Electronic Supplementary Material (ESI) for RSC Advances.

Structural Tuning Enables Piezochromic and Photochemical Properties in *N*-Aryl-β-Enaminones

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Supporting Information

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Piezochromic behavior of the synthesized *N*-aryl-β-enaminones

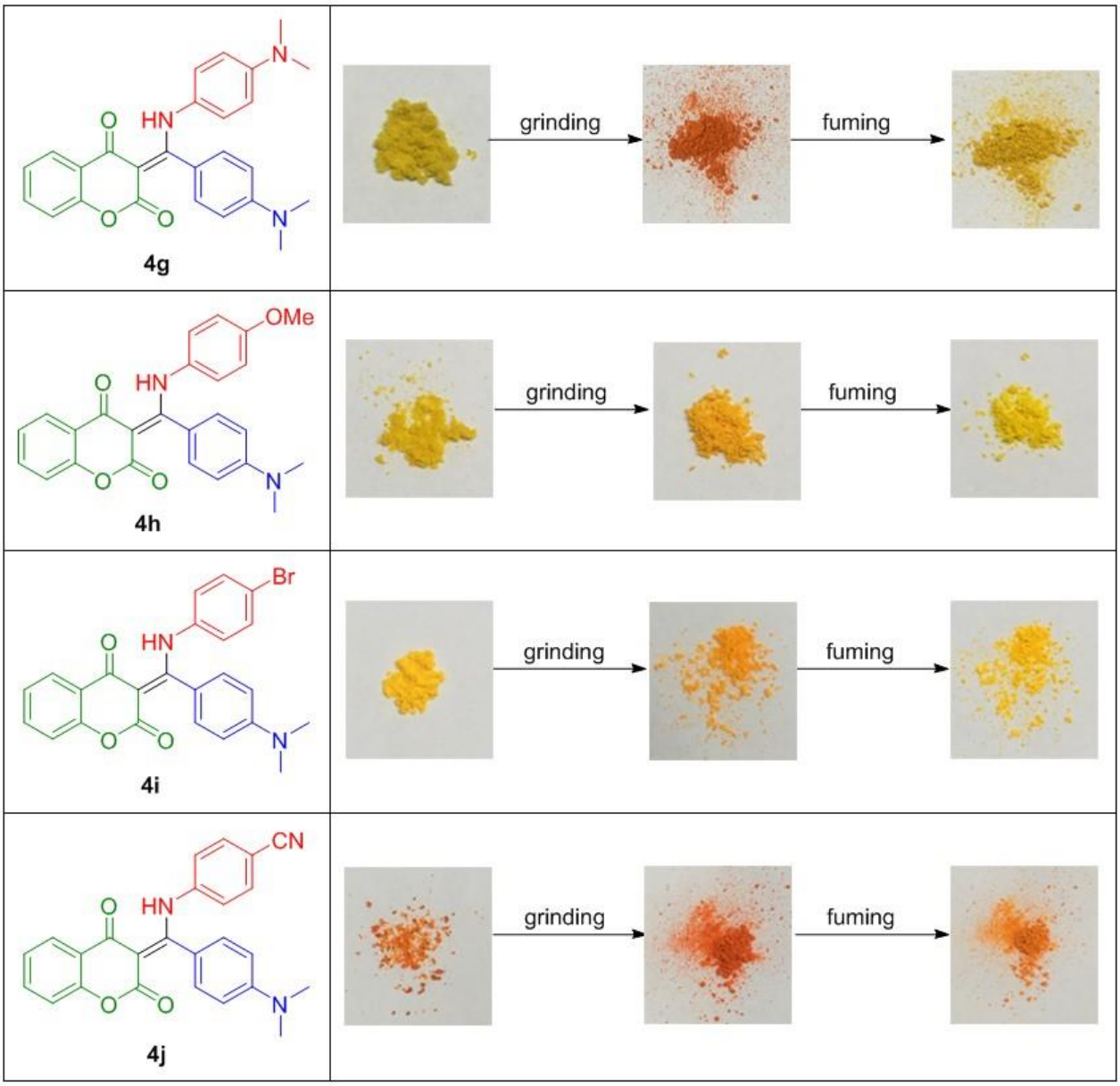
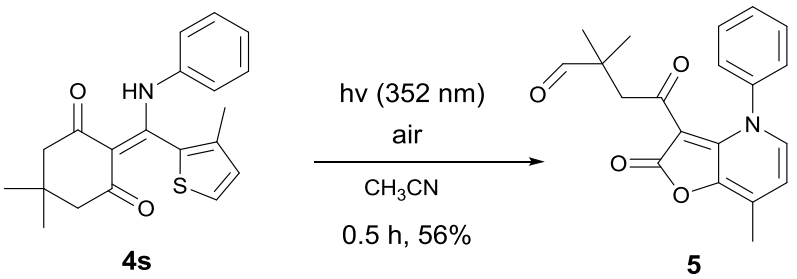


Figure S1. Color transition of the synthesized *N*-aryl-β-enaminones during grinding and fuming.

Photochemical reaction of *N*-aryl-β-enaminone 4s



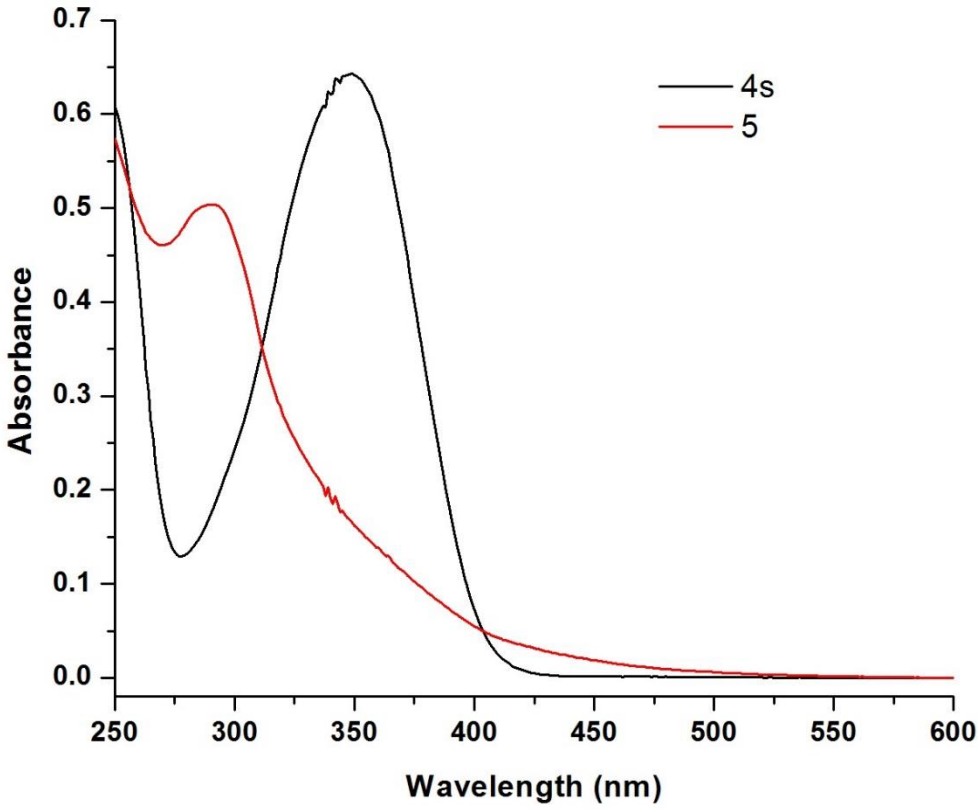
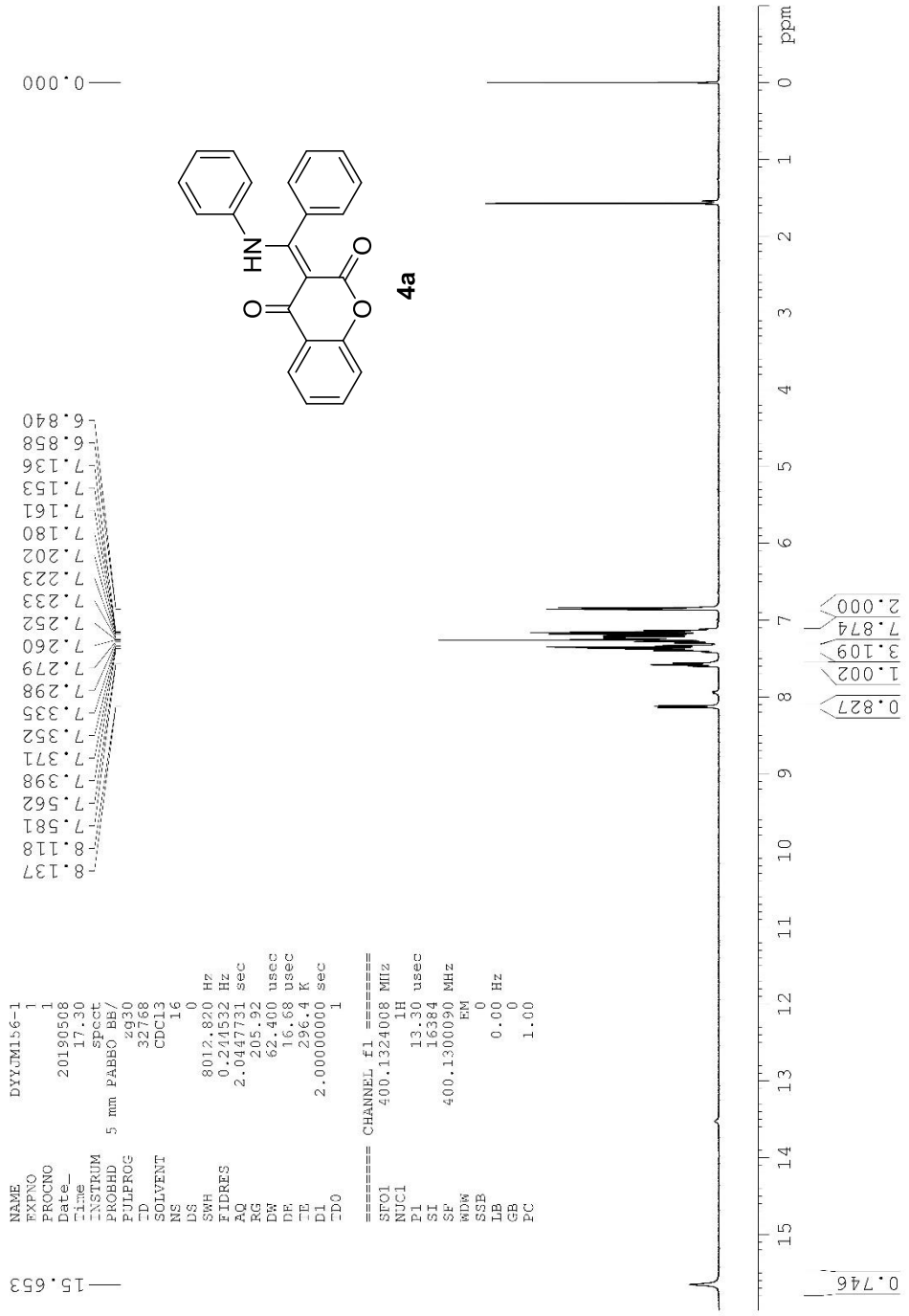


