Supplementary Material

Preparation of substituted alkoxypyridines via directed metalation and metal-halogen exchange

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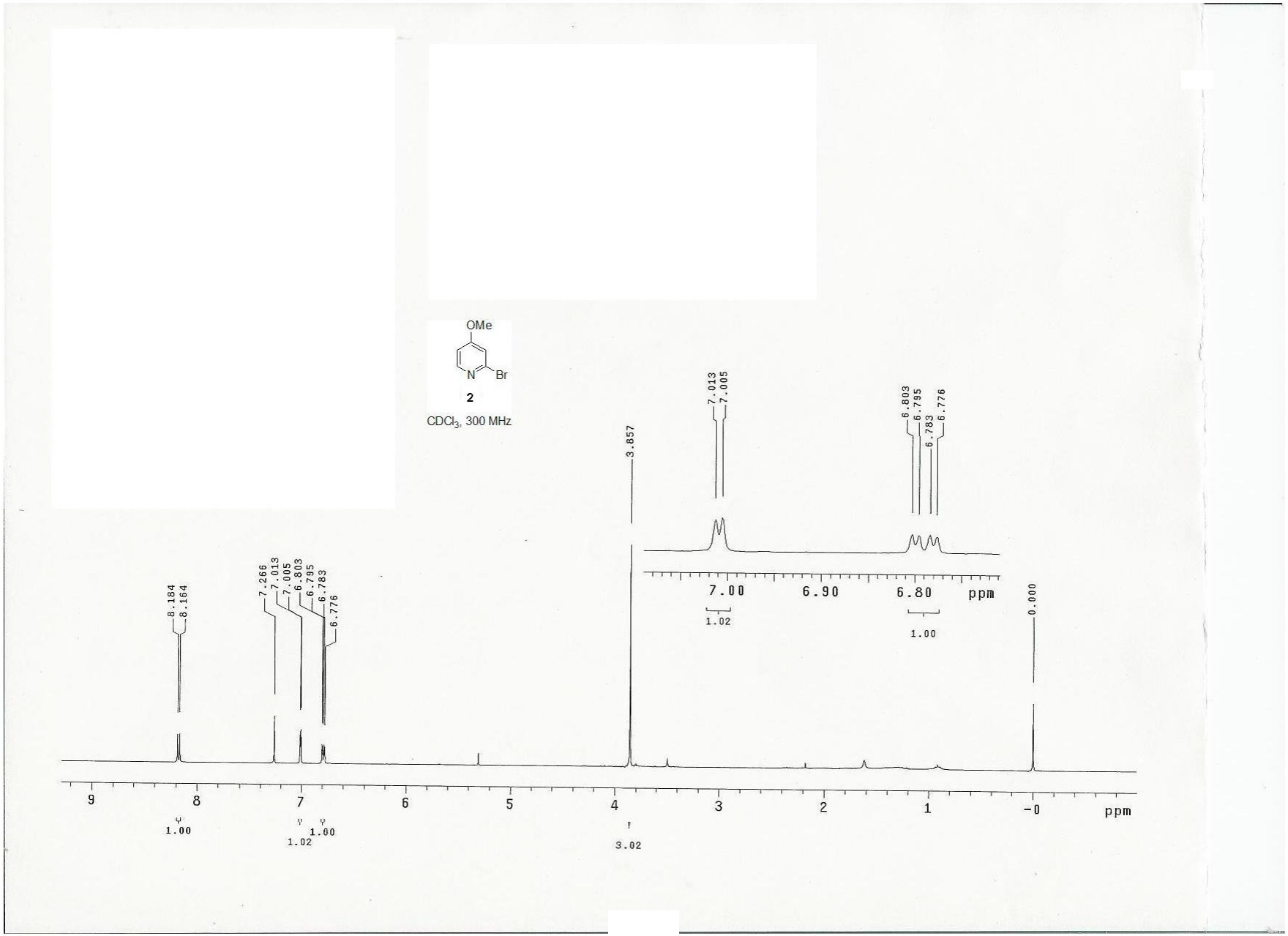
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7.005
6.803
6.795
6.783
6.776
7.00
6.90
6.80
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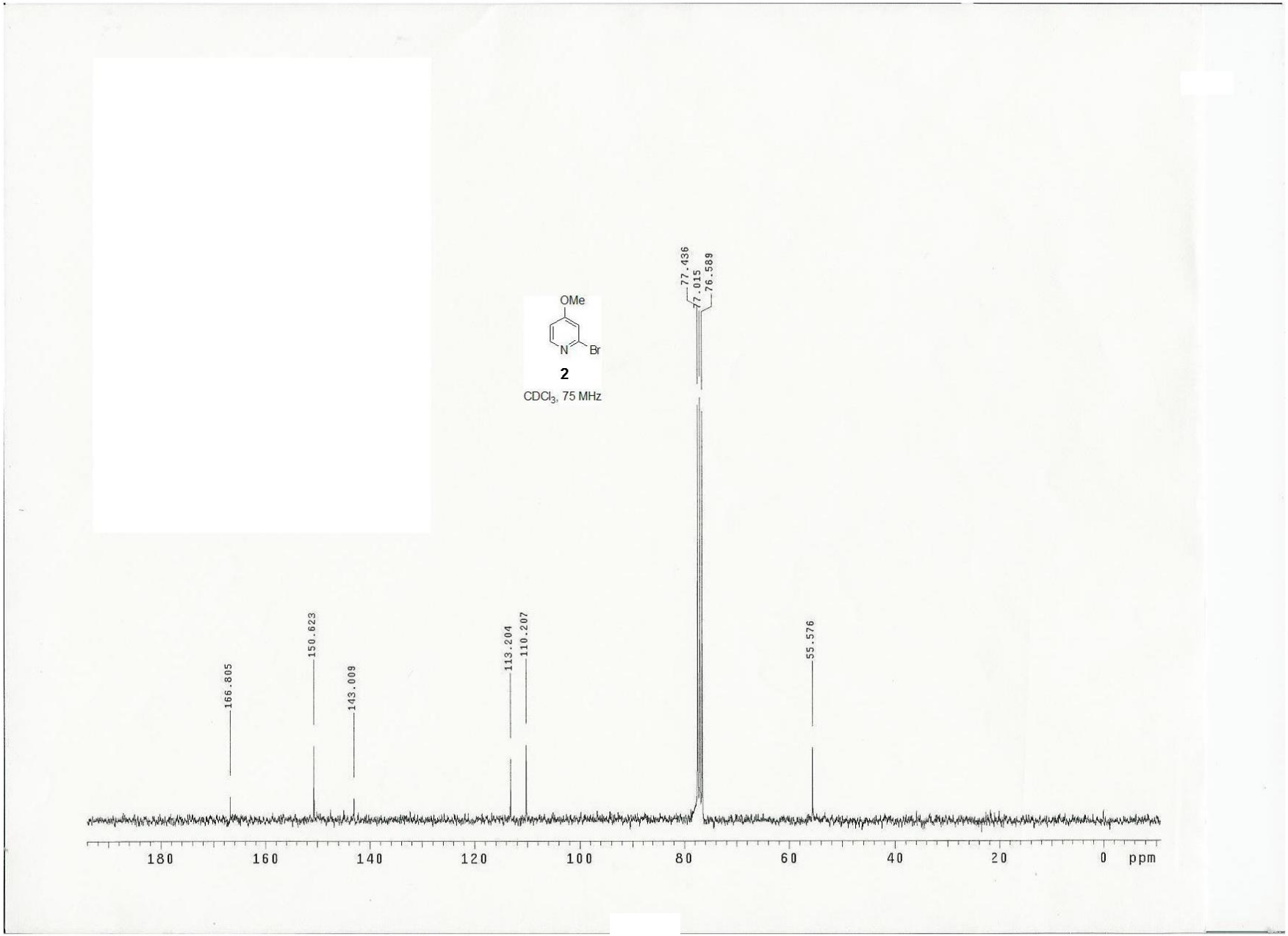
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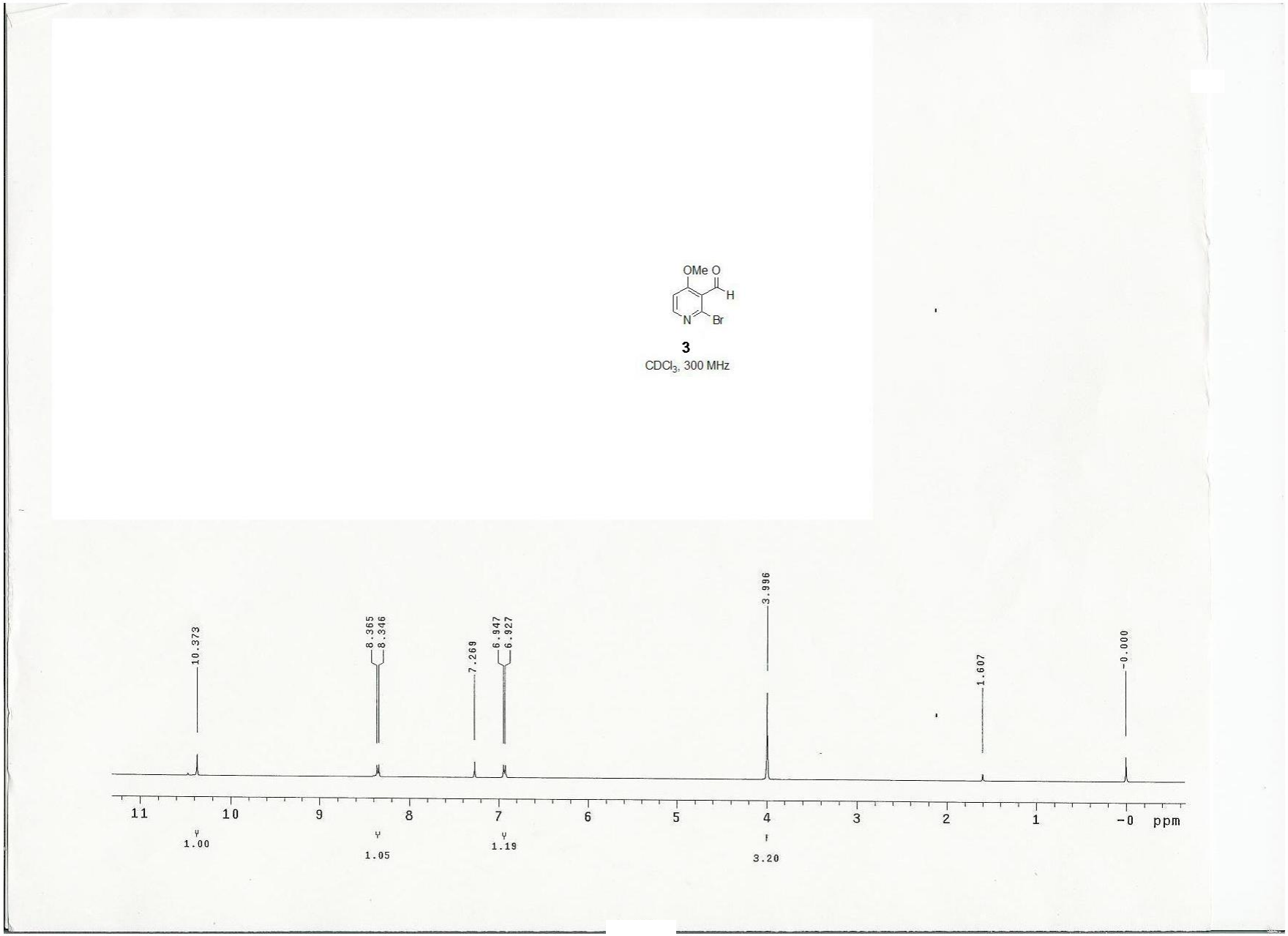
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7.269
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6.927
3.996
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-0.000
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7
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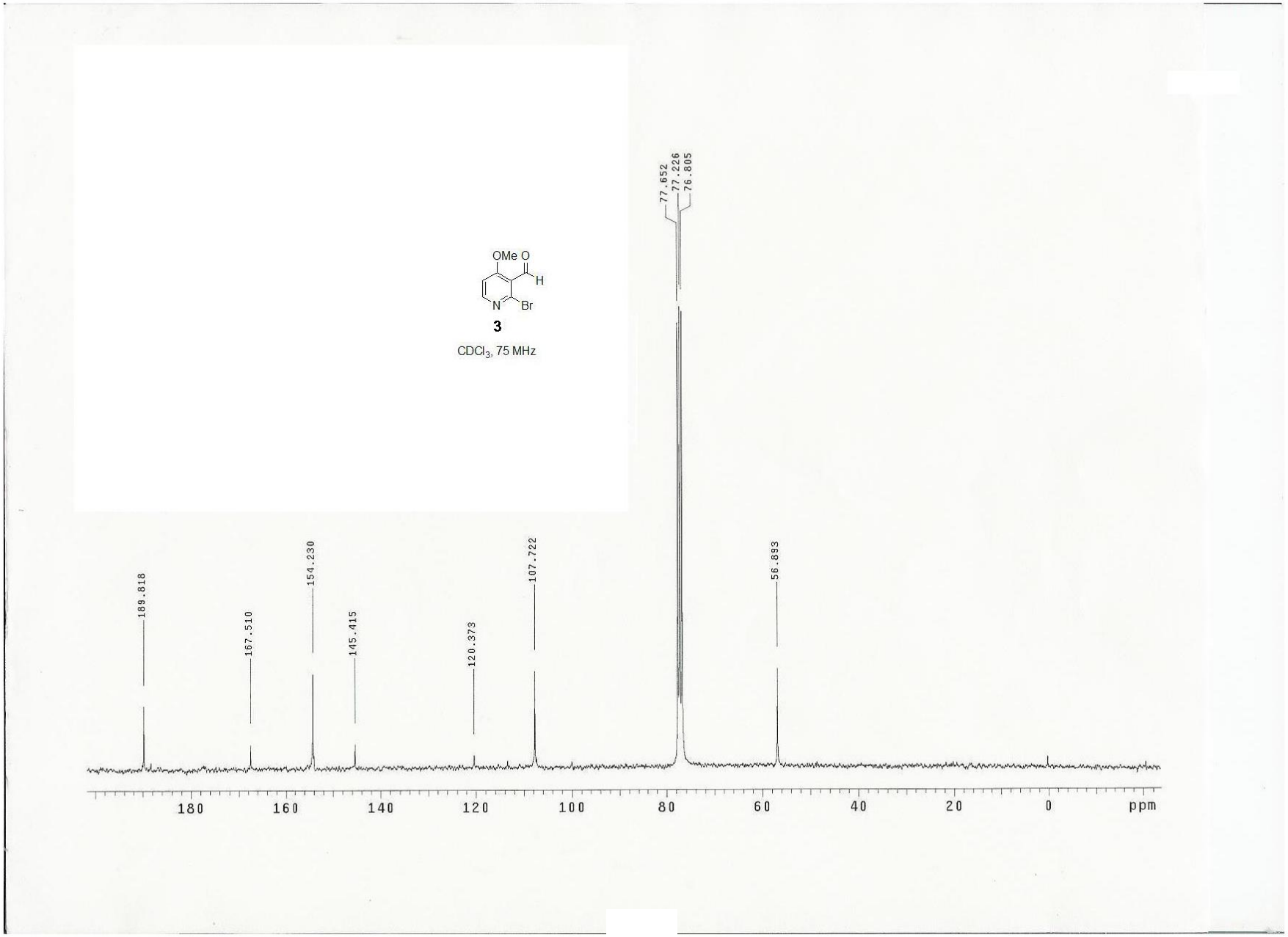
1.19
3.20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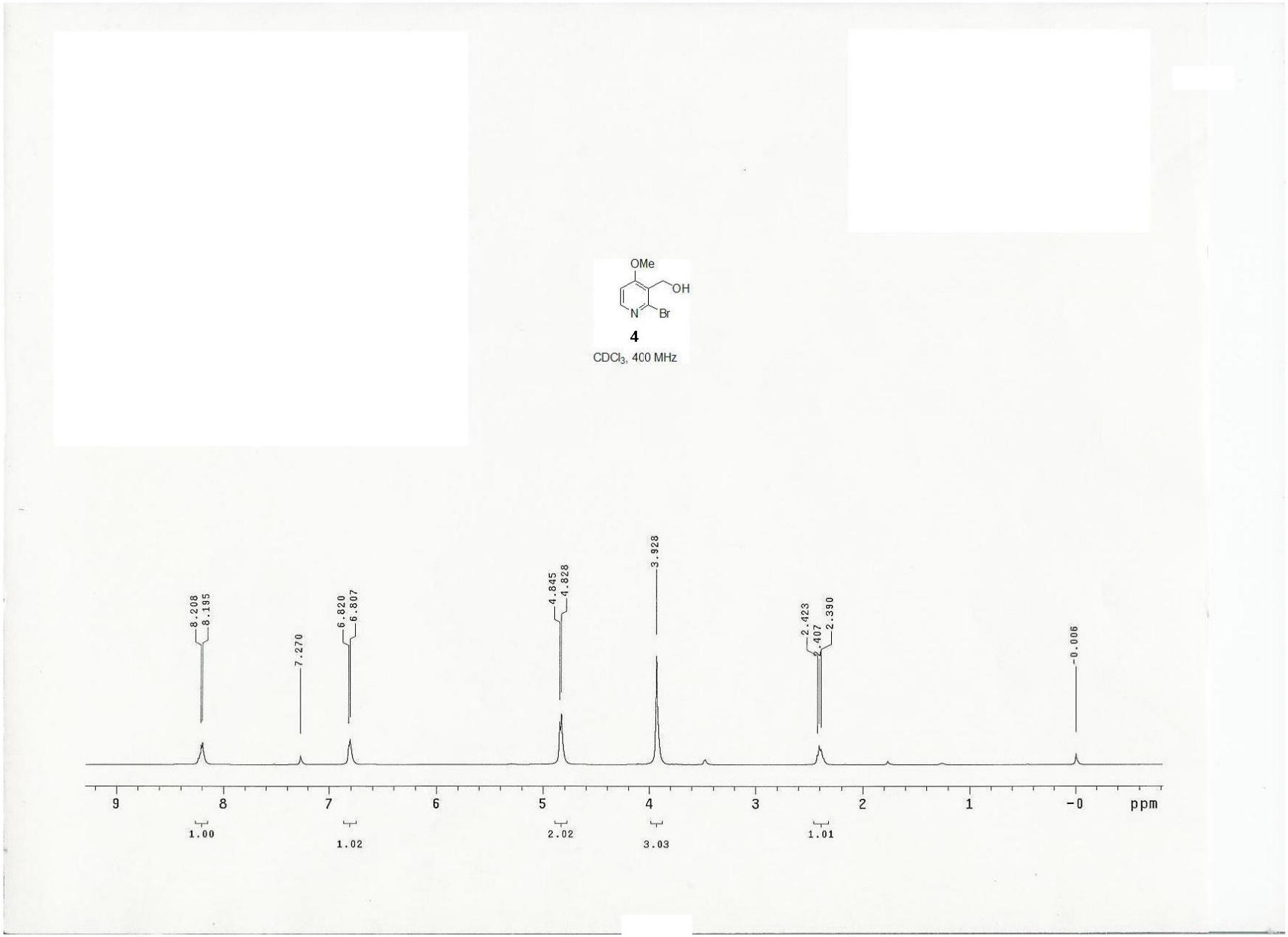
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2.390
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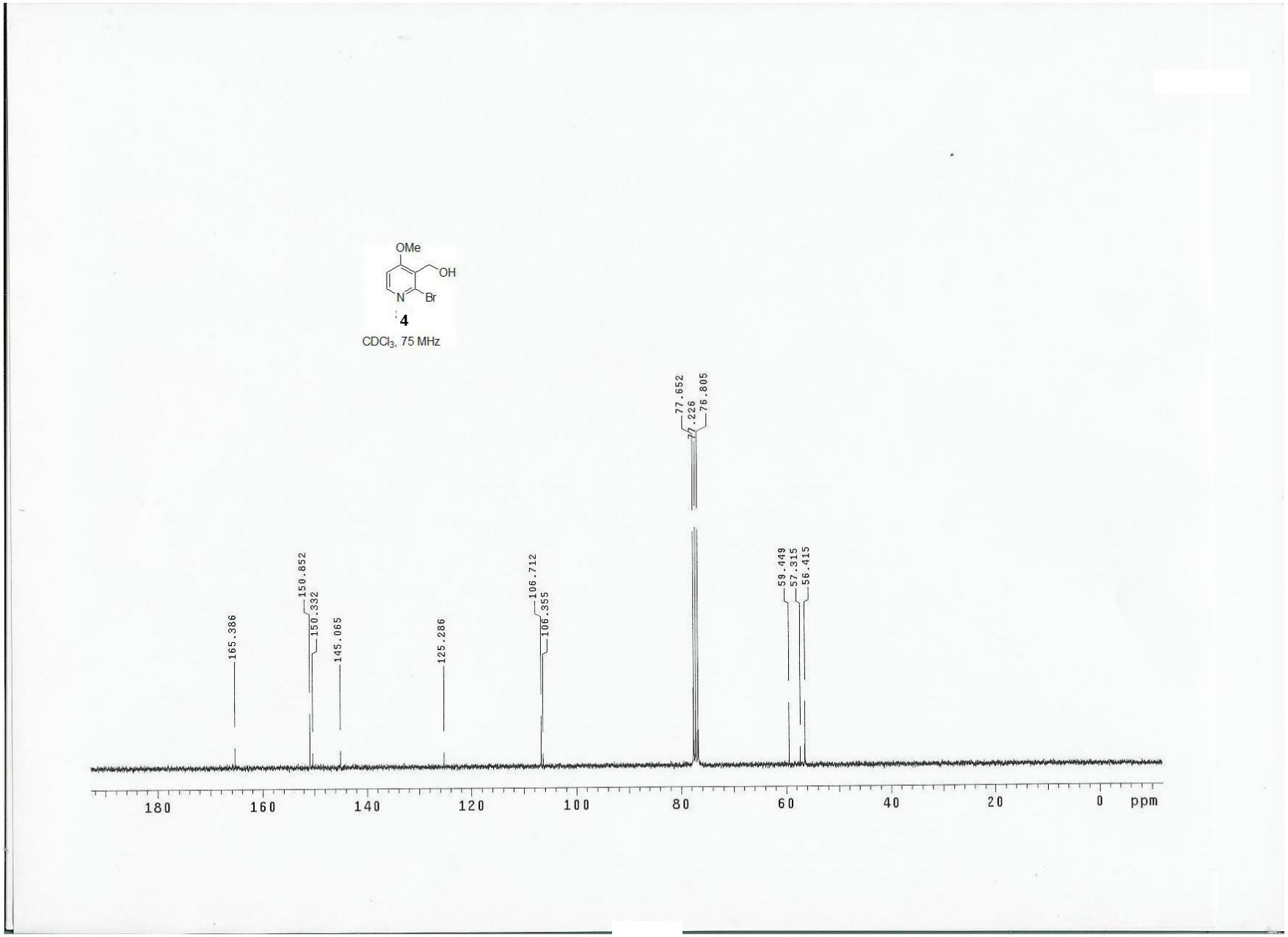
2.02
3.03
1.01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76.805
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150.332
145.065
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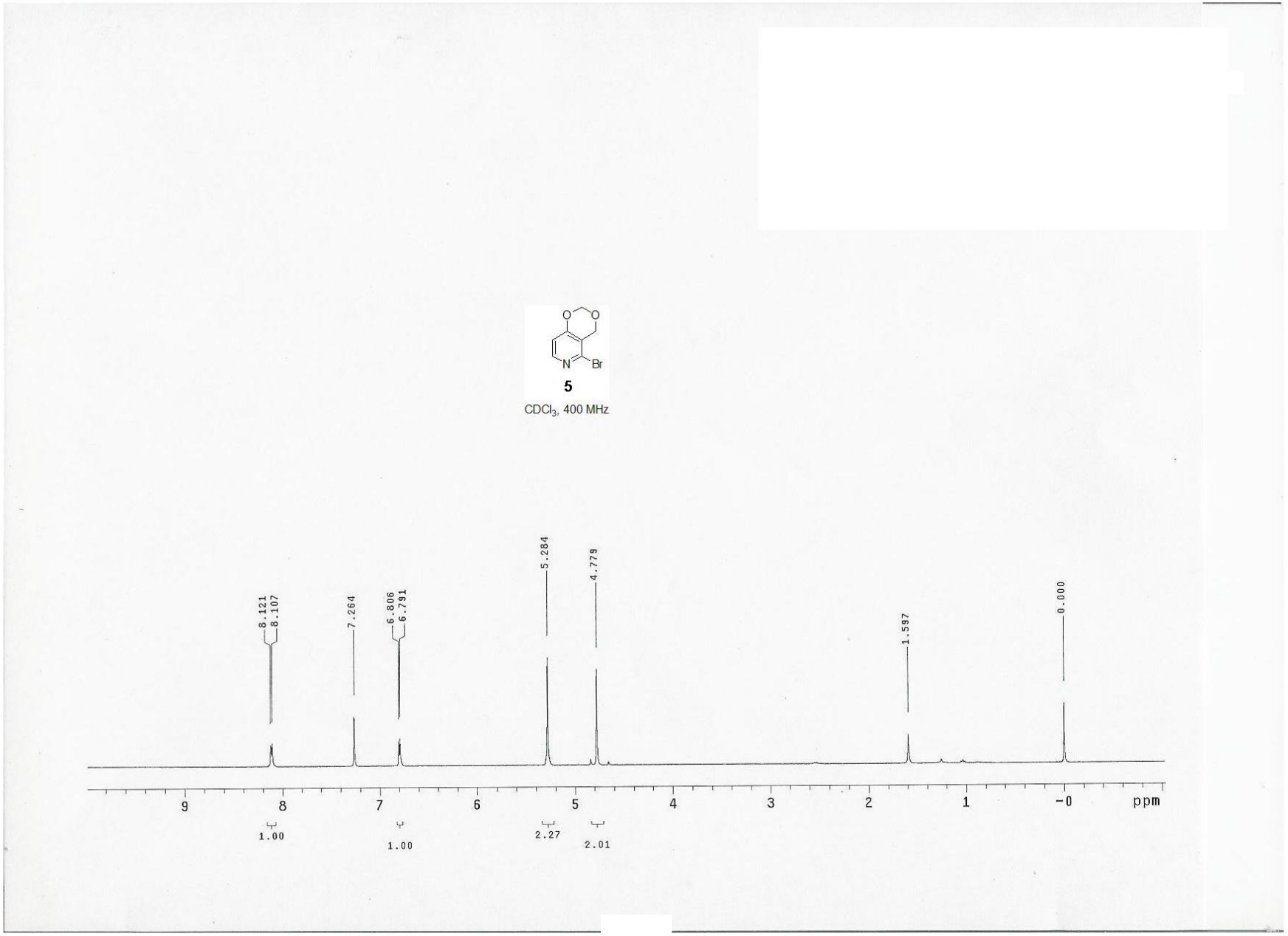
59.449
57.315
56.415
180
160
140
120
100
80
60
40
20
0
ppm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O
N
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1.597
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9
8
7
6
5
4
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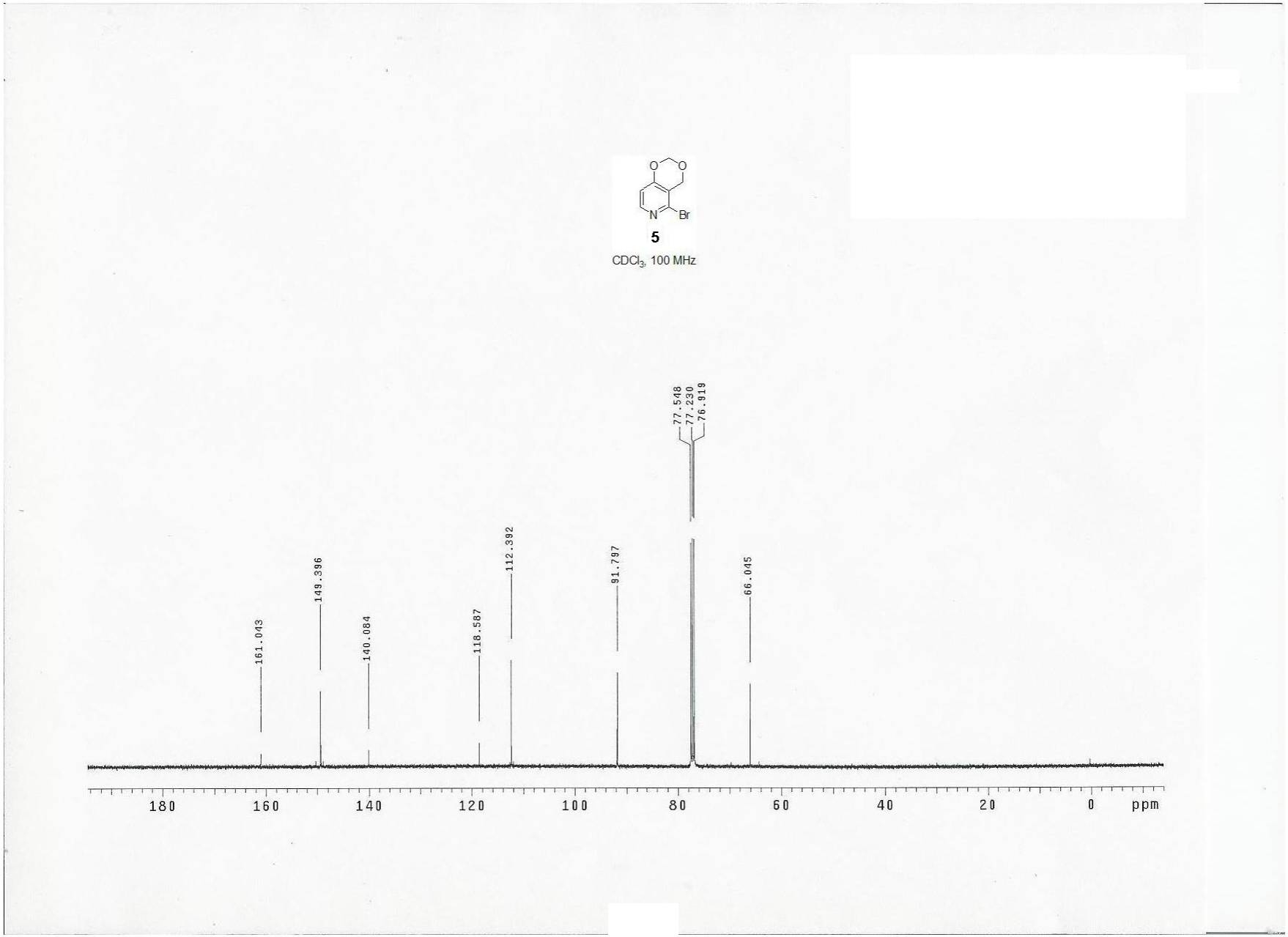
1.00
2.27
2.01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O
N
Br
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140.084
118.587
112.392
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77.230
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66.045
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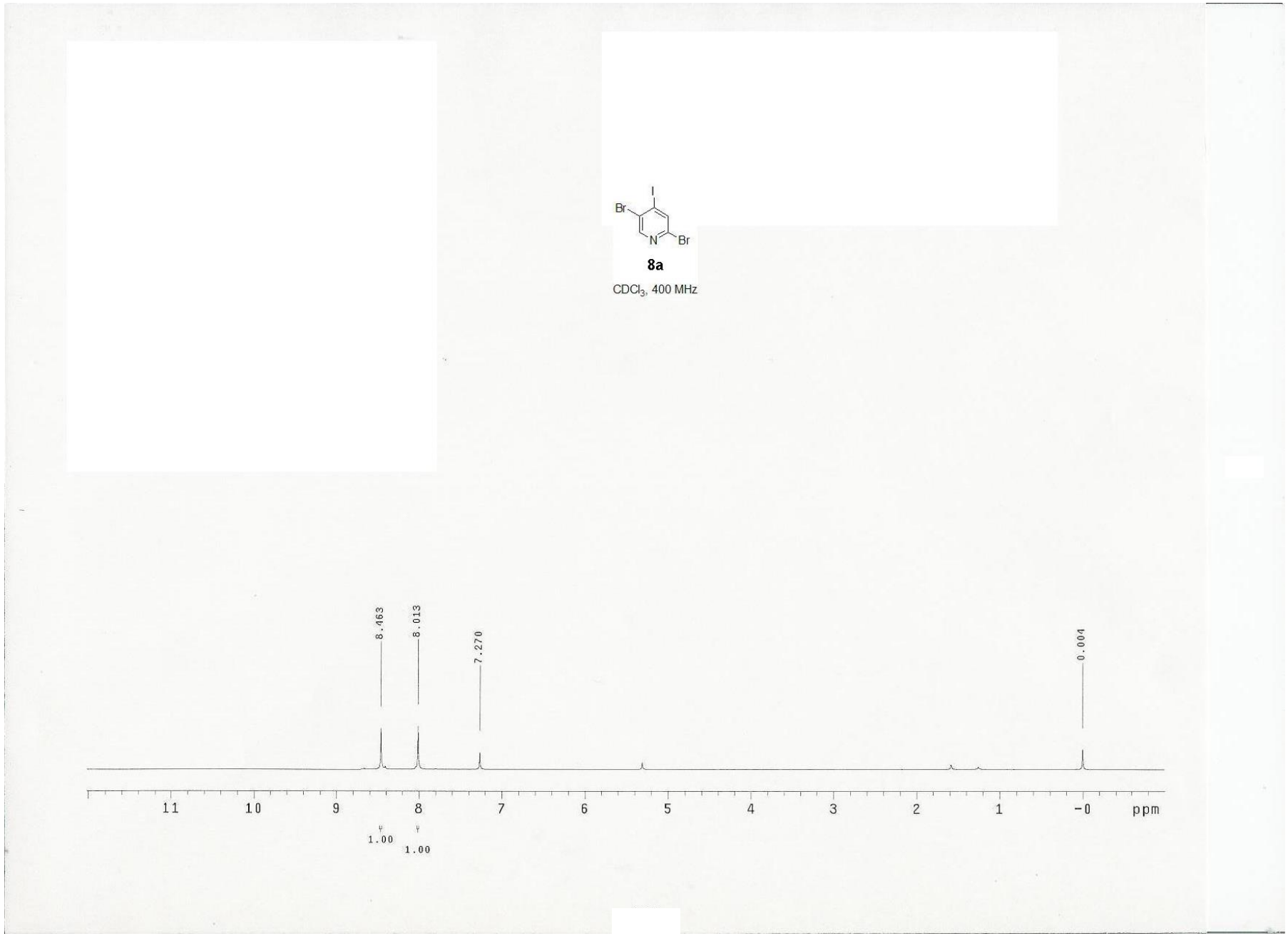
160
140
120
100
80
60
40
20
0
ppm


