

Supporting Information

For

**Synthesis of a Comprehensive Polyprenol
Library for Evaluation of Bacterial Enzyme
Lipid Substrate Specificity**

Baolin Wu,^{1,3} Robert Woodward,^{2,3} Liuqing Wen,¹ Xuan Wang,¹ Guohui Zhao,¹ Peng George Wang^{1}*

¹The Center for Therapeutics and Diagnostics (CDT), Department of Chemistry, Georgia State University, Atlanta, GA 30303.

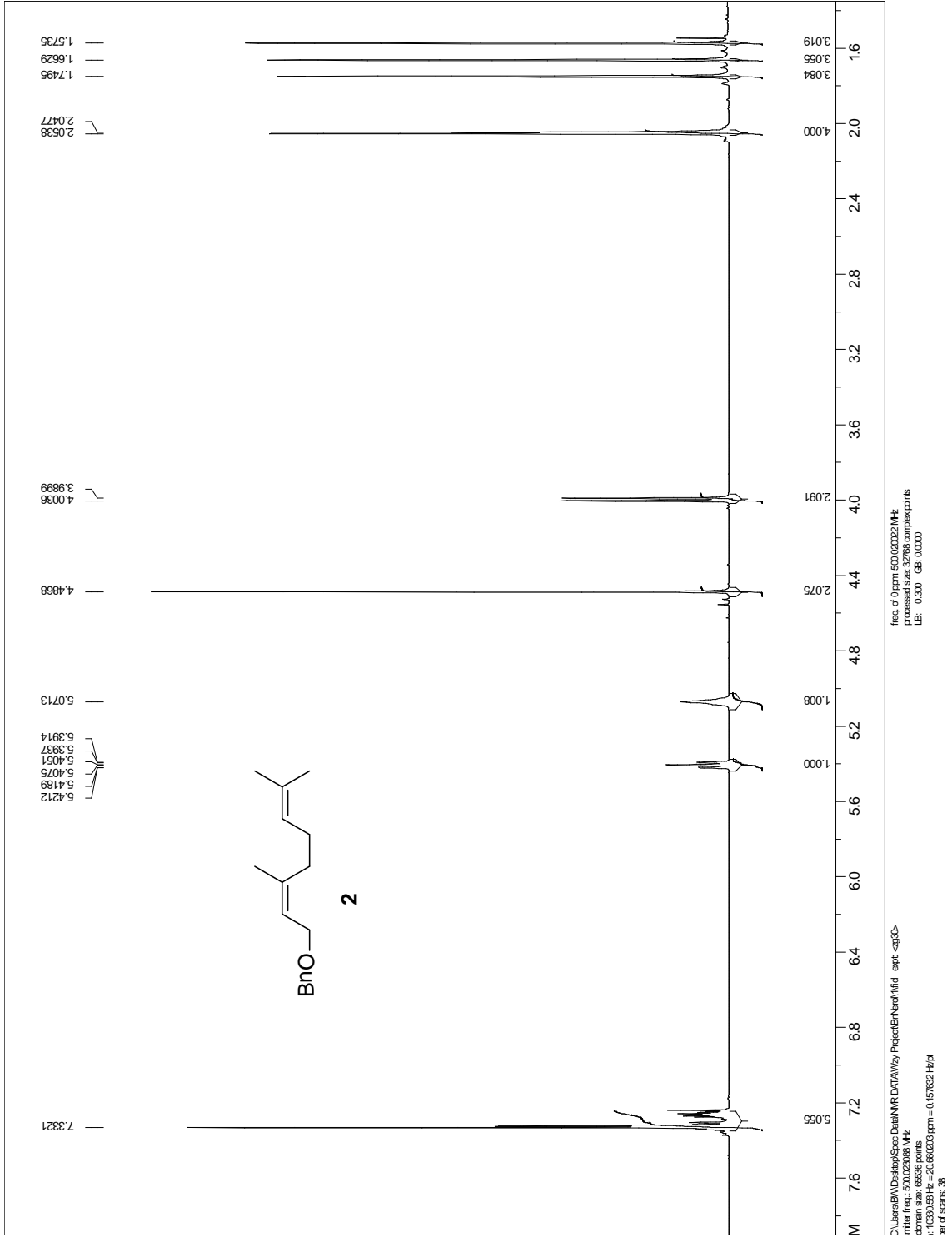
² Department of Chemistry and Biochemistry, University of Mount Union, Alliance, OH 44601

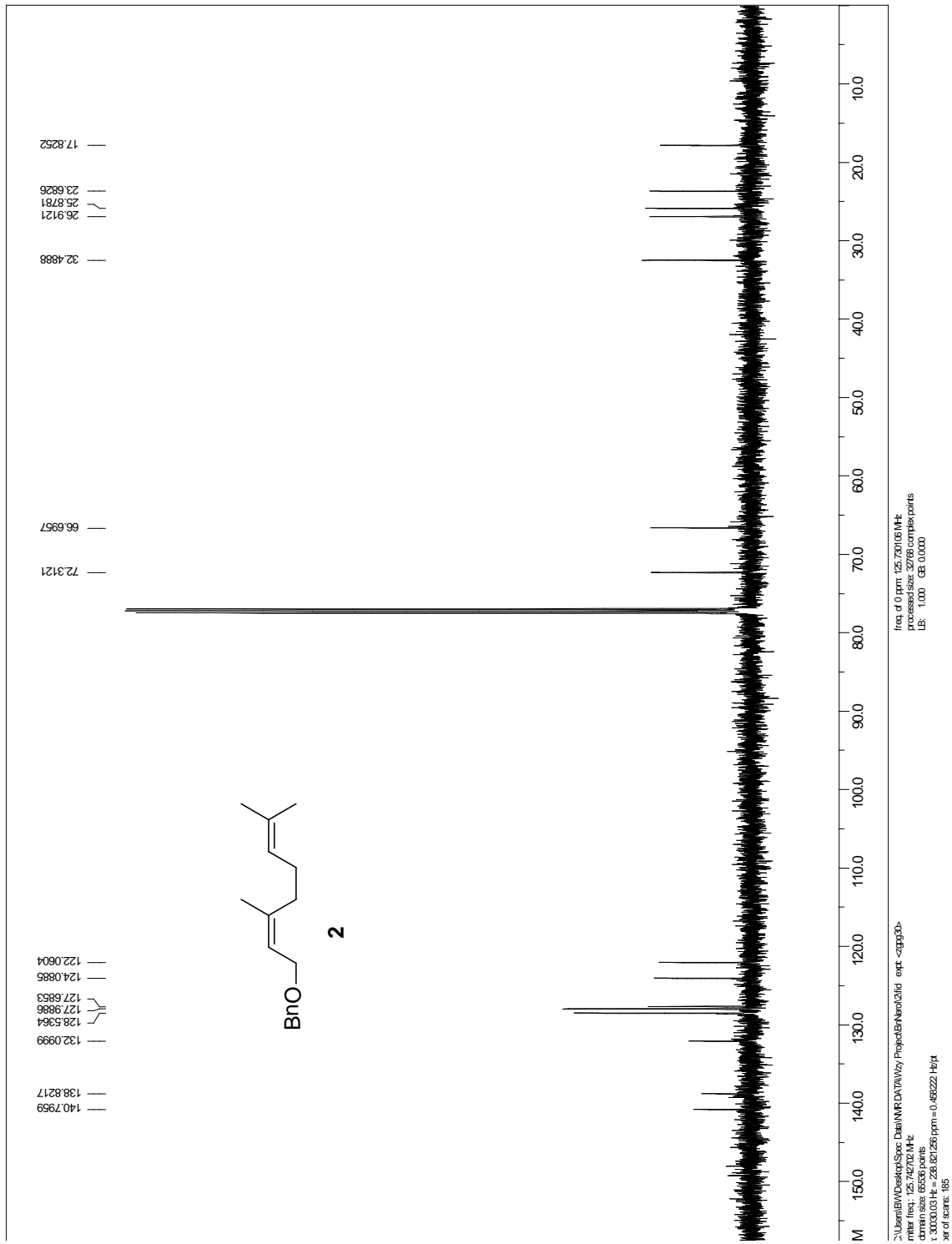
³ These authors contribute to this work equally

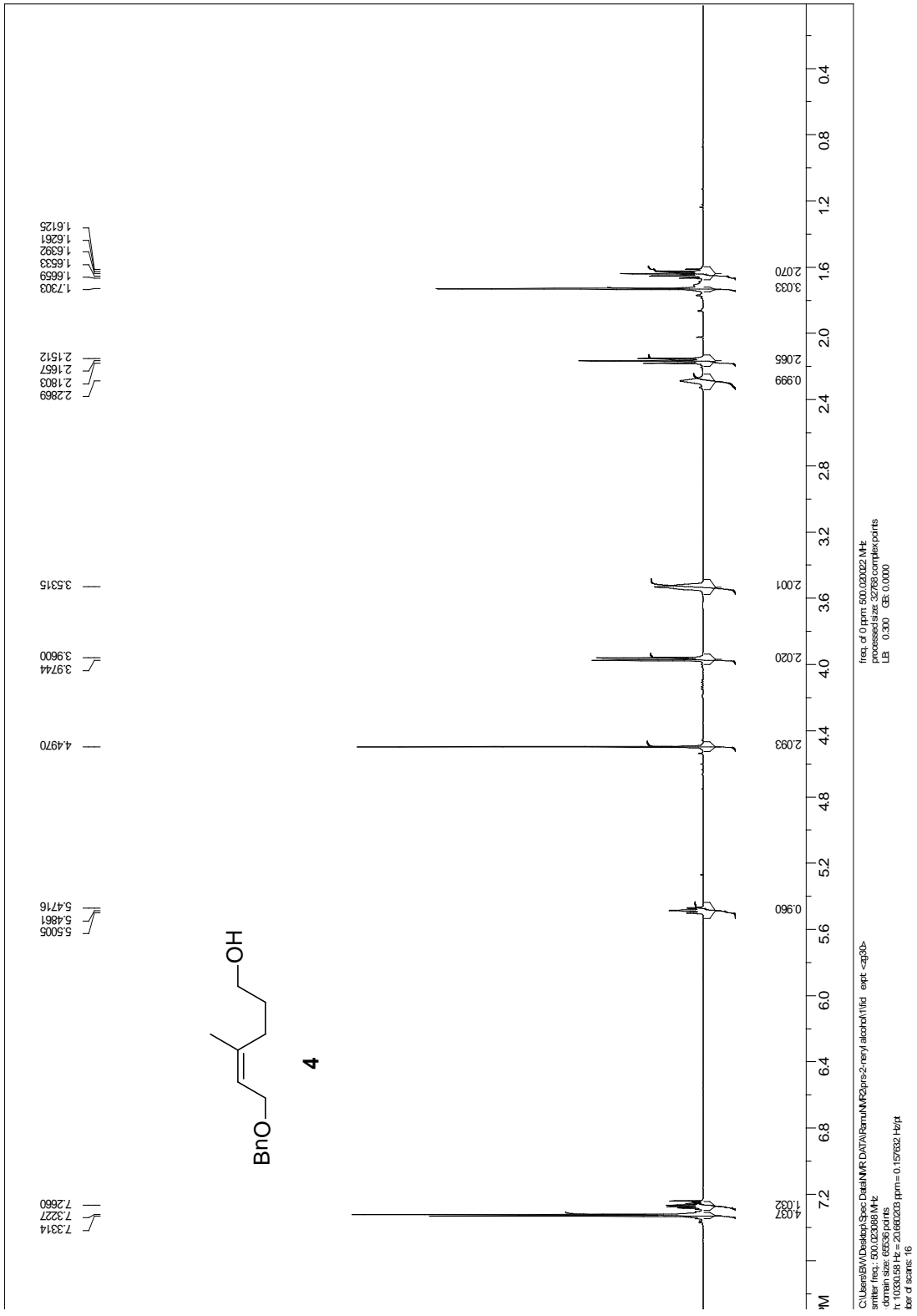
Corresponding author: pwang11@gsu.edu; Tel: 404-413-3591, Fax: 404-413-3580

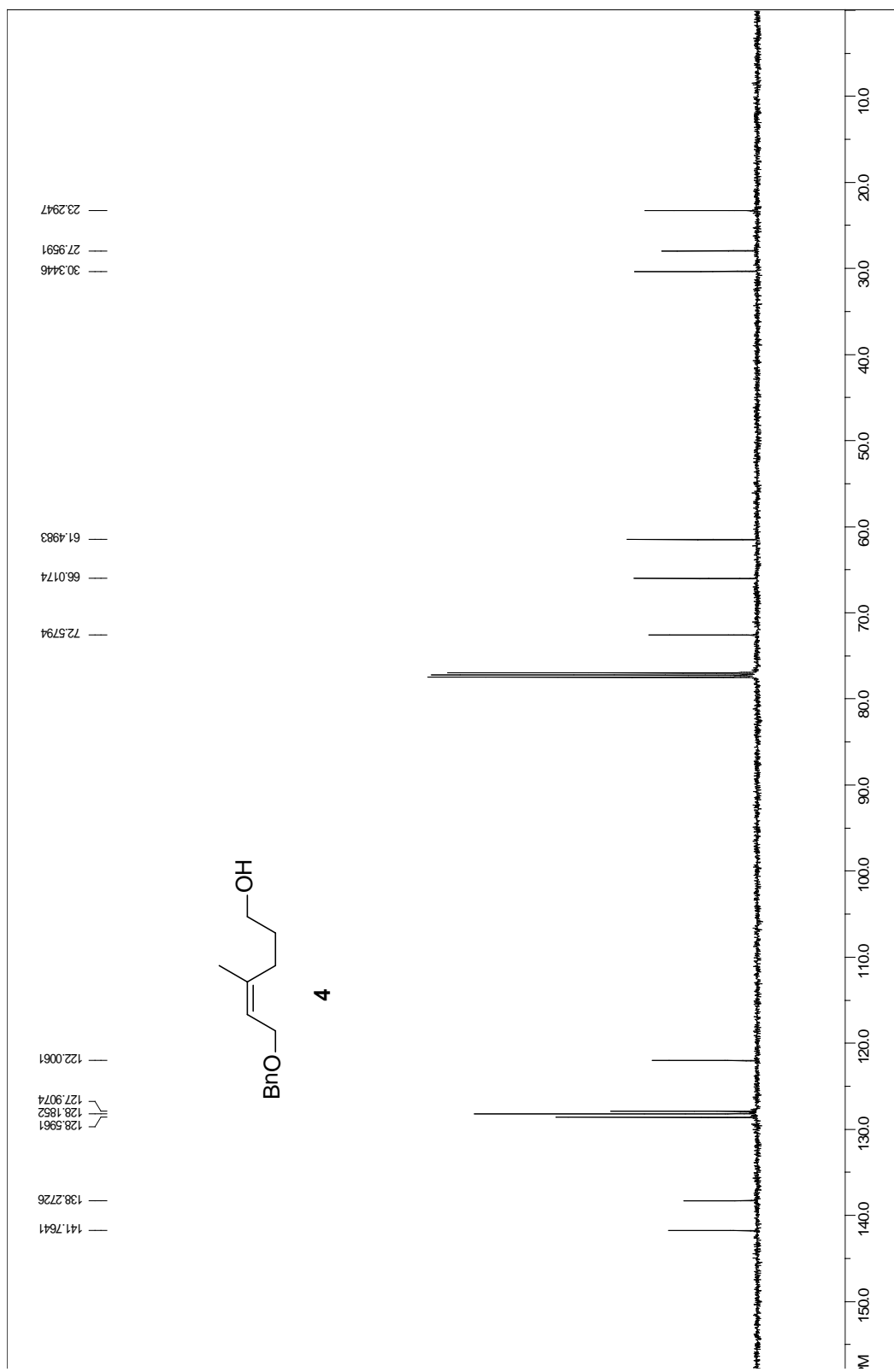
Table of Content

Compound #	NMR Spectra
Compound 2	P 3,4
Compound 4	P 5, 6
Compound 6	P 7, 8
Compound 7	P 9, 10
Compound 8	P 11, 12
Compound 9	P 13, 14
Compound 10	P 15, 16
Compound 12	P 17, 18
Compound 14	P 19, 20
Compound 15	P 21, 22
Compound 16	P 23, 24
Compound 18	P 25, 26
Compound 20	P 27, 28
Compound 22	P 29, 30
Compound 24	P 31, 32
Compound 25	P 33, 34
Compound 26	P 35, 36
Compound 27	P 37, 38
Compound 28	P 39, 40
Compound 29	P 41, 42
Compound 30	P 43, 44
Compound 31	P 45, 46, 47
Compound 32	P 48, 49, 50
Compound 33	P 51, 52, 53
Compound 34	P 54, 55, 56
Compound 35	P 57, 58, 59
Compound 36	P 60, 61, 62

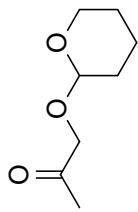




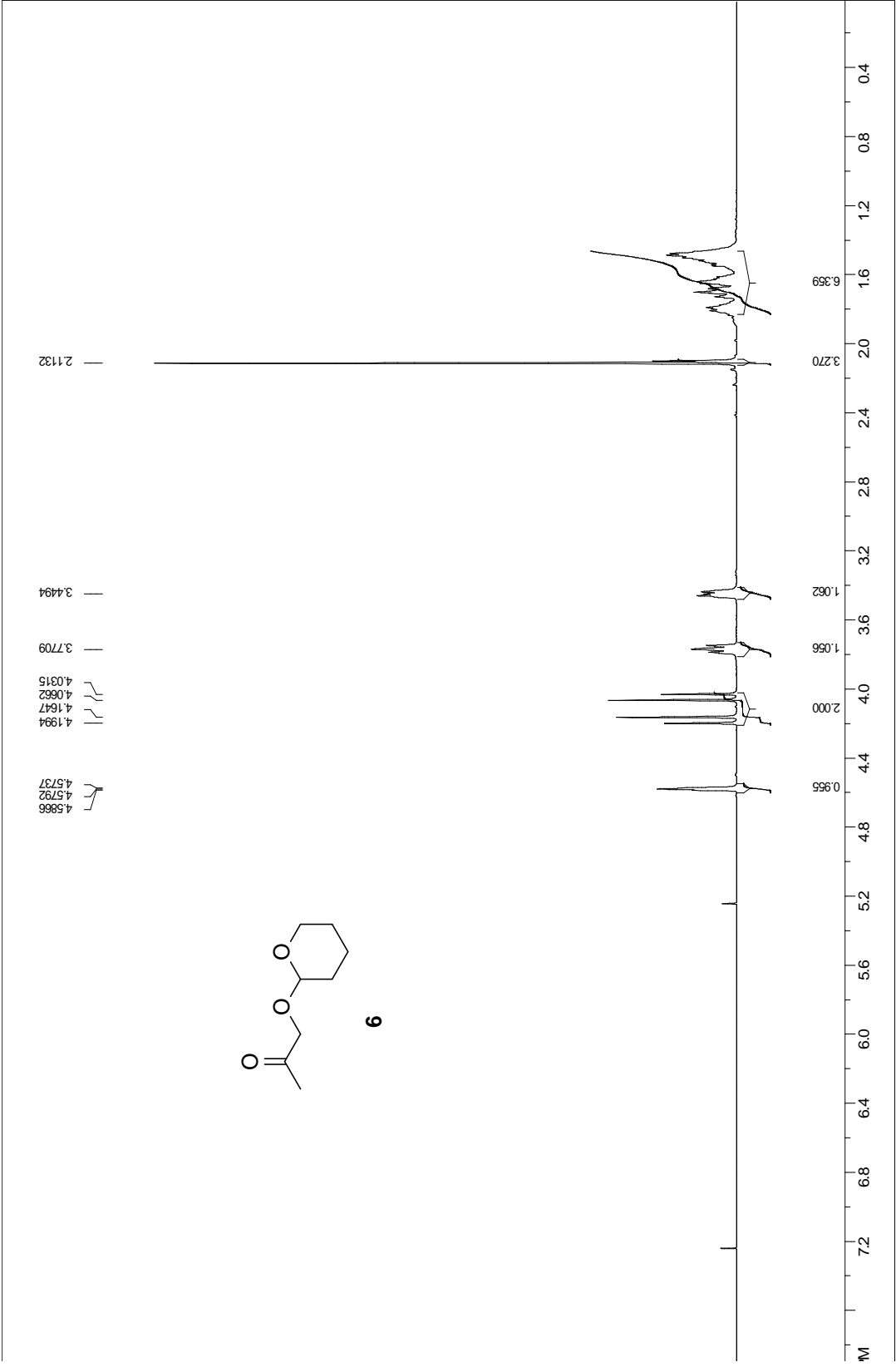


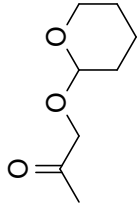


C:\Users\BMD\Desktop\Spec Data\NMR\DATA\Remu\NMR2\ps-2-nyl alcohol2\1d1 exp1 -<3>g30-
 smiler freq: 125.742702 MHz
 domain size: 65536 points
 x: 30000.00 Hz = 238.827259 ppm = 0.456222 Hqpt
 bar of scans: 145
 freq: 0.0 ppm 125.730706 MHz
 processed size: 32768 complex points
 LB: 1.000 GB: 0.0000

