Supplementary information

Magnetically Separable $CuFe_2O_4$ Nanoparticles as Recoverable Catalyst for Addition Reaction of C(sp3)-H Bond of Azaarenes to Aldehydes

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1. Instrument

All major chemicals and solvents were obtained from commercial sources and used without further purification. NMR spectra were recorded at 300 MHz for protons on JOEL JNM-ECA 300 spectrometers. ^{1}H NMR chemical shifts (δ) are given in ppm relative to TMS (δ = 0.0). Chemical shifts for ^{13}C NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent as the internal standard. Data Reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), integration, coupling constant and identification. copper ferrite ($CuFe_2O_4$) nanoparticle was obtained from Sigma Aldrich.

2. General procedure for C(sp^3)-H functionalization of azaarenes: A 25 mL Schlenk tube equipped with a magnetic stirring bar was charged with 2,6-lutidine (0.50 mmol), *p*-nitro-benzaldehyde (0.25 mmol), ethylene glycol (0.5ml), TBAC(1 equiv.) and $CuFe_2O_4$(0.1equiv.). The tube was sealed and heated at 100℃ for 24h. After completion of the reaction, the catalyst was separated with an external magnet and the resulting solution was extracted with ether (3×10 ml). The organic layer was dried with anhydrous Na_2SO_4, and concentrated under vacuum. The residue was chromatographed on a silica gel column eluted with a mixture of petroleum ether and ethyl acetate (1:1) to give pure products

3. Characterization data of products:

2-(6-methylpyridin-2-yl)-1-(4-nitrophenyl)ethanol (**3a**) ^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ 8.18 (s, 1H), 8.16 (s, 1H), 7.57 (d, *J*=5.7 Hz, 2H), 7.50 (t, *J*=8.0 Hz, 1H), 7.05 (d, *J*=8.0 Hz, 1H), 6.87 (d, *J*=8.0 Hz, 1H), 5.22 (d, *J*=4.8 Hz, 1H), 3.11-2.98 (m, 2H), 2.54 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) δ 158.2, 157.7, 151.7, 147.1, 137.5, 126.6, 123.6, 121.7, 120.7, 72.6, 44.5, 24.3 ;

1-(4-nitrophenyl)-2-(pyridin-2-yl)ethanol (**3b**) ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.51 (d, *J* = 4.9 Hz 1H), 8.17 (d, *J* = 8.6 Hz, 2H), 7.65 (td, *J* = 7.7, 15.36 Hz, 1H), 7.57 (d, *J* = 8.9 Hz, 2H), 7.25(m, 1H), 7.08 (d, *J*=7.8 Hz, 1H), 5.26 (dd, *J* = 3.1, 8.56 Hz, 1H), 3.18-3.06 (m, 2H)； ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ158.8, 151.6, 148.5, 147.2, 137.3, 126.7, 124.0, 123.7, 122.2, 72.6, 44.9.

1-(4-nitrophenyl)-2-(quinolin-2-yl)ethanol (**3c**) ^{1}H NMR (300 MHz, $CDCl_3$): *δ* 8.22 (d, *J* = 8.7 Hz,

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2H), 8.12 (d, *J* = 8.4 Hz, 1H), 8.06 (d, *J* = 8.7 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.74 (t, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.22 (d, *J* = 8.2 Hz, 1H), 5.44 (dd, *J* = 3.3 Hz, *J* = 8.4 Hz, 1H), 3.23-3.38 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): *δ* 159.7, 151.5, 147.2, 146.9, 137.3, 130.2, 128.6, 127.7, 126.7, 126.6, 123.7, 121.9, 72.1, 45.1;

2-(6-bromoquinolin-2-yl)-1-(4-nitrophenyl)ethanol (**3d**) ^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ 8.19 (d, *J*=8.2 Hz, 2H), 8.01 (d, *J*=8.3 Hz, 1H), 7.95 (d, *J*=8.2 Hz, 1H), 7.91 (d, *J*=8.9 Hz, 1H), 7.78 (dd, *J*=8.6, 1.6 Hz, 1H), 7.62 (d, *J*=8.5 Hz, 2H), 7.22 (d, *J*=8.6 Hz, 1H), 6.33 (s, 1H), 5.42 (dd, *J*=8.2 Hz, 1H), 3.34-3.21 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) δ 160.2, 151.2, 147.3, 145.6, 136.2, 133.6, 130.4, 129.8, 128.1, 126.7, 123.8, 122.9, 120.5, 72.1, 45.5;

2-(4,6-dimethylpyridin-2-yl)-1-(4-nitrophenyl)ethanol (**3e**) ^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ 8.17 (d, *J*=8.7, 2H), 7.57 (d, *J*=8.4 Hz, 2H), 6.88 (s, 1H), 6.72 (s, 1H), 5.20 (dd, *J*=3.0, 8.4 Hz, 1H), 3.08-2.93 (m, 2H), 2.50 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) δ 157.9, 157.1, 151.9, 148.8, 147.1, 126.6, 123.6, 122.7, 121.7, 72.7, 44.4, 24.1, 21.0;

2-(6-fluoroquinolin-2-yl)-1-(4-nitrophenyl)ethanol (**3f**) ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.19 (d, *J*=8.4 Hz, 2H), 8.02-8.06 (m, 2H), 7.62 (d, *J*=8.8 Hz, 2H), 7.47-7.50 (m, 1H), 7.41 (dd, *J*=8.8, 2.8 Hz, 1H), 7.21-7.24 (m, 2H), 5.42 (dd, *J*=2.8, 8.8Hz, 1H), 3.22-3.35 (m, 2H)； ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 161.6, 159.2, 151.3, 147.2, 144.0, 136.6 (d, *J*=5.3 Hz), 131.1 (d, *J*=9.0 Hz), 127.6, 126.7, 123.7, 122.7, 120.5 (d, *J*=102.4 Hz), 110.8(d, *J*=86.4 Hz), 72.1, 45.3;

1-(4-nitrophenyl)-2-(8-nitroquinolin-2-yl)ethanol (**3g**) ^{1}H NMR (300 MHz, DMSO-d_6): *δ* 8.41-8.44 (m, 1H), 8.11- 8.21 (m, 4H), 7.60-7.69 (m, 4H), 5.78 (br, 1H), 5.26 (s, 1H), 3.31 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): *δ* 162.6, 151.1, 147.2, 146.7, 138.5, 137.3, 132.9, 127.8, 126.7, 125.8, 125.3, 123.7, 123.6, 71.5, 45.6;

1-(4-nitrophenyl)-2-(quinoxalin-2-yl)ethanol (**3h**) ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 8.71 (s, 1H), 8.23 (d, *J* = 8.6 Hz, 2H), 8.10-8.06 (m, 2H), 7.83-7.78 (m, 2H), 7.66 (d, *J* = 8.6 Hz, 2H), 5.48 (dd, *J* = 2.8 Hz, *J* = 8.8 Hz, 1H), 3.45-3.32 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 154.1, 150.6, 147.4, 145.9, 141.7, 141.1, 130.8, 129.9, 128.6, 126.7, 123.9, 71.9, 43.3;

2-(6-methylquinolin-2-yl)-1-(4-nitrophenyl)ethanol (**3i**) ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.18 (d, *J* = 7.8 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.55 (m, 2H), 7.15 (d, *J* = 8.4 Hz, 1H), 5.41 (dd, *J* = 2.8, 8.7 Hz, 1H), 3.33-3.19 (m, 2H), 2.53(s, 3H)； ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 158.7, 151.6, 147.2, 145.5, 136.6, 136.5, 132.4, 128.3, 127.0, 126.7, 126.6, 123.7, 121.9, 72.3, 45.1, 21.6

1-(3-nitrophenyl)-2-(quinolin-2-yl)ethanol (**3j**) ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 8.36 (s, 1H), 8.06-8.14 (m, 3H), 7.82 (t, *J* = 8.6 Hz, 2H), 7.75 (t, *J* = 7.6 Hz, 1H), 7.57-7.50 (m, 2H), 7.23 (d, *J* = 2.4 Hz, 1H), 5.42 (dd, *J*=8.8 Hz, 1H), 3.37-3.27 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 159.7, 148.4, 146.2, 137.4, 132.1, 130.2, 129.4,128.6, 127.0, 127.0, 126.6, 122.4, 122.0, 121.1, 72.1, 45.3;

2-(6-methylpyridin-2-yl)-1-(3-nitrophenyl)ethanol (**3k**) ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.28 (s, 1H), 8.09 (d, *J*=8.0 Hz, 1H), 7.76 (d, *J*=7.6 Hz, 1H), 7.47-7.53 (m, 2H), 7.05 (d, *J*=8.0 Hz, 1H), 6.89 (d, *J*=8.4 Hz, 1H), 5.21 (dd, *J*=3.2, 8.8 Hz, 1H), 3.01-3.12 (m, 2H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 158.3, 157.5, 148.3, 146.5, 137.5, 132.1, 129.3, 122.2, 121.7, 121.0, 120.7, 72.5, 44.6, 24.4;

3-(1-hydroxy-2-(6-methylpyridin-2-yl)ethyl)benzonitrile (**3l**) ^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ 7.71 (s, 1H), 7.64 (d, *J*=8.2 Hz, 1H), 7.53 (m, 2H), 7.42 (t, *J*=8.6 Hz, 1H), 7.07 (d, *J*=6.8 Hz, 1H), 6.89 (d, *J*=7.8 Hz, 1H), 5.17 (dd, *J*=2.1, 8.0 Hz, 1H), 3.12-3.00 (m, 2H), 2.56 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) δ 158.0, 157.3, 145.7, 137.9, 130.9, 130.4, 129.6, 129.1, 121.9, 120.9,

119.0, 112.3, 72.4, 44.6, 24.1;

1-(4-nitrophenyl)-2-(pyrazin-2-yl)ethanol (**3m**) yellow solid, mp 137-139 ^{0}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.52 (s, 2H), 8.45 (s, 1H), 8.21 (d, *J* = 8.7 Hz, 2H), 7.78 (d, *J* = 8.7 Hz, 2H), 5.31 (dd, *J* = 3.9 Hz, *J* = 8.1 Hz, 1H), 3.25-3.11 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 154.3, 150.7, 147.4, 145.4, 143.4, 143.4, 126.6, 123.8, 72.2, 42.8;

4-(1-hydroxy-2-(6-methylpyridin-2-yl)ethyl)benzonitrile (**3n**) ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.60 -7.47 (m, 5H), 7.03 (d, *J*=7.6 Hz, 1H), 6.86 (d, *J*=7.6 Hz, 1H), 5.16 (dd, *J*=3.2, 8.8 Hz, 1H), 2.96-3.08 (m, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ158.8, 157.5, 149.7, 137.5, 132.2, 126.6, 121.7, 120.7, 119.0, 110.9, 72.7, 44.6, 24.3

4-(1-hydroxy-2-(quinolin-2-yl)ethyl)benzonitrile (**3o**) ^{1}H NMR (300 MHz, DMSO-d_6): δ 8.24 (d, *J* = 8.2 Hz, 1H), 7.94 (t, *J* = 8.2 Hz, 2H), 7.79-7.70 (m, 3H), 7.60-7.52 (m, 3H), 7.42 (d, *J* = 8.4 Hz, 1H), 5.72 (d, *J* = 4.8 Hz, 1H), 5.27-5.21 (m, 1H), 3.24 (d, *J* = 6.6Hz, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): δ 159.8, 151.7, 147.6, 136.3, 132.5, 129.8, 128.8, 128.2, 127.4, 127.0, 126.3, 123.1, 119.4, 110.0, 72.3, 48.2;

2-(benzo[d]thiazol-2-yl)-1-(3-nitrophenyl)ethanol(**3p**) White solid, mp 167-168°C, ^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ 8.36 (s, 1H), 8.15 (d, *J*=8.2 Hz, 1H), 8.02 (d, *J*=6.6 Hz, 1H), 7.87-7.80 (m, 2H), 7.57-7.38 (m, 3H), 5.44 (s, 1H), 3.54-3.38 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) δ 167.9, 152.6, 148.4, 144.8, 131.8, 129.4, 126.3, 125.3, 122.7, 122.6, 121.5, 120.9, 71.5, 42.4; HRMS (ESI) calculated for $C_{15}H_{13}N_2O_3S$: 301.06390 $(M+H)^+$, Found: 301.06414.

2-(benzo[d]thiazol-2-yl)-1-(2-nitrophenyl)ethanol(**3q**) Red solid, mp 160-161°C, ^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ 8.02-7.99 (m, 3H), 7.86 (d, *J*=7.9 Hz, 1H), 7.67 (t, *J*=7.9 Hz, 1H), 7.52-7.37 (m, 3H), 5.82 (d, *J*=8.8 Hz, 1H), 5.03(s, 1H), 3.73 (dd, *J*=15.3 Hz, *J*=1.9 Hz, 1H), 3.42-3.34 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) δ 168.5, 152.7, 147.5, 138.3, 134.6, 133.7, 128.4, 126.2, 125.1, 124.4, 122.7, 121.5, 68.4, 41.8; HRMS (ESI) calculated for $C_{15}H_{13}N_2O_3S$: 301.06396 $(M+H)^+$, Found: 301.06414.

2-(benzo[d]thiazol-2-yl)-1-(4-nitrophenyl)ethanol(**3r**) White solid, mp 178-180°C, ^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ 8.02-7.99 (m, 3H), 7.86 (d, *J*=7.9 Hz, 1H), 7.67 (t, *J*=7.9 Hz, 1H), 7.52-7.37 (m, 3H), 5.82 (d, *J*=8.8 Hz, 1H), 5.03(s, 1H), 3.73 (dd, *J*=15.3 Hz, *J*=1.9 Hz, 1H), 3.42-3.34 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) δ 168.5, 152.7, 147.5, 138.3, 134.6, 133.7, 128.4, 126.2, 125.1, 124.4, 122.7, 121.5, 68.4, 41.8; HRMS (ESI) calculated for $C_{15}H_{13}N_2O_3S$: 301.06390 $(M+H)^+$, Found: 301.06414.

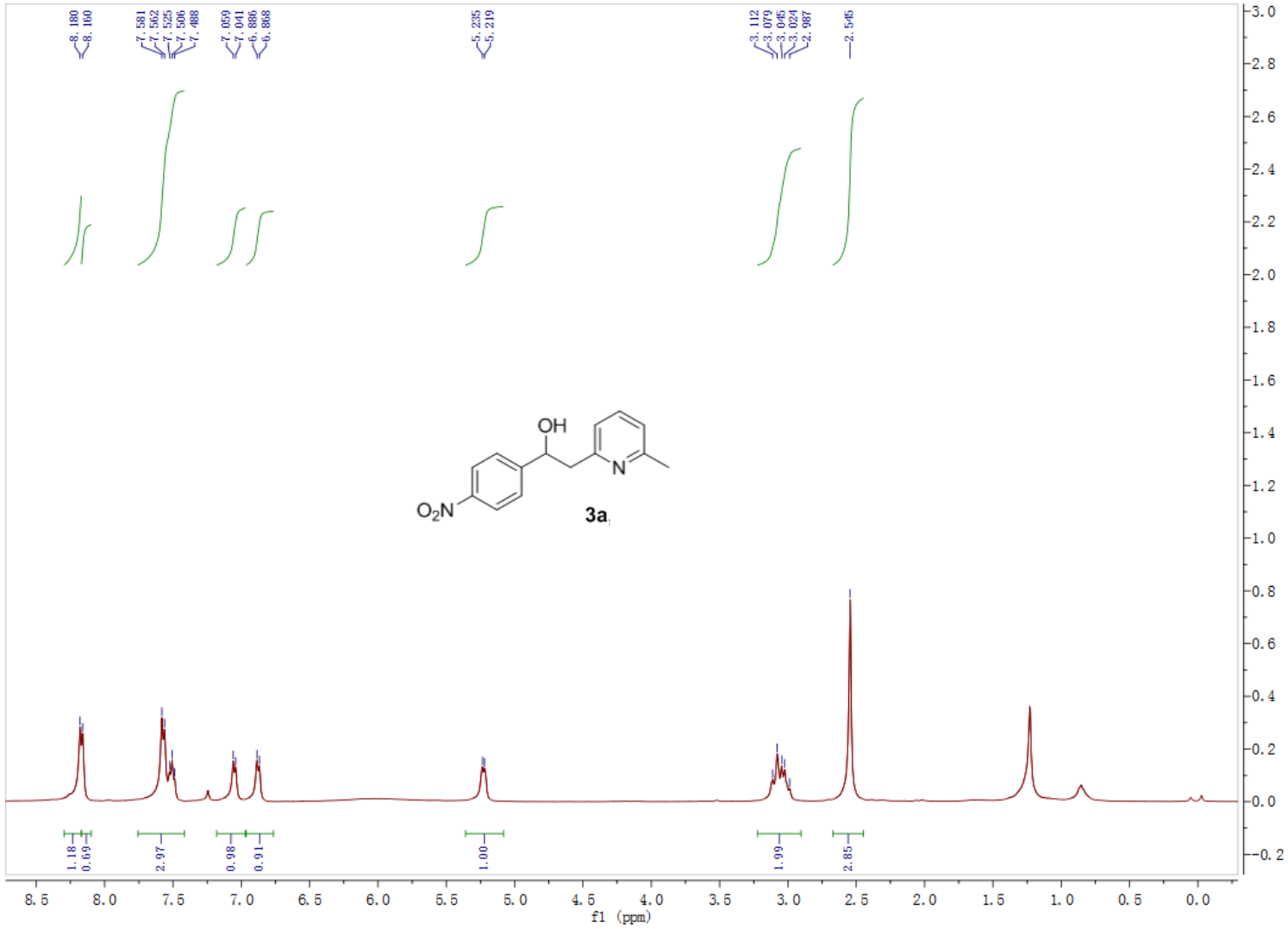
2-(6-methylpyridin-2-yl)-1-(pyridin-2-yl)ethanol (**3s**) ^{1}H NMR (600 MHz, $CDCl_3$, TMS) δ 8.50 (d, *J* = 4.7 Hz, 1H), 7.65 (td, *J* = 1.5, 8.0 Hz, 1H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 1H) ,7.13 (t, *J* = 6.2 Hz, 1H), 6.99 (d, *J* = 7.7 Hz,1H), 6.94(d, J = 7.7Hz, 1H), 5.19 (dd, *J* = 2.9, 9.1 Hz, 1H), 3.31 (dd, *J* = 3.4, 14.7 Hz, 1H), 3.05 (dd, *J* = 9.2, 14.7 Hz, 1H), 2.51 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, TMS) δ162.8, 158.8, 157.2, 148.4, 137.1, 136.7, 122.1, 121.2, 120.9, 120.3, 73.8, 44.0, 24.3.

ethyl 2-hydroxy-3-(6-methylpyridin-2-yl)propanoate (**3t**) ^{1}H NMR (600 MHz, $CDCl_3$, TMS) δ7.4 (t, *J* = 7.8 Hz, 1H), 7.00 (d, *J* = 7.7 Hz, 1H), 6.96 (d, *J* = 7.7Hz, 1H), 4.58 (dd, *J* = 3.9, 7.2 Hz, 1H), 4.16 (dd, *J* = 7.2, 14.4 Hz, 2H), 3.23 (dd, *J* = 4.05, 14.8 Hz, 1H), 3.11 (dd, *J* = 7.2, 14.8 Hz, 1H), 2.50 (s, 3H), 1.19 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, TMS) δ 173.7, 157.5, 157.2, 137.1, 121.5, 120.8, 70.6, 61.1, 40.3, 24.0, 14.1

4-(1-hydroxy-2-(6-methylpyridin-2-yl)ethyl)benzaldehyde (**3u**) ^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ 9.99 (s, 1H), 7.85 (d, *J*=8.4 Hz, 2H), 7.58 (d, *J*=8.5 Hz, 2H), 7.51 (t, *J*=7.8 Hz, 1H), 7.04

(d, *J*=8.0 Hz, 1H), 6.89 (d, *J*=7.8 Hz, 1H), 5.21 (dd, *J*=3.5, 9.0 Hz, 1H), 3.00-3.14 (m, 2H), 2.55 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) δ 192.2, 158.5, 157.5, 151.3, 137.5, 135.5, 129.9, 126.4, 121.6, 120.7, 73.0, 44.8, 24.3