Figure S2. Absorption spectra of compounds **4s** and **5** (3.0×10^{-5} M in CH_3CN)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DE 16.68 usec
TE 296.4 K
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SI 16384
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LB 0.00 Hz
GB 0
PC 1.00
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7.398
7.371
7.352
7.335
7.298
7.279
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7.233
7.223
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7.180
7.161
7.153
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2.000
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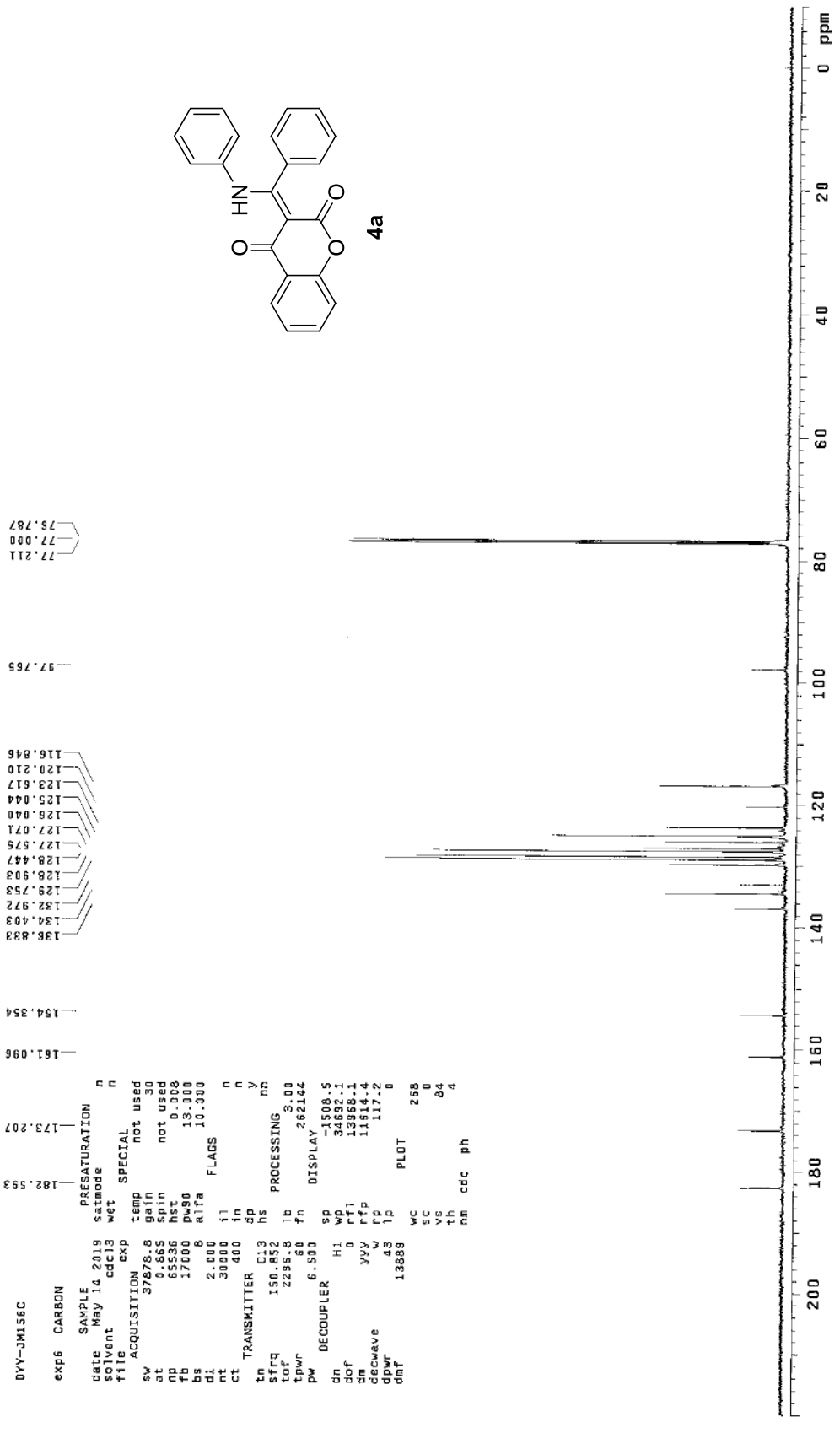
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tof 2295.8
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dmf 13889
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spin not used
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sc 0
vs 84
th 4
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161.096
154.354
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132.972
129.753
128.903
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123.617
120.210
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100
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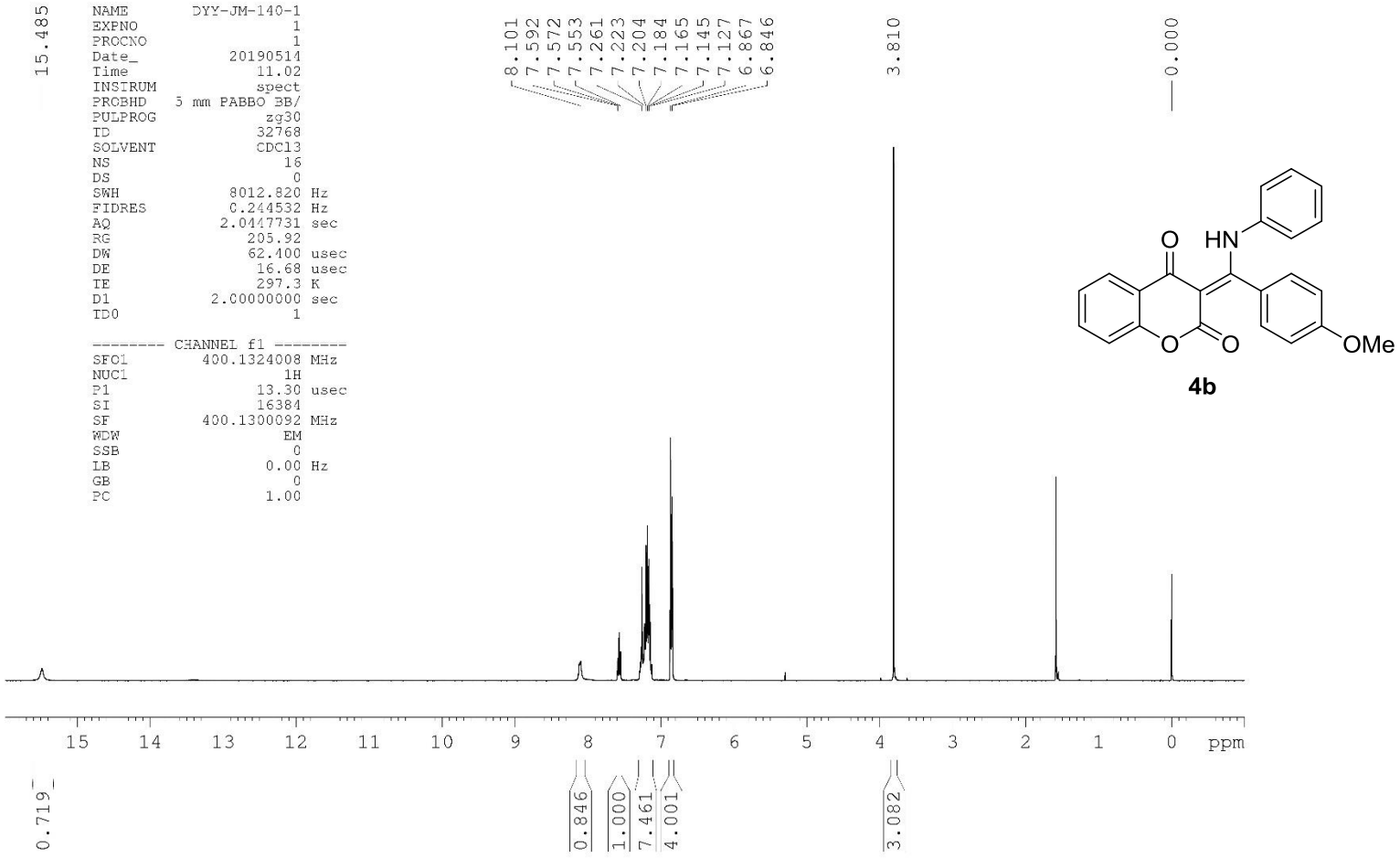
20
0 ppm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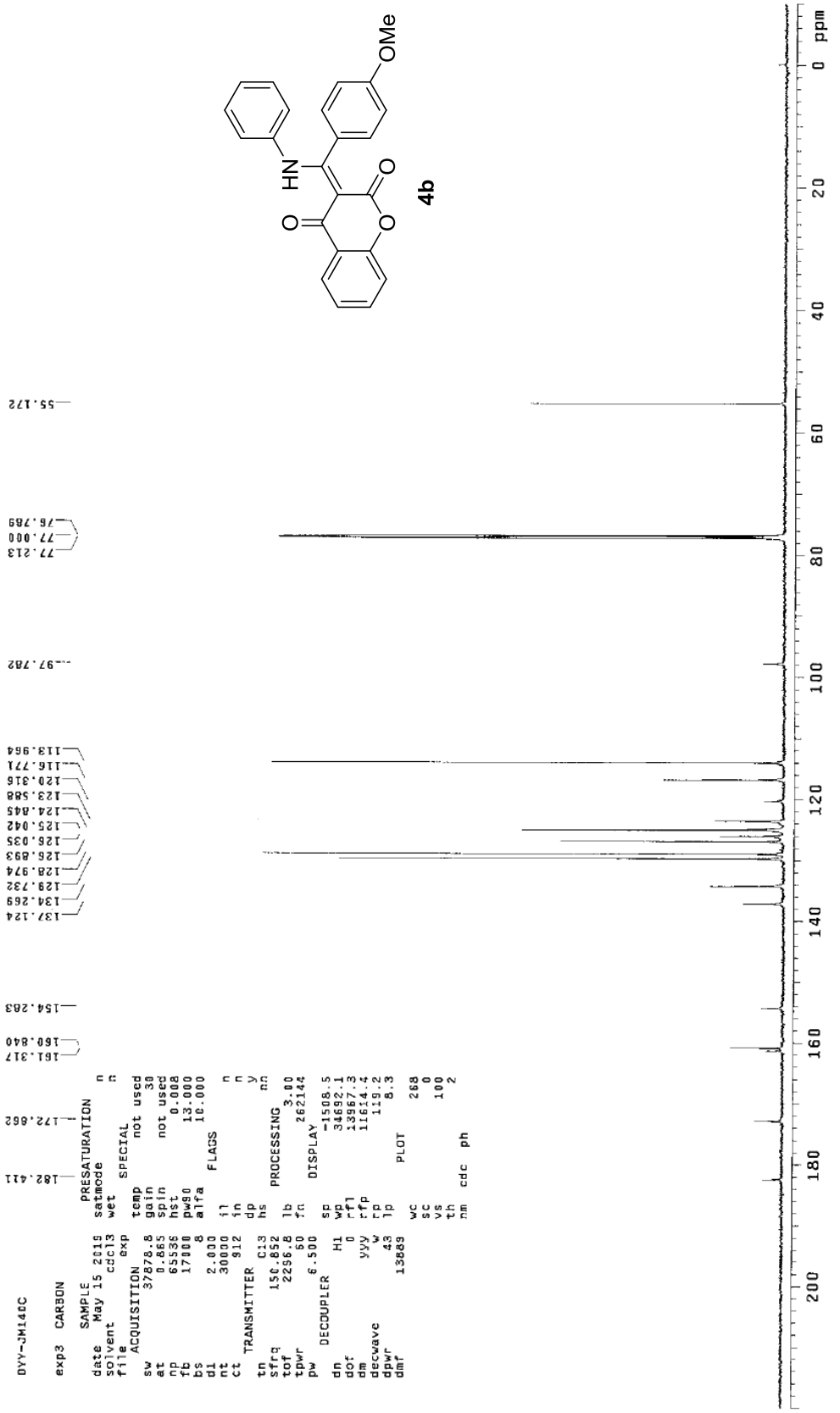
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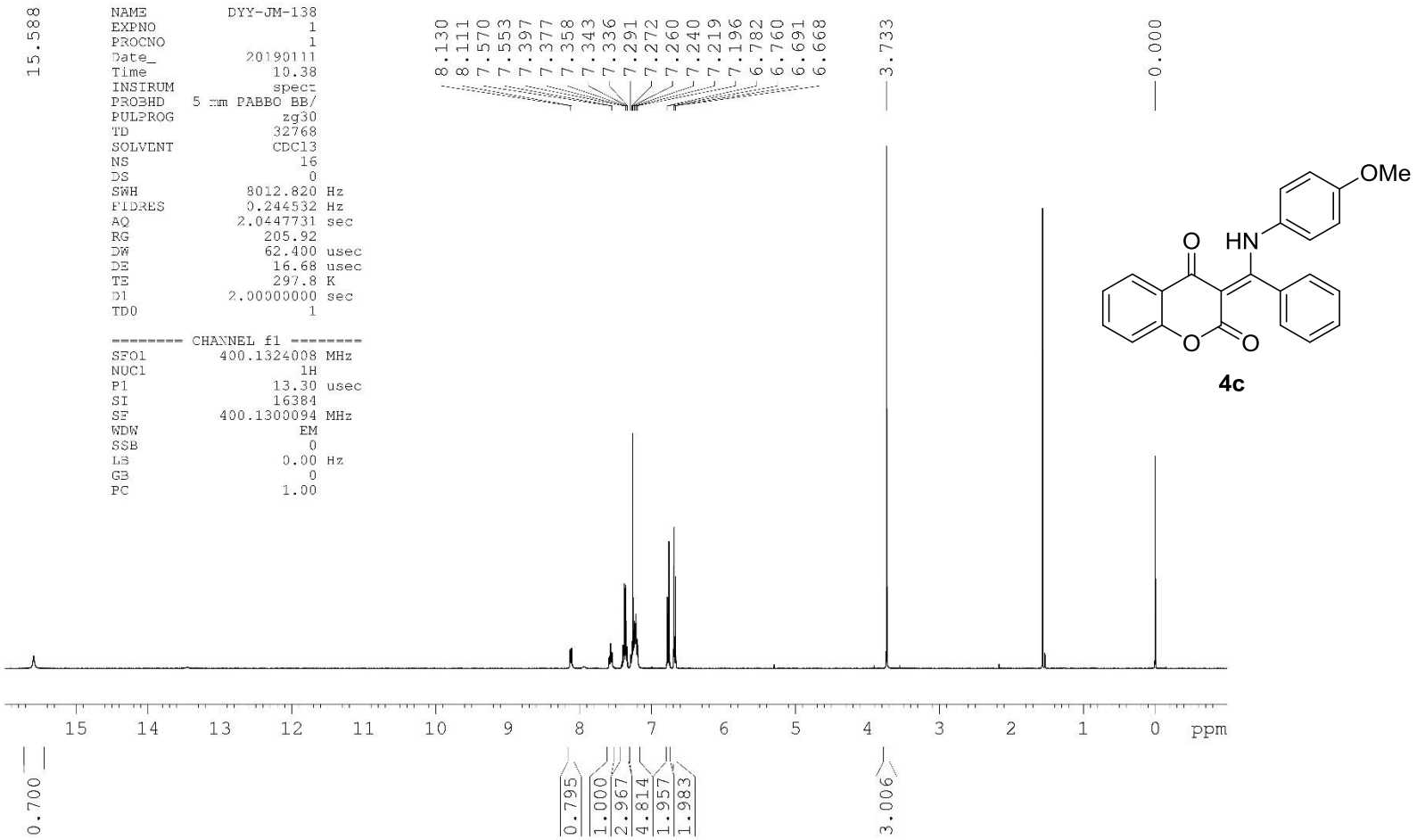
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SI 16384
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LB 0.00 Hz
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6.668
