Electronic Supplementary Material (ESI) for RSC Advances.

Crystallographic data for compound **3g** (AW71)

X-ray data for the compound were collected at room temperature using a Bruker Smart Apex CCD diffractometer with graphite monochromated MoKα radiation (λ=0.71073Å) with ω-scan method.[1] Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Unit cell dimensions were determined using 9047 reflections for AW71 data. Integration and scaling of intensity data were accomplished using SAINT program.[1] The structures were solved by Direct Methods using SHELXS97[2] and refinement was carried out by full-matrix least-squares technique using SHELXL97.[2] Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms, with C-H distances of 0.93--0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}$ (C) or $1.5U_{eq}$ for methyl atoms.

Crystal data for compound **3g** (AW71): $C_{12}H_{18}N_2O_5$, M = 414.30, yellow block, 0.41 x 0.26 x 0.15 mm^3, monoclinic, space group $P2_1/n$ (No. 14), a = 10.2802(8), b = 11.3015(9), c = 18.0590(14) Å, β = 104.2340(10)°, V = 2033.7(3) Å^3, Z = 4, D_c = 1.353 g/cm^3, F_{000} = 864, CCD area detector, MoKα radiation, λ = 0.71073 Å, T = 293(2)K, $2\theta_{max}$ = 50.0º, 18960 reflections collected, 3579 unique (R_{int} = 0.0255), Final *GooF* = 1.025, *R1* = 0.0377, *wR2* = 0.1000, *R* indices based on 3164 reflections with I >2σ(I) (refinement on F^2), 285 parameters, μ = 0.096 mm^{-1}. CCDC 1016218 contains supplementary crystallographic data. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk.

1. SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.
2. Sheldrick, G. M. SHELXS97 and SHELXL97, Programs for crystal structure solution and refinement; University of Gottingen: Germany, 1997.

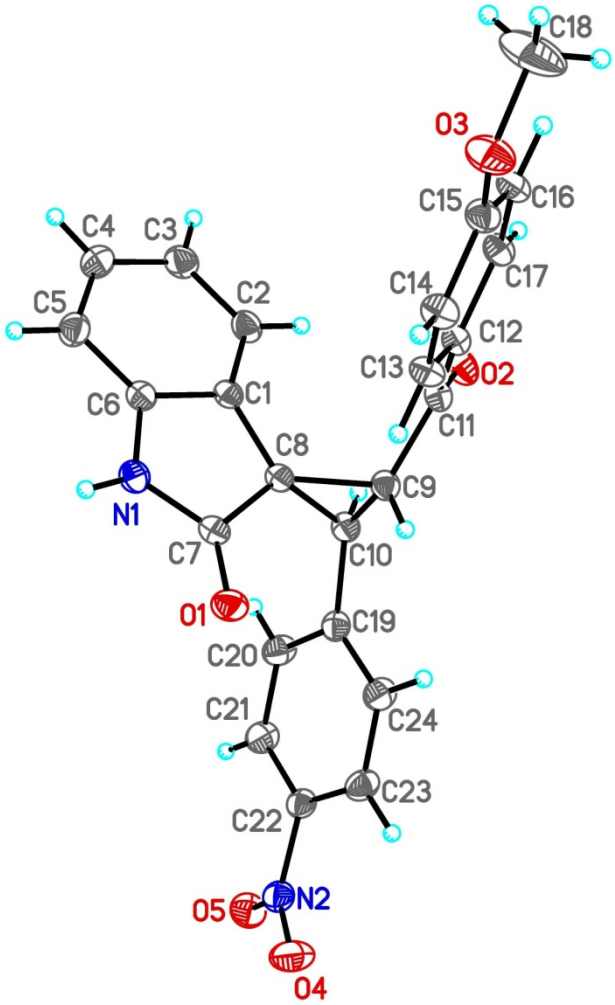
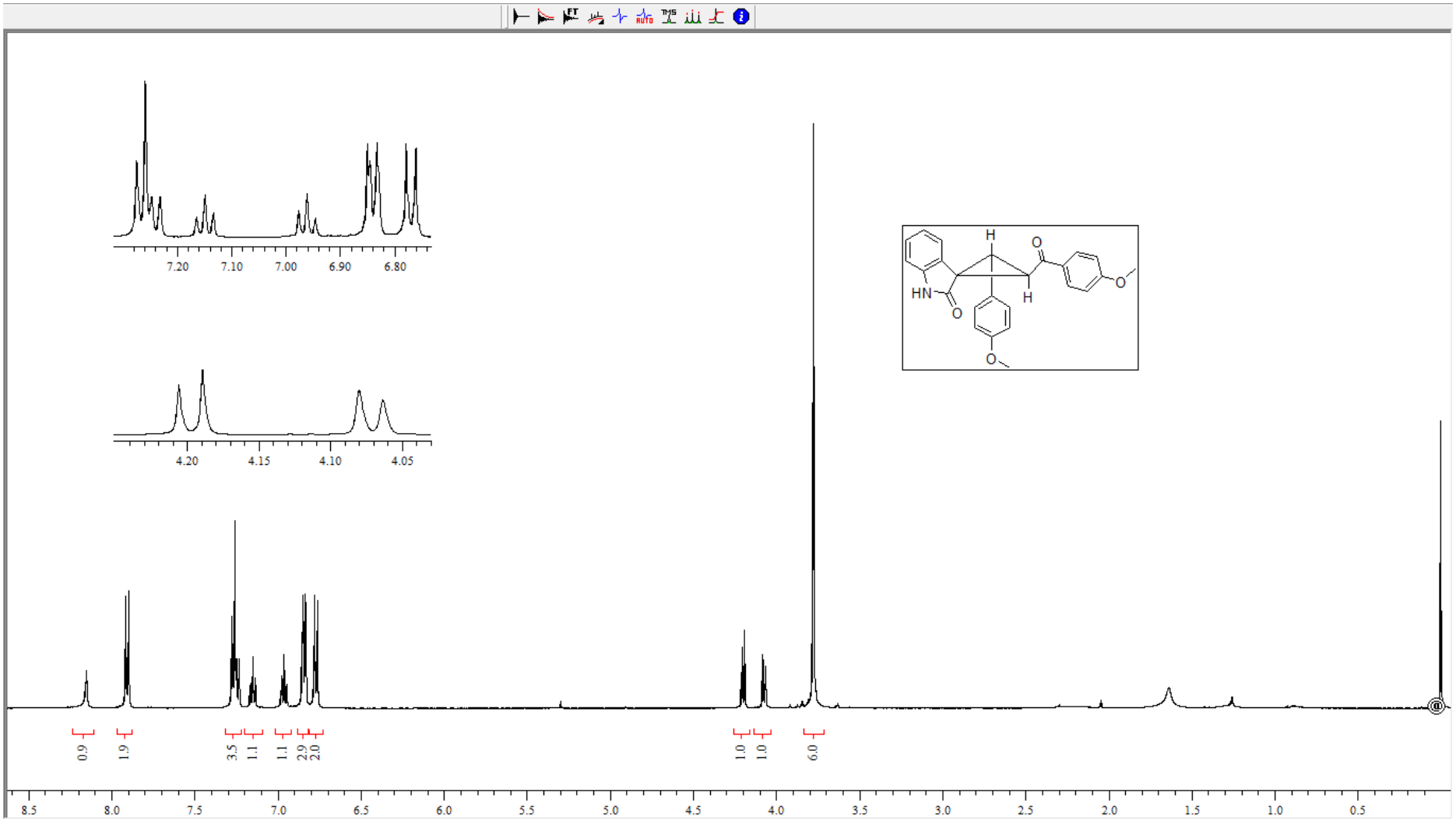


Figure caption: The molecular structure of compound **3g** (AW71) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 20% probability level and H atoms are shown as small spheres of arbitrary radius.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7.10
7.00
6.90
6.80
4.20
4.15
4.10
4.05
H
O
HN
O
H
O
O
0.9
1.9
3.5
1.1
1.1
2.9
2.0
1.0
1.0
6.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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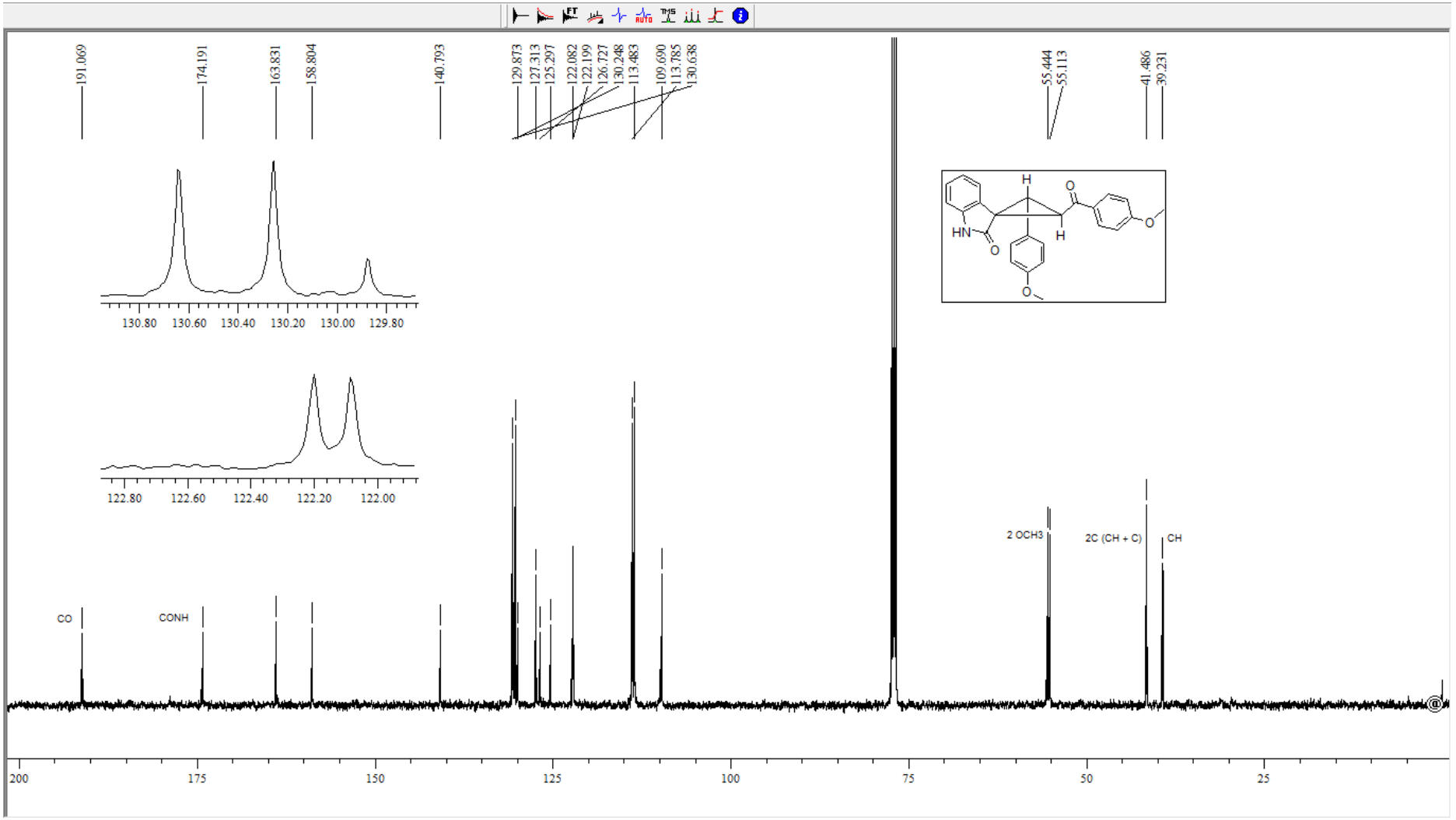
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5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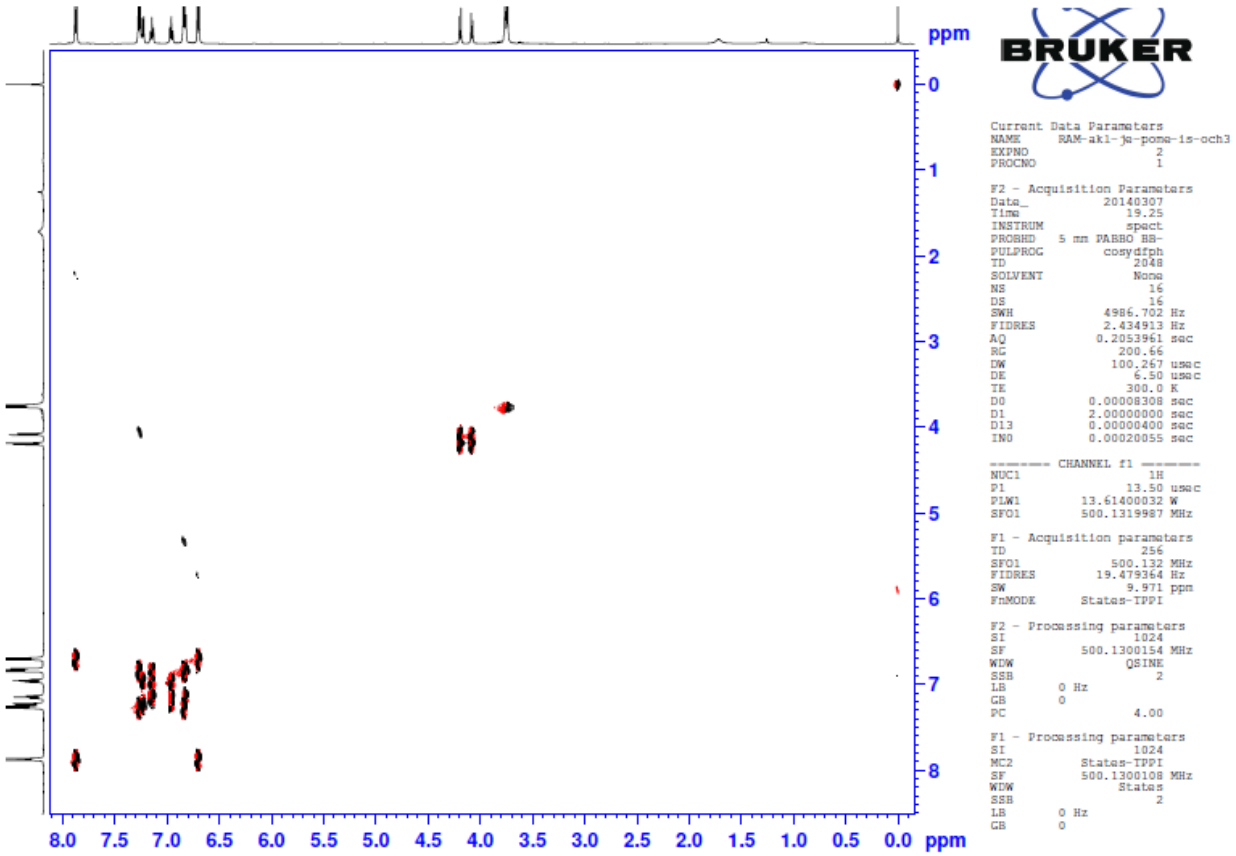
158.804
140.793
129.873
127.313
125.297
122.082
122.199
126.727
130.248
113.483
109.690
113.785
130.638
55.444
55.113
41.486
39.231
130.80
130.60
130.40
130.20
130.00
129.80
122.80
122.60
122.40
122.20
122.00
CO
CONH
2 OCH3
2C (CH + C)
CH
200
175
150
125
100
75
50
25



BRUKER

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PROCNO                          1

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DS                            16
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FIDRES                  2.434913 Hz
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D1                    2.00000000 sec
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======== CHANNEL f1 ========
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PLW1                13.61400032 W
SFO1                500.1319987 MHz

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FIDRES                 19.479364 Hz
SW                         9.971 ppm
FnMODE              States-TPPI

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WDW                       QSINE
SSB                           2
LB              0 Hz
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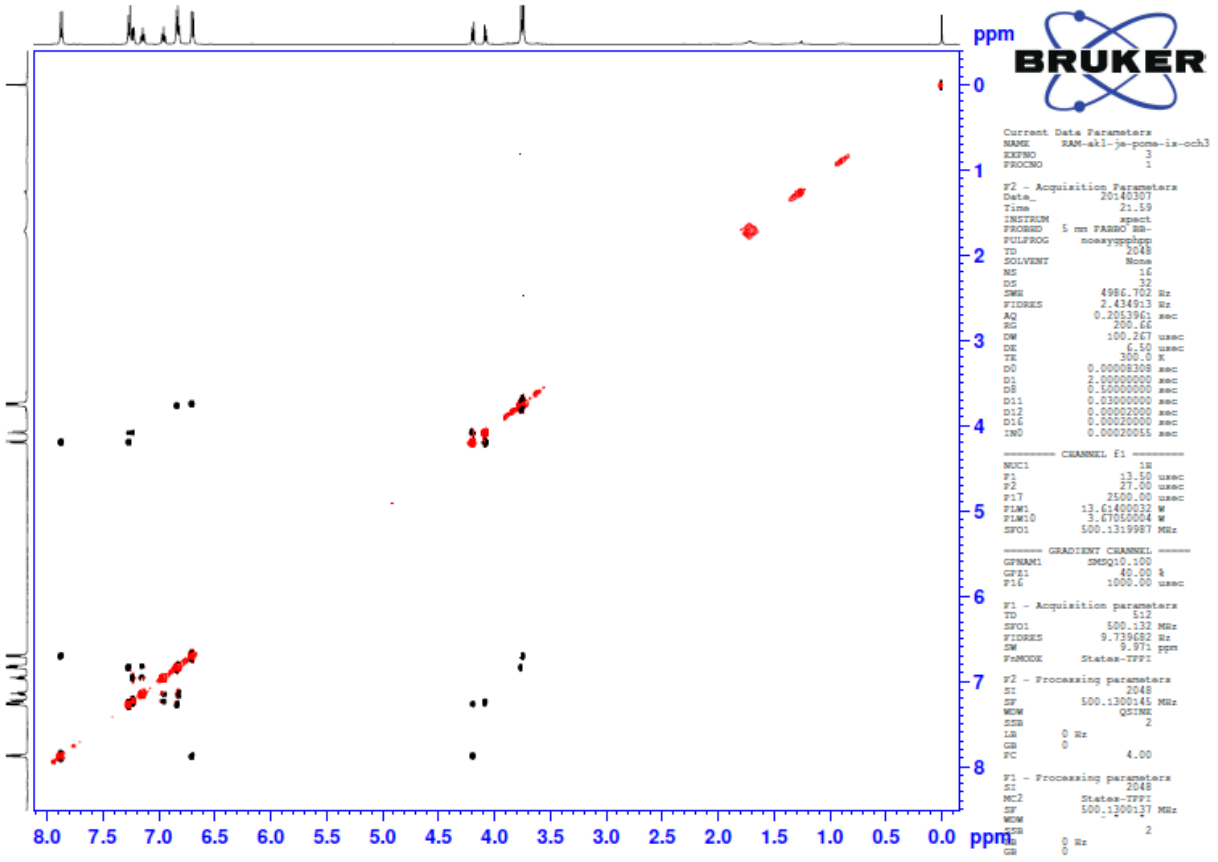
2D DQFCOSY (Double Quantum Filter Correlation spectroscopy) Spectrum of compound **3a** recorded on 500 MHz spectrometer.



