Supporting Information

H_2O_2-Mediated Oxidative Formation of Amides from Aromatic Amines and 1,3-Diketones as Novel Acylation Agents via C–C Bond Cleavage at Room Temperature in Water under Metal-Free Conditions

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1. General considerations

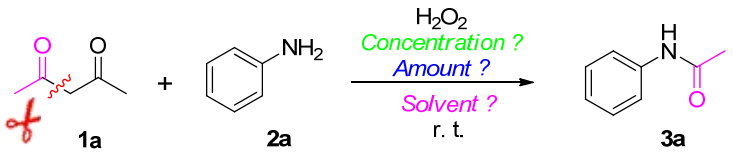
All reagents were purchased from commercial suppliers and used without further purification. All the reactions were carried out under an air atmosphere. ^{1}H NMR, ^{13}C NMR spectra were measured on a Bruker Avance NMR spectrometer (400 MHz or 100MHz, respectively) with $CDCl_3$ as solvent and recorded in ppm relative to internal tetramethylsilane standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, J, are reported in Hertz (Hz).

2. General procedure

A 10 mL of reaction tube was charged with aniline (0.50 mmol), 1,3-diketone (0.60 mmol) and H_2O_2 (30%, aq., 1.5 mmol) in the air. After the reaction was carried out at room temperature (about 25 °C) for 8 h, it was extracted twice with EtOAc. The organic layers were combined, dried over Na_2SO_4, and concentrated to yield the crude product, which was further purified by flash chromatography on silica gel to give the desired product.

3. Optimization of the solvent, and the concentration and amount of H_2O_2 in the reaction (Table S1)

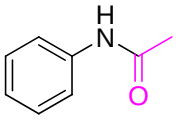
Table S1 Optimization of the solvent, and the concentration and amount of H_2O_2 in the model reaction[a]



Entry	H_2O_2 (concentration, amount)	Solvent	Yield (%)[b]
1	H_2O_2 (30% aq., 3.0 eq.)	Toluene	41
2	H_2O_2 (30% aq., 3.0 eq.)	DMF	0
3	H_2O_2 (30% aq., 3.0 eq.)	DMSO	0
4	H_2O_2 (30% aq., 3.0 eq.)	DME	0
5	H_2O_2 (30% aq., 3.0 eq.)	CH_3CN	0
6	H_2O_2 (30% aq., 3.0 eq.)	Dioxane	0
7	H_2O_2 (30% aq., 3.0 eq.)	THF	0
8	H_2O_2 (30% aq., 5.0 eq.)	Neat	88
9	H_2O_2 (30% aq., 4.0 eq.)	Neat	88
10	H_2O_2 (30% aq., 3.0 eq.)	Neat	88
11	H_2O_2 (30% aq., 2.0 eq.)	Neat	69
12	H_2O_2 (30% aq., 1.0 eq.)	Neat	37
13	H_2O_2 (35% aq., 3.0 eq.)	Neat	88
14	H_2O_2 (25% aq., 3.0 eq.)	Neat	82
15	H_2O_2 (20% aq., 3.0 eq.)	Neat	67
16	H_2O_2 (15% aq., 3.0 eq.)	Neat	56
17	H_2O_2 (6.0% aq., 3.0 eq.)	Neat	41

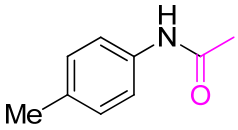
[a] Reaction conditions: **1a** (0.50 mmol), **2a** (0.60 mmol), H_2O_2 (aq. concentration, amount used in the reaction indicated in Table), solvent (2.0 mL) if needed, room temperature for 8 h. [b] Isolated yields.

4. Characterization data for all products



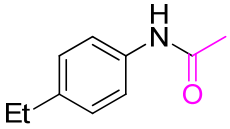
***N*-Phenylacetamide.**[1]

3a: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.78 (br, 1H), 7.52–7.50 (m, 2H), 7.32–7.28 (m, 2H), 7.12–7.08 (m, 1H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.6, 137.9, 128.9, 124.2, 120.0, 24.5.



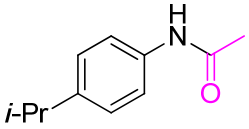
***N*-(*p*-Tolyl)acetamide.**[2]

3b: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.66 (br, 1H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 8.4 Hz, 2H), 2.31 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.5, 135.4, 133.9, 129.4, 120.1, 24.3, 20.8.



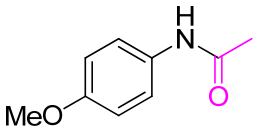
***N*-(4-Ethylphenyl)acetamide.**[3]

3c: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.00 (br, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 2.61 (q, *J* = 7.6 Hz, 2H), 2.13 (s, 3H), 1.21 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.8, 140.2, 135.6, 128.1, 120.3, 28.2, 24.2, 15.5.



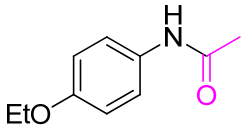
***N*-(4-*iso*-Propylphenyl)acetamide.**[3]

3d: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.86 (br, 1H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 2.90–2.84 (m, 1H), 2.14 (s, 3H), 1.23 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.7, 144.9, 135.6, 126.7, 120.3, 33.5, 24.3, 23.9.



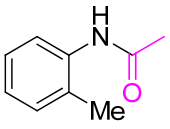
***N*-(4-Methoxyphenyl)acetamide.**[2]

3e: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.21 (br, 1H), 7.38 (d, *J* = 8.8 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 3.75 (s, 3H), 2.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.8, 156.3, 131.1, 122.0, 113.9, 55.3, 23.9.



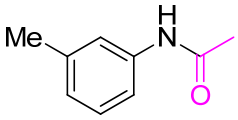
***N*-(4-Ethoxyphenyl)acetamide.**[4]

3f: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.13 (br, 1H), 7.36 (d, *J* = 8.8 Hz, 2H), 6.79 (d, *J* = 8.8 Hz, 2H), 3.97 (q, *J* = 7.2 Hz, 2H), 2.09 (s, 3H), 1.38 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.8, 155.6, 131.0, 122.0, 114.6, 63.6, 24.0, 14.7.



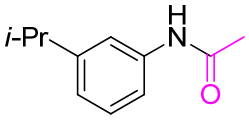
***N*-(*o*-Tolyl)acetamide.**[2]

3g: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.64–7.62 (m, 1H), 7.38 (br, 1H), 7.17–7.15 (m, 2H), 7.09–7.05 (m, 1H), 2.22 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.7, 135.6, 130.4, 130.0, 126.5, 125.4, 123.9, 23.9, 17.7.



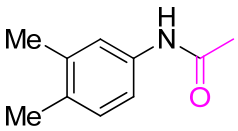
***N*-(*m*-Tolyl)acetamide.**[2]

3h: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.96 (br, 1H), 7.36 (s, 1H), 7.31–7.29 (m, 1H), 7.19–7.16 (m, 1H), 6.92–6.91 (m, 1H), 2.30 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.8, 138.7, 137.8, 128.6, 125.0, 120.7, 117.1, 24.4, 21.4.



***N*-(3-*iso*-Propylphenyl)acetamide.**[5]

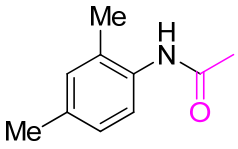
3i: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.48 (br, 1H), 7.36–7.35 (m, 2H), 7.26–7.22 (m, 1H), 6.99–6.97 (m, 1H), 2.91-2.84 (m, 1H), 2.17 (s, 3H), 1.24 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.6, 149.8, 137.9, 128.8, 122.4, 118.1, 117.5, 34.0, 24.4, 23.8.



***N*-(3,4-Dimethylphenyl)acetamide.**[3]

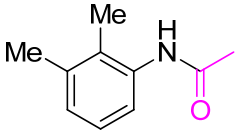
3j: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.15 (br, 1H), 7.29–7.23 (m, 2H), 7.04–7.02 (m, 1H), 2.20 (s, 3H), 2.19 (s, 3H), 2.13 (s, 3H); ^{13}C

NMR (100 MHz, $CDCl_3$) δ: 168.8, 136.9, 135.7, 132.4, 129.7, 121.6, 117.7, 24.1, 19.7, 19.0.



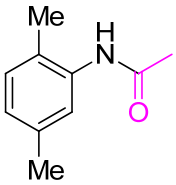
***N*-(2,4-Dimethylphenyl)acetamide.**[6]

3k: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.45–7.43 (m, 1H), 7.30 (br, 1H), 6.98–6.96 (m, 2H), 2.28 (s, 3H), 2.18 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.7, 135.2, 132.9, 131.0, 130.4, 127.0, 124.2, 23.8, 20.8, 17.6.



***N*-(2,3-Dimethylphenyl)acetamide.**[7]

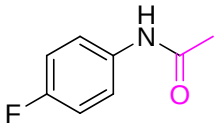
3l: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.34–7.32 (m, 1H), 7.14 (br, 1H), 7.09–7.05 (m, 1H), 7.02–6.99 (m, 1H), 2.28 (s, 3H), 2.16 (s, 3H), 2.11(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.8, 137.4, 135.2, 130.1, 127.6, 125.7, 122.7, 23.8, 20.5, 13.8.



***N*-(2,5-Dimethylphenyl)acetamide.**[7]

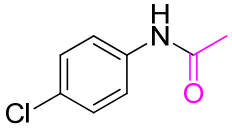
3m: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 (s, 1H), 7.34 (br, 1H), 7.05–7.03 (m, 1H), 6.89–6.88 (m, 1H), 2.29 (s, 3H), 2.18 (s, 3H), 2.14

(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.6, 136.2, 135.3, 130.1, 126.2, 124.5, 23.9, 20.9, 17.2.



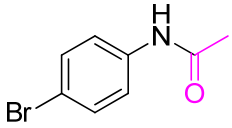
***N*-(4-Fluorophenyl)acetamide.**[8]

3n: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.77 (br, 1H), 7.46–7.43 (m, 2H), 7.00–6.96 (m, 2H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.7, 159.4 (d, J_{CF} = 242.1 Hz), 133.8 (d, J_{CF} = 2.8 Hz), 121.9 (d, J_{CF} = 7.9 Hz), 115.5 (d, J_{CF} = 22.4 Hz), 24.2.



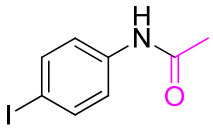
***N*-(4-Chlorophenyl)acetamide.**[2]

3o: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.47–7.45 (m, 2H), 7.33 (br, 1H), 7.31–7.27 (m, 2H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.3, 136.4, 129.3, 129.0, 121.1, 24.5.



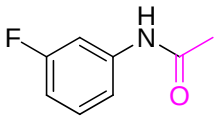
***N*-(4-Bromophenyl)acetamide.**[8]

3p: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.59 (br, 1H), 7.47–7.41 (m, 4H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.4, 136.9, 131.9, 121.4, 116.9, 24.5.



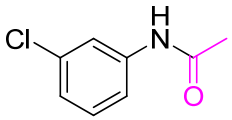
***N*-(4-Iodophenyl)acetamide.**[9]

3q: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.61 (d, J = 8.8 Hz, 2H), 7.36 (br, 1H), 7.29 (d, J = 8.4 Hz, 2H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.3, 137.9, 137.6, 121.6, 87.4, 24.6.



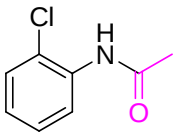
***N*-(3-Fluorophenyl)acetamide.**[8]

3r: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.32 (br, 1H), 7.48–7.46 (m, 1H), 7.23–7.19 (m, 1H), 7.17–7.15 (m, 1H), 6.80–6.77 (m, 1H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 169.3, 162.9 (d, J_{CF} = 243.1 Hz), 139.5 (d, J_{CF} = 10.8 Hz), 130.0 (d, J_{CF} = 9.3 Hz), 115.3 (d, J_{CF} = 2.8 Hz), 111.0 (d, J_{CF} = 21.2 Hz), 107.5 (d, J_{CF} = 25.9 Hz), 24.4.



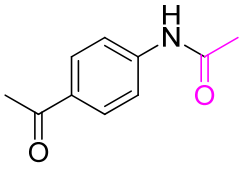
***N*-(3-Chlorophenyl)acetamide.**[8]

3s: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.28 (br, 1H), 7.64 (s, 1H), 7.35–7.33 (m, 1H), 7.22–7.17 (m, 1H), 7.09–7.05 (m, 1H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 169.2, 139.0, 134.4, 129.8, 124.3, 120.2, 118.0, 24.3.



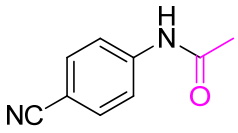
***N*-(2-Chlorophenyl)acetamide.**[8]

3t: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.32–8.30 (m, 1H), 7.68 (br, 1H), 7.36–7.34 (m, 1H), 7.27–7.23 (m, 1H), 7.05–7.01 (m, 1H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.3, 134.5, 128.9, 127.6, 124.6, 121.8, 121.1, 24.7.



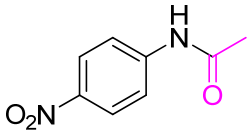
***N*-(4-Acetylphenyl)acetamide.**[3]

3u: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.17 (br, 1H), 7.91 (d, J = 8.4 Hz, 2H), 7.64 (d, J = 8.4 Hz, 2H), 2.57 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 197.3, 168.9, 142.5, 132.7, 129.7, 118.9, 26.4, 24.6.



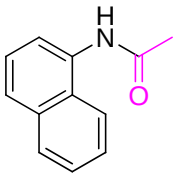
***N*-(4-Cyanophenyl)acetamide.**[8]

3v: Colorless solid. ^{1}H NMR (400 MHz, CD_3COCD_3) δ: 9.57 (br, 1H), 7.84 (d, J = 8.8 Hz, 2H), 7.69 (d, J = 8.8 Hz, 2H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ: 168.8, 143.6, 132.9, 119.1, 118.6, 105.9, 23.5.



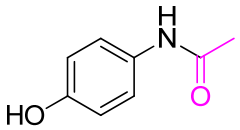
***N*-(4-Nitrophenyl)acetamide.**[10]

3w: Colorless solid. ^{1}H NMR (400 MHz, CD_3COCD_3) δ: 8.22 (br, 1H), 8.17 (d, *J* = 8.8 Hz, 2H), 7.88 (d, *J* = 8.8 Hz, 2H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ: 169.4, 145.4, 142.7, 124.7, 118.6, 23.5.



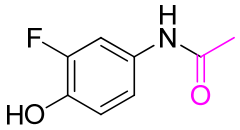
***N*-(Naphthalen-1-yl)acetamide.**[11]

3x: Colorless solid. ^{1}H NMR (400 MHz, CD_3COCD_3) δ: 9.22 (br, 1H), 8.15–8.13 (m, 1H), 7.91 (br, 2H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.52–7.45 (m, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ: 168.5, 134.2, 133.9, 128.1, 127.6, 125.6, 125.5, 125.3, 124.8, 121.9, 120.7, 22.9.



***N*-(4-Hydroxyphenyl)acetamide.**[10]

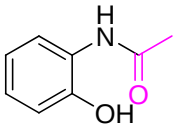
3y: Colorless solid. ^{1}H NMR (400 MHz, CD_3COCD_3) δ: 8.99 (br, 1H), 8.19 (s, 1H), 7.45 (d, *J* = 8.4 Hz, 2H), 6.76 (d, *J* = 8.4 Hz, 2H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ: 167.4, 153.3, 131.7, 120.7, 114.9, 23.0.



***N*-(3-Fluoro-4-hydroxyphenyl)acetamide.**[12]

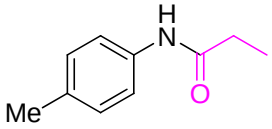
3z: Colorless solid. ^{1}H NMR (400 MHz, CD_3COCD_3) δ: 9.18 (br, 1H), 8.49 (s, 1H), 7.64 (d, *J* = 13.2 Hz, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 6.93–6.88 (m,

1H), 2.06 (s, 3H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ: 168.0, 150.7 (d, J_{CF} = 236.7 Hz), 140.5 (d, J_{CF} = 13.1 Hz), 132.0 (d, J_{CF} = 9.2 Hz), 117.3 (d, J_{CF} = 3.5 Hz), 115.2 (d, J_{CF} = 3.3 Hz), 107.8 (d, J_{CF} = 23.1 Hz), 23.0.



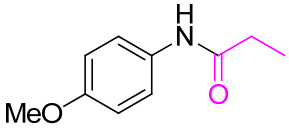
***N*-(2-Hydroxyphenyl)acetamide.**[13]

3aa: Colorless solid. ^{1}H NMR (400 MHz, CD_3COCD_3) δ: 9.41 (s, 1H), 9.27 (br, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.04–7.01 (m, 1H), 6.90 (d, J = 8.0 Hz, 1H), 6.82 –6.79 (m, 1H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ: 170.2, 148.4, 126.7, 125.5, 121.8, 119.5, 117.9, 22.5.



***N*-(*p*-Tolyl)propionamide.**[14]

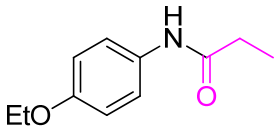
3ab: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.52 (br, 1H), 7.40 (d, J = 8.0 Hz, 2H), 7.10 (d, J = 8.0 Hz, 2H), 2.37 (q, J = 7.6 Hz, 2H), 2.31 (s, 3H), 1.23 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.1, 135.4, 133.7, 129.4, 119.9, 30.6, 20.8, 9.7.



***N*-(4-Methoxyphenyl)propionamide.**[14]

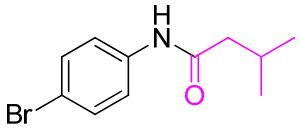
3ac: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (d, J = 8.8 Hz, 2H), 7.32 (br, 1H), 6.84 (d, J = 8.8 Hz, 2H), 3.78 (s, 3H), 2.36 (q, J = 7.6 Hz, 2H),

1.23 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.9, 156.3, 131.1, 121.8, 114.0, 55.4, 30.5, 9.7.



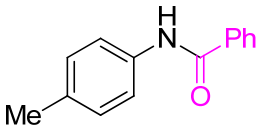
***N*-(4-Ethoxyphenyl)propionamide.**[15]

3ad: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40 (d, J = 8.8 Hz, 2H), 7.22 (br, 1H), 6.84 (d, J = 8.8 Hz, 2H), 4.00 (q, J = 7.2 Hz, 2H), 2.37 (q, J = 7.6 Hz, 2H), 1.40 (t, J = 6.8 Hz, 3H), 1.24 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.8, 155.7, 130.9, 121.7, 114.7, 63.7, 30.5, 14.8, 9.7.



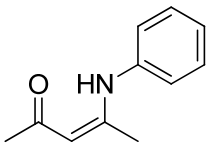
***N*-(4-Bromophenyl)-3-methylbutanamide.**[16]

3ag: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.48 (br, 1H), 7.44–7.39 (m, 4H), 2.21–2.16 (m, 3H), 1.00 (d, J = 6.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.0, 136.9, 131.9, 121.5, 116.7, 46.9, 26.2, 22.4.



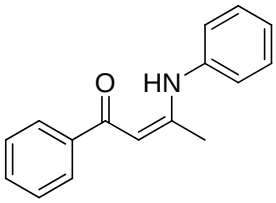
***N*-(*p*-Tolyl)benzamide.**[17]

3ah: Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.17 (br, 1H), 7.85–7.84 (m, 2H), 7.55–7.51 (m, 2H), 7.49 (s, 1H), 7.43–7.40 (m, 2H), 7.15–7.13 (m, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.8, 135.4, 134.9, 134.1, 131.5, 129.4, 128.5, 127.0, 120.5, 20.8.



4-(Phenylamino)pent-3-en-2-one.[18]

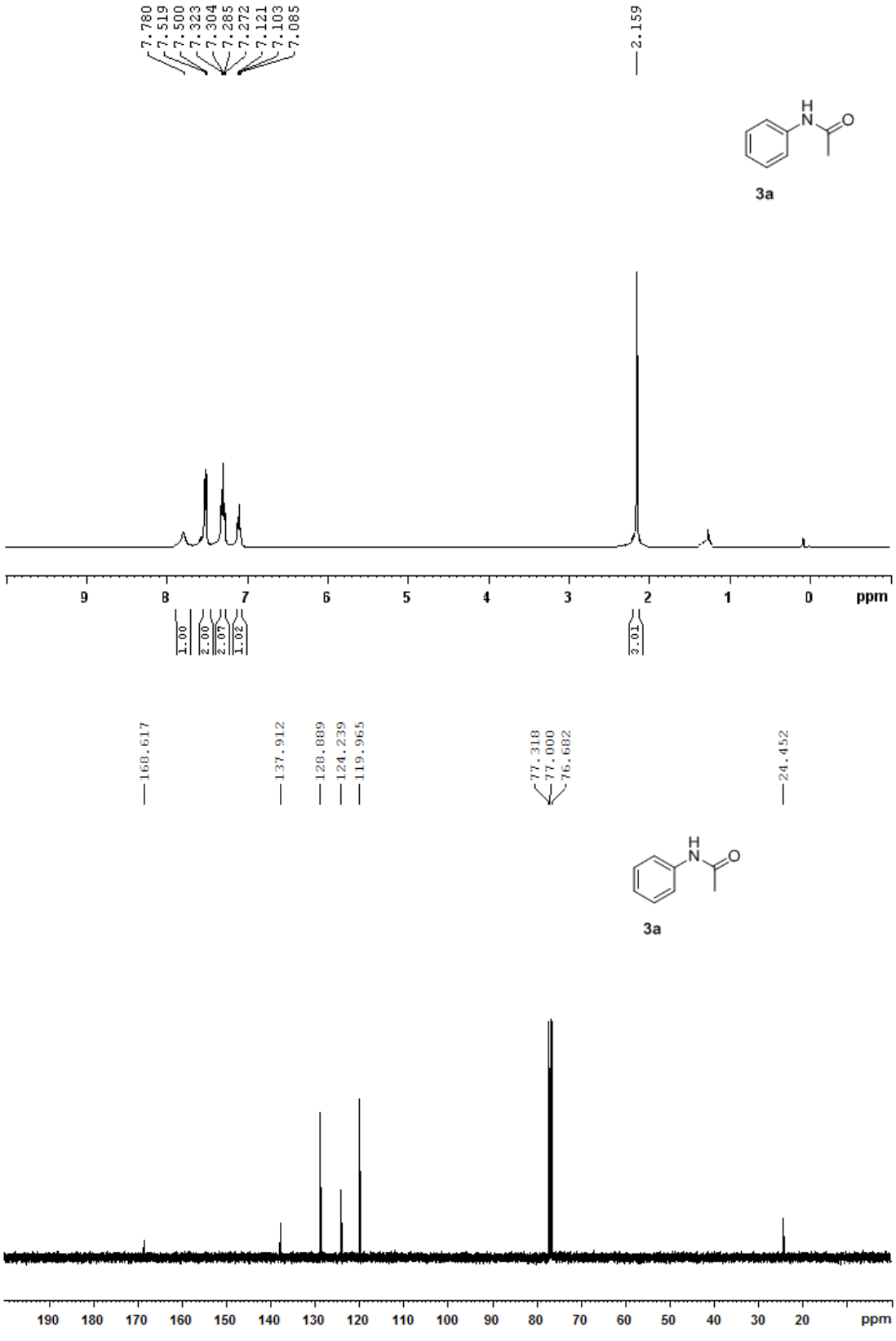
4a: Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 12.48 (br, 1H), 7.35–7.32 (m, 2H), 7.20–7.17 (m, 1H), 7.11 (d, *J* = 7.6 Hz, 2H), 5.19 (s, 1H), 2.10 (s, 3H), 1.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 196.1, 160.1, 138.7, 129.0, 125.5, 124.7, 97.6, 29.1, 19.7.

