Supporting information for

Palladium-Catalyzed Paraformaldehyde Insertion: A Three-Component Synthesis of Benzofurans

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General information:

All experiments were carried out under an atmosphere of air. Flash column chromatography was performed over silica gel 48-75 μm. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to $SiMe_4$ or chloroform signals. MS analyses were performed on an Agilent 5975 GC-MS instrument (EI). The new compounds were characterized by ^{1}H NMR, ^{13}C NMR, MS and HRMS. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. The substrates **1c**, **1d**, **1m**, **2j** were synthesized following the literature procedures. All other chemicals and solvents were used as received from commercial sources without further purification.

General Procedure for the preparation of substrates (1c, 1d, 1m, 2j):

Substrate **1c**[1]:

Bromine (11. 6 mL, 0. 23 mol) was added slowly to a cooled 0 ^{o}C of 4-ethylphenol (25 g, 0. 21 mol) dissolved in CH_2Cl_2 (125 mL). After the addition was complete the reaction mixture was stirred for 10 minutes and then quenched with 1 M NaOH. The reaction mixture was diluted with H_2O and the layers separated. The organic layer was concentrated to an orange oil. Purification by flash column chromatography (0 percent to 5% ethyl acetate in petroleum ether) gave the title compound **1c** as a clear oil.

Substrate **1d**[2]:

To a solution of 4-propylphenol (20 mmol) in chloroform (20 mL), $NaHCO_3$ (2 g, 24 mmol) was added. The resulting suspension was cooled to 0 ℃. While a solution of elementary bromine (1.12 mL, 22 mmol) in chloroform (8 mL) was slowly added, the suspension was vigorously stirred. After completion of the reaction, monitored by TLC the suspension was filtered. The filter with the solid residue was rinsed once with 50 mL of chloroform. The combined organic solution was evaporated under reduced pressure. The final work up of **1d** was done either by distillation or by column chromatography (petroleum ether: ethyl acetate = 9:1).

Substrate **1m**[3]:

To a solution of 3,4-dimethylphenol (2.48 g, 20.3 mmol, 1 equiv) in dichloromethane (200 mL) at -78 °C was added dropwise bromine (1.05 mL, 20.3 mmol, 1 equiv). After 1 h, 1 M Na_2SO_3 was added and the cold bath was removed. After warming to ambient temperature, the dichloromethane layer was separated, dried over Mg_2SO_4 and concentrated in vacuo to provide **1m** as a yellow solid.

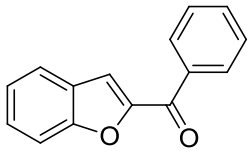
Substrate **2j**[4]:

2-Acetylthiophene (6 g, 47.6 mmol) was dissolved in chloroform (60 mL) and added to a slurry of $CuBr_2$ (13.5 g, 60.4 mmol) in ethyl acetate (120 mL). The mixture was refluxed for 6 h and then filtered while still hot through a celite pad. The filtrate cake was washed with ethyl acetate and the combined filtrate was evaporated to give **2j.**

General procedure for preparation of 3a:

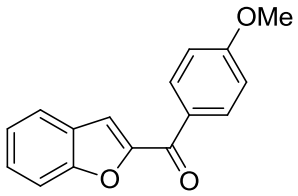
A 10 mL oven-dried reaction vessel was charged with $Pd(COD)Cl_2$ (2.9 mg, 0.01 mmol), diphenyl-2-pyridylphosphine (dpppy, 5.3 mg, 0.02 mmol), K_2CO_3 (83.0 mg, 0.6 mmol), 2-bromophenol (**1a**, 23 uL, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol), 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol) and DMSO (0.8 mL). The resulting solution was sealed under air and stirred at 140 ℃ for 24 h. After cooling to room temperature, the volatiles were removed under vacuum and the residue was purified by column chromatography (neutral aluminum oxide, petroleum ether/ethyl acetate = 40:1) to give **3a** as white solid; yield: 36.0 mg (81%).

Benzofuran-2-yl(phenyl)methanone (3a, CAS: 6272-40-8)[5]



^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.06-8.04 (m, 2H), 7.74 (d, J = 8.0 Hz, 1H), 7.66-7.63 (m, 2H), 7.56-7.49 (m, 4H), 7.34 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.4, 156.0, 152.3, 137.3, 132.9, 129.5, 128.5, 128.4, 127.0, 124.0, 123.3, 116.5, 112.6; MS (EI) m/z (%) 222 (100), 194, 145, 105, 77.

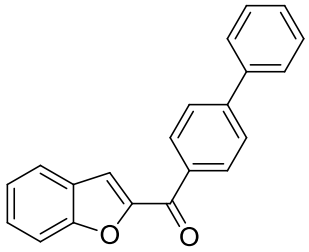
Benzofuran-2-yl(4-methoxyphenyl)methanone (3b, CAS: 63157-19-7)[6]



The reaction was conducted with methyl 2-bromophenol (**1a**, 34.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-(4-methoxyphenyl)ethanone (**2b**, 68.7 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3b** as white solid; yield 64%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.12 (d, J = 8.0 Hz, 2H), 8.28 (s, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.64 (d, J = 8.0 Hz, 1H）, 7.53-7.47 (m, 2H), 7.33 (t, J = 8.0 Hz, 1H), 7.03 (d, J = 8.0 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 182.2, 163.7, 155.9, 153.4, 132.0, 130.1, 127.8, 127.1, 123.9, 123.1, 114.8, 114.0, 112.5, 55.5; MS (EI) m/z (%) 252, 221, 135 (100), 107, 77.

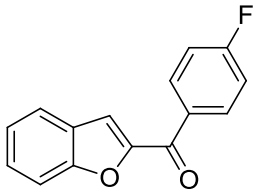
[1,1'-Biphenyl]-4-yl(benzofuran-2-yl)methanone (3c, CAS: 82158-42-7)[7]



The reaction was conducted with methyl 2-bromophenol (**1a**, 34.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 1-([1,1'-biphenyl]-4-yl)-2-bromoethanone (**2c**, 82.5 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3c** as white solid; yield 81%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.16 (d, J = 8.0 Hz, 2H), 7.78-7.74 (m, 3H), 7.68-7.66 (m, 3H), 7.59 (s, 1H), 7.54-7.48 (m, 3H), 7.44-7.41 (m, 1H), 7.35 (t, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 183.8, 156.0, 152.5, 145.7, 139.9, 135.9, 130.1, 129.0, 128.3, 128.3, 127.3 127.2, 127.1, 124.0, 123.3, 116.2, 112.6; MS (EI) m/z (%) 298, 221, 181 (100), 152, 77.

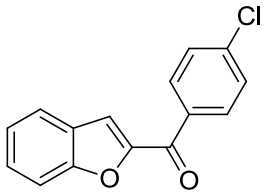
Benzofuran-2-yl(4-fluorophenyl)methanone (3d, CAS: 27044-77-5)[6]



The reaction was conducted with methyl 2-bromophenol (**1a**, 34.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-(4-fluorophenyl)ethanone (**2d**, 65.1 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3d** as white solid; yield 46%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.14 (dd, J_1 = 8.6 Hz, J_2 = 5.5 Hz, 2H), 7.71 (d, J = 8.0 Hz, 1H), 7.66-7.64 (m, 1H), 7.56-7.50 (m, 2H), 7.37-7.34 (m, 1H), 7.25-7.21 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 182.5, 165.5 (d, J = 253.3 Hz), 155.8, 151.9, 133.2 (d, J = 3.0 Hz), 132.0 (d, J = 9.2 Hz), 128.3, 126.7, 123.9, 123.2, 116.2, 115.6 (J = 21.8 Hz), 112.3; MS (EI) m/z (%) 240, 145, 123 (100), 95, 89.

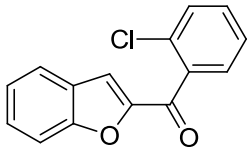
Benzofuran-2-yl(4-chlorophenyl)methanone (3e, CAS: 27052-20-6)[5]



The reaction was conducted with methyl 2-bromophenol (**1a**, 34.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-(4-chlorophenyl)ethanone (**2e**, 70.1 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3e** as white solid; yield 40%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.04 (d, J = 8.0 Hz, 2H), 7.75-7.74 (m, 1H), 7.66-7.64 (m, 1H), 7.56-7.52 (m, 4H), 7.37-7.35 (t, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 182.9, 156.0, 152.0, 139.4, 135.4, 130.9, 128.9, 128.5, 126.9, 124.1, 123.3, 116.5, 112.5; MS (EI) m/z (%) 256, 221, 139 (100), 89, 75.

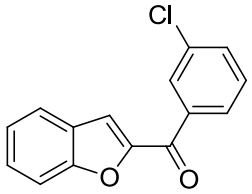
Benzofuran-2-yl(2-chlorophenyl)methanone (3f)[5]



The reaction was conducted with methyl 2-bromophenol (**1a**, 34.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-(2-chlorophenyl)ethanone (**2f**, 70.1 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3f** as yellow liquid; yield 40%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.79 (d, J = 8.0 Hz, 1H), 7.64-7.62 (m, 1H), 7.55-7.47 (m, 4H), 7.42-7.39 (m, 1H), 7.34-7.31 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 183.8, 156.4, 151.9, 137.4, 131.8, 131.7, 130.3, 129.3, 128.9, 127.0, 126.6, 124.1, 123.5, 117.7, 112.7; MS (EI) m/z (%) 256, 221, 145 (100), 111, 75.

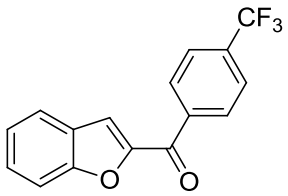
Benzofuran-2-yl(3-chlorophenyl)methanone (3g)



The reaction was conducted with methyl 2-bromophenol (**1a**, 34.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-(3-chlorophenyl)ethanone (**2g**, 70.1 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3g** as white solid; yield 41%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.04 (s, 1H), 7.95 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.67-7.61 (m, 2H), 7.57-7.47 (m, 3H), 7.36 (t, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 182.8, 156.1, 151.9, 138.7, 134.8, 132.8, 129.9, 129.4, 128.7, 127.6, 126.8, 124.1, 123.4, 116.8, 112.6; MS (EI) m/z (%) 256, 221, 145 (100), 89, 75; HRMS calcd. for: $C_{15}H_{10}ClO_2$ $[M+H]^+$ = 257.0369, found = 257.0365.

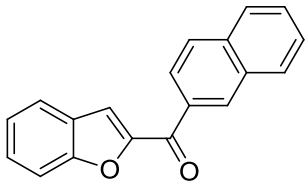
Benzofuran-2-yl(4-(trifluoromethyl)phenyl)methanone (3h, CAS: 512171-87-8)[8]



The reaction was conducted with methyl 2-bromophenol (**1a**, 34.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-(4-(trifluoromethyl)phenyl)ethanone (**2h**, 80.1 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3h** as white solid; yield 60%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.16 (d, J = 8.0 Hz, 2H), 7.82 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 1H), 7.66-7.64 (m, 1H), 7.58-7.52 (m, 2H), 7.36 (t, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 183.1, 156.2, 151.9, 140.1, 134.2 (q, J = 32.6), 129.8, 128.9, 126.9, 125.6 (q, J = 3.6), 125.0, 124.2, 123.4, 117.0, 112.6; MS (EI) m/z (%) 290, 221, 145 (100), 105, 89.

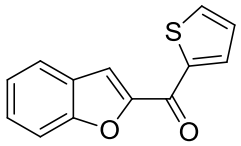
Benzofuran-2-yl(naphthalen-2-yl)methanone (3i)



The reaction was conducted with methyl 2-bromophenol (**1a**, 34.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-(naphthalen-2-yl)ethanone (**2i**, 74.7 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3i** as white solid; yield 45%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.62 (s, 1H), 8.10-8.08 (m, 1H), 8.02-7.92 (m, 3H), 7.77-7.75 (m, 1H), 7.70-7.60 (m, 4H), 7.52 (t, J = 8.0 Hz, 1H), 7.37-7.34 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.2, 156.0, 152.5, 135.5, 134.5, 132.4, 131.1, 129.5, 128.5, 128.5, 128.3, 127.8, 127.0, 126.9, 125.2, 124.0, 123.3, 116.4, 112.6; MS (EI) m/z (%) 272 (100), 244, 155, 127, 77; HRMS calcd. for: $C_{19}H_{12}O_2$ $[M+H]^+$ = 273.0916, found = 273.0912.

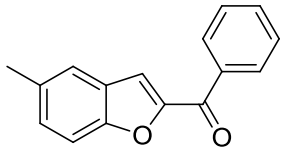
Benzofuran-2-yl(thiophen-2-yl)methanone (3j)[9]



The reaction was conducted with methyl 2-bromophenol (**1a**, 34.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-(thiophen-2-yl)ethanone (**2j**, 61.5 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3j** as brown solid; yield 52%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.34-8.33 (m, 1H), 7.78-7.73 (m, 3H), 7.66-7.64 (m, 1H), 7.51 (q, J = 8.0 Hz, 1H), 7.37-7.33 (m, 1H), 7.27-7.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 175.0, 155.8, 152.6, 142,3, 134.6, 134.5, 128.4, 128.2, 127.0, 124.0, 123.3, 114.6, 112.4; MS (EI) m/z (%) 228, 200, 145, 111 (100), 89.

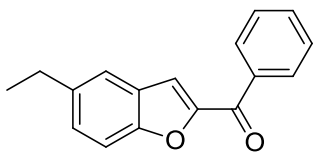
(5-Methylbenzofuran-2-yl)(phenyl)methanone (3k, CAS: 101277-97-8)[10]



The reaction was conducted with 2-bromo-4-methylphenol (**1b**, 37.4 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3k** as white solid; yield 51%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05-8.03 (m, 2H), 7.63-7.62 (m, 1H), 7.55-7.50 (m, 4H), 7.46 (s, 1H), 7.32-7.30 (m, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.4, 154.6, 152.4, 137.3, 133.6, 132.8, 120.0, 129.4, 128.5, 127.1, 122.7, 116.3, 112.1, 21.3; MS (EI) m/z (%) 236, 207 (100), 159, 105, 77.

(5-Ethylbenzofuran-2-yl)(phenyl)methanone (3l)

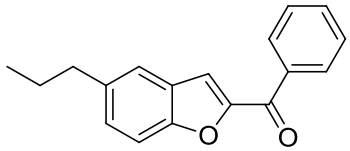


The reaction was conducted with 2-bromo-4-ethylphenol (**1c**, 40.2 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol).

The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3l** as yellow liquid; yield 62%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.04 (d, J = 8.0 Hz, 2H), 7.64-7.62 (m, 1H), 7.56-7.52 (m, 4H), 7.48 (s, 1H), 7.36-7.34 (m, 1H), 2.77 (d, J = 8.0 Hz, 2H), 1.31-1.28 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.4, 154.7, 152.4, 140.2, 137.3, 132.8, 129.4, 129.0, 128.5, 127.1, 121.5, 116.5, 112.2, 28.7, 16.3; MS (EI) m/z (%) 250, 235 (100), 207, 105, 77; HRMS calcd. for: $C_{17}H_{15}O_2$ $[M+H]^+$ = 251.1072, found = 251.1069.

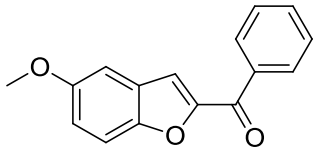
Phenyl(5-propylbenzofuran-2-yl)methanone (3m)



The reaction was conducted with 2-bromo-4-propylphenol (**1d**, 43.2 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3m** as yellow liquid; yield 77%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.04 (d, J = 8.0 Hz, 2H), 7.65-7.61 (m, 1H), 7.55-7.47 (m, 5H), 7.33-7.31 (m, 1H), 2.70 (t, J = 8.0 Hz, 2H), 1.73-1.64 (m, 2H), 0.96 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.4, 154.7, 152.4, 142.5, 137.3, 132.8, 129.5, 129.4, 128.5, 127.0, 122.2, 116.4, 112.1, 37.8, 24.9, 13.7; MS (EI) m/z (%) 264, 235 (100), 207, 105, 77; HRMS calcd. for: $C_{18}H_{17}O_2$ $[M+H]^+$ = 265.1229, found = 265.1218.

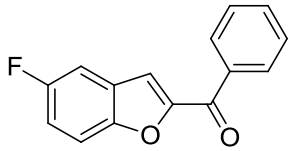
(5-Methoxybenzofuran-2-yl)(phenyl)methanone (3n, 383159-30-6)[11]



The reaction was conducted with 2-bromo-4-methoxyphenol (**1e**, 40.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3n** as white solid; yield 60%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05 (d, J = 8.0 Hz, 2H), 7.64 (t, J = 8.0 Hz, 1H), 7.56-7.52 (m, 3H), 7.48 (s, 1H), 7.13-7.11 (m, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.2, 156.7, 153.0, 151.2, 137.3, 132.8, 129.5, 128.5, 127.5, 118.5, 116.4, 113.2, 104.0, 55.9; MS (EI) m/z (%) 252 (100), 207, 175, 105, 77.

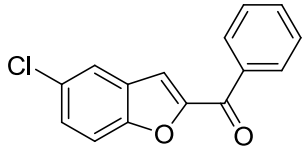
(5-Fluorobenzofuran-2-yl)(phenyl)methanone (3o)



The reaction was conducted with 2-bromo-4-fluorophenol (**1f**, 38.2 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3o** as white solid; yield 78%.

^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.05 (d, J = 8.0 Hz, 2H), 7.67-7.63 (m, 1H), 7.61-7.50 (m, 4H), 7.39-7.36 (m, 1H), 7.24-7.21 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 184.1, 159.6 (d, J = 239.6 Hz), 153.8, 152.3, 137.0, 133.1, 129.5, 128.6, 116.7 (d, J = 26.7 Hz), 116.1, 116.0, 113.6 (d, J = 9.5 Hz), 108.2 (d, J = 24.8 Hz); MS (EI) m/z (%) 240, 223, 163, 105 (100), 77; HRMS calcd. for: $C_{15}H_{10}FO_2$ $[M+H]^+$ = 241.0665, found = 241.0659.

(5-Chlorobenzofuran-2-yl)(phenyl)methanone (3p, CAS: 100914-68-9)[5]

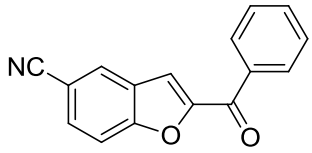


The reaction was conducted with 2-bromo-4-chlorophenol (**1g**, 41.4 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3p** as white solid; yield 68%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05-8.04 (m, 2H), 7.71-7.71 (m, 1H), 7.67-7.64 (m, 1H), 7.59-7.53 (m, 3H), 7.47-7.44 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.1, 154.2, 153.3,

136.8, 133.1, 129.6, 129.4, 128.6, 128.6, 128.2, 122.6, 115.4, 113.6; MS (EI) m/z (%) 256, 221, 179, 105 (100), 77.

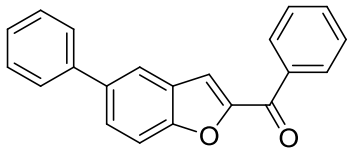
2-Benzoylbenzofuran-5-carbonitrile (3q)



The reaction was conducted with 3-bromo-4-hydroxybenzonitrile (**1h**, 39.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **3q** as white solid; yield 42%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.11 (s, 1H), 8.05 (d, J = 8.0 Hz, 2H), 7.76 (s, 2H), 7.70-7.67 (m, 1H), 7.59-7.55 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 183.7, 157.1, 154.0, 136.5, 133.5, 131.1, 129.5, 128.7, 128.5, 127.6, 118.6, 115.0, 113.9, 108.3; MS (EI) m/z (%) 247, 230, 190, 105 (100), 77; HRMS calcd. for: $C_{16}H_{10}NO_2$ $[M+H]^+$ = 248.0712, found = 248.0710.

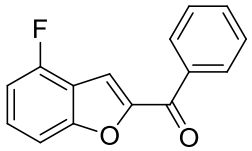
Phenyl(5-phenylbenzofuran-2-yl)methanone (3r, CAS: 102183-99-3)



The reaction was conducted with 3-bromo-(1,1'-biphenyl)-4-ol (**1i**, 49.8 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3r** as white solid; yield 70%.

^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.07 (d, J = 8.0 Hz, 2H), 7.90 (s, 1H), 7.75-7.71 (m, 2H), 7.69-7.61 (m, 3H), 7.58-7.54 (m, 3H), 7.47 (t, J = 8.0 Hz, 2H), 7.40-7.36 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.3, 155.5, 152.8, 140.8, 137.7, 137.1, 132.9, 129.4, 128.8, 128.5, 128.2, 127.5, 127.4, 127.3, 121.4, 116.6, 112.7; MS (EI) m/z (%) 298 (100), 221, 165, 105, 77.