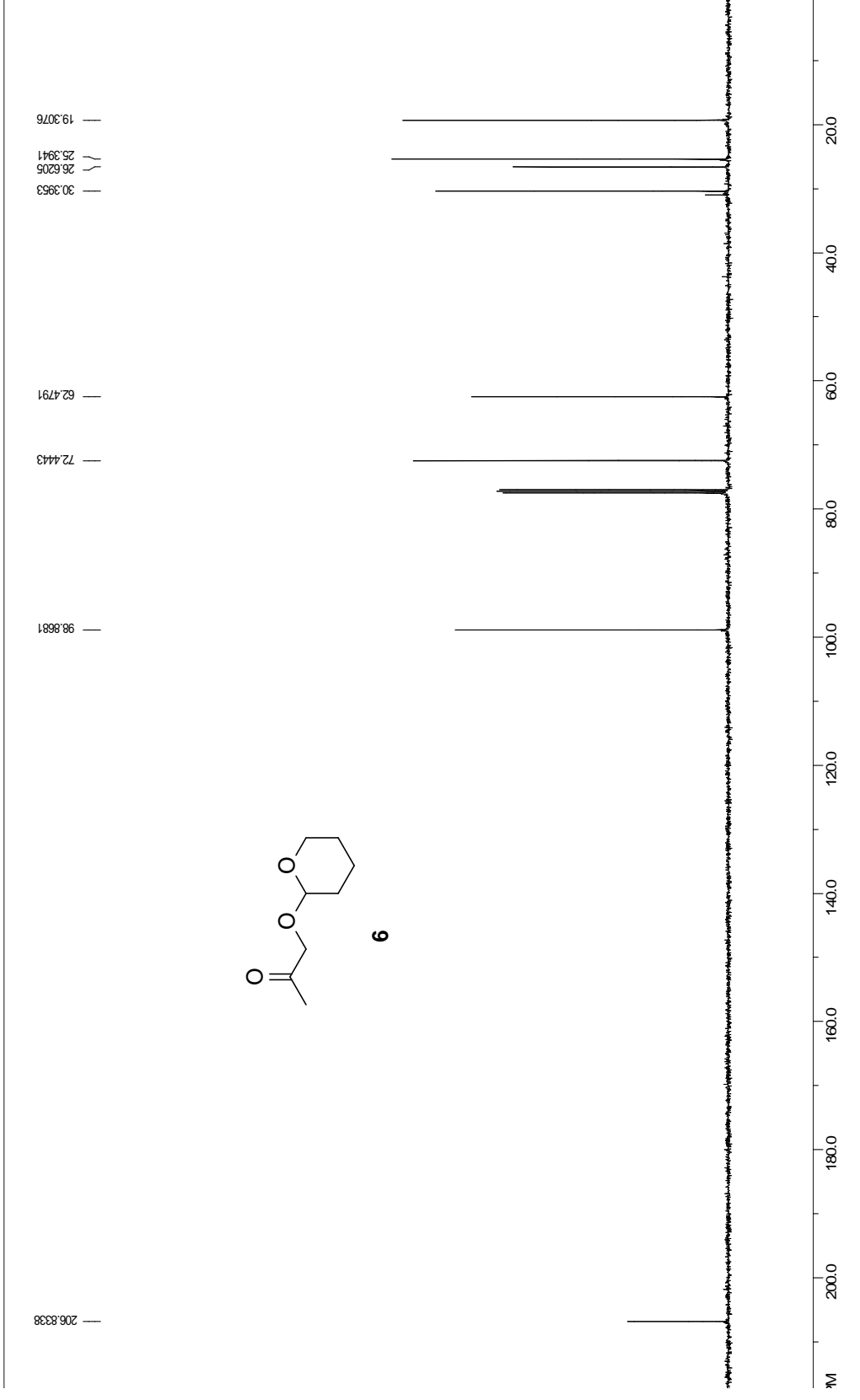


6



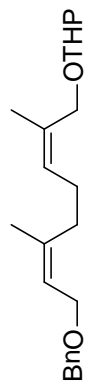


6

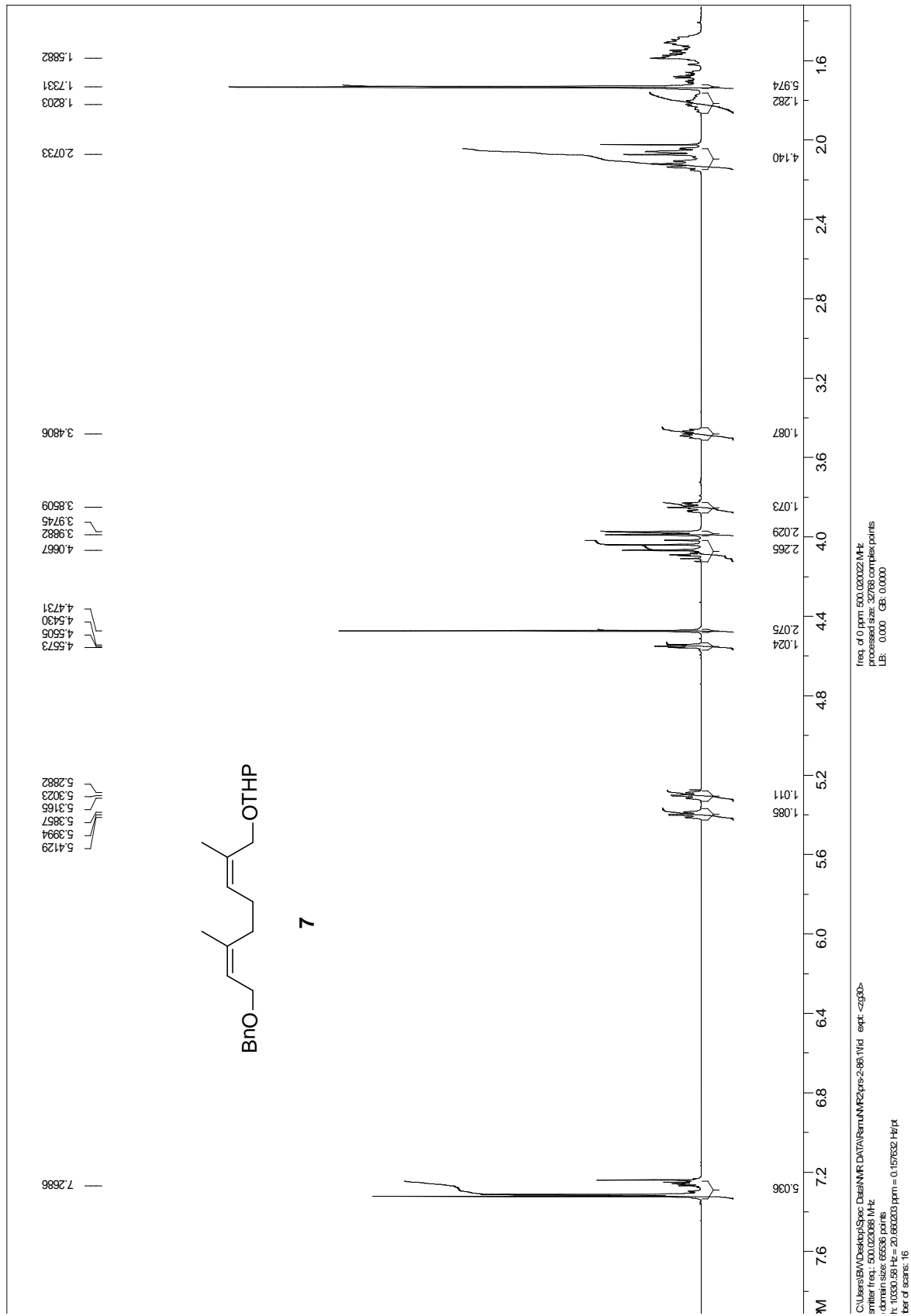


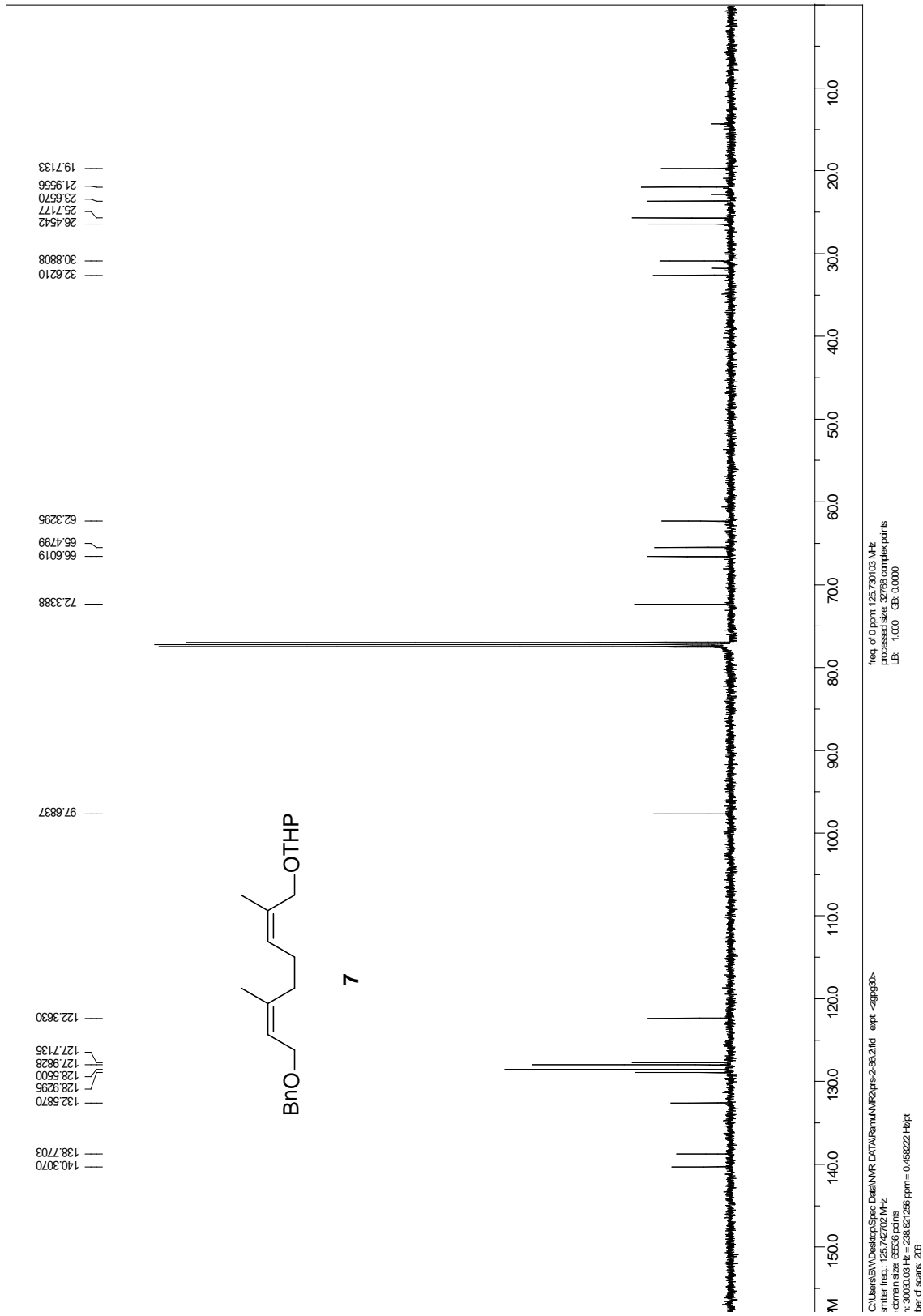
freq. of 0 ppm: 125.730110 MHz
 name: CDCl₃ sample: panis
 LB: 1.000 GB: 0.0000

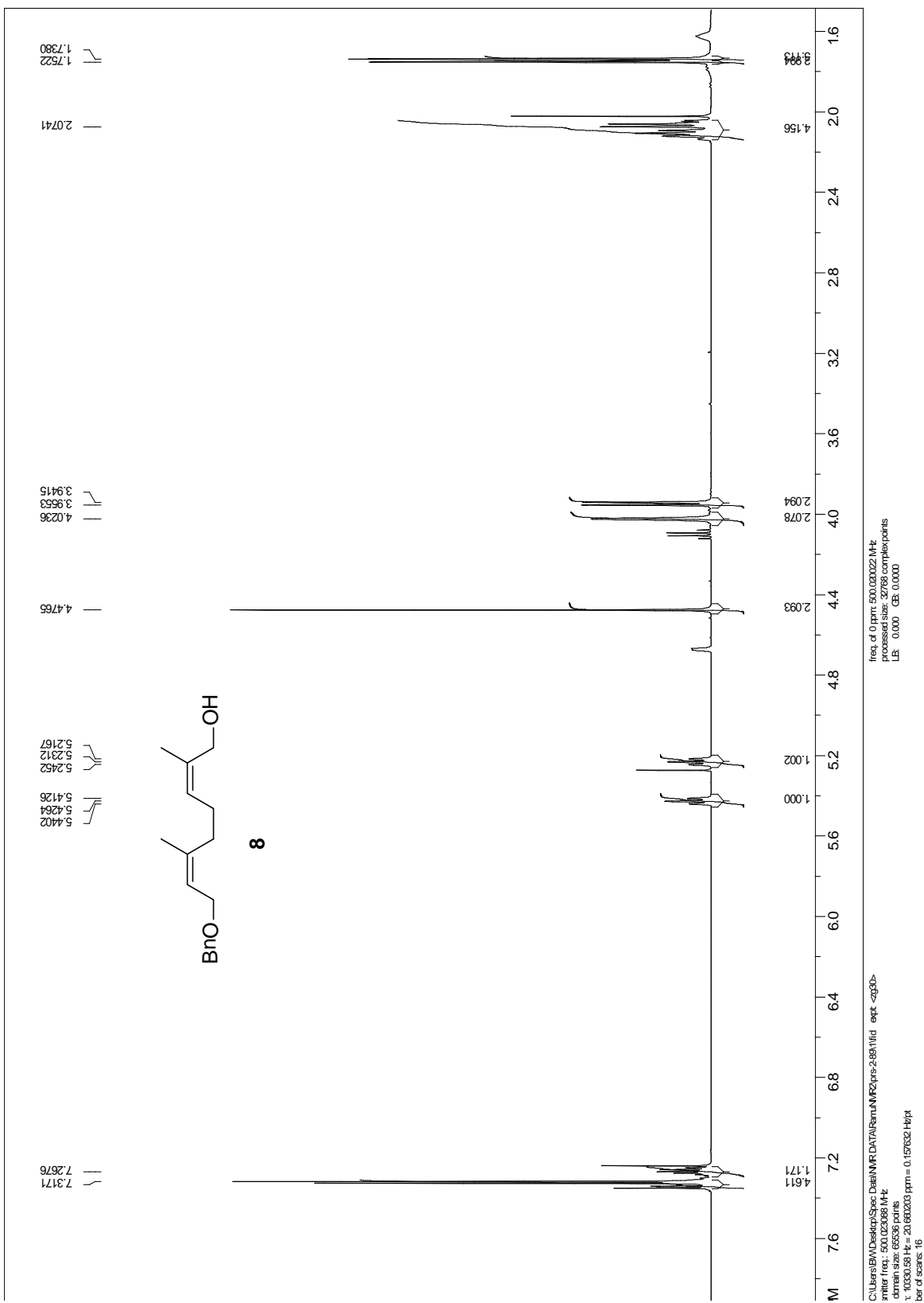
C:\Users\B\W\Desktop\Spec Data\NMR\DATA\pani\NMR2\ps-THP-hydroxy acetone\cdcl3\ exp1 <aggsg>
 f2: 125.760 MHz
 channel size: 66536 points
 h: 300.0000 Hz = 238.821256 ppm = 0.458222 Hz/pt
 no. of scans: 143

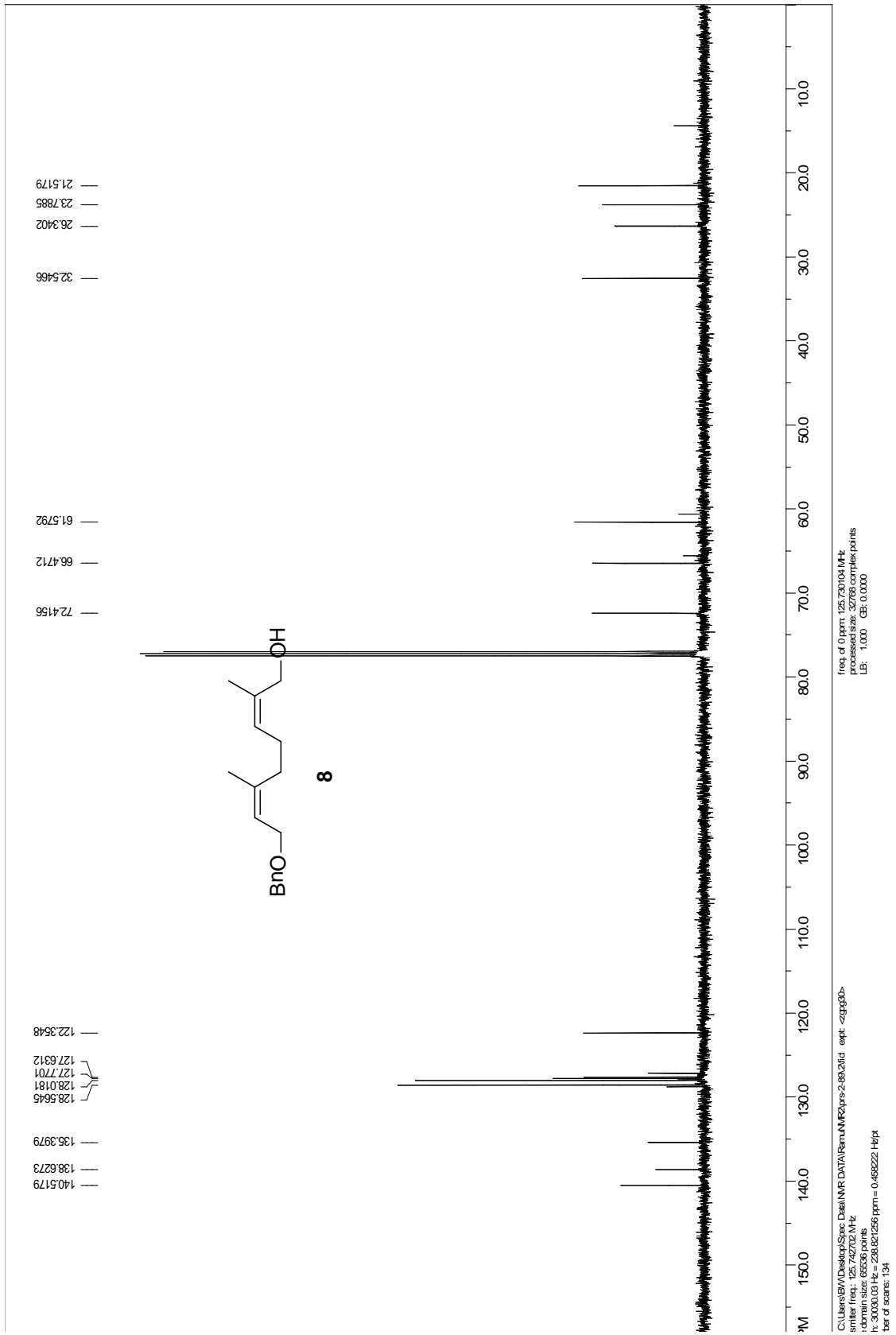


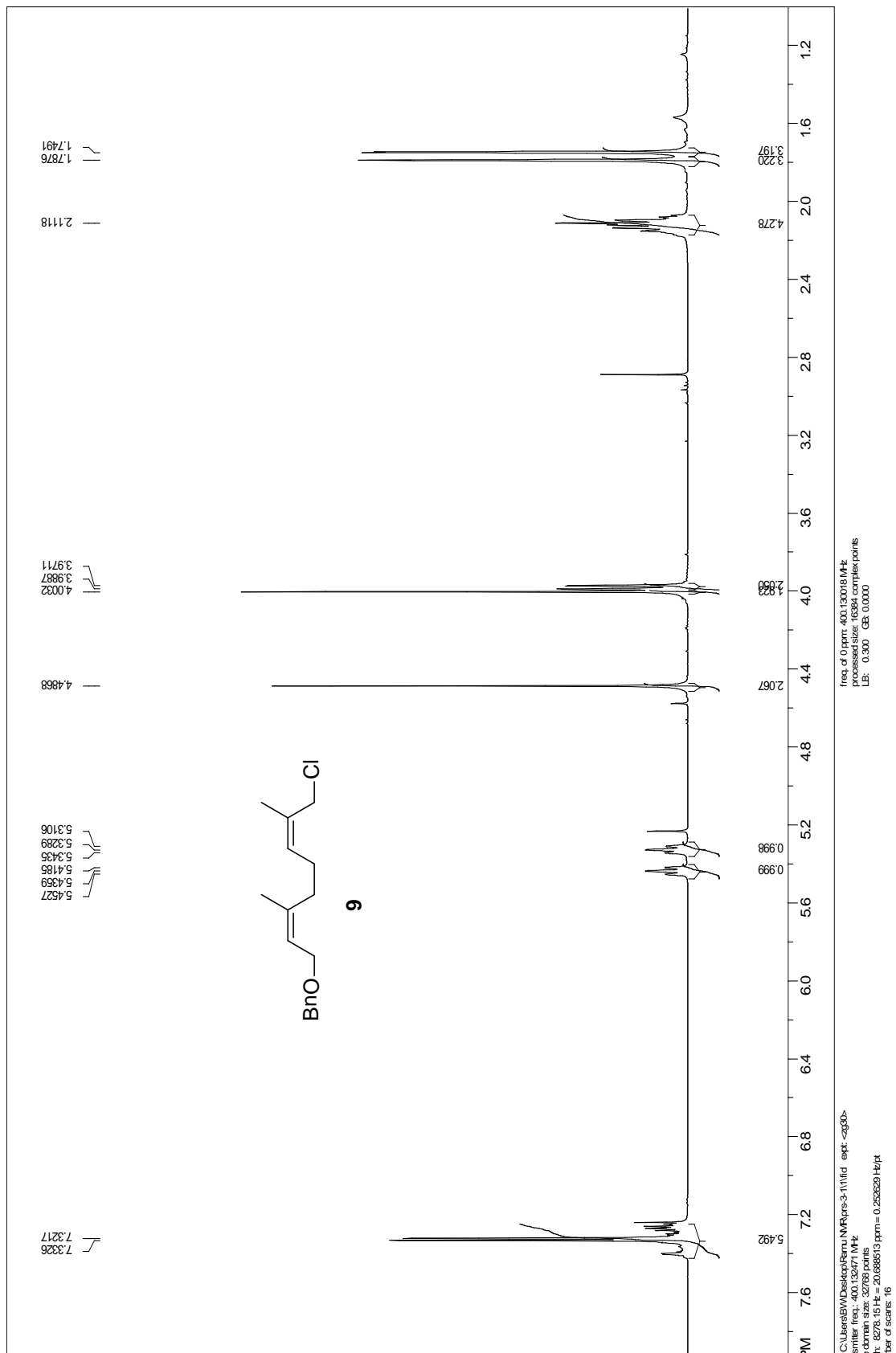
7

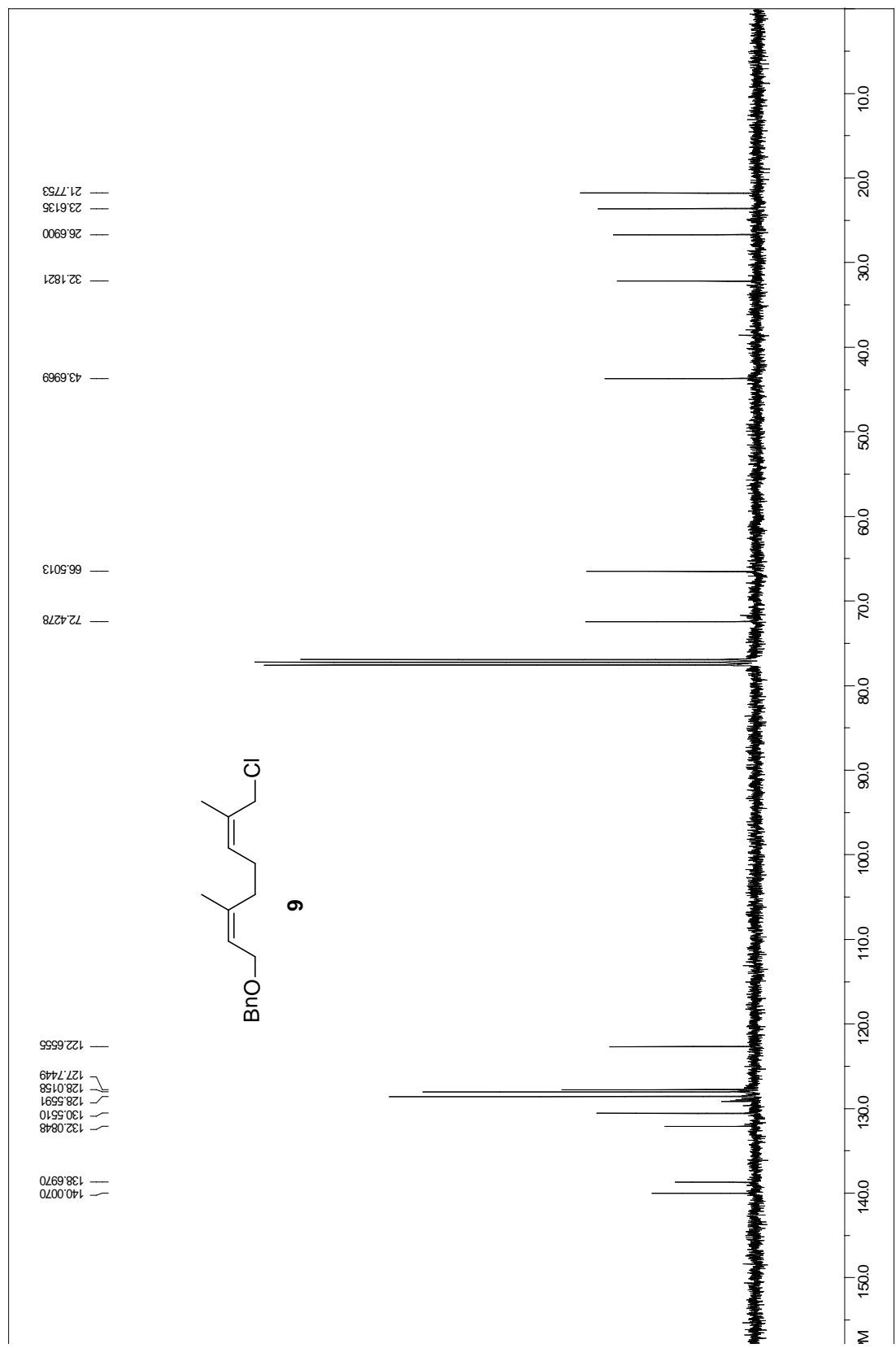






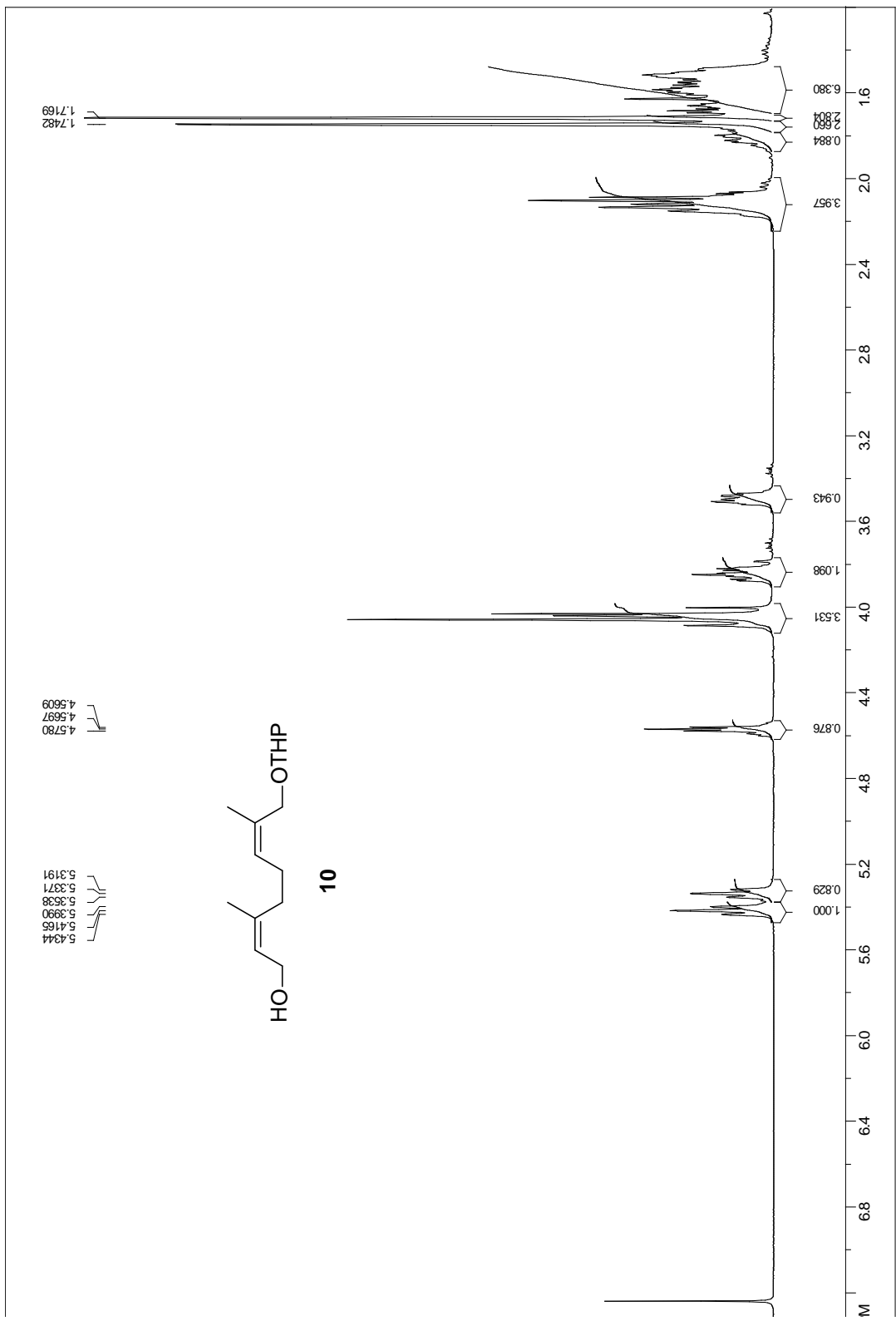






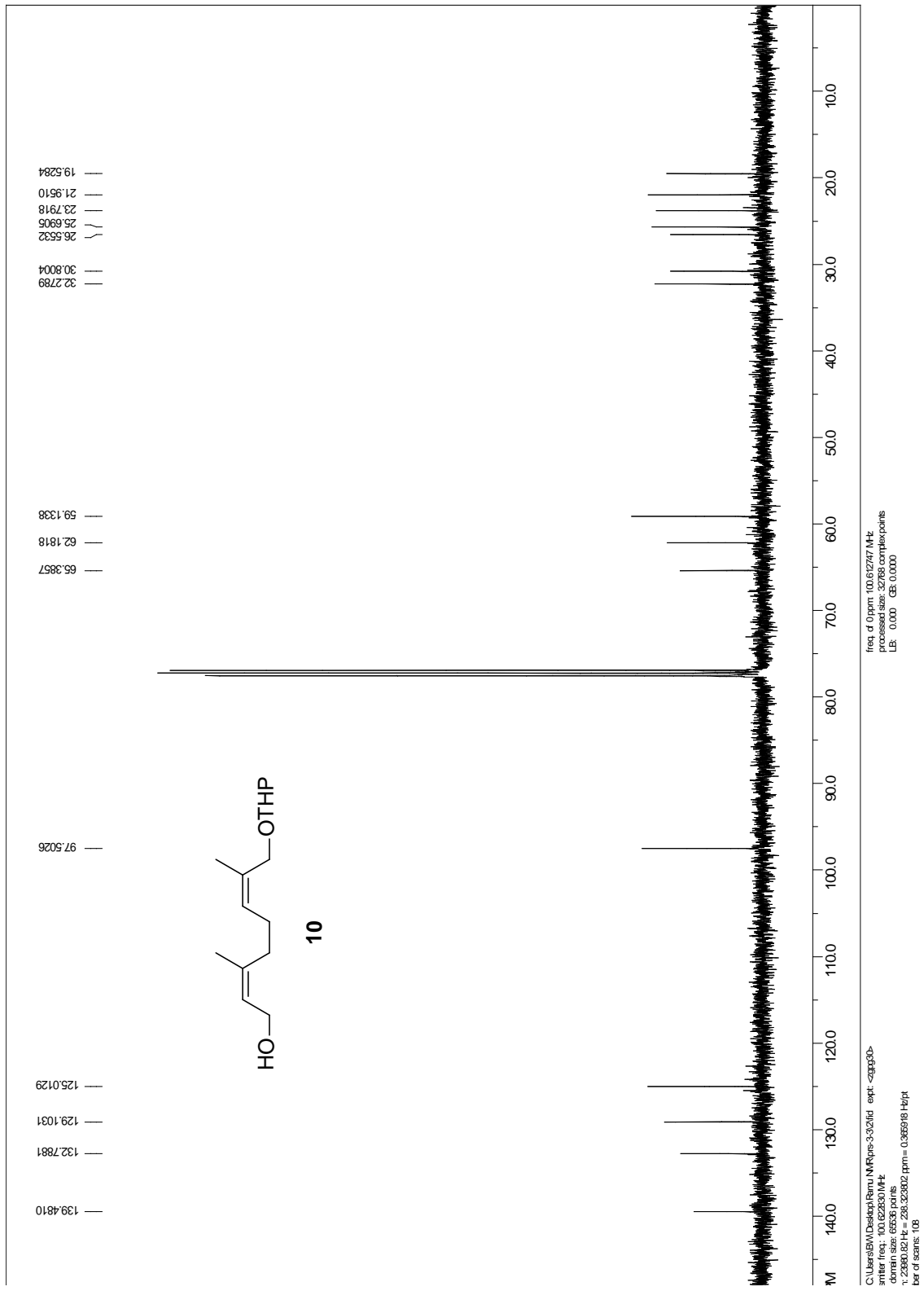
Trace of 0 ppm: 100.612749 MHz
 processed size: 32768 complex points
 LS: 1.00 GB 0.0000

