Supporting Information

Rhodium-Catalyzed *ortho*-Carboxylation of sp^2 C-H Bond

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1. General experimental details

Chemicals were either purchased or purified by standard techniques without special instructions. ^{1}H NMR and ^{13}C NMR spectra were measured on a 300 MHz Bruker spectrometer (^{1}H 300 MHz, ^{13}C 75 MHz), using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts are given in δ relative to TMS, the coupling constants J are given in Hz. All reactions were conducted under air atmosphere. Column chromatography was performed using EM Silica gel 60 (300-400 mesh).

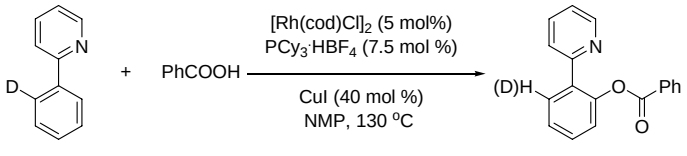
1.1 General procedure:

Under air atmosphere, a reaction tube was charged with 2-aryl pyridine (0.4 mmol), carboxylic acid (0.2 mmol), CuI (14.4 mg, 40 mol %), Rh(cod)Cl dimmer (4.9 mg, 5 mol %), $PCy_3{\cdot}HBF_4$ (5.5 mg, 7.5 mol %) and NMP (2 mL). The mixture was stired at 130 ^{o}C for 36 h. After the completion of the reaction, as monitored by TLC, 10 mL of ethyl acetate was added and the mixture was washed with water (3×5 mL) Then the organic layer was concentrated in vacuo and the residue was purified by flash column chromatography on a silica gel to give the desired product.

1.2 Preparation of 2-aryl pyridines:[1]

Under air atmosphere, a reaction tube was charged with 2-bromopyridine (0.5 mmol), aryl boronic acids (0.75 mmol), $PdCl_2$ (4.4 mg, 0.025 mmol), $K_3PO_4{\cdot}3H_2O$ (1.5 mmol) and toluene (3 mL). After the mixture was heated at 100 ^{o}C for 8 h, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on a silica gel to give the product.

1.3. kinetic isotope effect experiment



96% D

yield: 67%
D/H = 49/51

Under air atmosphere, a reaction tube was charged with 2-phenylpyridine (0.4 mmol, 96% D), benzoic acid (0.2 mmol), CuI (14.4 mg, 40 mol%), Rh(cod)Cl dimmer (4.9 mg, 5 mol %), $PCy_3{\cdot}HBF_4$ (5.5 mg, 7.5 mol %) and NMP (2 mL). The mixture was stired at 130 ^{o}C for 36 h. After the completion of the reaction, as monitored by TLC, 10 mL of ethyl acetate was added and the mixture was washed with water (3×5 mL) Then the organic layer was concentrated in vacuo and the

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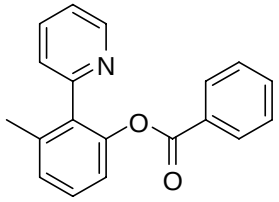
1.Pan, C.; Liu, M.; Zhang, L.; Wu, H.; Ding J.; Cheng, J. *Catal. Comm.* **2008**, *9*, 508.

residue was purified by flash column chromatography on a silica gel to give the desired product.
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.52-8.51 (m, 1H), 8.02-7.99 (m, 2H), 7.73-7.70 (m, 0.51H), 7.55-7.17 (m, 8H), 7.11-7.08 (m, 1H).

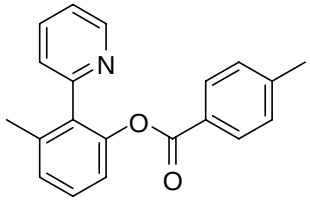
2. Experimental characterization data for compounds

3-Methyl-2-(pyridin-2-yl)phenyl benzoate (3aa)



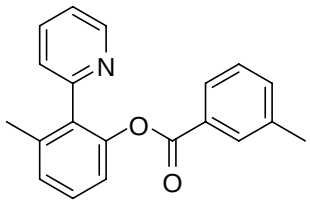
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.65-8.63 (m, 1H), 7.86-7.83 (m, 2H), 7.64-7.49 (m, 2H), 7.38-7.13 (m, 7H), 2.19 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.1, 155.8, 149.4, 148.6, 138.2, 136.0, 133.6, 133.3, 129.9, 129.3, 128.9, 128.3, 127.9, 124.8, 122.0, 120.1, 19.9.
IR (prism, cm^{-1}): ν 2984, 1741, 1373, 1241, 1047.
HRMS (EI) Calcd. for $C_{19}H_{15}NNaO_2$ $(M+Na)^+$ 312.1000, found 312.0995.

3-Methyl-2-(pyridin-2-yl)phenyl 4-methylbenzoate (3ab)



^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.65-8.63 (m, 1H), 7.74 (d, J = 8.2 Hz, 2H), 7.63-7.59 (m, 1H), 7.36-7.14 (m, 7H), 2.36 (s, 3H), 2.19 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.1, 155.8, 149.4, 148.7, 144.0, 138.1, 136.0, 133.2, 129.9, 129.0, 128.8, 127.8, 126.5, 124.8, 122.0, 120.1, 21.6, 19.9.
IR (prism, cm^{-1}): ν 3062, 2922, 1735, 1460, 1267, 1223, 1081.
HRMS (EI) Calcd. for $C_{20}H_{17}NNaO_2$ $(M+Na)^+$ 326.1157, found 326.1151.

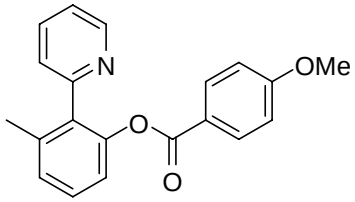
3-Methyl-2-(pyridin-2-yl)phenyl 3-methylbenzoate (3ac)



^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.66-8.64 (m, 1H), 7.65-7.62 (m, 3H), 7.36-7.14 (m, 7H), 2.33 (s, 3H), 2.19 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.2, 155.9, 149.4, 148.7, 138.2, 138.1, 136.0, 134.0, 133.7, 130.5, 129.2, 128.8, 128.2, 127.8, 127.0, 124.8, 122.0, 120.0, 21.1, 19.9.
IR (prism, cm^{-1}): ν 3014, 2923, 1736, 1460, 1275, 1224, 1187, 1093, 746.

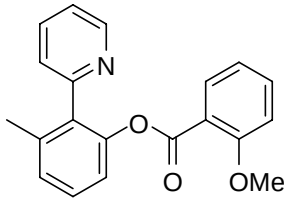
HRMS (EI) Calcd. for $C_{20}H_{17}NNaO_2$ $(M+Na)^+$ 326.1157, found 326.1151.

3-Methyl-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (3ad)



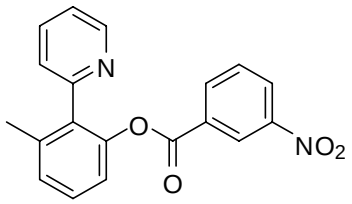
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.65-8.63 (m, 1H), 7.80 (d, *J* = 7.0 Hz, 2H), 7.63-7.59 (m, 1H), 7.37-7.12 (m, 5H), 6.83 (d, *J* = 7.0 Hz, 2H), 3.83 (s, 3H), 2.18 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 164.8, 163.6, 155.9, 149.4, 148.7, 138.1, 136.0, 133.7, 132.0, 128.8, 127.8, 124.8, 122.0, 121.6, 120.2, 113.5, 55.4, 19.9.
IR (prism, cm^{-1}): ν 3014, 2924, 1730, 1654, 1460, 1317, 1222, 1080.
HRMS (EI) Calcd. for $C_{20}H_{17}NNaO_3$ $(M+Na)^+$ 342.1106, found 342.1101.

3-Methyl-2-(pyridin-2-yl)phenyl 2-methoxybenzoate (3ae)



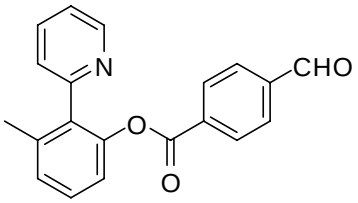
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.69-8.68 (m, 1H), 7.68-7.61 (m, 1H), 7.40-7.12 (m, 7H), 6.91-6.80 (m, 2H), 3.79 (s, 3H), 2.17 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 164.2, 159.6, 156.0, 149.4, 148.6, 138.1, 136.1, 133.9, 133.7, 131.8, 128.8, 127.8, 124.9, 122.0, 120.3, 119.9, 118.8, 111.9, 55.9, 19.9.
IR (prism, cm^{-1}): ν 3061, 2925, 1744, 1583, 1461, 1255, 1215, 1050, 745.
HRMS (EI) Calcd. for $C_{20}H_{17}NNaO_3$ $(M+Na)^+$ 342.1106, found 342.1101.

3-Methyl-2-(pyridin-2-yl)phenyl 3-nitrobenzoate (3af)



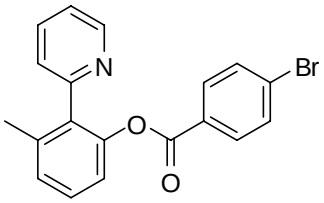
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.64-8.59 (m, 2H), 8.40-8.32 (m, 1H), 8.19-8.17 (d, *J* = 8.6 Hz, 1H), 7.80-7.58 (m, 2H), 7.39-7.18 (m, 5H), 2.20 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 162.9, 155.5, 149.6, 148.2, 148.1, 138.4, 136.2, 135.5, 133.4, 131.1, 129.6, 129.0, 128.4, 127.7, 124.8, 124.7, 122.3, 119.7, 19.9.
IR (prism, cm^{-1}): ν 3020, 2926, 1744, 1534, 1351, 1256, 1220, 1118, 758.
HRMS (EI) Calcd. for $C_{19}H_{14}N_2NaO_4$ $(M+Na)^+$ 357.0851, found 357.0846.

3-Methyl-2-(pyridin-2-yl)phenyl 4-formylbenzoate (3ag)



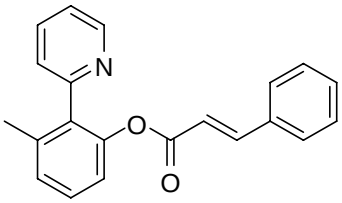
^{1}H NMR ($CDCl_3$, 300 MHz): δ 10.1 (s, 1H), 8.63-8.62 (m, 1H), 8.00 (d, *J* = 8.3 Hz, 2H), 7.87 (d, *J* = 8.3 Hz, 2H), 7.67-7.60 (m, 1H), 7.33-7.14 (m, 5H), 2.20 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.5, 164.1, 155.6, 149.6, 148.3, 139.3, 138.3, 136.1, 134.2, 133.4, 130.4, 129.4, 129.0, 128.2, 124.8, 122.2, 119.8, 19.9.
IR (prism, cm^{-1}): ν 3063, 2823, 1740, 1704, 1460, 1264, 1221, 1084.
HRMS (EI) Calcd. for $C_{20}H_{15}NNaO_3$ $(M+Na)^+$ 340.0950, found 340.0944.

3-Methyl-2-(pyridin-2-yl)phenyl 4-bromobenzoate (3ah)



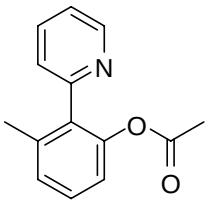
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.64-8.62 (m, 1H), 7.71-7.48 (m, 5H), 7.36-7.12 (m, 5H). 2.19 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 164.4, 155.7, 149.5, 148.4, 138.2, 137.7, 136.1, 131.6, 131.4, 131.3, 128.9, 128.5, 128.1, 124.7, 122.1, 119.9, 19.9.
IR (prism, cm^{-1}): ν 3063, 2923, 1738, 1586, 1460, 1265, 1222, 1082, 748.
HRMS (EI) Calcd. for $C_{19}H_{14}BrNNaO_2$ $(M+Na)^+$ 390.0106, found 390.0100.

3-Methyl-2-(pyridin-2-yl)phenyl cinnamate (3ai)



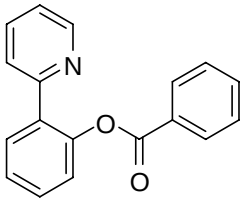
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.70-8.69 (m, 1H), 7.70-7.67 (m, 1H), 7.57 (d, *J* = 16.0 Hz, 1H), 7.46-7.10 (m, 10H), 6.34 (d, *J* = 16.0 Hz, 1H), 2.18 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.3, 155.8, 149.5, 148.4, 146.2, 138.2, 136.0, 134.1, 133.7, 130.5, 128.9, 128.9, 128.2, 127.9, 124.8, 122.1, 120.0, 116.9, 19.9.
IR (prism, cm^{-1}): ν 3060, 2924, 1729, 1634, 1459, 1220, 1140, 757.
HRMS (EI) Calcd. for $C_{21}H_{17}NNaO_2$ $(M+Na)^+$ 338.1157, found 338.1151.

3-Methyl-2-(pyridin-2-yl)phenyl acetate (3aj)



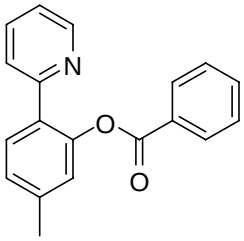
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.71-8.70 (m, 1H), 7.76-7.71 (m, 1H), 7.31-7.17 (m, 4H), 6.98 (d, J = 8.0 Hz, 1H), 2.15 (s, 3H), 1.95 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 169.5, 155.8, 149.5, 148.3, 138.2, 136.0, 133.6, 128.8, 128.0, 124.7, 122.1, 119.9, 20.5, 19.9.
IR (prism, cm^{-1}): ν 3061, 2924, 1765, 1461, 1201.
HRMS (EI) Calcd. for $C_{14}H_{13}NNaO_2$ $(M+Na)^+$ 250.0844, found 250.0838.

2-(Pyridin-2-yl)phenyl benzoate (3ba)[2]



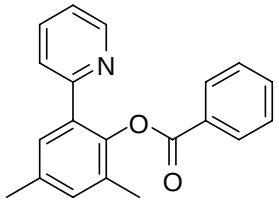
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.60-8.59 (m, 1H), 8.10-8.08 (m, 2H), 7.78-7.75 (m, 1H), 7.61-7.32 (m, 8H), 7.16-7.13 (m, 1H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.2, 155.5, 149.6, 148.3, 136.2, 133.5, 133.3, 130.9, 130.2, 129.7, 129.5, 128.5, 126.4, 123.7, 123.3, 122.2.

5-Methyl-2-(pyridin-2-yl)phenyl benzoate (3ca)



^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.58-8.57 (m, 1H), 8.11-8.08 (m, 2H), 7.70-7.43 (m, 6H), 7.20-7.11 (m, 3H), 2.44 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.3, 155.5, 149.5, 148.1, 140.2, 136.1, 133.4, 130.6, 130.3, 130.1, 129.5, 128.5, 127.3, 123.7, 123.5, 121.9, 21.2.
IR (prism, cm^{-1}): ν 3016, 1737, 1587, 1509, 1259, 1131, 1062, 755.
HRMS (EI) Calcd. for $C_{19}H_{15}NNaO_2$ $(M+Na)^+$ 312.1000, found 312.0995.

2,4-Dimethyl-6-(pyridin-2-yl)phenyl benzoate (3da)



^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.56-8.55 (m, 1H), 8.11-8.08 (m, 2H), 7.59-7.11 (m, 8H), 2.40 (s, 3H), 2.23 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 164.8, 156.1, 149.4, 144.7, 136.0, 135.8, 133.3, 132.2, 131.0, 130.1, 129.4, 128.9, 128.4, 128.2, 123.5, 121.9, 20.9, 16.5.

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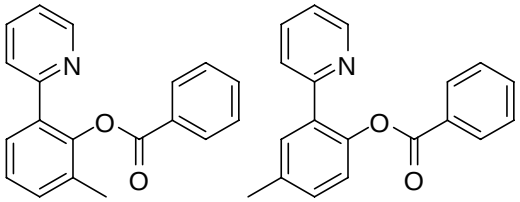
2. Dick, A. R.; Kampf, J. W.; Sanford, M. S. *J. Am. Chem Soc*. **2005**, *127*, 12790.

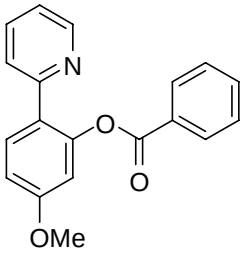
IR (prism, cm^{-1}): ν 3061, 2923, 1737, 1586, 1456, 1264, 1194, 1118, 1060, 708.
HRMS (EI) Calcd. for $C_{20}H_{17}NNaO_2$ $(M+Na)^+$ 326.1157, found 326.1151.

4-Methyl-2-(pyridin-2-yl)phenyl benzoate and 2-Methyl-6-(pyridin-2-yl)phenyl benzoate (**3ea**)



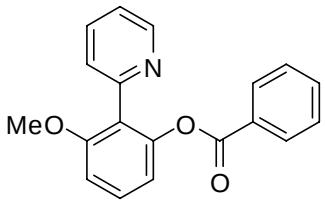
^1H NMR ($CDCl_3$, 300 MHz) See the Copies.

5-Methoxy-2-(pyridin-2-yl)phenyl benzoate (3fa)



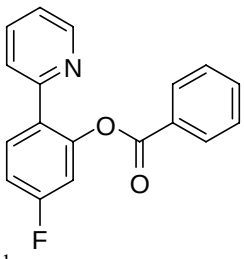
^1H NMR ($CDCl_3$, 300 MHz): δ 8.57-8.56 (m, 1H), 8.11-8.09 (m, 2H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.74-7.44 (m, 5H), 7.13-7.12 (m, 1H), 6.98-6.94 (m, 1H), 6.84 (d, *J* = 2.5 Hz, 1H), 3.86 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.0, 160.8, 155.1, 149.2, 149.2, 136.5, 133.5, 131.6, 130.2, 129.3, 128.5, 125.3, 123.5, 121.7, 112.6, 108.7, 55.6.
IR (prism, cm^{-1}): ν 3014, 2929, 1738, 1616, 1464, 1260, 1155, 1124, 757.
HRMS (EI) Calcd. for $C_{19}H_{15}NNaO_3$ $(M+Na)^+$ 328.0950, found 328.0944.

3-Methoxy-2-(pyridin-2-yl)phenyl benzoate (3ga)



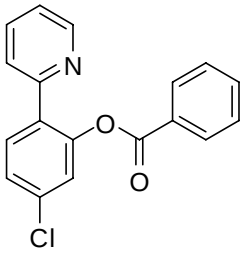
^1H NMR ($CDCl_3$, 300 MHz): δ 8.59-8.58 (m, 1H), 7.90-7.87 (m, 2H), 7.65-7.34 (m, 6H), 7.16-7.12 (m, 1H), 6.97-6.93 (m, 2H), 3.79 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.0, 157.9, 153.1, 149.5, 149.2, 135.8, 133.3, 130.0, 129.6, 129.3, 128.3, 125.8, 123.4, 122.0, 115.3, 108.8, 56.1.
IR (prism, cm^{-1}): ν 3007, 2929, 1738, 1608, 1584, 1464, 1264, 1223, 1094, 751, 707.
HRMS (EI) Calcd. for $C_{19}H_{15}NNaO_3$ $(M+Na)^+$ 328.0950, found 328.0944.

5-Fluoro-2-(pyridin-2-yl)phenyl benzoate (3ha)



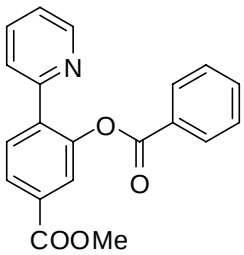
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.59-8.57 (m, 1H), 8.08-8.06 (m, 2H), 7.80-7.43 (m, 6H), 7.16-7.07 (m, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 164.7, 162.8 (d, J_{C-F} = 248.3 Hz), 154.7, 149.6, 148.9, 136.2, 133.7, 132.0 (d, J_{C-F} = 9.3 Hz), 130.2, 129.5, 129.0, 128.6, 123.6, 122.2, 113.6 (d, J_{C-F} = 21.1 Hz), 111.1 (d, J_{C-F} = 24.5 Hz).
IR (prism, cm^{-1}): ν 3065, 2925, 1742, 1601, 1464, 1257, 1177, 1145, 1057, 706.
HRMS (EI) Calcd. for $C_{18}H_{12}FNNaO_2$ $(M+Na)^+$ 316.0750, found 316.0744.

5-Chloro-2-(pyridin-2-yl)phenyl benzoate (3ia)



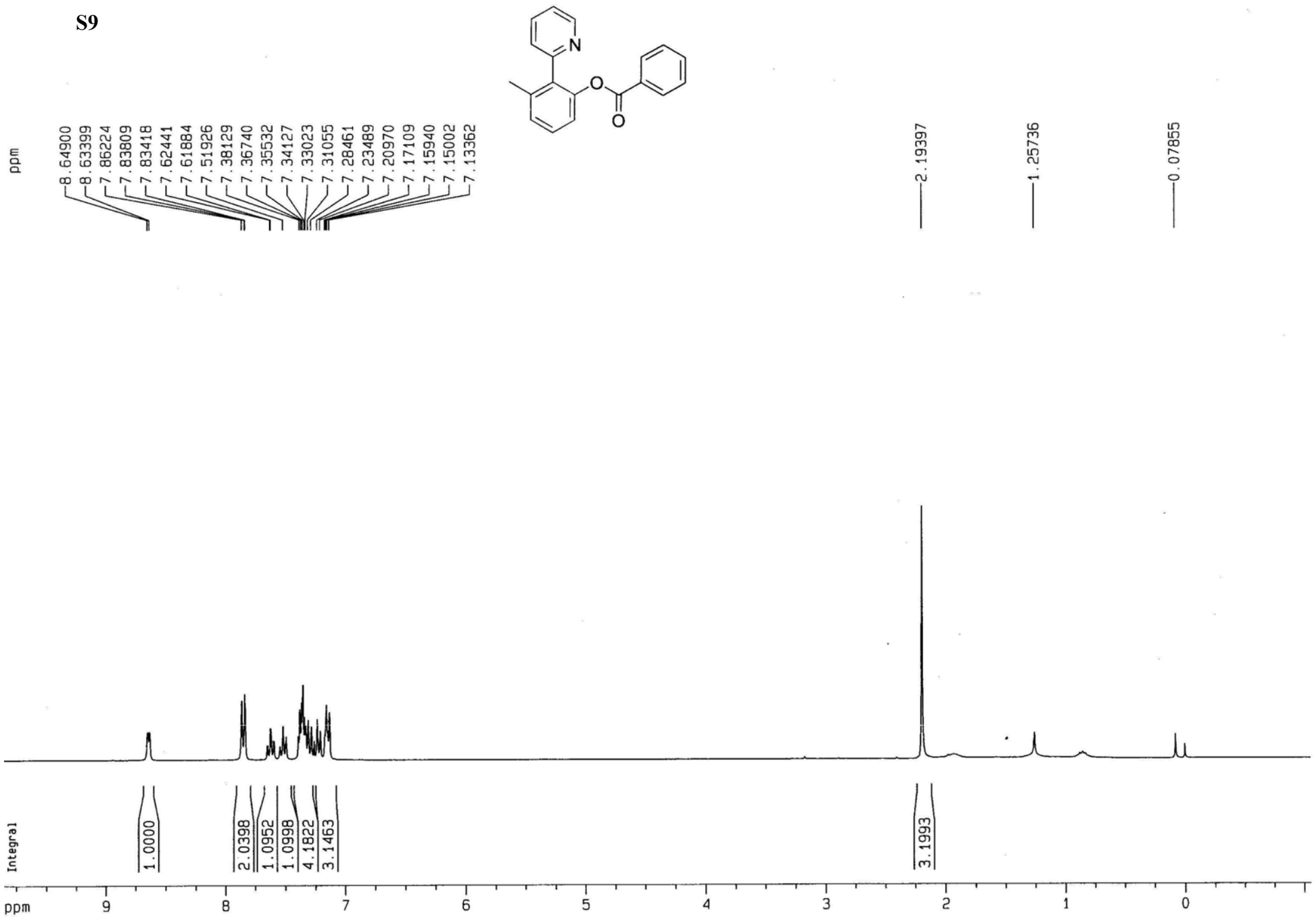
^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.59-8.58 (m, 1H), 8.08-8.05 (m, 2H), 7.75 (d, J = 8.3 Hz, 1H), 7.63-7.34 (m, 7H), 7.20-7.14 (m, 1H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 164.8, 154.5, 149.7, 148.6, 136.3, 134.9, 133.7, 131.9, 131.8, 130.2, 128.9, 128.6, 126.7, 123.8, 123.6, 122.4.
IR (prism, cm^{-1}): ν 3064, 2922, 1742, 1598, 1460, 1254, 1197, 1057, 706.
HRMS (EI) Calcd. for $C_{18}H_{12}ClNNaO_2$ $(M+Na)^+$ 332.0454, found 332.0449.

