Supporting Information

Synthesis of 3-[(Coumarinyl)carbonyl]-3a,8b-dihyroindeno[1,2-b]pyrrole-4(1*H*)-ones and Their Conversion to Coumarin Bearing Spiro[isobenzofuran-1,2'-pyrrole] Moiety compounds *via* Oxidative Cleavage Reaction

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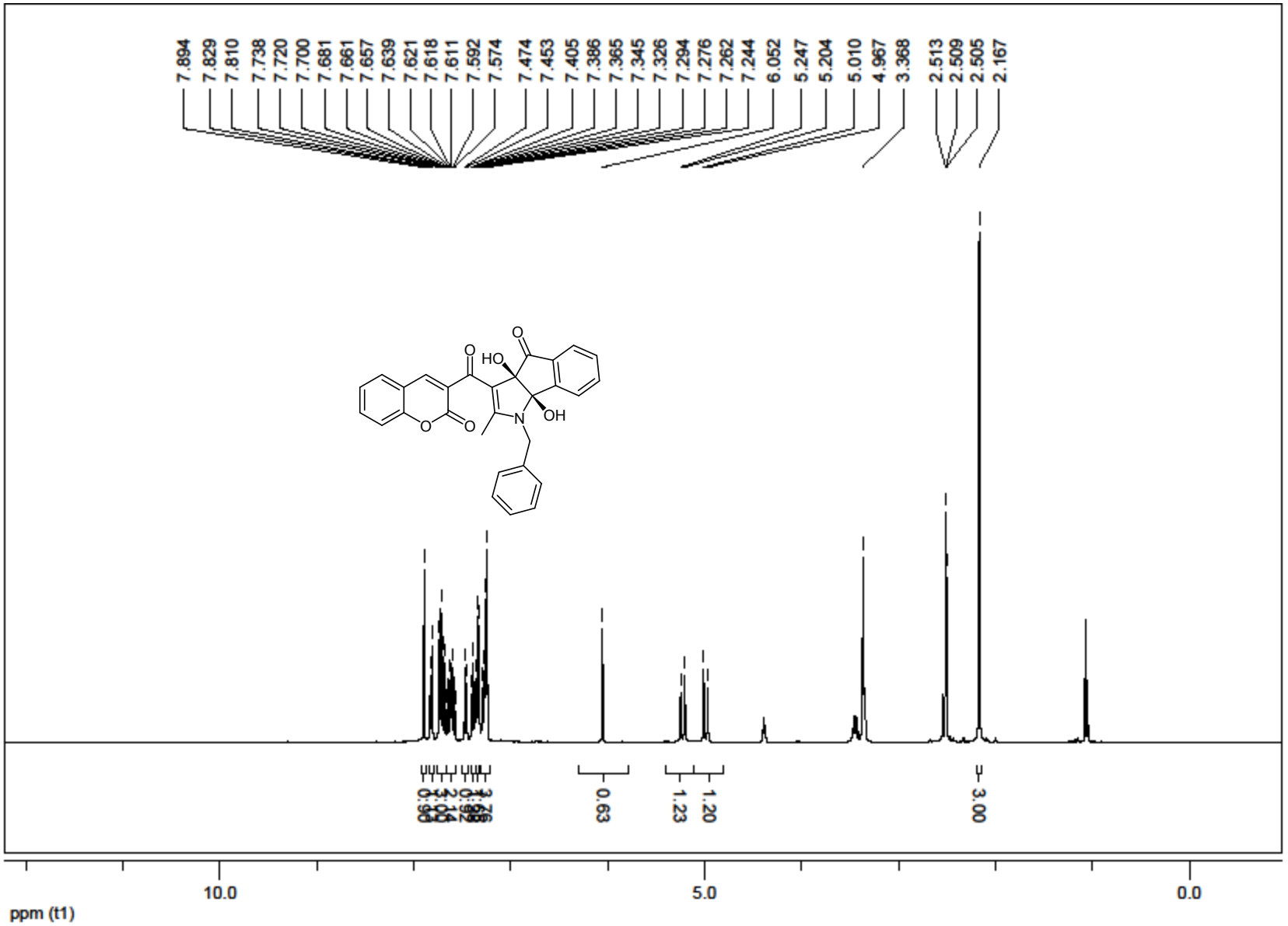
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7.345
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7.294
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7.262
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2.505
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O
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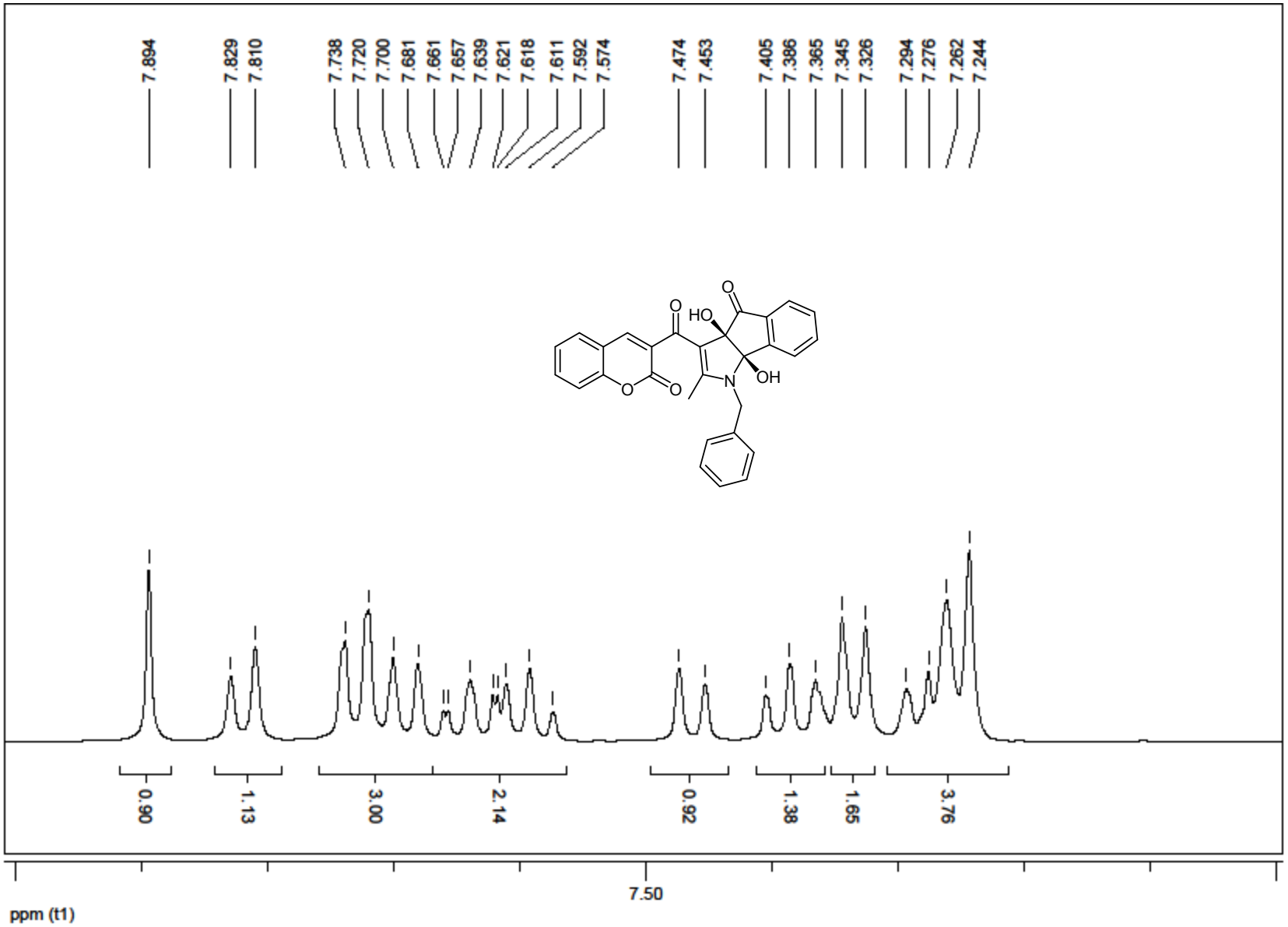
ppm (t1)

^{1}H NMR of 3a



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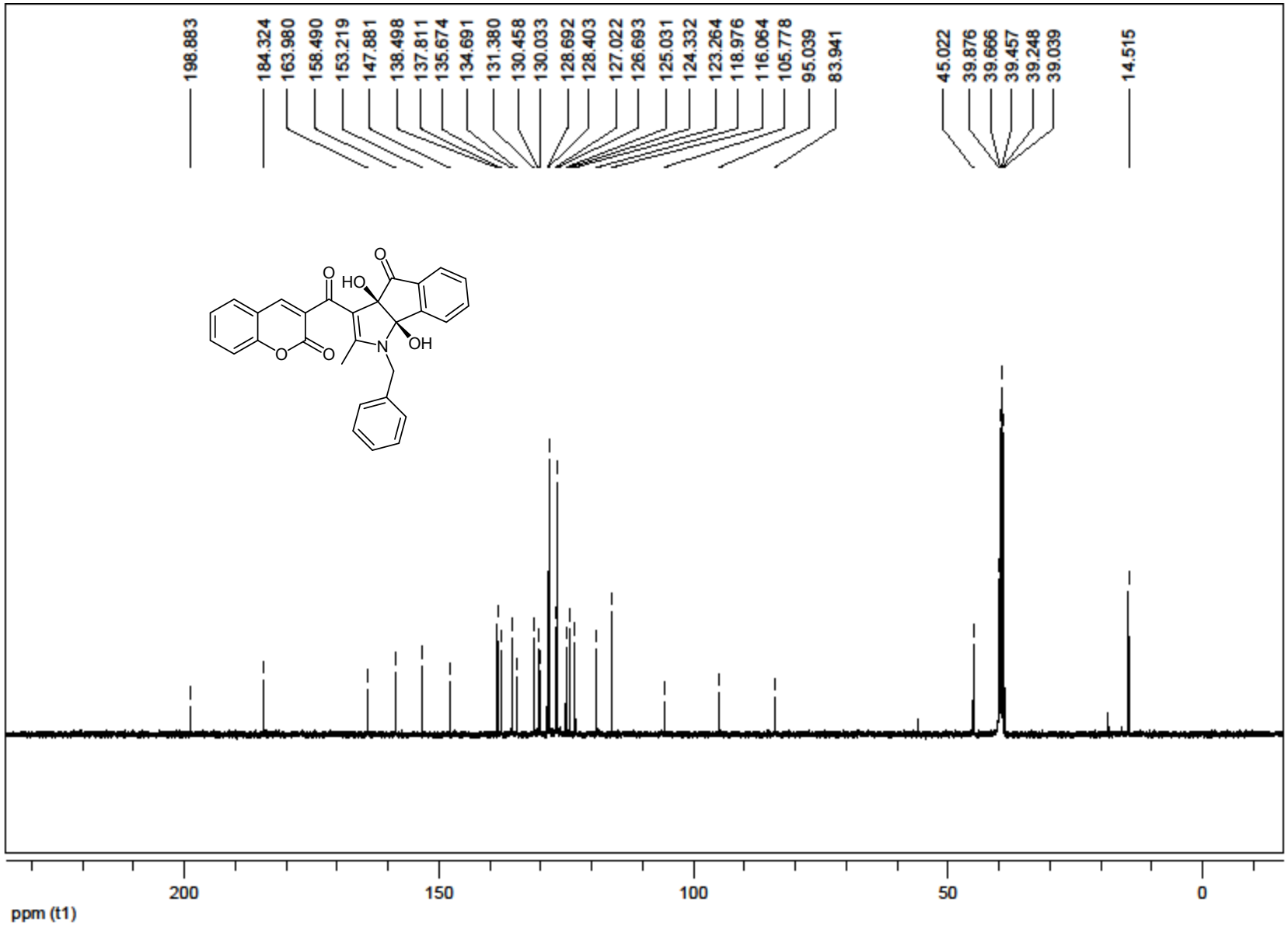
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128.692
128.403
127.022
126.693
125.031
124.332
123.264
118.976
116.064
105.778
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83.941
45.022
39.876
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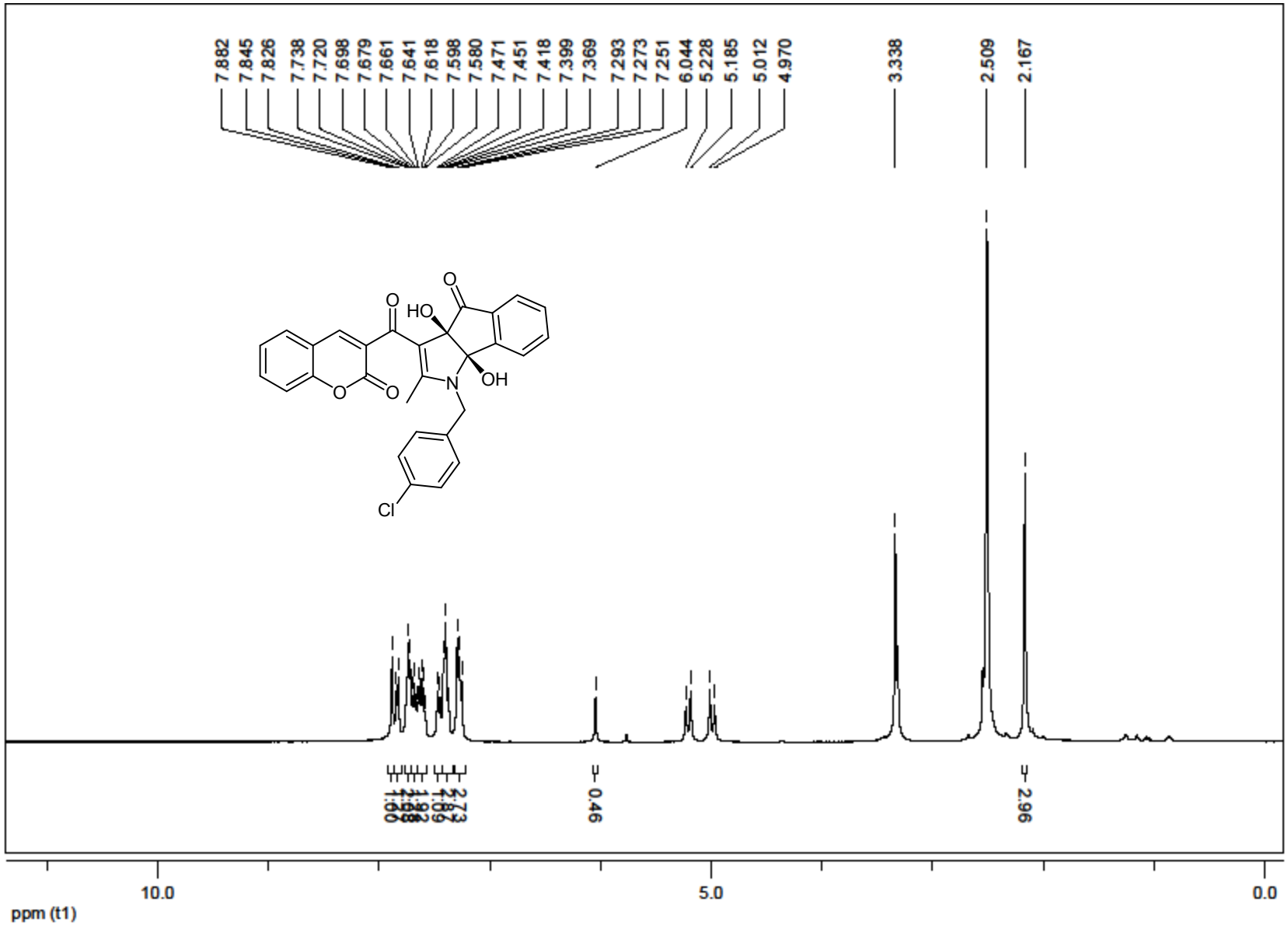
ppm (t1)

^{13}C NMR of 3a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7.418
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7.273
7.251
6.044
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5.185
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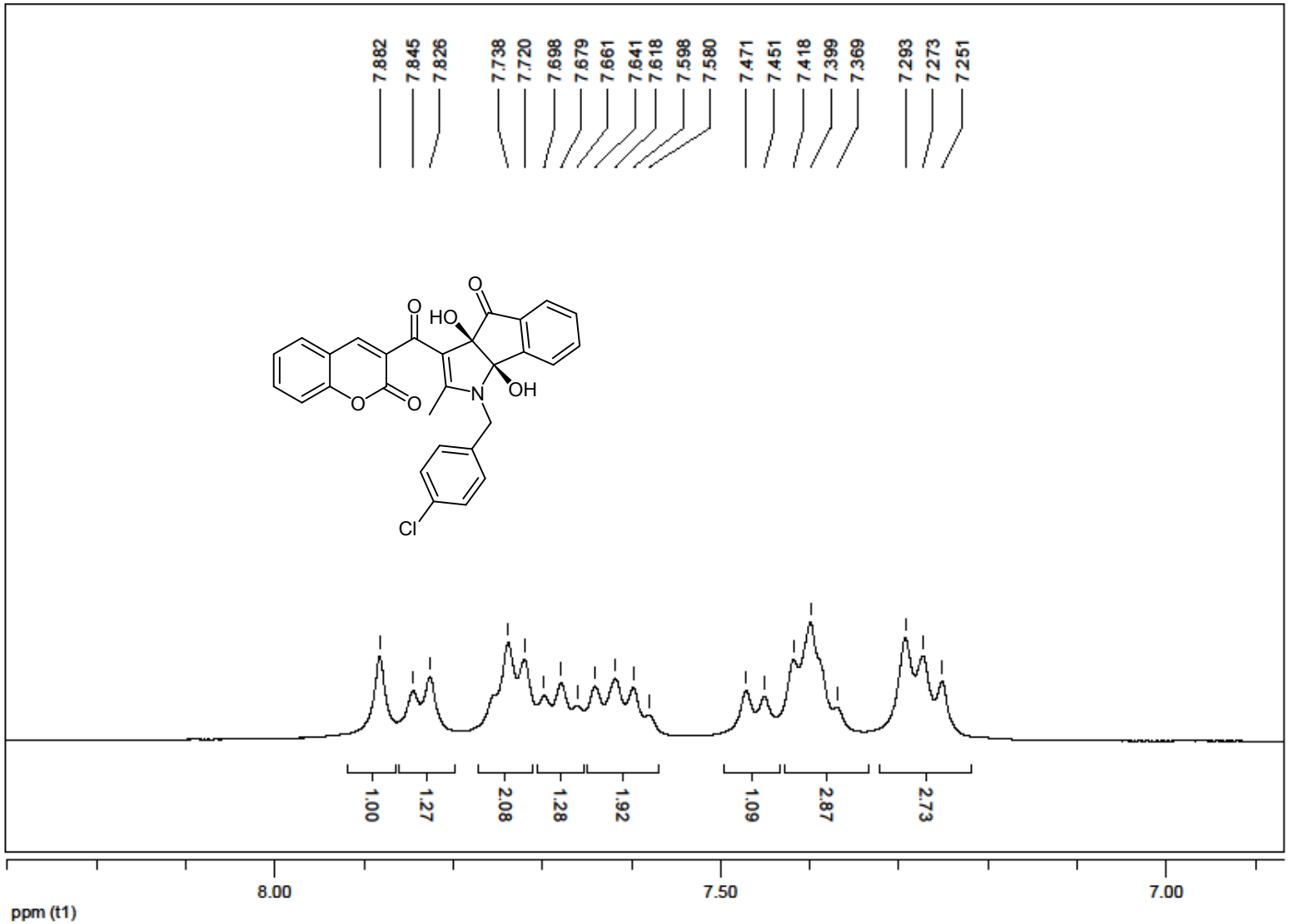
^{1}H NMR of 3b