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HN
O
O
O
4c
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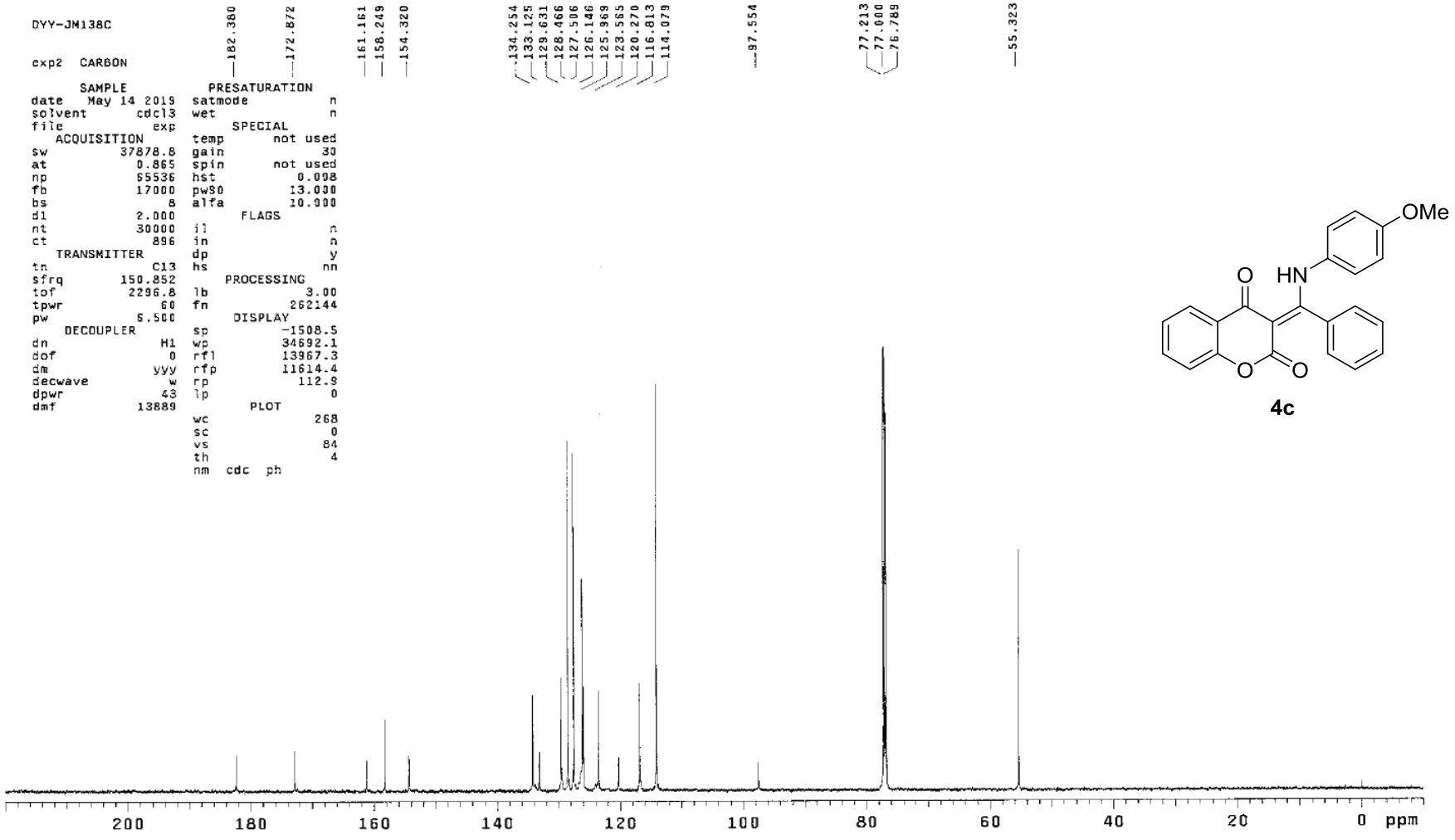
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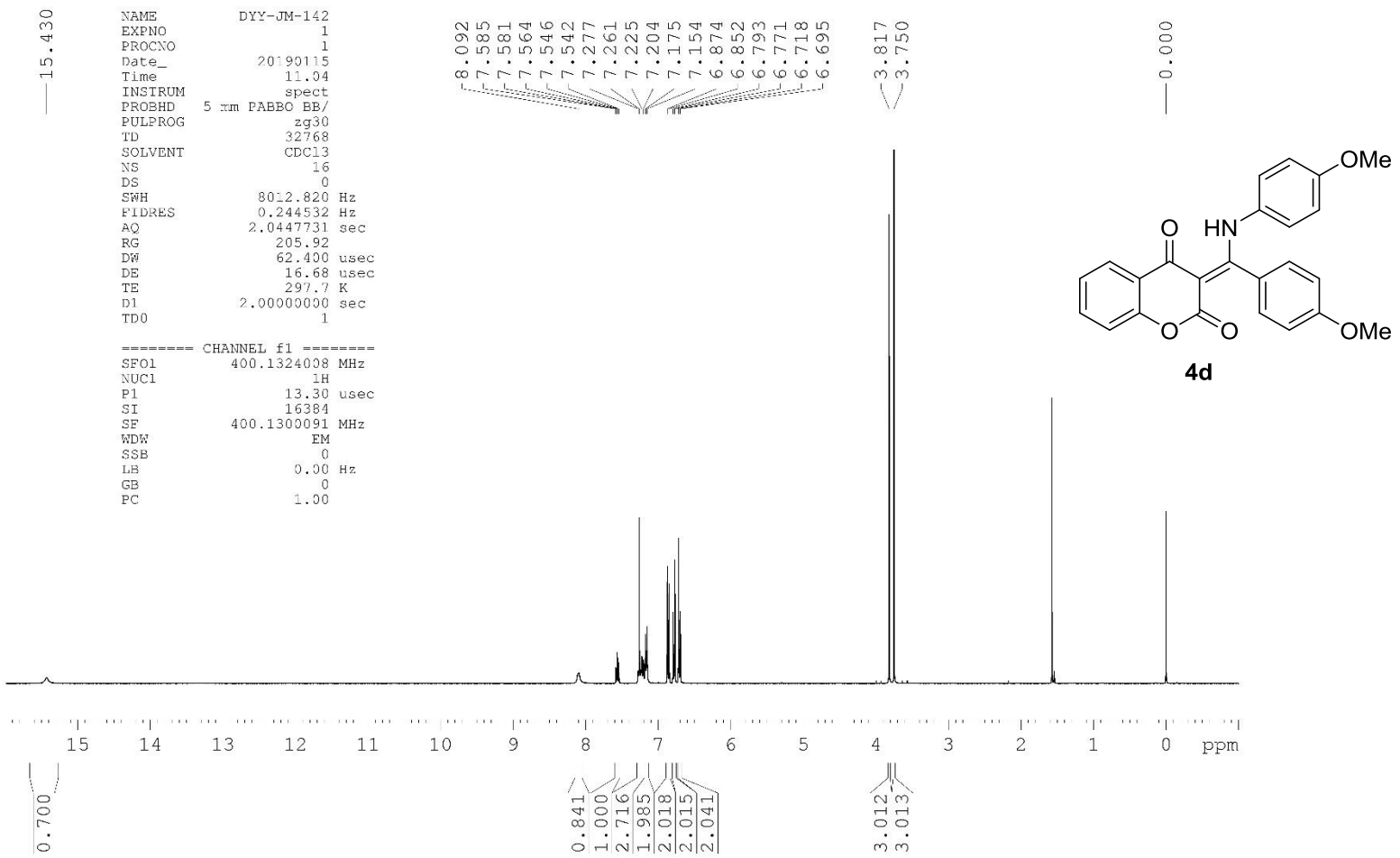
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RG 205.92
DW 62.400 usec
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SF 400.1300091 MHz
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SSB 0
LB 0.00 Hz
GB 0
PC 1.00
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HN
O
O
O
O
OMe
4d
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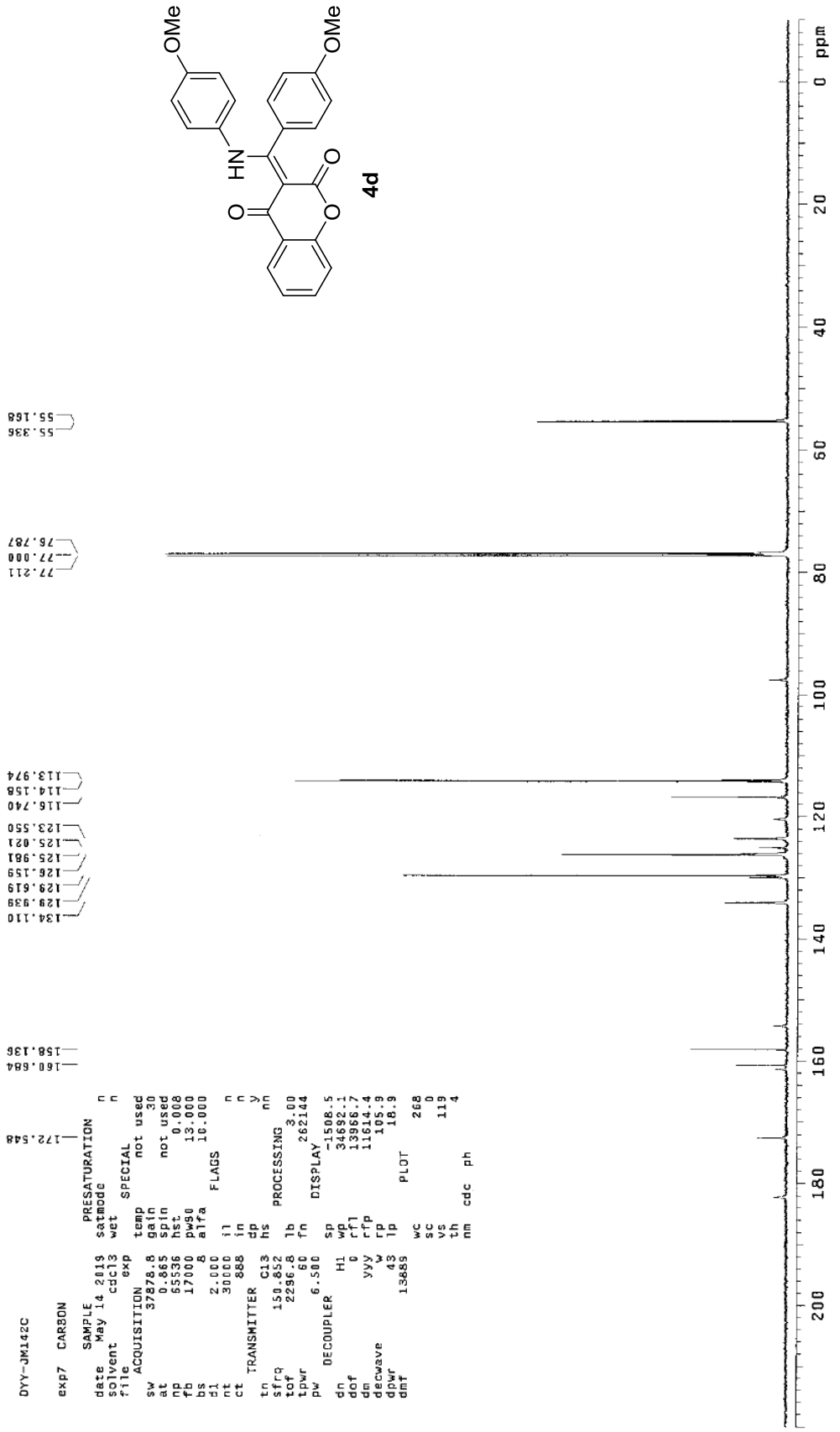
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O
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4d
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date May 14 2019
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113.974
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20
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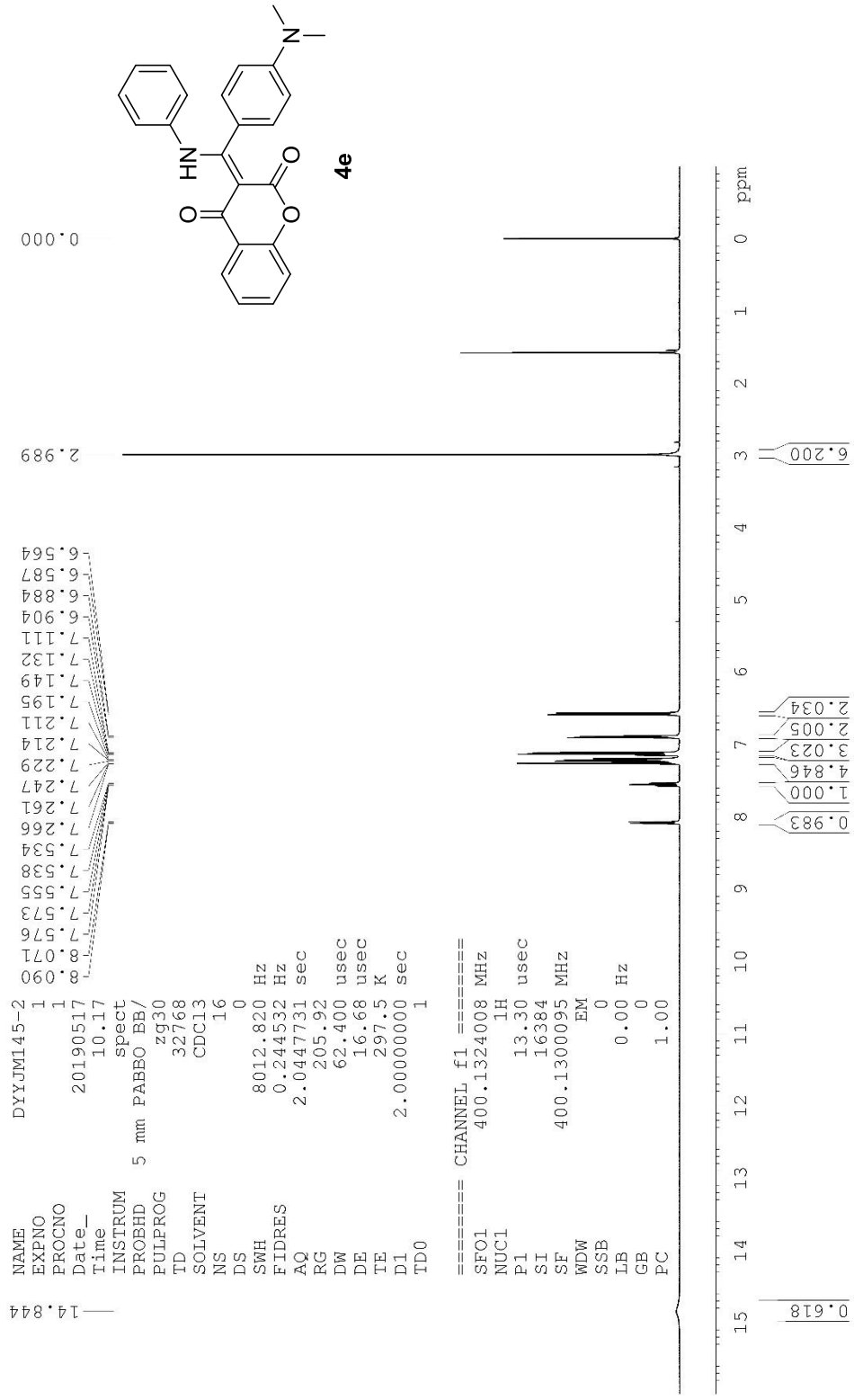
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SI 16384
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LB 0.00 Hz
GB 0
PC 1.00
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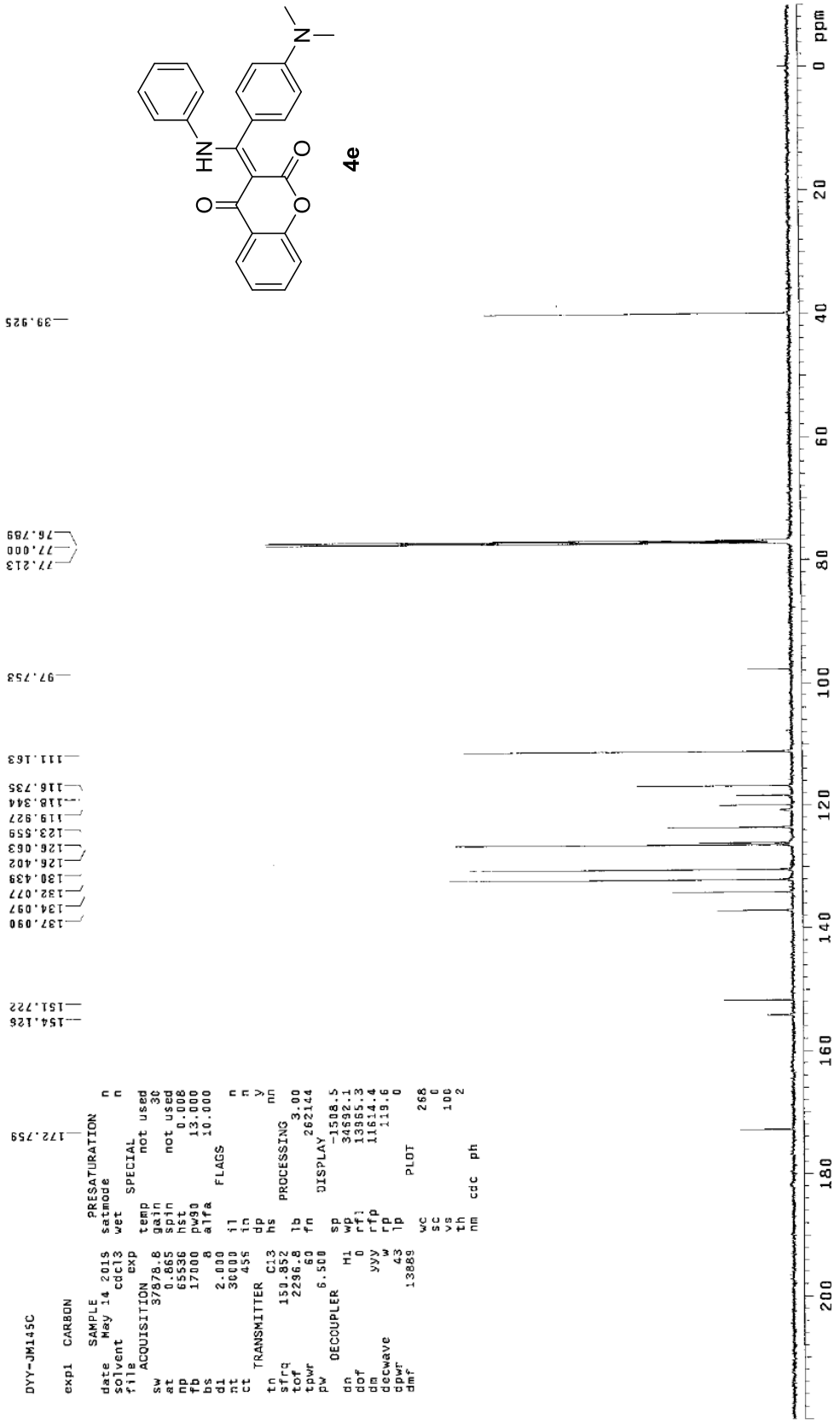
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tn C13
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tof 2296.8
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pw 6.500
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decwave w
dpwr 43
dmf 13889
PRESATURATION
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wet n
SPECIAL
