

Heterogeneous & Homogeneous & Bio-

CHEMCATCHEM

CATALYSIS

Supporting Information

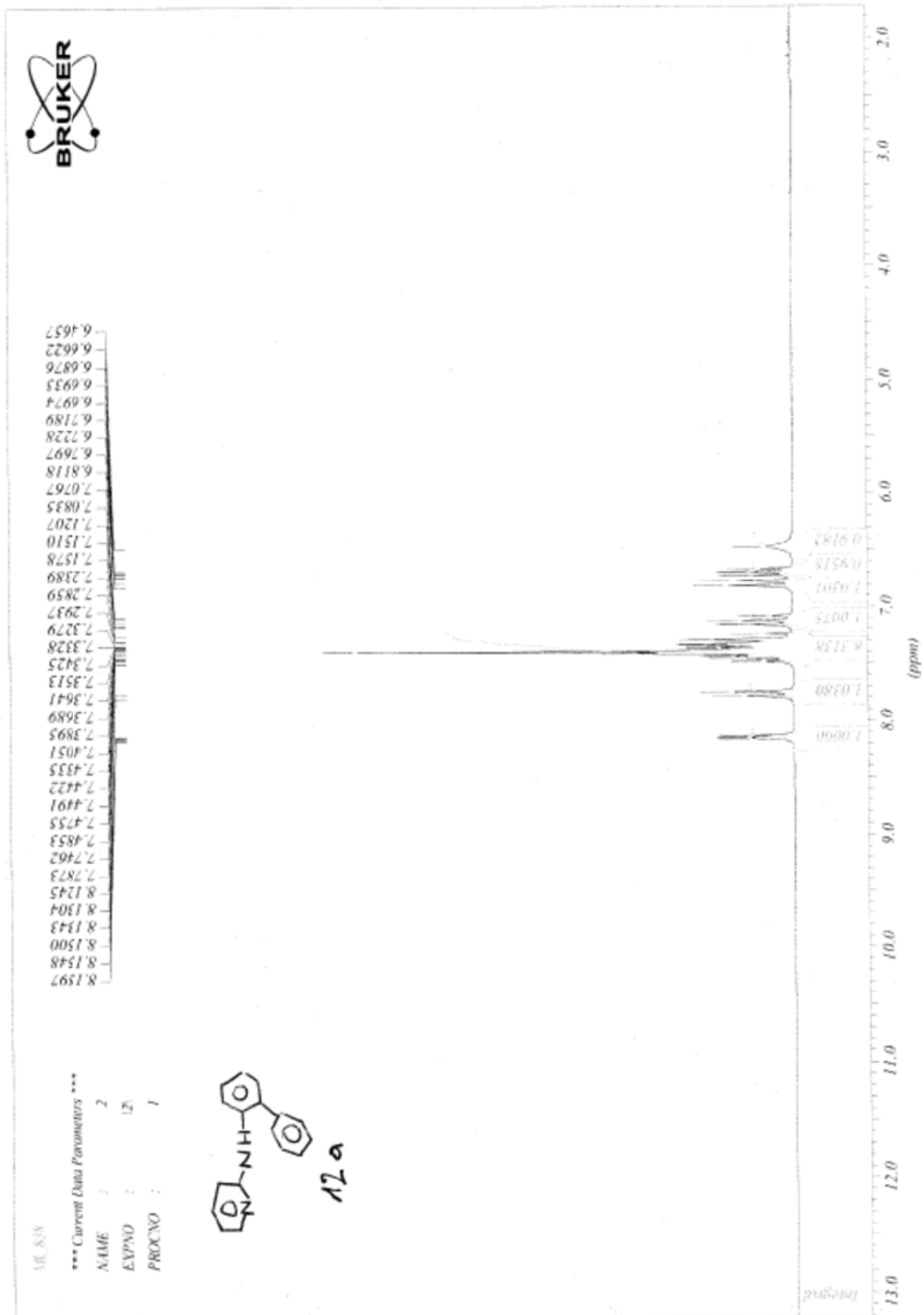
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Palladium(II)-Catalyzed Regioselective *Ortho* Arylation of sp^2 C–H Bonds of *N*-Aryl-2-amino Pyridine Derivatives

Moumita Koley, Navid Dastbaravardeh, Michael Schnürch,* and Marko D. Mihovilovic^[a]

cctc_201200155_sm_miscellaneous_information.pdf

N-([1,1'-biphenyl]-2-yl)pyridin-2-amine (12a):

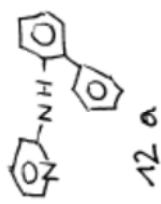




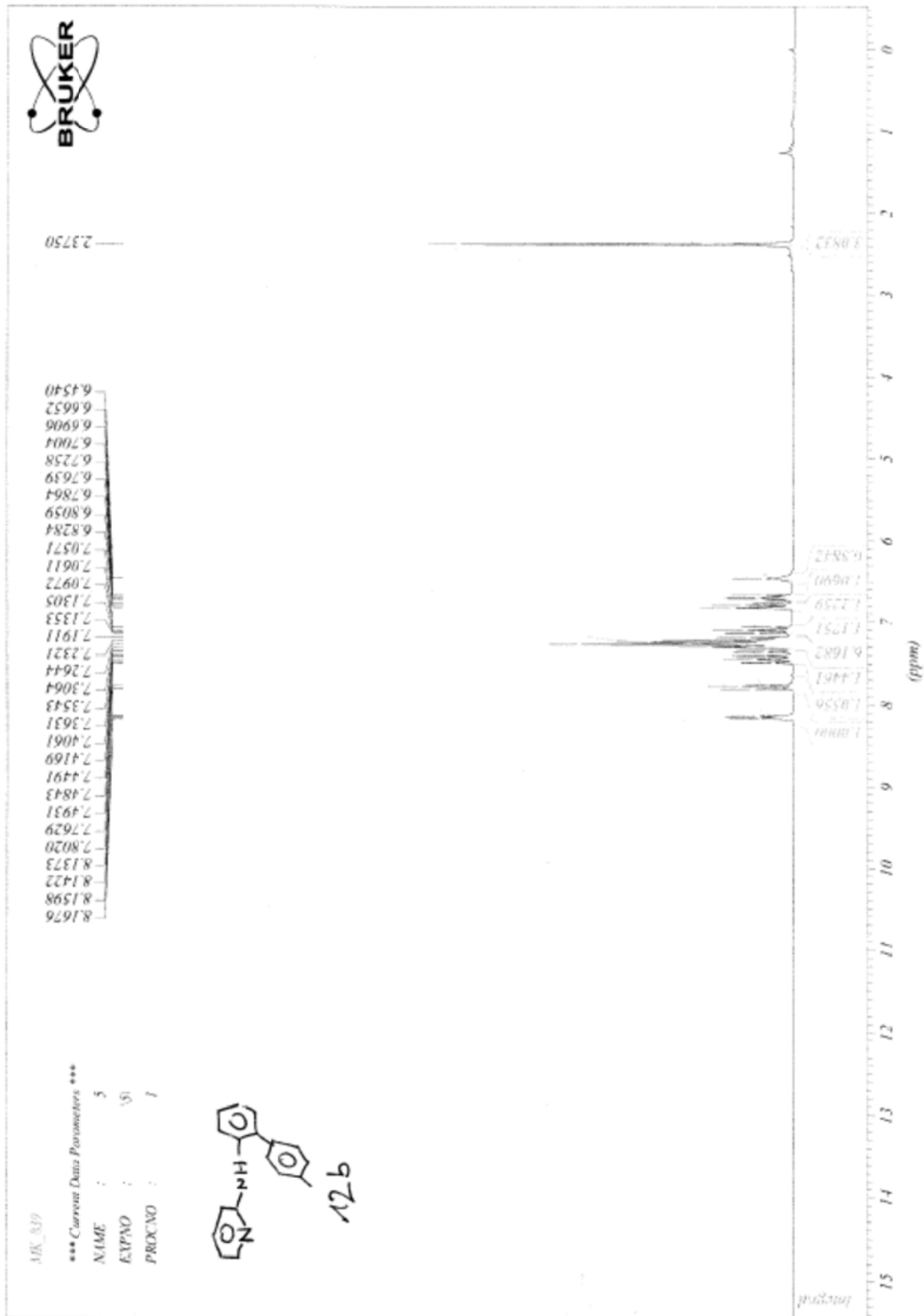
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EXPNO : H
PROCNO : 1

MR_331_2F

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- 137.4511
- 133.3170
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- 128.8529
- 128.2282
- 127.5755
- 122.9430
- 120.5986
- 115.0747
- 108.6173



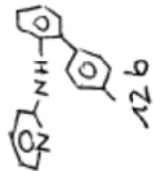
N-(4'-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12b):



16K 332

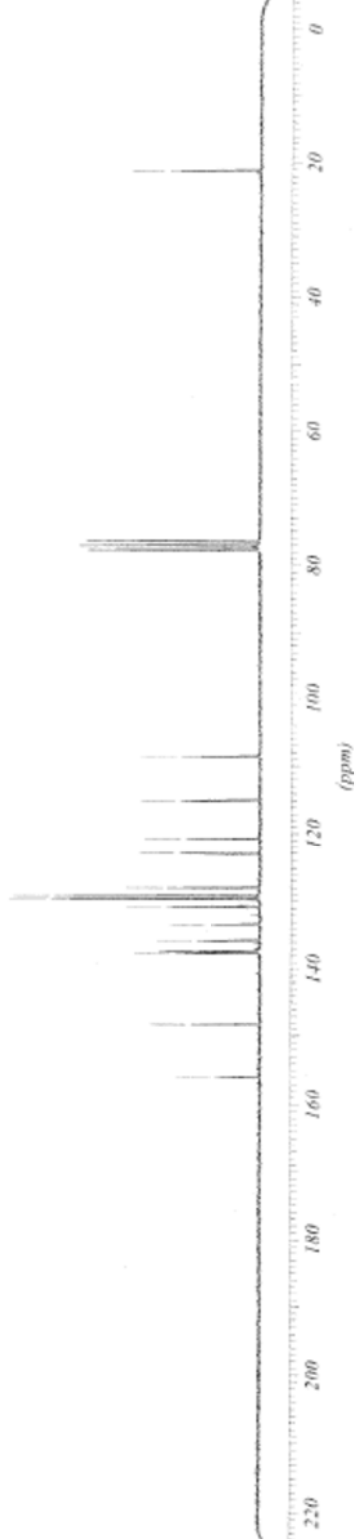
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EXPNO : 16
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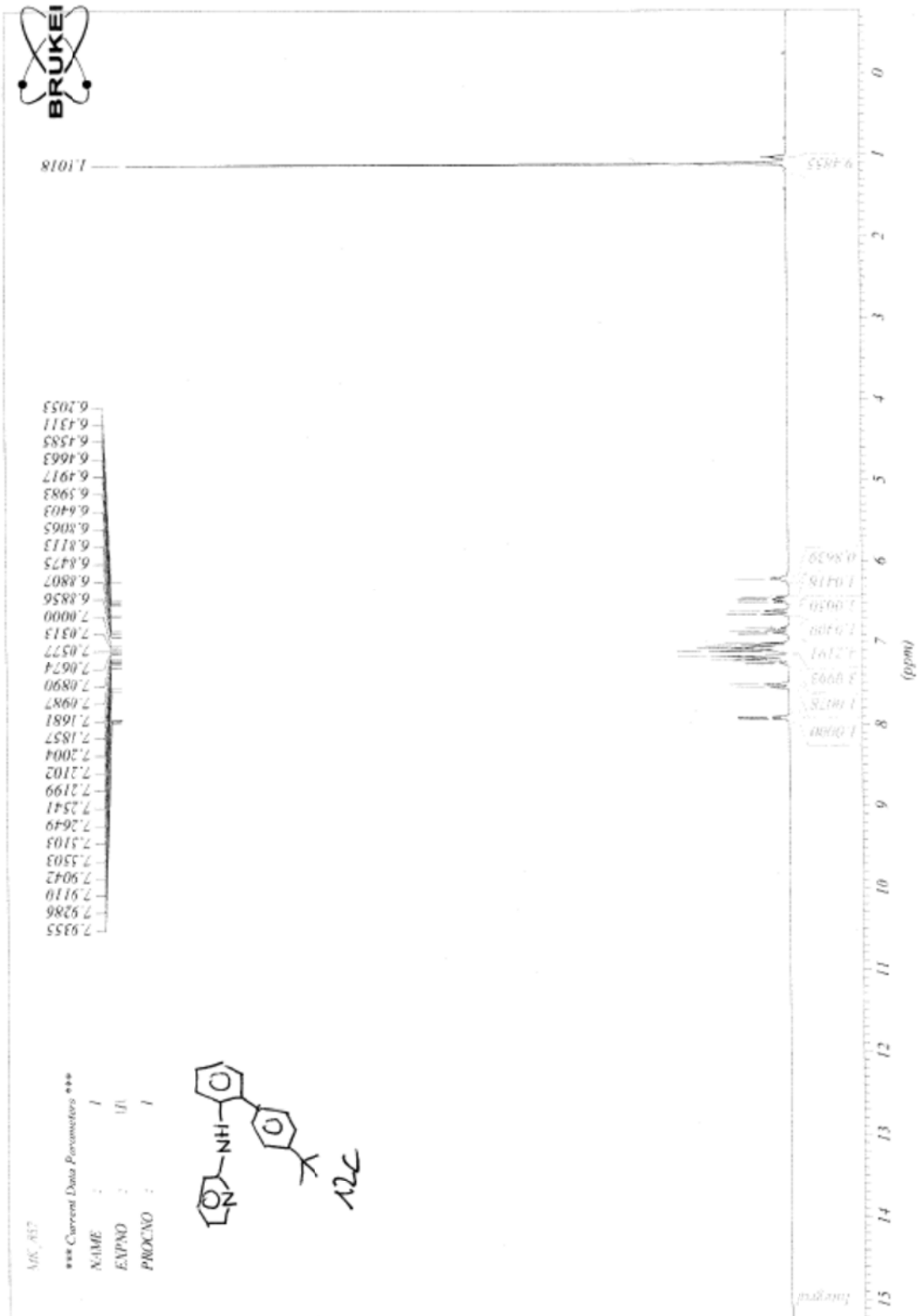