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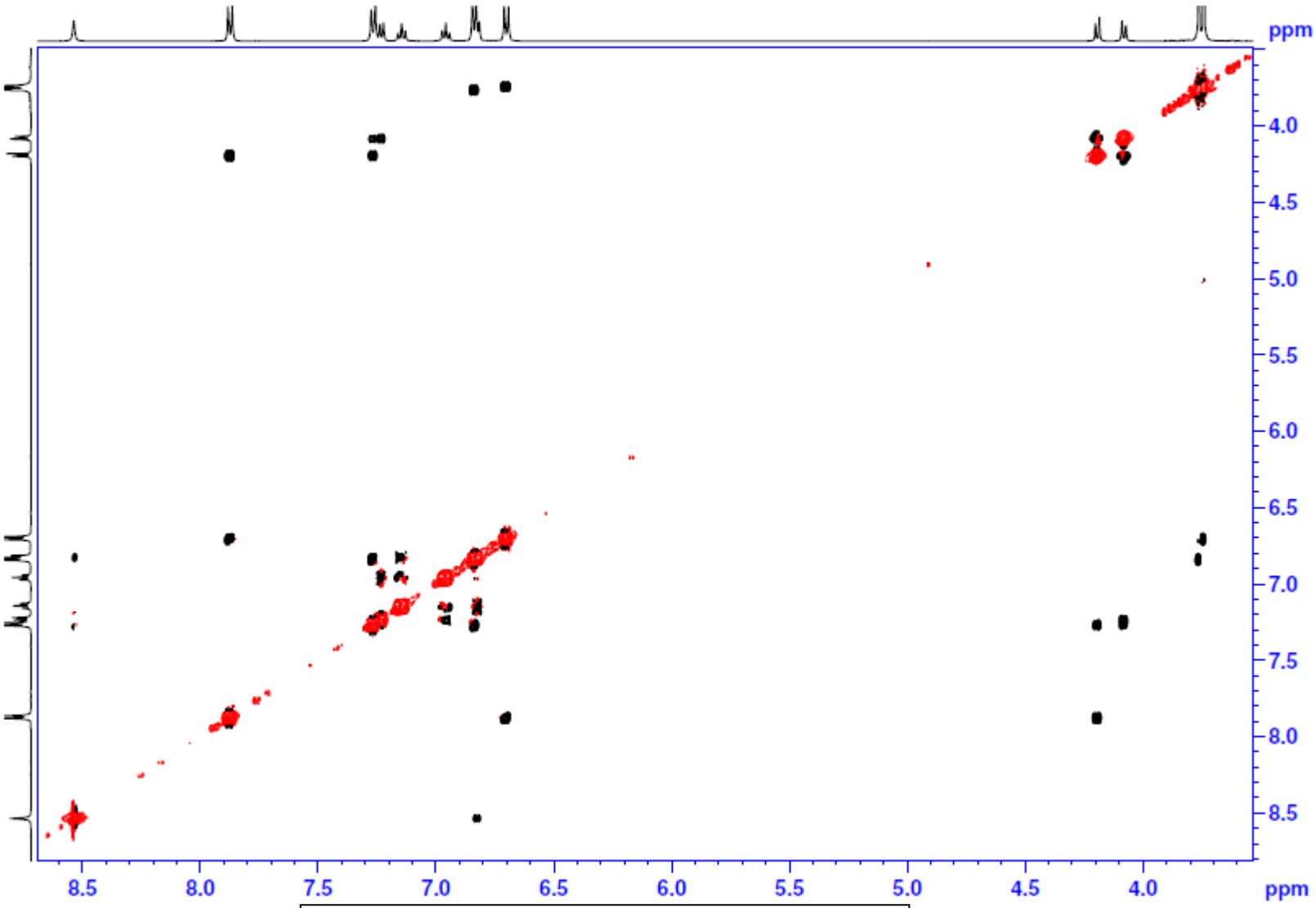

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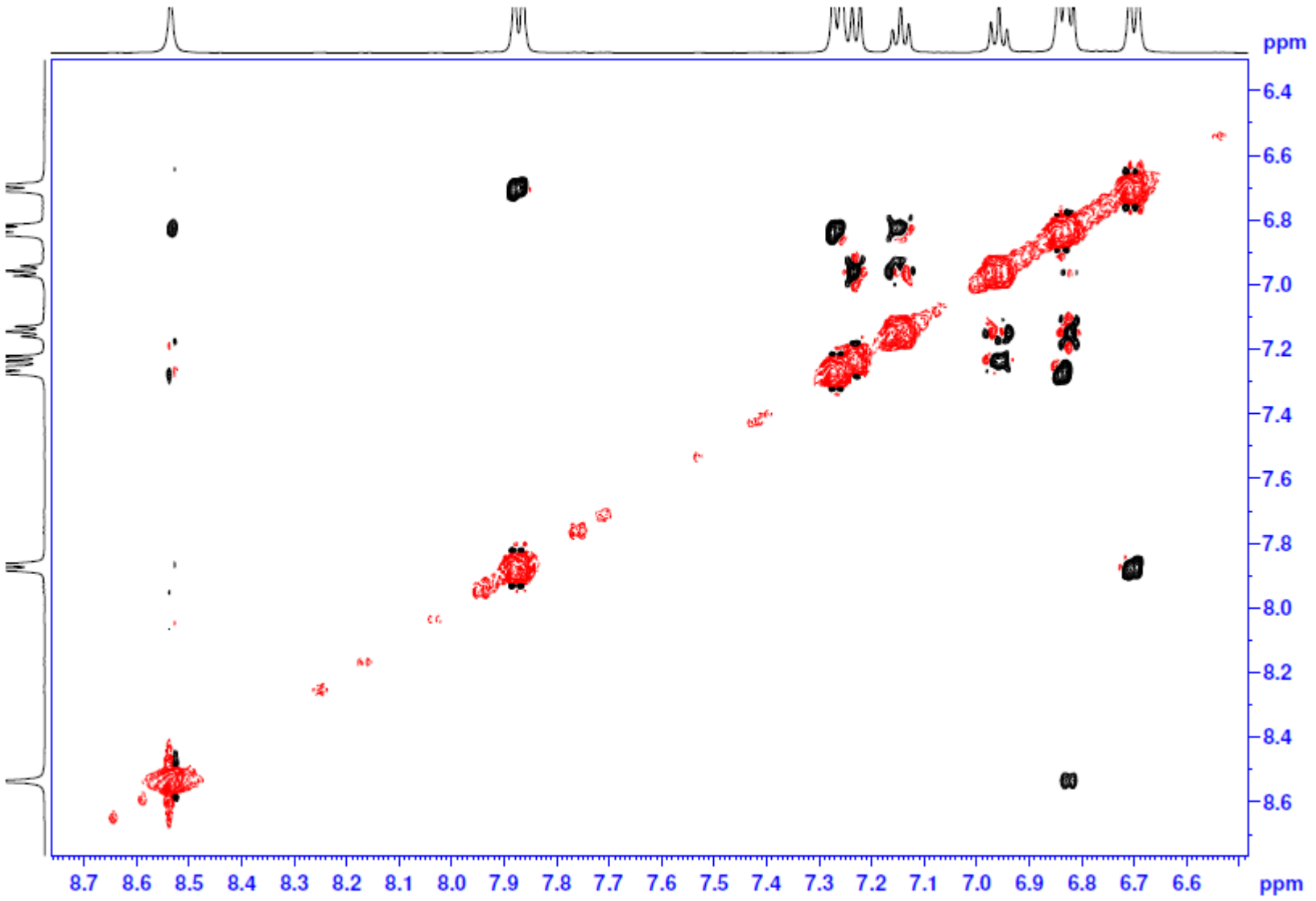

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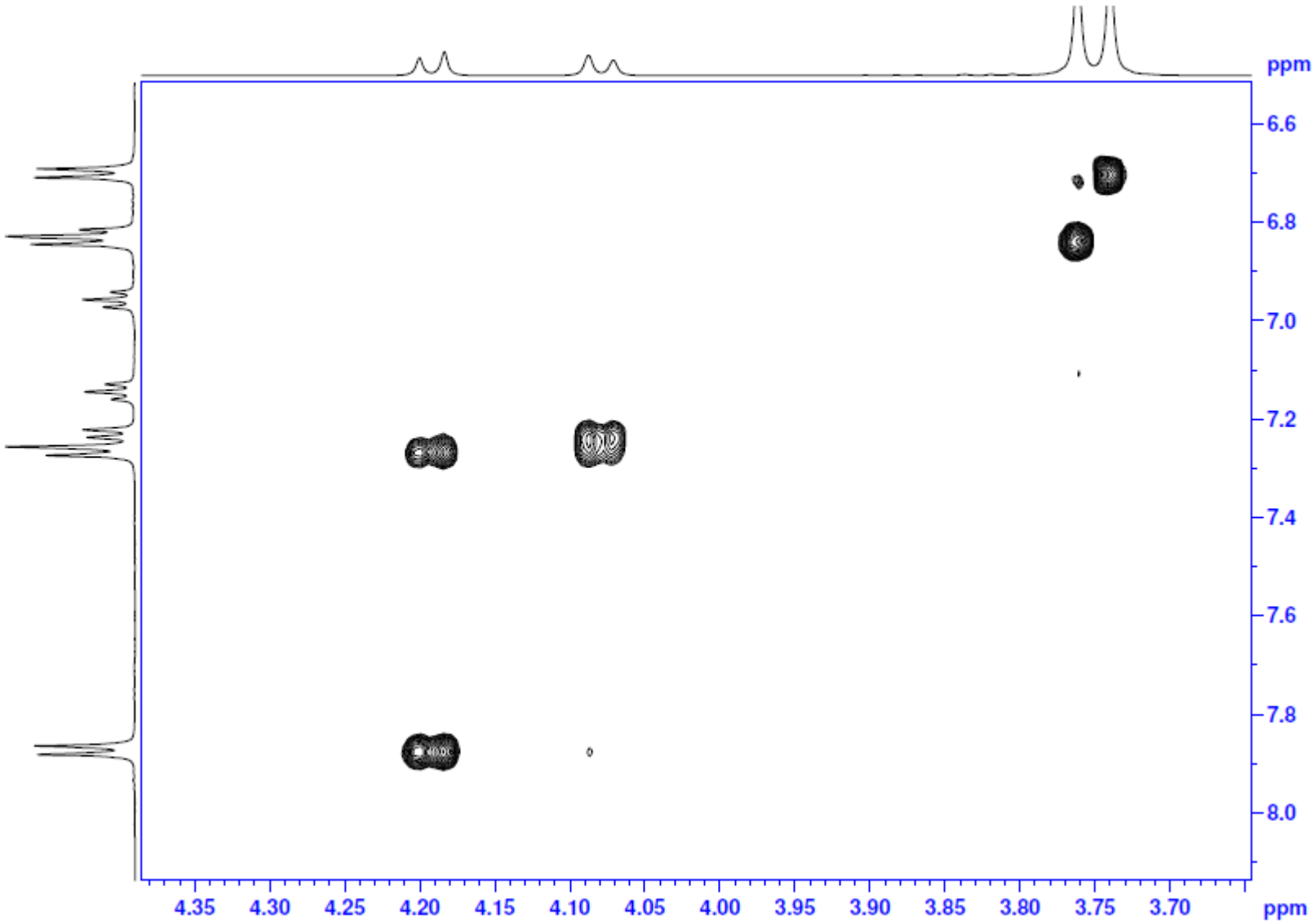

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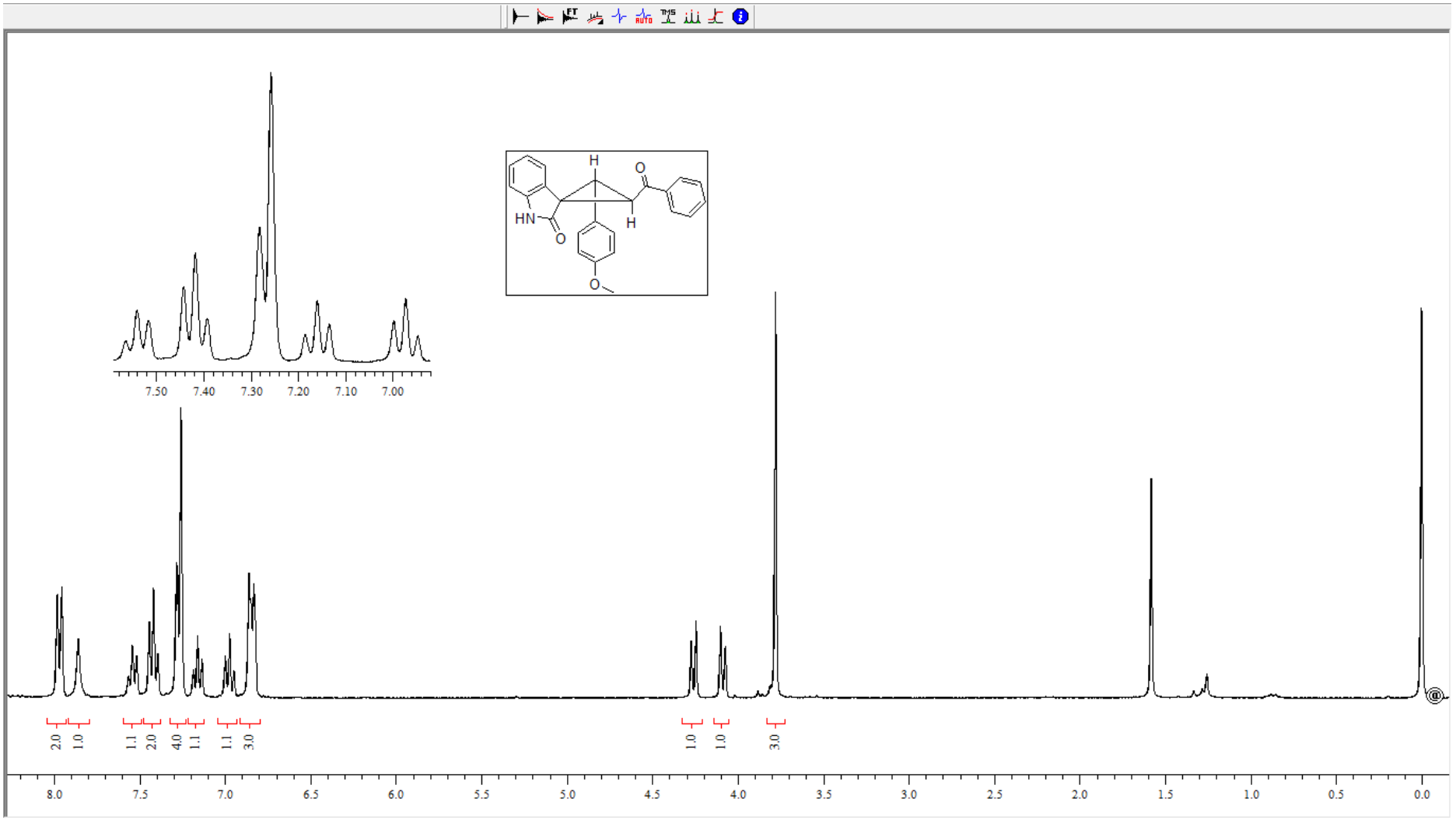
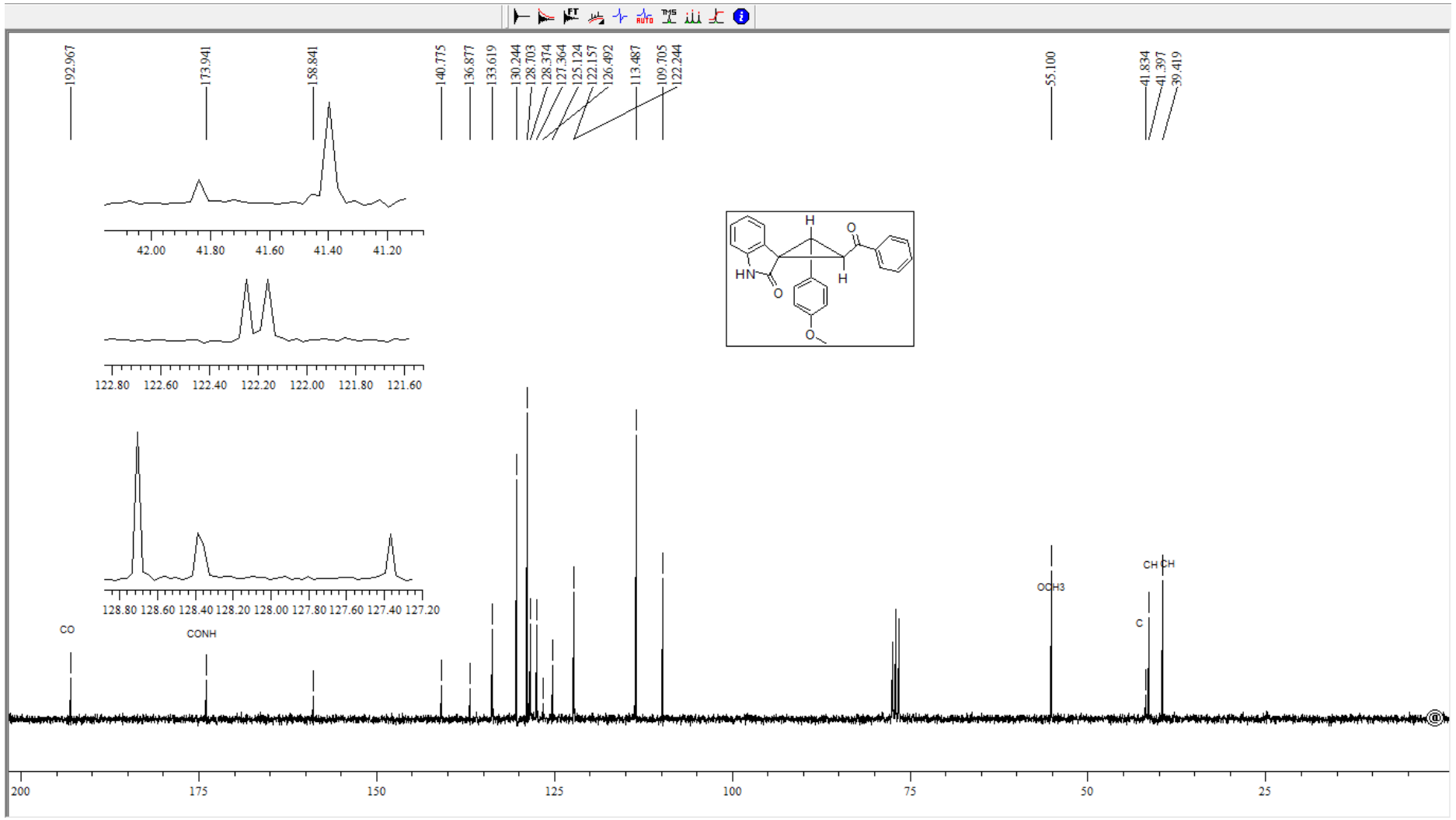