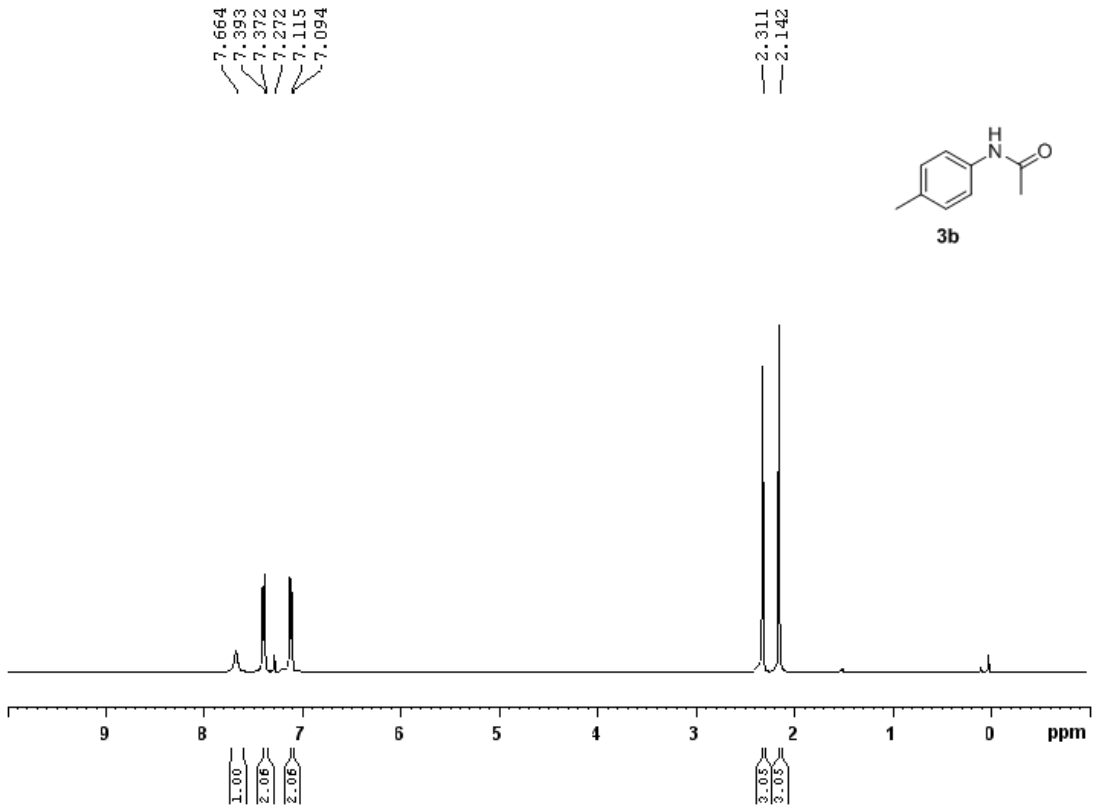


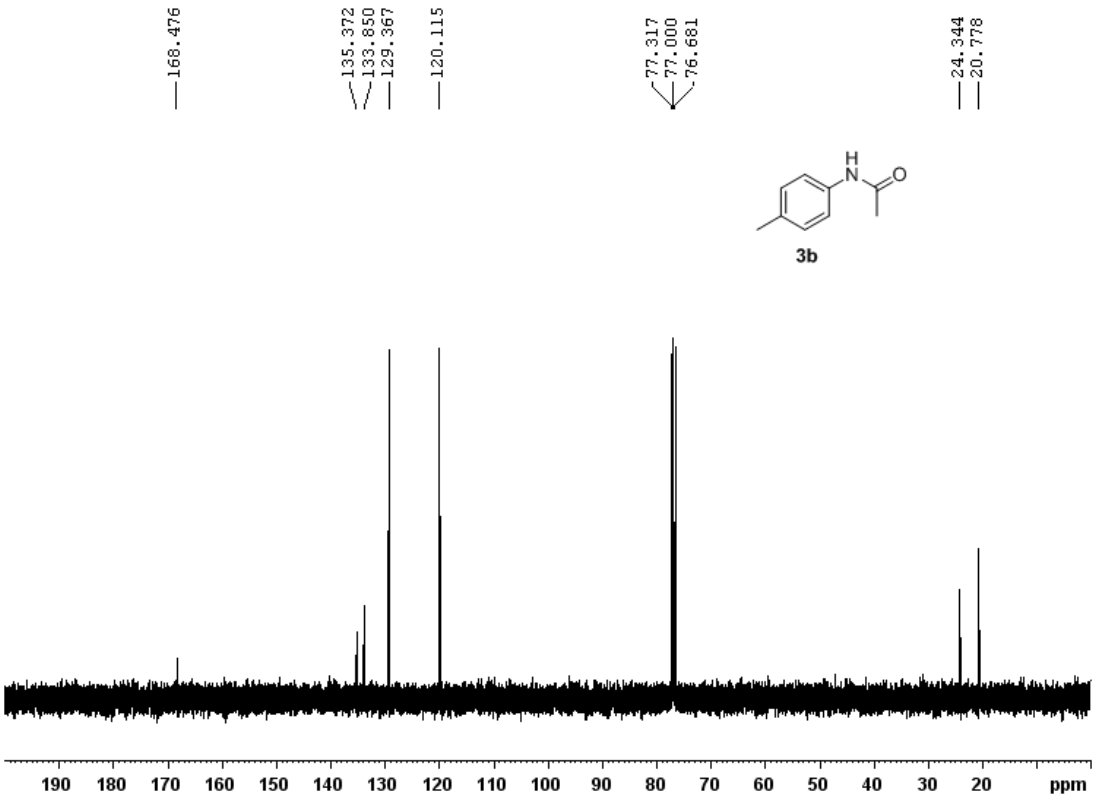
3-Anilino-1-phenyl-2-buten-1-one.[19]

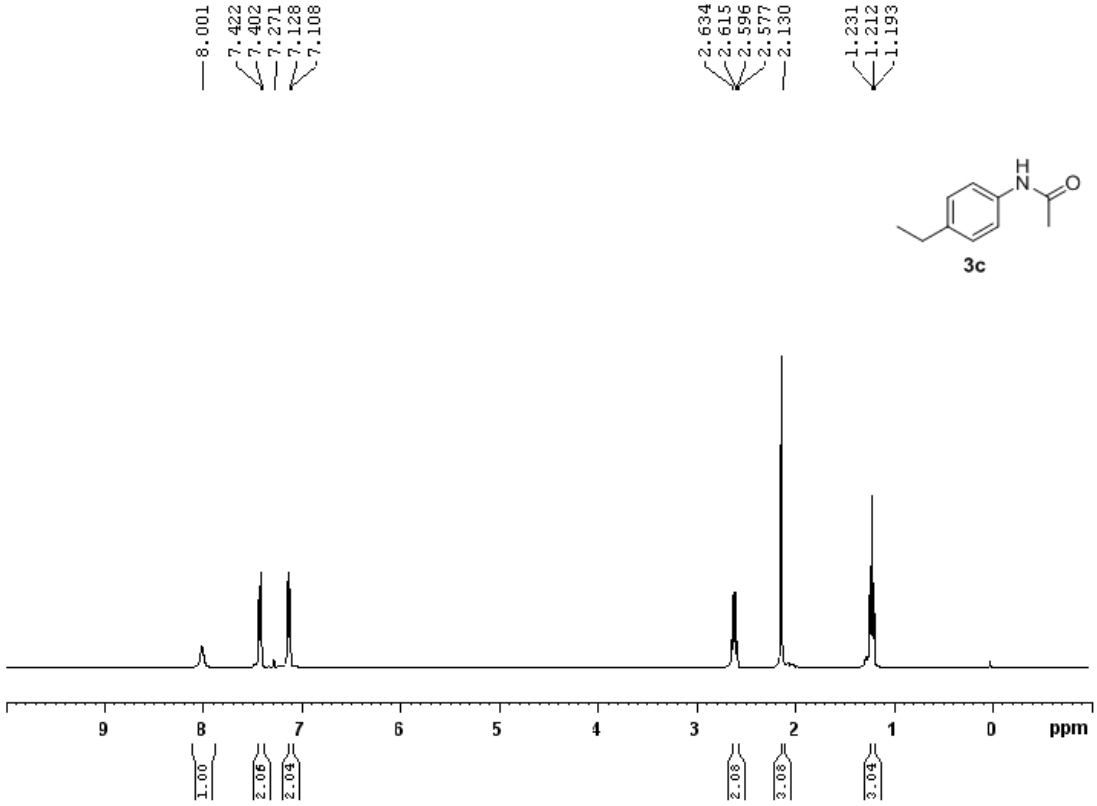
4k: Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 13.13 (br, 1H), 7.94 (d, *J* = 7.2 Hz, 2H), 7.50–7.42 (m, 3H), 7.40–7.37 (m, 2H), 7.25–7.19 (m, 3H), 5.91 (s, 1H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 188.6, 162.1, 139.9, 138.6, 130.8, 129.1, 128.2, 127.0, 125.7, 124.7, 94.2, 20.4.

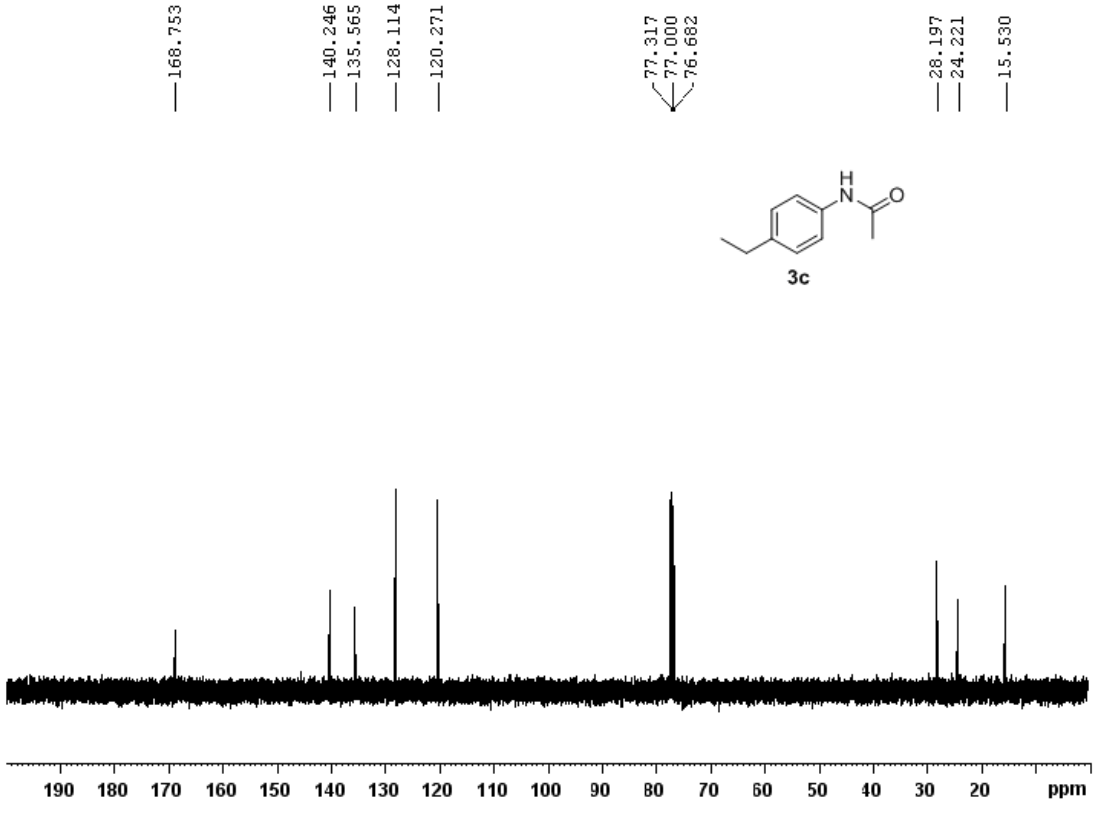
5. ^{1}H and ^{13}C NMR spectra of all products

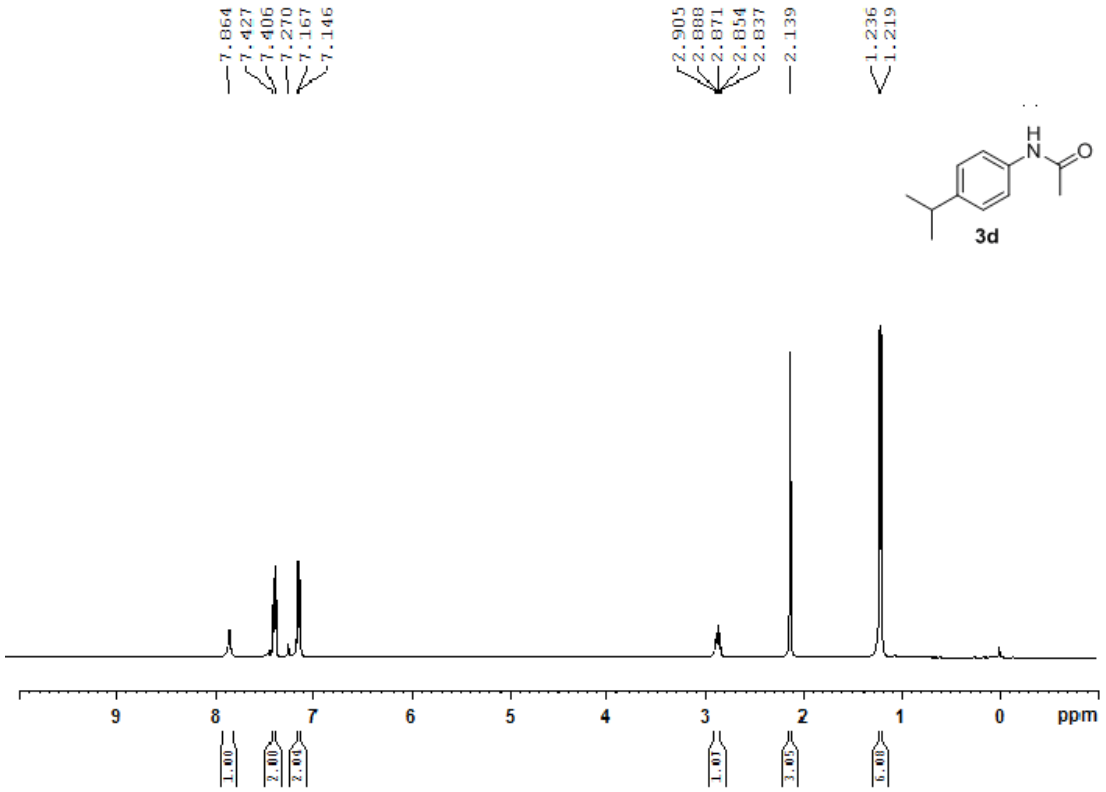








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2.888
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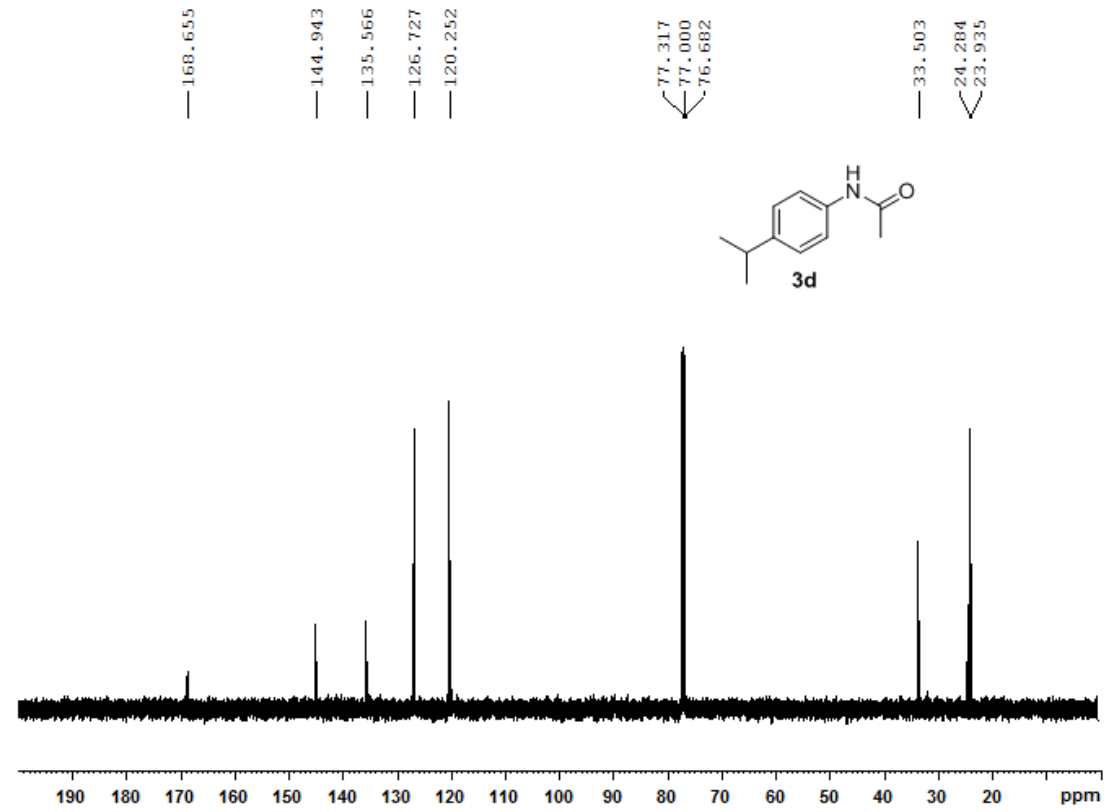
2.854
2.837
2.139
1.236
1.219
H
N
O
3d
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.00
2.04
1.07
3.05
6.00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76.682
33.503
24.284
23.935
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N
O
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190
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130
120
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80
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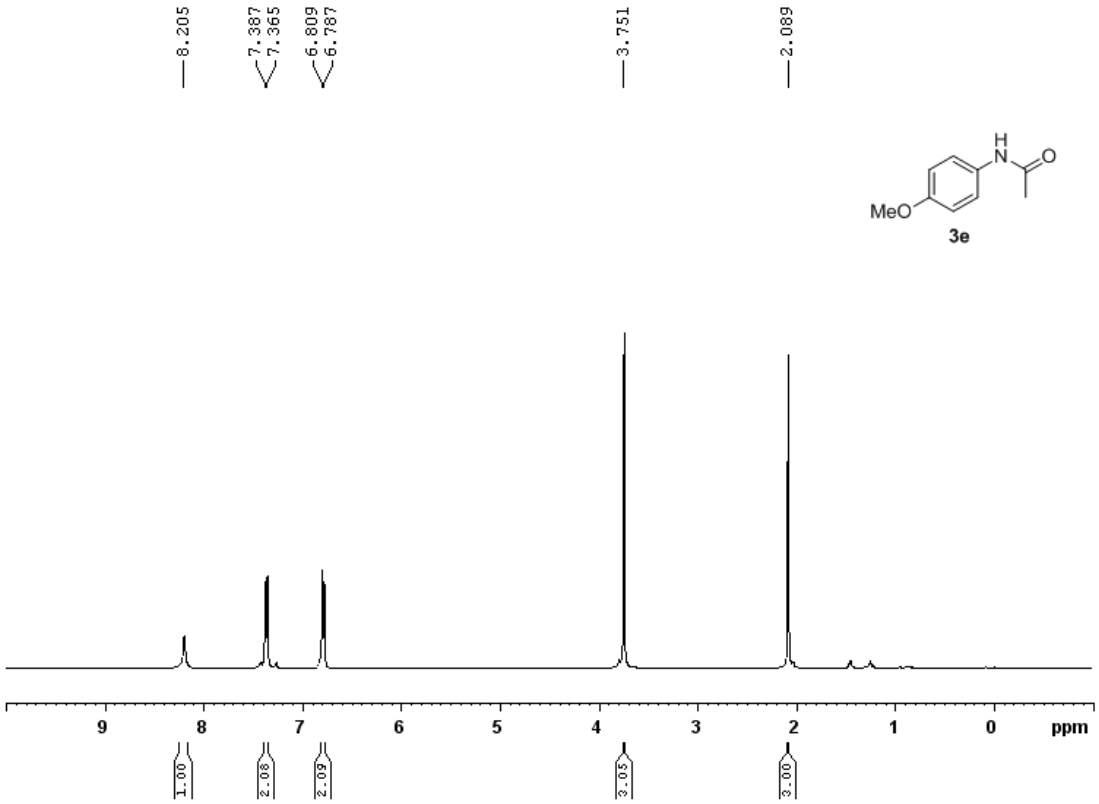
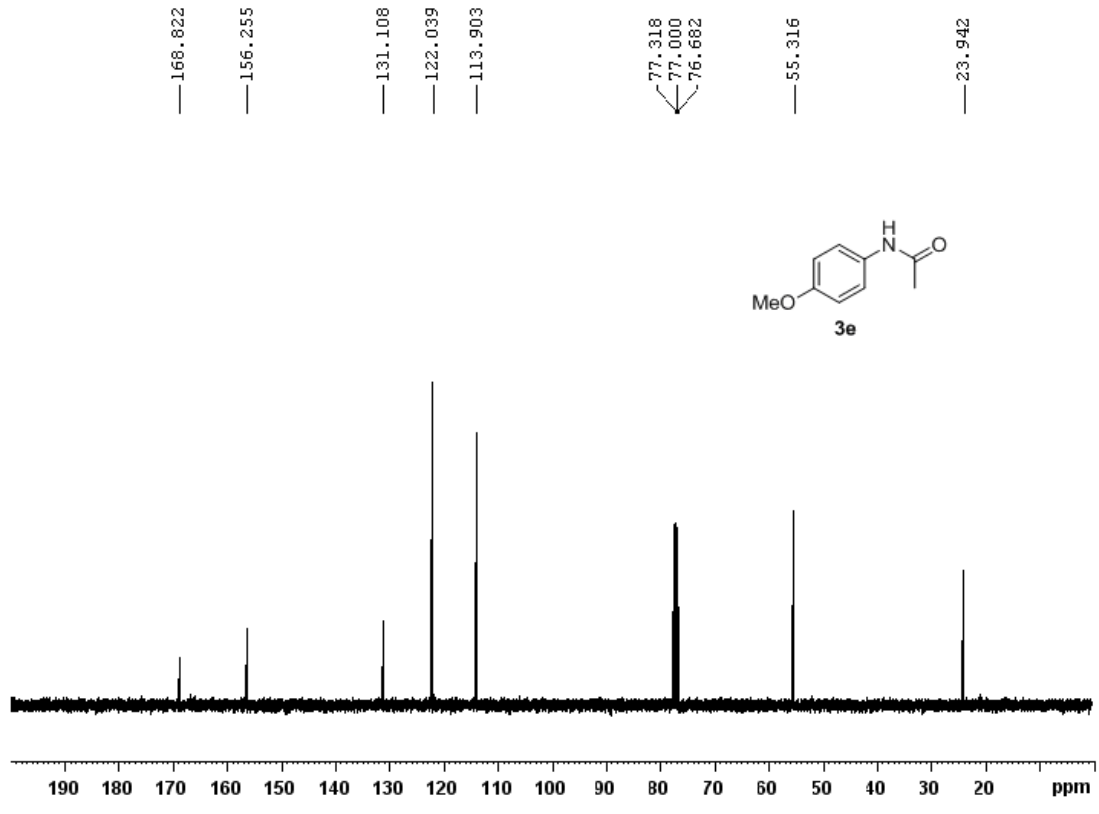
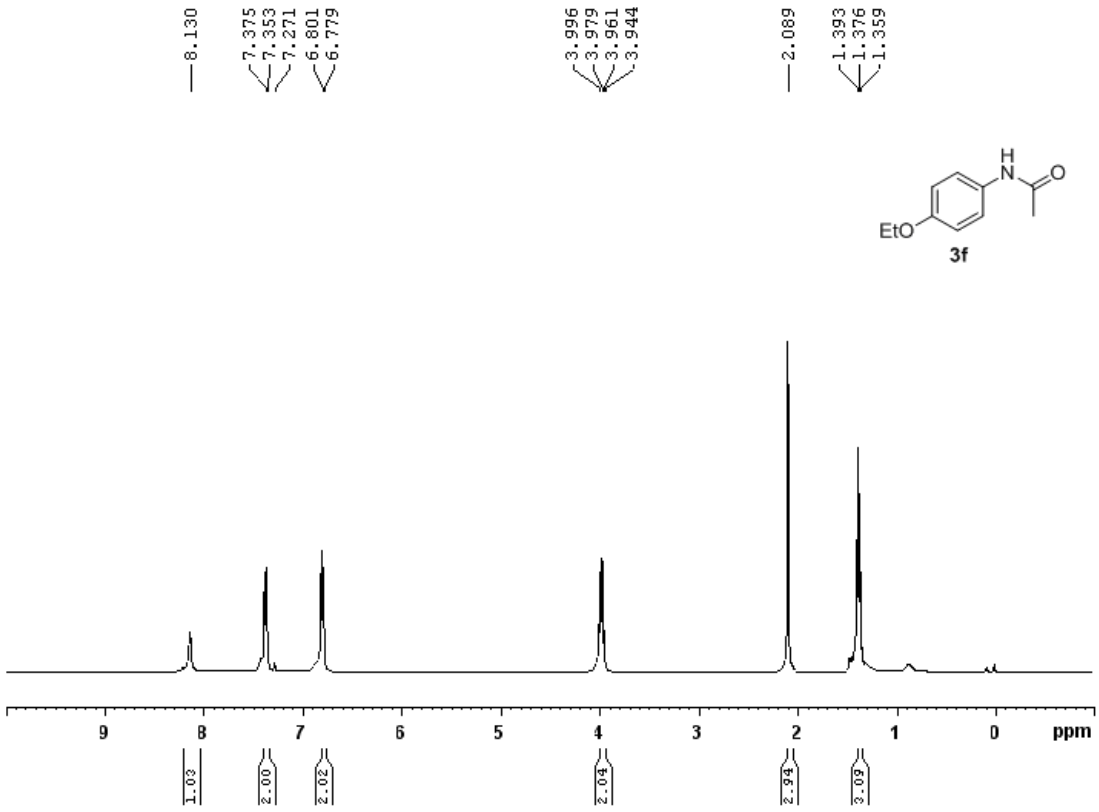
40
30
20
ppm