Br
I
N
Br
8a
CDCl3, 400 MHz
8.463
8.013
7.270
0.004
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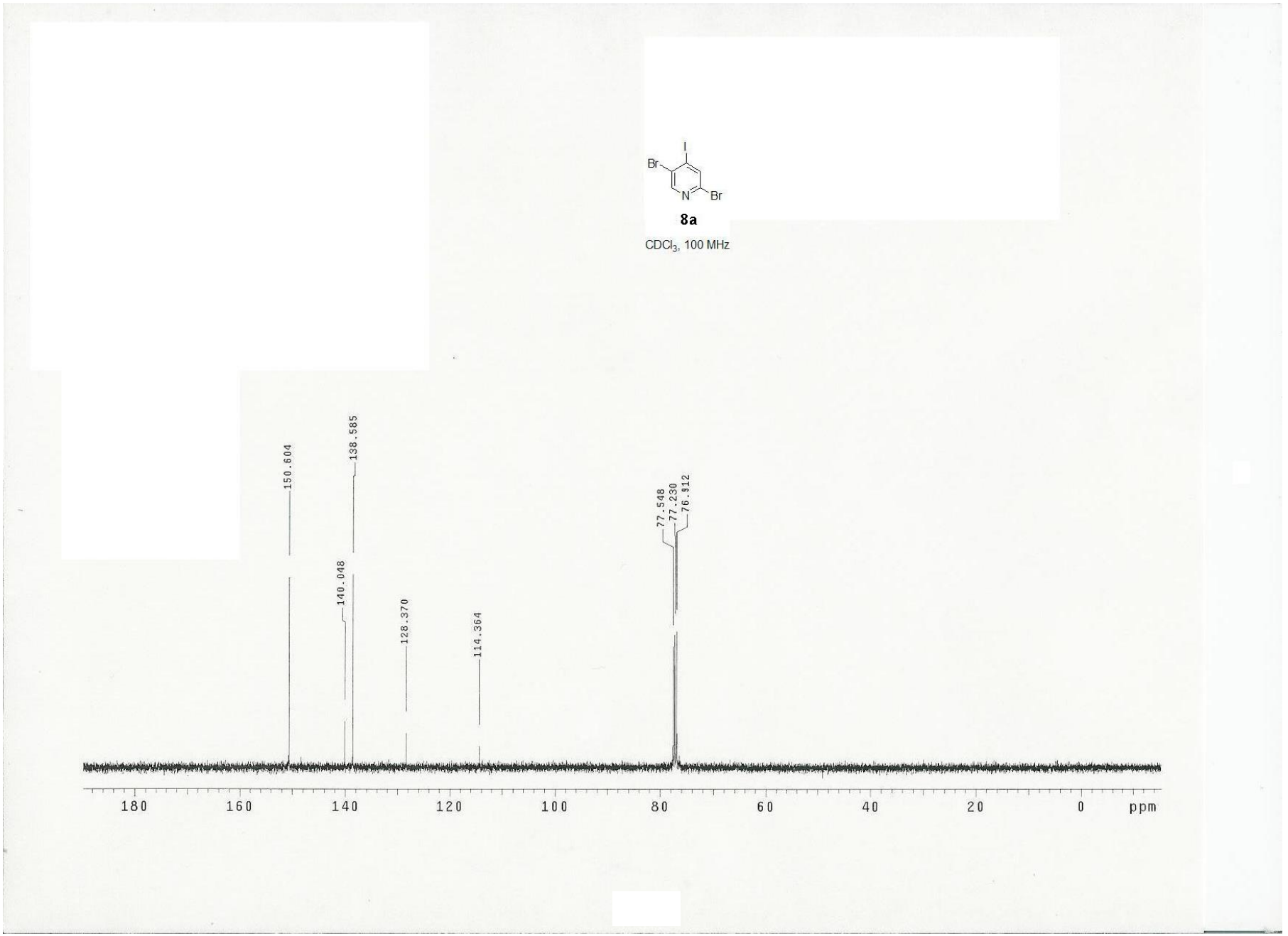
10
9
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.00


I
Br
N
Br
8a
CDCl3, 100 MHz
150.604
138.585
140.048
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114.364
77.548
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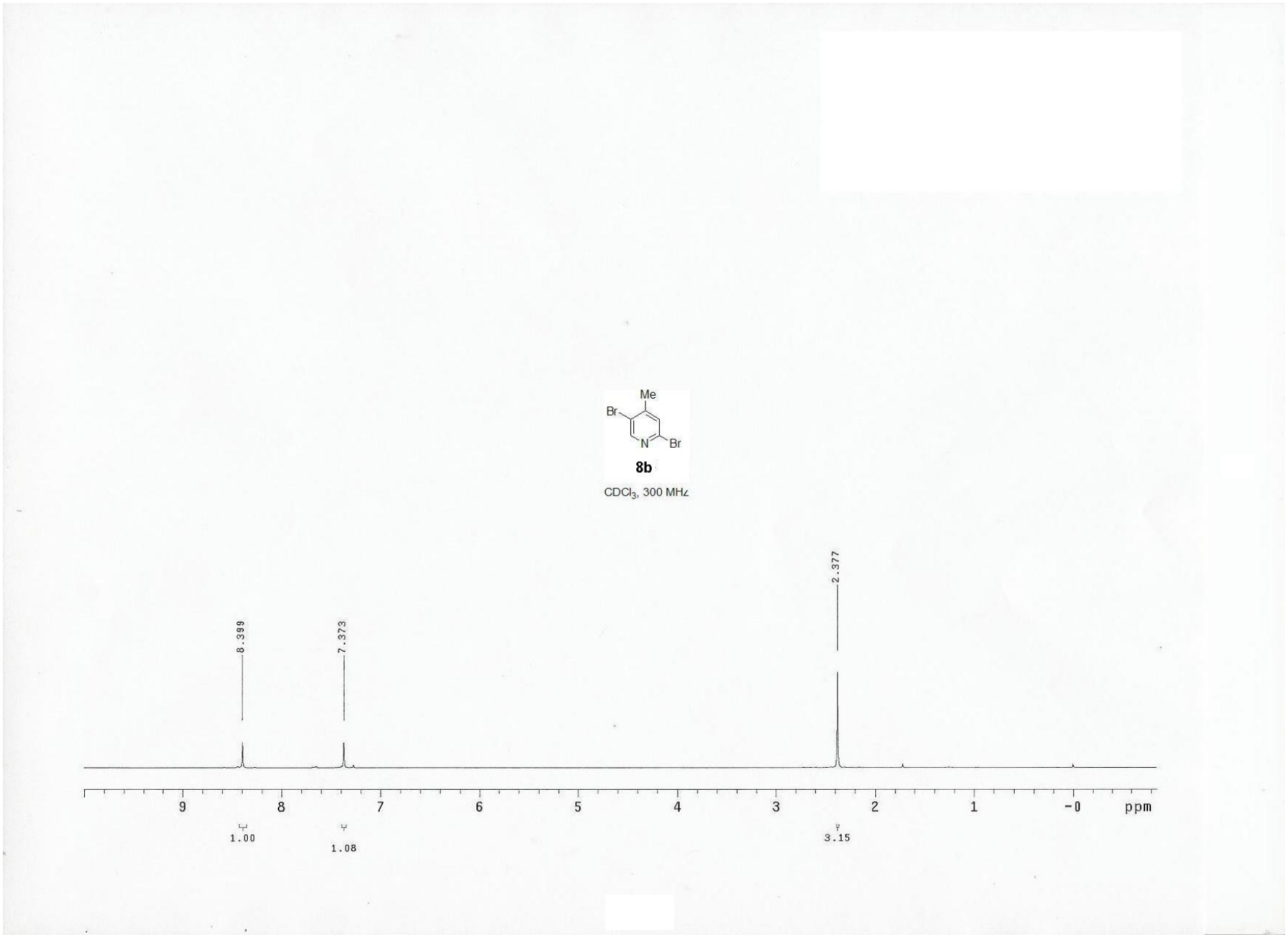
76.912
180
160
140
120
100
80
60
40
20
0
ppm


Me
Br
N
Br
8b
CDCl3, 300 MHz
8.399
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2.377
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8
7
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1
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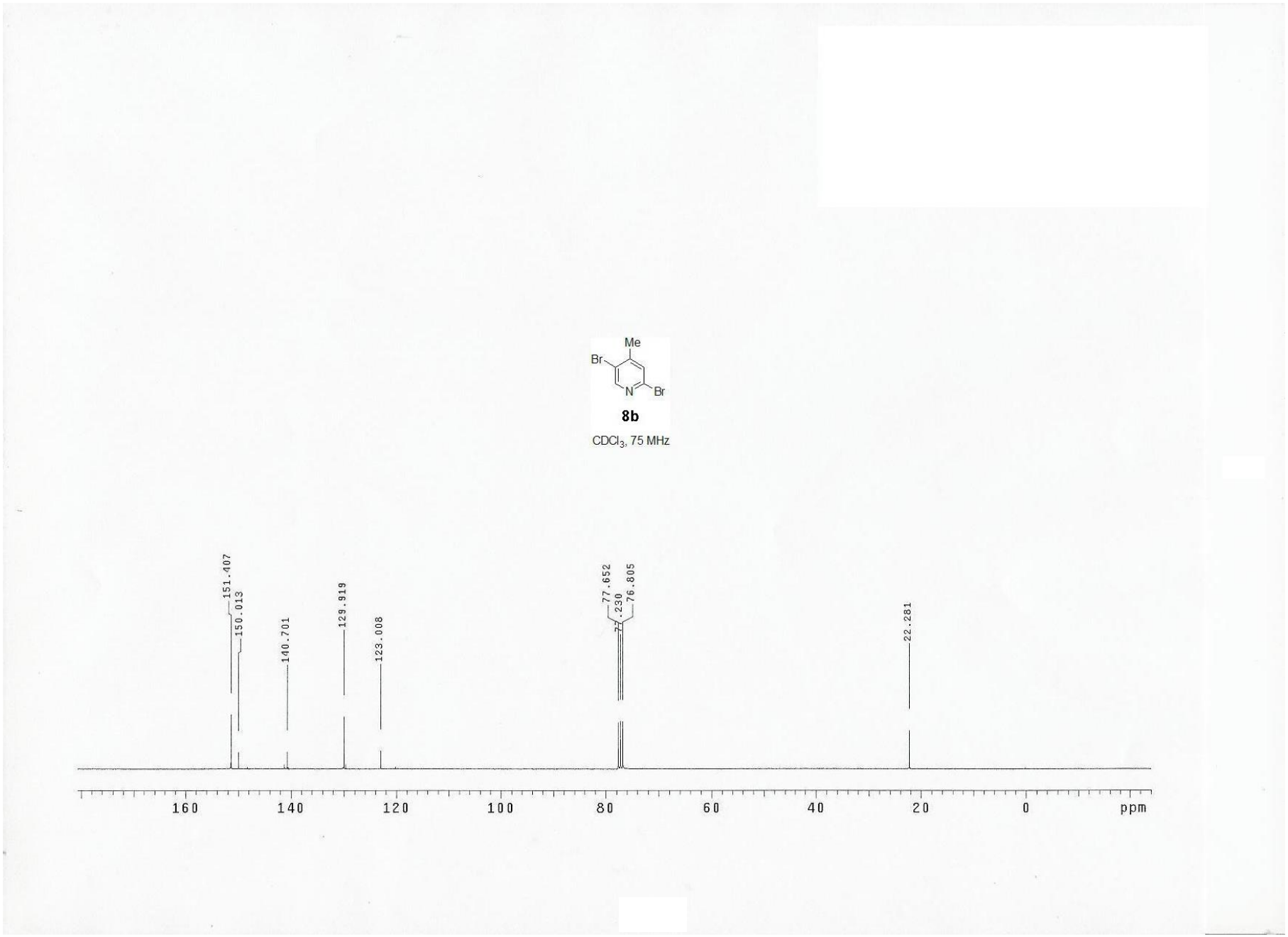
1.00
1.08
3.15


Me
Br
N
Br
8b
CDCl3, 75 MHz
151.407
150.013
140.701
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120
100
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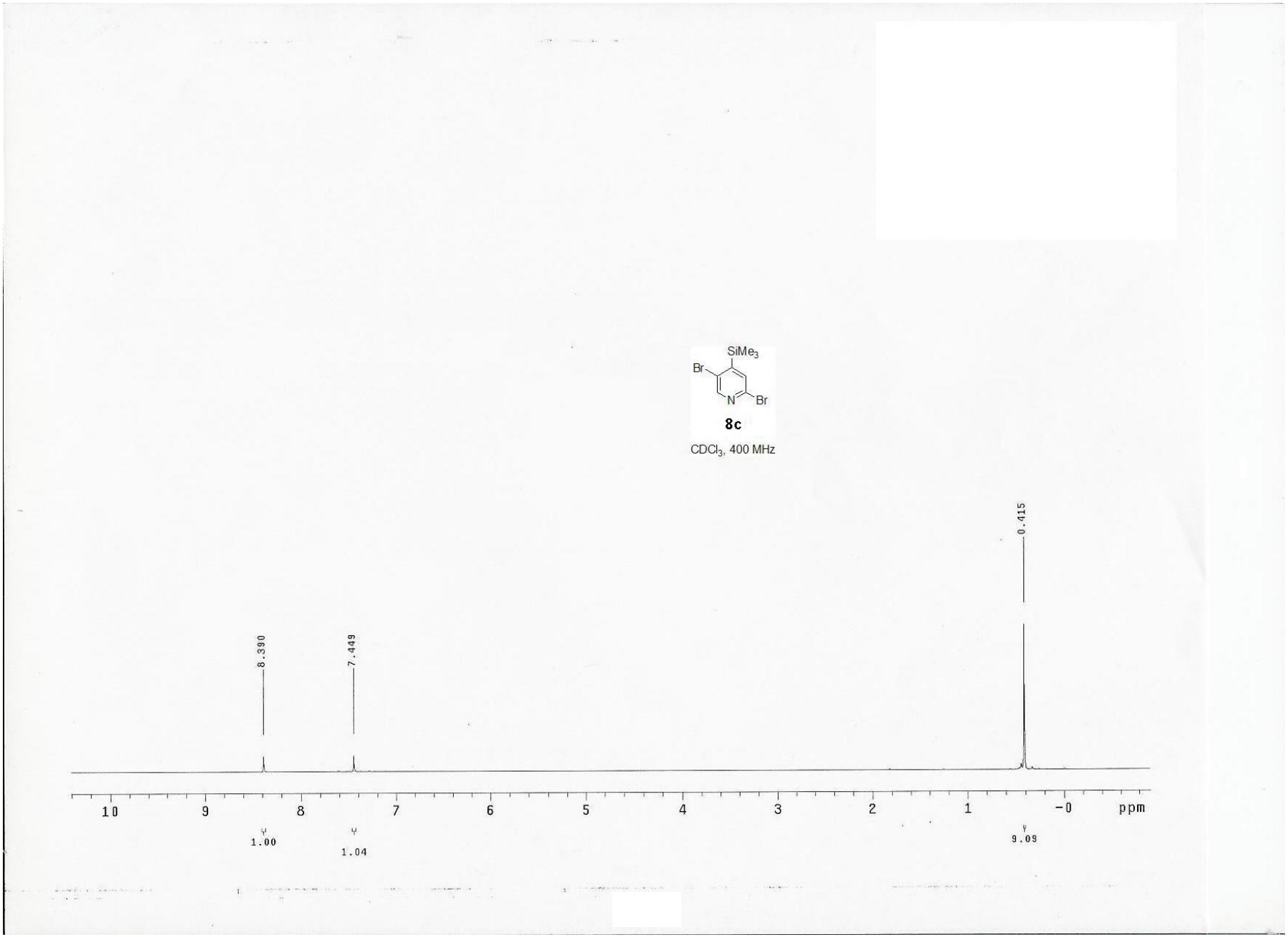
60
40
20
0
ppm


SiMe3
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N
Br
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CDCl3, 400 MHz
8.390
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10
9
8
7
6
5
4
3
2
1
-0
ppm
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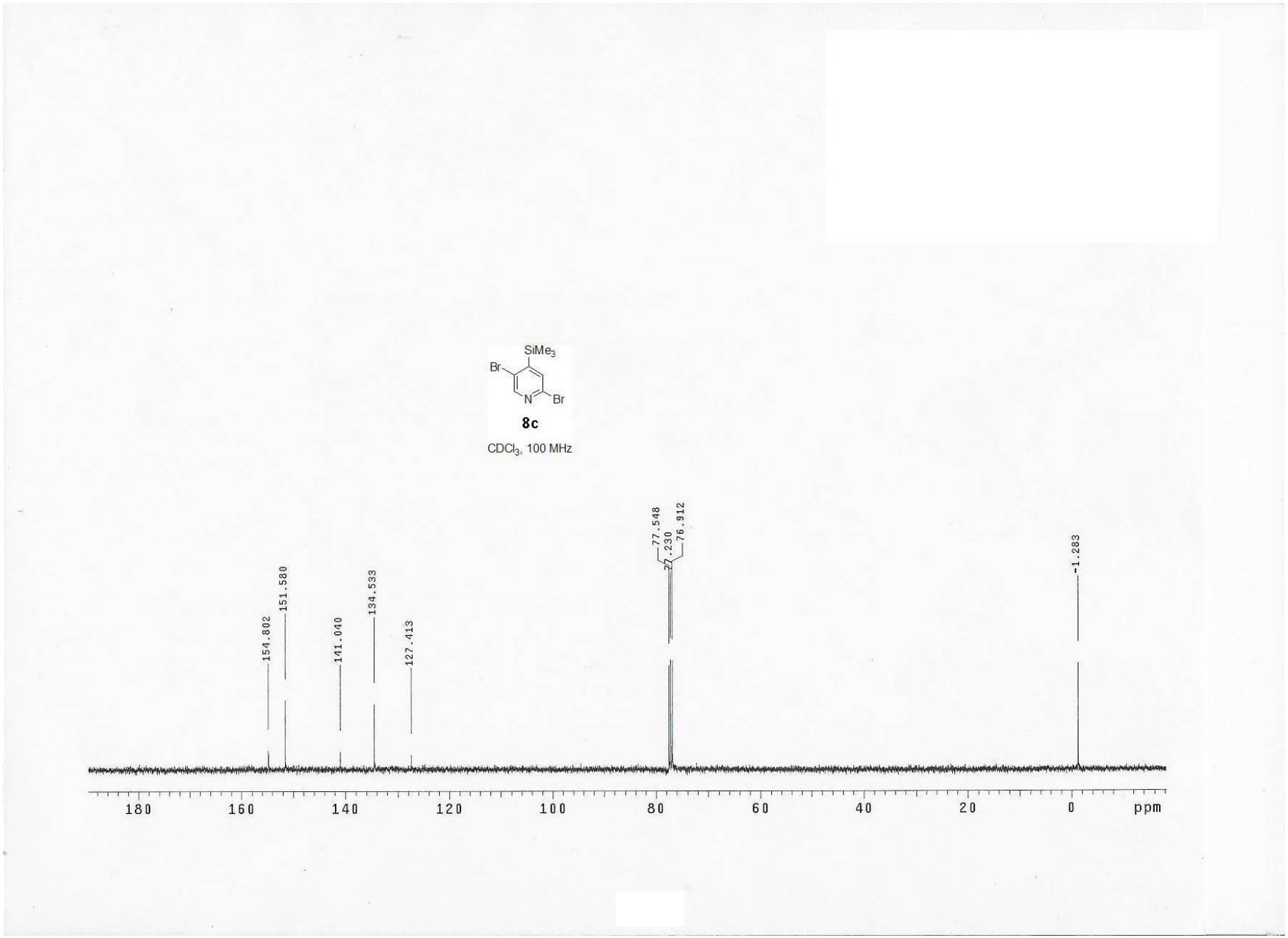
1.04
9.09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Br
8c
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120
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60
40
20
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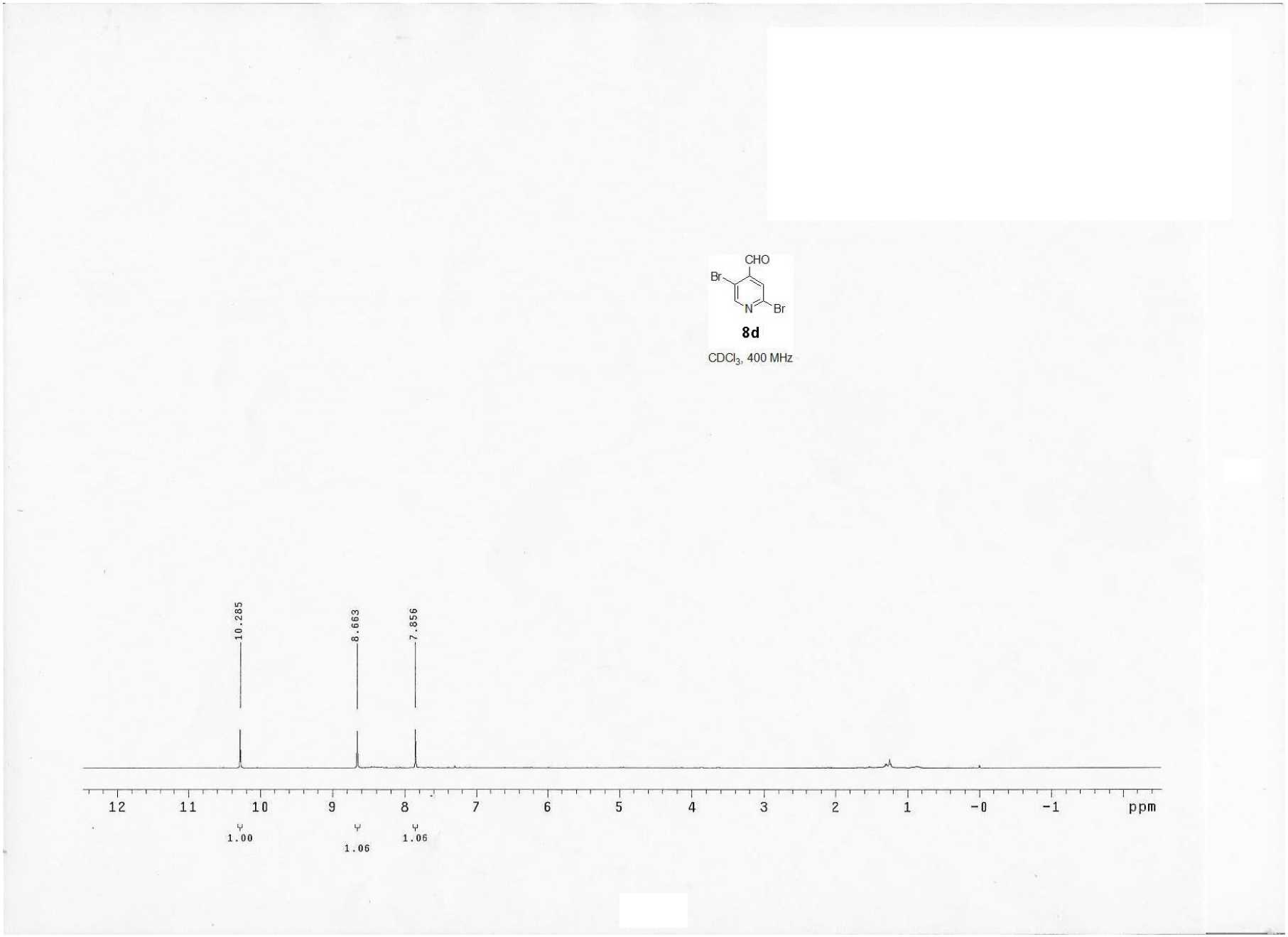
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11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
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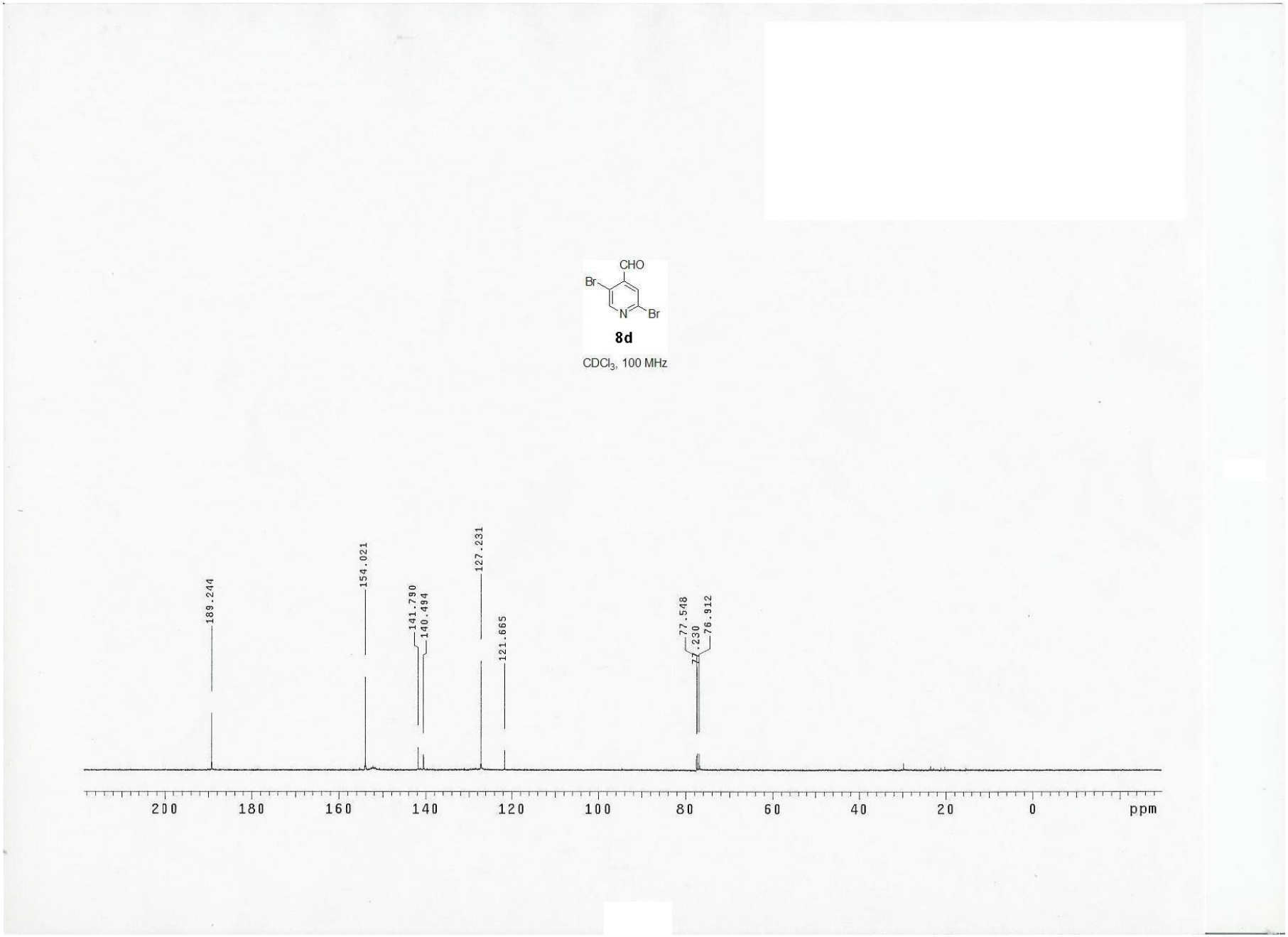
1.06
1.06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Br
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77.230
76.912
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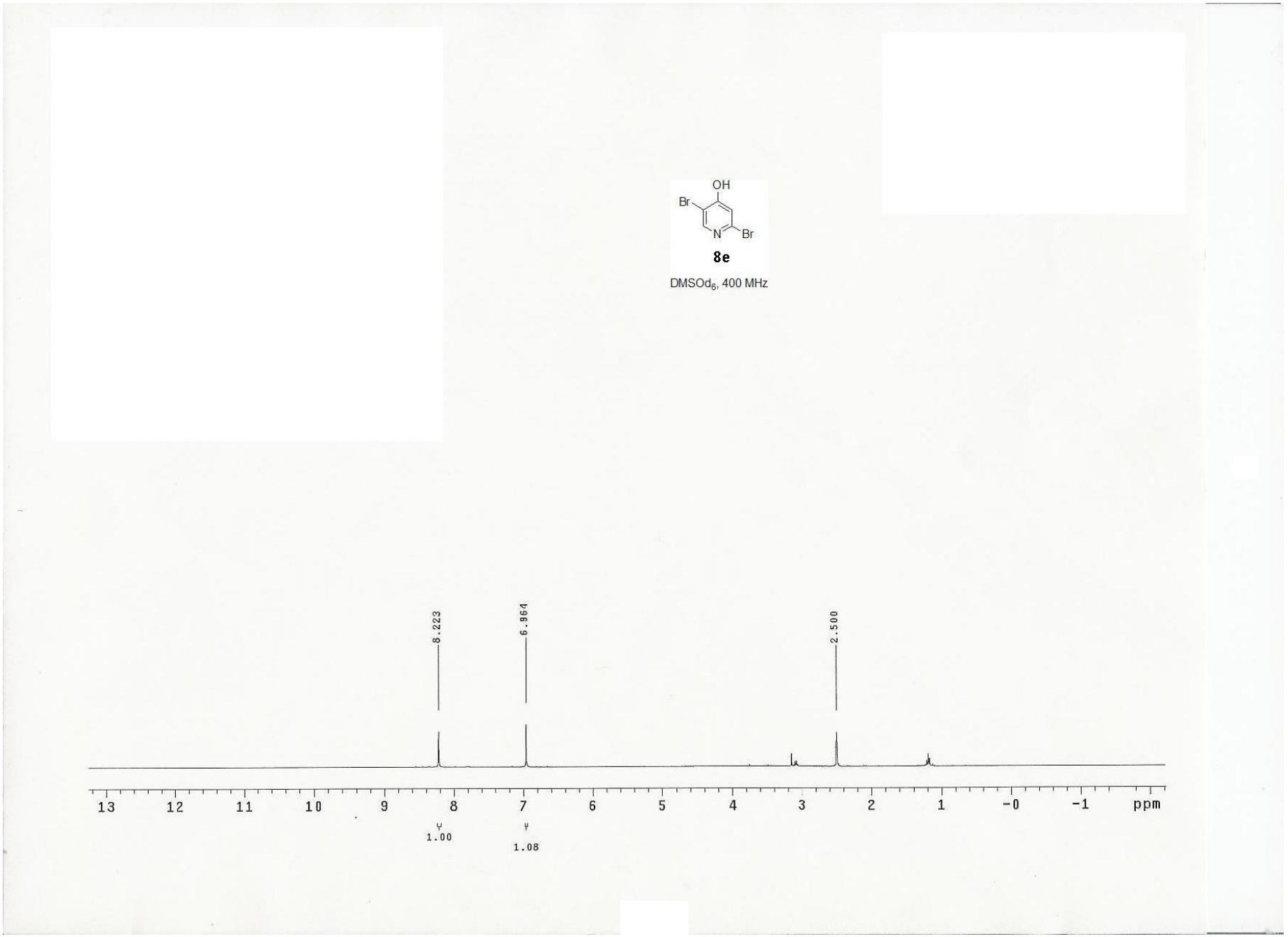
160
140
120
100
80
60
40
20
0
ppm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Br
8e
DMSOd6, 400 MHz
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9
8
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6
5
4
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1
-0
-1
ppm
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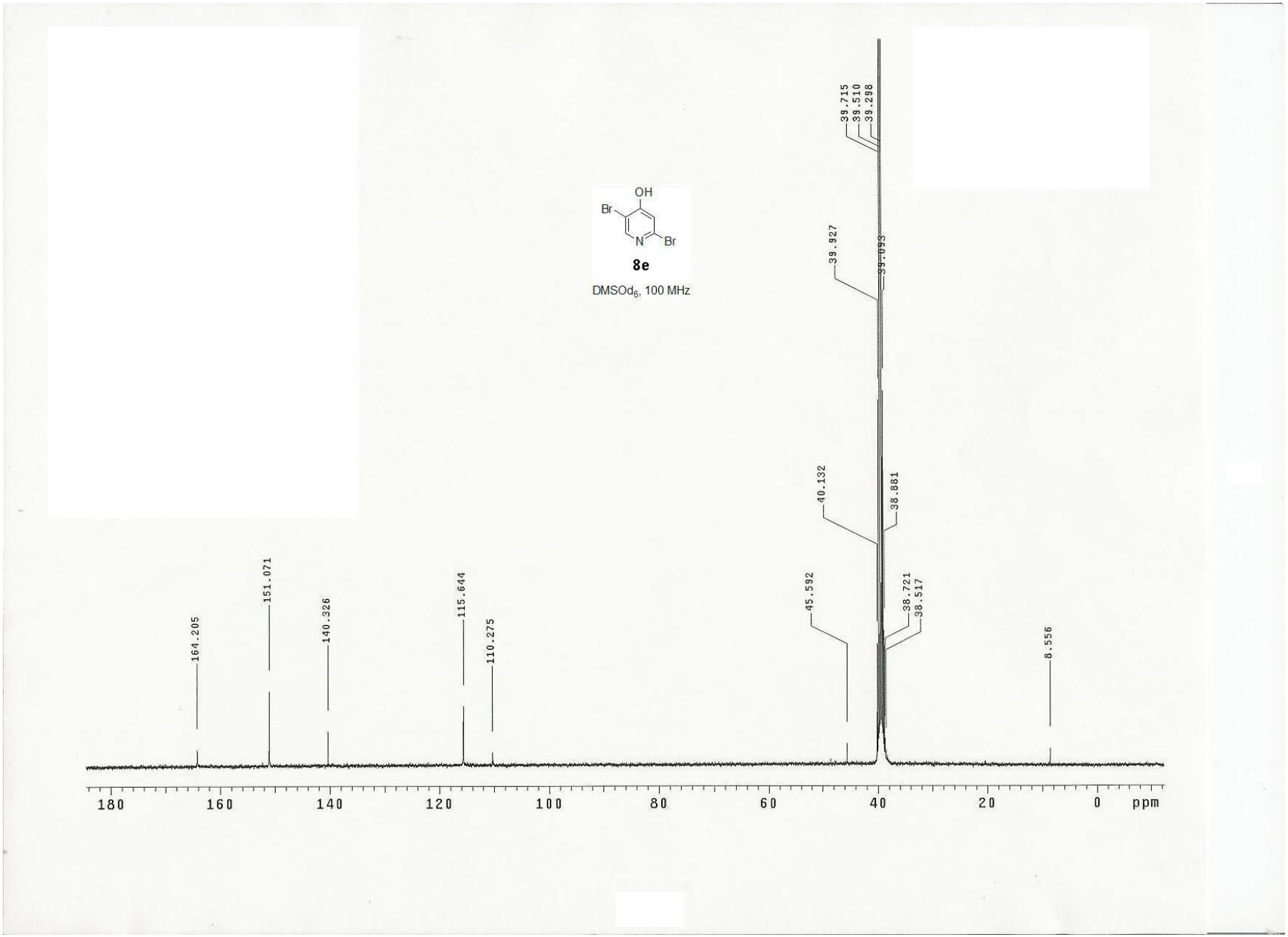
1.08


