Total Synthesis of (-)-4,8,10-Tridesmethyl Telithromycin

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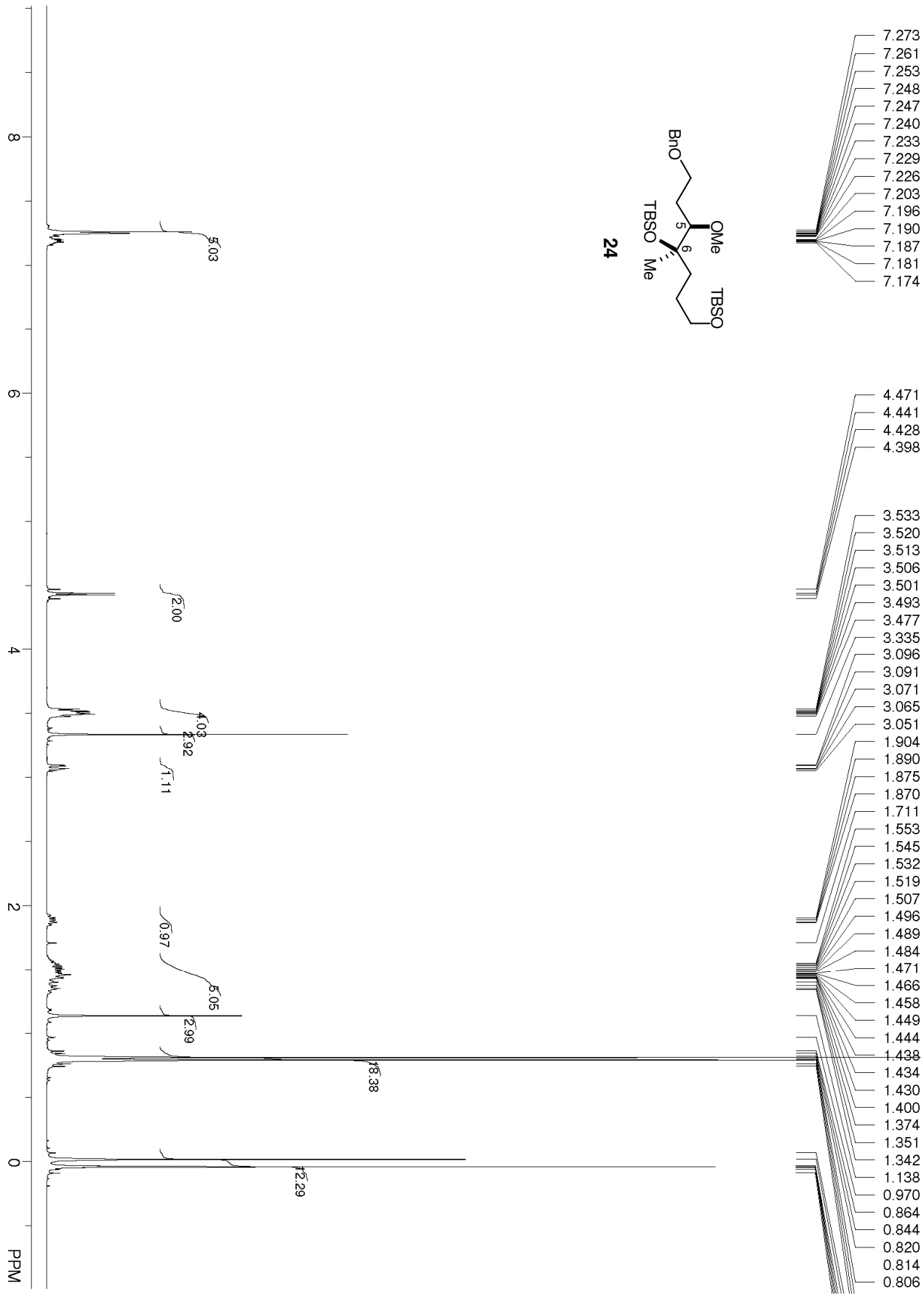
Department of Chemistry, Temple University, Philadelphia, PA 19122

Supporting Information

General. All reactions containing moisture or air sensitive reagents were performed in oven-dried glassware under nitrogen or Argon. Dimethylformamide, tetrahydrofuran, toluene and dichloromethane were passed through two columns of neutral alumina. Pyridine, 2,6-lutidine, acetone, *i*-Pr_2NEt and Et_3N were all distilled from CaH_2 prior to use. Molecular sieves (4Å) were activated by flame drying under vacuum prior to use. AgOTf was azeotroped with dry toluene. Compounds **3**,[1] **6**,[2] **7**,[3] **8**[4], **9**[5], [**11**, **19**, **20**, **39**, **41**, **43**, **49**, **50**, **51**, **48**, **58**, **60**, **61**, **62**, **63**, and **64**][1] were prepared according to known literature procedures. All other reagents were purchased from commercial sources and used without further purification. All solvents for work-up procedures were used as received. Flash column chromatography was performed according to the procedure of Still[6] using ICN Silitech 32-63 D 60Å silica gel with the indicated solvents. TBAF solution (1 M in THF) was prepared by adding 4Å molecular sieves (1 gm/mL) to a solution of TBAF•$3H_2O$ in THF and stirring for 4 h. For NHK reactions, DMSO was distilled under vaccum using CaH_2, and the solution was degassed (3 cycles of freeze-pump-thaw). $CrCl_2$ and $NiCl_2$ were weighed inside a glove box. For all RCM reactions, CH_2Cl_2 was deaerated by bubbling Argon (1 min/mL). Thin layer chromatography was performed on Analtech $60F_{254}$ silica gel plates. Detection was performed using UV light, $KMnO_4$ stain, PMA stain and subsequent heating. ^1H and ^{13}C NMR spectra were recorded at the indicated field strength in $CDCl_3$ at rt. Chemical shifts are indicated in parts per million (ppm) downfield from tetramethylsilane (TMS, δ = 0.00) and referenced to the $CDCl_3$. Splitting patterns are abbreviated as follows: s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet).

