Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information for **"Regio- and stereoselective synthesis of novel spiropyrrolidines through 1,3-dipolar cycloaddition reactions of azomethine ylides and 2-styrylquinazolin-4(3*H*)-ones"**

Contents

Crystallographic data for AU95 (compound **4a**)

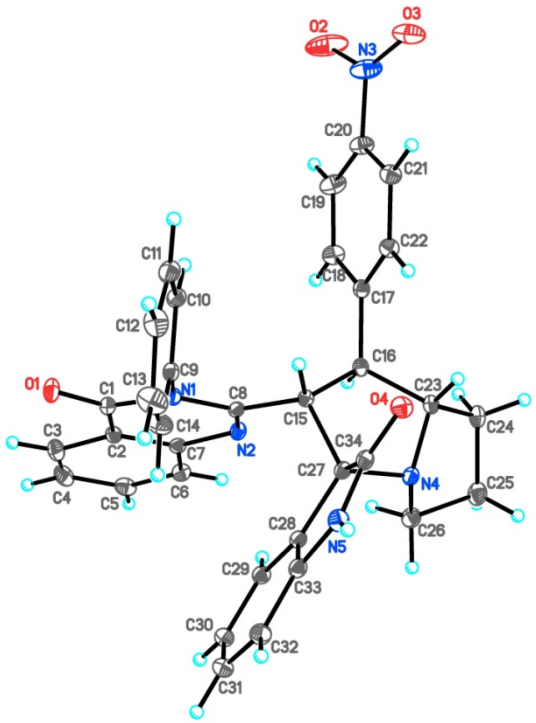


Figure caption: The molecular structure of AU95 (compound **4a**) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 10% probability level and H atoms are shown as small spheres of arbitrary radius.

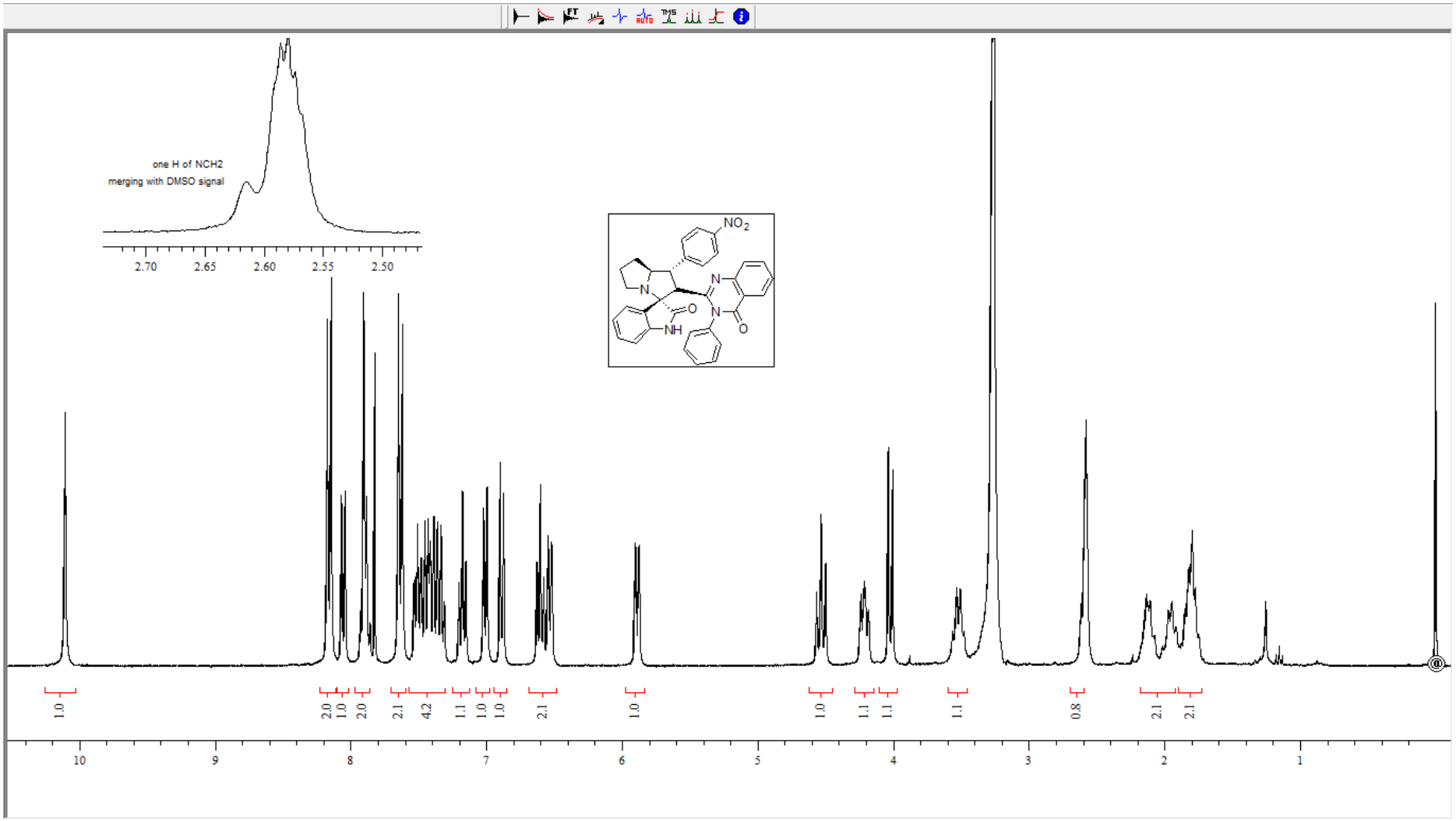
Crystal data for AU95: $C_{34}H_{27}N_5O_4$, M = 569.61, orange rectangle, 0.49 x 0.18 x 0.12 mm^3, monoclinic, space group $P2_1/c$ (No. 14), a = 15.9316(13), b = 11.8821(10), c = 15.2579(12) Å, β = 103.5740(10)˚, V = 2807.7(4) Å^3, Z = 4, D_c = 1.348 g/cm^3, F_{000} = 1192, CCD area detector, MoKα radiation, λ = 0.71073

