Supporting Information

Synthesis and Evaluation of a Series of C3-Substituted CBI Analogues of CC 1065 and the Duocarmycins

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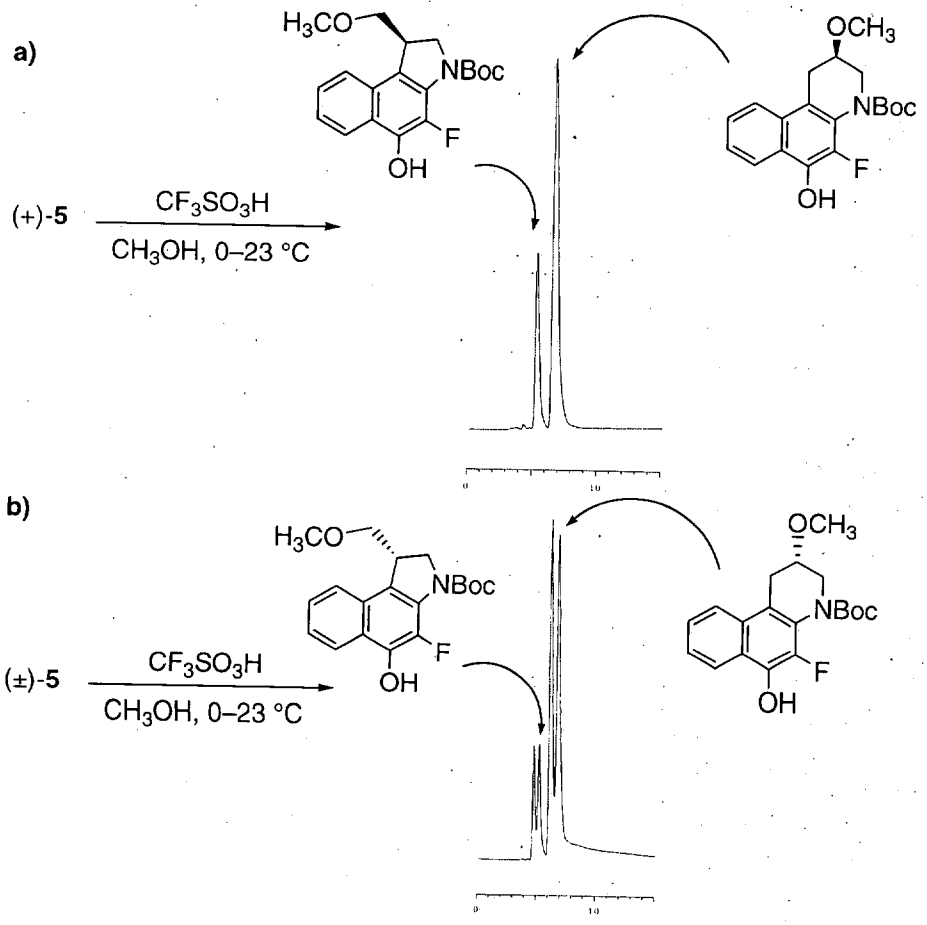


Figure 9. HPLC analysis (Chiralcel OD, 10% *i*-PrOH in hexanes) of the acid-catalyzed addition of methanol to a) (+)-**5** and b) (±)-**5**.

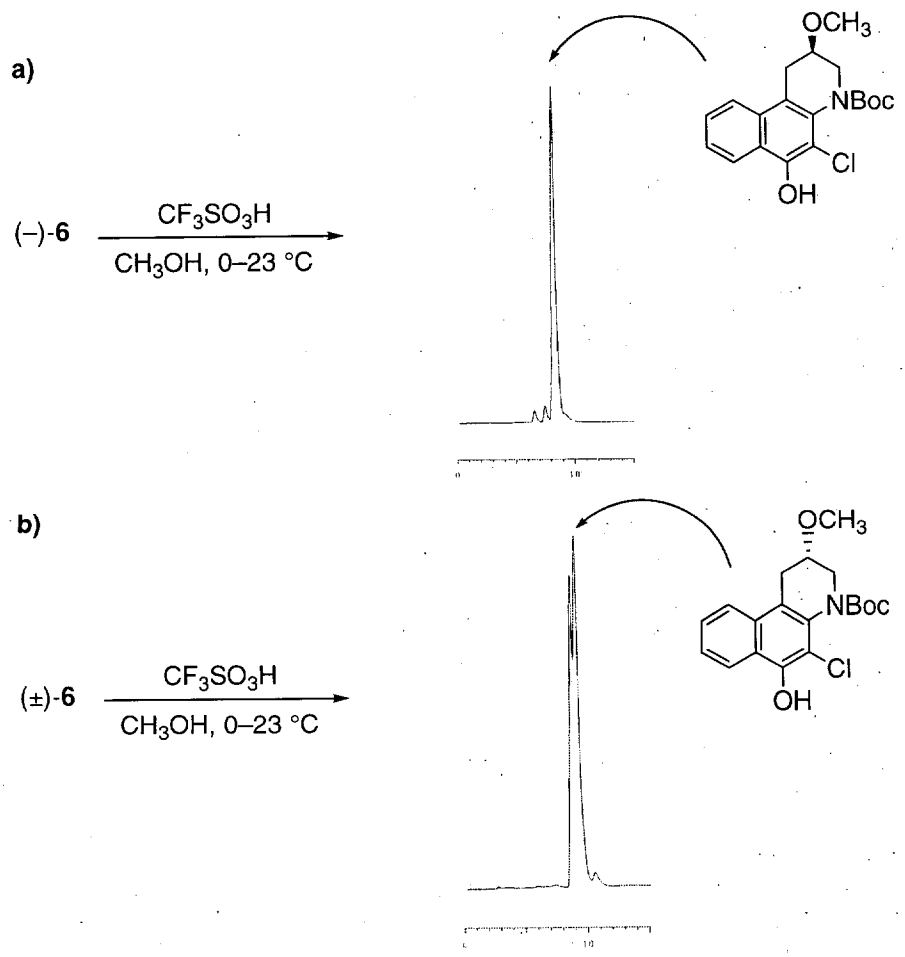


Figure 10. HPLC analysis (Chiralcel OD, 10% *i*-PrOH in hexanes) of the acid-catalyzed addition of methanol to a) (–)-**6** and b) (±)-**6**.

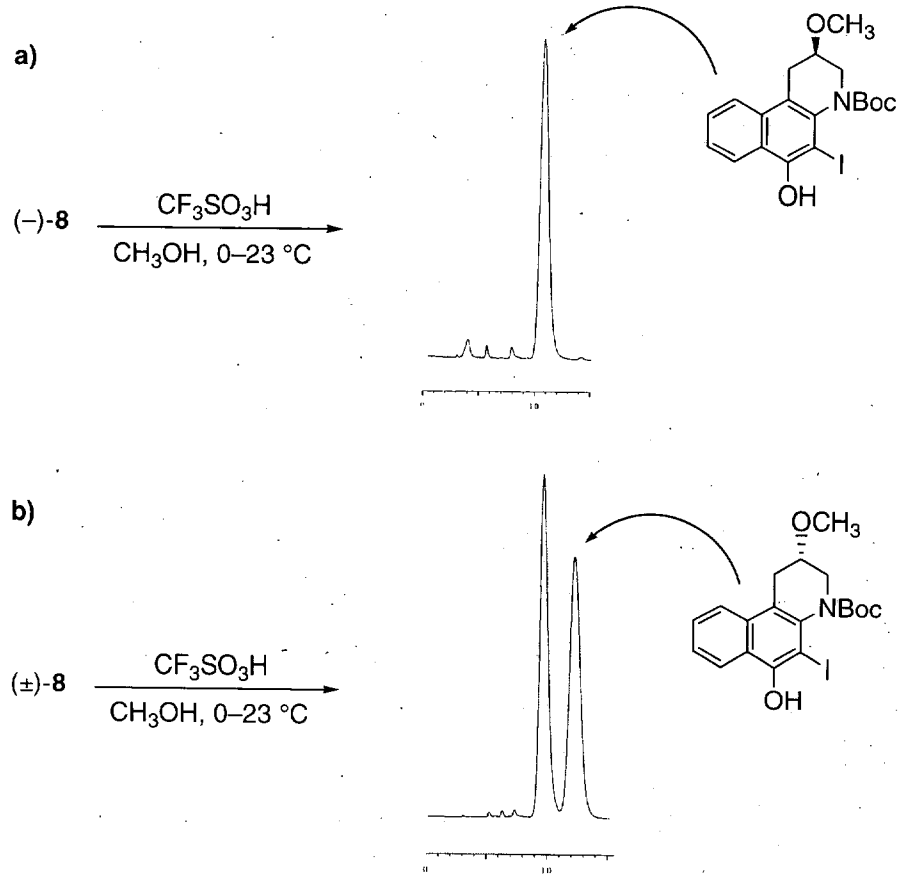


Figure 11. HPLC analysis (Chiralcel AD, 10% *i*-PrOH in hexanes) of the acid-catalyzed addition of methanol to a) (–)-**8** and b) (±)-**8**.

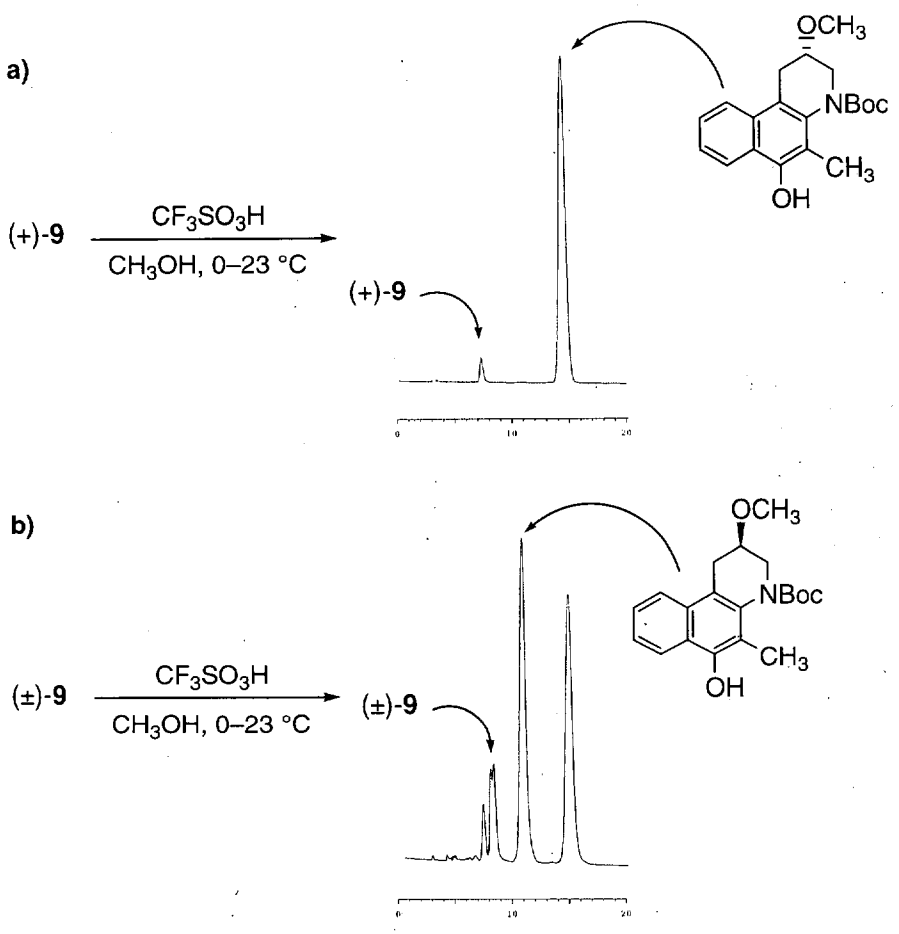
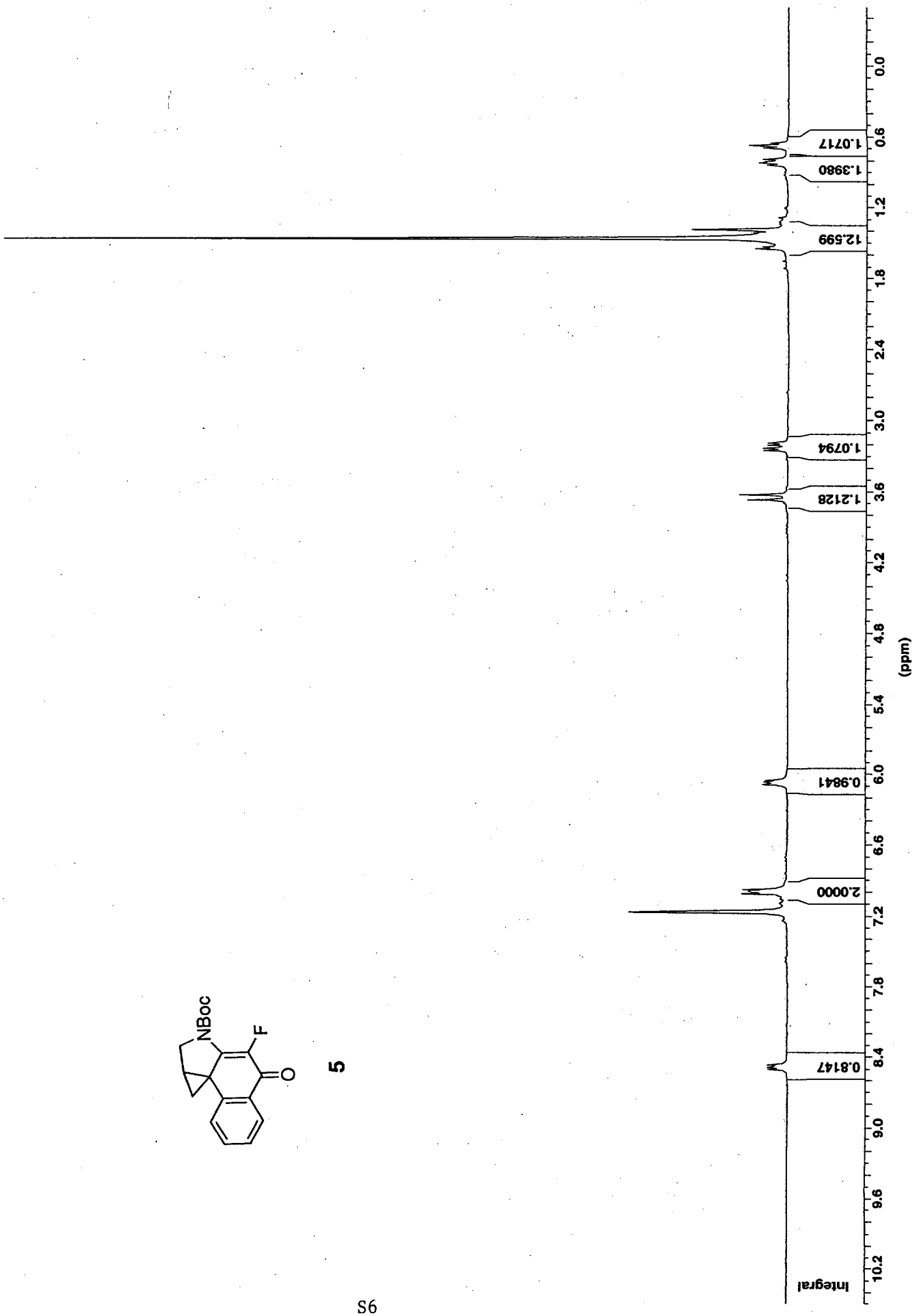


Figure 12. HPLC analysis (Chiralcel AD, 10% *i*-PrOH in hexanes) of the acid-catalyzed addition of methanol to a) (+)-**9** and b) (±)-**9**.