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137.4722
137.3248
135.7736
133.3802
130.7691
129.5689
129.1618
128.0247
122.9500
120.6267
114.9835
108.5752

21.1893



N-(4'-(*tert*-butyl)-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12c):

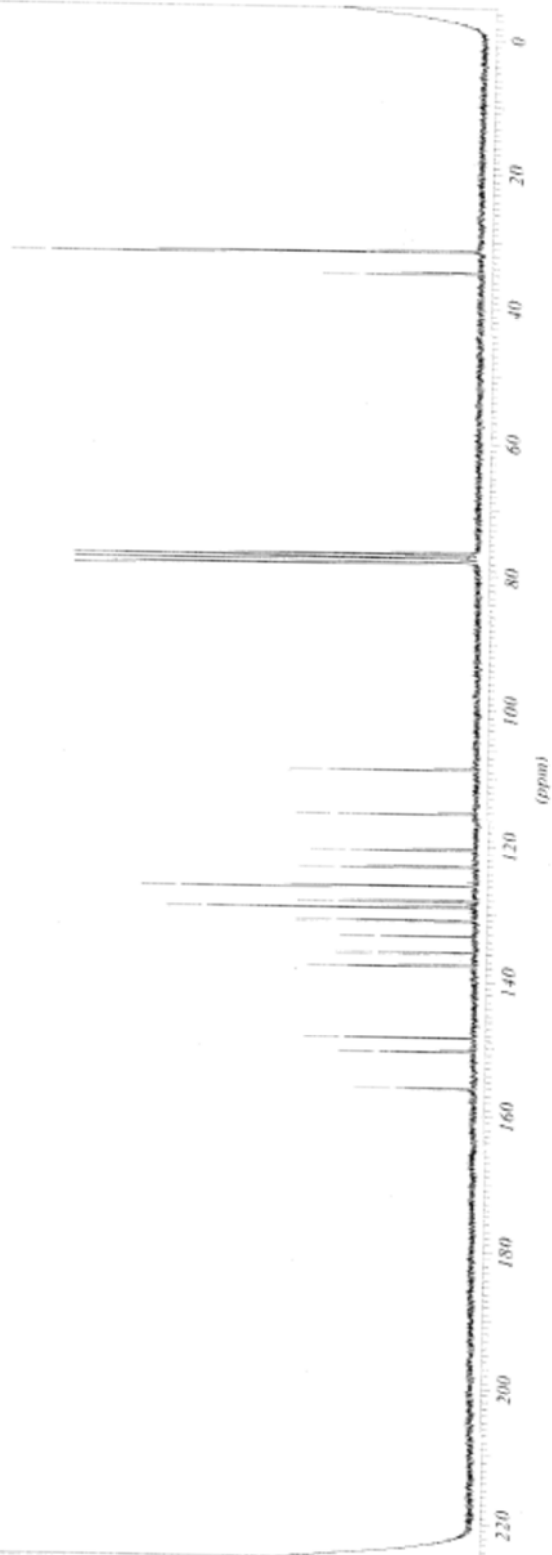
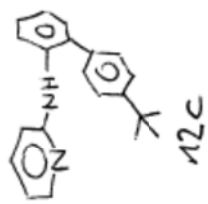




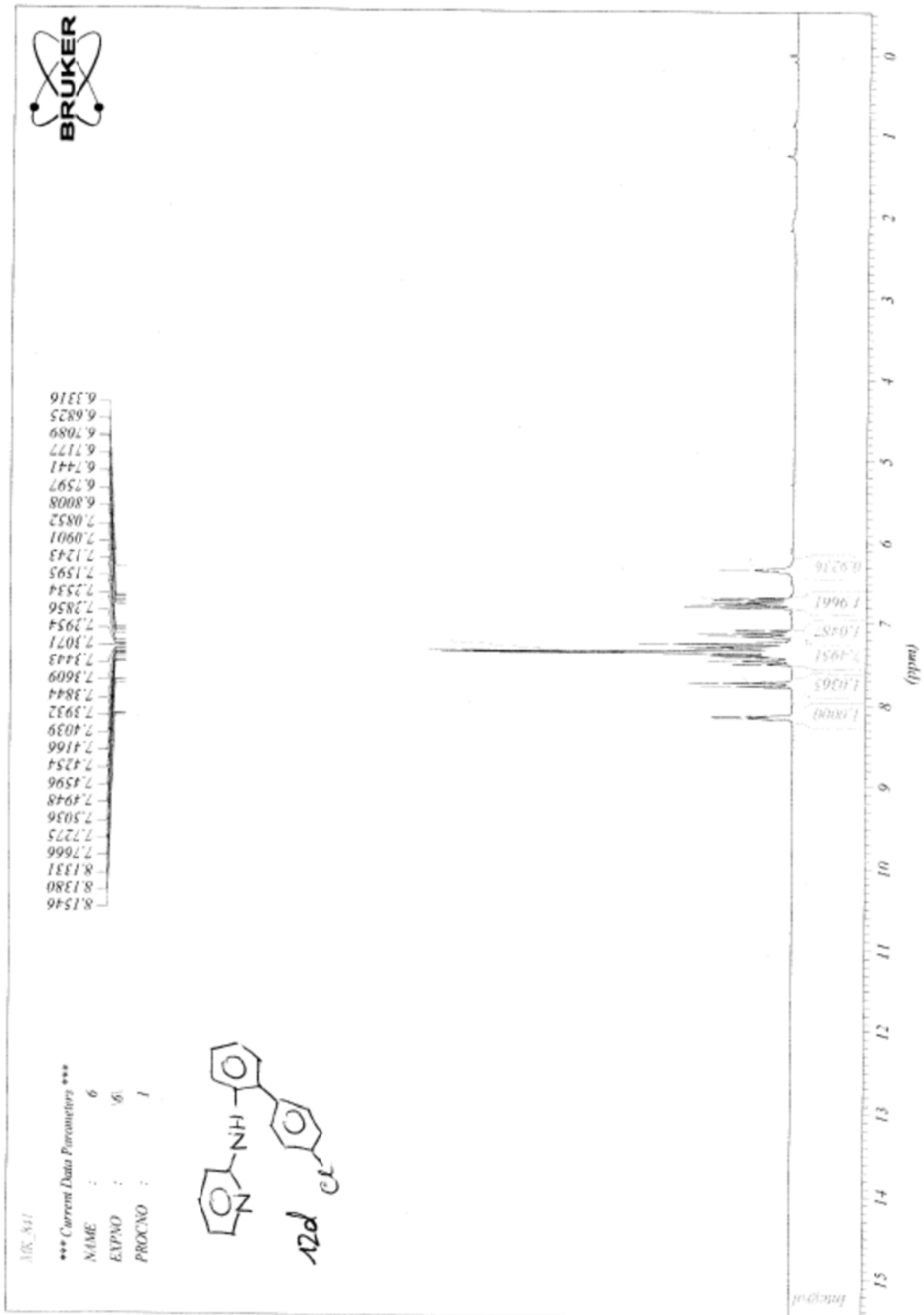
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31.3457

155.9250
150.4643
148.3586
137.6617
137.4933
135.6894
133.1696
130.8674
128.9512
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Product
*** Current Data Parameters ***
NAME : 2
EXPNO : 121
PROCNO : 1



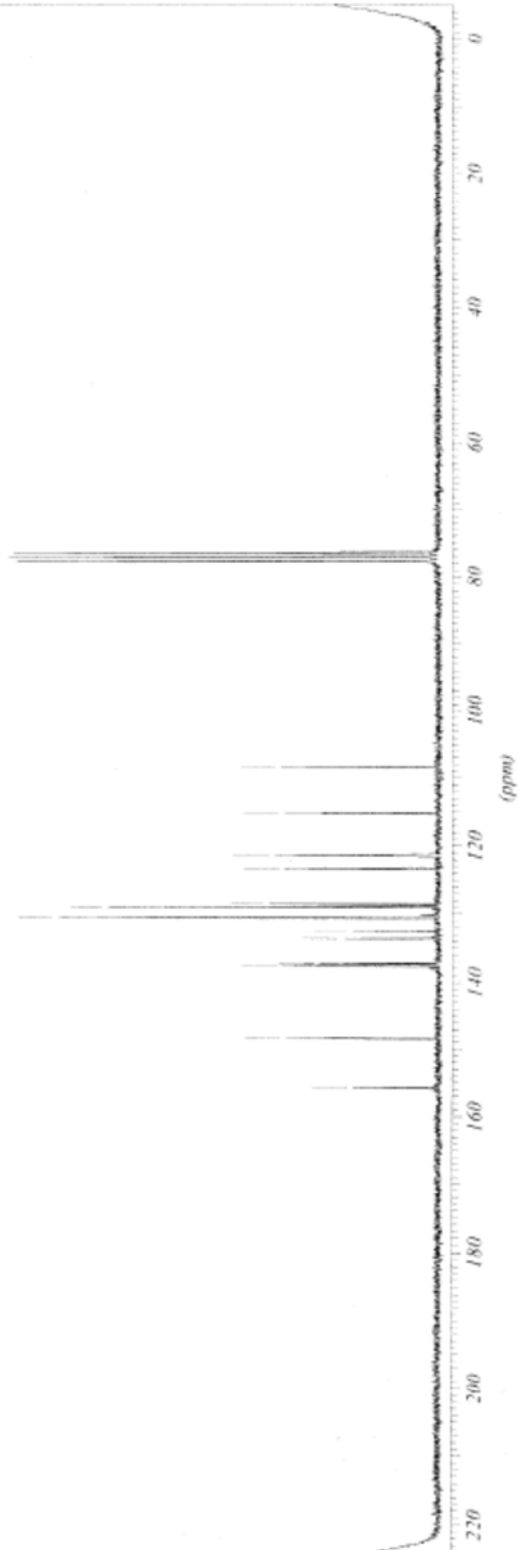
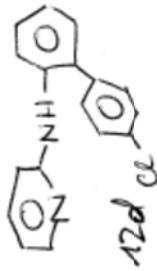
N-(4'-chloro-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12d):