H
O
HN
O
H
O
7.50
7.40
7.30
7.20
7.10
7.00
2.0
1.0
1.1
2.0
4.0
1.1
1.1
3.0
1.0
1.0
3.0
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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127.364
125.124
122.157
126.492
113.487
109.705
122.244
55.100
41.834
41.397
39.419
42.00 41.80 41.60 41.40 41.20
122.80 122.60 122.40 122.20 122.00 121.80 121.60
128.80 128.60 128.40 128.20 128.00 127.80 127.60 127.40 127.20
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O
HN
O
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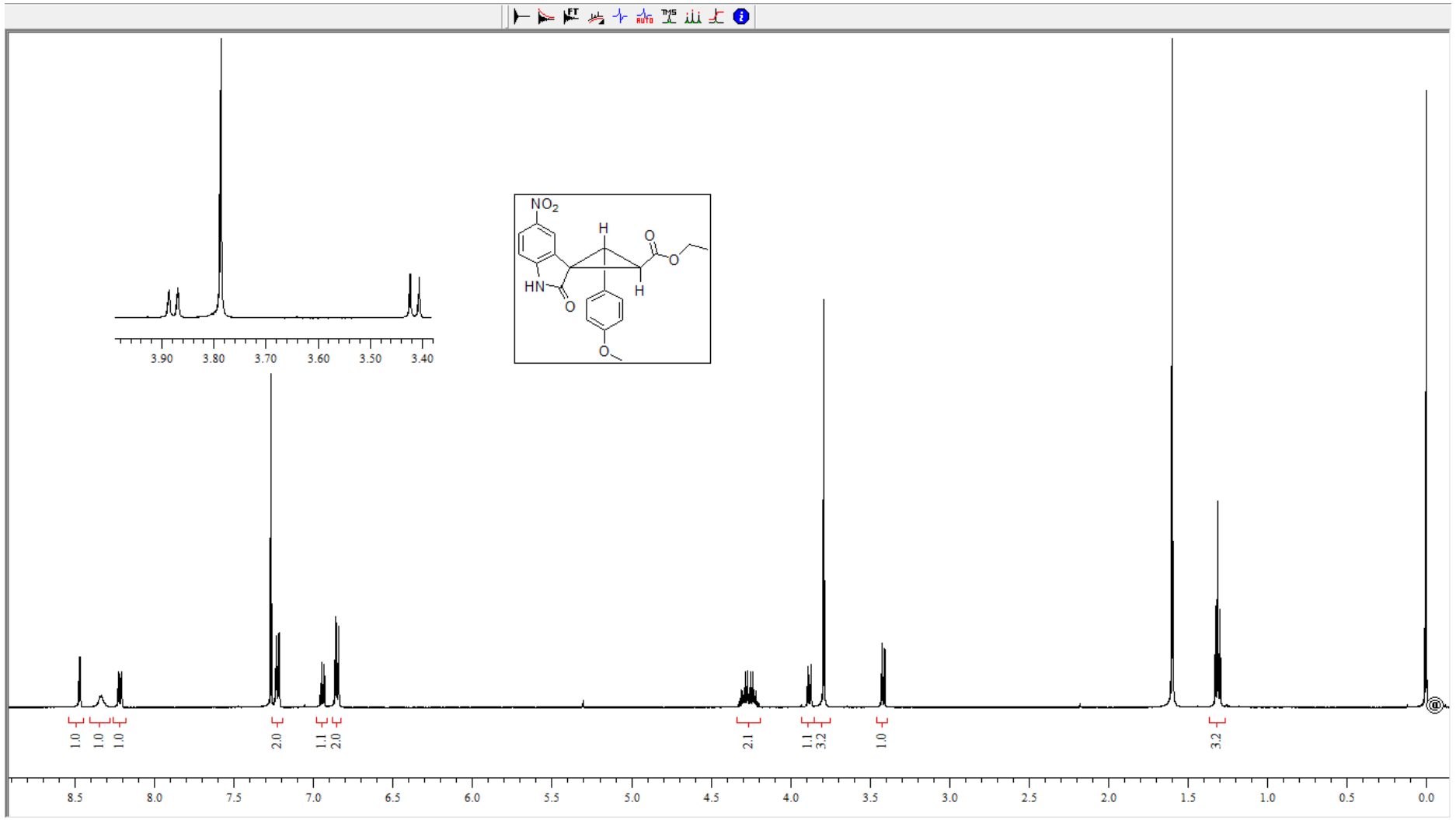
CO
CONH
OCH3
CH CH
C
200 175 150 125 100 75 50 25


NO2
H
O
O
HN
O
H
O
3.90
3.80
3.70
3.60
3.50
3.40
1.0
1.0
1.0
2.0
1.1
2.0
2.1
1.1
3.2
1.0
3.2
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
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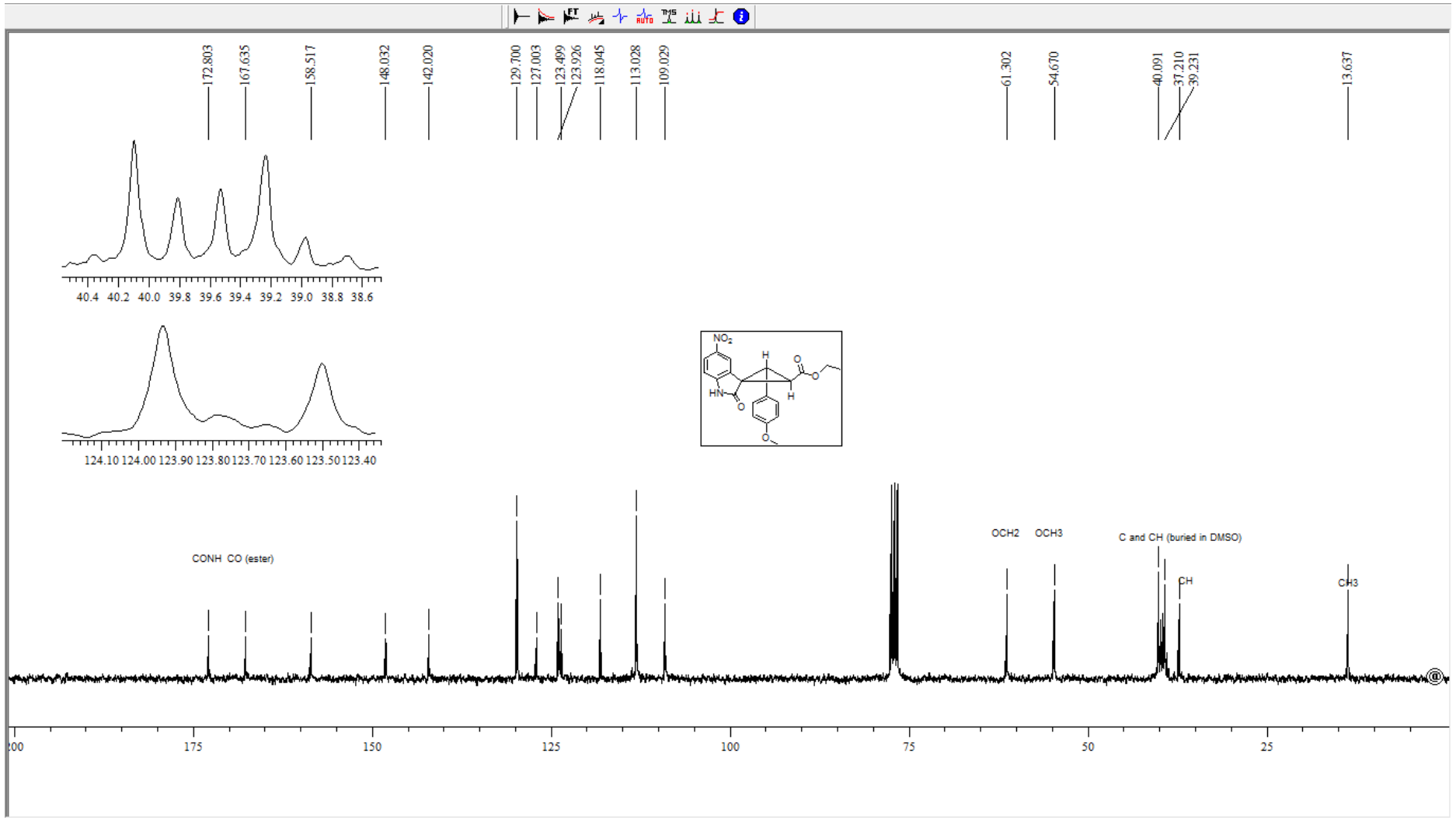
1.0
0.5
0.0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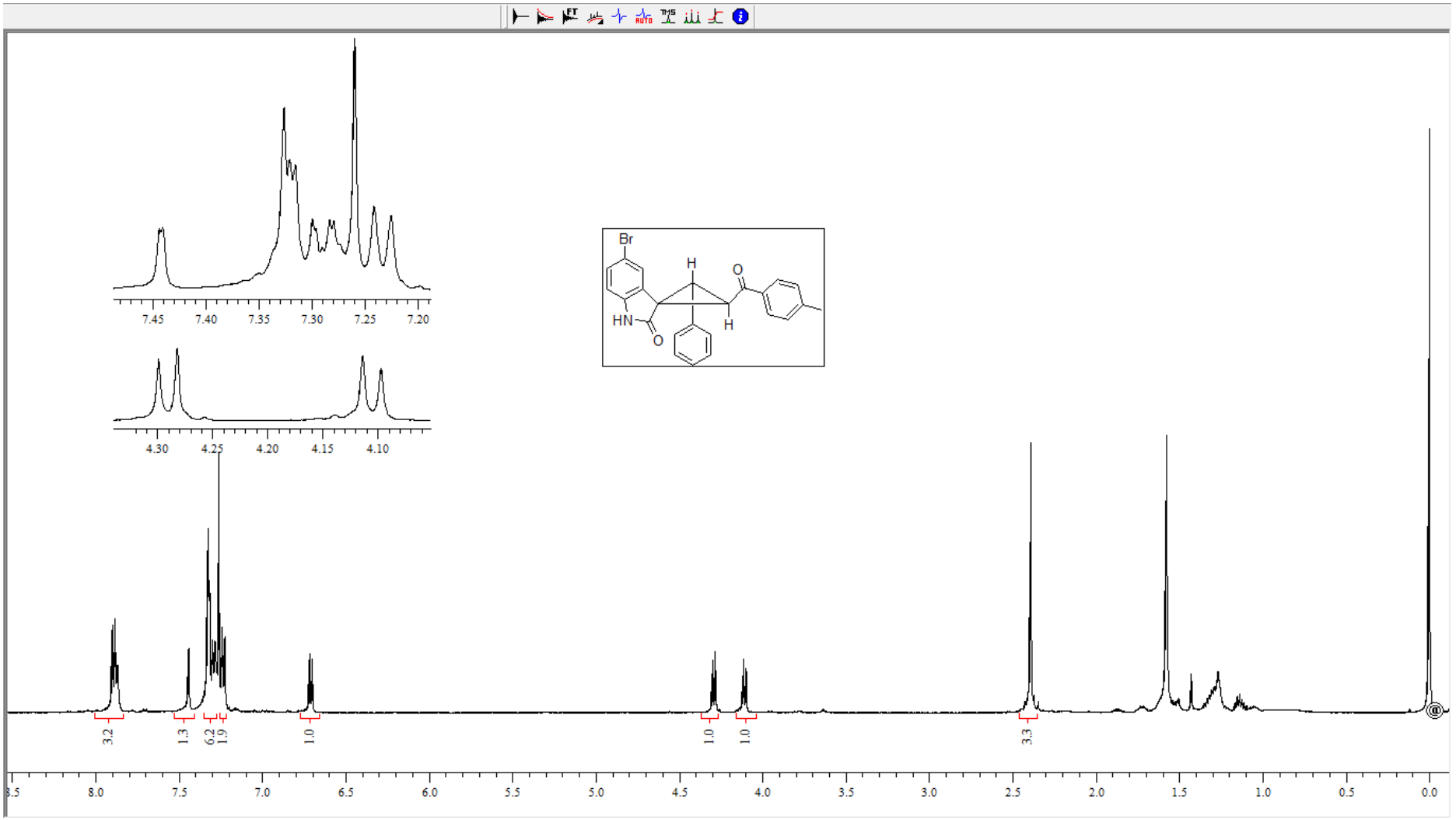
142.020
129.700
127.003
123.499
123.926
118.045
113.028
109.029
61.302
54.670
40.091
37.210
39.231
13.637
40.4 40.2 40.0 39.8 39.6 39.4 39.2 39.0 38.8 38.6
124.10 124.00 123.90 123.80 123.70 123.60 123.50 123.40
NO2
HN
O
H
O
O
H
O
CONH CO (ester)
OCH2
OCH3
C and CH (buried in DMSO)
CH
CH3
200
175
150
125
100
75
50
25


