Supplementary Information 1

Design and synthesis of lipid-coupled inositol 1,2,3,4,5,6-hexakisphosphate derivatives exhibiting high-affinity binding for HIV-1 MA domain

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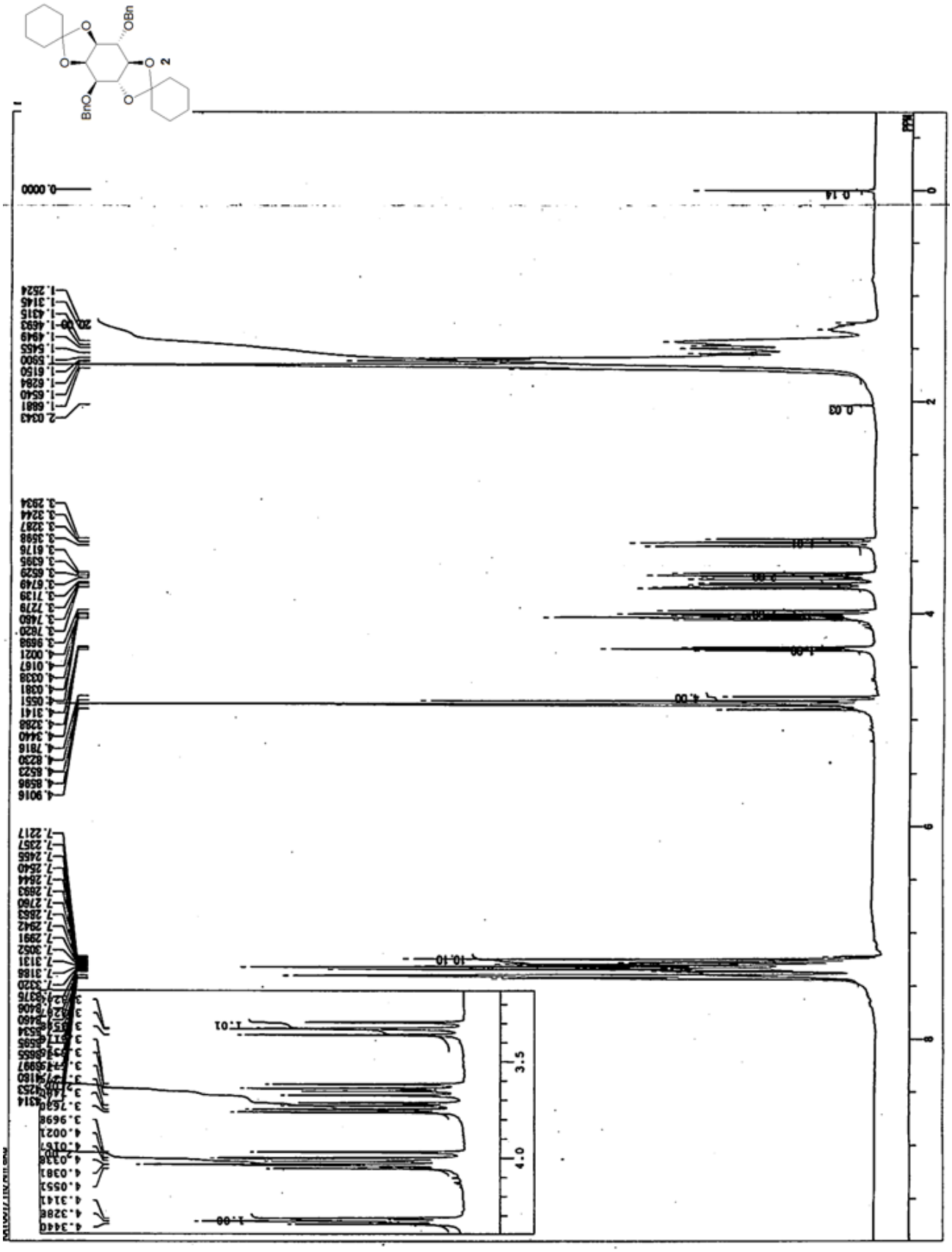
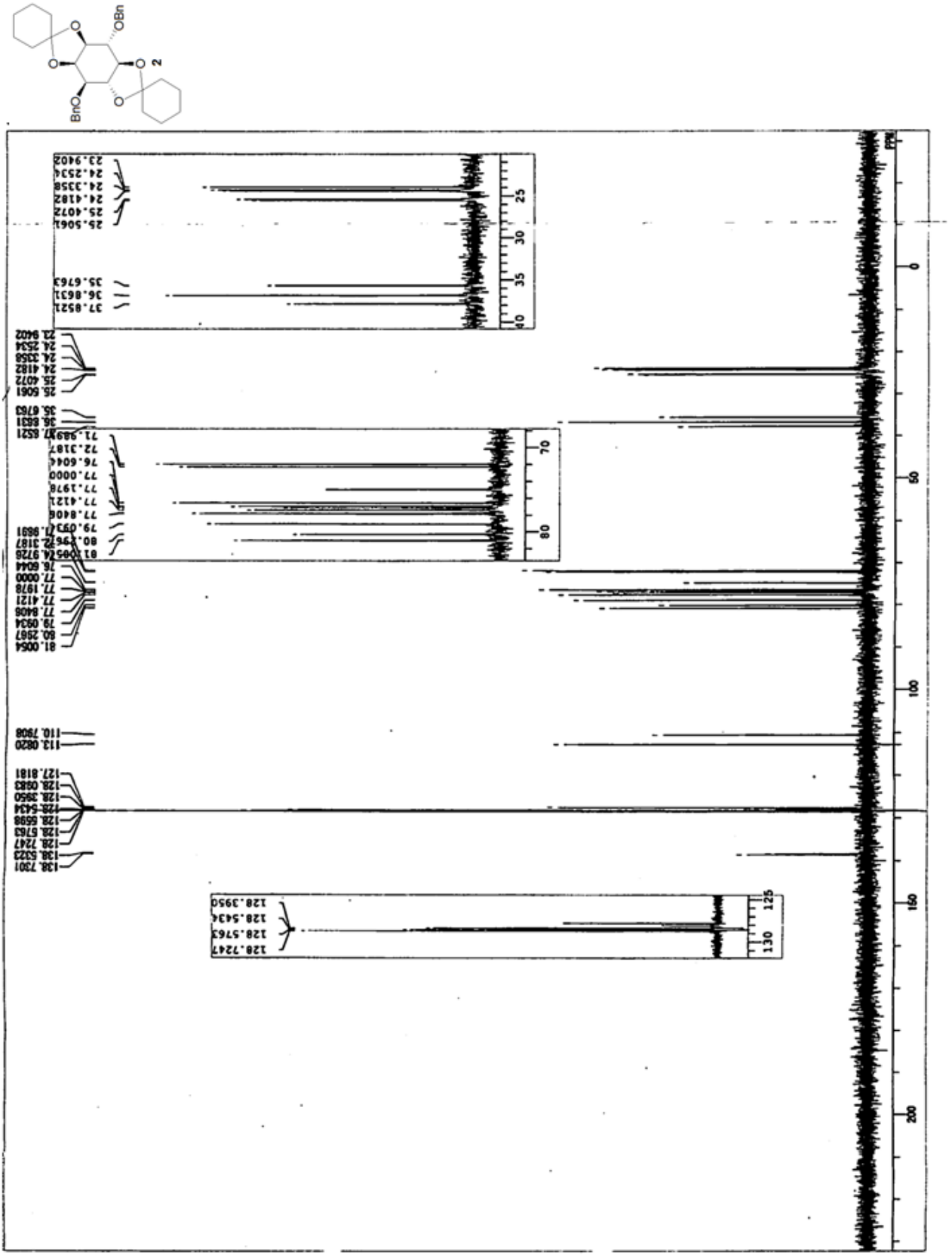
^{1}H, ^{13}C NMR (DEPT) spectra (Inositol moiety; compound 12-20)

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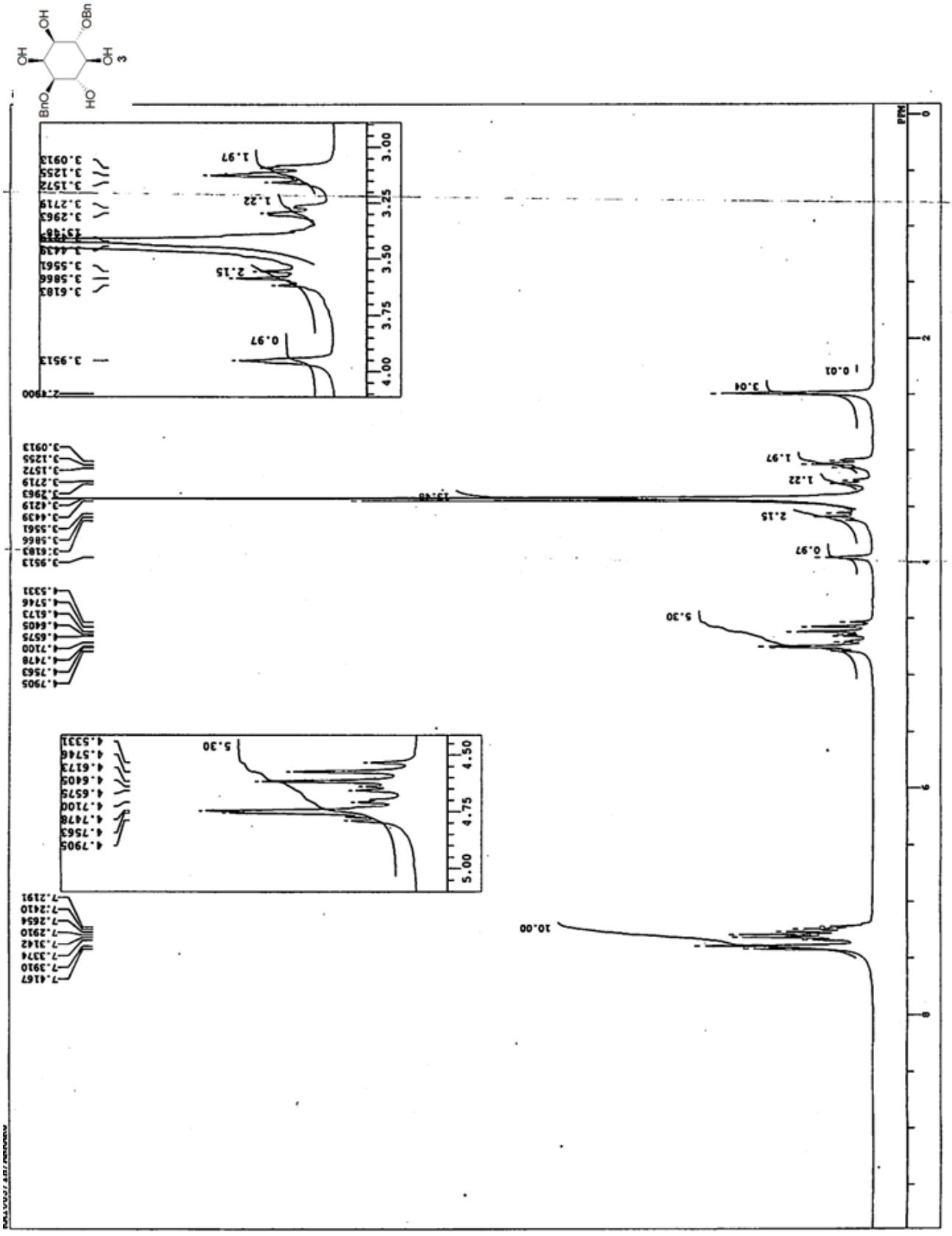
BnO
2
PPM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OBn
OH
OH
BnO
HO
3
PPM
0
2
4
6
8
10.00
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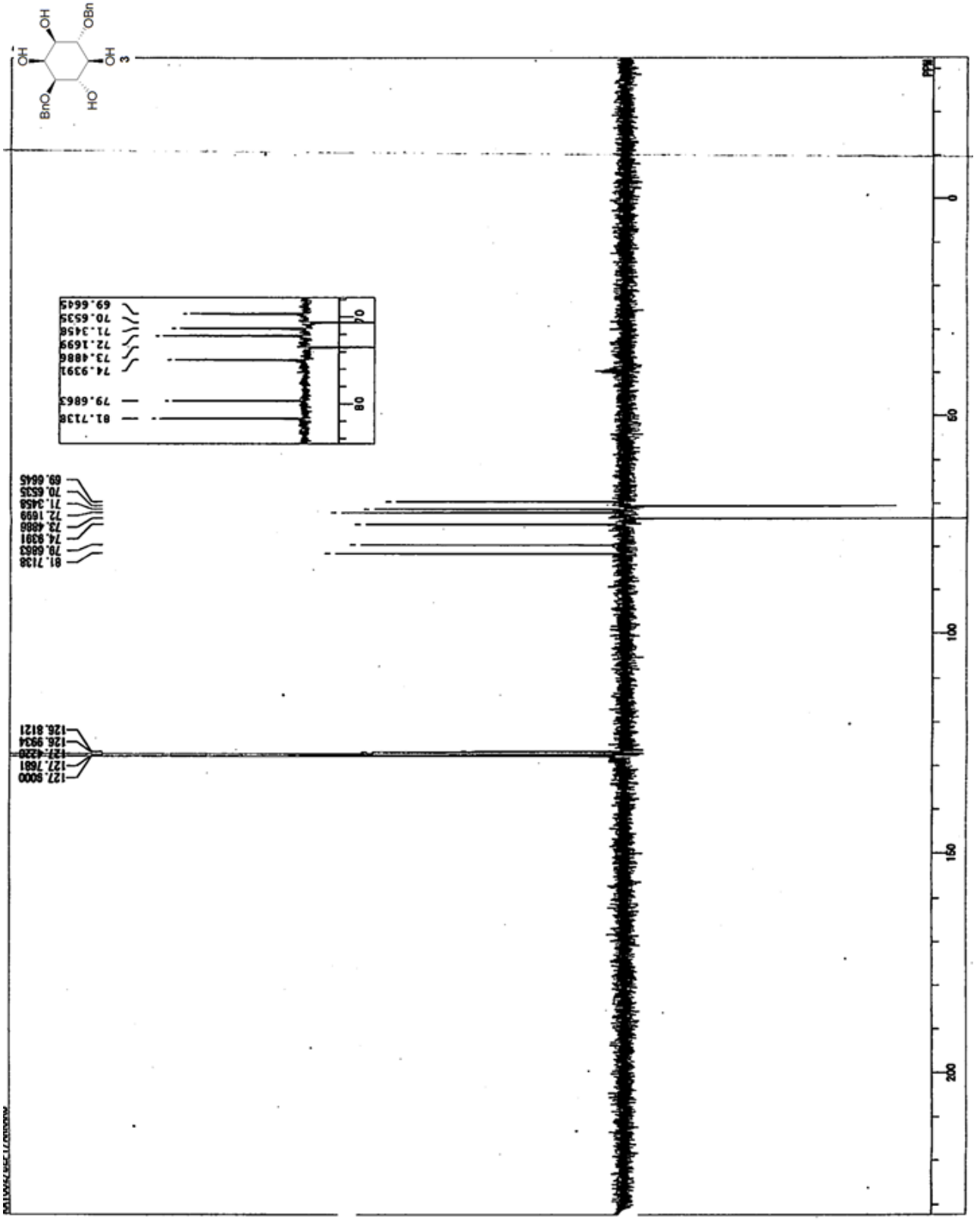
2.15
1.97
1.22
0.97
0.01
13.48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OBn
OH
3
BnO
HO
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79.6863
74.9391
73.4886
72.1699
71.3458
70.6535
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127.5000
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127.4230
126.9934
126.8121
ppm
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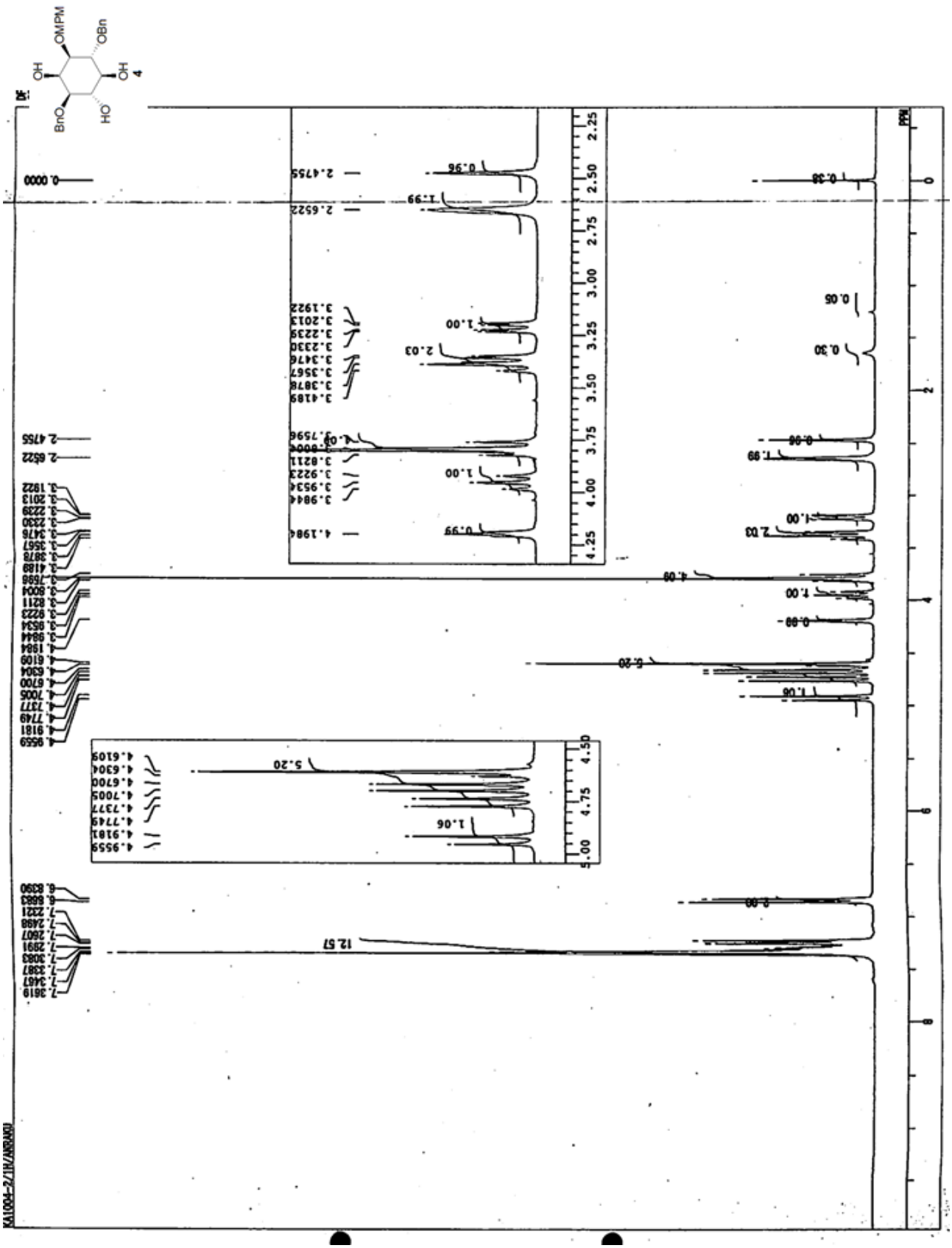
60
100
150
200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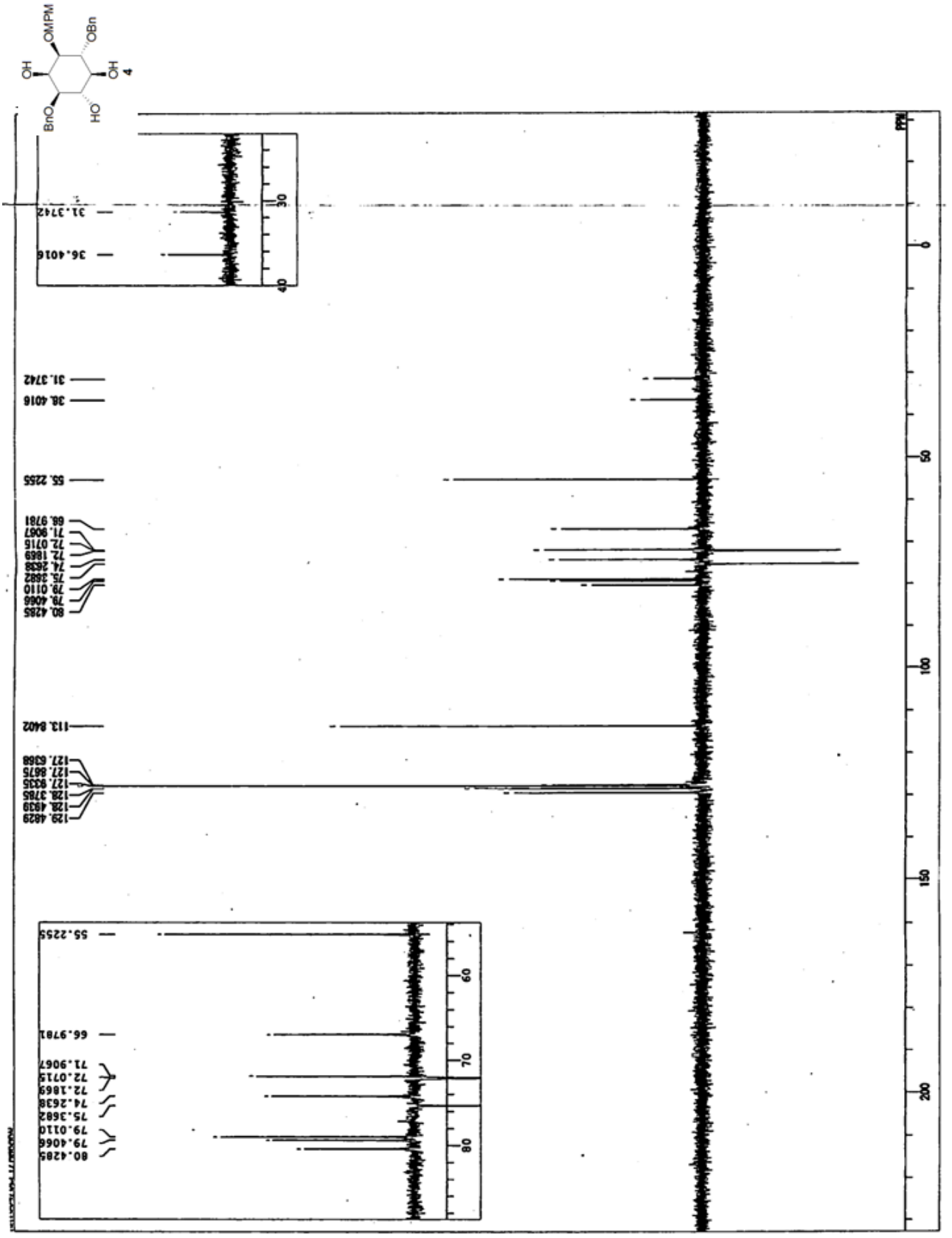
OBn
OH
OH
BnO
HO
4