4. Copies of ^{1}H and ^{13}C spectra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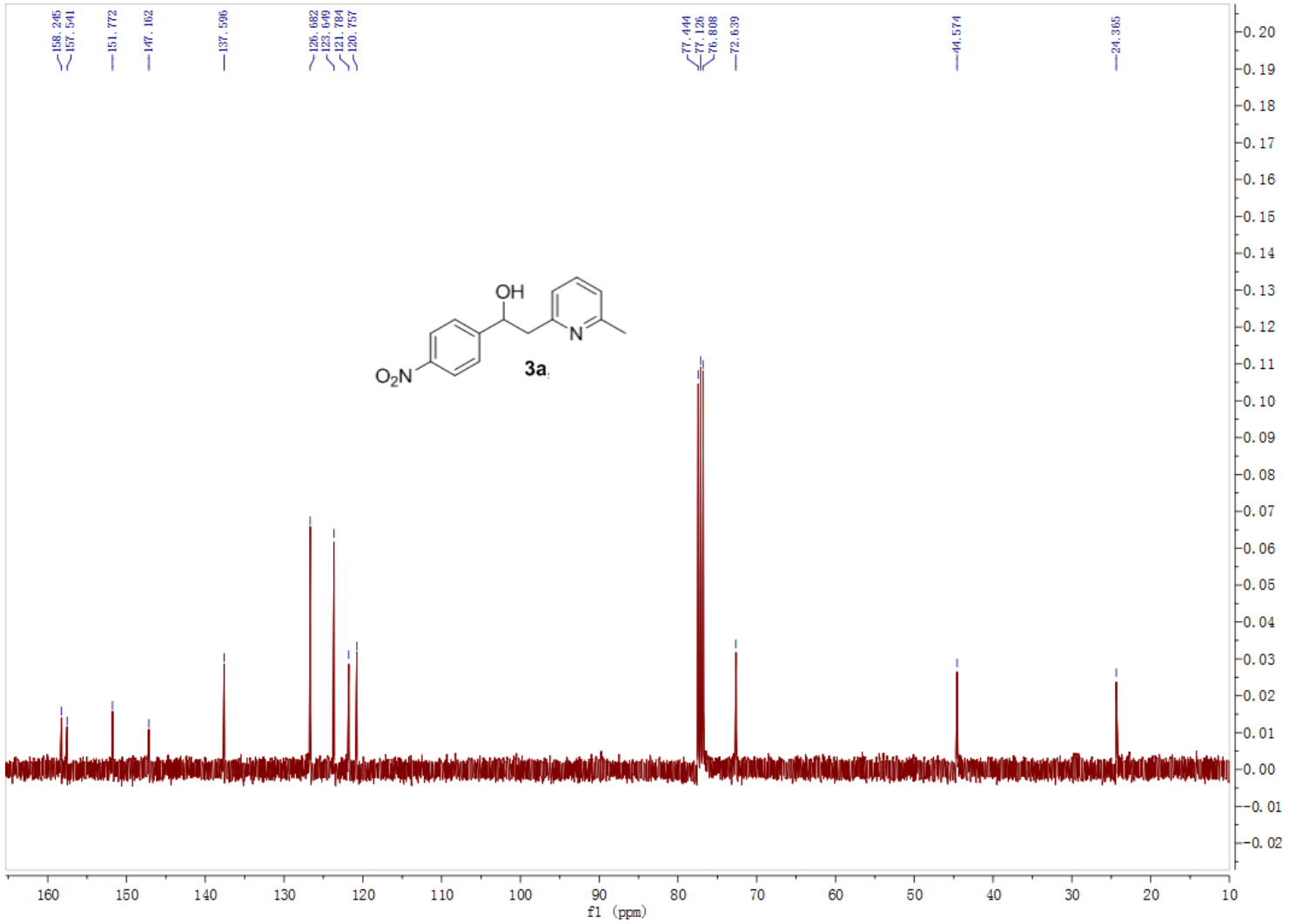
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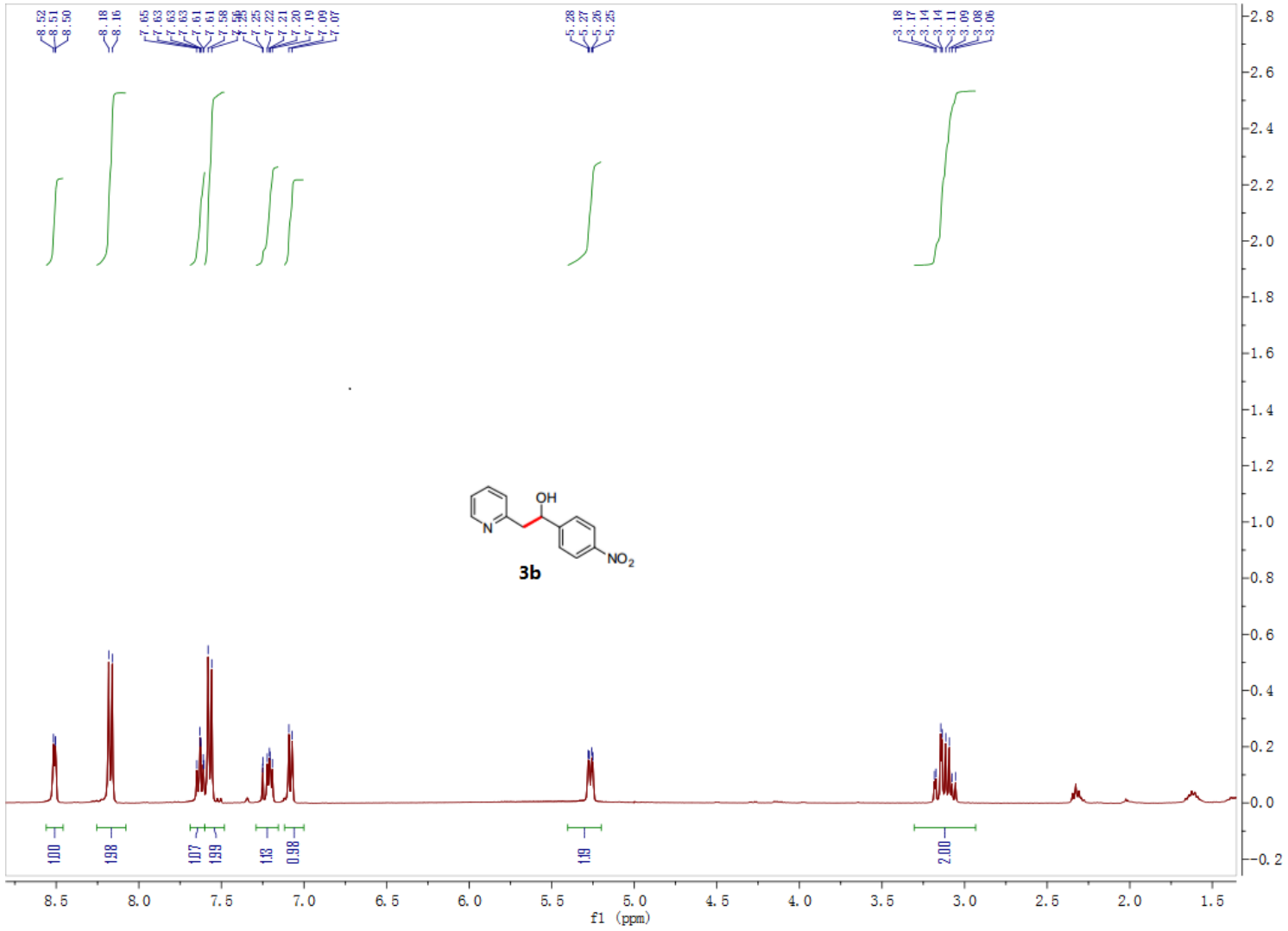
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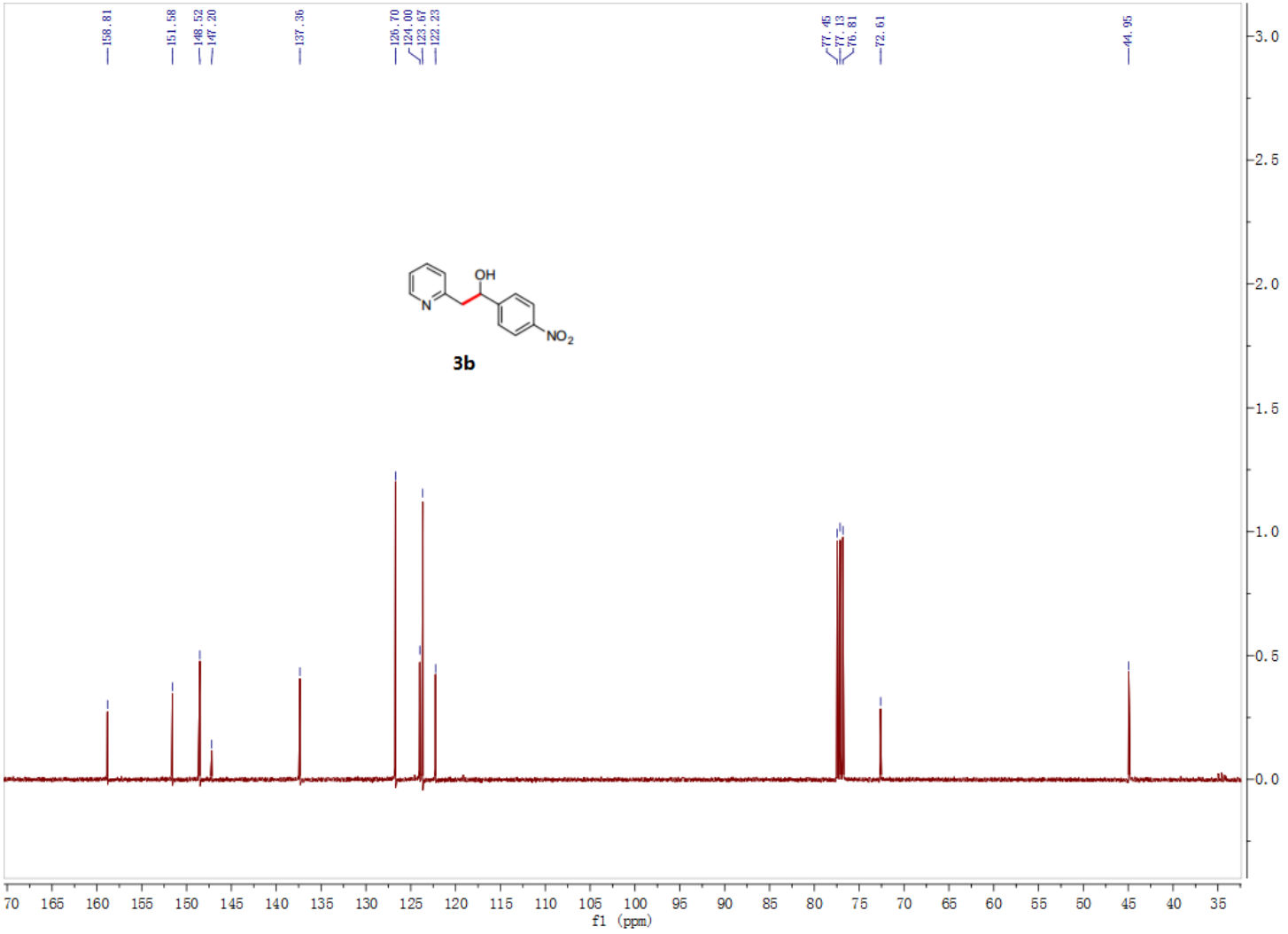
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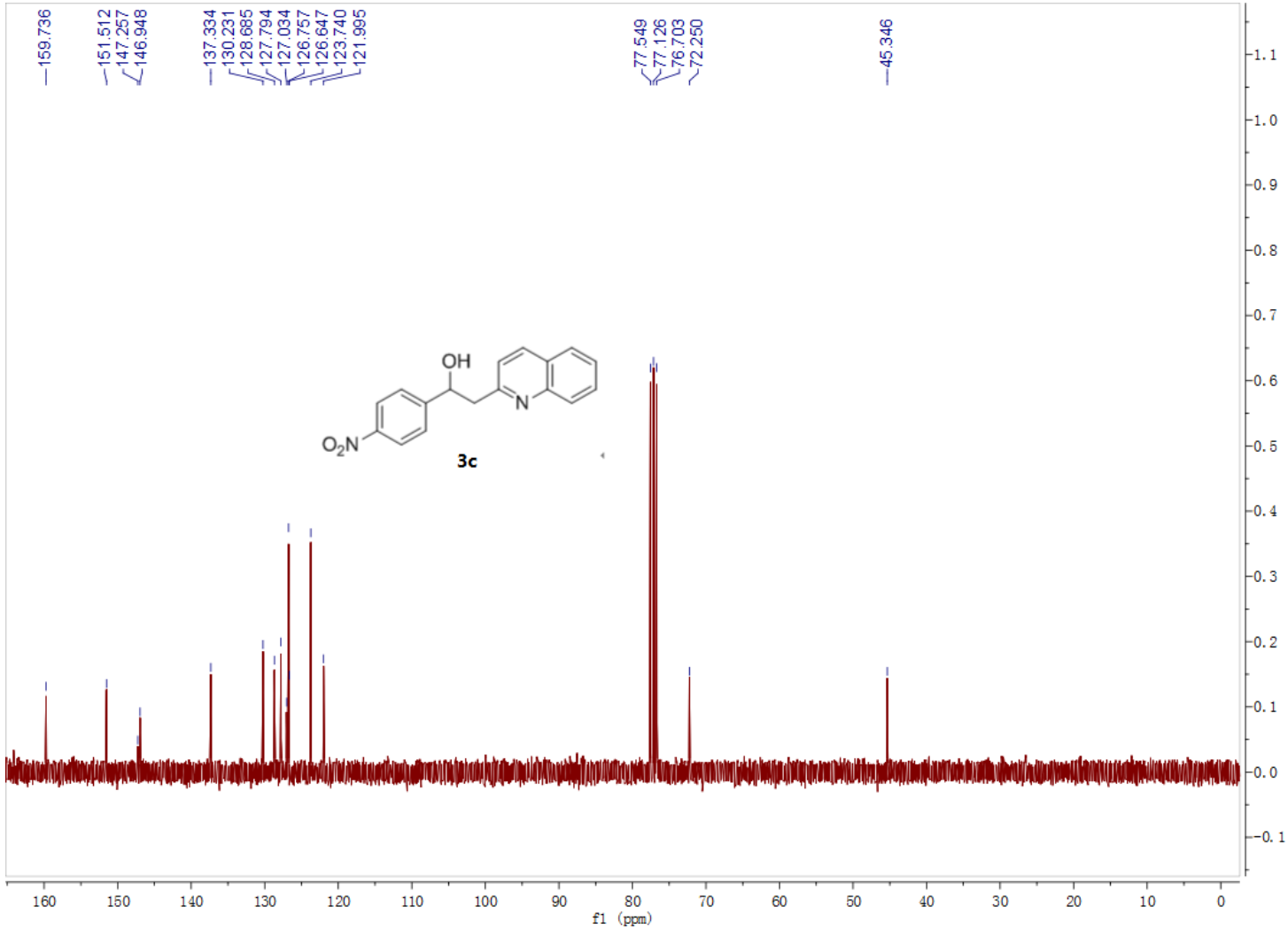
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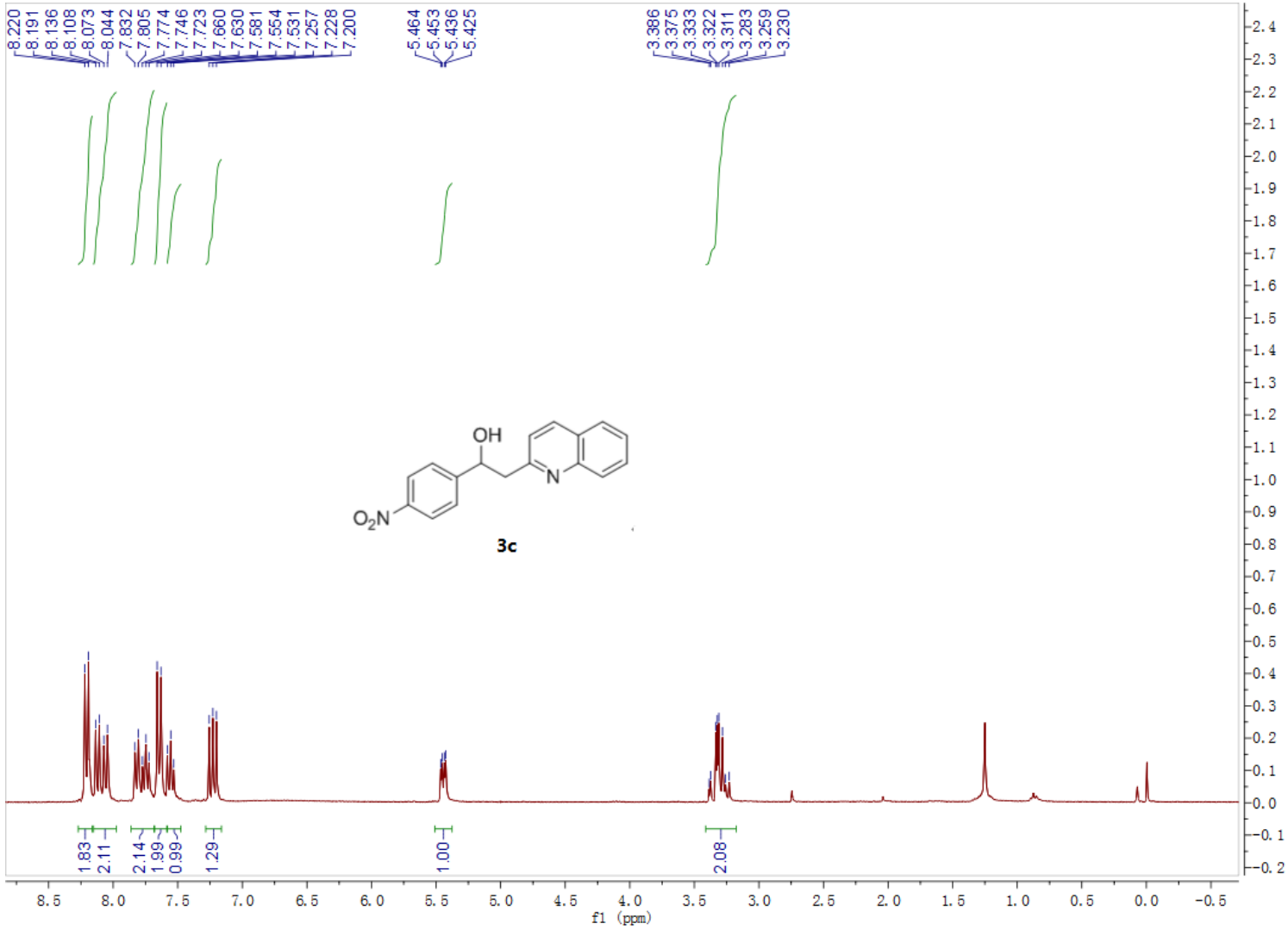
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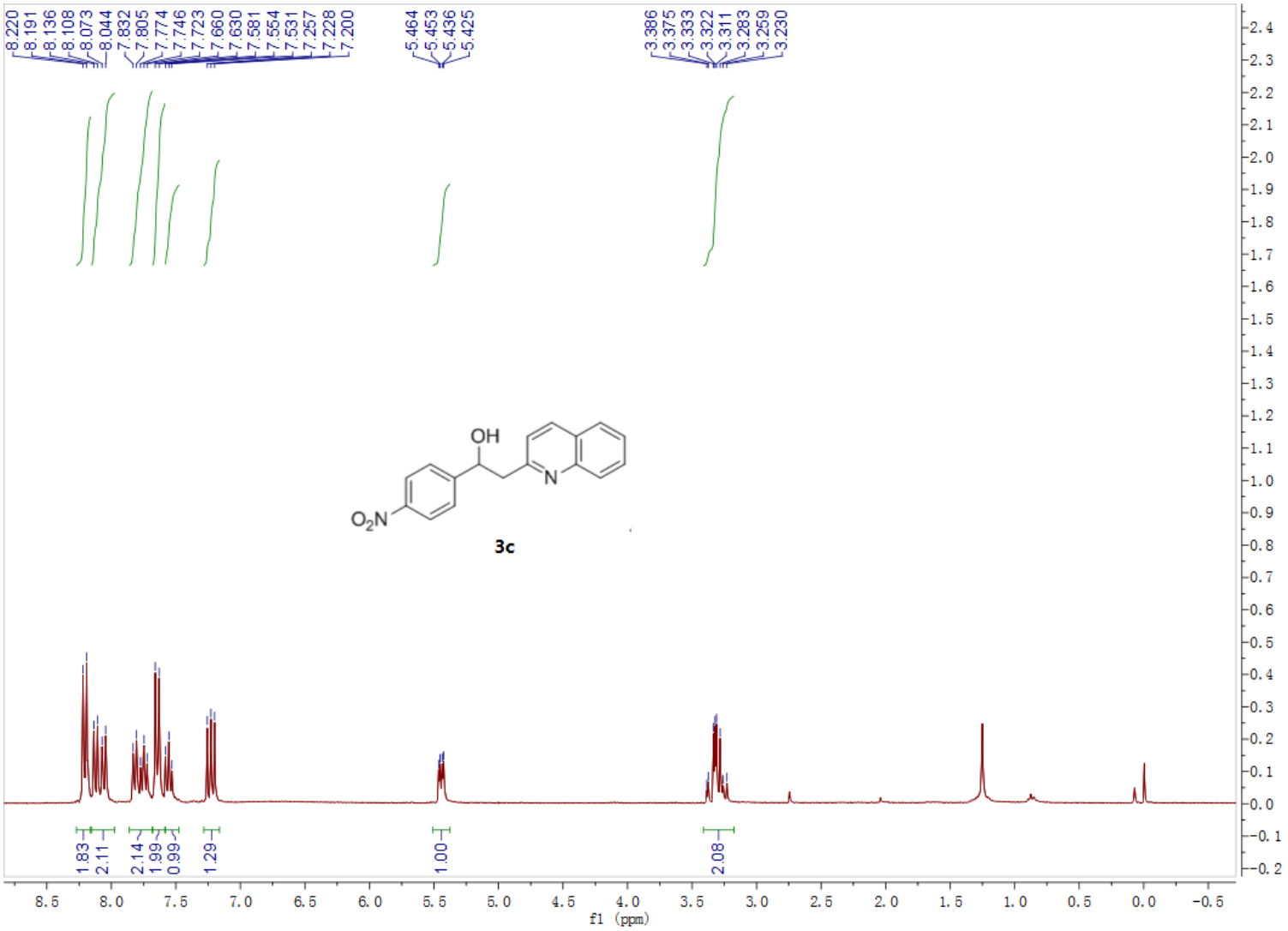
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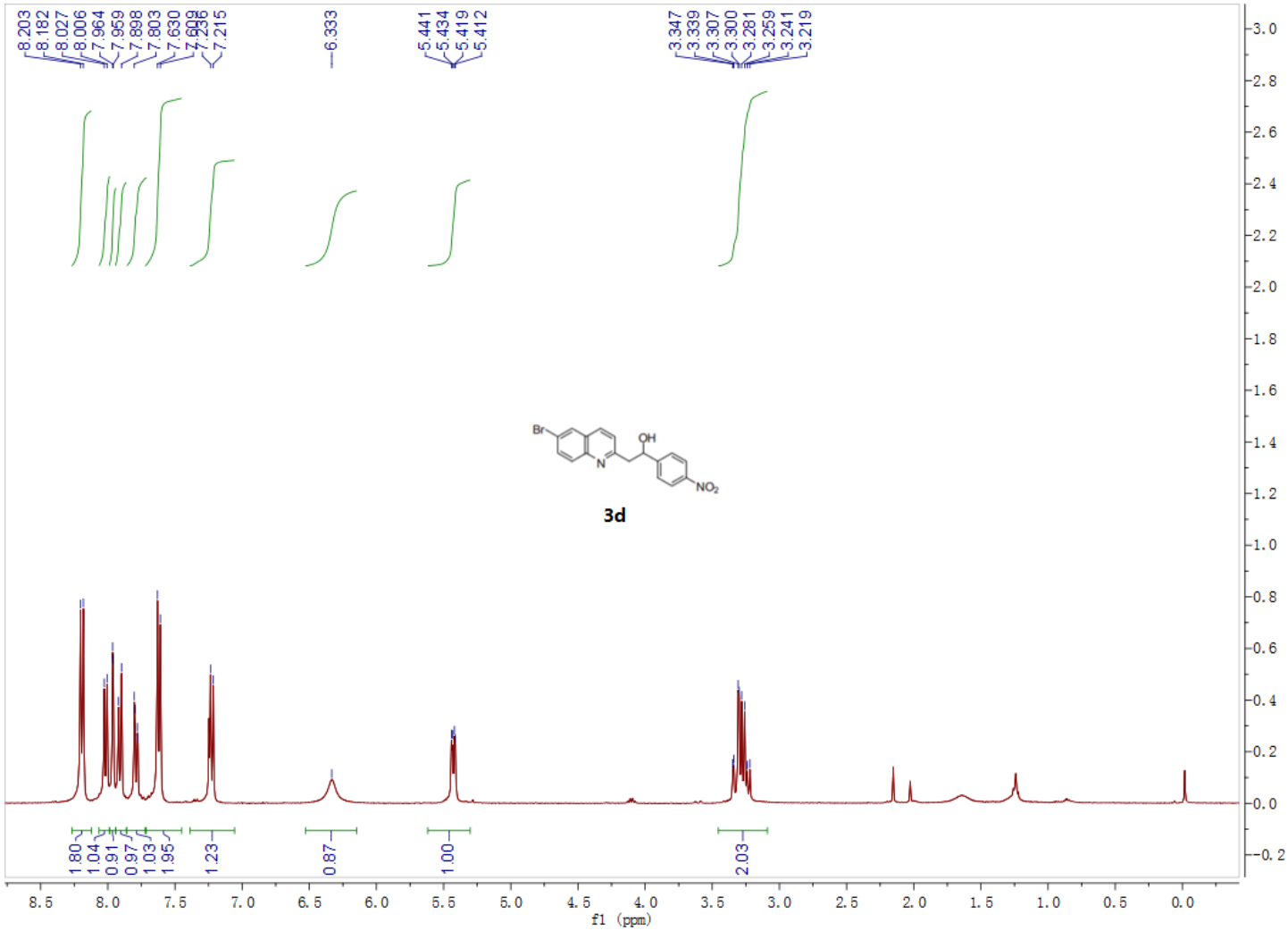
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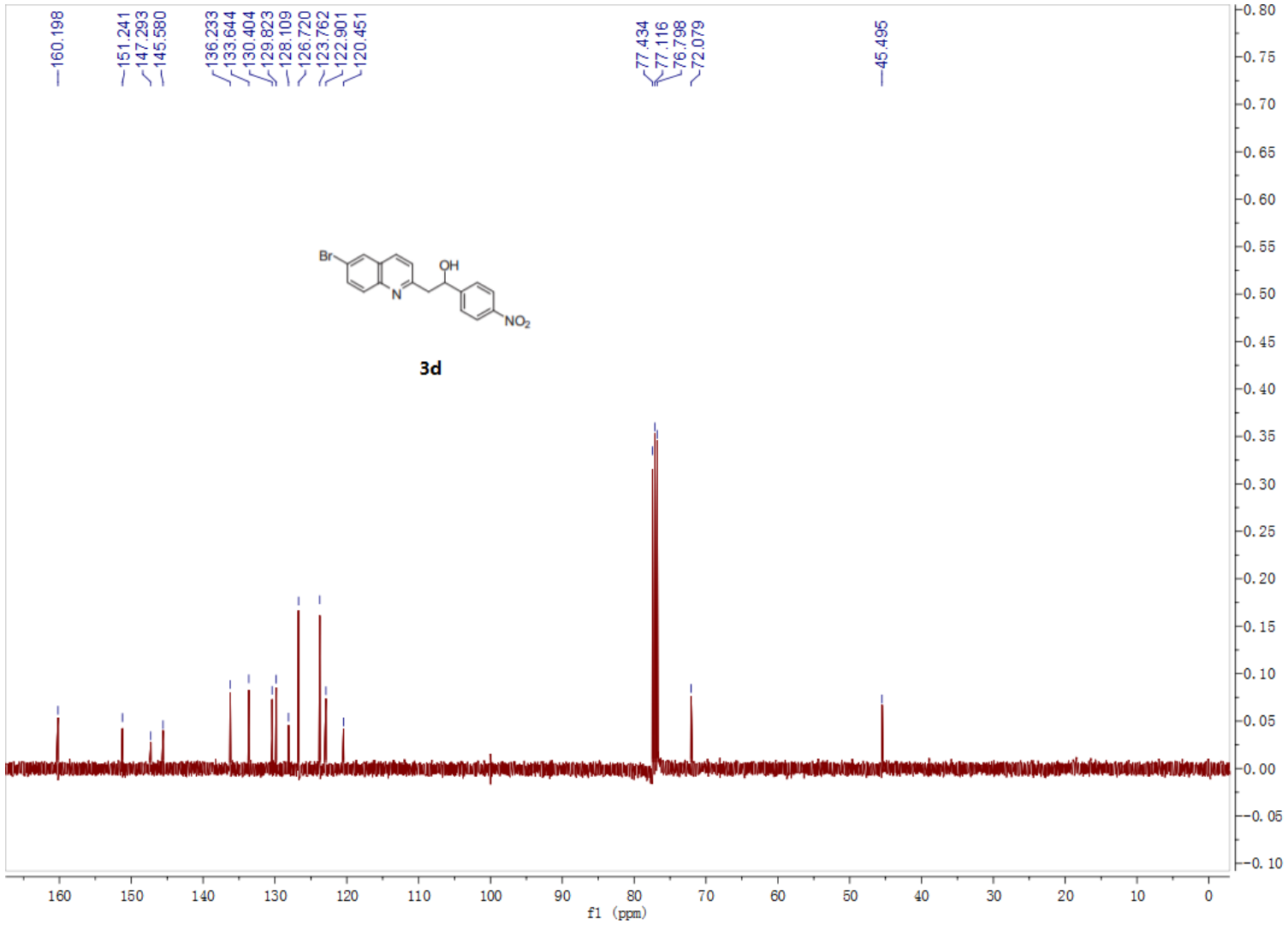
3.339
3.307
3.300
3.281
3.259
3.241
3.219
Br
OH
N
NO2
3d
1.80
1.04
0.91
0.97
1.03
1.95
1.23
0.87
1.00
2.03
f1 (ppm)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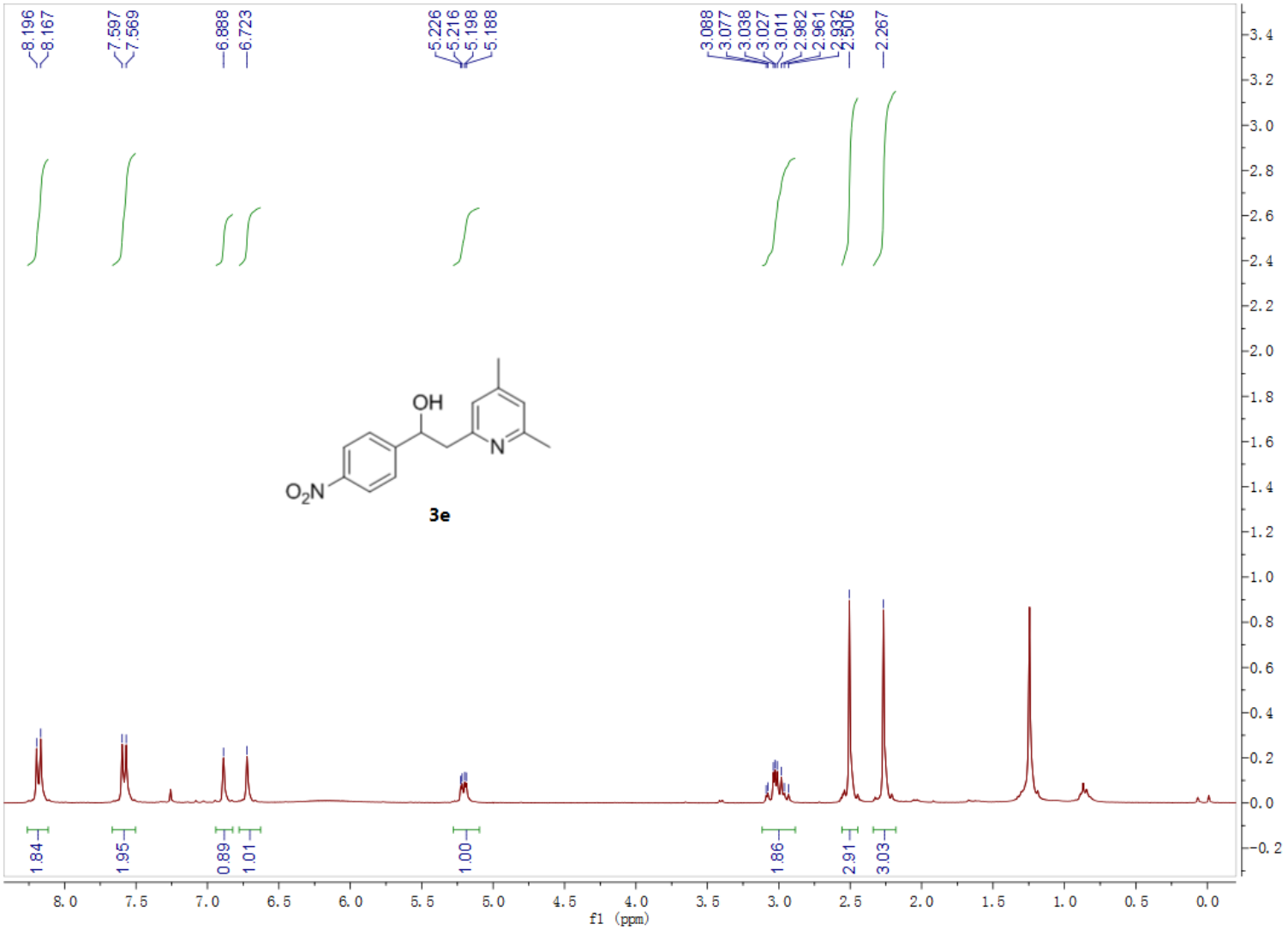
151.241
147.293
145.580
136.233
133.644
130.404
129.823
128.109
126.720
123.762
122.901
120.451
77.434
77.116
76.798
72.079
45.495
Br
OH
N
NO2
3d