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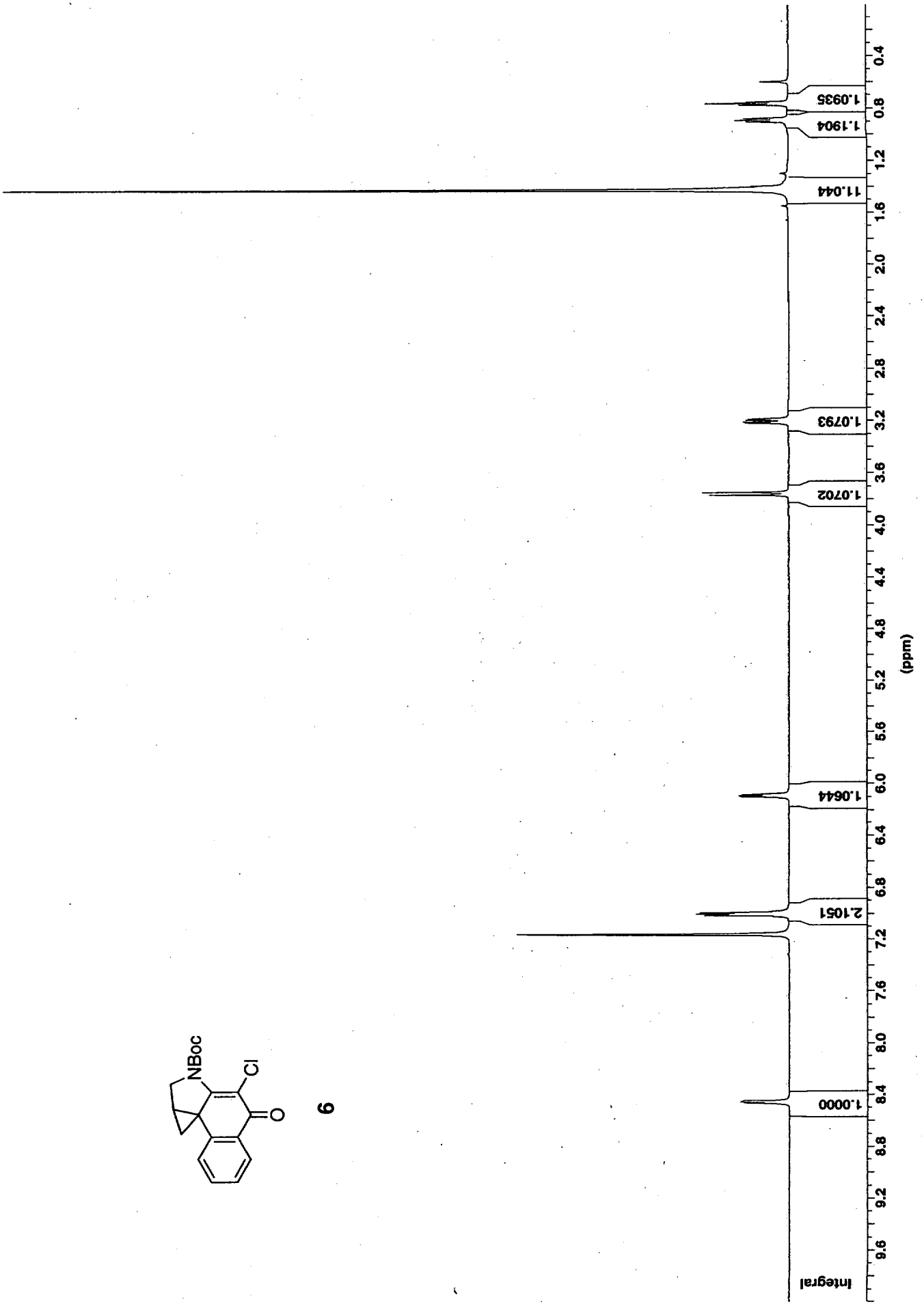
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11.044
1.0793
1.0702
1.0644
2.1051
1.0000
Integral
(ppm)
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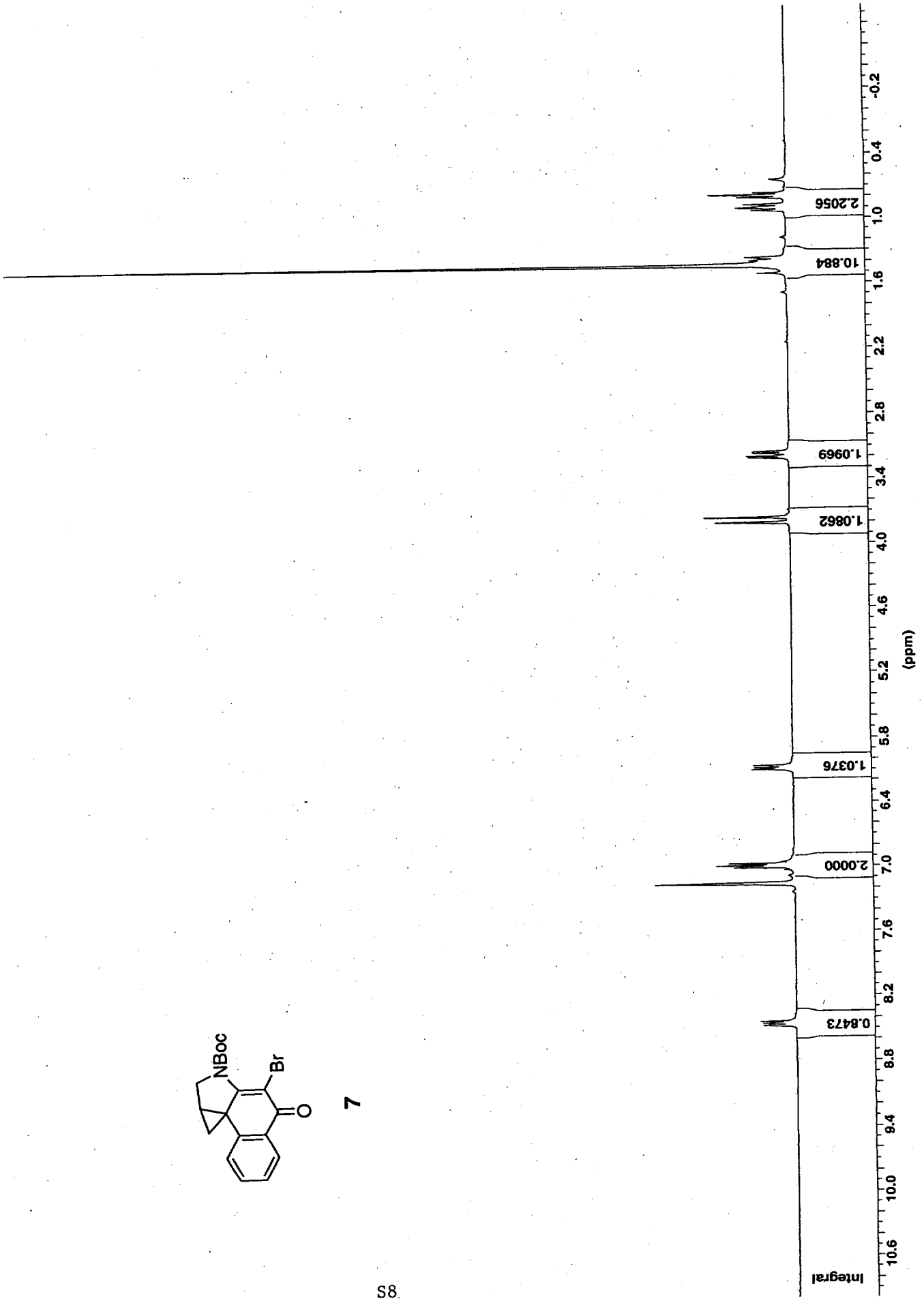
0.8
1.2
1.6
2.0
2.4
2.8
3.2
3.6
4.0
4.4
4.8
5.2
5.6
6.0
6.4
6.8
7.2
7.6
8.0
8.4
8.8
9.2
9.6

NBoc
Cl
O

6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1.0969
1.0862
1.0376
2.0000
0.8473
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(ppm)
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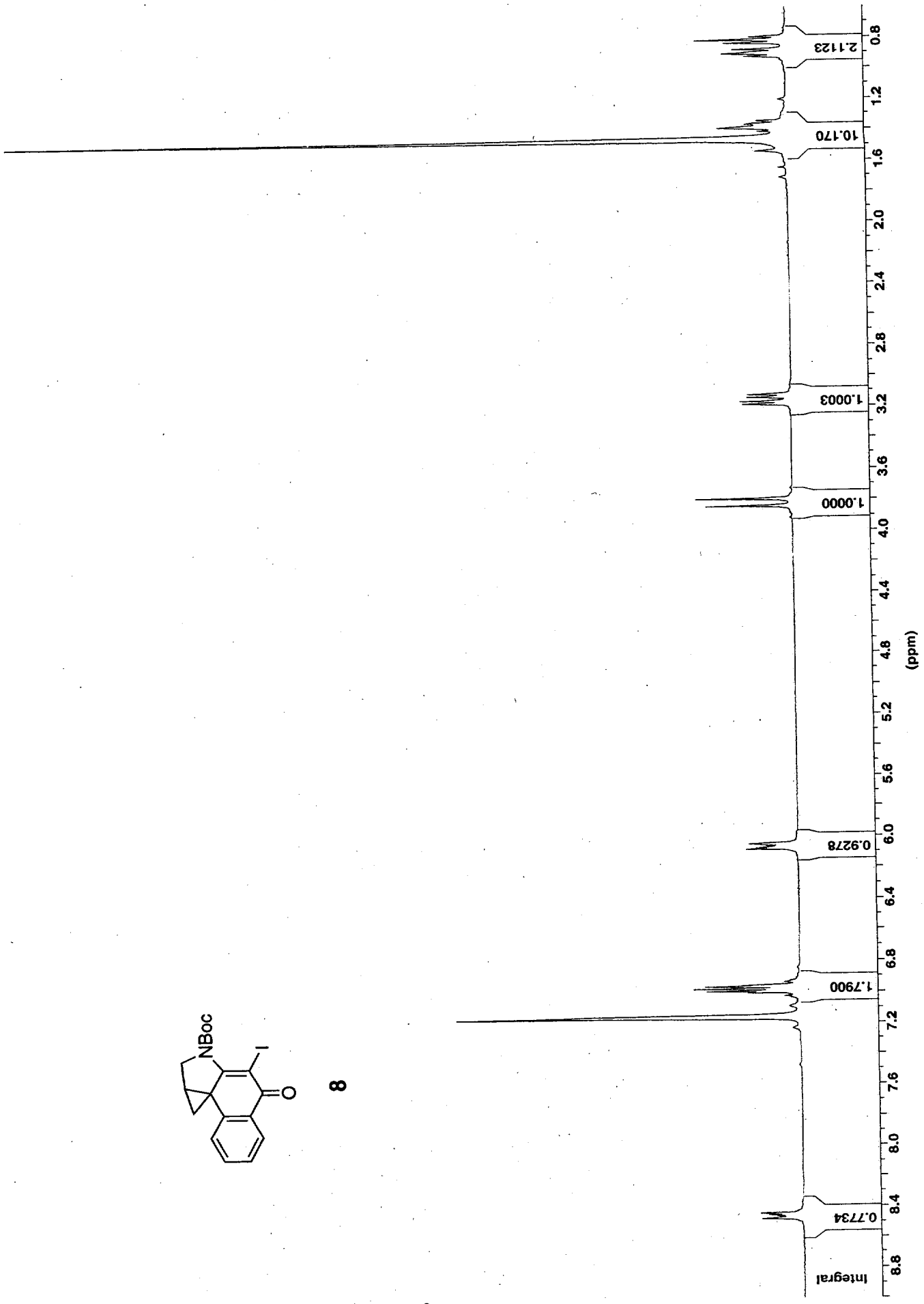
0.4
1.0
1.6
2.2
2.8
3.4
4.0
4.6
5.2
5.8
6.4
7.0
7.6
8.2
8.8
9.4
10.0
10.6

NBoc
Br
O

7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1.0003
1.0000
0.9278
1.7900
0.7734
Integral
(ppm)
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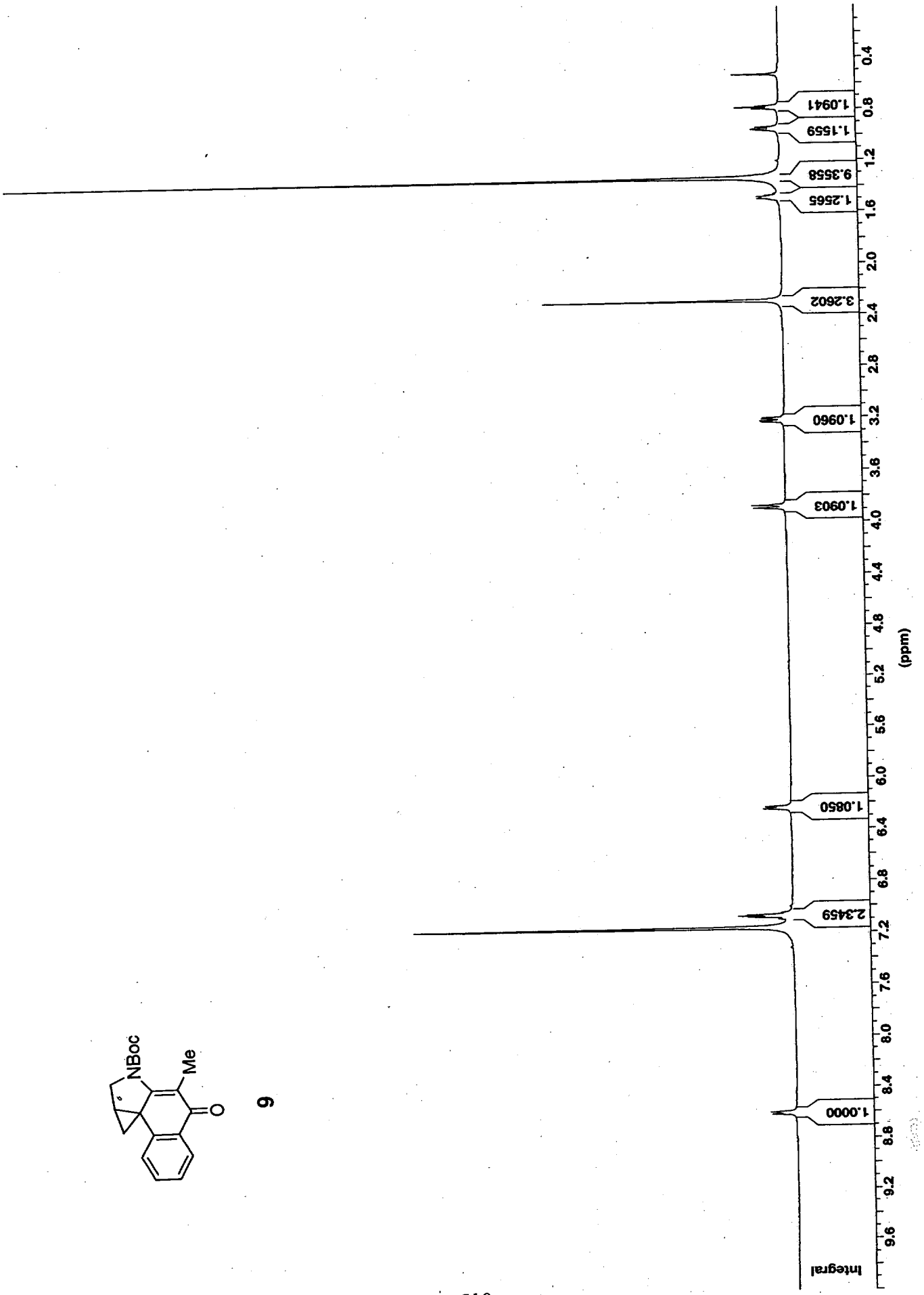
1.2
1.6
2.0
2.4
2.8
3.2
3.6
4.0
4.4
4.8
5.2
5.6
6.0
6.4
6.8
7.2
7.6
8.0
8.4
8.8
NBoc
O