OMPM
OBn
OH
OH
4
BnO
HO
31.3742
36.4016
55.2255
66.9781
71.9067
72.0715
72.1869
74.2638
75.3682
79.0110
79.4066
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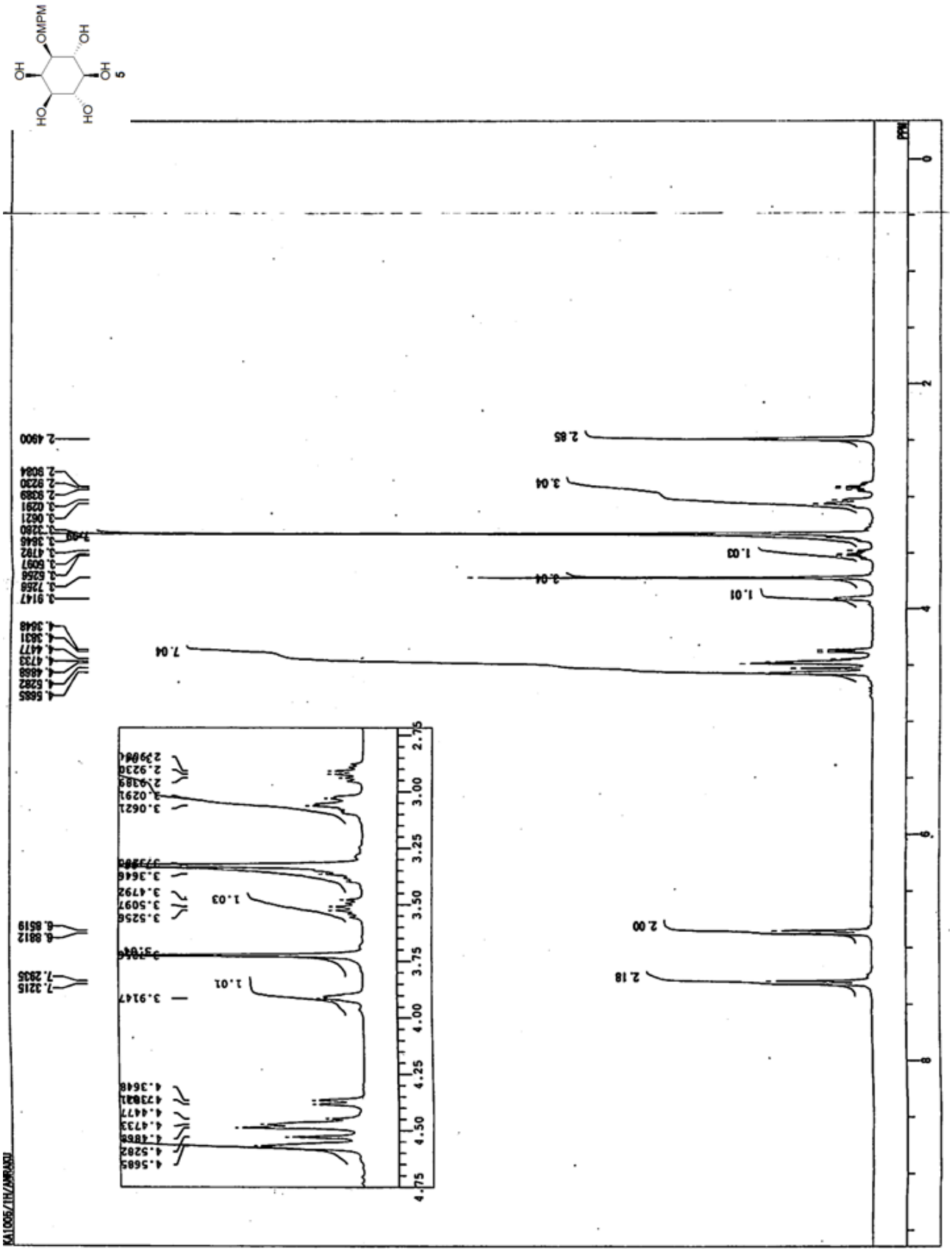
113.8402
127.6368
127.8675
127.8935
128.3785
128.4938
129.4829
PPM


OMPM
OH
HO
OH
OH
HO
5
PPM
0
2
4
6
8
2.85
3.04
1.03
3.04
1.01
7.04
2.00
2.18
1.01
1.03
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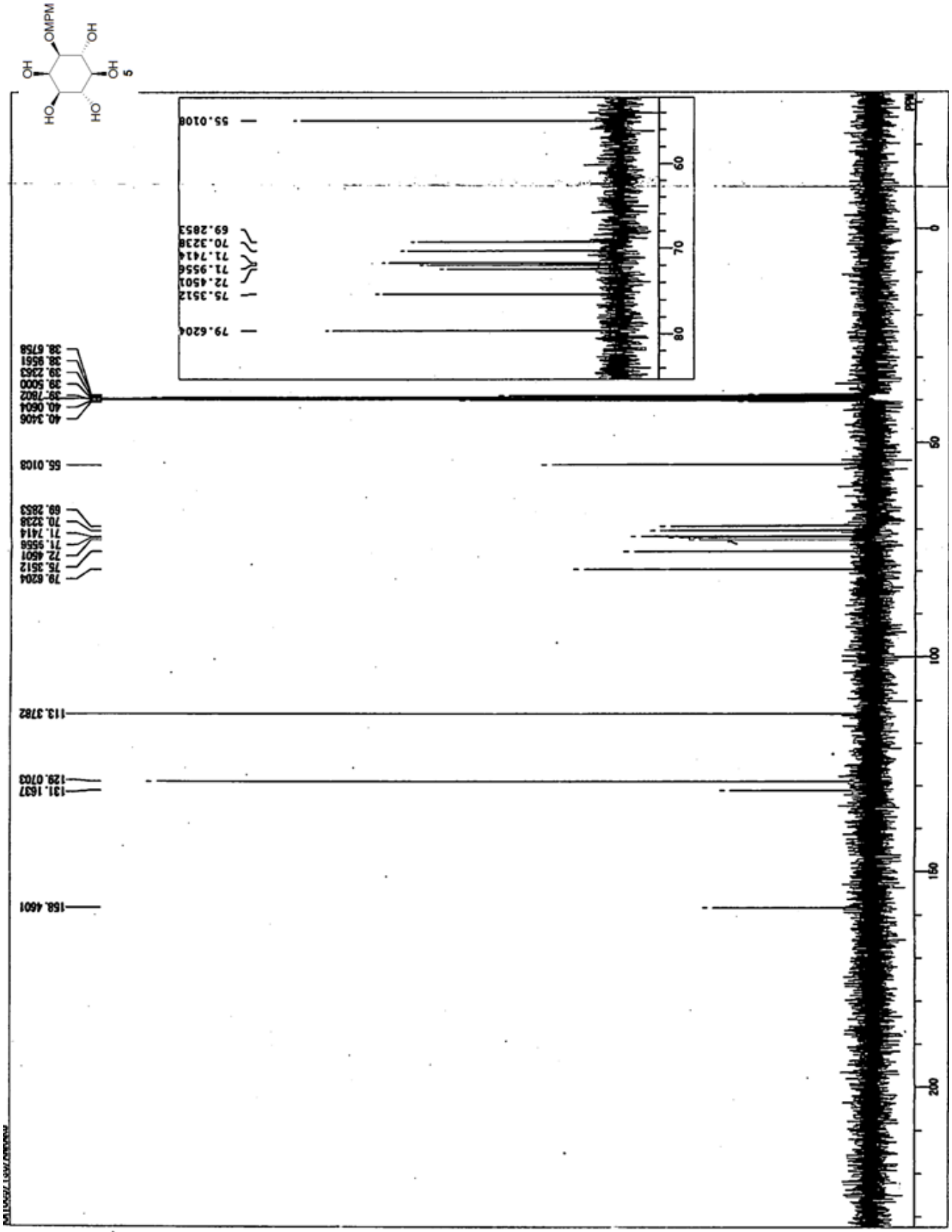
3.00
3.25
3.50
3.75
4.00
4.25
4.50
4.75


OMPM
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HO
OH
HO
OH
5
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69.2853
70.3238
71.7414
71.9556
72.4501
75.3512
79.6204
38.6758
38.8561
39.2363
39.5000
39.7802
40.0604
40.3406
55.0108
69.2853
70.3238
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129.0703
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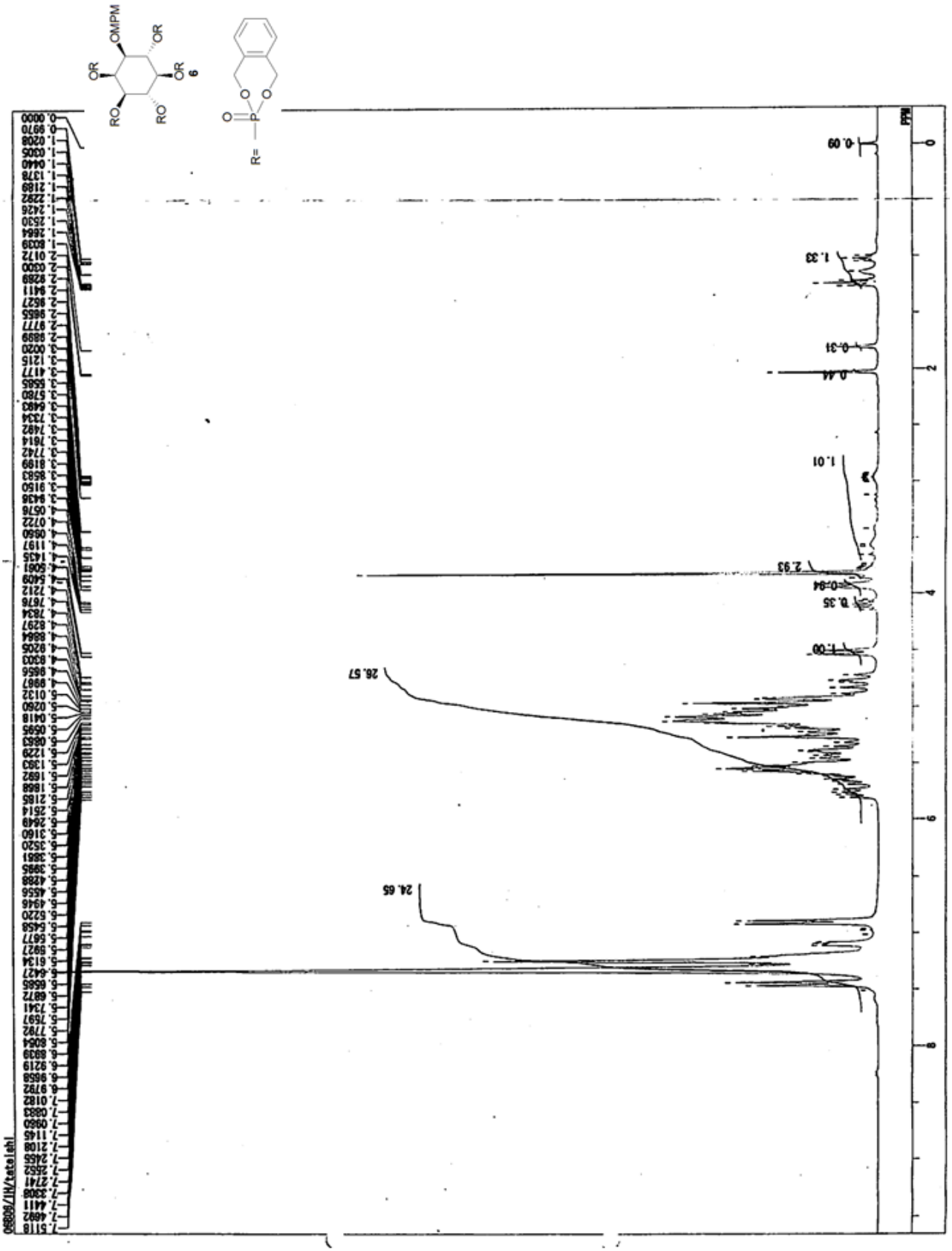
158.4601
PPM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OR
RO
RO
6
O
O
P
O
R=
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0.31
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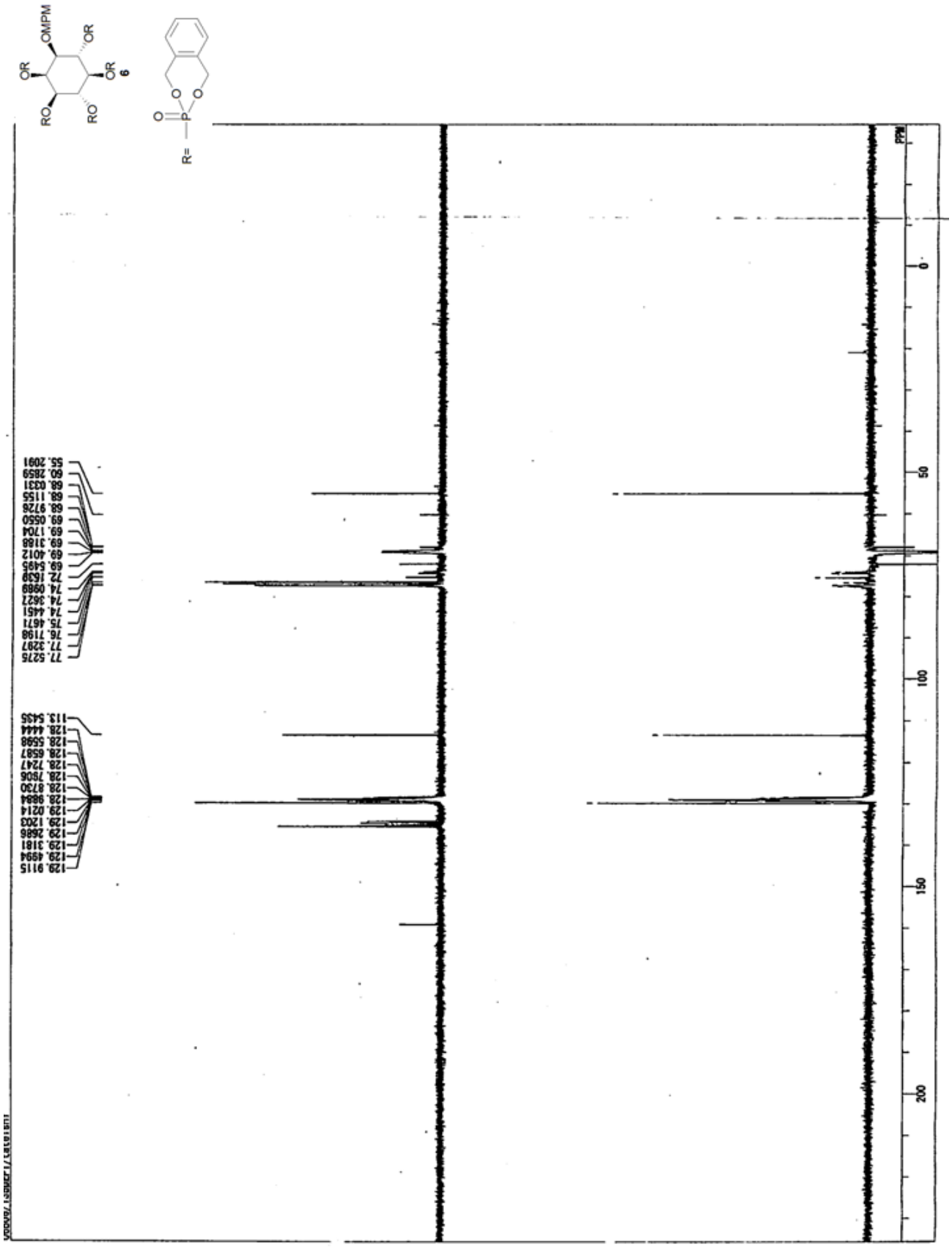
1.01
2.93
0.84
0.35
1.00
26.57
24.65
PPM
0
2
4
6
8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OR
OR
OR
RO
RO
6
R=
O
O
O
P
PPM
0
50
100
150
200
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77.3287
76.7198
75.4671
74.4451
74.3622
74.0989
72.1638
69.5495
69.4012
69.3186
69.1704
69.0550
68.9726
68.1155
68.0231
60.2859
55.2091
113.5455
128.4444
128.5598
128.6587
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129.0214
129.1203
129.2686
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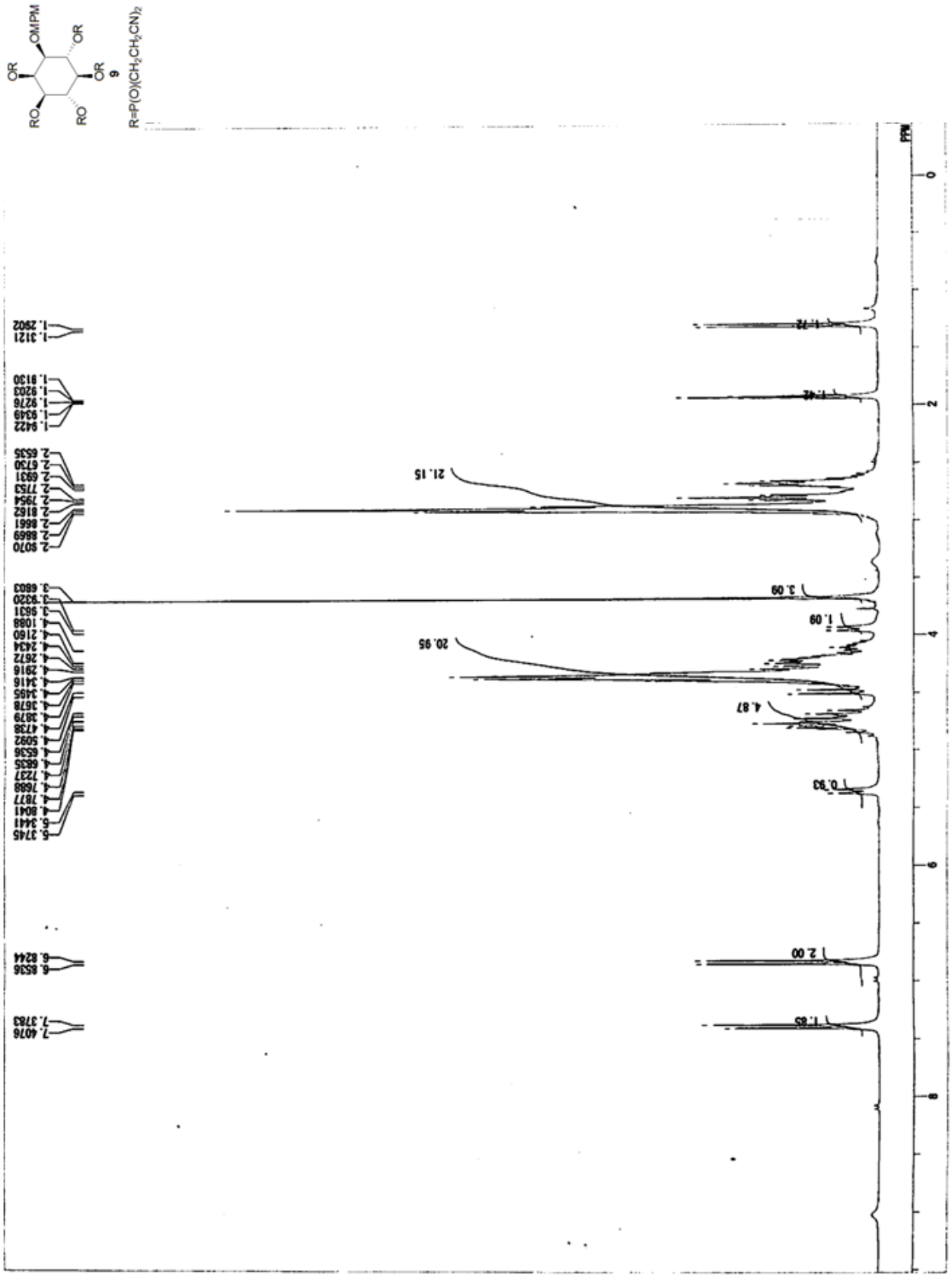
129.4594
129.9115


