Supporting Information

Asymmetric Synthesis of D-*ribo*-Phytosphingosine from 1-Tetradecyne and (4-Methoxyphenoxy)acetaldehyde

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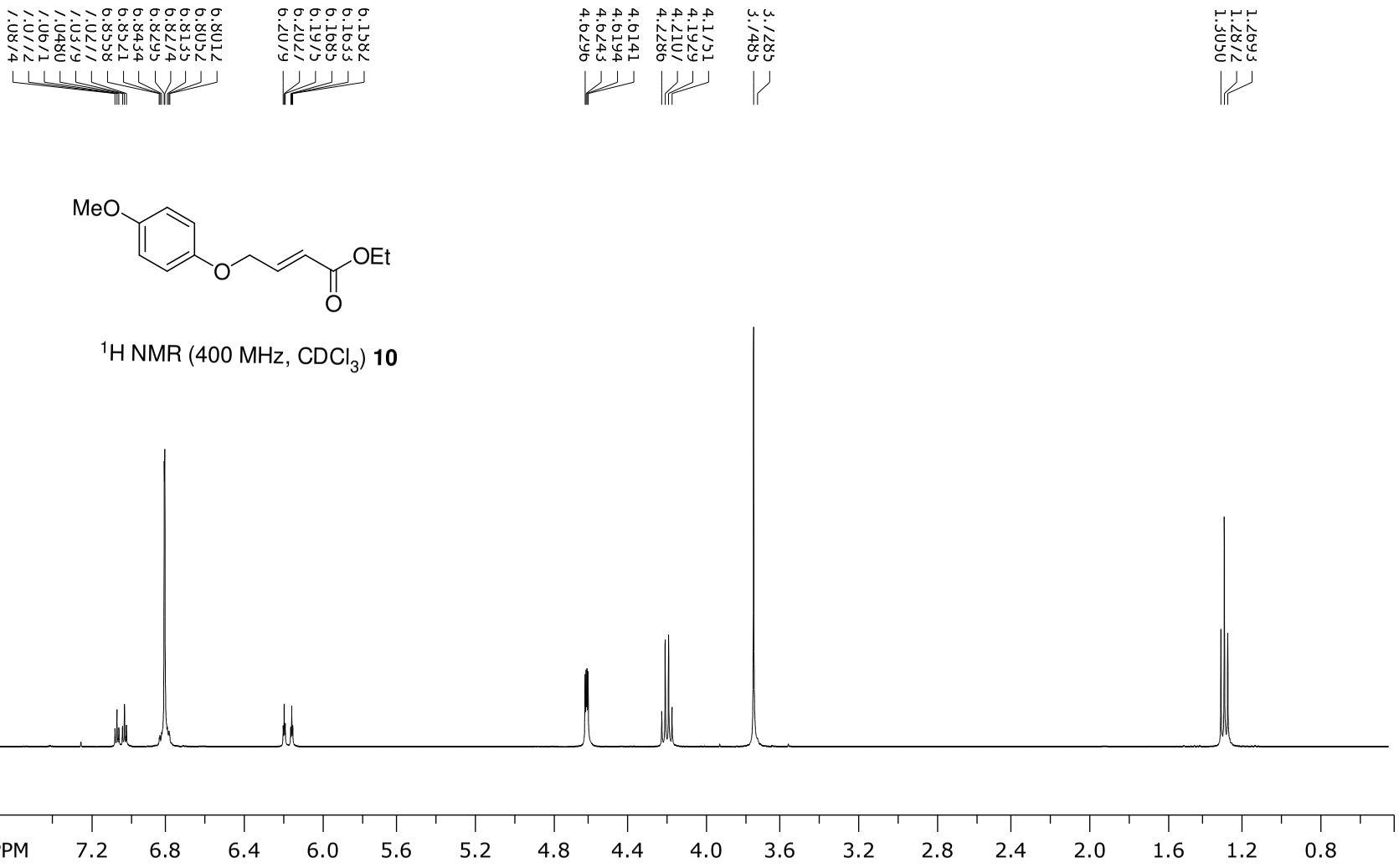
General Experimental Methods

All reactions were carried out under a dry nitrogen atmosphere using oven-dried glassware and magnetic stirring. The solvents were dried as follows: THF was heated at reflux over sodium benzophenone ketyl; toluene was heated at reflux over sodium; CH_2Cl_2 were dried over CaH_2. Silica gel 60 F254 aluminum TLC plates of 0.2 mm thickness were used to monitor the reactions. The spots were visualized with short wavelength ultraviolet light or by charring after spraying with 15% H_2SO_4. Flash chromatography was carried out with silica gel 60(230-400 ASTM mesh). ^1H NMR spectra were obtained on 400 or 500 MHz spectrometers. Chemical shifts were referenced on residual solvent peaks: $CDCl_3$ (δ = 7.26 ppm for ^1H NMR and 77.00 ppm for ^{13}C NMR), CD_3OD (δ = 4.78, 3.31 ppm for ^1H NMR and 49.1 ppm for ^{13}C NMR). Optical rotations were measured at room temperature in a 1.0-dm cell. High-resolution mass spectra were acquired by electrospray ionization.



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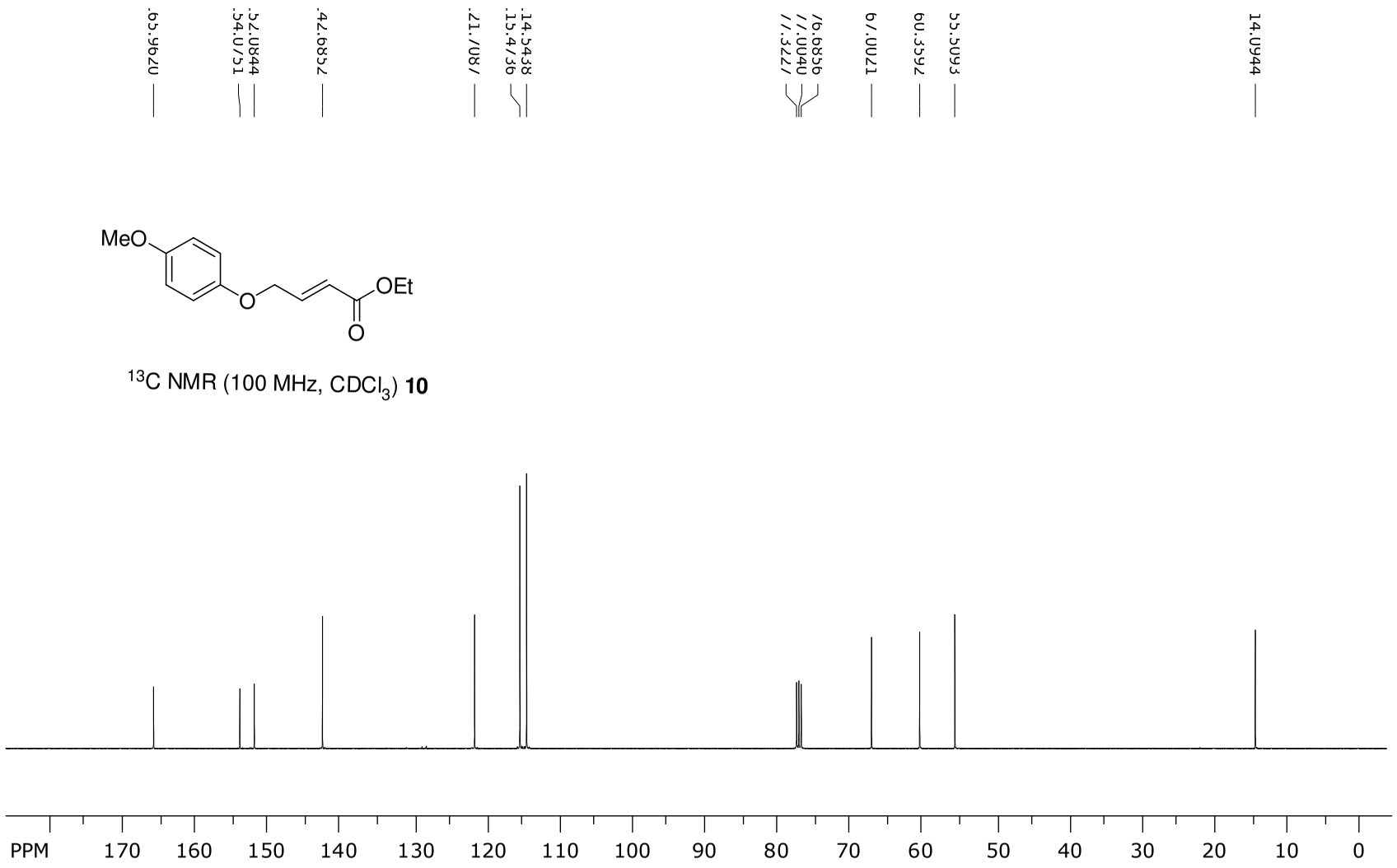

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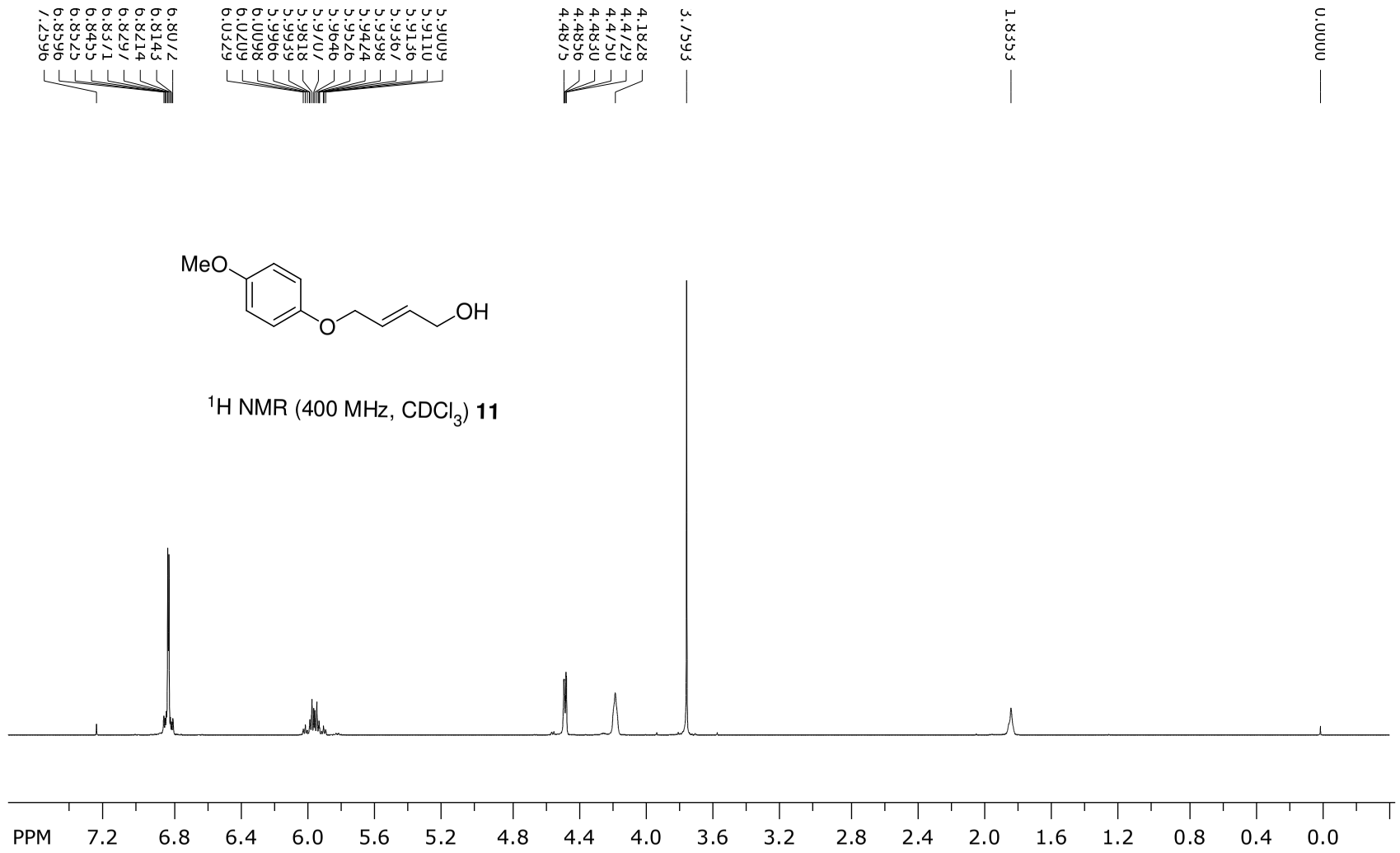

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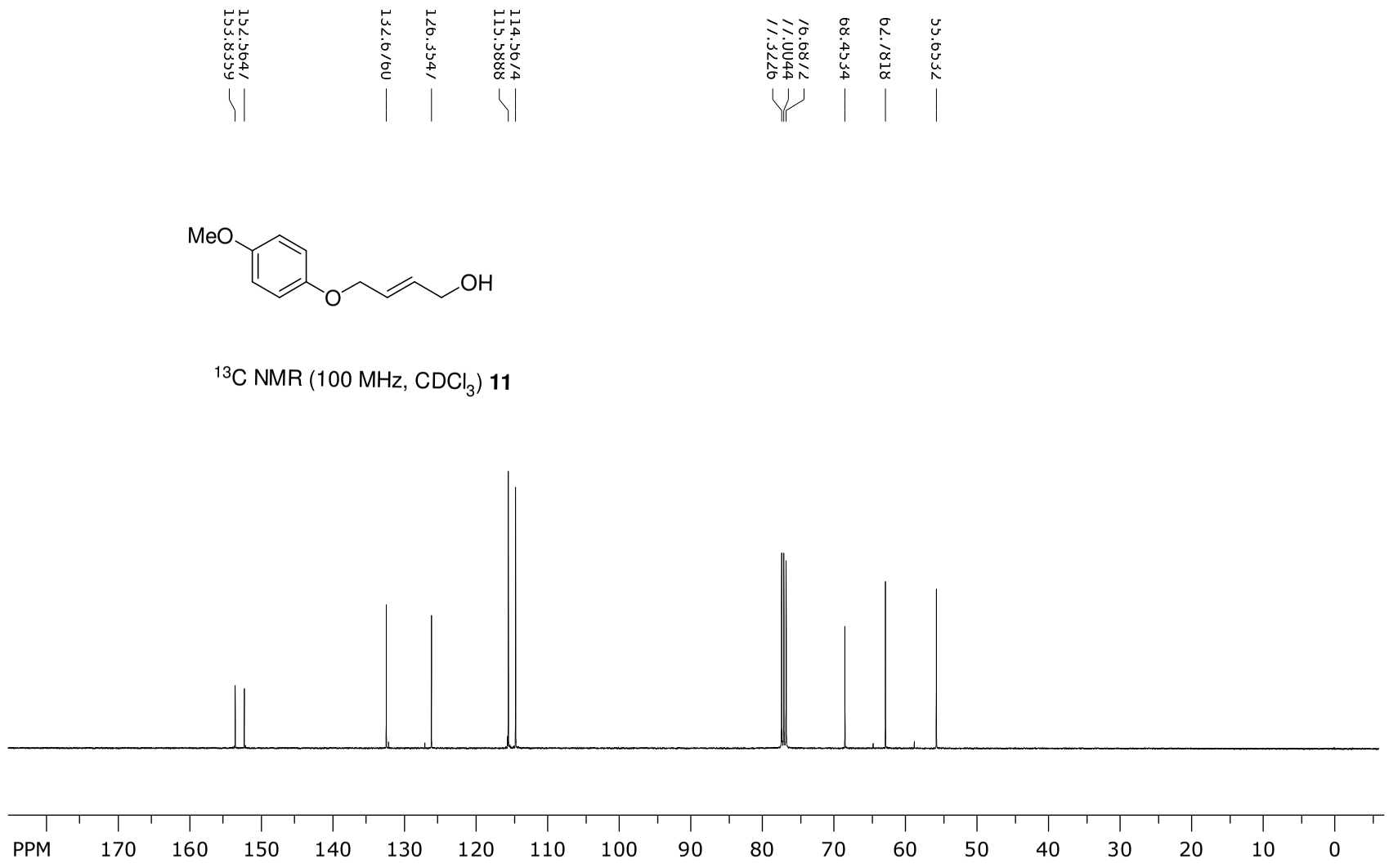

^{13}C NMR (100 MHz, $CDCl_3$) **11**

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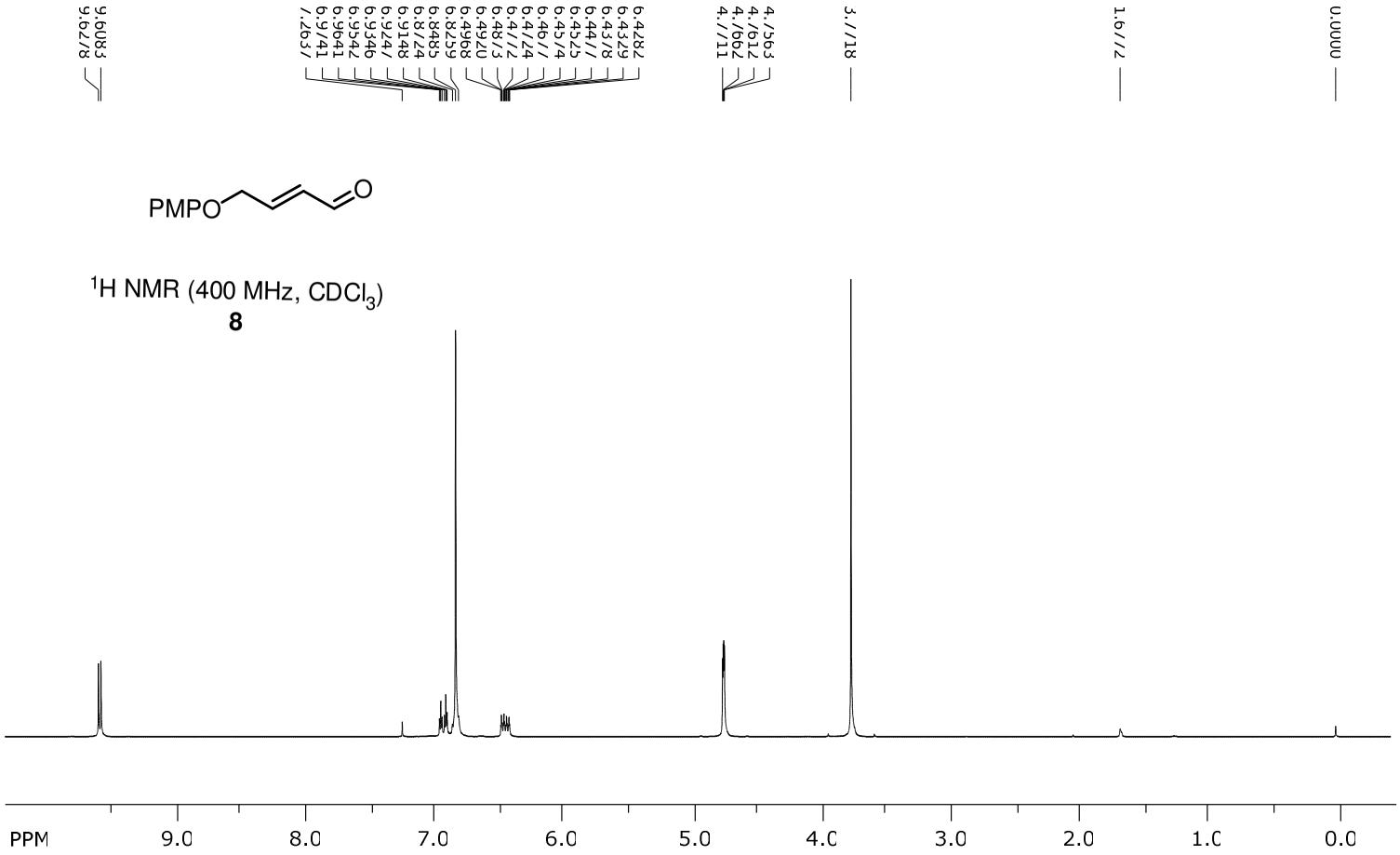