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spin not used
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in n
dp y
hs nn
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20
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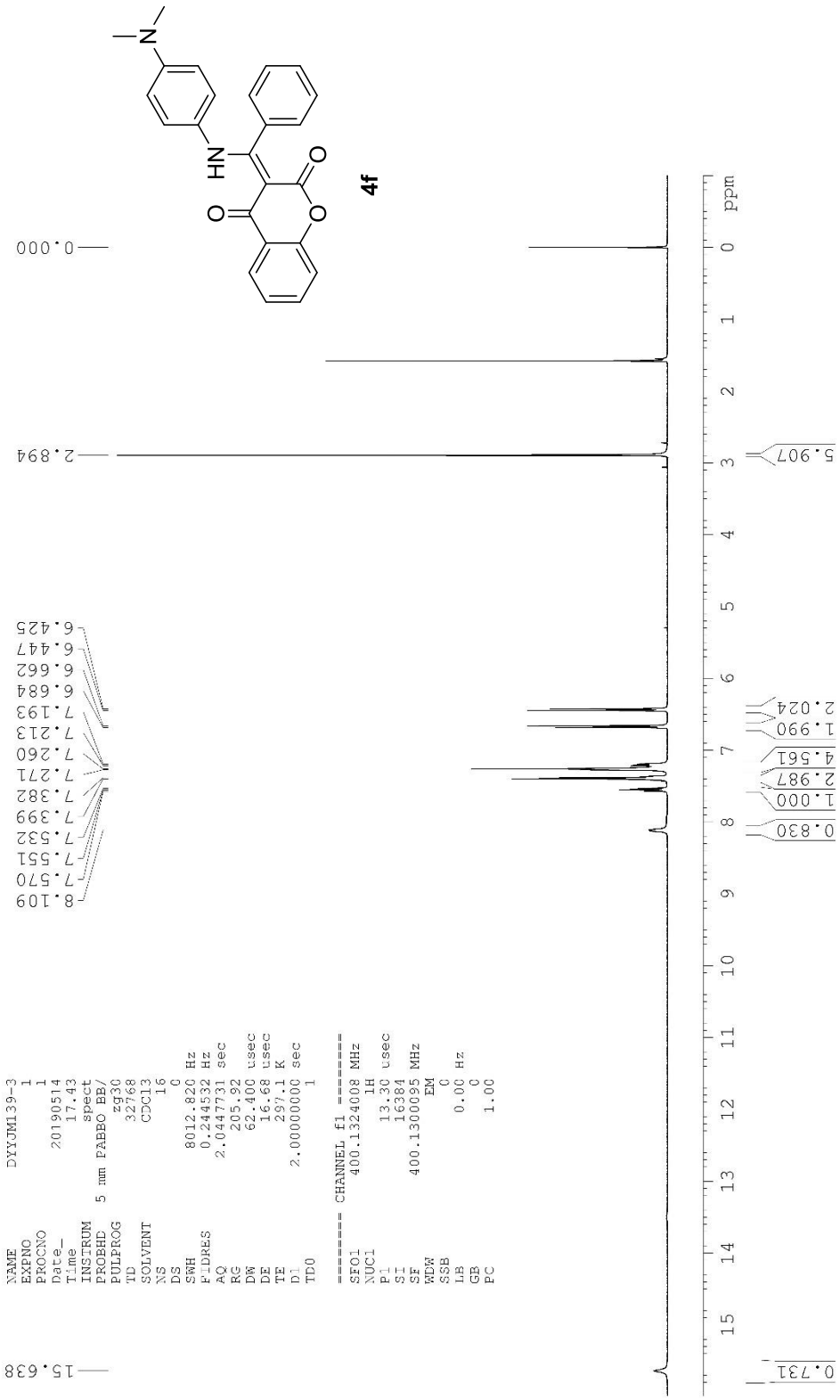
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NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
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2.894
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7.570
7.551
7.532
7.399
7.382
7.271
7.260
7.213
7.193
6.684
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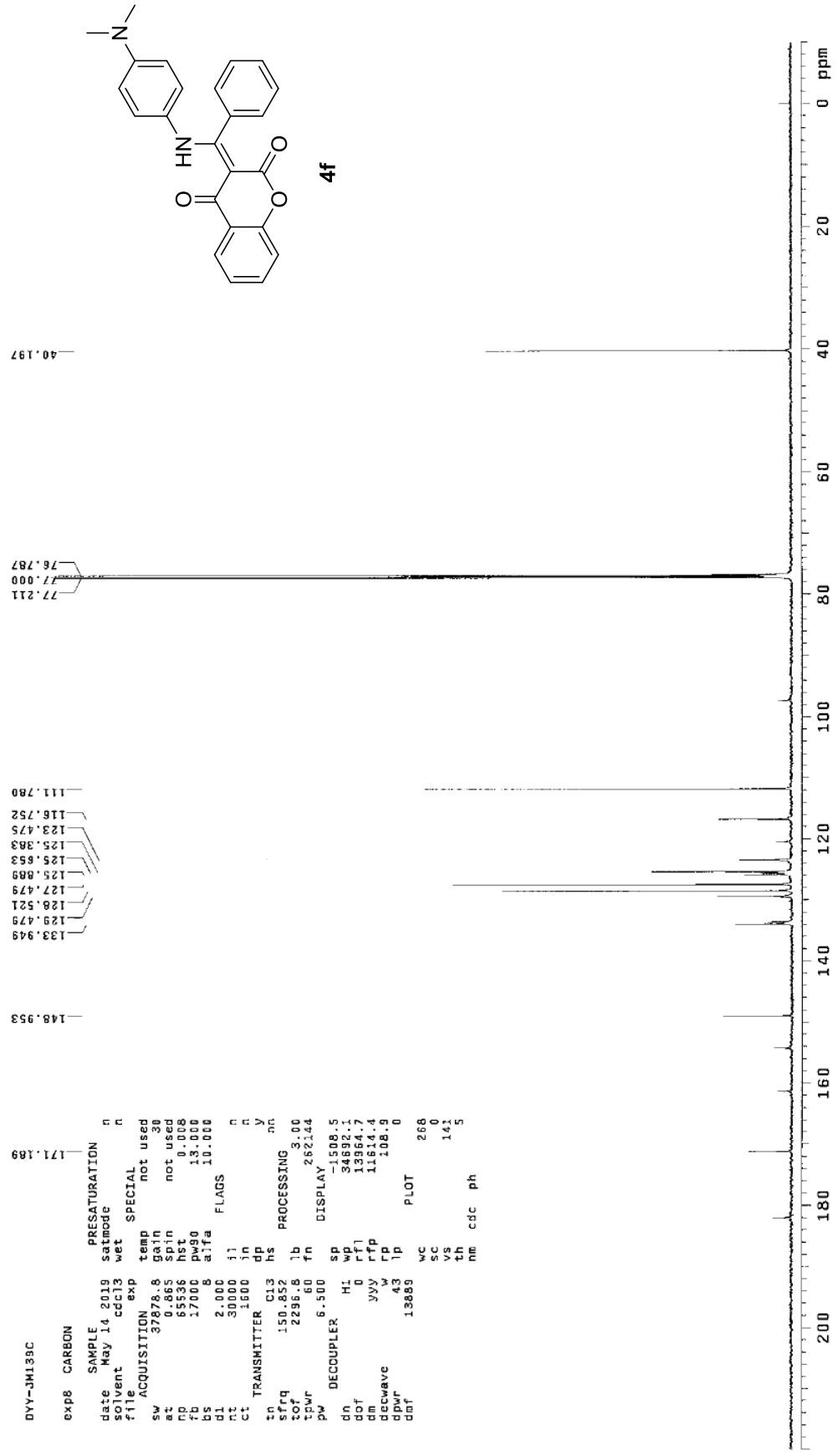
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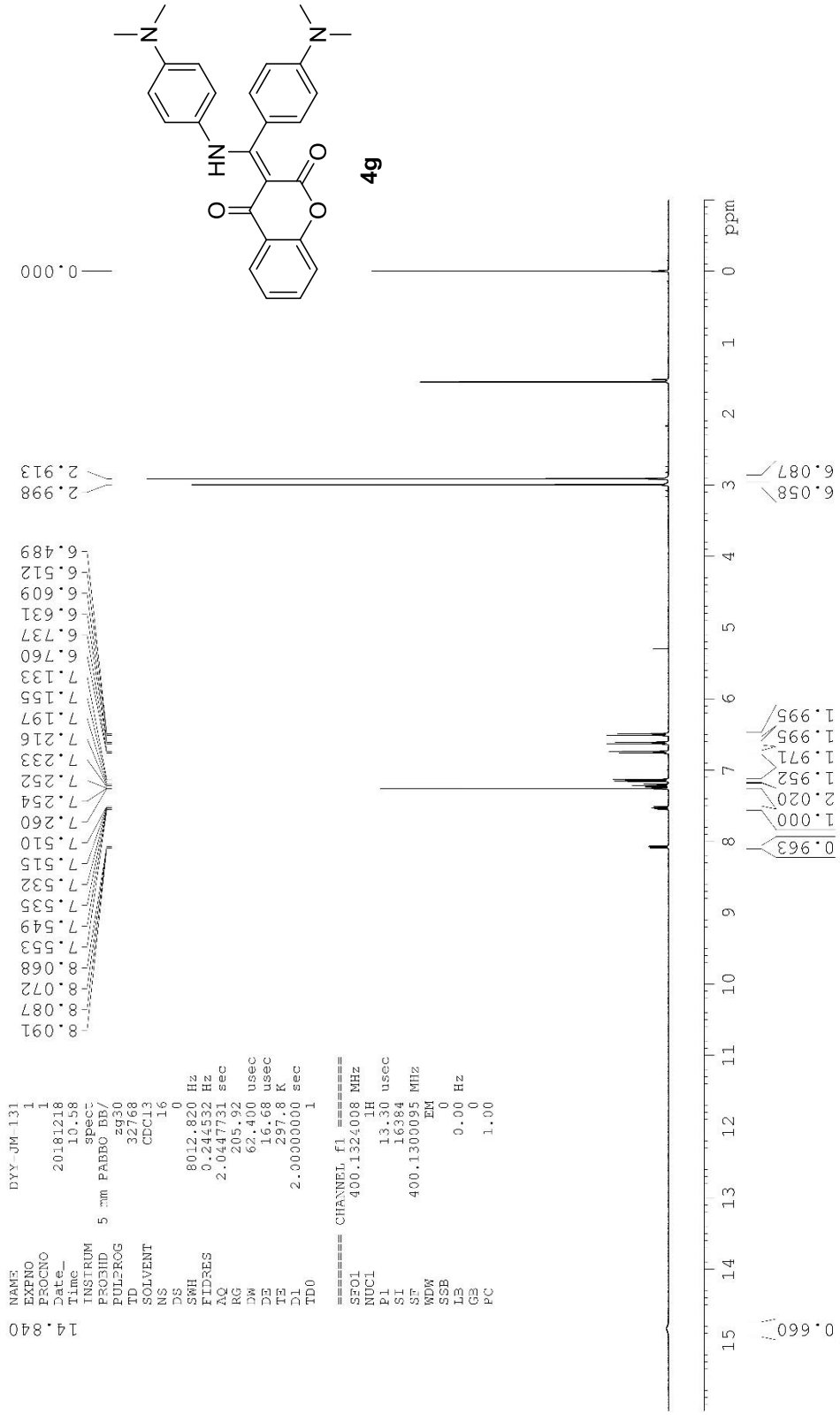
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NUC1 1H
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SI 16384
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PC 1.00
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8.072
8.068
7.553
7.549
7.535
7.532
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7.510
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7.155
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6.609
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6.489
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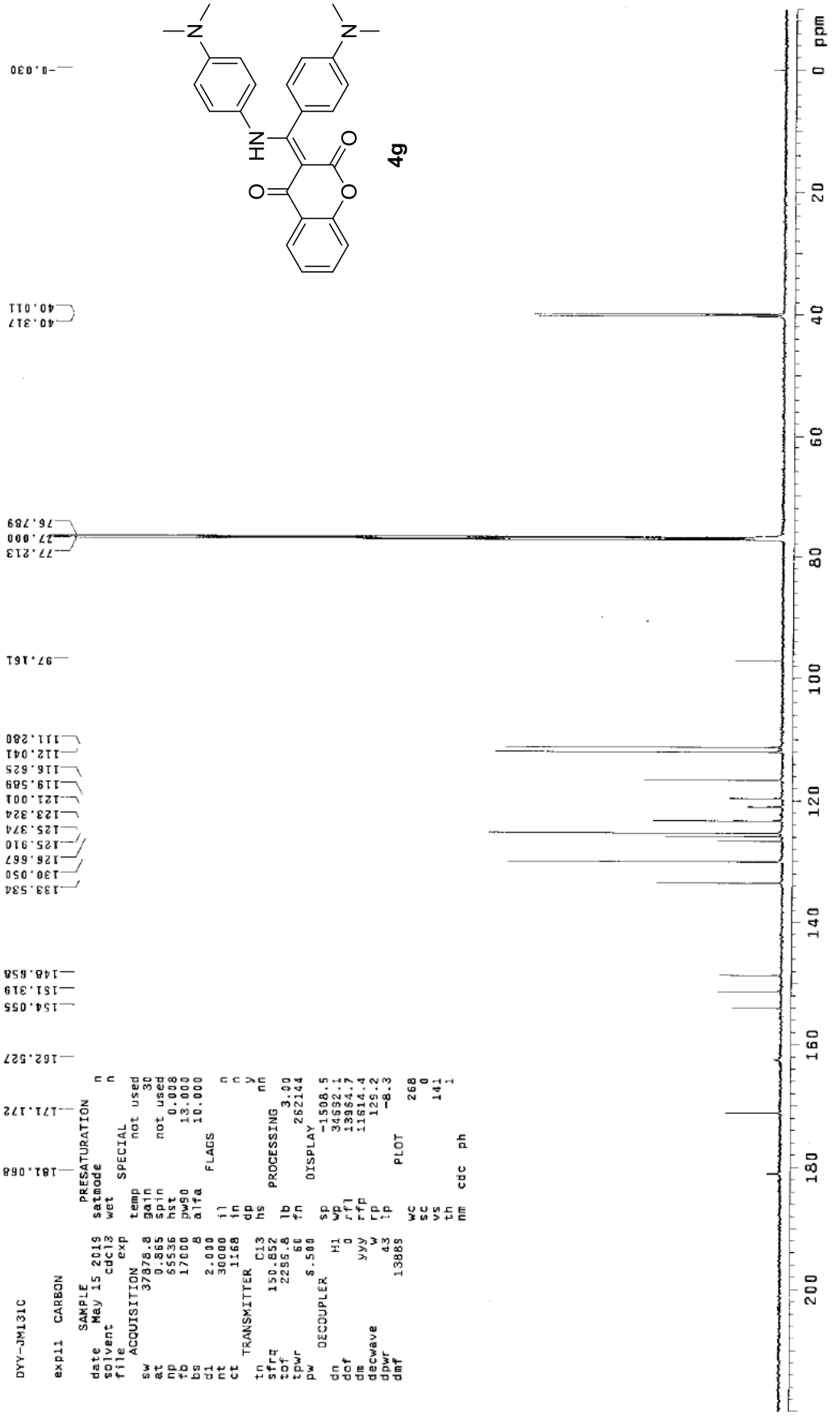
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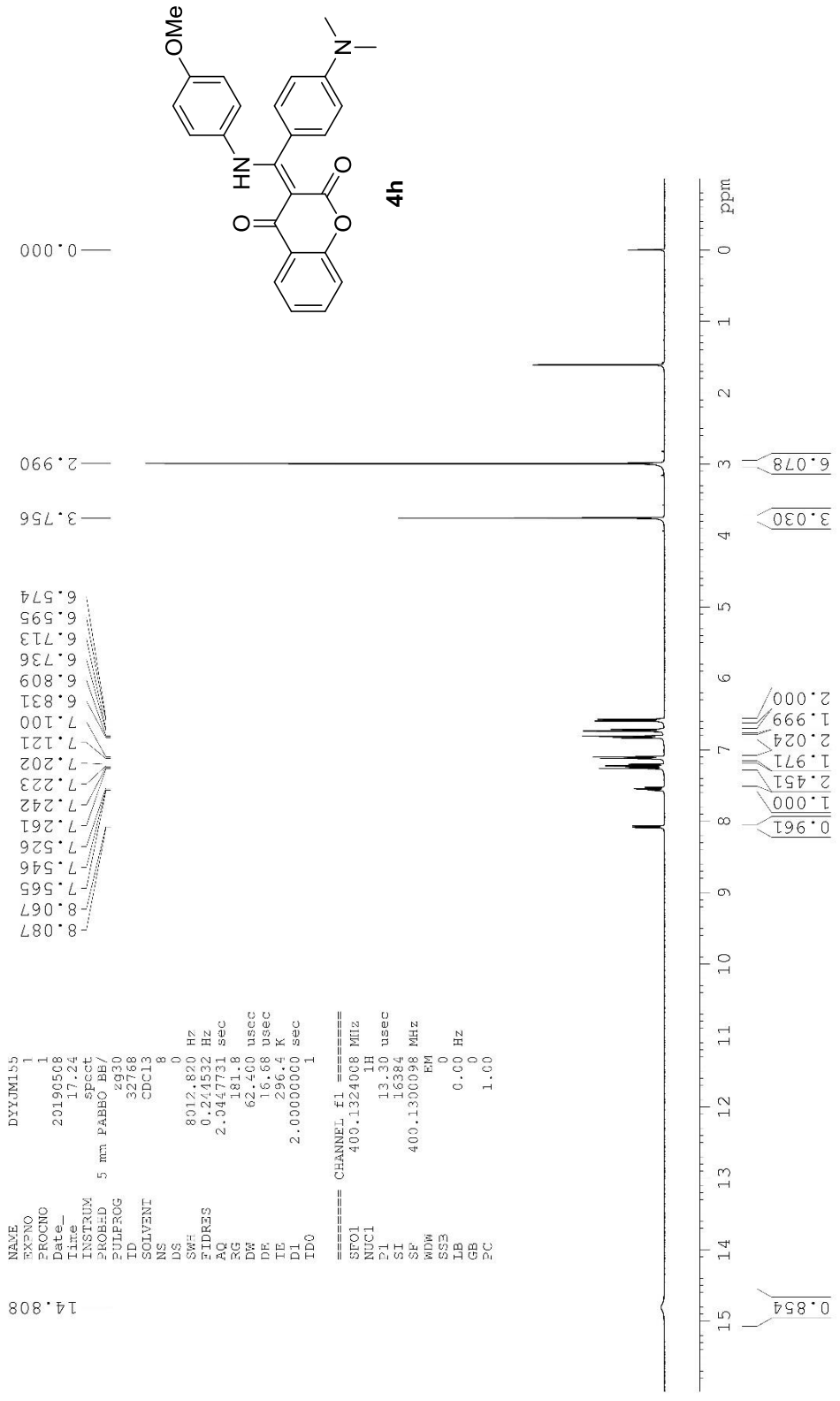
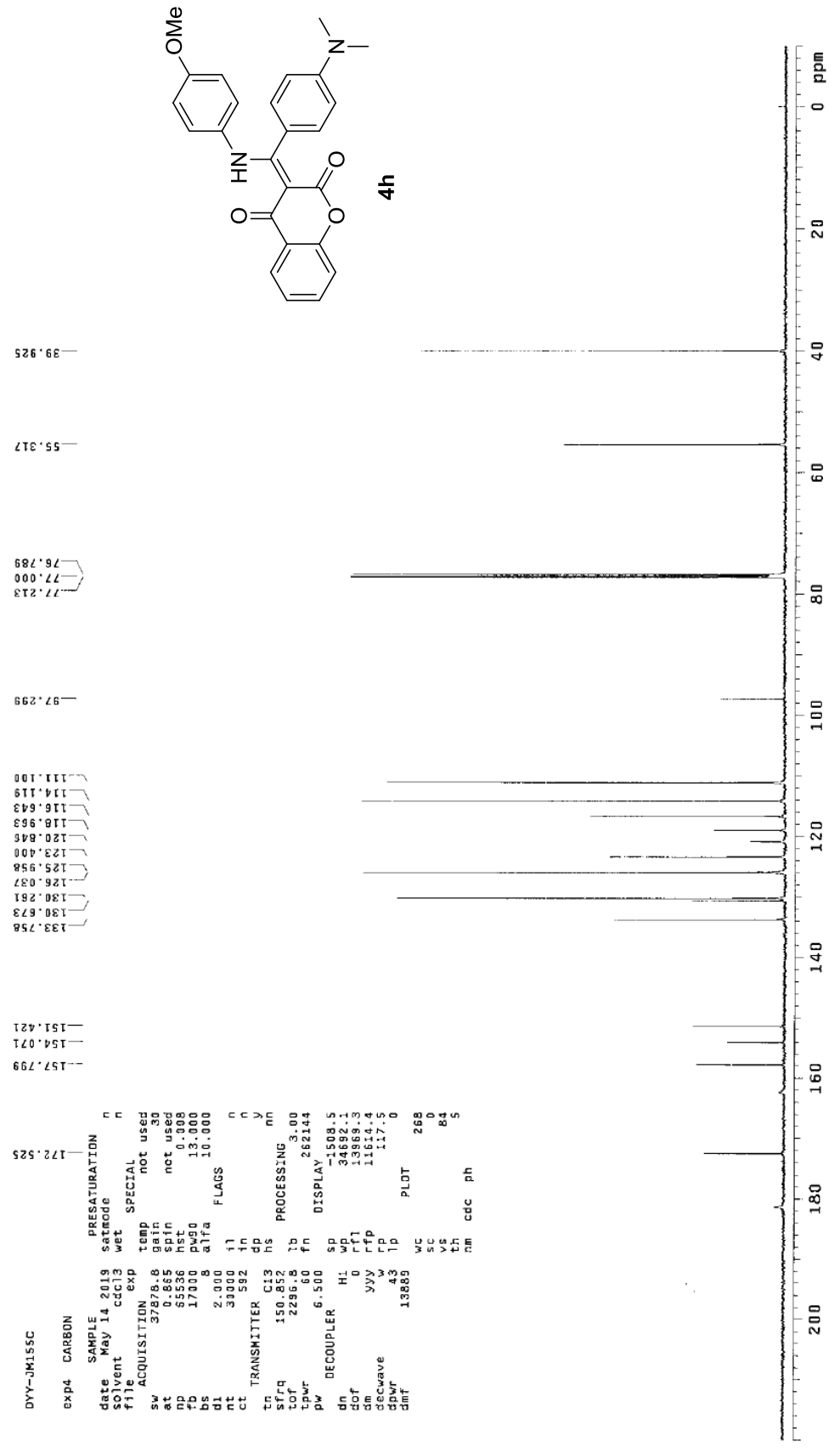
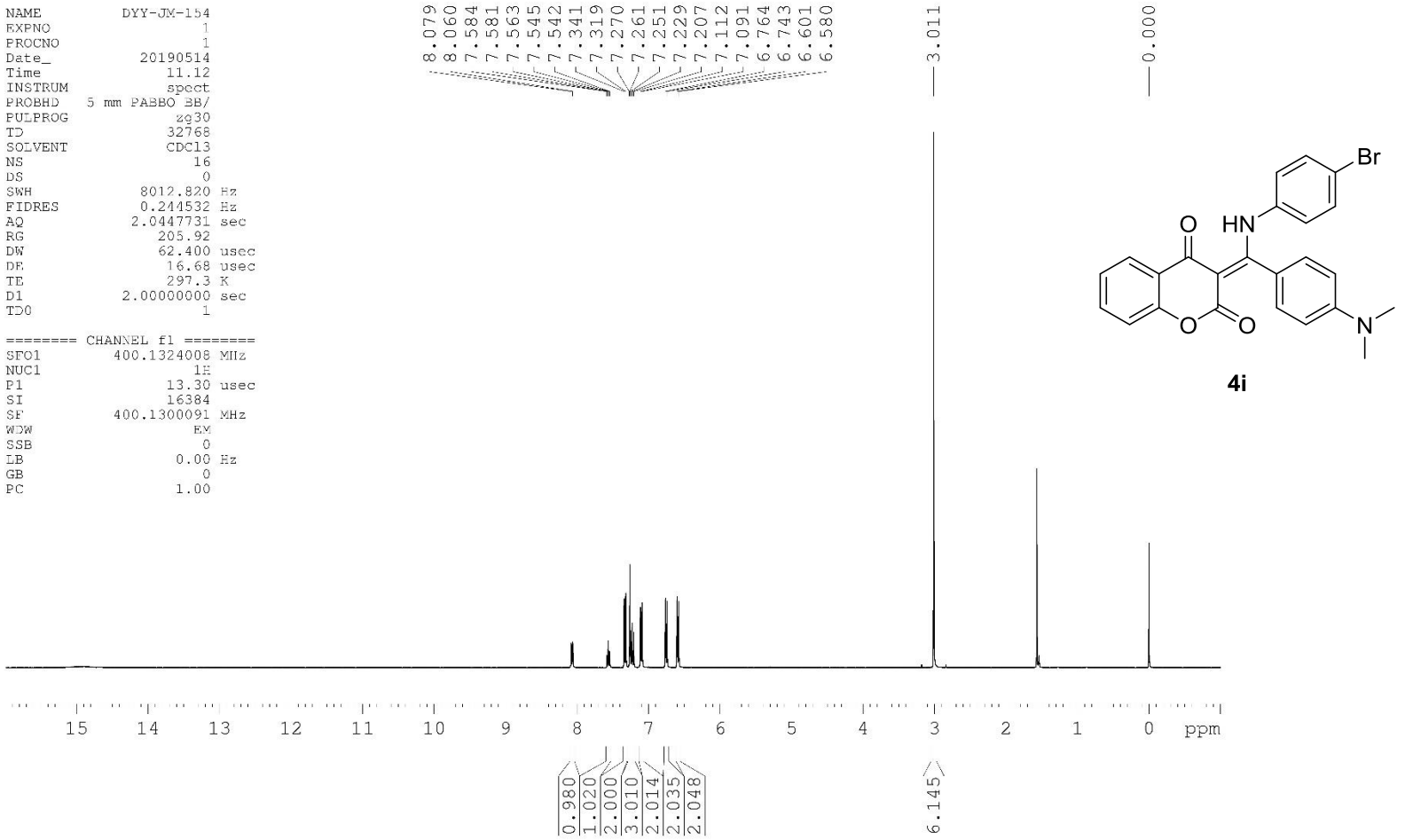
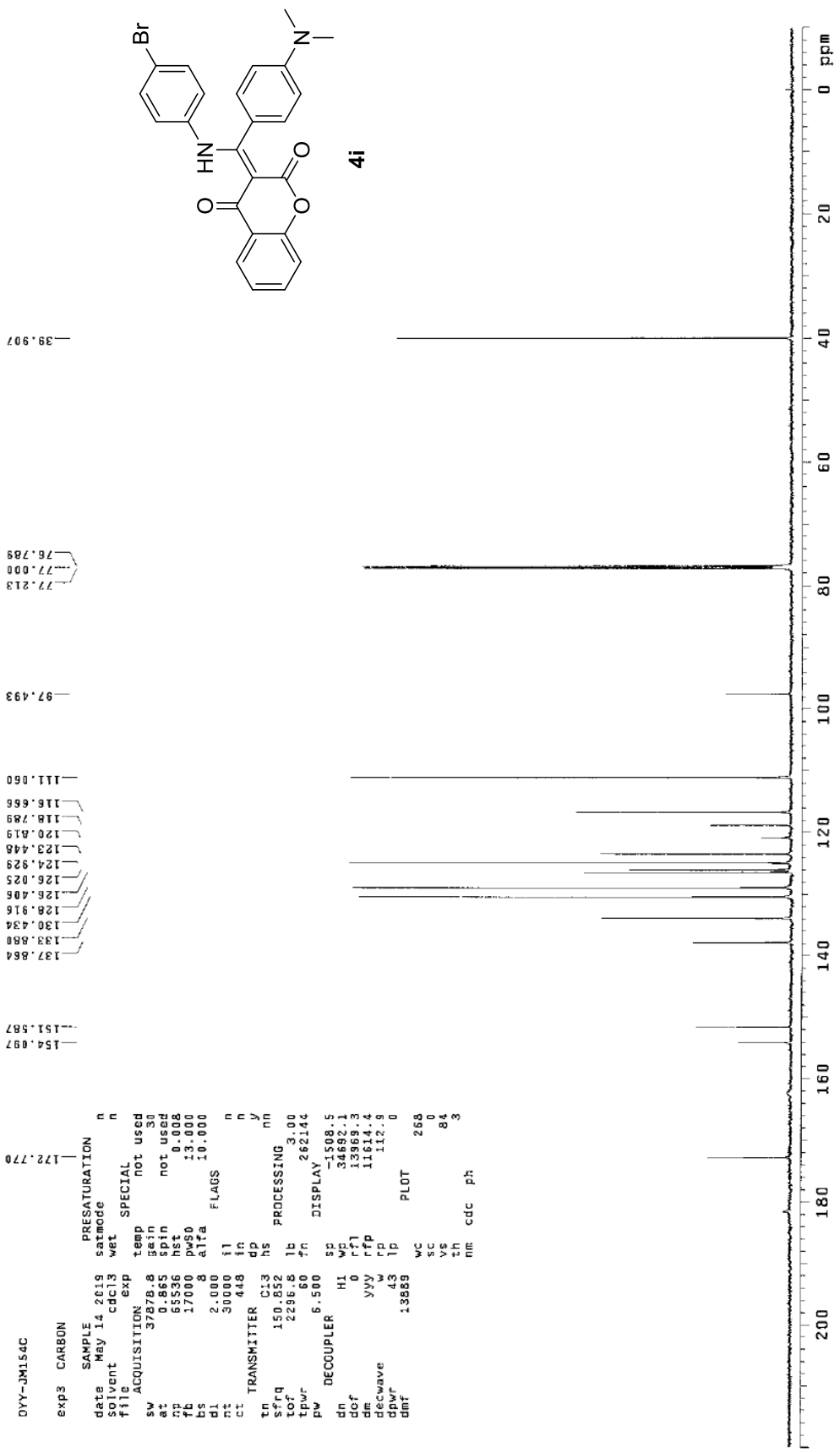
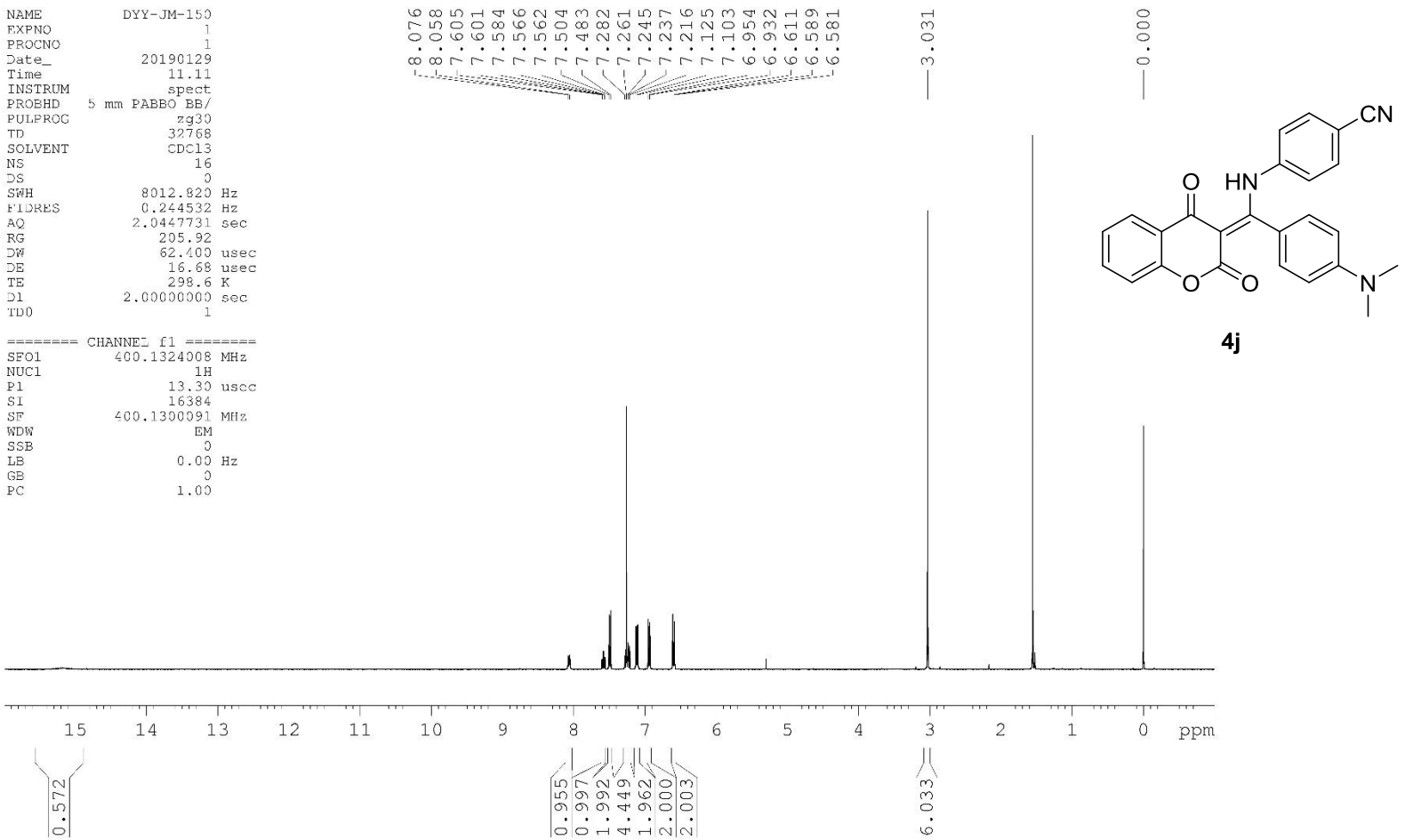
162.527
171.172
181.068
0 ppm
20
40
60
80
100
120
140
160
180
200