OH
Br
N
Br
8e
DMSOd6, 100 MHz
39.715
39.510
39.298
39.927
39.093
40.132
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45.592
38.721
38.517
8.556
164.205
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115.644
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160
140
120
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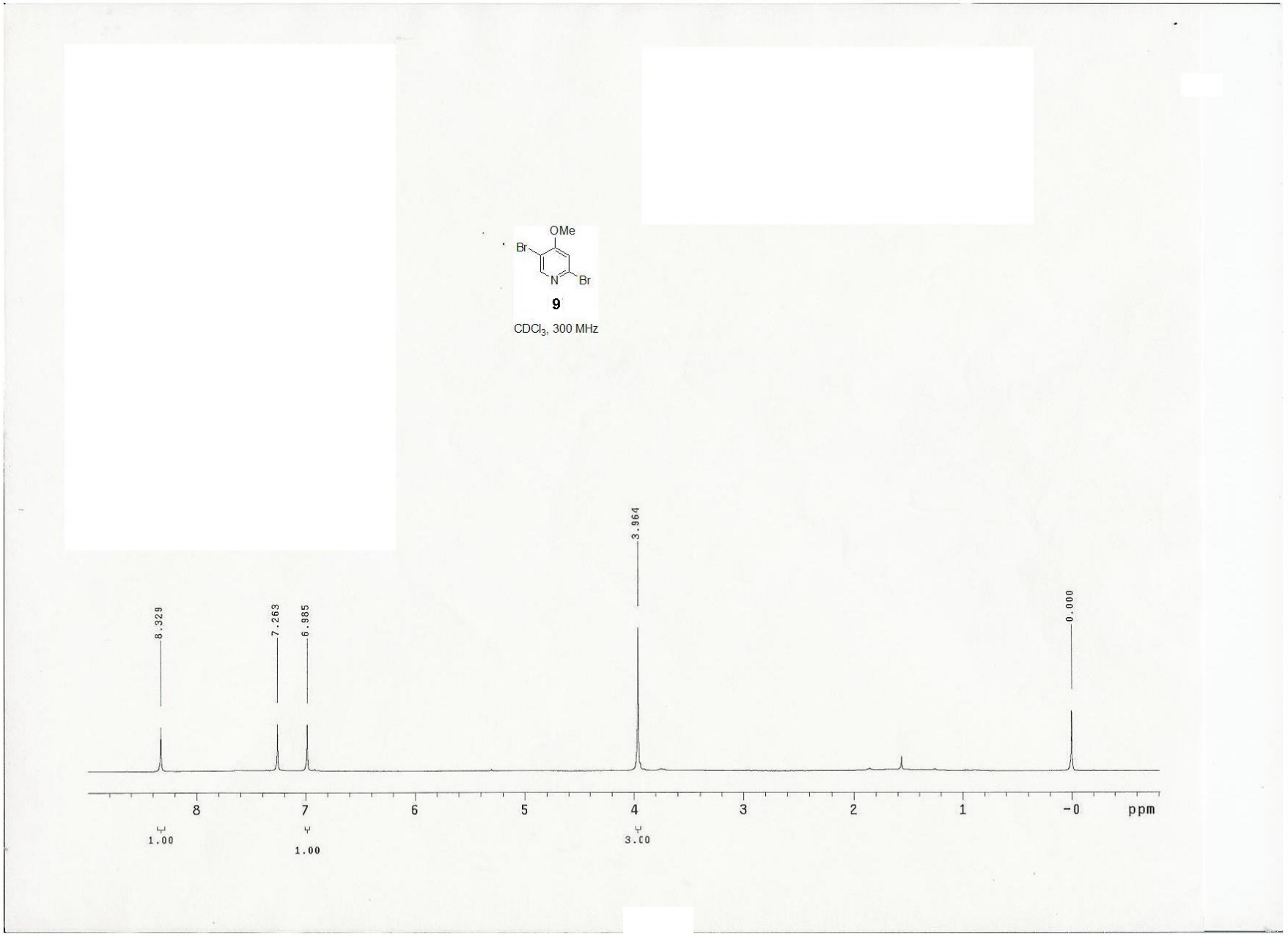
80
60
40
20
0
ppm

4e


OMe
Br
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Br
9
CDCl3, 300 MHz
8.329
7.263
6.985
3.964
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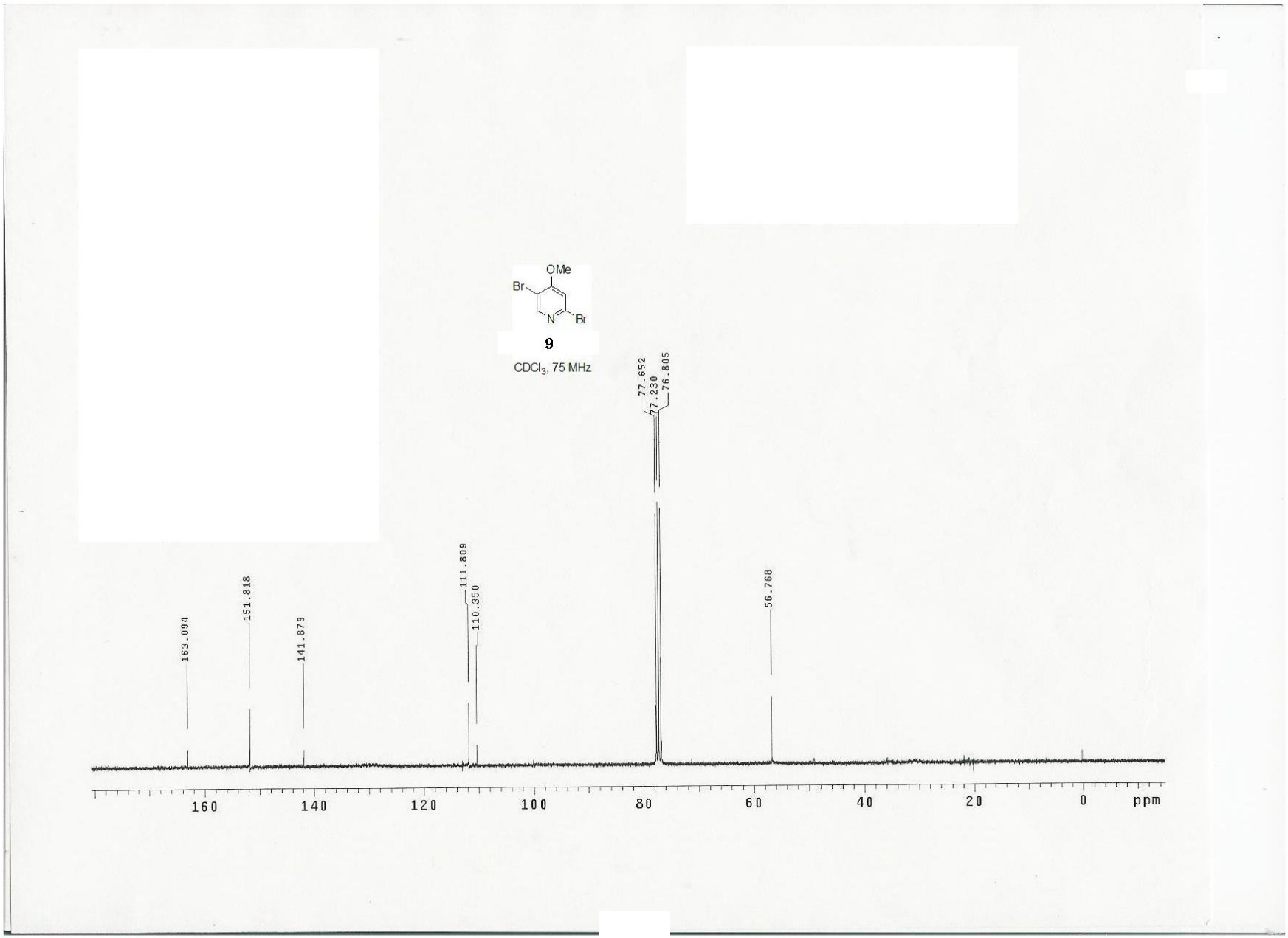
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.00
3.00


OMe
Br
N
Br
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CDCl3, 75 MHz
77.652
77.230
76.805
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111.809
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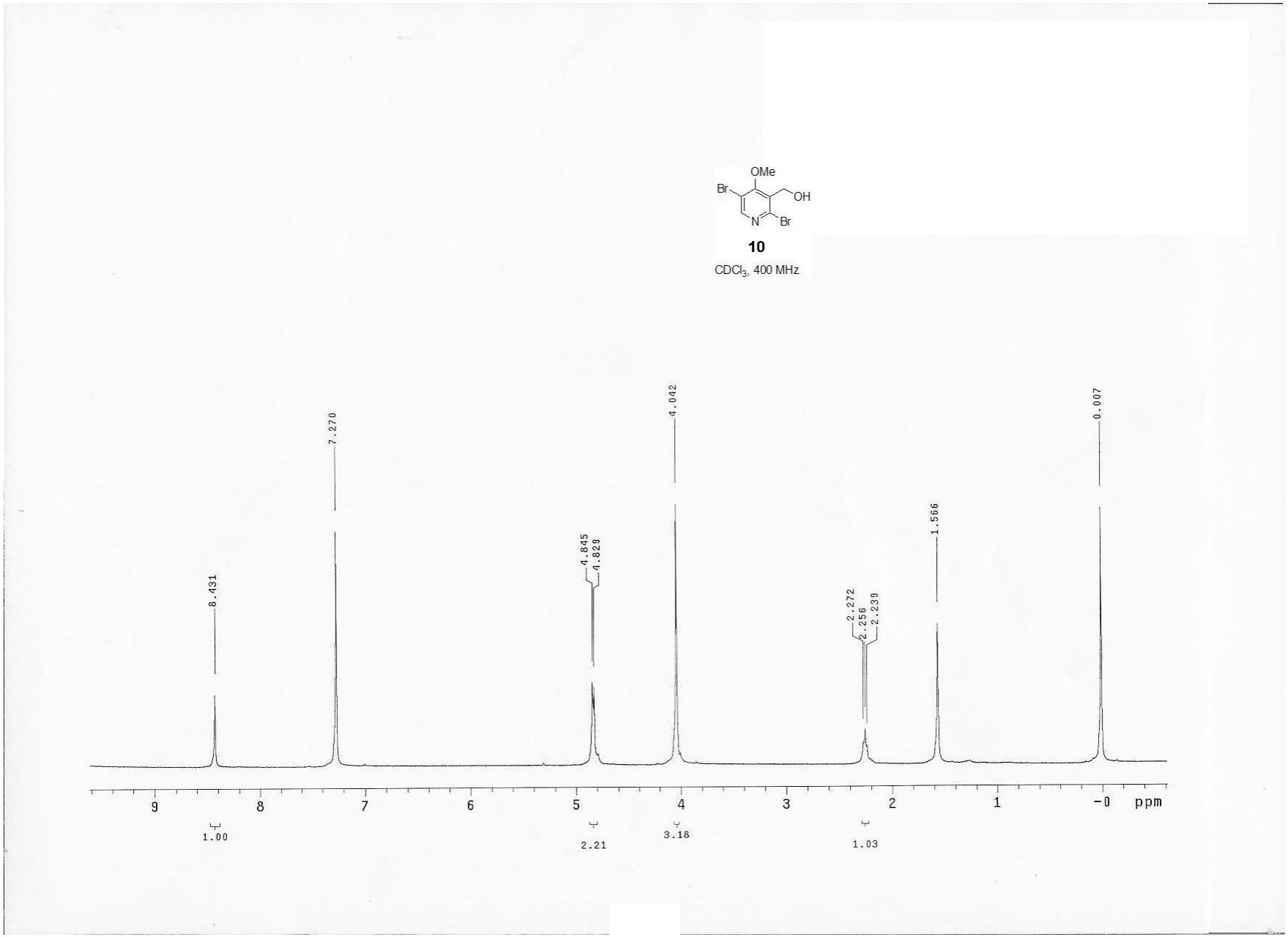
140
120
100
80
60
40
20
0
ppm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2.239
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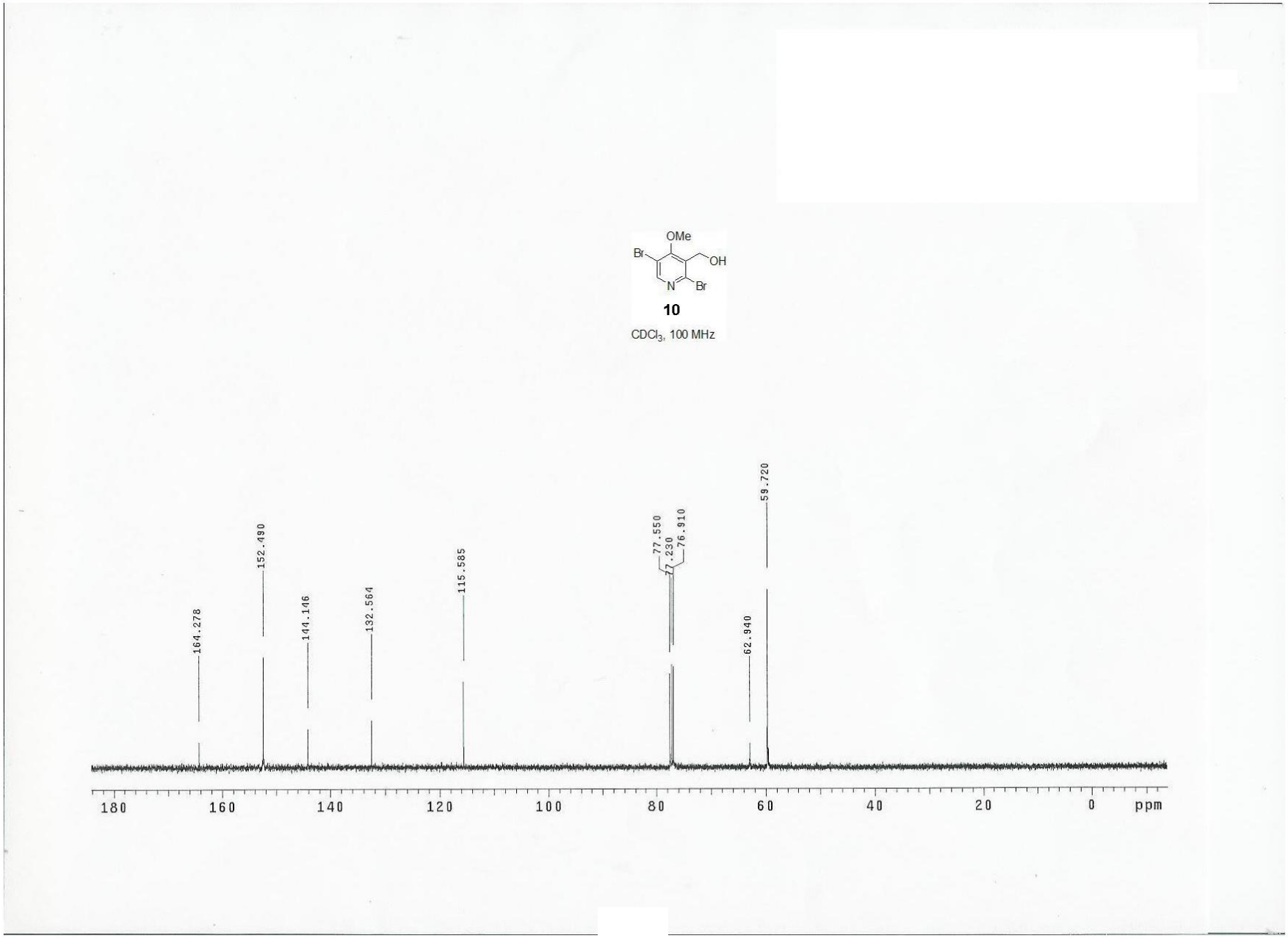
1.03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Br
OH
N
Br
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CDCl3, 100 MHz
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152.490
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132.564
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77.230
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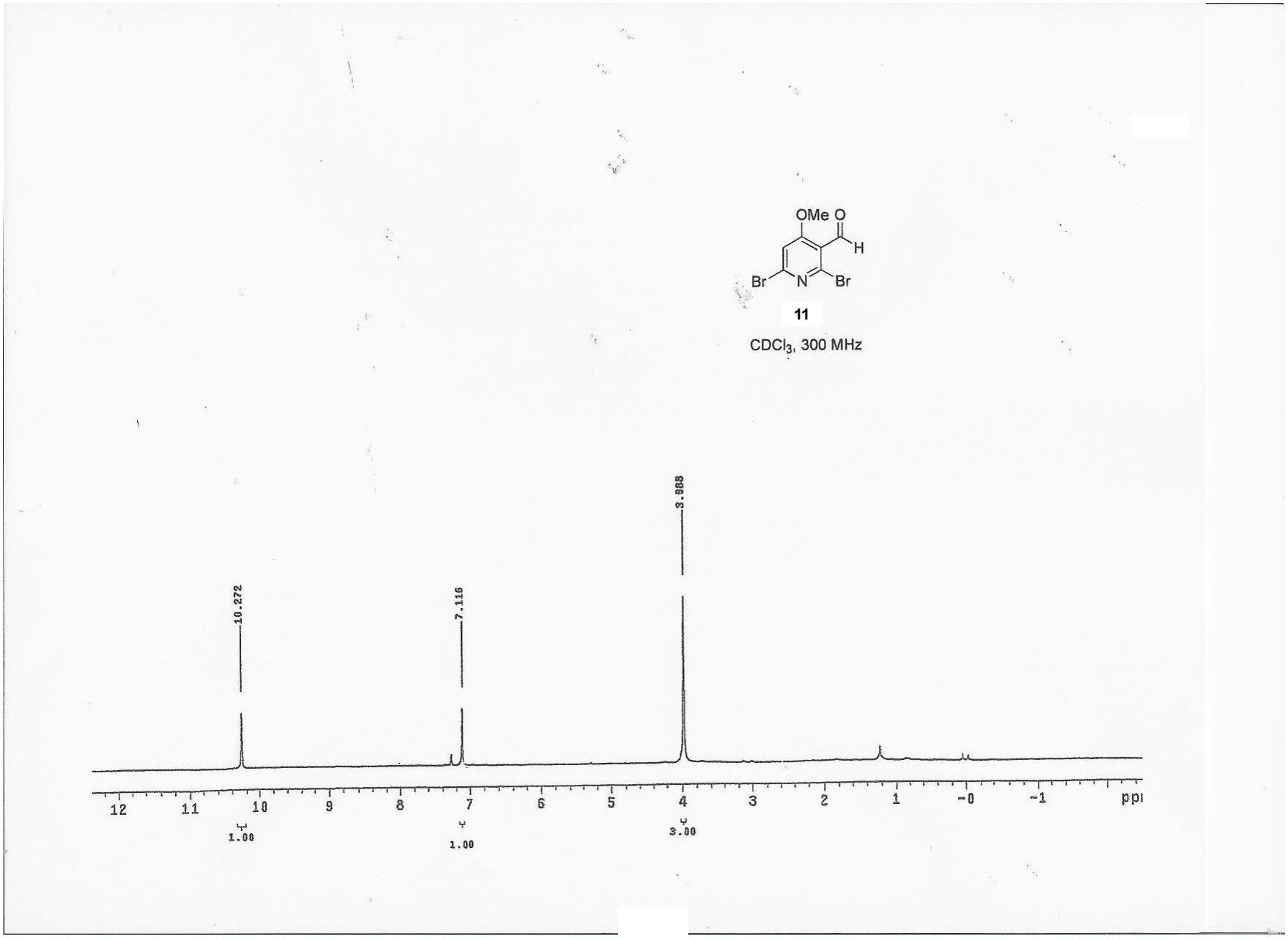
140
120
100
80
60
40
20
0
ppm


OMe O
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Br
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CDCl3, 300 MHz
10.272
7.116
3.988
12
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7
6
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4
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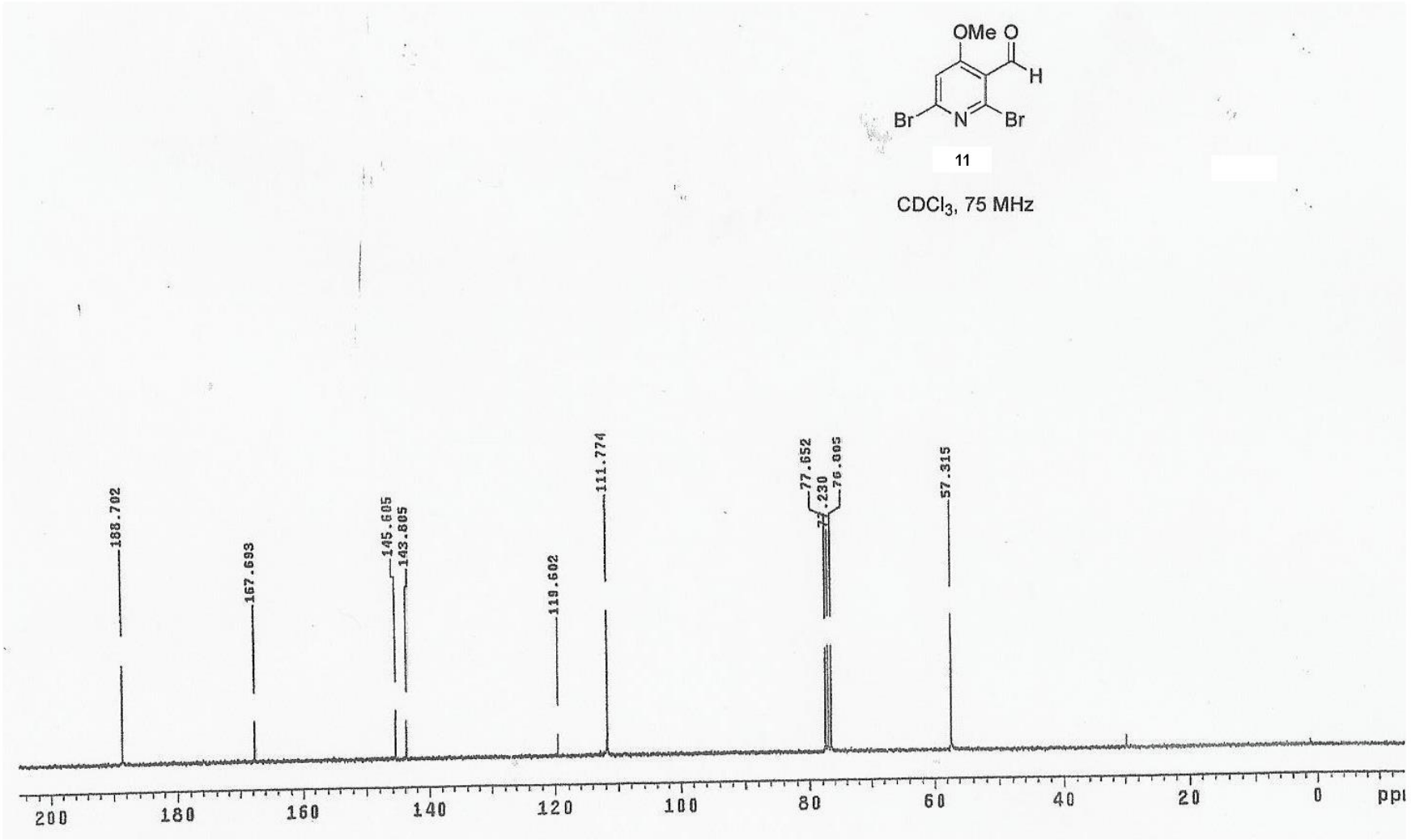
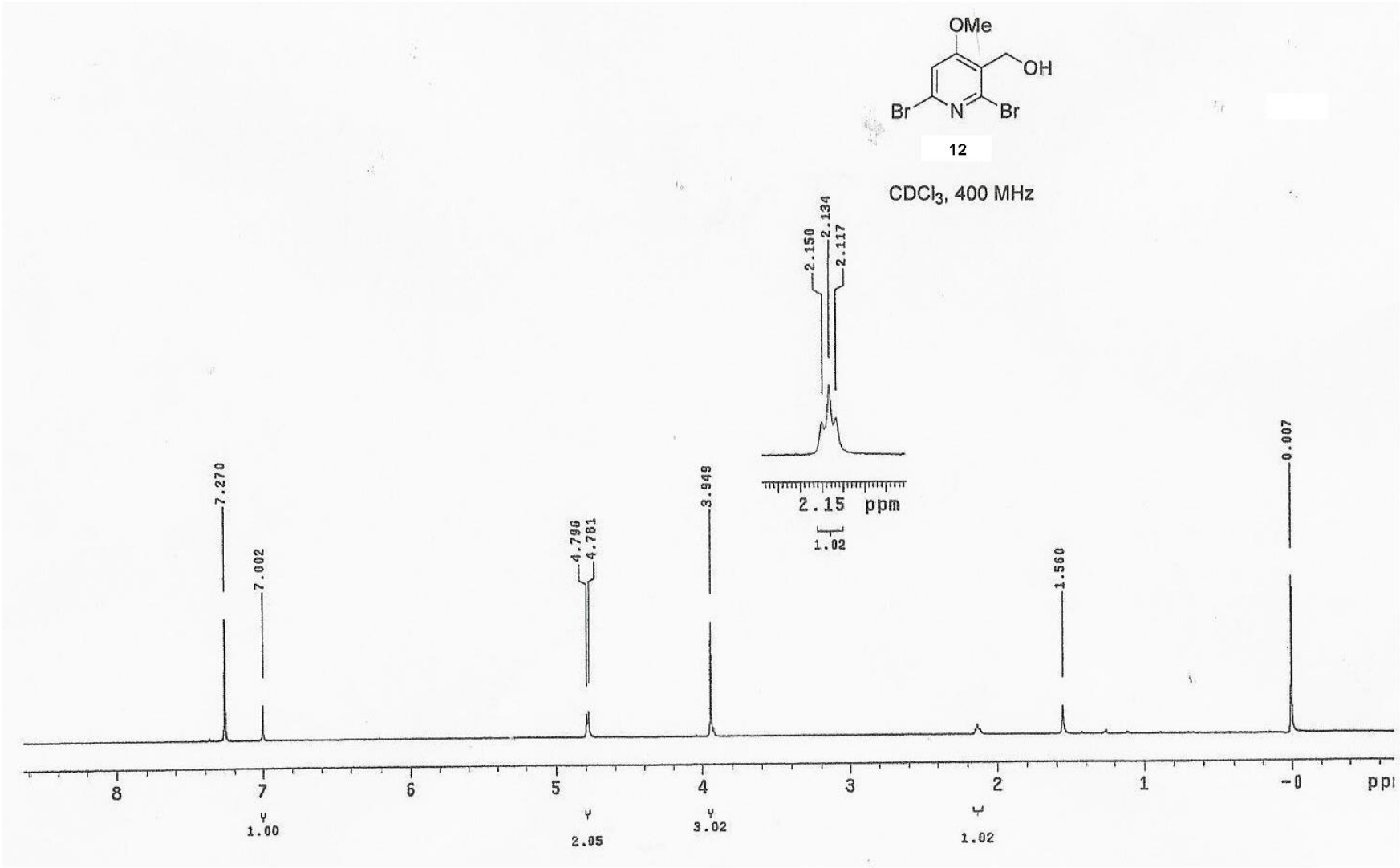
1
-0
-1
ppm
1.00
1.00
3.00


OMe
O
H
Br
N
Br
11
CDCl3, 75 MHz
188.702
167.693
145.605
143.805
119.602
111.774
77.652
77.230
76.805
57.315
200
180
160
140
120
100
80
60
40
20
0
ppm


OMe
OH
Br
N
Br
12
CDCl3, 400 MHz
7.270
7.002
4.796
4.781
3.949
2.150
2.134
2.117
2.15 ppm
1.02
1.560
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7
6
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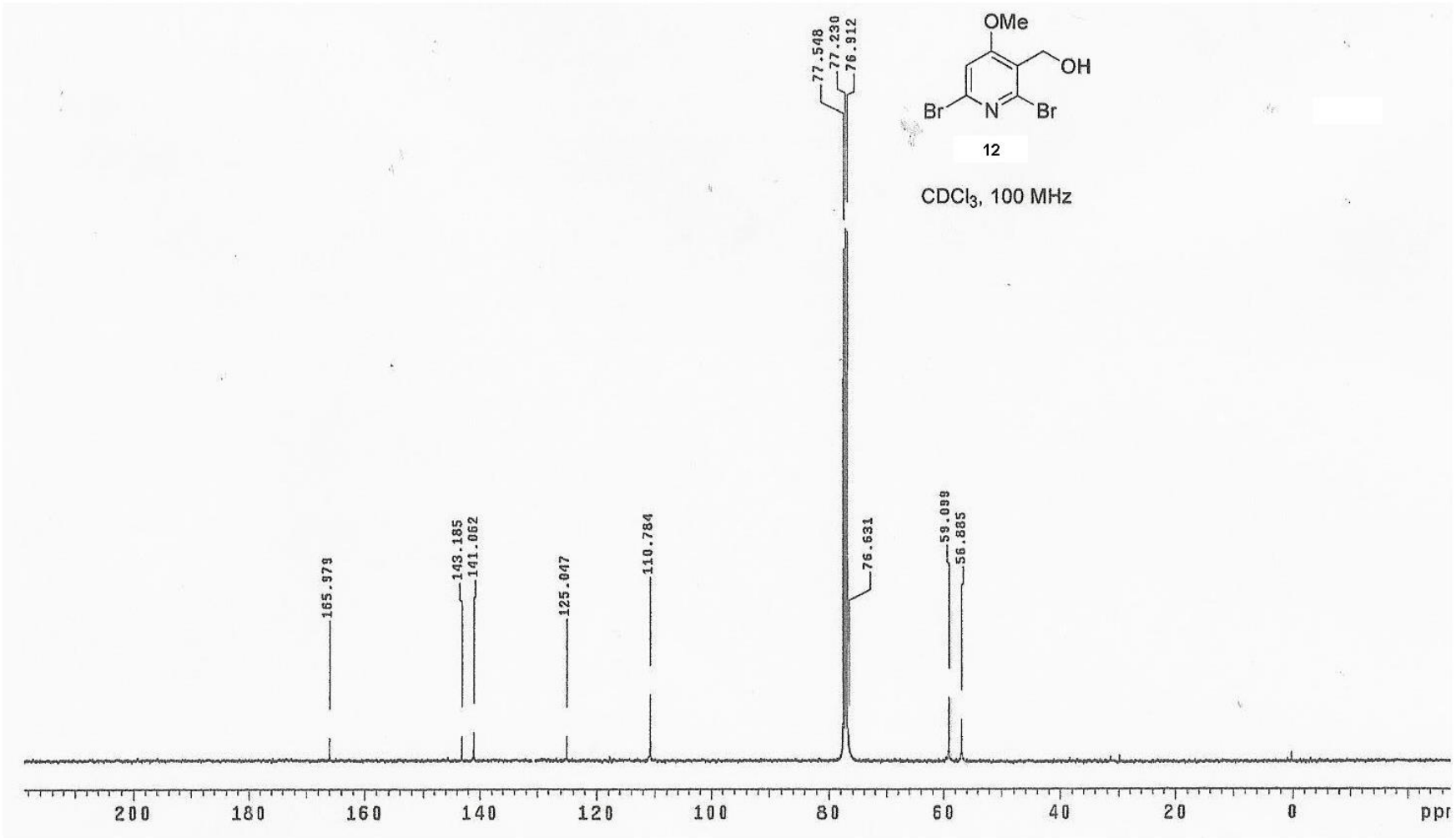
4
3
2
1
-0
ppm
1.00
2.05
3.02
1.02