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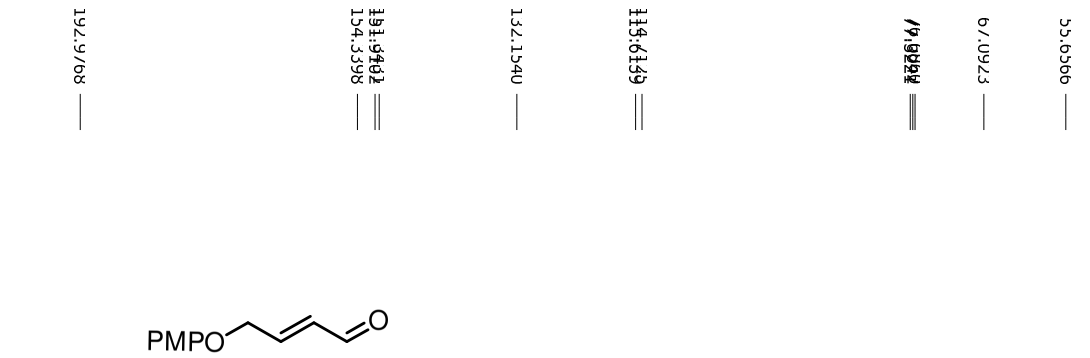
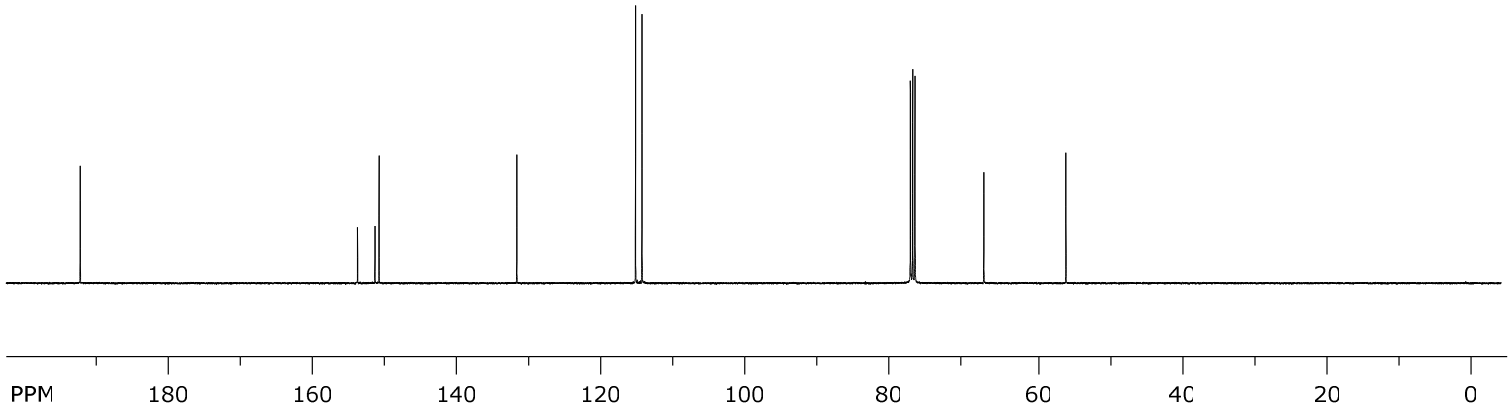


^{13}C NMR (100 MHz, $CDCl_3$)

8



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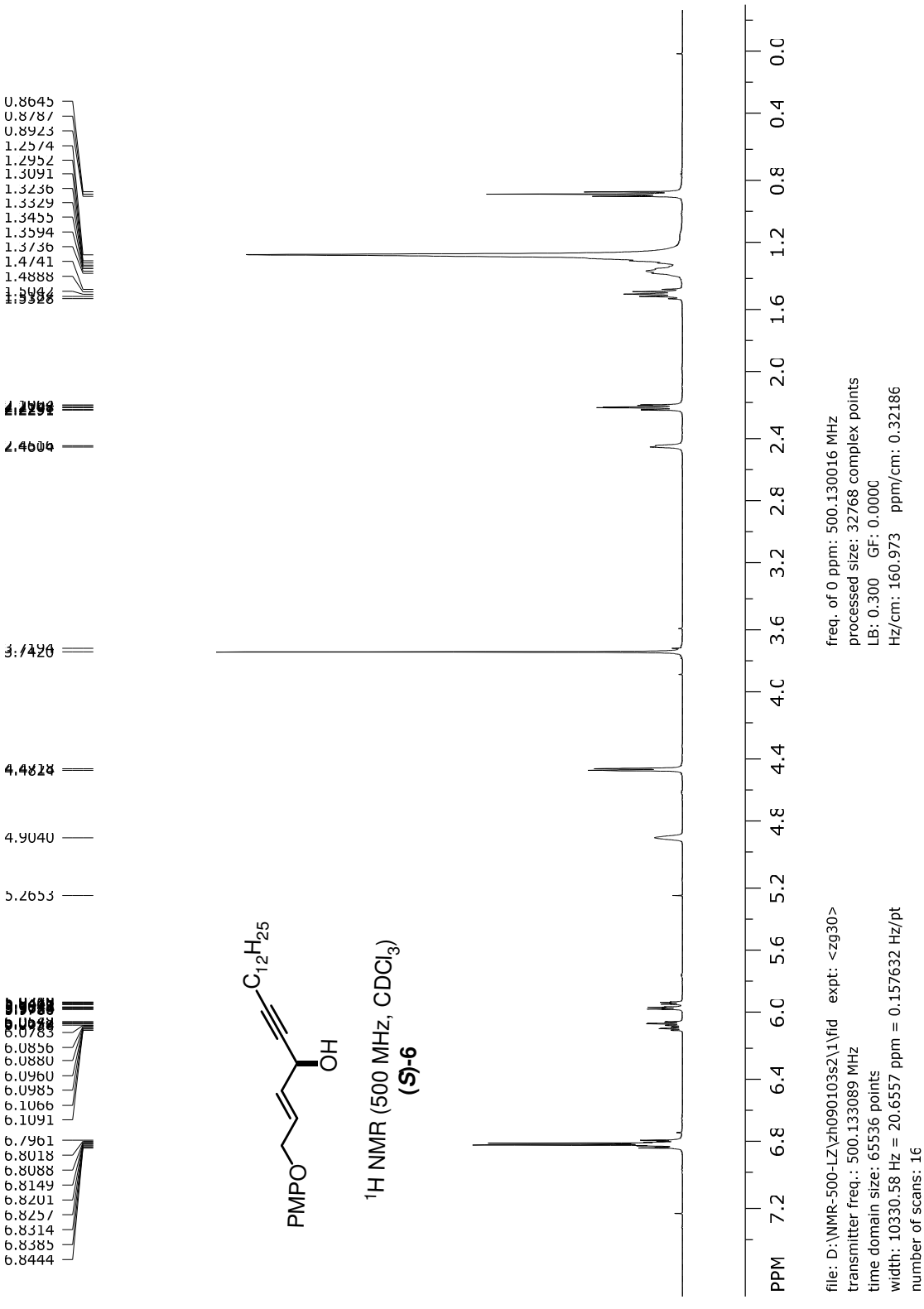
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OH
$C_{12}H_{25}$
^{1}H NMR (500 MHz, $CDCl_3$)
(S)-6
PPM
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
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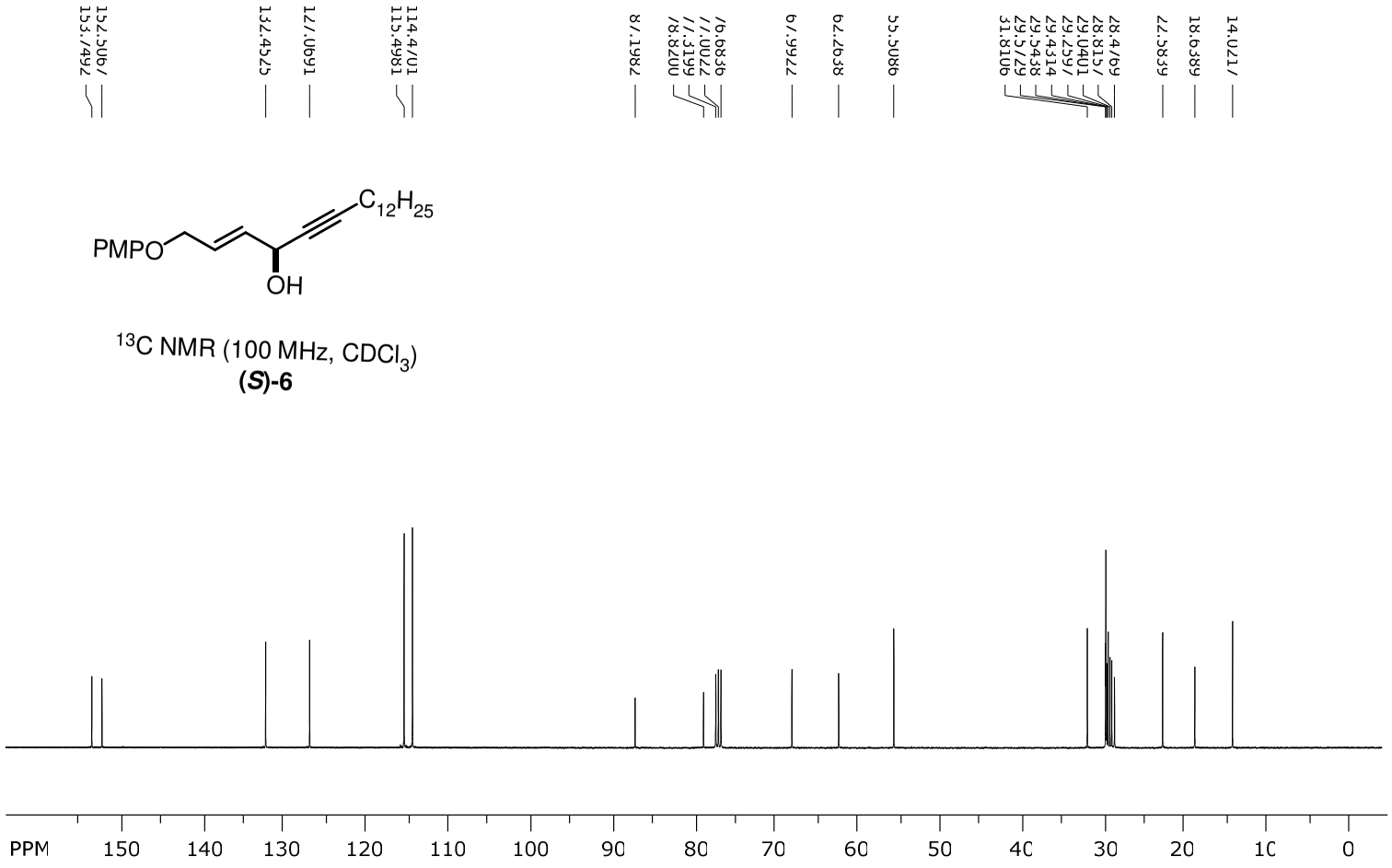

^{13}C NMR (100 MHz, $CDCl_3$)
(*S*)-6

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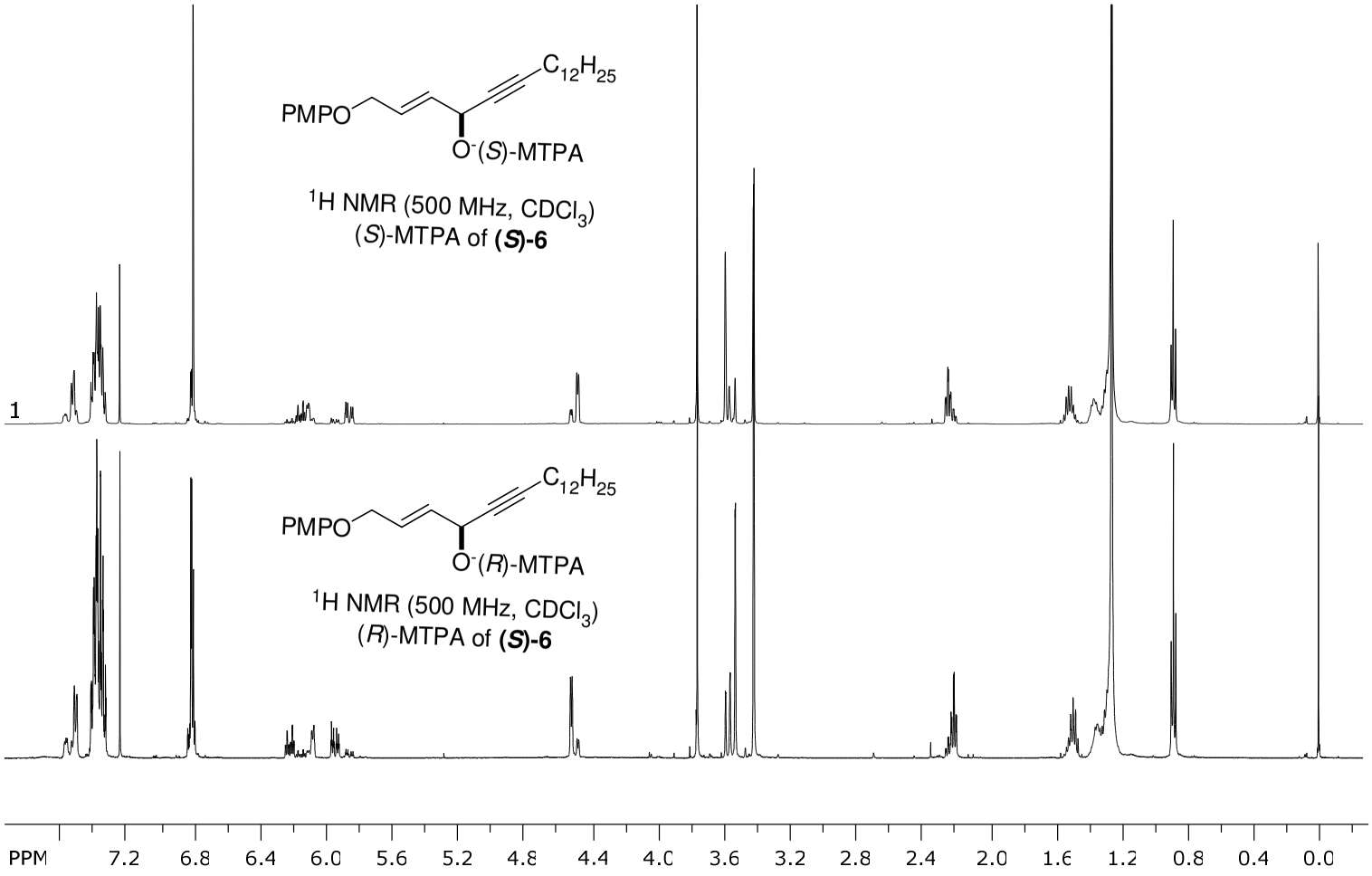

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number of scans: 16

freq. of 0 ppm: 500.130014 MHz
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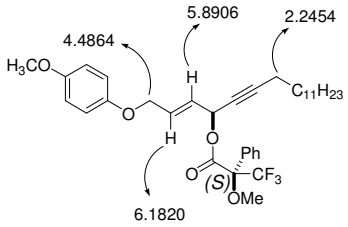
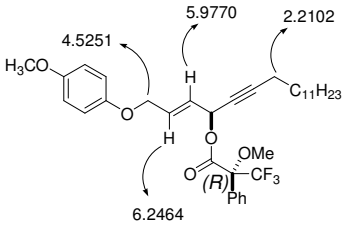
MTPA ester chemical shifts for determination of ee and absolute configuration:



(*S*)-MTPA of (***S***)-**6**



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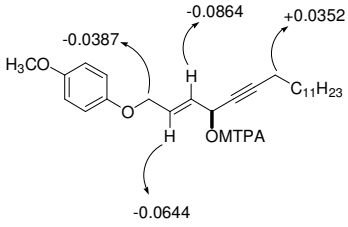

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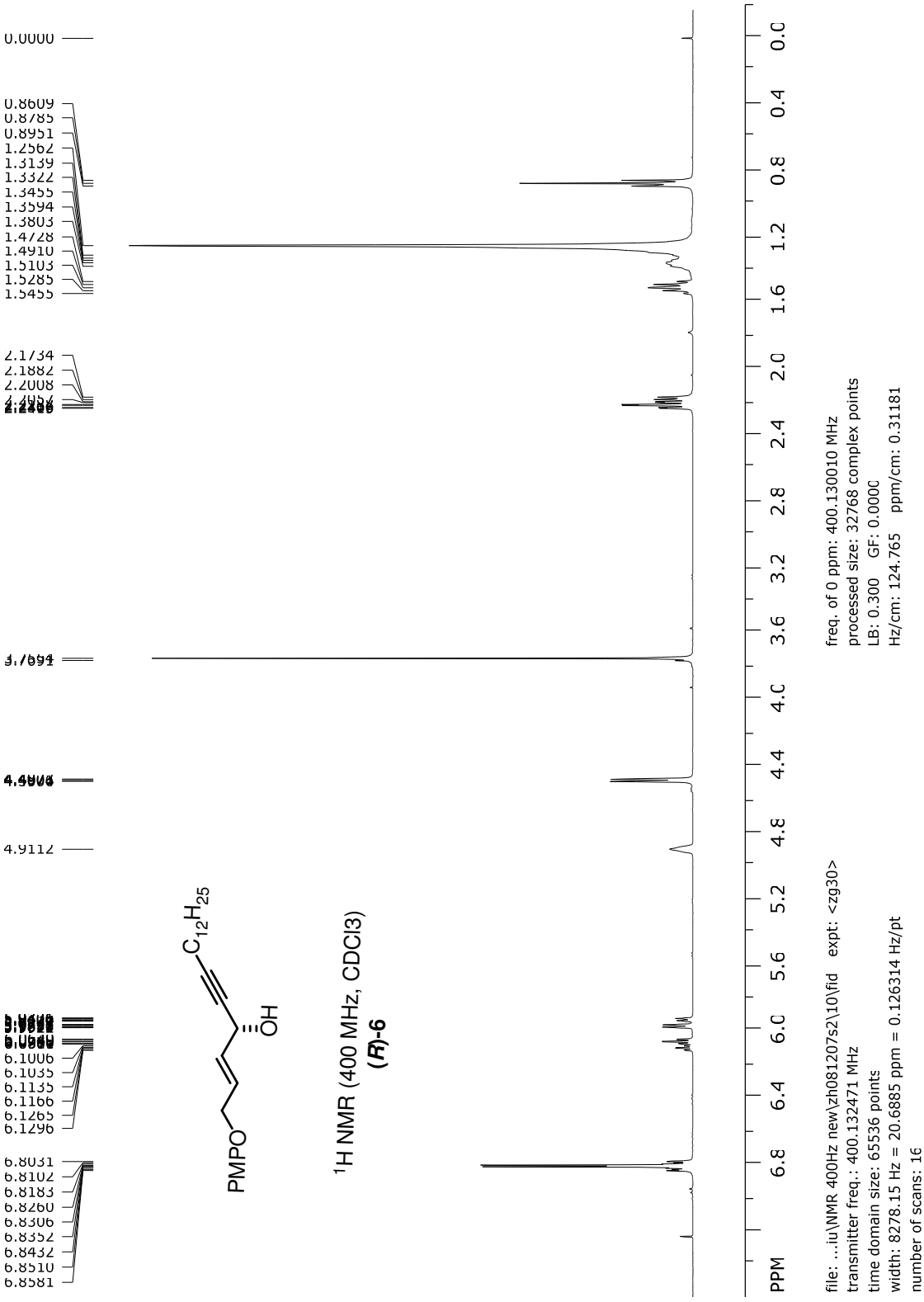
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$C_{12}H_{25}$
^{1}H NMR (400 MHz, CDCl3)
(R)-6
PPM
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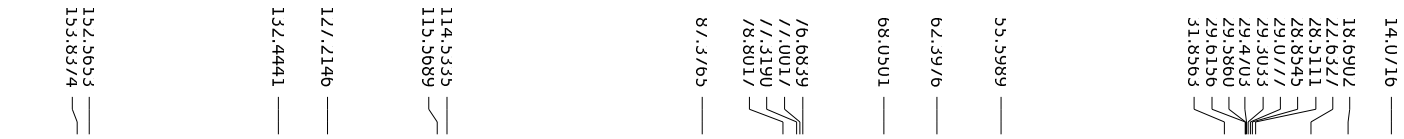
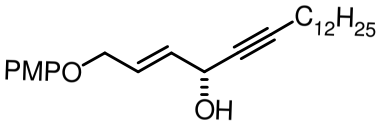
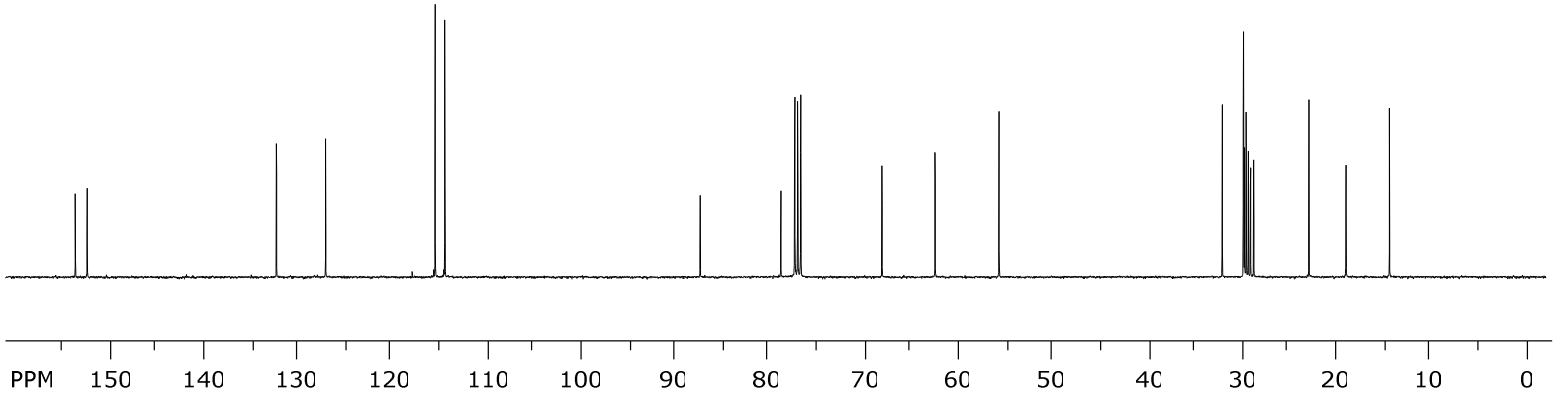