f1 (ppm)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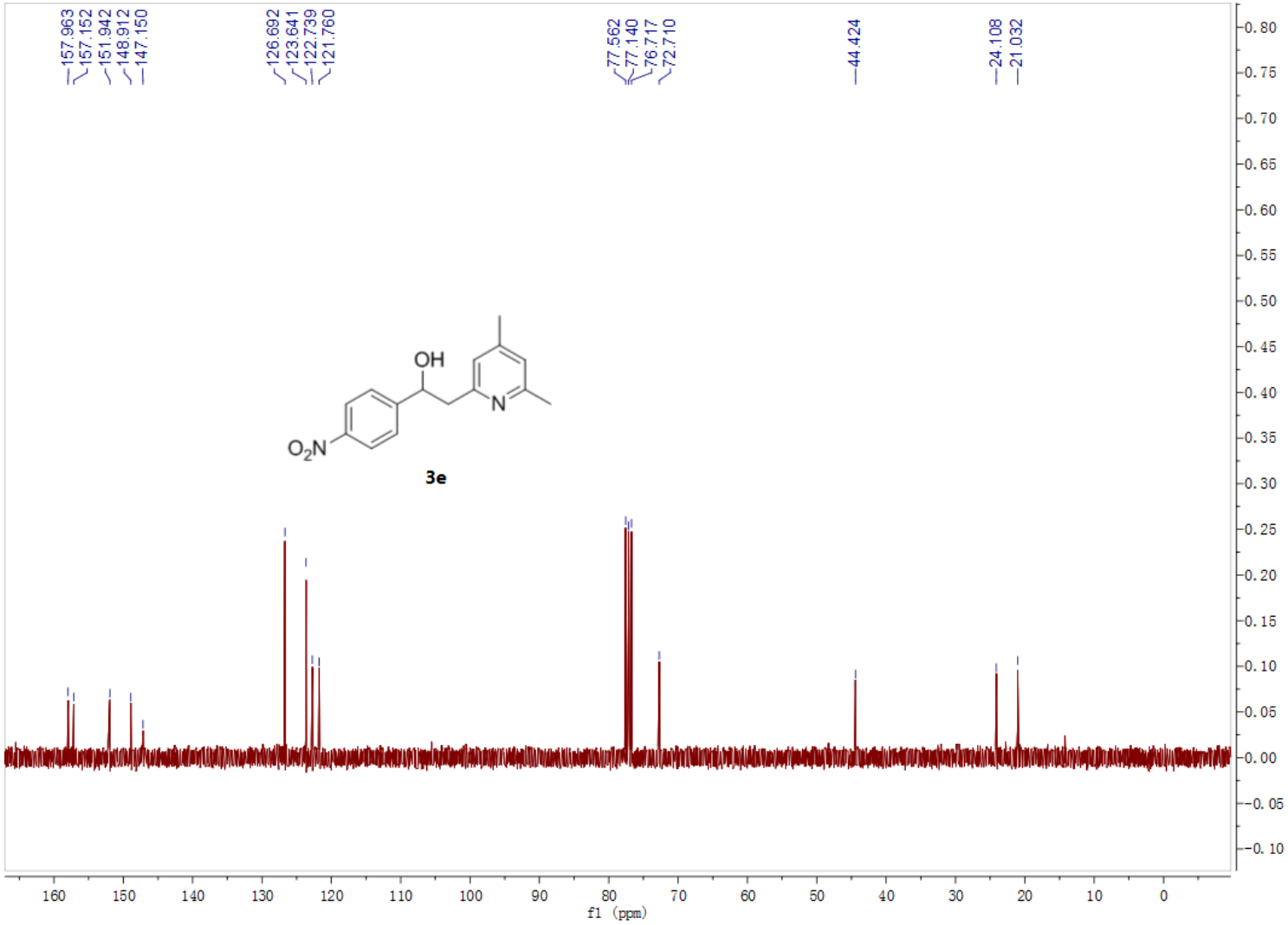
7.597
7.569
6.888
6.723
5.226
5.216
5.198
5.188
3.088
3.077
3.038
3.027
3.011
2.982
2.961
2.932
2.506
2.267
OH
N
O2N
3e
1.84
1.95
0.89
1.01
1.00
1.86
2.91
3.03
f1 (ppm)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157.152
151.942
148.912
147.150
126.692
123.641
122.739
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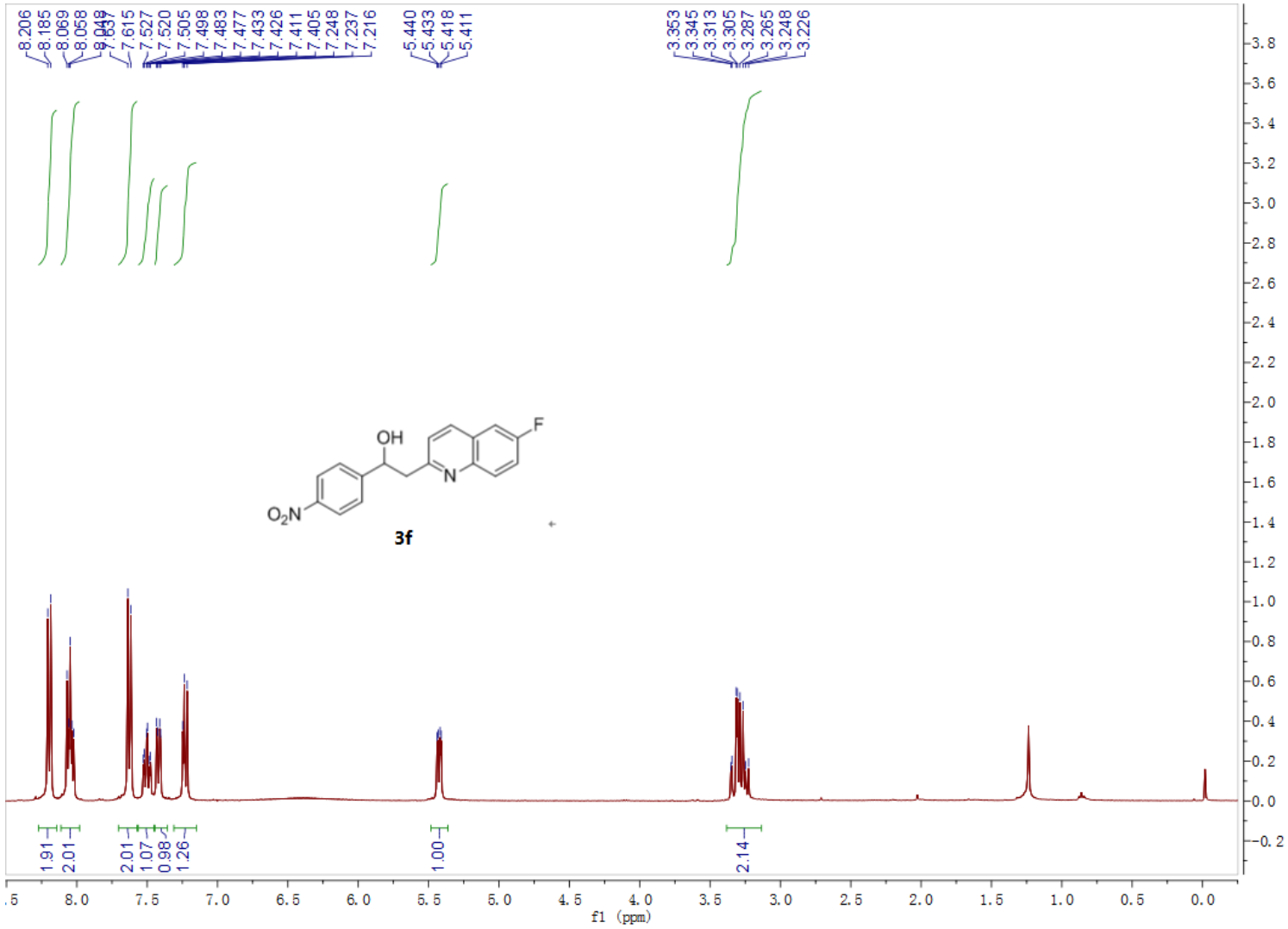
77.562
77.140
76.717
72.710
44.424
24.108
21.032
OH
N
O2N
3e
f1 (ppm)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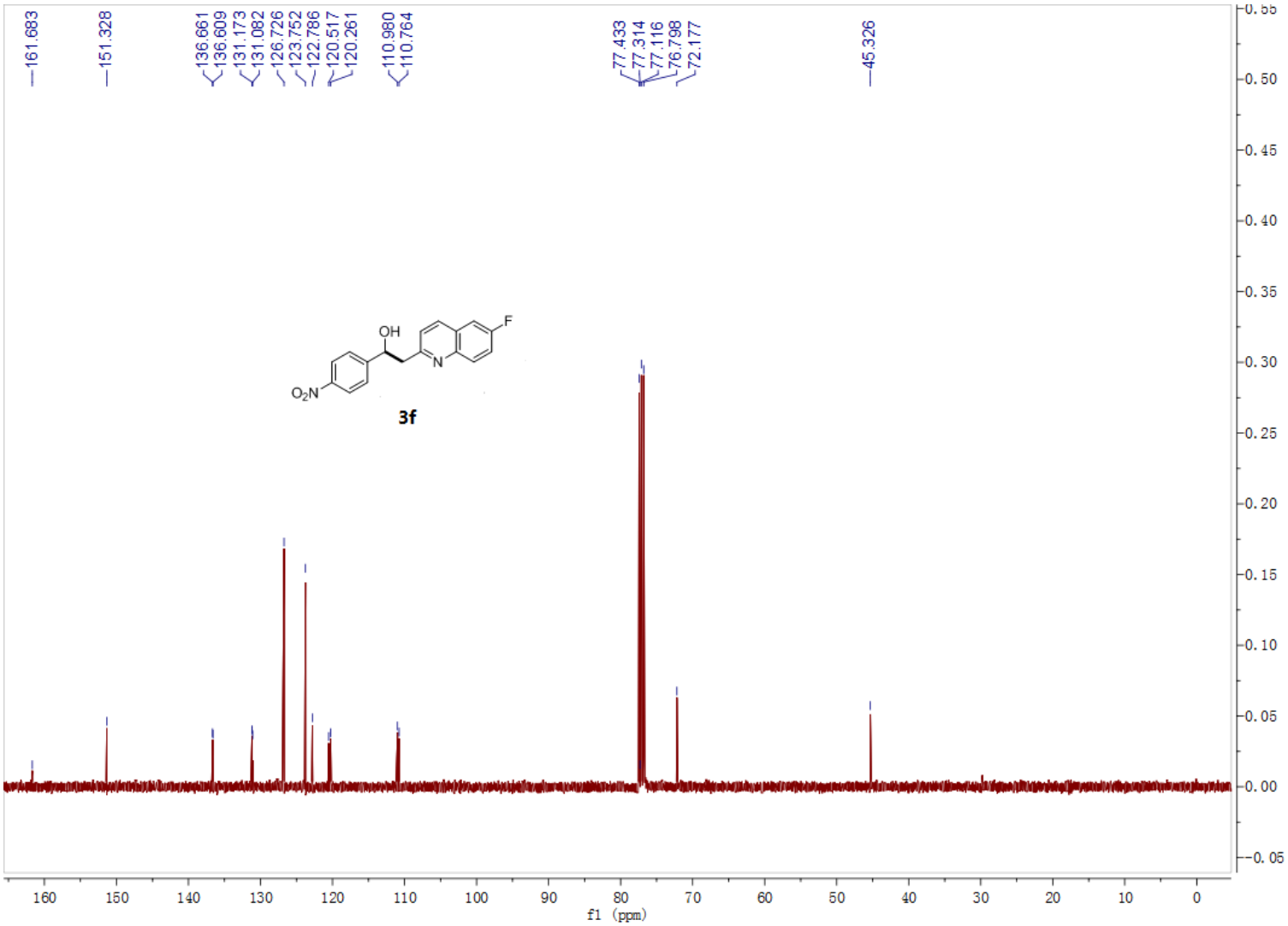
8.185
8.069
8.058
7.637
7.615
7.527
7.520
7.505
7.498
7.483
7.477
7.433
7.426
7.411
7.405
7.248
7.237
7.216
5.440
5.433
5.418
5.411
3.353
3.345
3.313
3.305
3.287
3.265
3.248
3.226
OH
F
N
O2N
3f
1.91
2.01
2.01
1.07
0.98
1.26
1.00
2.14
f1 (ppm)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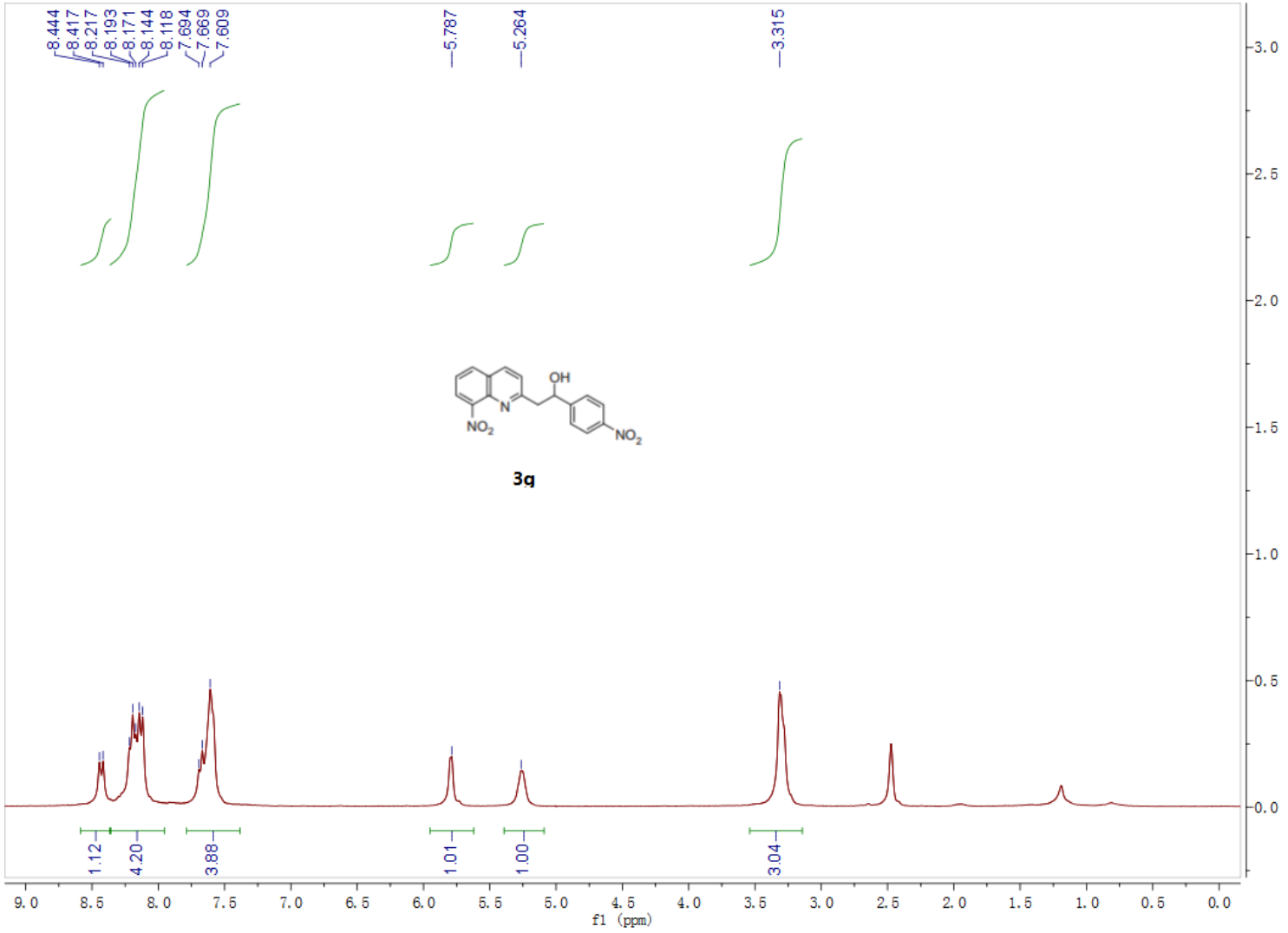
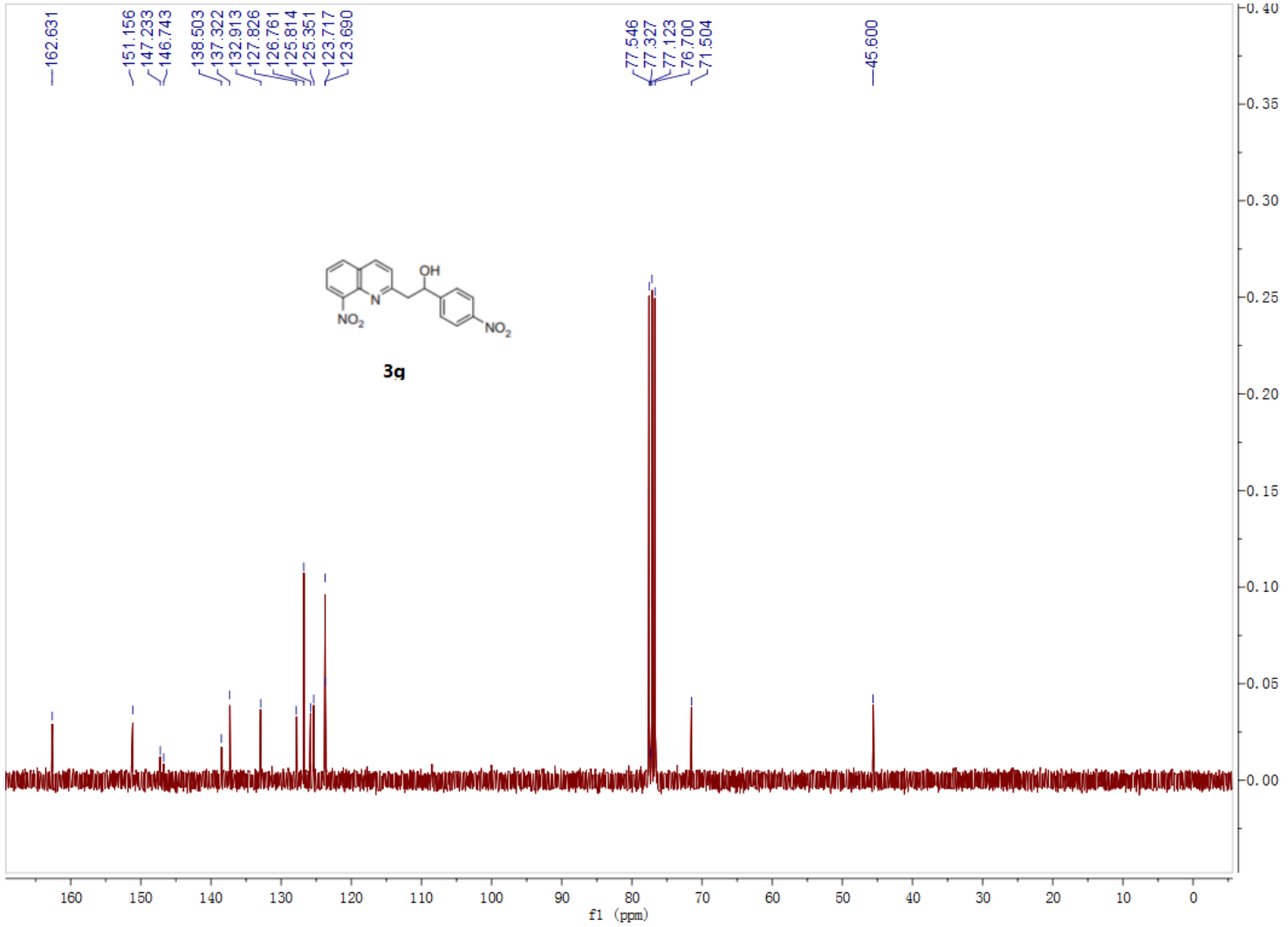
151.328
136.661
136.609
131.173
131.082
126.726
123.752
122.786
120.517
120.261
110.980
110.764
77.433
77.314
77.116
76.798
72.177
45.326
OH
F
N
O2N
3f
f1 (ppm)