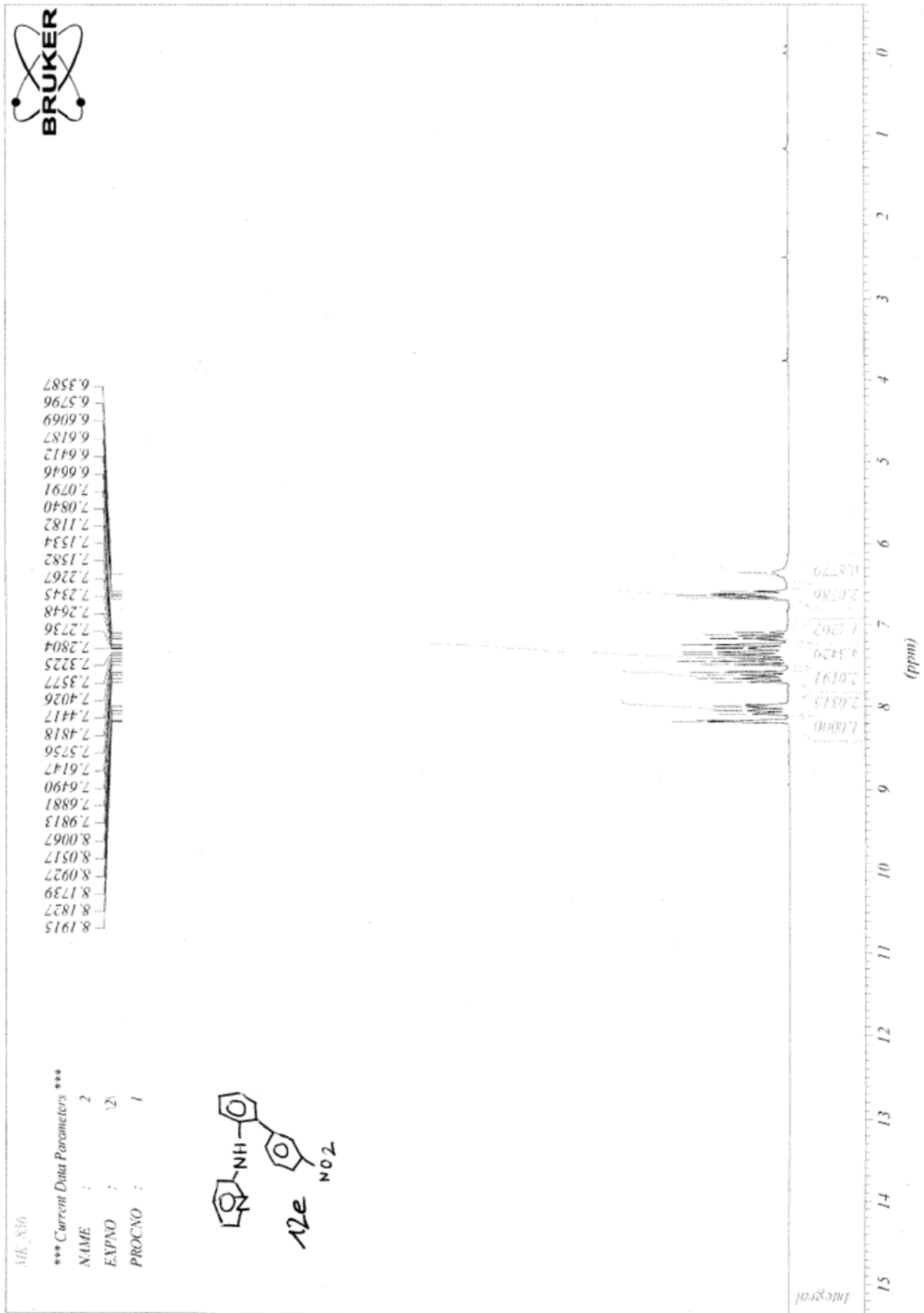


155.8478
148.4147
137.7249
137.3739
137.2546
133.6258
132.5028
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130.6428
129.0284
128.6143
123.5571
121.5005
115.1870
108.4278

*** Current Data Parameters ***
NAME : 7
EXPNO : 171
PROCNO : 1



N-(3'-nitro-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12e):

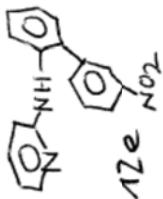




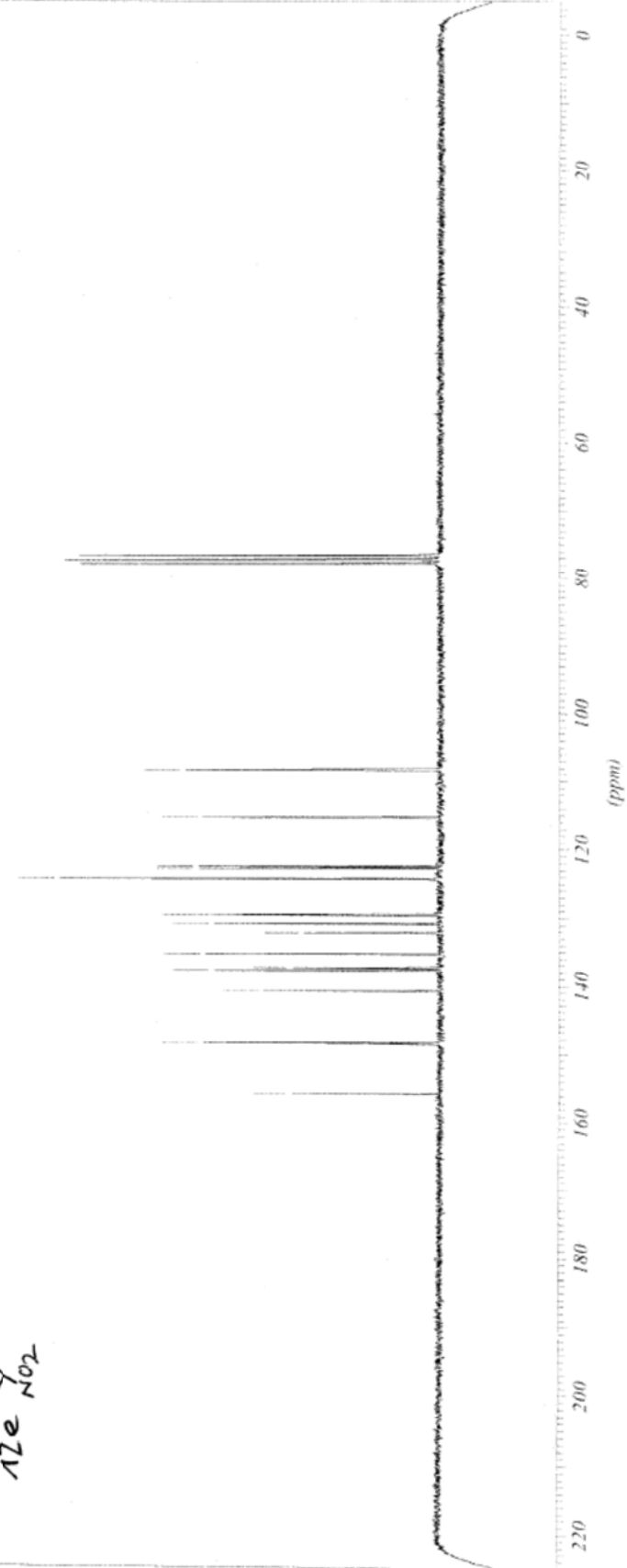
MAK 856

*** Current Data Parameters ***

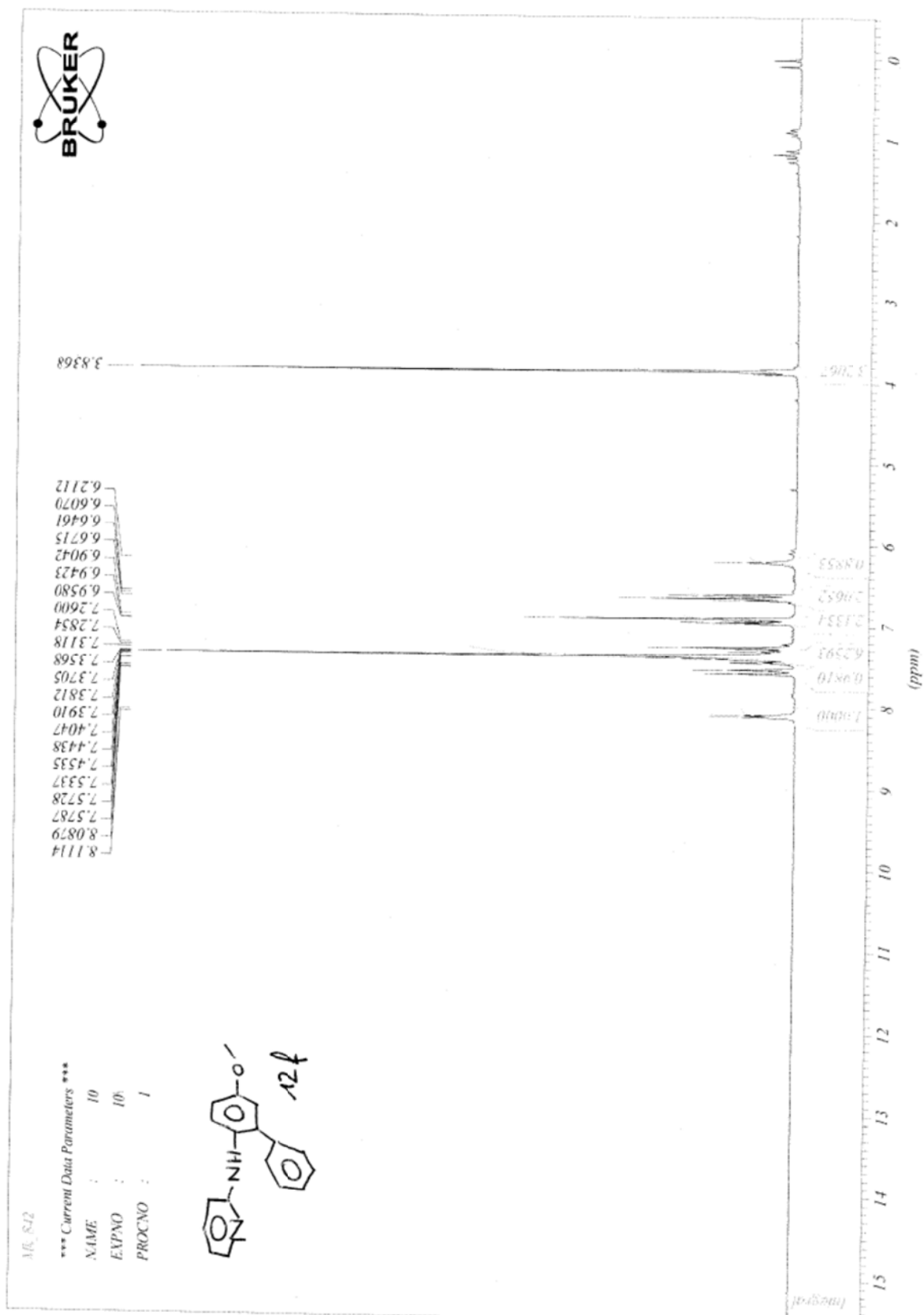
NAME : 3
EXPNO : 3
PROCNO : 1



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132.1659
130.7902
129.5689
129.4987
124.2204
122.6552
122.3674
115.3204
108.3085



N-(5-methoxy-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12f):