^{13}C NMR (100 MHz, CDCl3)
(*R*)-6



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number of scans: 1024

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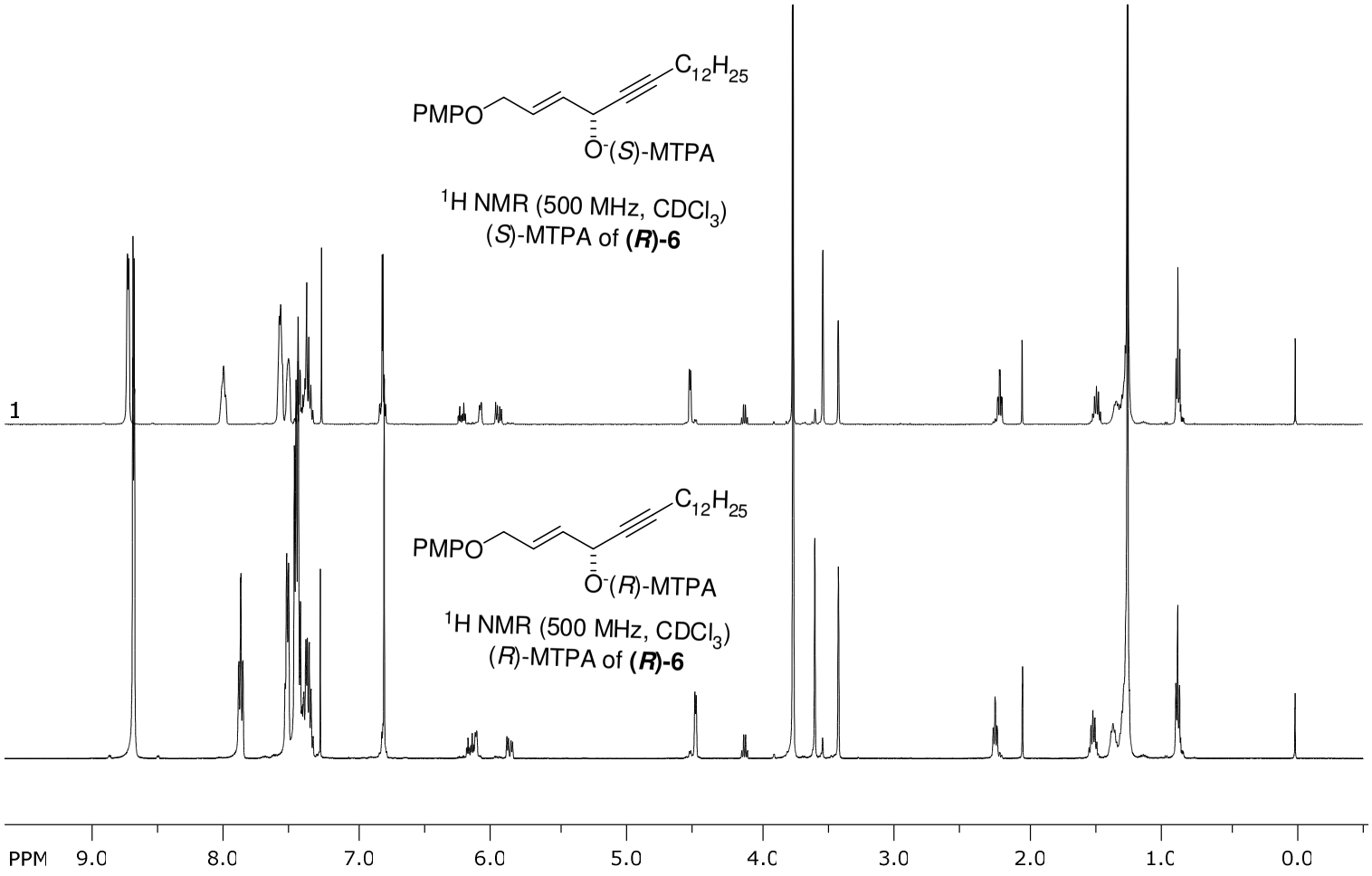

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number of scans: 16

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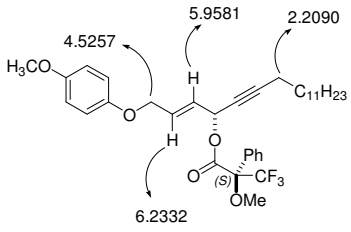
MTPA ester chemical shifts for determination of ee and absolute configuration:



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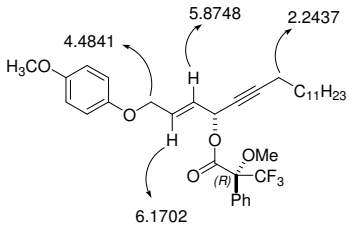

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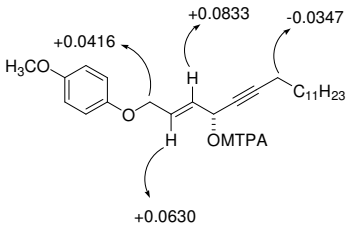

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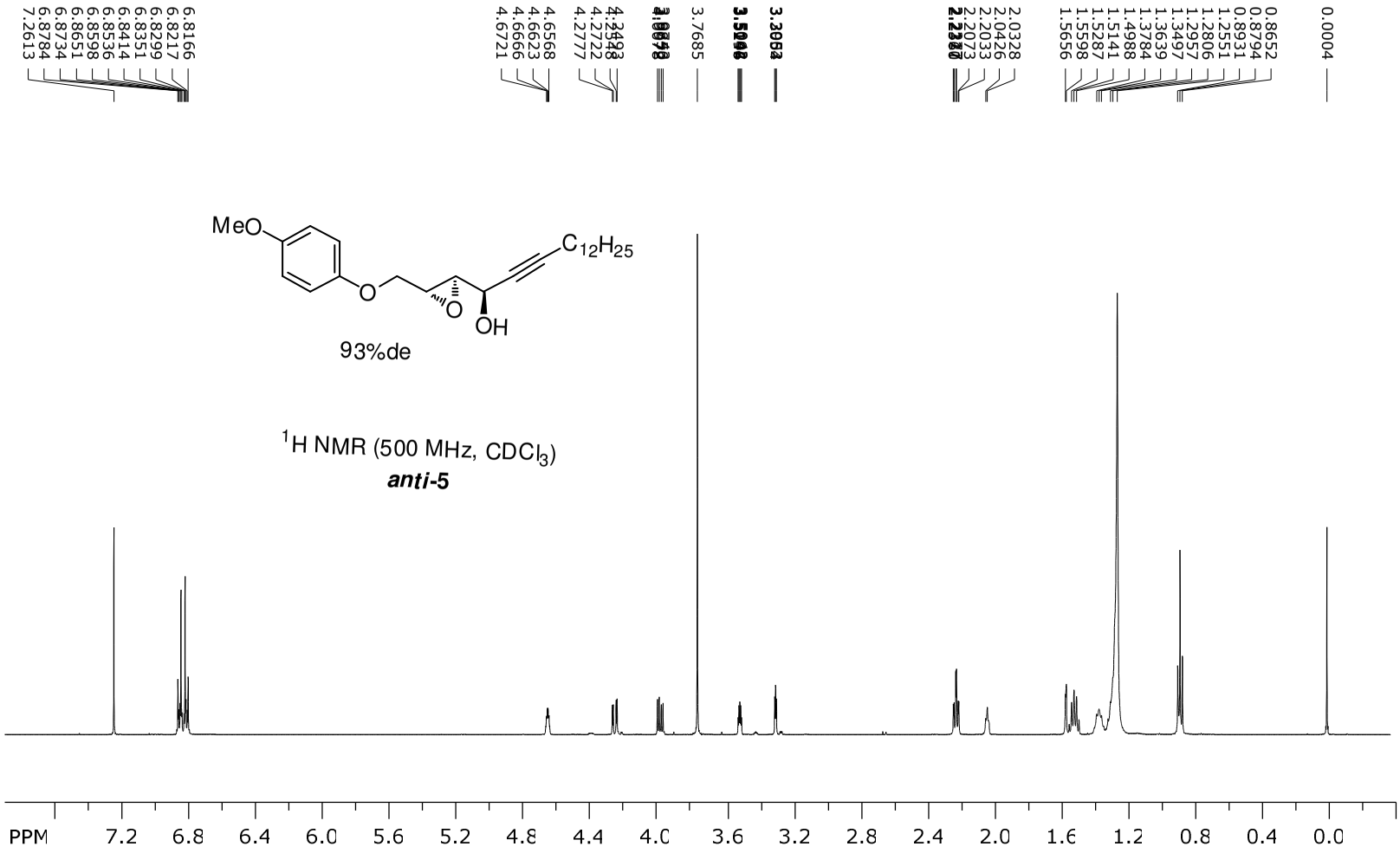

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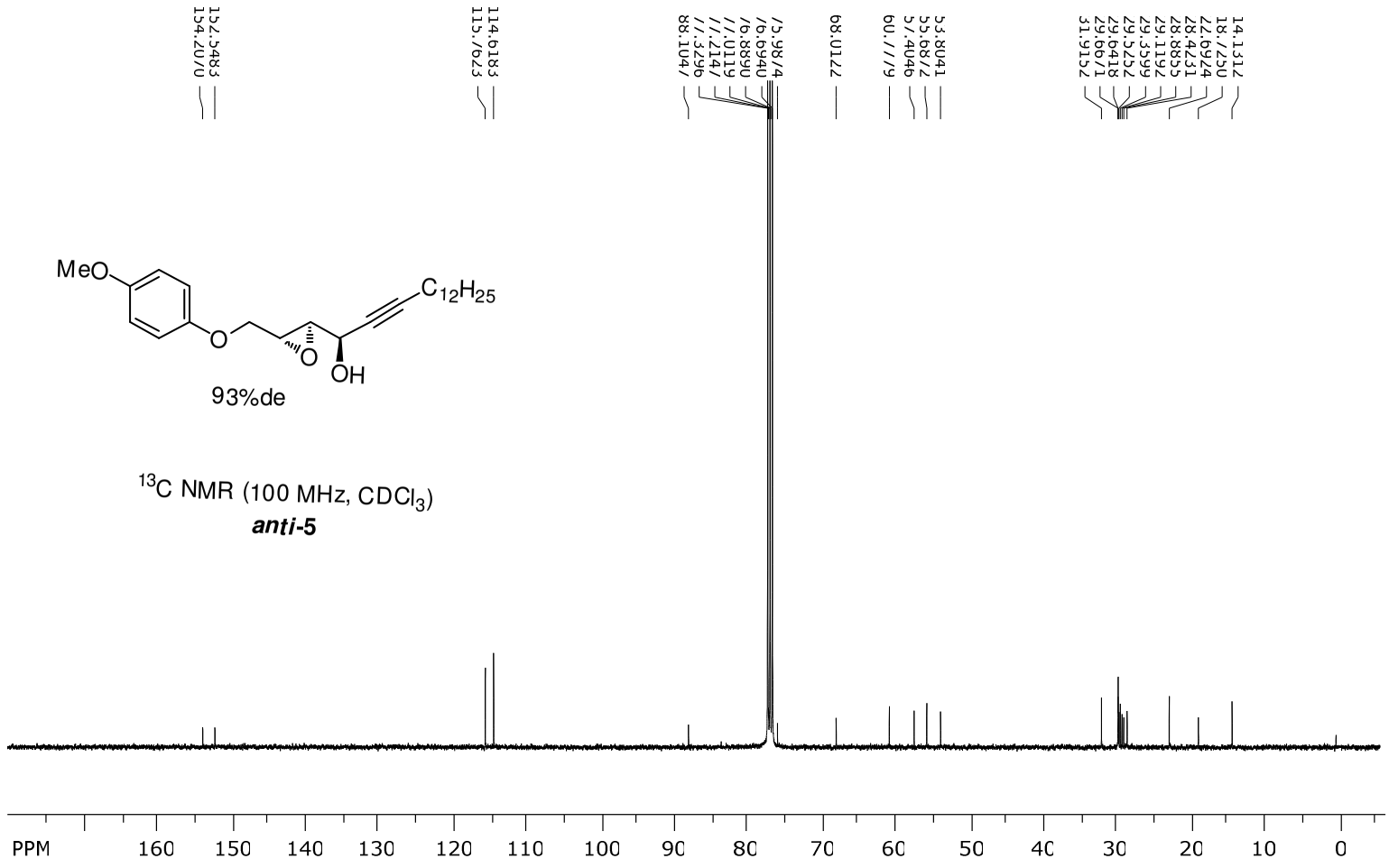

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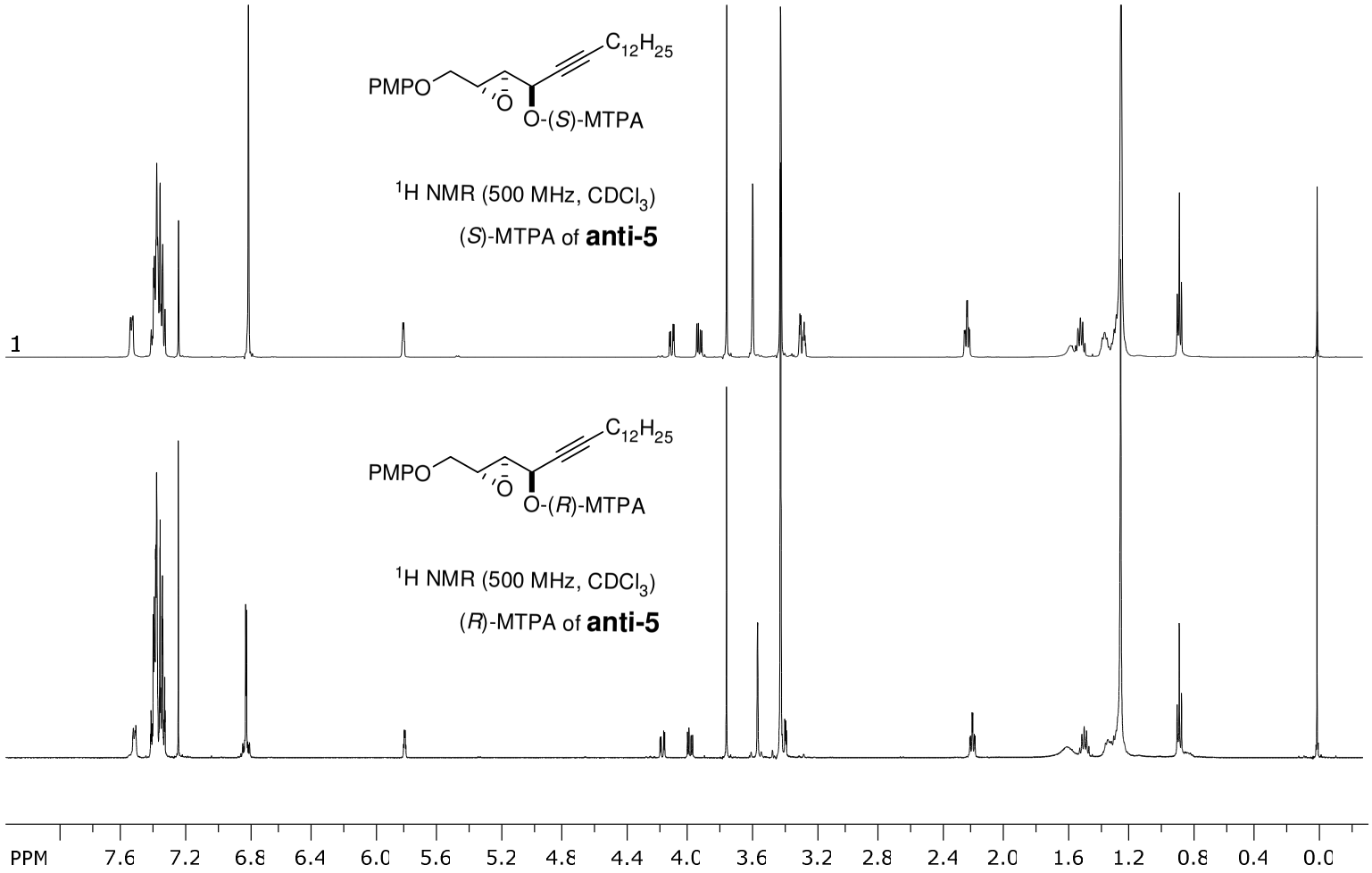

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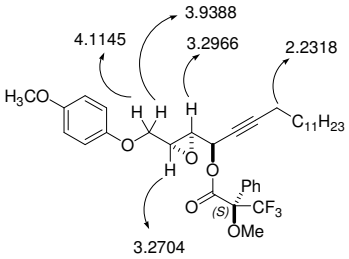
MTPA ester chemical shifts for determination of ee and absolute configuration:



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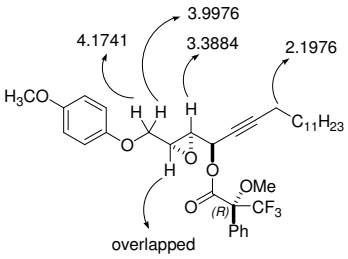

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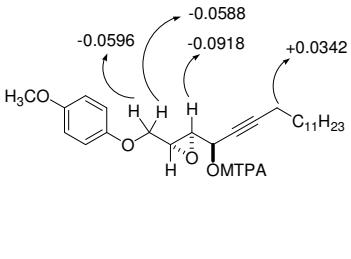

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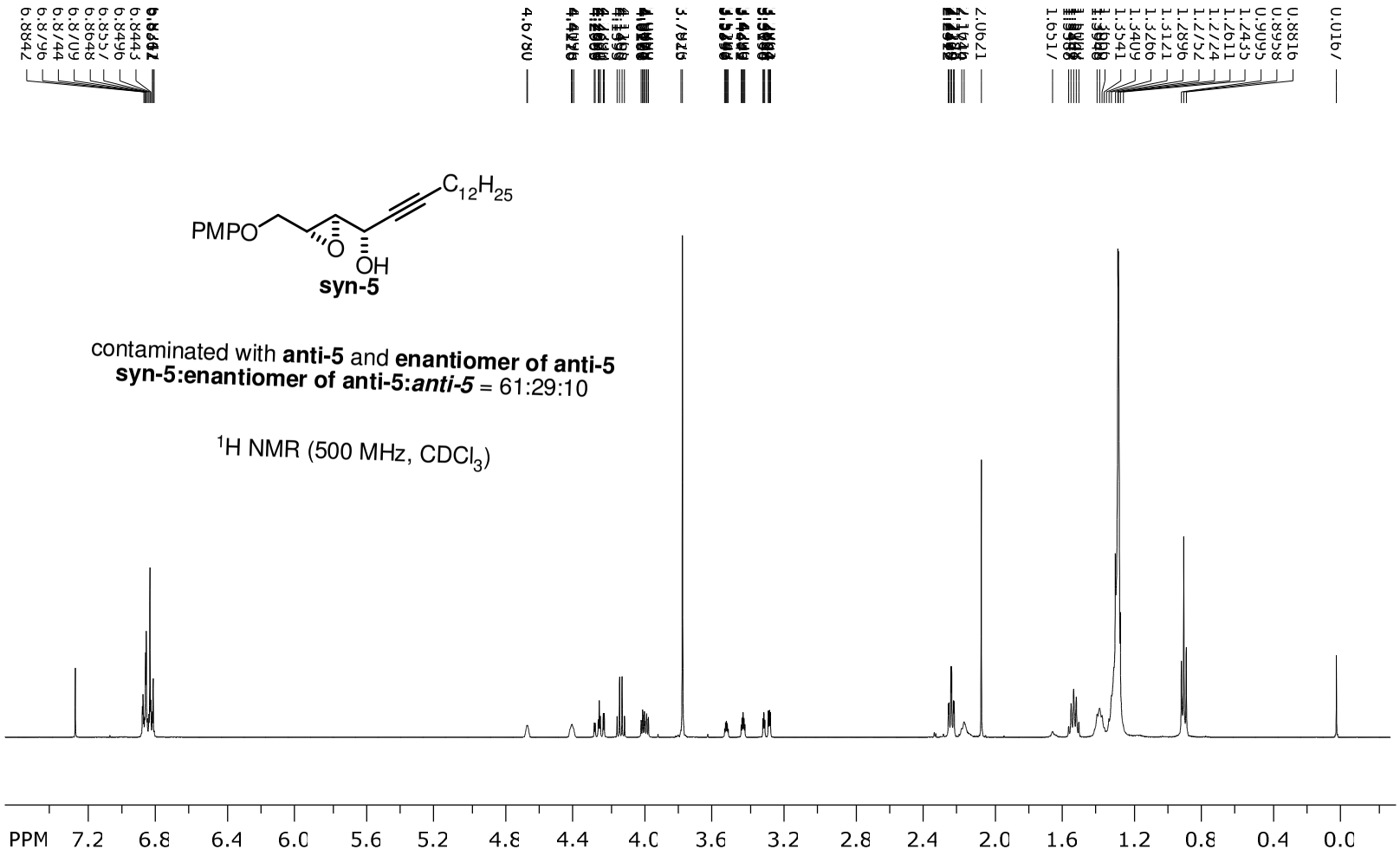