OM/PM
OR
OR
OR
RO
RO
9
R=P(O)(CH2CH2CN)2
PPM
0
2
4
6
8
1.85
2.00
0.93
4.87
20.95
1.09
3.09
21.15
1.3121
1.2902
1.9422
1.9349
1.9276
1.9203
1.8130
2.6535
2.6730
2.6931
2.7753
2.7954
2.8162
2.8661
2.8869
2.9070
3.6803
3.9220
3.9631
4.1088
4.2160
4.2434
4.2672
4.2916
4.3416
4.3495
4.3678
4.3879
4.4738
4.5092
4.6536
4.6635
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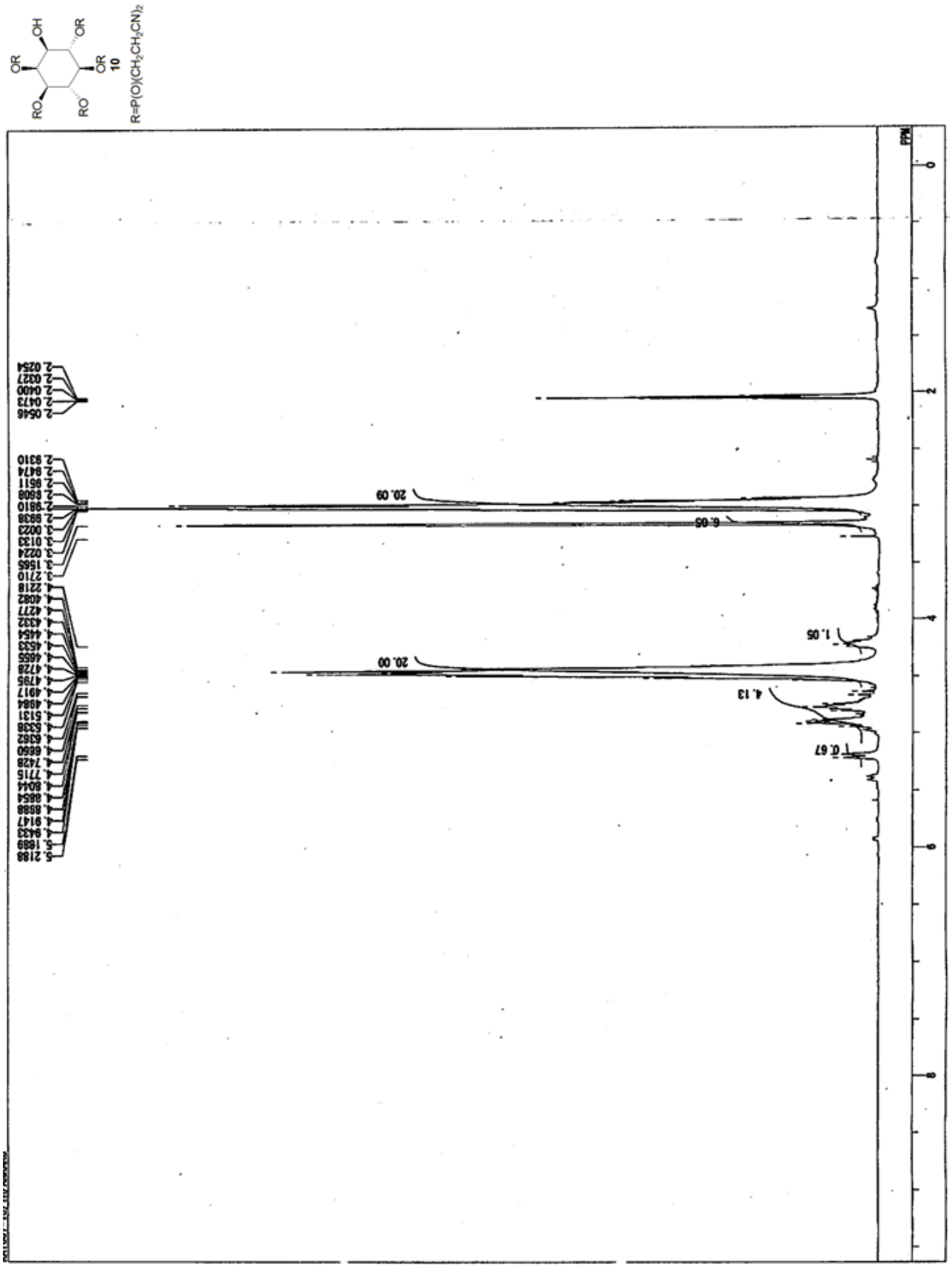
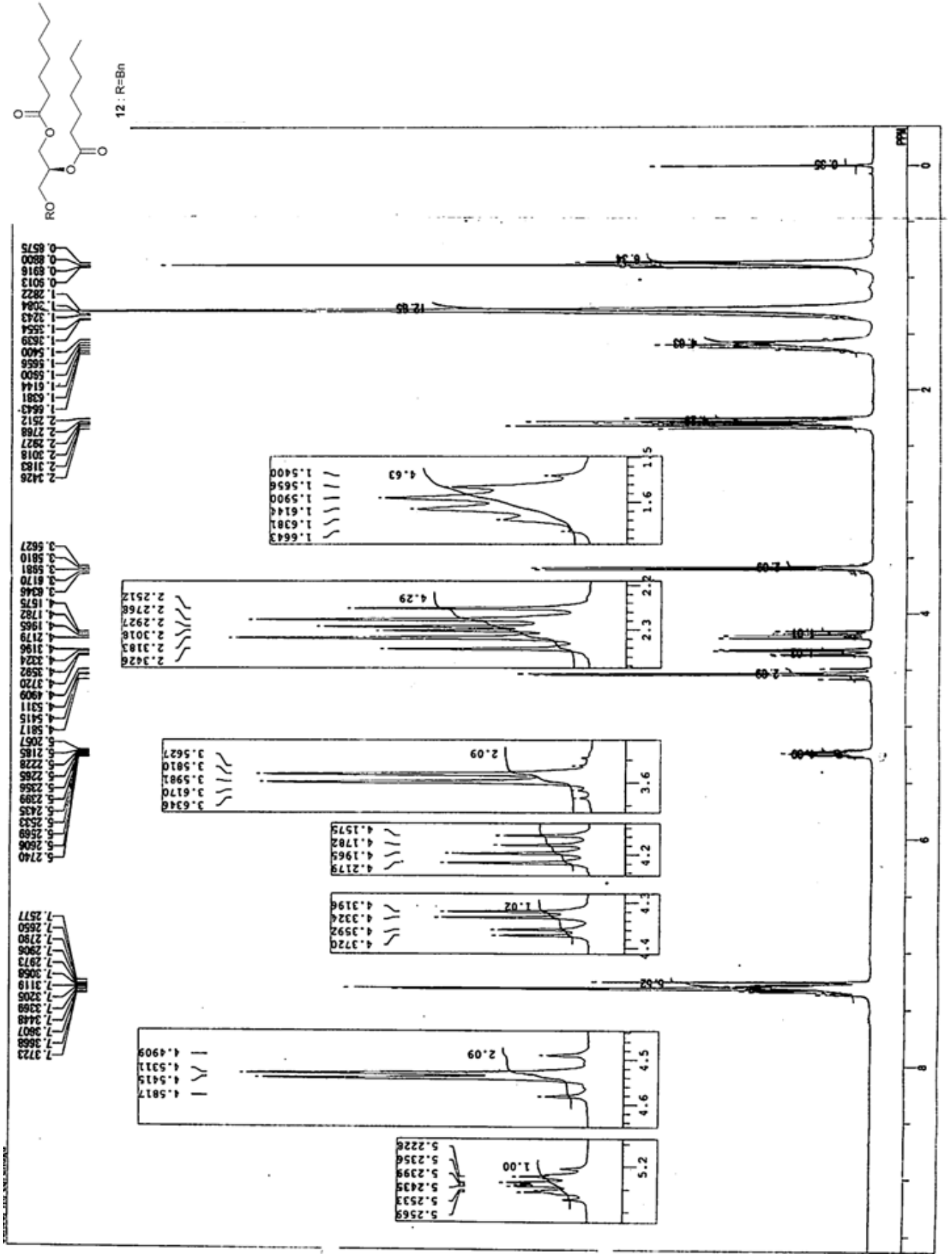
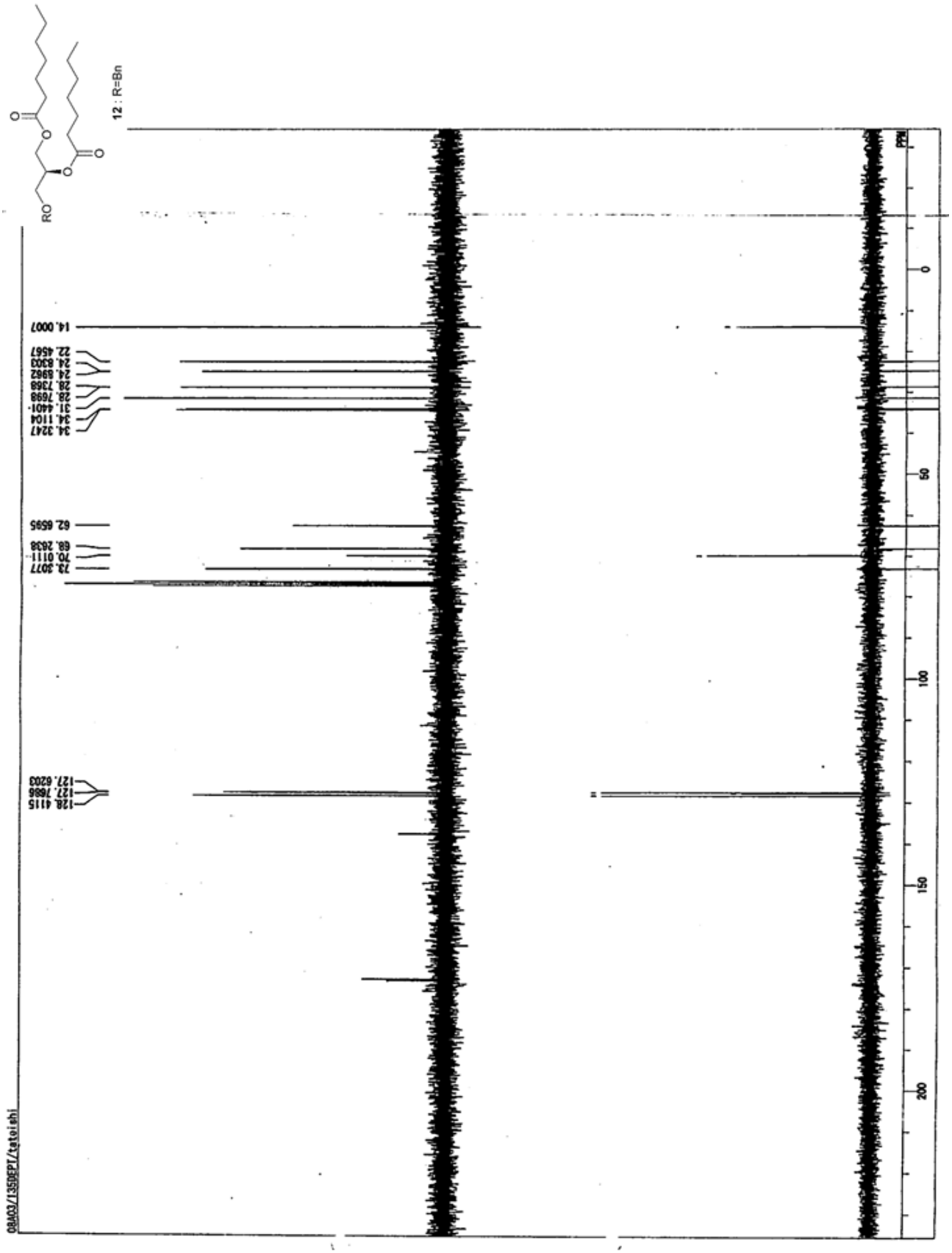
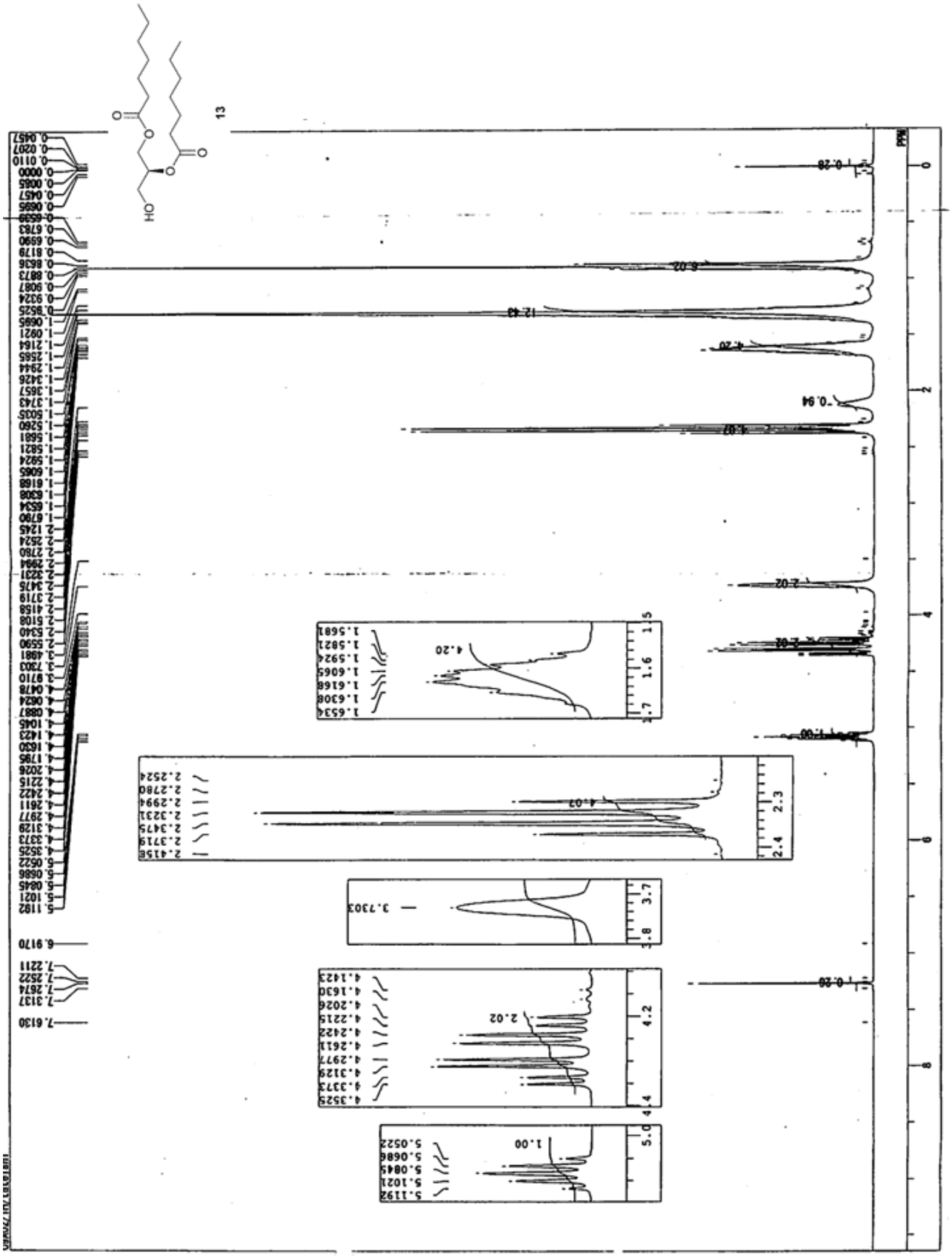
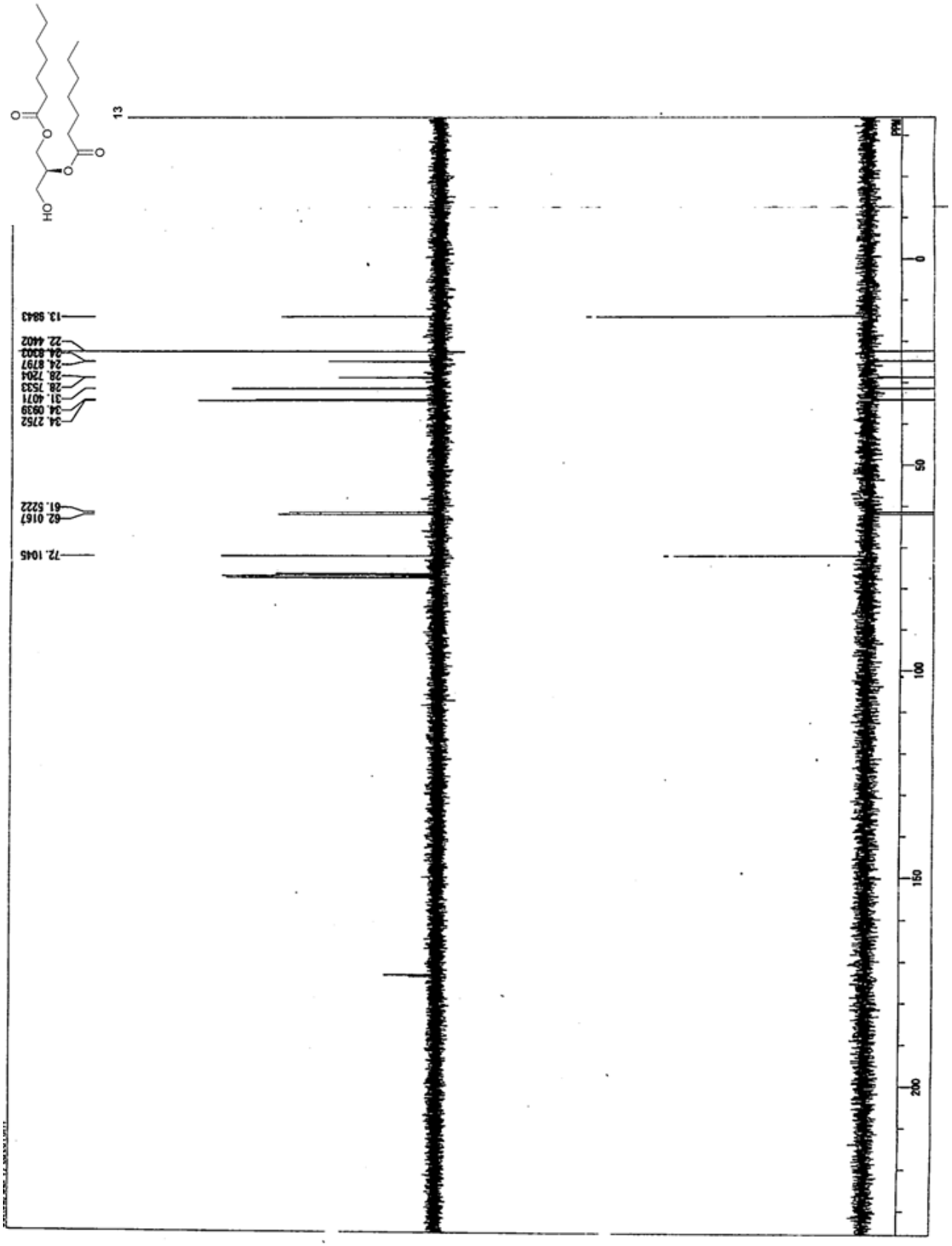