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3.979
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3.944
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1.376
1.359
EtO
3f
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7
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5
4
3
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1
0
ppm
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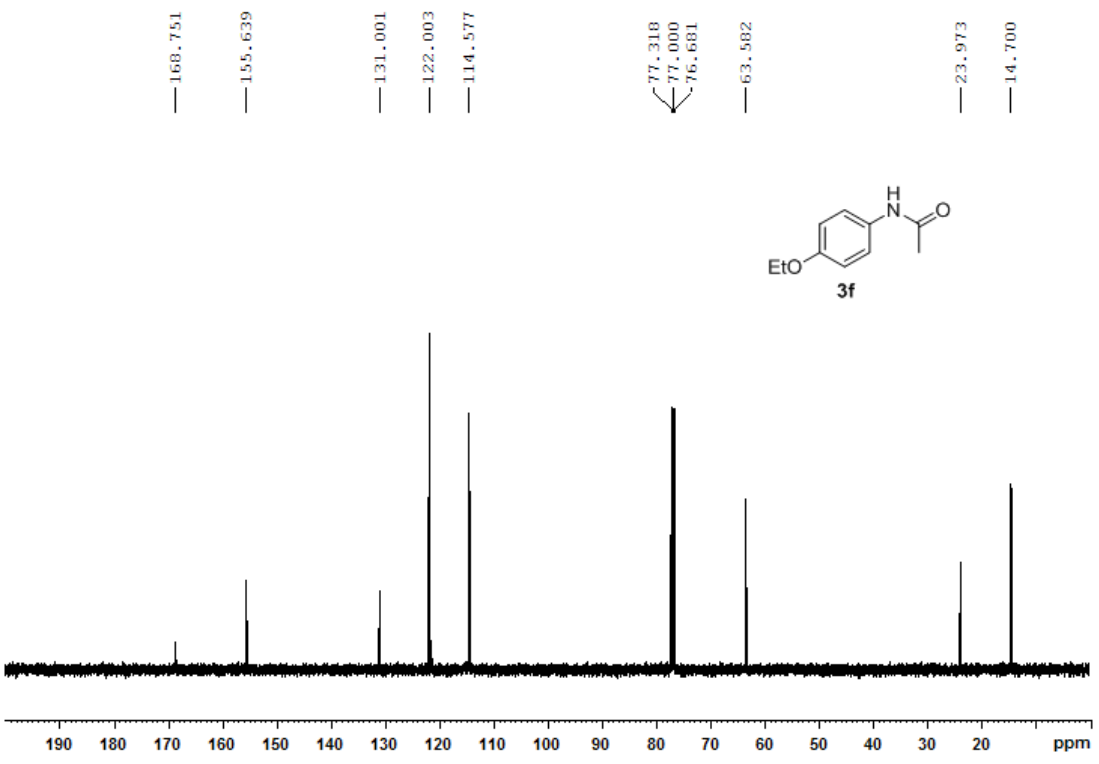
2.00
2.02
2.04
2.94
3.09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63.582
23.973
14.700
EtO
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160
150
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130
120
110
100
90
80
70
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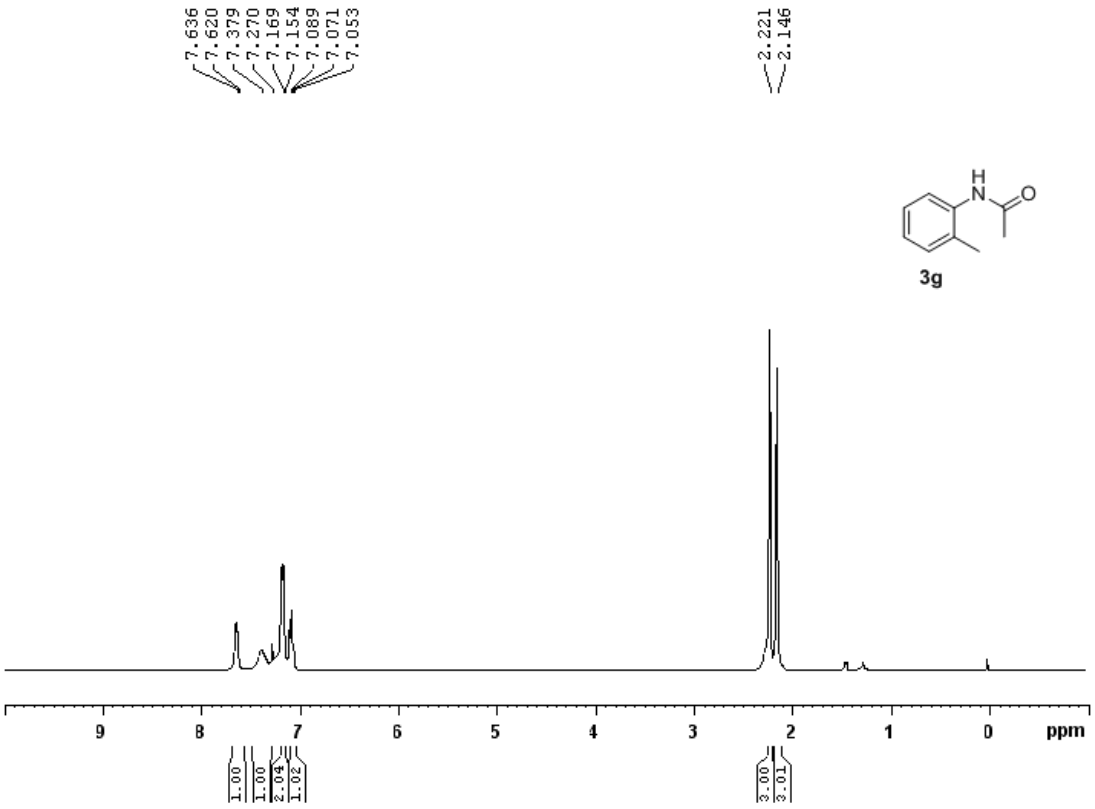
50
40
30
20
ppm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2.146
3g
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7
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5
4
3
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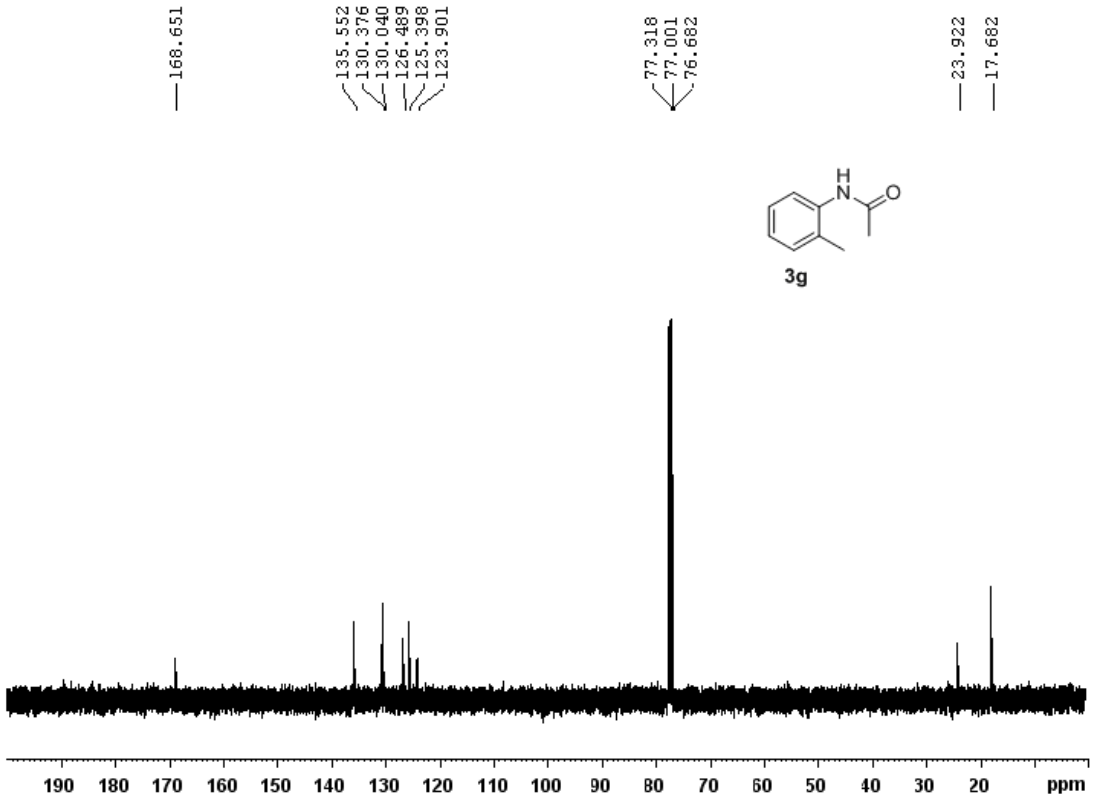
1
0
ppm
1.00
1.00
2.04
1.02
3.00
3.01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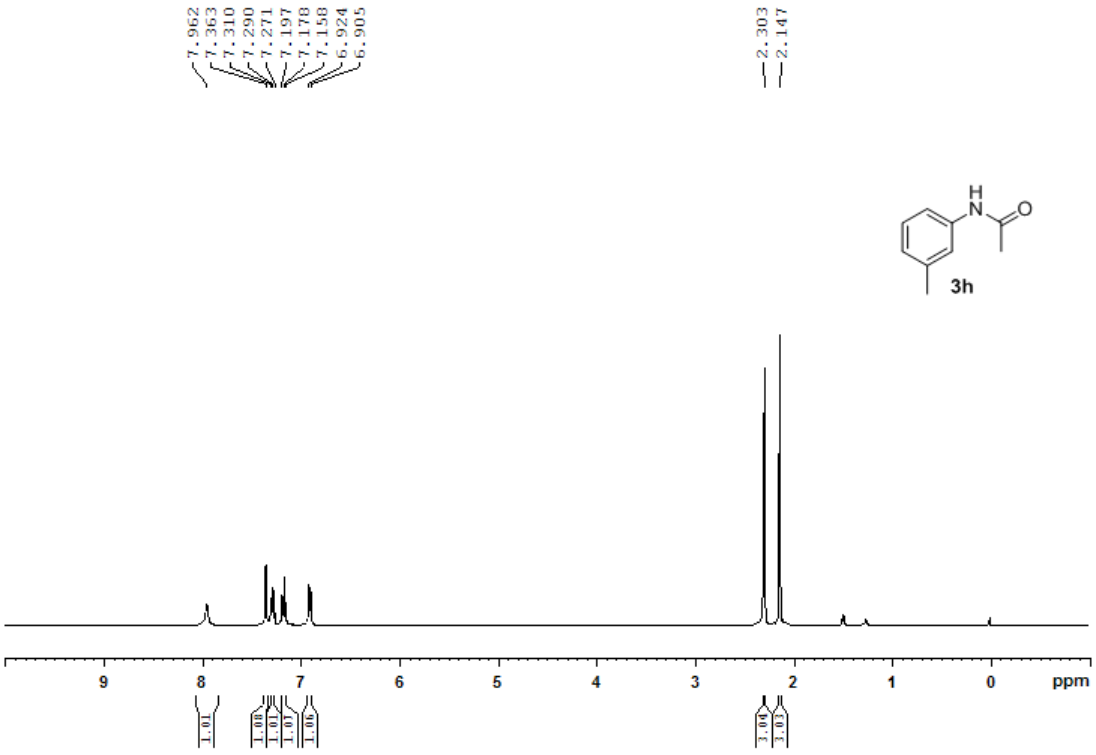
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N
O
3h
9
8
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0
ppm
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1.01
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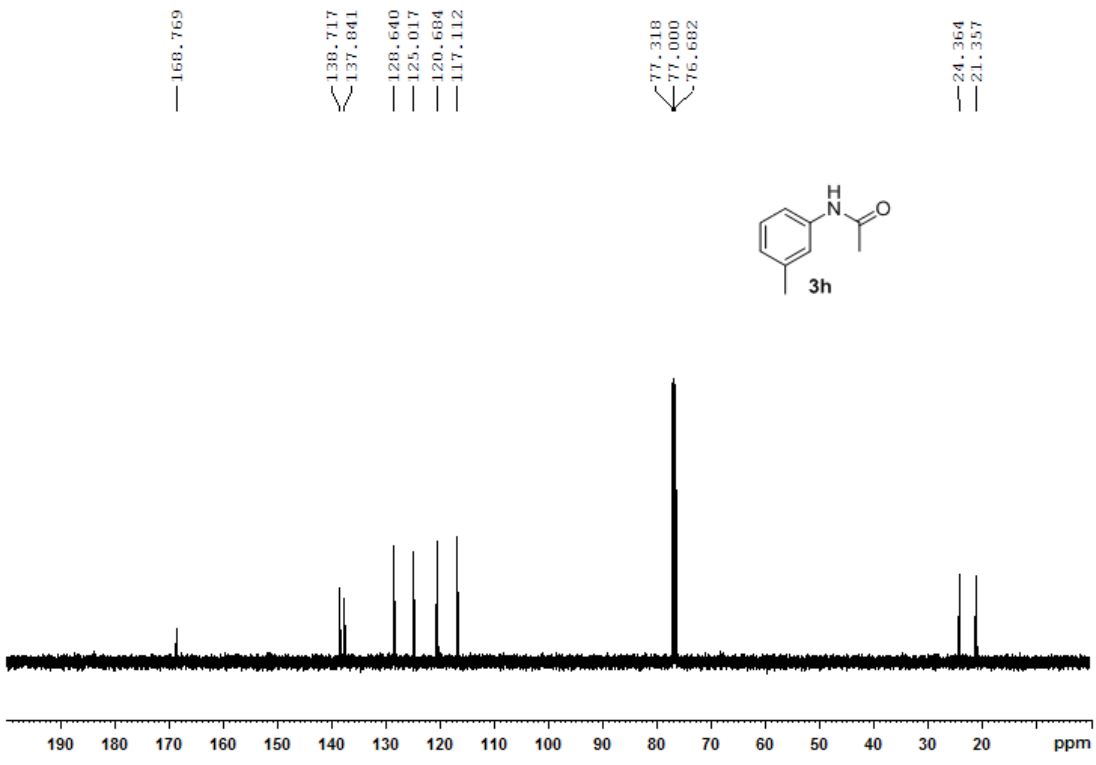
1.06
3.04
3.03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N
O
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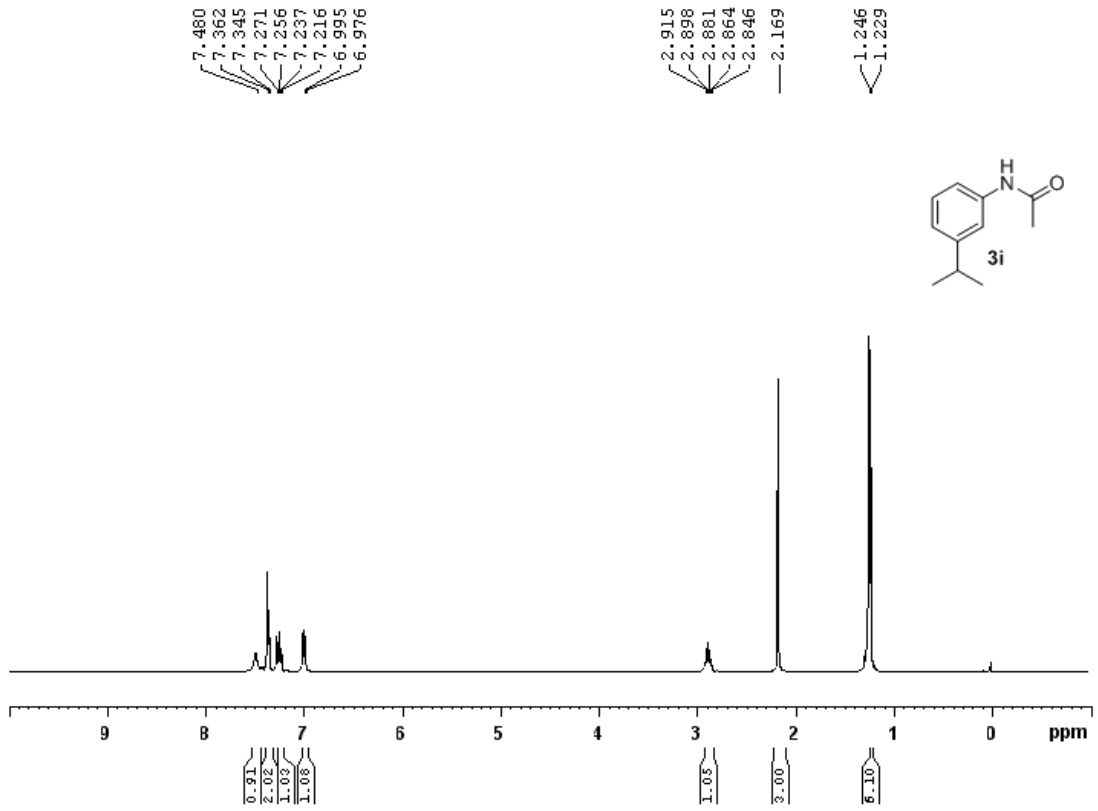