Supporting Information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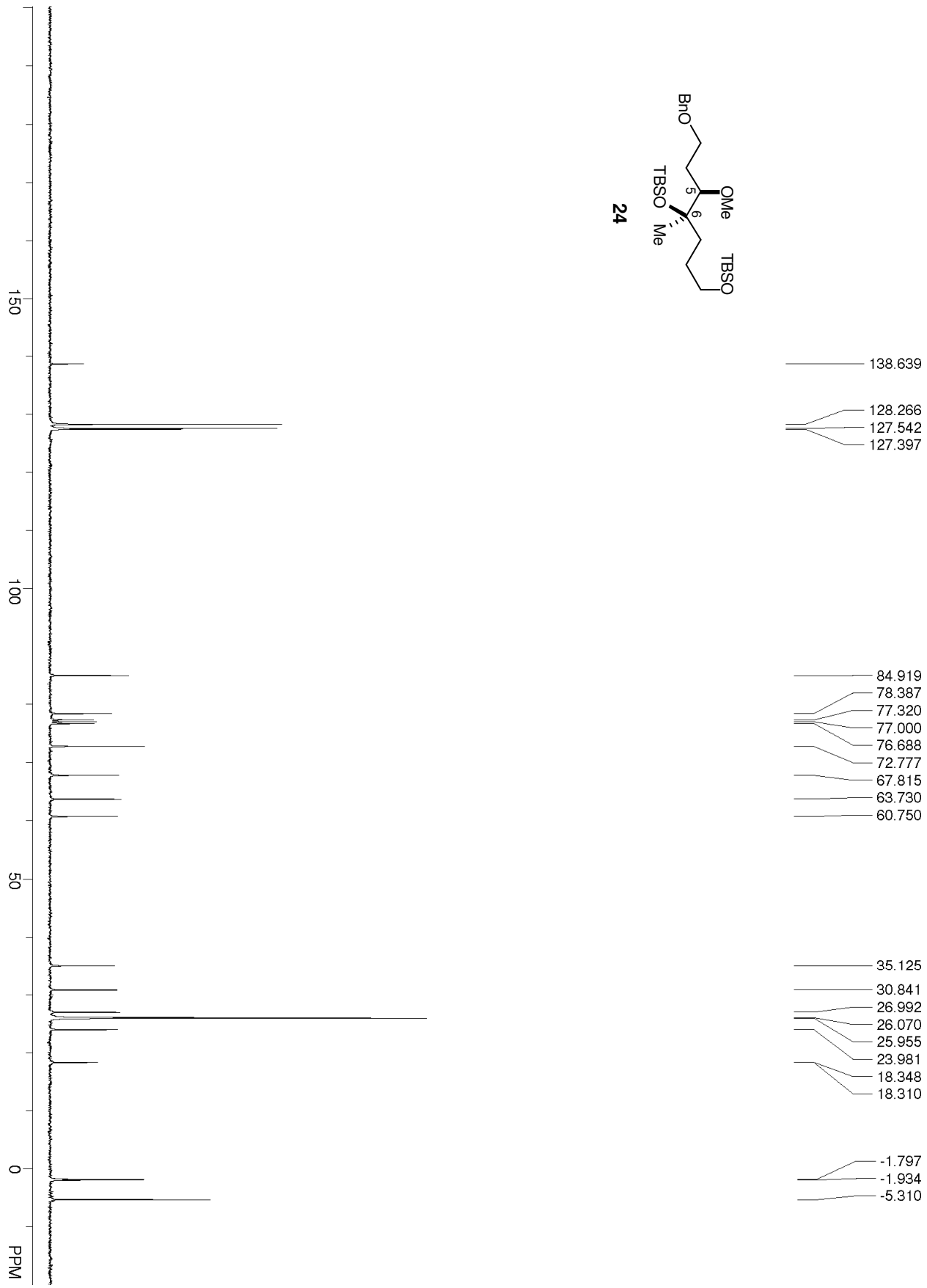
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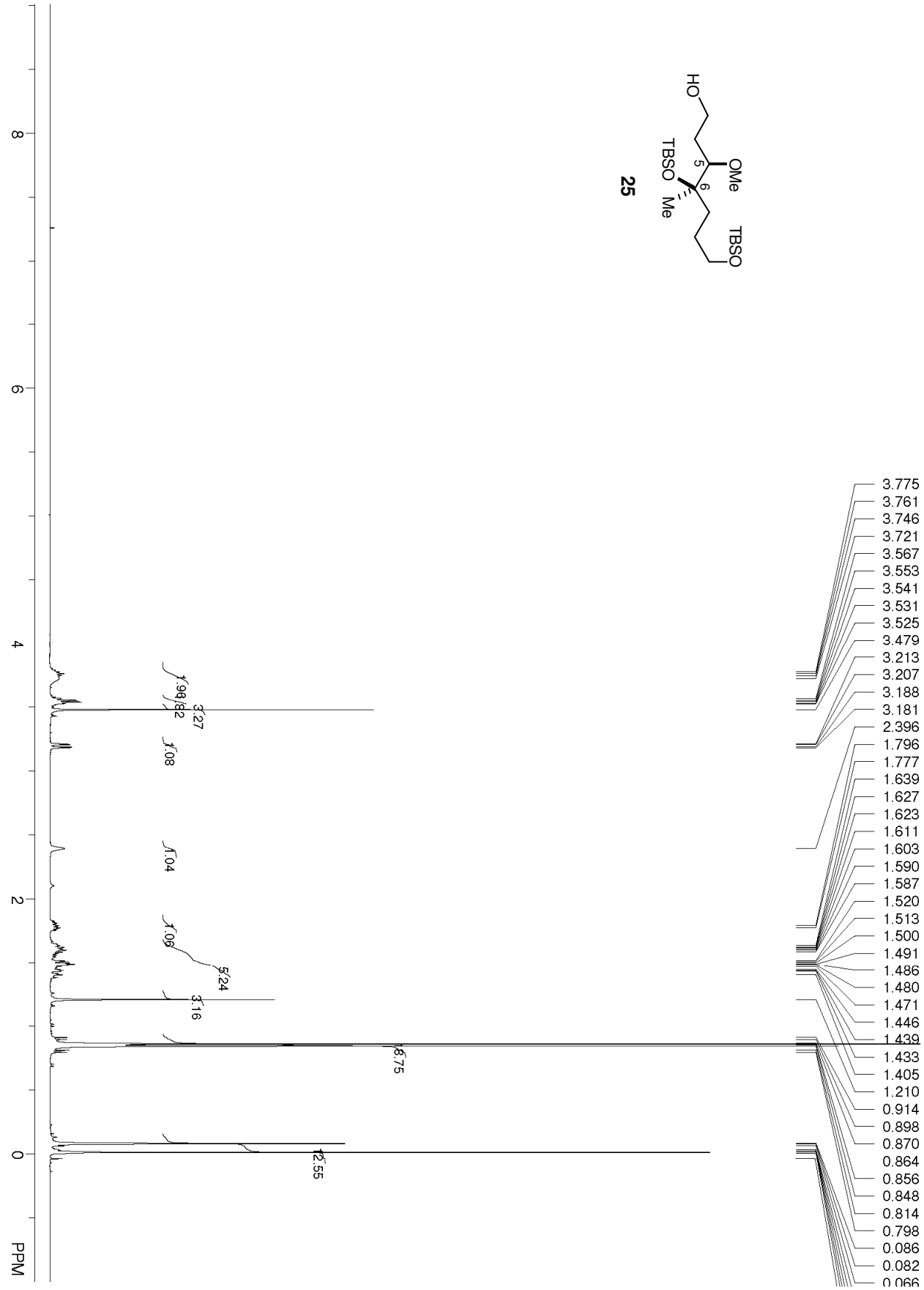
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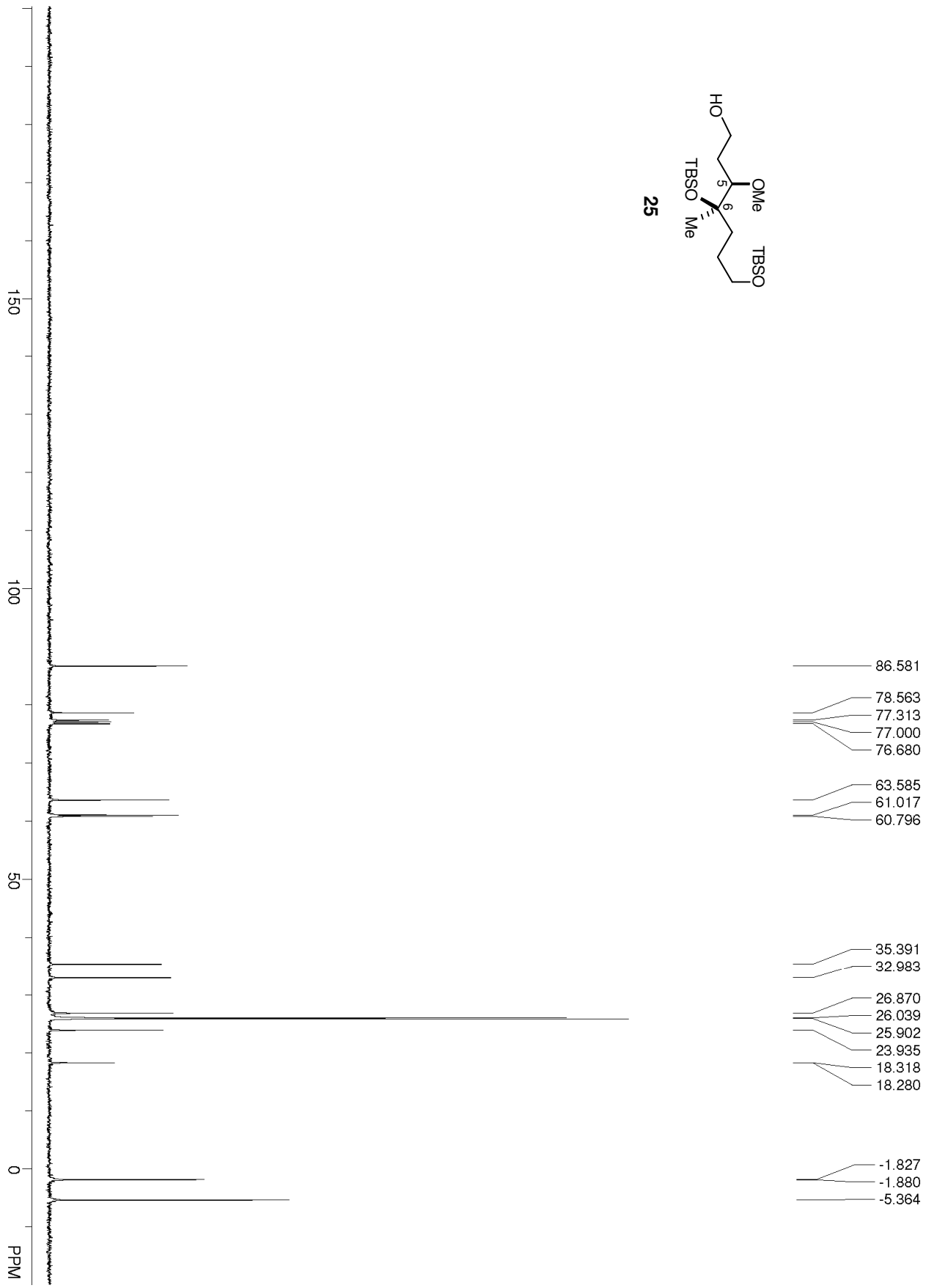
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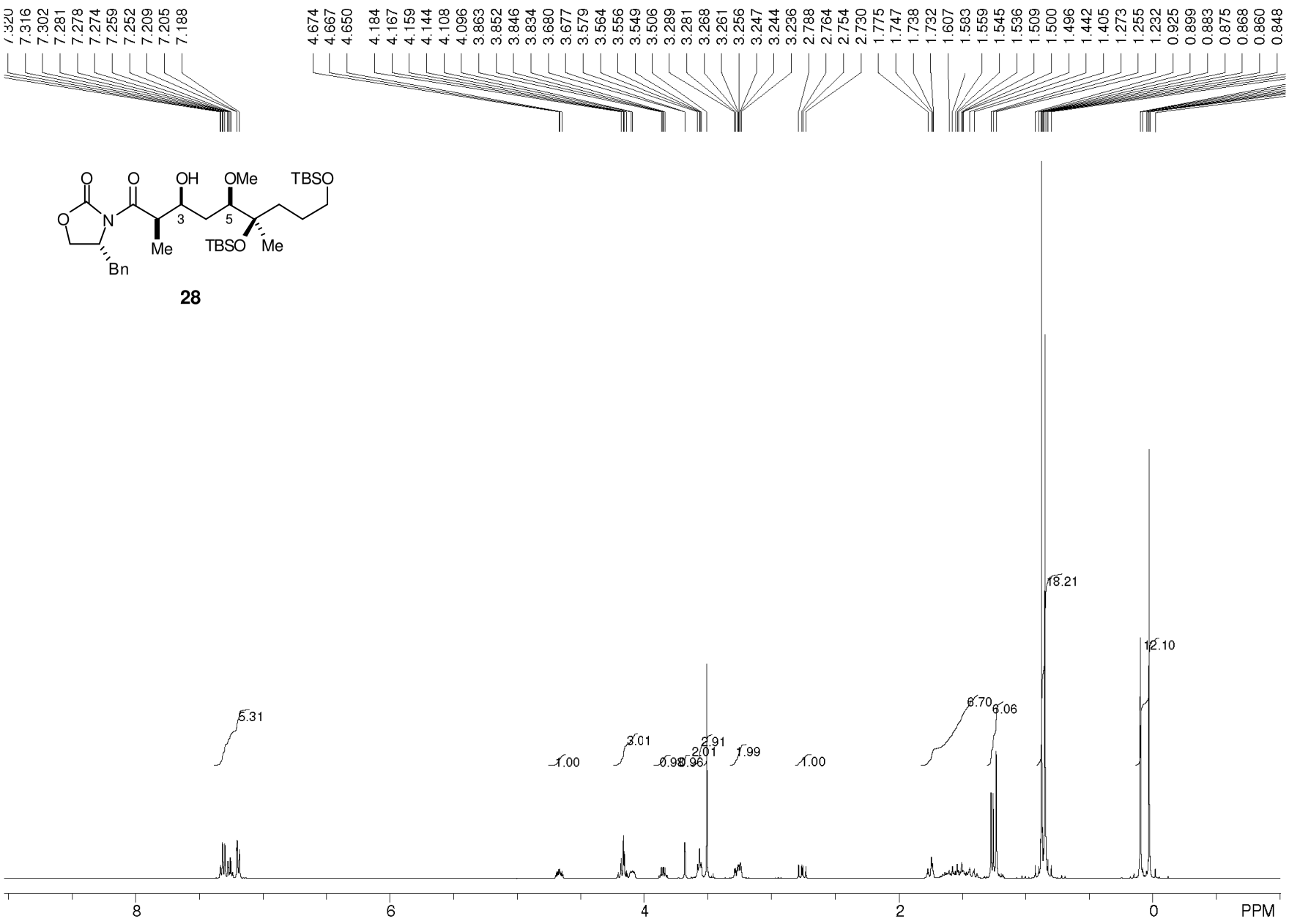
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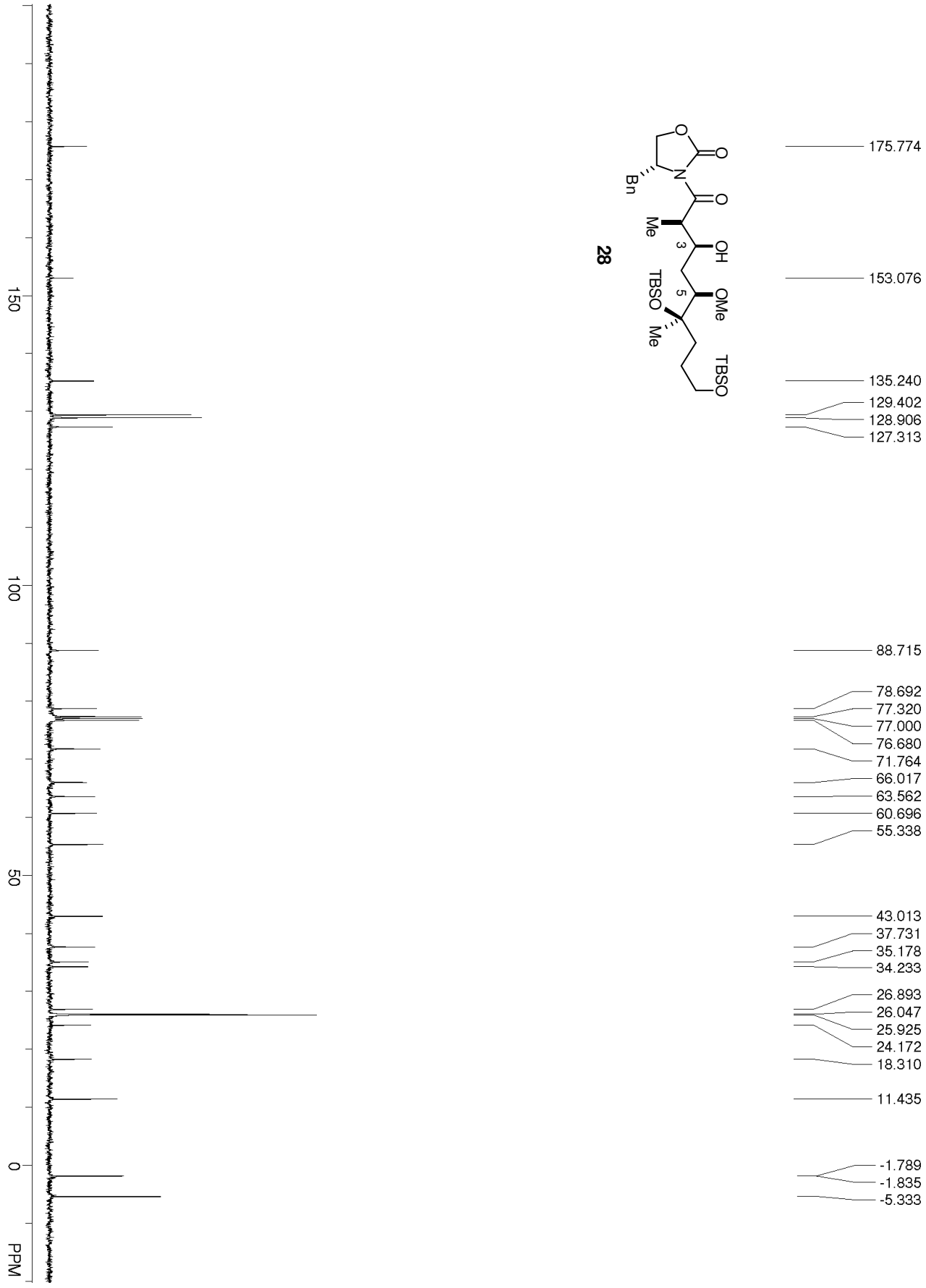
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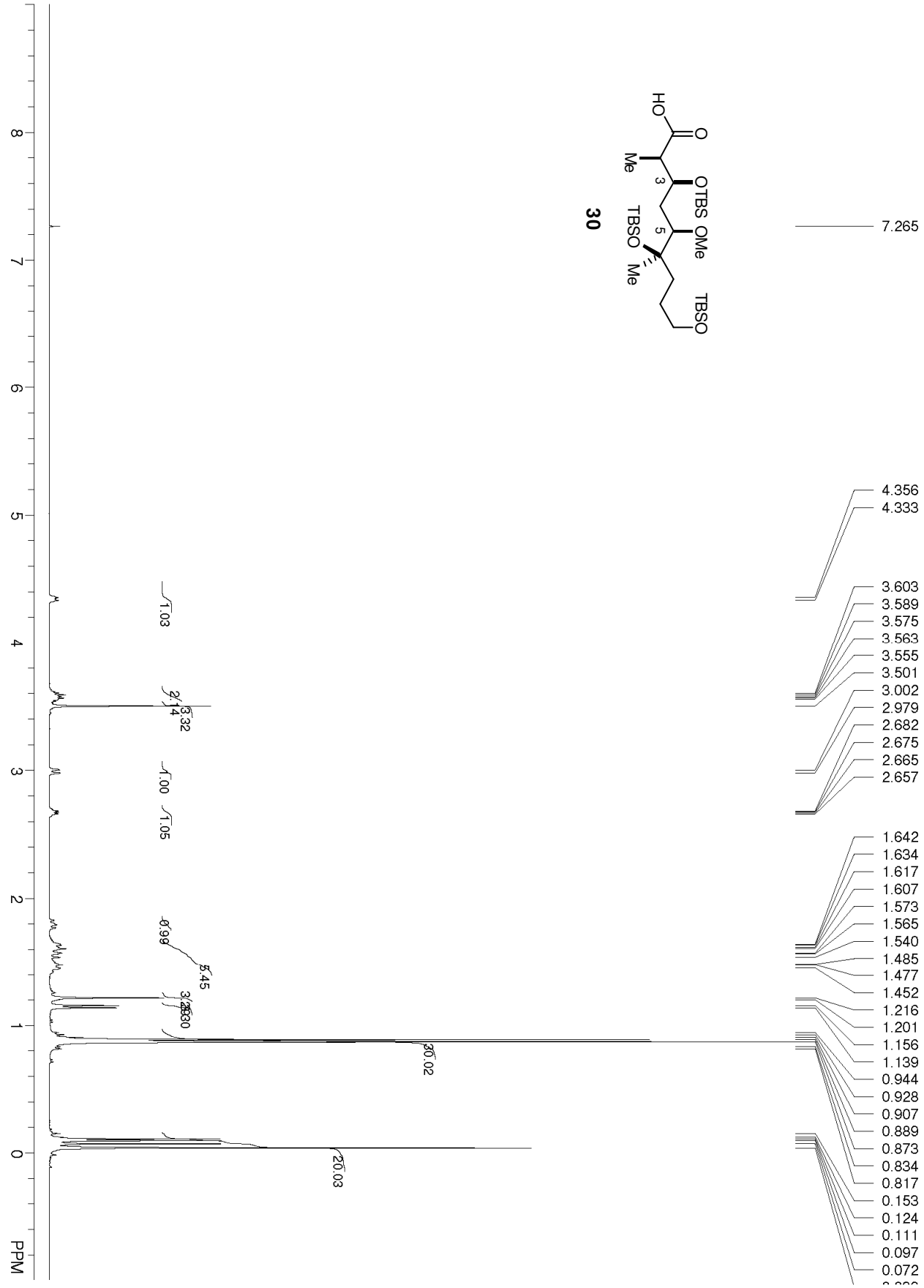
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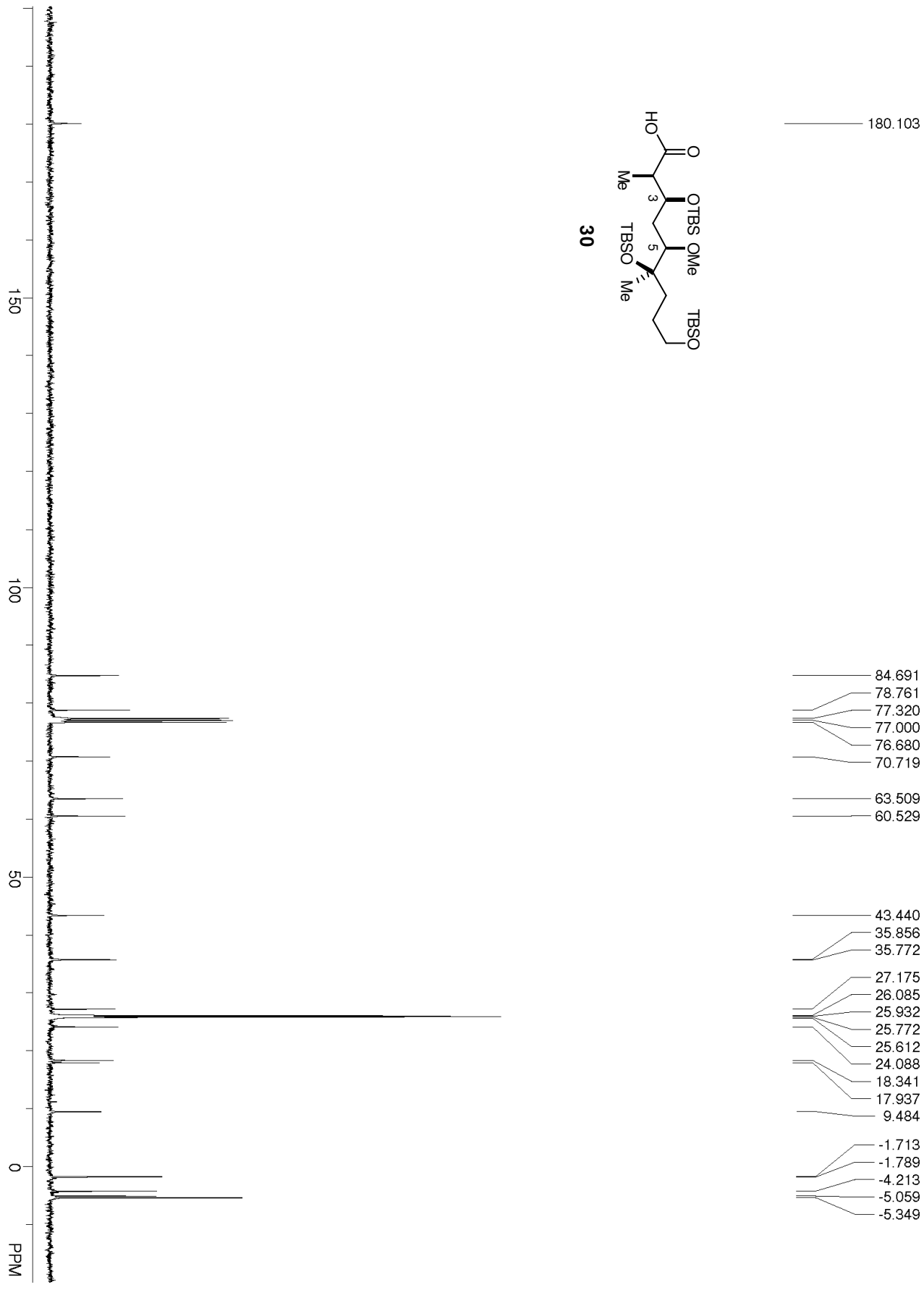
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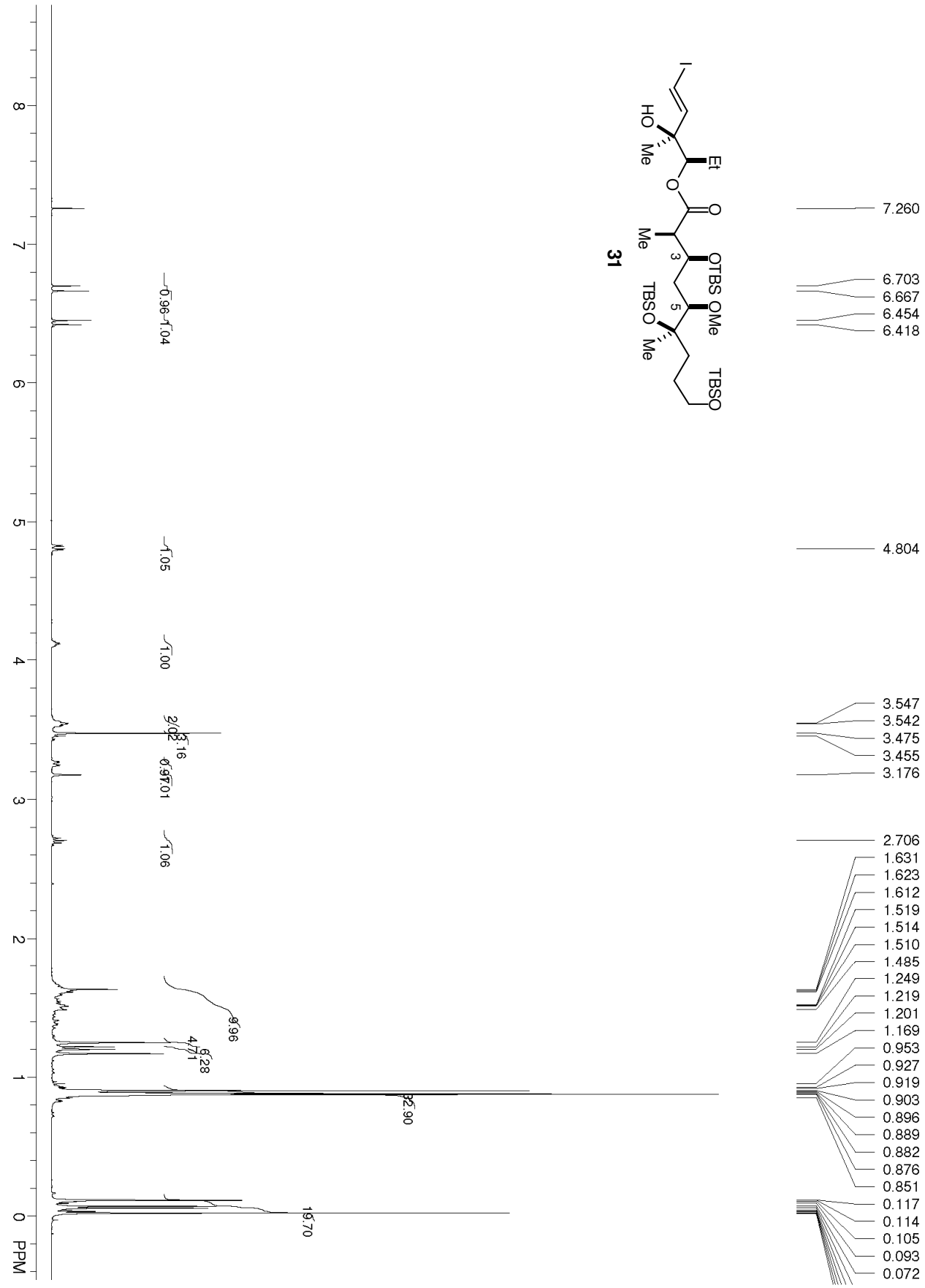
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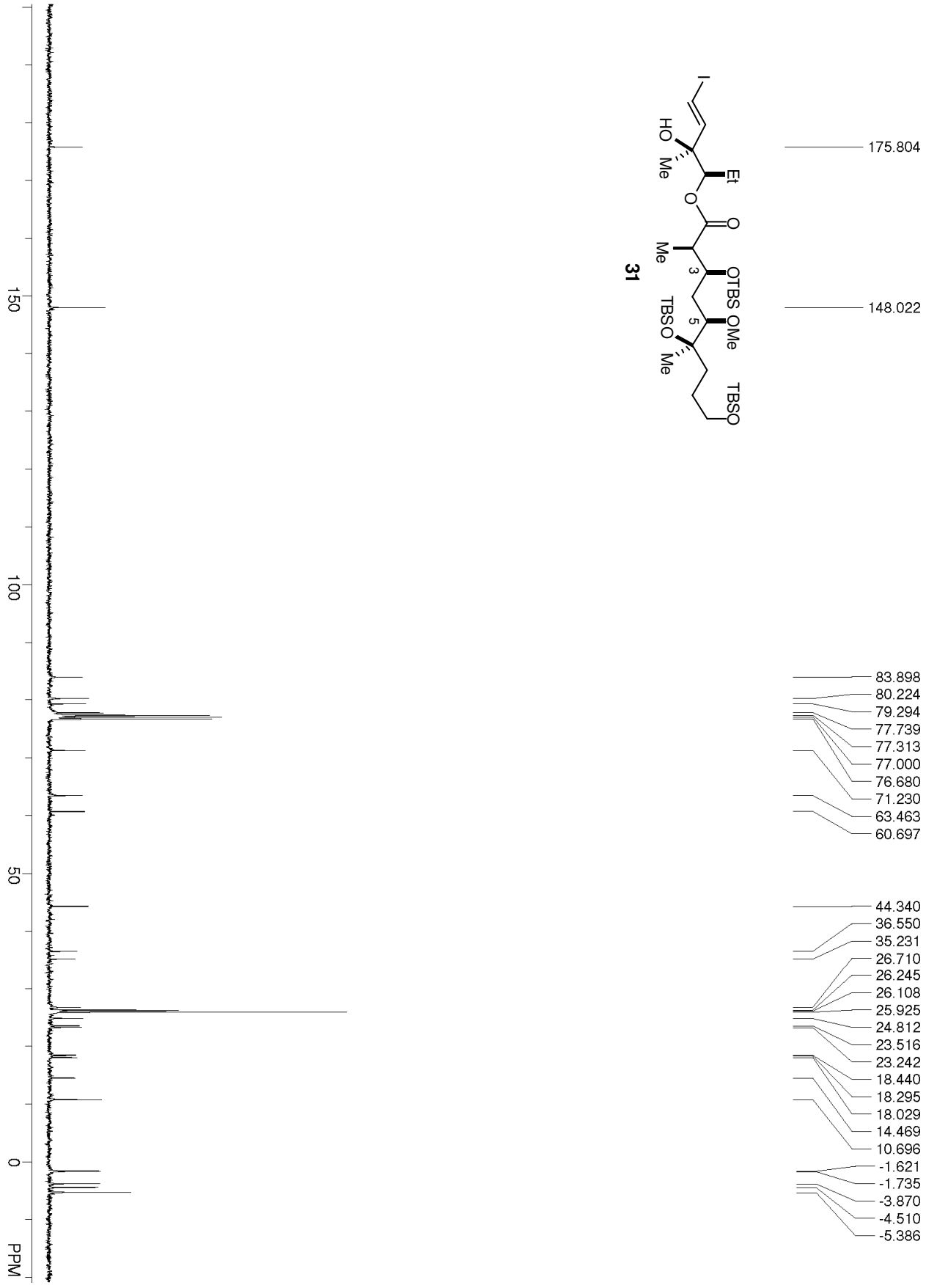
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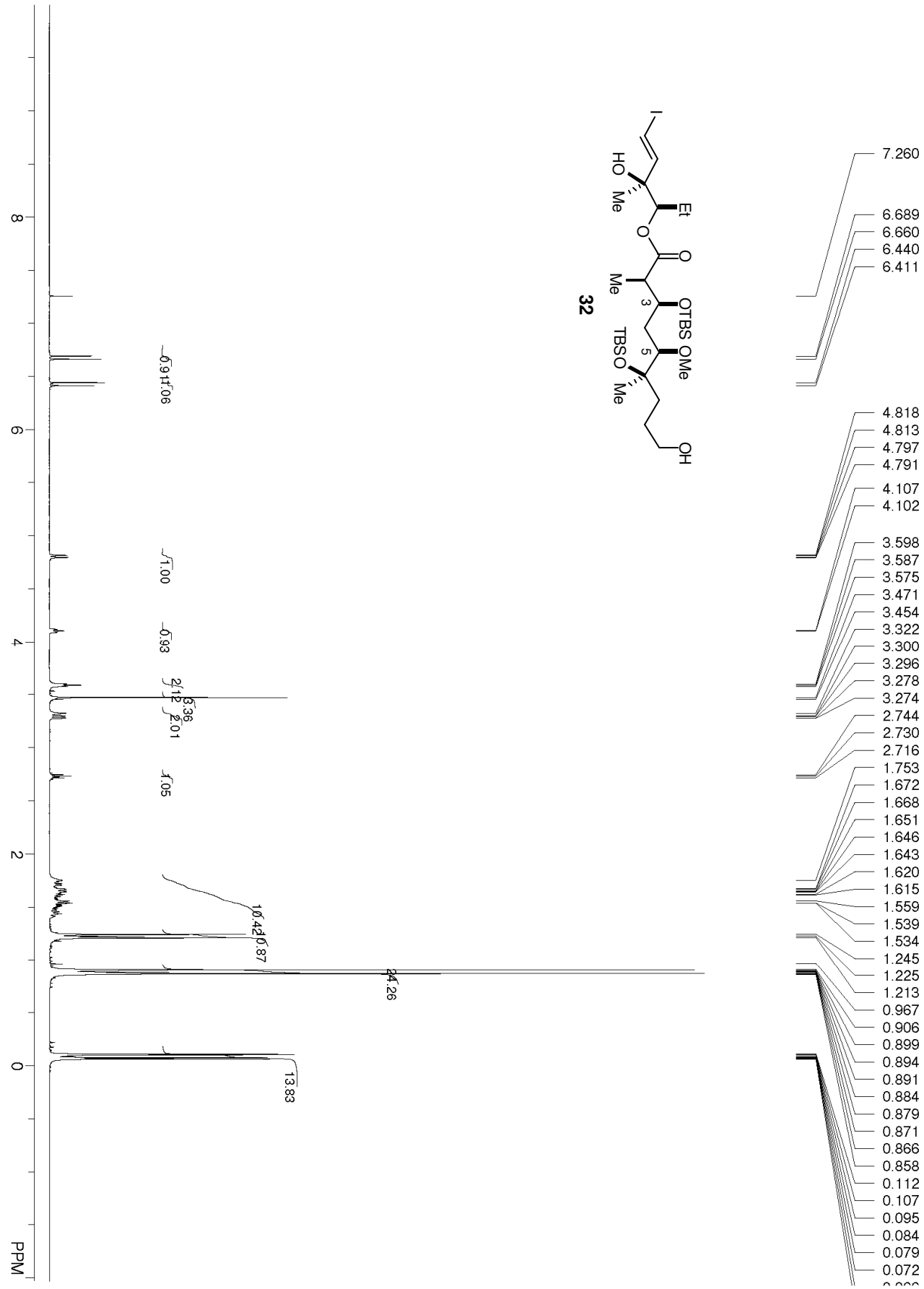
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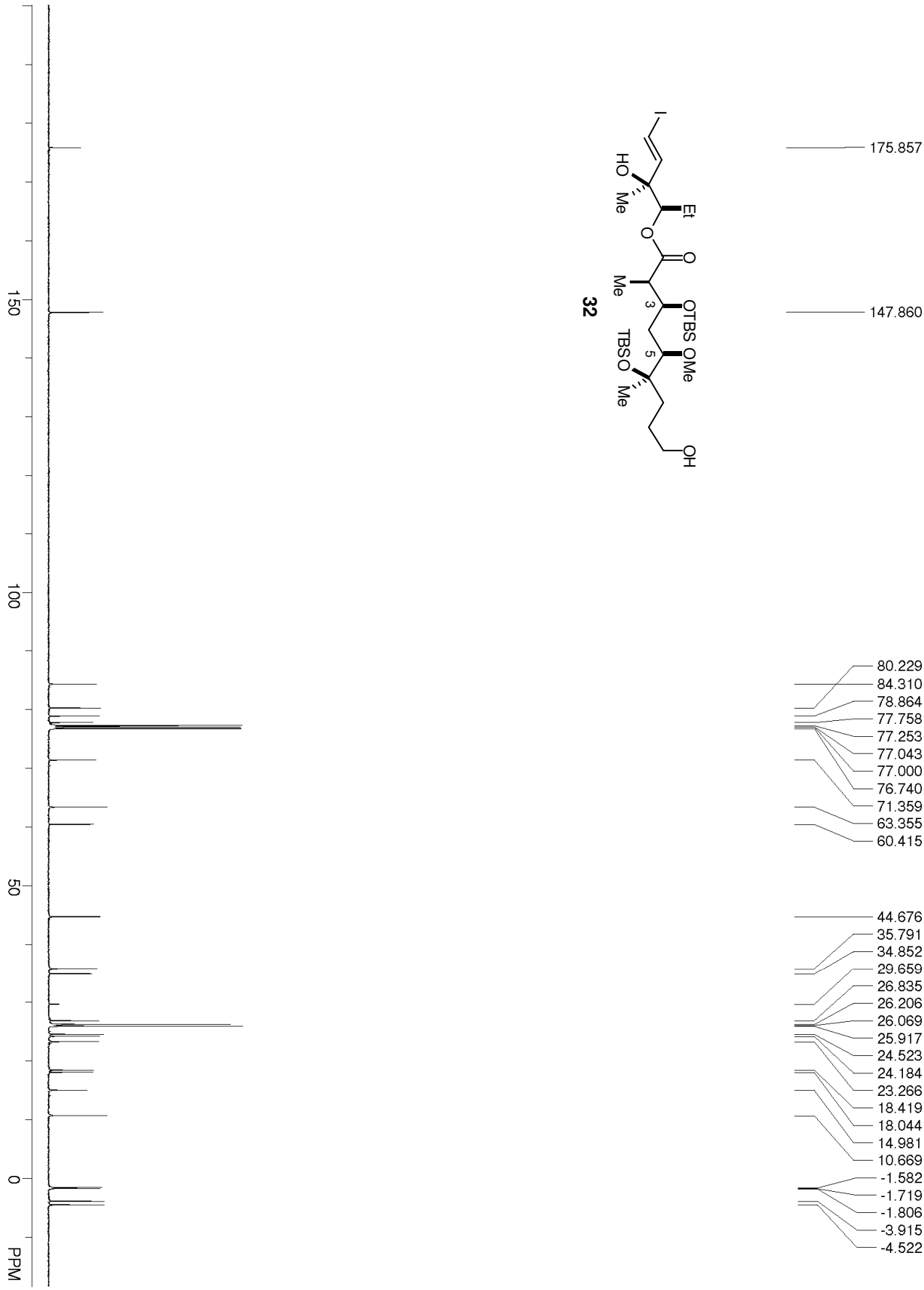
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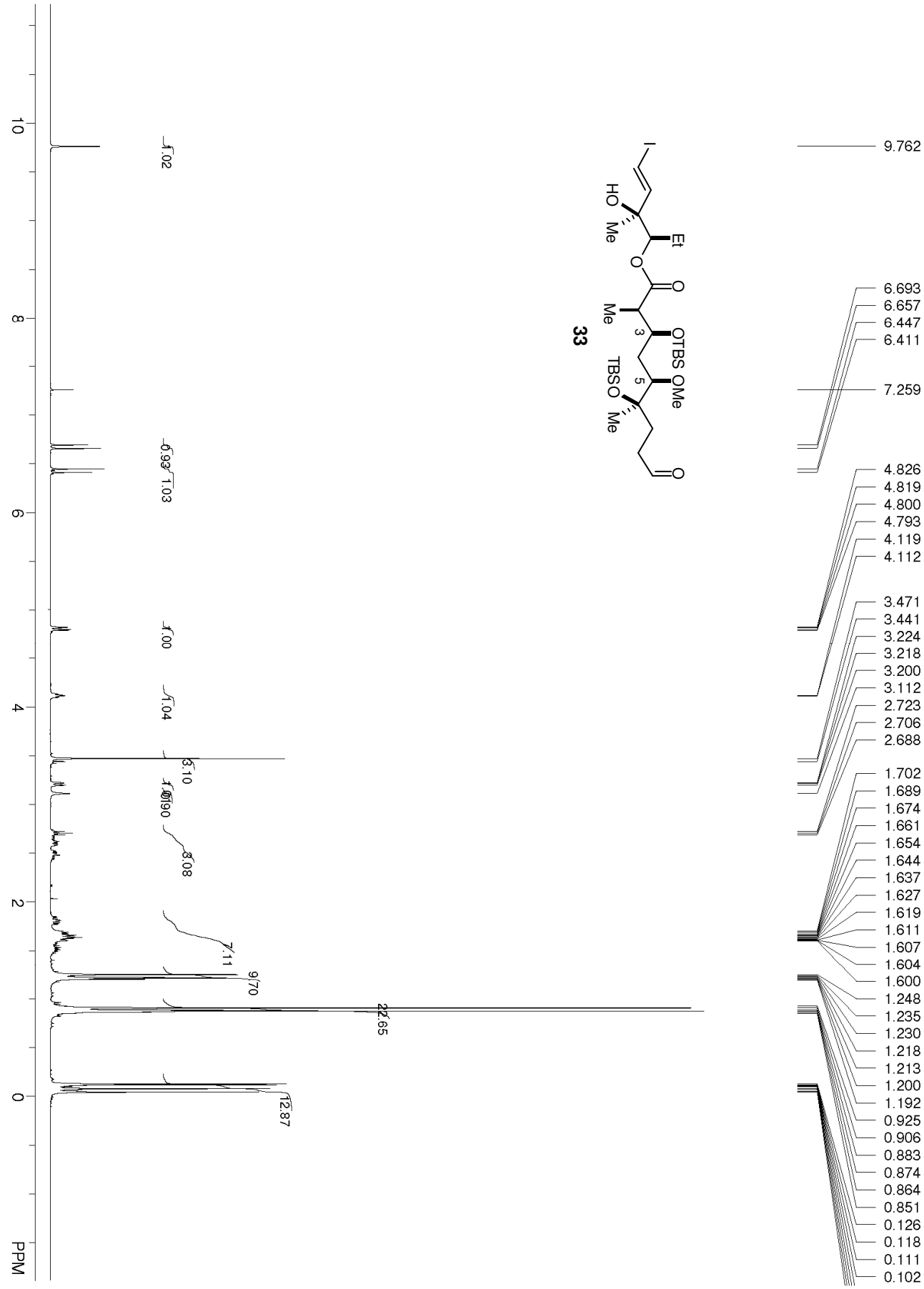
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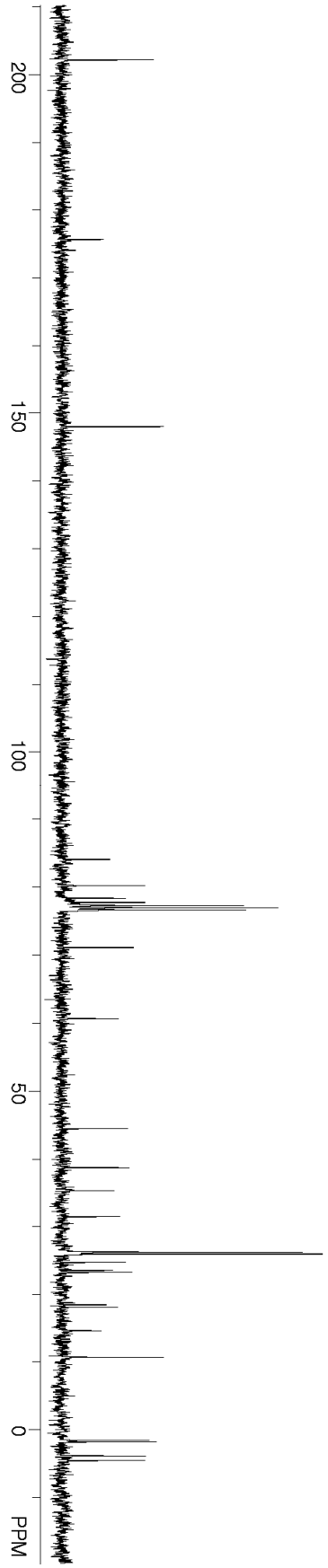
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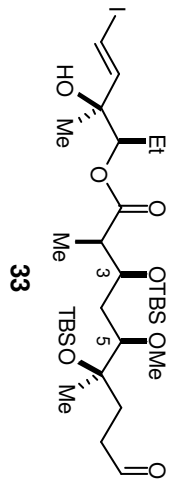
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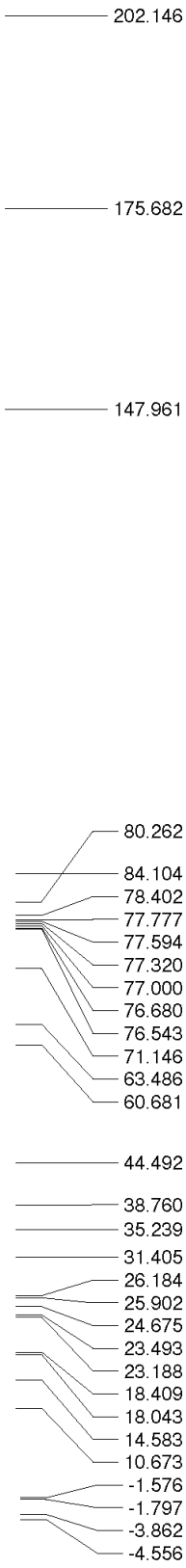
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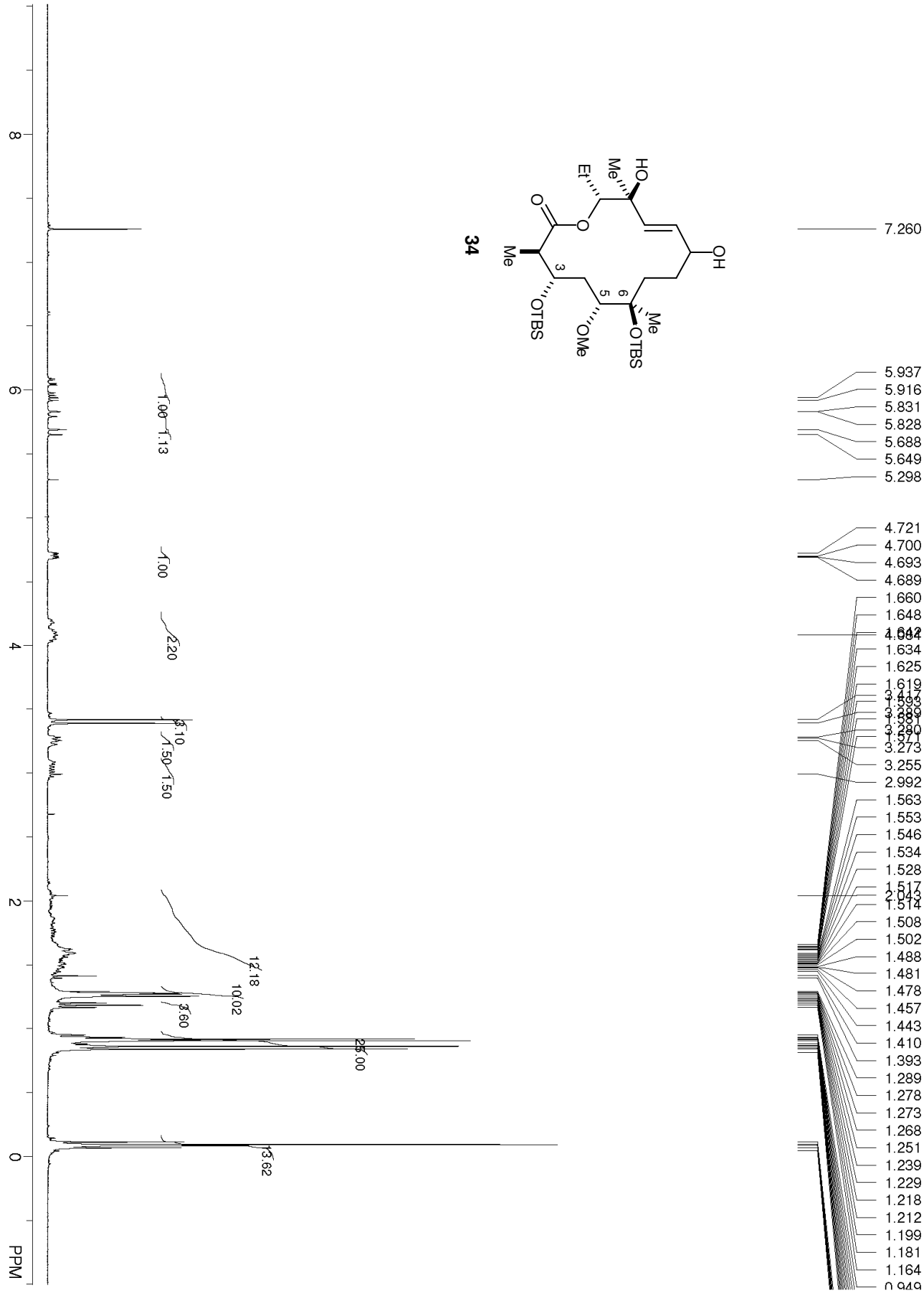
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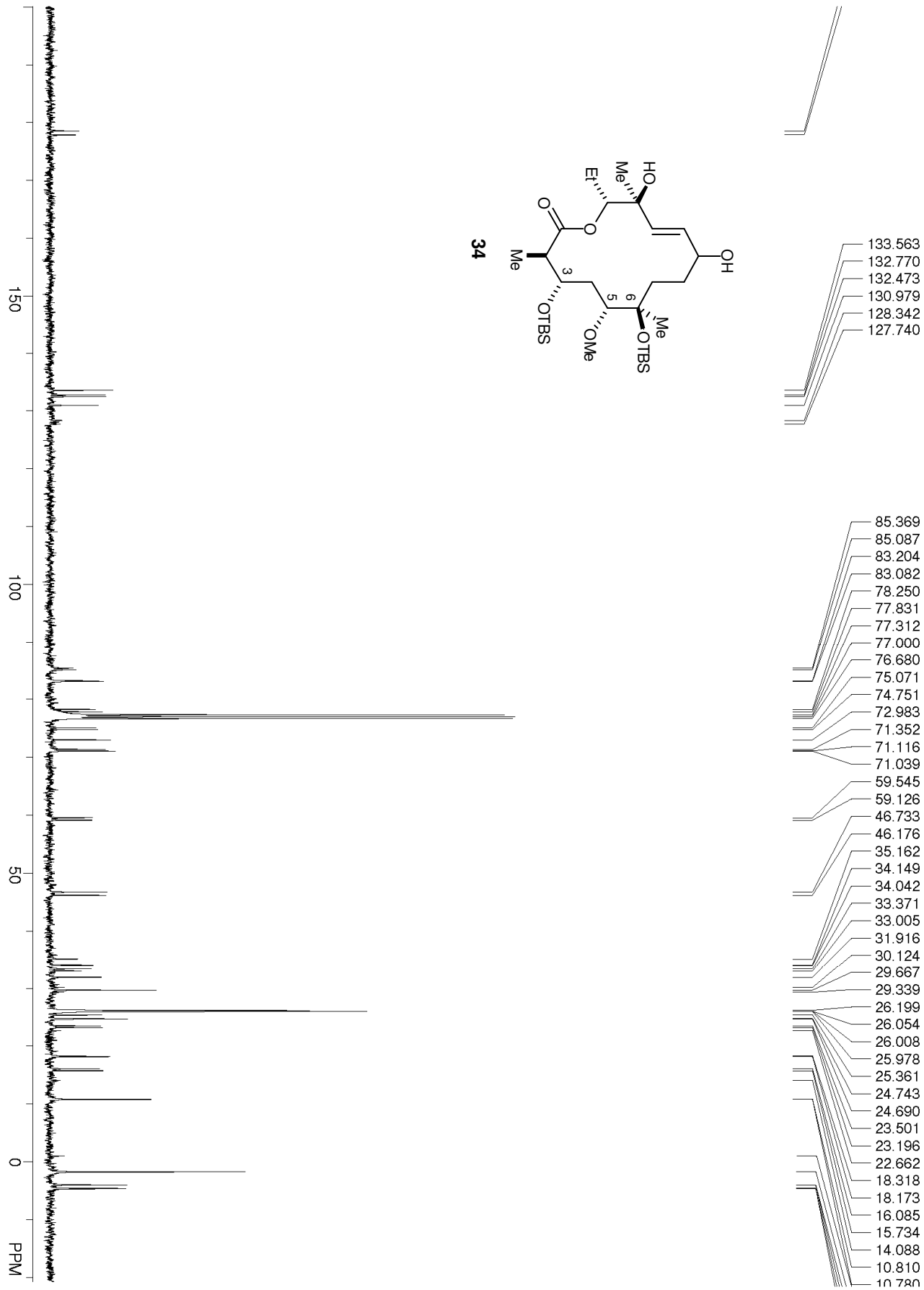
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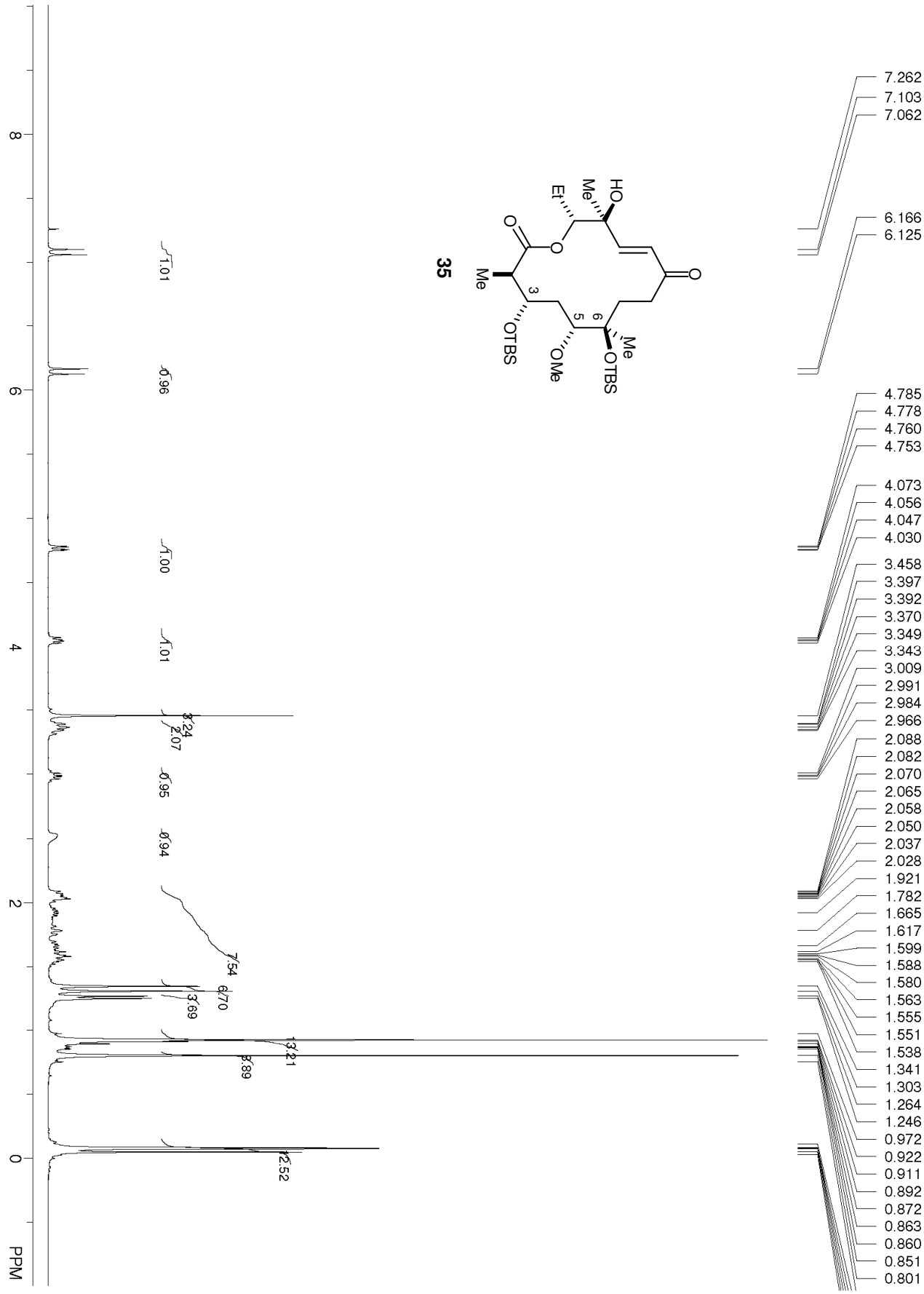
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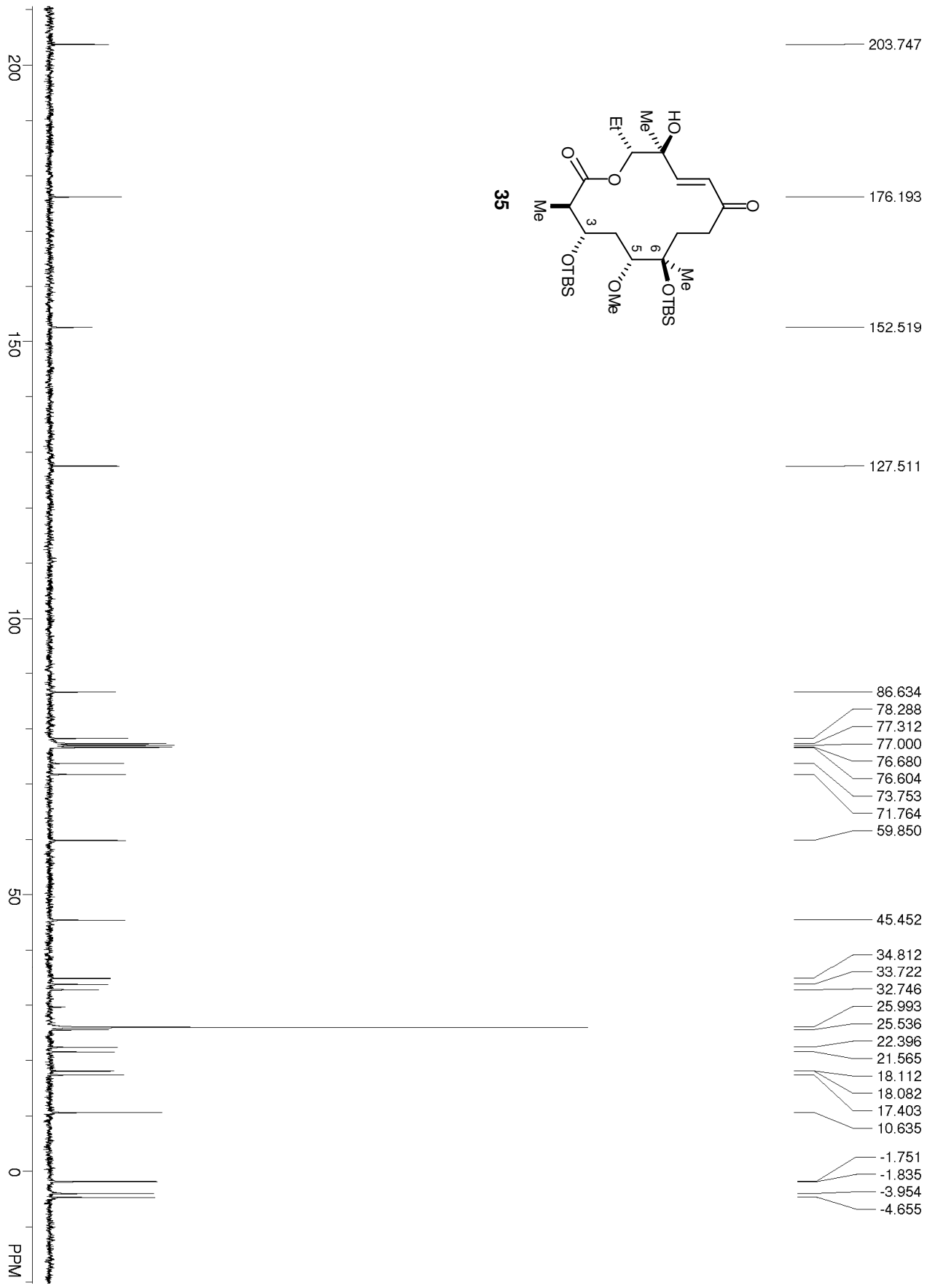
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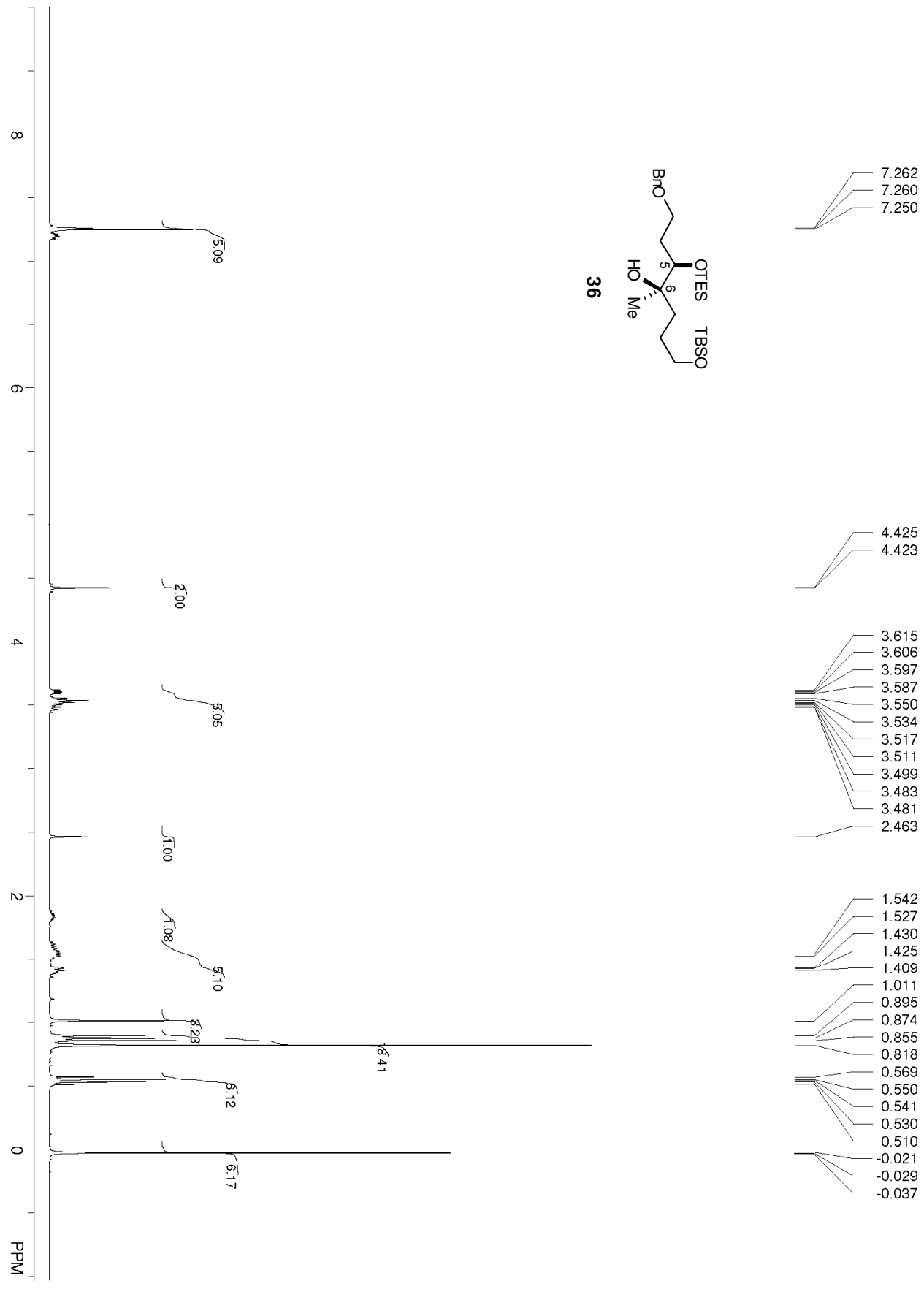
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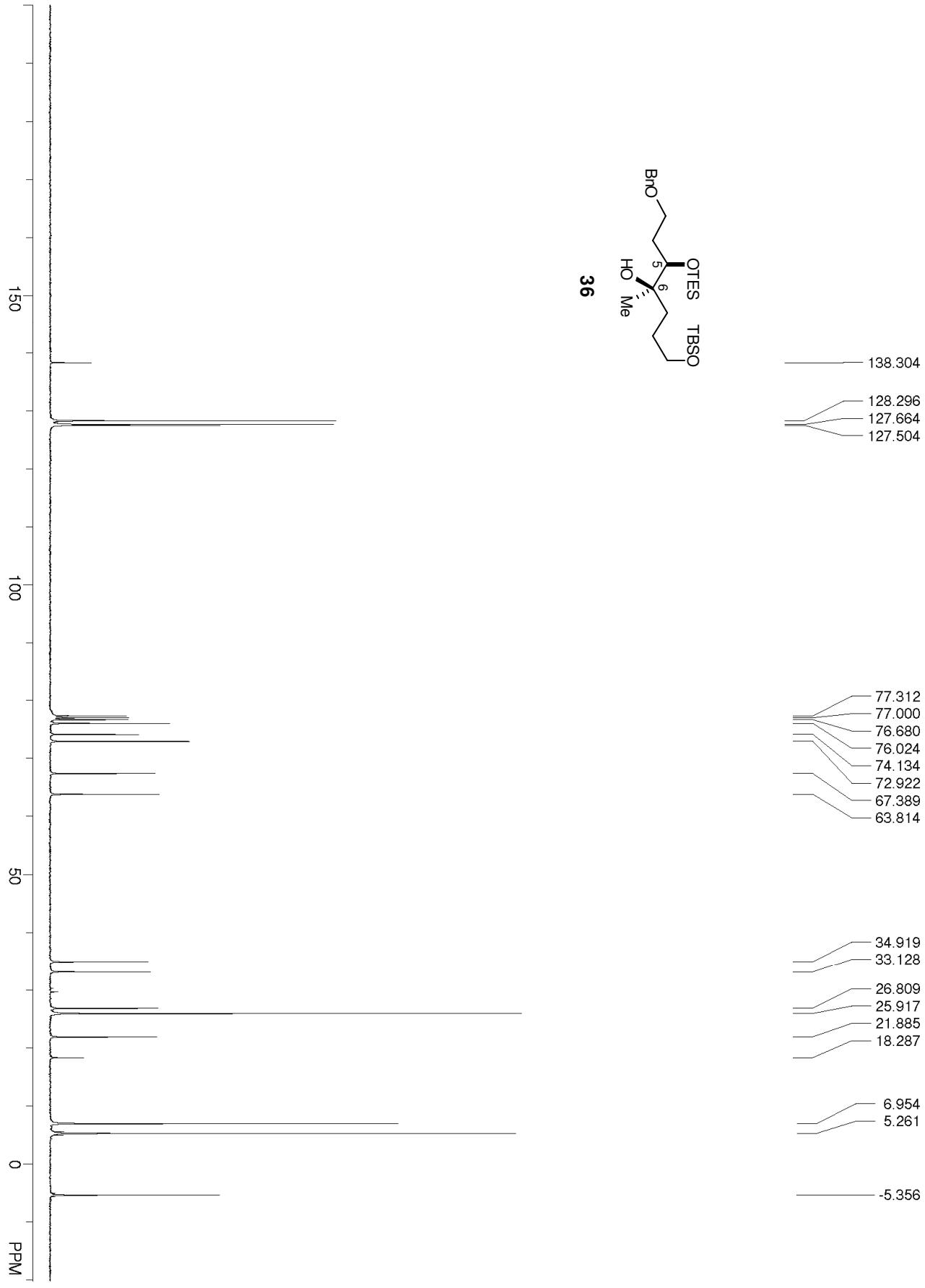
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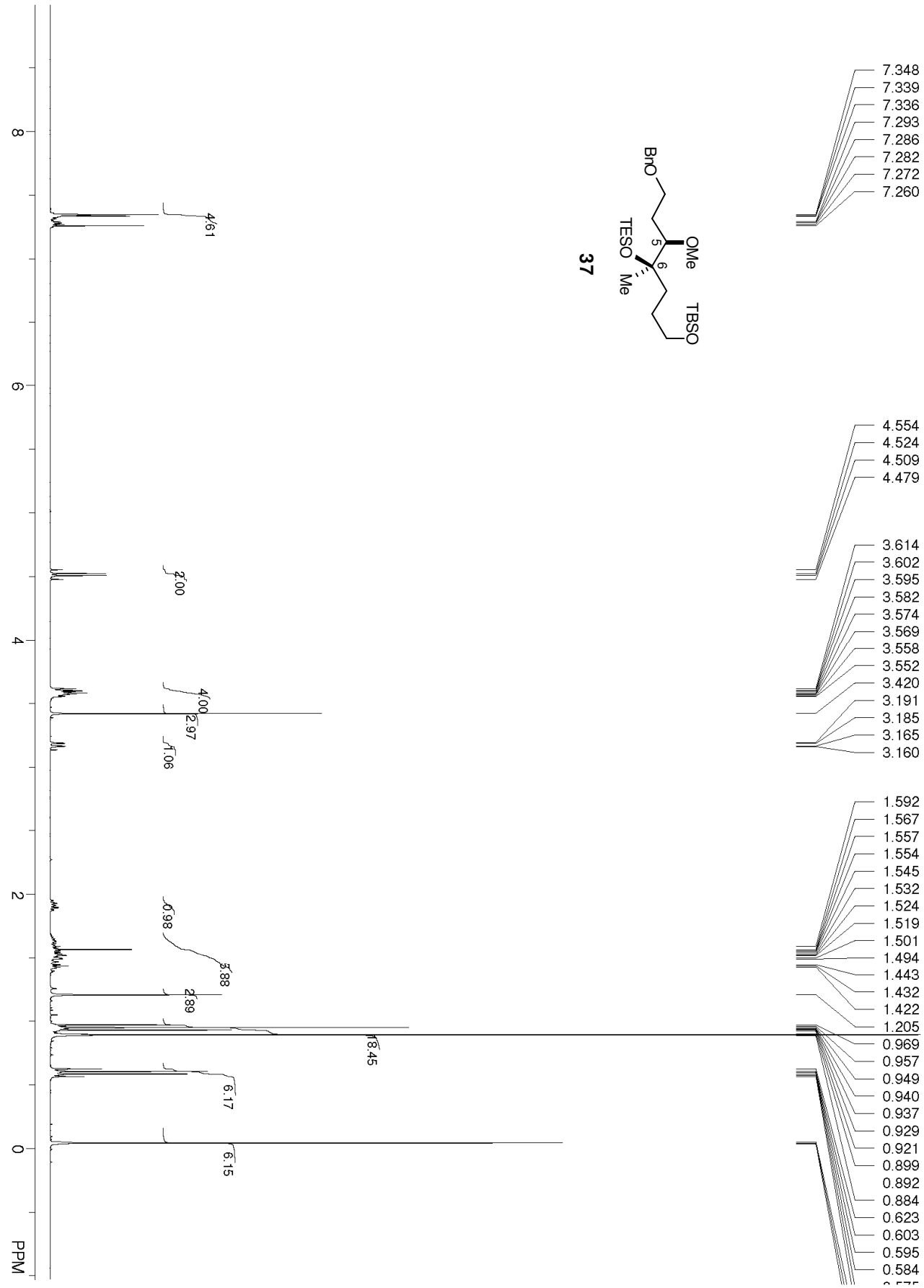
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OMe
TESO
Me
TBSO
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6