OMe
HN
O
O
O
N
4h
ppm


OMe
HN
O
O
O
O
N
4h
DYY-JM155C
exp4 CARBON
SAMPLE
date May 14 2019
solvent cdcl3
file exp
ACQUISITION
sw 37878.8
at 0.865
np 65536
fb 17000
bs 8
d1 2.000
nt 30000
ct 592
TRANSMITTER C13
tn
sfrq 150.852
tof 2296.8
tpwr 60
pw 6.500
DECOUPLER H1
dn
dof 0
dm yyy
decwave w
dpwr 43
dmf 13889
PRESATURATION n
satmode n
wet
SPECIAL
temp not used
gain 30
spin not used
hst 0.008
pw90 13.000
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 3.00
fn 262144
DISPLAY
sp -1508.5
wp 34692.1
rf1 13969.3
rfp 11614.4
rp 117.5
lp 0
PLOT
wc 268
sc 0
vs 84
th 5
nm cdc ph
172.525
157.799
154.071
151.421
133.758
130.673
130.261
126.037
125.958
123.408
120.846
118.963
116.643
114.119
111.100
97.299
77.213
77.000
76.789
55.317
39.925
200
180
160
140
120
100
80
60
40
20
0 ppm

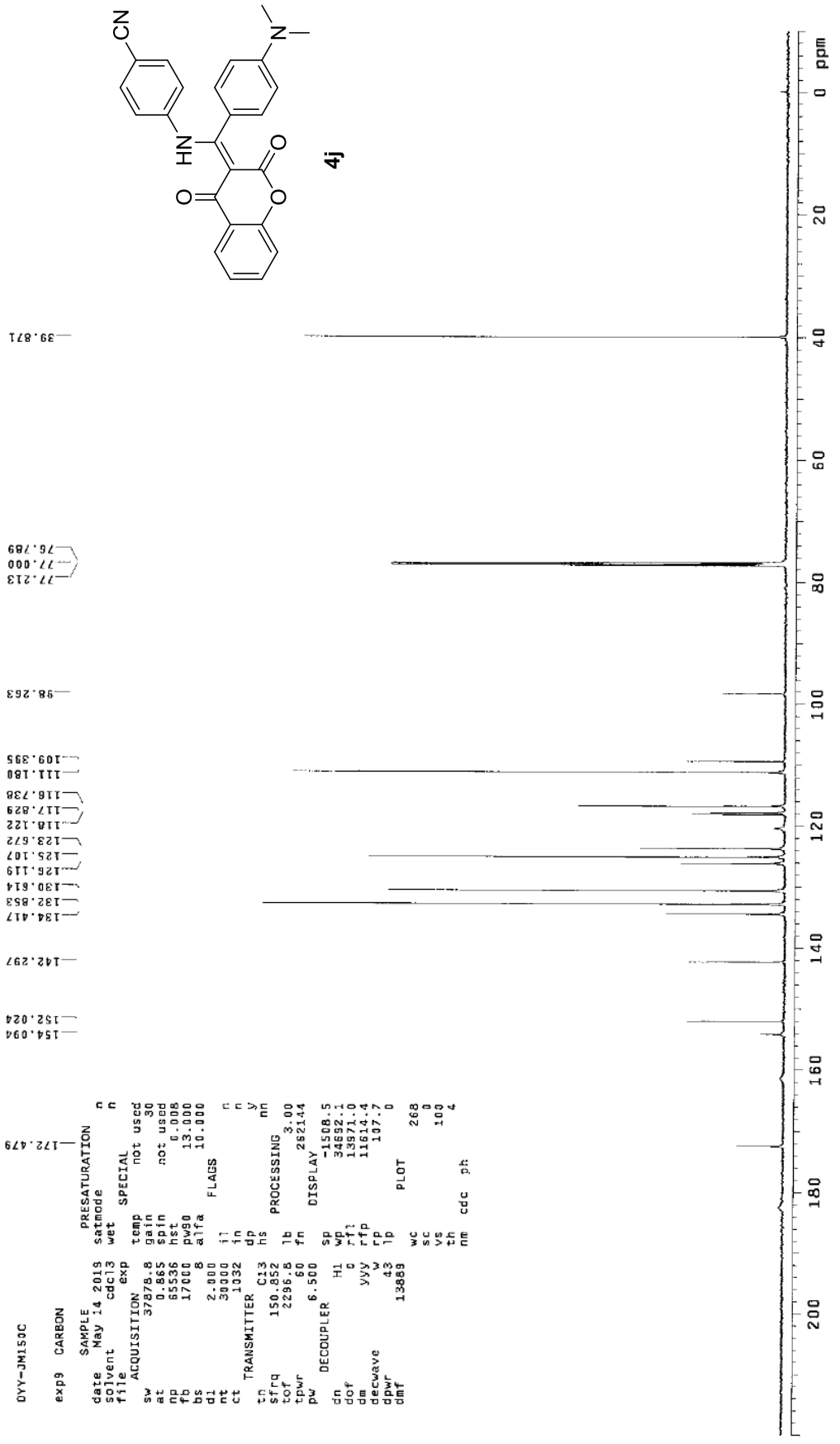

NAME DYY-JM-154
EXPNO 1
PROCNO 1
Date_ 20190514
Time 11.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 297.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.079
8.060
7.584
7.581
7.563
7.545
7.542
7.341
7.319
7.270
7.261
7.251
7.229
7.207
7.112
7.091
6.764
6.743
6.601
6.580
3.011
0.000
Br
O
HN
O
O
N
4i
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.980
1.020
2.000
3.010
2.014
2.035
2.048
6.145

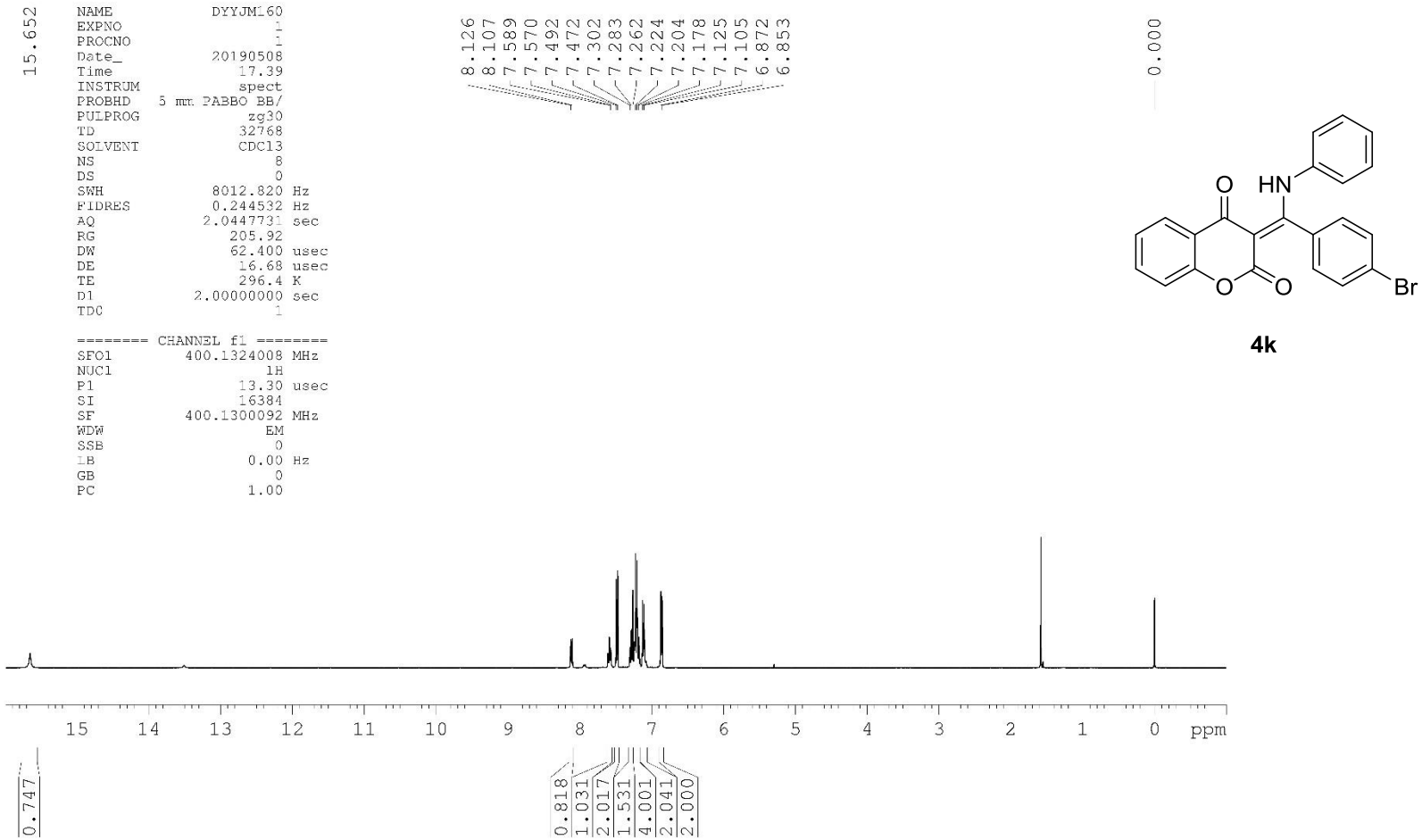

Br
HN
O
O
O
N
4i
DYY-JM154C
exp3 CARBON
SAMPLE
date May 14 2019
solvent cdcl3
file exp
ACQUISITION
sw 37878.8
at 0.865
np 65536
fb 17000
bs 8
d1 2.000
nt 30000
ct 448
TRANSMITTER
tn C13
sfrq 150.852
tof 2296.8
tpwr 60
pw 6.500
DECOUPLER
dn H1
dof 0
dm yyy
decwave w
dpwr 43
dmf 13889
PRESATURATION n
satmode n
wet SPECIAL
temp not used
gain 30
spin not used
hst 0.008
pw90 13.000
alfa 10.000
FLAGS
fl n
fn n
dp y
hs nn
PROCESSING
lb 3.00
fn 262144
DISPLAY
sp -1508.5
wp 34692.1
rf1 13969.3
rfp 11614.4
rp 112.9
lp 0
PLOT
wc 268
sc 0
vs 84
th 3
nm cdc ph
172.770
154.097
151.587
137.864
133.880
130.434
128.916
126.406
126.025
124.929
123.448
120.819
118.789
116.666
111.060
97.493
77.213
77.000
76.789
39.907
200
180
160
140
120
100
80
60
40
20
0 ppm

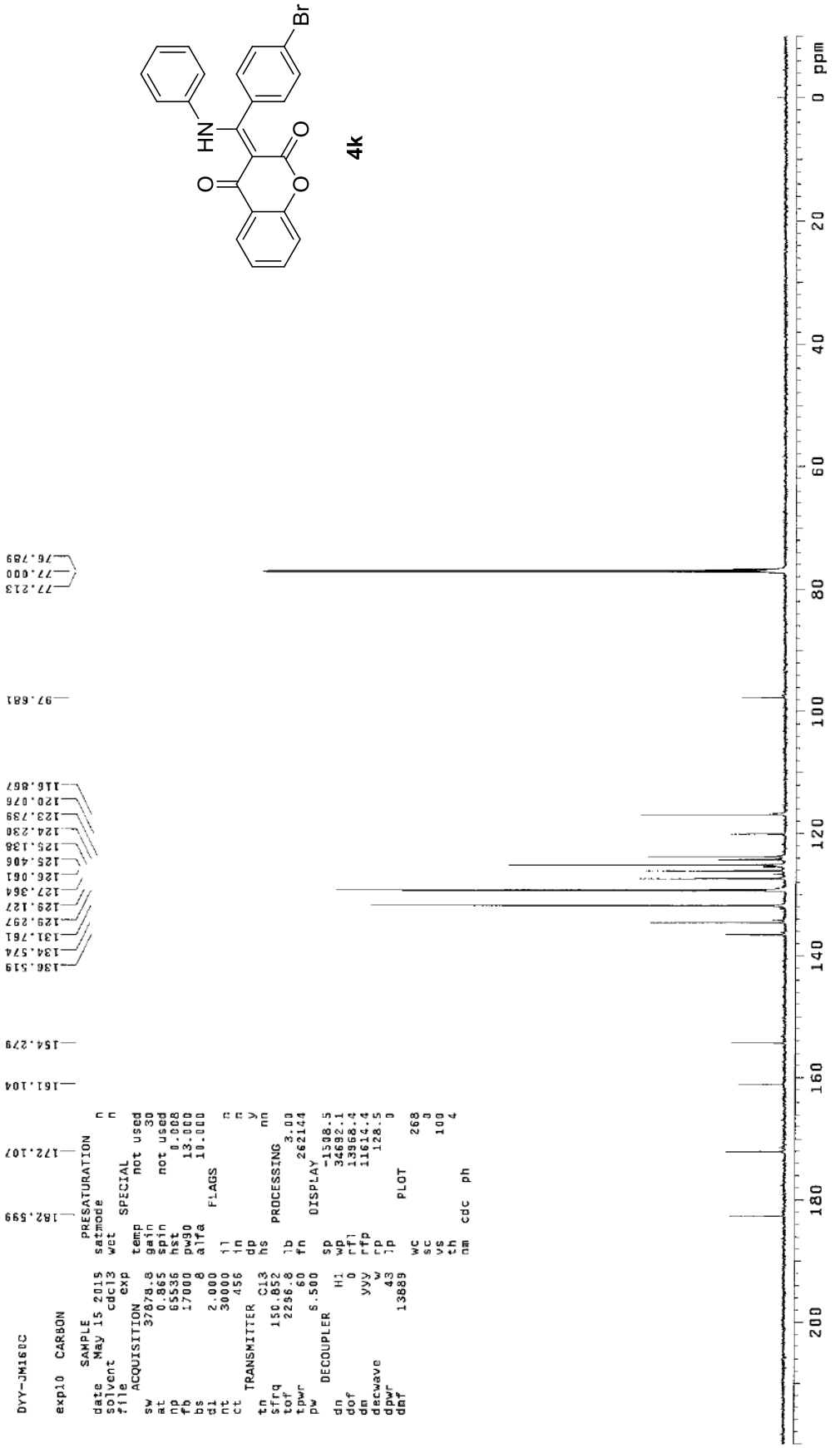

NAME DYY-JM-150
EXPNO 1
PROCNO 1
Date_ 20190129
Time 11.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 298.6 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.076
8.058
7.605
7.601
7.584
7.566
7.562
7.504
7.483
7.282
7.261
7.245
7.237
7.216
7.125
7.103
6.954
6.932
6.611
6.589
6.581
3.031
0.000
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.572
0.955
0.997
1.992
4.449
1.962
2.000
2.003
6.033

CN
HN
O
O
O
N

4j


4j
CN
HN
O
O
O
N
172.479
154.094
152.024
142.297
134.417
132.853
130.614
126.119
125.107
123.672
118.122
117.829
116.738
111.180
109.395
98.263
77.213
77.000
76.789
39.871
ppm


15.652
NAME DYYJM160
EXPNO 1
PROCNO 1
Date_ 20190508
Time 17.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 296.4 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.126
8.107
7.589
7.570
7.492
7.472
7.302
7.283
7.262
7.224
7.204
7.178
7.125
7.105
6.872
6.853
0.000
O
HN
O
O
Br
4k
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.747
0.818
1.031
2.017
1.531
4.001
2.041
2.000



DYY-JM160C

exp10 CARBON

SAMPLE
date May 15 2015
solvent cdcl3
file exp

ACQUISITION
sw 37878.8
at 0.865
np 65536
fb 17000
bs 8
d1 2.000
nt 30000
ct 456

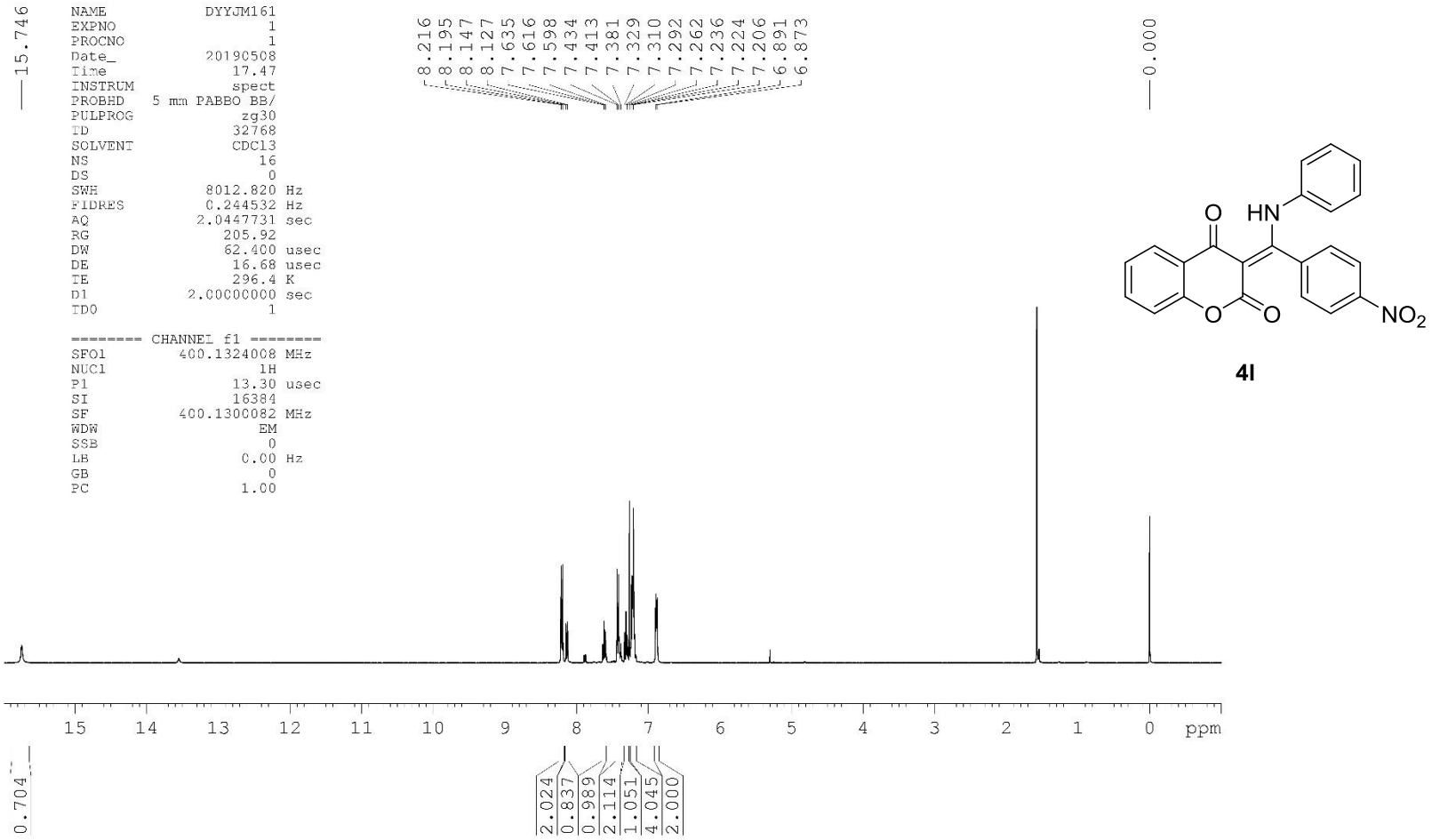
TRANSMITTER
tn C13
sfrq 150.852
tof 2296.8
tpwr 60
pw 8.500

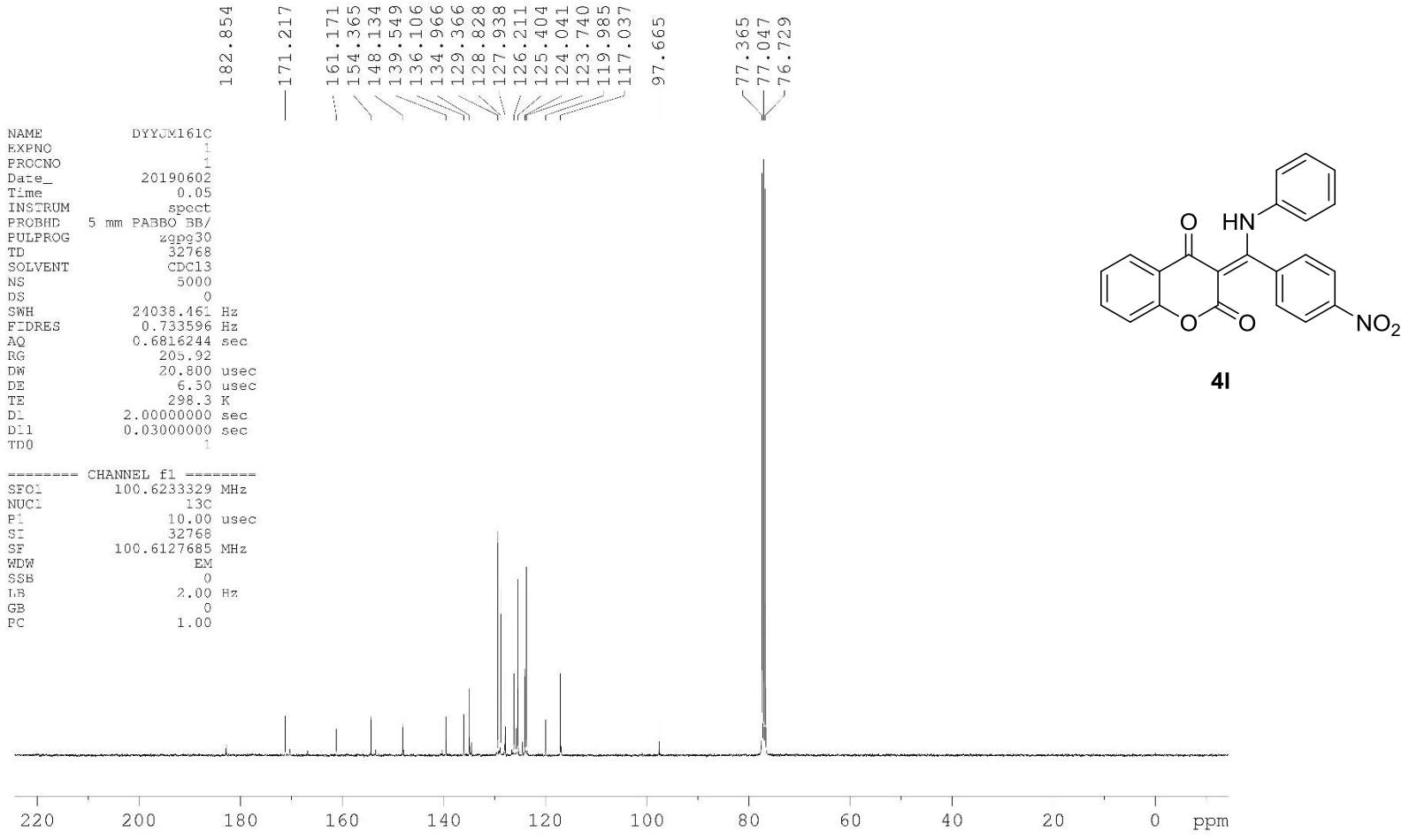
DECOUPLER
dn H1
dof 0
dm yyy
decwave w
dpwr 43
dmf 13889