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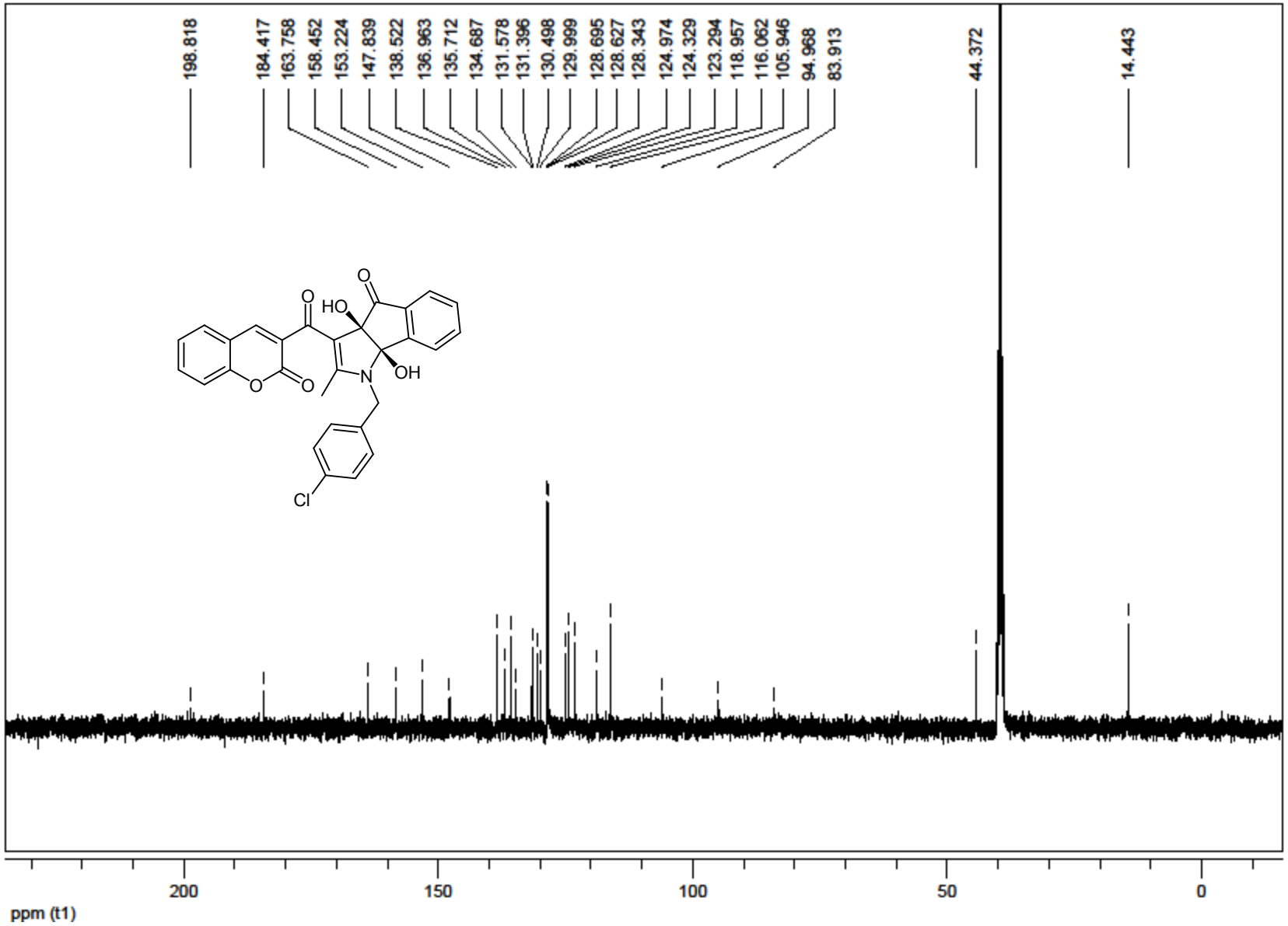
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124.329
123.294
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116.062
105.946
94.968
83.913
44.372
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O
Cl
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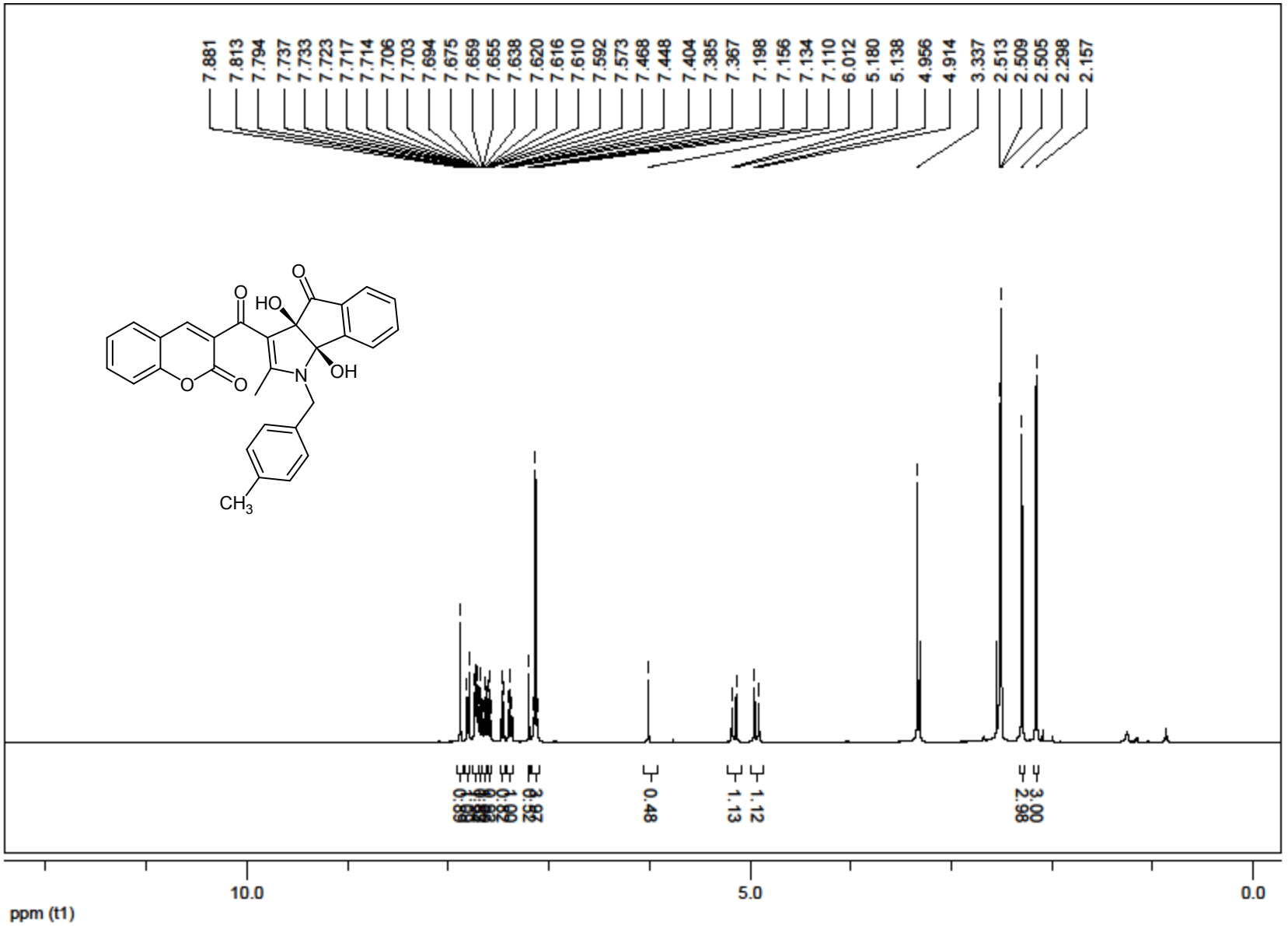
50
0
ppm (t1)

^{13}C NMR of 3b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7.655
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7.616
7.610
7.592
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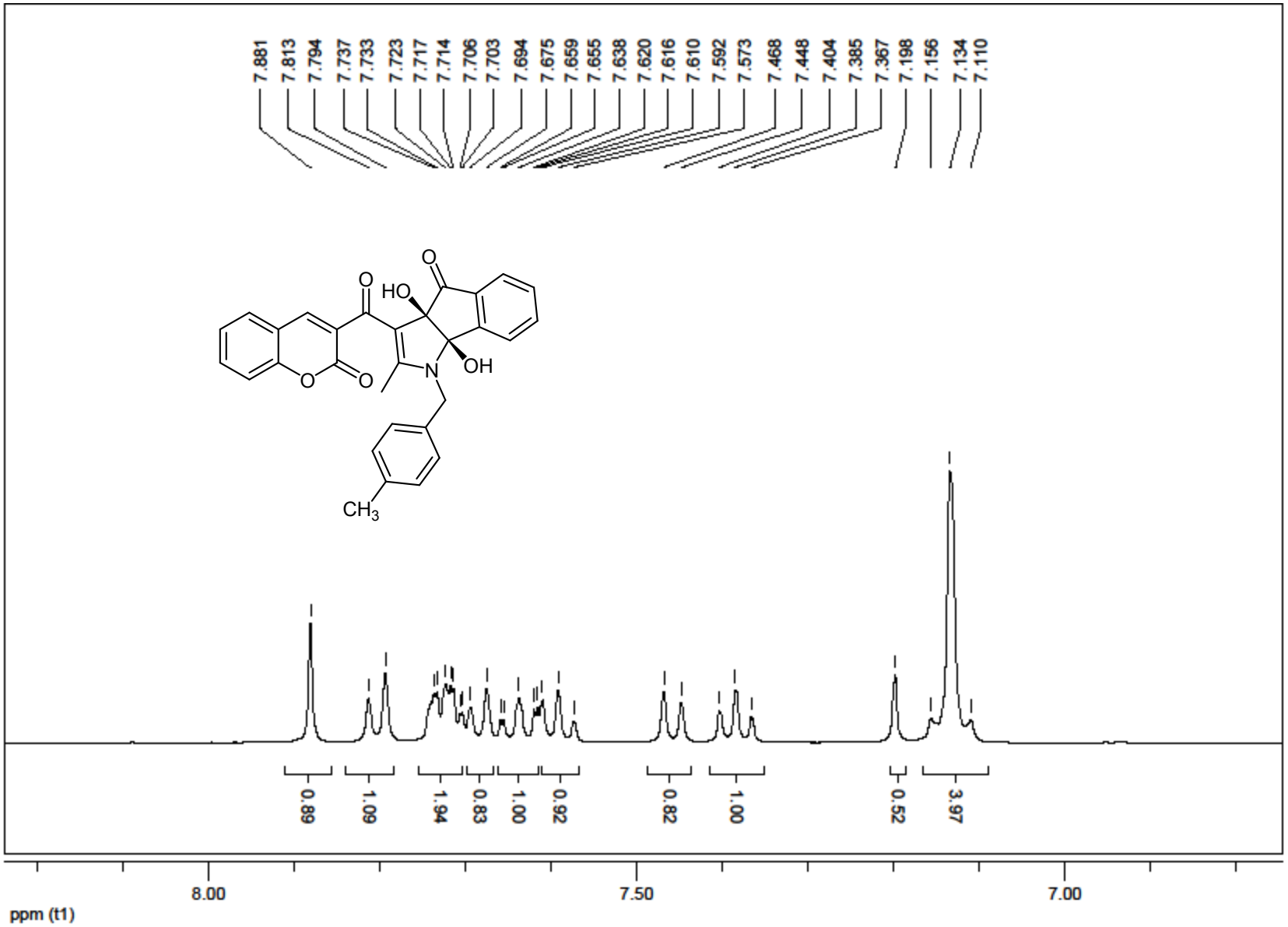

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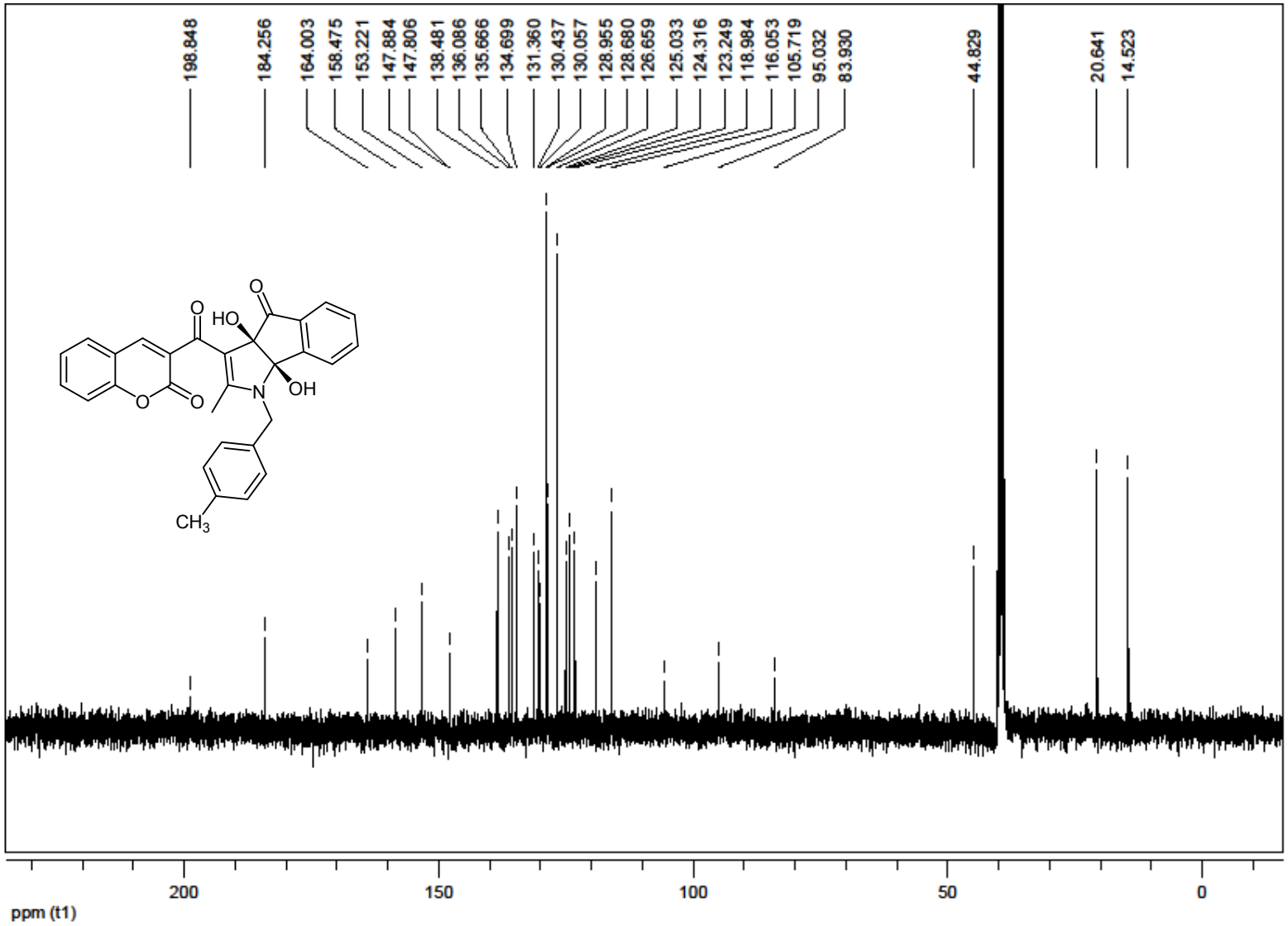
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126.659
125.033
124.316
123.249
118.984
116.053
105.719
95.032
83.930
44.829
20.641
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O
O
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OH
CH3
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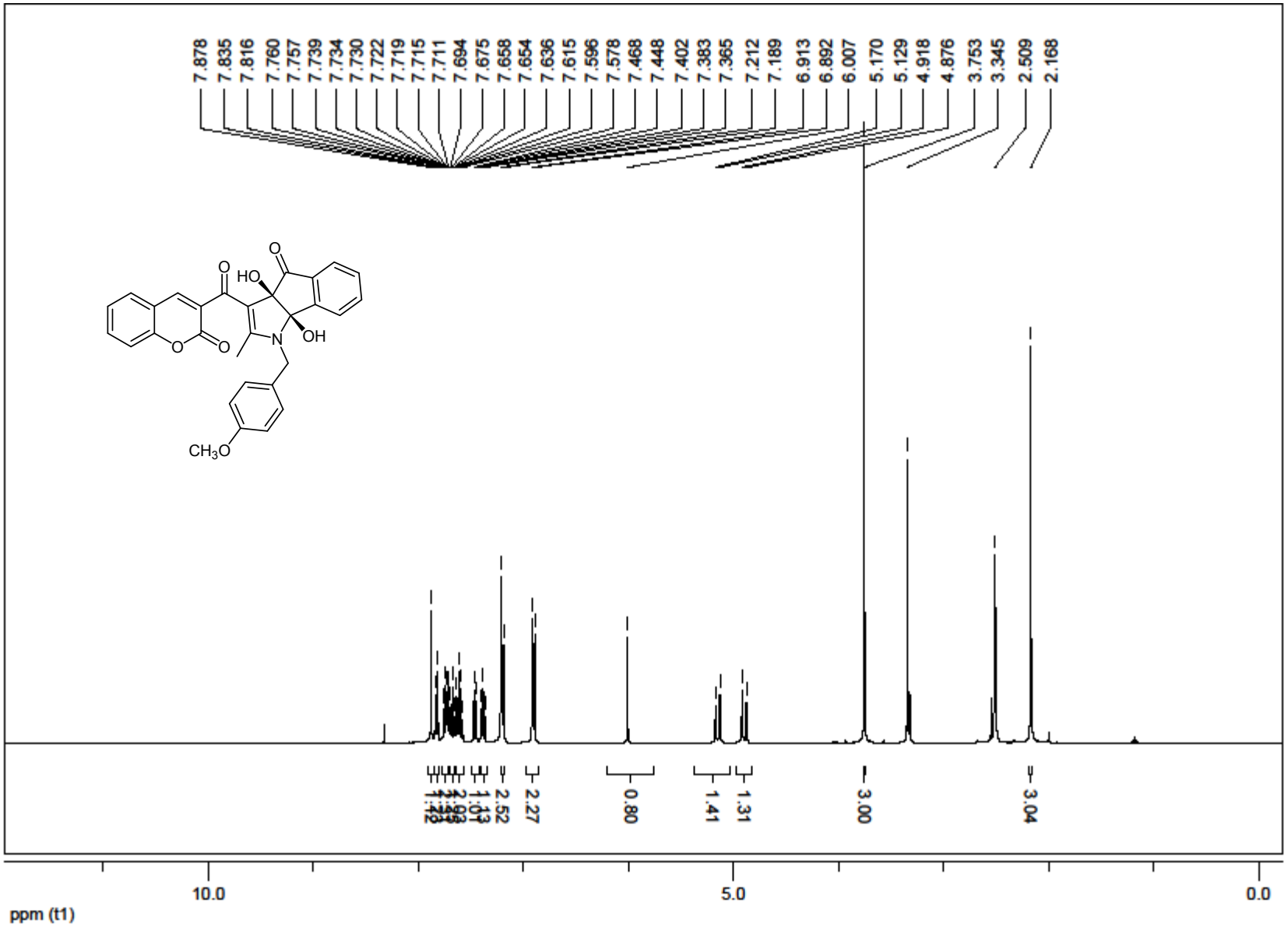
150
100
50
0
ppm (t1)