Å, T = 293(2)K, $2\vartheta_{max}$ = 50.0º, 26396 reflections collected, 4927 unique (R_{int} = 0.0238), Final GooF = 1.048, *R1* = 0.0384, *wR2* = 0.0979, *R* indices based on 4249 reflections with I >2σ(I) (refinement on F^2), 392 parameters, μ = 0.091 mm^{-1}. CCDC 994872 contains the supplementary crystallographic data for this paper. 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.

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 5516 reflections for AU95 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.

References:

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.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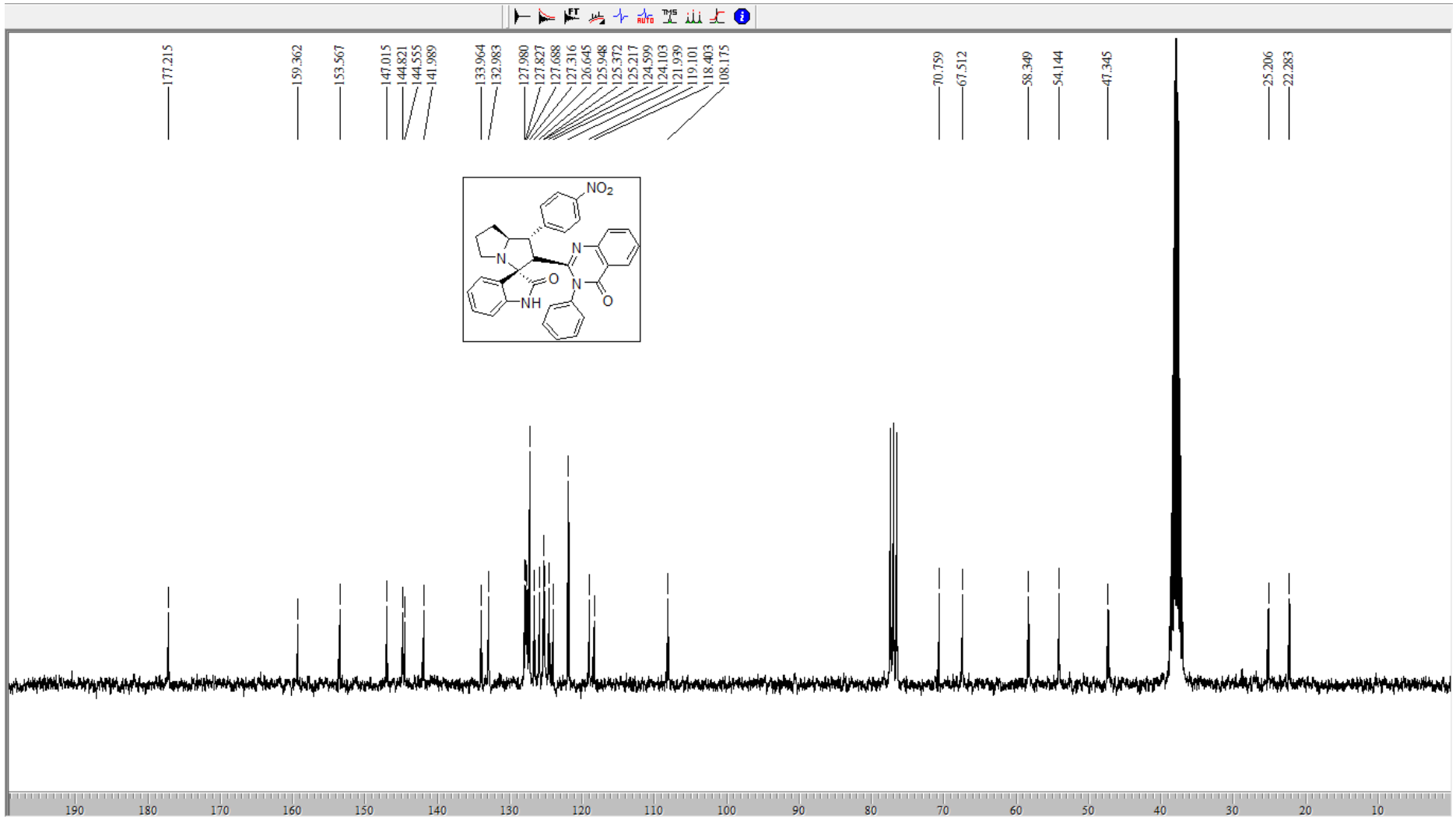
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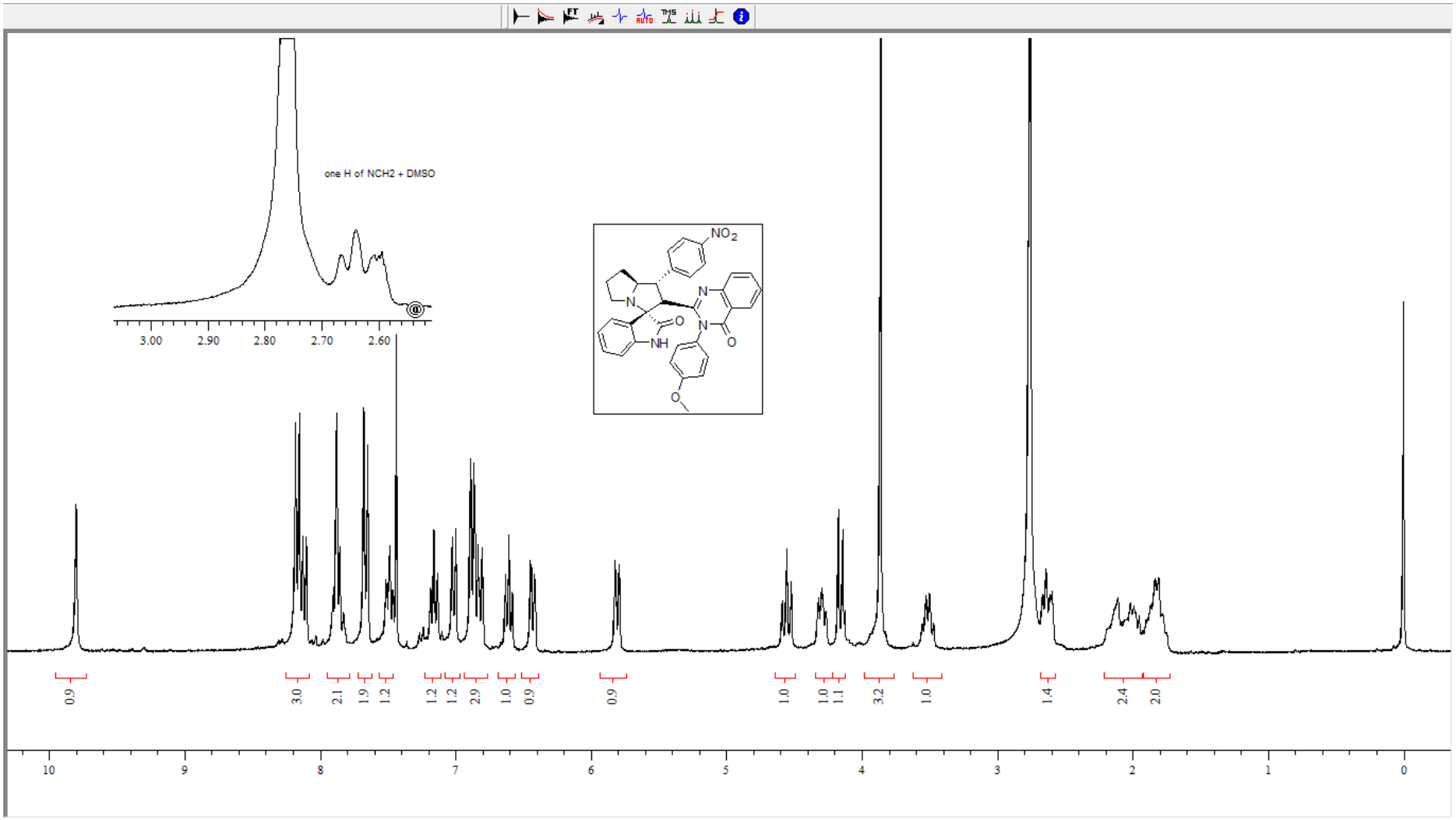
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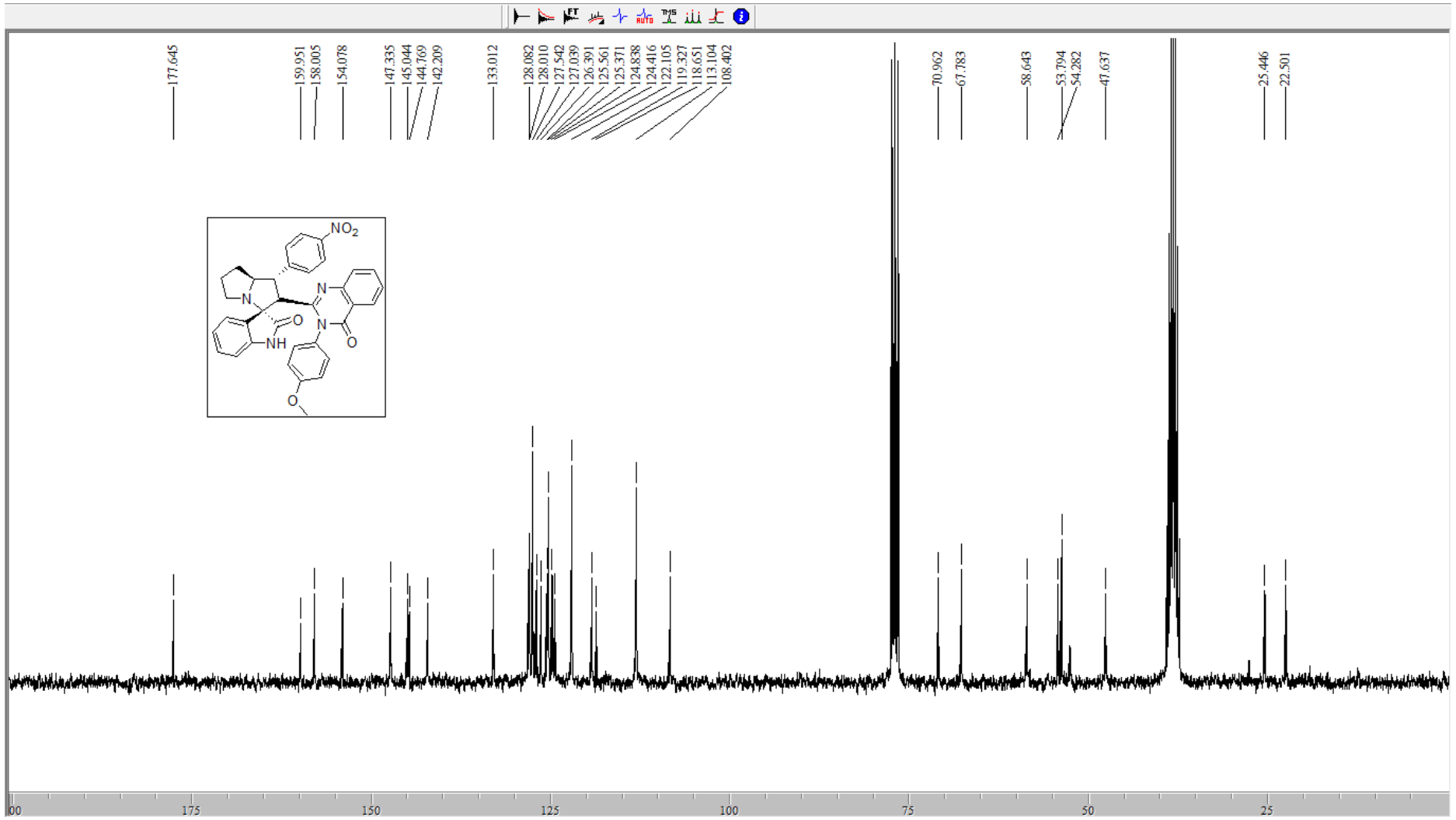
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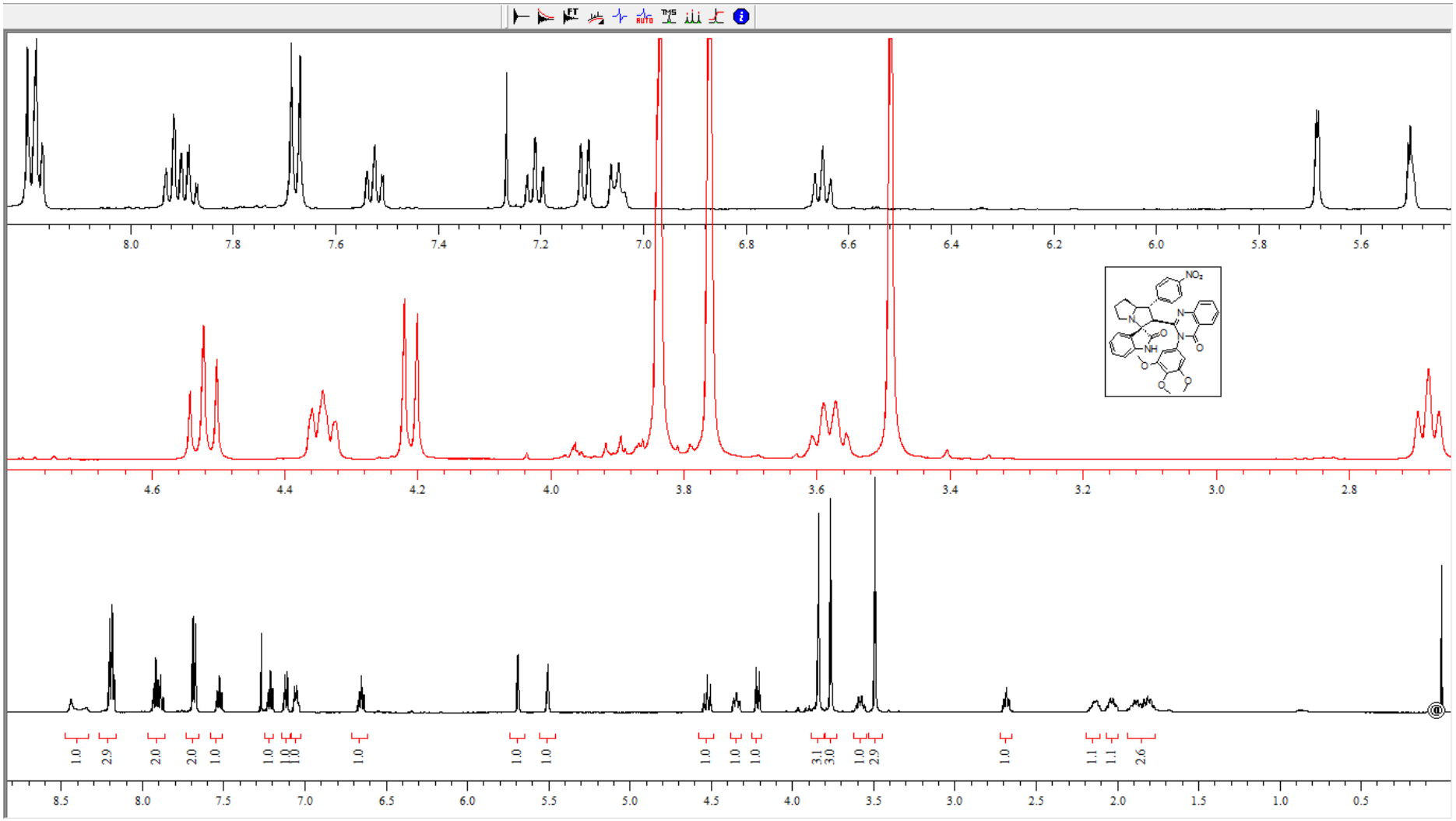
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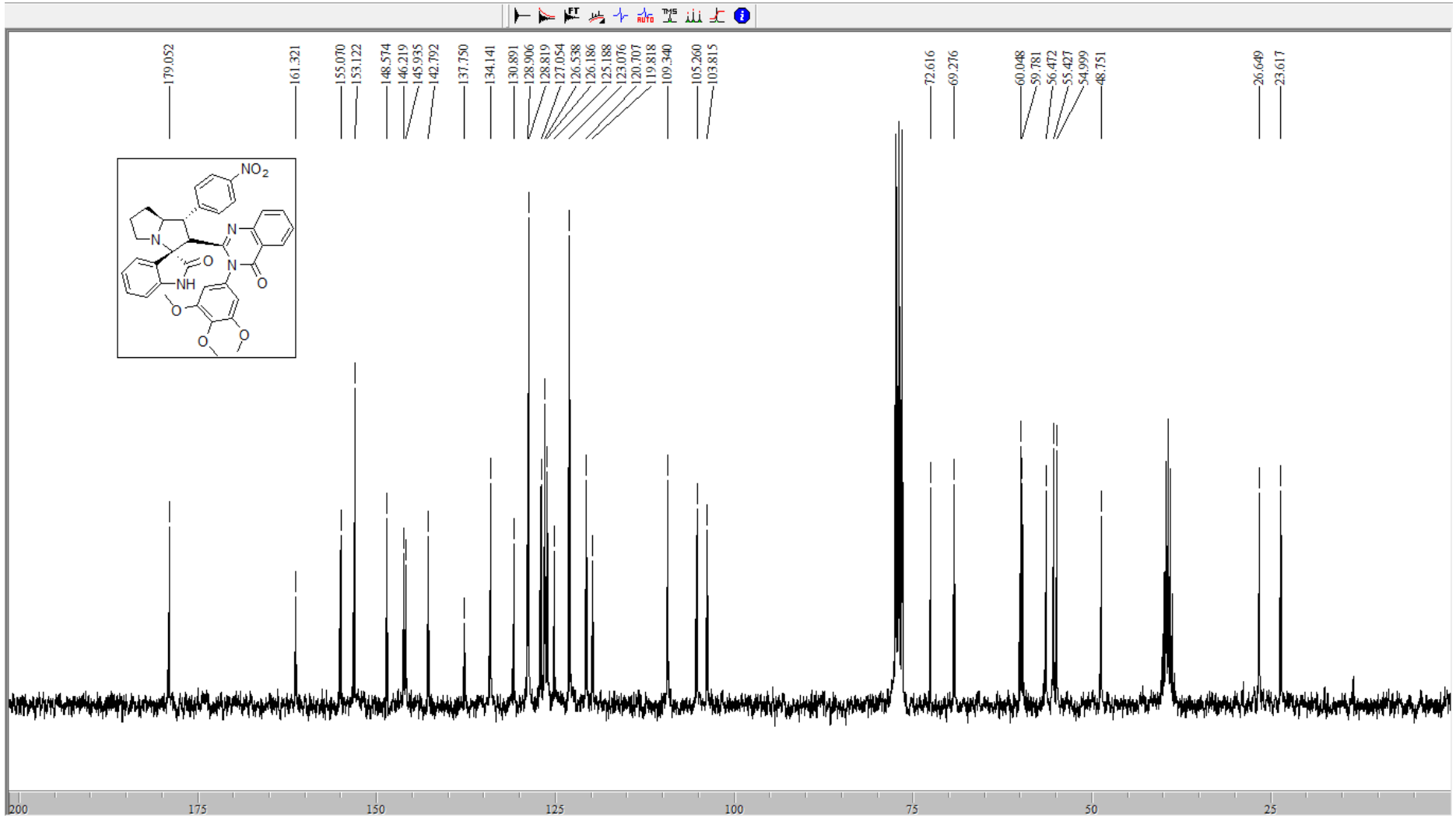