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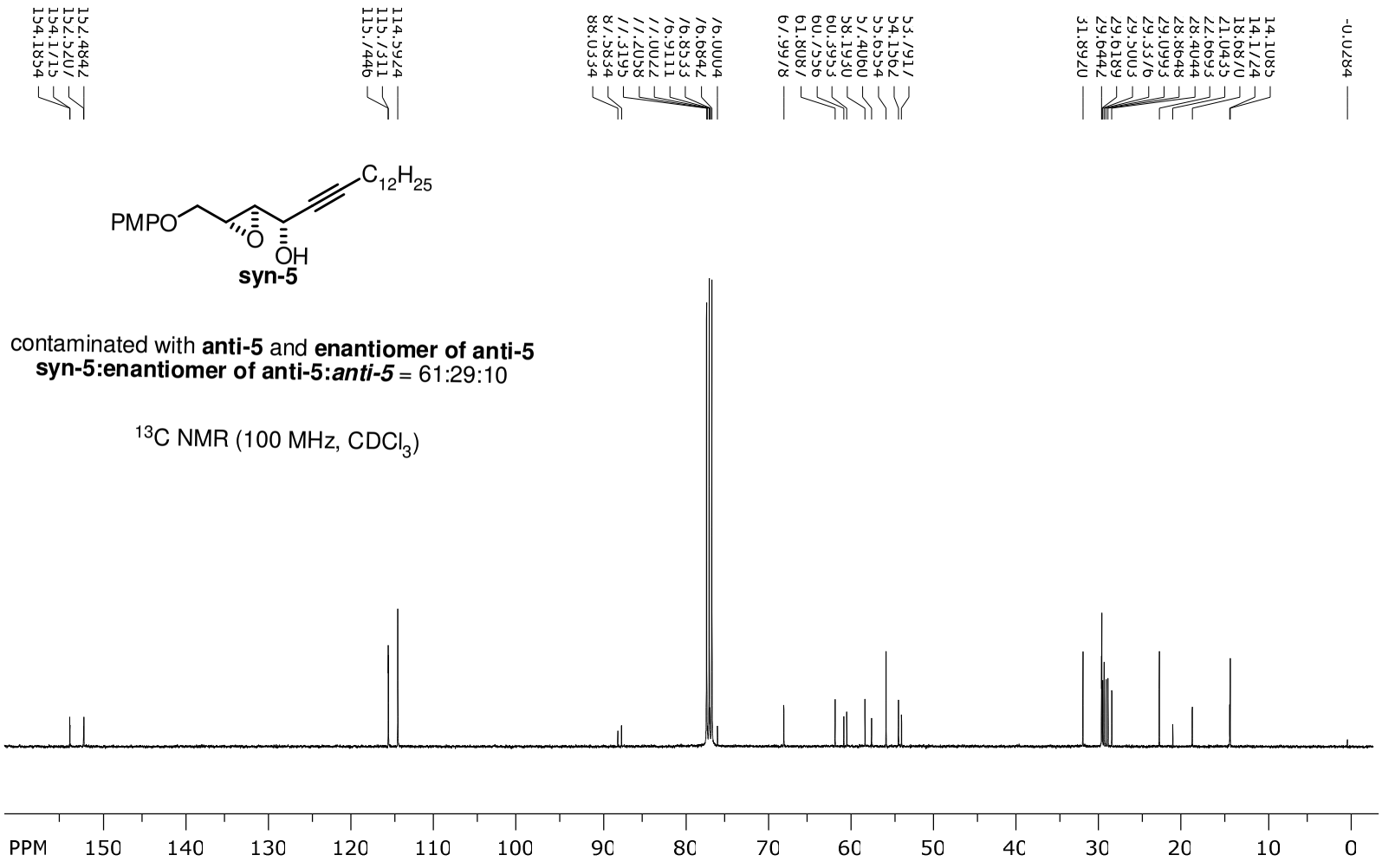

syn-5

contaminated with **anti-5** and **enantiomer of anti-5**
syn-5:enantiomer of anti-5:*anti-5* = 61:29:10

^{13}C NMR (100 MHz, $CDCl_3$)

file: ...\NMR-400(new)-LZ\zh090105s2\12\fid expt: <zgpg30>
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time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 4096

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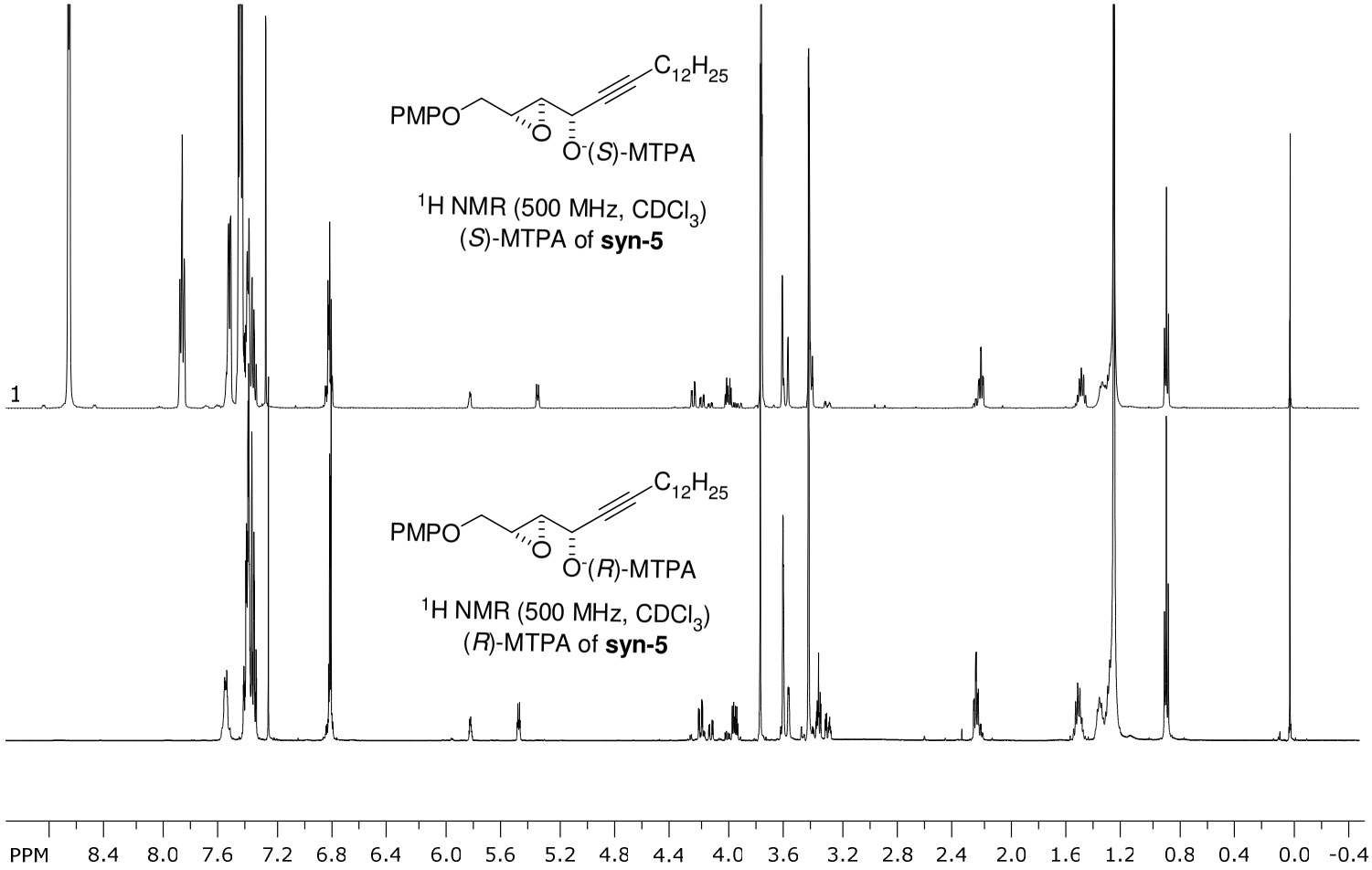

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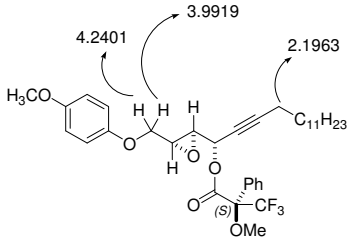
MTPA ester chemical shifts for determination of ee and absolute configuration:



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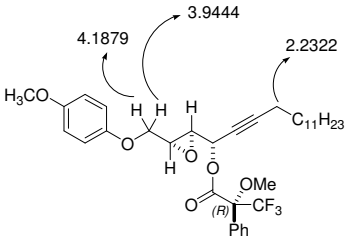

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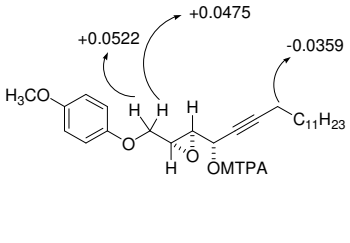

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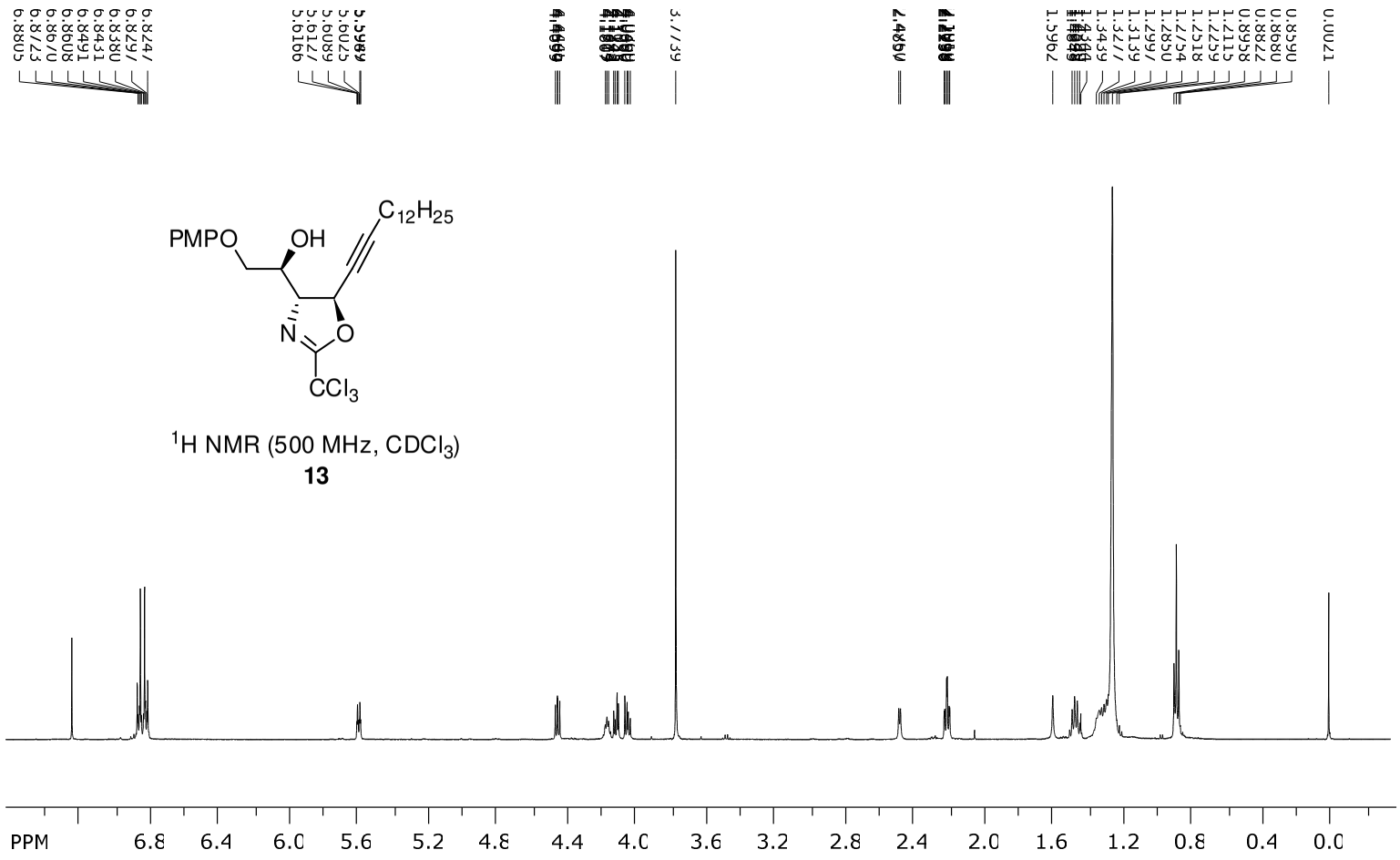

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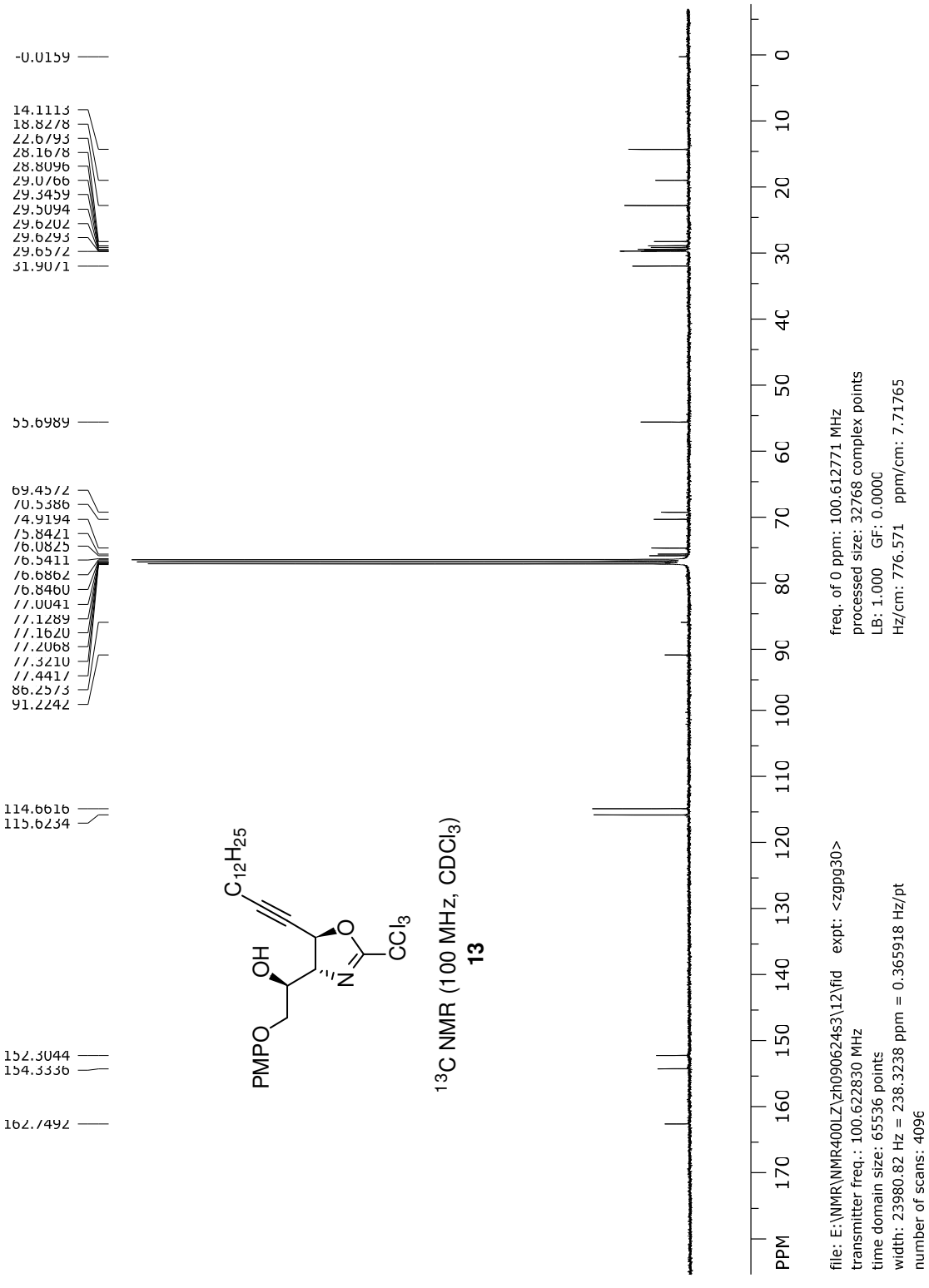
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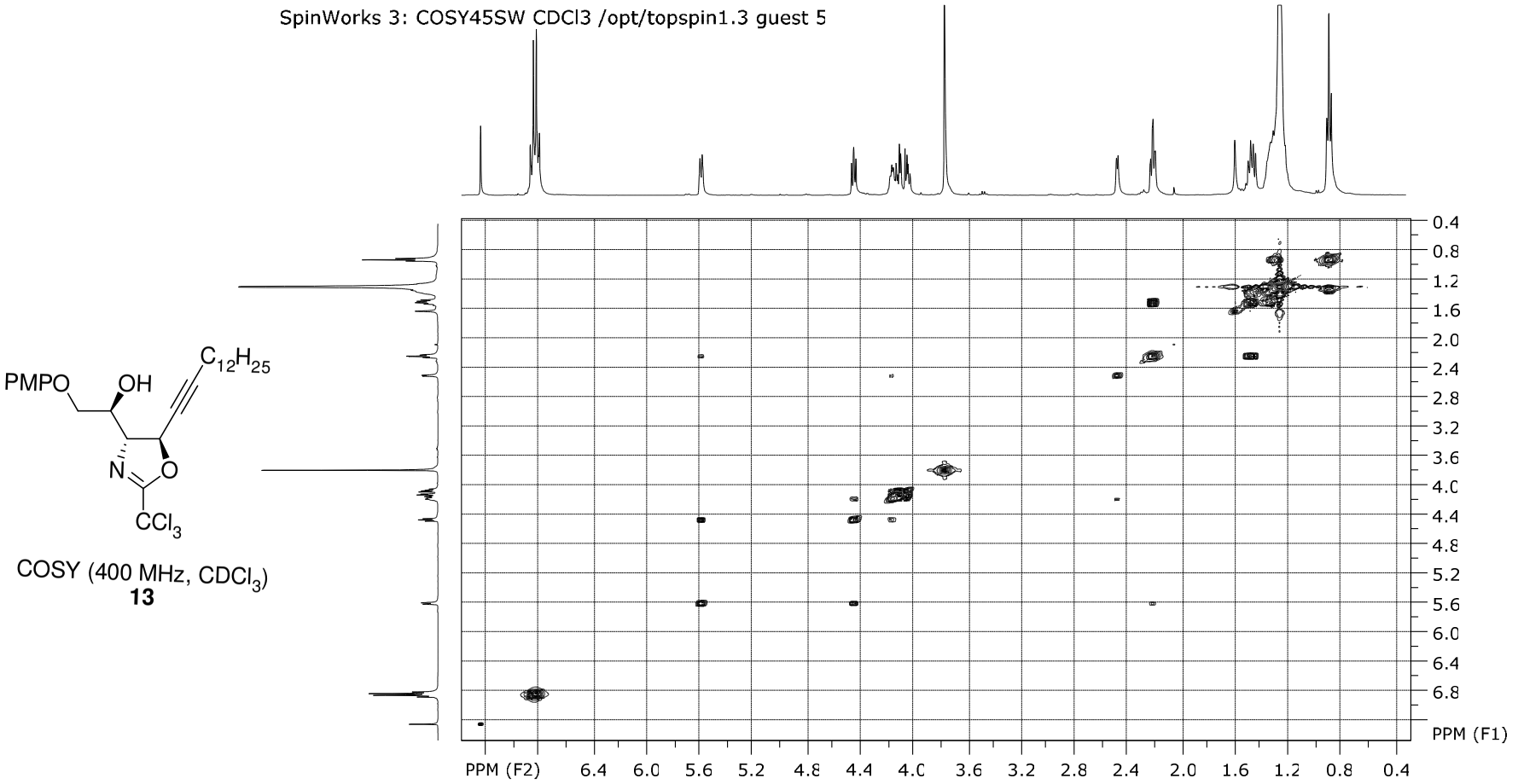
22.6793
28.1678
28.8096
29.0766
29.3459
29.5094
29.6202
29.6293
29.6572
31.9071
55.6989
69.4572
70.5386
74.9194
75.8421
76.0825
76.5411
76.6862
76.8460
77.0041
77.1289
77.1620
77.2068
77.3210
77.4417
86.2573
91.2242
114.6616
115.6234
152.3044
154.3336
162.7492
PMPO
OH
$C_{12}H_{25}$
CCl_3
^{13}C NMR (100 MHz, $CDCl_3$)
13
PPM
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
file: E:\NMR\NMR400LZ\zh090624s3\12\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 4096
freq. of 0 ppm: 100.612771 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 776.571 ppm/cm: 7.71765