OH
OR
OR
OR
RO
RO
10
R=P(O)(CH2CH2CN)2
PPM
0
2
4
6
8
20.09
6.05
20.00
1.05
4.13
1.67

^{1}H, ^{13}C NMR (DEPT) spectra (Glycerol moiety; compound 12-20)




12 : R=Bn
RO
14.0007
22.4567
24.8303
24.8962
28.7368
28.7698
31.4401
34.1104
34.3247
62.6595
68.2638
70.0111
73.3077
127.6203
127.7686
128.4115
PPM
0
50
100
150
200
08A03/135DEPT/tatsuishi




13.8843
22.4402
24.8797
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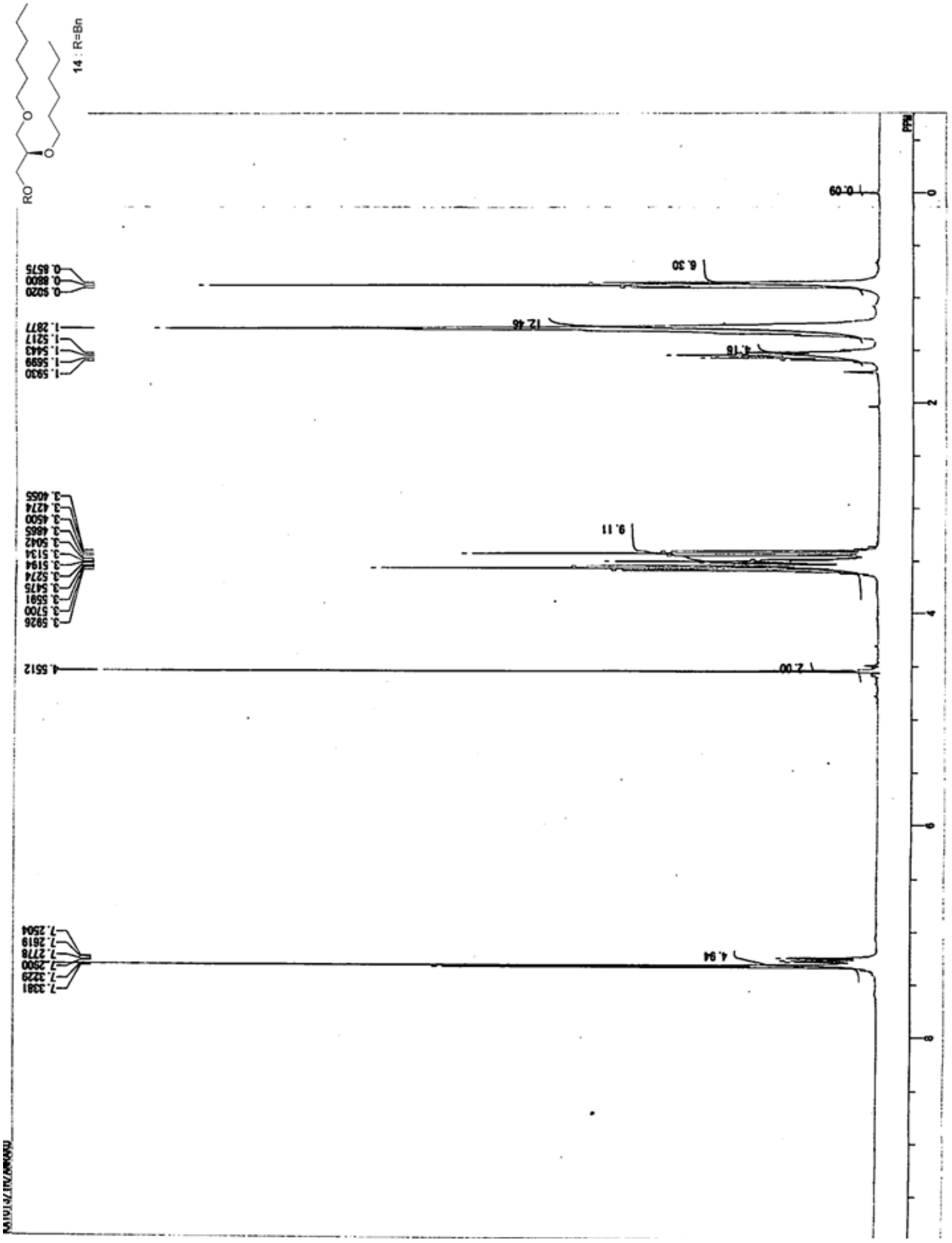
61.5222
62.0167
72.1045
PPM
0
50
100
150
200


14 : R=Bn
RO
0.09
6.30
12.46
4.18
9.11
2.00
4.94
4.5512
7.2504
7.2819
7.2778
7.2500
7.3229
7.3381
3.5926
3.5700
3.5591
3.5475
3.5274
3.5194
3.5134
3.5042
3.4865
3.4500
3.4274
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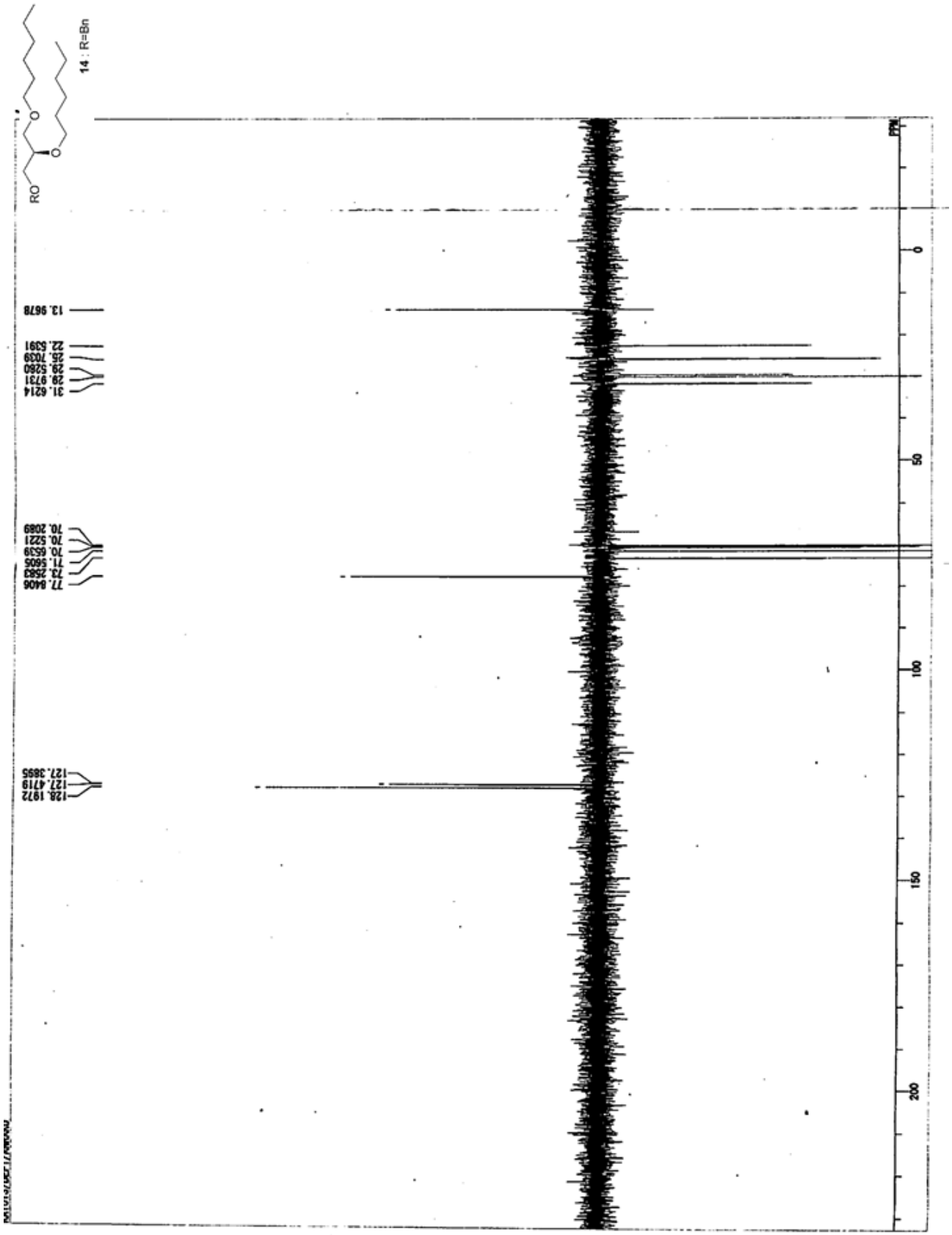
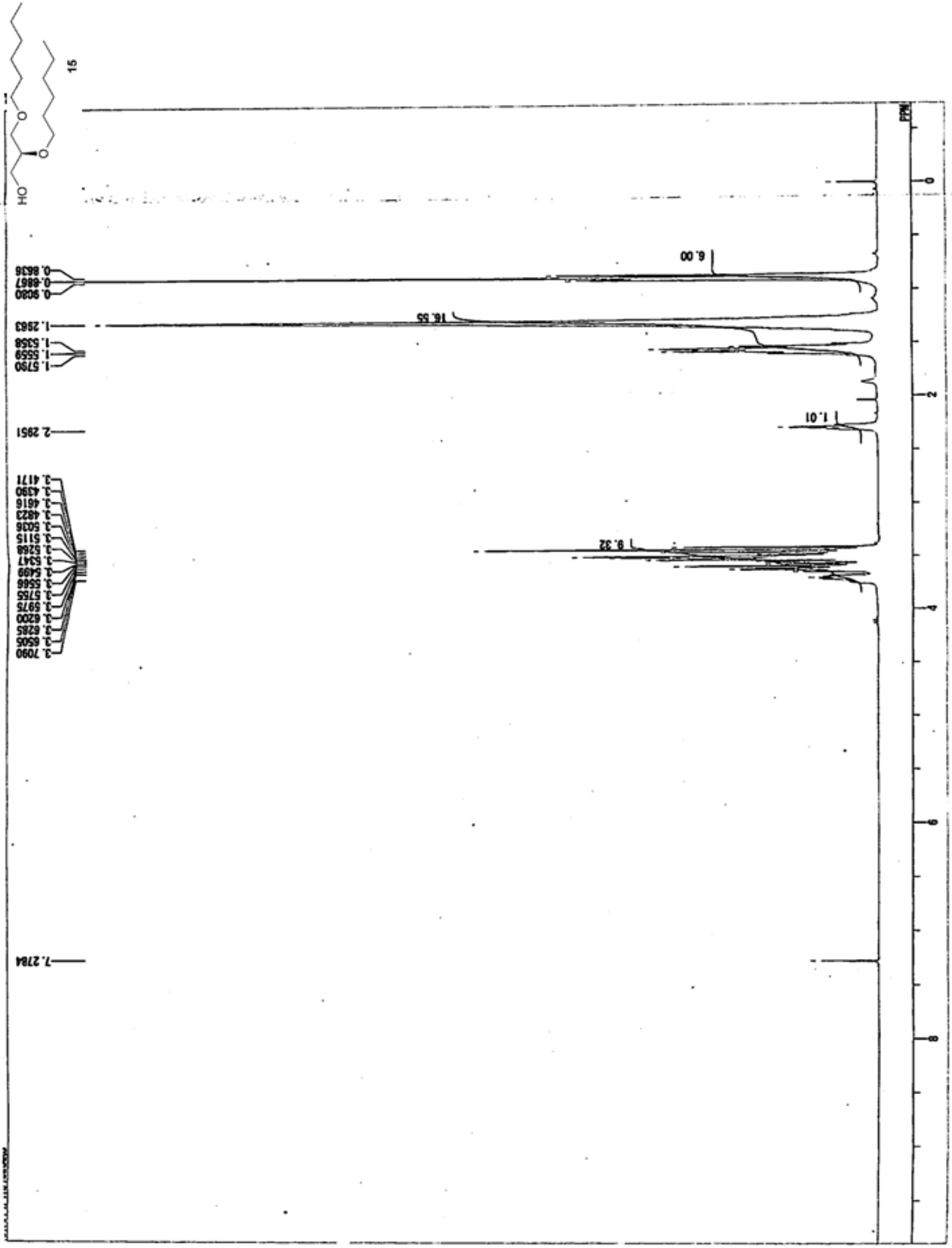
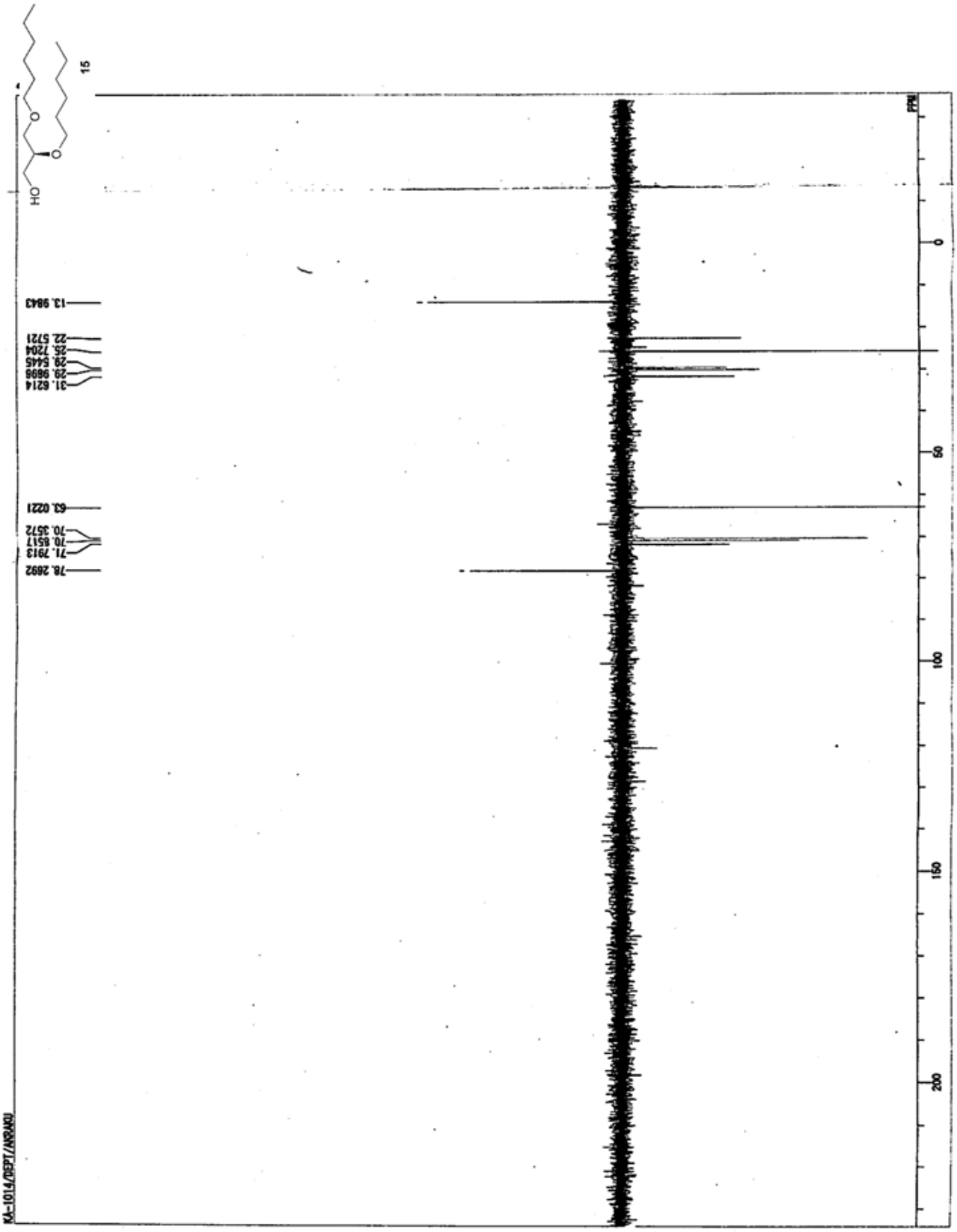
0.8920
0.8800
0.8575
PPM


14 : R=Bn
RO
13. 9678
22. 5391
25. 7039
29. 5280
29. 9731
31. 6214
70. 2089
70. 5221
70. 6539
71. 5605
73. 2563
77. 8406
127. 3895
127. 4719
128. 1972
PPM
0
50
100
150
200


15
HO
O
O
O
6.00
16.55
8.32
1.01
0.8636
0.8867
0.9080
1.2863
1.5750
1.5559
1.5356
2.2951
3.4171
3.4390
3.4616
3.4823
3.5036
3.5115
3.5268
3.5347
3.5499
3.5566
3.5755
3.5975
3.6200
3.6285
3.6506
3.7090
7.2784
PPM
0
2
4
6
8


15
HO
13.9843
22.5721
25.7204
29.5445
29.9896
31.6214
63.0221
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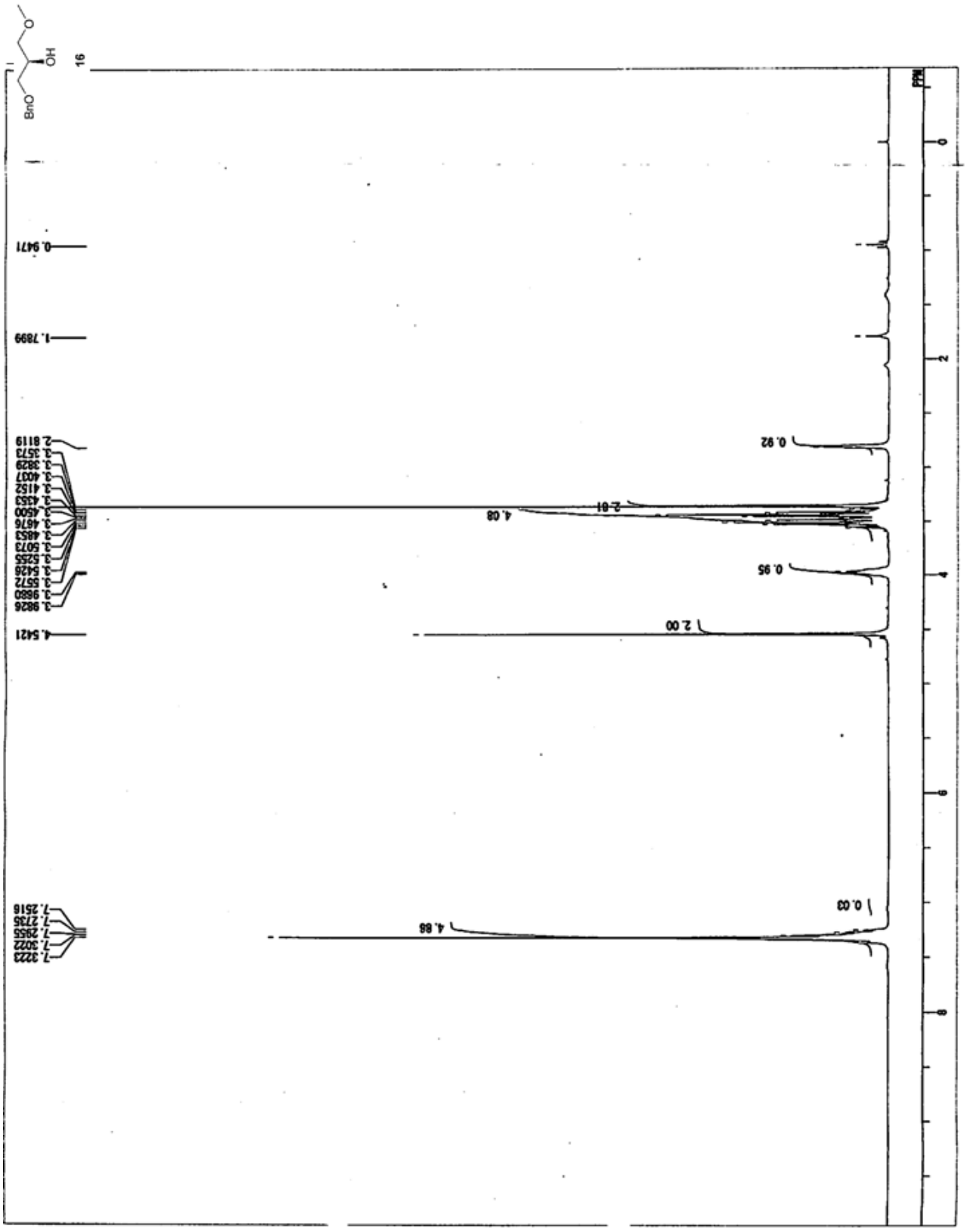
70.8517
71.7913
78.2892
KA-1014/DEPT/AVANCE
PPM
0
50
100
150
200