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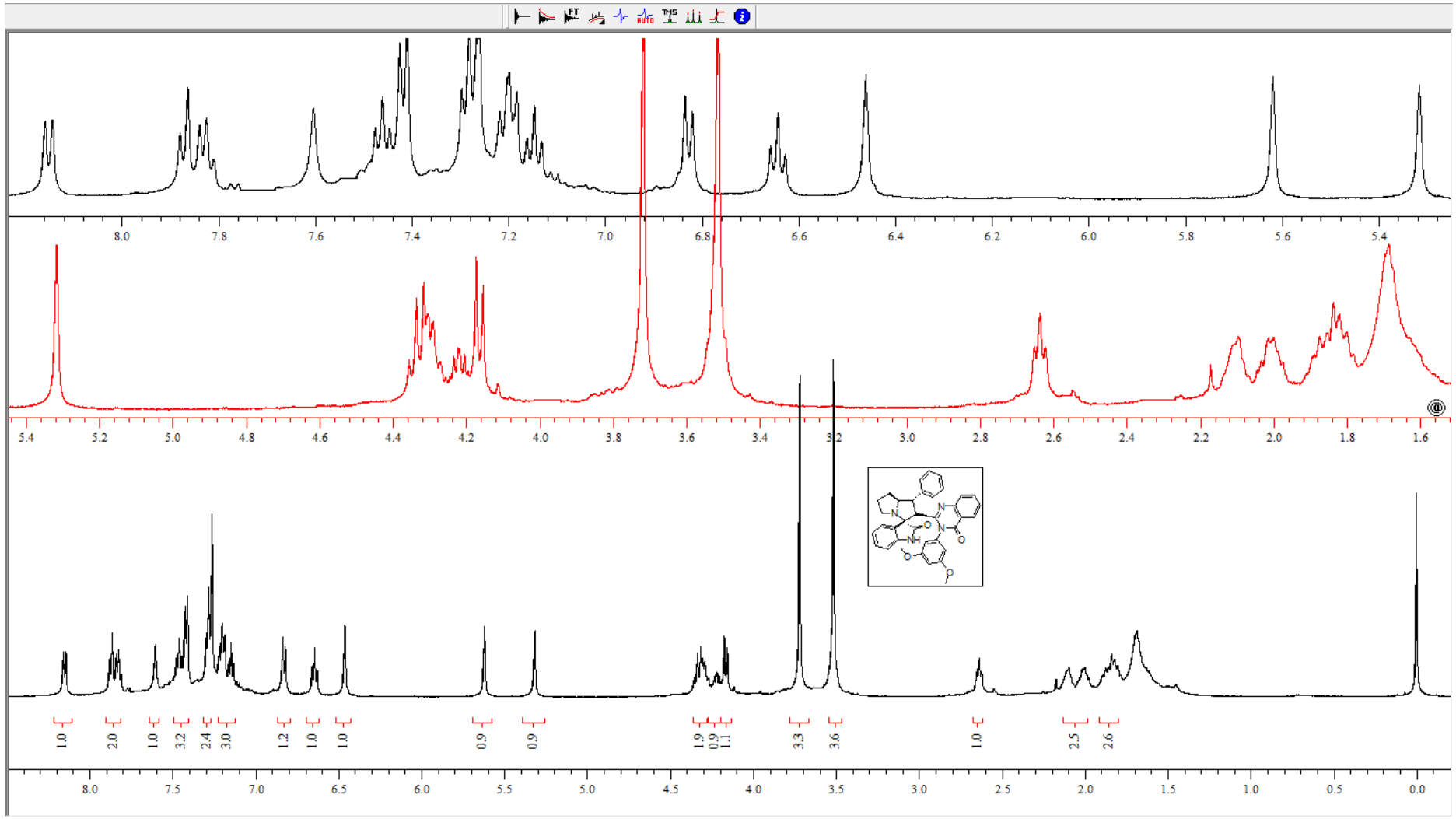
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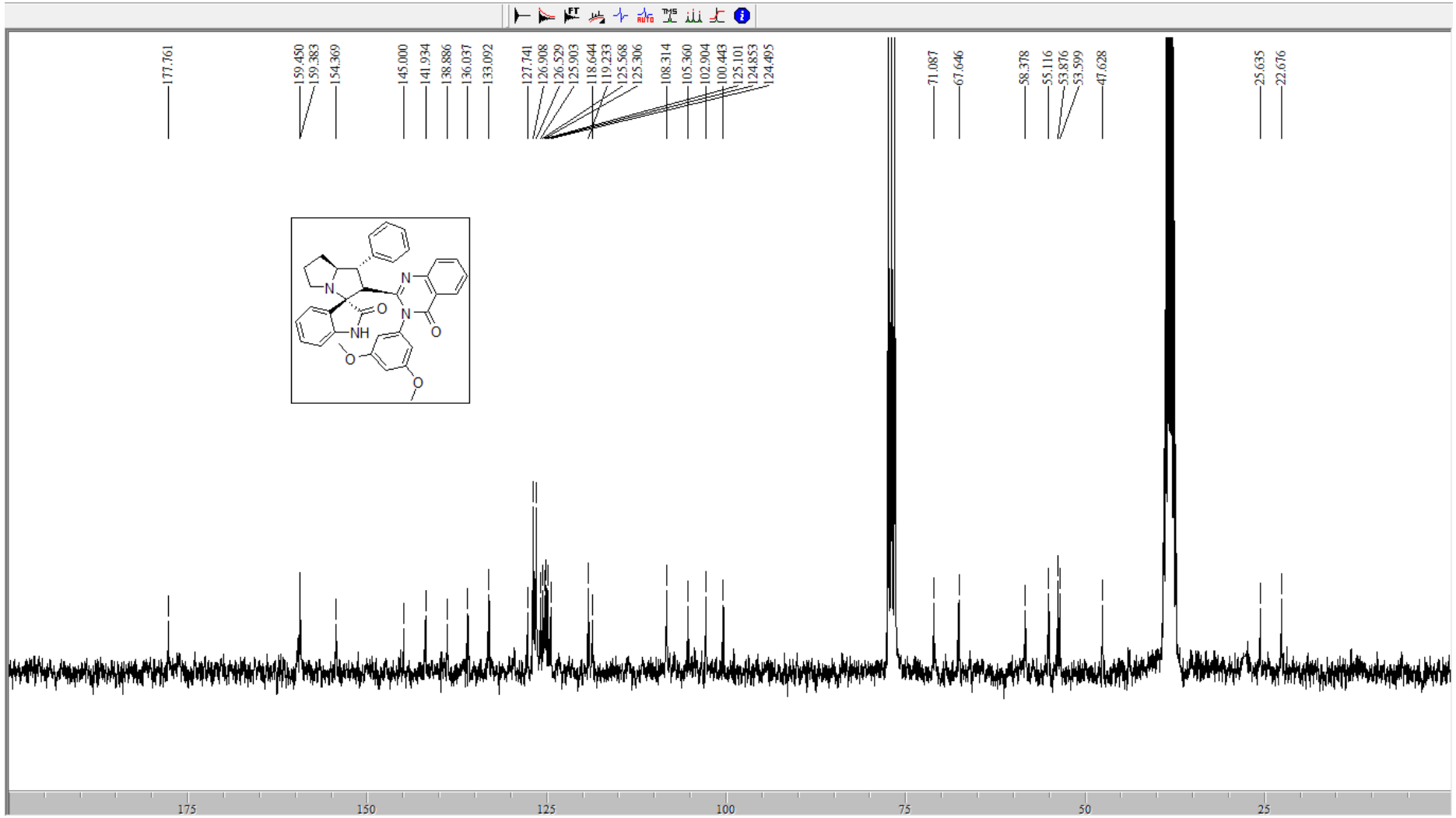
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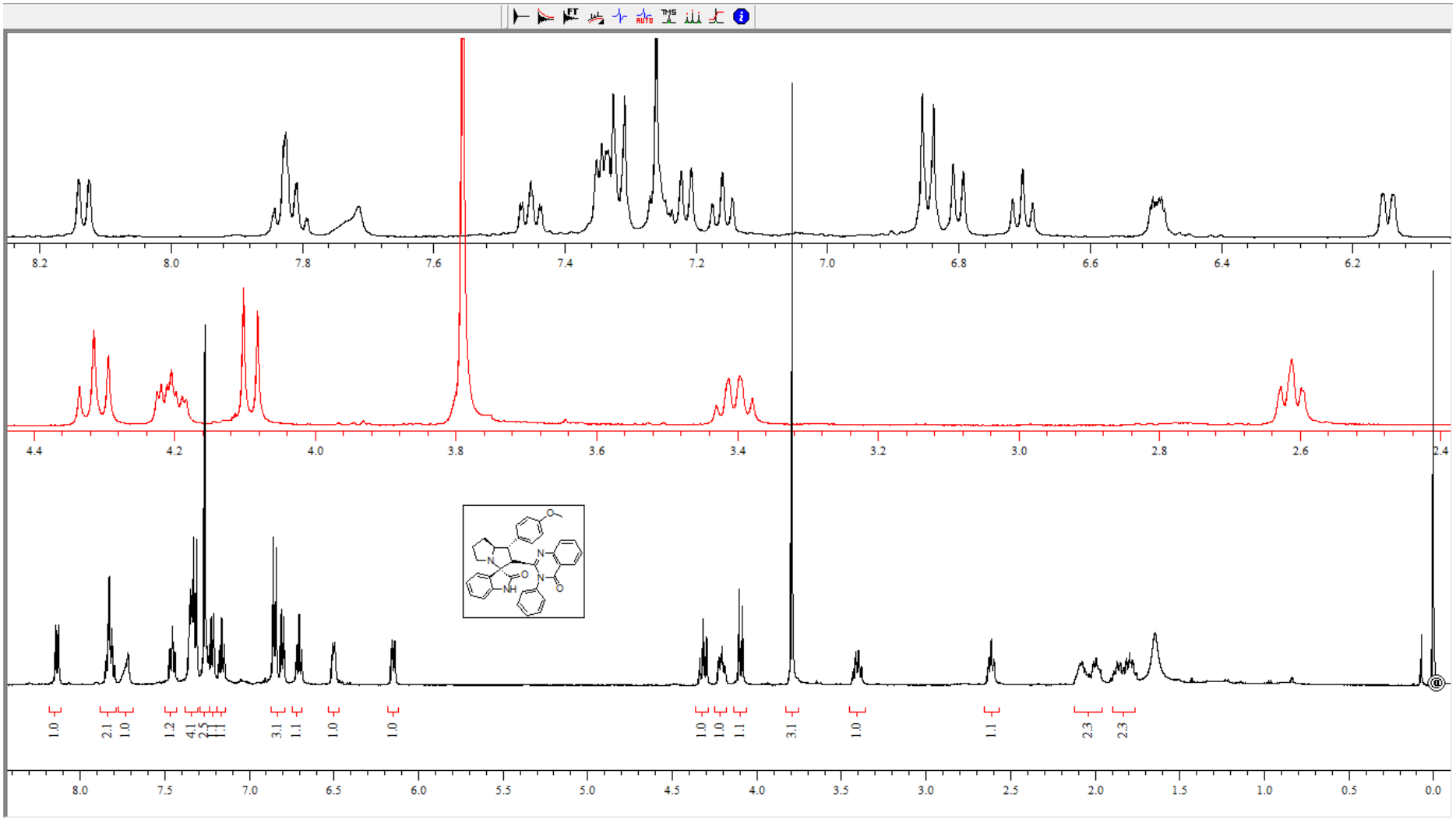
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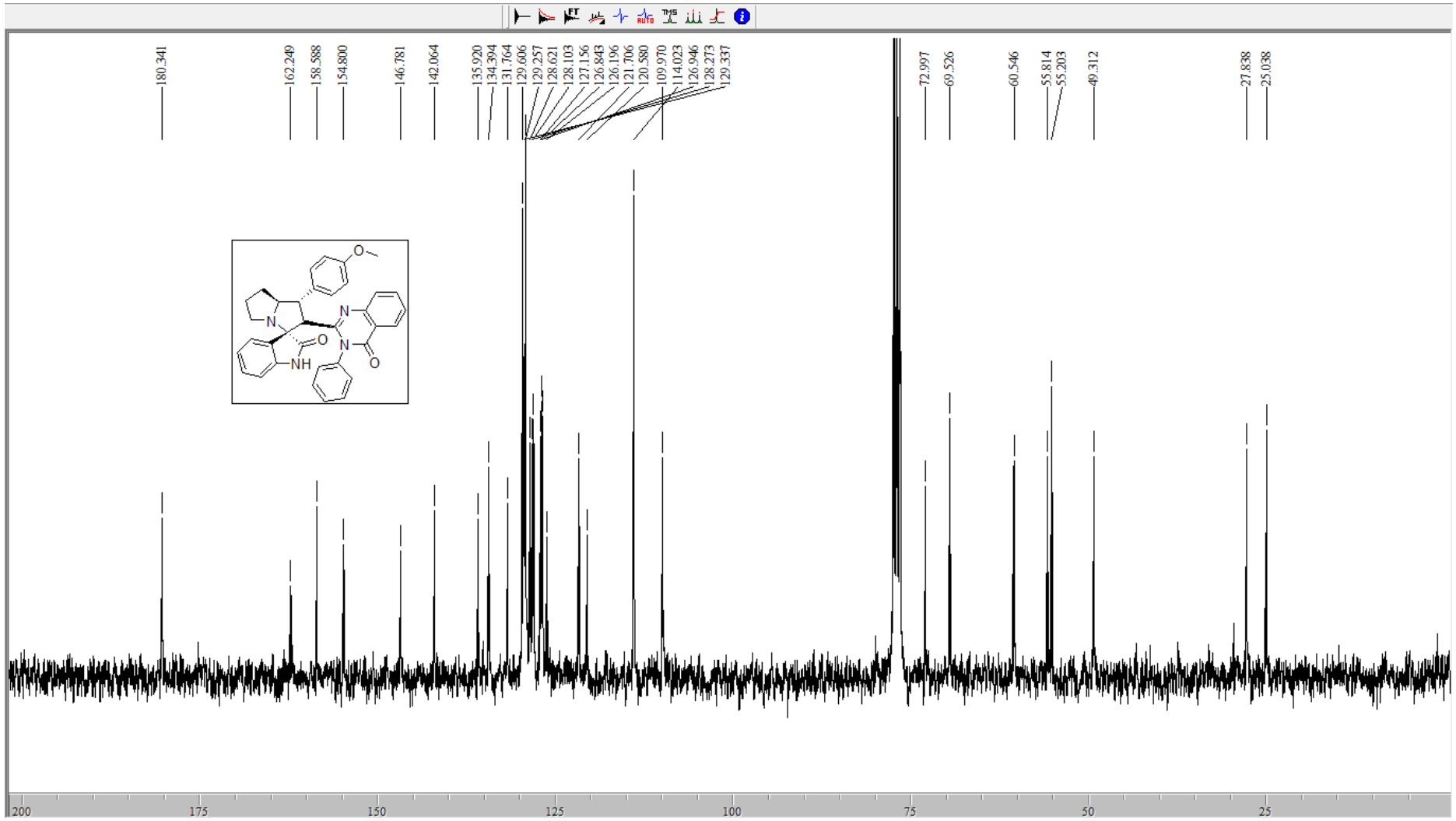
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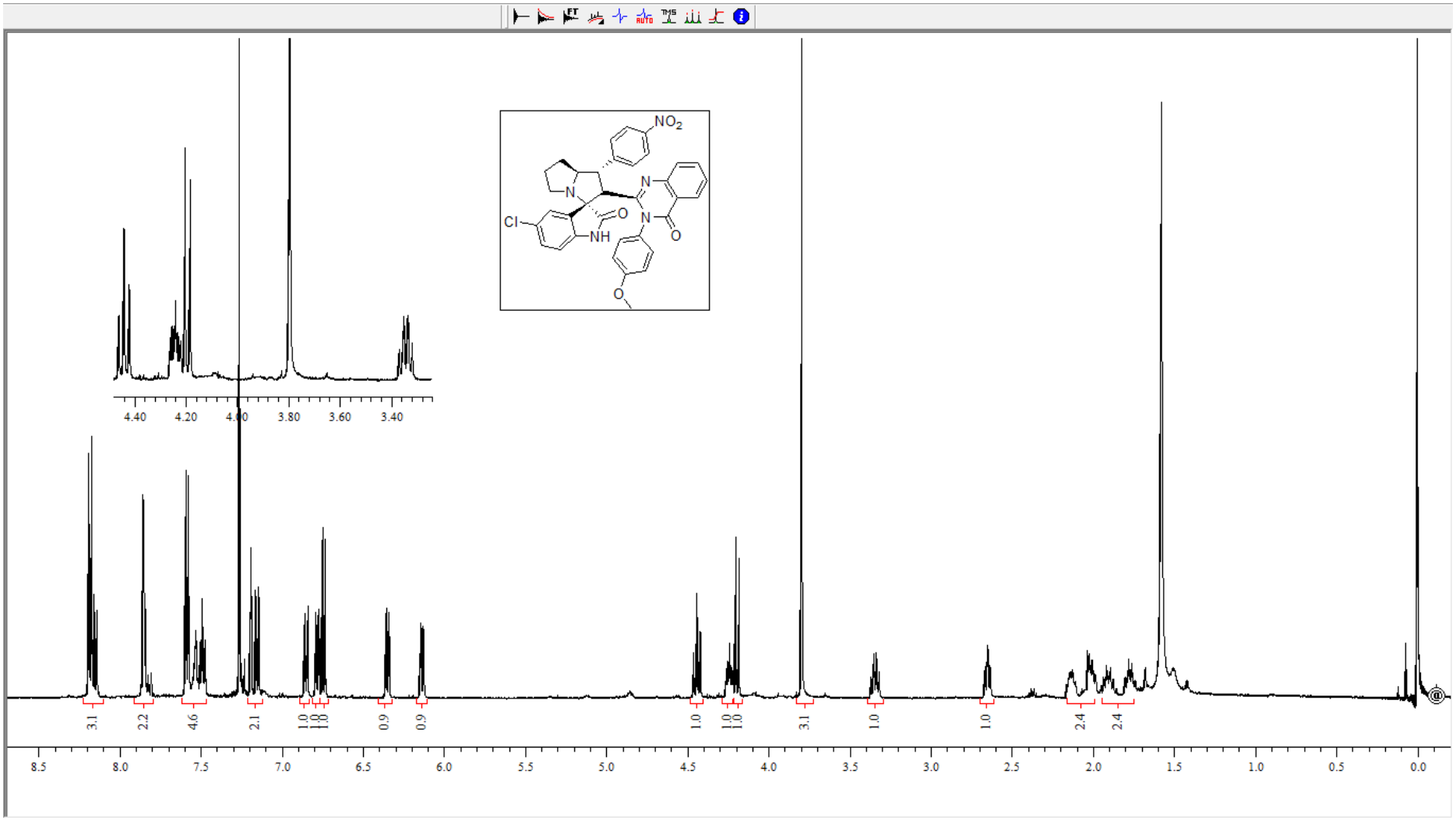
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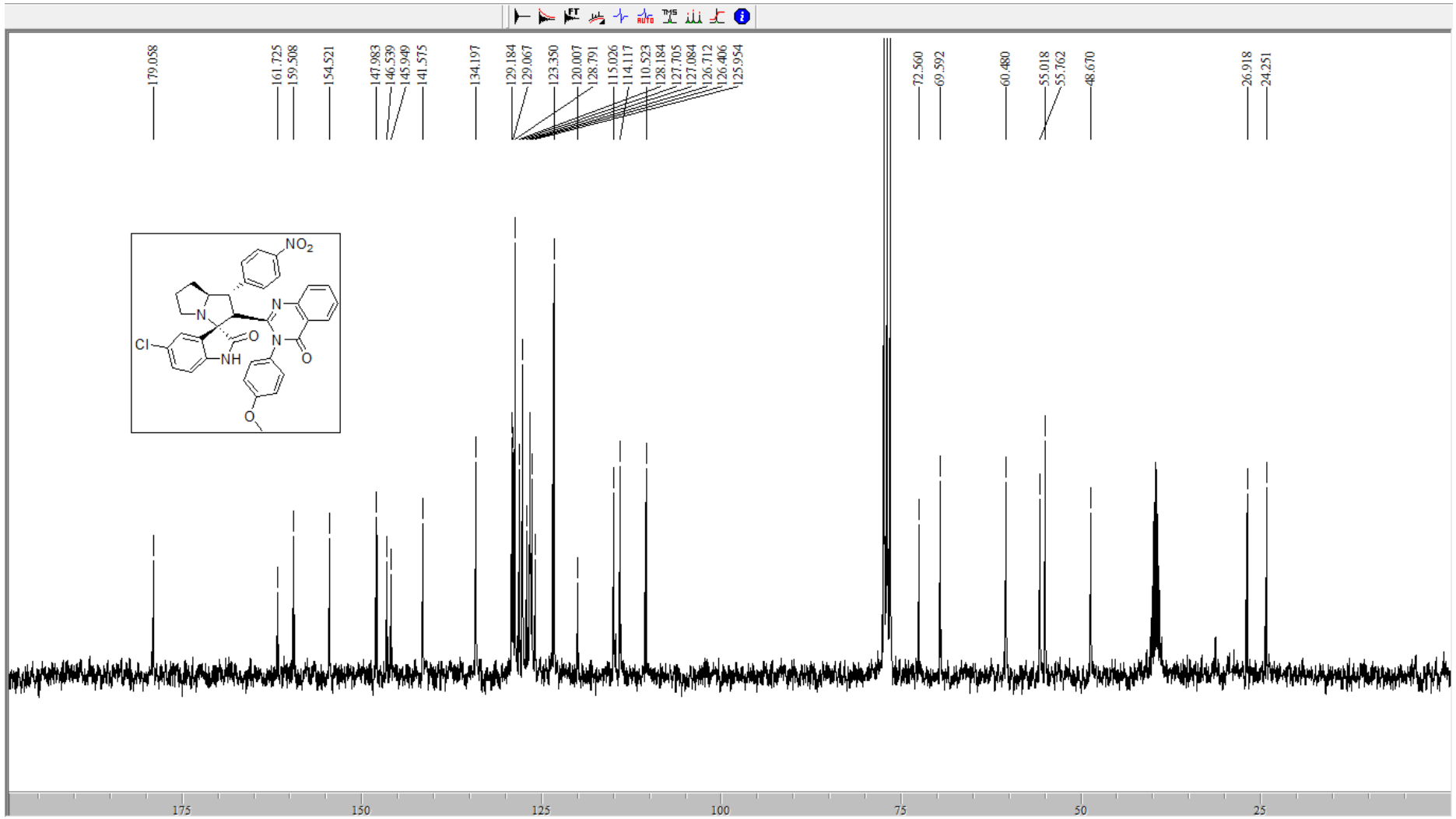
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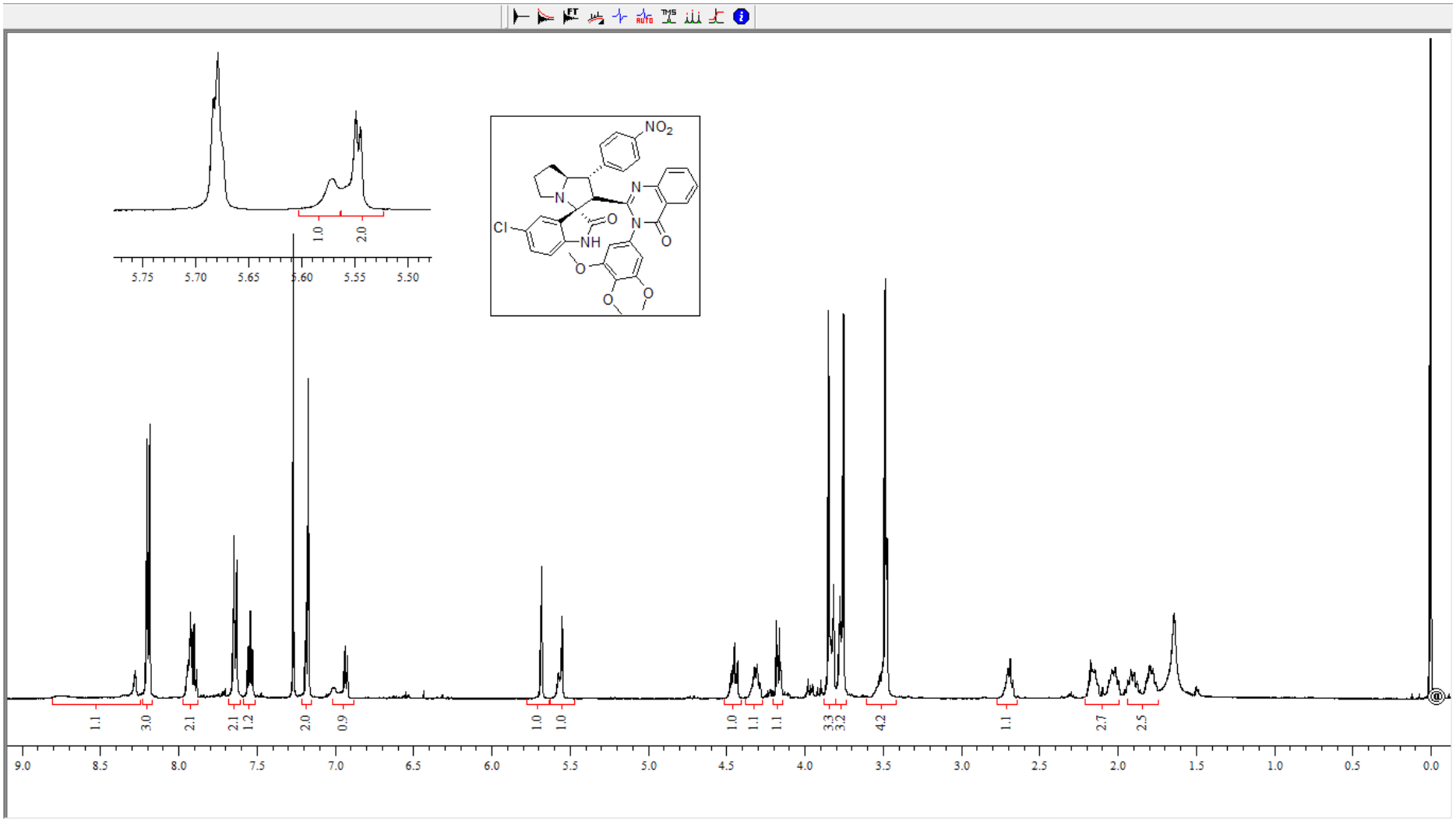
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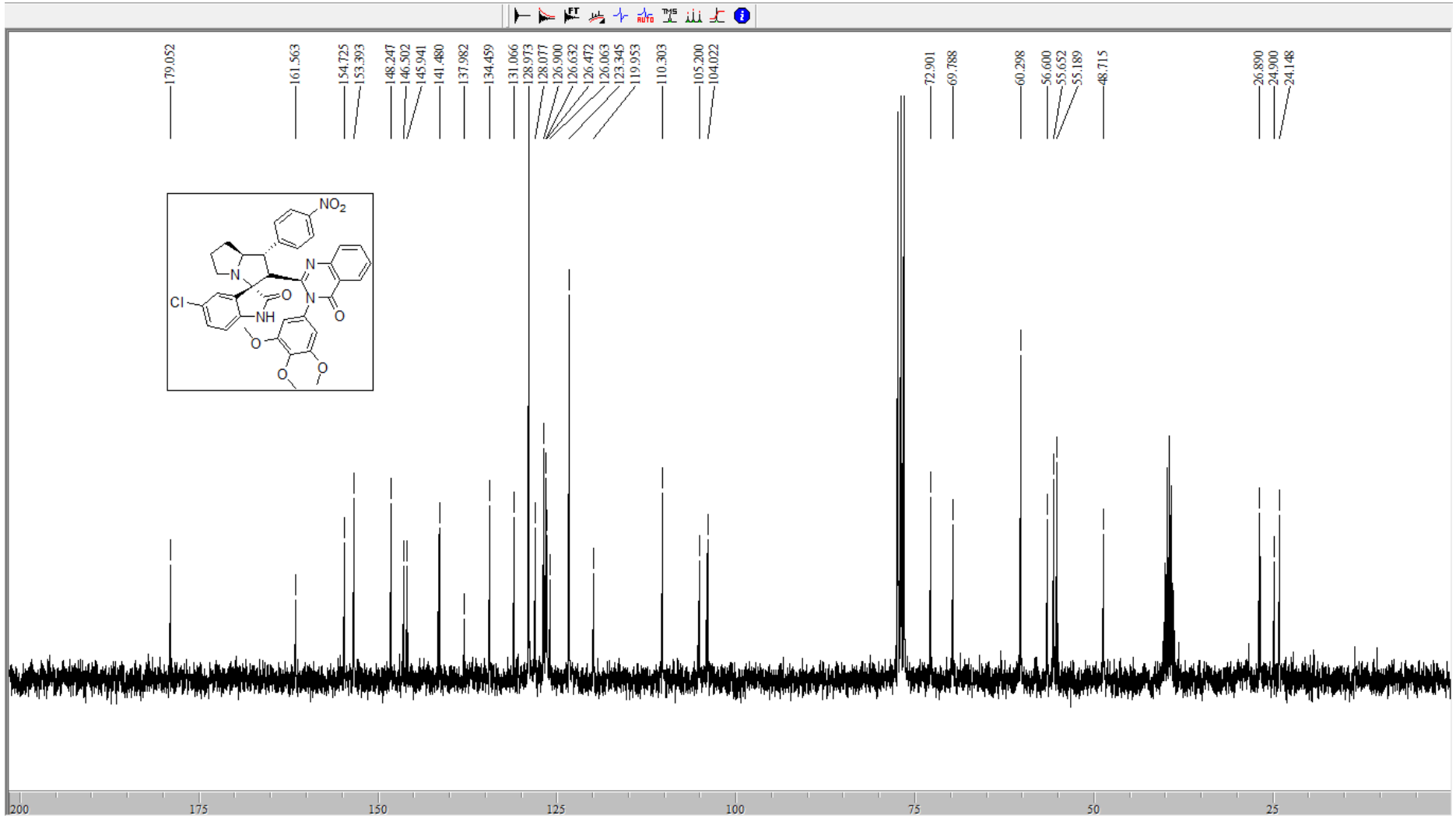
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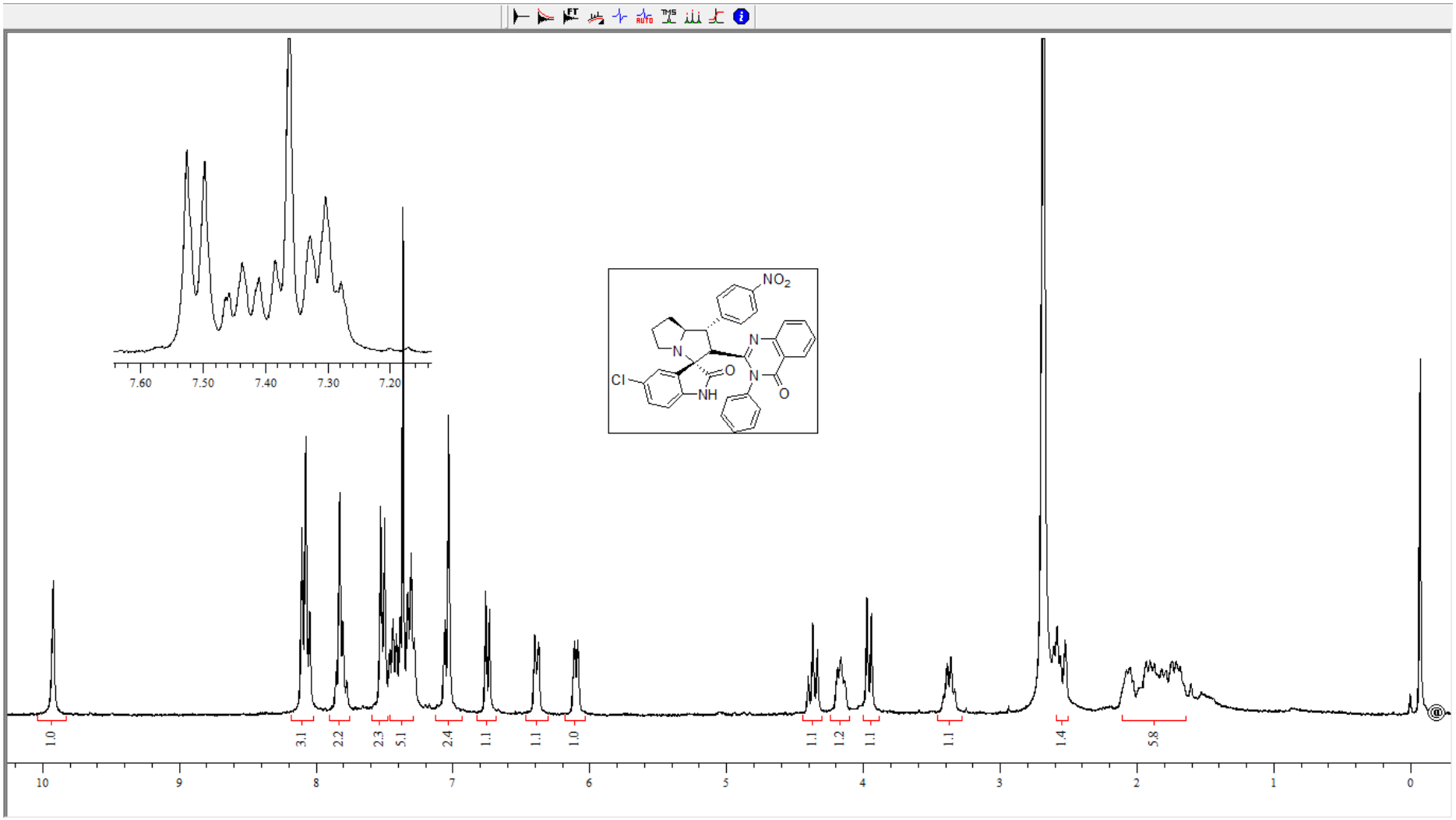
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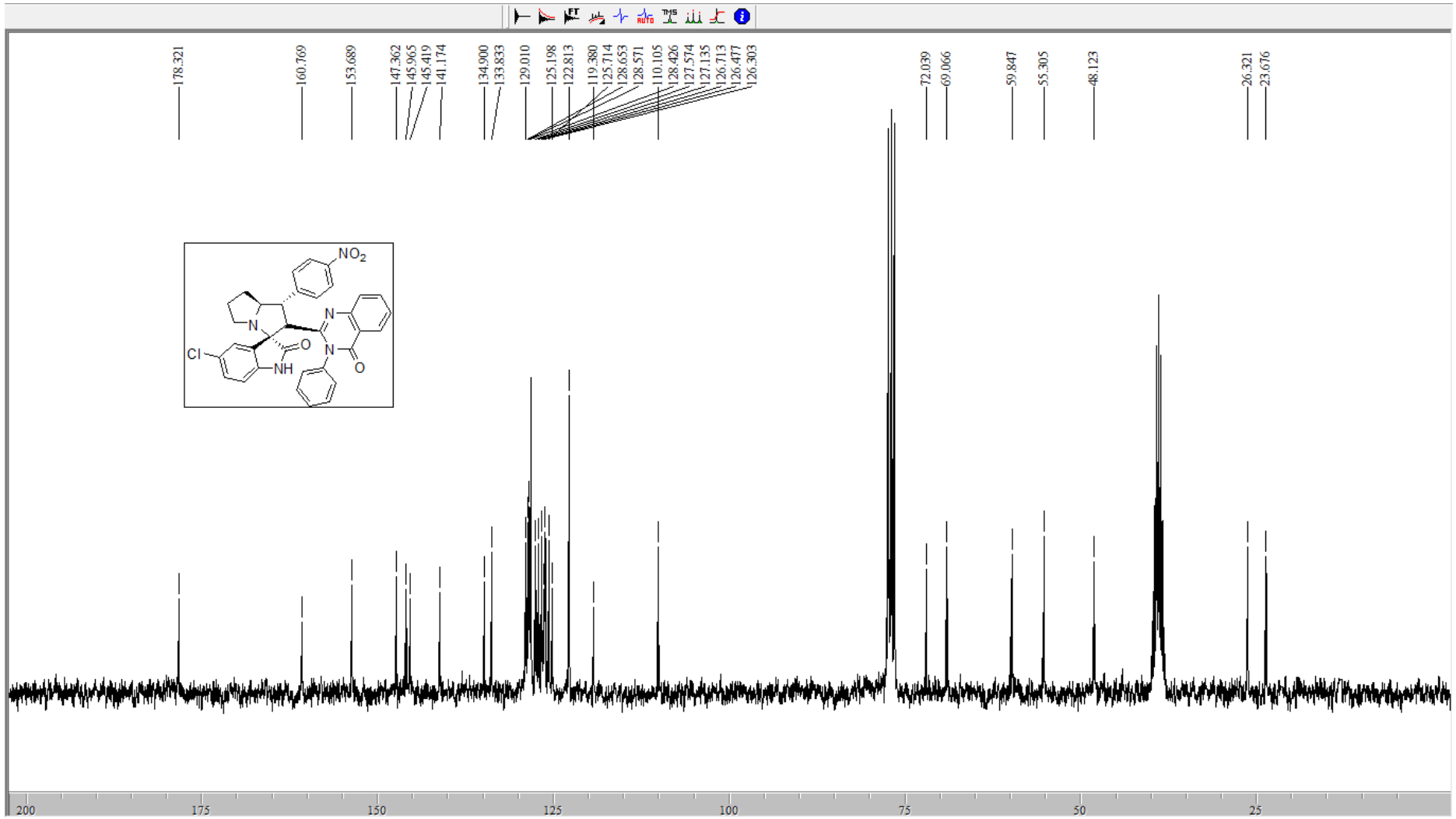