8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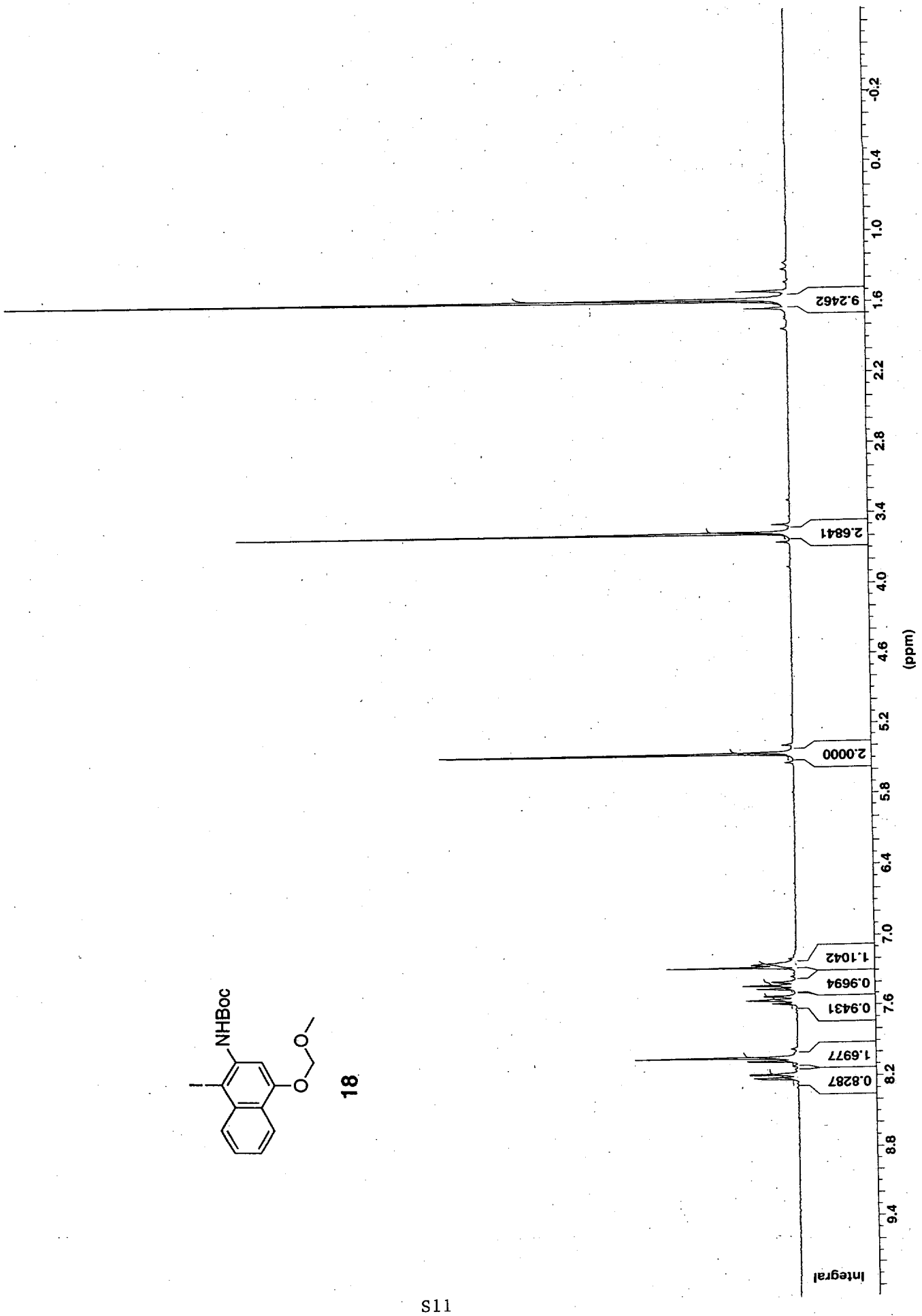
9.3558
1.2565
3.2602
1.0960
1.0903
1.0850
2.3459
1.0000
Integral
(ppm)
0.4
0.8
1.2
1.6
2.0
2.4
2.8
3.2
3.6
4.0
4.4
4.8
5.2
5.6
6.0
6.4
6.8
7.2
7.6
8.0
8.4
8.8
9.2
9.6

NBoc
Me
O

6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2.0000
1.1042
0.9694
0.9431
1.6977
0.8287
Integral
(ppm)
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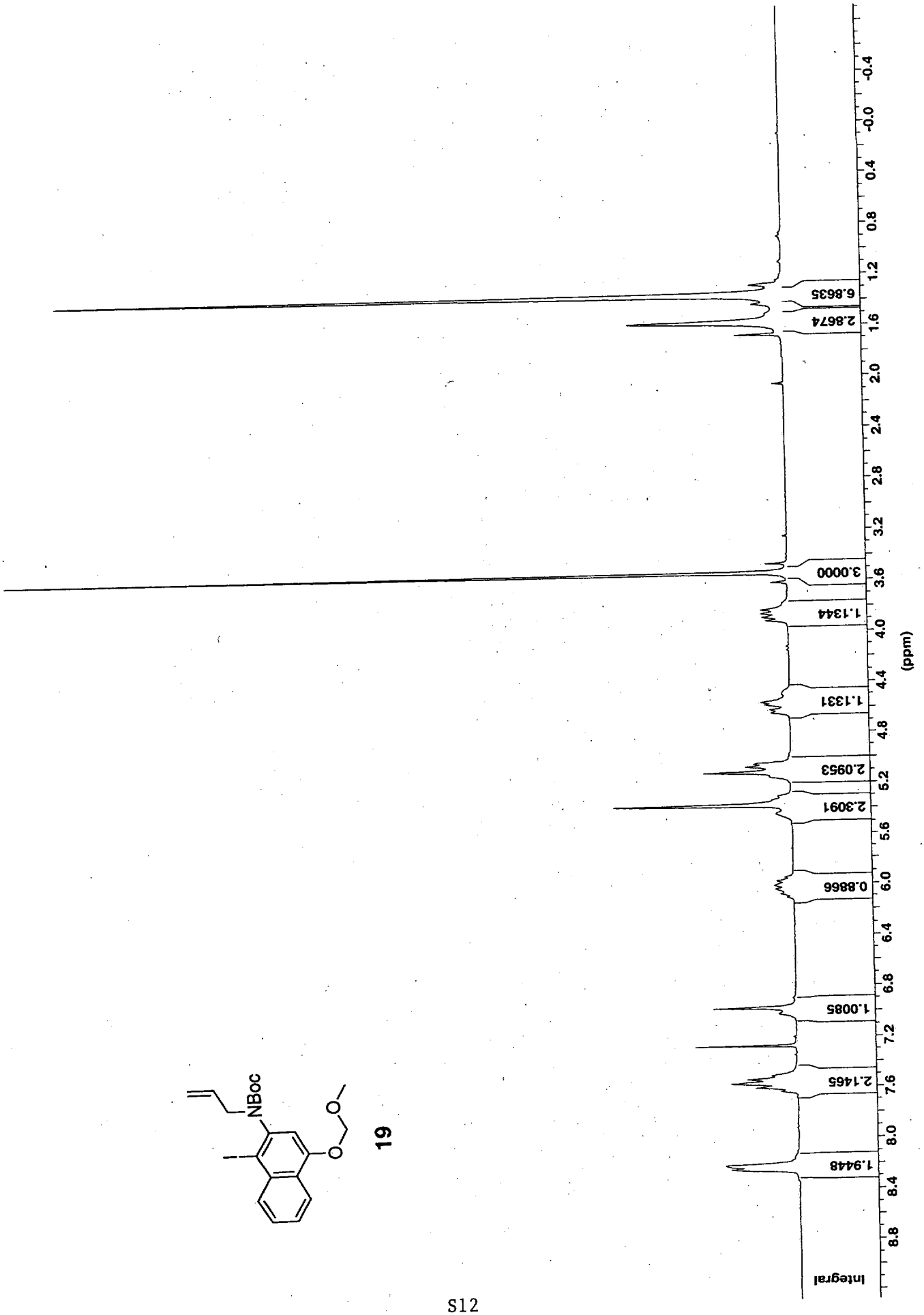
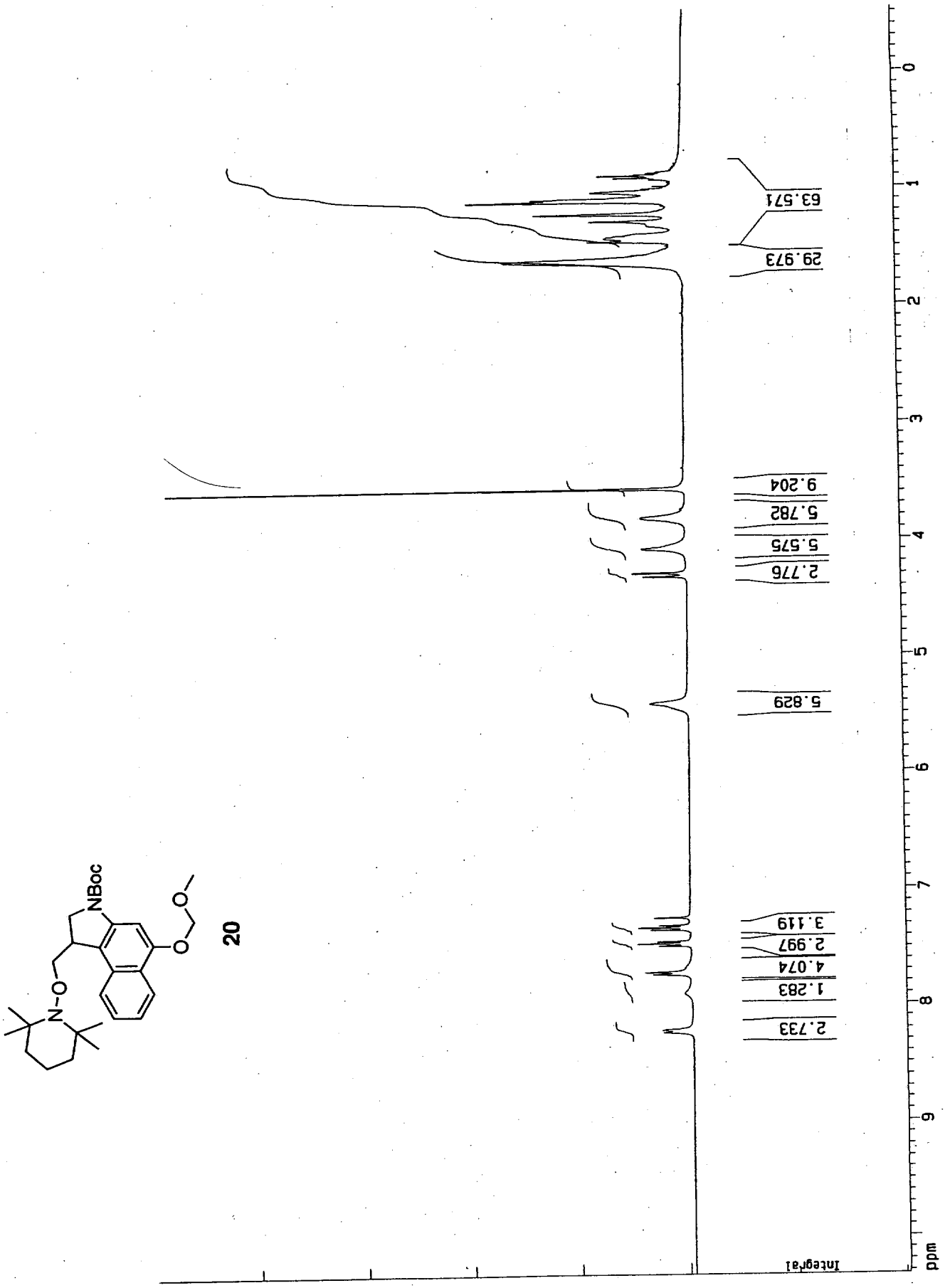
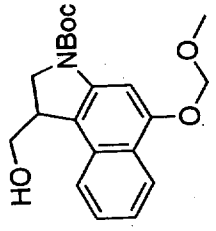
0.4
1.0
1.6
2.2
2.8
3.4
4.0
4.6
5.2
5.8
6.4
7.0
7.6
8.2
8.8
9.4