BnO
OH
16
PPM
0
2
4
6
8
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1.7899
2.8119
3.3573
3.3829
3.4037
3.4162
3.4353
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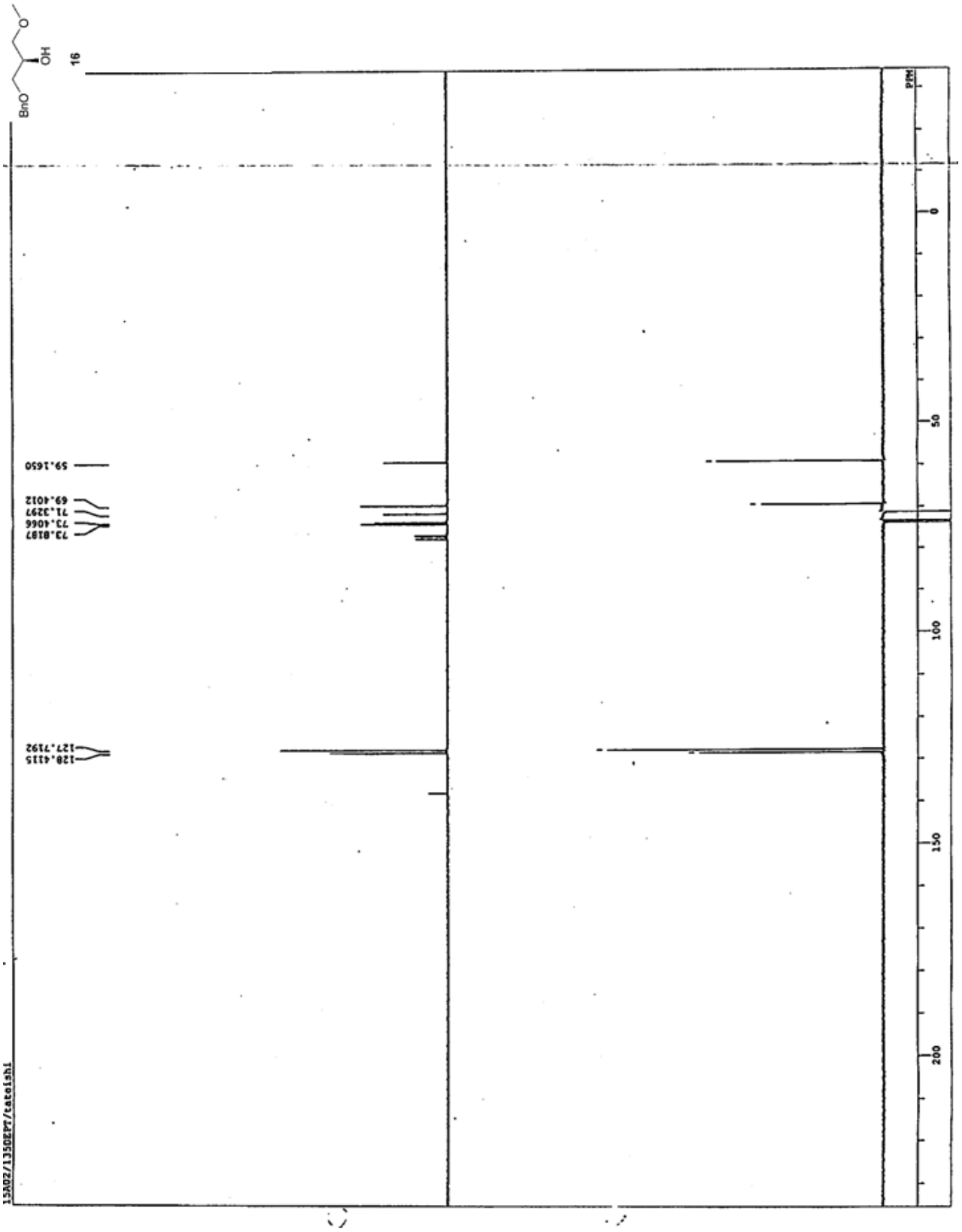
BnO
OH
O
16
59.1650
69.4012
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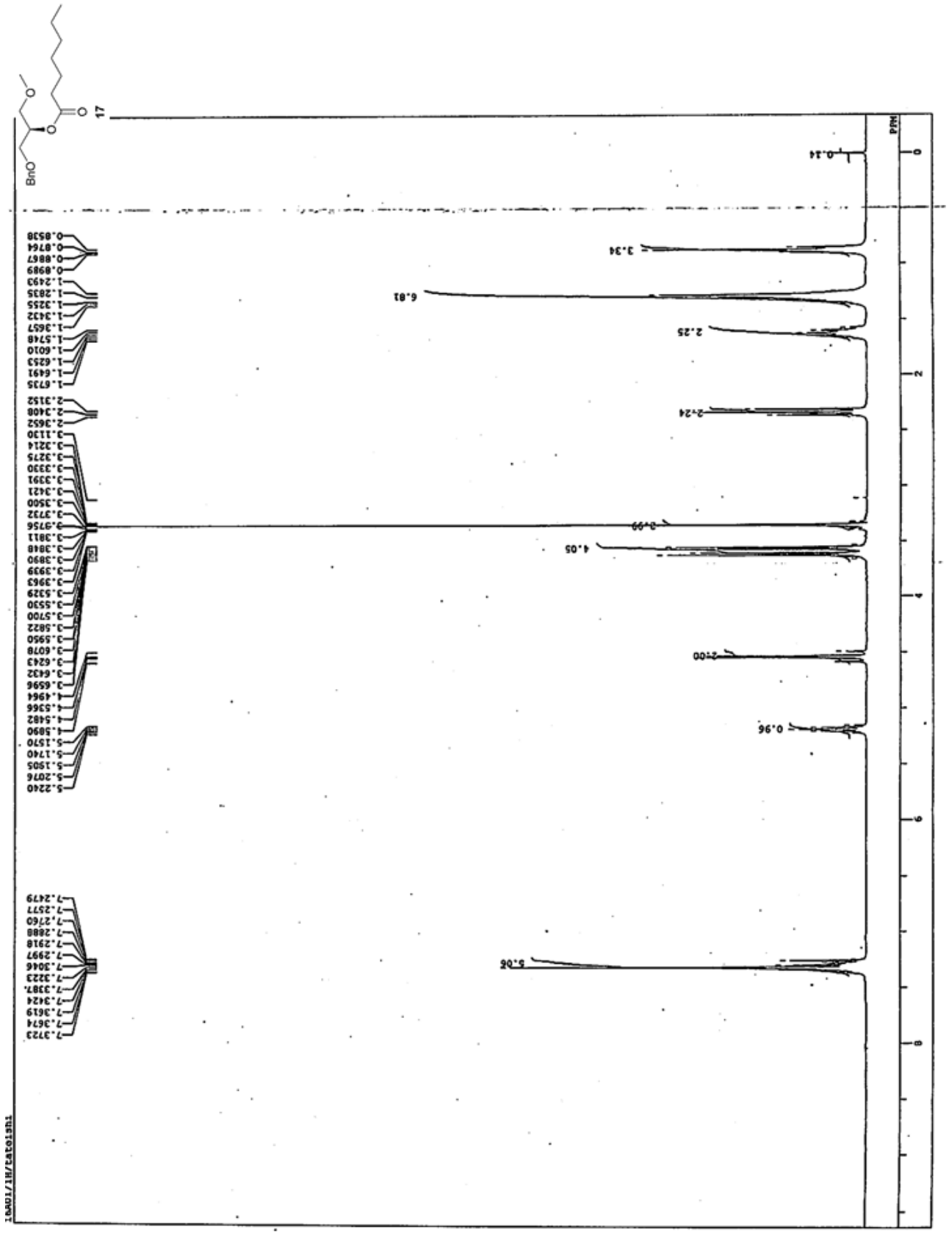
127.7192
128.4115
PPM
0
50
100
150
200
15A02/1350EPT/tatoishi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BnO
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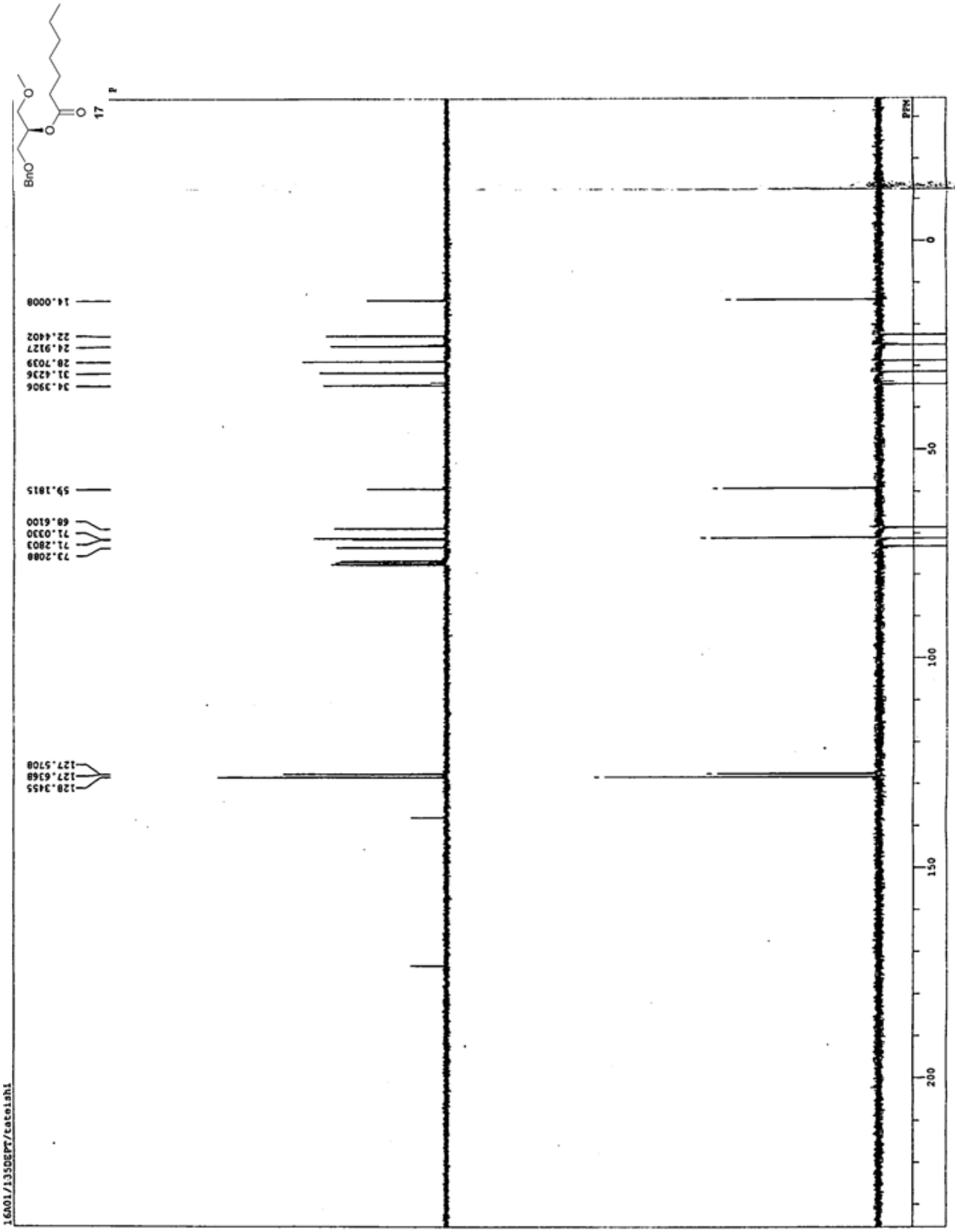
3.34
6.81
2.25
2.24
3.99
4.05
2.00
0.96
5.06