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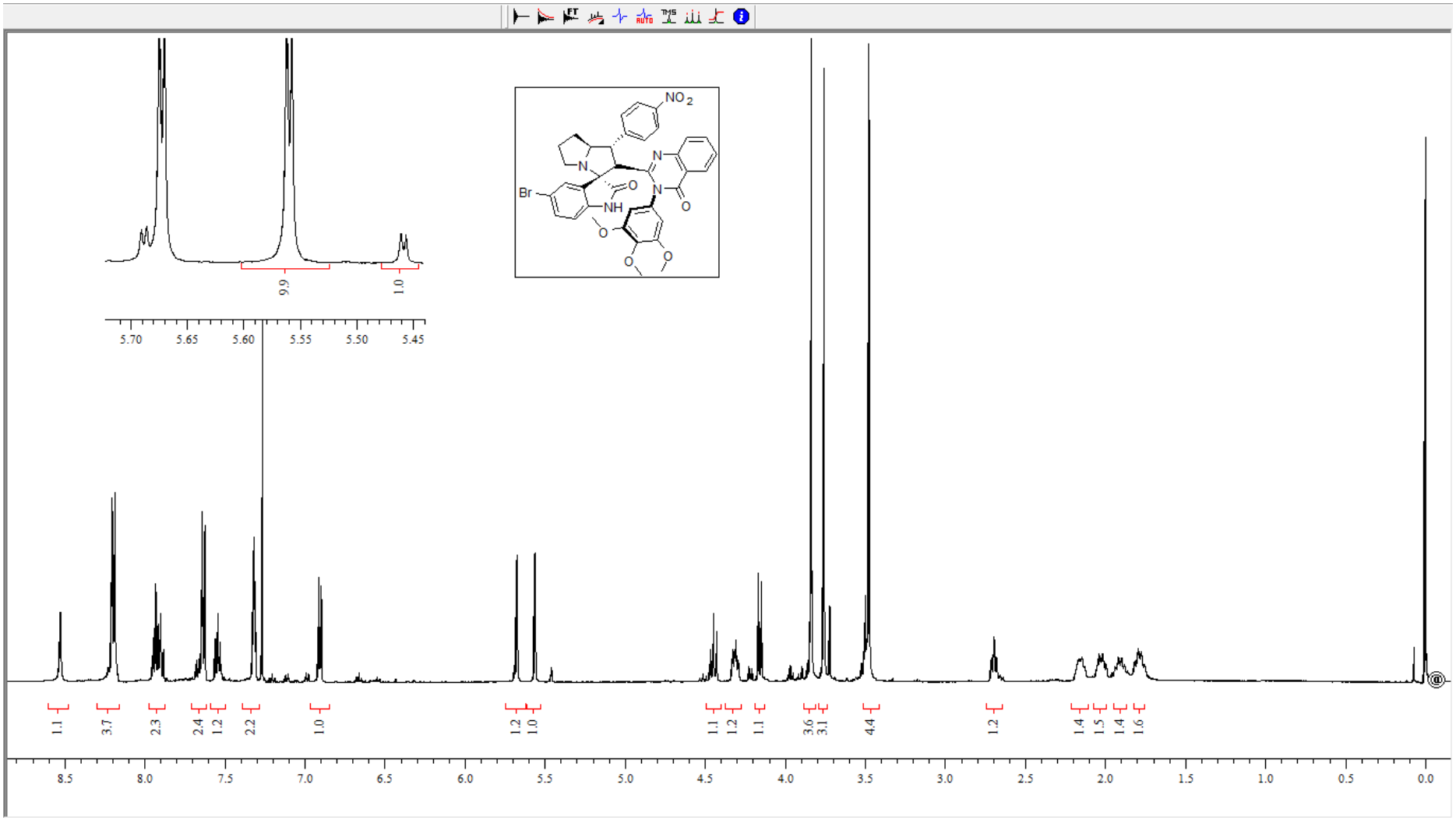
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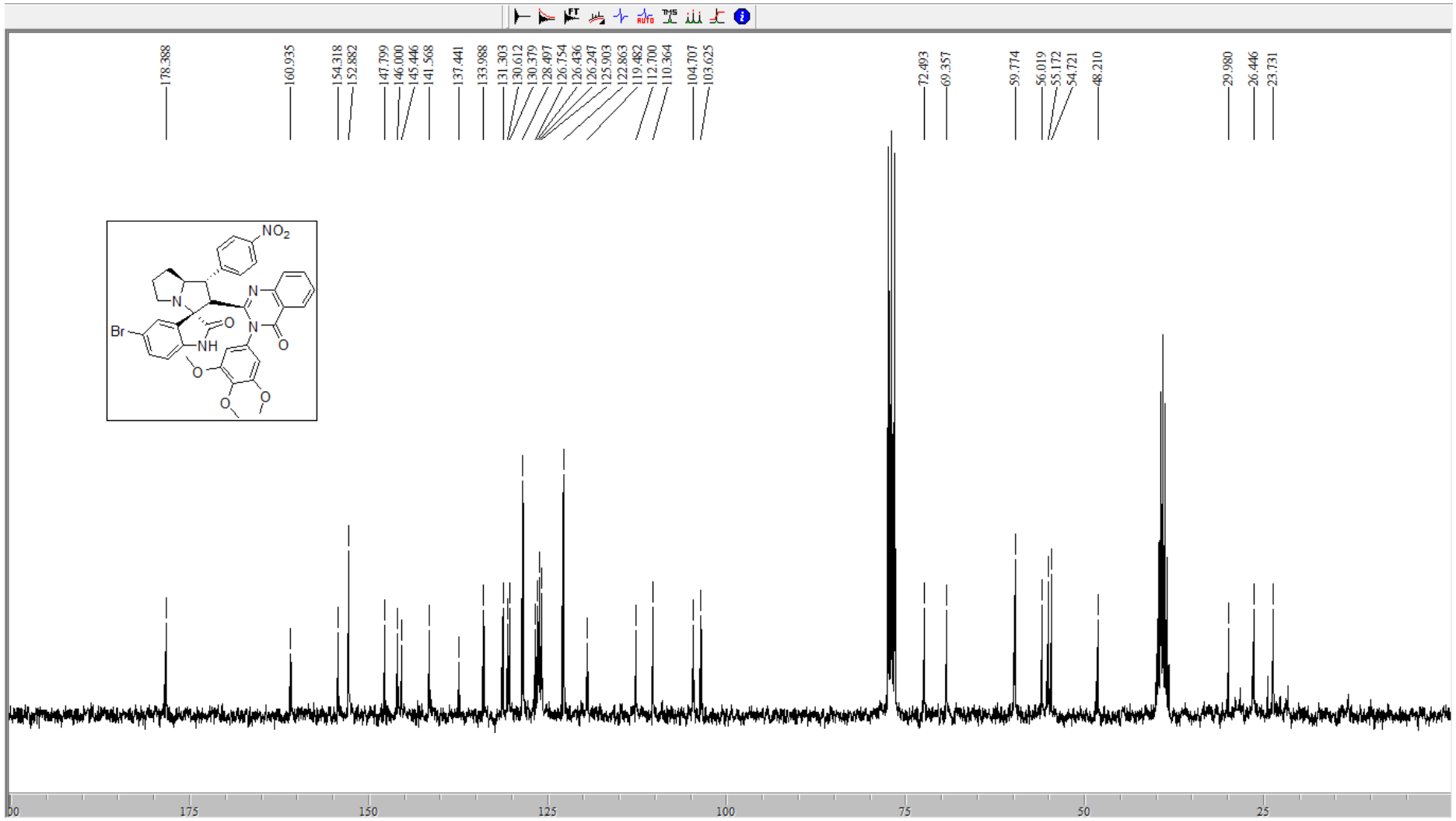
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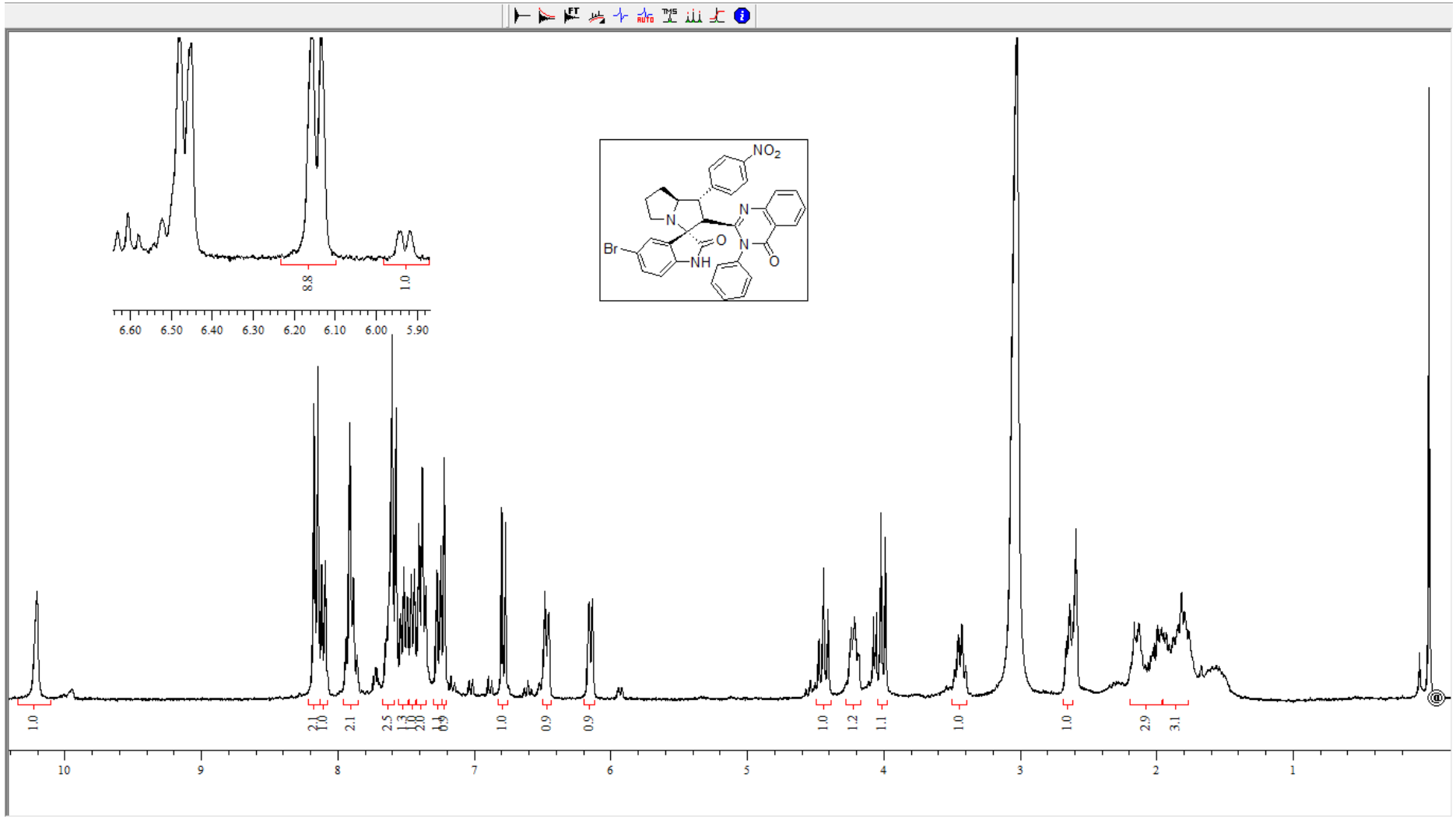
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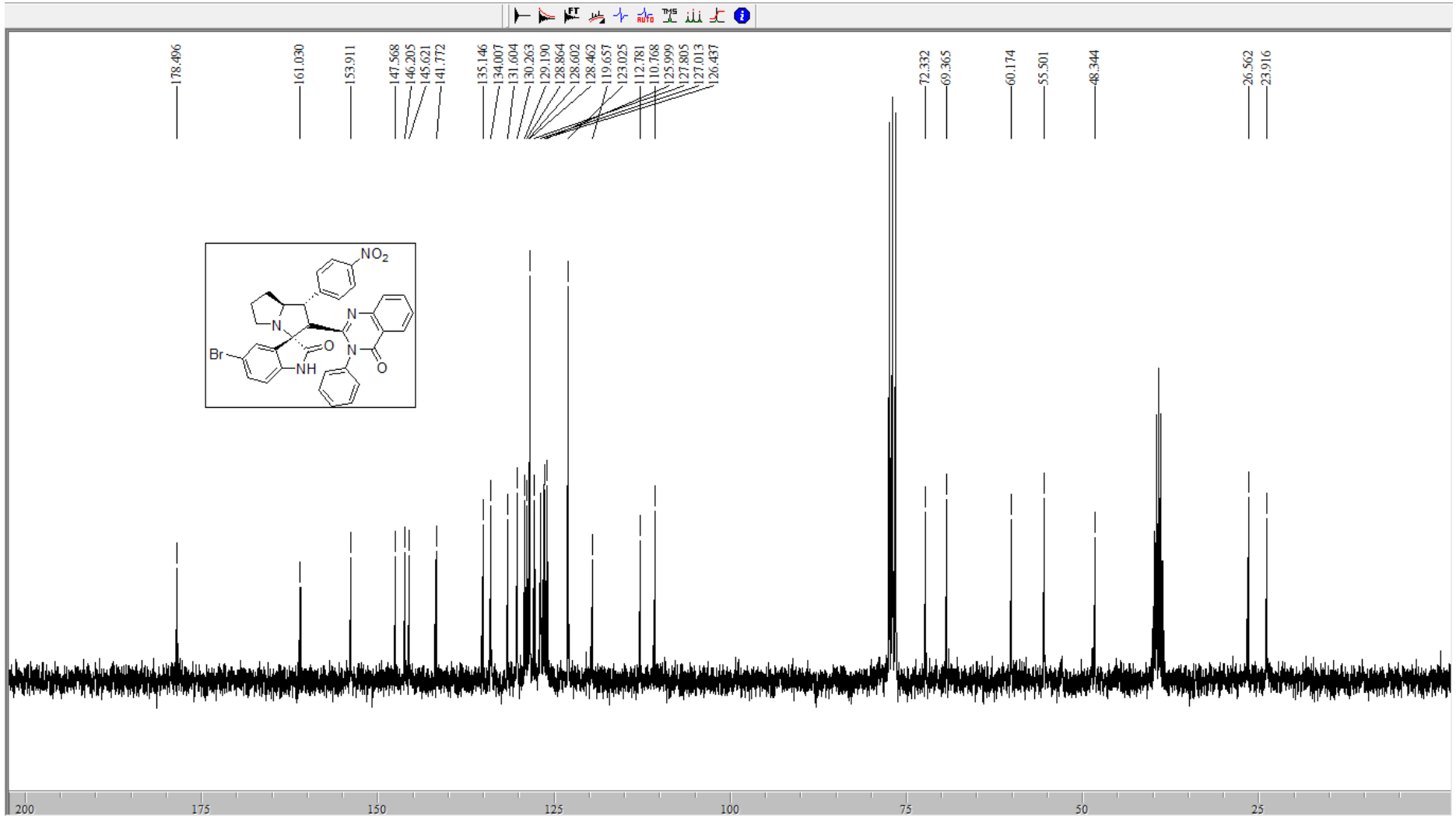
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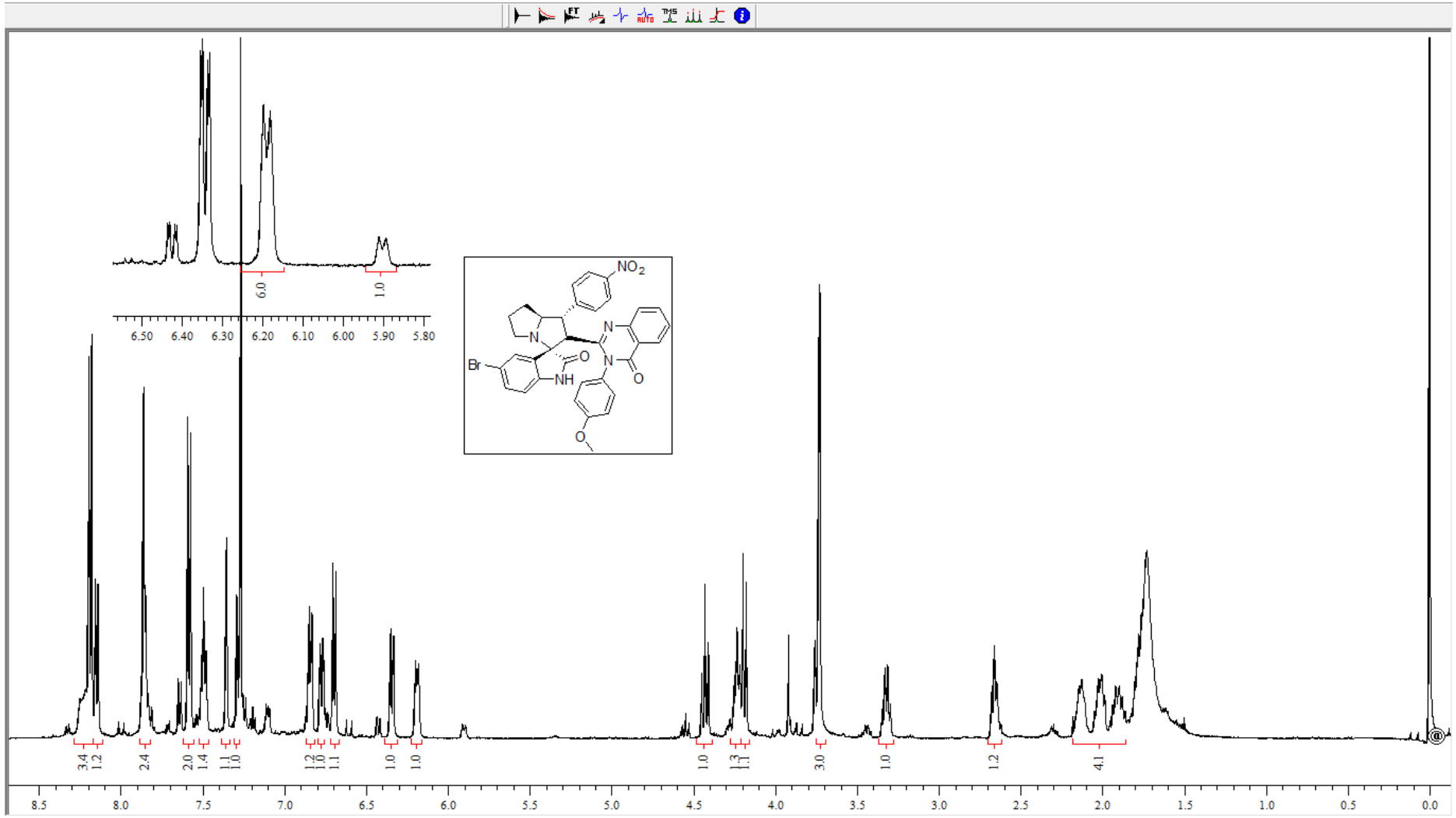
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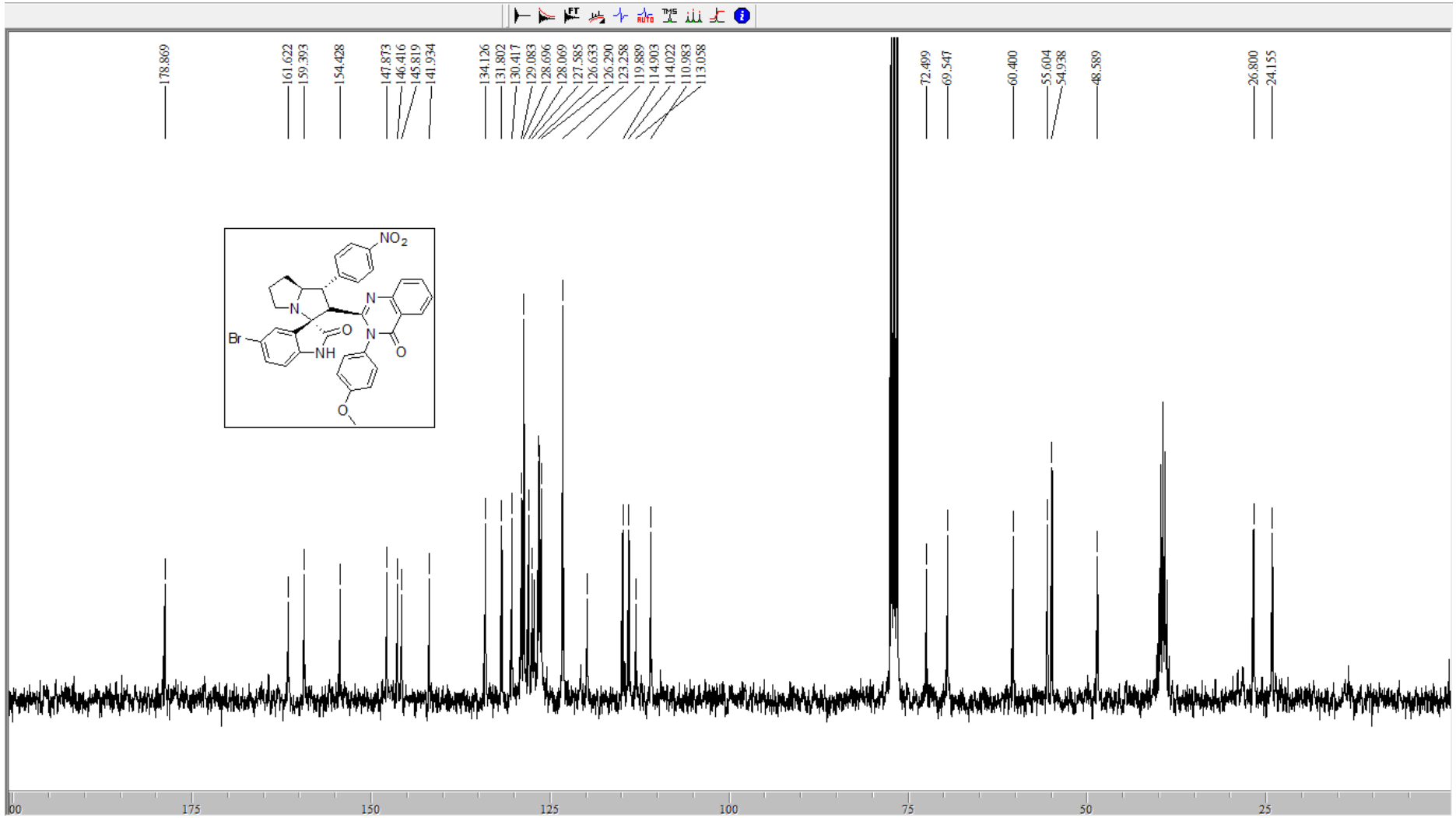
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128.069
127.585
126.633
126.290
123.258
119.889
114.903
114.022
110.983
113.058
72.499
69.547
60.400
55.604
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100
75
50
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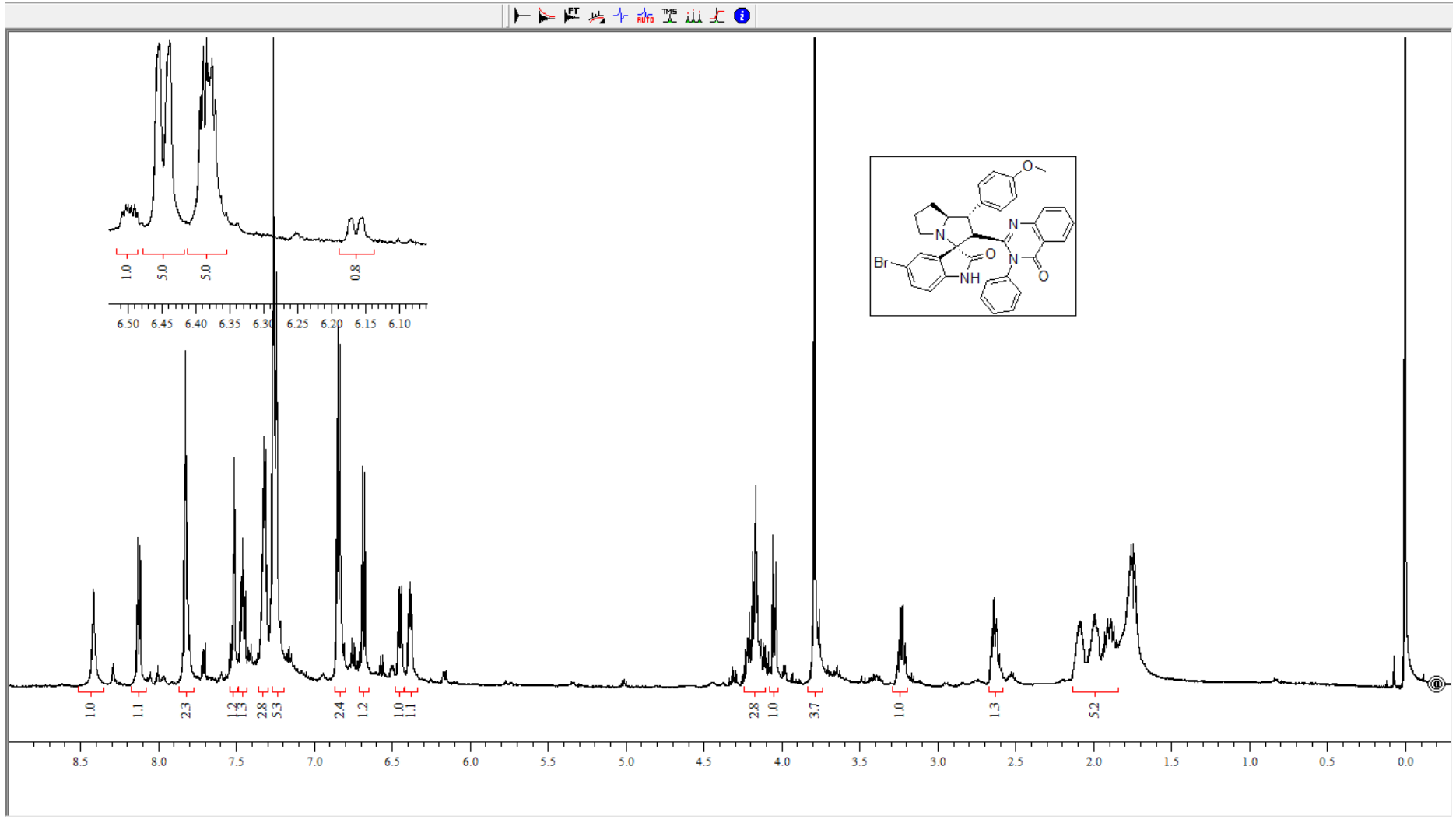
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5.0
5.0
0.8
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1.0 1.1 2.3 1.2 1.5 2.8 5.3 2.4 1.2 1.0 1.1 2.8 1.0 3.7 1.0 1.3 5.2