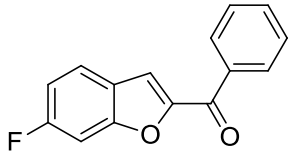
(4-Fluorobenzofuran-2-yl)(phenyl)methanone (3s)



The reaction was conducted with 2-bromo-3-fluorophenol (**1j**, 38.2 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3s** as white solid; yield 58%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05 (d, J = 8.0 Hz, 2H), 7.68-7.64 (m, 1H), 7.59-7.54 (m, 3H), 7.49-7.43 (m, 2H), 7.04-7.00 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 183.9, 157.0 (d, J = 252.6 Hz), 152.0, 136.8, 133.1, 129.4, 129.0 (d, J= 7.7 Hz), 128.6, 116.8, (d, J = 21.9 Hz), 112.3, 109.1 (d, J = 18.4 Hz), 108.7, 108.6; MS (EI) m/z (%) 240, 223, 163, 105 (100), 77; $C_{15}H_{10}FO_2$ $[M+H]^+$ = 241.0665, found = 241.0659.

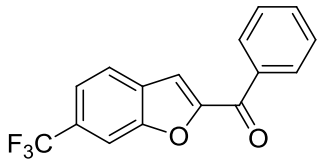
(6-Fluorobenzofuran-2-yl)(phenyl)methanone (3t)



The reaction was conducted with 2-bromo-5-fluorophenol (**1k**, 38.2 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3t** as white solid; yield 66%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05-8.03 (m, 2H), 7.71-7.64 (m, 2H), 7.57-7.51 (m, 3H), 7.37-7.35 (s, 1H), 7.15-7.11 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 183.9, 163.2 (d, J = 246.7 Hz), 137.1, 133.0, 129.4, 128.6, 128.6, 124.1 (d, J = 10.3 Hz), 123.4, 116.3, 116.2, 113.2 (d, J = 24.6 Hz), 100.0 (d, J = 26.5 Hz); MS (EI) m/z (%) 240, 223, 163, 105 (100), 77; HRMS calcd. for: $C_{15}H_{10}FO_2$ $[M+H]^+$ = 241.0665, found = 241.0660.

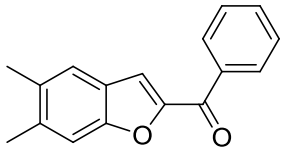
Phenyl(6-(trifluoromethyl)benzofuran-2-yl)methanone (3u)



The reaction was conducted with 2-bromo-5-(trifluoromethyl)phenol (**1l**, 48.2 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3u** as white solid; yield 50%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.08 (d, J = 8.0 Hz, 2H), 7.93 (s, 1H), 7.87-7.85 (m, 1H), 7.69-7.65 (s, 1H), 7.61-7.54 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 183.9, 154.8, 154.5, 136.7, 135.1, 134.5, 133.4, 129.6, 128.7, 123.9, 122.6, 120.8 (q, J = 3.6 Hz), 115.1, 110.3 (q, J =4.1 Hz); MS (EI) m/z (%) 290, 262, 213, 105 (100), 77.

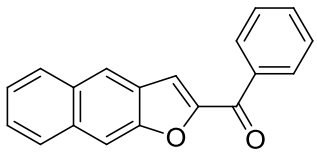
(5,6-Dimethylbenzofuran-2-yl)(phenyl)methanone (3v)



The reaction was conducted with 2-bromo-4,5-dimethylphenol (**1m**, 40.2 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3v** as white solid; yield 68%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.02 (d, J = 8.0 Hz, 2H), 7.64-7.61 (m, 1H), 7.55-7.51 (m, 2H), 7.45-7.42 (m, 3H), 2.41 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.3, 155.4, 151.9, 138.6, 137.5, 133.0, 132.6, 129.4, 128.4, 125.0, 122.9, 116.6, 112.7, 20.9, 20.0; MS (EI) m/z (%) 250 (100), 235, 173, 105, 77; HRMS calcd. for: $C_{17}H_{15}O_2$ $[M+H]^+$ = 251.1072, found = 251.1068.

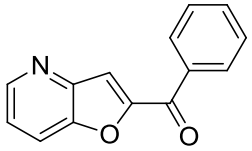
Naphtho[2,3-b]furan-2-yl(phenyl)methanone (3w, CAS: 82158-50-7)



The reaction was conducted with 3-bromonaphthalen-2-ol (**1n**, 44.6 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **3w** as yellow liquid; yield 52%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.18 (d, J = 8.0 Hz, 1H), 8.10 (d, J = 8.0 Hz, 2H), 8.02 (s, 2H), 7.98 (d, J = 8.0 Hz, 1H), 7.93-7.91 (m, 1H), 7.76-7.74 (m, 1H), 7.67-7.63 (m, 2H), 7.59-7.54(m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 183.8, 154.5, 151.9, 137.4, 132.7, 130.5, 130.1, 129.4, 129.1, 128.5, 128.2, 127,4, 125.5, 123.3, 122.9, 115.5, 112.8; MS (EI) m/z (%) 272 (100), 195, 139, 105, 77; HRMS calcd. for: $C_{19}H_{13}O_2$ $[M+H]^+$ = 273.0916, found = 273.0910.

Furo[3,2-b]pyridin-2-yl(phenyl)methanone (3x)[12]



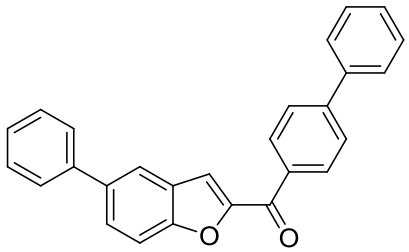
The reaction was conducted with 2-chloropyridin-3-ol (**1o**, 25.9 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 2-bromo-1-phenylethanone (**2a**, 60 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **3x** as white solid; yield 32%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.72-8.71 (m, 1H), 8.06 (d, J = 8.0 Hz, 2H), 7.95 (d, J = 8.0 Hz, 1H), 7.70-7.66 (m, 2H), 7.59-7.55 (m, 2H), 7.45-7.42 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 184.1, 154.4, 149.4, 147.9, 146.2, 136.6, 133.4, 129.5, 128.7, 122.3, 119.8, 116.5; MS (EI) m/z (%) 223, 207, 146, 105 (100), 77.

When 2-bromopyridin-3-ol (**1p**, 34.8 mg, 0.2 mmol) was used, the reaction yield for **3x** is 70%.

When 2-iodopyridin-3-ol (**1q**, 44.2 mg, 0.2 mmol) was used, the reaction yield for **3x** is 72%.

[1,1'-Biphenyl]-4-yl(5-phenylbenzofuran-2-yl)methanone (3y, 1370015-91-0)[13]



The reaction was conducted with 3-bromo-[1,1'-biphenyl]-4-ol (**1i**, 49.8 mg, 0.2 mmol), paraformaldehyde (15.0 mg, 0.5 mmol) and 1-([1,1'-biphenyl]-4-yl)-2-bromoethanone (**2c**, 82.5 mg, 0.3 mmol). The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 40:1) to give **3y** as white solid; yield 65%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.18 (d, J = 8.0 Hz, 2H), 7.92 (s, 1H), 7.79-7.77 (m, 2H), 7.74-7.73 (m, 1H),7.69-7.67 (m, 2H), 7.64-7.62 (m, 3H), 7.52-7.36 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 183.7, 155.5, 153.0, 145.8, 140.8, 139.8, 137.8, 135.8, 130.1, 129.0, 128.9, 128.3, 128.2, 127.6, 127.4, 127.3, 127.3 127.2, 121.5, 116.4, 112.7; HRMS calcd. for: $C_{27}H_{19}O_2$ $[M+H]^+$ = 375.1385, found = 375.1378.

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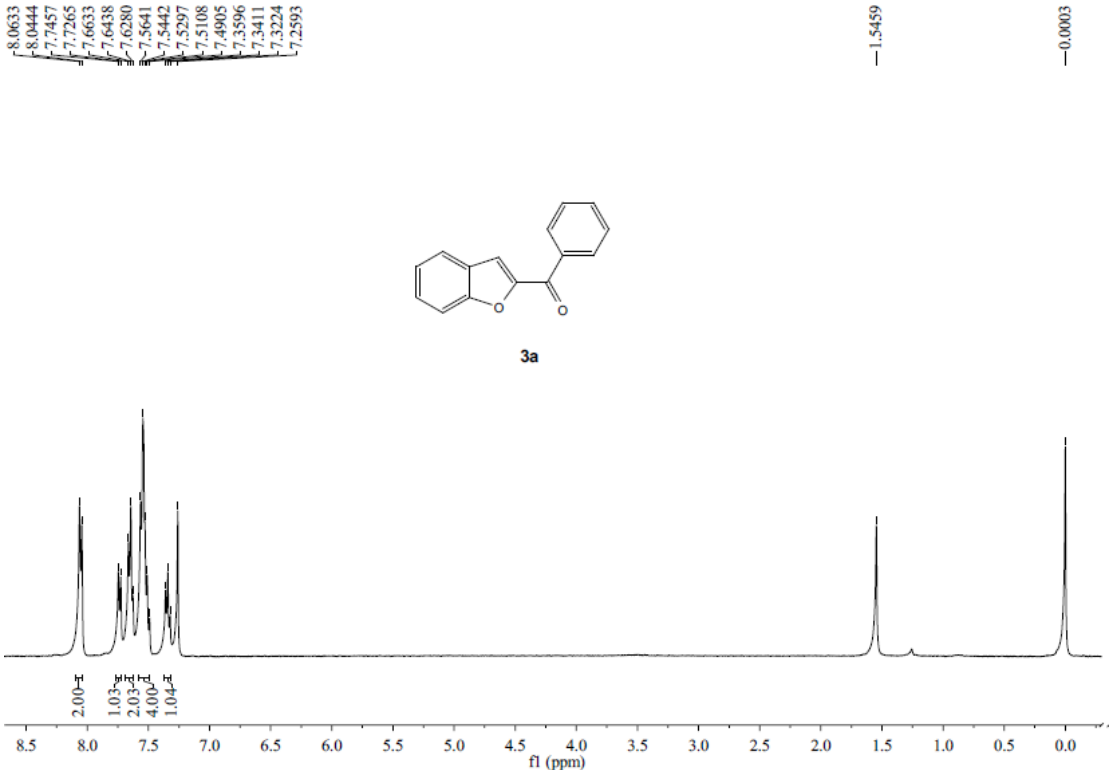
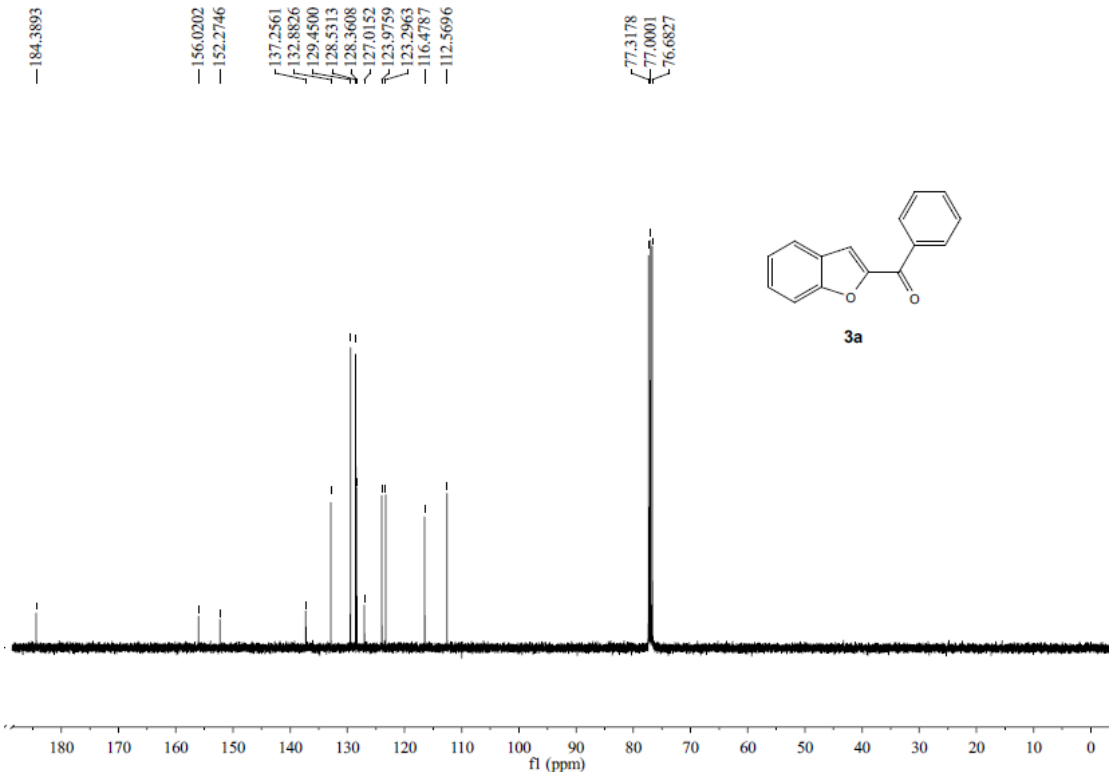
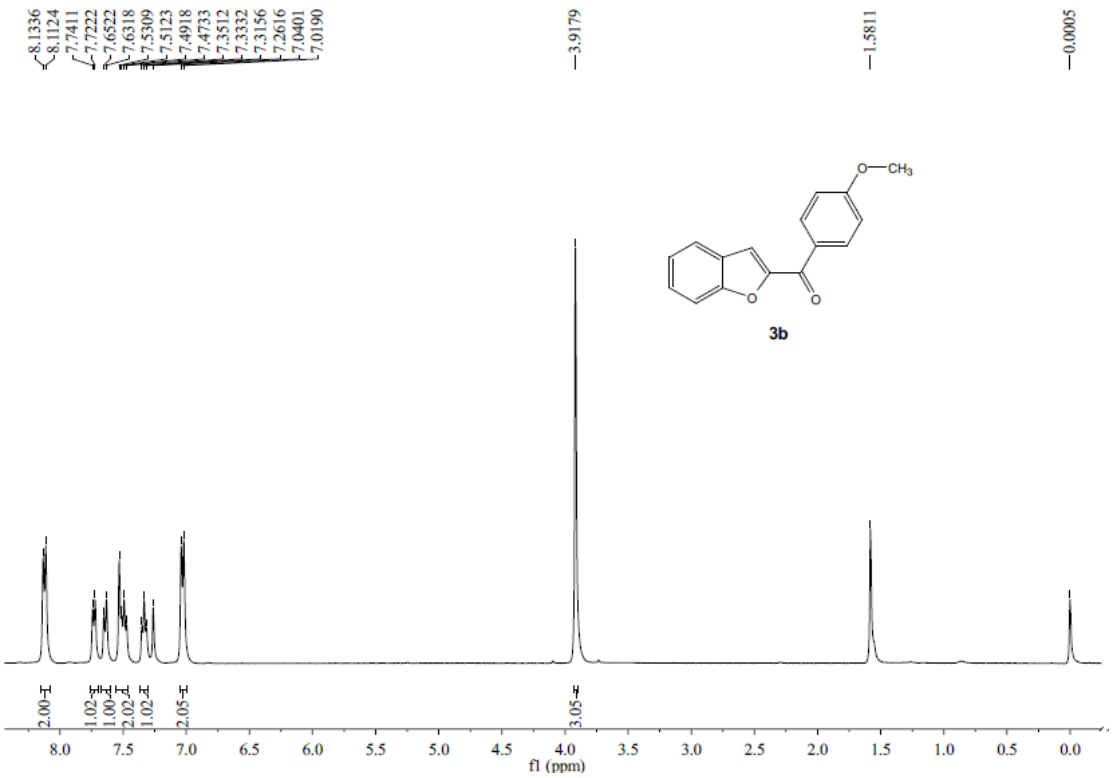
^{1}H NMR and ^{13}C NMR spectra for all products