Br
H
O
HN
O
H
7.45
7.40
7.35
7.30
7.25
7.20
4.30
4.25
4.20
4.15
4.10
3.2
1.3
6.2
1.9
1.0
1.0
1.0
3.3
8.5
8.0
7.5
7.0
6.5
6.0
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3.5
3.0
2.5
2.0
1.5
1.0
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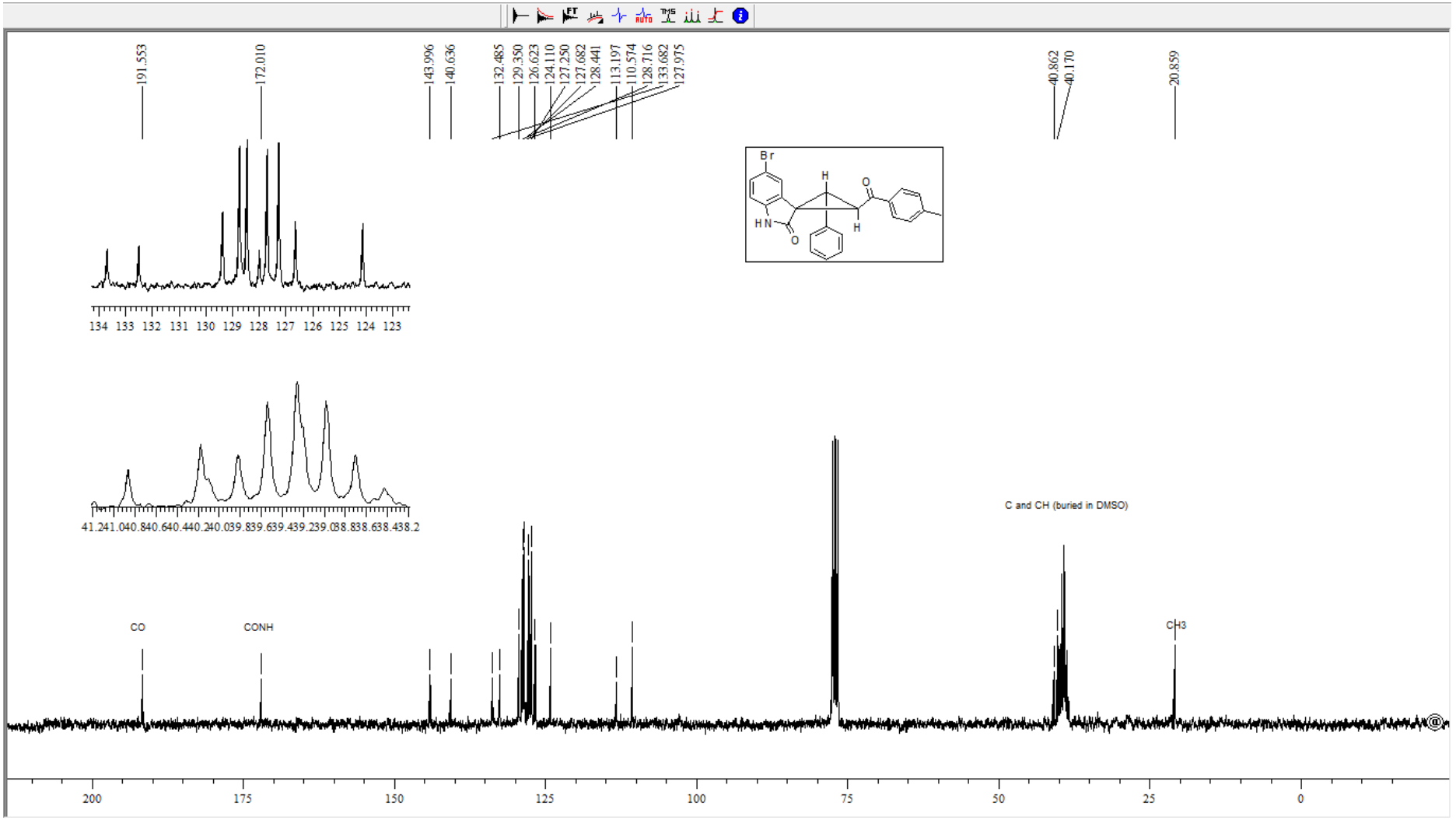
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124.110
127.250
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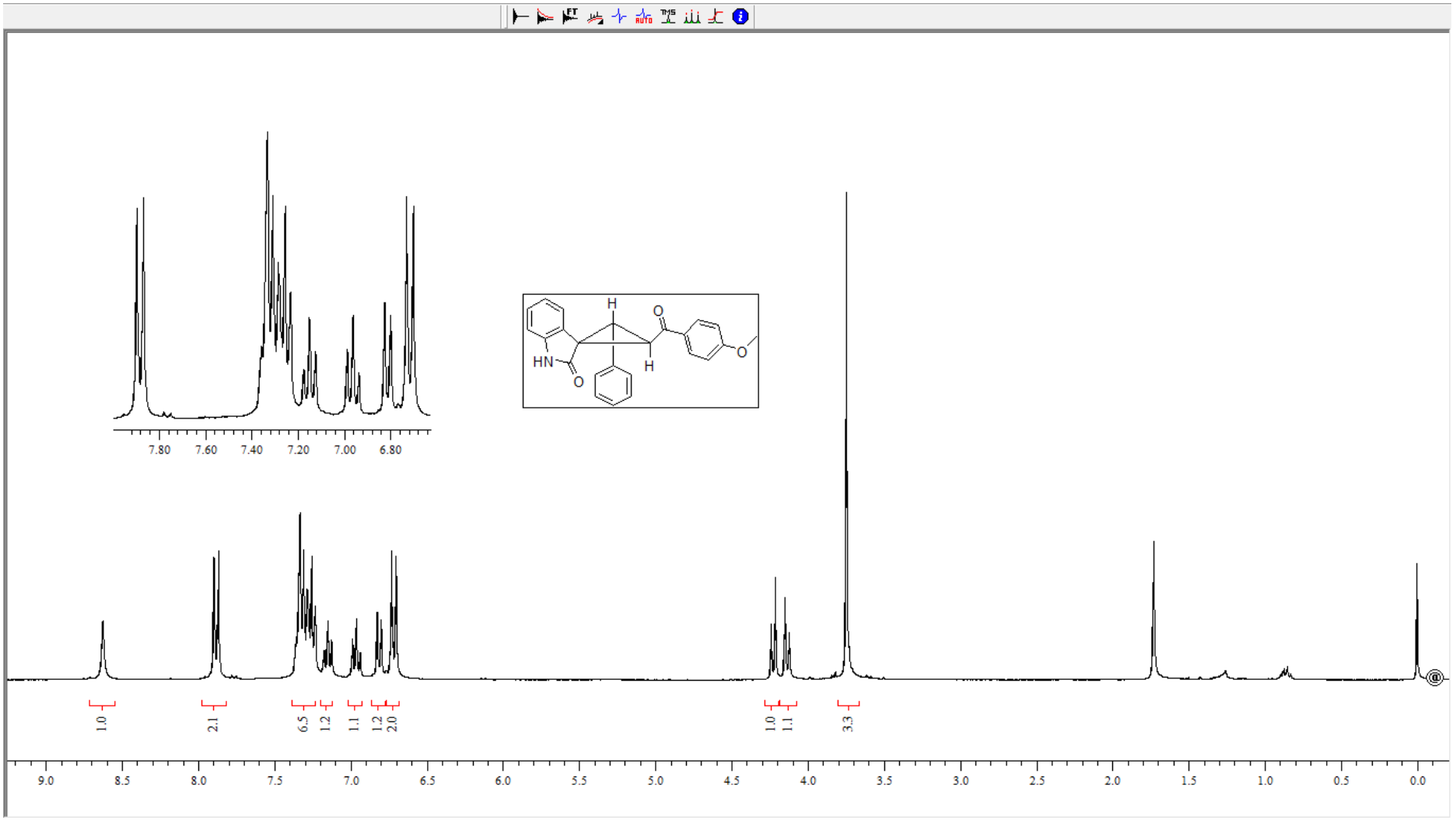
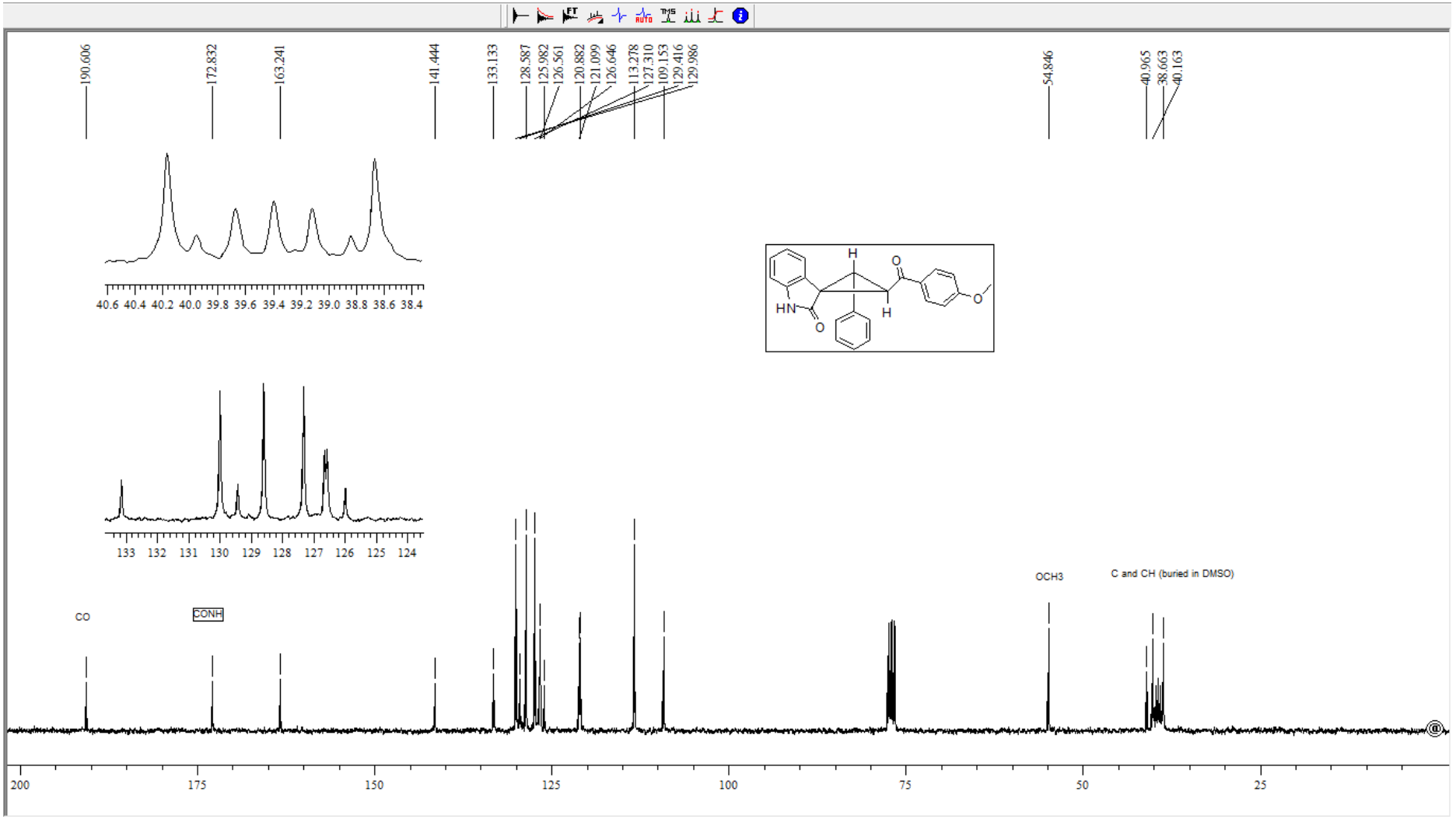
113.197
110.574
128.716
133.682
127.975
40.862
40.170
20.859
Br
H
O
HN
O
H
134 133 132 131 130 129 128 127 126 125 124 123
41.241.040.840.640.440.240.039.839.639.439.239.038.838.638.438.2
C and CH (buried in DMSO)
CO
CONH
CH3
200
175
150
125
100
75
50
25
0


7.80
7.60
7.40
7.20
7.00
6.80
HN
O
H
O
H
O
1.0
2.1
6.5
1.2
1.1
1.2
2.0
1.0
1.1
3.3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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163.241
141.444
133.133
128.587
125.982
126.561
120.882
121.099
126.646
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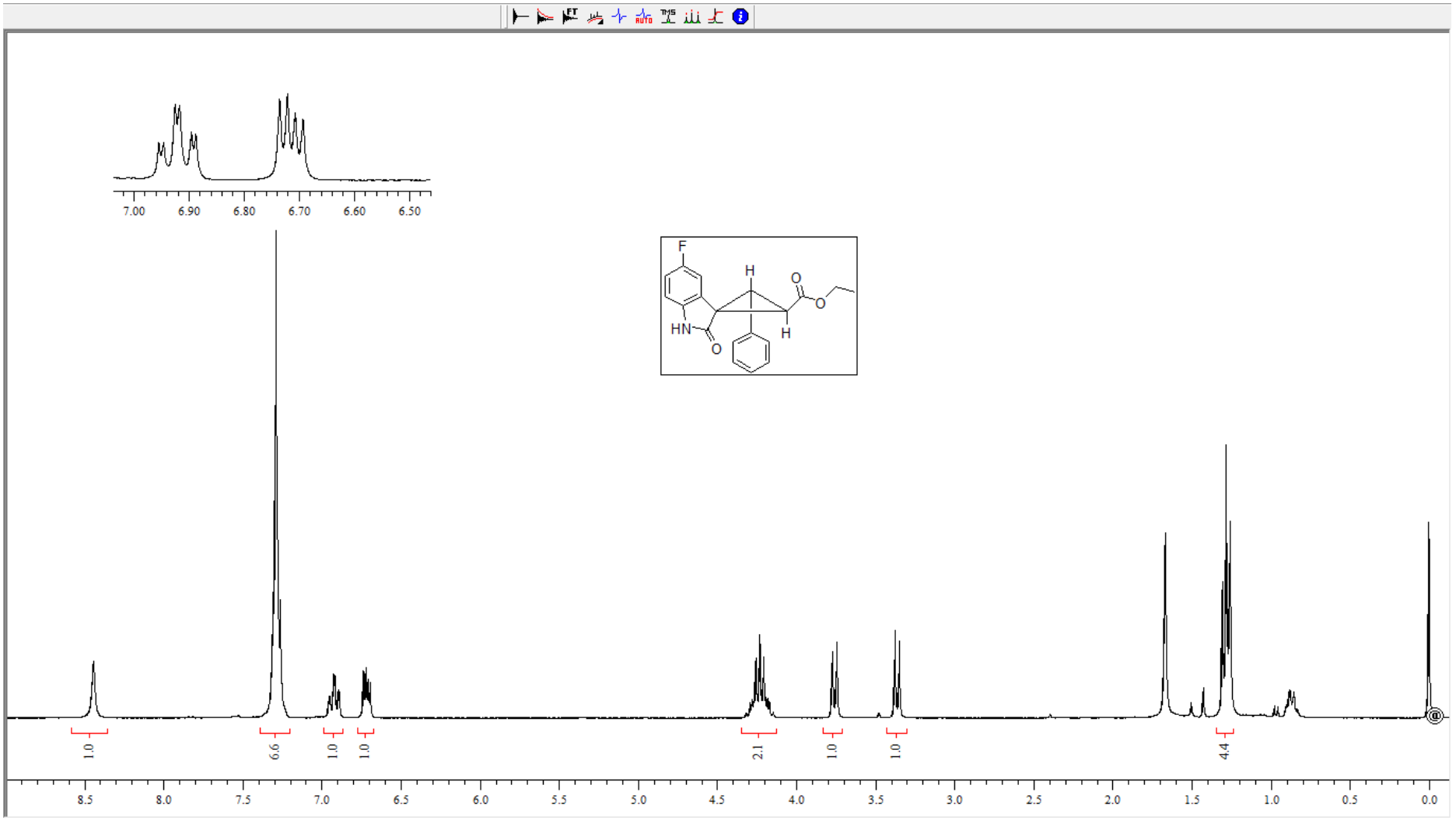
127.310
109.153
129.416
129.986
54.846
40.965
38.663
40.163
40.6 40.4 40.2 40.0 39.8 39.6 39.4 39.2 39.0 38.8 38.6 38.4
133 132 131 130 129 128 127 126 125 124
CO
CONH
OCH3
C and CH (buried in DMSO)
200 175 150 125 100 75 50 25


7.00
6.90
6.80
6.70
6.60
6.50
F
H
O
O
HN
O
H
1.0
6.6
1.0
1.0
2.1
1.0
1.0
4.4
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
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2.0
1.5
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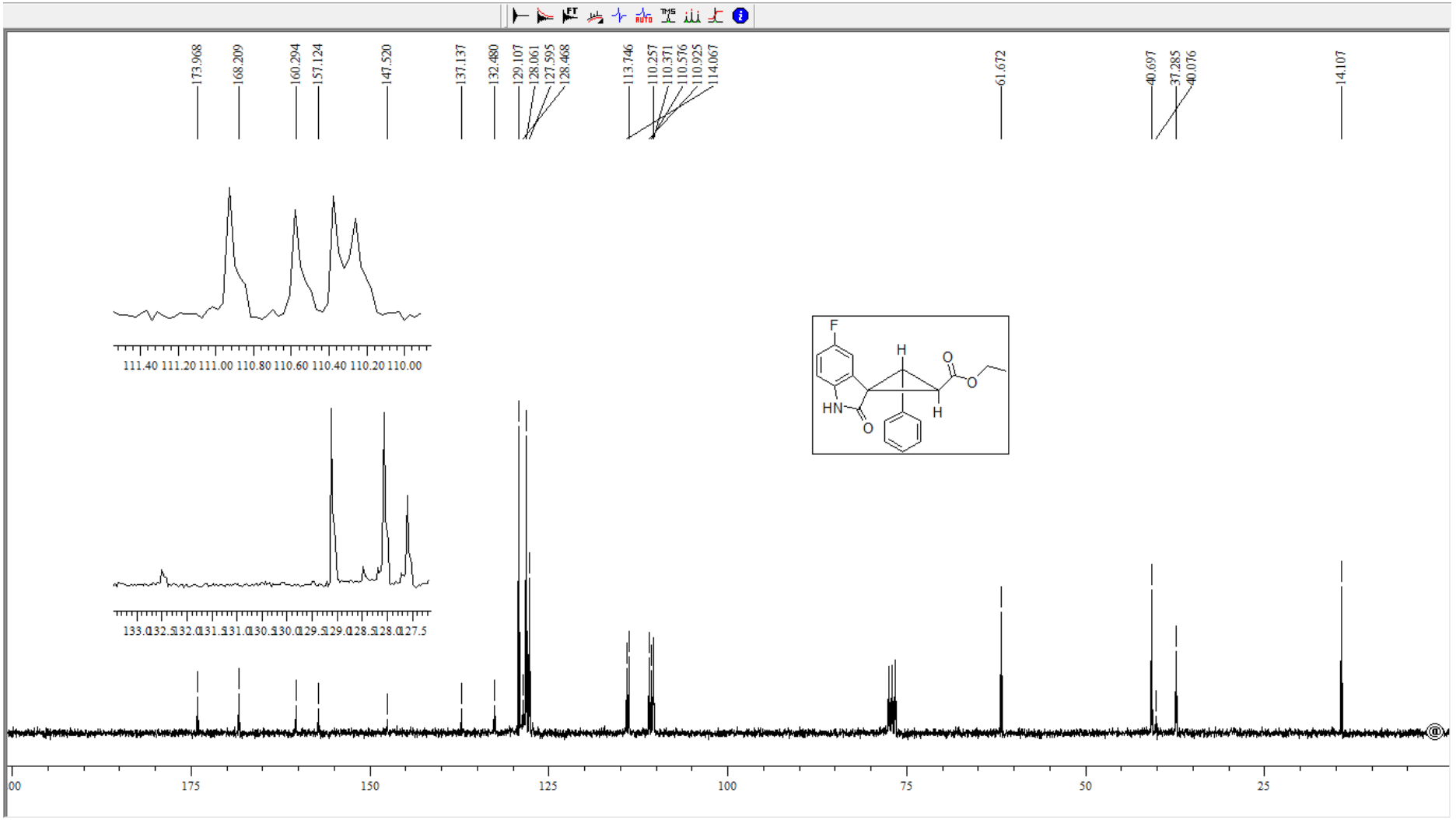
0.0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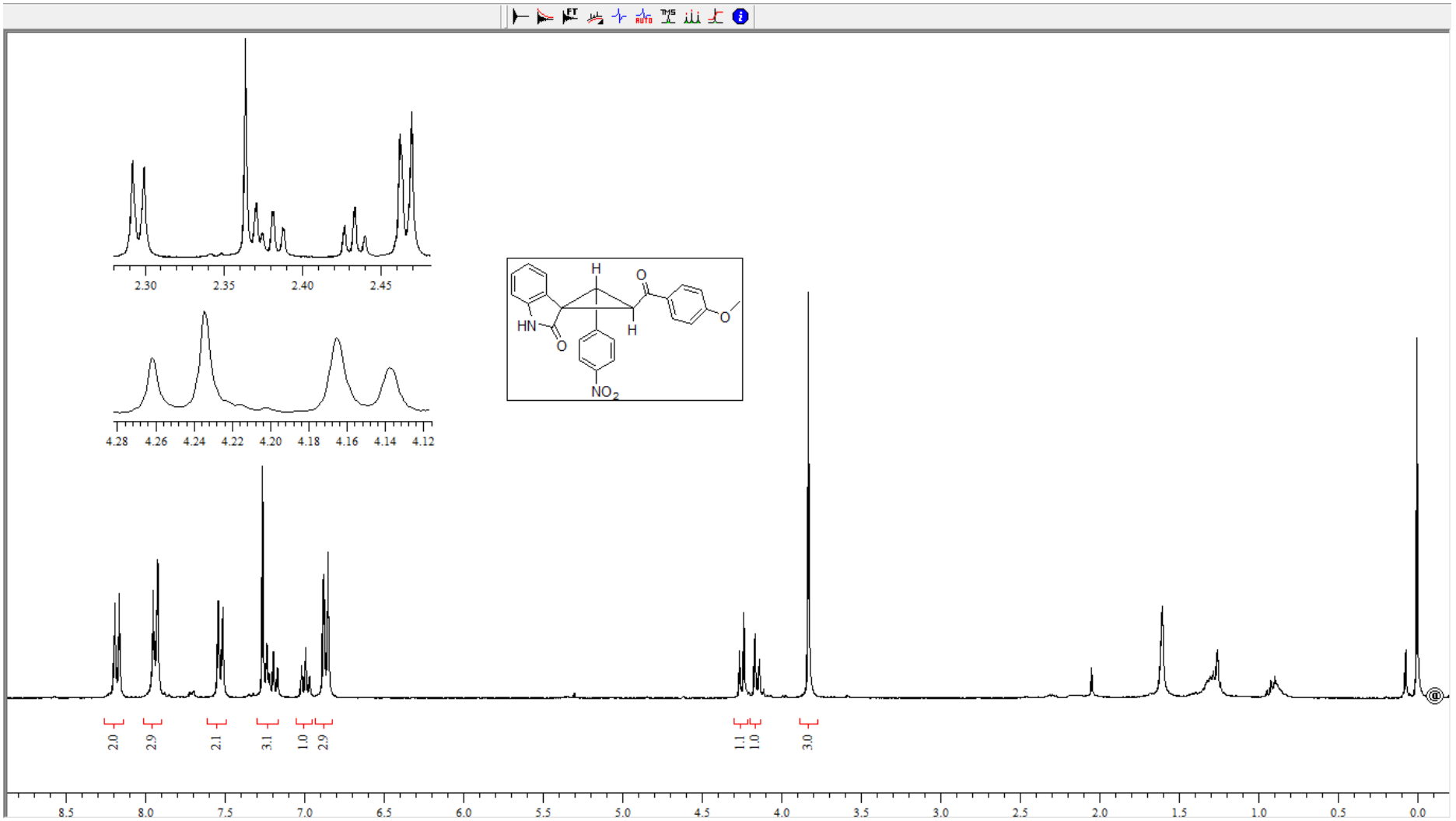
157.124
147.520
137.137
132.480
129.107
128.061
127.595
128.468
113.746
110.257
110.371
110.576
110.925
114.067
61.672
40.697
37.285
40.076
14.107
111.40 111.20 111.00 110.80 110.60 110.40 110.20 110.00
133.0 132.5 132.0 131.5 131.0 130.5 130.0 129.5 129.0 128.5 128.0 127.5
F
H
O
O
HN
O
H
00
175
150
125
100
75
50
25


