Supplementary Information

Metal-free radical C-H methylation of pyrimidinones and pyridinones with dicumyl peroxide

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1. General information

All reactions were performed in air. ^{1}H NMR (400 MHz or 300 MHz) and ^{13}C NMR (75 MHz or 101 MHz) spectra were determined on a Varian-Inova 300 MHz or 400 MHz spectrometer with $CDCl_3$ or DMSO-d_6 as solvent and tetramethylsilane (TMS) as internal standard. Chemical shifts were reported in parts per million (ppm) from internal TMS (δ), all coupling constants (J values) were reported in Hertz (Hz). High-resolution mass spectra were recorded on a TOF machine (CI and ESI). Column chromatography was performed with 300-400 mesh silica gel using flash column techniques. All of the reagents were obtained from commercial sources and used without further purification unless otherwise noted.

2. Experimental procedures

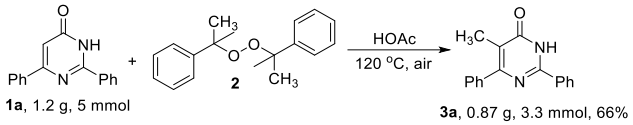
General procedure for the preparation of 5-methylpyrimidin-4-ones (3) and 3-methylpyridin-2-ones (5). To 1 mmol of pyrimidin-4-ones (**1**) or pyridin-2-ones (**4**) in 2 mL of acetic acid was added dicumyl peroxide (DCP, **2**) (0.81 g, 3 mmol). The mixture was stirred at 120 °C in air for 5 h. After the completion of the reaction (monitored by TLC), water (10 mL) was added, followed by extraction with ethyl acetate (10 mL × 3). The combined organic fractions were washed with aqueous saturated $NaHCO_3$ solution (15 mL × 3) and water (15 mL × 2), dried over anhydrous Na_2SO_4, and concentrated under vacuum to give the crude product, which was purified by flash column chromatography (silica gel, petroleum ether/ethyl acetate = 10:1) to give the corresponding products **3** or **5**.

Typical procedure for the preparation of 2,6-diphenyl-5-methylpyrimidinone (3a). To a solution of 2,6-diphenylpyrimidin-4-one (**1a**) (0.25 g, 1 mmol) in acetic acid (2 mL), dicumyl peroxide (DCP, **2**) (0.81 g, 3 mmol) was added. The mixture was stirred at 120 °C in air for 5 hours, after the completion of the reaction, water (10 mL) was added, extracted with ethyl acetate (10 mL × 3). The combined organic fractions were washed with aqueous saturated $NaHCO_3$ solution (15 mL × 3) and water (15 mL × 2), dried over anhydrous Na_2SO_4, and concentrated

under vacuum to give the crude product, which was purified by flash column chromatography (silica gel, petroleum ether/ethyl acetate = 10:1) to give 2,6-diphenyl-5-methyl pyrimidinone (**3a**) (191 mg, 73% yield).

Procedure for scale-up preparation of 2,6-diphenyl-5-methylpyrimidinone (3a)

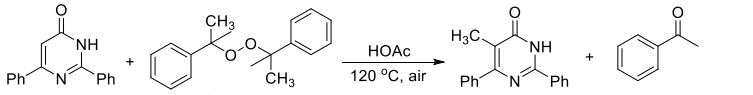
Procedure for 1 gram-scale preparation of 3a



1a, 1.2 g, 5 mmol　　**2**　　**3a**, 0.87 g, 3.3 mmol, 66%

To 2,6-diphenylpyrimidin-4-one (**1a**) (1.2 g, 5 mmol) in acetic acid (10 mL) was added DCP (**2**) (4.05 g, 15 mmol). The mixture was stirred at 120 °C in air for 5 hours. After the completion of the reaction (monitored by TLC), water (30 mL) was added, followed by extraction with ethyl acetate (20 mL × 3). The combined organic fractions were washed with aqueous saturated $NaHCO_3$ solution (30 mL × 3) and water (30 mL × 2), dried over anhydrous Na_2SO_4, and concentrated under vacuum to give the crude product, which was purified by flash column chromatography (silica gel, petroleum ether/ethyl acetate = 10:1) to give 2,6-diphenyl-5-methyl pyrimidinone (**3a**) (0.87 g, 66% yield).

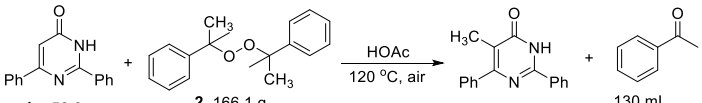
Procedure for 10 gram-scale preparation of 3a



1a, 10.0 g, 40 mmol　　**2**, 33.2 g, 123 mmol　　**3a**, 7.5 g, 28.4 mmol, 71%　　20.6 g, 172 mmol

To 2,6-diphenylpyrimidin-4-one (**1a**) (10.0 g, 40 mmol) in acetic acid (80 mL) was added DCP (**2**) (33.2 g, 123 mmol) in portions. The mixture was stirred at 120 °C under air. After the completion of reaction (monitored by TLC), acetic acid and acetophenone by-product were recovered by distillation under reduced pressure leaving behind a residue. To the residue was added water (50 mL), followed by extraction with ethyl acetate (25 mL × 4). The combined organic fractions were washed with aqueous saturated $NaHCO_3$ solution (50 mL × 2) and water (60 mL), dried over anhydrous Na_2SO_4, and concentrated under vacuum to give the crude product, which was recrystallized from ethyl acetate to afford the pure compound **3a** (7.5 g, 71% yield).

Procedure for 50 gram-scale preparation of 3a

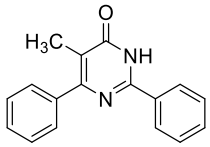


1a, 50.9 g, 205 mmol　　**2**, 166.1 g, 615 mmol　　**3a**, 37.7 g, 144 mmol, 70% yield　　130 mL

To 2,6-diphenylpyrimidin-4-one (**1a**) (50.9 g, 205 mmol) in acetic acid (400 mL) was added DCP (**2**) (166.1 g, 615 mmol) in batches. The mixture was stirred at 120 °C under air. After the completion of reaction (monitored by TLC), acetic acid (390 mL) and acetophenone by-product (130 mL, 133.9 g, 1.12 mol) were recovered by distillation under reduced pressure leaving behind a residue. To the residue was added water (200 mL), followed by extraction with ethyl acetate (100 mL × 4). The combined organic fractions were washed with aqueous saturated $NaHCO_3$ solution (200 mL × 2) and water (200 mL), dried over anhydrous Na_2SO_4, and concentrated under vacuum to give the crude product, which was recrystallized from ethyl acetate to afford the pure compound **3a** (37.7 g, 70% yield).

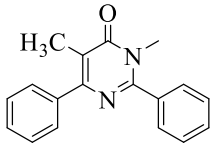
3. NMR and MS spectral data

*5-Methyl-2,6-diphenylpyrimidin-4(3H)-one (**3a**)*



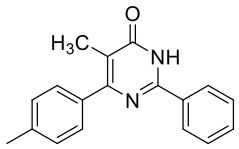
Colorless solid, mp 258−260 °C, 73% yield (191 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.85 (s, 1H), 8.17 (d, J = 7.1 Hz, 2H), 7.68 (d, J = 6.6 Hz, 2H), 7.53 (dd, J = 14.3, 6.8 Hz, 6H), 2.10 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.15, 152.97, 138.68, 132.26, 131.62, 129.11, 129.02, 128.86, 128.15, 127.45, 119.09, 12.65. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{17}H_{15}N_2O$ 263.1184, found 263.1194.

3,5-Dimethyl-2,6-diphenylpyrimidin-4(3H)-one (3a')



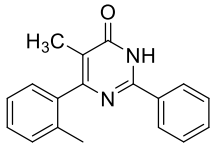
Colorless solid, mp 128−130 °C, 87% yield (240 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 – 7.51 (m, 4H), 7.50 – 7.45 (m, 3H), 7.44 – 7.36 (m, 3H), 3.50 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 163.78, 157.60, 156.37, 137.99, 134.58, 129.61, 128.51, 128.31, 128.23, 127.83, 127.69, 118.29, 34.14, 13.09. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{17}N_2O$ 277.1341, found 277.1330.

*5-Methyl-2-phenyl-6-(p-tolyl)pyrimidin-4(3H)-one (**3b**)*



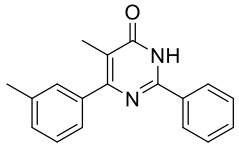
Colorless solid, mp 238−239 °C, 96% yield (265 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.69 (s, 1H), 8.17 (d, J = 7.2 Hz, 2H), 7.64 – 7.46 (m, 3H), 7.34 (d, J = 7.6 Hz, 2H), 7.28 – 7.20 (m, 1H), 7.09 – 6.98 (m, 1H), 2.41 (s, 3H), 2.10 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.76, 160.65, 152.48, 138.58, 135.43, 131.90, 131.03, 128.64, 128.35, 128.29, 127.10, 118.20, 20.92, 12.36. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{17}N_2O$ 277.1341, found 277.1350.

*5-Methyl-2-phenyl-6-(o-tolyl)pyrimidin-4(3H)-one (**3c**)*



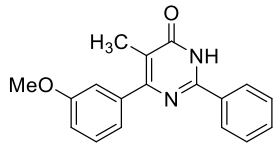
Colorless solid, mp 197−199 °C, 82% yield (226 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 13.11 (s, 1H), 8.30 – 8.10 (m, 2H), 7.42 (d, J = 6.9 Hz, 3H), 7.28 – 6.15 (m, 4H), 2.20 (s, 3H), 1.92 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.45, 162.46, 152.78, 137.93, 134.97, 131.80, 131.11, 129.98, 128.33, 128.09, 127.77, 127.18, 125.28, 119.73, 19.12, 11.62. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{17}N_2O$ 277.1341, found 277.1354.

5-Methyl-2-phenyl-6-(m-tolyl)pyrimidin-4(3H)-one ***(3d)***



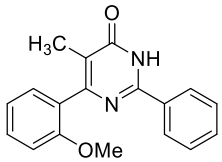
Colorless solid, mp 194−196 °C, 87% yield (226 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 13.21 (s, 1H), 8.35 (dd, J = 7.3, 2.0 Hz, 2H), 7.71 – 7.43 (m, 5H), 7.38 (t, J = 7.6 Hz, 1H), 7.27 (d, J = 7.4 Hz, 1H), 2.46 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.81, 161.02, 152.62, 138.21, 137.40, 131.86, 131.08, 129.28, 129.17, 128.32, 127.54, 127.16, 125.72, 118.48, 21.07, 12.32. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{17}N_2O$ 277.1341, found 277.1340.

6-(3-Methoxyphenyl)-5-methyl-2-phenylpyrimidin-4(3H)-one ***(3e)***



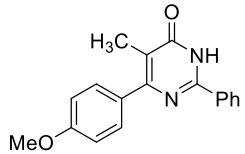
Colorless solid, mp 227−229 °C, 90% yield (263 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.74 (s, 1H), 8.44 – 7.96 (m, 2H), 7.61 – 7.51 (m, 3H), 7.44 (t, J = 7.9 Hz, 1H), 7.27 – 7.16 (m, 2H), 7.07 (ddd, J = 8.3, 2.6, 0.8 Hz, 1H), 3.84 (s, 3H), 2.09 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 158.92, 139.93, 132.56, 131.29, 129.16, 128.58, 127.54, 121.14, 118.32, 114.42, 114.24, 55.17, 12.64. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{17}N_2O_2$ 293.1290, found 293.1293.

6-(2-Methoxyphenyl)-2-phenylpyrimidin-4(3H)-one ***(3f)***



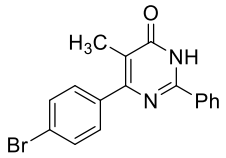
Colorless solid, mp 183−184 °C, 66% yield (193 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.73 (s, 1H), 8.11 (d, J = 7.2 Hz, 2H), 7.62 – 7.42 (m, 4H), 7.35 (dd, J = 7.4, 1.6 Hz, 1H), 7.17 (d, J = 8.3 Hz, 1H), 7.09 (t, J = 7.4 Hz, 1H), 3.81 (s, 2H), 1.82 (s, 2H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 156.30, 131.68, 130.54, 130.19, 129.61, 129.03, 128.19, 127.98, 120.83, 111.86, 55.86, 12.67. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{17}N_2O_2$ 293.1290, found 293.1291.

6-(4-Methoxyphenyl)-5-methyl-2-phenylpyrimidin-4(3H)-one ***(3g)***



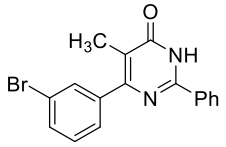
Colorless solid, mp 220−221 °C, 74% yield (216 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.91 (s, 1H), 8.31 (dd, J = 7.5, 2.0 Hz, 2H), 7.73 – 7.64 (m, 2H), 7.58 – 7.49 (m, 3H), 7.04 – 6.97 (m, 2H), 3.88 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.25, 160.70, 160.28, 152.79, 132.35, 131.53, 131.10, 130.79, 128.80, 127.51, 118.16, 113.52, 55.39, 12.95. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{17}N_2O_2$ 293.1290, found 293.1293.

6-(4-Bromophenyl)-5-methyl-2-phenylpyrimidin-4(3H)-one ***(3h)***



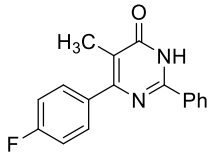
Colorless solid, mp 202−203 °C, 75% yield (255 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 13.11 (s, 1H), 8.32 (dd, J = 7.7, 1.7 Hz, 2H), 7.91 – 7.78 (m, 1H), 7.66 – 7.48 (m, 5H), 7.37 (d, J = 7.9 Hz, 1H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.52, 159.12, 152.89, 140.20, 131.59, 131.57, 131.53, 131.30, 129.19, 128.40, 127.24, 127.10, 121.88, 119.02, 12.22. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{17}H_{14}BrN_2O$ 341.0290, found 341.0299.

*6-(3-Bromophenyl)-5-methyl-2-phenylpyrimidin-4(3H)-one (**3i**)*



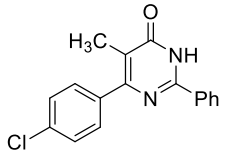
Colorless solid, mp 205−206 °C, 76% yield (258 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.55 (s, 1H), 8.27 (dd, J = 7.8, 1.7 Hz, 2H), 7.83 (t, J = 1.7 Hz, 1H), 7.56 (dt, J = 14.1, 5.5 Hz, 5H), 7.36 (t, J = 7.9 Hz, 1H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.71, 159.53, 153.26, 140.64, 132.06, 132.02, 132.01, 131.81, 129.67, 128.93, 127.71, 127.44, 122.36, 119.57, 12.73. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{17}H_{14}BrN_2O$ 341.0290, found 341.0281.

*6-(4-Fluorophenyl)-5-methyl-2-phenylpyrimidin-4(3H)-one (**3j**)*



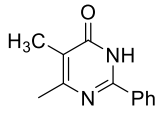
Colorless solid, mp 258−260 °C, 76% yield (213 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.93 (s, 1H), 8.30 (dd, J = 7.7, 1.8 Hz, 2H), 7.73 – 7.65 (m, 2H), 7.54 (t, J = 5.8 Hz, 3H), 7.18 (t, J = 8.7 Hz, 2H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.55, 163.90, 161.42, 159.60, 152.61, 134.20, 131.68, 131.23, 130.67 (d, J = 8 Hz), 128.40, 127.00, 118.45, 114.70 (d, J = 21 Hz), 12.34. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{17}H_{14}FN_2O$ 281.1090, found 281.1099.

*6-(4-Chlorophenyl)-5-methyl-2-phenylpyrimidin-4(3H)-one (**3k**)*



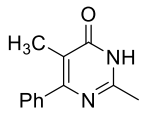
Colorless solid, mp 264−267 °C, 75% yield (222 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.66 (s, 1H), 8.26 (dd, J = 7.9, 1.6 Hz, 2H), 7.62 (d, J = 8.5 Hz, 2H), 7.52 (dt, J = 8.8, 4.4 Hz, 3H), 7.46 (d, J = 8.5 Hz, 2H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.83, 159.93, 153.12, 137.03, 135.14, 132.06, 131.78, 130.54, 128.92, 128.42, 127.39, 119.20, 12.78. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{17}H_{14}ClN_2O$ 297.0795, found 297.0794.

*5,6-Dimethyl-2-phenylpyrimidin-4(3H)-one (**3l**)*



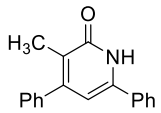
Colorless solid, mp 167−168 °C, 65% yield (130 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 13.28 (s, 1H), 8.30 – 8.20 (m, 2H), 7.50 (dd, J = 5.3, 1.8 Hz, 3H), 2.40 (s, 3H), 2.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 164.83, 161.13, 152.52, 131.87, 130.91, 128.28, 127.08, 118.12, 21.69, 10.40. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{12}H_{13}N_2O$ 201.1028, found 201.1035.

*2,5-Dimethyl-6-phenylpyrimidin-4(3H)-one (**3m**)*



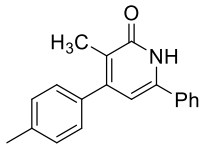
Colorless solid, mp 165−167 °C, 63% yield (126 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 13.19 (s, 1H), 7.60 – 7.40 (m, 5H), 2.54 (d, J = 3.5 Hz, 3H), 2.14 (d, J = 3.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.32, 161.61, 155.03, 138.50, 128.91, 128.71, 128.27, 117.94, 21.63, 12.46. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{12}H_{13}N_2O$ 201.1028, found 201.1034.

*3-Methyl-4,6-diphenylpyridin-2(1H)-one (**5a**)*



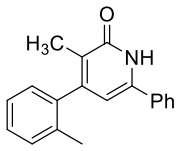
Colorless solid, mp 220−222 °C, 74% yield (193 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.38 (s, 1H), 7.73 (m, 2H), 7.45 – 7.28 (m, 8H), 6.42 (s, 1H), 2.04 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.05, 151.10, 141.95, 139.34, 133.05, 129.16, 128.54, 127.95, 127.80, 127.57, 126.02, 123.87, 106.93, 13.11. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{16}NO$ 262.1232, found 262.1236.

*3-Methyl-6-phenyl-4-(p-tolyl)pyridin-2(1H)-one (**5b**)*



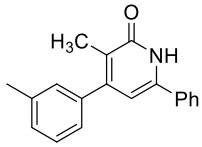
Colorless solid, mp 241−244 °C, 67% yield (179 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.40 (s, 1H), 7.52 – 7.30 (m, 9H), 6.24 (s, 1H), 2.47 (s, 3H), 2.11 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 164.33, 150.51, 142.13, 139.20, 135.59, 133.71, 130.41, 128.95, 128.86, 127.89, 127.86, 127.53, 125.62, 123.65, 109.07, 19.72, 13.08. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{19}H_{18}NO$ 276.1388, found 276.1395.

*3-Methyl-6-phenyl-4-(o-tolyl)pyridin-2(1H)-one (**5c**)*



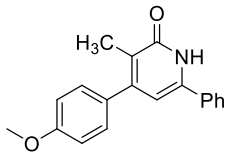
Colorless solid, mp 181−182 °C, 55% yield (151 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.40 (s, 1H), 7.61 – 7.26 (m, 9H), 6.24 (s, 1H), 2.47 (s, 3H), 2.11 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 164.33, 150.51, 142.13, 139.20, 135.59, 133.71, 130.41, 128.95, 128.86, 127.89, 127.86, 127.53, 125.62, 123.65, 109.07, 19.72, 13.08. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{19}H_{18}NO$ 276.1388, found 276.1393.

*3-Methyl-6-phenyl-4-(m-tolyl)pyridin-2(1H)-one (**5d**)*



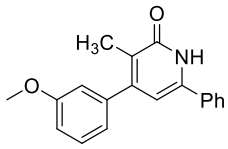
Colorless solid, mp 194−196 °C, 51% yield (140 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.29 (s, 1H), 7.60 (s, 1H), 7.54 – 7.34 (m, 7H), 7.24 (s, 1H), 6.48 (s, 1H), 2.43 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 151.44, 142.20, 139.84, 138.96, 133.50, 130.45, 129.00, 128.40, 128.27, 128.02, 126.90, 123.30, 107.07, 21.46, 13.69. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{19}H_{18}NO$ 276.1388, found 276.1399.

*4-(4-Methoxyphenyl)-3-methyl-6-phenylpyridin-2(1H)-one (**5e**)*



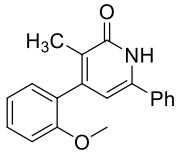
Colorless solid, mp 231−233 °C, 79% yield (230 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.23 (s, 1H), 7.76 (d, J = 8.8 Hz, 2H), 7.54 – 7.32 (m, 5H), 6.98 (d, J = 8.8 Hz, 2H), 6.43 (s, 1H), 3.84 (s, 3H), 2.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.51, 160.78, 151.64, 142.32, 139.99, 128.38, 128.27, 127.96, 127.88, 126.04, 123.29, 114.38, 106.46, 55.41, 13.56. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{19}H_{18}NO_2$ 292.1338, found 292.1346.