8.444
8.417
8.217
8.193
8.171
8.144
8.118
7.694
7.669
7.609
5.787
5.264
3.315
OH
N
NO2
NO2
3q
1.12
4.20
3.88
1.01
1.00
3.04
f1 (ppm)


162.631
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147.233
146.743
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137.322
132.913
127.826
126.761
125.814
125.351
123.717
123.690
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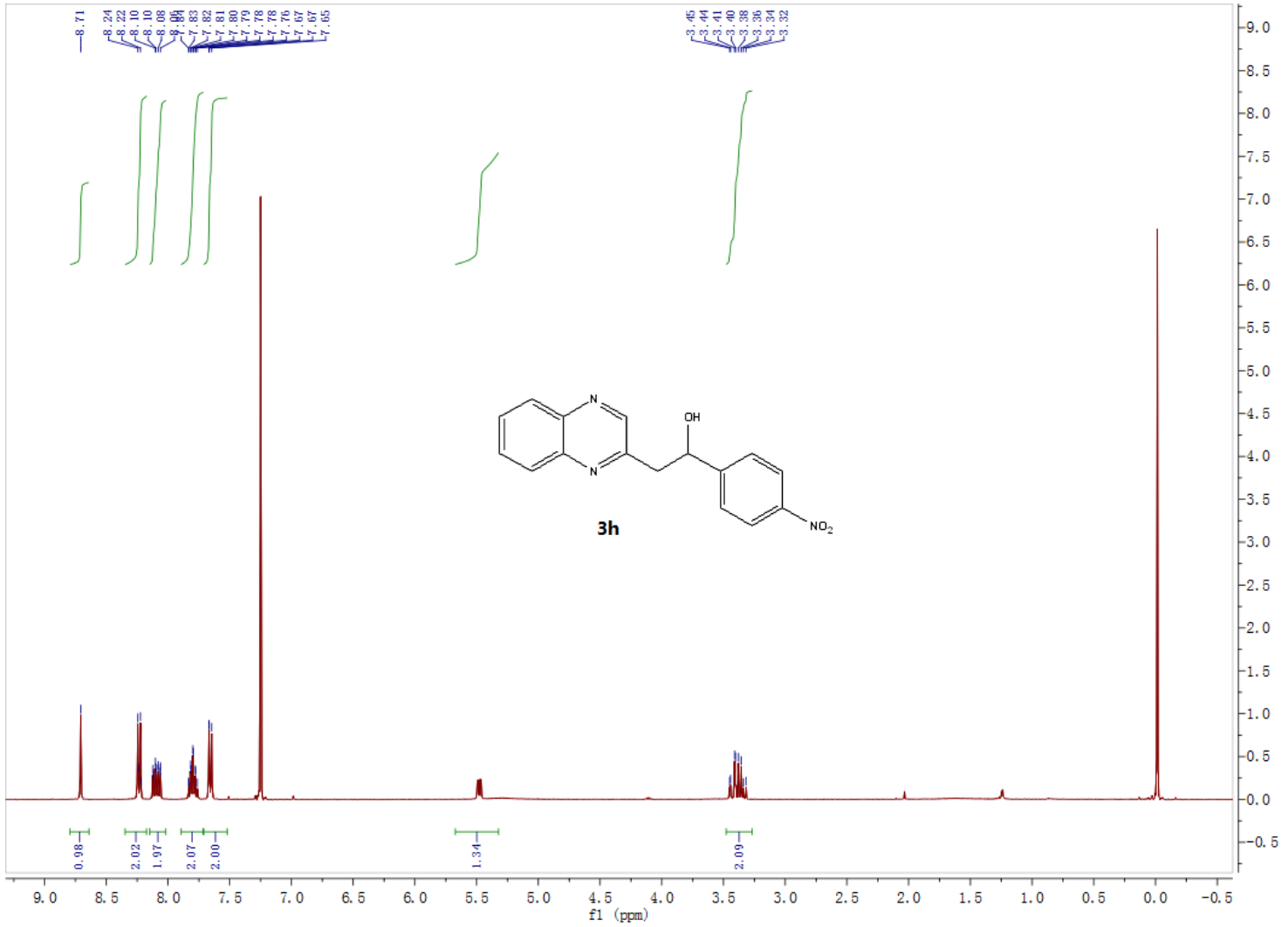
77.327
77.123
76.700
71.504
45.600
OH
N
NO2
NO2
3q
f1 (ppm)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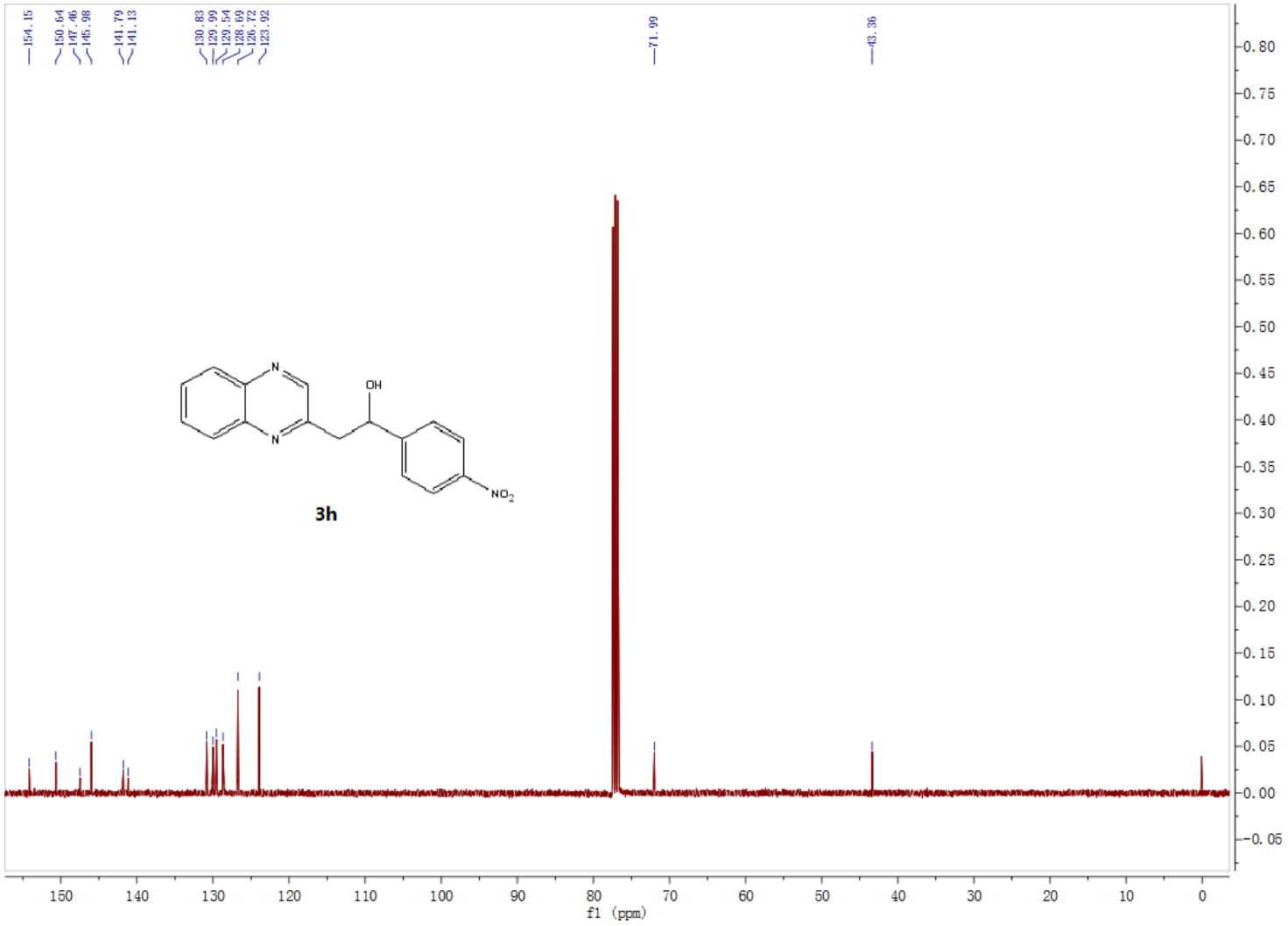
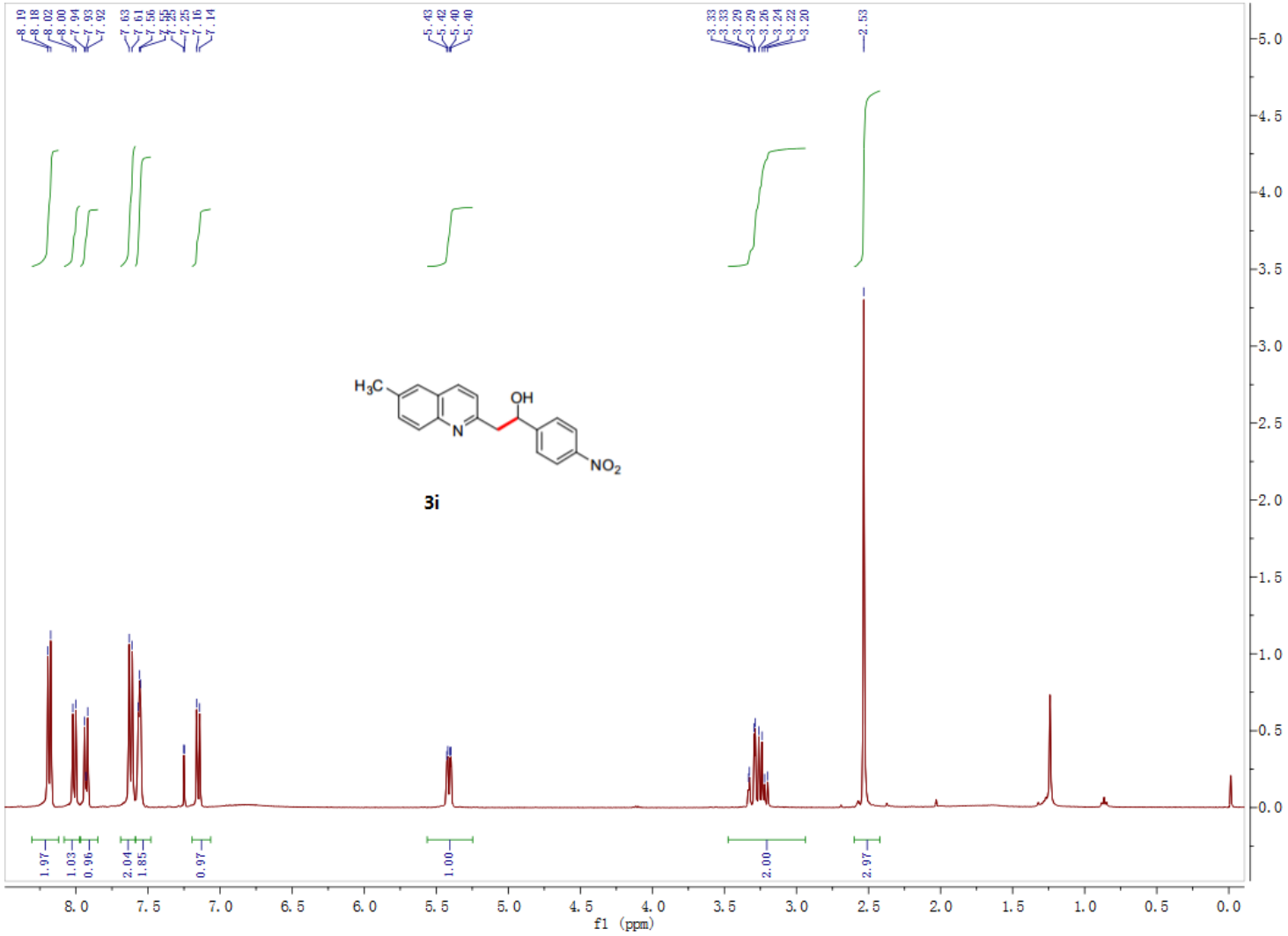
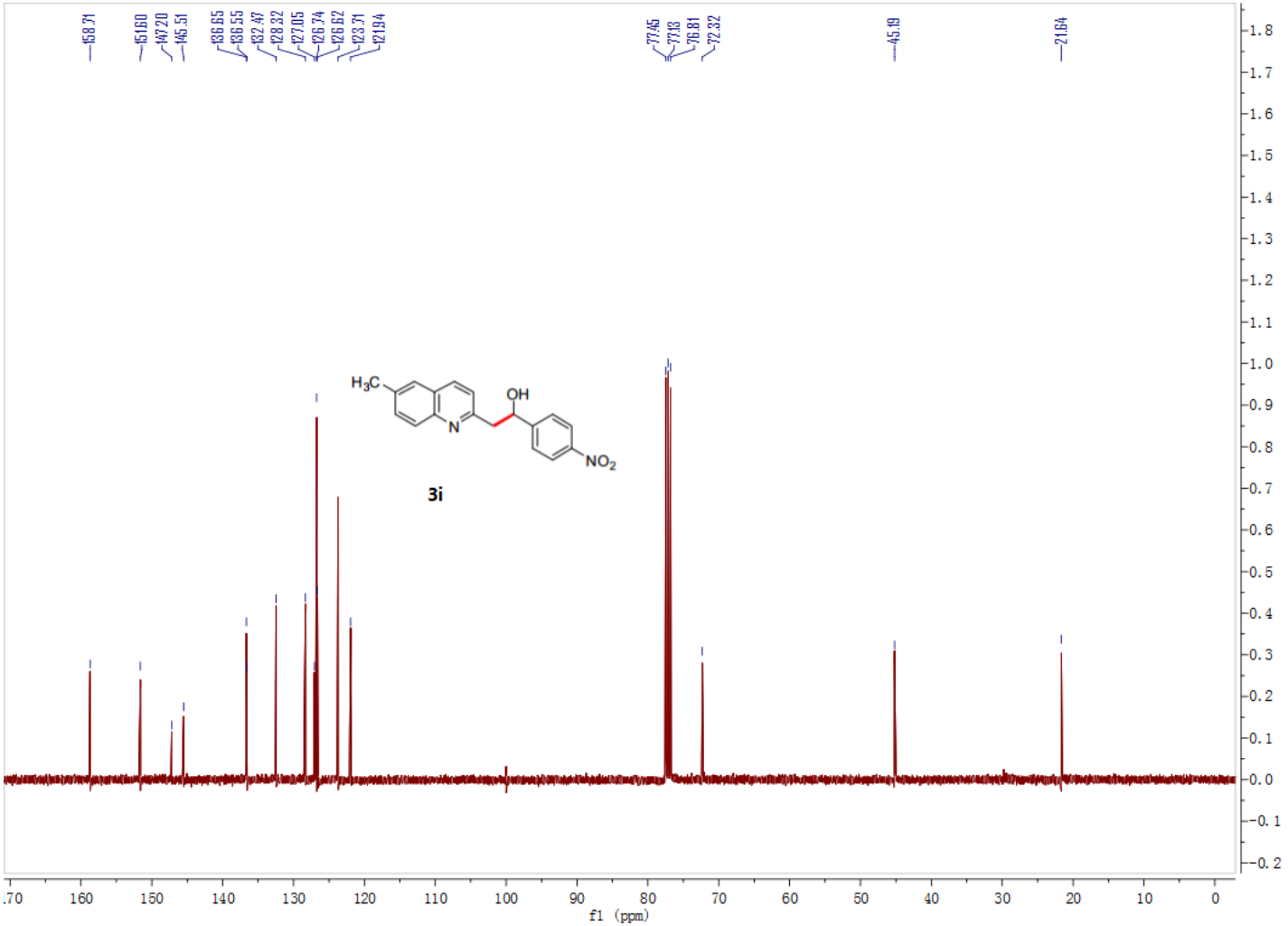
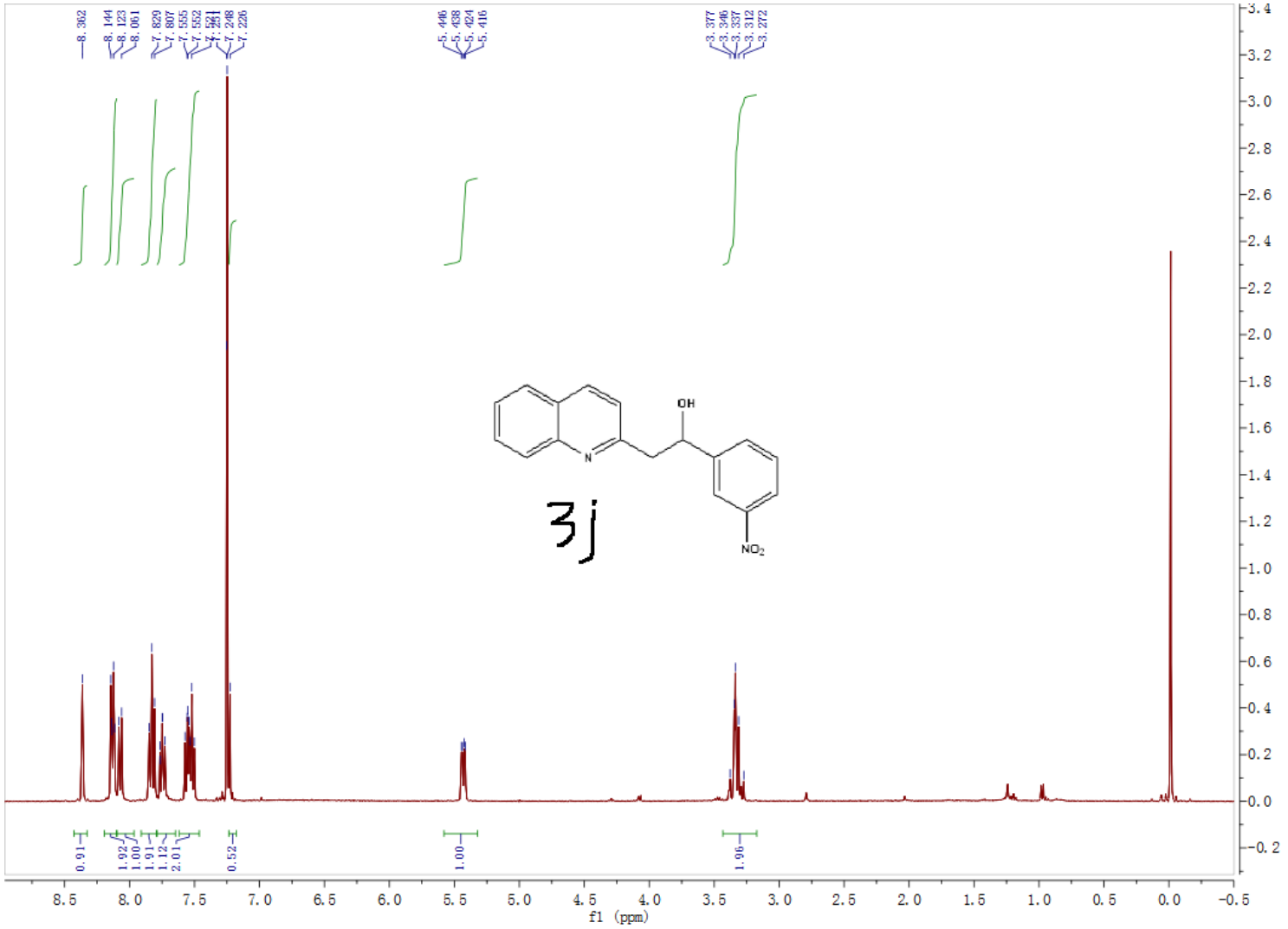
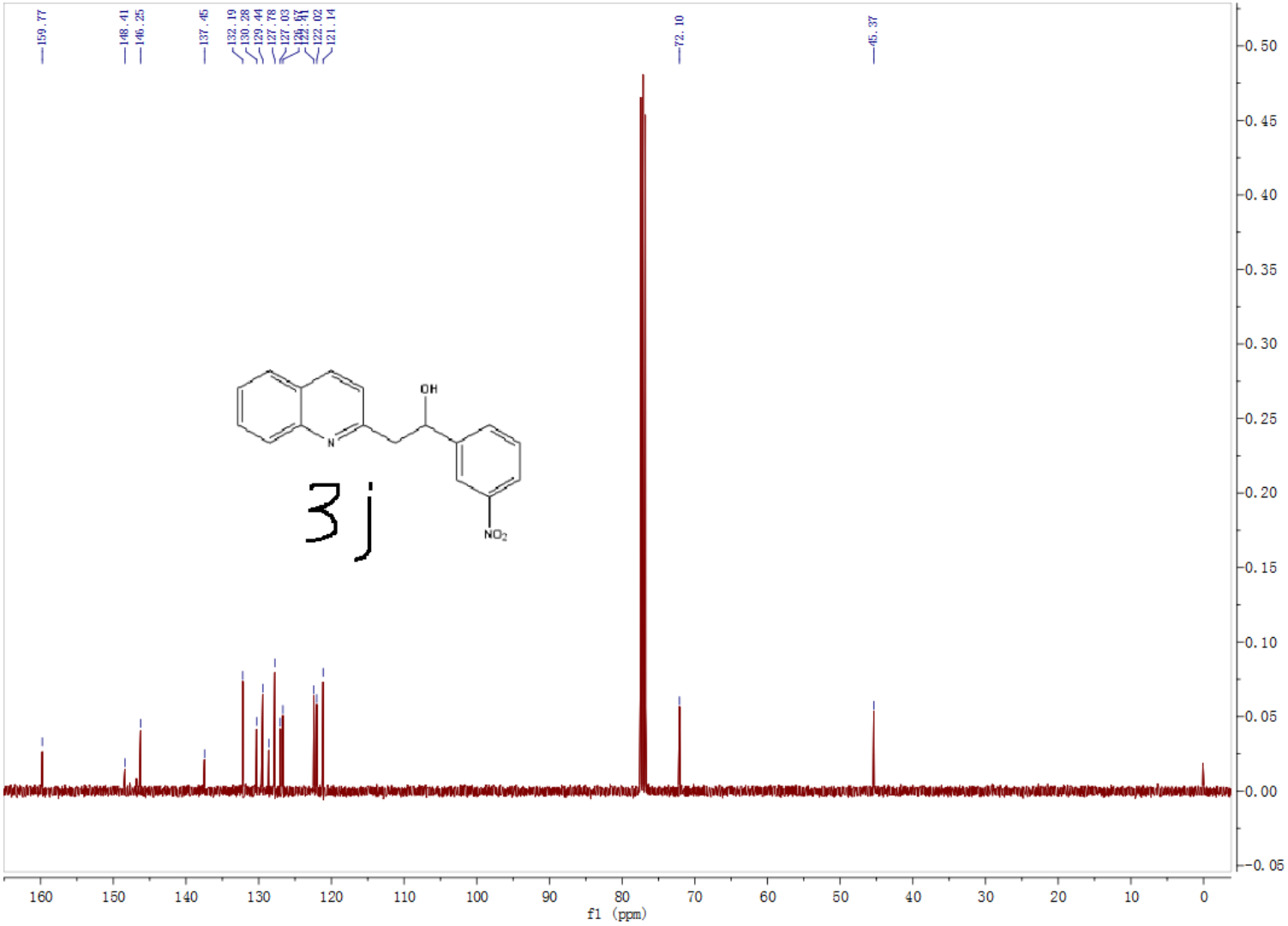
8.24
8.22
8.10
8.10
8.08
8.08
7.83
7.82
7.81
7.80
7.79
7.78
7.78
7.76
7.67
7.67
7.65
3.45
3.44
3.41
3.40
3.38
3.36
3.34
3.32
N
N
OH
NO2
3h
0.98
2.02
1.97
2.07
2.00
1.34
2.09
f1 (ppm)