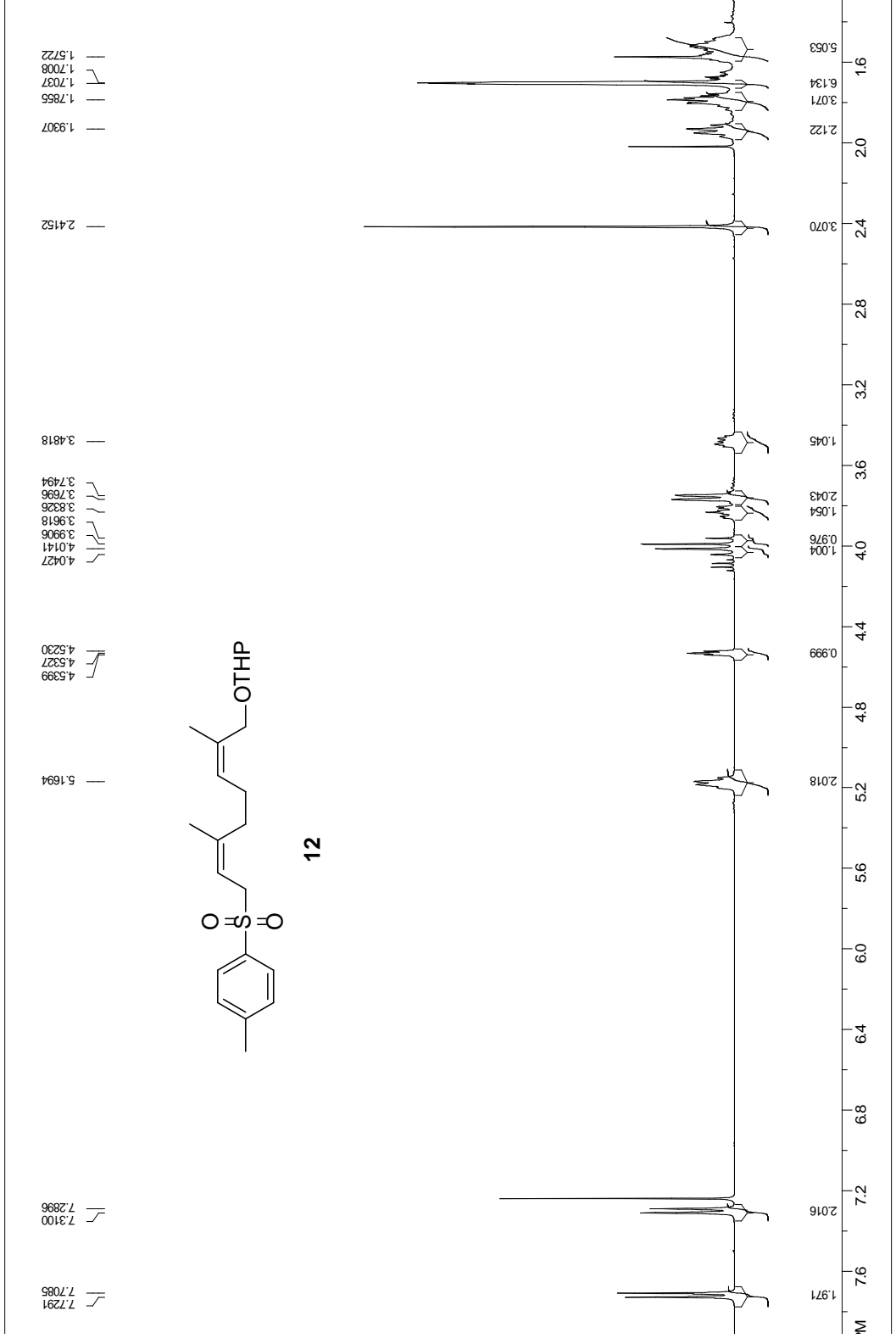
C:\Users\BMD\Desktop\Bamu\NMR\ps-5\12\fid exp1 ->psg00-
 antifer freq: 100.622830 MHz
 acq time: 14.25000000 ppm
 23000 Hz 230.00000000 ppm = 0.368918 Hz
 bot of scans: 137



C:\Users\BM\Desktop\item\NMR\ps-3-1\fid exp-0360-
 acq1.fid: 400.132671 MHz
 domain size: 32768 points
 40978.15114-20.000015 ppm - 0.25262946 pt
 box of scans: 16

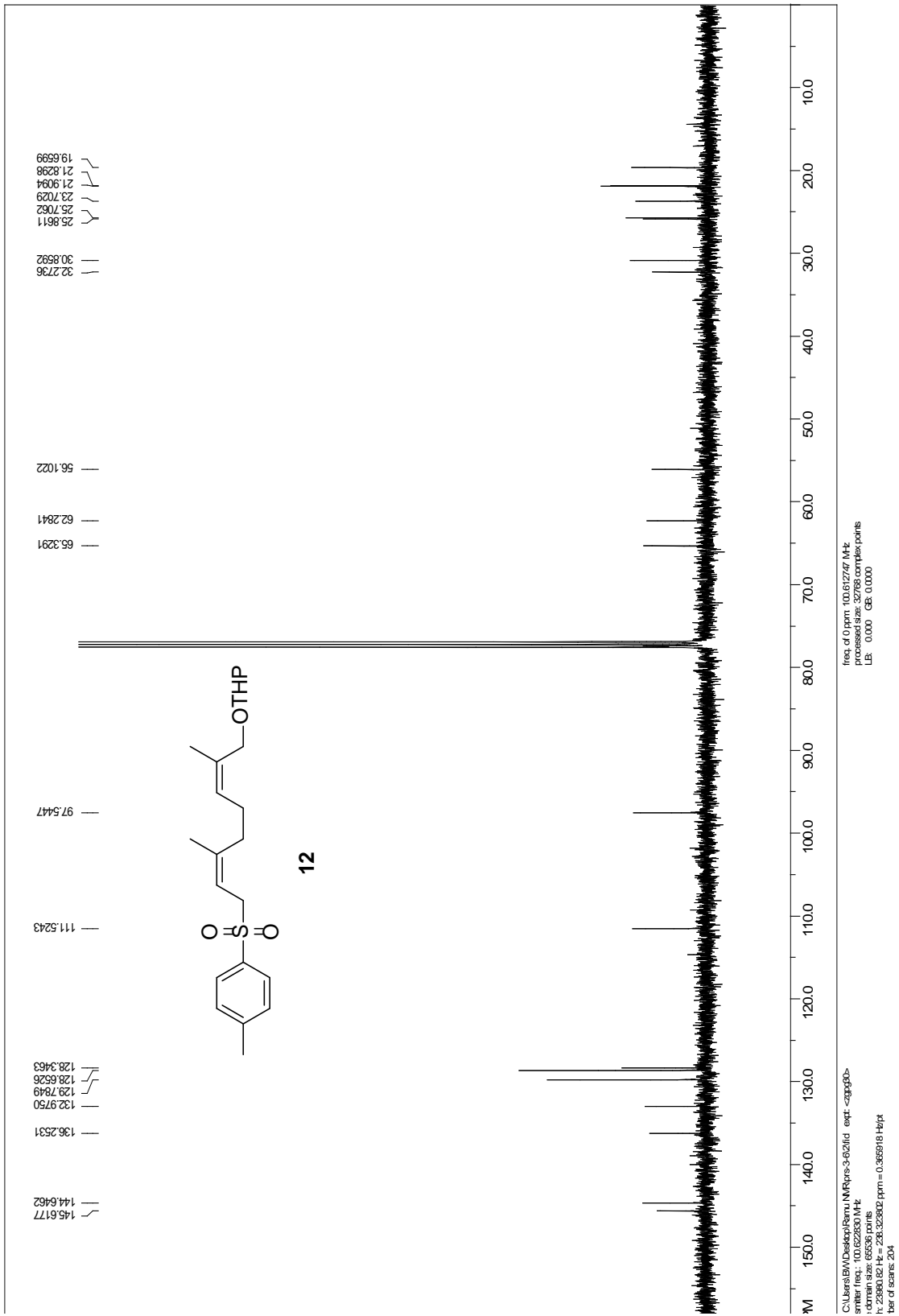
freq. of 0 ppm: 400.130018 MHz
 processed size: 16384 complex points
 LB: 0.000 GB: 0.0000

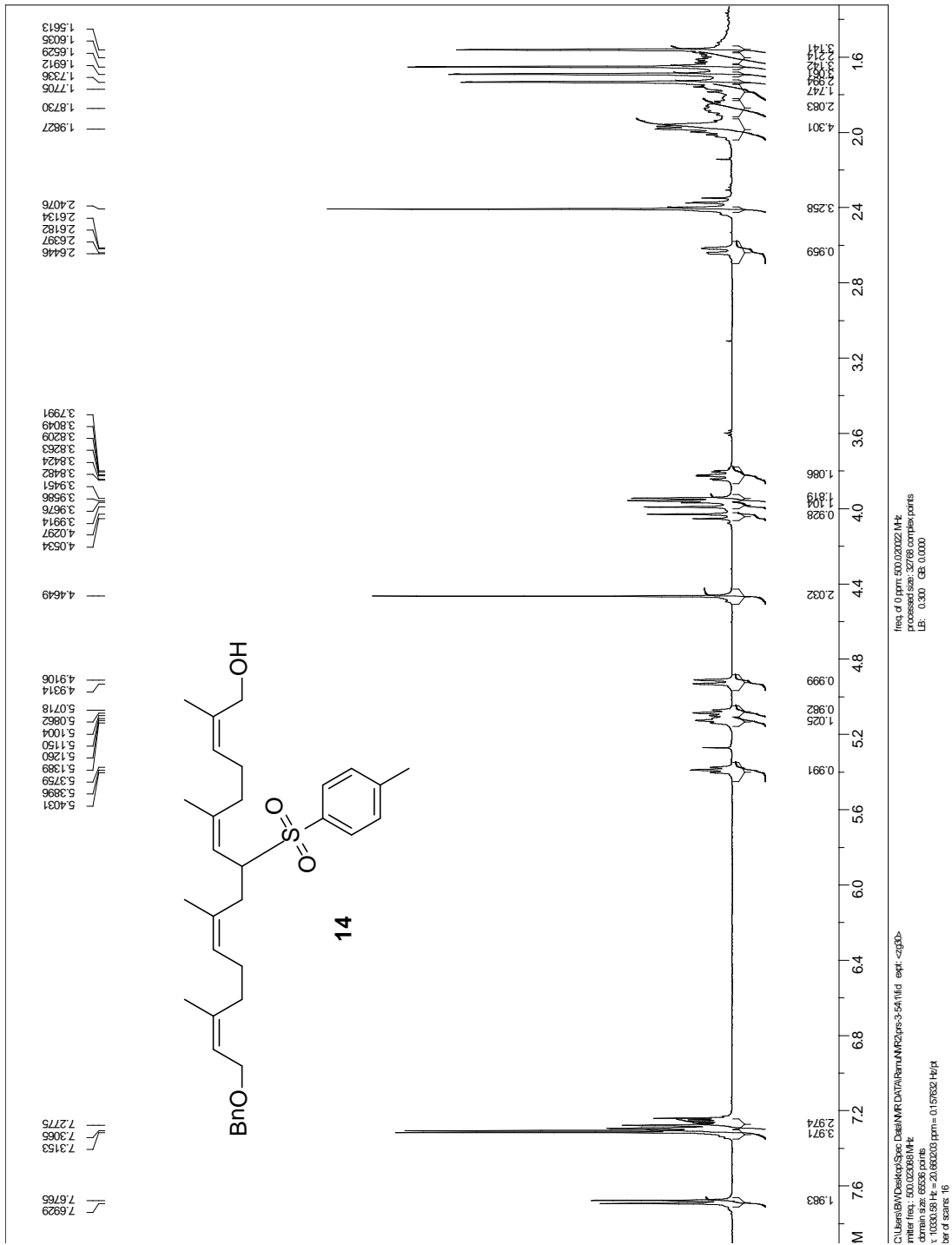


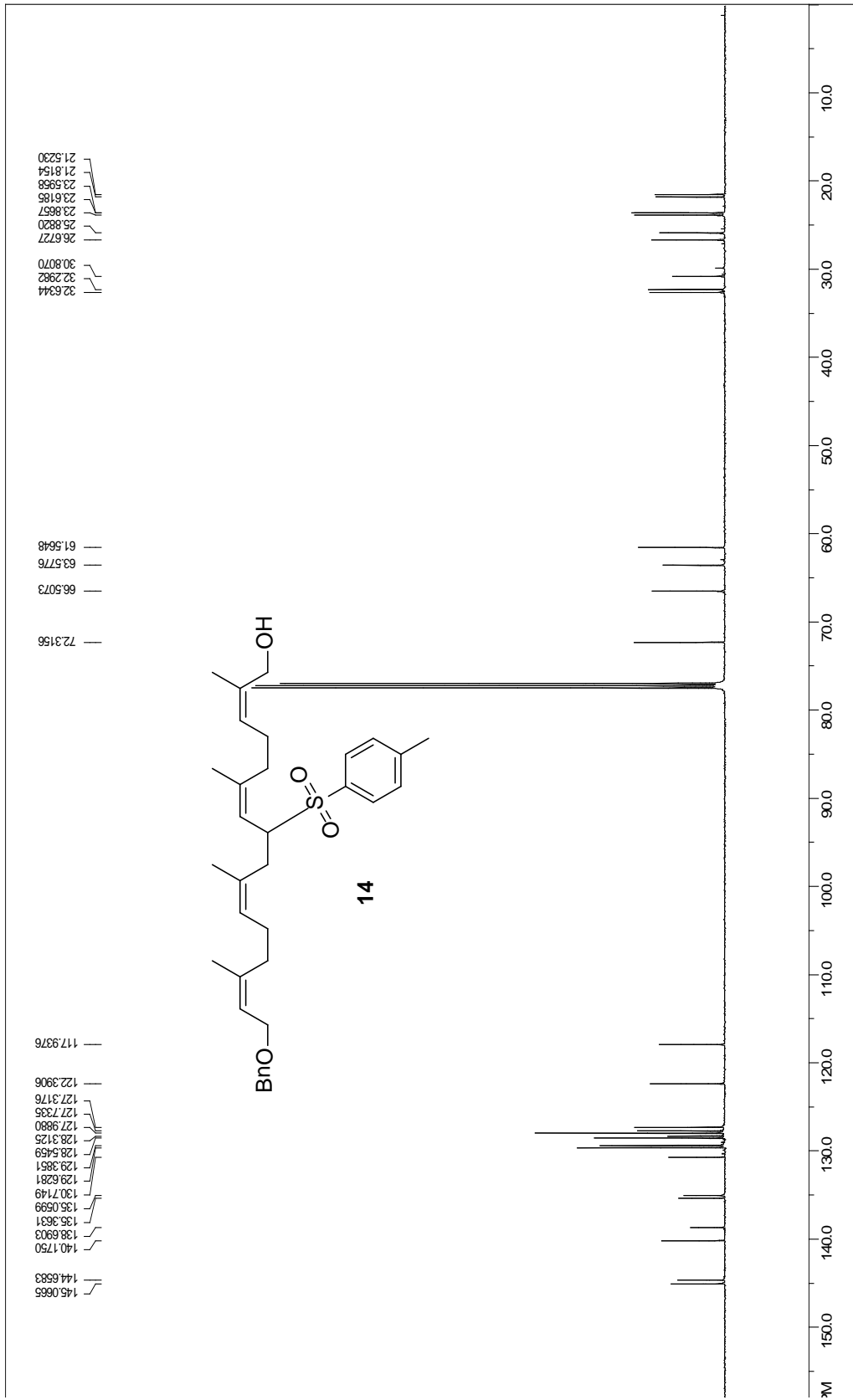


freq. of 0 ppm: 400.130018 MHz
 processed size: 1.6884 complex points
 LB: 0.000 GB: 0.0000

C:\Users\BWA\Desktop\BWA\NMR\BWA-3-B1\1d ext: -zgpgb-
 smilar freq: 400.132671 MHz
 domain size: 32768 points
 r: 32768 16 Hz = 201.686513 ppm = 0.252629146 pt
 bar of scans: 16







C:\Users\BAM\Desktop\Spec Data\MR DATA\Remun192\ps-3-5A21hd_ exp. <gpgb>

smiler_freq: 125.742702 MHz

r-domain size: 65536 points

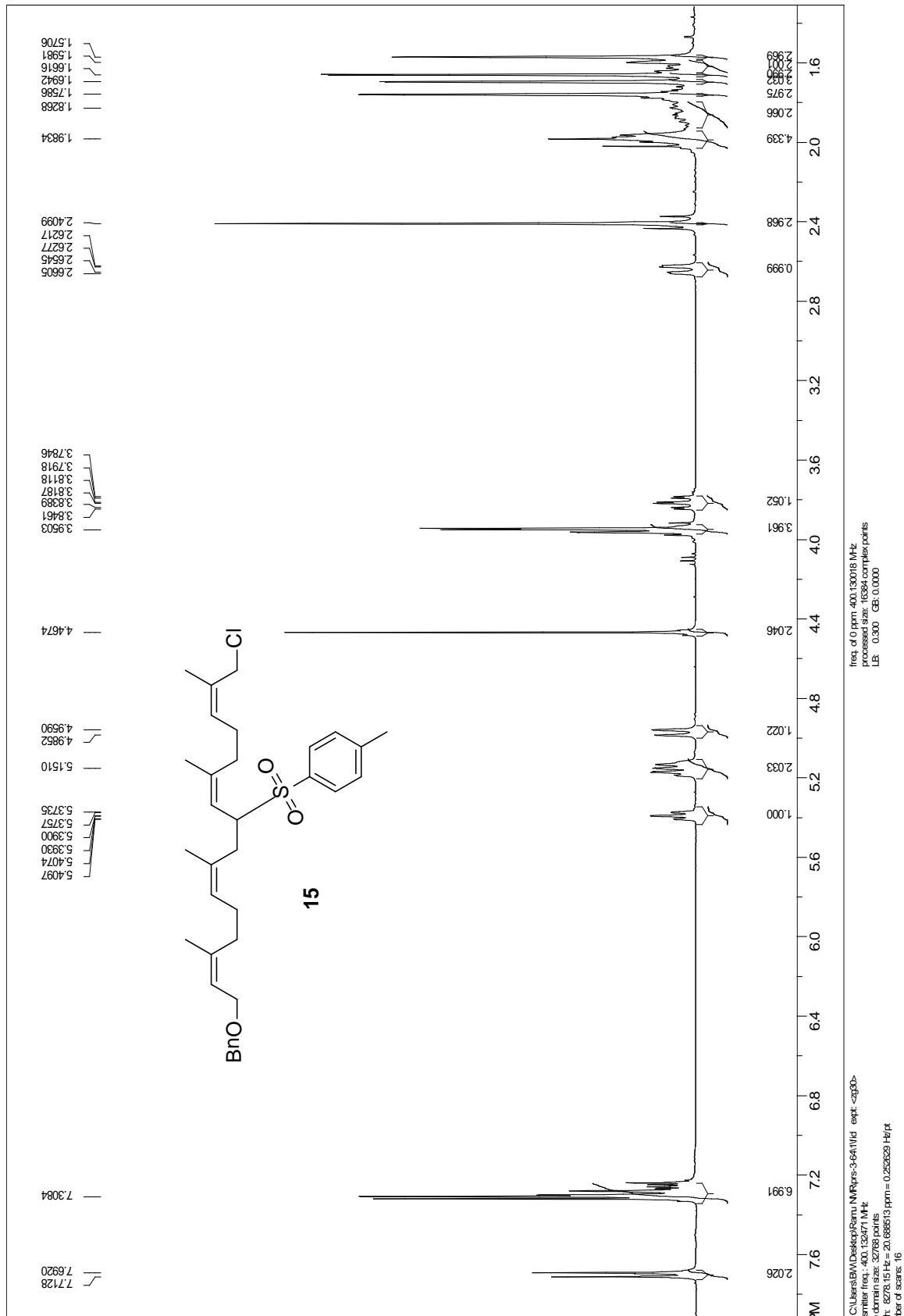
f1: 30000.03 Hz = 238.821256 ppm = 0.458222 Hz/pt