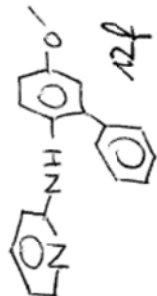




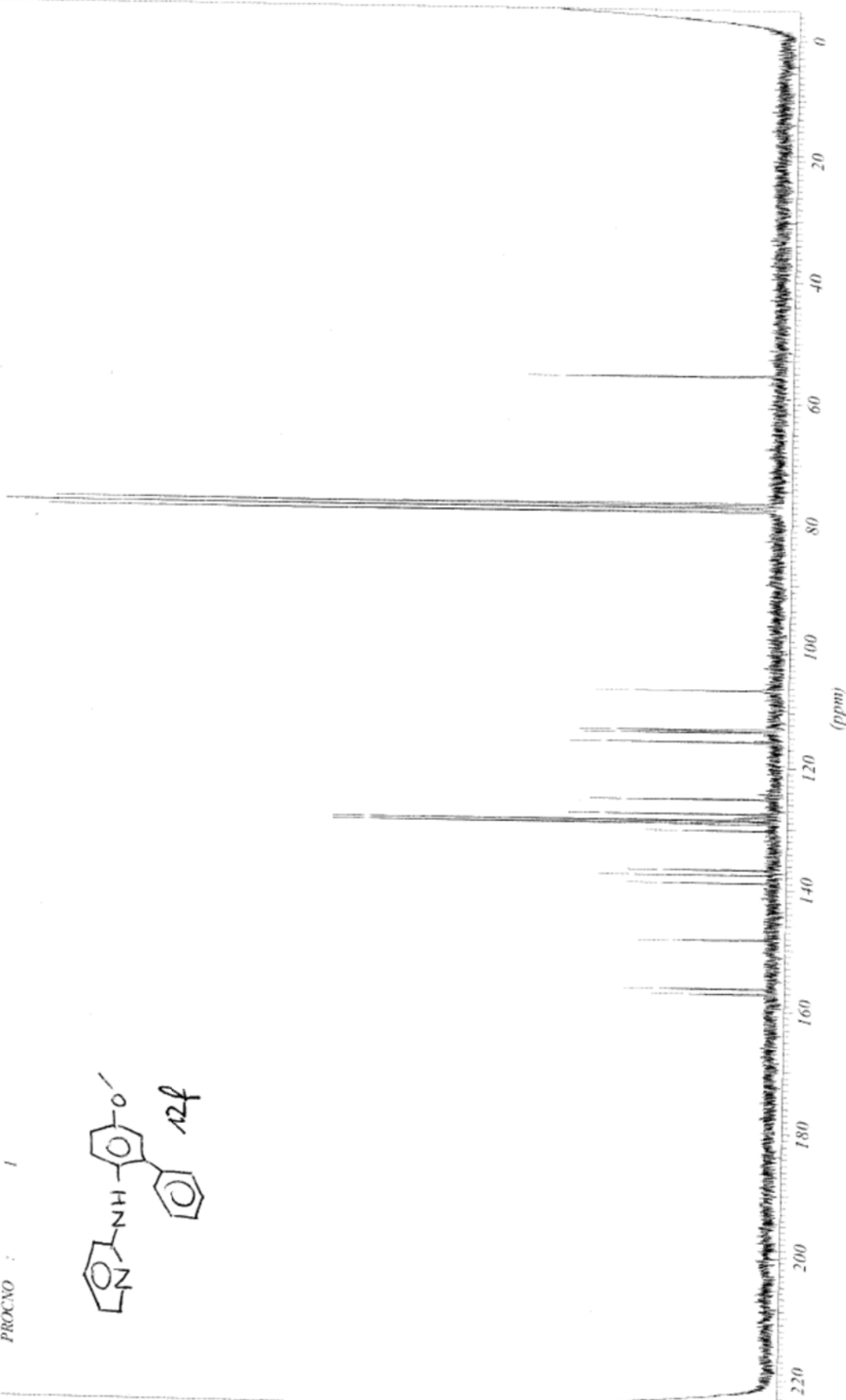
AME_8-12

*** Current Data Parameters ***

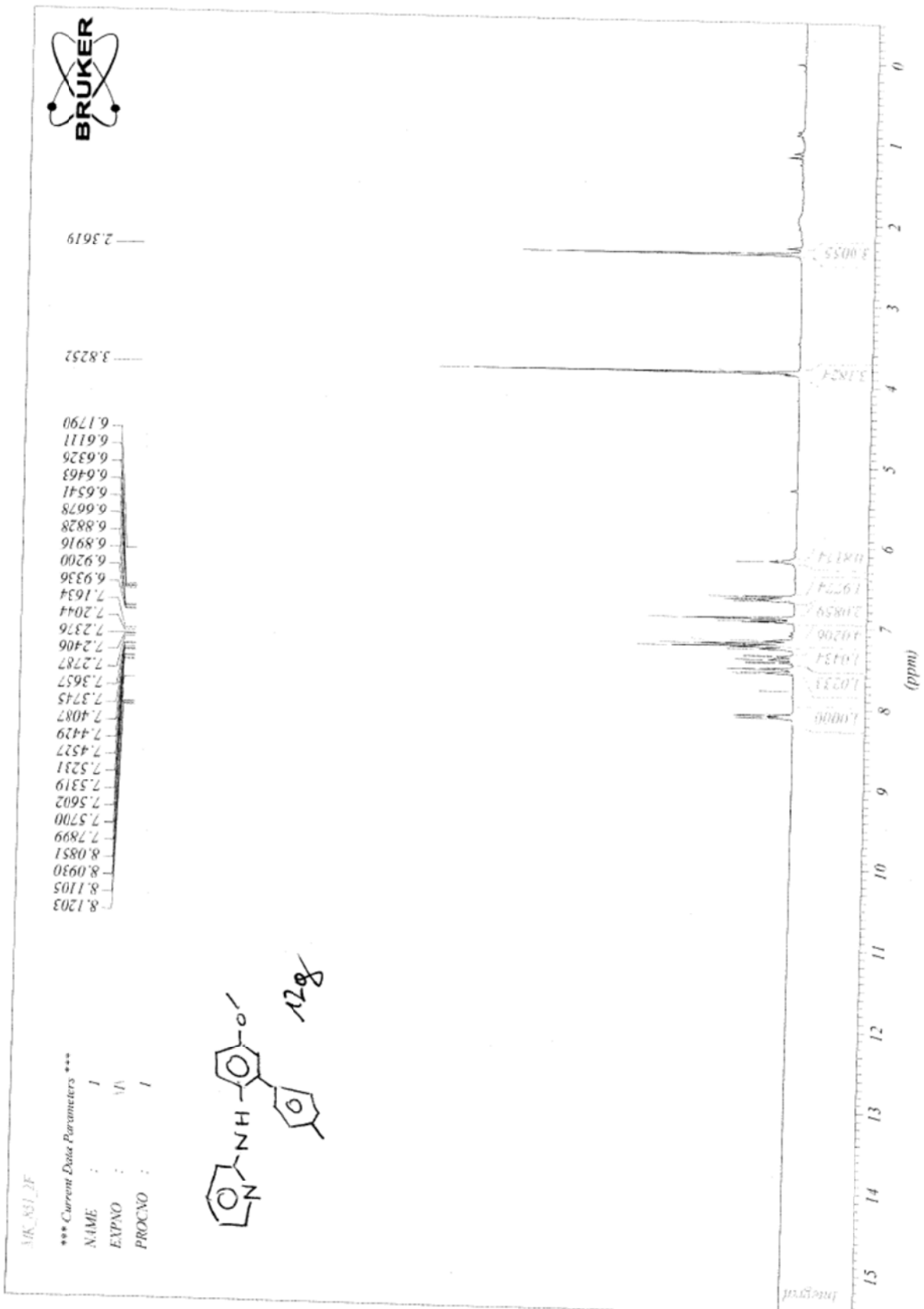
NAME : 11
EXPNO : 11
PROCNO : 1



- 157.1323
- 156.2900
- 148.1972
- 138.8479
- 137.6477
- 136.8545
- 130.1935
- 129.0635
- 128.6494
- 127.5895
- 125.1399
- 115.8258
- 114.2184
- 113.8464
- 107.4522
- 55.5891

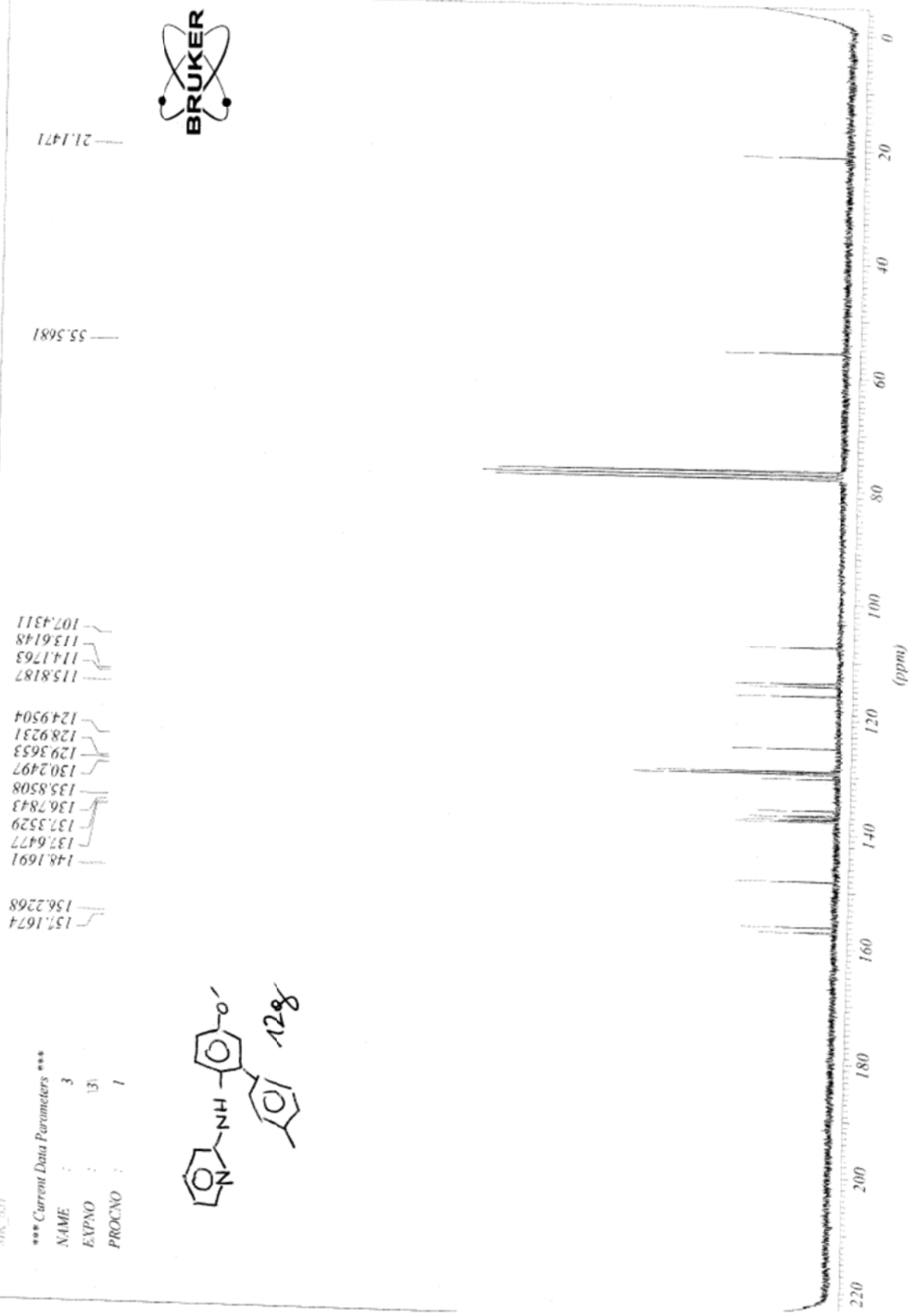
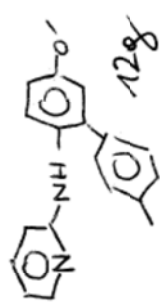


N-(5-methoxy-4'-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12g):

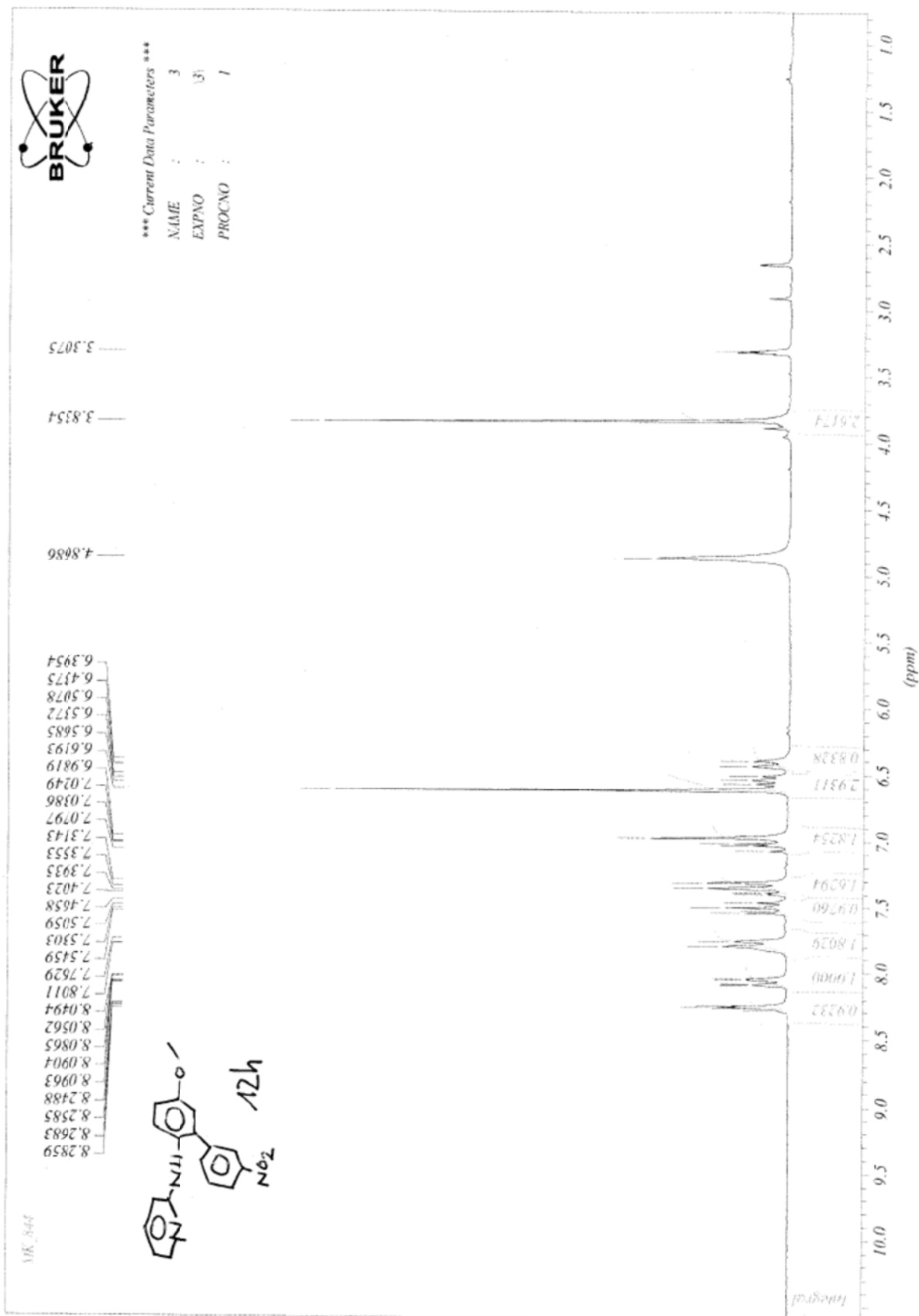


MK_551

*** Current Data Parameters ***
NAME : 3
EXPNO : 131
PROCNO : 1



N-(5-methoxy-3'-nitro-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12h):