NHBoc
O
O

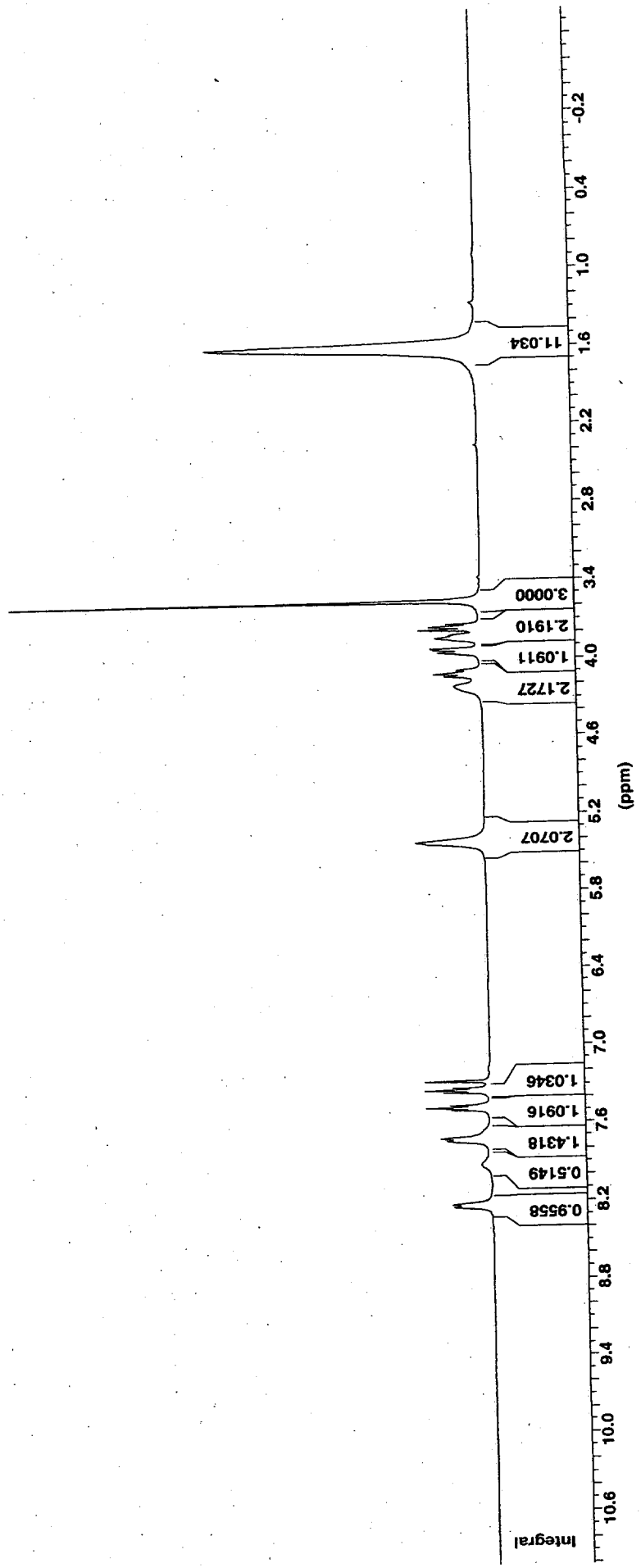
18






NBoc
O
O
HO

21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3.0000
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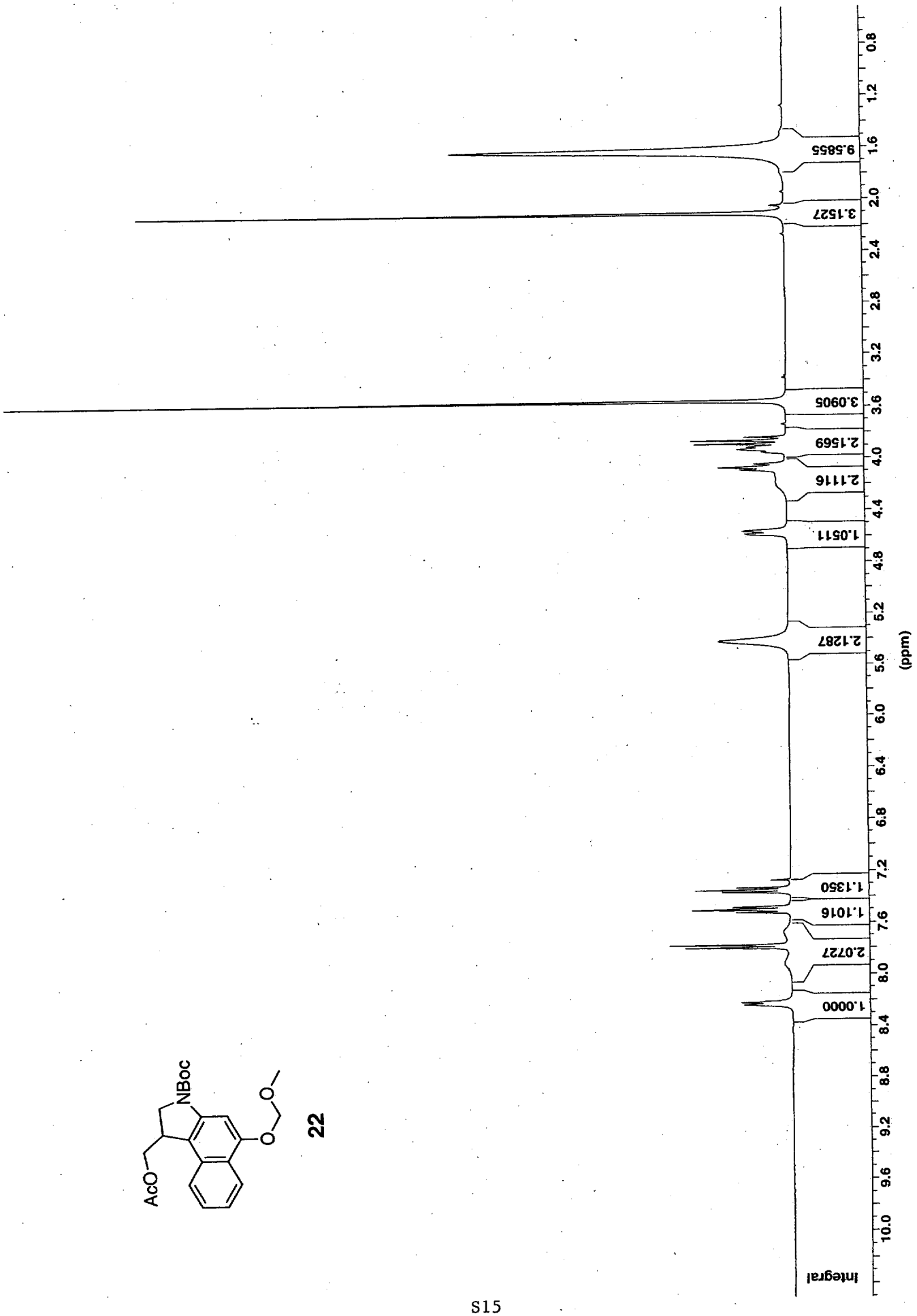
2.1727
2.0707
1.0346
1.0916
1.4318
0.5149
0.9558
Integral
(ppm)



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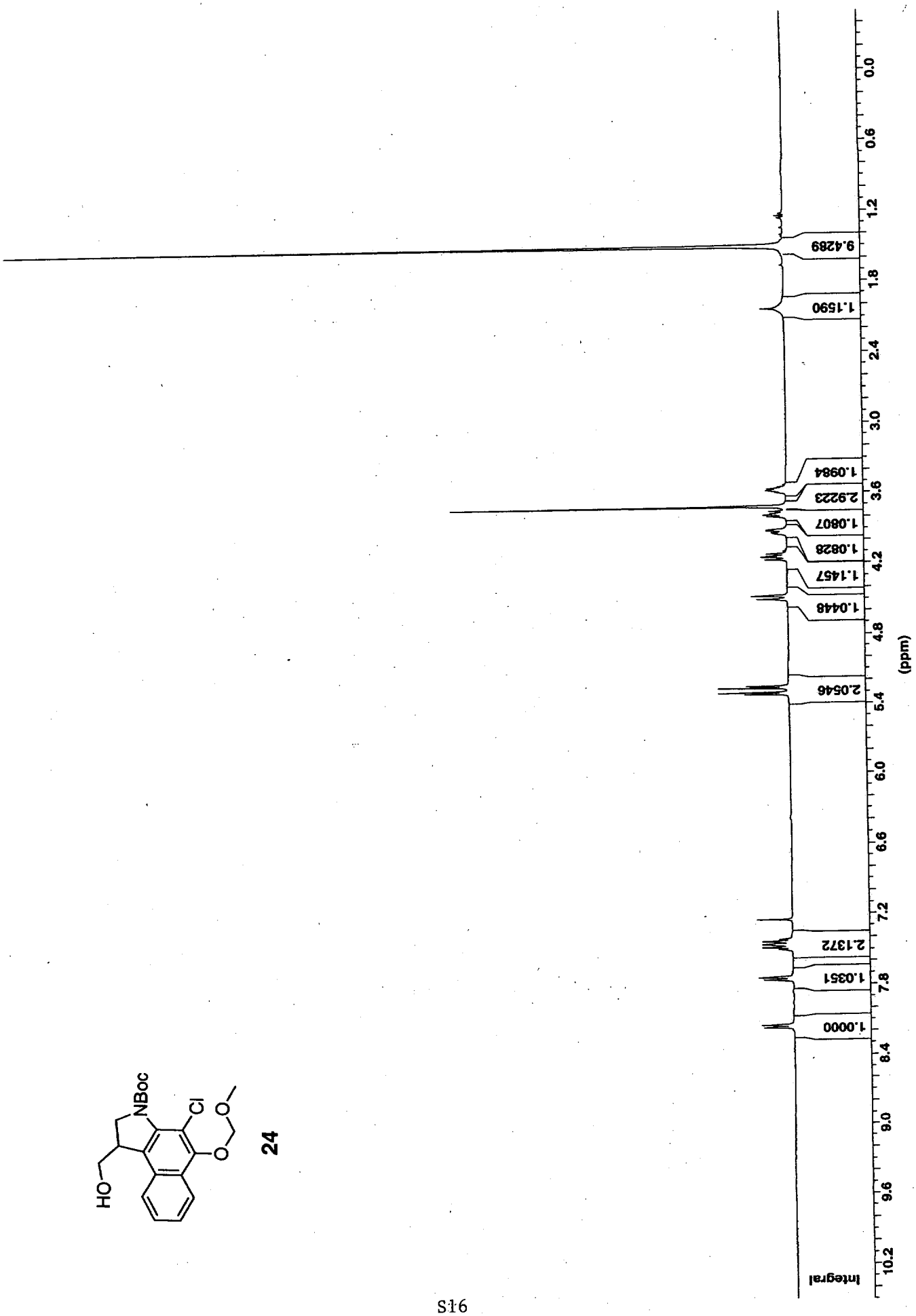

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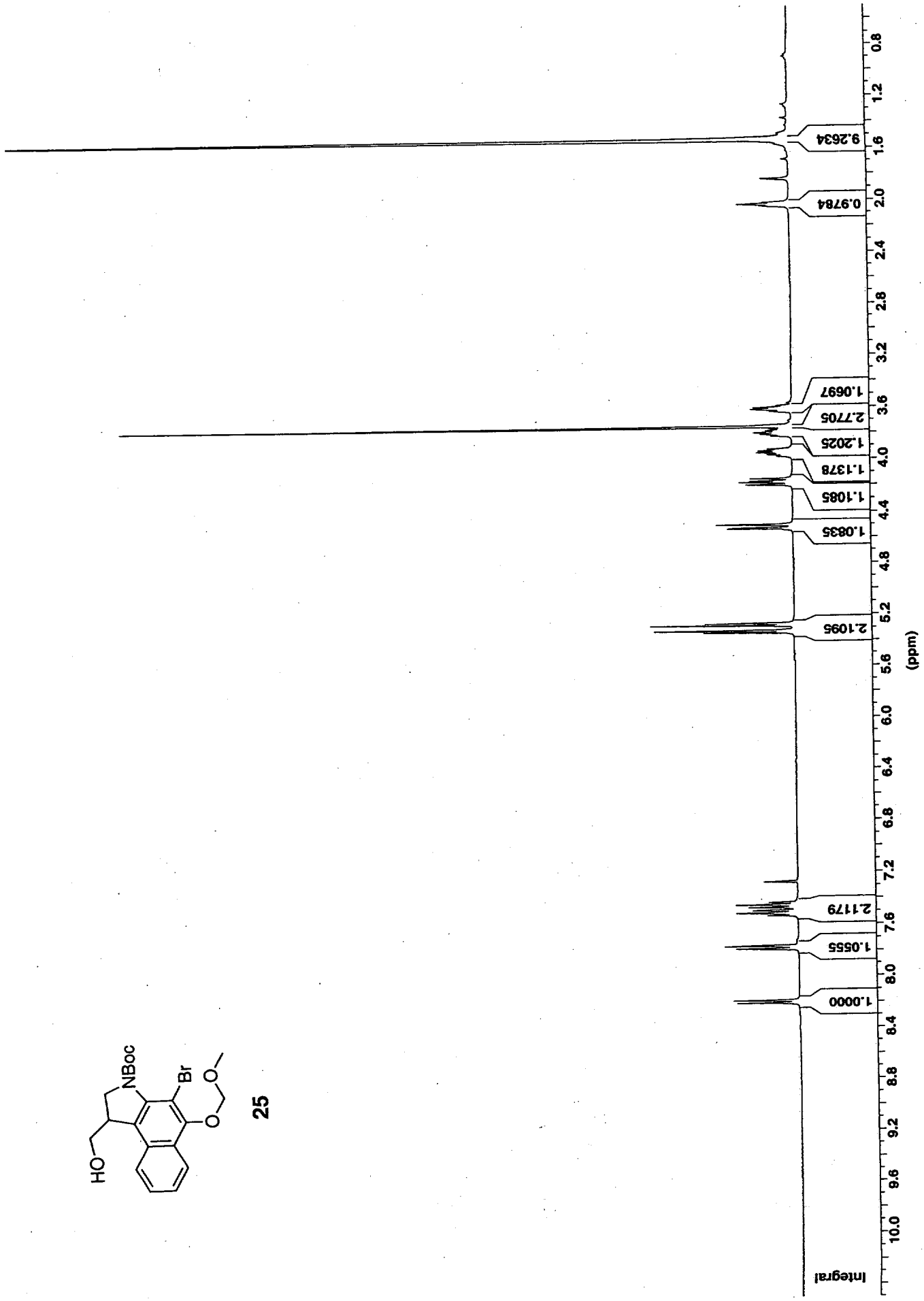
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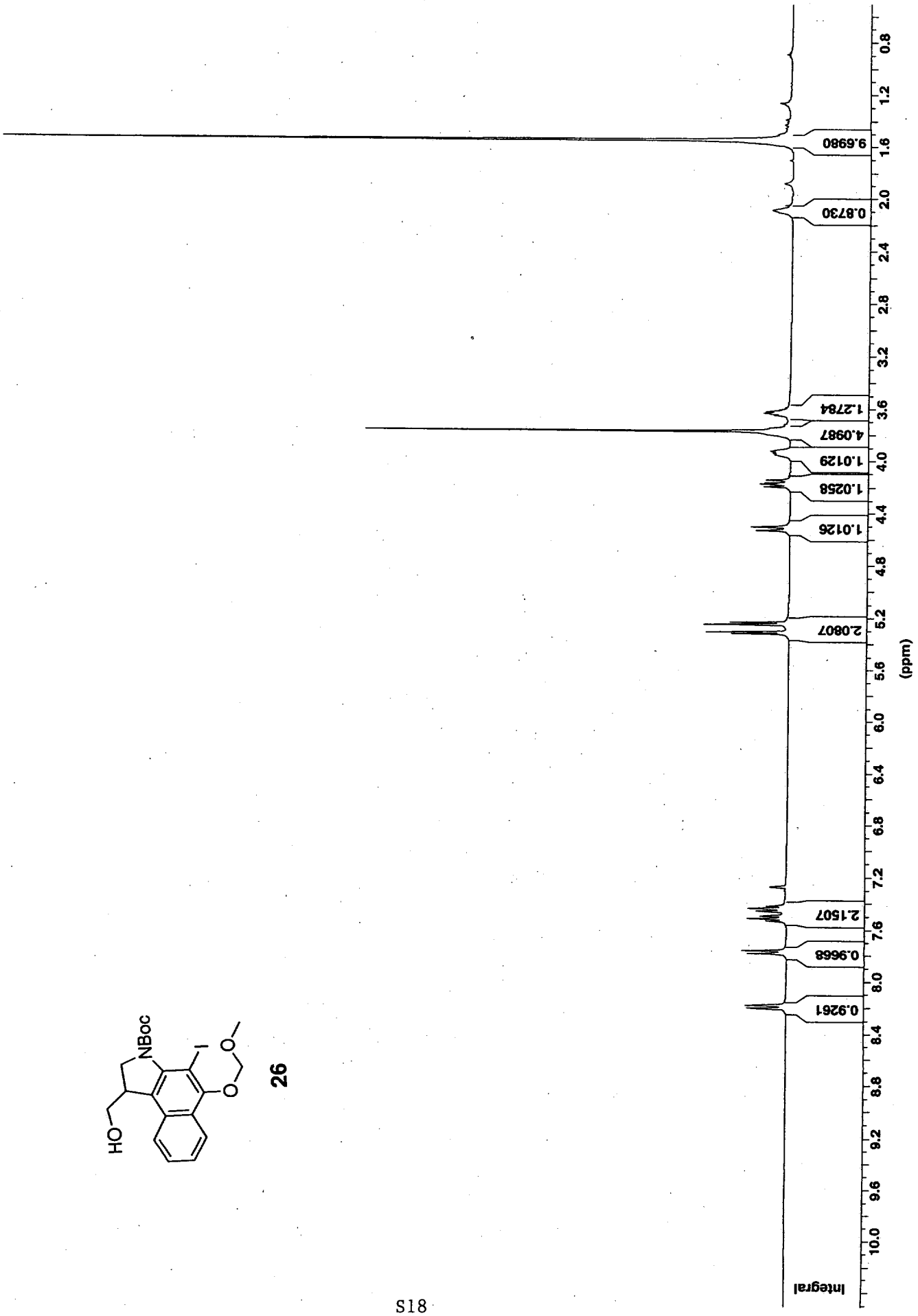
1.0697
2.7705
1.2025
1.1378
1.1085
1.0835
2.1095
2.1179
1.0555
1.0000
Integral
(ppm)
NBoc
Br
O
O
HO