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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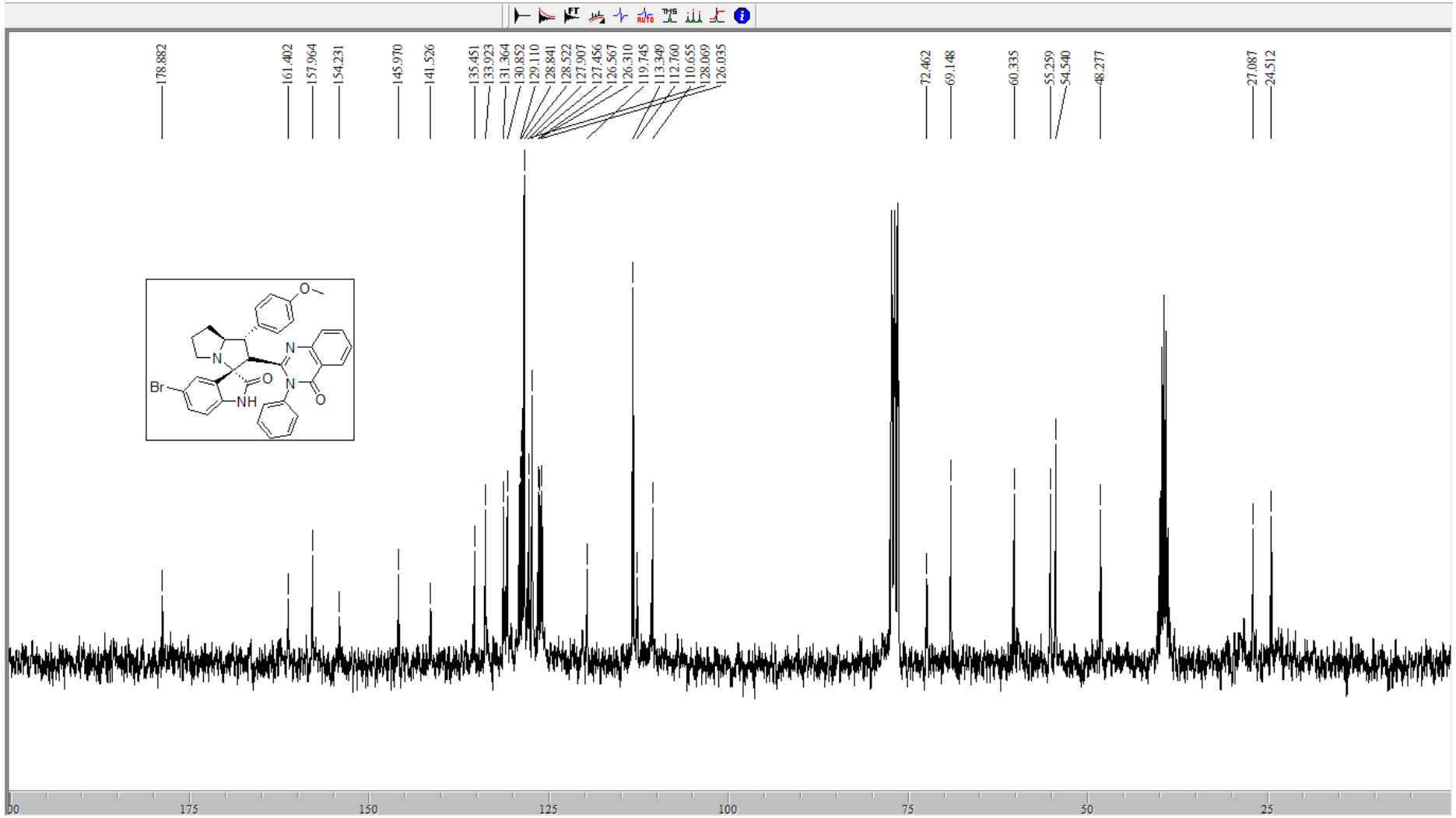
N
O
N
O
Br
NH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128.522
127.907
127.456
126.567
126.310
119.745
113.349
112.760
110.655
128.069
126.035
72.462
69.148
60.335
55.259
54.540
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N
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Br
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100
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50
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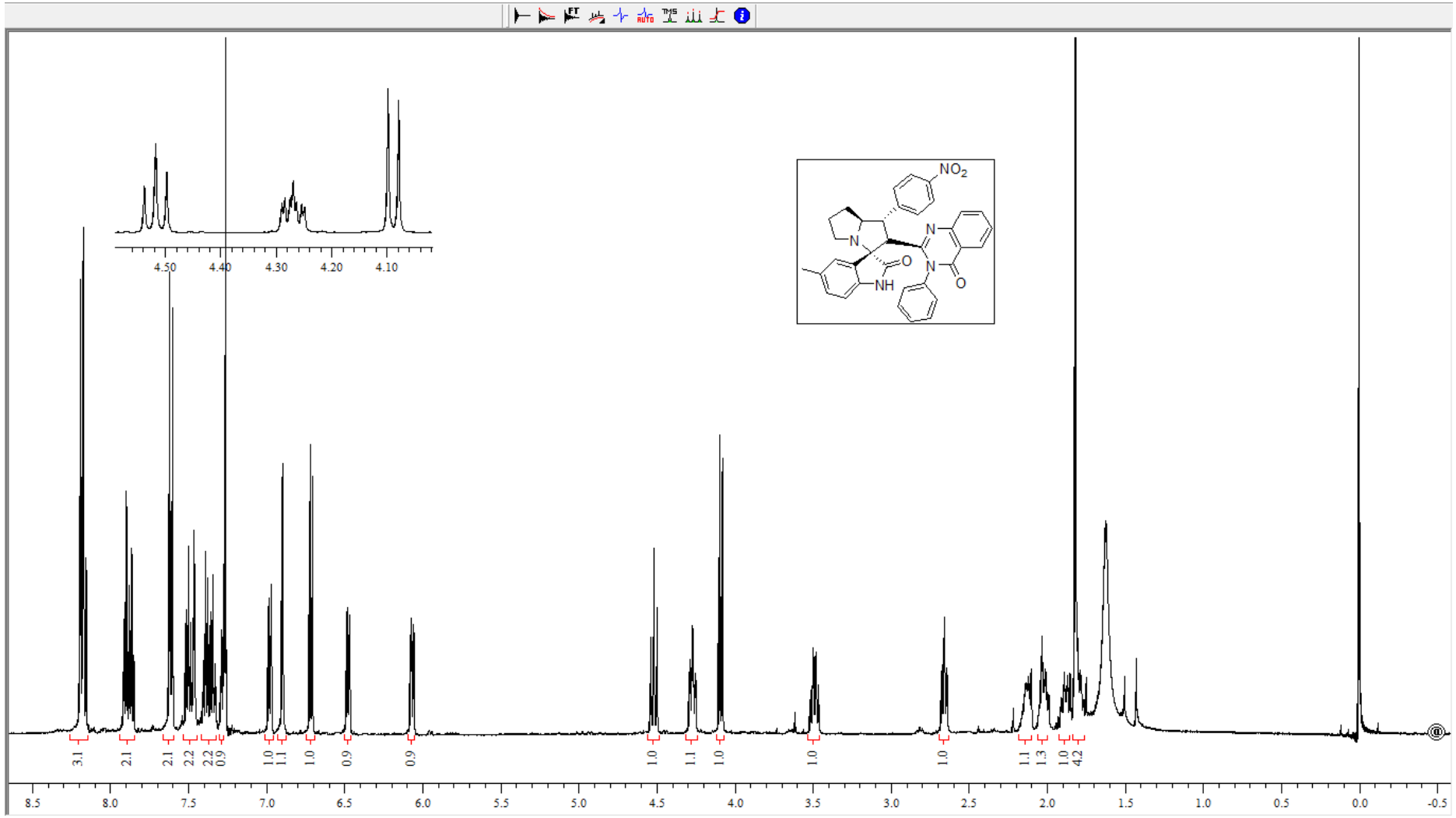
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NH
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O
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4.20
4.10
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2.1
2.2
2.2
0.9
1.0
1.1
1.0
0.9
0.9
1.0
1.1
1.0
1.0
1.0
1.1
1.3
1.0
4.2