Methyl 3-(benzoyloxy)-4-(pyridin-2-yl)benzoate (3ja)



^{1}H NMR ($CDCl_3$, 300 MHz): δ 8.63-8.61 (m, 1H), 8.10-8.06 (m, 3H), 7.99-7.98 (m, 1H), 7.89-7.87 (d, J = 8.1 Hz, 1H), 7.65-7.61 (m, 3H), 7.49-7.44 (m, 2H), 7.25-7.21 (m, 1H), 3.94 (s, 3H).
^{13}C NMR ($CDCl_3$, 75 MHz): δ 165.9, 164.9, 154.3, 149.6, 148.2, 137.2, 136.6, 133.7, 131.6, 131.1, 130.2, 129.0, 128.6, 127.4, 124.8, 123.9, 122.8, 52.4.
IR (prism, cm^{-1}): ν 3020, 1726, 1585, 1436, 1293, 1243, 758.
HRMS (EI) Calcd. for $C_{20}H_{15}NNaO_4$ $(M+Na)^+$ 356.0899, found 356.0893.

3aa ^{1}H NMR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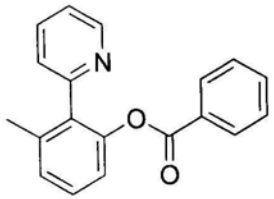
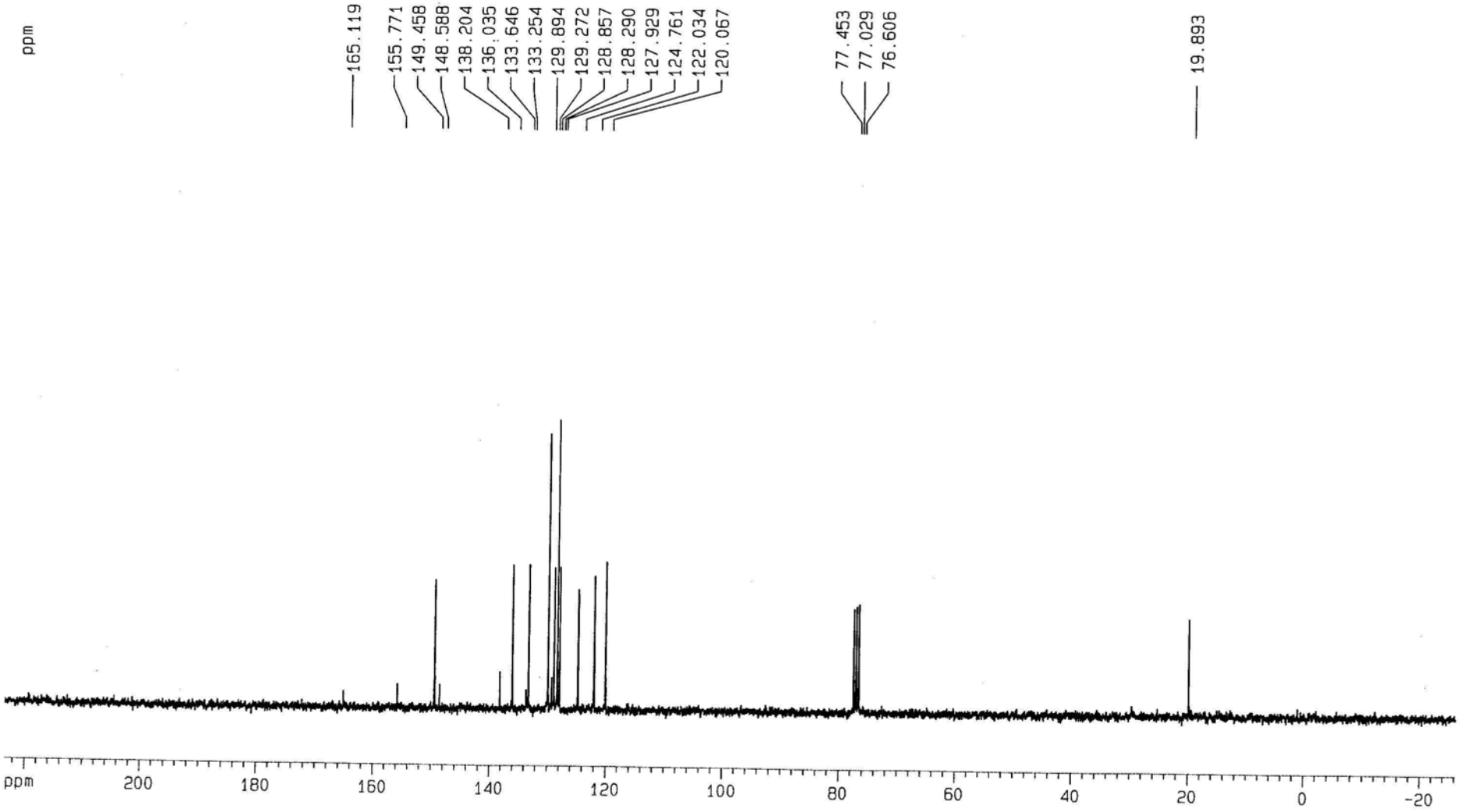
7.62441
7.61884
7.51926
7.38129
7.36740
7.35532
7.34127
7.33023
7.31055
7.28461
7.23489
7.20970
7.17109
7.15940
7.15002
7.13362
2.19397
1.25736
0.07855
Integral
1.0000
2.0398
1.0952
1.0998
4.1822
3.1463
3.1993
ppm
9
8
7
6
5
4
3
2
1
0

3aa ^{13}C NMR


N
O
O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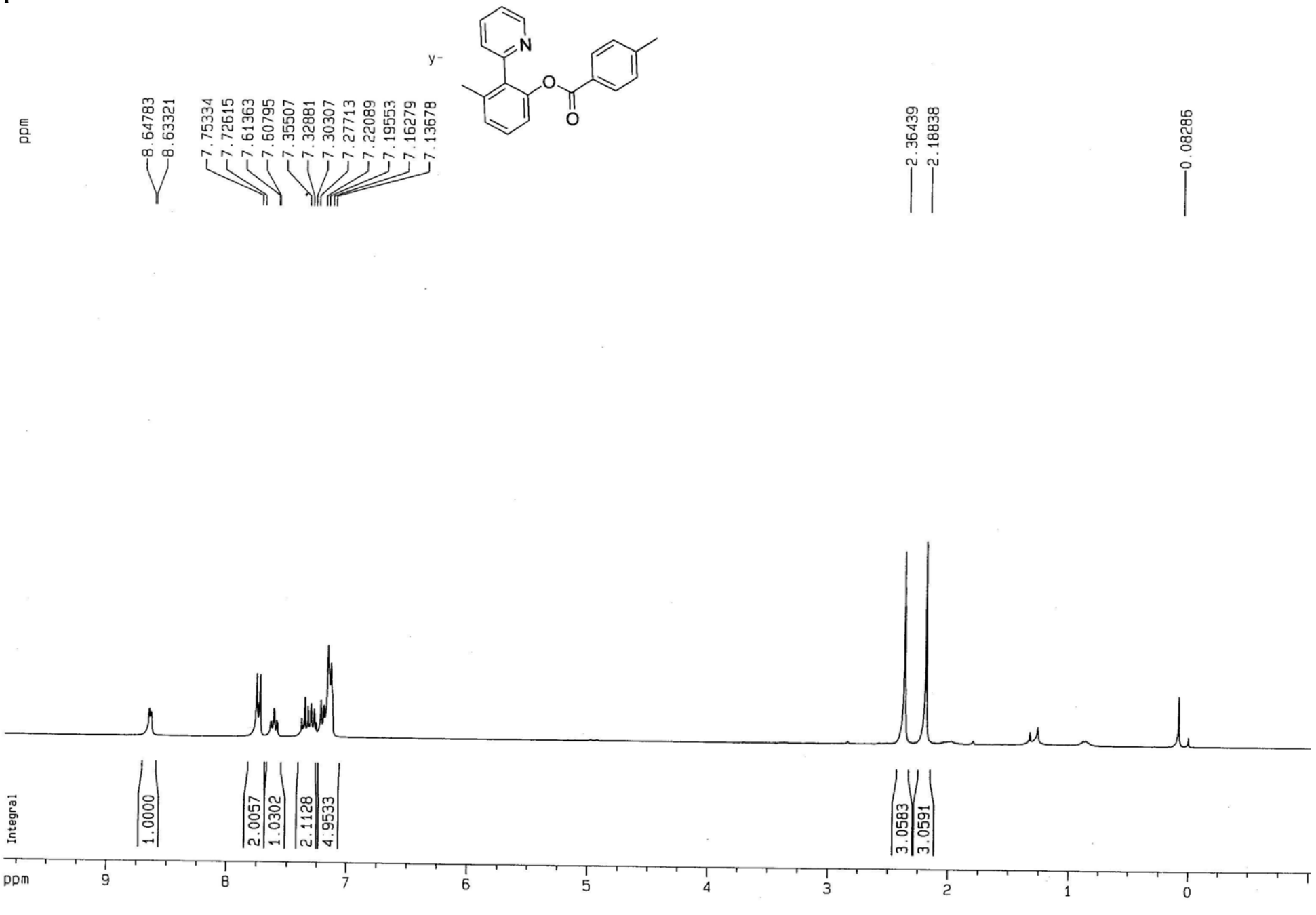
148.588
138.204
136.035
133.646
133.254
129.894
129.272
128.857
128.290
127.929
124.761
122.034
120.067
77.453
77.029
76.606
19.893
ppm
200
180
160
140
120
100
80
60
40
20
0
-20

3ab ^{1}H NMR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O
O
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7.35507
7.32881
7.30307
7.27713
7.22089
7.19553
7.16279
7.13678
2.36439
2.18838
0.08286
Integral
1.0000
2.0057
1.0302
2.1128
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3.0591
ppm
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8
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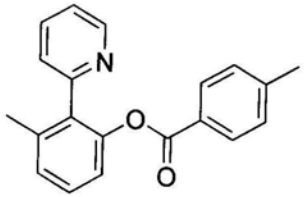
6
5
4
3
2
1
0

3ab ^{13}C NMR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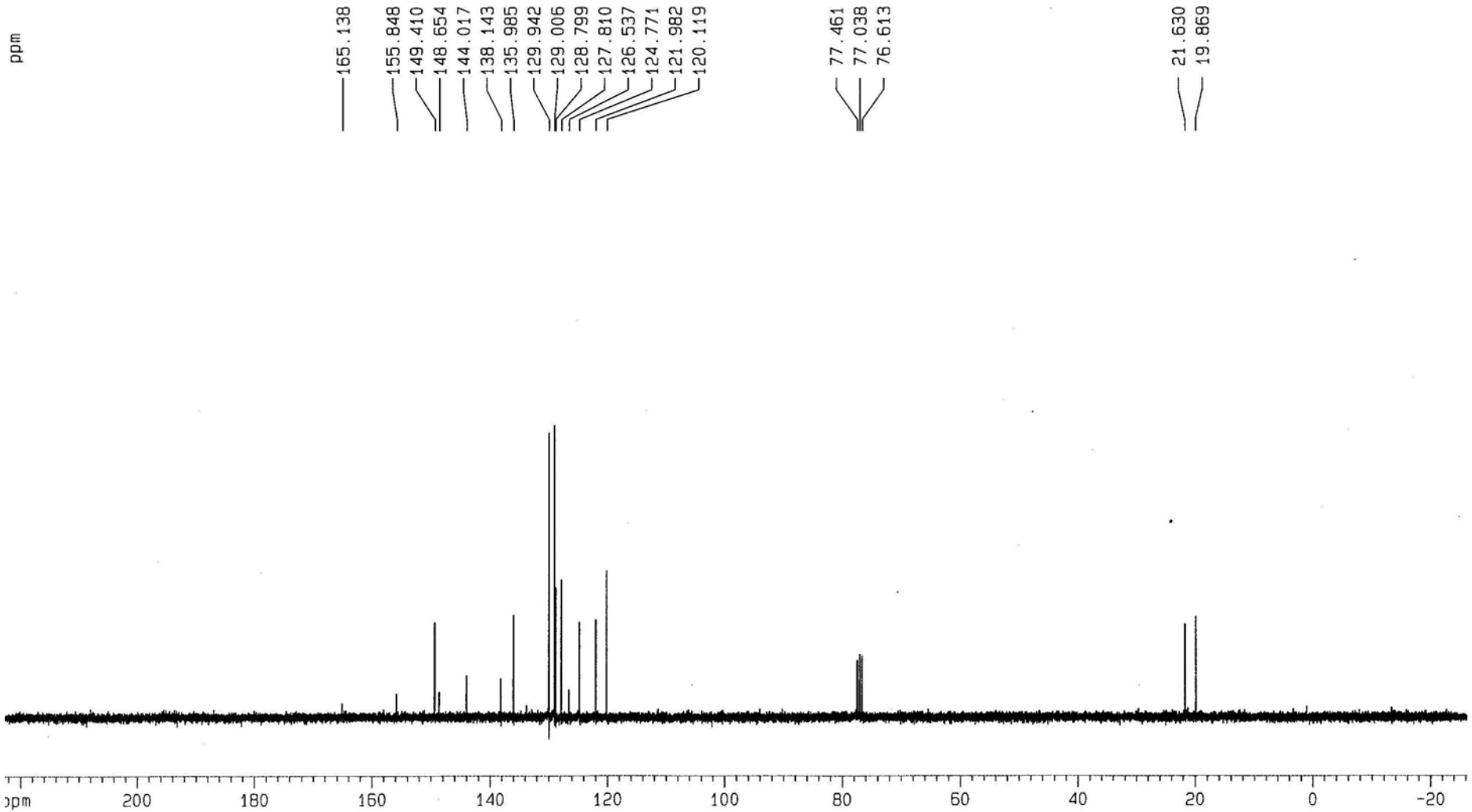
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129.006
128.799
127.810
126.537
124.771
121.982
120.119
77.461
77.038
76.613
21.630
19.869
200
180
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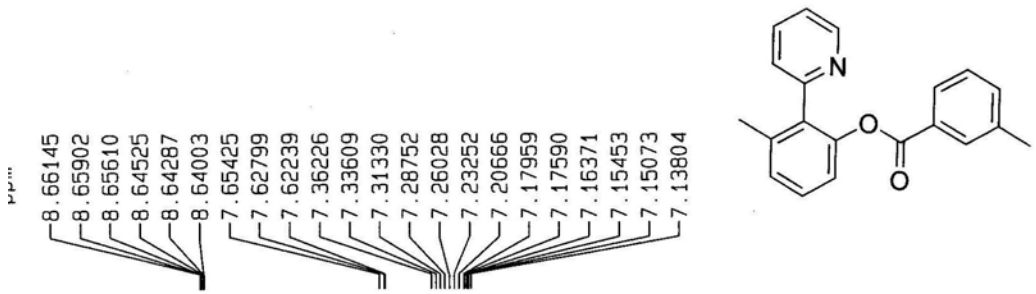
140
120
100
80
60
40
20
0
-20

3ac ^{1}H NMR


N
O
O

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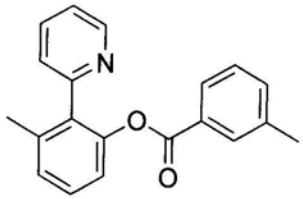
8.65610
8.64525
8.64287
8.64003
7.65425
7.62799
7.62239
7.36226
7.33609
7.31330
7.28752
7.26028
7.23252
7.20666
7.17959
7.17590
7.16371
7.15453
7.15073
7.13804
2.32817
2.19336
1.0000
3.0133
7.3500
3.0503
3.0588
pm
9
8
7
6
5
4
3
2
1
0

3ac ^{13}C NMR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O
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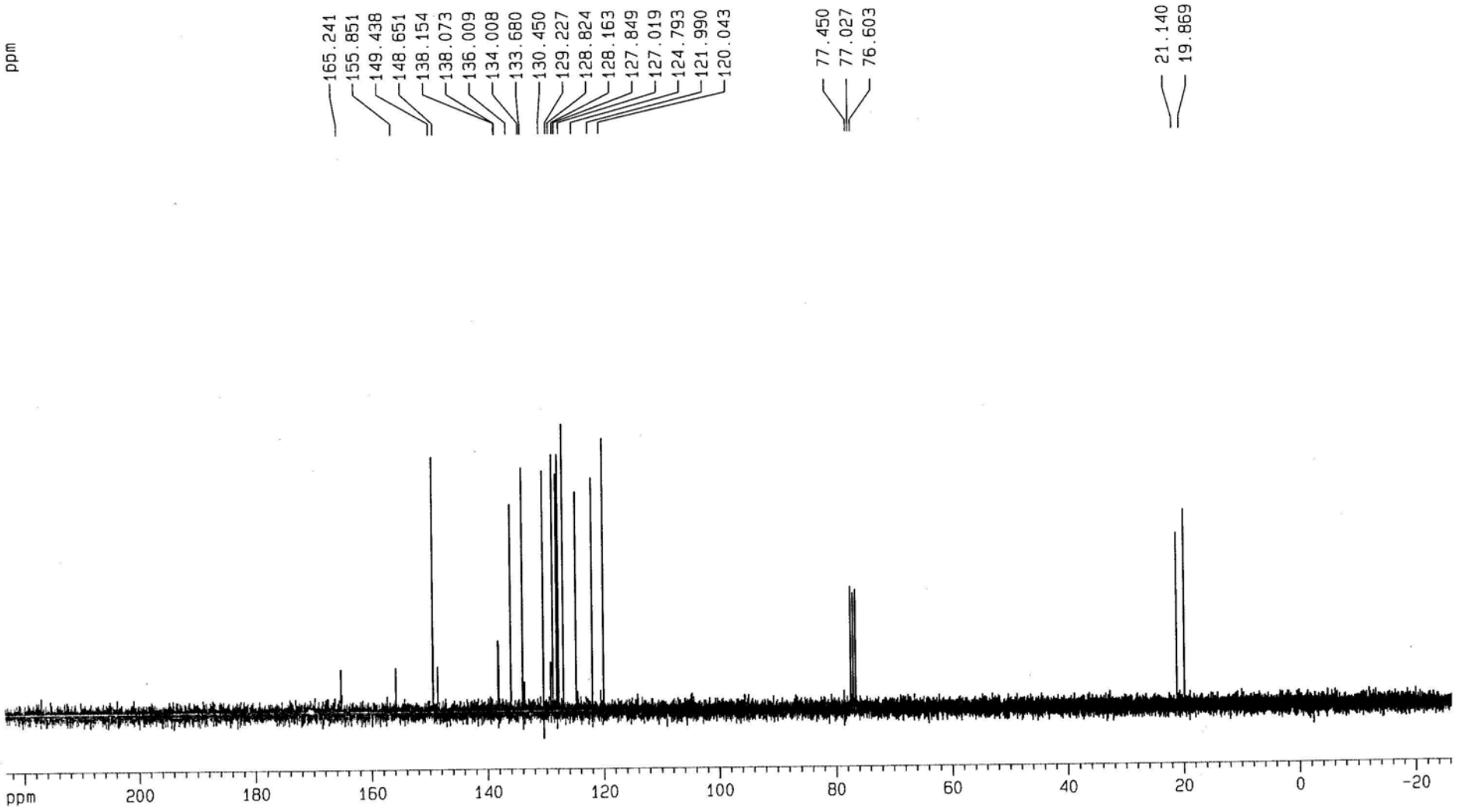
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128.163
127.849
127.019
124.793
121.990
120.043
77.450
77.027
76.603
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19.869
ppm
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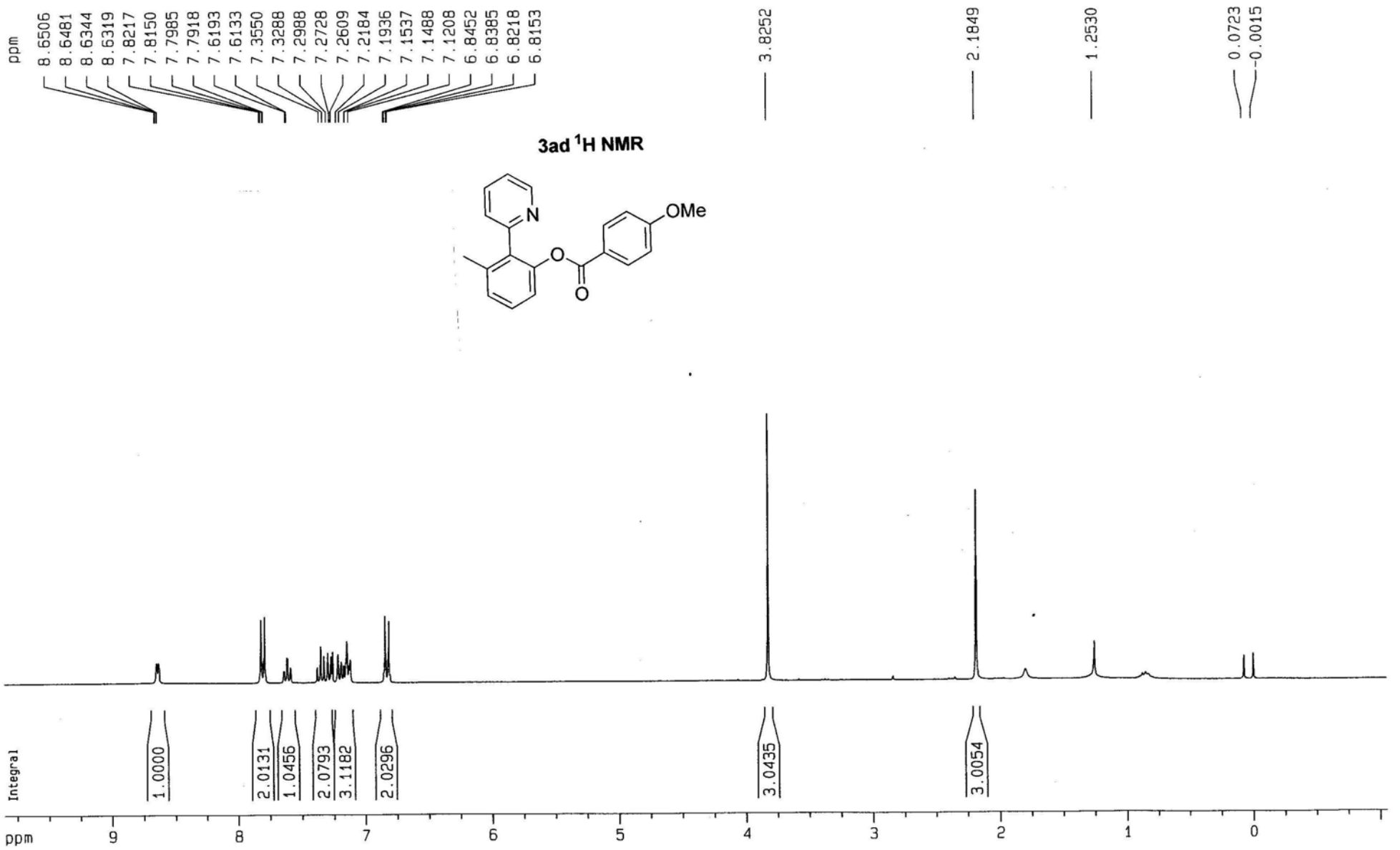
60
40
20
0
-20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8.6319
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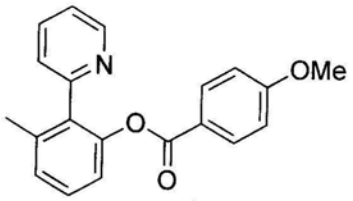
7.6193
7.6133
7.3550
7.3288
7.2988
7.2728
7.2609
7.2184
7.1936
7.1537
7.1488
7.1208
6.8452
6.8385
6.8218
6.8153
3.8252
2.1849
1.2530
0.0723
-0.0015
3ad ^{1}H NMR
N
O
O
OMe
Integral
1.0000
2.0131
1.0456
2.0793
3.1182
2.0296
3.0435
3.0054
ppm
9
8
7
6
5
4
3
2
1
0