77.548
77.230
76.912
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OH
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N
Br
12
CDCl3, 100 MHz
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143.185
141.062
125.047
110.784
76.631
59.099
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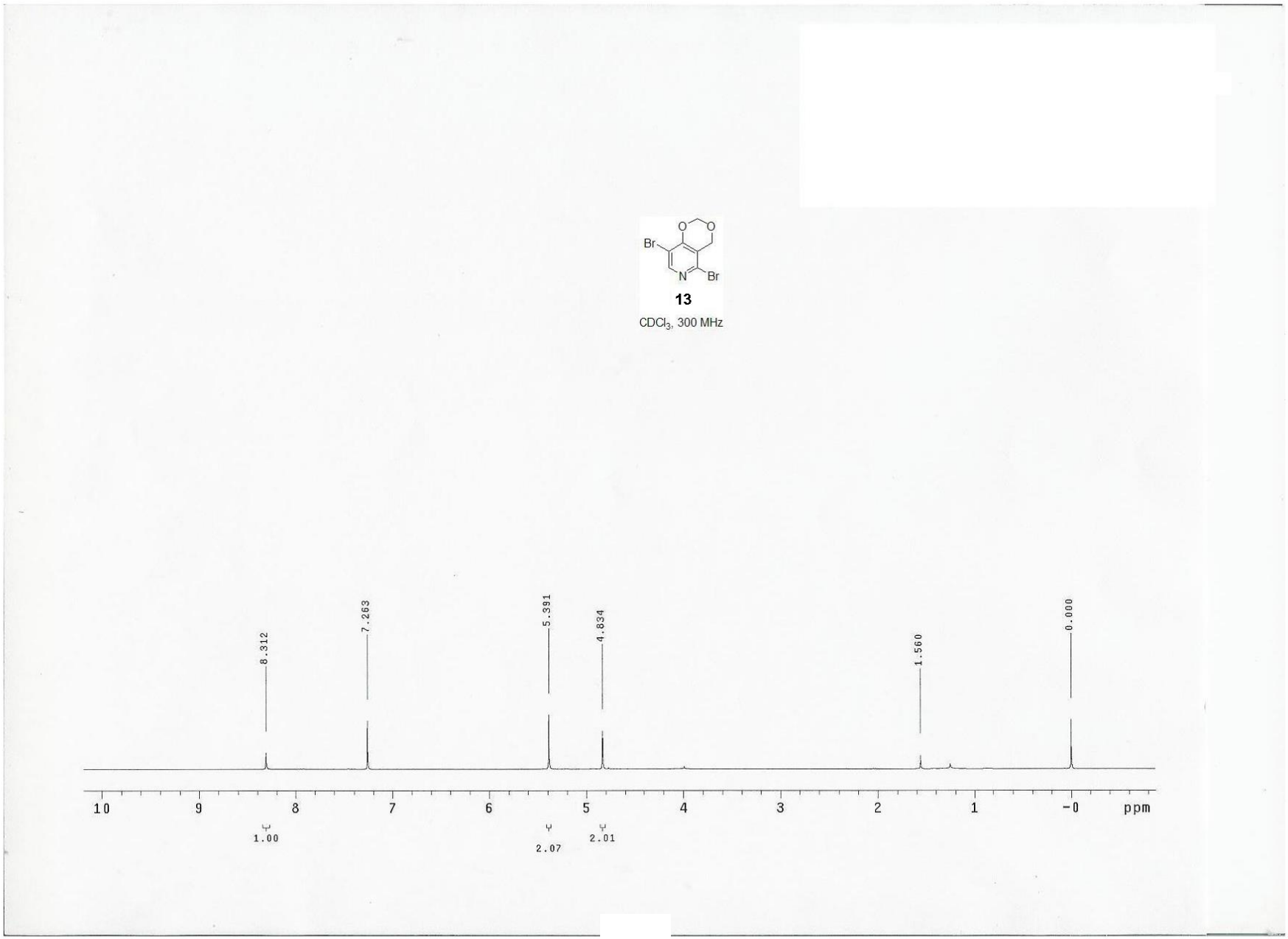
200
180
160
140
120
100
80
60
40
20
0
ppm


Br
O
O
N
Br
13
CDCl3, 300 MHz
8.312
7.263
5.391
4.834
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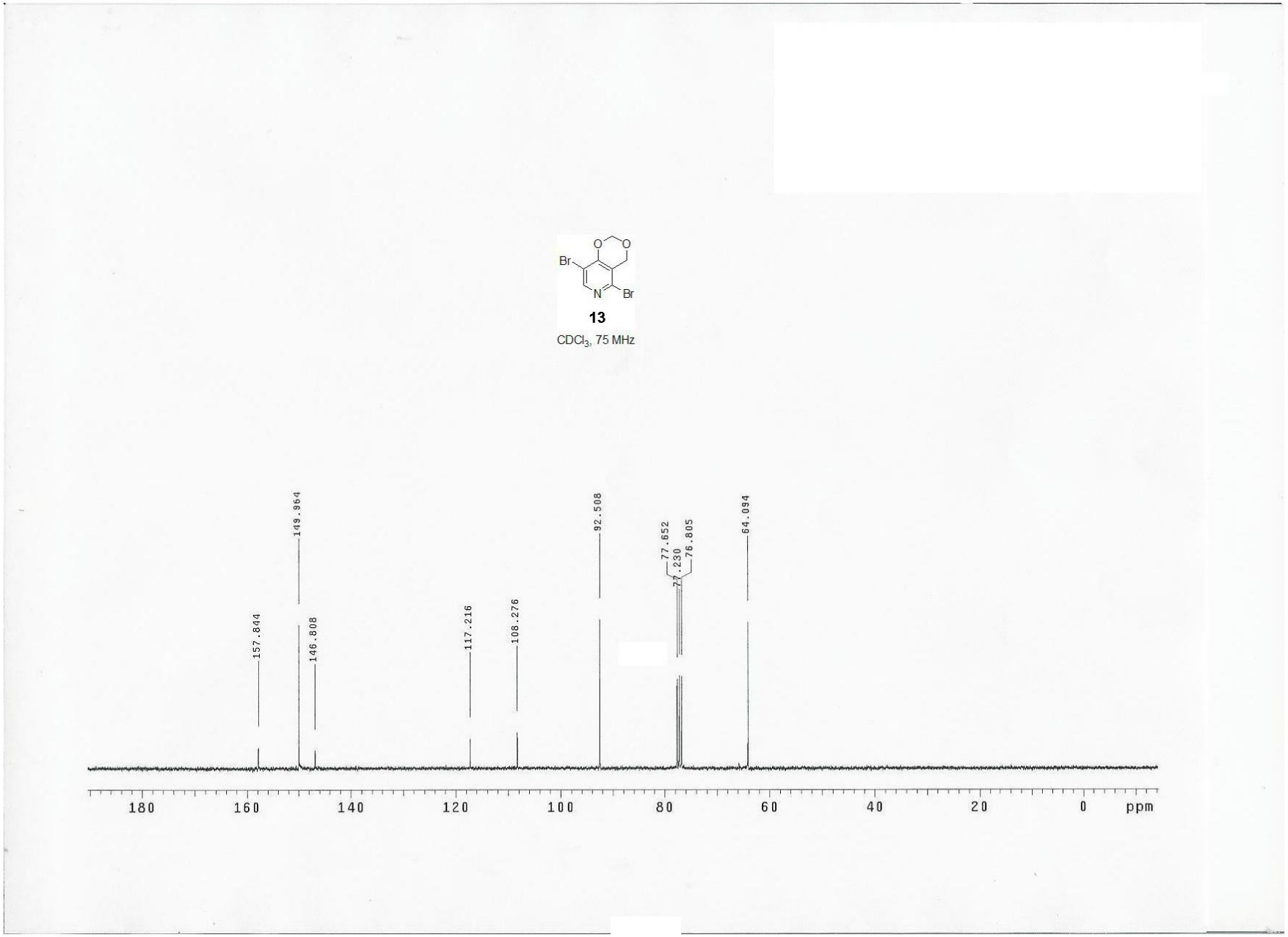
9
8
7
6
5
4
3
2
1
-0
ppm
1.00
2.07
2.01


Br
O
O
N
Br
13
CDCl3, 75 MHz
157.844
149.964
146.808
117.216
108.276
92.508
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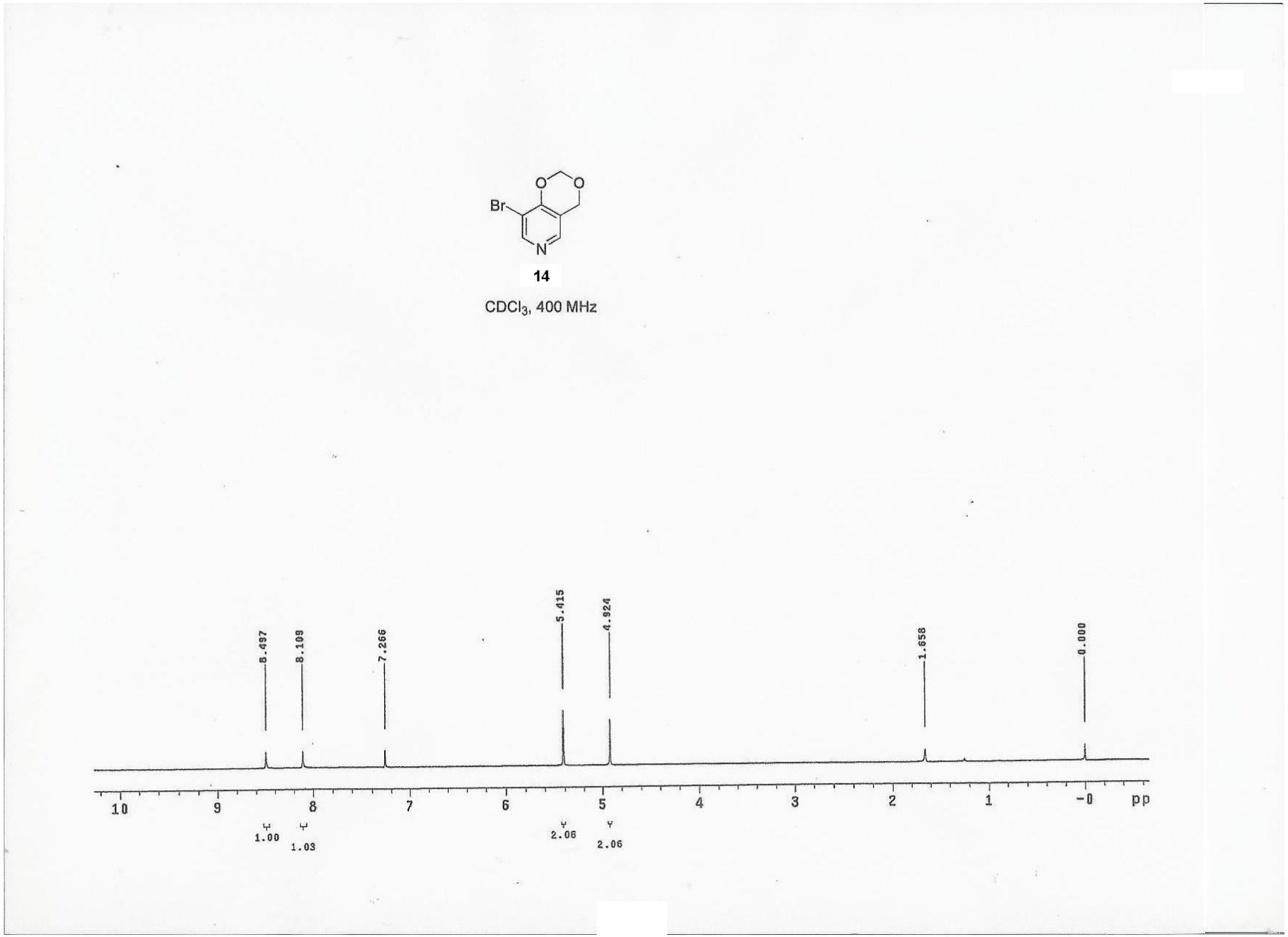
77.230
76.805
64.094
180
160
140
120
100
80
60
40
20
0
ppm


Br
O
O
N
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CDCl3, 400 MHz
8.497
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7.266
5.415
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1.658
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4
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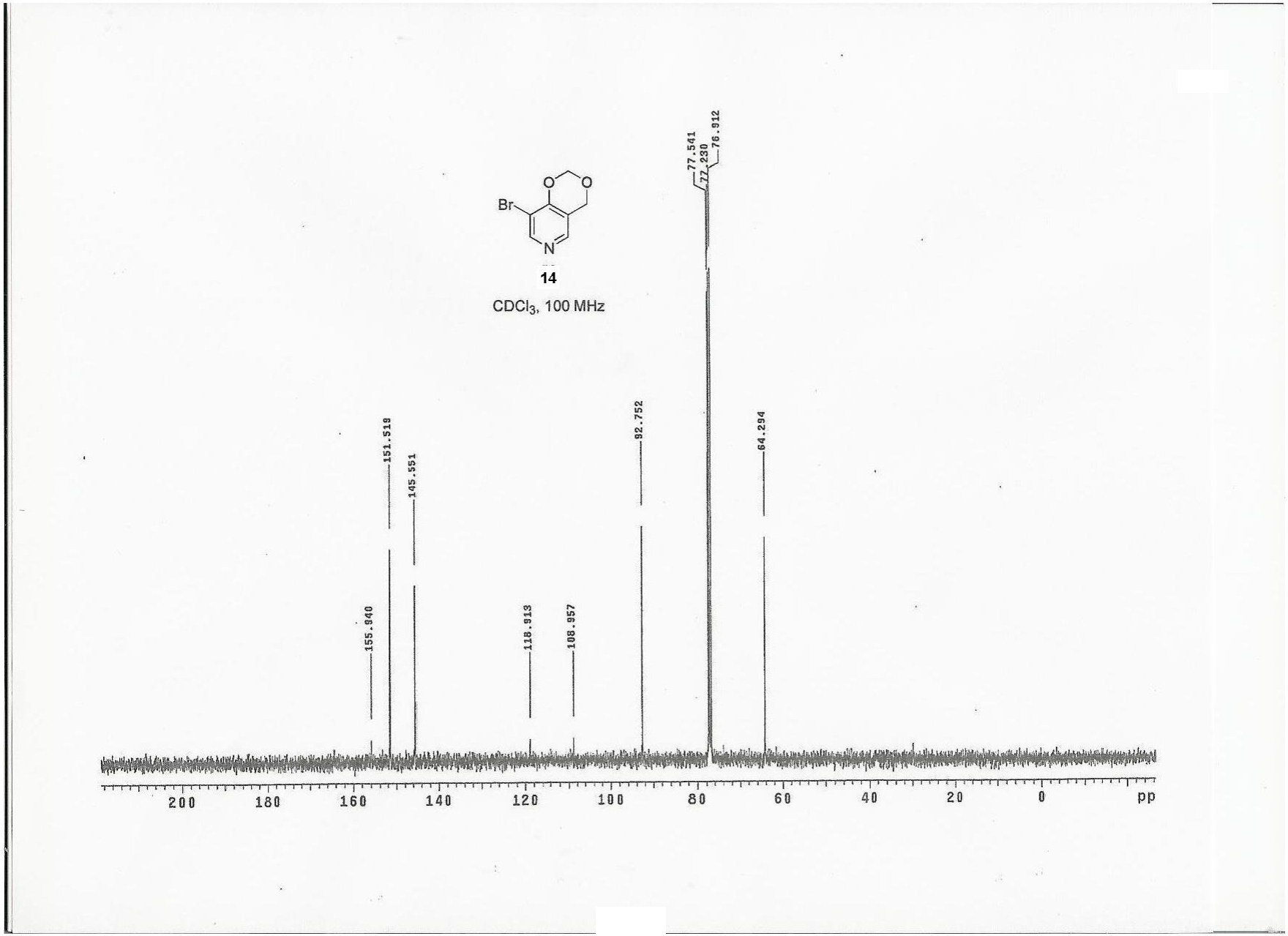
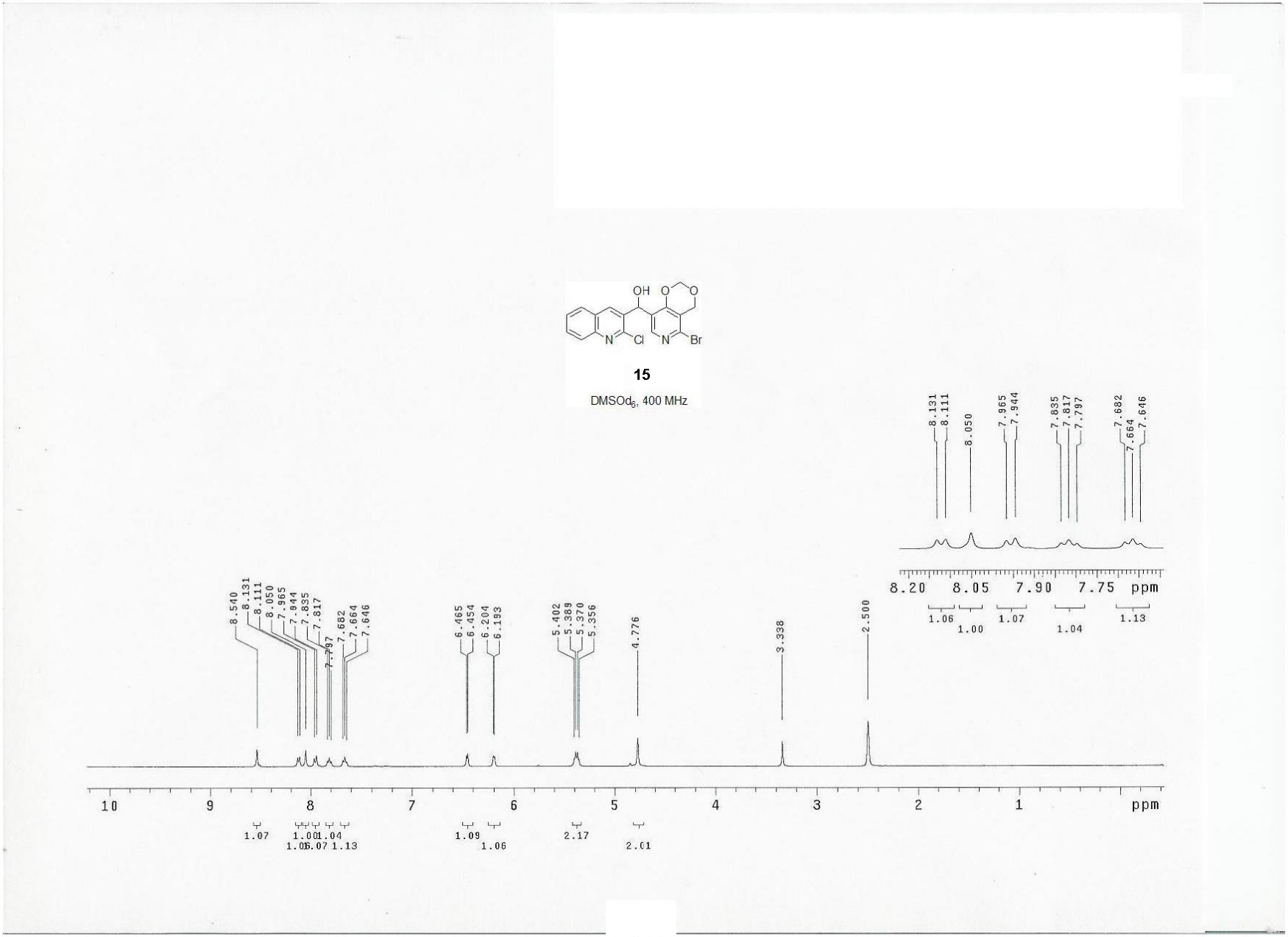
1
-0
pp
1.00
1.03
2.06
2.06


Br
O
O
N
14
CDCl3, 100 MHz
155.840
151.519
145.551
118.913
108.957
92.752
77.541
77.230
76.912
64.294
200
180
160
140
120
100
80
60
40
20
0
pp


OH
O
O
N
Cl
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Br
15
DMSOd6, 400 MHz
8.540
8.131
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7.965
7.944
7.835
7.817
7.797
7.682
7.664
7.646
6.465
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6.204
6.193
5.402
5.389
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2.500
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1.05
1.07
1.04
1.13
1.09
1.06
2.17
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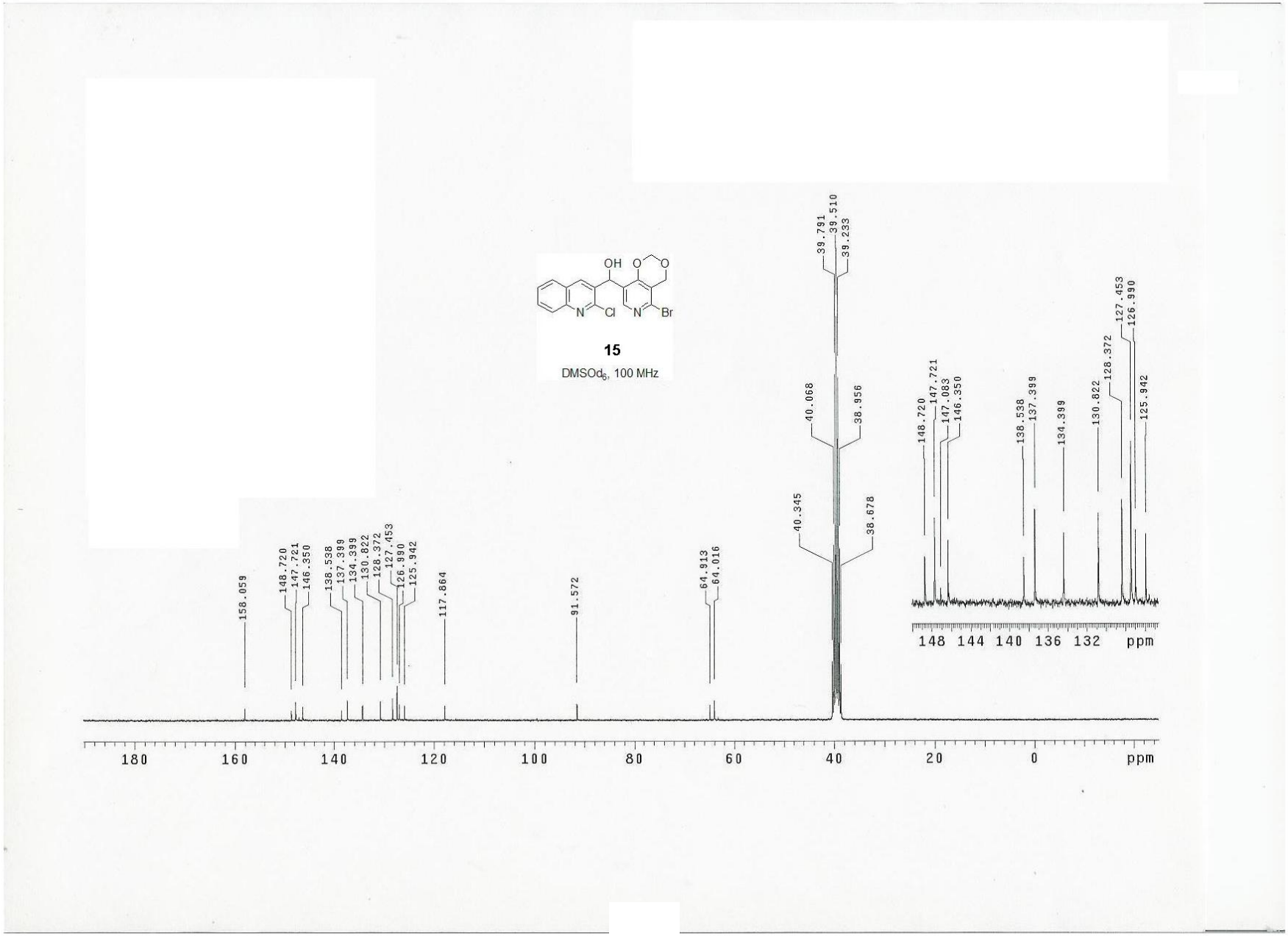
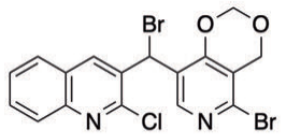
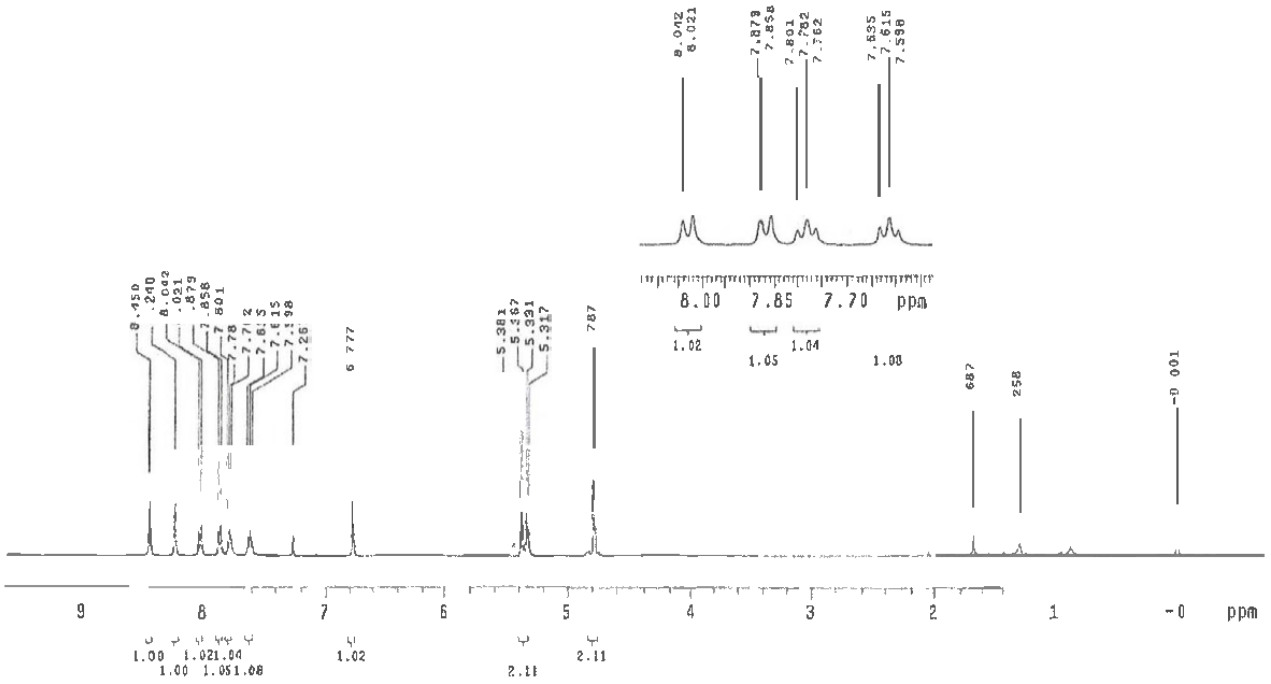
10
9
8
7
6
5
4
3
2
1
ppm
8.20
8.05
7.90
7.75
ppm
1.06
1.00
1.07
1.04
1.13

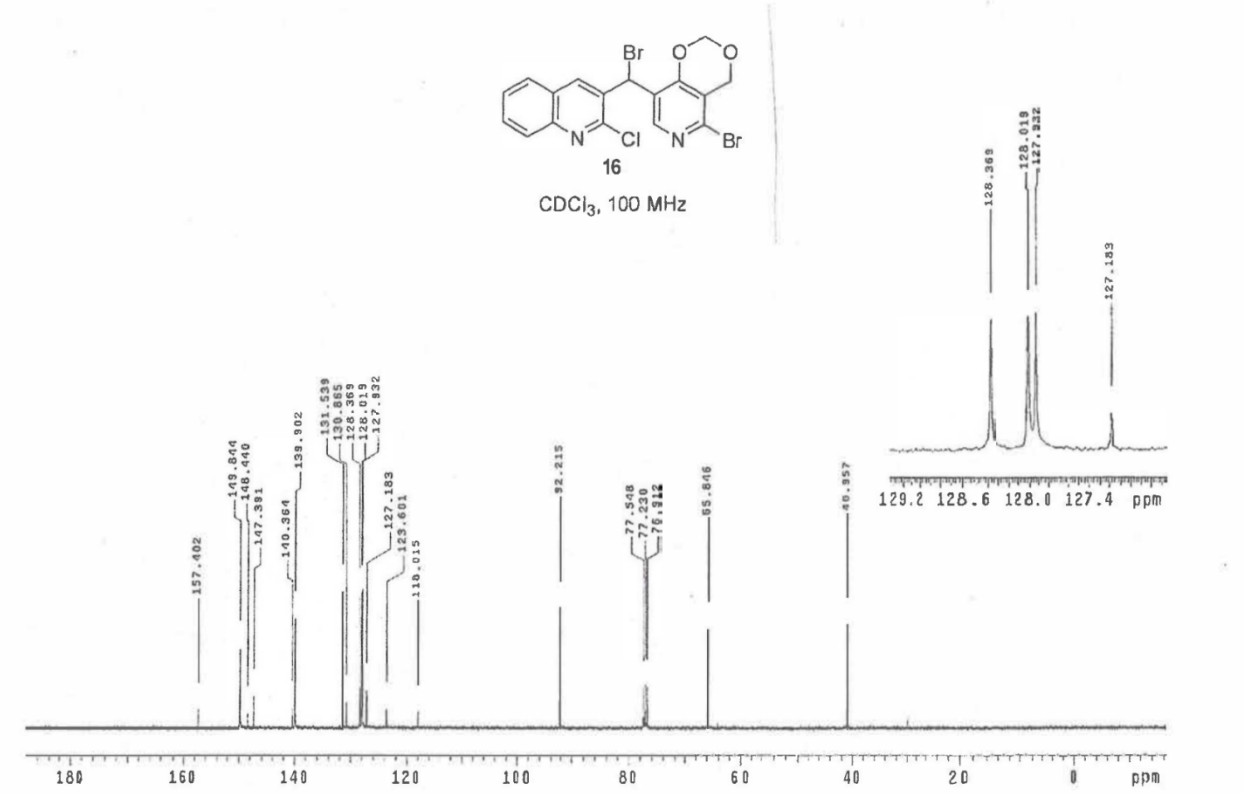

OH
O
O
N
Cl
N
Br
15
DMSOd6, 100 MHz
158.059
148.720
147.721
146.350
138.538
137.399
134.399
130.822
128.372
127.453
126.990
125.942
117.864
91.572
64.913
64.016
40.345
40.068
39.791
39.510
39.233
38.956
38.678
180
160
140
120
100
80
60
40
20
0
ppm
148 144 140 136 132 ppm

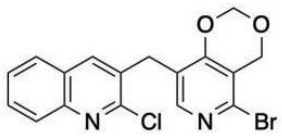


16

$CDCl_3$, 400 MHz

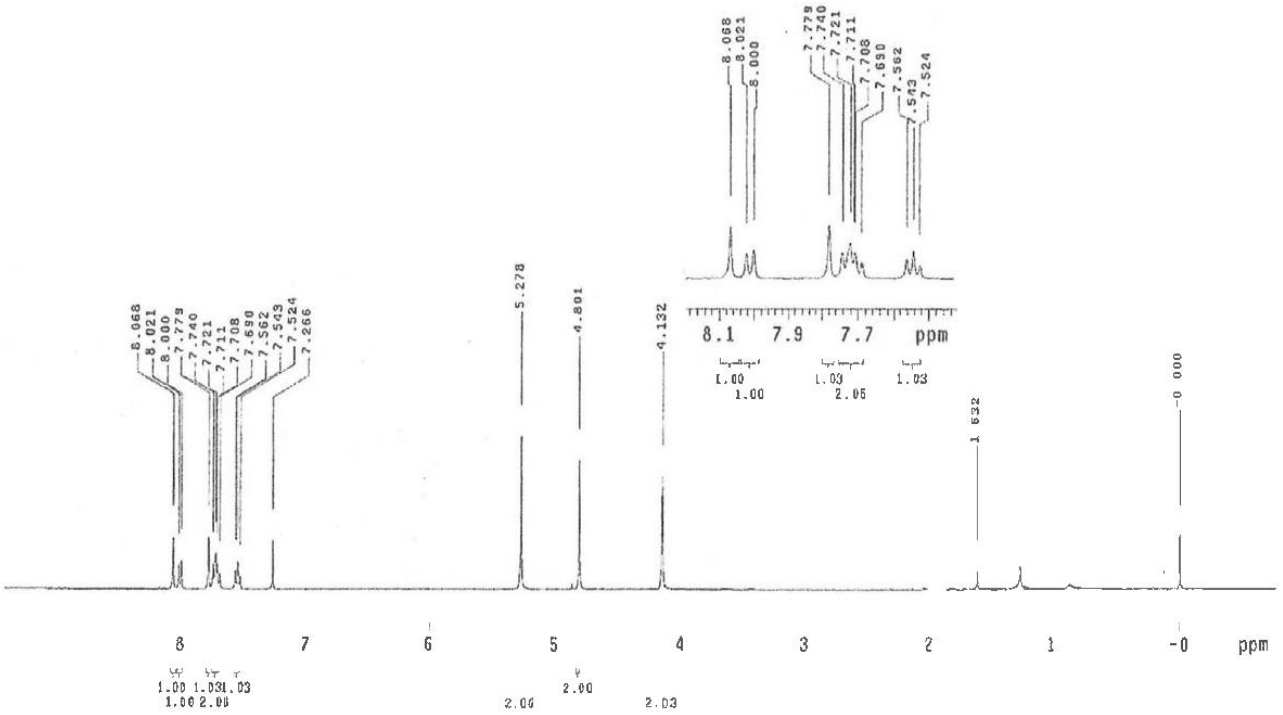


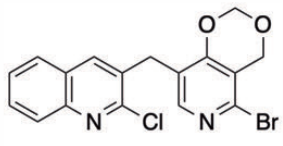

Br
O
O
N
Cl
N
Br
16
CDCl3, 100 MHz
157.402
149.844
148.440
147.391
140.364
139.902
131.539
130.885
128.369
128.019
127.832
127.183
123.601
110.015
92.215
77.548
77.230
76.912
65.846
40.957
128.369
128.019
127.832
127.183
129.2 128.6 128.0 127.4 ppm
180 160 140 120 100 80 60 40 20 0 ppm