^{13}C NMR of 3c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OH
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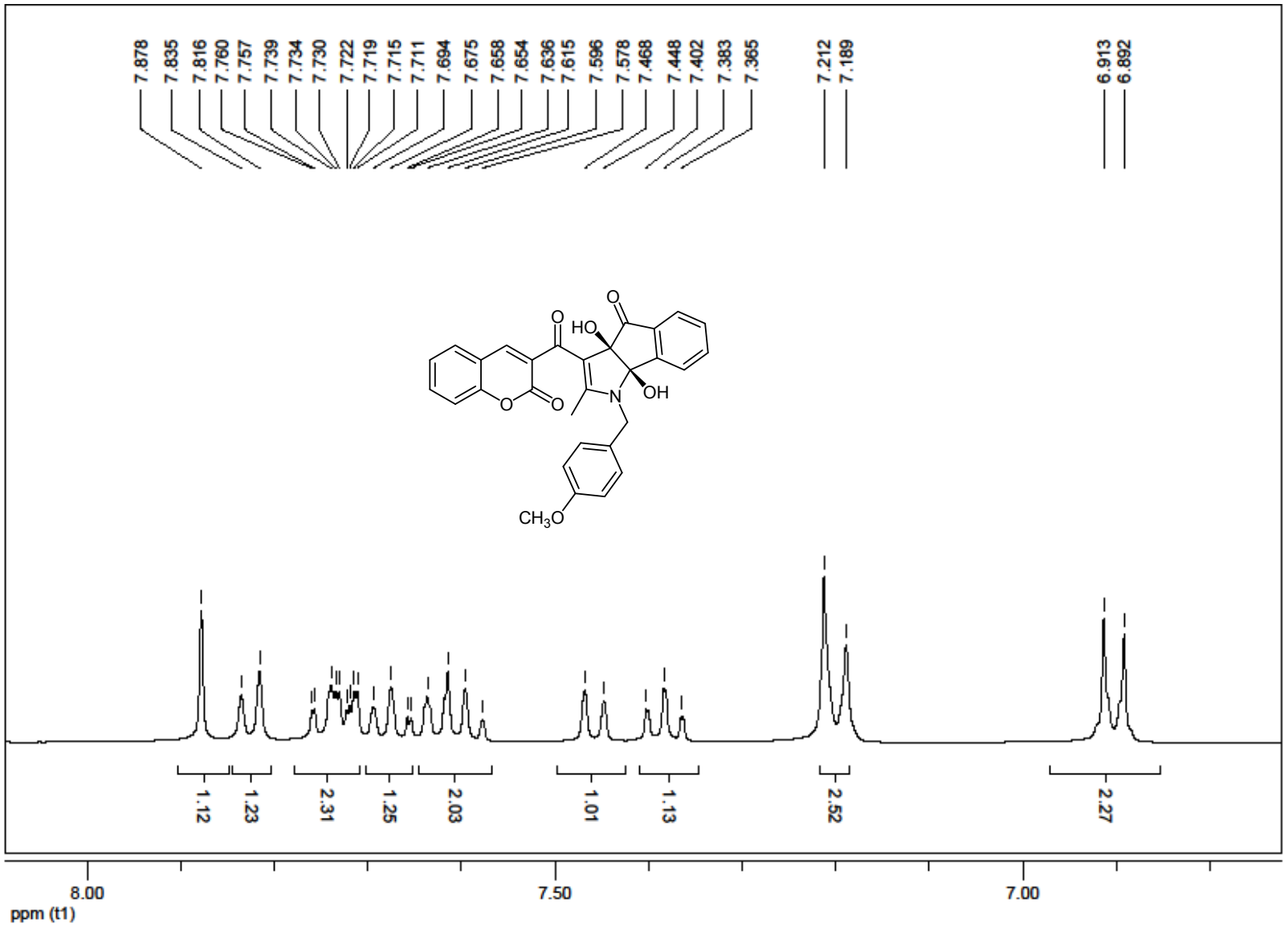
ppm (t1)

^{1}H NMR of 3d



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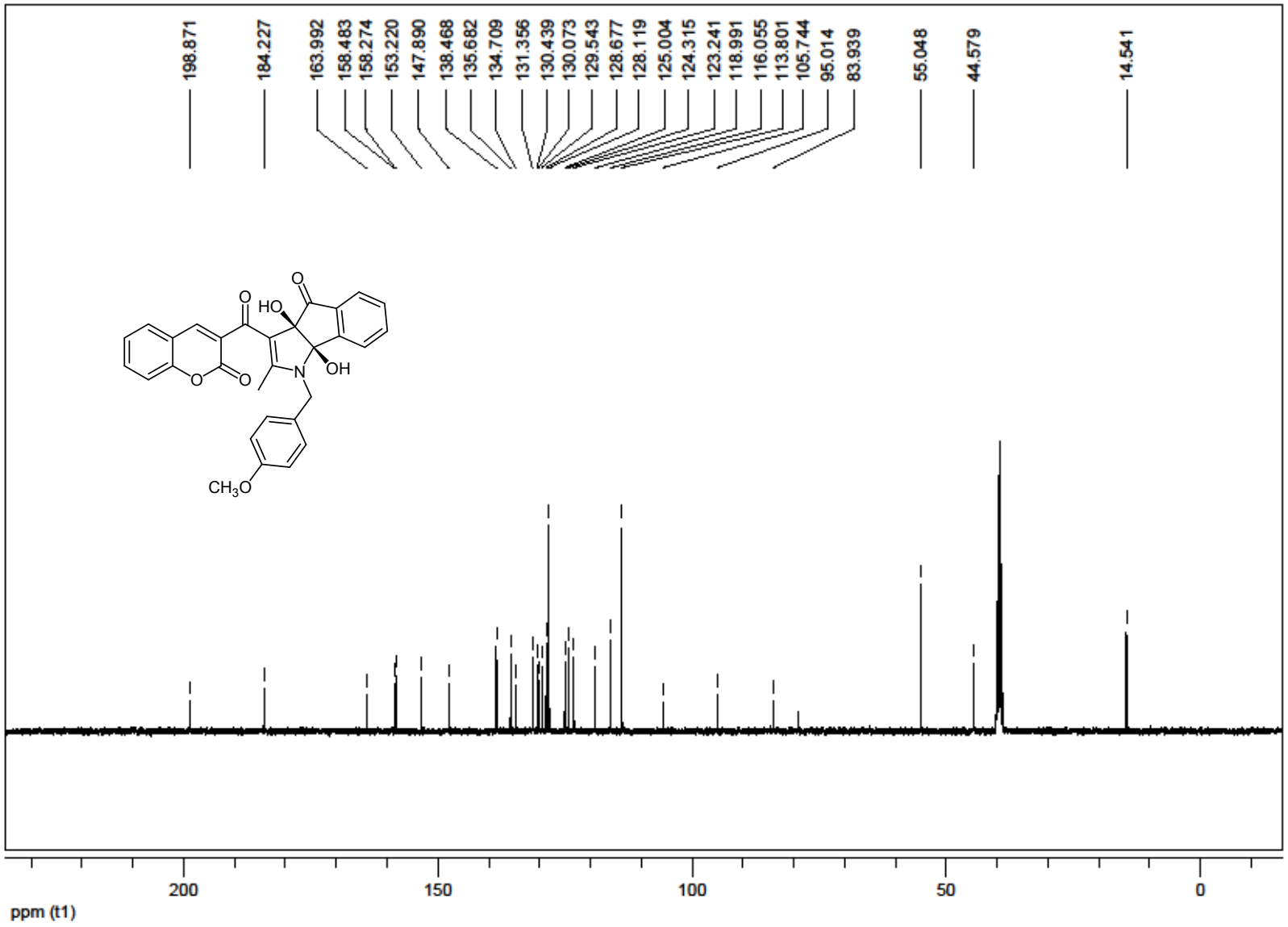
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83.939
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44.579
14.541
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O
O
CH3O
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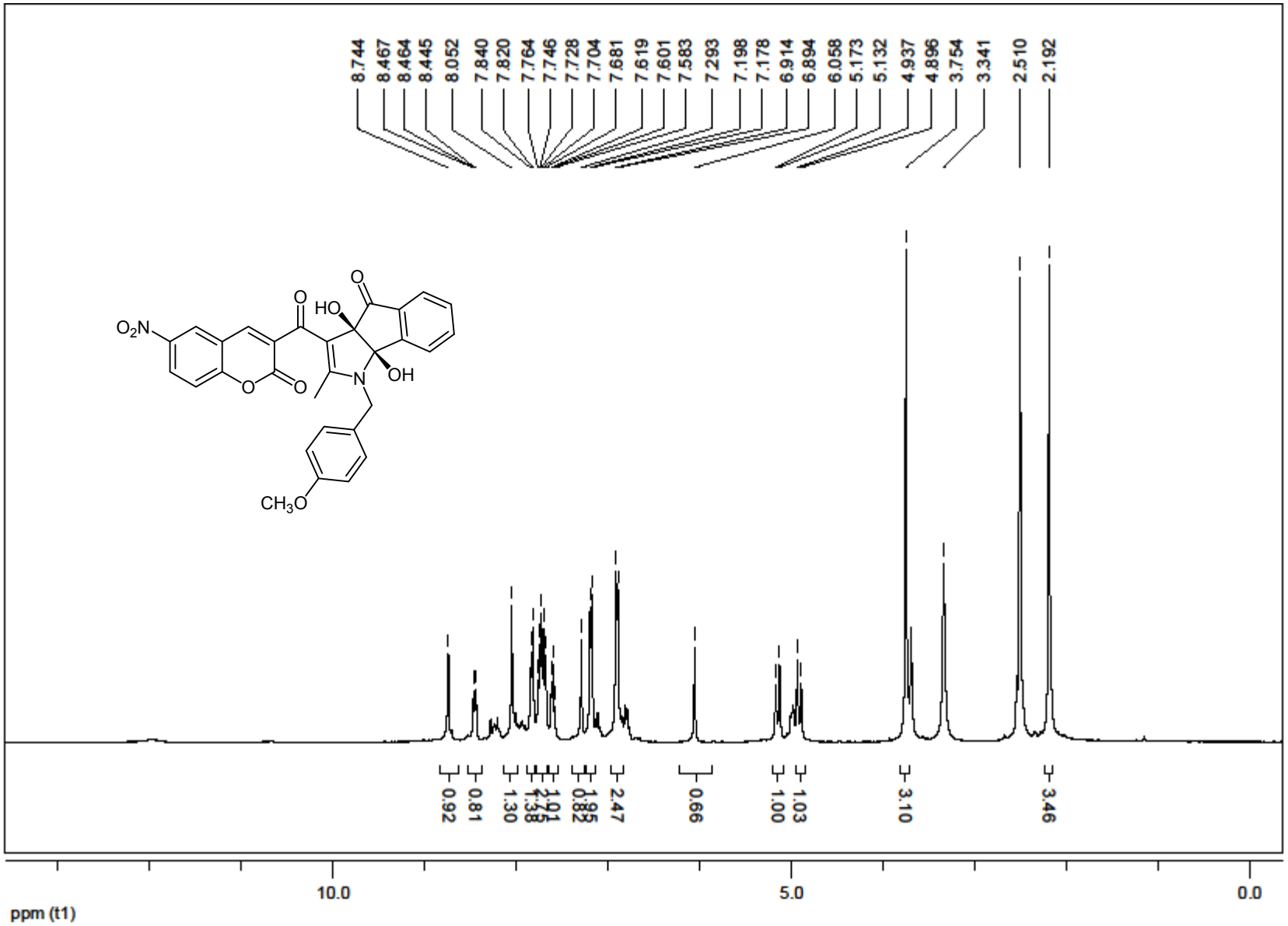
100
50
0
ppm (t1)

^{13}C NMR of 3d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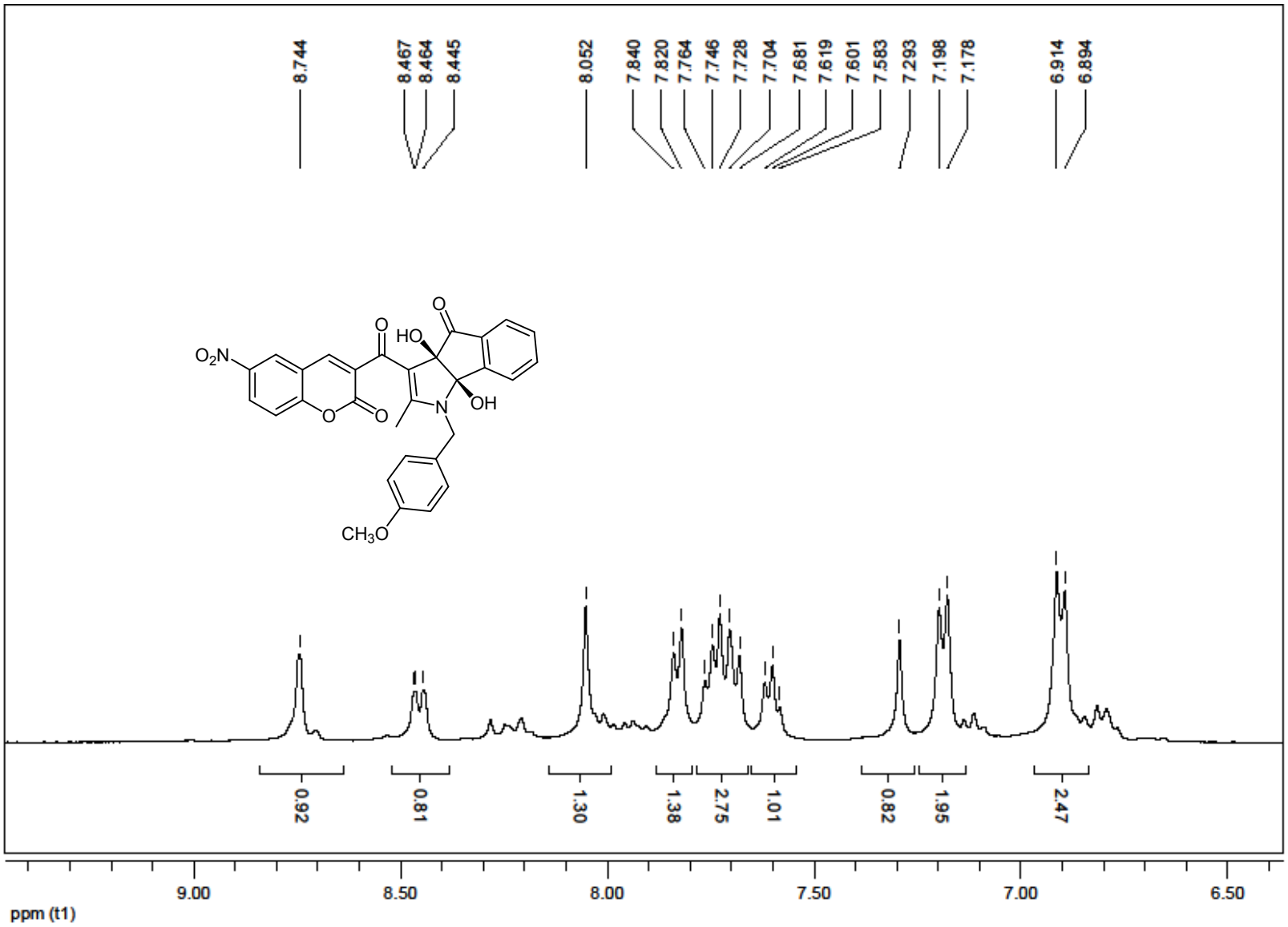
ppm (t1)