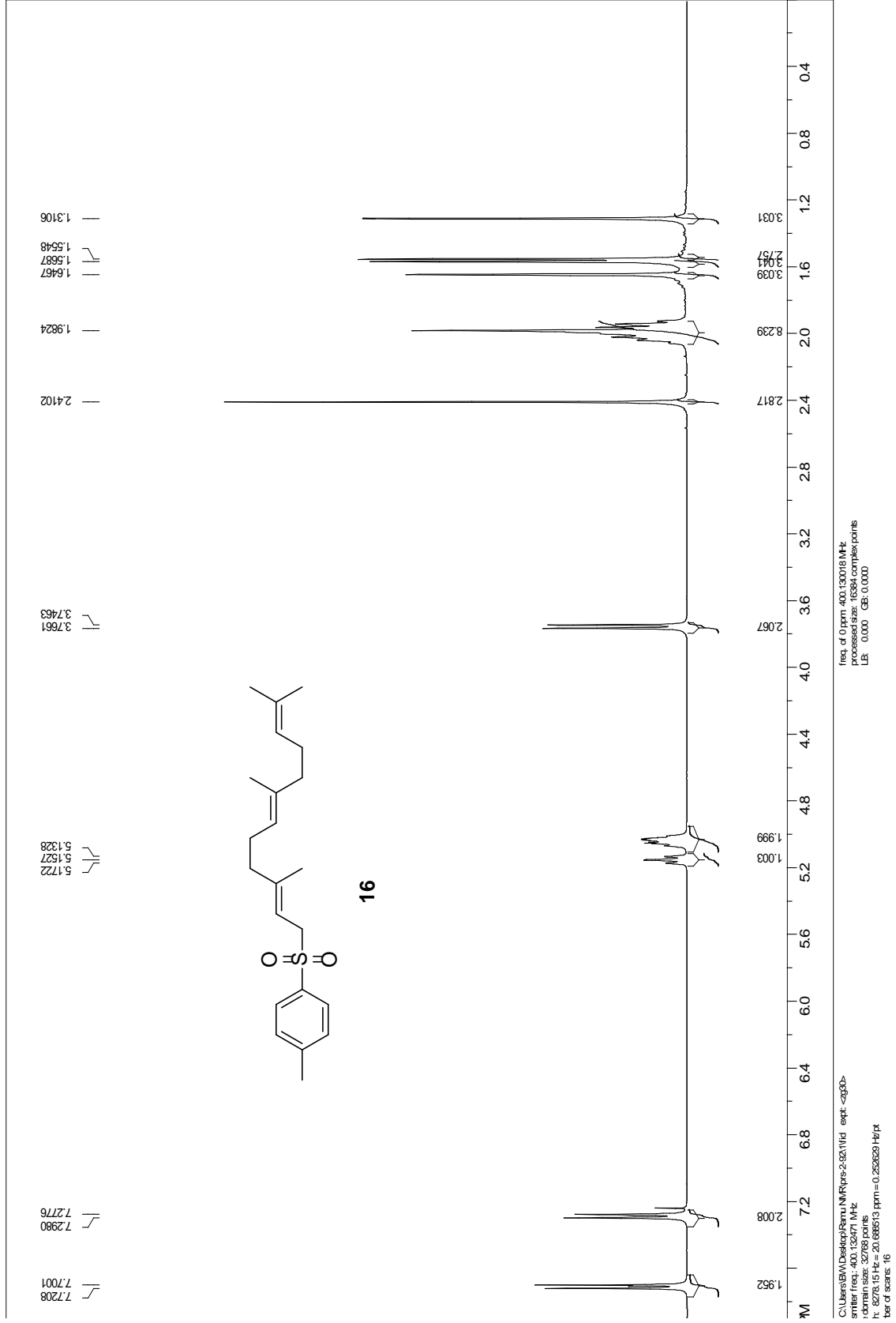
number of scans: 4442

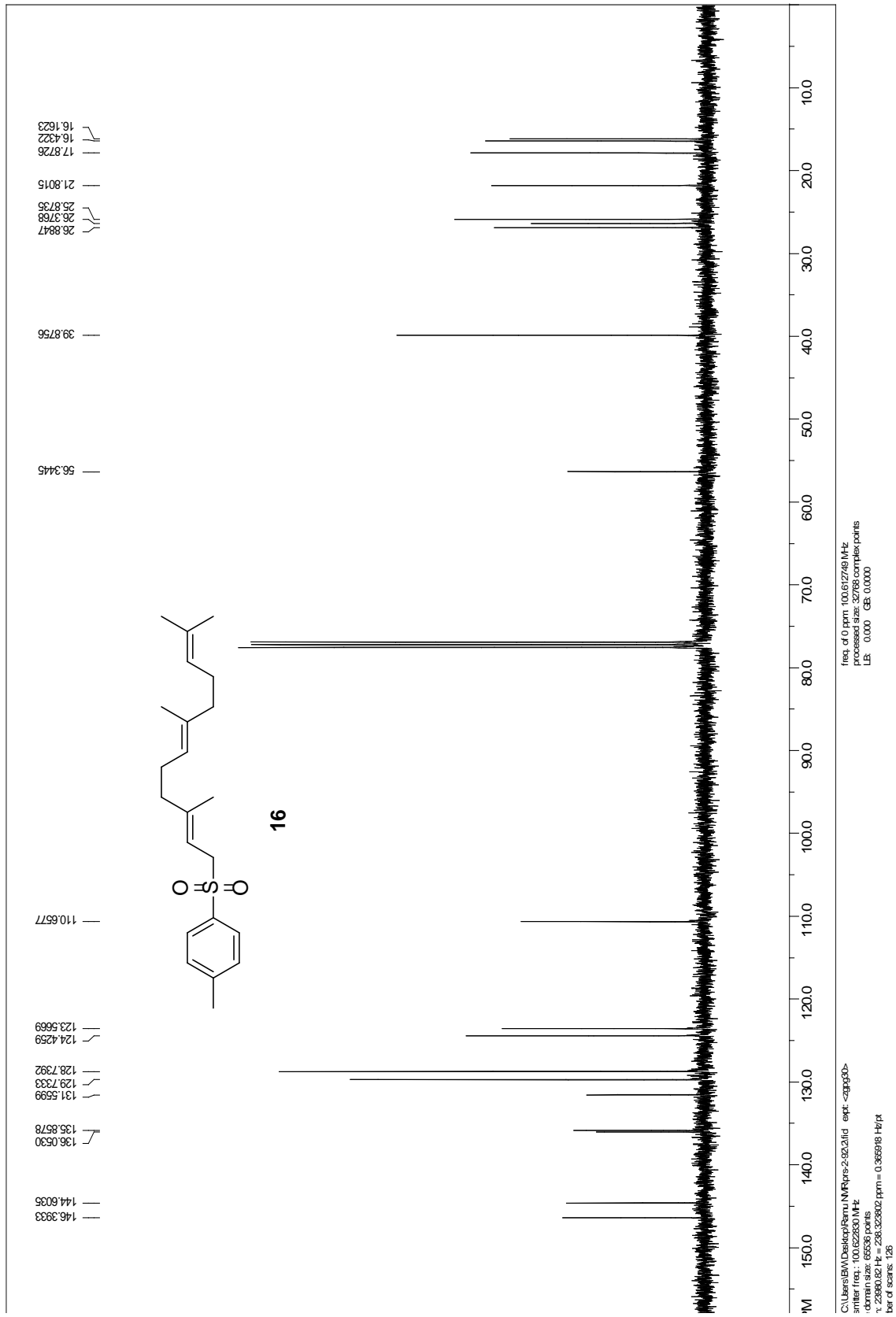
frec: of 0 ppm 125.730104 MHz

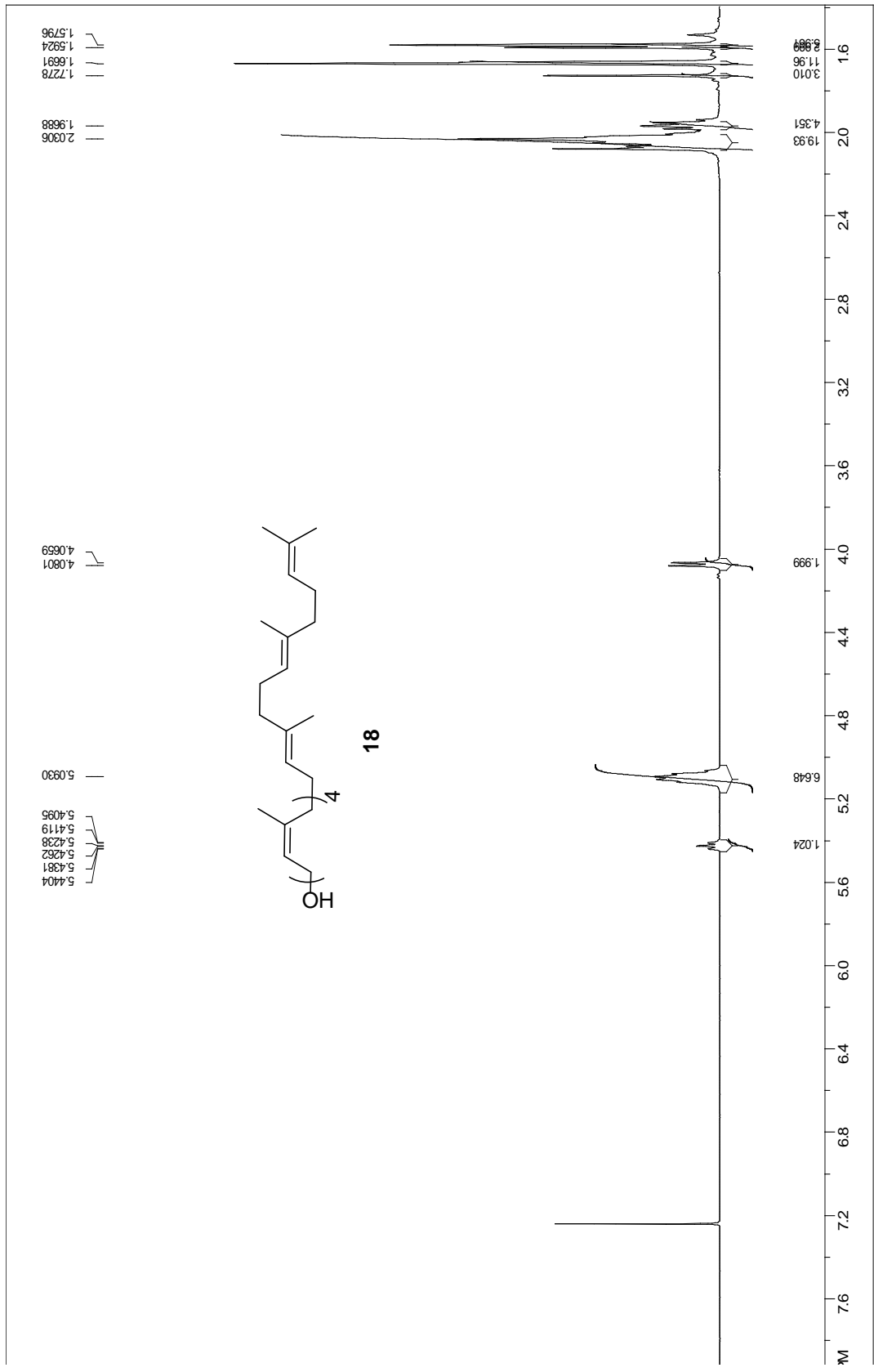
processed size: 32768 complex points

LB: 1.000 GB: 0.0000

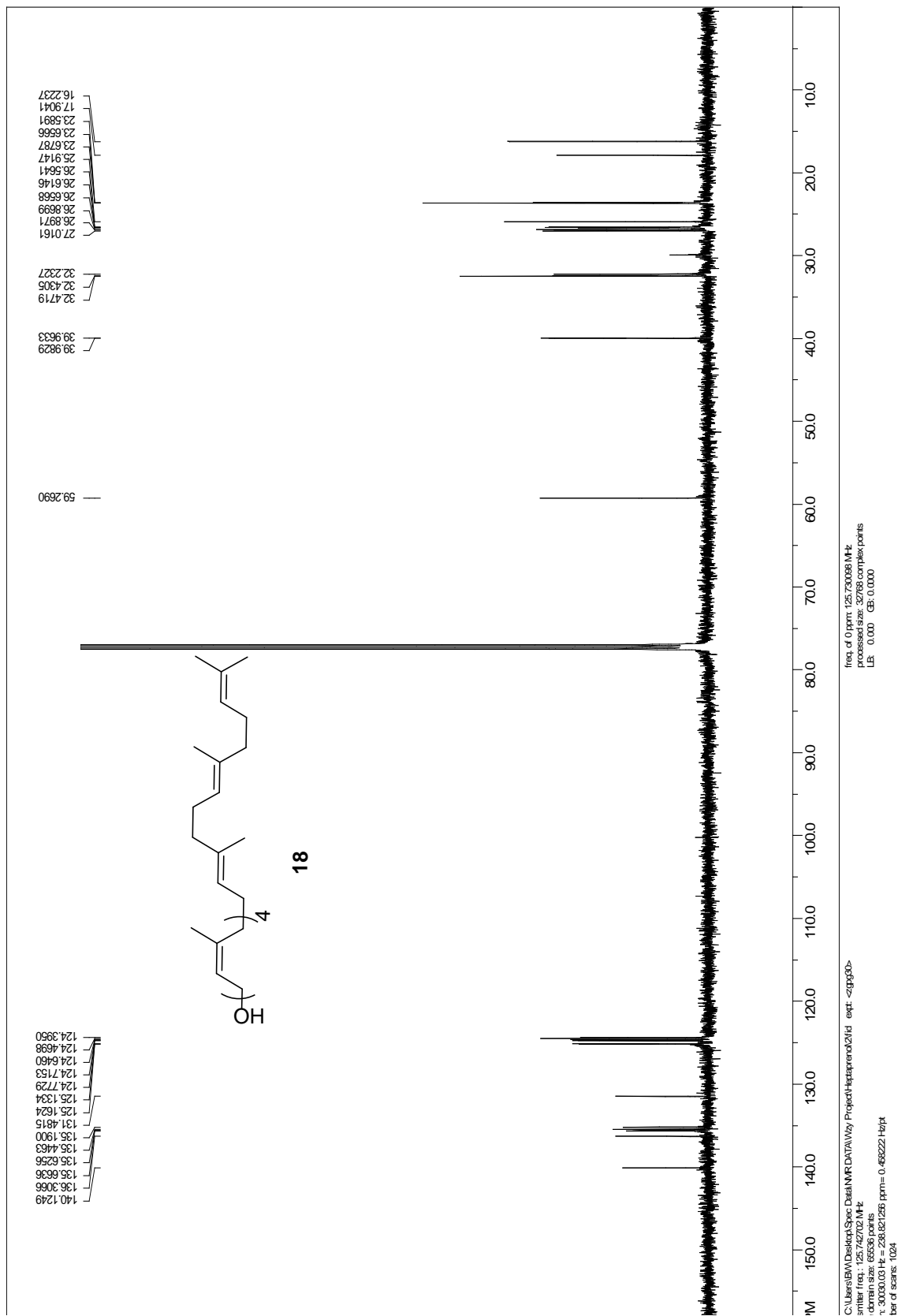


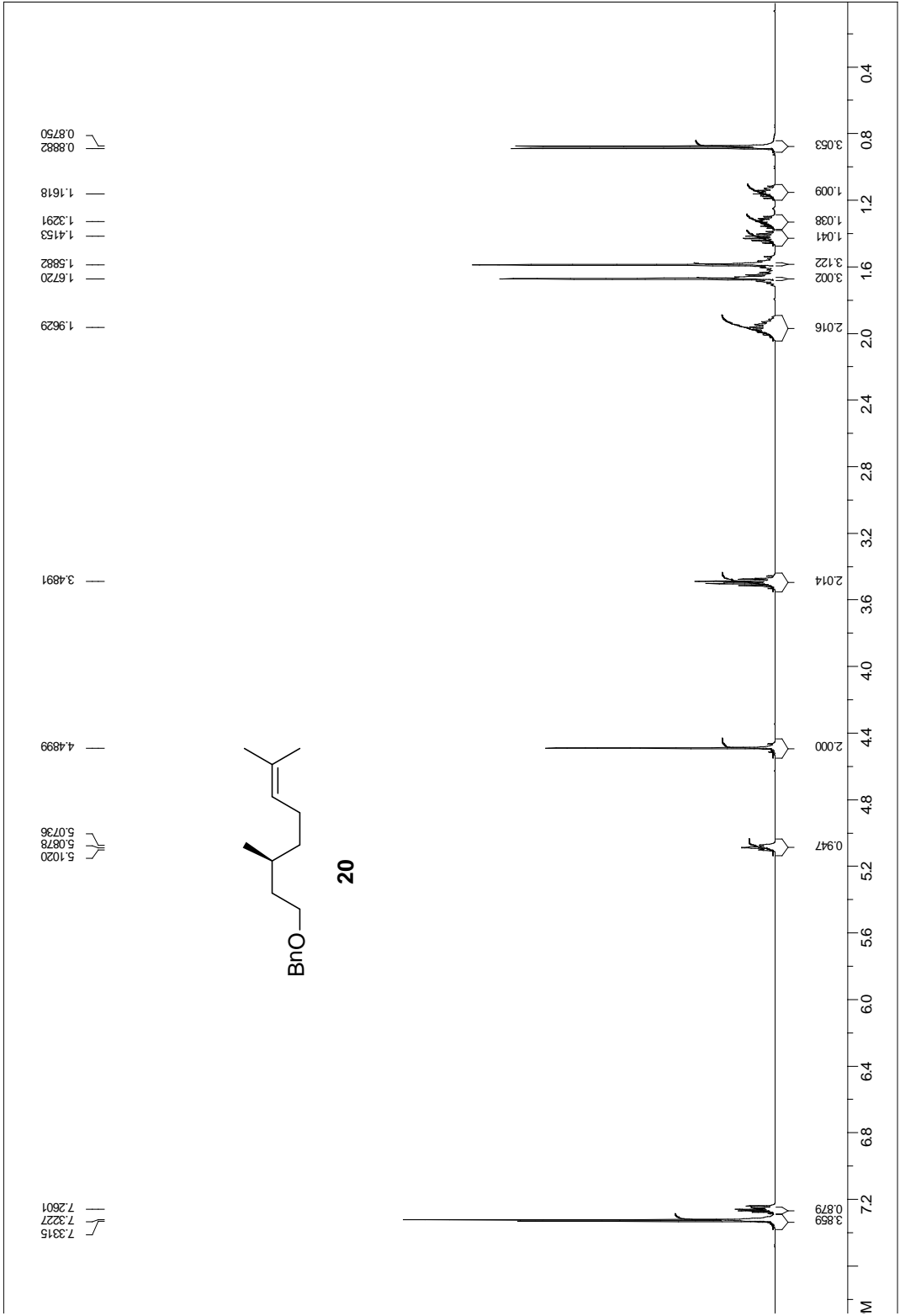






C:\Users\BVD\Desktop\Spec Data\NMR DATA\Wyz Project\Heptaprenol\1\1d exp1 ->g00-
 smilar file: 500.0202022.MHz
 carrier file: 65530.pcm.ms
 date: 20.06.2010 15:41:23
 bar of scans: 16
 freq of 0 ppm: 500.0202022.MHz
 processed size: 32788 complex.points
 LB: 0.000 GB: 0.0000

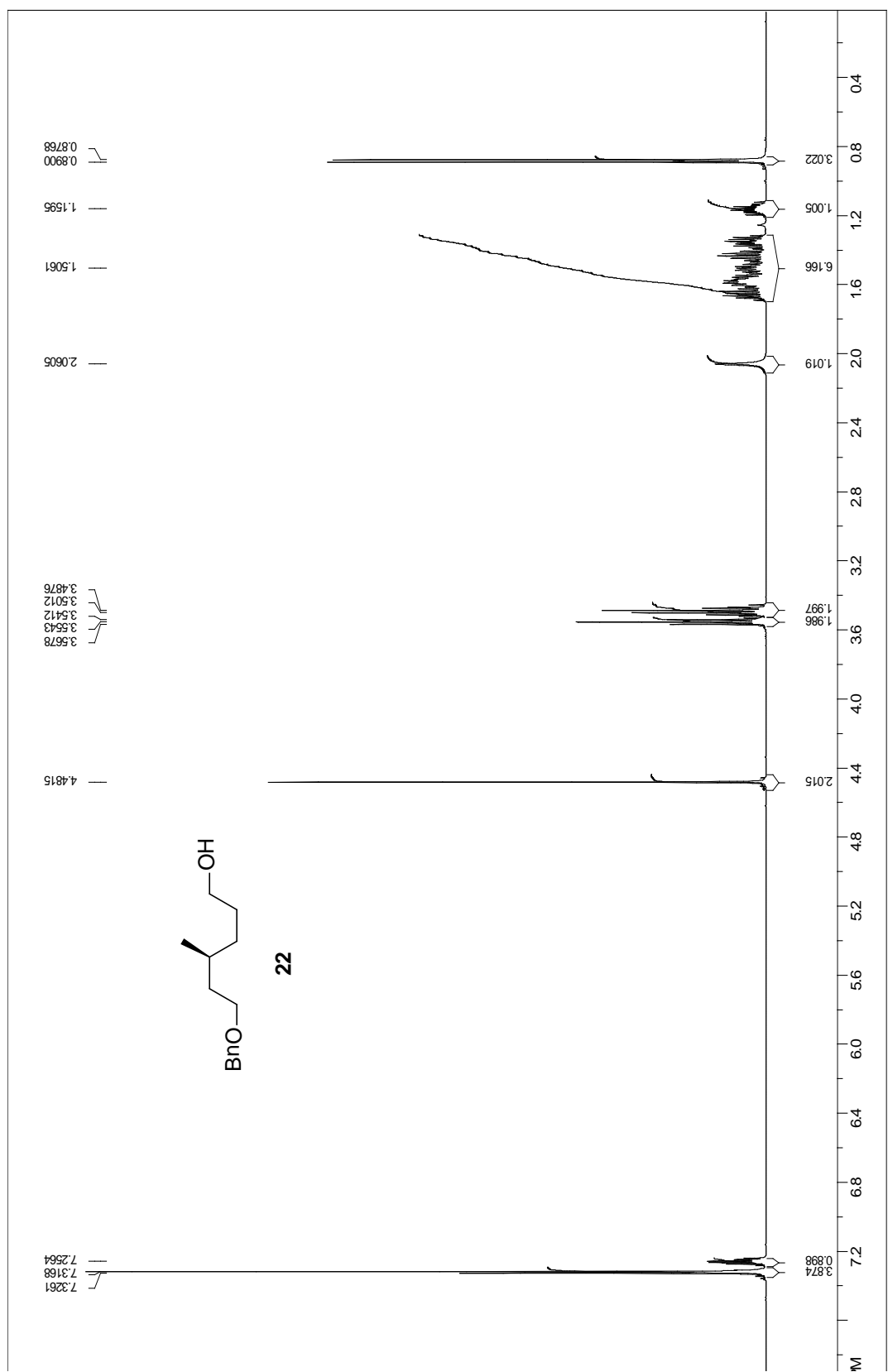




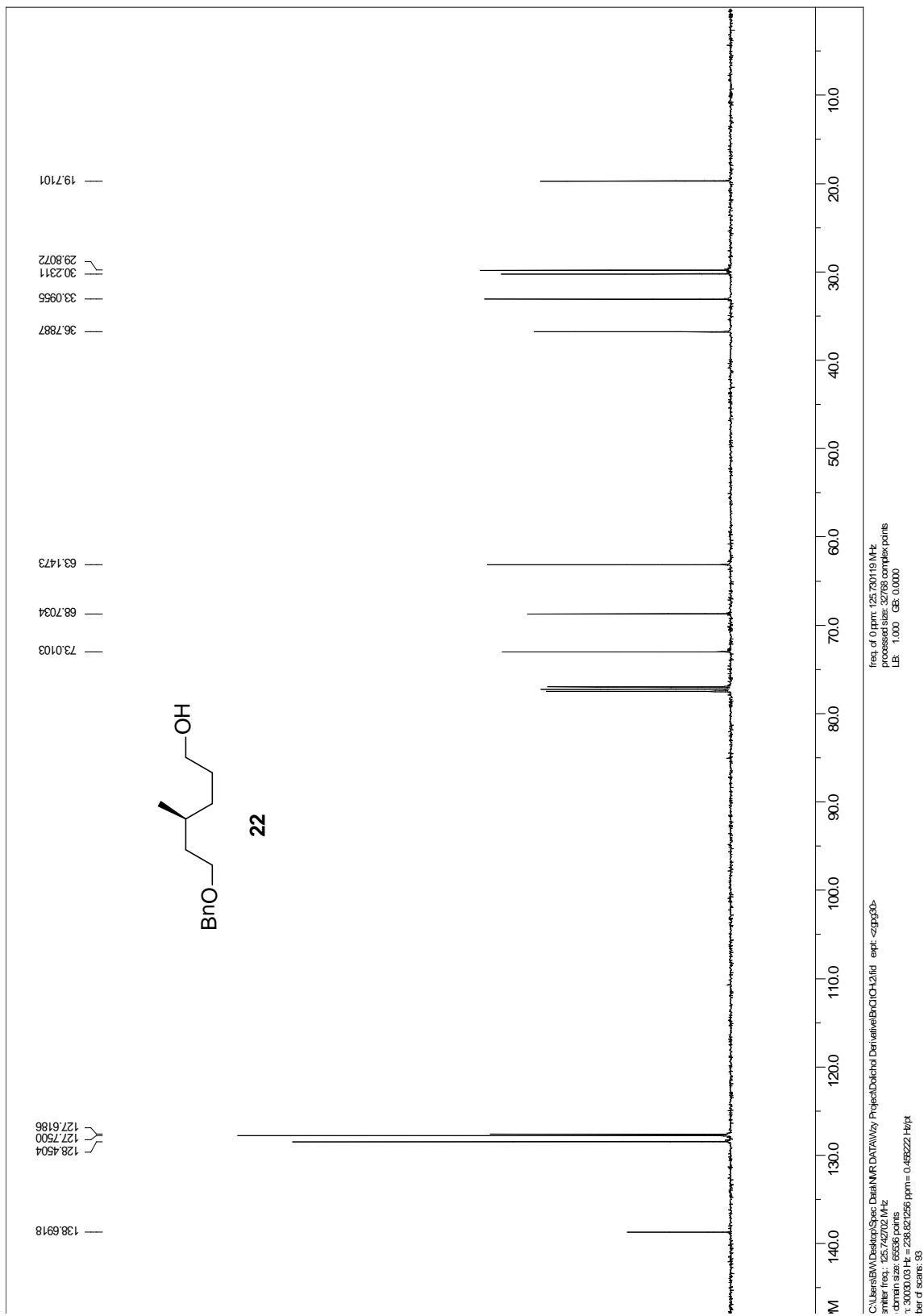
freq: 0 ppm; 50.02022 MHz
 Processed Size: 2768 complex points
 LS: 0.000 GB; 0.0000

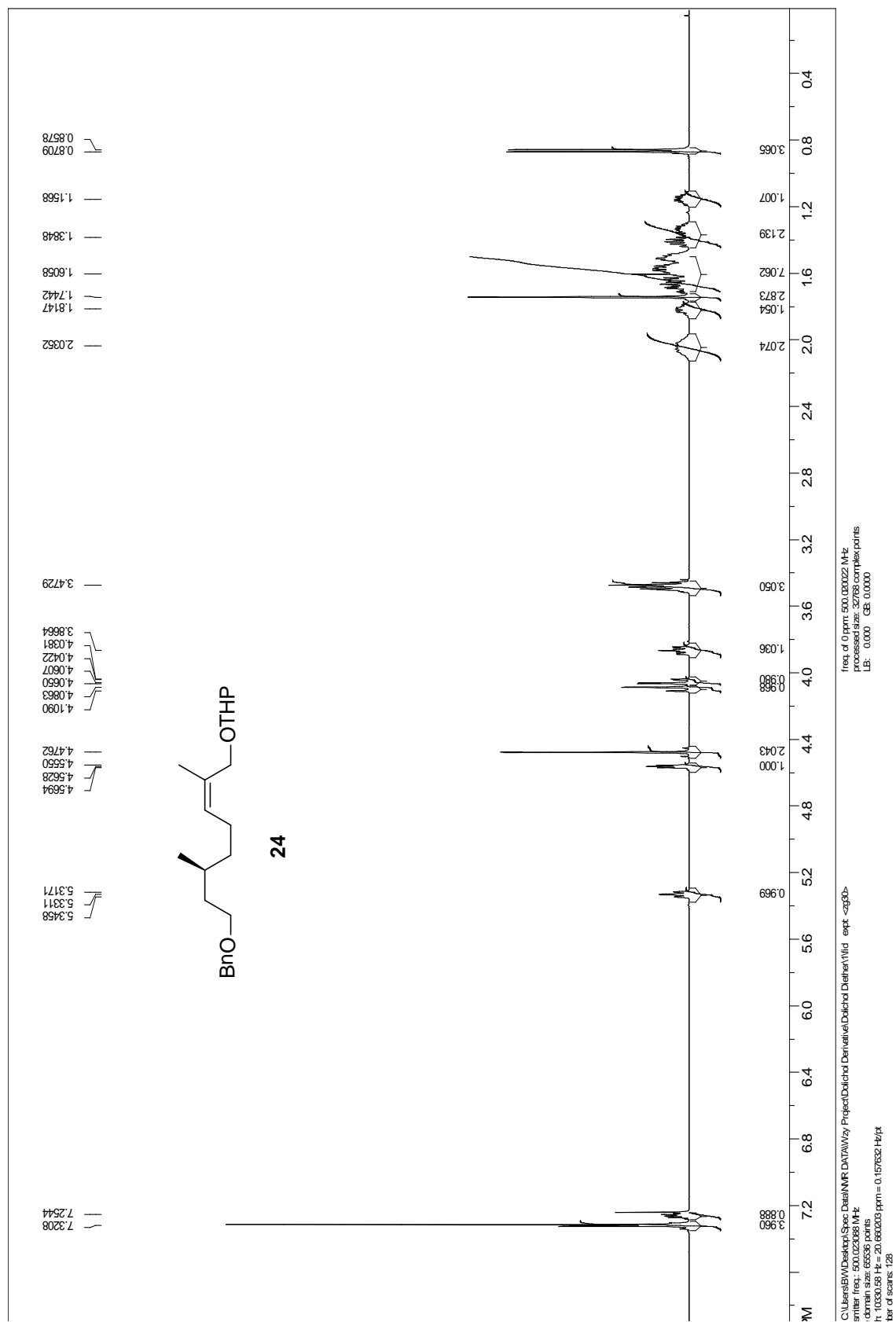
C:\Users\BVM\Desktop\Spec Data\NMR DATA\Wzy Project\Delchidol Derivative\BfCitronellol\11\td exp1 ->gfb->
 11/11/2011 10:30:58 AM
 Y: 10380.63 Hz = 20.692028 ppm = 0.157632 Hz/g
 ber of scans: 16

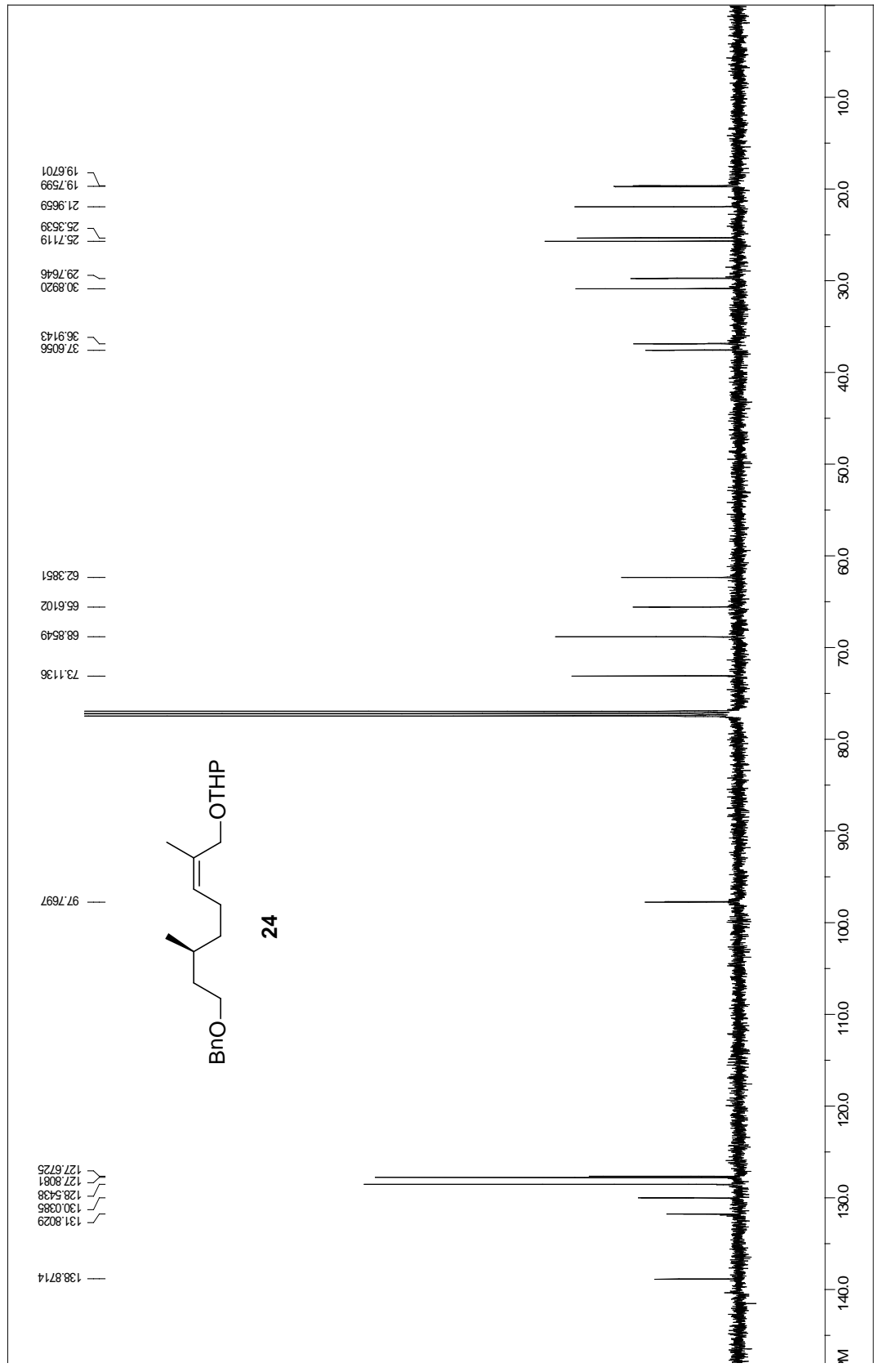




C:\Users\BWI\Desktop\Spec Data\NMR\DATA\Way Project\1Dolalol Derivative\BnOCH1\1d exp1 -srg50-
 smiter freq.: 500.022068 MHz
 domain size: 65636 points
 1: 10330.58 Hz = 20.660273 ppm = 0.157632 Hz/pt
 bar of scans: 128
 freq. of 0 ppm: 500.020021 MHz
 processed size: 32768 complex/points
 LB: 0.000 GB 0.0000