17

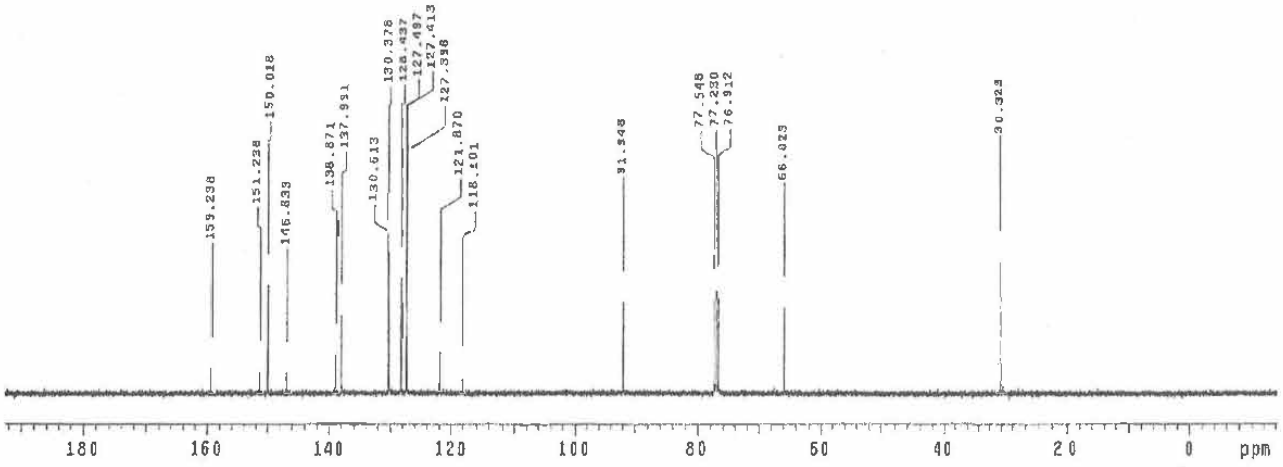
$CDCl_3$, 400 MHz

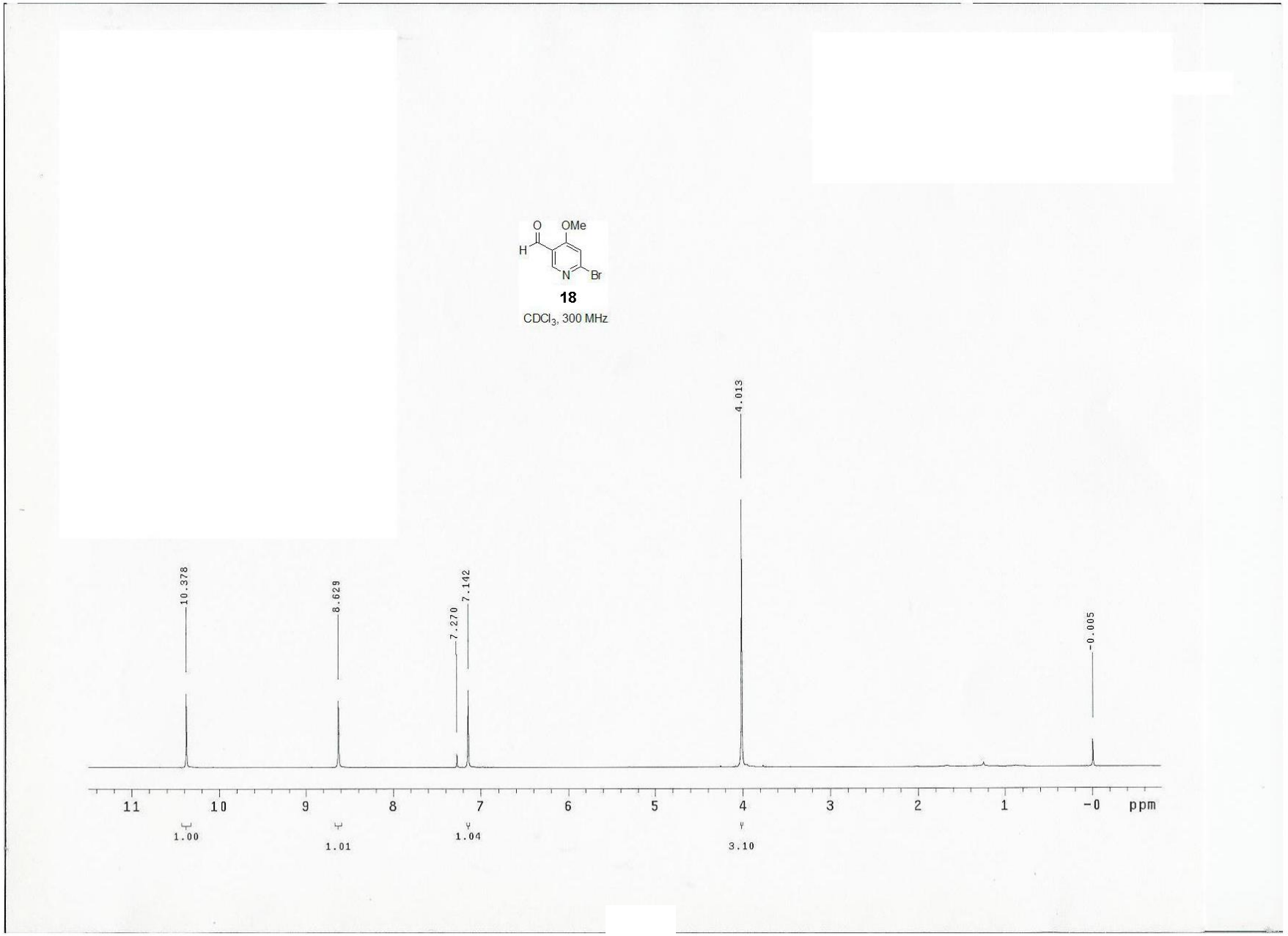


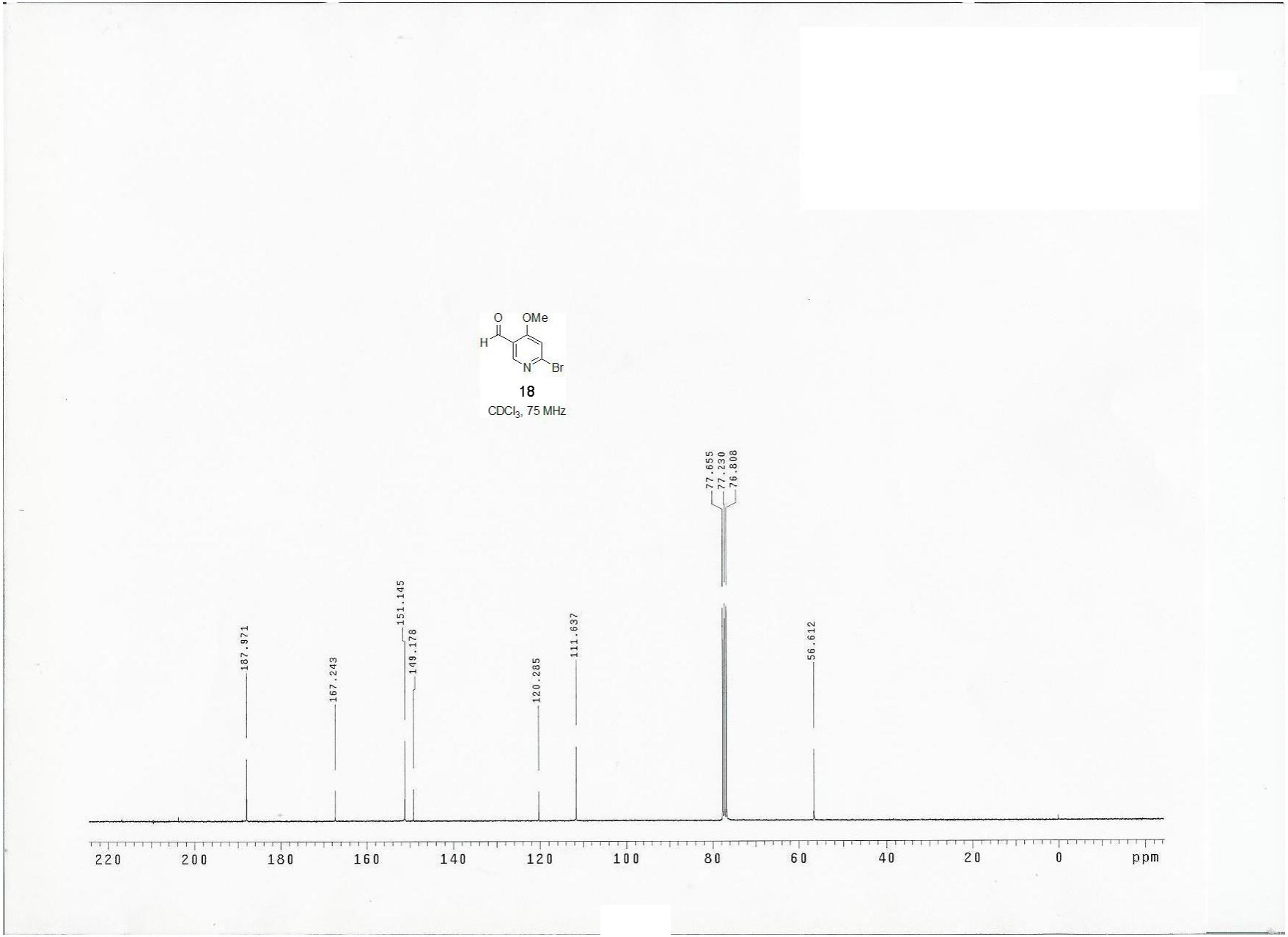


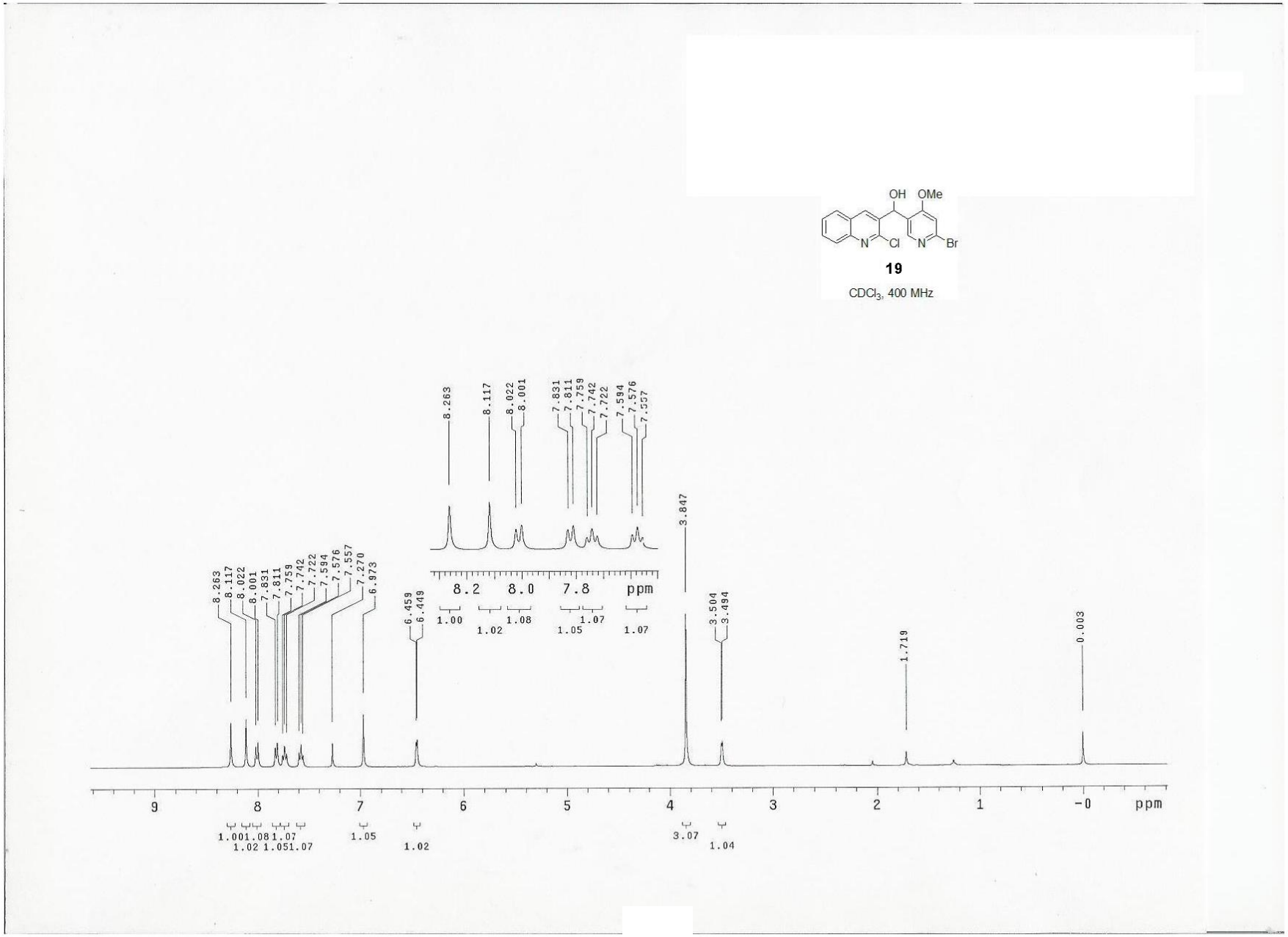
17

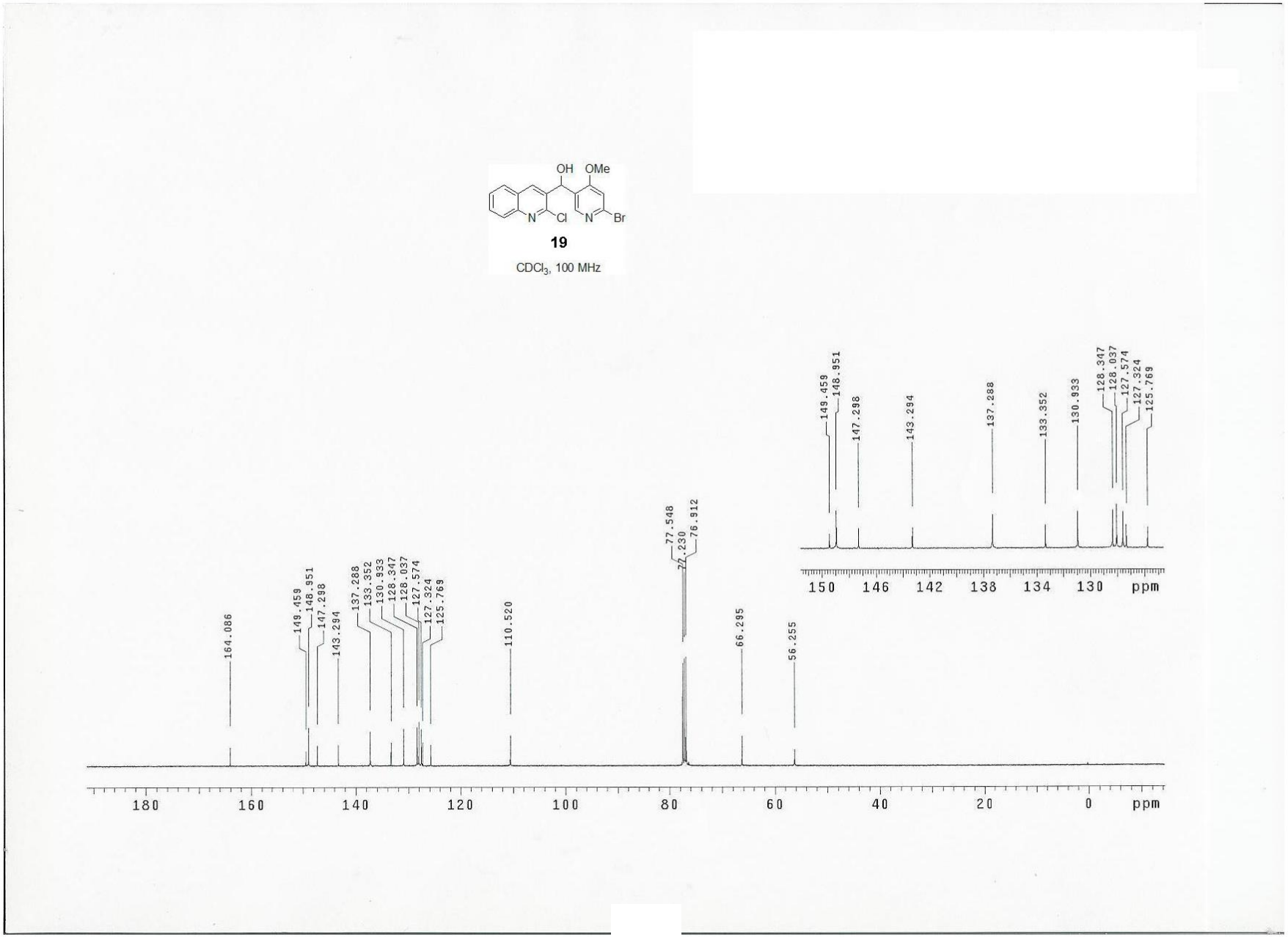
$CDCl_3$, 100 MHz

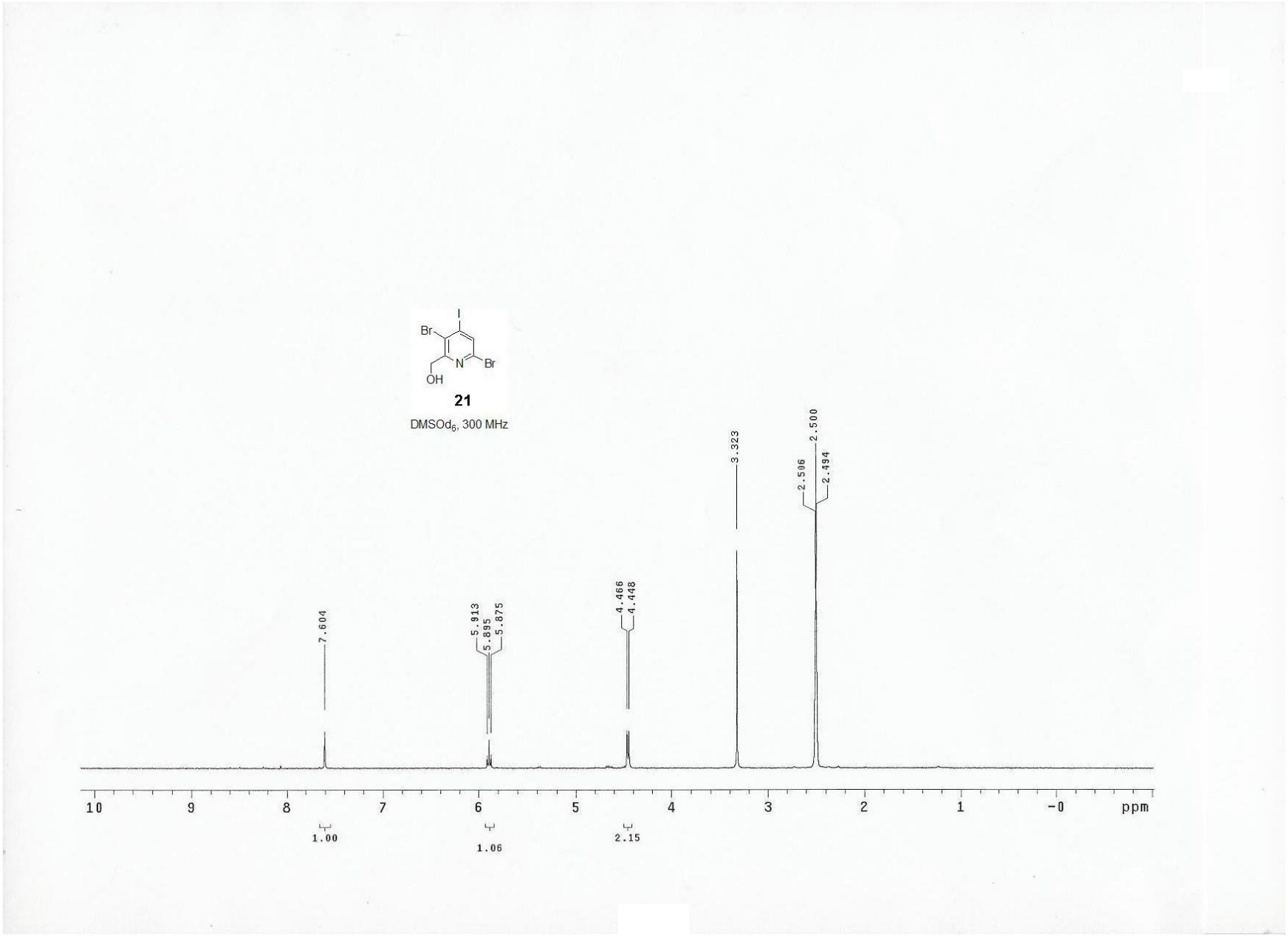


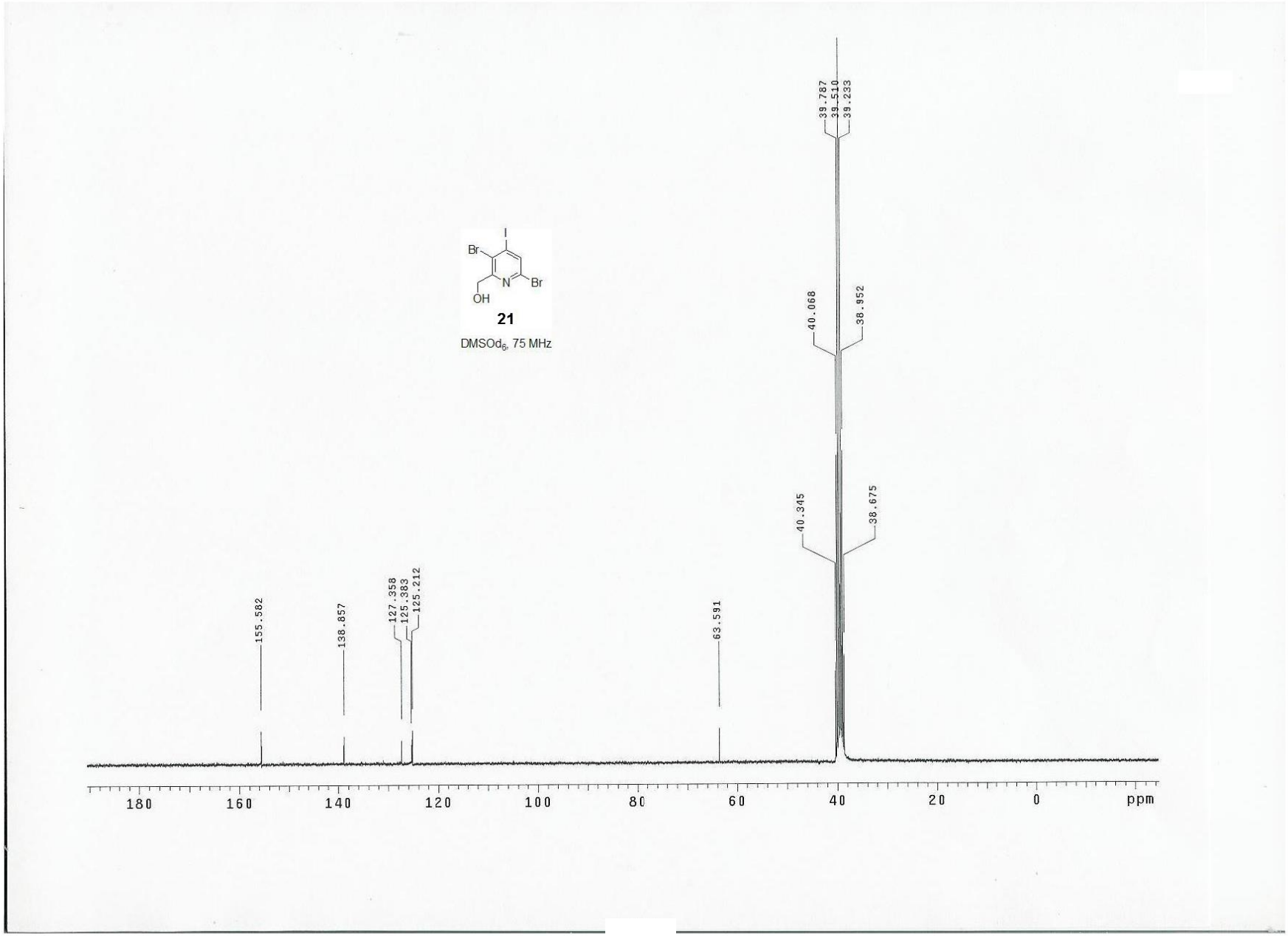

O
OMe
H
N
Br
18
CDCl3, 300 MHz
10.378
8.629
7.270
7.142
4.013
-0.005
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.01
1.04
3.10

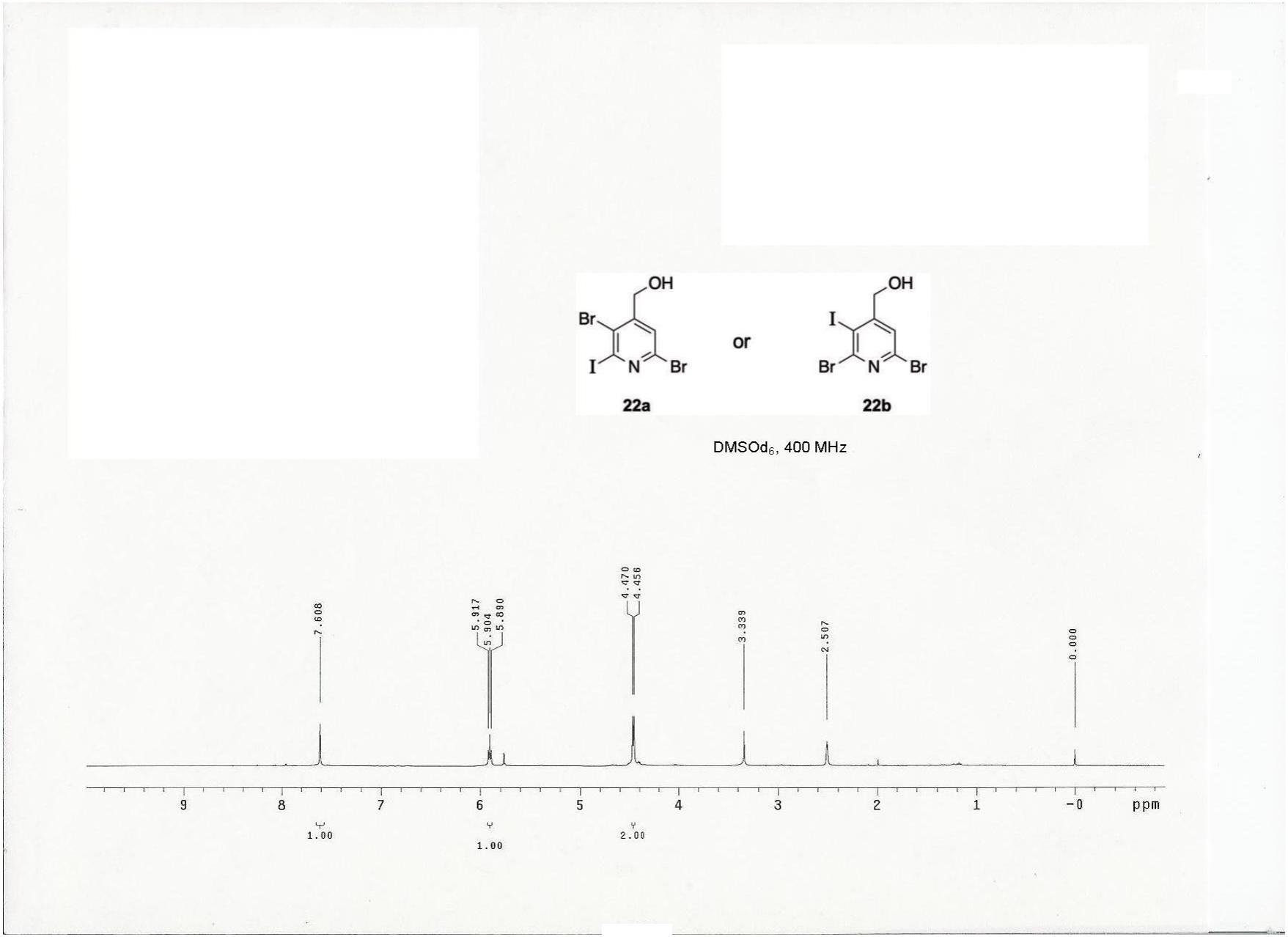

O
OMe
H
N
Br
18
CDCl3, 75 MHz
187.971
167.243
151.145
149.178
120.285
111.637
77.655
77.230
76.808
56.612
220
200
180
160
140
120
100
80
60
40
20
0
ppm

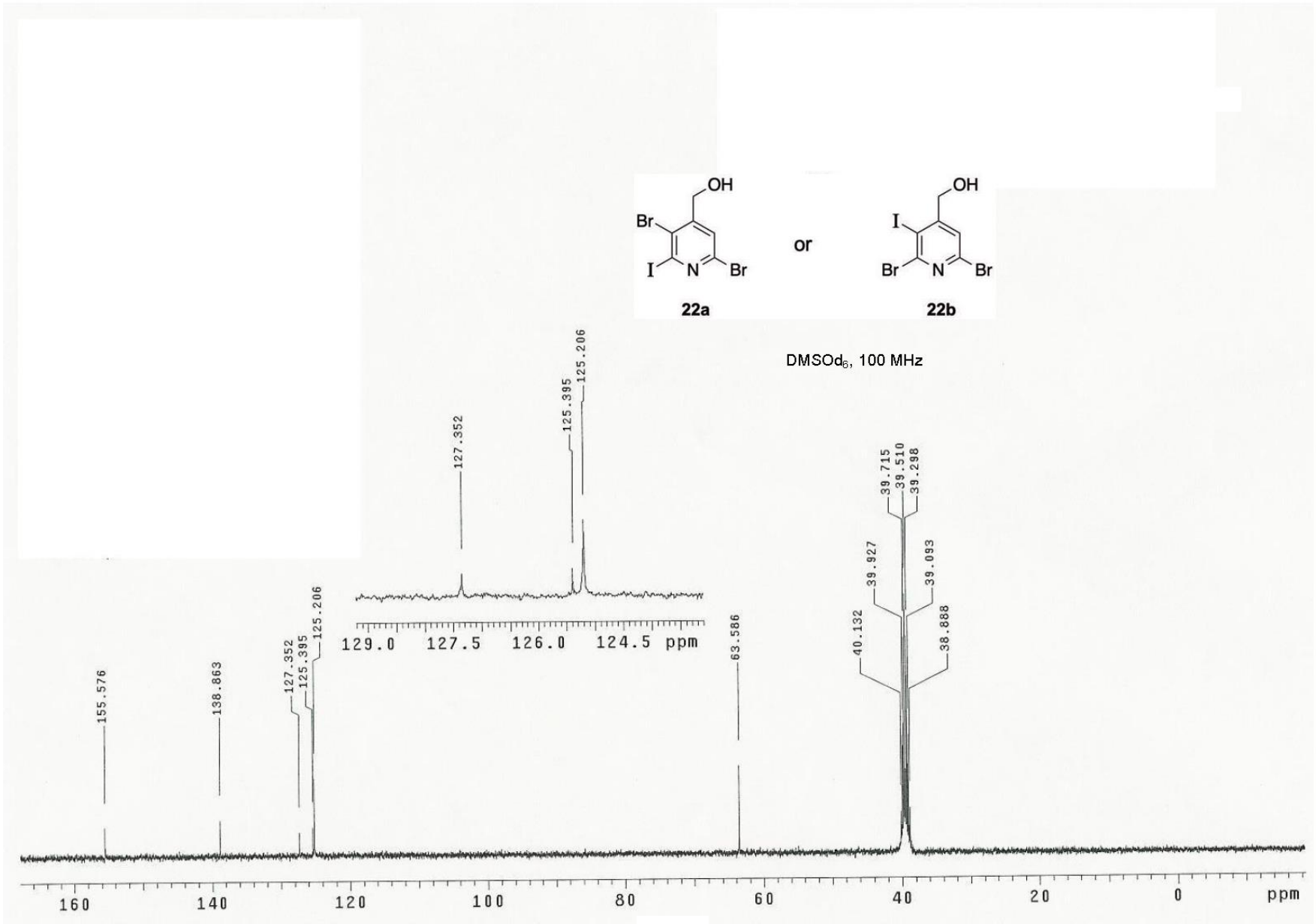

OH
OMe
N
Cl
N
Br
19
CDCl3, 400 MHz
8.263
8.117
8.022
8.001
7.831
7.811
7.759
7.742
7.722
7.594
7.576
7.557
7.270
6.973
6.459
6.449
3.847
3.504
3.494
1.719
0.003
8.2
8.0
7.8
ppm
1.00
1.02
1.08
1.05
1.07
1.07
9
8
7
6
5
4
3
2
1
-0
ppm
1.001.08 1.07
1.02 1.051.07
1.05
1.02
3.07
1.04

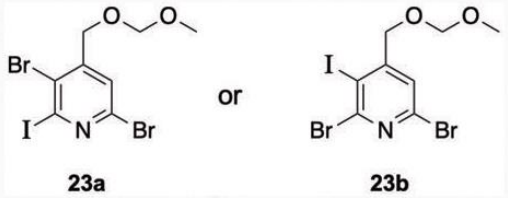

OH
OMe
N
Cl
N
Br
19
CDCl3, 100 MHz
164.086
149.459
148.951
147.298
143.294
137.288
133.352
130.933
128.347
128.037
127.574
127.324
125.769
110.520
77.548
77.230
76.912
66.295
56.255
180
160
140
120
100
80
60
40
20
0
ppm
150
146
142
138
134
130
ppm


Br
I
N
Br
OH
21
DMSOd6, 300 MHz
7.604
5.913
5.895
5.875
4.466
4.448
3.323
2.506
2.500
2.494
10
9
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.06
2.15


I
Br
N
Br
OH
21
DMSOd6, 75 MHz
39.787
39.510
39.233
40.068
38.952
40.345
38.675
155.582
138.857
127.358
125.383
125.212
63.591
180
160
140
120
100
80
60
40
20
0
ppm

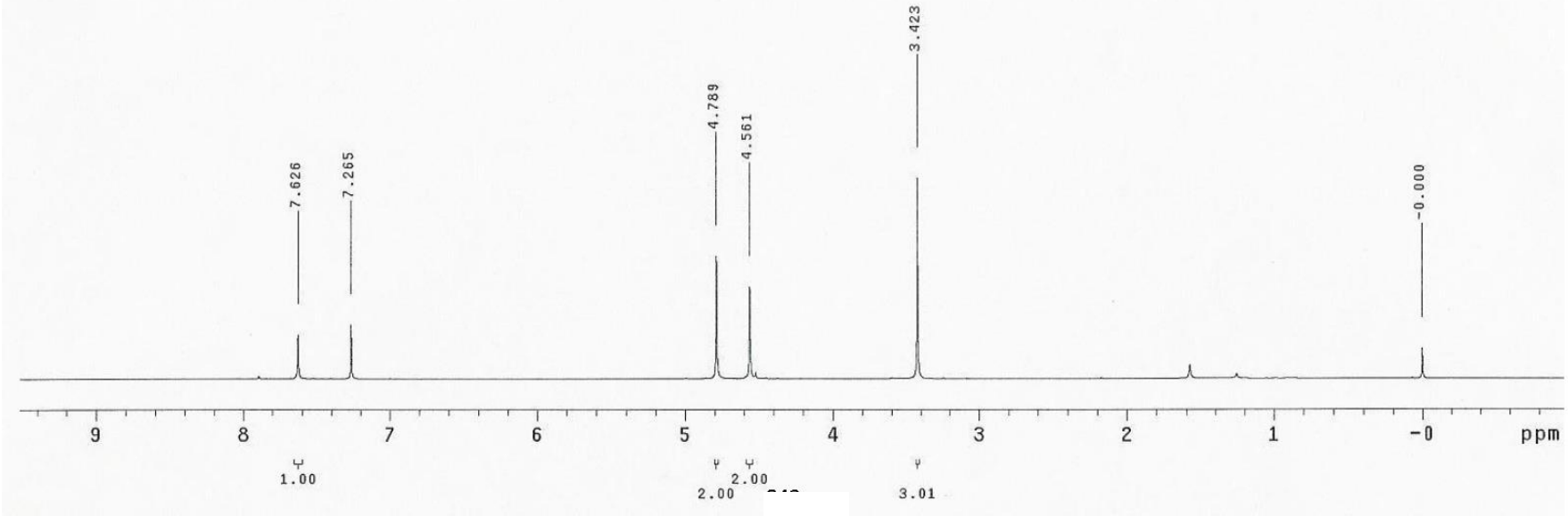

OH
Br
I
N
Br
or
OH
I
Br
N
Br
22a
22b
DMSOd6, 400 MHz
7.608
5.917
5.904
5.890
4.470
4.456
3.339
2.507
0.000
9
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.00
2.00