^{1}H NMR of 3e



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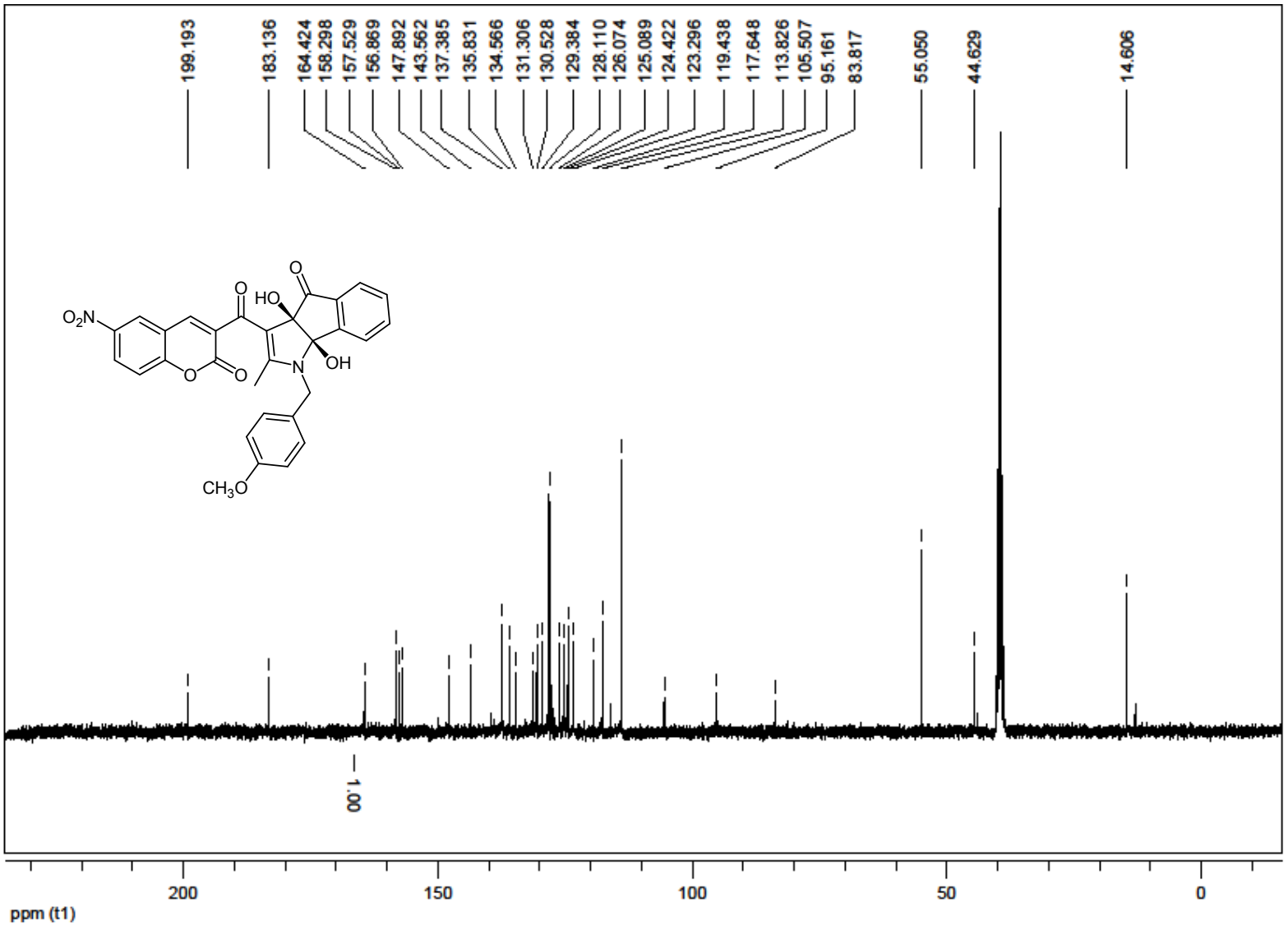
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83.817
55.050
44.629
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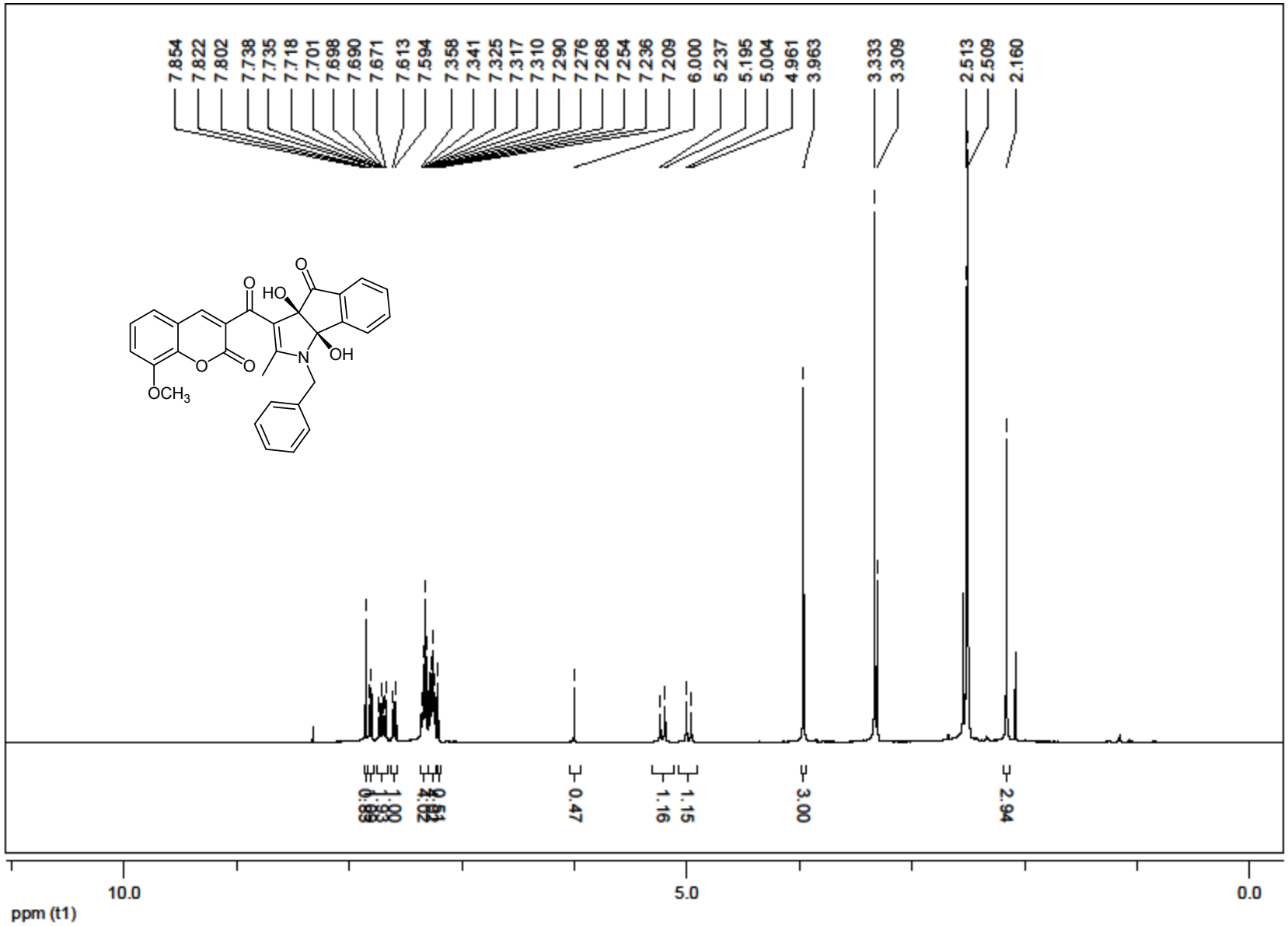
ppm (t1)

^{13}C NMR of 3e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7.254
7.236
7.209
6.000
5.237
5.195
5.004
4.961
3.963
3.333
3.309
2.513
2.509
2.160
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OH
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O
O
O
O
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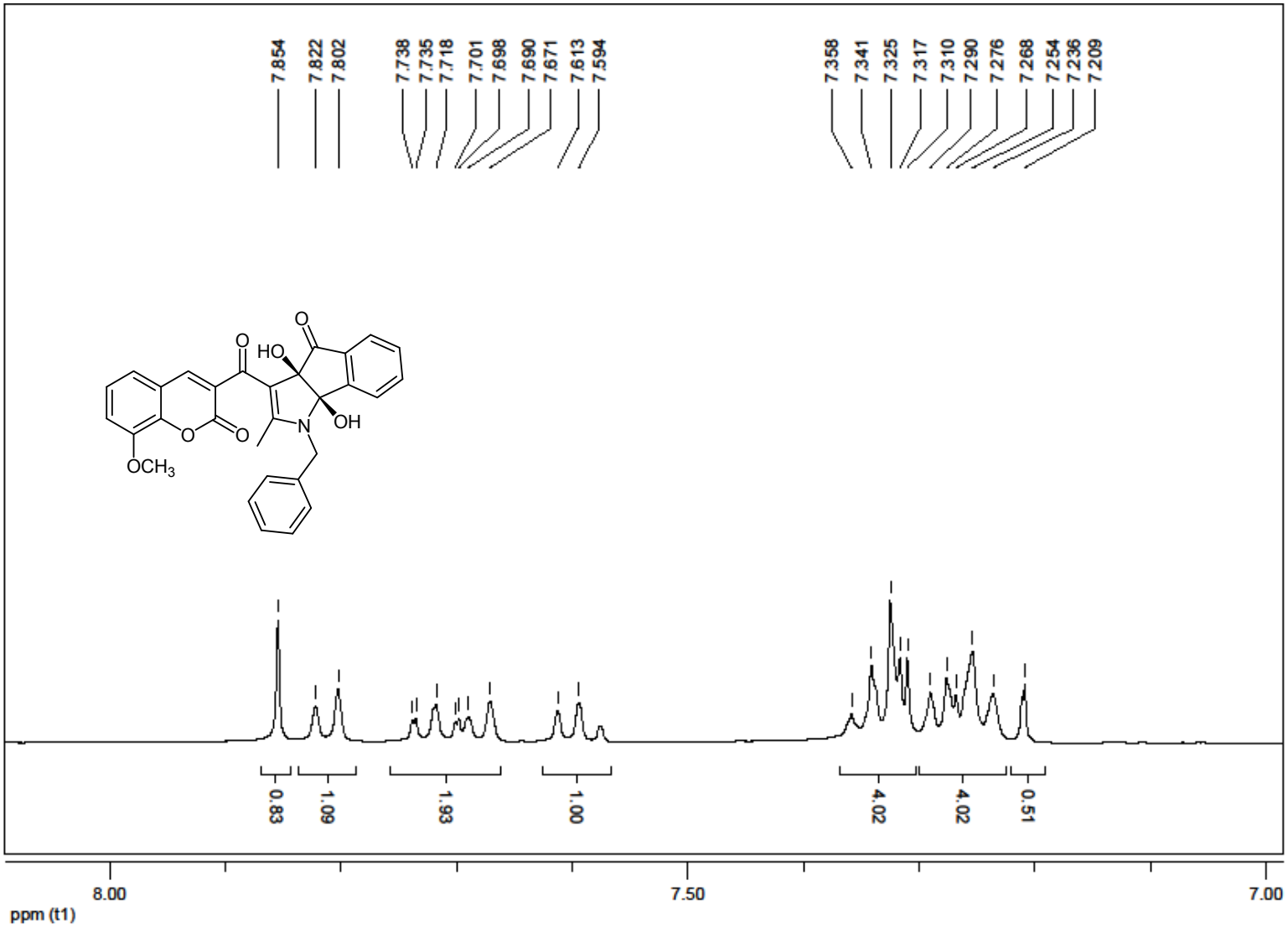
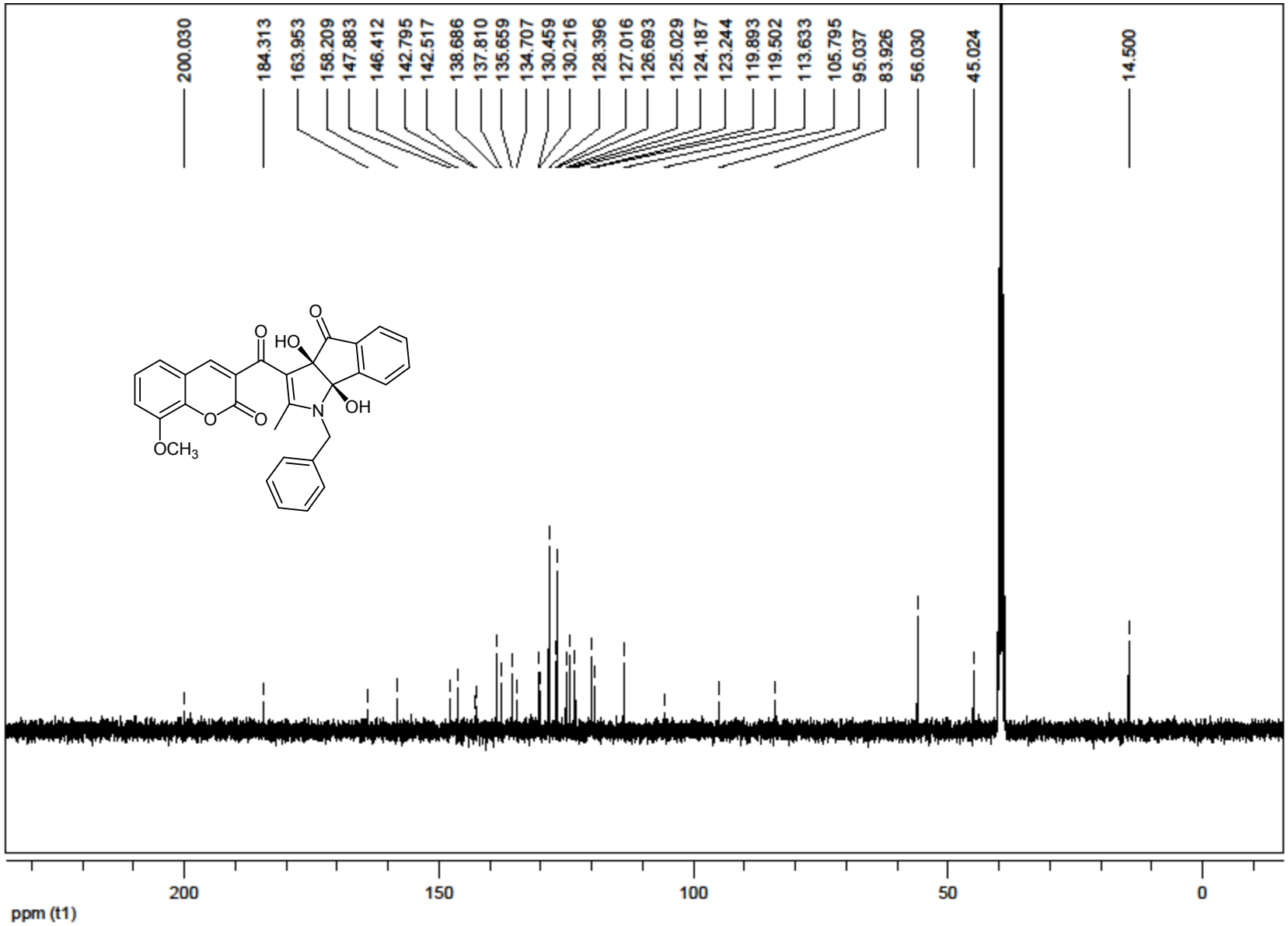
ppm (t1)