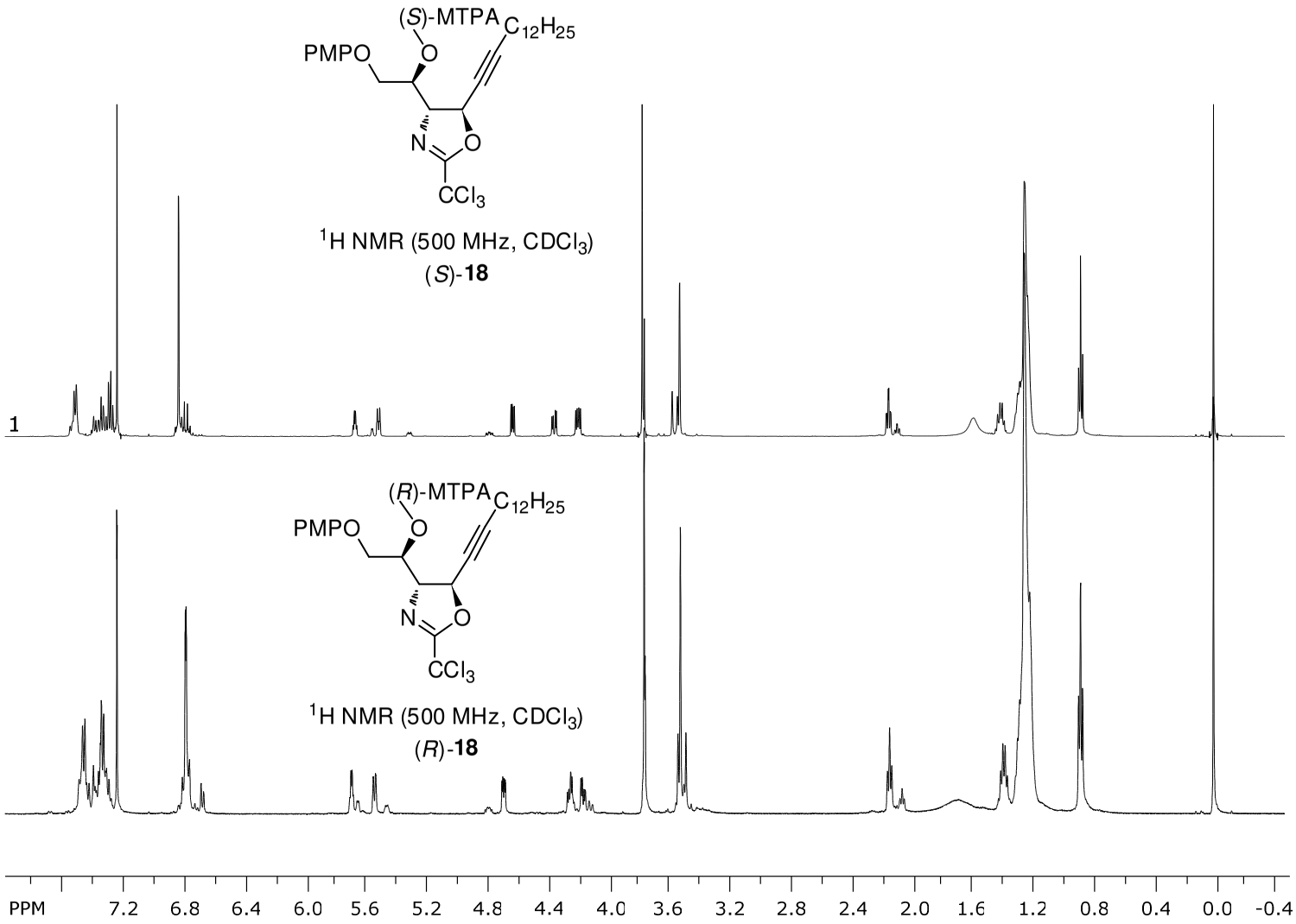


COSY (400 MHz, $CDCl_3$)
13

file: I:\NMR\NMR400LZ\zh090624s3\11\ser
expt: <cosyqf45>
transmitter freq: 400.131595 MHz
time domain size: 2048 by 128 points
width (F2): 3109.45 Hz = 7.7711 ppm = 1.5183 Hz/pt
number of scans: 8

F2: freq. of 0 ppm: 400.1300101 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 142.146 ppm/cm: 0.35525

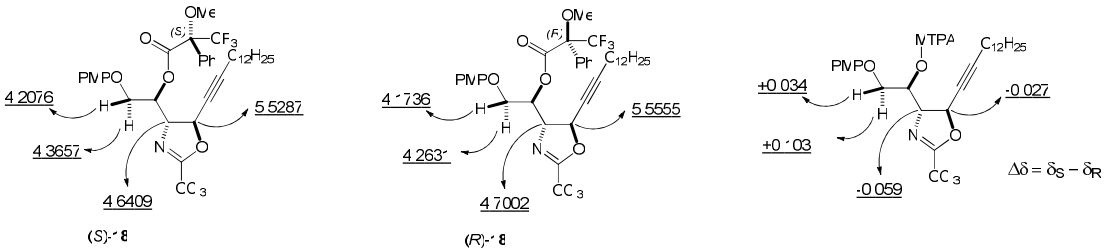
F1: freq. of 0 ppm: 400.1300101 MHz
processed size: 1024 complex points
window function: Sine
shift: 0.0 degrees
Hz/cm: 258.448 ppm/cm: 0.64591

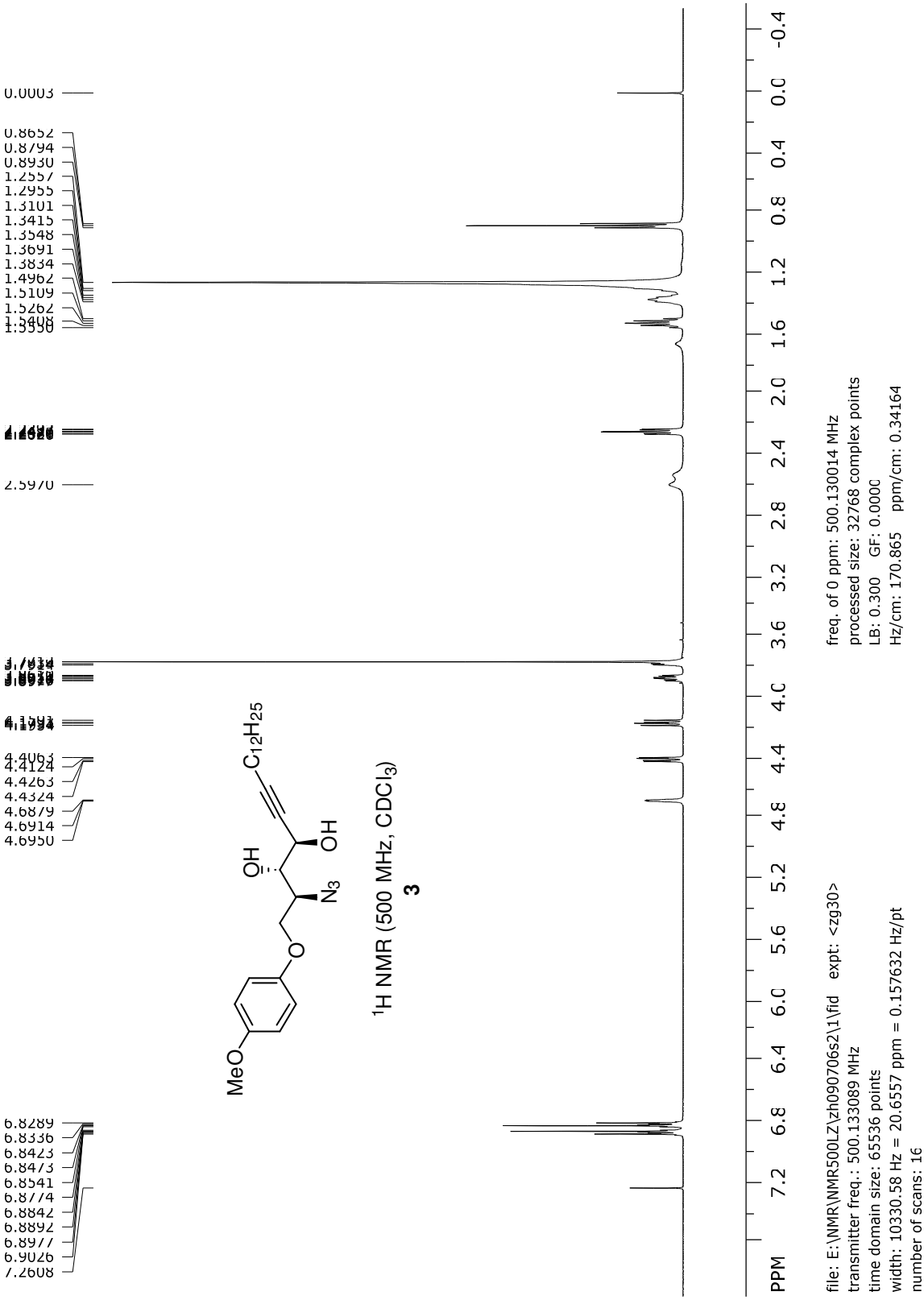


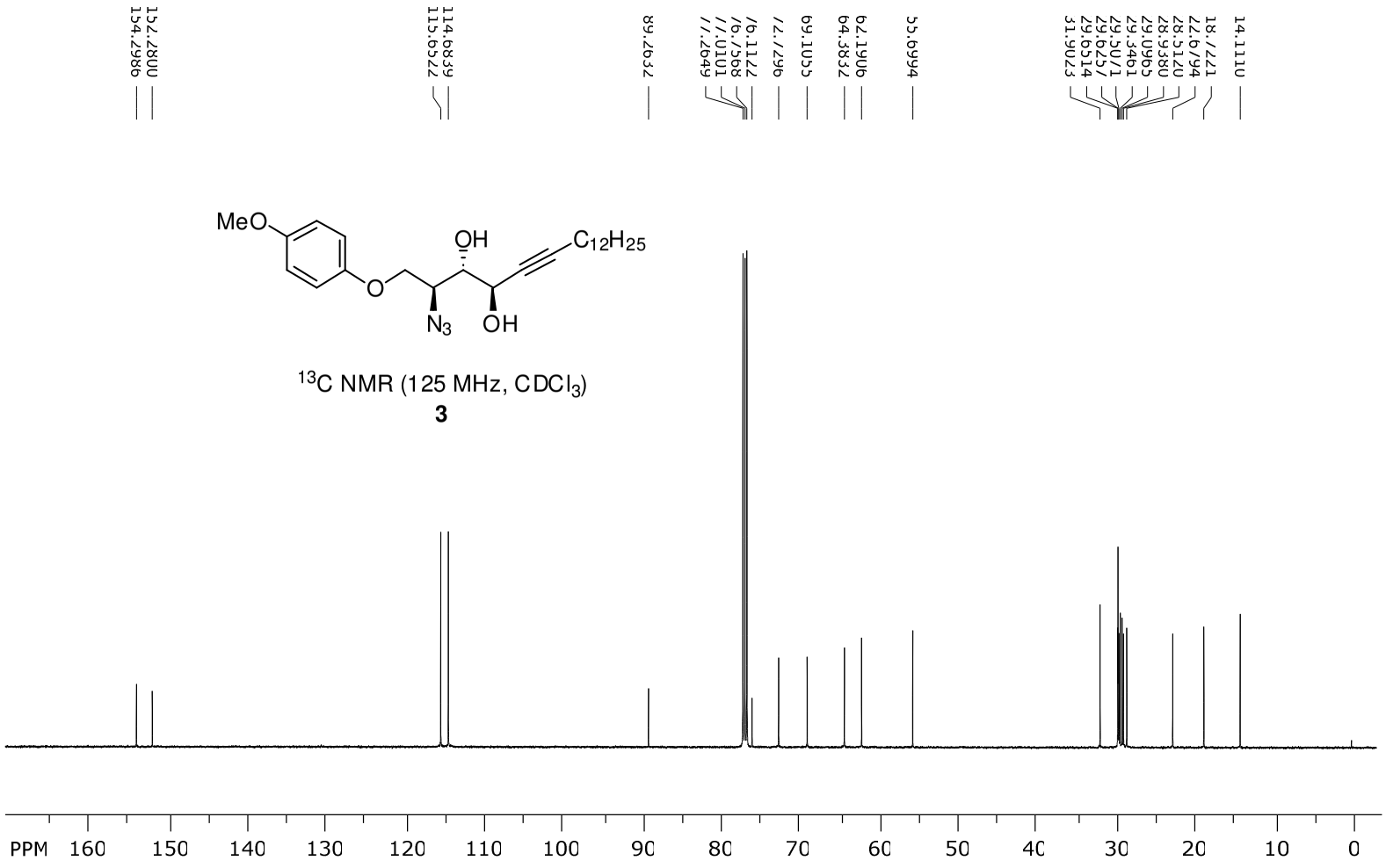
file: ...\NMR\NMR500LZ\zh090703s2-SCl\1\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130014 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 169.516 ppm/cm: 0.33894

MTPA ester chemical shifts for determination of ee and absolute configuration:




0.0003
0.8652
0.8794
0.8930
1.2557
1.2955
1.3101
1.3415
1.3548
1.3691
1.3834
1.4962
1.5109
1.5262
2.5970
4.4062
4.4124
4.4263
4.4324
4.6879
4.6914
4.6950
6.8289
6.8336
6.8423
6.8473
6.8541
6.8774
6.8842
6.8892
6.8977
6.9026
7.2608
MeO
OH
OH
N3
C12H25
1H NMR (500 MHz, CDCl3)
3
PPM
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
-0.4
file: E:\NMR\NMR500LZ\zh090706s2\1\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16
freq. of 0 ppm: 500.130014 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 170.865 ppm/cm: 0.34164

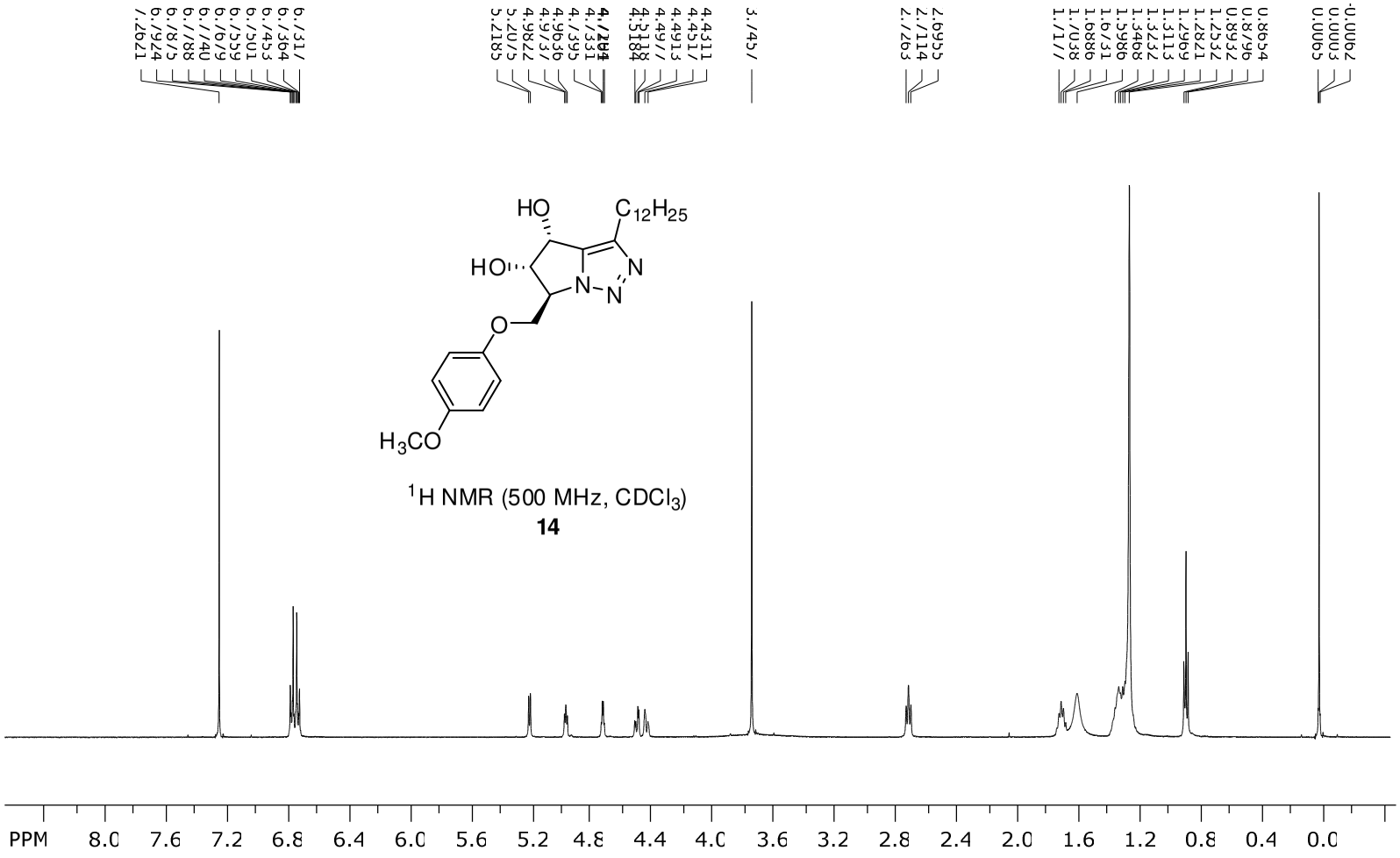


^{13}C NMR (125 MHz, $CDCl_3$)

3

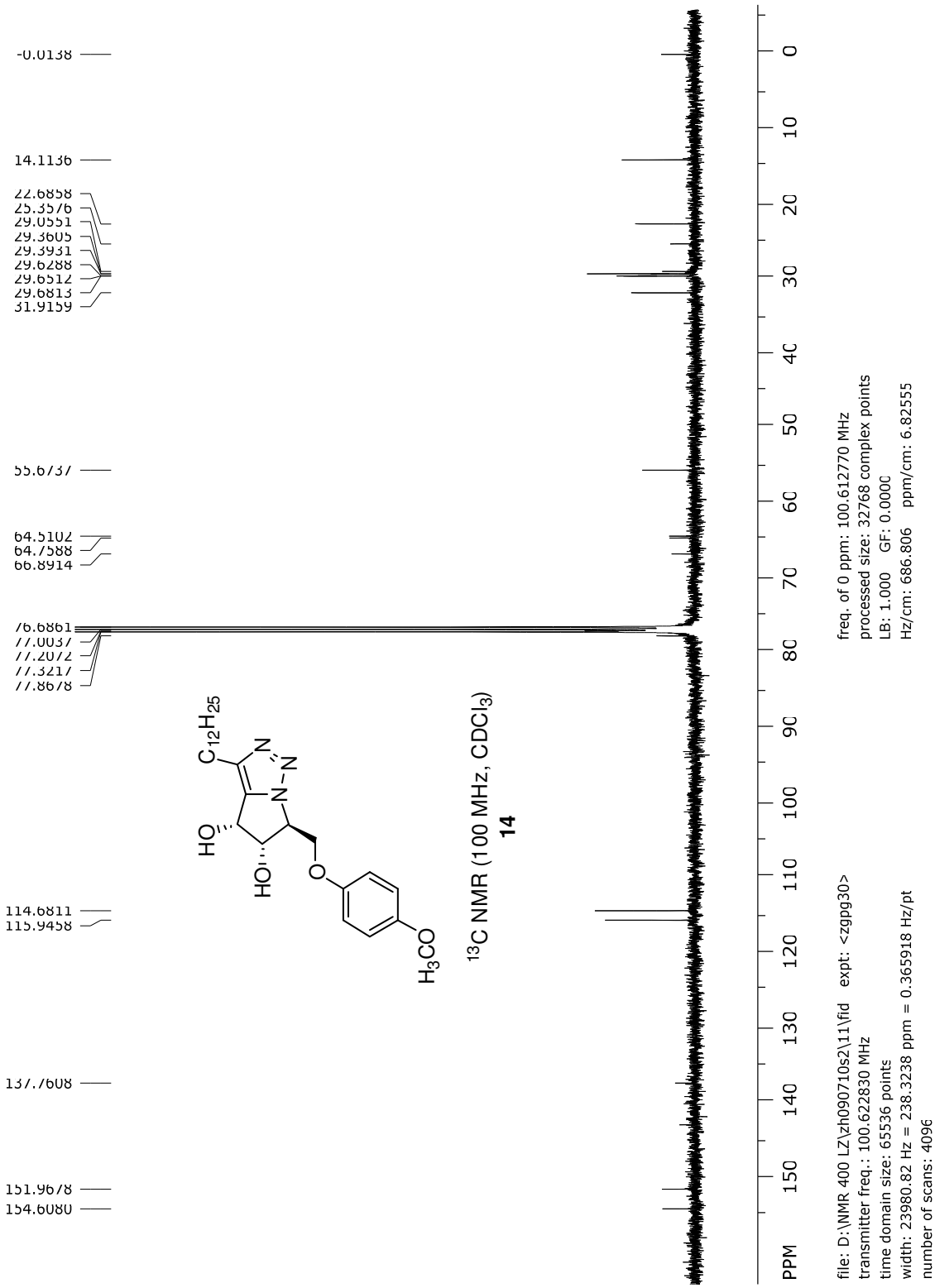
file: E:\NMR\NMR500LZ\zh090706s2\2\fid expt: <zgpg30>
transmitter freq.: 125.771622 MHz
time domain size: 65536 points
width: 31250.00 Hz = 248.4662 ppm = 0.476837 Hz/pt
number of scans: 8192