154.15
150.64
147.46
145.98
141.79
141.13
130.83
129.99
129.54
128.69
126.72
123.92
71.99
43.36
OH
N
N
NO2
3h
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.19
8.18
8.02
8.00
7.94
7.93
7.92
7.63
7.61
7.56
7.55
7.25
7.16
7.14
5.43
5.42
5.40
5.40
3.33
3.33
3.29
3.29
3.26
3.24
3.22
3.20
2.53
H3C
OH
N
NO2
3i
1.97
1.03
0.96
2.04
1.85
0.97
1.00
2.00
2.97
f1 (ppm)


158.71
151.60
147.20
145.51
136.65
135.55
132.47
128.32
127.05
126.74
126.62
123.71
121.94
77.45
77.13
76.81
72.32
45.19
21.64
H3C
OH
N
NO2
3i
f1 (ppm)


8.362
8.144
8.123
8.061
7.829
7.807
7.555
7.552
7.521
7.248
7.226
5.446
5.438
5.424
5.416
3.377
3.346
3.337
3.312
3.272
OH
N
NO2
3j
0.91
1.92
1.00
1.91
1.12
2.01
0.52
1.00
1.96
f1 (ppm)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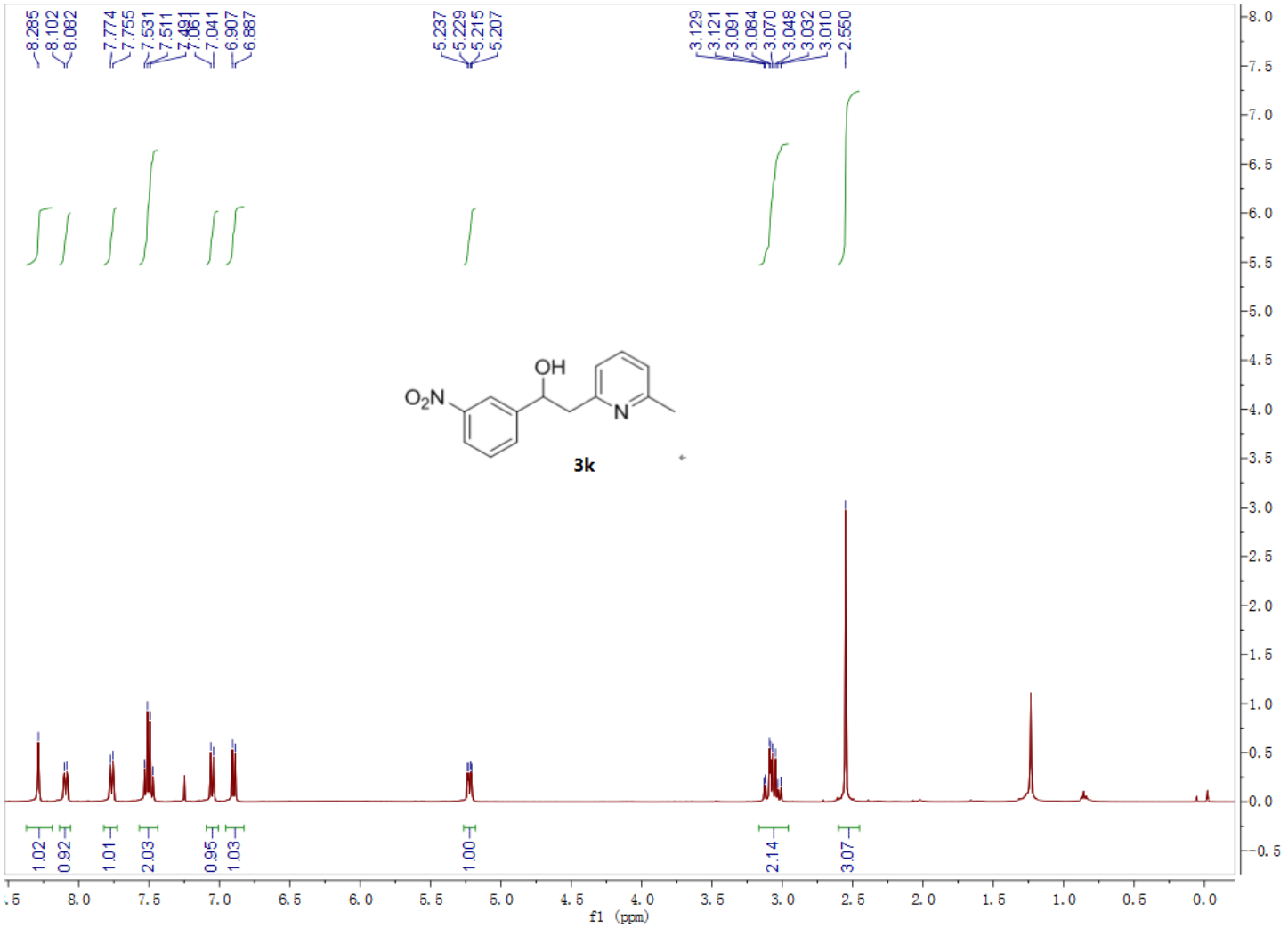
148.41
146.25
137.45
132.19
130.28
129.44
127.78
127.03
126.67
122.41
122.02
121.14
72.10
45.37
OH
N
NO2
3j
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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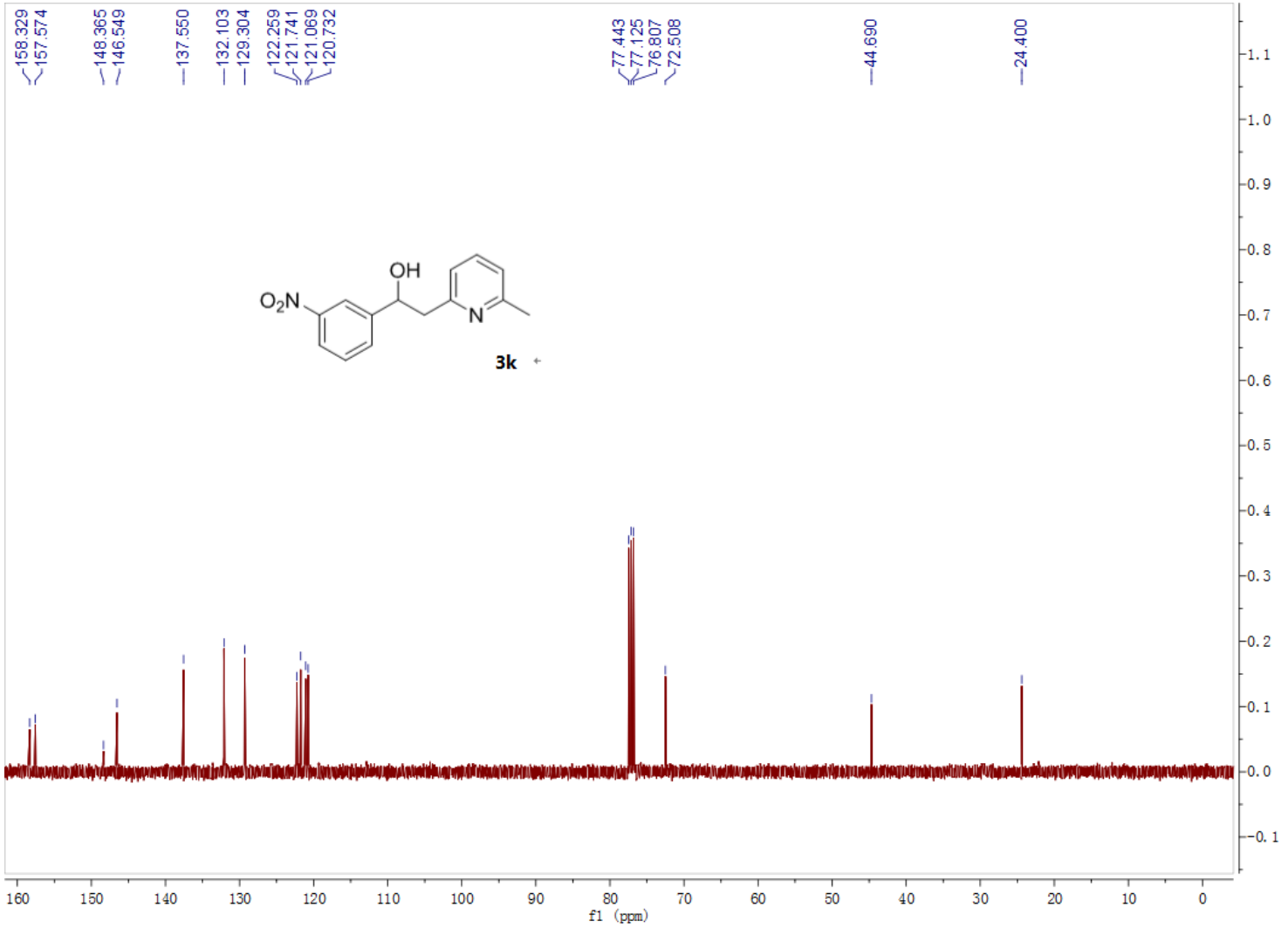
8.102
8.082
7.774
7.755
7.531
7.511
7.481
7.461
7.041
6.907
6.887
5.237
5.229
5.215
5.207
3.129
3.121
3.091
3.084
3.070
3.048
3.032
3.010
2.550
OH
O2N
N
3k
1.02
0.92
1.01
2.03
0.95
1.03
1.00
2.14
3.07
f1 (ppm)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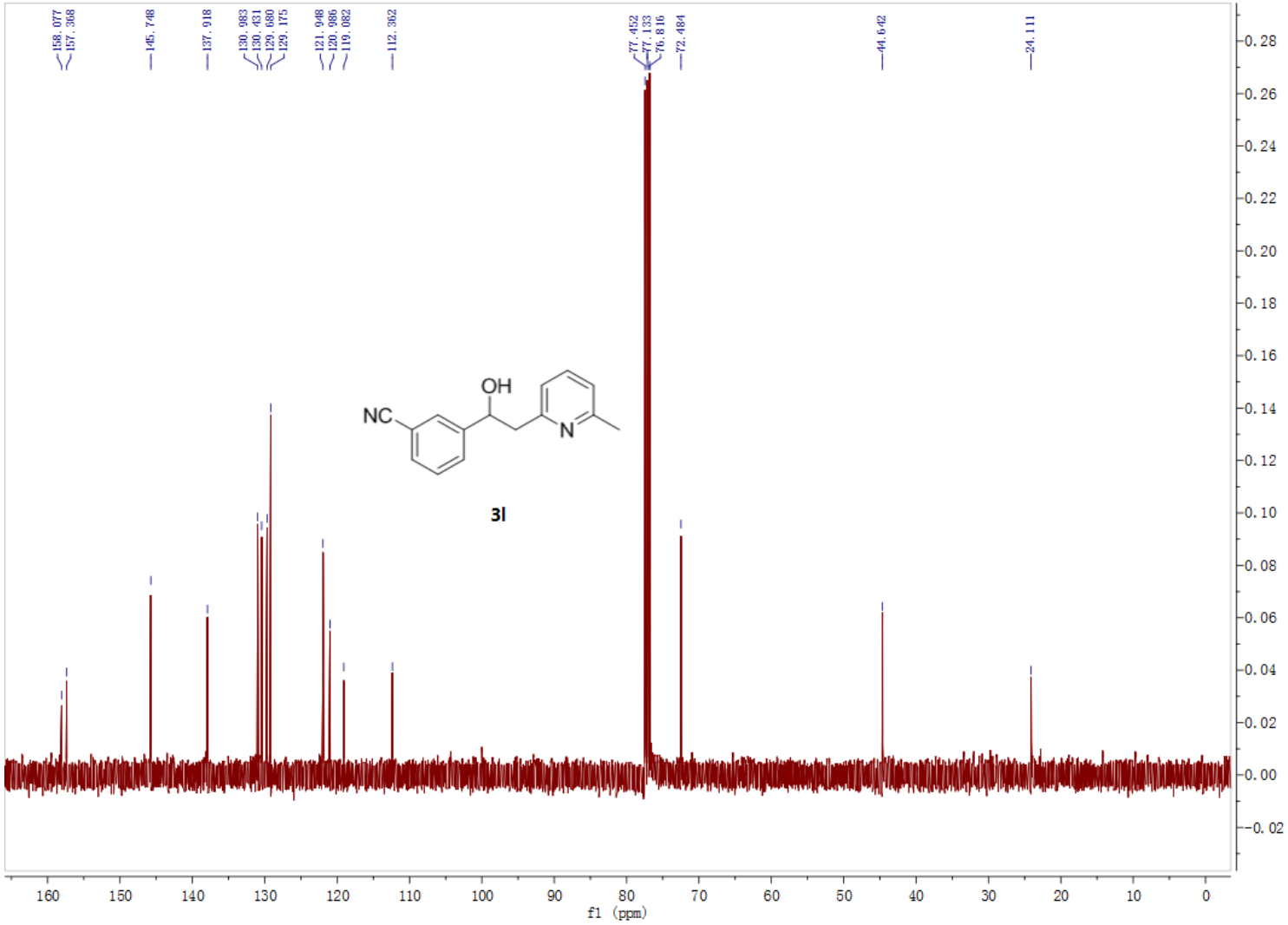
146.549
137.550
132.103
129.304
122.259
121.741
121.069
120.732
77.443
77.125
76.807
72.508
44.690
24.400
OH
O_2N
N
3k
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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145.748
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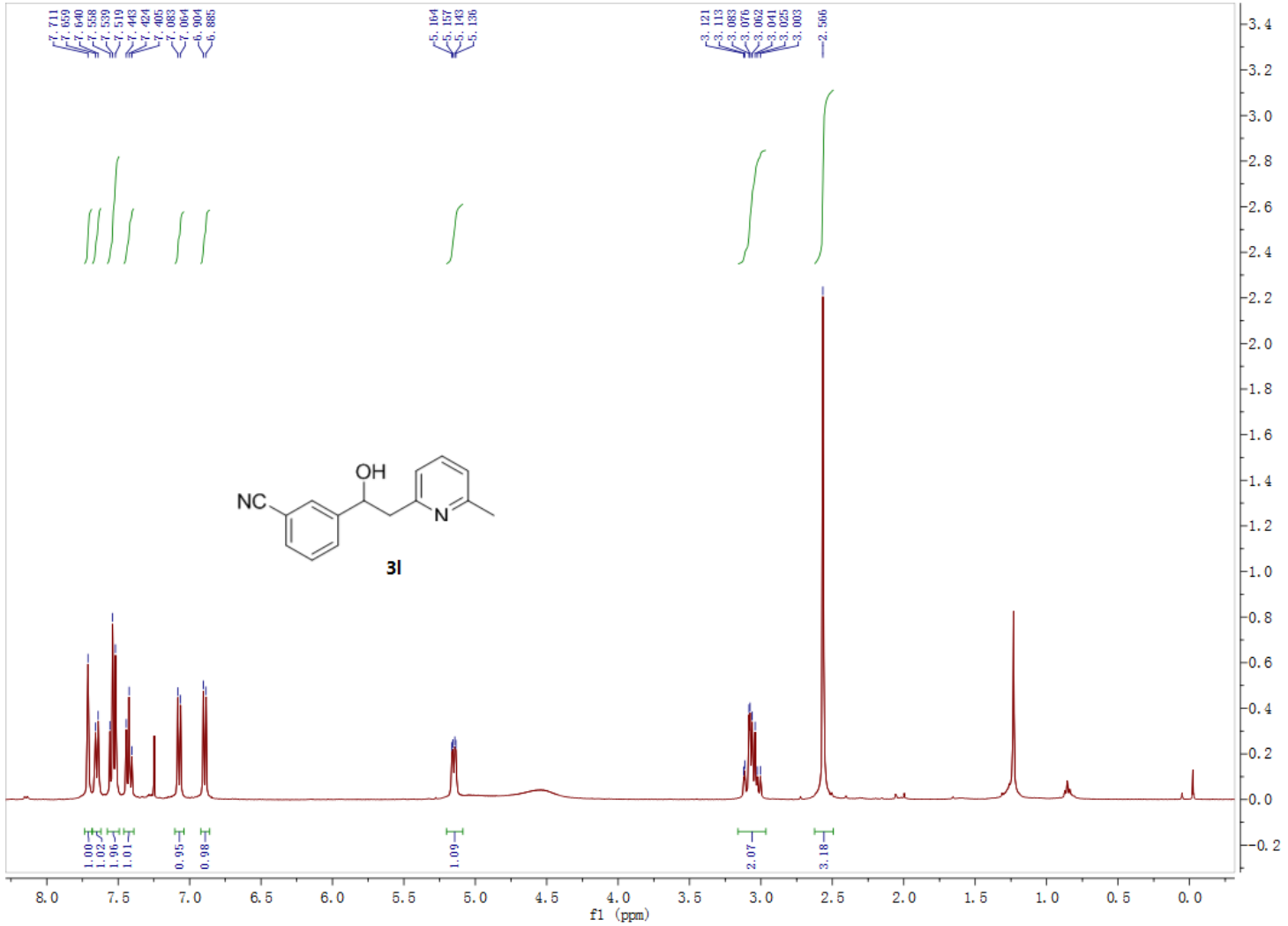
130.431
129.680
129.175
121.948
120.986
119.082
112.362
77.452
77.133
76.816
72.484
44.642
24.111
OH
NC
N
3l
f1 (ppm)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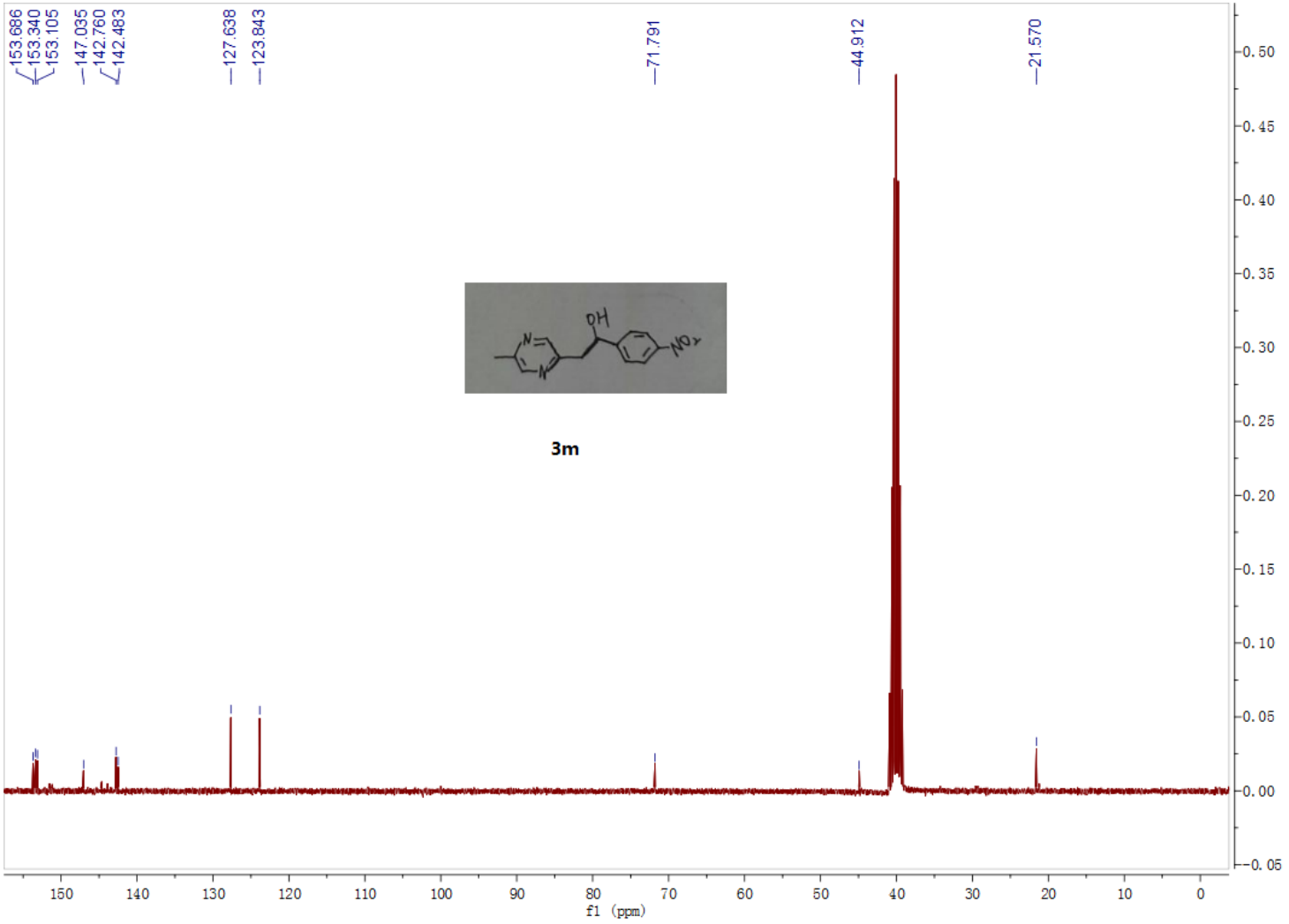
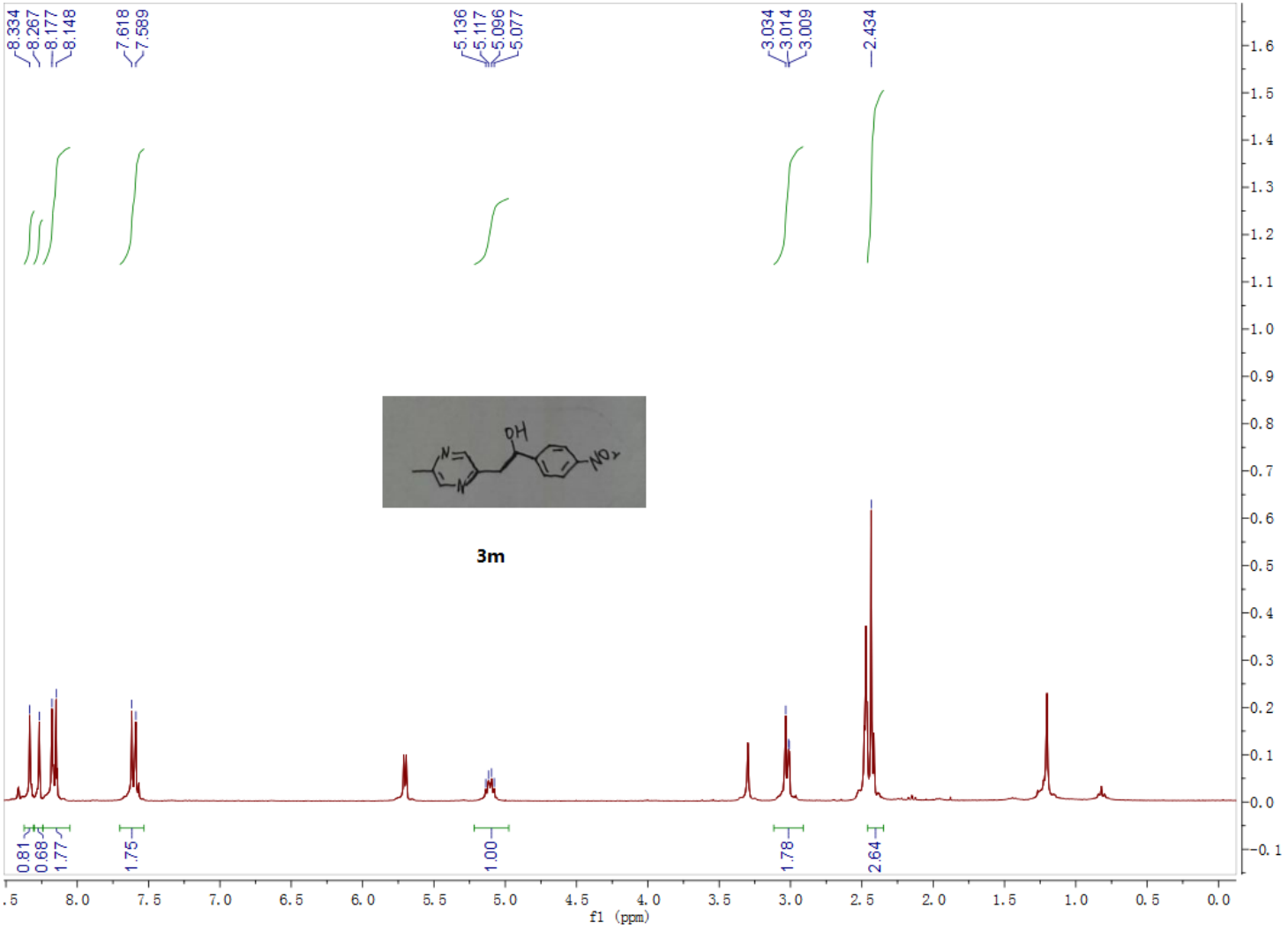
7.659
7.640
7.558
7.539
7.519
7.443
7.424
7.405
7.083
7.064
6.904
6.885
5.164
5.157
5.143
5.136
3.121
3.113
3.083
3.076
3.062
3.041
3.025
3.003
2.566
OH
NC
N
3l
1.00
1.02
1.96
1.01
0.95
0.98
1.09
2.07
3.18
f1 (ppm)