^{1}H NMR of 3f



^{1}H NMR of 3f (expand)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130.459
130.216
128.396
127.016
126.693
125.029
124.187
123.244
119.893
119.502
113.633
105.795
95.037
83.926
56.030
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100
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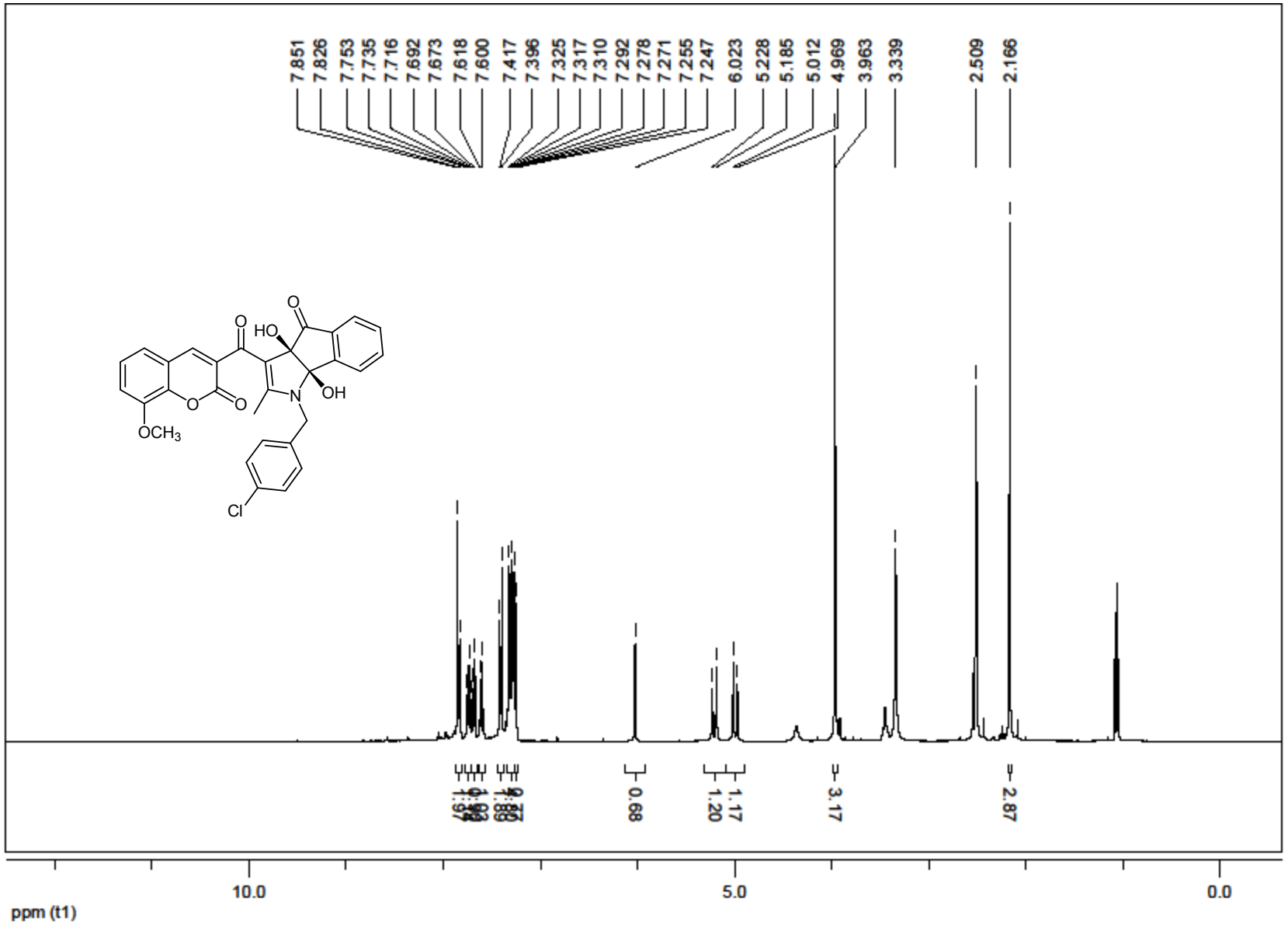
^{13}C NMR of 3f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7.292
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7.271
7.255
7.247
6.023
5.228
5.185
5.012
4.969
3.963
3.339
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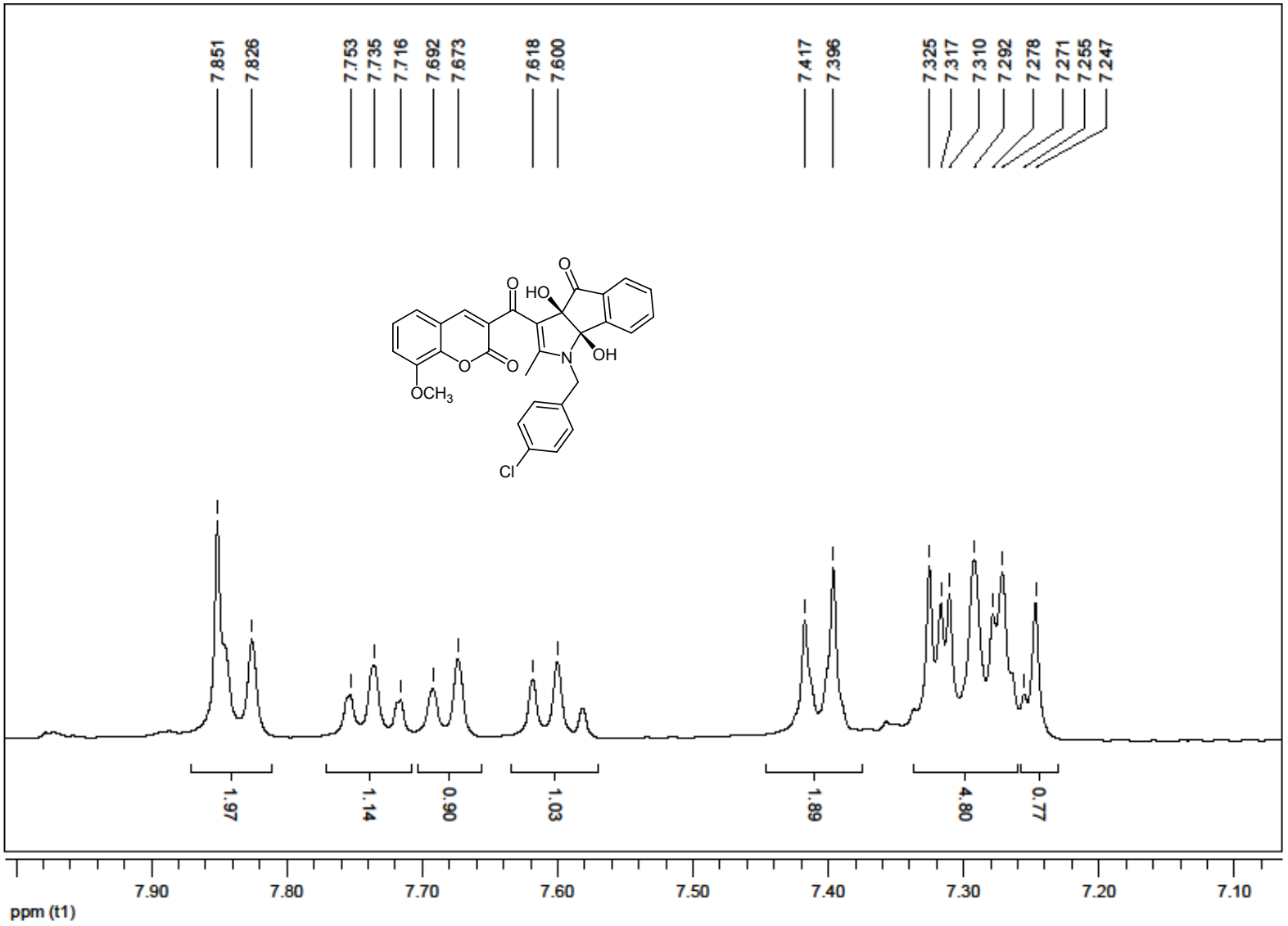
^{1}H NMR of 3g



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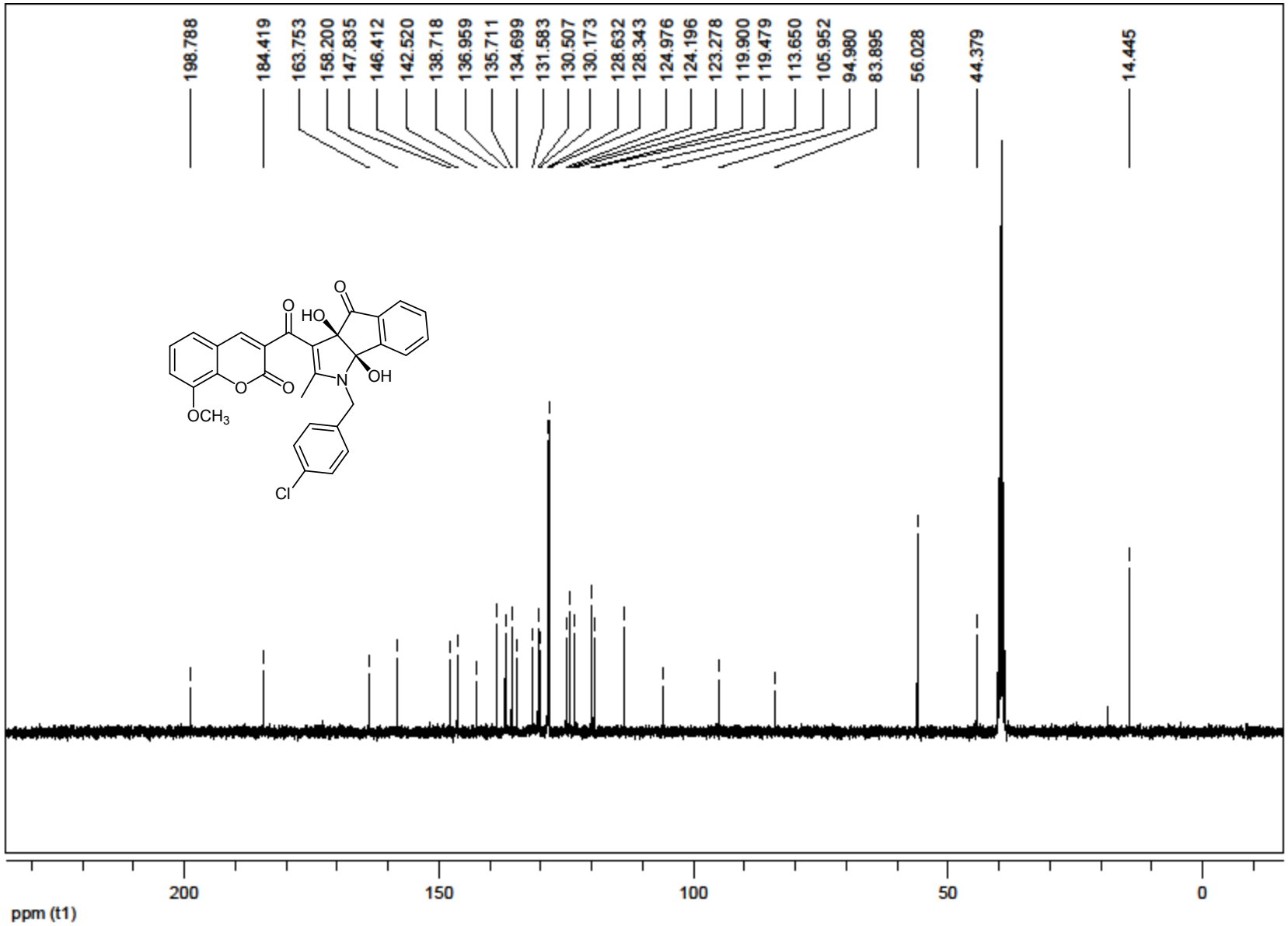
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131.583
130.507
130.173
128.632
128.343
124.976
124.196
123.278
119.900
119.479
113.650
105.952
94.980
83.895
56.028
44.379
14.445
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OH
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Cl
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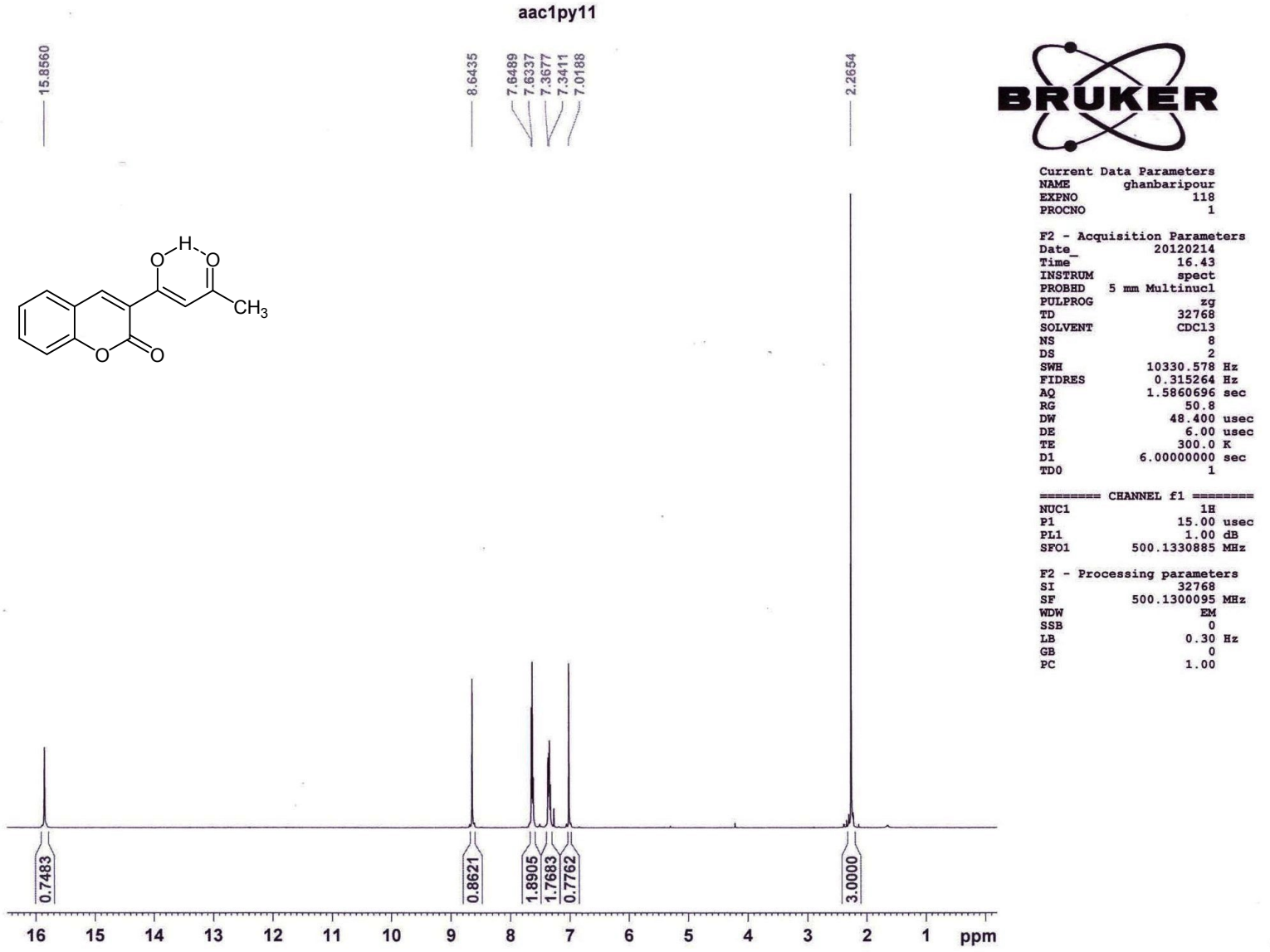
^{13}C NMR of 3g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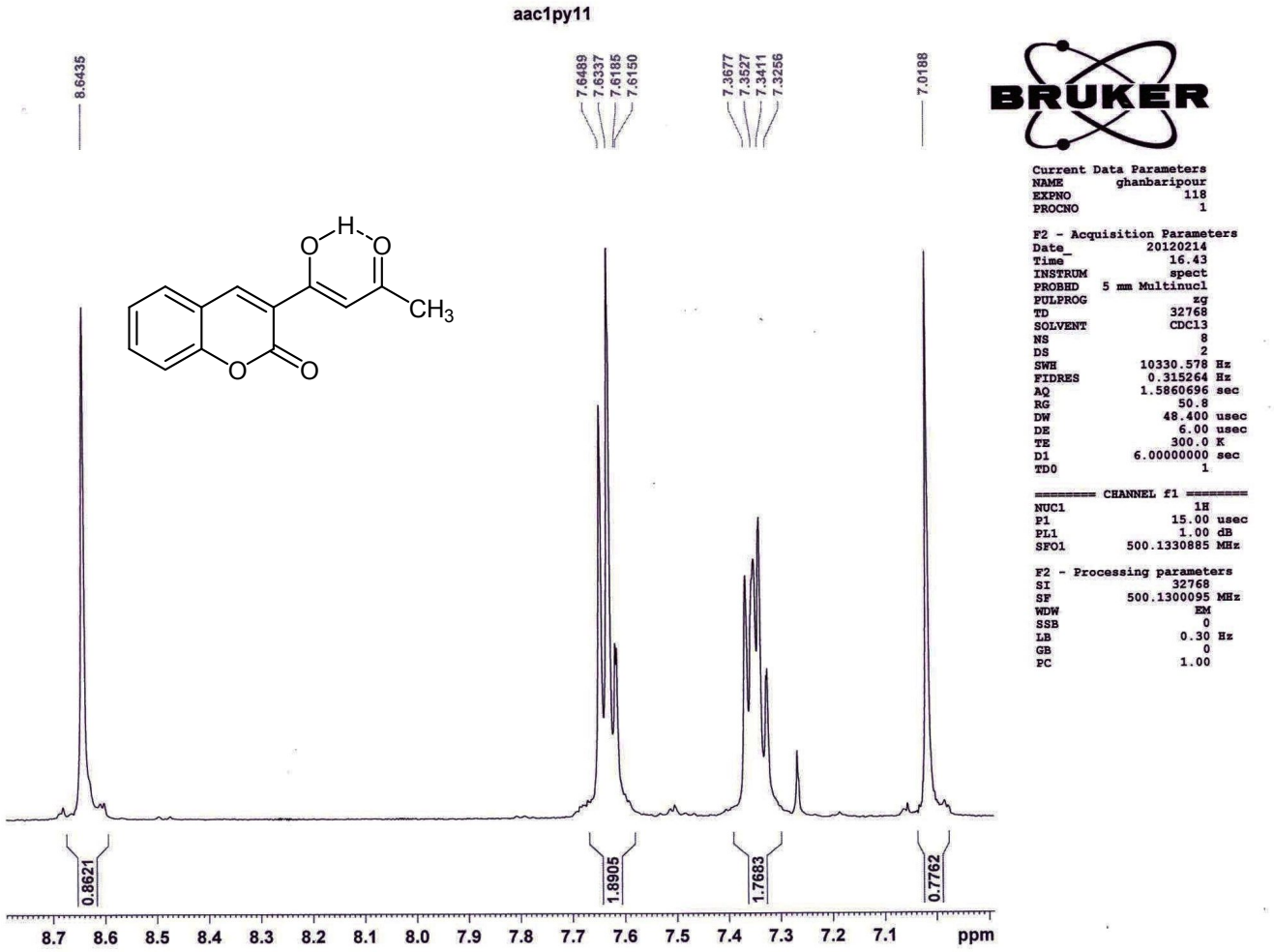
^{1}H NMR of 4a



