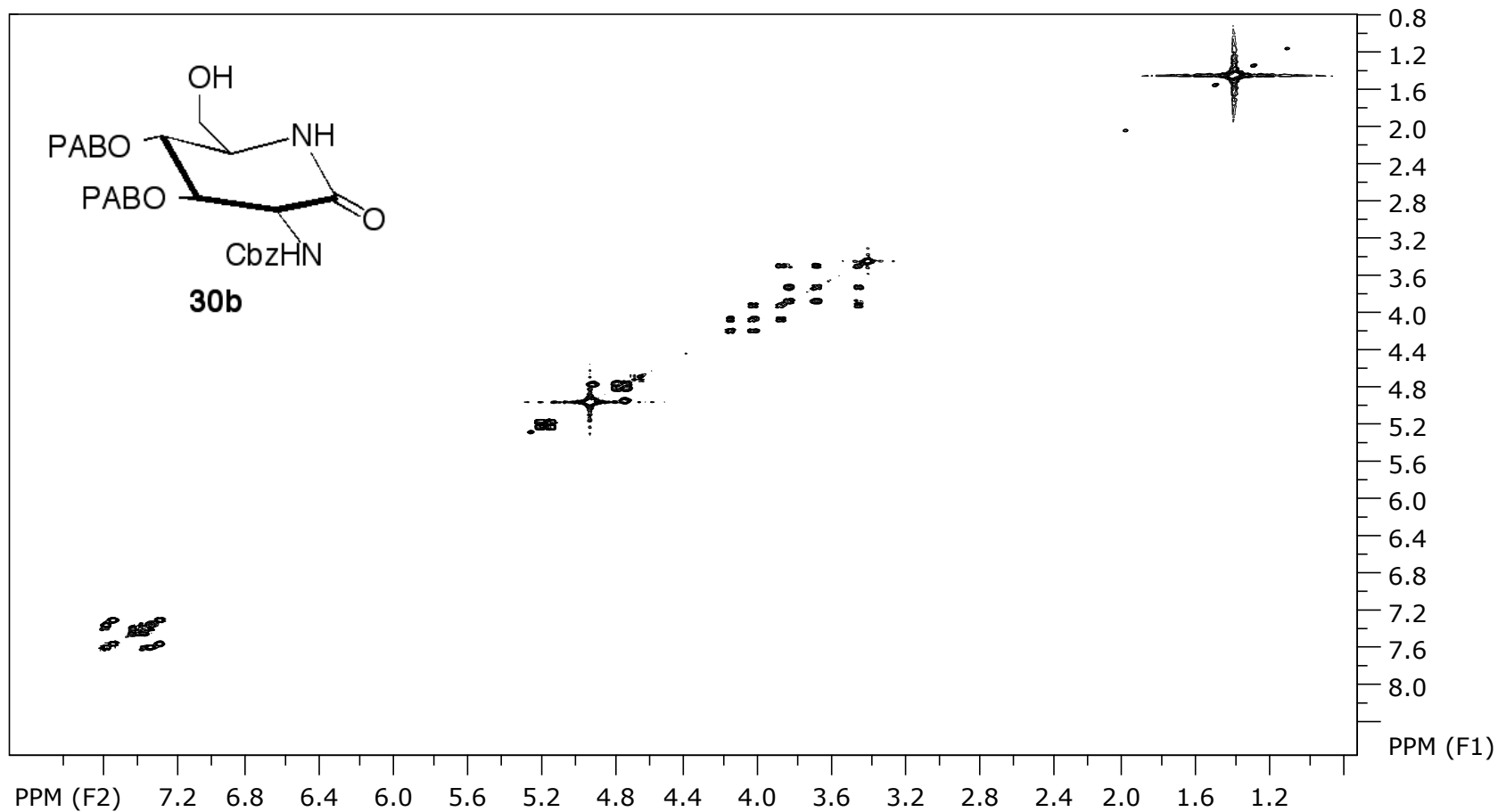
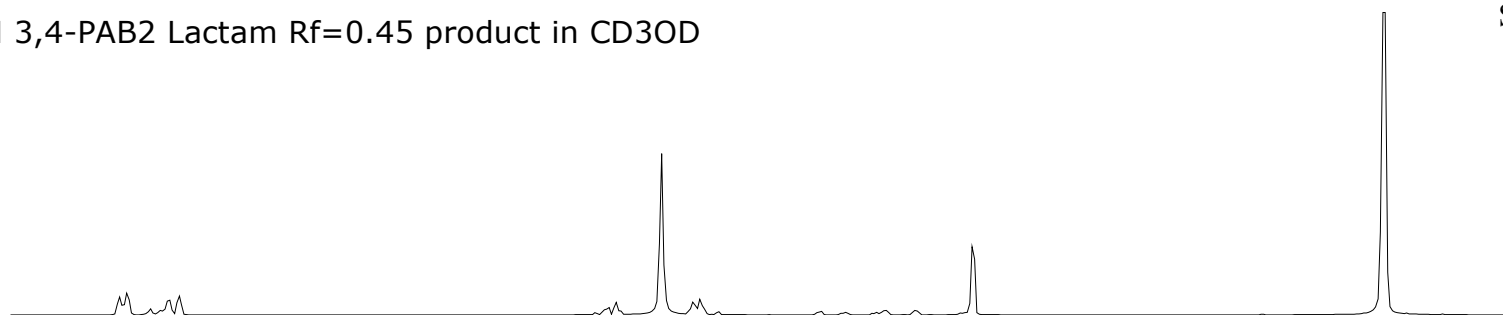
file: ...MR Data\6OHLactam0_45CD3OD1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 22.793 ppm/cm: 0.03795



file: ...MR Data\6OHLactam0_45CD3OD1H\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

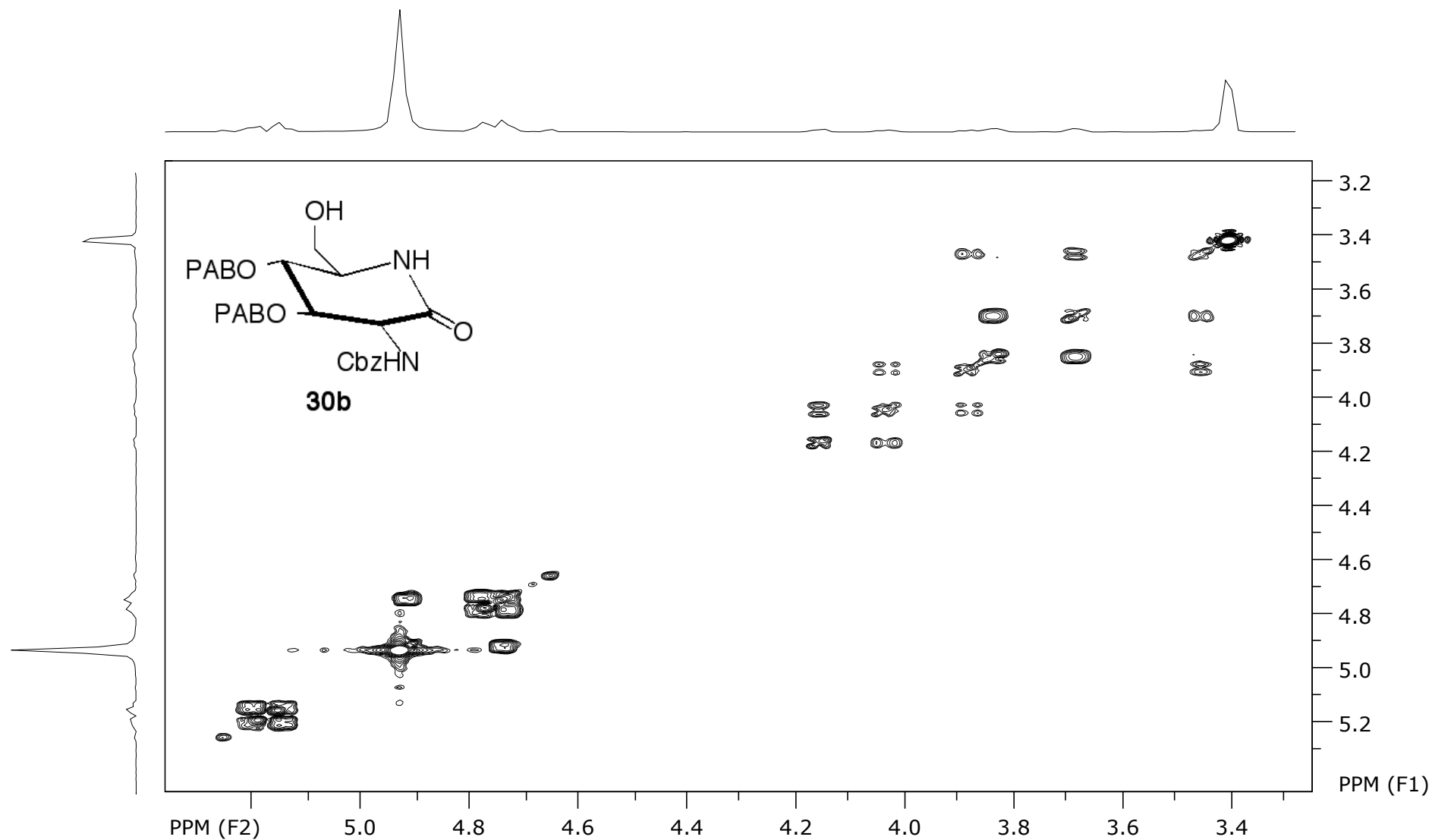
freq. of 0 ppm: 600.550023 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 11.260 ppm/cm: 0.01875



file: ... Data\6OHLactam0_45CD3ODCOSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
 number of scans: 1

F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 221.801 ppm/cm: 0.36933

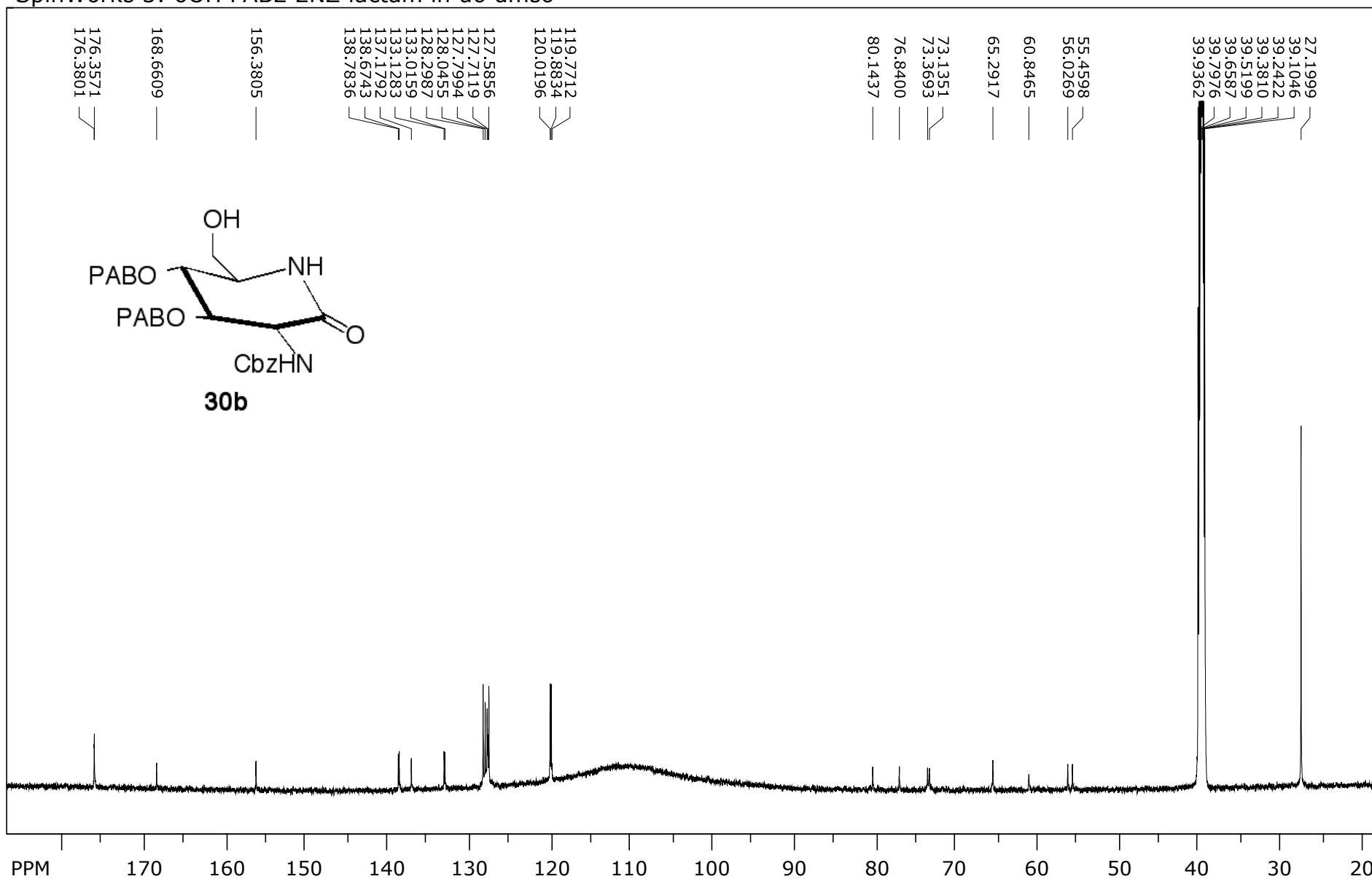
F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 435.143 ppm/cm: 0.72457



file: ... Data\6OHLactam0_45CD3ODCOSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
 number of scans: 1

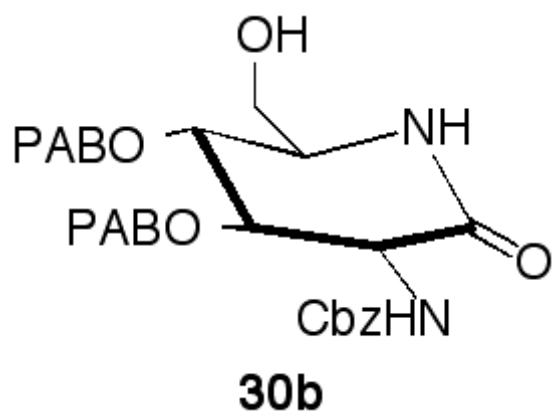
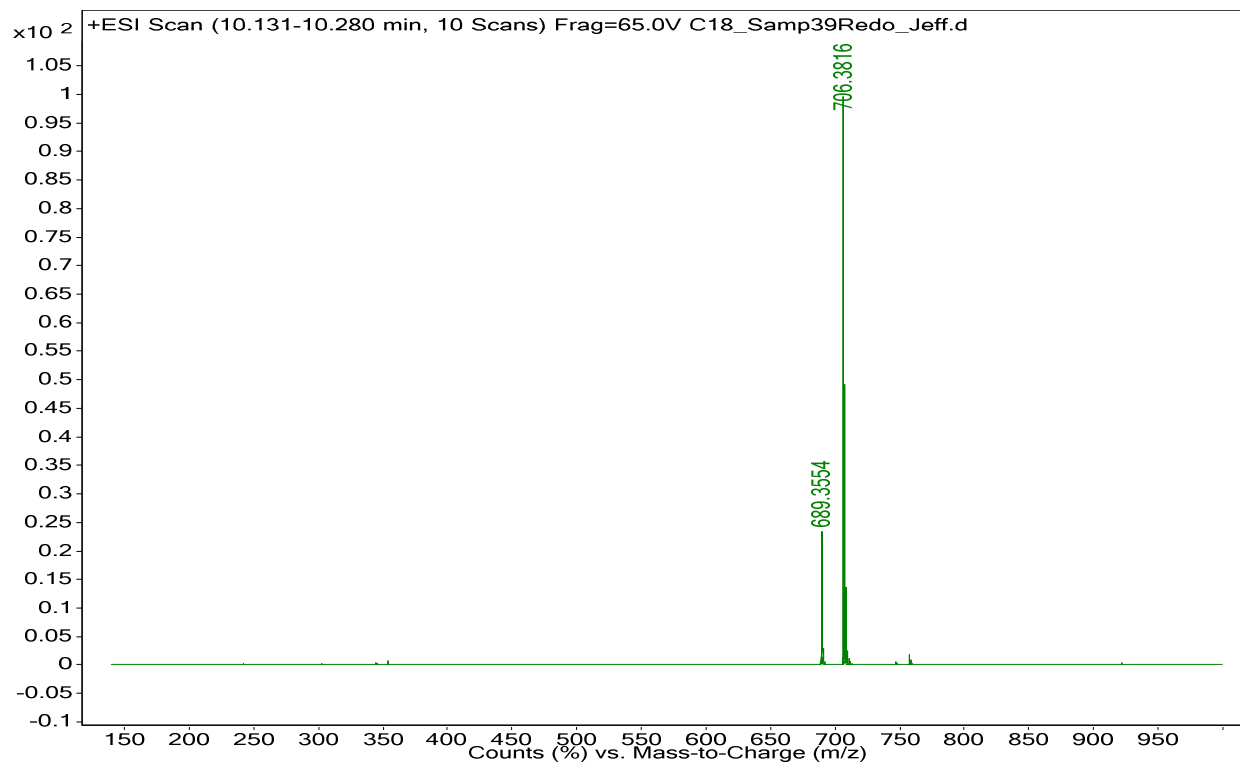
F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 63.288 ppm/cm: 0.10538

F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 127.375 ppm/cm: 0.21210

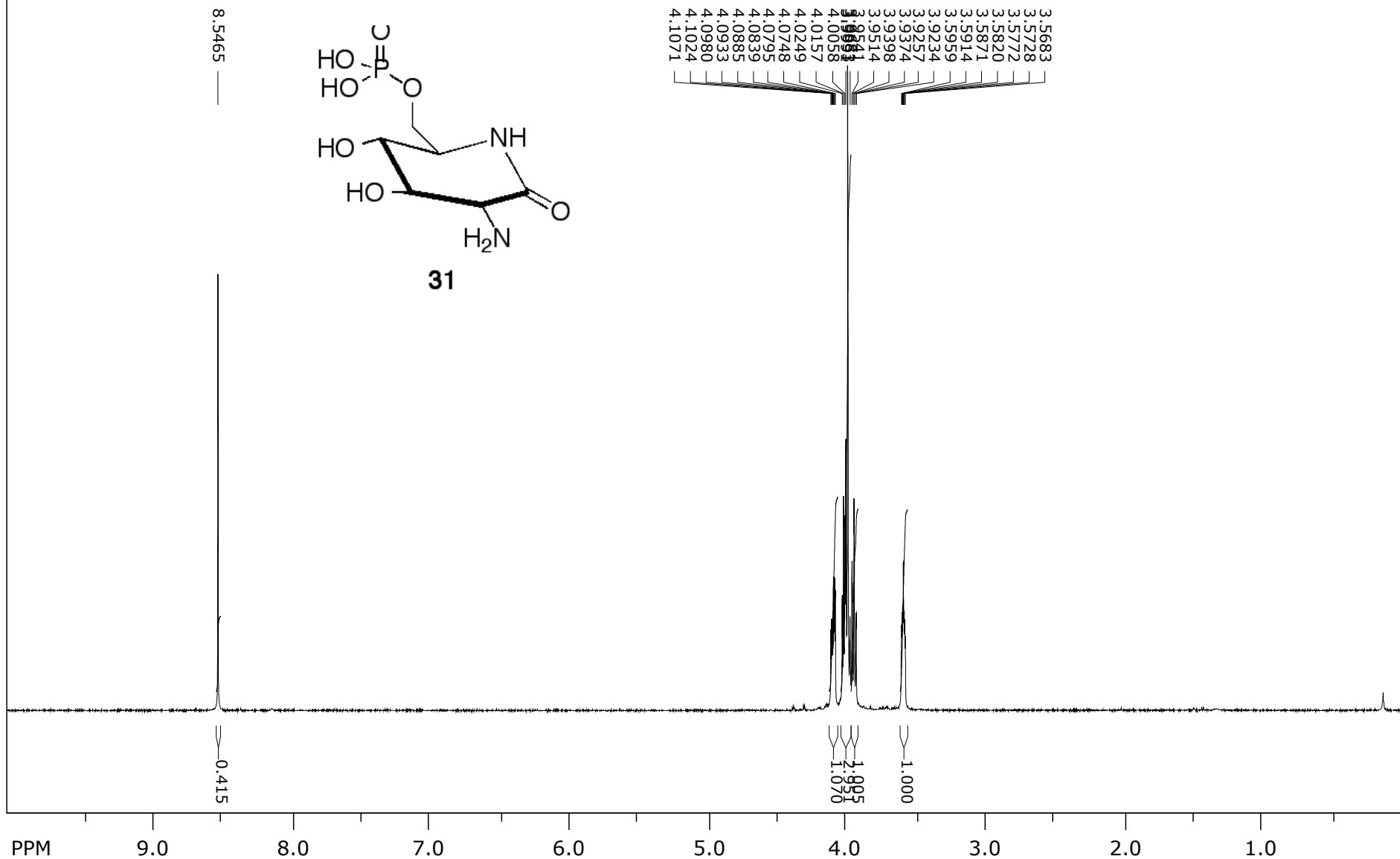


file: ...m spectra\6OHPiv2lactNZ_dmsol1\fid expt: <zgpg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 22528

freq. of 0 ppm: 151.008491 MHz
processed size: 32768 complex points
LB: 2.000 GF: 0.0000
Hz/cm: 1024.434 ppm/cm: 6.78328



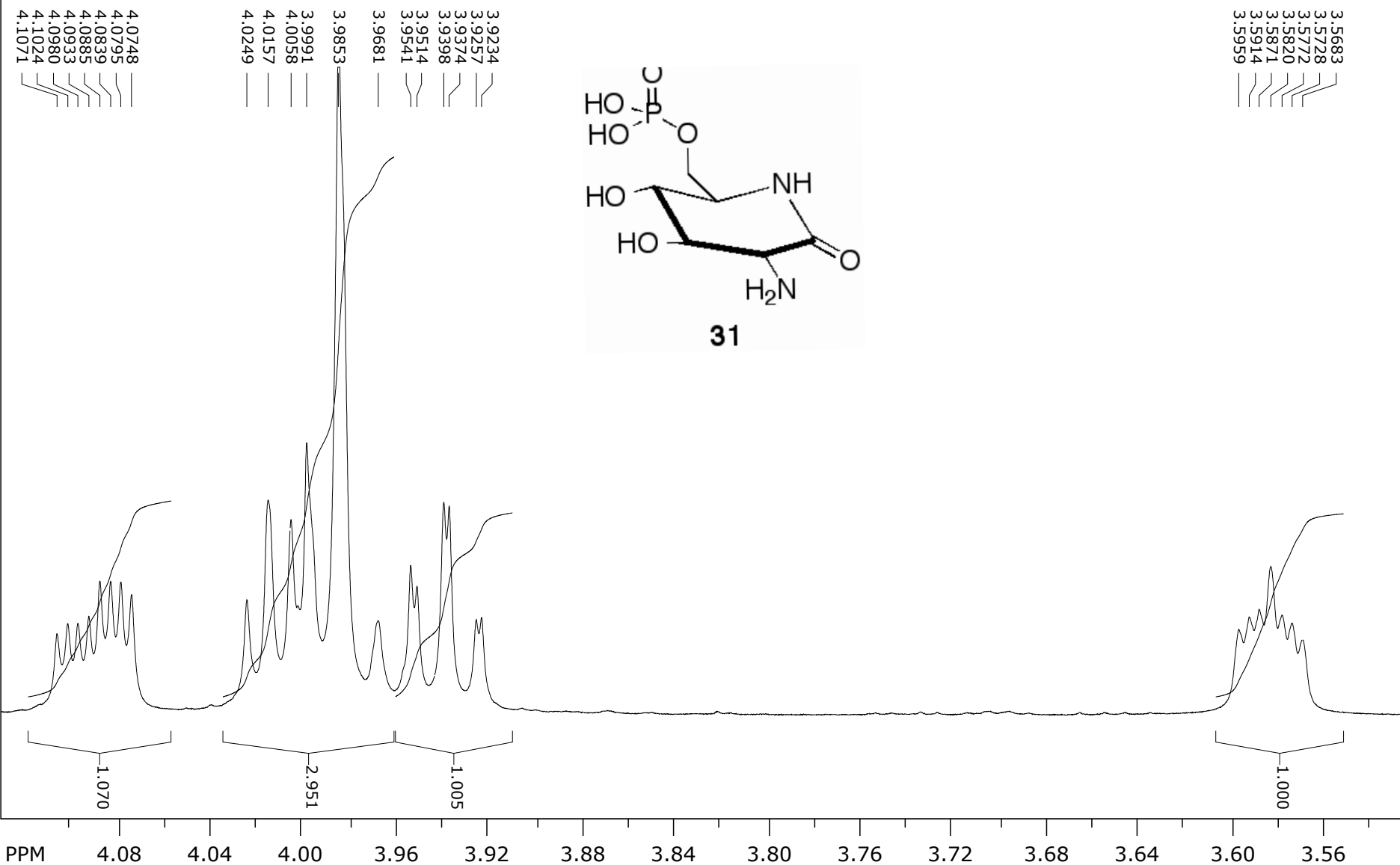
with residual Ammonium Formate



file: ...MR Data\Lactam6PinD2OwAmForm\2\fid expt: <zgpr>
 transmitter freq.: 600.552832 MHz
 time domain size: 65536 points
 width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
 number of scans: 32

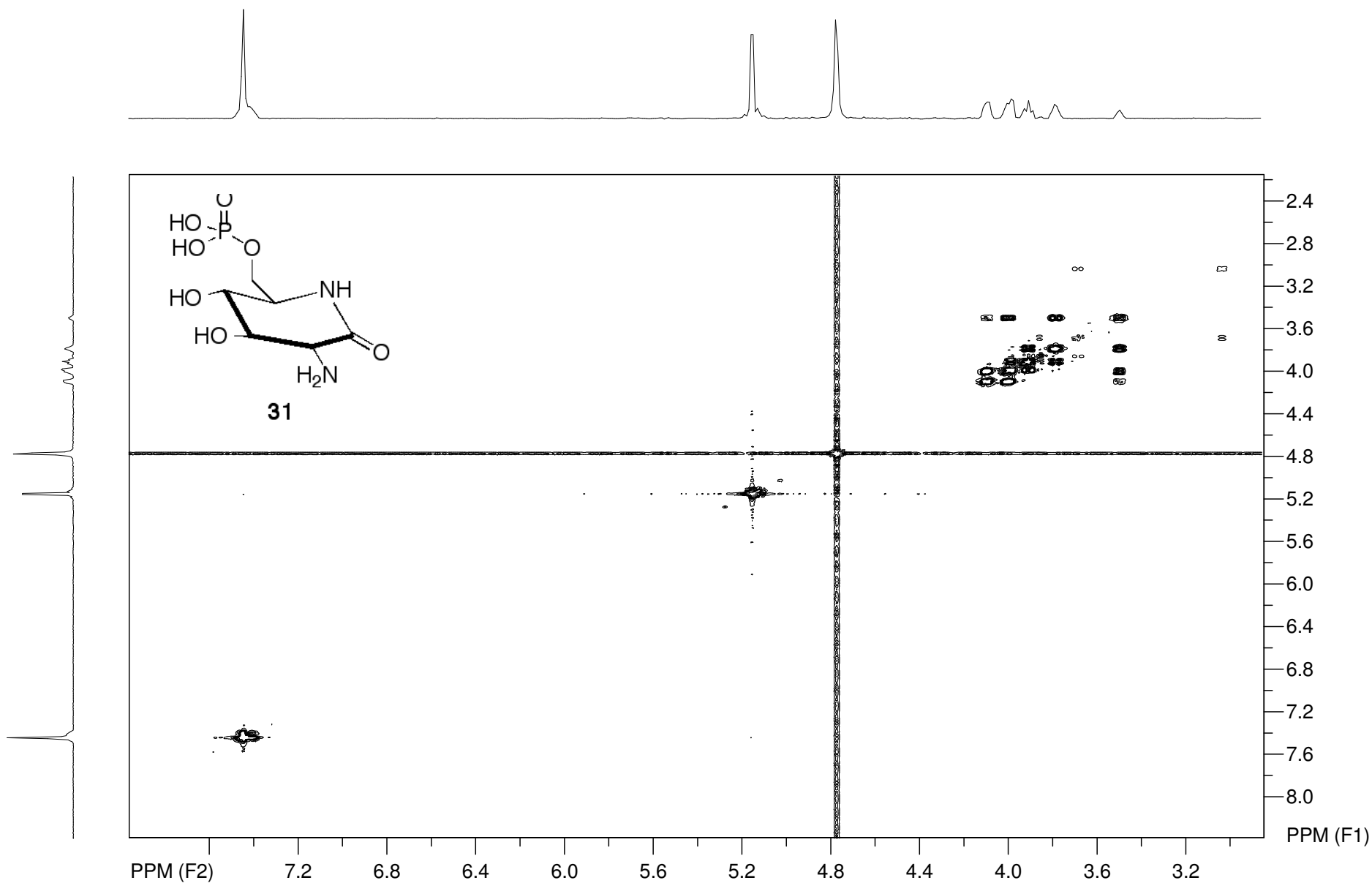
freq. of 0 ppm: 600.549962 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 243.604 ppm/cm: 0.40563

with residual Ammonium Formate



file: ...MR Data\Lactam6PinD2OwAmForm\2\fid exp: <zgpr>
 transmitter freq.: 600.552832 MHz
 time domain size: 65536 points
 width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
 number of scans: 32

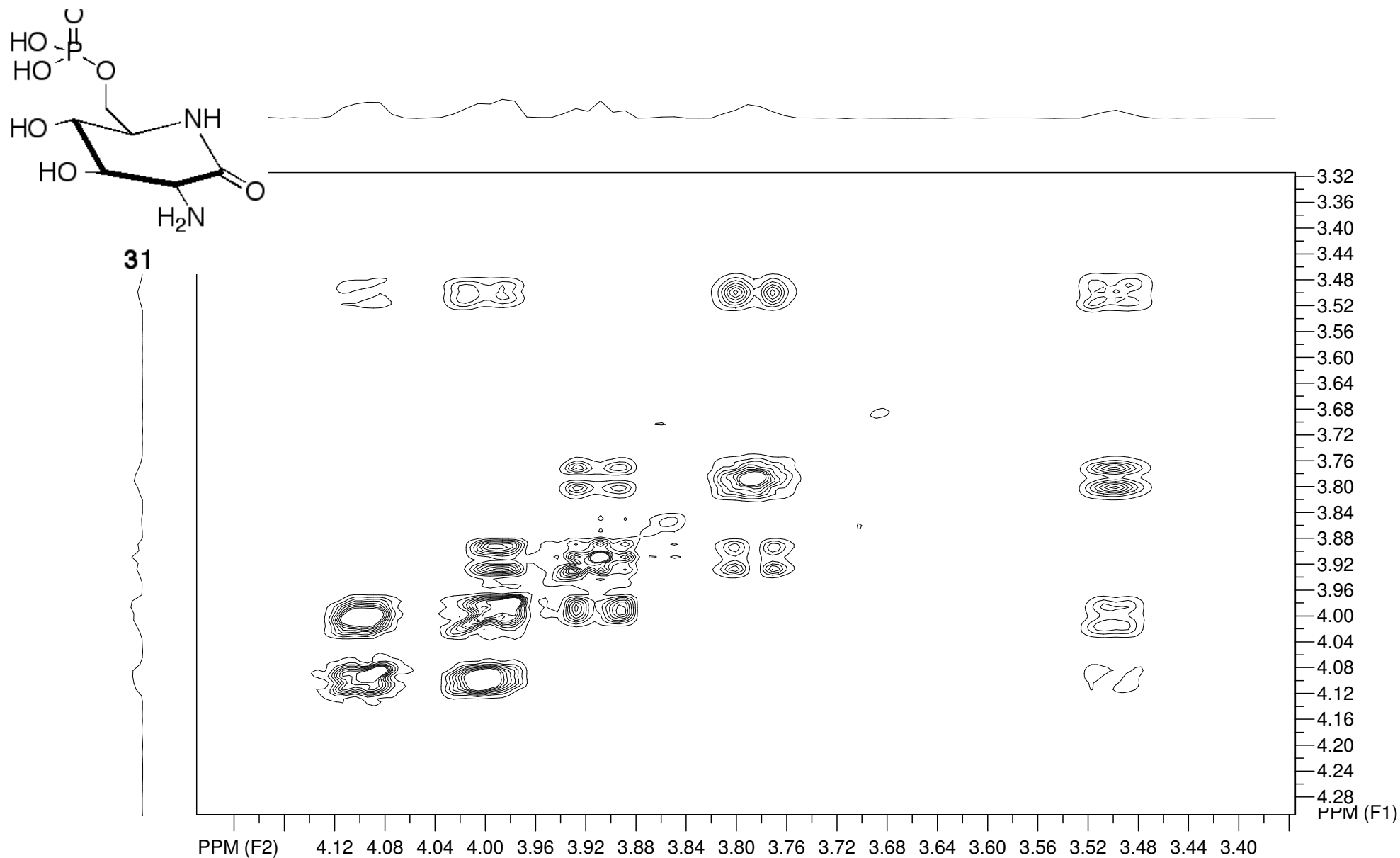
freq. of 0 ppm: 600.549962 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 14.624 ppm/cm: 0.02435



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\L6PNZ_D2O_COSY\1\ser exp: <cosygpqf>
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 149.805 ppm/cm: 0.24944

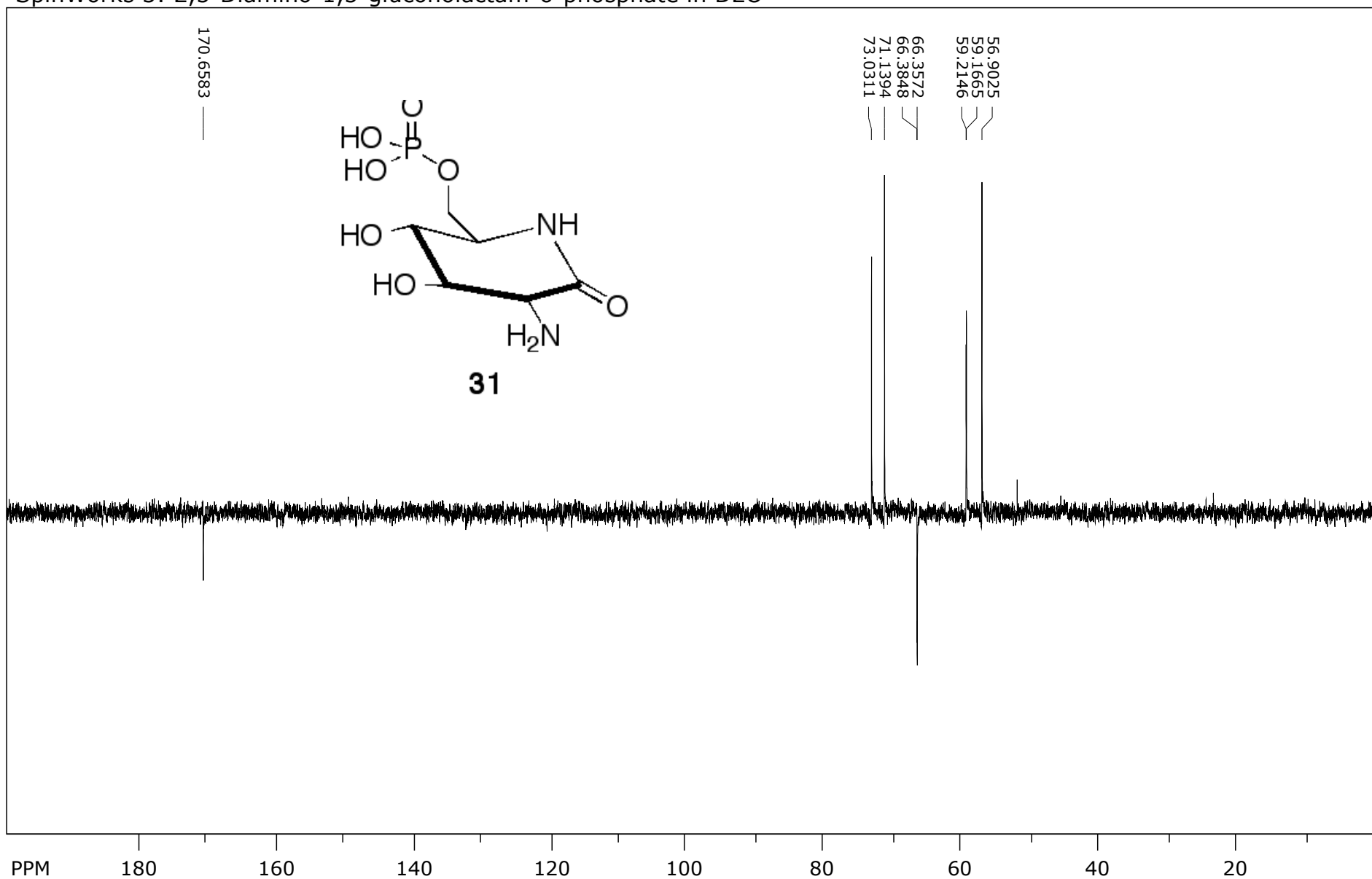
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 311.996 ppm/cm: 0.51951



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\L6PNZ_D2O_COSY\1\ser exp: <cosygpqf>
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 25.633 ppm/cm: 0.04268

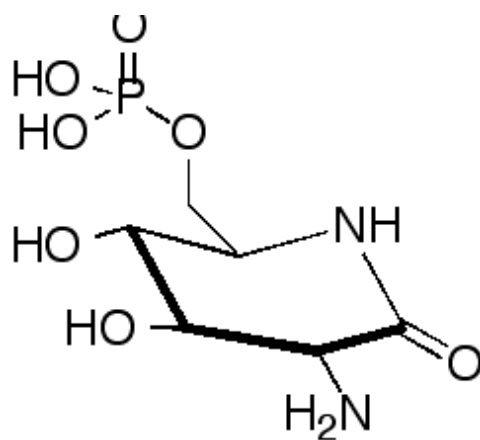
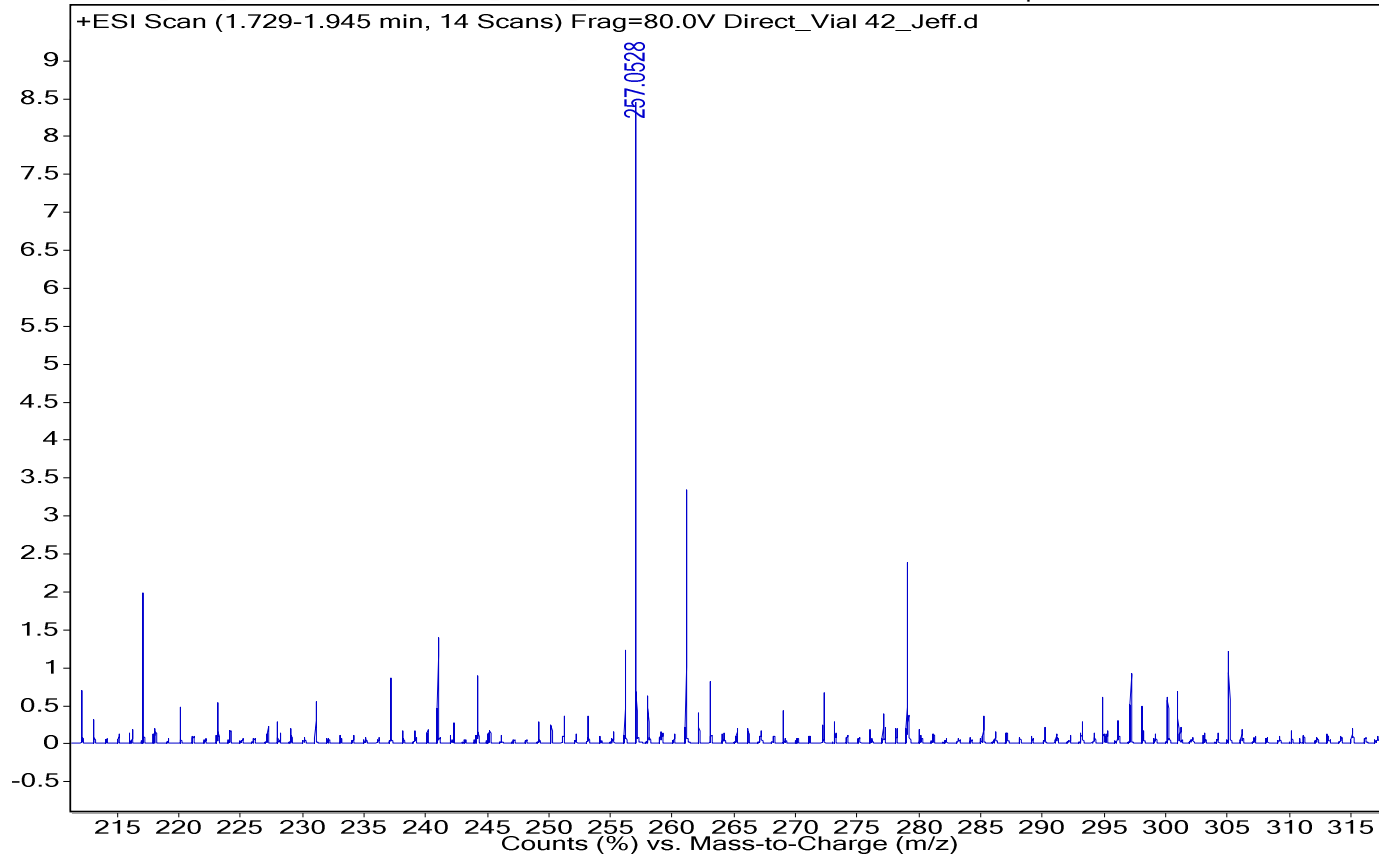
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 49.748 ppm/cm: 0.08284

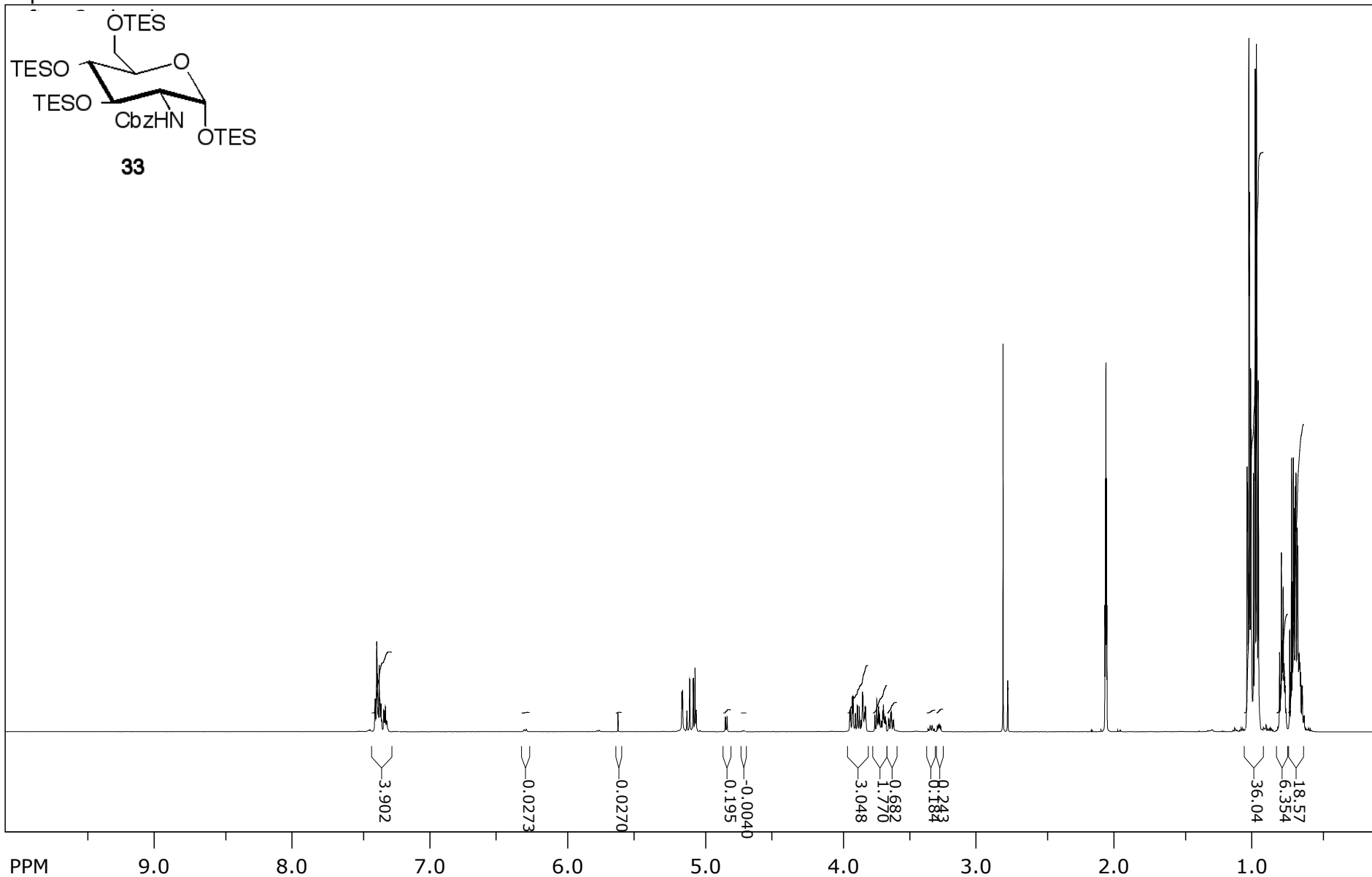


file: ...NMR Data\L6P_DEPTQ\L6P_DEPTQ\1\fid expt: <deptqgpp>
transmitter freq.: 151.023522 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 25600

freq. of 0 ppm: 151.008006 MHz
processed size: 32768 complex points
LB: 3.000 GF: 0.0000
Hz/cm: 1210.786 ppm/cm: 8.01720

Sample Name	Jeff 42	Position	Vial 42	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 42_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 1:51:49 PM

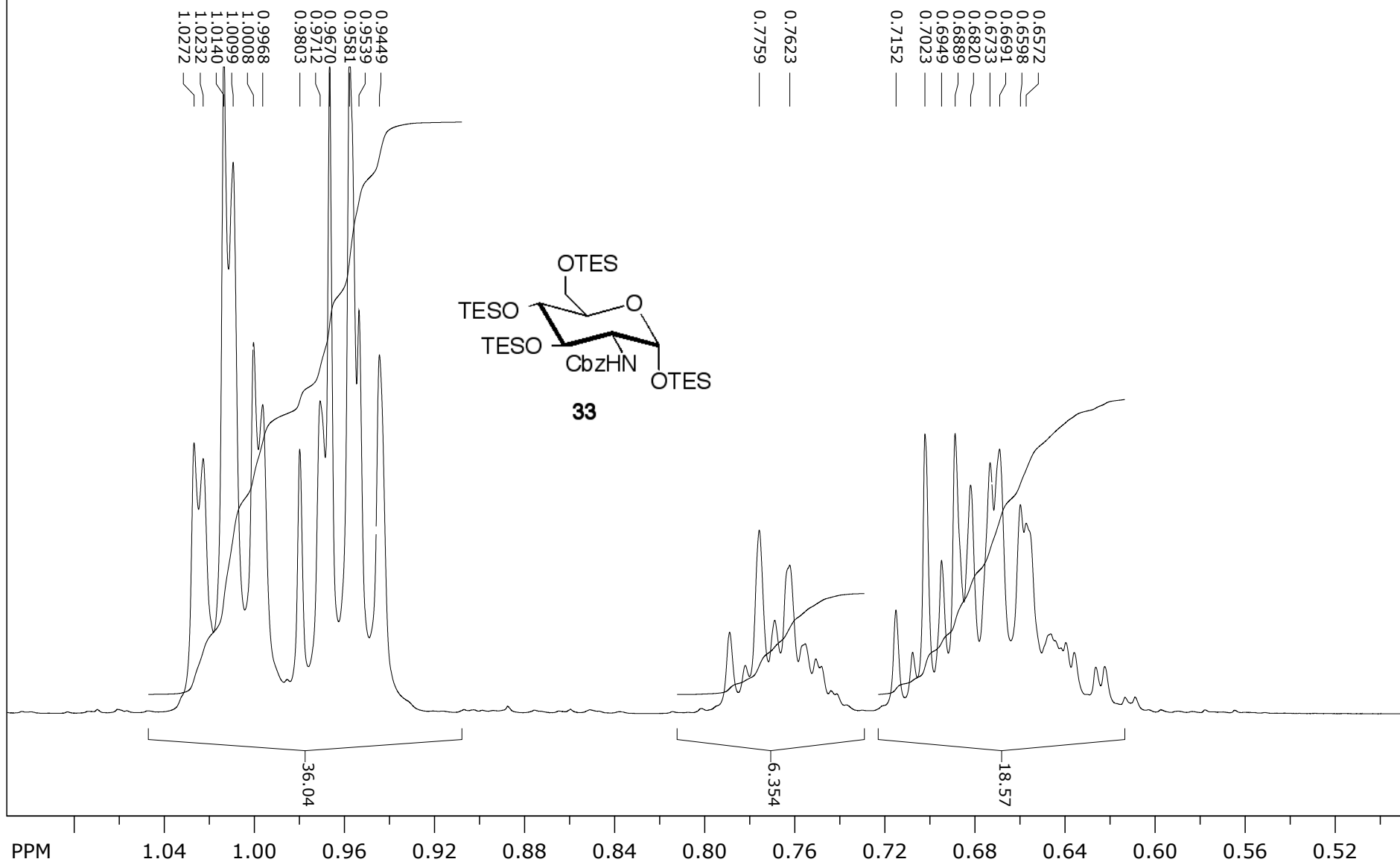
**31**



file: ... process\TES4GlcNZ_d6acetone\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 241.440 ppm/cm: 0.40203

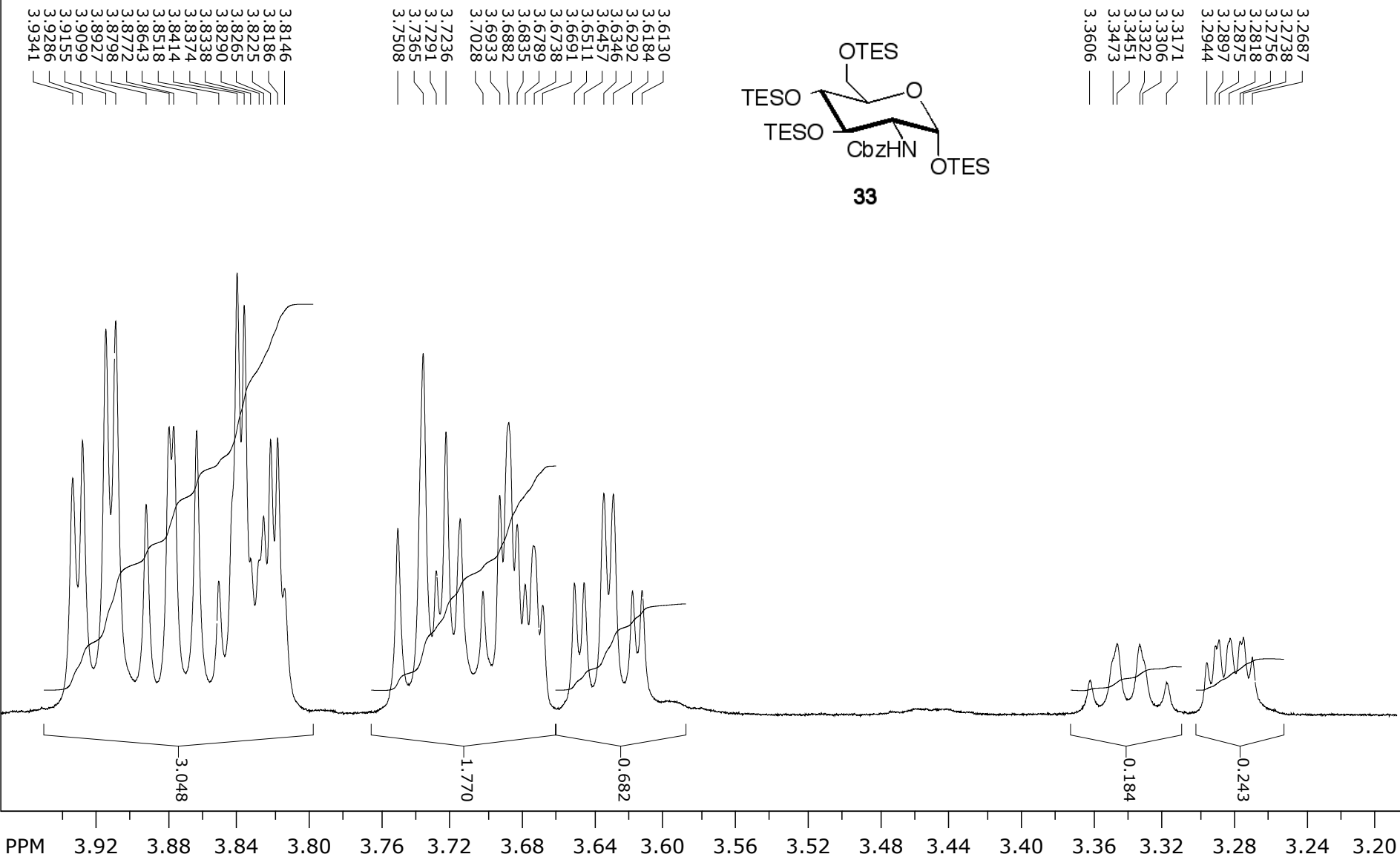
after 2nd column



file: ... process\TES4GlcNZ_d6acetone\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 14.971 ppm/cm: 0.02493

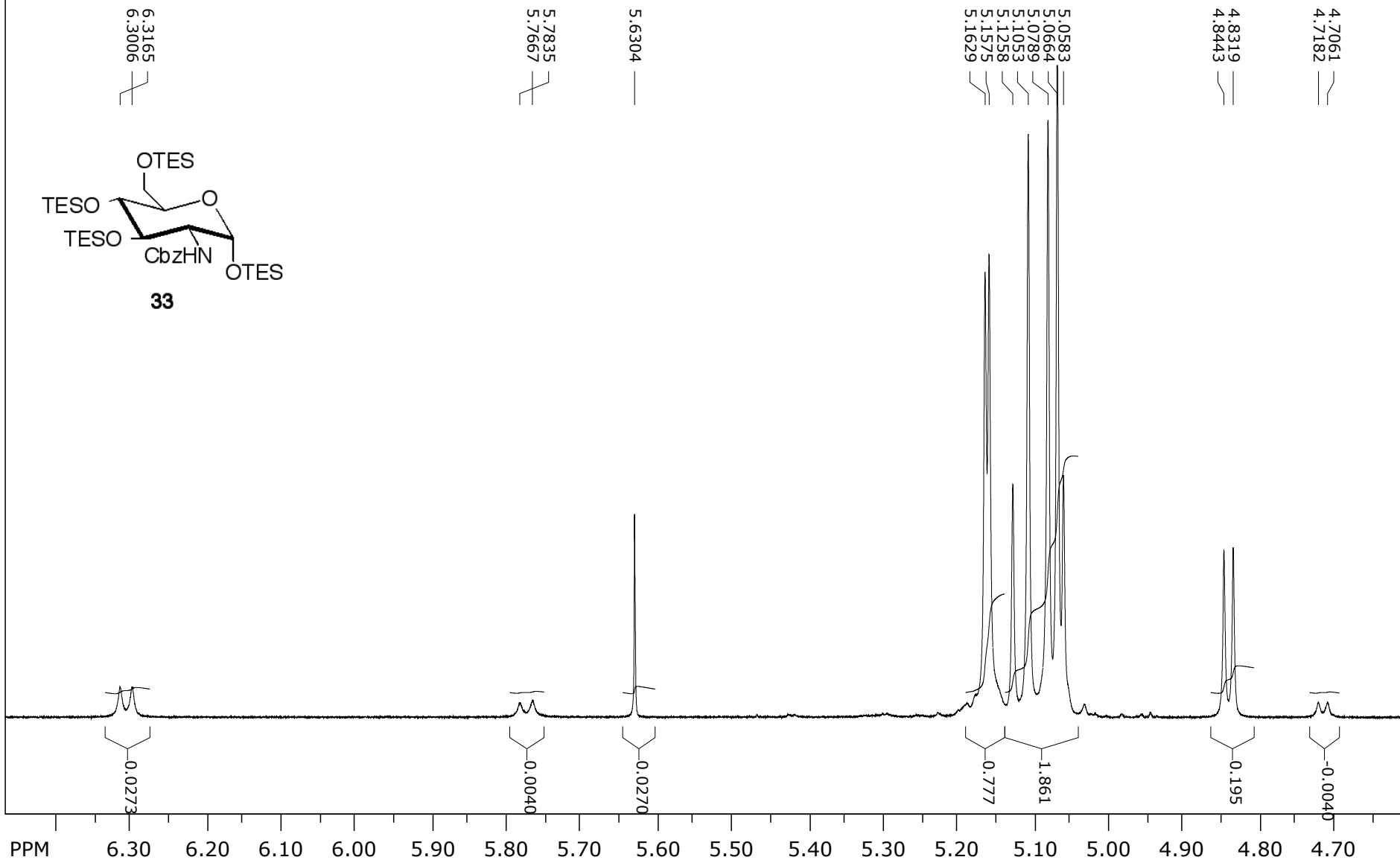
after 2nd column



file: ... process\TES4GlcNZ_d6acetone\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
 number of scans: 32

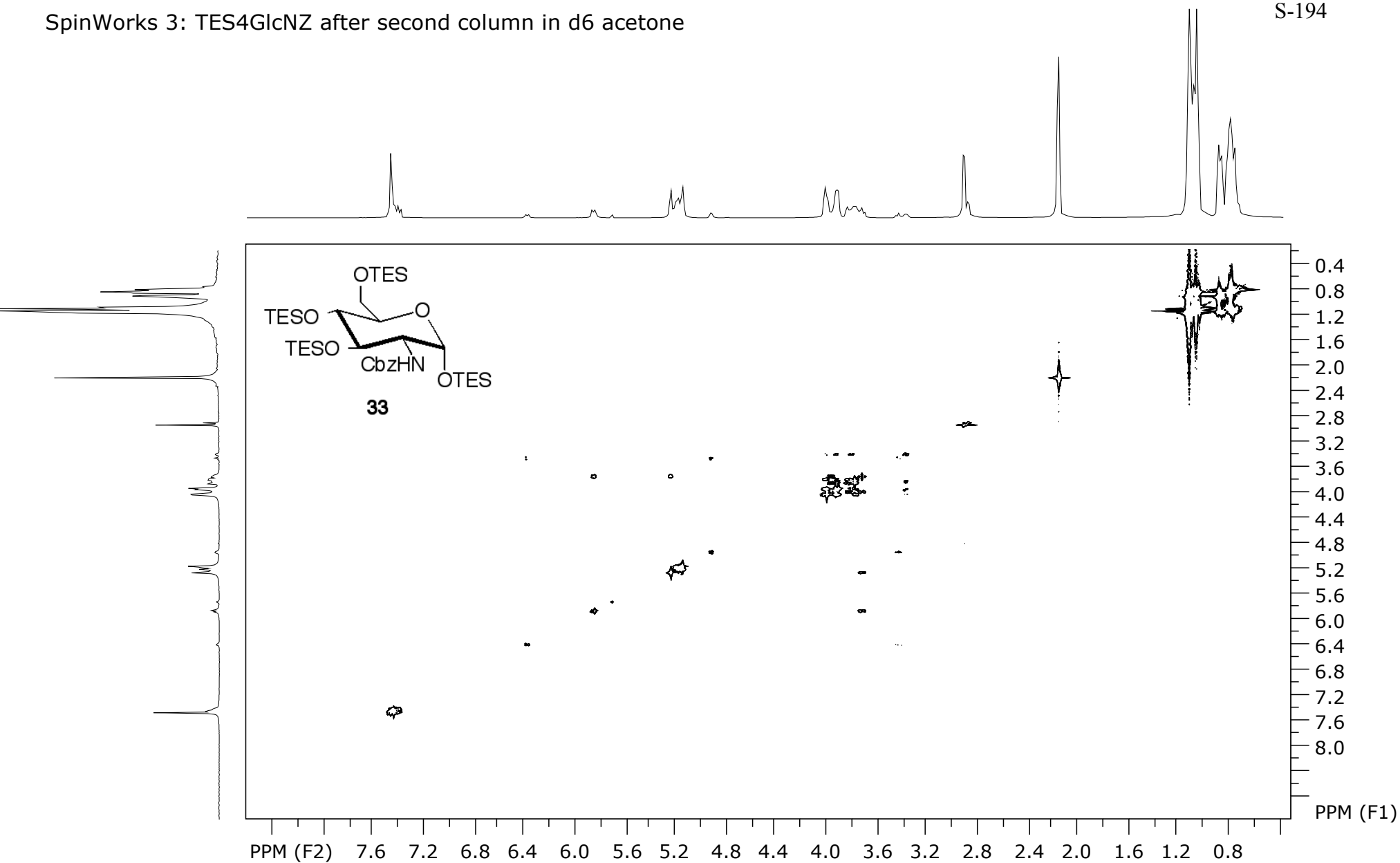
freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 18.922 ppm/cm: 0.03151

after 2nd column



file: ... process\TES4GlcNZ_d6acetone\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 32

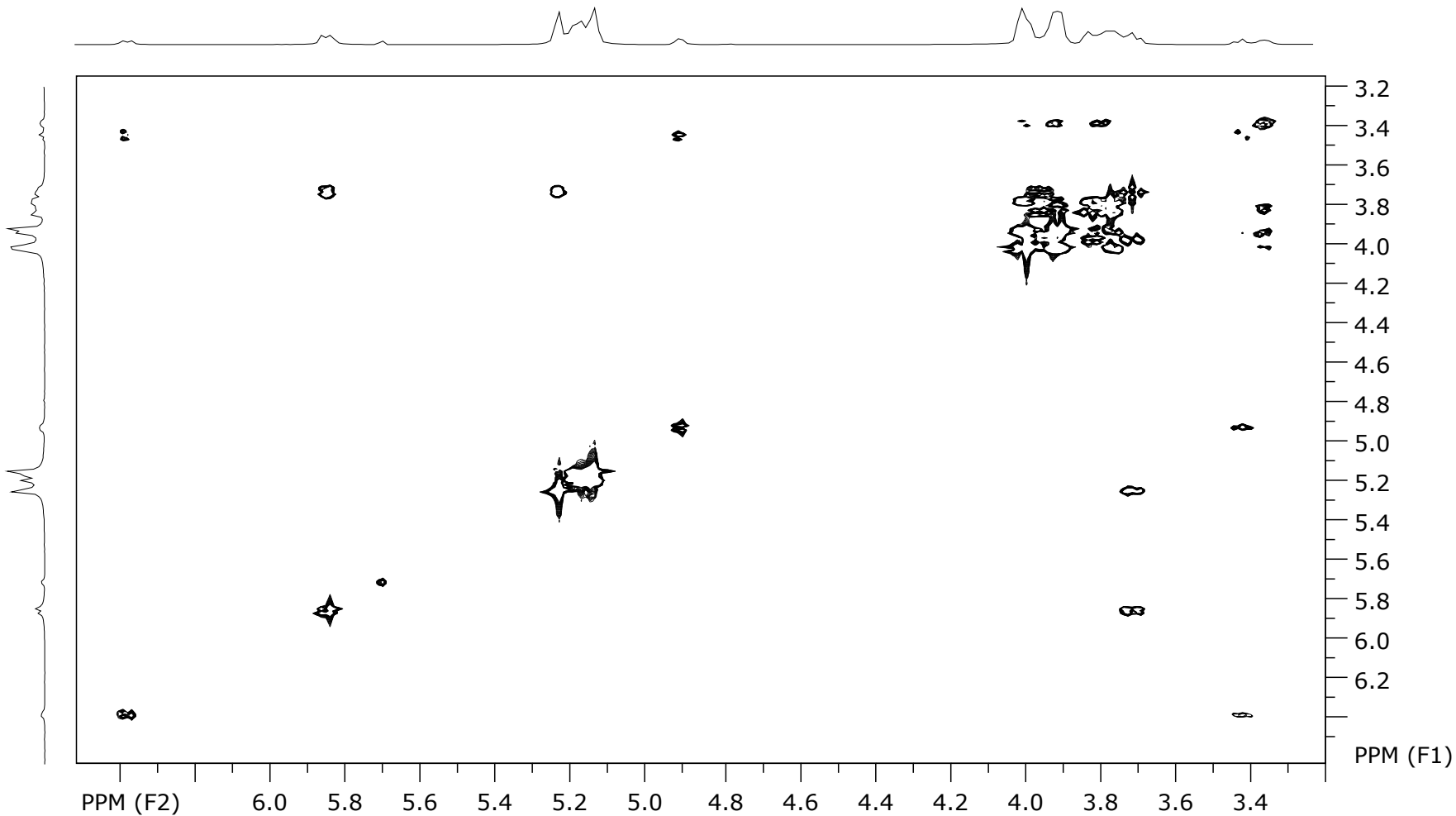
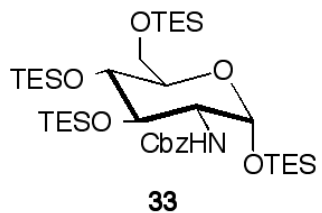
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 44.906 ppm/cm: 0.07477



file: ...ocess\TES4GlcNZd6acetoneCOSY\1\ser
expt: <cosygpqf>
transmitter freq: 600.552832 MHz
time domain size: 2048 by 2048 points
width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
number of scans: 2

F2: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 249.443 ppm/cm: 0.41536

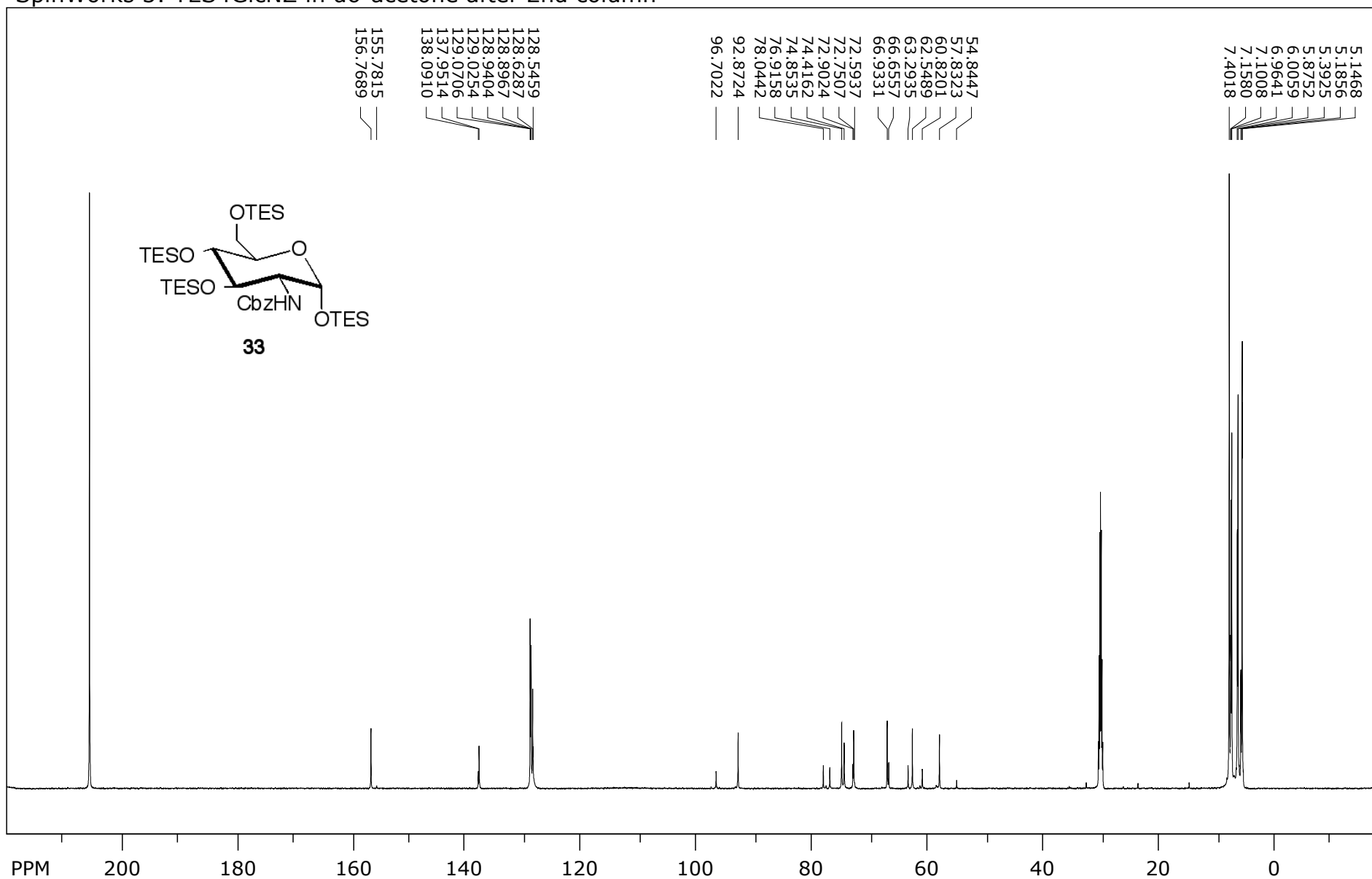
F1: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 495.237 ppm/cm: 0.82463



file: ...ocess\TES4GlcNZd6acetoneCOSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
 number of scans: 2

F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 99.306 ppm/cm: 0.16536

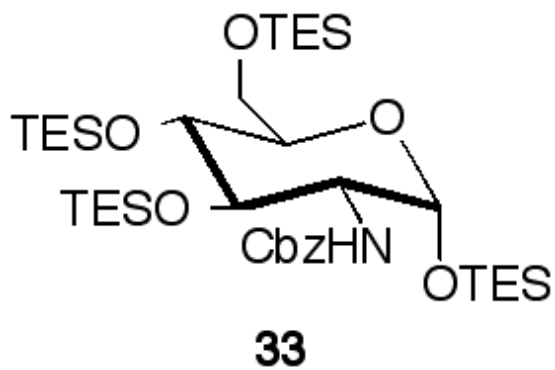
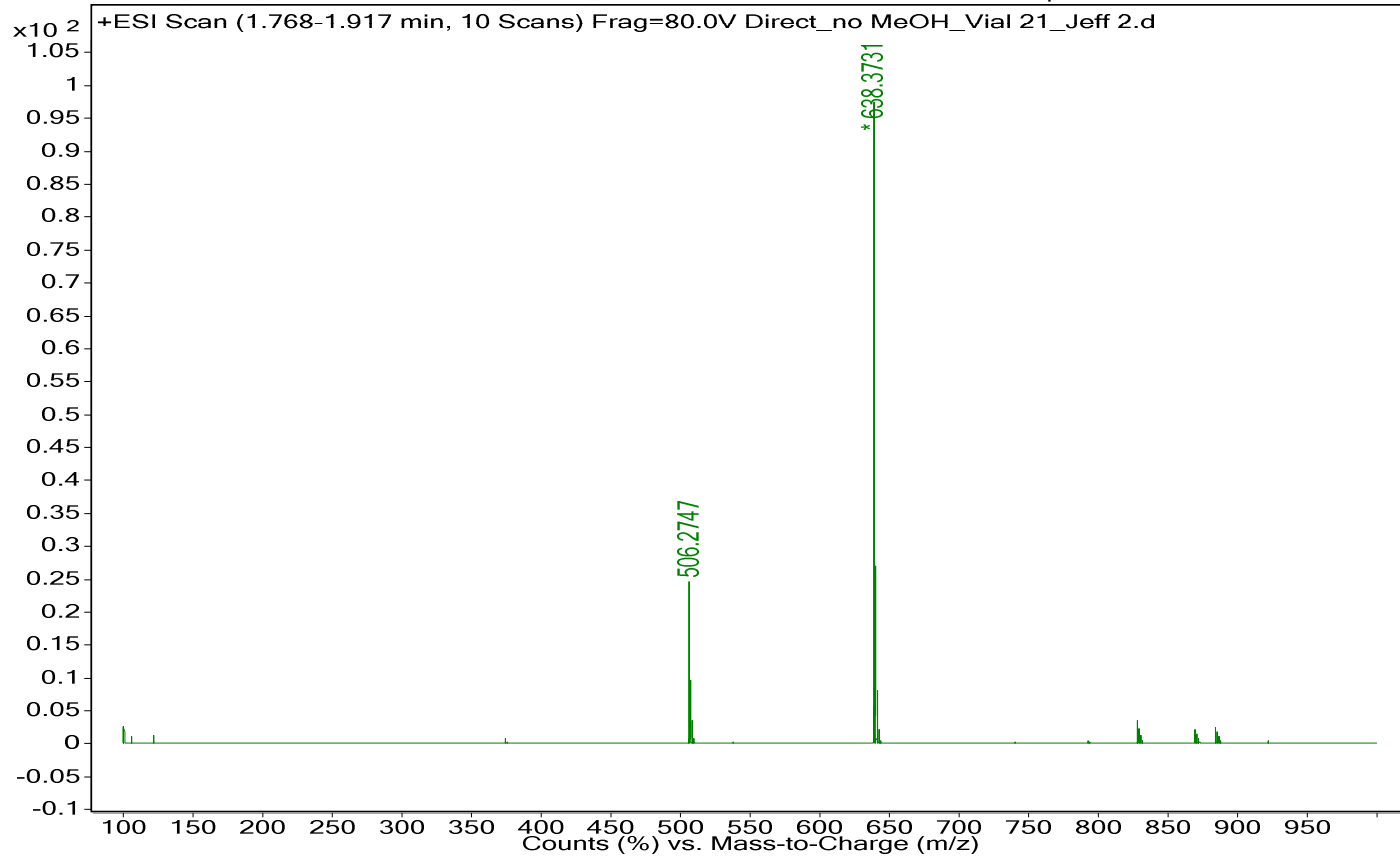
F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 190.359 ppm/cm: 0.31697

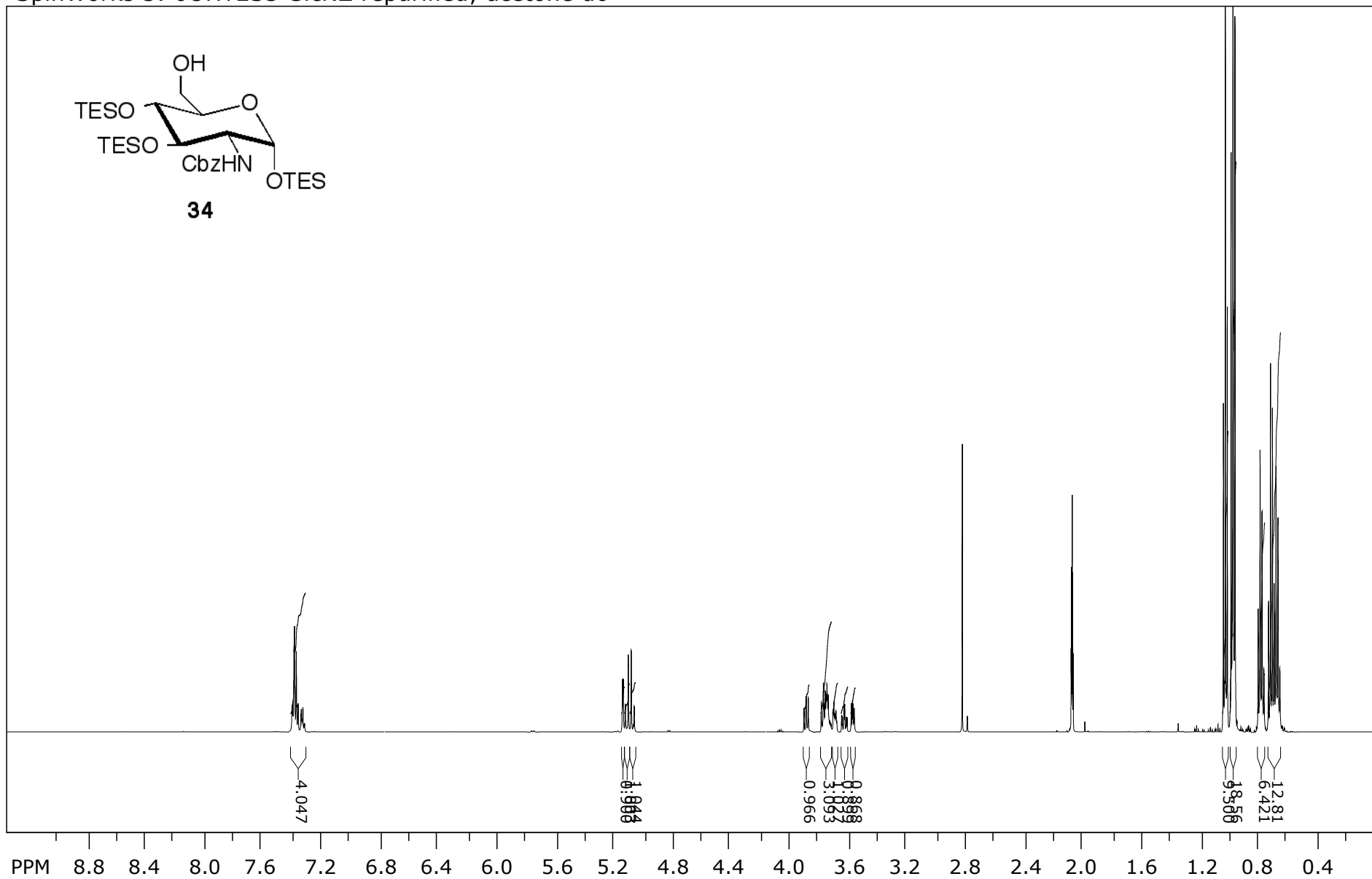
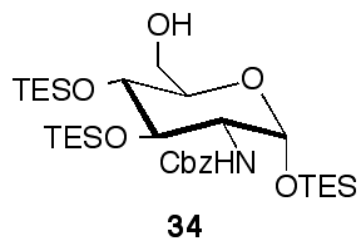


file: ...process\TES4GlcNZ_d6Acet_C13\1\fid expt: <zgpg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 4000

freq. of 0 ppm: 151.008298 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 1442.308 ppm/cm: 9.55022