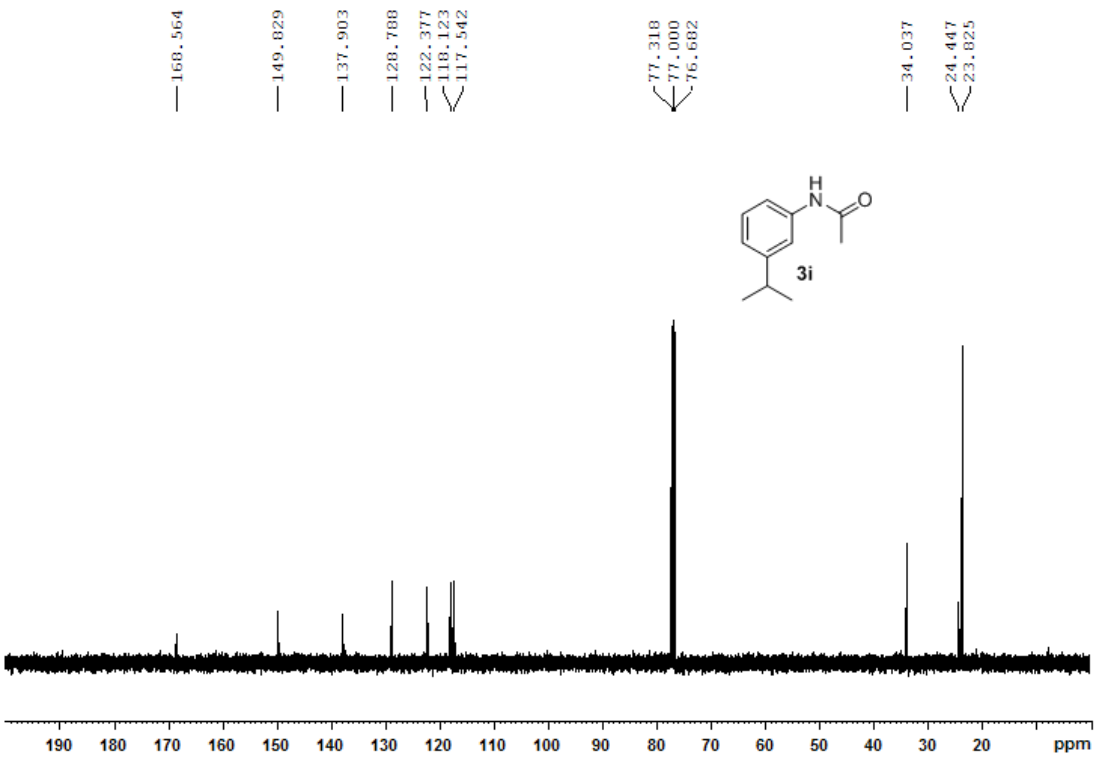

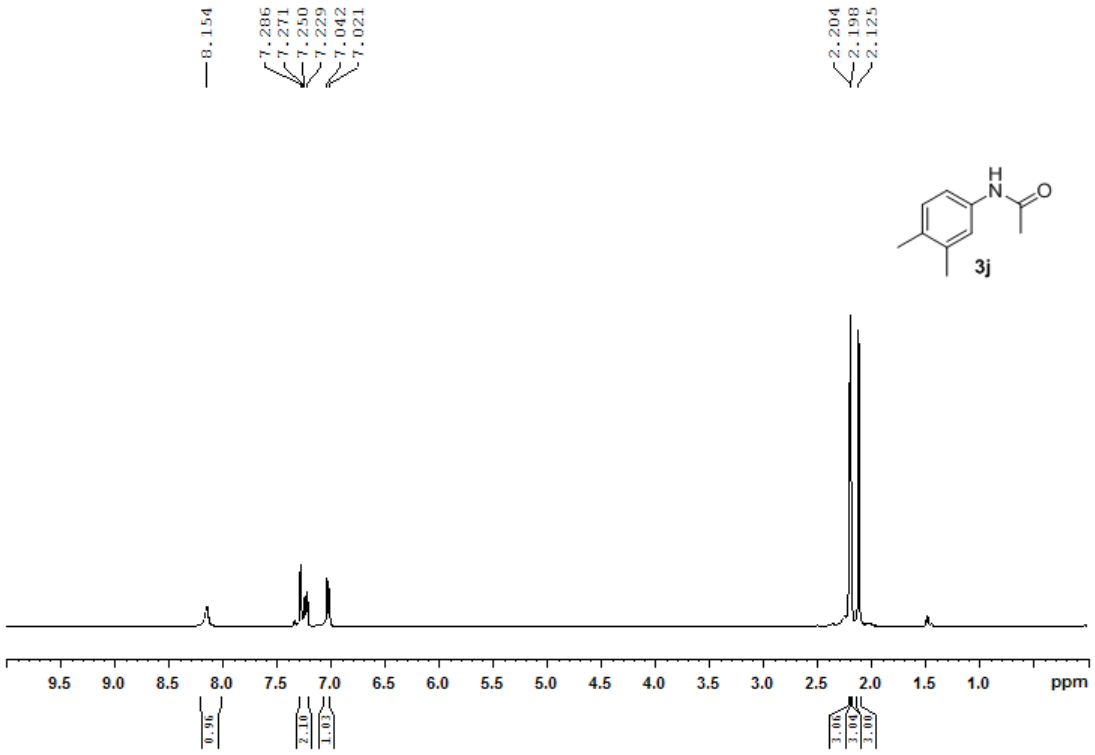
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7.042
7.021
2.204
2.198
2.125
3j
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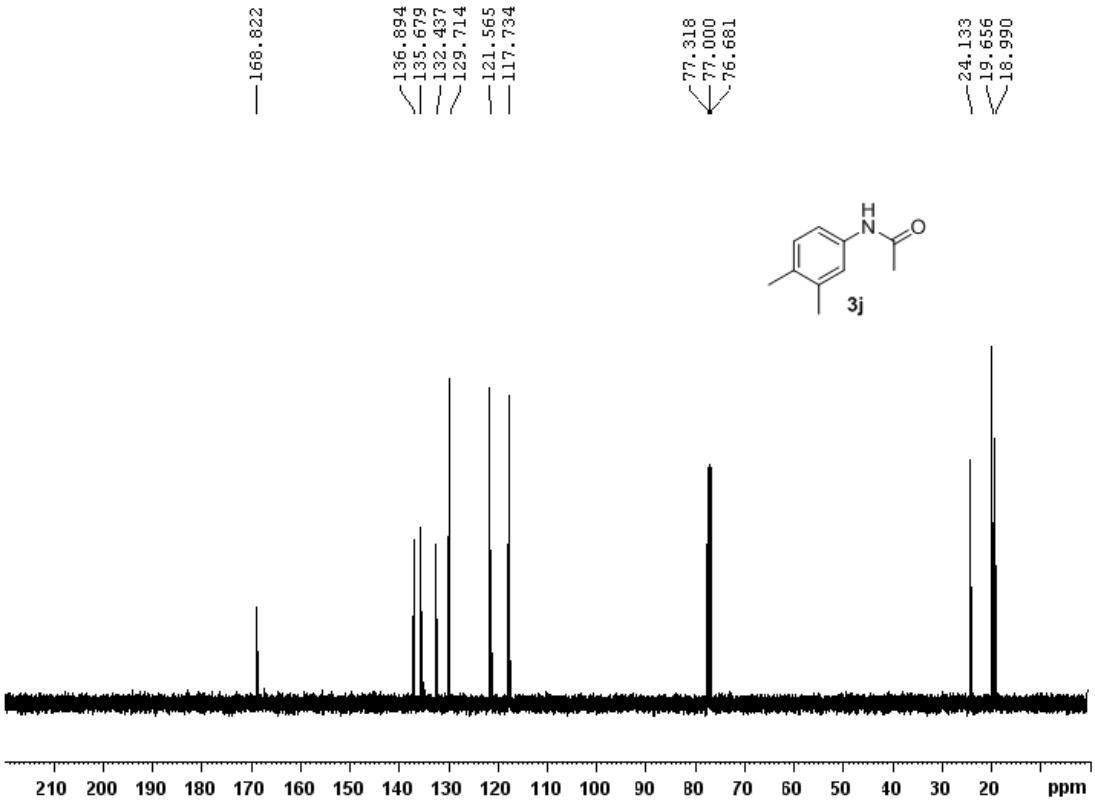
0.96
2.10
1.03
3.06
3.04
3.00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3j
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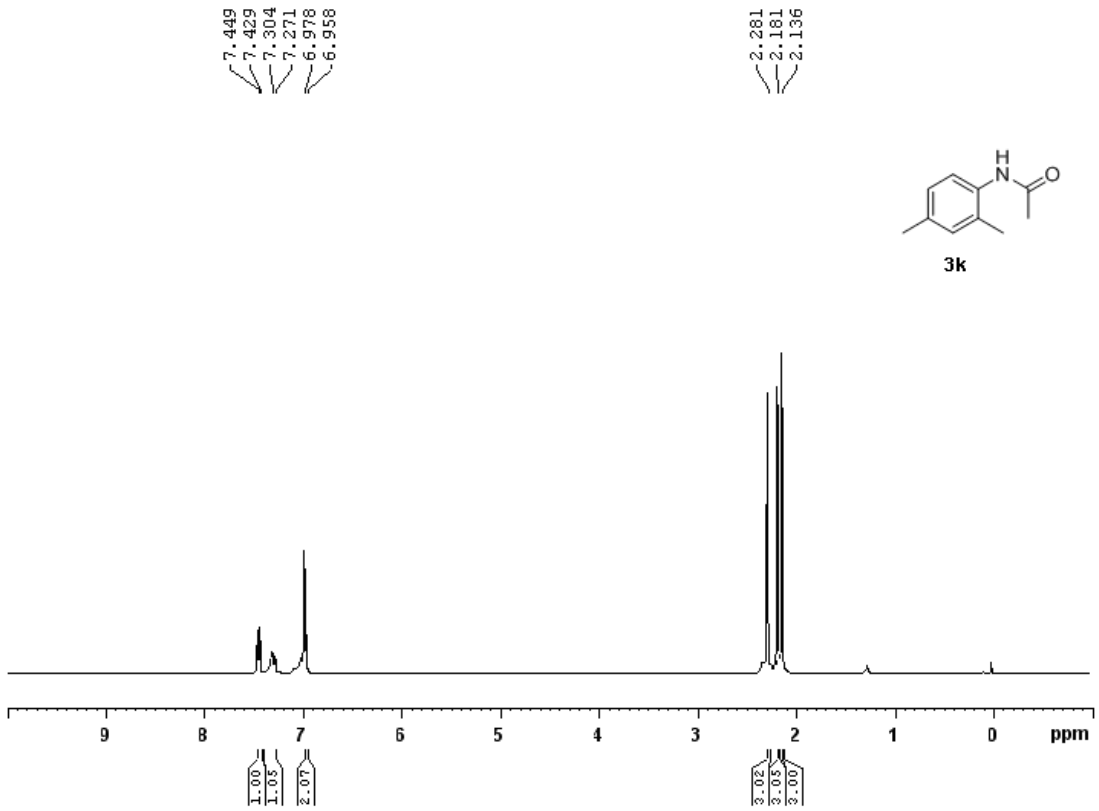
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ppm
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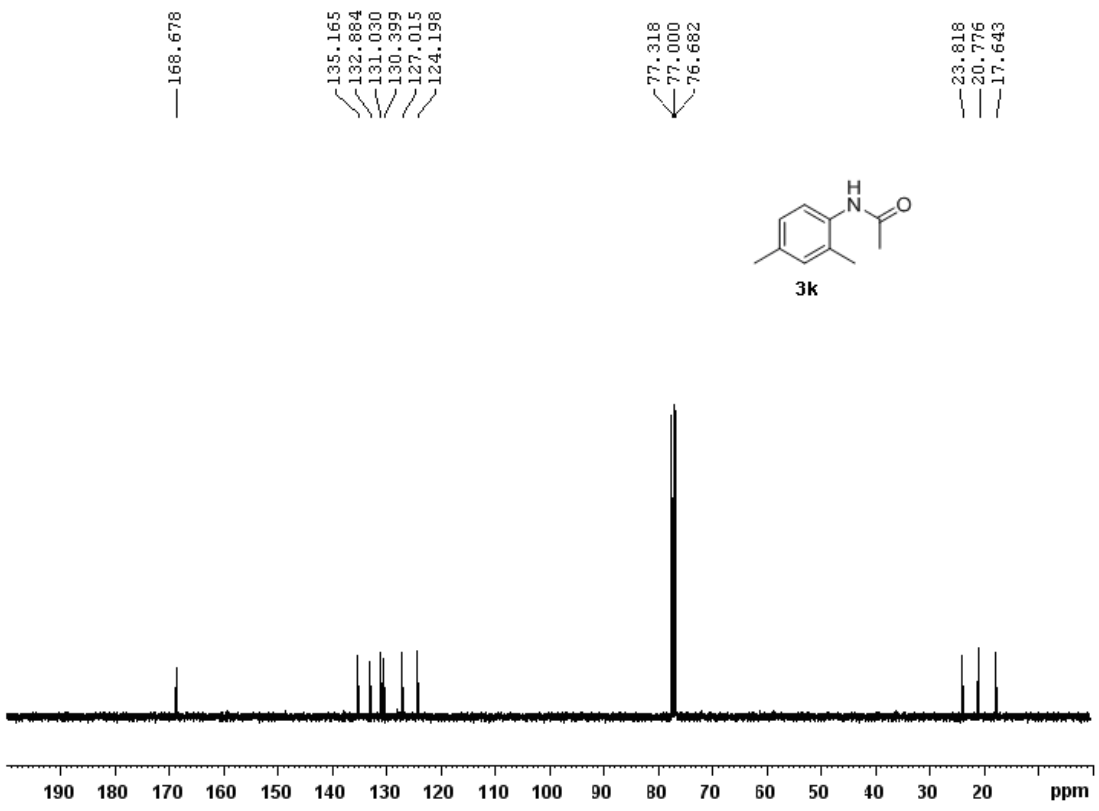
3.00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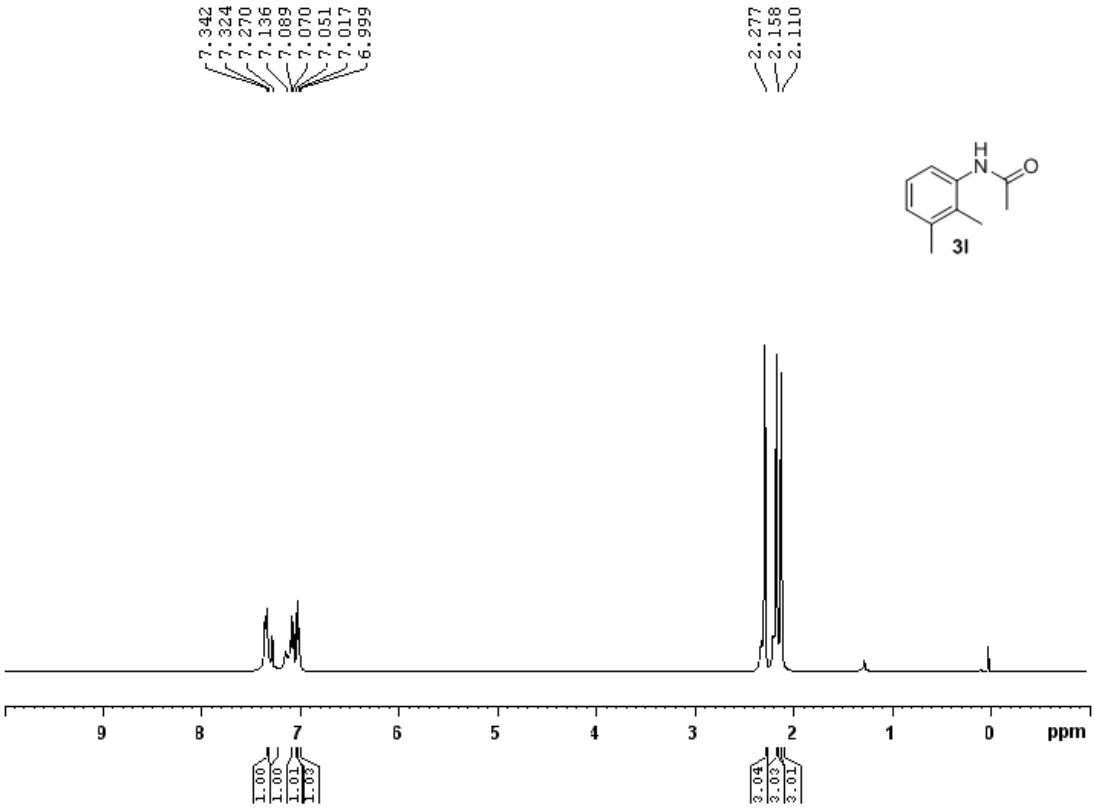
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9
8
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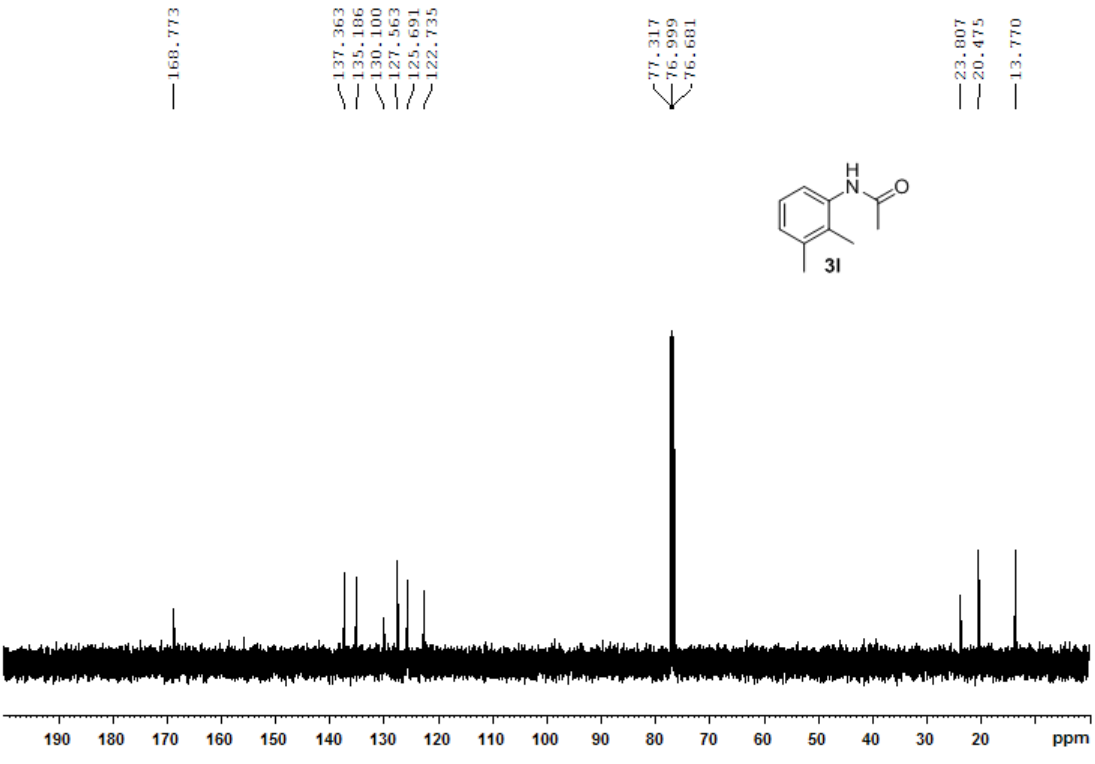
3.01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3l
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180
170
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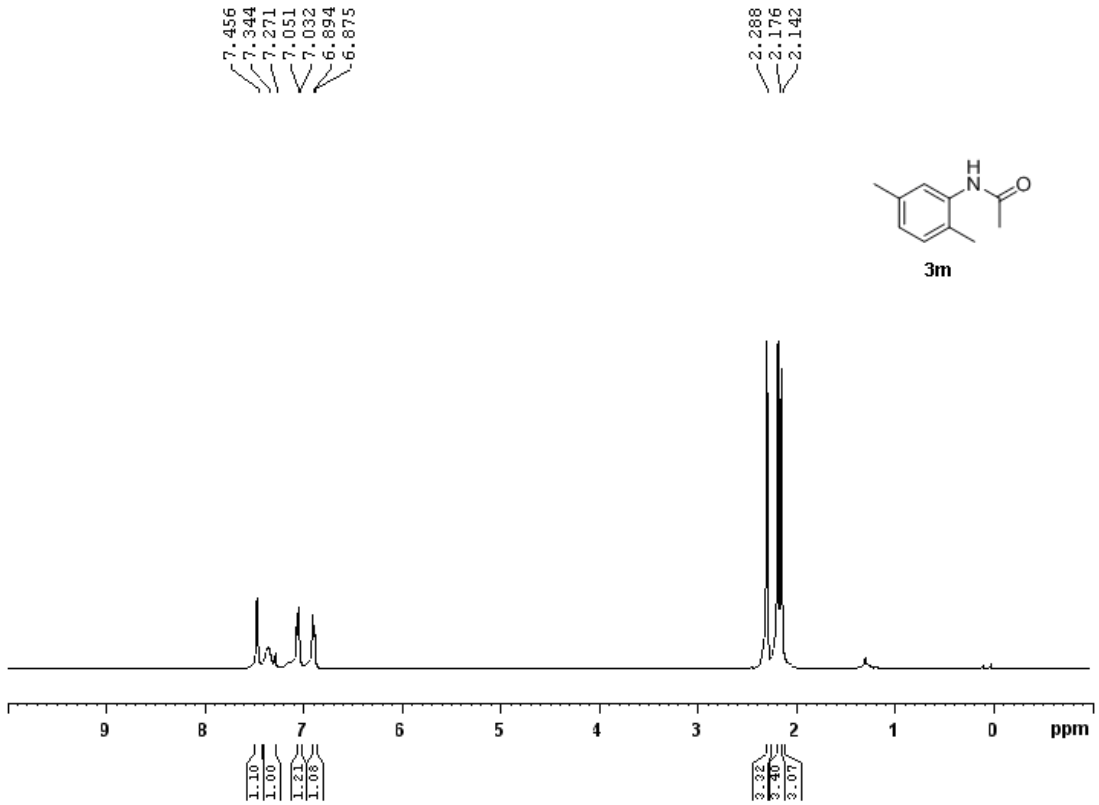
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2.288
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3m
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8
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1.21
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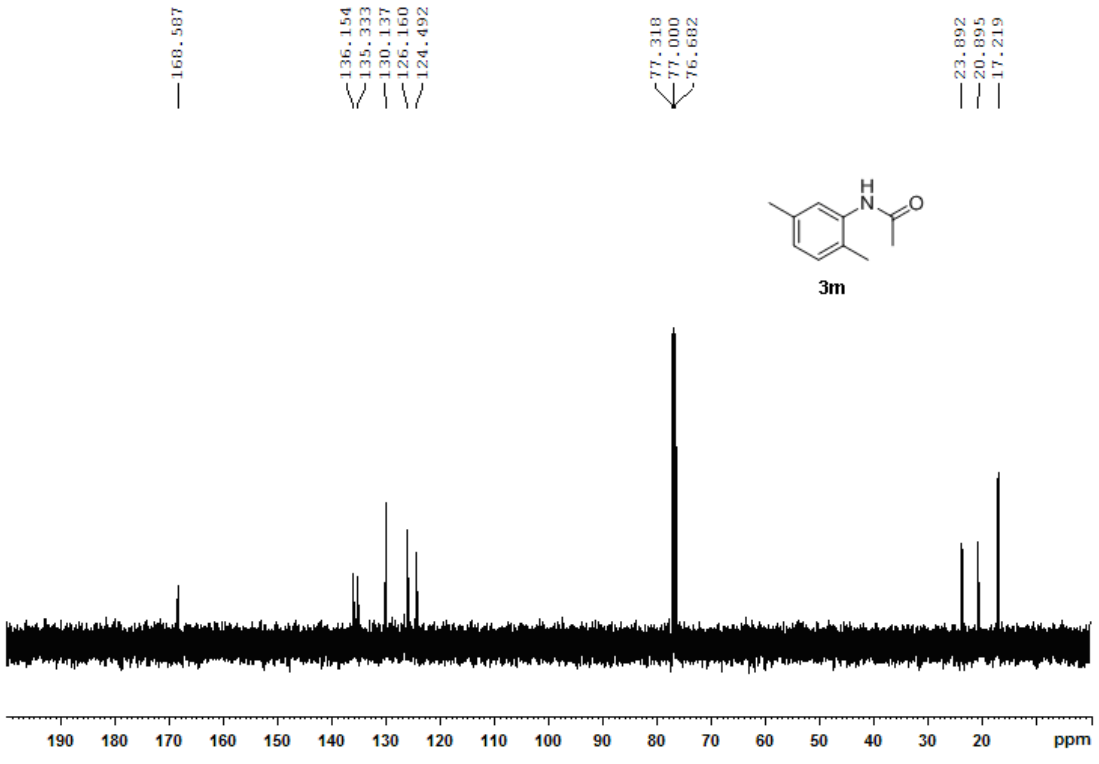
3.40
3.07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124.492
77.318
77.000
76.682
23.892
20.895
17.219
3m
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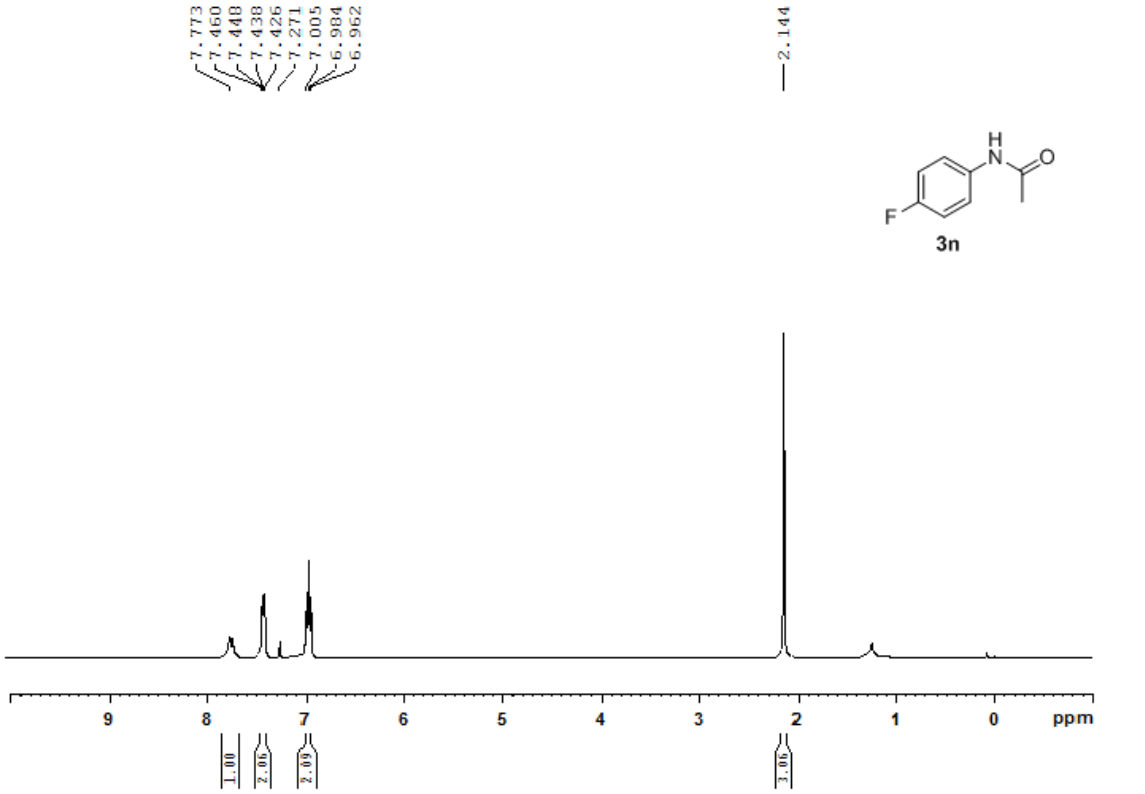
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6.984
6.962
2.144
H
N
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8
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ppm
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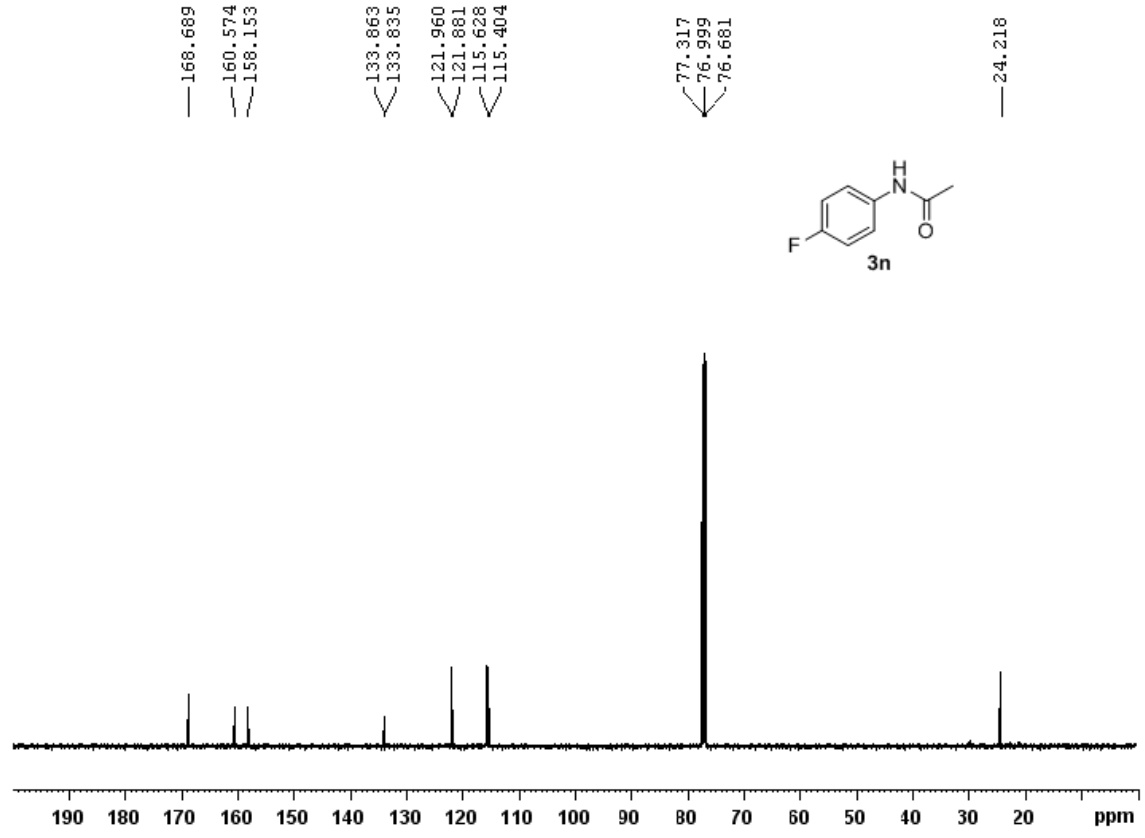
2.06
2.09
3.06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121.881
115.628
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76.999
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24.218
H
N
O
F
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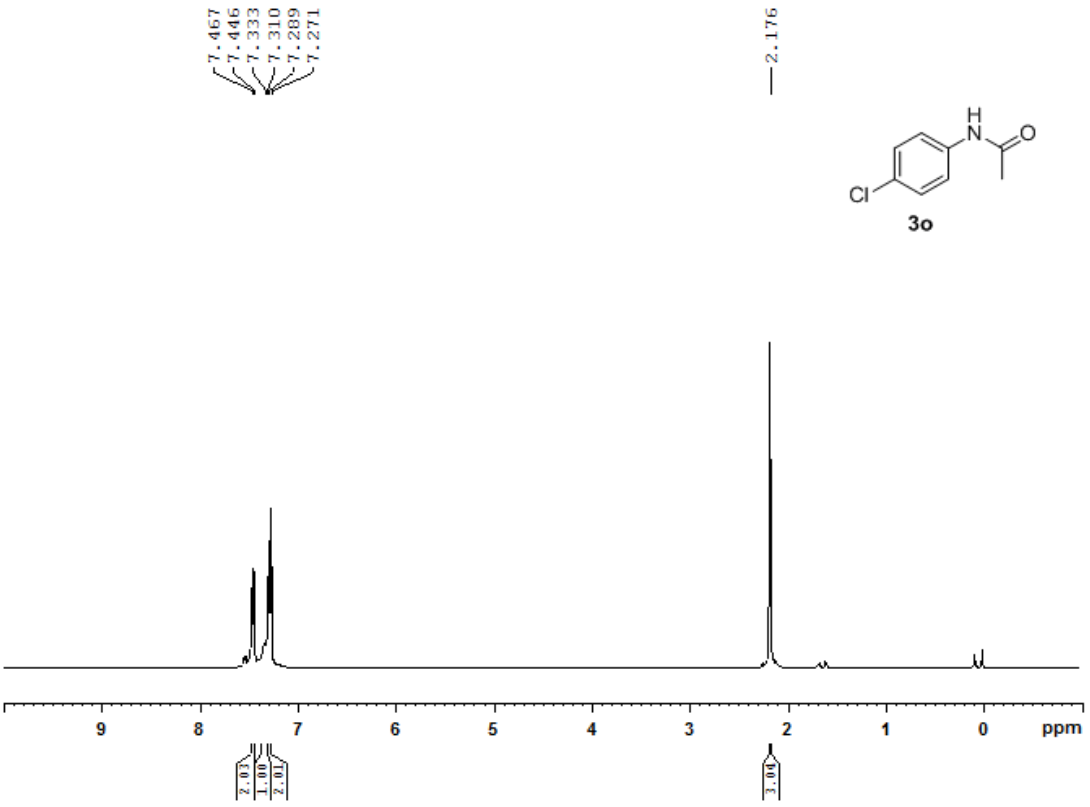
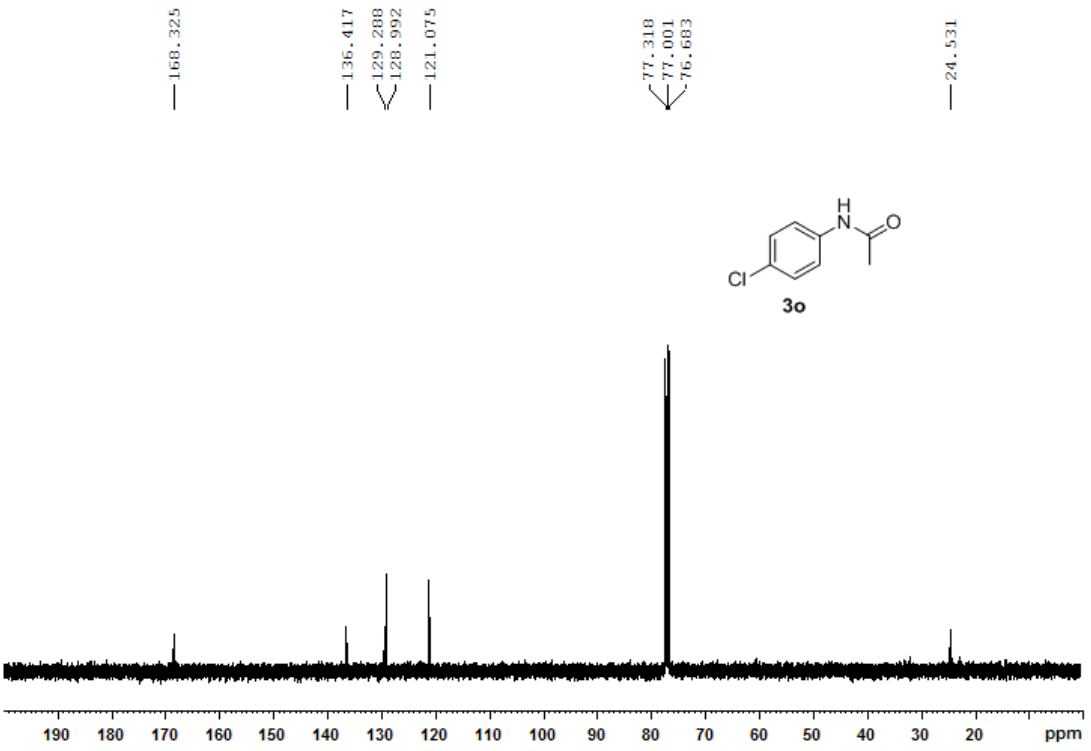
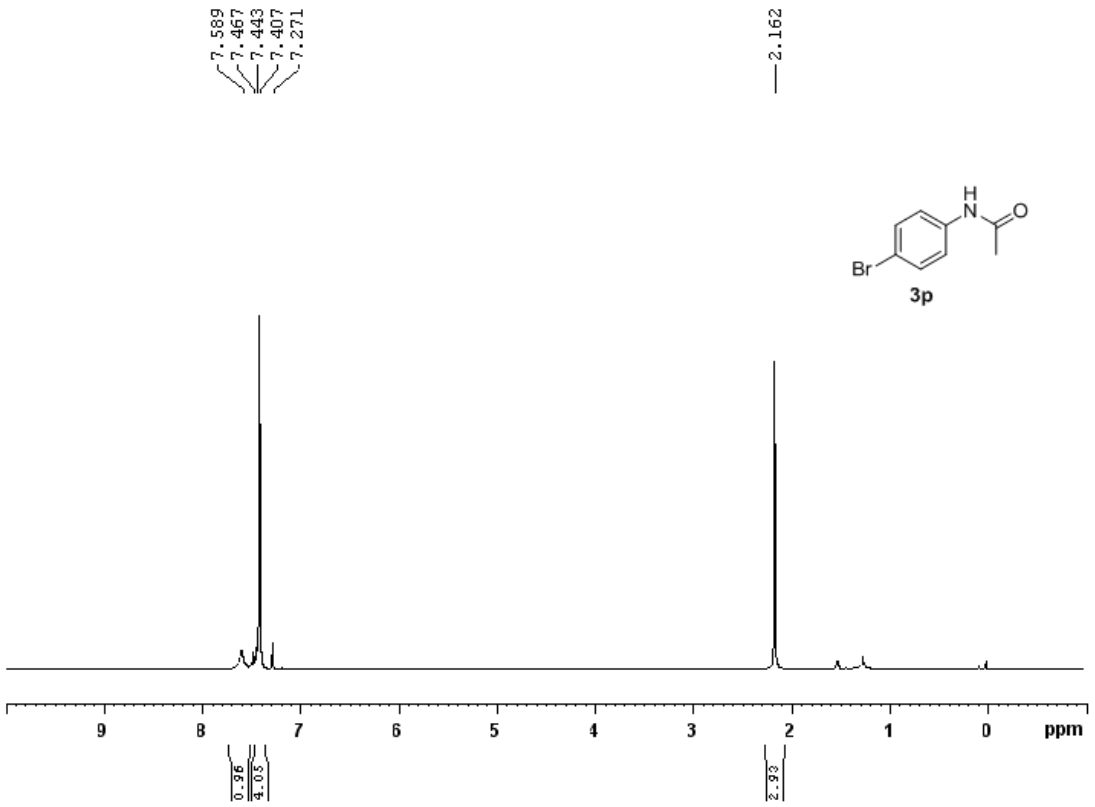
ppm