25



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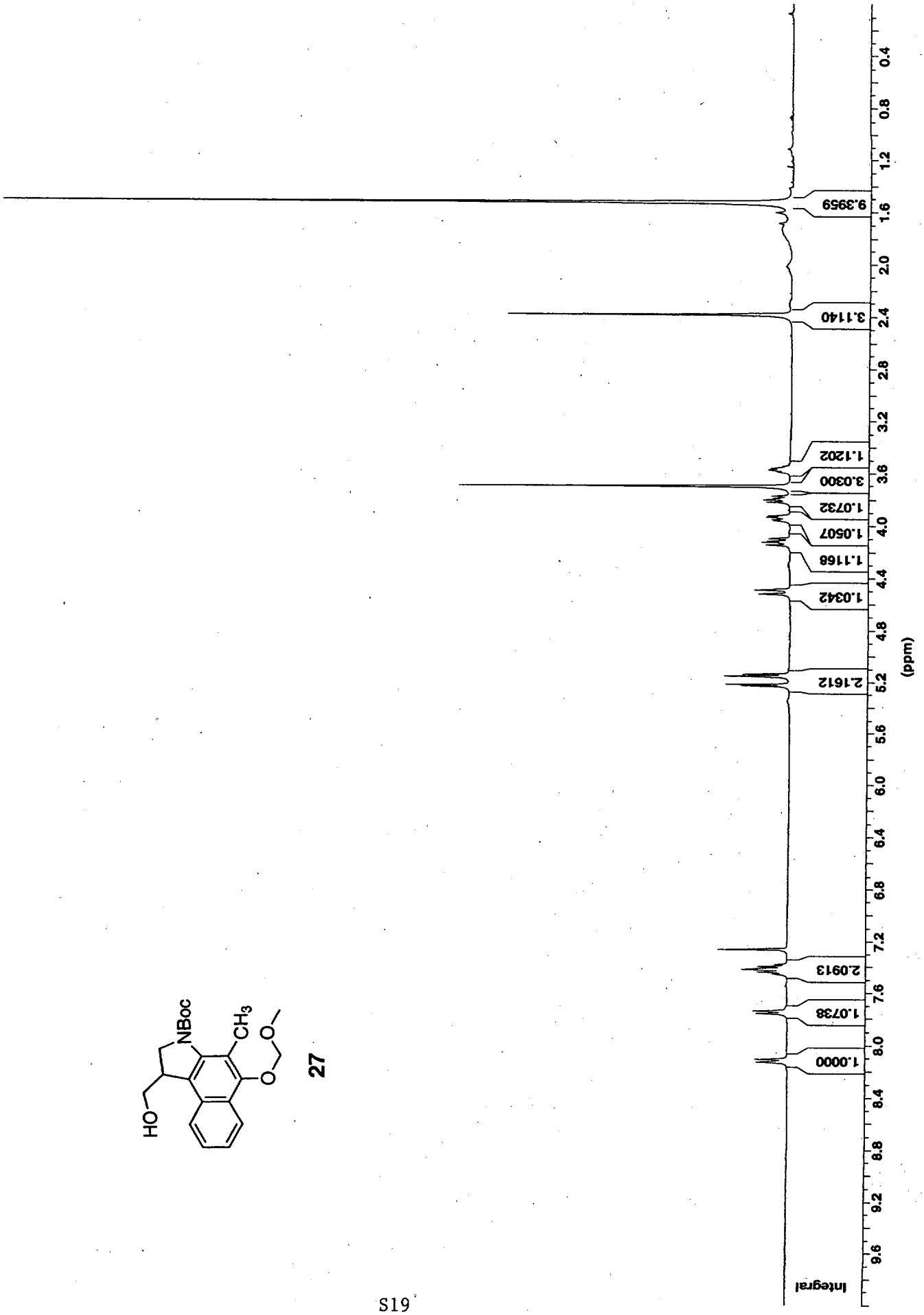

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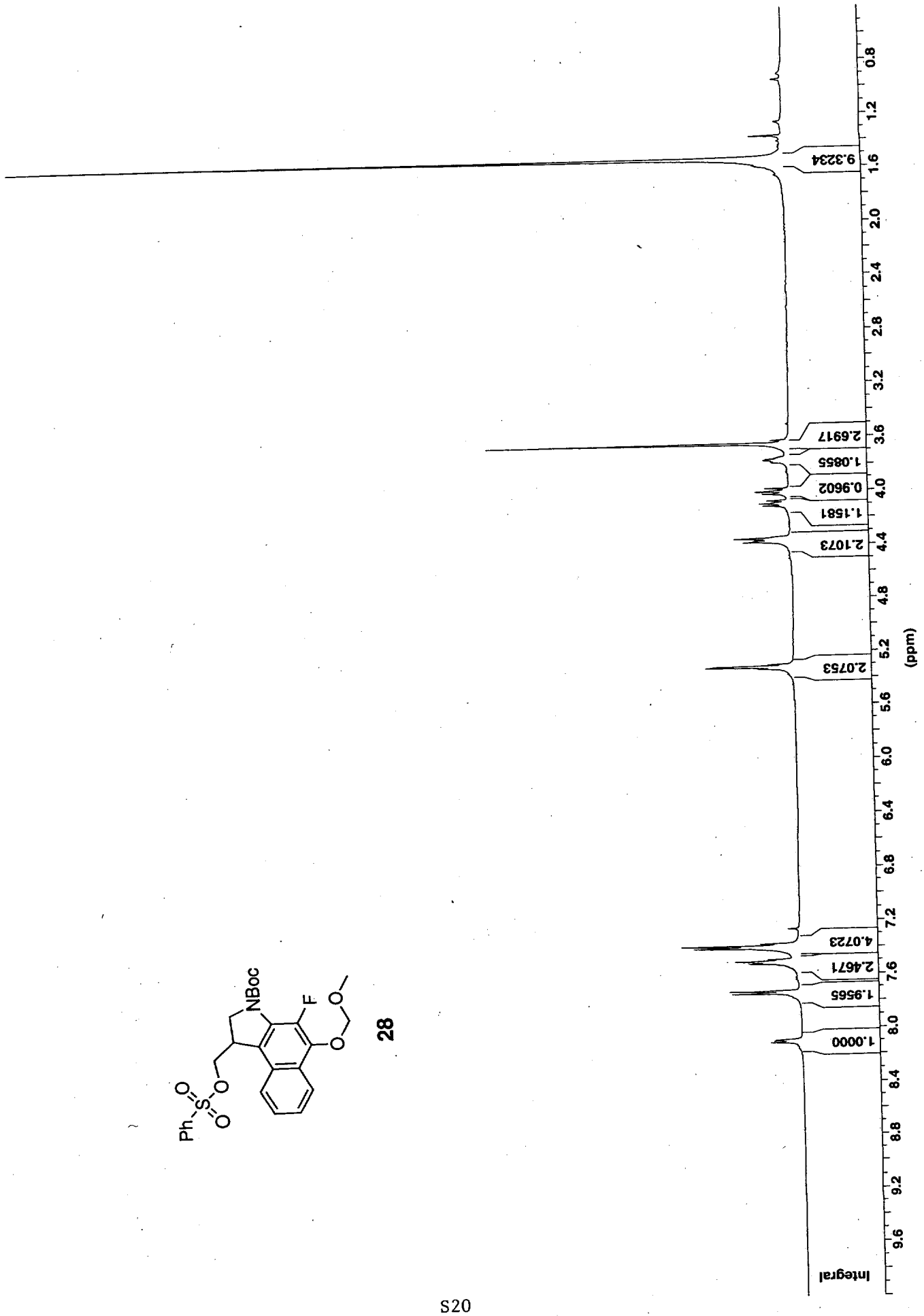

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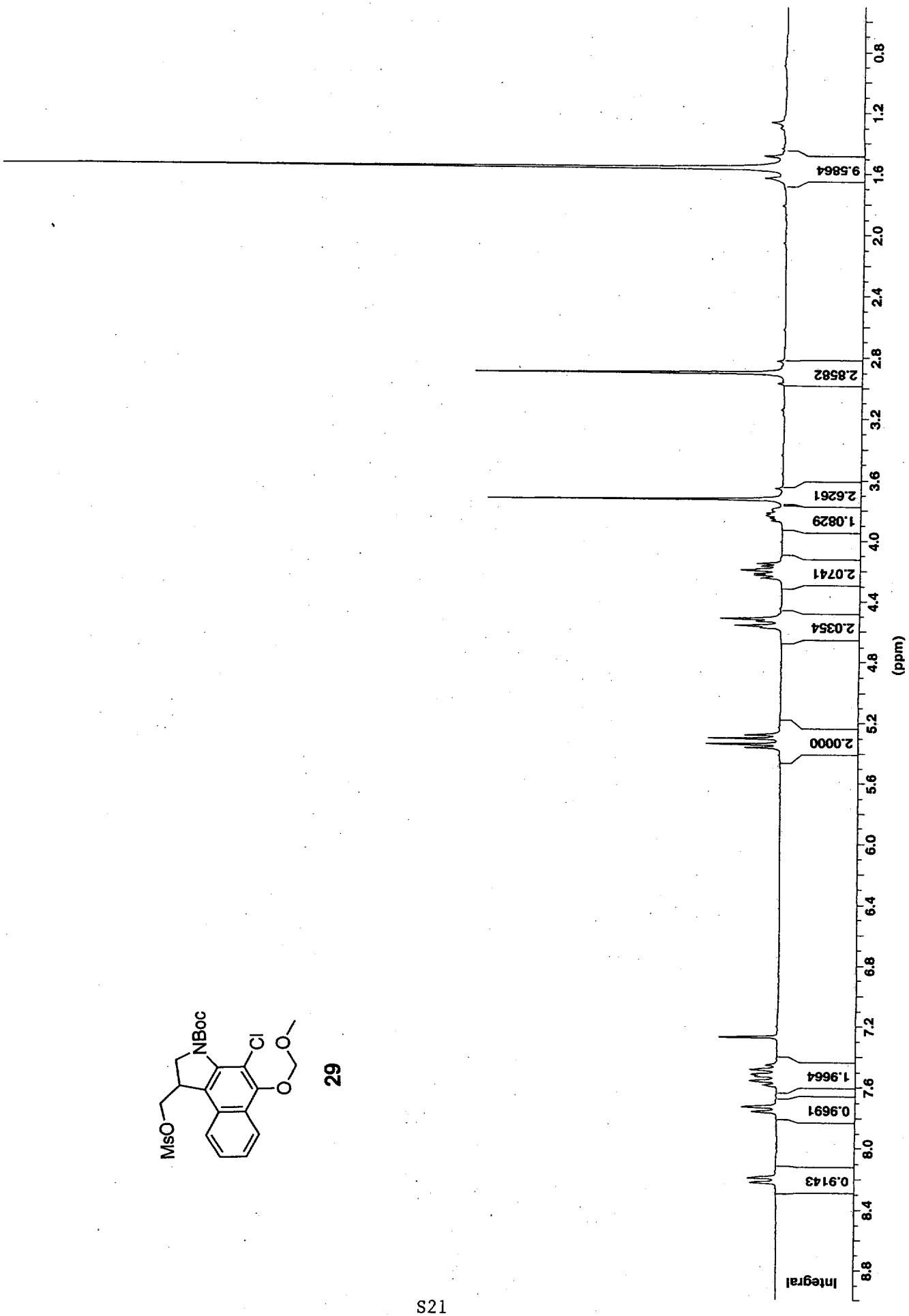
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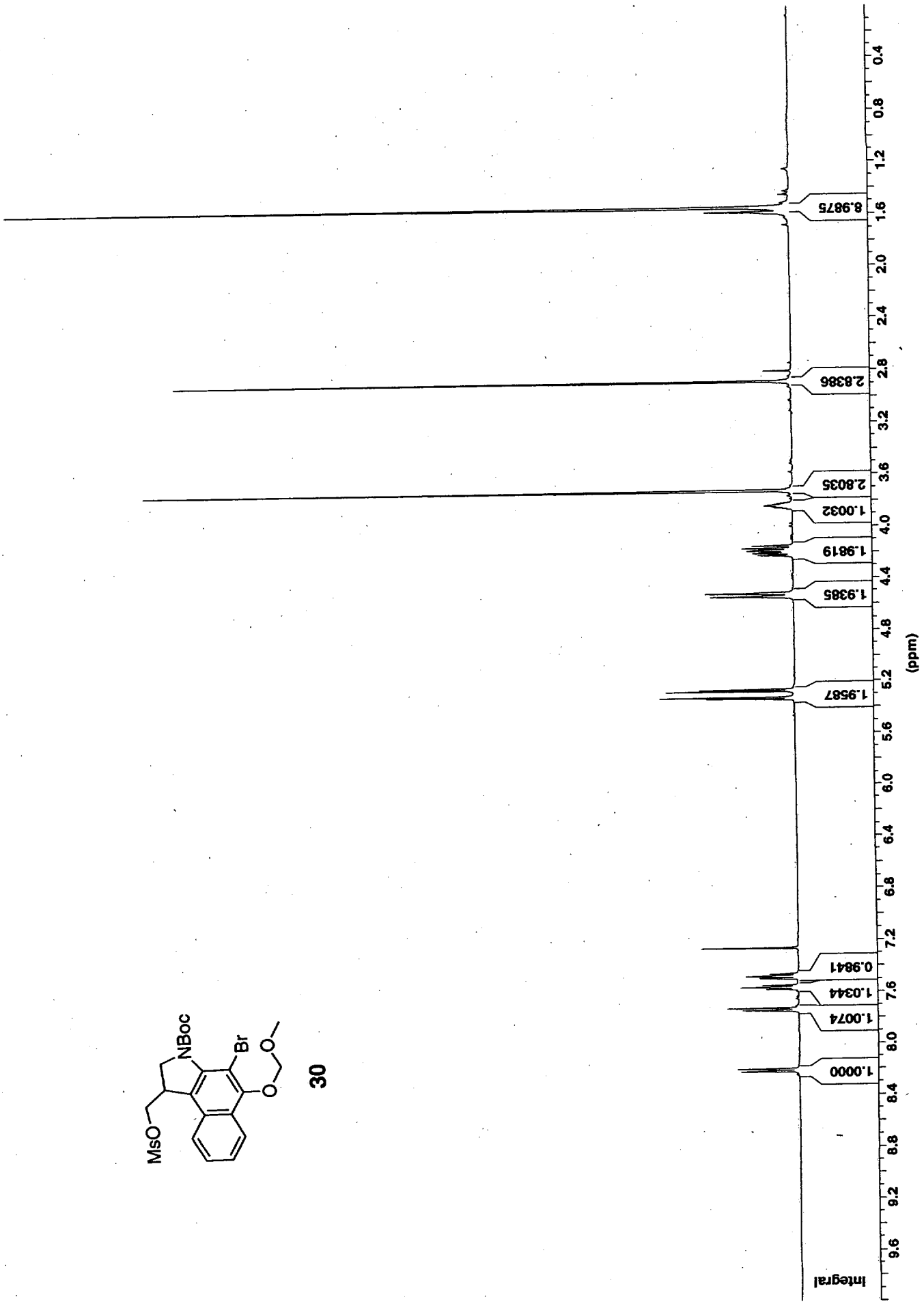
2.8582
2.6261
1.0829
2.0741
2.0354
2.0000
1.9664
0.9691
0.9143
Integral
(ppm)