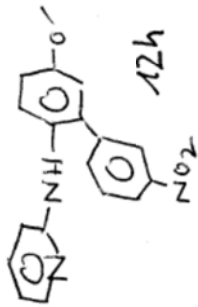




MK 844

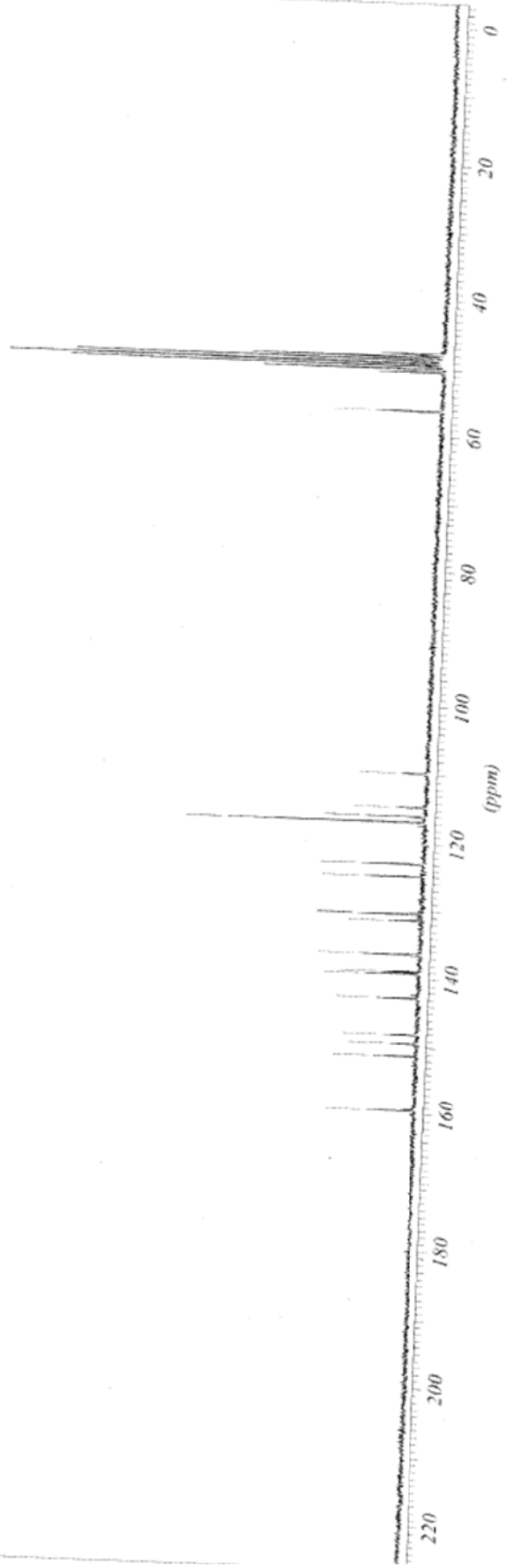
*** Current Data Parameters ***

NAME : KOSBIB-1
EXPNO : 4
PROCNO : 1



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- 149.4138
- 148.0942
- 142.7949
- 139.1942
- 138.8081
- 136.3936
- 131.2698
- 130.3713
- 130.2871
- 124.8264
- 122.9453
- 116.8388
- 116.0176
- 114.6840
- 109.7356

56.1318

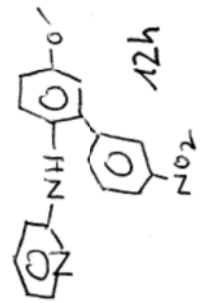




56.1318

- 159.3526
- 151.2528
- 149.4138
- 148.0942
- 142.7949
- 139.1942
- 138.8081
- 136.3936
- 131.2698
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- 124.8264
- 122.9453
- 116.8388
- 116.0176
- 114.6840
- 109.7356

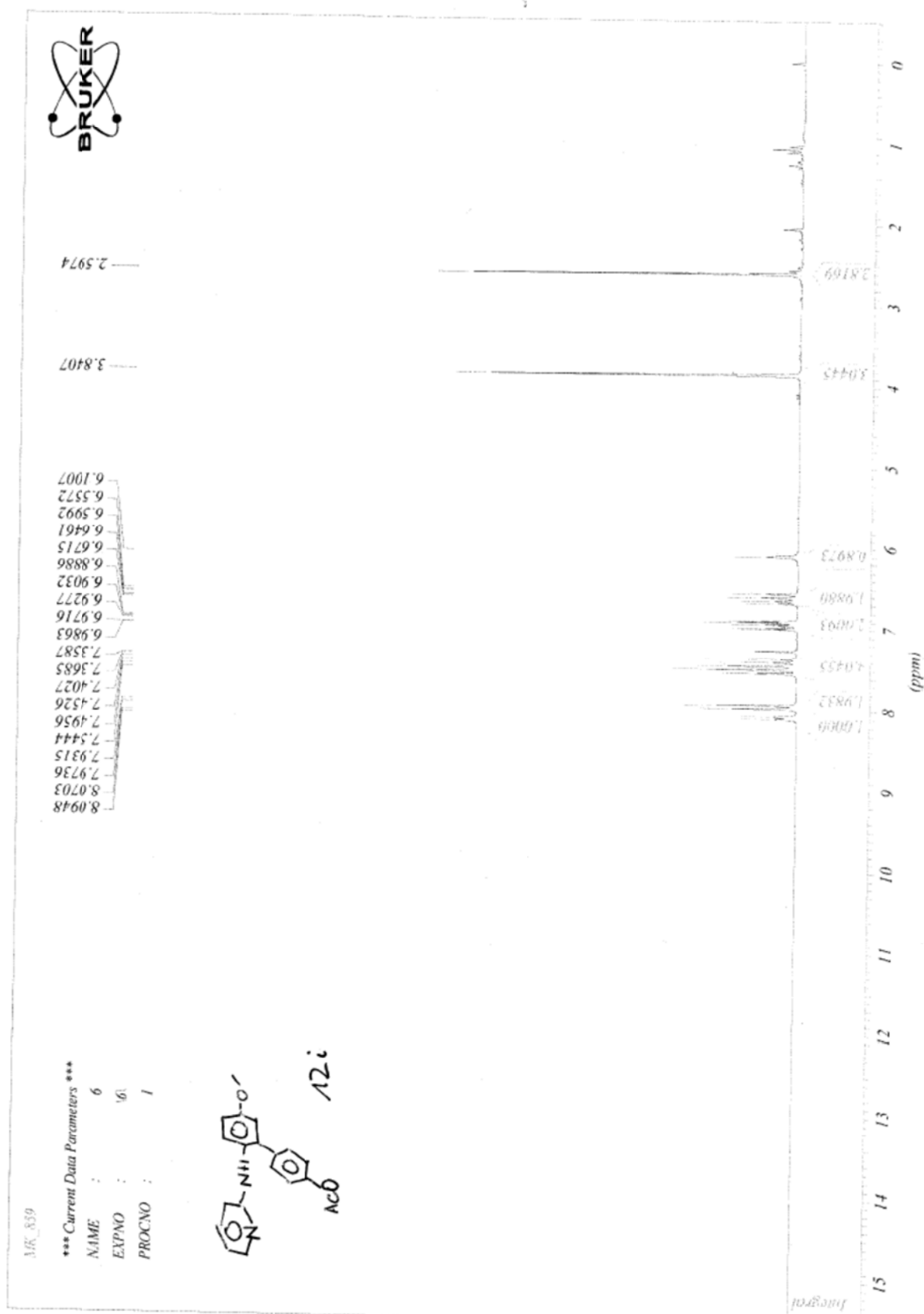
*** Current Data Parameters ***
NAME : K05B08-1
EXPNO : 4
PROCNO : 1



(ppm)



5'-Methoxy-2'-(pyridin-2-ylamino)-[1,1'-biphenyl]-4-yl acetate (12i):





26.6570

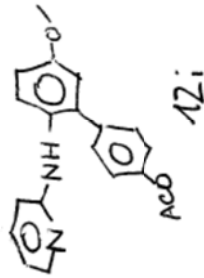
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107.1854
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126.1155
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148.4779

156.6339
157.1674

197.6667



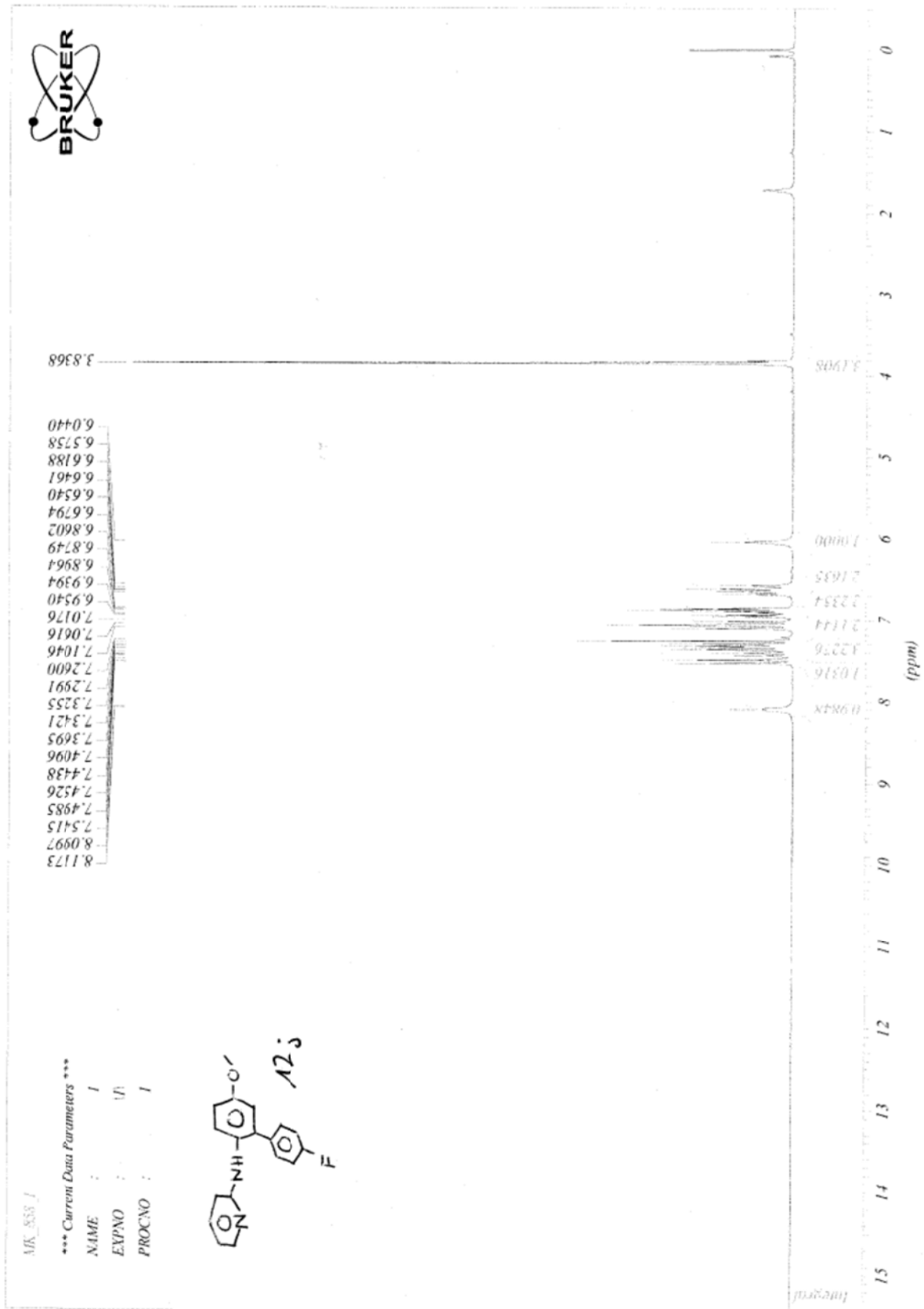
*** Current Data Parameters ***

NAME : 8
EXPNO : 181
PROCNO : 1

(ppm)

220 200 180 160 140 120 100 80 60 40 20 0

N-(4'-fluoro-5-methoxy-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12j):