3ad ^{13}C NMR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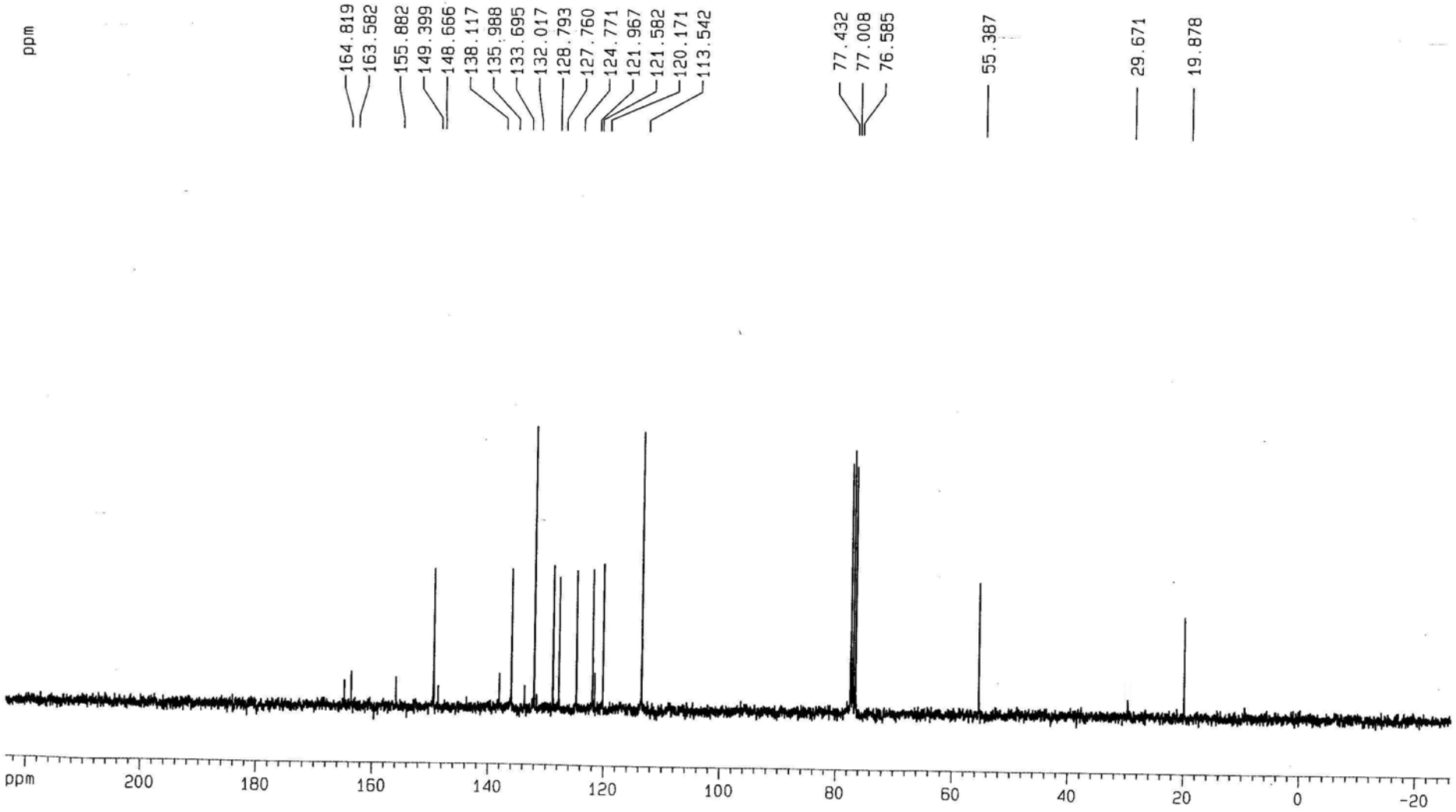
OMe
O
O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121.582
120.171
113.542
77.432
77.008
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120
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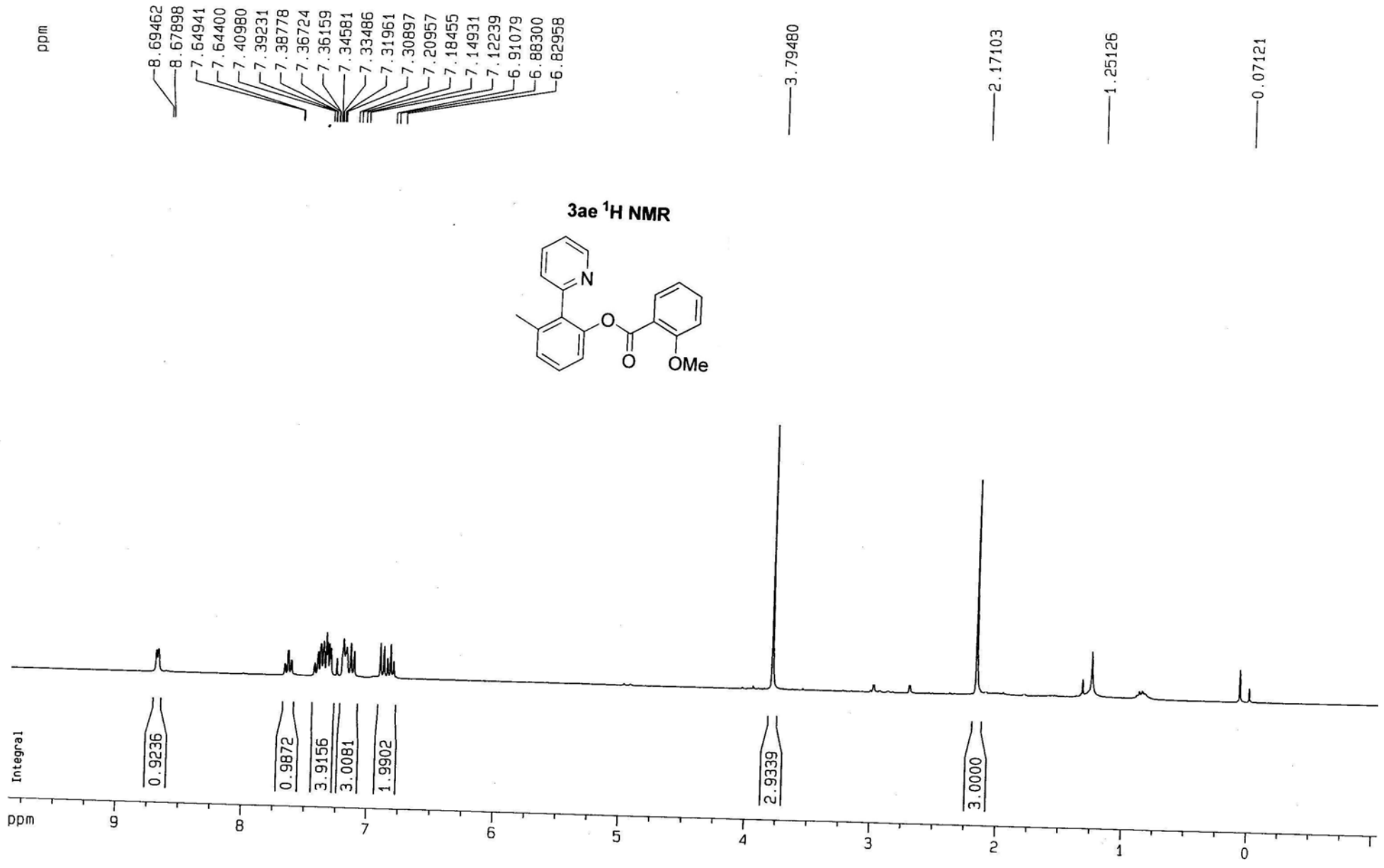
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7.30897
7.20957
7.18455
7.14931
7.12239
6.91079
6.88300
6.82958
3.79480
2.17103
1.25126
0.07121
3ae ^{1}H NMR
N
O
O
OMe
Integral
0.9236
0.9872
3.9156
3.0081
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3.0000
ppm
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8
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4
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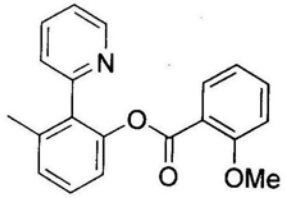
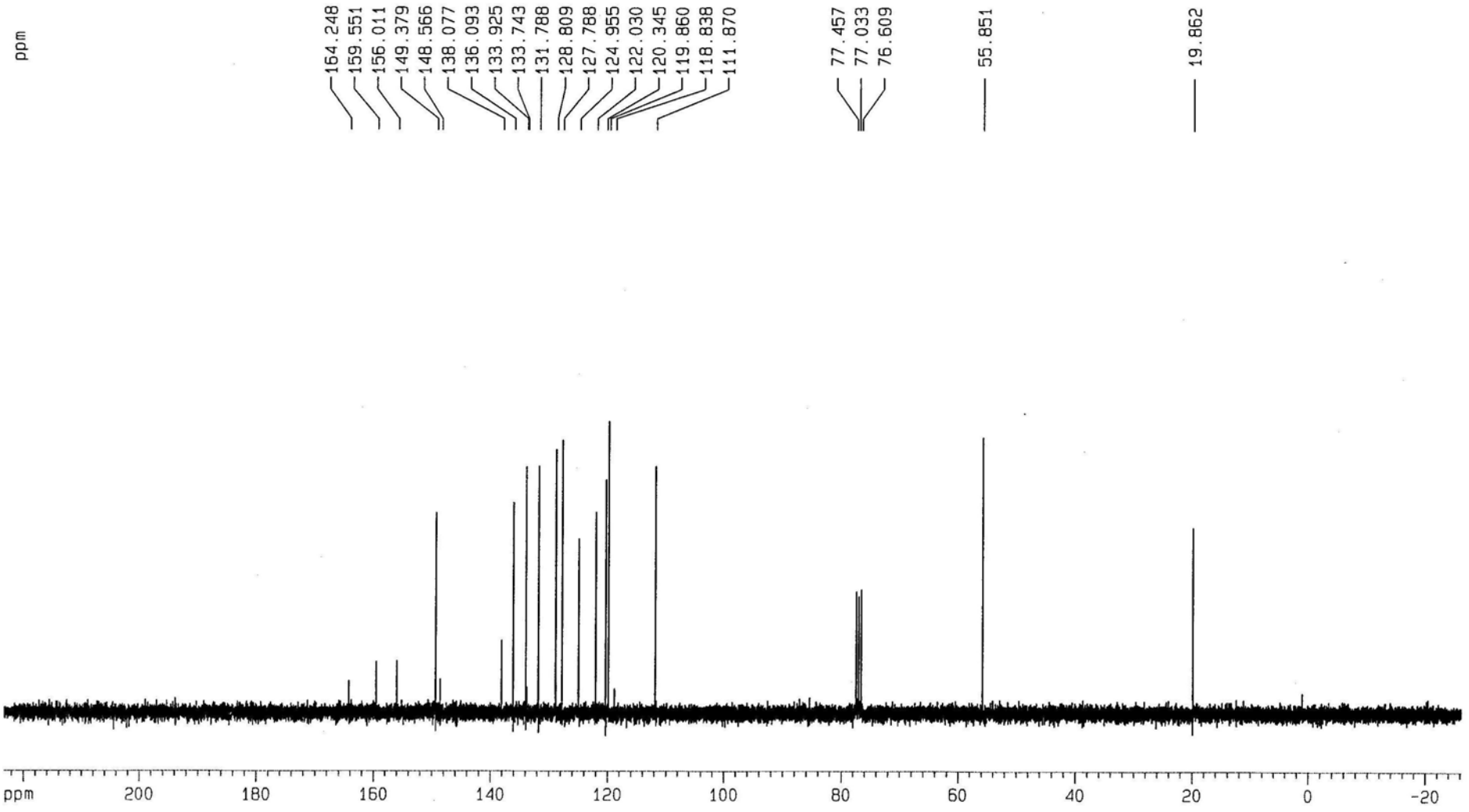
3ae ^{13}C NMR


N
O
O
OMe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127.788
124.955
122.030
120.345
119.860
118.838
111.870
77.457
77.033
76.609
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19.862
ppm
200
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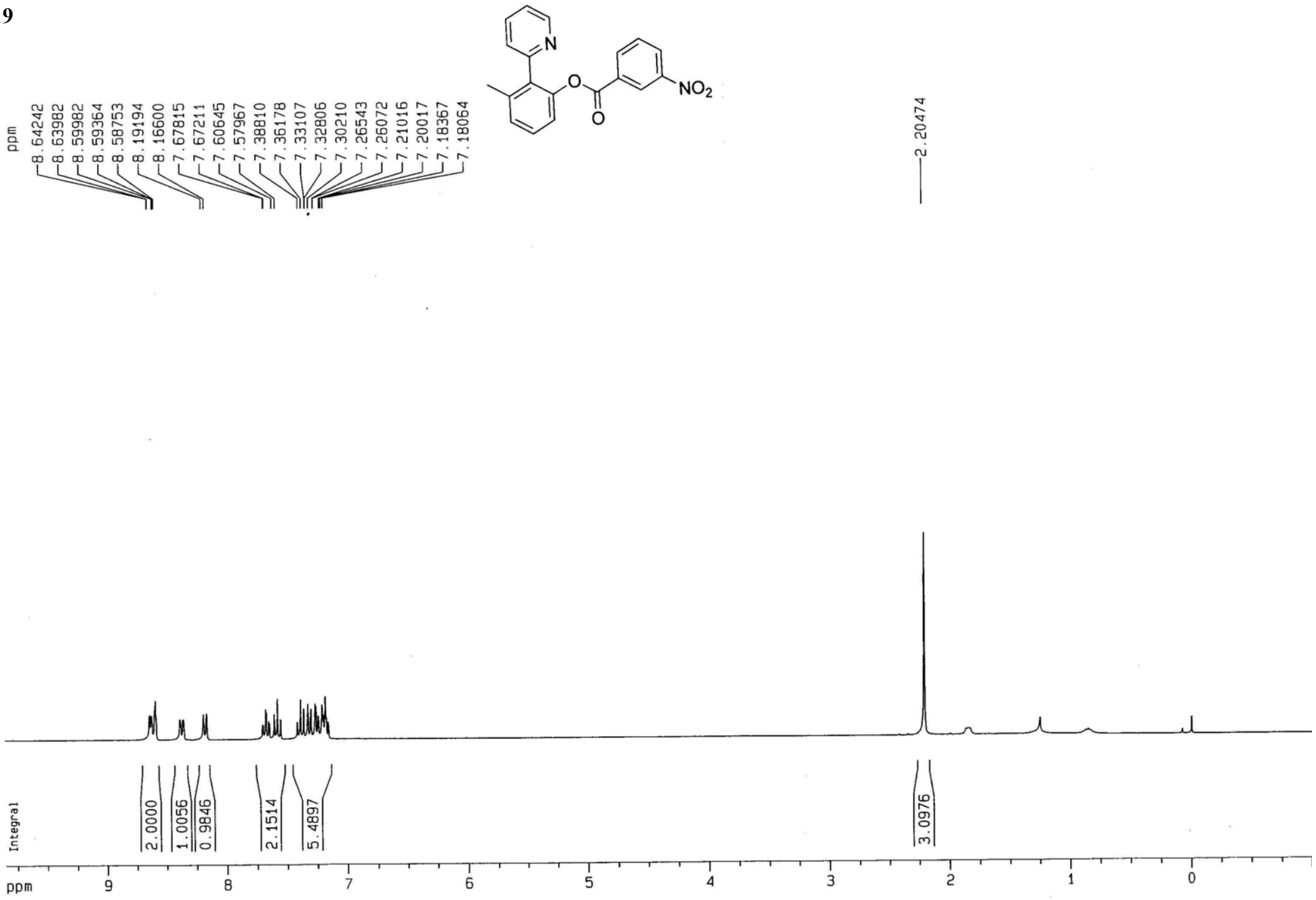
140
120
100
80
60
40
20
0
-20

3af ^{1}H NMR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7.33107
7.32806
7.30210
7.26543
7.26072
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7.18064
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Integral
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ppm
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4
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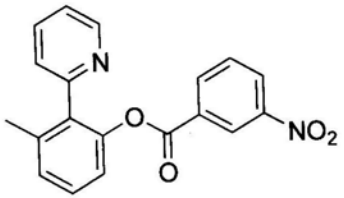
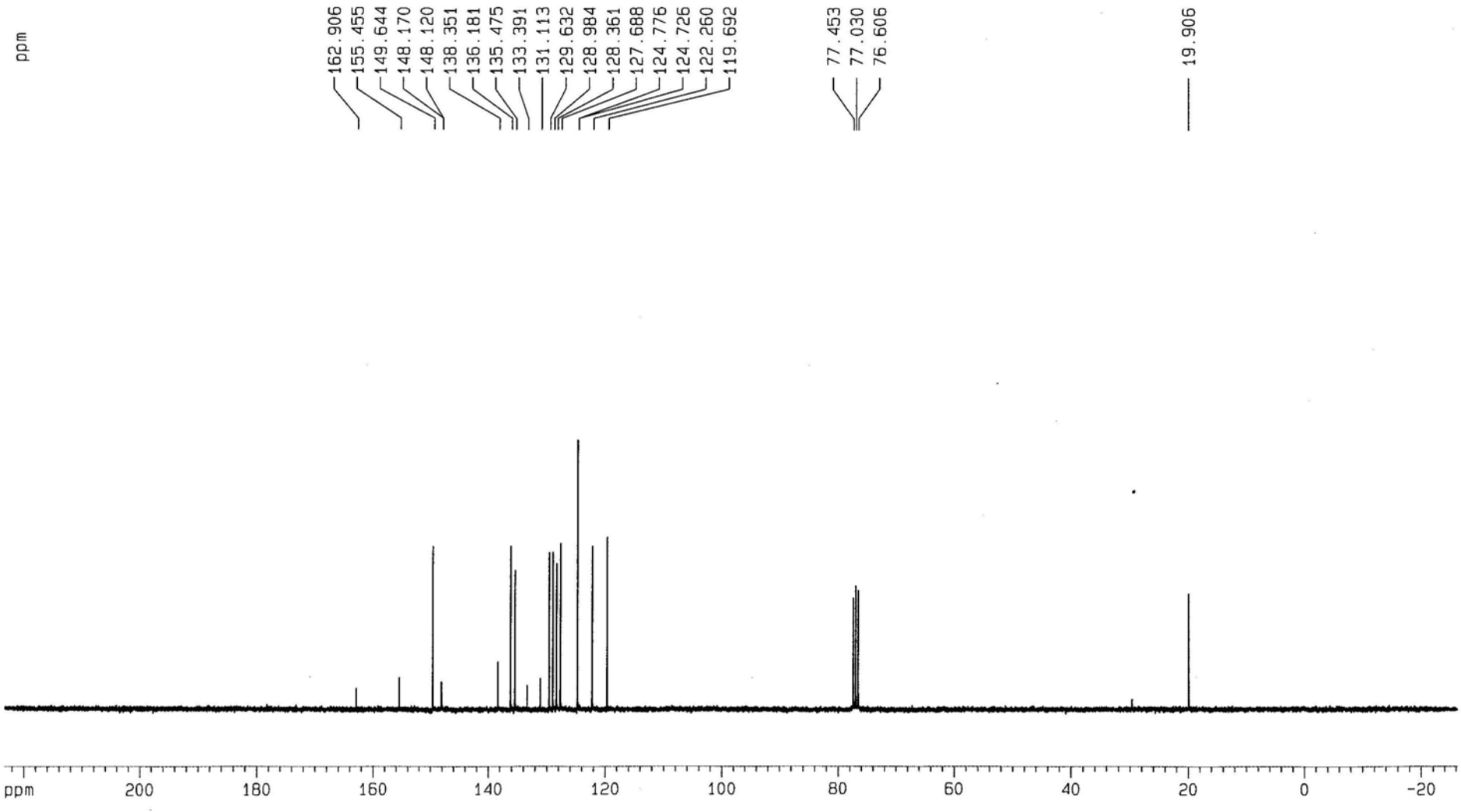
0