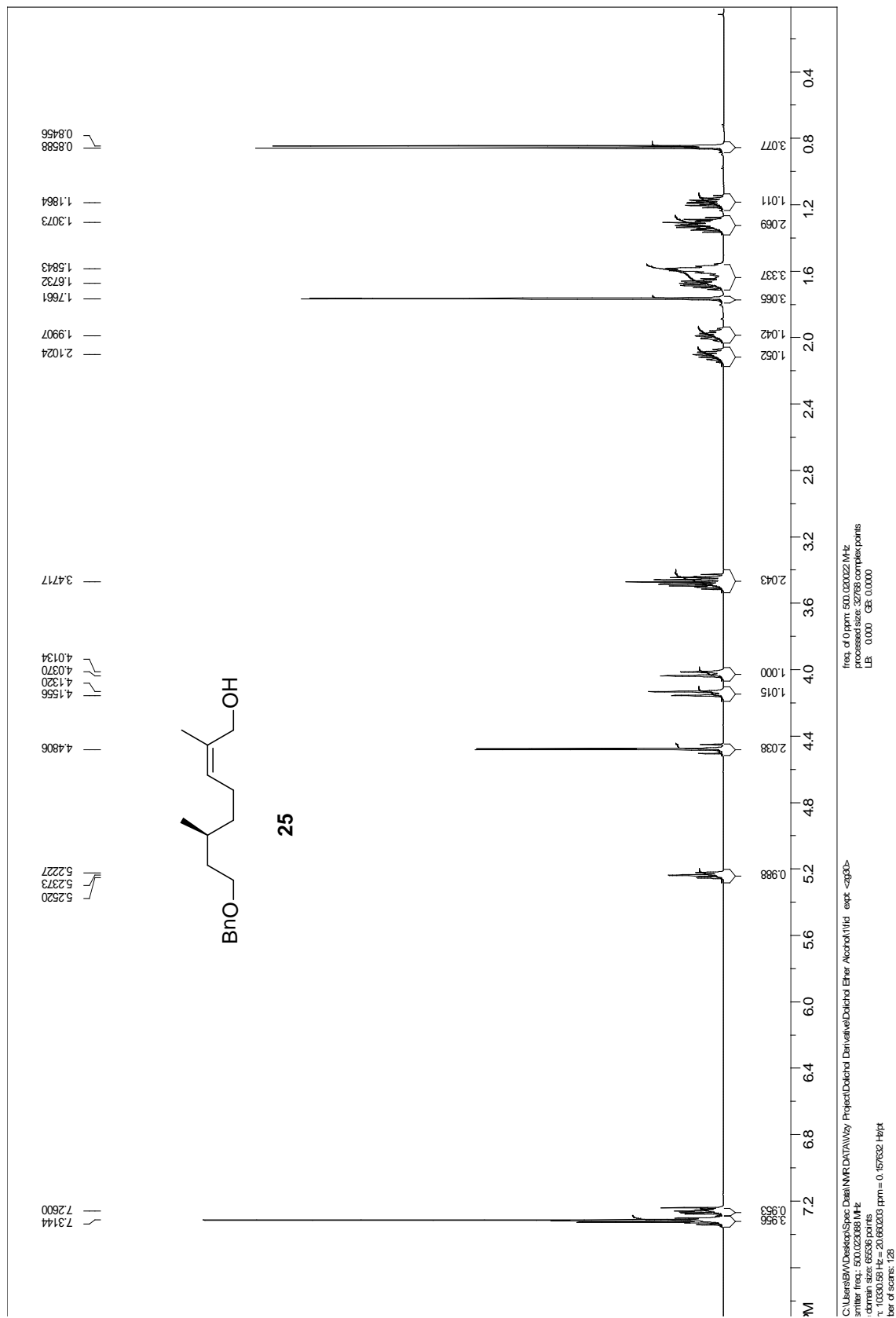


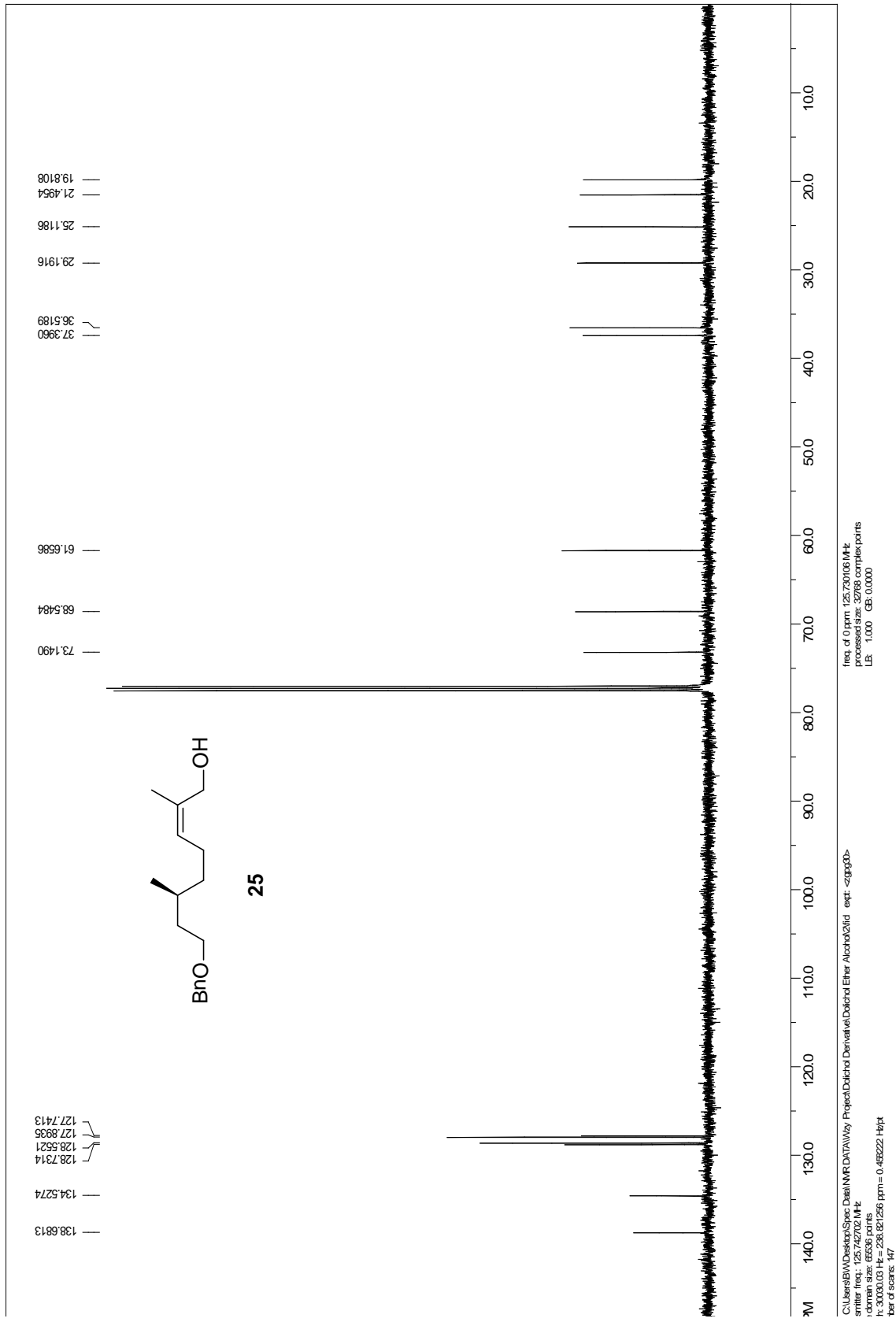


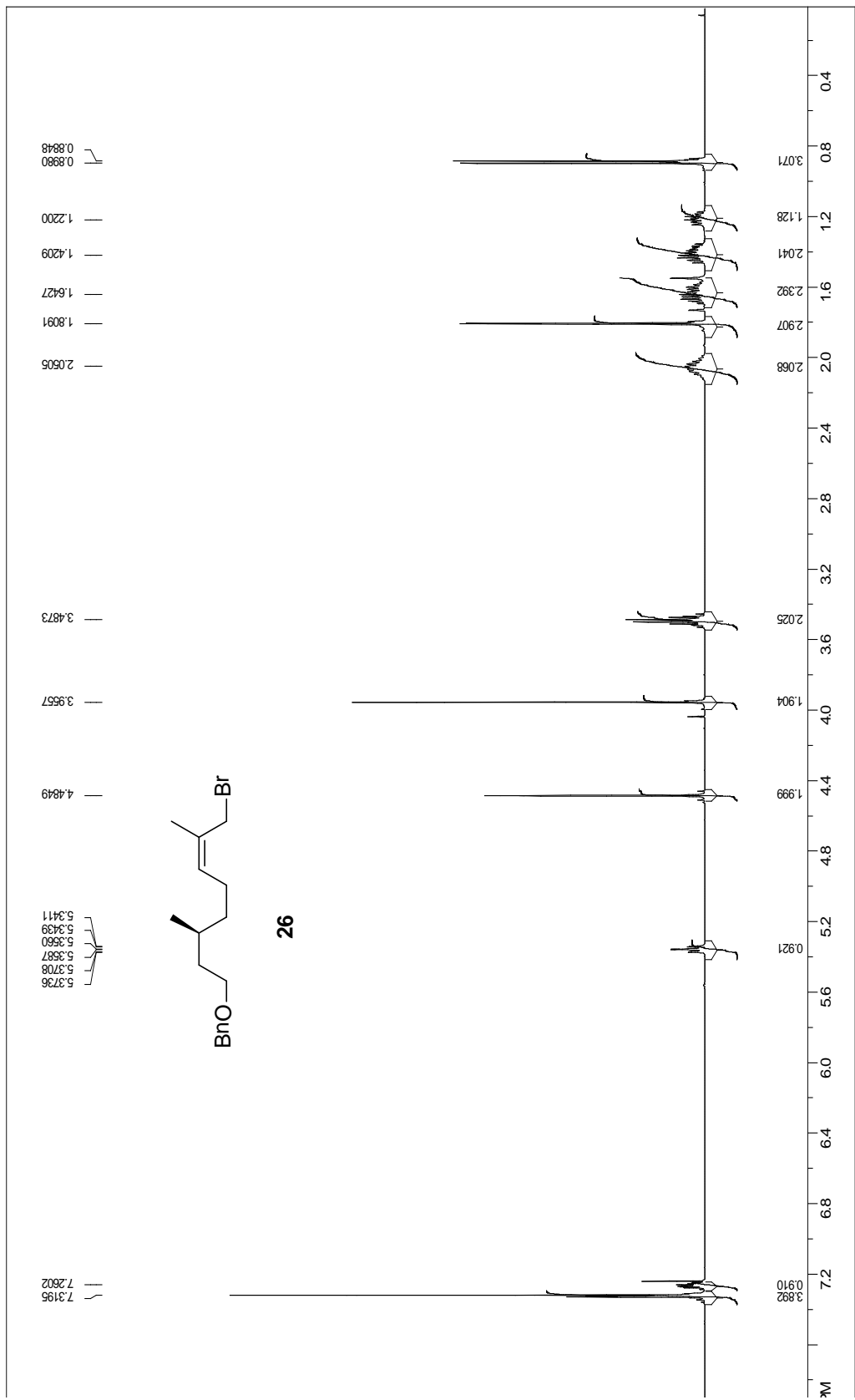


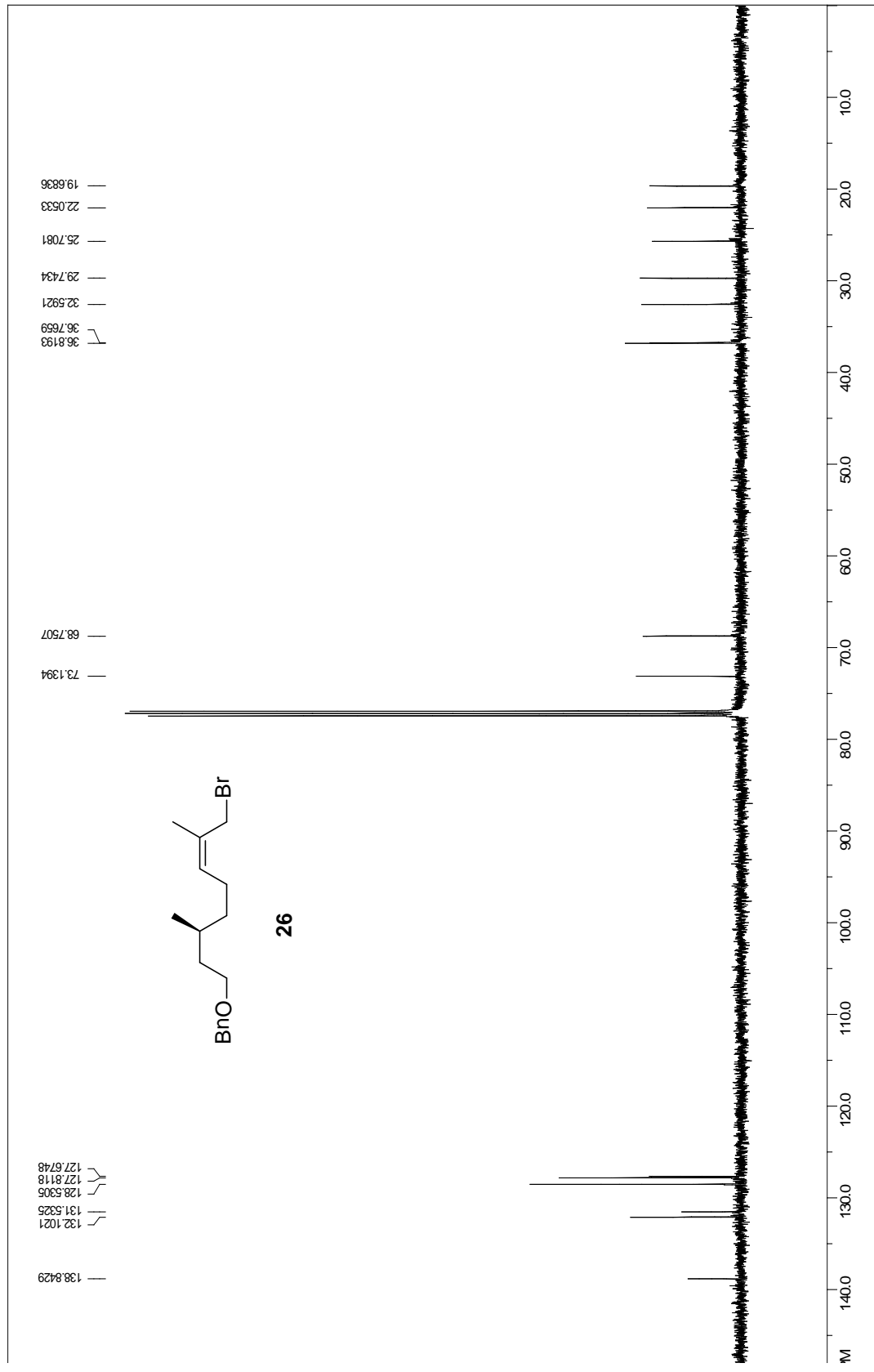
freq. of 0 ppm: 125.730108 MHz
 processed size: 327788 complex points
 LB: 1.000 GB 0.00000

C:\Users\BWD\Desktop\Spec Data\NMR DATA\Wzy Project\Dalchini Derivative\Dalchini Diether\2\1d exp1 -s3g3g3-
 smiler freq.: 125.742702 MHz
 channel: 600.131415
 compound: 24
 date: 2018.08.12 08:12:56 ppm= 0.468222 Hzpt
 bar of scans: 256



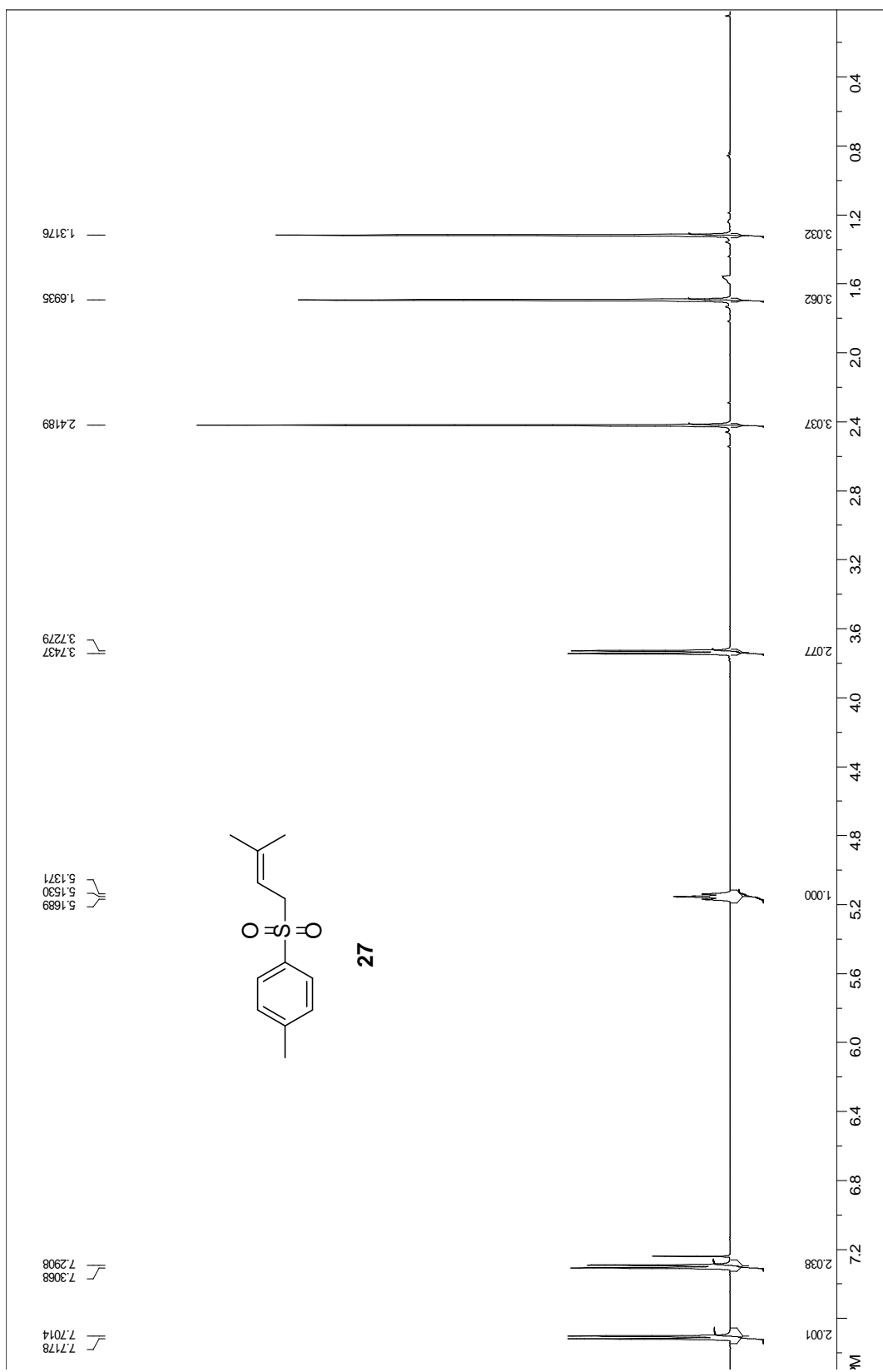




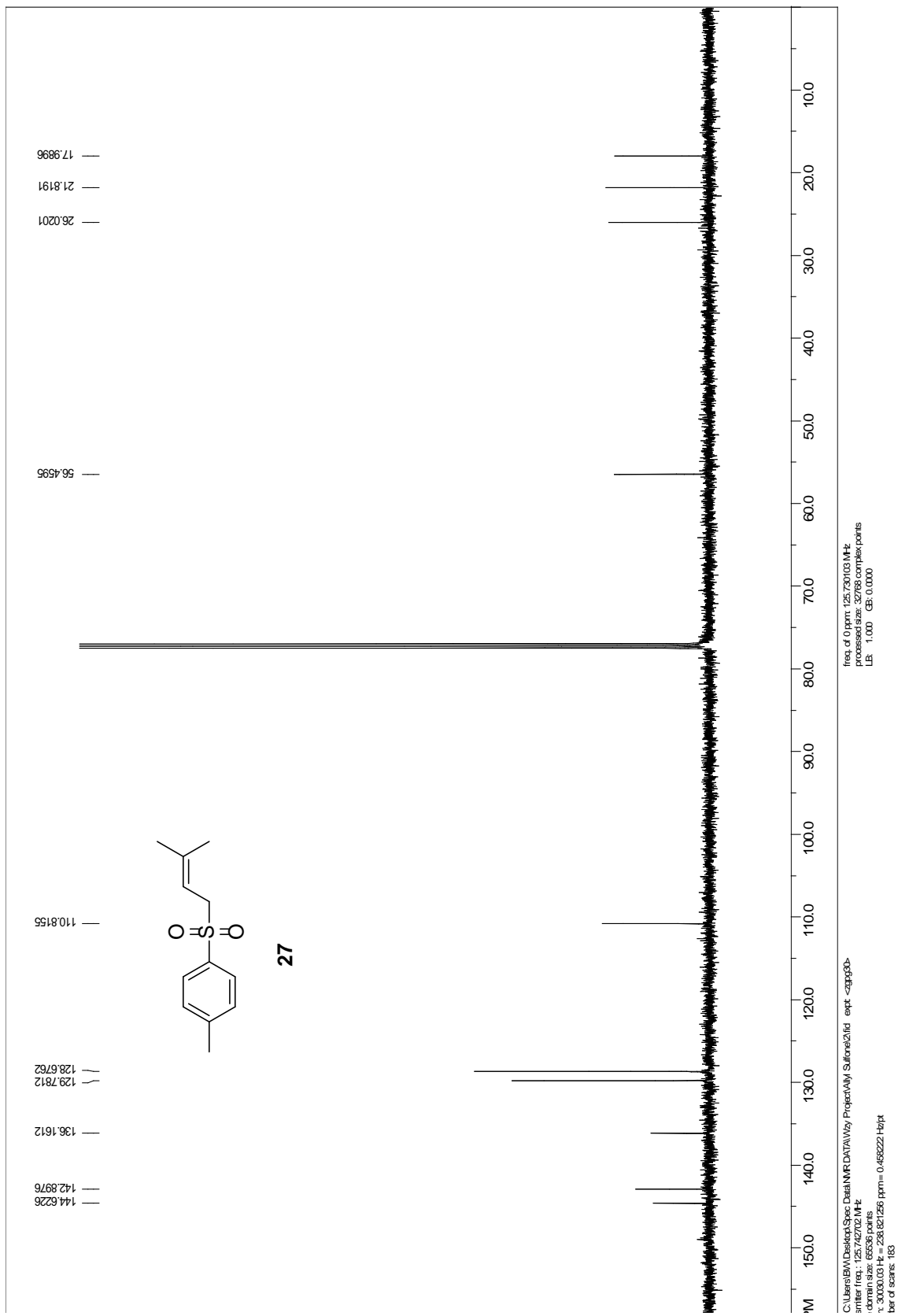


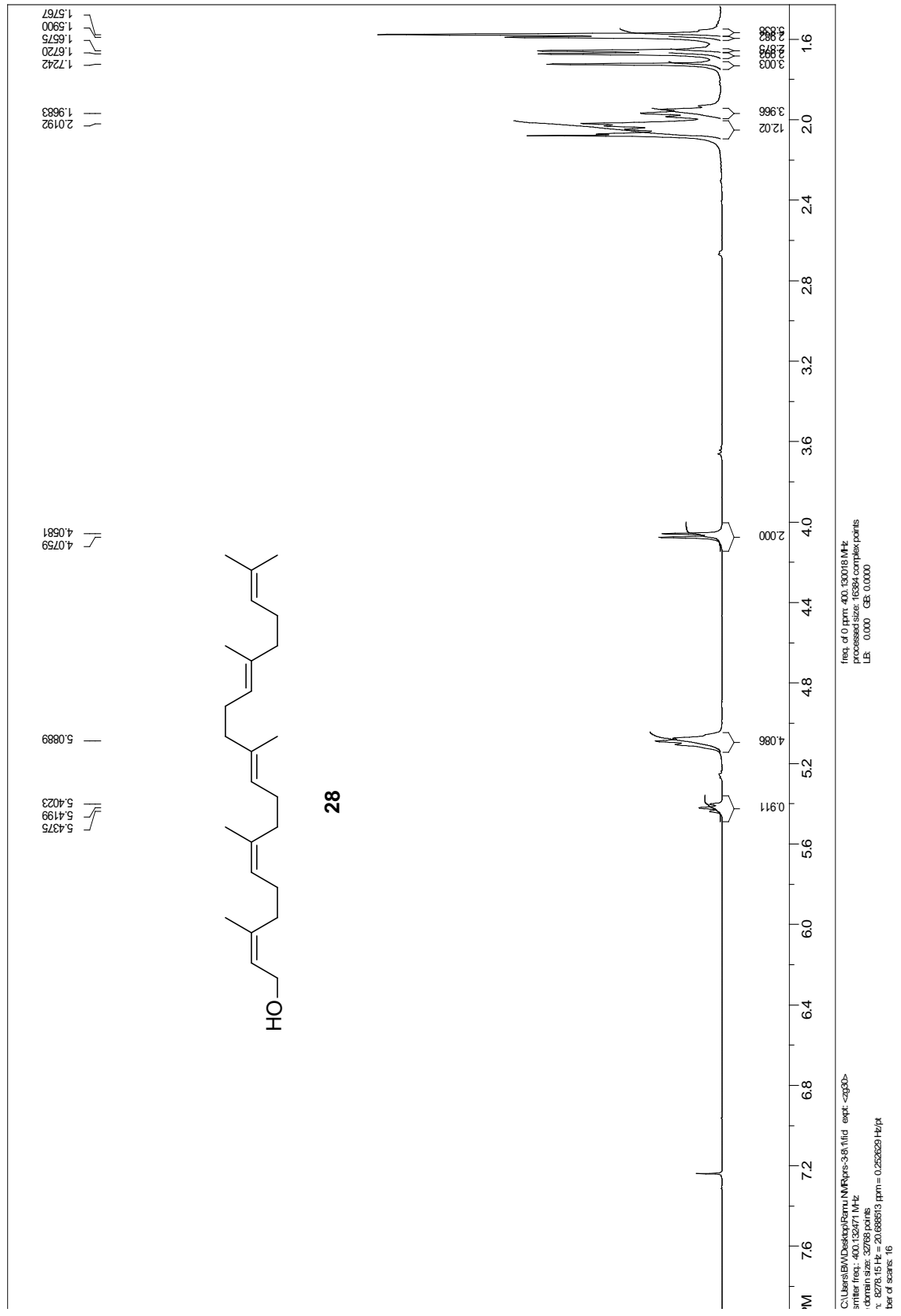
freq. of 0 ppm: 125.730105 MHz
 processed size: 327788 complexpoints
 LB: 1.000 GB: 0.00000

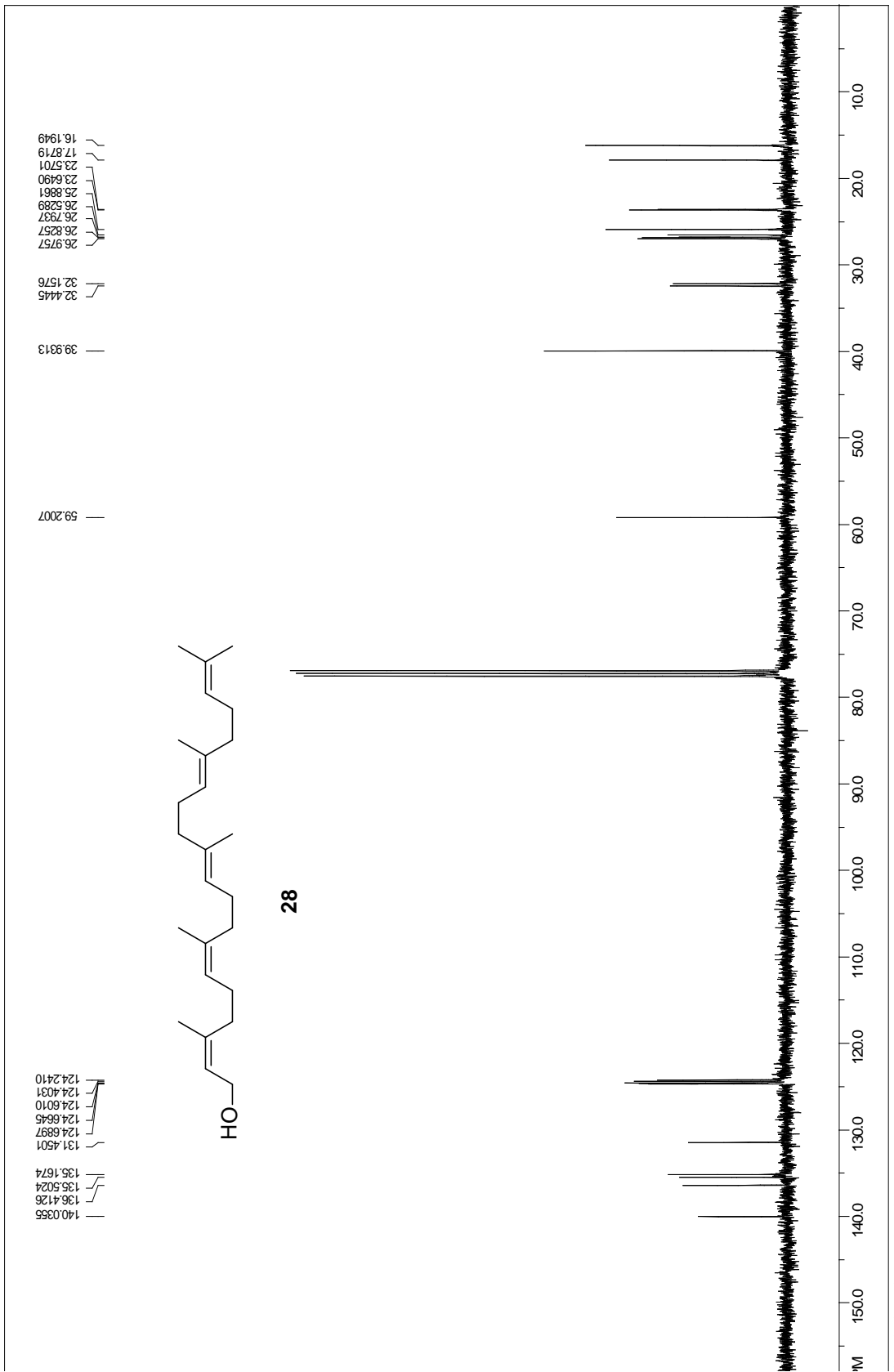
C:\Users\BWD\Desktop\Spec Data\NMR\DATA\Wzy Project\Delta1chd Derivative\Delta1chd Coupling Bromide\21id exp1 -z9g95d-
 smiler freq.: 125.742702 MHz
 domain size: 65536 points
 T: 3000.031 Hz = 238.627256 ppm = 0.459222 Hz
 bar of scans: 170