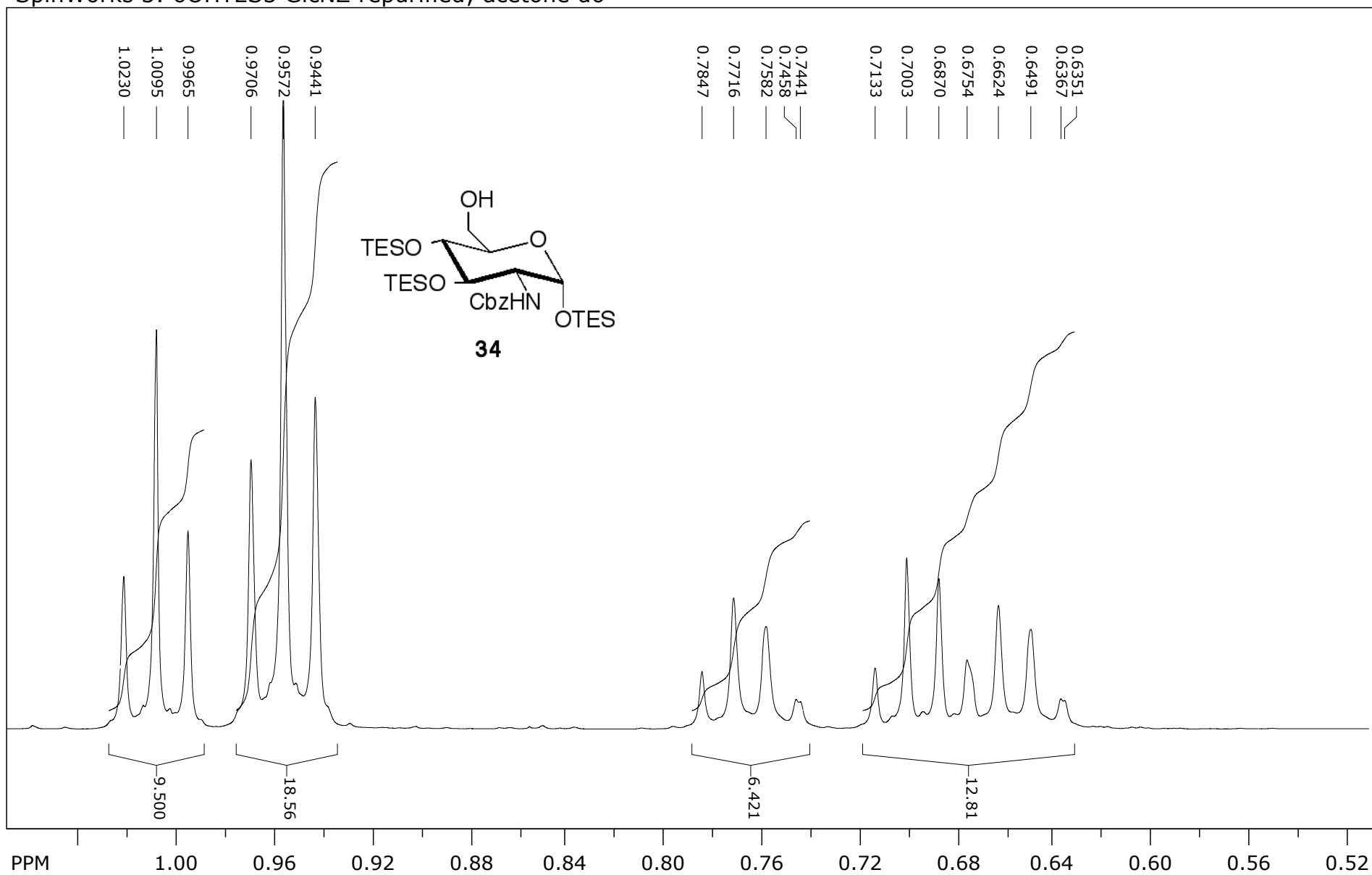
Sample Name	Jeff 21	Position	Vial 73	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_no MeOH_Vial	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/21/2012 1:39:28 PM





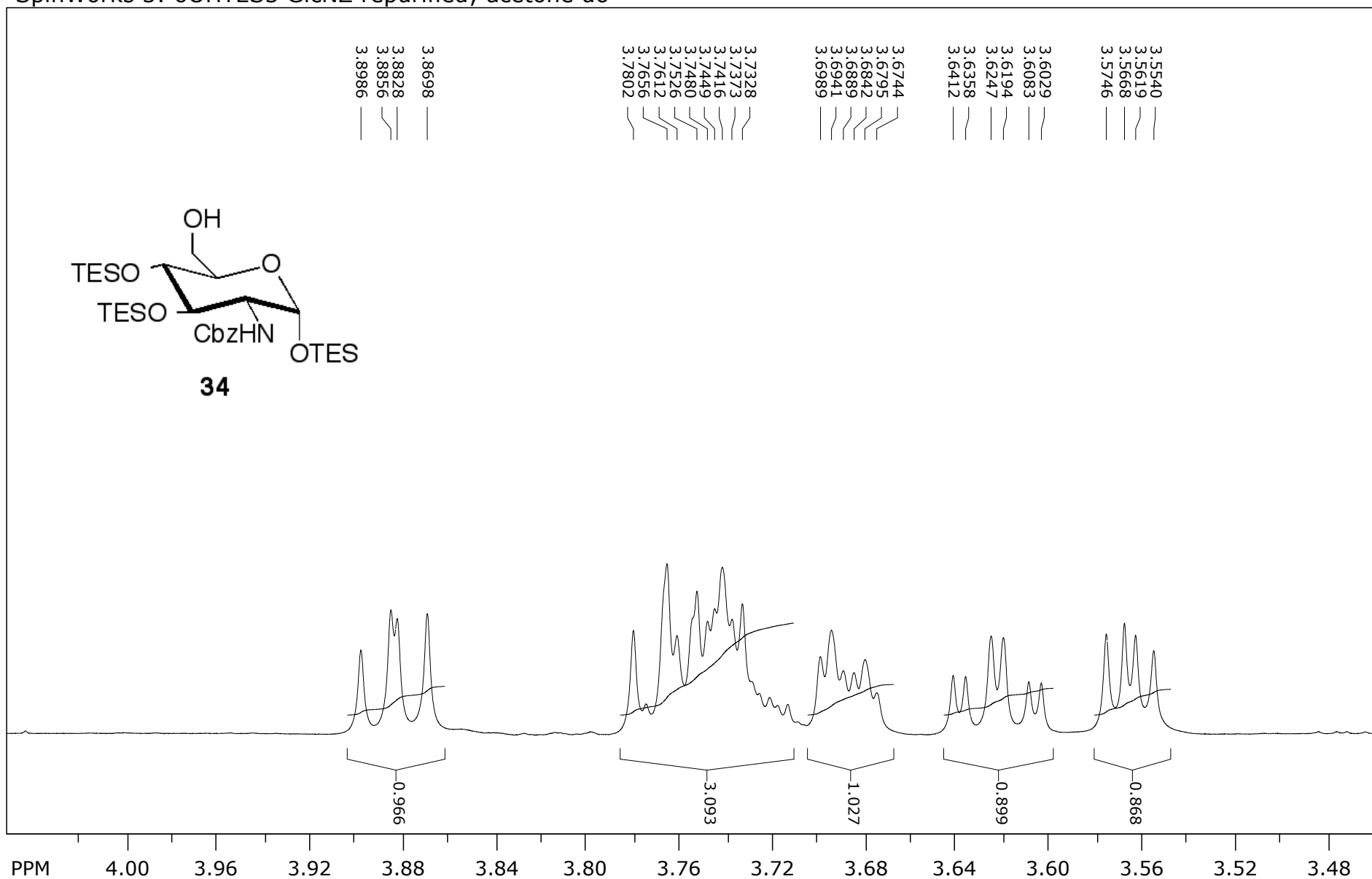
file: ... process\6OHTES3NZrepur_acet\1\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 226.004 ppm/cm: 0.37633



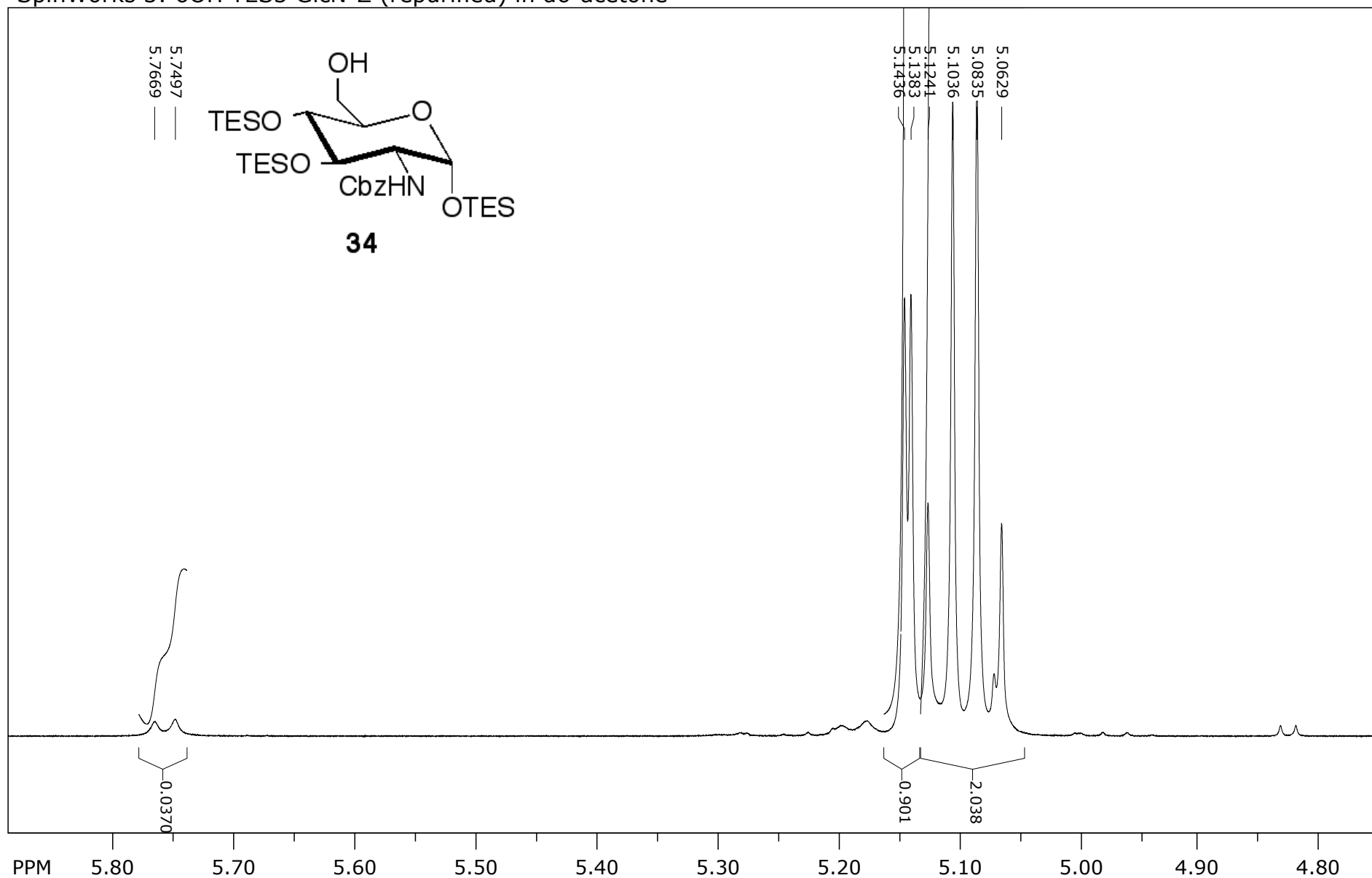
file: ... process\6OHTES3NZrepur_acet\1\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 13.495 ppm/cm: 0.02247



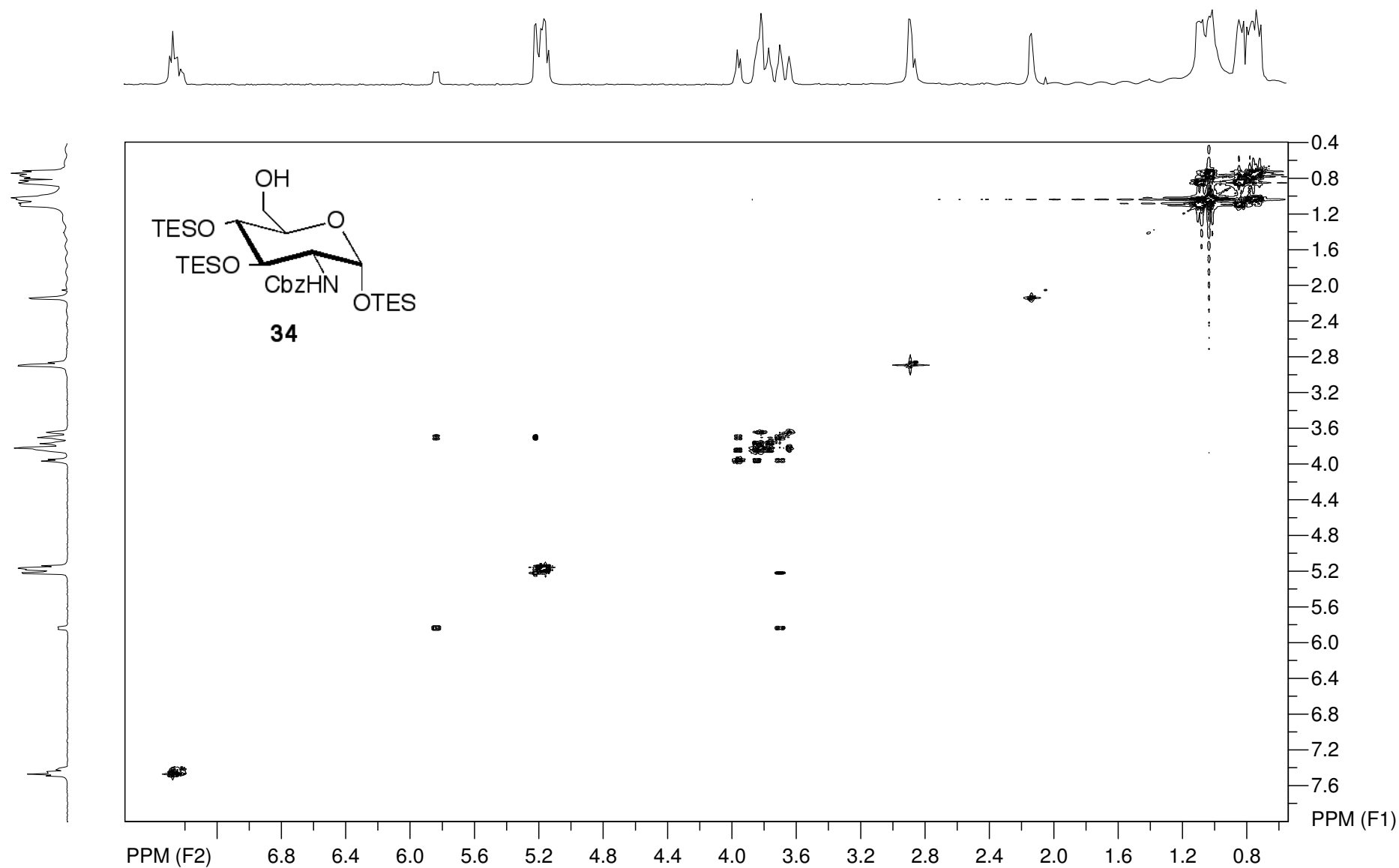
file: ... process\6OHTES3NZrepur_acet\1\fid exp: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 14.326 ppm/cm: 0.02386



file: ...NMR Data\6OHTES3NZrepur_acet\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

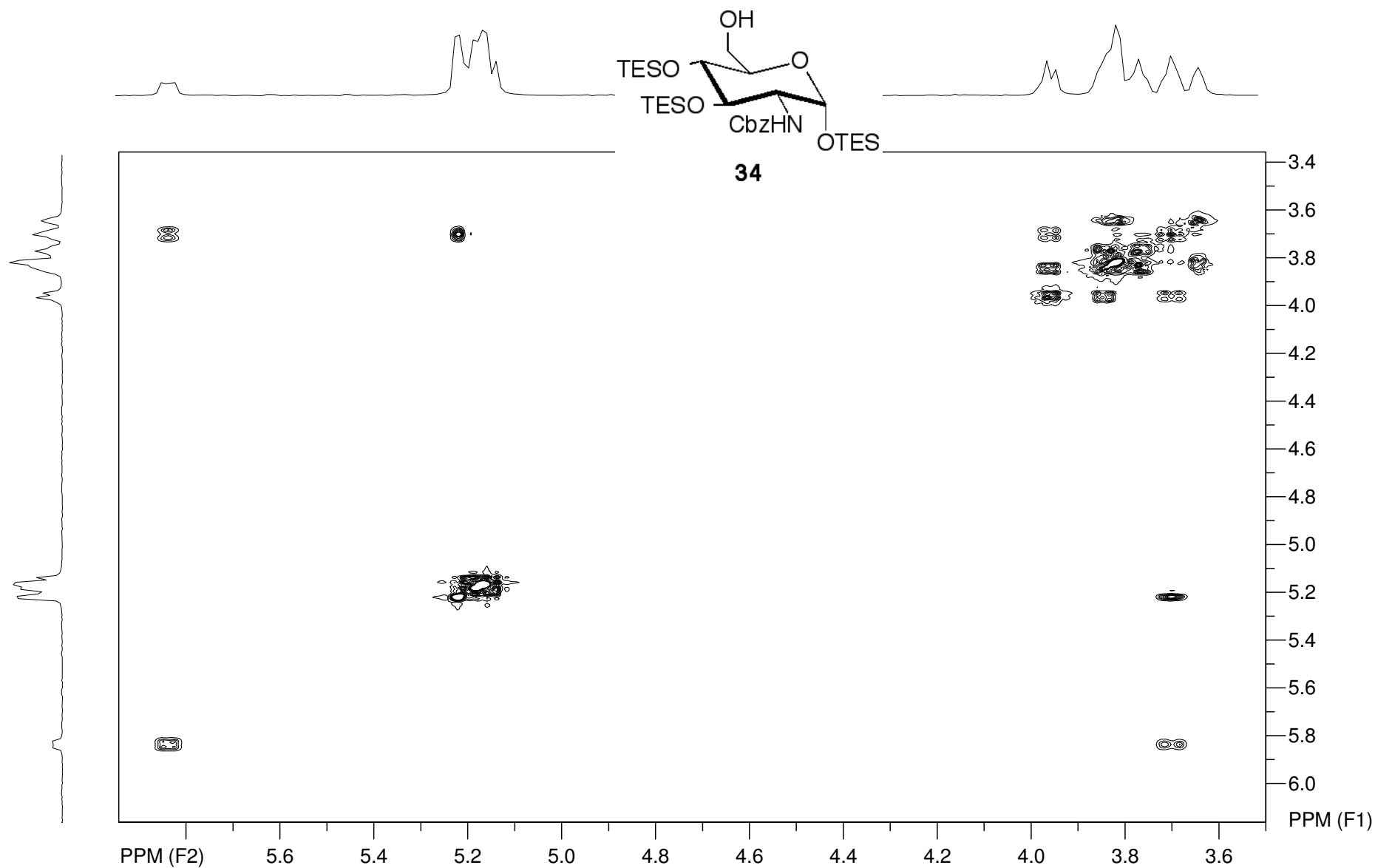
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 27.365 ppm/cm: 0.04557



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\6OHTES3NZrepur_COSYF2.:
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 211.793 ppm/cm: 0.35266

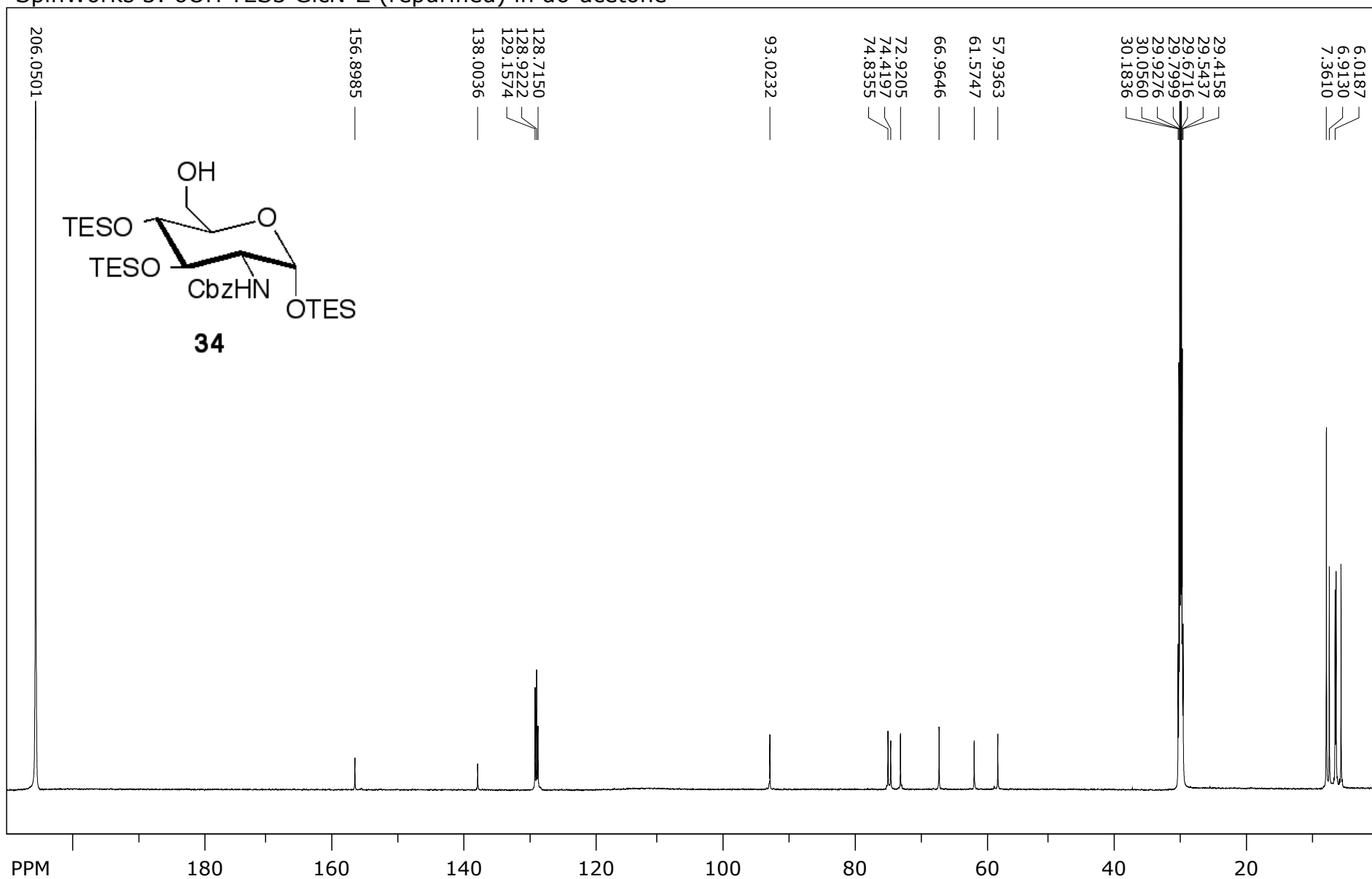
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 380.889 ppm/cm: 0.63423



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\6OHTES3NZrepur_COSYF2.:
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 71.575 ppm/cm: 0.11918

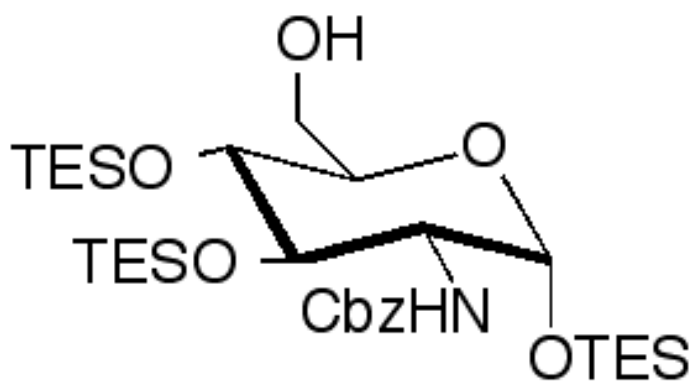
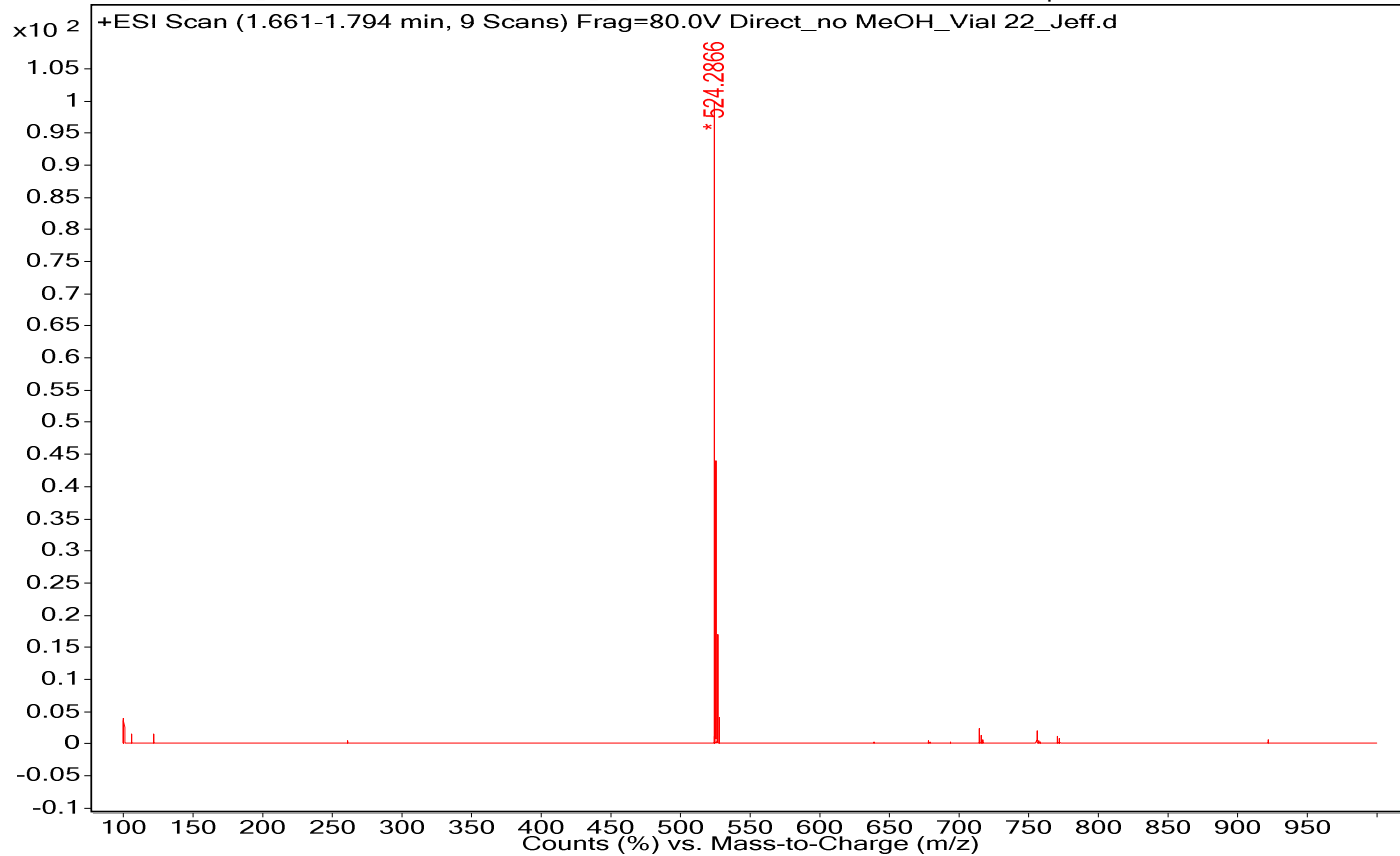
F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 140.423 ppm/cm: 0.23382

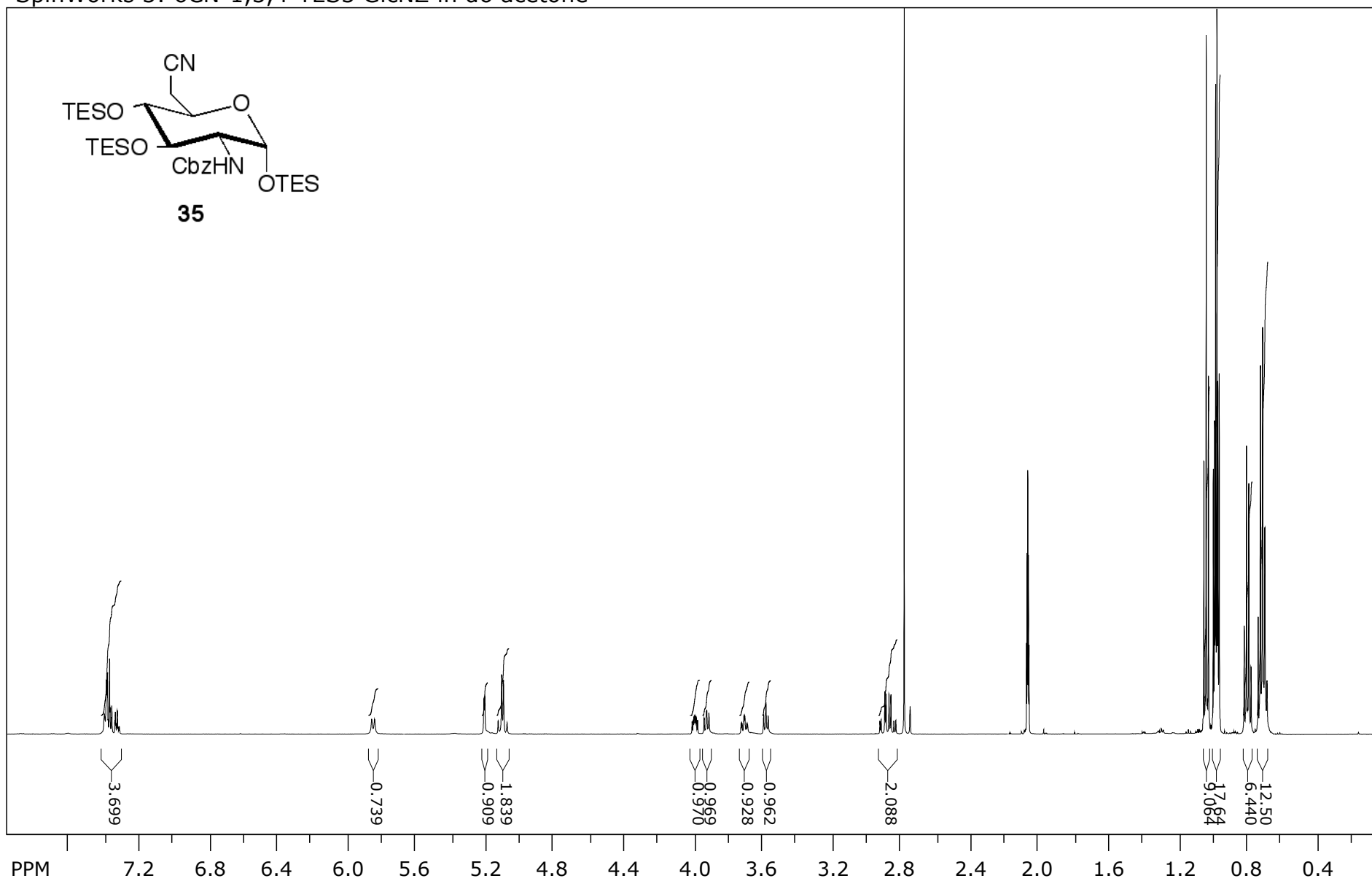


file: ... Data\6OHTES3NZrepur_acet13C\1\fid expt: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 22528

freq. of 0 ppm: 151.008289 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 1275.702 ppm/cm: 8.44704

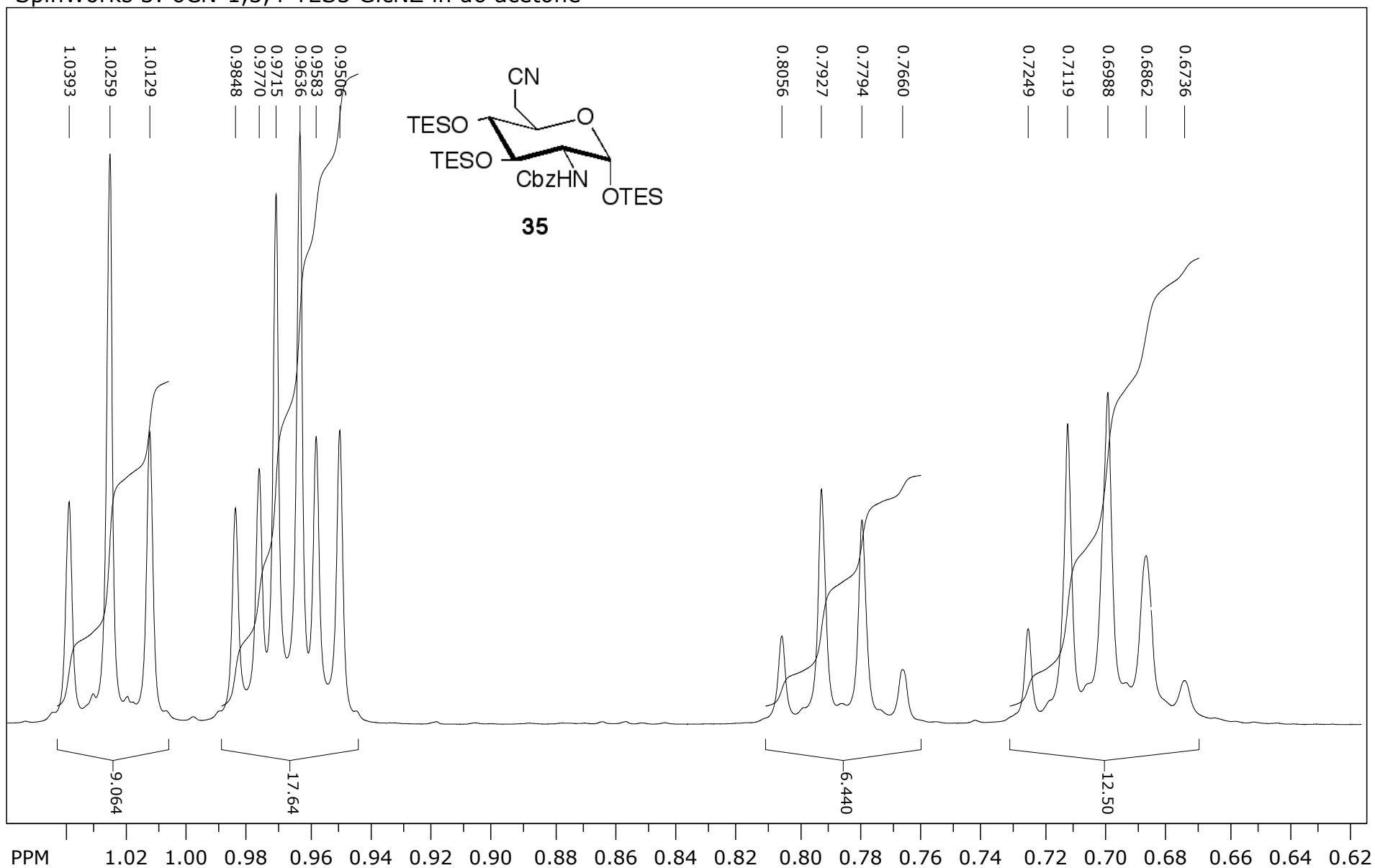
Sample Name	Jeff 22	Position	Vial 74	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_no MeOH_Vial	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/21/2012 1:48:46 PM

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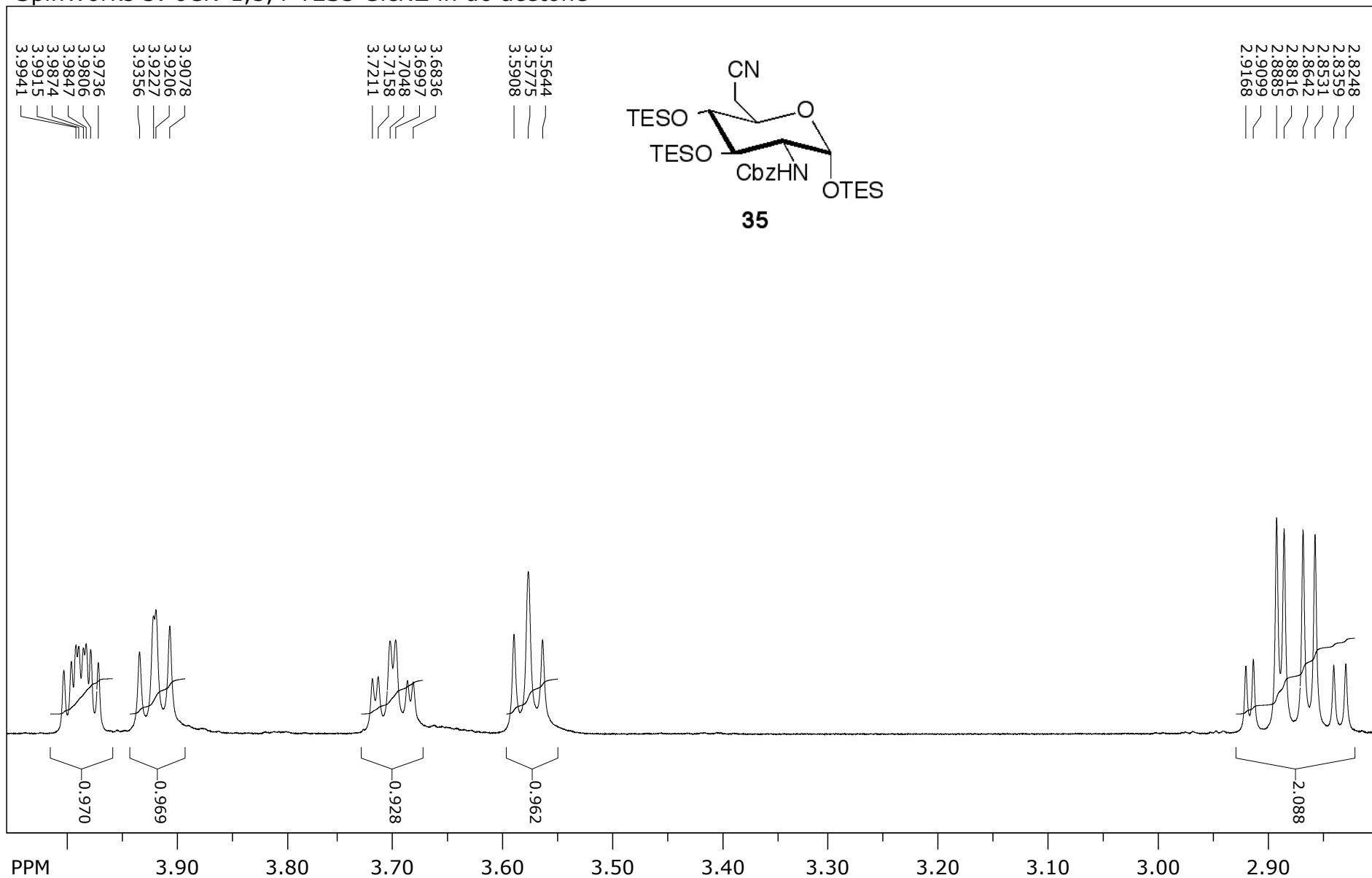
file: ...CNTES3GlcNZ_acet_p1optimized\2\fid expt: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 65536 points
width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
number of scans: 16

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 191.020 ppm/cm: 0.31807



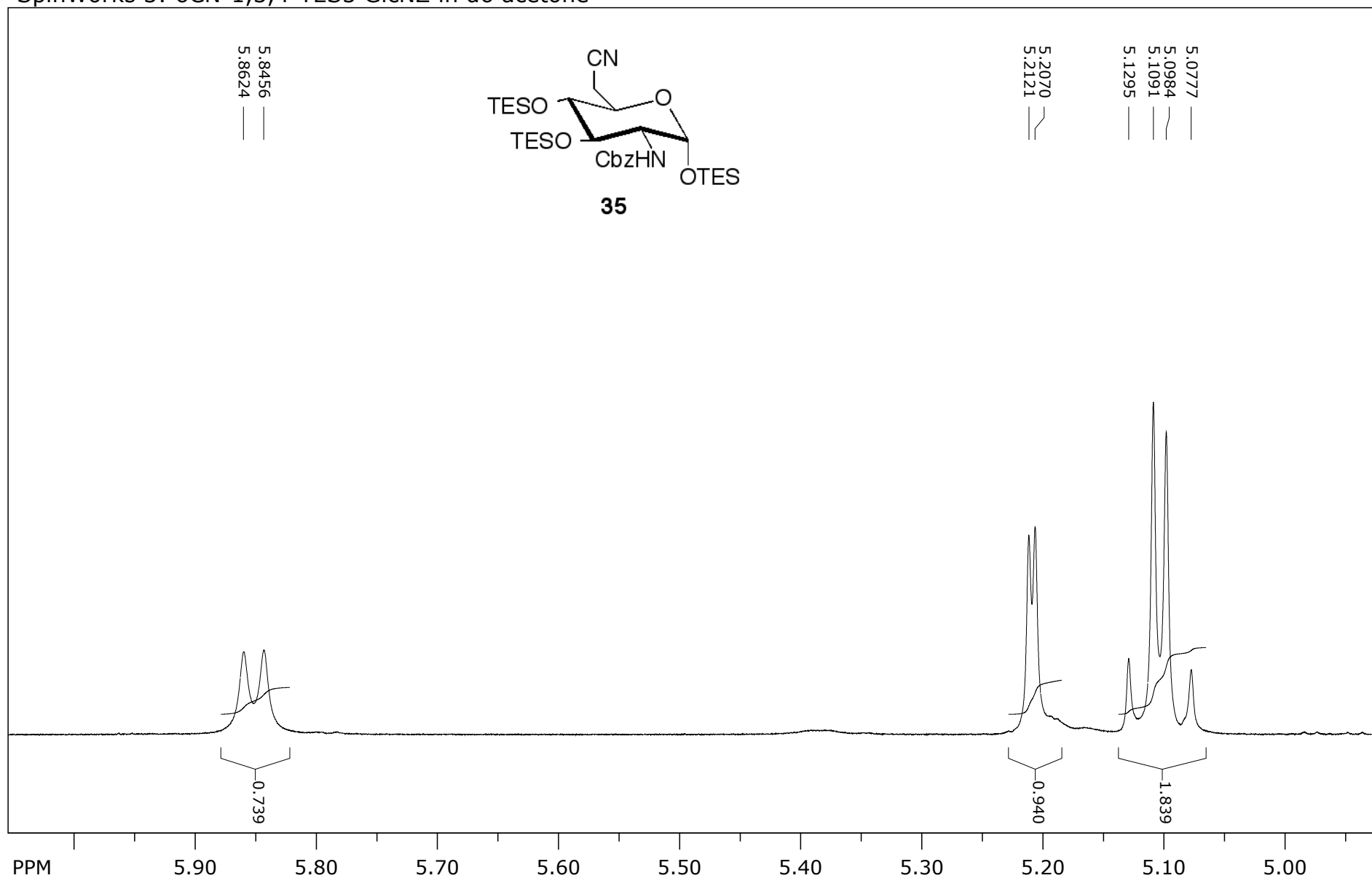
file: ...CNTES3GlcNZ_acet_p1optimized\2\fid expt: <zgpr>
 transmitter freq.: 600.552832 MHz
 time domain size: 65536 points
 width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
 number of scans: 16

freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 10.671 ppm/cm: 0.01777



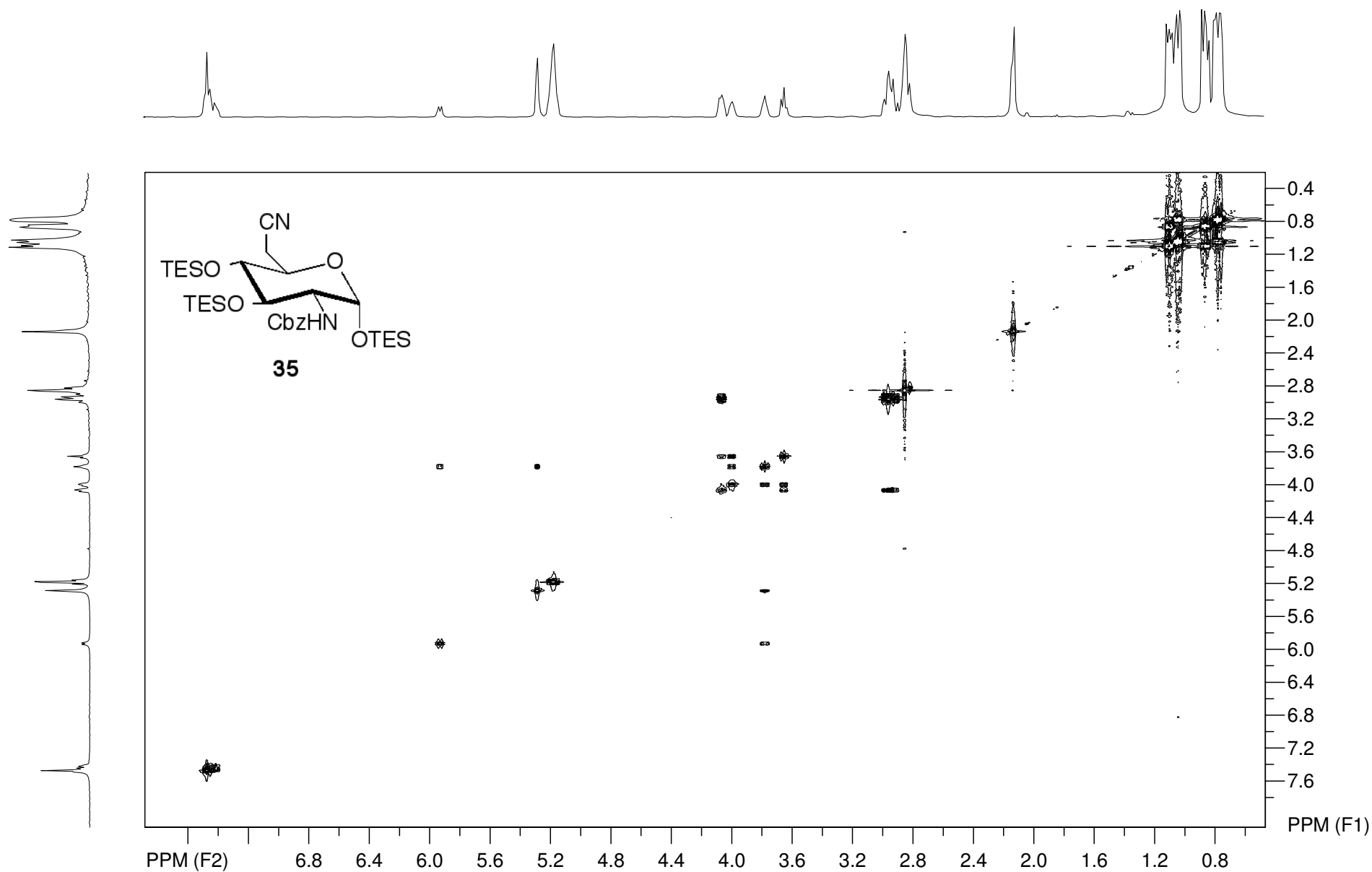
file: ...CNTES3GlcNZ_acet_p1optimized\2\fid expt: <zgpr>
 transmitter freq.: 600.552832 MHz
 time domain size: 65536 points
 width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
 number of scans: 16

freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 30.352 ppm/cm: 0.05054



file: ...CNTES3GlcNZ_acet_p1optimized\2\fid expt: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 65536 points
width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
number of scans: 16

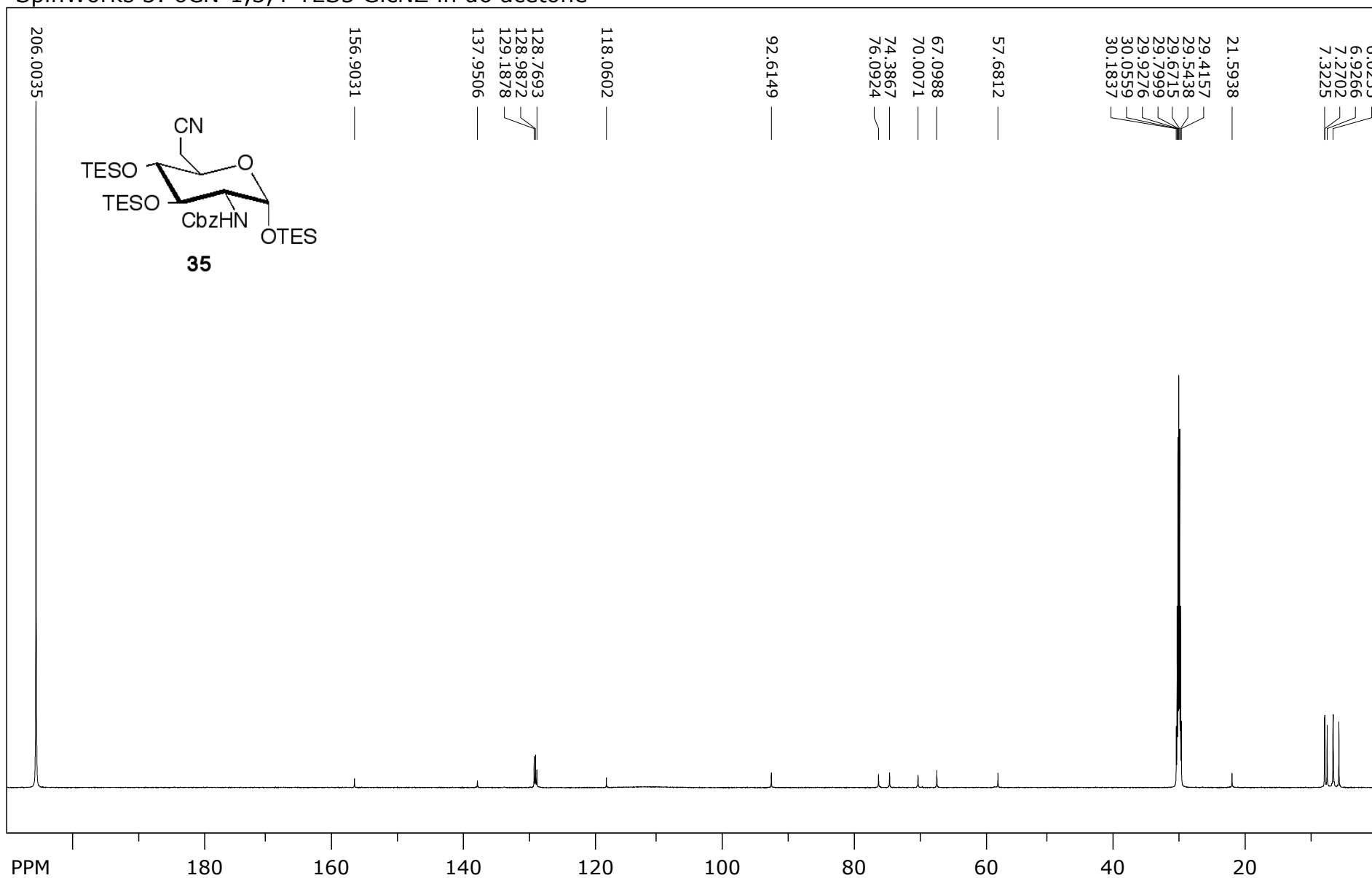
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 27.258 ppm/cm: 0.04539



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\6CNTES3GlcNZ_COSY_f2:\freq. of 0 ppm: 600.549962 MHz
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

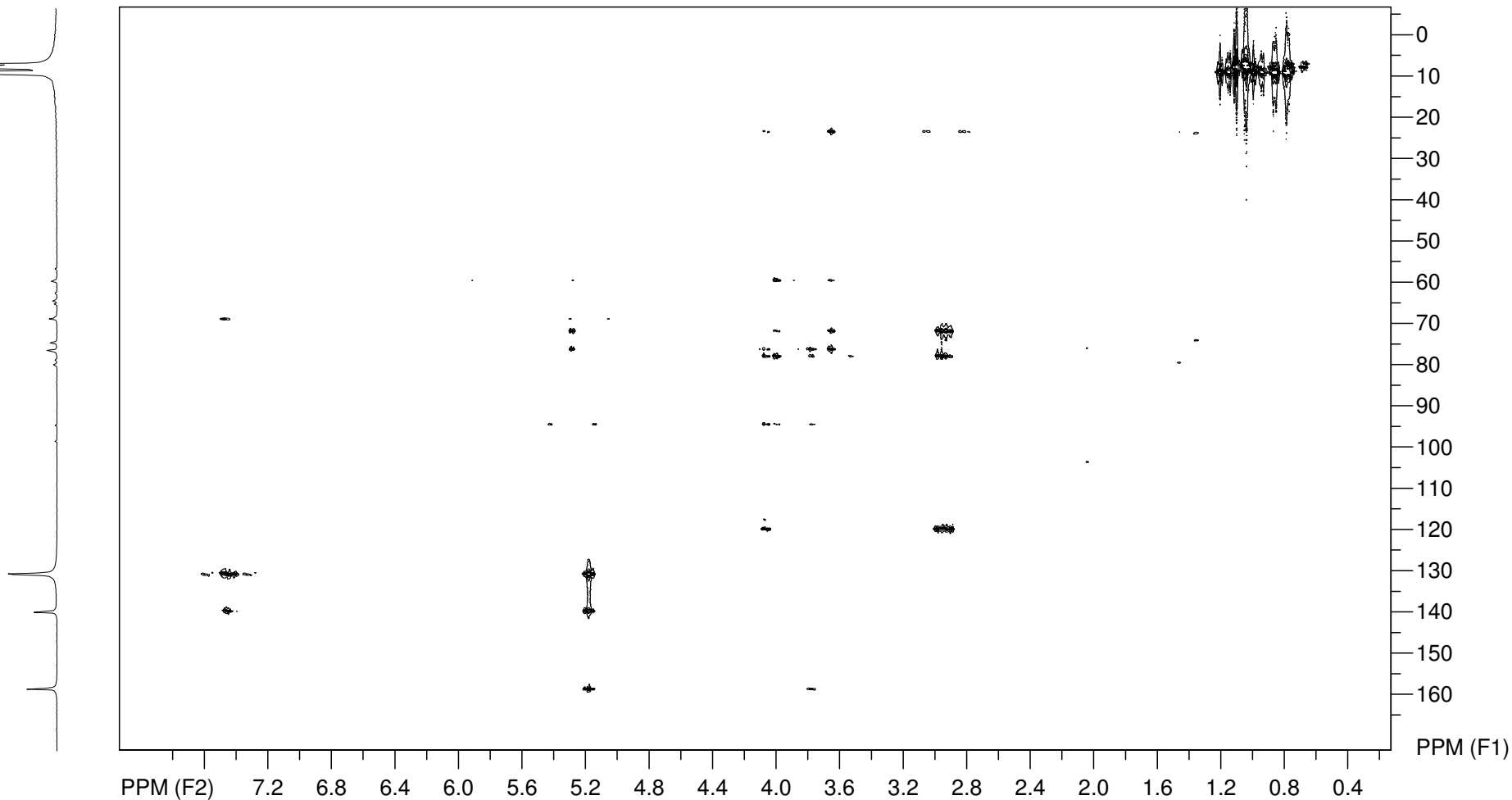
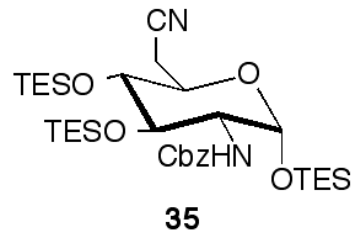
processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 217.327 ppm/cm: 0.36188

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 398.310 ppm/cm: 0.66324



file: ...ess\6CNTES3GlcNZ_13C_acetone\1\fid expt: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 25600

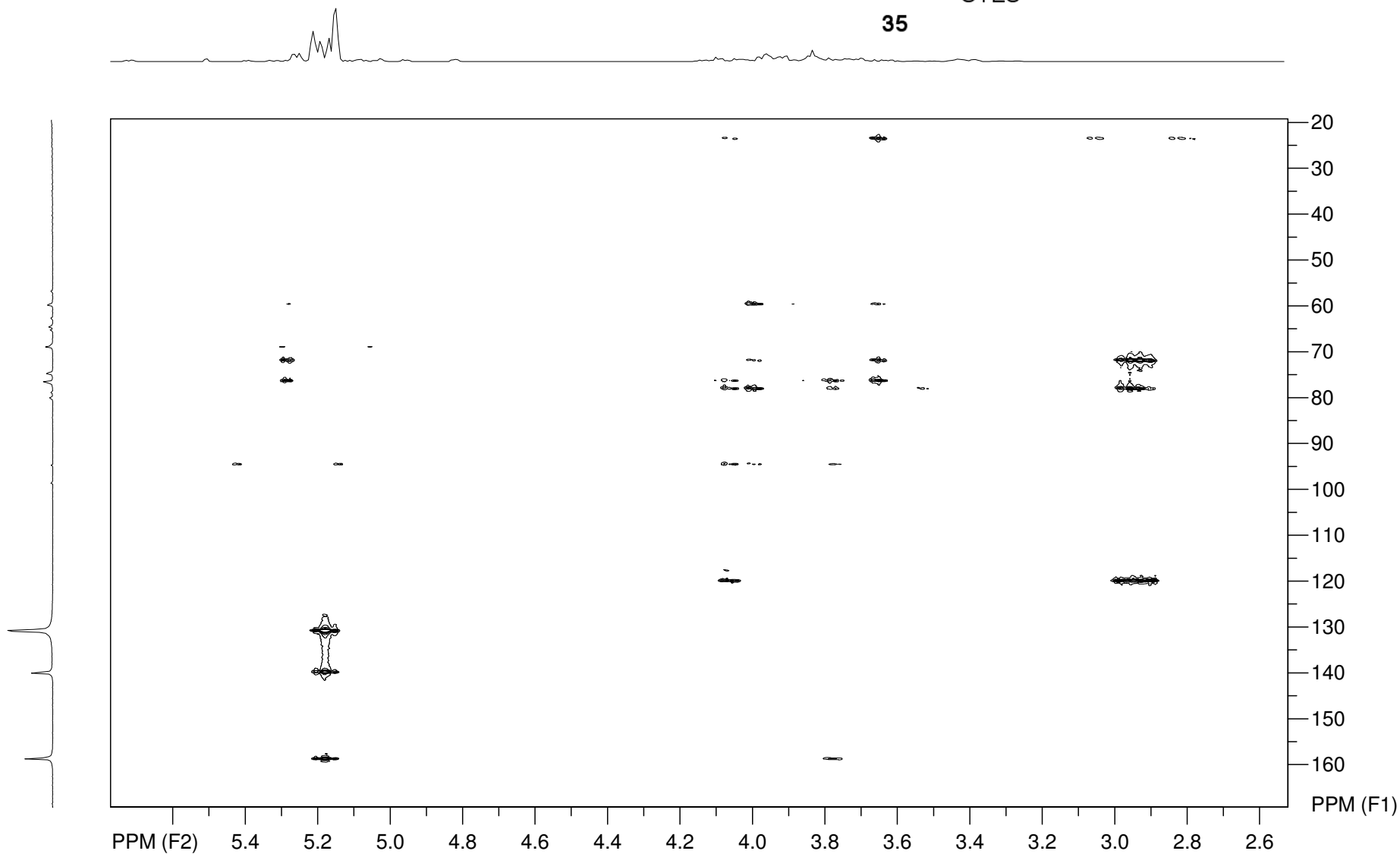
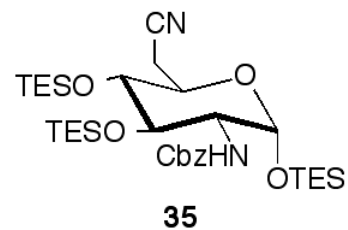
freq. of 0 ppm: 151.008284 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 1276.507 ppm/cm: 8.45237



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\6CNTES3GlcNZ_HMBC_F2:tfreq. of 0 ppm: 600.549962 MHz
 transmitter freq.: 600.553783 MHz
 time domain size: 4096 by 4096 points
 width (F2): 7812.45 Hz = 13.008827 ppm = 1.907336 Hz/pt
 number of scans: 2

processed size: 2048 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 234.558 ppm/cm: 0.39057

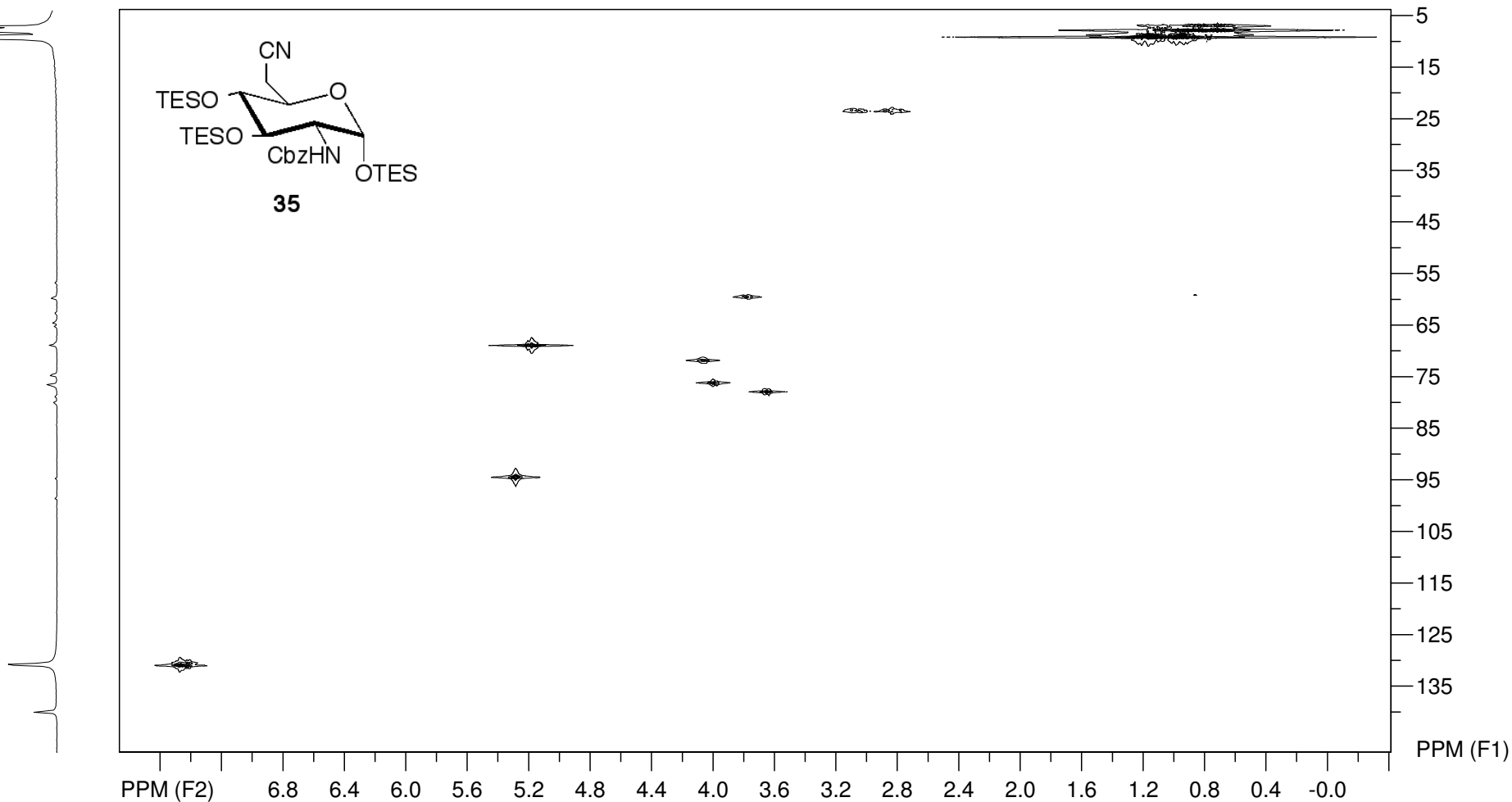
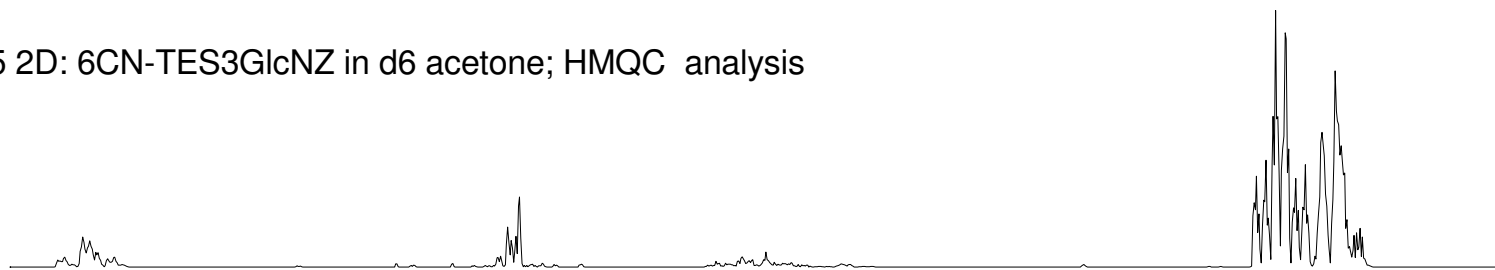
F1: freq. of 0 ppm: 151.008006 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 2268.833 ppm/cm: 15.02304



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\6CNTES3GlcNZ_HMBC_F2:tfreq. of 0 ppm: 600.549962 MHz
transmitter freq.: 600.553783 MHz
time domain size: 4096 by 4096 points
width (F2): 7812.45 Hz = 13.008827 ppm = 1.907336 Hz/pt
number of scans: 2

processed size: 2048 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 95.211 ppm/cm: 0.15854

F1: freq. of 0 ppm: 151.008006 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 1888.301 ppm/cm: 12.50336

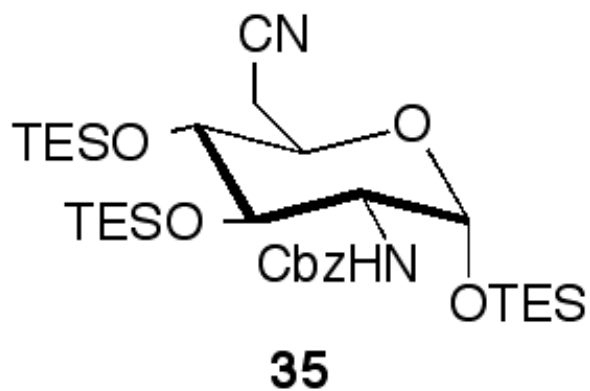
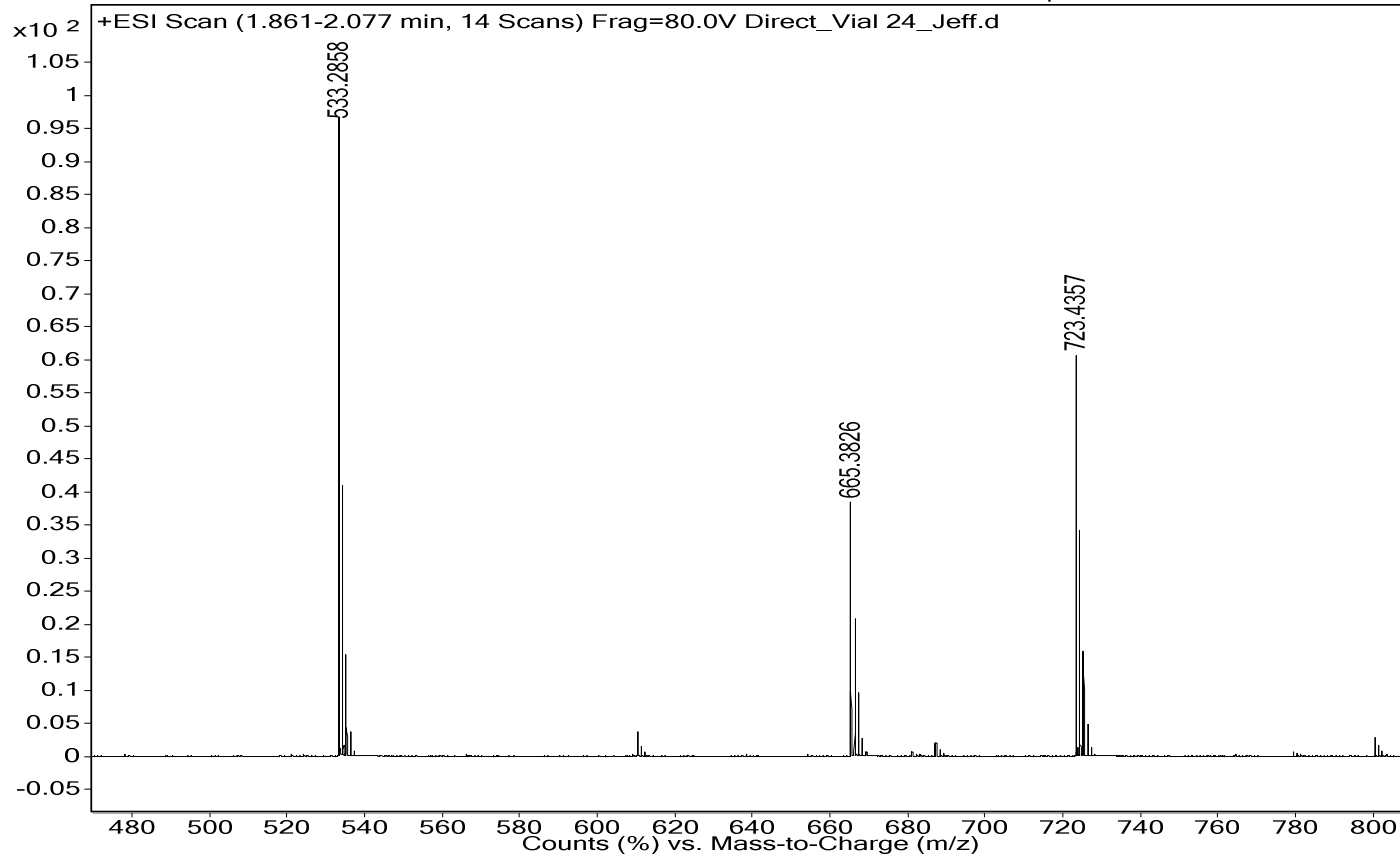


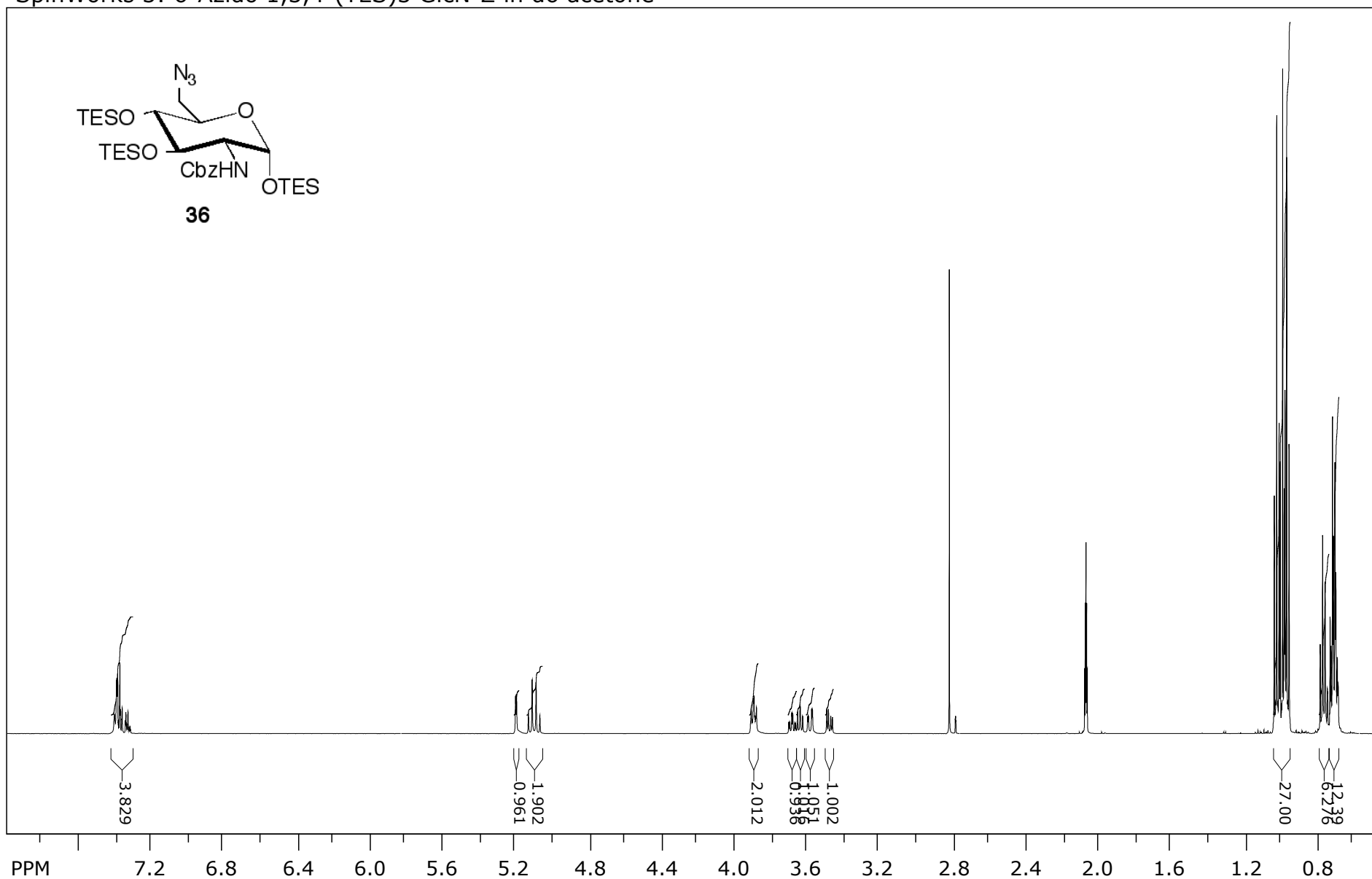
file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\6CNTES3GlcNZ_HMQCaF2;.freq. of 0 ppm: 600.549962 MHz
transmitter freq.: 600.552721 MHz
time domain size: 4096 by 4096 points
width (F2): 6067.93 Hz = 10.103961 ppm = 1.481429 Hz/pt
number of scans: 2

processed size: 1024 complex points
window function: Sine Squared
shift: 90.0 degrees
Hz/cm: 242.536 ppm/cm: 0.40385

F1: freq. of 0 ppm: 151.008006 MHz
processed size: 1024 complex points
window function: Sine Squared
shift: 90.0 degrees
Hz/cm: 1812.123 ppm/cm: 11.99895

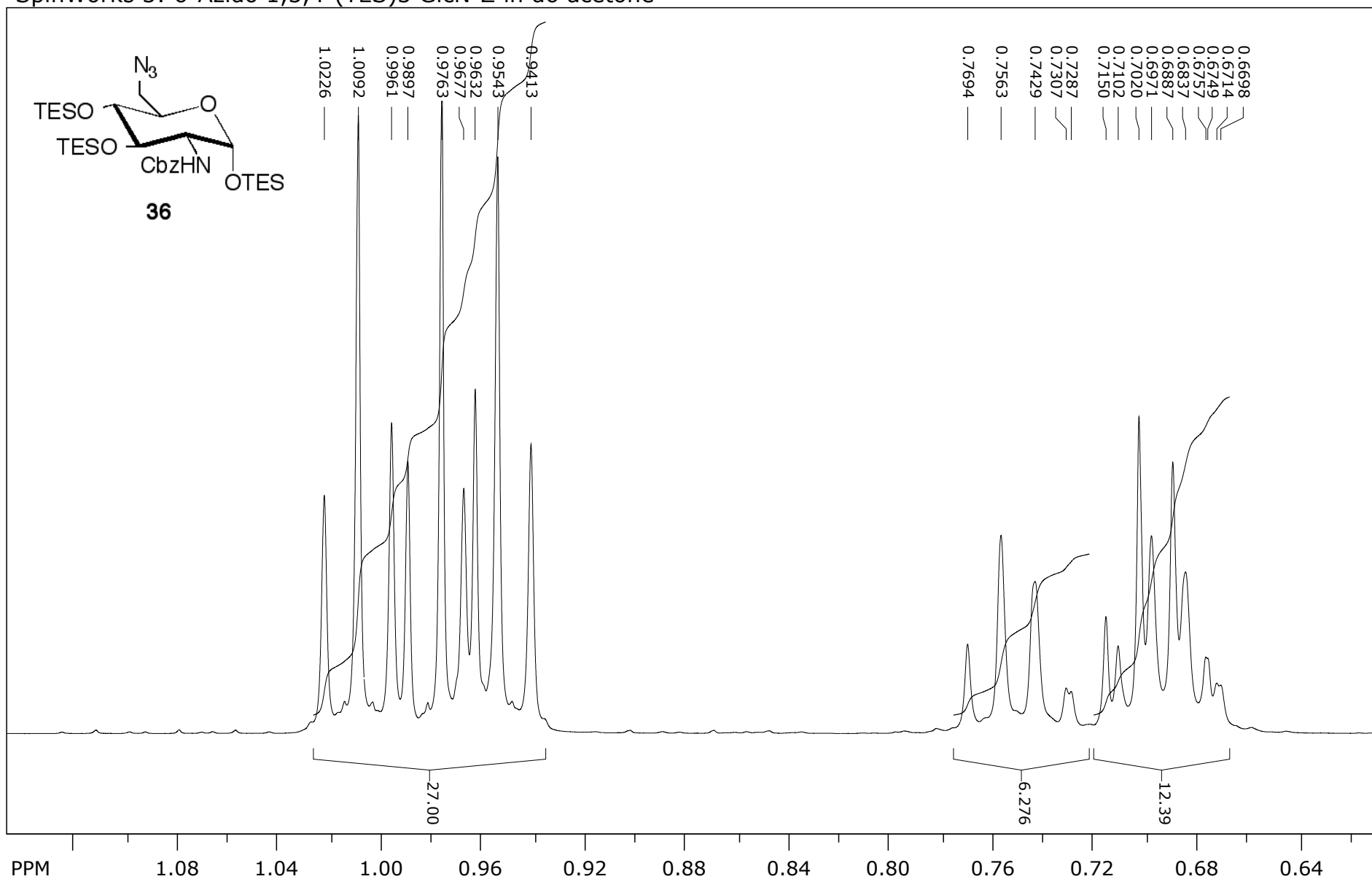
Sample Name	Jeff 24	Position	Vial 24	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 24_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 12:27:48 PM