PRESATURATION n
satmode n
wet SPECIAL
temp not used
gain 30
spin not used
hst 0.008
pw90 13.000
alfa 10.000
FLAGS
il n
in n
dp y
hs nn

PROCESSING
lb 3.00
fn 262144

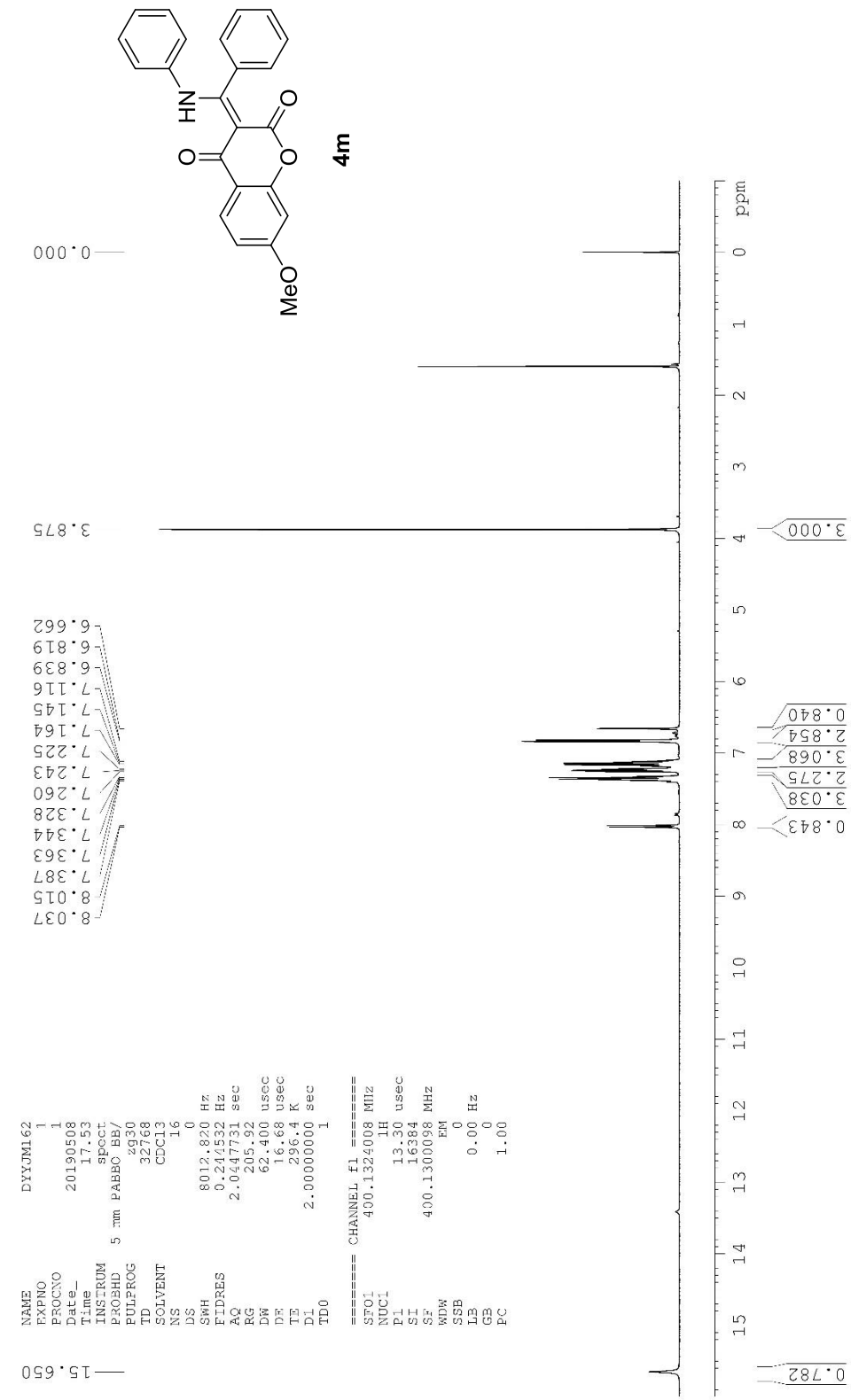
DISPLAY
sp -1508.5
wp 34692.1
rfl 13968.4
rfp 11614.4
rp 128.5
lp 0
PLOT
wc 268
sc 0
vs 100
th 4
nm cdc ph

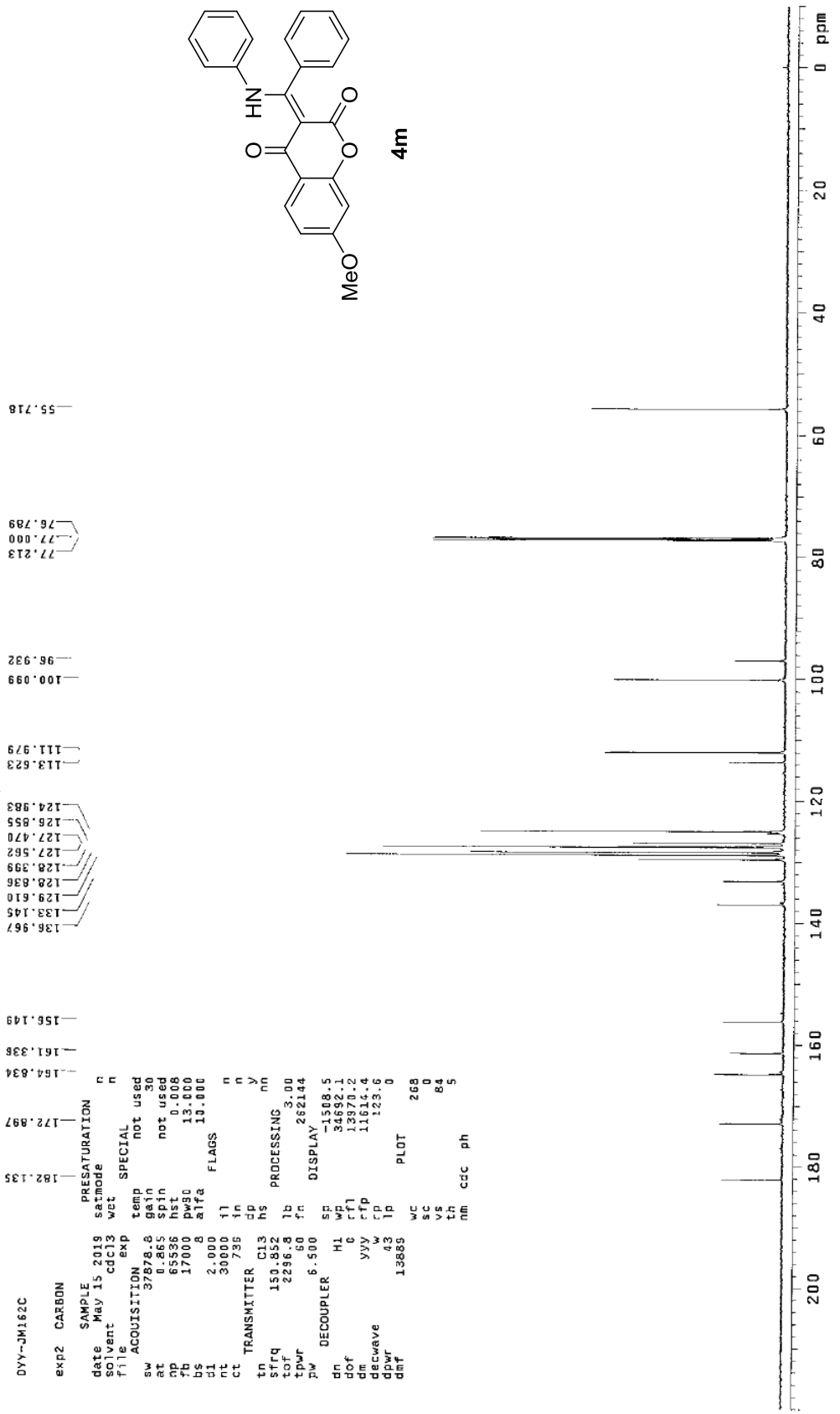

15.746
NAME DYYJM161
EXPNO 1
PROCNO 1
Date_ 20190508
Time 17.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 296.4 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300082 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.216
8.195
8.147
8.127
7.635
7.616
7.598
7.434
7.413
7.381
7.329
7.310
7.292
7.262
7.236
7.224
7.206
6.891
6.873
0.000
O
HN
O
O
NO2
4l
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.704
2.024
0.837
0.989
2.114
1.051
4.045
2.000

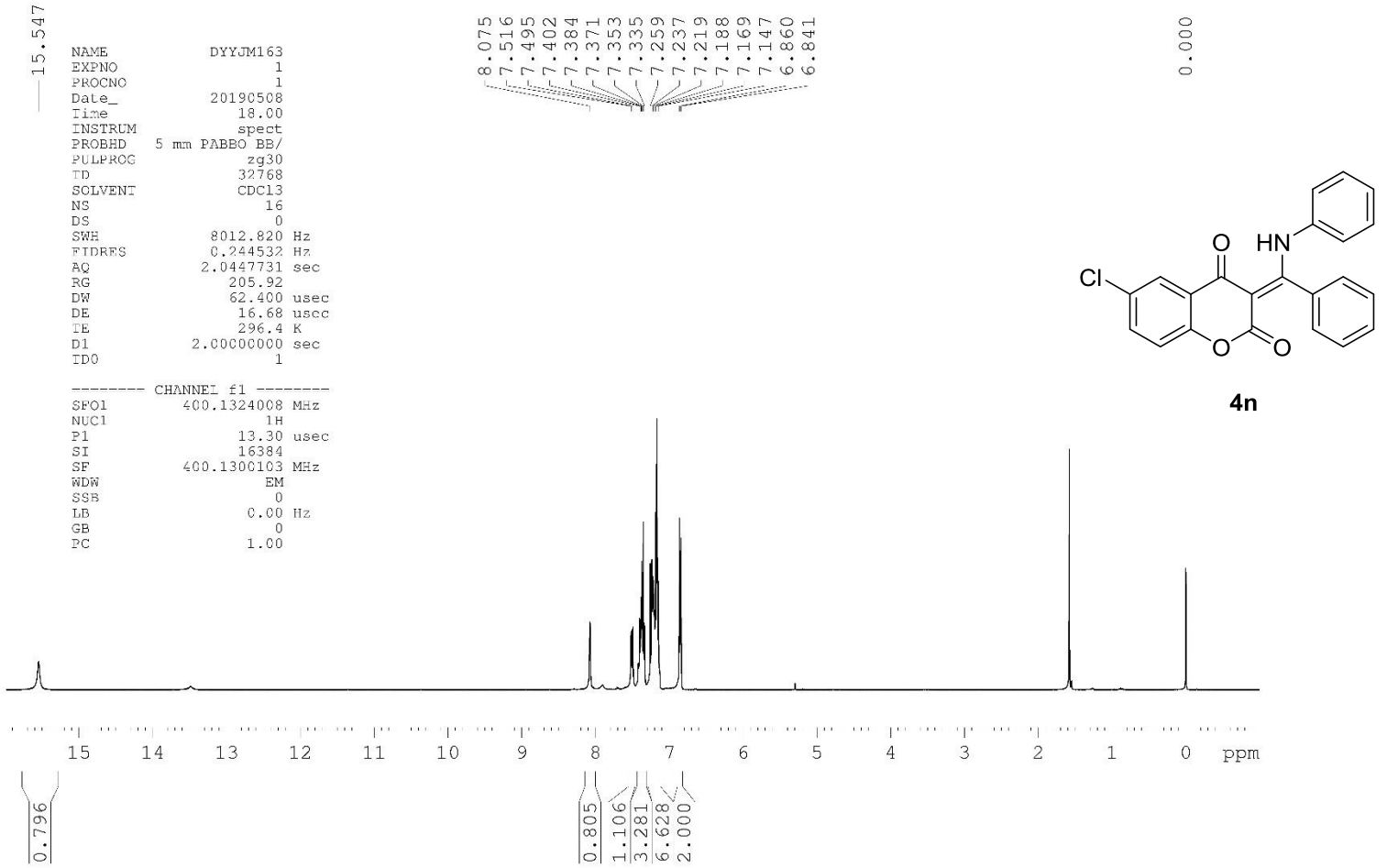

182.854
171.217
161.171
154.365
148.134
139.549
136.106
134.966
129.366
128.828
127.938
126.211
125.404
124.041
123.740
119.985
117.037
97.665
77.365
77.047
76.729
NAME DYYJM161C
EXPNO 1
PROCNO 1
Date_ 20190602
Time 0.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 5000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 203.92
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
220
200
180
160
140
120
100
80
60
40
20
0
ppm

O
HN
O
O
NO2

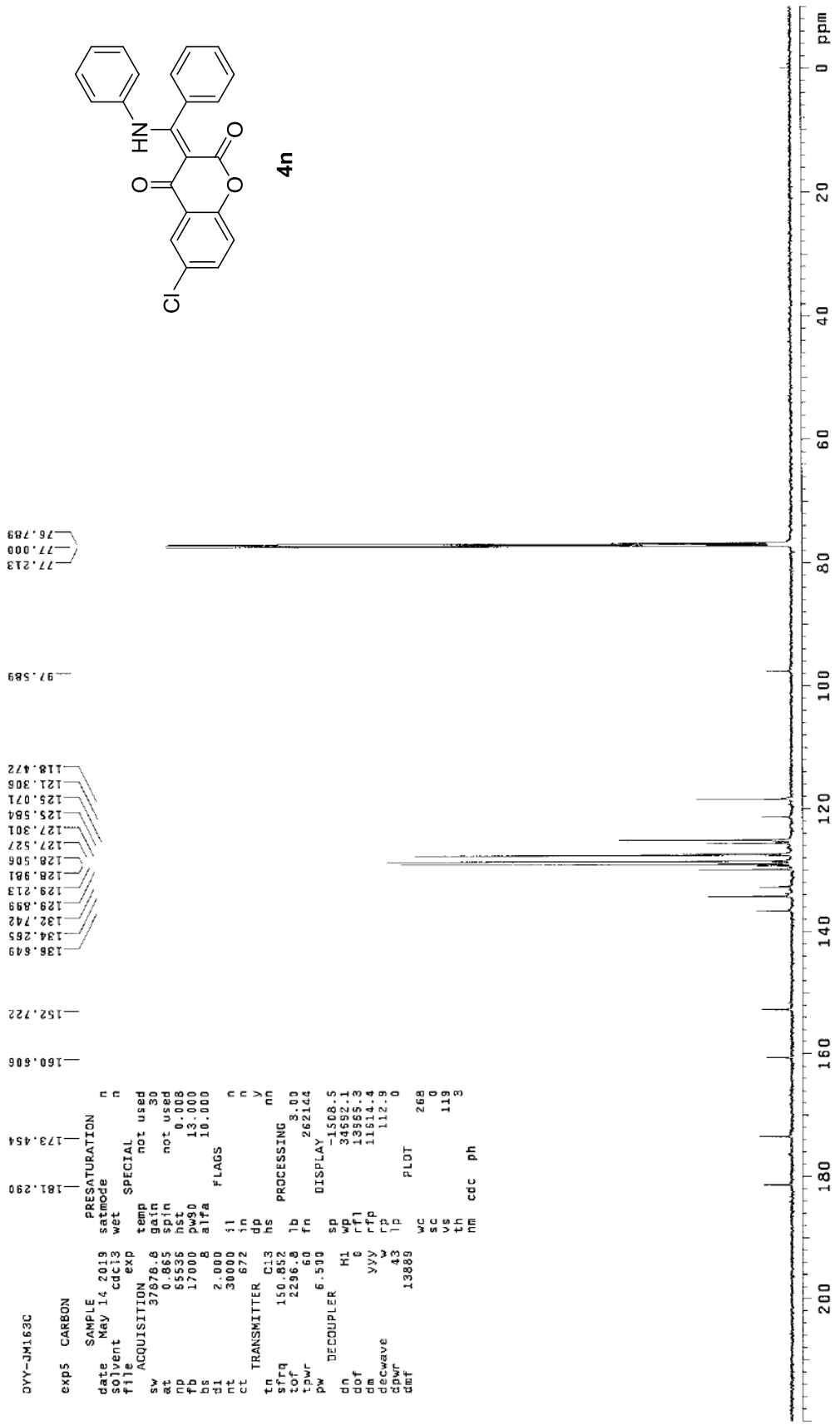
4l

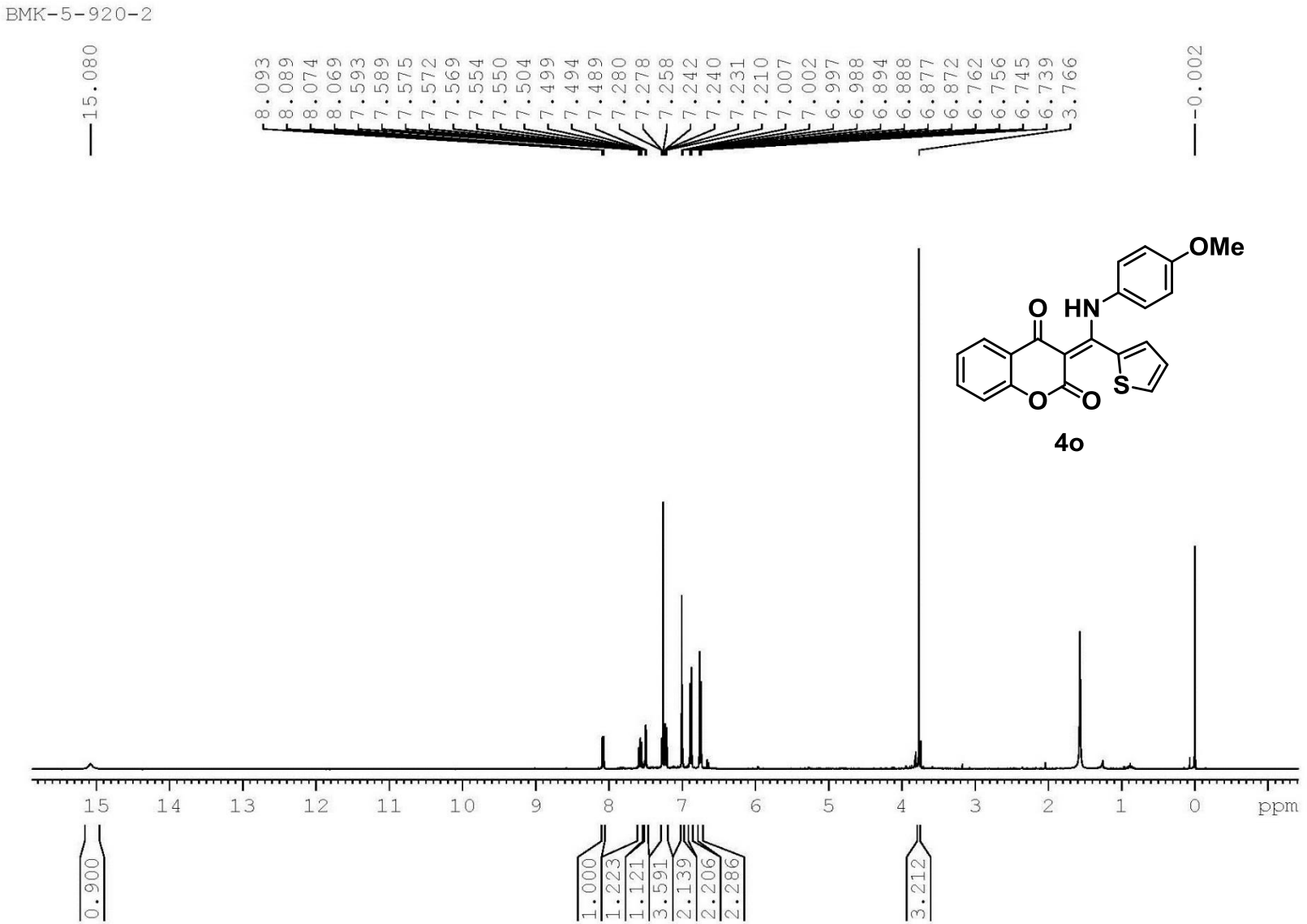

4m
HN
O
O
O
MeO
0.000
3.875
8.037
8.015
7.387
7.363
7.344
7.328
7.260
7.243
7.225
7.164
7.145
7.116
6.839
6.819
6.662
15.650
0.782
0.843
3.038
2.275
3.068
2.854
0.840
3.000
ppm