3af ^{13}C NMR


N
O
O
NO2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127.688
124.776
124.726
122.260
119.692
77.453
77.030
76.606
19.906
ppm
200
180
160
140
120
100
80
60
40
20
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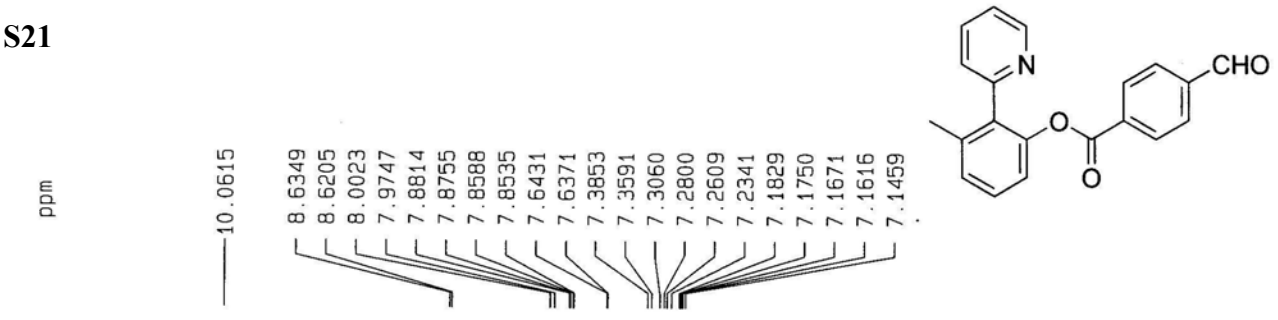
-20

3ag ^{1}H NMR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CHO
O
O

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7.3591
7.3060
7.2800
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7.2341
7.1829
7.1750
7.1671
7.1616
7.1459
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1.2476
1.2292
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Integral
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2.0780
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ppm
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4
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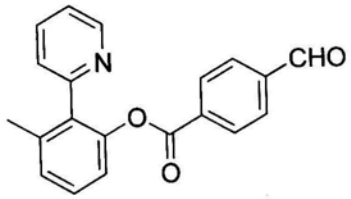
3ag ^{13}C NMR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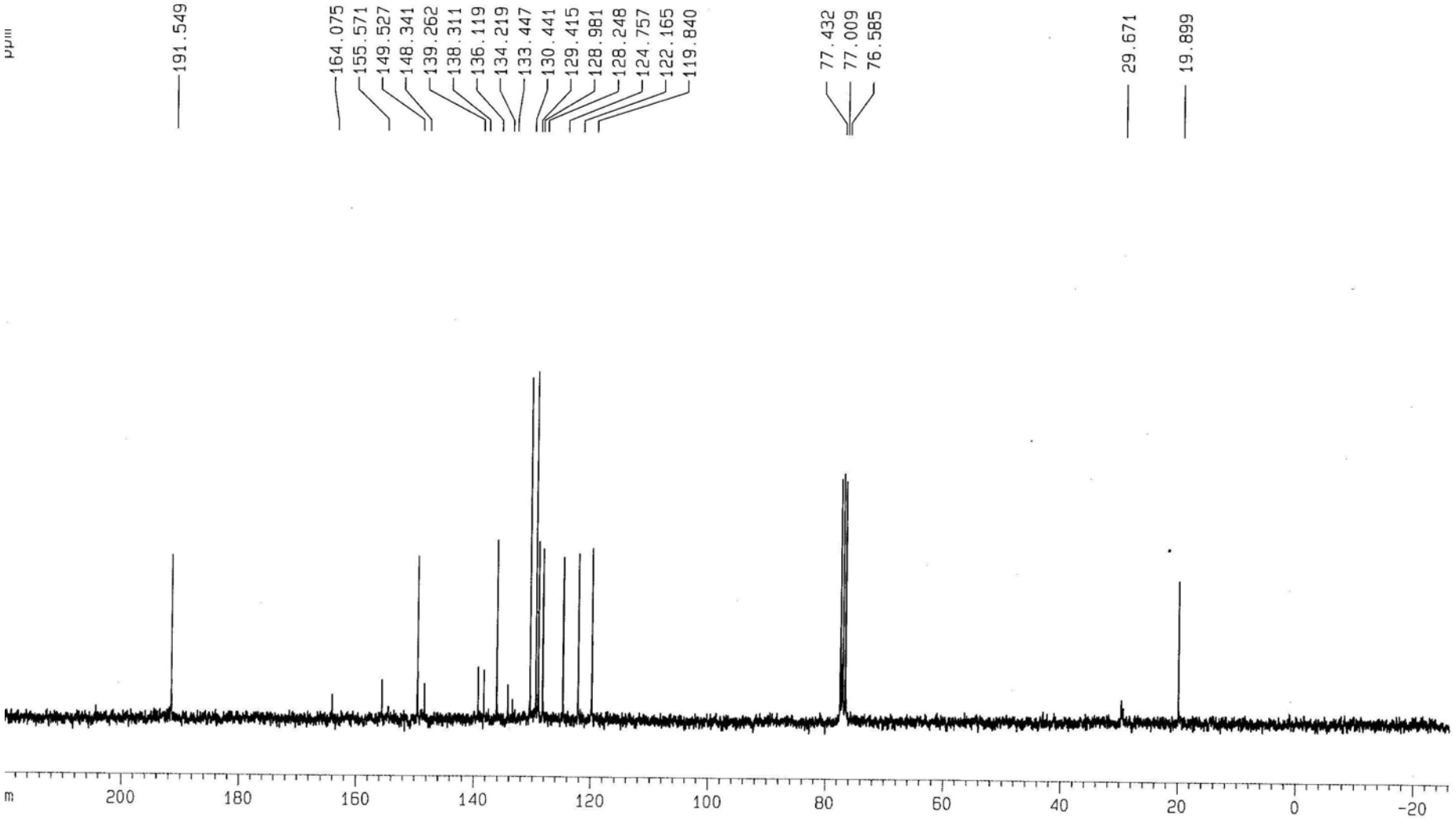
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128.248
124.757
122.165
119.840
77.432
77.009
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100
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60
40
20
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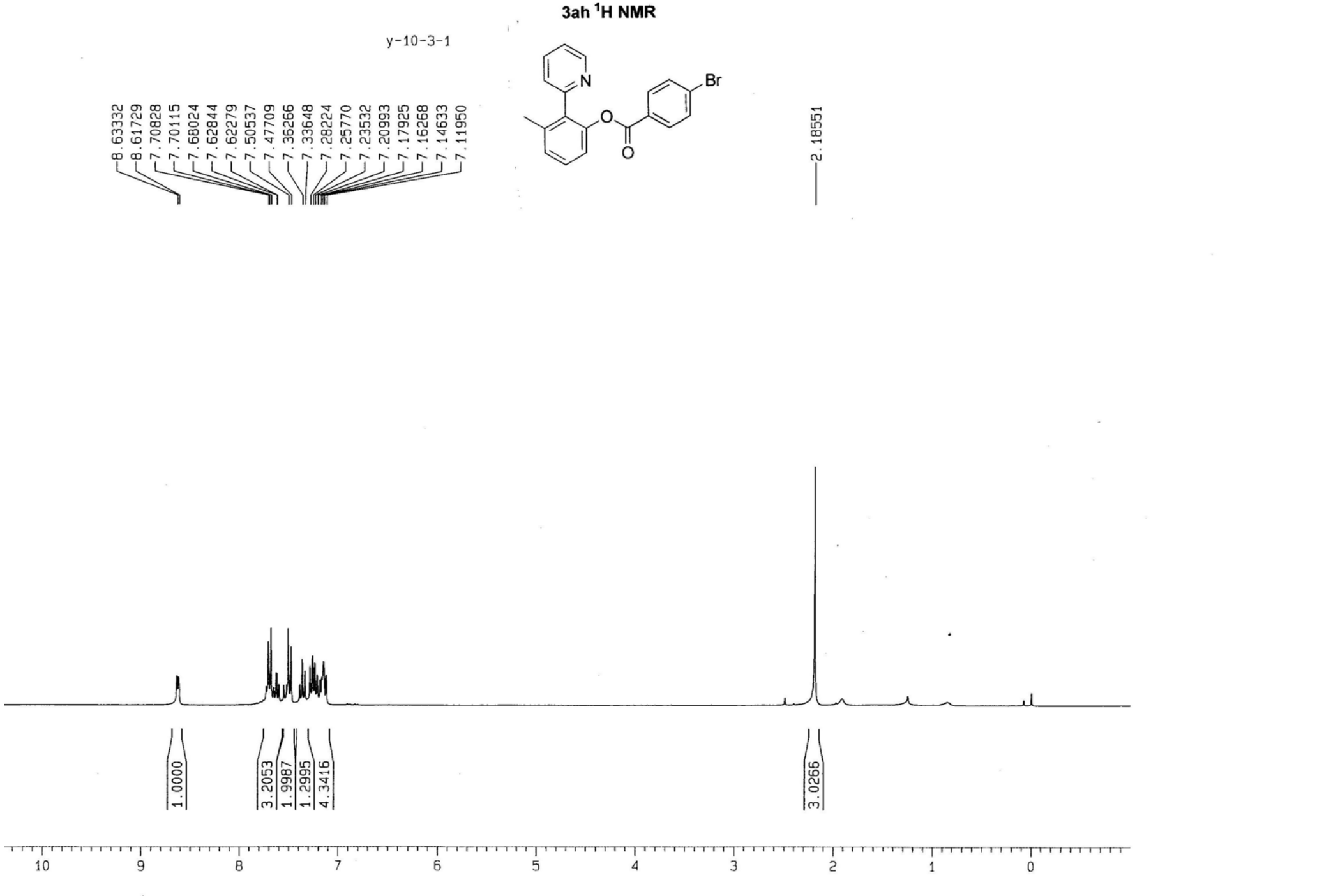
-20

3ah ^{1}H NMR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7.50537
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7.33648
7.28224
7.25770
7.23532
7.20993
7.17925
7.16268
7.14633
7.11950
2.18551
N
O
O
Br
1.0000
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7
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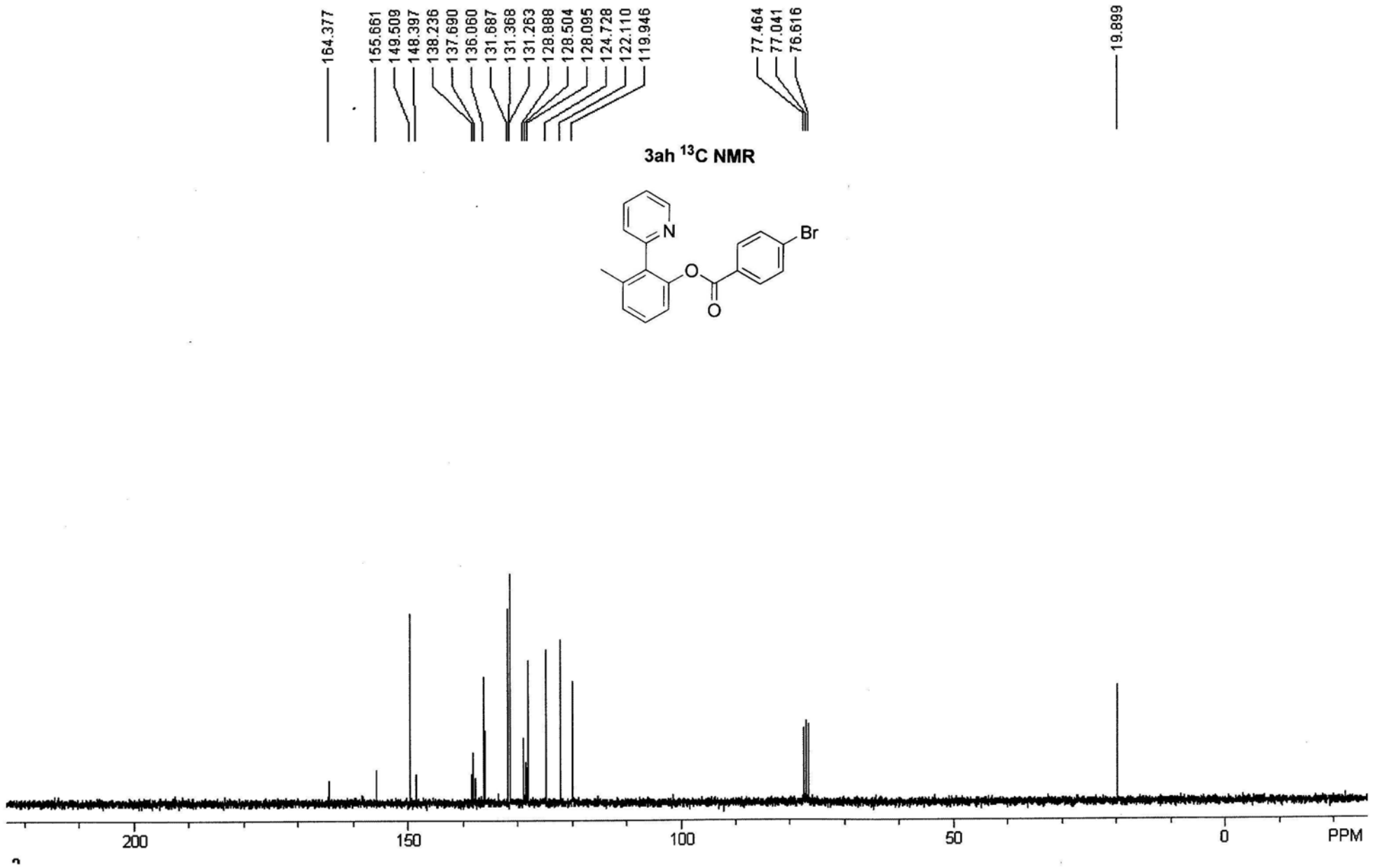
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137.690
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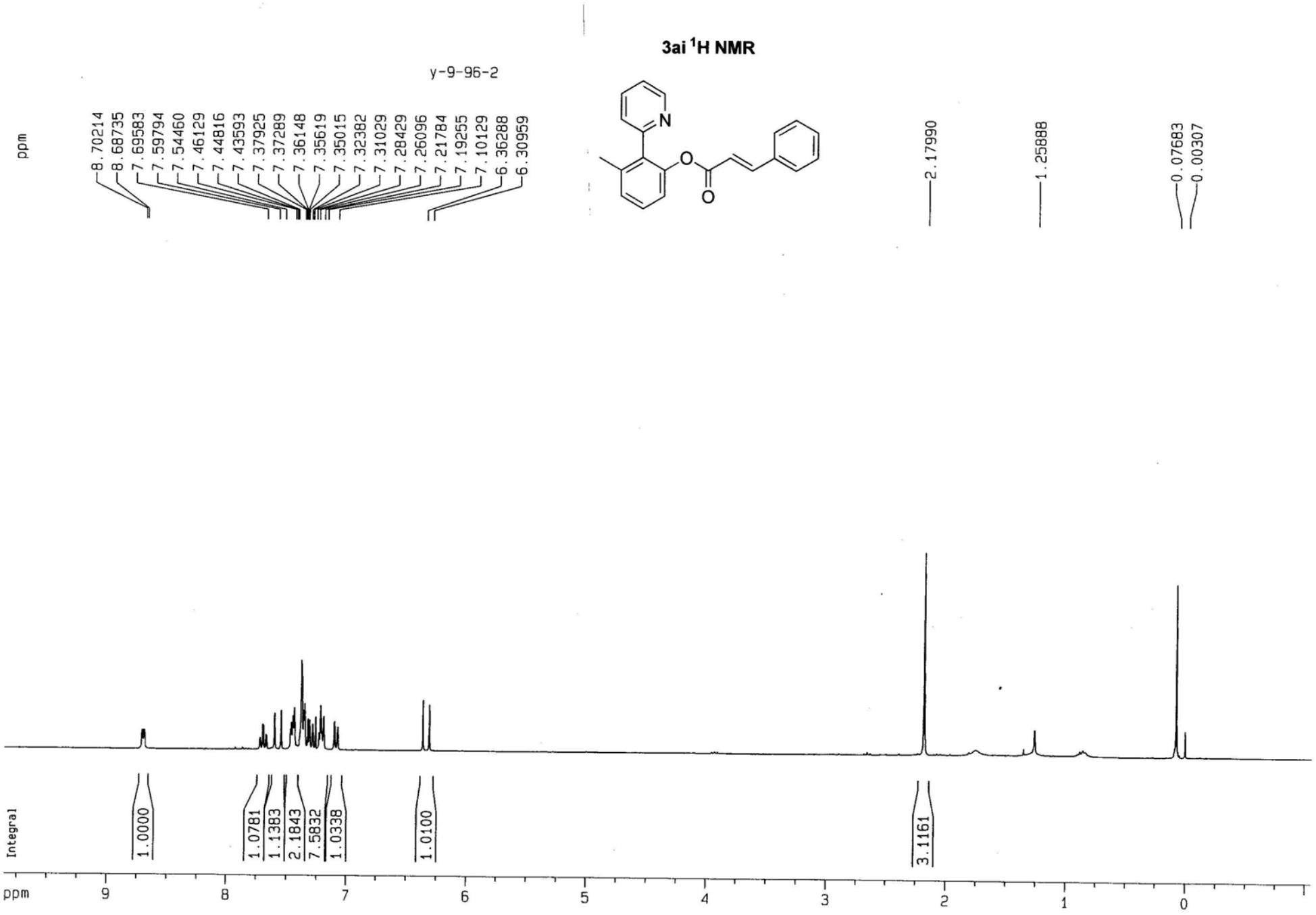
131.687
131.368
131.263
128.888
128.504
128.095
124.728
122.110
119.946
77.464
77.041
76.616
19.899
3ah ^{13}C NMR
N
Br
O
O
200
150
100
50
0
PPM


3ai ^{1}H NMR
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7.36148
7.35619
7.35015
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7.19255
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0.00307
Integral
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4
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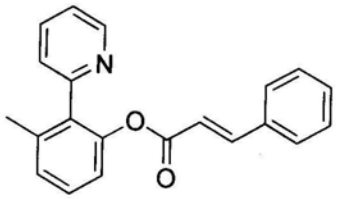
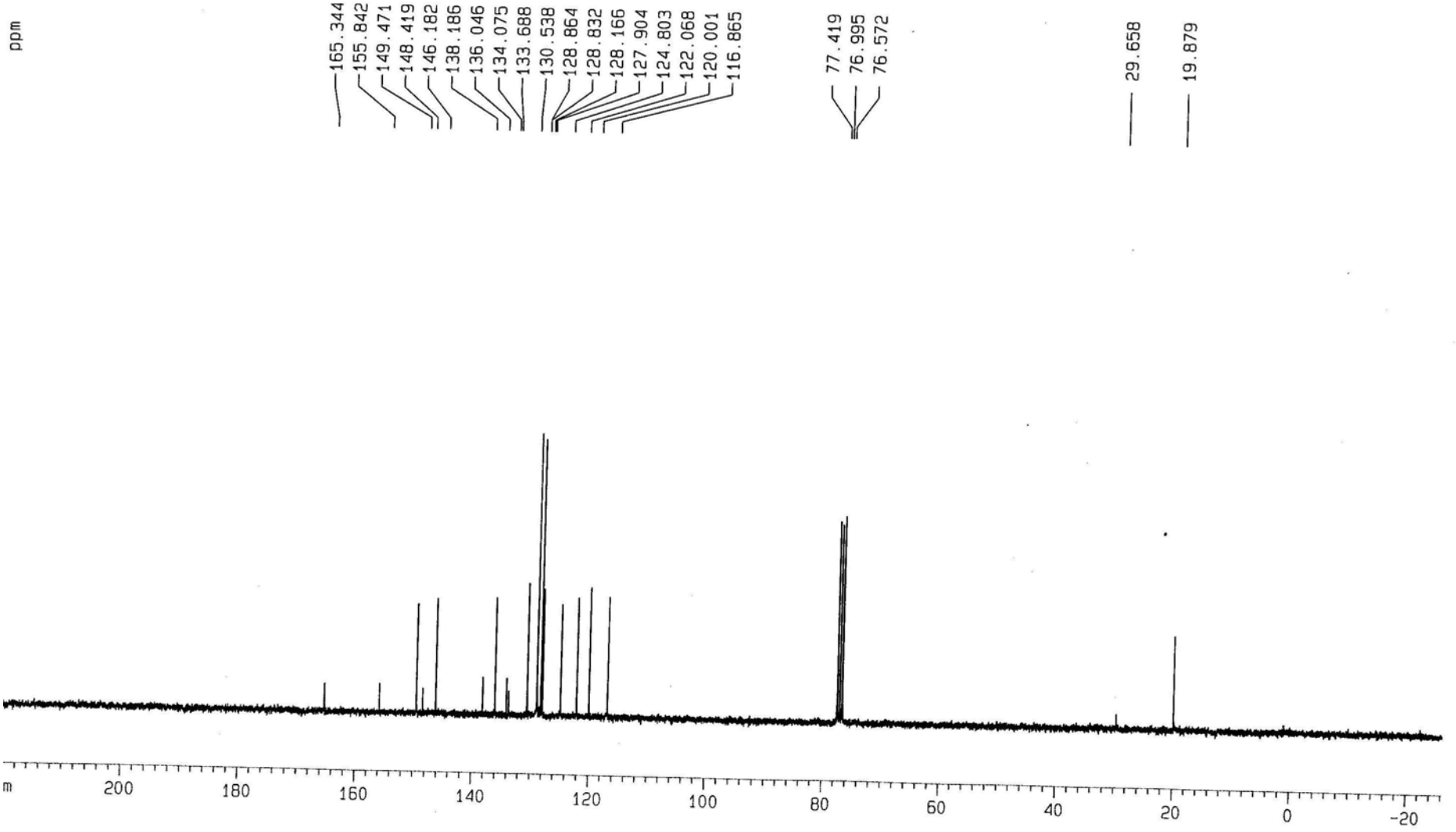
0