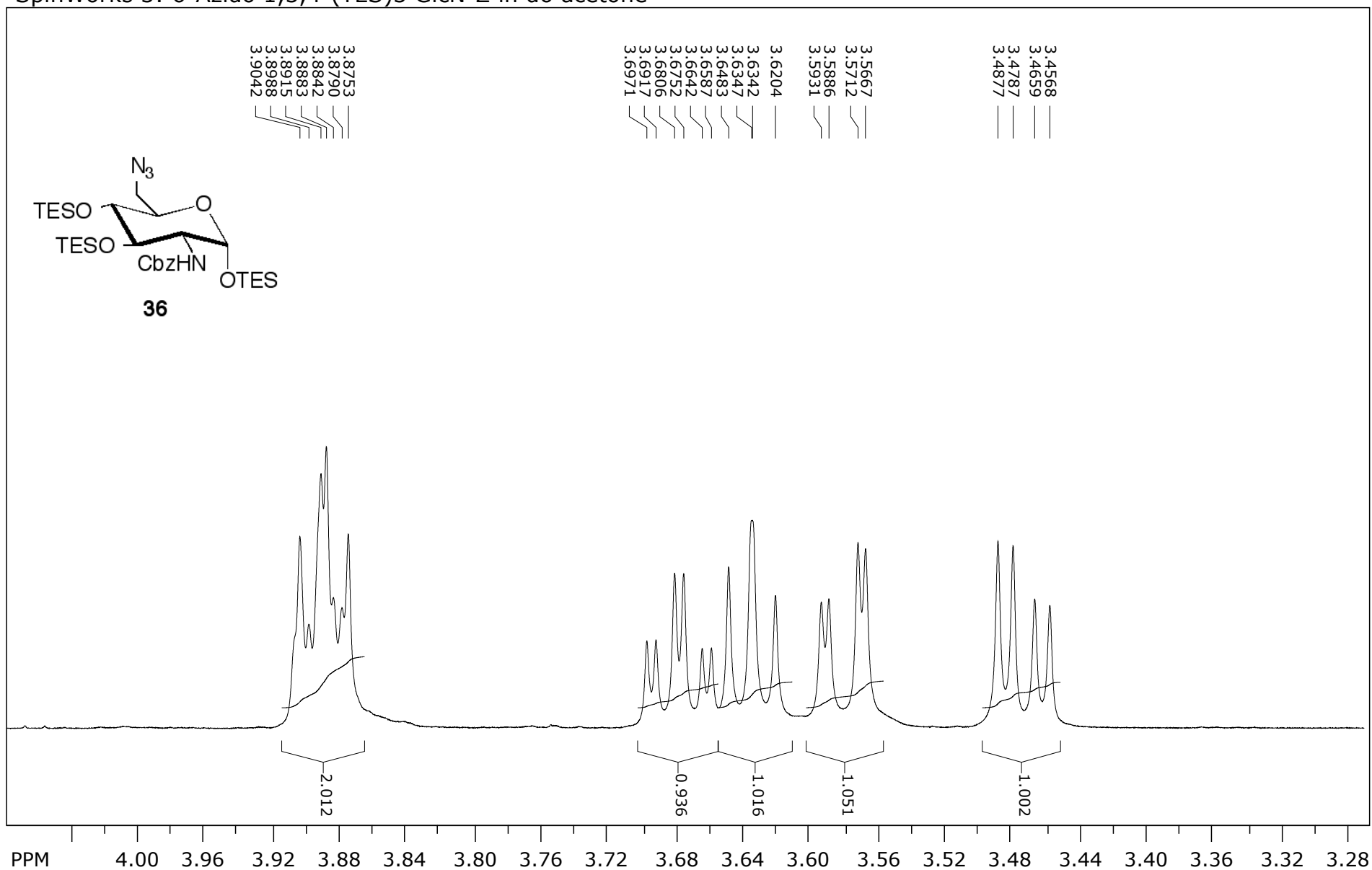
file: ...ng to process\6N3TES3NZ_acet\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 181.576 ppm/cm: 0.30235



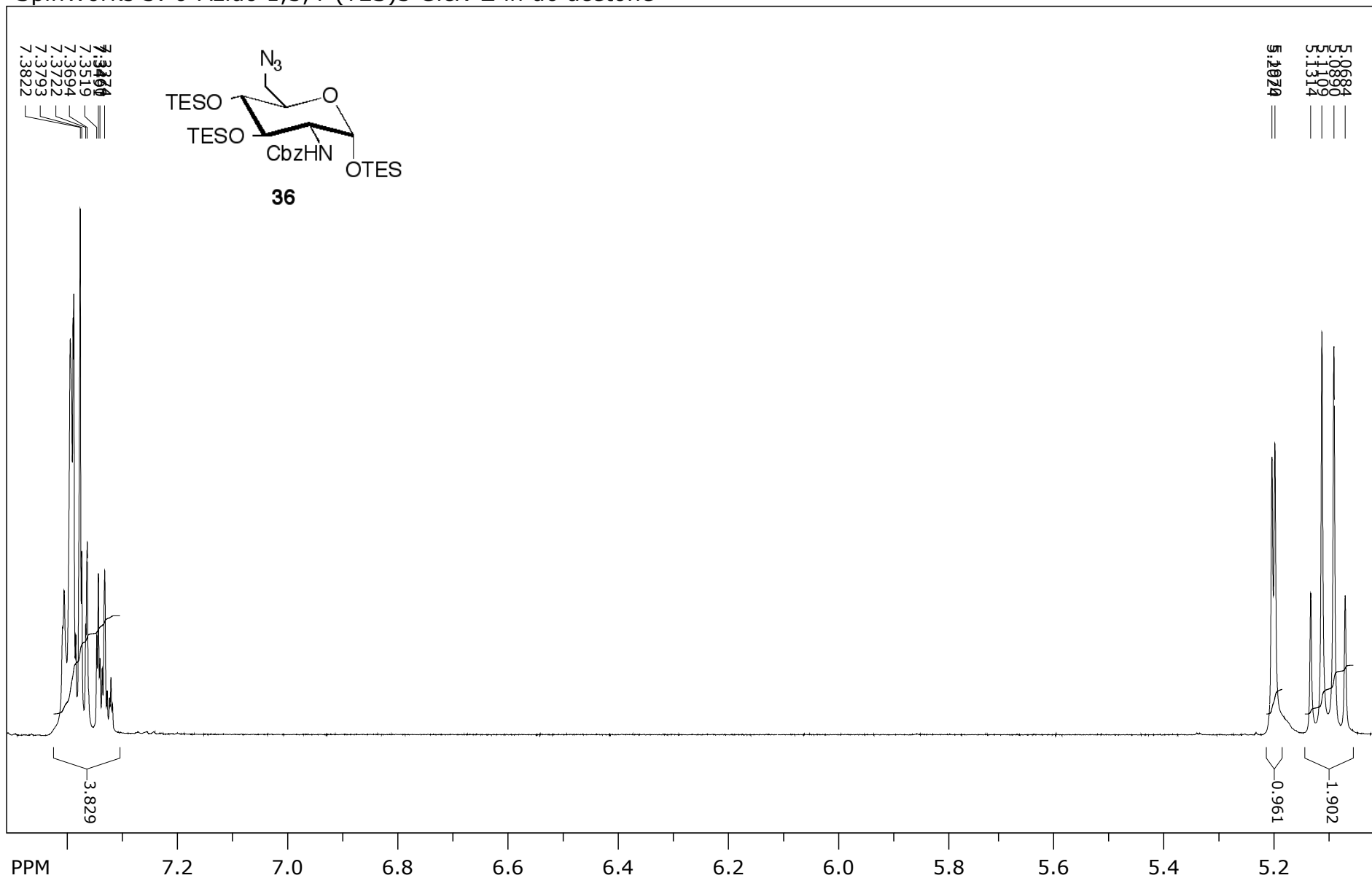
file: ...ng to process\6N3TES3NZ_acet\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 12.970 ppm/cm: 0.02160



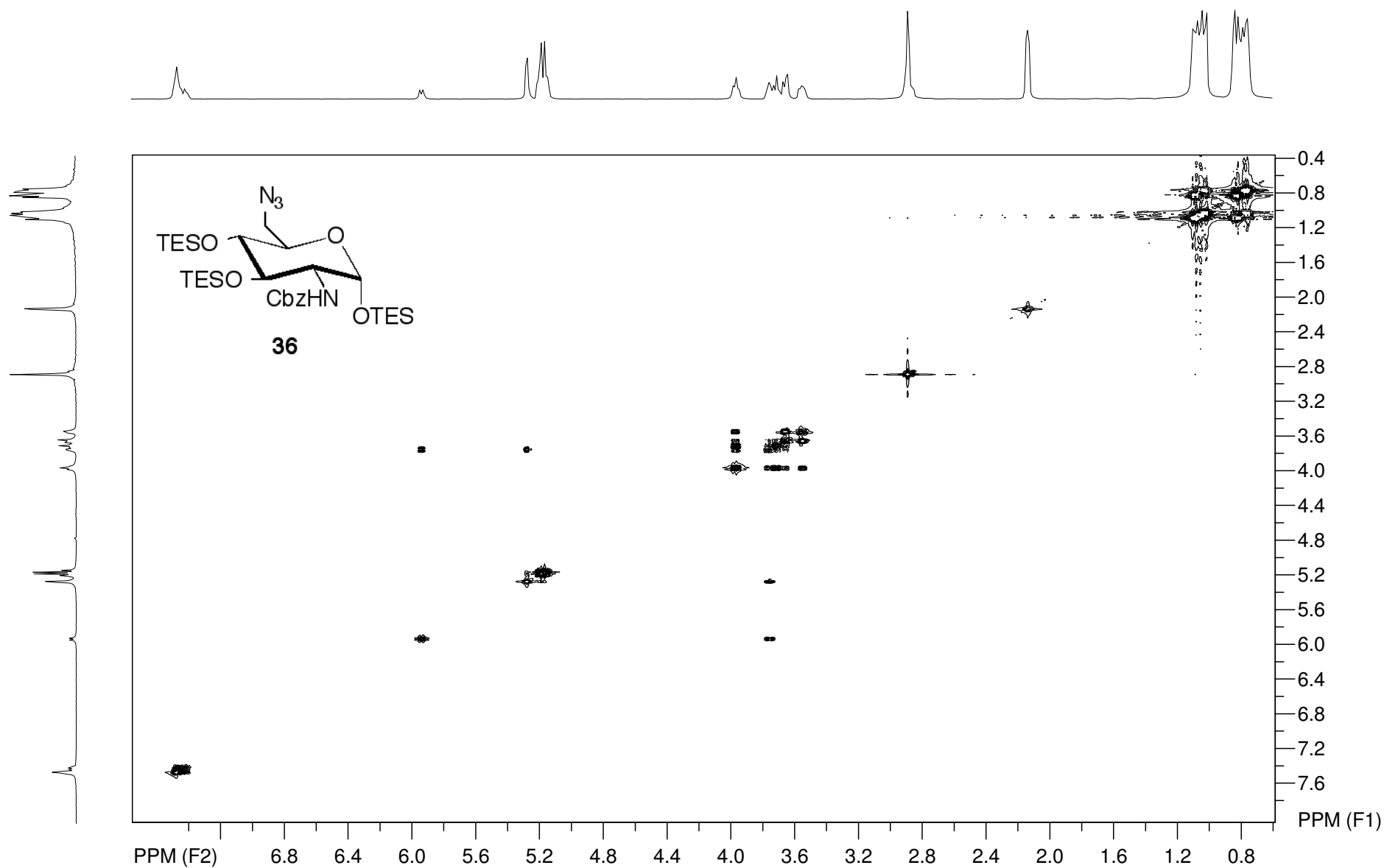
file: ...ng to process\6N3TES3NZ_acet\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550010 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 19.455 ppm/cm: 0.03239



file: ...ng to process\6N3TES3NZ_acet\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

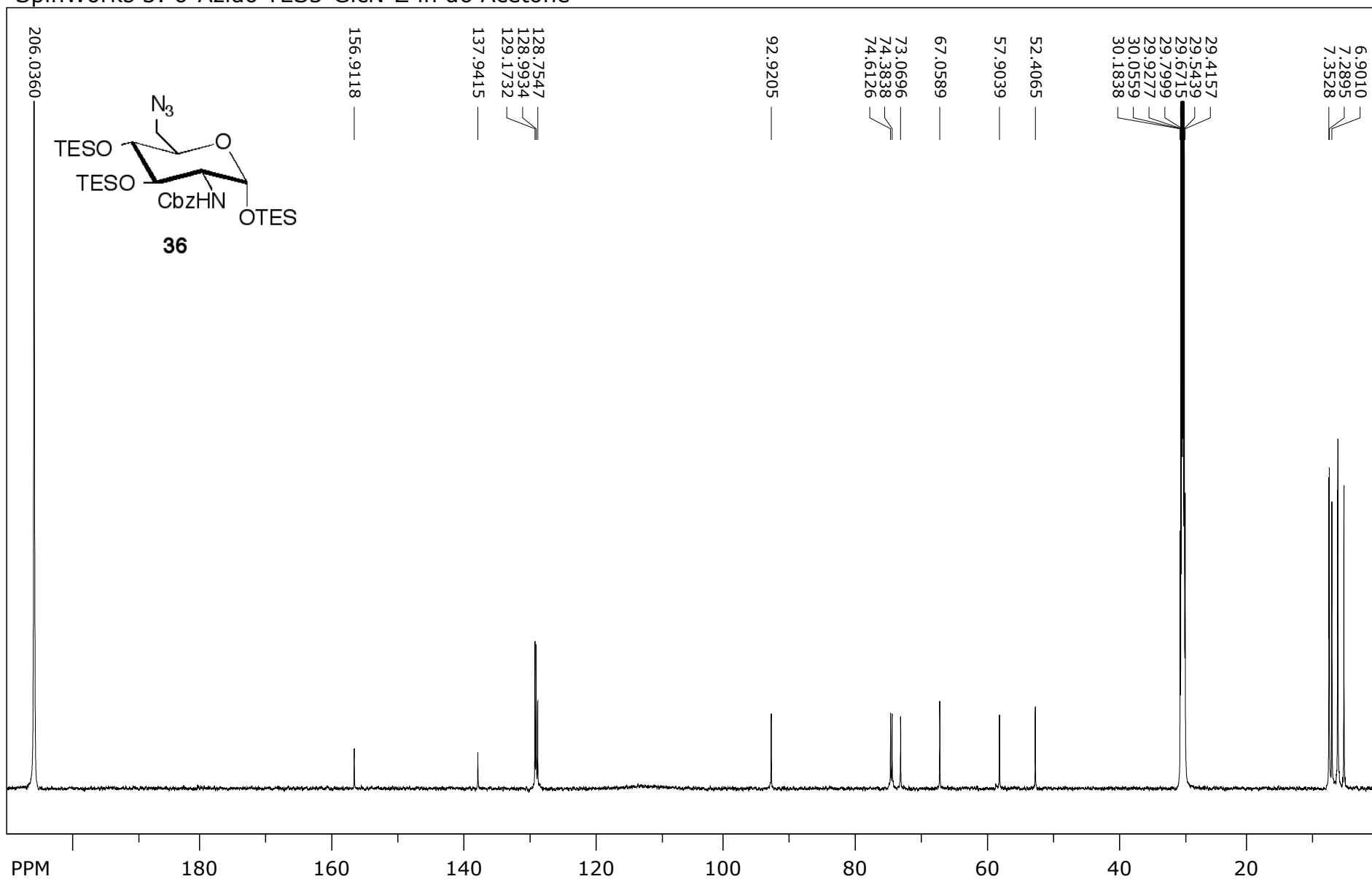
freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 60.289 ppm/cm: 0.10039



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\6N3TES3NZ_COSY\1\serF2.xfreq. of 0 ppm: 600.549962 MHz
transmitter freq.: 600.552832 MHz
time domain size: 2048 by 2048 points
width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
number of scans: 1

processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 209.948 ppm/cm: 0.34959

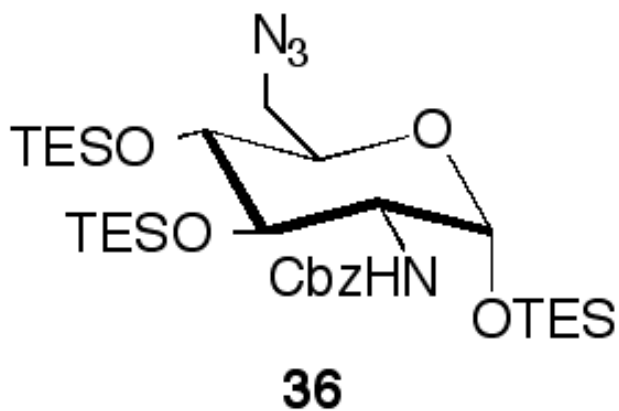
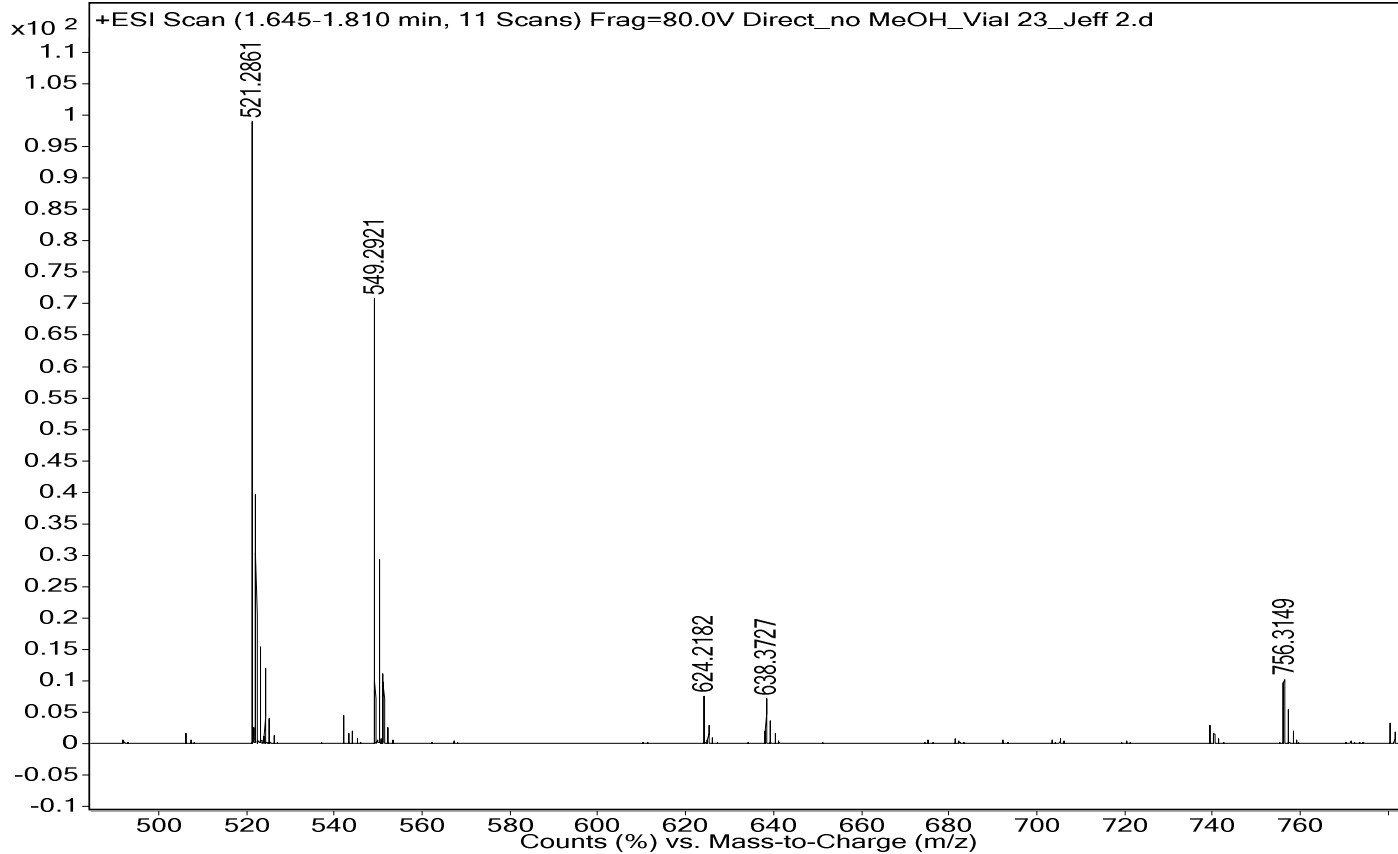
F1: freq. of 0 ppm: 600.549962 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 384.848 ppm/cm: 0.64082

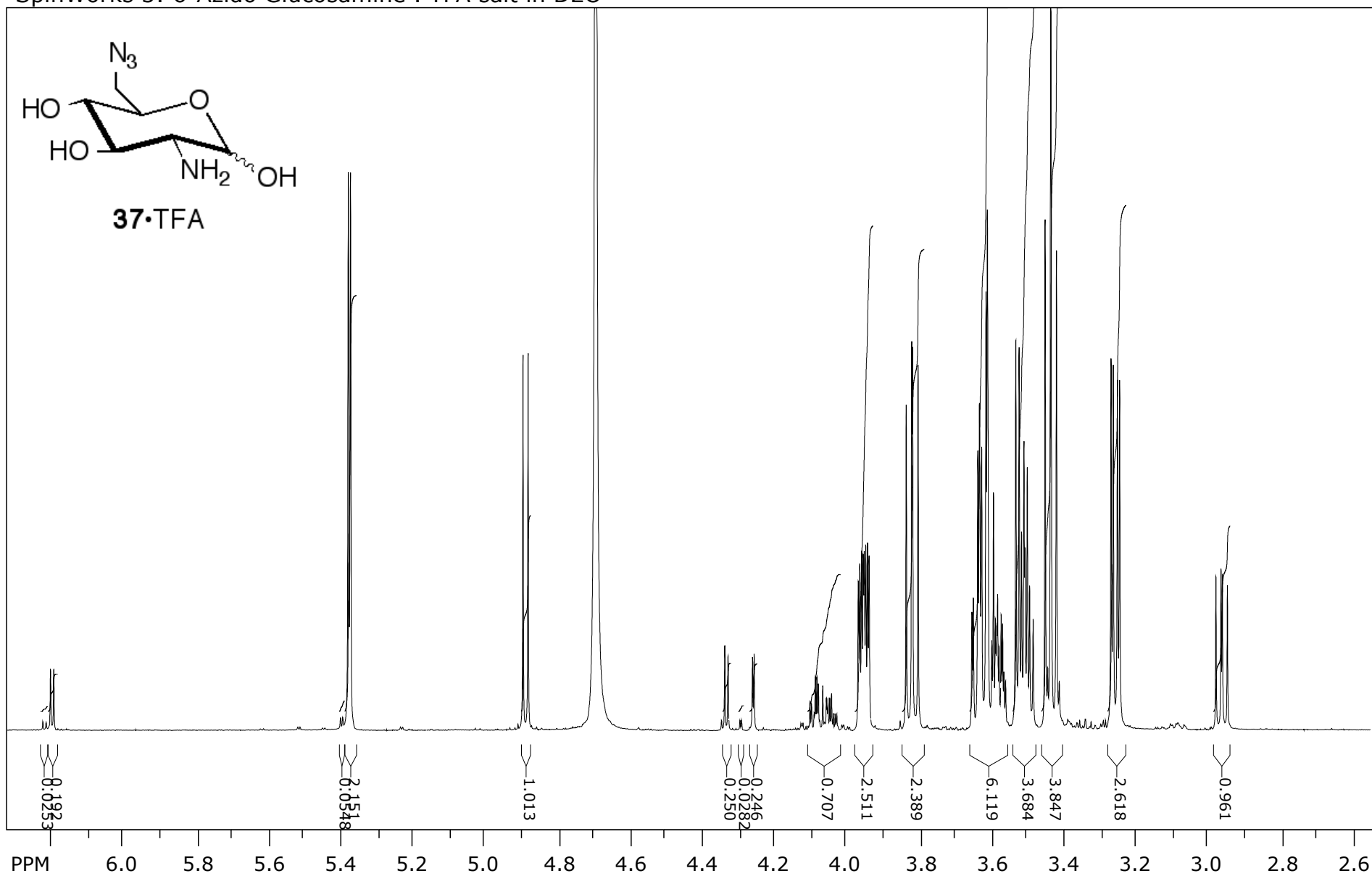


file: ...ing to process\6N3TES3NZ_13C\1\fid exp: <zpgg30>
transmitter freq.: 151.023519 MHz
time domain size: 65536 points
width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
number of scans: 6144

freq. of 0 ppm: 151.008288 MHz
processed size: 32768 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 1271.678 ppm/cm: 8.42039

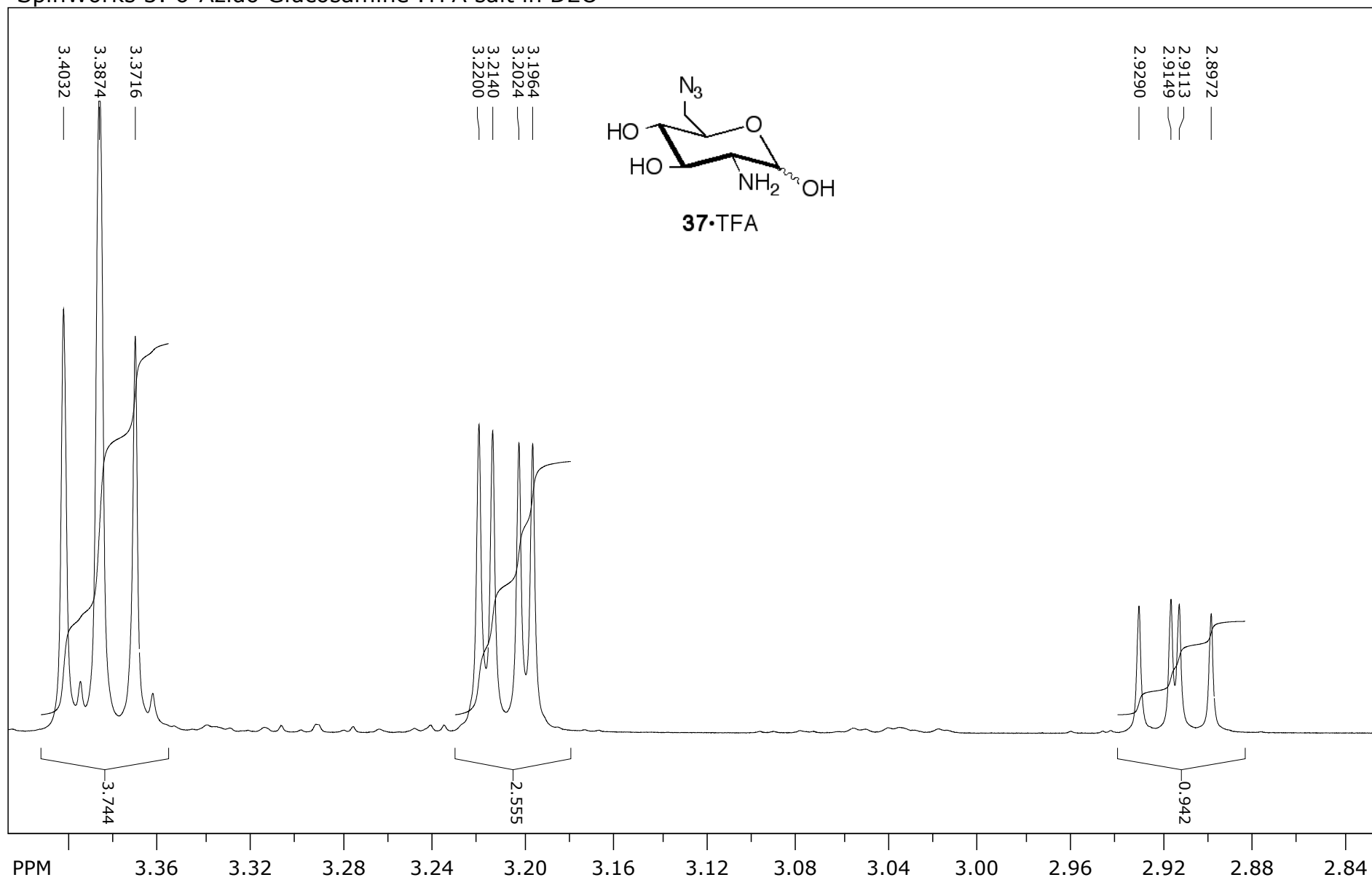
Sample Name	Jeff 23	Position	Vial 75	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_no MeOH_Vial	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/21/2012 1:53:31 PM





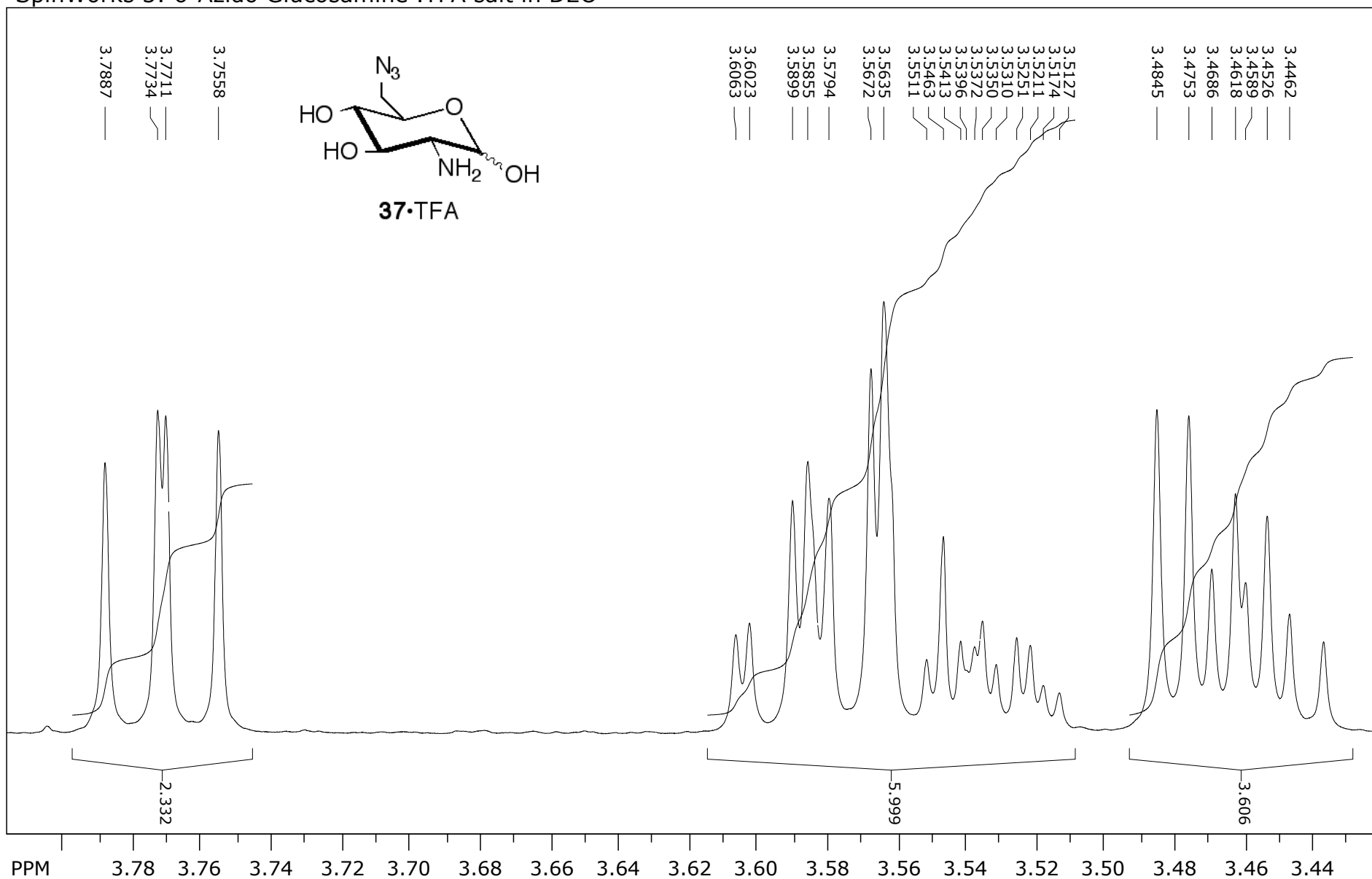
file: ...r\NMR Data\6N3GlcNH2_TFA_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 90.949 ppm/cm: 0.15144



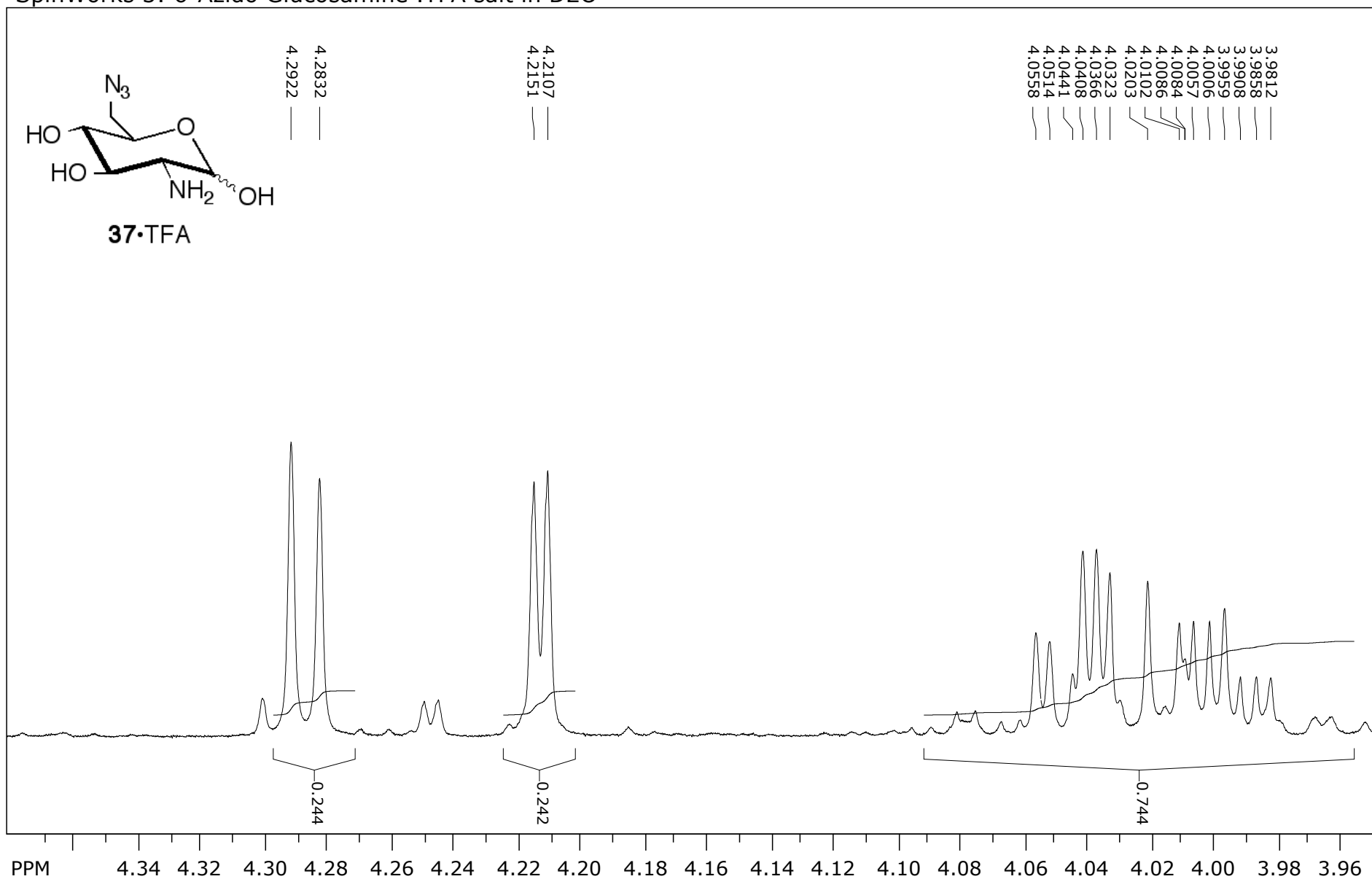
file: ...to process\6N3GlcNH2_TFA_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550037 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 14.518 ppm/cm: 0.02417



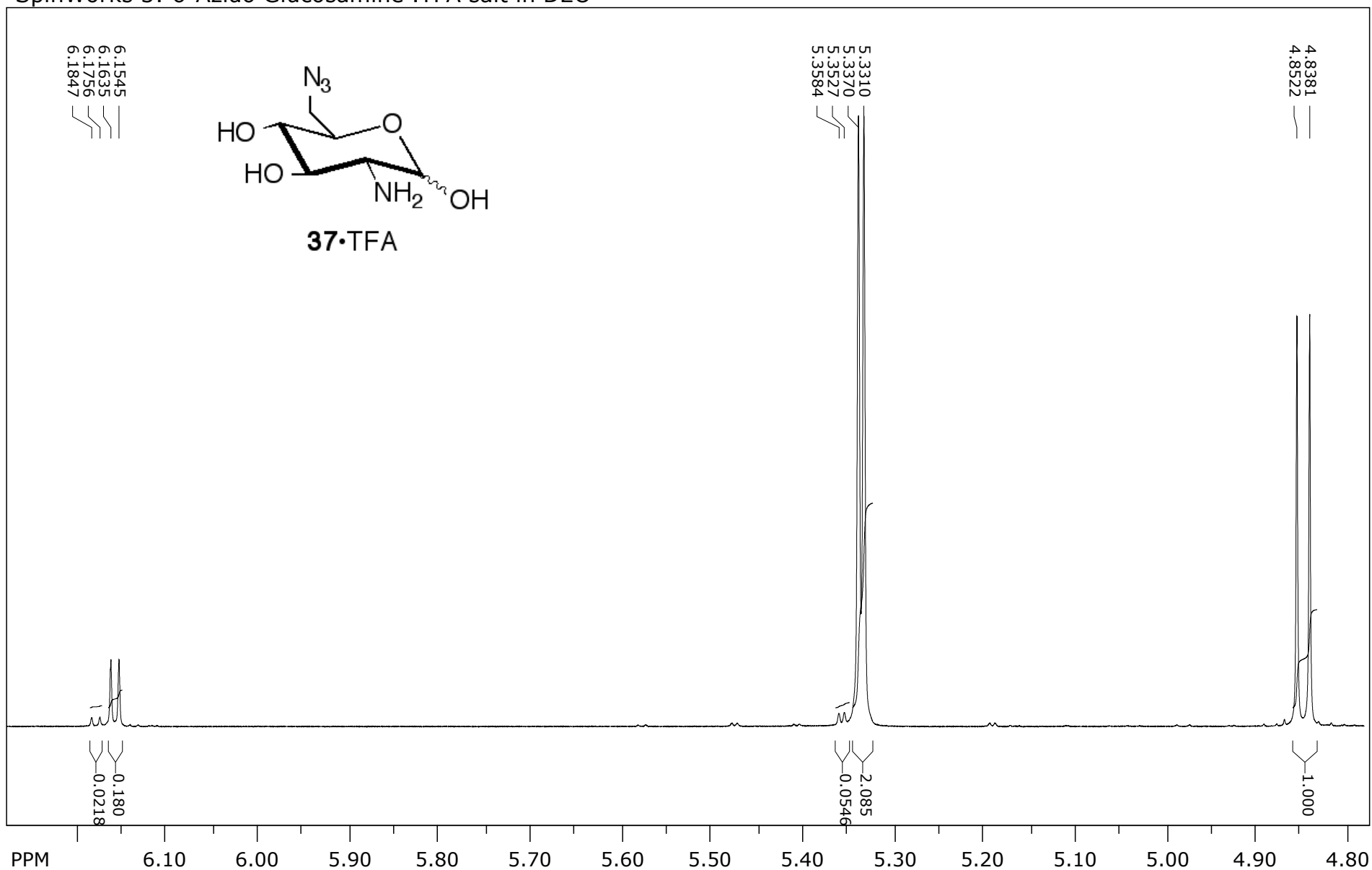
file: ...to process\6N3GlcNH2_TFA_D2O\1\fid expt: <zgpr>
 transmitter freq.: 600.553538 MHz
 time domain size: 65536 points
 width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550037 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 9.530 ppm/cm: 0.01587



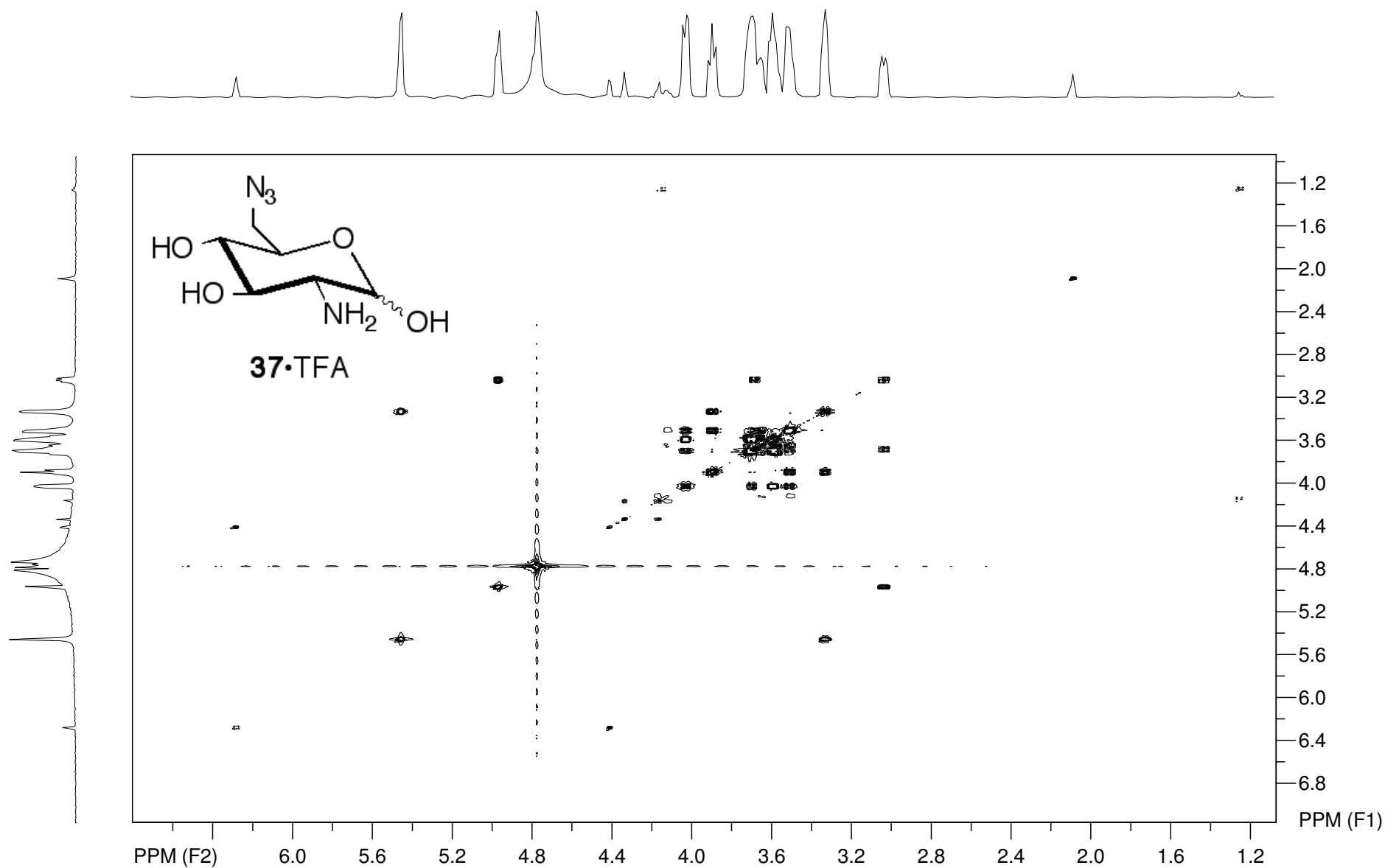
file: ...to process\6N3GlcNH2_TFA_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550037 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 10.463 ppm/cm: 0.01742



file: ...to process\6N3GlcNH2_TFA_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 7211.54 Hz = 12.0082 ppm = 0.110039 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550037 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 36.058 ppm/cm: 0.06004

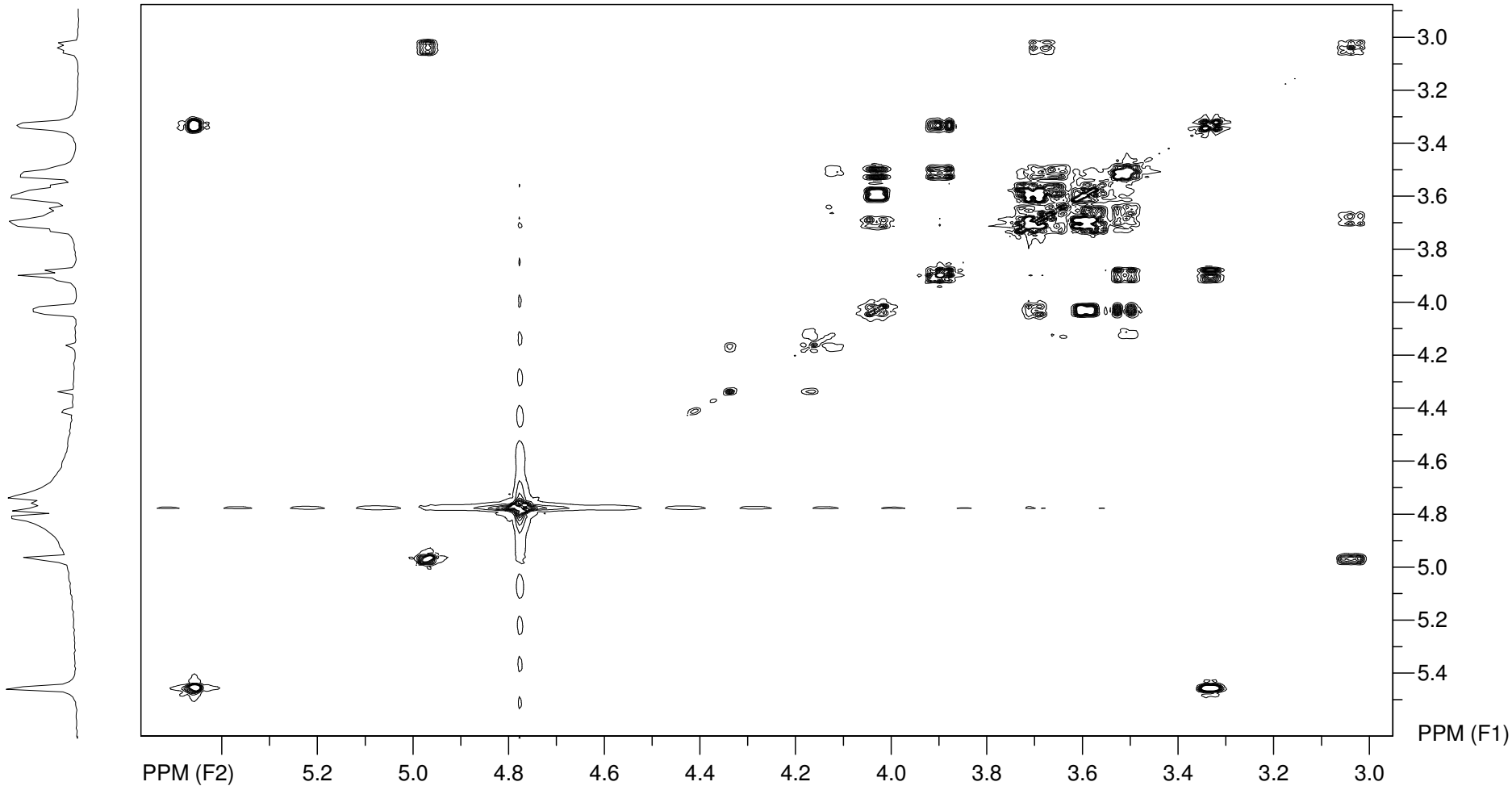
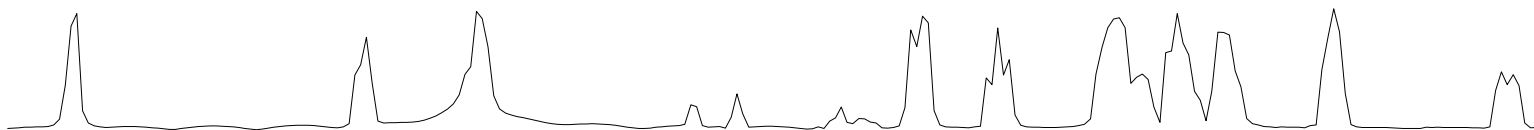
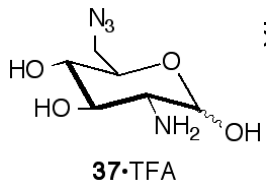


file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\6N3GlcNH2_TFA_D2O\F2:\freq. of 0 ppm: 600.549962 MHz
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 167.884 ppm/cm: 0.27955

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 311.996 ppm/cm: 0.51951

; 2D: 6N3 GlcNH2.TFA salt in D2O

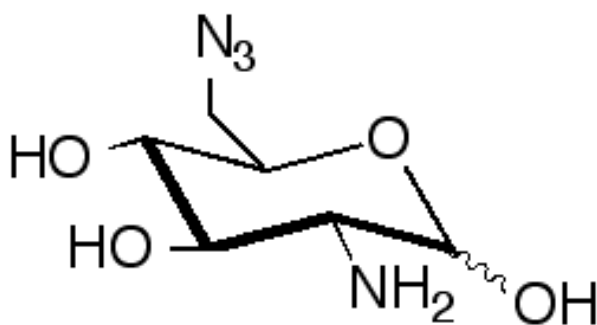
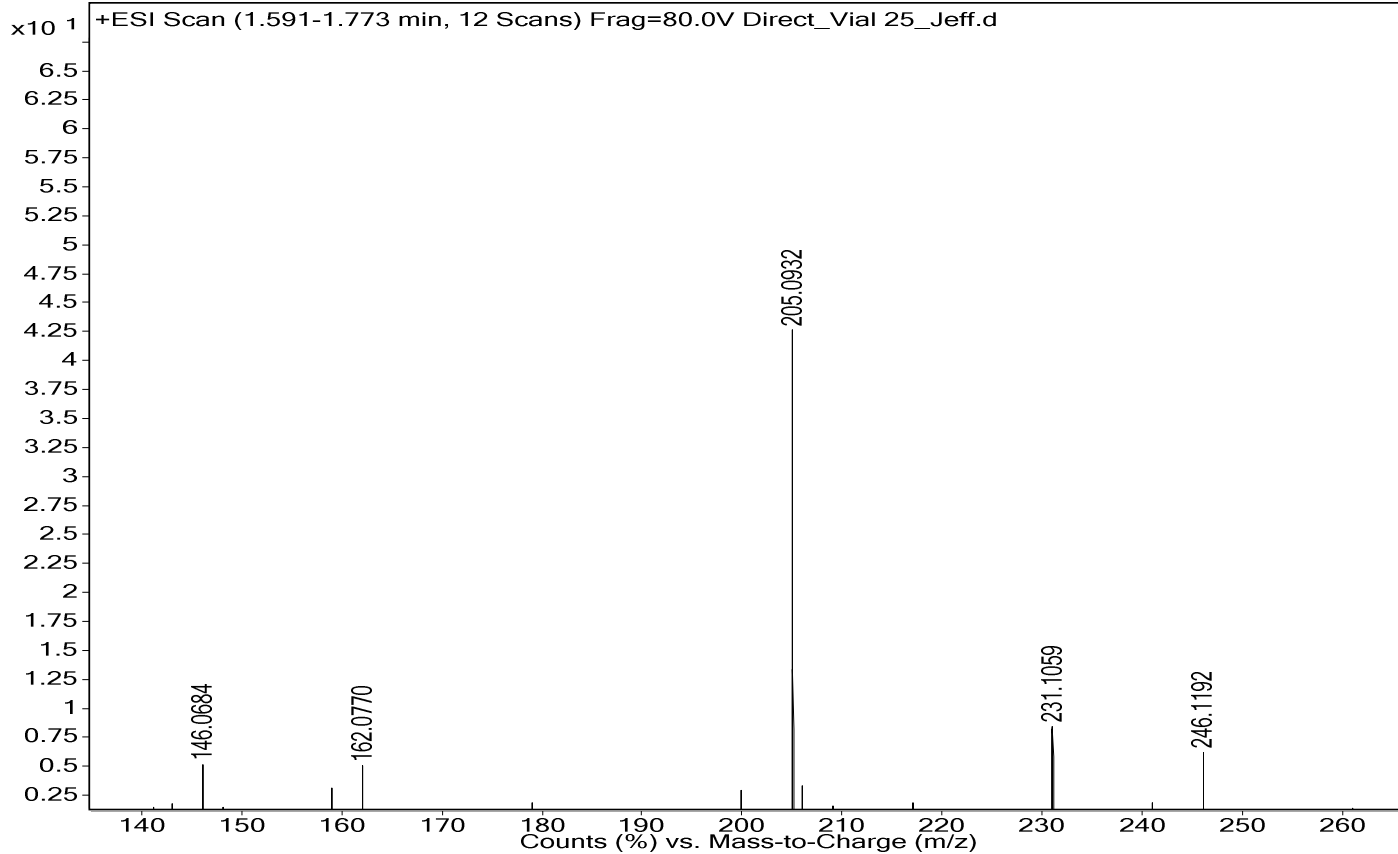


file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\remaining to process\6N3GlcNH2_TFA_D2O\F2:\freq. of 0 ppm: 600.549962 MHz
 transmitter freq.: 600.552832 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.59 Hz = 10.006806 ppm = 2.934368 Hz/pt
 number of scans: 2

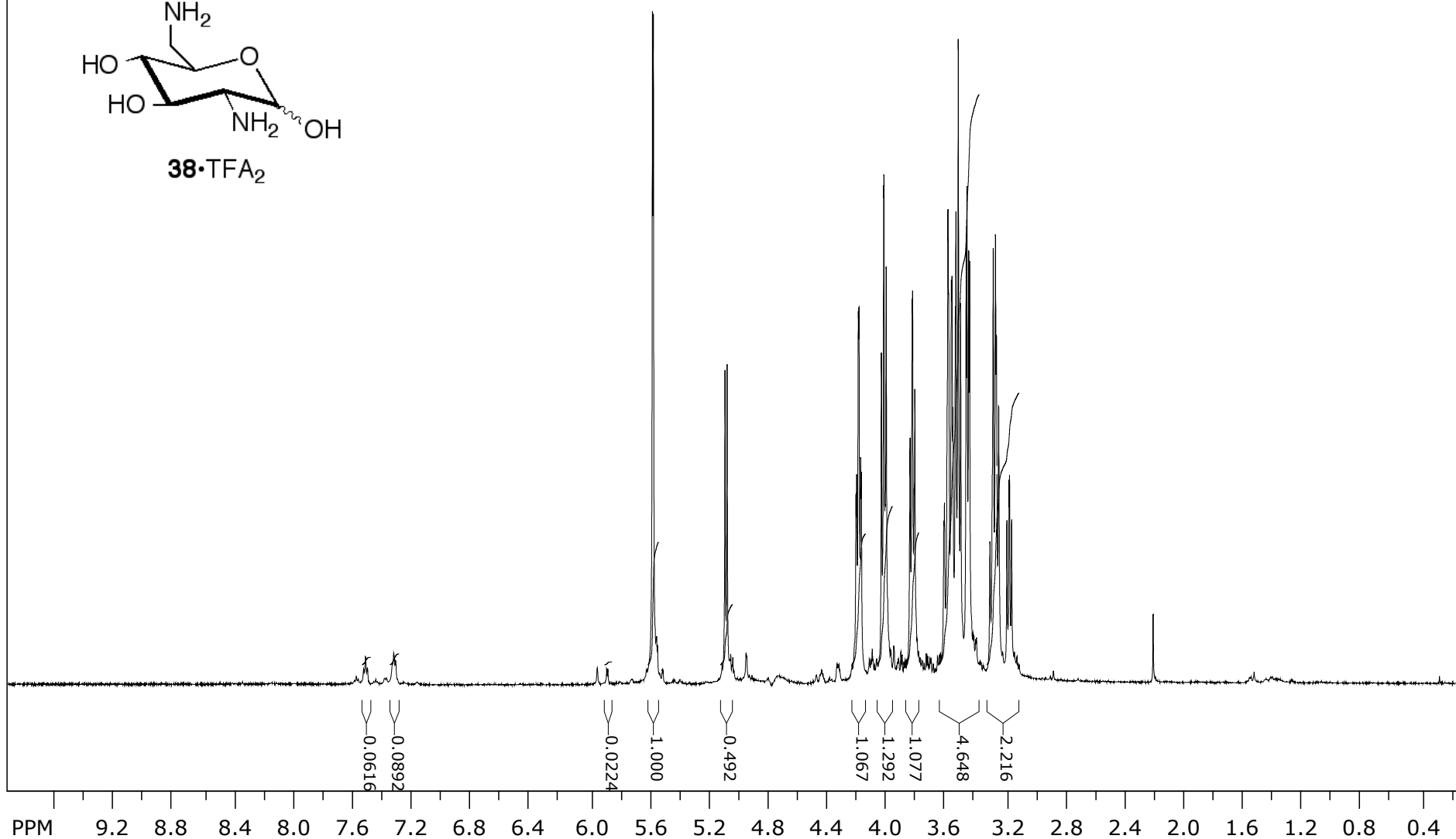
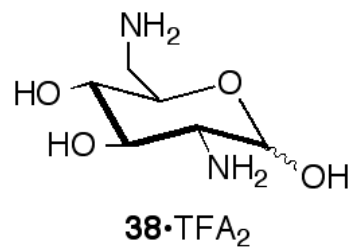
processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 76.705 ppm/cm: 0.12772

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 138.226 ppm/cm: 0.23016

Sample Name	Jeff 25	Position	Vial 25	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 25_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 12:32:26 PM



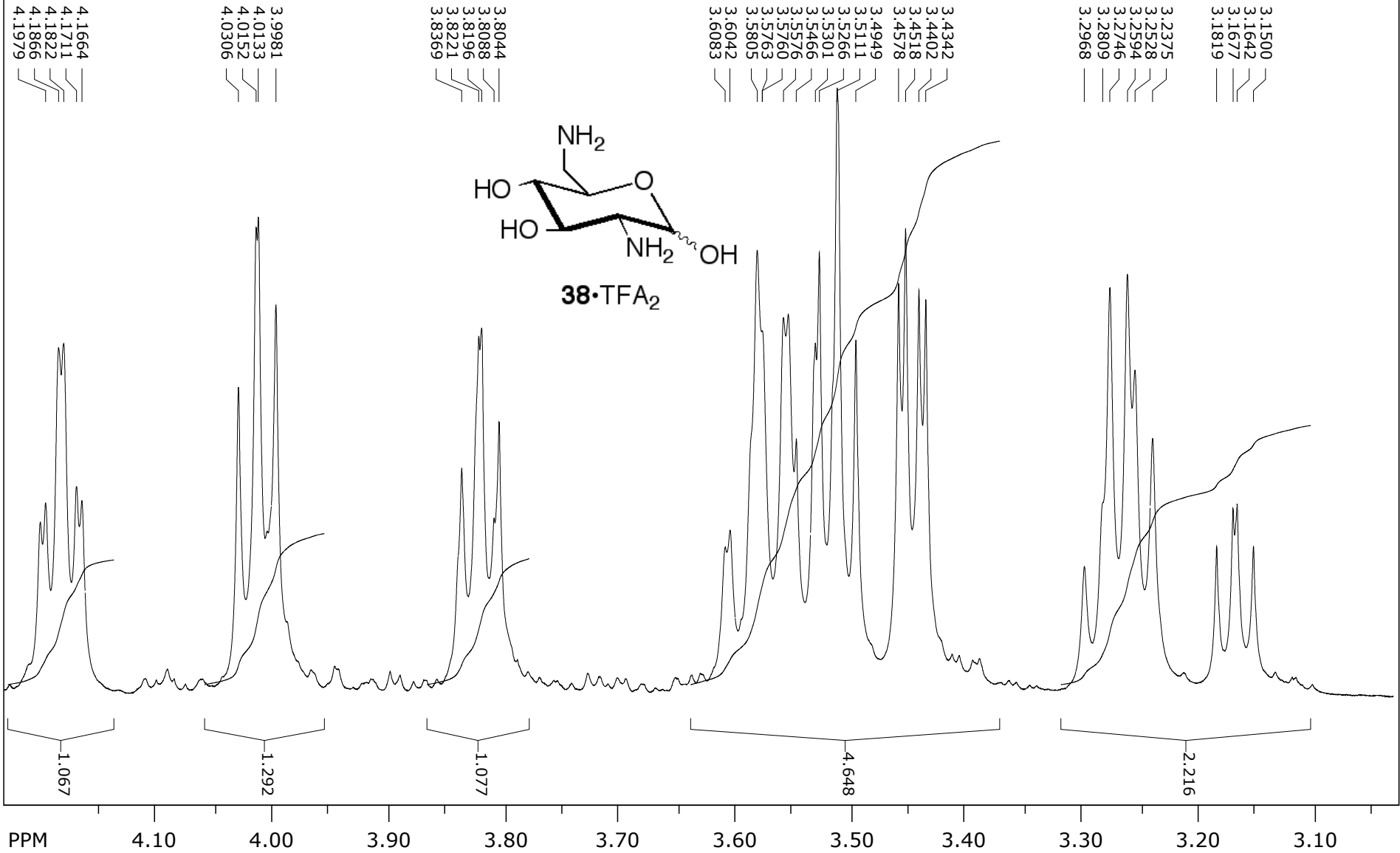
37-TFA



file: ...R Data\26DiAmGlu_TFAsalt_D2O\2\fid expt: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 65536 points
width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
number of scans: 32

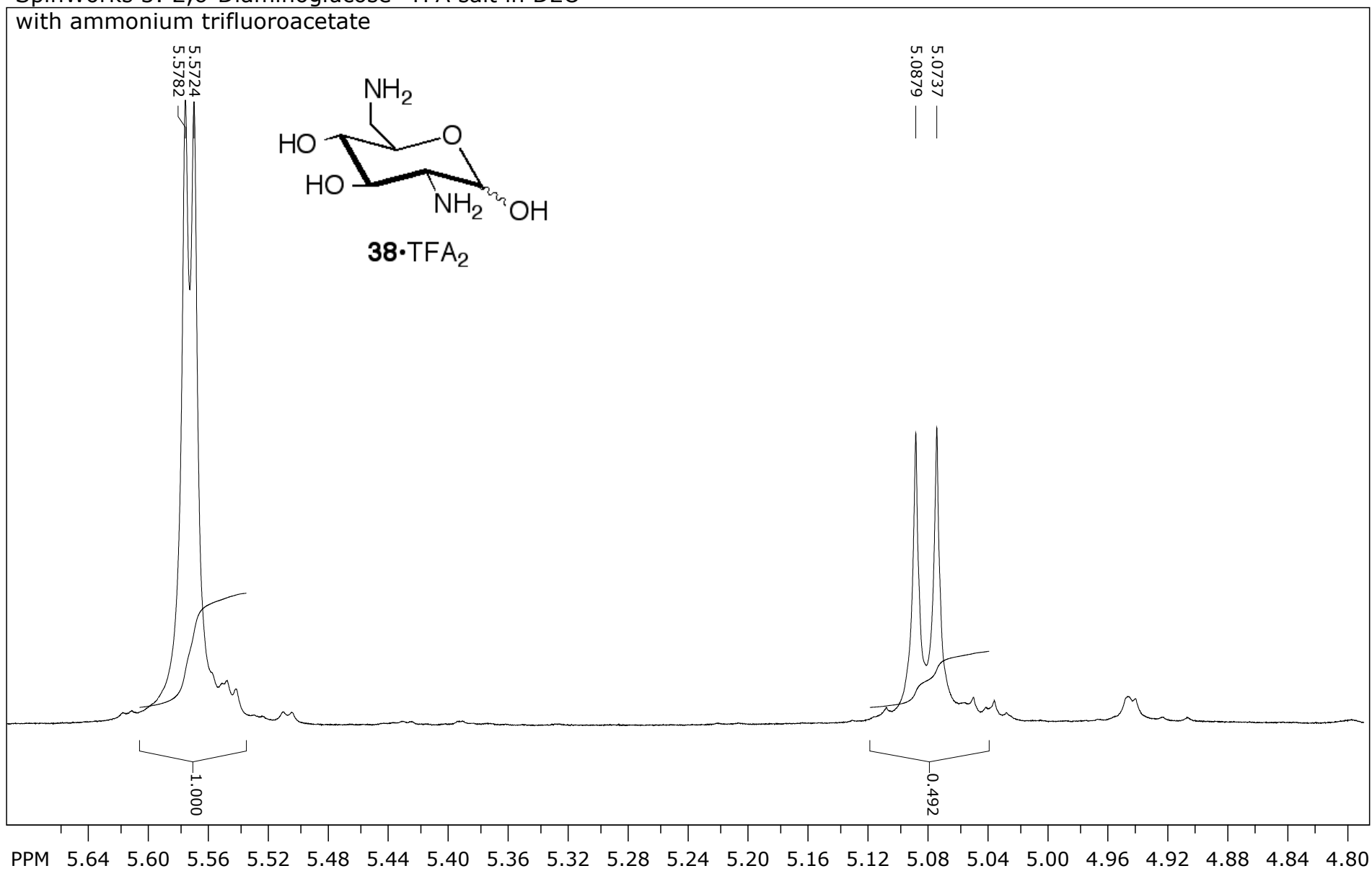
freq. of 0 ppm: 600.549962 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 236.736 ppm/cm: 0.39420

with ammonium trifluoroacetate



file: ...R Data\26DiAmGlu_TFA salt_D2O\2\fid expt: <zgpr>
 transmitter freq.: 600.552832 MHz
 time domain size: 65536 points
 width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
 number of scans: 32

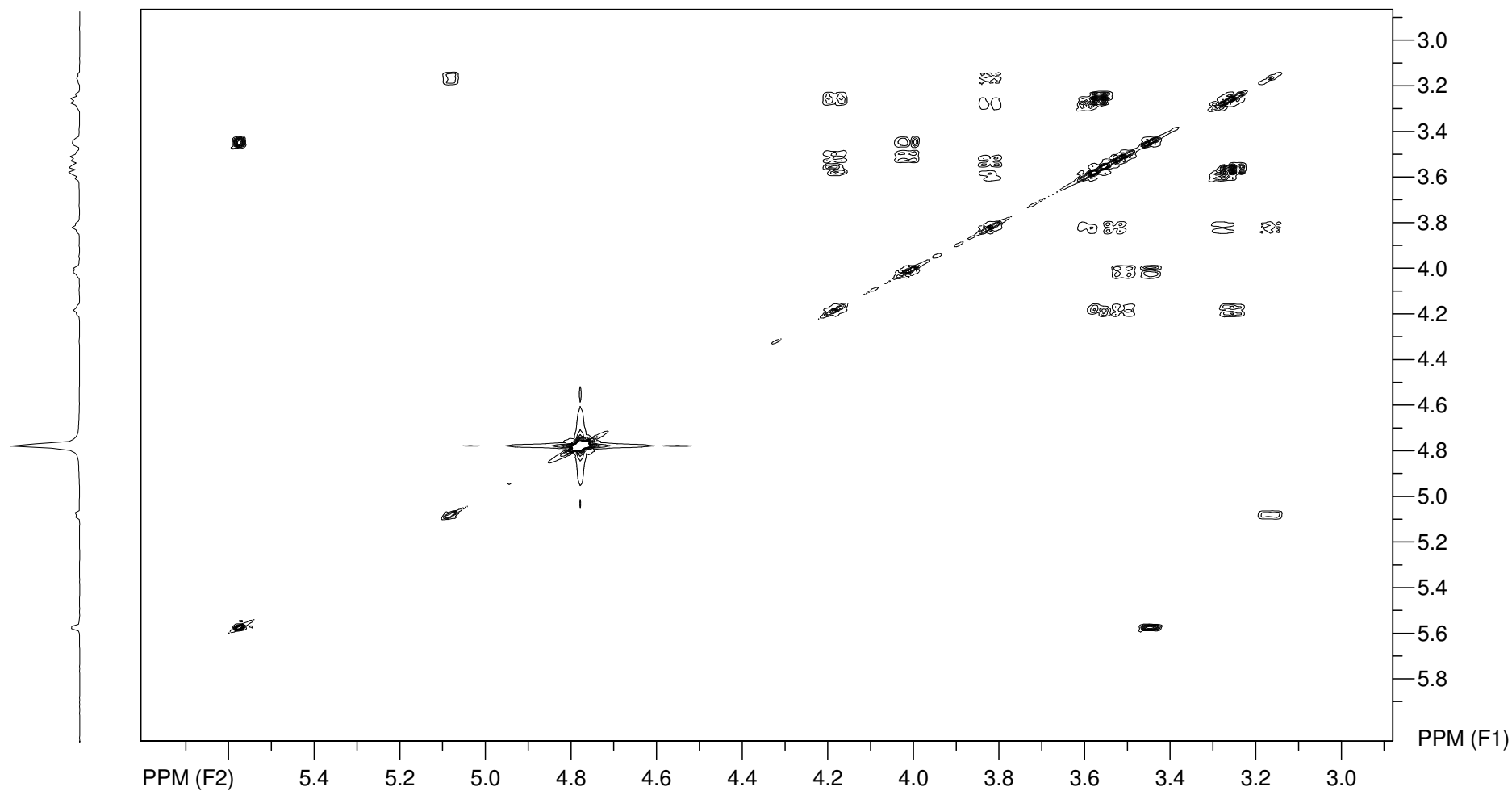
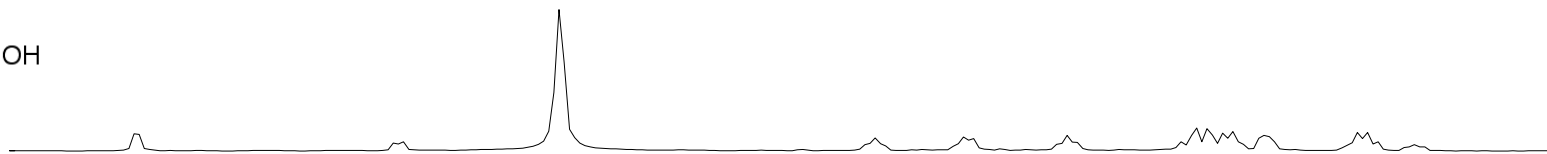
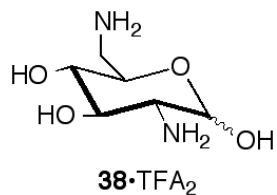
freq. of 0 ppm: 600.549962 MHz
 processed size: 262144 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 28.962 ppm/cm: 0.04823



file: ...R Data\26DiAmGlu_TFA salt_D2O\2\fid expt: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 65536 points
width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.549962 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 21.892 ppm/cm: 0.03645

D: 2,6-Diaminoglucose -TFA salt in D2O with ammoniumTFA

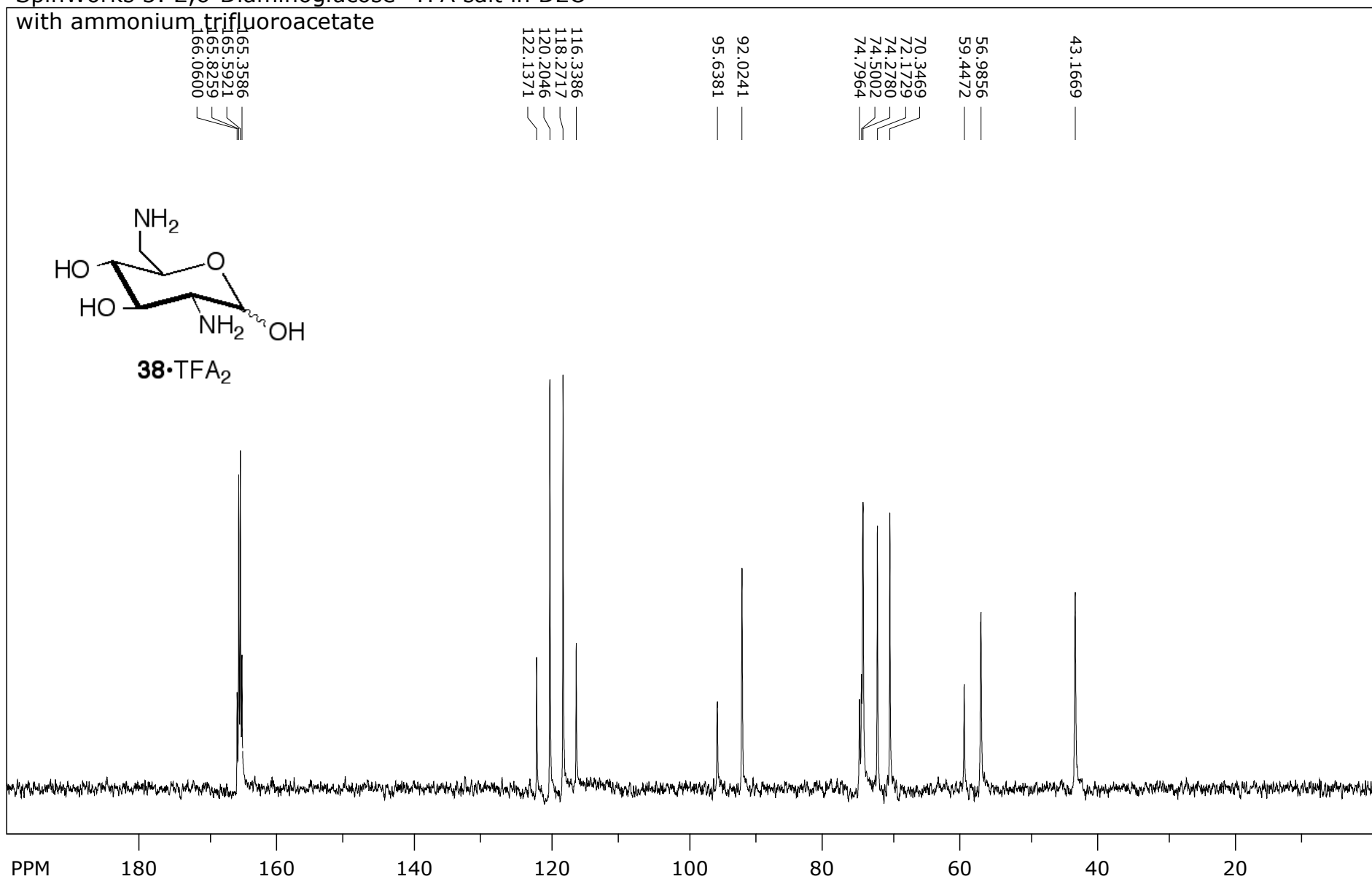


file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\26DiAmGlu_D2O_COSY\2\ser
 transmitter freq.: 600.553566 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.58 Hz = 10.006793 ppm = 2.934365 Hz/pt
 number of scans: 2

expt: <cosygp
 F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 85.693 ppm/cm: 0.14269

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 160.574 ppm/cm: 0.26738

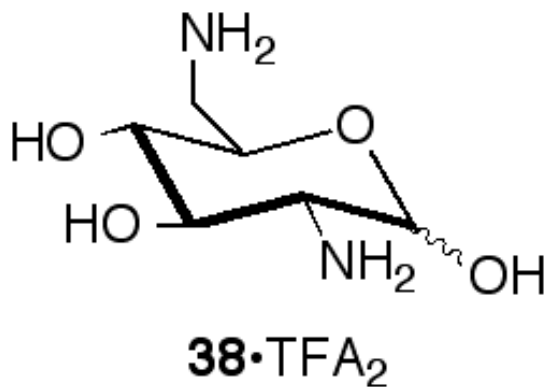
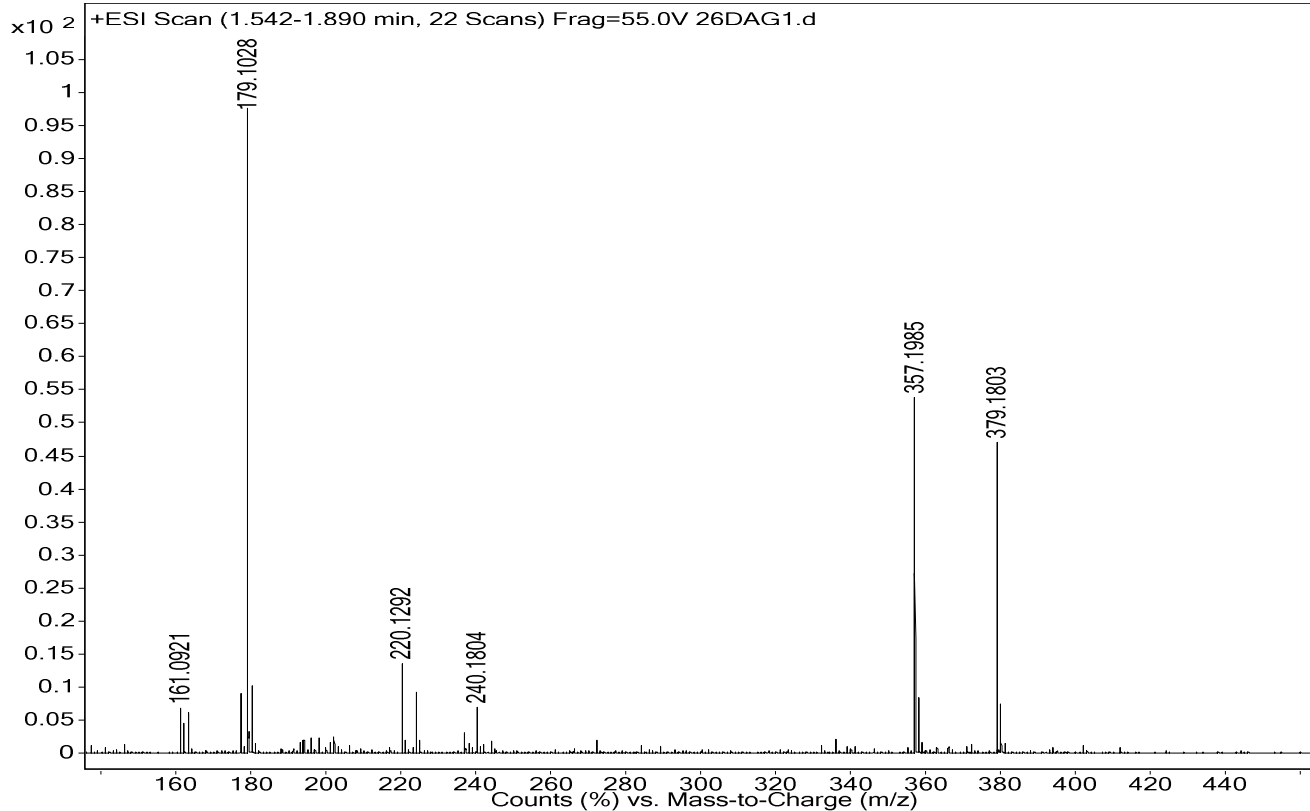
with ammonium trifluoroacetate