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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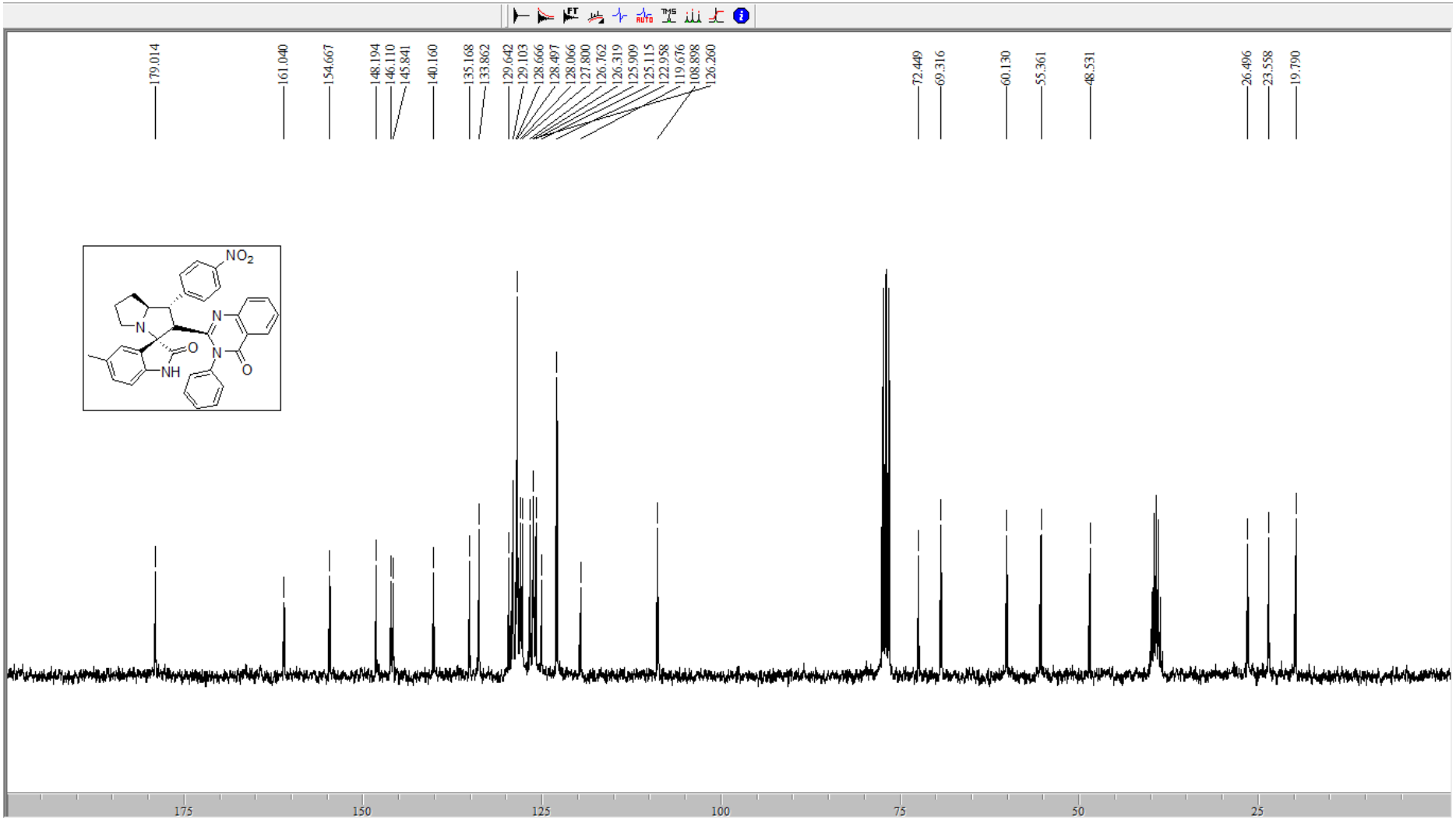
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NH
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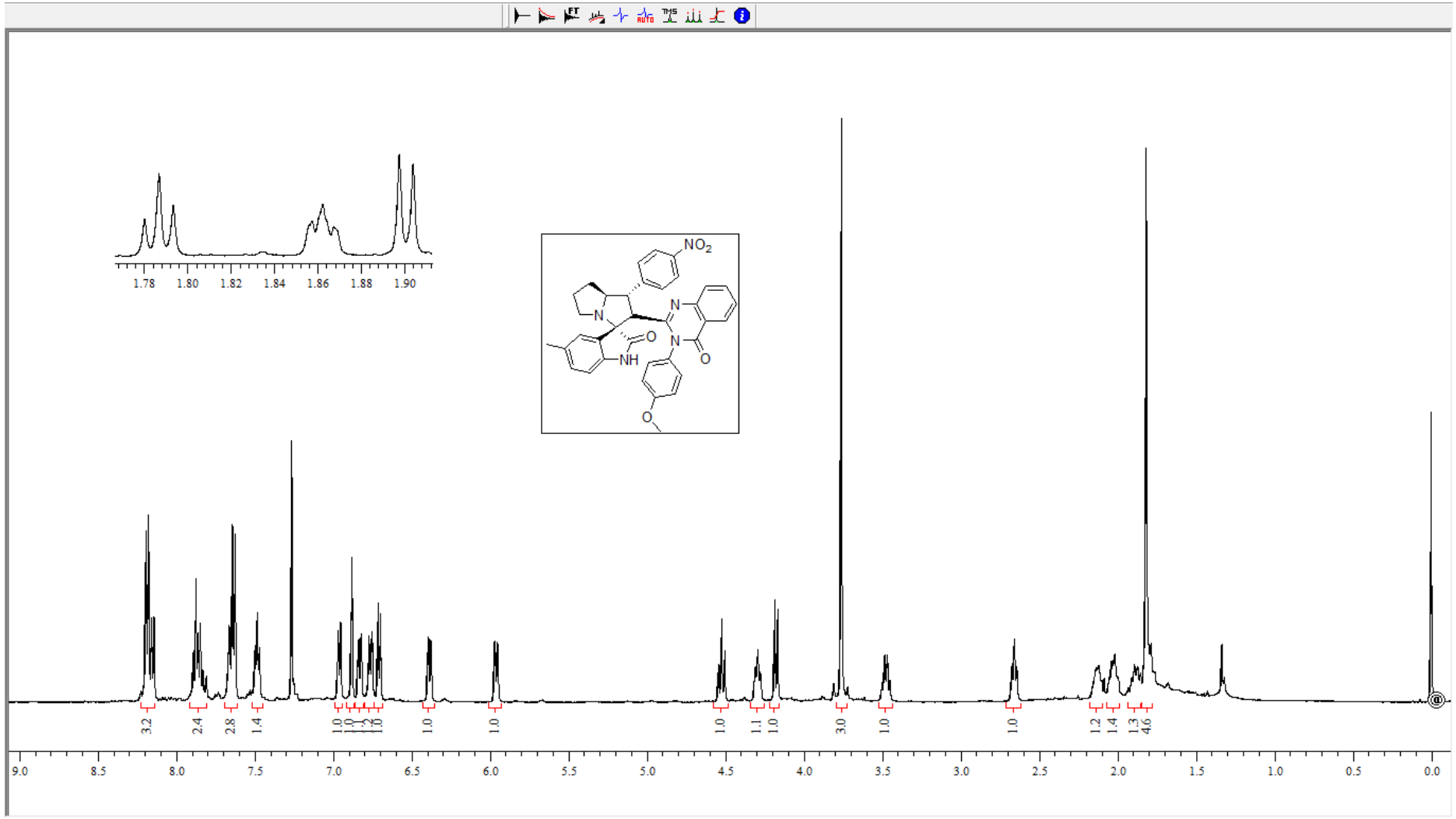
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1.90
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N
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NH
O
3.2
2.4
2.8
1.4
1.0
1.0
1.1
1.2
1.0
1.0
1.0
1.1
1.0
3.0
1.0
1.0
1.2
1.4
1.3
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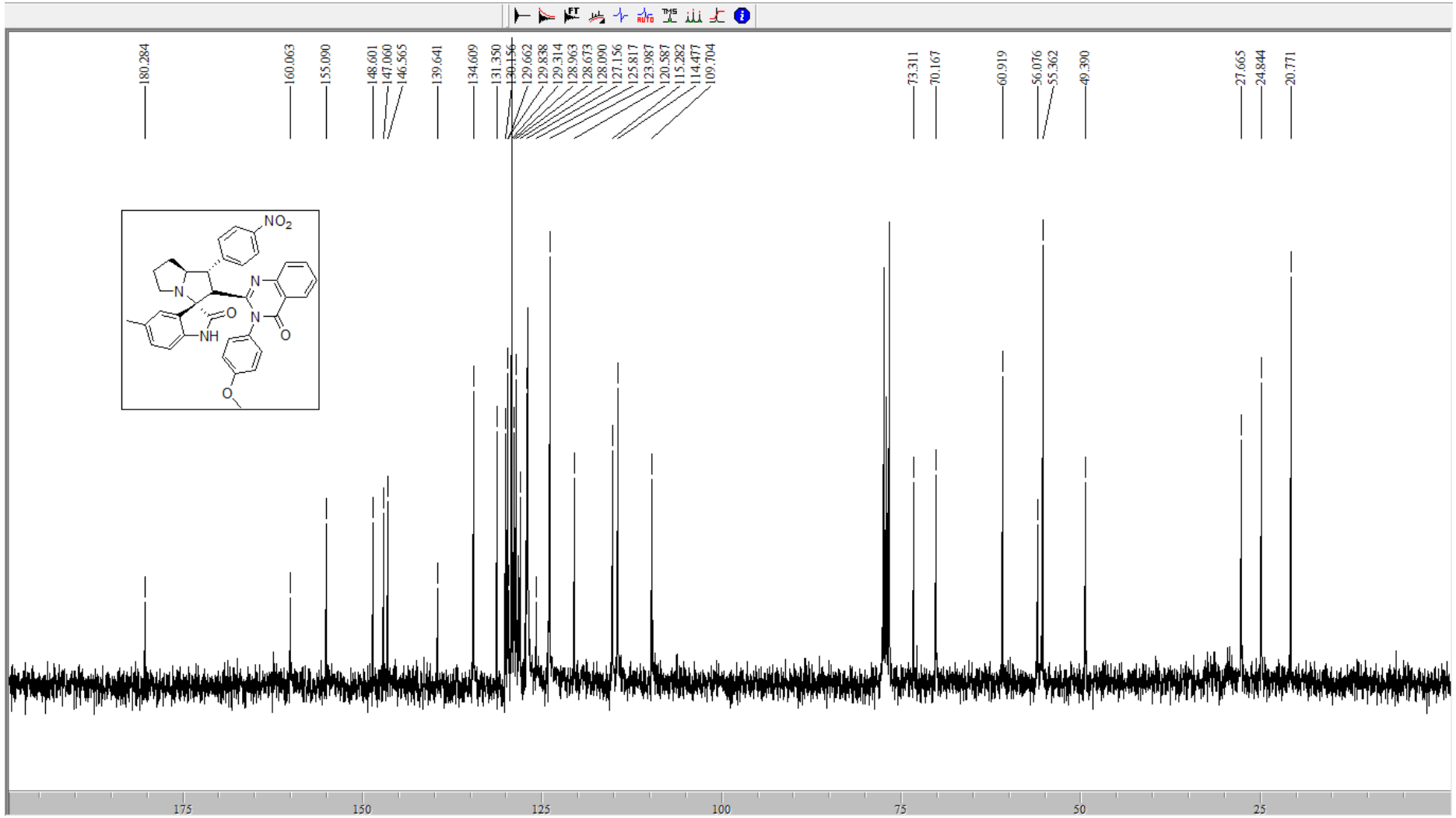
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134.609
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128.963
128.673
128.090
127.156
125.817
123.987
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115.282
114.477
109.704
73.311
70.167
60.919
56.076
55.362
49.390
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24.844