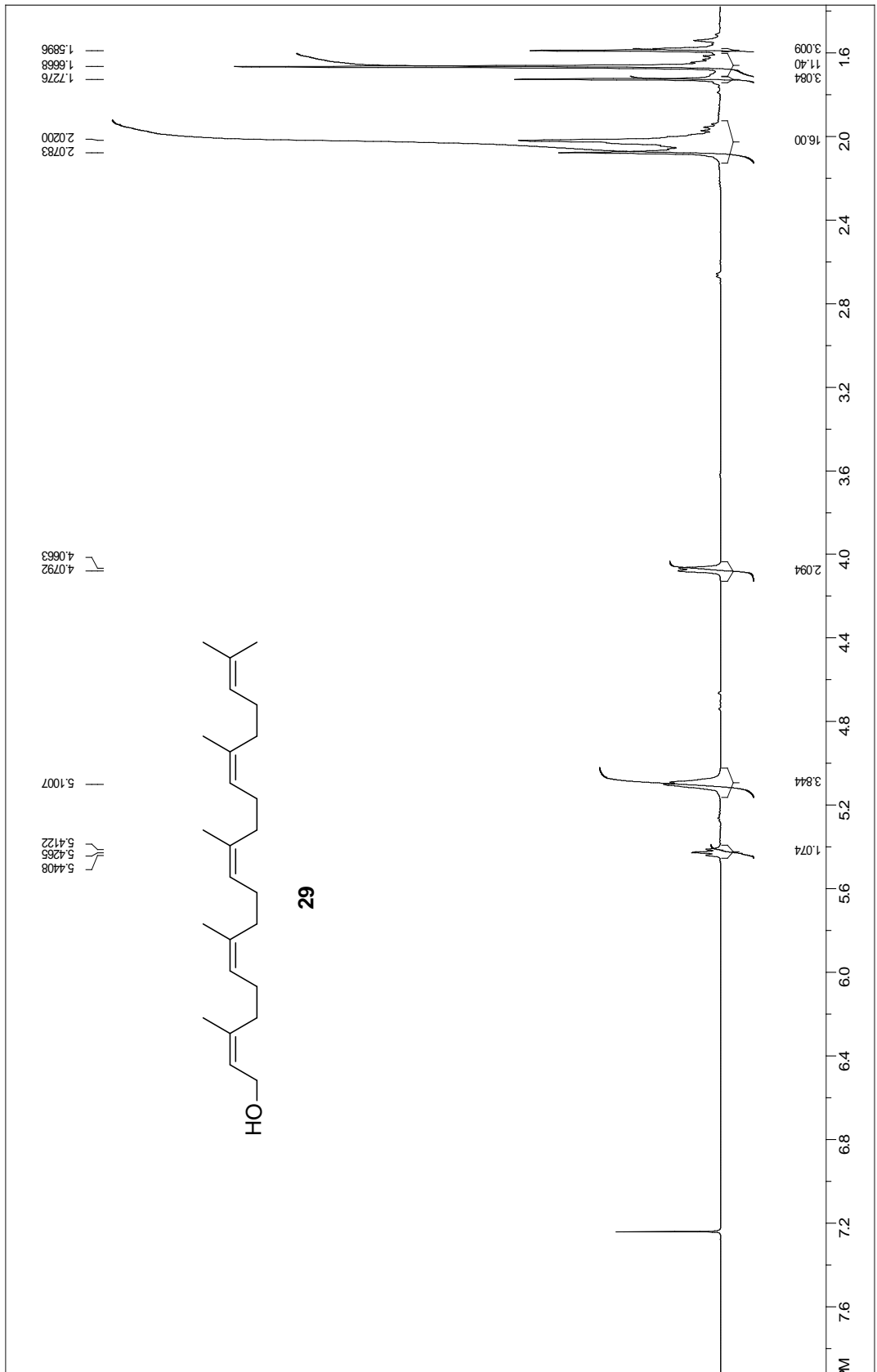
C:\Users\BVA\Desktop\Spec Data\NMR DATA\Wzy Project\NMR\111d exp1 -zgg0-
 smiler freq.: 600.023088 MHz
 domain size: 65536 points
 Ir: 10350.58 Hz = 20.66203 ppm = 0.157632 Hz/pt
 Bar of scale: 36
 freq. of 0 ppm: 500.020021 MHz
 processed size: 32768 complex points
 LB: 0.300 GB 0.0000



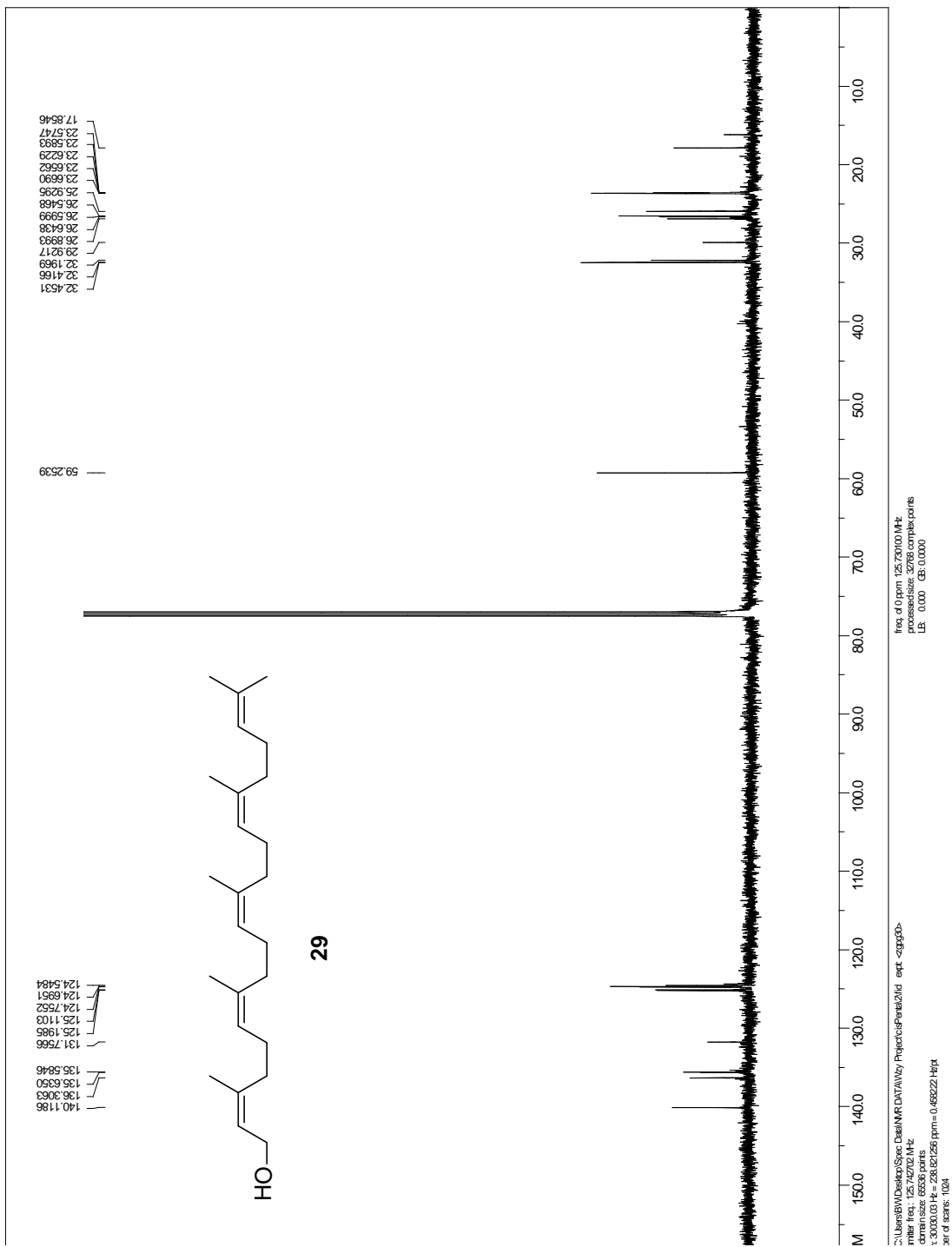


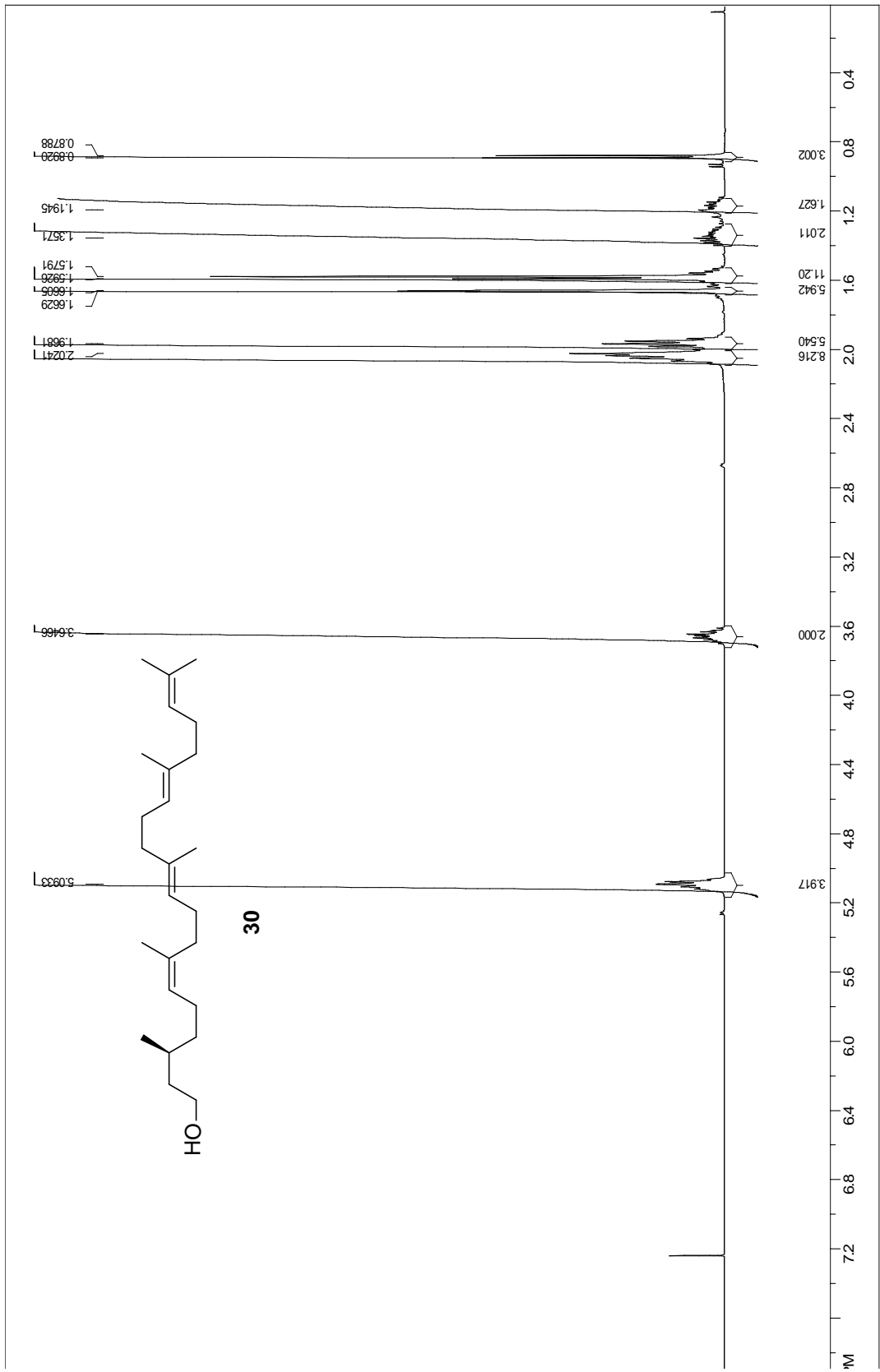


C:\Users\BVM\Desktop\p18anu\NMR\ps-3-8-21\rd_apt_
 -smile: 100.612748 MHz
 -domain size: 65536 points
 -f: 23880.02 Hz = 238.328802 ppm = 0.365161 Hz
 -bar of scans: 160
 freq: 0 ppm: 100.612748 MHz
 processed size: 32768 complex points
 LB: 1.000 GB 0.0000



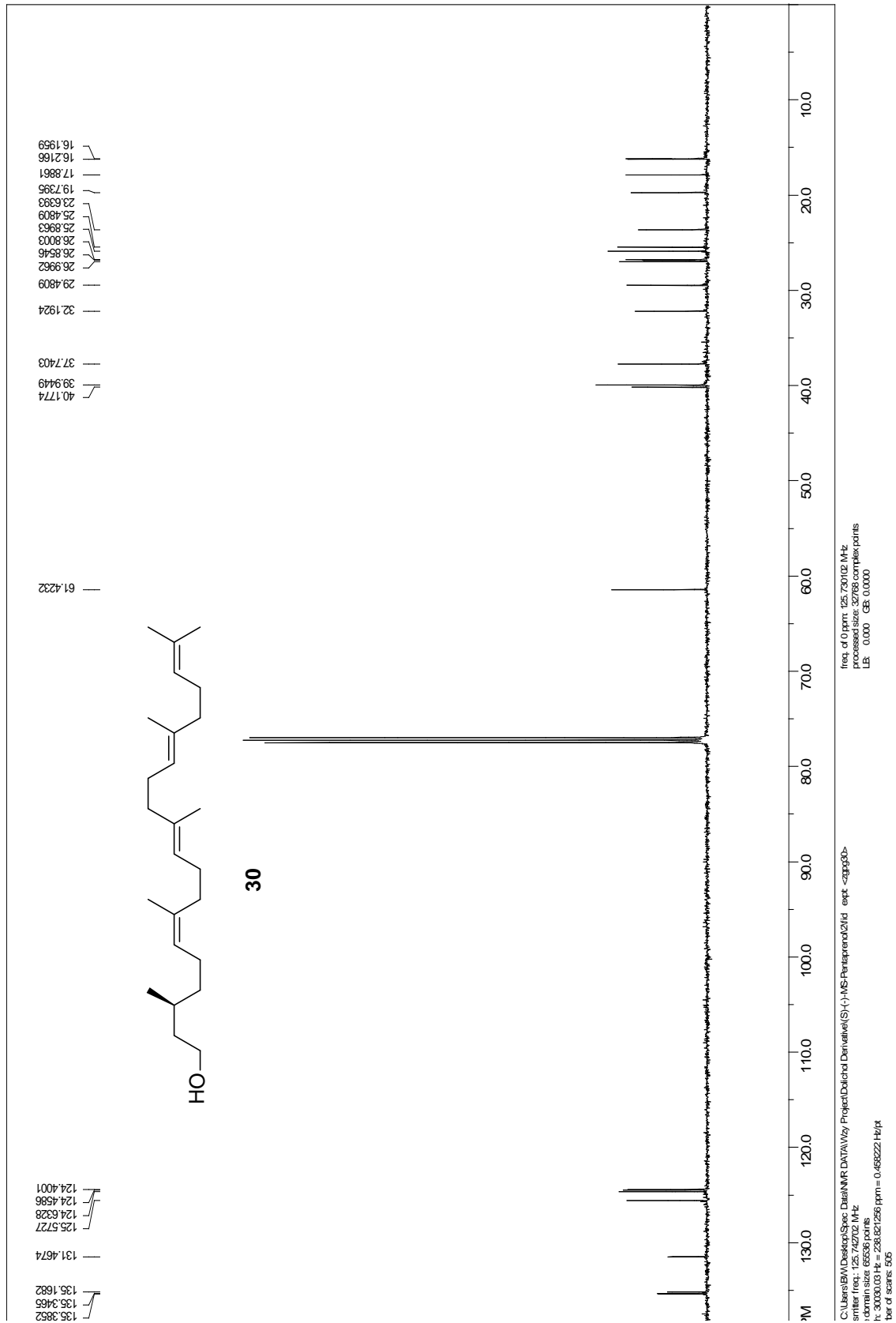
C:\Users\BAM\Desktop\Spec Data\NMR\DATA\Wzy Project\cis\Panel\1\ld exp1 - <zg00>
 smiller (freq.: 500.022038 MHz)
 - domain size: 65536 points
 fr: 10330.88 Hz = 20.662003 ppm = 0.157632 Hz/pt
 tot of scans: 16
 freq. of 0 ppm: 500.022022 MHz
 processed size: 32768 complex points
 LB: 0.000 GB: 0.0000

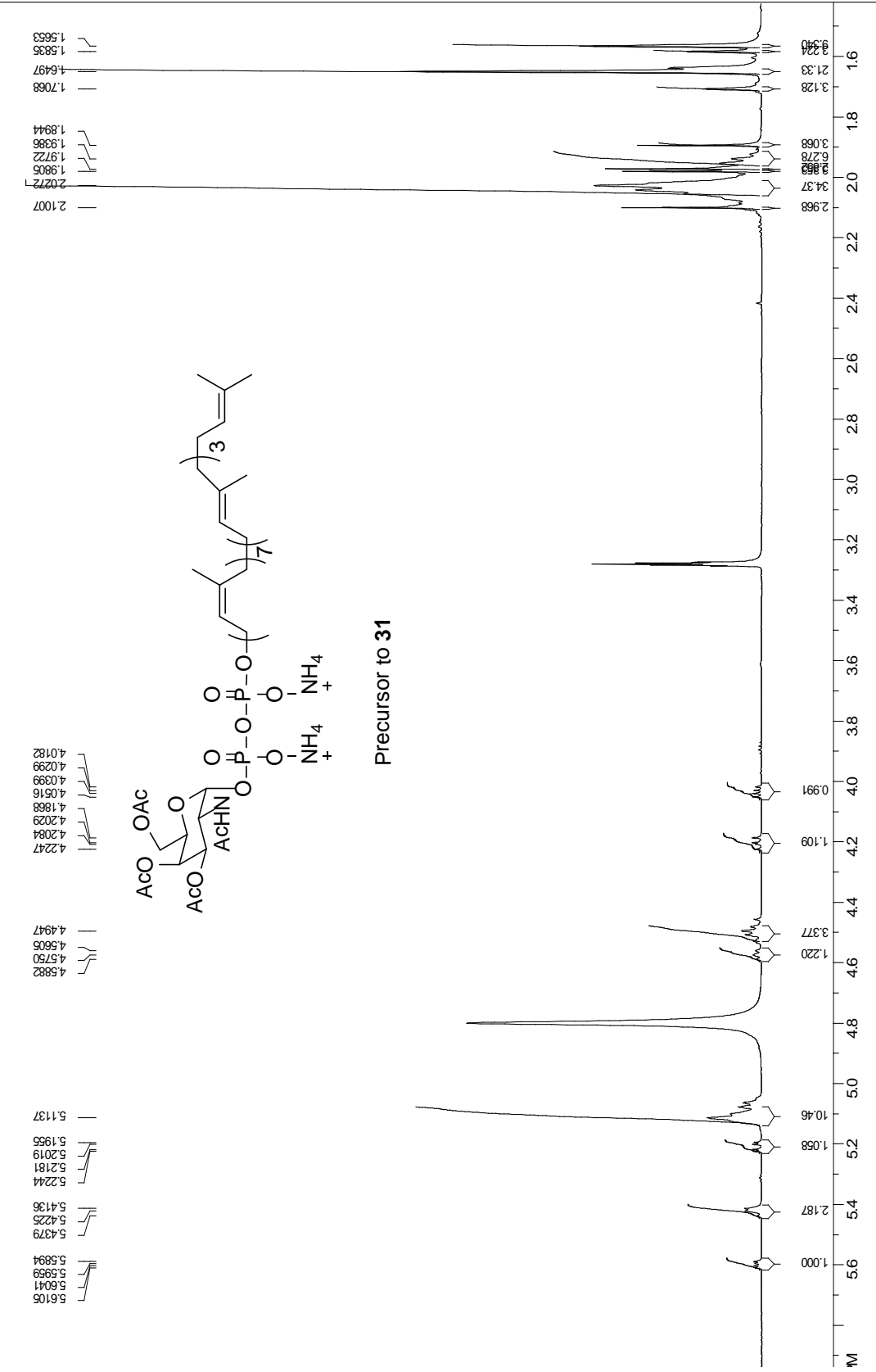




File: 01000022 MHz
 processed size: 32768 complex points
 LS: 0.000 GB: 0.0000

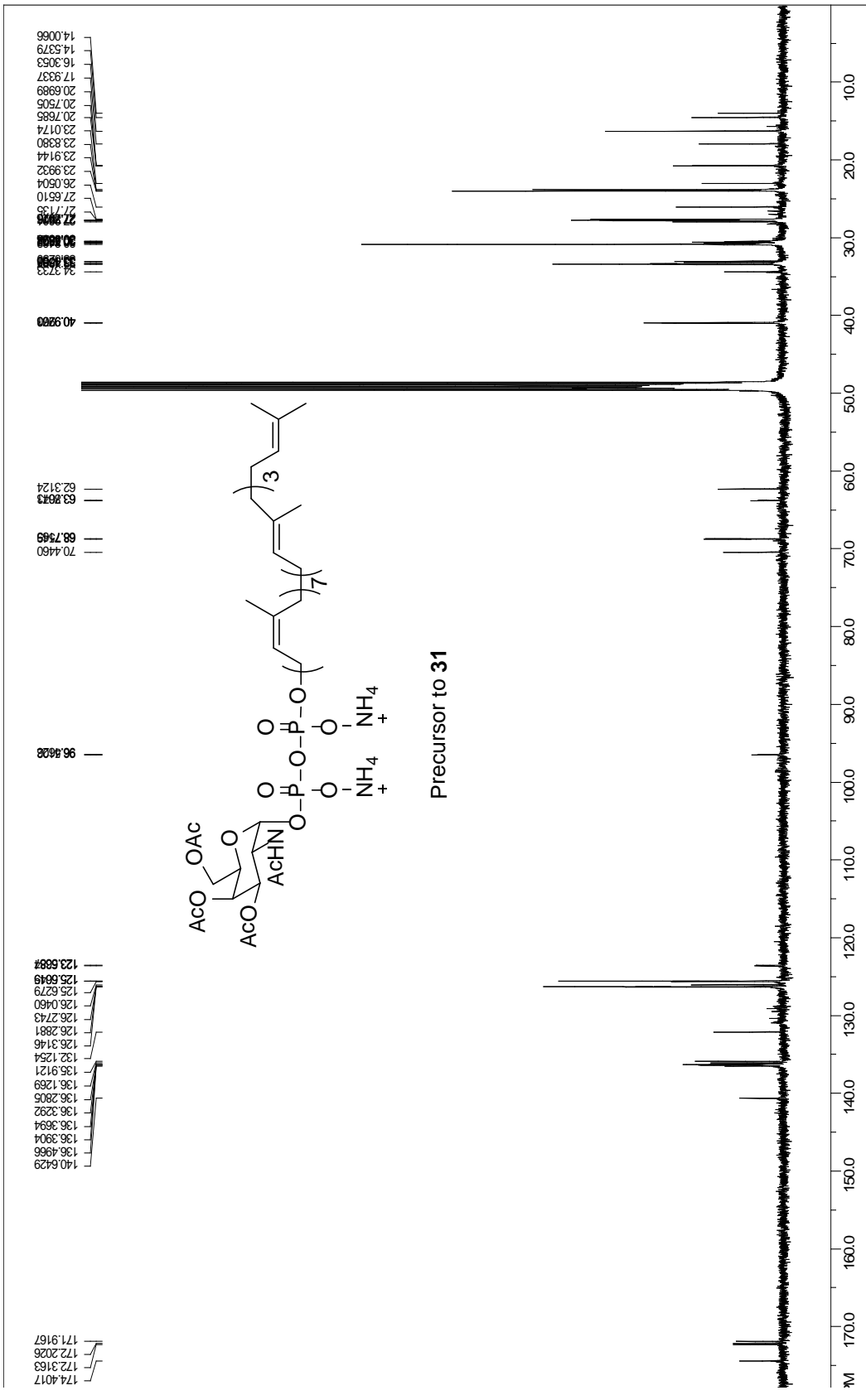
C:\Users\BMD\Desktop\Spec Data\NMR DATA\Way Project\Baldich\Derivative(S)-(-)-MS-Pentiprenol\1\fid exp1 <2>g30>
 smiter freq: 500.022000 MHz
 65530 points
 101800.591 Hz 21.000000 ppm = 0.157652 Hz/pt
 bar of scans: 1/28





freq. of 0 ppm: 500.000204 MHz
processed size: 32788 complex points
LB: 0.000 GB: 0.0000

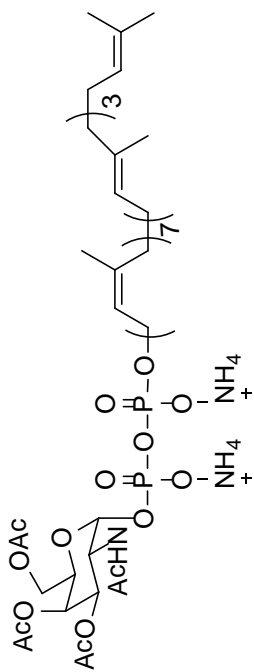
MACOSY-PR1.tic1.tif, exp: <g>
acifur freq.: 500.020388 MHz
domain size: 65536 points
gamma: 10030.59 Hz = 20.662023 ppm = 0.157632 Hz/pt
bar of scans: 64



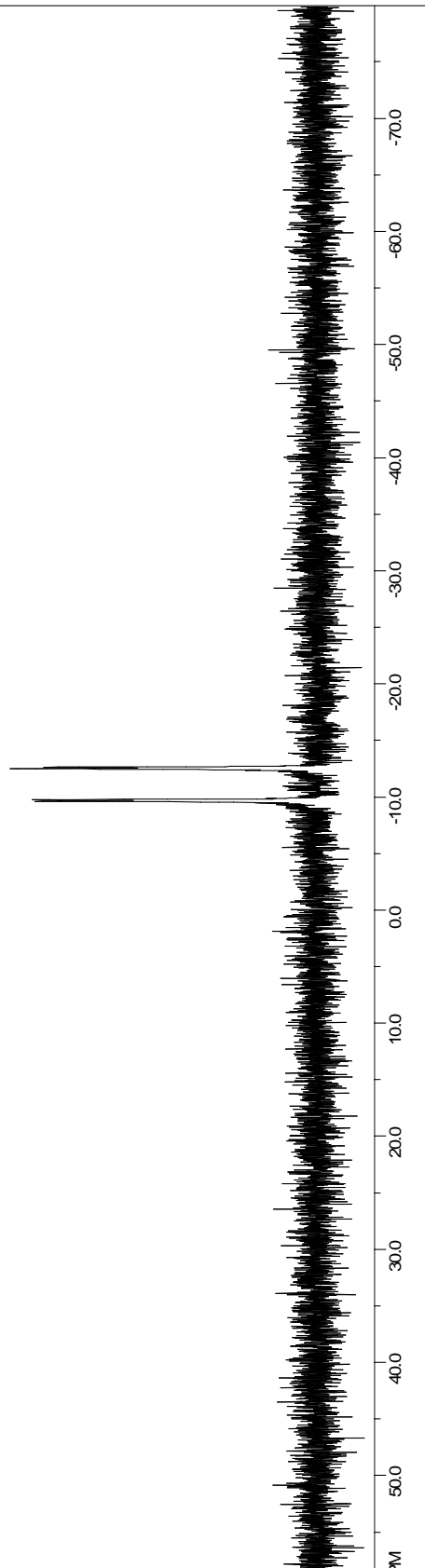
J:\AccG\1\NMR\1257252\2\data exp1 ->3pp030-
 emitter freq.: 125.742702 MHz
 domain size: 65536 points
 time resolution: 0.2821250 ppm = 0.455222 Hz
 bar of scales: 15086

freq. of 0 ppm: 125.725839 MHz
 processed size: 32768 complex points
 LB: 1.000 GB 0.0000