3ai ^{13}C NMR


N
O
O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127.904
124.803
122.068
120.001
116.865
77.419
76.995
76.572
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m
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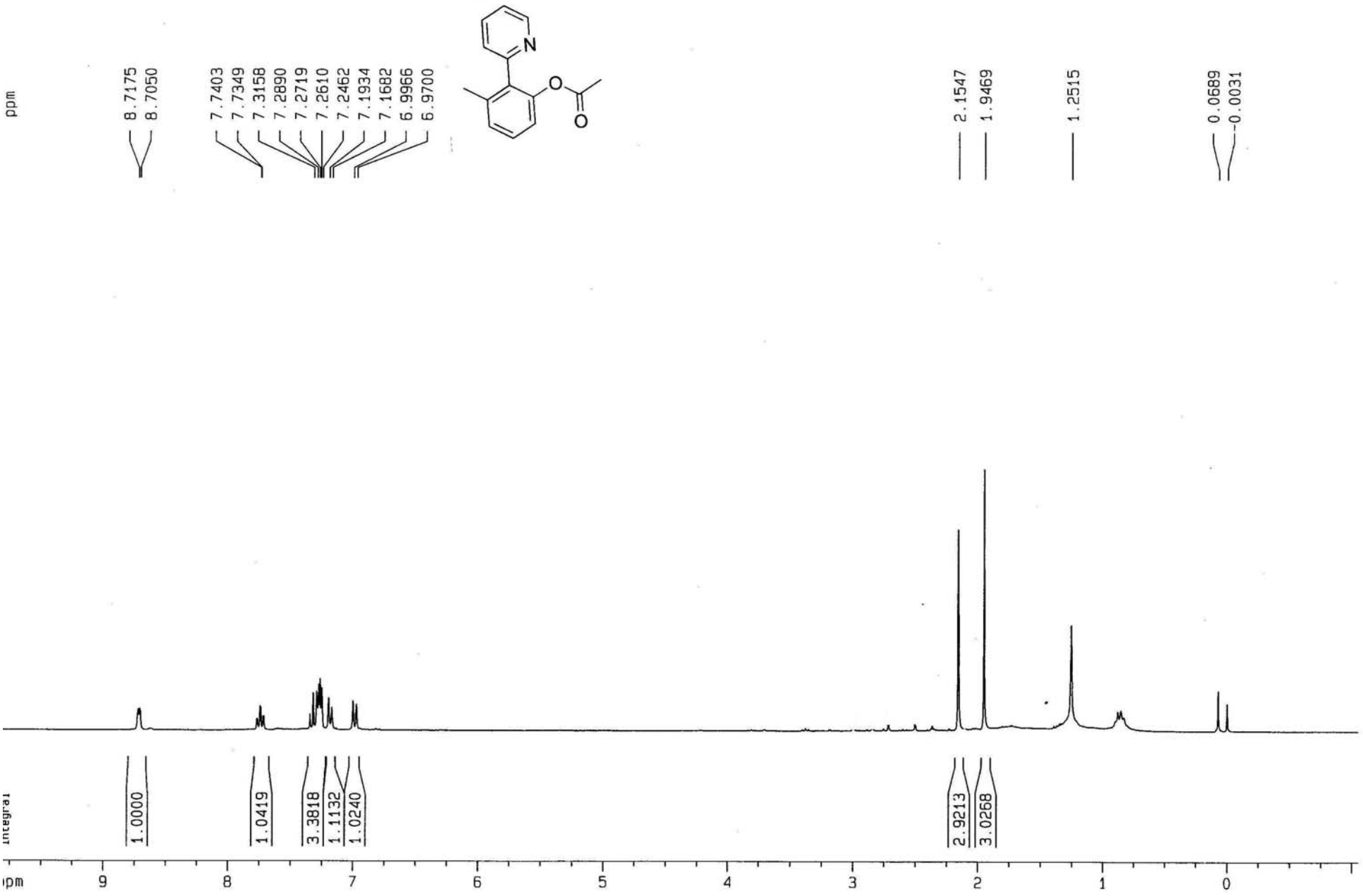
180
160
140
120
100
80
60
40
20
0
-20

3aj ^{1}H NMR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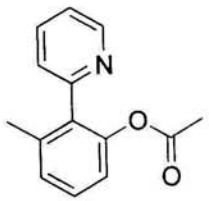
7.1682
6.9966
6.9700
2.1547
1.9469
1.2515
0.0689
0.0031
N
O
O
Integral
1.0000
1.0419
3.3818
1.1132
1.0240
2.9213
3.0268
ppm
9
8
7
6
5
4
3
2
1
0

3aj ^{13}C NMR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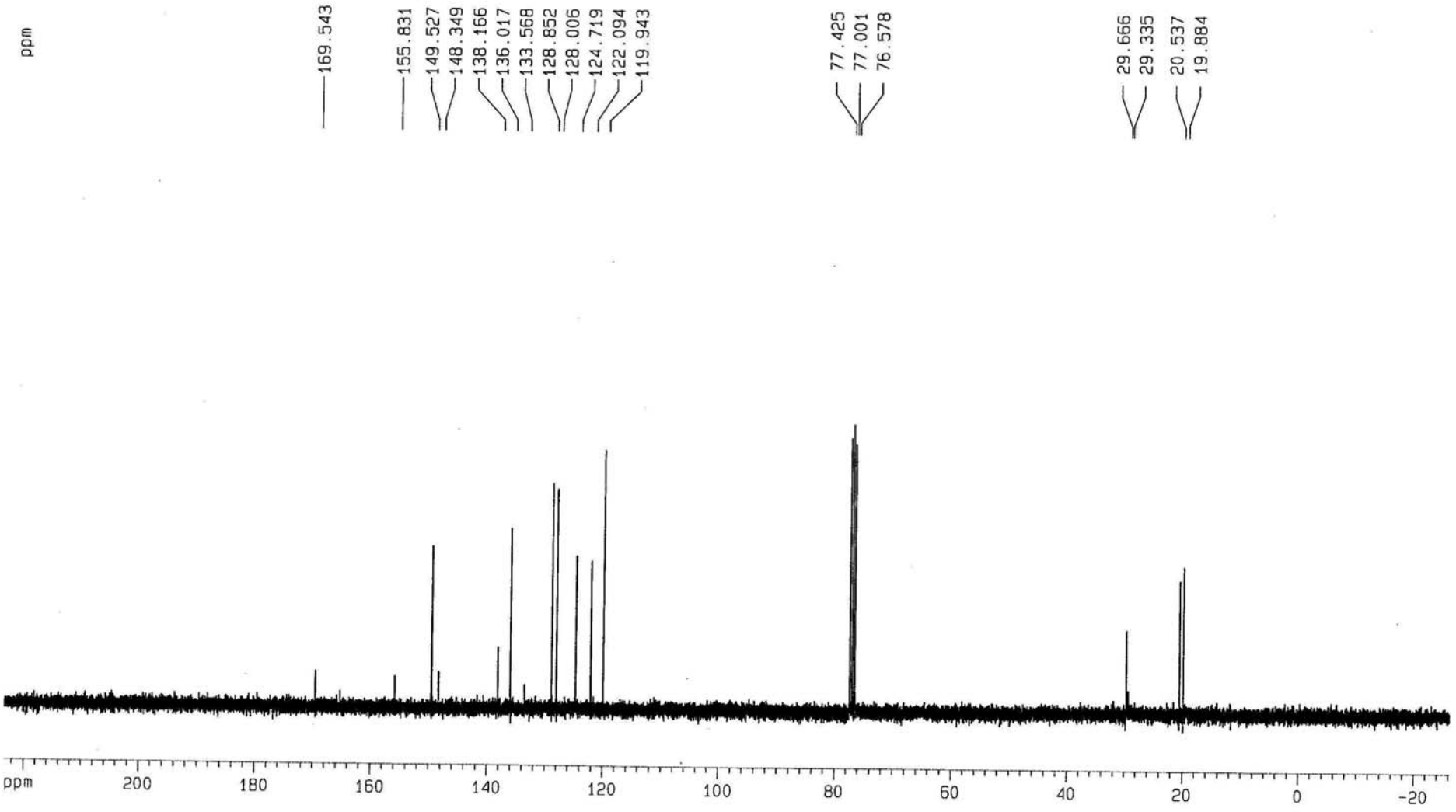
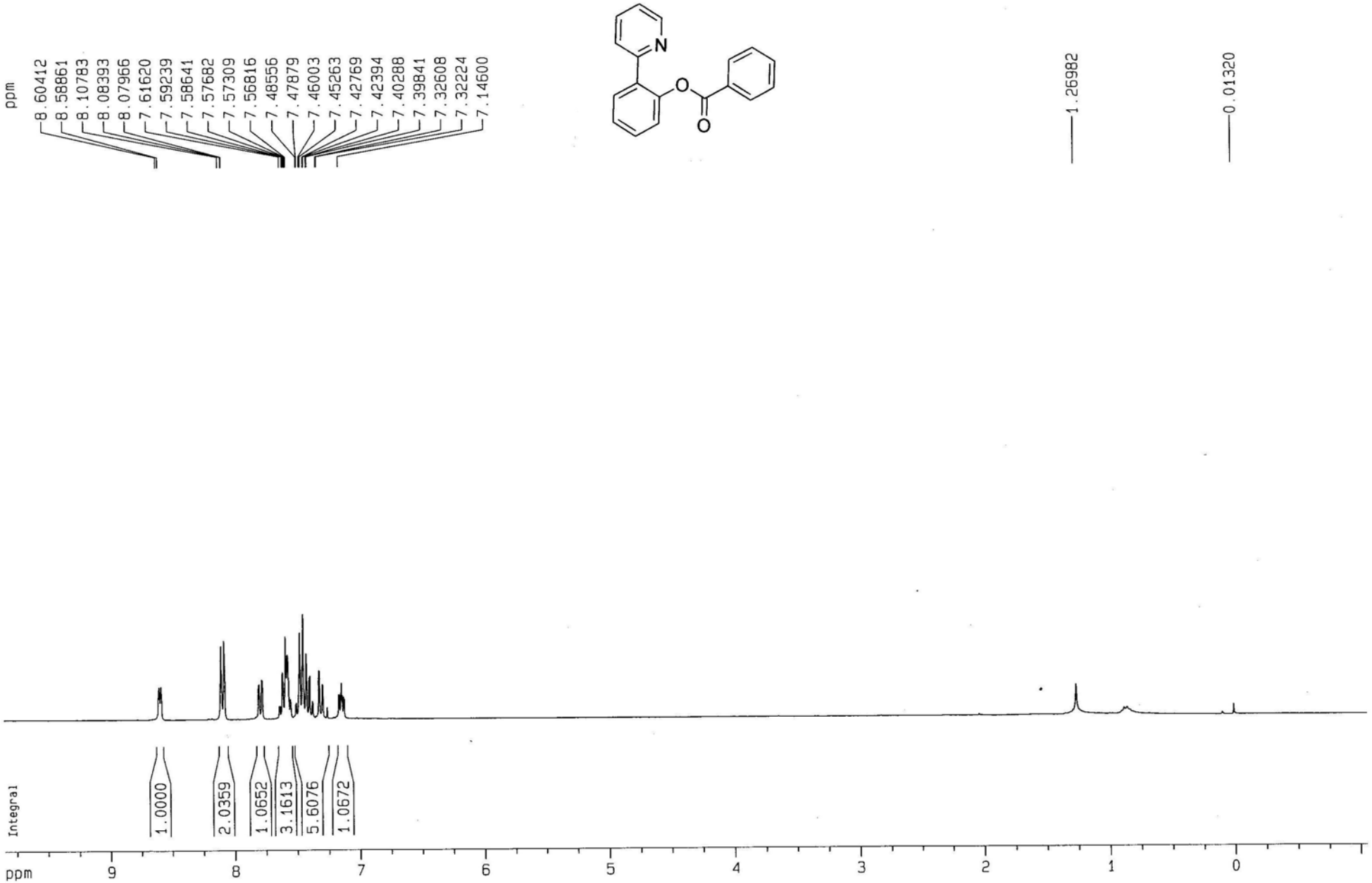
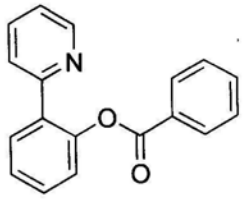
O
O

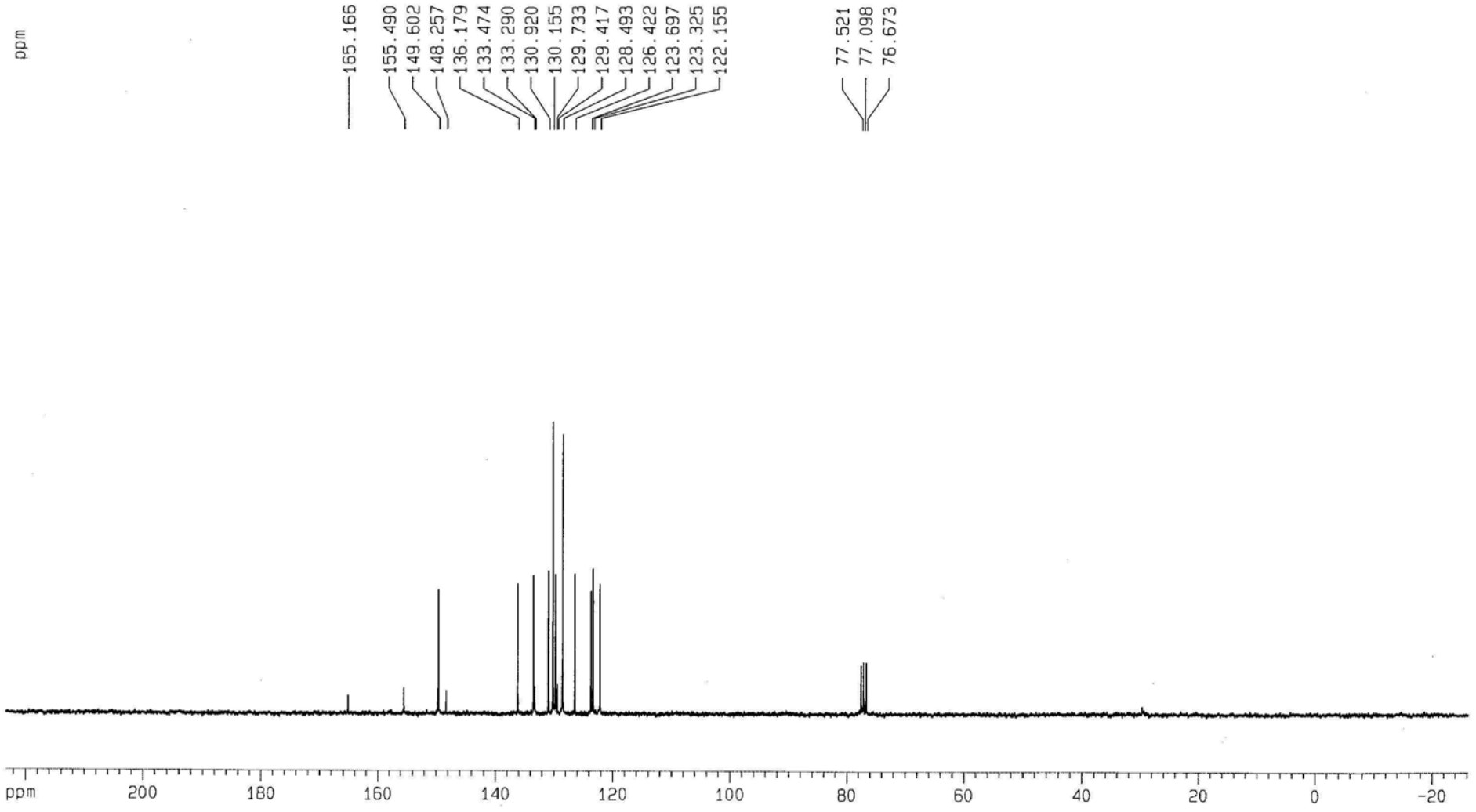

ppm
169.543
155.831
149.527
148.349
138.166
136.017
133.568
128.852
128.006
124.719
122.094
119.943
77.425
77.001
76.578
29.666
29.335
20.537
19.884
ppm
200
180
160
140
120
100
80
60
40
20
0
-20

3ba ^{1}H NMR

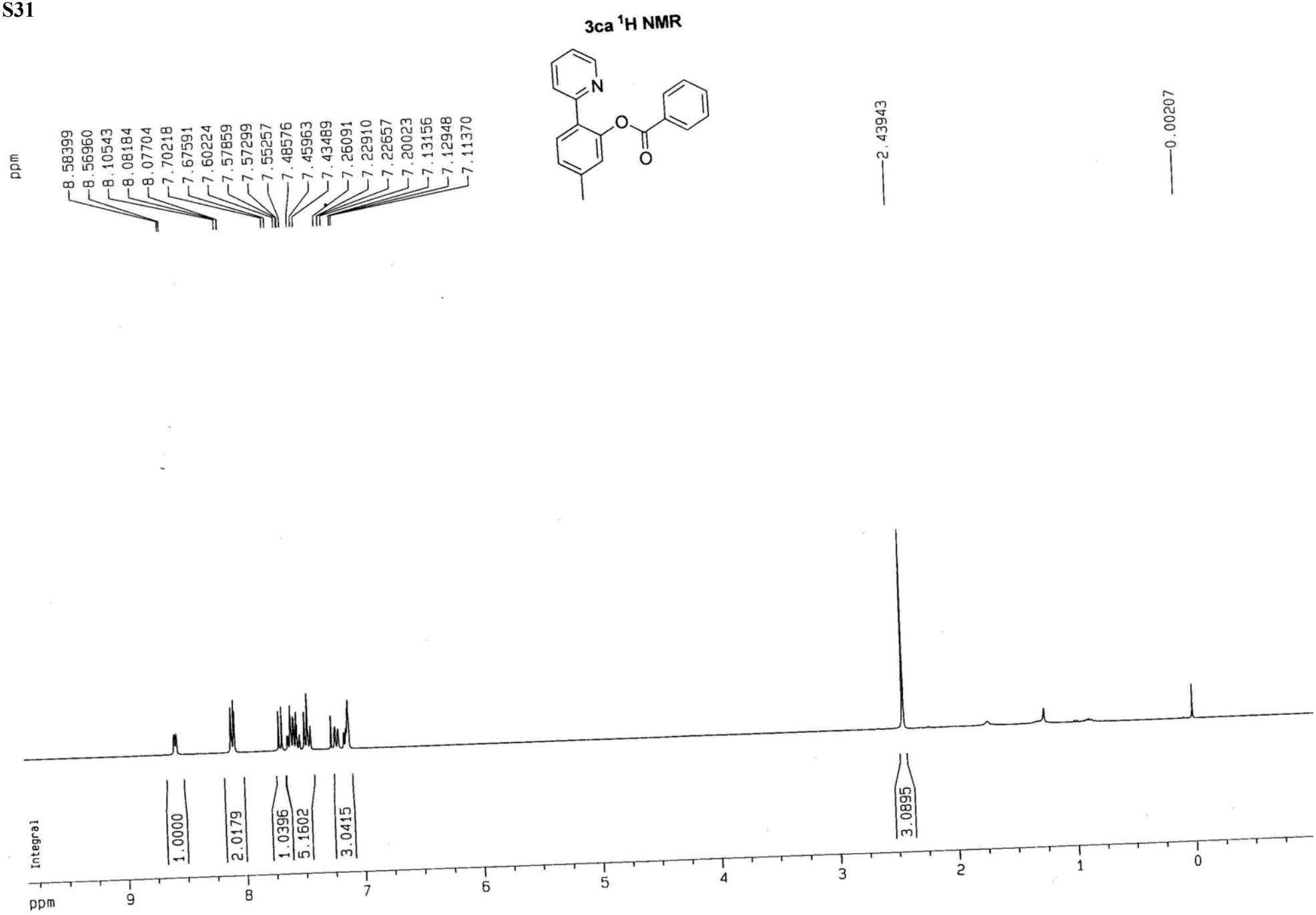

ppm
8.60412
8.58861
8.10783
8.08393
8.07966
7.61620
7.59239
7.58641
7.57682
7.57309
7.56816
7.48556
7.47879
7.46003
7.45263
7.42769
7.42394
7.40288
7.39841
7.32608
7.32224
7.14600
1.26982
0.01320
Integral
1.0000
2.0359
1.0652
3.1613
5.6076
1.0672
ppm
9
8
7
6
5
4
3
2
1
0

3ba ^{13}C NMR

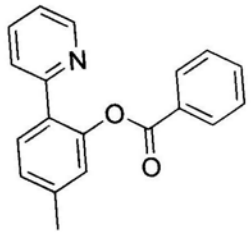

N
O
O


ppm
165.166
155.490
149.602
148.257
136.179
133.474
133.290
130.920
130.155
129.733
129.417
128.493
126.422
123.697
123.325
122.155
77.521
77.098
76.673
ppm
200
180
160
140
120
100
80
60
40
20
0
-20

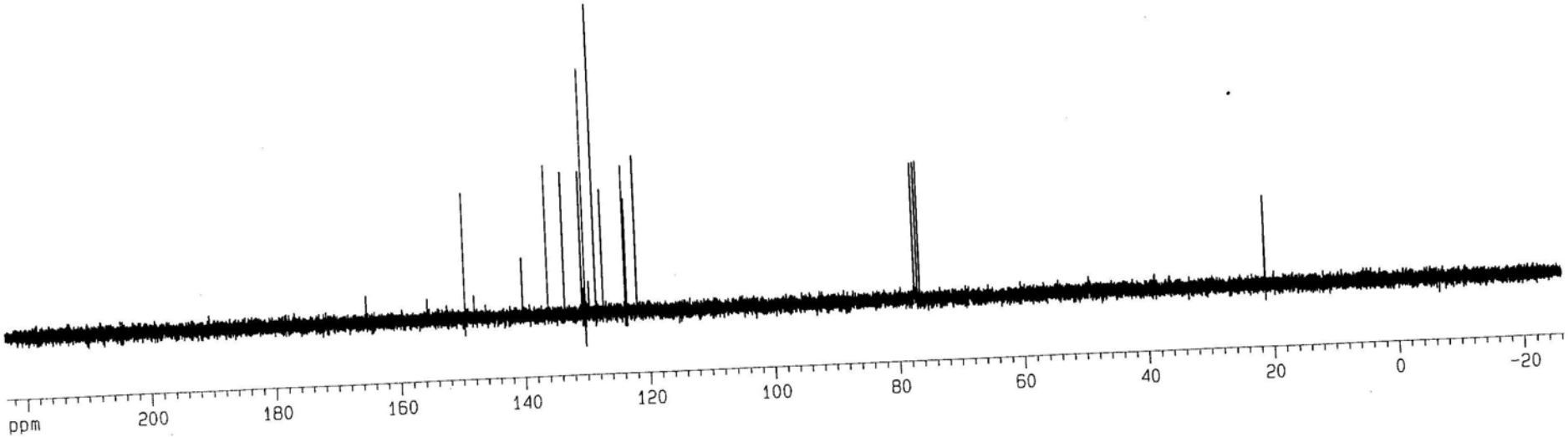
3ca ^{1}H NMR


ppm
8.58399
8.56960
8.10543
8.08184
8.07704
7.70218
7.67591
7.60224
7.57859
7.57299
7.55257
7.48576
7.45963
7.43489
7.26091
7.22910
7.22657
7.20023
7.13156
7.12948
7.11370
2.43943
0.00207
Integral
1.0000
2.0179
1.0396
5.1602
3.0415
3.0895
ppm
9
8
7
6
5
4
3
2
1
0