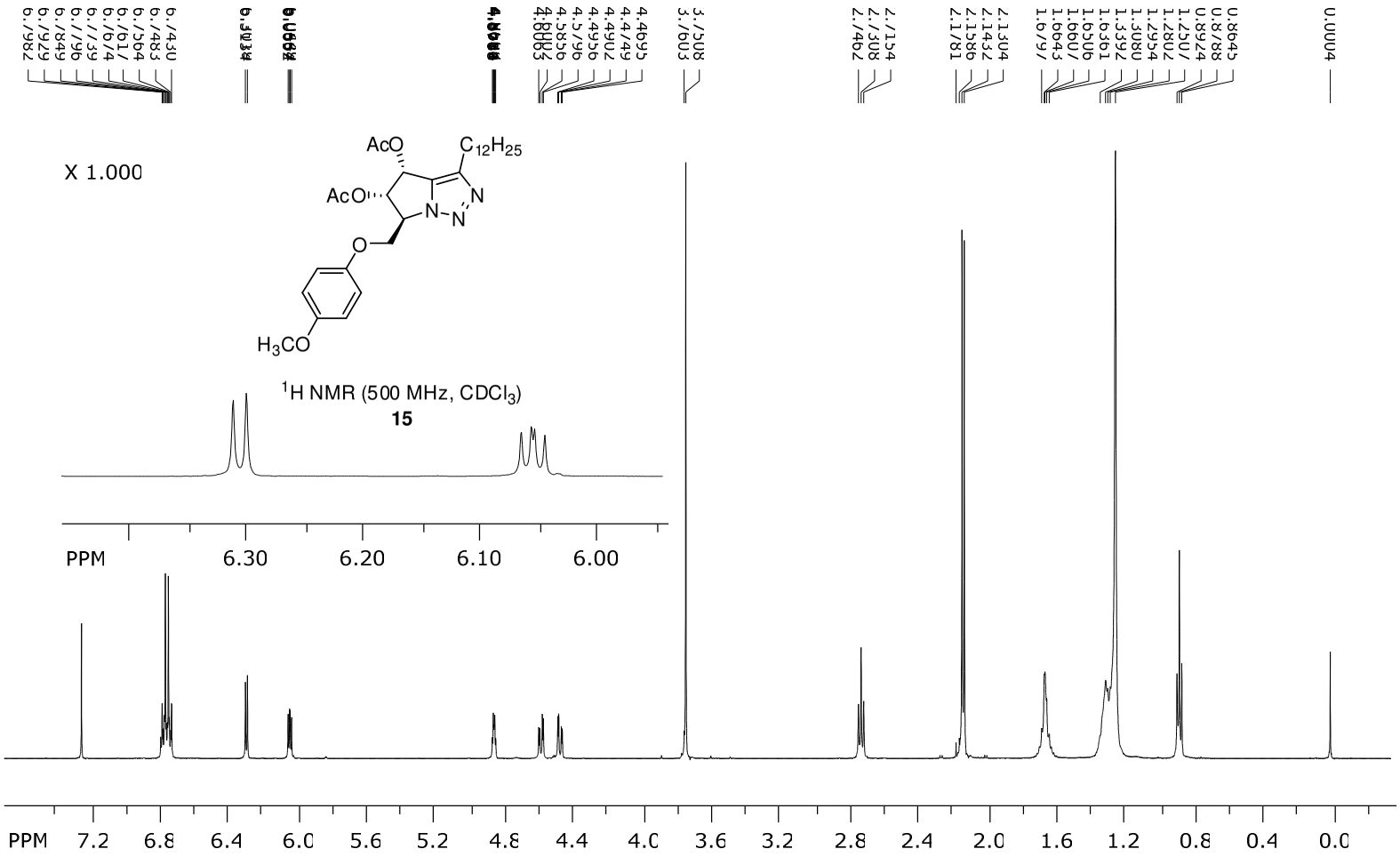
freq. of 0 ppm: 125.757793 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 875.952 ppm/cm: 6.96462



file: D:\NMR 500 LZ\zh090710s2\1\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16

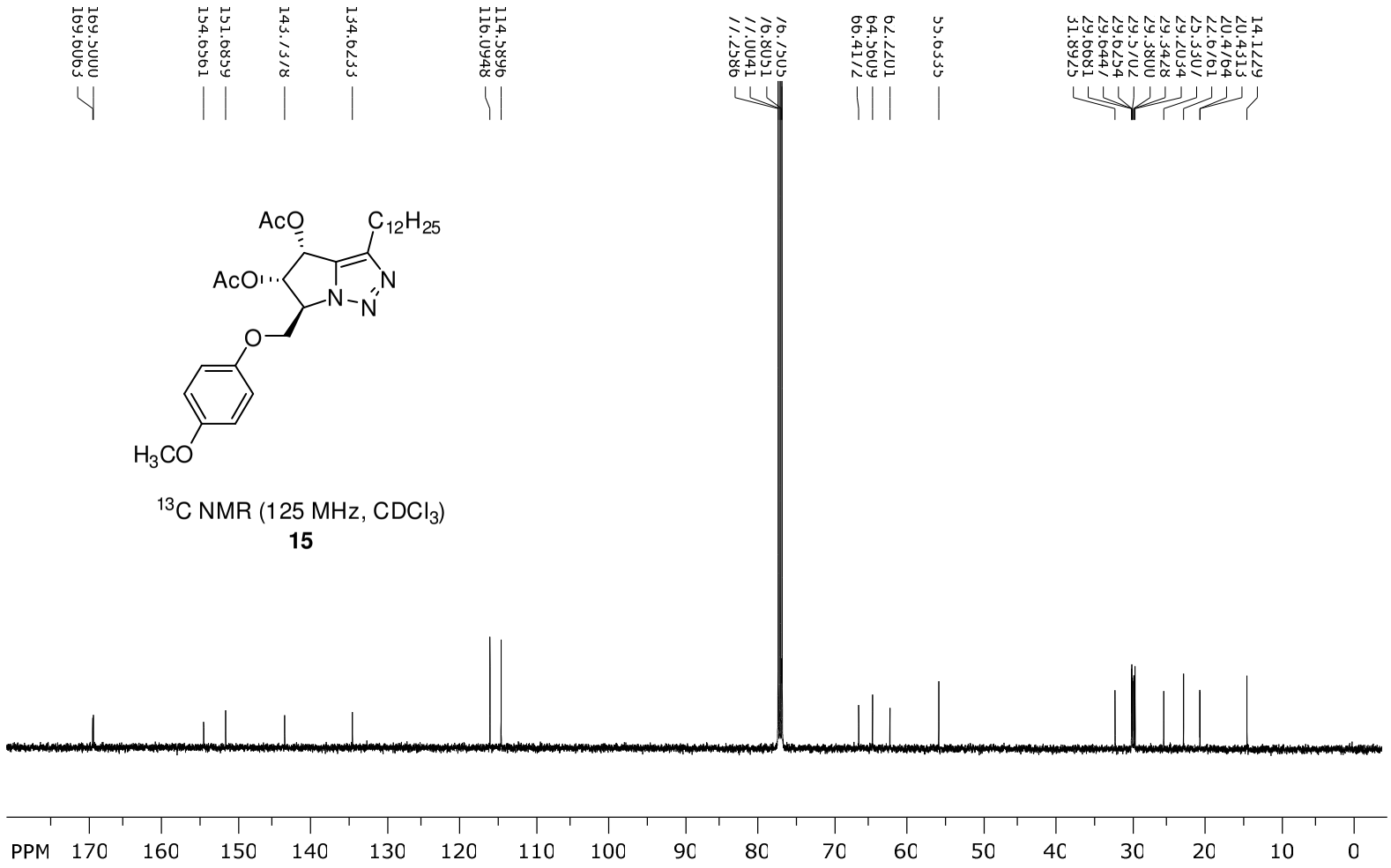
freq. of 0 ppm: 500.130013 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 183.005 ppm/cm: 0.36591


-0.0138
14.1136
22.6858
25.3576
29.0351
29.3605
29.3931
29.6288
29.6512
29.6813
31.9159
55.6737
64.5102
64.7588
66.8914
76.6861
77.0037
77.2072
77.3217
77.8678
114.6811
115.9458
137.7608
151.9678
154.6080
PPM
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
HO
HO
O
$C_{12}H_{25}$
H_3CO
N
N
N
^{13}C NMR (100 MHz, $CDCl_3$)
14
file: D:\NMR 400 LZ\zh090710s2\11\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 4096
freq. of 0 ppm: 100.612770 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 686.806 ppm/cm: 6.82555



file: D:\NMR 500 LZ\zh090805s2\1\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130010 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 161.422 ppm/cm: 0.32276

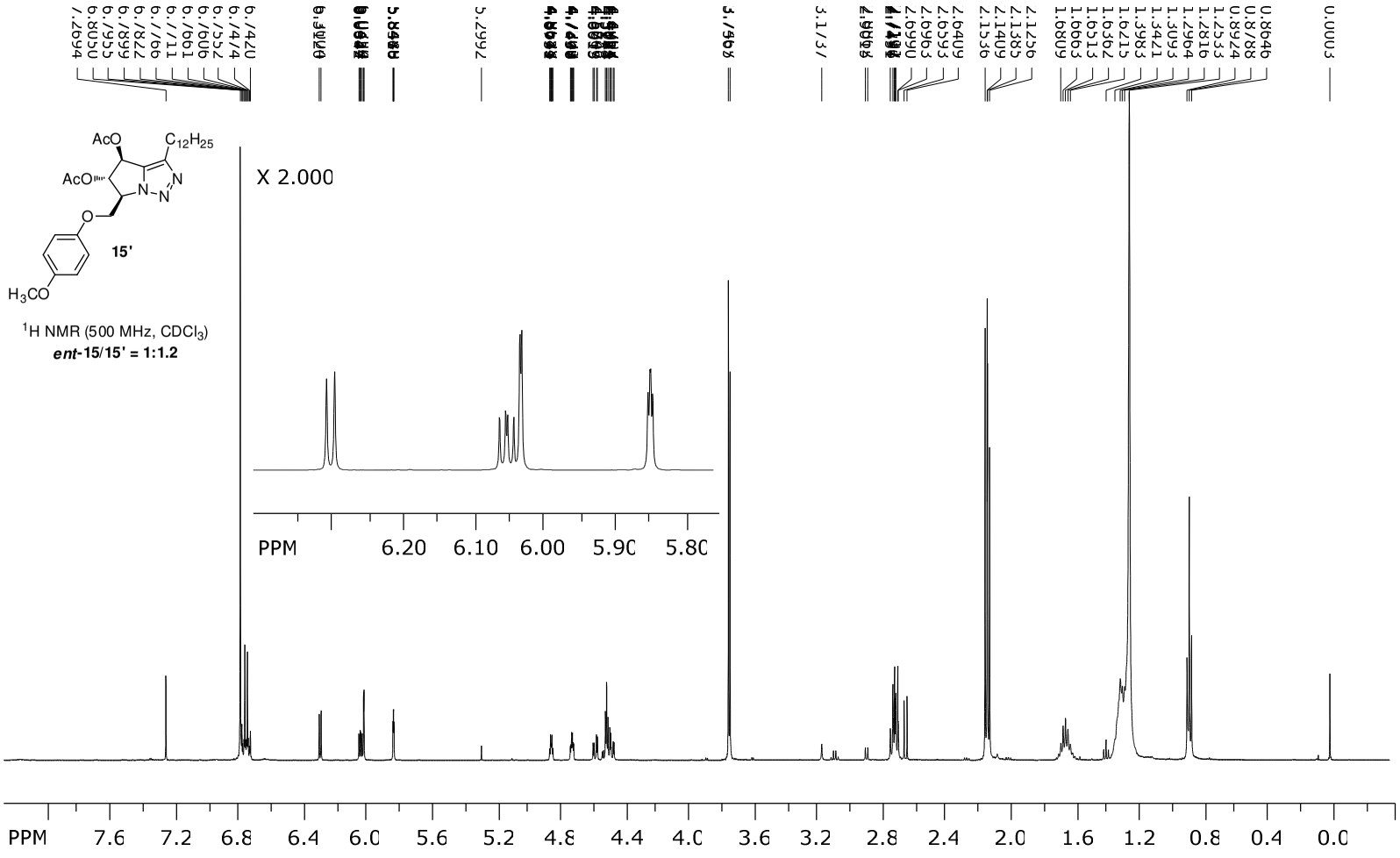


^{13}C NMR (125 MHz, $CDCl_3$)

15

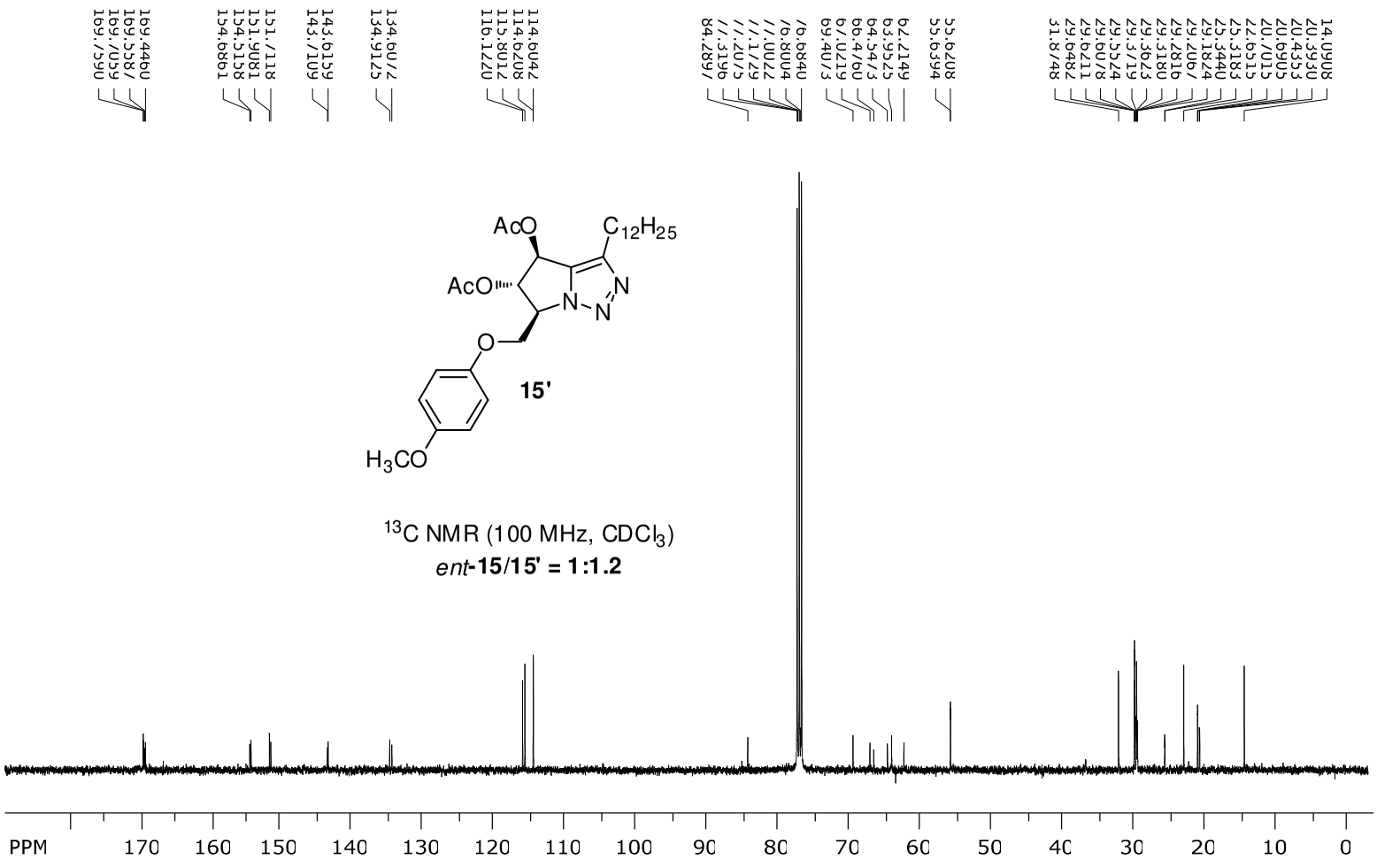
file: D:\NMR 500 LZ\zh090805s2\2\fid expt: <zgpg30>
transmitter freq.: 125.771622 MHz
time domain size: 65536 points
width: 31250.00 Hz = 248.4662 ppm = 0.476837 Hz/pt
number of scans: 1024

freq. of 0 ppm: 125.757796 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 931.719 ppm/cm: 7.40802



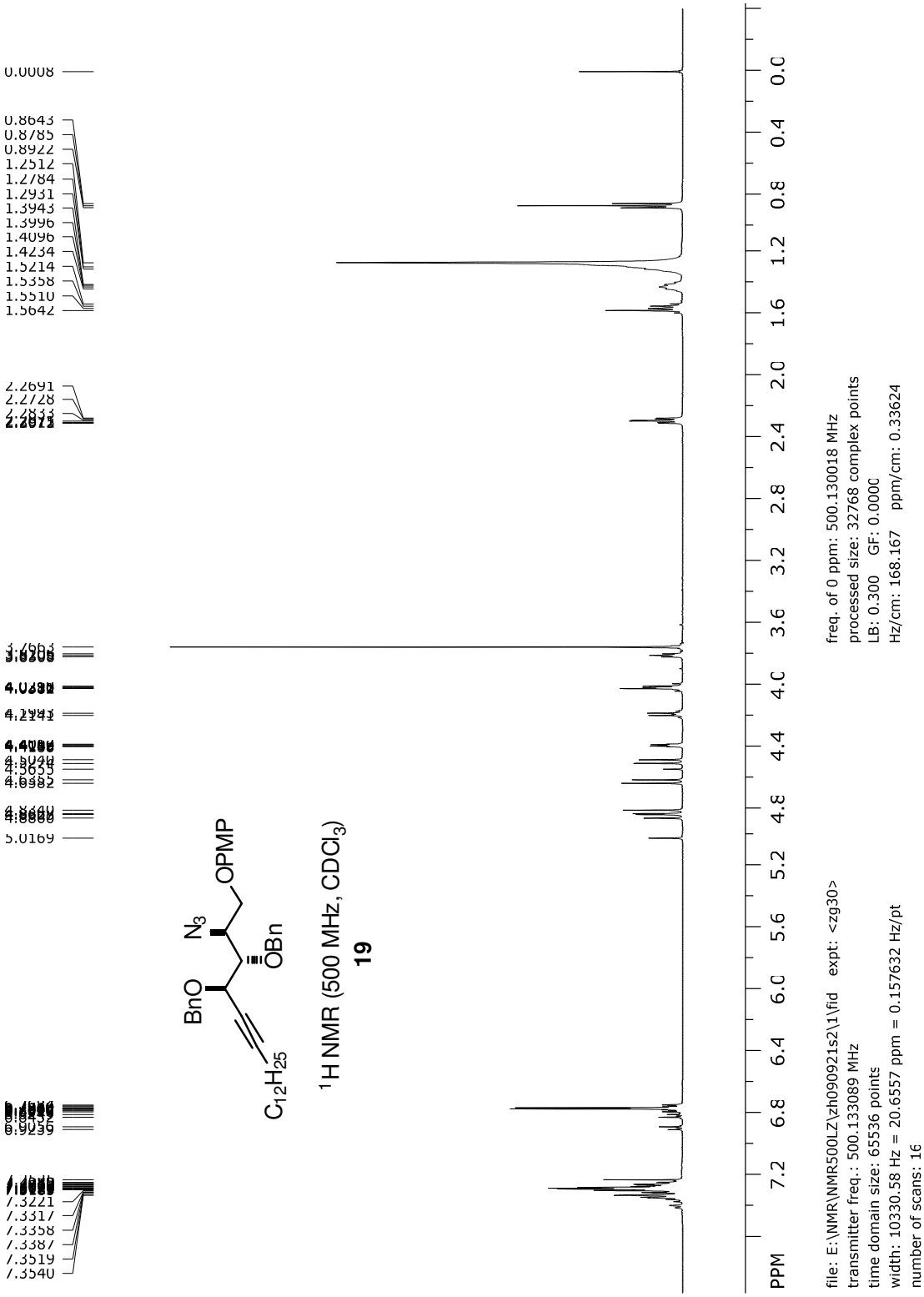
file: E:\NMR\NMR500LZ\zh090226s2\1\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16