2.30
2.35
2.40
2.45
4.28
4.26
4.24
4.22
4.20
4.18
4.16
4.14
4.12
H
O
HN
O
H
O
NO2
2.0
2.9
2.1
3.1
1.0
2.9
1.1
1.0
3.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
4.0
3.5
3.0
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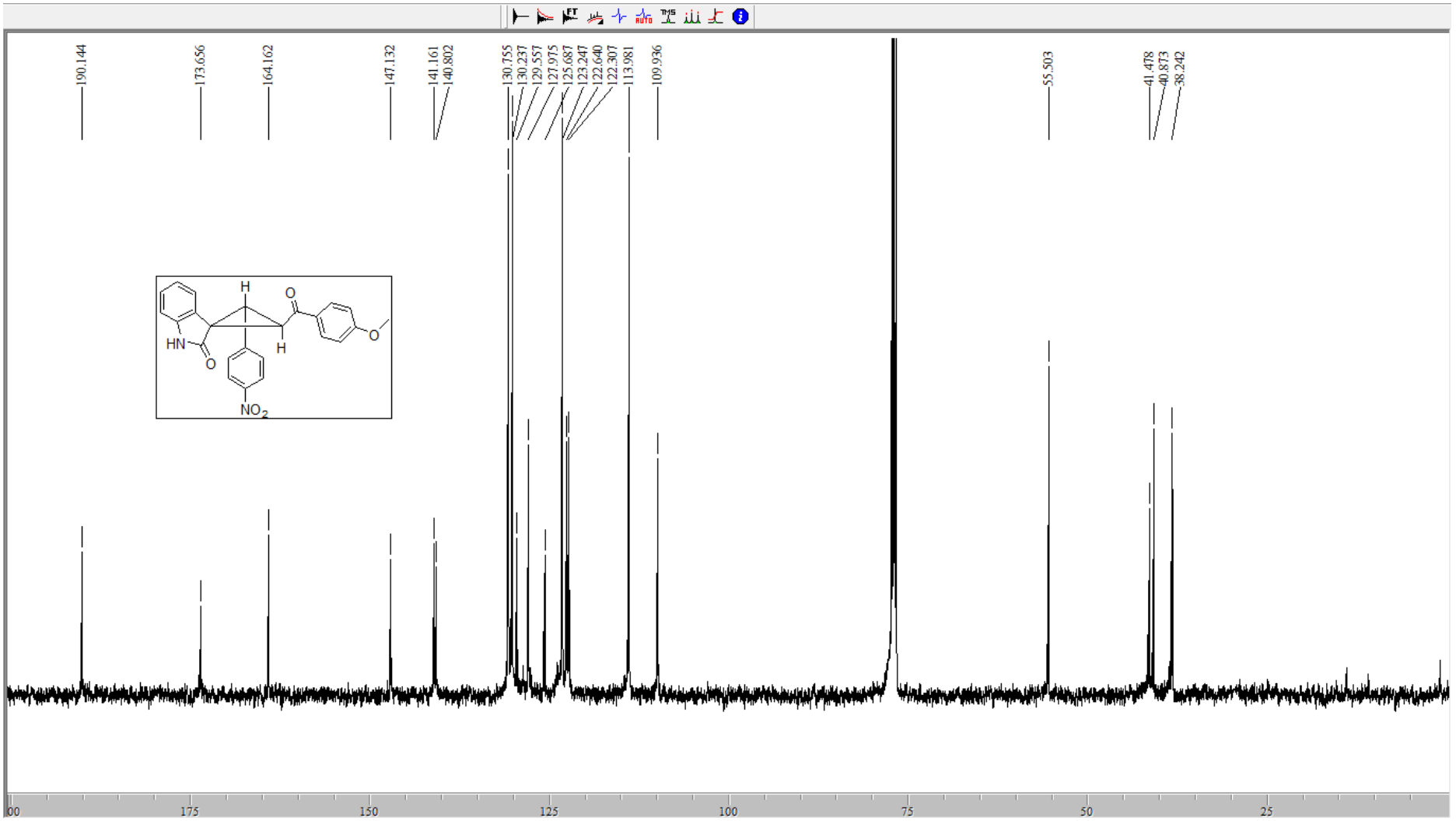
2.0
1.5
1.0
0.5
0.0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173.656
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141.161
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127.975
125.687
123.247
122.640
122.307
113.981
109.936
55.503
41.478
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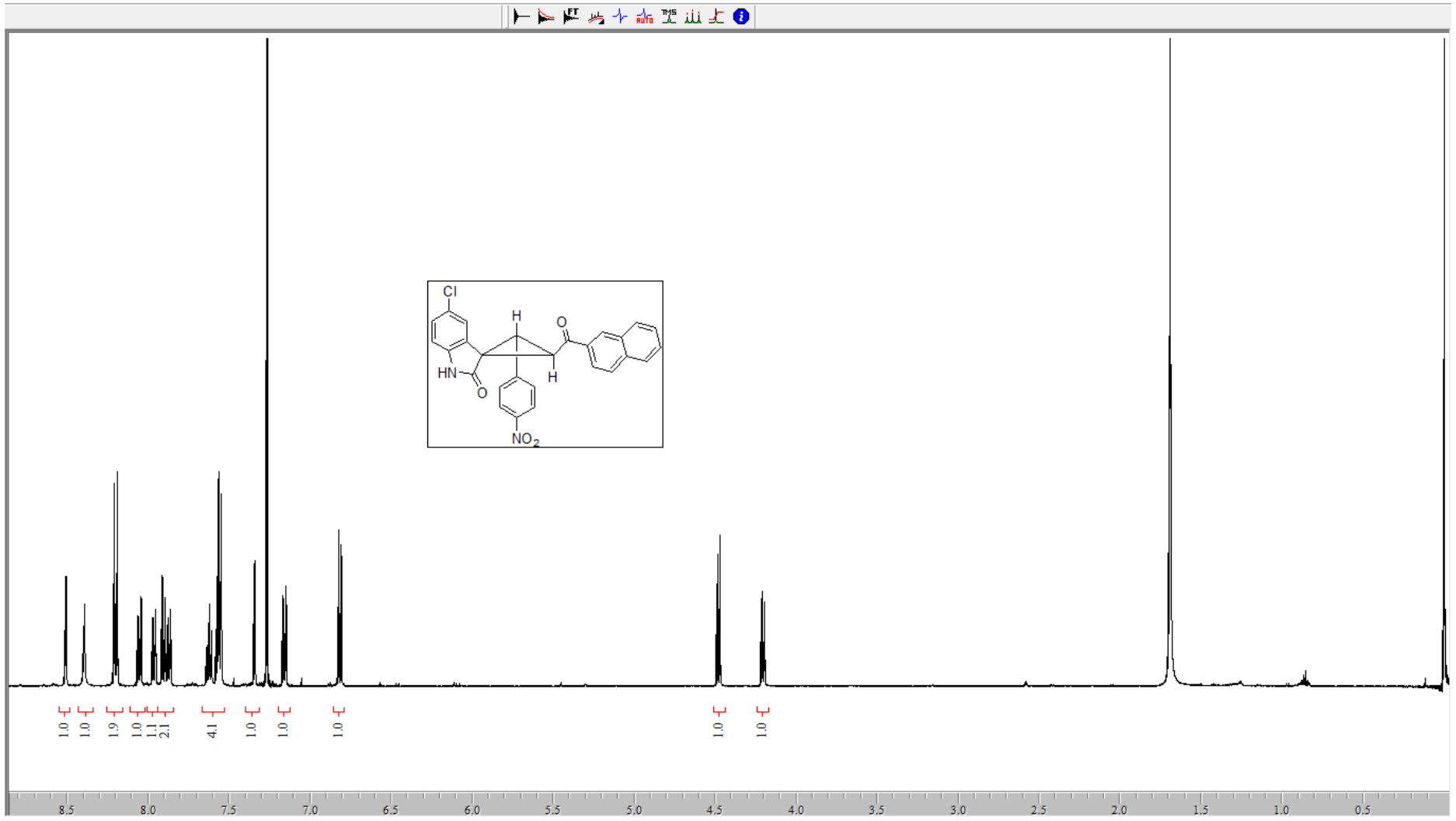
38.242
H
O
HN
O
H
O
NO2
175
150
125
100
75
50
25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H
O
HN
O
H
NO2
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1.0
1.9
1.0
1.1
2.1
4.1
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1.0
1.0
1.0
1.0
8.5
8.0
7.5
7.0
6.5
6.0
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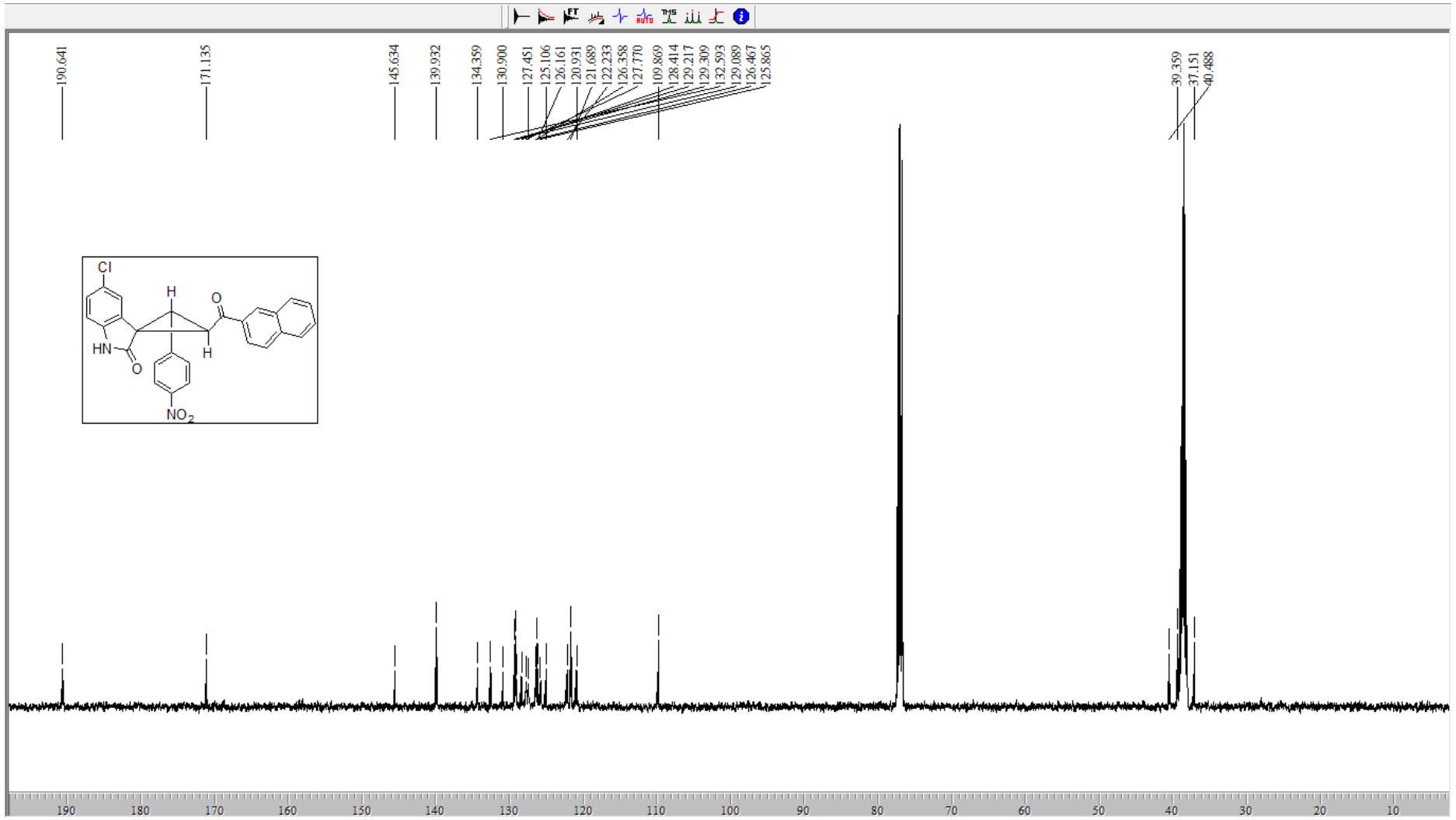
0.5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130.900
127.451
125.106
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120.931