153.686
153.340
153.105
147.035
142.760
142.483
127.638
123.843
71.791
44.912
21.570
OH
NO2
3m
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.267
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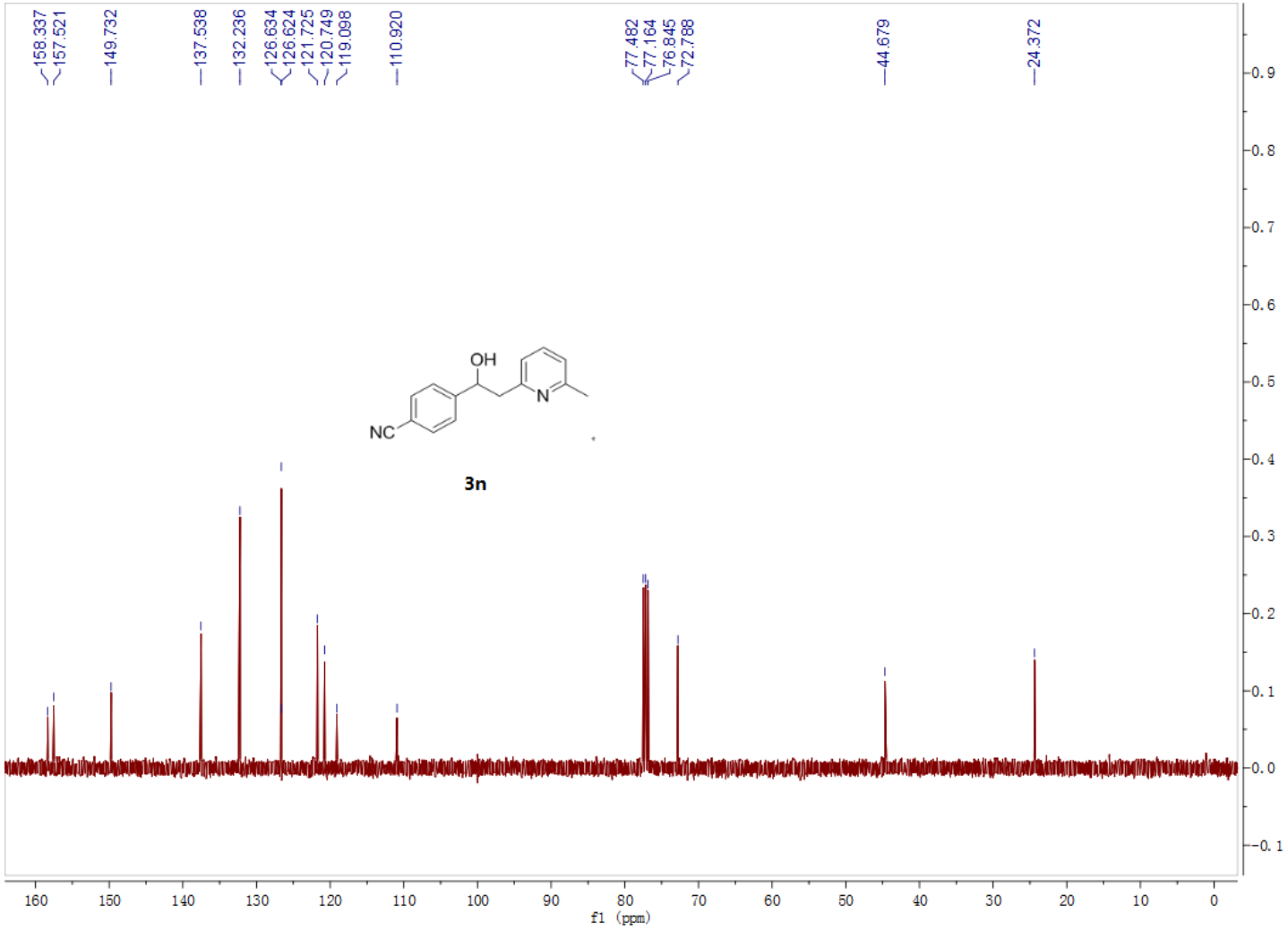
8.148
7.618
7.589
5.136
5.117
5.096
5.077
3.034
3.014
3.009
2.434
OH
NO2
N
N
3m
0.81
0.68
1.77
1.75
1.00
1.78
2.64
f1 (ppm)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132.236
126.634
126.624
121.725
120.749
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76.845
72.788
44.679
24.372
OH
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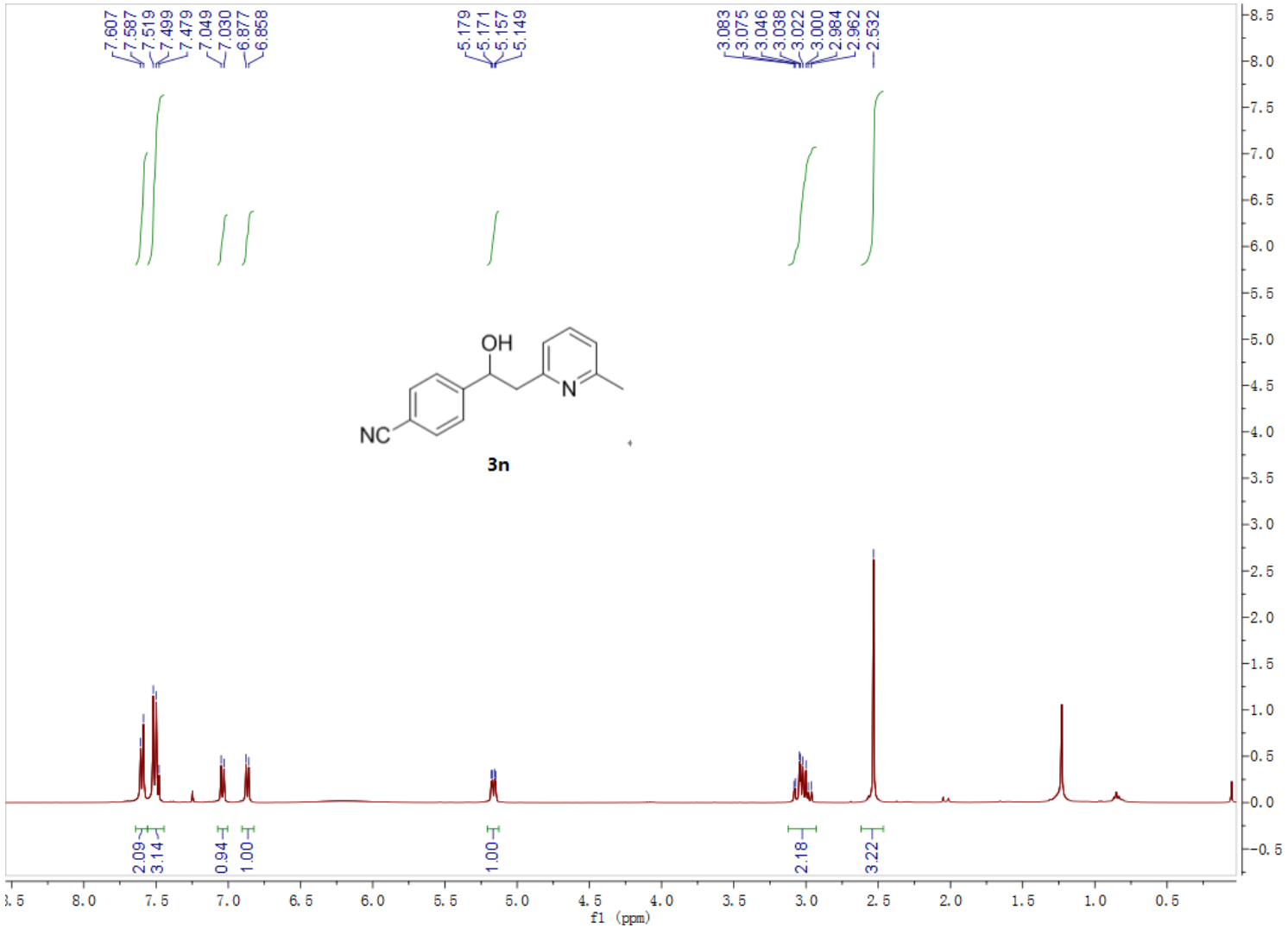
NC
3n
f1 (ppm)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7.587
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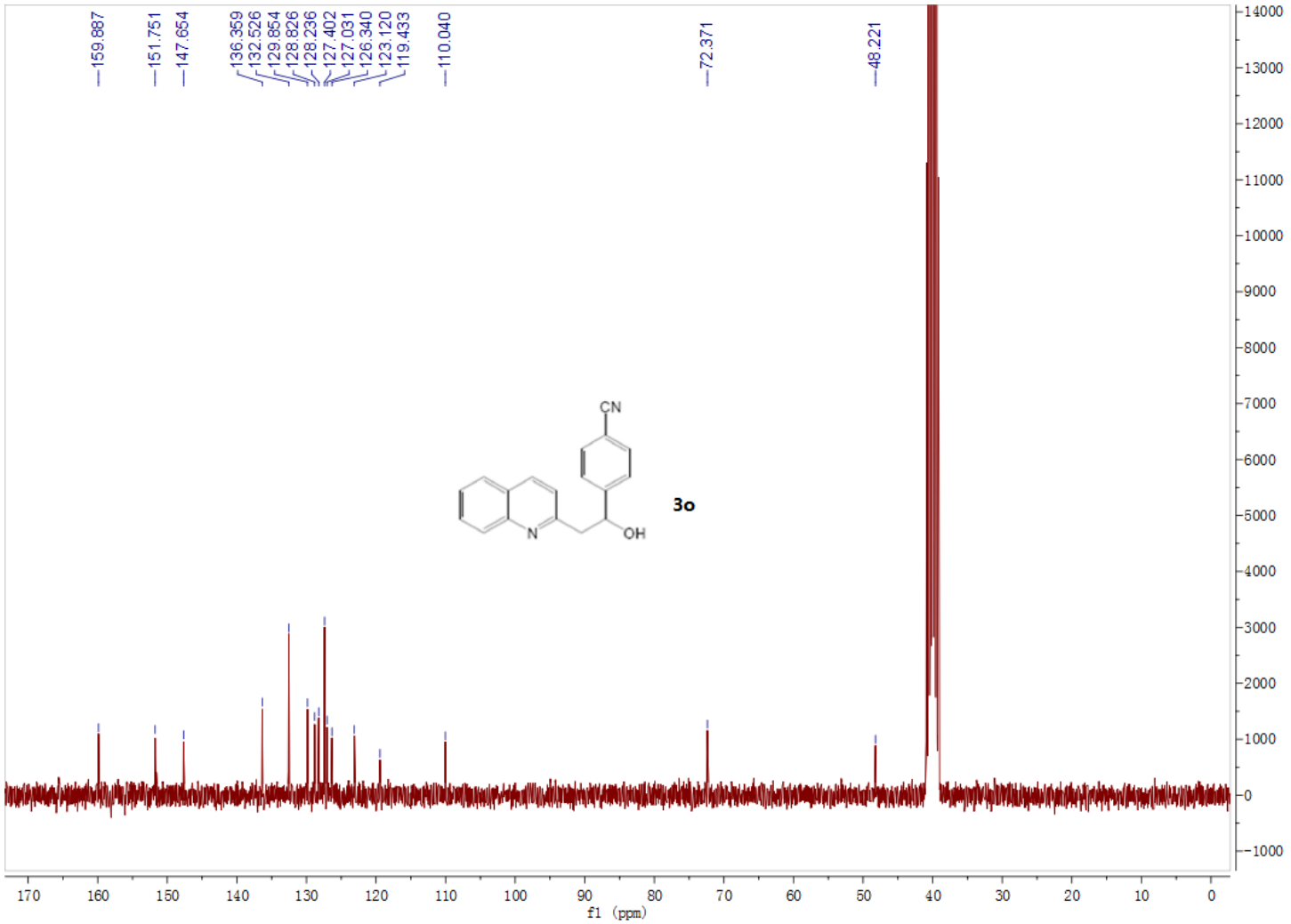
7.499
7.479
7.049
7.030
6.877
6.858
5.179
5.171
5.157
5.149
3.083
3.075
3.046
3.038
3.022
3.000
2.984
2.962
2.532
OH
N
NC
3n
2.09
3.14
0.94
1.00
1.00
2.18
3.22
f1 (ppm)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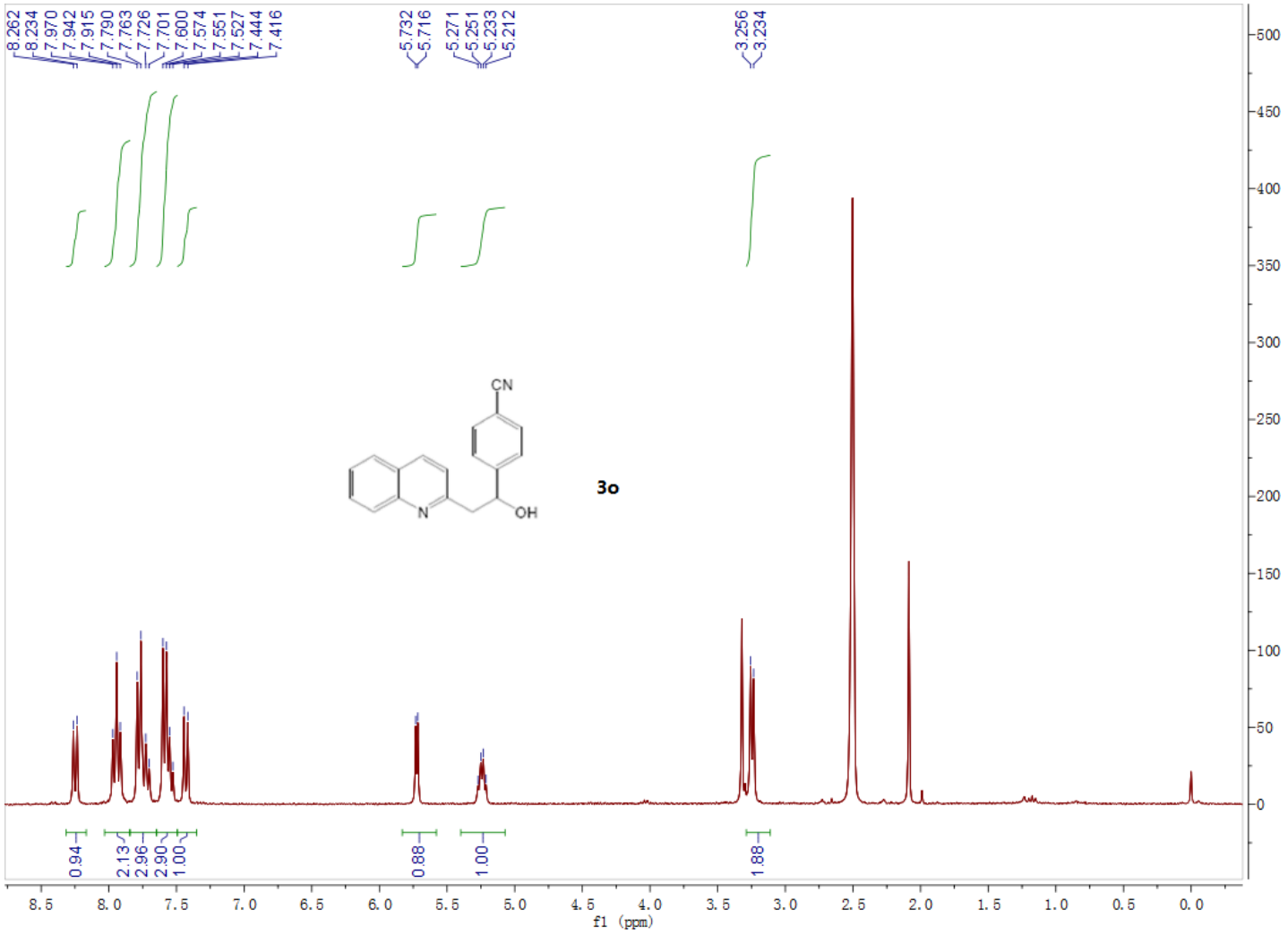
136.359
132.526
129.854
128.826
128.236
127.402
127.031
126.340
123.120
119.433
110.040
72.371
48.221
CN
N
OH
3o
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.915
7.790
7.763
7.726
7.701
7.600
7.574
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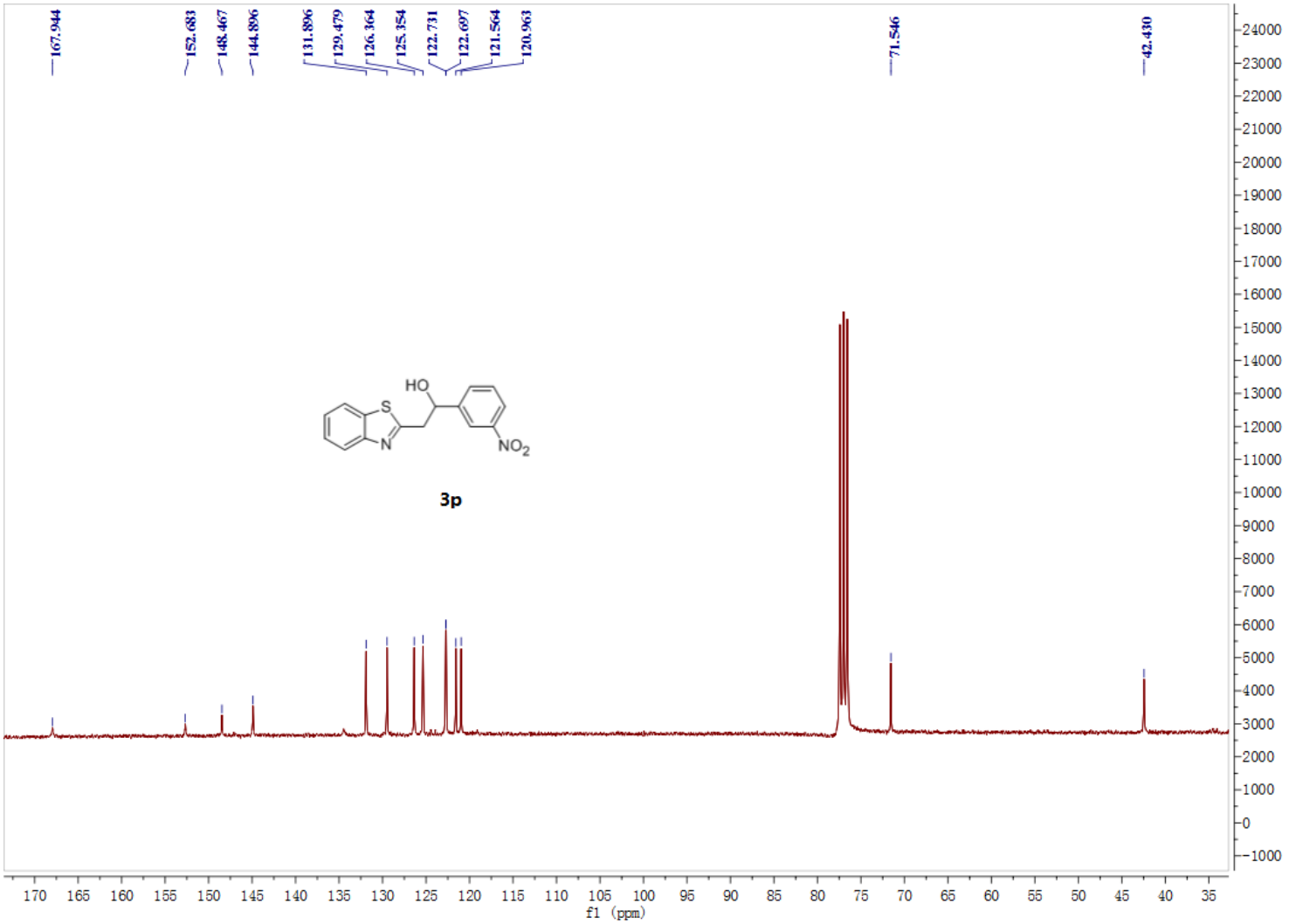