*4-(3-Methoxyphenyl)-3-methyl-6-phenylpyridin-2(1H)-one (**5f**)*



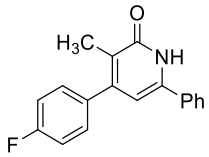
Colorless solid, mp 213−215 °C, 61% yield (178 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.84 (s, 1H), 7.60 – 7.18 (m, 8H), 6.97 (dd, J = 7.9, 1.2 Hz, 1H), 6.49 (s, 1H), 3.90 (s, 3H), 2.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.31, 160.14, 151.41, 142.20, 139.80, 134.96, 130.08, 128.41, 128.28, 128.04, 124.58, 118.74, 115.77, 111.58, 107.38, 55.52, 13.72. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{19}H_{18}NO_2$ 292.1338, found 292.1342.

*4-(2-Methoxyphenyl)-3-methyl-6-phenylpyridin-2(1H)-one (**5g**)*



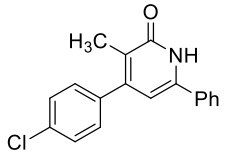
Colorless solid, mp 175−177 °C, 61% yield (178 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.22 (s, 1H), 7.55 – 7.30 (m, 7H), 7.03 (t, J = 7.5 Hz, 2H), 6.41 (s, 1H), 3.93 (s, 3H), 2.11 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 163.16, 155.97, 150.72, 139.72, 139.34, 130.73, 129.04, 127.90, 127.80, 127.50, 124.09, 120.99, 120.95, 111.22, 107.73, 55.32, 13.35. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{19}H_{18}NO_2$ 292.1338, found 292.1343.

*4-(4-Fluorophenyl)-3-methyl-6-phenylpyridin-2(1H)-one (**5h**)*



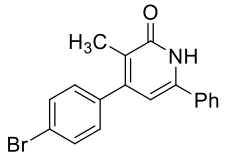
Colorless solid, mp 233−235 °C, 35% yield (119 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.22 (s, 1H), 7.90 – 7.70 (m, 2H), 7.49 – 7.33 (m, 5H), 7.16 (t, J = 8.5 Hz, 2H), 6.45 (s, 1H), 2.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 164.85, 162.37, 151.60, 141.50, 139.69, 129.82, 128.53 (d, J = 9 Hz), 128.45, 128.23, 128.11, 116.07 (d, J = 22 Hz), 107.30, 13.56. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{15}FNO$ 280.1138, found 280.1149.

*4-(4-Chlorophenyl)-3-methyl-6-phenylpyridin-2(1H)-one (**5i**)*



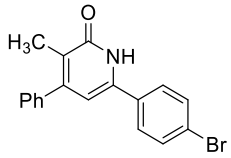
Colorless solid, mp 252−253 °C, 62% yield (183 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.90 (s, 1H), 7.72 (d, J = 8.5 Hz, 2H), 7.42 (ddd, J = 24.7, 16.7, 7.4 Hz, 7H), 6.41 (s, 1H), 2.06 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 151.54, 141.23, 139.59, 135.77, 132.01, 129.26, 128.47, 128.23, 128.15, 127.76, 124.79, 107.52, 13.63. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{15}ClNO$ 296.0842, found 296.0840.

*4-(4-Bromophenyl)-3-methyl-6-phenylpyridin-2(1H)-one (**5j**)*



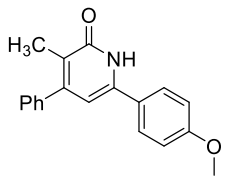
Colorless solid, mp 216−217 °C, 61% yield (170 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.15 (s, 1H), 7.67 (d, J = 8.0 Hz, 2H), 7.57 (d, J = 8.0 Hz, 2H), 7.50 – 7.40 (m, 3H), 7.36 (d, J = 6.8 Hz, 2H), 6.49 (s, 1H), 2.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.45, 150.58, 142.90, 138.98, 133.74, 132.00, 130.31, 130.16, 129.46, 126.70, 122.64, 107.09, 13.92. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{15}BrNO$ 340.0337, found 340.0329.

*6-(4-Bromophenyl)-3-methyl-4-phenylpyridin-2(1H)-one (**5k**)*



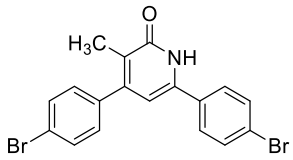
Colorless solid, mp 263−265 °C, 41% yield (139 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.79 (s, 1H), 7.85 – 7.76 (m, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.56 – 7.47 (m, 3H), 7.38 – 7.26 (m, 2H), 6.48 (s, 1H), 2.16 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 164.62, 149.75, 142.07, 138.15, 132.92, 131.17, 129.48, 129.33, 128.64, 125.87, 121.82, 106.27, 13.10. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{15}BrNO$ 340.0337, found 340.0341.

*6-(4-Methoxyphenyl)-3-methyl-4-phenylpyridin-2(1H)-one (**5l**)*



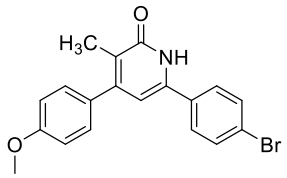
Colorless solid, mp 223−224 °C, 66% yield (192 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.77 (s, 1H), 7.78 (d, J = 5.9 Hz, 2H), 7.48 (d, J = 15.9 Hz, 5H), 7.04 (d, J = 5.4 Hz, 2H), 6.44 (s, 1H), 3.84 (s, 3H), 1.99 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 163.70, 160.19, 149.94, 142.76, 139.49, 128.37, 128.28, 128.02, 127.93, 125.96, 121.70, 114.11, 105.32, 55.28, 13.51. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{19}H_{18}NO_2$ 292.1338, found 292.1345.

*4,6-Bis(4-bromophenyl)-3-methylpyridin-2(1H)-one (**5m**)*



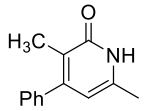
Colorless solid, mp 260−262 °C, 33% yield (138 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.60 (s, 1H), 7.53 – 7.49 (m, 5H), 7.30 – 7.28 (m, 1H), 7.21 – 7.10 (m, 2H), 6.30 (s, 1H), 2.02 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 164.78, 149.91, 142.23, 138.30, 133.07, 131.32, 129.63, 129.49, 128.79, 126.03, 121.97, 106.42, 13.25. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{18}H_{14}Br_2NO$ 419.9422, found 419.9427.

*6-(4-Bromophenyl)-4-(4-methoxyphenyl)-3-methylpyridin-2(1H)-one (**5n**)*



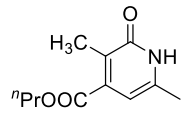
Colorless solid, mp 251−253 °C, 74% yield (273 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.79 (s, 1H), 7.78 (d, J = 7.1 Hz, 2H), 7.67 (d, J = 7.2 Hz, 2H), 7.41 (d, J = 7.2 Hz, 2H), 7.07 (d, J = 6.8 Hz, 2H), 6.58 (s, 1H), 3.84 (s, 3H), 2.03 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 163.61, 159.03, 149.55, 142.26, 133.34, 131.57, 131.31, 129.81, 128.70, 122.65, 122.28, 113.76, 107.33, 55.16, 13.65. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{19}H_{17}BrNO_2$ 370.0443, found 370.0445.

*3,6-Dimethyl-4-phenylpyridin-2(1H)-one (**5o**)*



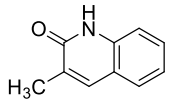
Colorless solid, mp 170−173 °C, 65% yield (129 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.67 (s, 1H), 7.50 – 7.30 (m, 5H), 5.91 (s, 1H), 2.19 (s, 3H), 1.89 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 168.35, 154.56, 145.81, 144.32, 133.05, 132.76, 132.52, 125.72, 110.82, 22.93, 18.04. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{13}H_{14}NO$ 200.1075, found 200.1080.

*Propyl 6-methyl-2-oxo-1,2-dihydropyridine-4-carboxylate (**5p**)*



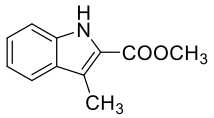
Colorless solid, mp 178−179 °C, 51% yield (107 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.88 (s, 1H), 6.14 (s, 1H), 4.23 (t, J = 6.6 Hz, 2H), 2.19 (s, 3H), 2.10 (s, 3H), 1.71 (dt, J = 11.4, 5.7 Hz, 2H), 0.97 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6): δ 166.65, 163.35, 142.40, 139.27, 125.31, 102.17, 66.57, 21.42, 18.21, 12.90, 10.34. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{11}H_{16}NO_3$ 210.1130, found 210.1125.

*3-Methylquinolin-2(1H)-one (**5q**)*



Colorless solid, mp 210−213 °C, 45% yield (72 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.10 (s, 1H), 7.65 (s, 1H), 7.52 – 7.39 (m, 3H), 7.22 – 7.15 (m, 1H), 2.31 (d, J = 0.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 164.70, 137.52, 137.49, 130.02, 129.27, 126.83, 122.43, 120.33, 115.68, 16.85. HRMS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{10}H_{10}NO$ 160.0762, found 160.0757.

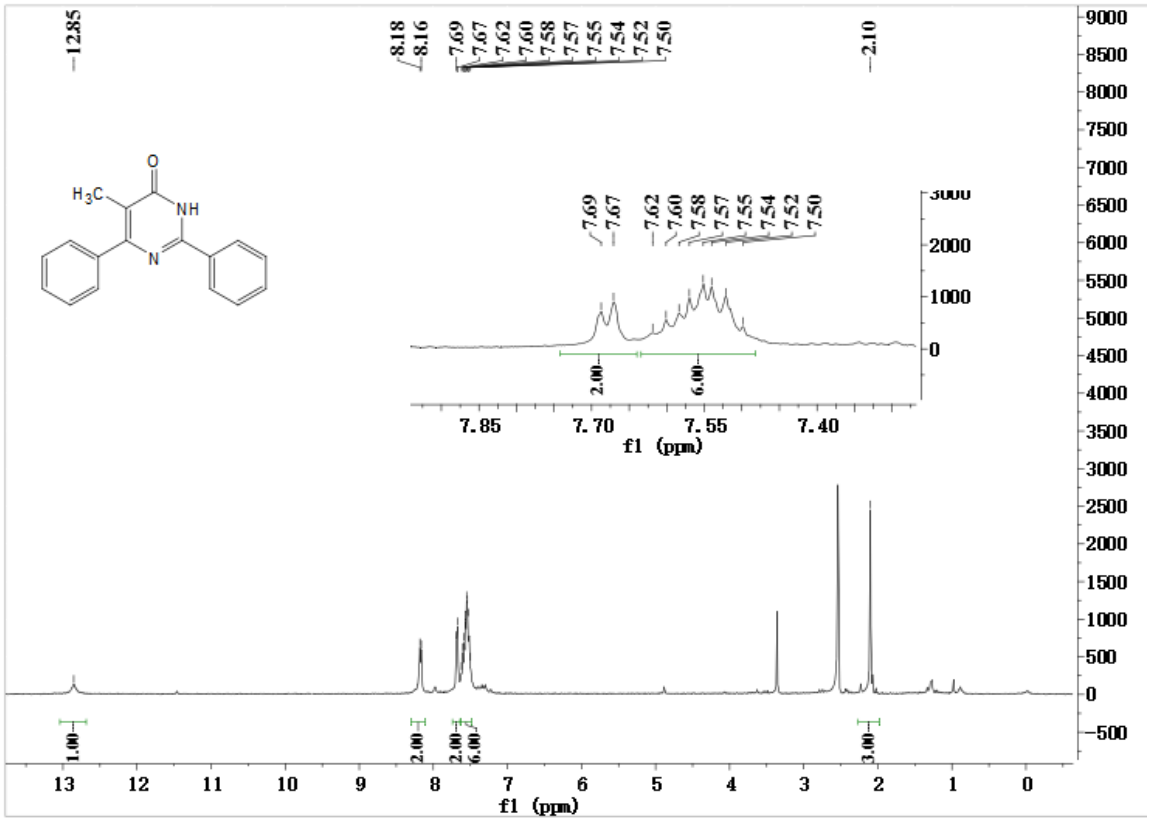
*Methyl 3-methyl-1H-indole-2-carboxylate (**5r**)*

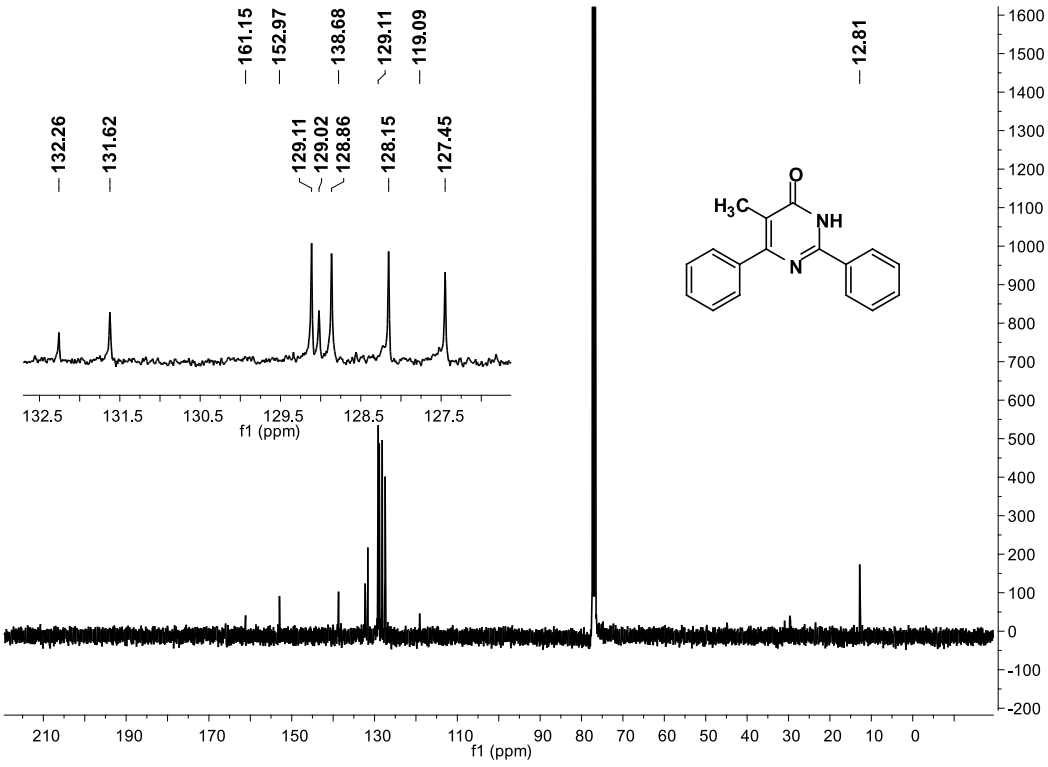


Colorless solid, mp 146−148 °C, 22% yield (42 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.51 (s, 1H), 7.71 (d, J = 8.1 Hz, 1H), 7.43 (dd, J = 15.8, 8.7 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 7.17 (t, J = 7.4 Hz, 1H), 3.97 (s, 3H), 1.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.32, 136.62, 127.00, 126.62, 124.95, 122.17, 120.34, 111.56, 108.40, 51.61, 29.27. MS (ESI-TOF) *m/z*: $(M+H)^+$ Calcd for $C_{11}H_{12}NO_2$ 190.1, found 190.1.

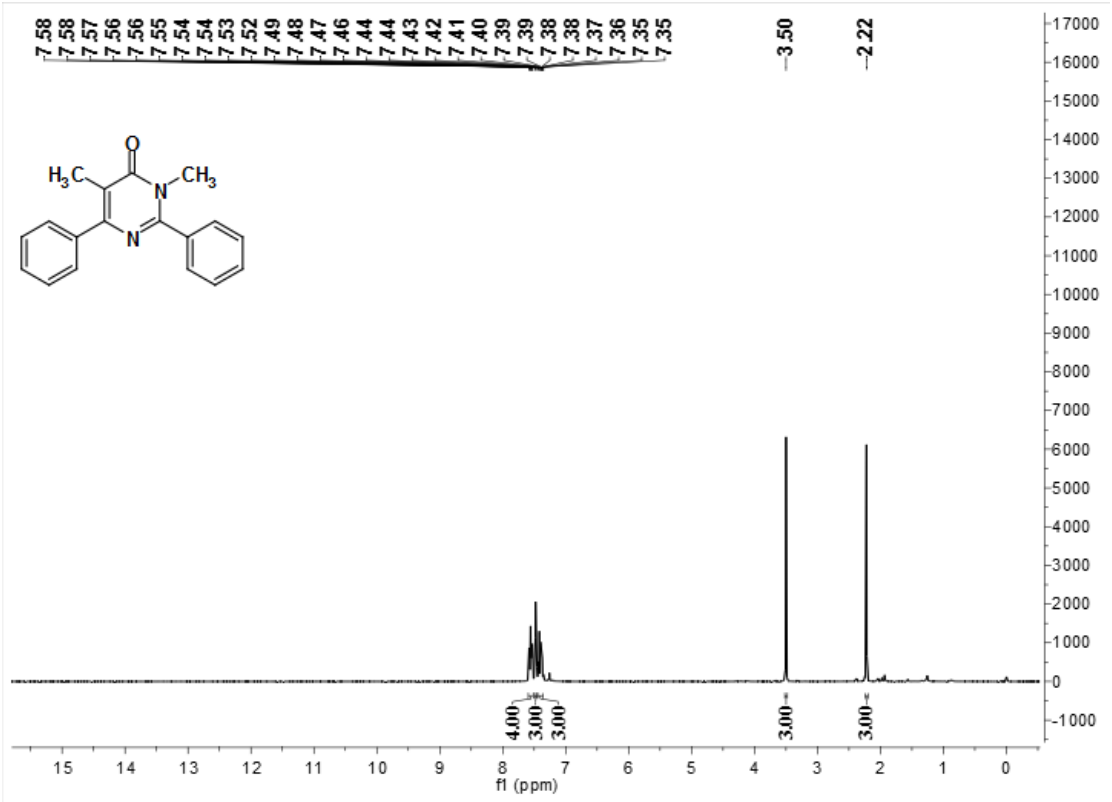
4. NMR spectra

Compound **3a**





Compound **3a'**


7.58
7.58
7.57
7.56
7.56
7.55
7.54
7.54
7.53
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7.49
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7.46
7.44
7.44
7.43
7.42
7.41
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7.39
7.38
7.38
7.37
7.36
7.35
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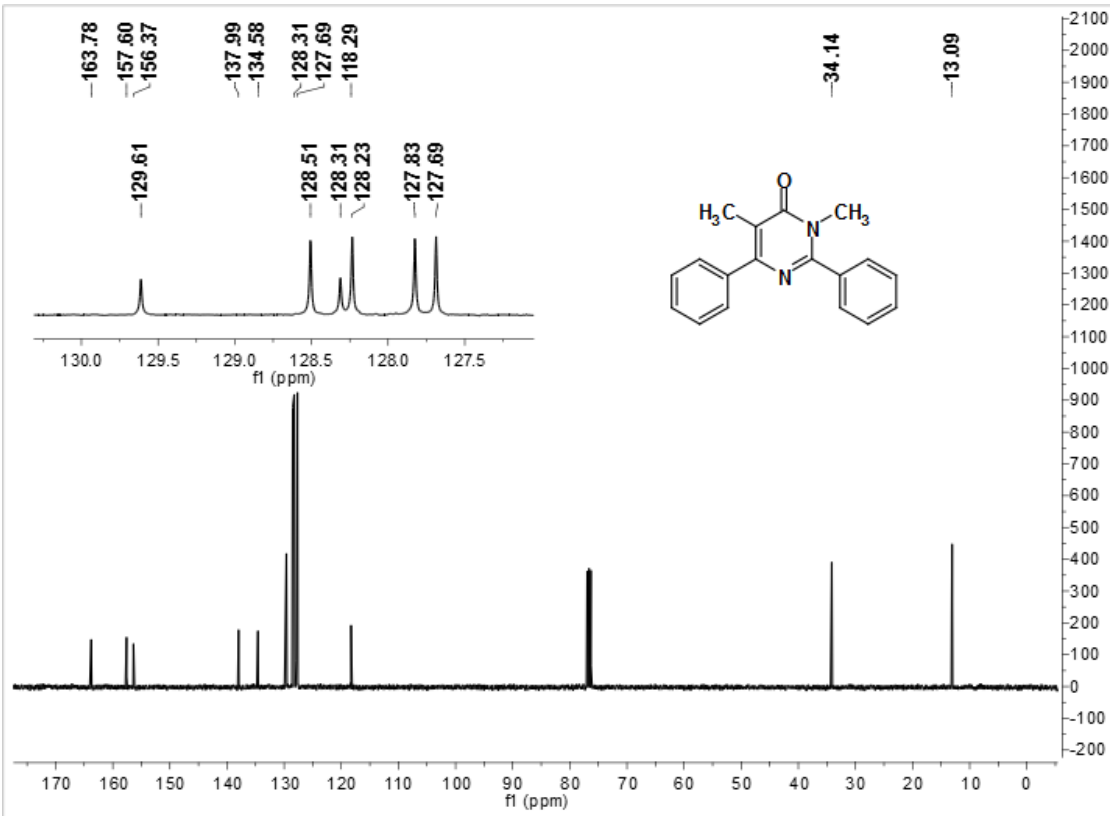
3.00
3.00
3.00
3.00
f1 (ppm)