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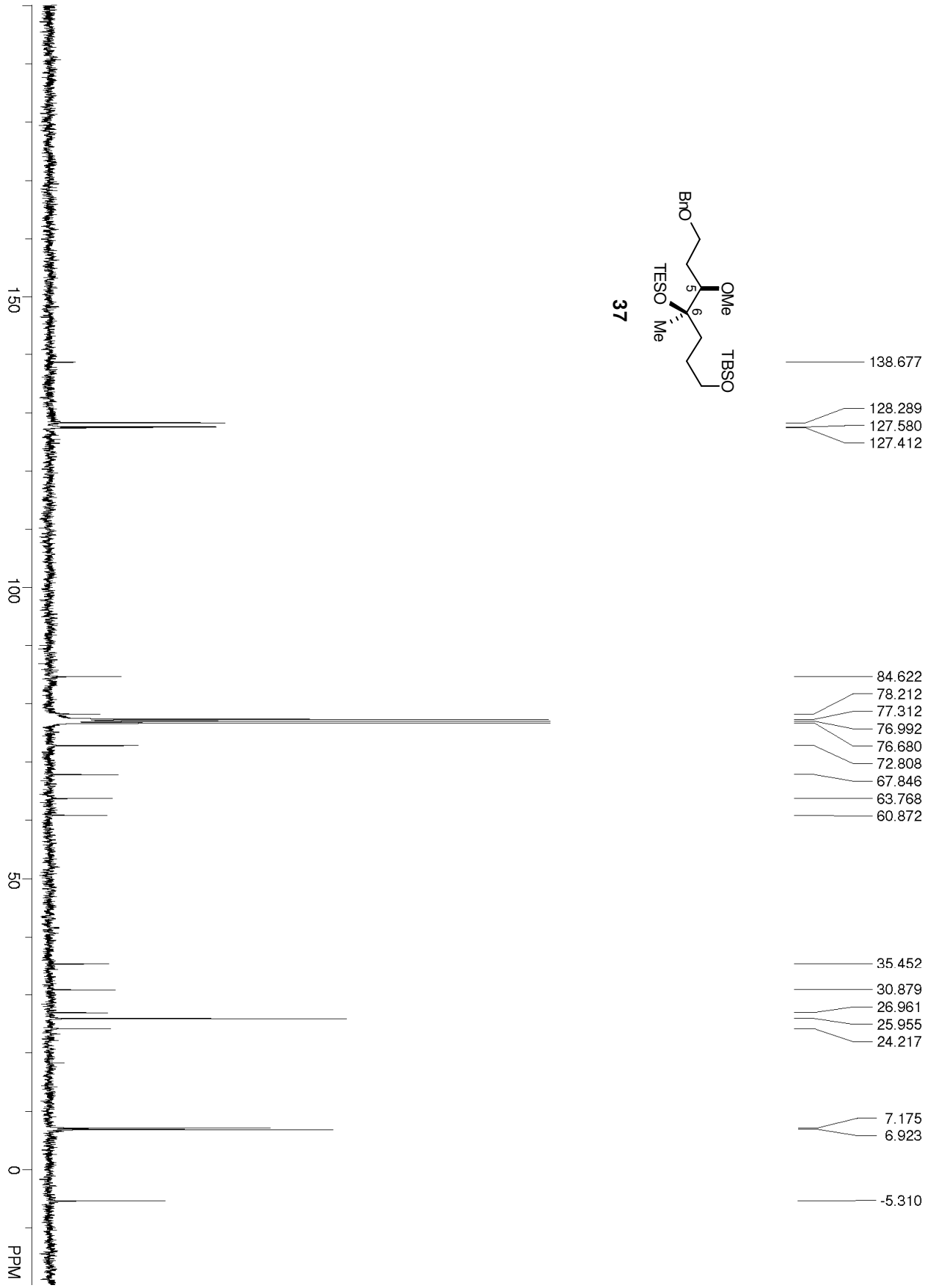
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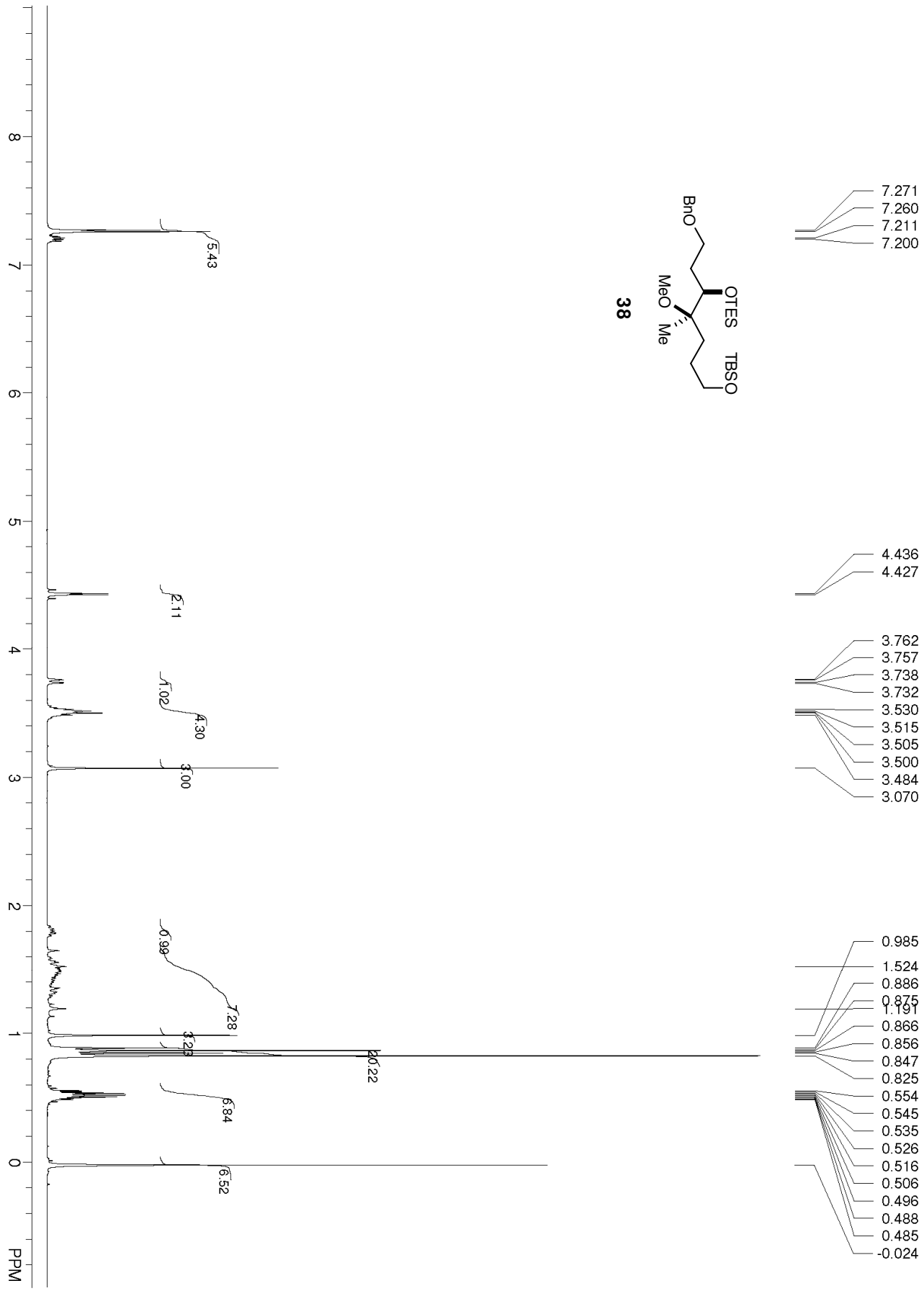
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Me
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3.530
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3.500
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1.191
0.866
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0.554
0.545
0.535
0.526
0.516
0.506
0.496
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0.485
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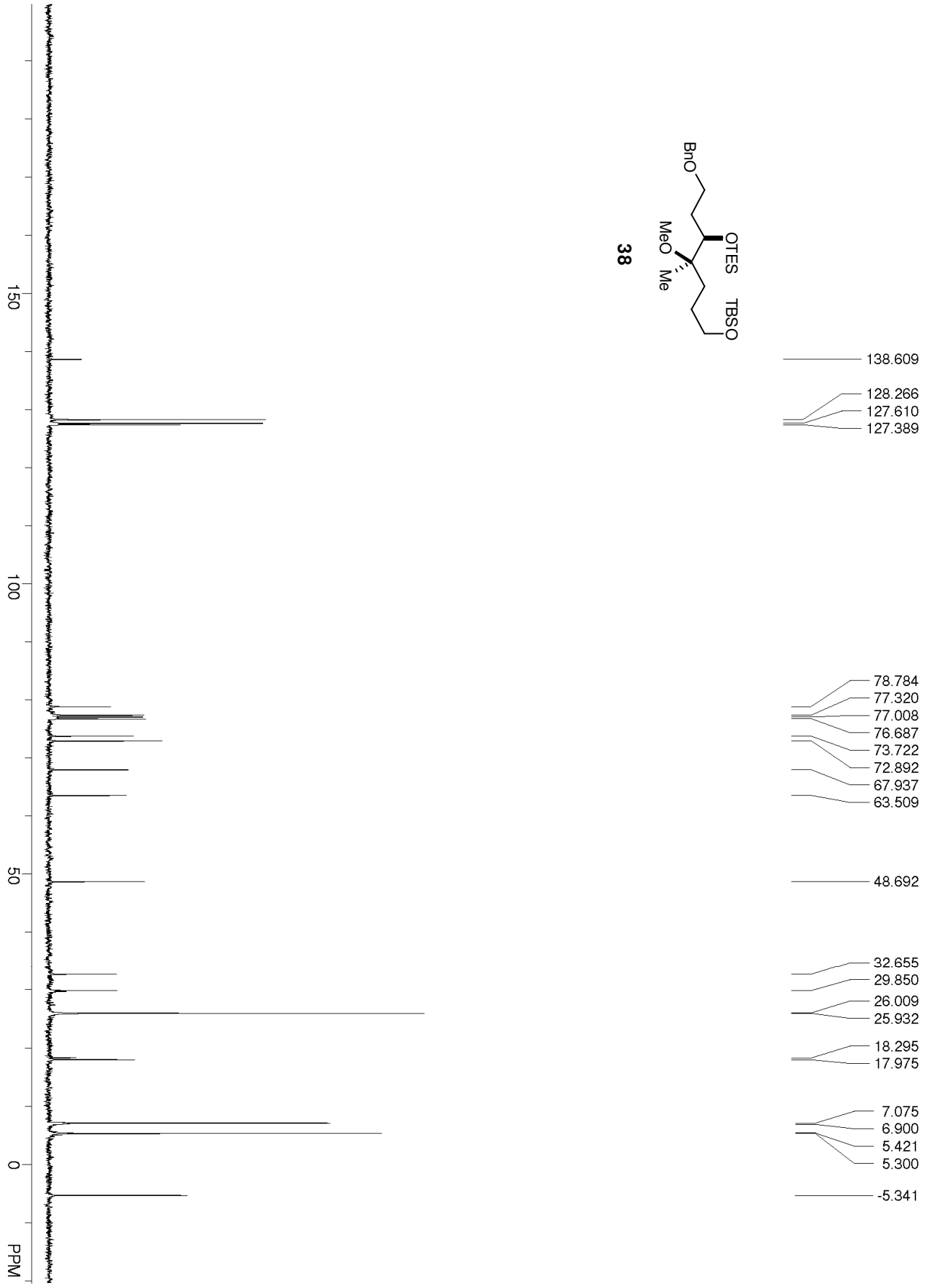
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MeO
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TBSO
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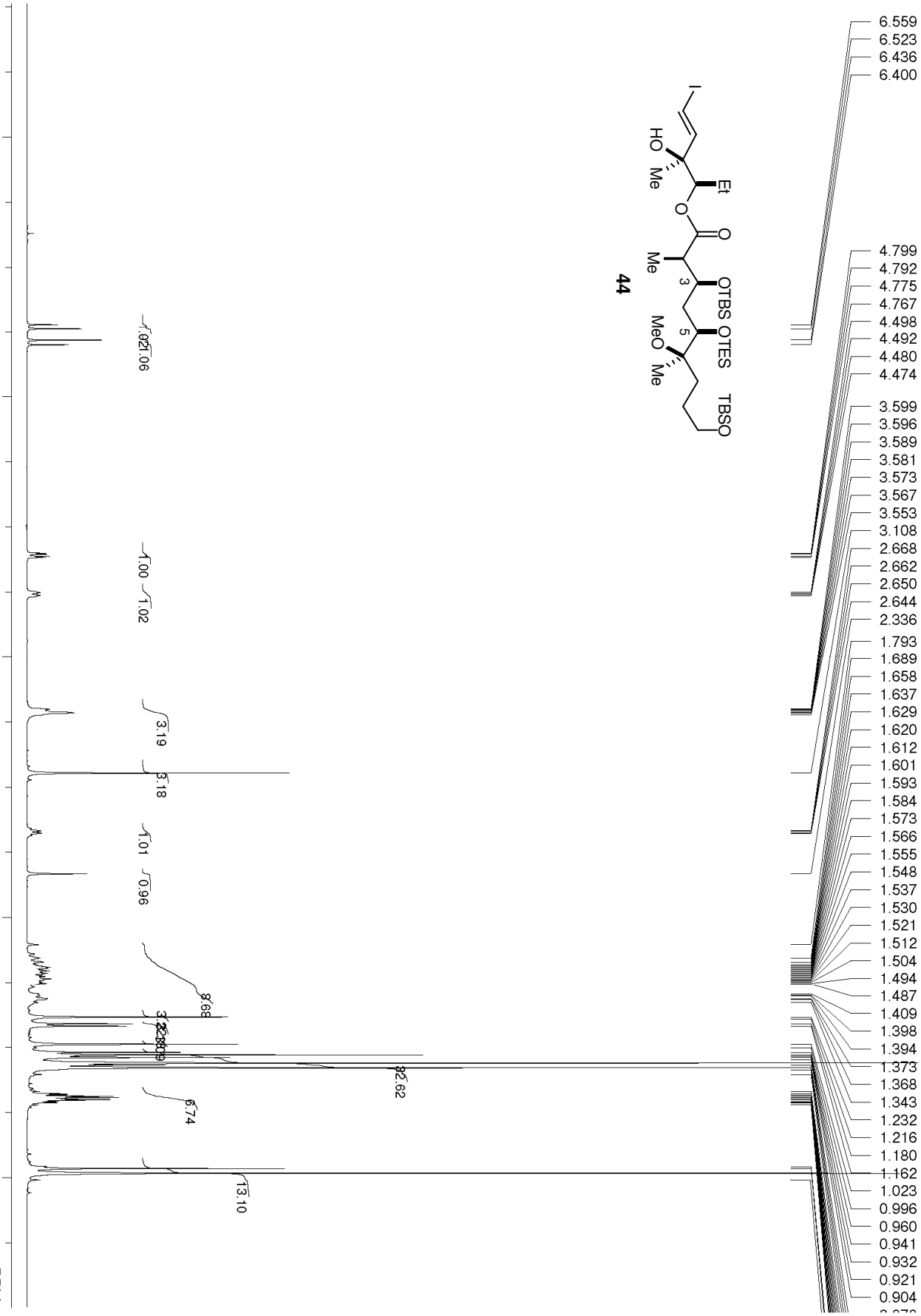
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2.662
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2.644
2.336
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1.658
1.637
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1.620
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1.601
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1.573
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1.512
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0.932
0.921
0.904
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Me
Et
O
O
Me
3
OTBS
OTES
5
MeO
Me
TBSO
I
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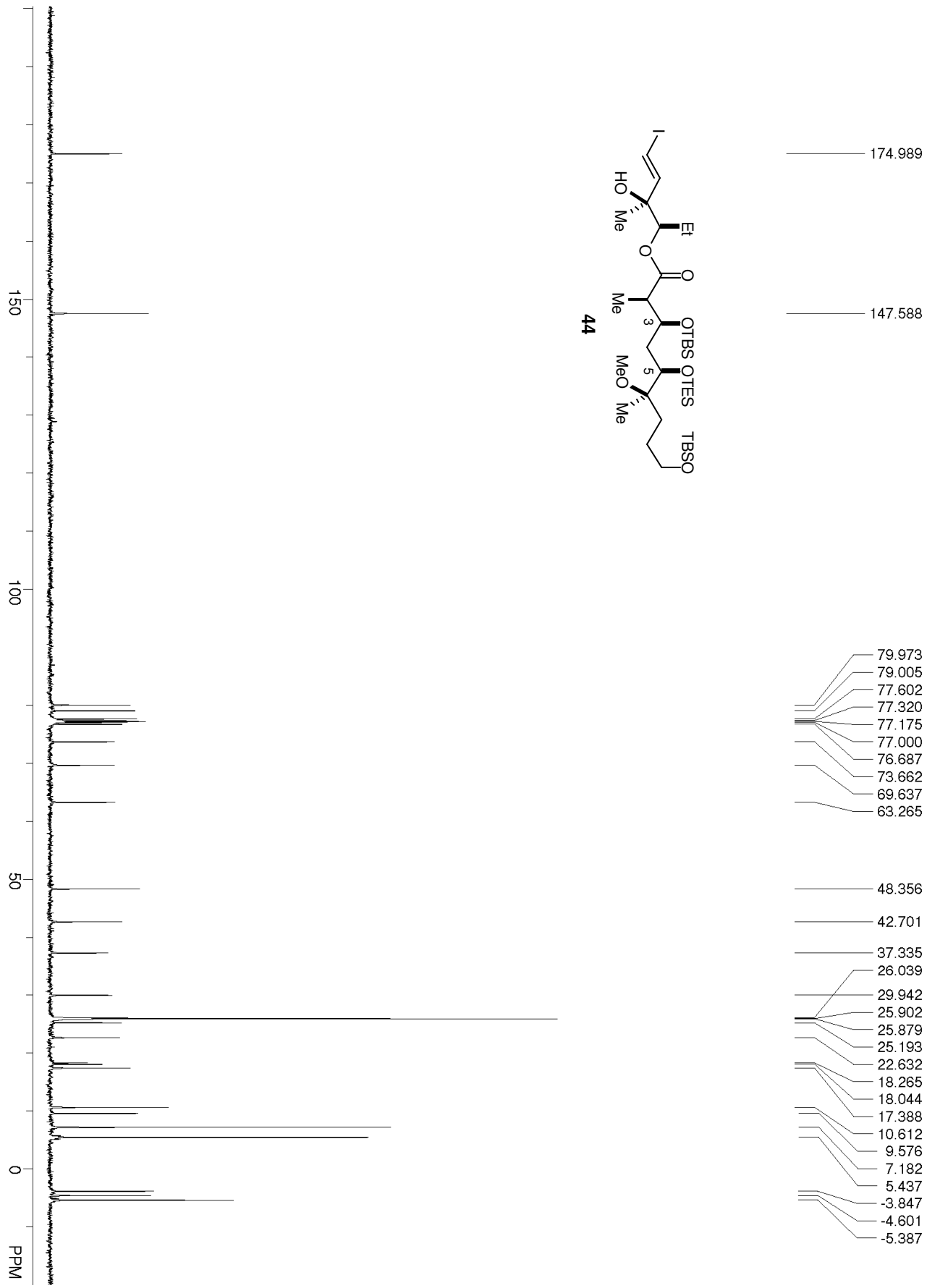
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O
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MeO
Me
TBSO
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77.000
76.687
73.662
69.637
63.265
48.356
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22.632
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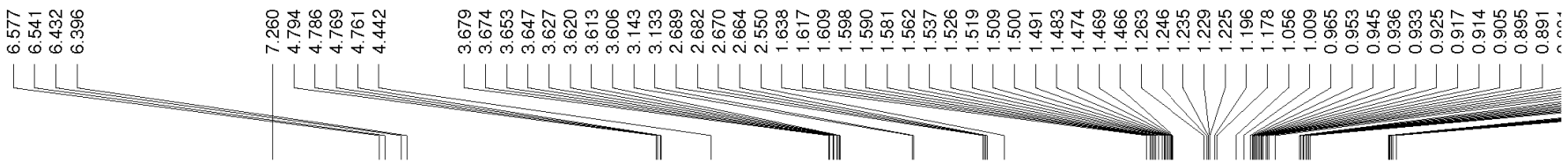
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3.143
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1.590
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1.519
1.509
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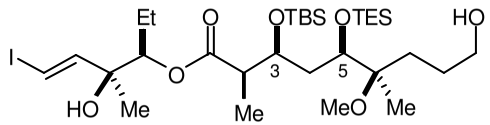
Et
O
OTBS
OTES
HO
I
O
3
5
HO
Me
Me
MeO
Me