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7.7411
7.7222
7.6522
7.6318
7.5309
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7.4918
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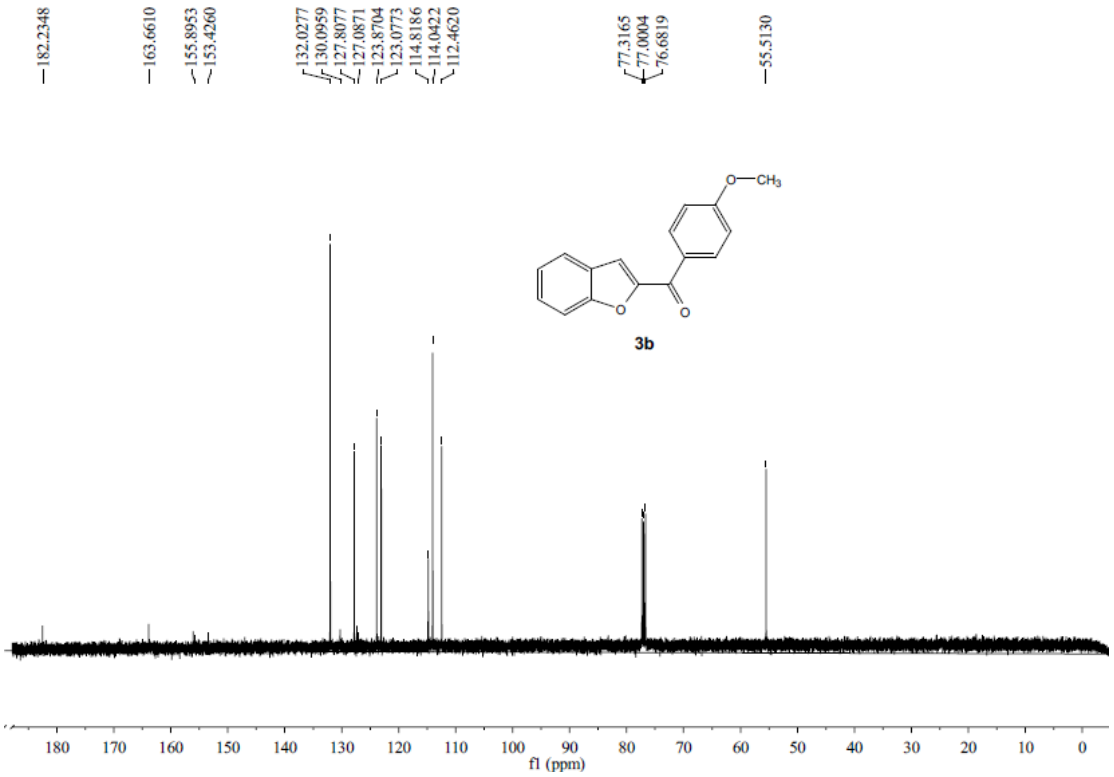
7.3512
7.3332
7.3156
7.2616
7.0401
7.0190
3.9179
1.5811
0.0005
O—CH3
O
O
3b
2.00
1.02
1.00
2.02
1.02
2.05
3.05
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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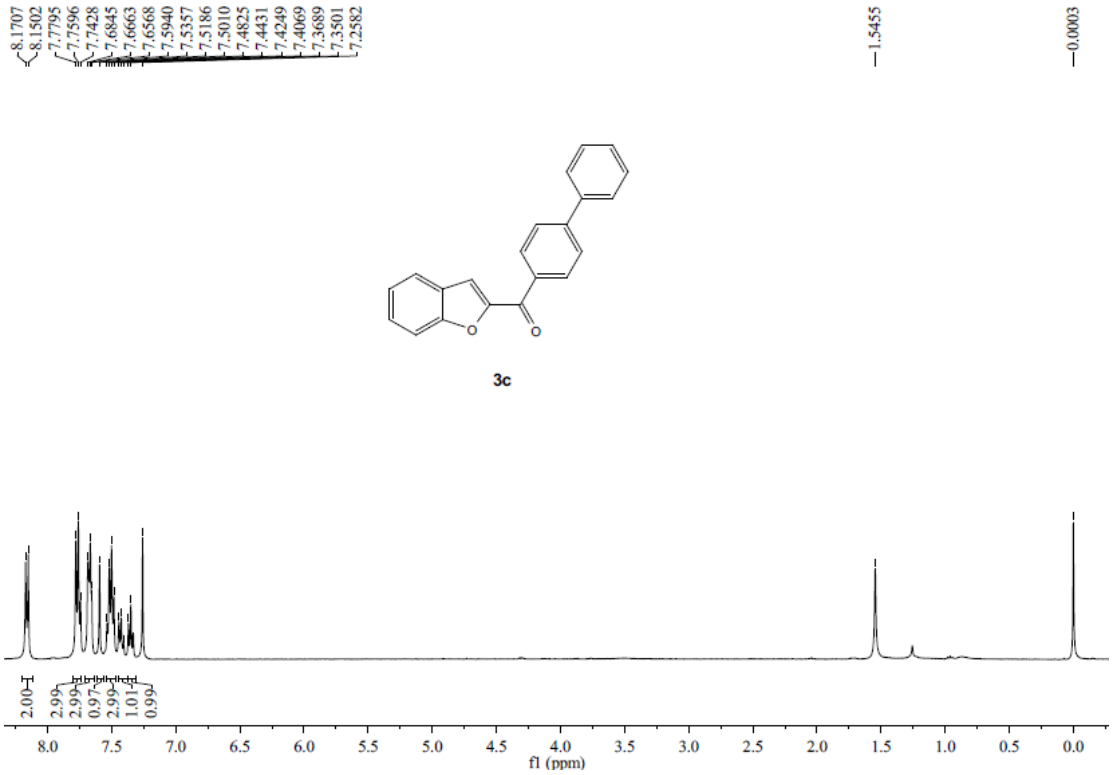
155.8953
153.4260
132.0277
130.0959
127.8077
127.0871
123.8704
123.0773
114.8186
114.0422
112.4620
77.3165
77.0004
76.6819
55.5130
O—CH3
O
O
3b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.5010
7.4825
7.4431
7.4249
7.4069
7.3689
7.3501
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3c
2.00
2.99
2.94
0.97
2.99
1.01
0.99
8.0
7.5
7.0
6.5
6.0
5.5
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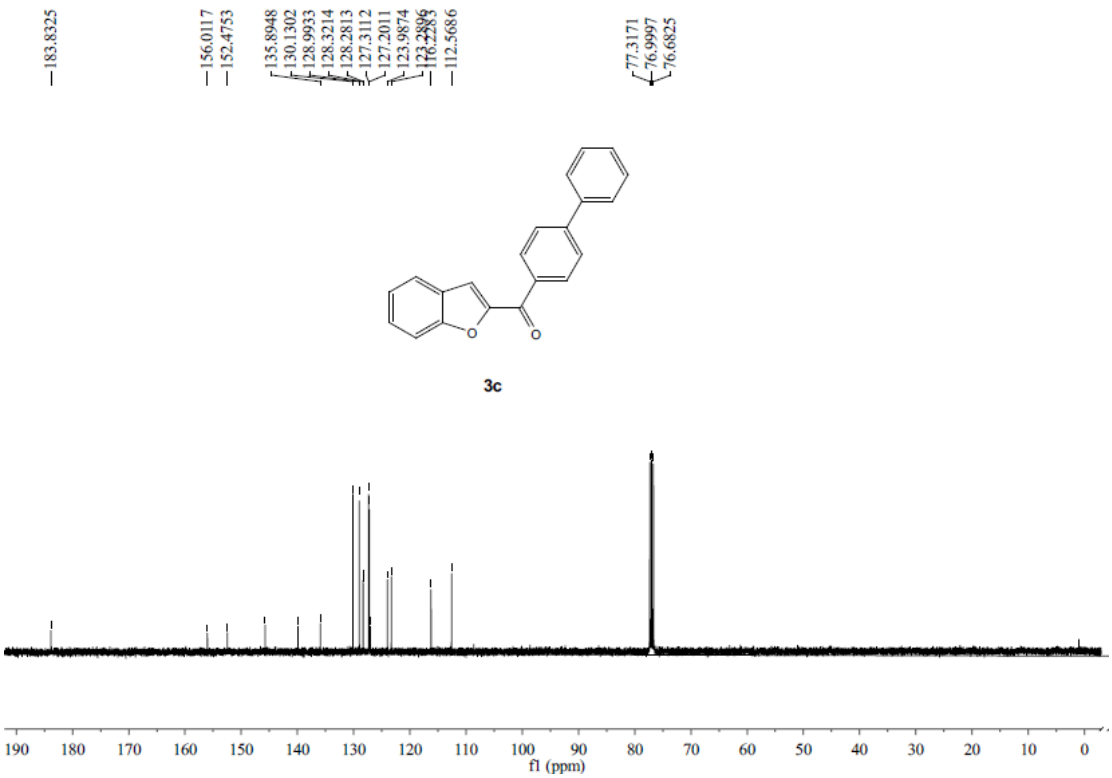
f1 (ppm)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152.4753
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130.1302
128.9933
128.3214
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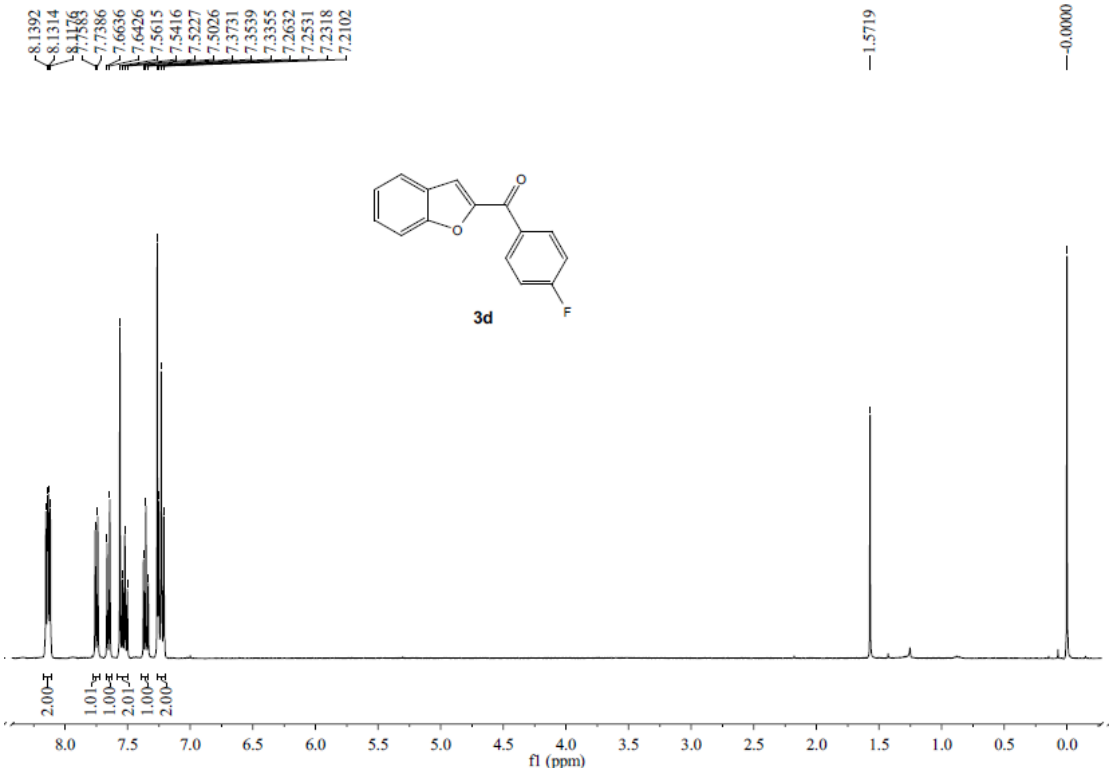
127.2011
123.9874
112.5686
77.3171
76.9997
76.6825
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.3355
7.2632
7.2531
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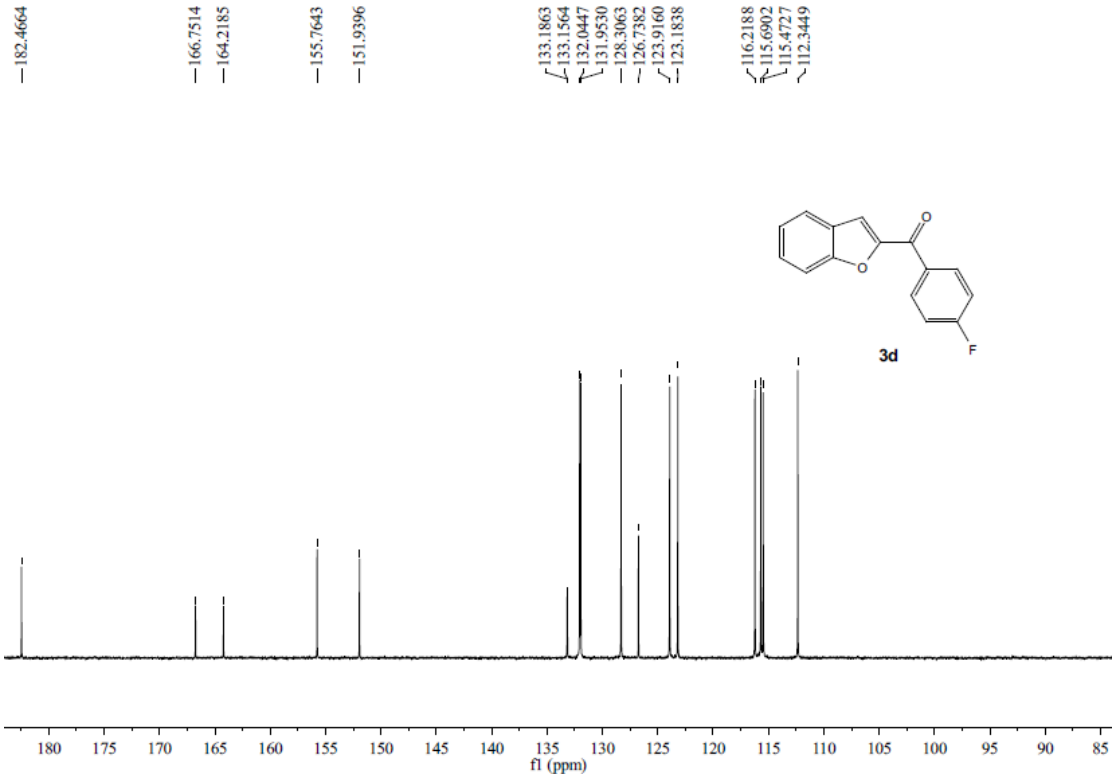
3d
2.00
1.01
1.00
2.01
1.00
2.00
f1 (ppm)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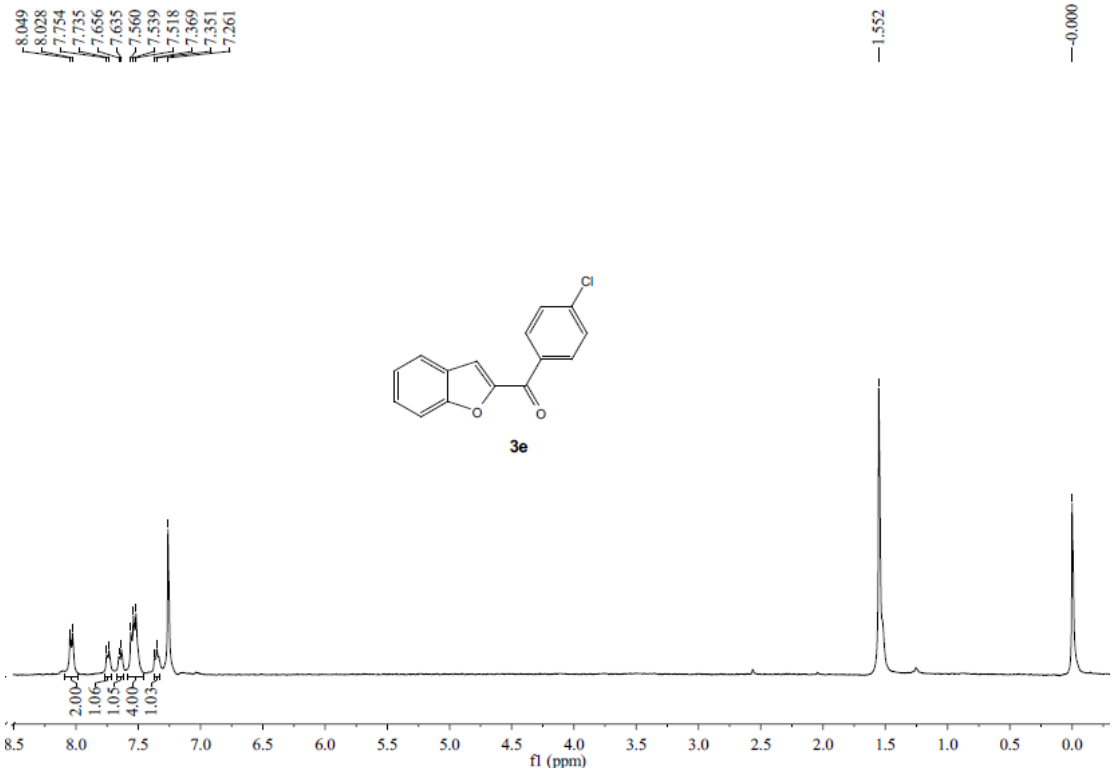
133.1863
133.1564
132.0447
131.9530
128.3063
126.7382
123.9160
123.1838
116.2188
115.6902
115.4727
112.3449
3d
f1 (ppm)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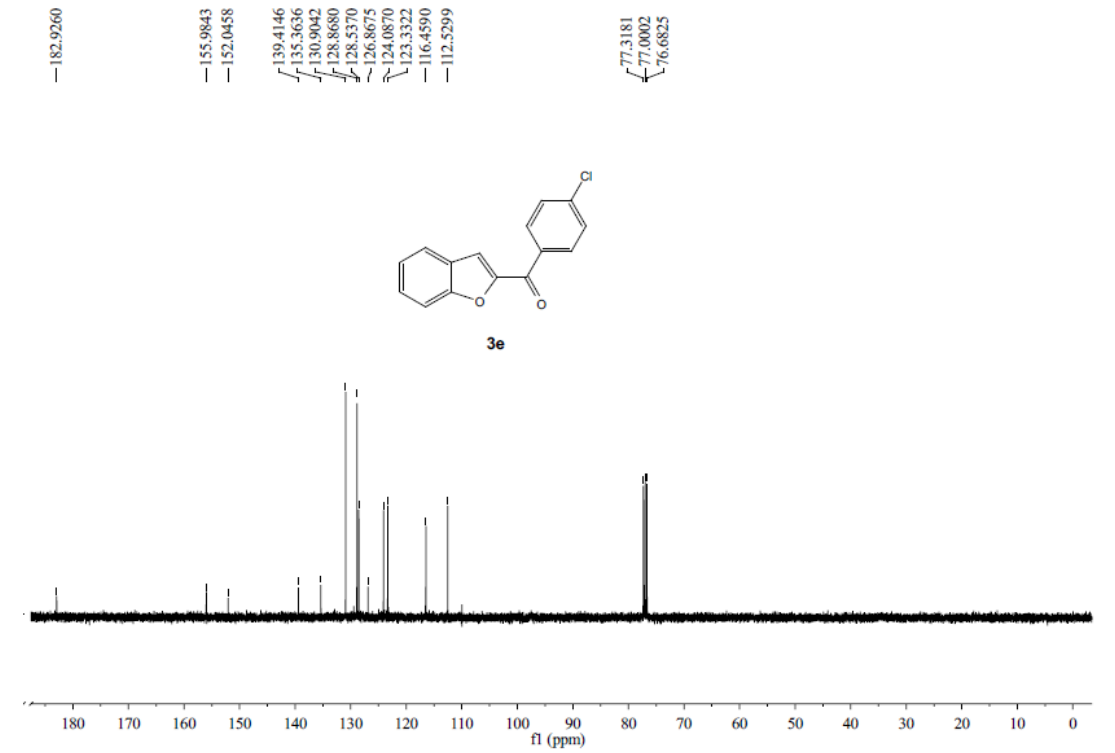
8.028
7.754
7.735
7.656
7.635
7.560
7.539
7.518
7.369
7.351
7.261
1.552
0.000
Cl
O
O
3e
2.00
1.06
1.05
4.00
1.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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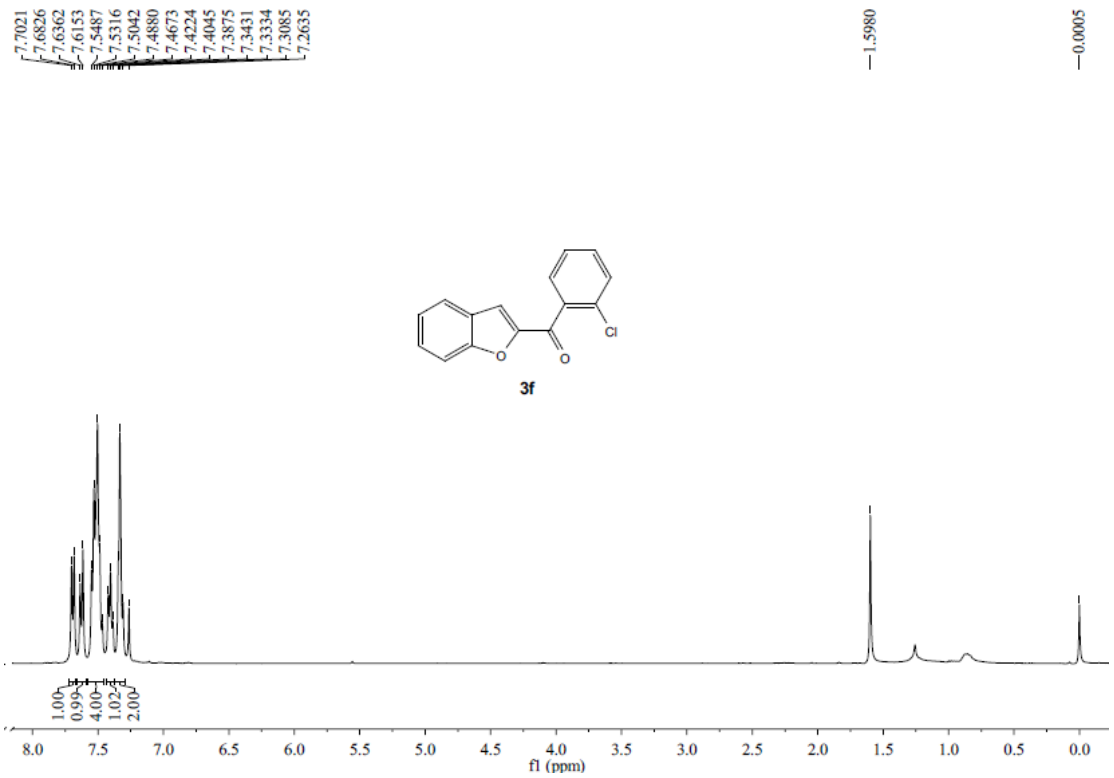
126.8675
124.0870
123.3322
116.4590
112.5299
77.3181
77.0002
76.6825
Cl
O
O
3e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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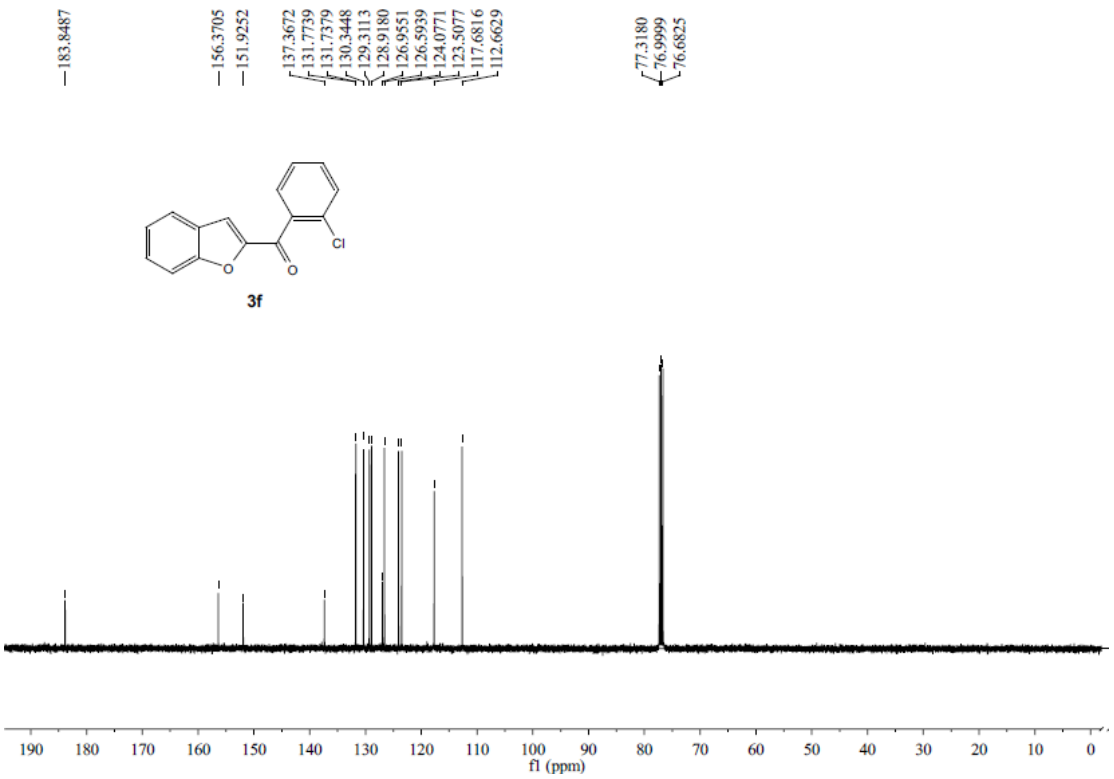
7.5487
7.5316
7.5042
7.4880
7.4673
7.4224
7.4045
7.3875
7.3431
7.3334
7.3085
7.2635
1.5980
0.0005
Cl
O
O
3f
1.00
0.99
4.00
1.02
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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137.3672
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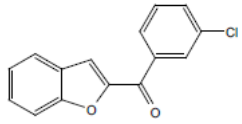
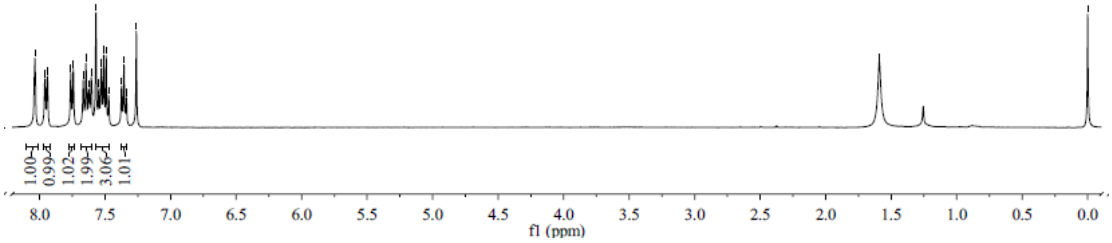
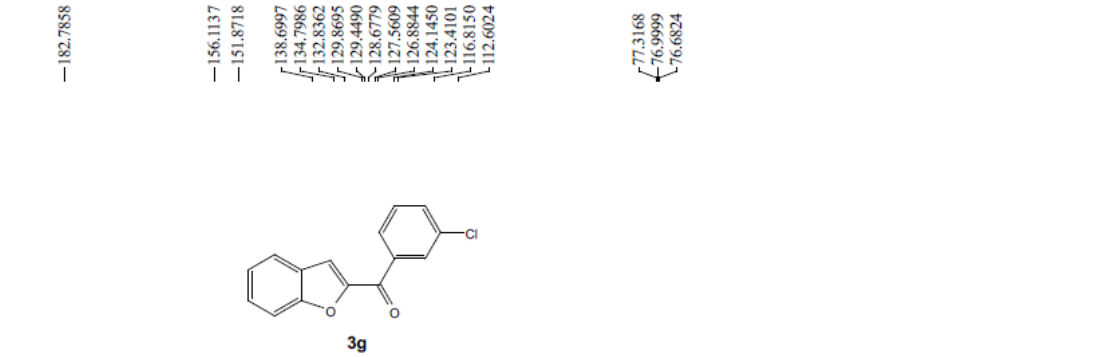
131.7379
130.3448
129.3113
128.9180
126.9551
126.5939
124.0771
123.5077
117.6816
112.6629
77.3180
76.9999
76.6825
Cl
O
O
3f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.0357
7.9591
7.9399
7.7621
7.7425
7.6670
7.6460
7.6255
7.6056
7.5697
7.5478
7.5288
7.5107
7.4915
7.4718
7.3745
7.3558
7.3370
7.2613
1.5903
0.0004