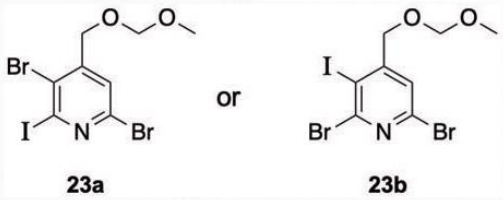

OH
Br
I
N
Br
22a
or
OH
I
Br
N
Br
22b
DMSOd6, 100 MHz
155.576
138.863
127.352
125.395
125.206
63.586
40.132
39.927
39.715
39.510
39.298
39.093
38.888
129.0
127.5
126.0
124.5 ppm
160
140
120
100
80
60
40
20
0
ppm



23a **23b**

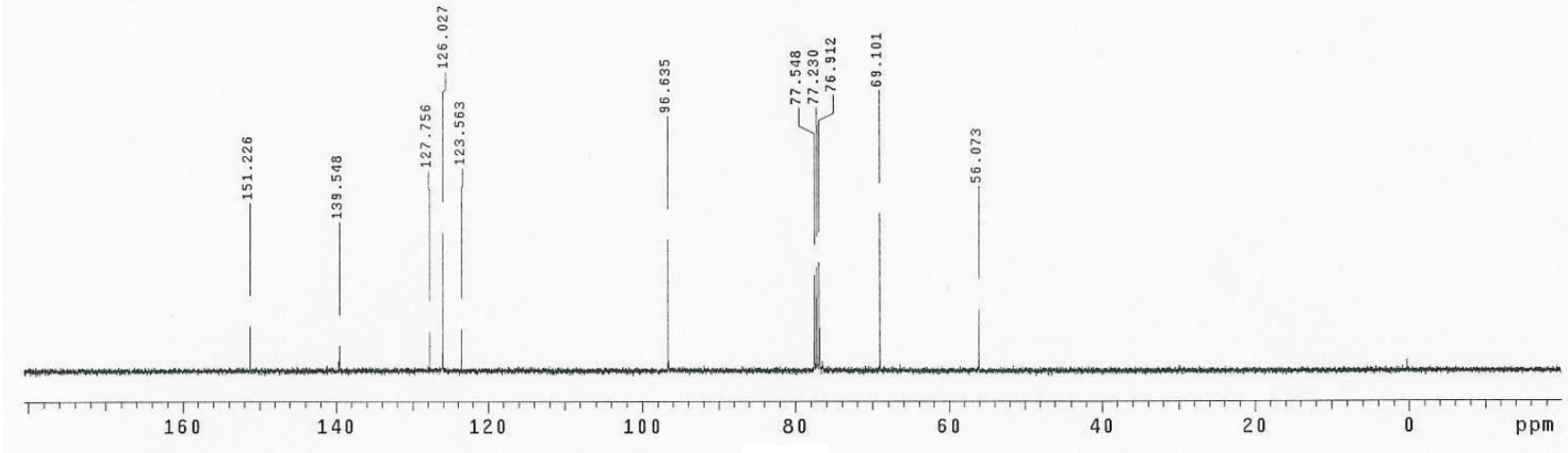
$CDCl_3$, 400 MHz

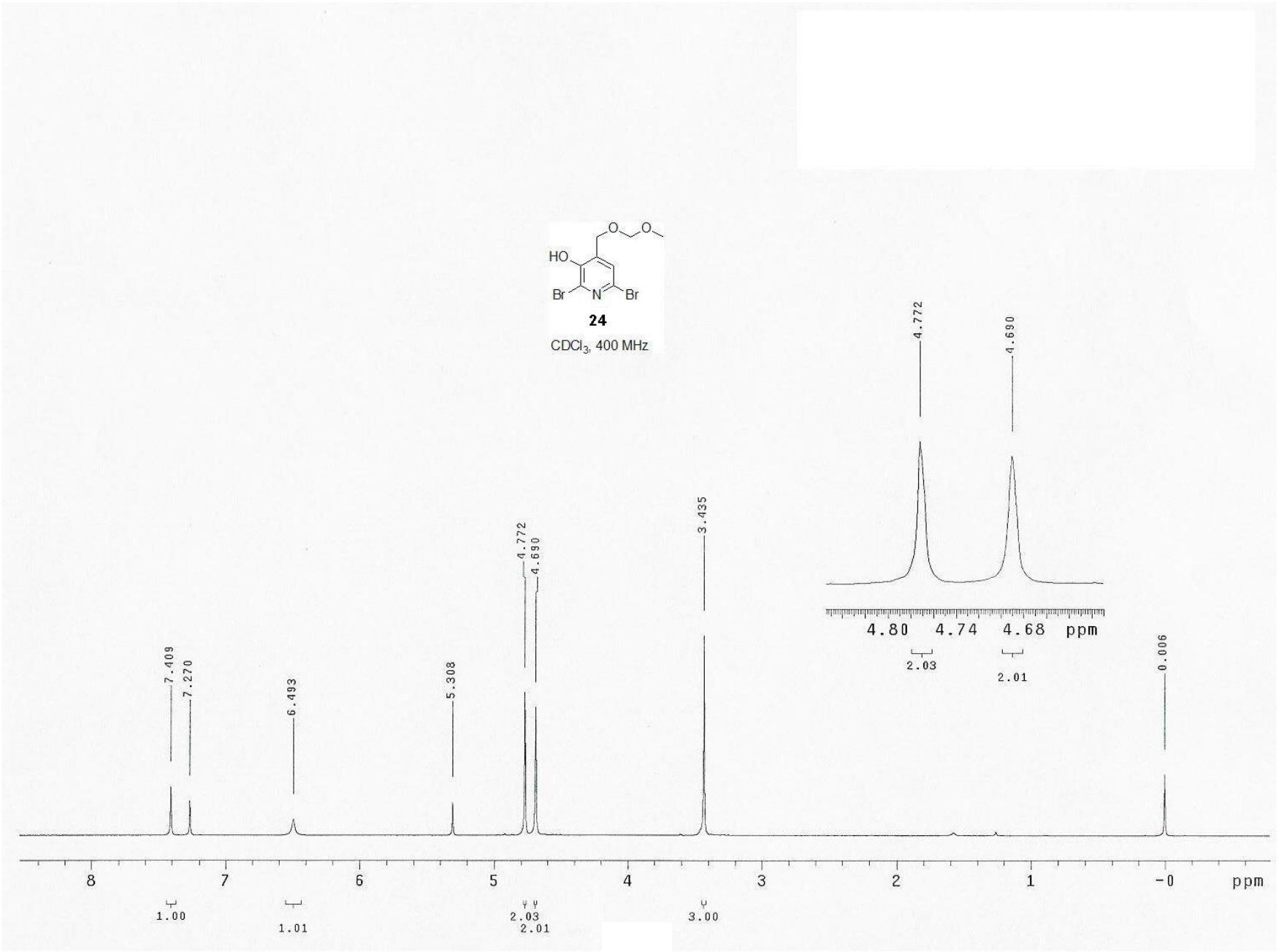


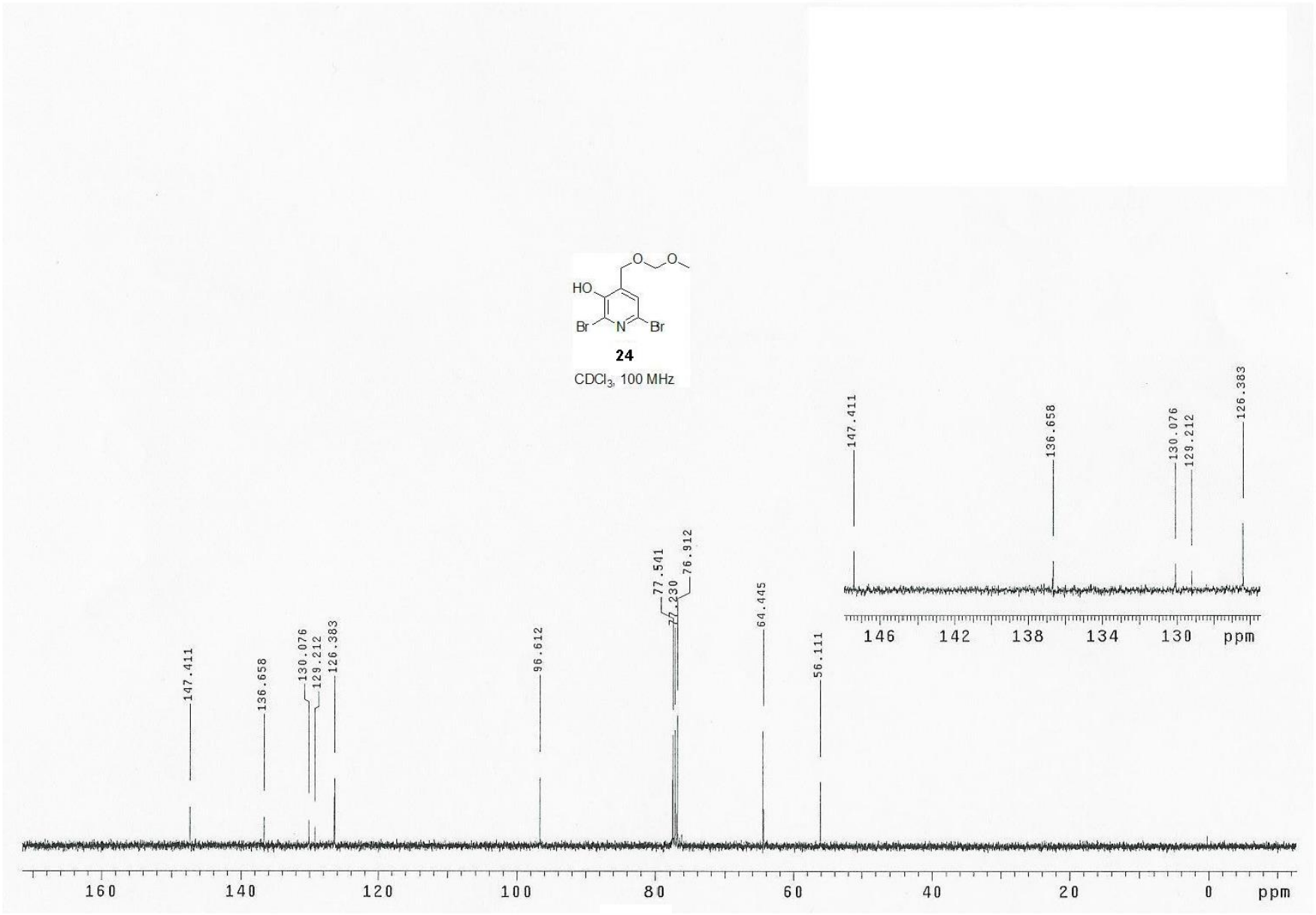


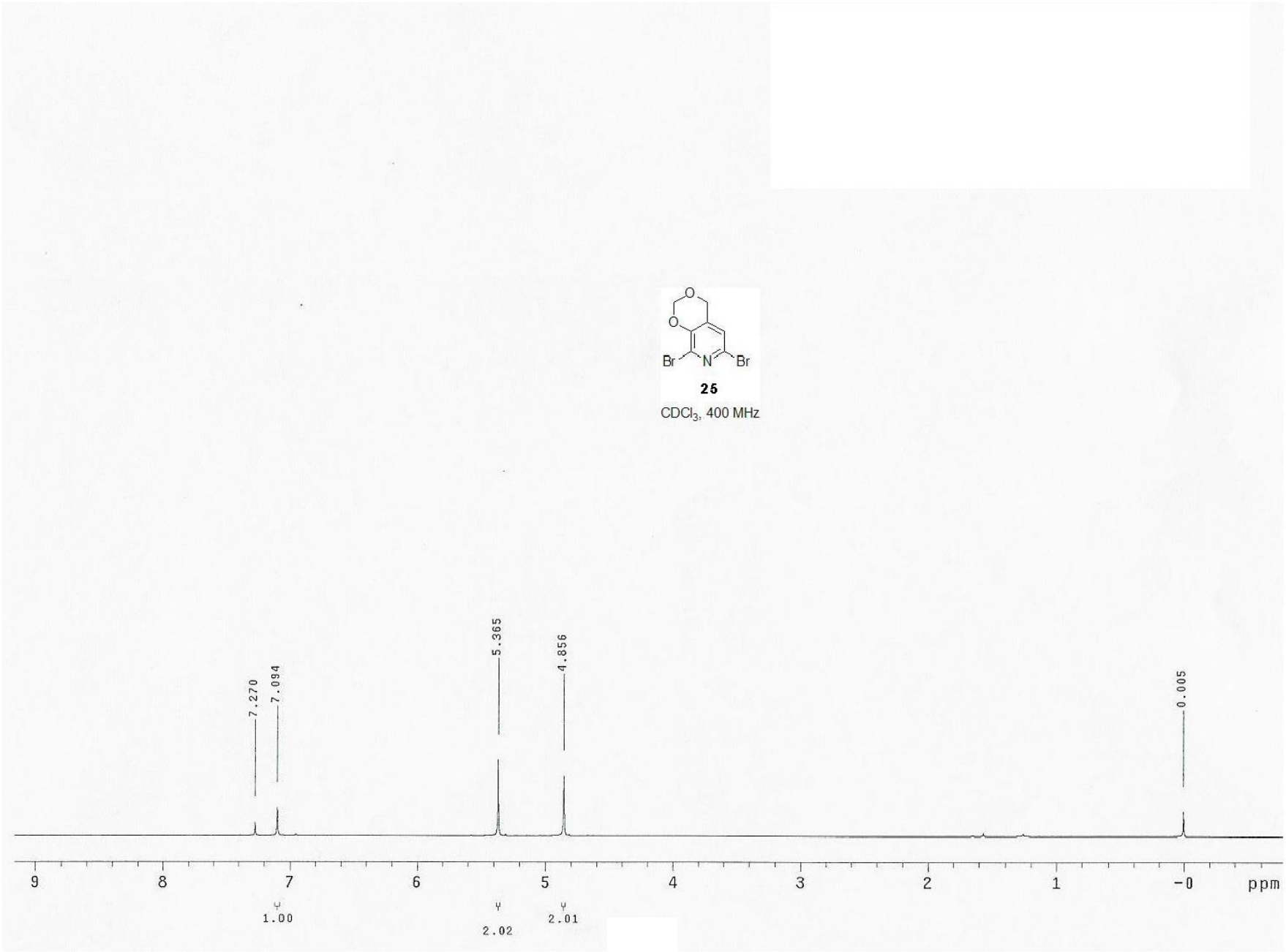
23a **23b**

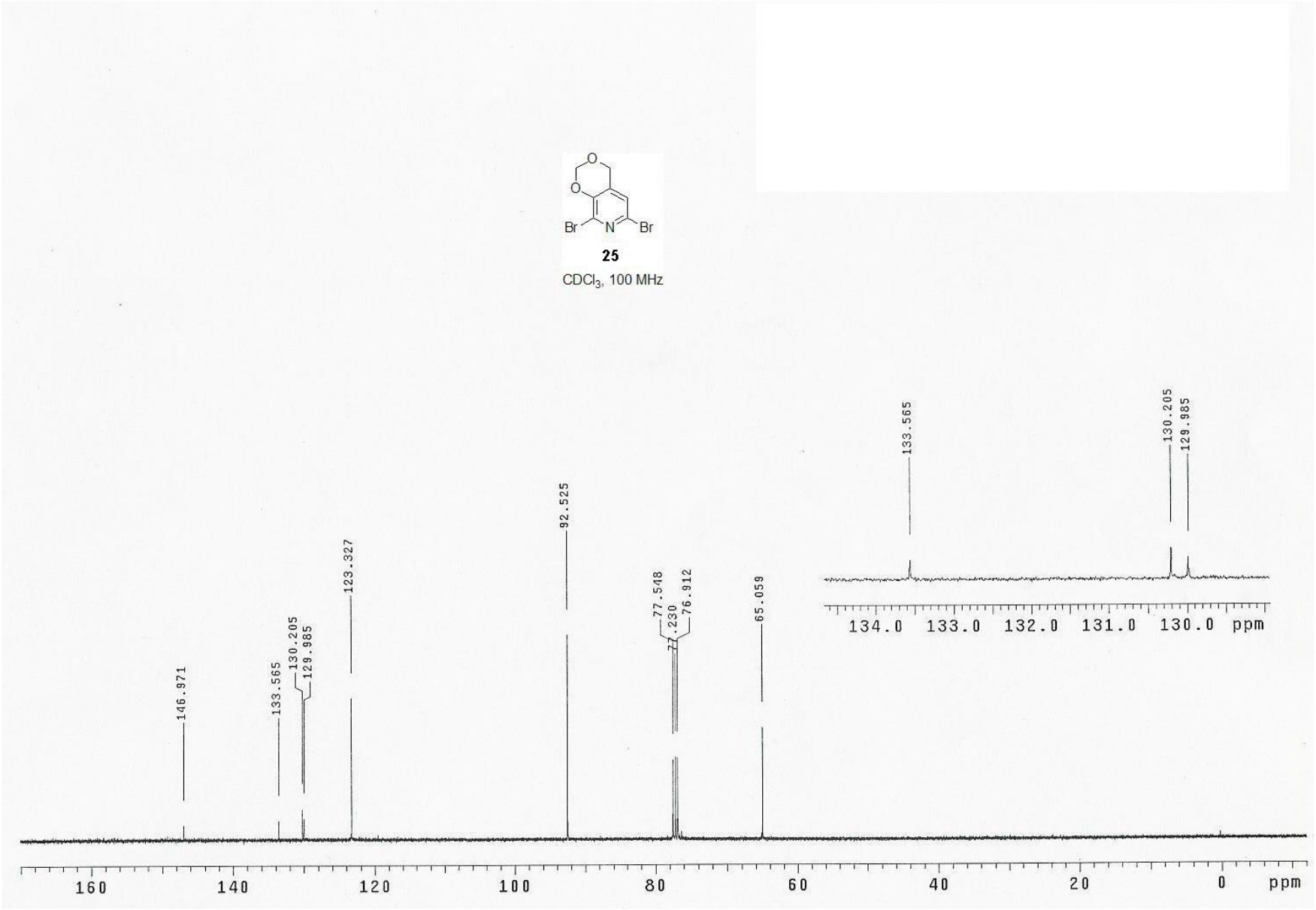
$CDCl_3$, 100 MHz

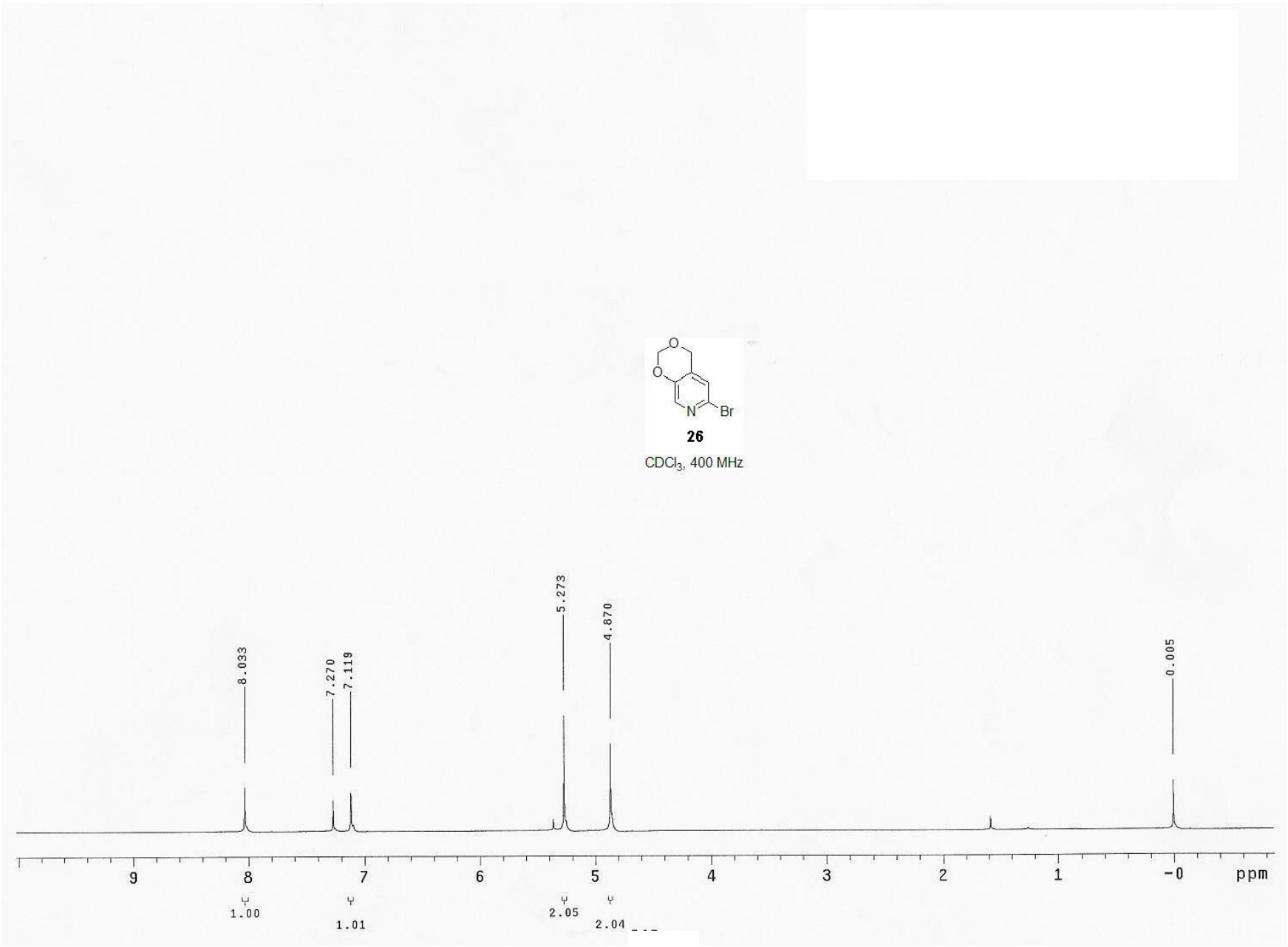


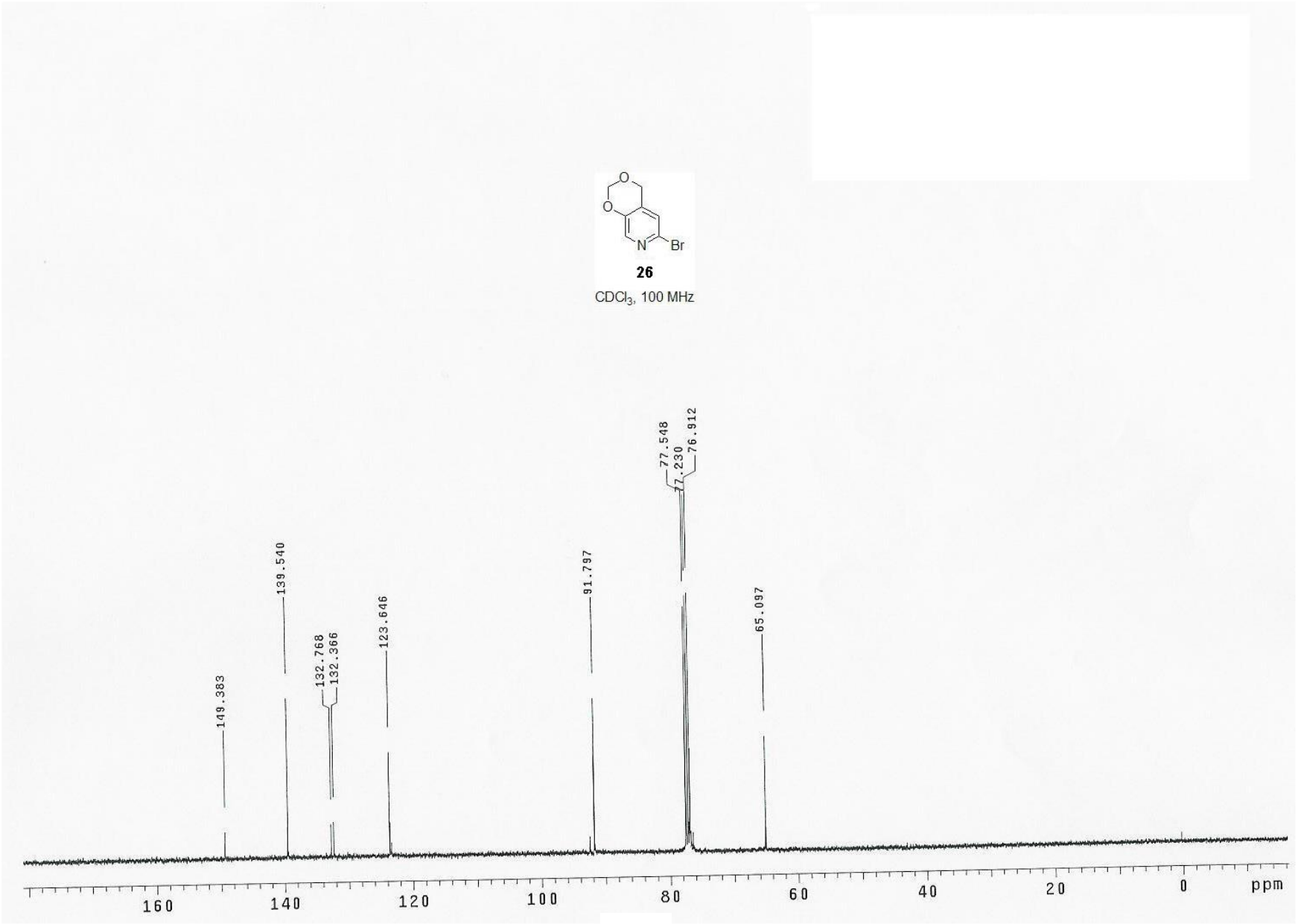

HO
Br
N
Br
O
O
24
CDCl3, 400 MHz
7.409
7.270
6.493
5.308
4.772
4.690
3.435
0.006
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.01
2.03
2.01
3.00
4.772
4.690
4.80
4.74
4.68
ppm
2.03
2.01


HO
Br
N
Br
O
O
24
CDCl3, 100 MHz
147.411
136.658
130.076
129.212
126.383
96.612
77.541
77.230
76.912
64.445
56.111
160
140
120
100
80
60
40
20
0
ppm
146
142
138
134
130
ppm


O
O
Br
N
Br
25
CDCl3, 400 MHz
7.270
7.094
5.365
4.856
0.005
9
8
7
6
5
4
3
2
1
-0
ppm
1.00
2.02
2.01


O
O
Br
N
Br
25
CDCl3, 100 MHz
146.971
133.565
130.205
129.985
123.327
92.525
77.548
77.230
76.912
65.059
160
140
120
100
80
60
40
20
0
ppm
133.565
130.205
129.985
134.0
133.0
132.0
131.0
130.0
ppm


O
O
N
Br
26
CDCl3, 400 MHz
8.033
7.270
7.119
5.273
4.870
0.005
9
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.01
2.05
2.04


O
O
N
Br
26
CDCl3, 100 MHz
149.383
139.540
132.768
132.366
123.646
91.797
77.548
77.230
76.912
65.097
160
140
120
100
80
60
40
20
0
ppm

General Experimental: (for $C_7H_{7.33}Br_2NO_{2.17}$ (x07093)

Data Collection and Processing. The sample (x07093) was submitted by Ibrahim Bori of the Comins research group at North Carolina State University. The sample was mounted on a nylon loop with a small amount of NVH immersion oil. All X-ray measurements were made on a Bruker-Nonius X8 Apex2 diffractometer at a temperature of 110 K. The unit cell dimensions were determined from a symmetry constrained fit of 9933 reflections with 4.8° <211<56.04°. The data collection strategy was a number of 11 and 11 scans which collected data up to 57.54° (211). The frame integration was performed using SAINT+.[1] The resulting raw data was scaled and absorption corrected using a multi-scan averaging of symmetry equivalent data using SADABS.[2]

Structure Solution and Refinement. The structure was solved by direct methods using the SIR92 program.[3] All non-hydrogen atoms were obtained from the initial E-map. The hydrogen atoms were introduced at idealized positions and were allowed to refine isotropically. The structural model was fit to the data using full matrix least-squares based on F. The calculated structure factors included corrections for anomalous dispersion from the usual tabulation. The structure was refined using LSTSQ program from NRCVAX,[4] graphic plots were produced using the NRCVAX crystallographic program suite. Additional information and other relevant literature references can be found in the reference section of the Facility's Web page (http://www.xray.ncsu.edu).

Additional Notes: There are two of the organic molecules (designated 'A' and 'B') and one third of a water in the asymmetric unit. The water molecule site on a 3 (i.e. a site with crystallographic three-fold symmetry) site which forces a disorder in the water's hydrogen atom positions. The fractional number of hydrogens and oxygens in the formula is correct and arises from this circumstance.

Acknowledgement The authors wish to thank the Department of Chemistry of North Carolina State University and the State of North Carolina for funding the purchase of the Apex2 diffractometer.

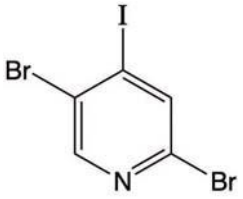
1 . Bruker-Nonius, SAINT+ version 7.34A, **2006**, Bruker-Nonius, Madison, WI 53711, USA

2 . Bruker-Nonius, SADABS version 2.10, **2004**, Bruker-Nonius, Madison, WI 53711, USA

3 . Altomare, A.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.; Burla, M. C.; Polidori, G.; Camalli, M. *J. Appl. Cryst.* **1994**, *27*, 435

4 .Gabe, E. J.; Le Page, Y.; Charland, J. P.; Lee, F. L. and White, P. S. *J. Appl. Cryst*. **1989**, *22*, 384- 387.

X-ray Crystal Data and Structure Refinement for 8a



8a

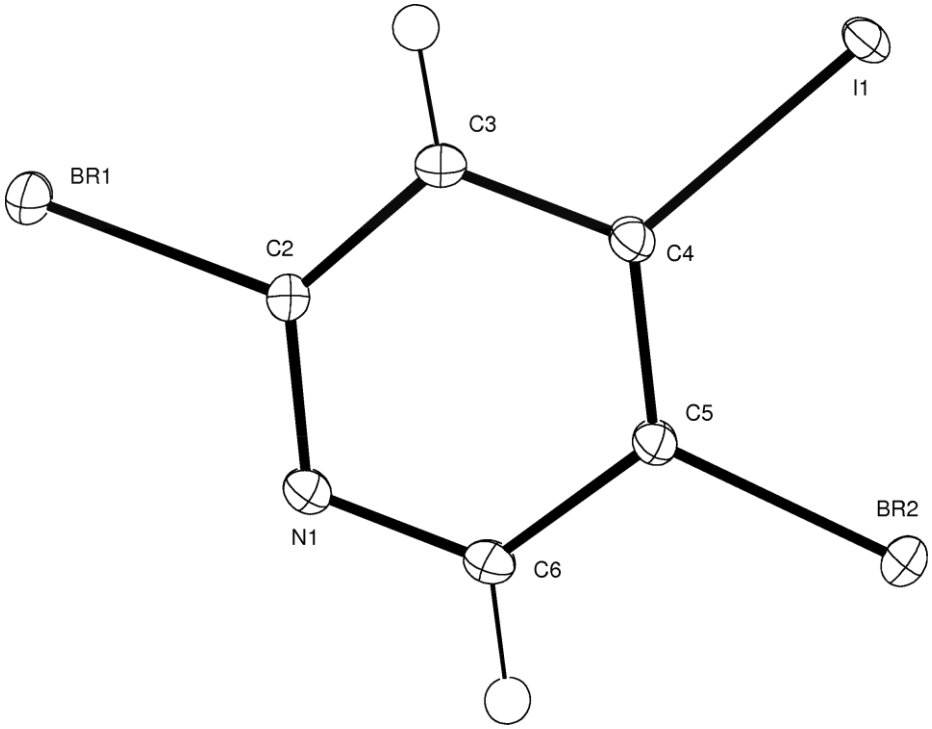


Figure 1. ORTEP drawing of ***x08083*** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity.