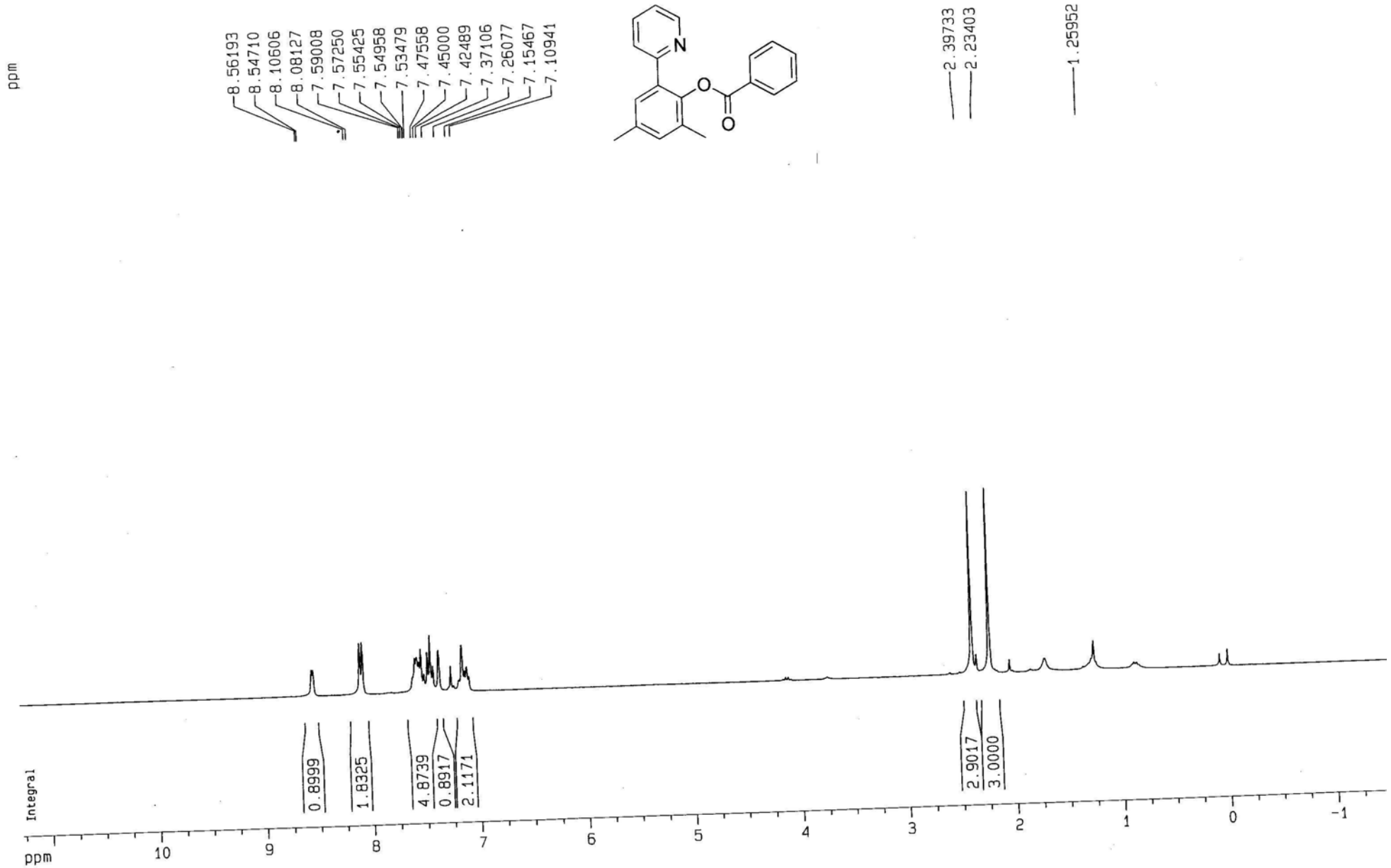
3ca ^{13}C NMR



165.287
155.537
149.539
148.055
140.178
136.095
133.399
130.627
130.338
130.143
129.509
128.456
127.287
123.737
123.527
121.878
77.434
77.011
76.587
21.196



3da ^{1}H NMR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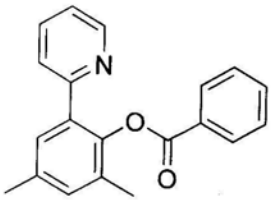
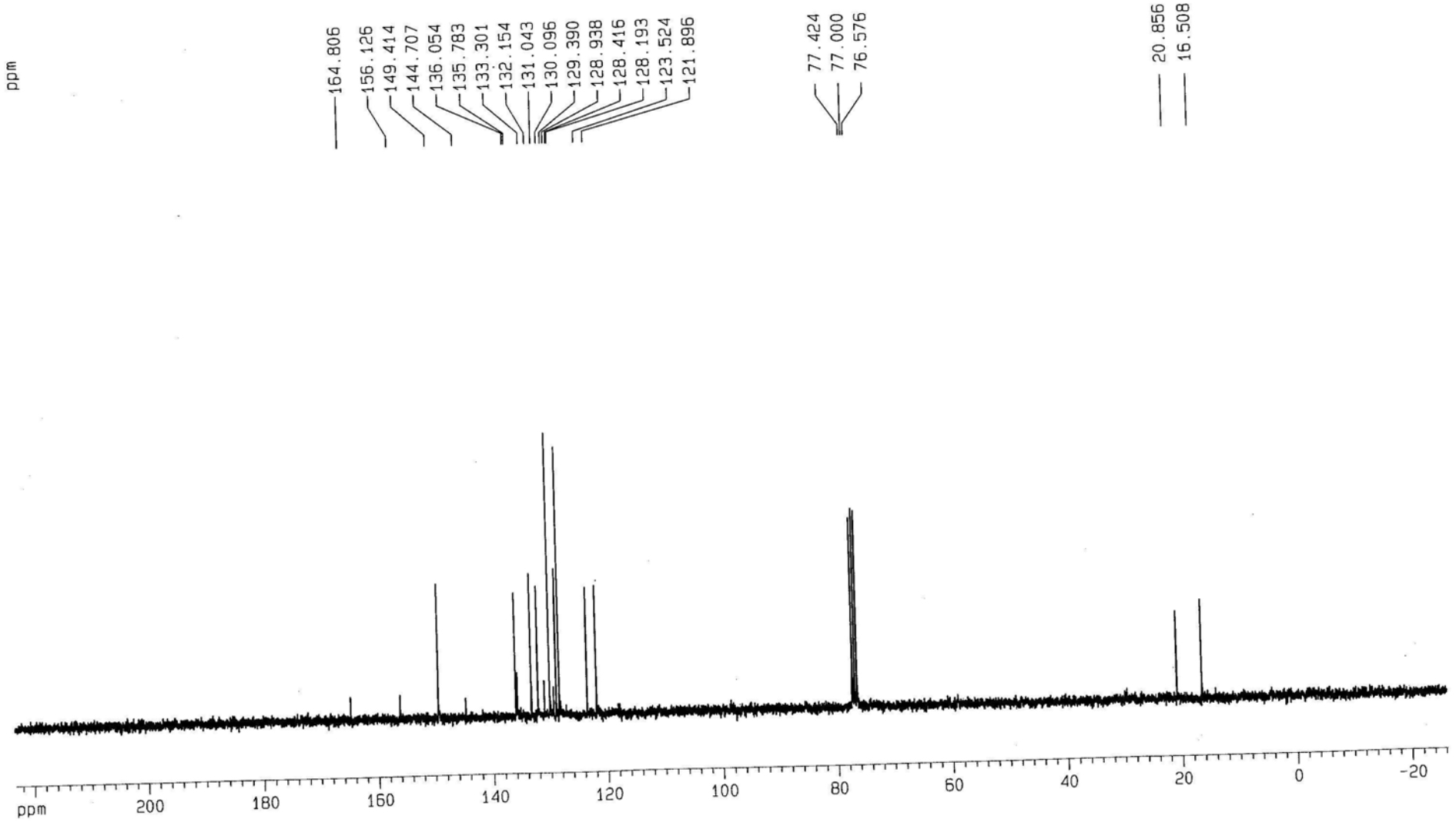
8.54710
8.10606
8.08127
7.59008
7.57250
7.55425
7.54958
7.53479
7.47558
7.45000
7.42489
7.37106
7.26077
7.15467
7.10941
N
O
O
2.39733
2.23403
1.25952
Integral
0.8999
1.8325
4.8739
0.8917
2.1171
2.9017
3.0000
ppm
10
9
8
7
6
5
4
3
2
1
0
-1

3da ^{13}C NMR


N
O
O


ppm
164.806
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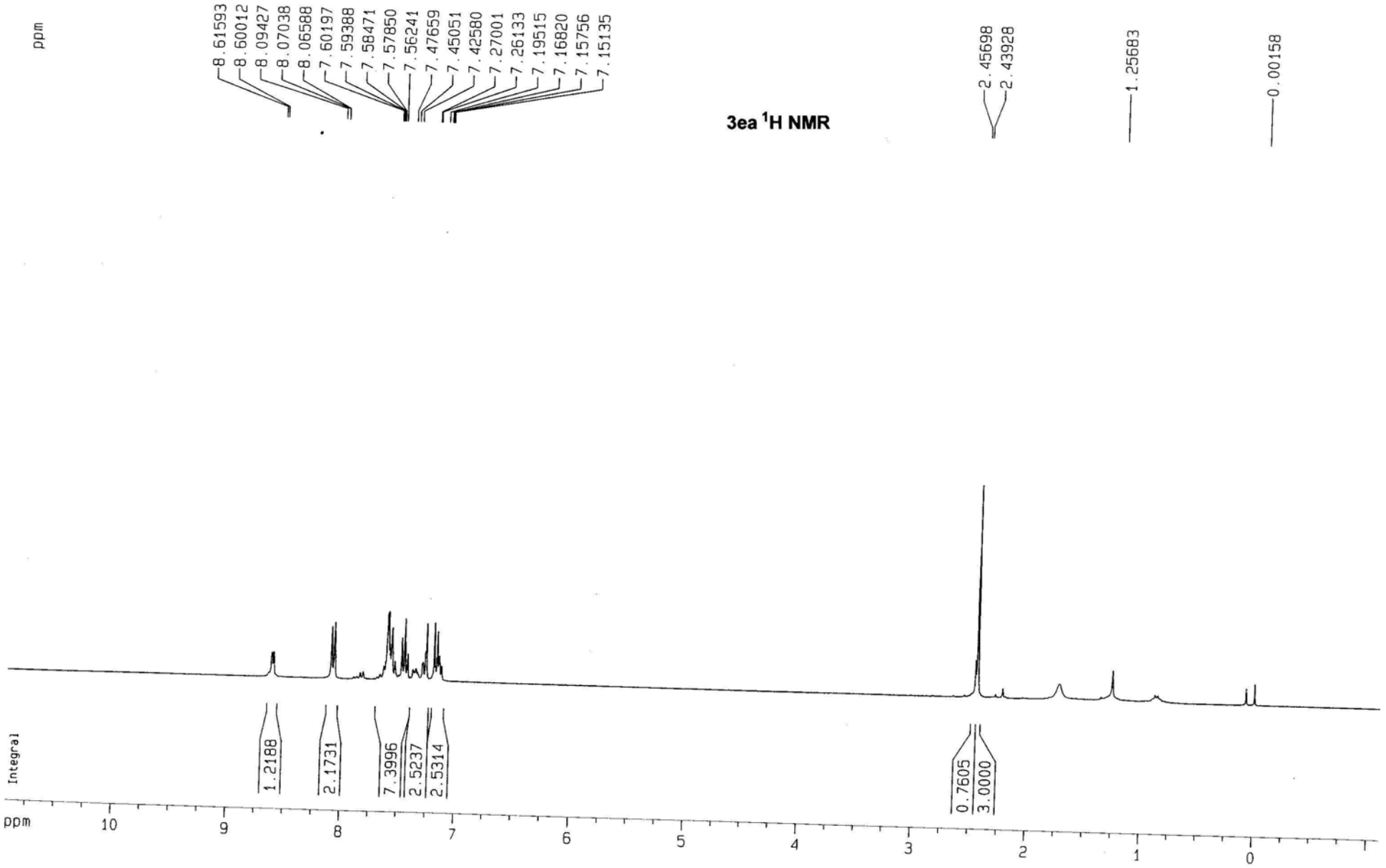
149.414
144.707
136.054
135.783
133.301
132.154
131.043
130.096
129.390
128.938
128.416
128.193
123.524
121.896
77.424
77.000
76.576
20.856
16.508
ppm
200
180
160
140
120
100
80
60
40
20
0
-20


ppm
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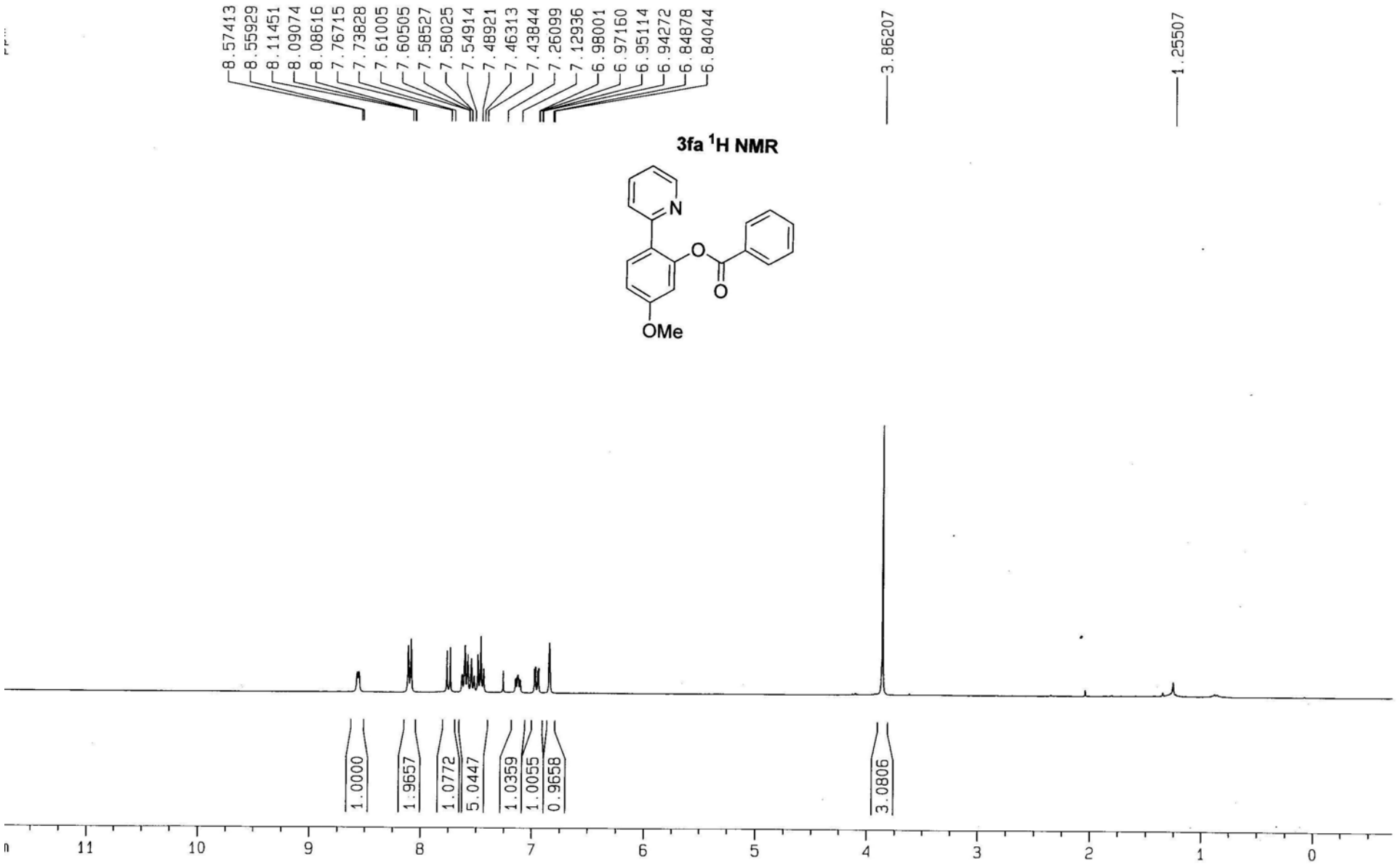
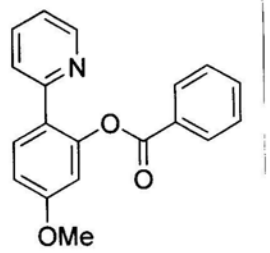
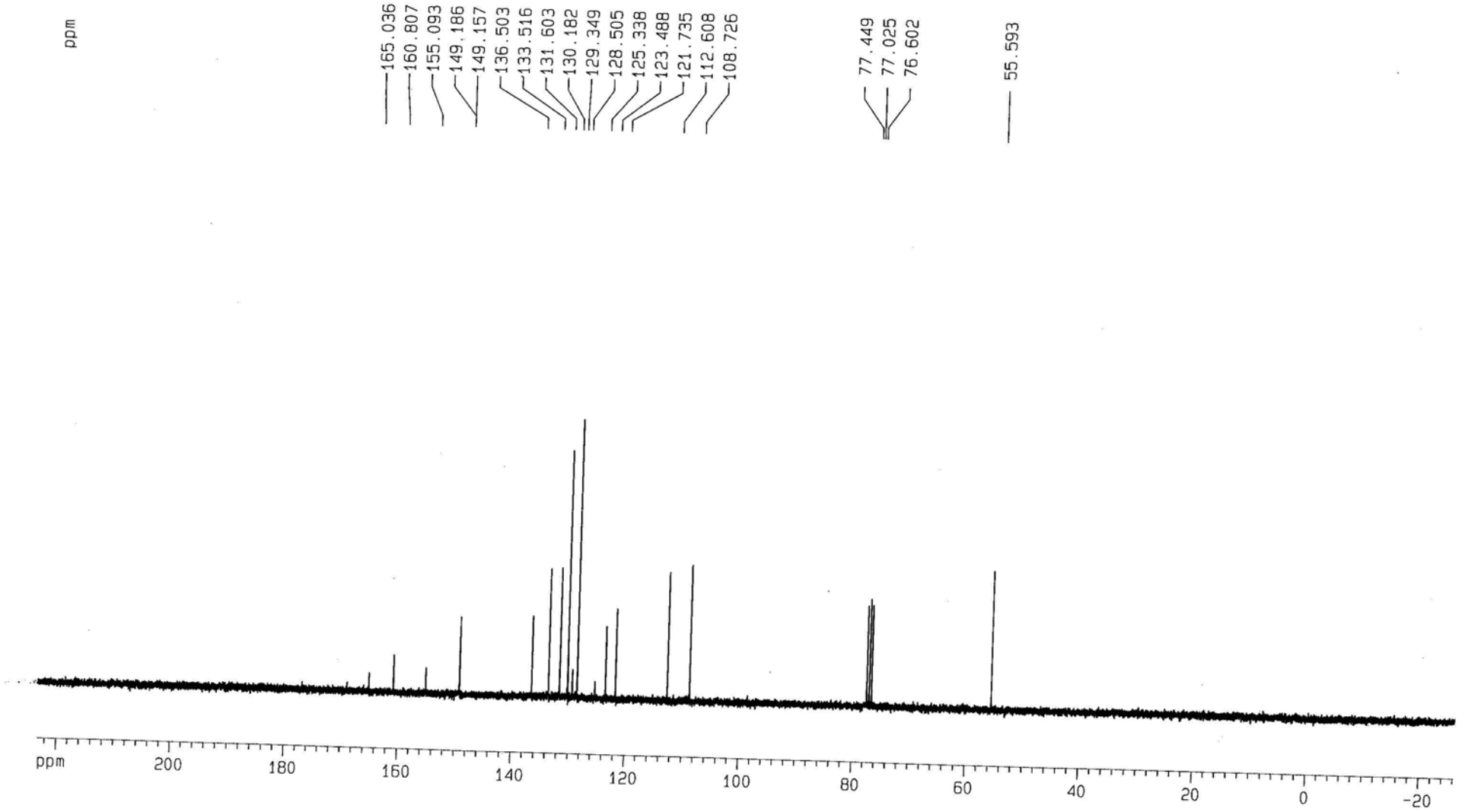
8.60012
8.09427
8.07038
8.06588
7.60197
7.59388
7.58471
7.57850
7.56241
7.47659
7.45051
7.42580
7.27001
7.26133
7.19515
7.16820
7.15756
7.15135
3ea ^{1}H NMR
2.45698
2.43928
1.25683
0.00158
Integral
1.2188
2.1731
7.3996
2.5237
2.5314
0.7605
3.0000
ppm
10
9
8
7
6
5
4
3
2
1
0


8.57413
8.55929
8.11451
8.09074
8.08616
7.76715
7.73828
7.61005
7.60505
7.58527
7.58025
7.54914
7.48921
7.46313
7.43844
7.26099
7.12936
6.98001
6.97160
6.95114
6.94272
6.84878
6.84044
3.86207
1.25507
3fa ^{1}H NMR
N
O
O
OMe
1.0000
1.9657
1.0772
5.0447
1.0359
1.0055
0.9658
3.0806
11
10
9
8
7
6
5
4
3
2
1
0