7.527
7.444
7.416
5.732
5.716
5.271
5.251
5.233
5.212
3.256
3.234
CN
N
OH
3o
0.94
2.13
2.96
2.90
1.00
0.88
1.00
1.88
f1 (ppm)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152.683
148.467
144.896
131.896
129.479
126.364
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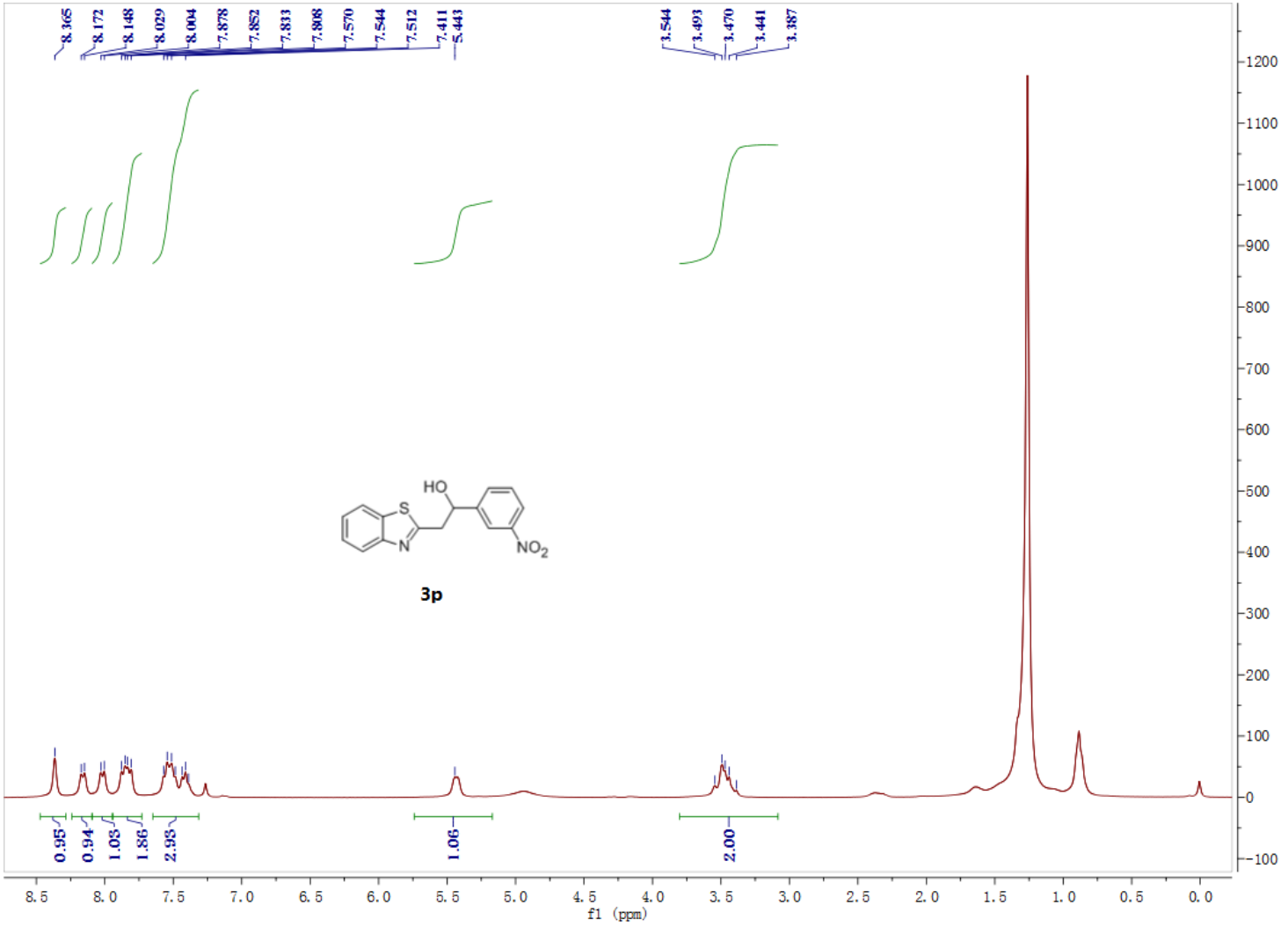
122.697
121.564
120.963
71.546
42.430
HO
S
N
NO2
3p
f1 (ppm)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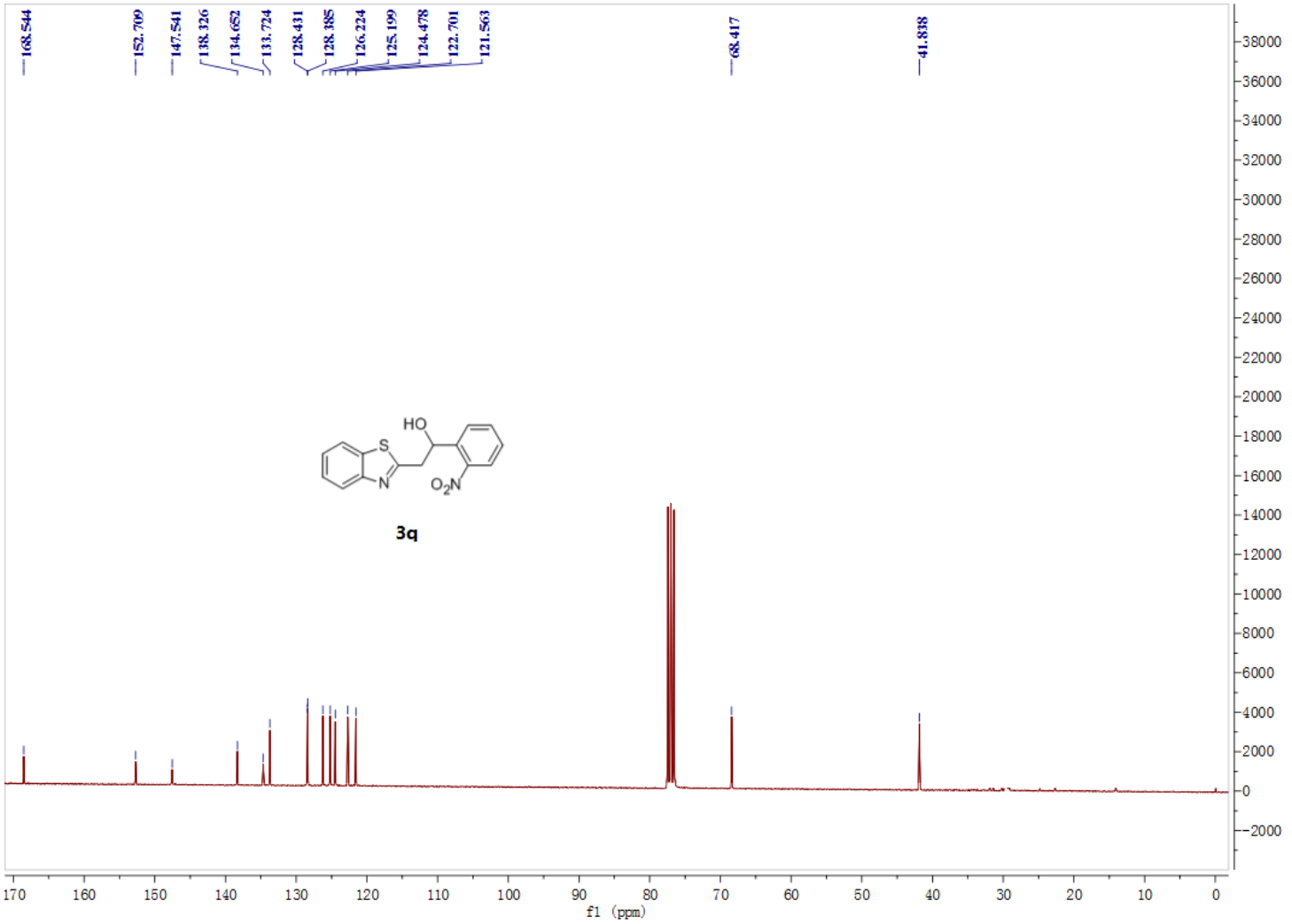
8.172
8.148
8.029
8.004
7.878
7.852
7.833
7.808
7.570
7.544
7.512
7.411
5.443
3.544
3.493
3.470
3.441
3.387
HO
S
N
NO2
3p
0.95
0.94
1.03
1.86
2.93
1.06
2.00
f1 (ppm)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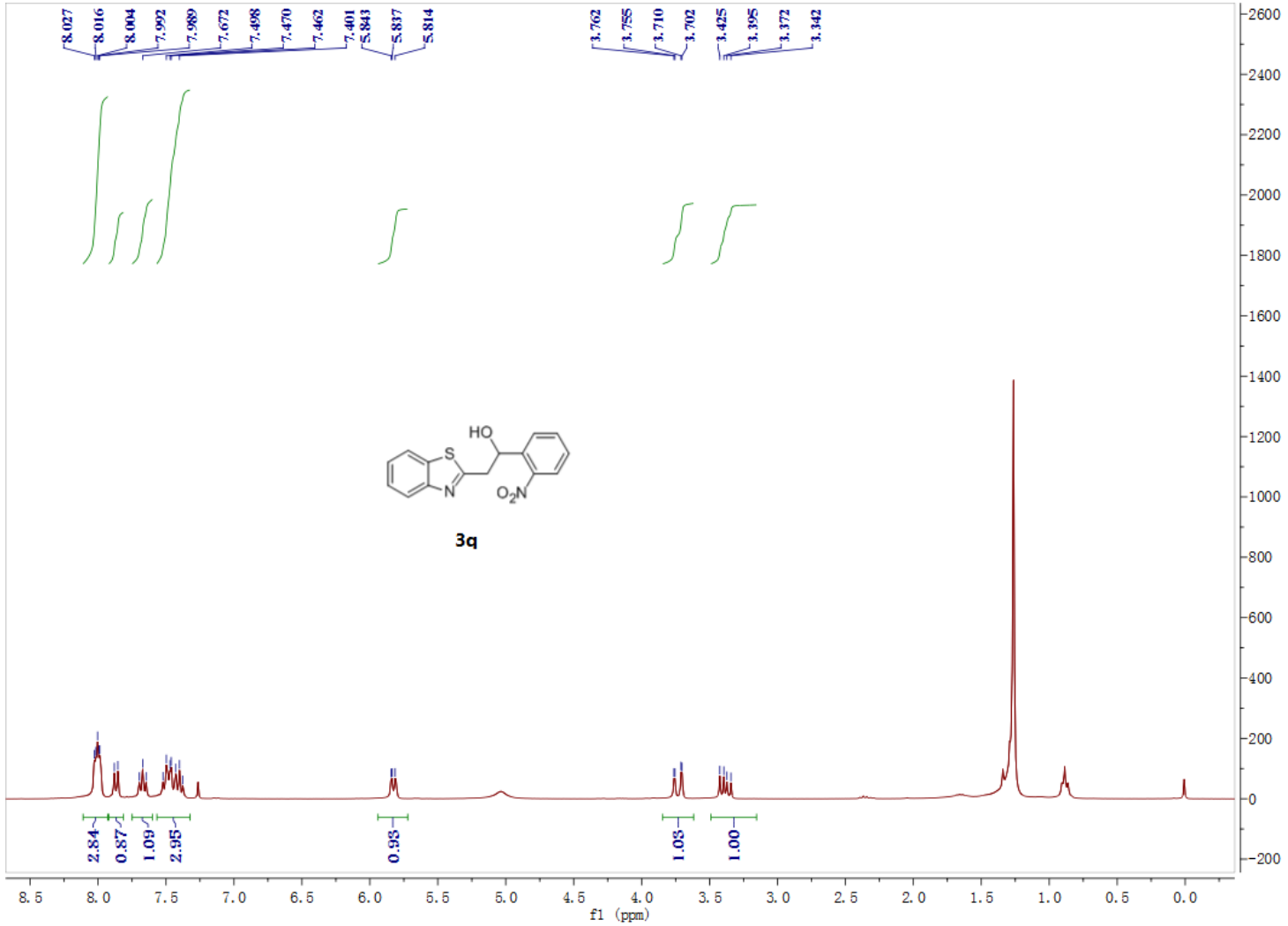
147.541
138.326
134.652
133.724
128.431
128.385
126.224
125.199
124.478
122.701
121.563
68.417
41.838
HO
S
N
O2N
3q
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.027
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7.672
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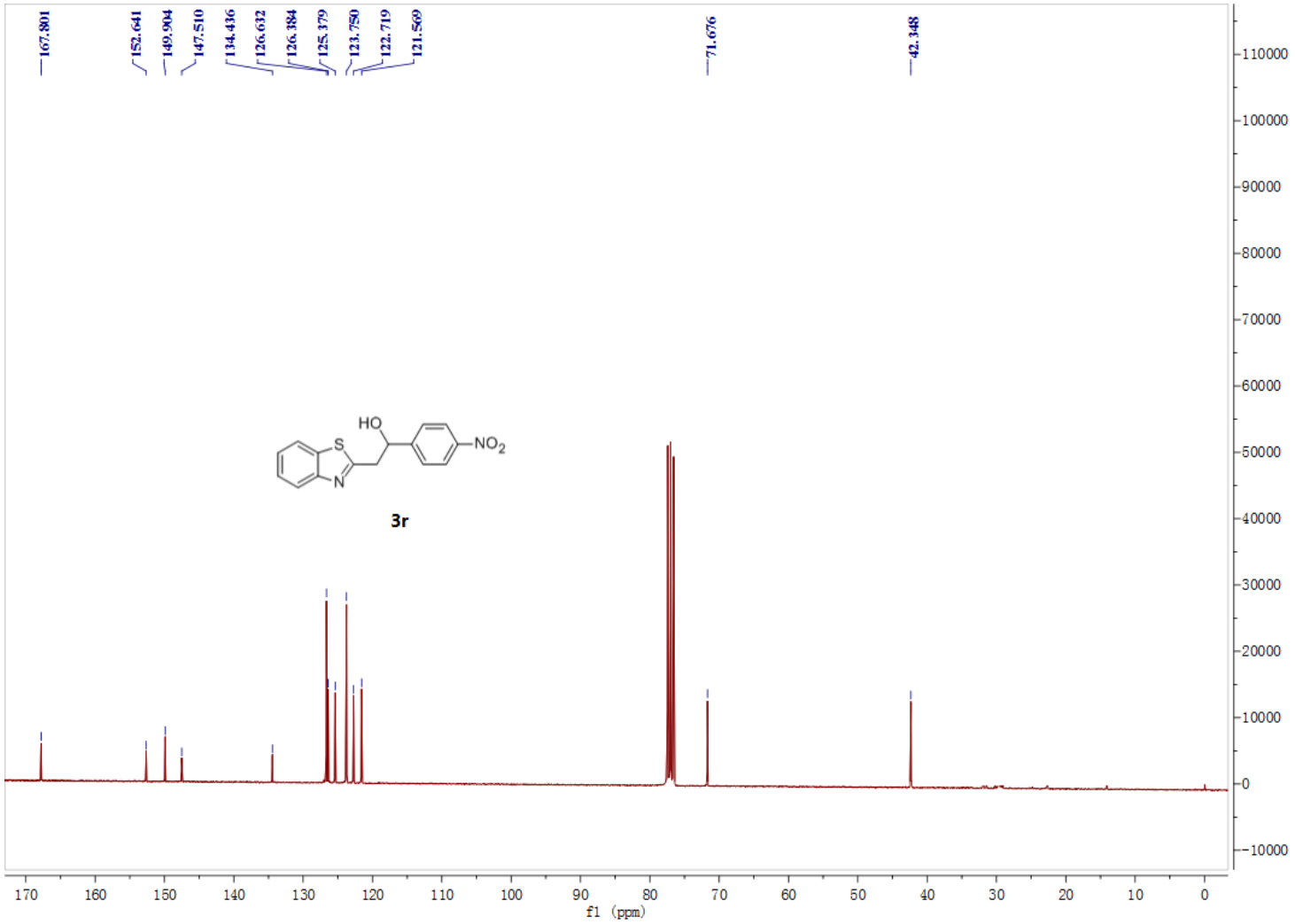
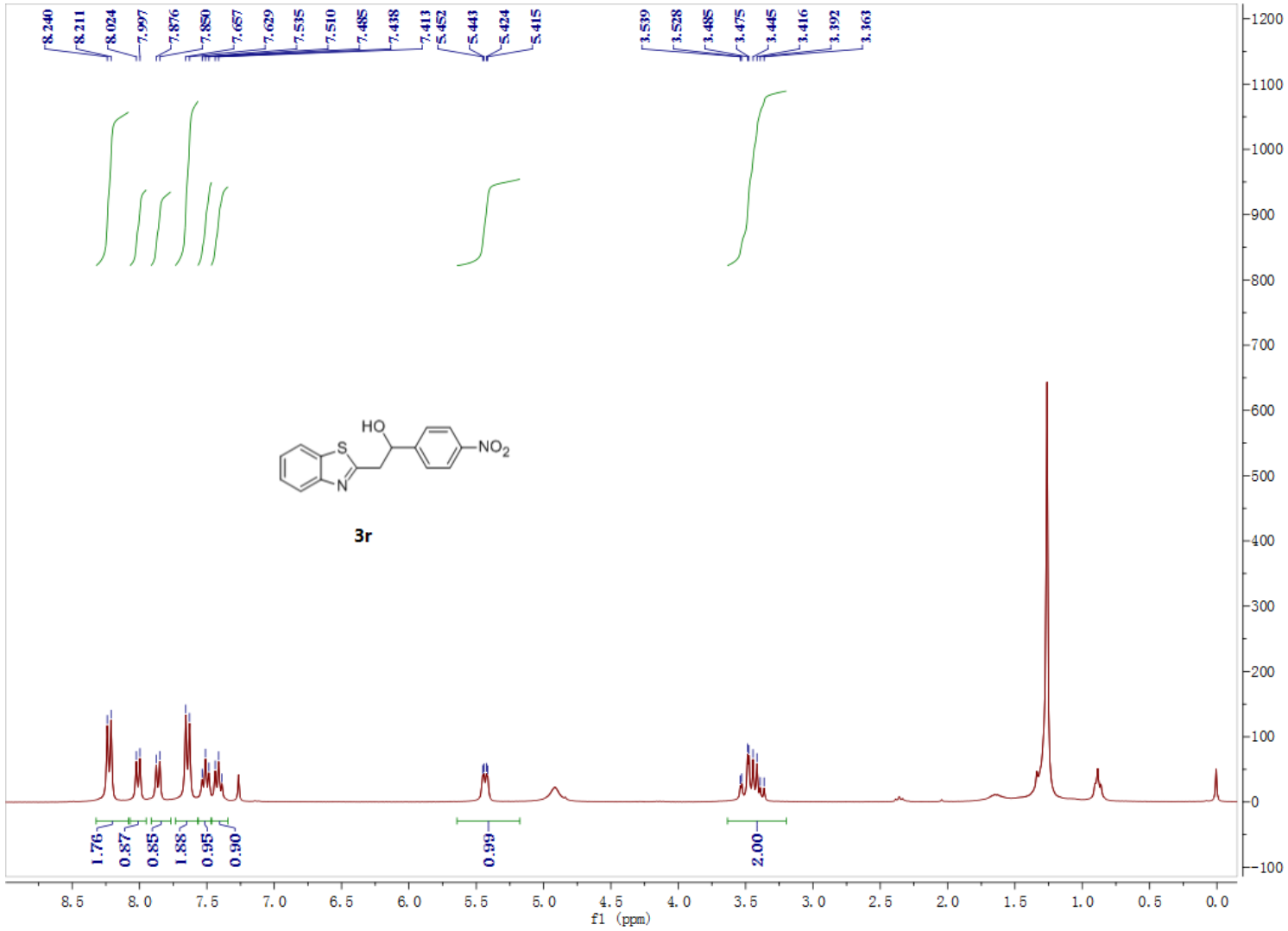
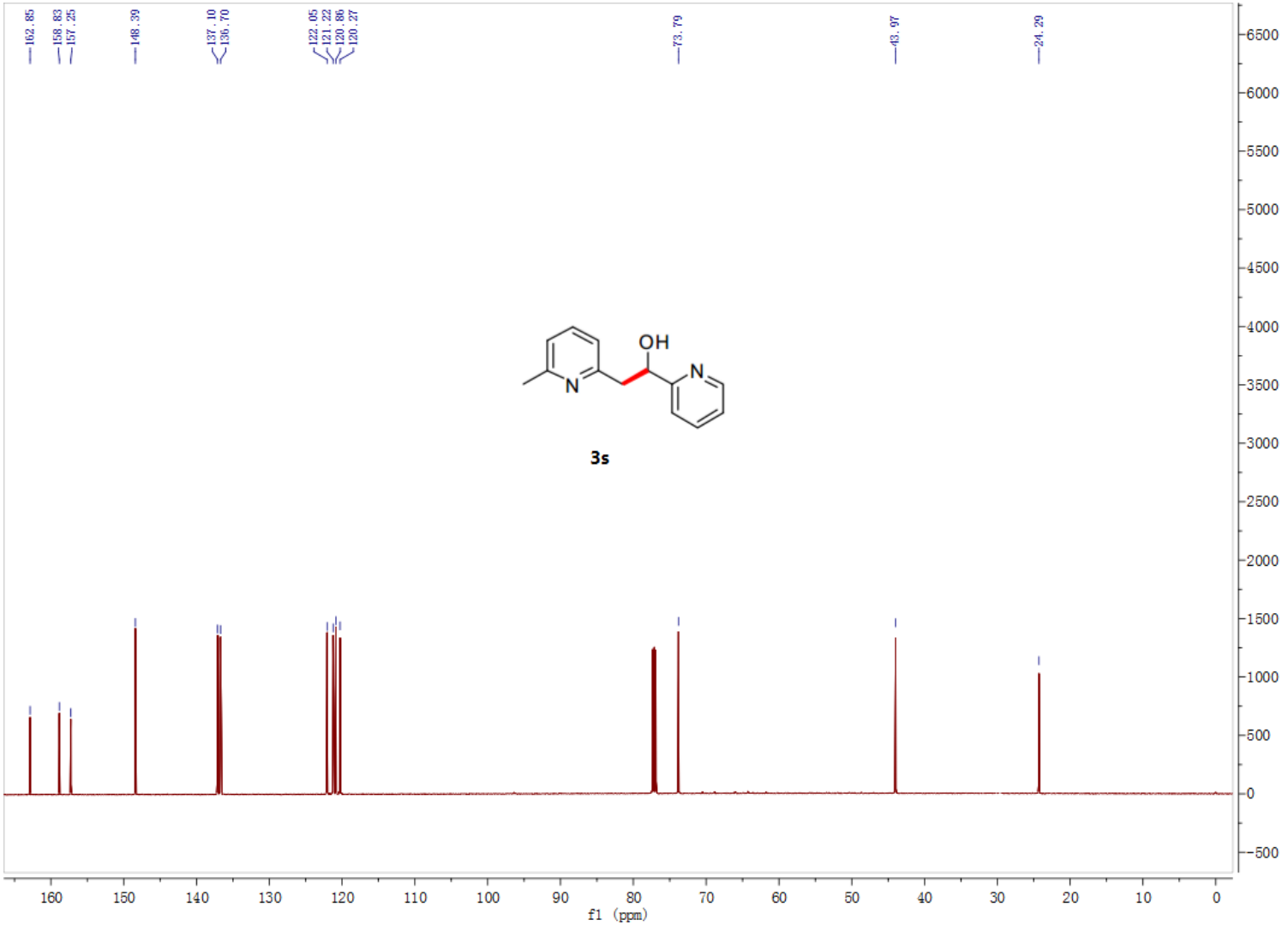
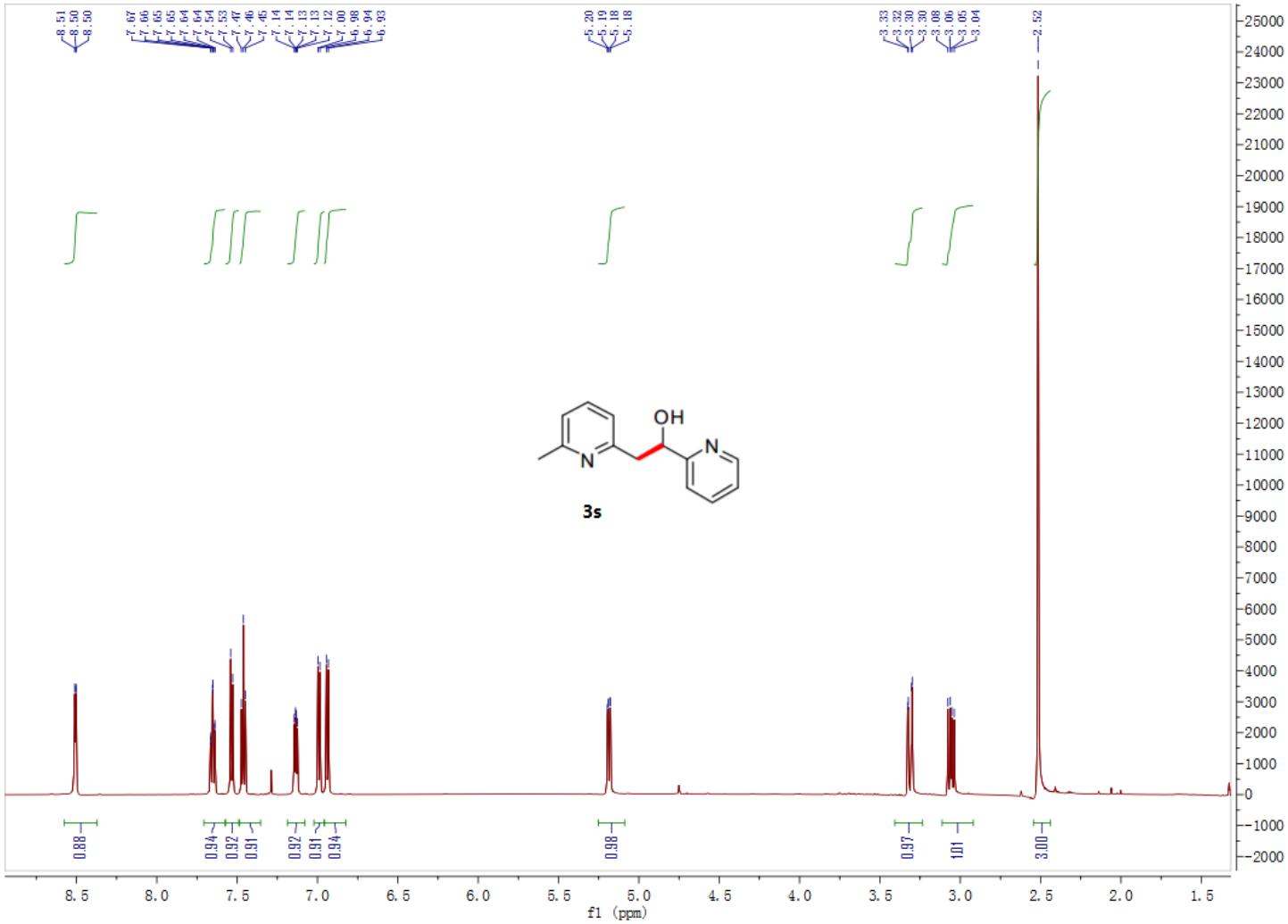
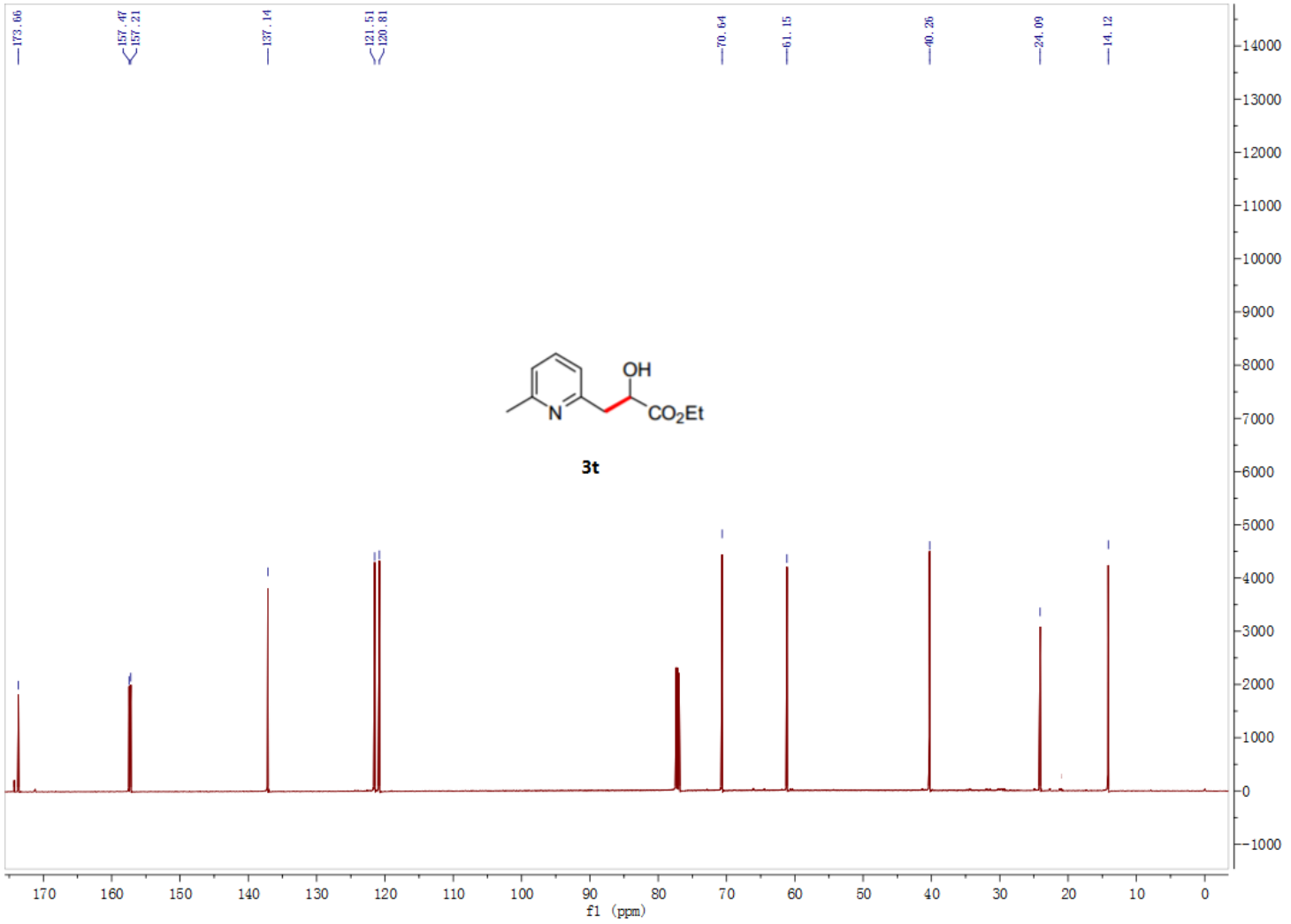
7.470
7.462
7.401
5.843
5.837
5.814
3.762
3.755
3.710
3.702
3.425
3.395
3.372
3.342
HO
S
N
O2N
3q
2.84
0.87
1.09
2.95
0.93
1.03
1.00
f1 (ppm)