163.78
157.60
156.37
137.99
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127.69
118.29
34.14
13.09
129.61
128.51
128.31
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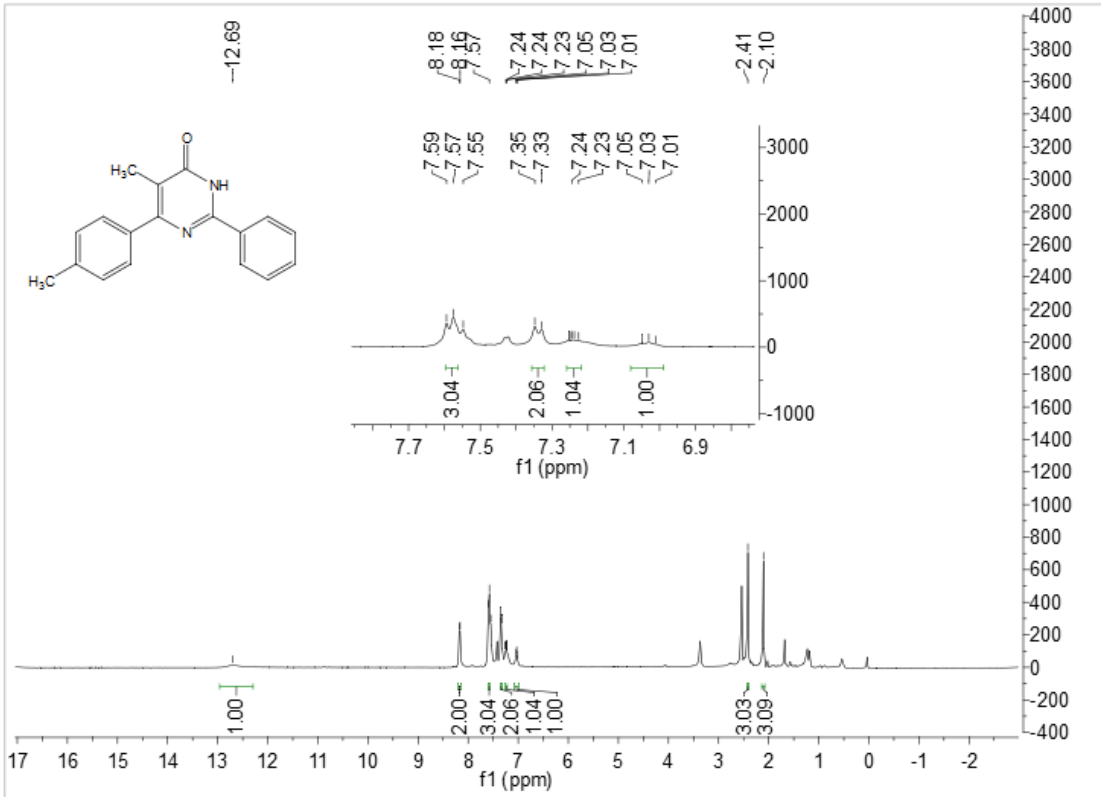
127.83
127.69
H3C
CH3
O
N
N
f1 (ppm)
f1 (ppm)

Compound **3b**


12.69
8.18
8.16
7.57
7.24
7.24
7.23
7.05
7.03
7.01
2.41
2.10
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7.57
7.55
7.35
7.33
7.24
7.23
7.05
7.03
7.01
3.04
2.06
1.04
1.00
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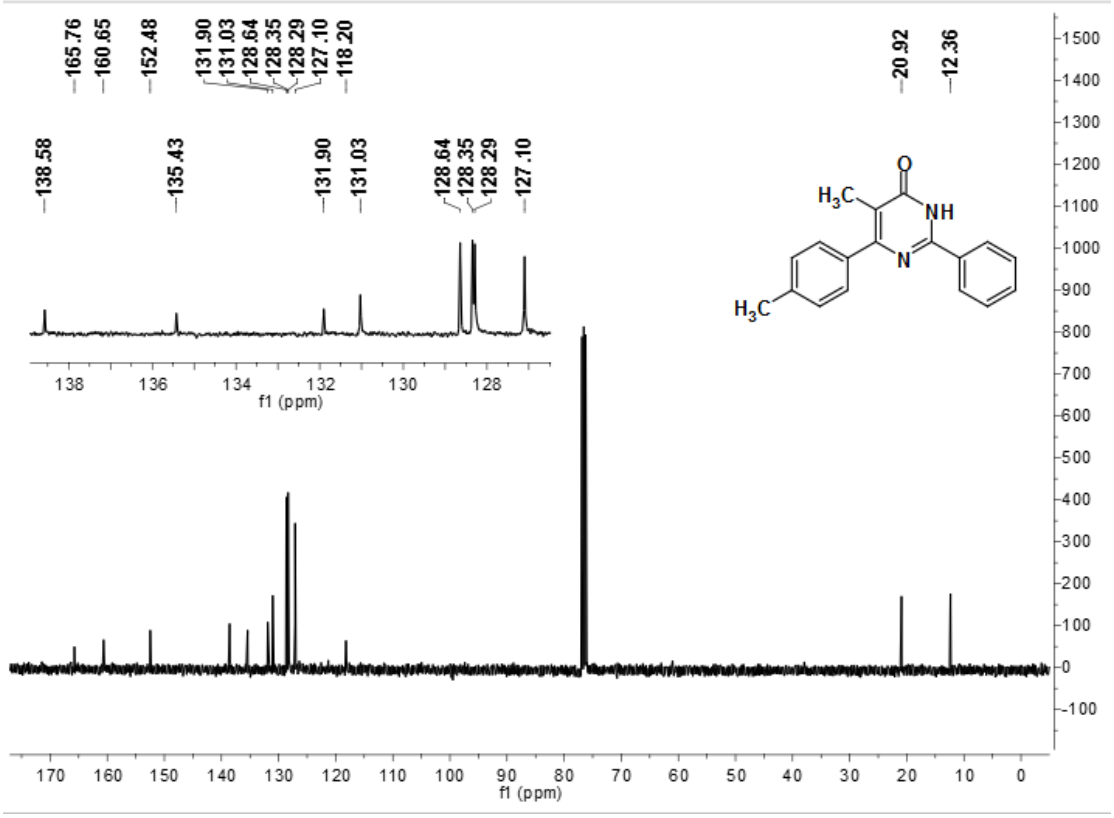
2.00
3.04
2.06
1.04
1.00
3.03
3.09
f1 (ppm)


165.76
160.65
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131.90
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128.29
127.10
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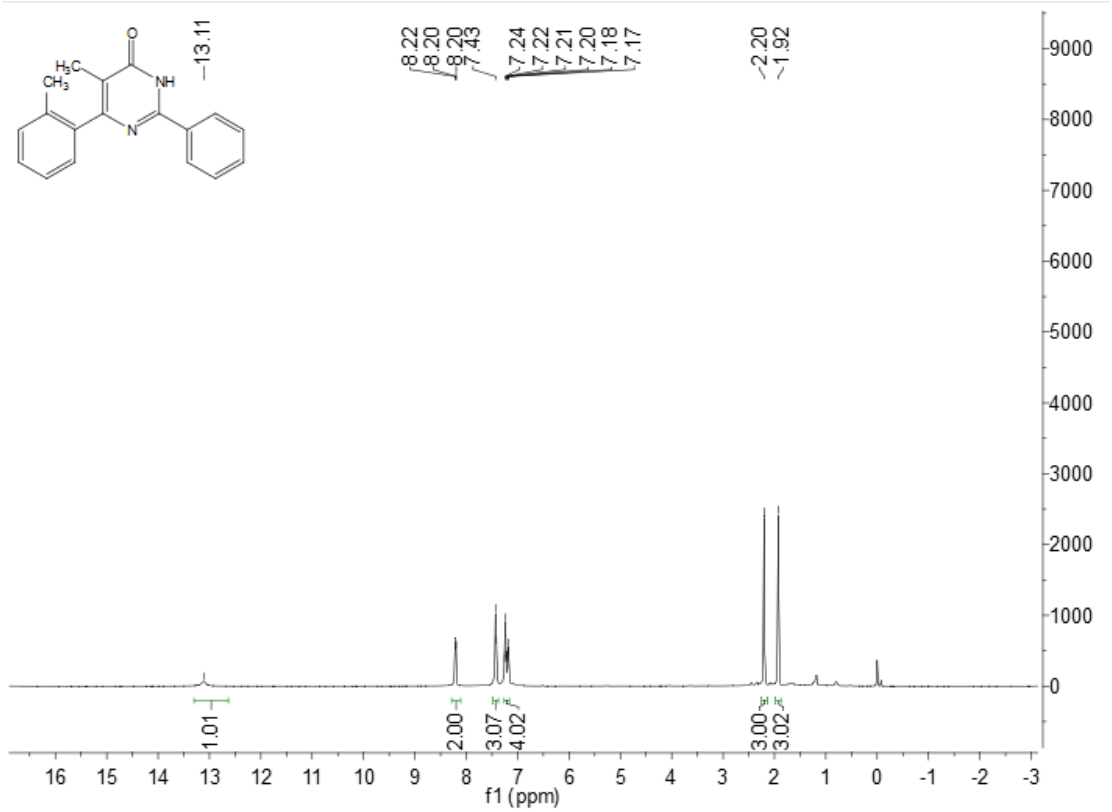
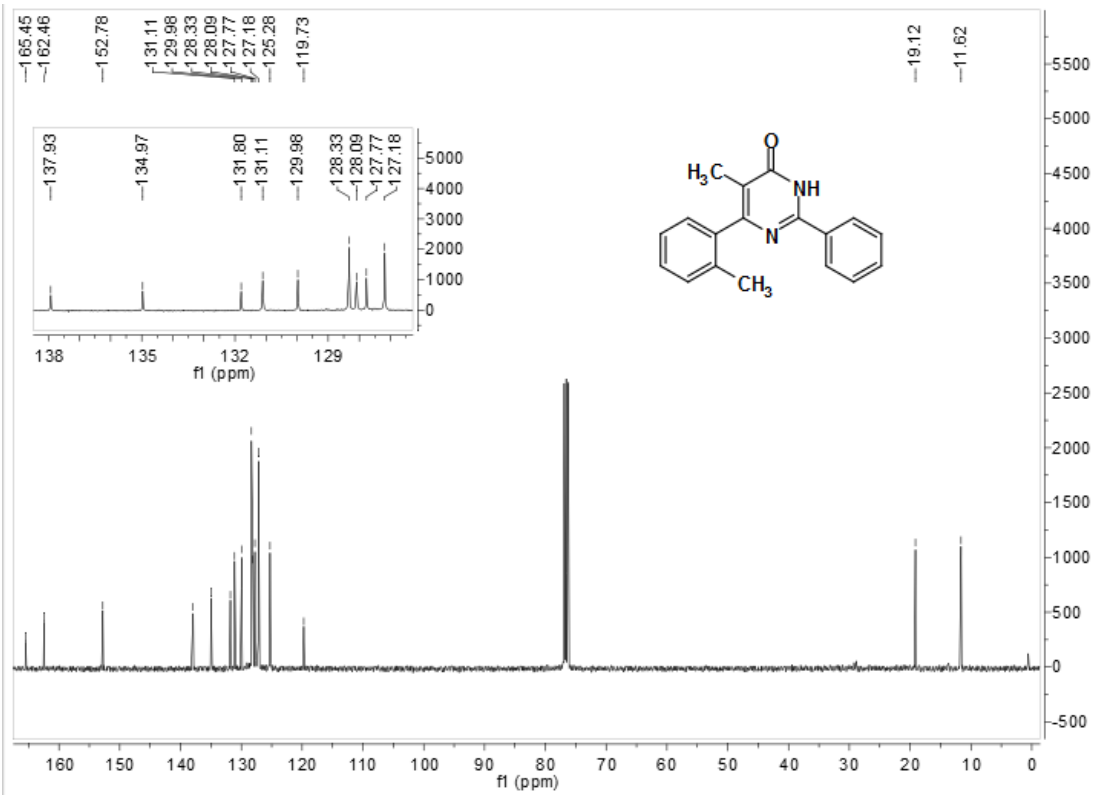
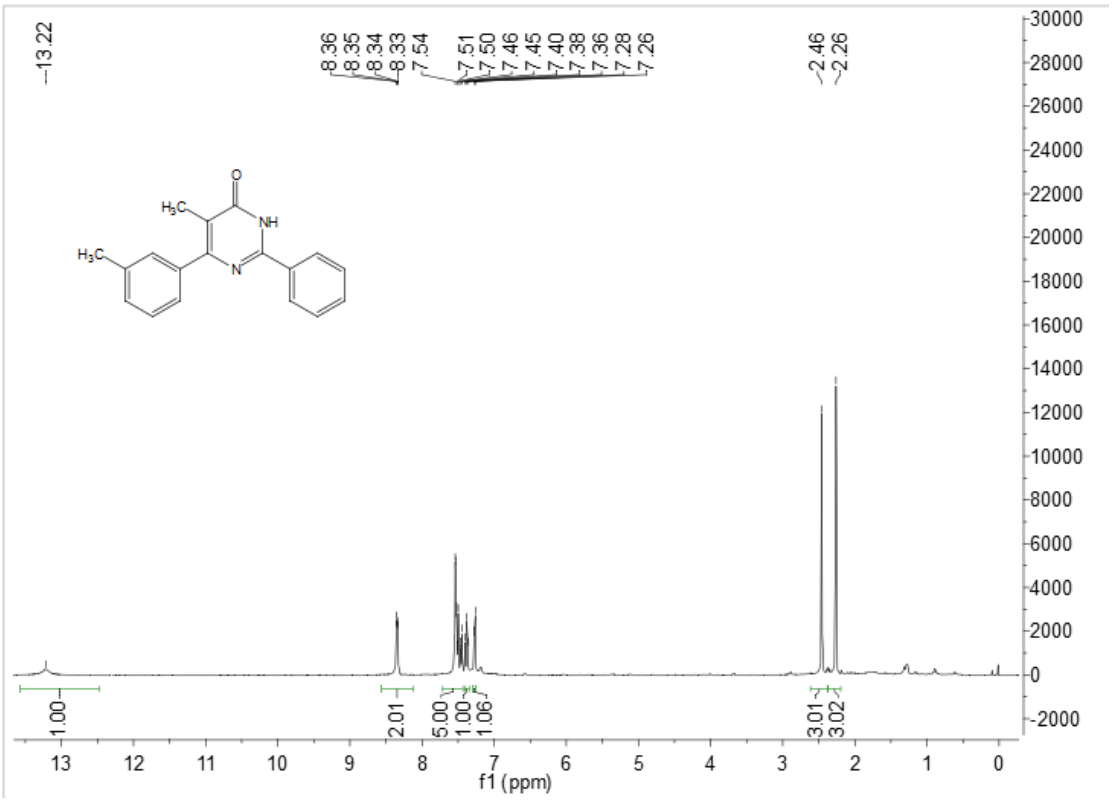
138.58
135.43
131.90
131.03
128.64
128.35
128.29
127.10
20.92
12.36
f1 (ppm)
f1 (ppm)

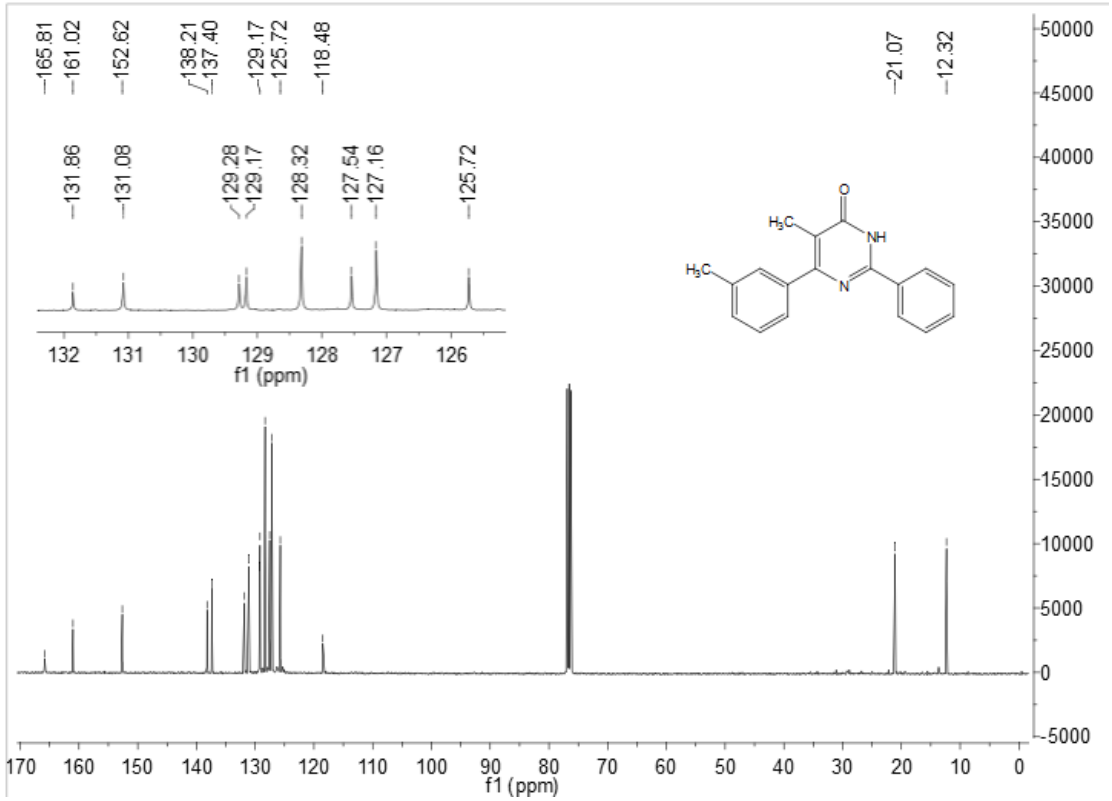
Compound **3c**


13.11
8.22
8.20
8.20
7.43
7.24
7.22
7.21
7.20
7.18
7.17
2.20
1.92
1.01
2.00
3.07
4.02
3.00
3.02
f1 (ppm)

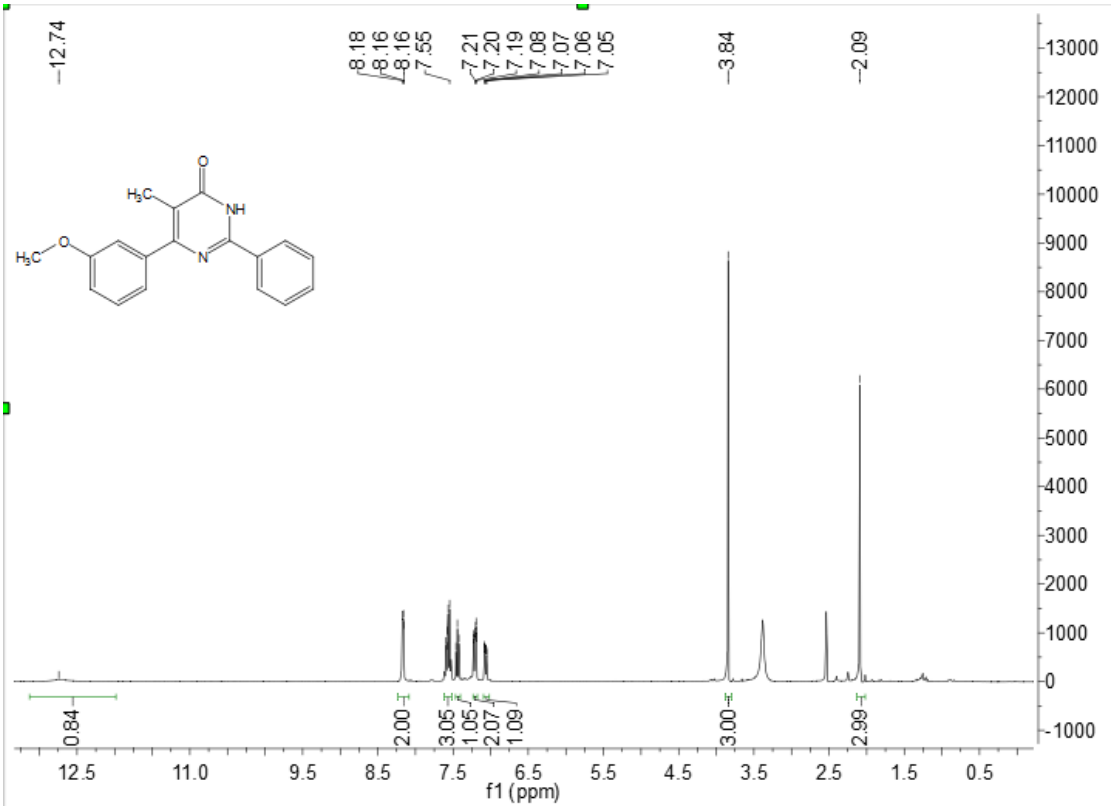

165.45
162.46
152.78
131.11
129.98
128.33
128.09
127.77
127.18
125.28
119.73
19.12
11.62
137.93
134.97
131.80
131.11
129.98
128.33
128.09
127.77
127.18
f1 (ppm)
f1 (ppm)