-12.6260
 -9.6206
 -9.7581

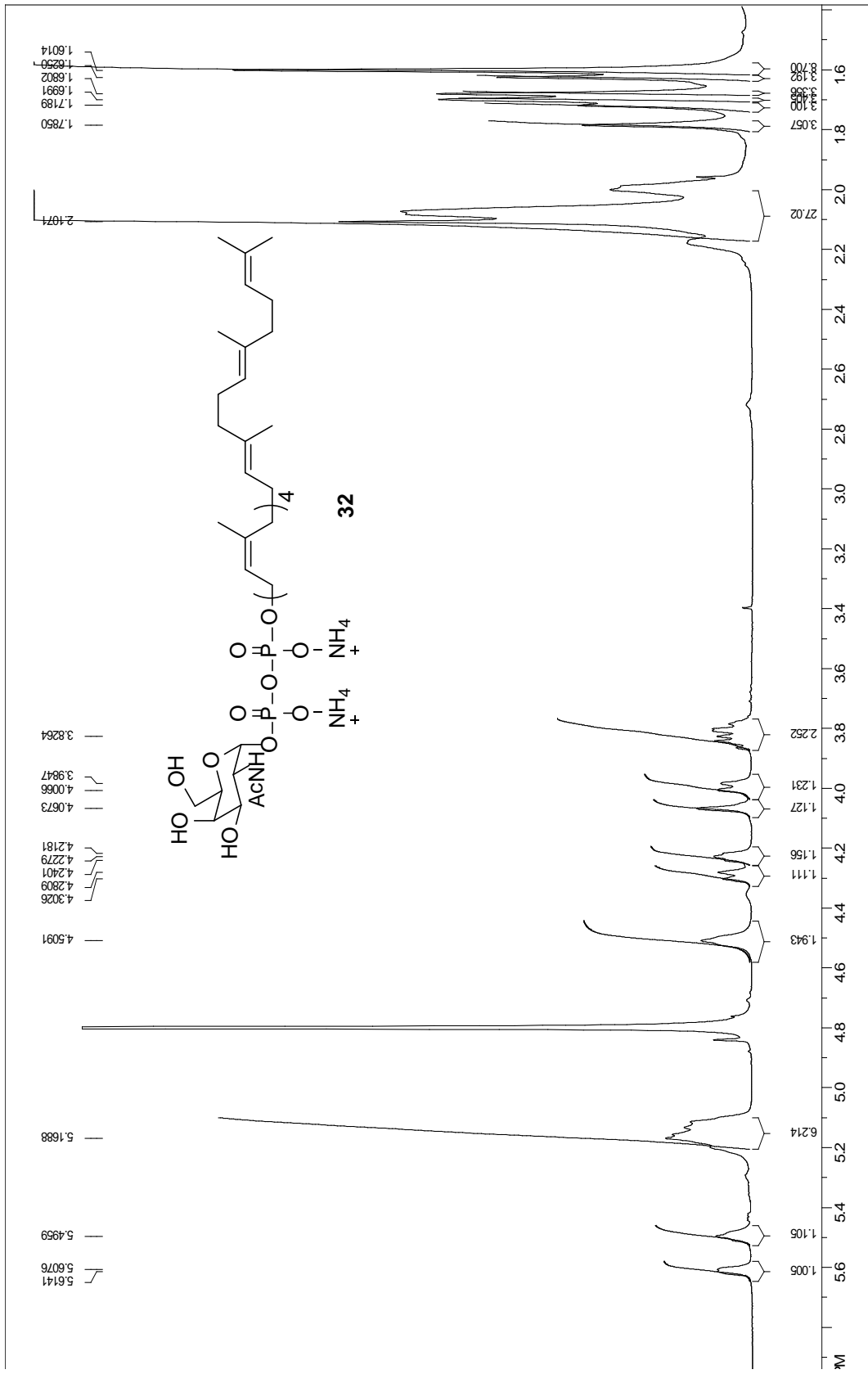


Precursor to **31**

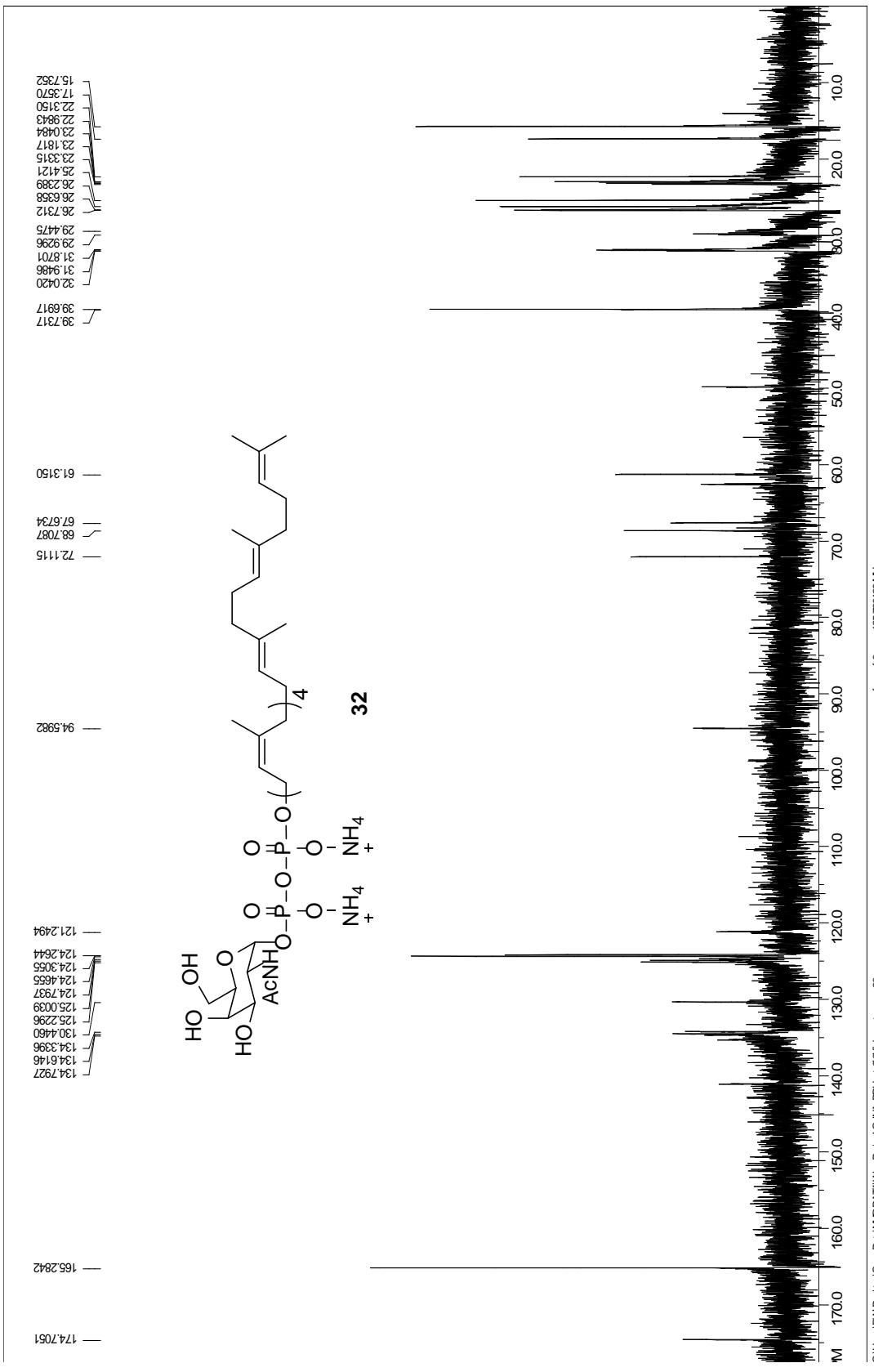


J:\Gait\NMR\1h\PC\res\1h1.f exp: <agg33>
 Date_ Acq: 20130714
 Chem: 31
 Chem: 31
 Conv: 1000 Hz = 400.914228 ppm = 0.9800630 Hz
 Num of scans: 728

freq. of 0 ppm: 61.975488 MHz
 Processed: 20130714
 Gain: 1.000 GB 0.0000



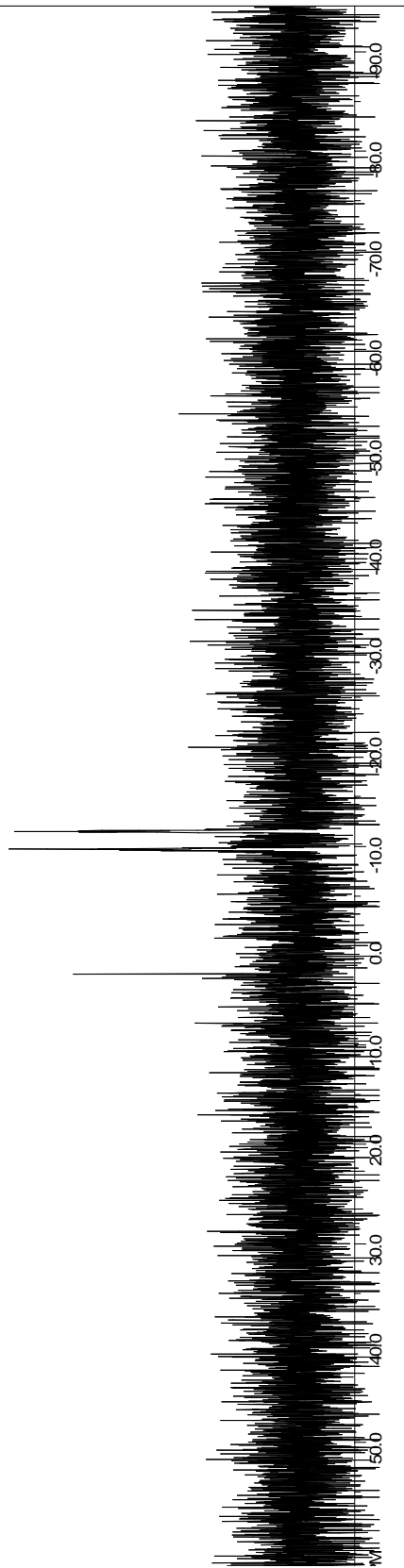
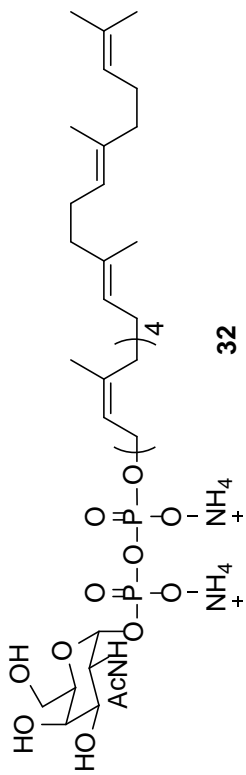
C:\Users\BMD\Desktop\Spec Data\NMR\DATA\Wzy Project\GAIN\CPPT\Hpt2\1161 exp1 <3g30>
 smilar freq.: 500.132069 MHz
 domain size: 65536 points
 ft: 10330.59 Hz = 20.662003 ppm = 0.157632 Hz/pt
 no. of scans: 64
 LB: 0.000 GB: 0.0000
 processed size: 32788 complex points
 freq.: 410 ppm: 500.132069 MHz



freq. of 0 ppm: 125.730125 MHz
 processed size: 32788 complex points
 LB: 0.000 GB: 0.0000

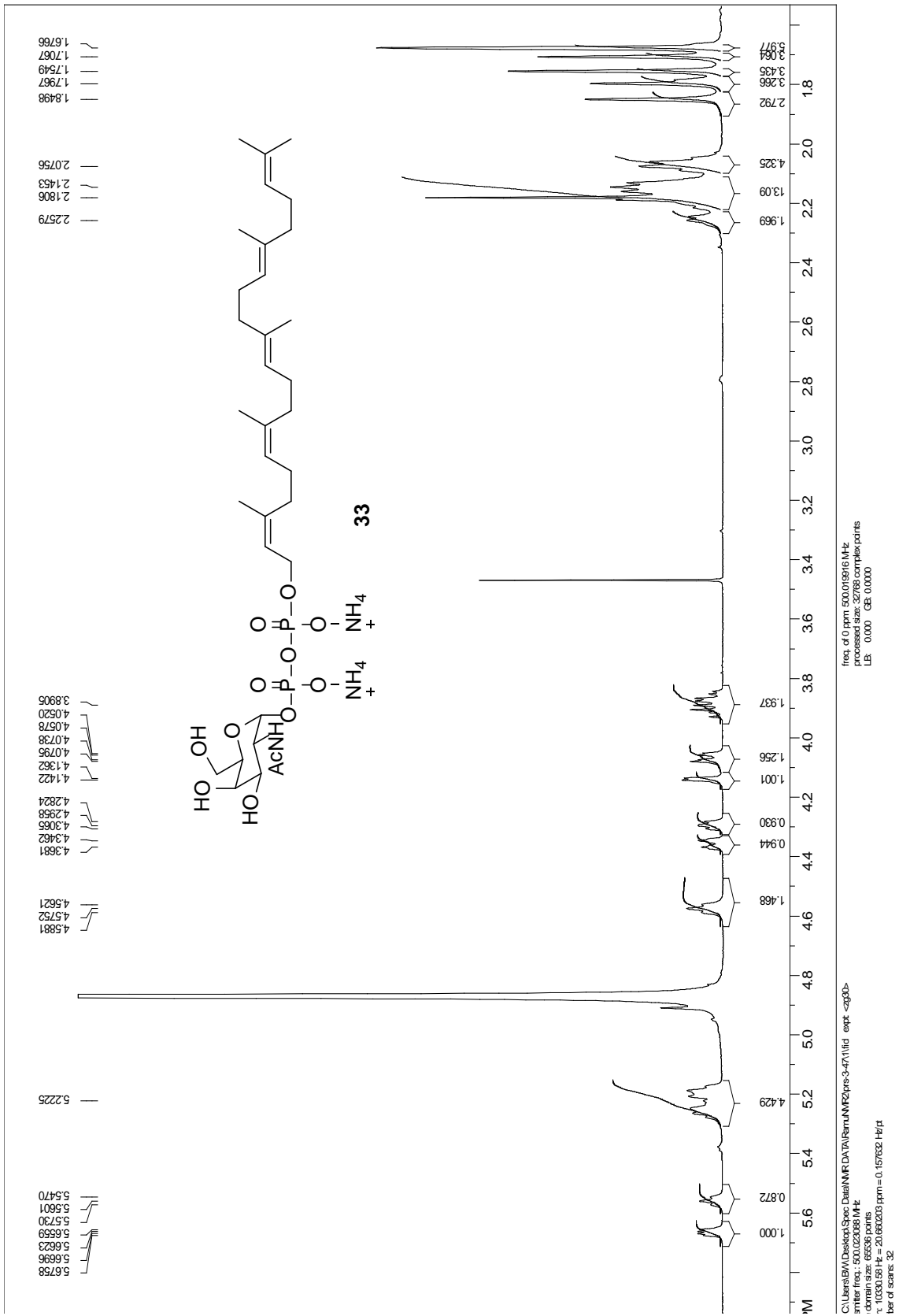
C:\Users\BWI\Desktop\Spec Data\NMR\DATA\Wzy Project\Gal\GalMcPFP\pp2\21\fid_esp1--ppg30-
 smiter freq.: 125.742702 MHz
 domain size: 65536 points
 x: 30000.03 Hz = 238.821256 ppm = 0.458222 Hz/pt
 ber of scans: 12505

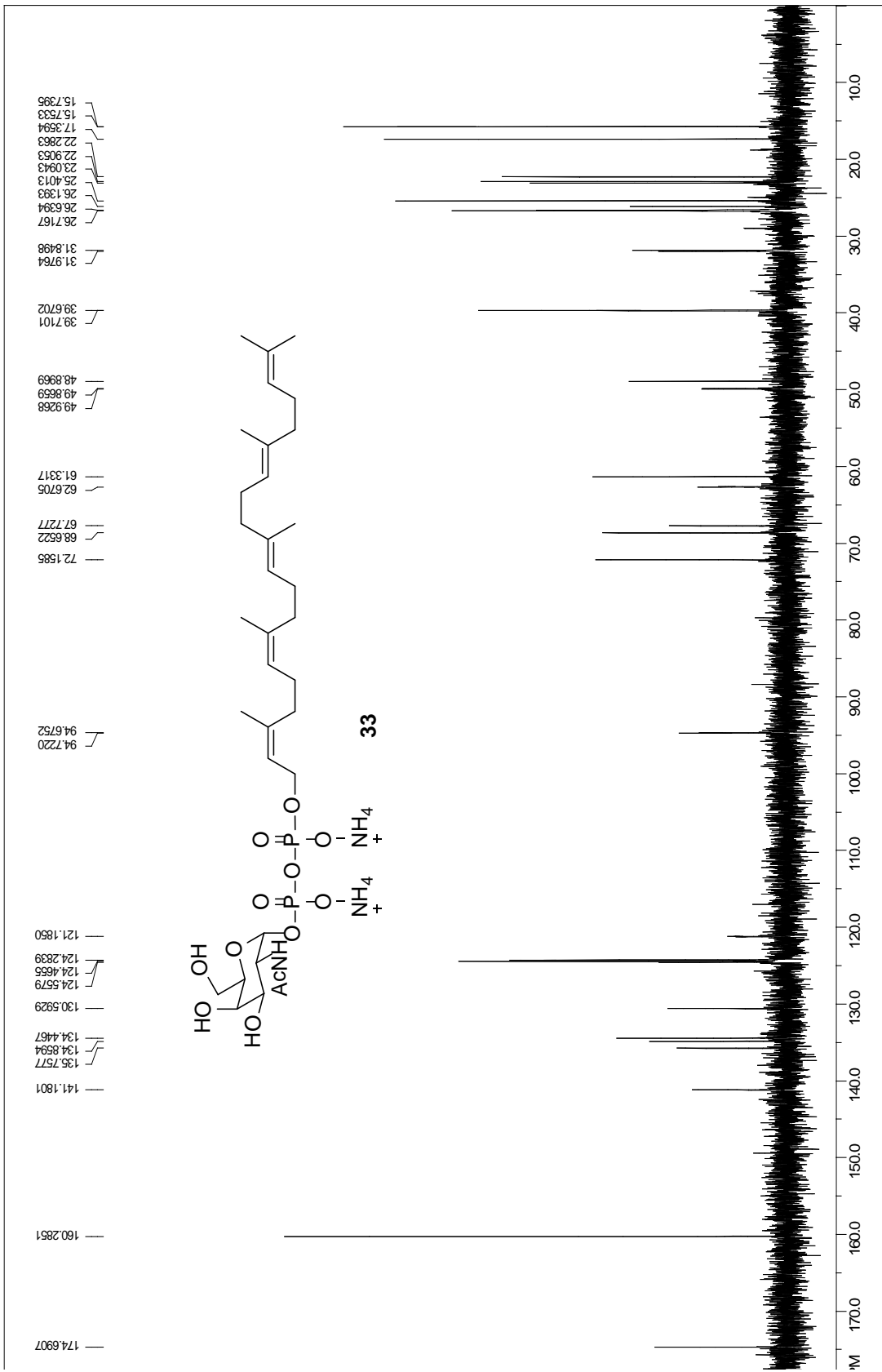
-9.7064
 -11.4192
 -11.4783



J:\Galk\NCP\Phos\1\vid exp1 <agg3>
 31P NMR
 161.562774 MHz
 32768 complex points
 1.000 GB 0.0000

J:\Galk\NCP\Phos\1\vid exp1 <agg3>
 31P NMR
 161.562774 MHz
 32768 complex points
 1.000 GB 0.0000

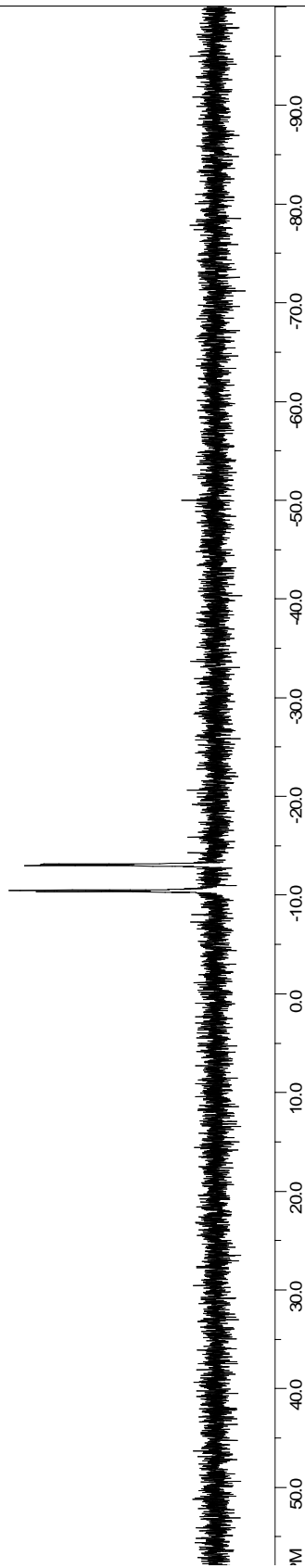
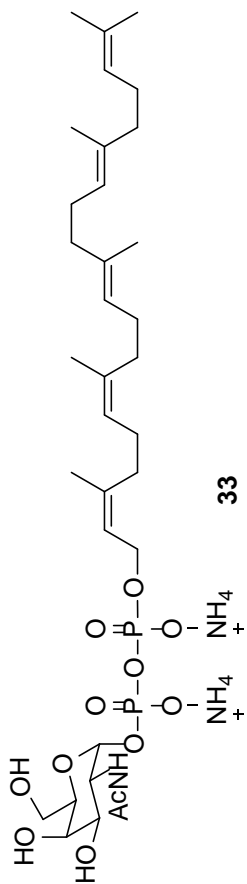




freq. of 0 ppm 125.730129 MHz
 processed size: 32768 complex points
 LB: 1.000 GB 0.0000

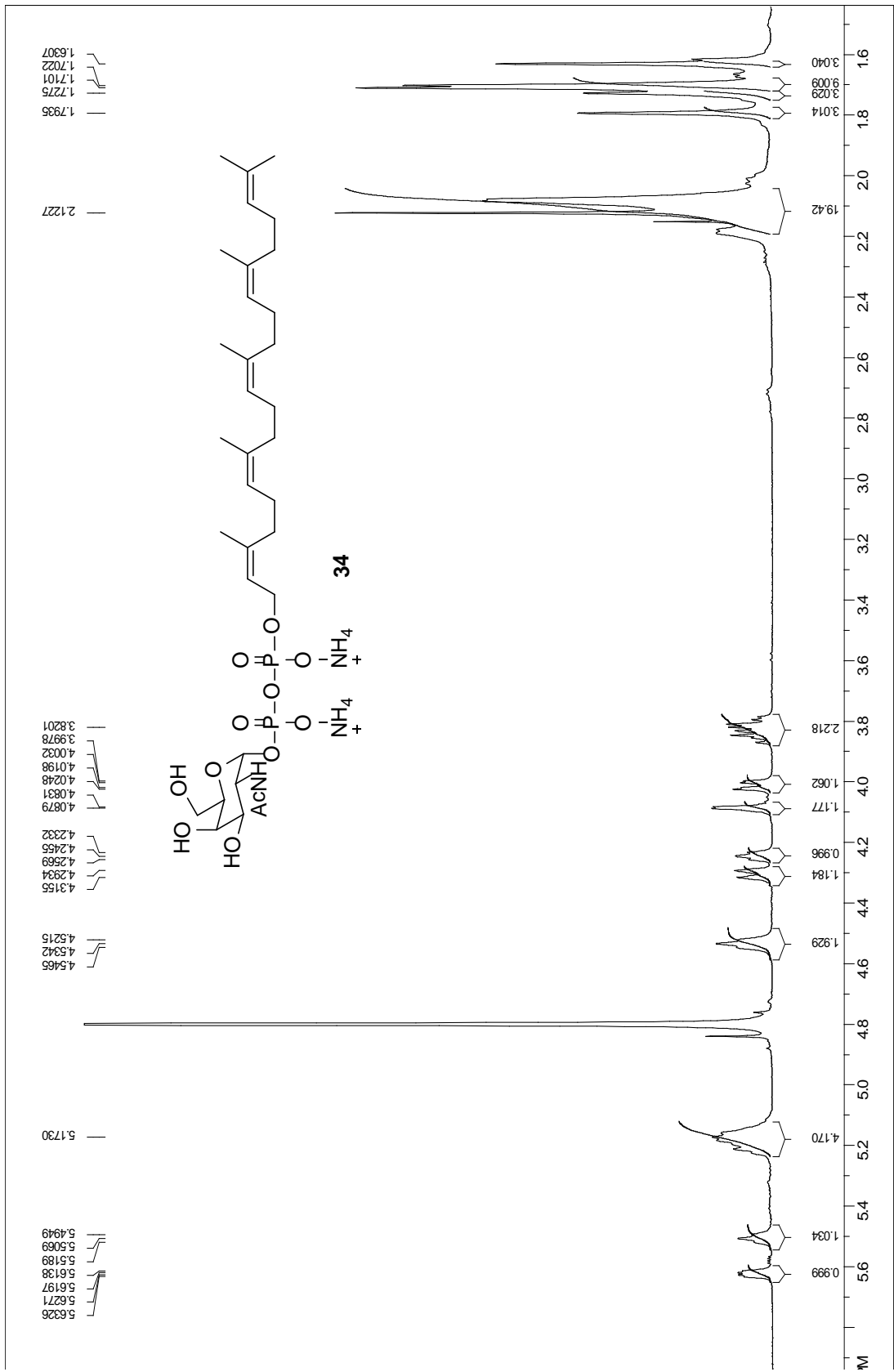
C:\Users\BMD\Desktop\Spec Data\NMR\DATA\Ram\NMR2\pns-3-47\2\fid exp: -zggp30-
 simlar (freq.: 125.742702 MHz
 domain size: 65536 points
 * 30030.03 Hz = 238.821256 ppm = 0.458222 Hz/pt
 tot of scans: 11242

-10.3510
-10.4872
-13.0017
-13.1314



freq. of 0 ppm: 161.97573 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

C:\Users\BWD\Desktop\Ramu\NMR\amesy\pentasaccharide\1\fid exp1 <ppp30>
smile: freq.: 161.967474 MHz
domain size: 65336 points
r: 64565.06 Hz = 400.914228 ppm = 0.990650 Hz/pt
bar of scale: 161



CVUsers\BWI\Desktop\Spc Data\NMR DATA\Way Project\GAINC\PP8a\PerinNew\1.fid exp1 -cg3b-
 acqname: 500.023038 MHz
 acqfreq: 500.023038 MHz
 domain size: 65536 points
 f1: 1.033038 Hz = 20.662003 ppm = 0.157632 Hz/pt
 lb: 0.000 GB 0.0000
 processed size: 32768 complex points
 freq. of 0 ppm: 500.019561 MHz

15.6883
17.3296
22.2789
22.9981
23.0380
23.1781
23.2285
25.4060
25.4504
26.2231
26.3539
26.5855
31.8439
32.0590
32.1021