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8
7
6
5
4
3
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1
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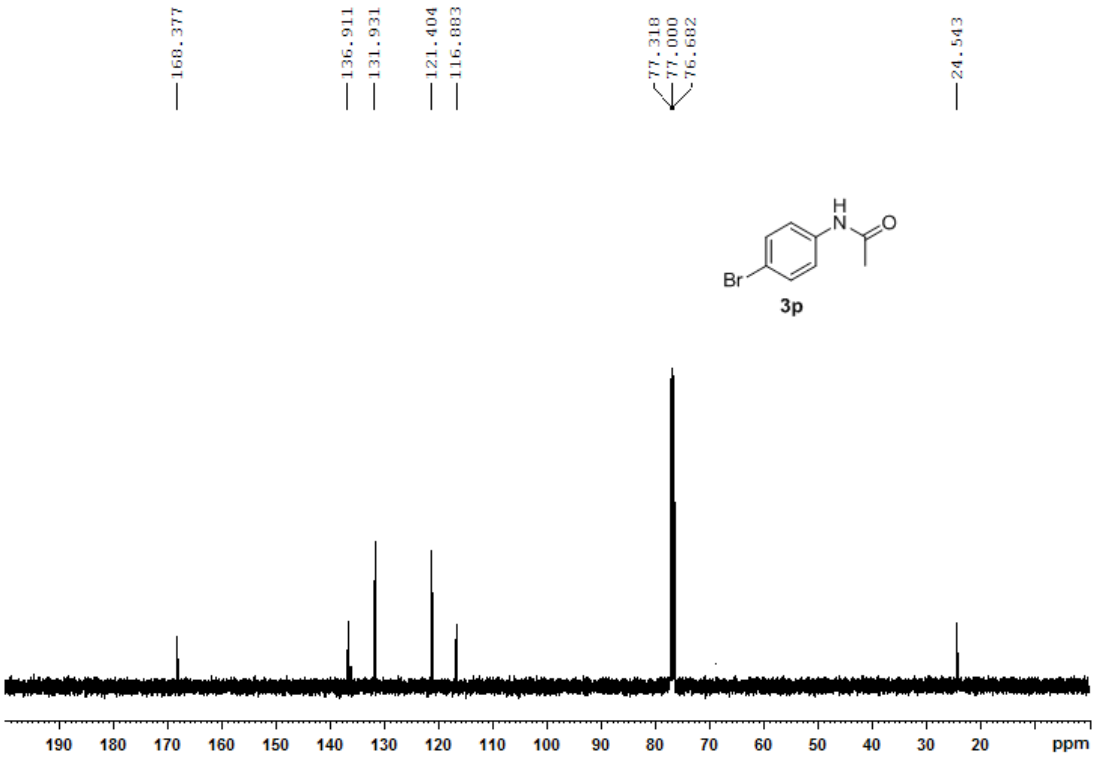
4.05
2.93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76.682
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Br
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80
70
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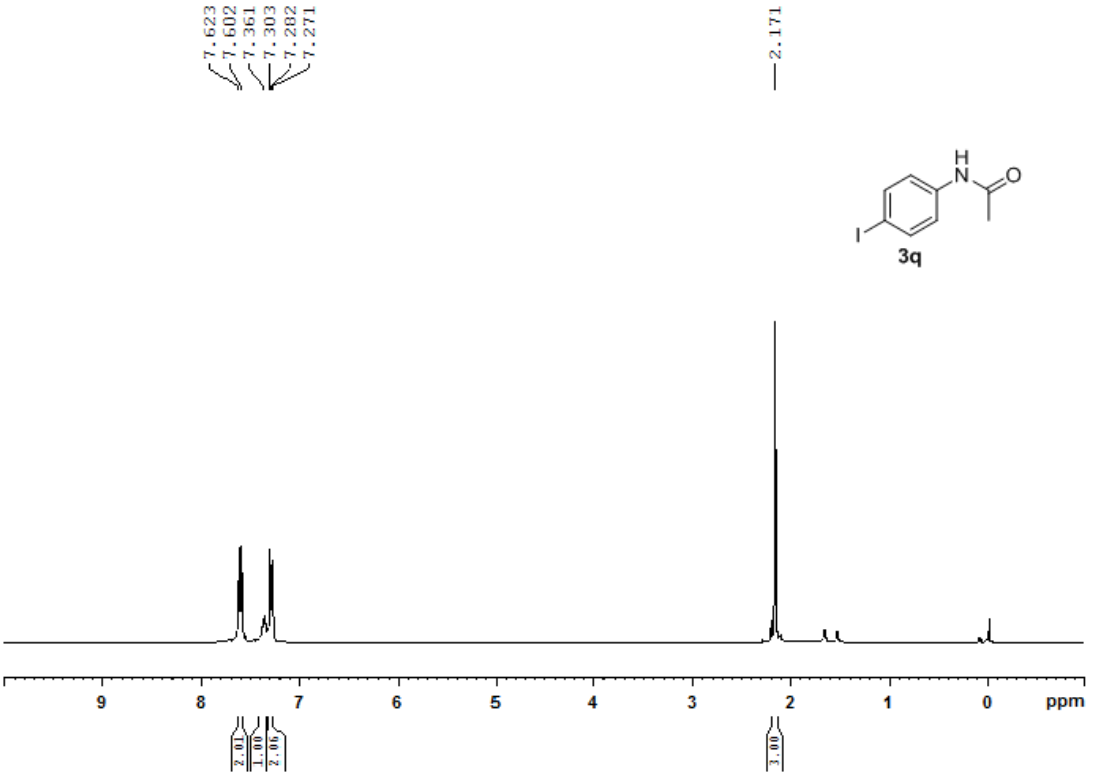
20
ppm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7.361
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6
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ppm
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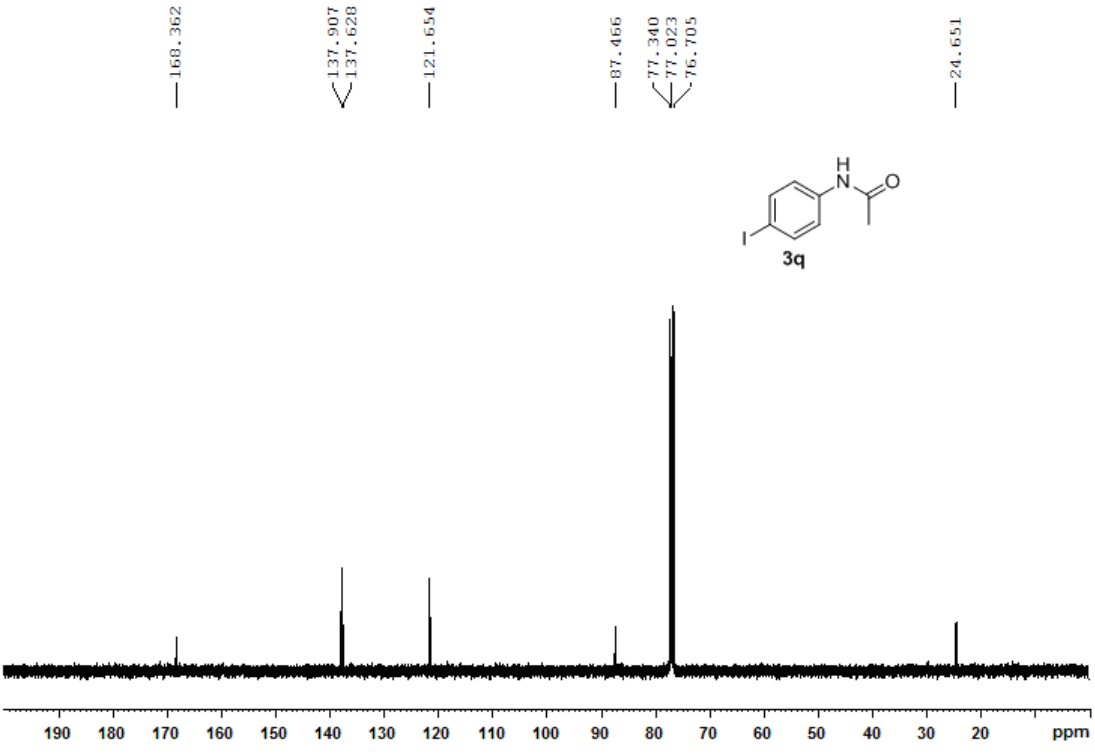
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77.340
77.023
76.705
24.651
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80
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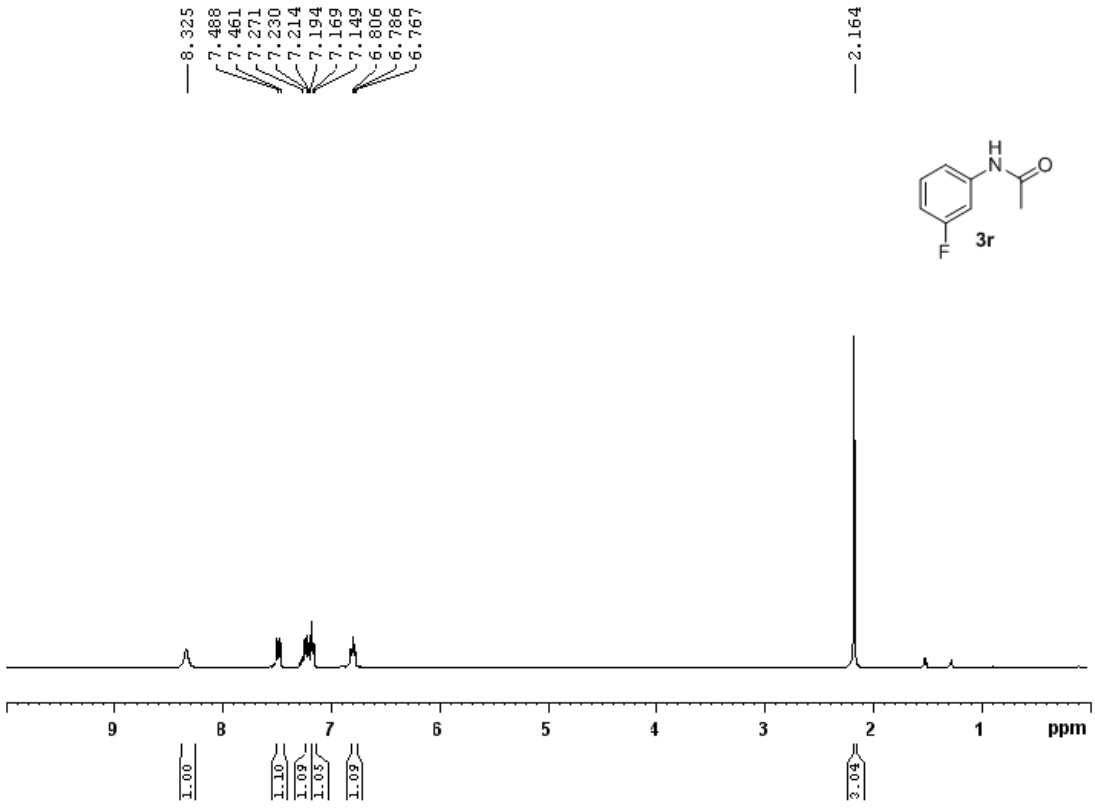
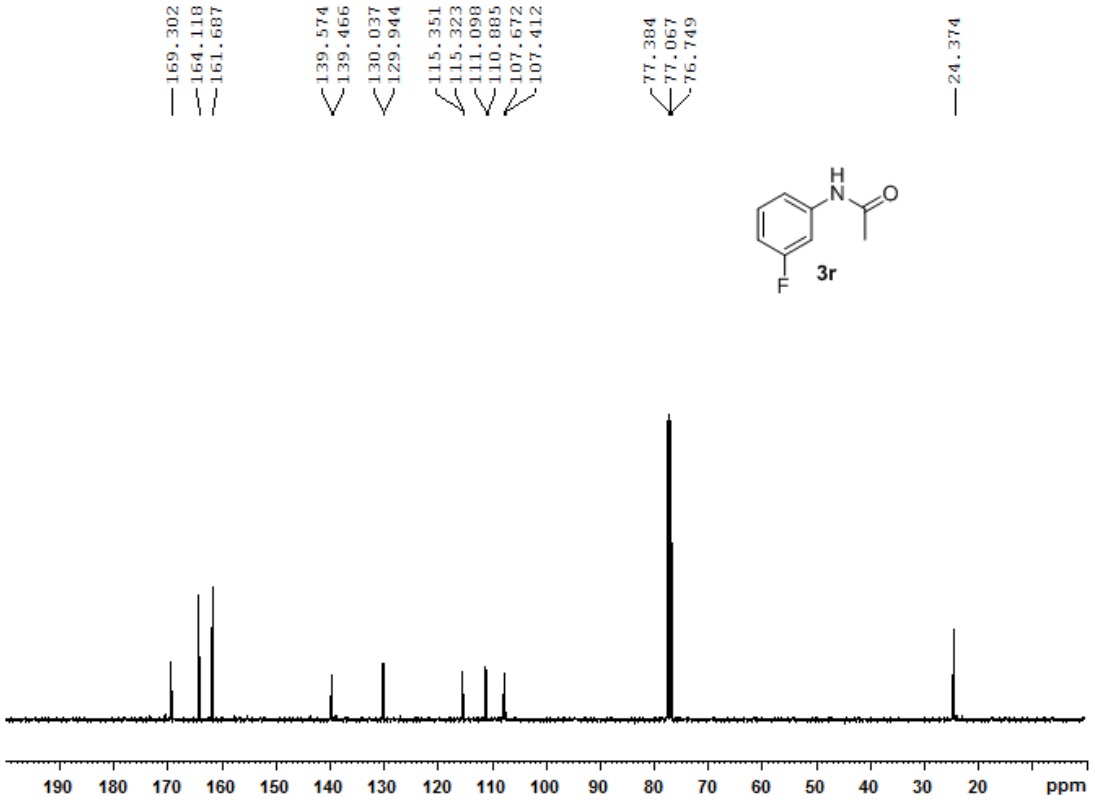
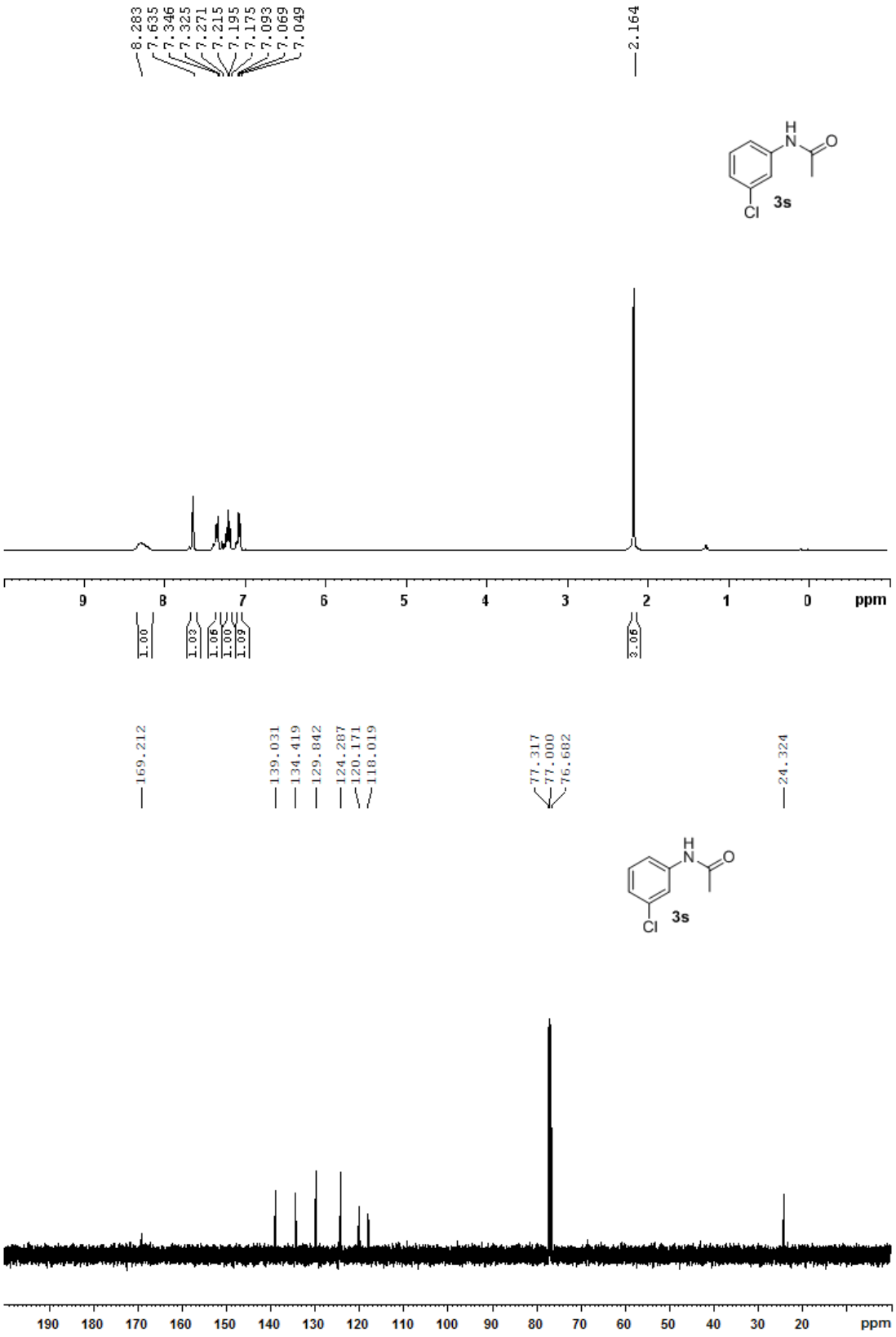
20
ppm



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7.271
7.215
7.195
7.175
7.093
7.069
7.049
2.164
3s
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
1.06
1.00
1.09
3.06
169.212
139.031
134.419
129.842
124.287
120.171
118.019
77.317
77.000
76.682
24.324
3s
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150
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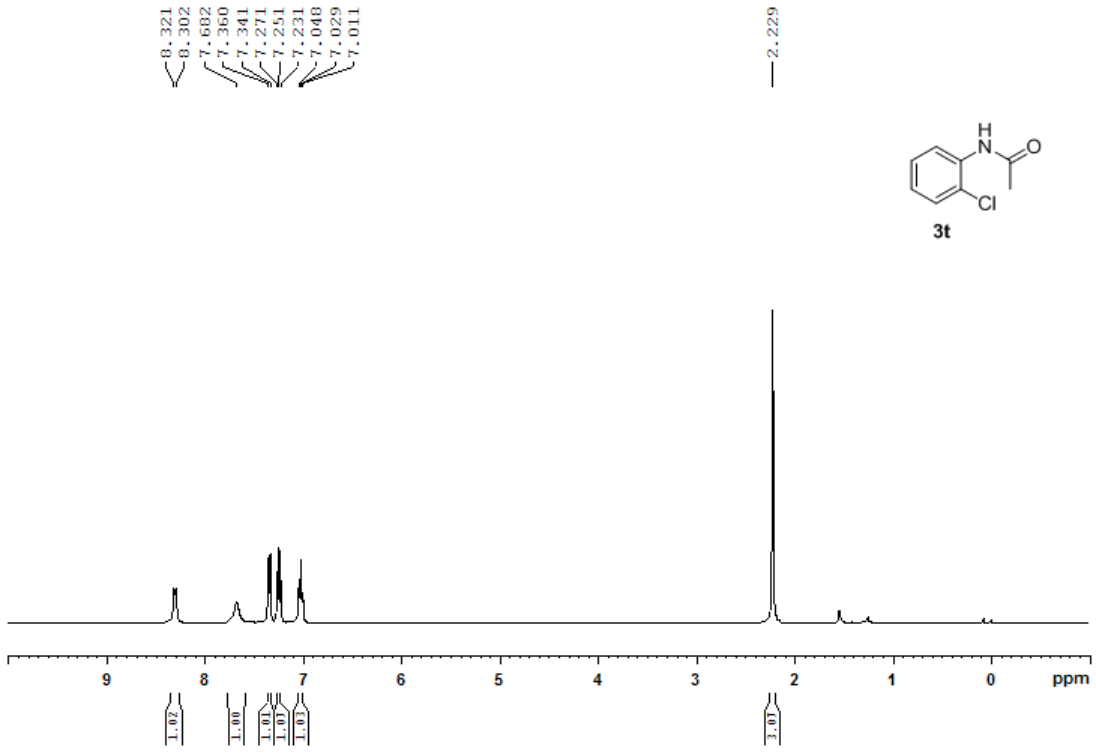
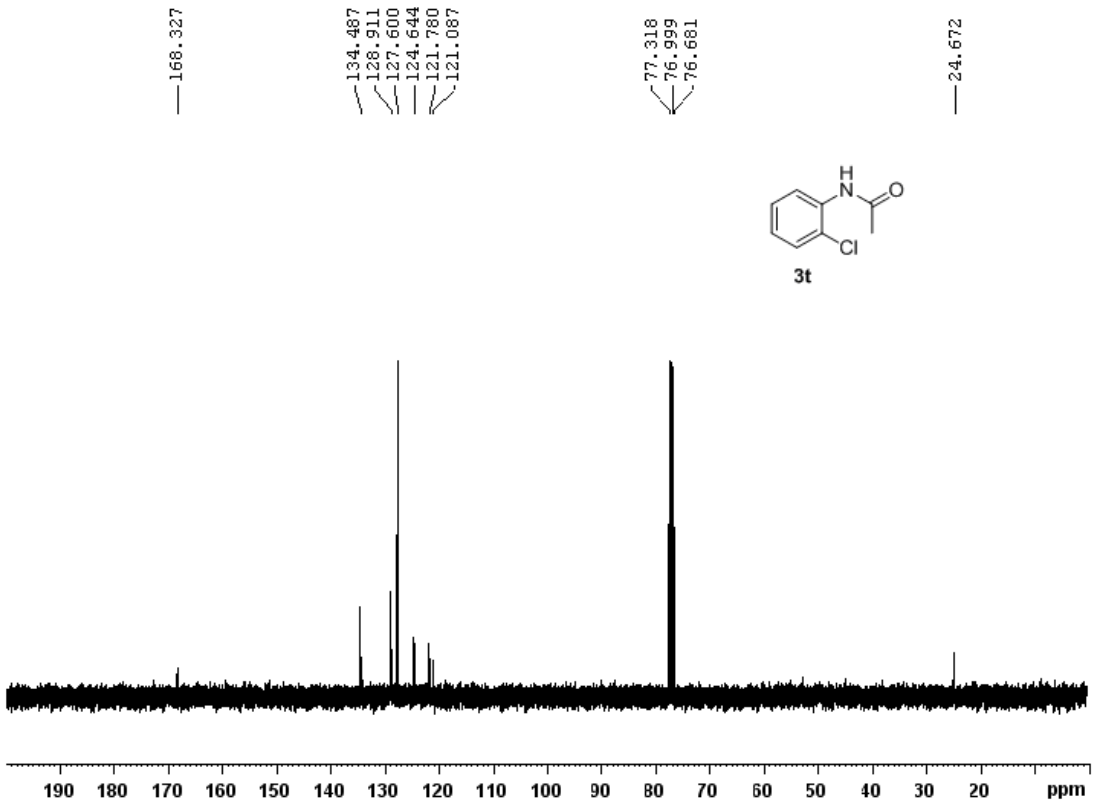
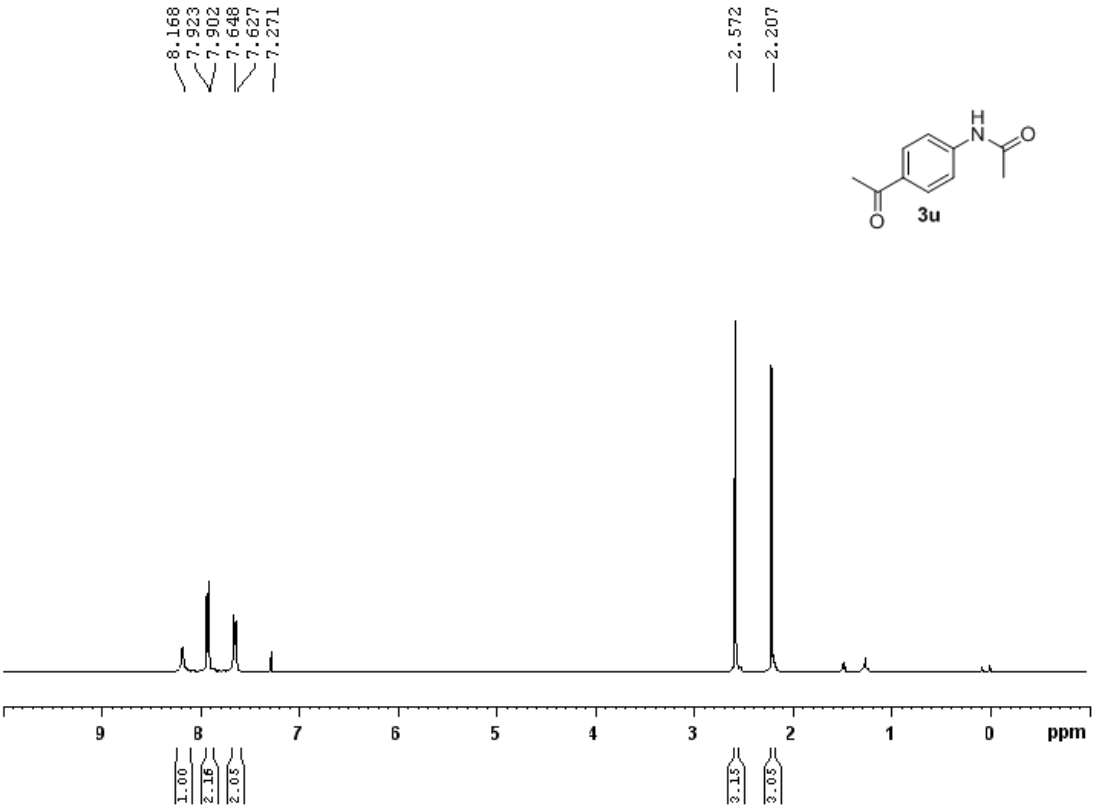
40
30
20
ppm