3fa ^{13}C NMR


N
O
O
OMe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165.036
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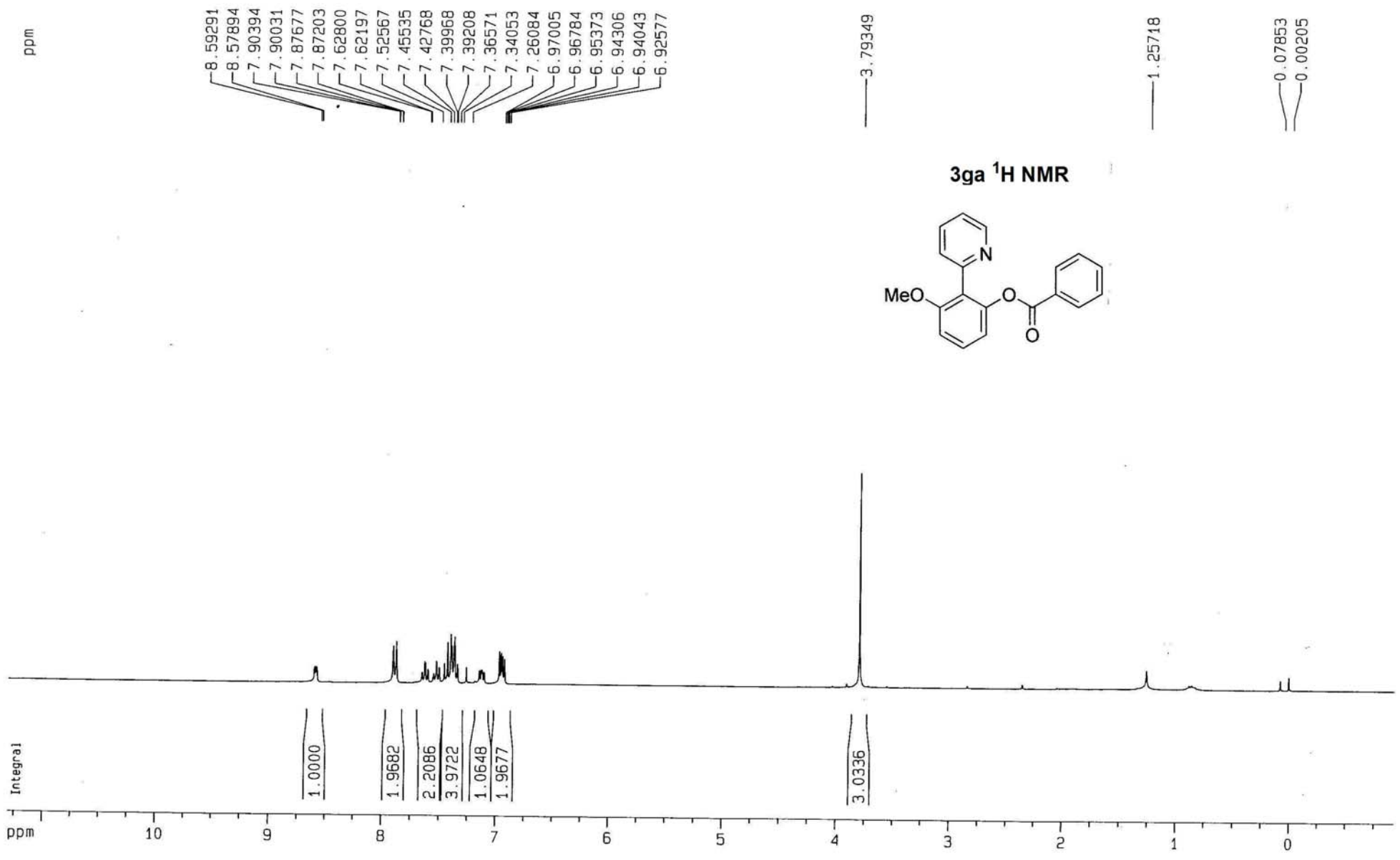
155.093
149.186
149.157
136.503
133.516
131.603
130.182
129.349
128.505
125.338
123.488
121.735
112.608
108.726
77.449
77.025
76.602
55.593
ppm
200
180
160
140
120
100
80
60
40
20
0
-20


ppm
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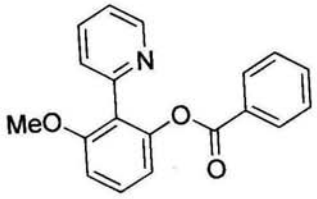
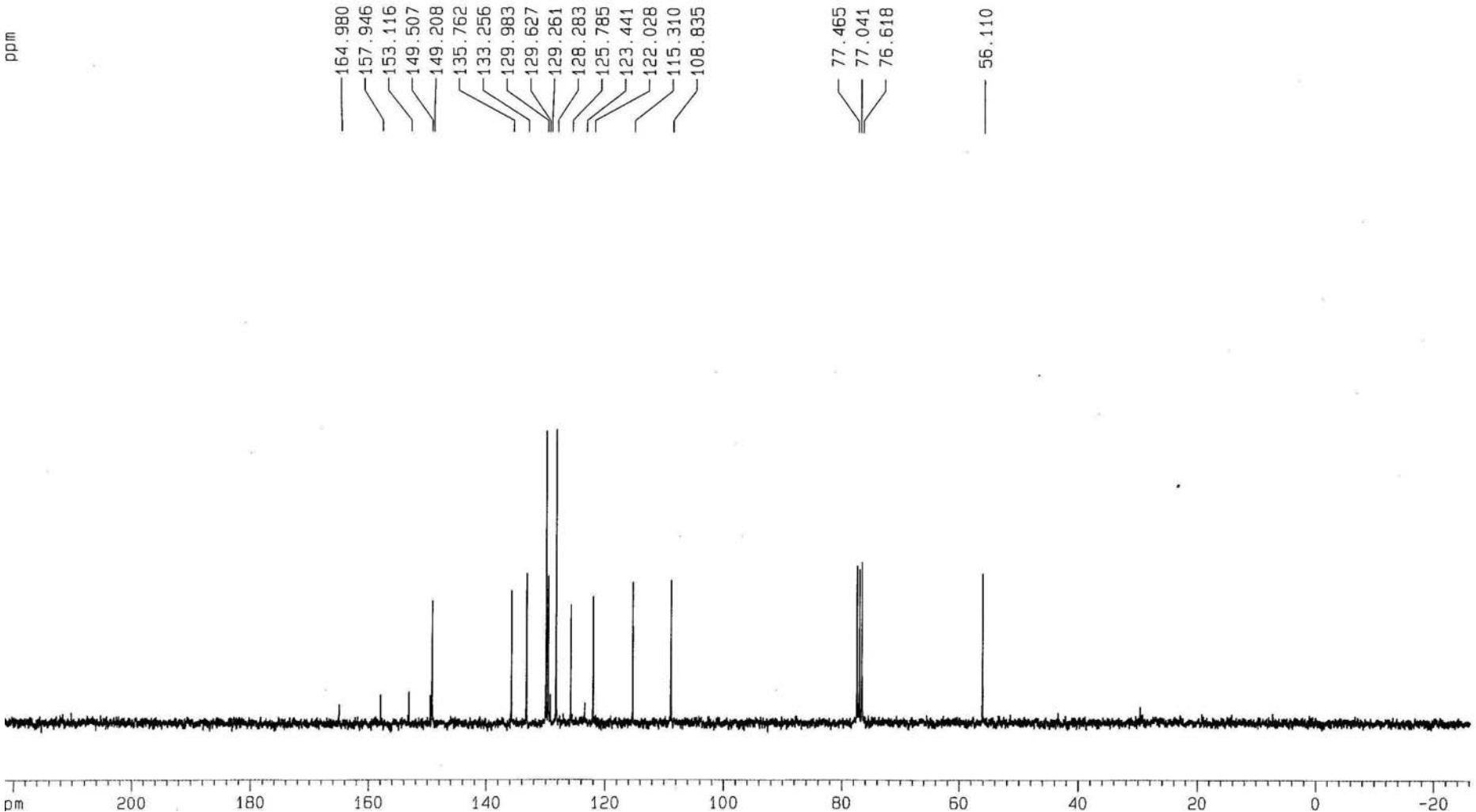
8.57894
7.90394
7.90031
7.87677
7.87203
7.62800
7.62197
7.52567
7.45535
7.42768
7.39968
7.39208
7.36571
7.34053
7.26084
6.97005
6.96784
6.95373
6.94306
6.94043
6.92577
3.79349
1.25718
0.07853
0.00205
3ga ^{1}H NMR
N
MeO
O
O
Integral
1.0000
1.9682
2.2086
3.9722
1.0648
1.9677
3.0336
ppm
10
9
8
7
6
5
4
3
2
1
0

3ga ^{13}C NMR


N
MeO
O
O


ppm
164.980
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149.208
135.762
133.256
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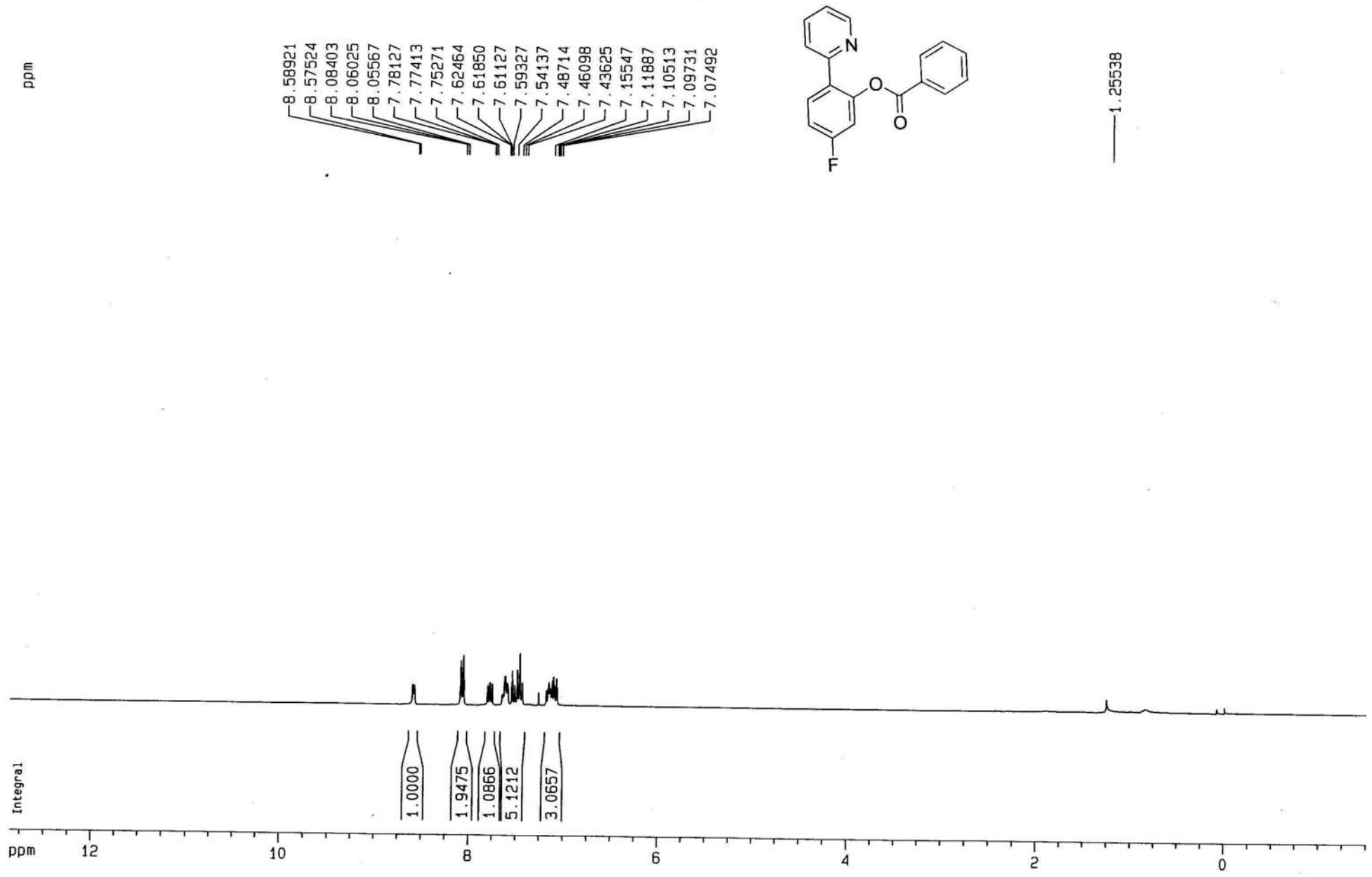
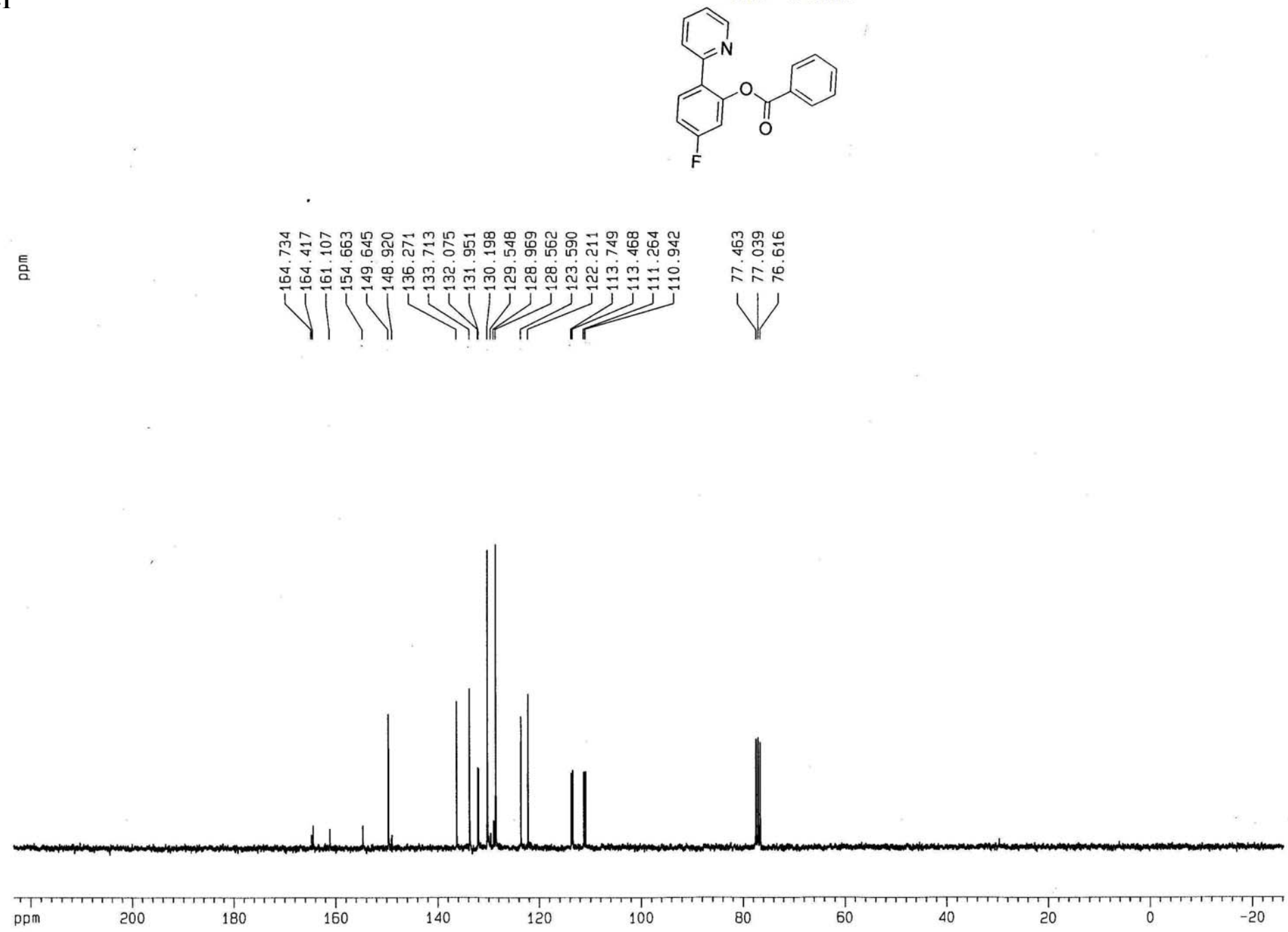
129.627
129.261
128.283
125.785
123.441
122.028
115.310
108.835
77.465
77.041
76.618
56.110
pm
200
180
160
140
120
100
80
60
40
20
0
-20

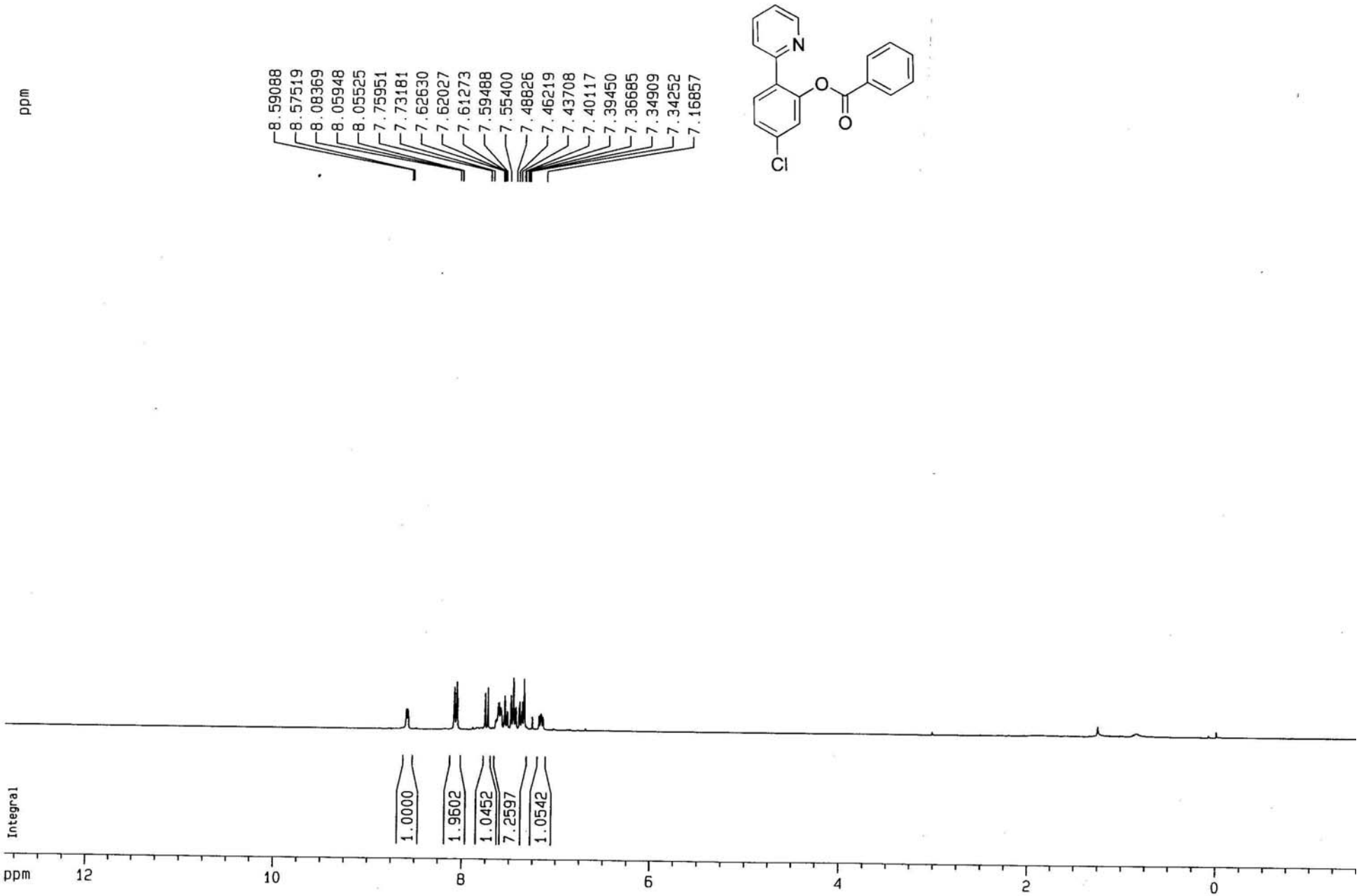
3ha ^{1}H NMR


ppm
8.58921
8.57524
8.08403
8.06025
8.05567
7.78127
7.77413
7.75271
7.62464
7.61850
7.61127
7.59327
7.54137
7.48714
7.46098
7.43625
7.15547
7.11887
7.10513
7.09731
7.07492
1.25538
N
O
O
F
Integral
1.0000
1.9475
1.0866
5.1212
3.0657
ppm
12
10
8
6
4
2
0

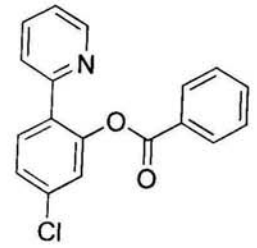
3ha ^{13}C NMR

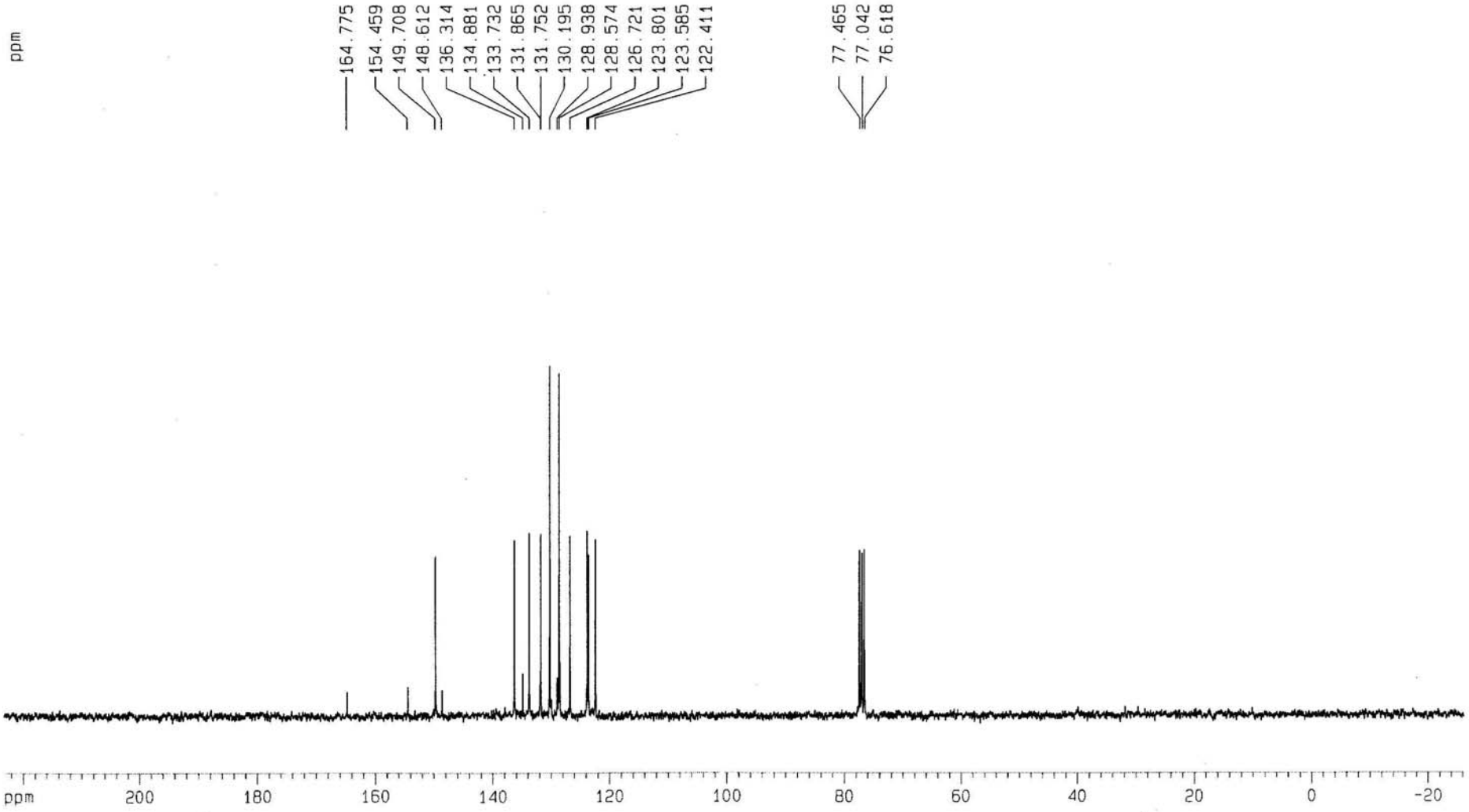

N
O
O
F
ppm
164.734
164.417
161.107
154.663
149.645
148.920
136.271
133.713
132.075
131.951
130.198
129.548
128.969
128.562
123.590
122.211
113.749
113.468
111.264
110.942
77.463
77.039
76.616
ppm
200
180
160
140
120
100
80
60
40
20
0
-20