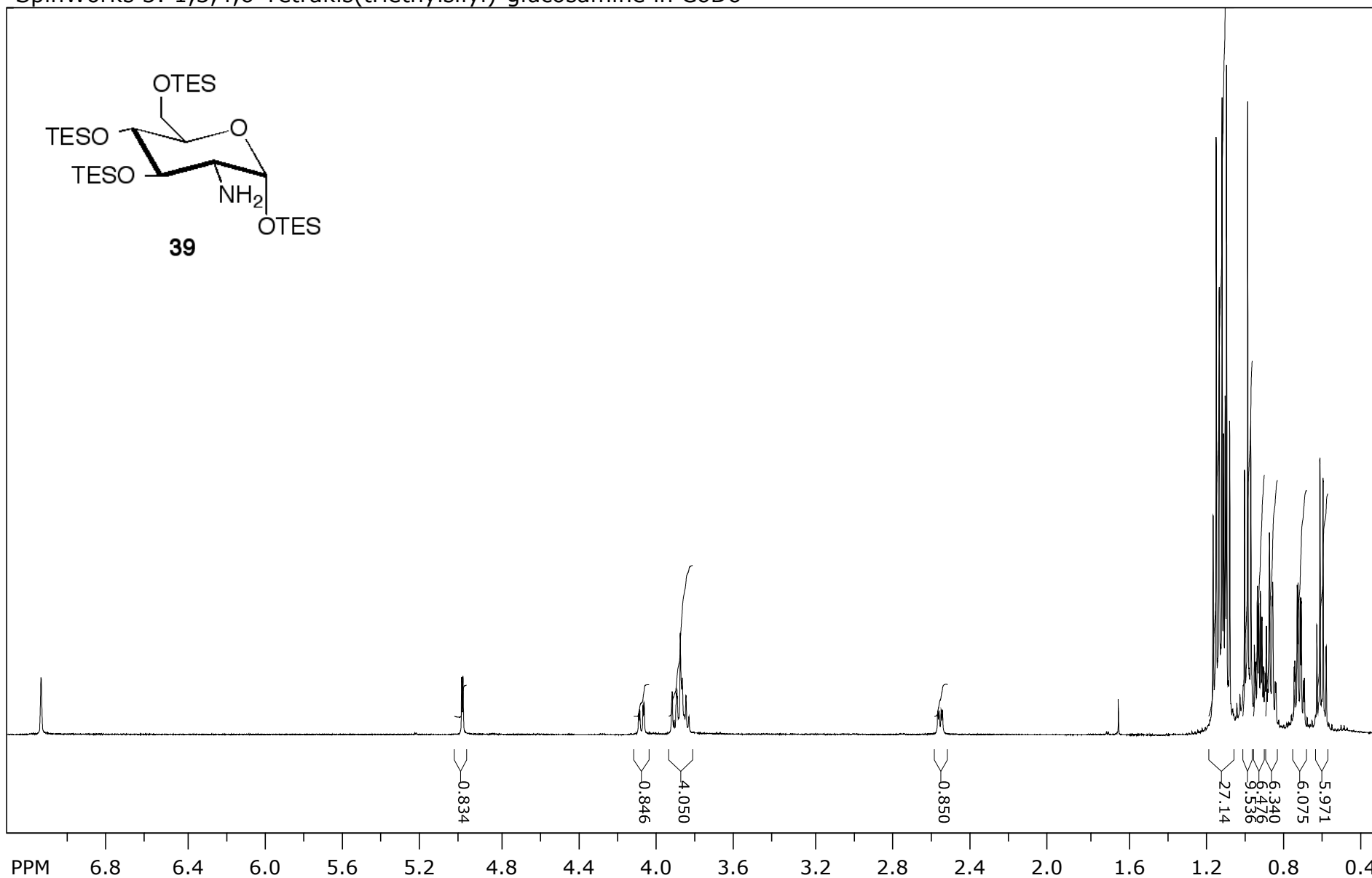


file: ...ata\26DiAmGlu_TFA salt_D2O13C\1\fid expt: <zpgg30>
 transmitter freq.: 151.023519 MHz
 time domain size: 65536 points
 width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
 number of scans: 18432

freq. of 0 ppm: 151.008006 MHz
 processed size: 32768 complex points
 LB: 10.000 GF: 0.0000
 Hz/cm: 1215.337 ppm/cm: 8.04734

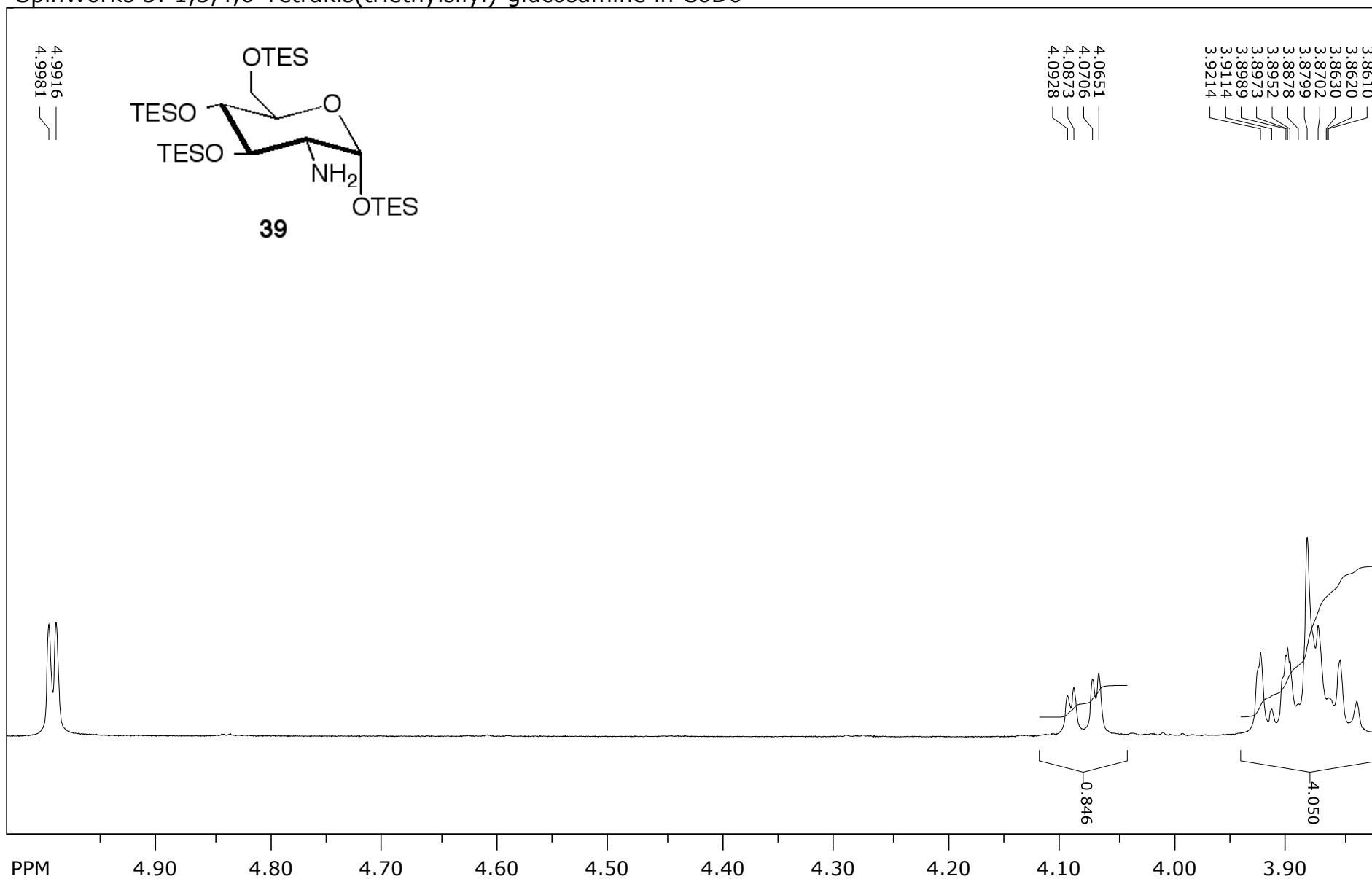
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	26DAG1.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable





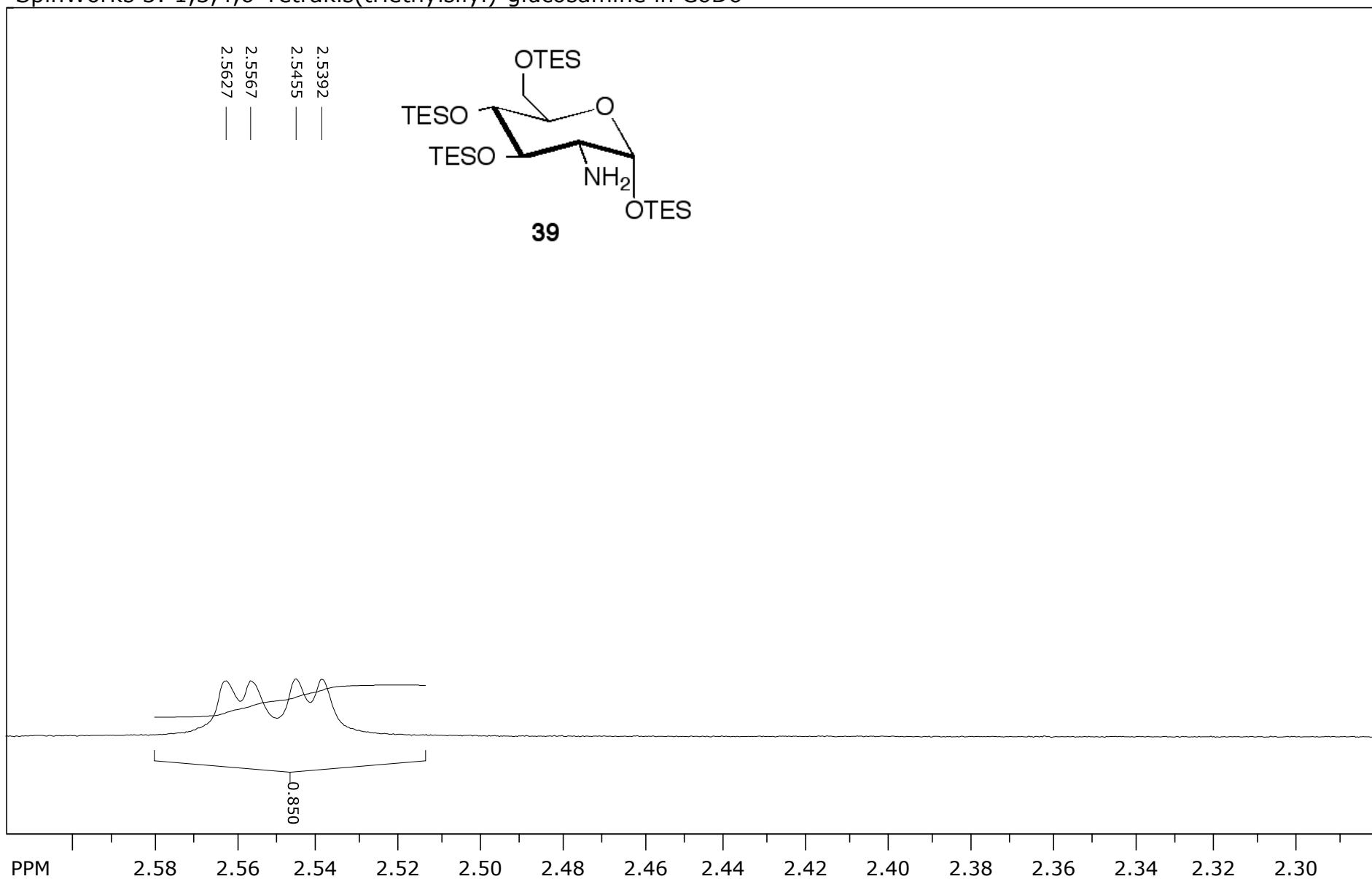
file: ..._10\TES4GlcNH2 in d6 benzene\1\fid expt: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 6009.62 Hz = 12.0181 ppm = 0.091699 Hz/pt
number of scans: 32

freq. of 0 ppm: 500.046065 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 140.235 ppm/cm: 0.28044



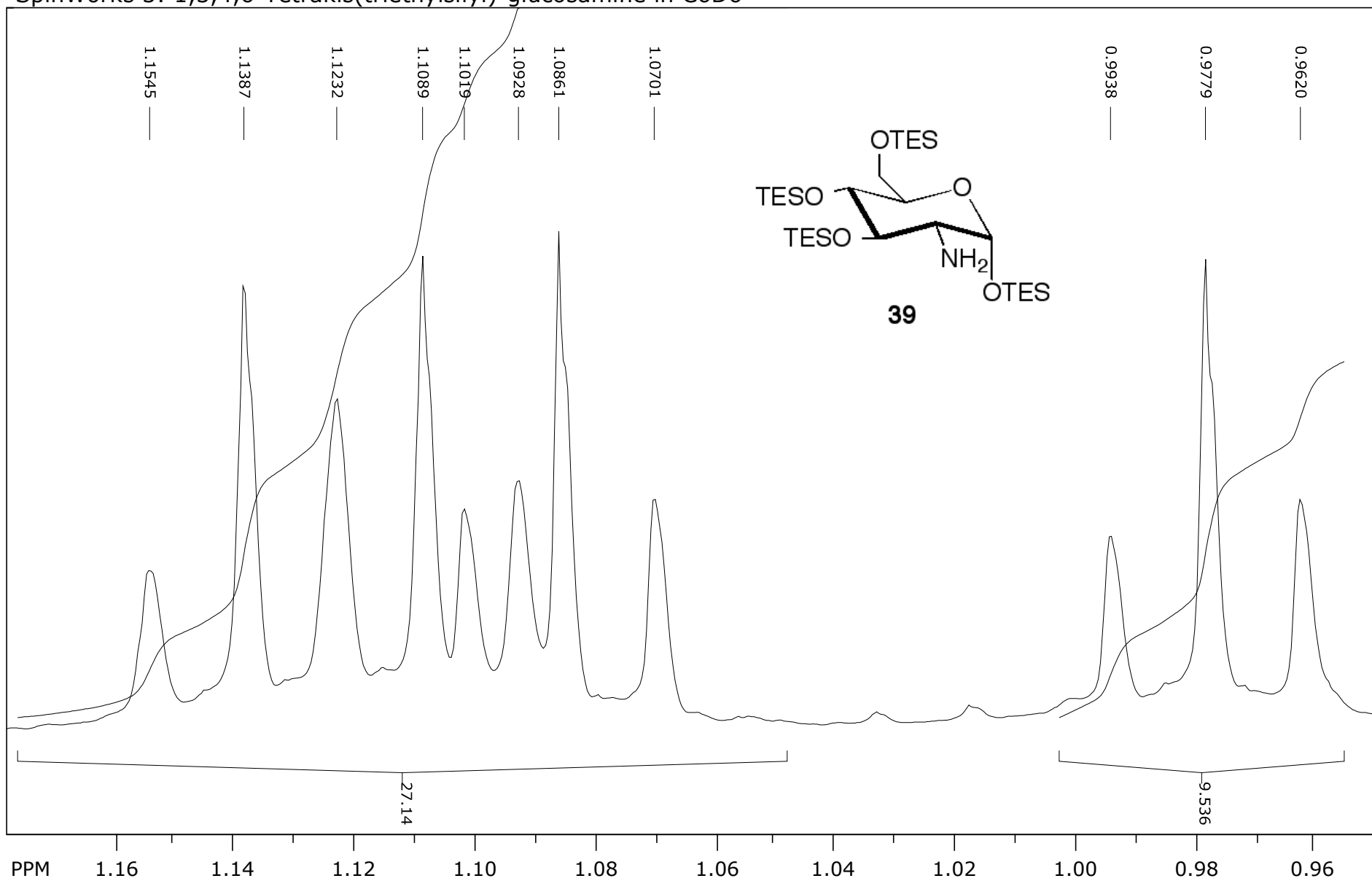
file: ..._10\TES4GlcNH2 in d6 benzene\1\fid expt: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 6009.62 Hz = 12.0181 ppm = 0.091699 Hz/pt
number of scans: 32

freq. of 0 ppm: 500.046065 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 24.387 ppm/cm: 0.04877



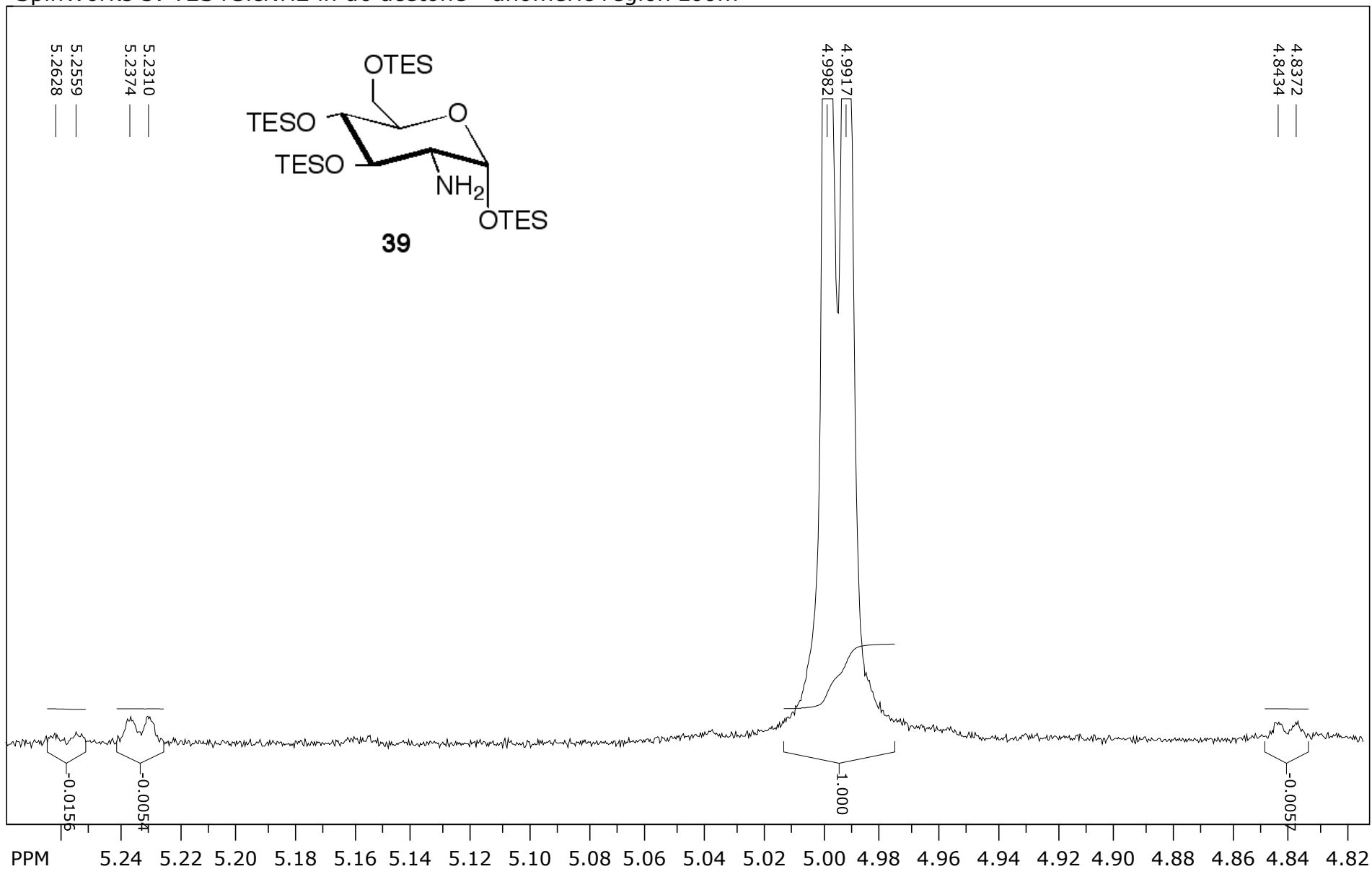
file: ..._10\TES4GlcNH2 in d6 benzene\1\fid expt: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 6009.62 Hz = 12.0181 ppm = 0.091699 Hz/pt
number of scans: 32

freq. of 0 ppm: 500.046065 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 6.747 ppm/cm: 0.01349



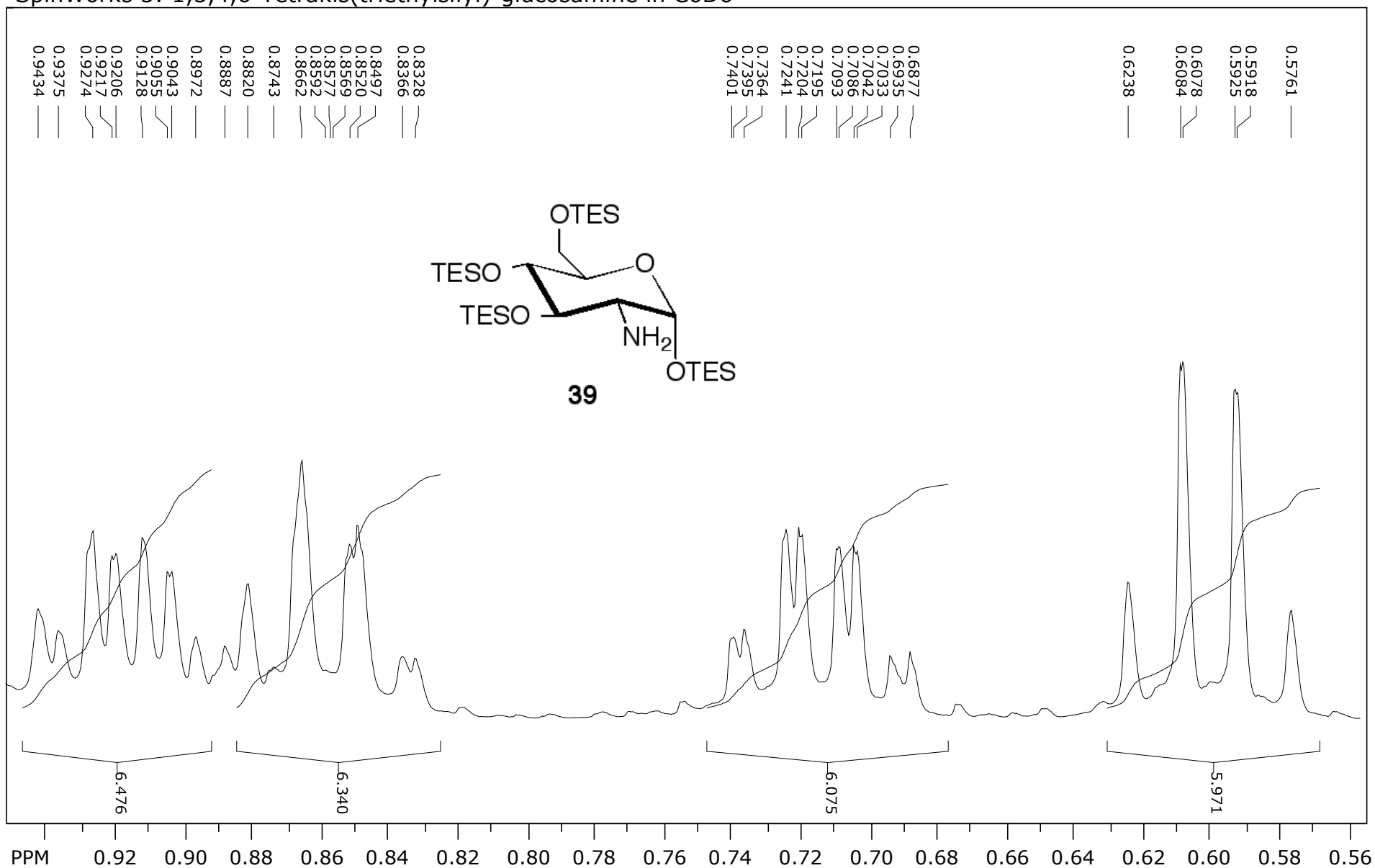
file: ..._10\TES4GlcNH2 in d6 benzene\1\fid expt: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 6009.62 Hz = 12.0181 ppm = 0.091699 Hz/pt
number of scans: 32

freq. of 0 ppm: 500.046065 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 4.590 ppm/cm: 0.00918



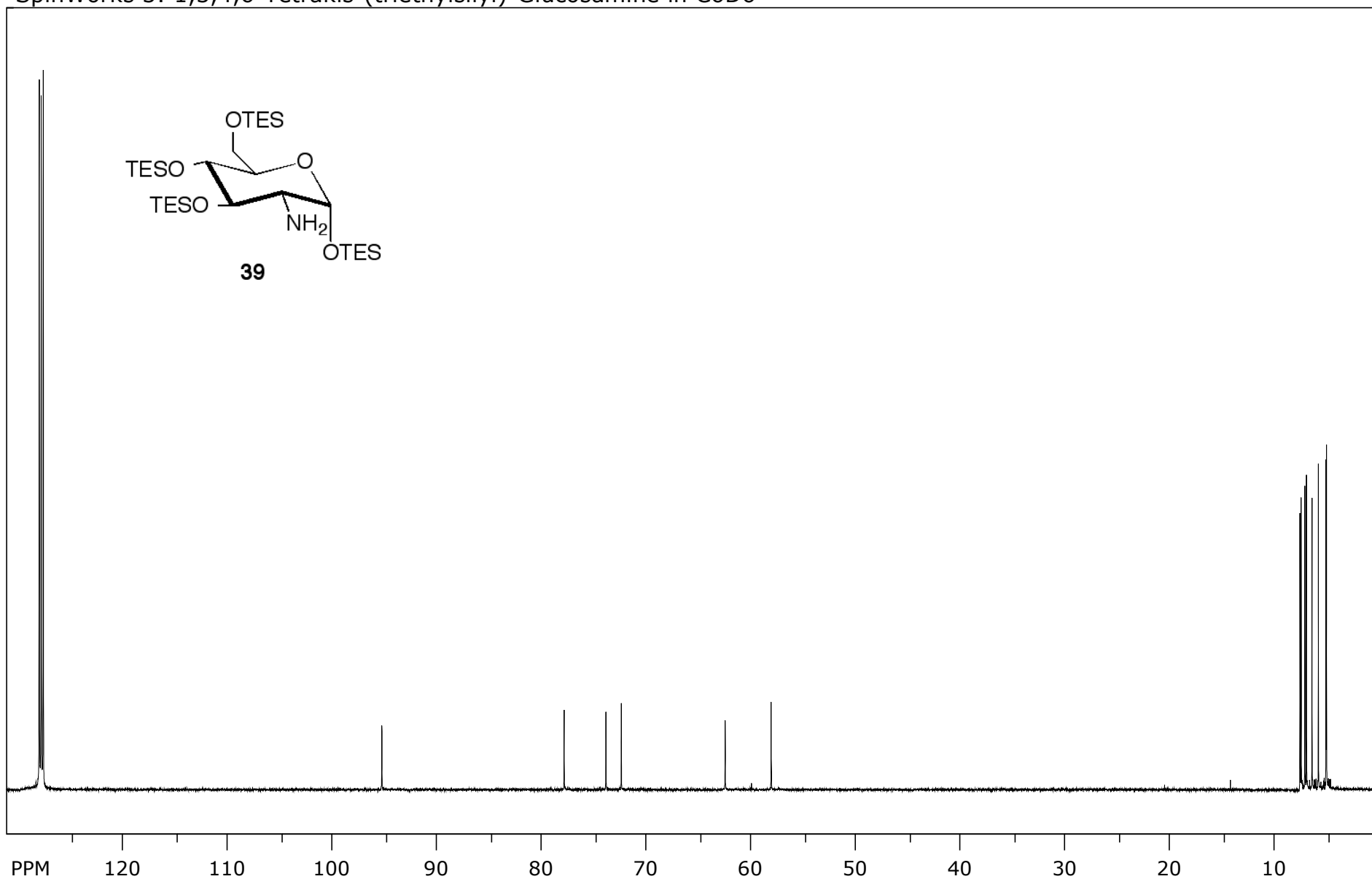
file: ..._10\TES4GlcNH2 in d6 benzene\1\fid expt: <zg>
 transmitter freq.: 500.049088 MHz
 time domain size: 65536 points
 width: 6009.62 Hz = 12.0181 ppm = 0.091699 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.046065 MHz
 processed size: 32768 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 9.317 ppm/cm: 0.01863



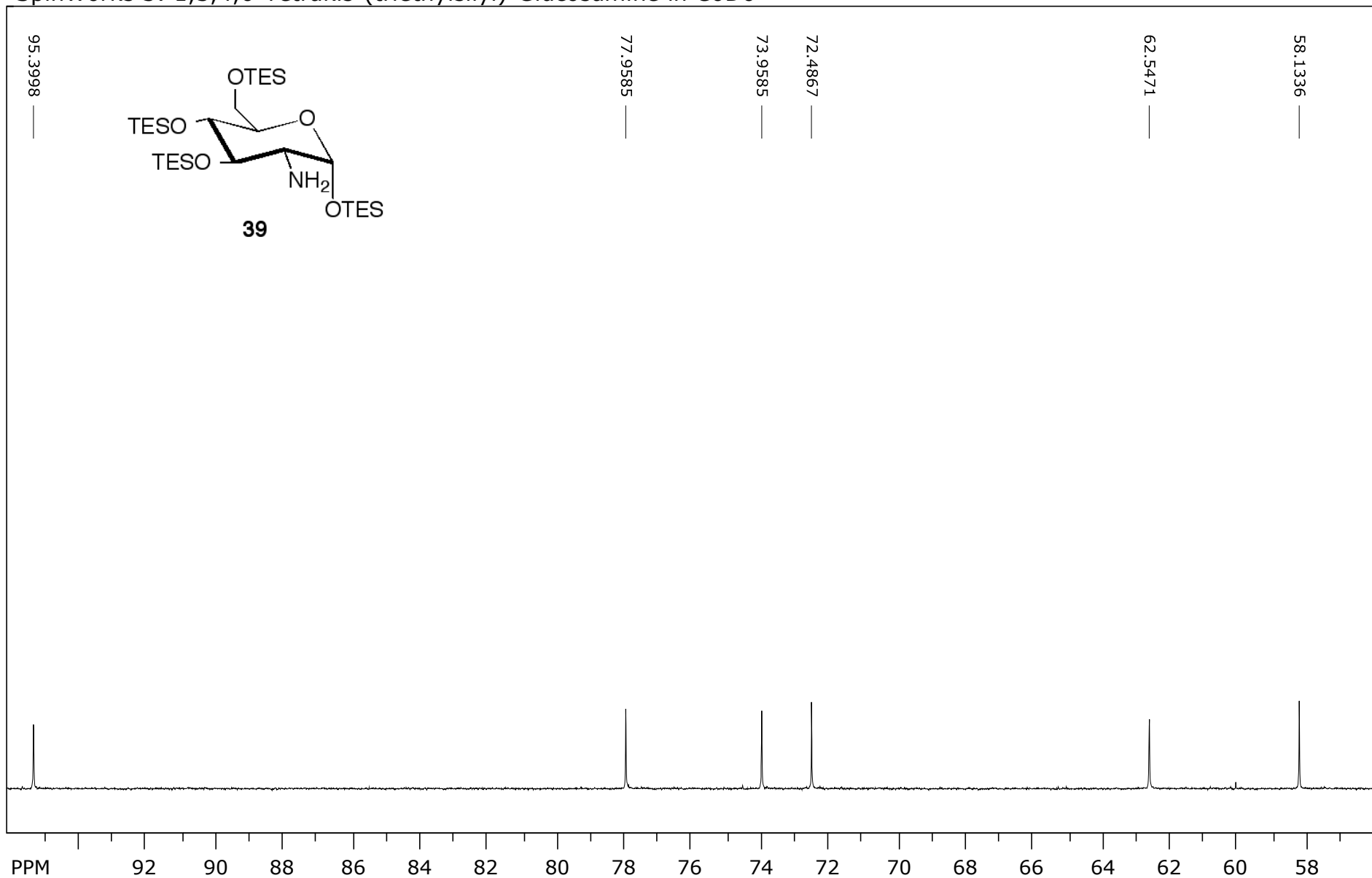
file: ..._10\TES4GlcNH2 in d6 benzene\1\fid expt: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 6009.62 Hz = 12.0181 ppm = 0.091699 Hz/pt
number of scans: 32

freq. of 0 ppm: 500.046065 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 7.947 ppm/cm: 0.01589



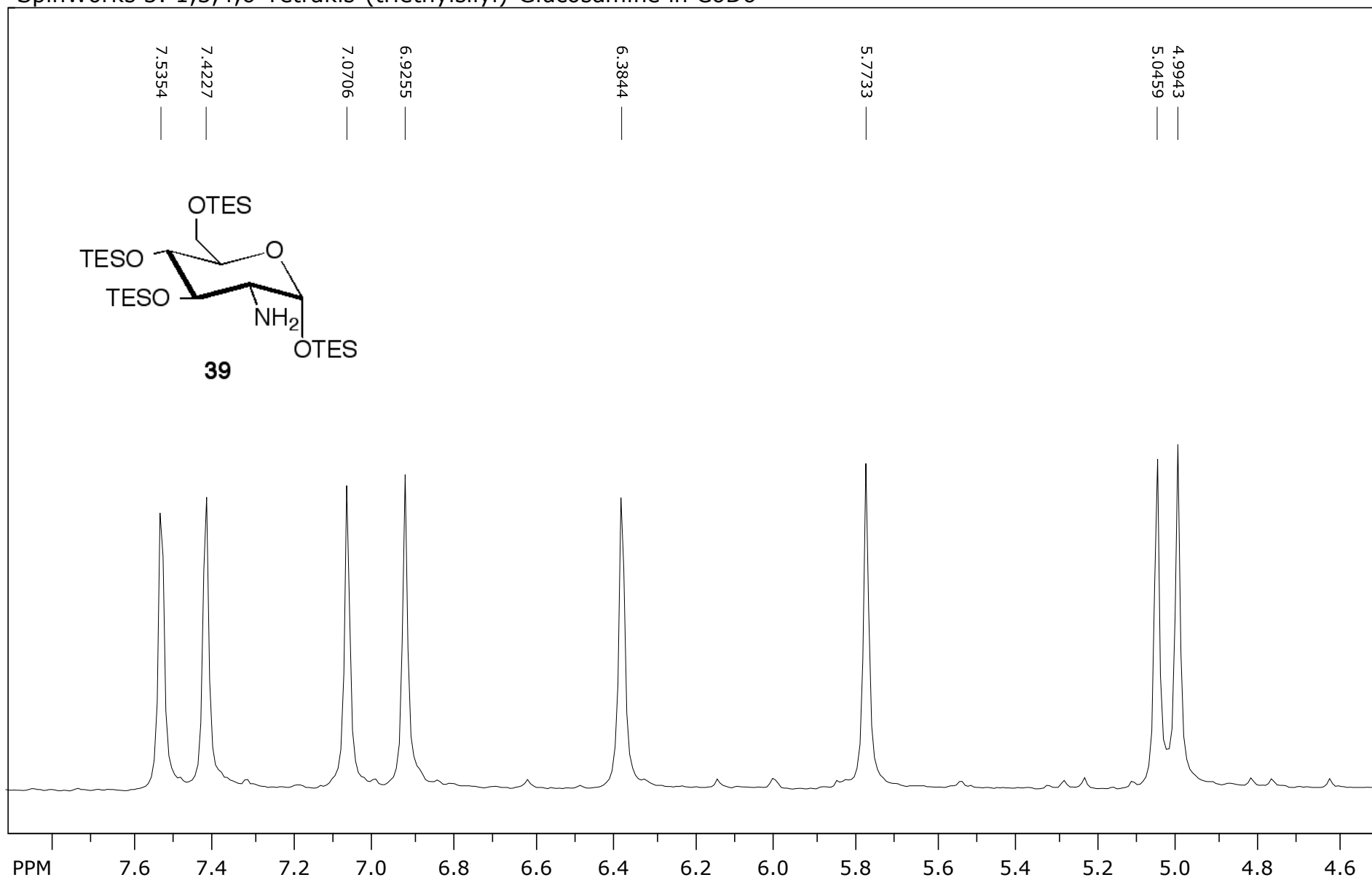
file: ..._10\TES4GlcNH2 in d6 benzene\2\fid exp: <zpgg30>
transmitter freq.: 125.749240 MHz
time domain size: 65536 points
width: 30030.03 Hz = 238.8088 ppm = 0.458222 Hz/pt
number of scans: 256

freq. of 0 ppm: 125.736637 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 660.429 ppm/cm: 5.25195



file: ..._10\TES4GlcNH2 in d6 benzene\2\fid expt: <zpgg30>
transmitter freq.: 125.749240 MHz
time domain size: 65536 points
width: 30030.03 Hz = 238.8088 ppm = 0.458222 Hz/pt
number of scans: 256

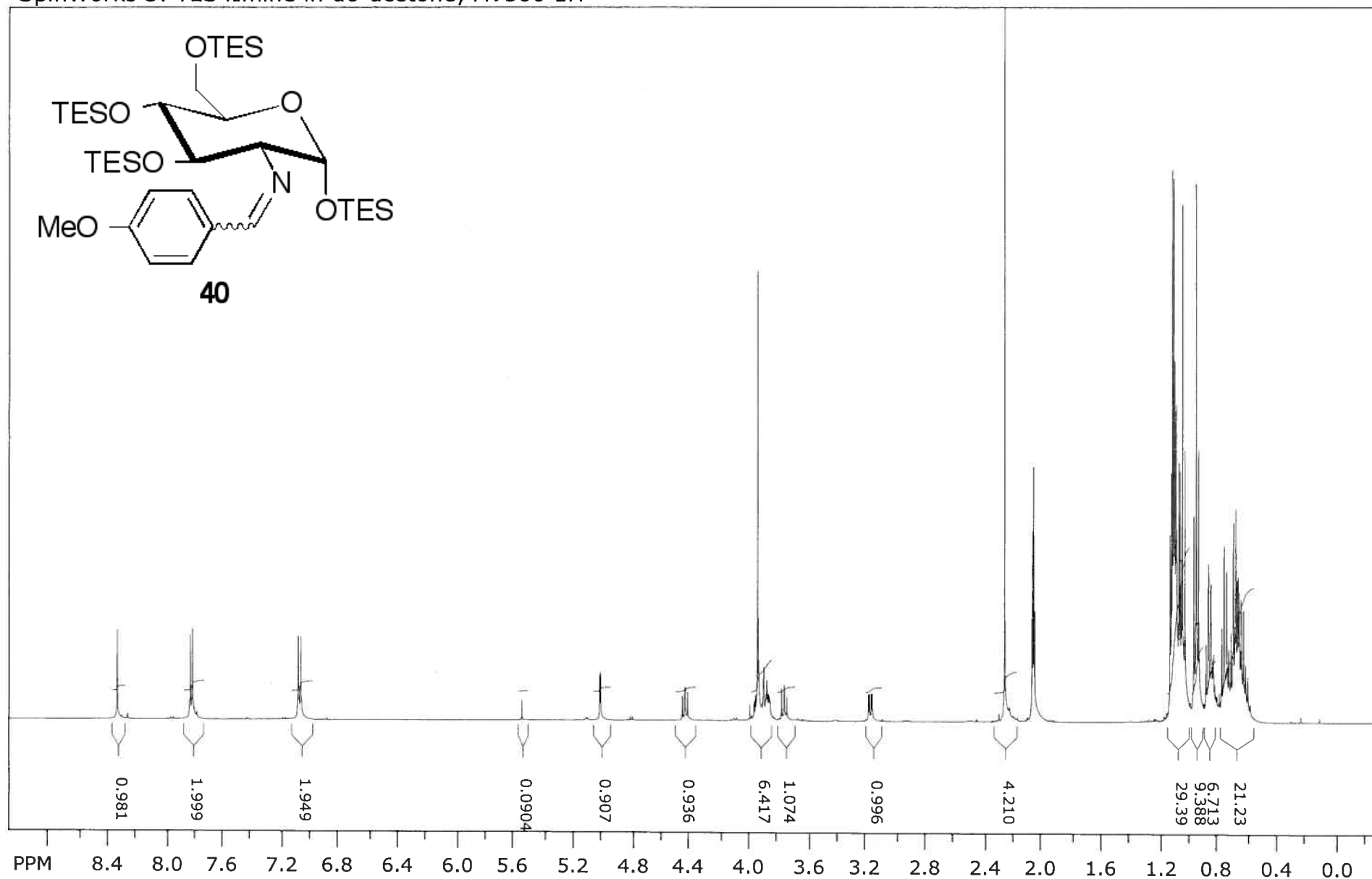
freq. of 0 ppm: 125.736637 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 203.181 ppm/cm: 1.61576



file: ..._10\TES4GlcNH2 in d6 benzene\2\fid expt: <zpgg30>
transmitter freq.: 125.749240 MHz
time domain size: 65536 points
width: 30030.03 Hz = 238.8088 ppm = 0.458222 Hz/pt
number of scans: 256

freq. of 0 ppm: 125.736637 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 17.227 ppm/cm: 0.13699

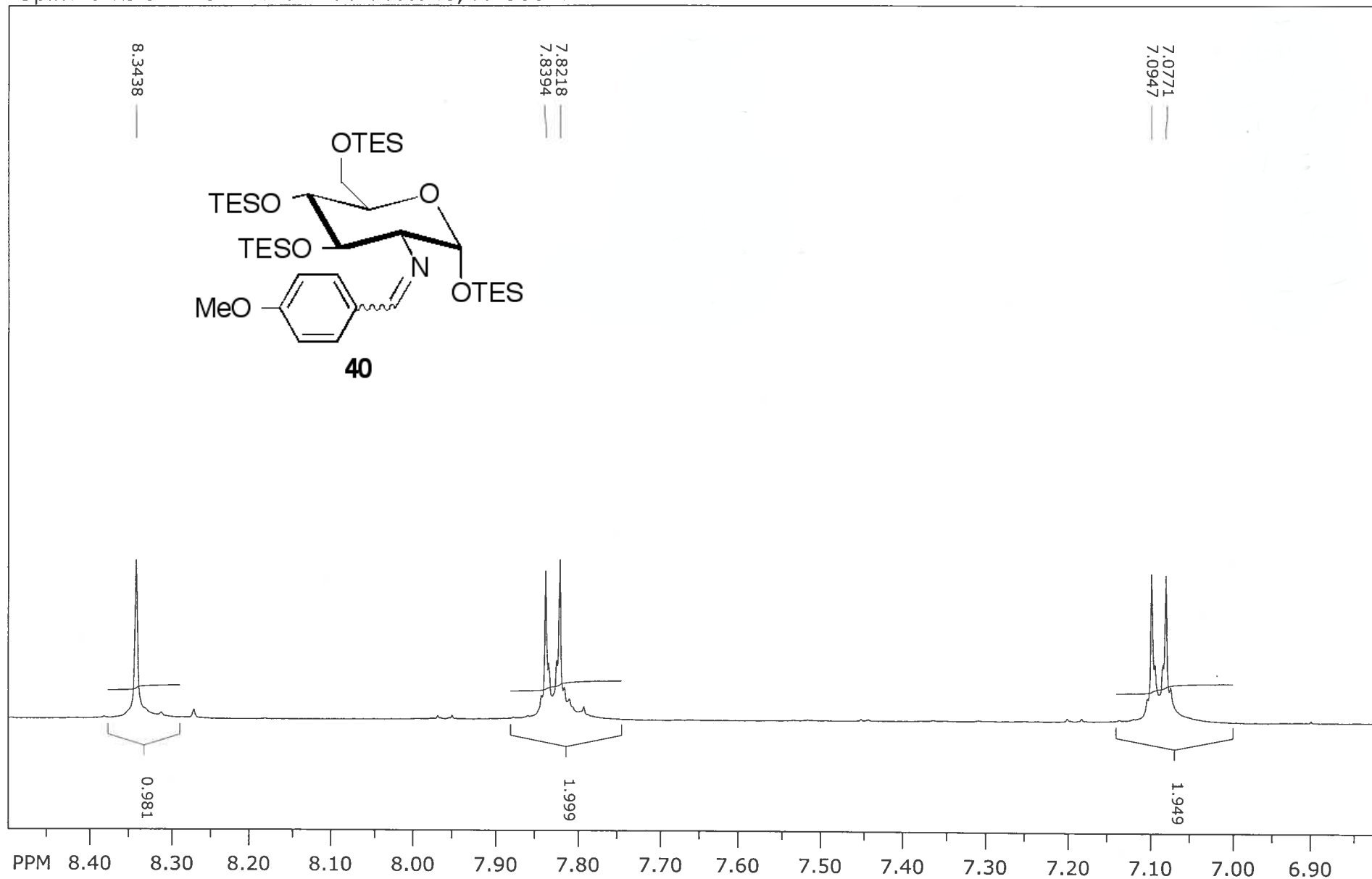
SpinWorks 3: TES4Imine in d6-acetone; AV500 1H



file: ...\\nmr\Posakony\nmr\imine_7_09\1\fid expt: <zg>
 transmitter freq.: 500.049088 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.045964 MHz
 processed size: 32768 complex points
 LB: 0.300 GF: 0.0000
 Hz/cm: 187.772 ppm/cm: 0.37551

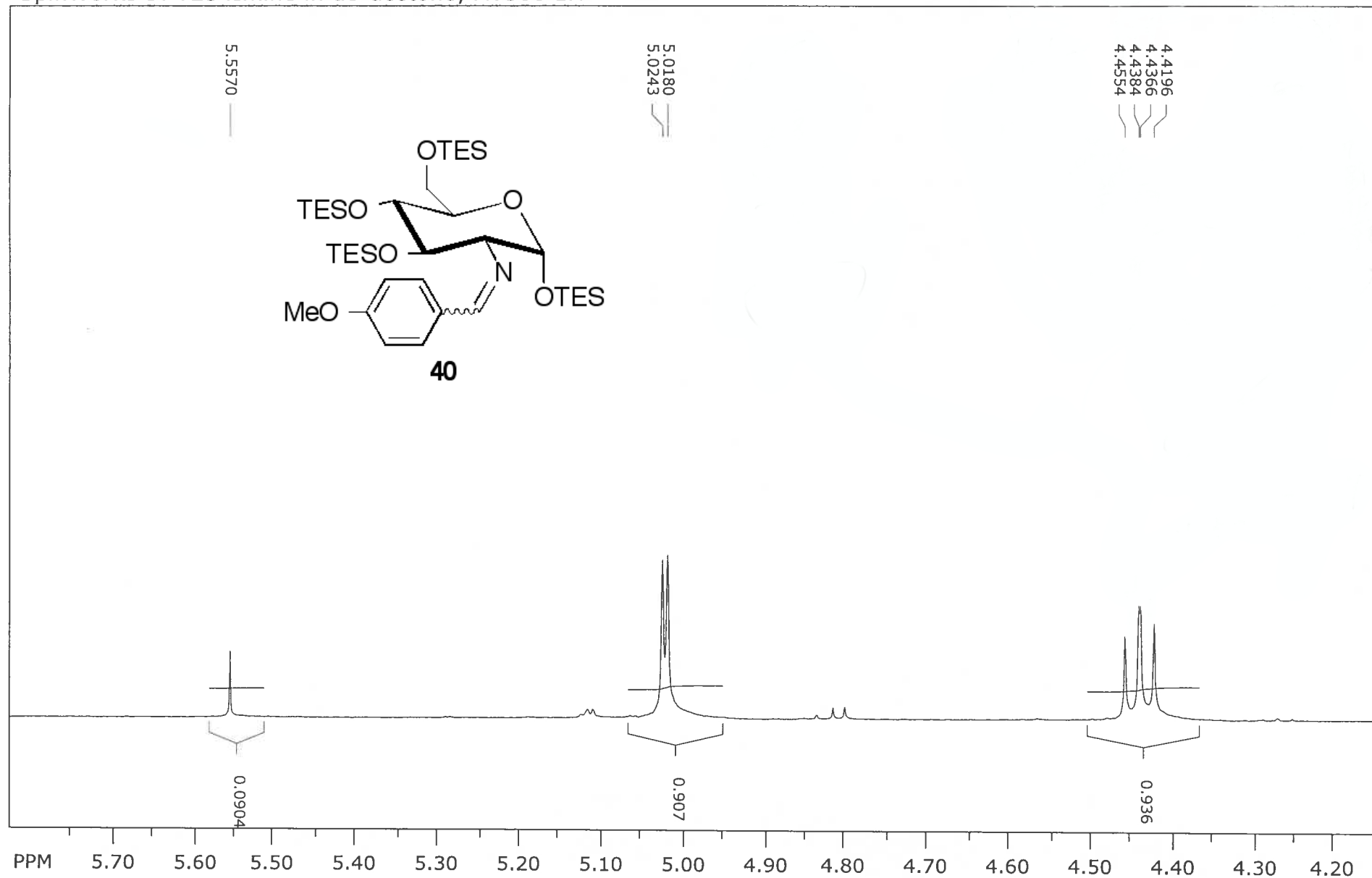
SpinWorks 3: TES4Imine in d6-acetone; AV500 1H



file: ...\\nmr\Posakony\nmr\imine_7_09\1\fid expt: <zg>
 transmitter freq.: 500.049088 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.045964 MHz
 processed size: 32768 complex points
 LB: 0.300 GF: 0.0000
 Hz/cm: 33.677 ppm/cm: 0.06735

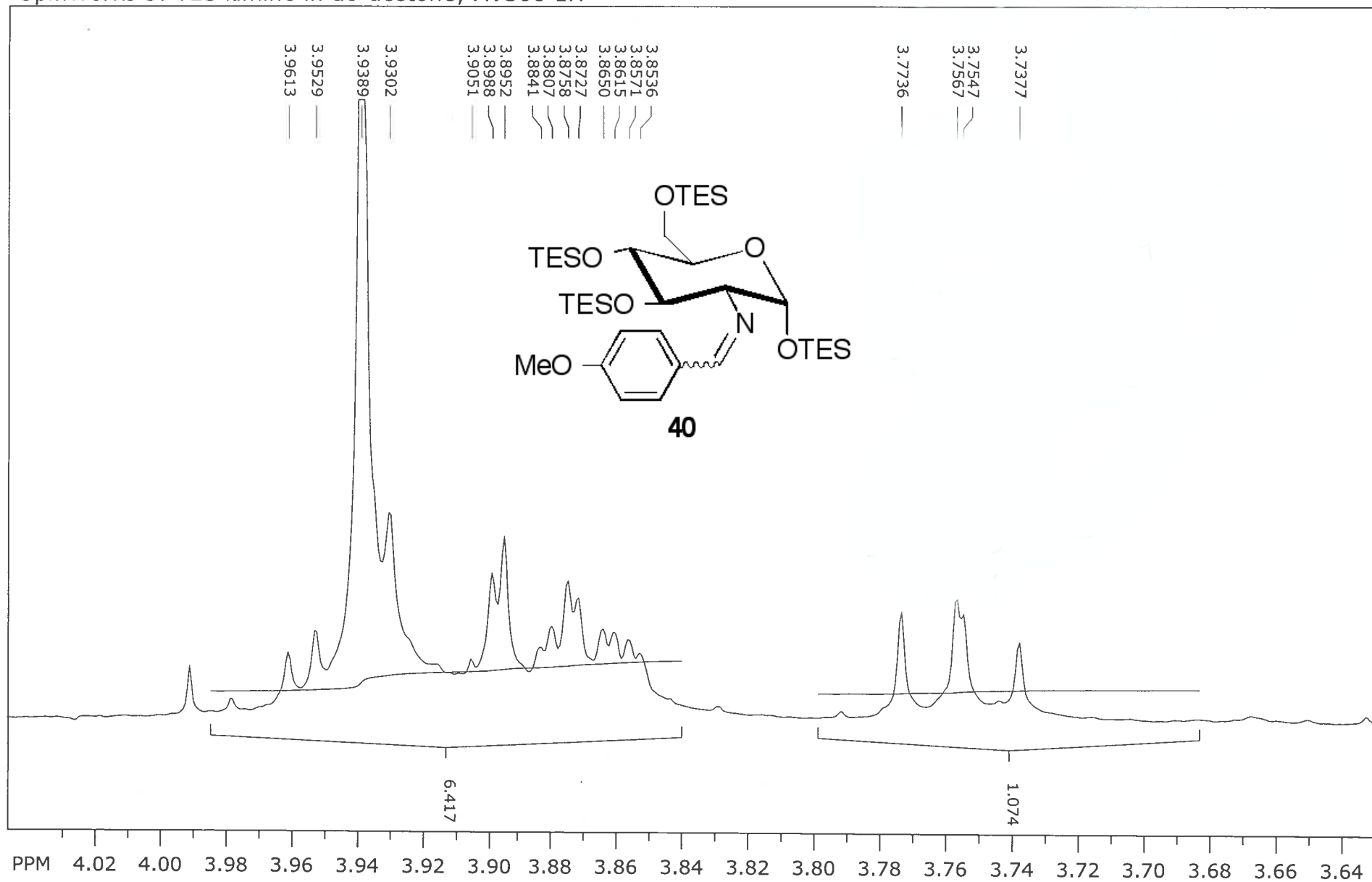
SpinWorks 3: TES4Imine in d6-acetone; AV500 1H



file: ...\\nmr\Posakony\nmr\imine_7_09\1\fid expt: <zg>
 transmitter freq.: 500.049088 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.045964 MHz
 processed size: 32768 complex points
 LB: 0.300 GF: 0.0000
 Hz/cm: 33.677 ppm/cm: 0.06735

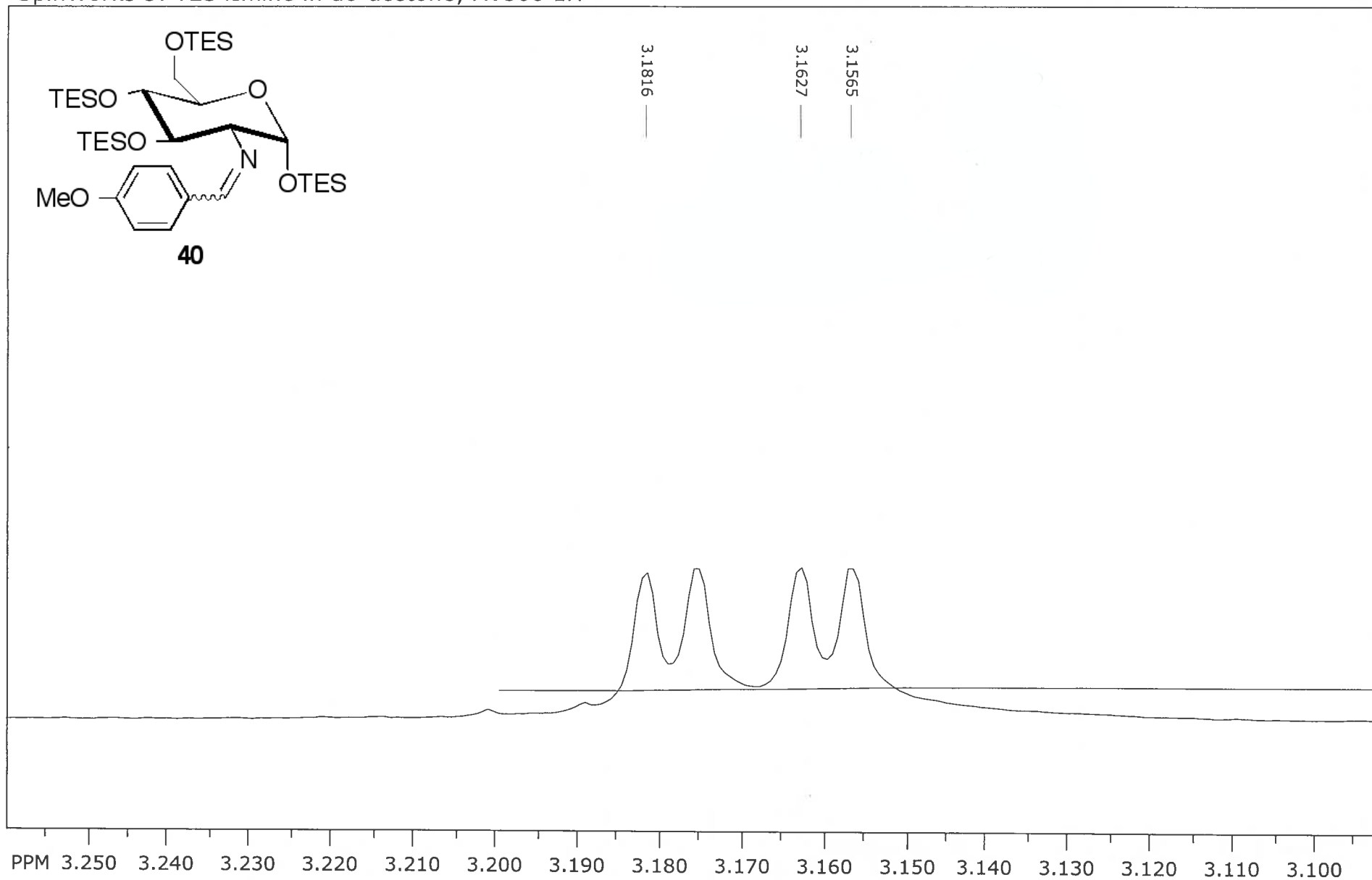
SpinWorks 3: TES4Imine in d6-acetone; AV500 1H



file: ...\\nmr\Posakony\nmr\imine_7_09\1\fid expt: <zg>
 transmitter freq.: 500.049088 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.045964 MHz
 processed size: 32768 complex points
 LB: 0.300 GF: 0.0000
 Hz/cm: 8.375 ppm/cm: 0.01675

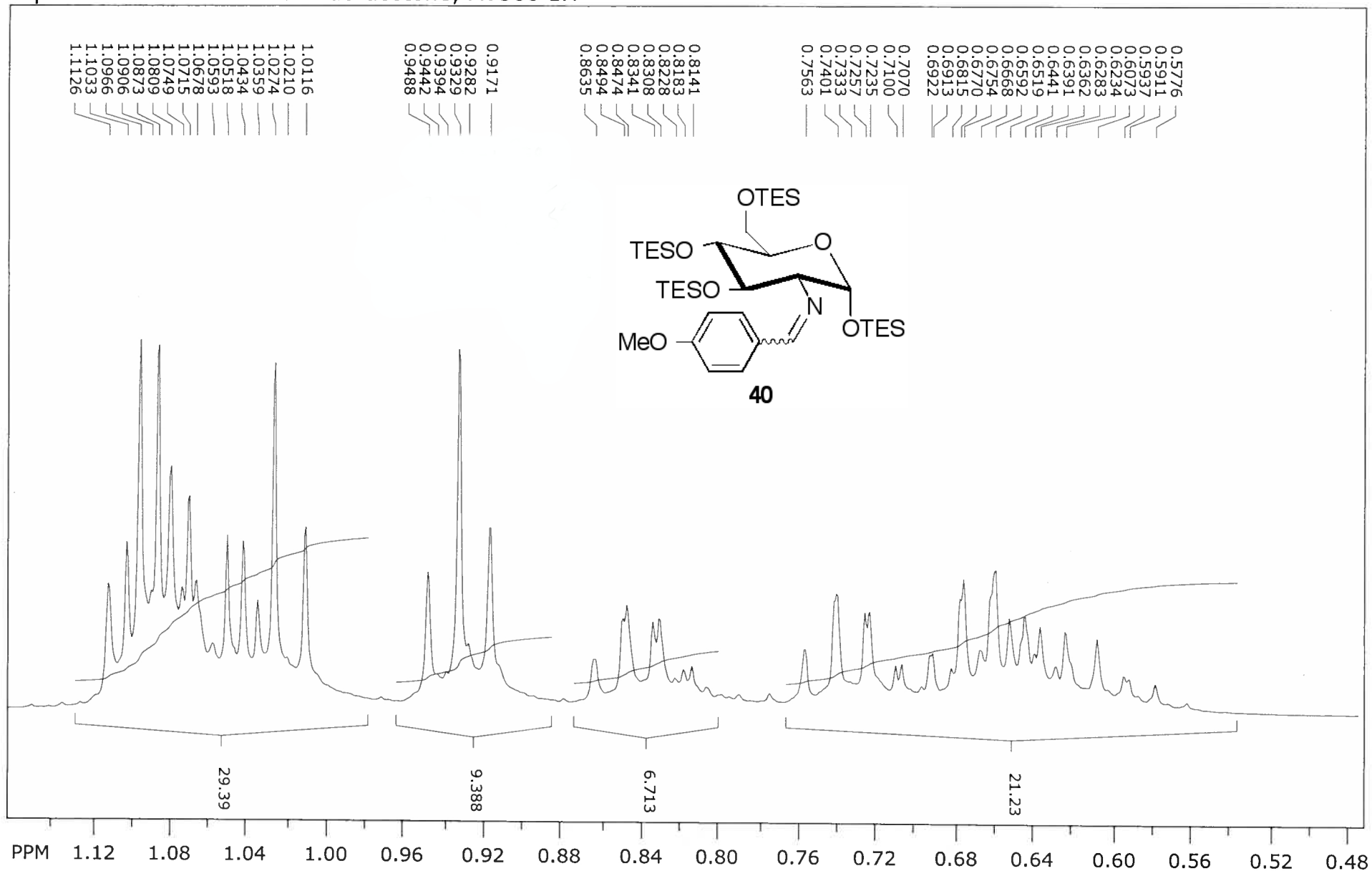
SpinWorks 3: TES4Imine in d6-acetone; AV500 1H



file: ...\\nrmr\Posakony\nmr\imine_7_09\1\fid expt: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
number of scans: 32

freq. of 0 ppm: 500.045964 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 3.358 ppm/cm: 0.00671

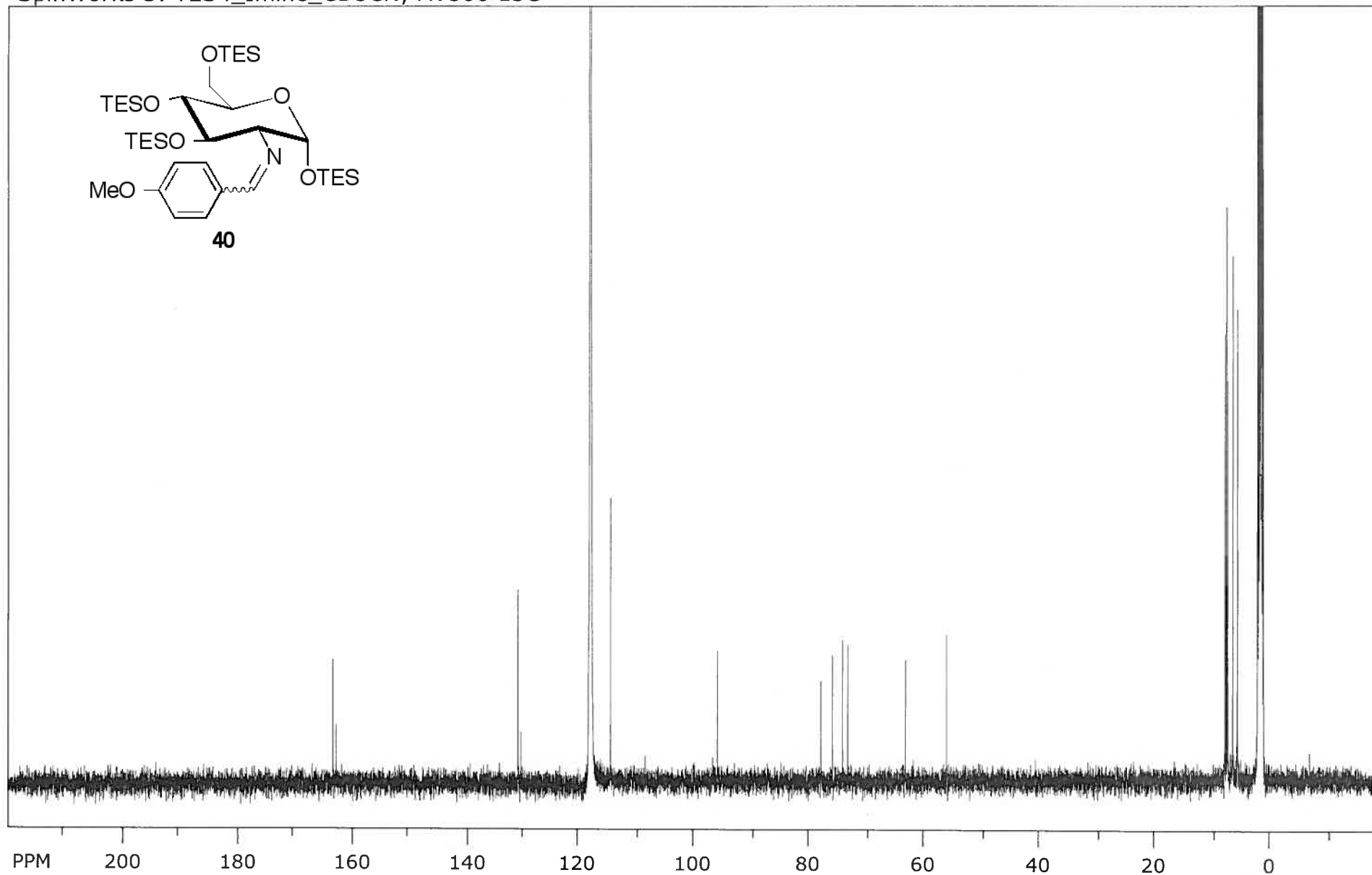
SpinWorks 3: TES4Imine in d6-acetone; AV500 1H



file: ...\\nrm\Posakony\nmr\imine_7_09\1\fid expt: <zg>
 transmitter freq.: 500.049088 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
 number of scans: 32

freq. of 0 ppm: 500.045964 MHz
 processed size: 32768 complex points
 LB: 0.300 GF: 0.0000
 Hz/cm: 13.818 ppm/cm: 0.02763

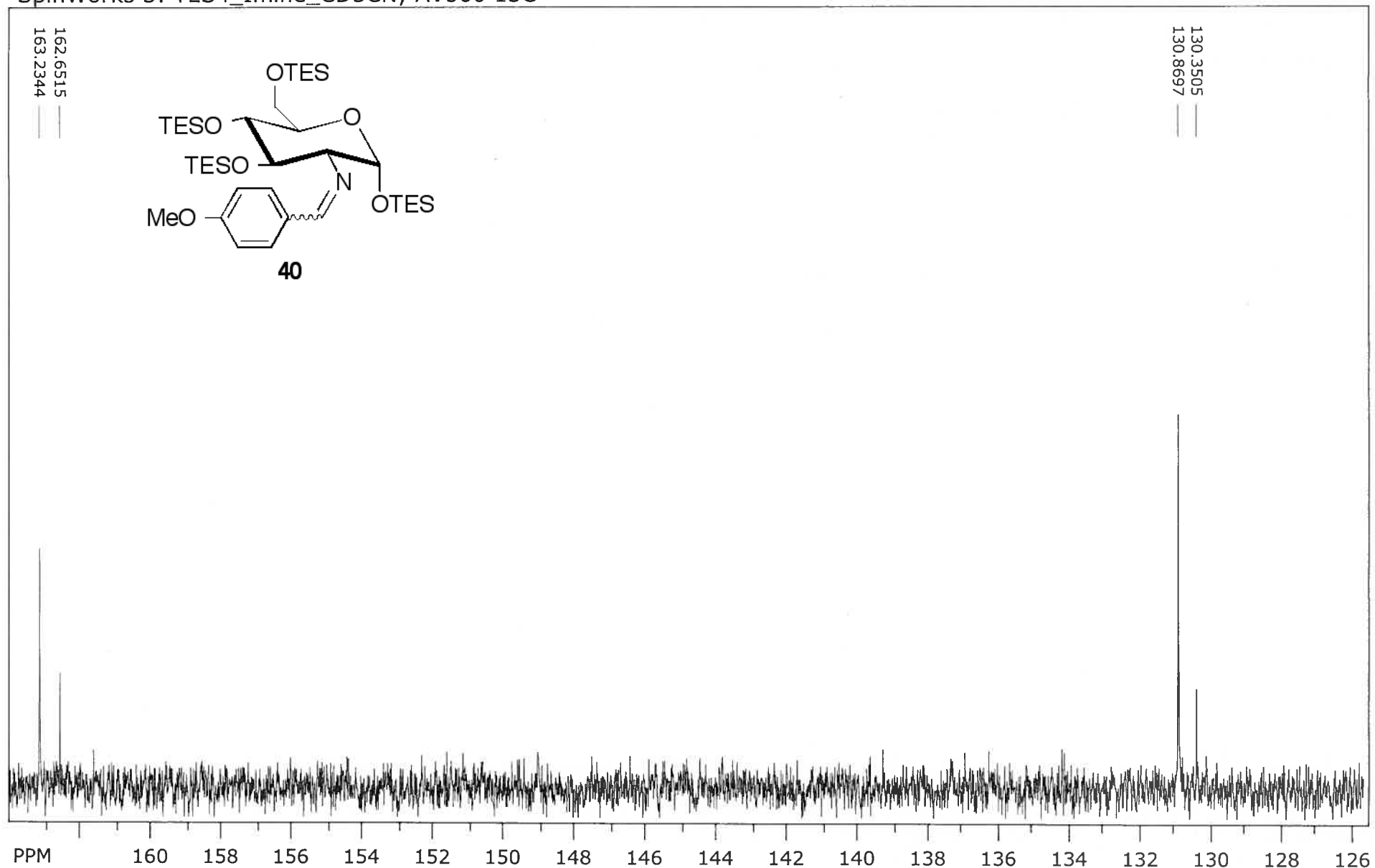
SpinWorks 3: TES4_Imine_CD3CN; AV500 13C



file: ...\\nmr\Posakony\nmr\imine_7_09\2\fid expt: <zpgg30>
transmitter freq.: 125.749240 MHz
time domain size: 65536 points
width: 30030.03 Hz = 238.8088 ppm = 0.458222 Hz/pt
number of scans: 2700

freq. of 0 ppm: 125.736558 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 1201.201 ppm/cm: 9.55235

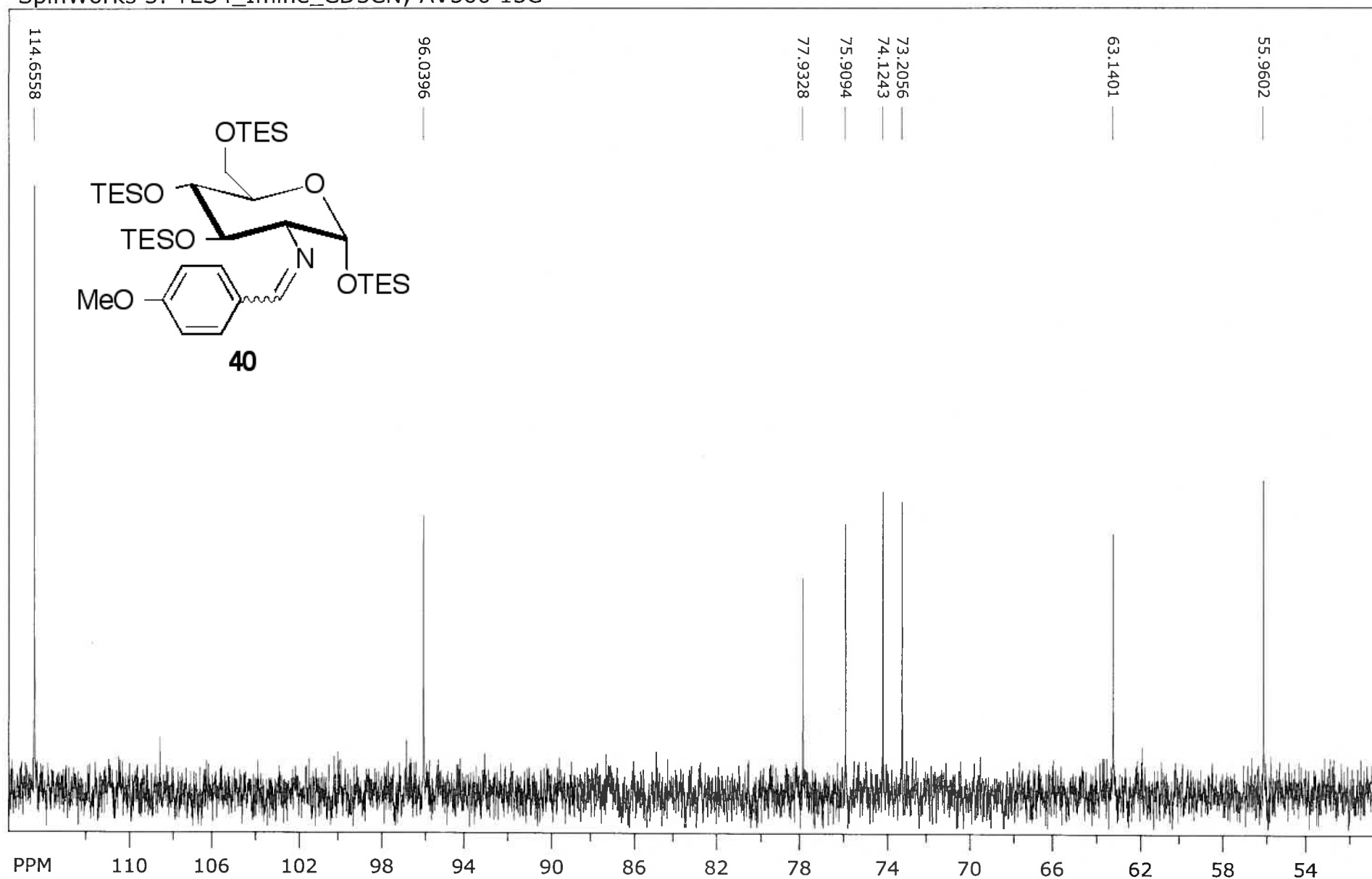
SpinWorks 3: TES4_Imine_CD3CN; AV500 13C



file: ...\\nmr\Posakony\nmr\imine_7_09\2\fid expt: <zpgg30>
transmitter freq.: 125.749240 MHz
time domain size: 65536 points
width: 30030.03 Hz = 238.8088 ppm = 0.458222 Hz/pt
number of scans: 2700

freq. of 0 ppm: 125.736558 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 193.713 ppm/cm: 1.54047

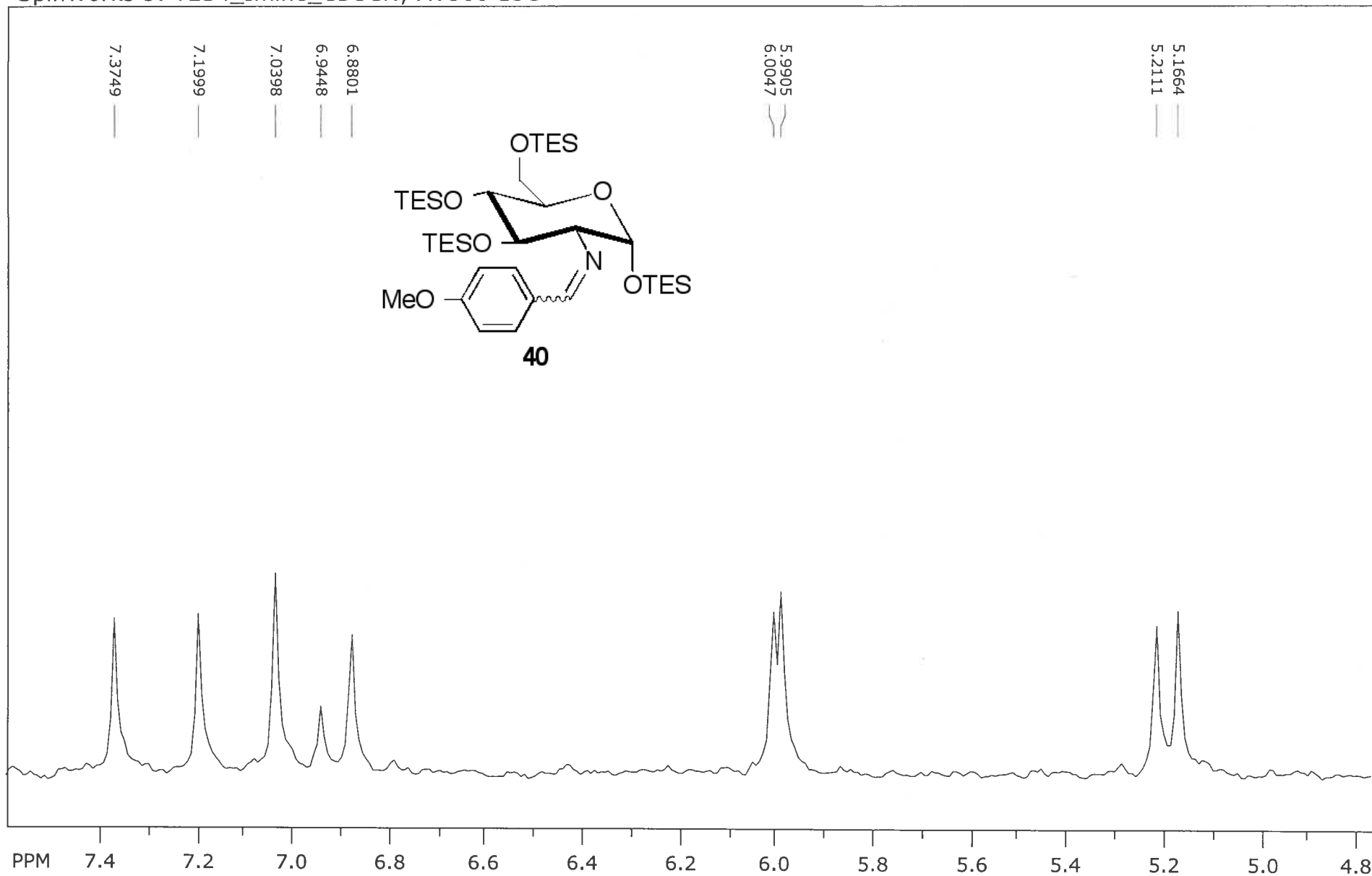
SpinWorks 3: TES4_Imine_CD3CN; AV500 13C



file: ...\\nmr\Posakony\nmr\imine_7_09\2\fid expt: <zgpg30>
 transmitter freq.: 125.749240 MHz
 time domain size: 65536 points
 width: 30030.03 Hz = 238.8088 ppm = 0.458222 Hz/pt
 number of scans: 2700

freq. of 0 ppm: 125.736558 MHz
 processed size: 32768 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 328.588 ppm/cm: 2.61304