4m
MeO
O
O
HN
O
DYY-JW162C
exp2 CARBON
SAMPLE
date May 15 2019
solvent cdcl3
file exp
ACQUISITION
sw 37878.8
at 0.865
np 65536
fb 17000
bs 8
d1 2.000
nt 30000
ct 735
TRANSMITTER C13
tn
sfrq 150.852
tof 2296.8
tpwr 60
pw 6.500
DECOUPLER H1
dn
dof 0
dm yyy
decwave w
dpwr 43
dmf 13889
PRESATURATION n
satmode n
wet SPECIAL
temp not used
gain 30
spin not used
hst 0.008
pw90 13.000
alfa 10.000
FLAGS
fl n
in n
dp y
hs nn
PROCESSING
lb 3.00
fn 262144
DISPLAY
sp -1508.5
wp 34692.1
rfl 13870.2
rfp 11614.4
rp 123.6
lp 0
PLOT
wc 268
sc 0
vs 84
th 5
nm cdc ph
182.135
172.897
164.834
161.336
156.149
136.967
133.145
129.610
128.836
128.399
127.562
127.470
126.855
124.983
113.623
111.979
100.099
96.932
77.213
77.000
76.789
55.718
0 ppm
20
40
60
80
100
120
140
160
180
200

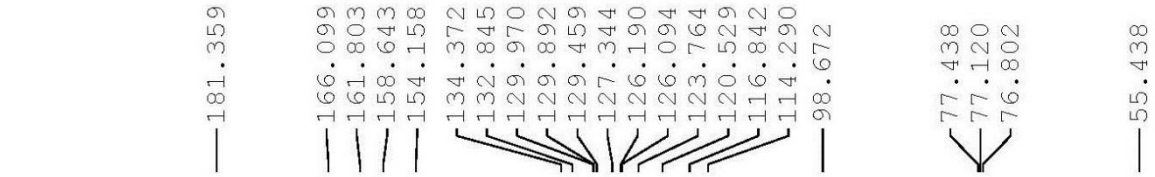

15.547
8.075
7.516
7.495
7.402
7.384
7.371
7.353
7.335
7.259
7.237
7.219
7.188
7.169
7.147
6.860
6.841
0.000
NAME DYYJM163
EXPNO 1
PROCNO 1
Date_ 20190508
Time 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 296.4 K
D1 2.00000000 sec
TD0 1
-------- CHANNEL f1 --------
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
HN
Cl
O
O
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.796
0.805
1.106
3.281
6.628
2.000

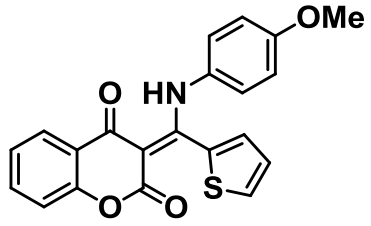
4n


4n
DYY-JM163C
exp5 CARBON
SAMPLE
date May 14 2019
solvent cdcl3
file exp
ACQUISITION
sw 37878.8
at 0.865
np 65536
fb 17000
bs 8
d1 2.000
nt 30000
ct 672
TRANSMITTER C13
tn
sfrq 150.852
tof 2296.8
tpwr 60
pw 6.500
DECOUPLER H1
dn
dof 0
dm yyy
decwave y
dpwr 43
dmf 13889
PRESATURATION n
satmode n
wet SPECIAL
temp
gain not used
spin not used
hst 0.008
pw90 13.000
alfa 10.000
FLAGS
i1 n
in n
dp y
hs nn
PROCESSING
lb 3.00
fn 262144
DISPLAY
sp -1508.5
wp 34692.1
rf1 13865.3
rfp 11614.4
rp 112.9
lp 0
PLOT
wc 268
sc 0
vs 119
th 3
nm cdc ph
181.290
173.454
160.606
152.722
136.649
134.285
132.742
129.899
129.213
128.981
128.506
127.527
127.301
125.584
125.071
121.305
118.472
97.589
77.213
77.000
76.789
200
180
160
140
120
100
80
60
40
20
0 ppm

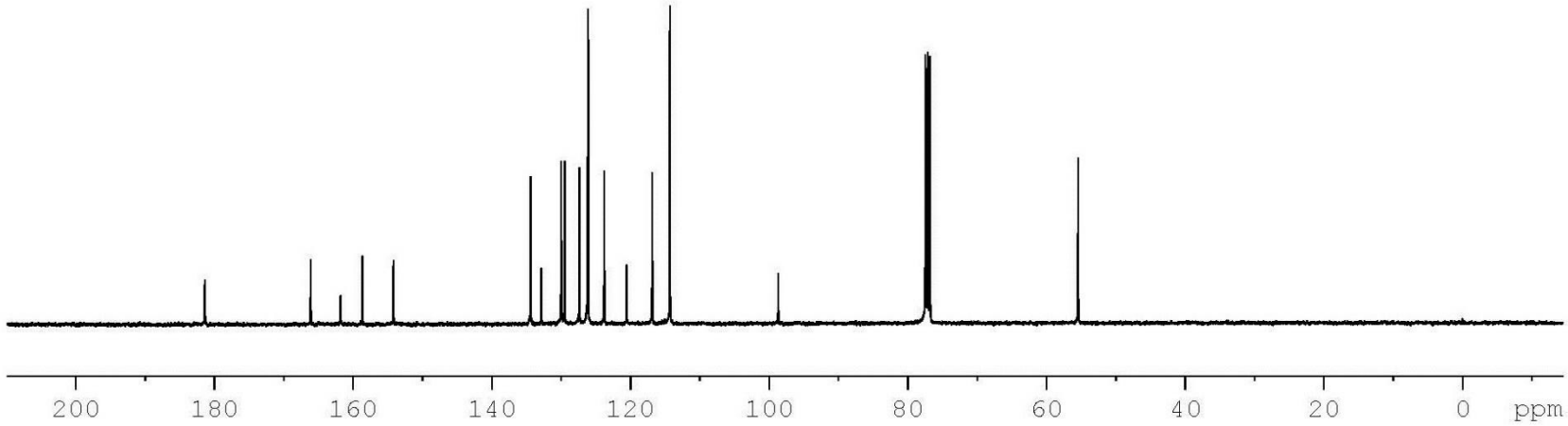

BMK-5-920-2
15.080
8.093
8.089
8.074
8.069
7.593
7.589
7.575
7.572
7.569
7.554
7.550
7.504
7.499
7.494
7.489
7.280
7.278
7.258
7.242
7.240
7.231
7.210
7.007
7.002
6.997
6.988
6.894
6.888
6.877
6.872
6.762
6.756
6.745
6.739
3.766
-0.002
OMe
O
HN
S
O
O
4o
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.900
1.000
1.223
1.121
3.591
2.139
2.206
2.286
3.212

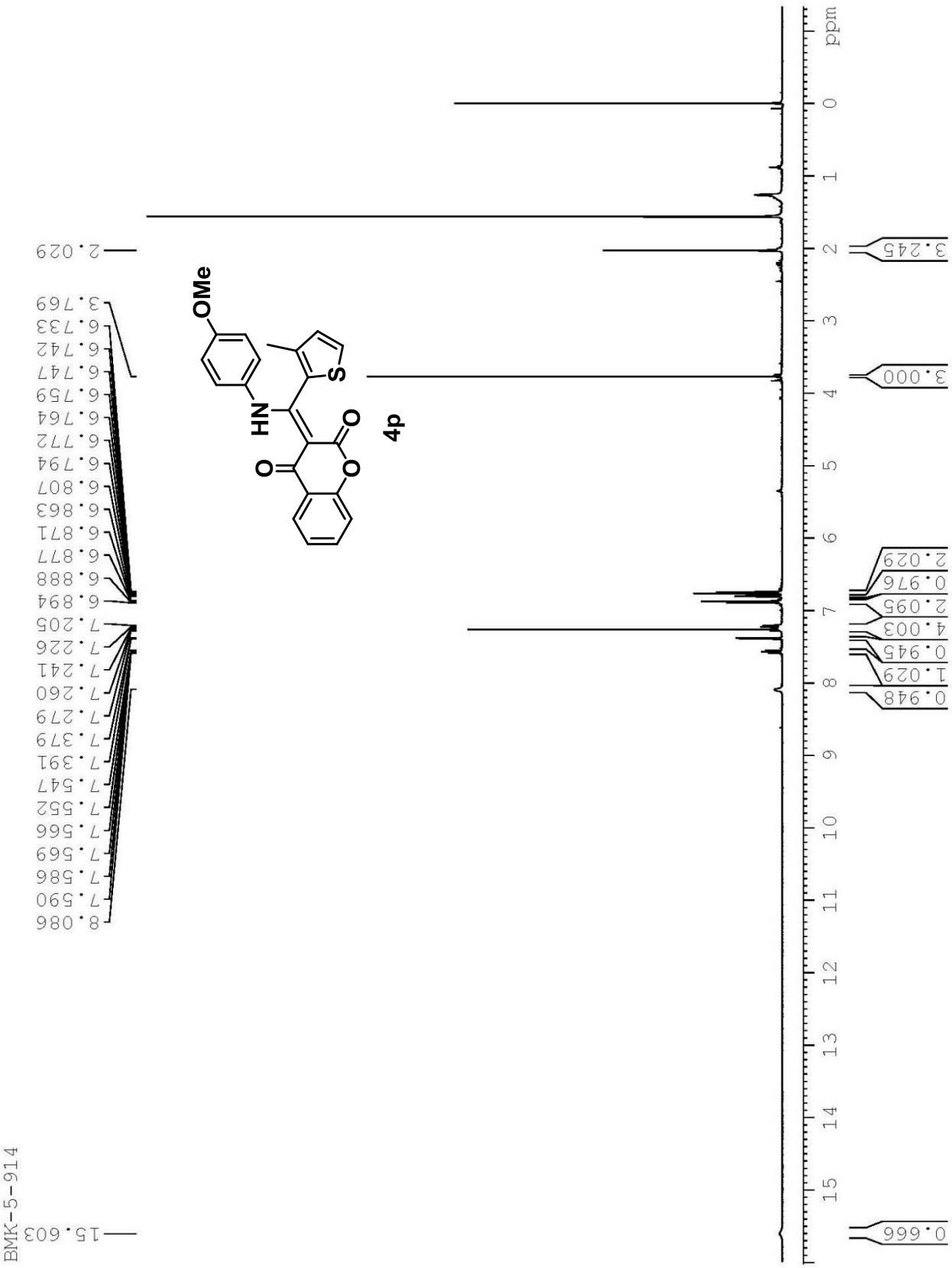
BMK-5-920-C

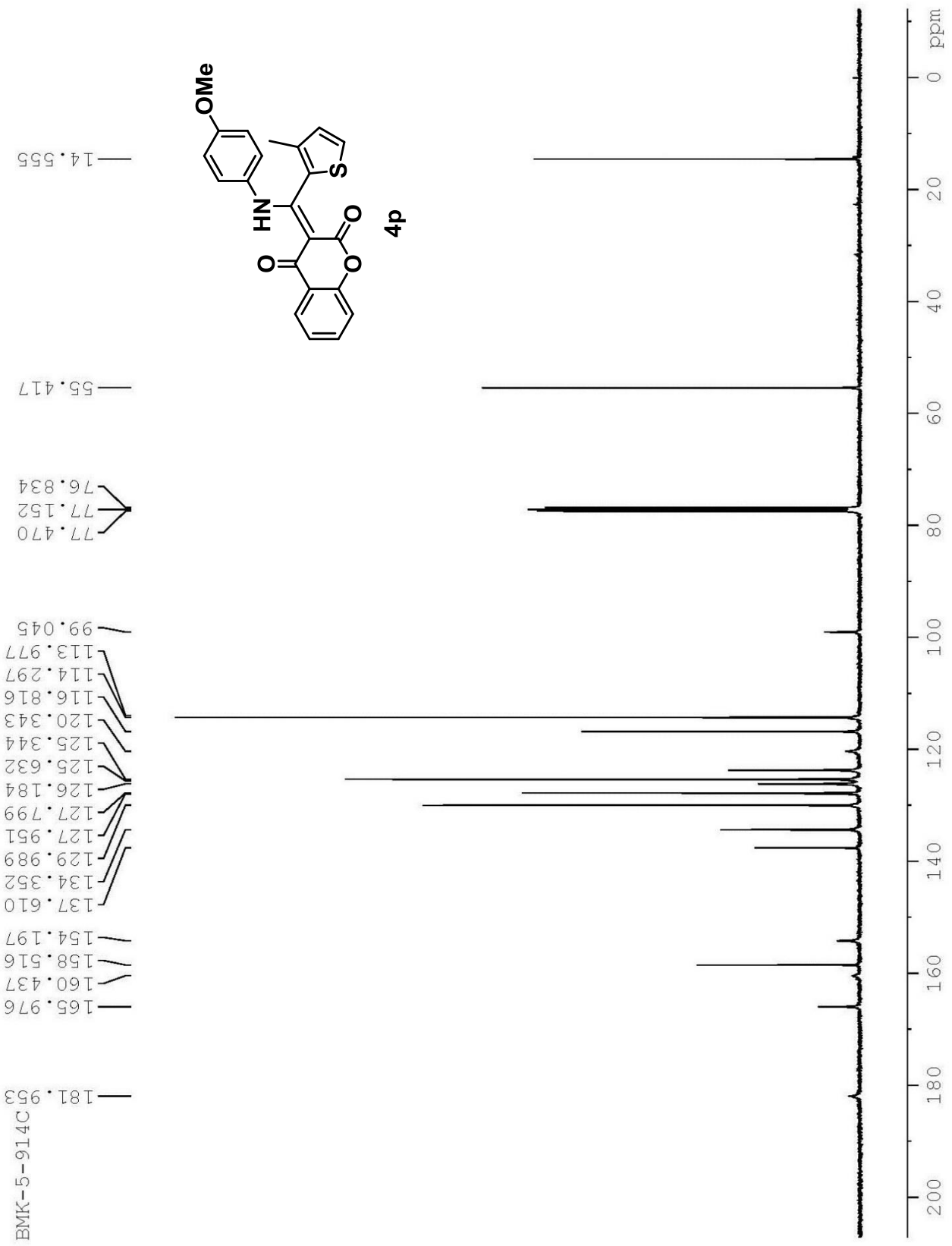

181.359
166.099
161.803
158.643
154.158
134.372
132.845
129.970
129.892
129.459
127.344
126.190
126.094
123.764
120.529
116.842
114.290
98.672
77.438
77.120
76.802
55.438


OMe
O
HN
S
O
O

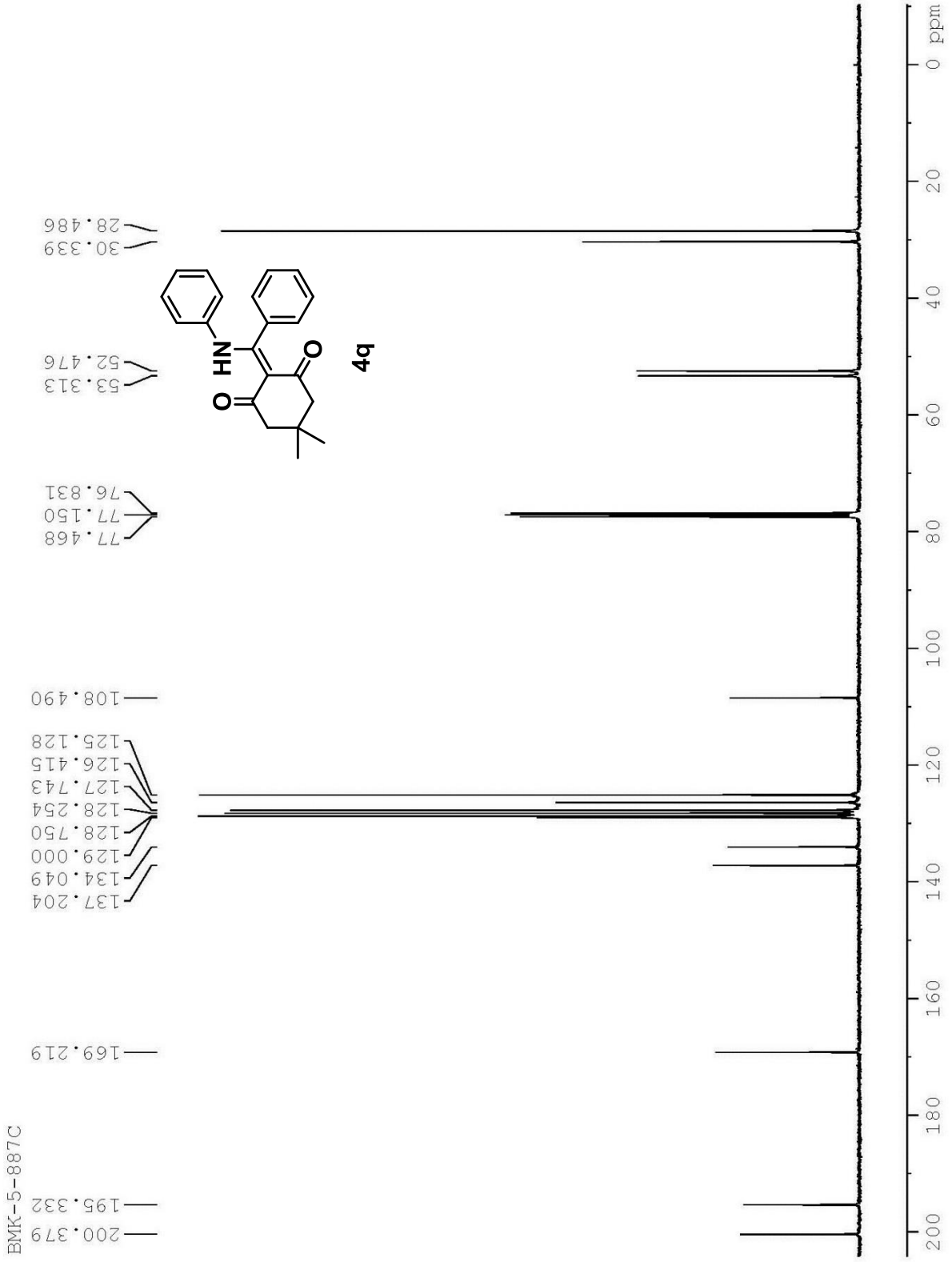
4o


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

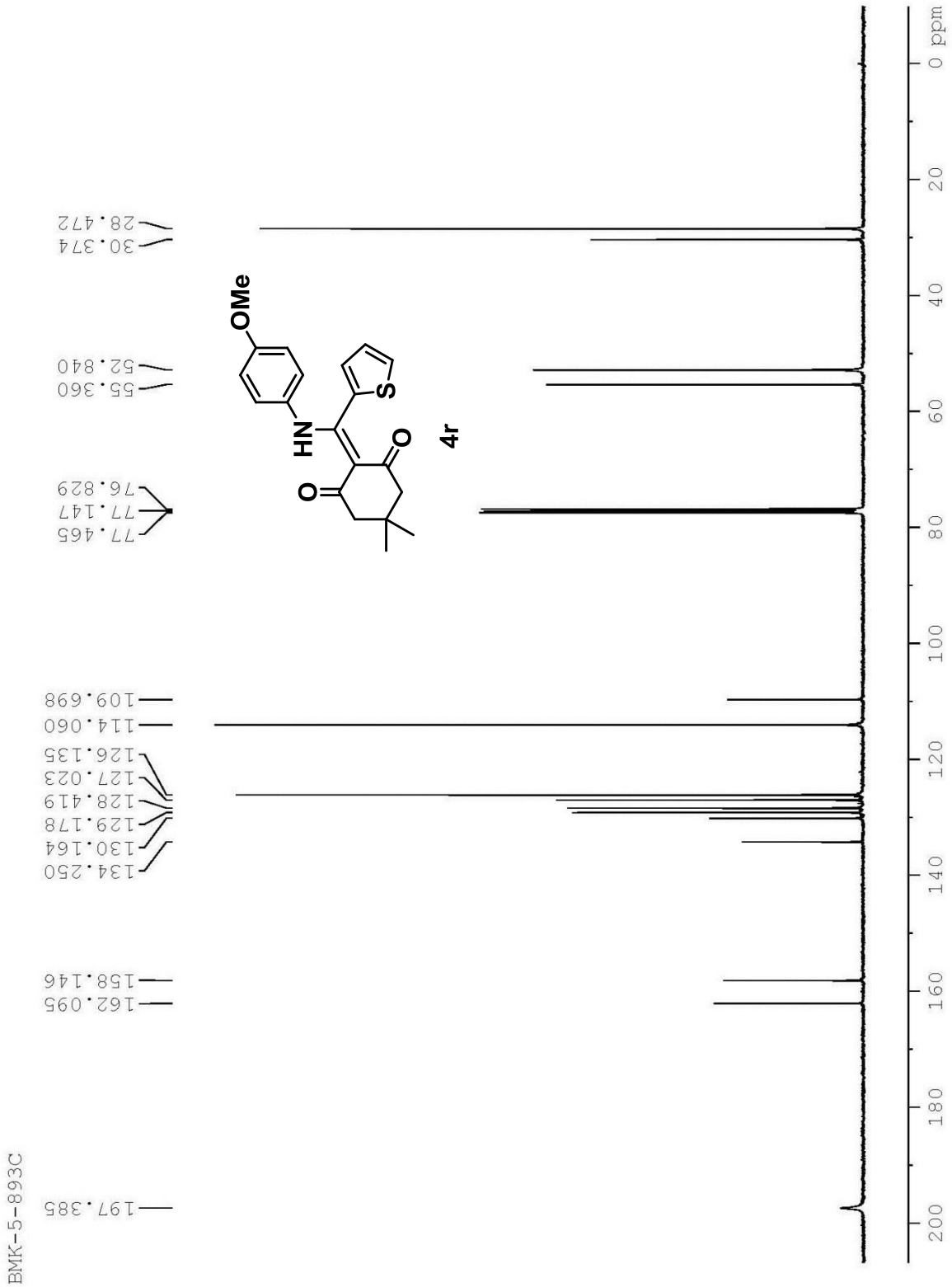

BMK-5-914
15.603
8.086
7.590
7.586
7.569
7.566
7.552
7.547
7.391
7.379
7.279
7.260
7.241
7.226
7.205
6.894
6.888
6.877
6.871
6.863
6.807
6.794
6.772
6.764
6.759
6.747
6.742
6.733
6.769
2.029
OMe
HN
S
O
O
O
4p
0.948
1.029
0.945
4.003
2.095
0.976
2.029
3.000
3.245
0.666
ppm
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15