45

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6.56
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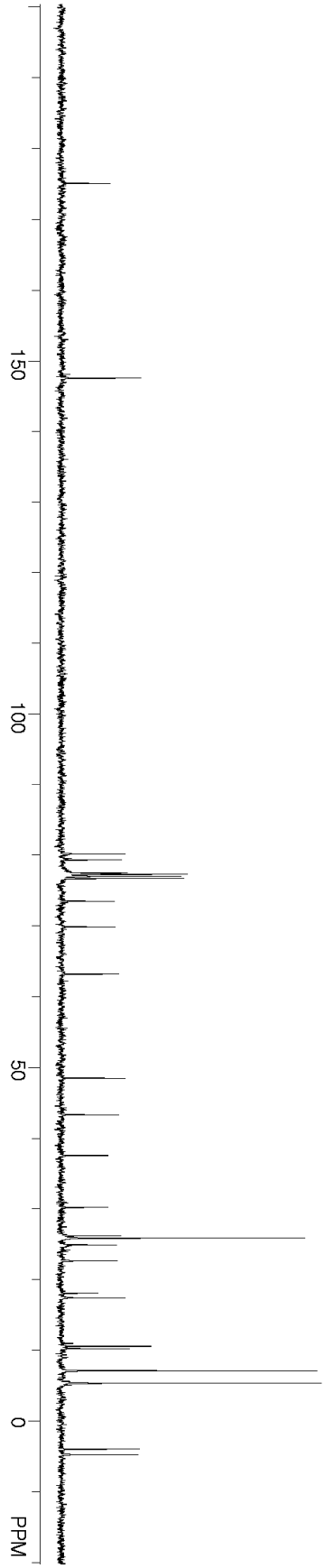

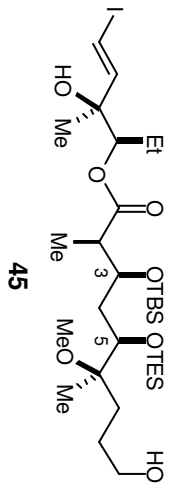

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63.227
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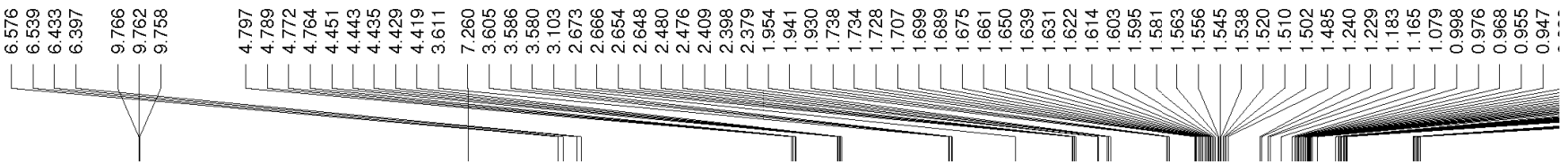
-4.662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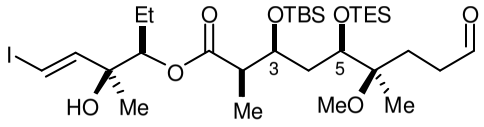
Et
O
OTBS
OTES
O
I
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3
5
HO
Me
Me
MeO
Me

46

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1.00
1.00
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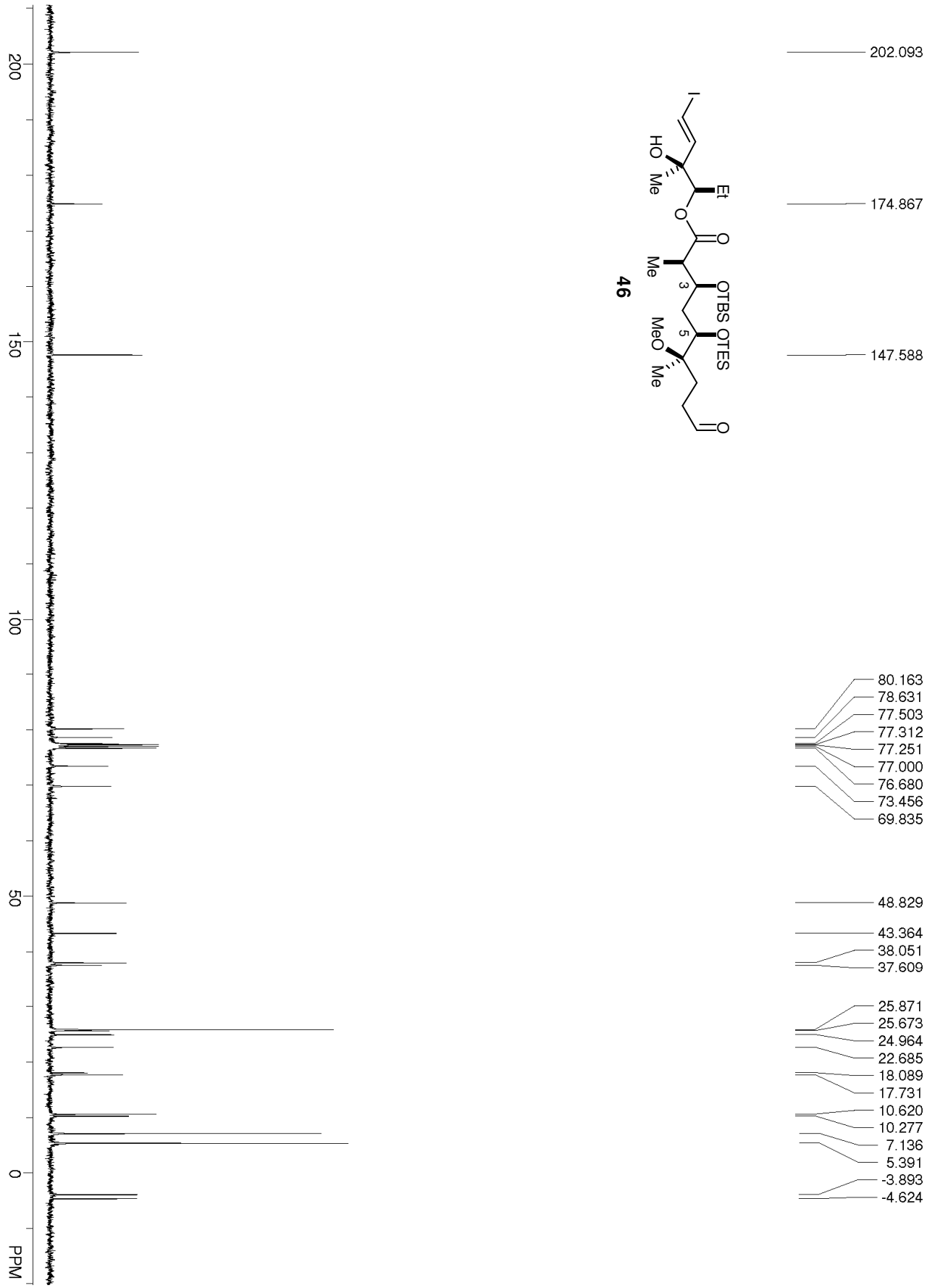
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OTES
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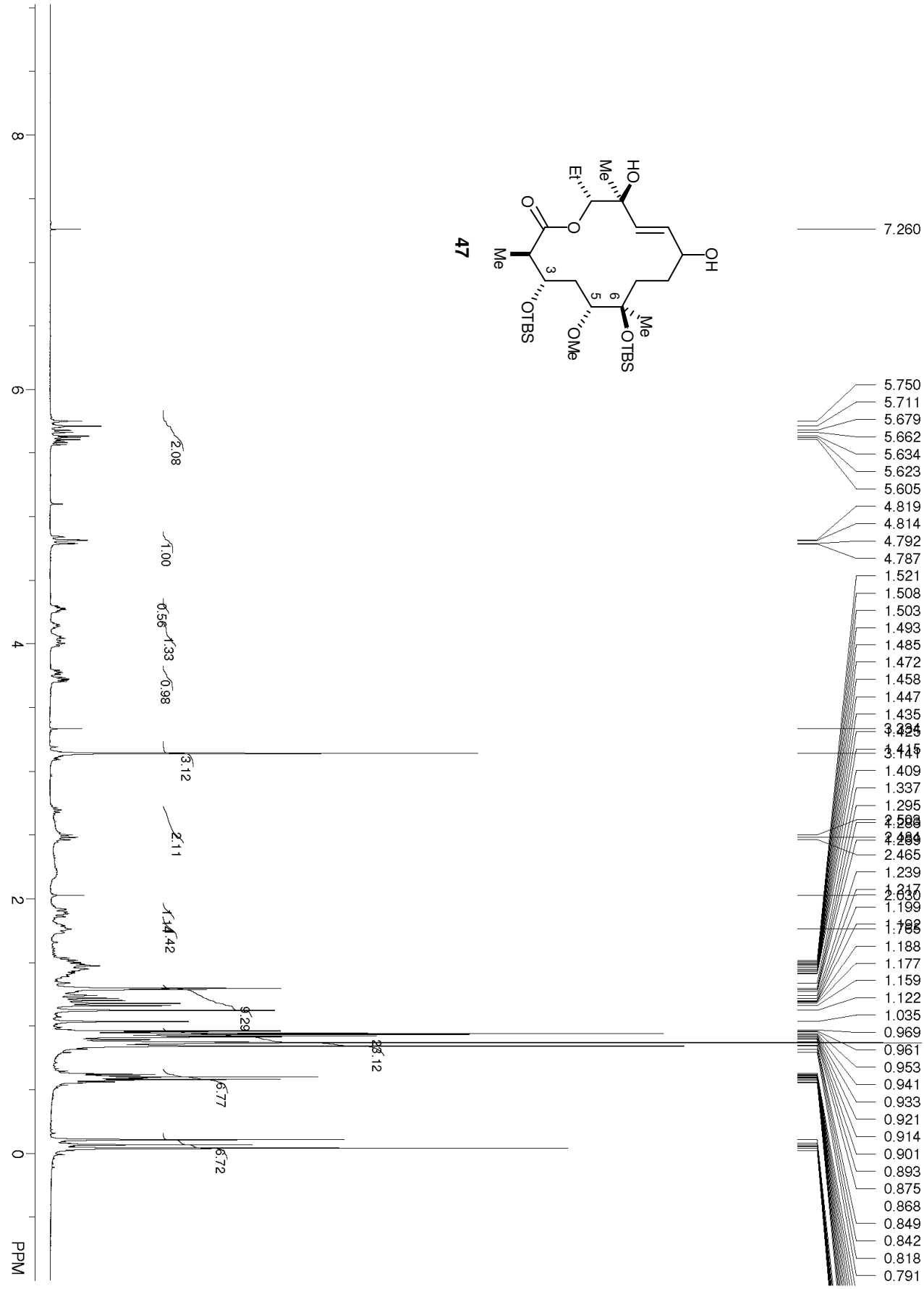
Me
O
I

46


47
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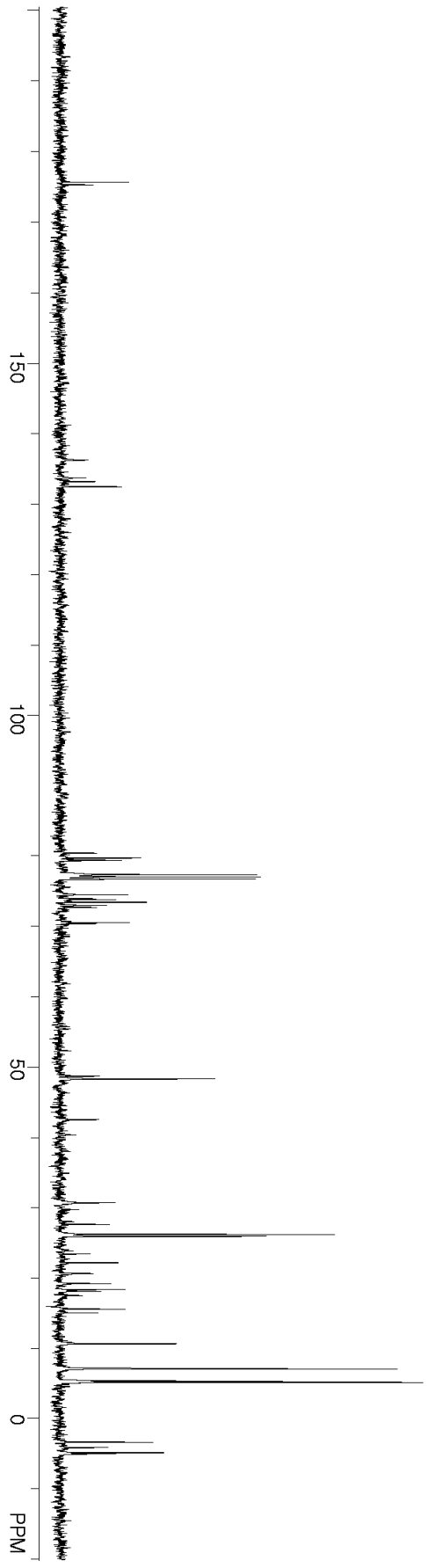
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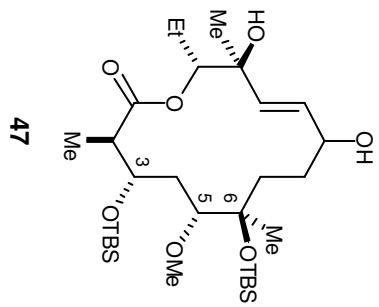
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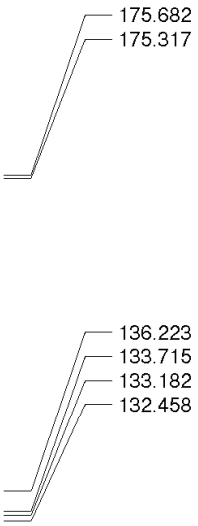
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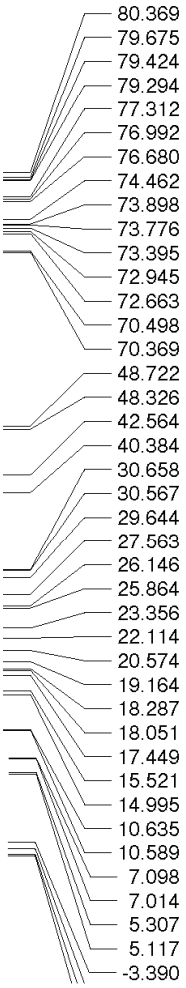
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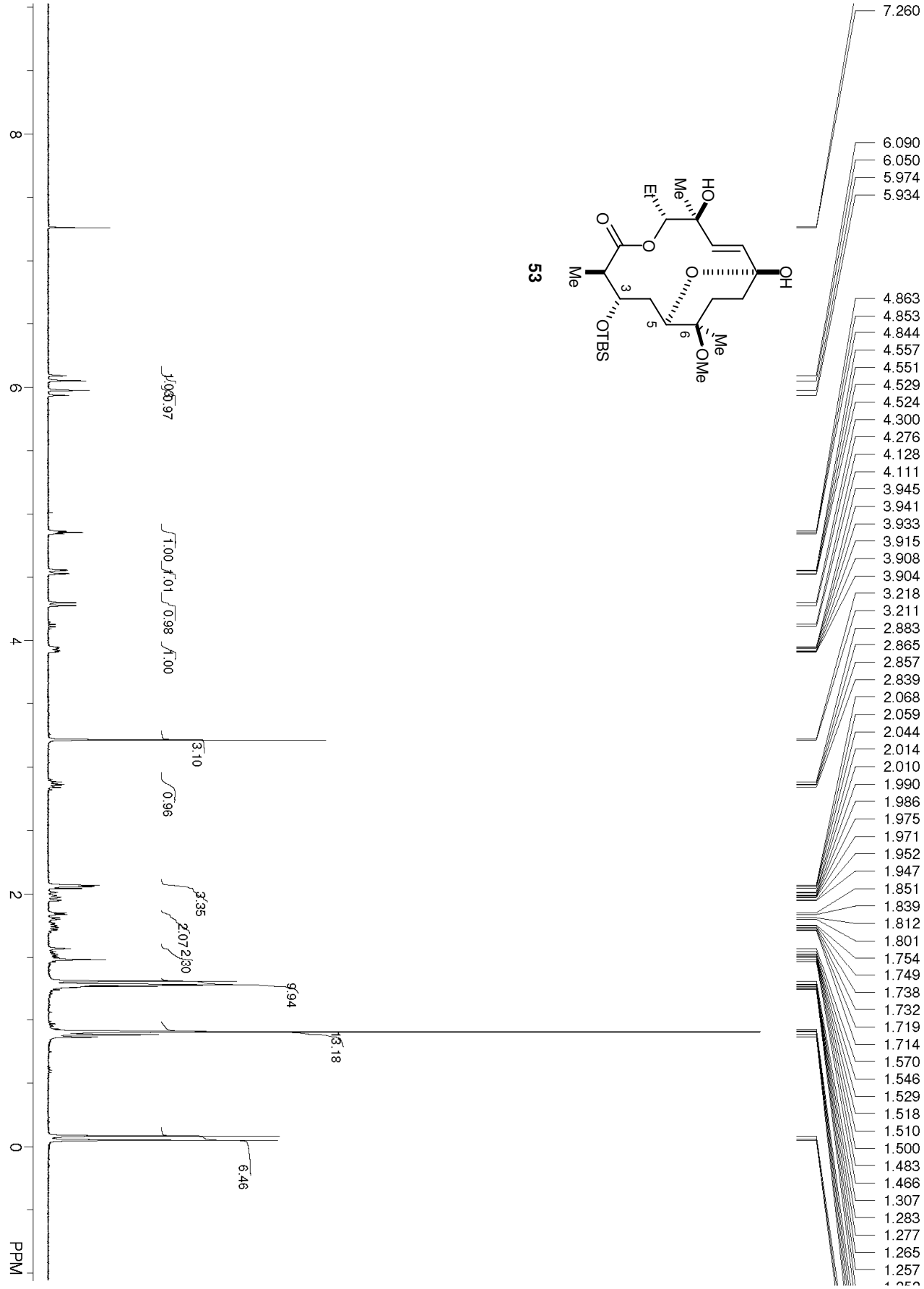
53
HO
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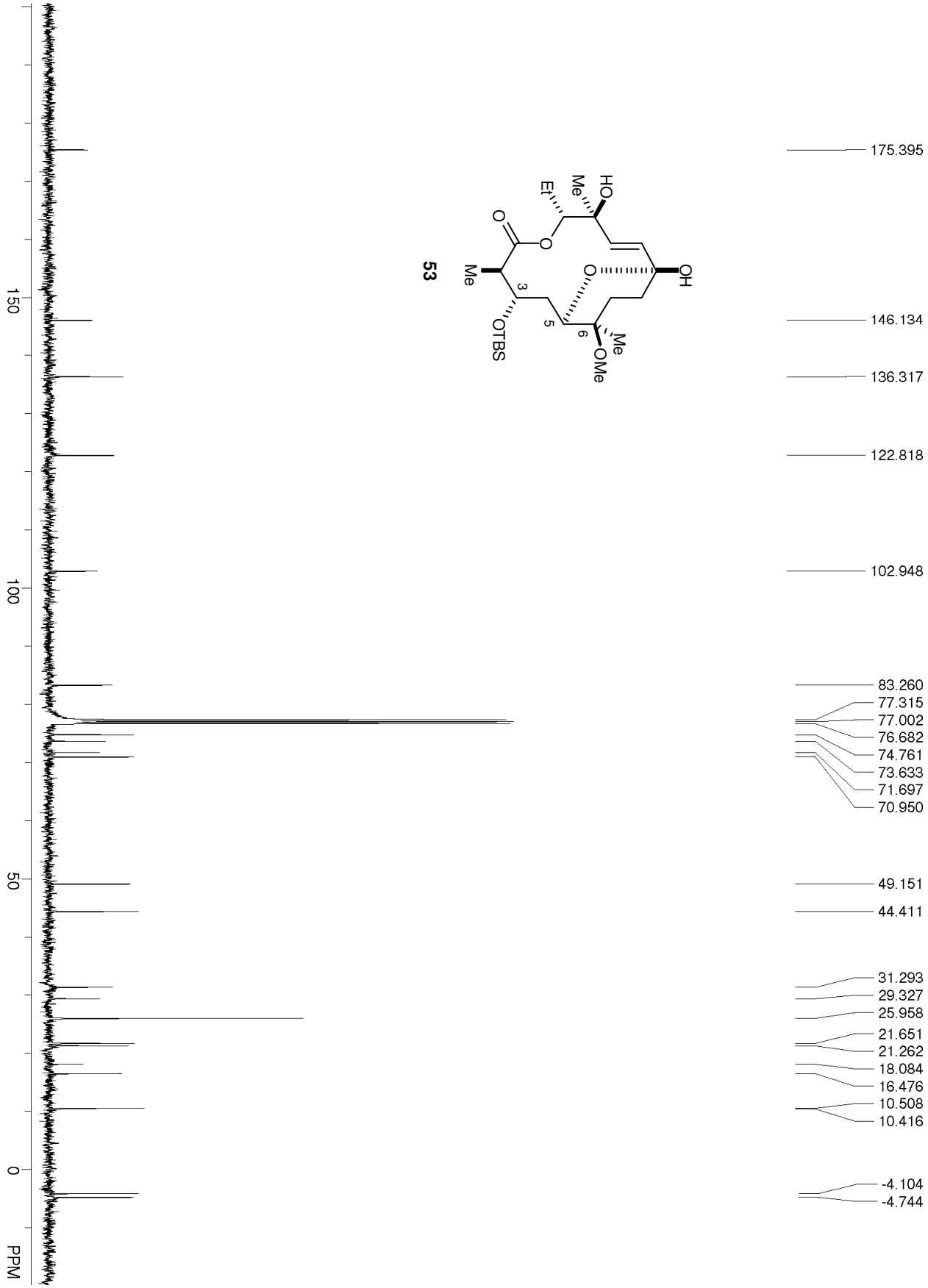
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-4.104
-4.744
150
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PPM
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Et
Me
HO
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OTBS
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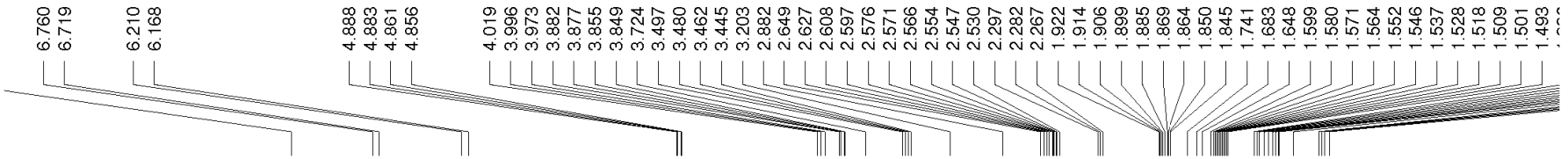
OH
Me
OMe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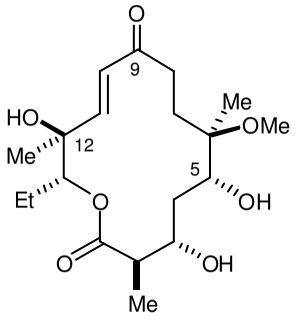
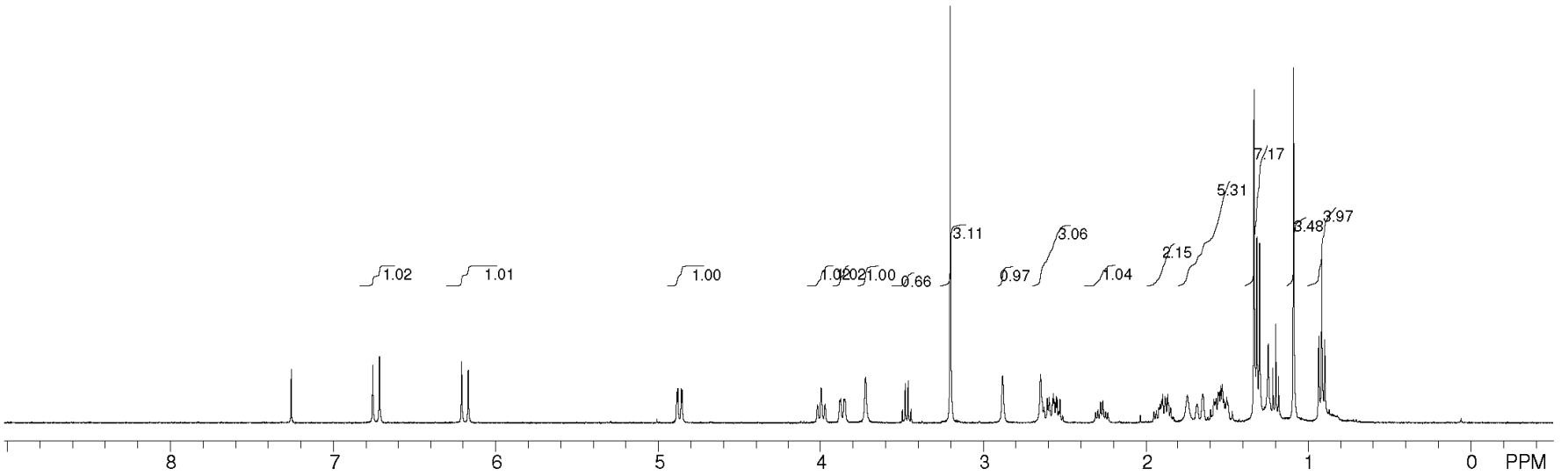
6.719
6.210
6.168
4.888
4.883
4.861
4.856
4.019
3.996
3.973
3.882
3.877
3.855
3.849
3.724
3.497
3.480
3.462
3.445
3.203
2.882
2.649
2.627
2.608
2.597
2.576
2.571
2.566
2.554
2.547
2.530
2.297
2.282
2.267
1.922
1.914
1.906
1.899
1.885
1.869
1.864
1.850
1.845
1.741
1.683
1.648
1.599
1.580
1.571
1.564
1.552
1.546
1.537
1.528
1.518
1.509
1.501
1.493