BnO
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14.0008
22.4402
24.9127
28.7039
31.4236
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59.1815
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71.2803
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127.5708
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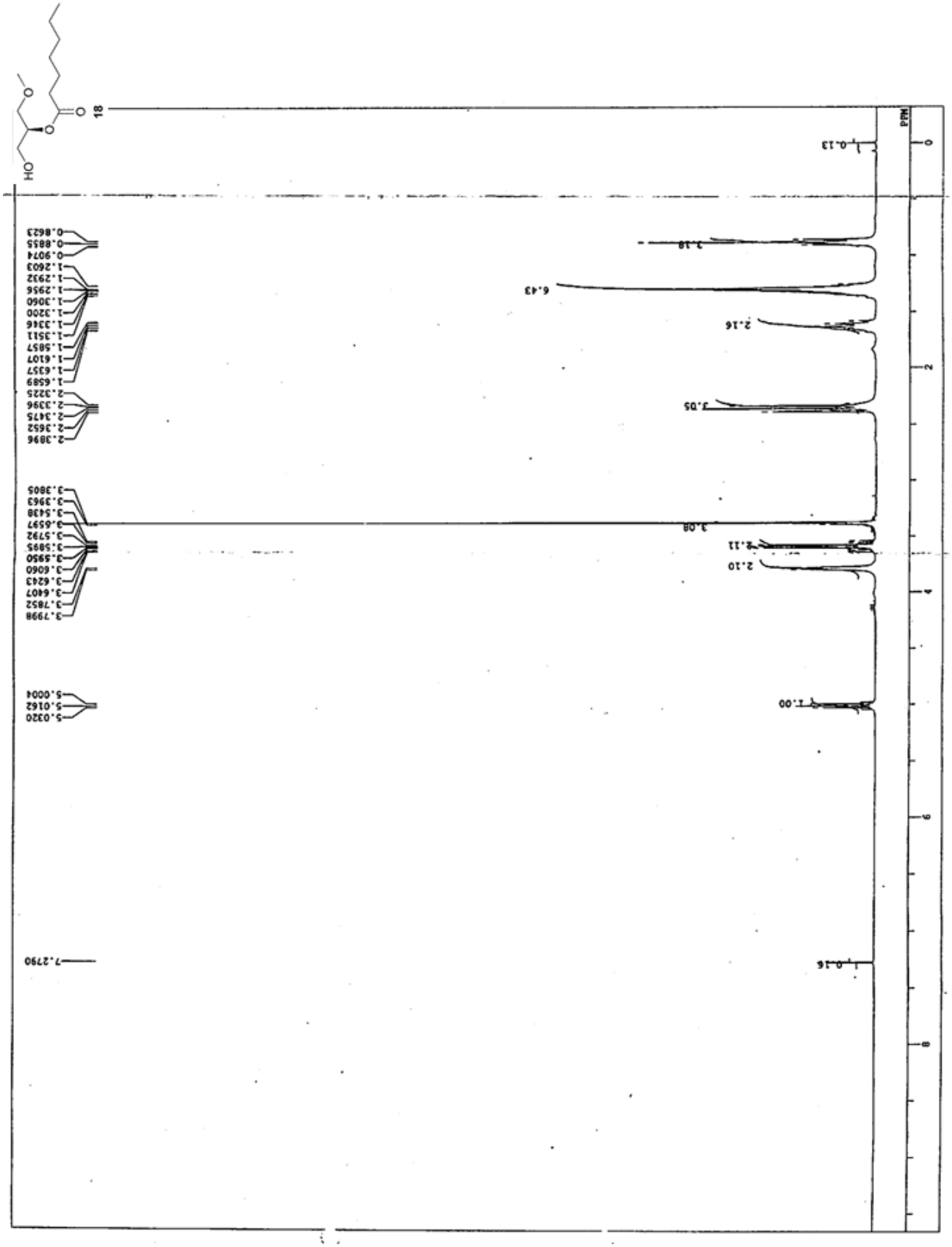
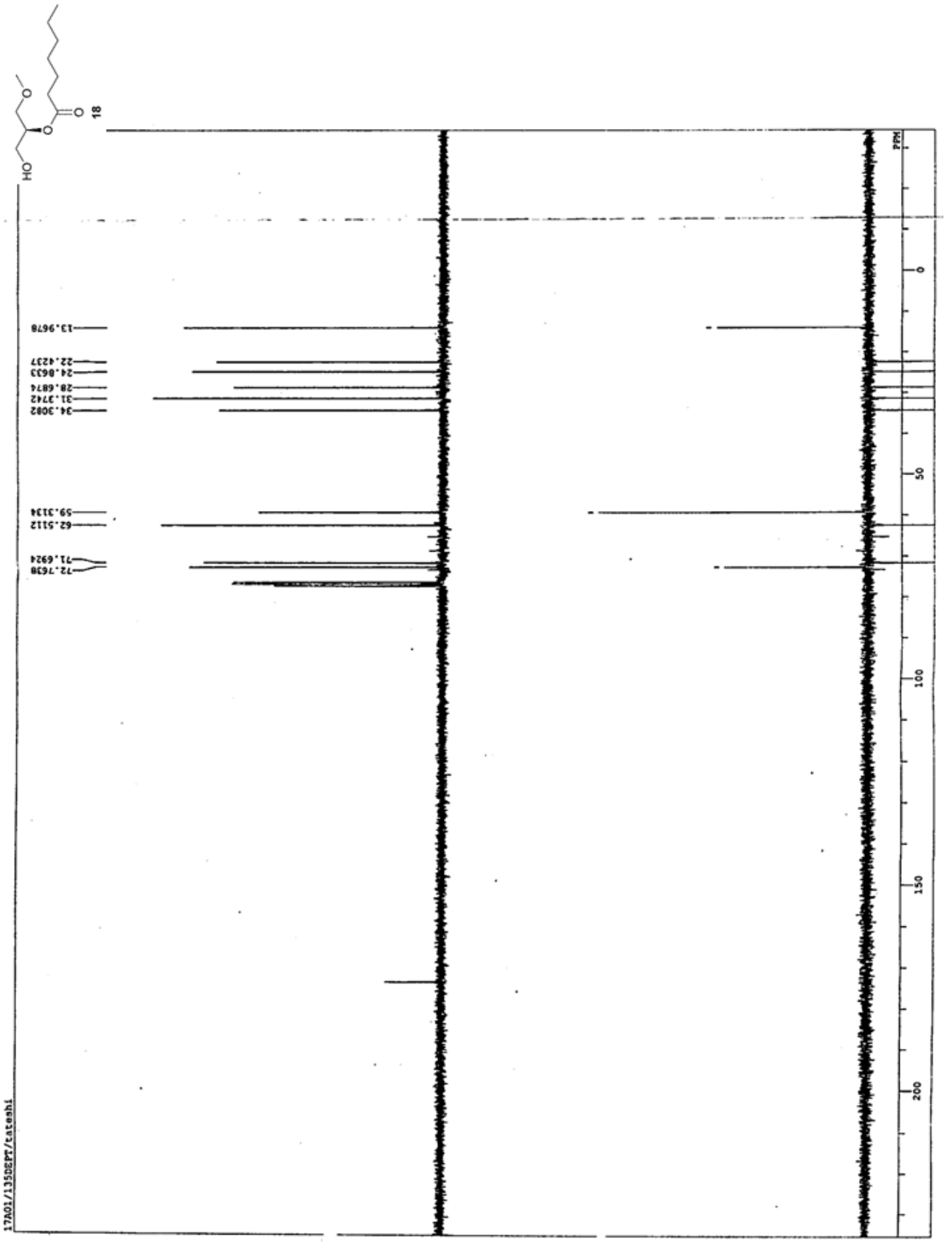
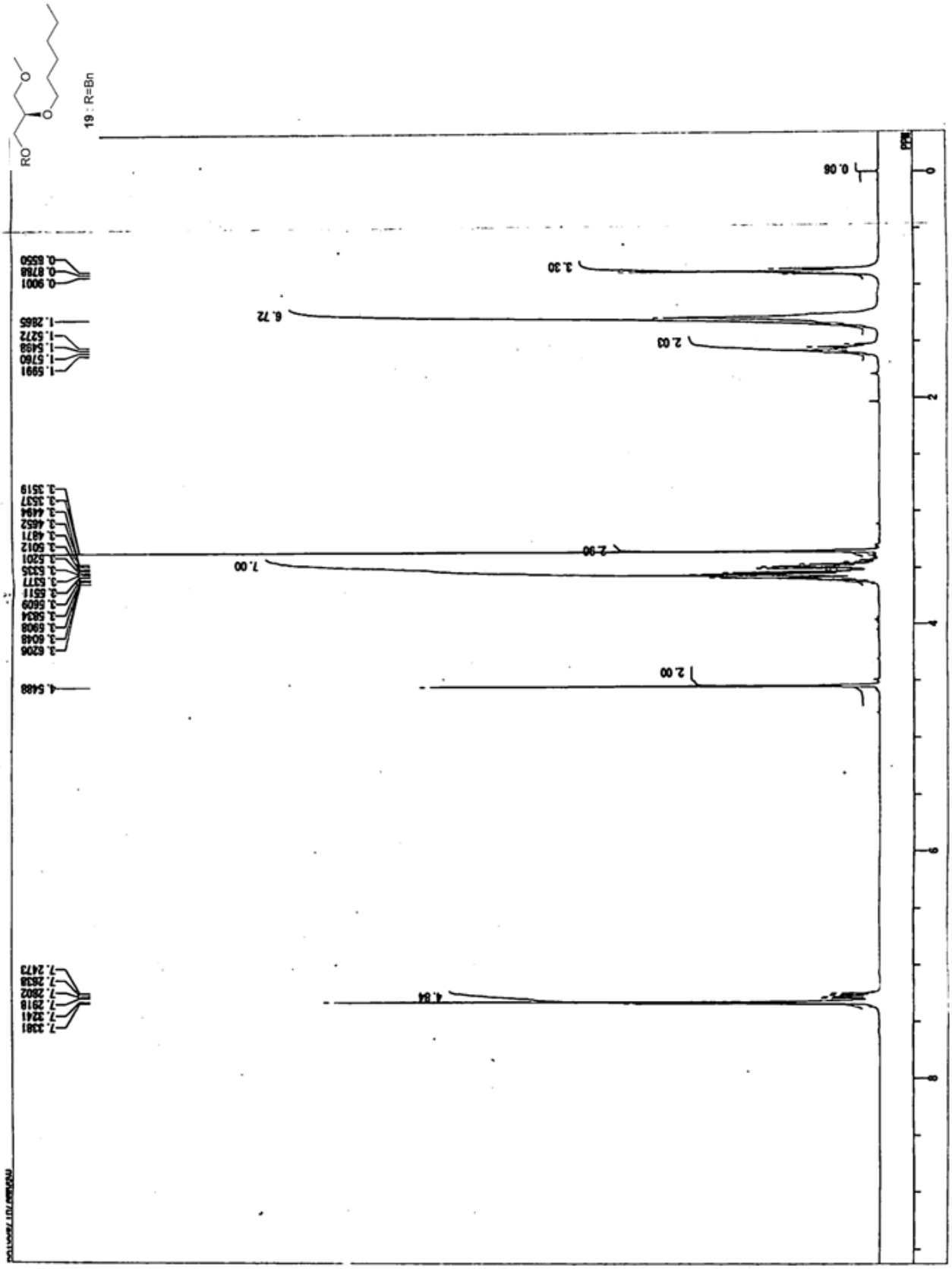
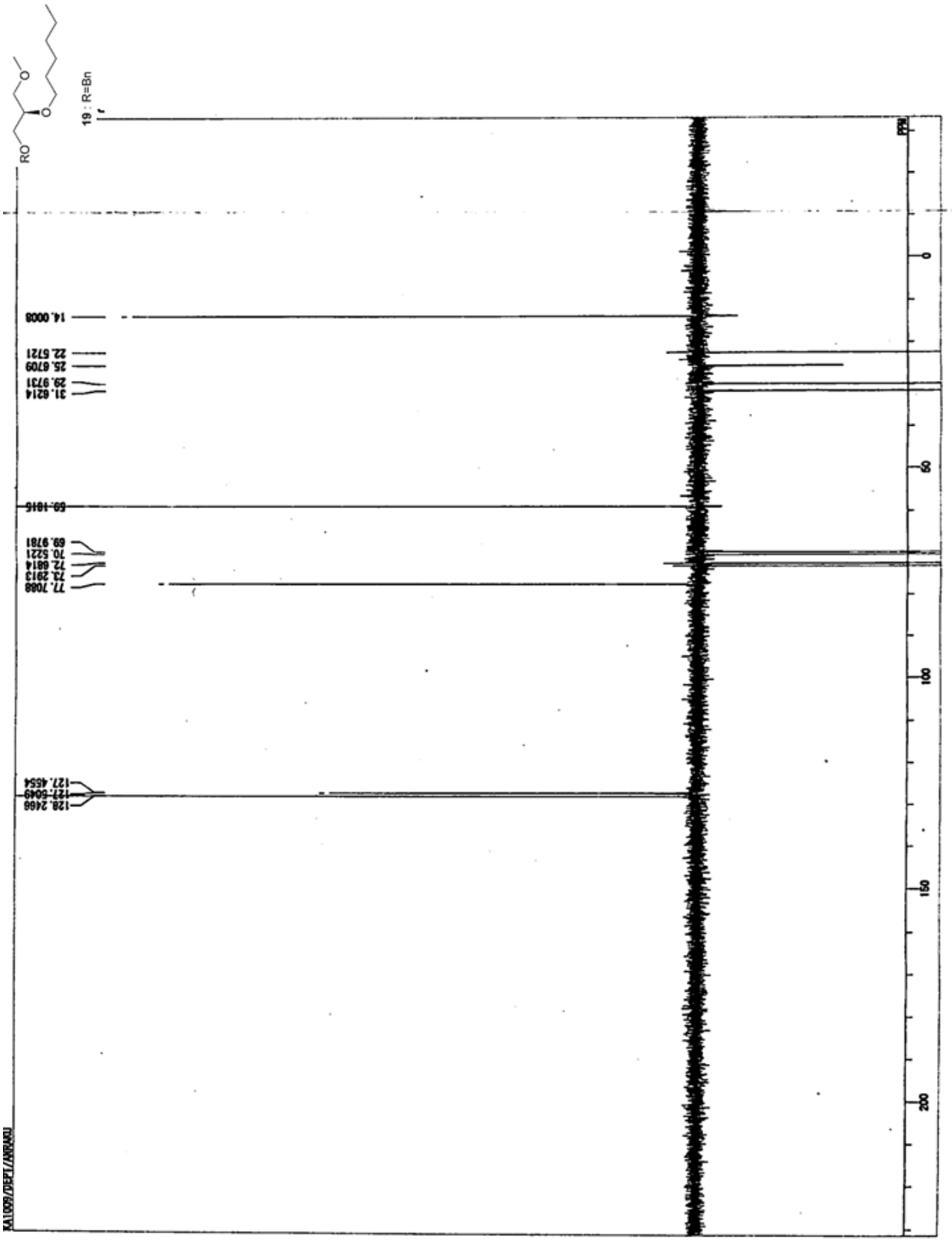
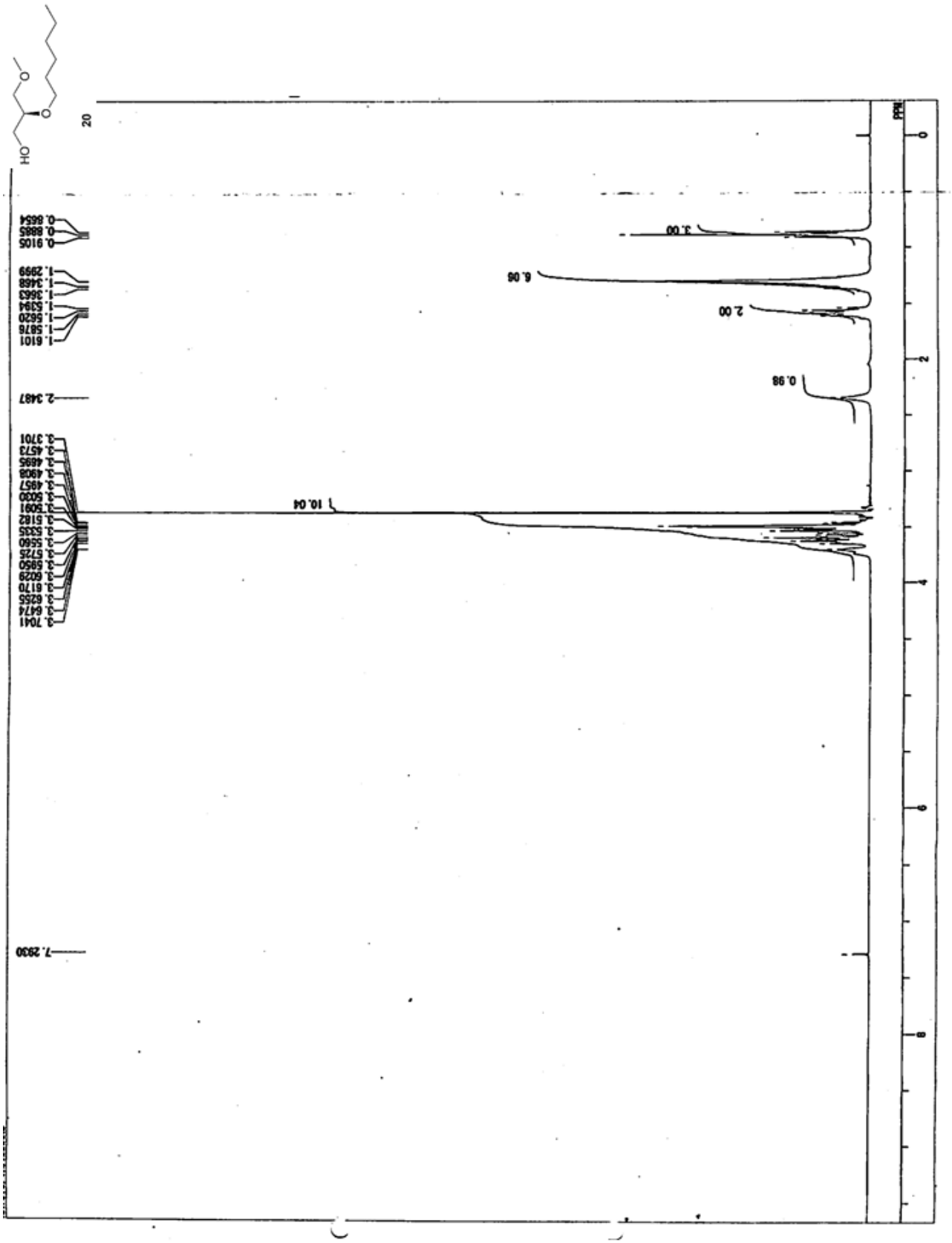



18
HO
13.9678
22.4237
24.0633
28.6874
31.3742
34.3082
59.3134
62.5112
71.6924
72.7638
PPM
0
50
100
150
200
17A01/135DEPT/tateshi


19 : R=Bn
RO
0.06
3.30
6.72
2.03
2.90
7.00
2.00
4.84
4.5488


19 : R=Bn
RO
O
O
14.0008
22.5721
25.6709
29.9731
31.8214
59.1816
69.9781
70.5221
72.8814
73.2913
77.7088
127.4554
127.6049
128.2466
0
50
100
150
200
PPM


O
O
HO
20
0
2
4
6
8
PPM
3.00
6.06
2.00
0.98
10.04
7.2930
2.3487
0.9105
0.8885
0.8654
1.6101
1.5876
1.5620
1.5394
1.3663
1.3468
1.2999
3.7041
3.6474
3.6255
3.6170
3.6029
3.5950
3.5725
3.5560
3.5335
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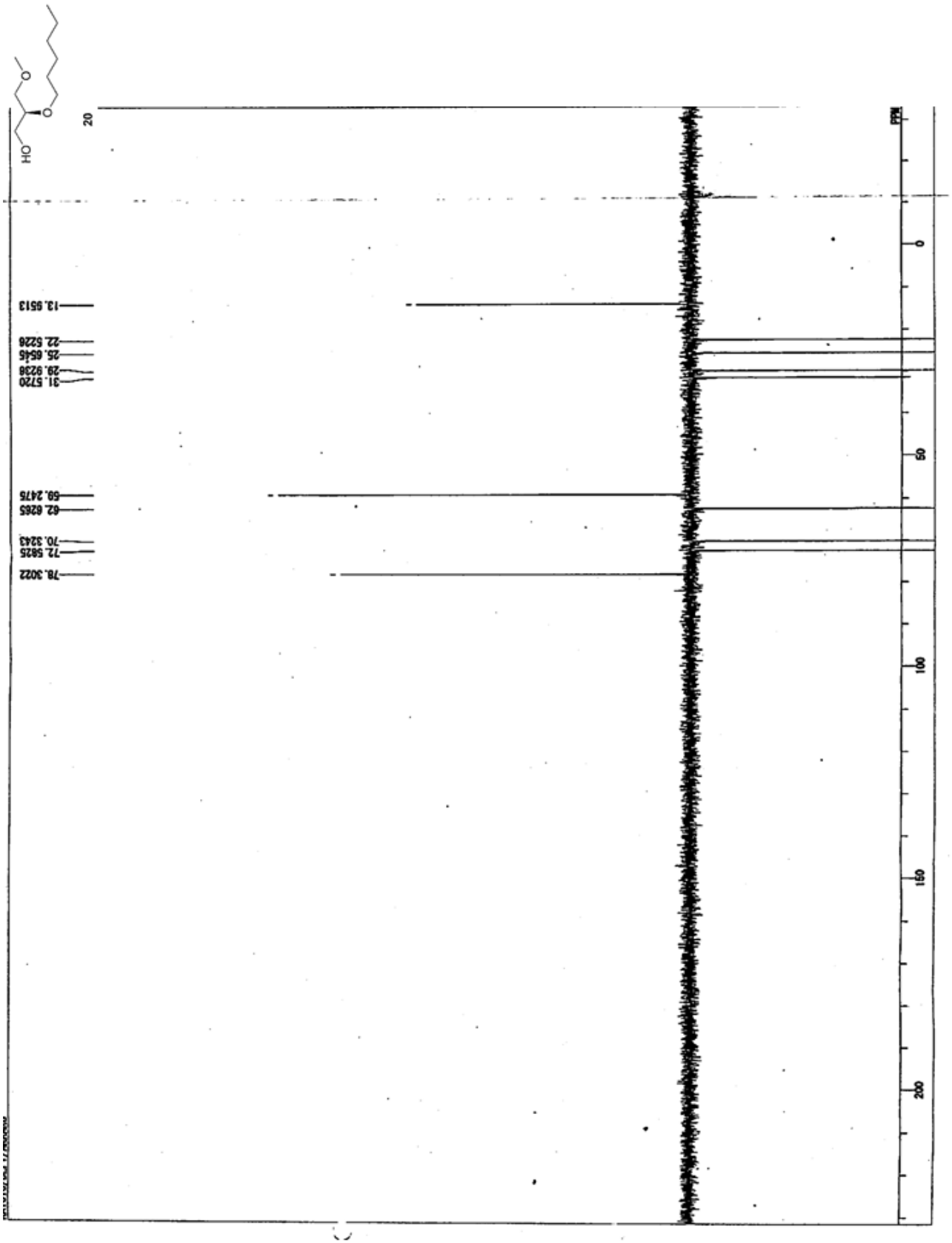
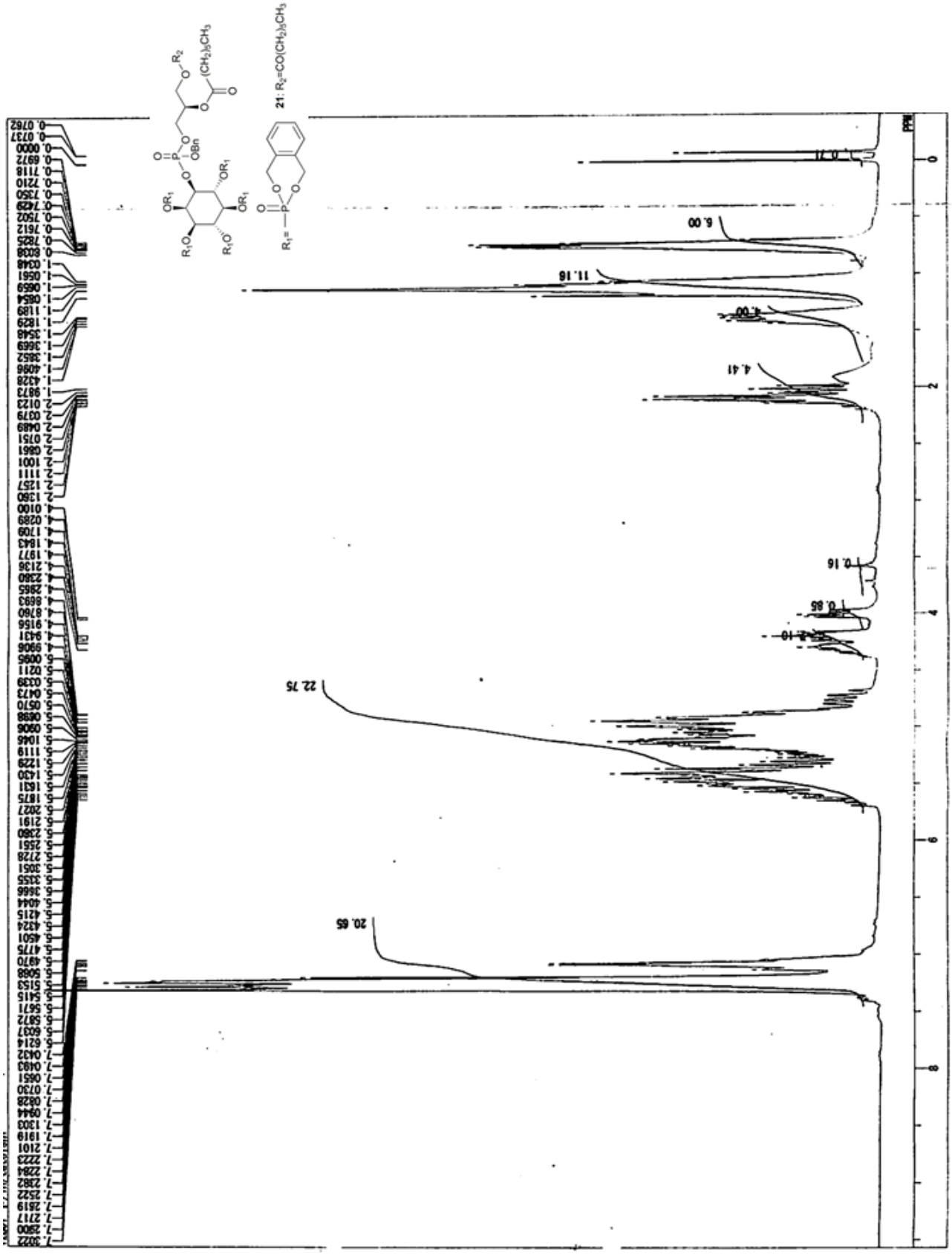
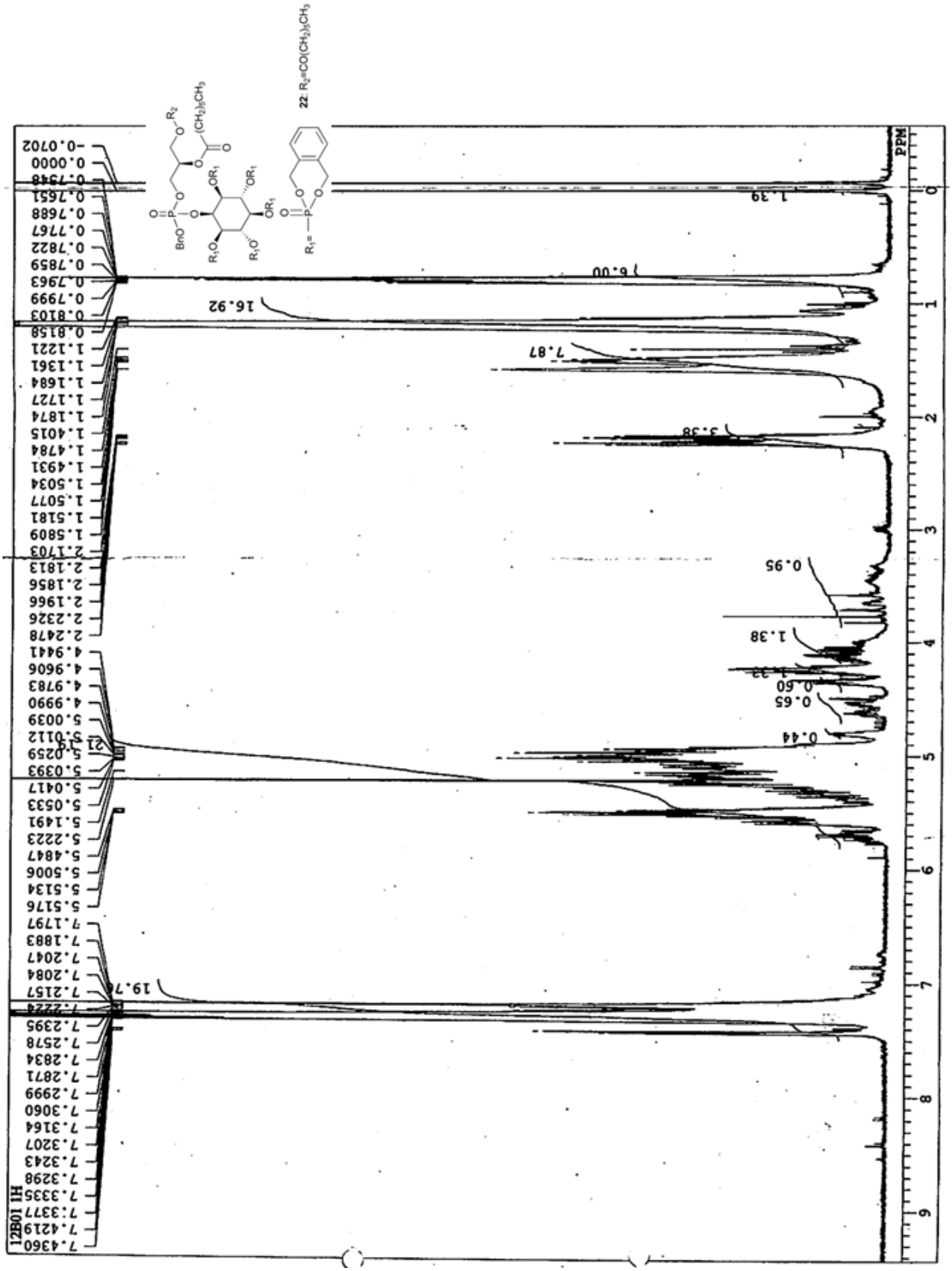
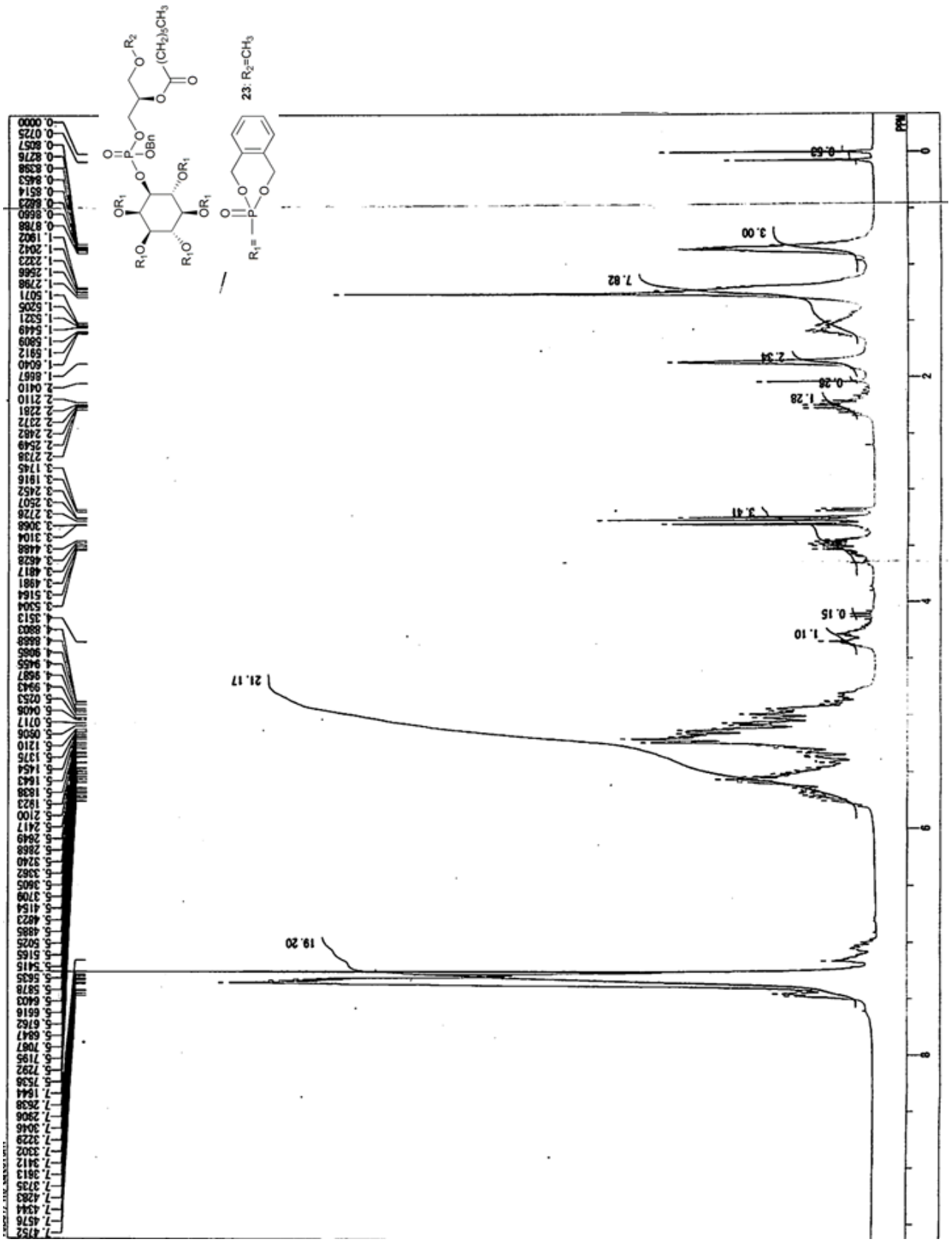
3.5091
3.5030
3.4957
3.4908
3.4695
3.4573
3.3701