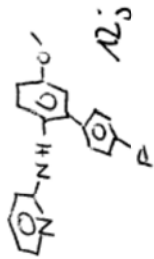




AK_858_1

*** Current Data Parameters ***

NAME : 4
EXPNO : 4
PROCNO : 1



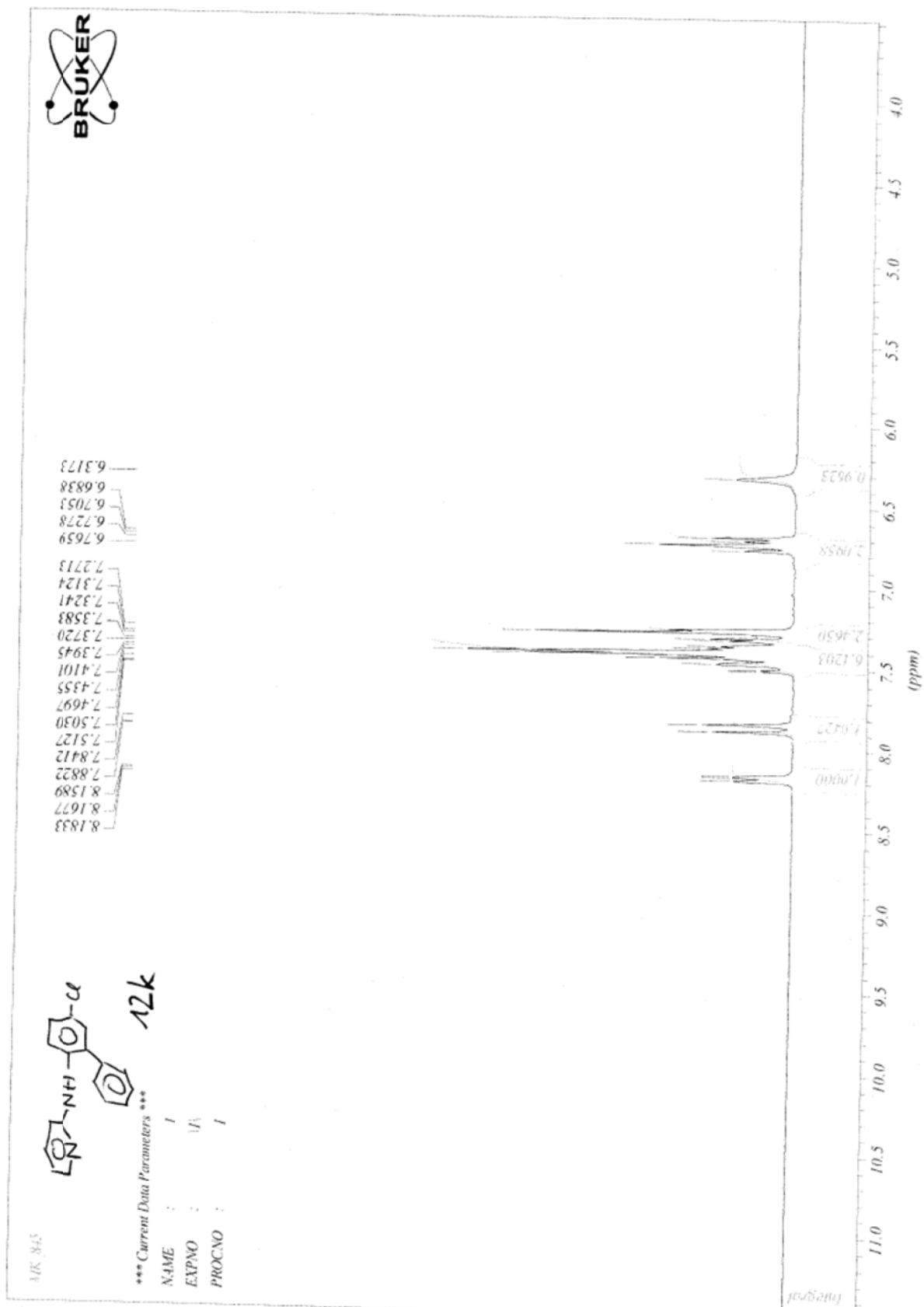
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159.8556
157.1533
156.4374
148.4288
137.6407
136.1597
134.8261
134.7629
130.8112
130.6568
130.2006
125.5681
115.8819
115.7907
115.3625
114.3377
113.9026
107.2205

55.5962

(ppm)

220 200 180 160 140 120 100 80 60 40 20 0

N-(5-chloro-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12k):

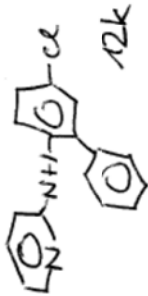




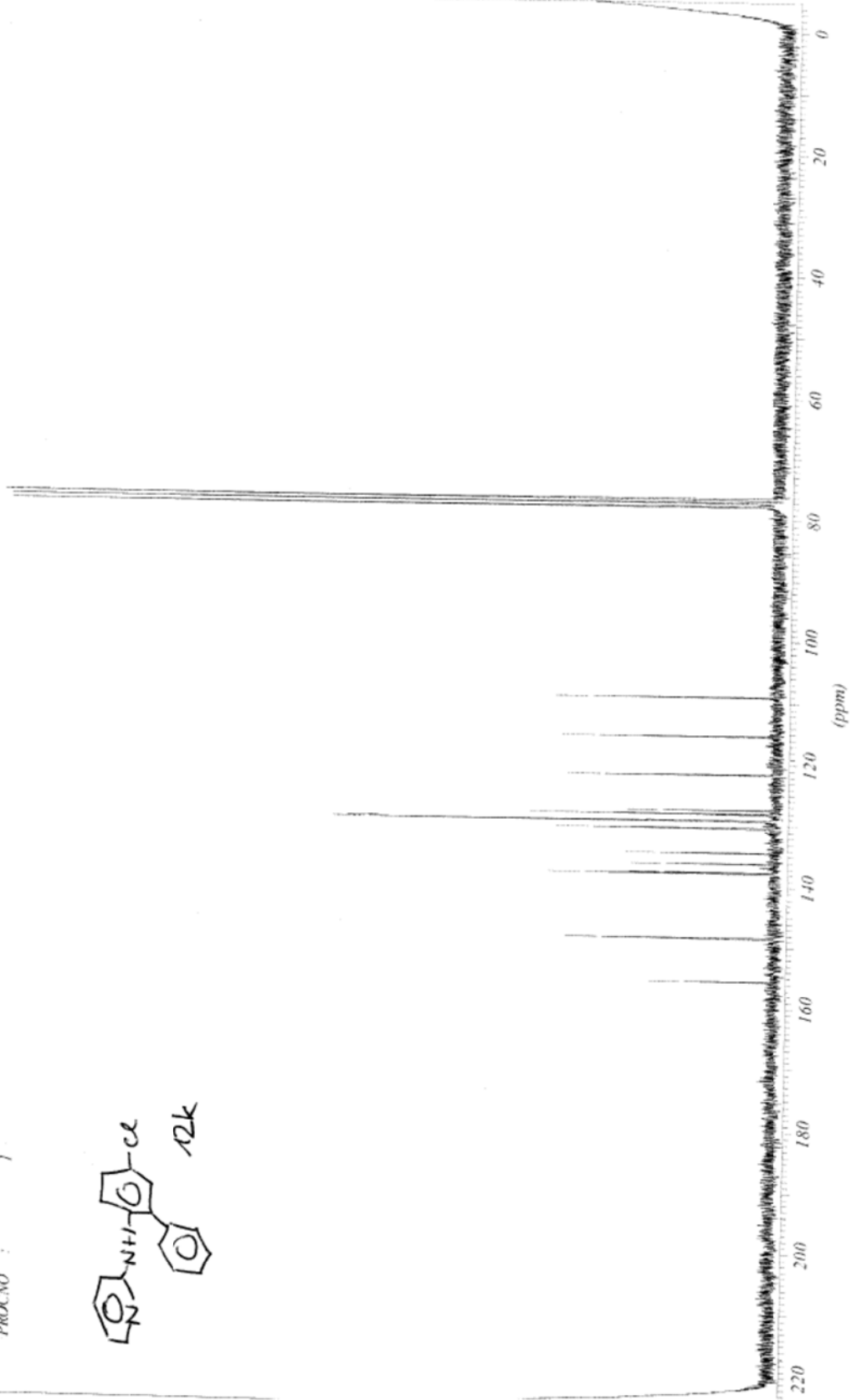
AK_845

*** Current Data Parameters ***

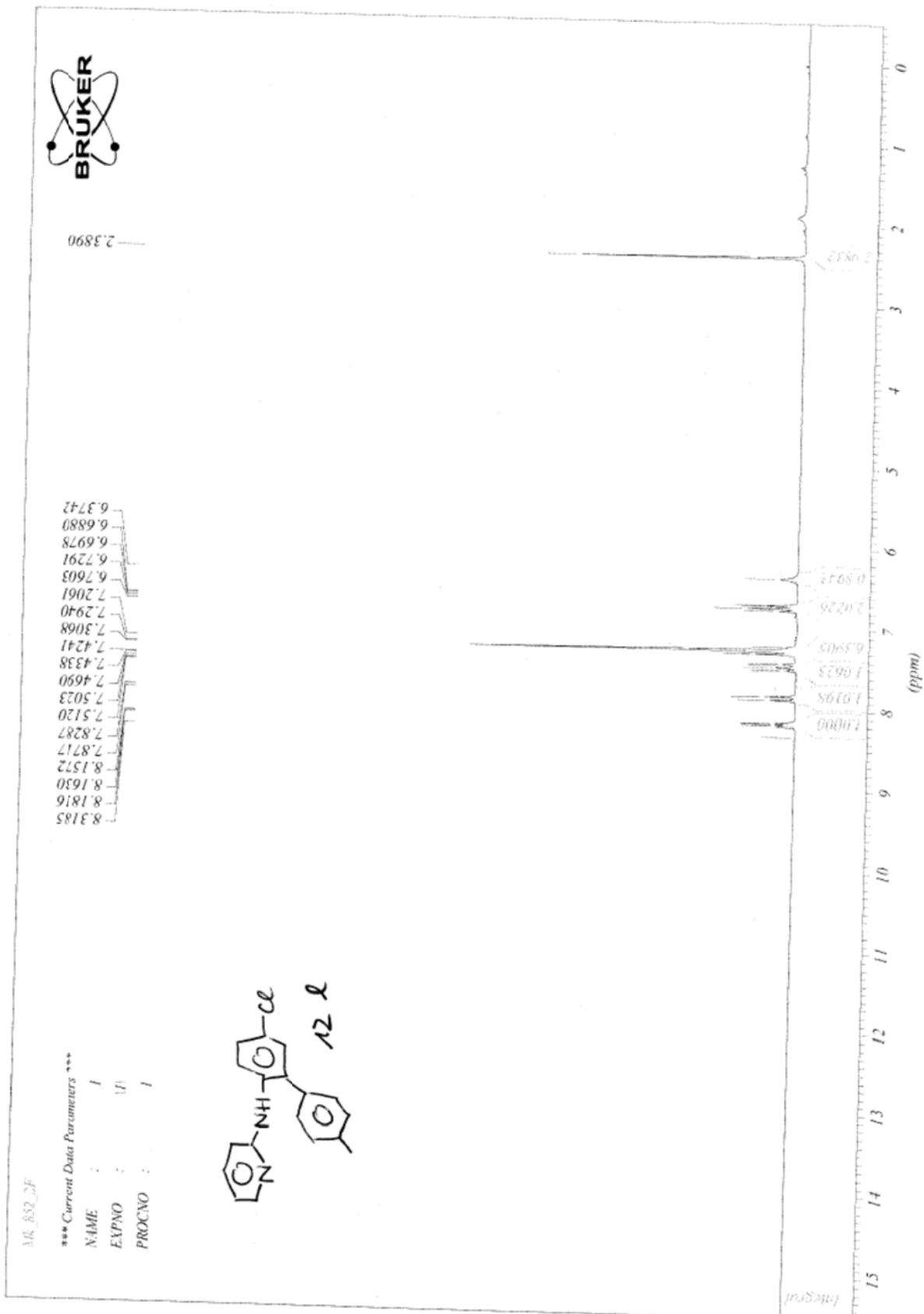
NAME : 2
EXPNO : 121
PROCNO : 1



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137.5494
136.2018
134.3909
130.3409
129.1618
129.0495
128.1019
128.0598
127.4281
121.6024
115.4327
109.0876



N-(5-chloro-4'-methyl-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12l):