O
9
HO
Me
OMe
12
Me
5
Et
O
OH
O
OH
Me

54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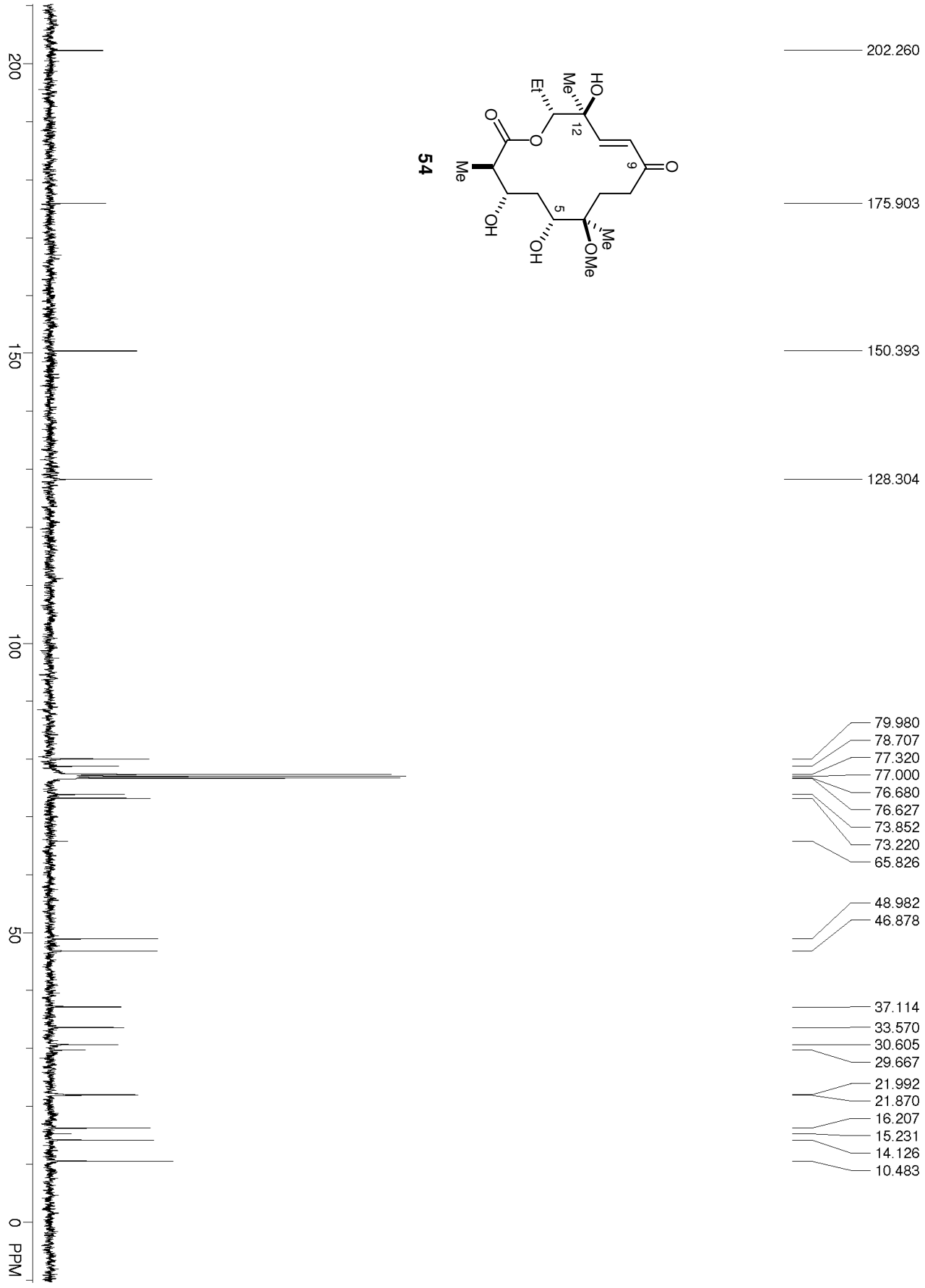
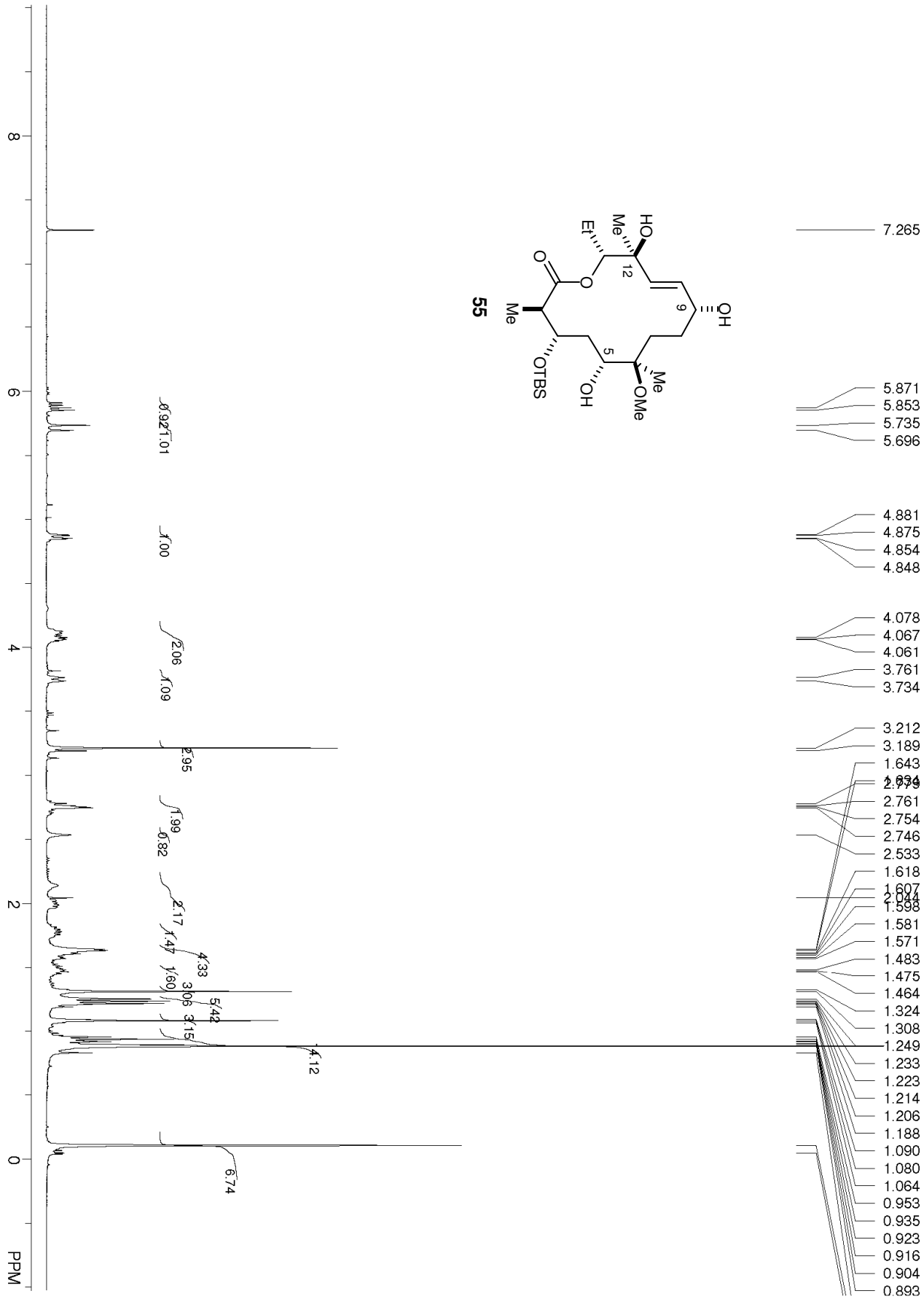
1.01
1.00
1.00
0.66
3.11
0.97
3.06
1.04
2.15
5.31
7.17
3.48
3.97
8
7
6
5
4
3
2
1
0
PPM


200
150
100
50
0 PPM
202.260
175.903
150.393
128.304
79.980
78.707
77.320
77.000
76.680
76.627
73.852
73.220
65.826
48.982
46.878
37.114
33.570
30.605
29.667
21.992
21.870
16.207
15.231
14.126
10.483

54


55
HO
Me
Et
O
O
12
9
OH
Me
OTBS
5
OH
Me
OMe
7.265
5.871
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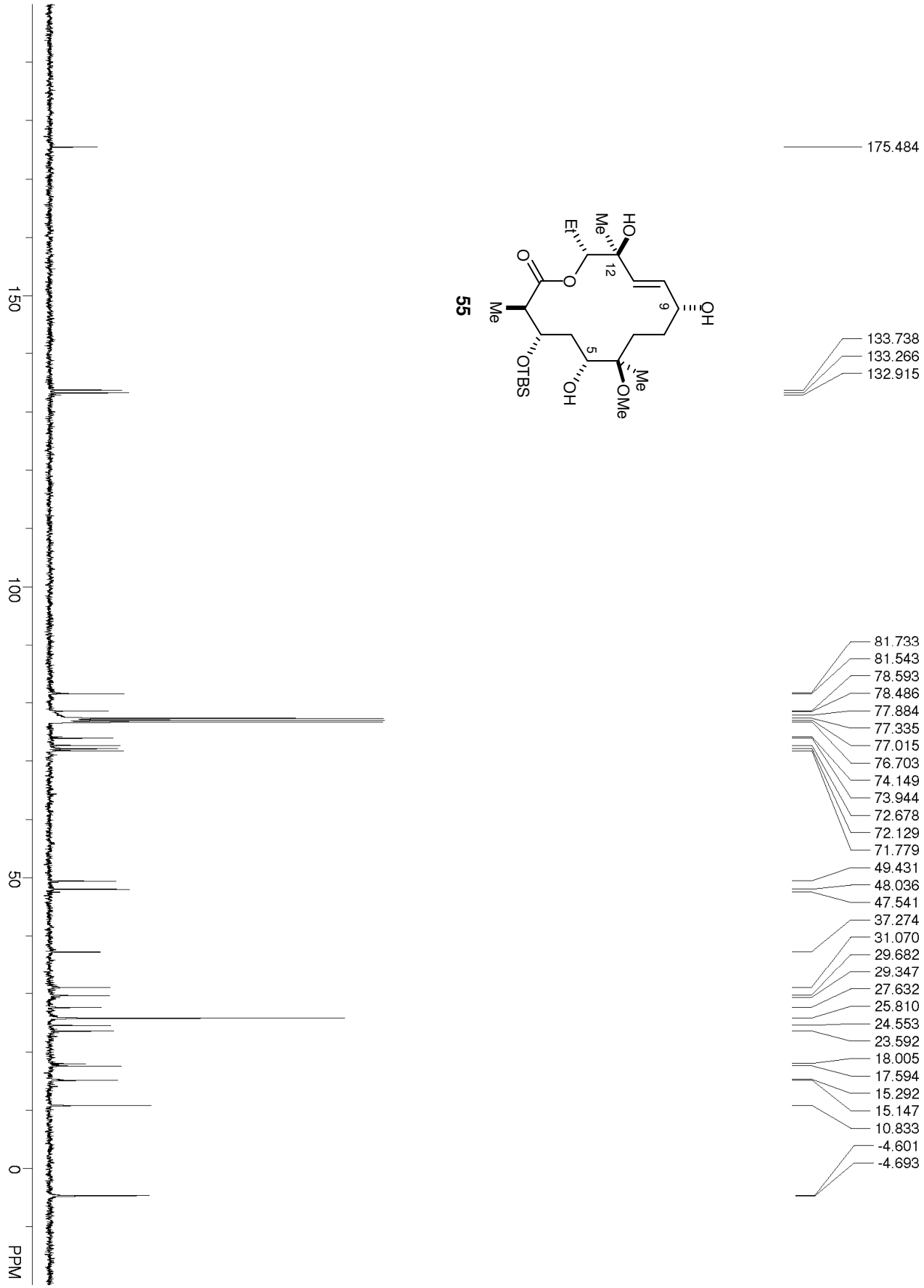
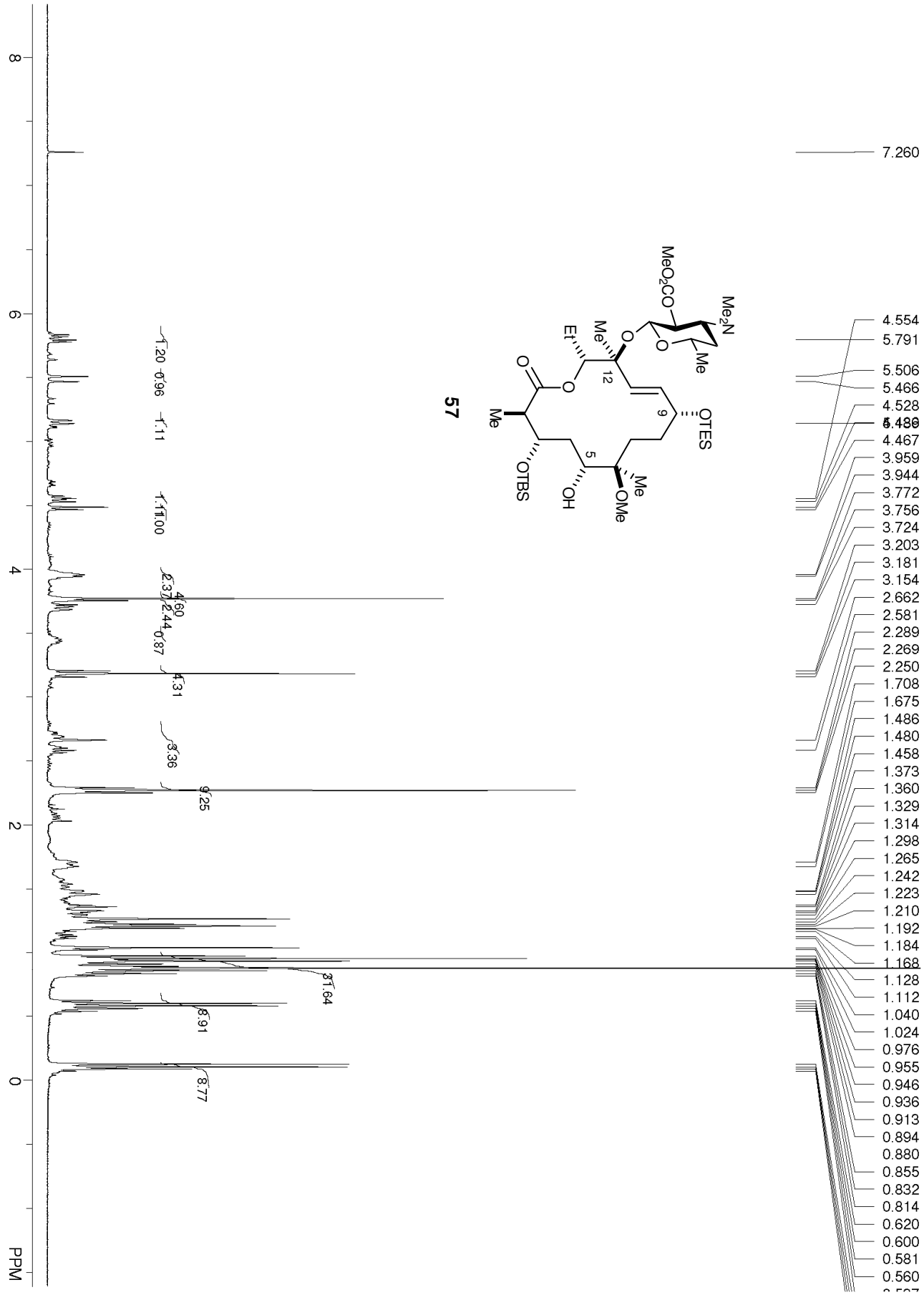
5.735
5.696
4.881
4.875
4.854
4.848
4.078
4.067
4.061
3.761
3.734
3.212
3.189
1.643
2.761
2.754
2.746
2.533
1.618
1.607
1.581
1.571
1.483
1.475
1.464
1.324
1.308
1.249
1.233
1.223
1.214
1.206
1.188
1.090
1.080
1.064
0.953
0.935
0.923
0.916
0.904
0.893
0.92
1.01
1.00
2.06
1.09
2.95
1.99
0.82
2.17
1.47
4.33
1.60
3.06
5.42
3.15
4.12
6.74
8
6
4
2
0
PPM


175.484
133.738
133.266
132.915
81.733
81.543
78.593
78.486
77.884
77.335
77.015
76.703
74.149
73.944
72.678
72.129
71.779
49.431
48.036
47.541
37.274
31.070
29.682
29.347
27.632
25.810
24.553
23.592
18.005
17.594
15.292
15.147
10.833
-4.601
-4.693
150
100
50
0
PPM

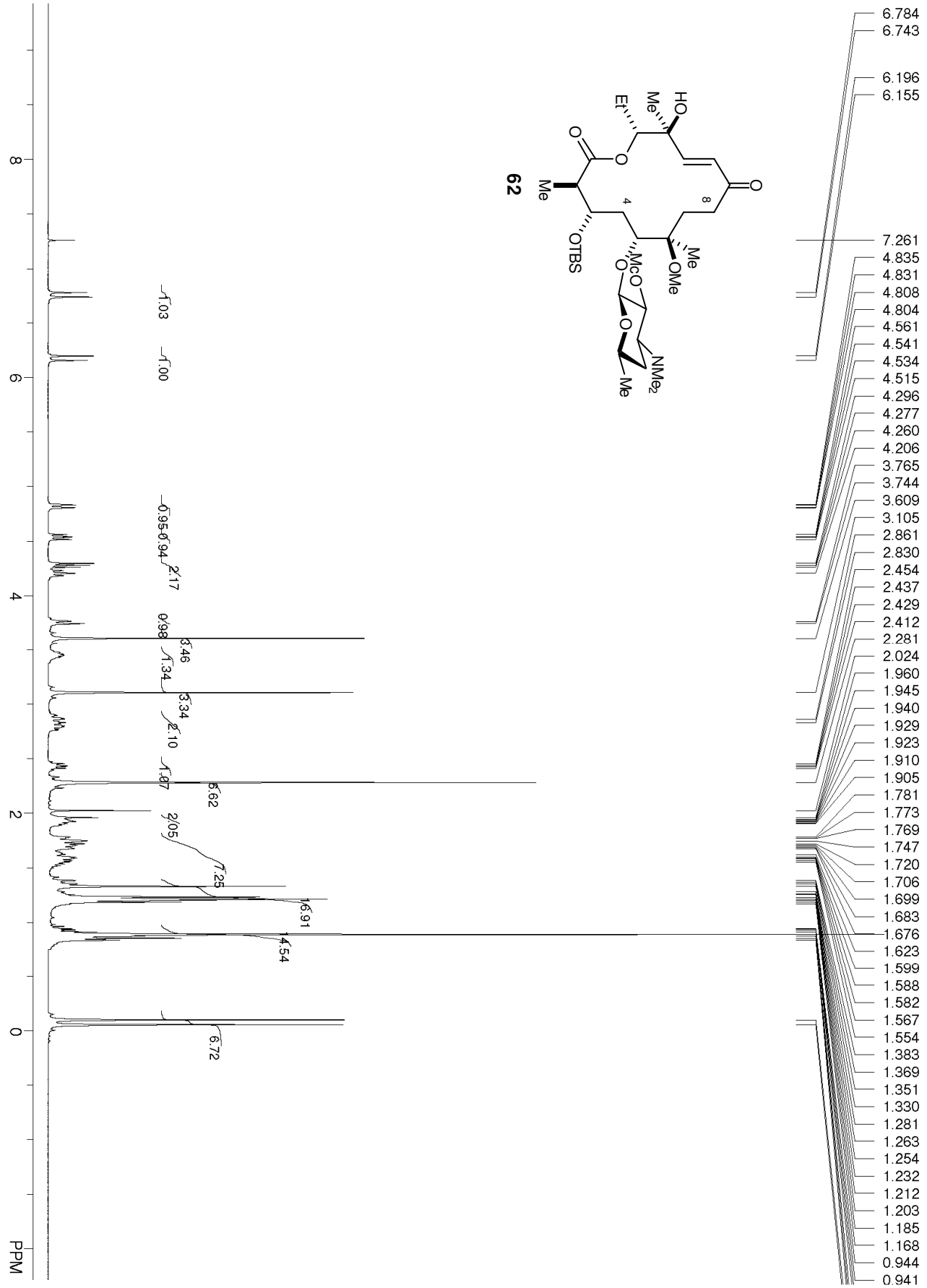
55

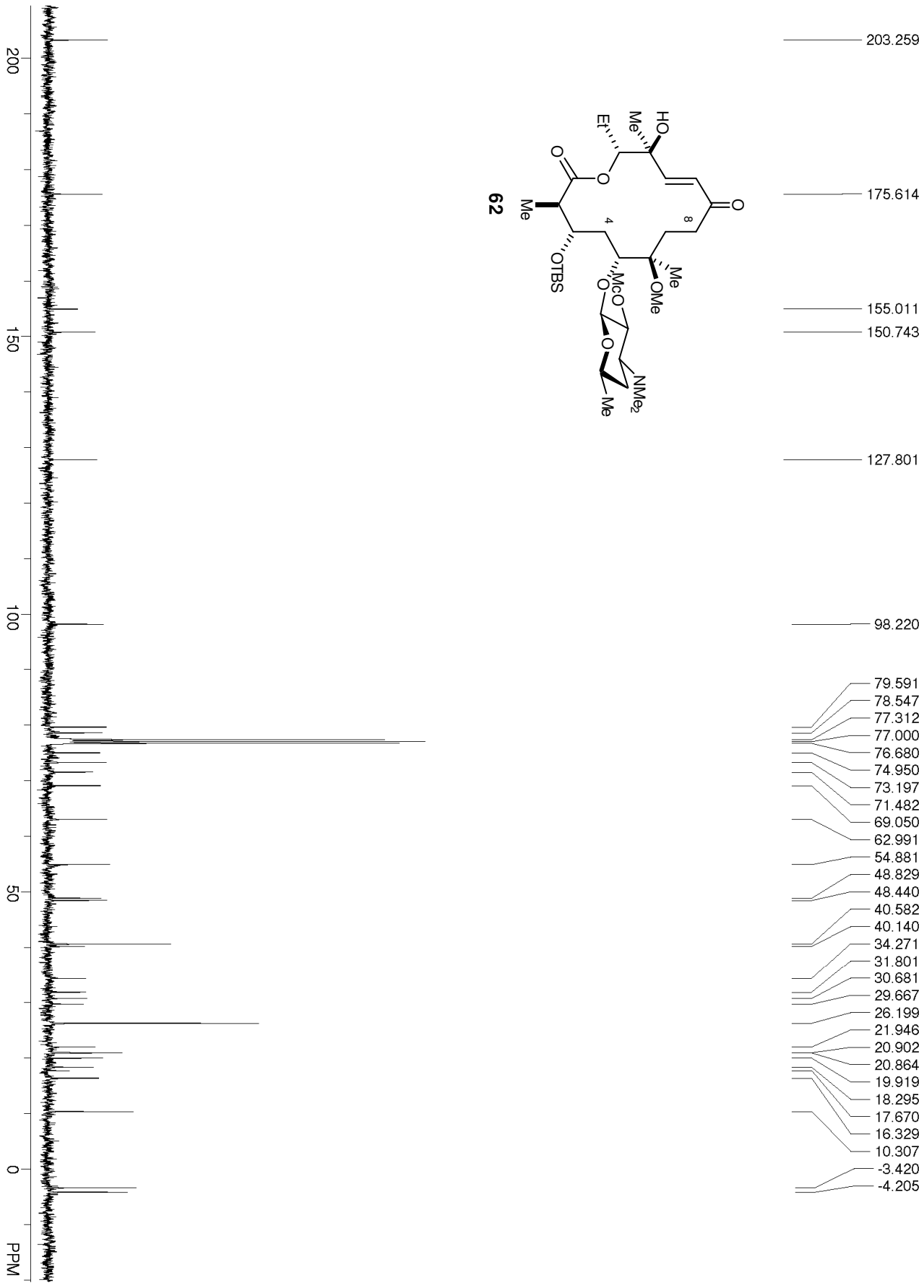

57
Me2N
MeO2CO
Me
Et
Me
12
9
OTES
OTBS
OH
5
Me
OMe
Me
7.260
4.554
5.791
5.506
5.466
4.528
4.467
3.959
3.944
3.772
3.756
3.724
3.203
3.181
3.154
2.662
2.581
2.289
2.269
2.250
1.708
1.675
1.486
1.480
1.458
1.373
1.360
1.329
1.314
1.298
1.265
1.242
1.223
1.210
1.192
1.184
1.168
1.128
1.112
1.040
1.024
0.976
0.955
0.946
0.936
0.913
0.894
0.880
0.855
0.832
0.814
0.620
0.600
0.581
0.560
1.20
0.96
1.11
1.11
1.00
2.37
4.60
2.44
0.87
4.31
3.36
9.25
31.64
8.91
8.77
8
6
4
2
0
PPM

57

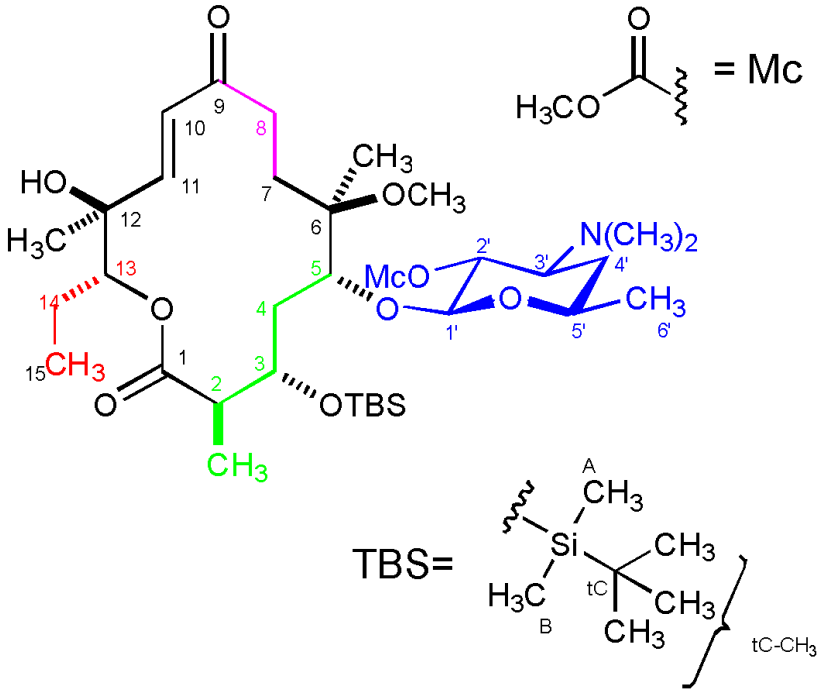
174.379
155.309
135.850
131.261

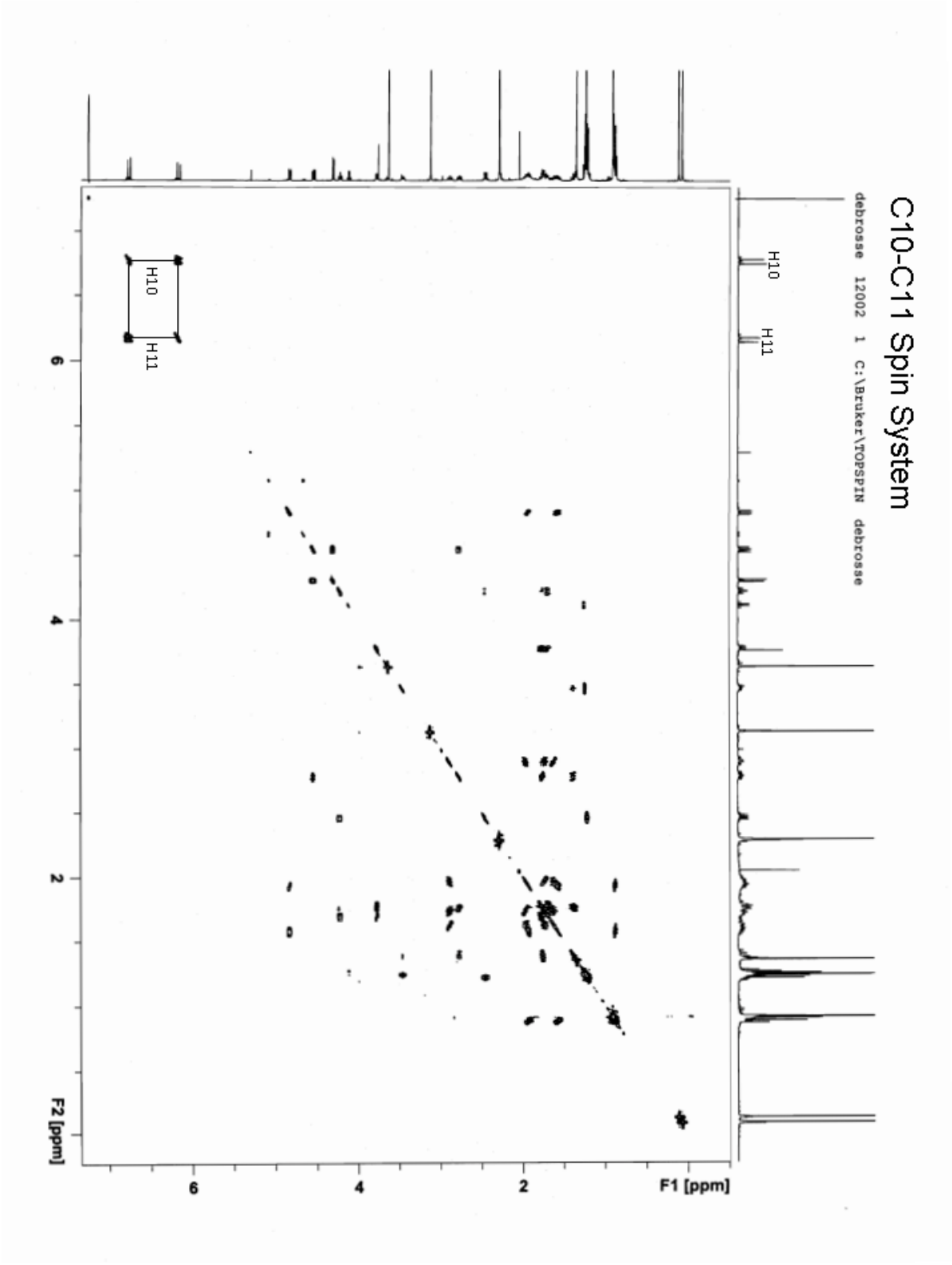
79.774
96.657
78.753
77.854
77.320
77.000
76.687
75.110
74.065
73.966
73.639
73.021
68.844
63.143
63.029
54.637
49.149
48.684
40.612
40.483
37.693
31.710
30.833
29.652
28.143
25.864
25.734
24.667
22.929
21.252
20.864
20.688
17.998
16.694
15.605
10.627
6.954
6.778
4.972
4.850
4.804