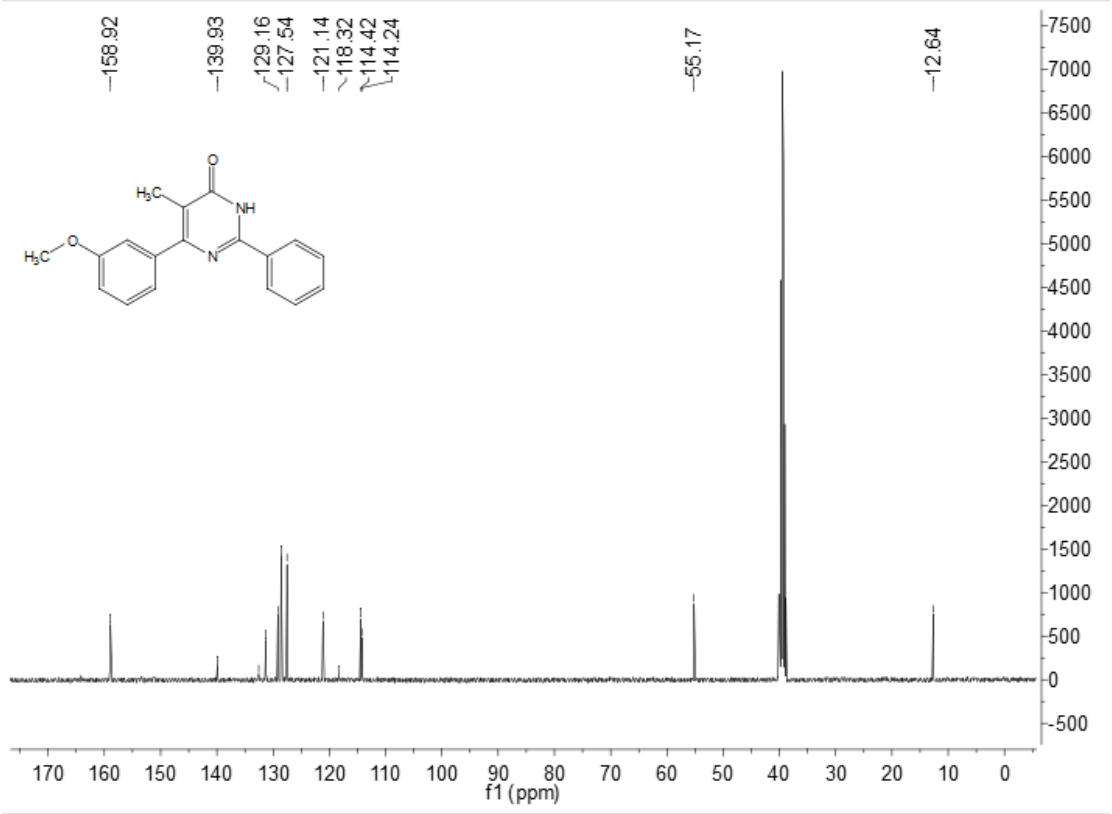
Compound **3d**


13.22
8.36
8.35
8.34
8.33
7.54
7.51
7.50
7.46
7.45
7.40
7.38
7.36
7.28
7.26
2.46
2.26
1.00
2.01
5.00
1.00
1.06
3.01
3.02
f1 (ppm)

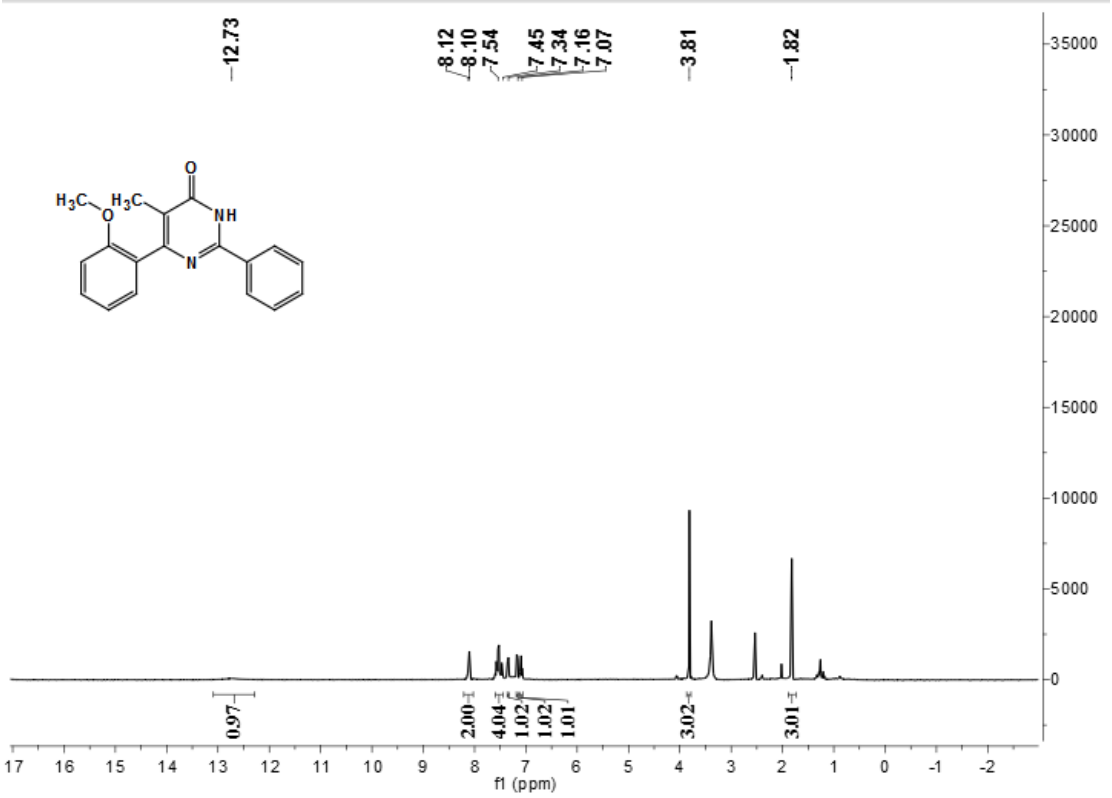

165.81
161.02
152.62
138.21
137.40
129.17
125.72
118.48
131.86
131.08
129.28
129.17
128.32
127.54
127.16
125.72
21.07
12.32
f1 (ppm)

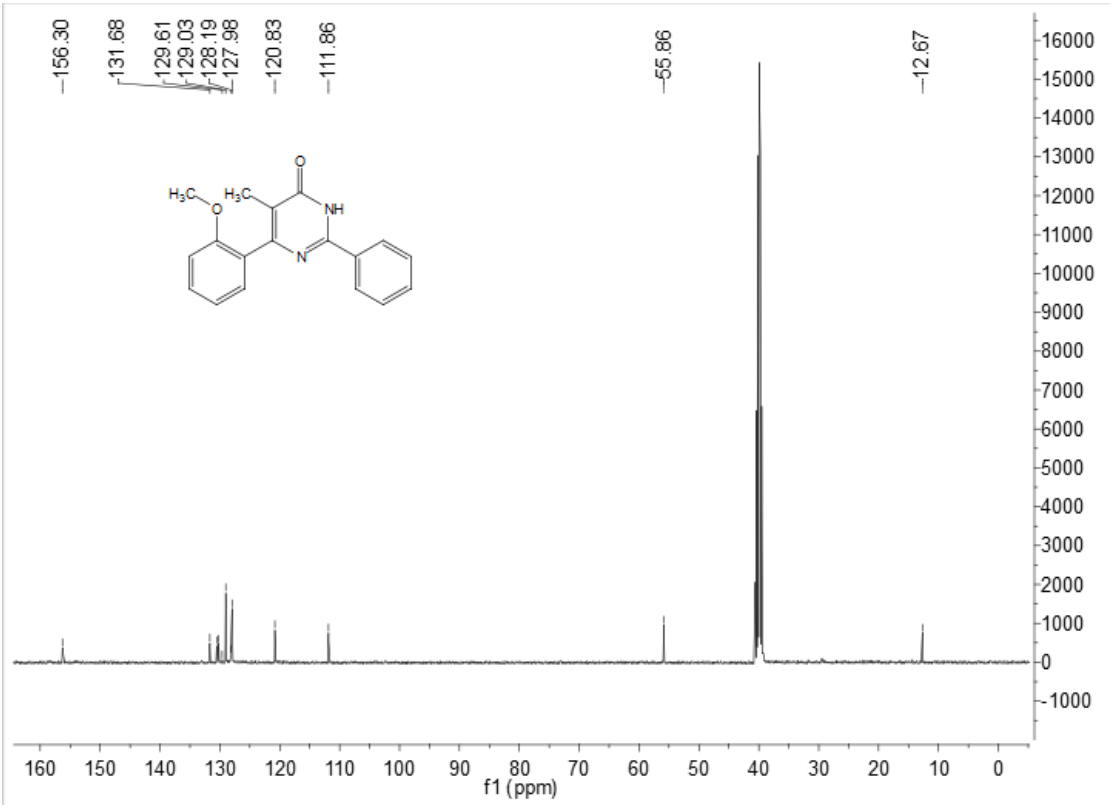
Compound **3e**


12.74
8.18
8.16
8.16
7.55
7.21
7.20
7.19
7.08
7.07
7.06
7.05
3.84
2.09
0.84
2.00
3.05
1.05
2.07
1.09
3.00
2.99
f1 (ppm)

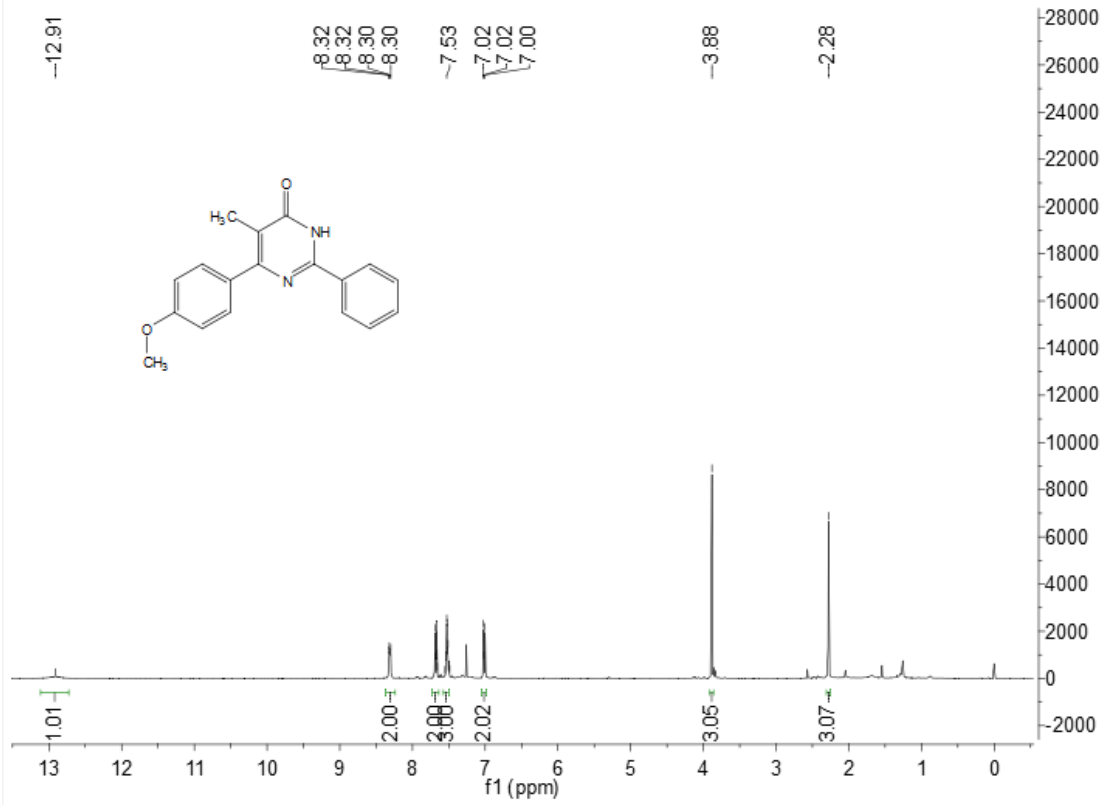

158.92
139.93
129.16
127.54
121.14
118.32
114.42
114.24
55.17
12.64
f1 (ppm)

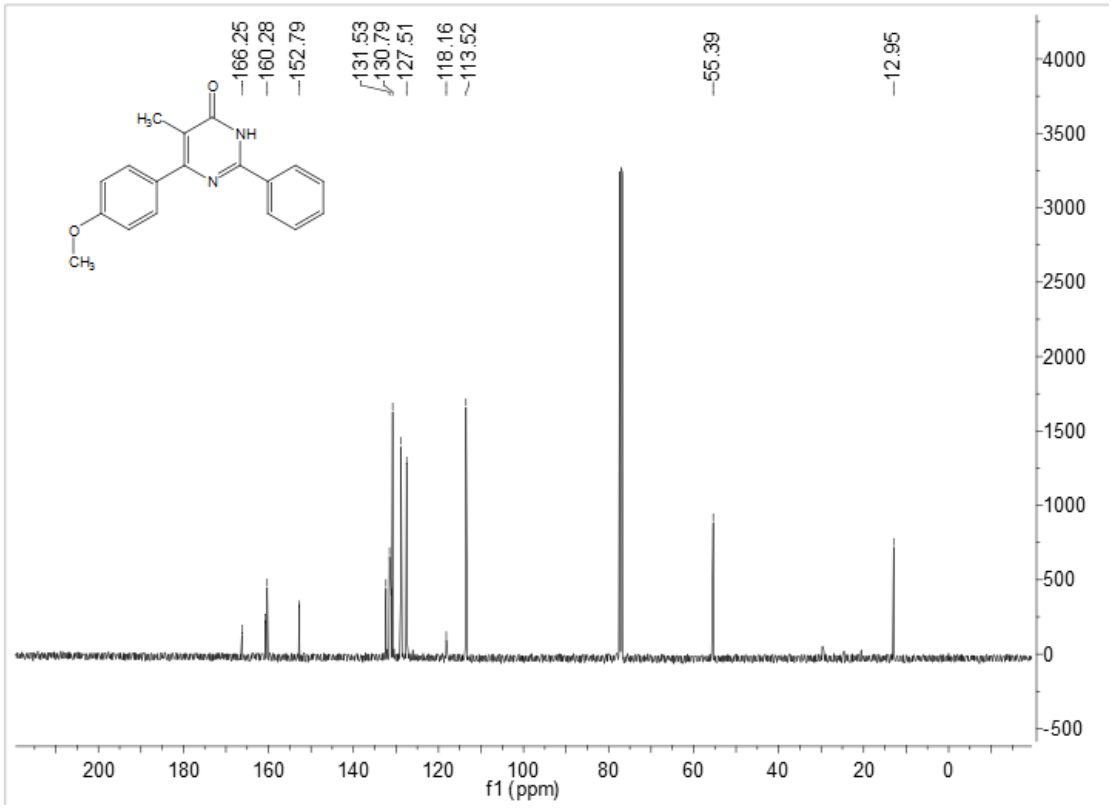
Compound **3f**


12.73
8.12
8.10
7.54
7.45
7.34
7.16
7.07
3.81
1.82
0.97
2.00
4.04
1.02
1.02
1.01
3.02
3.01
f1 (ppm)

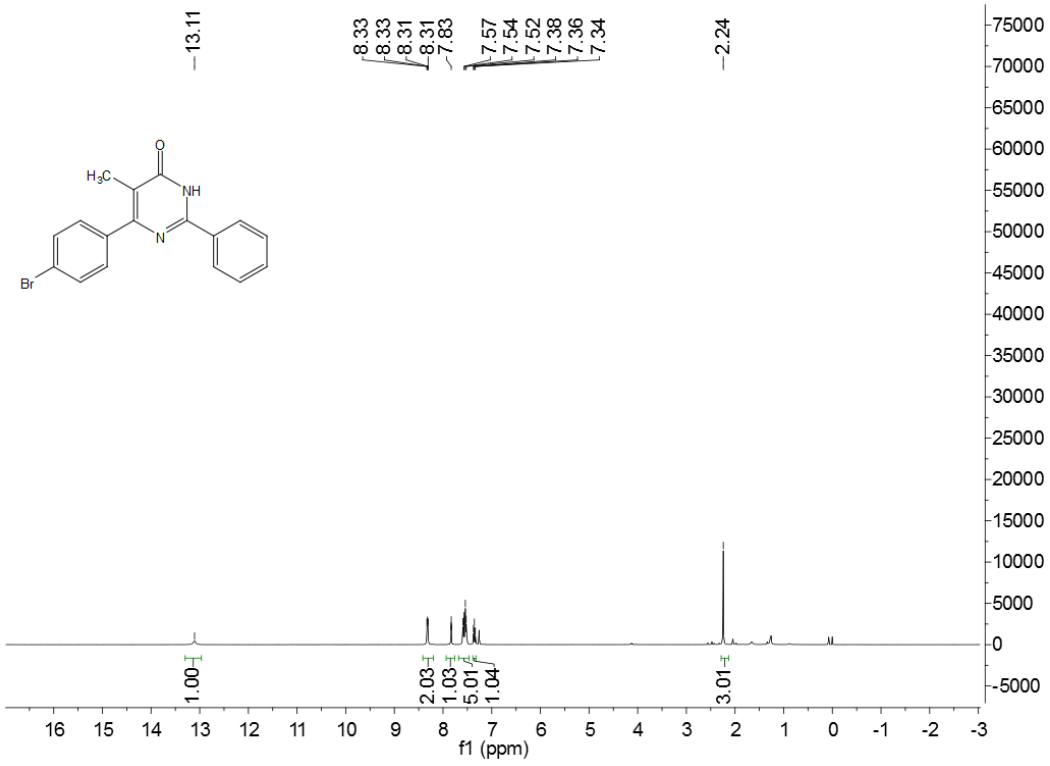

156.30
131.68
129.61
129.03
128.19
127.98
120.83
111.86
55.86
12.67
f1 (ppm)

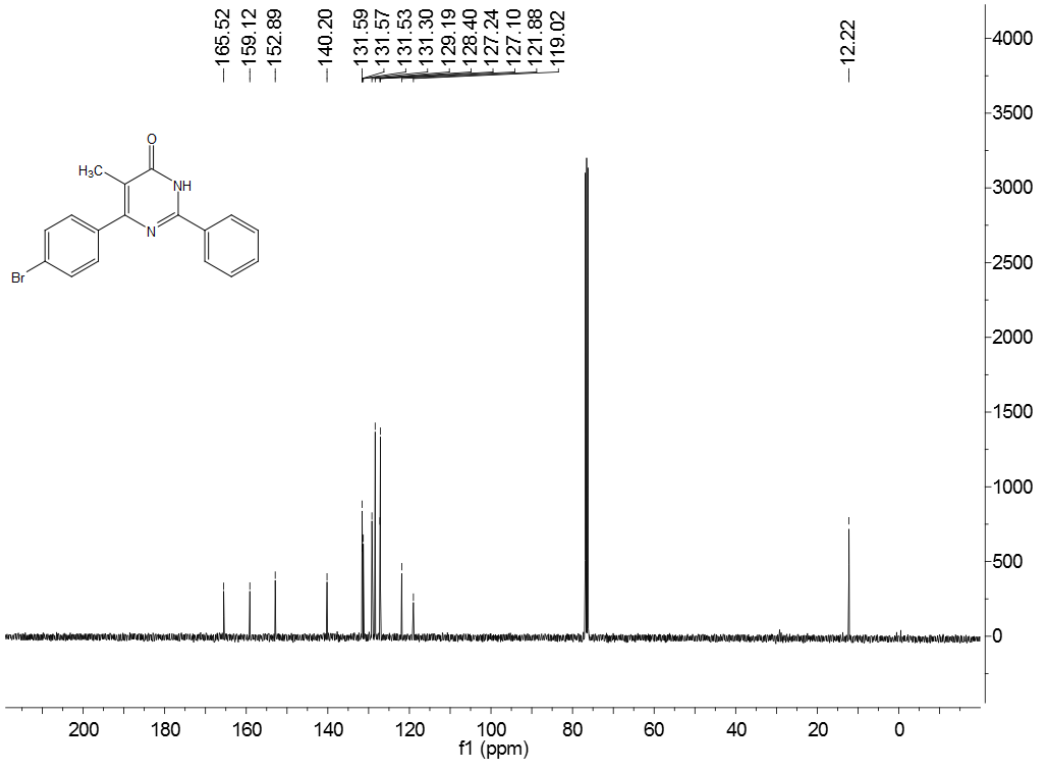
Compound **3g**


12.91
8.32
8.32
8.30
8.30
7.53
7.02
7.02
7.00
3.88
2.28
1.01
2.00
2.00
3.00
2.02
3.05
3.07
f1 (ppm)

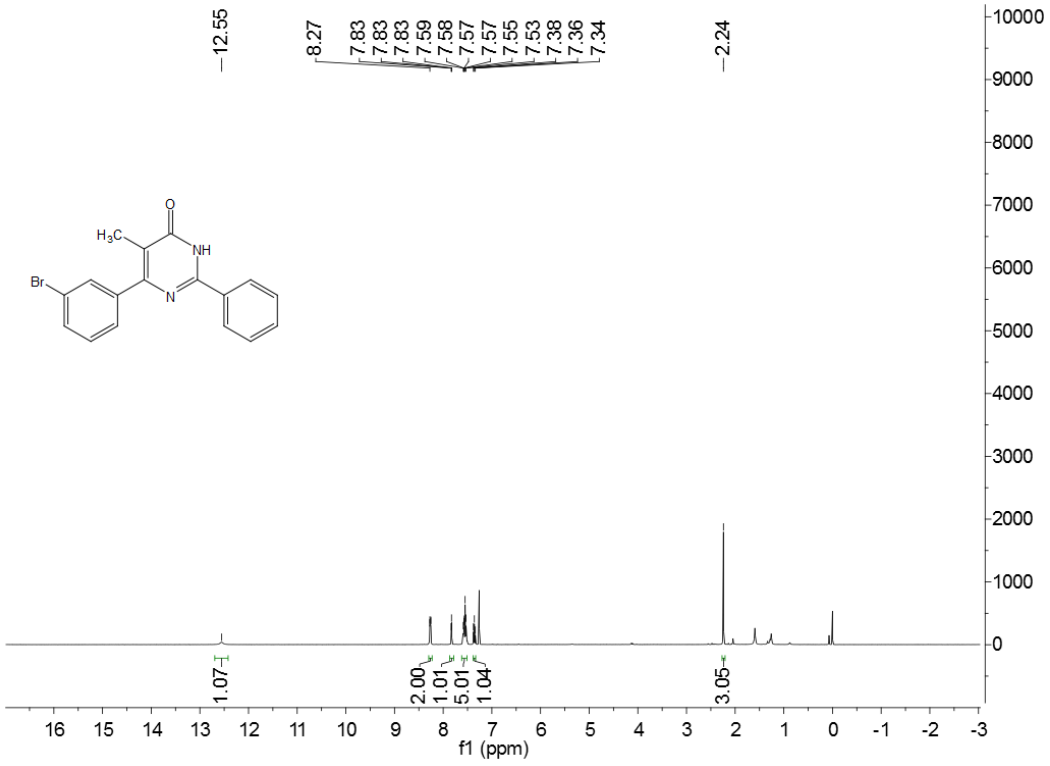

166.25
160.28
152.79
131.53
130.79
127.51
118.16
113.52
55.39
12.95
f1 (ppm)