3ia ^{1}H NMR


ppm
8.59088
8.57519
8.08369
8.05948
8.05525
7.75951
7.73181
7.62630
7.62027
7.61273
7.59488
7.55400
7.48826
7.46219
7.43708
7.40117
7.39450
7.36685
7.34909
7.34252
7.16857
N
O
O
Cl
Integral
1.0000
1.9602
1.0452
7.2597
1.0542
ppm
12
10
8
6
4
2
0

3ia ^{13}C NMR


N
O
O
Cl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149.708
148.612
136.314
134.881
133.732
131.865
131.752
130.195
128.938
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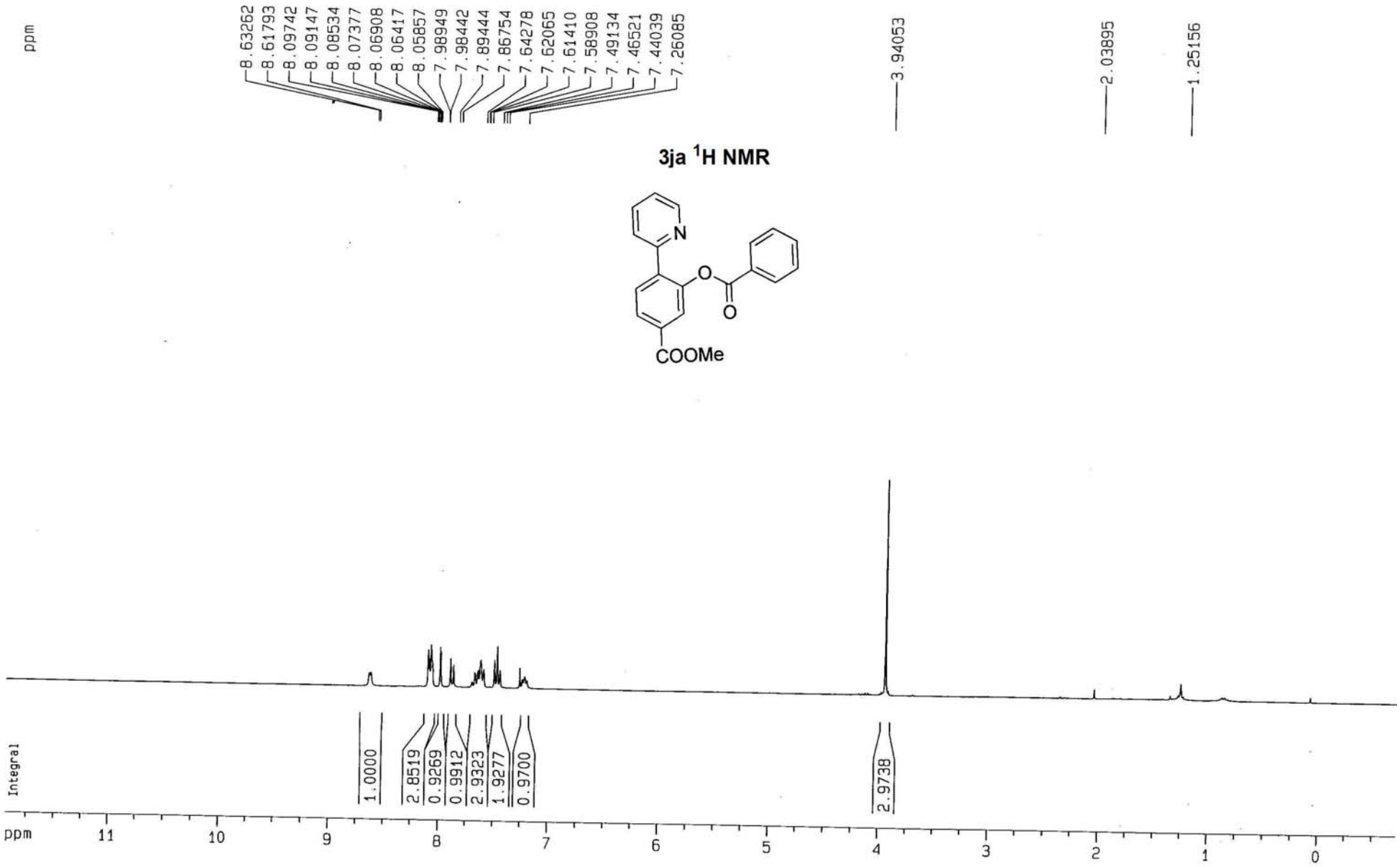
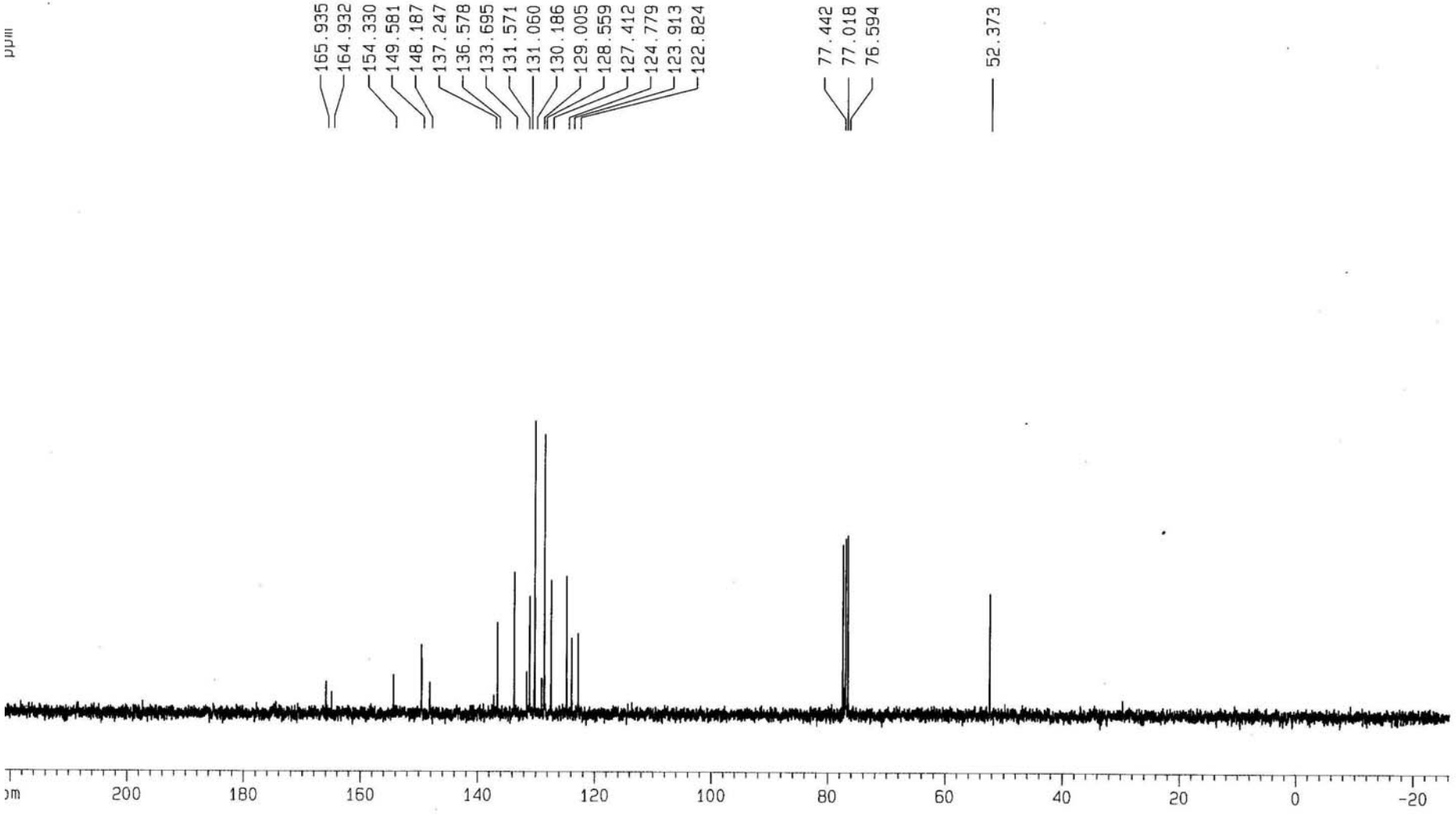
123.801
123.585
122.411
77.465
77.042
76.618
ppm
200
180
160
140
120
100
80
60
40
20
0
-20

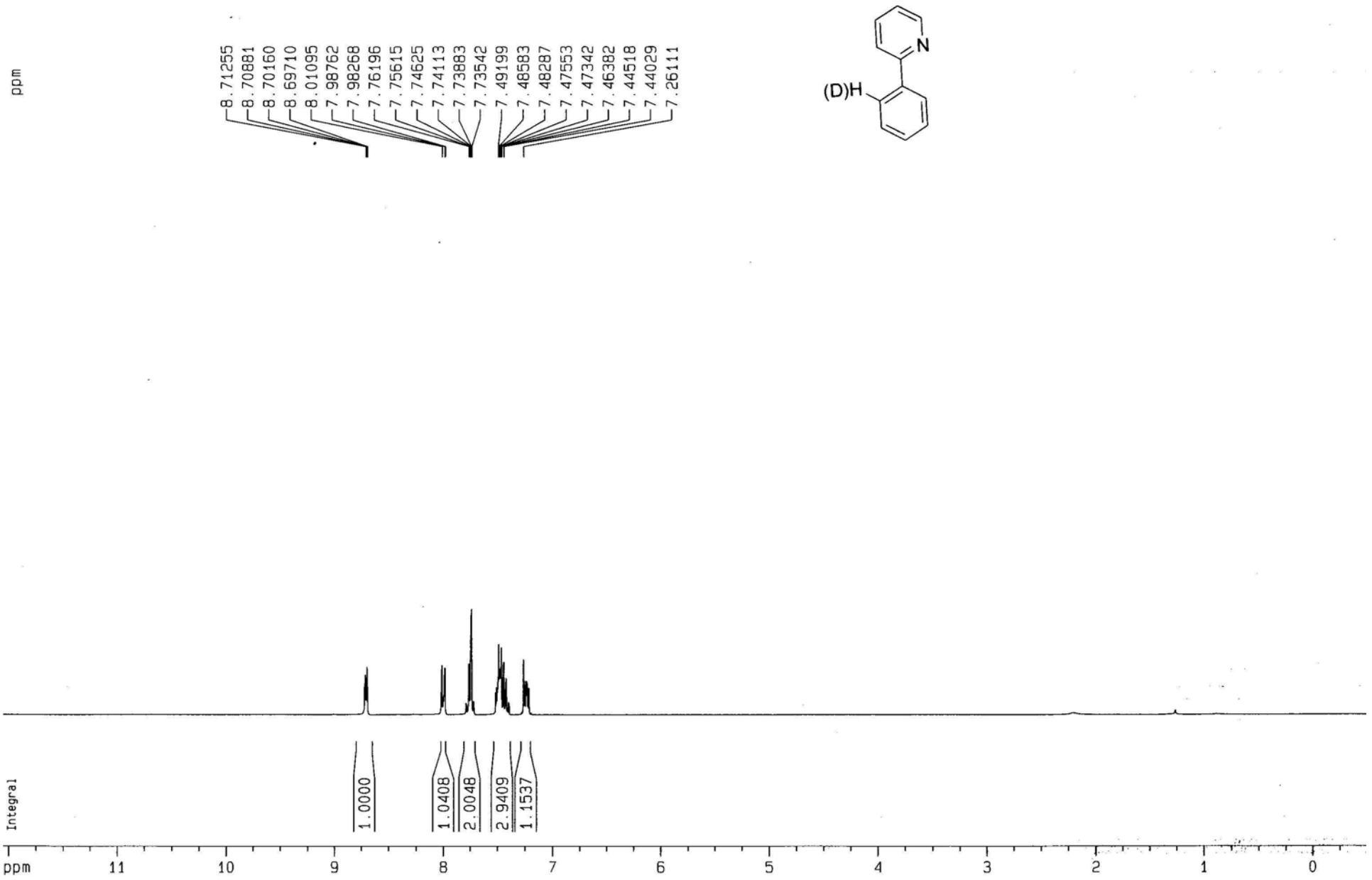

ppm
8.63262
8.61793
8.09742
8.09147
8.08534
8.07377
8.06908
8.06417
8.05857
7.98949
7.98442
7.89444
7.86754
7.64278
7.62065
7.61410
7.58908
7.49134
7.46521
7.44039
7.26085
3.94053
2.03895
1.25156
3ja ^{1}H NMR
N
O
O
COOMe
Integral
1.0000
2.8519
0.9269
0.9912
2.9323
1.9277
0.9700
2.9738
ppm
11
10
9
8
7
6
5
4
3
2
1
0

3ja ^{13}C NMR


N
O
O
COOMe


165.935
164.932
154.330
149.581
148.187
137.247
136.578
133.695
131.571
131.060
130.186
129.005
128.559
127.412
124.779
123.913
122.824
77.442
77.018
76.594
52.373
200
180
160
140
120
100
80
60
40
20
0
-20

3b' ^{1}H NMR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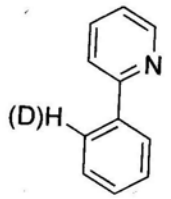
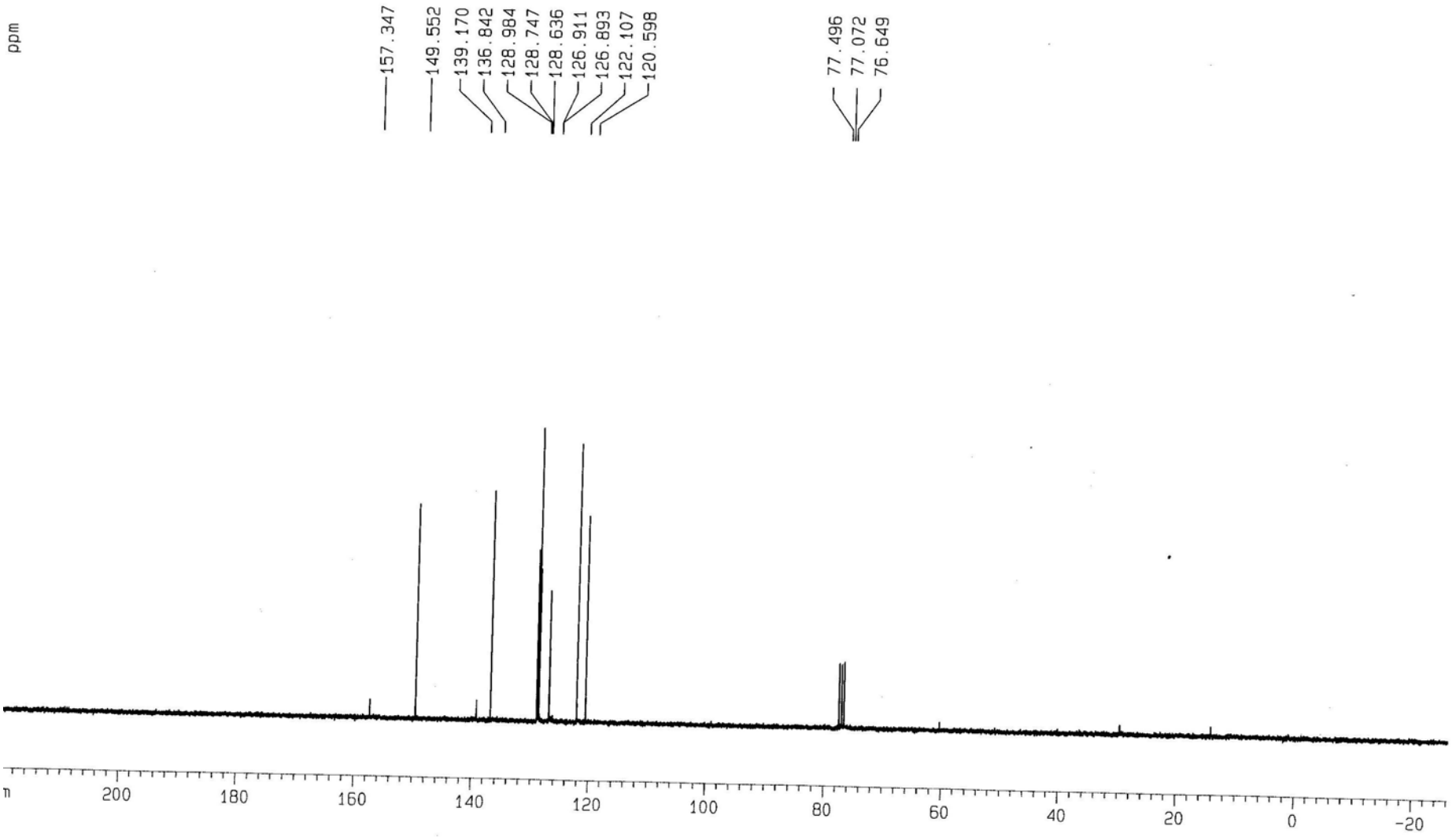
8.70160
8.69710
8.01095
7.98762
7.98268
7.76196
7.75615
7.74625
7.74113
7.73883
7.73542
7.49199
7.48583
7.48287
7.47553
7.47342
7.46382
7.44518
7.44029
7.26111
N
(D)H
Integral
1.0000
1.0408
2.0048
2.9409
1.1537
ppm
11
10
9
8
7
6
5
4
3
2
1
0

3b' ^{13}C NMR


N
(D)H


ppm
157.347
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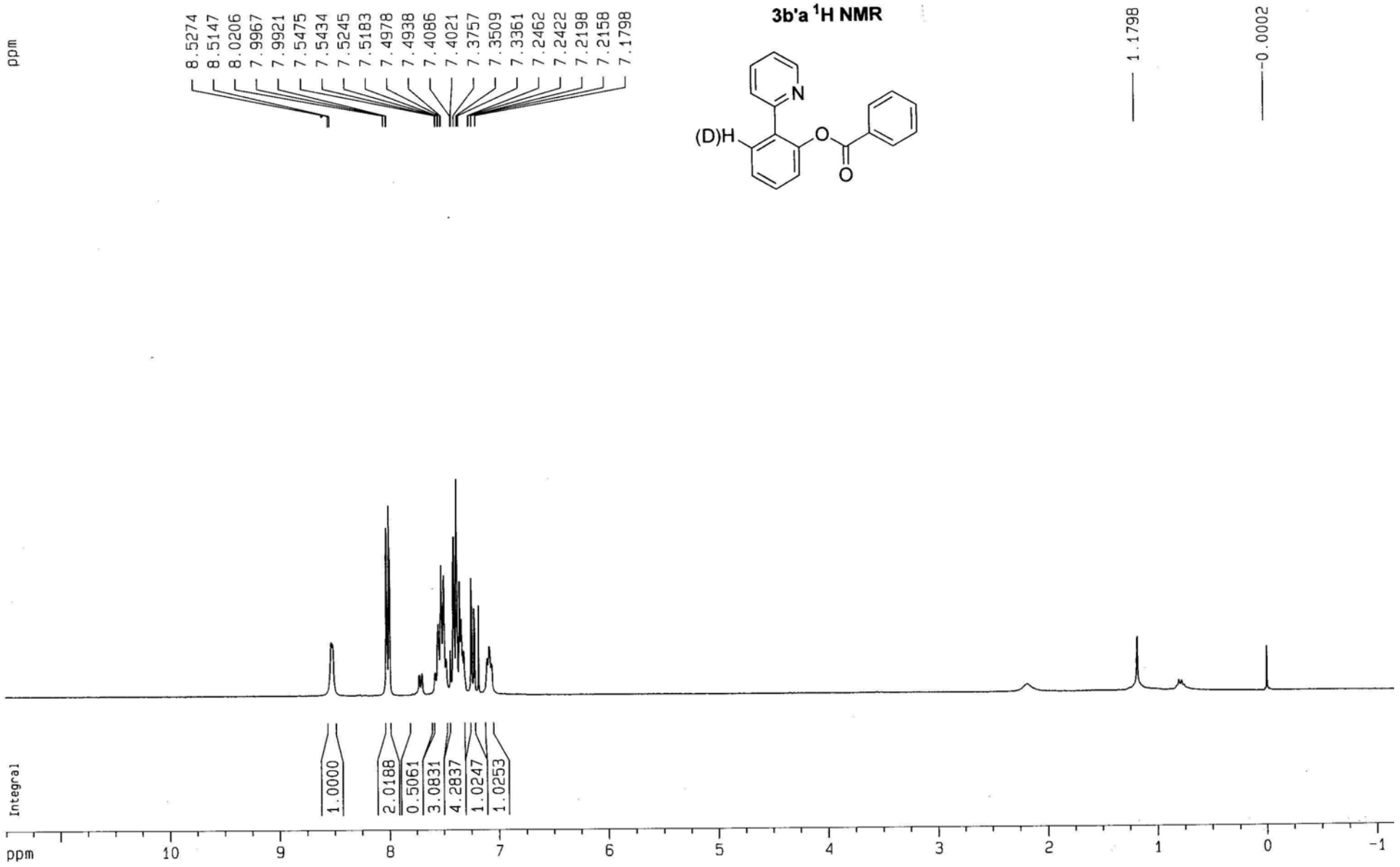
139.170
136.842
128.984
128.747
128.636
126.911
126.893
122.107
120.598
77.496
77.072
76.649
200
180
160
140
120
100
80
60
40
20
0
-20


3b'a ^{1}H NMR
ppm
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8.5147
8.0206
7.9967
7.9921
7.5475
7.5434
7.5245
7.5183
7.4978
7.4938
7.4086
7.4021
7.3757
7.3509
7.3361
7.2462
7.2422
7.2198
7.2158
7.1798
1.1798
-0.0002
(D)H
N
O
O
Integral
1.0000
2.0188
0.5061
3.0831
4.2837
1.0247
1.0253
ppm
10
9
8
7
6
5
4
3
2
1
0
-1