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126.358
127.770
109.869
128.414
129.217
129.309
132.593
129.089
126.467
125.865
39.359
37.151
40.488
Cl
H
O
HN
O
H
NO2
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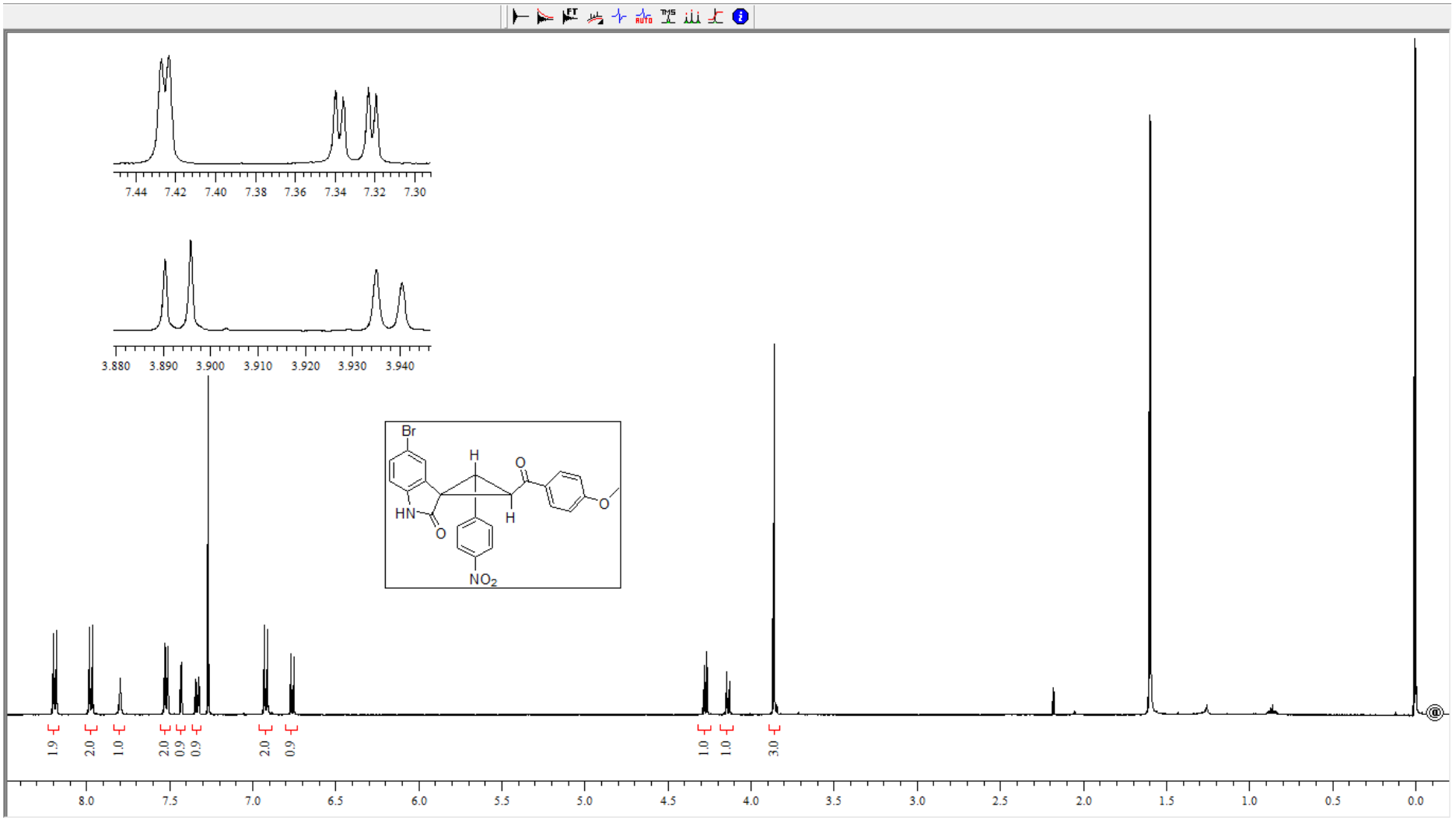
10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Br
H
O
HN
O
H
O
NO2
1.9 2.0 1.0 2.0 0.9 0.9 2.0 0.9 1.0 1.0 3.0
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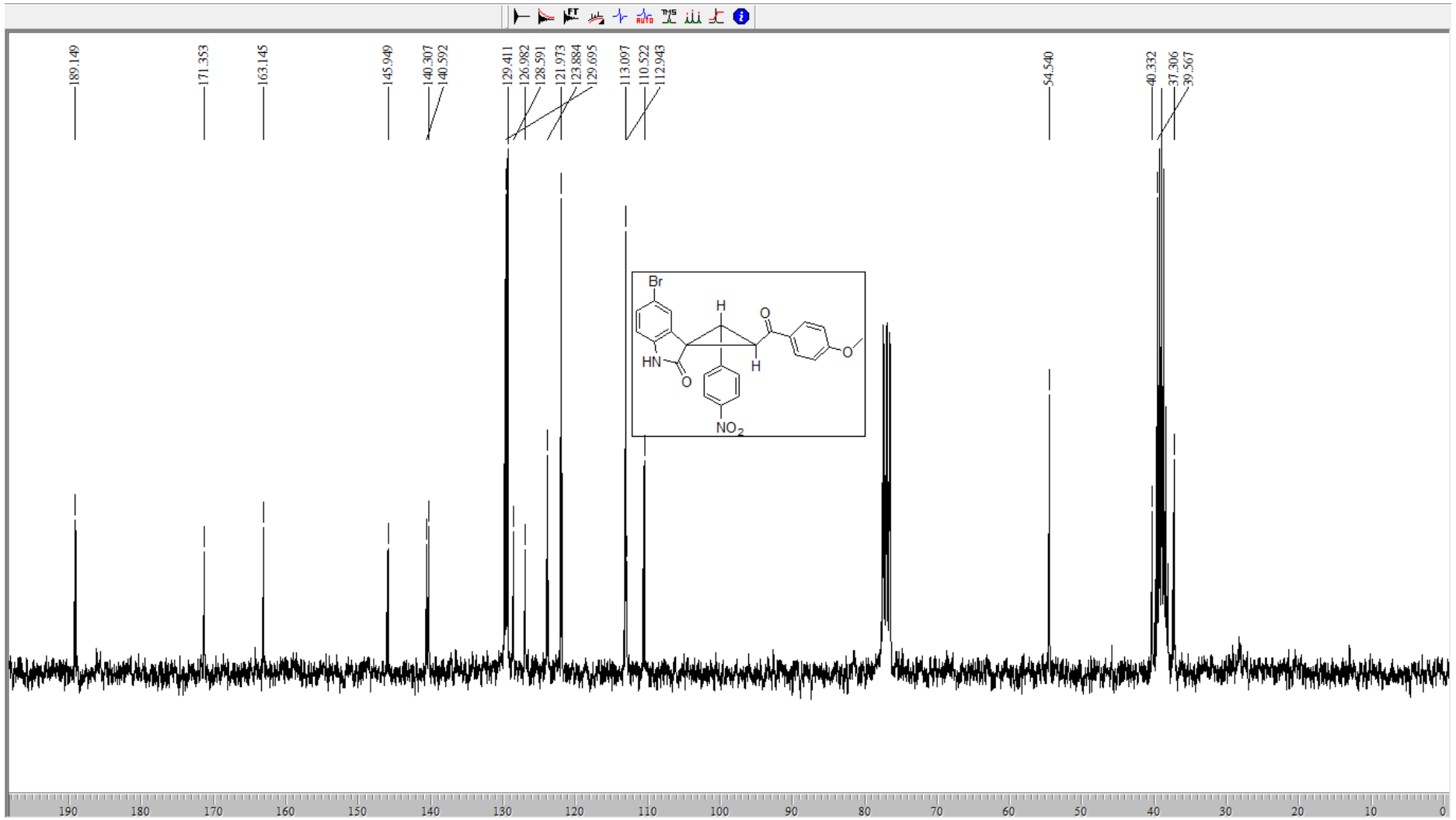
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129.695
113.097
110.522
112.943
54.540
40.332
37.306
39.567
Br
H
O
HN
O
H
O
NO2
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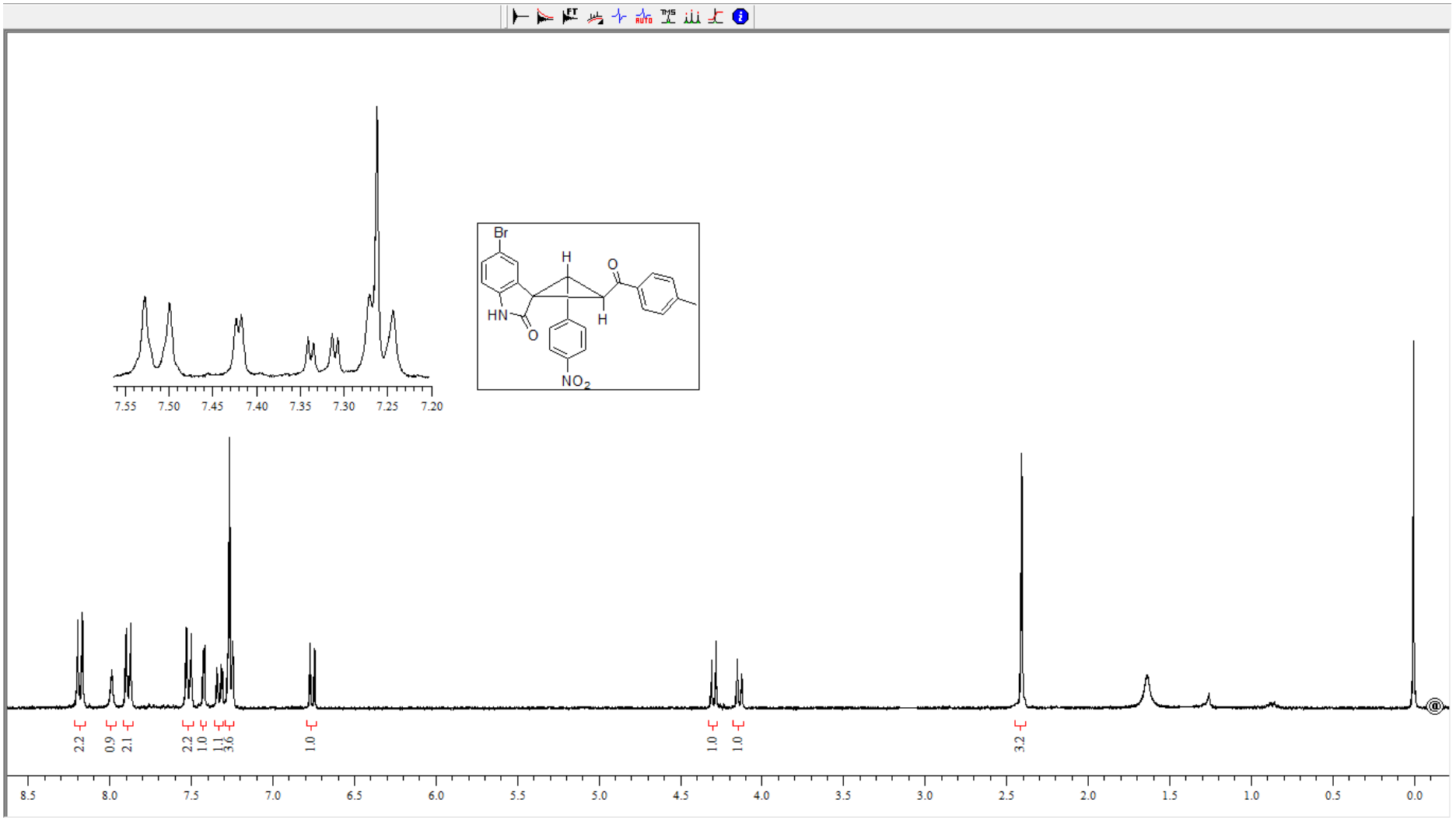
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H
O
HN
O
H
NO2
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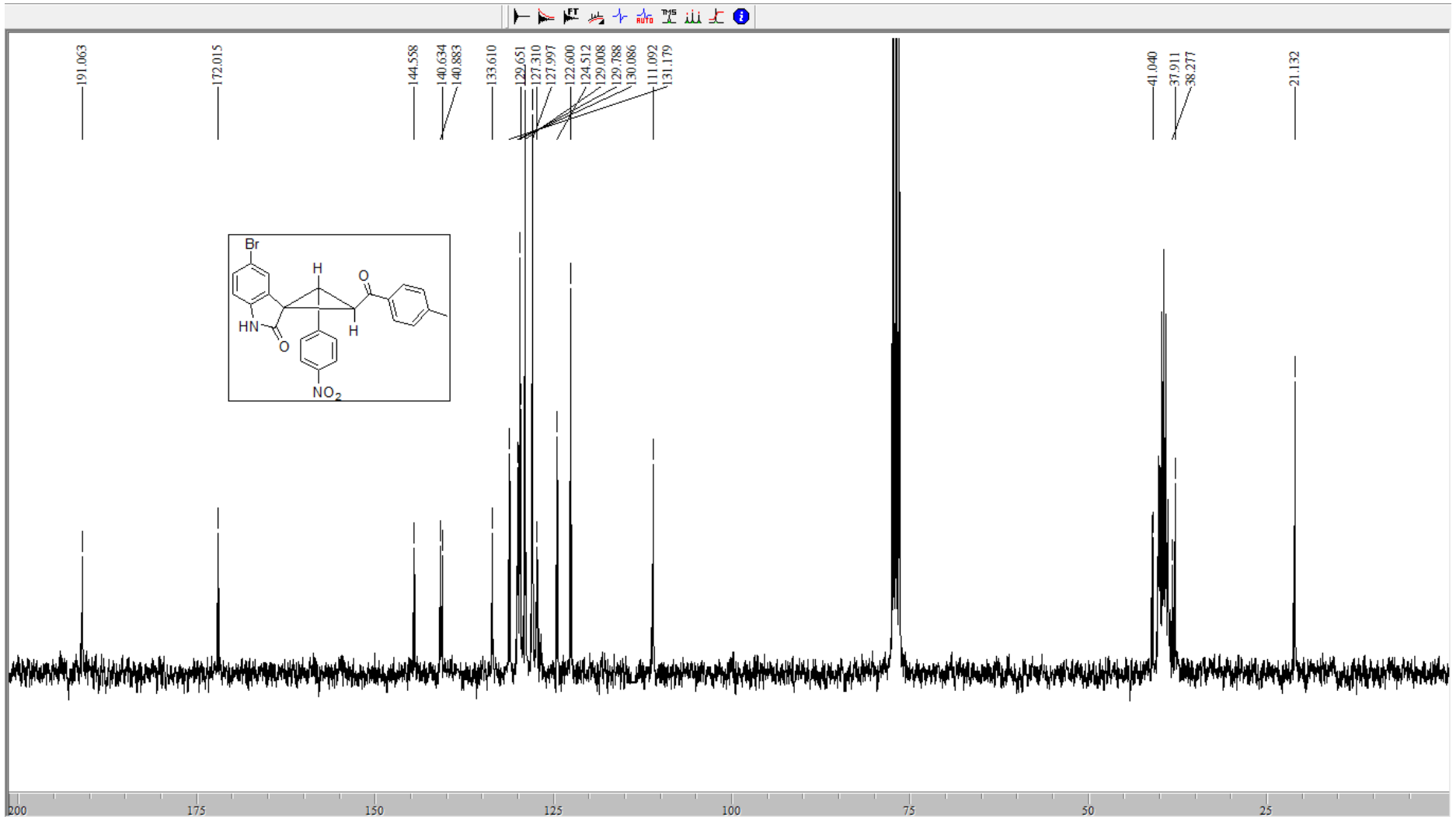
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130.086
111.092
131.179
41.040
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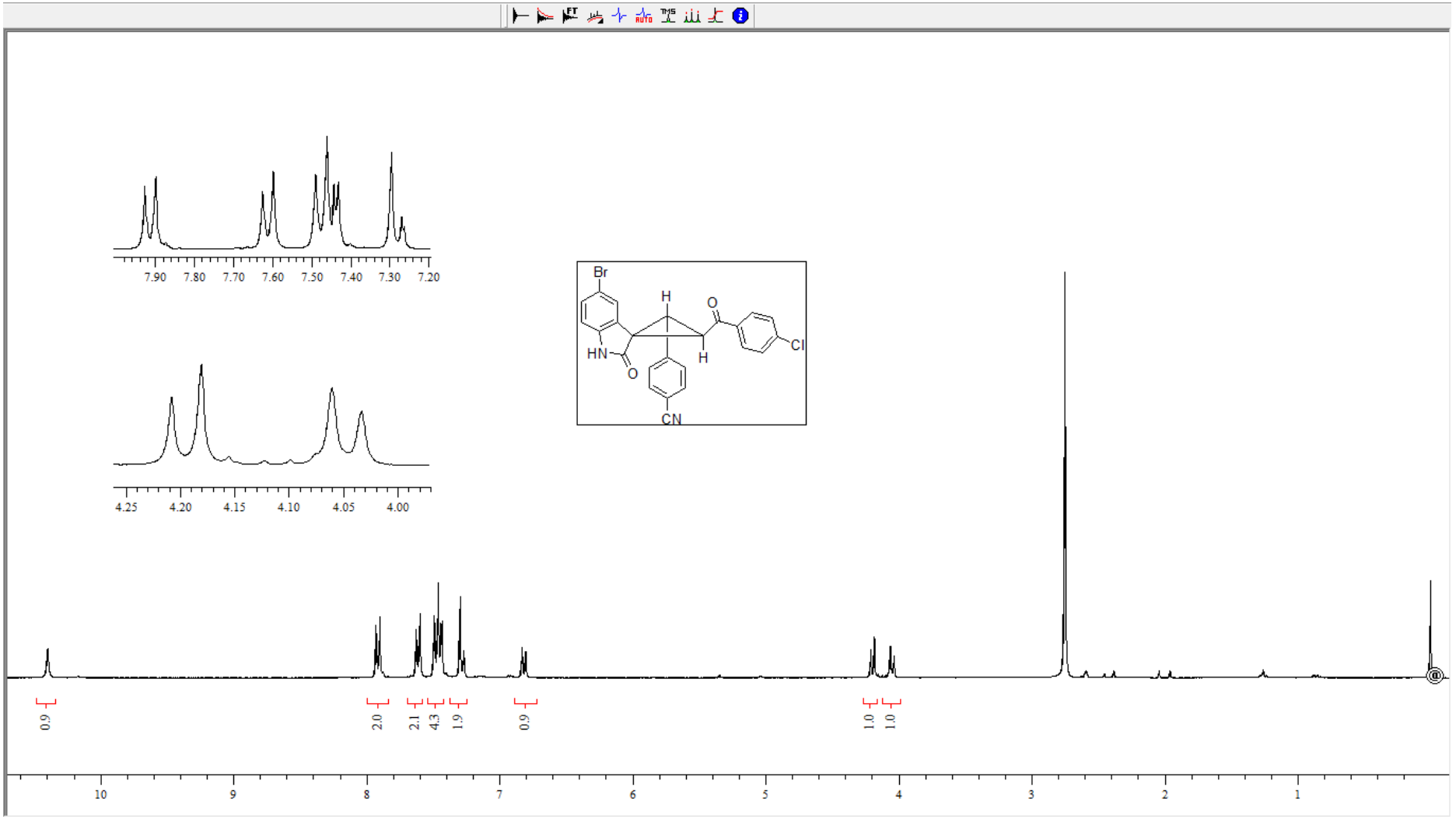
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2.1
4.3
1.9
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1.0