NBoc
Cl
O
O
MsO

29



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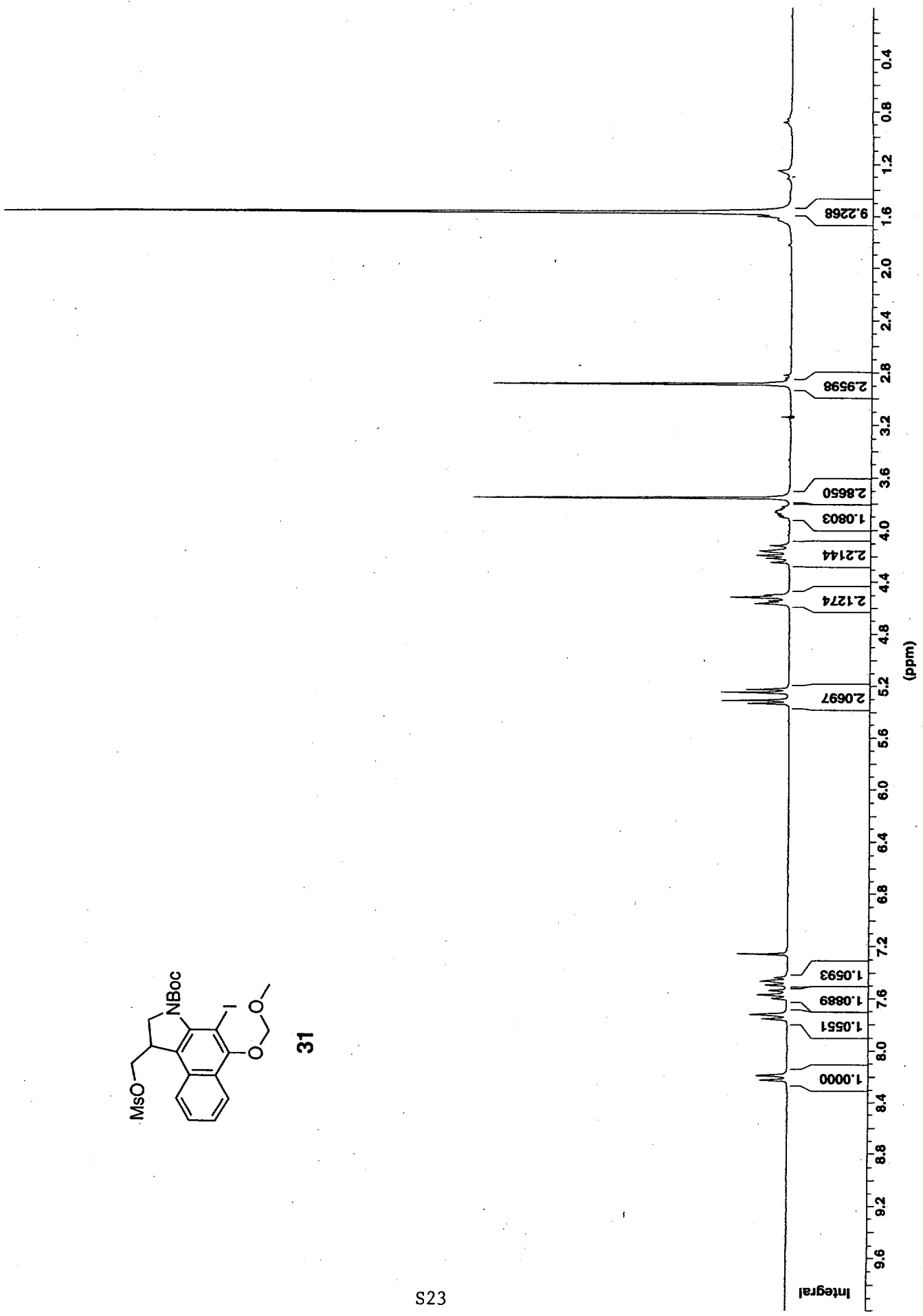

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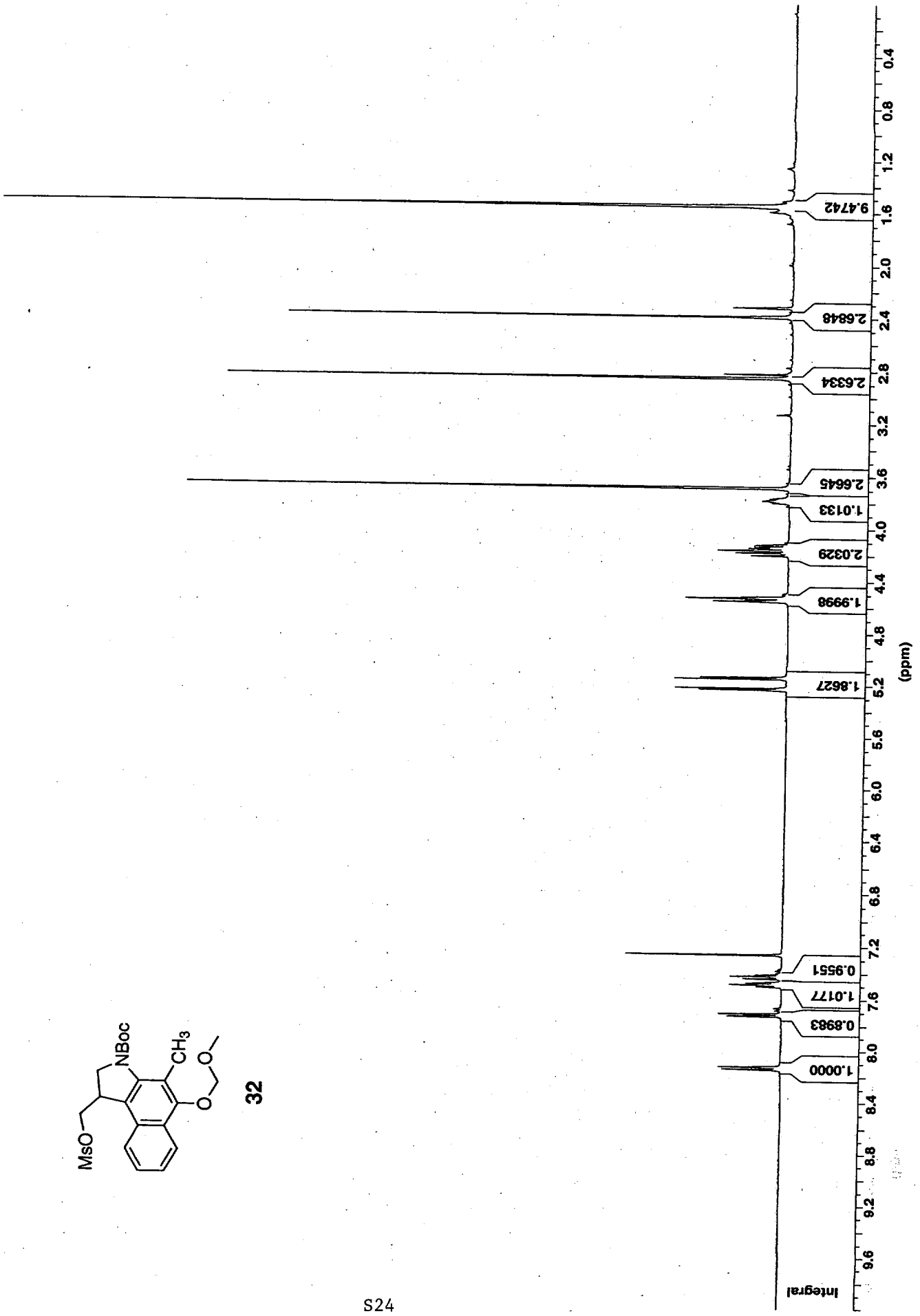

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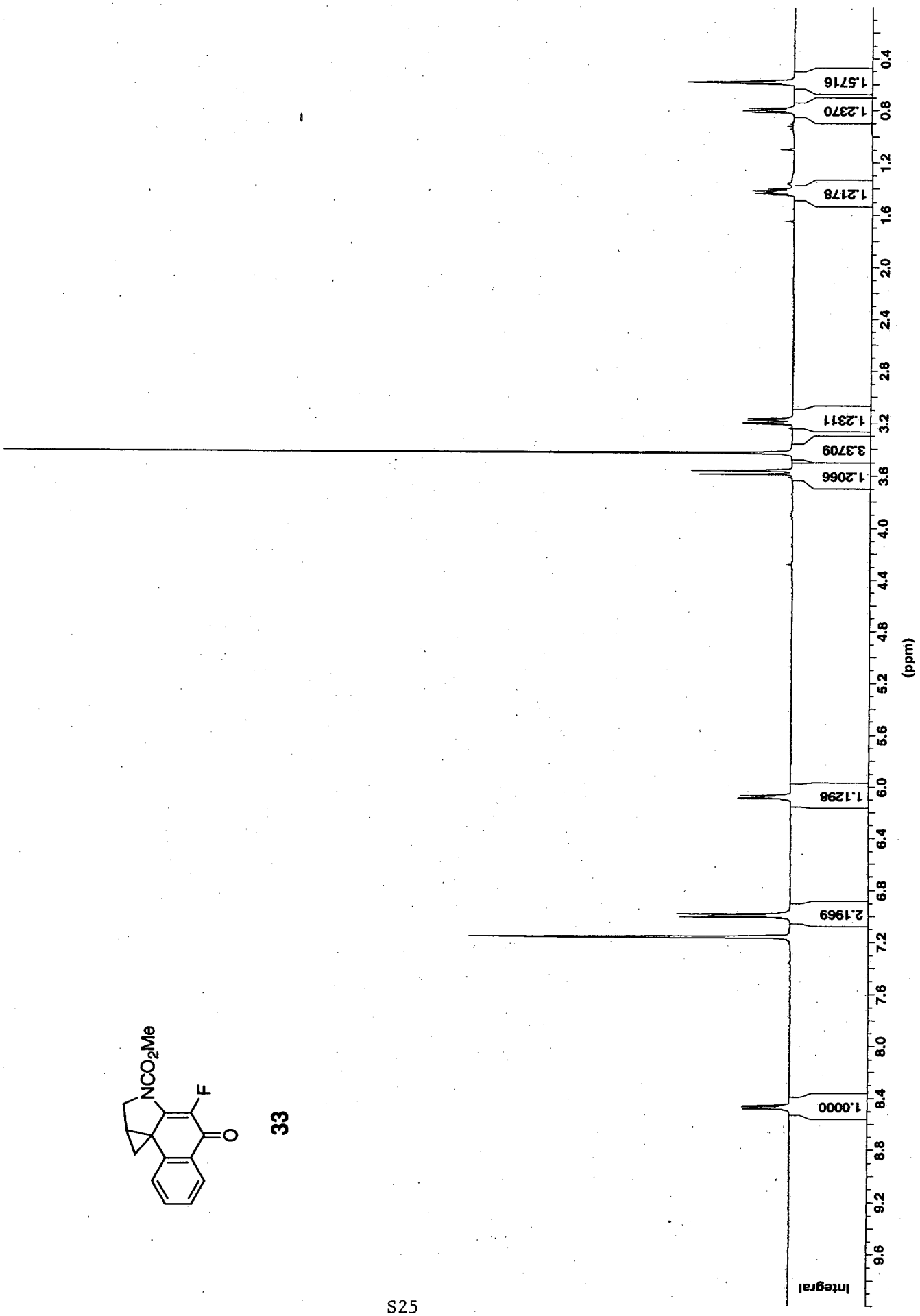
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1.2370
1.2178
1.2311
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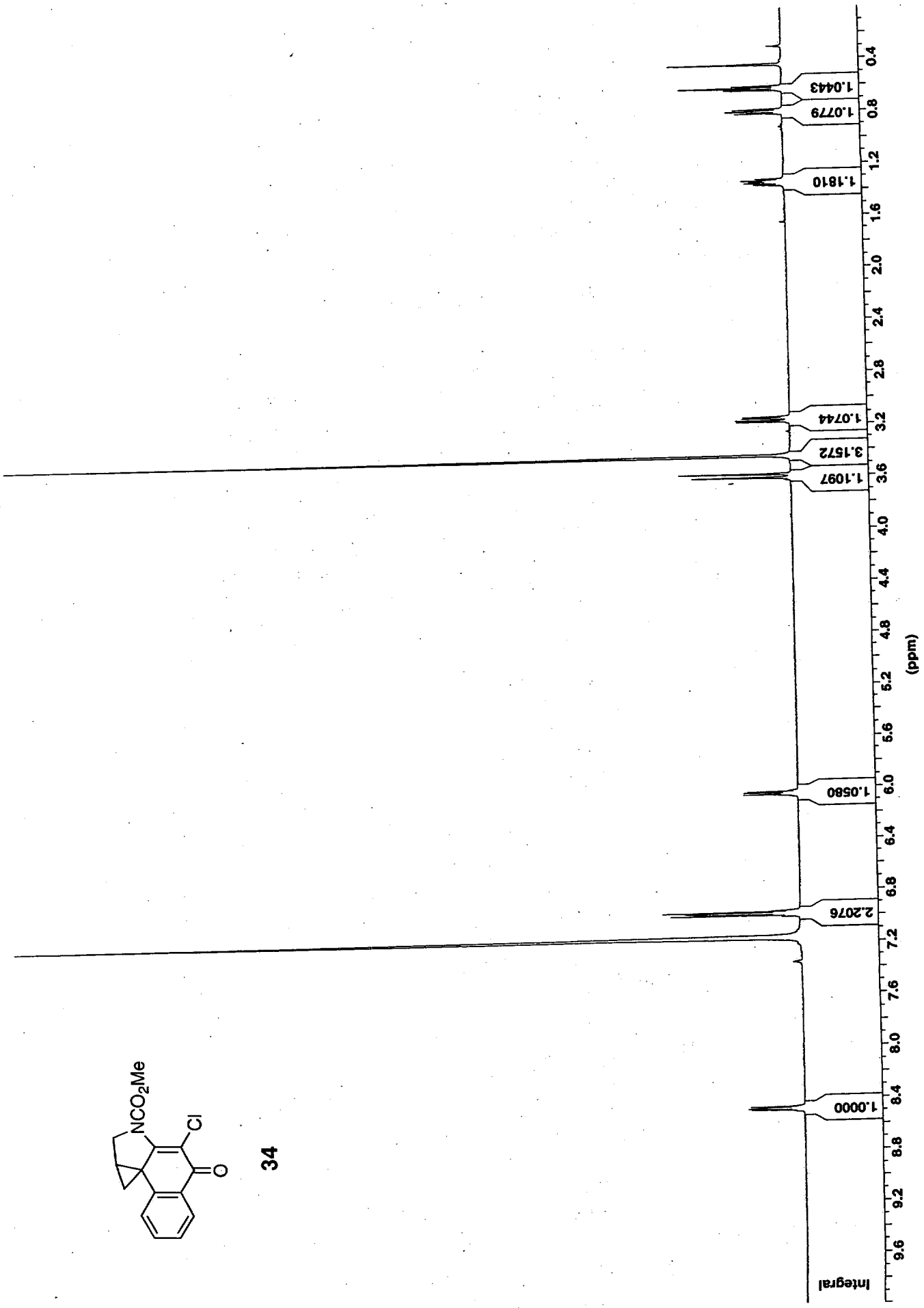
1.2066
1.1298
2.1969
1.0000
Integral
(ppm)