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7.627
7.271
2.572
2.207
3u
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8
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6
5
4
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ppm
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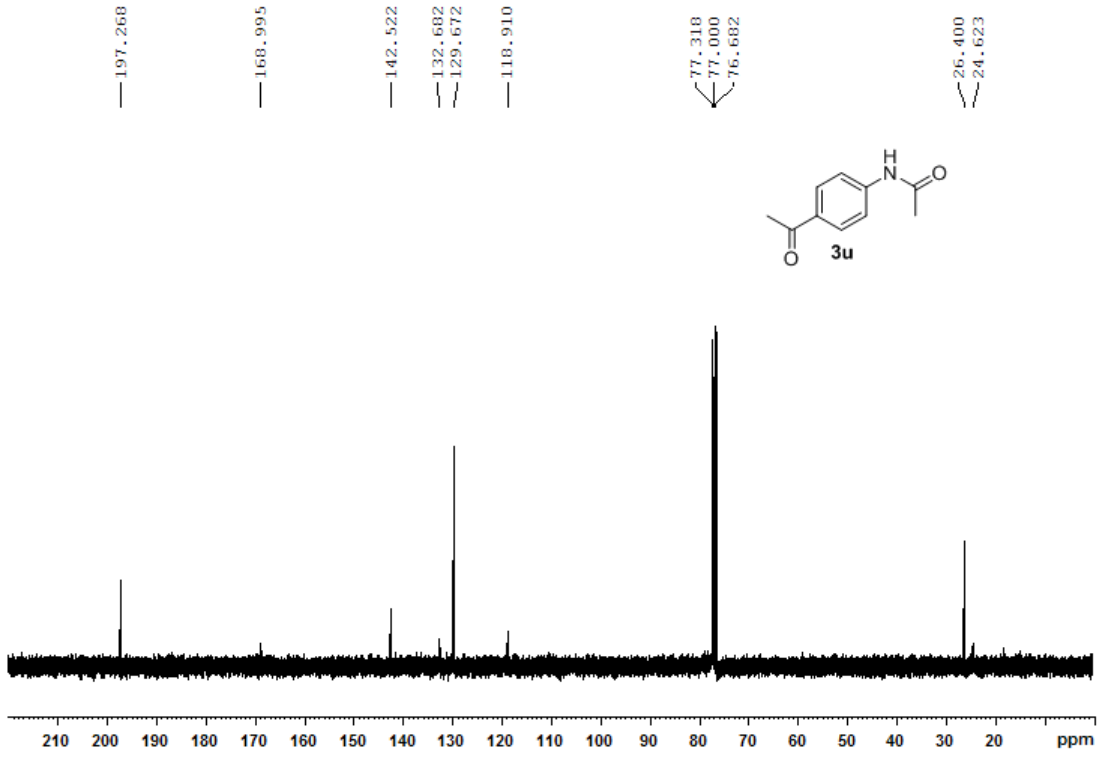
2.16
2.05
3.15
3.03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26.400
24.623
3u
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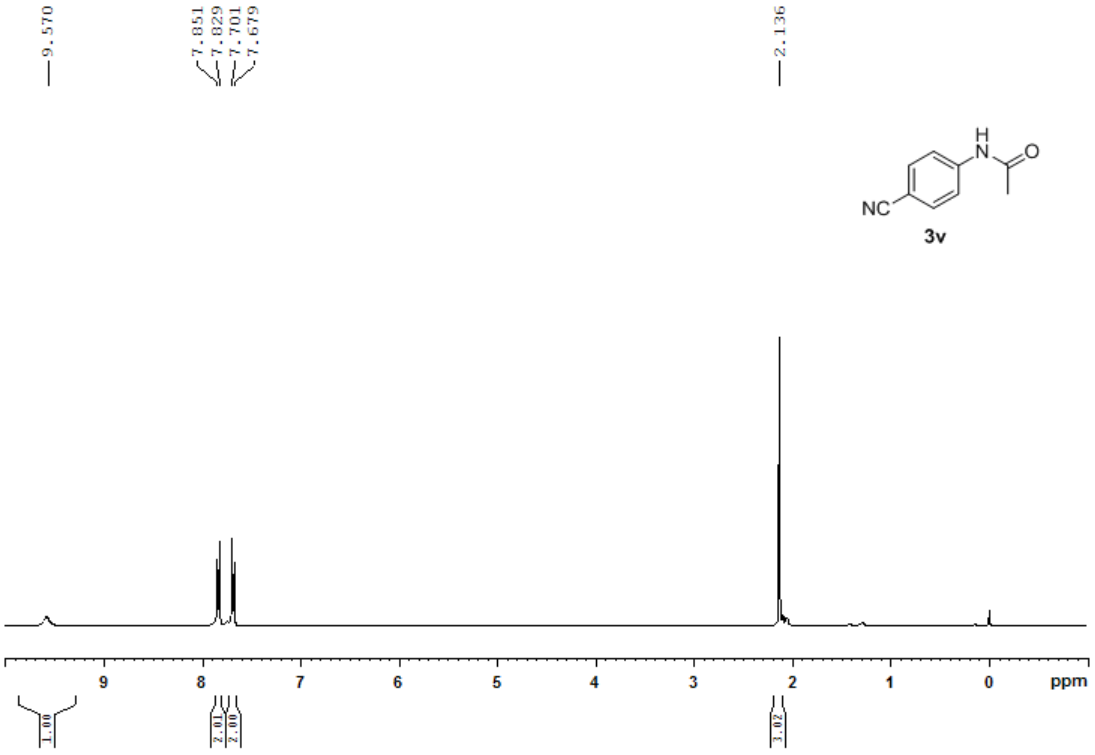
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7
6
5
4
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ppm
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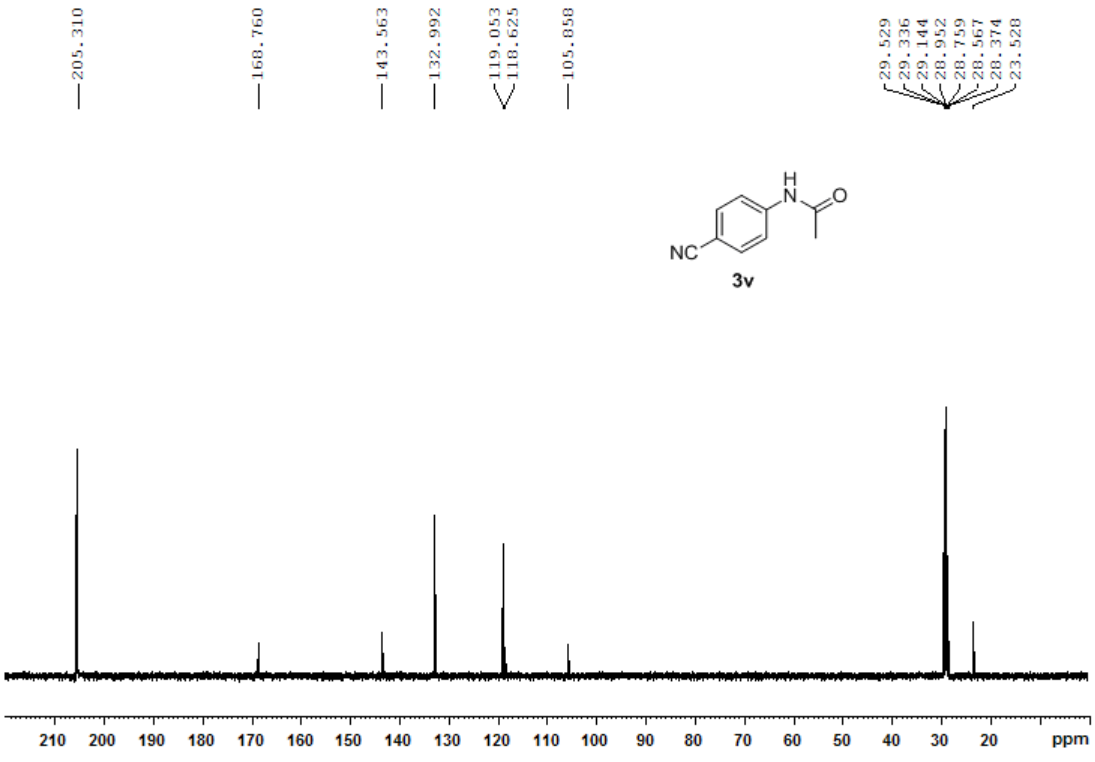
2.00
3.07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28.567
28.374
23.528
NC
3v
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150
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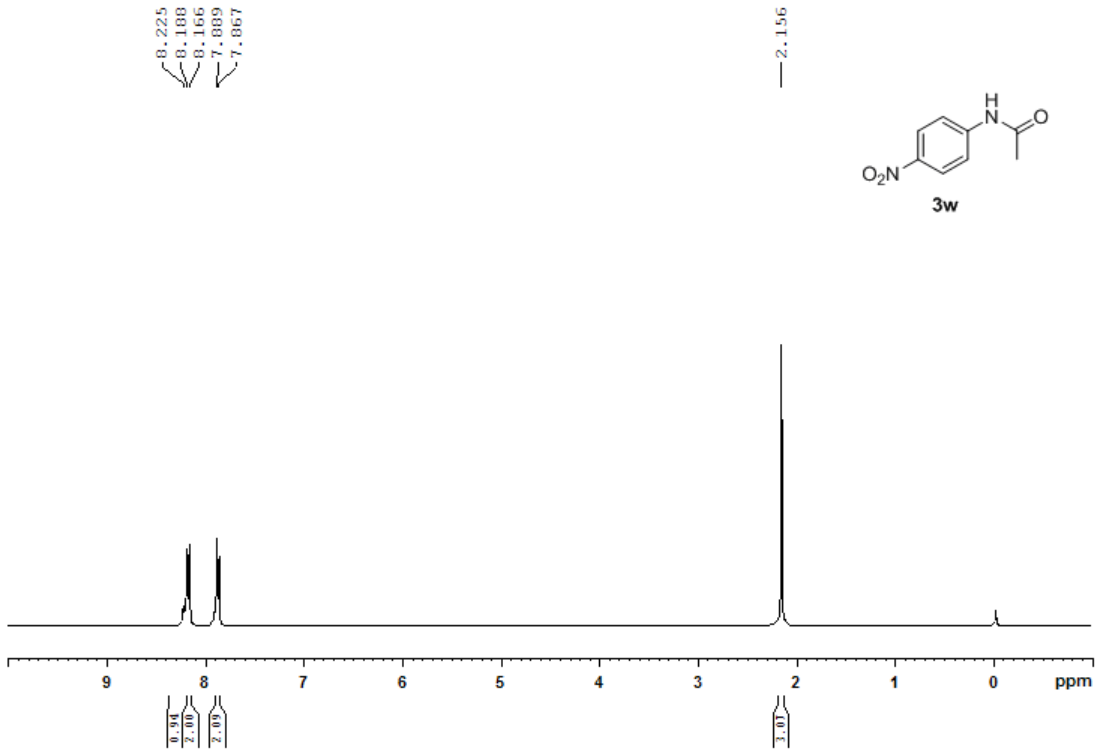
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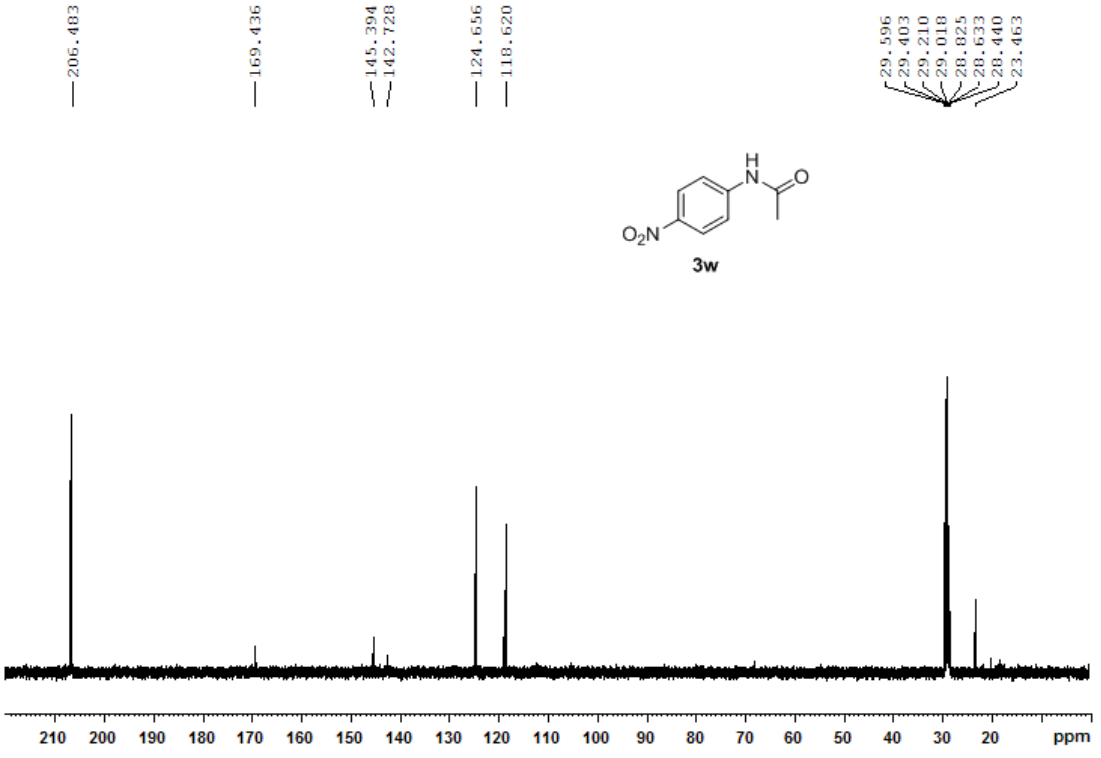
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29.210
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28.825
28.633
28.440
23.463
3w
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80
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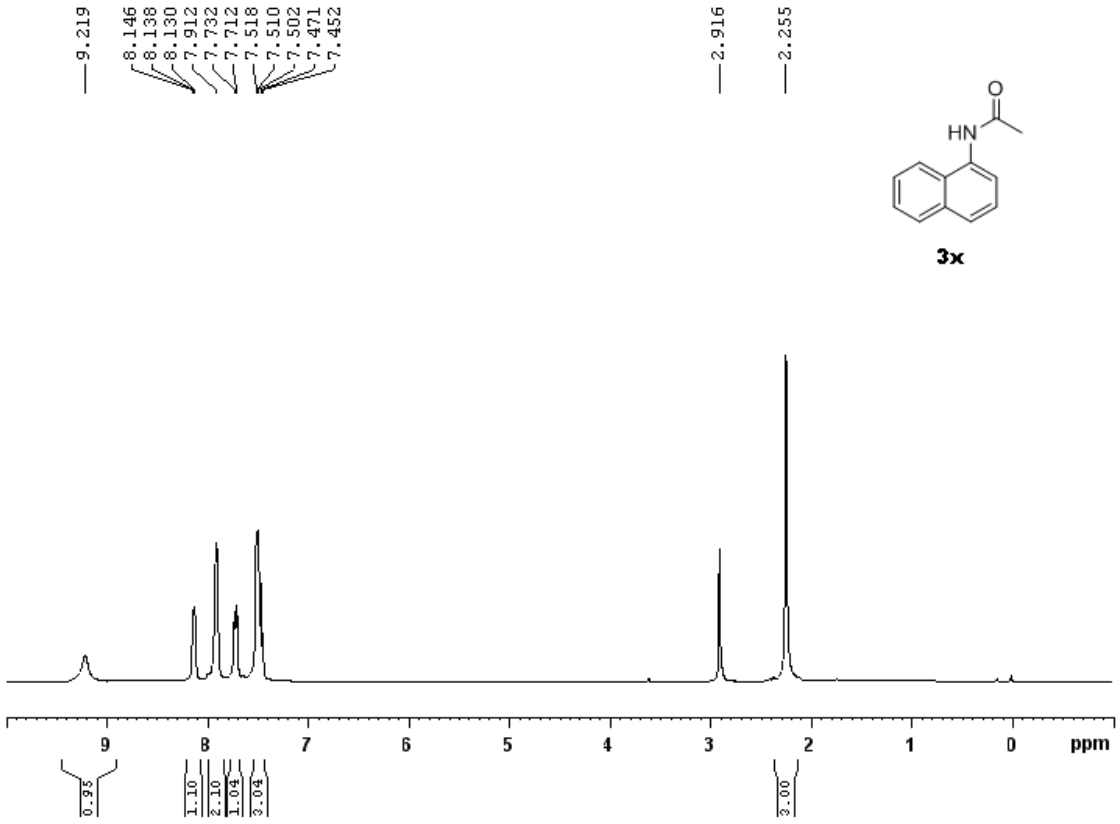
20
ppm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7.502
7.471
7.452
2.916
2.255
HN
O
3x
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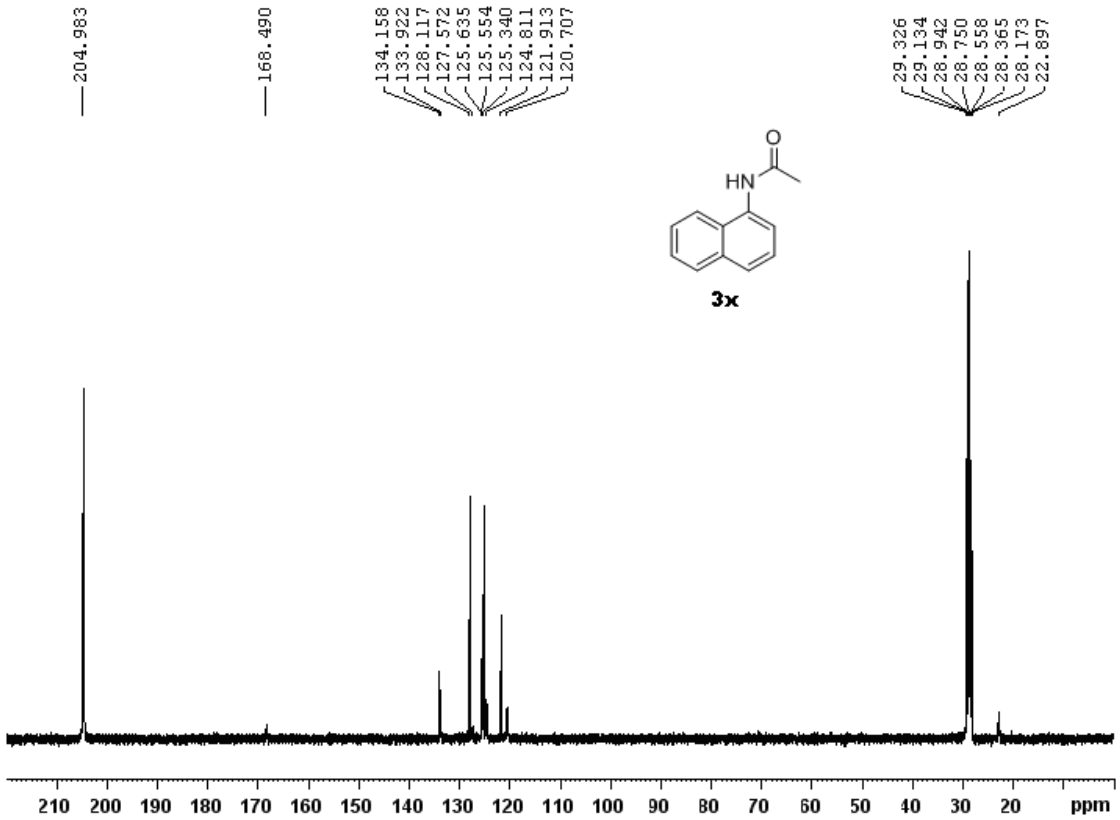
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125.554
125.340
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121.913
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29.134
28.942
28.750
28.558
28.365
28.173
22.897
HN
O
3x
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20
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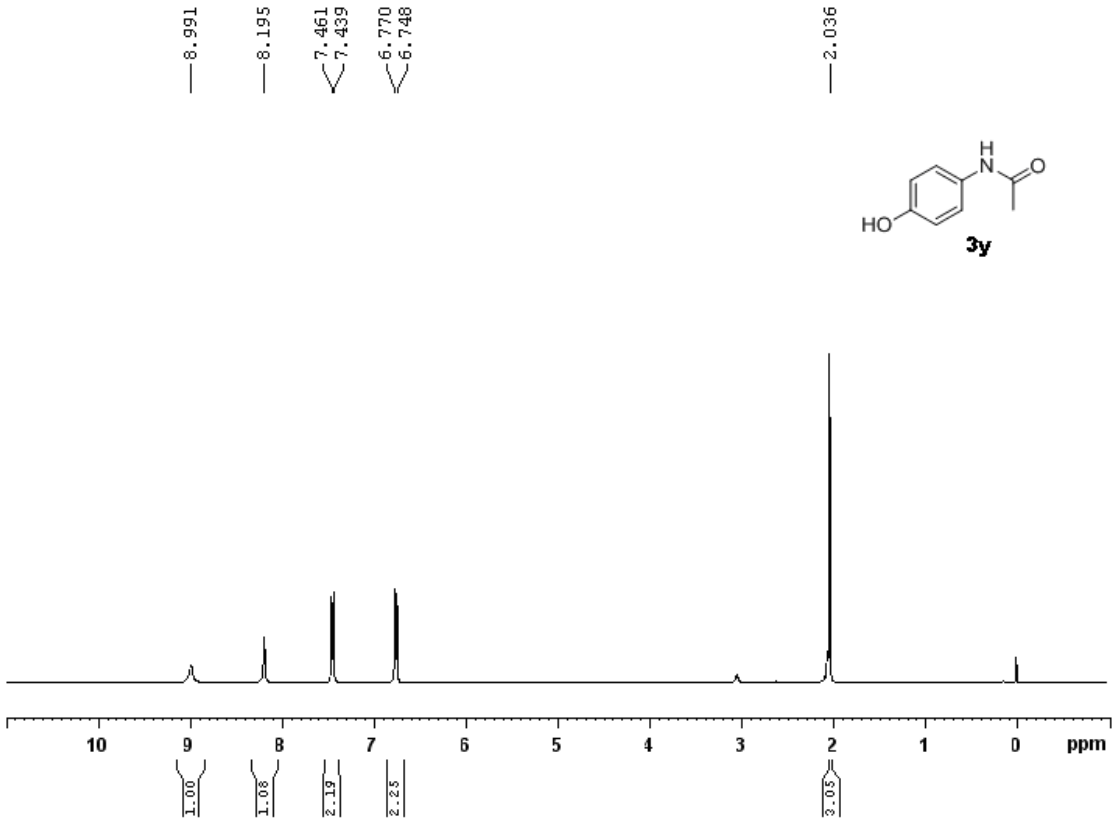
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O
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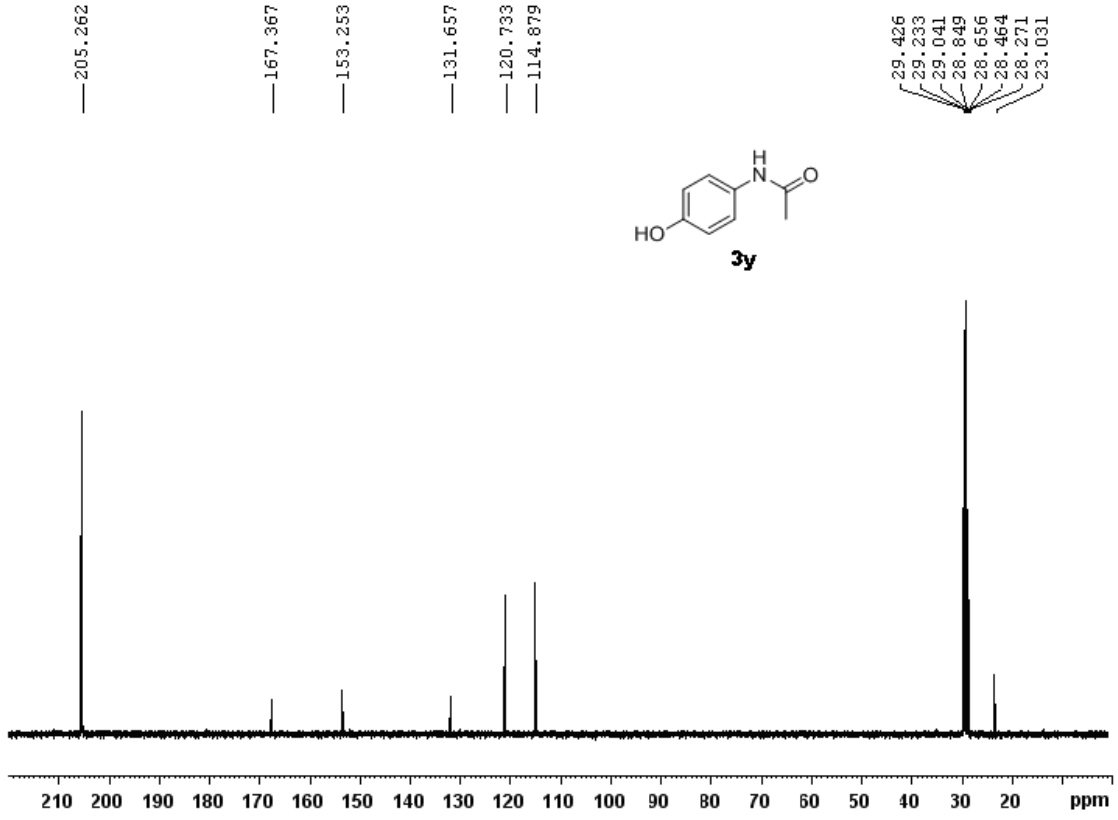
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28.271
23.031
HO
H
N
O
3y
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80
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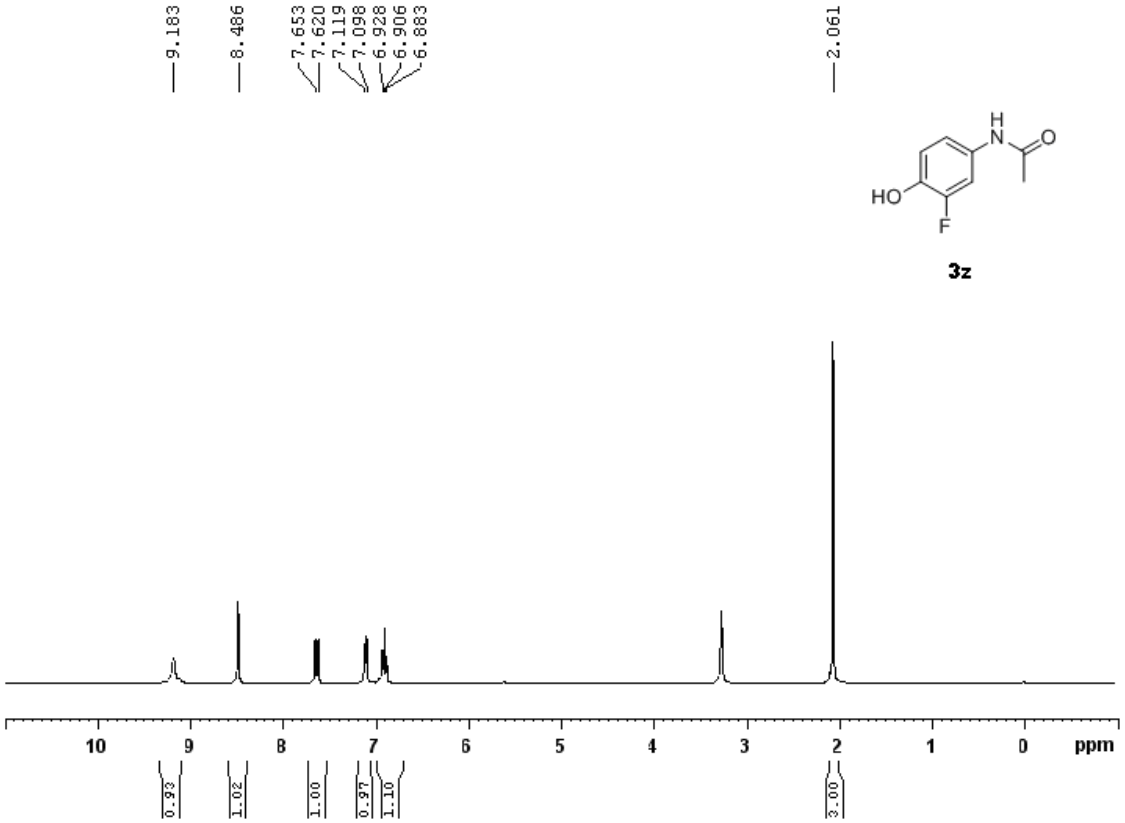
20
ppm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6.906
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H