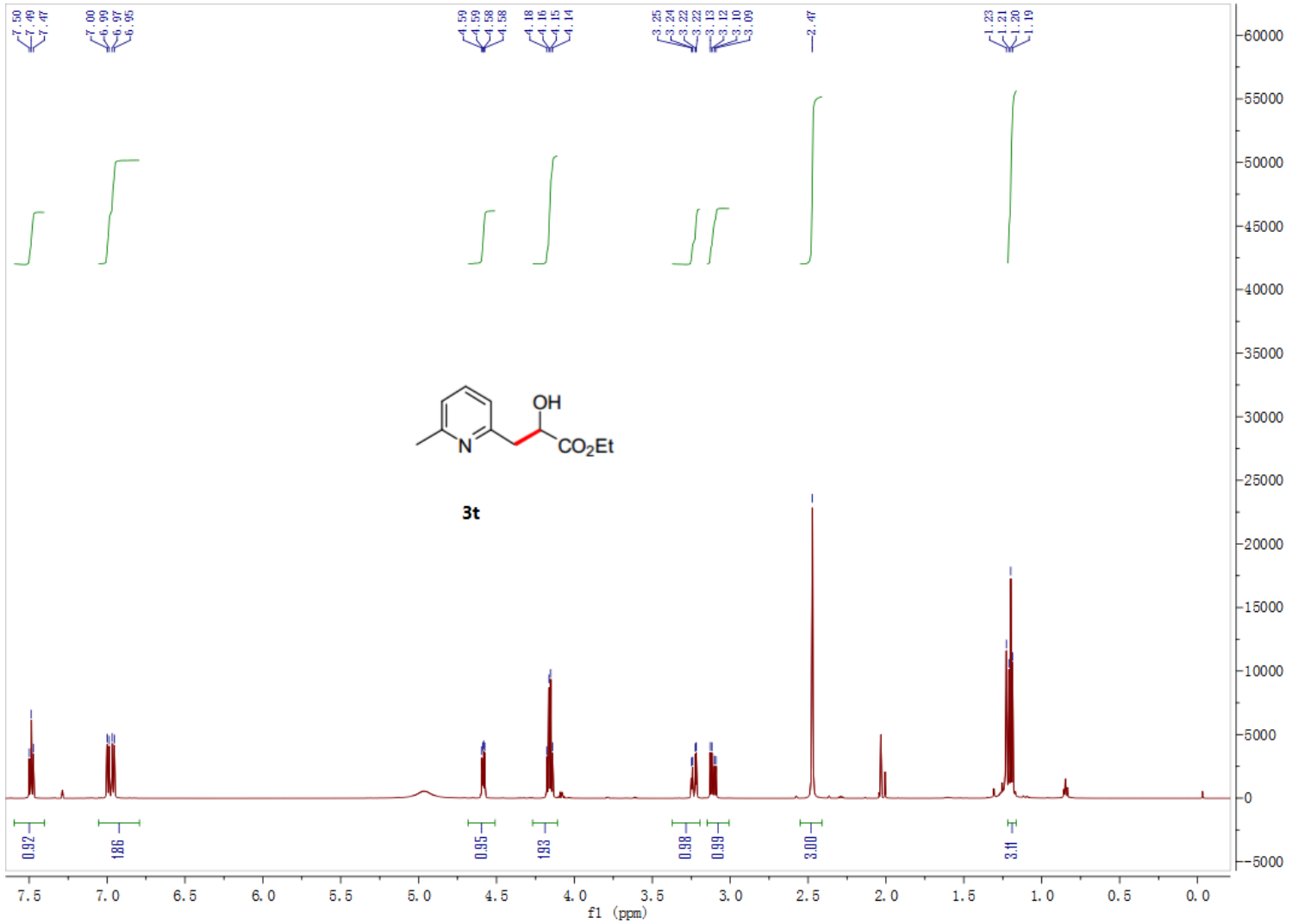

167.801
152.641
149.904
147.510
134.436
126.632
126.384
125.379
123.750
122.719
121.569
71.676
42.348
HO
S
N
NO2
3r
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

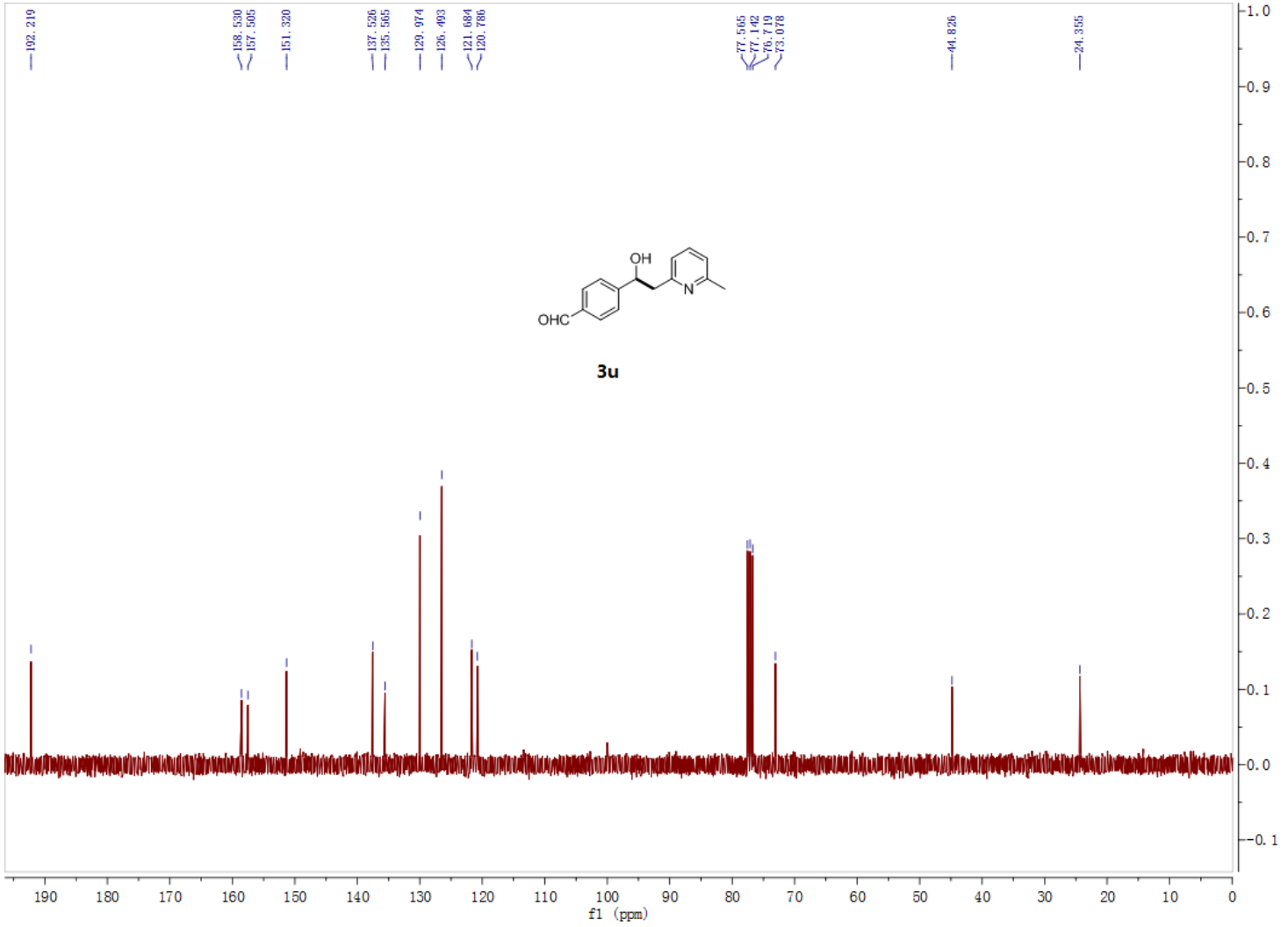

8.240
8.211
8.024
7.997
7.876
7.850
7.657
7.629
7.535
7.510
7.485
7.438
7.413
5.452
5.443
5.424
5.415
3.539
3.528
3.485
3.475
3.445
3.416
3.392
3.363
HO
S
N
NO2
3r
1.76
0.87
0.85
1.88
0.95
0.90
0.99
2.00
f1 (ppm)

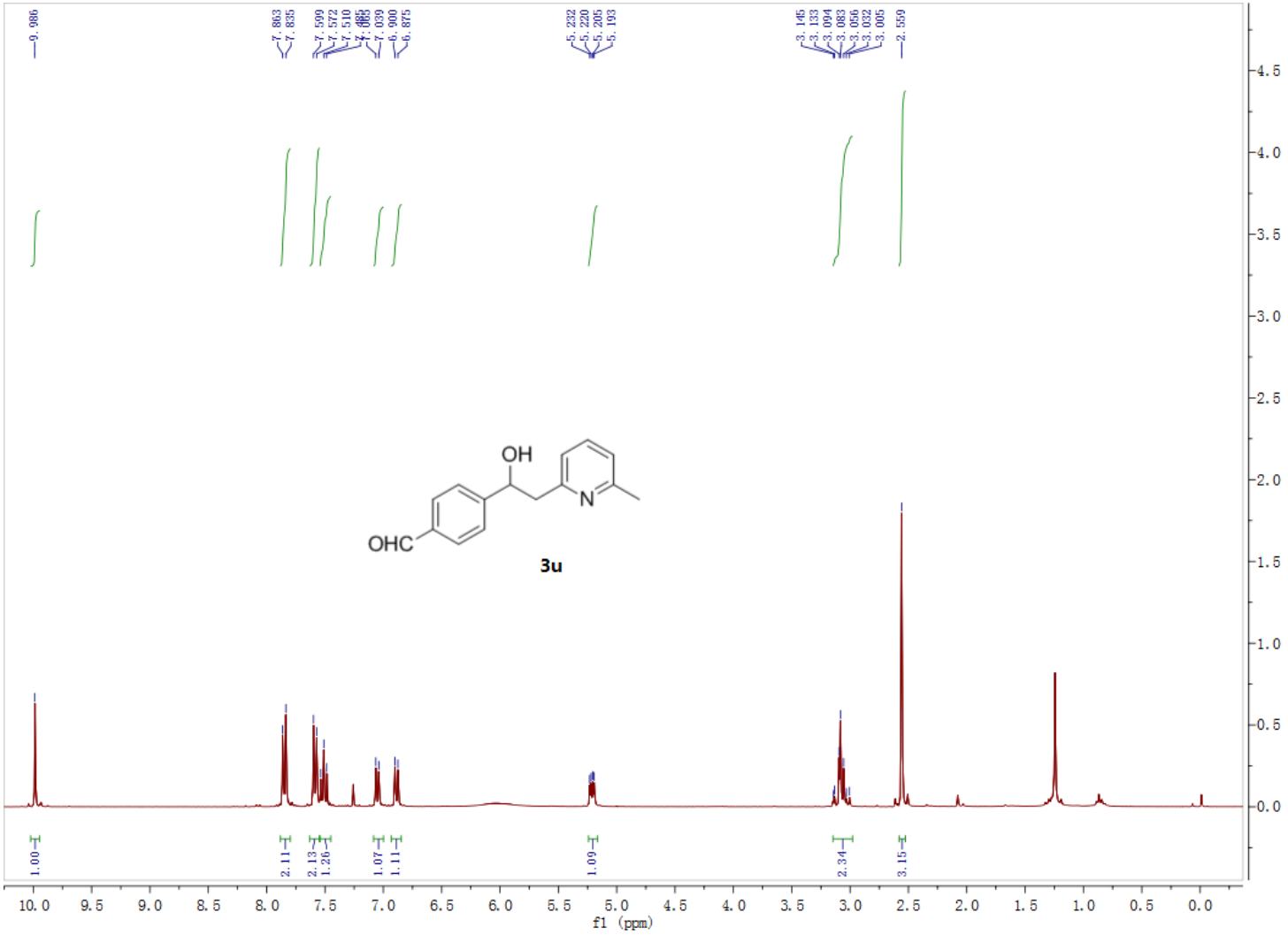

162.85
158.83
157.25
148.39
137.10
136.70
122.05
121.22
120.86
120.27
73.79
43.97
24.29
OH
N
N
3s
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.51
8.50
8.50
7.67
7.66
7.65
7.65
7.64
7.64
7.54
7.53
7.47
7.46
7.45
7.14
7.14
7.13
7.13
7.12
7.00
6.98
6.94
6.93
5.20
5.19
5.18
5.18
3.33
3.32
3.30
3.30
3.08
3.06
3.05
3.04
2.52
OH
N
N
3s
0.88
0.94
0.92
0.91
0.92
0.91
0.94
0.98
0.97
1.01
3.00
f1 (ppm)


173.66
157.47
157.21
137.14
121.51
120.81
70.64
61.15
40.26
24.09
14.12
OH
N
CO2Et
3t
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.50
7.49
7.47
7.00
6.99
6.97
6.95
4.59
4.59
4.58
4.58
4.18
4.16
4.15
4.14
3.25
3.24
3.22
3.22
3.13
3.12
3.10
3.09
2.47
1.23
1.21
1.20
1.19
OH
N
CO2Et
3t
0.92
1.86
0.95
1.93
0.98
0.99
3.00
3.11
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
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
f1 (ppm)


192.219
158.530
157.505
151.320
137.526
135.565
129.974
126.493
121.684
120.786
77.565
77.142
76.719
73.078
44.826
24.355
OH
N
OHC
3u
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.986
7.863
7.835
7.599
7.572
7.510
7.039
6.900
6.875
5.232
5.220
5.205
5.193
3.145
3.133
3.094
3.083
3.056
3.032
3.005
2.559
OH
N
OHC
3u
1.00
2.11
2.13
1.26
1.07
1.11
1.09
2.34
3.15
f1 (ppm)