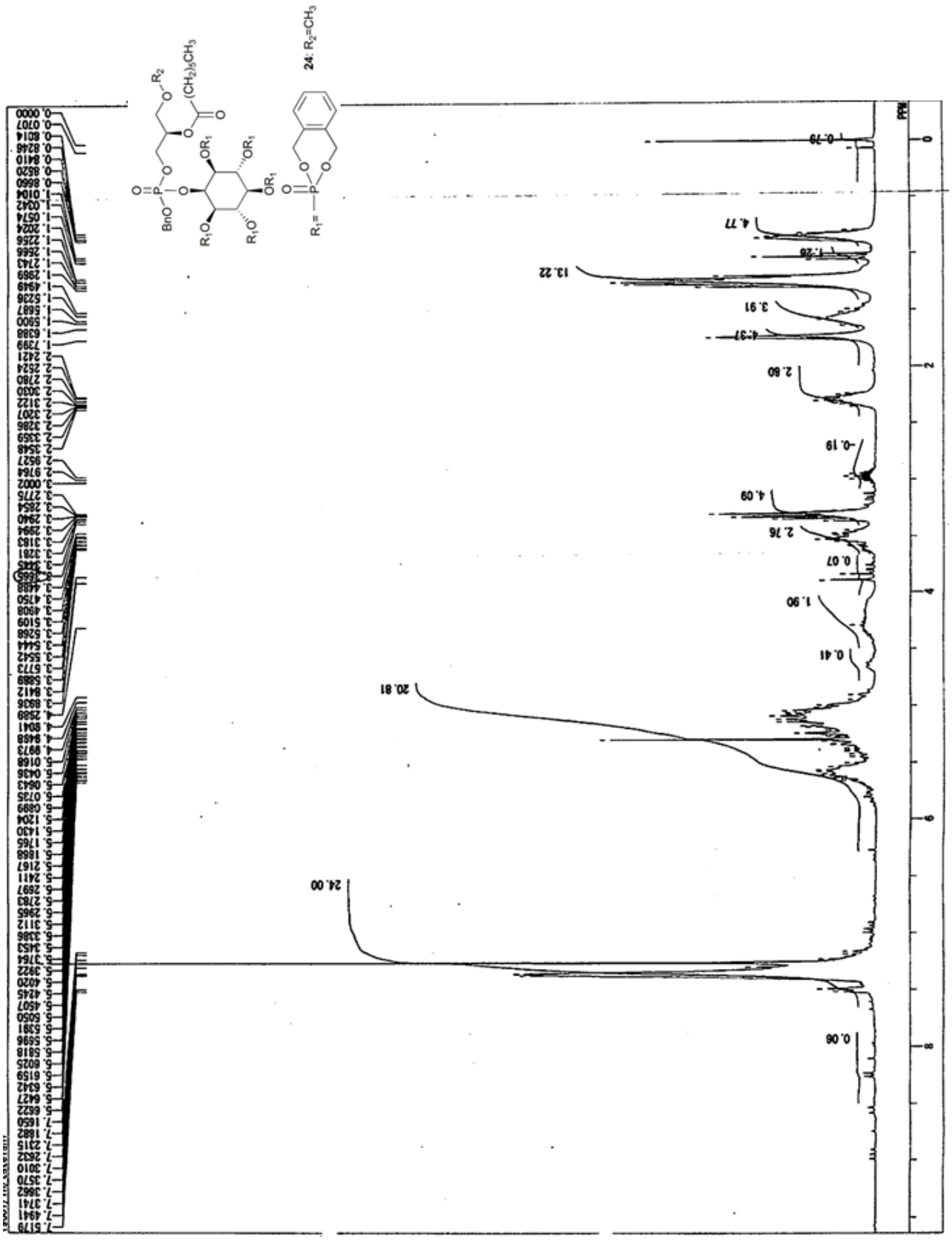

HO
O
O
20
13.9513
22.5226
25.6546
29.9236
31.5720
59.2475
62.6265
70.3243
72.5825
78.3022
PPM
0
50
100
150
200

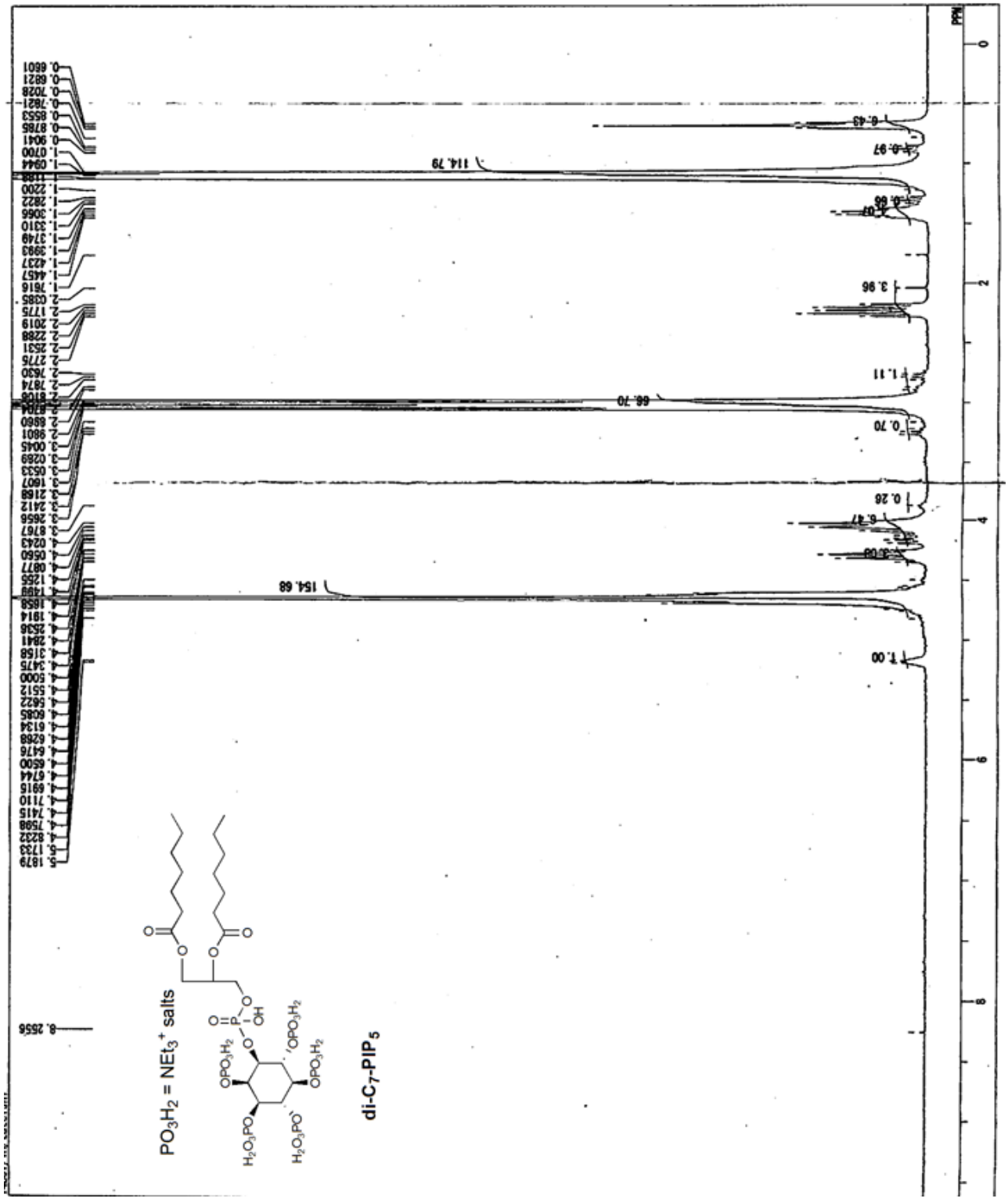
^{1}H NMR spectra (compound 21-26 and PIP_5 derivatives)