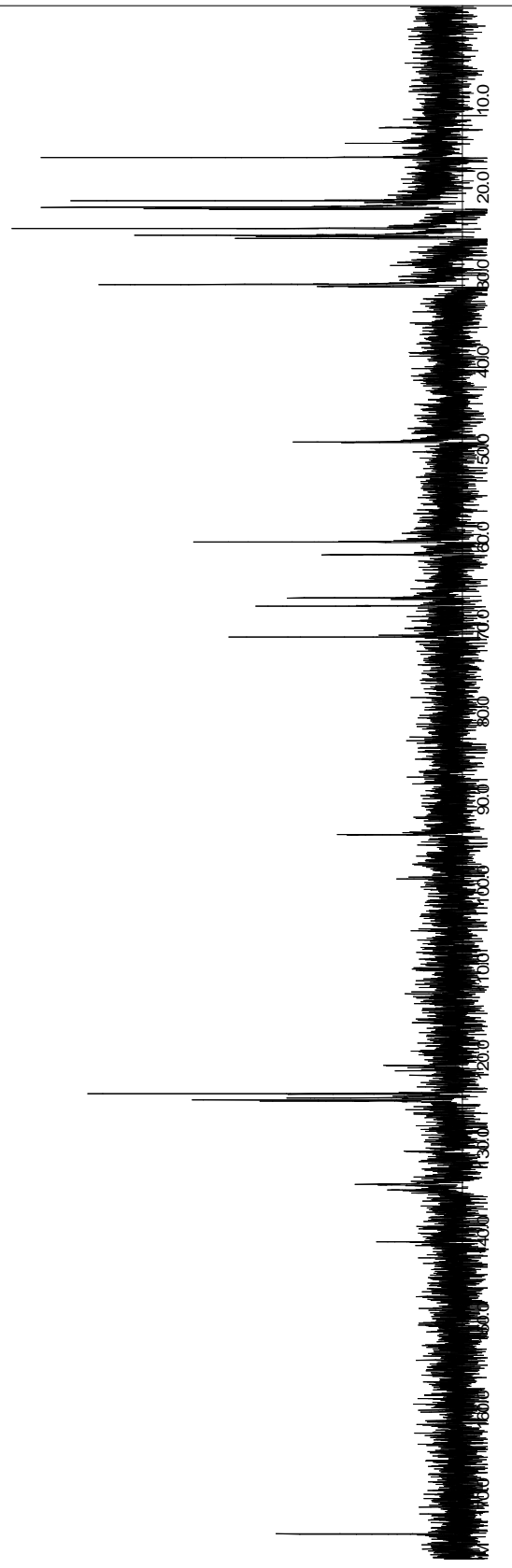
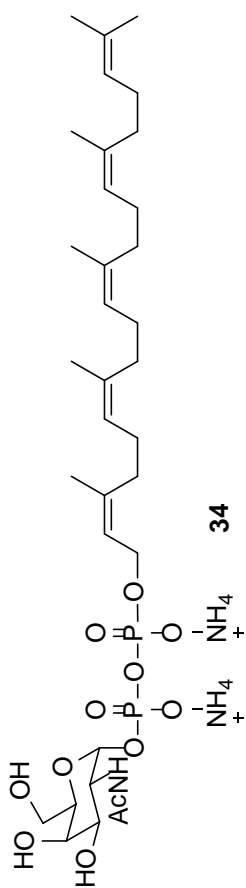
49.9018
49.8403

61.2933
62.7695
67.6790
68.6257
72.1580

94.7986

124.3522
124.4122
124.8524
125.1027
125.2276
134.7113
134.7963
135.3969
135.4229
141.3172

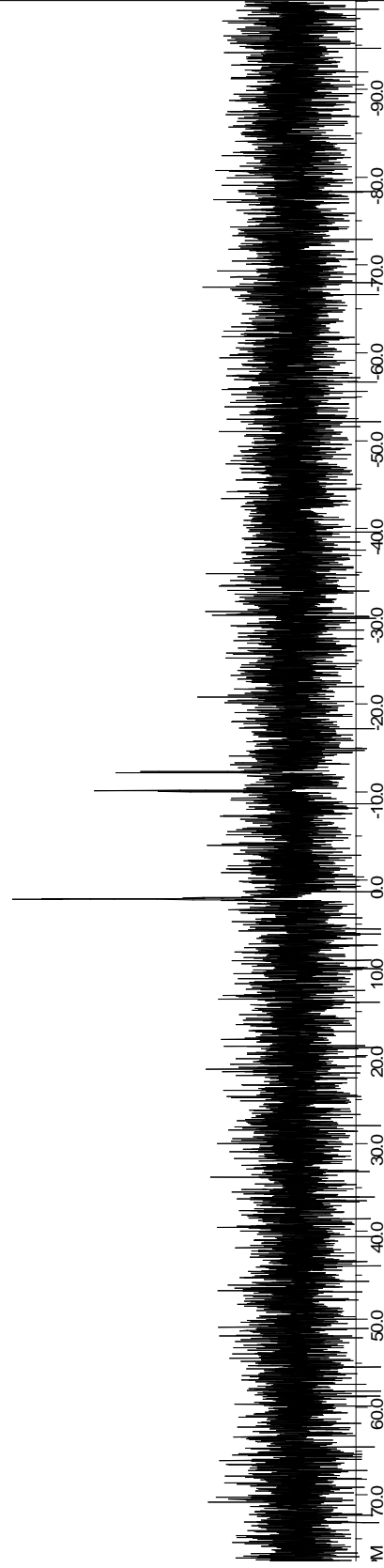
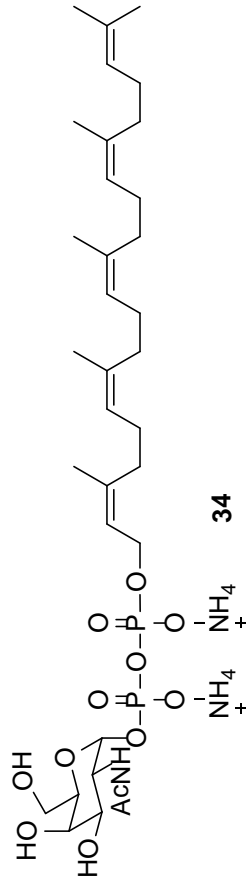
174.7238



freq. of 0 ppm: 125.730125 MHz
 125.730125 MHz
 LB: 0.000 GB: 0.0000

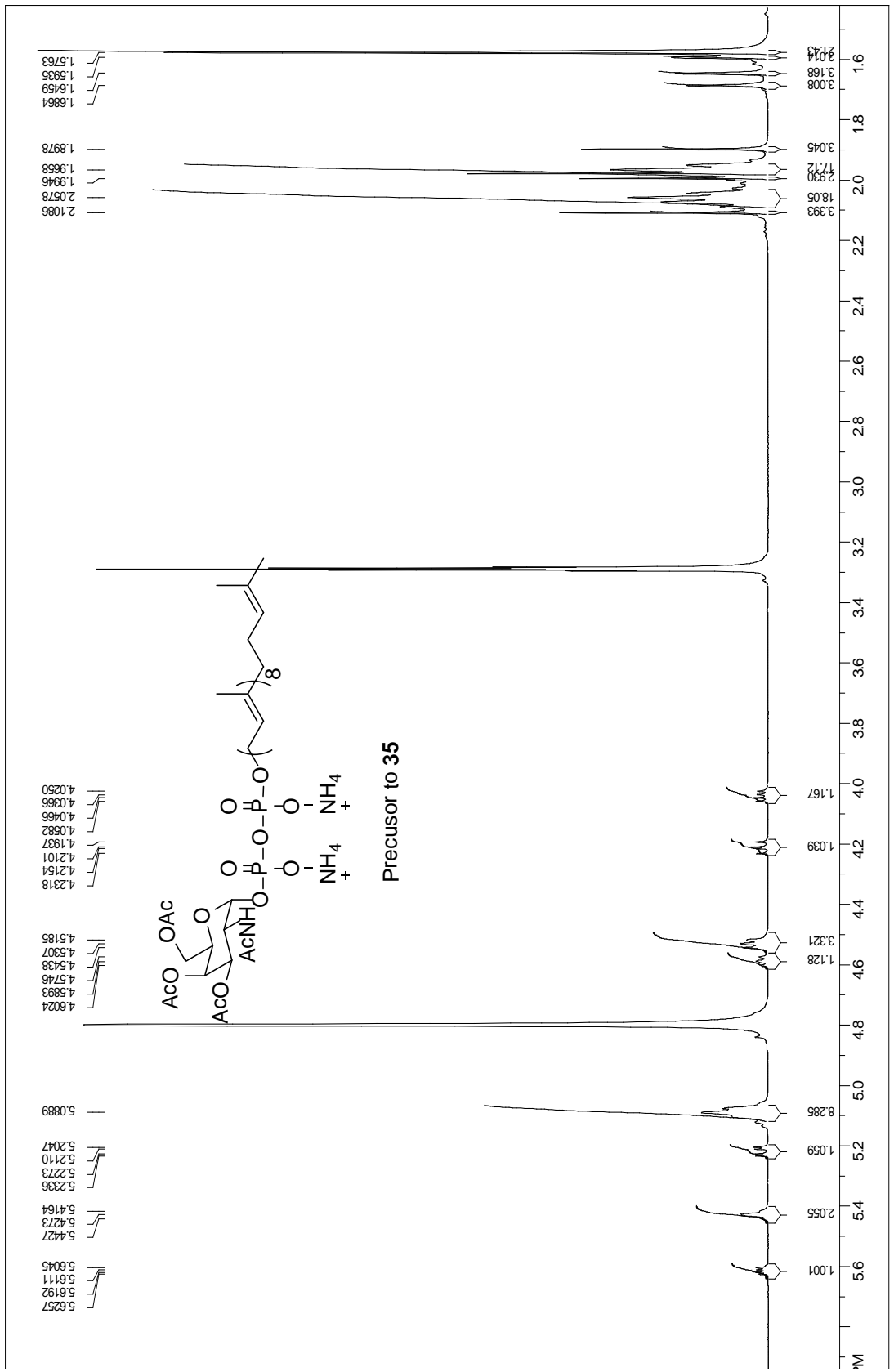
C:\Users\BVD\Desktop\Spec: Data\NMR DATA\Wzy Project\GalNAc6SPePsefNew2\fid exp1 -3ppg98-
 name: 1347963-1353969-1354229-1413172-1248524-1244122-1243522
 h: 30000.00 Hz = 288.821256 ppm = 0.458222 Hz/tt
 bar of scans: 15111

-10.0612
-10.1785
-12.1939
-12.3245



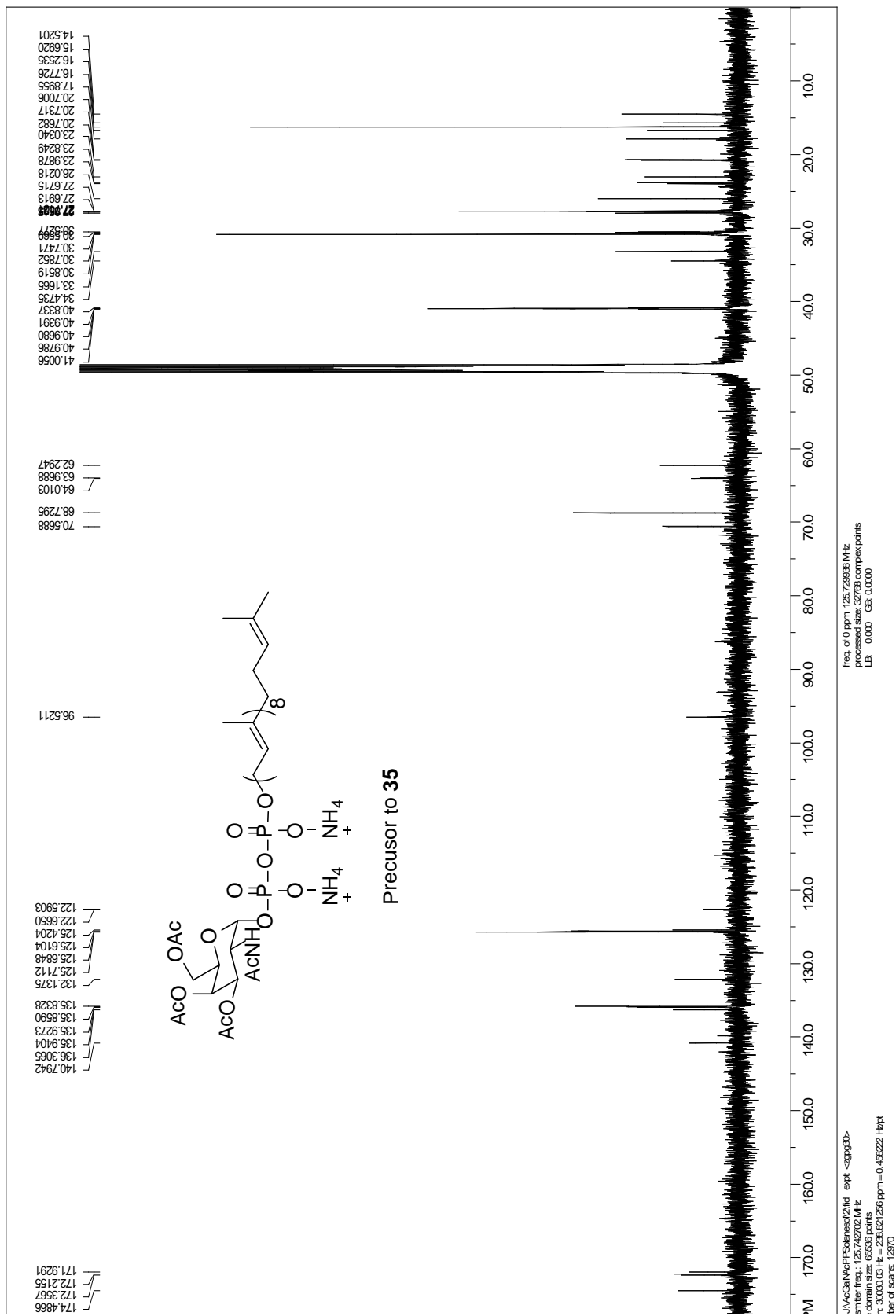
J:\Gai\Nc\FFam\Phos\1\vid exp1 <g3p3d>
 acqfile: 1613674741.viz
 Date_UTC: 2011-08-11 10:00:00
 X: 64635.00 Hz Y: 400.914228 ppm = 0.998830 Hz/pt
 ber of scans: 246

freq. of 0 ppm: 161.375485 MHz
 process size: 32788 complex points
 LS: 1.00 GB 0.0000

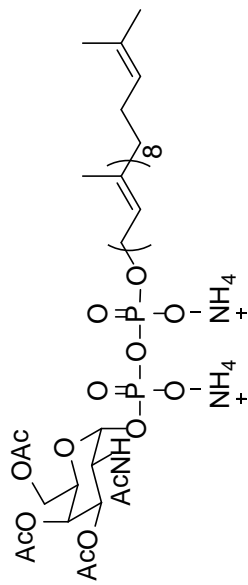


freq: 0 ppm: 500.02020 MHz
 processed size: 32788 complex points
 LB: 0.000 GB: 0.0000

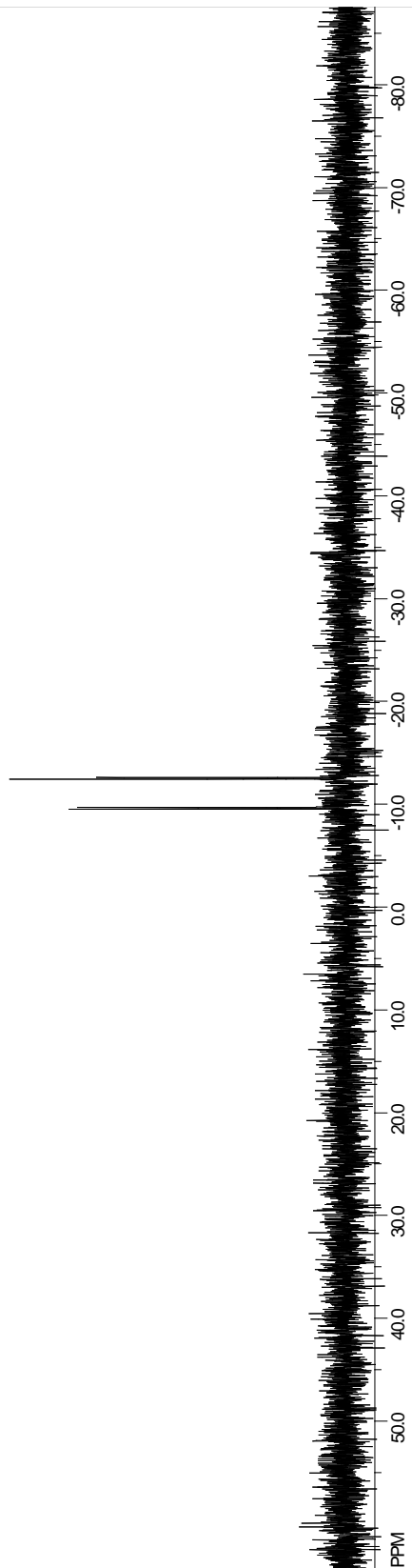
J:\AccG\NMR\PPS\data\011\1d exp1 <g>gde</g>
 similar freq: 500.020388 MHz
 domain size: 65936 points
 r: 10350.98 Hz = 20.66203 ppm = 0.15763214 pt
 bar of scans: 64



-9.5562
-9.6994
-12.4672
-12.6090

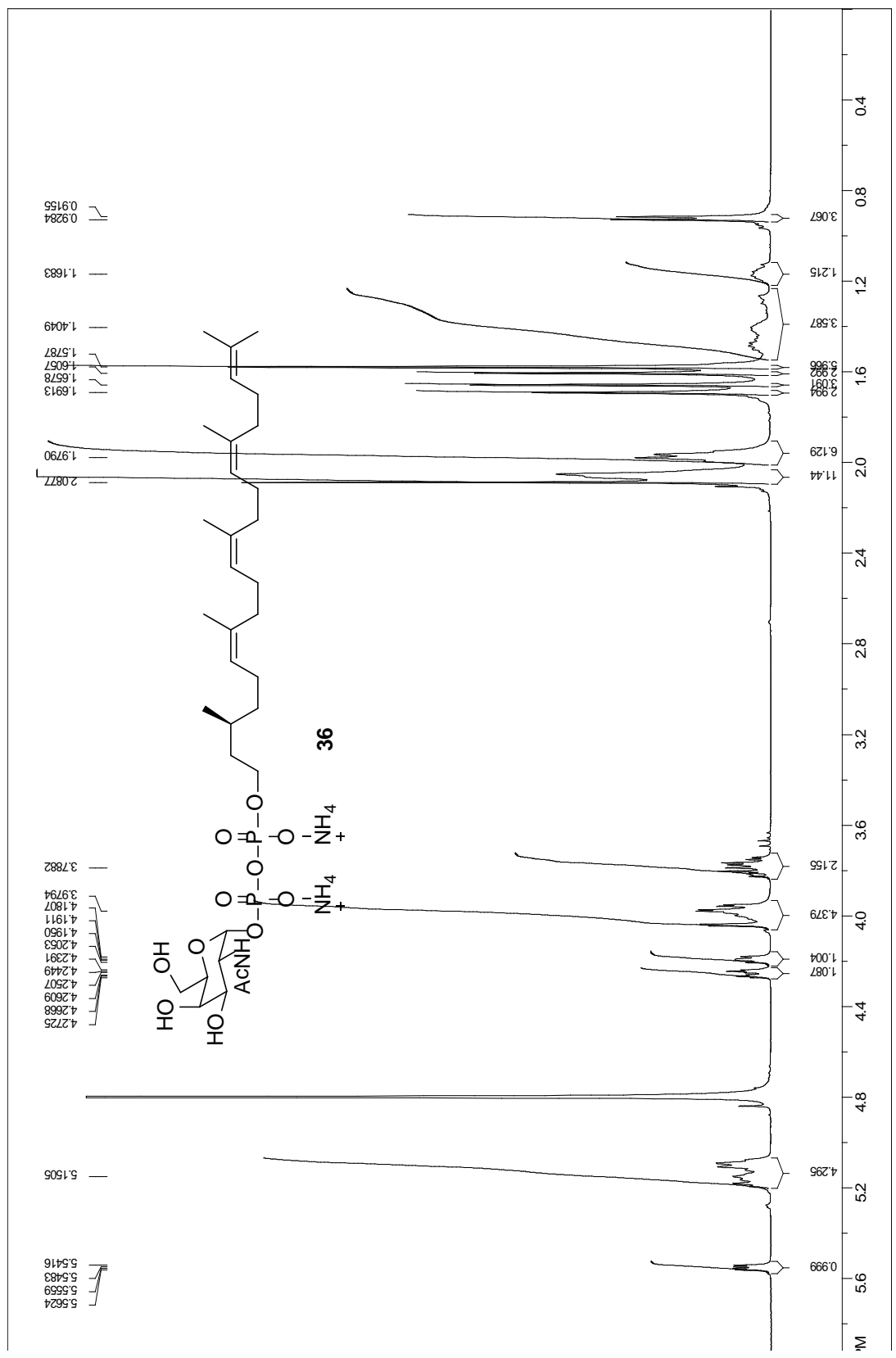


Precursor to 35



freq. of 0 ppm: 161.575460 MHz
processed size: 32768 complex points
LB: 1.000 GE: 0.0000

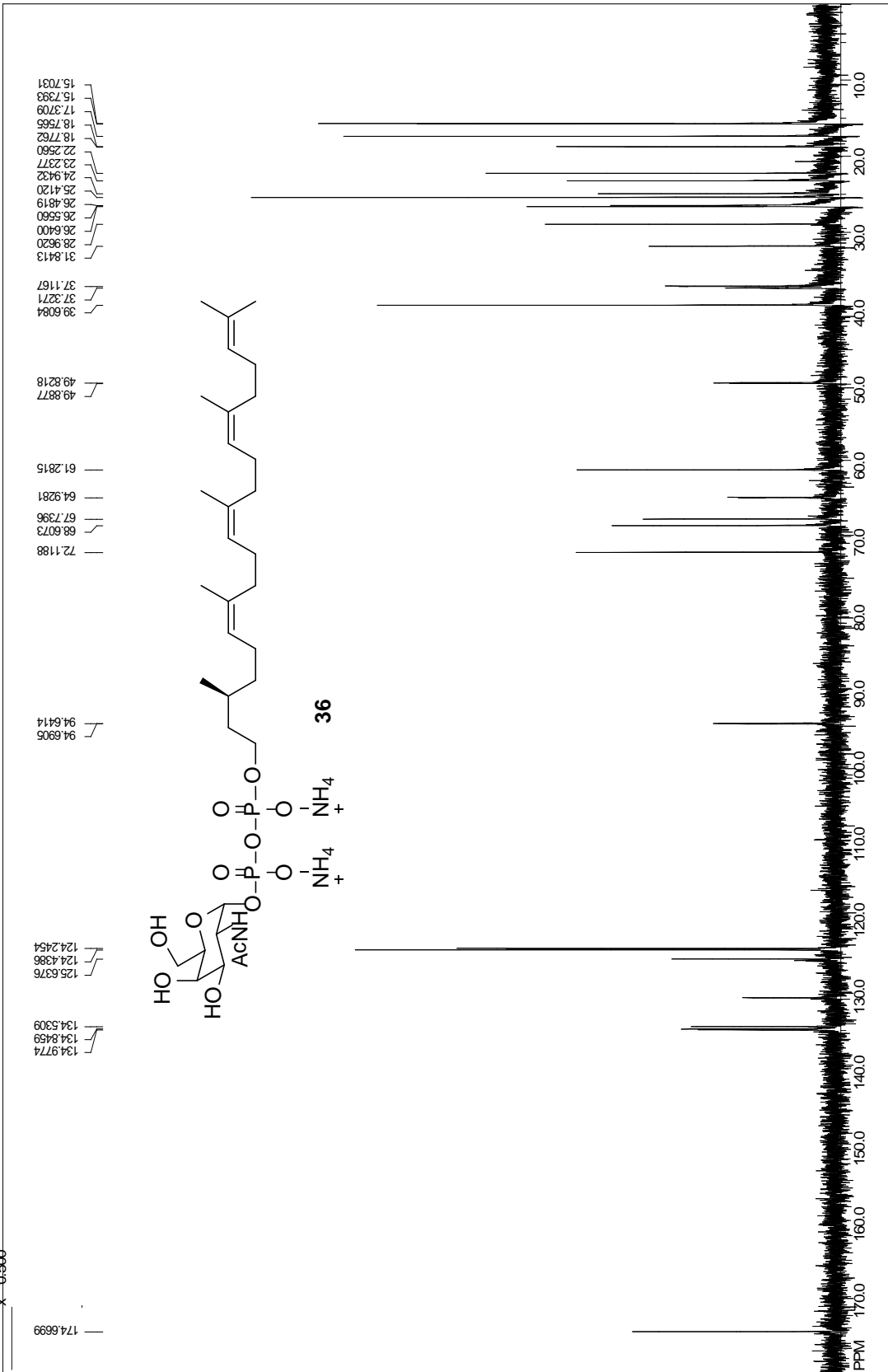
file: J:\ACSI\AcFPOden\003\fid_ expt_ <2>g3d>
transmitter freq.: 161.367474 MHz
time domain size: 65536 points
width: 64935.06 Hz = 400.914228 ppm = 0.990030 Hz/pt
number of scans: 211



freq. of 0 ppm: 500.019850 MHz
 processed size: 32788 complex points
 LB: 0.300 GB: 0.0000

J:\GAIN\PM\SP\entia\1\vid exp1 <exp>
 smiller freq.: 500.023288 MHz
 domain size: 65536 points
 τ: 10.030.091 Hz = 20.60203 ppm = 0.157632 Hz pt
 bar of scans: 64

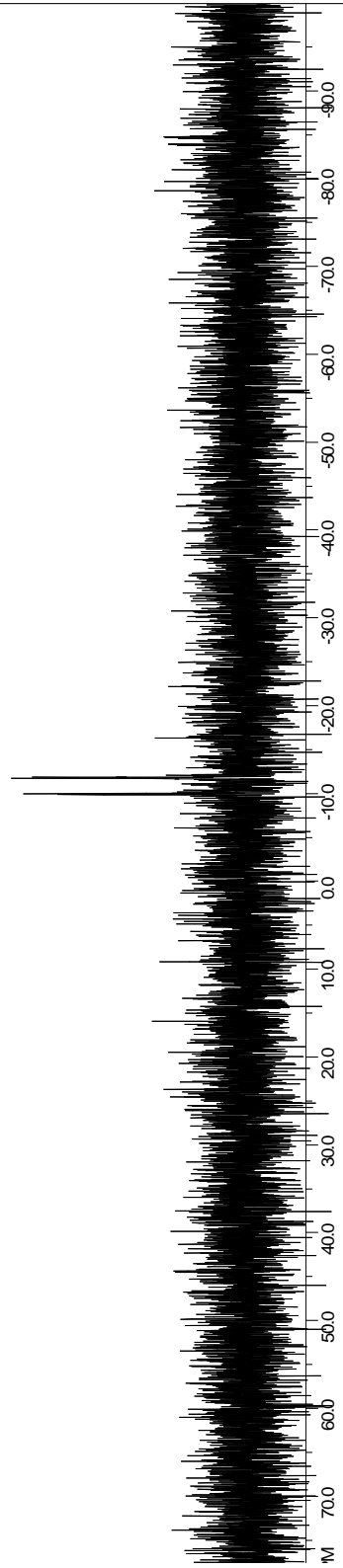
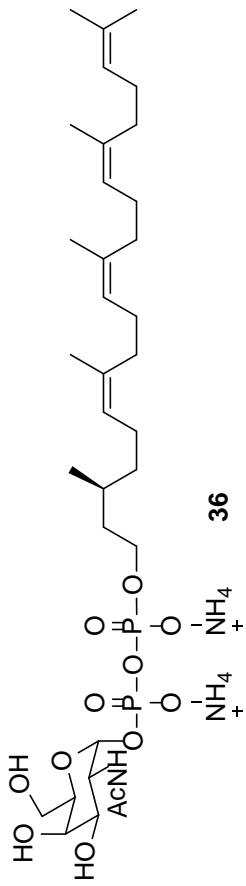
SpinWorks 2.3
X 0.500



file: J:\GAIN\PPMS\Panel\2\fid_ext_<ggg30>
transmitter freq.: 125.742702 MHz
time domain size: 66536 points
width: 30030.03 Hz = 236.821256 ppm = 0.465221 Hz/pt
number of scans: 13338

freq. of 0 ppm: 125.730129 MHz
processed size: 32768 complex points
LB: 1.000 GB: 0.0000

9.8927
10.0040
11.7383
11.8513



J:\GAIN\MSPeria2\fid exp - <ppp30>
smile: freq: 161.97744 MHz
domain size: 6536 points
r: 64635.06 Hz = 403.94228 ppm = 0.930830 Hz/pt
bar of scans: 58

freq: 0 ppm: 161.975460 MHz
processed size: 32768 complex points
LE: 0.000 GB: 0.0000