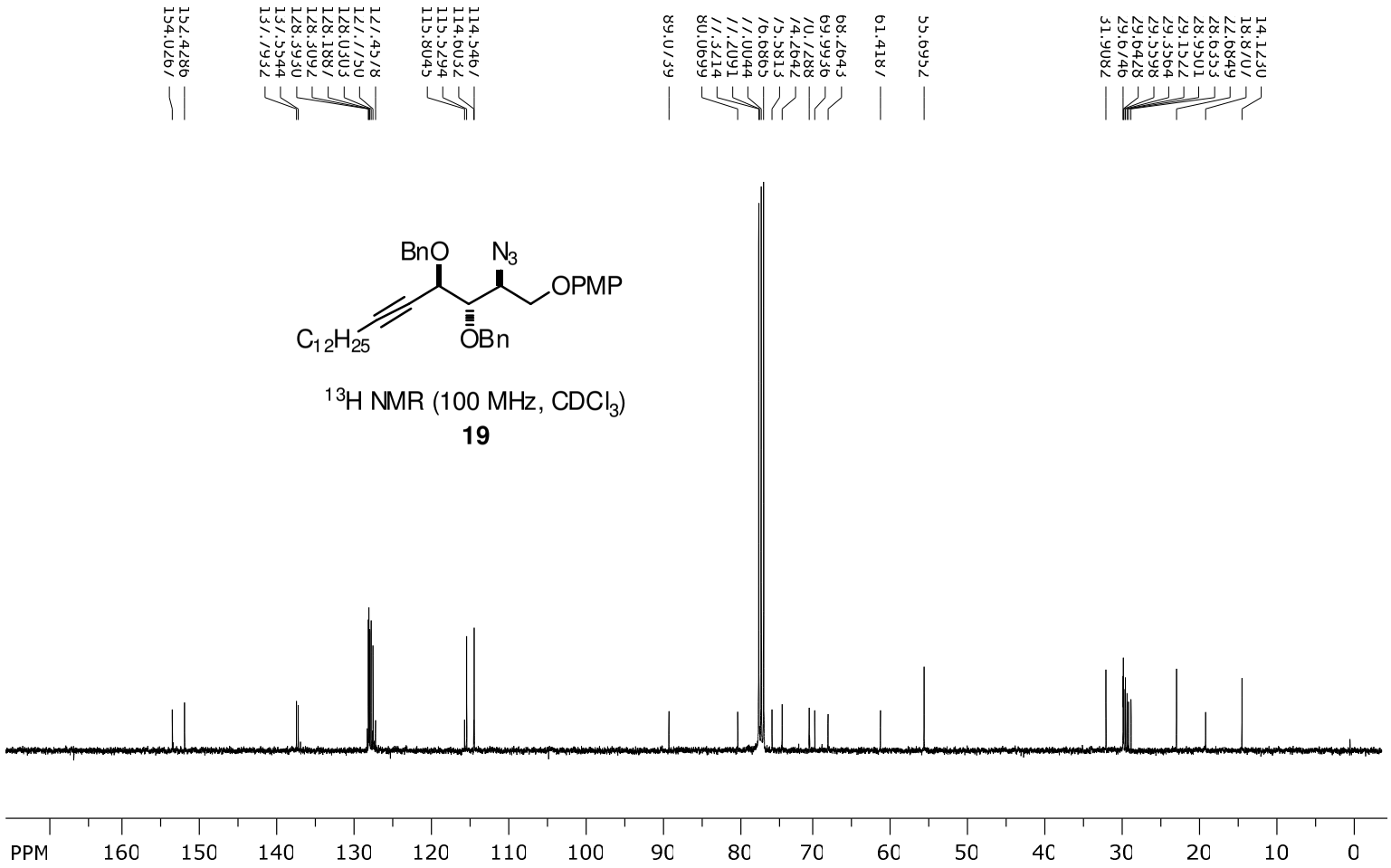
freq. of 0 ppm: 500.130009 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 173.113 ppm/cm: 0.34613



file: E:\NMR\NMR400LZ\zh090226s2\10\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 1024

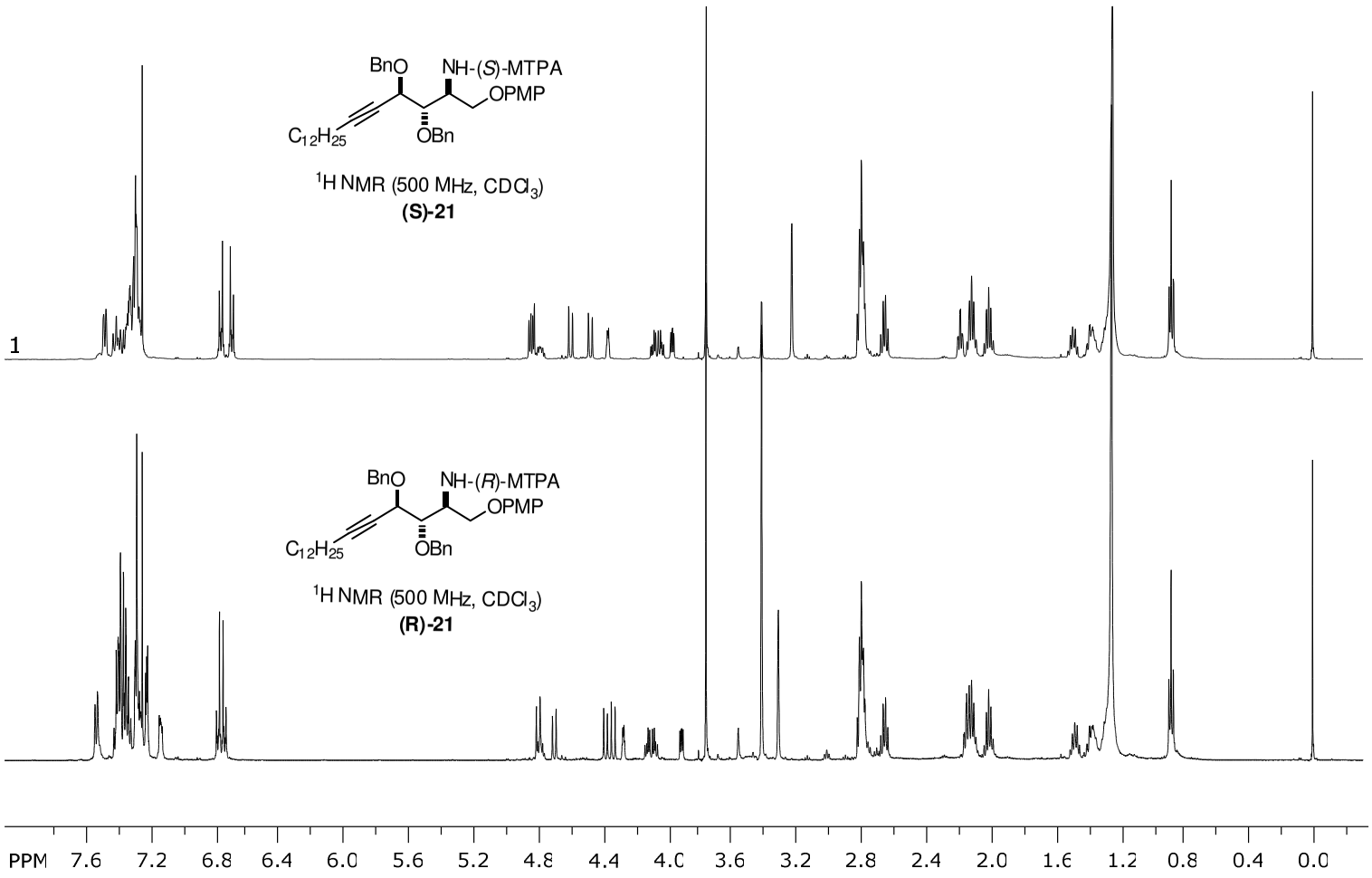
freq. of 0 ppm: 100.612774 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 775.528 ppm/cm: 7.70727


0.0008
0.8643
0.8785
0.8922
1.2512
1.2784
1.2931
1.3943
1.3996
1.4096
1.4234
1.5214
1.5358
1.5510
1.5642
2.2691
2.2728
5.0169
7.3221
7.3317
7.3358
7.3387
7.3519
7.3540
BnO
N3
OPMP
OBn
C12H25
1H NMR (500 MHz, CDCl3)
19
PPM
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
file: E:\NMR\NMR500LZ\zh090921s2\1\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16
freq. of 0 ppm: 500.130018 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 168.167 ppm/cm: 0.33624



file: E:\NMR\NMR400LZ\zh090921s2\10\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 1024

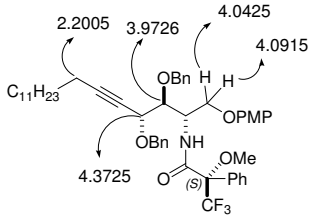
freq. of 0 ppm: 100.612773 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 724.382 ppm/cm: 7.19899



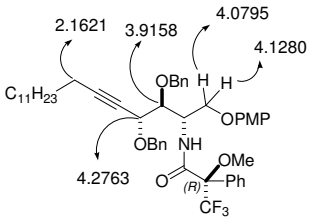
file: E:\NMR\NMR500LZ\zh090929-SCl\1\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130014 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 168.617 ppm/cm: 0.33714

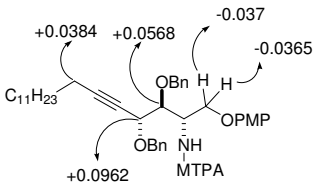
MTPA amide chemical shifts for determination of ee and absolute configuration:



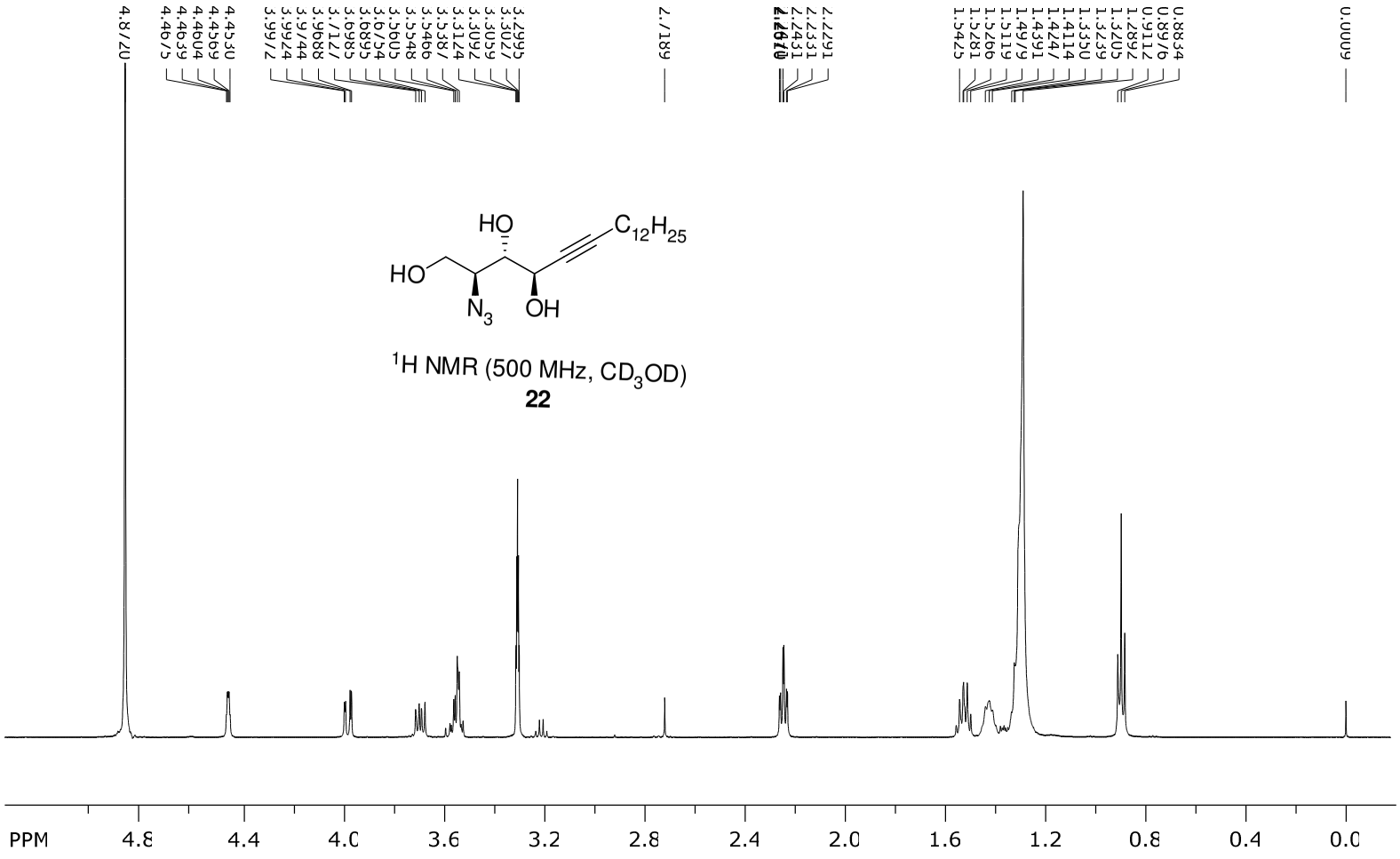
(*S*)-**21**



(*R*)-**21**

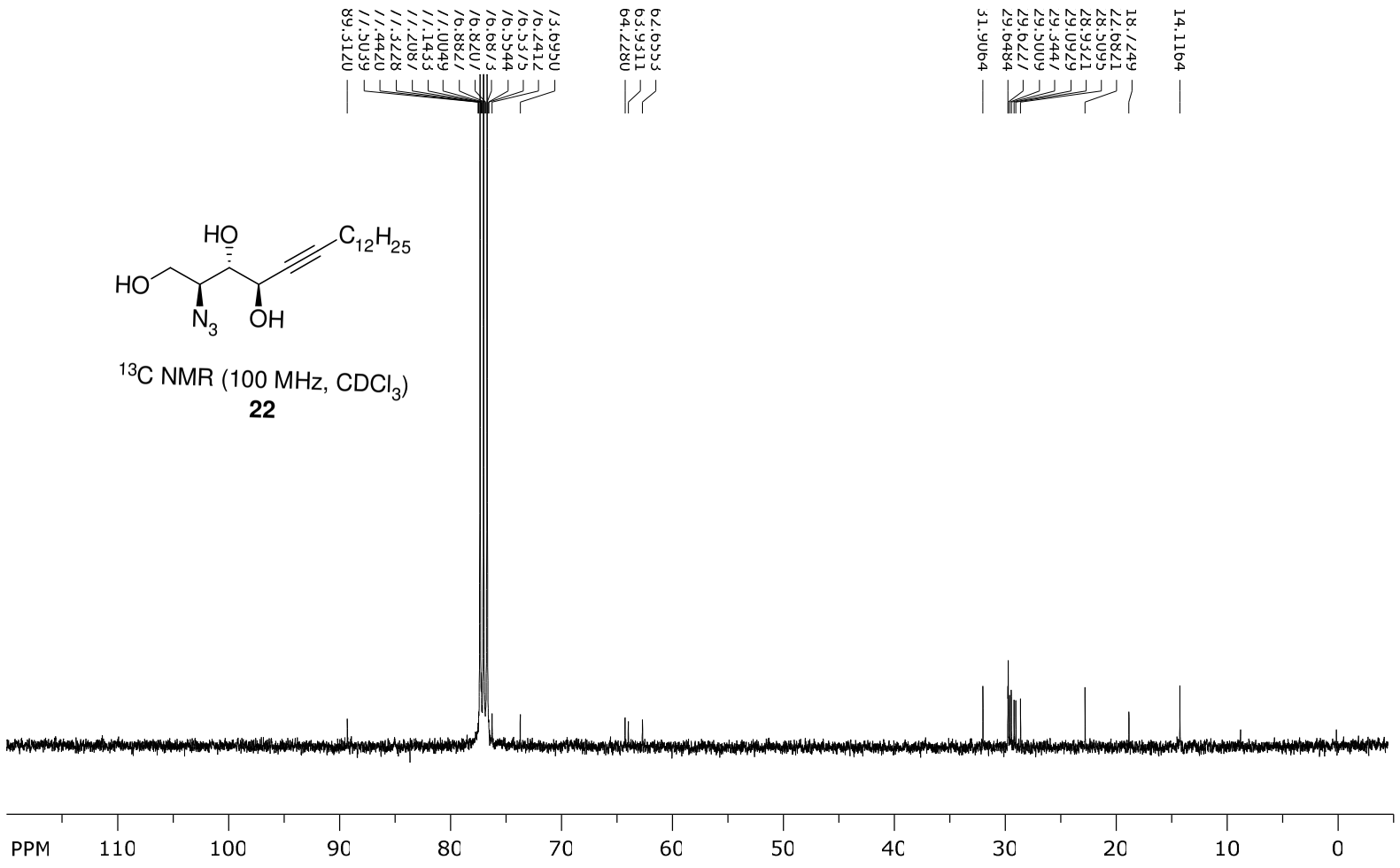


$\Delta\delta = \delta_S - \delta_R$



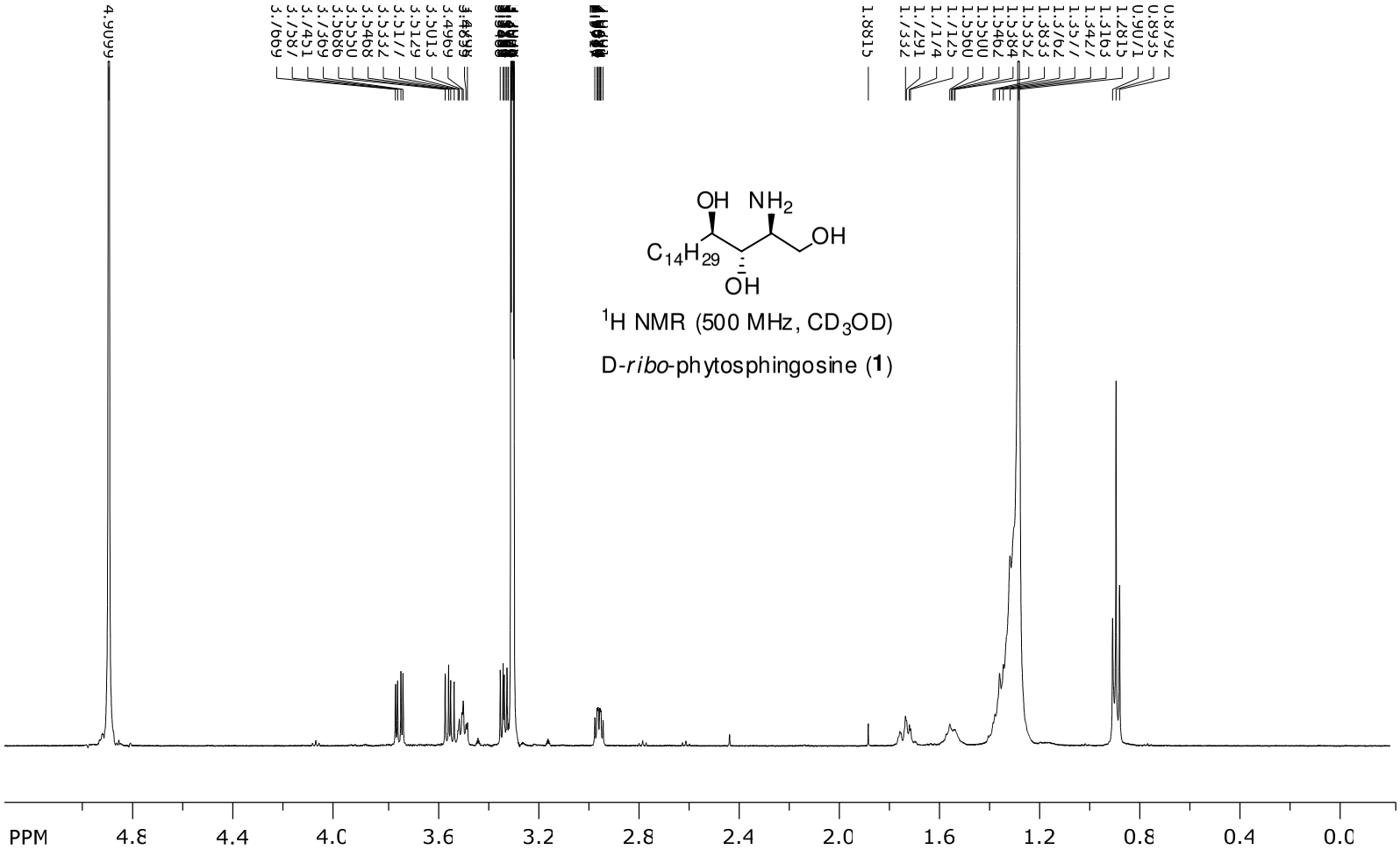
file: E:\NMR\NMR500LZ\zh090709s2\3\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130013 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 110.608 ppm/cm: 0.22116