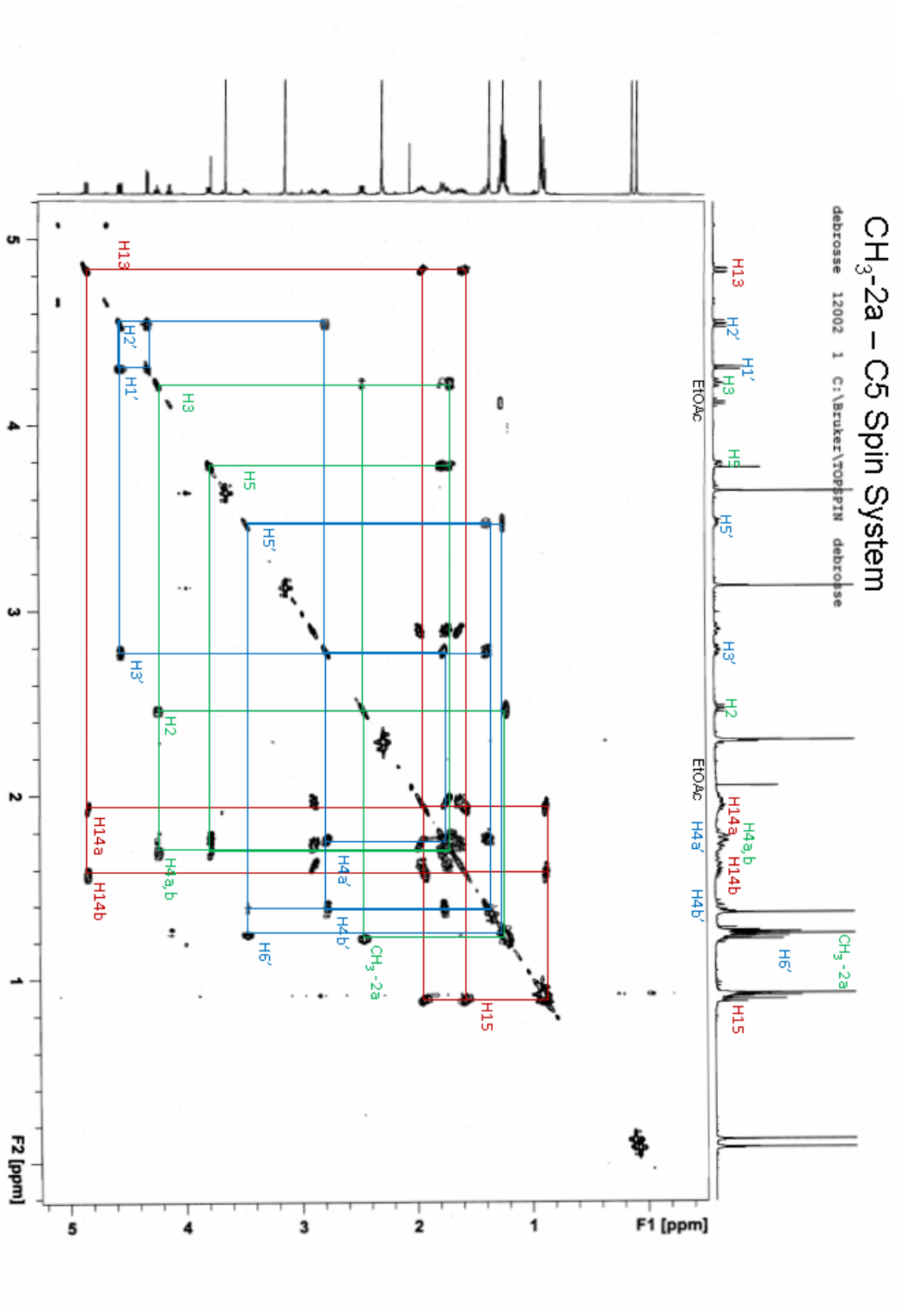

62
HO
Me
Et
O
O
O
O
Me
4
8
OTBS
Me
OMe
McO
O
O
NMe2
Me
6.784
6.743
6.196
6.155
7.261
4.835
4.831
4.808
4.804
4.561
4.541
4.534
4.515
4.296
4.277
4.260
4.206
3.765
3.744
3.609
3.105
2.861
2.830
2.454
2.437
2.429
2.412
2.281
2.024
1.960
1.945
1.940
1.929
1.923
1.910
1.905
1.781
1.773
1.769
1.747
1.720
1.706
1.699
1.683
1.676
1.623
1.599
1.588
1.582
1.567
1.554
1.383
1.369
1.351
1.330
1.281
1.263
1.254
1.232
1.212
1.203
1.185
1.168
0.944
0.941
1.03
1.00
0.95
0.94
2.17
0.98
3.46
1.34
3.34
2.10
1.87
5.62
2.05
7.25
6.91
4.54
6.72
8
6
4
2
0
PPM

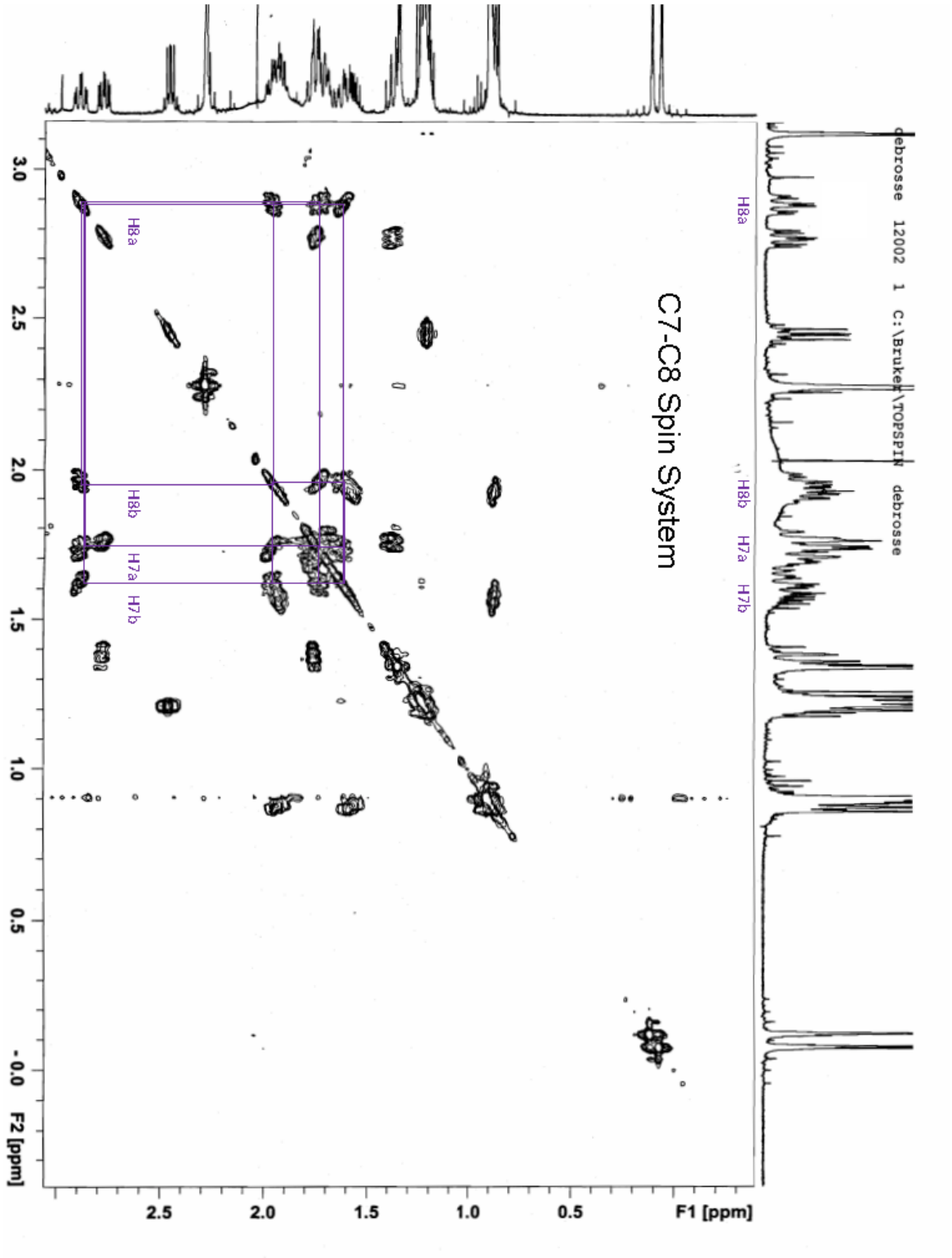

200
150
100
50
0
PPM
203.259
175.614
155.011
150.743
127.801
98.220
79.591
78.547
77.312
77.000
76.680
74.950
73.197
71.482
69.050
62.991
54.881
48.829
48.440
40.582
40.140
34.271
31.801
30.681
29.667
26.199
21.946
20.902
20.864
19.919
18.295
17.670
16.329
10.307
-3.420
-4.205
62
Et
Me
HO
O
O
O
Me
4
8
O
OTBS
McO
O
Me
OMe
O
O
NMe2
Me

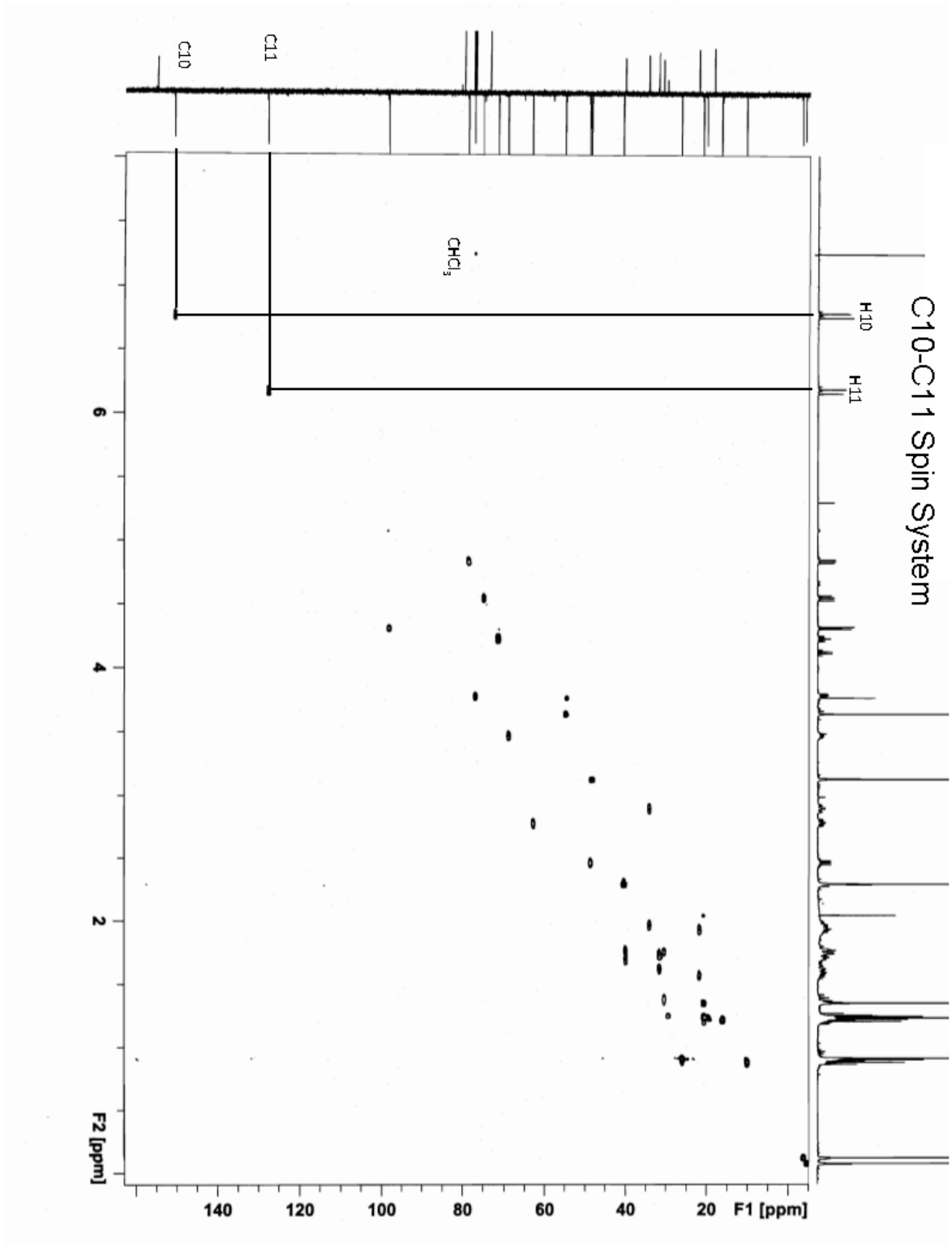
Structural assignments for 4,8,10-tridesmethyl 3-OTBS intermediate

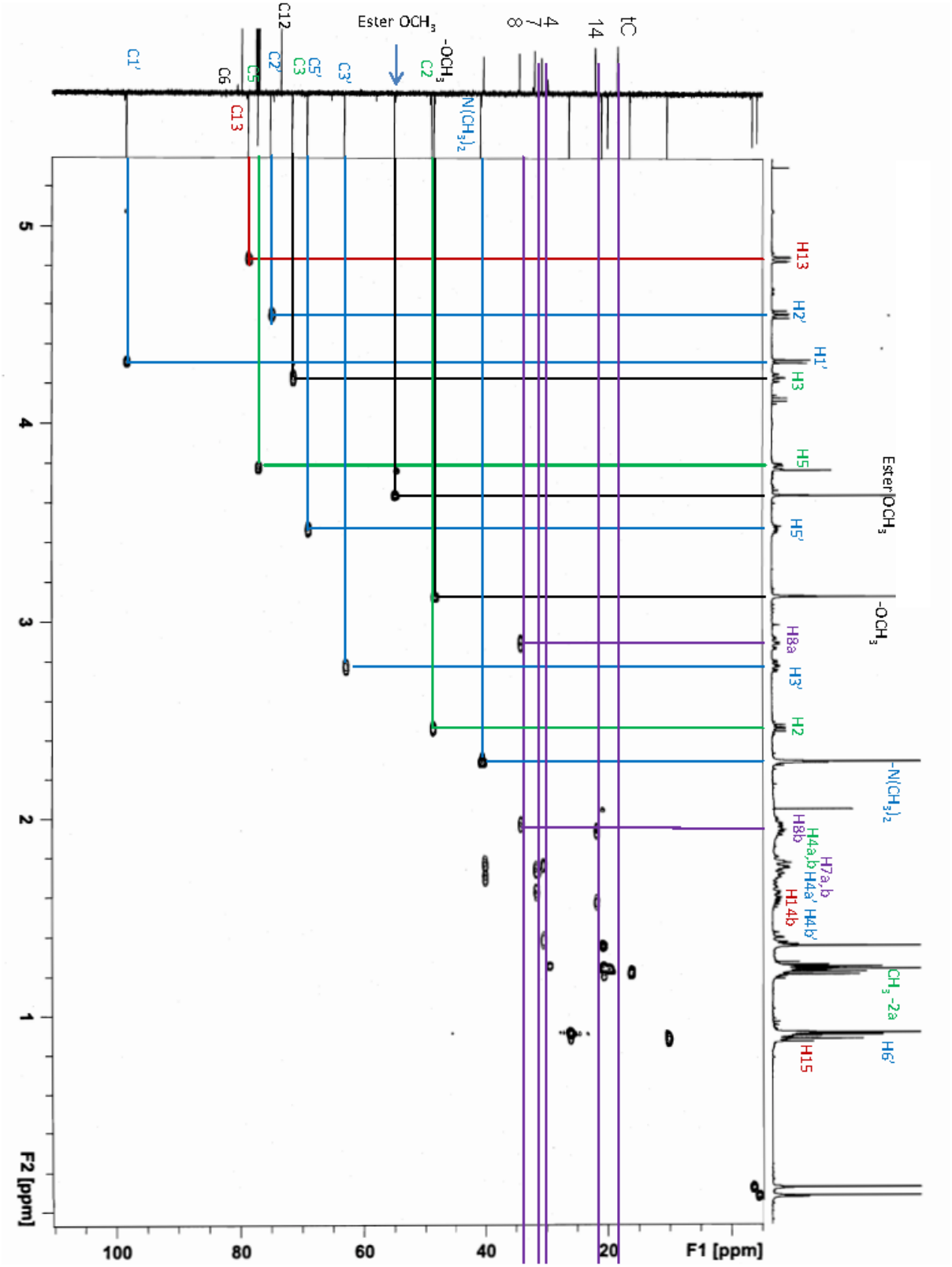


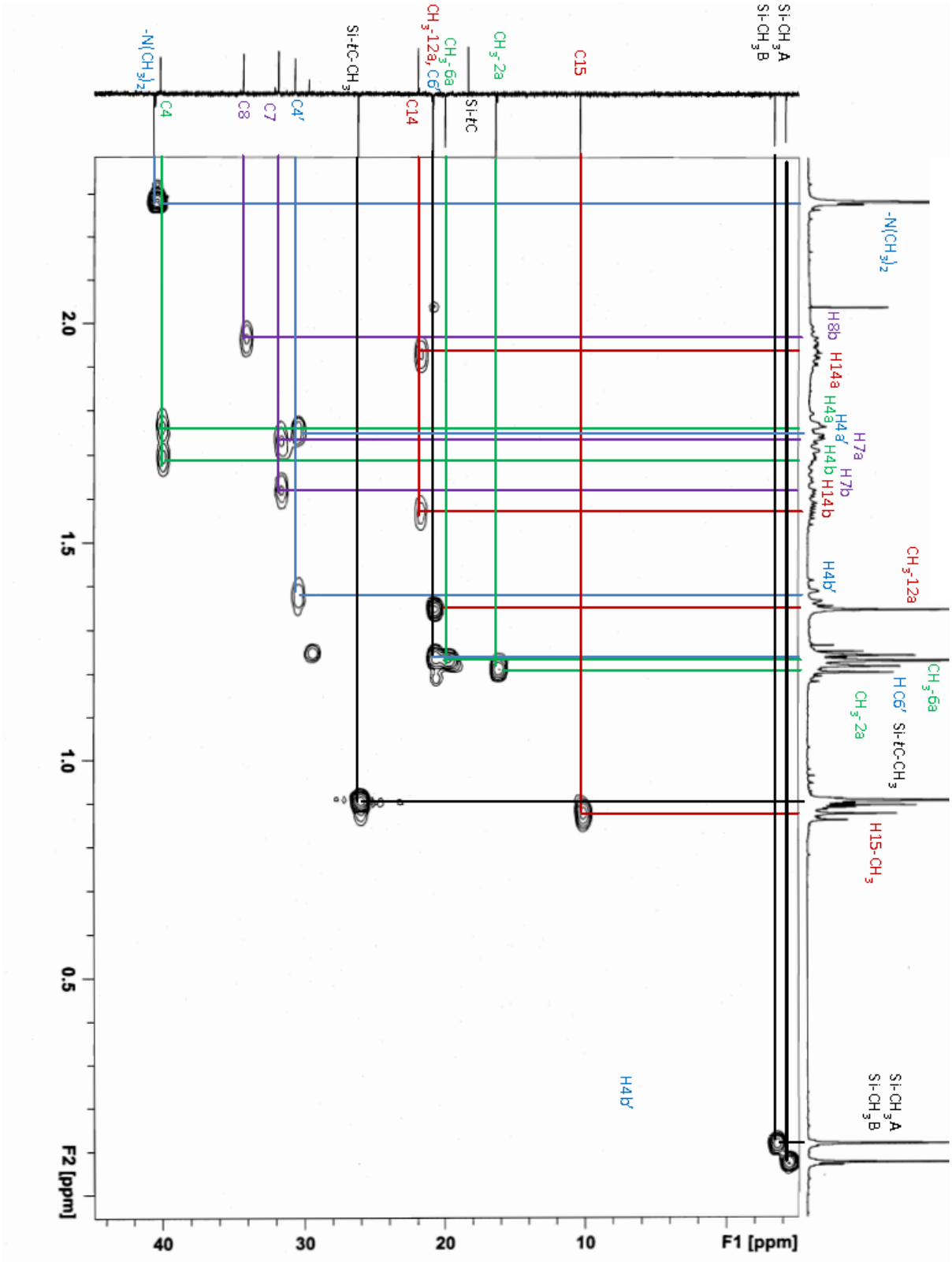

C10-C11 Spin System
debrosse 12002 1 C:\Bruker\TOPSPIN debrosse
H10
H11
H10
H11
F2 [ppm]
F1 [ppm]
6
4
2
6
4
2

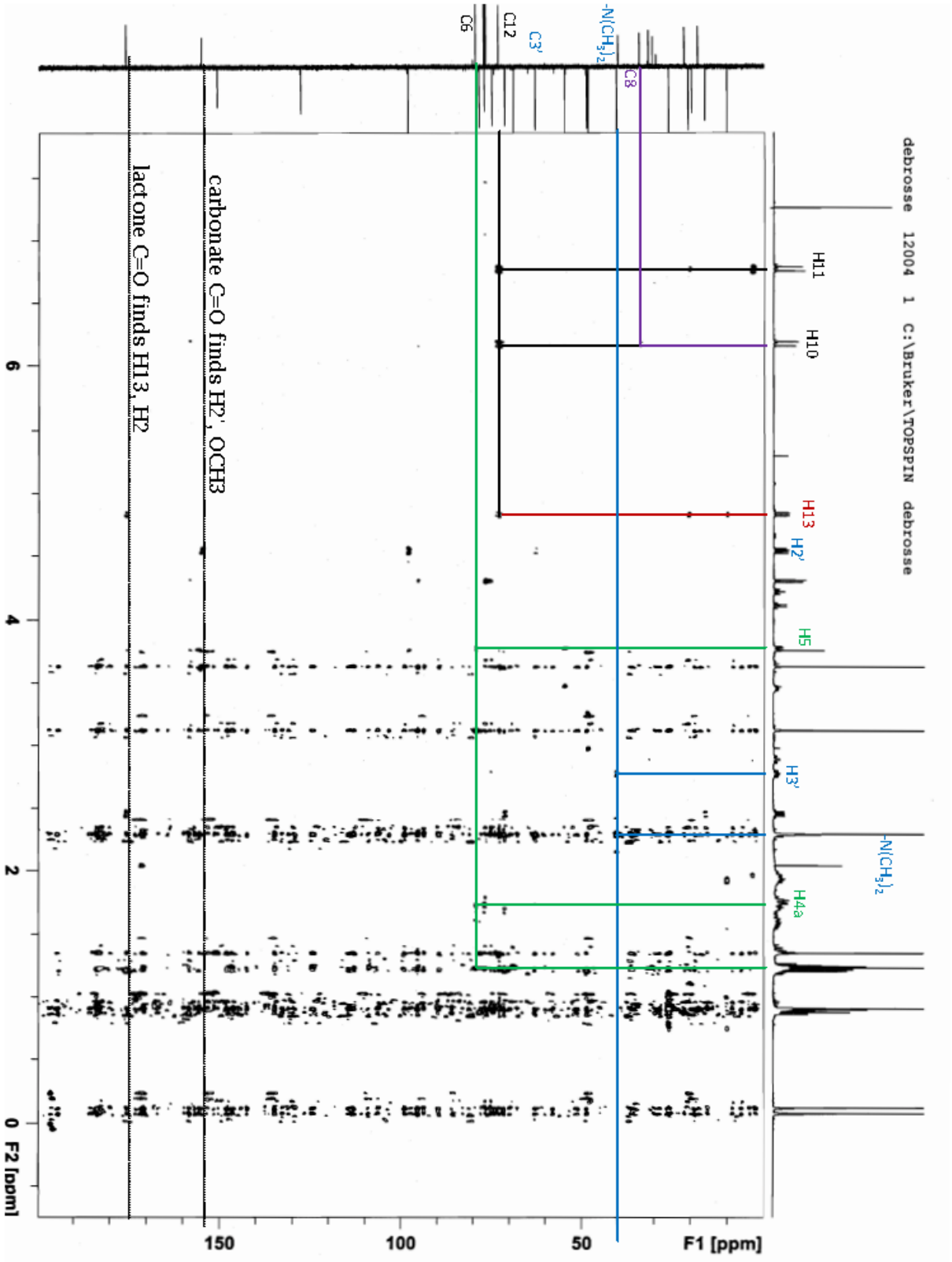

CH3-2a – C5 Spin System
debrosse 12002 1 C:\Bruker\TOPSPIN debrosse
F1 [ppm]
F2 [ppm]
H13
H2'
H1'
H3
H5
H5'
H3'
H2
H14a
H14b
H4a,b
H4a'
H4b'
H6'
CH3-2a
H15
EtOAc


C7-C8 Spin System
H8a
H8b
H7a
H7b
F1 [ppm]
F2 [ppm]
debrosse 12002 1 C:\Bruker\TOPSPIN debrosse

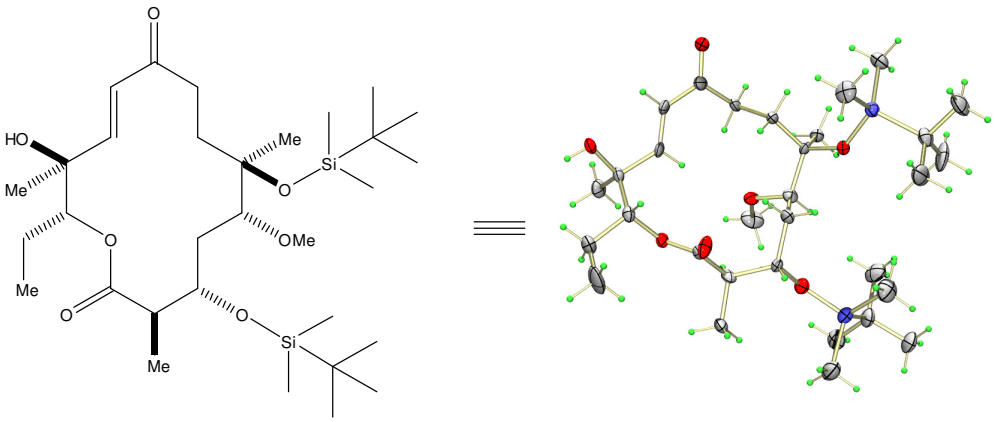

C10-C11 Spin System
C10
C11
CHCl3
H10
H11
F2 [ppm]
F1 [ppm]
6
4
2
140
120
100
80
60
40
20


F2 [ppm]
F1 [ppm]
100
80
60
40
20
1
2
3
4
5
C1'
C6
C13
C5
C12
C2'
C5'
C3
C3'
Ester OCH3
-OCH3
C2
N(CH3)2
4
7
8
14
tC
H13
H2'
H1'
H3
H5
Ester OCH3
H5'
-OCH3
H8a
H3'
H2
-N(CH3)2
H8b
H4a,b H4a' H4b'
H7a,b
H14b
CH3 -2a
H6'
H15


F2 [ppm]
F1 [ppm]
2.0
1.5
1.0
0.5
40
30
20
10
-N(CH3)2
H8b
H14a
H4a
H4a'
H7a
H4b
H7b
H14b
H4b'
CH3-12a
CH3-6a
H6'
Si-tC-CH3
CH3-2a
H15-CH3
Si-CH3A
Si-CH3B
C4
C8
C7
C4'
Si-tC-CH3
C14
CH3-12a, C6'
CH3-6a
Si-tC
CH3-2a
C15
Si-CH3A
Si-CH3B


debrosse 12004 1 C:\Bruker\TOPSPIN debrosse
C6
C12
C3'
-N(CH3)2
C8
H11
H10
H13
H2'
H5
H3'
-N(CH3)2
H4a
carbonate C=O finds H2', OCH3
lactone C=O finds H13, H2
F2 [ppm]
F1 [ppm]
150
100
50
6
4
2
0

X-ray Structure Determination of Compound 35



Compound 99085, $C_{31}H_{60}Si_2O_7$, crystallizes in the triclinic space group P1 with a=14.540(2)Å, b=15.889(2)Å, c=18.453(2)Å, α=86.760(5)°, β=79.926(5)°, γ=64.920(5)°, V=3800.8(6)Å^3, Z=4 and d_{calc}=1.050 g/cm^3. X-ray intensity data were collected on a Rigaku Mercury CCD area detector employing graphite-monochromated Mo-K_α radiation (λ=0.71073 Å) at a temperature of 143K. Preliminary indexing was performed from a series of twelve 0.5° rotation images with exposures of 30 seconds. A total of 578 rotation images were collected with a crystal to detector distance of 35 mm, a 2θ swing angle of -12°, rotation widths of 0.5° and exposures of 20 seconds: scan no. 1 was a ϕ-scan from 315° to 525° at ω = 10° and χ = 20°; scan no. 2 an ω-scan from -20° to 5° at χ = -90° and ϕ = 315°; scan no. 3 was an ω-scan from -20° to 12° at χ = -90° and ϕ = 135°; scan no. 4 was an ω-scan from -20° to 2° at χ = -90° and ϕ = 225°. Rotation images were processed using CrystalClear[7], producing a listing of unaveraged F^2 and $\sigma(F^2)$ values which were then passed to the CrystalStructure[8] program package for further processing and structure solution on a Dell Pentium III computer. A total of 26883 reflections were measured over the ranges $5.02 \le 2\theta \le 45.1$ °, $-15 \le h \le 15$, $-17 \le k \le 17$, $-19 \le l \le 19$ yielding 26883 unique reflections (R_{int} = 0.0000). The intensity data were corrected for Lorentz and polarization effects and for absorption using REQAB[9] (minimum and maximum transmission 0.393, 1.000).

The structure was solved by direct methods (SIR2004[10]). The asymmetric unit includes four molecules of the title compound. Initial refinement yielded an R-factor over 25%; analysis by the TwinSolve module of CrystalClear indicated that the crystal was twinned by rotation of 180° about the b* reciprocal axis. A data file with F^2 values for two twin components was prepared for use in the least squares program. Refinement was by full-matrix least squares based on F^2 using SHELXL-97[11]. All reflections were used during refinement. The weighting scheme used was $w=1/[\sigma^2(F_o^2)+ 0.1165P^2 + 4.9260P]$ where $P = (F_o^2 + 2F_c^2)/3$. Non-hydrogen atoms were refined using a "riding" model. Refinement converged to R_1=0.0770 and wR_2=0.1958 for 23395 reflections for which $F > 4\sigma(F)$ and R_1=0.0944, wR_2=0.2169 and GOF = 1.117 for all 26883 unique, non-zero reflections and 1443 variables[12]. The maximum Δ/σ in the final cycle of least squares was 0.025 and the two most prominent peaks in the final difference Fourier were +0.895 and -0.361 e/Å^3. The twinning parameter refined to a value of 0.497(1).

Table 1. lists cell information, data collection parameters, and refinement data. Final positional and equivalent isotropic thermal parameters are given in Table 2. Anisotropic thermal parameters are in Table 3. Tables 4. and 5. list bond distances and bond angles. Figure 1. is a numbered ChemDraw of the molecule. Figure 2. is ORTEP[13] representations of the molecule with 30% probability thermal ellipsoids displayed.

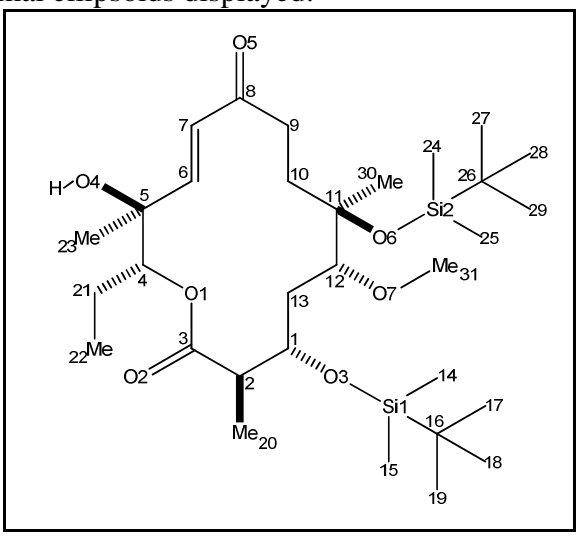


Figure 1. Numbered ChemDraw of the molecule.

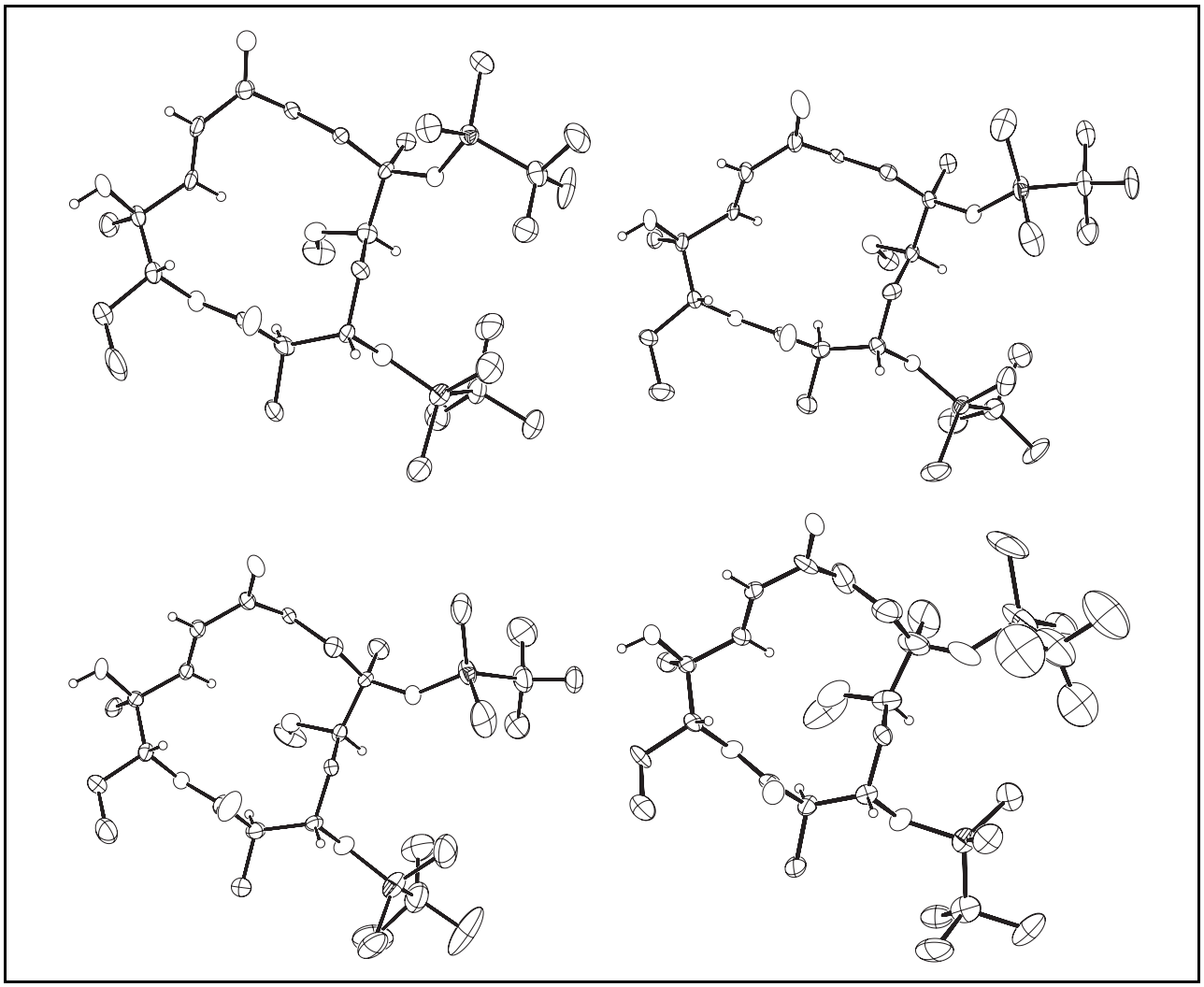


Figure 2. ORTEP drawings of the four molecules in the asymmetric unit with 30% probability thermal ellipsoids.