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NO2
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N
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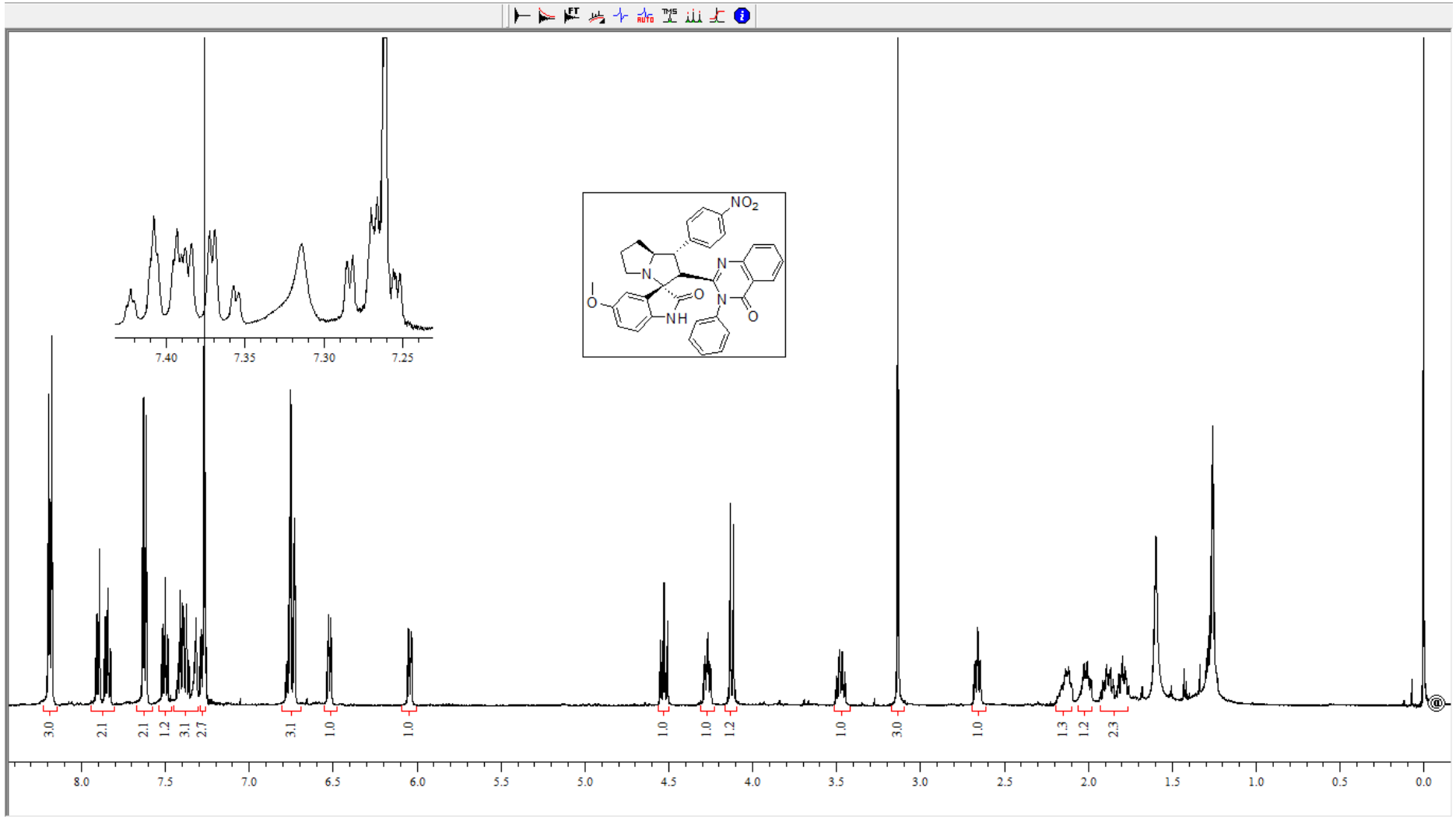
150
125
100
75
50
25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O
O
NH
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7.30
7.25
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2.1
2.1
1.2
3.1
2.7
3.1
1.0
1.0
1.0
1.0
1.2
1.0
3.0
1.0
1.3
1.2
2.3
8.0
7.5
7.0
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6.0
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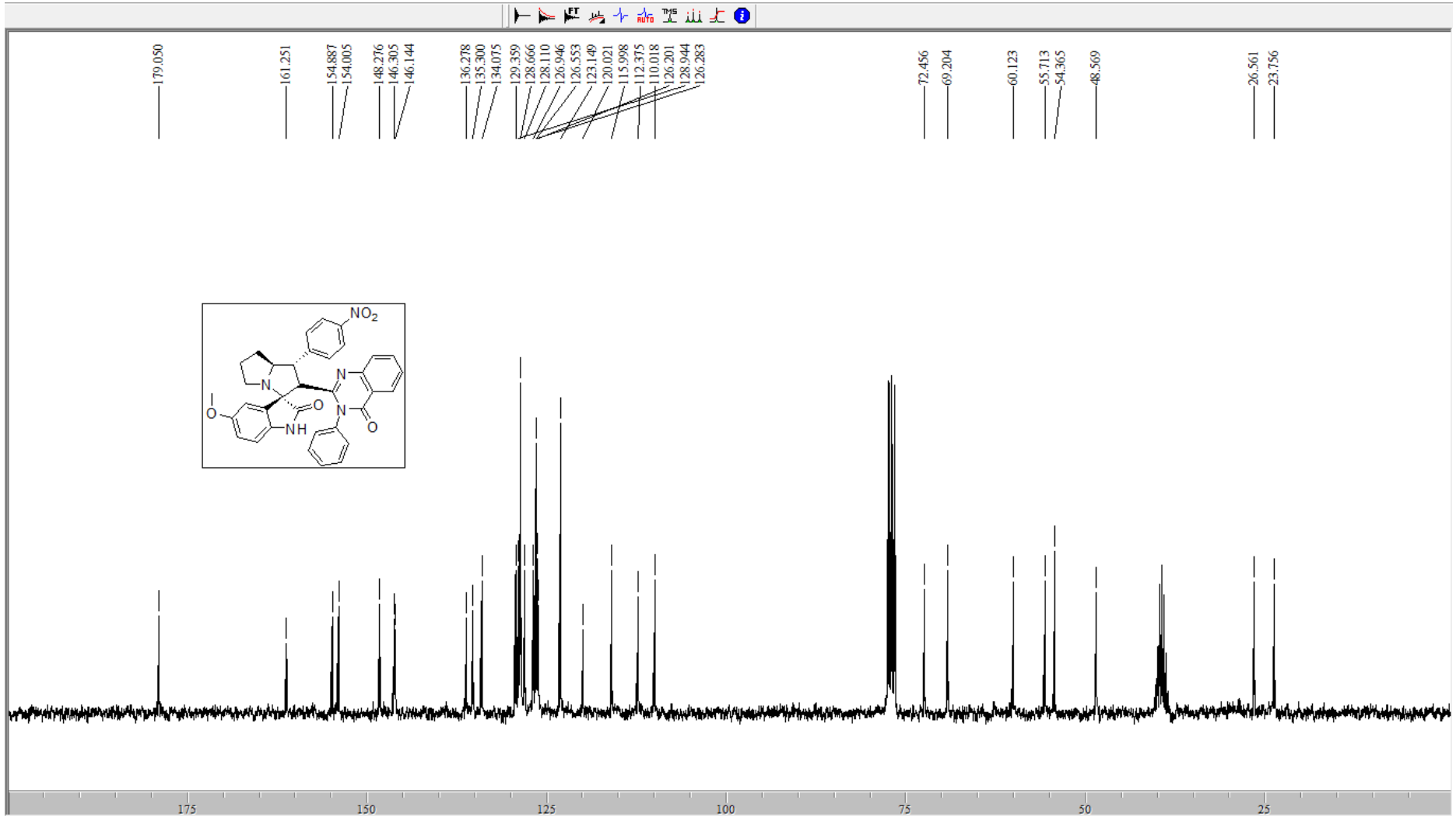
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128.110
126.946
126.553
123.149
120.021
115.998
112.375
110.018
126.201
128.944
126.283
72.456
69.204
60.123
55.713
54.365
48.569
26.561
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NH
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100
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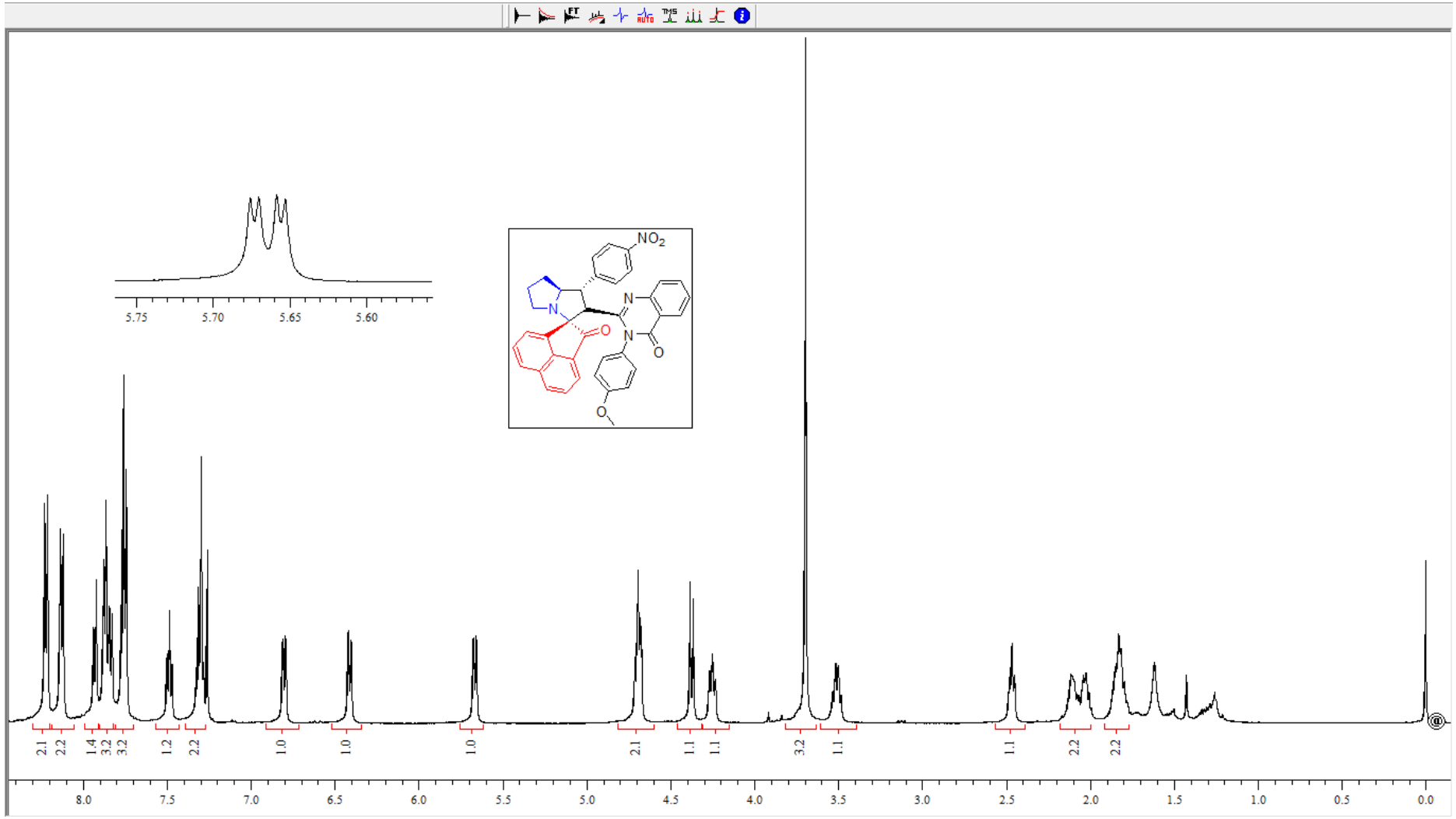