Cl
O
O

3g


1.00
0.99
1.02
1.99
3.06
1.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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138.6997
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132.8362
129.8695
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128.6779
127.5609
126.8844
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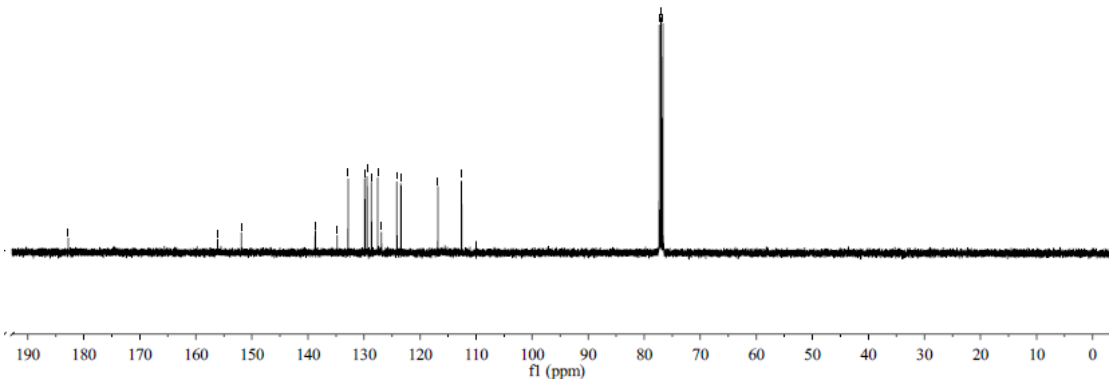
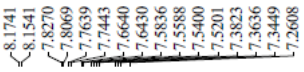
123.4101
116.8150
112.6024
77.3168
76.9999
76.6824

Cl
O
O

3g


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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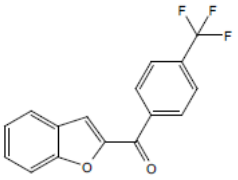
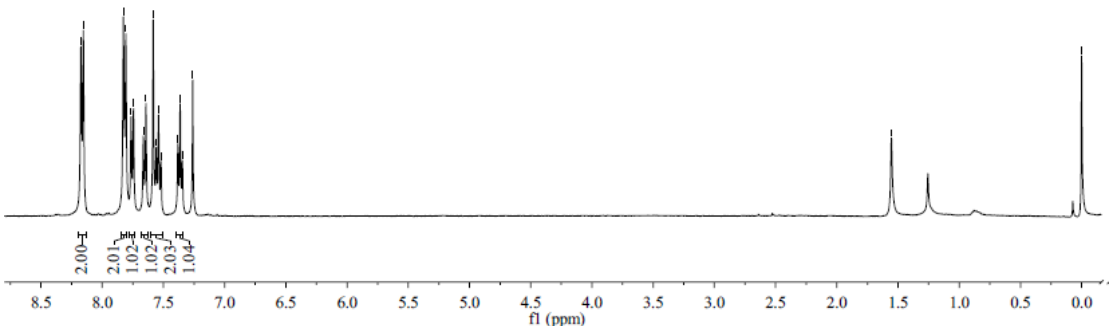
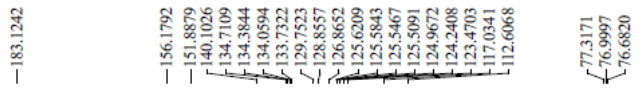
8.1541
7.8270
7.8069
7.7639
7.7443
7.6640
7.6430
7.5836
7.5588
7.5400
7.5201
7.3823
7.3636
7.3449
7.2608
1.5539
0.0004


F
F
F
O
O

3h


2.00
2.01
1.02
1.02
2.03
1.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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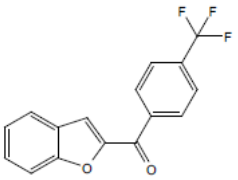
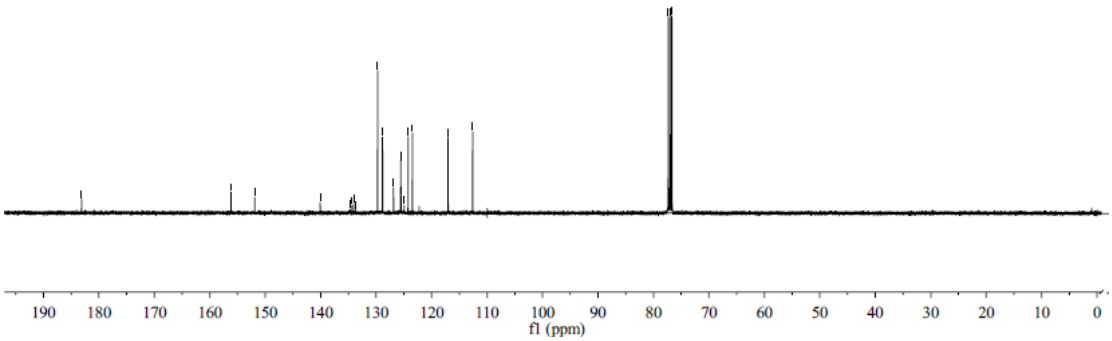
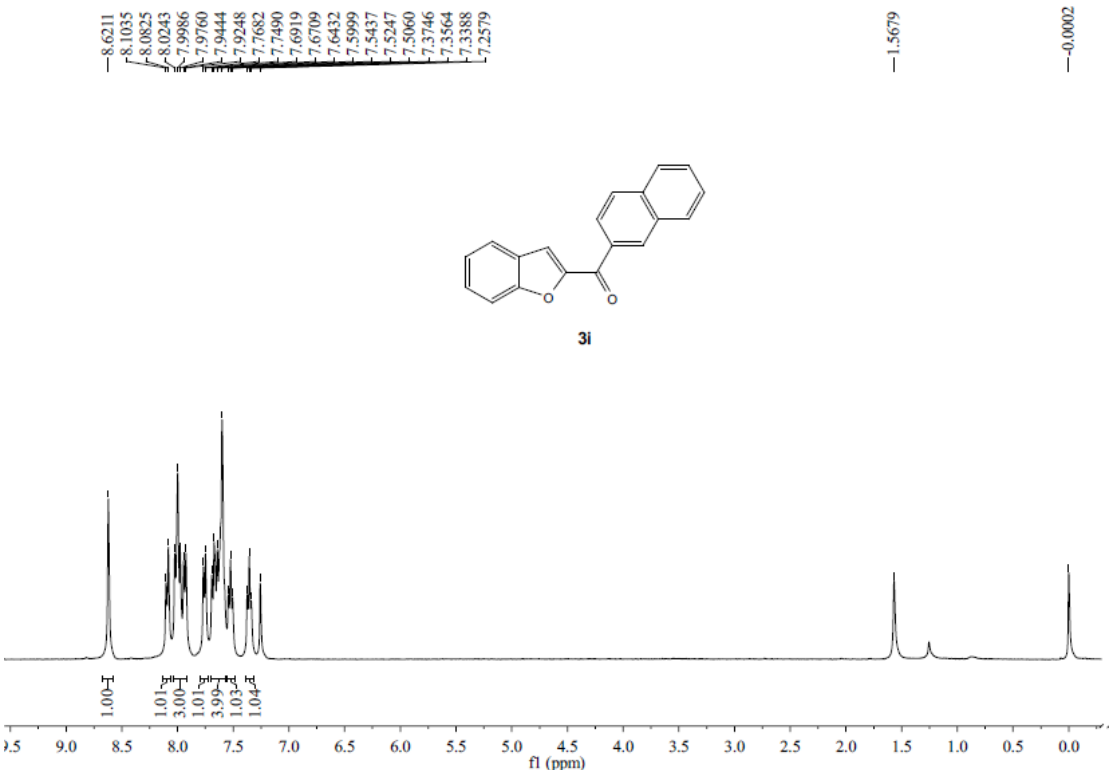
140.1026
134.7109
134.3844
134.0594
133.7322
129.7523
128.8557
126.8652
125.6209
125.5843
125.5467
125.5091
124.9672
124.2408
123.4703
117.0341
112.6068
77.3171
76.9997
76.6820


F
F
F
O
O

3h


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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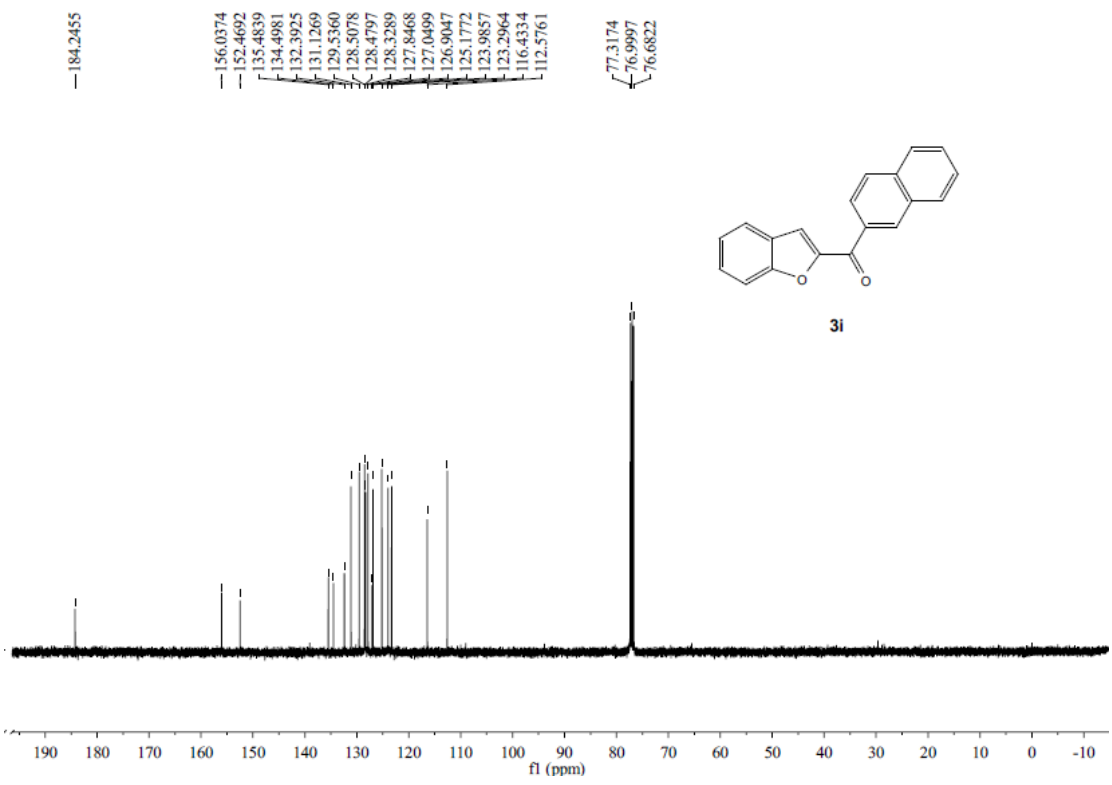
8.1035
8.0825
8.0243
7.9986
7.9760
7.9444
7.9248
7.7682
7.7490
7.6919
7.6709
7.6432
7.5999
7.5437
7.5247
7.5060
7.3746
7.3564
7.3388
7.2579
1.5679
-0.0002
1.00
1.01
3.00
1.01
3.99
1.03
1.04
f1 (ppm)

3i


184.2455
156.0374
152.4692
135.4839
134.4981
132.3925
131.1269
129.5360
128.5078
128.4797
128.3289
127.8468
127.0499
126.9047
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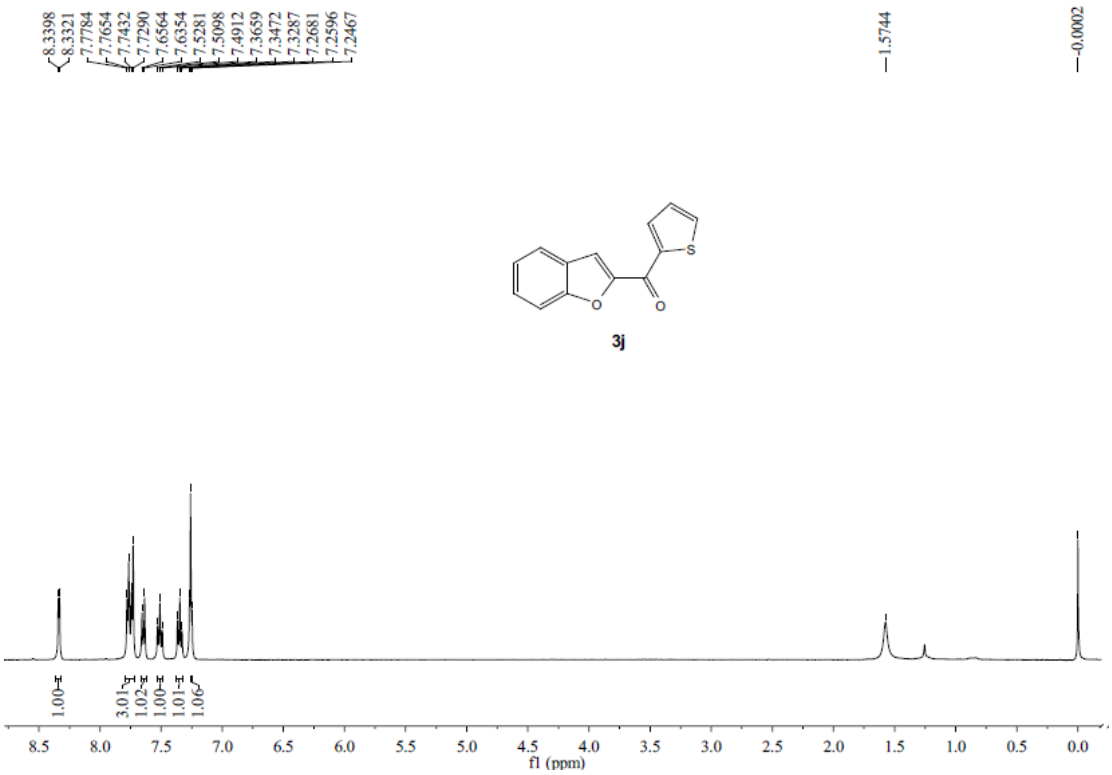
123.2964
116.4334
112.5761
77.3174
76.9997
76.6822
f1 (ppm)