Table 1. Summary of Structure Determination of Compound 99085

Formula:	$C_{31}H_{60}Si_2O_7$
Formula weight:	600.97
Crystal class:	triclinic
Space group:	P1 (#1)
Z	4
Cell constants:	
a	14.540(2)Å
b	15.889(2)Å
c	18.453(2)Å
α	86.760(5)°
β	79.926(5)°
γ	64.920(5)°
V	3800.8(6)Å^3
μ	1.31 cm^{-1}
crystal size, mm	0.40 x 0.22 x 0.06
D_{calc}	1.050 g/cm^3
F(000)	1320
Radiation:	Mo-K_α (λ=0.71073Å)
2θ range	5.02 – 45.1 °
hkl collected:	-15≤ h ≤15; -17≤ k ≤17; -19≤ l ≤19
No. reflections measured:	26883
No. unique reflections:	26883 (R_{int}=0.0000)
No. observed reflections	23395 (F>4σ)
No. reflections used in refinement	26883
No. parameters	1443
R indices (F>4σ)	R_1=0.0770
	wR_2=0.1958
R indices (all data)	R_1=0.0944
	wR_2=0.2169
GOF:	1.117
Final Difference Peaks, e/Å^3	+0.895, -0.361

Table 2. Refined Positional Parameters for Compound 99085

Atom	x	y	z	U_{eq}, Å^2
Molecule No. 1				
Si1	0.2194(2)	0.7766(2)	1.22399(11)	0.0531(6)
Si2	0.5091(2)	0.50718(14)	0.94335(10)	0.0377(5)
O1	0.3511(3)	1.0264(3)	0.9968(2)	0.0360(11)
O2	0.4673(4)	0.9204(4)	1.0599(3)	0.0522(14)
O3	0.2304(4)	0.8329(4)	1.1465(3)	0.0484(13)
O4	0.4994(4)	1.0493(3)	0.8201(3)	0.0459(12)
H4	0.5027	1.0980	0.8283	0.069
O5	0.5129(5)	0.7696(4)	0.7147(3)	0.058(2)
O6	0.4105(4)	0.6089(3)	0.9689(2)	0.0378(11)
O7	0.2499(4)	0.8571(3)	0.9623(2)	0.0416(12)
C1	0.3217(6)	0.8416(5)	1.1100(3)	0.036(2)
H1	0.3706	0.8245	1.1445	0.047
C2	0.2892(6)	0.9468(5)	1.0909(4)	0.039(2)
H2	0.2342	0.9669	1.0612	0.052
C3	0.3816(6)	0.9601(5)	1.0479(3)	0.034(2)
C4	0.4301(5)	1.0464(5)	0.9471(4)	0.035(2)
H4a	0.4979	0.9974	0.9521	0.046
C5	0.4134(5)	1.0440(5)	0.8679(4)	0.034(2)
C6	0.4112(6)	0.9520(5)	0.8496(3)	0.036(2)
H6	0.3665	0.9332	0.8812	0.047
C7	0.4687(6)	0.8968(5)	0.7918(4)	0.043(2)
H7	0.5195	0.9113	0.7636	0.057
C8	0.4576(7)	0.8148(5)	0.7693(4)	0.045(2)
C9	0.3788(6)	0.7852(5)	0.8118(3)	0.038(2)
H9a	0.3551	0.7565	0.7786	0.051
H9b	0.3199	0.8391	0.8350	0.051
C10	0.4271(6)	0.7141(5)	0.8722(3)	0.034(2)
H10a	0.4760	0.6561	0.8476	0.045
H10b	0.4655	0.7378	0.8966	0.045
C11	0.3519(6)	0.6932(5)	0.9312(3)	0.032(2)
C12	0.2995(6)	0.7695(5)	0.9947(4)	0.038(2)
H12	0.2461	0.7557	1.0262	0.051
C13	0.3716(6)	0.7739(5)	1.0432(4)	0.038(2)
H13a	0.4224	0.7911	1.0128	0.051
H13b	0.4082	0.7120	1.0611	0.051
C14	0.3245(8)	0.6584(7)	1.2253(6)	0.078(3)
H14a	0.3283	0.6228	1.1836	0.118
H14b	0.3110	0.6283	1.2698	0.118
H14c	0.3888	0.6629	1.2230	0.118
C15	0.2107(9)	0.8465(8)	1.3051(5)	0.076(3)
H15a	0.1567	0.9078	1.3037	0.113

H15b	0.2750	0.8507	1.3035	0.113
H15c	0.1960	0.8170	1.3496	0.113
C16	0.0954(7)	0.7630(6)	1.2259(4)	0.059(2)
C17	0.1025(9)	0.7102(9)	1.1544(5)	0.080(3)
H17a	0.1109	0.7459	1.1121	0.120
H17b	0.0404	0.7019	1.1564	0.120
H17c	0.1604	0.6506	1.1510	0.120
C18	0.0813(8)	0.7063(7)	1.2953(5)	0.070(3)
H18a	0.0763	0.7394	1.3387	0.104
H18b	0.1393	0.6468	1.2925	0.104
H18c	0.0194	0.6976	1.2973	0.104
C19	0.0034(7)	0.8616(7)	1.2297(5)	0.068(2)
H19a	-0.0017	0.8938	1.2738	0.102
H19b	-0.0594	0.8552	1.2301	0.102
H19c	0.0150	0.8963	1.1876	0.102
C20	0.2503(8)	1.0066(6)	1.1625(4)	0.066(3)
H20a	0.1915	0.9996	1.1898	0.098
H20b	0.2313	1.0707	1.1504	0.098
H20c	0.3041	0.9867	1.1918	0.098
C21	0.4247(7)	1.1398(6)	0.9721(4)	0.057(2)
H21a	0.4656	1.1602	0.9343	0.076
H21b	0.3539	1.1860	0.9770	0.076
C22	0.4624(11)	1.1348(7)	1.0442(6)	0.099(4)
H22a	0.4568	1.1949	1.0566	0.148
H22b	0.5330	1.0905	1.0395	0.148
H22c	0.4213	1.1160	1.0823	0.148
C23	0.3107(6)	1.1228(5)	0.8544(4)	0.047(2)
H23a	0.3098	1.1817	0.8648	0.071
H23b	0.2547	1.1155	0.8859	0.071
H23c	0.3035	1.1204	0.8039	0.071
C24	0.4982(7)	0.4553(6)	0.8594(4)	0.051(2)
H24a	0.5004	0.4947	0.8183	0.077
H24b	0.4343	0.4493	0.8668	0.077
H24c	0.5545	0.3950	0.8496	0.077
C25	0.6345(6)	0.5190(7)	0.9258(5)	0.062(2)
H25a	0.6358	0.5573	0.8838	0.093
H25b	0.6906	0.4586	0.9165	0.093
H25c	0.6411	0.5471	0.9682	0.093
C26	0.5058(6)	0.4326(5)	1.0255(4)	0.048(2)
C27	0.5852(8)	0.3322(6)	1.0087(6)	0.079(3)
H27a	0.6525	0.3310	0.9941	0.118
H27b	0.5684	0.3069	0.9695	0.118
H27c	0.5847	0.2957	1.0519	0.118
C28	0.3982(8)	0.4343(8)	1.0484(7)	0.094(3)
H28a	0.3483	0.4972	1.0590	0.141
H28b	0.3976	0.3976	1.0915	0.141

H28c	0.3816	0.4092	1.0090	0.141
C29	0.5334(9)	0.4687(7)	1.0913(5)	0.079(3)
H29a	0.4842	0.5314	1.1037	0.118
H29b	0.6010	0.4670	1.0780	0.118
H29c	0.5321	0.4299	1.1329	0.118
C30	0.2725(6)	0.6762(5)	0.8984(4)	0.041(2)
H30a	0.2270	0.6634	0.9371	0.061
H30b	0.3067	0.6241	0.8647	0.061
H30c	0.2335	0.7304	0.8728	0.061
C31	0.1394(7)	0.8987(7)	0.9782(5)	0.072(3)
H31a	0.1132	0.9570	0.9537	0.108
H31b	0.1171	0.9090	1.0304	0.108
H31c	0.1139	0.8580	0.9612	0.108
		Molecule No. 2		
Si1	0.7514(2)	0.2121(2)	0.29831(10)	0.0440(5)
Si2	0.7361(2)	-0.0654(2)	0.55262(12)	0.0503(6)
O1	0.4196(3)	0.5025(3)	0.5299(2)	0.0295(10)
O2	0.3914(4)	0.3917(4)	0.4784(3)	0.0489(14)
O3	0.7045(3)	0.2699(3)	0.3787(2)	0.0330(11)
O4	0.2380(4)	0.5461(3)	0.7037(2)	0.0407(12)
H4	0.1946	0.5983	0.6972	0.061
O5	0.4425(6)	0.2312(4)	0.7773(4)	0.091(2)
O6	0.7153(4)	0.0444(3)	0.5435(2)	0.0444(13)
O7	0.7029(4)	0.2768(3)	0.5544(2)	0.0401(12)
C1	0.6039(5)	0.2925(5)	0.4198(3)	0.032(2)
H1	0.5612	0.2859	0.3869	0.042
C2	0.5583(5)	0.3964(5)	0.4439(3)	0.034(2)
H2	0.6001	0.4035	0.4774	0.045
C3	0.4480(5)	0.4271(4)	0.4846(3)	0.028(2)
C4	0.3175(6)	0.5358(5)	0.5763(3)	0.036(2)
H4a	0.2856	0.4943	0.5688	0.047
C5	0.3325(5)	0.5310(5)	0.6575(3)	0.034(2)
C6	0.4127(5)	0.4332(4)	0.6710(3)	0.0249(14)
H6	0.4795	0.4152	0.6455	0.033
C7	0.3939(6)	0.3727(5)	0.7160(4)	0.041(2)
H7	0.3269	0.3914	0.7410	0.055
C8	0.4693(6)	0.2777(5)	0.7306(4)	0.049(2)
C9	0.5767(6)	0.2410(5)	0.6897(3)	0.040(2)
H9a	0.6240	0.2251	0.7245	0.053
H9b	0.5853	0.2891	0.6583	0.053
C10	0.6040(6)	0.1541(5)	0.6418(4)	0.040(2)
H10a	0.6101	0.1025	0.6742	0.053
H10b	0.5470	0.1659	0.6161	0.053
C11	0.7037(6)	0.1243(4)	0.5843(3)	0.036(2)
C12	0.7004(6)	0.1960(4)	0.5230(3)	0.030(2)
H12	0.7626	0.1674	0.4860	0.040

C13	0.6073(6)	0.2261(5)	0.4841(3)	0.034(2)
H13a	0.5455	0.2560	0.5202	0.046
H13b	0.6056	0.1709	0.4657	0.046
C14	0.7438(7)	0.0971(6)	0.3074(5)	0.068(2)
H14a	0.6729	0.1069	0.3186	0.102
H14b	0.7791	0.0631	0.3463	0.102
H14c	0.7754	0.0623	0.2620	0.102
C15	0.6766(7)	0.2799(8)	0.2249(4)	0.081(3)
H15a	0.6805	0.3388	0.2196	0.121
H15b	0.6059	0.2899	0.2387	0.121
H15c	0.7052	0.2457	0.1791	0.121
C16	0.8887(6)	0.2012(6)	0.2750(4)	0.051(2)
C17	0.9518(7)	0.1343(7)	0.3318(5)	0.069(3)
H17a	0.9500	0.0748	0.3289	0.103
H17b	0.9221	0.1601	0.3806	0.103
H17c	1.0219	0.1268	0.3208	0.103
C18	0.9376(7)	0.1585(9)	0.1983(4)	0.086(3)
H18a	0.9358	0.0990	0.1959	0.130
H18b	1.0078	0.1508	0.1881	0.130
H18c	0.9002	0.1987	0.1627	0.130
C19	0.8910(8)	0.2971(8)	0.2801(5)	0.077(3)
H19a	0.8521	0.3382	0.2455	0.116
H19b	0.9609	0.2900	0.2691	0.116
H19c	0.8613	0.3227	0.3290	0.116
C20	0.5554(7)	0.4616(6)	0.3797(4)	0.054(2)
H20a	0.6238	0.4444	0.3530	0.081
H20b	0.5283	0.5243	0.3982	0.081
H20c	0.5122	0.4574	0.3476	0.081
C21	0.2525(6)	0.6329(6)	0.5501(4)	0.051(2)
H21a	0.2893	0.6715	0.5499	0.068
H21b	0.1886	0.6608	0.5846	0.068
C22	0.2279(7)	0.6311(7)	0.4727(4)	0.076(3)
H22a	0.1883	0.6934	0.4584	0.113
H22b	0.1890	0.5950	0.4730	0.113
H22c	0.2909	0.6037	0.4383	0.113
C23	0.3725(6)	0.6024(5)	0.6748(4)	0.037(2)
H23a	0.3232	0.6641	0.6667	0.056
H23b	0.4369	0.5903	0.6432	0.056
H23c	0.3824	0.5971	0.7253	0.056
C24	0.6833(11)	-0.0913(8)	0.6454(6)	0.107(4)
H24a	0.7195	-0.0825	0.6809	0.160
H24b	0.6915	-0.1546	0.6462	0.160
H24c	0.6115	-0.0504	0.6571	0.160
C25	0.6643(8)	-0.0833(7)	0.4825(6)	0.088(3)
H25a	0.6911	-0.0694	0.4343	0.132
H25b	0.5924	-0.0428	0.4946	0.132

H25c	0.6731	-0.1467	0.4832	0.132
C26	0.8785(6)	-0.1466(6)	0.5261(5)	0.052(2)
C27	0.9395(8)	-0.1573(7)	0.5891(5)	0.082(3)
H27a	0.9325	-0.0973	0.6030	0.122
H27b	1.0109	-0.1968	0.5728	0.122
H27c	0.9130	-0.1844	0.6306	0.122
C28	0.8900(8)	-0.2430(6)	0.5027(6)	0.081(3)
H28a	0.8599	-0.2690	0.5431	0.122
H28b	0.9618	-0.2834	0.4892	0.122
H28c	0.8556	-0.2364	0.4615	0.122
C29	0.9263(7)	-0.1026(7)	0.4611(5)	0.072(3)
H29a	0.9203	-0.0436	0.4768	0.108
H29b	0.8904	-0.0939	0.4204	0.108
H29c	0.9977	-0.1432	0.4463	0.108
C30	0.7979(6)	0.0987(5)	0.6214(4)	0.050(2)
H30a	0.7983	0.0544	0.6592	0.075
H30b	0.7951	0.1535	0.6429	0.075
H30c	0.8593	0.0719	0.5855	0.075
C31	0.7957(6)	0.2899(5)	0.5240(4)	0.043(2)
H31a	0.7935	0.3438	0.5466	0.065
H31b	0.7992	0.2982	0.4719	0.065
H31c	0.8554	0.2362	0.5337	0.065
Molecule No. 3				
Si1	0.7499(3)	0.7114(2)	1.1990(2)	0.0865(9)
Si2	1.0700(2)	0.4488(2)	0.96413(14)	0.0557(6)
O1	0.7960(3)	1.0009(3)	0.9724(2)	0.0351(11)
O2	0.9163(5)	0.9295(5)	1.0454(3)	0.071(2)
O3	0.7435(4)	0.7717(4)	1.1215(2)	0.0509(13)
O4	0.9158(4)	1.0621(3)	0.7968(3)	0.0464(13)
H4	0.8933	1.1183	0.8040	0.070
O5	1.1194(4)	0.7347(4)	0.7361(3)	0.062(2)
O6	0.9824(4)	0.5574(3)	0.9637(2)	0.0398(12)
O7	0.7882(4)	0.7853(3)	0.9295(2)	0.0458(13)
C1	0.8172(6)	0.8047(5)	1.0882(3)	0.038(2)
H1	0.8578	0.8036	1.1257	0.051
C2	0.7579(6)	0.9088(5)	1.0681(4)	0.041(2)
H2	0.7103	0.9126	1.0351	0.055
C3	0.8335(6)	0.9452(6)	1.0288(4)	0.045(2)
C4	0.8621(6)	1.0398(5)	0.9271(3)	0.034(2)
H4a	0.9337	1.0039	0.9341	0.046
C5	0.8523(5)	1.0262(5)	0.8448(3)	0.034(2)
C6	0.8958(5)	0.9233(5)	0.8299(3)	0.033(2)
H6	0.8581	0.8910	0.8521	0.044
C7	0.9867(6)	0.8753(5)	0.7859(4)	0.045(2)
H7	1.0240	0.9079	0.7639	0.060
C8	1.0308(6)	0.7739(5)	0.7707(4)	0.042(2)

C9	0.9691(6)	0.7169(5)	0.7993(3)	0.039(2)
H9a	0.9753	0.6750	0.7607	0.052
H9b	0.8968	0.7585	0.8128	0.052
C10	1.0096(6)	0.6596(6)	0.8679(4)	0.043(2)
H10a	1.0721	0.6048	0.8512	0.057
H10b	1.0267	0.6969	0.8982	0.057
C11	0.9300(6)	0.6288(5)	0.9154(3)	0.033(2)
C12	0.8455(6)	0.7079(5)	0.9711(3)	0.036(2)
H12	0.7984	0.6836	0.9989	0.048
C13	0.8925(6)	0.7394(5)	1.0246(3)	0.036(2)
H13a	0.9318	0.7707	0.9972	0.049
H13b	0.9407	0.6846	1.0457	0.049
C14	0.8718(11)	0.6001(8)	1.1870(7)	0.110(4)
H14a	0.9305	0.6145	1.1811	0.165
H14b	0.8752	0.5666	1.1442	0.165
H14c	0.8718	0.5626	1.2297	0.165
C15	0.7560(10)	0.7817(9)	1.2790(5)	0.093(3)
H15a	0.8182	0.7906	1.2686	0.139
H15b	0.7551	0.7482	1.3239	0.139
H15c	0.6976	0.8410	1.2841	0.139
C16	0.6408(11)	0.6869(8)	1.2097(6)	0.095(3)
C17	0.6262(11)	0.6559(10)	1.1367(6)	0.110(4)
H17a	0.6253	0.7014	1.1000	0.164
H17b	0.5622	0.6500	1.1437	0.164
H17c	0.6820	0.5971	1.1210	0.164
C18	0.634(2)	0.625(2)	1.2767(9)	0.193(8)
H18a	0.6396	0.6525	1.3200	0.290
H18b	0.6893	0.5643	1.2680	0.290
H18c	0.5693	0.6209	1.2837	0.290
C19	0.5393(11)	0.7888(13)	1.2385(7)	0.136(5)
H19a	0.5329	0.8339	1.2006	0.204
H19b	0.5502	0.8109	1.2822	0.204
H19c	0.4774	0.7793	1.2491	0.204
C20	0.6967(7)	0.9689(6)	1.1360(4)	0.056(2)
H20a	0.6477	0.9467	1.1607	0.084
H20b	0.6611	1.0320	1.1218	0.084
H20c	0.7427	0.9660	1.1686	0.084
C21	0.8270(7)	1.1412(5)	0.9501(4)	0.048(2)
H21a	0.8610	1.1699	0.9138	0.063
H21b	0.7534	1.1741	0.9505	0.063
C22	0.8495(9)	1.1518(7)	1.0243(5)	0.078(3)
H22a	0.8252	1.2166	1.0360	0.118
H22b	0.9225	1.1213	1.0239	0.118
H22C	0.8154	1.1243	1.0607	0.118
C23	0.7414(6)	1.0725(5)	0.8328(4)	0.041(2)
H23a	0.7147	1.1382	0.8420	0.062

H23b	0.7013	1.0472	0.8658	0.062
H23c	0.7381	1.0615	0.7829	0.062
C24	1.1704(9)	0.4168(8)	0.8843(7)	0.123(5)
H24a	1.1969	0.4632	0.8766	0.184
H24b	1.1427	0.4124	0.8418	0.184
H24c	1.2249	0.3578	0.8921	0.184
C25	1.1326(10)	0.4462(8)	1.0469(7)	0.106(4)
H25a	1.0814	0.4622	1.0906	0.159
H25b	1.1626	0.4900	1.0405	0.159
H25c	1.1852	0.3849	1.0514	0.159
C26	1.0079(8)	0.3637(7)	0.9865(6)	0.077(2)
C27	0.9811(12)	0.3388(10)	0.9139(6)	0.119(4)
H27a	1.0430	0.3107	0.8786	0.178
H27b	0.9341	0.3945	0.8940	0.178
H27c	0.9498	0.2961	0.9248	0.178
C28	1.0832(8)	0.2754(7)	1.0176(5)	0.083(3)
H28a	1.1469	0.2504	0.9837	0.125
H28b	1.0545	0.2306	1.0249	0.125
H28c	1.0956	0.2897	1.0638	0.125
C29	0.9089(7)	0.4055(7)	1.0370(6)	0.075(3)
H29a	0.8639	0.4615	1.0162	0.113
H29b	0.9204	0.4197	1.0835	0.113
H29c	0.8778	0.3624	1.0440	0.113
C30	0.8777(7)	0.5925(6)	0.8688(4)	0.051(2)
H30a	0.8288	0.5752	0.9004	0.076
H30b	0.9285	0.5392	0.8405	0.076
H30c	0.8427	0.6401	0.8363	0.076
C31	0.6820(7)	0.7997(8)	0.9321(6)	0.082(3)
H31a	0.6483	0.8520	0.9027	0.123
H31b	0.6468	0.8114	0.9821	0.123
H31c	0.6808	0.7452	0.9132	0.123
Molecule No. 4				
Si1	1.2507(2)	0.2643(2)	0.36584(13)	0.0601(7)
Si2	1.2341(3)	0.0448(3)	0.6189(2)	0.1166(14)
O1	0.8314(4)	0.5434(3)	0.5407(2)	0.0415(12)
O2	0.8251(4)	0.4600(4)	0.4468(3)	0.055(2)
O3	1.1564(4)	0.3531(4)	0.4145(3)	0.0490(13)
O4	0.6187(4)	0.5732(3)	0.6935(2)	0.0424(12)
H4	0.5781	0.6261	0.6855	0.064
O5	0.8059(4)	0.2565(4)	0.7748(3)	0.058(2)
O6	1.1647(5)	0.1497(6)	0.5937(4)	0.089(2)
O7	1.0487(5)	0.4047(5)	0.6060(3)	0.073(2)
C1	1.0535(6)	0.3675(5)	0.4433(4)	0.038(2)
H1	1.0294	0.3459	0.4048	0.051
C2	0.9856(6)	0.4718(5)	0.4532(4)	0.049(2)
H2	1.0080	0.4969	0.4905	0.066

C3	0.8711(7)	0.4896(6)	0.4790(4)	0.047(2)
C4	0.7240(6)	0.5657(5)	0.5742(4)	0.036(2)
H4a	0.7040	0.5193	0.5576	0.047
C5	0.7221(6)	0.5579(5)	0.6579(3)	0.036(2)
C6	0.7913(6)	0.4592(5)	0.6755(4)	0.044(2)
H6	0.8599	0.4373	0.6531	0.058
C7	0.7655(6)	0.3996(5)	0.7196(4)	0.038(2)
H7	0.6967	0.4190	0.7407	0.051
C8	0.8370(7)	0.3076(6)	0.7366(4)	0.054(2)
C9	0.9571(8)	0.2905(7)	0.7264(5)	0.085(3)
H9a	0.9649	0.3479	0.7162	0.113
H9b	0.9873	0.2624	0.7695	0.113
C10	1.0026(9)	0.2259(8)	0.6620(5)	0.096(3)
H10a	0.9586	0.2447	0.6247	0.128
H10b	1.0151	0.1627	0.6763	0.128
C11	1.1160(8)	0.2362(9)	0.6318(5)	0.100(3)
C12	1.1042(7)	0.3135(7)	0.5717(4)	0.065(2)
H12	1.1733	0.3068	0.5493	0.086
C13	1.0489(6)	0.3063(5)	0.5100(4)	0.040(2)
H13a	0.9772	0.3227	0.5305	0.053
H13b	1.0790	0.2420	0.4930	0.053
C14	1.3541(8)	0.1985(7)	0.4224(5)	0.071(3)
H14a	1.3264	0.1721	0.4638	0.106
H14b	1.3784	0.2401	0.4394	0.106
H14c	1.4101	0.1497	0.3927	0.106
C15	1.2027(8)	0.1833(8)	0.3336(5)	0.082(3)
H15a	1.1752	0.1573	0.3754	0.123
H15b	1.2586	0.1341	0.3041	0.123
H15c	1.1498	0.2167	0.3048	0.123
C16	1.3026(8)	0.3135(9)	0.2868(5)	0.079(3)
C17	1.4113(9)	0.2332(11)	0.2438(6)	0.113(4)
H17a	1.3998	0.1811	0.2309	0.169
H17b	1.4622	0.2131	0.2755	0.169
H17c	1.4352	0.2585	0.1999	0.169
C18	1.2206(10)	0.3564(11)	0.2294(5)	0.112(4)
H18a	1.2028	0.3089	0.2149	0.168
H18b	1.2513	0.3785	0.1868	0.168
H18c	1.1596	0.4070	0.2530	0.168
C19	1.3272(8)	0.3963(8)	0.3076(5)	0.078(3)
H19a	1.2655	0.4449	0.3326	0.116
H19b	1.3529	0.4201	0.2636	0.116
H19c	1.3782	0.3741	0.3393	0.116
C20	0.9910(8)	0.5248(7)	0.3808(5)	0.089(3)
H20a	0.9484	0.5899	0.3895	0.133
H20b	0.9672	0.5018	0.3444	0.133
H20c	1.0610	0.5154	0.3634	0.133

C21	0.6549(7)	0.6629(5)	0.5472(4)	0.052(2)
H21a	0.5870	0.6833	0.5769	0.069
H21b	0.6828	0.7060	0.5569	0.069
C22	0.6431(10)	0.6704(8)	0.4718(6)	0.103(4)
H22a	0.5992	0.7334	0.4621	0.154
H22b	0.6128	0.6302	0.4613	0.154
H22c	0.7093	0.6526	0.4413	0.154
C23	0.7597(6)	0.6230(5)	0.6888(4)	0.047(2)
H23a	0.7165	0.6863	0.6788	0.071
H23b	0.8294	0.6084	0.6659	0.071
H23c	0.7566	0.6153	0.7410	0.071
C24	1.1823(11)	0.0191(12)	0.7135(8)	0.164(6)
H24a	1.1865	0.0589	0.7488	0.246
H24b	1.2222	-0.0446	0.7244	0.246
H24c	1.1118	0.0297	0.7158	0.246
C25	1.3715(8)	0.0266(9)	0.6198(6)	0.098(4)
H25a	1.4005	0.0403	0.5723	0.146
H25b	1.4117	-0.0368	0.6313	0.146
H25c	1.3720	0.0671	0.6563	0.146
C26	1.2263(12)	-0.0281(10)	0.5495(8)	0.145(4)
C27	1.276(2)	-0.1328(13)	0.569(2)	0.232(8)
H27a	1.2380	-0.1429	0.6142	0.349
H27b	1.3461	-0.1501	0.5755	0.349
H27c	1.2754	-0.1698	0.5303	0.349
C28	1.2959(14)	-0.0237(12)	0.4757(9)	0.155(5)
H28a	1.3637	-0.0371	0.4849	0.233
H28b	1.2667	0.0373	0.4558	0.233
H28c	1.3001	-0.0687	0.4411	0.233
C29	1.1172(14)	-0.006(2)	0.5375(14)	0.224(8)
H29a	1.0769	-0.0115	0.5831	0.335
H29b	1.1198	-0.0490	0.5018	0.335
H29c	1.0862	0.0561	0.5199	0.335
C30	1.1890(11)	0.2435(12)	0.6813(7)	0.156(6)
H30a	1.1965	0.1994	0.7202	0.234
H30b	1.1603	0.3051	0.7022	0.234
H30c	1.2552	0.2303	0.6521	0.234
C31	1.1044(10)	0.4597(12)	0.6077(6)	0.128(6)
H31a	1.0589	0.5188	0.6309	0.192
H31b	1.1321	0.4691	0.5583	0.192
H31c	1.1596	0.4284	0.6351	0.192