Table 1*. Summary of Crystal Data for *x08083(8a)

Identification	x08083
code Formula	$C_5H_2Br_2IN$
Formula Weight (*g/mol*)	362.80
Crystal Dimensions (*mm*)	0.40 × 0.26 × 0.20
Crystal Color and Habit	colourless prism
Crystal System	Triclinic
Space Group	P -1
Temperature, K	110
a, Å	7.2260(2)
b, Å	7.9444(2)
c, Å	8.0985(2)
α,°	61.2390(14)
β,°	70.5395(15)
γ,°	76.2013(15)
V, $Å^3$	382.544(17)
Number of reflections to determine final unit cell	5452
Min and Max 2θ for cell determination, °	6.26, 84.54
Z	2
F(000)	324
ρ (*g/cm*)	3.150
λ, Å, (MoKα)	0.71070
μ, (cm^{-1})	14.539
Diffractometer Type	Bruker-Nonius X8 Apex2
Scan Type(s)	omega and phi scans
Max 2θfor data collection, °	85.06
Measured fraction of data	0.930
Number of reflections measured	12538
Unique reflections measured	5127
R_{merge}	0.0330
Number of reflections included in refinement	5127
Cut off Threshold Expression	>2sigma(I)
Structure refined using	full matrix least-squares using F^2
Weighting Scheme	calc
	$w=1/[sigma^2(Fo^2)+(0.0377P)^2+0.0$

	000P] where P=(Fo^2+2Fc^2)/3
Number of parameters in least-squares	82
R_1	0.0313
wR_2	0.0710
R_1 (all data)	0.0414
wR_2 (all data)	0.0745
GOF	1.016
Maximum shift/error	0.001
Min & Max peak heights on final ΔF Map (e^-/Å)	-2.734, 3.600

Where:

$R_1 = \sum(|Fo| - |Fc|) / \sum Fo$

$wR_2 = [\sum(w(Fo^2 - Fc^2)^2) / \sum(w Fo^4)]^{½}$

GOF = $[\sum(w(Fo^2 - Fc^2)^2) / (\text{No. of reflns.} - \text{No. of params.})]^{½}$

Table 2*. Atomic Coordinates for *x08083 (8a)

Atom	X	Y	z	$U_{iso/equiv}$
I1	0.20918(2)	0.16236(2)	0.73700(2)	0.01247(3)
Br1	-0.19314(3)	0.88868(3)	0.73524(3)	0.01273(4)
Br2	0.60649(3)	0.31217(3)	0.78747(3)	0.01453(5)
N1	0.1904(3)	0.7694(3)	0.7620(3)	0.0128(3)
C2	0.0398(3)	0.7164(3)	0.7449(3)	0.0102(3)
C3	0.0393(3)	0.5477(3)	0.7354(3)	0.0120(3)
C4	0.2093(3)	0.4203(3)	0.7466(3)	0.0107(3)
C5	0.3687(3)	0.4727(3)	0.7660(3)	0.0109(3)
C6	0.3537(3)	0.6482(3)	0.7712(3)	0.0131(3)
H3	-0.0737	0.5195	0.7215	0.014
H6	0.4648	0.6830	0.7817	0.016

***Table 3*. Anisotropic Displacement Parameters for *x08083* (8a)**

Atom	u^{11}	u^{22}	u^{33}	u^{12}	u^{13}	u^{23}
I1	0.01510(6)	0.00993(6)	0.01632(6)	-0.00086(4)	-0.00627(4)	-0.00747(5)
Br1	0.01178(8)	0.01153(9)	0.01521(9)	0.00160(6)	-0.00469(7)	-0.00653(7)
Br2	0.01040(8)	0.01381(10)	0.02143(10)	0.00161(7)	-0.00639(7)	-0.00904(8)
N1	0.0140(7)	0.0102(7)	0.0176(7)	-0.0008(6)	-0.0066(6)	-0.0071(6)
C2	0.0102(7)	0.0089(7)	0.0110(7)	0.0000(6)	-0.0034(6)	-0.0040(6)
C3	0.0119(7)	0.0125(8)	0.0141(8)	-0.0014(6)	-0.0050(6)	-0.0066(7)
C4	0.0123(7)	0.0099(7)	0.0119(7)	-0.0006(6)	-0.0045(6)	-0.0056(6)
C5	0.0117(7)	0.0105(8)	0.0137(7)	0.0003(6)	-0.0053(6)	-0.0070(6)
C6	0.0127(8)	0.0128(8)	0.0182(8)	-0.0018(6)	-0.0053(7)	-0.0091(7)

Table 4. Bond Lengths for x08083 (8a)

I1-C4	2.088(2)	C3-C4	1.391(3)
Br1-C2	1.897(2)	C3-H3	0.9500
Br2-C5	1.884(2)	C4-C5	1.392(3)
N1-C2	1.325(3)	C5-C6	1.392(3)
N1-C6	1.331(3)	C6-H6	0.9500
C2-C3	1.379(3)		

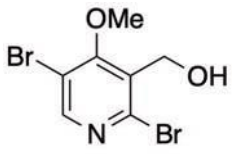
Table 5*. Bond Angles for *x08083 (8a)

C2-N1-C6	116.62(19)	C3-C4-I1	118.42(15)
N1-C2-C3	125.42(19)	C5-C4-I1	124.13(15)
N1-C2-Br1	116.23(16)	C4-C5-C6	119.66(19)
C3-C2-Br1	118.35(15)	C4-C5-Br2	122.02(16)
C2-C3-C4	118.00(19)	C6-C5-Br2	118.31(15)
C2-C3-H3	121.0	N1-C6-C5	122.8(2)
C4-C3-H3	121.0	N1-C6-H6	118.6
C3-C4-C5	117.44(19)	C5-C6-H6	118.6

Table 6*. Torsion Angles for *x08083 (8a)

C6-N1-C2-C3	-0.2(3)	I1-C4-C5-C6	-179.90(16)
C6-N1-C2-Br1	179.24(16)	C3-C4-C5-Br2	178.86(15)
N1-C2-C3-C4	0.8(3)	I1-C4-C5-Br2	-0.4(3)
Br1-C2-C3-C4	-178.70(15)	C2-N1-C6-C5	-0.8(3)
C2-C3-C4-C5	-0.3(3)	C4-C5-C6-N1	1.3(3)
C2-C3-C4-I1	179.00(15)	Br2-C5-C6-N1	-178.28(17)
C3-C4-C5-C6	-0.7(3)		

X-ray Crystal Data and Structure Refinement for 10



10

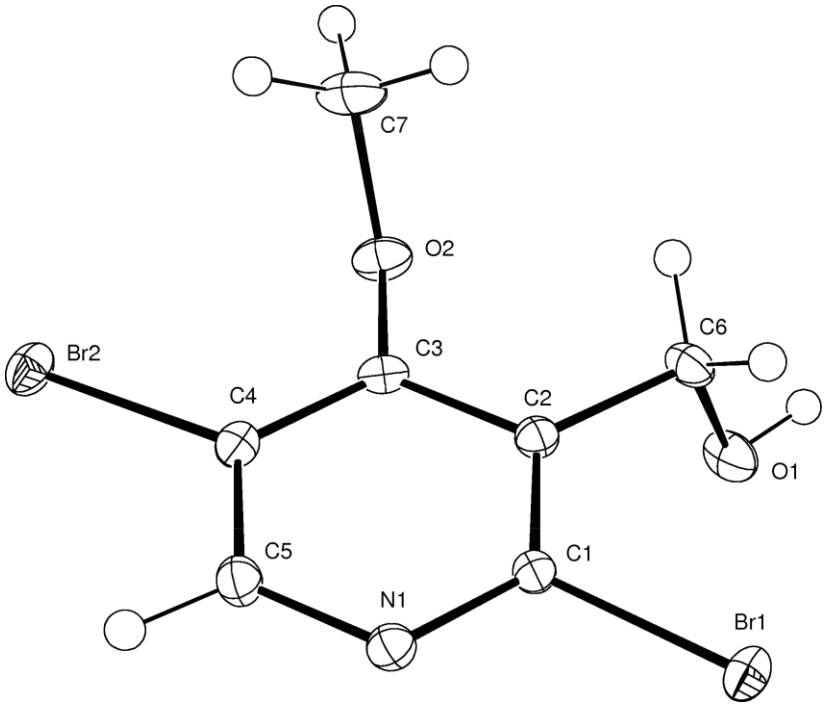


Figure 2. ORTEP drawing of ***x07109*** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity.

Table 1. Summary of Crystal Data for x07109 (10)

Identification code	x07109
Formula	$C_7H_7Br_2NO_2$
Formula Weight (*g/mol*)	296.94
Crystal Dimensions (*mm*)	0.28 × 0.16 × 0.06
Crystal Color and Habit	colorless prism
Crystal System	monoclinic
Space Group	P n
Temperature, K	110
a, Å	8.1615(2)
b, Å	4.81360(10)
c, Å	11.2770(2)
α°	90.0
β,°	93.2778(10)
γ,°	90.0
V, Å3	442.306(16)
Number of reflections to determine final unit cell	9891
Min and Max 2θ for cell determination, °	6.0, 72.68 Z 2
F(000)	283.29
ρ (*g/cm*)	2.230
λ, Å, (MoKα)	0.71073
μ, (*cm-1*)	9.15
Diffractometer Type	Bruker-Nonius X8 Apex2
Scan Type(s)	omega and phi scans
Max 2θ for data collection, °	77.24
Measured fraction of data	0.93
Number of reflections measured	25452
Unique reflections measured	4118
Rmerge	0.027
Number of reflections included in refinement	3993
Cut off Threshold Expression	Inet > 1.0sigma(Inet)
Structure refined using	full matrix least-squares using F

Weighting Scheme	1/(sigma^2(F)+0.00025F^2)
Number of parameters in least-squares	108
Rf	0.020
Rw	0.024
Rf (all data)	0.022
Rw (all data)	0.024
GOF	1.04
Maximum shift/error	0.000
Min & Max peak heights on final ΔF Map (e^-/Å)	-0.85, 1.15

Where:

Rf = $\sum$(|Fo - Fc|) / $\sum$ Fo

Rw = [$\sum$(w(Fo - Fc)^2) / $\sum$(Fo^2)]½

GOF = [$\sum$(w(Fo - Fc)^2) / (No. of reflns. - No. of params.)]½

Table 2*. Atomic Coordinates for *x07109 (10)

Atom	X	y	z	Uiso/equiv
Br1	0.24410	0.20741(3)	0.88435	0.01583(7)
Br2	0.59414(2)	-0.72633(3)	0.573511(15)	0.01677(7)
O1	0.55352(17)	-0.1808(3)	1.04824(12)	0.0213(5)
O2	0.73979(12)	-0.4496(3)	0.80638(10)	0.0184(4)
N1	0.27432(16)	-0.1602(3)	0.70162(12)	0.0141(5)
C1	0.35681(17)	-0.0667(3)	0.79884(13)	0.0117(5)
C2	0.51310(18)	-0.1479(3)	0.83846(13)	0.0131(5)
C3	0.58872(18)	-0.3507(3)	0.76942(13)	0.0133(5)
C4	0.50340(18)	-0.4528(3)	0.66954(13)	0.0131(5)
C5	0.34699(19)	-0.3542(3)	0.63750(14)	0.0154(6)
C6	0.60219(16)	-0.0302(3)	0.94845(12)	0.0167(5)
C7	0.8738(2)	-0.3275(4)	0.74483(19)	0.0249(7)
H1	0.615	-0.117	1.106	0.0312
H5	0.295	-0.439	0.568	0.0255
H6a	0.575	0.164	0.945	0.0266
H6b	0.719	-0.050	0.946	0.0266
H7a	0.976	-0.419	0.764	0.0350

H7b	0.860	-0.336	0.660	0.0350
H7c	0.877	-0.138	0.772	0.0350

Table 3*. Anisotropic Displacement Parameters for *x07109 (10)

Atom	u11	u22	u33	u12	u13	u23
Br1	0.01945(8)	0.01327(6)	0.01526(8)	0.00246(6)	0.00527(6)	0.00054(6)
Br2	0.02171(9)	0.01255(6)	0.01668(8)	0.00138(6)	0.00664(6)	-0.00001(6)
O1	0.0228(6)	0.0283(6)	0.0123(5)	-0.0067(5)	-0.0035(4)	0.0030(4)
O2	0.0118(4)	0.0232(5)	0.0201(5)	0.0032(4)	-0.0002(3)	0.0063(4)
N1	0.0134(5)	0.0143(5)	0.0147(6)	0.0011(4)	0.0004(4)	0.0004(4)
C1	0.0129(6)	0.0116(5)	0.0106(6)	-0.0010(4)	0.0011(4)	0.0010(4)
C2	0.0134(6)	0.0135(5)	0.0125(6)	-0.0015(5)	0.0017(4)	0.0005(4)
C3	0.0105(6)	0.0139(6)	0.0155(6)	0.0004(5)	0.0017(4)	0.0034(5)
C4	0.0151(6)	0.0113(5)	0.0131(6)	0.0006(4)	0.0028(5)	0.0006(4)
C5	0.0171(6)	0.0145(6)	0.0148(7)	-0.0014(5)	0.0013(5)	-0.0020(5)
C6	0.0150(6)	0.0196(6)	0.0152(6)	-0.0045(5)	-0.0022(5)	-0.0001(5)
C7	0.0125(6)	0.0333(9)	0.0292(9)	-0.0016(6)	0.0029(6)	0.0050(7)

Table 4*. Bond Lengths for *x07109 (10)

Br1-C1	1.9021(14)	C2-C6	1.512(2)
Br2-C4	1.8833(15)	C3-C4	1.380(2)
O1-C6	1.4146(20)	C4-C5	1.390(2)
O1-H1	0.86	C5-H5	0.96
O2-C3	1.3646(18)	C6-H6a	0.96
O2-C7	1.453(2)	C6-H6b	0.96
N1-C1	1.332(2)	C7-H7a	0.96
N1-C5	1.340(2)	C7-H7b	0.96
C1-C2	1.384(2)	C7-H7c	0.96
C2-C3	1.412(2)		

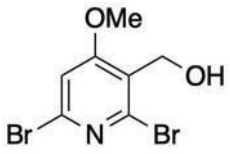
***Table 5*. Bond Angles for *x07109* (10)**

C6-O1-H1	104.22	N1-C5-C4	121.73(15)
C3-O2-C7	113.86(12)	N1-C5-H5	123.11
C1-N1-C5	117.46(13)	C4-C5-H5	115.14
Br1-C1-N1	114.55(11)	O1-C6-C2	108.47(12)
Br1-C1-C2	119.73(11)	O1-C6-H6a	116.77
N1-C1-C2	125.72(14)	O1-C6-H6b	107.32
C1-C2-C3	116.17(14)	C2-C6-H6a	103.63
C1-C2-C6	123.40(13)	C2-C6-H6b	111.81
C3-C2-C6	120.43(14)	H6a-C6-H6b	108.89
O2-C3-C2	119.25(14)	O2-C7-H7a	112.03
O2-C3-C4	121.98(14)	O2-C7-H7b	114.26
C2-C3-C4	118.69(14)	O2-C7-H7c	103.86
Br2-C4-C3	121.44(11)	H7a-C7-H7b	104.97
Br2-C4-C5	118.34(11)	H7a-C7-H7c	110.94
C3-C4-C5	120.22(14)	H7b-C7-H7c	110.94

Table 6*. Torsion Angles for *x07109 (10)

C7-O2-C3-C2	-100.9(3)	C6-C2-C3-O2	3.31(12)
C7-O2-C3-C4	82.5(2)	C6-C2-C3-C4	-179.9(3)
C5-N1-C1-Br1	-179.9(3)	C1-C2-C6-O1	85.1(2)
C5-N1-C1-C2	1.48(16)	C3-C2-C6-O1	-95.3(3)
C1-N1-C5-C4	-0.86(15)	O2-C3-C4-Br2	-2.63(9)
Br1-C1-C2-C3	-179.5(3)	O2-C3-C4-C5	177.4(3)
Br1-C1-C2-C6	0.17(10)	C2-C3-C4-Br2	-179.3(3)
N1-C1-C2-C3	-0.93(14)	C2-C3-C4-C5	0.76(15)
N1-C1-C2-C6	178.8(3)	Br2-C4-C5-N1	179.8(3)
C1-C2-C3-O2	-177.0(3)	C3-C4-C5-N1	-0.22(15)
C1-C2-C3-C4	-0.23(14)		

X-ray Crystal Data and Structure Refinement for 12



12

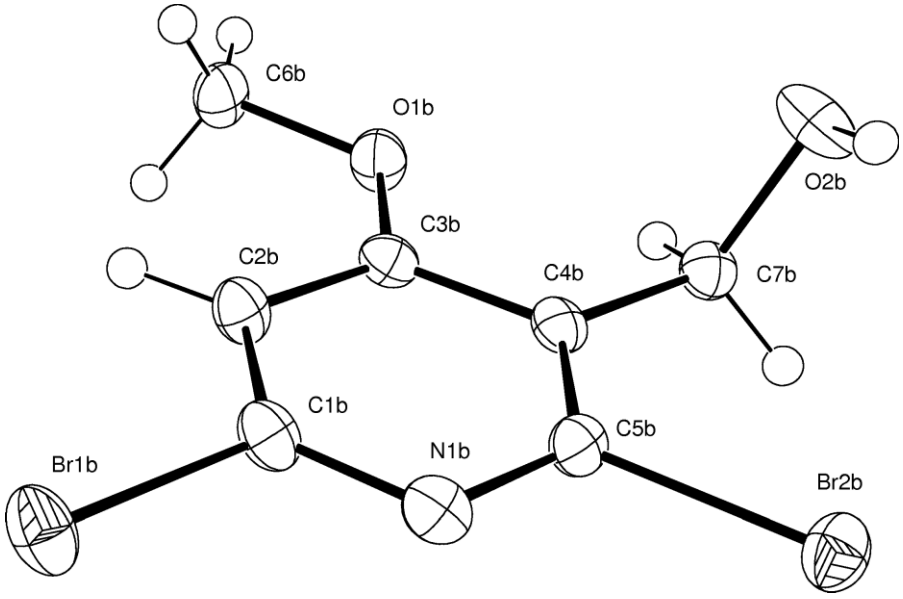


Figure 3. ORTEP drawing of ***x07093 molecule B*** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity.

Table 1*. Summary of Crystal Data for *x07093 (12)

Identification	x07093
code Formula	$C_7H_{7.33}Br_2NO_{2.17}$
Formula Weight (*g/mol*)	299.95
Crystal Dimensions (*mm*)	0.11 × 0.12 × 0.42
Crystal Color and Habit	colorless prism
Crystal System	Trigonal
Space Group	P -3
Temperature, K	110
a, Å	19.6153(3)
b, Å	19.6153(3)
c, Å	8.4067(2)
α,°	90.0
β,°	90.0
γ,°	120.0
V, Å^3	2801.21(8)
Number of reflections to determine final unit cell	9933
Min and Max 2θ for cell determination, °	4.8, 56.04
Z	12
F(000)	1719.75
ρ (*g/cm*)	2.134
λ, Å, (MoKα)	0.71073
μ, (*cm^{-1}*)	8.67
Diffractometer Type	Bruker-Nonius X8 Apex2
Scan Type(s)	omega and phi scans
Max 2θ for data collection, °	57.54
Measured fraction of data	1.00
Number of reflections measured	67179
Unique reflections measured	4868
R_{merge}	0.033

Number of reflections included in refinement	4073
Cut off Threshold Expression	Inet > 1.0sigma(Inet)
Structure refined using	full matrix least-squares using F
Weighting Scheme	$1/(sigma^2(F)+0.0005F^2)$
Number of parameters in least-squares	220
Rf	0.030
Rw	0.036
Rf (all data)	0.045
Rw (all data)	0.037
GOF	1.13
Maximum shift/error	0.002
Min & Max peak heights on final ΔF Map (e^-/Å)	-0.62, 1.16

Where:

$Rf = \sum(|Fo - Fc|) / \sum Fo$

$Rw = [\sum(w(Fo - Fc)^2) / \sum(Fo^2)]^{½}$

$GOF = [\sum(w(Fo - Fc)^2) / (No. of reflns. - No. of params.)]$

Table 2*. Atomic Coordinates for *x07093 (12)

Atom	X	y	z	Uiso/equiv
Br1a	0.907310(17)	0.115841(17)	0.06846(4)	0.03019(18)
Br2a	0.740345(17)	0.263653(16)	-0.04299(4)	0.02808(17)
O1a	0.60965(10)	-0.00868(11)	0.2341(2)	0.0221(11)
O2a	0.54472(12)	0.07886(14)	-0.0097(2)	0.0379(15)
N1a	0.80701(13)	0.17427(13)	0.0276(3)	0.0235(14)
C1a	0.80845(16)	0.11292(16)	0.0874(3)	0.0236(16)
C2a	0.74611(15)	0.04827(15)	0.1593(3)	0.0204(16)
C3a	0.67582(15)	0.04936(15)	0.1693(3)	0.0196(15)
C4a	0.67078(15)	0.11343(15)	0.1100(3)	0.0190(15)
C5a	0.73889(16)	0.17293(15)	0.0414(3)	0.0209(15)
C6a	0.61287(16)	-0.07513(16)	0.2973(3)	0.0234(16)
C7a	0.59524(15)	0.11487(15)	0.1219(3)	0.0204(15)

Br1b	0.900136(16)	0.116991(16)	0.55321(4)	0.02911(18)
Br2b	0.733136(17)	0.262843(16)	0.41394(3)	0.02588(17)
O1b	0.60339(11)	-0.00367(11)	0.7159(2)	0.0247(11)
O2b	0.58366(11)	0.16100(12)	0.7107(2)	0.0310(13)
N1b	0.80007(13)	0.17512(13)	0.4986(3)	0.0218(13)
C1b	0.80164(15)	0.11543(16)	0.5659(3)	0.0220(16)
C2b	0.73980(16)	0.05278(15)	0.6432(3)	0.0221(16)
C3b	0.66878(15)	0.05307(15)	0.6471(3)	0.0195(14)
C4b	0.66308(15)	0.11496(15)	0.5758(3)	0.0185(15)
C5b	0.73148(16)	0.17308(14)	0.5069(3)	0.0194(15)
C6b	0.60921(17)	-0.06624(16)	0.7961(3)	0.0259(17)
C7b	0.58757(16)	0.11708(15)	0.5810(3)	0.0204(15)
O1w	0.66667	0.33333	0.7146(5)	0.0483(17)
H2a	0.751	0.005	0.200	0.0301
H2ha	0.555	0.089	-0.109	0.0512
H6aa	0.562	-0.113	0.340	0.0327
H6ab	0.627	-0.099	0.214	0.0327
H6ac	0.652	-0.058	0.380	0.0327
H7aa	0.607	0.169	0.129	0.0302
H7ab	0.568	0.087	0.217	0.0302
H2b	0.745	0.011	0.691	0.0319
H2hb	0.622	0.209	0.703	0.0415
H6ba	0.559	-0.103	0.840	0.0360
H6bb	0.625	-0.093	0.721	0.0360
H6bc	0.648	-0.044	0.880	0.0360
H7ba	0.545	0.064	0.592	0.0304
H7bb	0.582	0.139	0.483	0.0304
H1w	0.647	0.284	0.699	0.0583

Table 3*. Anisotropic Displacement Parameters for *x07093 (12)

Atom	u11	u22	u33	u12	u13	u23
Br1a	0.01821(15)	0.02372(16)	0.04503(19)	0.00777(12)	0.00441(12)	0.00070(13)
Br2a	0.02670(16)	0.01824(14)	0.03362(16)	0.00698(12)	-0.00442(12)	0.00577(11)
O1a	0.0178(9)	0.0173(10)	0.0290(10)	0.0072(8)	0.0021(8)	0.0036(8)
O2a	0.0350(13)	0.0629(16)	0.0256(10)	0.0319(12)	-0.0149(9)	-0.0194(10)
N1a	0.0202(12)	0.0180(11)	0.0282(12)	0.0065(10)	-0.0009(9)	-0.0001(9)
C1a	0.0188(14)	0.0224(14)	0.0275(14)	0.0088(12)	-0.0026(11)	-0.0047(11)
C2a	0.0198(13)	0.0165(13)	0.0240(13)	0.0085(11)	-0.0008(11)	-0.0022(11)
C3a	0.0195(13)	0.0164(13)	0.0197(12)	0.0066(11)	-0.0007(10)	-0.0026(10)
C4a	0.0188(13)	0.0163(13)	0.0187(12)	0.0065(11)	-0.0020(10)	-0.0010(10)
C5a	0.0228(14)	0.0156(13)	0.0213(13)	0.0073(11)	-0.0029(11)	-0.0006(10)
C6a	0.0188(14)	0.0180(13)	0.0313(14)	0.0076(11)	0.0012(11)	0.0042(11)
C7a	0.0210(14)	0.0187(13)	0.0209(12)	0.0094(11)	-0.0020(11)	-0.0016(10)
Br1b	0.01872(15)	0.02129(15)	0.04552(18)	0.00866(12)	0.00424(12)	-0.00140(12)
Br2b	0.02906(16)	0.01816(14)	0.02952(15)	0.01112(12)	-0.00219(11)	0.00029(11)
O1b	0.0213(10)	0.0233(10)	0.0303(10)	0.0118(9)	0.0074(8)	0.0066(8)
O2b	0.0250(11)	0.0350(12)	0.0344(11)	0.0160(10)	-0.0019(9)	-0.0169(9)
N1b	0.0194(12)	0.0175(11)	0.0247(11)	0.0064(10)	0.0007(9)	-0.0032(9)
C1b	0.0188(14)	0.0187(13)	0.0279(14)	0.0089(11)	-0.0003(11)	-0.0048(11)
C2b	0.0201(14)	0.0172(13)	0.0285(14)	0.0089(12)	0.0019(11)	-0.0004(11)
C3b	0.0190(13)	0.0182(13)	0.0194(12)	0.0079(11)	0.0015(10)	-0.0023(10)
C4b	0.0206(13)	0.0170(13)	0.0184(12)	0.0097(11)	-0.0022(10)	-0.0055(10)
C5b	0.0234(14)	0.0137(12)	0.0199(12)	0.0085(11)	-0.0018(11)	-0.0026(10)
C6b	0.0255(15)	0.0206(14)	0.0318(15)	0.0117(12)	0.0059(12)	0.0072(12)
C7b	0.0217(14)	0.0190(13)	0.0206(13)	0.0102(12)	-0.0030(10)	-0.0038(10)
O1w	0.0518(14)	0.0518	0.042(2)	0.0259	0.00000	0.00000

Table 4*. Bond Lengths for *x07093 (12)

Br1a-C1a	1.918(3)	O1b-C3b	1.338(3)
Br2a-C5a	1.903(3)	O1b-C6b	1.454(3)
O1a-C3a	1.342(3)	O2b-C7b	1.415(3)
O1a-C6a	1.438(3)	O2b-H2hb	0.86
O2a-C7a	1.416(3)	N1b-C1b	1.315(4)
O2a-H2ha	0.86	N1b-C5b	1.328(4)
N1a-C1a	1.317(4)	C1b-C2b	1.383(4)
N1a-C5a	1.328(4)	C2b-C3b	1.396(4)
C1a-C2a	1.385(4)	C2b-H2b	0.96
C2a-C3a	1.392(4)	C3b-C4b	1.407(4)
C2a-H2a	0.96	C4b-C5b	1.381(4)
C3a-C4a	1.401(4)	C4b-C7b	1.503(4)
C4a-C5a	1.386(4)	C6b-H6ba	0.96
C4a-C7a	1.499(4)	C6b-H6bb	0.96
C6a-H6aa	0.96	C6b-H6bc	0.96
C6a-H6ab	0.96	C7b-H7ba	0.96
C6a-H6ac	0.96	C7b-H7bb	0.96
C7a-H7aa	0.96	O1w-H1w	0.86
C7a-H7ab	0.96	O1w-H1w[1]	0.86
Br1b-C1b	1.920(3)	O1w-H1w[2]	0.86
Br2b-C5b	1.912(3)		

1. 1-y,x-y,z

2. 1-x+y,1-x,z

Table 5*. Bond Angles for *x07093(12)

C3a-O1a-C6a	117.2(2)	C1b-N1b-C5b	115.2(2)
C7a-O2a-H2ha	128.3(2)	Br1b-C1b-N1b	115.69(19)
C1a-N1a-C5a	115.4(2)	Br1b-C1b-C2b	118.0(2)
Br1a-C1a-N1a	115.09(20)	N1b-C1b-C2b	126.4(2)
Br1a-C1a-C2a	118.7(2)	C1b-C2b-C3b	116.2(2)
N1a-C1a-C2a	126.2(3)	C1b-C2b-H2b	121.8
C1a-C2a-C3a	116.1(2)	C3b-C2b-H2b	122.0
C1a-C2a-H2a	121.9	O1b-C3b-C2b	123.4(2)
C3a-C2a-H2a	122.0	O1b-C3b-C4b	116.4(2)
O1a-C3a-C2a	123.8(2)	C2b-C3b-C4b	120.2(2)
O1a-C3a-C4a	115.7(2)	C3b-C4b-C5b	115.3(2)
C2a-C3a-C4a	120.5(2)	C3b-C4b-C7b	121.1(2)
C3a-C4a-C5a	115.7(2)	C5b-C4b-C7b	123.6(2)
C3a-C4a-C7a	120.5(2)	Br2b-C5b-N1b	113.61(18)
C5a-C4a-C7a	123.9(2)	Br2b-C5b-C4b	119.61(20)
Br2a-C5a-N1a	113.86(19)	N1b-C5b-C4b	126.8(2)
Br2a-C5a-C4a	120.0(2)	O1b-C6b-H6ba	109.3
N1a-C5a-C4a	126.1(2)	O1b-C6b-H6bb	109.4
O1a-C6a-H6aa	109.5	O1b-C6b-H6bc	109.7
O1a-C6a-H6ab	109.6	H6ba-C6b-H6bb	109.5
O1a-C6a-H6ac	109.3	H6ba-C6b-H6bc	109.5
H6aa-C6a-H6ab	109.5	H6bb-C6b-H6bc	109.5
H6aa-C6a-H6ac	109.5	O2b-C7b-C4b	113.2(2)
H6ab-C6a-H6ac	109.5	O2b-C7b-H7ba	107.5
O2a-C7a-C4a	113.0(2)	O2b-C7b-H7bb	109.5
O2a-C7a-H7aa	108.6	C4b-C7b-H7ba	108.6
O2a-C7a-H7ab	108.5	C4b-C7b-H7bb	108.6
C4a-C7a-H7aa	108.8	H7ba-C7b-H7bb	109.5
C4a-C7a-H7ab	108.5	H1w-O1w-H1w^{1}	117.67(13)
H7aa-C7a-H7ab	109.5	H1w-O1w-H1w^{2}	117.67(13)

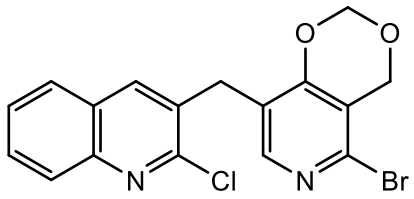
C3b-O1b-C6b	117.1(2)	H1w[1]-O1w-H1w[2]	117.67(13)
C7b-O2b-H2hb	108.74		

1. 1-y,x-y,z
2. 1-x+y,1-x,z

Table 6*. Torsion Angles for *x07093 (12)

C6a-O1a-C3a-C2a	0.5(2)	C6b-O1b-C3b-C2b	2.9(2)
C6a-O1a-C3a-C4a	-179.5(4)	C6b-O1b-C3b-C4b	-177.4(4)
C5a-N1a-C1a-Br1a	-179.5(4)	C5b-N1b-C1b-Br1b	179.5(4)
C5a-N1a-C1a-C2a	1.1(2)	C5b-N1b-C1b-C2b	-0.4(2)
C1a-N1a-C5a-Br2a	178.9(4)	C1b-N1b-C5b-Br2b	177.9(4)
C1a-N1a-C5a-C4a	-0.8(2)	C1b-N1b-C5b-C4b	-1.0(2)
Br1a-C1a-C2a-C3a	-179.8(4)	Br1b-C1b-C2b-C3b	-178.8(4)
N1a-C1a-C2a-C3a	-0.4(2)	N1b-C1b-C2b-C3b	1.1(2)
C1a-C2a-C3a-O1a	179.5(5)	C1b-C2b-C3b-O1b	179.4(5)
C1a-C2a-C3a-C4a	-0.5(2)	C1b-C2b-C3b-C4b	-0.4(2)
O1a-C3a-C4a-C5a	-179.3(5)	O1b-C3b-C4b-C5b	179.5(5)
O1a-C3a-C4a-C7a	0.48(19)	O1b-C3b-C4b-C7b	1.25(19)
C2a-C3a-C4a-C5a	0.7(2)	C2b-C3b-C4b-C5b	-0.8(2)
C2a-C3a-C4a-C7a	-179.5(5)	C2b-C3b-C4b-C7b	-179.0(5)
C3a-C4a-C5a-Br2a	-179.7(4)	C3b-C4b-C5b-Br2b	-177.3(4)
C3a-C4a-C5a-N1a	0.0(2)	C3b-C4b-C5b-N1b	1.6(2)
C7a-C4a-C5a-Br2a	0.57(16)	C7b-C4b-C5b-Br2b	0.85(16)
C7a-C4a-C5a-N1a	-179.8(5)	C7b-C4b-C5b-N1b	179.7(5)
C3a-C4a-C7a-O2a	-88.4(4)	C3b-C4b-C7b-O2b	93.4(4)
C5a-C4a-C7a-O2a	91.3(4)	C5b-C4b-C7b-O2b	-84.7(4)

X-ray Crystal Data and Structure Refinement for 17



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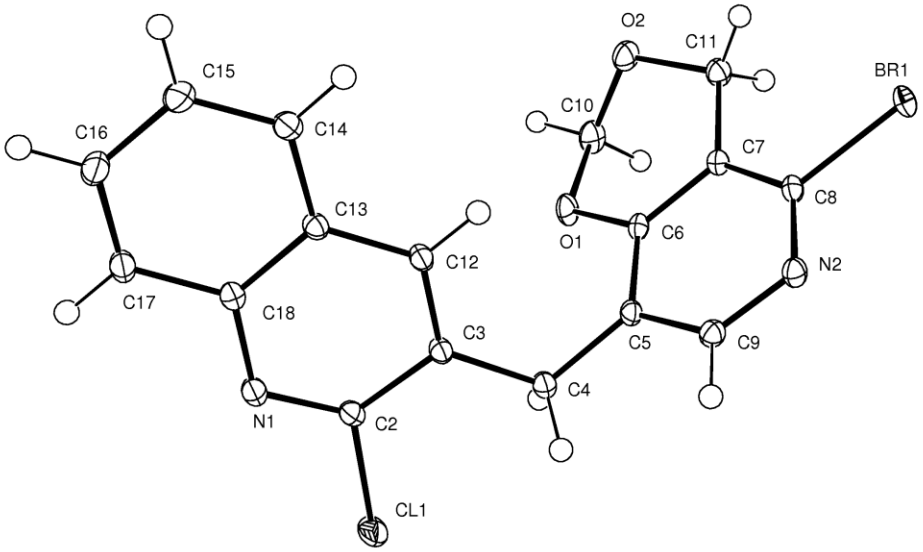


Figure 4. ORTEP drawing of ***x08116*** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity.