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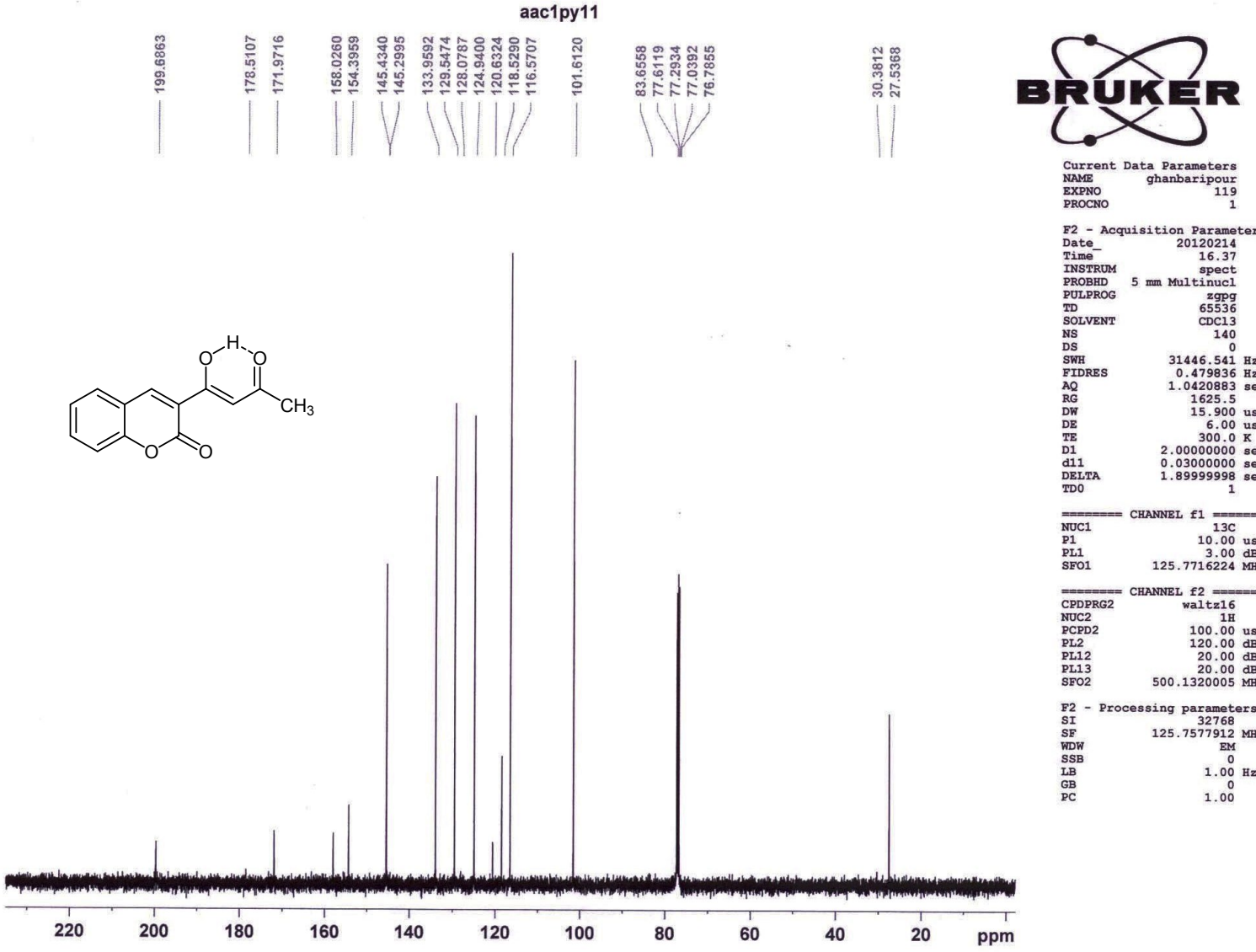
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20
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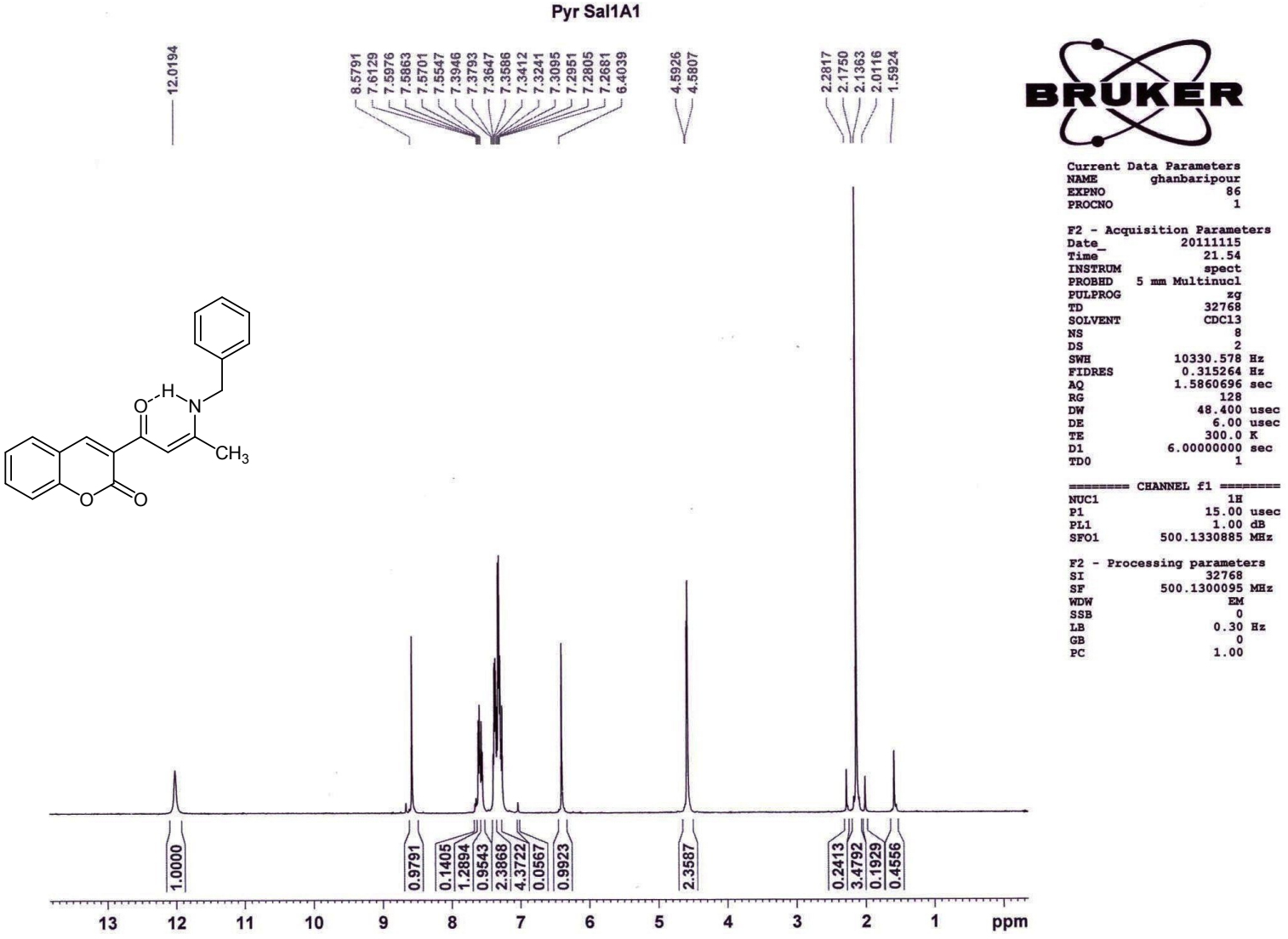
^{13}C NMR of 4a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5
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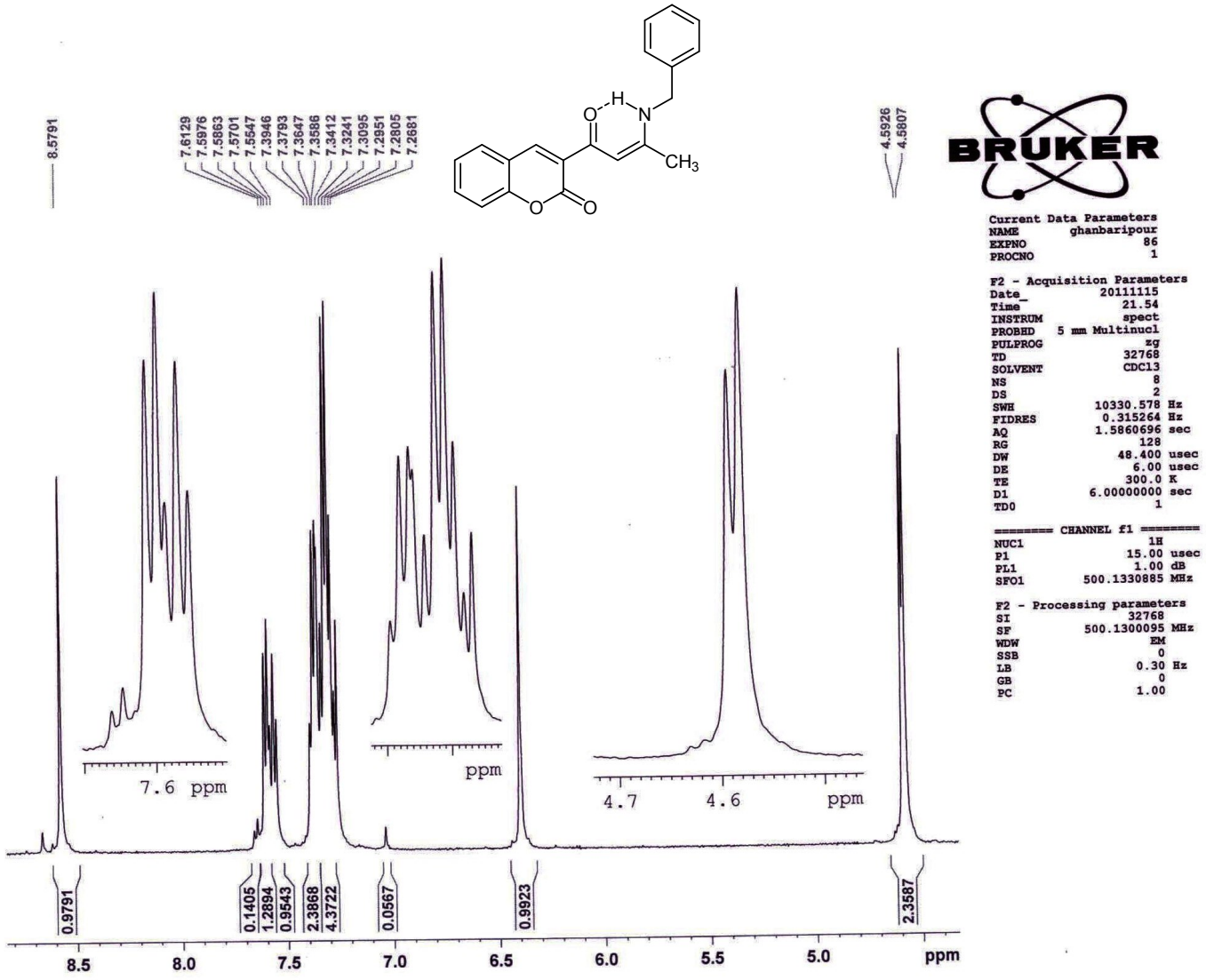
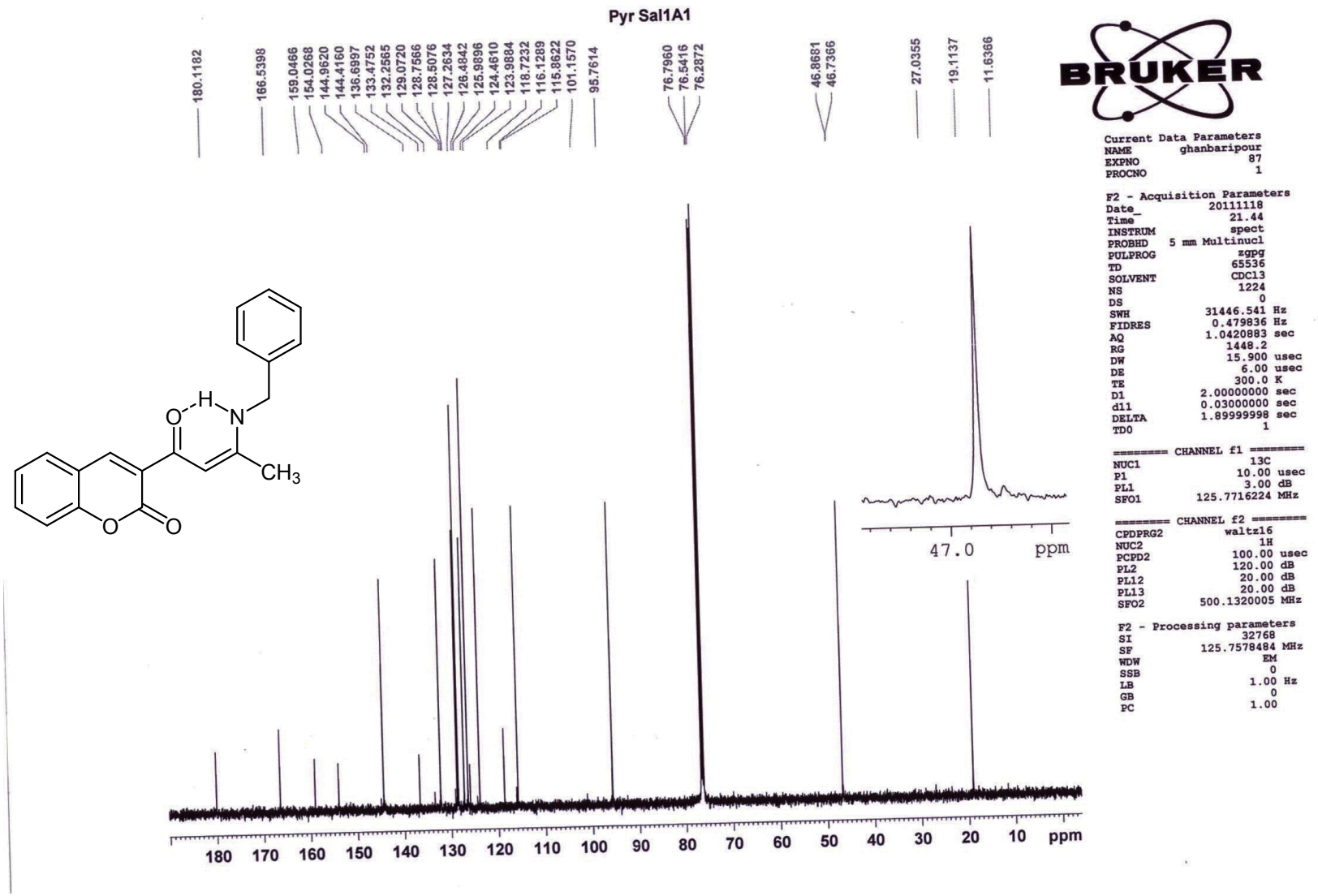
ppm

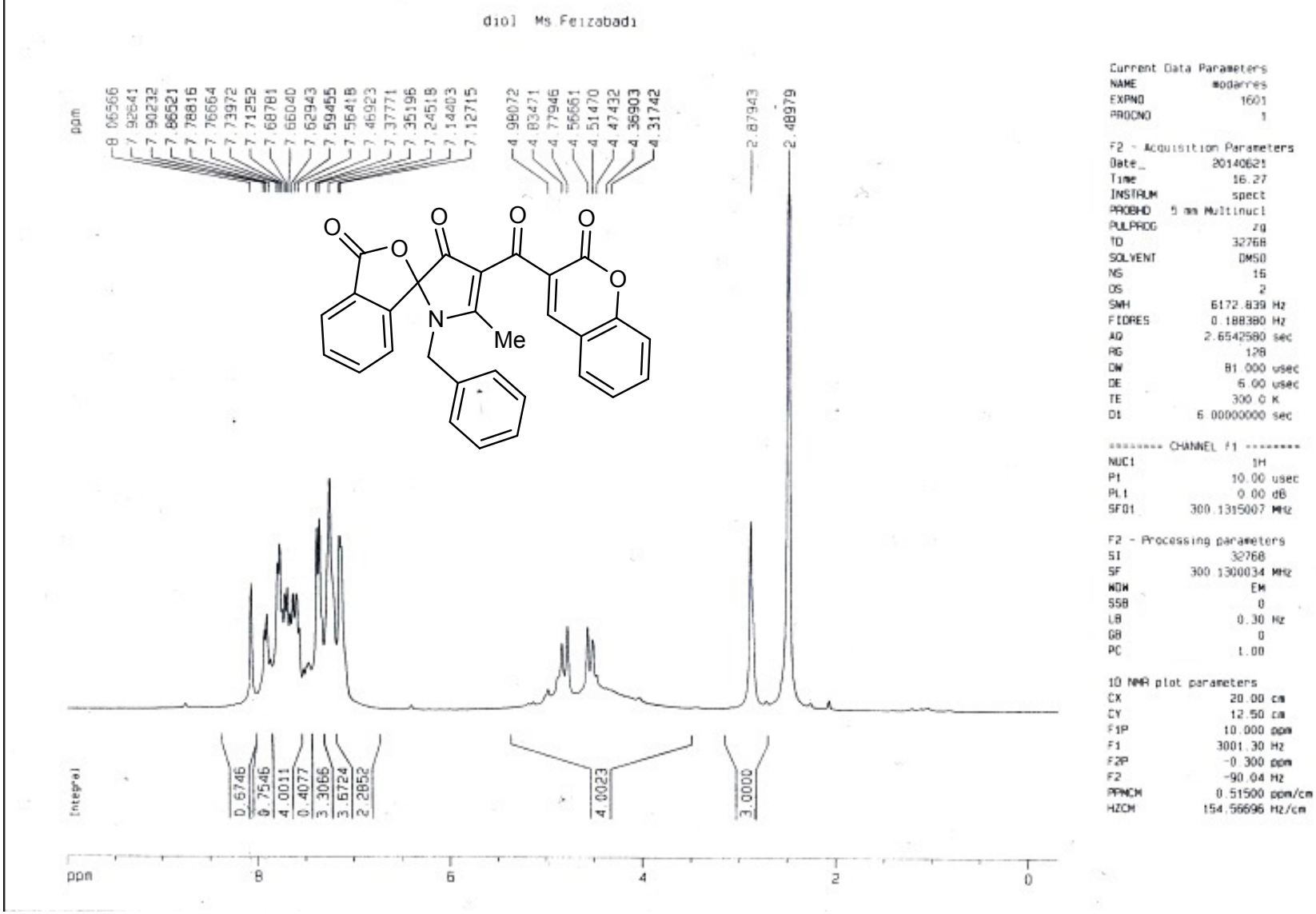
^{1}H NMR of 5a



^{1}H NMR of 5a (expand)