$U_{eq}={}^{1}/_{3}[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$

Table 3. Refined Thermal Parameters (U's) for Compound 99085

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Molecule No. 1						
Si1	0.065(2)	0.053(2)	0.0421(12)	0.0038(10)	0.0019(11)	-0.0297(13)
Si2	0.0366(13)	0.0348(12)	0.0403(11)	0.0009(9)	-0.0057(9)	-0.0139(10)
O1	0.034(3)	0.025(3)	0.042(3)	0.003(2)	-0.001(2)	-0.007(2)
O2	0.039(3)	0.048(3)	0.066(3)	0.029(3)	-0.015(3)	-0.016(3)
O3	0.051(3)	0.049(3)	0.049(3)	-0.002(2)	0.005(2)	-0.030(3)
O4	0.049(3)	0.021(3)	0.059(3)	-0.004(2)	0.011(2)	-0.014(2)
O5	0.082(4)	0.036(3)	0.045(3)	-0.004(2)	0.015(3)	-0.023(3)
O6	0.043(3)	0.030(3)	0.037(2)	0.003(2)	-0.002(2)	-0.014(2)
O7	0.037(3)	0.033(3)	0.036(3)	0.000(2)	-0.002(2)	0.002(2)
C1	0.044(5)	0.032(4)	0.030(3)	0.004(3)	0.003(3)	-0.019(4)
C2	0.031(4)	0.027(4)	0.047(4)	-0.010(3)	0.007(3)	-0.003(3)
C3	0.044(4)	0.023(4)	0.035(4)	-0.003(3)	-0.001(3)	-0.017(4)
C4	0.030(4)	0.029(4)	0.045(4)	0.004(3)	-0.005(3)	-0.014(3)
C5	0.032(4)	0.020(4)	0.047(4)	0.002(3)	-0.002(3)	-0.010(3)
C6	0.050(5)	0.031(4)	0.031(3)	0.015(3)	-0.009(3)	-0.022(4)
C7	0.056(5)	0.026(4)	0.034(4)	0.012(3)	0.006(3)	-0.011(4)
C8	0.061(5)	0.026(4)	0.034(4)	0.005(3)	-0.005(4)	-0.006(4)
C9	0.059(5)	0.020(4)	0.030(3)	0.000(3)	-0.007(3)	-0.011(4)
C10	0.046(5)	0.024(4)	0.027(3)	0.000(2)	-0.001(3)	-0.011(3)
C11	0.046(5)	0.033(4)	0.021(3)	0.009(3)	-0.009(3)	-0.020(3)
C12	0.028(4)	0.033(4)	0.044(4)	-0.001(3)	-0.002(3)	-0.006(3)
C13	0.048(5)	0.034(4)	0.038(4)	-0.004(3)	-0.005(3)	-0.023(4)
C14	0.061(6)	0.066(6)	0.089(7)	0.015(5)	-0.014(5)	-0.009(5)
C15	0.107(8)	0.089(7)	0.053(5)	0.007(4)	-0.010(5)	-0.064(6)
C16	0.068(5)	0.056(5)	0.063(5)	0.011(4)	-0.001(4)	-0.040(4)
C17	0.086(7)	0.111(8)	0.064(5)	-0.002(5)	0.010(5)	-0.069(7)
C18	0.077(7)	0.077(7)	0.067(5)	0.021(4)	-0.002(5)	-0.049(6)
C19	0.059(5)	0.072(6)	0.082(6)	0.001(4)	-0.003(5)	-0.040(4)
C20	0.097(7)	0.032(5)	0.058(5)	-0.013(3)	0.026(5)	-0.030(5)
C21	0.077(7)	0.041(5)	0.060(5)	-0.004(4)	-0.004(4)	-0.033(5)
C22	0.176(13)	0.062(7)	0.107(8)	0.015(6)	-0.068(8)	-0.081(8)
C23	0.053(5)	0.036(4)	0.051(4)	0.013(3)	-0.023(4)	-0.014(4)
C24	0.046(5)	0.043(5)	0.062(5)	-0.012(4)	-0.006(4)	-0.016(4)
C25	0.041(5)	0.078(7)	0.079(6)	0.002(5)	-0.010(4)	-0.037(5)
C26	0.037(4)	0.033(4)	0.066(4)	0.003(3)	-0.009(4)	-0.008(4)
C27	0.085(7)	0.035(5)	0.098(7)	0.000(4)	-0.025(6)	-0.005(5)
C28	0.067(6)	0.076(7)	0.132(9)	0.058(7)	0.004(6)	-0.037(5)
C29	0.118(9)	0.051(6)	0.055(5)	0.015(4)	-0.035(6)	-0.018(6)
C30	0.055(5)	0.038(5)	0.031(4)	-0.002(3)	-0.005(3)	-0.022(4)

C31	0.043(5)	0.068(7)	0.080(6)	-0.011(5)	-0.014(5)	0.004(5)
Molecule No. 2						
Si1	0.0365(13)	0.0512(14)	0.0323(11)	-0.0067(9)	0.0006(9)	-0.0083(11)
Si2	0.0489(14)	0.0275(12)	0.0638(14)	-0.0047(9)	0.0136(11)	-0.0139(11)
O1	0.032(3)	0.025(3)	0.028(2)	0.003(2)	-0.003(2)	-0.010(2)
O2	0.031(3)	0.046(3)	0.070(3)	-0.025(3)	-0.002(3)	-0.016(3)
O3	0.030(3)	0.034(3)	0.029(2)	0.000(2)	-0.001(2)	-0.009(2)
O4	0.031(3)	0.027(3)	0.048(3)	-0.004(2)	0.005(2)	-0.001(2)
O5	0.110(5)	0.026(3)	0.093(4)	0.020(3)	0.037(4)	-0.008(3)
O6	0.069(4)	0.021(3)	0.034(2)	-0.002(2)	0.009(2)	-0.017(3)
O7	0.058(3)	0.029(3)	0.041(3)	0.003(2)	-0.011(2)	-0.025(3)
C1	0.028(4)	0.031(4)	0.037(4)	0.002(3)	-0.009(3)	-0.012(3)
C2	0.031(4)	0.043(4)	0.031(4)	0.002(3)	-0.002(3)	-0.019(3)
C3	0.033(4)	0.021(4)	0.031(3)	0.001(3)	-0.009(3)	-0.009(3)
C4	0.039(4)	0.023(4)	0.035(3)	0.000(3)	-0.002(3)	-0.006(3)
C5	0.031(4)	0.024(4)	0.034(3)	-0.004(3)	0.006(3)	-0.005(3)
C6	0.015(3)	0.024(3)	0.030(3)	-0.005(3)	0.009(3)	-0.008(3)
C7	0.052(5)	0.020(3)	0.045(4)	-0.001(3)	0.008(4)	-0.013(3)
C8	0.061(5)	0.024(4)	0.044(4)	-0.001(3)	0.012(4)	-0.010(4)
C9	0.056(5)	0.020(4)	0.027(3)	0.008(2)	-0.004(3)	-0.002(3)
C10	0.050(4)	0.029(4)	0.036(4)	0.008(3)	-0.002(3)	-0.016(4)
C11	0.052(5)	0.017(4)	0.034(4)	-0.001(2)	-0.006(3)	-0.009(3)
C12	0.039(4)	0.019(4)	0.032(3)	-0.002(2)	0.003(3)	-0.015(3)
C13	0.044(5)	0.039(4)	0.030(3)	-0.001(3)	-0.007(3)	-0.026(4)
C14	0.061(6)	0.060(5)	0.079(6)	-0.030(4)	-0.005(5)	-0.021(5)
C15	0.058(6)	0.134(9)	0.043(5)	0.006(5)	-0.023(4)	-0.028(6)
C16	0.033(4)	0.068(6)	0.046(4)	-0.004(4)	-0.007(3)	-0.015(4)
C17	0.039(5)	0.081(7)	0.071(5)	0.003(5)	-0.014(4)	-0.010(5)
C18	0.045(6)	0.144(10)	0.042(4)	-0.028(5)	0.021(4)	-0.020(6)
C19	0.072(7)	0.095(7)	0.076(6)	0.013(5)	-0.006(5)	-0.049(6)
C20	0.058(6)	0.041(5)	0.049(4)	0.016(3)	0.005(4)	-0.015(4)
C21	0.048(5)	0.047(5)	0.033(4)	0.013(3)	0.003(4)	0.000(4)
C22	0.060(6)	0.096(8)	0.042(5)	0.015(4)	-0.015(4)	-0.004(6)
C23	0.042(5)	0.027(4)	0.040(4)	-0.003(3)	-0.001(3)	-0.013(4)
C24	0.150(10)	0.062(7)	0.096(6)	-0.002(5)	0.061(6)	-0.063(8)
C25	0.076(7)	0.055(7)	0.148(8)	-0.006(6)	-0.037(7)	-0.035(6)
C26	0.042(4)	0.031(4)	0.072(5)	-0.009(4)	0.000(4)	-0.007(4)
C27	0.074(6)	0.053(6)	0.083(6)	-0.011(5)	-0.017(5)	0.010(5)
C28	0.079(7)	0.026(5)	0.114(8)	-0.022(4)	0.001(6)	-0.002(4)
C29	0.046(5)	0.066(6)	0.084(6)	-0.001(5)	0.018(5)	-0.015(5)
C30	0.056(5)	0.034(5)	0.043(4)	-0.001(3)	-0.005(4)	-0.004(4)
C31	0.046(5)	0.042(5)	0.051(4)	0.007(3)	-0.015(4)	-0.024(4)
Molecule No. 3						
Si1	0.117(3)	0.082(2)	0.062(2)	0.024(2)	-0.004(2)	-0.051(2)

Si2	0.0390(14)	0.0346(13)	0.084(2)	0.0029(11)	0.0009(12)	-0.0112(11)
O1	0.035(3)	0.030(3)	0.033(2)	0.004(2)	-0.004(2)	-0.007(2)
O2	0.063(4)	0.096(5)	0.074(4)	0.046(3)	-0.039(3)	-0.047(4)
O3	0.061(3)	0.056(3)	0.038(3)	0.005(2)	0.003(2)	-0.032(3)
O4	0.049(3)	0.026(3)	0.054(3)	0.013(2)	0.004(2)	-0.013(3)
O5	0.054(4)	0.027(3)	0.074(4)	-0.002(3)	0.022(3)	-0.001(3)
O6	0.043(3)	0.031(3)	0.042(3)	0.004(2)	-0.007(2)	-0.014(2)
O7	0.033(3)	0.041(3)	0.042(3)	0.005(2)	-0.005(2)	0.004(2)
C1	0.054(5)	0.042(4)	0.023(3)	0.001(3)	-0.007(3)	-0.024(4)
C2	0.039(4)	0.045(4)	0.032(4)	0.001(3)	-0.001(3)	-0.012(3)
C3	0.043(5)	0.046(5)	0.040(4)	0.012(3)	-0.009(3)	-0.015(4)
C4	0.032(4)	0.031(4)	0.039(3)	0.007(3)	-0.004(3)	-0.013(3)
C5	0.028(4)	0.029(4)	0.032(3)	0.002(3)	0.002(3)	-0.004(3)
C6	0.032(4)	0.029(4)	0.033(4)	0.007(3)	0.000(3)	-0.012(3)
C7	0.050(5)	0.030(4)	0.044(4)	0.003(3)	0.016(4)	-0.016(3)
C8	0.035(4)	0.028(4)	0.042(4)	0.001(3)	0.002(3)	0.002(3)
C9	0.054(5)	0.020(4)	0.032(4)	-0.002(3)	-0.003(3)	-0.007(3)
C10	0.033(4)	0.043(5)	0.050(4)	0.004(3)	-0.010(3)	-0.012(4)
C11	0.044(4)	0.032(4)	0.024(3)	0.004(2)	-0.003(3)	-0.018(3)
C12	0.041(4)	0.032(4)	0.033(4)	0.010(3)	-0.008(3)	-0.014(3)
C13	0.045(5)	0.023(4)	0.032(4)	0.002(3)	-0.005(3)	-0.006(3)
C14	0.139(8)	0.076(7)	0.112(9)	0.031(5)	-0.059(8)	-0.030(6)
C15	0.125(10)	0.130(9)	0.051(5)	0.022(5)	-0.036(6)	-0.075(8)
C16	0.138(8)	0.086(7)	0.088(7)	0.026(5)	-0.031(7)	-0.070(6)
C17	0.150(12)	0.149(12)	0.081(6)	-0.006(6)	0.000(7)	-0.118(11)
C18	0.23(2)	0.26(2)	0.169(12)	0.15(2)	-0.08(2)	-0.19(2)
C19	0.102(7)	0.183(12)	0.104(9)	-0.027(8)	0.013(8)	-0.051(8)
C20	0.068(6)	0.045(5)	0.042(4)	-0.001(3)	-0.003(4)	-0.014(4)
C21	0.054(5)	0.037(4)	0.046(4)	-0.007(3)	-0.002(4)	-0.015(4)
C22	0.110(9)	0.050(6)	0.077(6)	-0.005(4)	-0.027(6)	-0.031(6)
C23	0.040(4)	0.040(5)	0.034(4)	0.014(3)	-0.015(3)	-0.006(4)
C24	0.095(8)	0.054(7)	0.142(8)	0.027(6)	0.060(7)	0.009(6)
C25	0.091(9)	0.076(8)	0.146(8)	0.025(7)	-0.078(8)	-0.011(7)
C26	0.084(7)	0.045(5)	0.095(6)	0.003(4)	0.011(5)	-0.031(5)
C27	0.173(14)	0.104(10)	0.107(8)	-0.015(7)	-0.018(7)	-0.085(10)
C28	0.093(7)	0.041(5)	0.092(7)	0.014(5)	0.020(5)	-0.021(5)
C29	0.060(6)	0.071(7)	0.099(7)	-0.003(5)	0.009(5)	-0.040(5)
C30	0.051(5)	0.049(5)	0.054(5)	-0.004(4)	-0.011(4)	-0.021(4)
C31	0.045(5)	0.087(8)	0.087(7)	-0.036(6)	-0.029(5)	0.009(5)
Molecule no. 4						
Si1	0.056(2)	0.067(2)	0.0595(14)	-0.0077(12)	-0.0087(12)	-0.0273(14)
Si2	0.070(2)	0.124(3)	0.165(3)	0.101(3)	-0.050(2)	-0.050(2)
O1	0.049(3)	0.043(3)	0.038(3)	0.002(2)	0.004(2)	-0.028(3)
O2	0.058(4)	0.050(4)	0.054(3)	-0.009(3)	-0.009(3)	-0.021(3)

O3	0.042(3)	0.062(4)	0.045(3)	-0.011(2)	0.000(2)	-0.025(3)
O4	0.041(3)	0.029(3)	0.050(3)	0.004(2)	0.001(2)	-0.011(2)
O5	0.061(4)	0.030(3)	0.068(3)	0.011(2)	0.002(3)	-0.011(3)
O6	0.058(4)	0.111(4)	0.107(4)	0.074(3)	-0.034(3)	-0.045(3)
O7	0.067(4)	0.123(5)	0.055(3)	-0.022(3)	-0.002(3)	-0.065(4)
C1	0.041(4)	0.047(4)	0.039(4)	-0.002(3)	-0.009(3)	-0.030(3)
C2	0.057(4)	0.033(4)	0.052(4)	-0.003(3)	0.017(4)	-0.023(4)
C3	0.062(5)	0.035(5)	0.040(4)	0.012(3)	0.002(4)	-0.023(4)
C4	0.044(4)	0.025(4)	0.045(4)	0.008(3)	-0.007(3)	-0.022(3)
C5	0.046(4)	0.027(4)	0.033(3)	0.001(3)	-0.002(3)	-0.016(3)
C6	0.038(4)	0.041(4)	0.045(4)	0.012(3)	-0.001(3)	-0.013(3)
C7	0.031(4)	0.041(4)	0.040(4)	0.004(3)	0.007(3)	-0.018(3)
C8	0.074(5)	0.044(5)	0.051(5)	0.027(4)	-0.029(4)	-0.026(4)
C9	0.092(5)	0.052(5)	0.099(6)	0.008(4)	-0.041(5)	-0.011(4)
C10	0.141(6)	0.071(6)	0.072(5)	0.014(4)	-0.007(5)	-0.047(5)
C11	0.068(6)	0.138(5)	0.076(5)	0.053(5)	-0.036(4)	-0.022(5)
C12	0.042(5)	0.112(6)	0.050(5)	0.021(4)	-0.018(4)	-0.040(5)
C13	0.032(4)	0.040(4)	0.050(4)	0.006(3)	-0.014(3)	-0.014(4)
C14	0.071(6)	0.074(7)	0.075(6)	-0.003(5)	-0.034(5)	-0.029(5)
C15	0.077(7)	0.106(8)	0.077(6)	-0.017(5)	-0.019(5)	-0.046(6)
C16	0.055(6)	0.117(8)	0.073(6)	0.006(5)	-0.021(4)	-0.042(6)
C17	0.077(7)	0.167(11)	0.084(7)	-0.043(7)	0.028(5)	-0.051(7)
C18	0.122(9)	0.169(13)	0.053(6)	0.025(6)	-0.037(6)	-0.062(9)
C19	0.082(7)	0.104(8)	0.065(6)	0.017(5)	-0.008(5)	-0.061(7)
C20	0.083(7)	0.053(6)	0.080(6)	0.020(5)	0.047(5)	-0.007(5)
C21	0.066(5)	0.026(4)	0.065(5)	0.020(3)	-0.028(4)	-0.016(4)
C22	0.135(11)	0.058(7)	0.079(6)	0.016(5)	-0.013(7)	-0.011(7)
C23	0.054(5)	0.043(5)	0.043(4)	0.004(3)	-0.010(4)	-0.019(4)
C24	0.107(9)	0.187(13)	0.183(8)	0.147(8)	-0.024(8)	-0.065(9)
C25	0.067(6)	0.120(9)	0.110(8)	0.046(7)	-0.034(6)	-0.041(6)
C26	0.143(8)	0.127(6)	0.221(8)	0.079(6)	-0.078(6)	-0.102(7)
C27	0.28(2)	0.139(8)	0.32(2)	0.087(9)	-0.110(14)	-0.113(11)
C28	0.191(12)	0.121(11)	0.208(9)	-0.003(8)	-0.064(8)	-0.105(10)
C29	0.166(10)	0.25(2)	0.32(2)	0.027(14)	-0.098(11)	-0.134(11)
C30	0.120(9)	0.181(12)	0.111(9)	-0.001(8)	-0.088(8)	0.017(8)
C31	0.118(11)	0.23(2)	0.093(8)	-0.069(9)	0.005(7)	-0.131(12)

The form of the anisotropic displacement parameter is:
$ep[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

Table 4. Bond Distances in Compound 99085, Å

Molecule no. 1					
Si1-O3	1.663(5)	Si1-C14	1.854(10)	Si1-C15	1.869(9)
Si1-C16	1.898(9)	Si2-O6	1.666(5)	Si2-C24	1.856(7)
Si2-C26	1.877(8)	Si2-C25	1.882(8)	O1-C3	1.354(8)
O1-C4	1.472(8)	O2-C3	1.190(8)	O3-C1	1.437(9)
O4-C5	1.430(8)	O5-C8	1.218(9)	O6-C11	1.462(8)
O7-C12	1.421(8)	O7-C31	1.436(10)	C1-C13	1.543(10)
C1-C2	1.569(10)	C2-C3	1.526(10)	C2-C20	1.548(10)
C4-C5	1.526(10)	C4-C21	1.545(10)	C5-C6	1.534(10)
C5-C23	1.540(10)	C6-C7	1.334(10)	C7-C8	1.469(11)
C8-C9	1.501(11)	C9-C10	1.572(9)	C10-C11	1.531(10)
C11-C30	1.517(9)	C11-C12	1.577(10)	C12-C13	1.518(9)
C16-C18	1.558(11)	C16-C17	1.569(13)	C16-C19	1.566(13)
C21-C22	1.510(12)	C26-C27	1.531(12)	C26-C28	1.536(13)
C26-C29	1.552(12)				
Molecule no. 2					
Si1-O3	1.666(5)	Si1-C14	1.873(10)	Si1-C15	1.880(8)
Si1-C16	1.902(8)	Si2-O6	1.644(5)	Si2-C24	1.849(9)
Si2-C25	1.901(10)	Si2-C26	1.908(8)	O1-C3	1.370(8)
O1-C4	1.469(8)	O2-C3	1.201(8)	O3-C1	1.428(8)
O4-C5	1.417(8)	O5-C8	1.222(9)	O6-C11	1.445(8)
O7-C12	1.454(8)	O7-C31	1.463(9)	C1-C13	1.536(9)
C1-C2	1.553(10)	C2-C3	1.526(10)	C2-C20	1.523(10)
C4-C21	1.532(10)	C4-C5	1.544(9)	C5-C6	1.537(9)
C5-C23	1.547(10)	C6-C7	1.319(9)	C7-C8	1.486(10)
C8-C9	1.488(11)	C9-C10	1.547(10)	C10-C11	1.546(10)
C11-C30	1.527(10)	C11-C12	1.551(9)	C12-C13	1.526(9)
C16-C18	1.522(11)	C16-C19	1.547(14)	C16-C17	1.567(12)
C21-C22	1.537(11)	C26-C27	1.540(12)	C26-C28	1.547(12)
C26-C29	1.560(12)				
Molecule No. 3					
Si1-O3	1.668(6)	Si1-C16	1.764(13)	Si1-C14	1.889(13)
Si1-C15	1.937(10)	Si2-O6	1.654(5)	Si2-C24	1.806(11)
Si2-C25	1.899(10)	Si2-C26	1.912(10)	O1-C3	1.360(8)
O1-C4	1.473(8)	O2-C3	1.212(8)	O3-C1	1.417(9)
O4-C5	1.436(8)	O5-C8	1.237(9)	O6-C11	1.433(8)
O7-C12	1.429(8)	O7-C31	1.454(11)	C1-C13	1.542(10)
C1-C2	1.566(10)	C2-C3	1.512(11)	C2-C20	1.516(10)
C4-C21	1.530(10)	C4-C5	1.585(9)	C5-C6	1.504(10)
C5-C23	1.513(10)	C6-C7	1.353(10)	C7-C8	1.482(10)
C8-C9	1.542(11)	C9-C10	1.565(9)	C10-C11	1.557(10)
C11-C30	1.518(10)	C11-C12	1.594(10)	C12-C13	1.509(9)
C16-C18	1.55(2)	C16-C17	1.54(2)	C16-C19	1.70(2)
C21-C22	1.497(11)	C26-C29	1.474(13)	C26-C28	1.523(14)

C26-C27	1.574(14)				
Molecule No. 4					
Si1-O3	1.658(6)	Si1-C16	1.815(11)	Si1-C15	1.868(10)
Si1-C14	1.880(9)	Si2-O6	1.633(7)	Si2-C26	1.824(14)
Si2-C24	1.870(11)	Si2-C25	1.897(10)	O1-C3	1.351(9)
O1-C4	1.472(9)	O2-C3	1.208(9)	O3-C1	1.421(9)
O4-C5	1.455(9)	O5-C8	1.222(9)	O6-C11	1.412(12)
O7-C31	1.426(13)	O7-C12	1.444(12)	C1-C2	1.529(11)
C1-C13	1.535(10)	C2-C20	1.547(11)	C2-C3	1.555(12)
C4-C5	1.538(9)	C4-C21	1.554(9)	C5-C6	1.515(10)
C5-C23	1.532(10)	C6-C7	1.345(10)	C7-C8	1.445(11)
C8-C9	1.628(12)	C9-C10	1.480(12)	C10-C11	1.719(13)
C11-C30	1.559(13)	C11-C12	1.582(11)	C12-C13	1.539(10)
C16-C19	1.58(2)	C16-C18	1.637(14)	C16-C17	1.65(2)
C21-C22	1.423(12)	C26-C29	1.53(2)	C26-C27	1.56(2)
C26-C28	1.57(2)				

Table 5. Bond Angles in Compound 99085, °

Molecule No. 1					
O3-Si1-C14	113.8(4)	O3-Si1-C15	110.3(4)	C14-Si1-C15	109.9(5)
O3-Si1-C16	104.0(3)	C14-Si1-C16	107.5(5)	C15-Si1-C16	111.2(5)
O6-Si2-C24	113.5(3)	O6-Si2-C26	103.3(3)	C24-Si2-C26	111.2(4)
O6-Si2-C25	111.0(4)	C24-Si2-C25	108.0(4)	C26-Si2-C25	109.8(4)
C3-O1-C4	118.6(5)	C1-O3-Si1	126.3(5)	C11-O6-Si2	135.5(4)
C12-O7-C31	115.7(6)	O3-C1-C13	109.6(6)	O3-C1-C2	107.0(6)
C13-C1-C2	114.8(5)	C3-C2-C20	108.6(6)	C3-C2-C1	109.8(6)
C20-C2-C1	110.0(6)	O2-C3-O1	125.1(6)	O2-C3-C2	124.5(6)
O1-C3-C2	110.4(6)	O1-C4-C5	108.7(5)	O1-C4-C21	108.0(6)
C5-C4-C21	114.7(6)	O4-C5-C4	107.8(5)	O4-C5-C6	106.9(5)
C4-C5-C6	111.3(5)	O4-C5-C23	111.9(6)	C4-C5-C23	111.6(6)
C6-C5-C23	107.3(6)	C7-C6-C5	124.9(7)	C6-C7-C8	124.8(7)
O5-C8-C7	119.8(7)	O5-C8-C9	118.6(7)	C7-C8-C9	121.5(7)
C8-C9-C10	109.9(6)	C11-C10-C9	116.6(6)	O6-C11-C30	107.9(5)
O6-C11-C10	108.4(5)	C30-C11-C10	112.1(5)	O6-C11-C12	103.7(5)
C30-C11-C12	111.5(6)	C10-C11-C12	112.8(6)	O7-C12-C13	110.3(6)
O7-C12-C11	108.3(5)	C13-C12-C11	115.0(6)	C12-C13-C1	116.6(6)
C18-C16-C17	110.2(7)	C18-C16-C19	110.8(8)	C17-C16-C19	109.2(8)
C18-C16-Si1	107.7(6)	C17-C16-Si1	109.9(6)	C19-C16-Si1	109.1(6)
C22-C21-C4	113.7(7)	C27-C26-C28	109.3(8)	C27-C26-C29	107.5(7)
C28-C26-C29	108.6(9)	C27-C26-Si2	110.6(6)	C28-C26-Si2	110.8(6)
C29-C26-Si2	109.9(6)				
Molecule No. 2					
O3-Si1-C14	109.9(3)	O3-Si1-C15	110.8(4)	C14-Si1-C15	108.9(5)
O3-Si1-C16	104.5(3)	C14-Si1-C16	113.2(4)	C15-Si1-C16	109.4(4)
O6-Si2-C24	112.9(4)	O6-Si2-C25	103.4(4)	C24-Si2-C25	109.2(6)
O6-Si2-C26	111.9(3)	C24-Si2-C26	111.0(5)	C25-Si2-C26	108.0(4)
C3-O1-C4	117.2(5)	C1-O3-Si1	125.4(4)	C11-O6-Si2	142.3(4)
C12-O7-C31	112.9(5)	O3-C1-C13	111.2(5)	O3-C1-C2	107.2(5)
C13-C1-C2	113.8(5)	C3-C2-C20	107.3(6)	C3-C2-C1	110.1(6)
C20-C2-C1	113.4(6)	O2-C3-O1	123.0(6)	O2-C3-C2	125.7(6)
O1-C3-C2	111.3(6)	O1-C4-C21	107.2(5)	O1-C4-C5	108.0(5)
C21-C4-C5	115.2(6)	O4-C5-C6	108.6(5)	O4-C5-C4	109.1(6)
C6-C5-C4	108.3(5)	O4-C5-C23	111.1(5)	C6-C5-C23	108.4(5)
C4-C5-C23	111.2(6)	C7-C6-C5	124.8(6)	C6-C7-C8	126.5(7)
O5-C8-C7	119.3(7)	O5-C8-C9	120.8(7)	C7-C8-C9	119.9(6)
C8-C9-C10	112.4(6)	C11-C10-C9	116.0(6)	O6-C11-C30	109.2(6)
O6-C11-C10	108.3(6)	C30-C11-C10	111.2(5)	O6-C11-C12	102.6(5)
C30-C11-C12	110.8(6)	C10-C11-C12	114.2(6)	O7-C12-C13	110.0(5)
O7-C12-C11	109.1(5)	C13-C12-C11	113.8(6)	C12-C13-C1	115.8(6)
C18-C16-C19	110.3(8)	C18-C16-C17	108.2(8)	C19-C16-C17	109.5(7)
C18-C16-Si1	110.3(6)	C19-C16-Si1	110.7(6)	C17-C16-Si1	107.8(6)
C4-C21-C22	112.6(7)	C27-C26-C28	109.8(7)	C27-C26-C29	106.2(7)

C28-C26-C29	110.3(7)	C27-C26-Si2	112.3(6)	C28-C26-Si2	109.8(6)
C29-C26-Si2	108.2(6)				
Molecule no. 3					
O3-Si1-C16	103.9(4)	O3-Si1-C14	109.7(4)	C16-Si1-C14	110.4(6)
O3-Si1-C15	110.1(4)	C16-Si1-C15	115.5(6)	C14-Si1-C15	107.1(6)
O6-Si2-C24	113.7(4)	O6-Si2-C25	103.8(4)	C24-Si2-C25	107.1(7)
O6-Si2-C26	111.6(4)	C24-Si2-C26	114.7(6)	C25-Si2-C26	104.9(5)
C3-O1-C4	117.9(5)	C1-O3-Si1	125.2(5)	C11-O6-Si2	142.4(4)
C12-O7-C31	113.8(7)	O3-C1-C13	111.1(6)	O3-C1-C2	108.0(6)
C13-C1-C2	116.1(5)	C3-C2-C20	109.2(7)	C3-C2-C1	109.6(6)
C20-C2-C1	111.7(6)	O2-C3-O1	123.4(7)	O2-C3-C2	125.4(6)
O1-C3-C2	111.2(7)	O1-C4-C21	109.6(6)	O1-C4-C5	104.8(5)
C21-C4-C5	114.1(5)	O4-C5-C6	107.9(5)	O4-C5-C23	111.7(5)
C6-C5-C23	110.2(6)	O4-C5-C4	108.1(5)	C6-C5-C4	107.2(5)
C23-C5-C4	111.6(6)	C7-C6-C5	123.3(6)	C6-C7-C8	124.1(7)
O5-C8-C7	119.1(7)	O5-C8-C9	120.0(6)	C7-C8-C9	120.8(6)
C8-C9-C10	110.6(6)	C11-C10-C9	113.0(6)	O6-C11-C30	109.3(6)
O6-C11-C10	108.5(6)	C30-C11-C10	112.4(5)	O6-C11-C12	102.8(5)
C30-C11-C12	109.9(6)	C10-C11-C12	113.4(6)	O7-C12-C13	109.5(6)
O7-C12-C11	108.7(5)	C13-C12-C11	112.4(6)	C12-C13-C1	116.6(6)
C18-C16-C17	115.8(12)	C18-C16-C19	100.6(13)	C17-C16-C19	108.9(10)
C18-C16-Si1	113.1(9)	C17-C16-Si1	112.0(9)	C19-C16-Si1	105.1(8)
C22-C21-C4	113.2(7)	C29-C26-C28	111.6(8)	C29-C26-C27	105.3(9)
C28-C26-C27	109.4(10)	C29-C26-Si2	111.9(7)	C28-C26-Si2	109.4(7)
C27-C26-Si2	109.1(7)				
Molecule No. 4					
O3-Si1-C16	106.5(5)	O3-Si1-C15	111.7(4)	C16-Si1-C15	109.5(5)
O3-Si1-C14	110.2(4)	C16-Si1-C14	109.7(5)	C15-Si1-C14	109.2(5)
O6-Si2-C26	102.8(6)	O6-Si2-C24	112.4(6)	C26-Si2-C24	111.3(8)
O6-Si2-C25	111.3(5)	C26-Si2-C25	112.2(7)	C24-Si2-C25	106.9(6)
C3-O1-C4	118.0(6)	C1-O3-Si1	130.0(5)	C11-O6-Si2	132.3(6)
C31-O7-C12	117.5(8)	O3-C1-C2	109.3(6)	O3-C1-C13	111.5(6)
C2-C1-C13	117.1(6)	C1-C2-C20	112.1(6)	C1-C2-C3	110.2(6)
C20-C2-C3	107.3(7)	O2-C3-O1	125.8(7)	O2-C3-C2	123.8(7)
O1-C3-C2	110.4(7)	O1-C4-C5	106.2(5)	O1-C4-C21	107.9(6)
C5-C4-C21	115.5(6)	O4-C5-C6	105.8(6)	O4-C5-C23	112.2(6)
C6-C5-C23	107.8(6)	O4-C5-C4	108.4(5)	C6-C5-C4	109.2(6)
C23-C5-C4	113.2(6)	C7-C6-C5	127.9(7)	C6-C7-C8	124.8(7)
O5-C8-C7	120.3(8)	O5-C8-C9	120.9(7)	C7-C8-C9	115.7(7)
C10-C9-C8	101.1(8)	C9-C10-C11	101.9(9)	O6-C11-C30	109.3(9)
O6-C11-C12	106.6(8)	C30-C11-C12	106.2(9)	O6-C11-C10	94.5(8)
C30-C11-C10	126.1(9)	C12-C11-C10	112.3(7)	O7-C12-C13	108.8(7)
O7-C12-C11	110.0(7)	C13-C12-C11	113.5(8)	C12-C13-C1	115.3(6)
C19-C16-C18	105.8(10)	C19-C16-C17	106.9(8)	C18-C16-C17	109.3(8)
C19-C16-Si1	113.5(7)	C18-C16-Si1	110.9(7)	C17-C16-Si1	110.1(8)
C22-C21-C4	117.5(7)	C29-C26-C27	107(2)	C29-C26-C28	111.2(14)

C27-C26-C28	103(2)	C29-C26-Si2	114.8(14)	C27-C26-Si2	111.2(12)
C28-C26-Si2	109.1(8)				

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[12]. $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$

$wR_2 = \{ \sum w (F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2 \}^{1/2}$

$GOF = \{ \sum w (F_o^2 - F_c^2)^2 / (n - p) \}^{1/2}$

where n = the number of reflections and p = the number of parameters refined.

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