NCO2Me
F
O

33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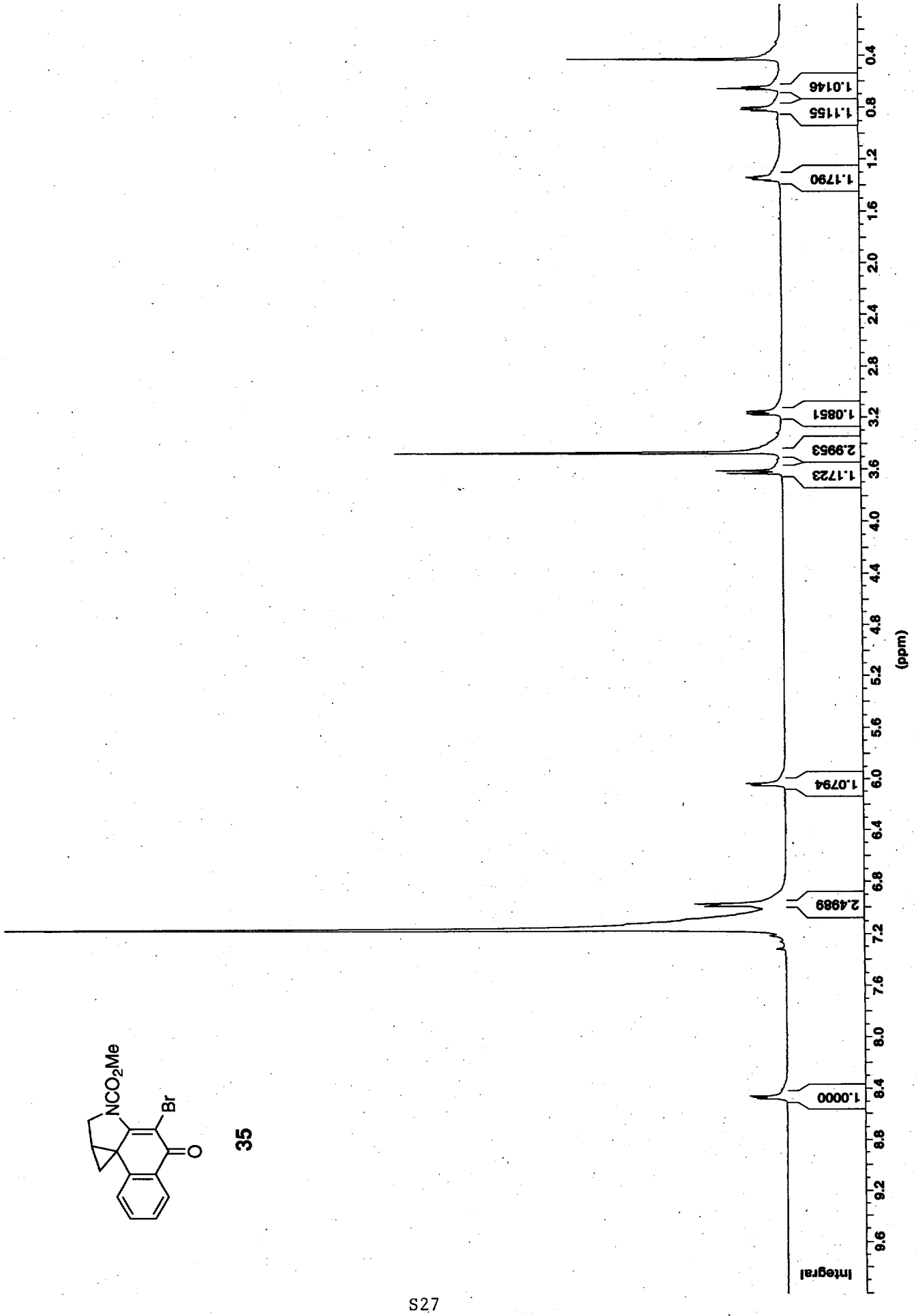
3.1572
1.1097
1.0580
2.2076
1.0000
Integral
(ppm)
0.4
0.8
1.2
1.6
2.0
2.4
2.8
3.2
3.6
4.0
4.4
4.8
5.2
5.6
6.0
6.4
6.8
7.2
7.6
8.0
8.4
8.8
9.2
9.6

NCO2Me
Cl
O

34



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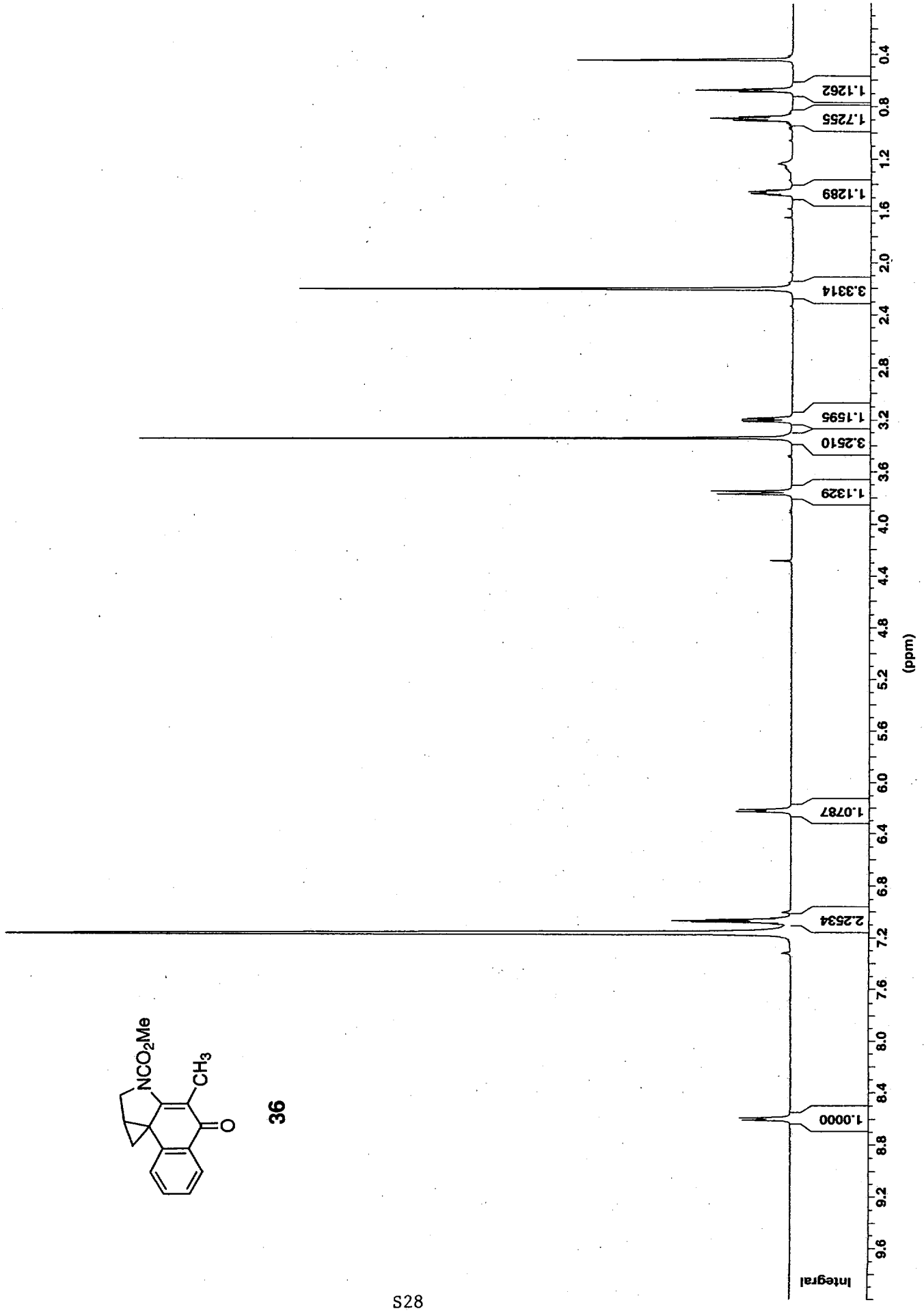

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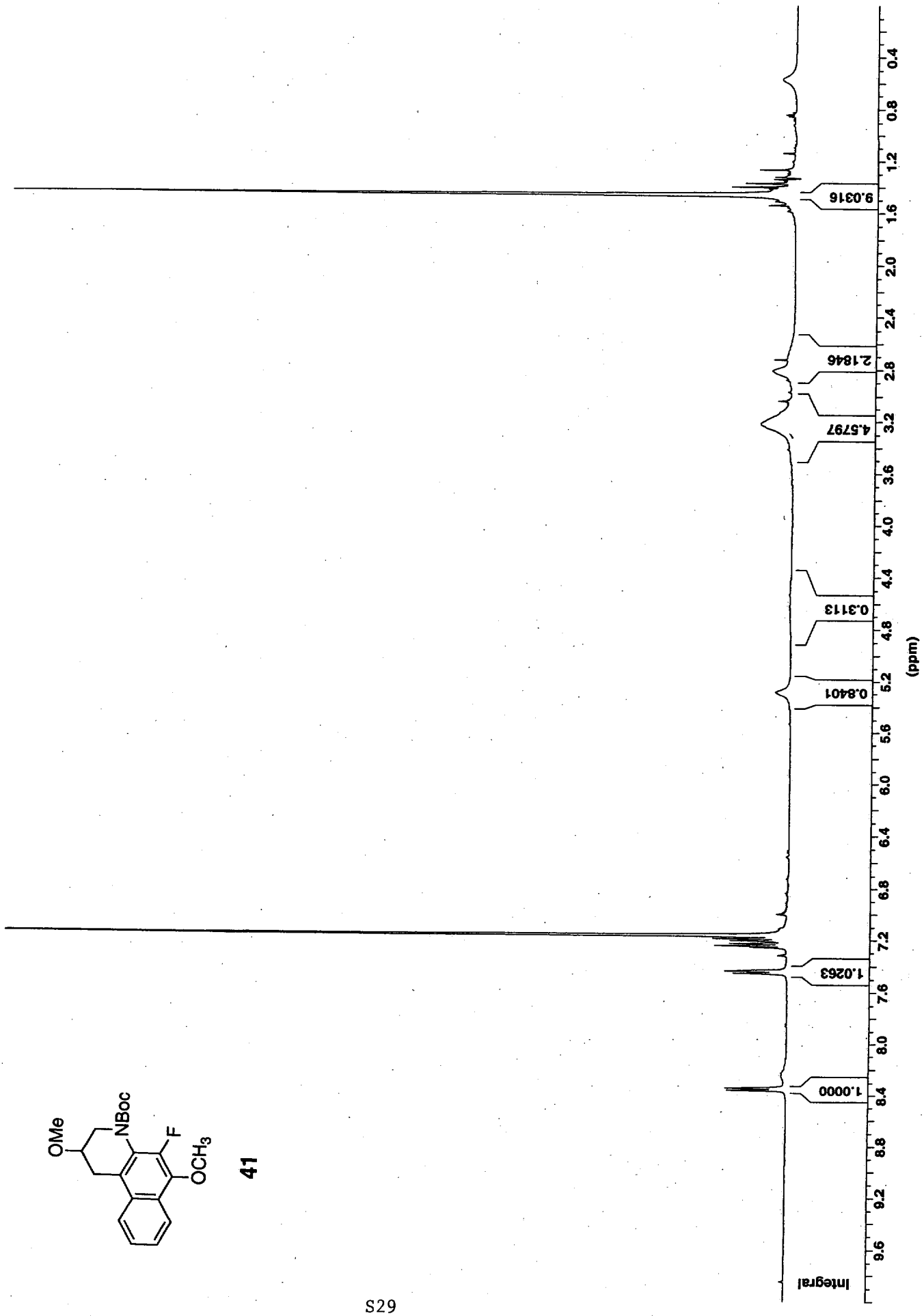
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4.5797
0.3113
0.8401
1.0263
1.0000
Integral
(ppm)
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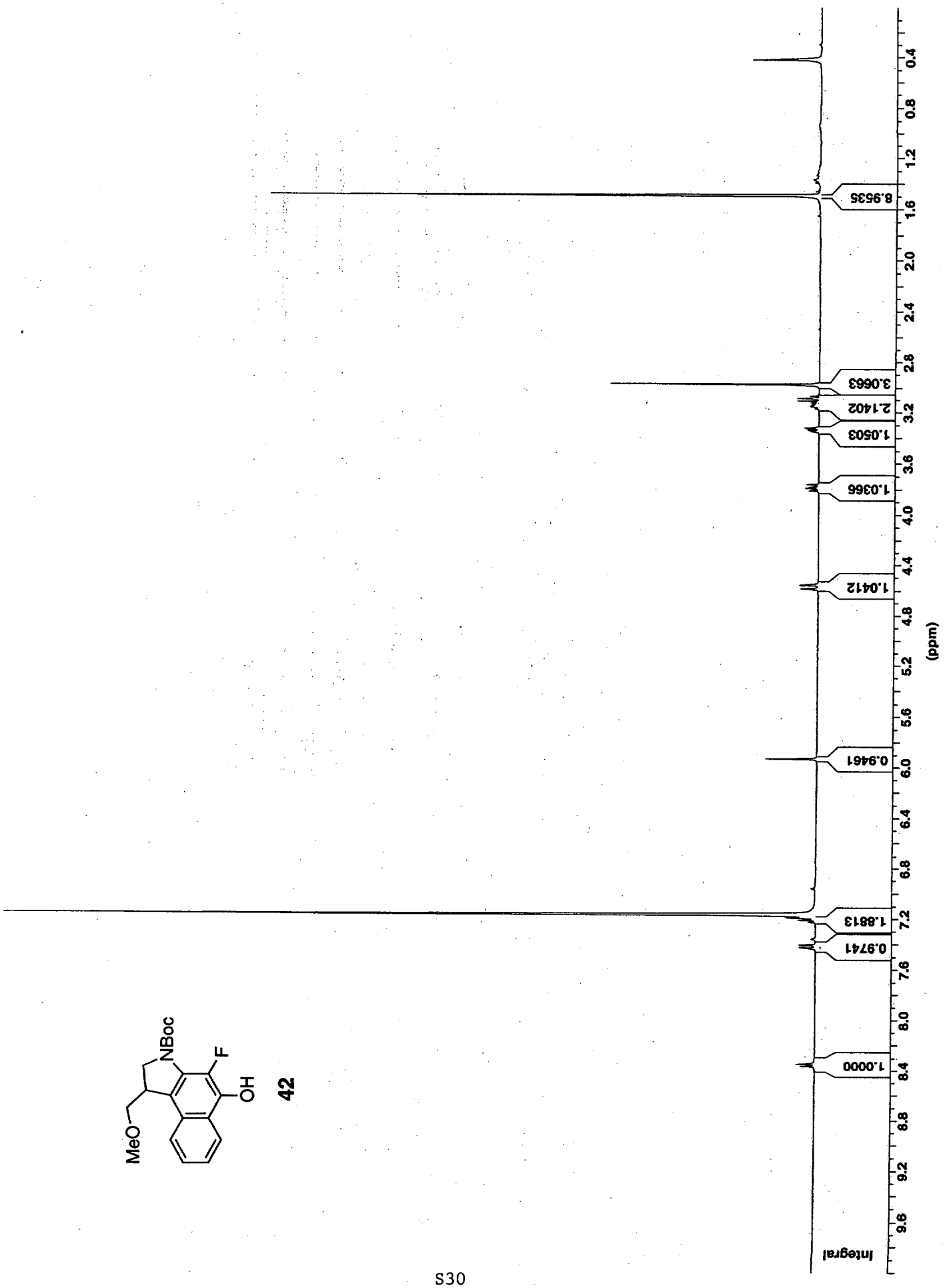
0.8
1.2
1.6
2.0
2.4
2.8
3.2
3.6
4.0
4.4
4.8
5.2
5.6
6.0
6.4
6.8
7.2
7.6
8.0
8.4
8.8
9.2
9.6