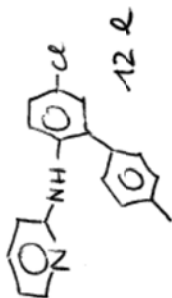
MK_851

*** Current Data Parameters ***

NAME : KOSBEZ-1

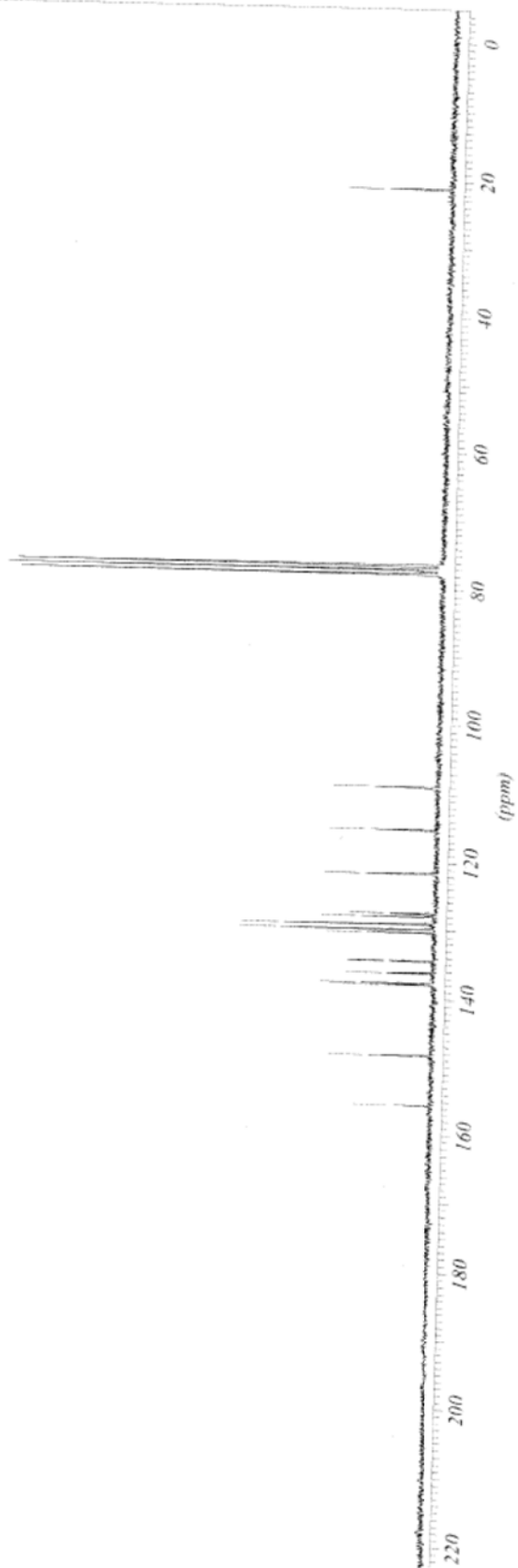
EXPNO : 2

PROCNO : 1

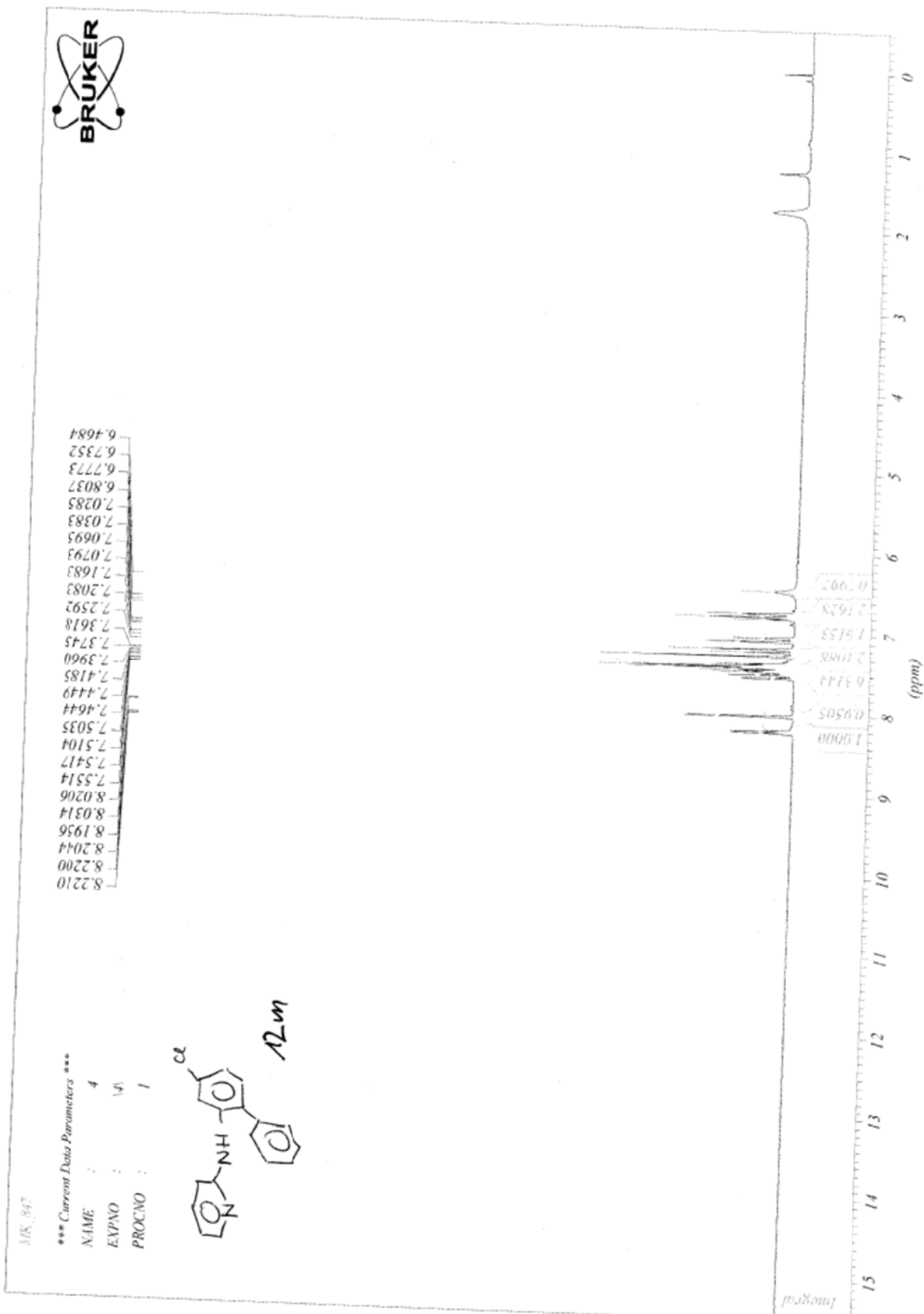


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137.9284
137.7038
136.2018
134.5242
134.4470
130.2988
129.7303
129.0003
127.8282
127.4000
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115.3134
109.0595

21.1822



N-(4-chloro-[1,1'-biphenyl]-2-yl)pyridin-2-amine (12m):

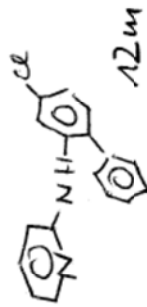




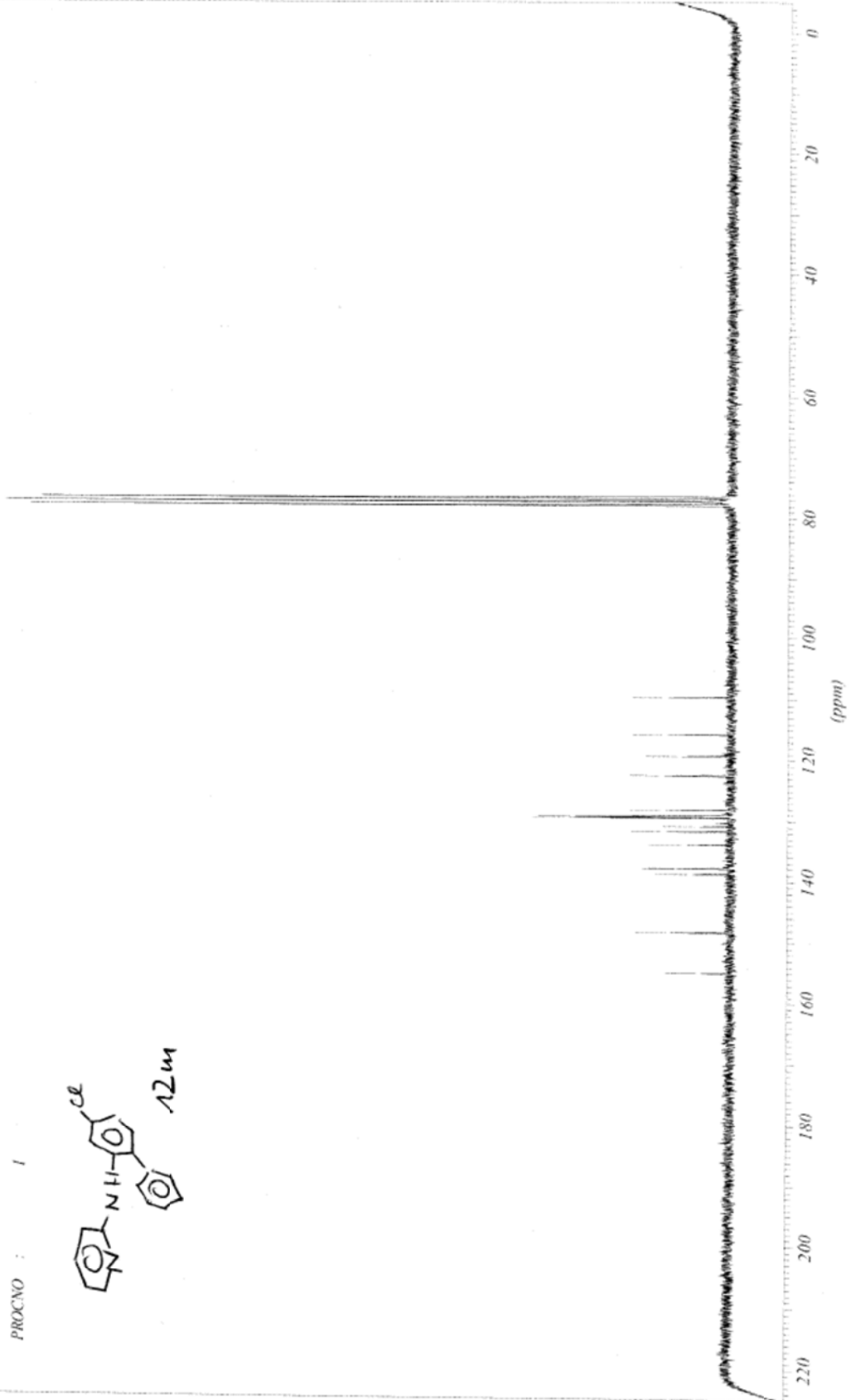
MR_847

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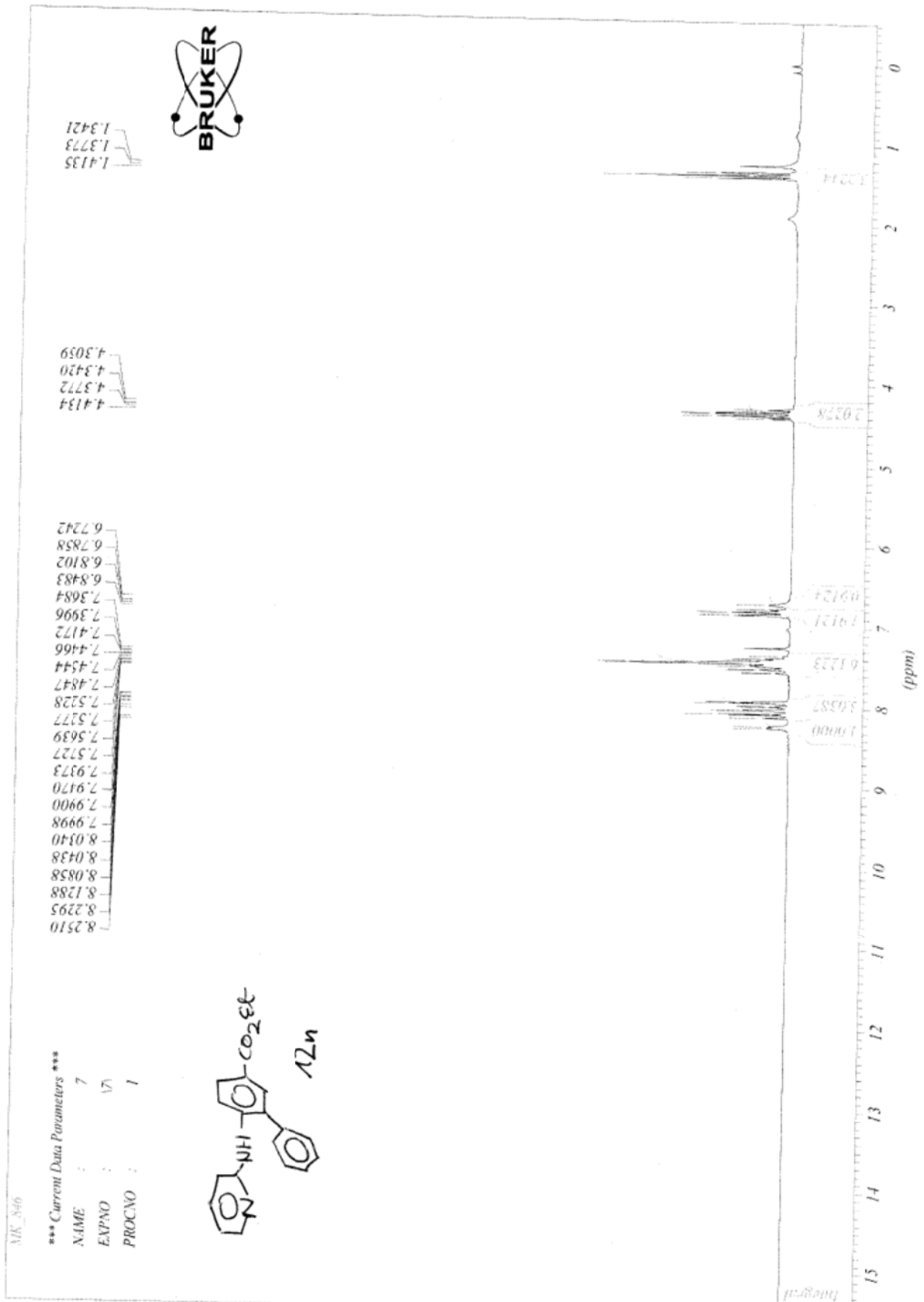
NAME : 5
EXPNO : (5)
PROCNO : 1