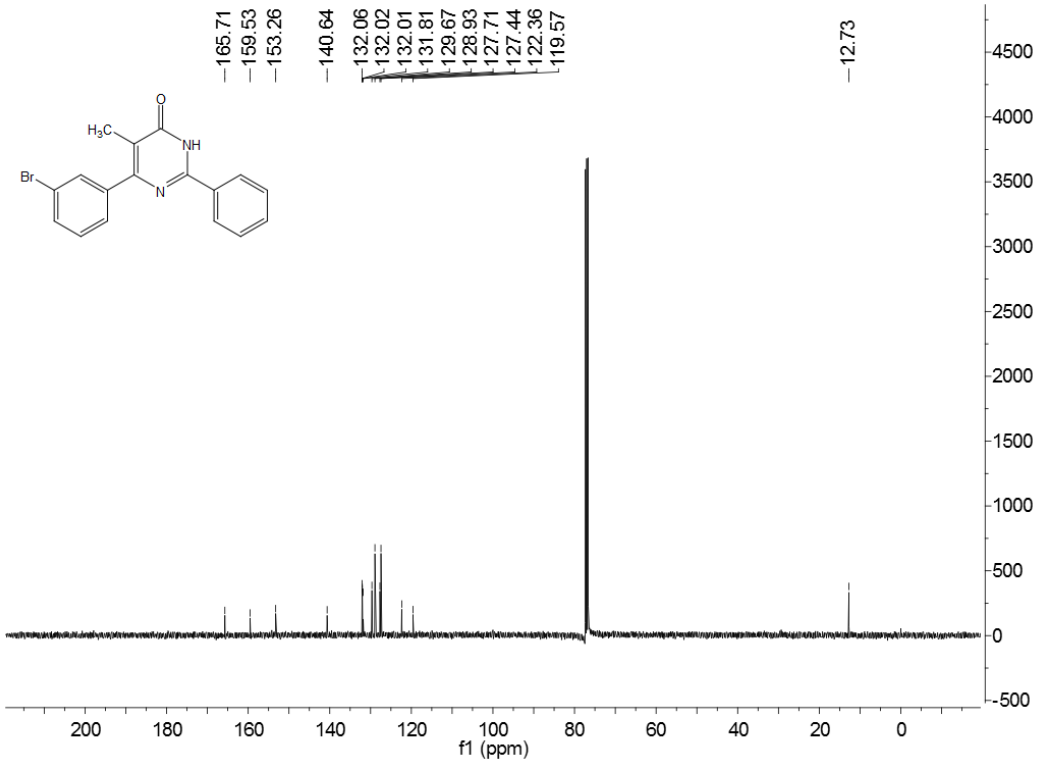
Compound **3h**


13.11
8.33
8.33
8.31
8.31
7.83
7.57
7.54
7.52
7.38
7.36
7.34
2.24
O
H3C
NH
N
Br
1.00
2.03
1.03
5.01
1.04
3.01
f1 (ppm)

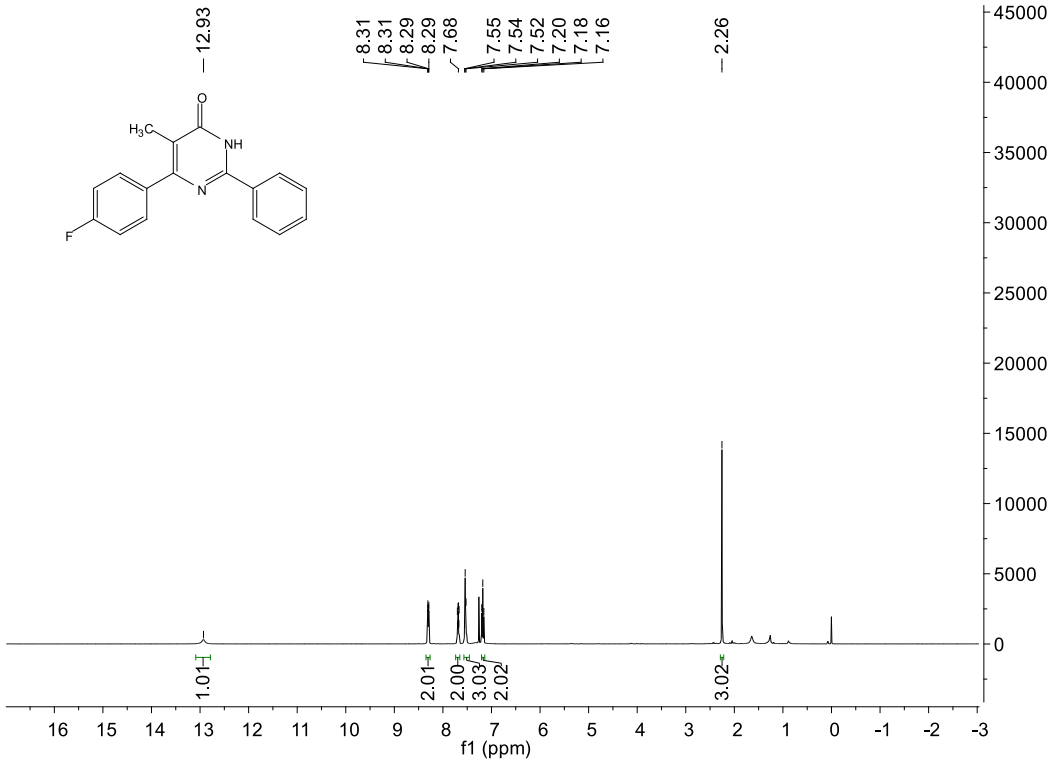

165.52
159.12
152.89
140.20
131.59
131.57
131.53
131.30
129.19
128.40
127.24
127.10
121.88
119.02
12.22
O
H3C
NH
N
Br
f1 (ppm)

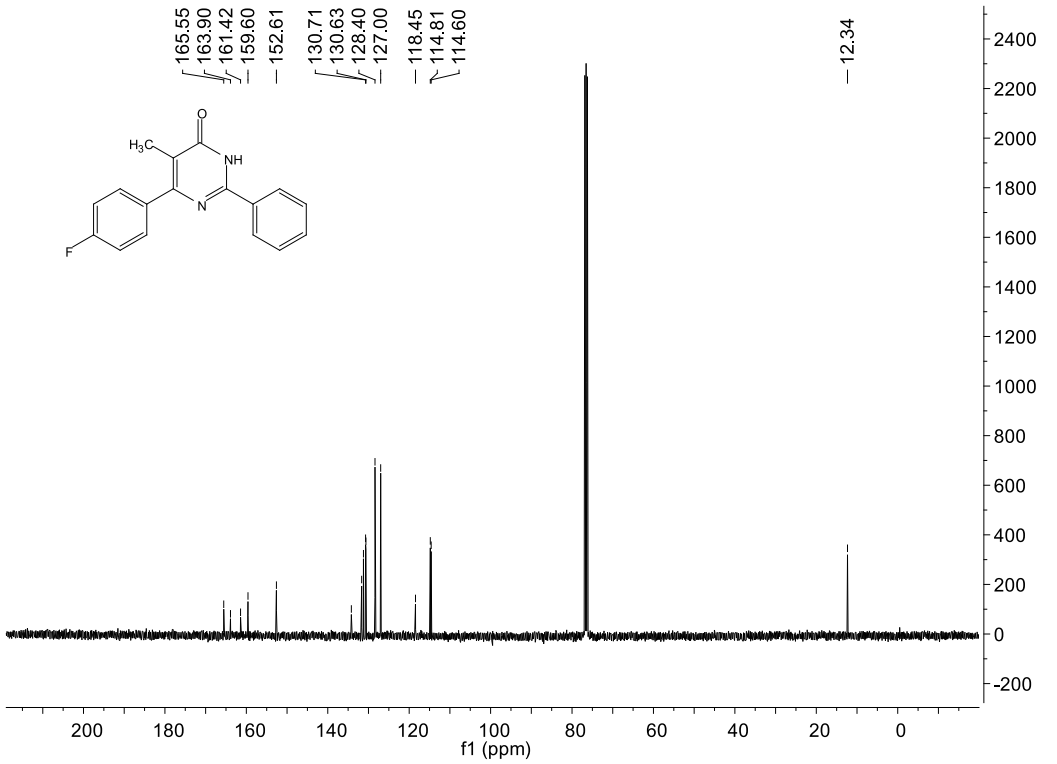
Compound **3i**


12.55
8.27
7.83
7.83
7.83
7.59
7.58
7.57
7.57
7.55
7.53
7.38
7.36
7.34
2.24
O
H3C
NH
Br
N
1.07
2.00
1.01
5.01
1.04
3.05
f1 (ppm)

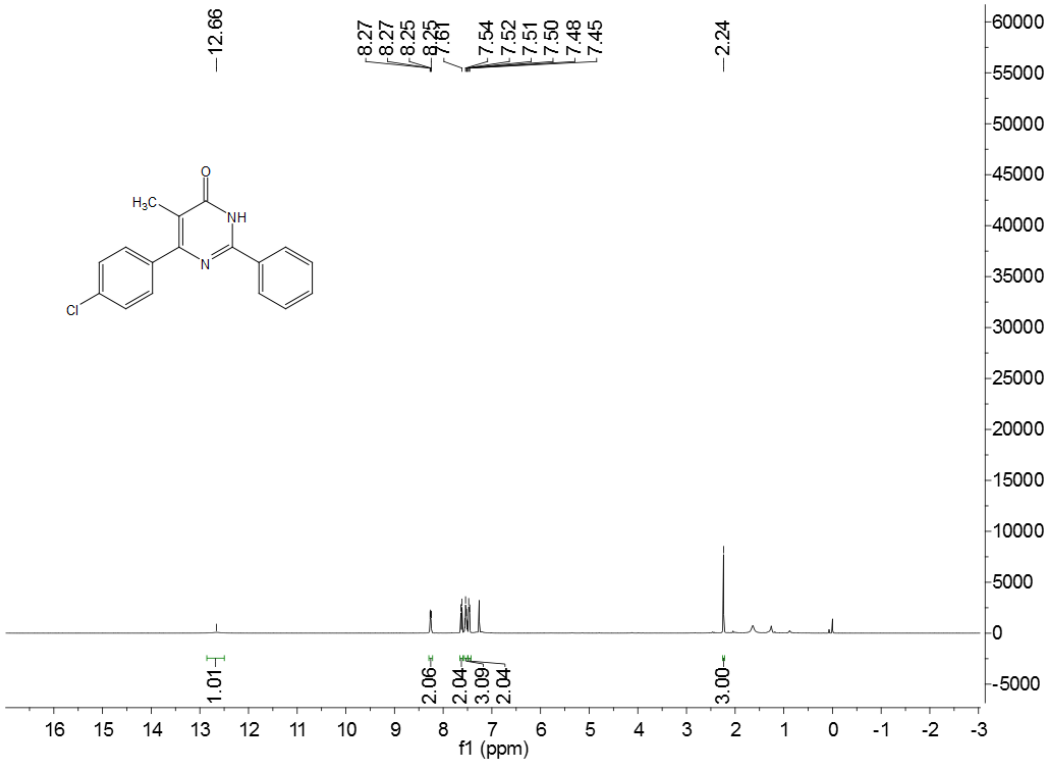

165.71
159.53
153.26
140.64
132.06
132.02
132.01
131.81
129.67
128.93
127.71
127.44
122.36
119.57
12.73
O
H3C
NH
Br
N
f1 (ppm)

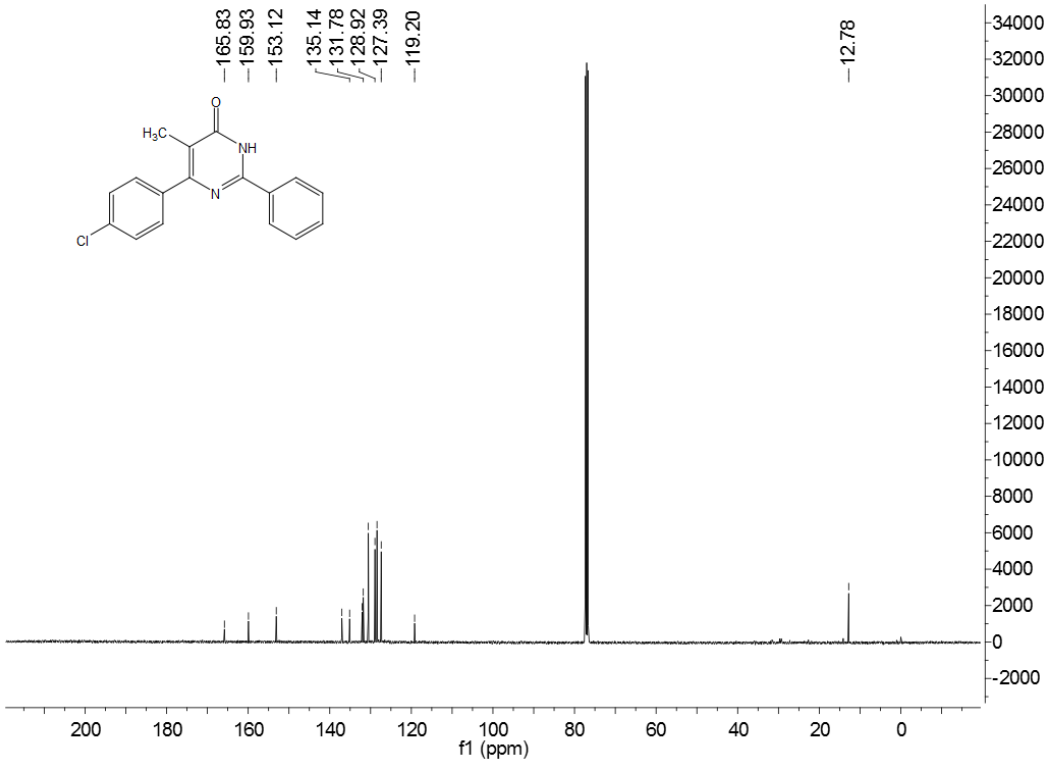
Compound **3j**


12.93
8.31
8.31
8.29
8.29
7.68
7.55
7.54
7.52
7.20
7.18
7.16
2.26
O
H3C
NH
N
F
1.01
2.01
2.00
3.03
2.02
3.02
f1 (ppm)

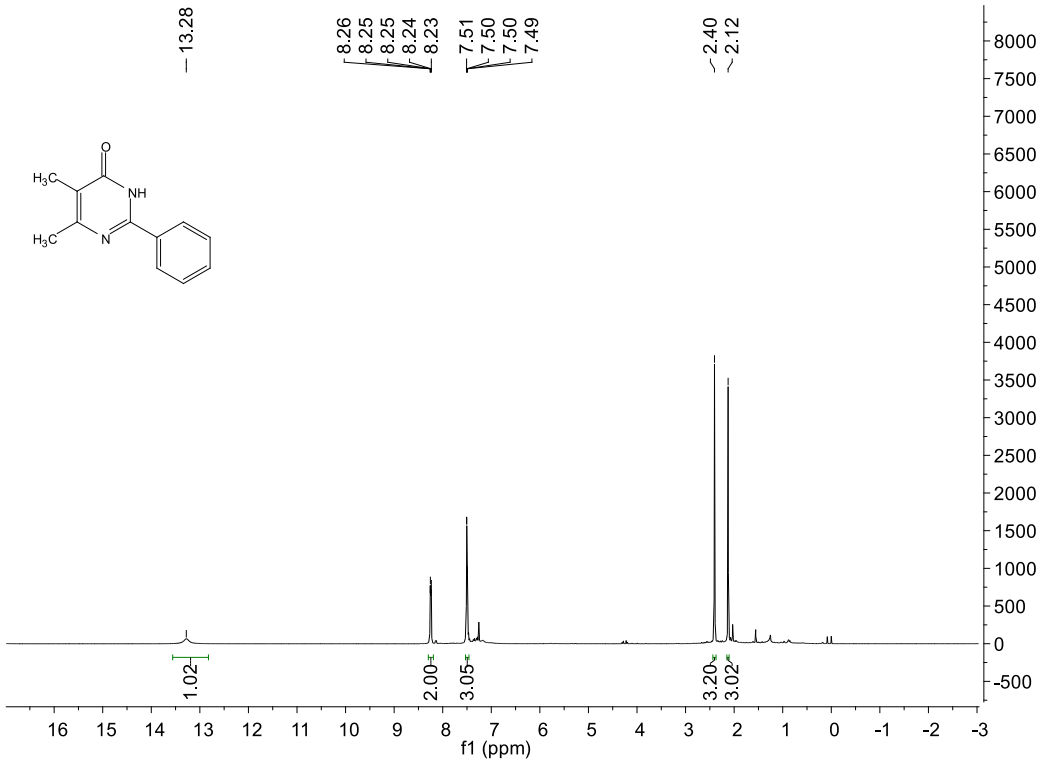

165.55
163.90
161.42
159.60
152.61
130.71
130.63
128.40
127.00
118.45
114.81
114.60
12.34
O
H3C
NH
N
F
f1 (ppm)

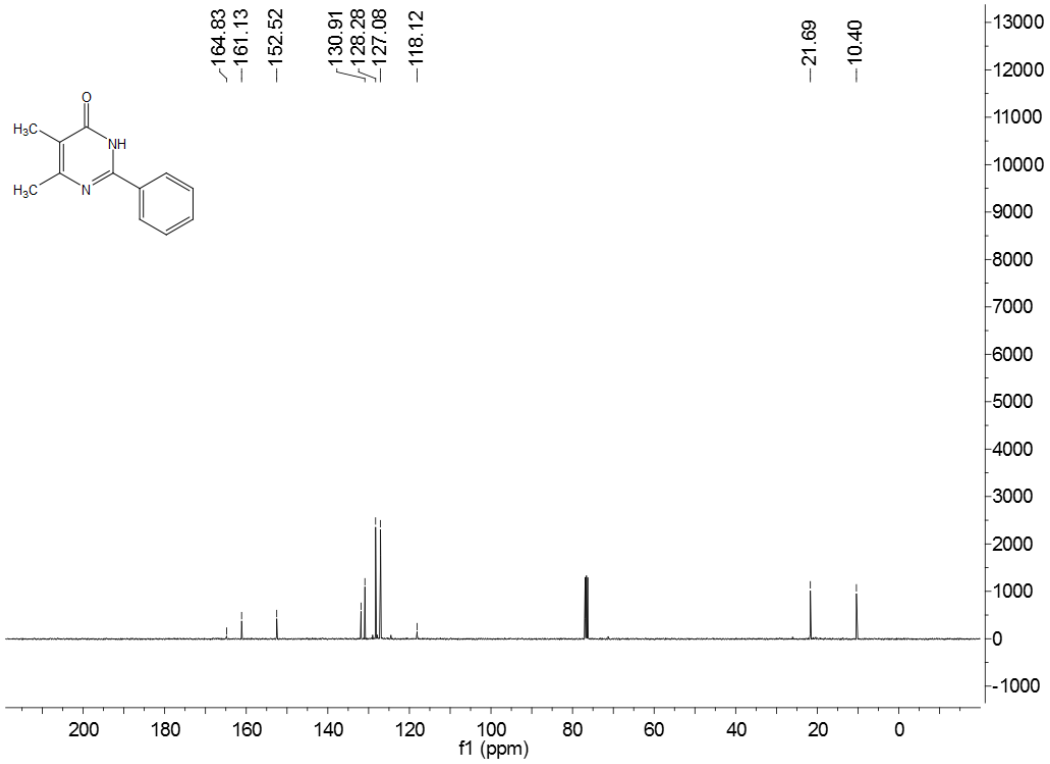
Compound **3k**


12.66
8.27
8.27
8.25
8.25
7.61
7.54
7.52
7.51
7.50
7.48
7.45
2.24
O
H3C
NH
N
Cl
1.01
2.06
2.04
3.09
2.04
3.00
f1 (ppm)