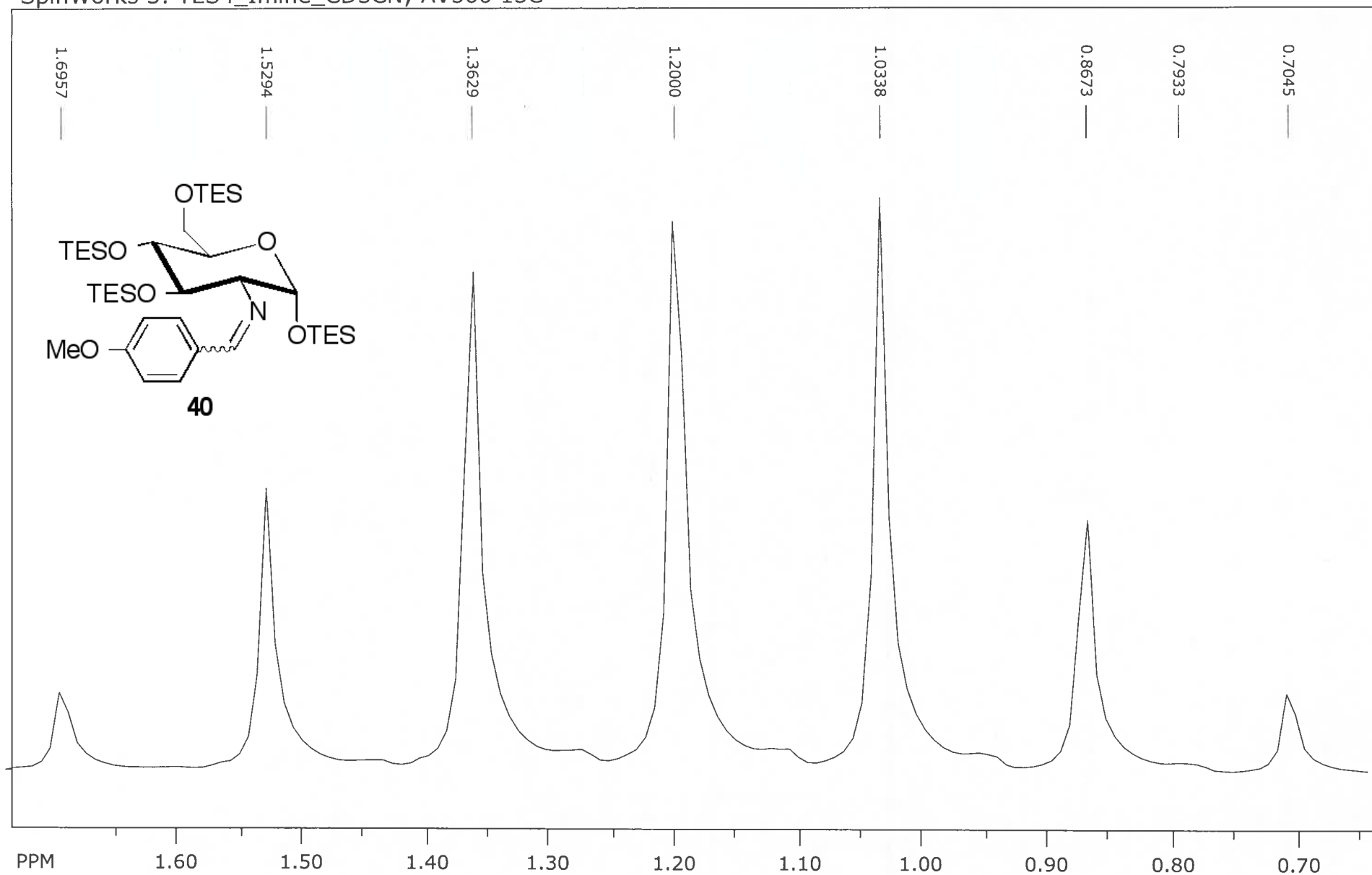
SpinWorks 3: TES4_Imine_CD3CN; AV500 13C



file: ...\\nmr\Posakony\nmr\imine_7_09\2\fid expt: <zpgg30>
 transmitter freq.: 125.749240 MHz
 time domain size: 65536 points
 width: 30030.03 Hz = 238.8088 ppm = 0.458222 Hz/pt
 number of scans: 2700

freq. of 0 ppm: 125.736558 MHz
 processed size: 32768 complex points
 LB: 1.000 GF: 0.0000
 Hz/cm: 14.259 ppm/cm: 0.11340

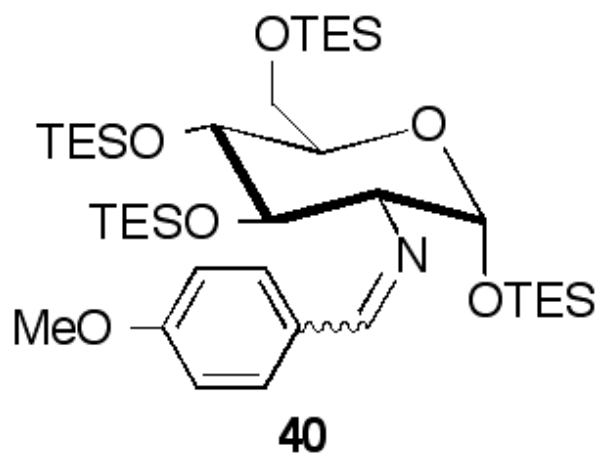
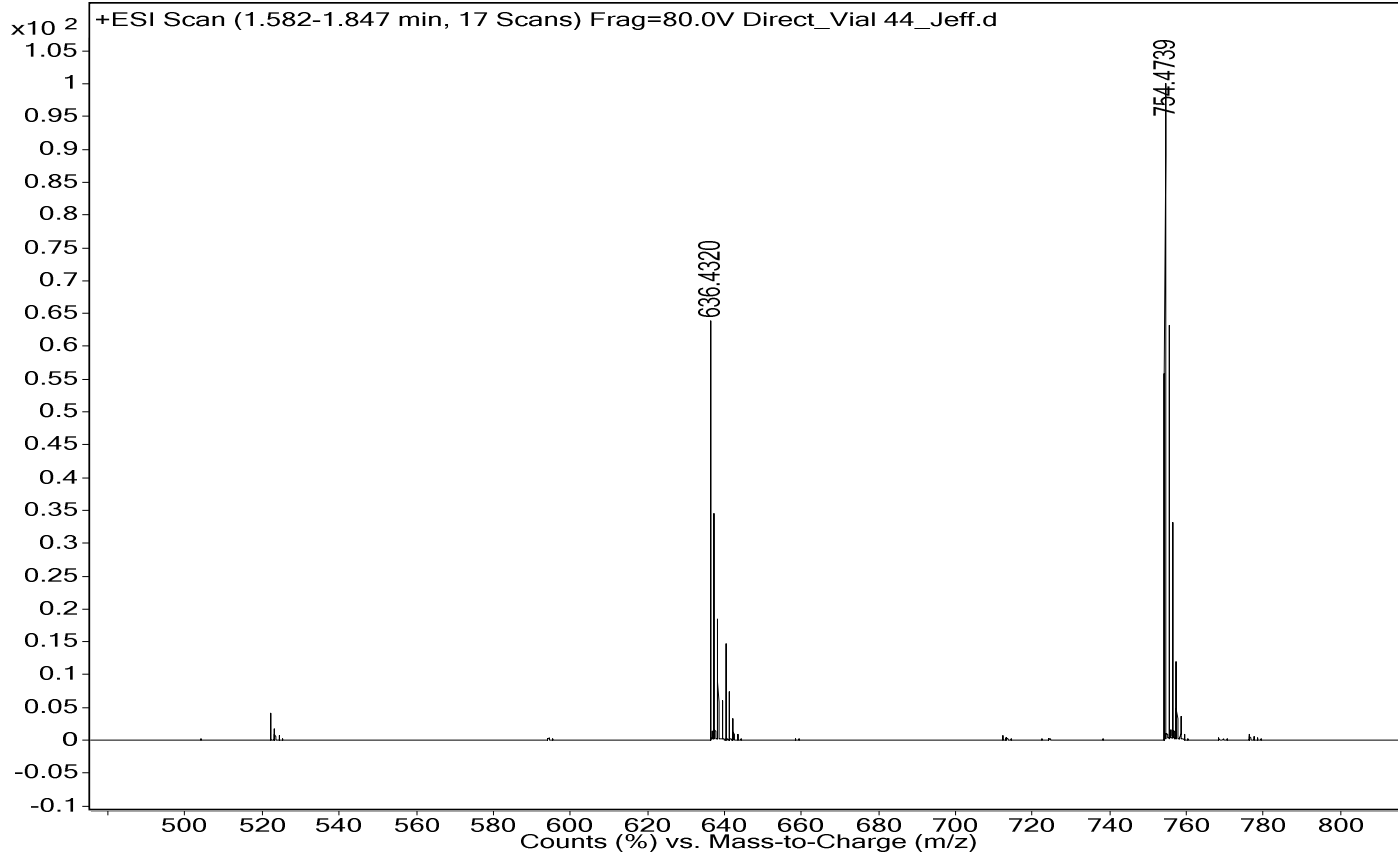
SpinWorks 3: TES4_Imine_CD3CN; AV500 13C

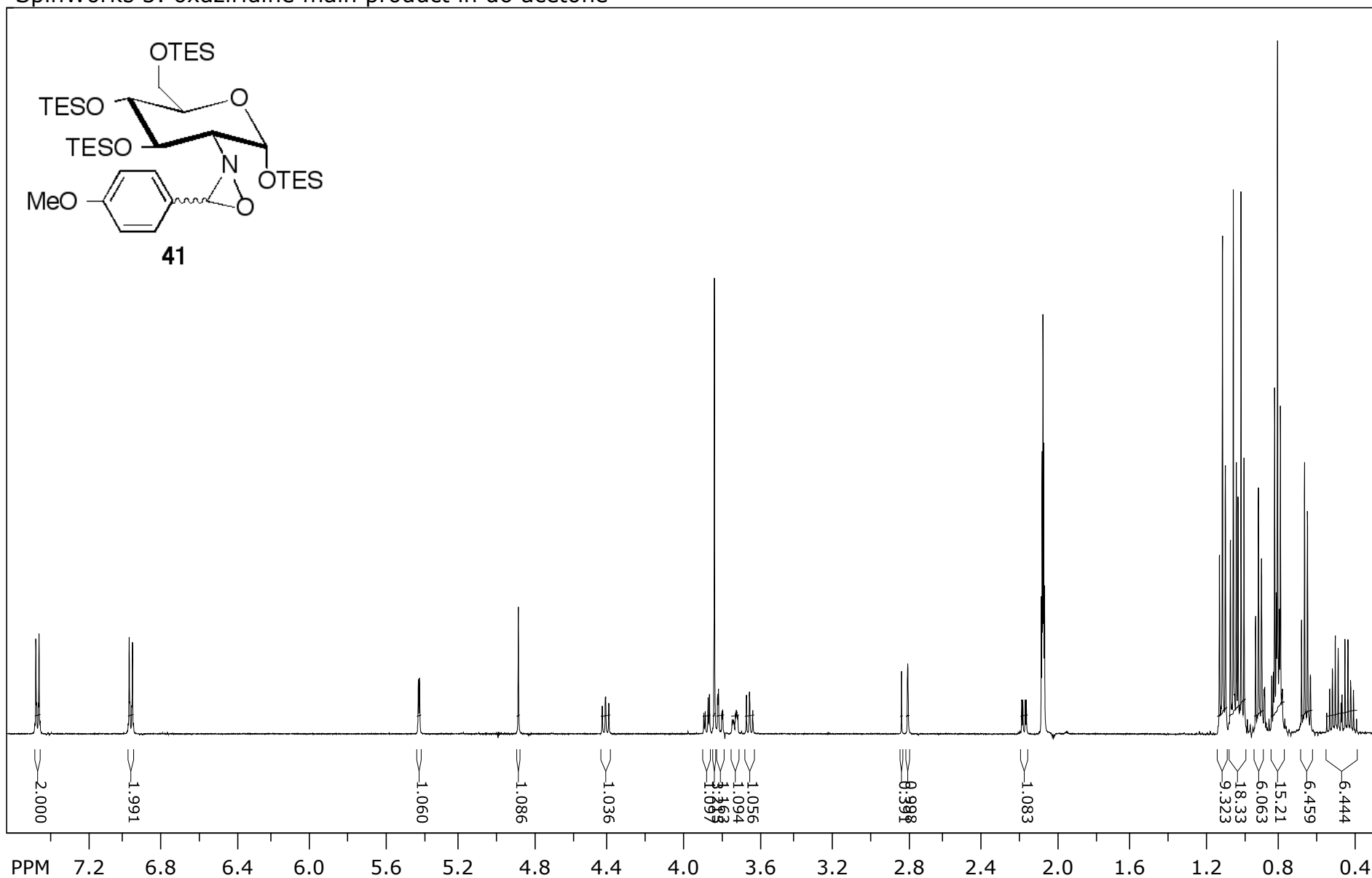


file: ...\\nrmr\Posakony\nmr\imine_7_09\2\fid expt: <zpgg30>
transmitter freq.: 125.749240 MHz
time domain size: 65536 points
width: 30030.03 Hz = 238.8088 ppm = 0.458222 Hz/pt
number of scans: 2700

freq. of 0 ppm: 125.736558 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 5.541 ppm/cm: 0.04406

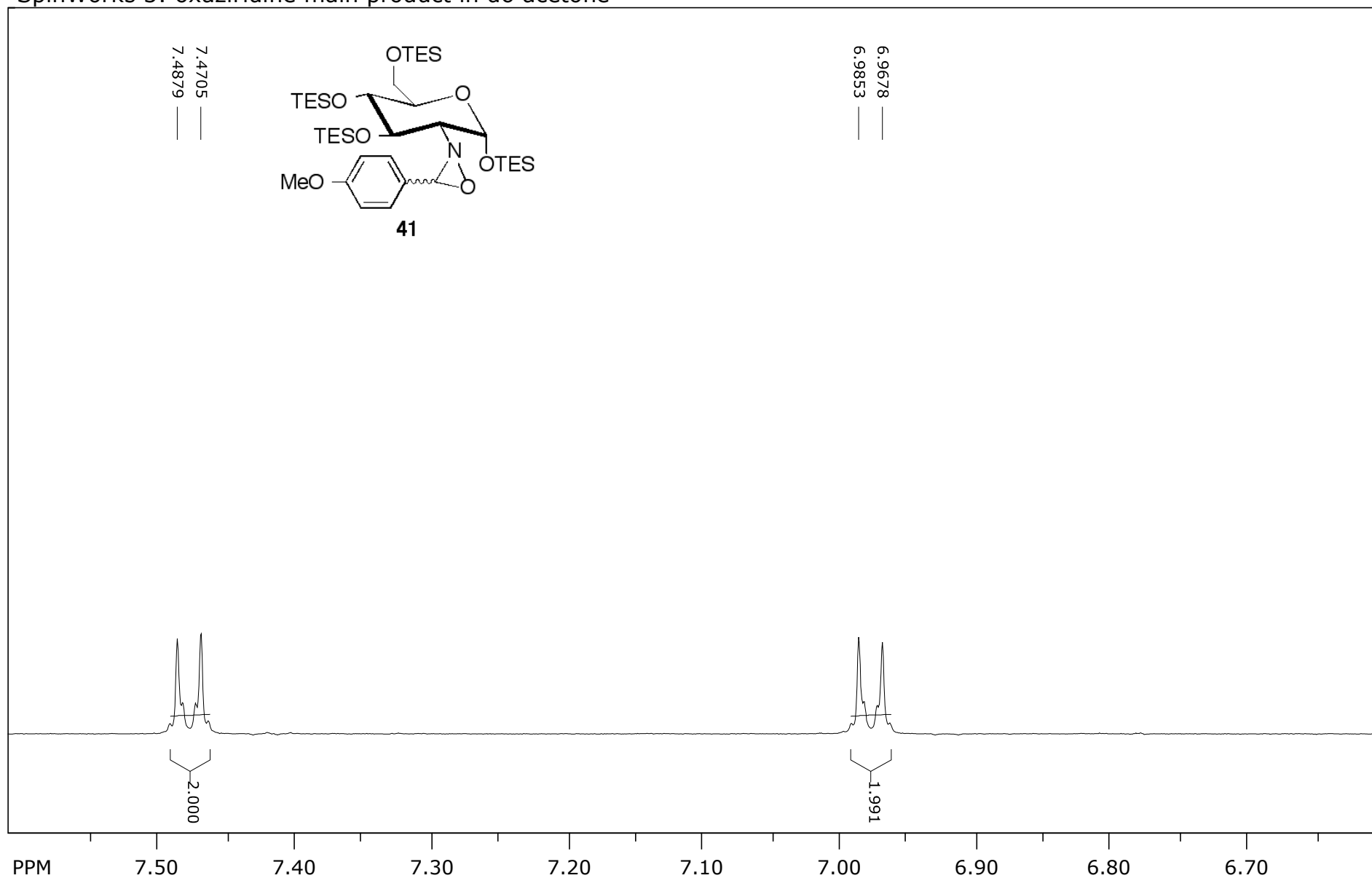
Sample Name	Jeff 44	Position	Vial 44	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 44_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 2:01:09 PM





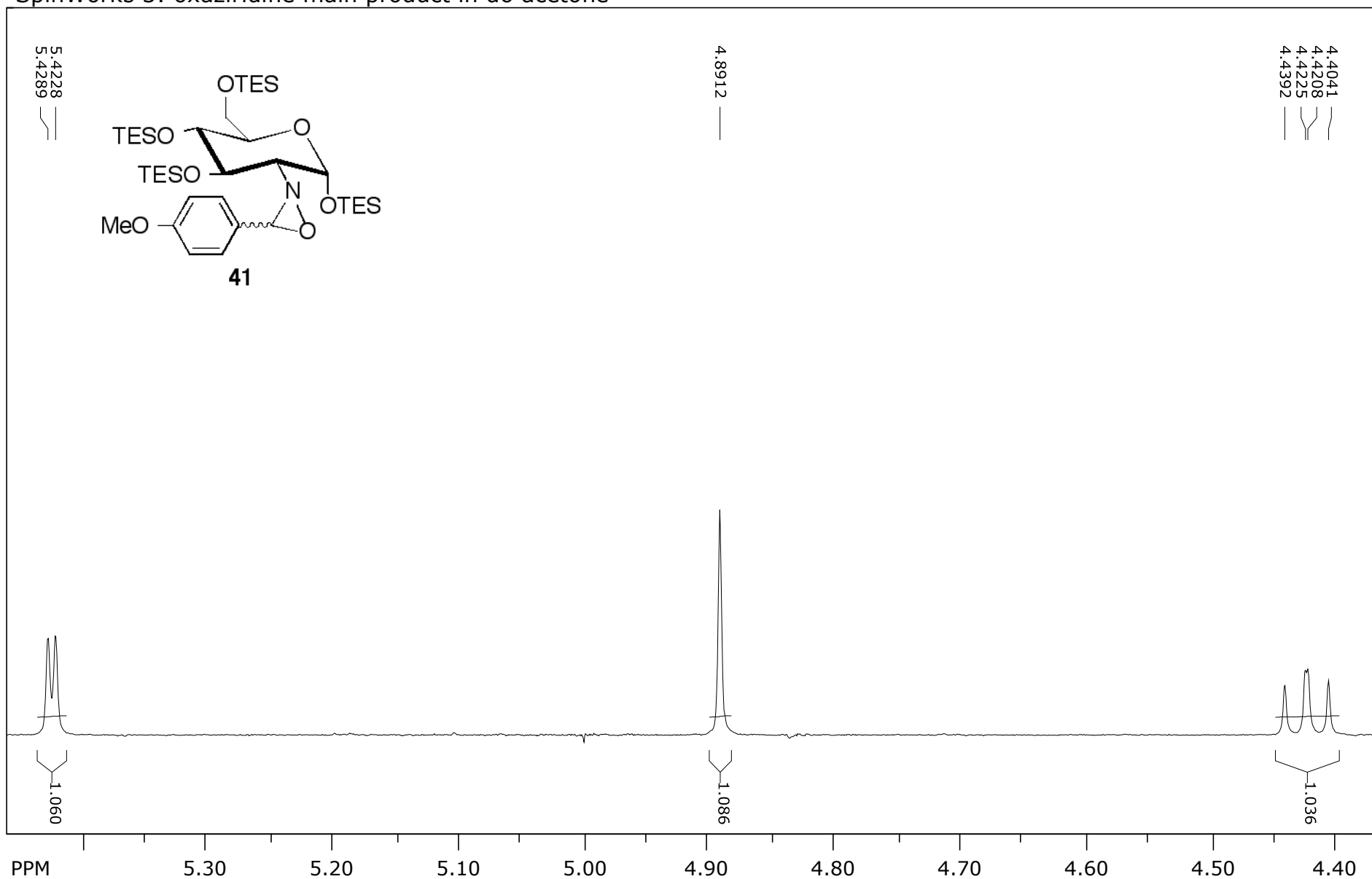
file: ...ir main in acetone-d6 dilute\1\fid expt: <zg>
transmitter freq.: 499.852499 MHz
time domain size: 32768 points
width: 5000.00 Hz = 10.0030 ppm = 0.152588 Hz/pt
number of scans: 128

freq. of 0 ppm: 499.850000 MHz
processed size: 16384 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 147.496 ppm/cm: 0.29508



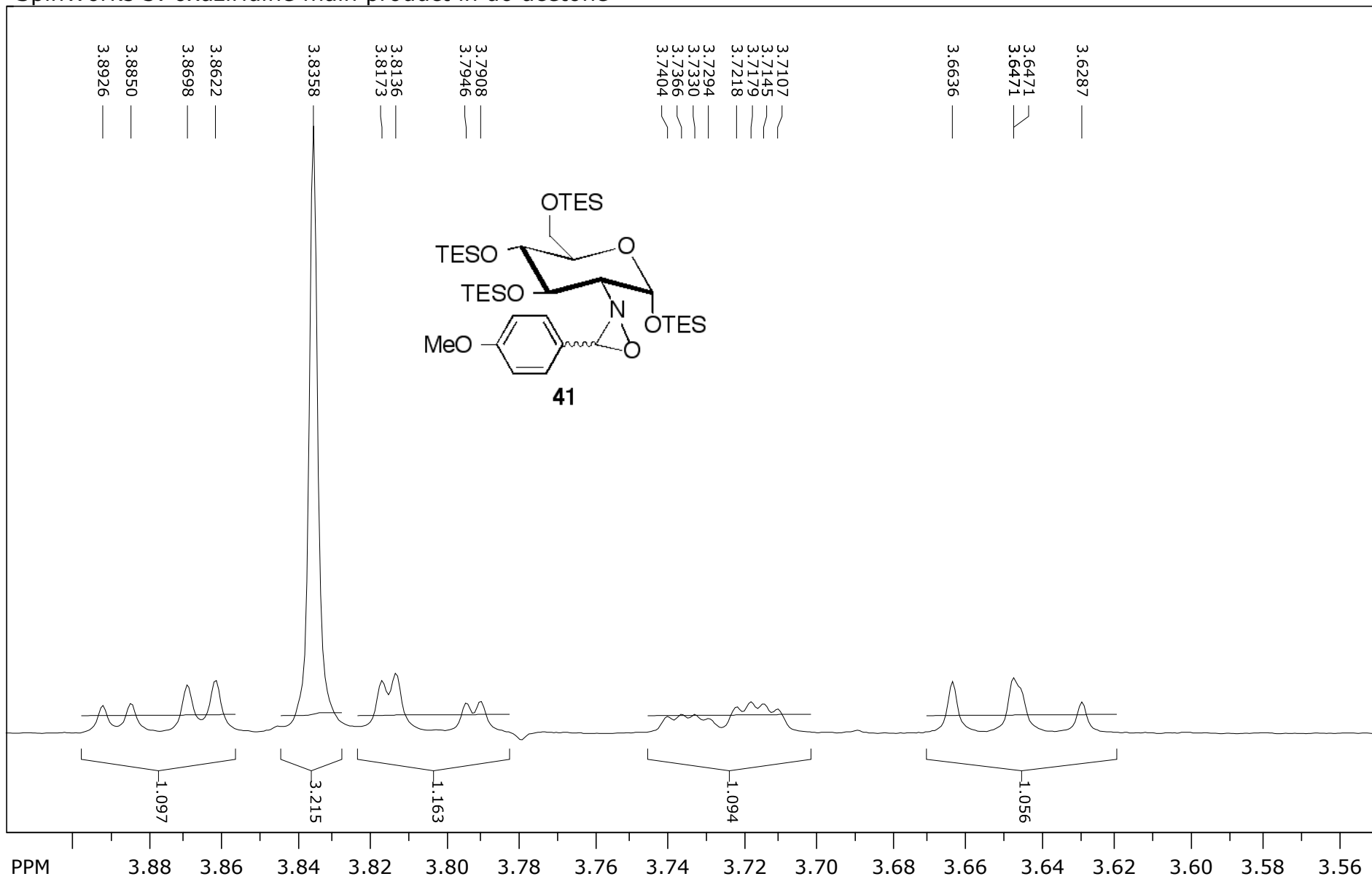
file: ...ir main in acetone-d6 dilute\1\fid expt: <zg>
transmitter freq.: 499.852499 MHz
time domain size: 32768 points
width: 5000.00 Hz = 10.0030 ppm = 0.152588 Hz/pt
number of scans: 128

freq. of 0 ppm: 499.850000 MHz
processed size: 16384 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 20.213 ppm/cm: 0.04044



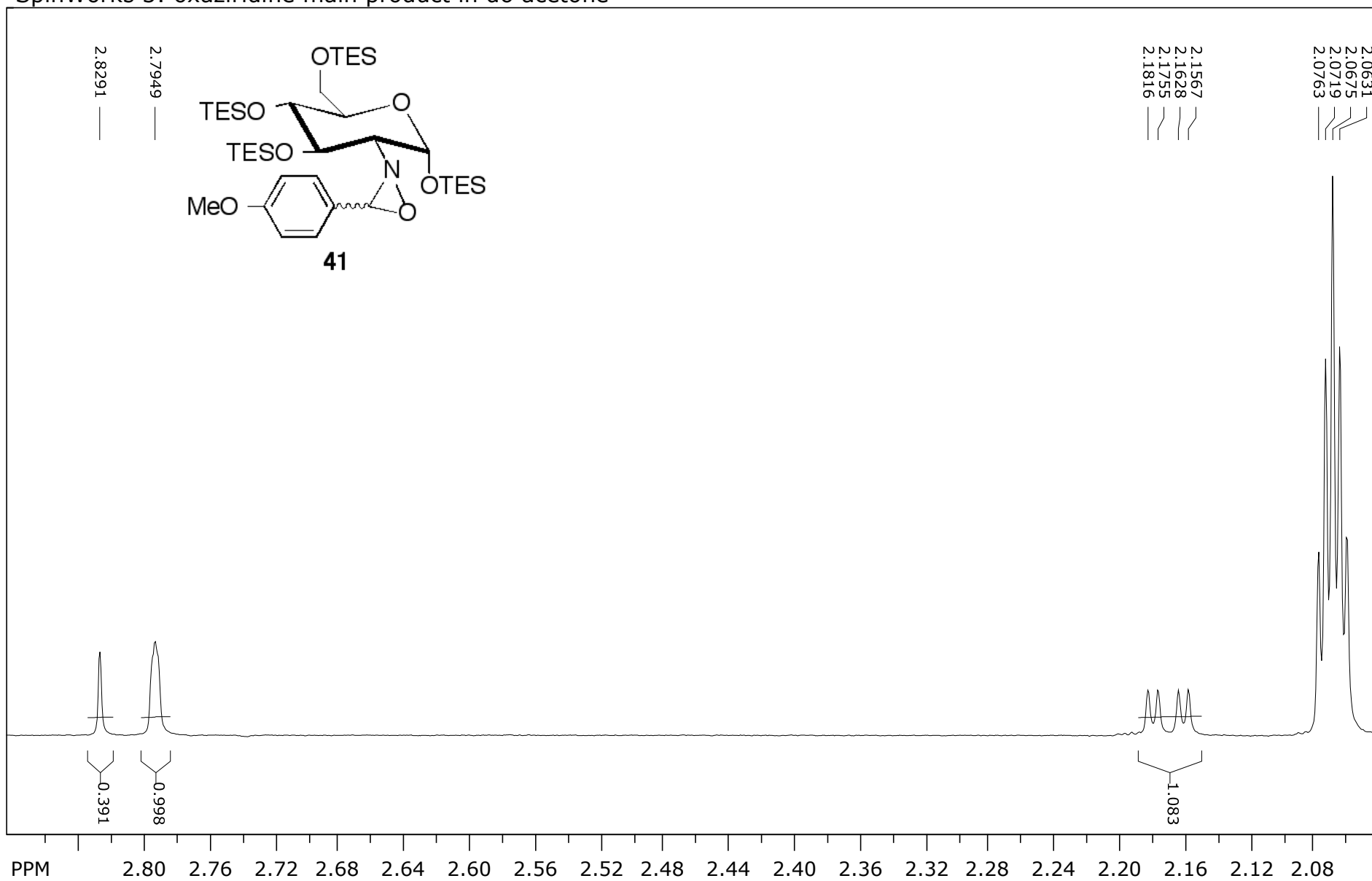
file: ...ir main in acetone-d6 dilute\1\fid expt: <zg>
transmitter freq.: 499.852499 MHz
time domain size: 32768 points
width: 5000.00 Hz = 10.0030 ppm = 0.152588 Hz/pt
number of scans: 128

freq. of 0 ppm: 499.850000 MHz
processed size: 16384 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 21.954 ppm/cm: 0.04392



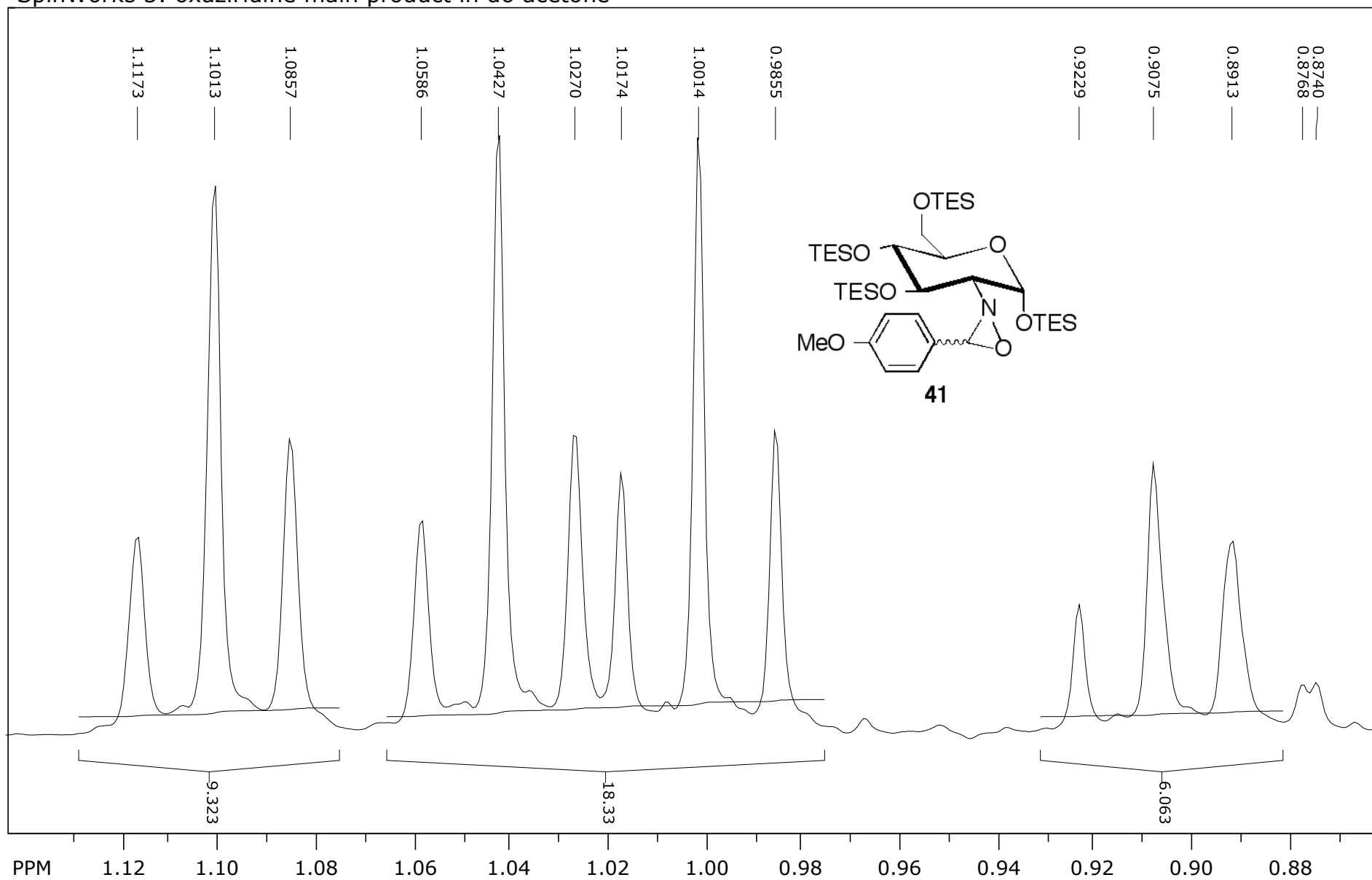
file: ...ir main in acetone-d6 dilute\1\fid expt: <zg>
transmitter freq.: 499.852499 MHz
time domain size: 32768 points
width: 5000.00 Hz = 10.0030 ppm = 0.152588 Hz/pt
number of scans: 128

freq. of 0 ppm: 499.850000 MHz
processed size: 16384 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 7.393 ppm/cm: 0.01479



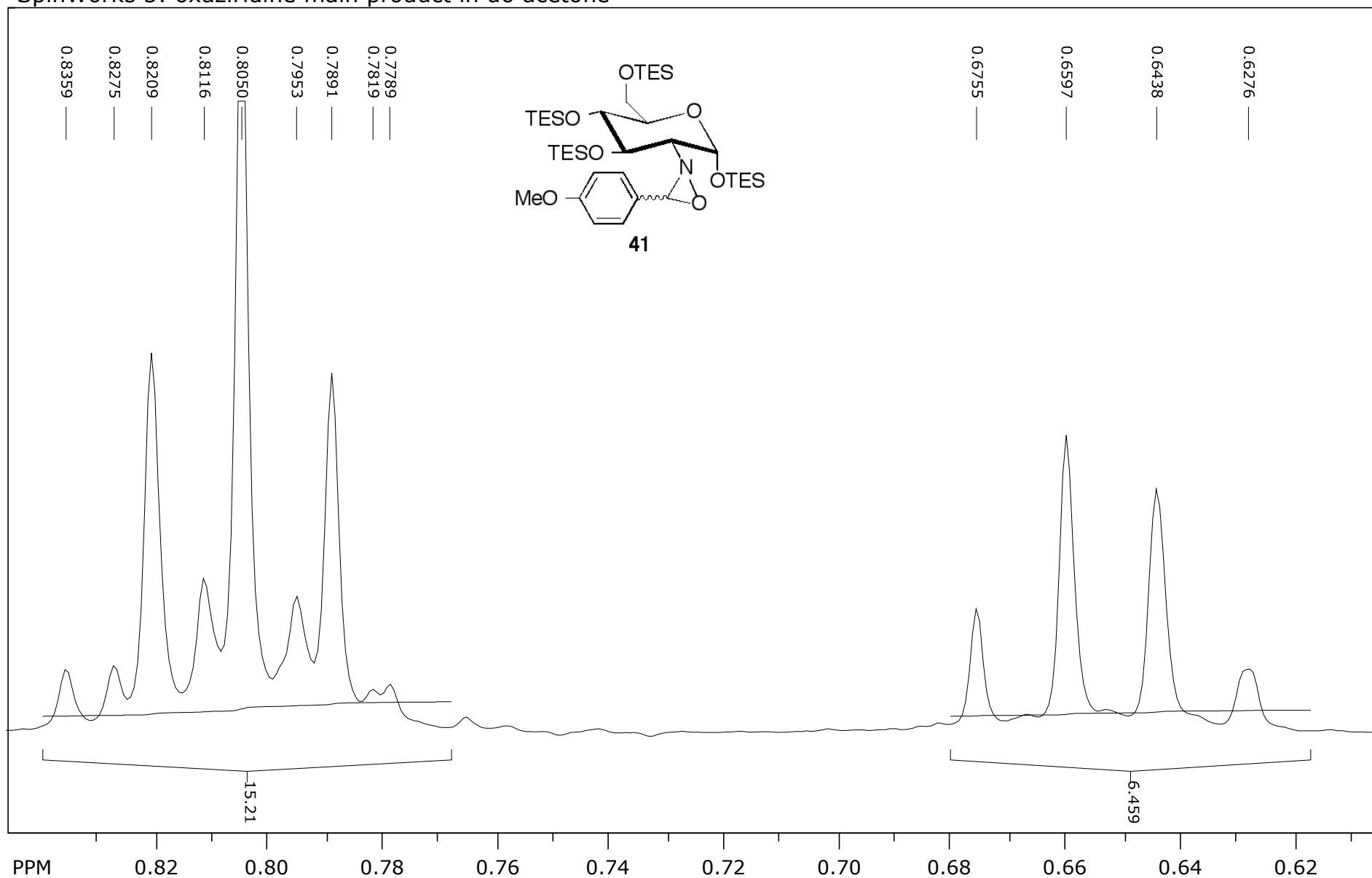
file: ...ir main in acetone-d6 dilute\1\fid expt: <zg>
transmitter freq.: 499.852499 MHz
time domain size: 32768 points
width: 5000.00 Hz = 10.0030 ppm = 0.152588 Hz/pt
number of scans: 128

freq. of 0 ppm: 499.850000 MHz
processed size: 16384 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 16.945 ppm/cm: 0.03390



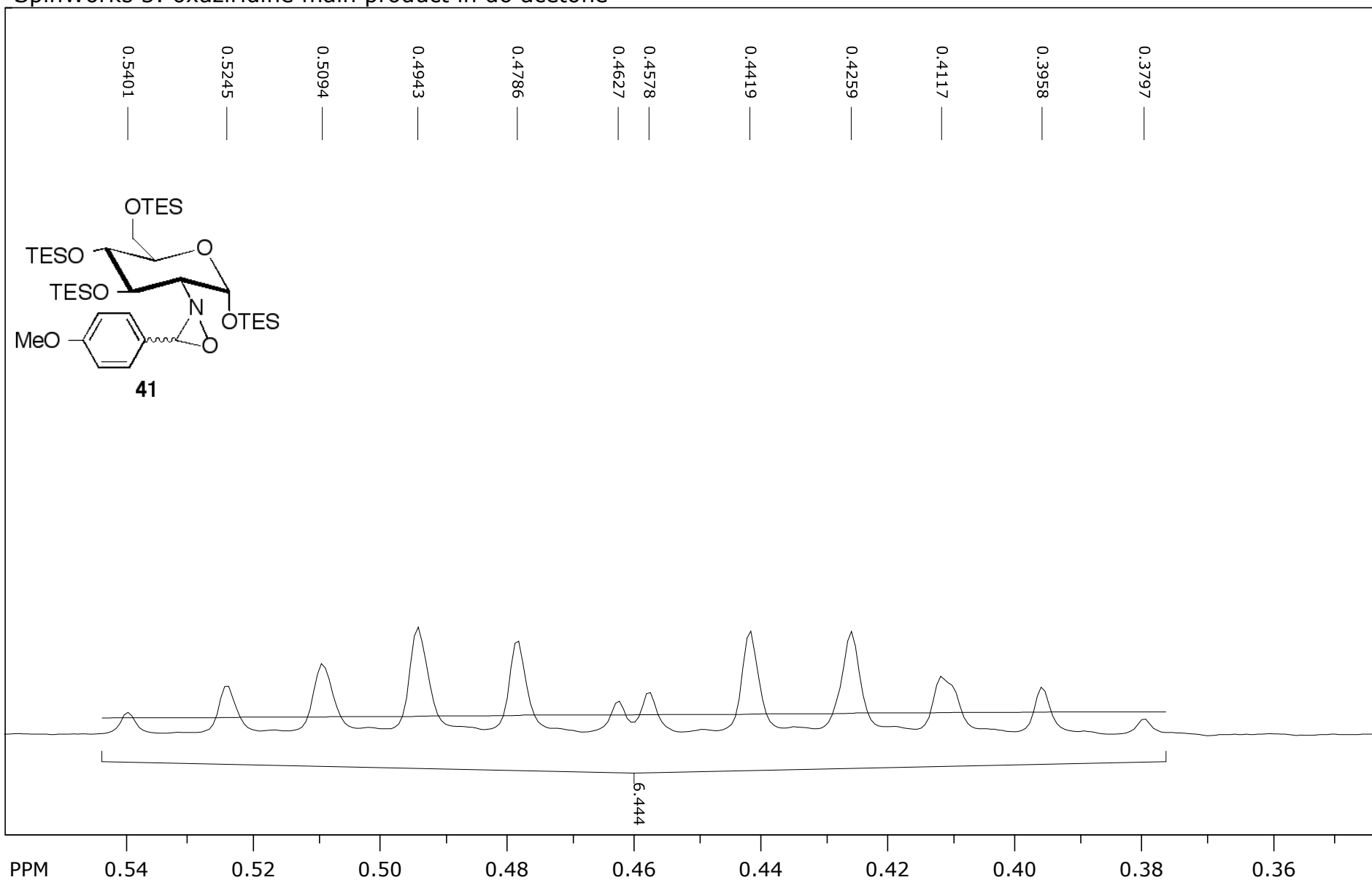
file: ...ir main in acetone-d6 dilute\1\fid expt: <zg>
transmitter freq.: 499.852499 MHz
time domain size: 32768 points
width: 5000.00 Hz = 10.0030 ppm = 0.152588 Hz/pt
number of scans: 128

freq. of 0 ppm: 499.850000 MHz
processed size: 16384 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 5.656 ppm/cm: 0.01132



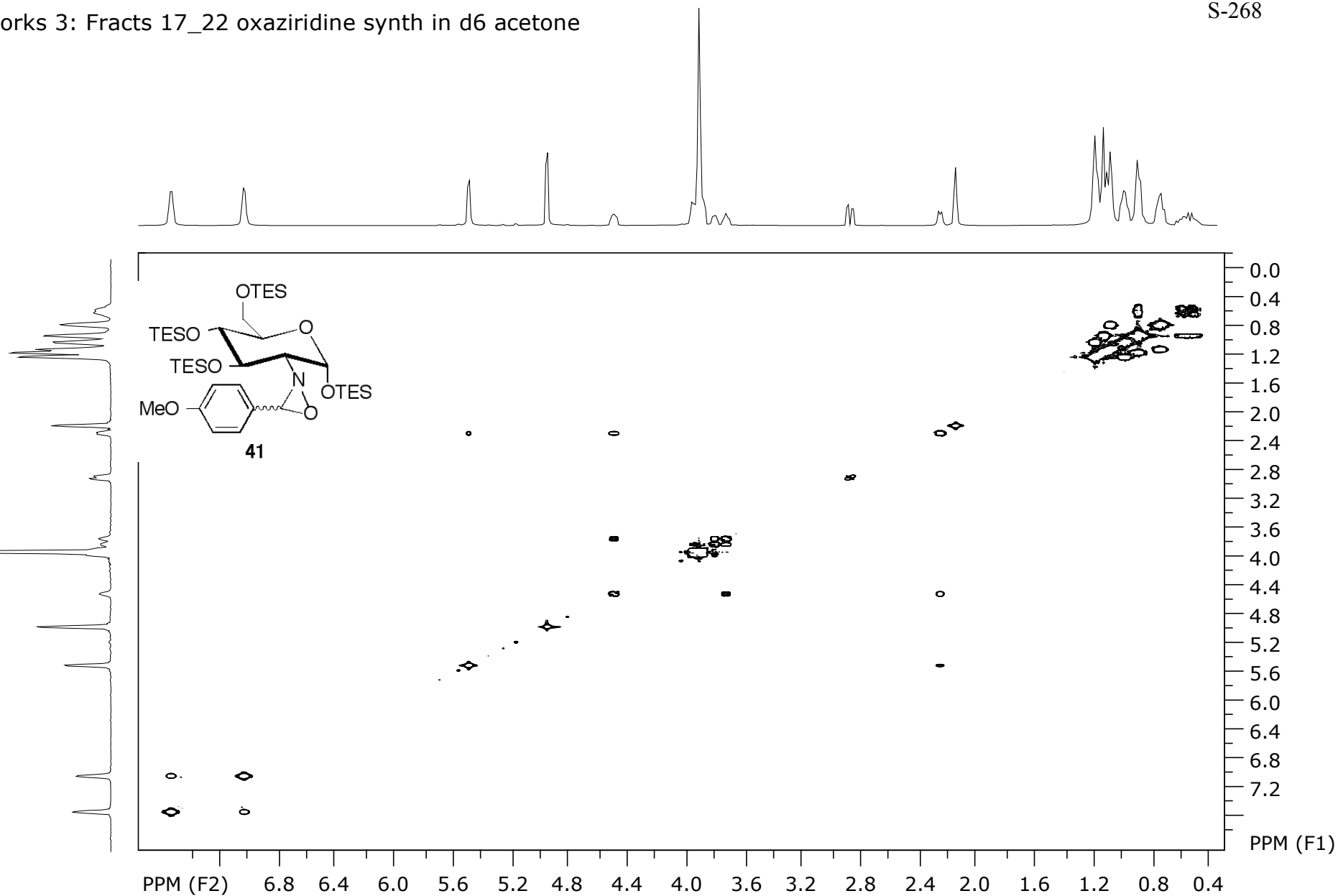
file: ...ir main in acetone-d6 dilute\1\fid expt: <zg>
transmitter freq.: 499.852499 MHz
time domain size: 32768 points
width: 5000.00 Hz = 10.0030 ppm = 0.152588 Hz/pt
number of scans: 128

freq. of 0 ppm: 499.850000 MHz
processed size: 16384 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 4.829 ppm/cm: 0.00966



file: ...ir main in acetone-d6 dilute\1\fid expt: <zg>
transmitter freq.: 499.852499 MHz
time domain size: 32768 points
width: 5000.00 Hz = 10.0030 ppm = 0.152588 Hz/pt
number of scans: 128

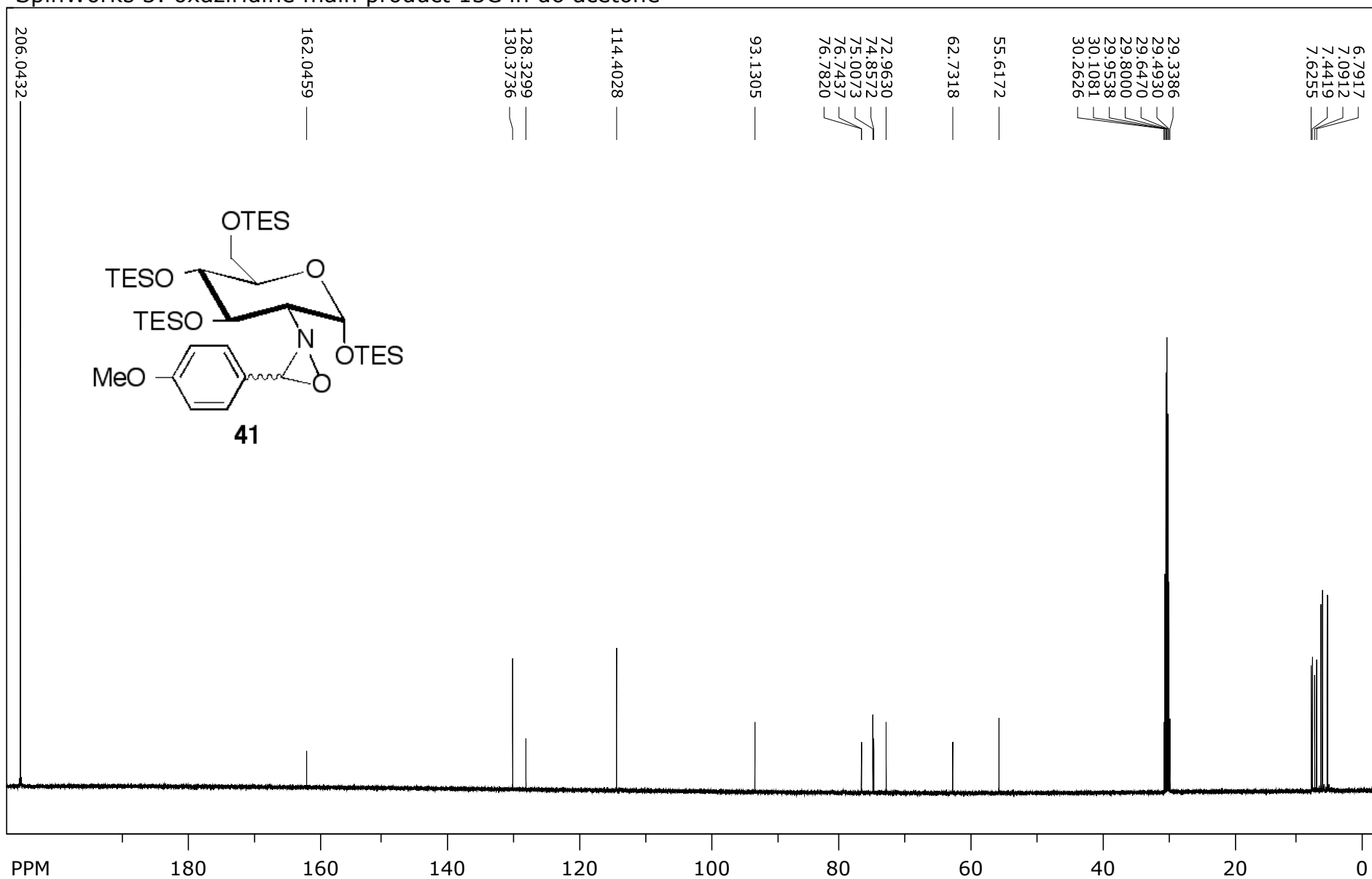
freq. of 0 ppm: 499.850000 MHz
processed size: 16384 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 4.333 ppm/cm: 0.00867



file: ...r\NMR Data\nmr6_10\cosy17_22\1\ser
expt: <cosygpqf>
transmitter freq: 600.552832 MHz
time domain size: 2048 by 512 points
width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
number of scans: 1

F2: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 223.955 ppm/cm: 0.37291

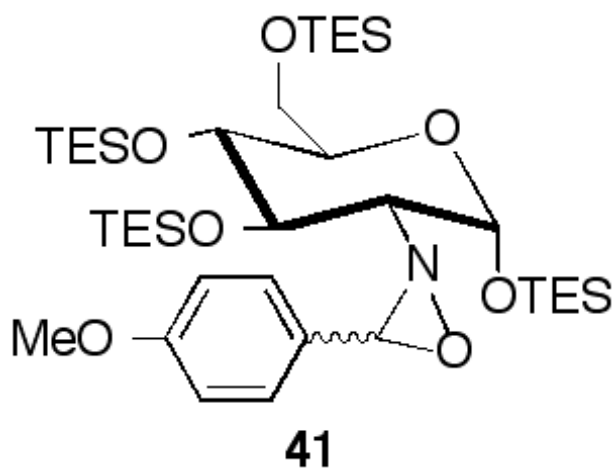
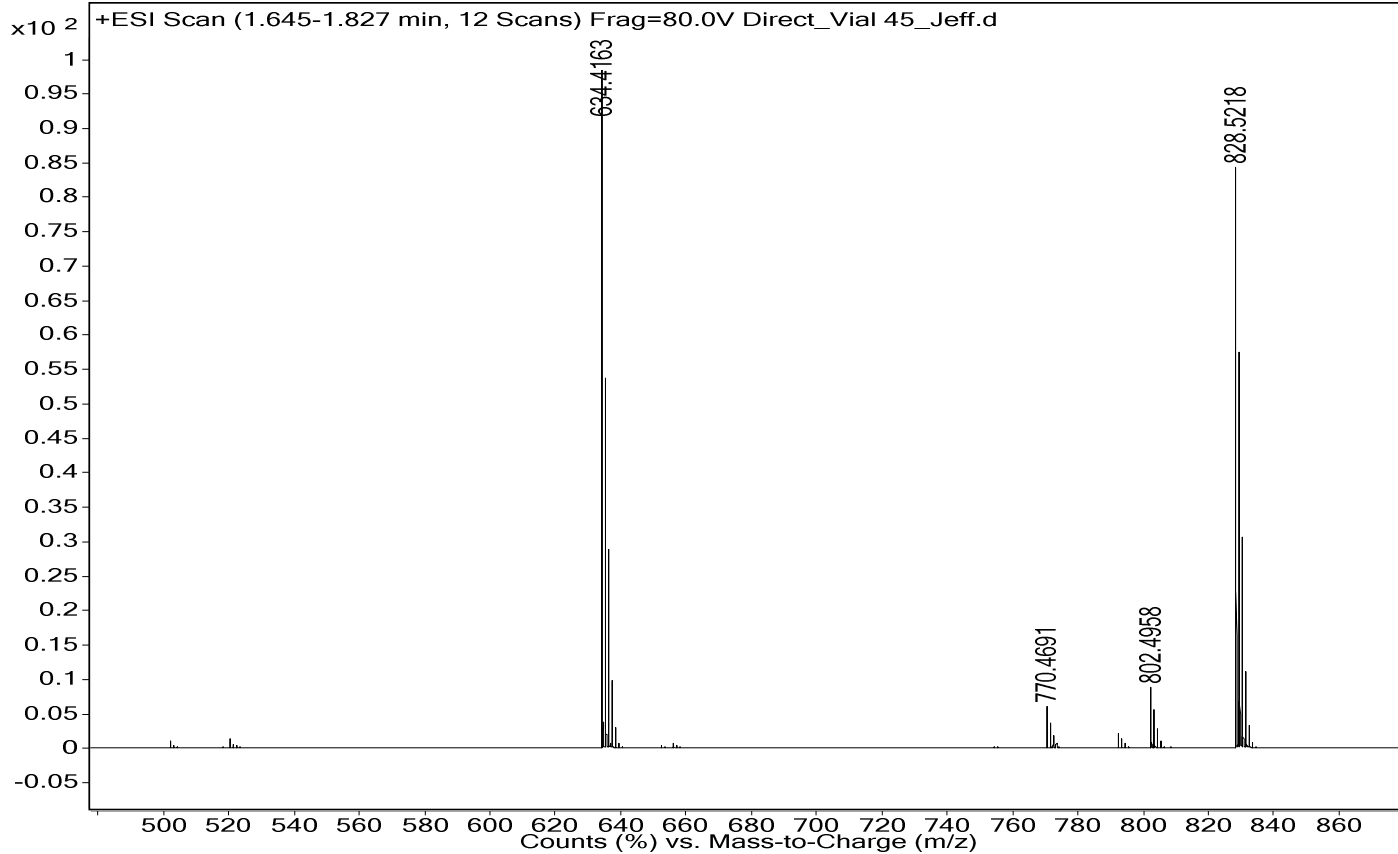
F1: freq. of 0 ppm: 600.5499623 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 452.666 ppm/cm: 0.75375

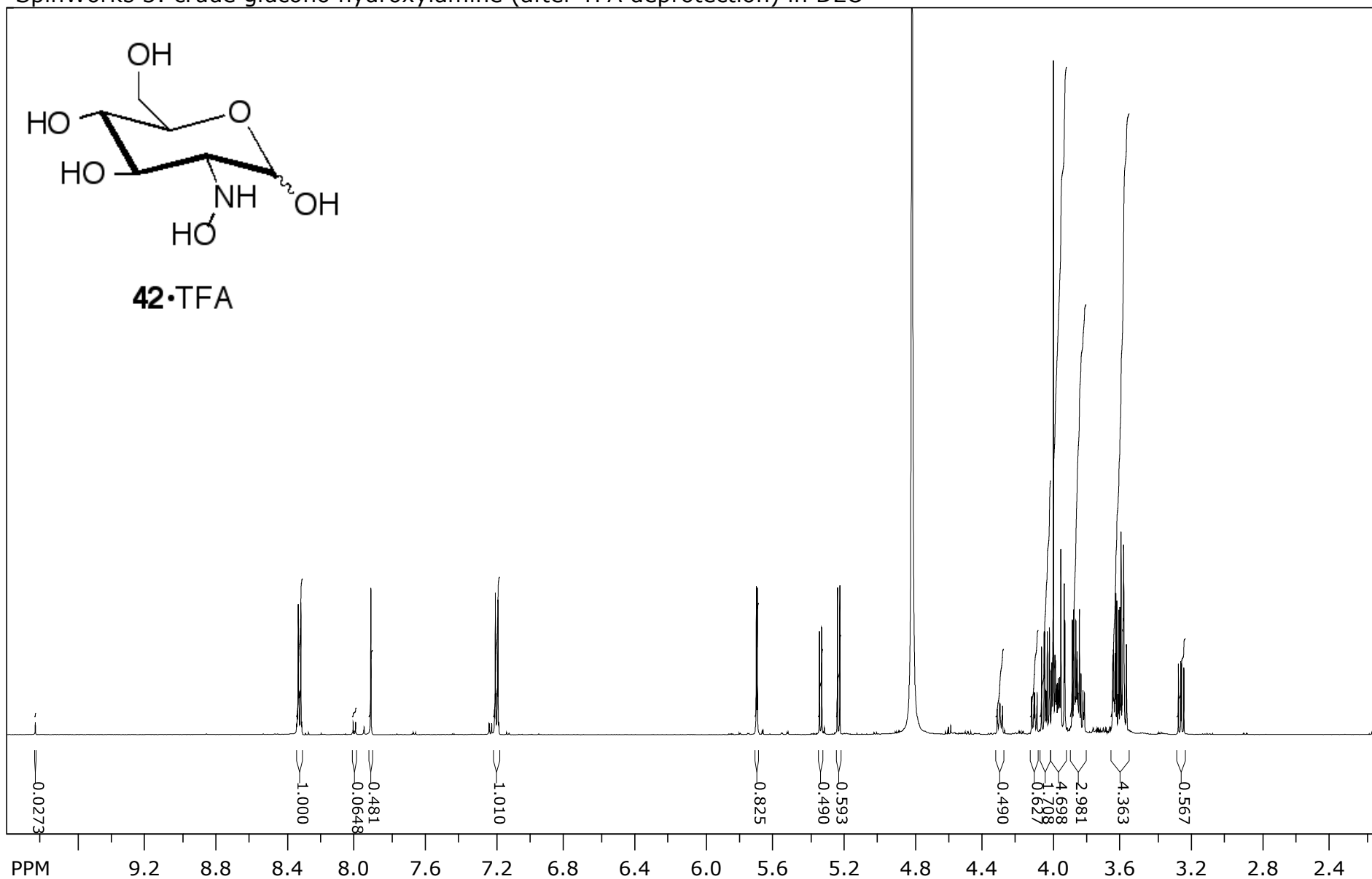


file: ..._4\oxazir main in acetone-d6\2\fid expt: <zgpg>
transmitter freq.: 125.699901 MHz
time domain size: 65536 points
width: 27777.78 Hz = 220.9849 ppm = 0.423855 Hz/pt
number of scans: 4096

freq. of 0 ppm: 125.687273 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 1060.356 ppm/cm: 8.43561

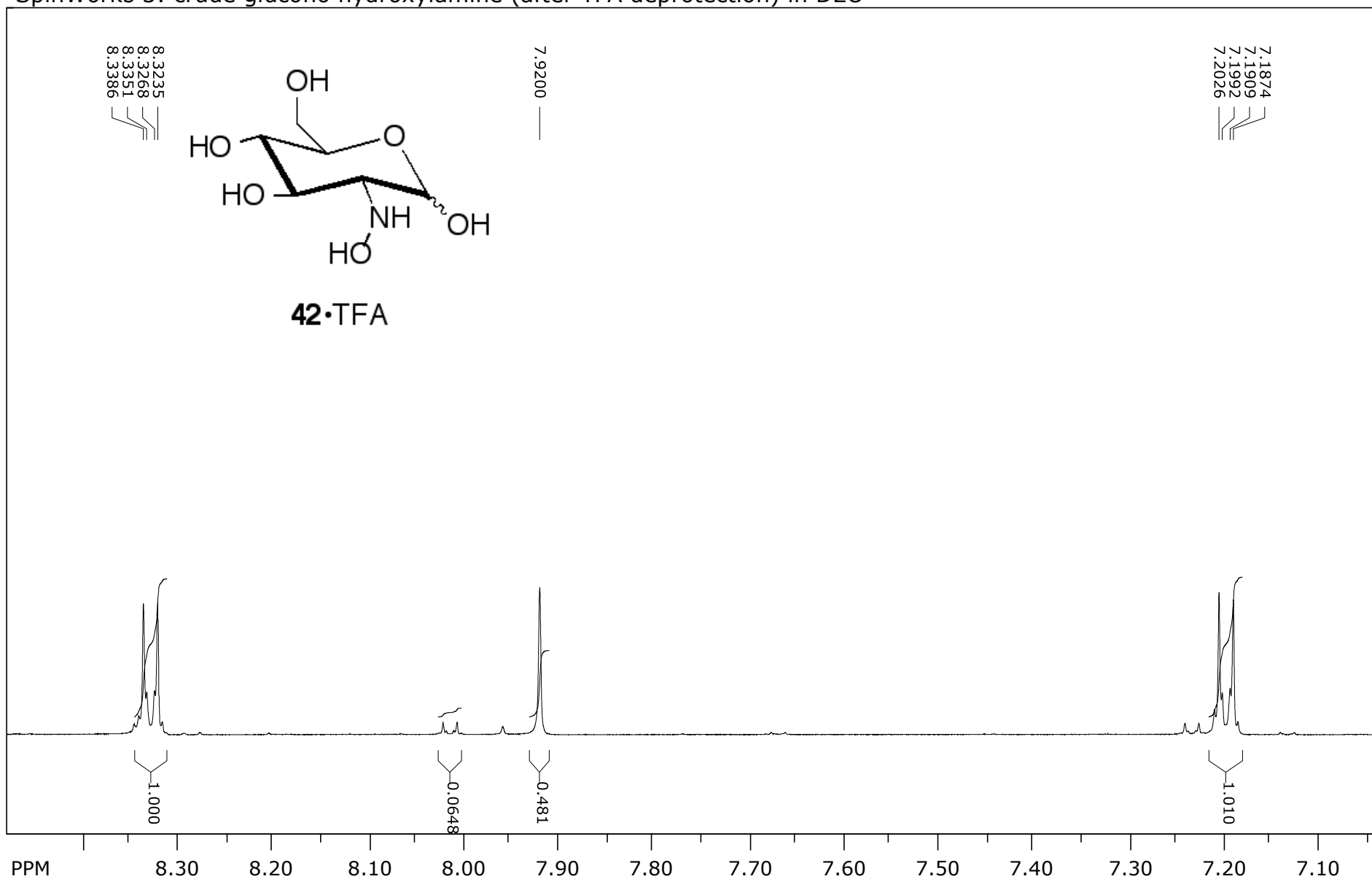
Sample Name	Jeff 45	Position	Vial 45	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 45_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 2:05:52 PM





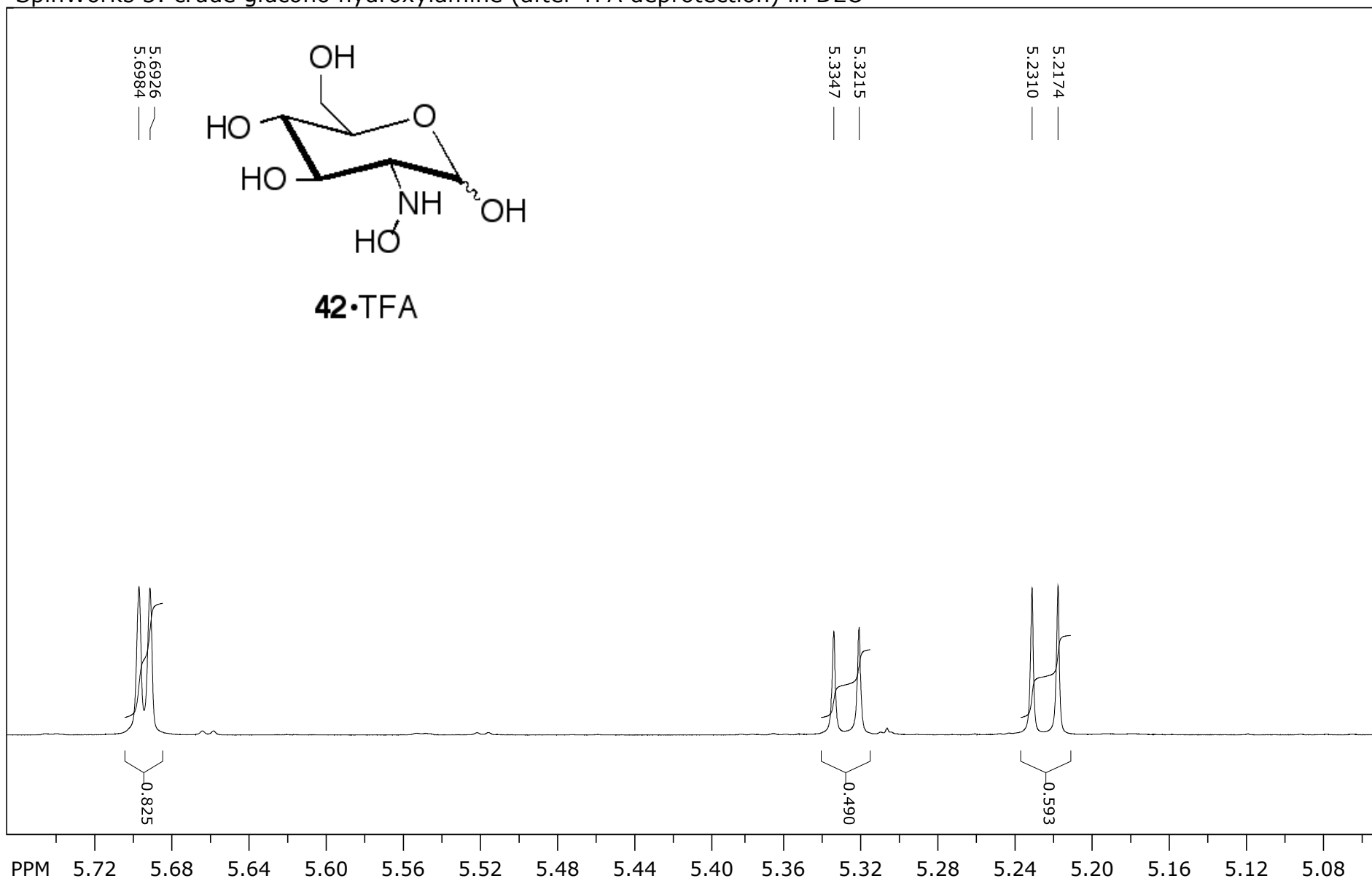
file: ...and 6P\GlcNOHpostTFADpro_D2O\1\fid expt: <zgr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 16

freq. of 0 ppm: 600.549946 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 189.938 ppm/cm: 0.31627



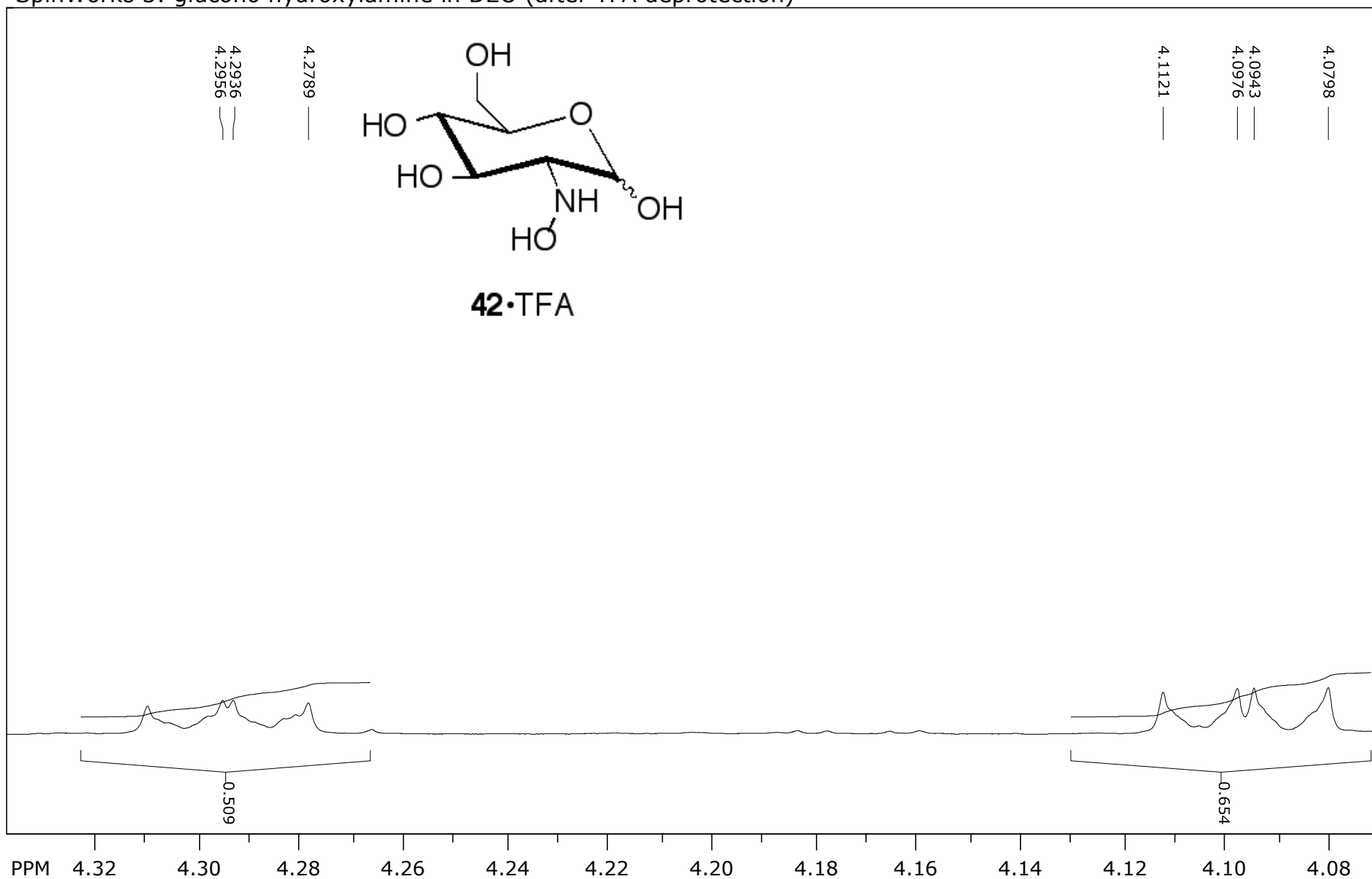
file: ...and 6P\GlcNOHpostTFADpro_D2O\1\fid expt: <zgr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 16

freq. of 0 ppm: 600.549946 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 34.810 ppm/cm: 0.05796



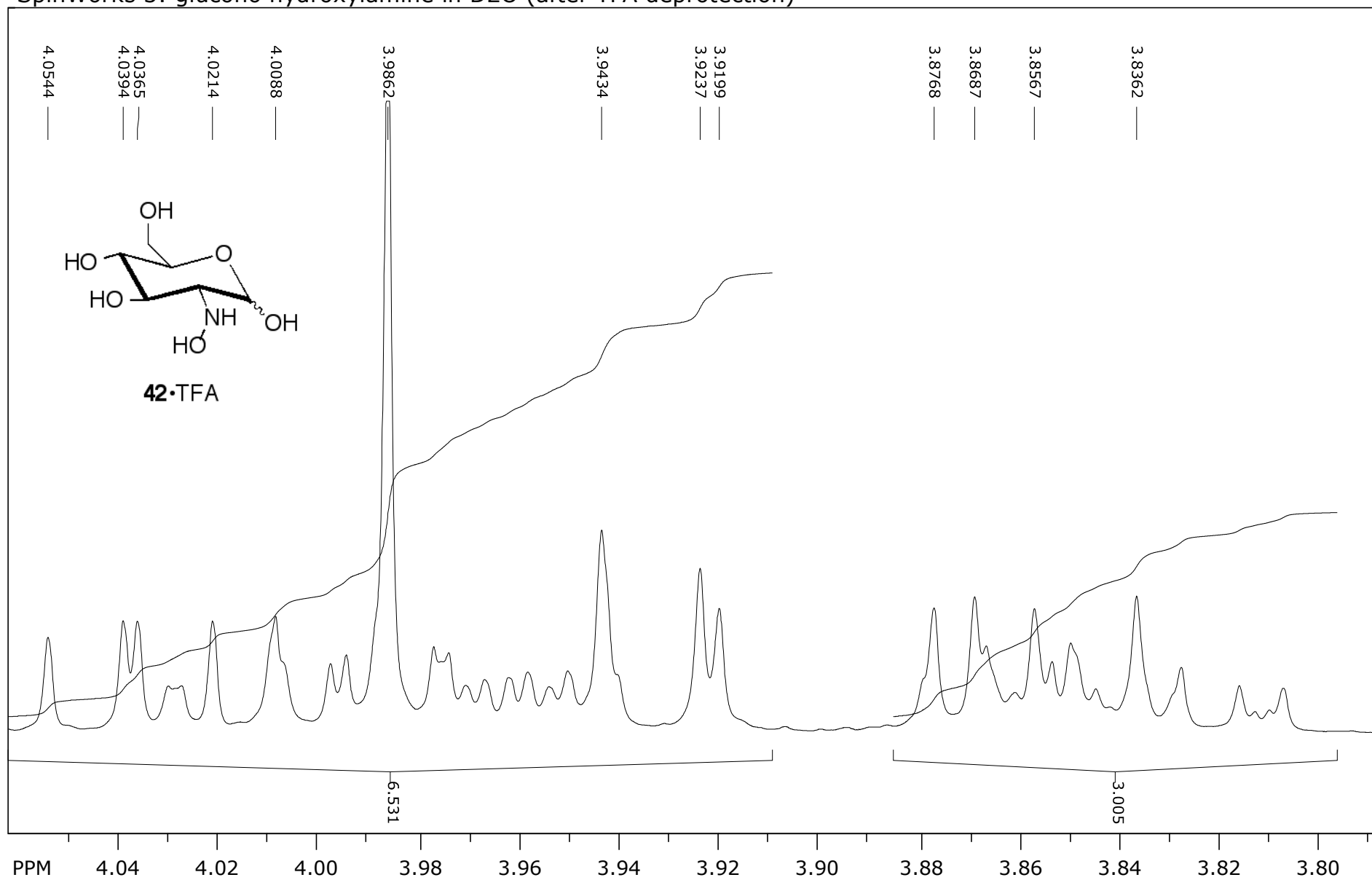
file: ...and 6P\GlcNOHpostTFADpro_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 16

freq. of 0 ppm: 600.549946 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 17.248 ppm/cm: 0.02872



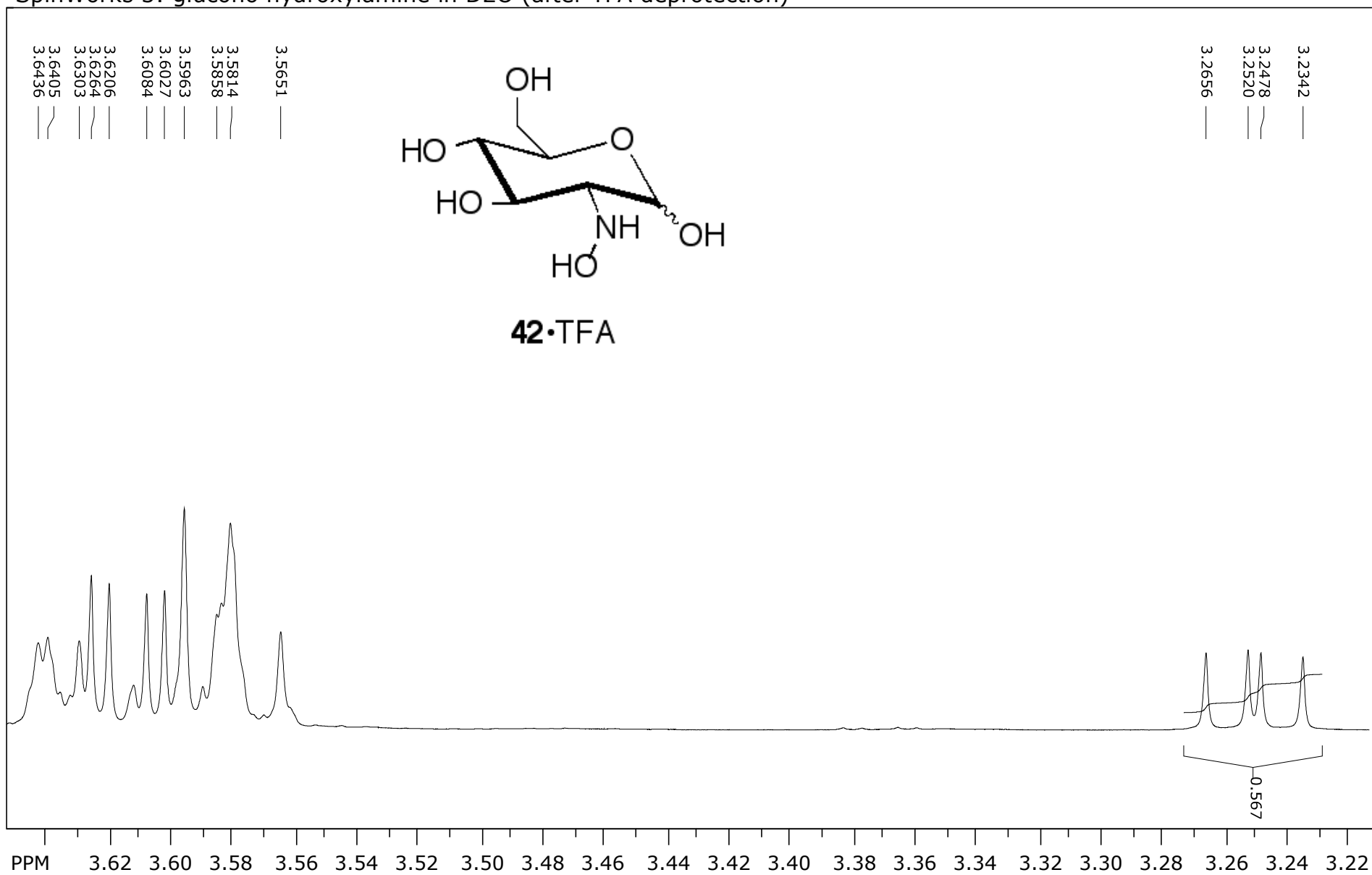
file: ...and 6P\GlcNOHpostTFADpro_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 16

freq. of 0 ppm: 600.549947 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 6.433 ppm/cm: 0.01071