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129.2881
129.0775
127.9405
122.2832
119.2791
115.7486
109.6421



Ethyl 6-(pyridin-2-ylamino)-[1,1'-biphenyl]-3-carboxylate (12n):



PCL XL Error

Subsystem:
Error:
Operator:
Position:



I/O
InputReadError
ReadChar
12285

14.4019

60.6709

110.6317

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117.0751

123.3220

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130.8603

132.0957

137.8091

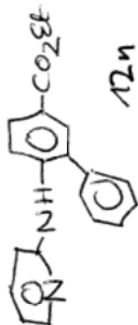
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154.4230

166.3973

*** Current Data Parameters ***
NAME : 8
EXPNO : 8
PROCNO : 1



(ppm)

0

20

40

60

80

100

120

140

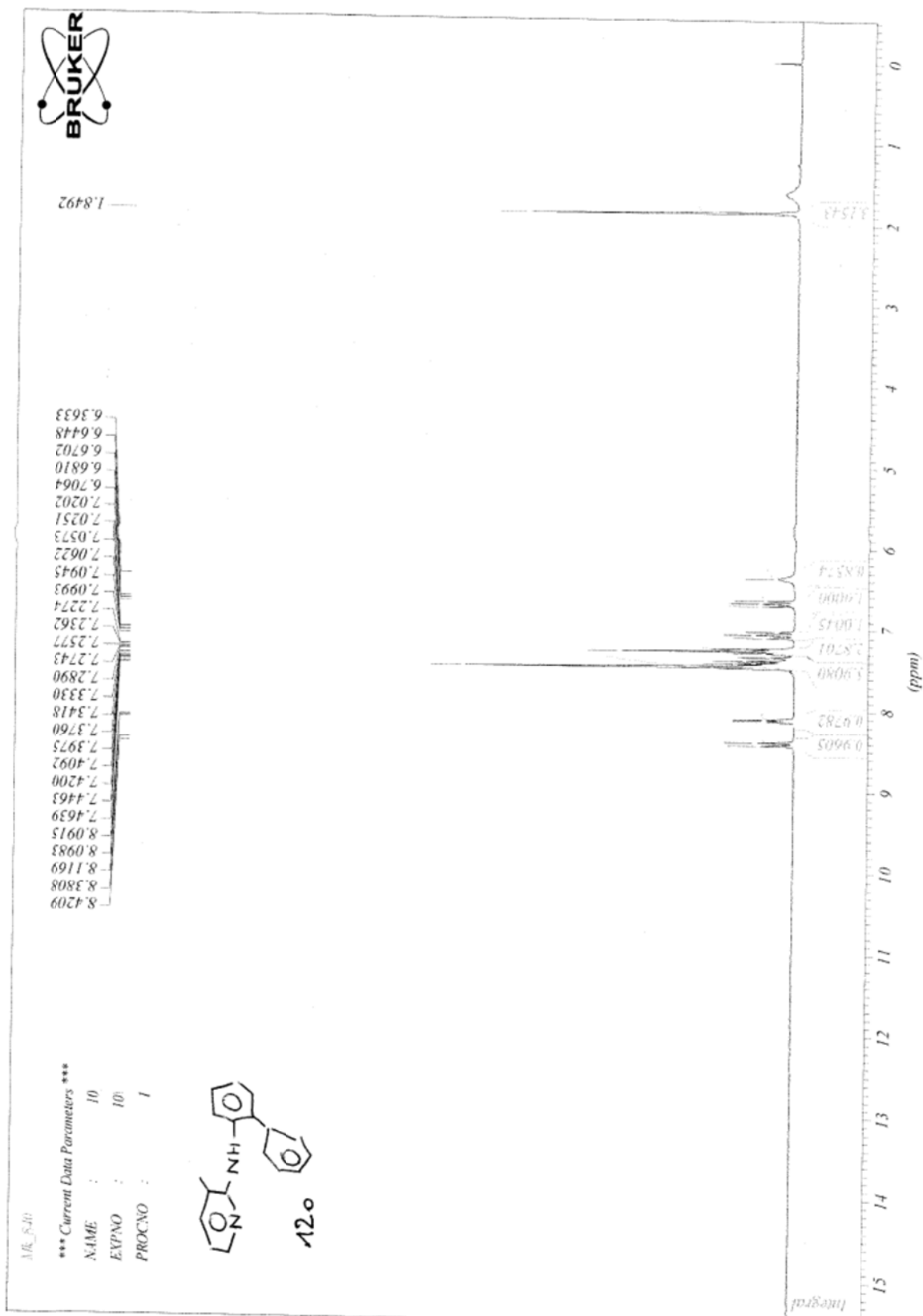
160

180

200

220

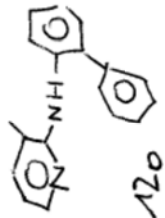
N-([1,1'-biphenyl]-2-yl)-3-methylpyridin-2-amine (12o):



MR_S40

*** Current Data Parameters ***

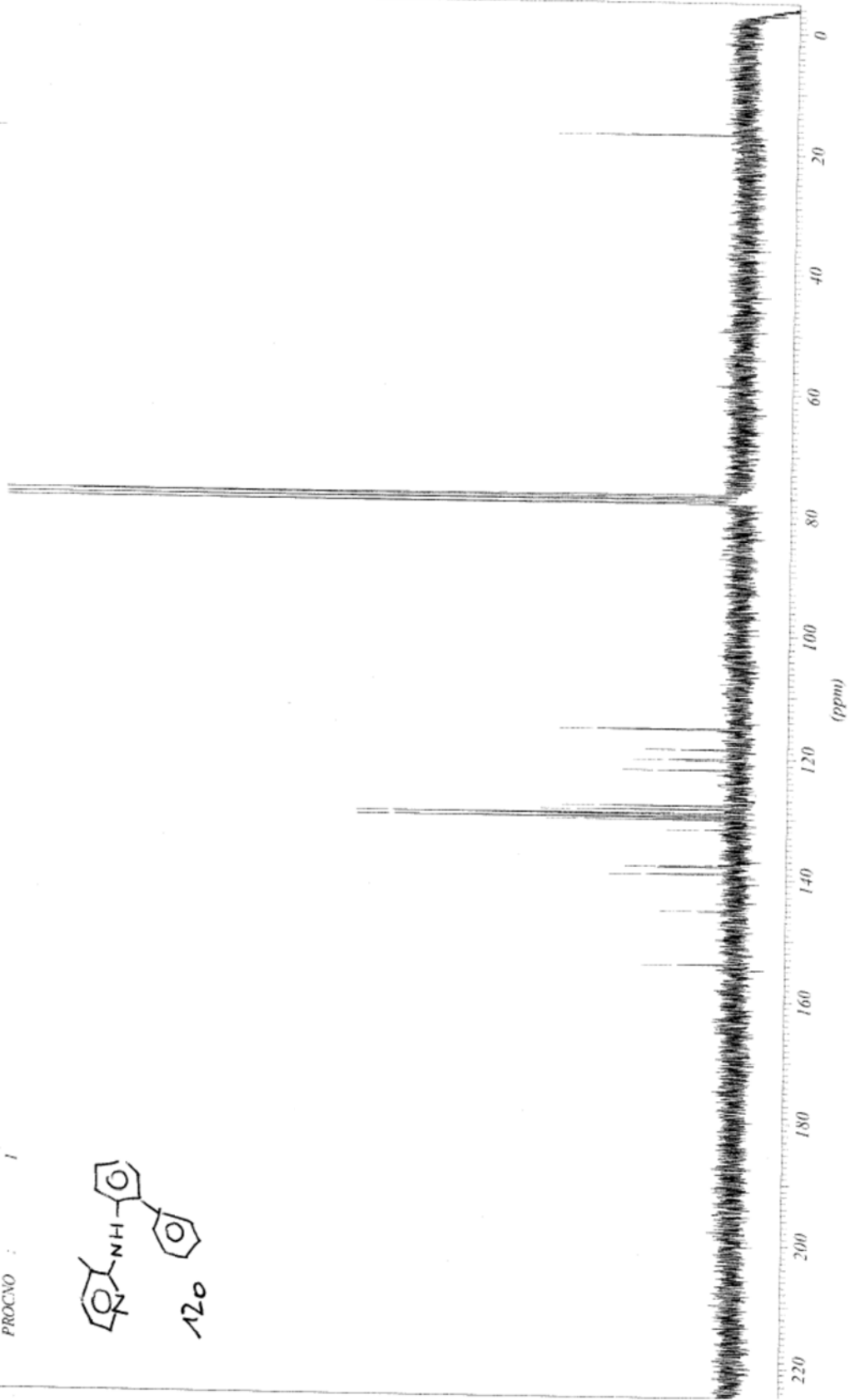
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EXPNO : 111
PROCNO : 1



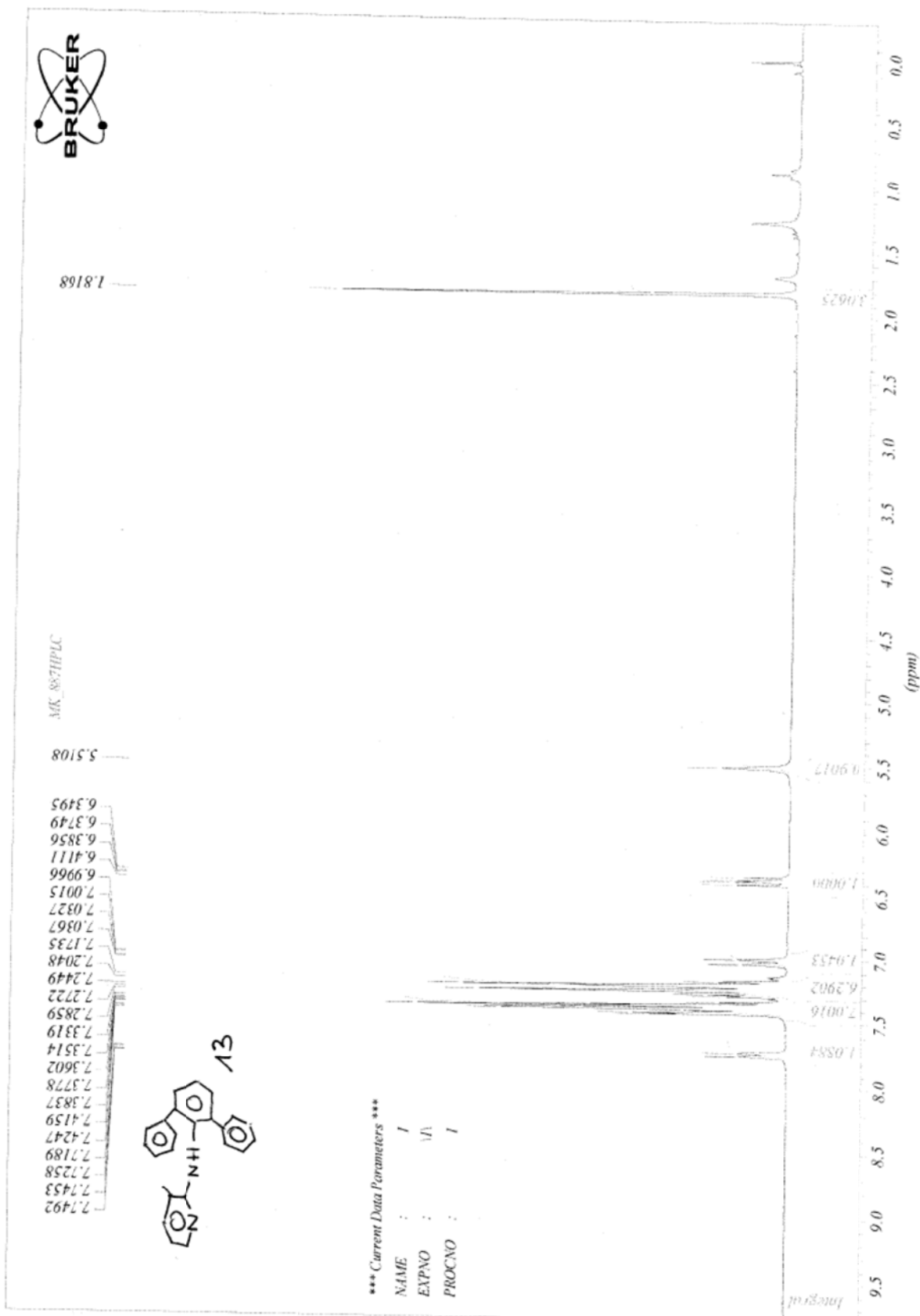
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139.0374
137.7530
131.6324
129.8917
129.4425
128.9512
128.2844
127.6597
121.7076
119.9740
118.4859
115.0677



16.9428



N-([1,1':3',1''-terphenyl]-2'-yl)-3-methylpyridin-2-amine (13):



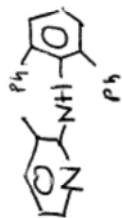
MK_880-1PLC

*** Current Data Parameters ***

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EXPNO : 21

PROCNO : 1



13