N
O
3z
10
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7
6
5
4
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0
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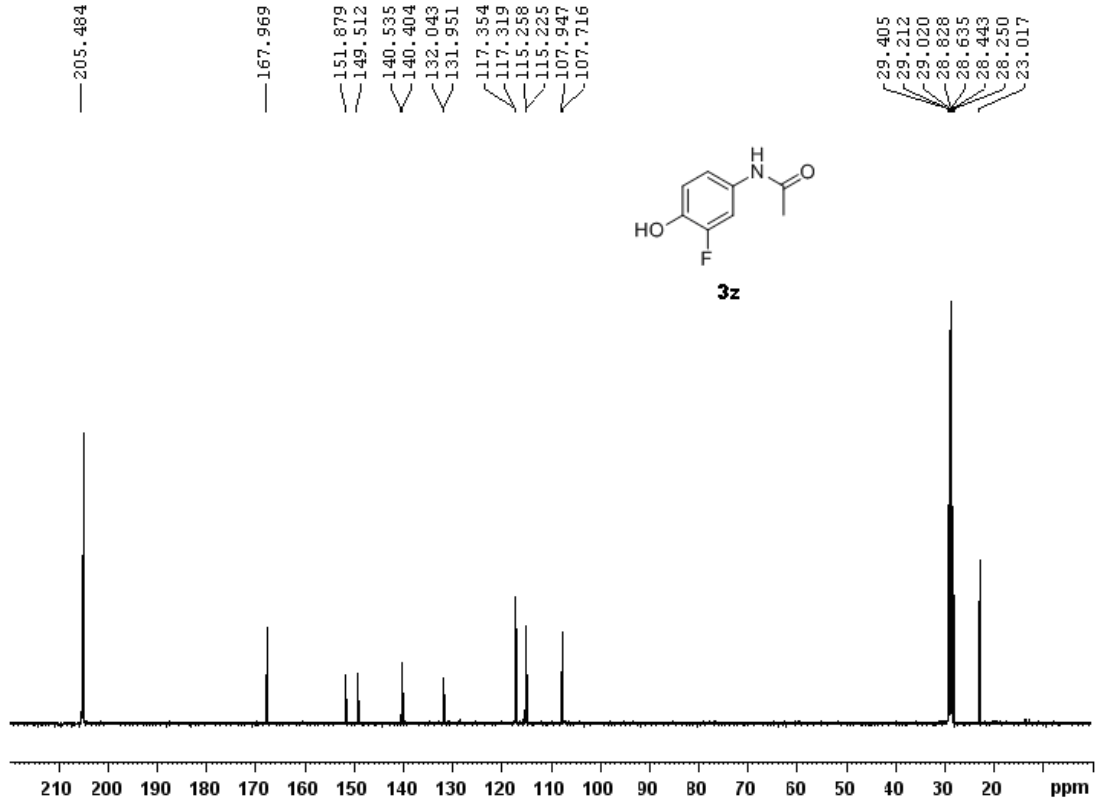
3.00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107.716
29.405
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29.020
28.828
28.635
28.443
28.250
23.017
HO
F
H
N
O
3z
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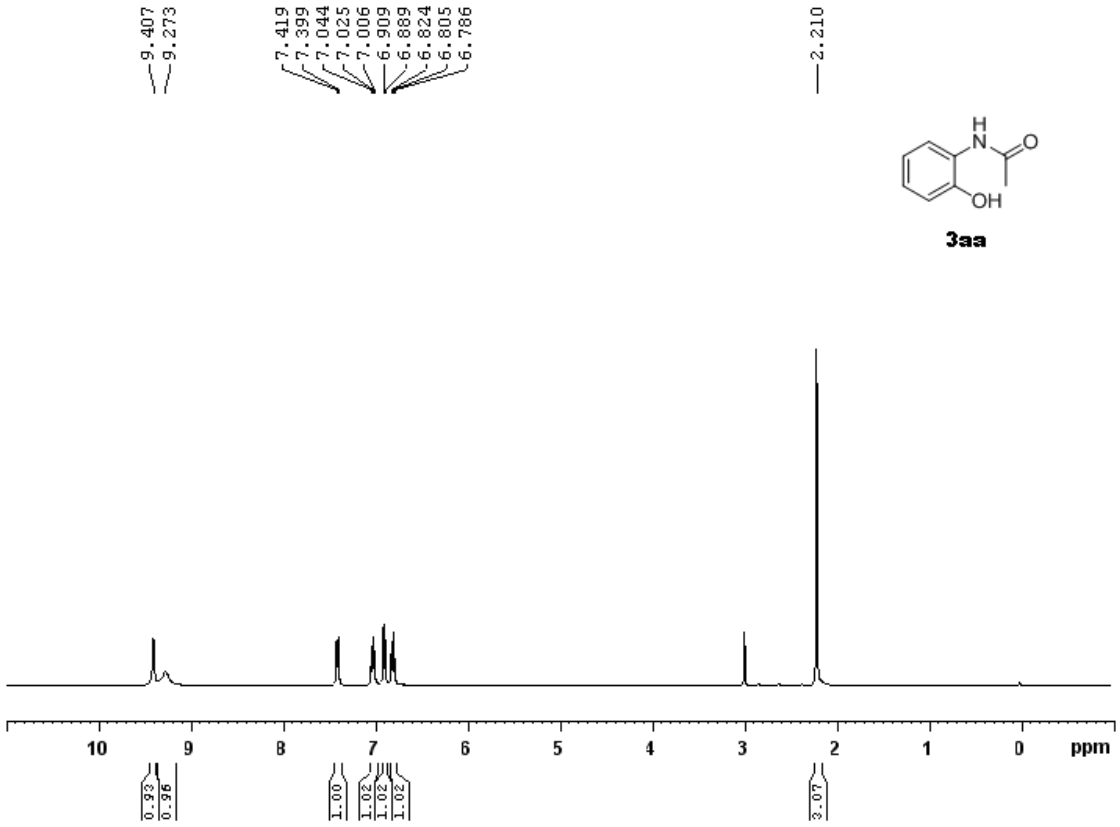
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6.824
6.805
6.786
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10
9
8
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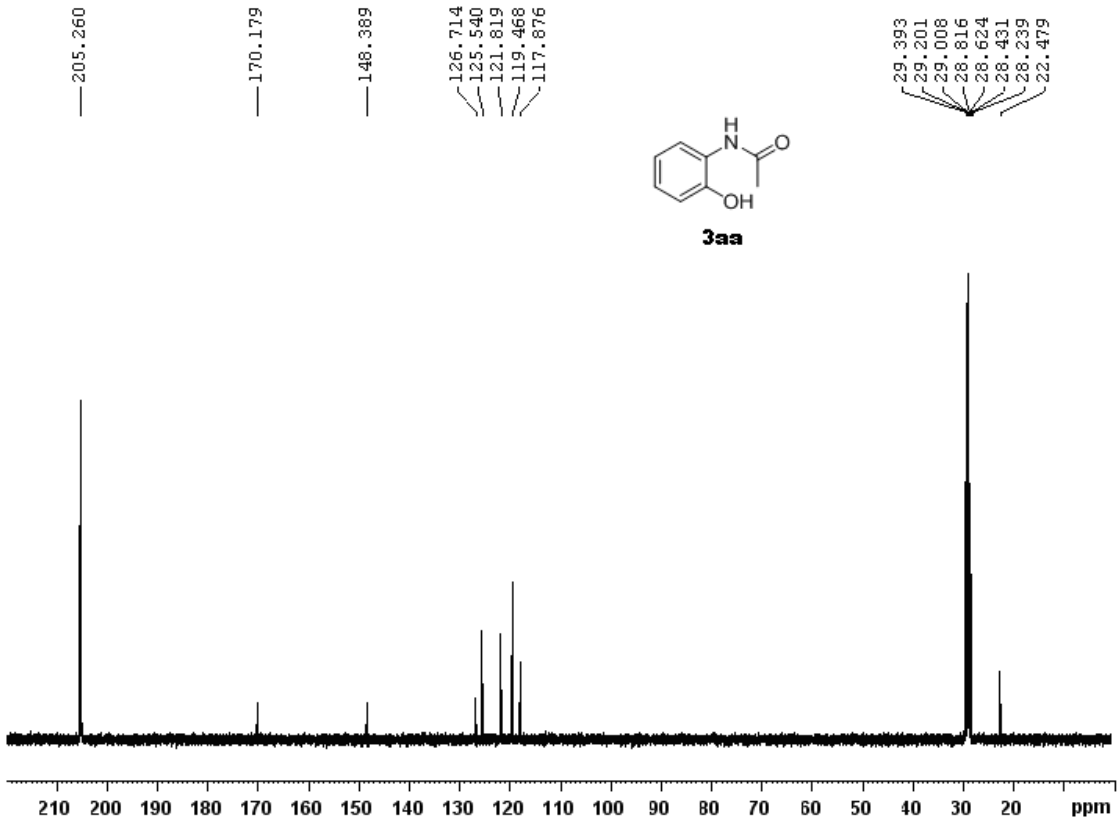
1.02
1.02
3.07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28.624
28.431
28.239
22.479
3aa
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20
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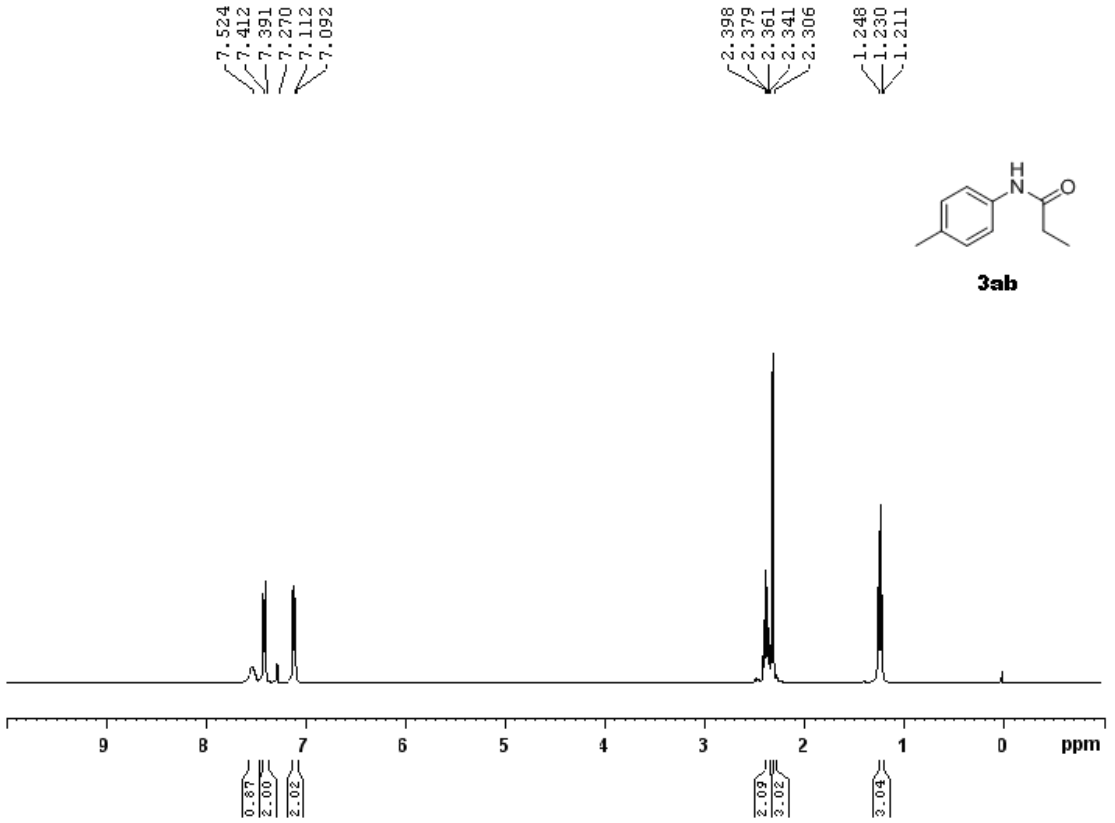
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1.211
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N
O
3ab
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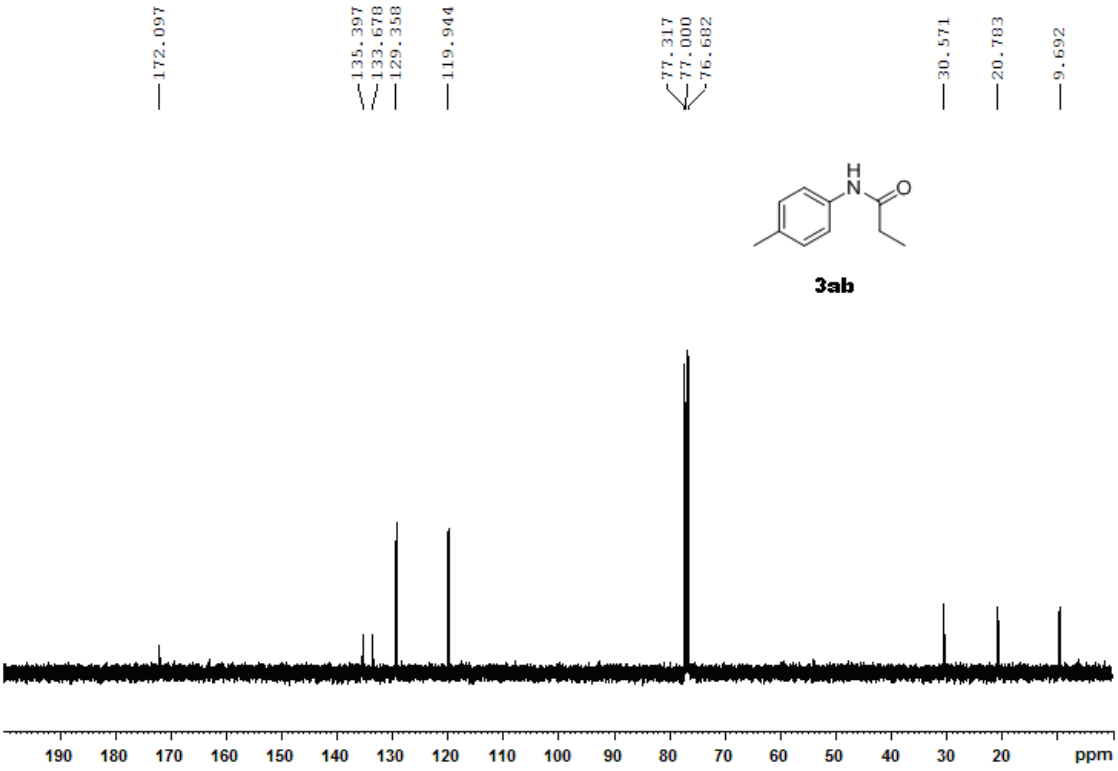
3.04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H
N
O
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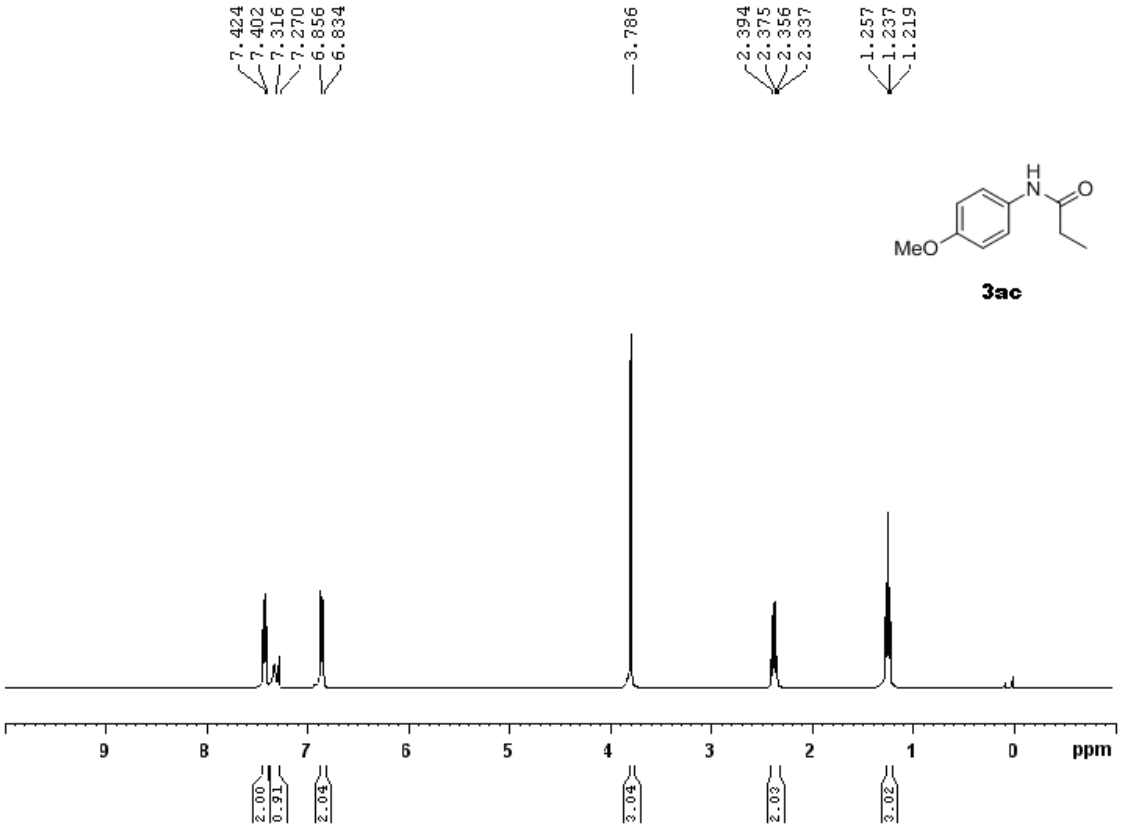
20
ppm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1.219
MeO
H
N
O
3ac
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4
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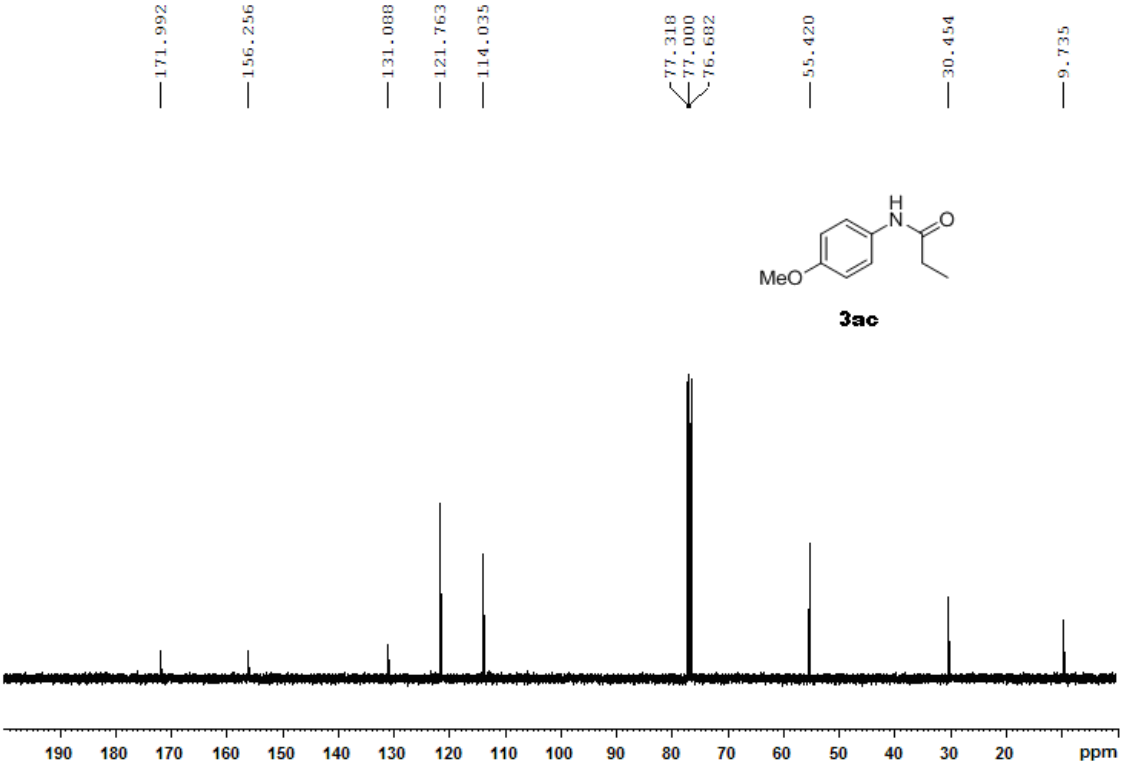
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77.000
76.682
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30.454
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MeO
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N
O
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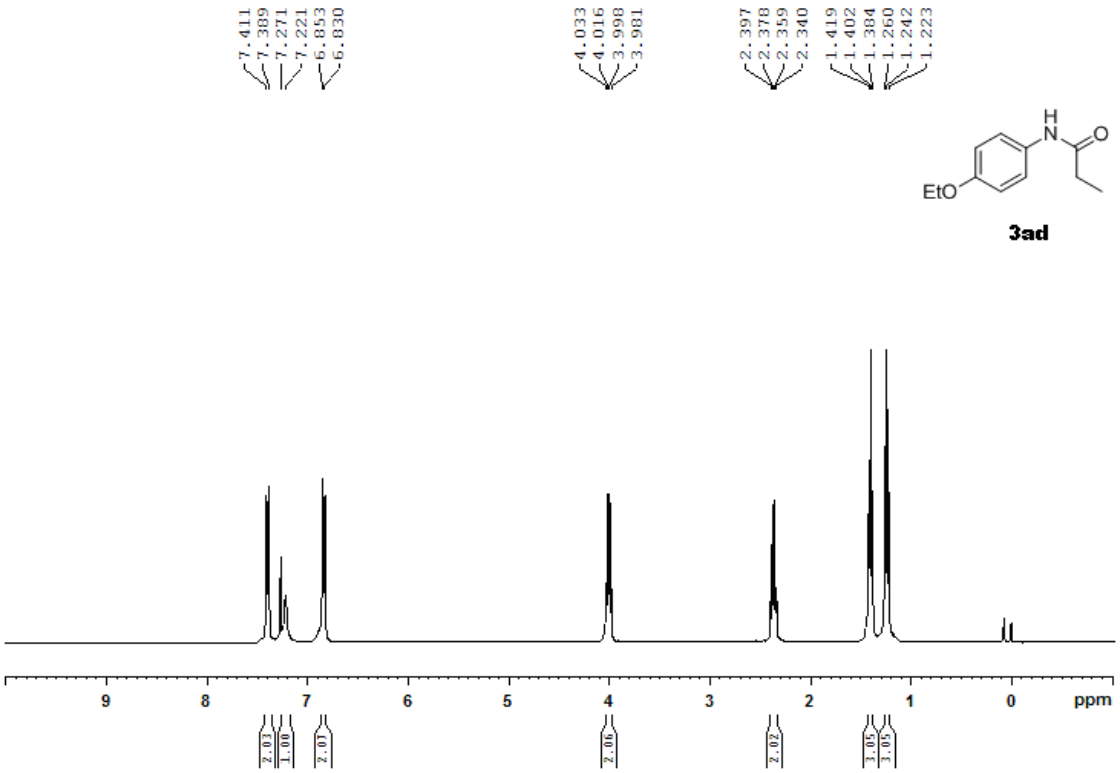
ppm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2.340
1.419
1.402
1.384
1.260
1.242
1.223
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N
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EtO
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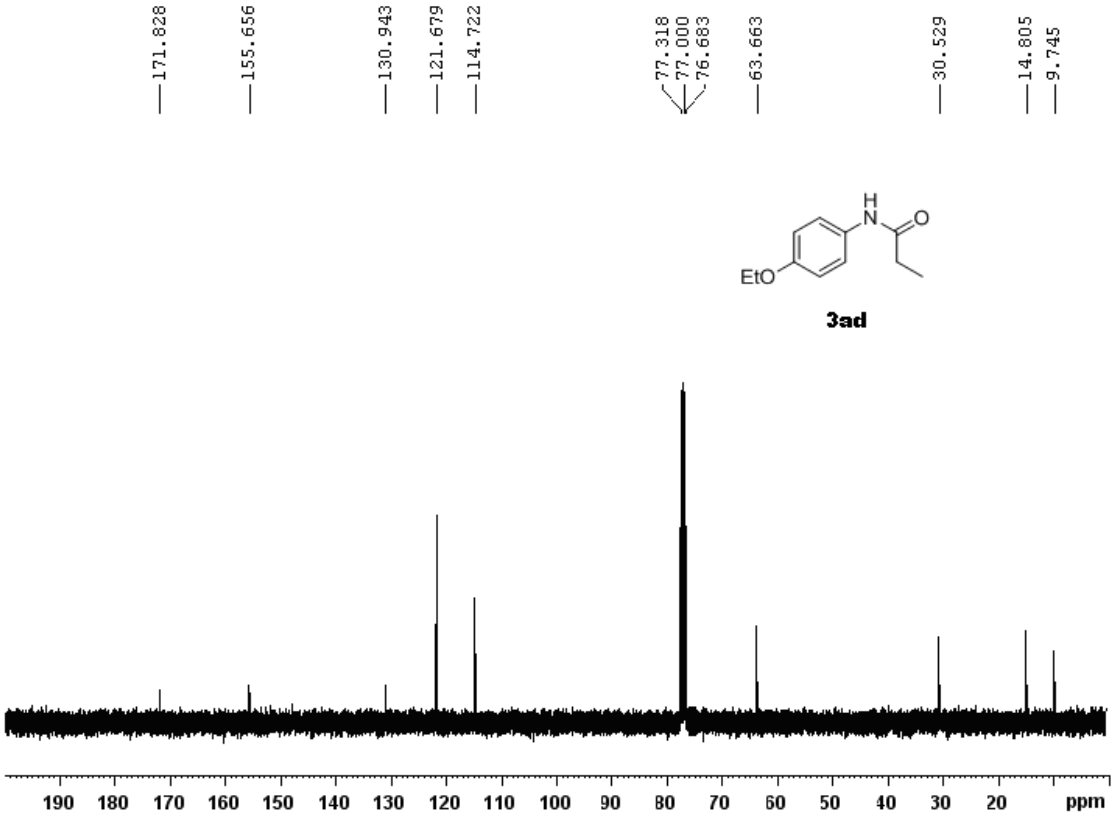
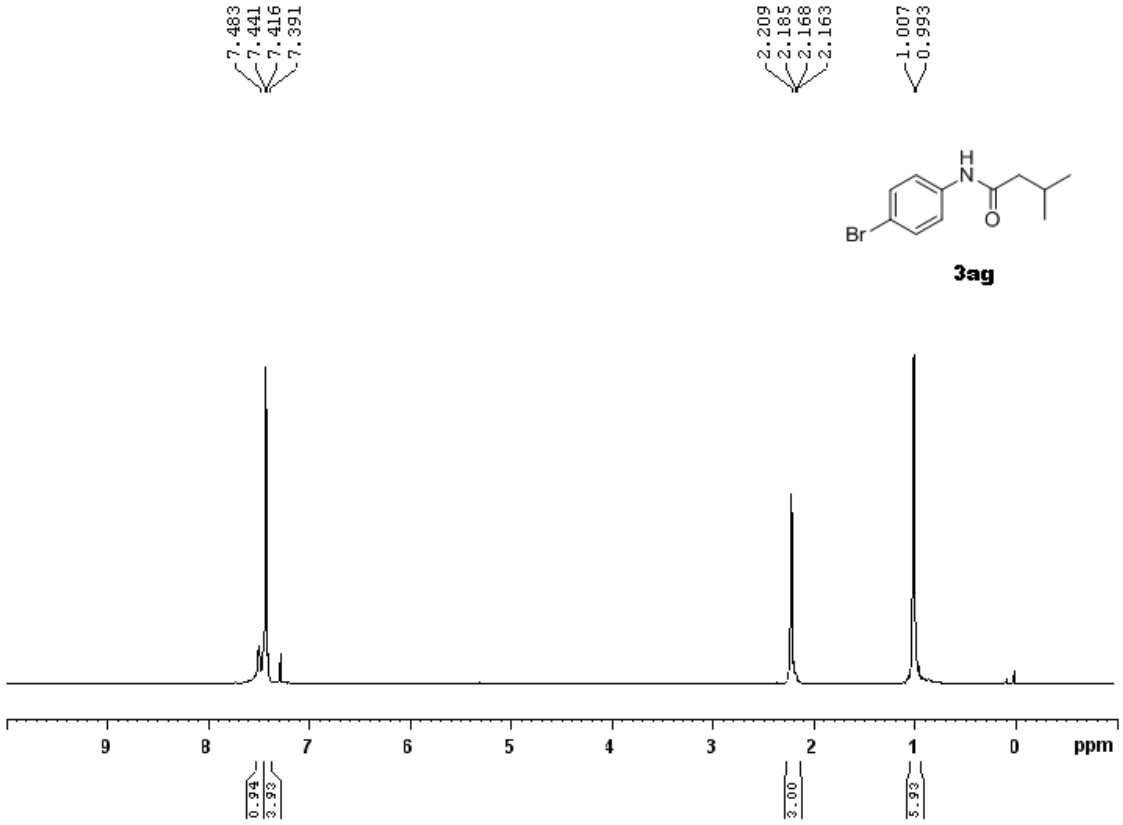
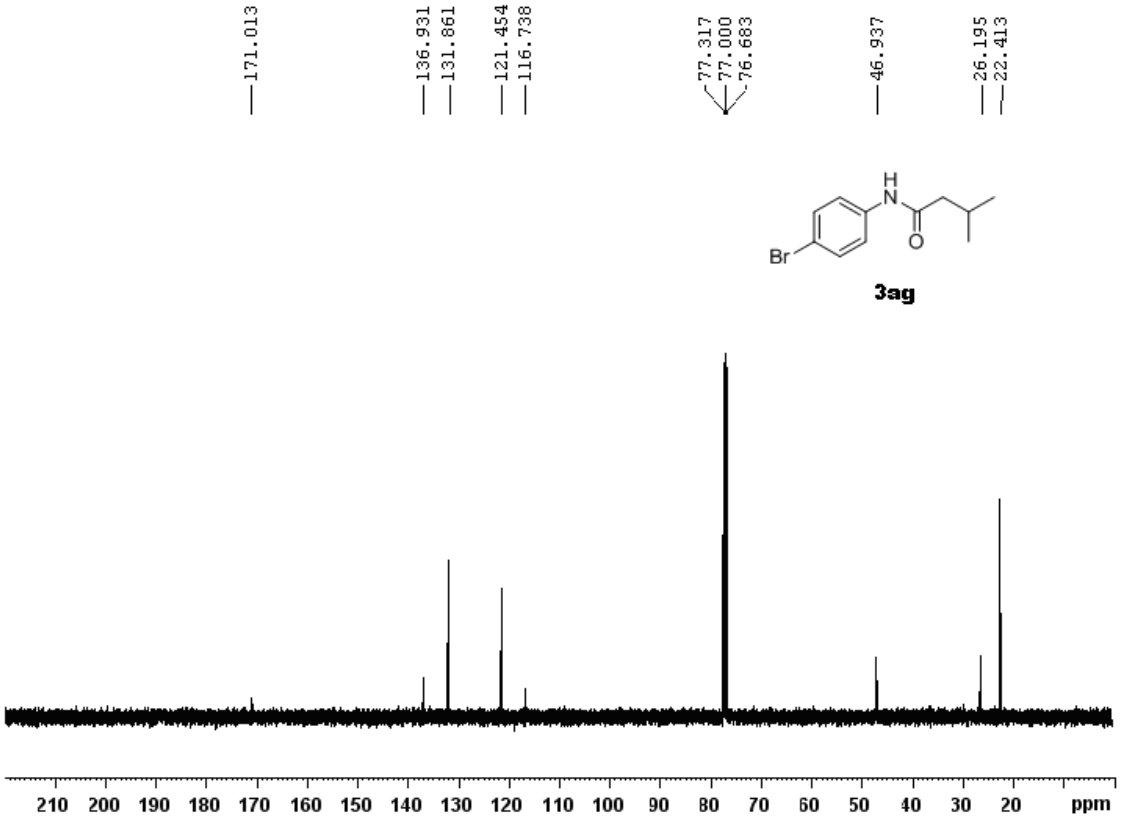
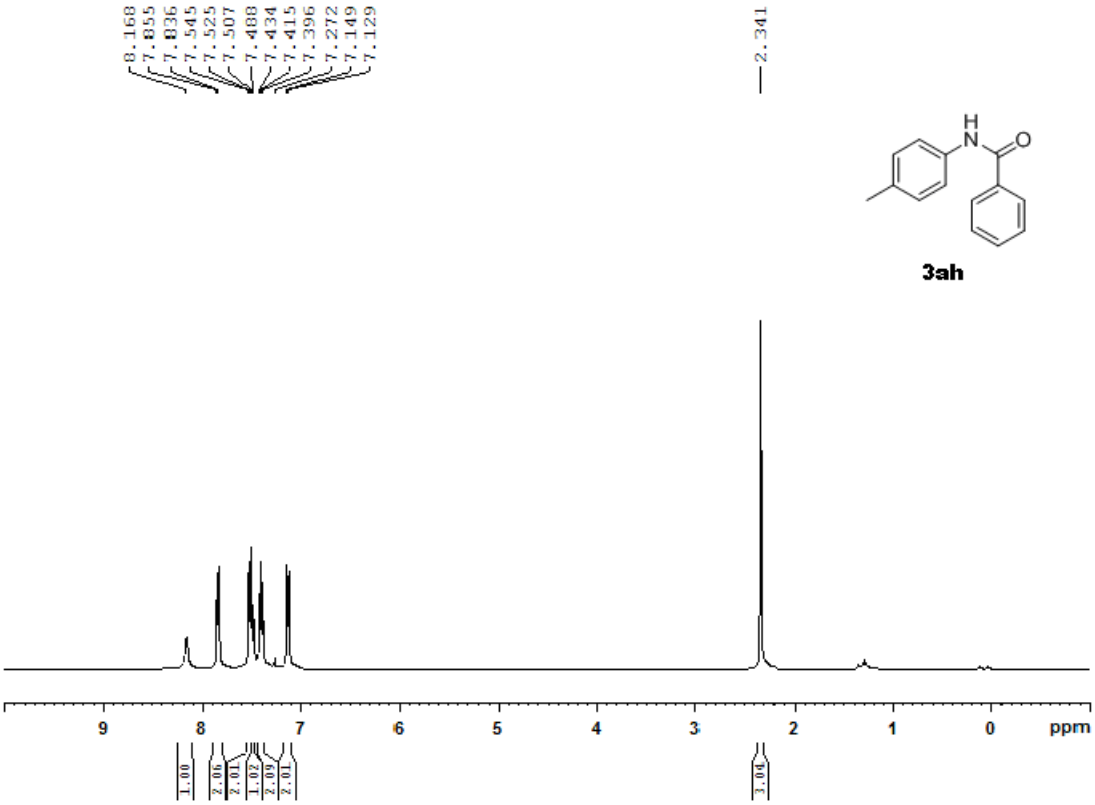
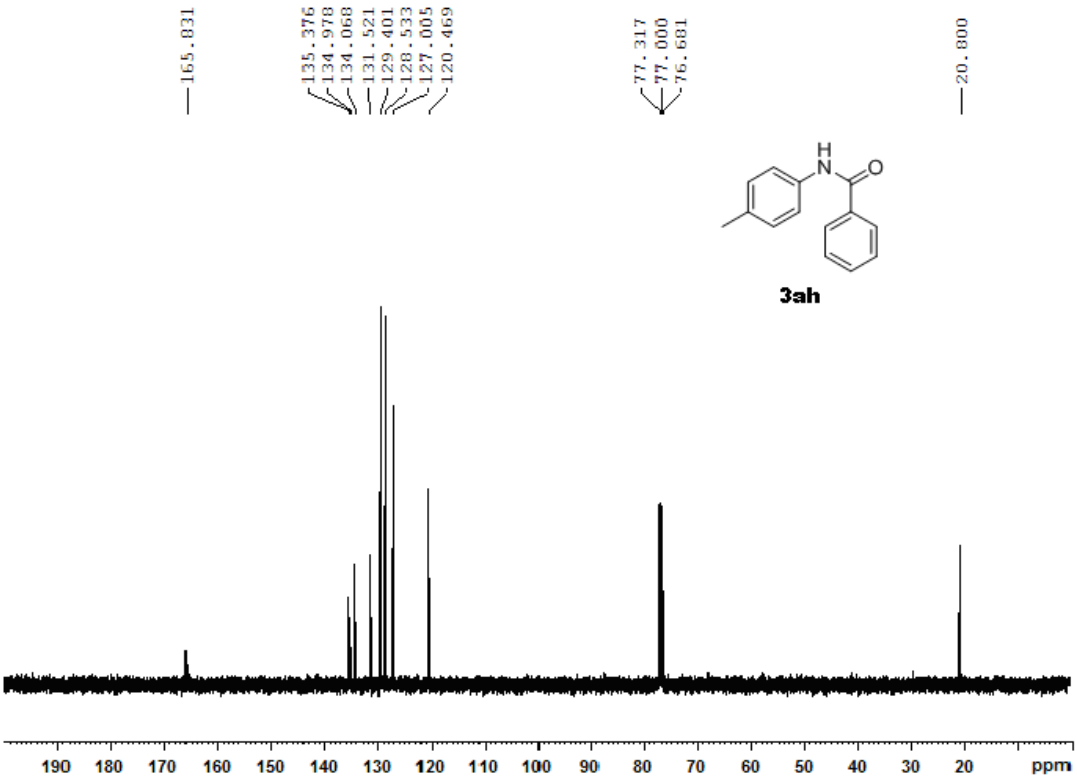
7
6
5
4
3
2
1
0
ppm
2.03
1.00
2.07
2.06
2.02
3.05
3.05