Pyr Sal1A1
180.1182
166.5398
159.0466
154.0268
144.9620
144.4160
136.6997
133.4752
132.2565
129.0720
128.7566
128.5076
127.2634
126.4842
125.9896
124.4610
123.9884
118.7232
116.1289
115.8622
101.1570
95.7614
76.7960
76.5416
76.2872
46.8681
46.7366
27.0355
19.1137
11.6366
BRUKER
Current Data Parameters
NAME ghanbaripour
EXPNO 87
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111118
Time 21.44
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1224
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 1448.2
DW 15.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 3.00 dB
SFO1 125.7716224 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7578484 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
47.0
ppm
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{13}C NMR of 5a


diol Ms Feizabadi
ppm
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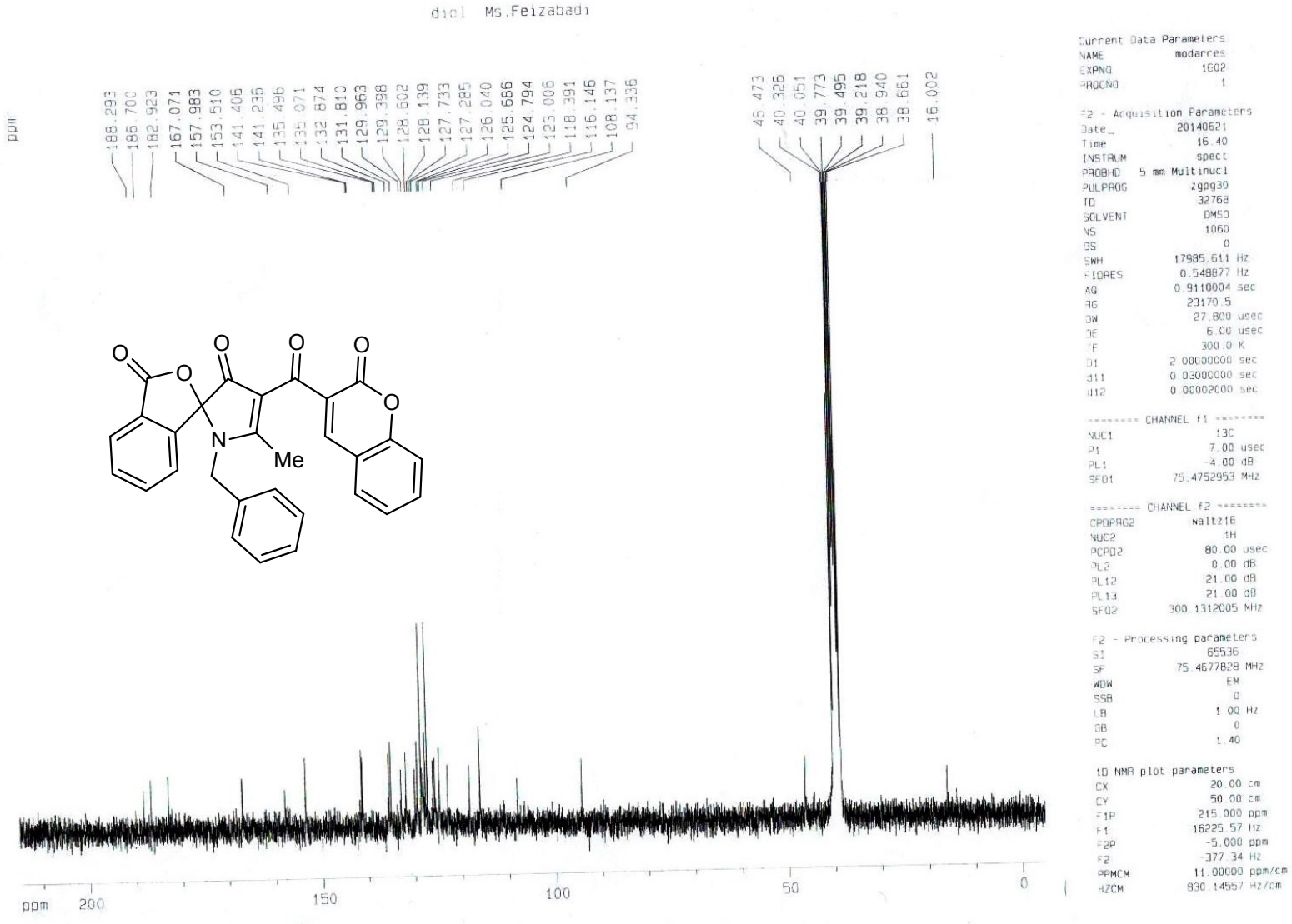
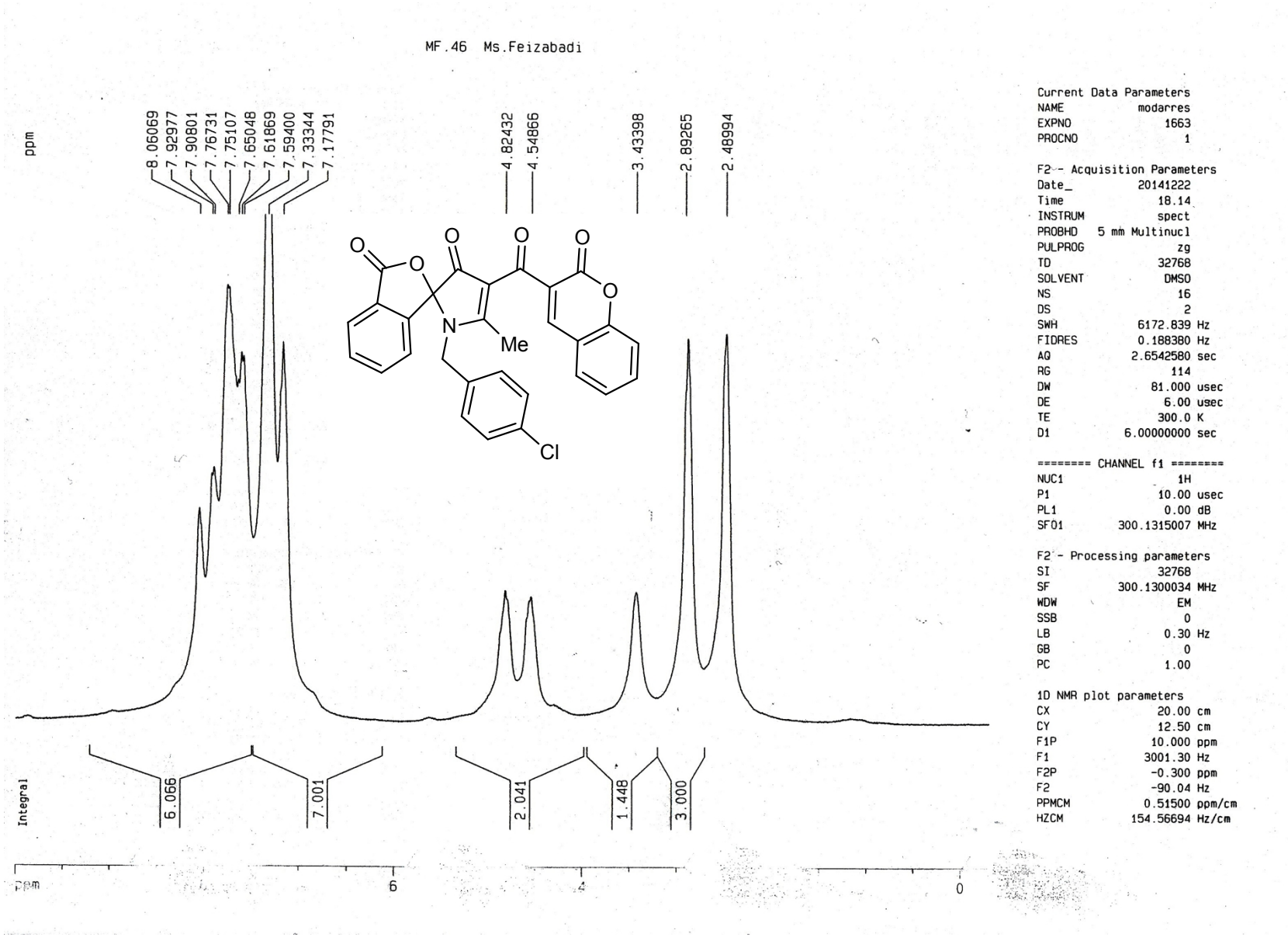
7.92641
7.90232
7.86521
7.78816
7.76664
7.73972
7.71252
7.68781
7.66040
7.62943
7.59455
7.56418
7.46923
7.37771
7.35196
7.24518
7.14403
7.12715
4.98072
4.83471
4.77946
4.56661
4.51470
4.47432
4.36903
4.31742
2.87943
2.48979
O
O
O
O
O
N
Me
Integral
0.6746
0.7546
4.0011
0.4077
3.3066
3.6724
2.2852
4.0023
3.0000
ppm
8
6
4
2
0
Current Data Parameters
NAME modarres
EXPNO 1601
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140621
Time 16.27
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 128
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz
F2 - Processing parameters
SI 32768
SF 300.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.300 ppm
F2 -90.04 Hz
PPMCM 0.51500 ppm/cm
HZCM 154.56696 Hz/cm

^{1}H NMR of 7a


dicl Ms.Feizabadi
ppm
188.293
186.700
182.923
167.071
157.983
153.510
141.406
141.236
135.496
135.071
132.674
131.810
129.963
129.398
128.602
128.139
127.733
127.285
126.040
125.686
124.794
123.006
118.391
116.146
108.137
94.336
46.473
40.326
40.051
39.773
39.495
39.218
38.940
38.661
16.002
O
O
O
O
O
N
Me
ppm 200
150
100
50
0
Current Data Parameters
NAME modarres
EXPNO 1602
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140621
Time 16.40
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1060
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 23170.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SF01 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677828 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 50.00 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 11.00000 ppm/cm
HZCM 830.14557 Hz/cm

^{13}C NMR of 7a


MF.46 Ms.Feizabadi
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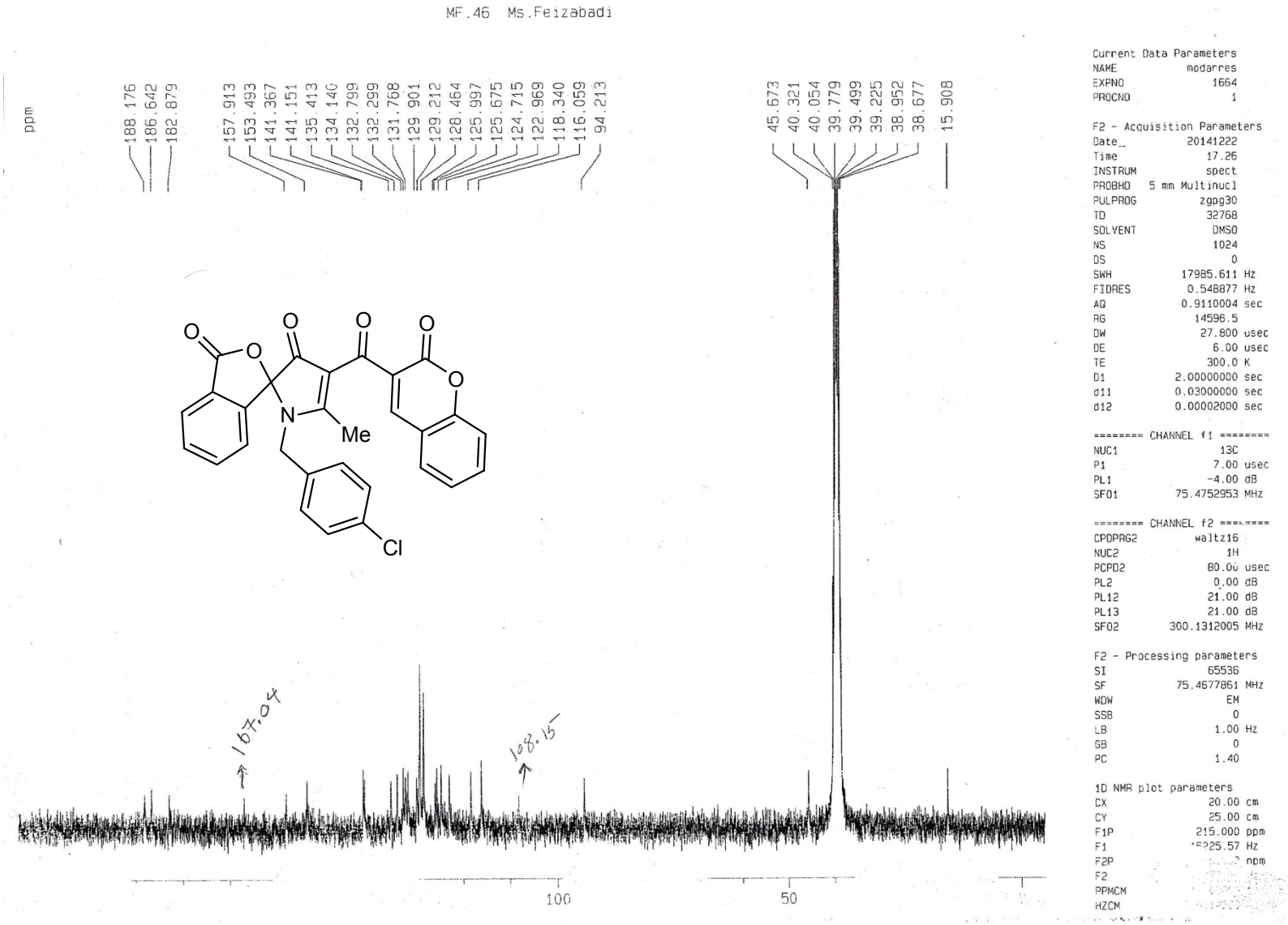
7.92977
7.90801
7.76731
7.75107
7.65048
7.61869
7.59400
7.33344
7.17791
4.82432
4.54866
3.43398
2.89265
2.48994
Me
Cl
Integral
6.066
7.001
2.041
1.448
3.000
6
4
0
Current Data Parameters
NAME modarres
EXPNO 1663
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141222
Time 18.14
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 114
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SF01 300.1315007 MHz
F2 - Processing parameters
SI 32768
SF 300.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.300 ppm
F2 -90.04 Hz
PPMCM 0.51500 ppm/cm
HZCM 154.56694 Hz/cm

^{1}H NMR of 7b


MF.46 Ms.Feizabadi
ppm
188.176
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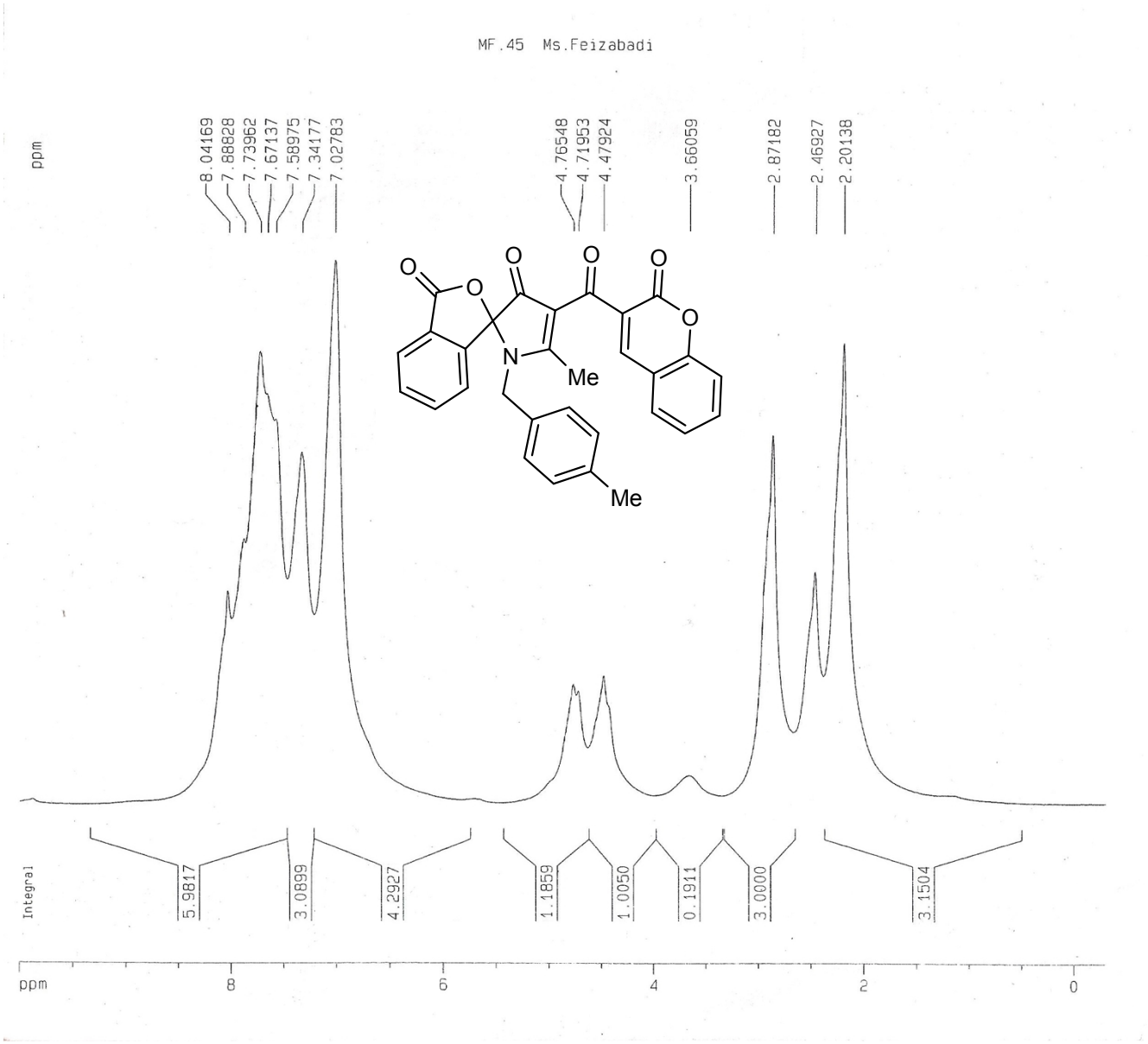
182.879
157.913
153.493
141.367
141.151
135.413
134.140
132.799
132.299
131.768
129.901
129.212
128.464
125.997
125.675
124.715
122.969
118.340
116.059
94.213
45.673
40.321
40.054
39.779
39.499
39.225
38.952
38.677
15.908
O
O
O
O
O
O
N
Me
Cl
167.04
168.15
100
50
Current Data Parameters
NAME modarres
EXPNO 1664
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141222
Time 17.26
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1024
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 14596.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SF01 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677861 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 25.00 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P
F2
PPMCM
HZCM