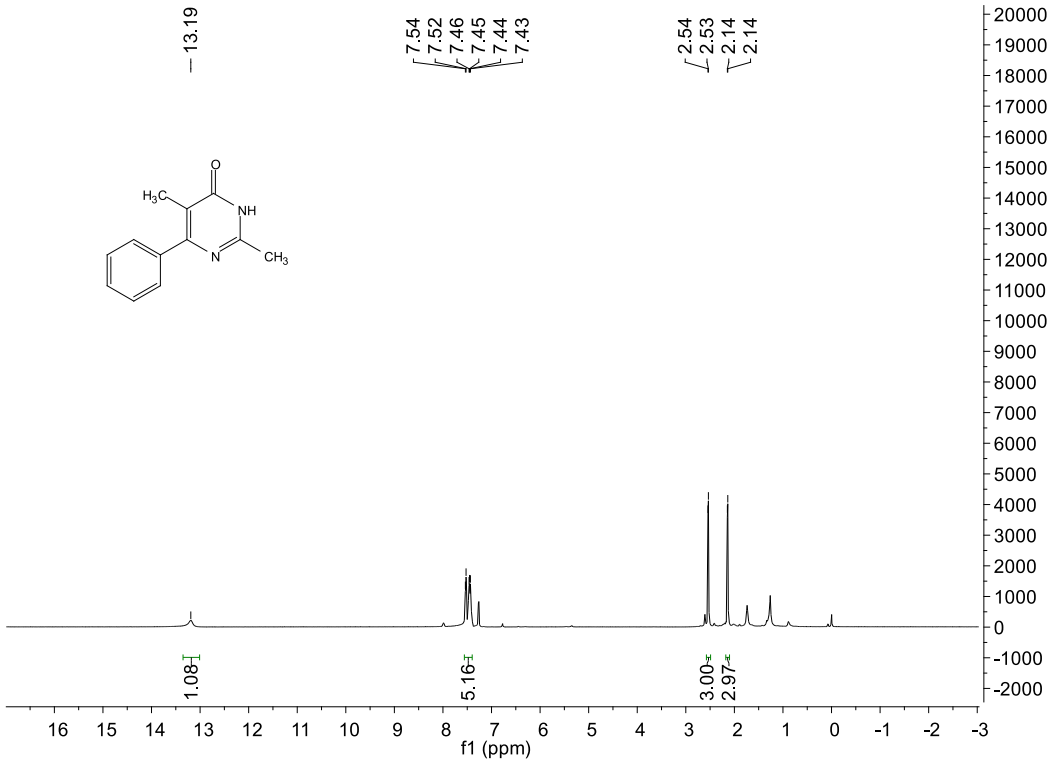

165.83
159.93
153.12
135.14
131.78
128.92
127.39
119.20
12.78
O
H3C
NH
N
Cl
f1 (ppm)

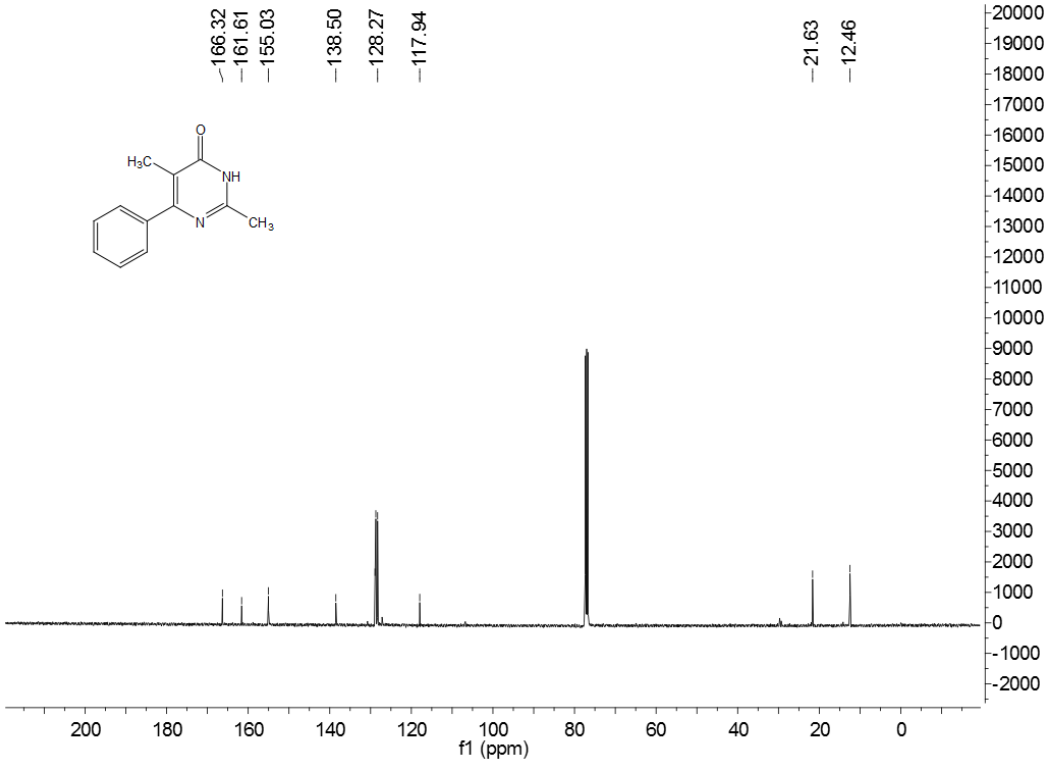
Compound **3l**


13.28
8.26
8.25
8.25
8.24
8.23
7.51
7.50
7.50
7.49
2.40
2.12
1.02
2.00
3.05
3.20
3.02
f1 (ppm)

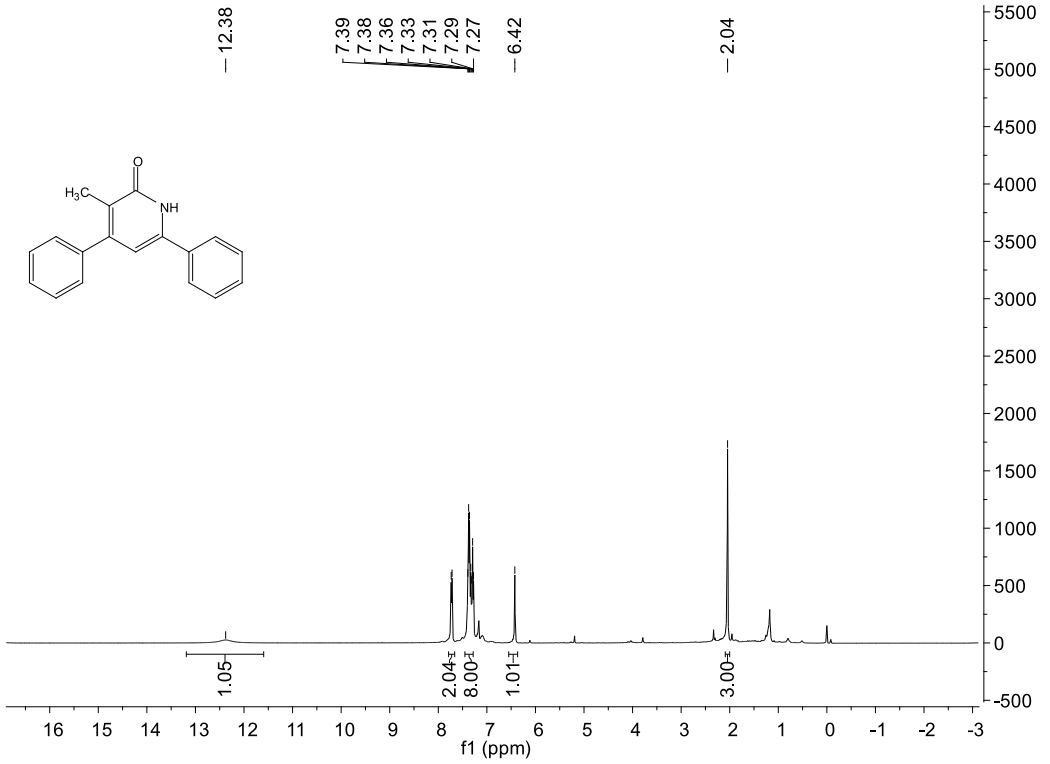

164.83
161.13
152.52
130.91
128.28
127.08
118.12
21.69
10.40
f1 (ppm)

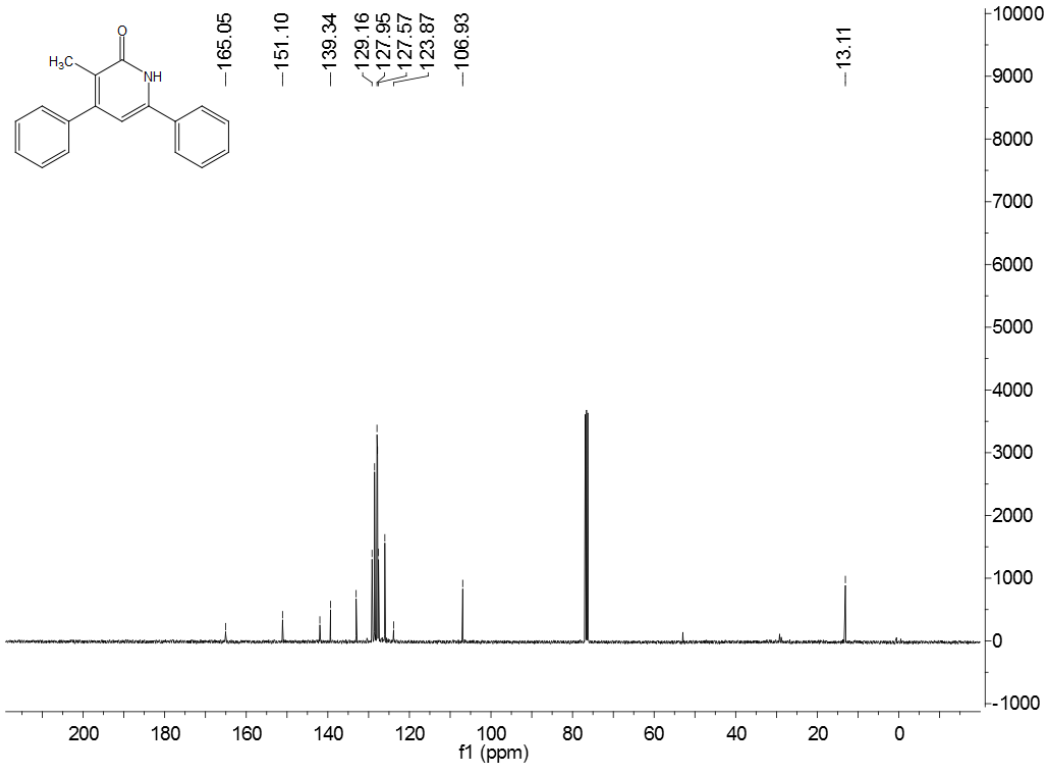
Compound **3m**


13.19
7.54
7.52
7.46
7.45
7.44
7.43
2.54
2.53
2.14
2.14
1.08
5.16
3.00
2.97
f1 (ppm)

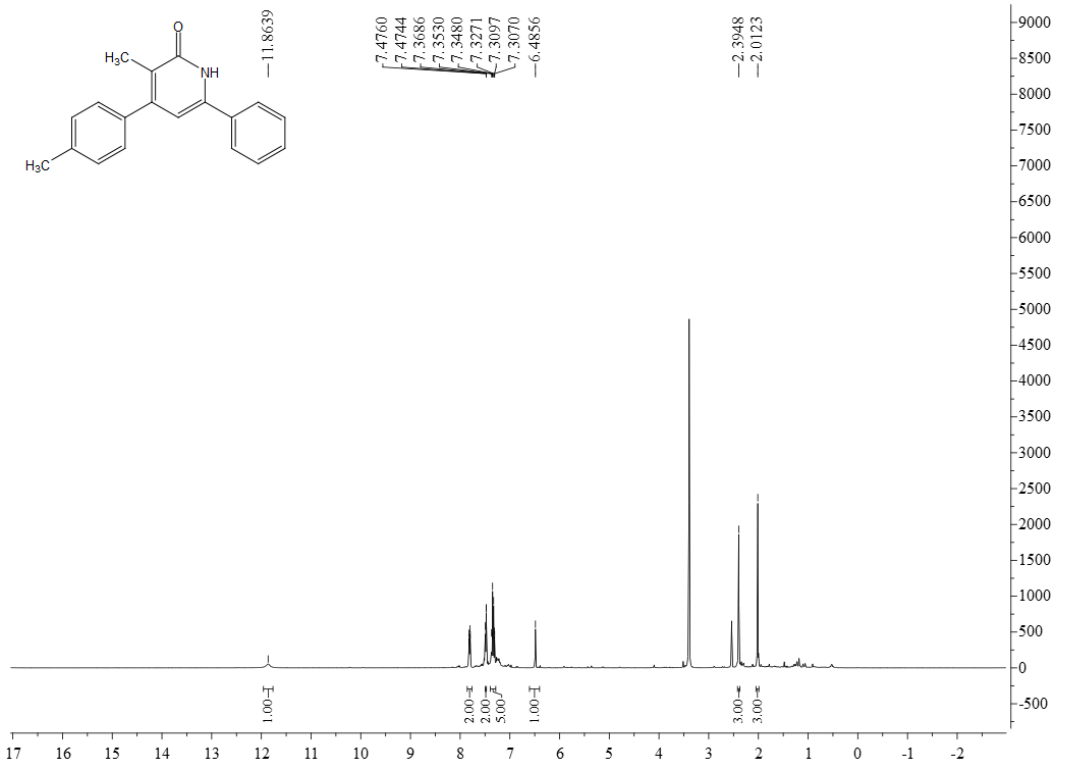

166.32
161.61
155.03
138.50
128.27
117.94
21.63
12.46
f1 (ppm)

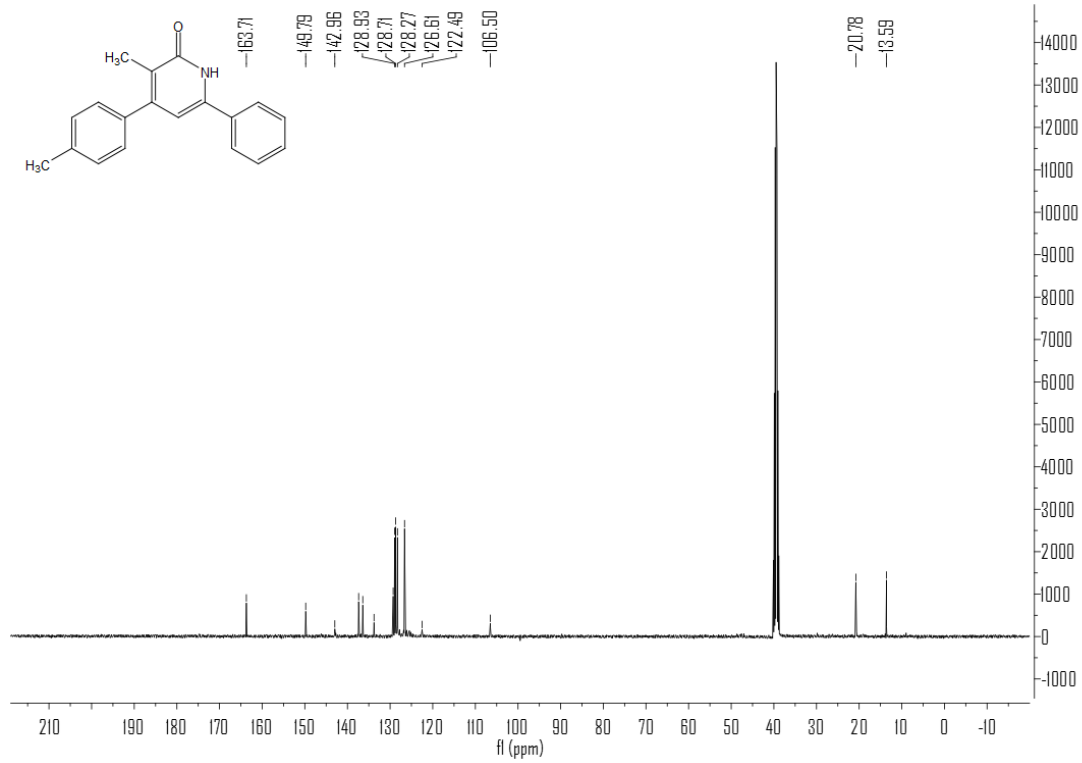
Compound **5a**


12.38
7.39
7.38
7.36
7.33
7.31
7.29
7.27
6.42
2.04
1.05
2.04
8.00
1.01
3.00
f1 (ppm)

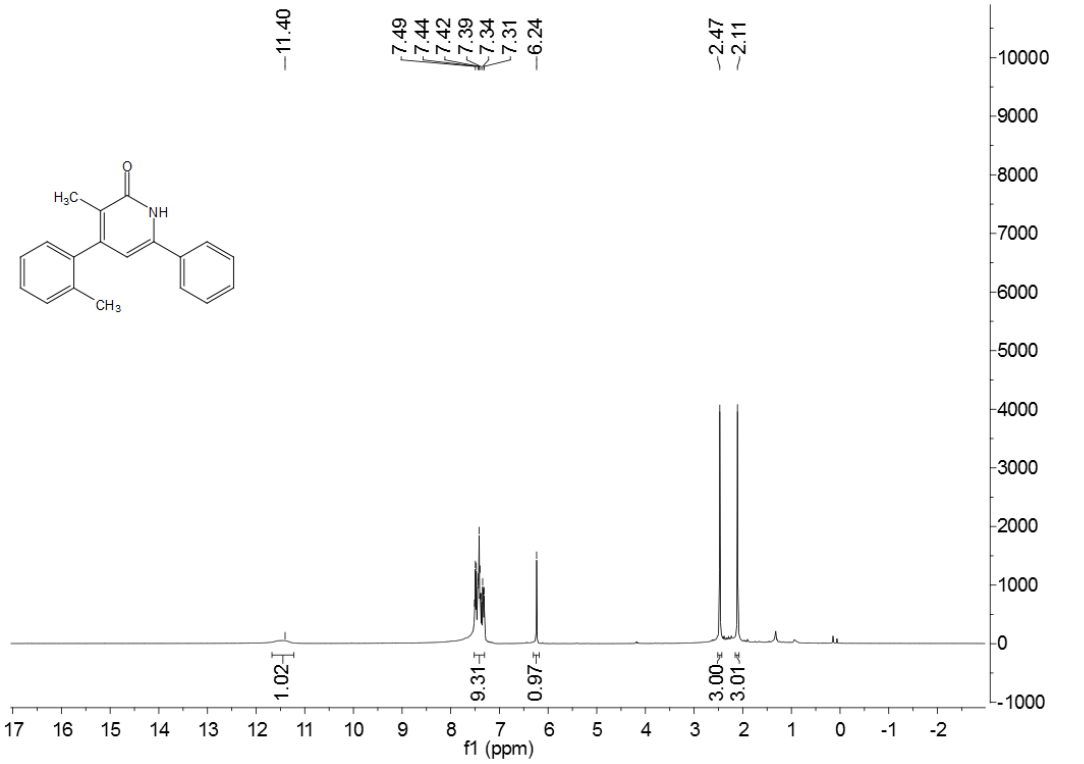

165.05
151.10
139.34
129.16
127.95
127.57
123.87
106.93
13.11
f1 (ppm)

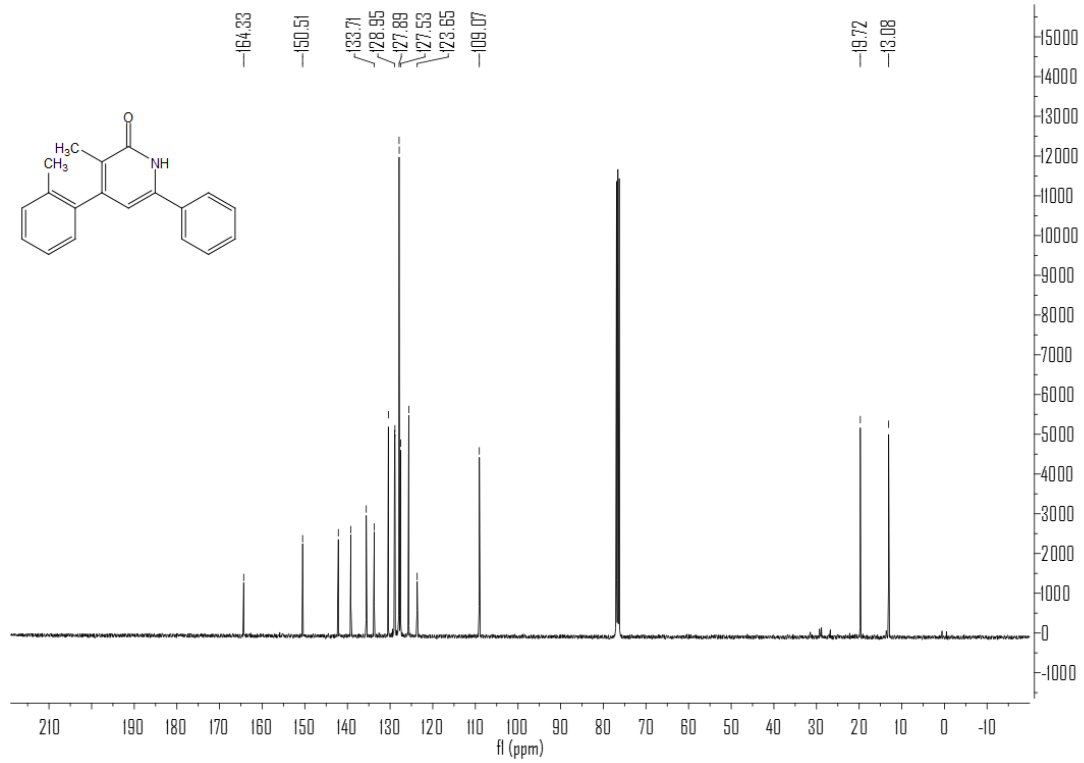
Compound **5b**


11.8639
7.4760
7.4744
7.3686
7.3530
7.3480
7.3271
7.3097
7.3070
6.4856
2.3948
2.0123
1.00
2.00
2.00
5.00
1.00
3.00
3.00