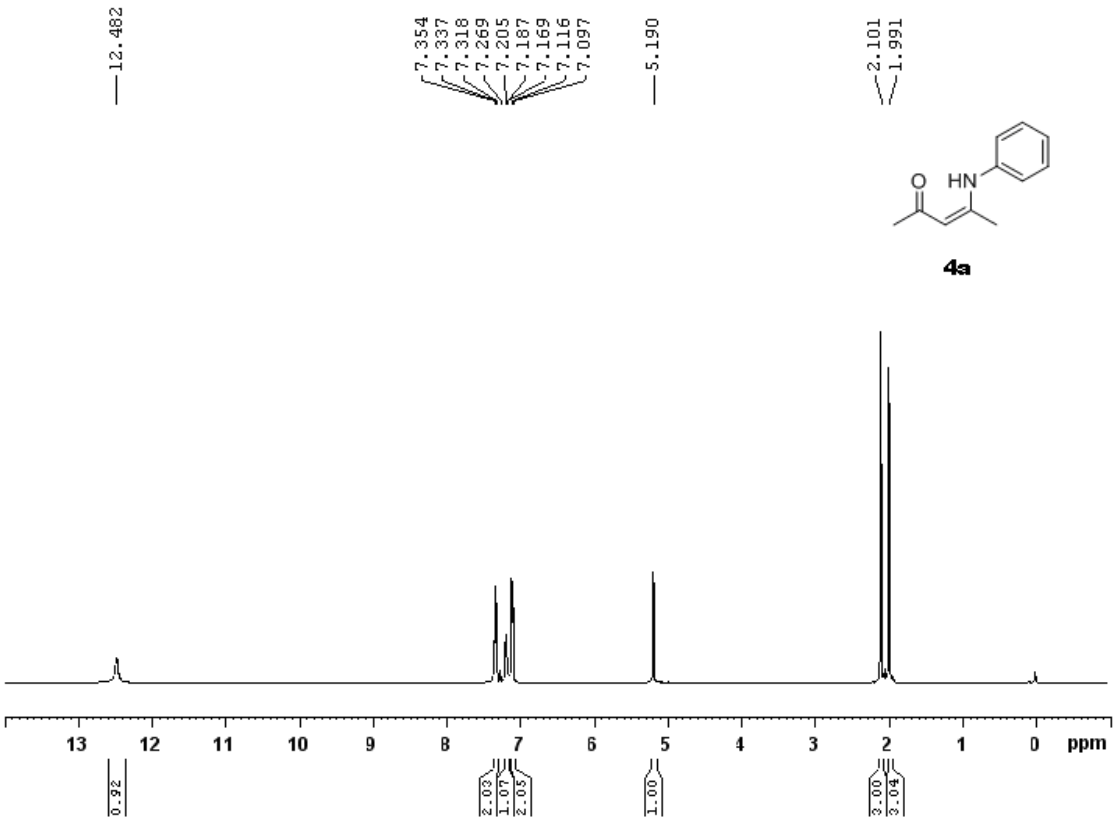

171.828
155.656
130.943
121.679
114.722
77.318
77.000
76.683
63.663
30.529
14.805
9.745
H
N
O
EtO
3ad
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

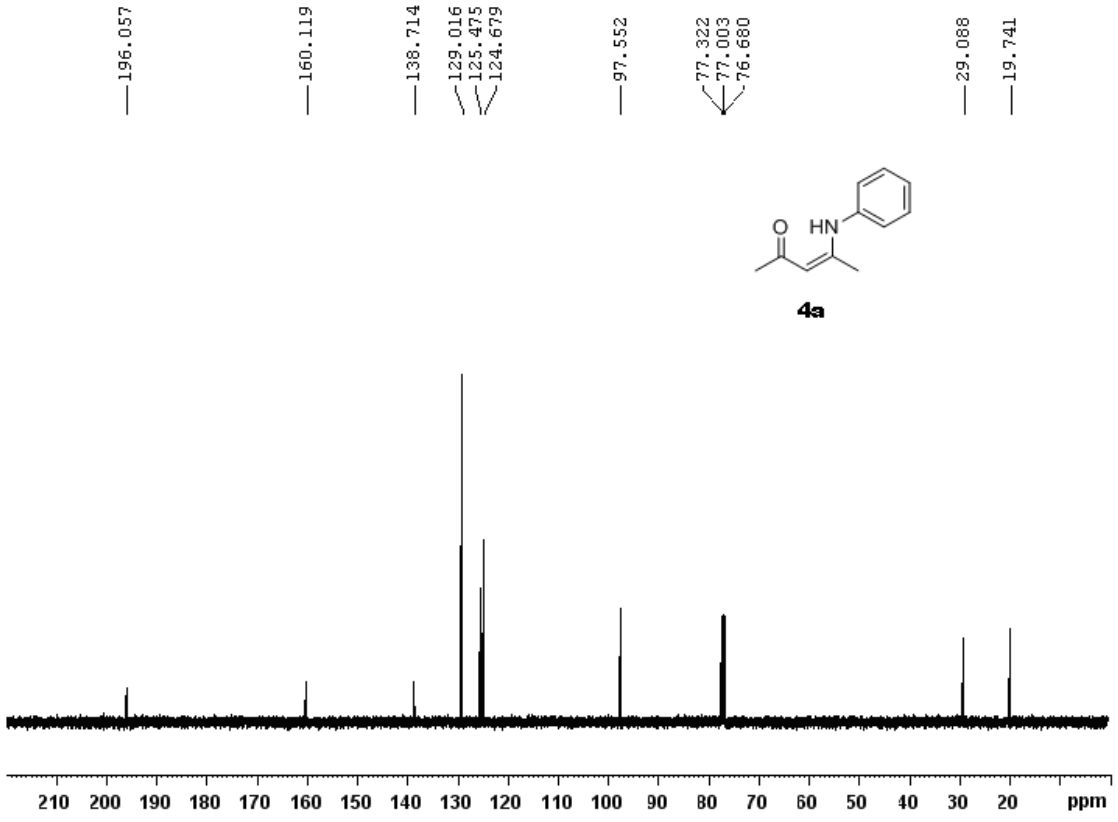

7.483
7.441
7.416
7.391
2.209
2.185
2.168
2.163
1.007
0.993
Br
H
N
O
3ag
9
8
7
6
5
4
3
2
1
0
ppm
0.94
3.93
3.00
5.93

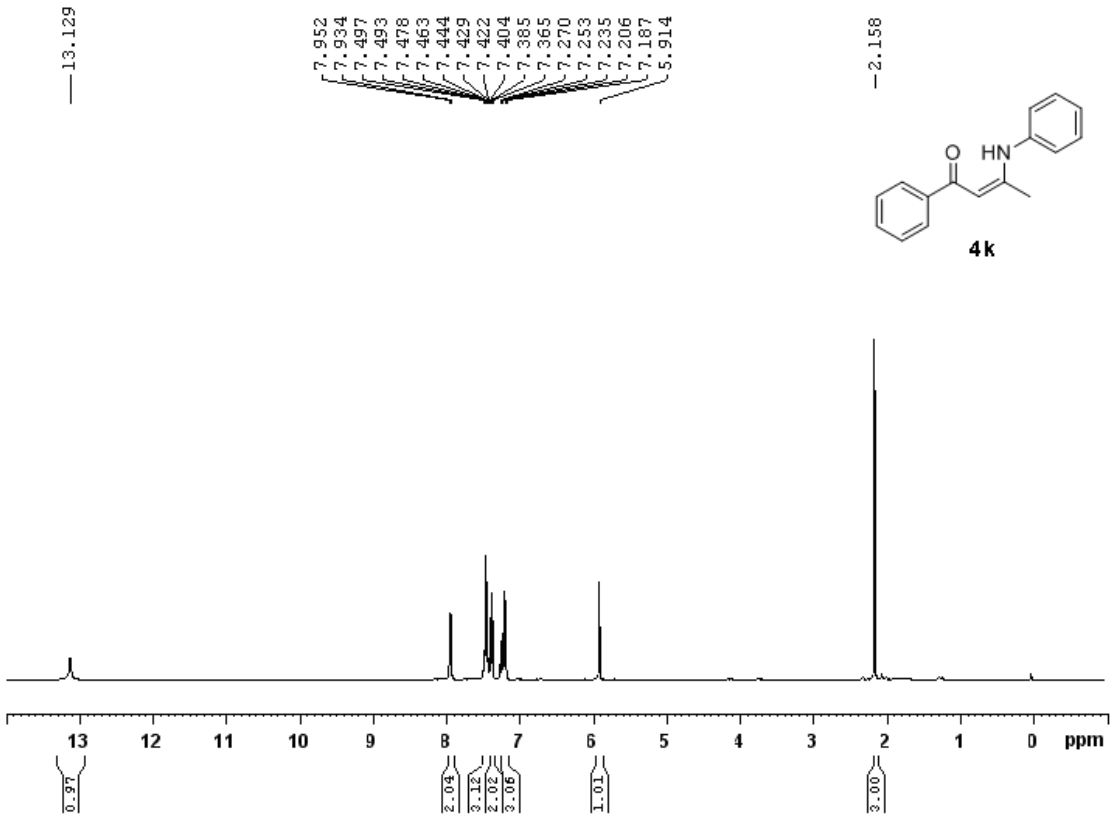

171.013
136.931
131.861
121.454
116.738
77.317
77.000
76.683
46.937
26.195
22.413
Br
H
N
O
3ag
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.168
7.855
7.836
7.545
7.525
7.507
7.488
7.434
7.415
7.396
7.272
7.149
7.129
2.341
3ah
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.06
2.01
1.02
2.09
2.01
3.04


165.831
135.376
134.978
134.068
131.521
129.401
128.533
127.005
120.469
77.317
77.000
76.681
20.800
3ah
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm



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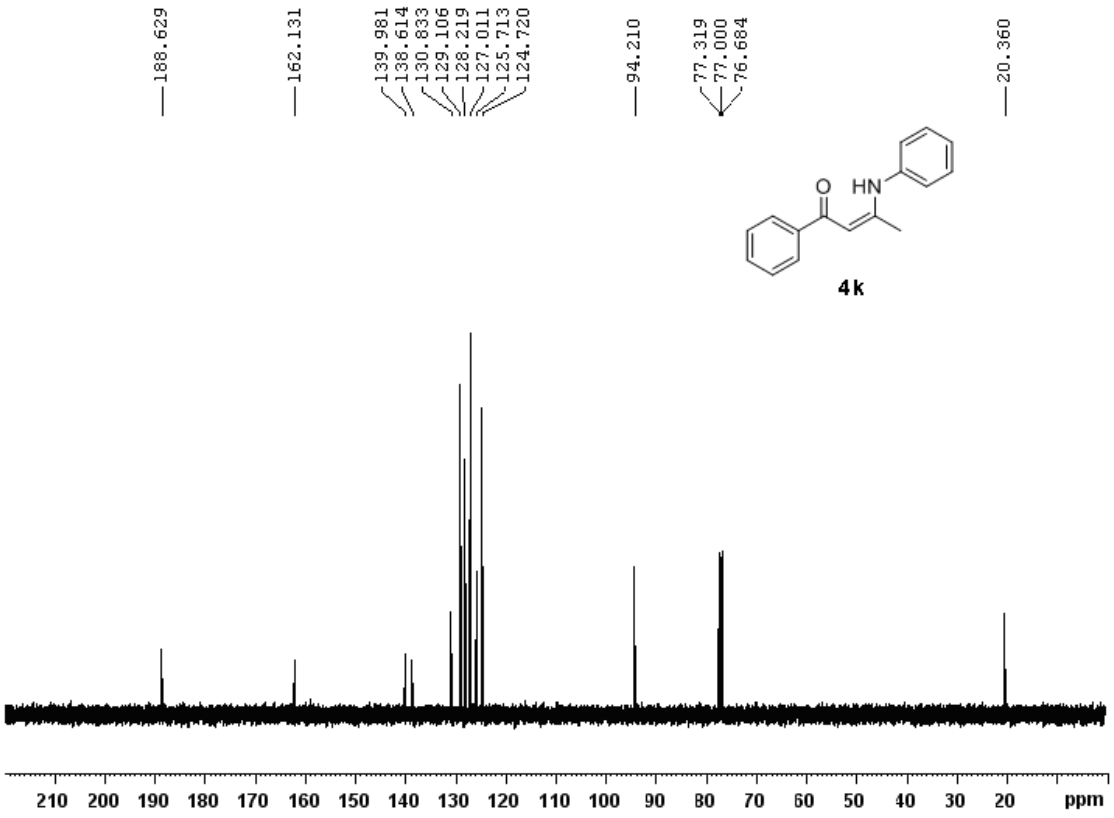
7.952
7.934
7.497
7.493
7.478
7.463
7.444
7.429
7.422
7.404
7.385
7.365
7.270
7.253
7.235
7.206
7.187
5.914
2.158
O
HN
4k
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
2.04
3.12
2.02
3.06
1.01
3.00


188.629
162.131
139.981
138.614
130.833
129.106
128.219
127.011
125.713
124.720
94.210
77.319
77.000
76.684
20.360
O
HN
4k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

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