3i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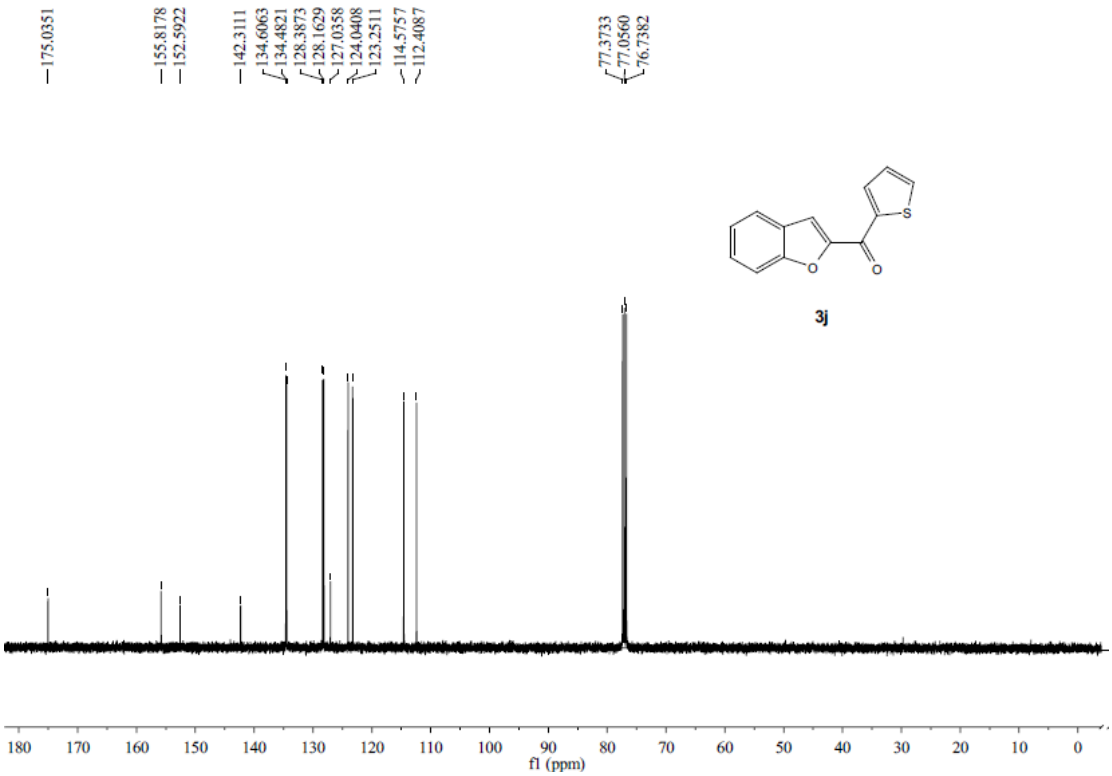
8.3321
7.7784
7.7654
7.7432
7.7290
7.6564
7.6354
7.5281
7.5098
7.4912
7.3659
7.3472
7.3287
7.2681
7.2596
7.2467
1.5744
0.0002
3j
1.00
3.01
1.02
1.00
1.01
1.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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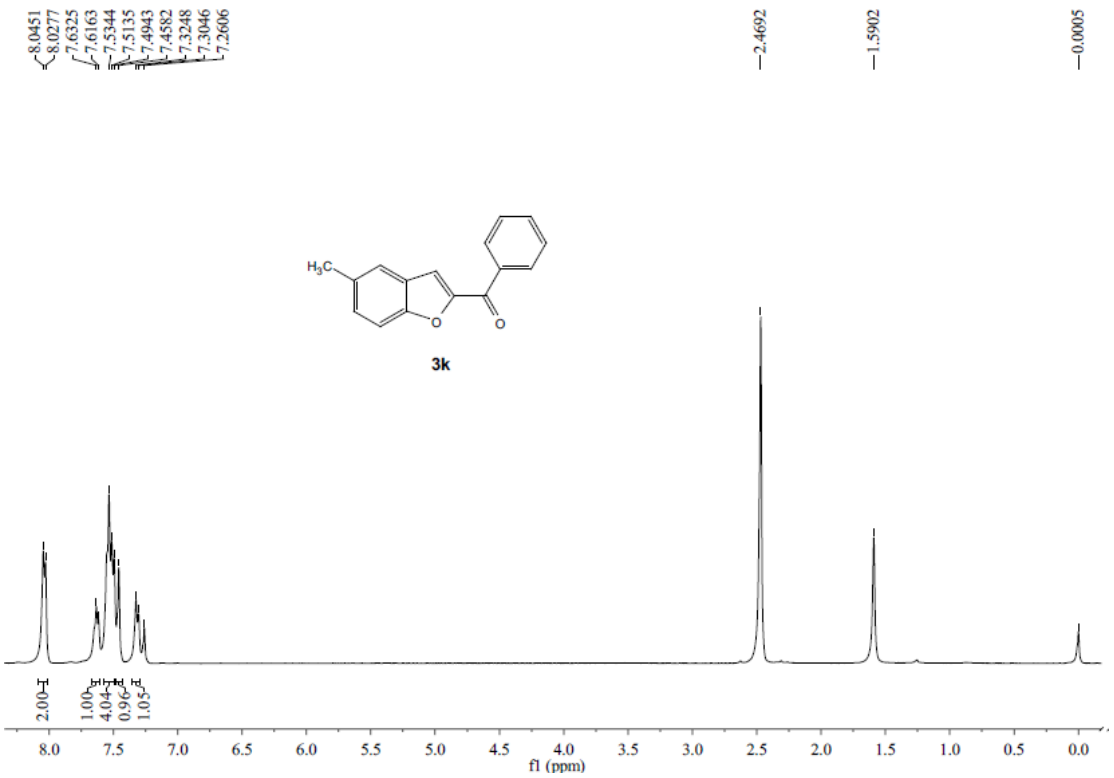
152.5922
142.3111
134.6063
134.4821
128.3873
128.1629
127.0358
124.0408
123.2511
114.5757
112.4087
77.3733
77.0560
76.7382
3j
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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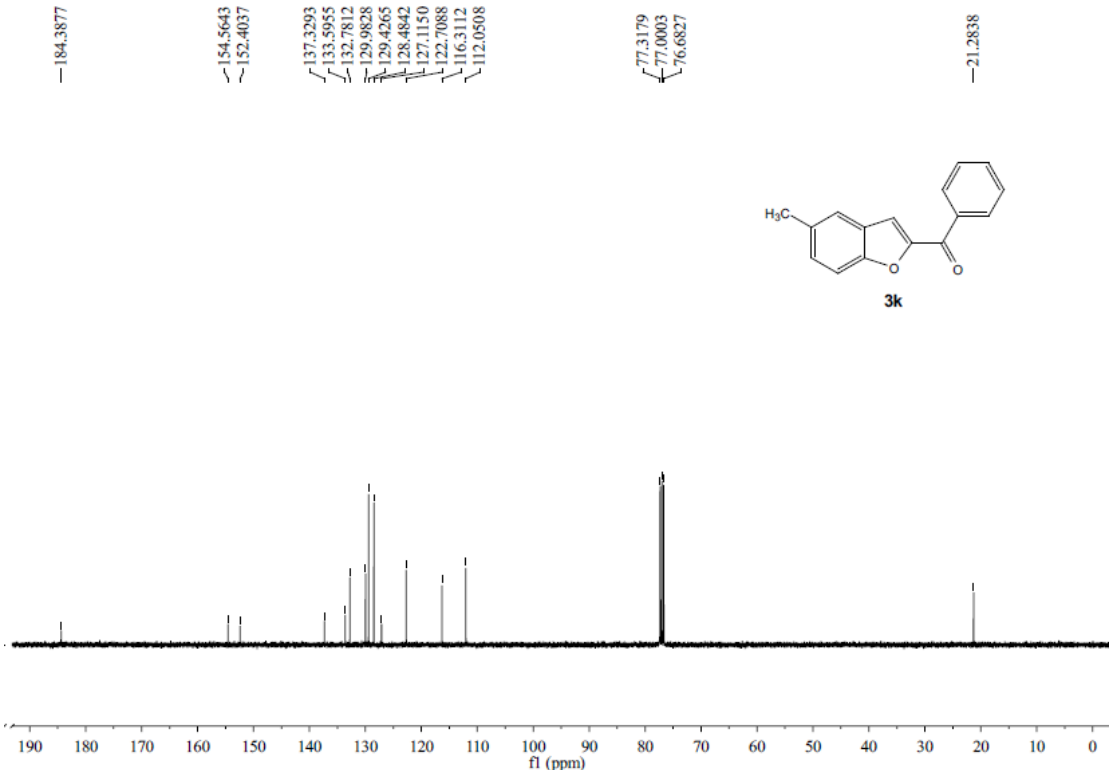
7.6325
7.6163
7.5344
7.5135
7.4943
7.4582
7.3248
7.3046
7.2606
2.4692
1.5902
0.0005
H3C
O
O
3k
2.00
1.00
4.04
0.96
1.05
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.5955
132.7812
129.9828
129.4265
128.4842
127.1150
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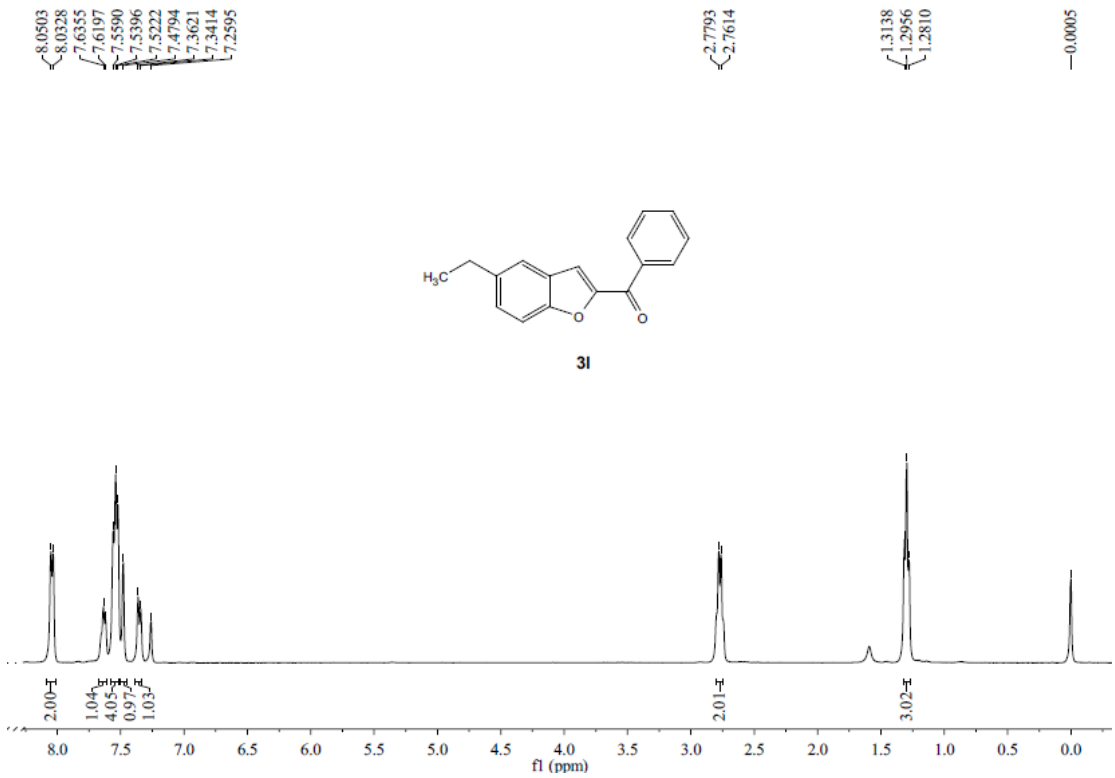
112.0508
77.3179
77.0003
76.6827
21.2838
H3C
O
O
3k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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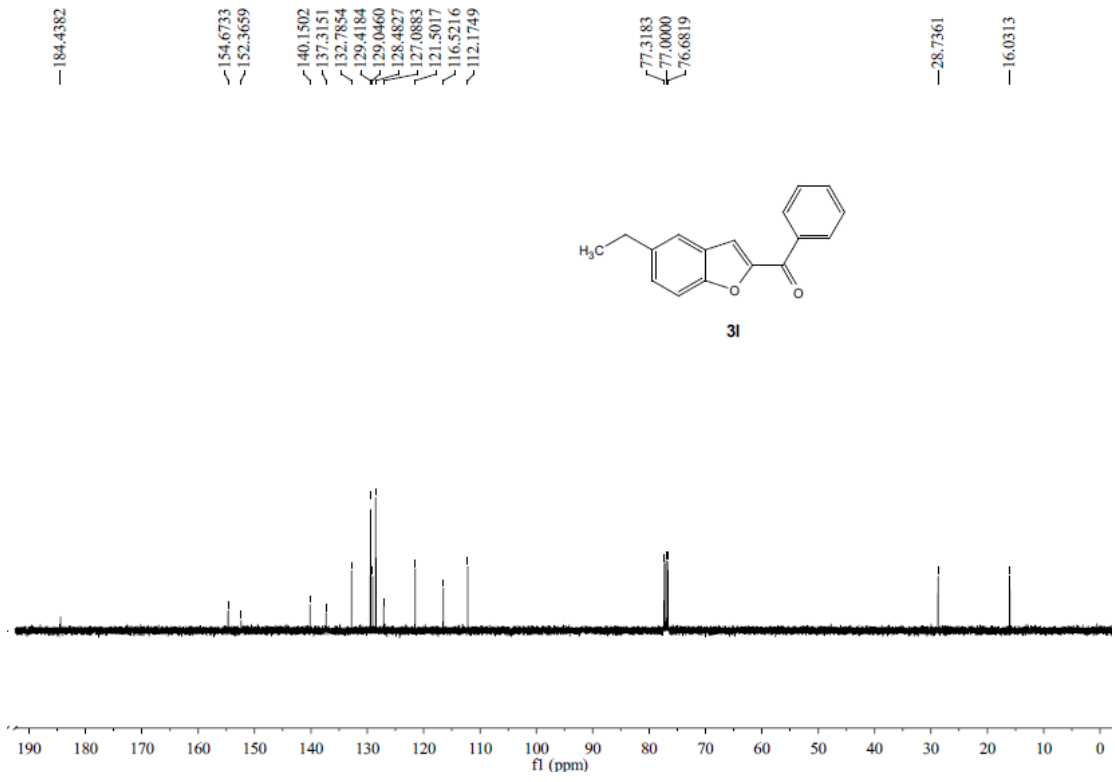
7.6355
7.6197
7.5590
7.5396
7.5222
7.4794
7.3621
7.3414
7.2595
2.7793
2.7614
1.3138
1.2956
1.2810
0.0005
H3C
O
O
3l
2.00
1.04
4.05
0.97
1.03
2.01
3.02
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.3151
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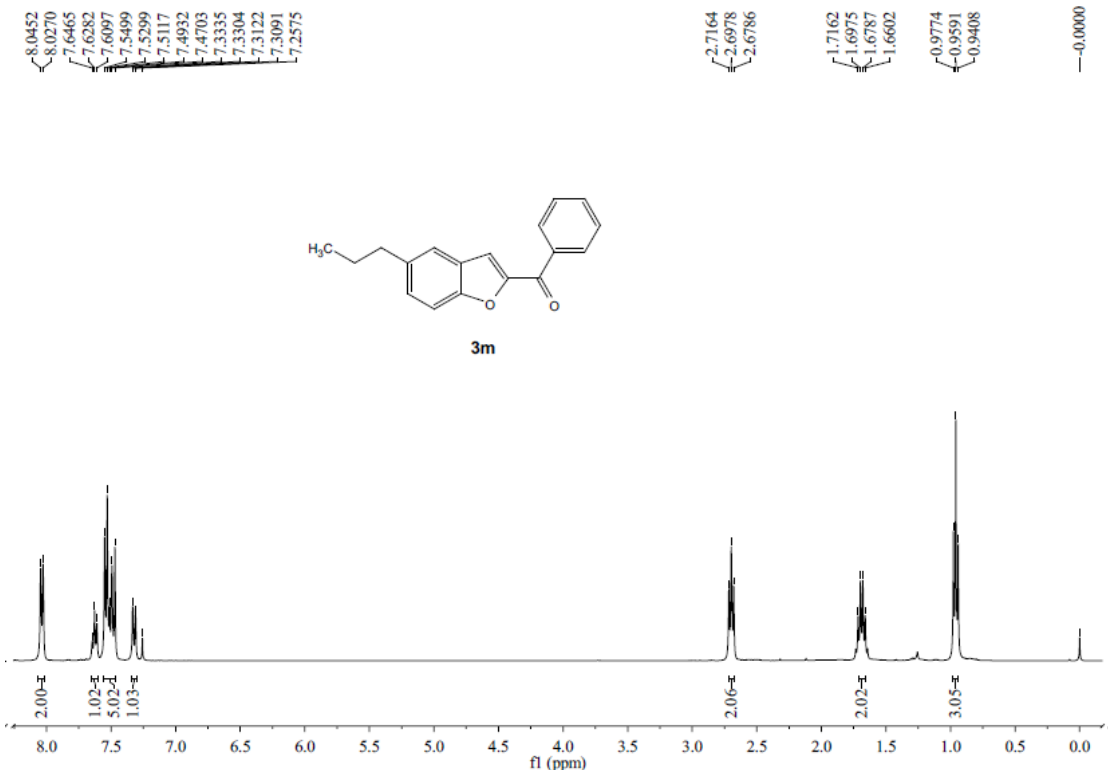
129.4184
129.0460
128.4827
127.0883
121.5017
116.5216
112.1749
77.3183
77.0000
76.6819
28.7361
16.0313
H3C
O
O
3l
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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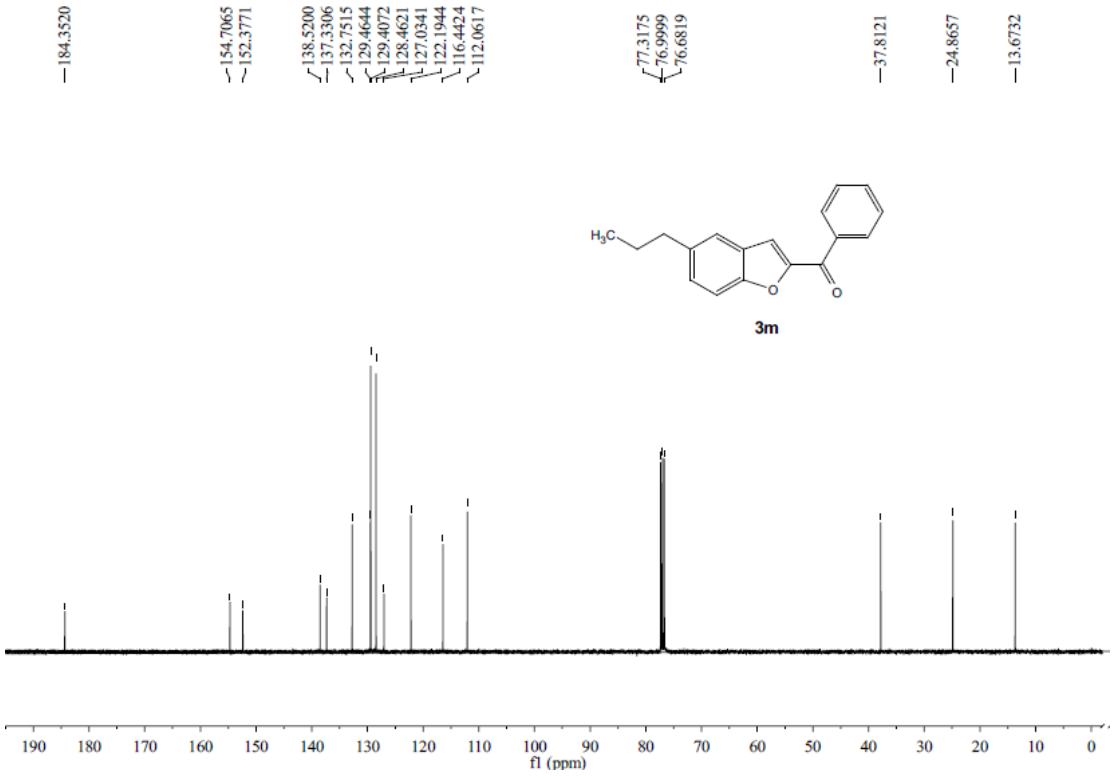
7.6097
7.5499
7.5299
7.5117
7.4932
7.4703
7.3335
7.3304
7.3122
7.3091
7.2575
2.7164
2.6978
2.6786
1.7162
1.6975
1.6787
1.6602
0.9774
0.9591
0.9408
0.0000
H3C
O
O
3m
2.00
1.02
5.02
1.03
2.06
2.02
3.05
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.4644
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128.4621
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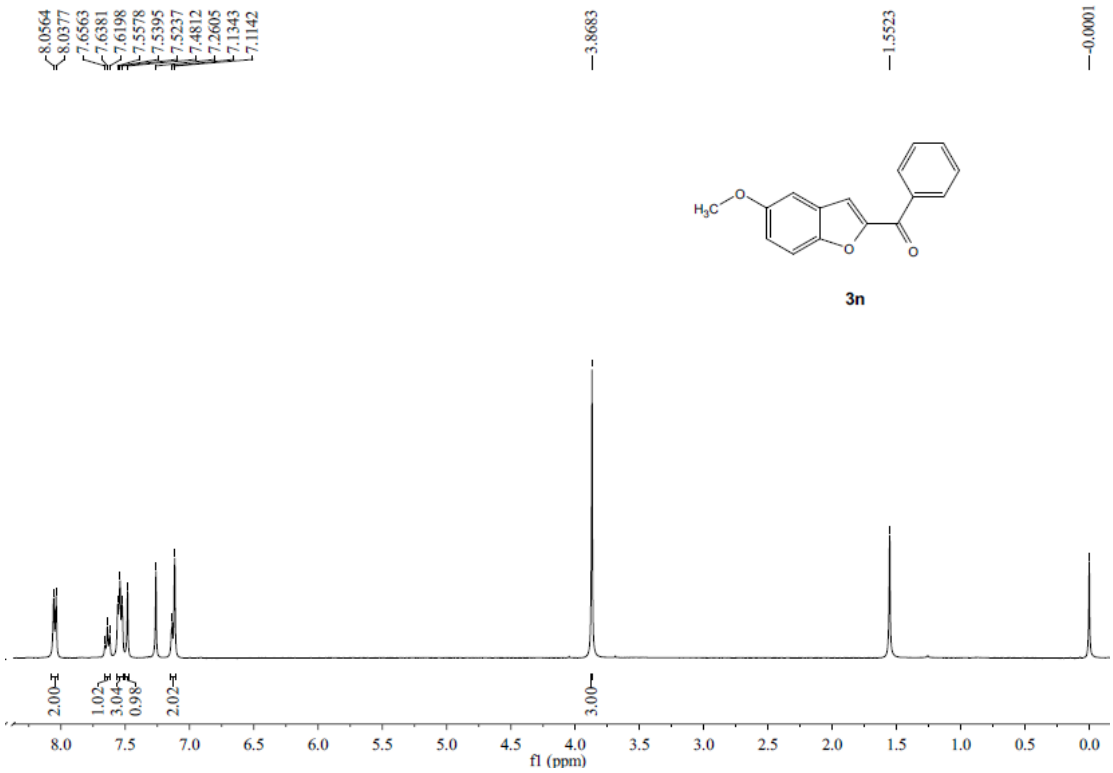
122.1944
116.4424
112.0617
77.3175
76.9999
76.6819
37.8121
24.8657
13.6732
H3C
O
O
3m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.4812
7.2605
7.1343
7.1142
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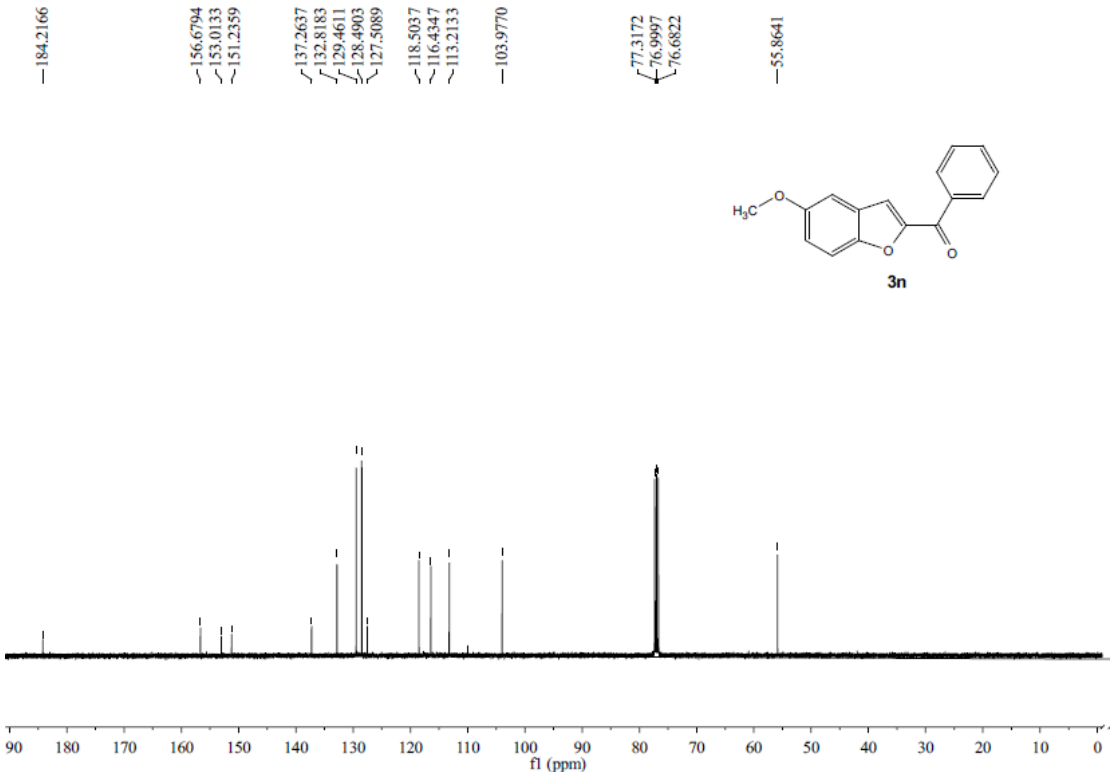
-0.0001
3n
2.00
1.02
3.04
0.98
2.02
3.00