1.0
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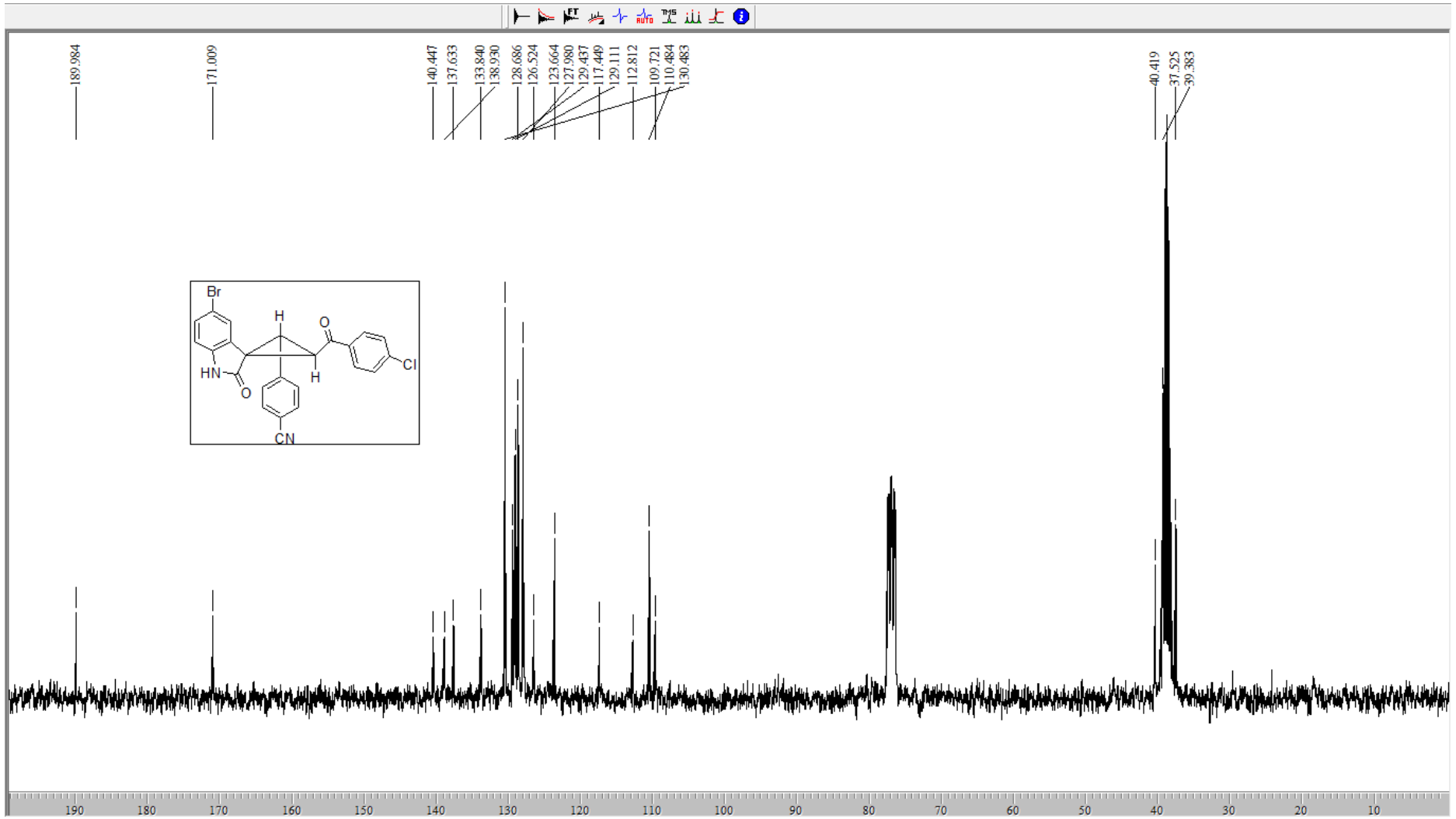
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112.812
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110.484
130.483
40.419
37.525
39.383
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O
HN
O
H
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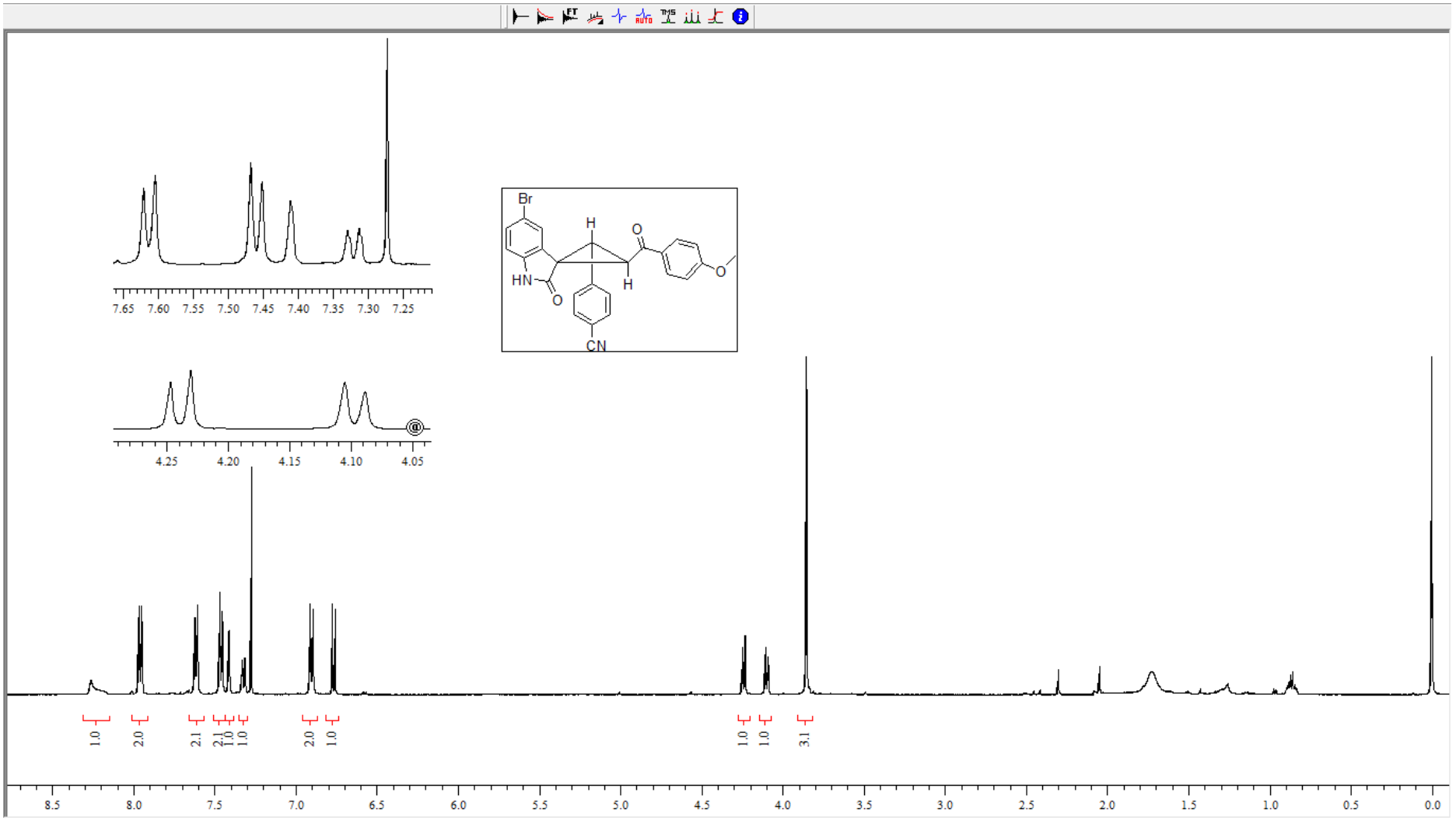
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4.25 4.20 4.15 4.10 4.05
1.0 2.0 2.1 2.1 1.0 1.0 2.0 1.0 1.0 1.0 3.1
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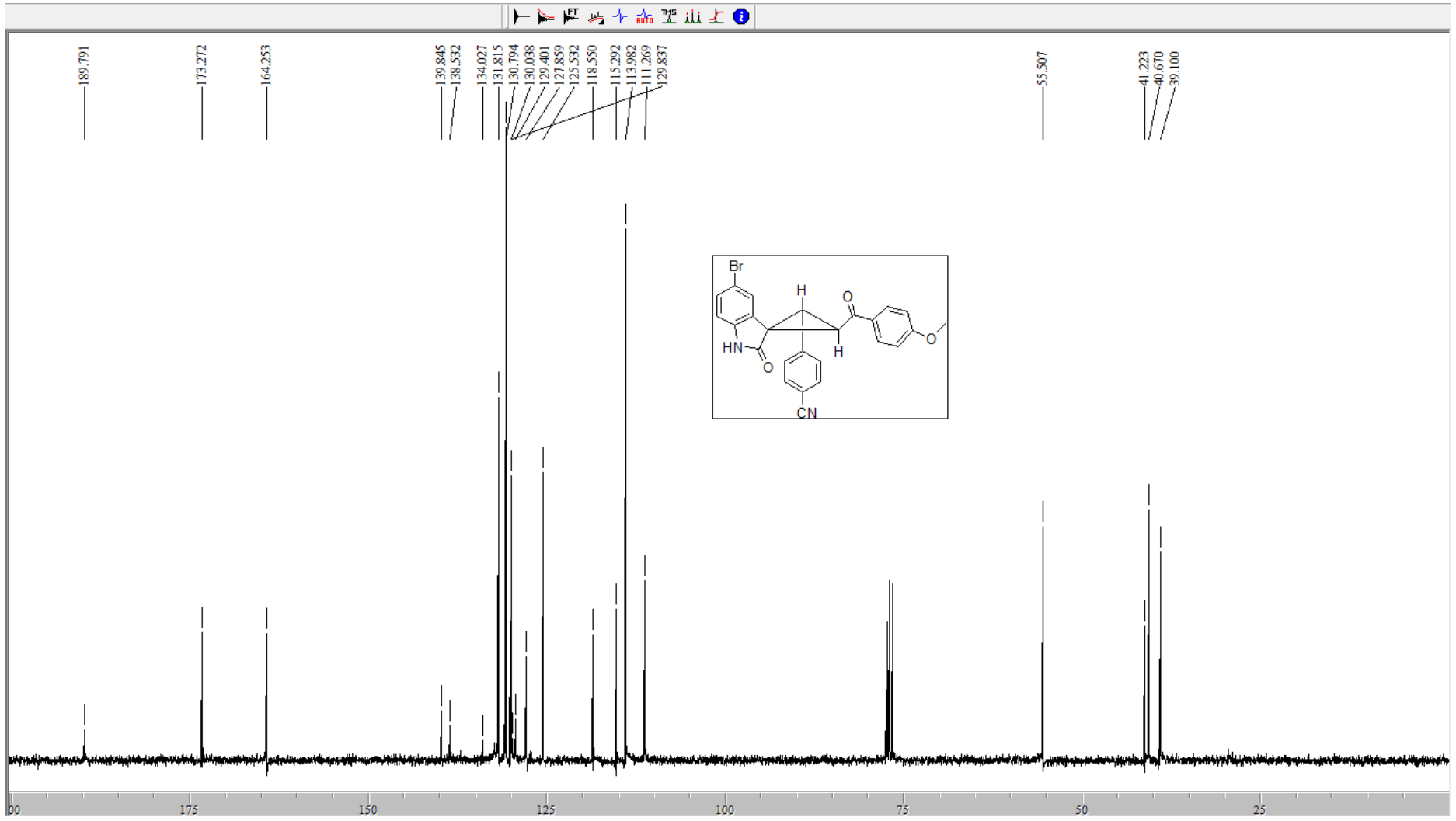
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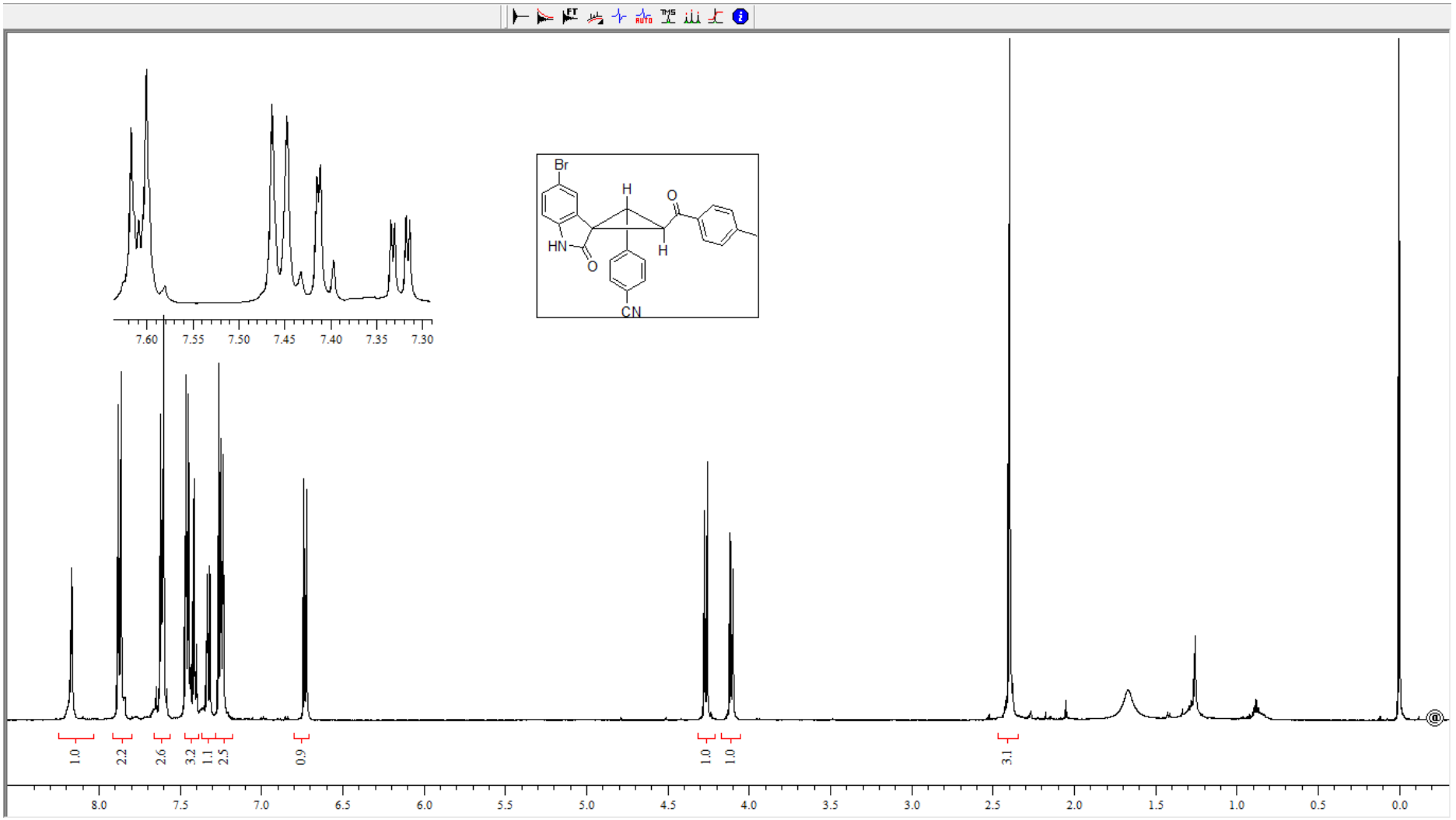
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7.35
7.30
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2.2
2.6
3.2
1.1
2.5
0.9
1.0
1.0
3.1
8.0
7.5
7.0
6.5
6.0
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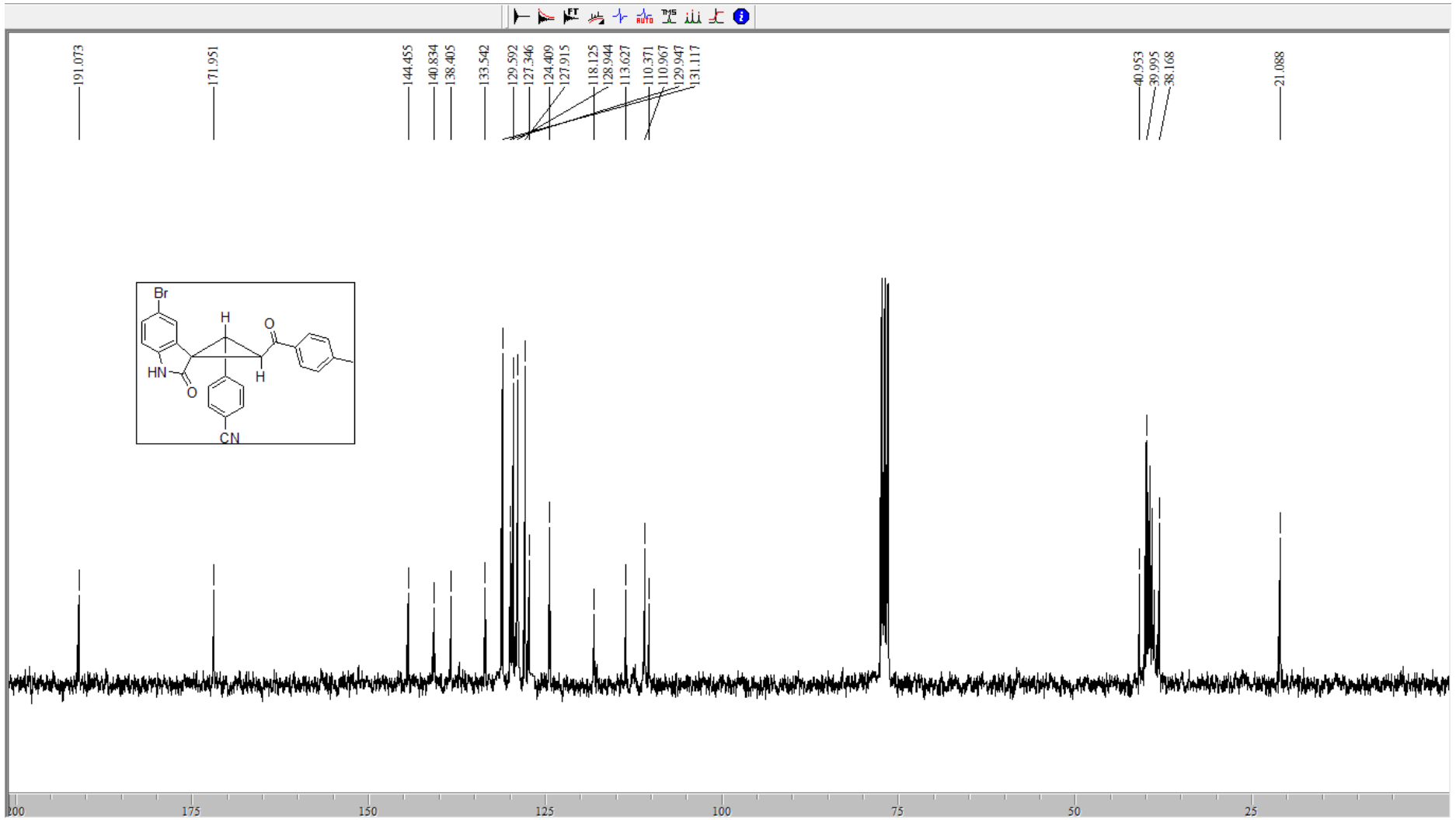
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131.117
40.953
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O
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125