Table 1*. Summary of Crystal Data for *x08116 (17)

Identification code	x08116
Formula	$C_{17}H_{12}BrClN_2O_2$
Formula Weight (*g/mol*)	391.65
Crystal Dimensions (*mm*)	0.38 × 0.18 × 0.10
Crystal Color and Habit	colourless prism
Crystal System	Monoclinic
Space Group	C 2/c
Temperature, K	110
a, Å	22.8934(8)
b, Å	9.5504(4)
c, Å	16.1581(6)
α,°	90.00
β,°	123.3268(14)
γ,°	90.00
V, Å3	2951.85(19)
Number of reflections to determine final unit cell	9255
Min and Max 2θ for cell determination, °	4.76, 72.02
Z	8
F(000)	1568
ρ (*g/cm*)	1.763
λ, Å, (MoKα)	0.71070
μ, (cm^{-1})	2.977
Diffractometer Type	Bruker-Nonius X8 Apex2
Scan Type(s)	omega and phi scans
Max 2θ for data collection, °	75.06
Measured fraction of data	0.997
Number of reflections measured	81967
Unique reflections measured	7769

R_{merge}	0.0381
Number of reflections included in refinement	7769
Cut off Threshold Expression	>2sigma(I)
Structure refined using	full matrix least-squares using F^2
Weighting Scheme	calc w=1/[sigma^2(Fo^2)+(0.0334P)^2+1.2879P] where P=(Fo^2+2Fc^2)/3
Number of parameters in least-squares	208
R_1	0.0252
wR_2	0.0602
R_1 (all data)	0.0379
wR_2 (all data)	0.0642
GOF	1.025
Maximum shift/error	0.004
Min & Max peak heights on final ΔF Map (e^-/Å)	-0.363, 0.651

Where:

$R_1 = \sum(|Fo| - |Fc|) / \sum Fo$

$wR_2 = [\sum(w(Fo^2 - Fc^2)^2) / \sum(w Fo^4)]^{½}$

$GOF = [\sum(w(Fo^2 - Fc^2)^2) / (\text{No. of reflns.} - \text{No. of params.})]^{½}$

Table 2*. Atomic Coordinates for *x08116 (17)

Atom	X	y	z	$U_{iso/equiv}$
Br1	0.643278(5)	0.861021(10)	0.095395(7)	0.01511(3)
Cl1	0.977470(14)	1.39424(3)	0.10330(2)	0.02386(6)
O1	0.77813(4)	1.03081(8)	-0.06391(5)	0.01529(13)
O2	0.70806(4)	0.83051(8)	-0.12497(6)	0.01745(14)
N1	1.03882(4)	1.15927(9)	0.11890(7)	0.01452(14)
N2	0.74737(4)	1.05939(9)	0.16486(6)	0.01369(14)
C2	0.98416(5)	1.21159(10)	0.11240(7)	0.01366(15)
C3	0.93008(5)	1.13638(9)	0.11165(7)	0.01188(14)
C4	0.86696(5)	1.21389(10)	0.09536(8)	0.01422(16)

C5	0.81118(5)	1.12518(9)	0.09125(7)	0.01152(14)
C6	0.76824(5)	1.03599(10)	0.01152(7)	0.01104(14)
C7	0.71722(5)	0.95433(9)	0.01063(7)	0.01119(14)
C8	0.71057(5)	0.97172(10)	0.09055(7)	0.01182(14)
C9	0.79718(5)	1.13320(10)	0.16445(7)	0.01358(15)
C10	0.72275(5)	0.95904(12)	-0.15038(7)	0.01726(17)
C11	0.67536(5)	0.85166(10)	-0.07203(7)	0.01531(16)
C12	0.93965(5)	0.99432(10)	0.12393(7)	0.01221(15)
C13	0.99842(5)	0.92970(10)	0.13214(7)	0.01219(15)
C14	1.01062(5)	0.78307(10)	0.14355(8)	0.01579(16)
C15	1.06731(5)	0.72702(11)	0.14768(8)	0.01797(18)
C16	1.11403(5)	0.81383(11)	0.14013(8)	0.01770(17)
C17	1.10370(5)	0.95594(11)	0.12906(7)	0.01571(16)
C18	1.04619(5)	1.01638(10)	0.12637(7)	0.01264(15)
H4A	0.8832	1.2831	0.1494	0.017
H4B	0.8456	1.2667	0.0325	0.017
H9	0.8248	1.1954	0.2182	0.016
H10A	0.6802	1.0179	-0.1833	0.021
H10B	0.7368	0.9439	-0.1978	0.021
H11A	0.6722	0.7615	-0.0446	0.018
H11B	0.6274	0.8879	-0.1176	0.018
H12	0.9065	0.9385	0.1270	0.015
H14	0.9794	0.7235	0.1483	0.019
H15	1.0752	0.6289	0.1557	0.022
H16	1.1530	0.7736	0.1427	0.021
H17	1.1351	1.0136	0.1232	0.019

Table 3*. Anisotropic Displacement Parameters for *x08116 (!7)

Atom	u^{11}	u^{22}	u^{33}	u^{12}	u^{13}	u^{23}
Br1	0.01419(4)	0.01852(5)	0.01642(5)	-0.00222(3)	0.01082(4)	0.00175(3)
Cl1	0.02061(11)	0.01120(9)	0.04513(16)	-0.00100(8)	0.02147(12)	0.00211(10)

O1	0.0148(3)	0.0228(3)	0.0129(3)	-0.0024(3)	0.0105(3)	-0.0015(2)
O2	0.0185(3)	0.0208(3)	0.0164(3)	-0.0013(3)	0.0117(3)	-0.0047(3)
N1	0.0117(3)	0.0146(3)	0.0183(4)	-0.0010(3)	0.0089(3)	0.0004(3)
N2	0.0139(3)	0.0169(3)	0.0125(3)	-0.0004(3)	0.0087(3)	-0.0002(3)
C2	0.0122(3)	0.0112(3)	0.0181(4)	-0.0014(3)	0.0087(3)	0.0001(3)
C3	0.0095(3)	0.0128(3)	0.0133(4)	-0.0006(3)	0.0062(3)	0.0004(3)
C4	0.0118(3)	0.0122(4)	0.0204(4)	0.0000(3)	0.0099(3)	0.0005(3)
C5	0.0096(3)	0.0121(3)	0.0135(4)	0.0012(3)	0.0068(3)	0.0008(3)
C6	0.0109(3)	0.0133(3)	0.0114(3)	0.0017(3)	0.0077(3)	0.0016(3)
C7	0.0107(3)	0.0127(4)	0.0112(3)	0.0003(3)	0.0066(3)	0.0003(3)
C8	0.0114(3)	0.0135(4)	0.0129(4)	0.0007(3)	0.0081(3)	0.0021(3)
C9	0.0130(4)	0.0150(4)	0.0131(4)	-0.0003(3)	0.0074(3)	-0.0017(3)
C10	0.0171(4)	0.0248(5)	0.0120(4)	-0.0007(4)	0.0092(3)	-0.0013(3)
C11	0.0146(4)	0.0180(4)	0.0146(4)	-0.0025(3)	0.0088(3)	-0.0032(3)
C12	0.0100(3)	0.0126(4)	0.0143(4)	-0.0006(3)	0.0068(3)	0.0012(3)
C13	0.0099(3)	0.0128(4)	0.0127(4)	-0.0006(3)	0.0055(3)	0.0003(3)
C14	0.0132(4)	0.0132(4)	0.0201(4)	-0.0003(3)	0.0086(3)	0.0007(3)
C15	0.0150(4)	0.0152(4)	0.0218(5)	0.0019(3)	0.0089(4)	-0.0005(3)
C16	0.0137(4)	0.0195(4)	0.0203(4)	0.0024(3)	0.0096(4)	-0.0018(4)
C17	0.0116(4)	0.0192(4)	0.0174(4)	-0.0008(3)	0.0086(3)	-0.0010(3)
C18	0.0105(3)	0.0142(4)	0.0130(4)	-0.0007(3)	0.0064(3)	-0.0002(3)

***Table 4*. Bond Lengths for *x08116* (17)**

Br1-C8	1.9051(9)	C7-C8	1.3909(12)
Cl1-C2	1.7502(10)	C7-C11	1.5023(13)
O1-C6	1.3575(11)	C9-H9	0.9500
O1-C10	1.4432(12)	C10-H10A	0.9900
O2-C10	1.3930(13)	C10-H10B	0.9900
O2-C11	1.4271(12)	C11-H11A	0.9900
N1-C2	1.2970(12)	C11-H11B	0.9900
N1-C18	1.3722(12)	C12-C13	1.4188(13)
N2-C8	1.3195(12)	C12-H12	0.9500

N2-C9	1.3438(13)	C13-C18	1.4148(13)
C2-C3	1.4257(13)	C13-C14	1.4200(14)
C3-C12	1.3712(13)	C14-C15	1.3712(14)
C3-C4	1.5124(13)	C14-H14	0.9500
C4-C5	1.5032(13)	C15-C16	1.4106(15)
C4-H4A	0.9900	C15-H15	0.9500
C4-H4B	0.9900	C16-C17	1.3724(15)
C5-C9	1.3872(13)	C16-H16	0.9500
C5-C6	1.4000(13)	C17-C18	1.4163(13)
C6-C7	1.3979(13)	C17-H17	0.9500

***Table 5*. Bond Angles for *x08116* (17)**

C6-O1-C10	113.29(7)	O2-C10-H10A	109.4
C10-O2-C11	110.06(8)	O1-C10-H10A	109.4
C2-N1-C18	117.18(8)	O2-C10-H10B	109.4
C8-N2-C9	116.60(8)	O1-C10-H10B	109.4
N1-C2-C3	126.96(9)	H10A-C10-H10B	108.0
N1-C2-Cl1	115.27(7)	O2-C11-C7	109.69(8)
C3-C2-Cl1	117.77(7)	O2-C11-H11A	109.7
C12-C3-C2	115.36(8)	C7-C11-H11A	109.7
C12-C3-C4	124.81(8)	O2-C11-H11B	109.7
C2-C3-C4	119.81(8)	C7-C11-H11B	109.7
C5-C4-C3	116.04(8)	H11A-C11-H11B	108.2
C5-C4-H4A	108.3	C3-C12-C13	120.78(8)
C3-C4-H4A	108.3	C3-C12-H12	119.6
C5-C4-H4B	108.3	C13-C12-H12	119.6
C3-C4-H4B	108.3	C18-C13-C12	117.84(8)
H4A-C4-H4B	107.4	C18-C13-C14	118.79(8)
C9-C5-C6	116.34(8)	C12-C13-C14	123.35(8)
C9-C5-C4	121.32(9)	C15-C14-C13	120.31(9)
C6-C5-C4	122.25(8)	C15-C14-H14	119.8

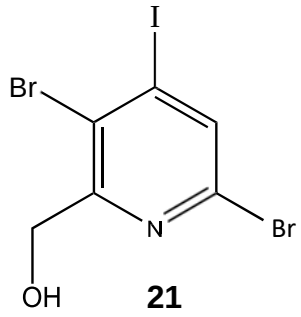
O1-C6-C7	121.40(8)	C13-C14-H14	119.8
O1-C6-C5	117.98(8)	C14-C15-C16	120.58(9)
C7-C6-C5	120.62(8)	C14-C15-H15	119.7
C8-C7-C6	116.15(8)	C16-C15-H15	119.7
C8-C7-C11	124.17(8)	C17-C16-C15	120.54(9)
C6-C7-C11	119.64(8)	C17-C16-H16	119.7
N2-C8-C7	125.44(8)	C15-C16-H16	119.7
N2-C8-Br1	116.18(7)	C16-C17-C18	119.85(9)
C7-C8-Br1	118.38(7)	C16-C17-H17	120.1
N2-C9-C5	124.72(9)	C18-C17-H17	120.1
N2-C9-H9	117.6	N1-C18-C13	121.71(8)
C5-C9-H9	117.6	N1-C18-C17	118.38(9)
O2-C10-O1	111.05(8)	C13-C18-C17	119.91(9)

Table 6*. Torsion Angles for *x08116 (17)

C18-N1-C2-C3	-0.33(16)	C8-N2-C9-C5	1.28(14)
C18-N1-C2-Cl1	179.87(7)	C6-C5-C9-N2	1.92(14)
N1-C2-C3-C12	3.33(15)	C4-C5-C9-N2	178.67(9)
Cl1-C2-C3-C12	-176.87(7)	C11-O2-C10-O1	70.02(10)
N1-C2-C3-C4	-175.14(10)	C6-O1-C10-O2	-49.14(11)
Cl1-C2-C3-C4	4.65(13)	C10-O2-C11-C7	-50.04(10)
C12-C3-C4-C5	-0.95(14)	C8-C7-C11-O2	-163.08(9)
C2-C3-C4-C5	177.38(9)	C6-C7-C11-O2	14.63(12)
C3-C4-C5-C9	112.74(10)	C2-C3-C12-C13	-2.68(14)
C3-C4-C5-C6	-70.70(12)	C4-C3-C12-C13	175.71(9)
C10-O1-C6-C7	12.45(12)	C3-C12-C13-C18	-0.54(14)
C10-O1-C6-C5	-168.04(8)	C3-C12-C13-C14	-179.09(9)
C9-C5-C6-O1	176.77(8)	C18-C13-C14-C15	-0.75(14)
C4-C5-C6-O1	0.05(13)	C12-C13-C14-C15	177.79(10)
C9-C5-C6-C7	-3.72(13)	C13-C14-C15-C16	-0.35(16)
C4-C5-C6-C7	179.56(8)	C14-C15-C16-C17	0.36(17)

O1-C6-C7-C8	-178.14(8)	C15-C16-C17-C18	0.76(15)
C5-C6-C7-C8	2.37(13)	C2-N1-C18-C13	-3.32(14)
O1-C6-C7-C11	3.98(13)	C2-N1-C18-C17	177.19(9)
C5-C6-C7-C11	-175.51(8)	C12-C13-C18-N1	3.75(14)
C9-N2-C8-C7	-2.88(14)	C14-C13-C18-N1	-177.63(9)
C9-N2-C8-Br1	177.01(7)	C12-C13-C18-C17	-176.77(9)
C6-C7-C8-N2	1.09(14)	C14-C13-C18-C17	1.85(14)
C11-C7-C8-N2	178.87(9)	C16-C17-C18-N1	177.63(9)
C6-C7-C8-Br1	-178.80(6)	C16-C17-C18-C13	-1.87(14)
C11-C7-C8-Br1	-1.01(12)		

X-ray Crystal Data and Structure Refinement for 21



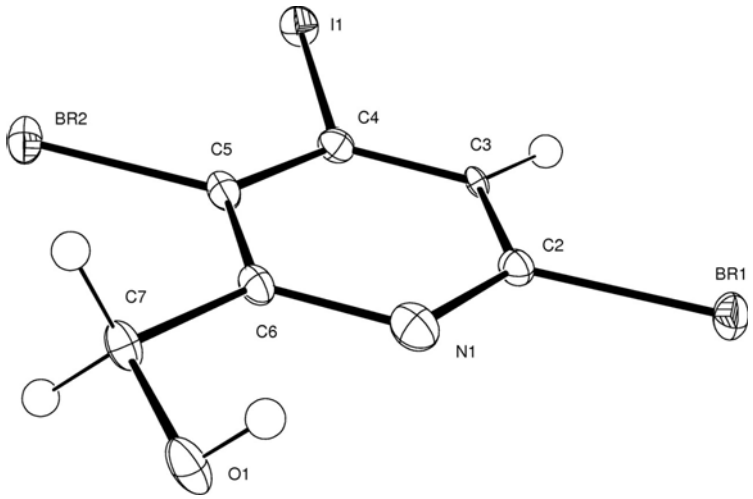


Figure 5. ORTEP drawing of ***x08099*** showing naming and numbering scheme.
Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity.

***Table 1*. Summary of Crystal Data for *x08099* (21)**

Identification code	x08099
Formula	$C_6H_4Br_2INO$
Formula Weight (*g/mol*)	392.82
Crystal Dimensions (*mm*)	0.30 × 0.20 × 0.08
Crystal Color and Habit	colourless prism
Crystal System	Monoclinic
Space Group	P 2_1/c
Temperature, K	110
a, Å	4.36900(10)
b, Å	13.9316(3)
c, Å	14.7442(3)
α,°	90.00
β,°	92.8342(11)
γ,°	90.00
V, $Å^3$	896.34(3)
Number of reflections to determine final unit cell	9265
Min and Max 2θ for cell determination, °	5.54, 75.98
Z	4
F(000)	712
ρ (*g/cm*)	2.911
λ, Å, (MoKα)	0.71070
μ, (cm^{-1})	12.430
Diffractometer Type	Bruker-Nonius X8 Apex2
Scan Type(s)	omega and phi scans
Max 2θ for data collection, °	81.22
Measured fraction of data	0.868
Number of reflections measured	23005
Unique reflections measured	4986
R_{merge}	0.0384
Number of reflections included in refinement	4986

Cut off Threshold Expression	>2sigma(I)
Structure refined using	full matrix least-squares using F^2
Weighting Scheme	calc w=1/[sigma^2(Fo^2)+(0.0372P)^2+1.7342P] where P=(Fo^2+2Fc^2)/3
Number of parameters in least-squares	100
R_1	0.0329
wR_2	0.0786
R_1 (all data)	0.0490
wR_2 (all data)	0.0835
GOF	1.045
Maximum shift/error	0.001
Min & Max peak heights on final ΔF Map (e^-/Å)	-1.986, 1.921

Where:

$R_1 = \sum(|Fo| - |Fc|) / \sum Fo$

$wR_2 = [\sum(w(Fo^2 - Fc^2)^2) / \sum(w Fo^4)]^{½}$

$GOF = [\sum(w(Fo^2 - Fc^2)^2) / (\text{No. of reflns.} - \text{No. of params.})]^{½}$

***Table 2*. Atomic Coordinates for *x08099* (21)**

Atom	X	y	z	$U_{iso/equiv}$
I1	0.05665(4)	0.015841(14)	0.867342(12)	0.01441(5)
Br1	-0.66752(6)	0.34818(2)	0.878557(18)	0.01423(6)
Br2	0.16084(6)	0.07017(2)	0.638474(19)	0.01470(6)
O1	-0.3436(5)	0.33771(16)	0.54028(14)	0.0167(4)
N1	-0.3955(6)	0.2929(2)	0.71647(18)	0.0174(5)
C2	-0.4308(6)	0.2672(2)	0.80609(17)	0.0109(4)
C3	-0.3069(5)	0.19102(17)	0.84662(15)	0.0065(4)
C4	-0.1312(6)	0.13407(19)	0.79740(17)	0.0107(4)
C5	-0.0793(6)	0.1533(2)	0.70697(17)	0.0113(4)
C6	-0.2133(6)	0.2343(2)	0.66489(17)	0.0112(4)

C7	-0.1605(7)	0.2579(2)	0.56735(17)	0.0138(5)
H1	-0.2953	0.3852	0.5731	0.025
H3	-0.3409	0.1770	0.9084	0.008
H7A	0.0585	0.2730	0.5605	0.017
H7B	-0.2147	0.2019	0.5284	0.017

Table 3*. Anisotropic Displacement Parameters for *x08099 (21)

Atom	u^{11}	u^{22}	u^{33}	u^{12}	u^{13}	u^{23}
I1	0.01831(8)	0.01281(8)	0.01207(8)	0.00217(6)	0.00018(6)	0.00259(6)
Br1	0.01646(12)	0.01515(13)	0.01139(11)	0.00247(9)	0.00387(9)	-0.00096(9)
Br2	0.01639(12)	0.01446(13)	0.01360(11)	-0.00006(9)	0.00427(9)	-0.00274(9)
O1	0.0274(11)	0.0151(10)	0.0075(8)	0.0009(8)	-0.0007(7)	0.0002(7)
N1	0.0194(11)	0.0189(12)	0.0139(10)	-0.0016(9)	-0.0001(8)	0.0004(9)
C2	0.0110(10)	0.0133(11)	0.0085(9)	-0.0009(8)	0.0009(7)	-0.0002(8)
C3	0.0095(9)	0.0073(9)	0.0028(8)	-0.0007(7)	0.0009(6)	0.0001(7)
C4	0.0123(10)	0.0099(10)	0.0099(10)	-0.0004(8)	-0.0009(8)	0.0007(8)
C5	0.0129(10)	0.0123(11)	0.0088(9)	-0.0031(8)	0.0016(8)	-0.0017(8)
C6	0.0129(10)	0.0125(11)	0.0081(9)	-0.0021(8)	0.0011(8)	-0.0004(8)
C7	0.0190(12)	0.0157(12)	0.0069(9)	-0.0006(9)	0.0021(8)	0.0000(9)

Table 4*. Bond Lengths for *x08099 (21)

I1-C4	2.090(3)	C3-C4	1.342(4)
Br1-C2	1.895(3)	C3-H3	0.9500
Br2-C5	1.889(3)	C4-C5	1.390(4)
O1-C7	1.416(4)	C5-C6	1.401(4)
O1-H1	0.8400	C6-C7	1.504(4)
N1-C2	1.385(4)	C7-H7A	0.9900
N1-C6	1.392(4)	C7-H7B	0.9900
C2-C3	1.321(4)		

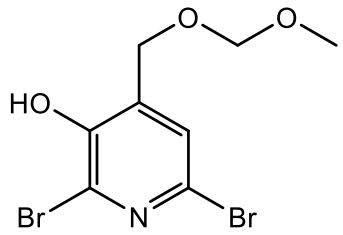
Table 5*. Bond Angles for *x08099 (21)

C7-O1-H1	109.5	C4-C5-Br2	121.1(2)
C2-N1-C6	117.6(2)	C6-C5-Br2	119.19(19)
C3-C2-N1	125.2(3)	N1-C6-C5	117.9(2)
C3-C2-Br1	116.49(19)	N1-C6-C7	120.9(2)
N1-C2-Br1	118.3(2)	C5-C6-C7	121.3(2)
C2-C3-C4	117.6(2)	O1-C7-C6	109.3(2)
C2-C3-H3	121.2	O1-C7-H7A	109.8
C4-C3-H3	121.2	C6-C7-H7A	109.8
C3-C4-C5	122.0(2)	O1-C7-H7B	109.8
C3-C4-I1	114.86(18)	C6-C7-H7B	109.8
C5-C4-I1	123.2(2)	H7A-C7-H7B	108.3
C4-C5-C6	119.7(2)		

Table 6*. Torsion Angles for *x08099 (21)

C6-N1-C2-C3	-0.5(4)	I1-C4-C5-Br2	1.8(3)
C6-N1-C2-Br1	178.07(19)	C2-N1-C6-C5	0.2(4)
N1-C2-C3-C4	0.4(4)	C2-N1-C6-C7	-179.2(2)
Br1-C2-C3-C4	-178.17(19)	C4-C5-C6-N1	0.0(4)
C2-C3-C4-C5	-0.1(4)	Br2-C5-C6-N1	178.38(19)
C2-C3-C4-I1	179.70(18)	C4-C5-C6-C7	179.5(2)
C3-C4-C5-C6	-0.1(4)	Br2-C5-C6-C7	-2.1(3)
I1-C4-C5-C6	-179.89(19)	N1-C6-C7-O1	-5.7(4)
C3-C4-C5-Br2	-178.4(2)	C5-C6-C7-O1	174.8(2)

X-ray Crystal Data and Structure Refinement for 24



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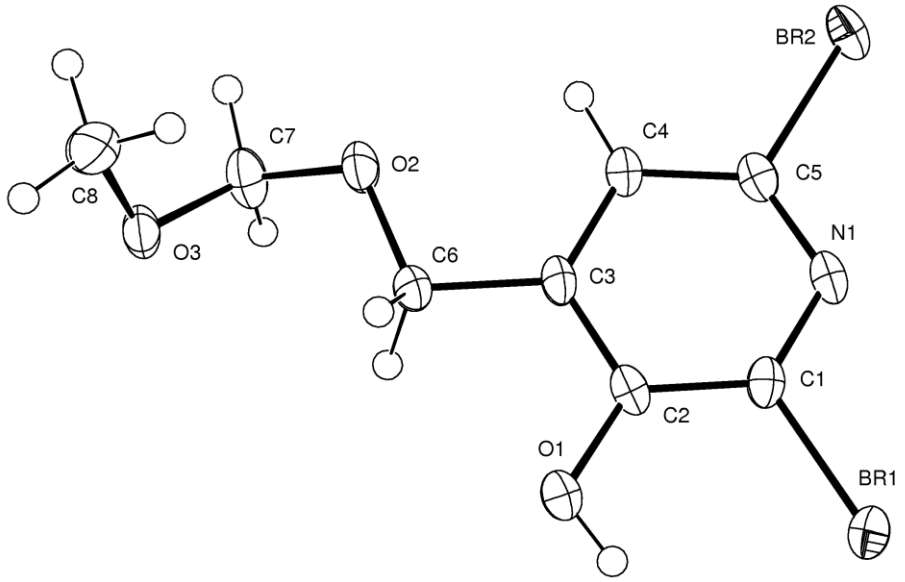

Figure 6. ORTEP drawing of ***x08131*** showing naming and numbering scheme. Ellipsoids are at the 50% probability level and hydrogen atoms were drawn with arbitrary radii for clarity.

Table 1*. Summary of Crystal Data for *x08131 (24)

Identification code	x08131
Formula	$C_8H_9Br_2NO_3$
Formula Weight (*g/mol*)	326.98
Crystal Dimensions (*mm*)	0.34 × 0.16 × 0.03
Crystal Color and Habit	colourless prism
Crystal System	Monoclinic
Space Group	P 2_1/c
Temperature, K	110
a, Å	10.8948(7)
b, Å	13.6076(8)
c, Å	7.0966(4)
α,°	90.00
β,°	97.323(4)
γ,°	90.00
V, Å^3	1043.51(11)
Number of reflections to determine final unit cell	5263
Min and Max 2θ for cell determination, °	4.82, 55.4
Z	4
F(000)	632
ρ (*g/cm*)	2.081
λ, Å, (MoKα)	0.71070
μ, (cm^{-1})	7.749
Diffractometer Type	Bruker-Nonius X8 Apex2
Scan Type(s)	omega and phi scans
Max 2θ for data collection, °	56.12
Measured fraction of data	0.994
Number of reflections measured	18540
Unique reflections measured	2519
R_{merge}	0.0709
Number of reflections included in refinement	2519

Cut off Threshold Expression	>2sigma(I)
Structure refined using	full matrix least-squares using F^2
Weighting Scheme	calc w=1/[sigma^2(Fo^2)+(0.0347P)^2+1.9214P] where P=(Fo^2+2Fc^2)/3
Number of parameters in least-squares	163
R_1	0.0328
wR_2	0.0703
R_1 (all data)	0.0658
wR_2 (all data)	0.0864
GOF	1.000
Maximum shift/error	0.001
Min & Max peak heights on final ΔF Map (e^-/Å)	-0.750, 0.597

Where:

$R_1 = \sum(|Fo| - |Fc|) / \sum Fo$

$wR_2 = [\sum(w(Fo^2 - Fc^2)^2) / \sum(w Fo^4)]^{½}$

$GOF = [\sum(w(Fo^2 - Fc^2)^2) / (\text{No. of reflns.} - \text{No. of params.})]^{½}$

Table 2*. Atomic Coordinates for *x08131 (24)

Atom	X	y	z	$U_{iso/equiv}$
Br1	0.08602(4)	0.13226(3)	0.91472(6)	0.02666(13)
Br2	-0.39765(4)	0.09292(3)	1.03971(6)	0.02905(14)
O1	0.0194(3)	0.3576(2)	0.9178(4)	0.0263(6)
O2	-0.3138(3)	0.47684(19)	1.0254(4)	0.0264(6)
O3	-0.2737(3)	0.64611(19)	1.0414(4)	0.0266(6)
N1	-0.1600(3)	0.1350(2)	0.9751(4)	0.0217(7)
C1	-0.0661(4)	0.1937(3)	0.9503(5)	0.0212(8)
C2	-0.0728(4)	0.2961(3)	0.9501(5)	0.0207(8)
C3	-0.1843(4)	0.3387(3)	0.9839(5)	0.0208(8)
C4	-0.2829(4)	0.2786(3)	1.0112(6)	0.0211(8)
C5	-0.2642(4)	0.1779(3)	1.0024(5)	0.0204(8)

C6	-0.1918(4)	0.4486(3)	0.9975(6)	0.0241(9)
C7	-0.3185(5)	0.5629(3)	1.1318(7)	0.0289(10)
C8	-0.3505(5)	0.6724(4)	0.8712(8)	0.0370(11)
H1	0.086(4)	0.325(4)	0.932(7)	0.039(15)
H4	-0.361(3)	0.305(3)	1.031(5)	0.007(9)
H6A	-0.123(4)	0.473(3)	1.098(6)	0.026(11)
H6B	-0.170(4)	0.477(3)	0.880(6)	0.018(10)
H7A	-0.269(4)	0.555(3)	1.256(6)	0.024(11)
H7B	-0.408(4)	0.570(3)	1.145(6)	0.028(12)
H8A	-0.358(6)	0.614(5)	0.781(9)	0.08(2)
H8B	-0.308(5)	0.725(4)	0.822(8)	0.060(17)
H8C	-0.433(5)	0.685(4)	0.892(7)	0.056(16)

***Table 3*. Anisotropic Displacement Parameters for *x08131* (24)**

Atom	u^{11}	u^{22}	u^{33}	u^{12}	u^{13}	u^{23}
Br1	0.0304(2)	0.0205(2)	0.0294(2)	0.00354(16)	0.00498(18)	-0.00322(17)
Br2	0.0358(3)	0.0191(2)	0.0328(3)	-0.00942(17)	0.00637(19)	-0.00028(17)
O1	0.0279(17)	0.0172(15)	0.0339(17)	-0.0025(13)	0.0044(13)	0.0032(12)
O2	0.0297(16)	0.0151(14)	0.0349(17)	-0.0009(11)	0.0065(13)	-0.0043(12)
O3	0.0319(16)	0.0148(14)	0.0337(16)	-0.0003(12)	0.0065(13)	-0.0009(12)
N1	0.0325(19)	0.0143(16)	0.0178(17)	-0.0039(14)	0.0015(15)	-0.0001(13)
C1	0.029(2)	0.0159(19)	0.0182(19)	0.0025(16)	0.0021(17)	0.0010(15)
C2	0.029(2)	0.0157(19)	0.0181(19)	-0.0049(15)	0.0043(17)	-0.0012(15)
C3	0.028(2)	0.0128(18)	0.021(2)	-0.0007(16)	0.0014(17)	0.0017(15)
C4	0.027(2)	0.0146(19)	0.022(2)	0.0003(16)	0.0038(17)	0.0007(15)
C5	0.028(2)	0.0177(19)	0.0151(19)	-0.0032(16)	0.0019(16)	0.0011(15)
C6	0.024(2)	0.016(2)	0.034(2)	-0.0011(16)	0.0061(19)	0.0027(18)
C7	0.042(3)	0.018(2)	0.028(2)	-0.0027(19)	0.013(2)	-0.0033(18)
C8	0.028(3)	0.032(3)	0.050(3)	0.003(2)	0.002(2)	0.011(2)

Table 4*. Bond Lengths for *x08131 (24)

Br1-C1	1.902(4)	C3-C4	1.383(5)
Br2-C5	1.903(4)	C3-C6	1.501(5)
O1-C2	1.349(5)	C4-C5	1.388(5)
O1-H1	0.85(5)	C4-H4	0.95(4)
O2-C7	1.398(5)	C6-H6A	1.02(4)
O2-C6	1.422(5)	C6-H6B	0.97(4)
O3-C7	1.418(5)	C7-H7A	0.98(4)
O3-C8	1.424(6)	C7-H7B	0.99(5)
N1-C5	1.313(5)	C8-H8A	1.01(6)
N1-C1	1.328(5)	C8-H8B	0.95(6)
C1-C2	1.395(5)	C8-H8C	0.94(6)
C2-C3	1.395(5)		

***Table 5*. Bond Angles for *x08131* (24)**

C2-O1-H1	108(3)	O2-C6-C3	109.7(3)
C7-O2-C6	113.6(3)	O2-C6-H6A	116(2)
C7-O3-C8	112.6(4)	C3-C6-H6A	109(2)
C5-N1-C1	116.5(3)	O2-C6-H6B	110(2)
N1-C1-C2	124.1(4)	C3-C6-H6B	109(2)
N1-C1-Br1	116.9(3)	H6A-C6-H6B	104(3)
C2-C1-Br1	119.0(3)	O2-C7-O3	112.7(3)
O1-C2-C1	125.4(4)	O2-C7-H7A	110(3)
O1-C2-C3	117.0(3)	O3-C7-H7A	108(3)
C1-C2-C3	117.5(3)	O2-C7-H7B	104(3)
C4-C3-C2	119.1(3)	O3-C7-H7B	111(3)
C4-C3-C6	122.1(3)	H7A-C7-H7B	111(4)
C2-C3-C6	118.7(3)	O3-C8-H8A	109(4)
C3-C4-C5	117.1(4)	O3-C8-H8B	104(3)
C3-C4-H4	121(2)	H8A-C8-H8B	112(5)

C5-C4-H4	122(2)	O3-C8-H8C	112(3)
N1-C5-C4	125.6(4)	H8A-C8-H8C	104(5)
N1-C5-Br2	116.1(3)	H8B-C8-H8C	116(5)
C4-C5-Br2	118.3(3)		

Table 6*. Torsion Angles for *x08131 (24)

C5-N1-C1-C2	-0.6(6)	C6-C3-C4-C5	-177.6(4)
C5-N1-C1-Br1	179.0(3)	C1-N1-C5-C4	-1.4(6)
N1-C1-C2-O1	-177.2(4)	C1-N1-C5-Br2	-179.5(3)
Br1-C1-C2-O1	3.3(5)	C3-C4-C5-N1	1.8(6)
N1-C1-C2-C3	2.0(6)	C3-C4-C5-Br2	179.9(3)
Br1-C1-C2-C3	-177.6(3)	C7-O2-C6-C3	149.1(3)
O1-C2-C3-C4	177.8(3)	C4-C3-C6-O2	-4.7(5)
C1-C2-C3-C4	-1.5(6)	C2-C3-C6-O2	177.9(3)
O1-C2-C3-C6	-4.8(5)	C6-O2-C7-O3	63.0(5)
C1-C2-C3-C6	176.0(4)	C8-O3-C7-O2	66.6(5)
C2-C3-C4-C5	-0.2(6)		