f1 (ppm)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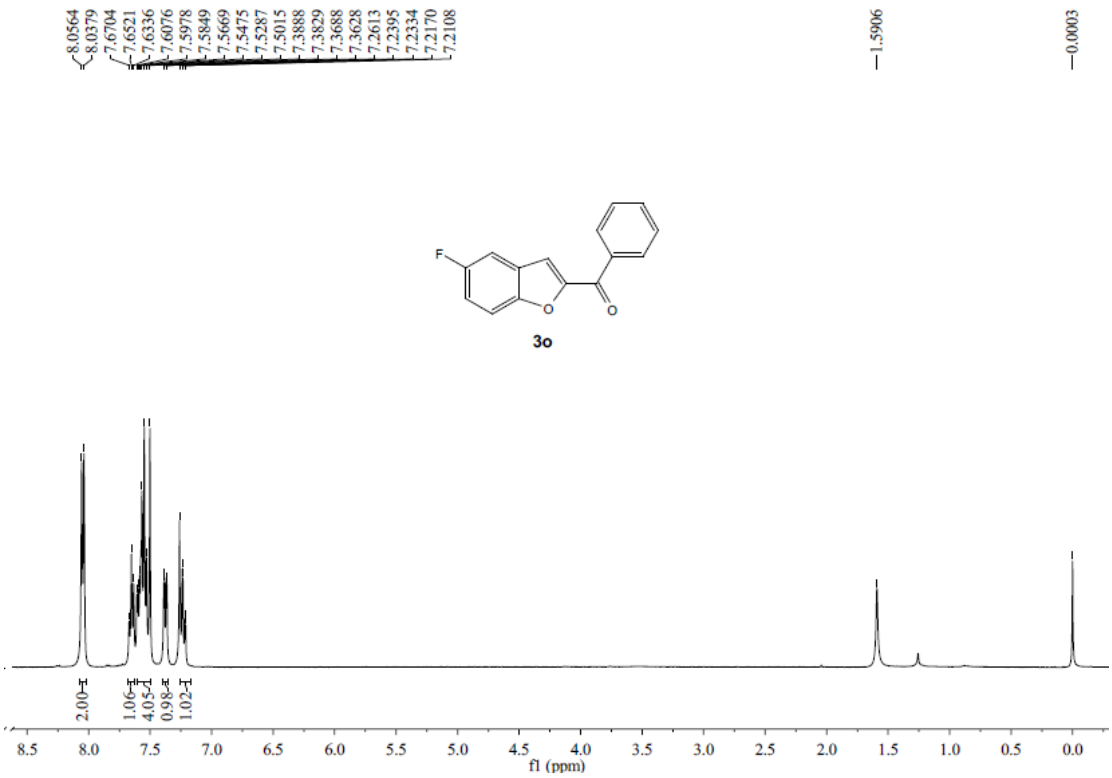
76.6822
55.8641
3n
f1 (ppm)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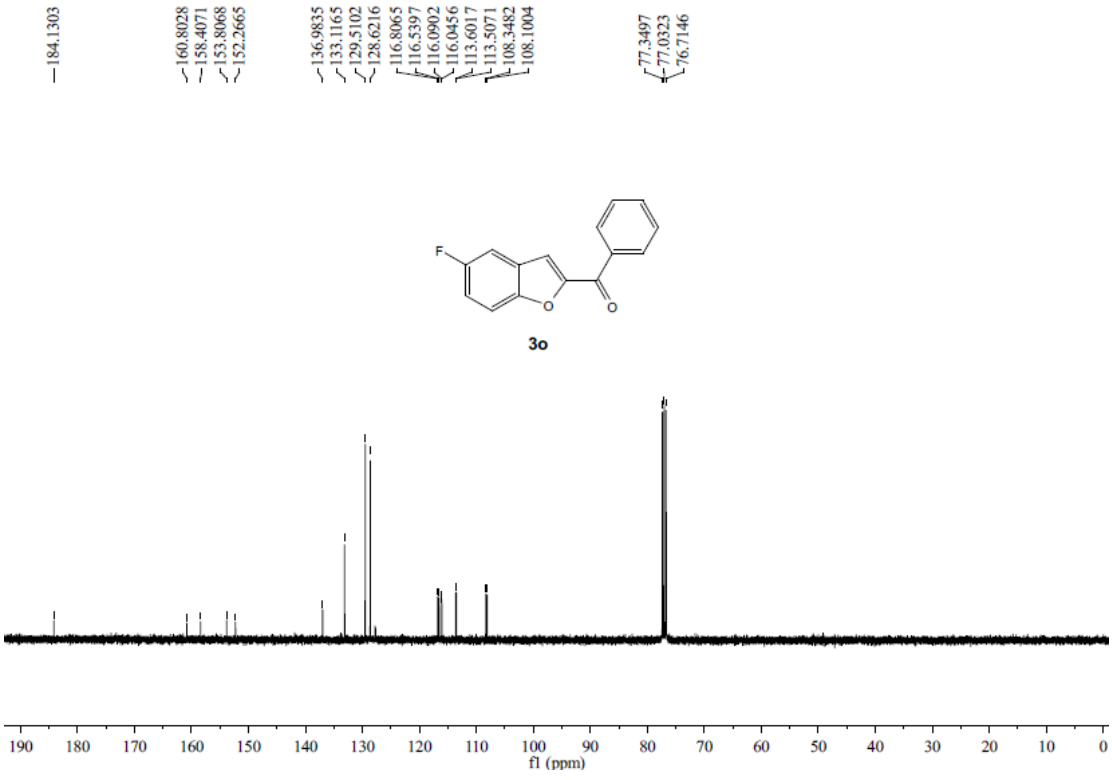
7.5015
7.3888
7.3829
7.3688
7.3628
7.2613
7.2395
7.2334
7.2170
7.2108
1.5906
0.0003
F
O
O
3o
2.00
1.06
4.05
0.98
1.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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153.8068
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133.1165
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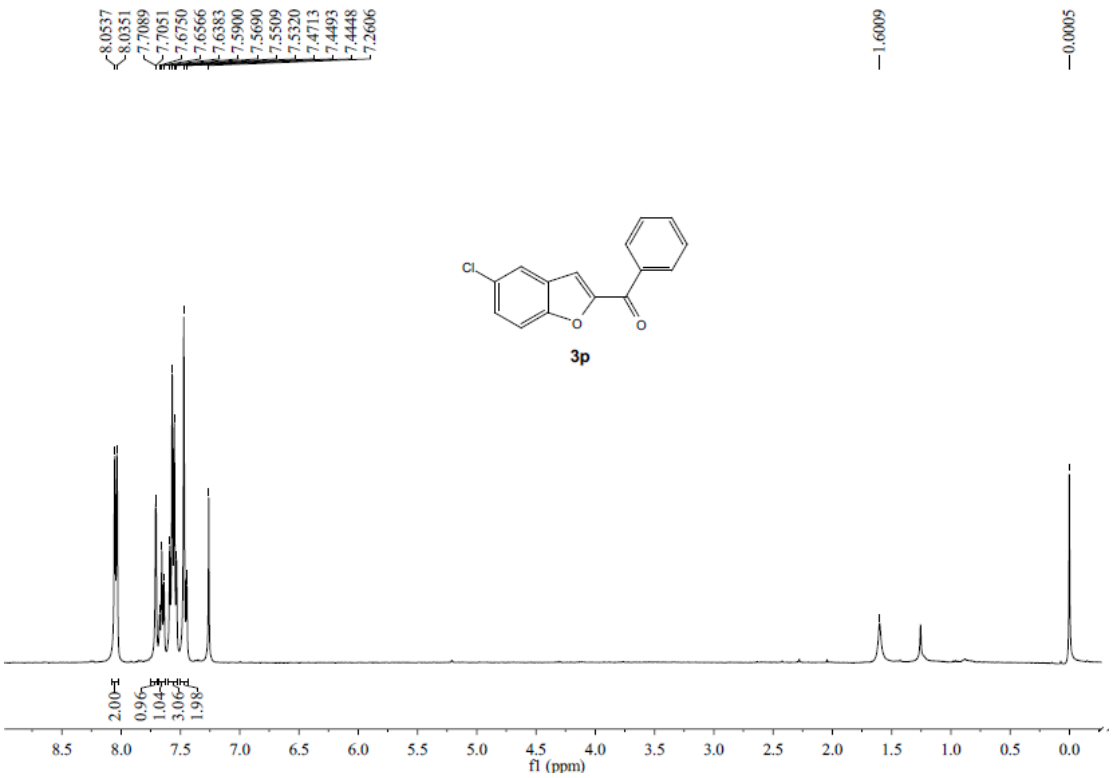
128.6216
116.8065
116.5397
116.0902
116.0456
113.6017
113.5071
108.3482
108.1004
77.3497
77.0323
76.7146
F
O
O
3o
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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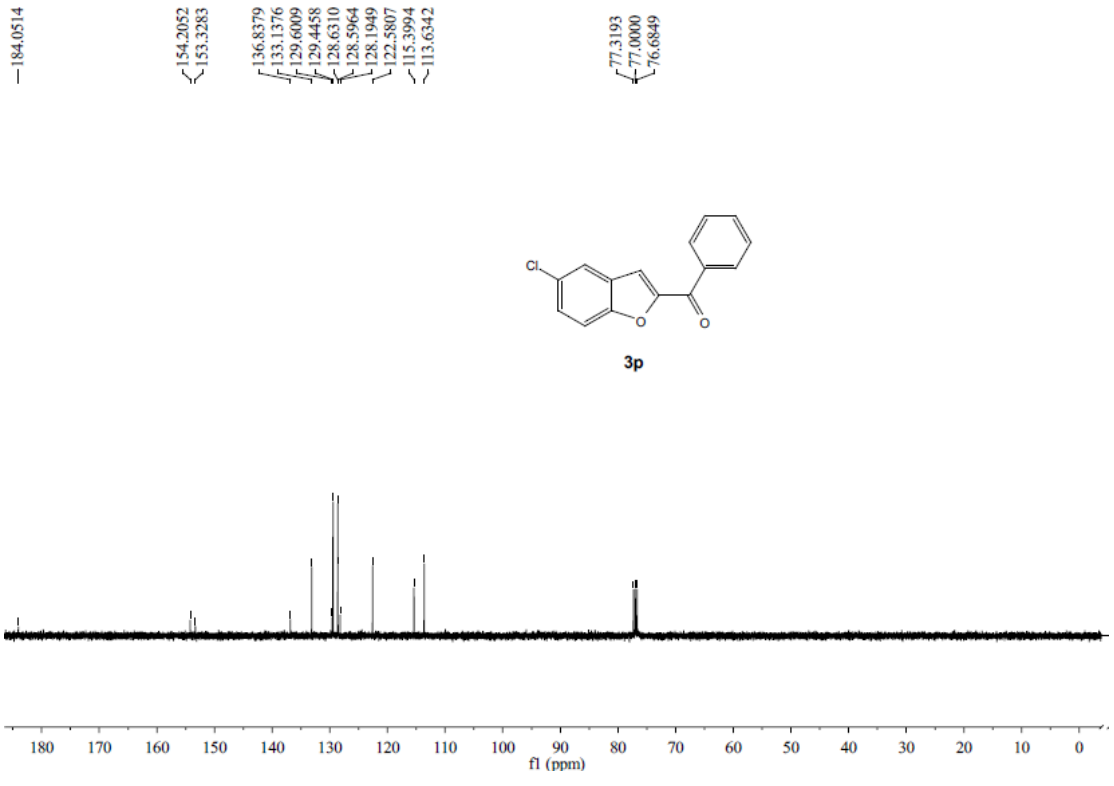
8.0351
7.7089
7.7051
7.6750
7.6566
7.6383
7.5900
7.5690
7.5509
7.5320
7.4713
7.4493
7.4448
7.2606
1.6009
0.0005
Cl
O
O
3p
2.00
0.96
1.04
3.06
1.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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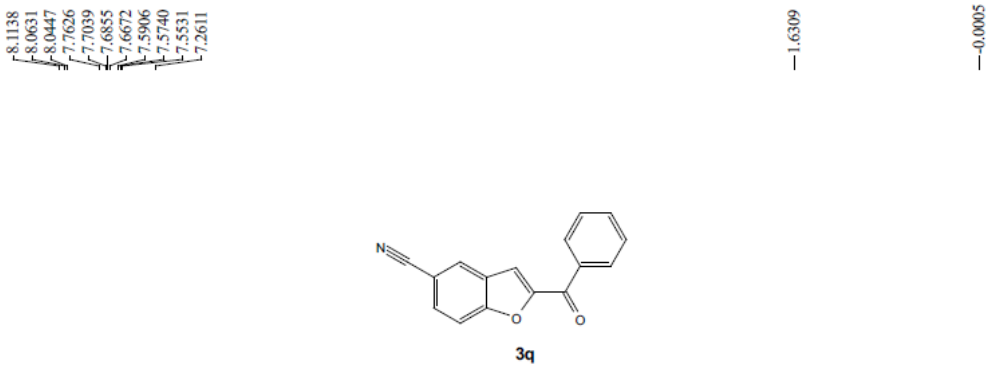
154.2052
153.3283
136.8379
133.1376
129.6009
129.4458
128.6310
128.5964
128.1949
122.5807
115.3994
113.6342
77.3193
77.0000
76.6849
Cl
O
O
3p
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.0631
8.0447
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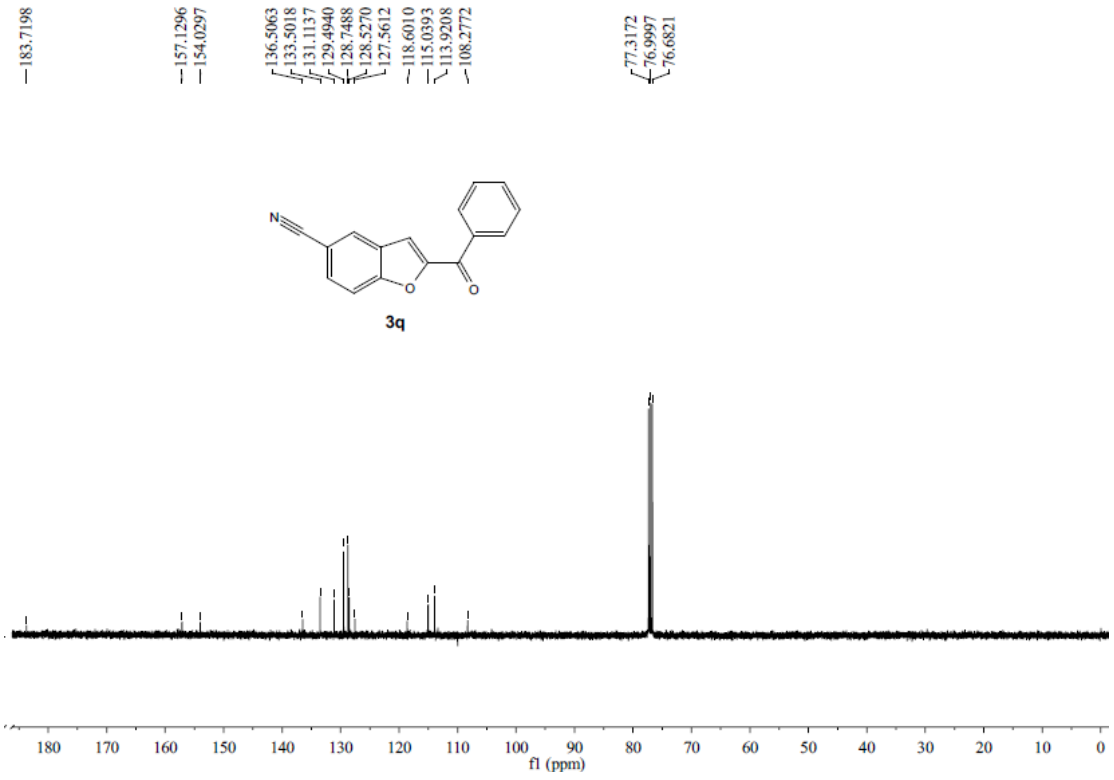
7.7039
7.6855
7.6672
7.5906
7.5740
7.5531
7.2611
1.6309
0.0005
N
O
O
3q
1.00
2.05
2.01
1.07
2.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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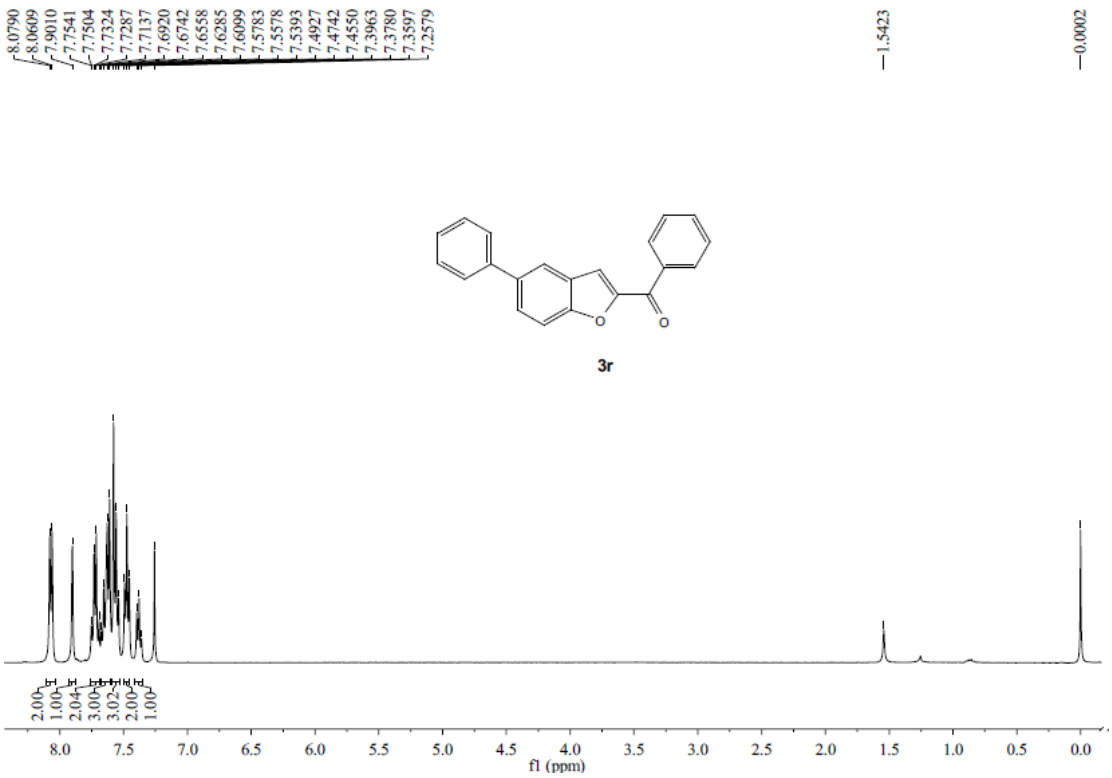
154.0297
136.5063
133.5018
131.1137
129.4940
128.7488
128.5270
127.5612
118.6010
115.0393
113.9208
108.2772
77.3172
76.9997
76.6821
N
O
O
3q
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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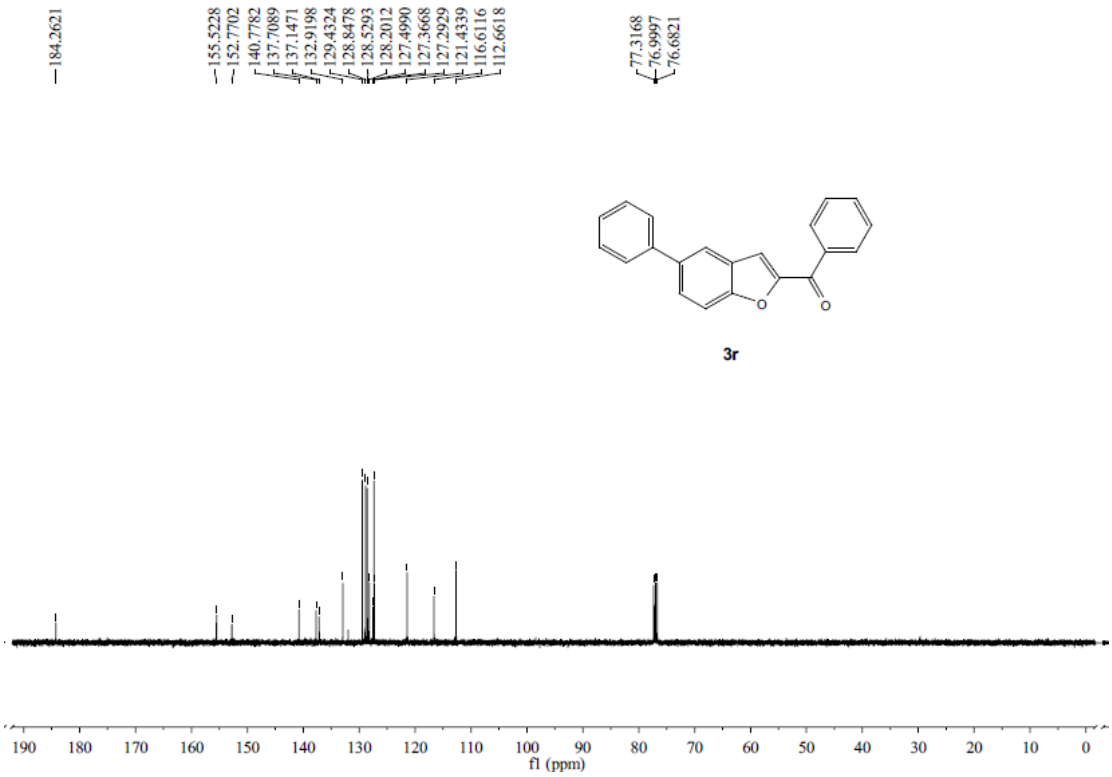
8.0609
7.9010
7.7541
7.7504
7.7324
7.7287
7.7137
7.6920
7.6742
7.6558
7.6285
7.6099
7.5783
7.5578
7.5393
7.4927
7.4742
7.4550
7.3963
7.3780
7.3597
7.2579
1.5423
0.0002
3r
2.00
1.00
2.04
3.00
3.02
2.00
1.00
f1 (ppm)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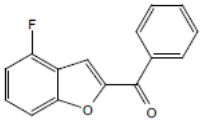
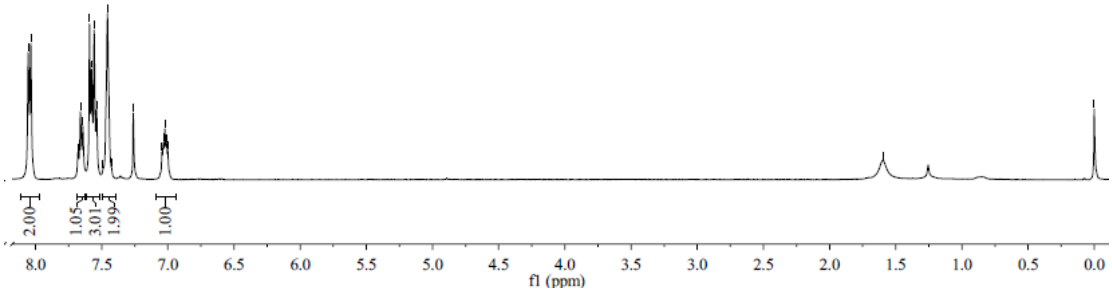
152.7702
140.7782
137.7089
137.1471
132.9198
129.4324
128.8478
128.5293
128.2012
127.4990
127.3668
127.2929
121.4339
116.6116
112.6618
77.3168
76.9997
76.6821
3r
f1 (ppm)