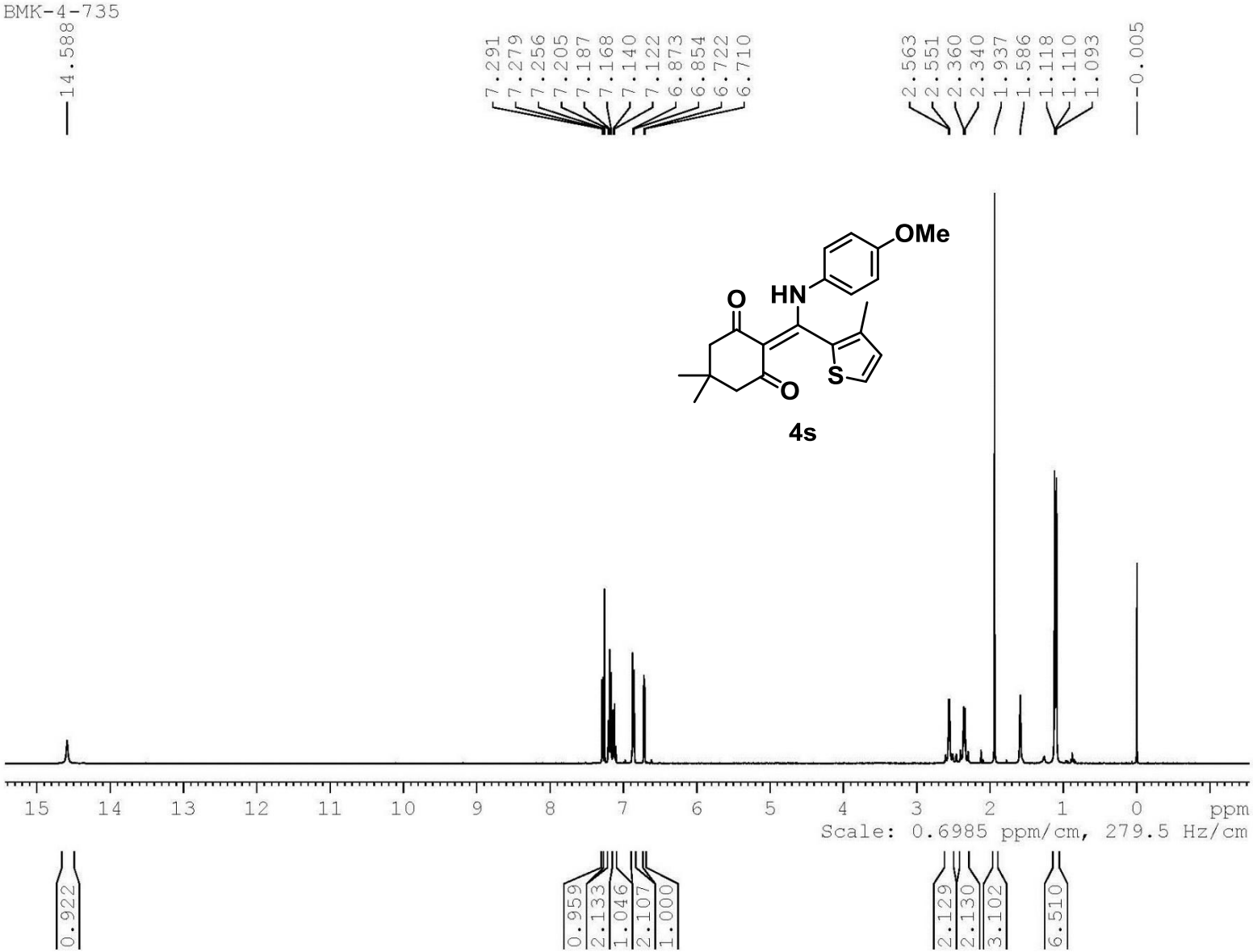

OMe
HN
S
O
O
O
4p
BMK-5-914C
181.953
165.976
160.437
158.516
154.197
137.610
134.352
129.989
127.951
127.799
126.184
125.632
125.344
120.343
116.816
114.297
113.977
99.045
77.470
77.152
76.834
55.417
14.555
ppm
0
20
40
60
80
100
120
140
160
180
200

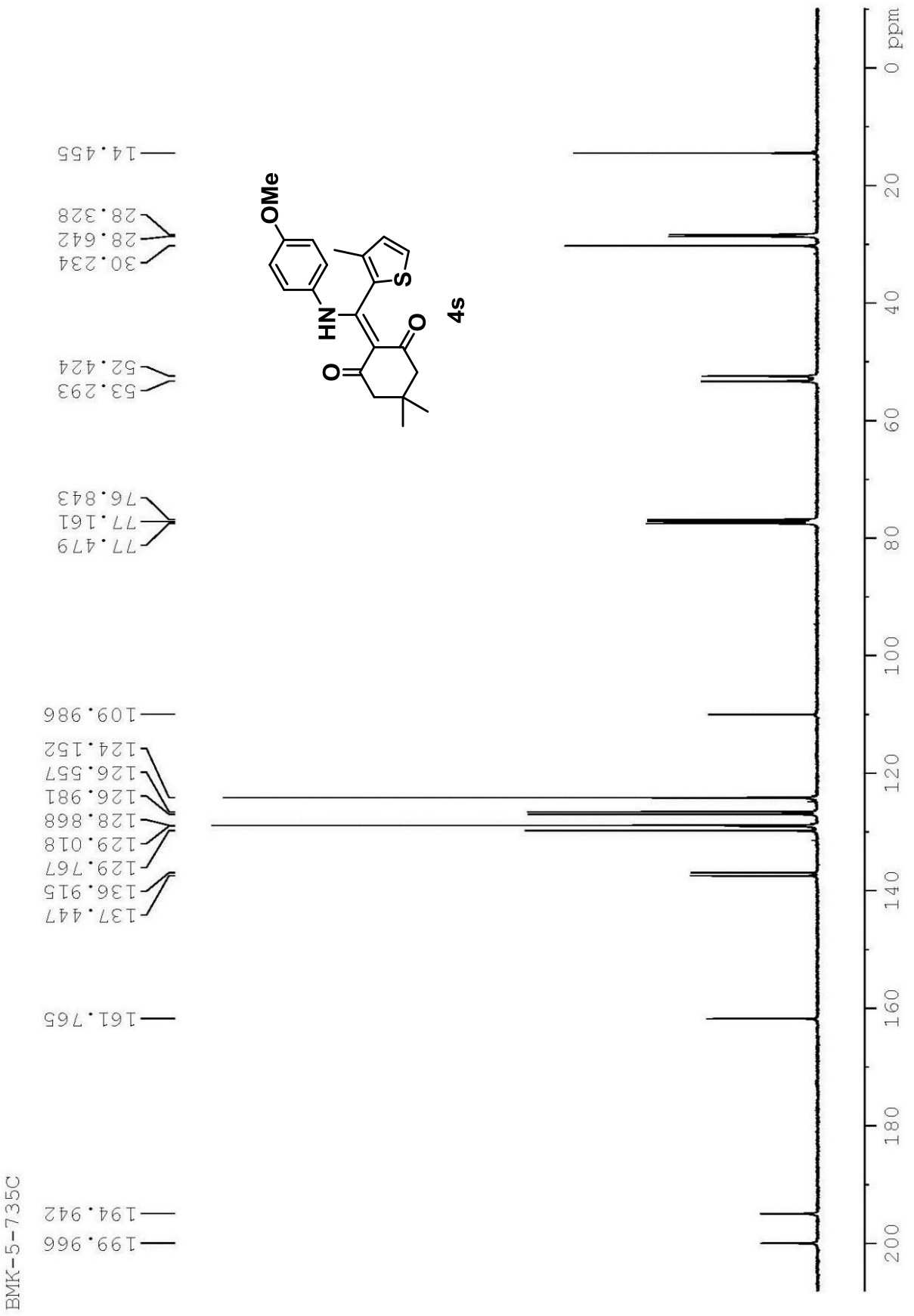
BMK-5-287
14.708
0.000
1.115
2.329
2.573
6.749
6.768
7.047
7.050
7.058
7.066
7.072
7.083
7.087
7.095
7.101
7.115
7.119
7.133
7.138
7.142
7.261
7.266
7.279
7.282
7.297
7.302
7.306
7.311
7.318
7.334
7.337
HN
O
O
4q
0.768
2.653
4.789
1.950
2.000
1.980
5.886
Scale: 0.6809 ppm/cm, 272.4 Hz/cm
0 ppm
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15


BMK-5-887C
200.379
195.332
169.219
137.204
134.049
129.000
128.750
128.254
127.743
126.415
125.128
108.490
77.468
77.150
76.831
53.313
52.476
30.339
28.486
HN
O
O
4q
0 ppm
20
40
60
80
100
120
140
160
180
200

BMK-5-893-1
14.394
1.128
2.472
3.759
6.712
6.717
6.729
6.734
6.806
6.814
6.819
6.836
6.844
6.922
6.931
6.934
6.943
7.280
7.404
7.417
7.419
OMe
HN
O
O
S
4r
ppm
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
6.386
4.390
3.000
2.163
3.136
1.058
1.027
1.109

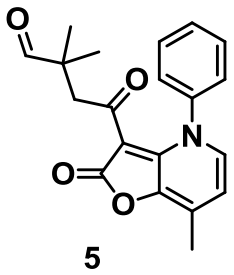

BMK-5-893C
197.385
162.095
158.146
134.250
130.164
129.178
128.419
127.023
126.135
114.060
109.698
76.829
77.147
77.465
55.360
52.840
30.374
28.472
OMe
HN
O
O
S
4r
0 ppm
20
40
60
80
100
120
140
160
180
200


BMK-4-735
14.588
7.291
7.279
7.256
7.205
7.187
7.168
7.140
7.122
6.873
6.854
6.722
6.710
2.563
2.551
2.360
2.340
1.937
1.586
1.118
1.110
1.093
0.005
OMe
HN
O
O
S
4s
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
Scale: 0.6985 ppm/cm, 279.5 Hz/cm
0.922
0.959
2.133
1.046
2.107
1.000
2.129
2.130
3.102
6.510

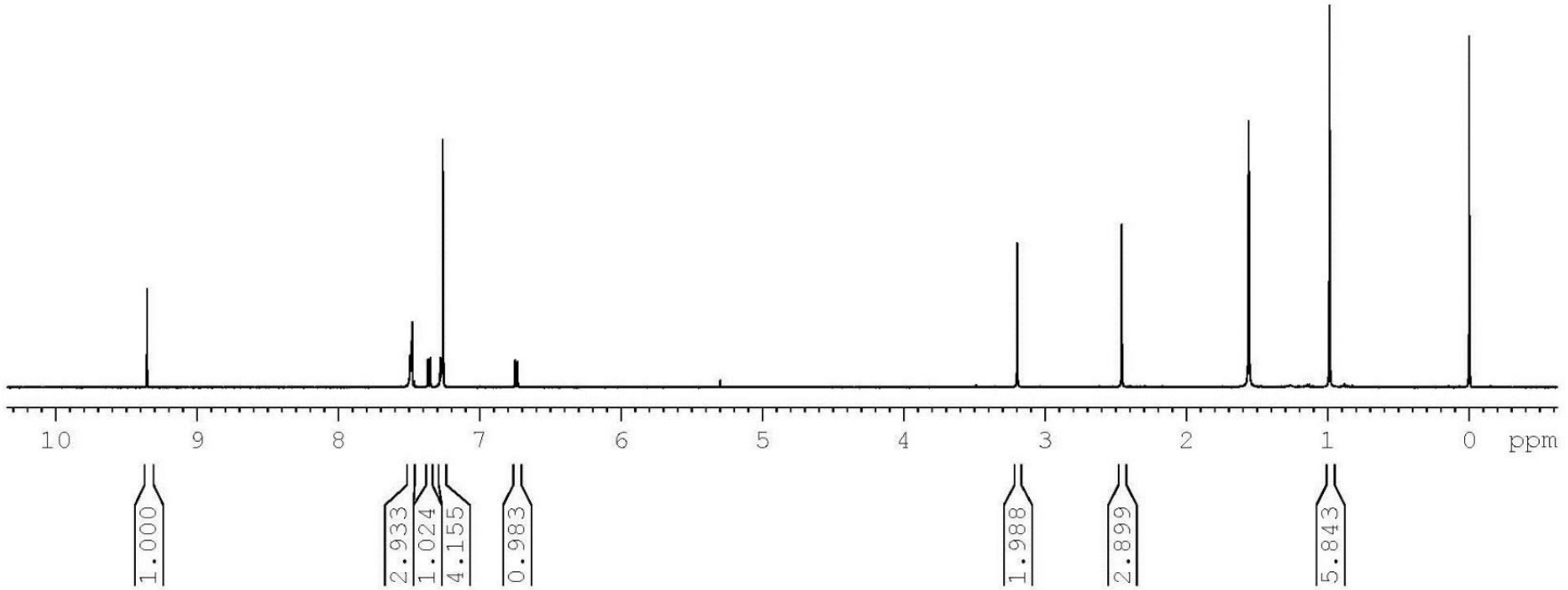

BMK-5-735C
199.966
194.942
161.765
137.447
136.915
129.767
129.018
128.868
126.981
126.557
124.152
109.986
77.479
77.161
76.843
53.293
52.424
30.234
28.642
28.328
14.455
OMe
HN
O
O
S
4s
0 ppm
20
40
60
80
100
120
140
160
180
200

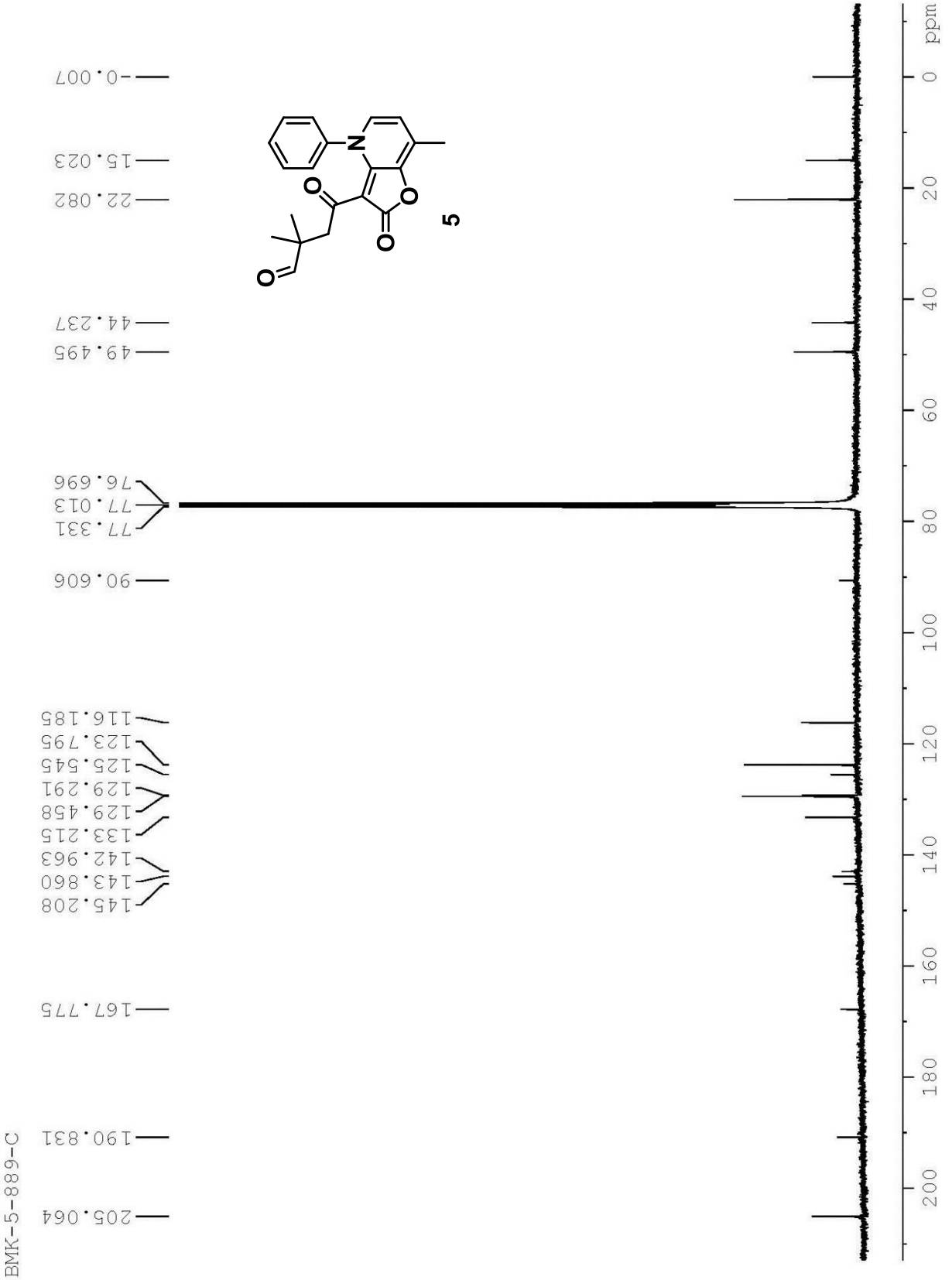
BMK-5-889-N


9.354
7.495
7.489
7.485
7.478
7.368
7.350
7.280
7.271
7.267
7.262
7.256
6.751
6.734
3.199
2.459
1.561
0.989
0.000


O
O
N
O
O

5


10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
2.933
1.024
4.155
0.983
1.988
2.899
5.843


BMK-5-889-C
205.064
190.831
167.775
145.208
143.860
142.963
133.215
129.458
129.291
125.545
123.795
116.185
90.606
77.331
77.013
76.696
49.495
44.237
22.082
15.023
-0.007
ppm
0
20
40
60
80
100
120
140
160
180
200
O
O
O
O
N
5