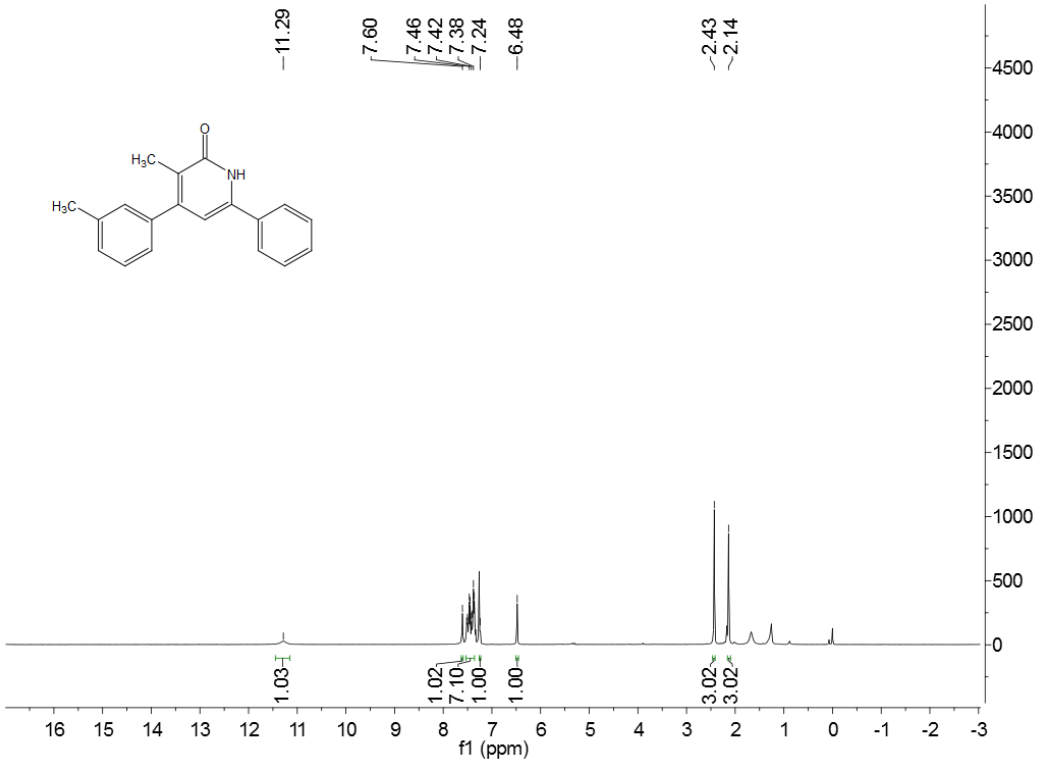

163.71
149.79
142.96
128.83
128.71
128.27
126.61
122.49
106.50
20.78
13.59
f1 (ppm)

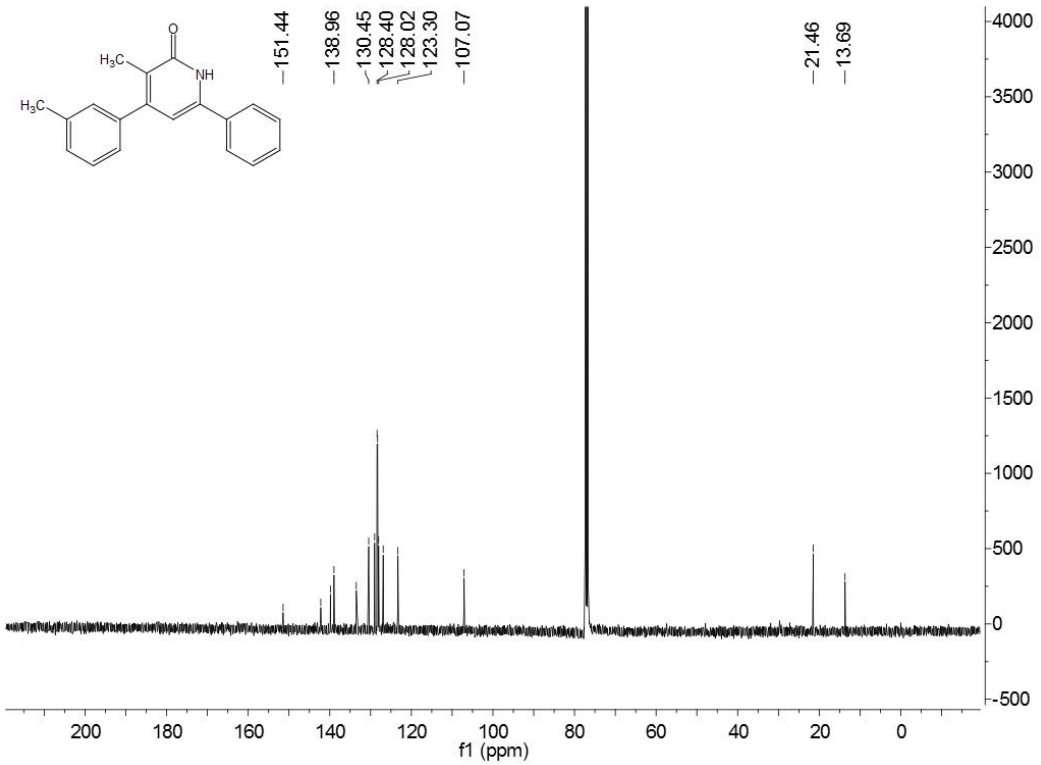
Compound **5c**


11.40
7.49
7.44
7.42
7.39
7.34
7.31
6.24
2.47
2.11
1.02
9.31
0.97
3.00
3.01
f1 (ppm)

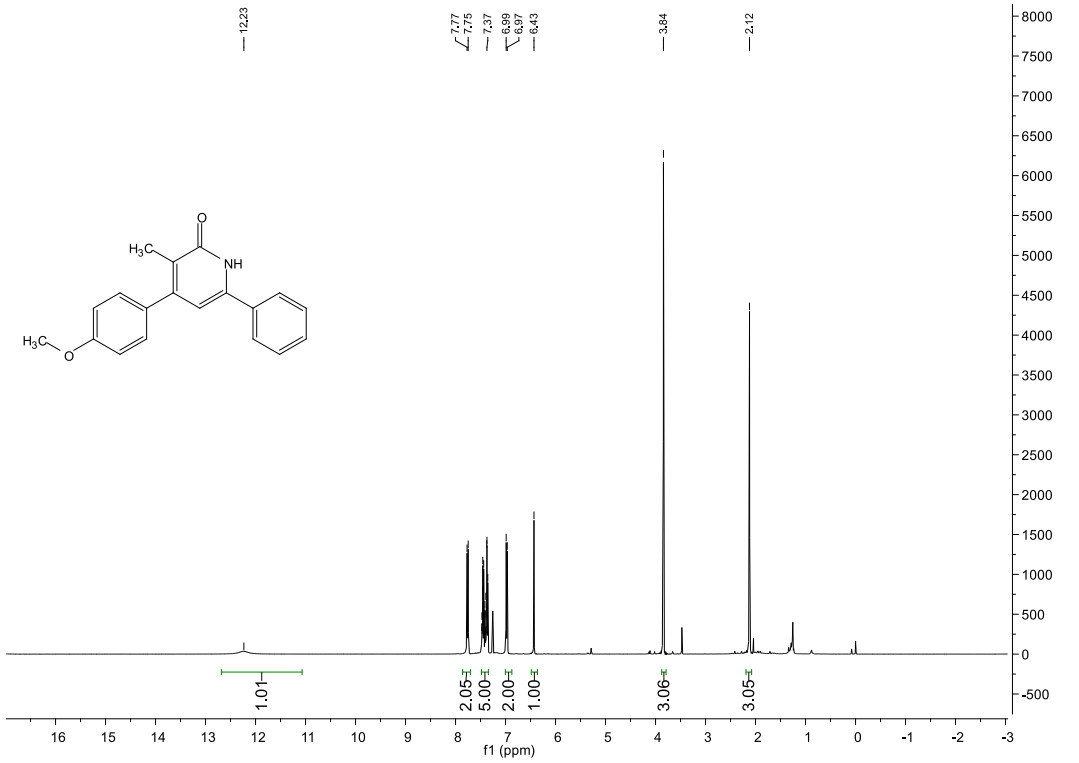

164.33
150.51
133.71
128.95
127.89
127.53
123.65
109.07
19.72
13.08
f1 (ppm)

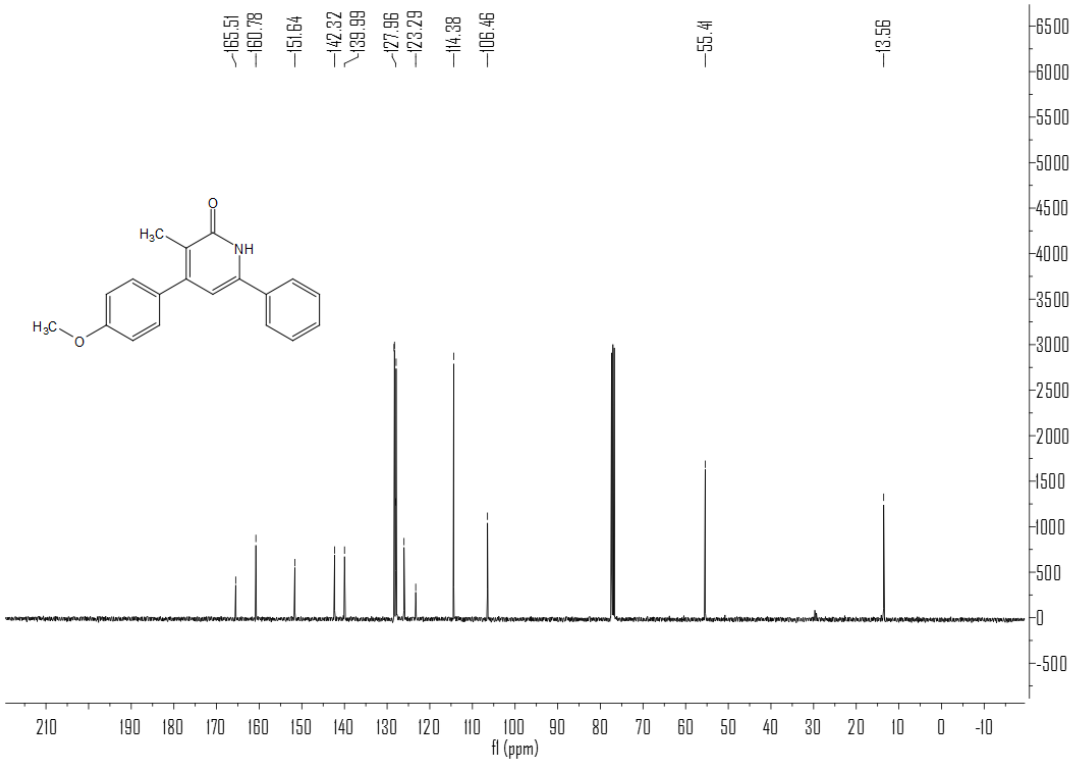
Compound **5d**


11.29
7.60
7.46
7.42
7.38
7.24
6.48
2.43
2.14
O
H3C
NH
H3C
1.03
1.02
7.10
1.00
1.00
3.02
3.02
f1 (ppm)

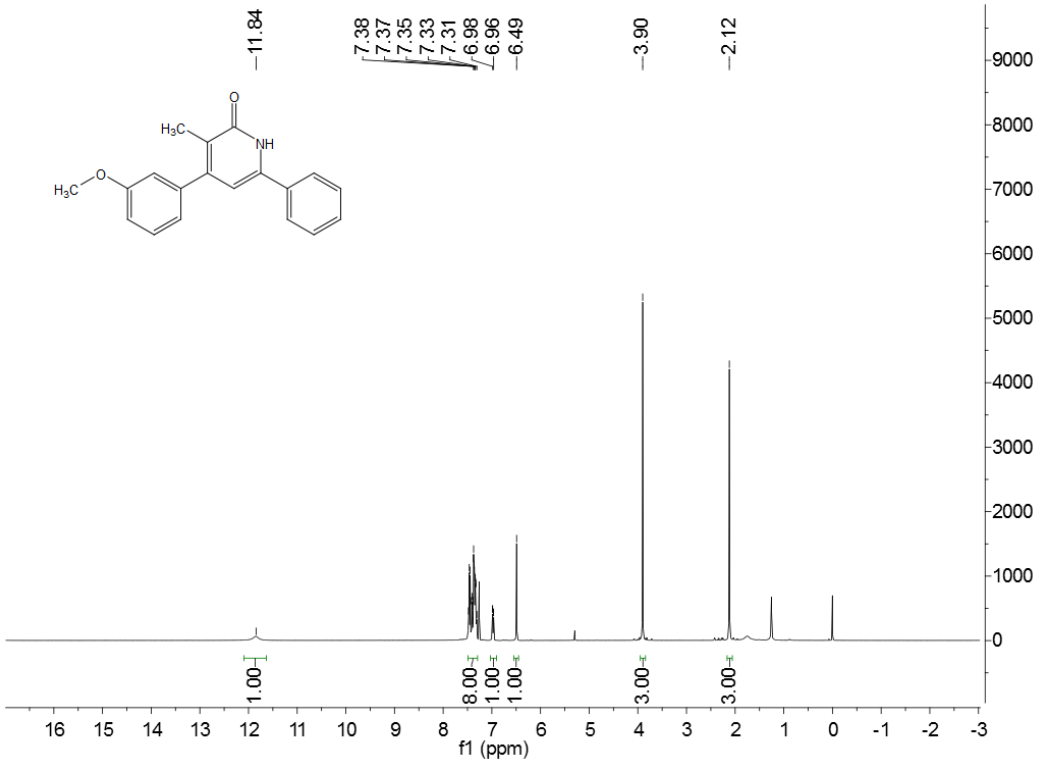

151.44
138.96
130.45
128.40
128.02
123.30
107.07
21.46
13.69
O
H3C
NH
H3C
f1 (ppm)

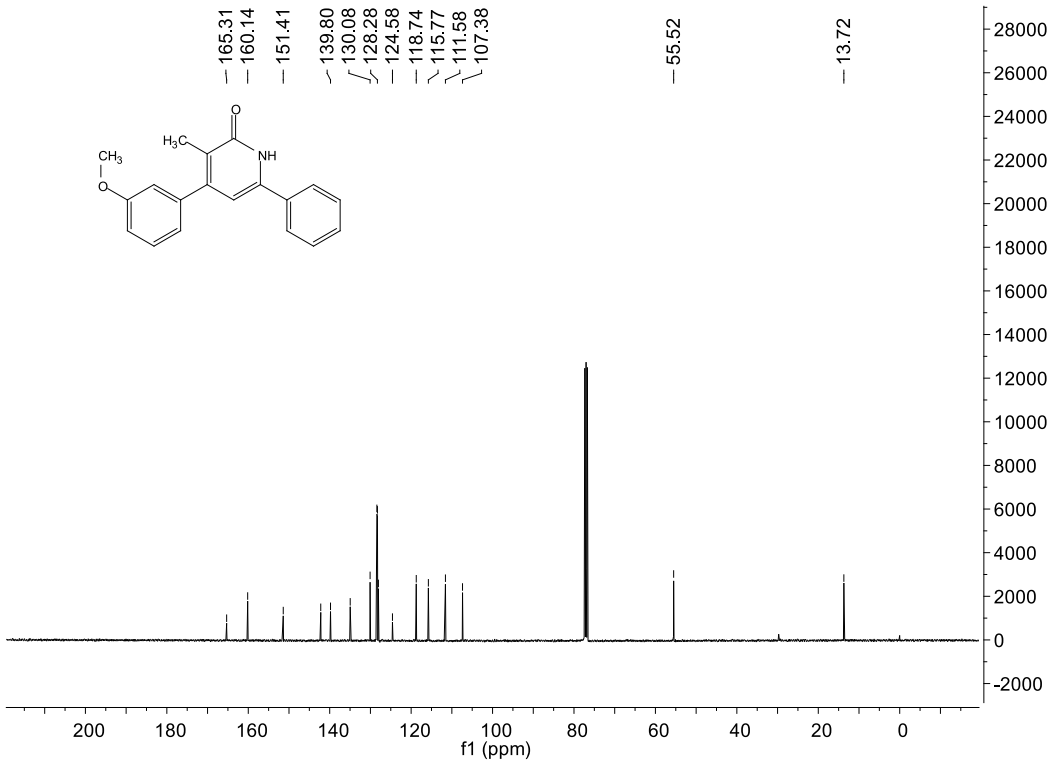
Compound **5e**


12.23
7.77
7.75
7.37
6.99
6.97
6.43
3.84
2.12
1.01
2.05
5.00
2.00
1.00
3.06
3.05
f1 (ppm)

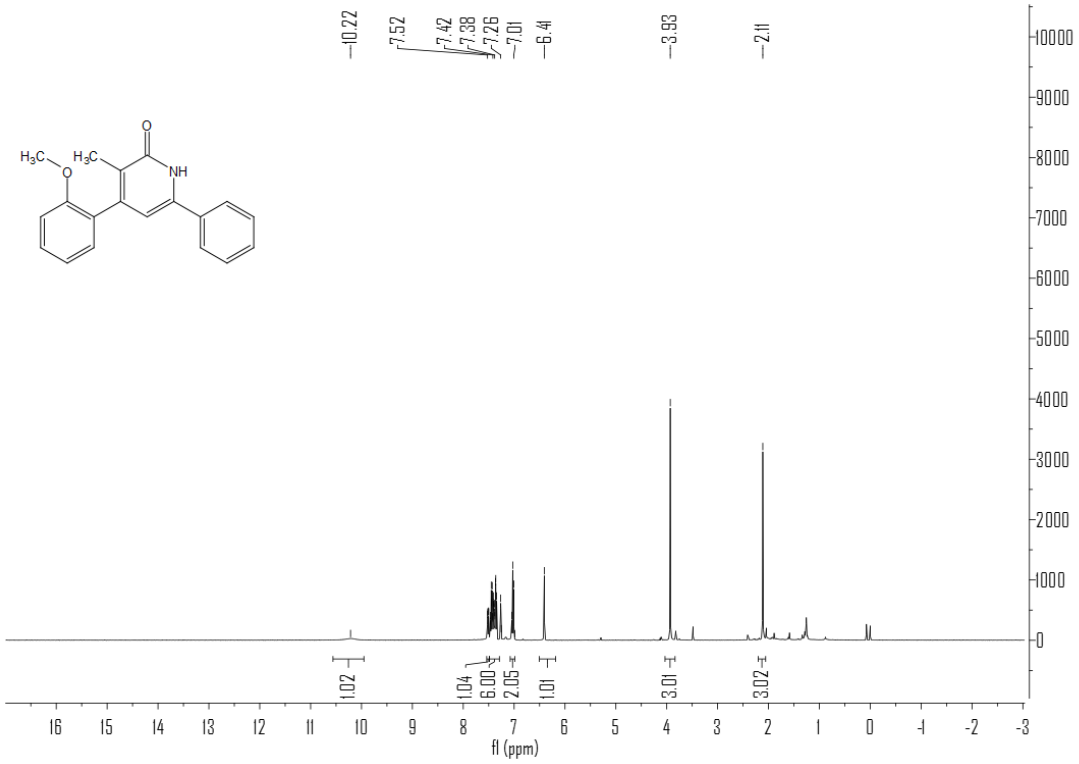

165.51
160.78
151.64
142.32
139.99
127.96
123.29
114.38
106.46
55.41
13.56
f1 (ppm)

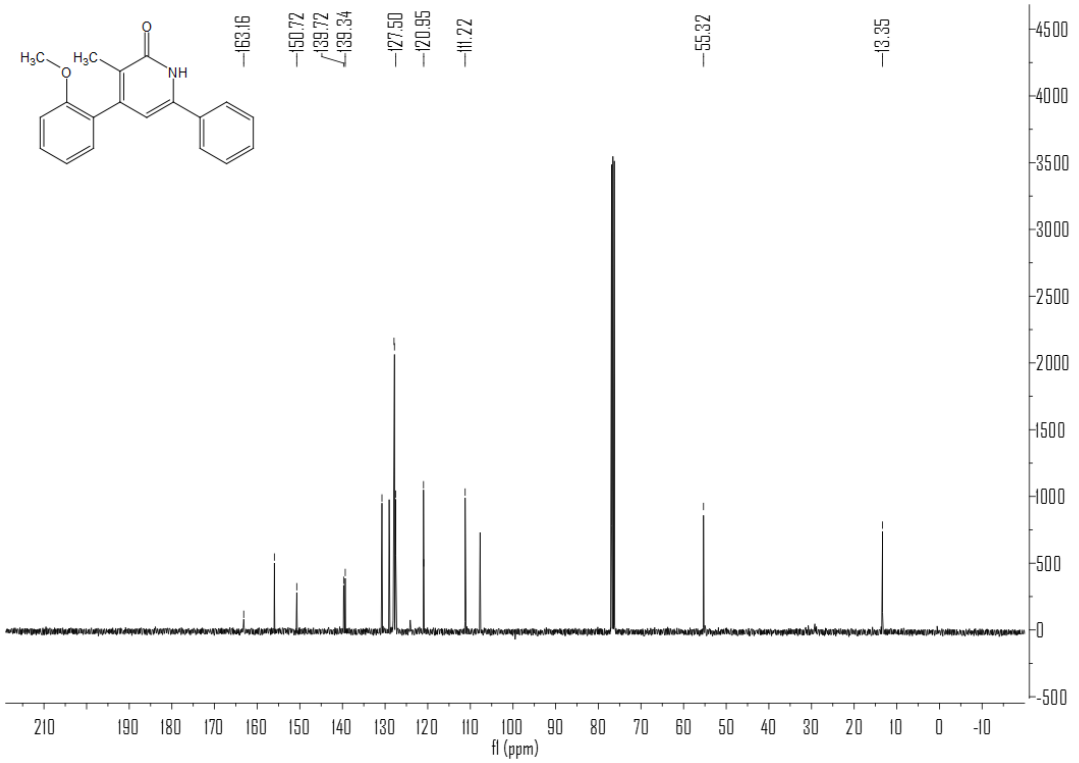
Compound **5f**


11.84
7.38
7.37
7.35
7.33
7.31
6.98
6.96
6.49
3.90
2.12
1.00
8.00
1.00
1.00
3.00
3.00
f1 (ppm)