8.0353
7.6782
7.6610
7.6428
7.5922
7.5765
7.5572
7.5386
7.4893
7.4562
7.4261
7.2615
7.0450
7.0325
7.0227
7.0140
7.0098
7.0007
1.5972
0.0003


F
O
O

3s


2.00
1.05
3.01
1.99
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


183.9153
158.2237
155.6974
152.0126
136.8348
133.1041
129.3854
128.9629
128.8858
128.5958
116.9438
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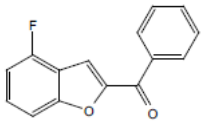
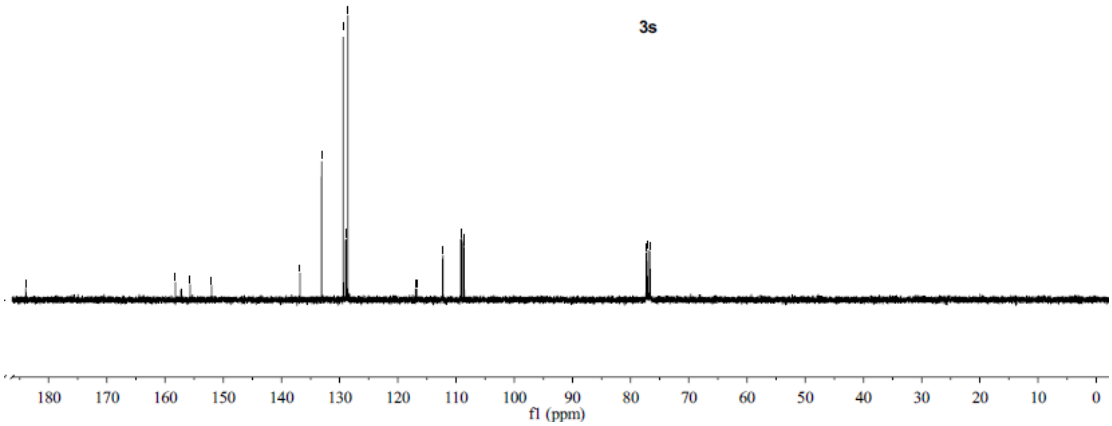
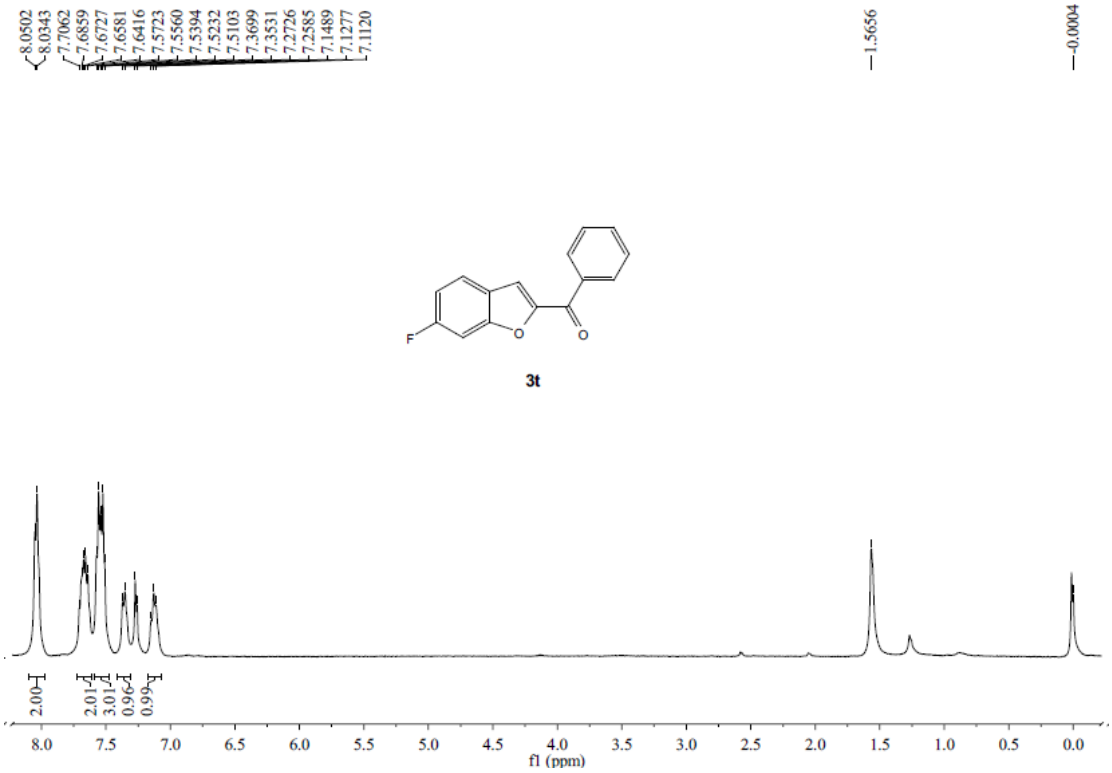
112.2689
109.1815
108.9980
108.6546
108.6092
77.3142
76.9996
76.6805