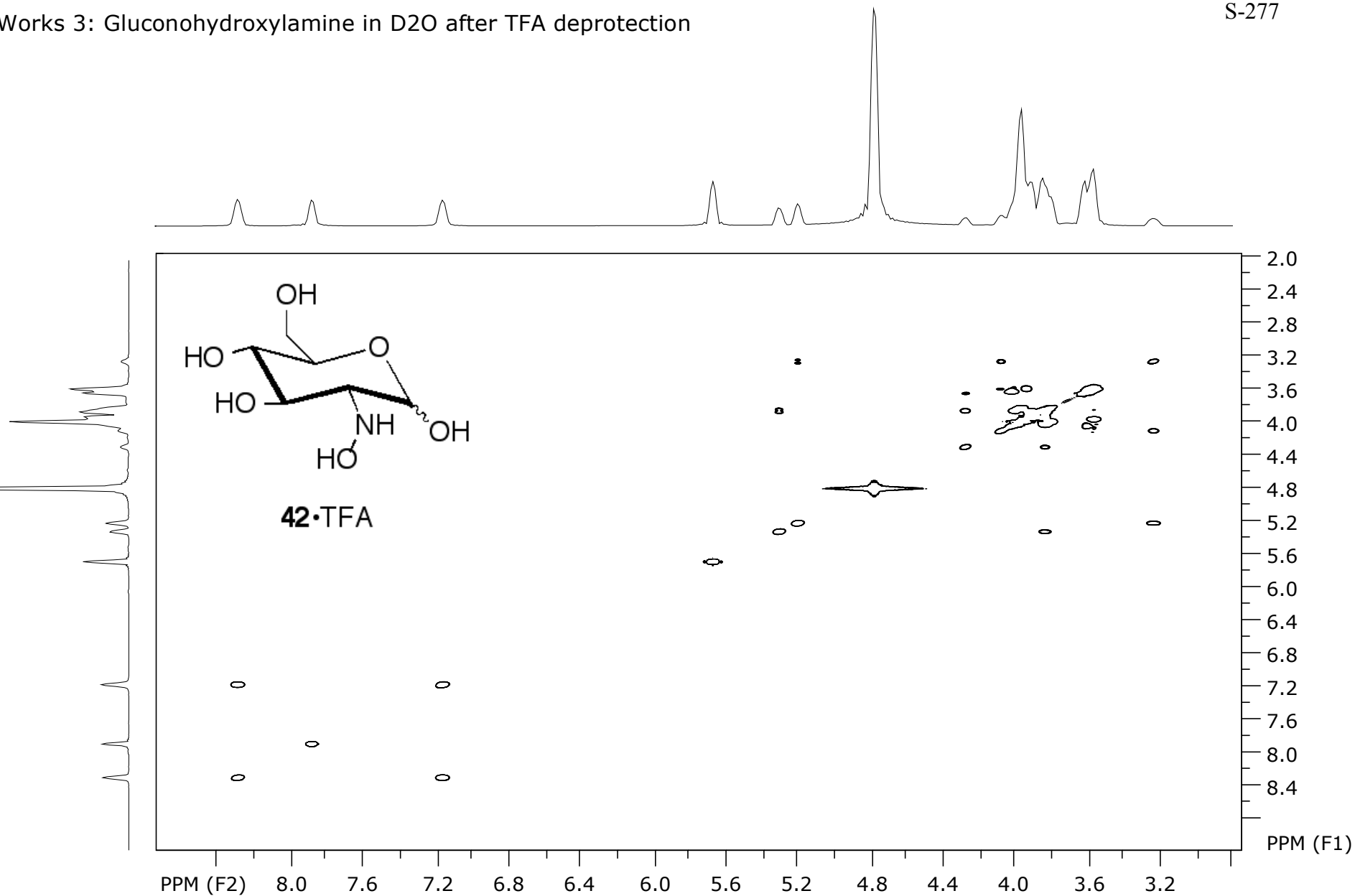
file: ...and 6P\GlcNOHpostTFADpro_D2O\1\fid expt: <zgpr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 16

freq. of 0 ppm: 600.549947 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 6.599 ppm/cm: 0.01099



file: ...and 6P\GlcNOHpostTFADpro_D2O\1\fid expt: <zgr>
transmitter freq.: 600.553538 MHz
time domain size: 65536 points
width: 8417.51 Hz = 14.0162 ppm = 0.128441 Hz/pt
number of scans: 16

freq. of 0 ppm: 600.549947 MHz
processed size: 262144 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 10.594 ppm/cm: 0.01764

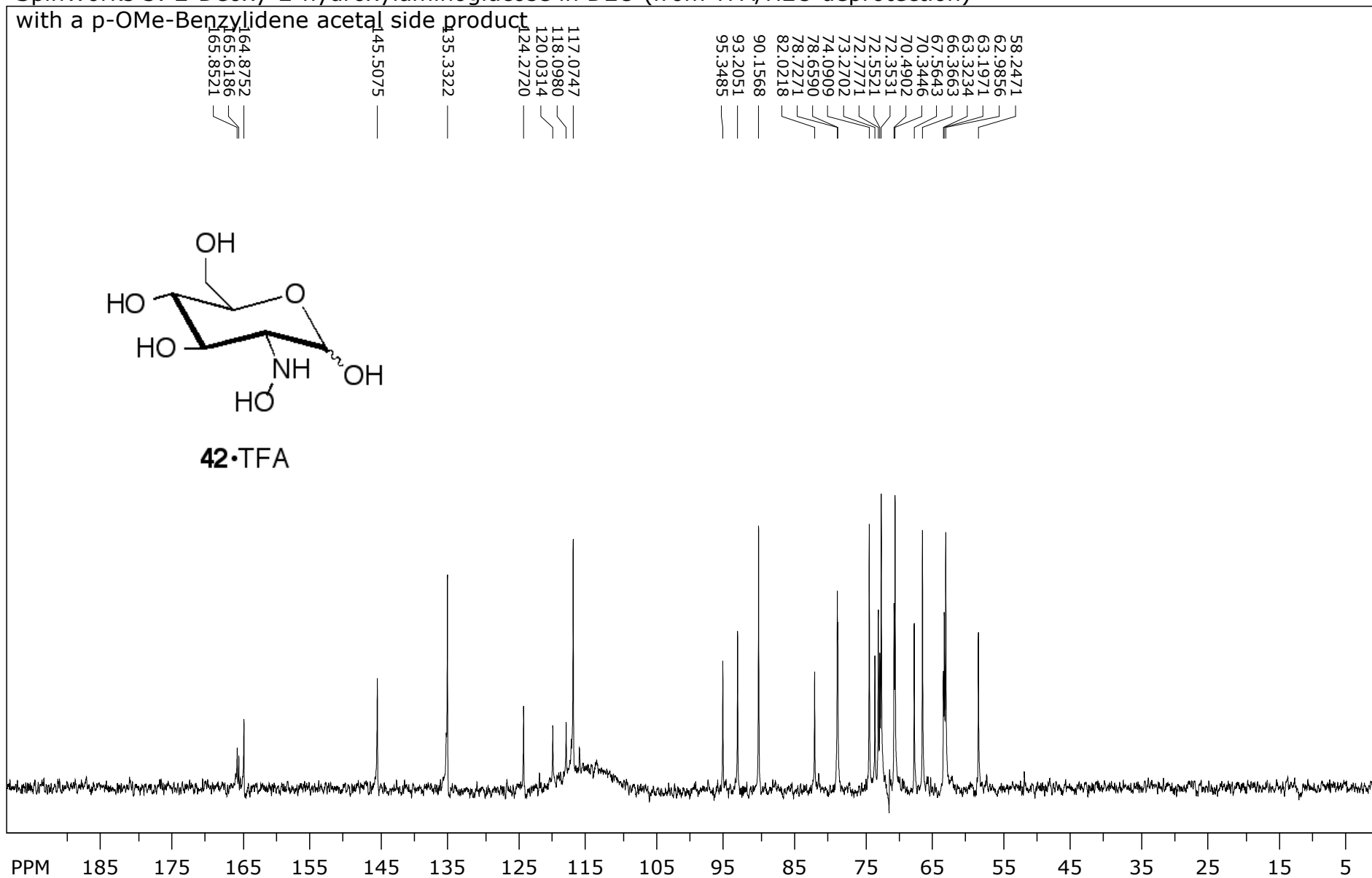


file: ...and 6P\GlcNOH_frTFApro_COSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 1024 by 512 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 7.0425 Hz/pt
 number of scans: 1

F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 179.930 ppm/cm: 0.29961

F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 394.257 ppm/cm: 0.65649

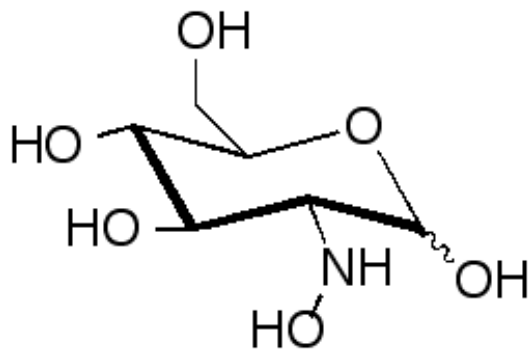
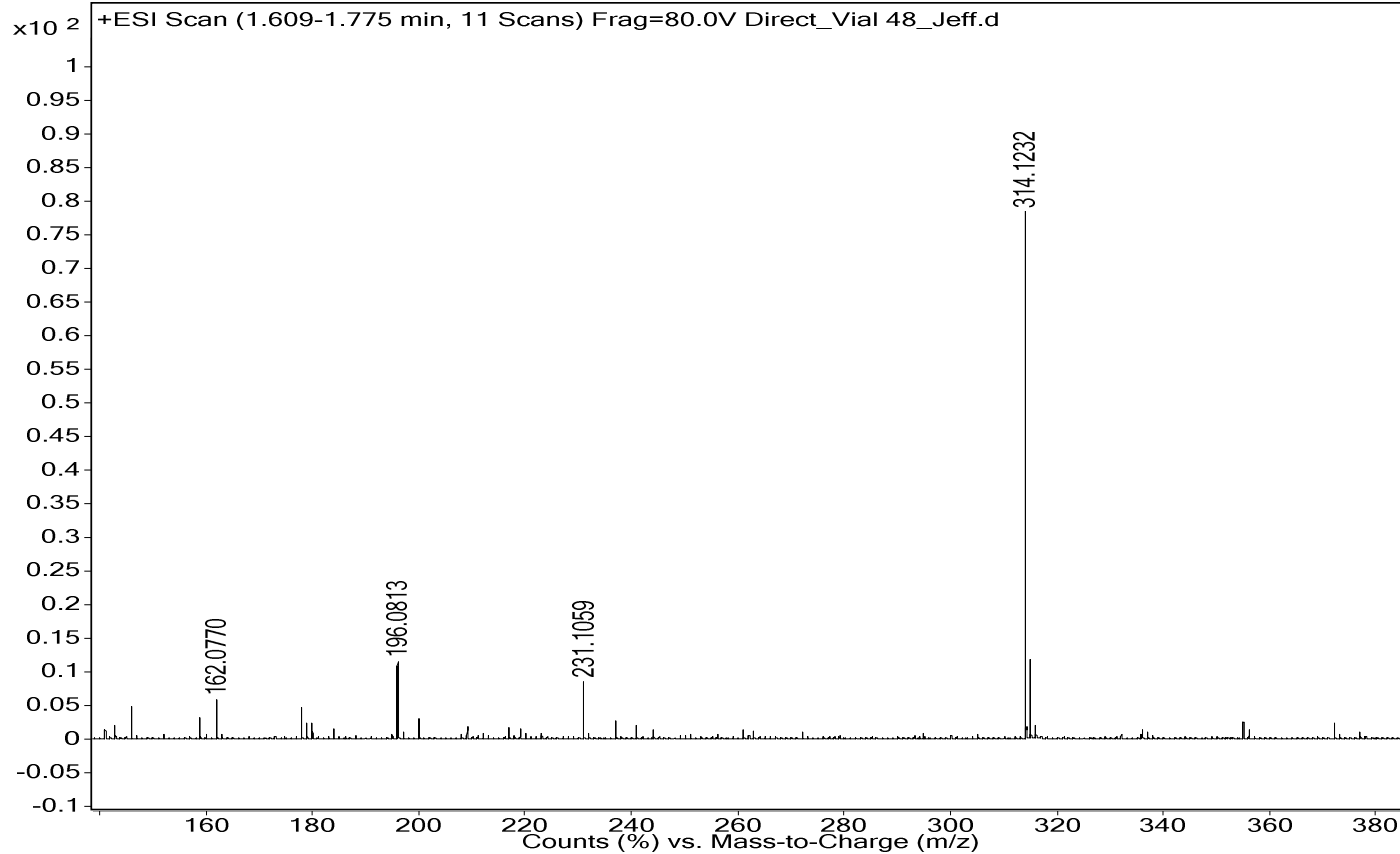
with a p-OMe-Benzylidene acetal side product



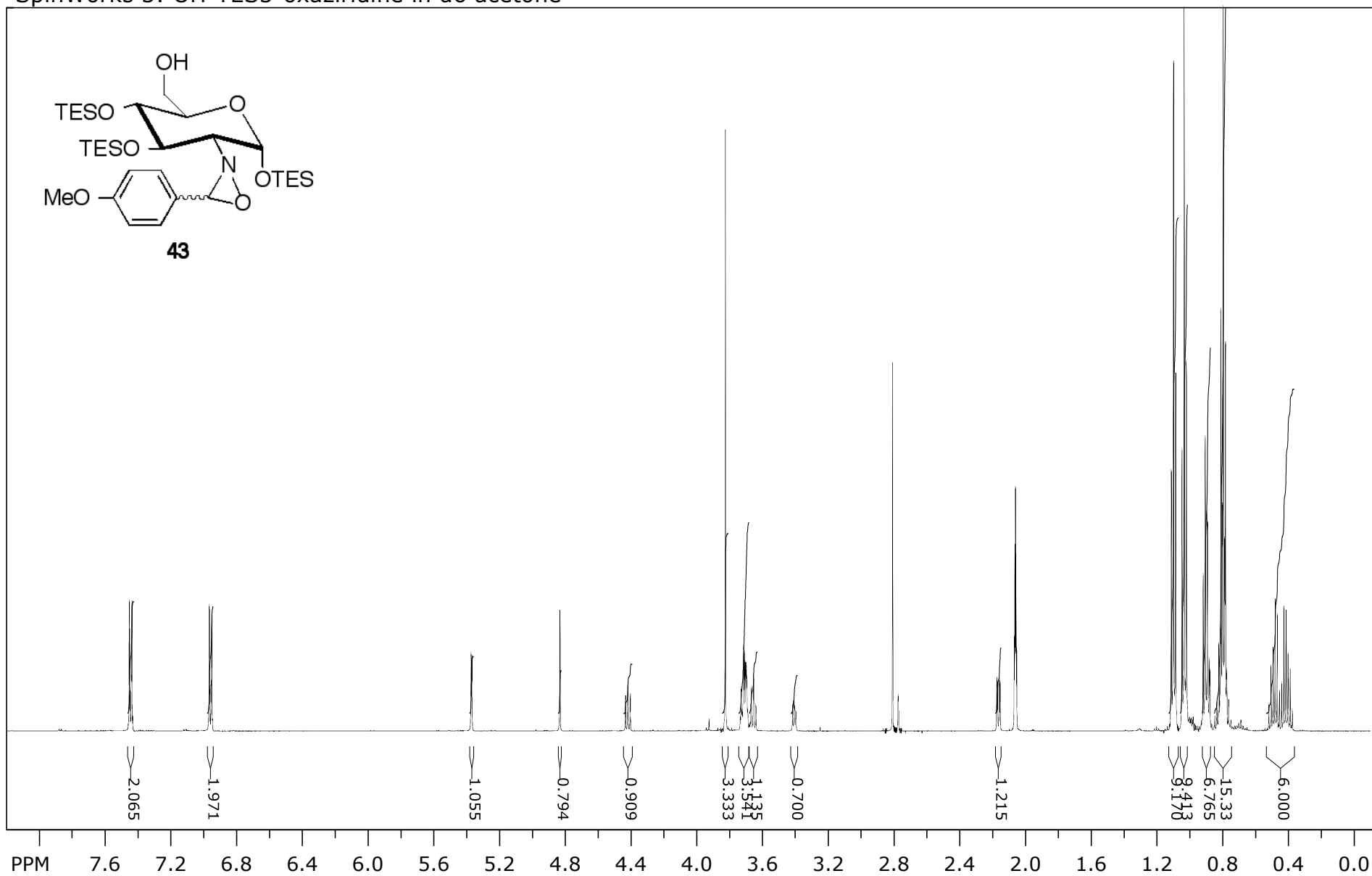
file: ...r\NMR Data\GlcNOHmix_13C_D2O\1\fid expt: <zgpg30>
 transmitter freq.: 151.023519 MHz
 time domain size: 65536 points
 width: 36057.69 Hz = 238.7555 ppm = 0.550197 Hz/pt
 number of scans: 38912

freq. of 0 ppm: 151.008006 MHz
 processed size: 32768 complex points
 LB: 10.000 GF: 0.0000
 Hz/cm: 1203.265 ppm/cm: 7.96740

Sample Name	Jeff 48	Position	Vial 48	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 48_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 2:20:01 PM

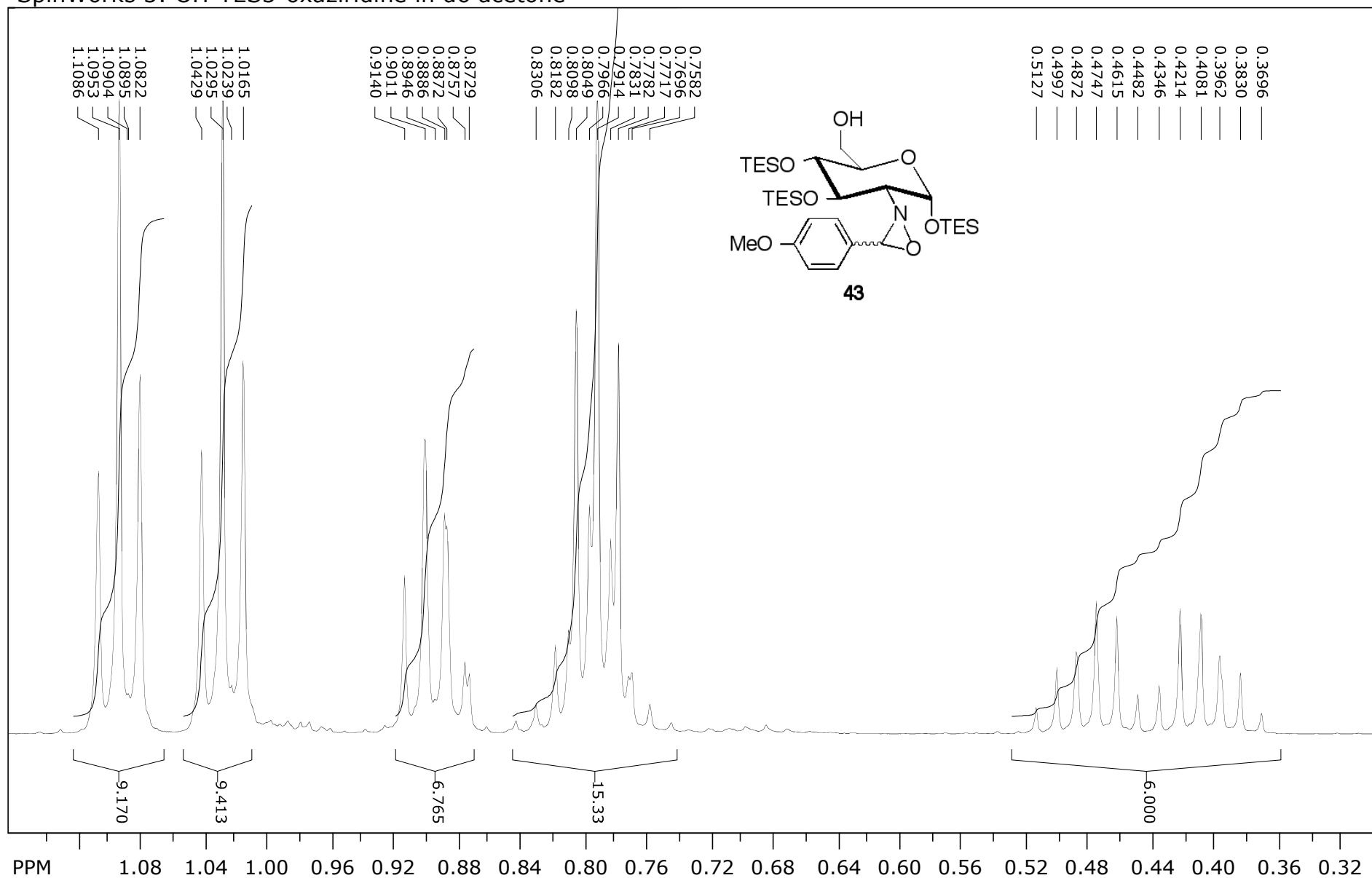


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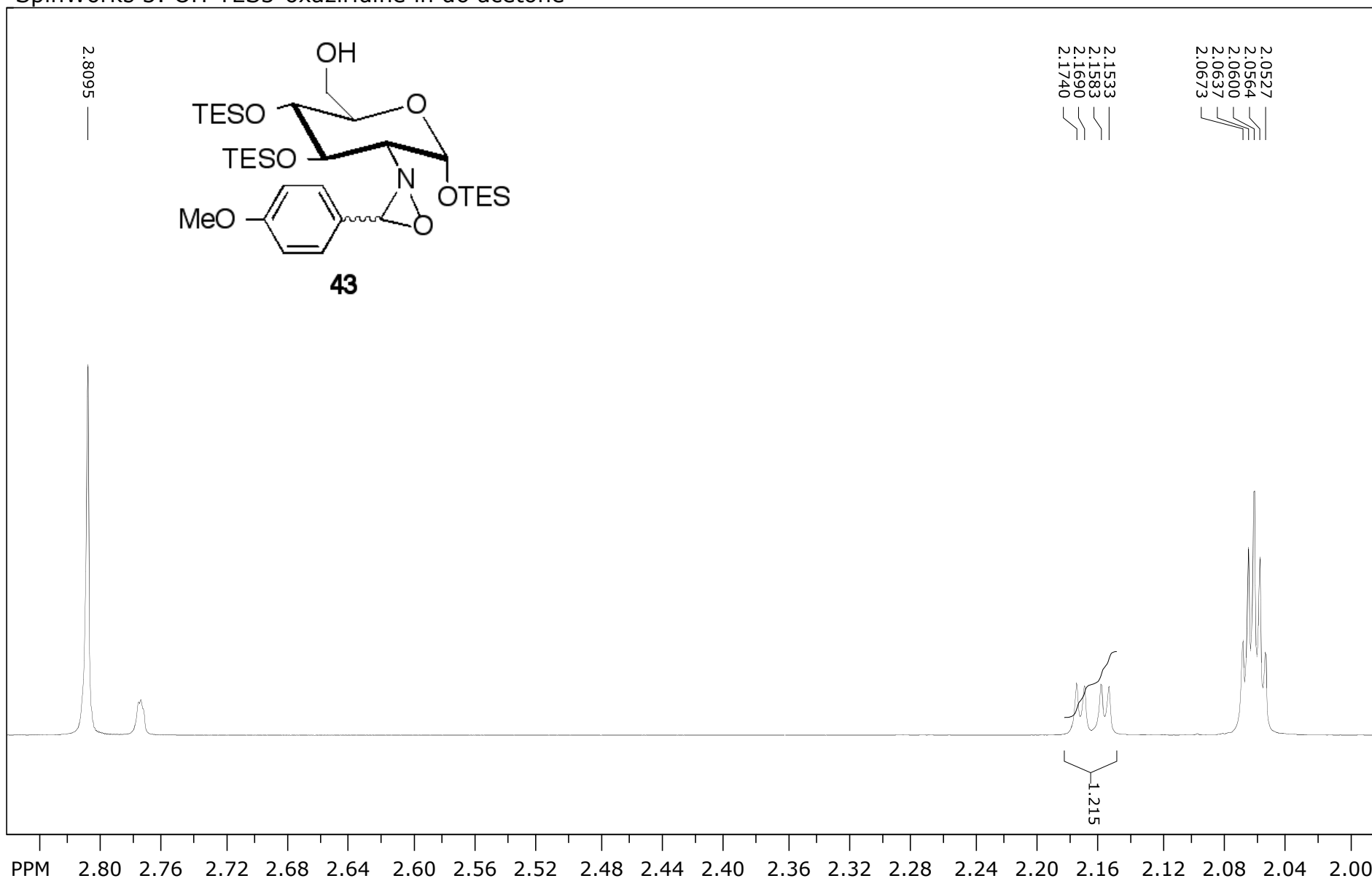
file: ...\Oxaziridines\mainTES3oxazir\1\fid expt: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 32768 points
width: 9615.38 Hz = 16.0109 ppm = 0.293438 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 200.034 ppm/cm: 0.33308



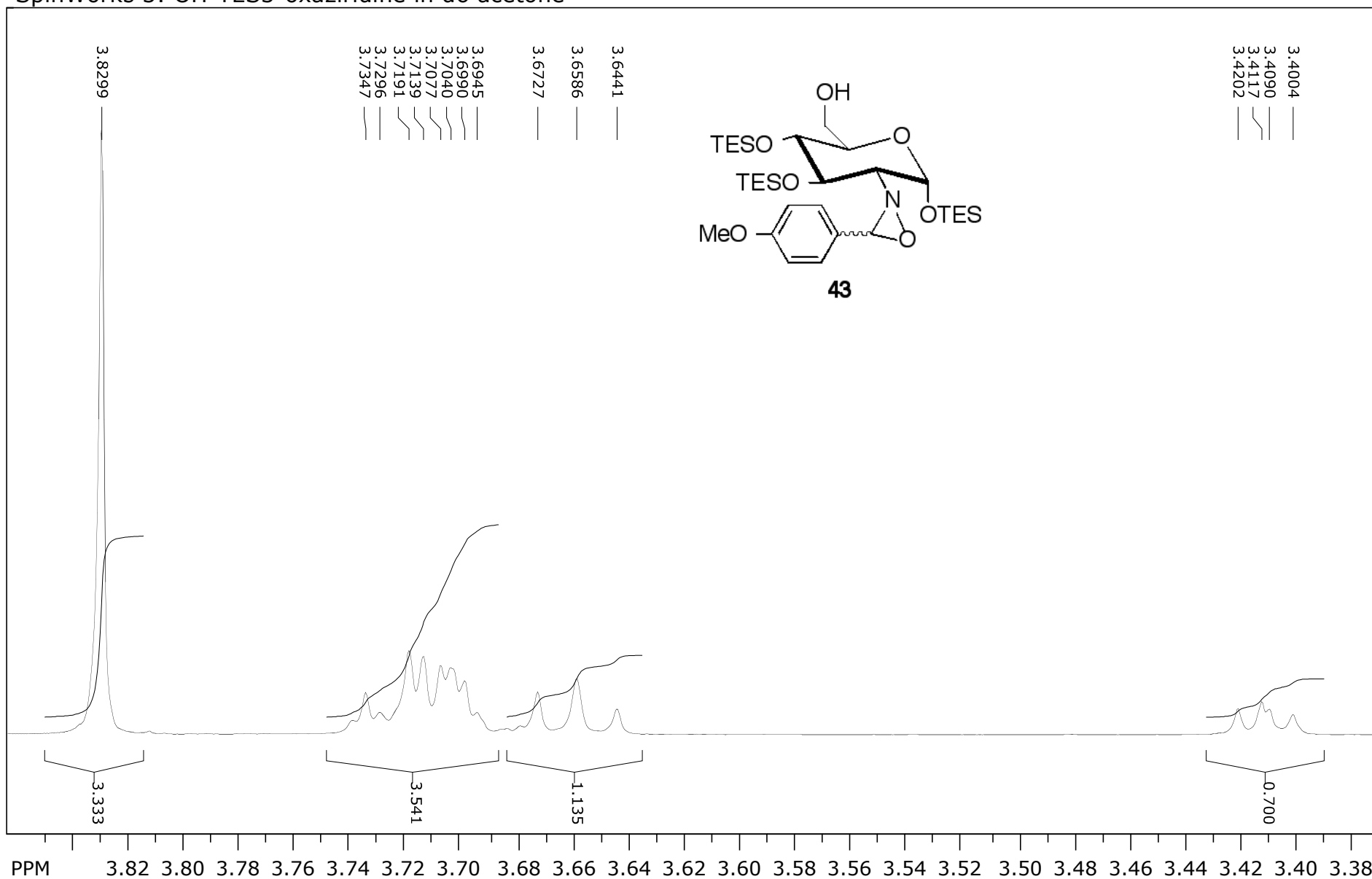
file: ...\Oxaziridines\mainTES3oxazir\1\fid expt: <zgr>
 transmitter freq.: 600.552832 MHz
 time domain size: 32768 points
 width: 9615.38 Hz = 16.0109 ppm = 0.293438 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550010 MHz
 processed size: 32768 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 20.917 ppm/cm: 0.03483



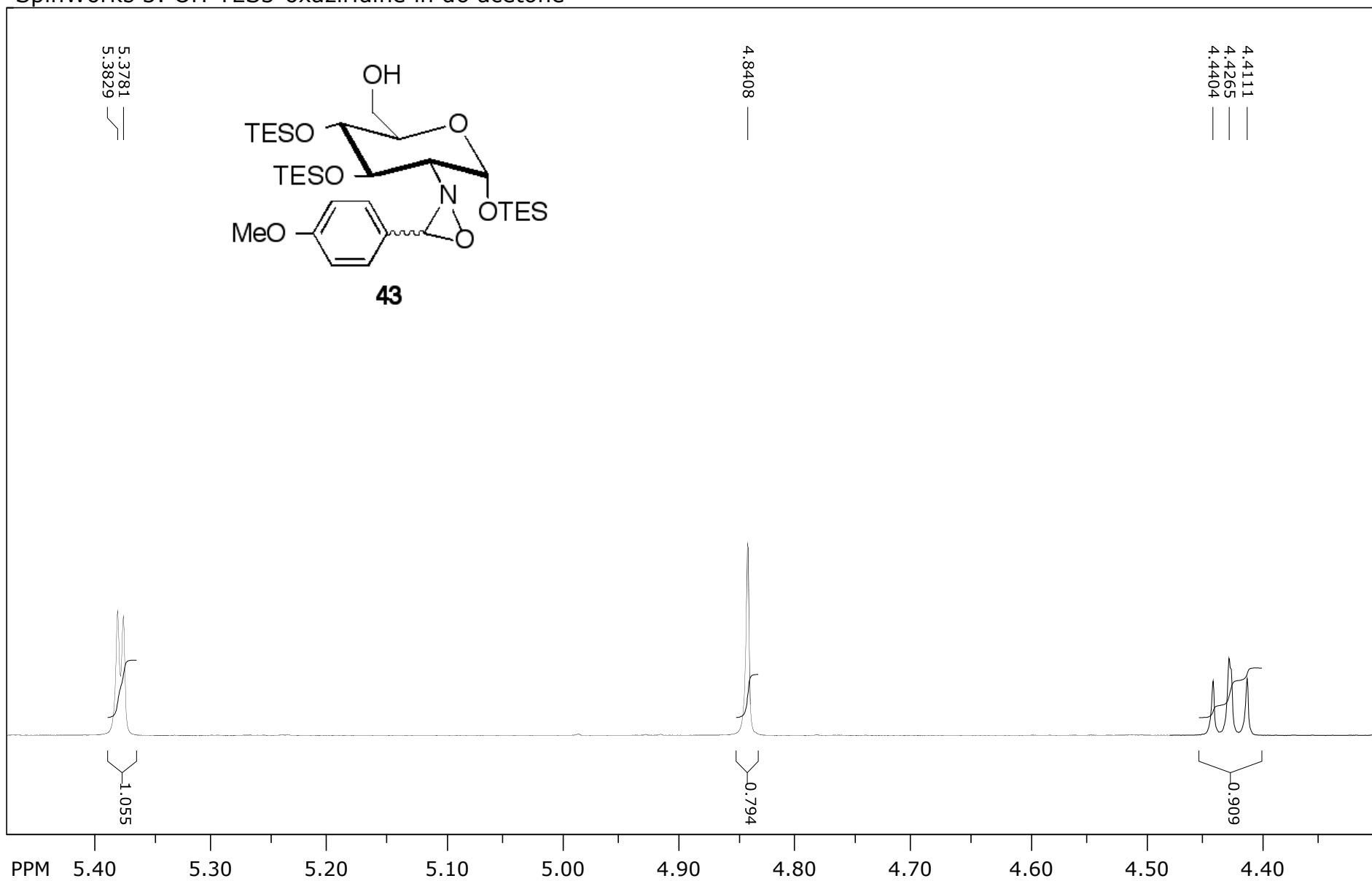
file: ...\Oxaziridines\mainTES3oxazir\1\fid expt: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 32768 points
width: 9615.38 Hz = 16.0109 ppm = 0.293438 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 21.179 ppm/cm: 0.03527



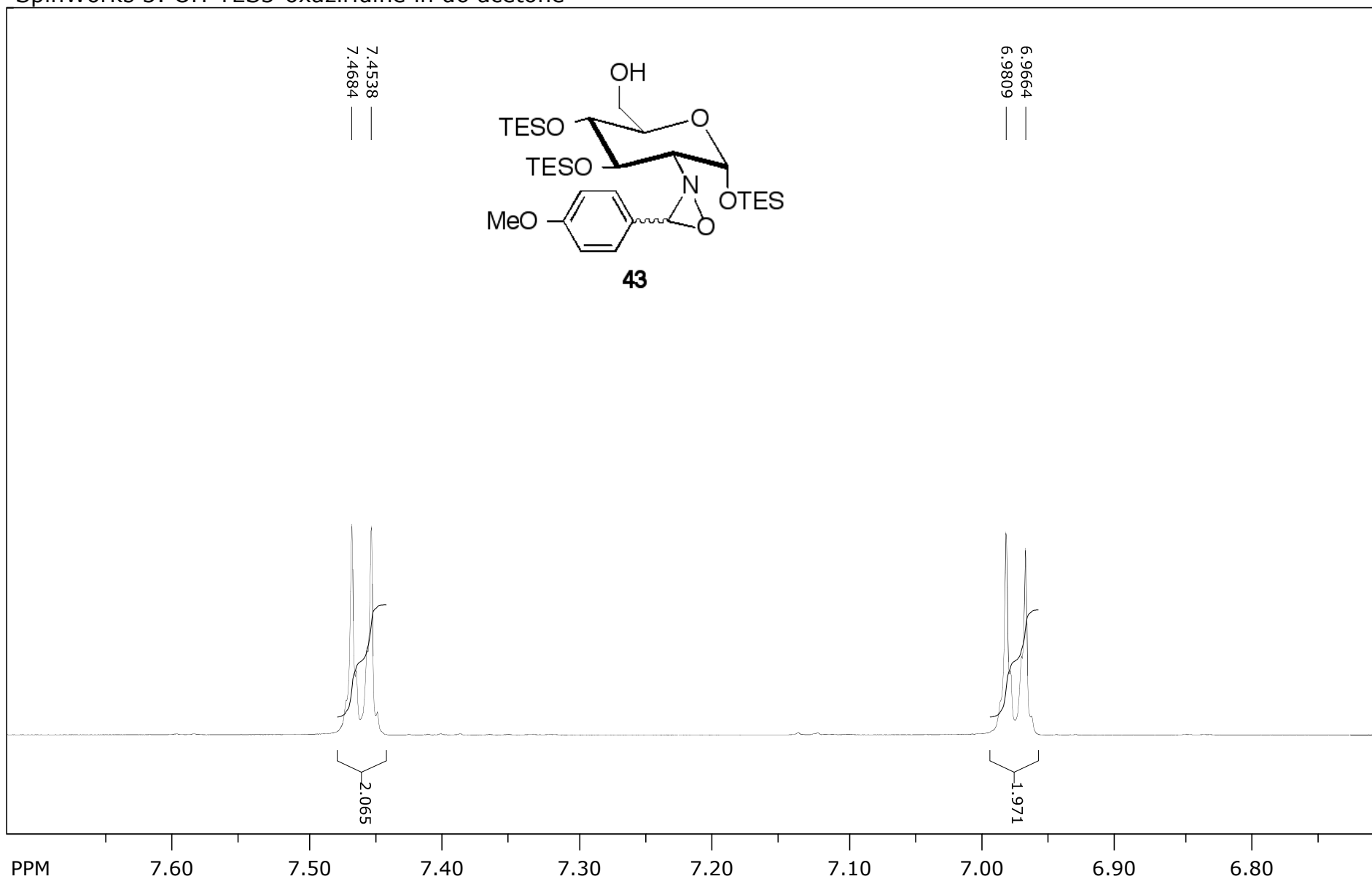
file: ...\Oxaziridines\mainTES3oxazir\1\fid expt: <zgpr>
 transmitter freq.: 600.552832 MHz
 time domain size: 32768 points
 width: 9615.38 Hz = 16.0109 ppm = 0.293438 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.550010 MHz
 processed size: 32768 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 11.882 ppm/cm: 0.01978



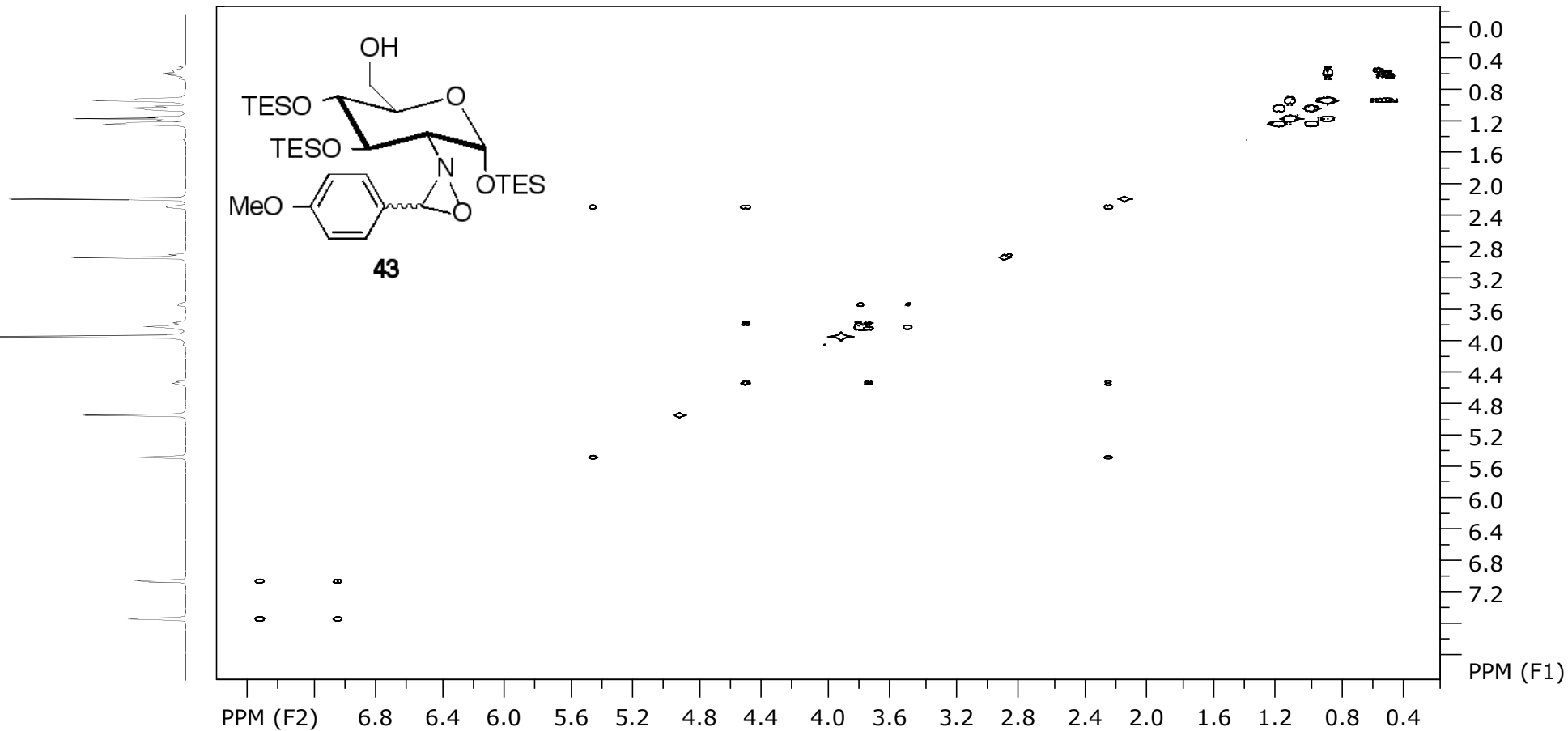
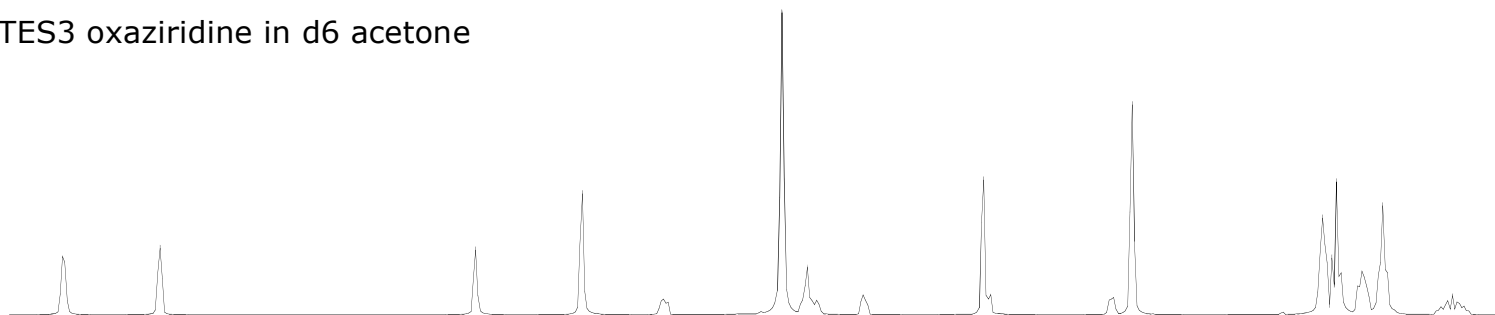
file: ...\Oxaziridines\mainTES3oxazir\1\fid expt: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 32768 points
width: 9615.38 Hz = 16.0109 ppm = 0.293438 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 28.365 ppm/cm: 0.04723



file: ...\Oxaziridines\mainTES3oxazir\1\fid expt: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 32768 points
width: 9615.38 Hz = 16.0109 ppm = 0.293438 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.550010 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 24.554 ppm/cm: 0.04089

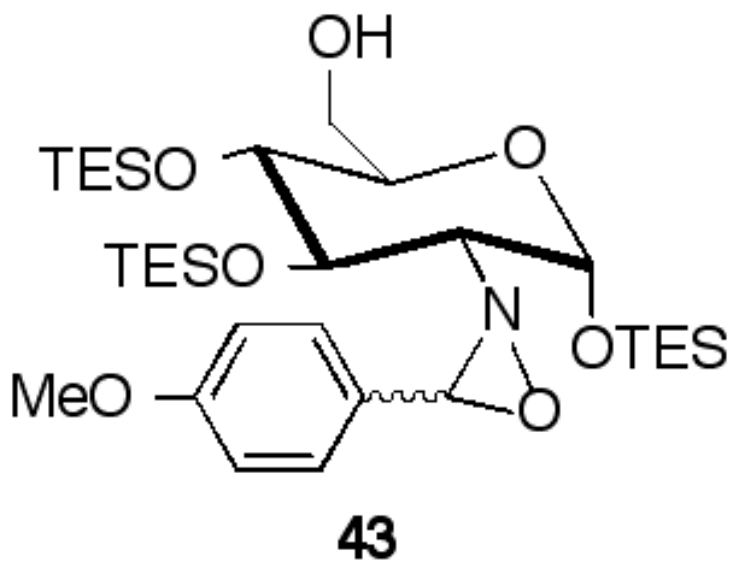
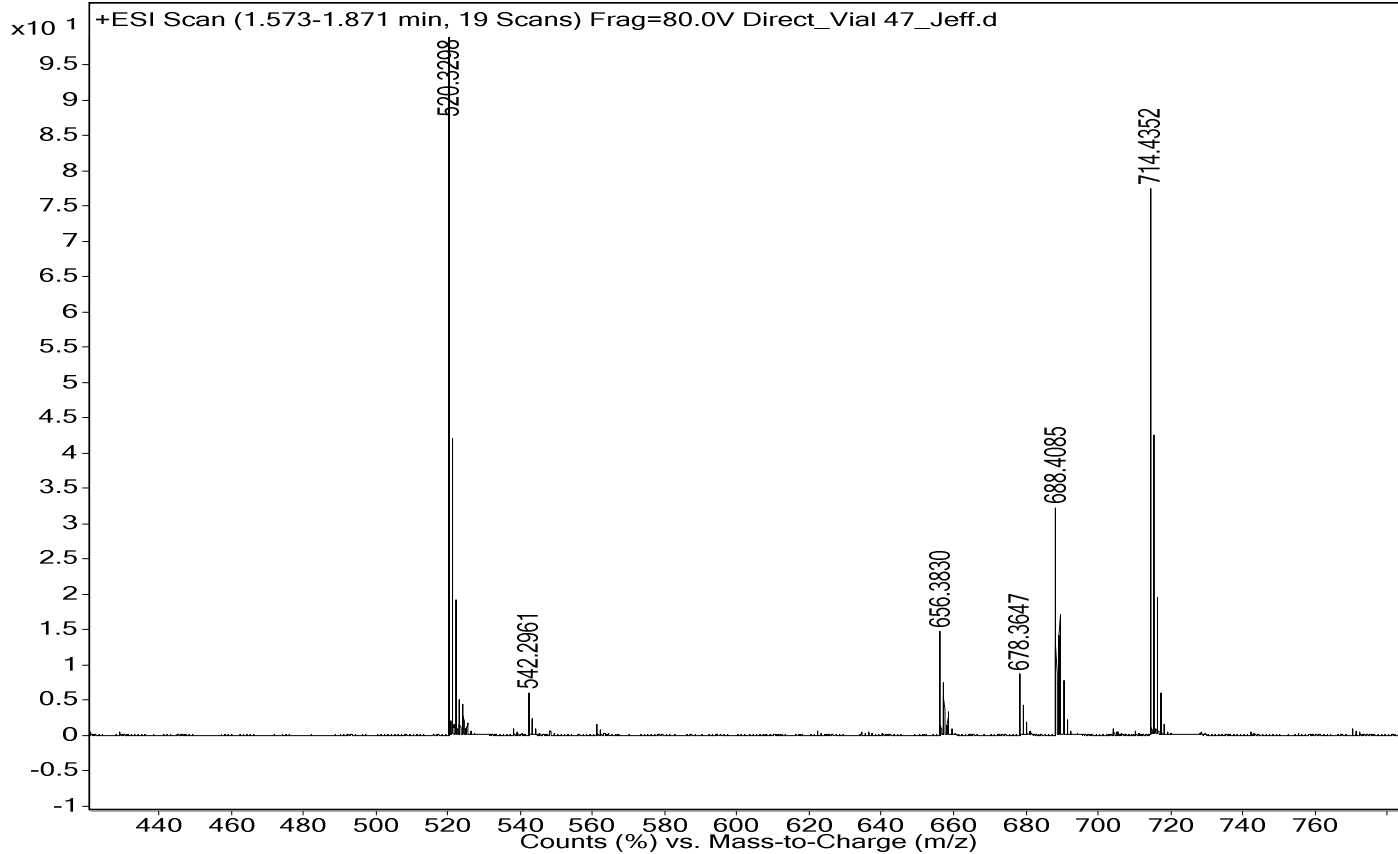


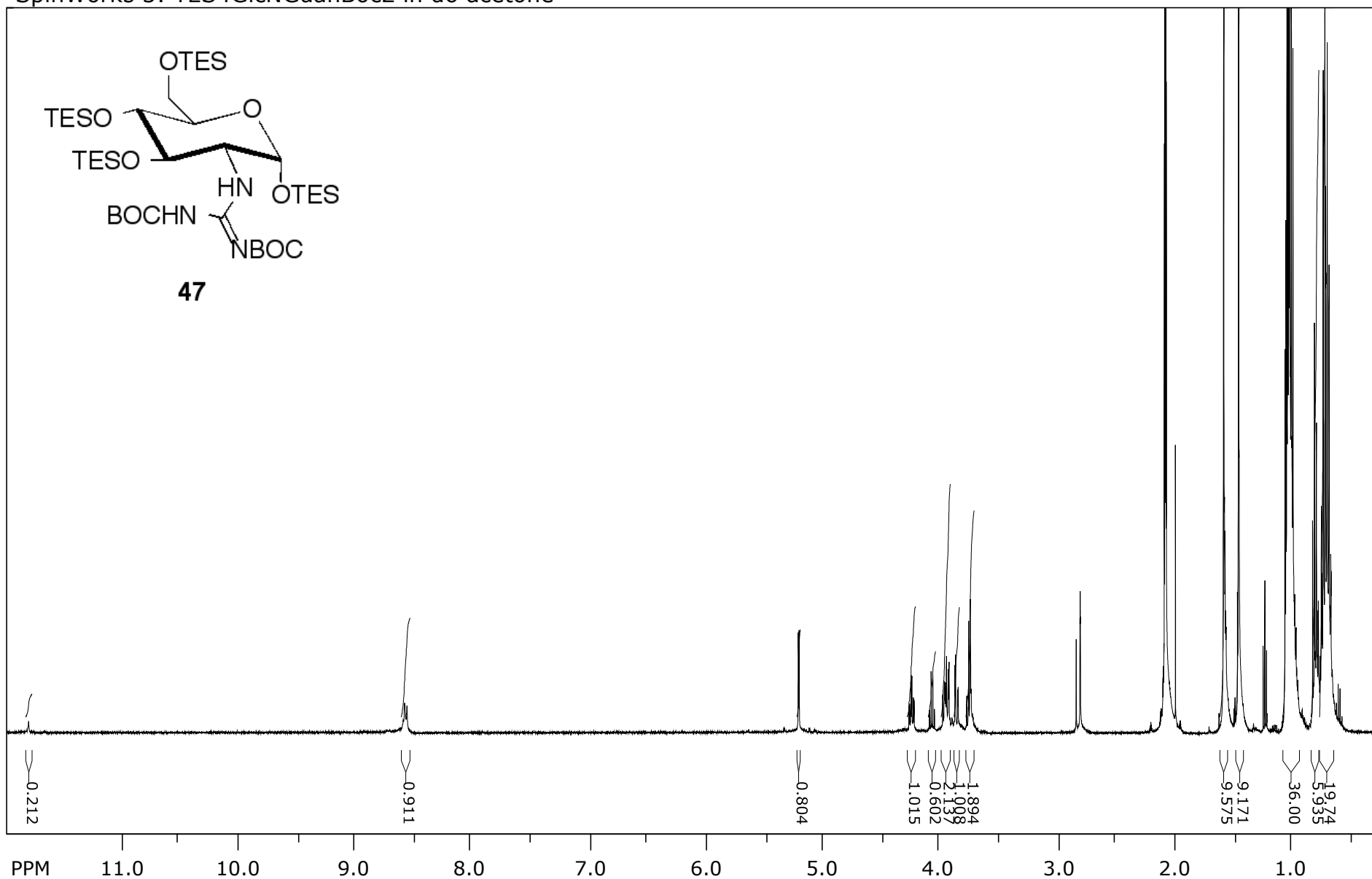
file: ...ziridines\mainTES3oxazirCOSY\1\ser
 expt: <cosygpqf>
 transmitter freq: 600.552832 MHz
 time domain size: 2048 by 1024 points
 width (F2): 7211.54 Hz = 12.0082 ppm = 3.5213 Hz/pt
 number of scans: 4

F2: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 228.262 ppm/cm: 0.38009

F1: freq. of 0 ppm: 600.5499623 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 468.241 ppm/cm: 0.77968

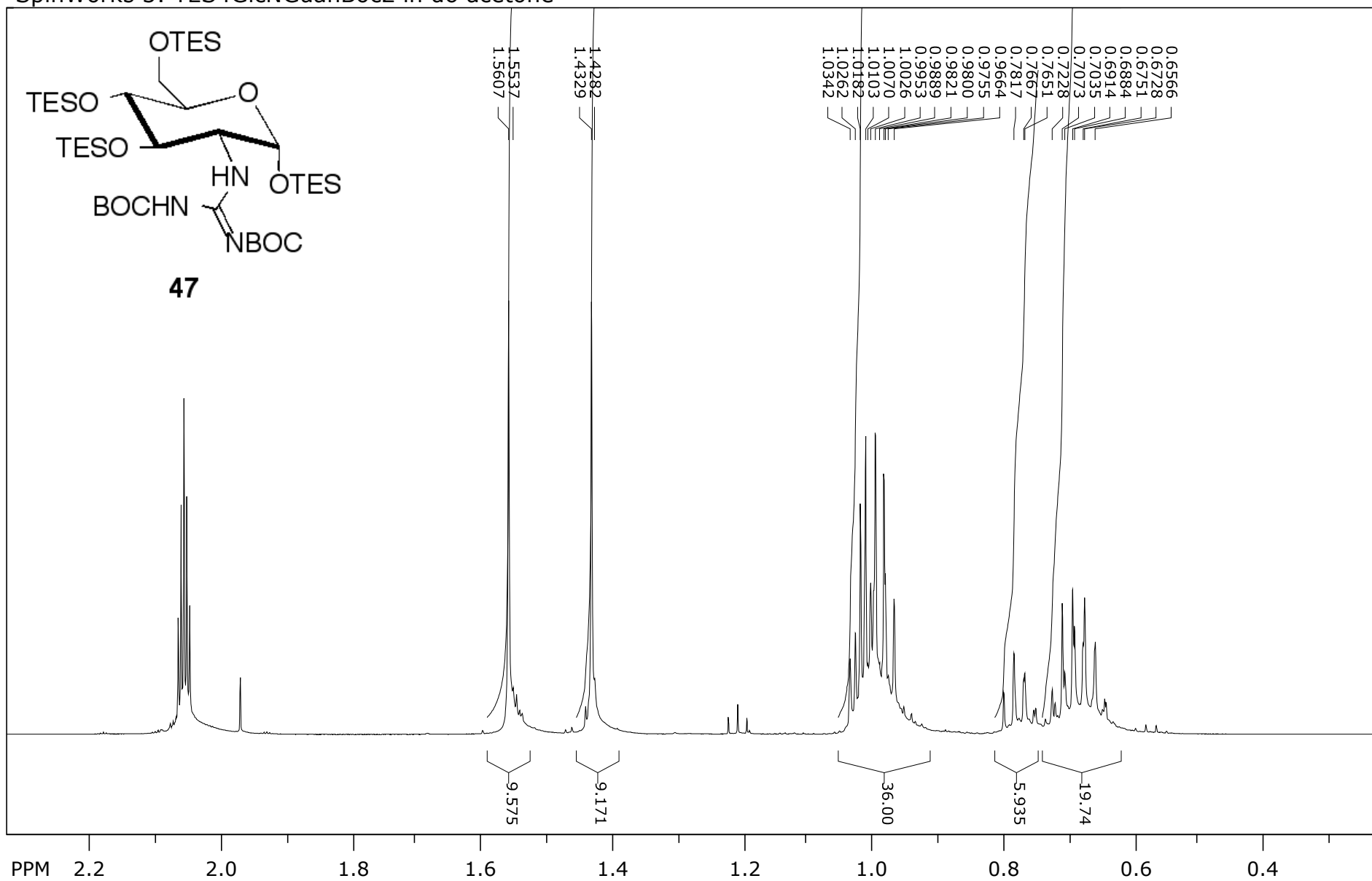
Sample Name	Jeff 47	Position	Vial 47	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 47_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 2:15:15 PM





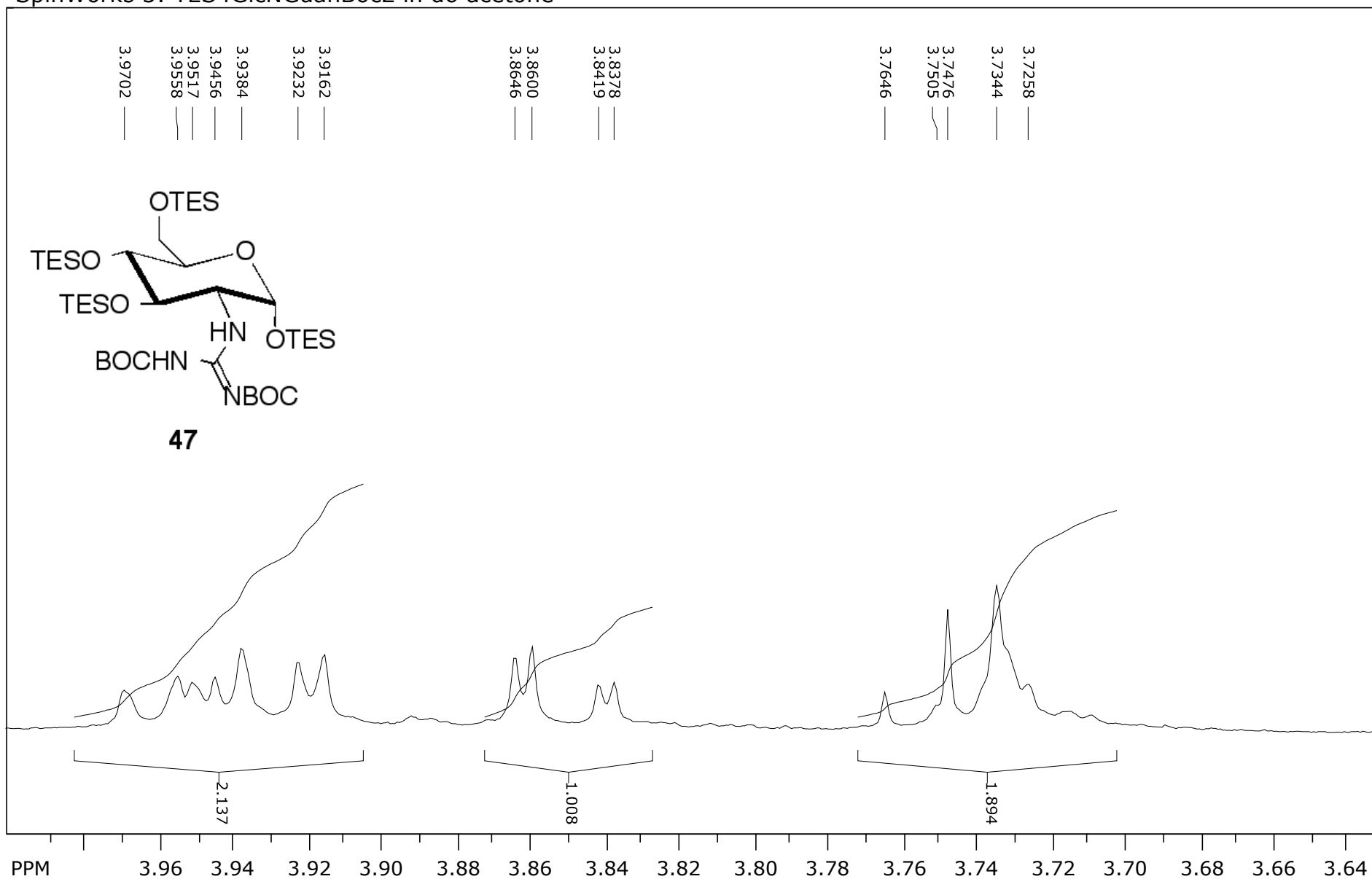
file: ...akony\nmr\TES4GB2_10_09_main\1\fid expt: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
number of scans: 164

freq. of 0 ppm: 500.046007 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 235.380 ppm/cm: 0.47071



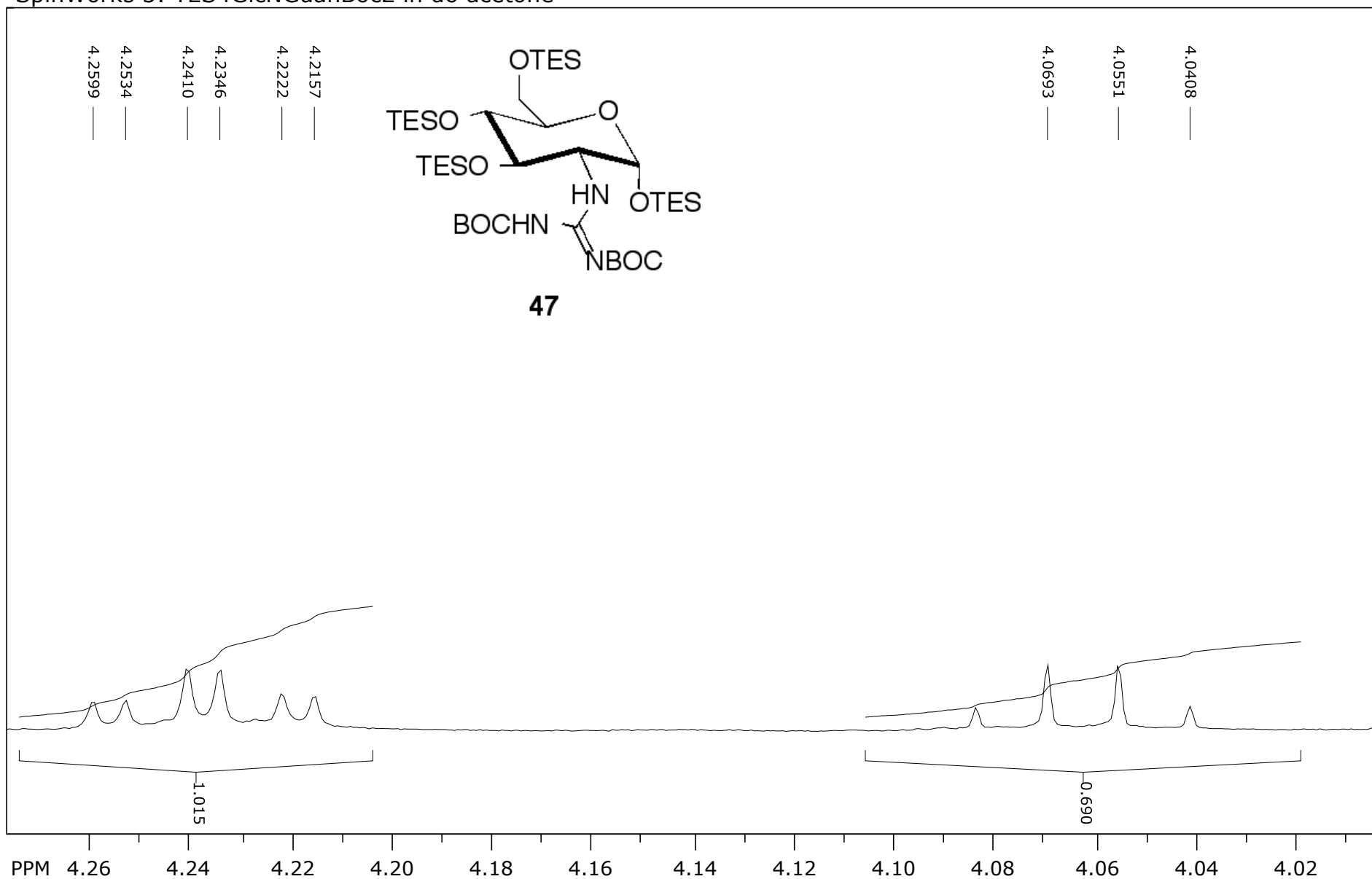
file: ...akony\nmr\TES4GB2_10_09_main\1\fid expt: <zg>
 transmitter freq.: 500.049088 MHz
 time domain size: 65536 points
 width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
 number of scans: 164

freq. of 0 ppm: 500.046007 MHz
 processed size: 32768 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 42.300 ppm/cm: 0.08459



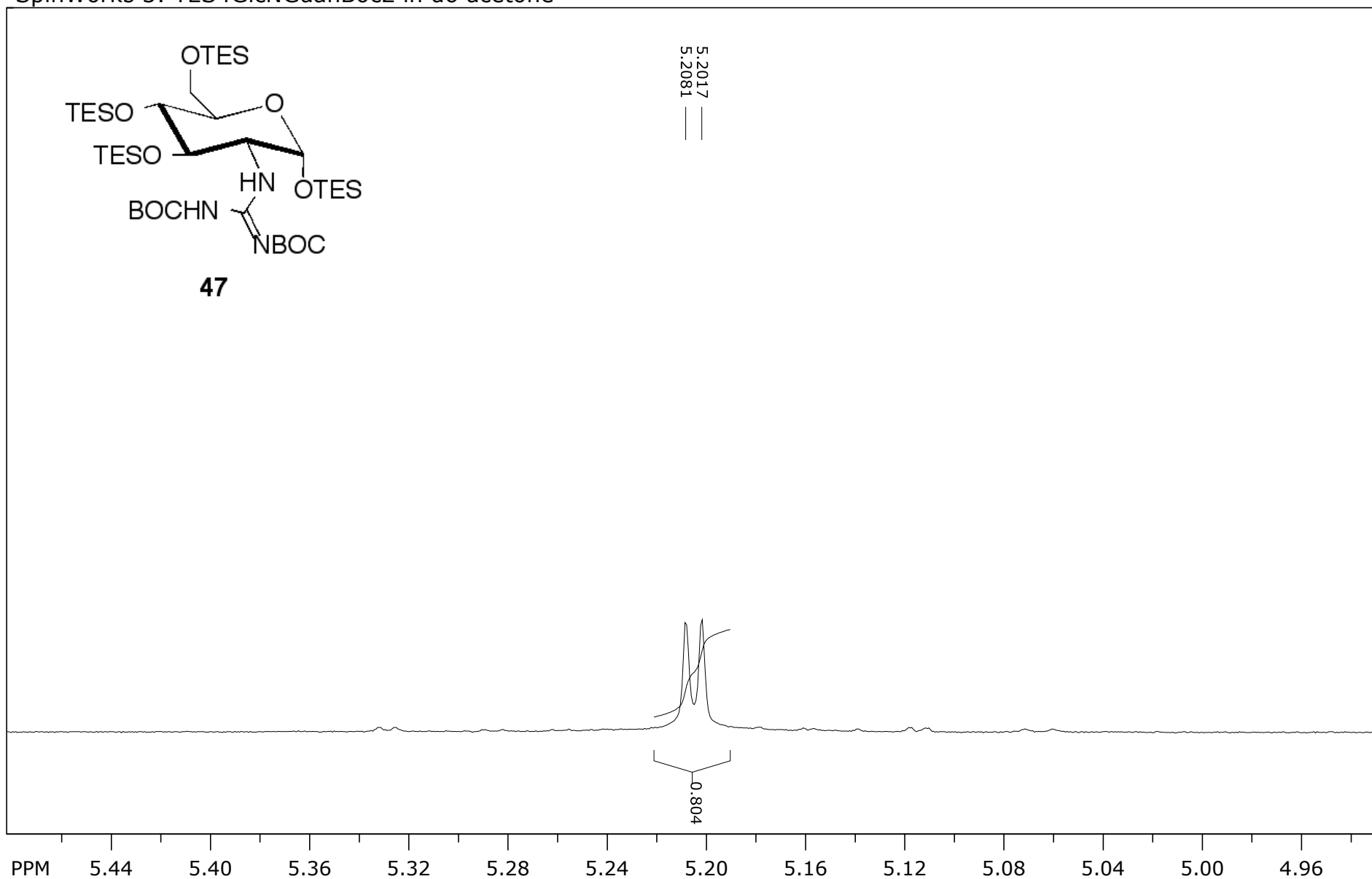
file: ...akony\nmr\TES4GB2_10_09_main\1\fid exp: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
number of scans: 164

freq. of 0 ppm: 500.046007 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 7.419 ppm/cm: 0.01484



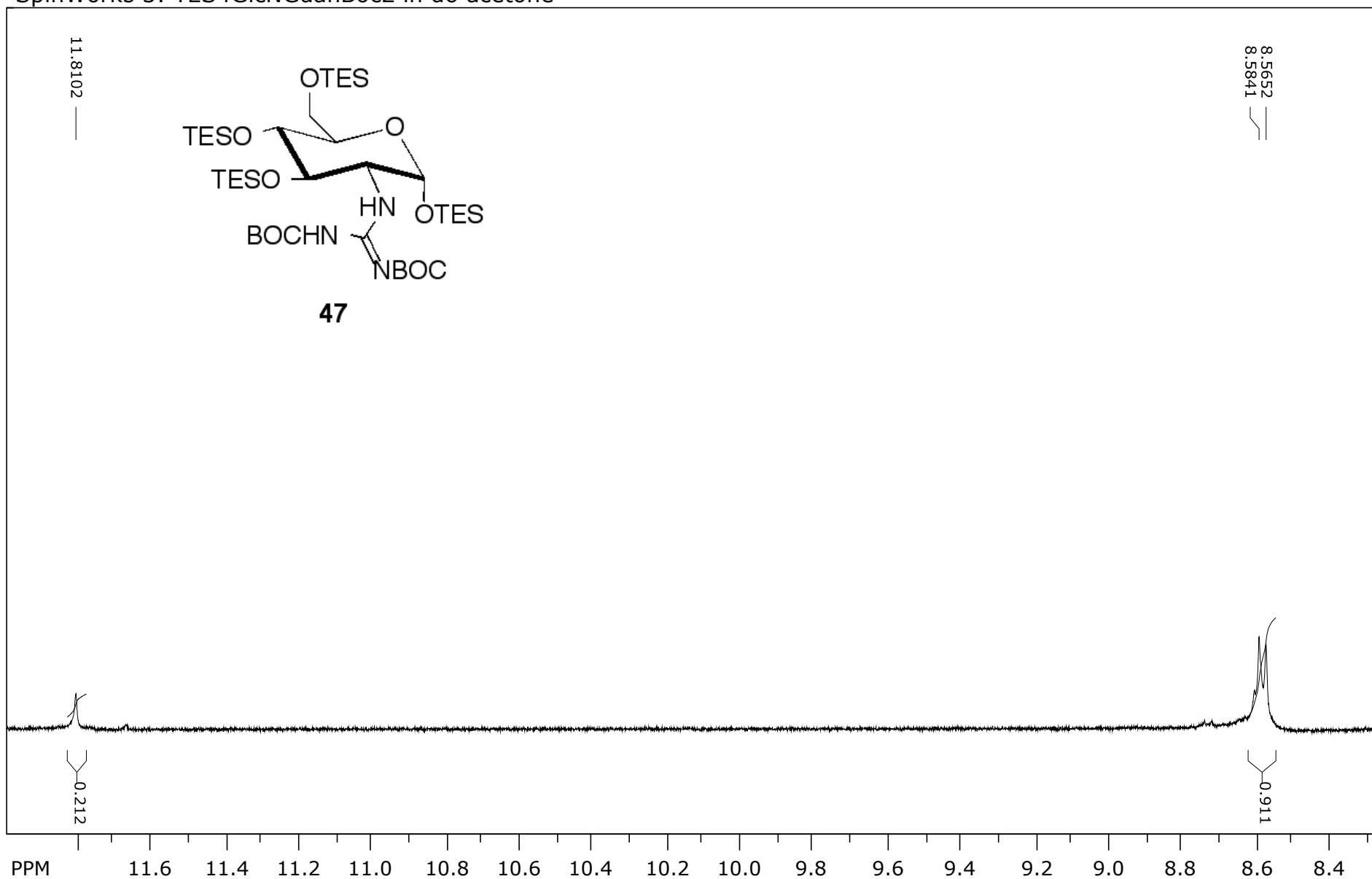
file: ...akony\nmr\TES4GB2_10_09_main\1\fid expt: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
number of scans: 164

freq. of 0 ppm: 500.046007 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 5.481 ppm/cm: 0.01096



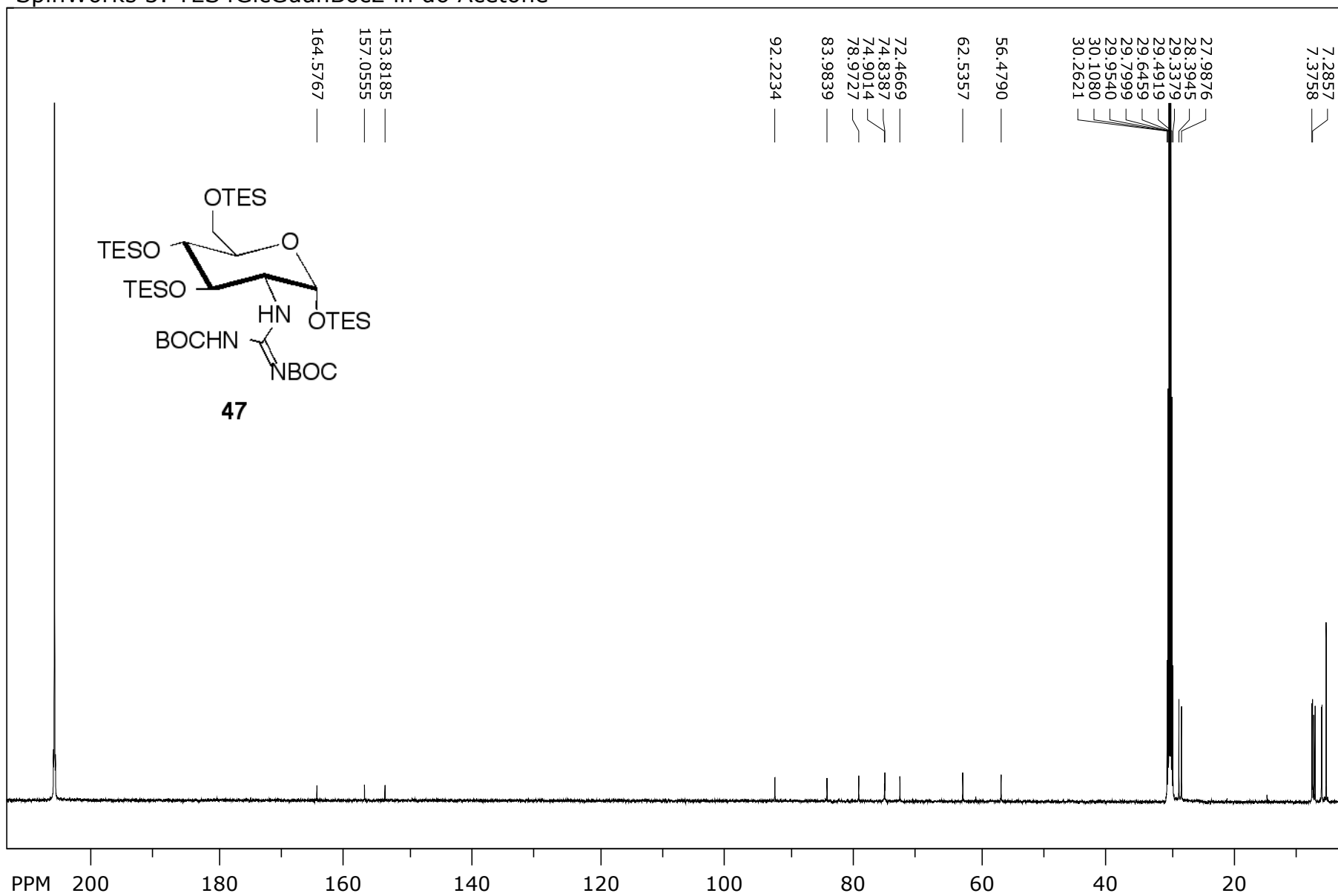
file: ...akony\nmr\TES4GB2_10_09_main\1\fid exp: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
number of scans: 164

freq. of 0 ppm: 500.046007 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 11.144 ppm/cm: 0.02229



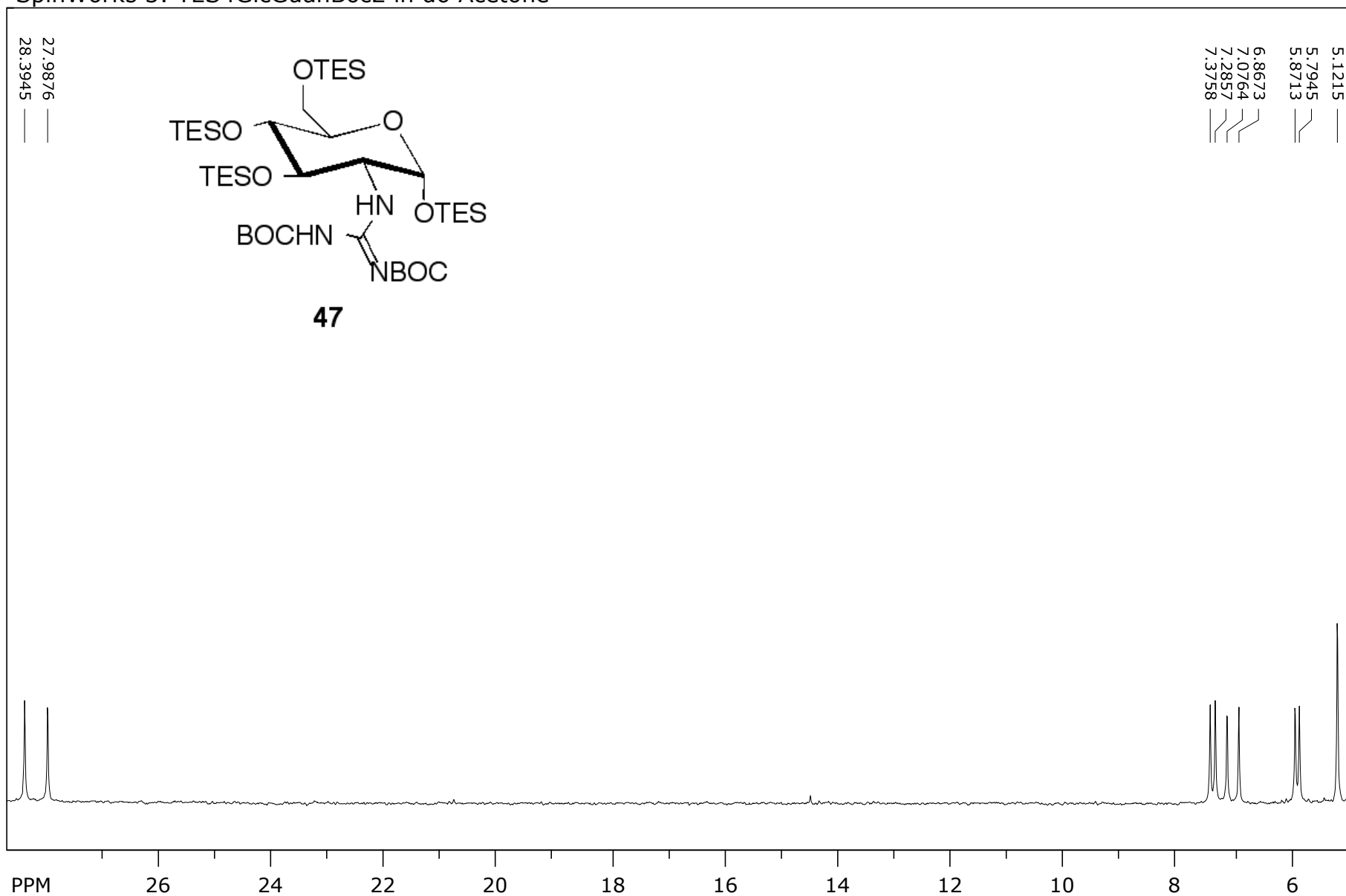
file: ...akony\nmr\TES4GB2_10_09_main\1\fid expt: <zg>
transmitter freq.: 500.049088 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6591 ppm = 0.157632 Hz/pt
number of scans: 164

freq. of 0 ppm: 500.046007 MHz
processed size: 32768 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 74.821 ppm/cm: 0.14963