100
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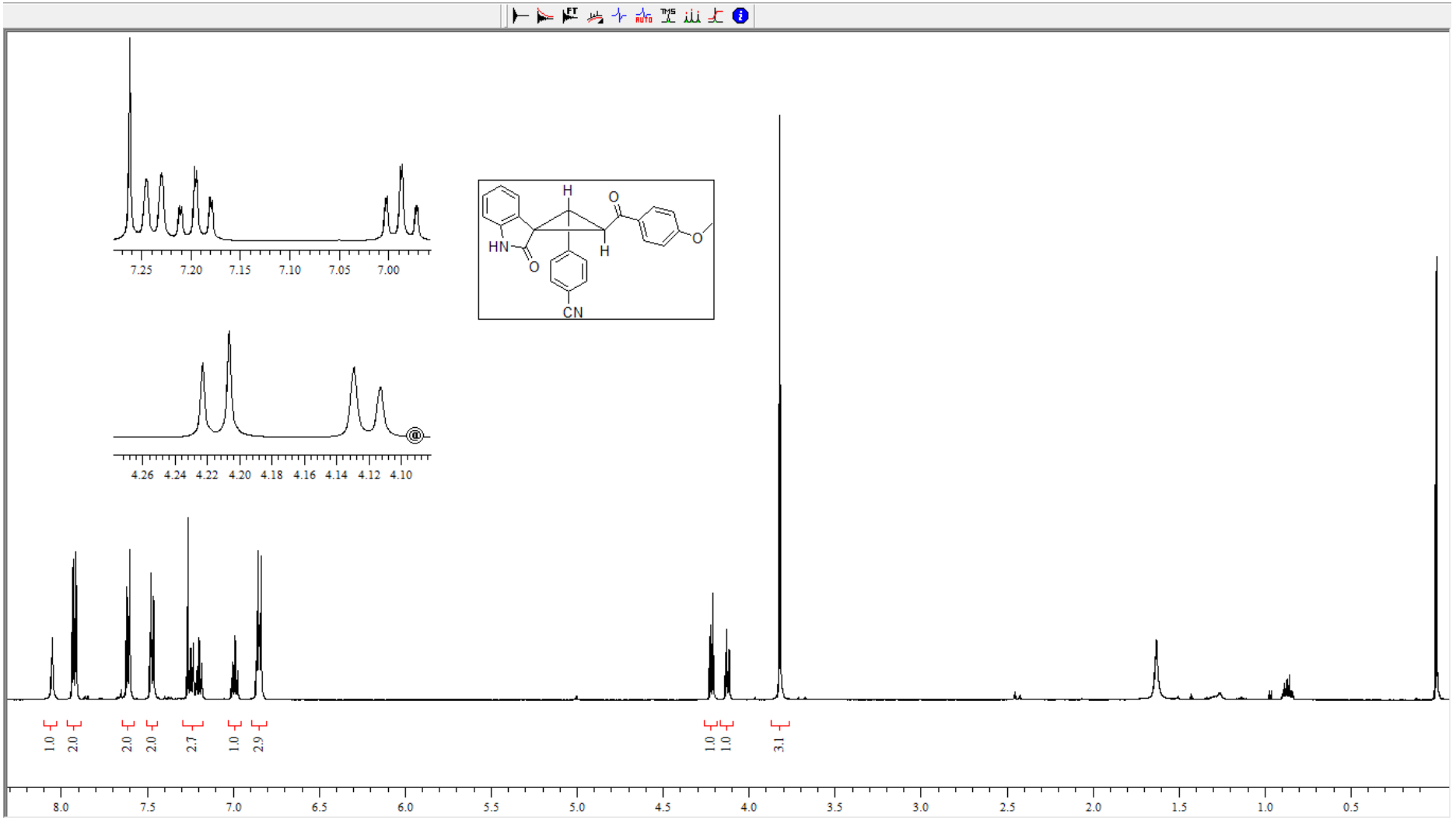
50
25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HN
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CN
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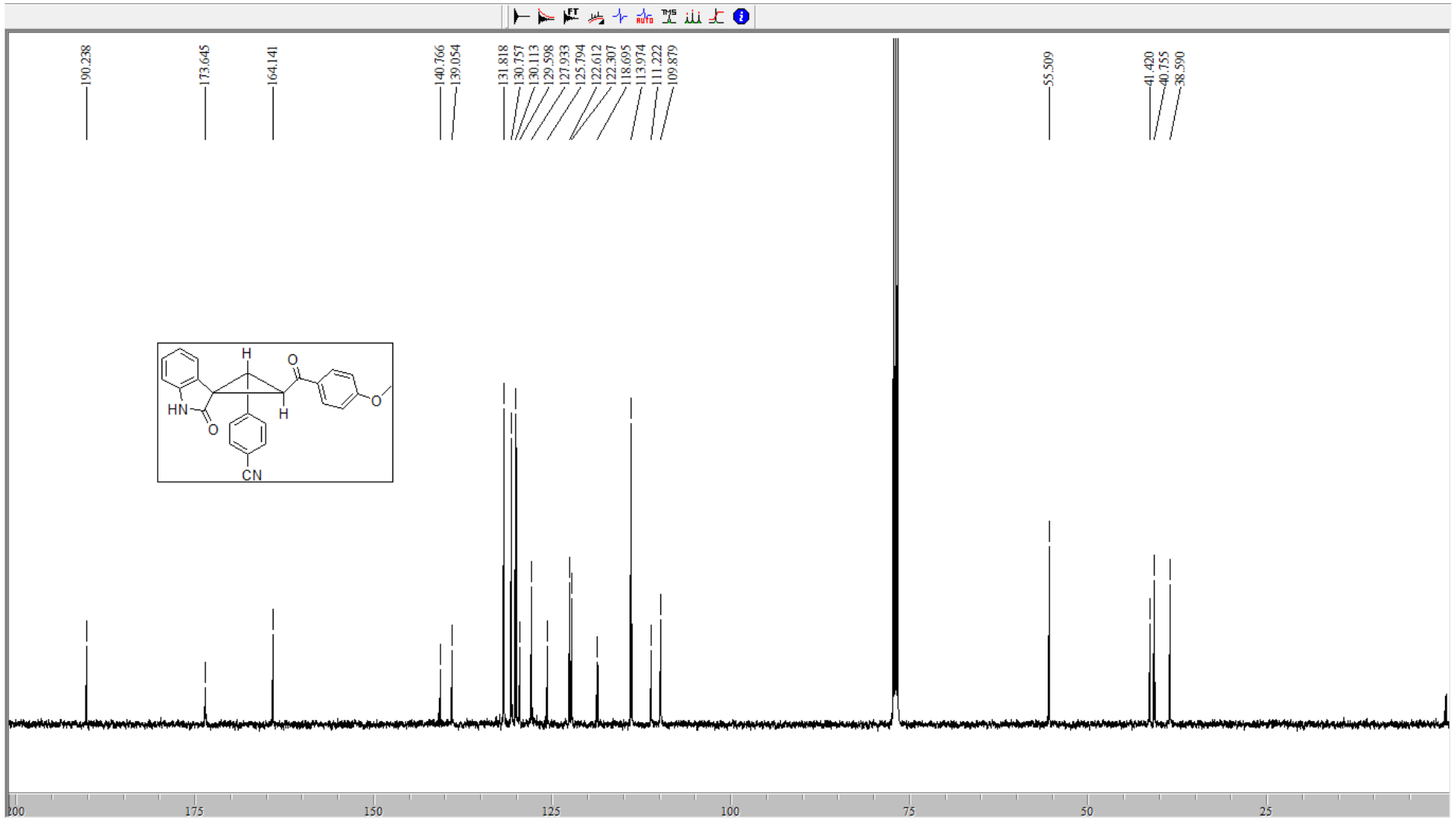
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55.509
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200
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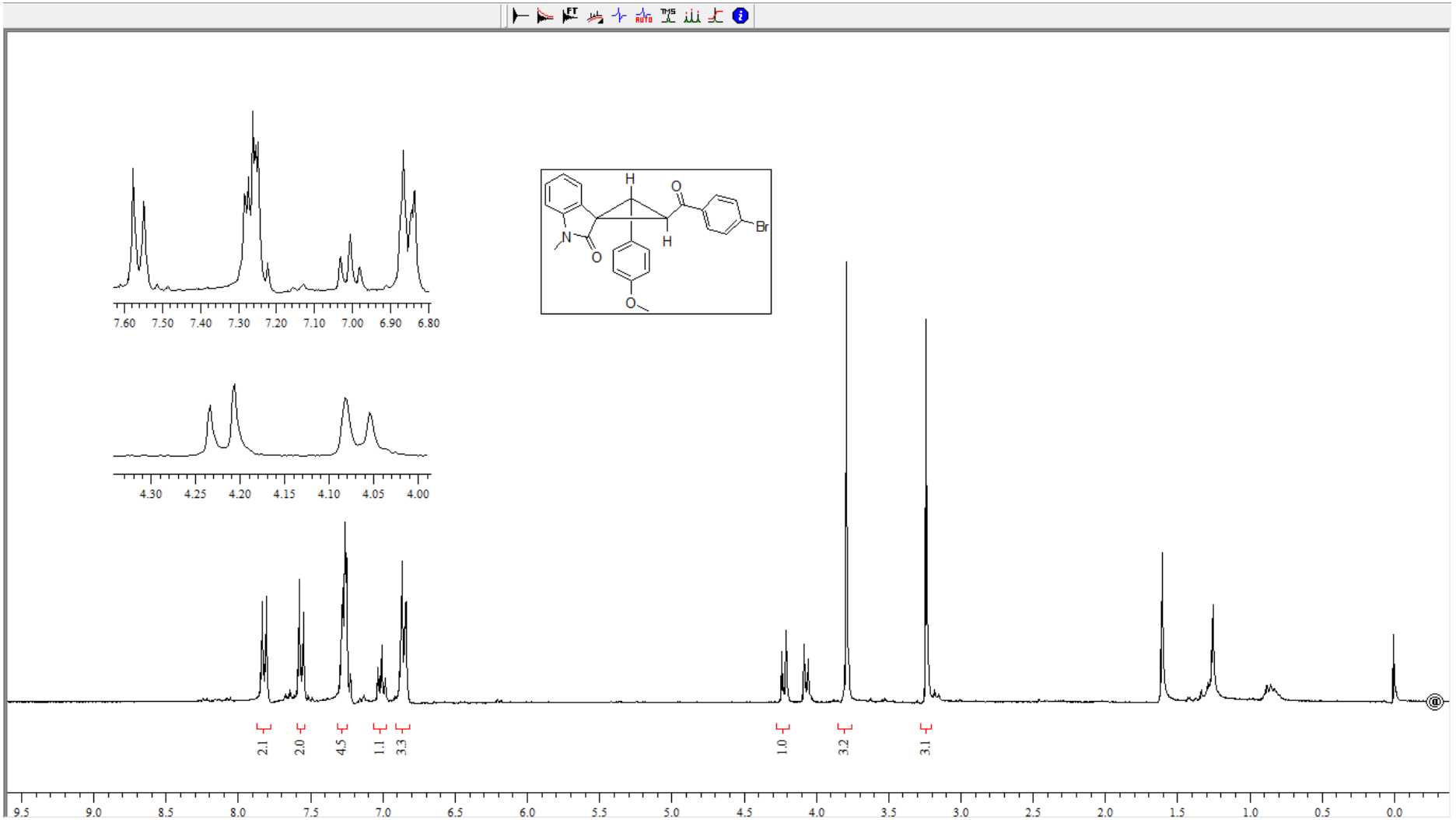
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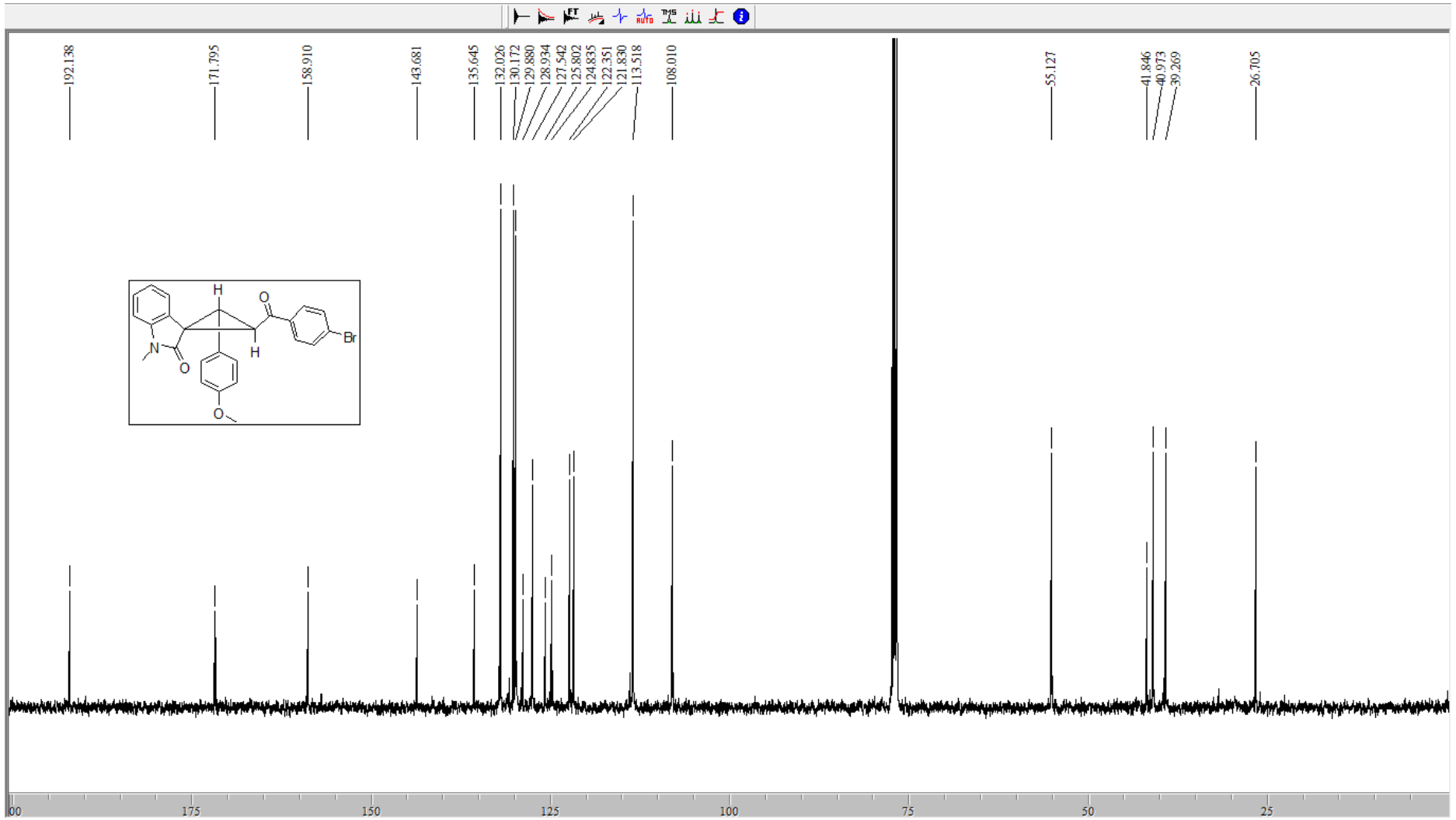
N
O
H
Br
O
2.1
2.0
4.5
1.1
3.3
1.0
3.2
3.1
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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41.846
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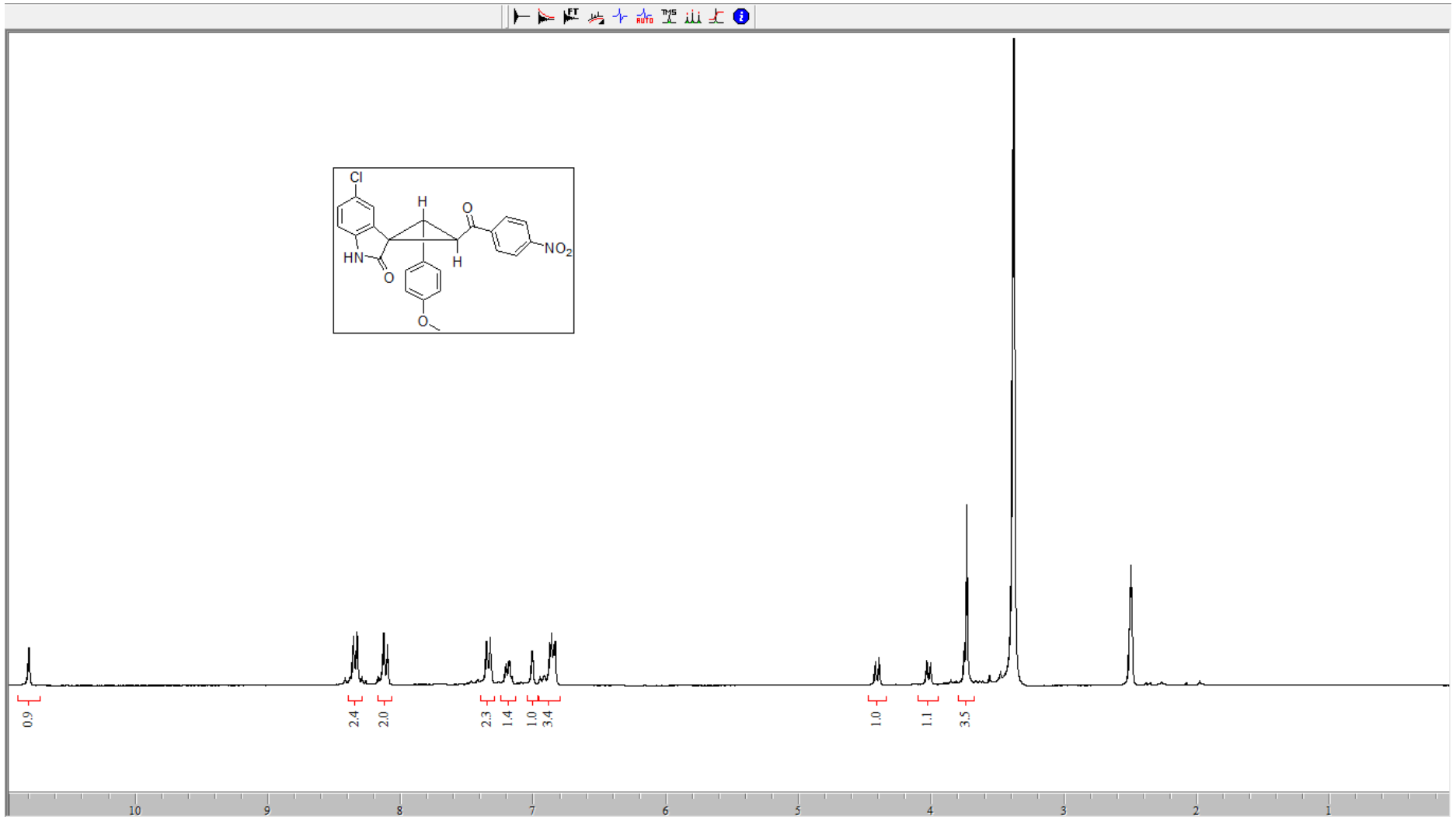
25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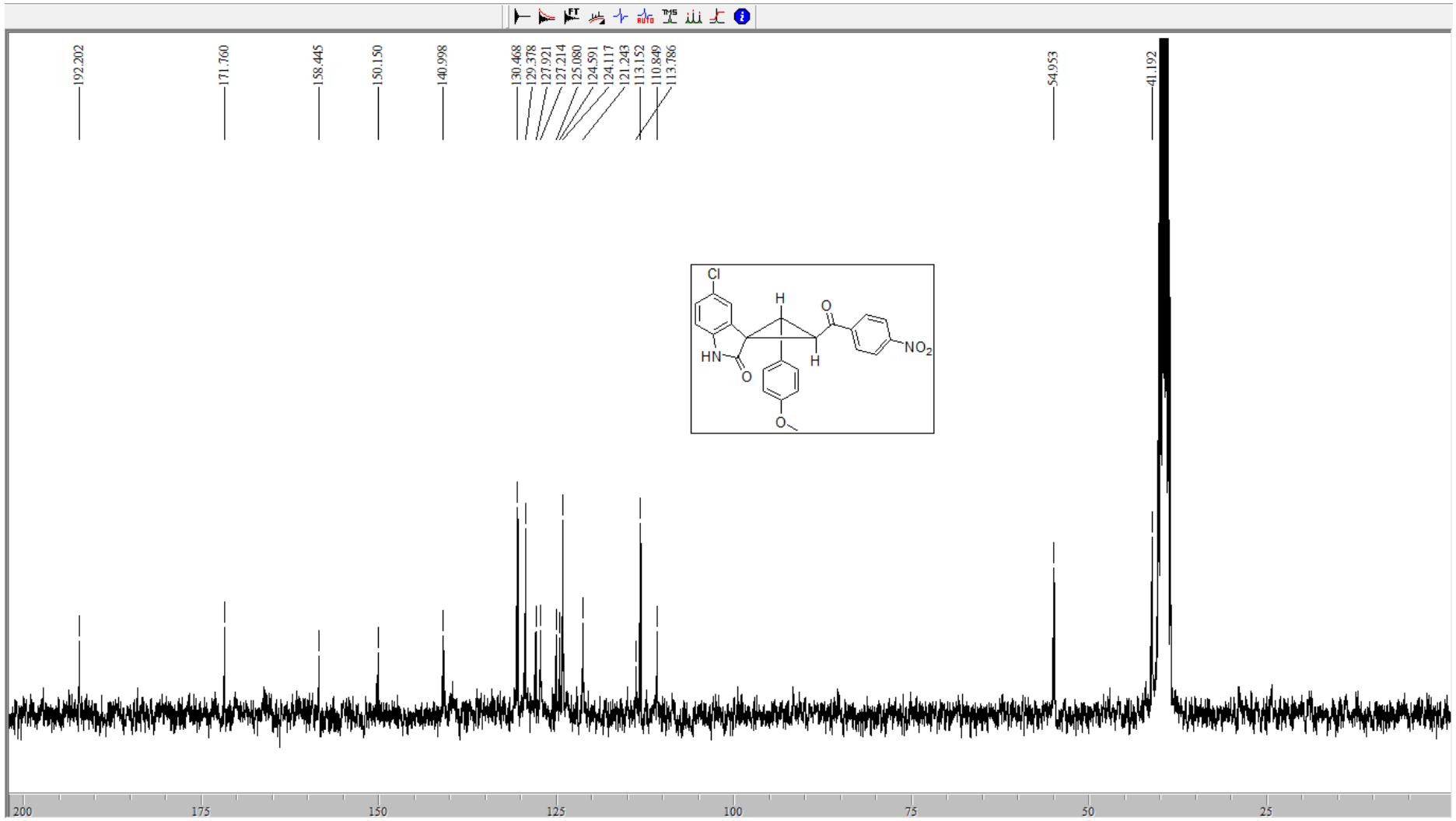
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113.786
54.953
41.192
Cl
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NO2
HN
O
H
O
200
175
150
125
100
75
50
25