^{13}C NMR of 7b



Current Data Parameters
NAME modarres
EXPNO 1655
PROCNO 1

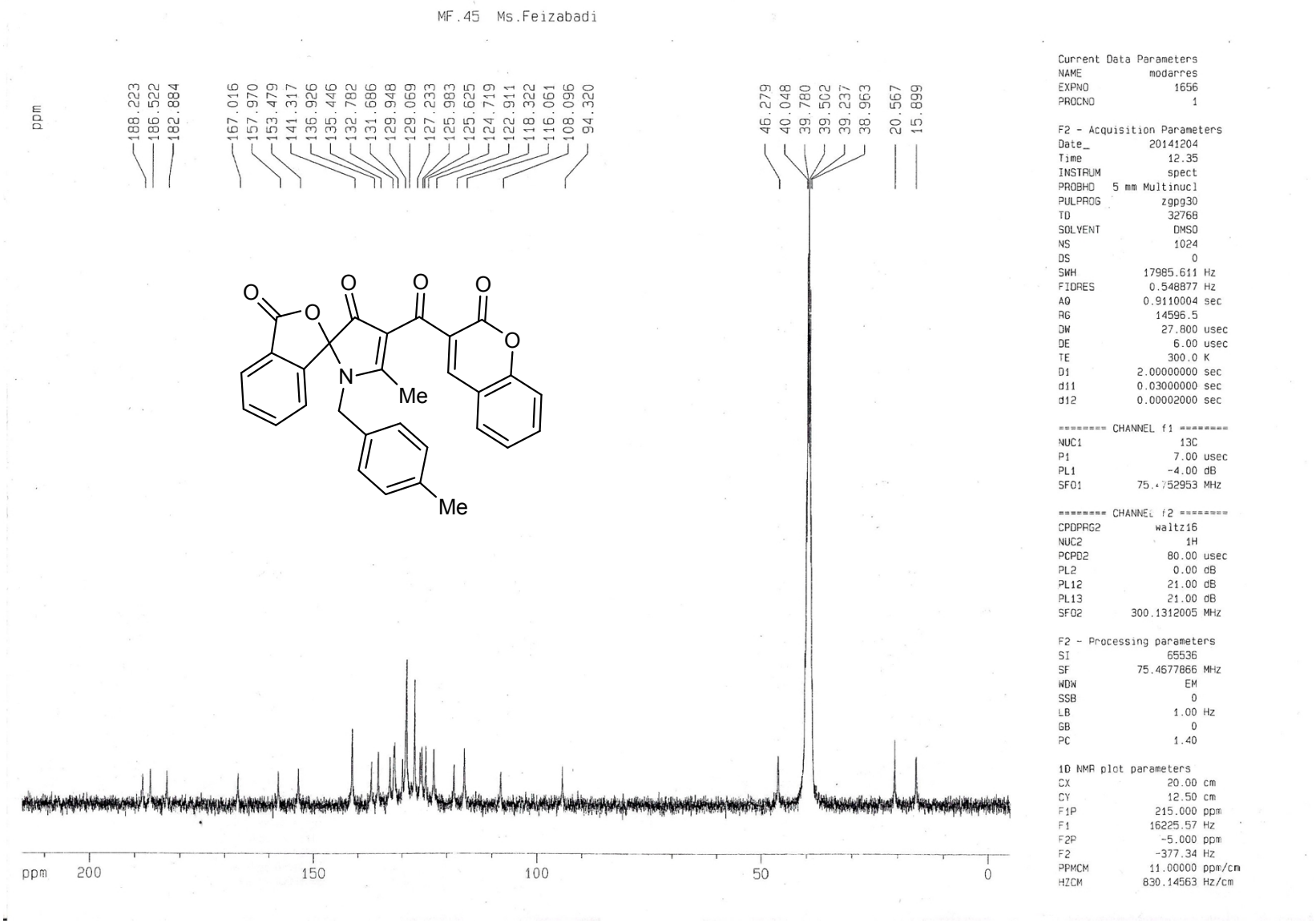
F2 - Acquisition Parameters
Date_ 20141204
Time 13.27
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 40.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 300.1300043 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.300 ppm
F2 -90.04 Hz
PPMCM 0.51500 ppm/cm
HZCM 154.56696 Hz/cm

^{1}H NMR of 7c


MF.45 Ms.Feizabadi
ppm
188.223
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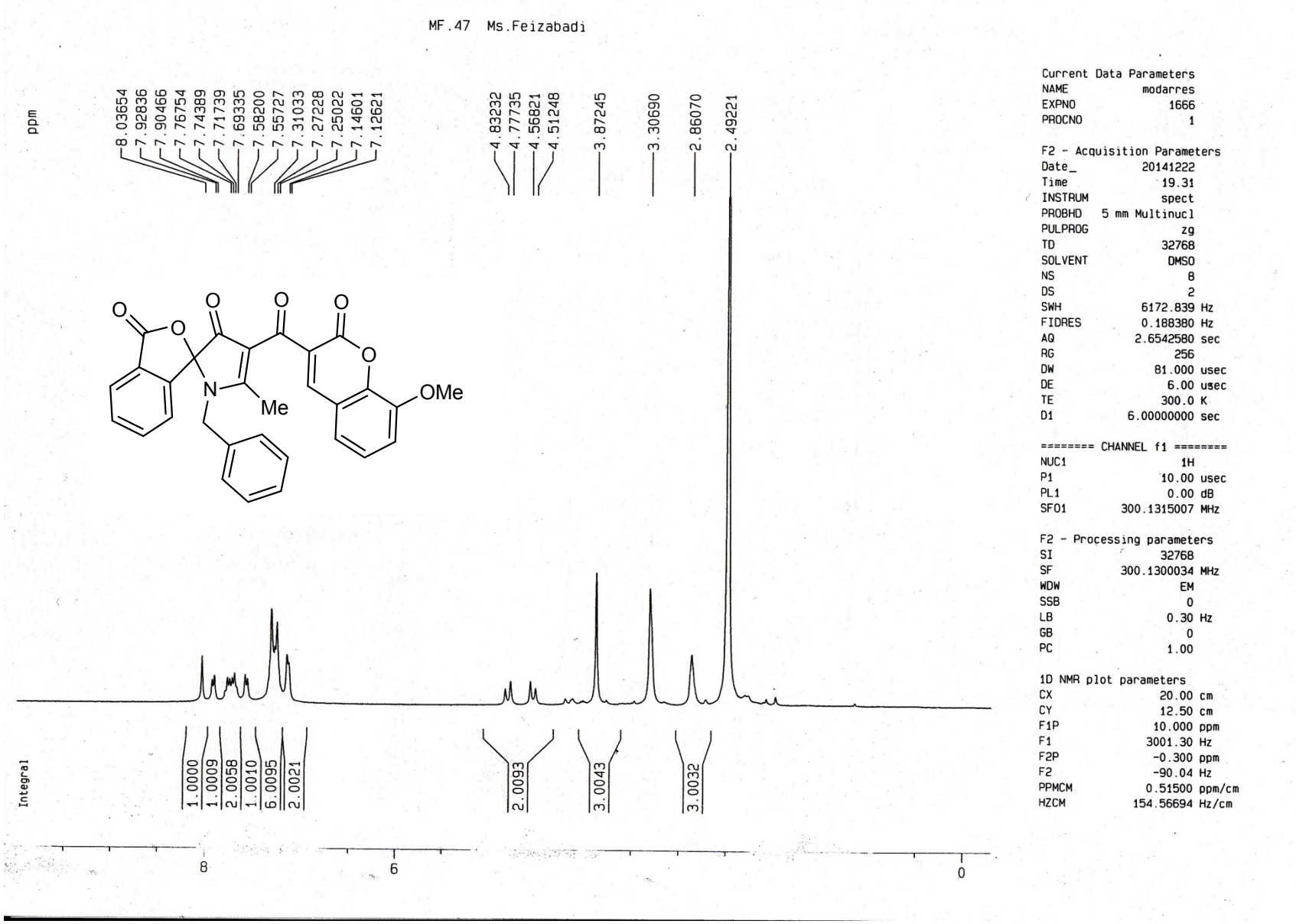
182.884
167.016
157.970
153.479
141.317
136.926
135.446
132.782
131.686
129.948
129.069
127.233
125.983
125.625
124.719
122.911
118.322
116.061
108.096
94.320
46.279
40.048
39.780
39.502
39.237
38.963
20.567
15.899
O
O
O
O
O
O
N
Me
Me
ppm 200
150
100
50
0
Current Data Parameters
NAME modarres
EXPNO 1656
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141204
Time 12.35
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1024
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 14596.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677866 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 11.00000 ppm/cm
HZCM 830.14563 Hz/cm

^{13}C NMR of 7c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7.90466
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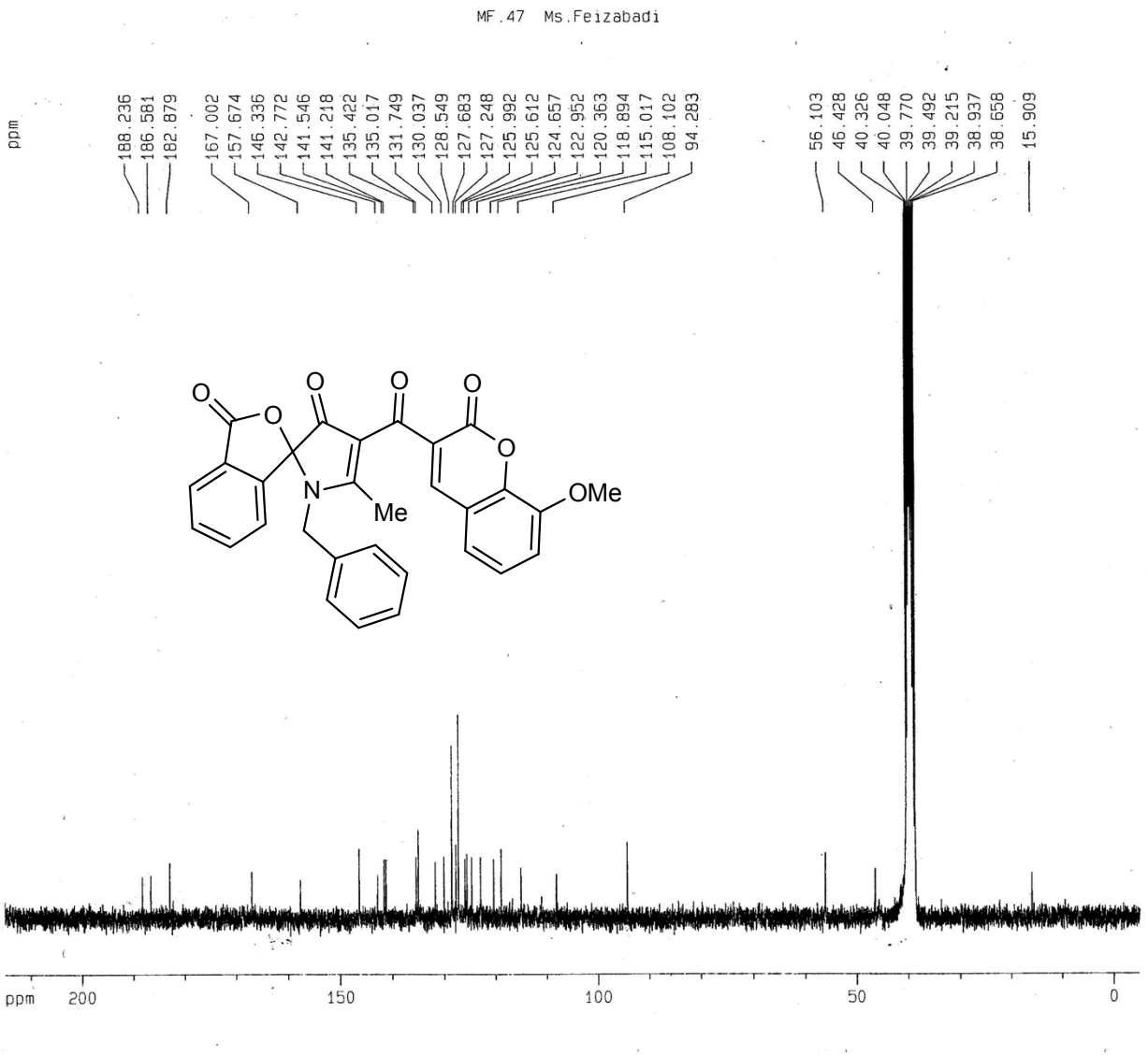
7.71739
7.69335
7.58200
7.55727
7.31033
7.27228
7.25022
7.14601
7.12621
4.83232
4.77735
4.56821
4.51248
3.87245
3.30690
2.86070
2.49221
O
O
O
O
O
O
N
Me
OMe
Integral
1.0000
1.0009
2.0058
1.0010
6.0095
2.0021
2.0093
3.0043
3.0032
8
6
0
Current Data Parameters
NAME modarres
EXPNO 1666
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141222
Time 19.31
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 32768
SOLVENT DMSO
NS 8
DS 2
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 256
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 300.1315007 MHz
F2 - Processing parameters
SI 32768
SF 300.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.300 ppm
F2 -90.04 Hz
PPMCM 0.51500 ppm/cm
HZCM 154.56694 Hz/cm

^{1}H NMR of 7f

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Current Data Parameters
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EXPNO               1669
PROCNO                 1

F2 - Acquisition Parameters
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Time               18.10
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PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                32768
SOLVENT            DMSO
NS                10240
DS                    0
SWH           17985.611 Hz
FIDRES         0.548877 Hz
AQ             0.9110004 sec
RG                14596.5
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 7.00 usec
PL1               -4.00 dB
SFO1          75.4752953 MHz

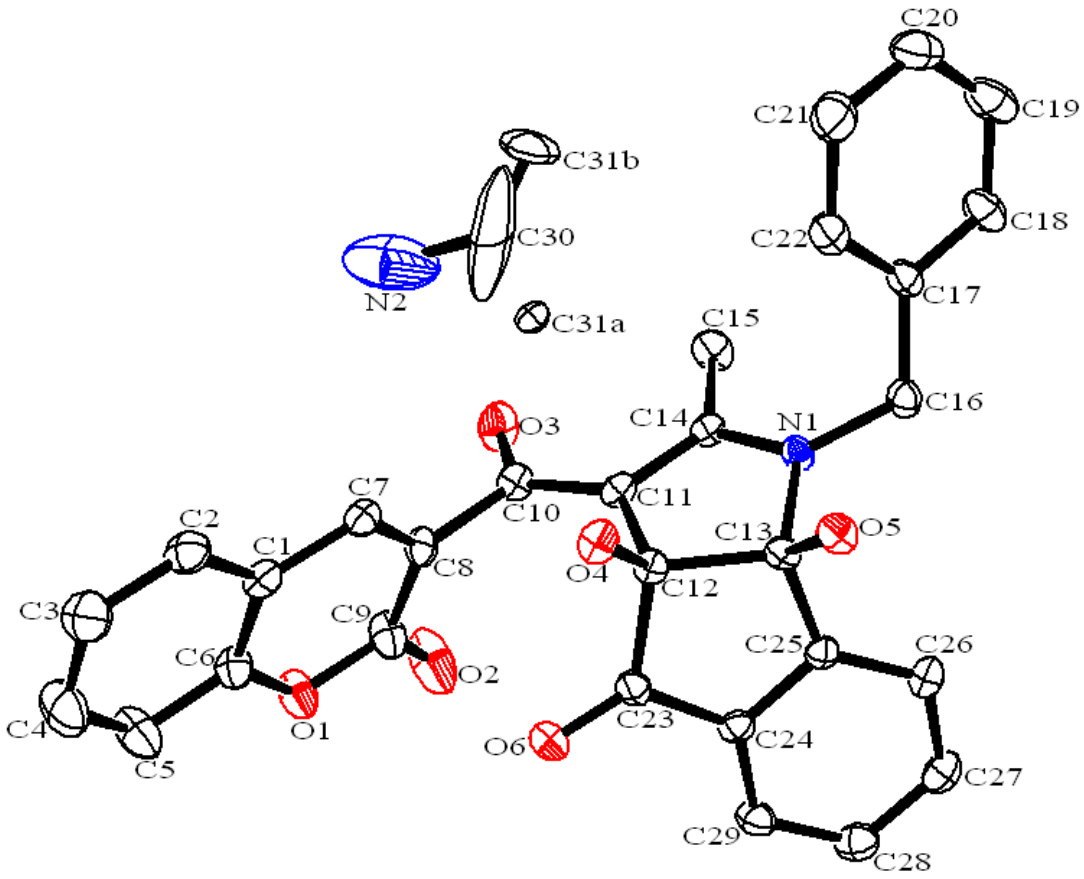
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              21.00 dB
PL13              21.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 65536
SF            75.4677861 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                120.00 cm
F1P              215.000 ppm
F1              16225.57 Hz
F2P               -5.000 ppm
F2               -377.34 Hz
PPMCM          11.00000 ppm/cm
HZCM          830.14563 Hz/cm
```

^{13}C NMR of 7f

ORTEP diagram for 3a



ORTEP diagram for 7a