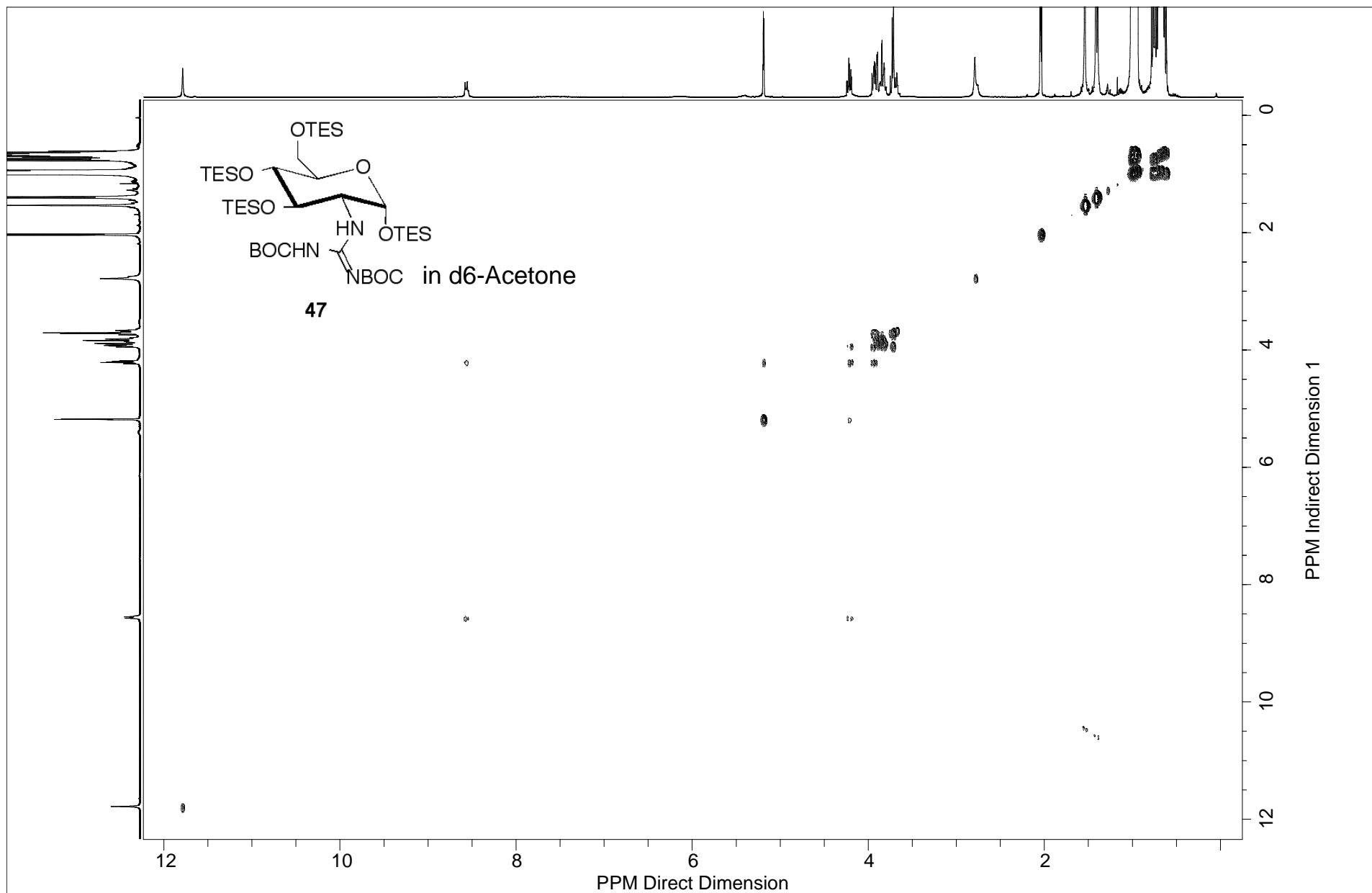
file: ...Data\jjp 11_05\TES4GB2 11_05\2\fid exp: <zgpg30>
transmitter freq.: 125.749582 MHz
time domain size: 65536 points
width: 30303.03 Hz = 240.9792 ppm = 0.462388 Hz/pt
number of scans: 3600

freq. of 0 ppm: 125.736559 MHz
processed size: 32768 complex points
LB: 2.500 GF: 0.0000
Hz/cm: 1109.054 ppm/cm: 8.81955



file: ...Data\jjp 11_05\TES4GB2 11_05\2\fid exp: <zgpg30>
transmitter freq.: 125.749582 MHz
time domain size: 65536 points
width: 30303.03 Hz = 240.9792 ppm = 0.462388 Hz/pt
number of scans: 3600

freq. of 0 ppm: 125.736559 MHz
processed size: 32768 complex points
LB: 2.500 GF: 0.0000
Hz/cm: 124.645 ppm/cm: 0.99122



TES4GB2_in_CO(CD3)2 (32993)

USER: JR -- DATE: Sep 21, 2009 17:51:49

F1: 399.785 F2: 399.785 SW1: 5597 SW2: 5597 OF1: 2398.7 OF2: 2398.7 PTS1d: 1024 , 1024 PTS2d: 256 , 512

EX: cosy_pfg.ex2

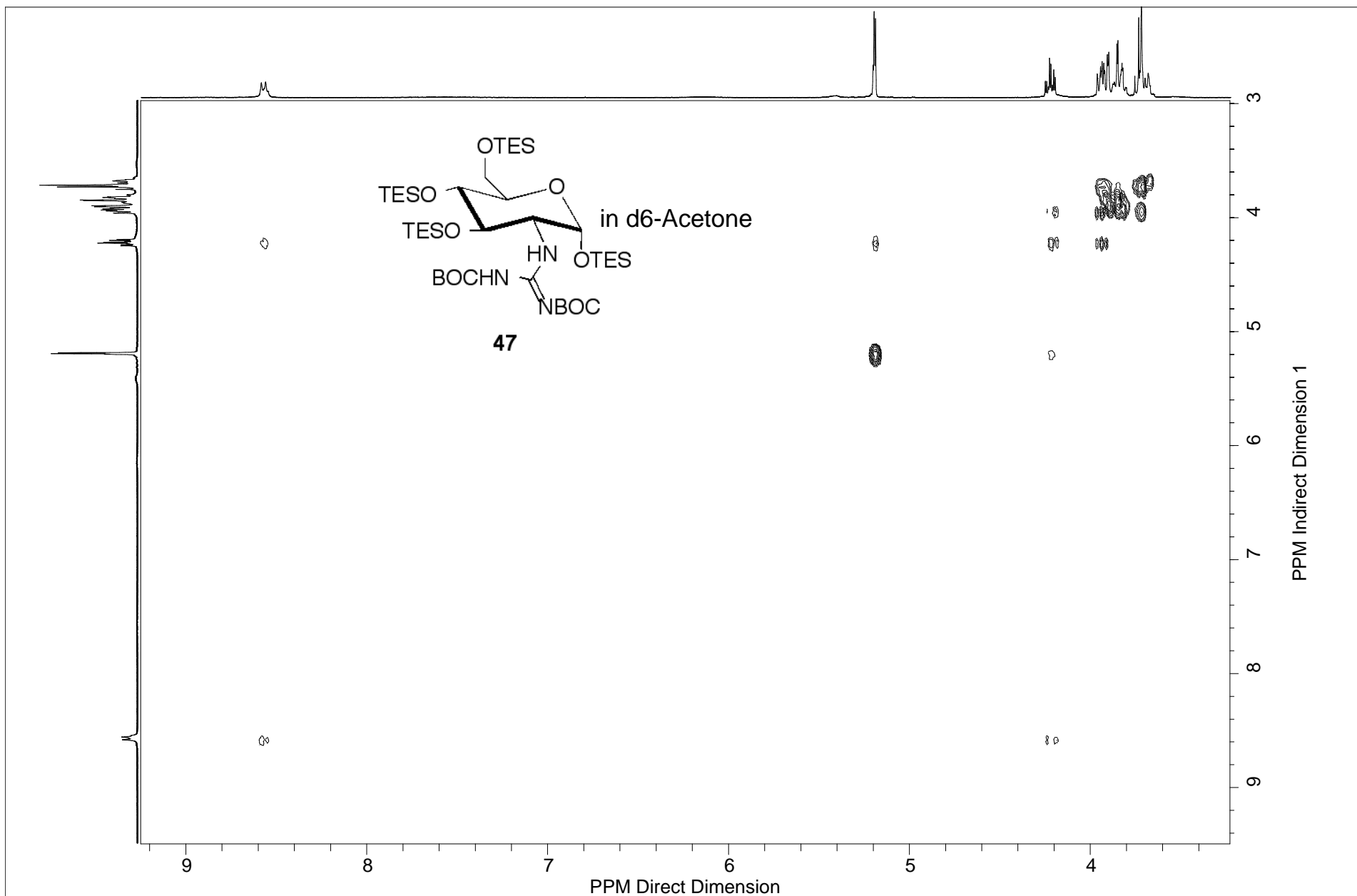
PW: 13.9us, 90deg

PD: 2.0 sec

NA: 2

LB: 0.0

Nuts - \$\$fh090921_COSY-1.jdf



TES4GB2_in_CO(CD3)2 (32993)

USER: JR -- DATE: Sep 21, 2009 17:51:49

F1: 399.785

F2: 399.785

SW1: 5597

SW2: 5597

OF1: 2398.7

OF2: 2398.7

PTS1d: 1024 , 1024 PTS2d: 256 , 512

EX: cosy_pfg.ex2

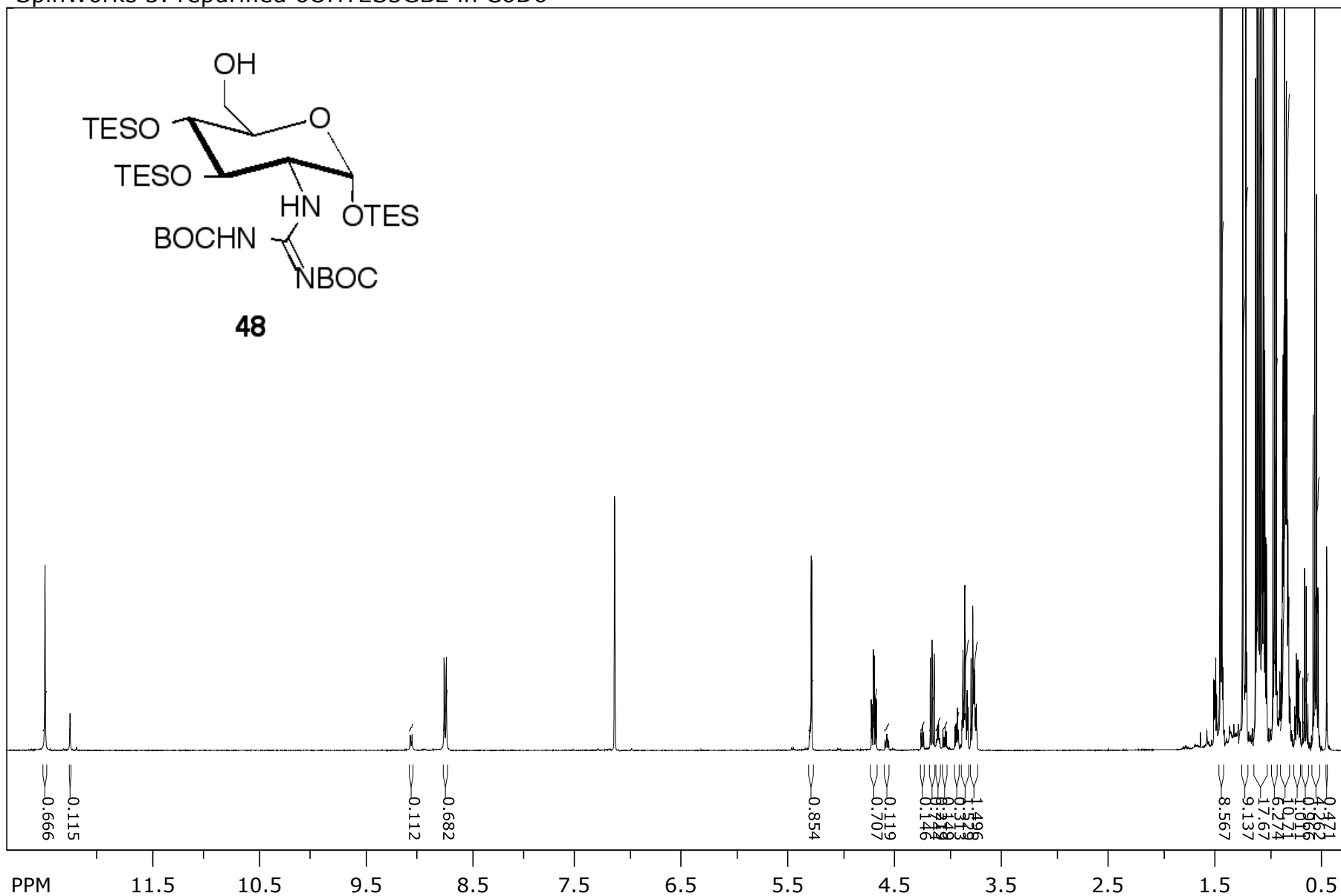
PW: 13.9us, 90deg

PD: 2.0 sec

NA: 2

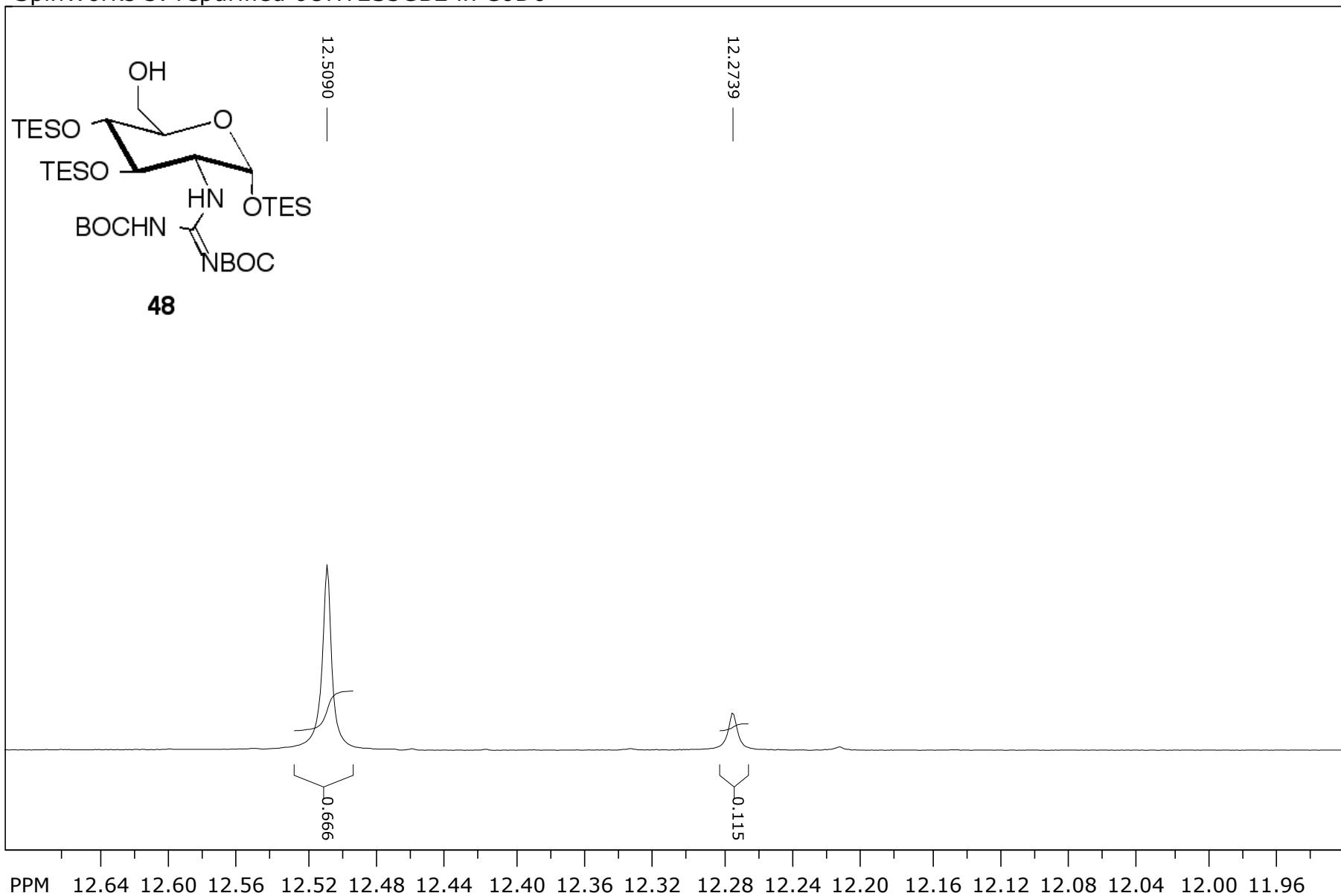
LB: 0.0

Nuts - \$\$fh090921_COSY-1.jdf



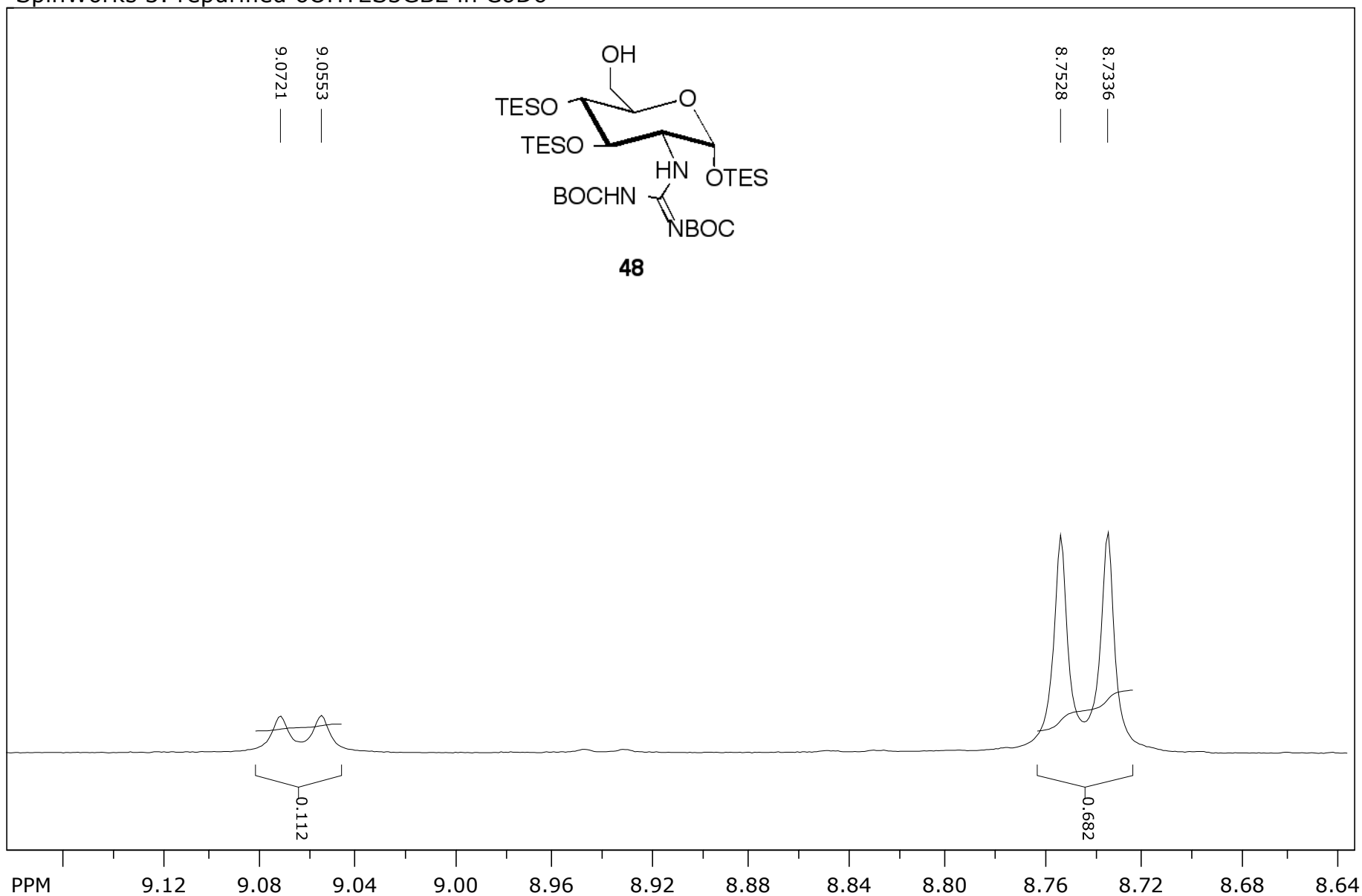
file: ..._11\6OHTES3GB2 repur in C6D6\1\fid expt: <zg>
 transmitter freq.: 499.853228 MHz
 time domain size: 32768 points
 width: 8012.82 Hz = 16.0303 ppm = 0.244532 Hz/pt
 number of scans: 64

freq. of 0 ppm: 499.850061 MHz
 processed size: 16384 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 263.125 ppm/cm: 0.52640



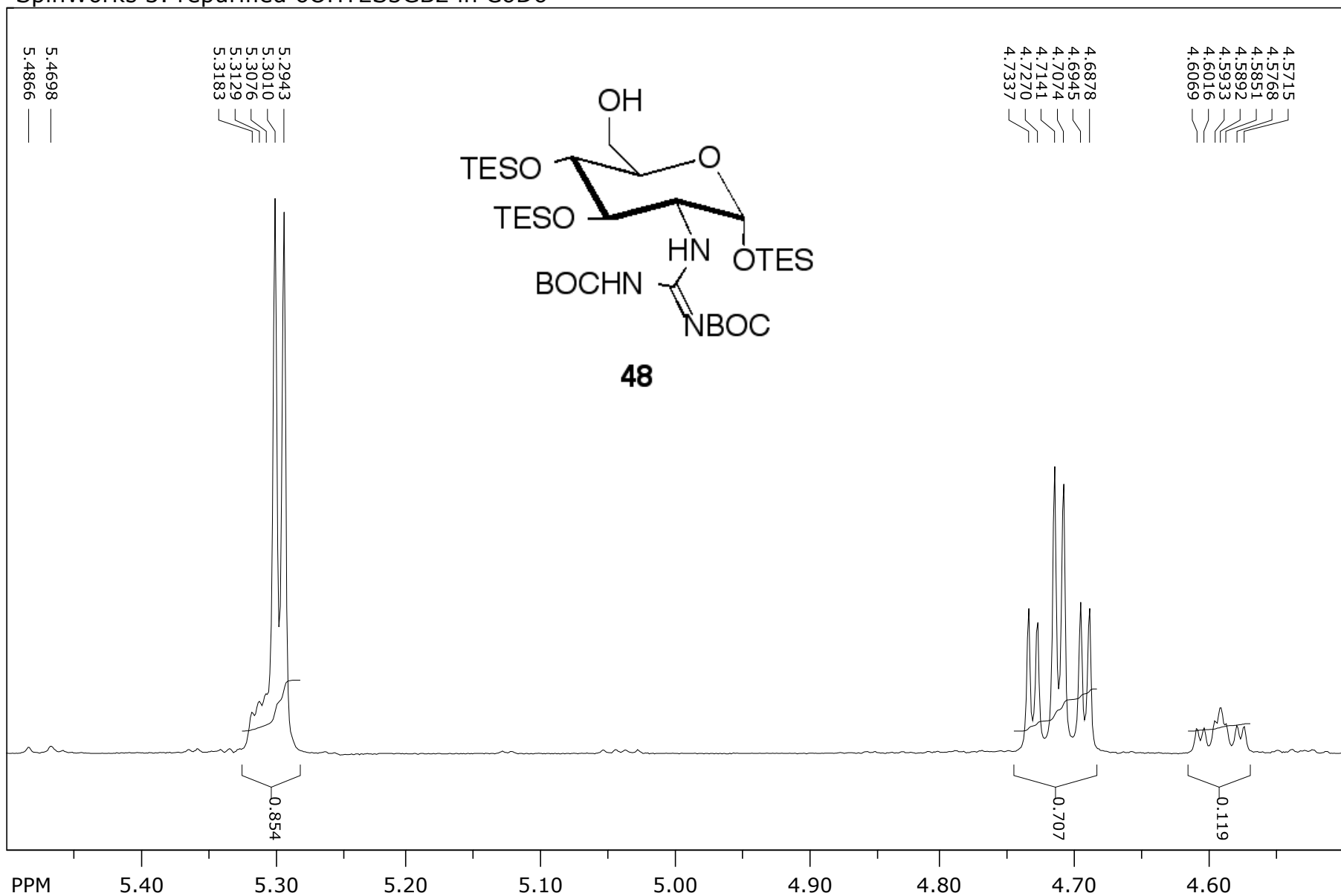
file: ..._11\6OHTES3GB2 repur in C6D6\1\fid expt: <zg>
transmitter freq.: 499.853228 MHz
time domain size: 32768 points
width: 8012.82 Hz = 16.0303 ppm = 0.244532 Hz/pt
number of scans: 64

freq. of 0 ppm: 499.850061 MHz
processed size: 16384 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 16.219 ppm/cm: 0.03245



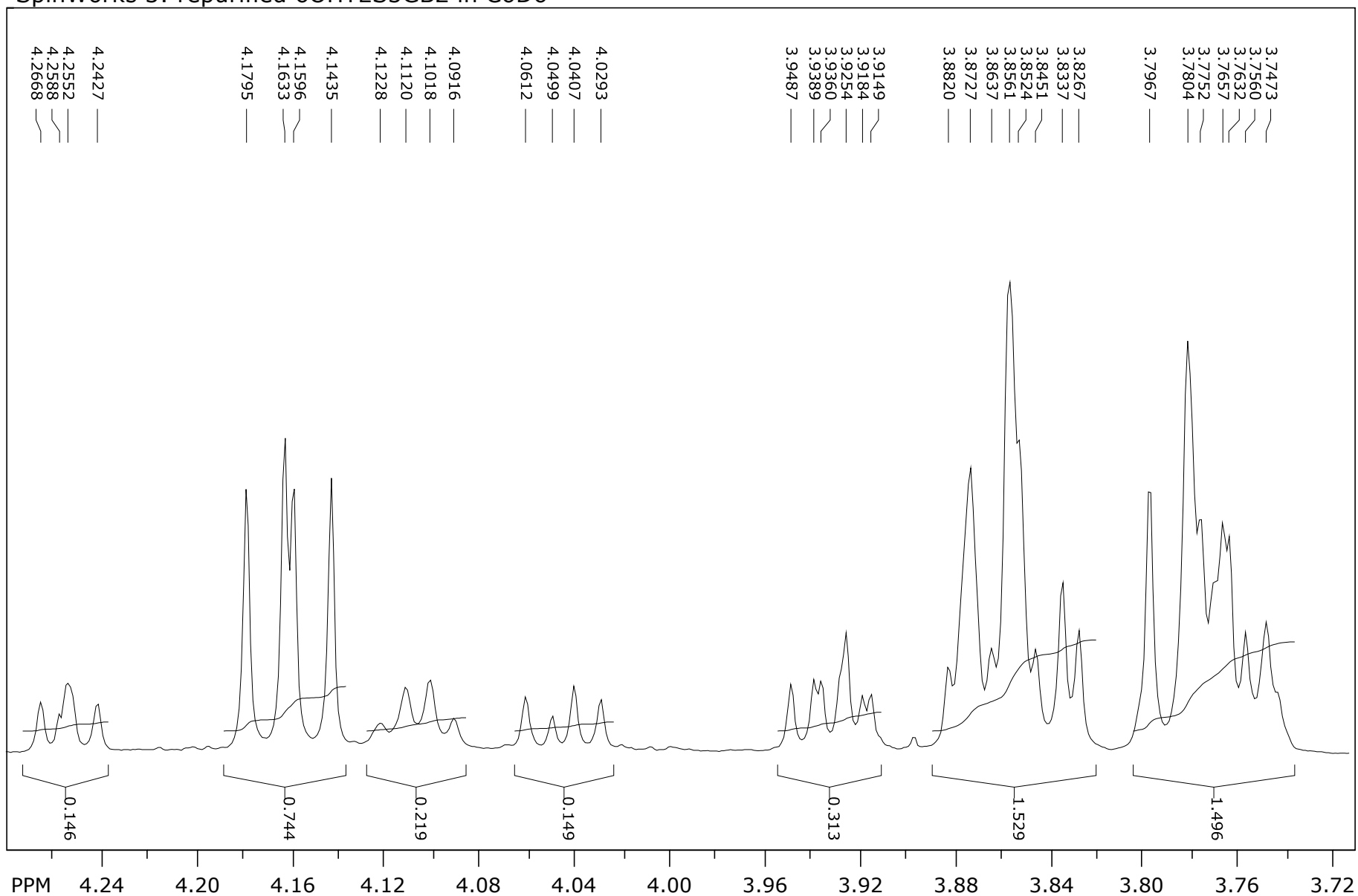
file: ..._11\6OHTES3GB2 repur in C6D6\1\fid expt: <zg>
transmitter freq.: 499.853228 MHz
time domain size: 32768 points
width: 8012.82 Hz = 16.0303 ppm = 0.244532 Hz/pt
number of scans: 64

freq. of 0 ppm: 499.850061 MHz
processed size: 16384 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 11.440 ppm/cm: 0.02289



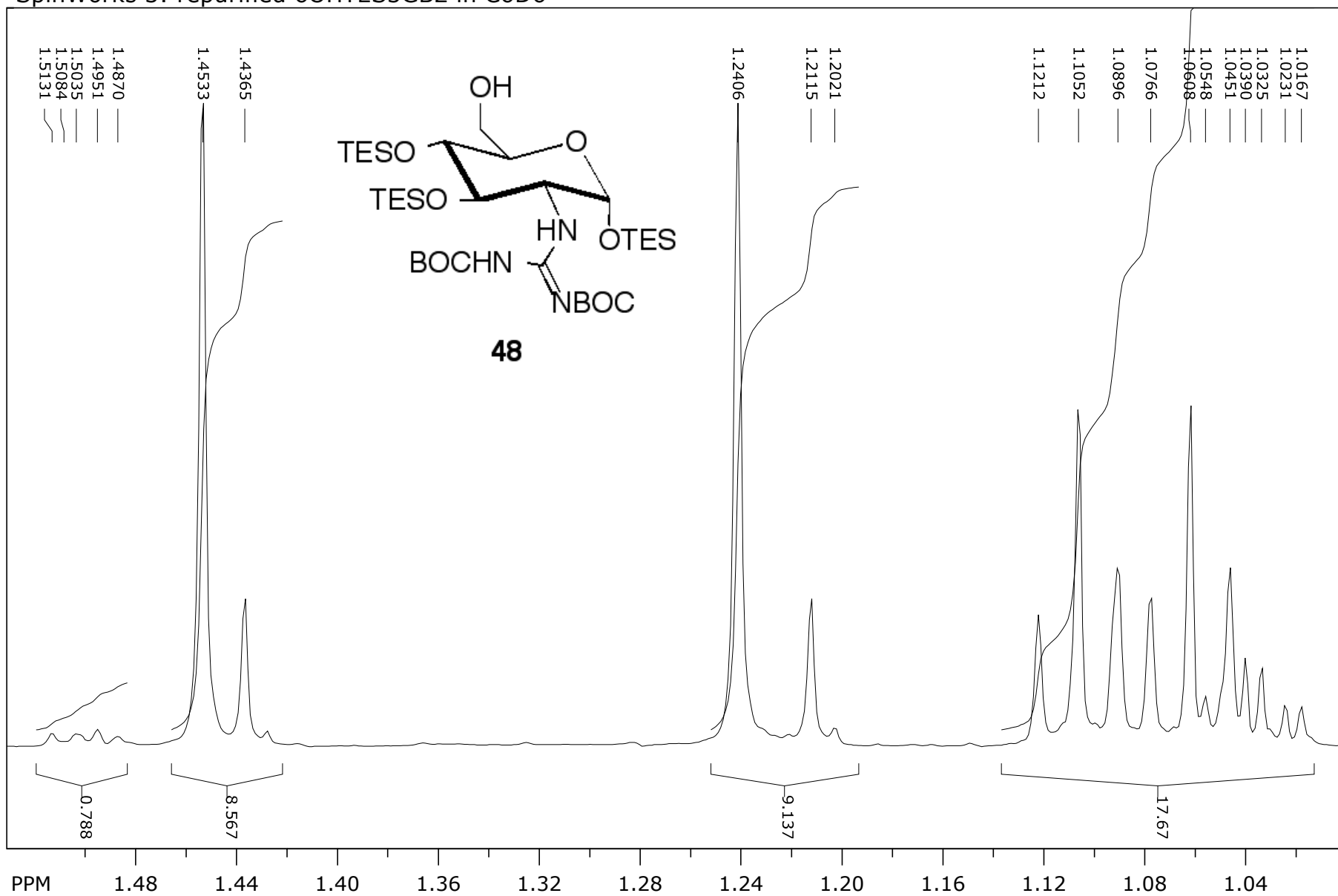
file: ..._11\6OHTES3GB2 repur in C6D6\1\fid expt: <zg>
 transmitter freq.: 499.853228 MHz
 time domain size: 32768 points
 width: 8012.82 Hz = 16.0303 ppm = 0.244532 Hz/pt
 number of scans: 64

freq. of 0 ppm: 499.850061 MHz
 processed size: 16384 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 21.059 ppm/cm: 0.04213



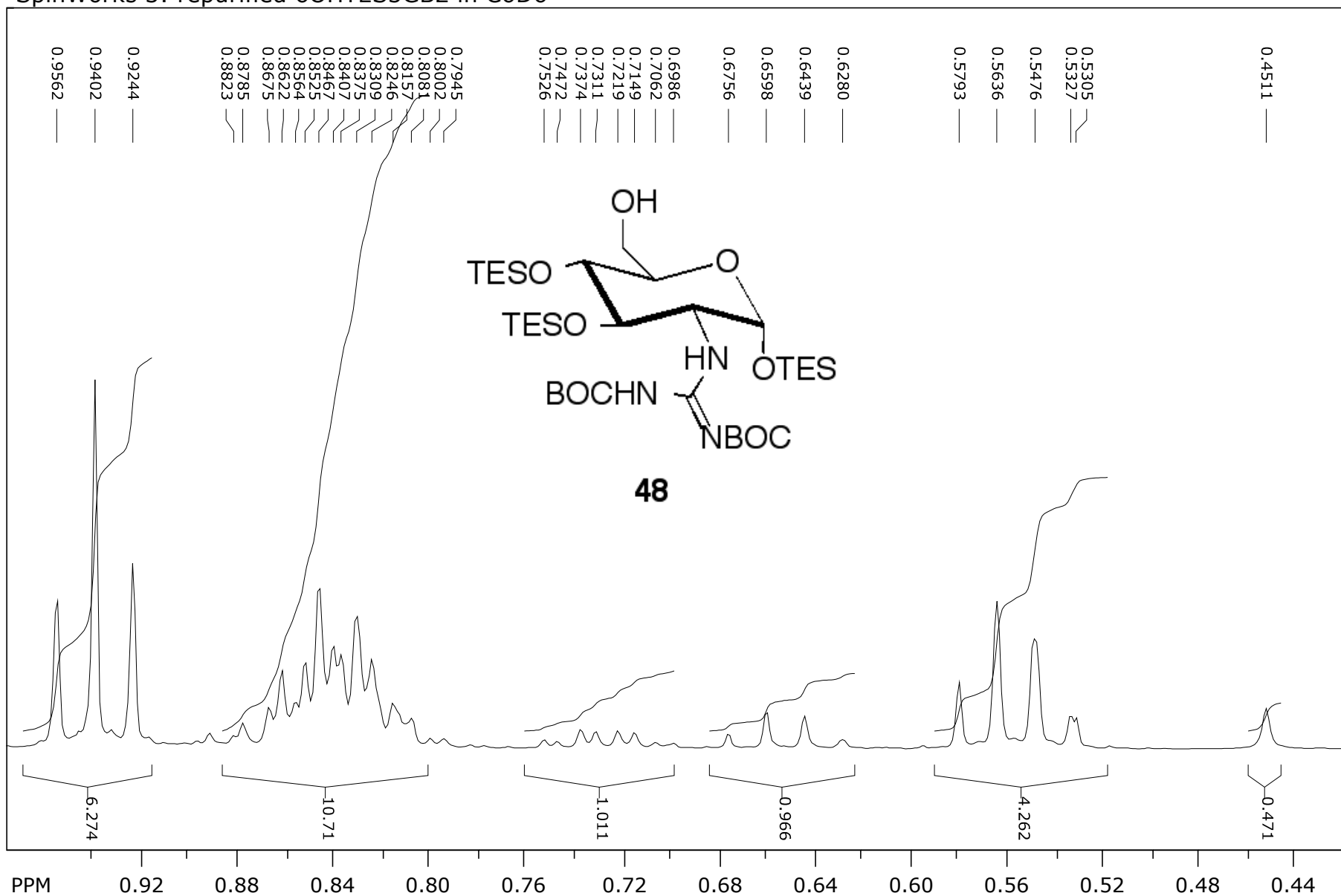
file: ..._11\6OHTES3GB2 repur in C6D6\1\fid expt: <zg>
transmitter freq.: 499.853228 MHz
time domain size: 32768 points
width: 8012.82 Hz = 16.0303 ppm = 0.244532 Hz/pt
number of scans: 64

freq. of 0 ppm: 499.850061 MHz
processed size: 16384 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 11.855 ppm/cm: 0.02372



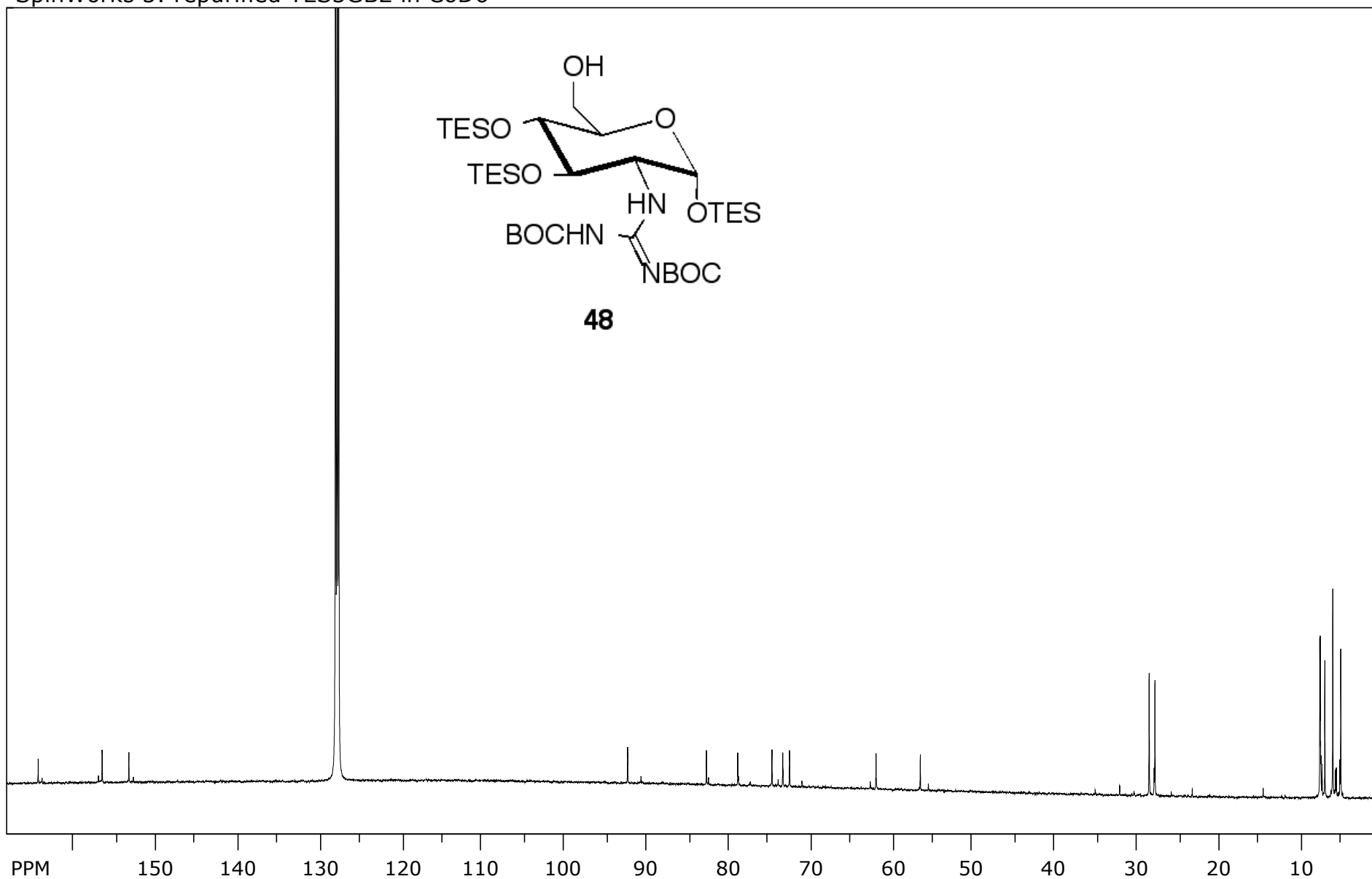
file: ..._11\6OHTES3GB2 repur in C6D6\1\fid expt: <zg>
 transmitter freq.: 499.853228 MHz
 time domain size: 32768 points
 width: 8012.82 Hz = 16.0303 ppm = 0.244532 Hz/pt
 number of scans: 64

freq. of 0 ppm: 499.850061 MHz
 processed size: 16384 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 11.088 ppm/cm: 0.02218



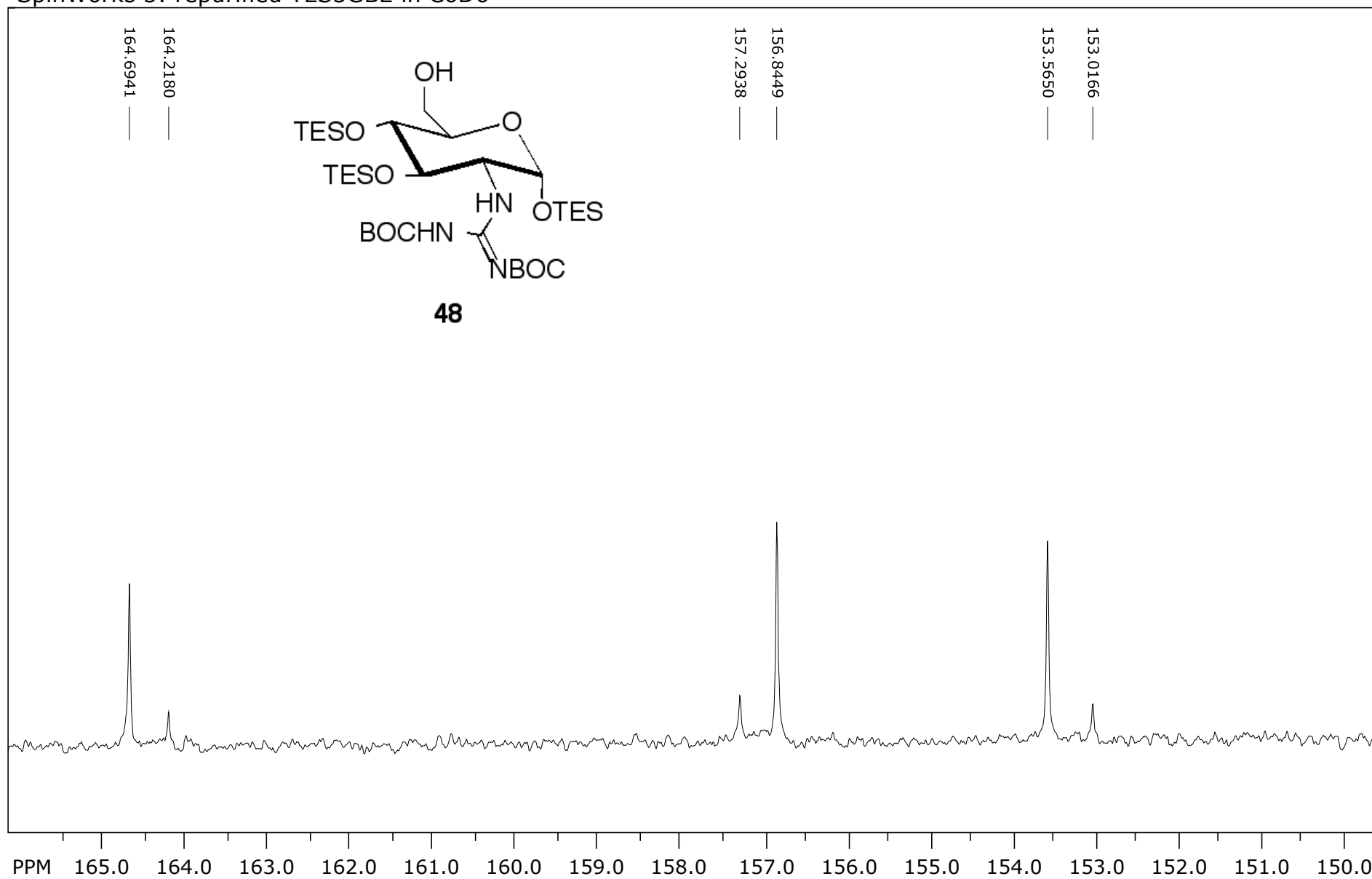
file: ..._11\6OHTES3GB2 repur in C6D6\1\fid expt: <zg>
 transmitter freq.: 499.853228 MHz
 time domain size: 32768 points
 width: 8012.82 Hz = 16.0303 ppm = 0.244532 Hz/pt
 number of scans: 64

freq. of 0 ppm: 499.850061 MHz
 processed size: 16384 complex points
 LB: 0.000 GF: 0.0000
 Hz/cm: 11.682 ppm/cm: 0.02337



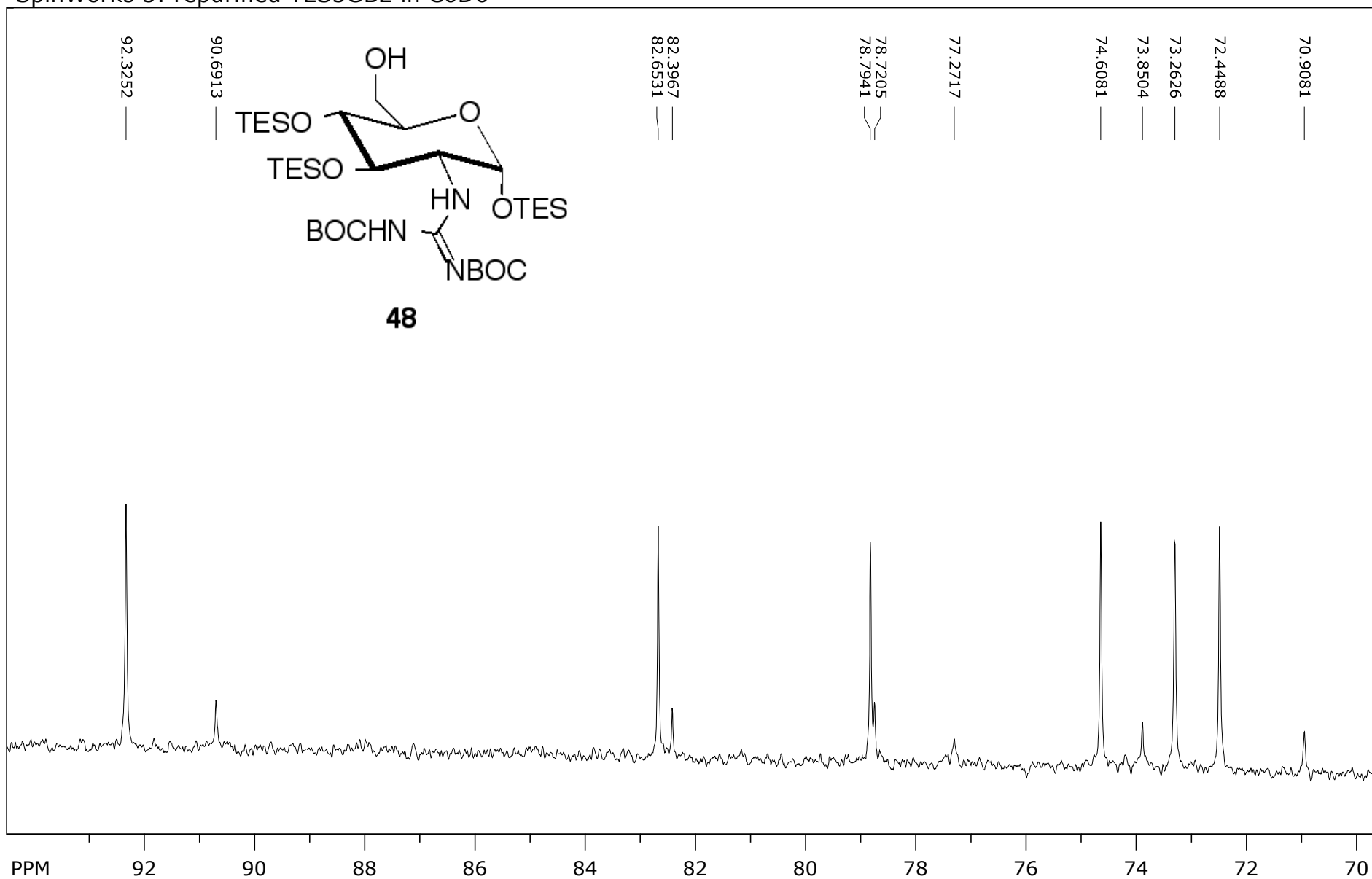
file: ..._11\6OHTES3GB2 repur in C6D6\2\fid expt: <zgpg>
transmitter freq.: 125.699901 MHz
time domain size: 65536 points
width: 27777.78 Hz = 220.9849 ppm = 0.423855 Hz/pt
number of scans: 5120

freq. of 0 ppm: 125.687357 MHz
processed size: 32768 complex points
LB: 3.500 GF: 0.0000
Hz/cm: 846.939 ppm/cm: 6.73779



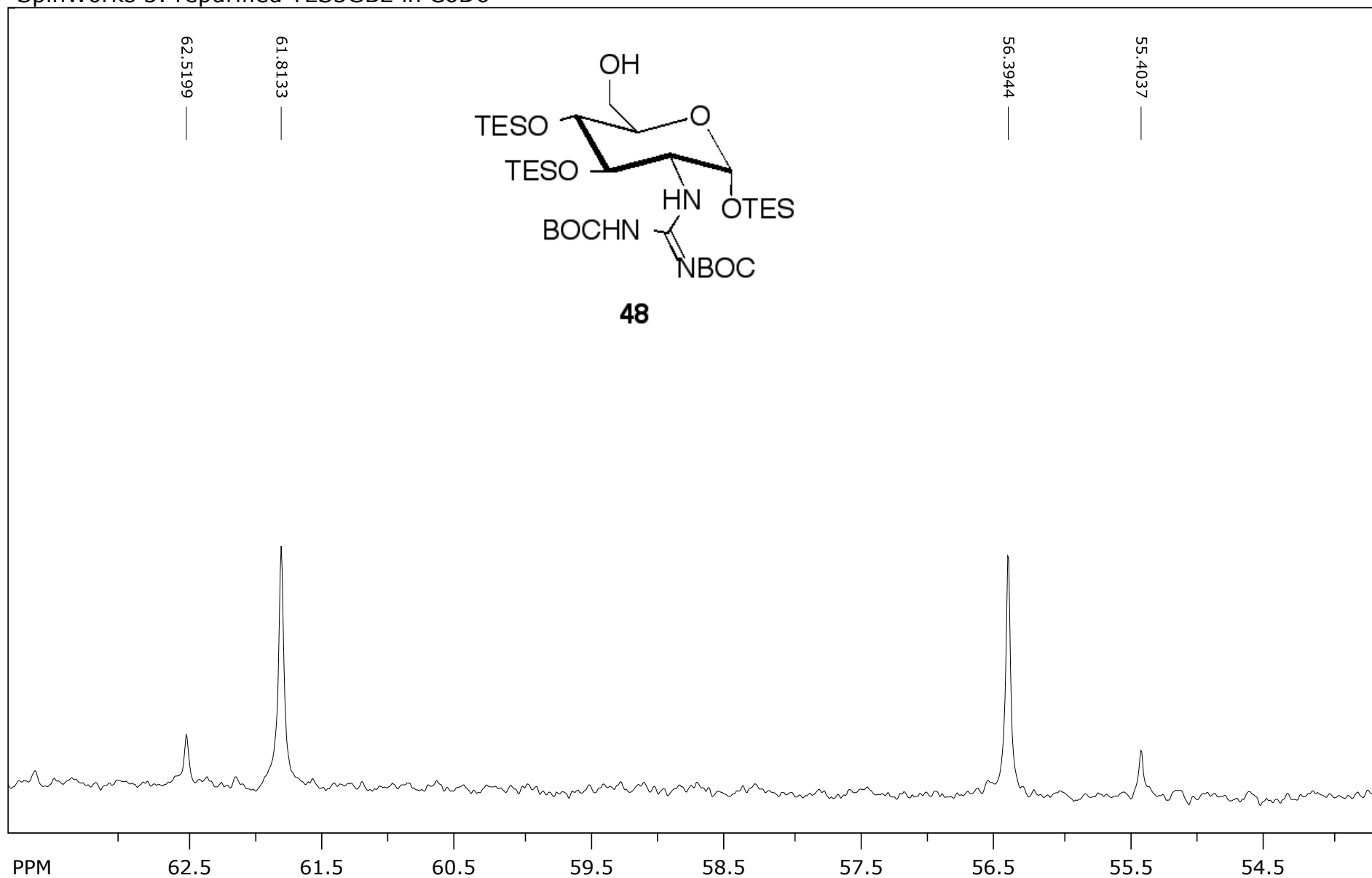
file: ..._11\6OHTES3GB2 repur in C6D6\2\fid expt: <zpgg>
transmitter freq.: 125.699901 MHz
time domain size: 65536 points
width: 27777.78 Hz = 220.9849 ppm = 0.423855 Hz/pt
number of scans: 5120

freq. of 0 ppm: 125.687357 MHz
processed size: 32768 complex points
LB: 3.500 GF: 0.0000
Hz/cm: 83.435 ppm/cm: 0.66377



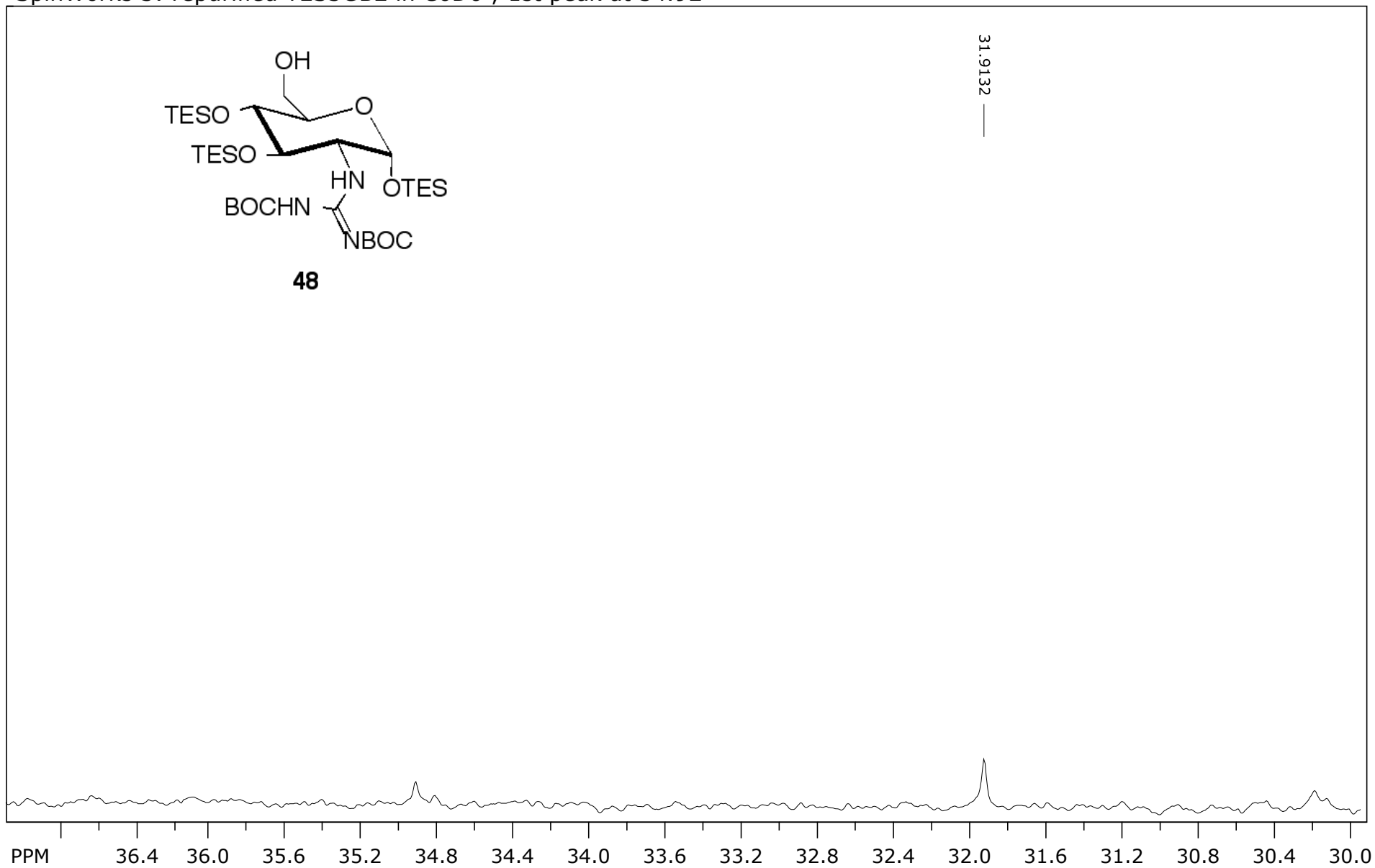
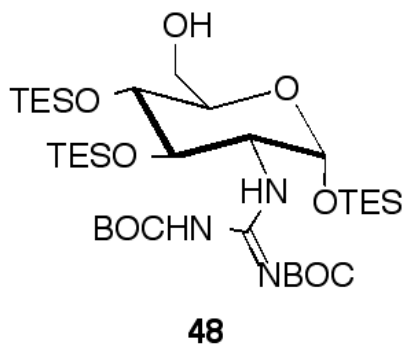
file: ..._11\6OHTES3GB2 repur in C6D6\2\fid expt: <zpgp>
transmitter freq.: 125.699901 MHz
time domain size: 65536 points
width: 27777.78 Hz = 220.9849 ppm = 0.423855 Hz/pt
number of scans: 5120

freq. of 0 ppm: 125.687357 MHz
processed size: 32768 complex points
LB: 3.500 GF: 0.0000
Hz/cm: 125.386 ppm/cm: 0.99750



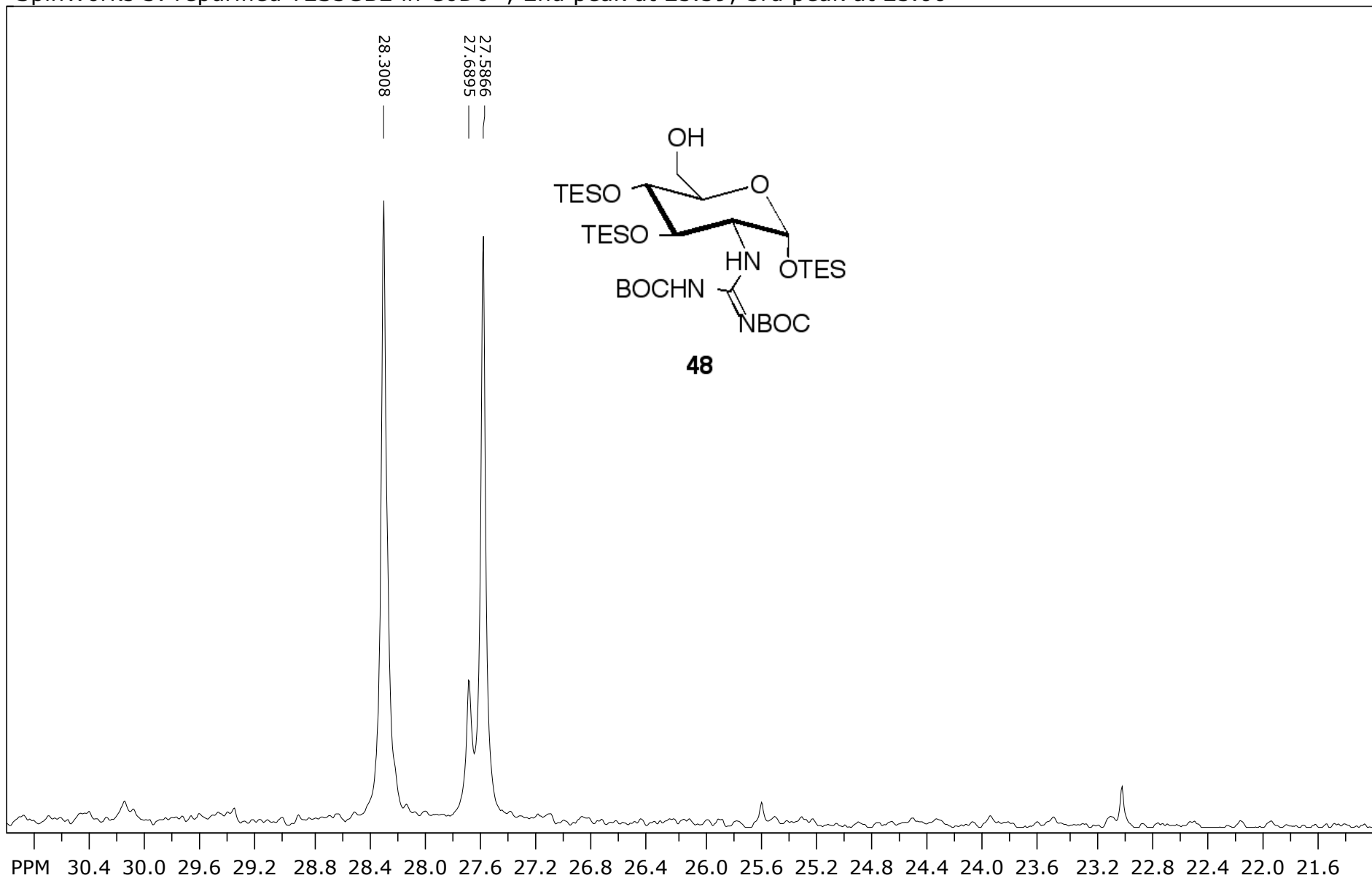
file: ..._11\6OHTES3GB2 repur in C6D6\2\fid expt: <zgpg>
transmitter freq.: 125.699901 MHz
time domain size: 65536 points
width: 27777.78 Hz = 220.9849 ppm = 0.423855 Hz/pt
number of scans: 5120

freq. of 0 ppm: 125.687357 MHz
processed size: 32768 complex points
LB: 3.500 GF: 0.0000
Hz/cm: 51.367 ppm/cm: 0.40865



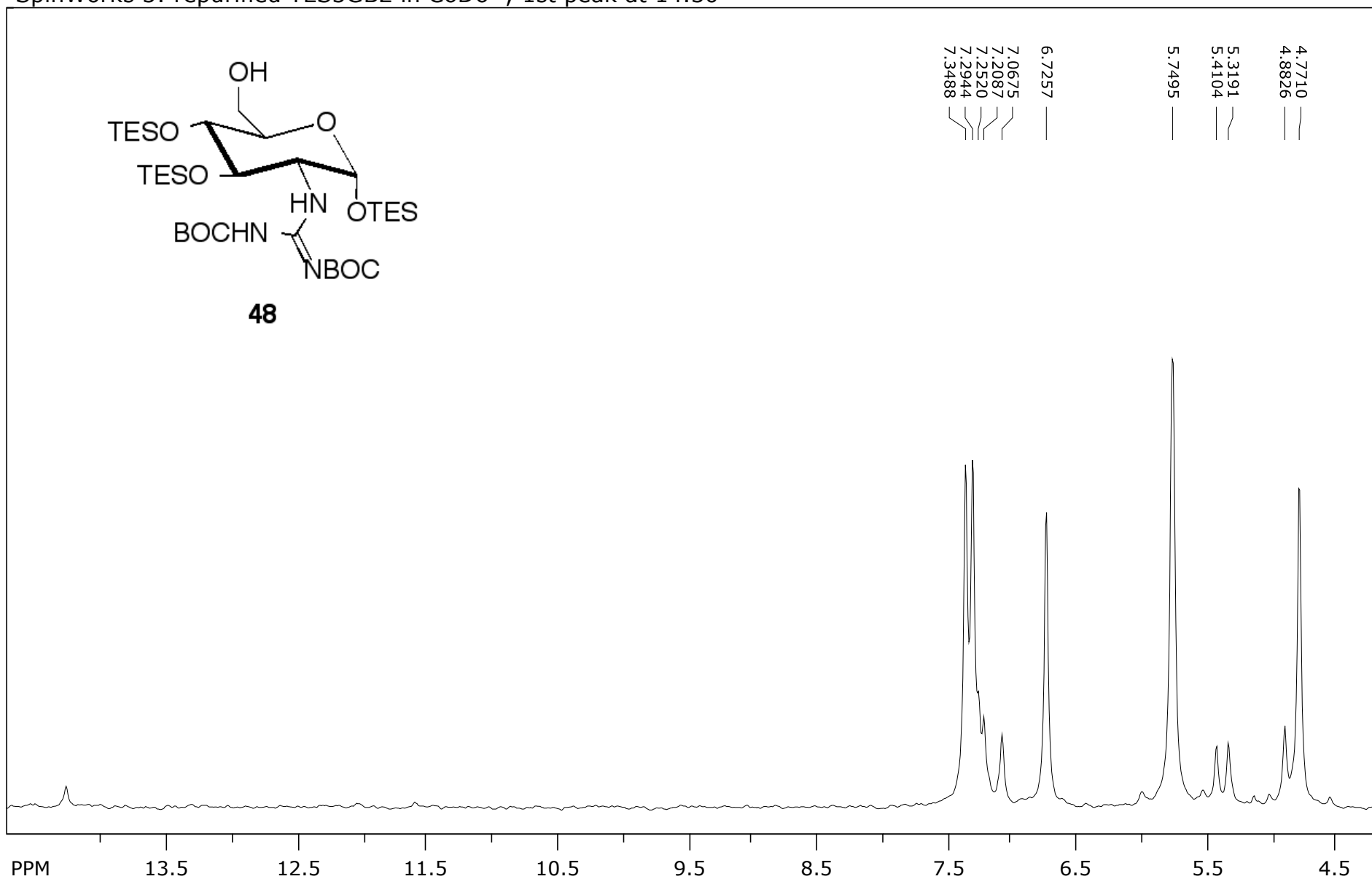
file: ..._11\6OHTES3GB2 repur in C6D6\2\fid expt: <zggp>
transmitter freq.: 125.699901 MHz
time domain size: 65536 points
width: 27777.78 Hz = 220.9849 ppm = 0.423855 Hz/pt
number of scans: 5120

freq. of 0 ppm: 125.687357 MHz
processed size: 32768 complex points
LB: 3.500 GF: 0.0000
Hz/cm: 36.079 ppm/cm: 0.28702



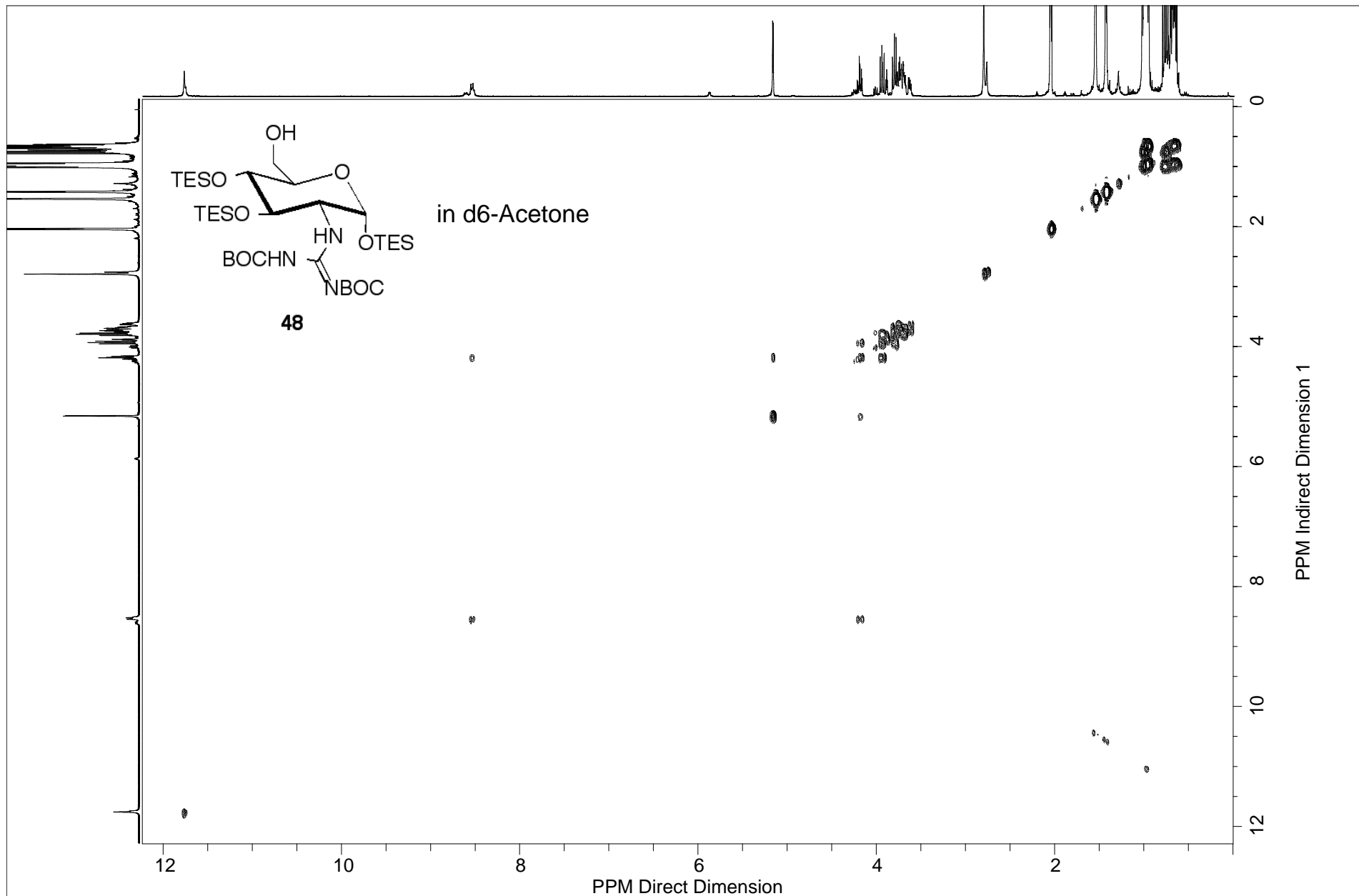
file: ..._11\6OHOTES3GB2 repur in C6D6\2\fid expt: <zpgg>
transmitter freq.: 125.699901 MHz
time domain size: 65536 points
width: 27777.78 Hz = 220.9849 ppm = 0.423855 Hz/pt
number of scans: 5120

freq. of 0 ppm: 125.687357 MHz
processed size: 32768 complex points
LB: 3.500 GF: 0.0000
Hz/cm: 49.532 ppm/cm: 0.39405



file: ..._11\6OHTES3GB2 repur in C6D6\2\fid expt: <zpgg>
transmitter freq.: 125.699901 MHz
time domain size: 65536 points
width: 27777.78 Hz = 220.9849 ppm = 0.423855 Hz/pt
number of scans: 5120

freq. of 0 ppm: 125.687357 MHz
processed size: 32768 complex points
LB: 3.500 GF: 0.0000
Hz/cm: 53.297 ppm/cm: 0.42400



6-OH-TES3GB2_in_CO(CD3)2 (32993)

USER: JR -- DATE: Sep 21, 2009 18:14:58

F1: 399.785

F2: 399.785

SW1: 5597

SW2: 5597

OF1: 2398.7

OF2: 2398.7

PTS1d: 1024

1024

PTS2d: 256

512

EX: cosy_pfg.ex2

PW: 13.9us, 90deg

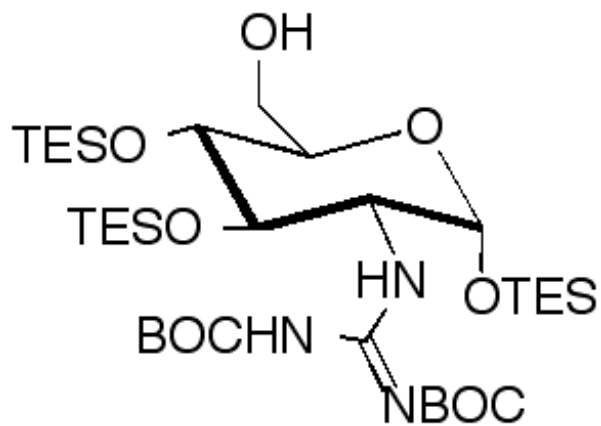
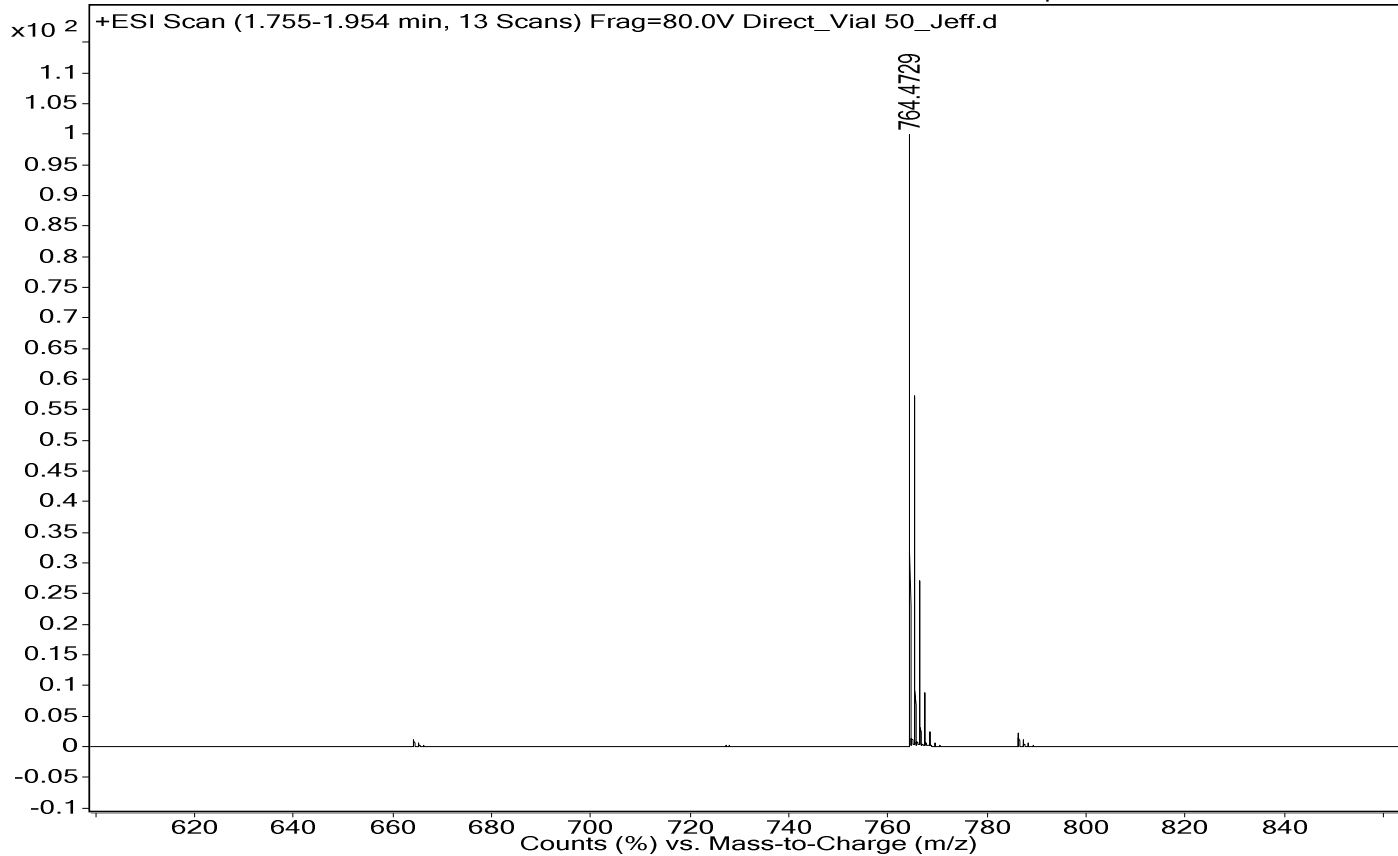
PD: 2.0 sec