OMe
NBoc
F
OCH3

41



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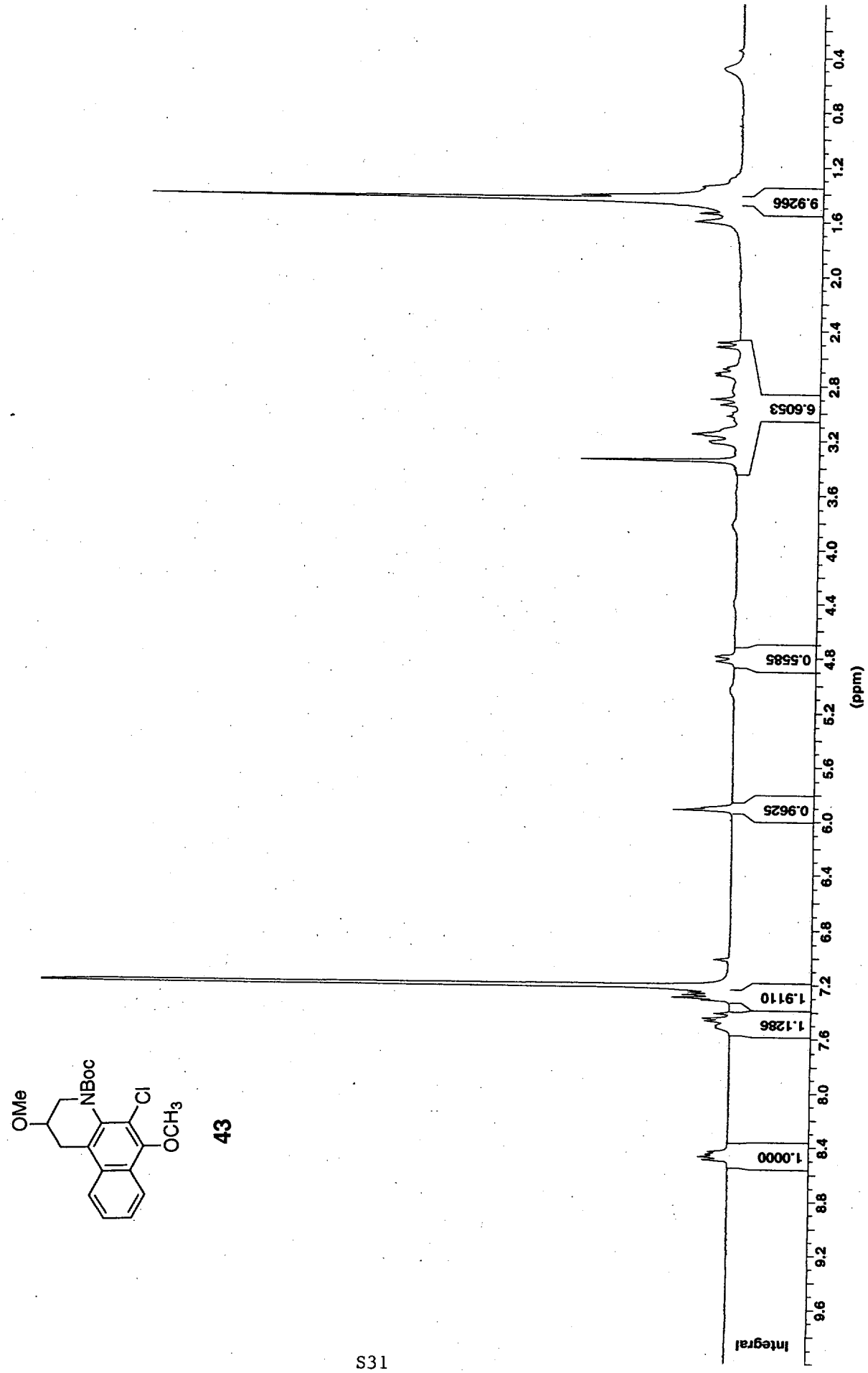
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1.0000
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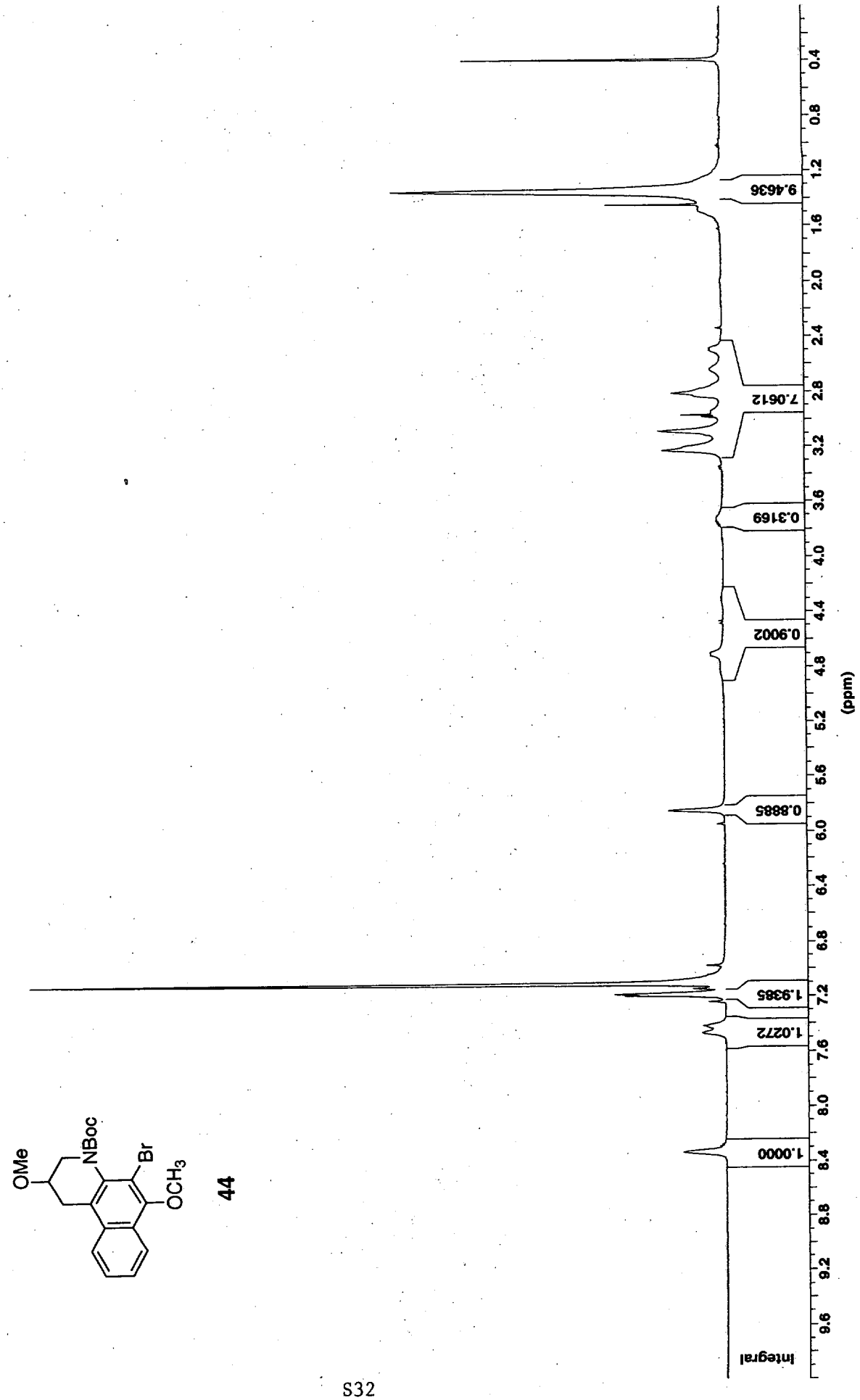
(ppm)
OMe
NBoc
Cl
OCH3

43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1.0272
1.0000
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(ppm)
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1.2
1.6
2.0
2.4
2.8
3.2
3.6
4.0
4.4
4.8
5.2
5.6
6.0
6.4
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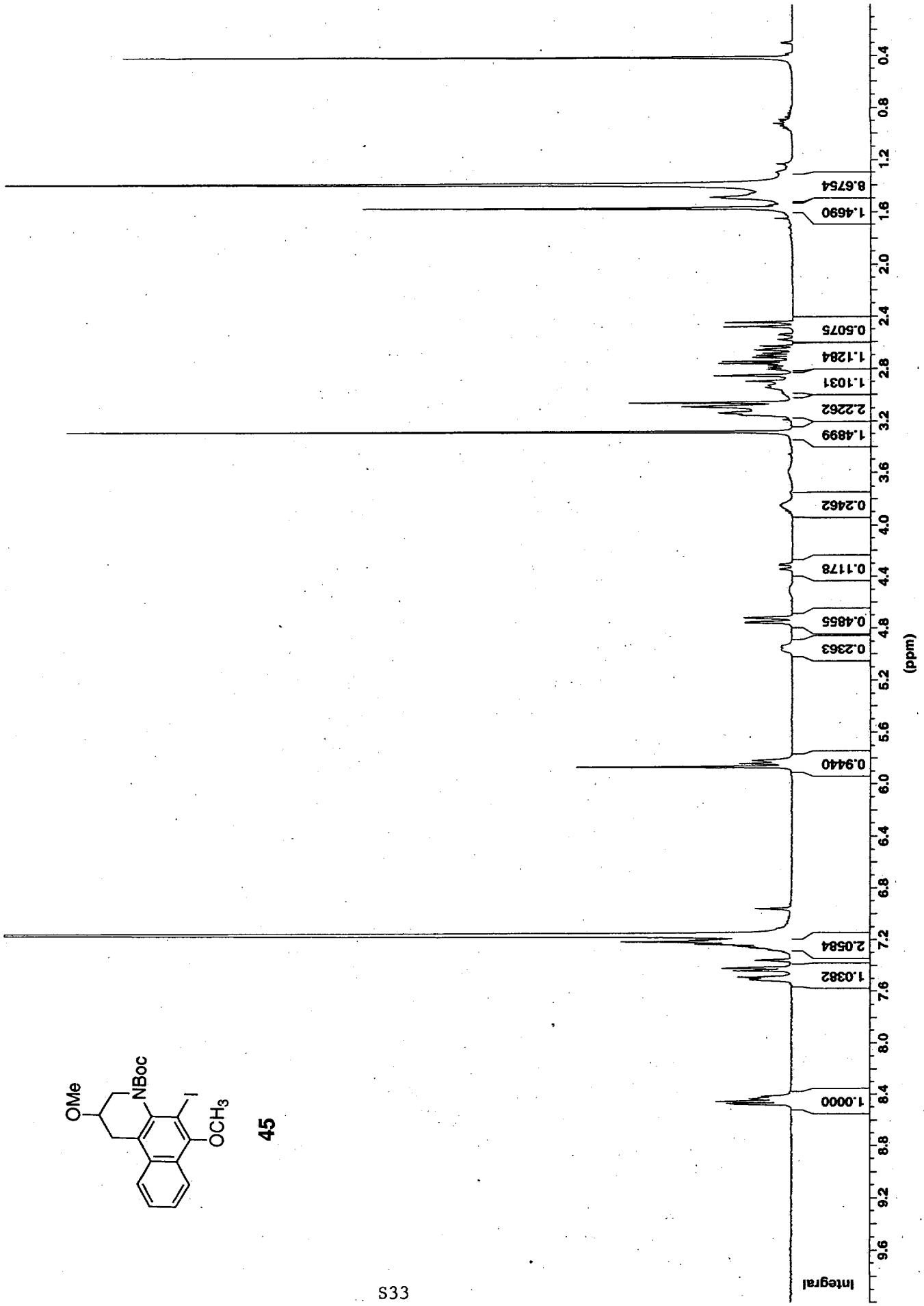
7.6
8.0
8.4
8.8
9.2
9.6

OMe
NBoc
Br
OCH3

44



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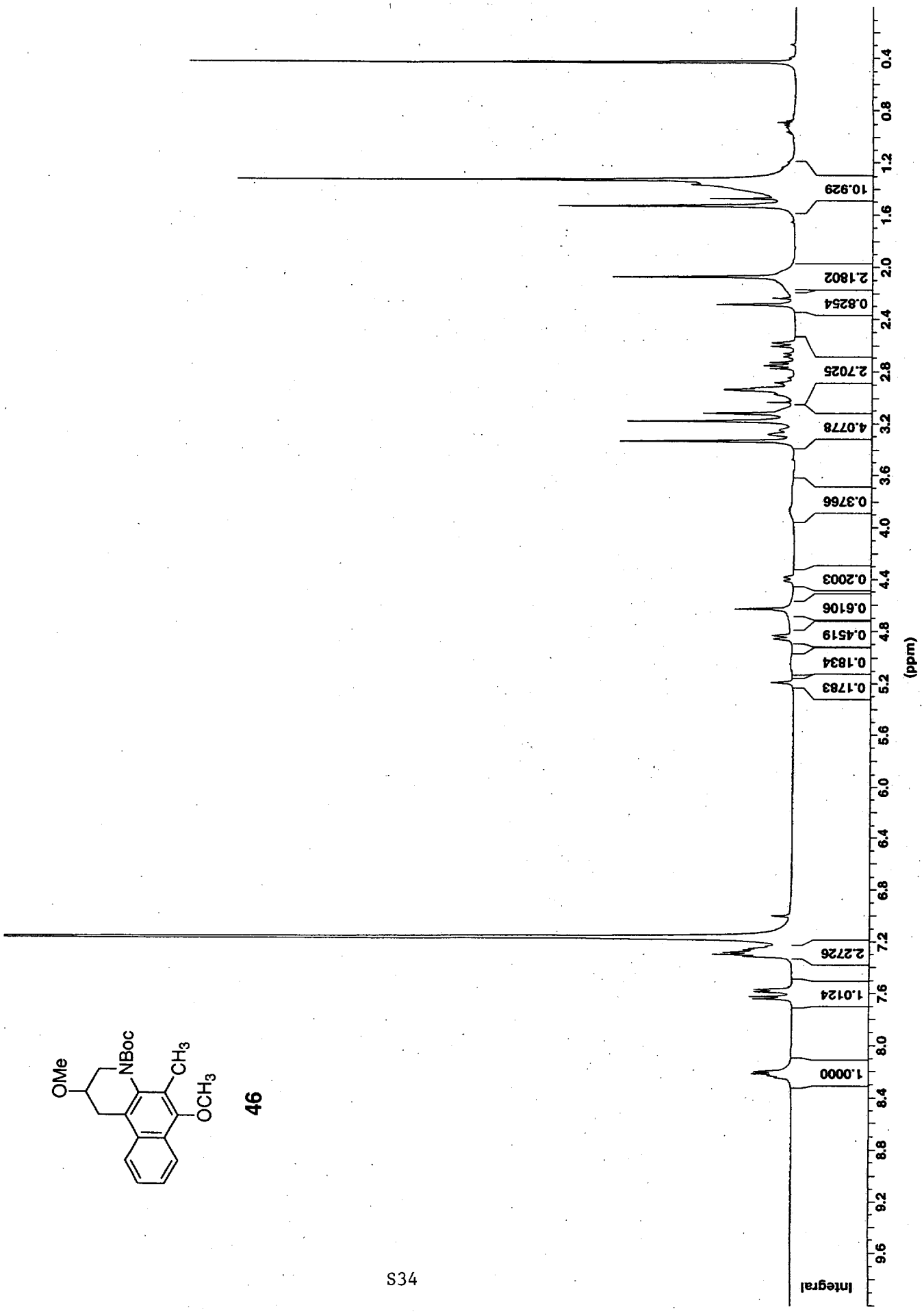

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