50
25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5.65
5.60
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N
O
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2.2
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3.2
1.2
2.2
1.0
1.0
1.0
2.1
1.1
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3.2
1.1
1.1
2.2
2.2
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7.5
7.0
6.5
6.0
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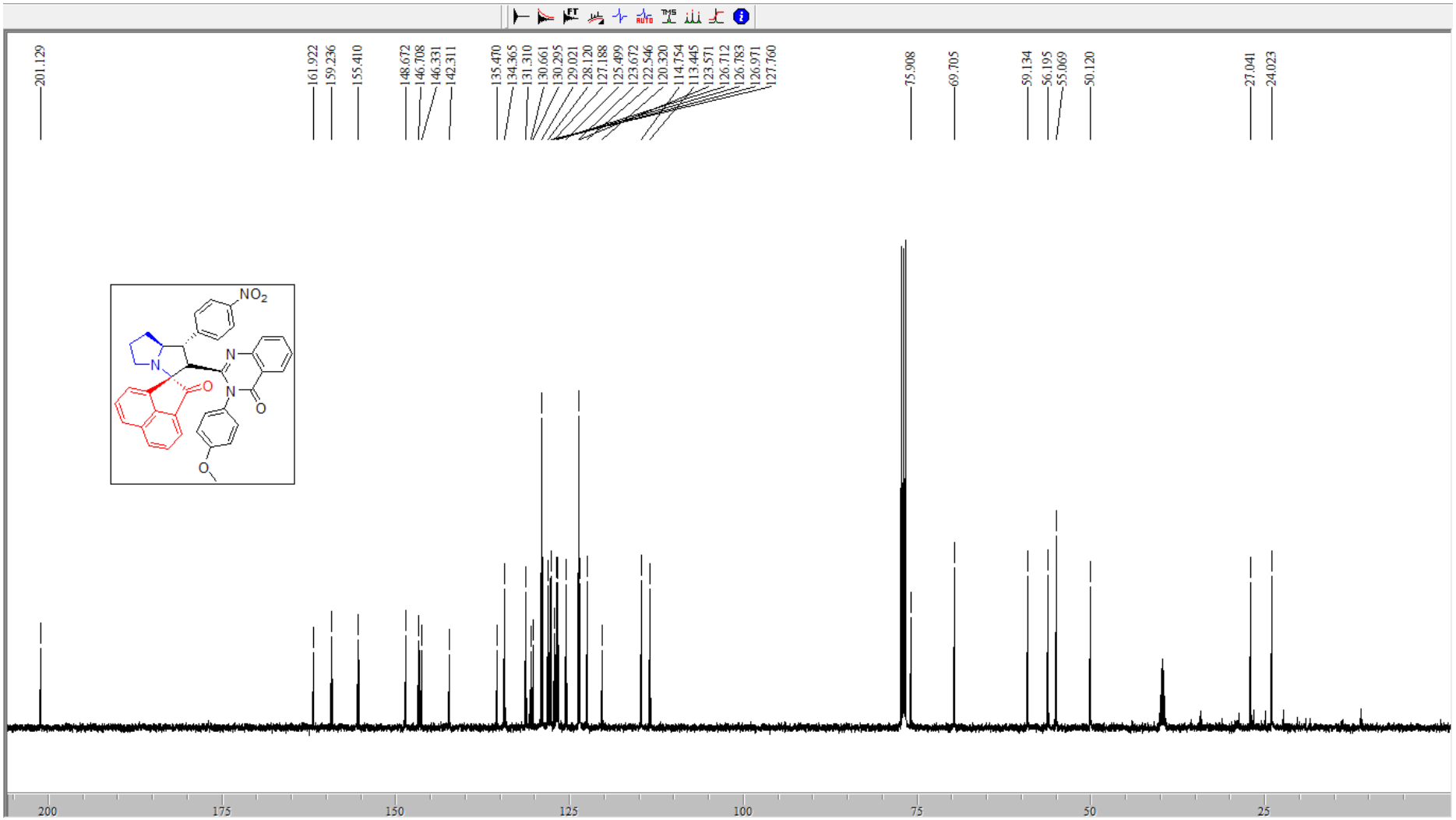
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56.195
55.069
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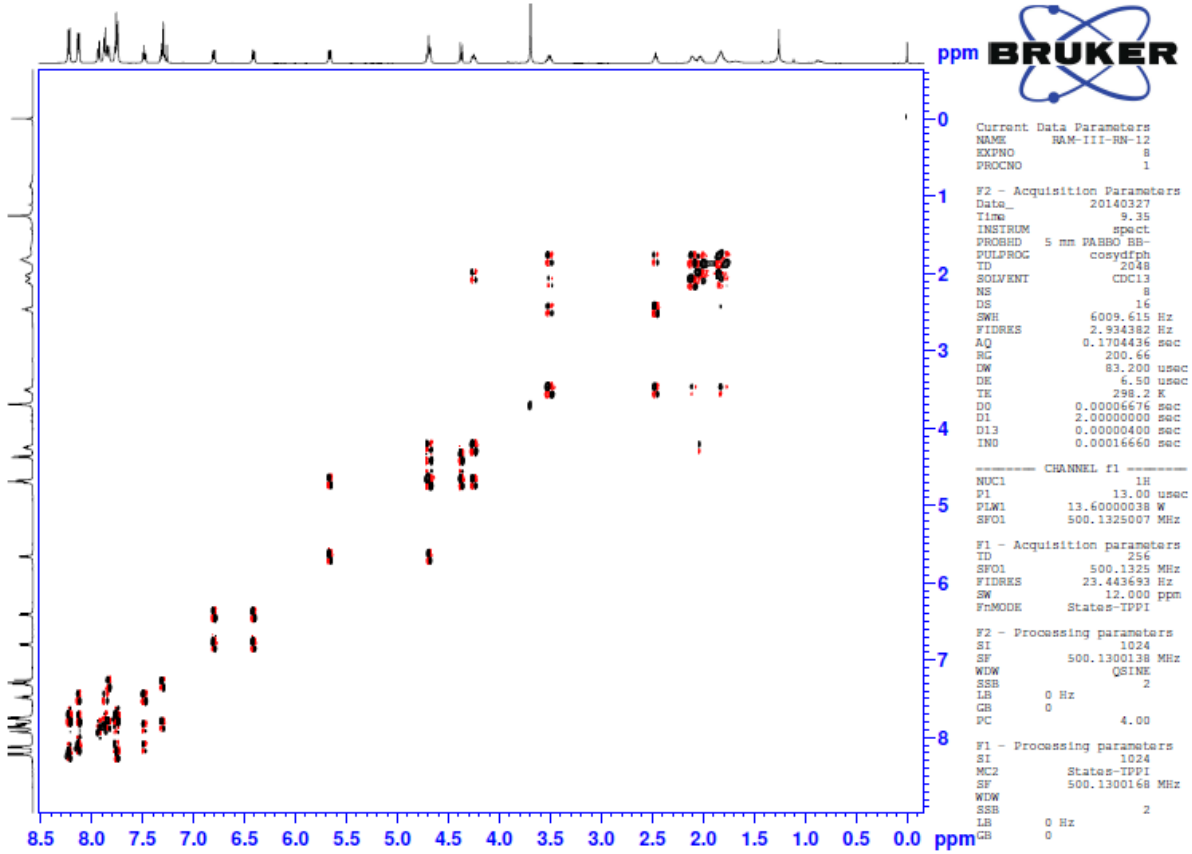
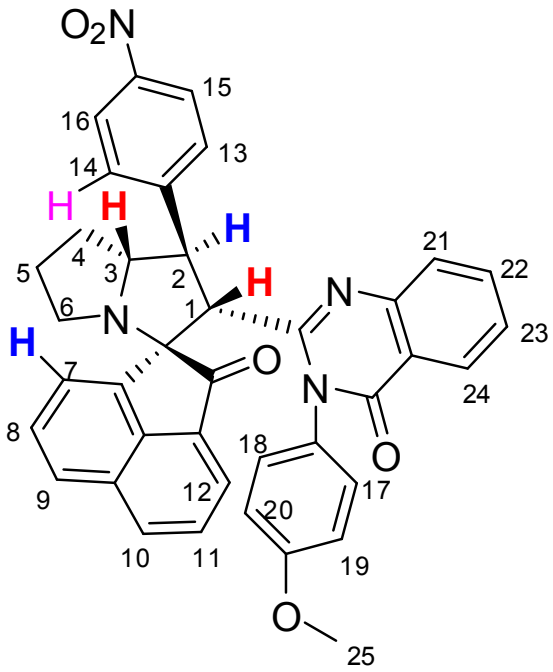
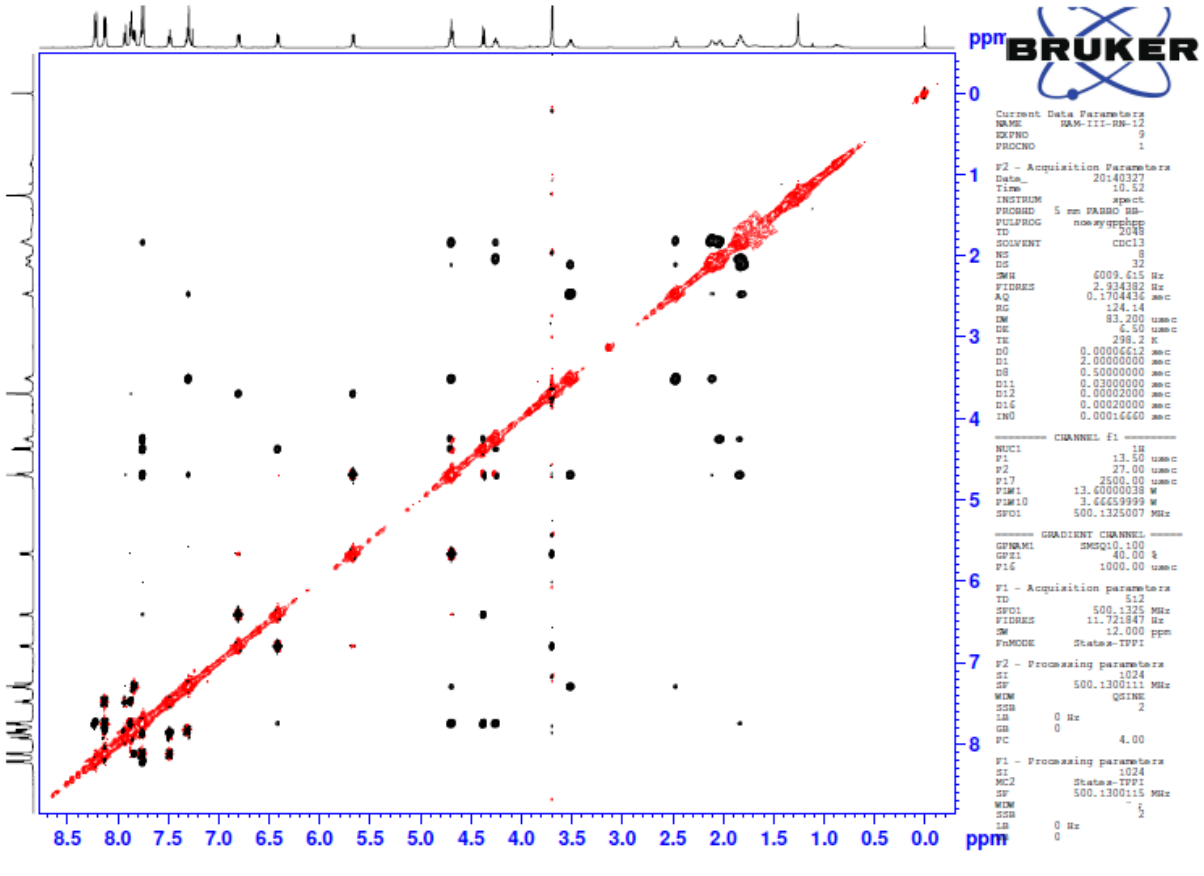
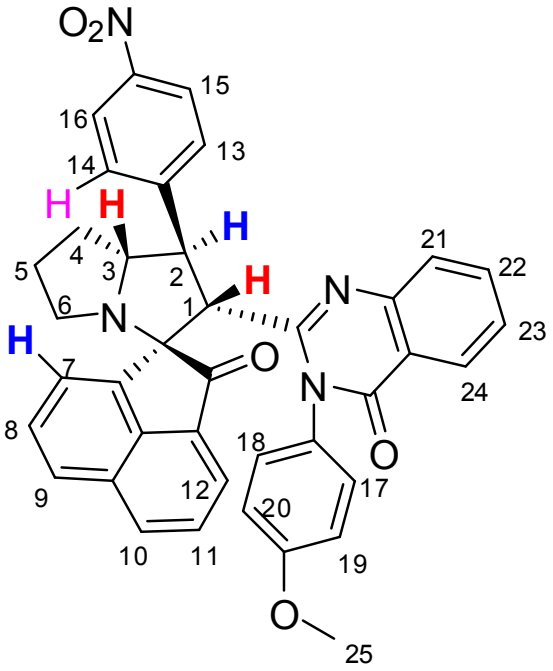




2D Double Quantum Filtered Correlation Spectroscopy (DQFCOSY) spectrum of compound **4p**





2D NOESY (Nuclear Overhauser effect spectroscopy) of compound **4p**