NA: 2

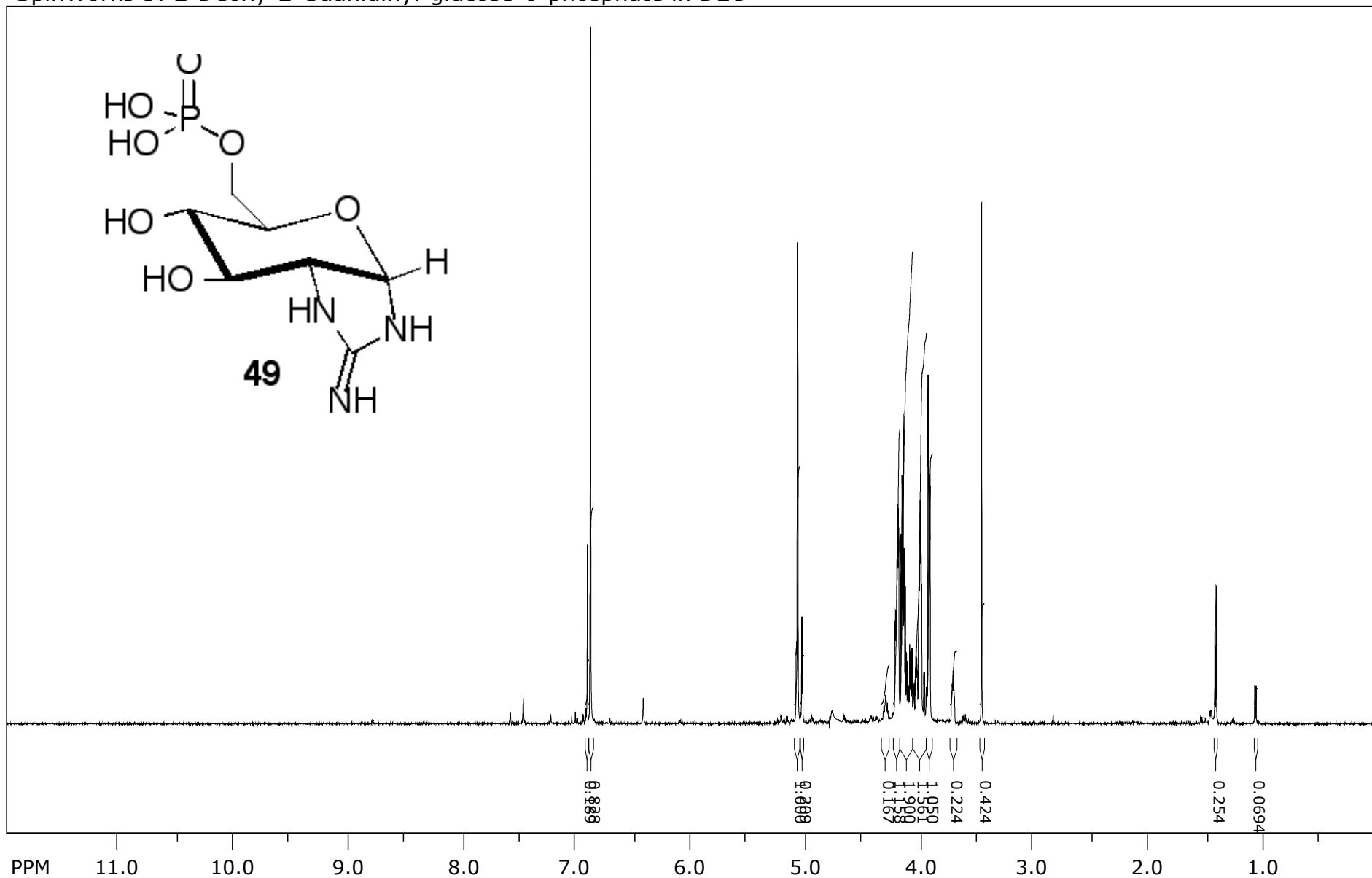
LB: 0.0

Nuts - \$\$fh090921_COSY-2.jdf

Sample Name	Jeff 50	Position	Vial 50	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 50_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 2:29:31 PM

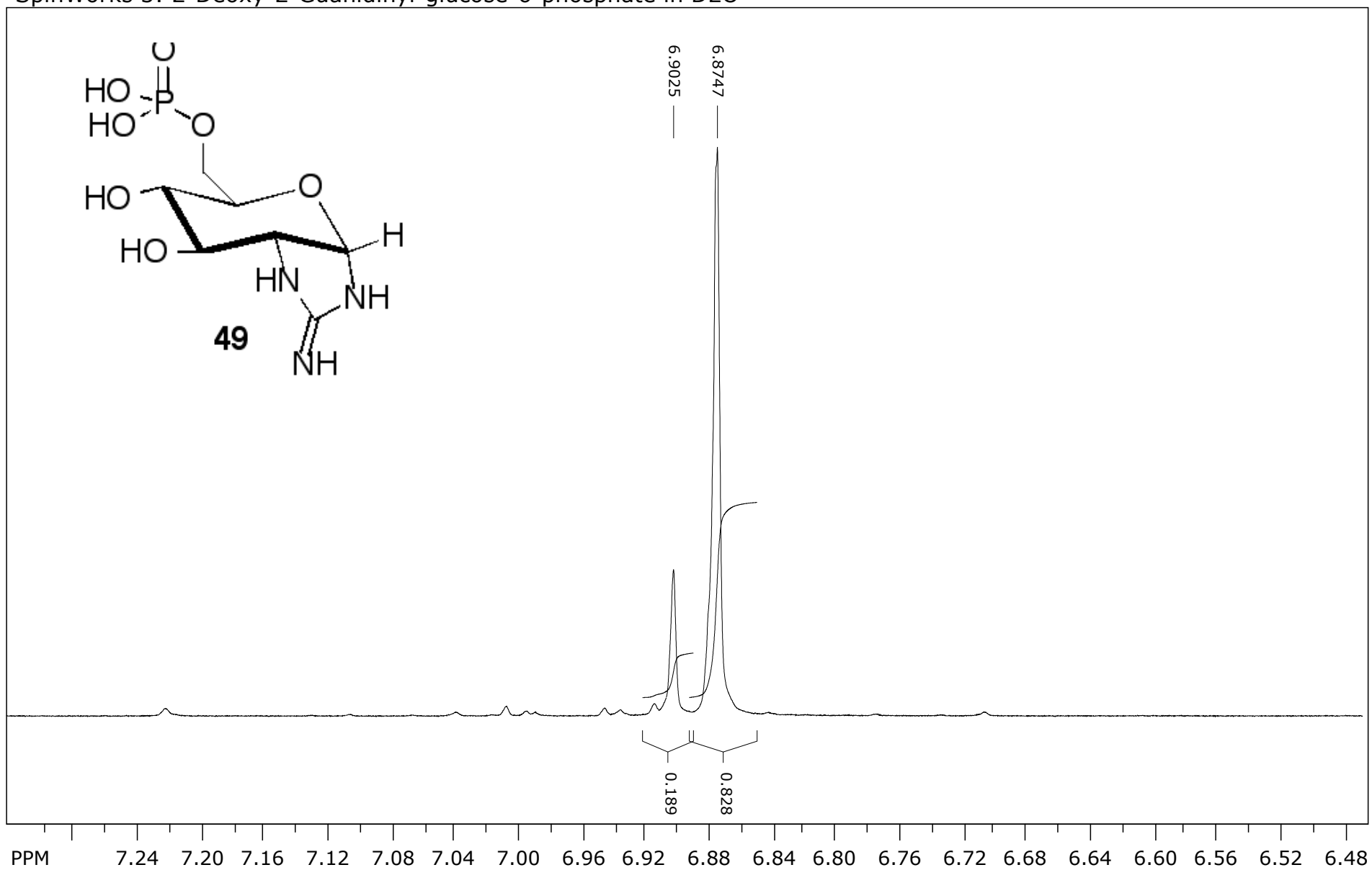


48



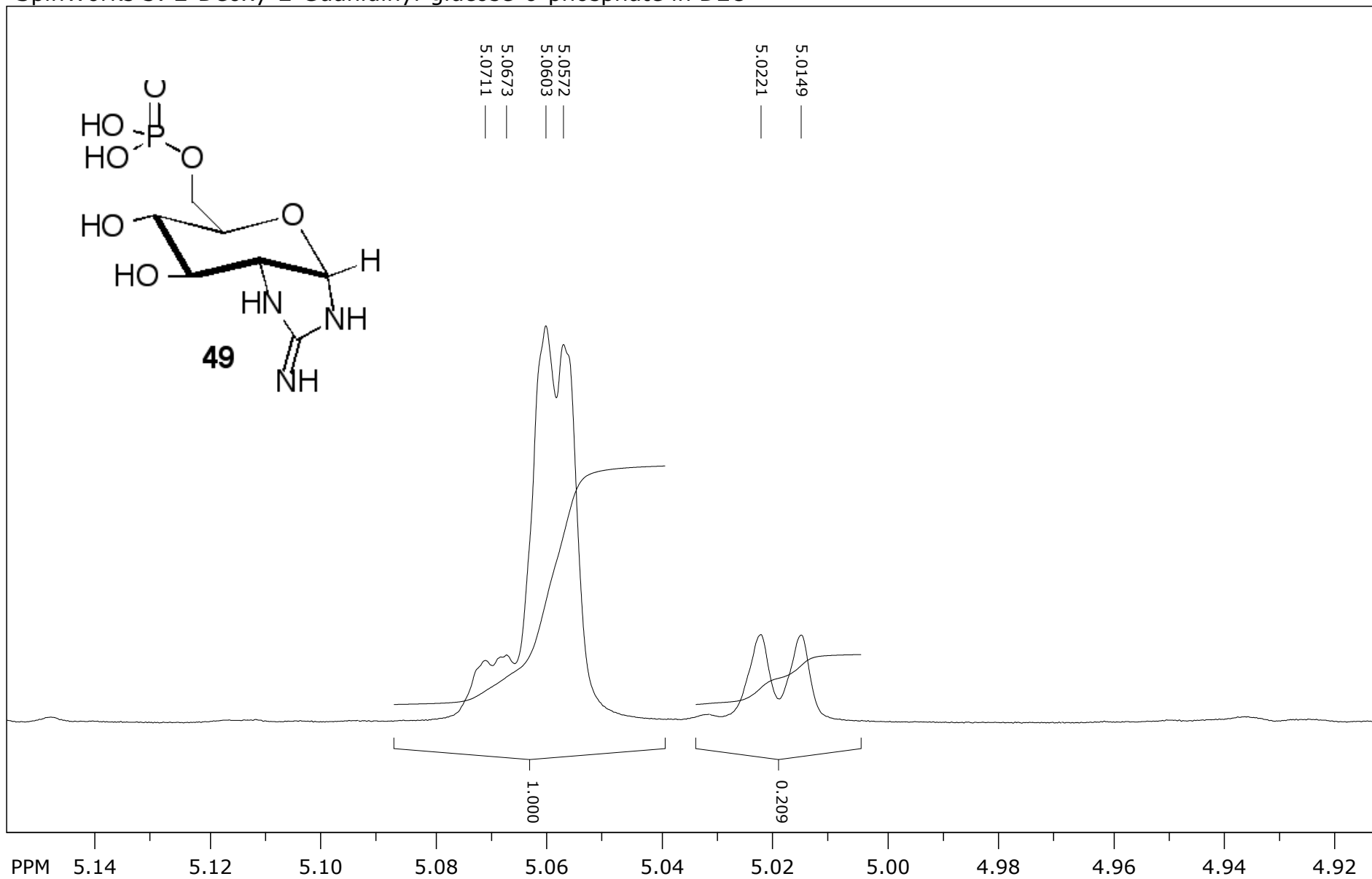
file: ...der\NMR Data\Guan6P_finalD2O\2\fid expt: <zgr>
transmitter freq.: 600.552832 MHz
time domain size: 65536 points
width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.549962 MHz
processed size: 262144 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 289.105 ppm/cm: 0.48140



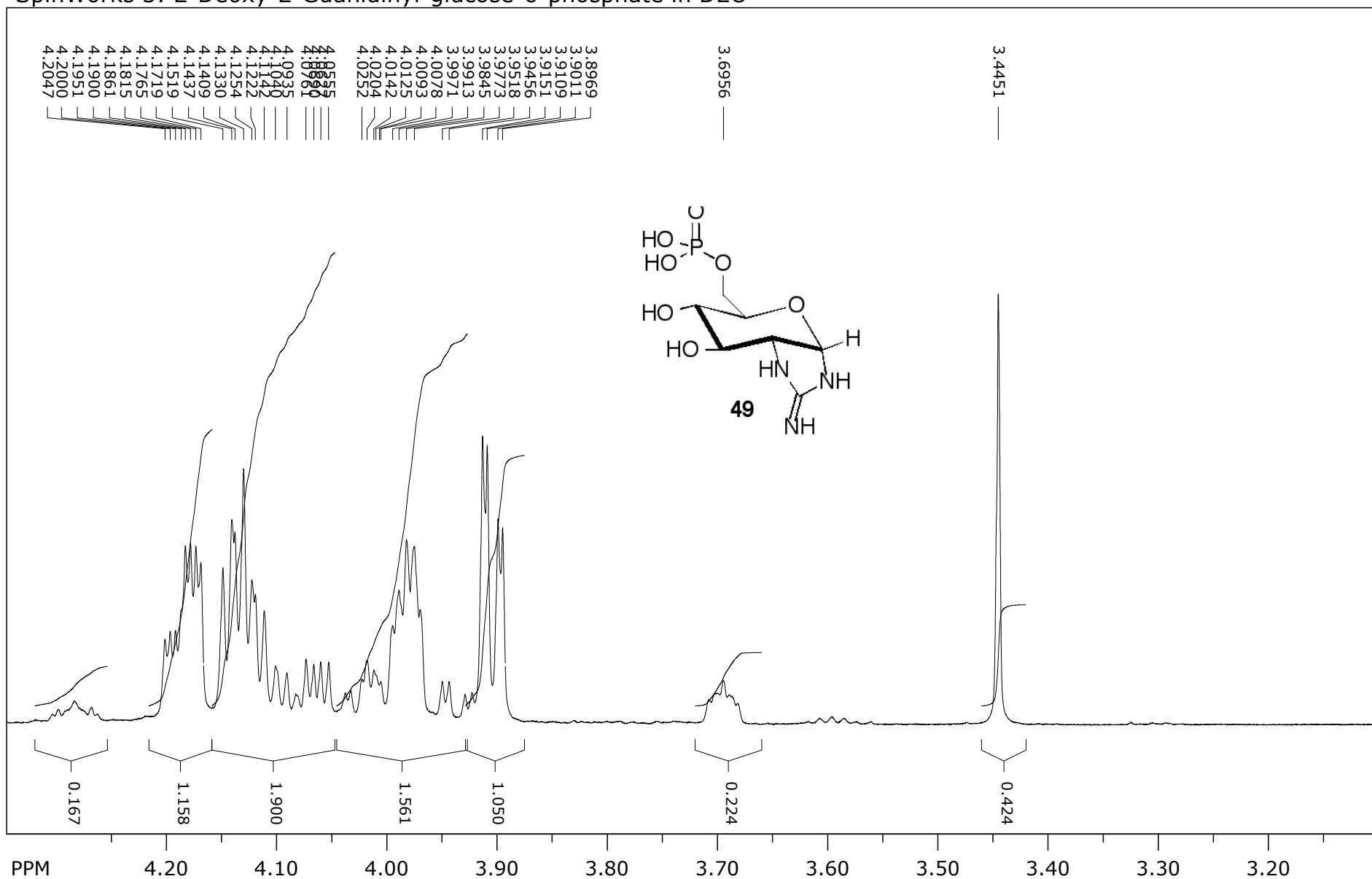
file: ...der\NMR Data\Guan6P_finalD2O\2\fid exp: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 65536 points
width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.549962 MHz
processed size: 262144 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 20.604 ppm/cm: 0.03431



file: ...der\NMR Data\Guan6P_finalD2O\2\fid expt: <zgpr>
transmitter freq.: 600.552832 MHz
time domain size: 65536 points
width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
number of scans: 32

freq. of 0 ppm: 600.549962 MHz
processed size: 262144 complex points
LB: 5.000 GF: 0.0000
Hz/cm: 5.863 ppm/cm: 0.00976

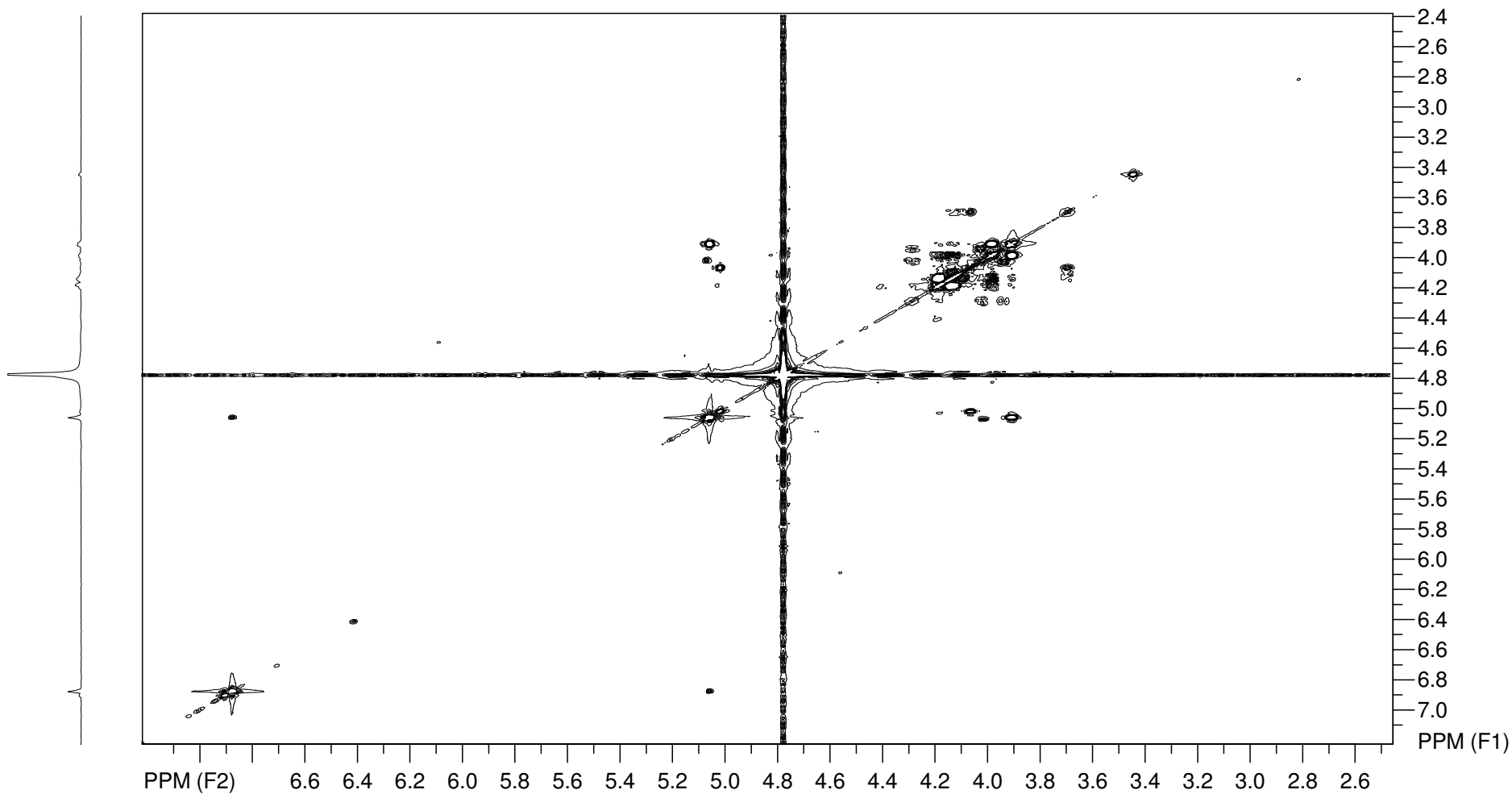
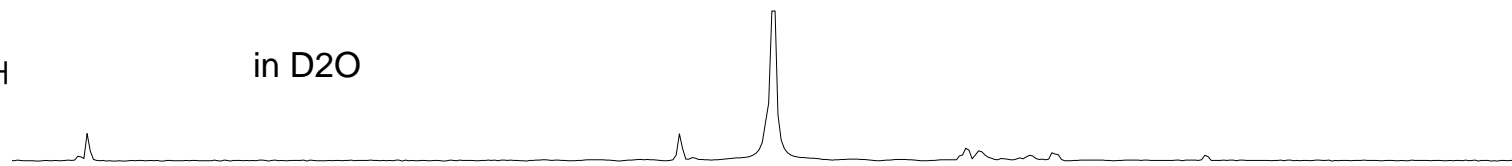
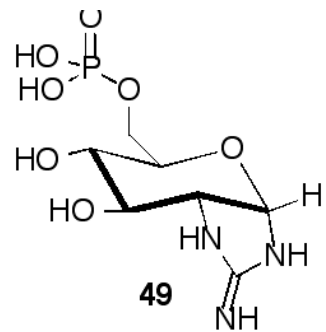


file: ...der\NMR Data\Guan6P_finalD2O\2\fid exp: <zgpr>
 transmitter freq.: 600.552832 MHz
 time domain size: 65536 points
 width: 9615.38 Hz = 16.0109 ppm = 0.146719 Hz/pt
 number of scans: 32

freq. of 0 ppm: 600.549962 MHz
 processed size: 262144 complex points
 LB: 5.000 GF: 0.0000
 Hz/cm: 30.048 ppm/cm: 0.05003

): COSYPHPR

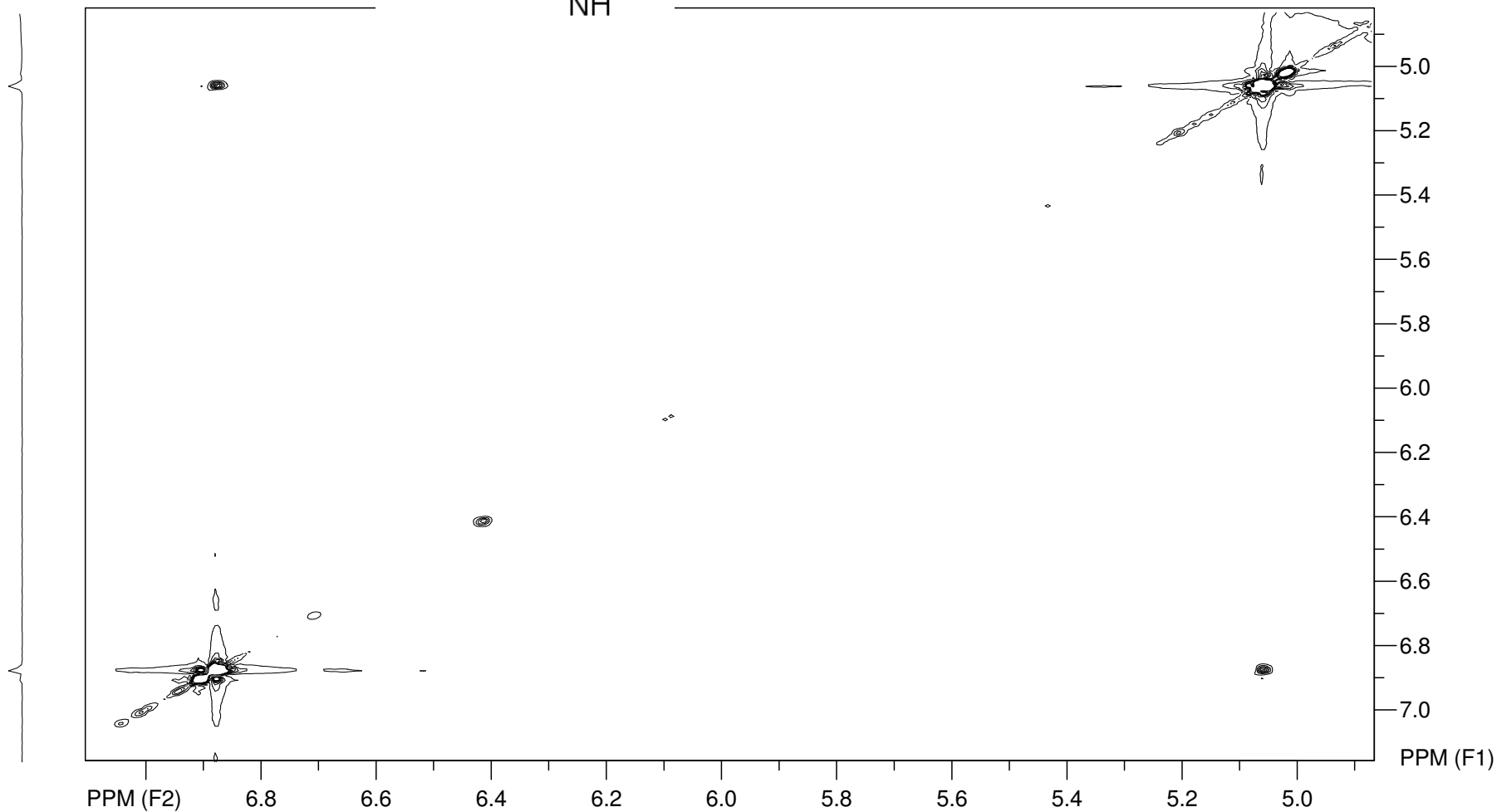
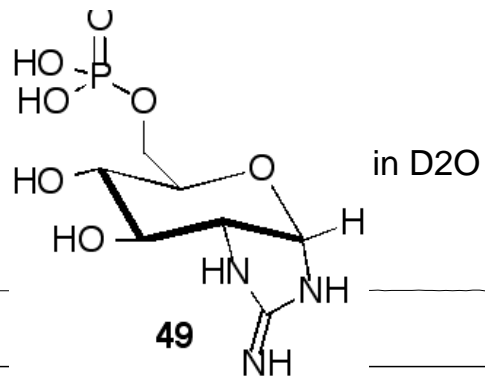
in D2O



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\Guan6PCOSY9_21_2\ser exp: <cosygpqf>
 transmitter freq.: 600.553566 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.58 Hz = 10.006793 ppm = 2.934365 Hz/pt
 number of scans: 1

F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 139.532 ppm/cm: 0.23234

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 242.633 ppm/cm: 0.40402

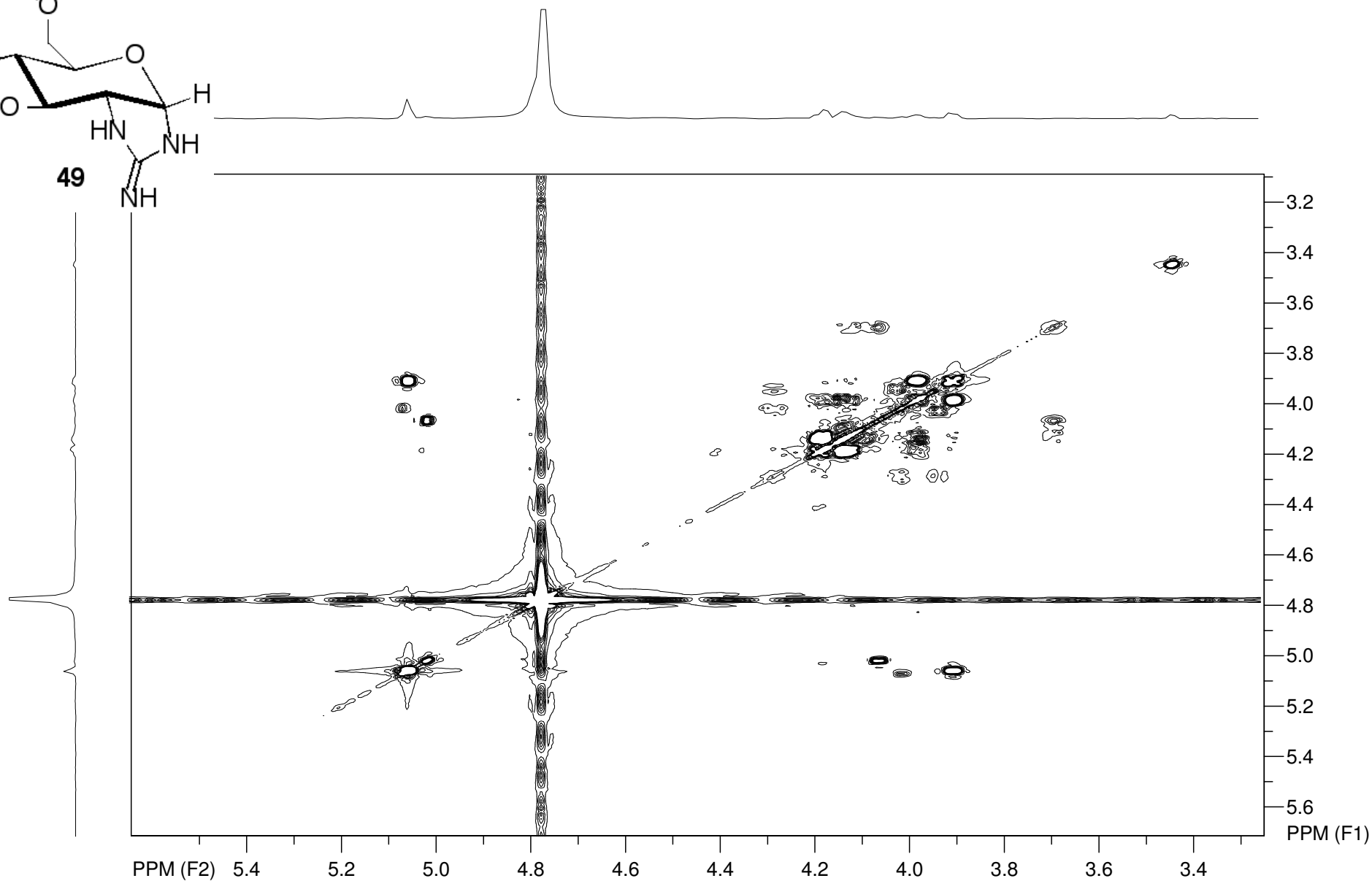
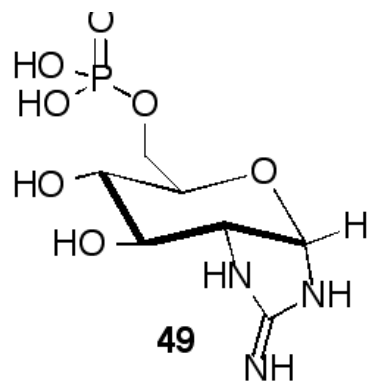


file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\Guan6PCOSY9_21_2\ser exp: <cosygpqf>
 transmitter freq.: 600.553566 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.58 Hz = 10.006793 ppm = 2.934365 Hz/pt
 number of scans: 1

F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 65.595 ppm/cm: 0.10922

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 117.093 ppm/cm: 0.19498

2-Deoxy-2-Guanidinyglucose-6-phosphate in D2O



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\Guan6PCOSY9_21\2\ser exp: <cosygpqf>
 transmitter freq.: 600.553566 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.58 Hz = 10.006793 ppm = 2.934365 Hz/pt
 number of scans: 1

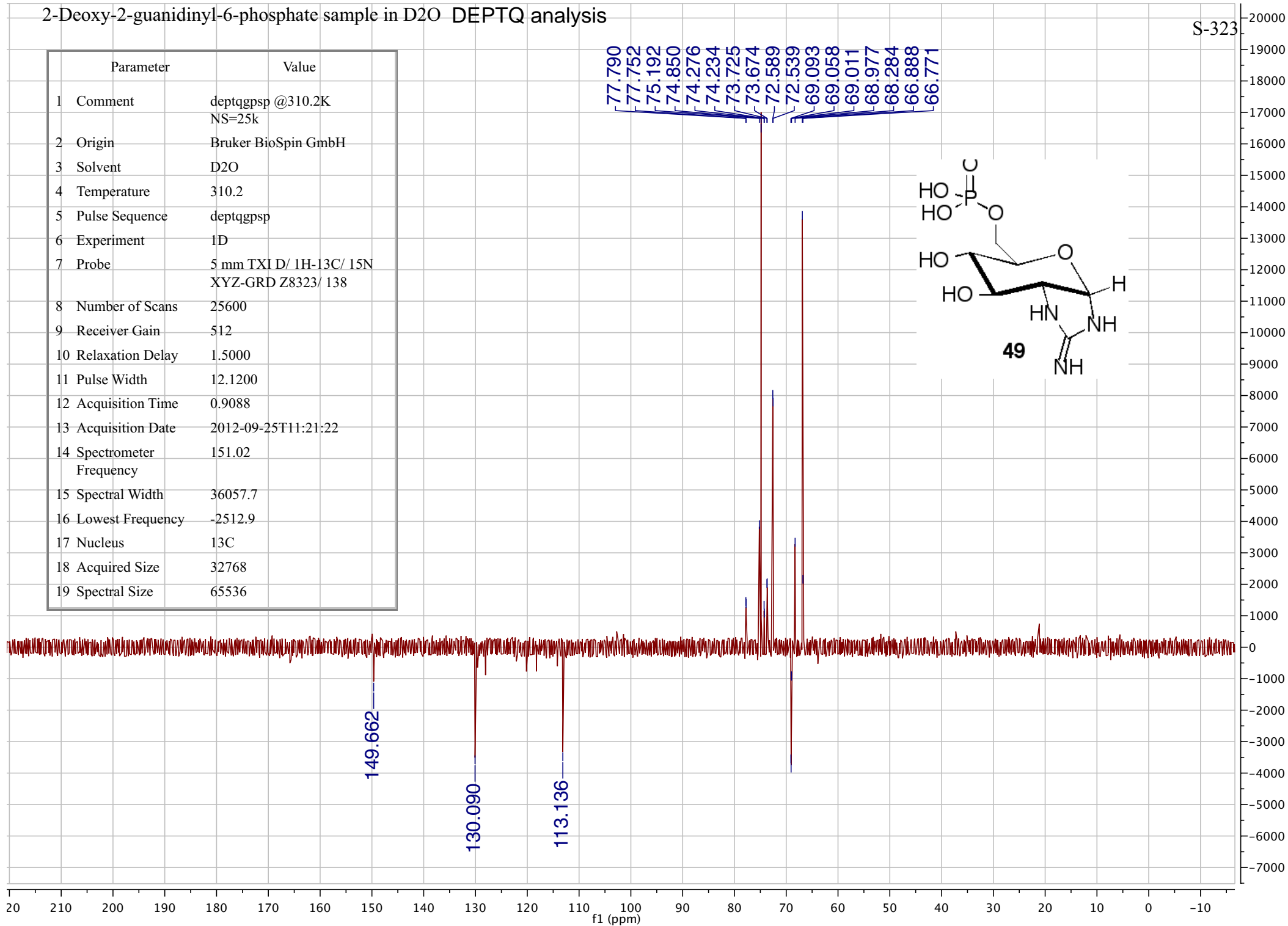
F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 70.106 ppm/cm: 0.11673

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 131.450 ppm/cm: 0.21888

2-Deoxy-2-guanidiny-6-phosphate sample in D2O DEPTQ analysis

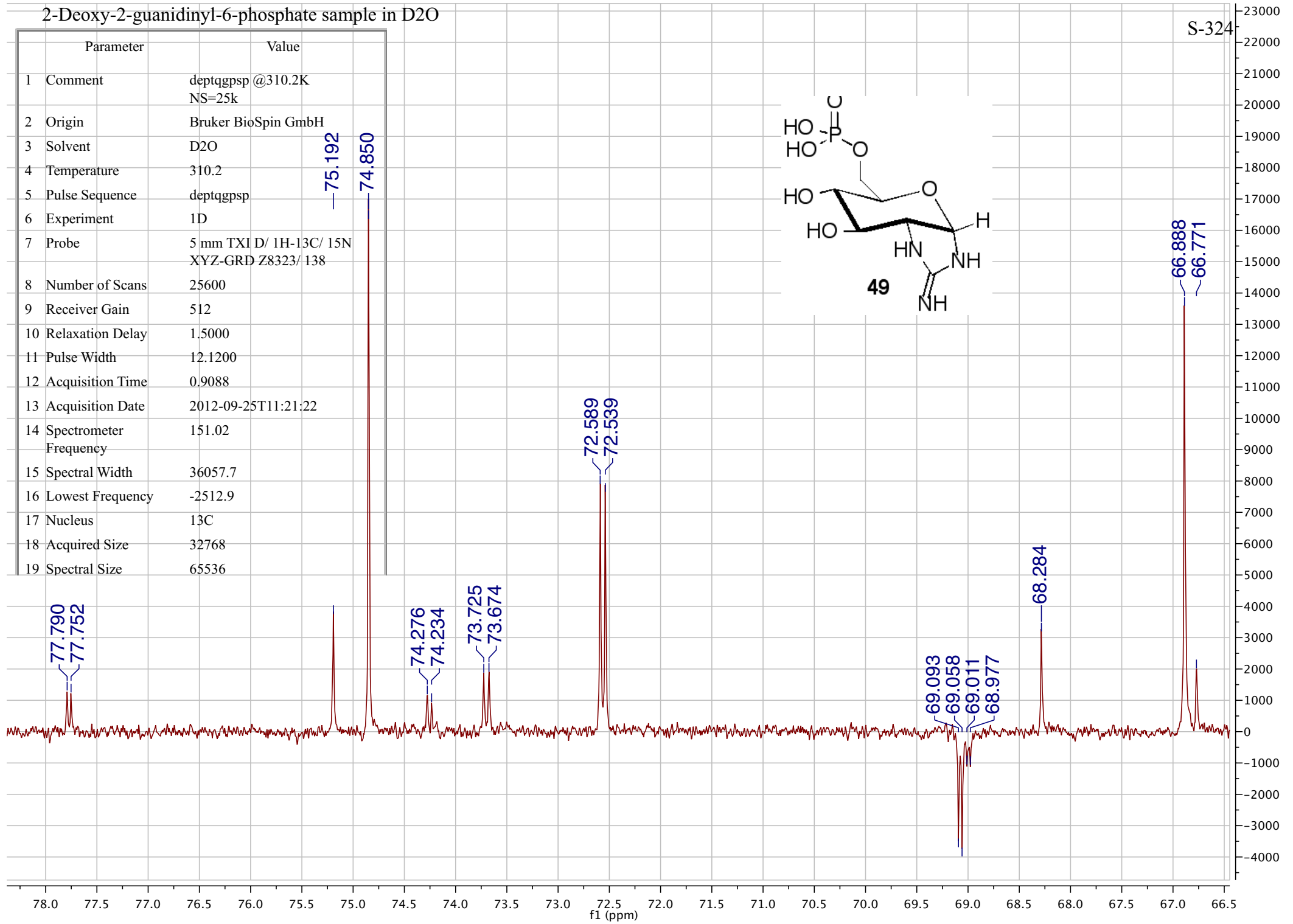
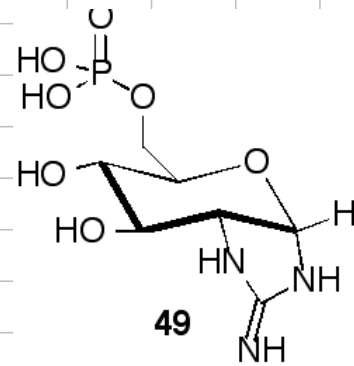
S-323

Parameter	Value
1 Comment	deptqgsp @310.2K NS=25k
2 Origin	Bruker BioSpin GmbH
3 Solvent	D2O
4 Temperature	310.2
5 Pulse Sequence	deptqgsp
6 Experiment	1D
7 Probe	5 mm TXI D/ 1H-13C/ 15N XYZ-GRD Z8323/ 138
8 Number of Scans	25600
9 Receiver Gain	512
10 Relaxation Delay	1.5000
11 Pulse Width	12.1200
12 Acquisition Time	0.9088
13 Acquisition Date	2012-09-25T11:21:22
14 Spectrometer Frequency	151.02
15 Spectral Width	36057.7
16 Lowest Frequency	-2512.9
17 Nucleus	13C
18 Acquired Size	32768
19 Spectral Size	65536

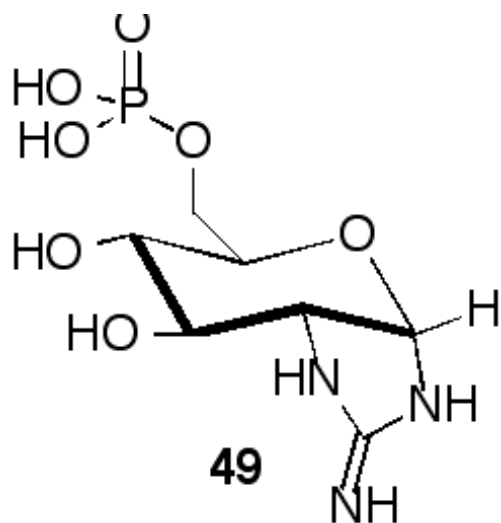
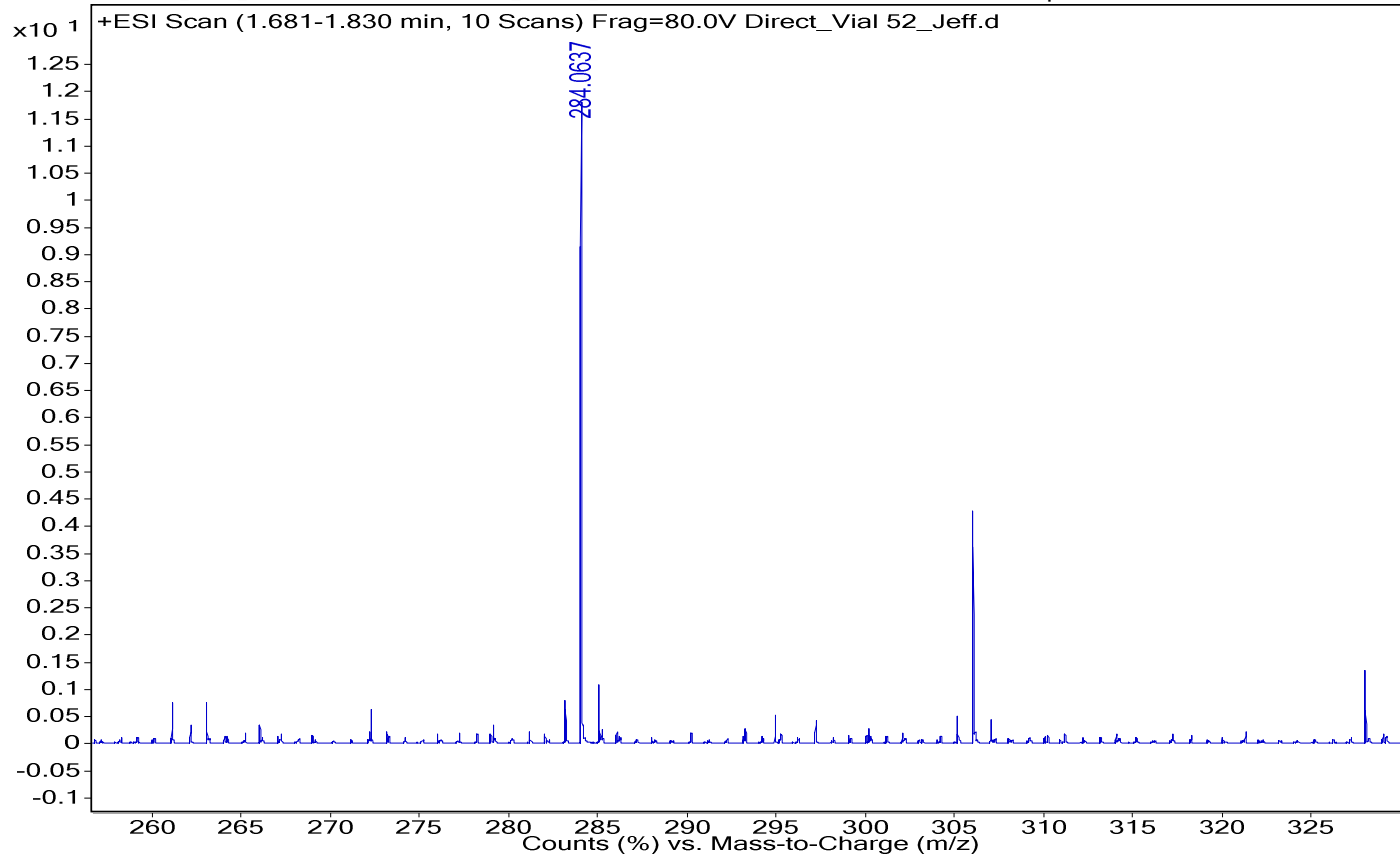


2-Deoxy-2-guanidiny-6-phosphate sample in D2O

Parameter	Value
1 Comment	deptqgsp @310.2K NS=25k
2 Origin	Bruker BioSpin GmbH
3 Solvent	D2O
4 Temperature	310.2
5 Pulse Sequence	deptqgsp
6 Experiment	1D
7 Probe	5 mm TXI D/ 1H-13C/ 15N XYZ-GRD Z8323/ 138
8 Number of Scans	25600
9 Receiver Gain	512
10 Relaxation Delay	1.5000
11 Pulse Width	12.1200
12 Acquisition Time	0.9088
13 Acquisition Date	2012-09-25T11:21:22
14 Spectrometer Frequency	151.02
15 Spectral Width	36057.7
16 Lowest Frequency	-2512.9
17 Nucleus	13C
18 Acquired Size	32768
19 Spectral Size	65536

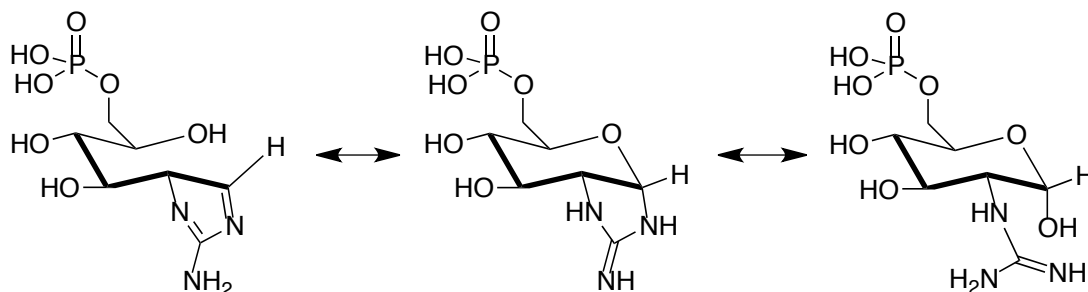


Sample Name	Jeff 52	Position	Vial 52	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	Success
Data Filename	Direct_Vial 52_Jeff.	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	8/17/2012 2:38:49 PM



Discussion of the NMR spectra of compound 49. The three doublets at 5-5.1 ppm are consistent with the C_1H of **49**, based on their COSY correlations and chemical shifts. The coupling values between 2.3-4.3 Hz indicate a shallow dihedral angle with C_2H . The (-) doublets at 69-69.1 ppm in the DEPTQ spectrum match that expected for (at least two) phosphate esters at C_6 with two attached protons and J_{C-P} of 5-5.3 Hz. 1C_5 (single attached proton) is also expected to exhibit J_{C-P} coupling and thus the three (+) doublets at 72.6 (d, $J=7.5$ Hz), 73.7 (d, $J=7.6$ Hz), and 74.3 (d, $J=7.5$ Hz) can plausibly be assigned to three distinct C_5 's. Finally, the (-) peaks at 113.1, 130.1 and 150.0 are consistent with three distinct central C 's, originating from the 'guanidine', which have no attached protons.

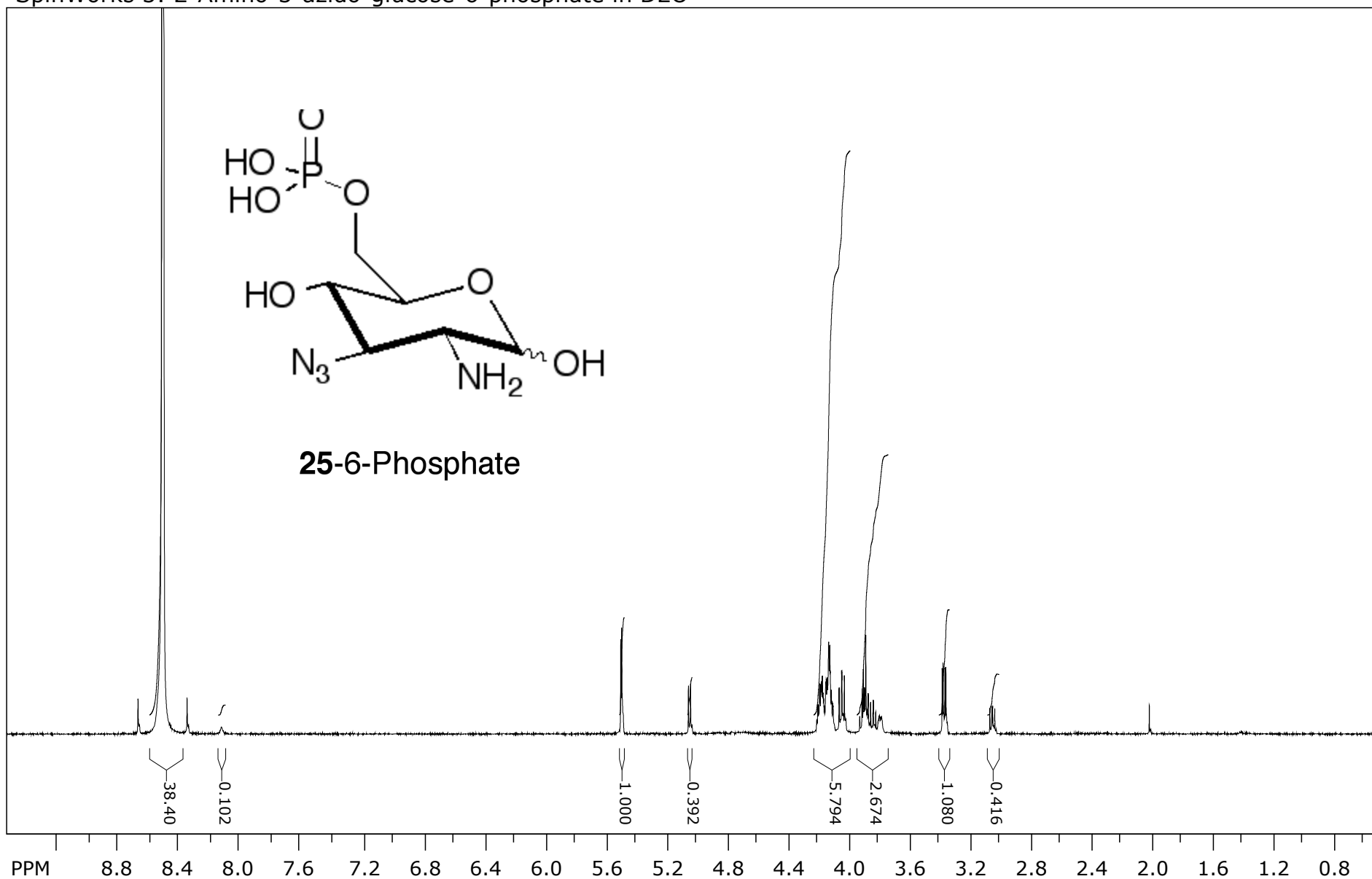
Figure S1. Proposed structures for the 3 species observed in the NMR spectra in **49**.



- (1) Gács-Baitz, E.; Sági, G.; Kajtár-Peredy, M. *Nucleosides, Nucleotides and Nucleic Acids* **2005**, *24*, 247-257.

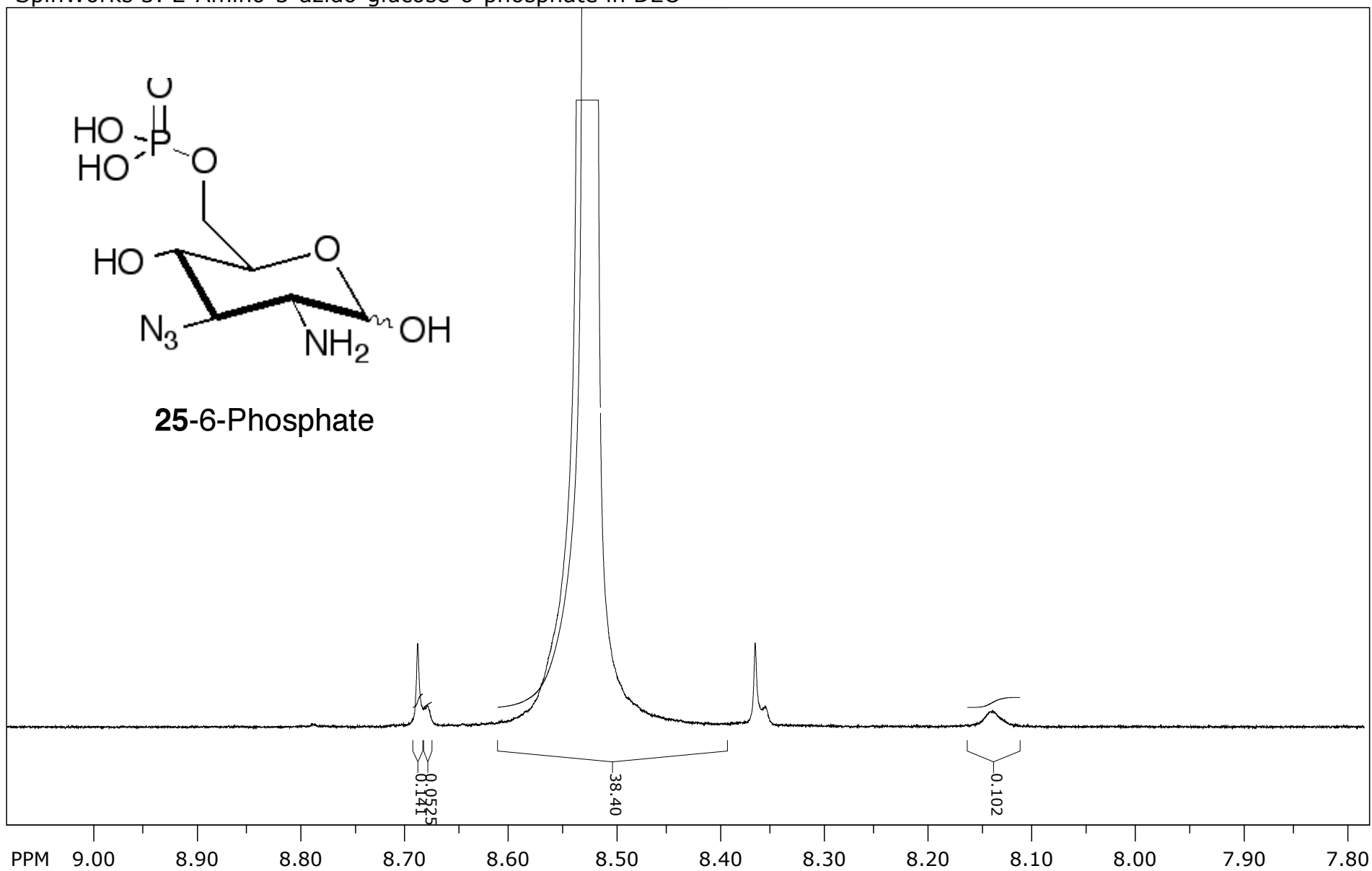
2-Amino-3-azido-2,3-dideoxyglucose-6-phosphate. The enzymatic phosphorylation followed that described by Guo and Frost.¹ A solution of **25** (as the TFA salt, 10 mg, 32 μmol), ATP (0.1 g), $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ (45 mg) and citric acid $\cdot \text{H}_2\text{O}$ (18 mg) in deionized H_2O (5 mL) was adjusted to $\text{pH}=8.0$ with 0.5N KOH. Three additions of yeast hexokinase (100 UN each) were made; one at the start, then at 10 h and 20 h. The pH was re-adjusted to 8 with 0.1N KOH after each addition. After 36 h, the sample was lyophilized and the phosphorylated product was isolated by anion exchange chromatography using ammonium formate. Final lyophilization (2x) afforded 12 mg of a white powder, which contained 24.5 equiv of ammonium formate, based on integration of the formate C-H and the combined anomeric protons; yield of 2-Amino-3-azido-2,3-dideoxyglucose-6-phosphate was 6.6 μmol (21%). ^1H NMR (D_2O , 600 MHz) δ : [α : β ratio = 1:0.4] 3.04 (dd, $J=11.0, 8.4$ Hz, 0.4H, $\text{H}\beta_2$), 3.36 (dd, $J=11.1, 3.6$ Hz, 1H, $\text{H}\alpha_2$), 3.75 to 3.93 (m, 2.8 H), 4.04 (dd, $J=11.0, 9.4$ Hz, 1H, $\text{H}\alpha_3$), 4.09 to 4.20 (m, 3.5 H), 5.04 (d, $J=8.4$ Hz, 0.4H, $\text{H}\beta_1$), 5.50 (d, $J=3.6$ Hz, 1H, $\text{H}\alpha_1$). The sample decomposed in solution over a period of days at room temperature and a ^{13}C -NMR spectrum was not obtained. HRMS $^m/z$ $[\text{C}_6\text{H}_{14}\text{N}_4\text{O}_7\text{P}]^+$ 285.0595 = Found 285.05860

- (1) Guo, J.; Frost, J. *Journal of the American Chemical Society* **2002**, *124*, 10642-10643.



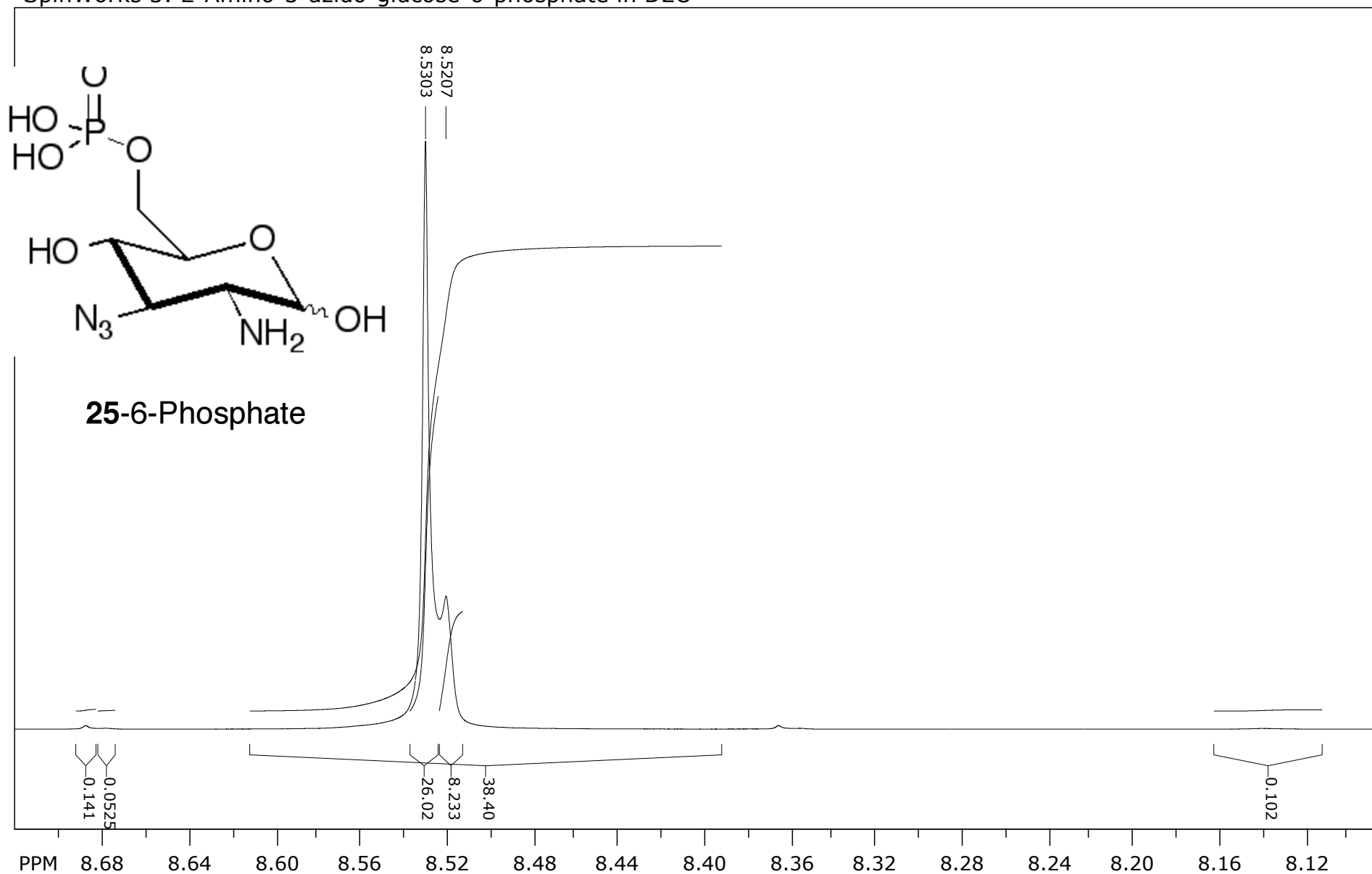
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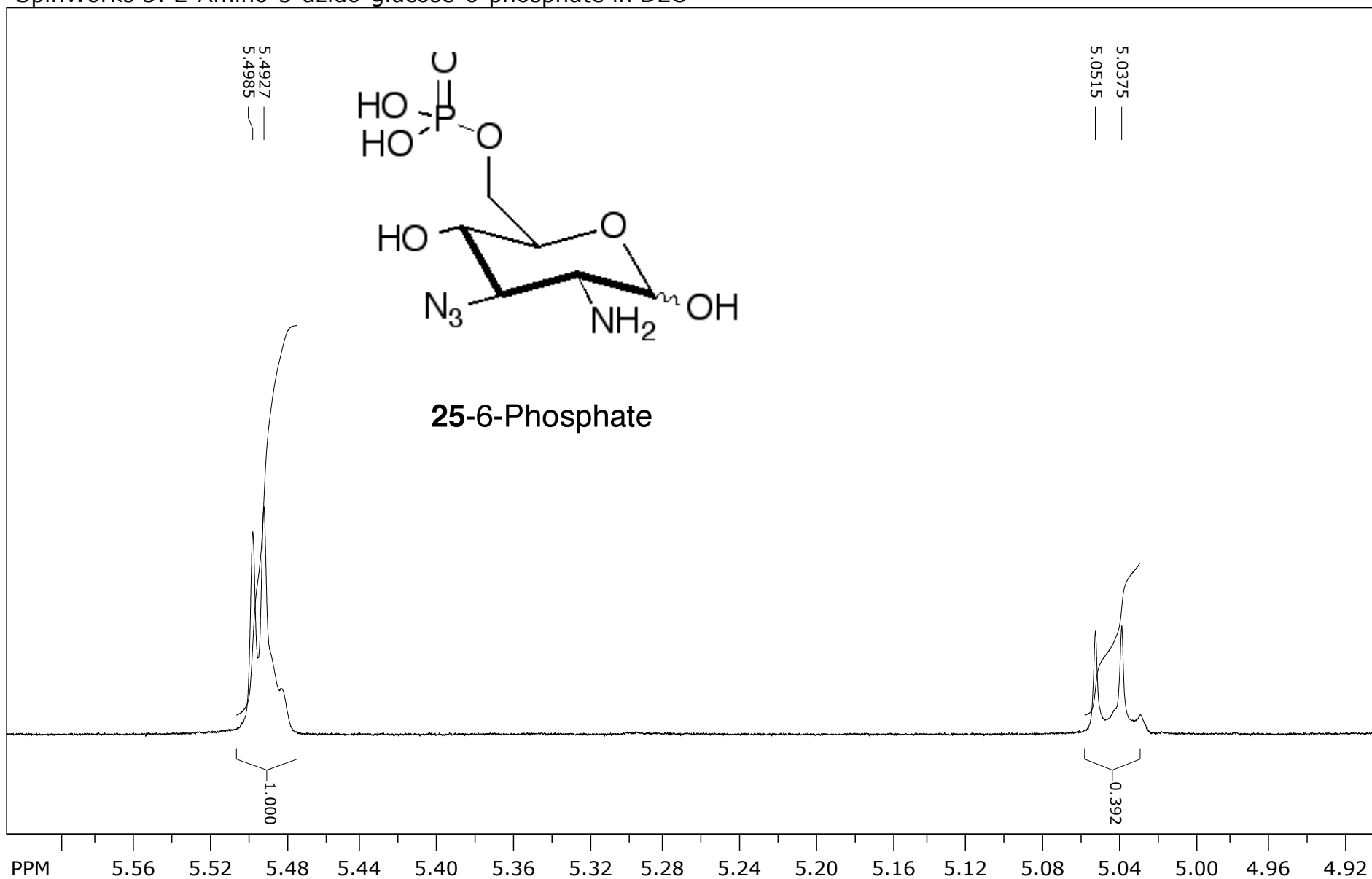
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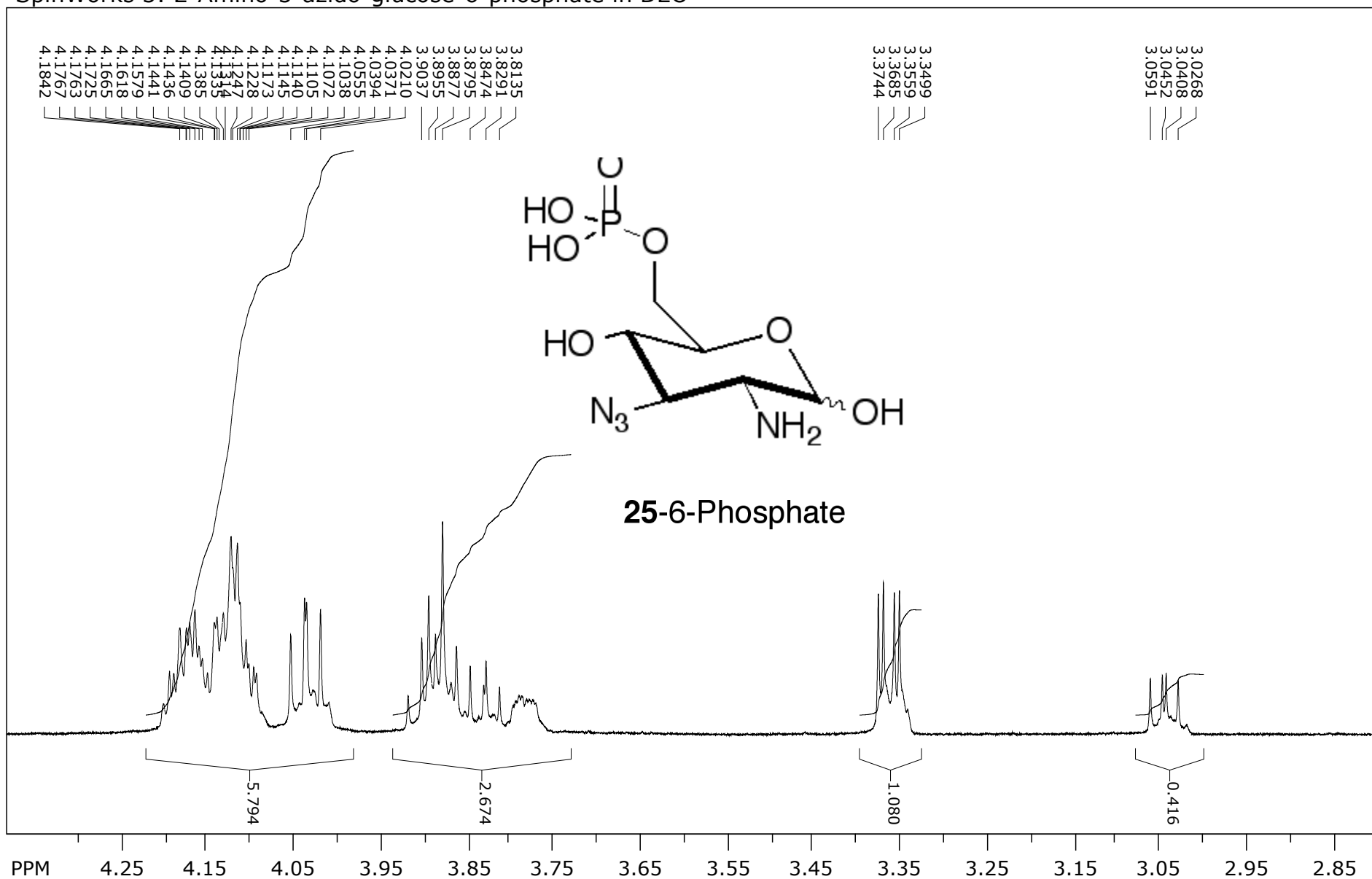
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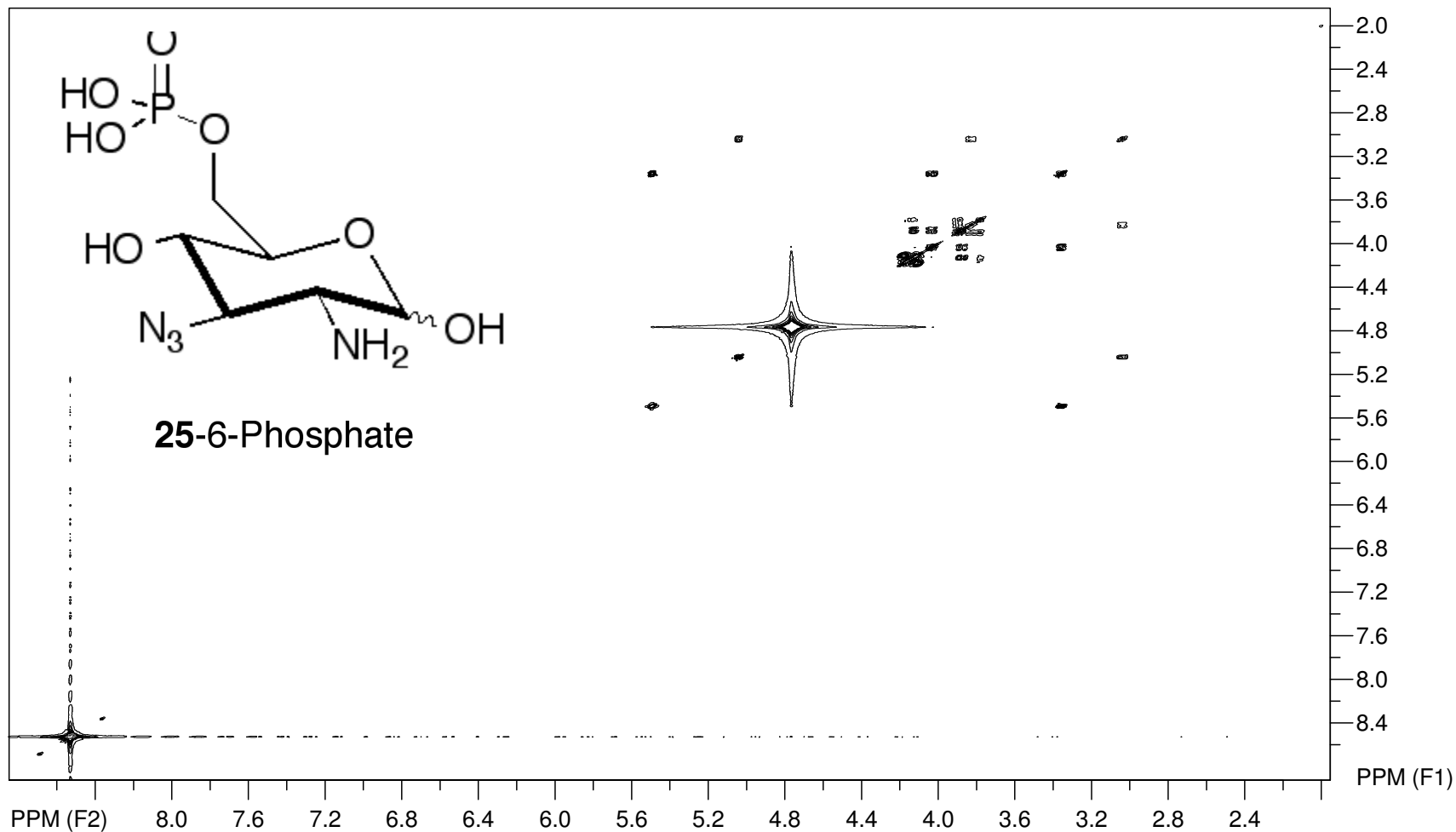
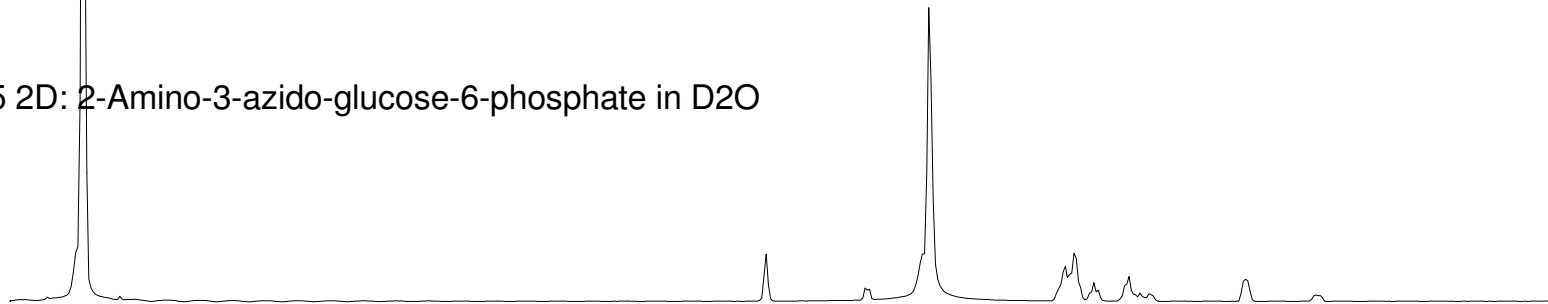
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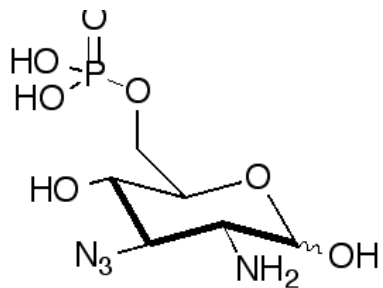
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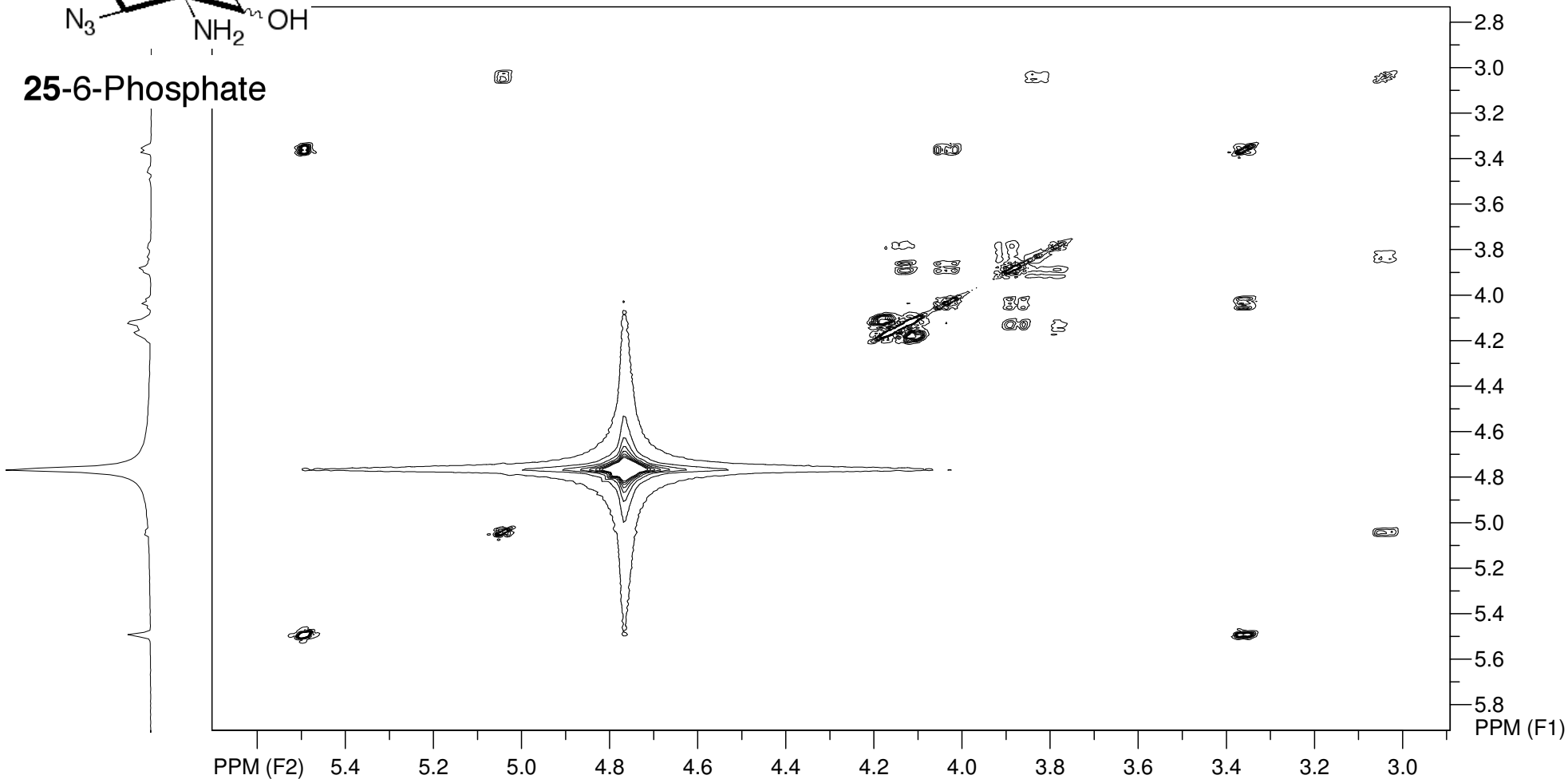
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 transmitter freq.: 600.553566 MHz
 time domain size: 2048 by 2048 points
 width (F2): 6009.58 Hz = 10.006793 ppm = 2.934365 Hz/pt
 number of scans: 1

F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 202.015 ppm/cm: 0.33638

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 354.757 ppm/cm: 0.59072



25-6-Phosphate



file: C:\Users\Jeff\Documents\NMR Folder\NMR Data\3N3GlcN6P_COSY\2\ser exp: <cosygpqf>
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 time domain size: 2048 by 2048 points
 width (F2): 6009.58 Hz = 10.006793 ppm = 2.934365 Hz/pt
 number of scans: 1

F2: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 82.344 ppm/cm: 0.13711

F1: freq. of 0 ppm: 600.549962 MHz
 processed size: 1024 complex points
 window function: Sine
 shift: 0.0 degrees
 Hz/cm: 159.188 ppm/cm: 0.26507

Sample Name	Jeff_isolHK	Position	Vial 1	Instrument Name	Instrument 1	User Name	DYL
Inj Vol	1	InjPosition		SampleType	Unknown	IRM Calibration Status	S-335 Success
Data Filename	AECisoprod2.d	ACQ Method	Direct_small mol_Jef	Comment		Acquired Time	1/6/2013 2:53:00 P