F
O
O

3s


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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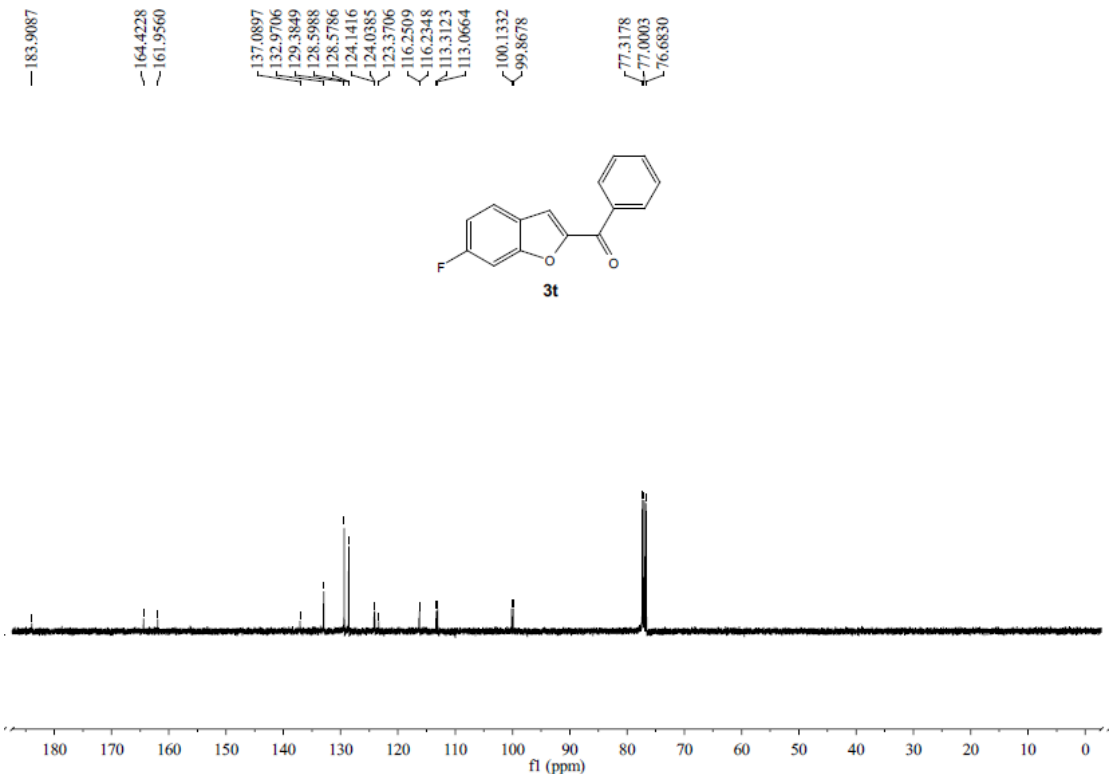
8.0343
7.7062
7.6859
7.6727
7.6581
7.6416
7.5723
7.5560
7.5394
7.5232
7.5103
7.3699
7.3531
7.2726
7.2585
7.1489
7.1277
7.1120
1.5656
0.0004
F
O
O
3t
2.00
2.01
3.01
0.96
0.99
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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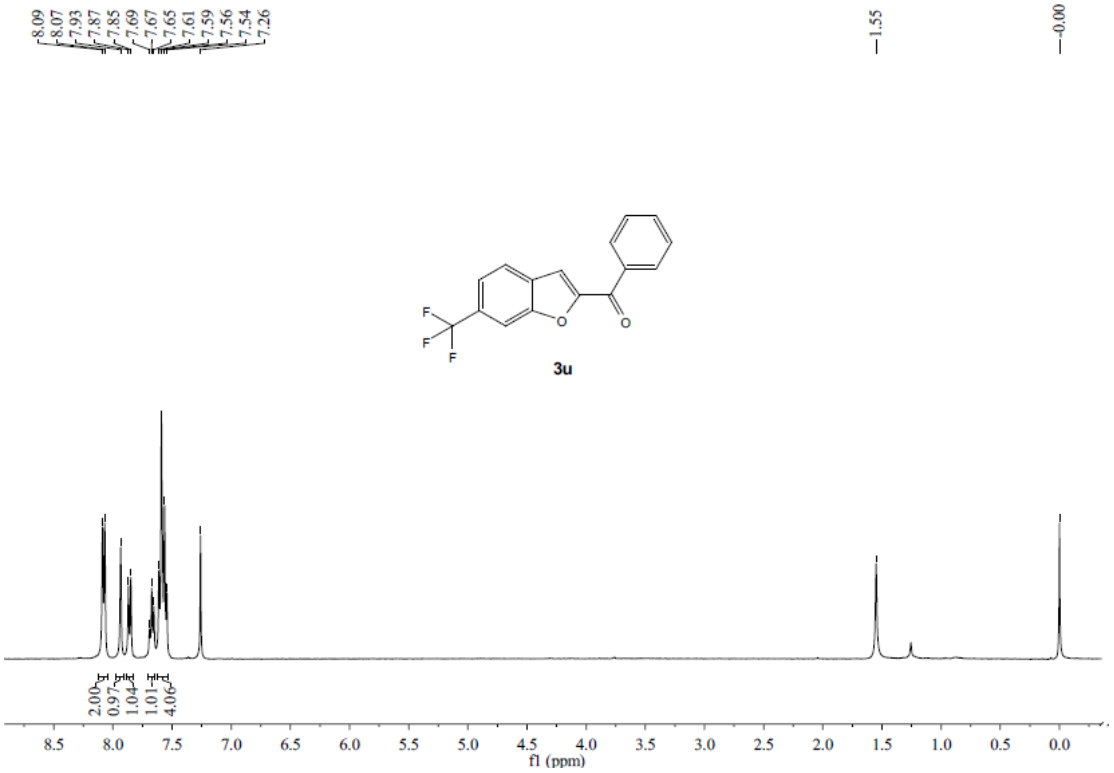
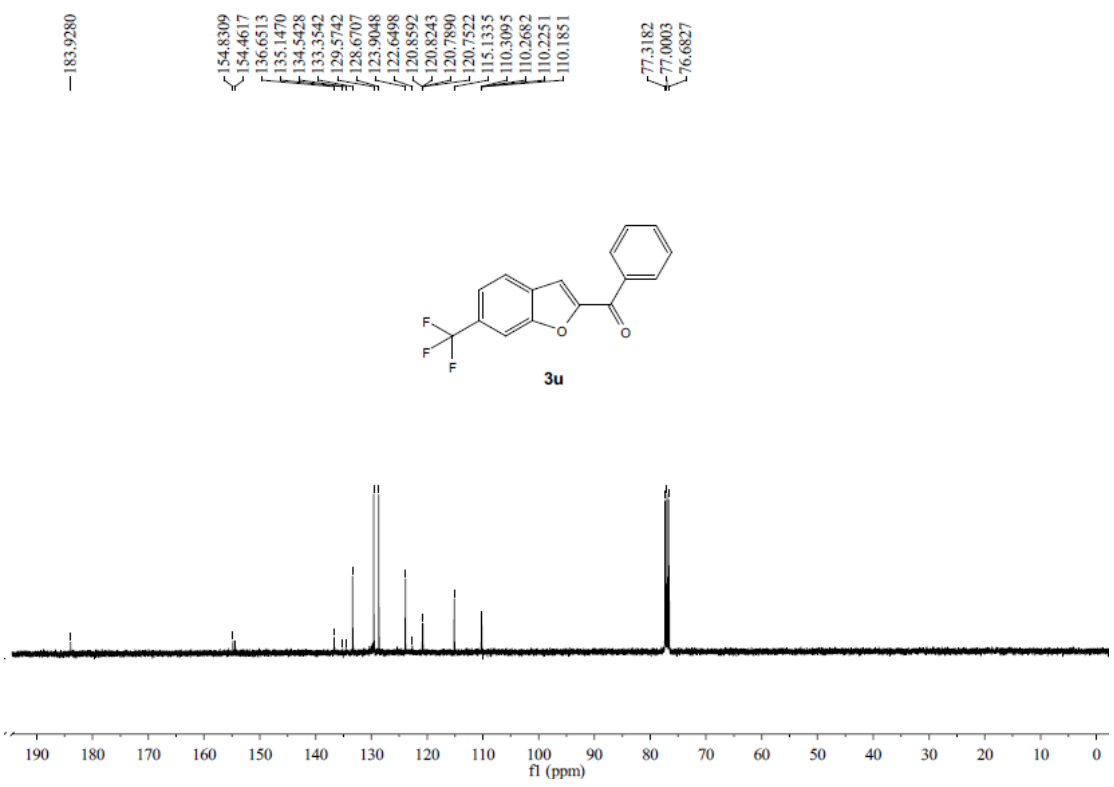
164.4228
161.9560
137.0897
132.9706
129.3849
128.5988
128.5786
124.1416
124.0385
123.3706
116.2509
116.2348
113.3123
113.0664
100.1332
99.8678
77.3178
77.0003
76.6830
F
O
O
3t
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.09
8.07
7.93
7.87
7.85
7.69
7.67
7.65
7.61
7.59
7.56
7.54
7.26
1.55
0.00
3u
2.00
0.97
1.04
1.01
4.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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154.4617
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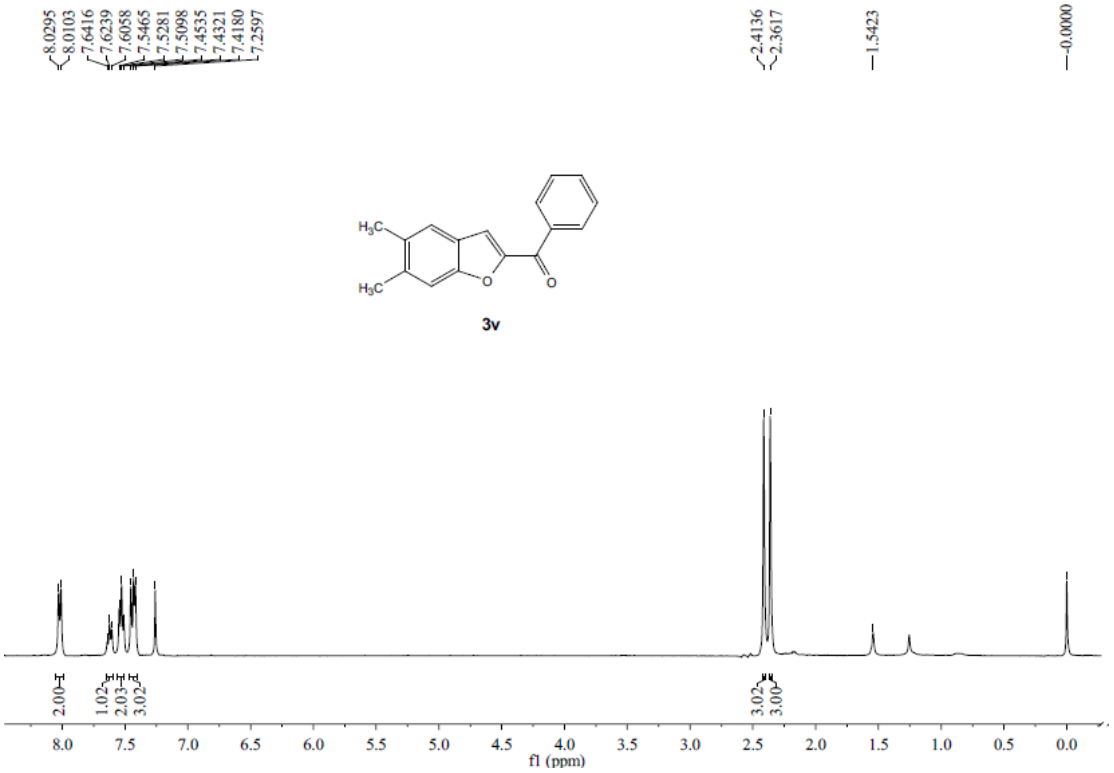
135.1470
134.5428
133.3542
129.5742
128.6707
123.9048
122.6498
120.8592
120.8243
120.7890
120.7522
115.1335
110.3095
110.2682
110.2251
110.1851
77.3182
77.0003
76.6827
3u
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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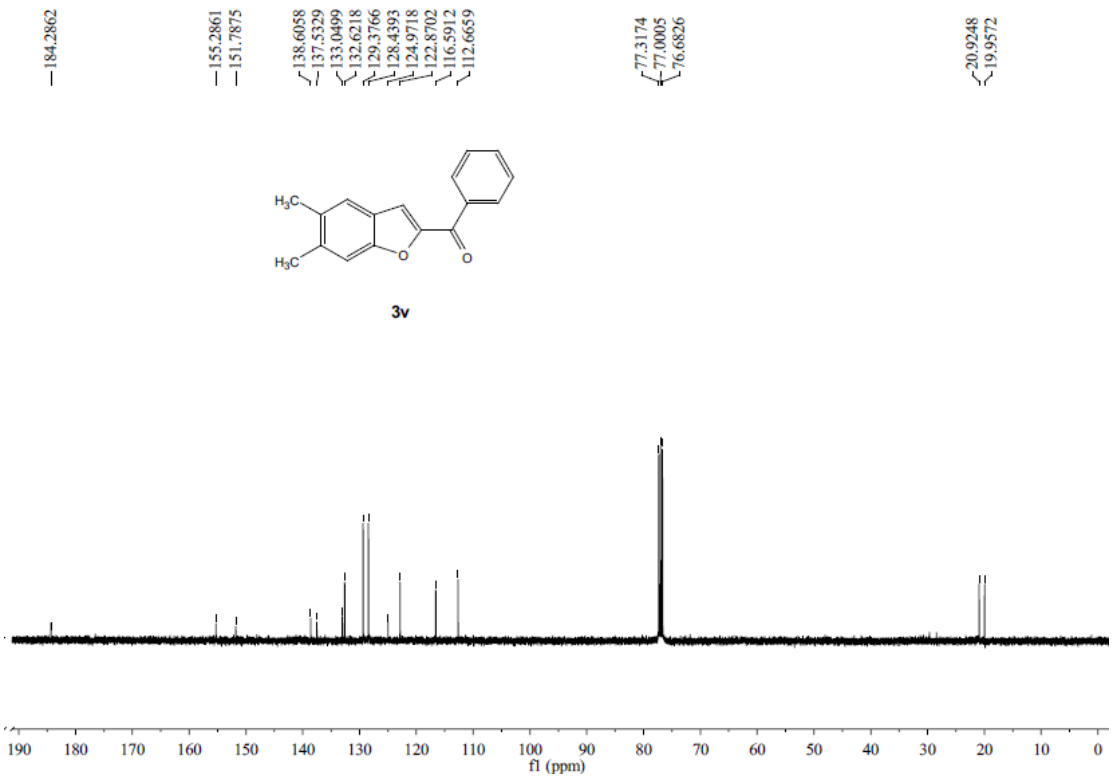
7.6239
7.6058
7.5465
7.5281
7.5098
7.4535
7.4321
7.4180
7.2597
2.4136
2.3617
1.5423
0.0000
H3C
H3C
O
O
3v
2.00
1.02
2.03
3.02
3.02
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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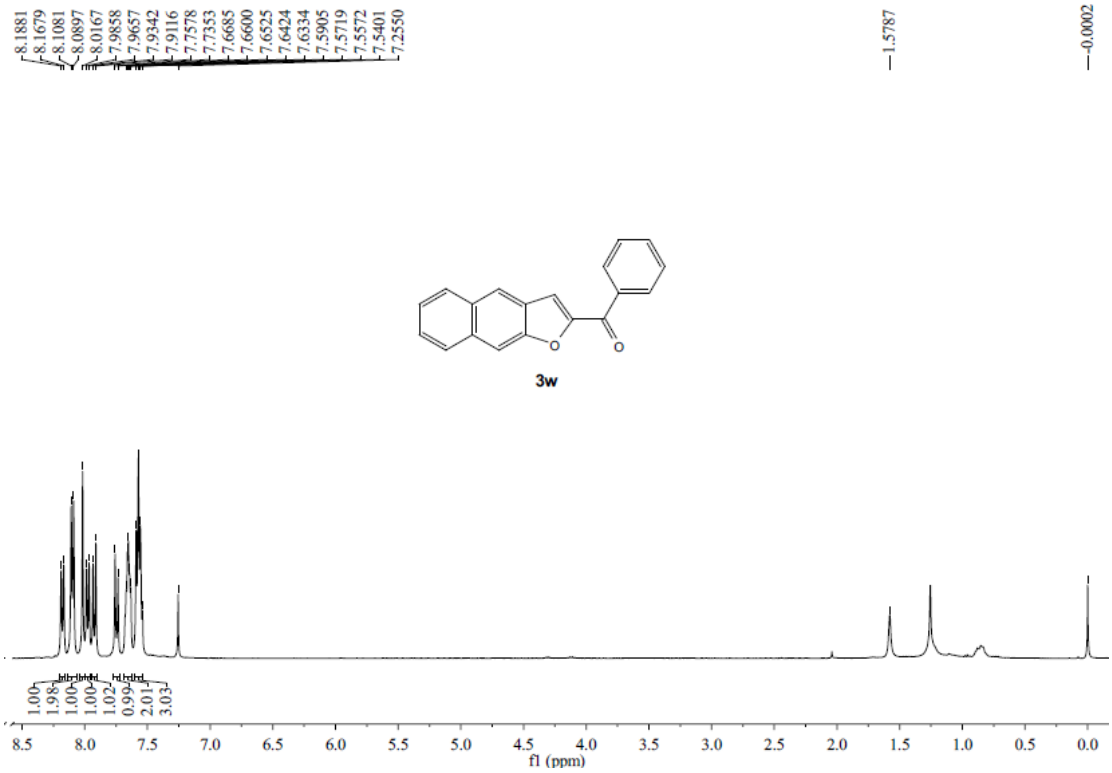
133.0499
132.6218
129.3766
128.4393
124.9718
122.8702
116.5912
112.6659
77.3174
77.0005
76.6826
20.9248
19.9572
H3C
H3C
O
O
3v
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.1081
8.0897
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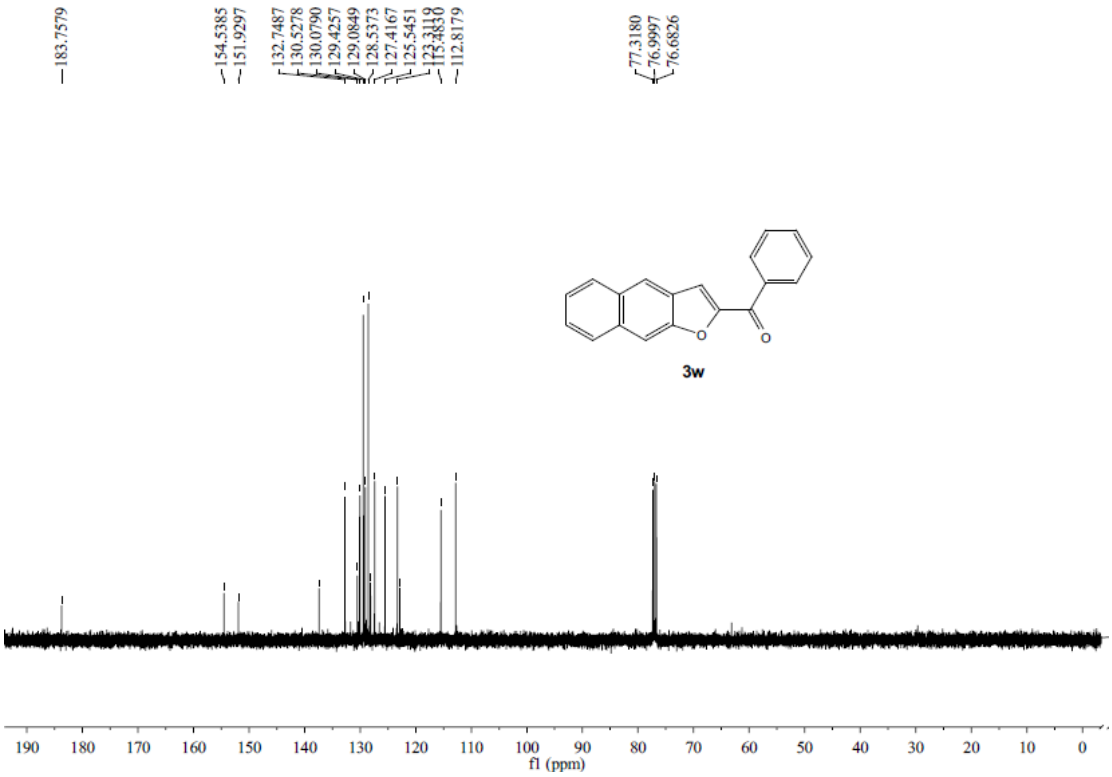
7.9657
7.9342
7.9116
7.7578
7.7353
7.6685
7.6600
7.6525
7.6424
7.6334
7.5905
7.5719
7.5572
7.5401
7.2550
1.5787
0.0002
3w
1.00
1.98
1.00
1.00
1.02
0.99
2.01
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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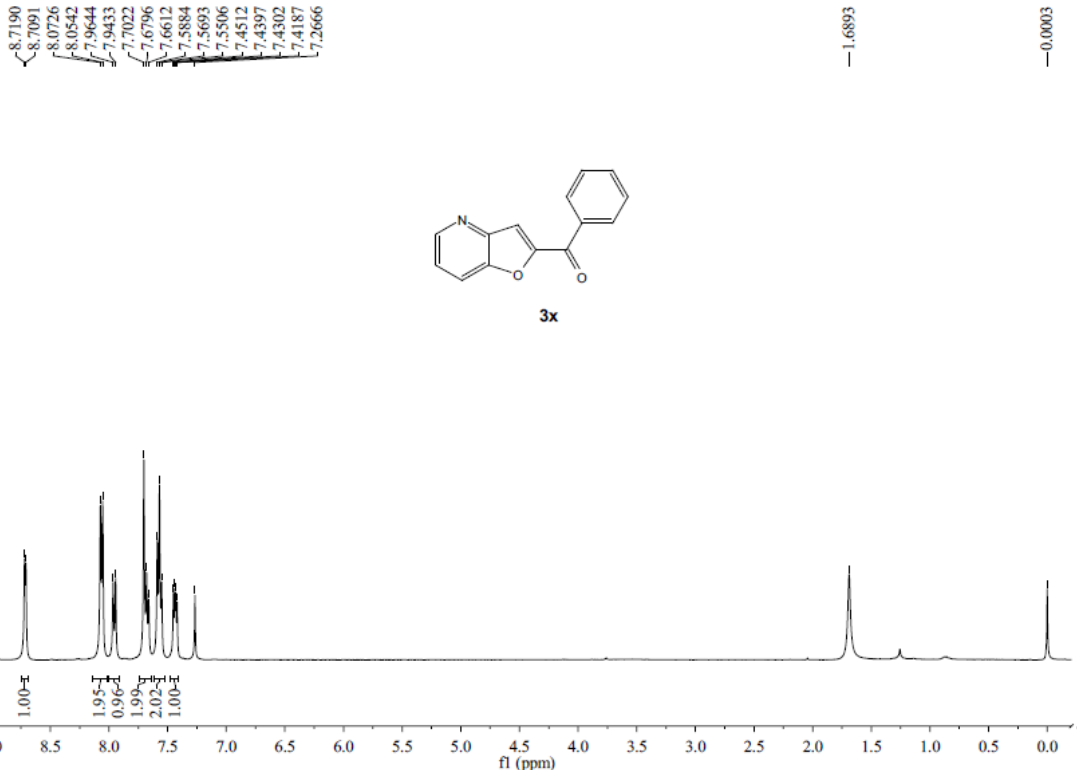
151.9297
132.7487
130.5278
130.0790
129.4257
129.0849
128.5373
127.4167
125.5451
123.3119
115.4830
112.8179
77.3180
76.9997
76.6826
3w
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.9644
7.9433
7.7022
7.6796
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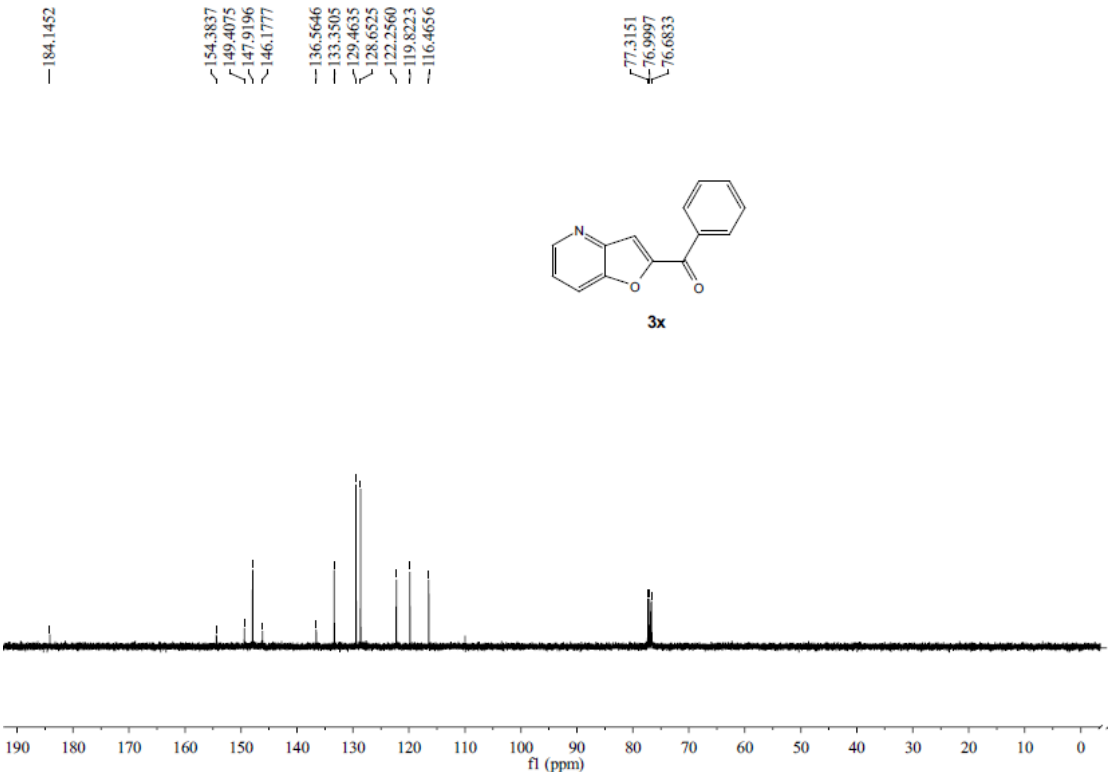
7.5693
7.5506
7.4512
7.4397
7.4302
7.4187
7.2666
1.6893
0.0003
N
O
O
3x
1.00
1.95
0.96
1.99
2.02
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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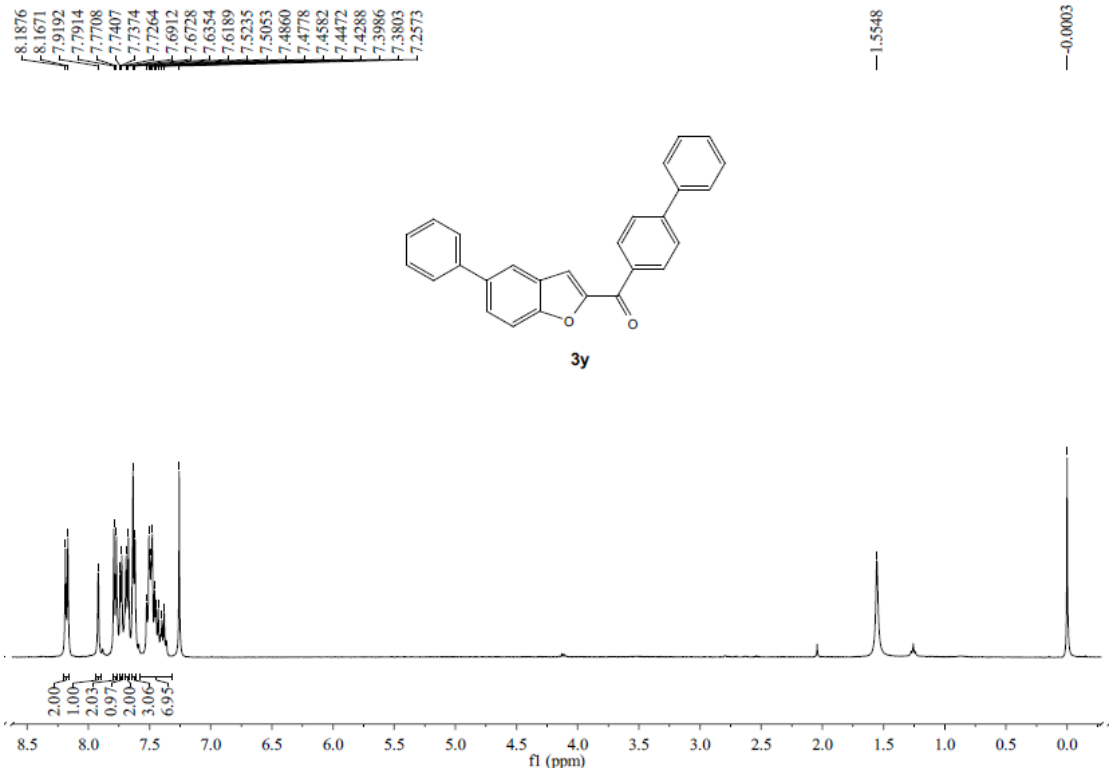
128.6525
122.2560
119.8223
116.4656
77.3151
76.9997
76.6833
N
O
O
3x
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.7374
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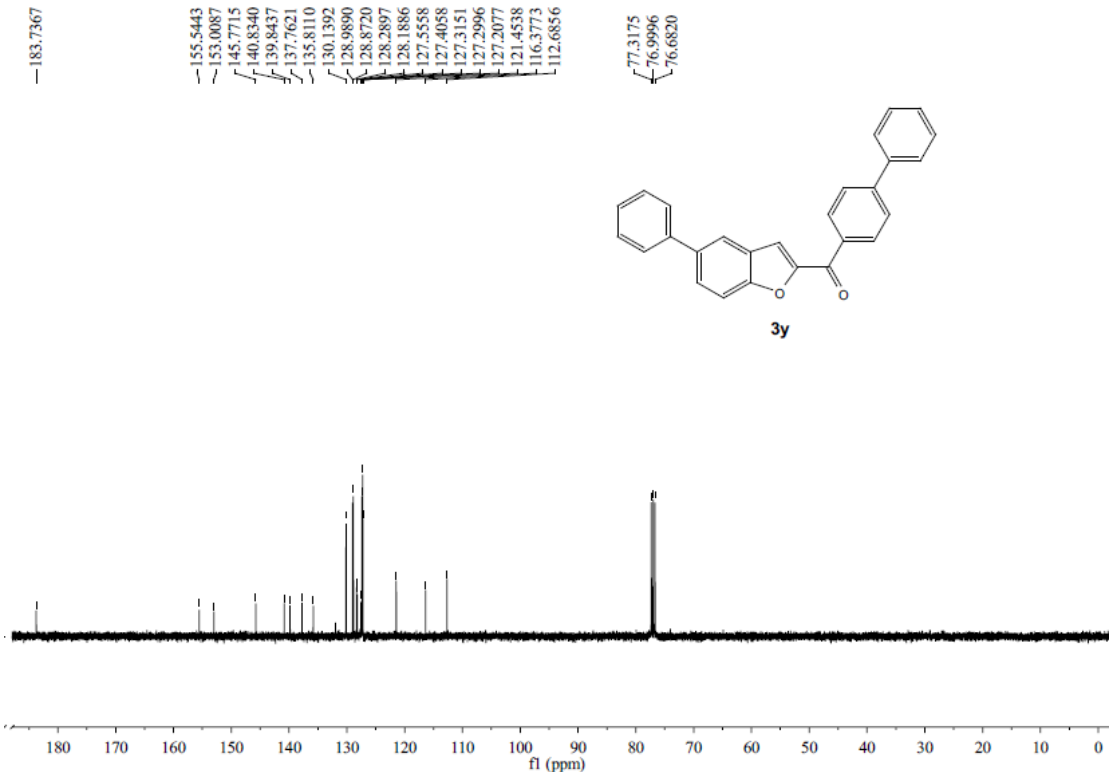
7.6189
7.5235
7.5053
7.4860
7.4778
7.4582
7.4472
7.4288
7.3986
7.3803
7.2573
1.5548
0.0003
3y
2.00
1.00
2.03
0.97
2.00
3.06
6.95
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.7621
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128.8720
128.2897
128.1886
127.5558
127.4058
127.3151
127.2996
127.2077
121.4538
116.3773
112.6856
77.3175
76.9996
76.6820
3y
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)