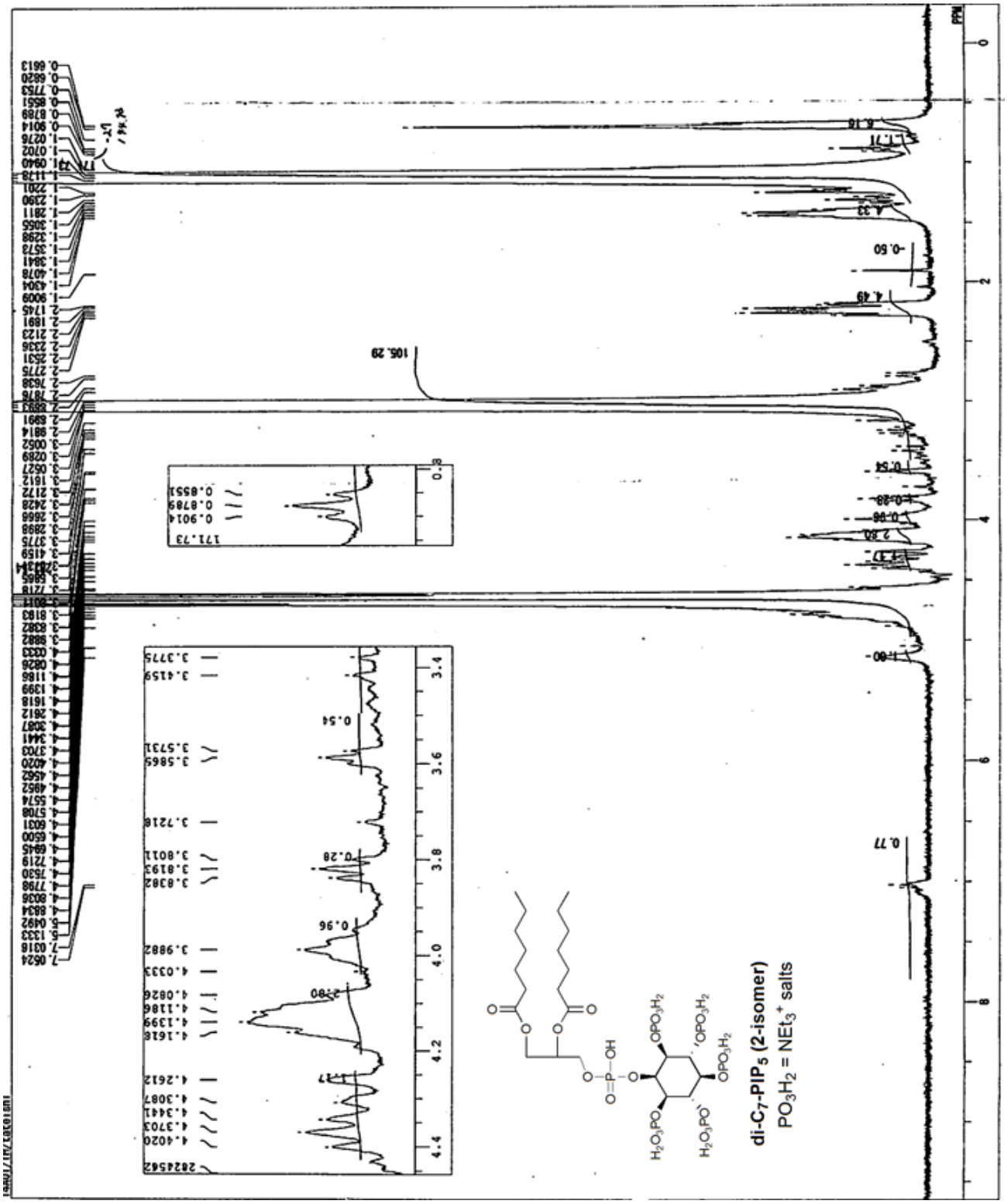


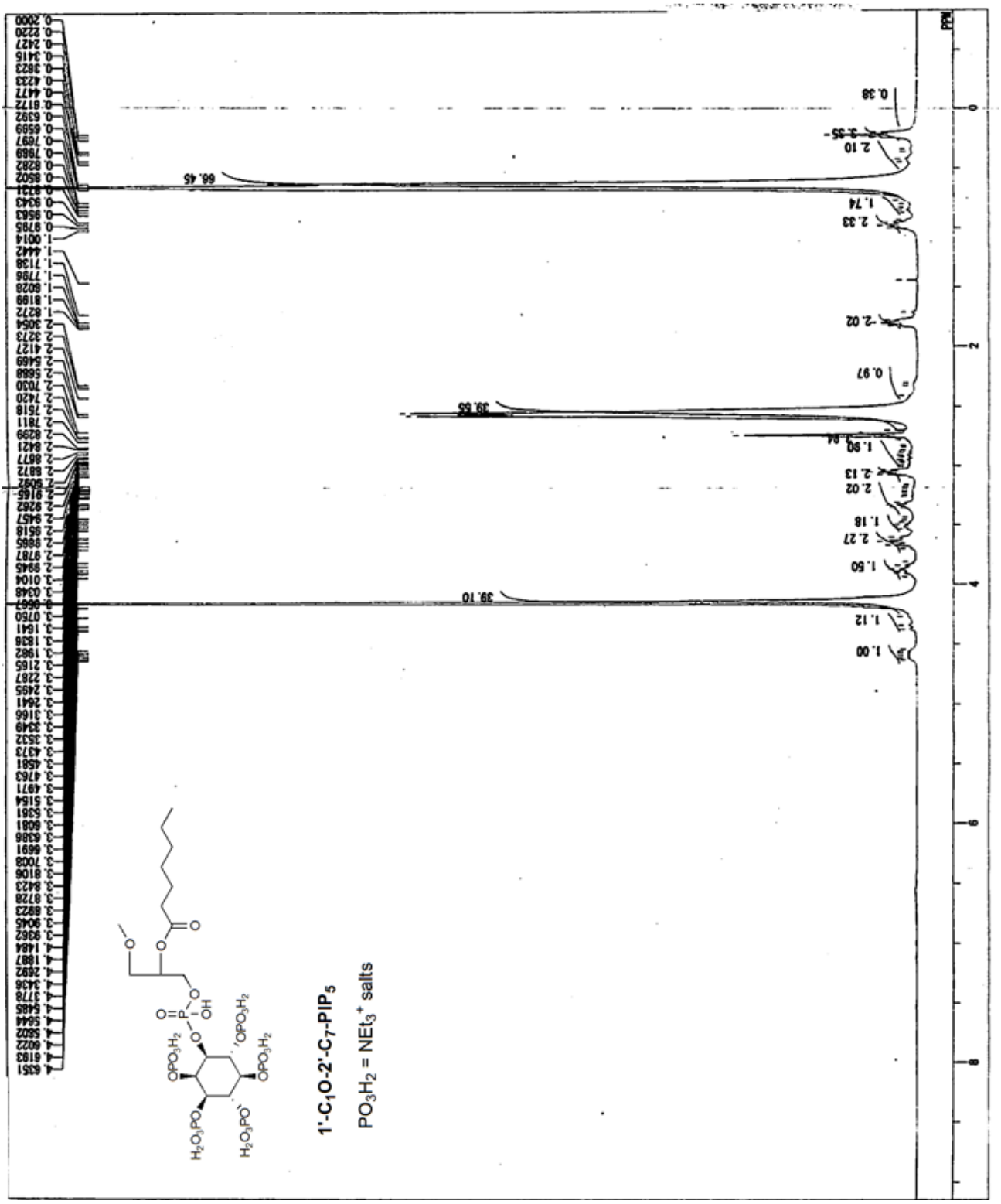

22: R2=CO(CH2)6CH3
PPM
1.39
16.00
16.92
7.87
3.38
0.95
1.38
0.65
0.60
0.44
19.76
12B01 1H

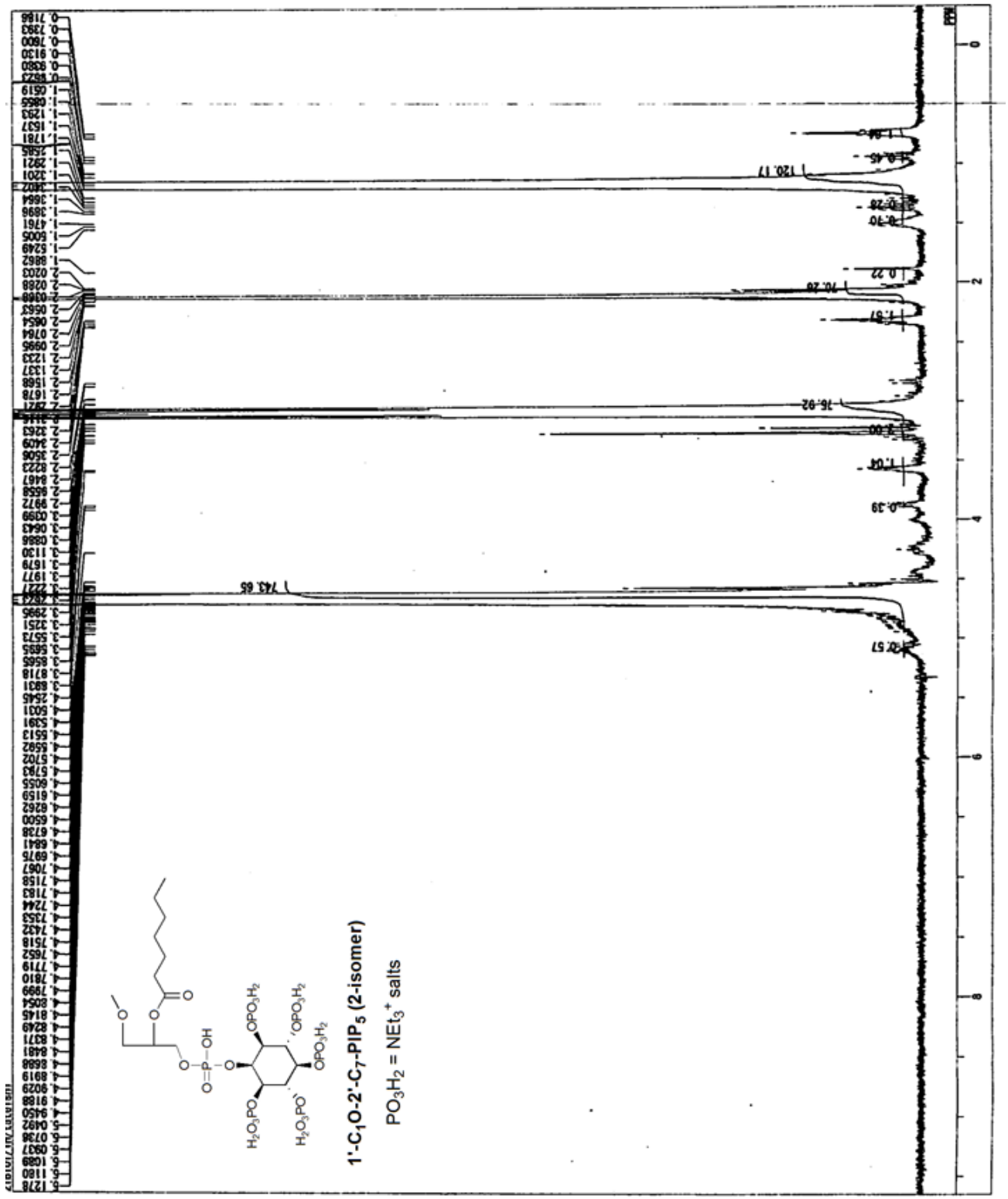

23: R2=CH3
0.63
3.00
7.82
2.34
0.28
1.28
3.41
0.15
1.10
21.17
19.20

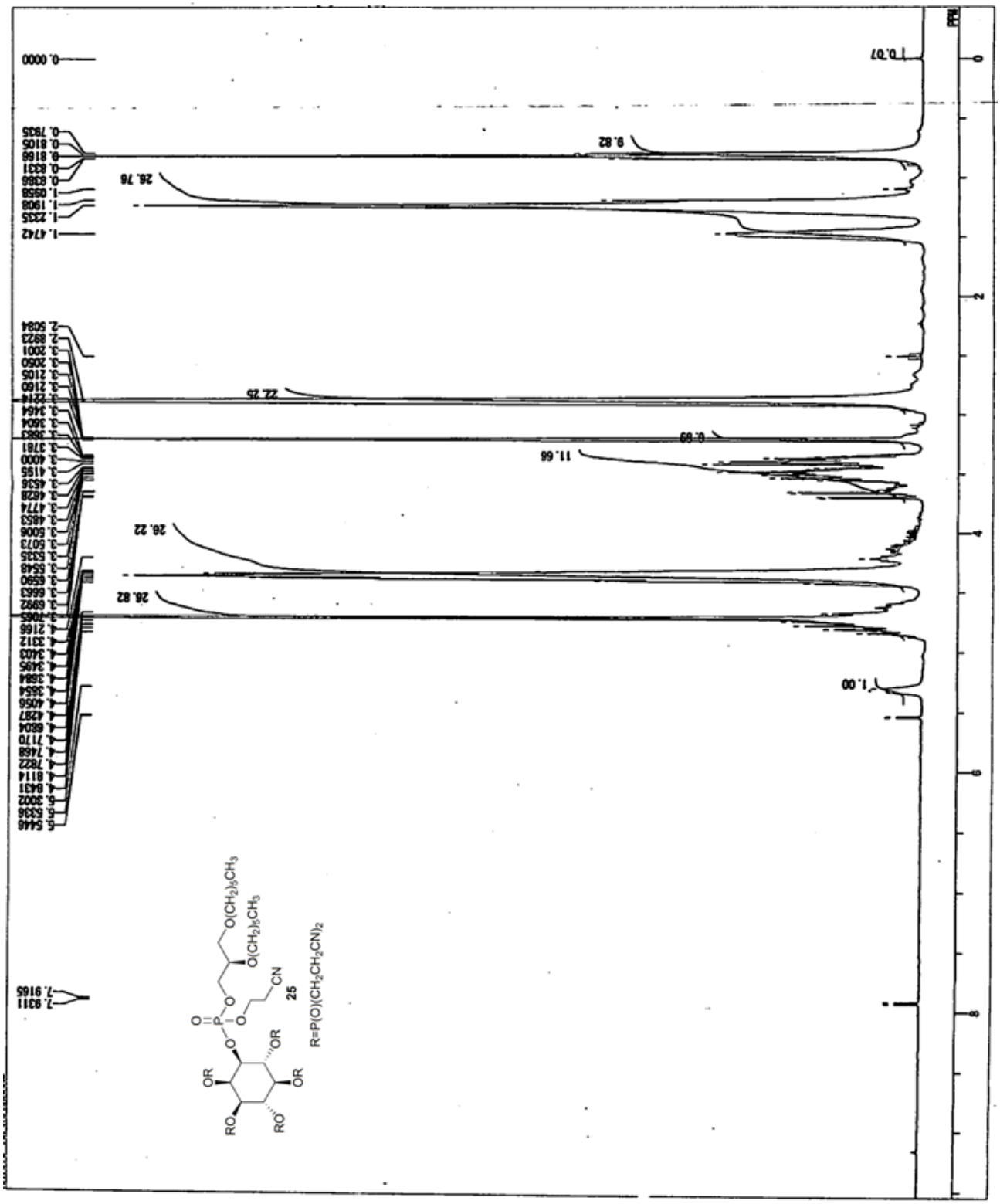

24: R2=CH3
R1=
BnO
R1O
OR1
(CH2)5CH3
R2
PPM
0.79
4.77
1.26
13.22
3.91
4.37
2.80
0.19
4.09
2.76
0.07
1.90
0.41
20.81
24.00
0.06

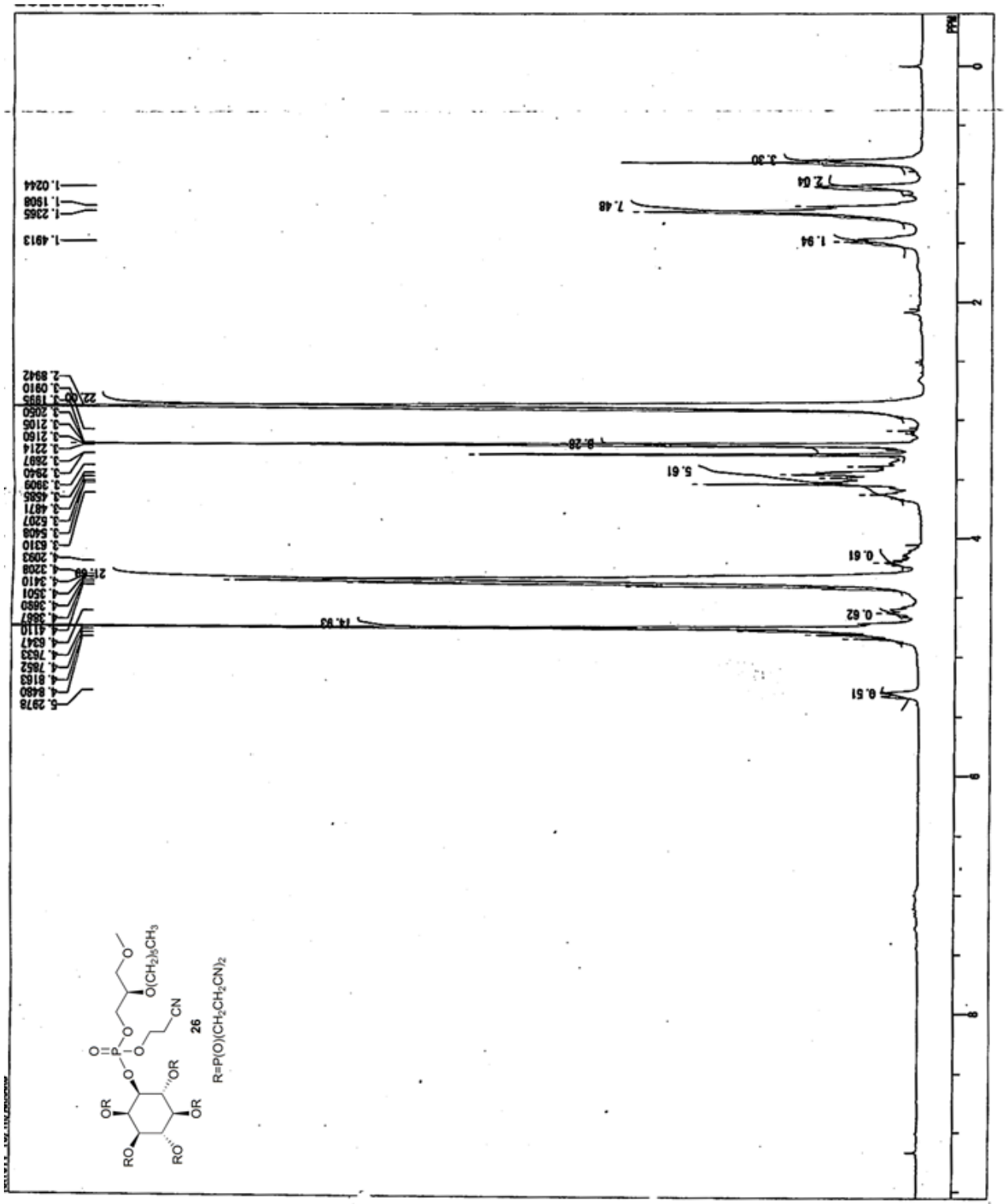

PPM
0
2
4
6
8
154.68
114.79
66.70
8.2556
1.00
0.26
0.70
1.11
3.86
6.47
6.43
6.97
6.86
PO3H2 = NEt3+ salts
di-C7-PIP5

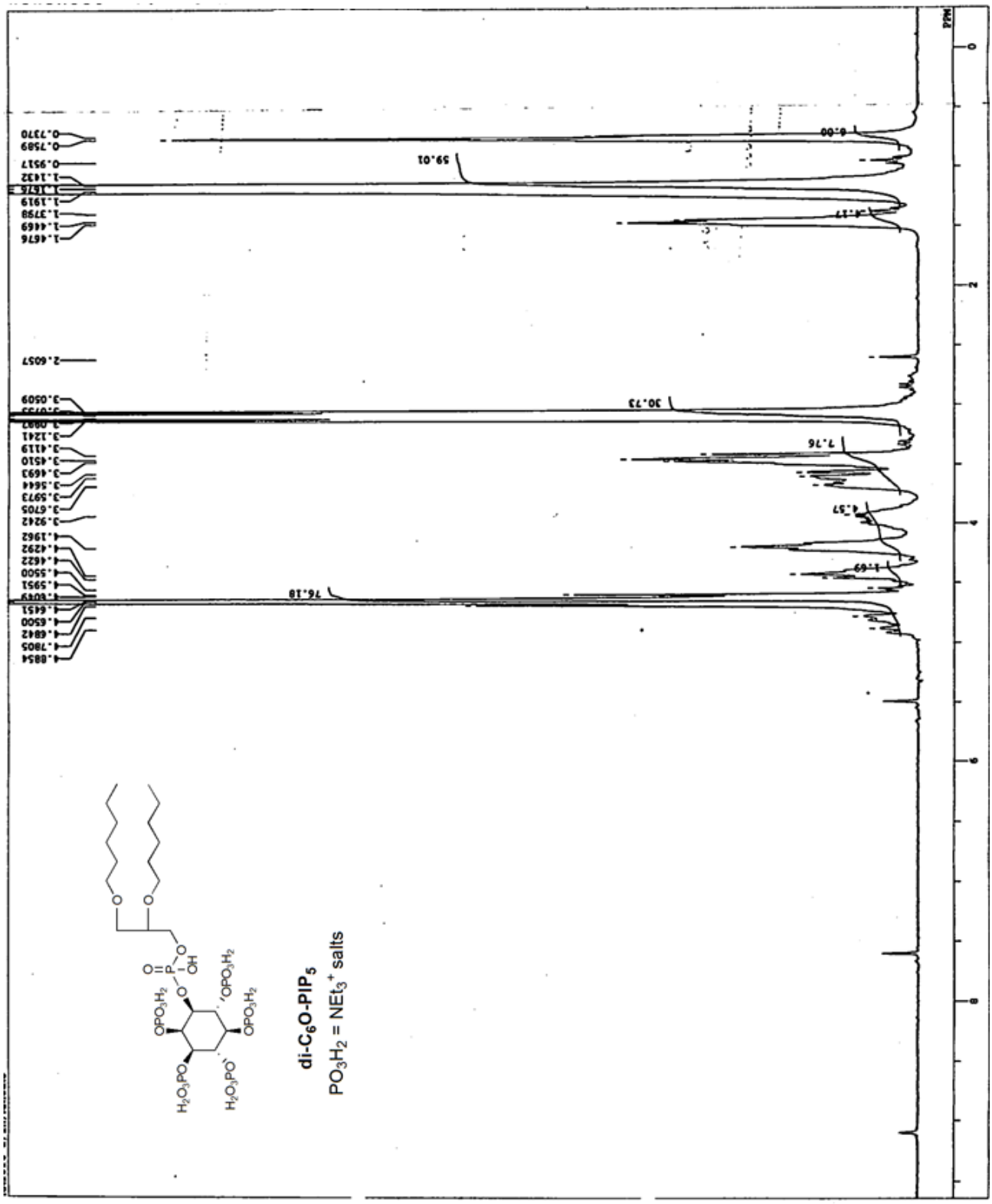

di-C7-PIP5 (2-isomer)
PO3H2 = NEt3+ salts

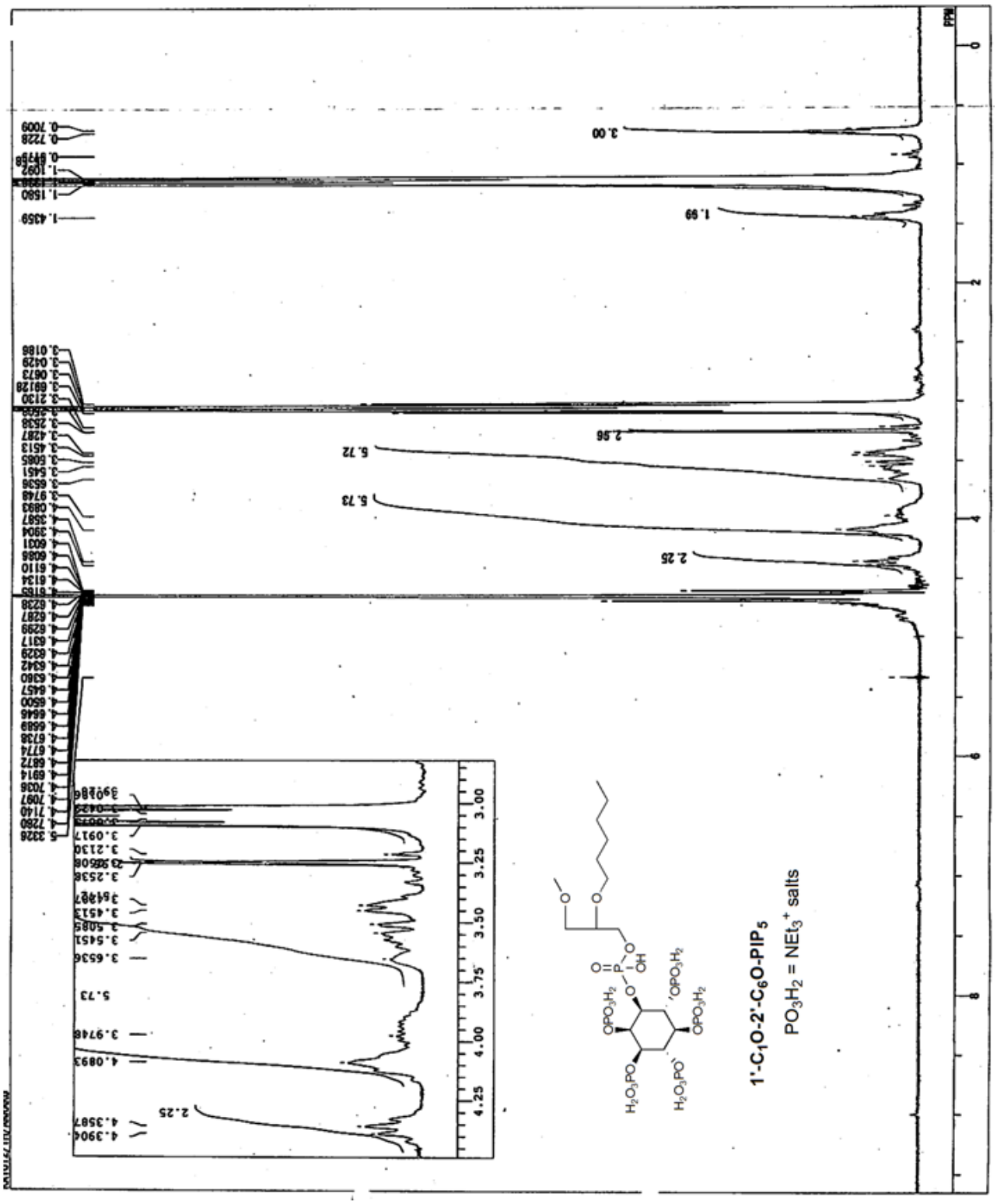

1'-C1O-2'-C7-PIP5
PO3H2 = NEt3+ salts


1'-C1O-2'-C7-PIP5 (2-isomer)
PO3H2 = NEt3+ salts


0.0000
0.7835
0.8105
0.8166
0.8231
0.8386
1.0958
1.1908
1.2235
1.4742
2.5084
2.8923
3.2001
3.2060
3.2105
3.2160
3.2214
3.3464
3.3604
3.3883
3.3781
3.4000
3.4195
3.4536
3.4628
3.4774
3.4853
3.5006
3.5073
3.5325
3.5548
3.5590
3.6663
3.6992
3.7065
4.2166
4.3312
4.3403
4.3495
4.3584
4.3654
4.4056
4.4287
4.6804
4.7170
4.7468
4.7822
4.8114
5.8431
5.3002
5.5236
5.5446
7.8311
7.9165
7.0.07
9.82
26.76
22.25
0.89
11.66
26.22
26.82
1.00
PPM
0
2
4
6
8
O(CH2)5CH3
O(CH2)5CH3
CN
25
R=P(O)(CH2CH2CN)2
OR
RO


26
R=P(O)(CH2CH2CN)2


di-C6O-PIP5
PO3H2 = NEt3+ salts


1'-C10-2'-C6O-PIP5
PO3H2 = NEt3+ salts