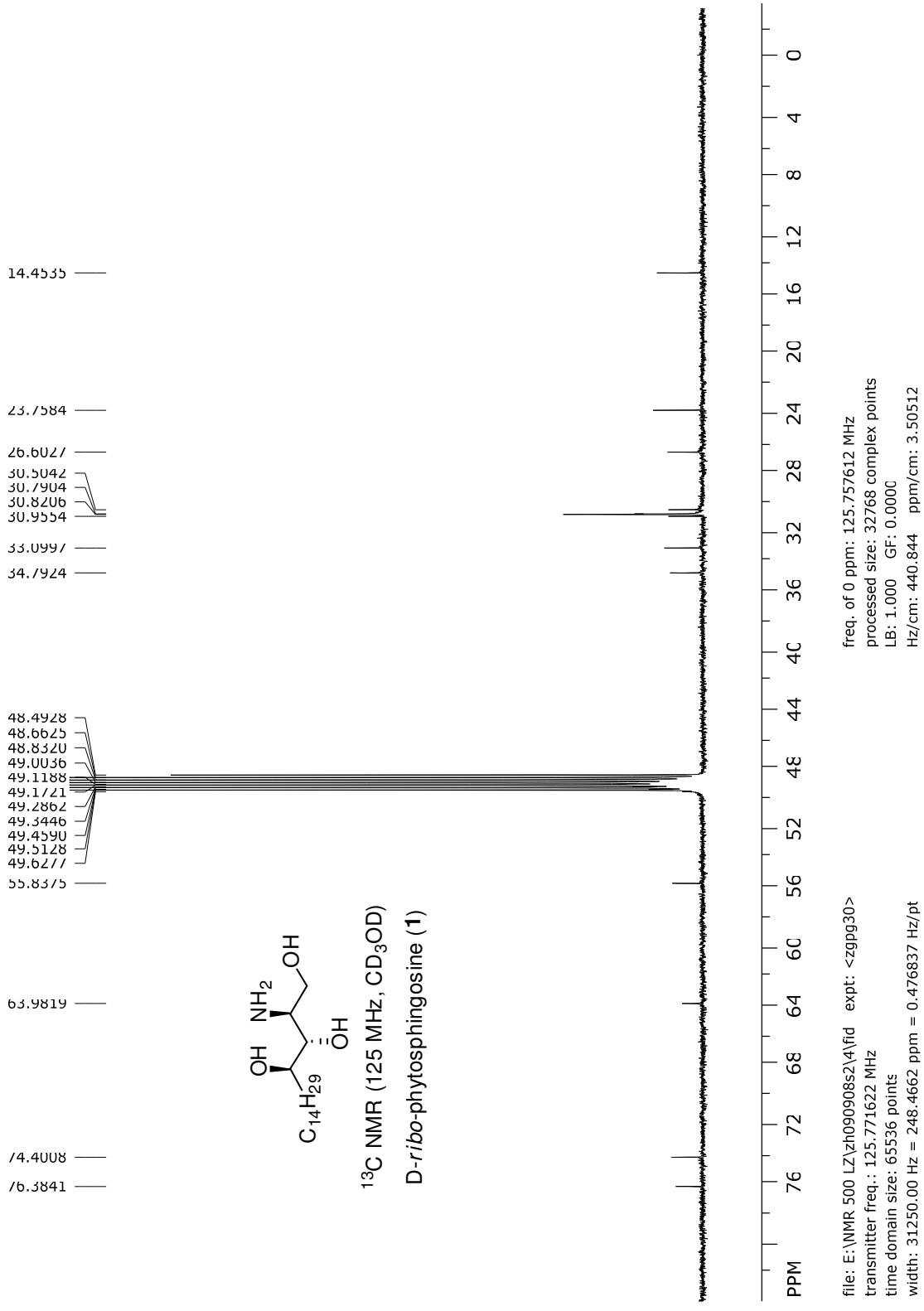
file: E:\NMR\NMR400LZ\zh090709s2\10\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 2048

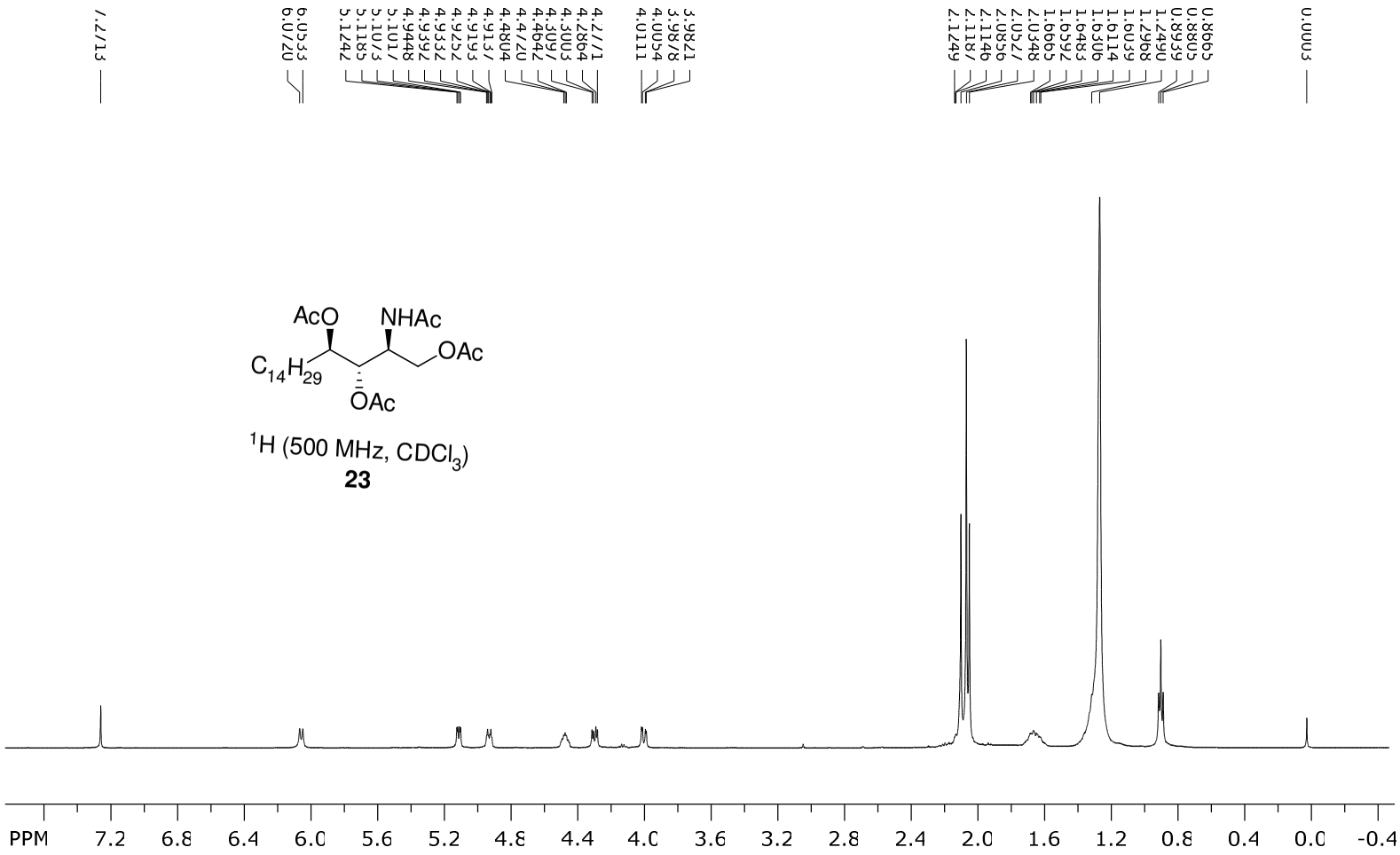
freq. of 0 ppm: 100.612771 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 502.058 ppm/cm: 4.98950



file: E:\NMR 500 LZ\zh090908s2\3\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16

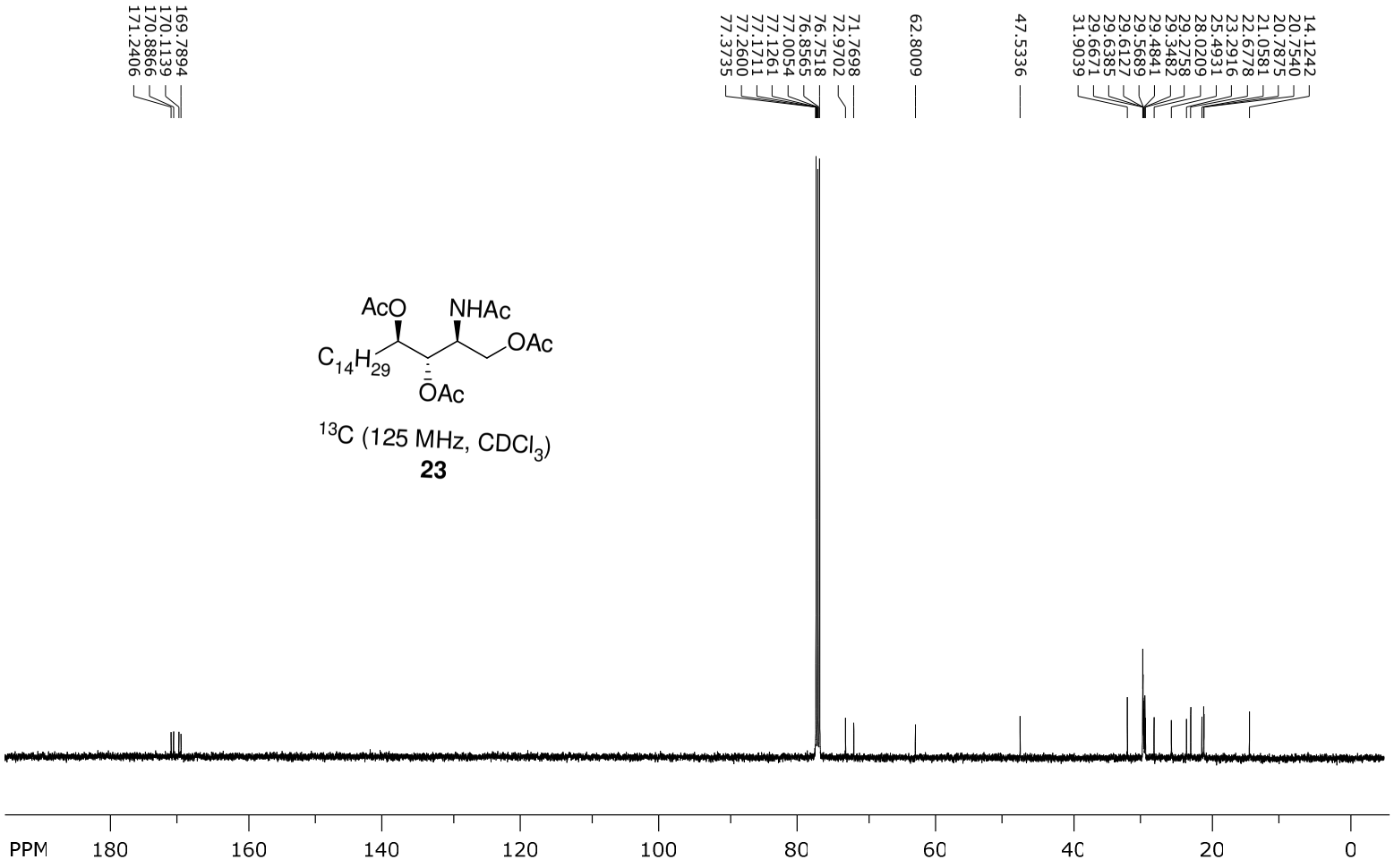
freq. of 0 ppm: 500.130016 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 110.546 ppm/cm: 0.22103


14.4535
23.7584
26.6027
30.5042
30.7904
30.8206
30.9554
33.0997
34.7924
48.4928
48.6625
48.8320
49.0036
49.1188
49.1721
49.2862
49.3446
49.4590
49.5128
49.6277
55.8375
63.9819
74.4008
76.3841
OH NH2 OH
C14H29
OH
13C NMR (125 MHz, CD3OD)
D-ribo-phytosphingosine (1)
PPM
76 72 68 64 60 56 52 48 44 40 36 32 28 24 20 16 12 8 4 0
file: E:\NMR 500 LZ\zh090908s2\4\fid expt: <zgpg30>
transmitter freq.: 125.771622 MHz
time domain size: 65536 points
width: 31250.00 Hz = 248.4662 ppm = 0.476837 Hz/pt
number of scans: 12288
freq. of 0 ppm: 125.757612 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 440.844 ppm/cm: 3.50512



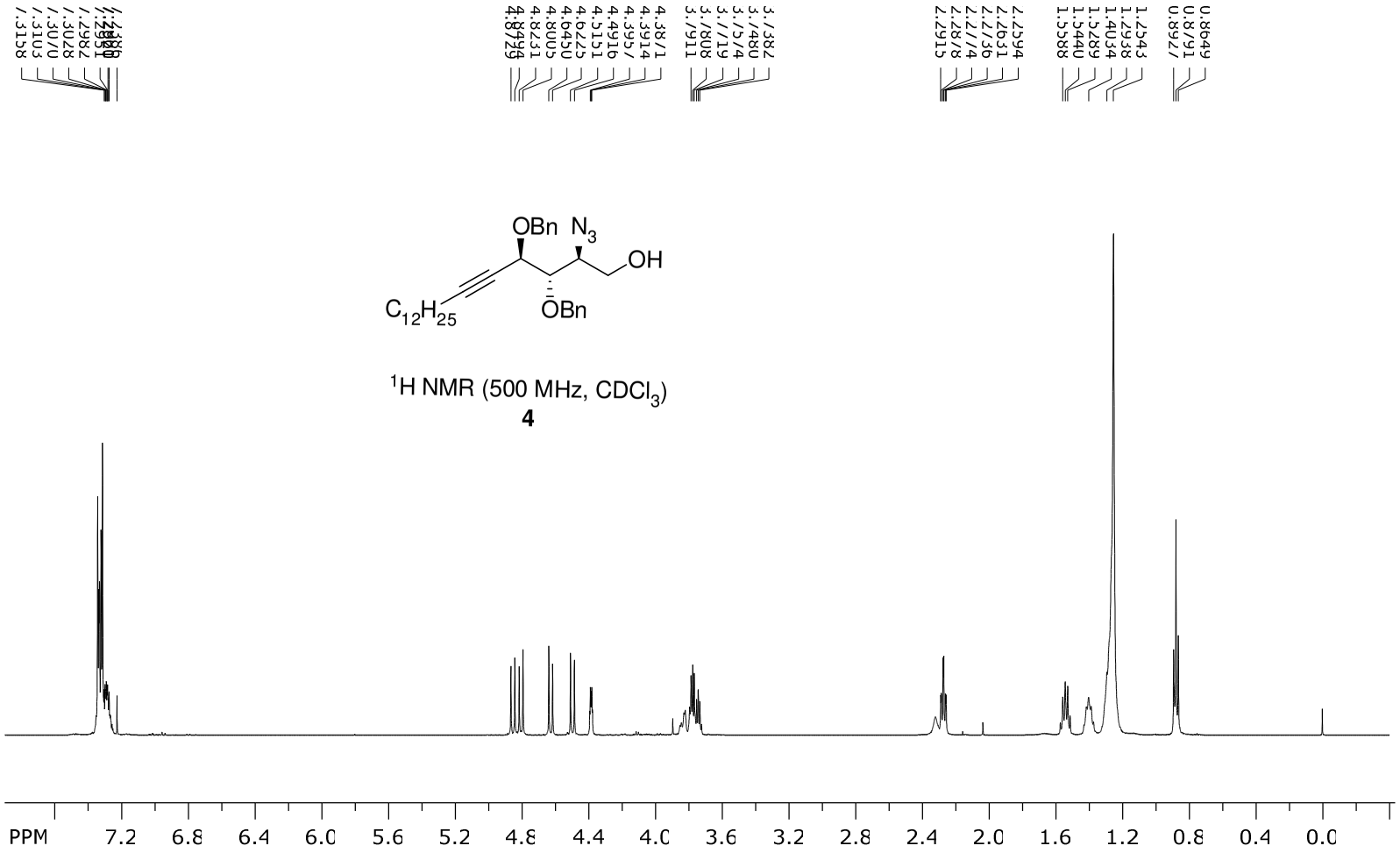
file: E:\NMR 500 LZ\zh090908s3\2\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16

freq. of 0 ppm: 500.130008 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 166.909 ppm/cm: 0.33373



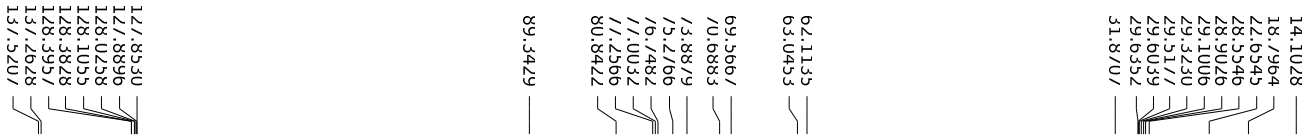
file: E:\NMR 500 LZ\zh090908s3\3\fid expt: <zgpg30>
transmitter freq.: 125.771622 MHz
time domain size: 65536 points
width: 31250.00 Hz = 248.4662 ppm = 0.476837 Hz/pt
number of scans: 1024

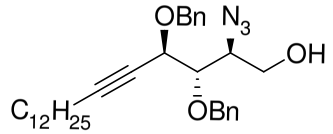
freq. of 0 ppm: 125.757795 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 1010.739 ppm/cm: 8.03630



file: D:\NMR 500 LZ\zh090930s2\1\fid expt: <zg30>
transmitter freq.: 500.133089 MHz
time domain size: 65536 points
width: 10330.58 Hz = 20.6557 ppm = 0.157632 Hz/pt
number of scans: 16

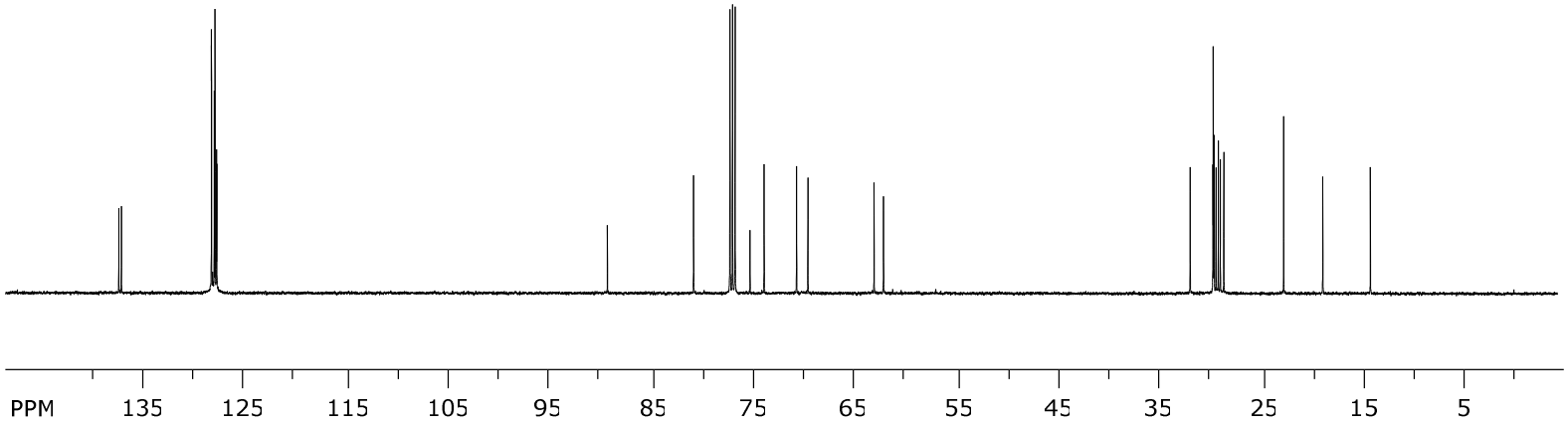
freq. of 0 ppm: 500.130025 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 166.368 ppm/cm: 0.33265





^{13}C NMR (100 MHz, $CDCl_3$)

4



file: D:\NMR 500 LZ\zh090930s2\2\fid expt: <zgpg30>
transmitter freq.: 125.771622 MHz
time domain size: 65536 points
width: 31250.00 Hz = 248.4662 ppm = 0.476837 Hz/pt
number of scans: 1024

freq. of 0 ppm: 125.757802 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 769.859 ppm/cm: 6.12108