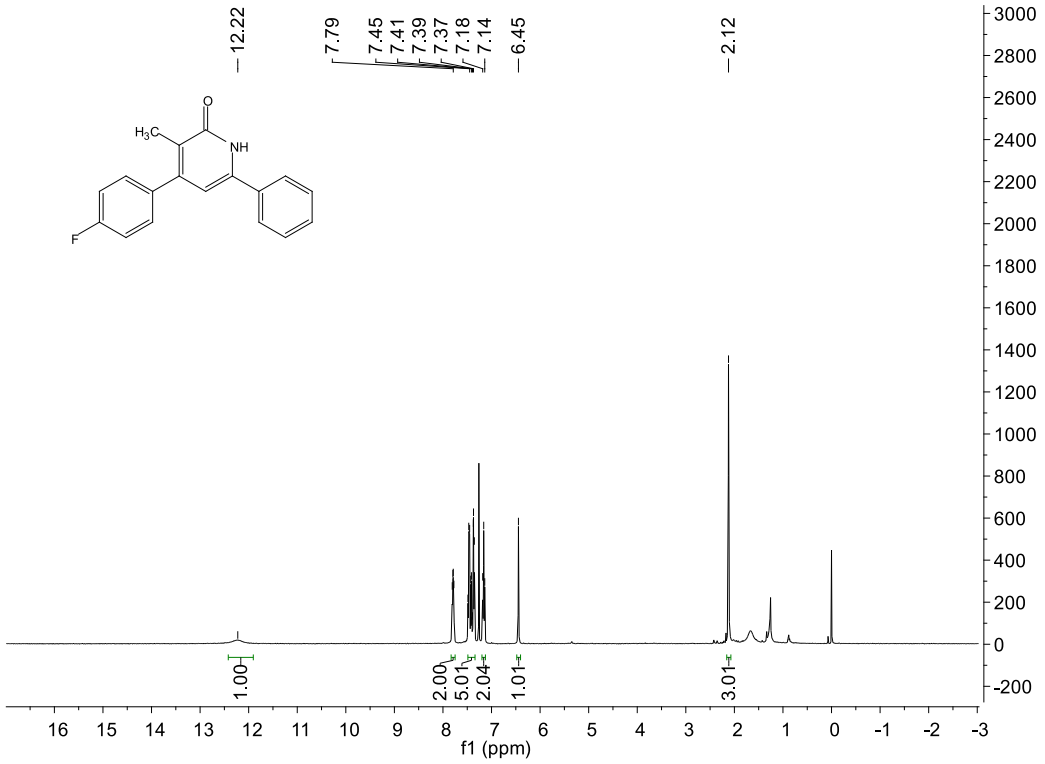

165.31
160.14
151.41
139.80
130.08
128.28
124.58
118.74
115.77
111.58
107.38
55.52
13.72
f1 (ppm)

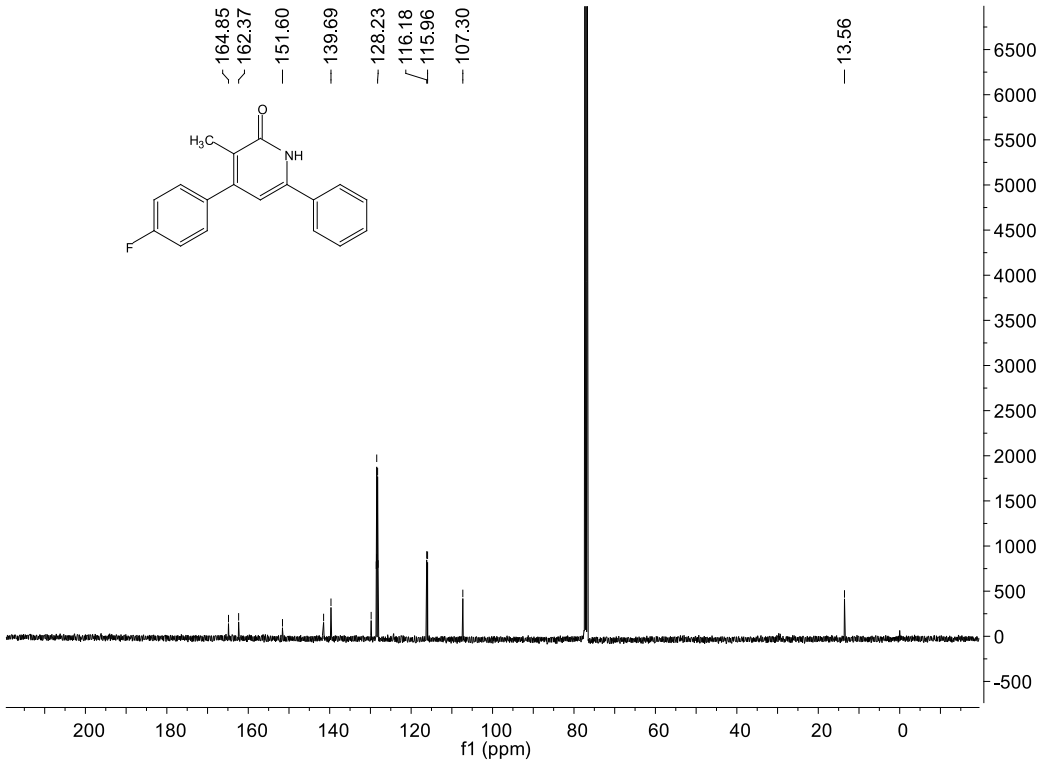
Compound **5g**


10.22
7.52
7.42
7.38
7.26
7.01
6.41
3.93
2.11
1.02
1.04
6.00
2.05
1.01
3.01
3.02
f1 (ppm)

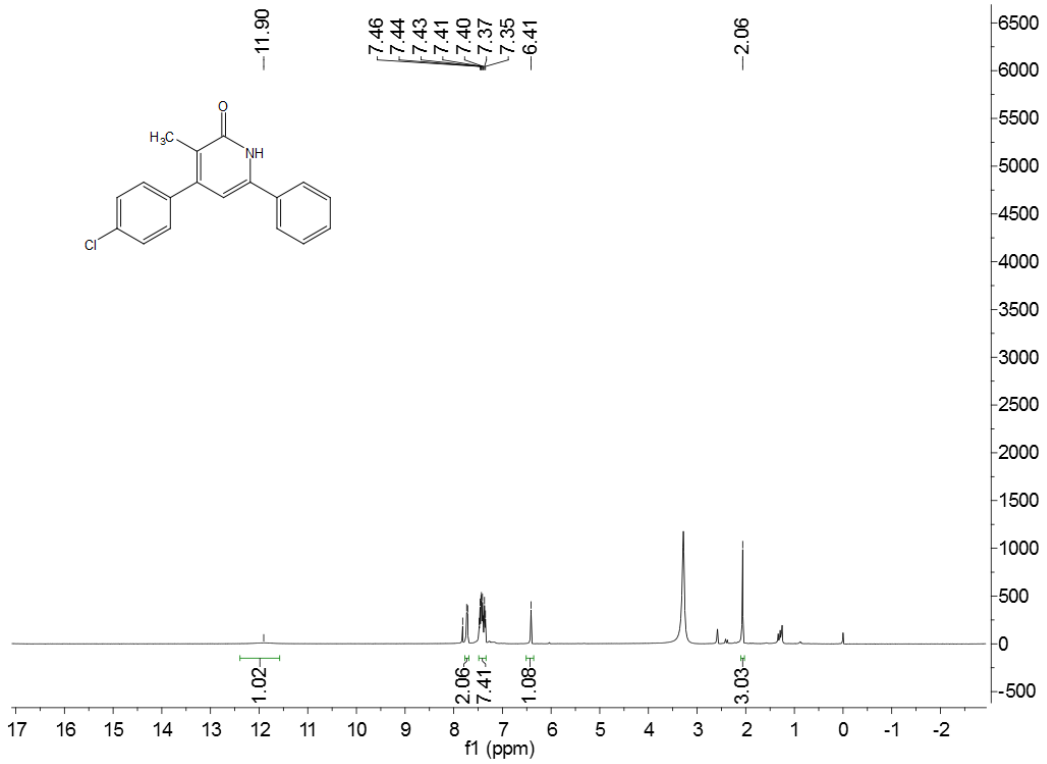

163.16
150.72
139.72
139.34
127.50
120.95
111.22
55.32
13.35
f1 (ppm)

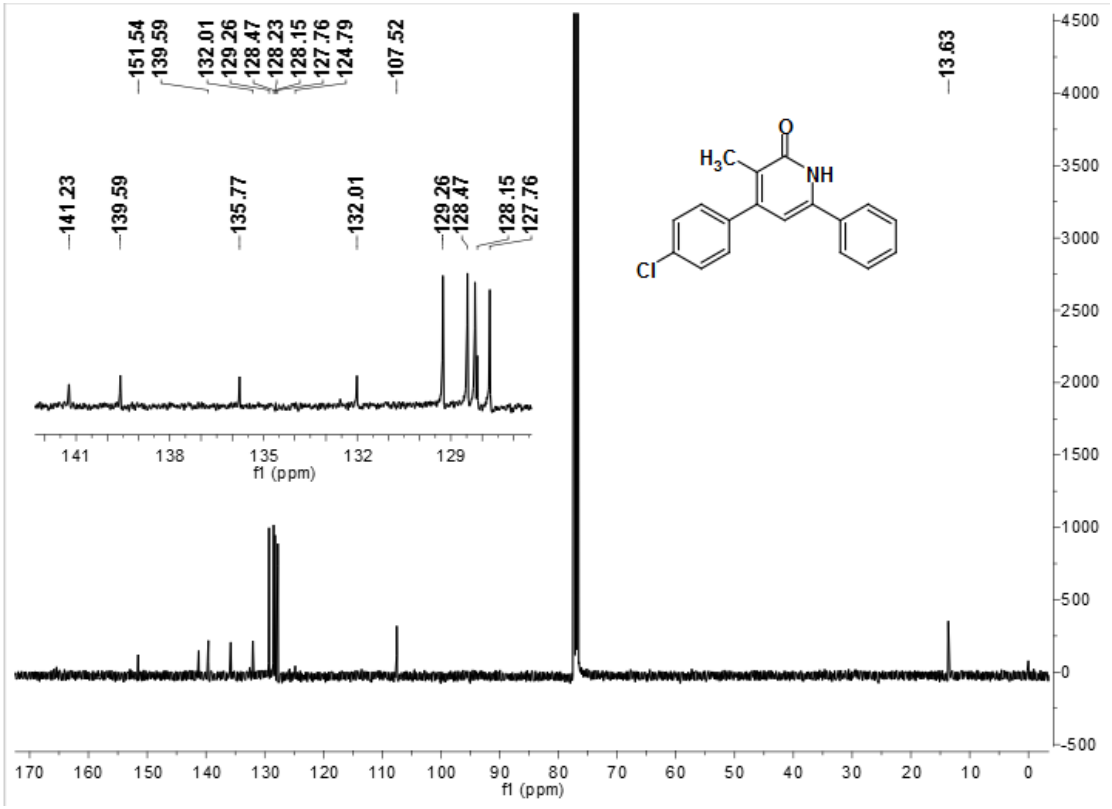
Compound **5h**


12.22
7.79
7.45
7.41
7.39
7.37
7.18
7.14
6.45
2.12
O
H3C
NH
F
1.00
2.00
5.01
2.04
1.01
3.01
f1 (ppm)

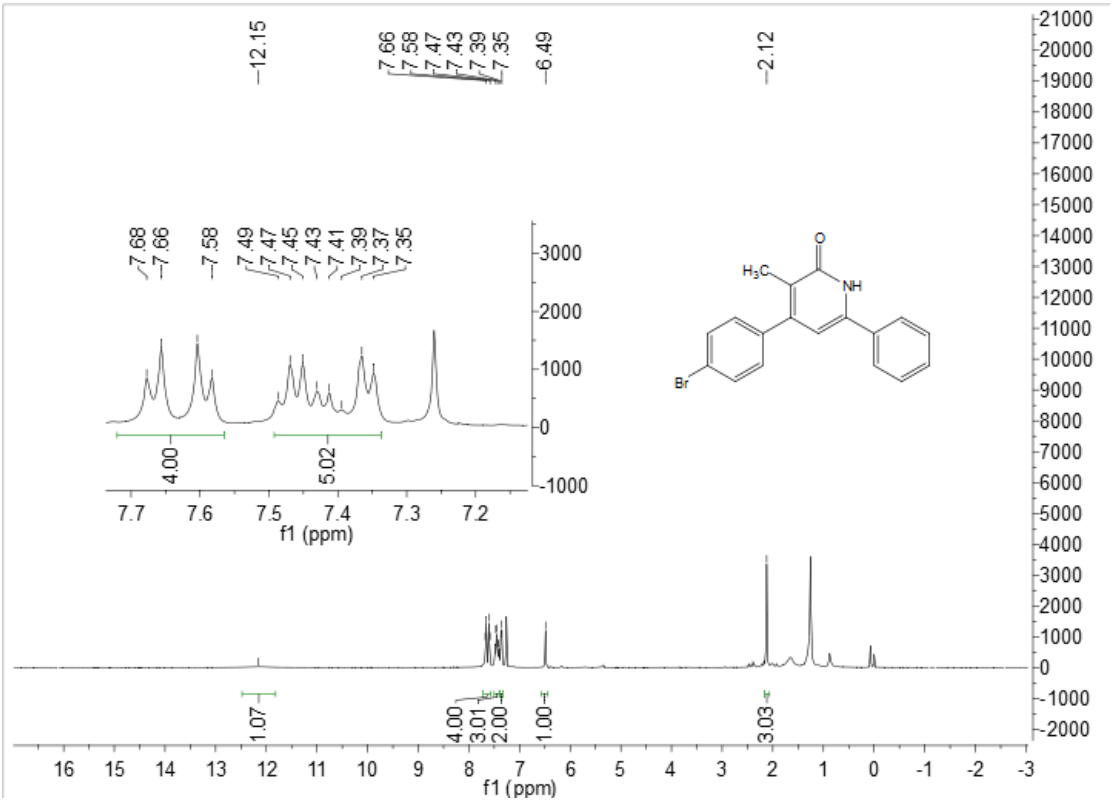

164.85
162.37
151.60
139.69
128.23
116.18
115.96
107.30
13.56
O
H3C
NH
F
f1 (ppm)

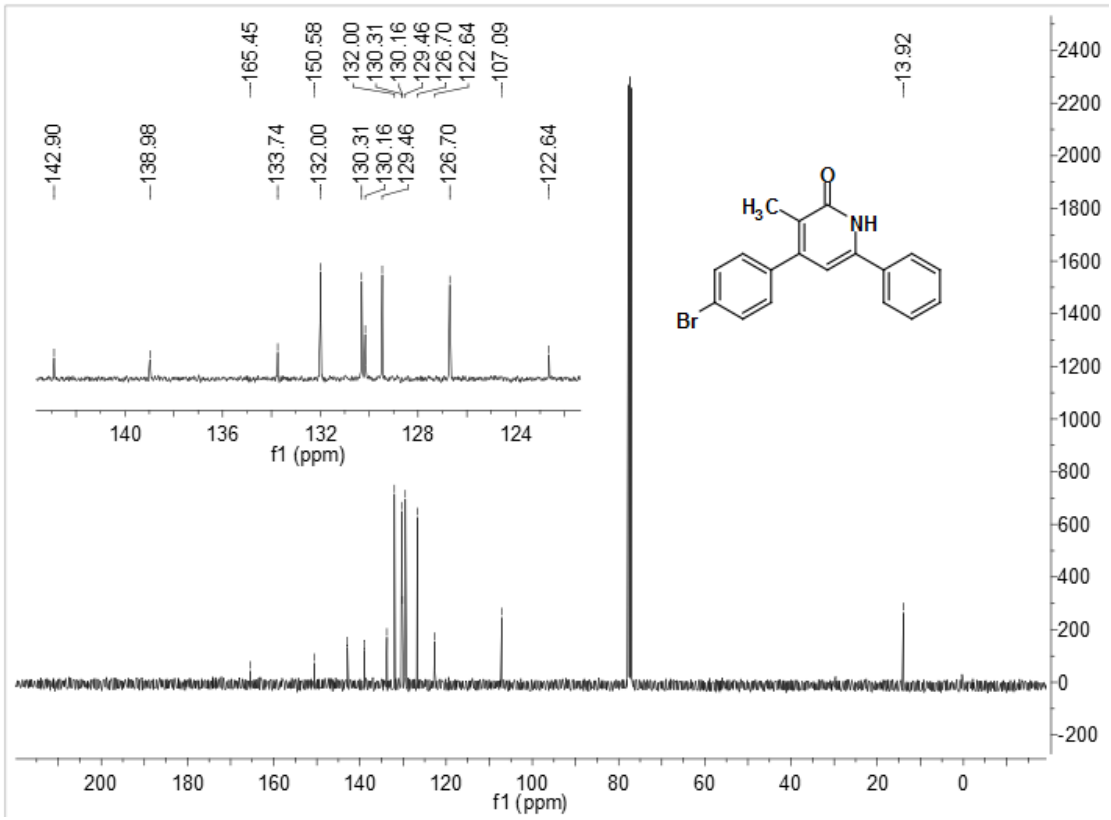
Compound **5i**


11.90
7.46
7.44
7.43
7.41
7.40
7.37
7.35
6.41
2.06
O
H3C
NH
Cl
1.02
2.06
7.41
1.08
3.03
f1 (ppm)

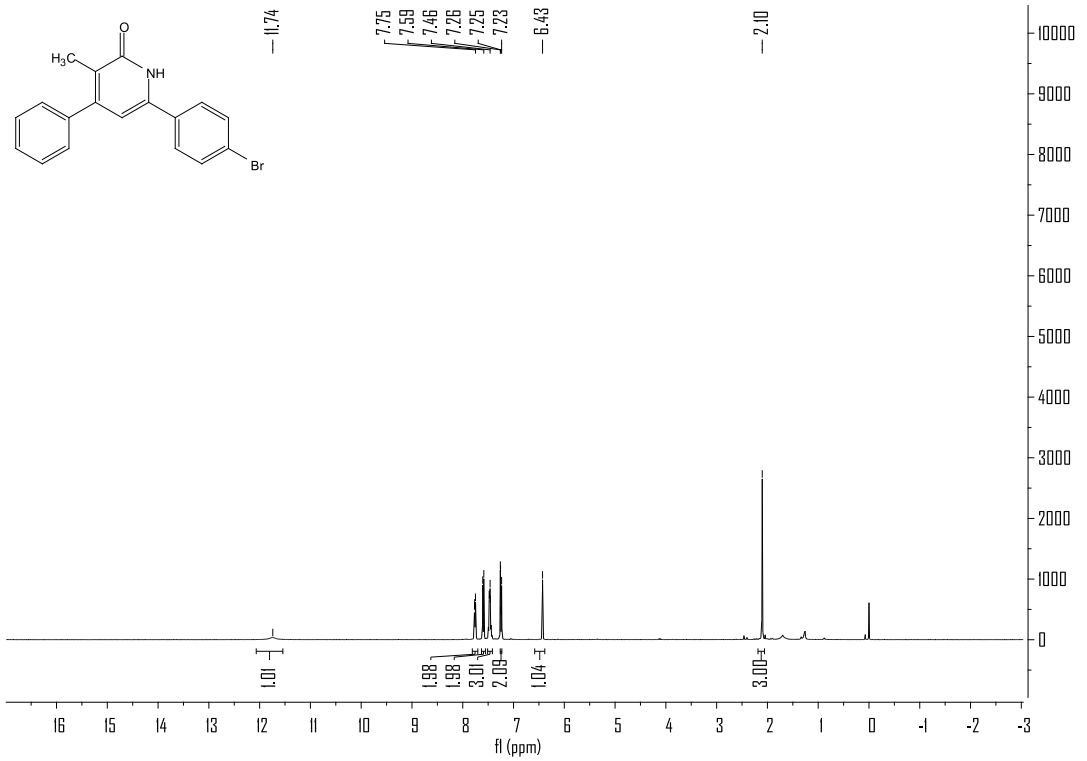

151.54
139.59
132.01
129.26
128.47
128.23
128.15
127.76
124.79
107.52
13.63
141.23
139.59
135.77
132.01
129.26
128.47
128.15
127.76
O
H3C
NH
Cl
f1 (ppm)
f1 (ppm)

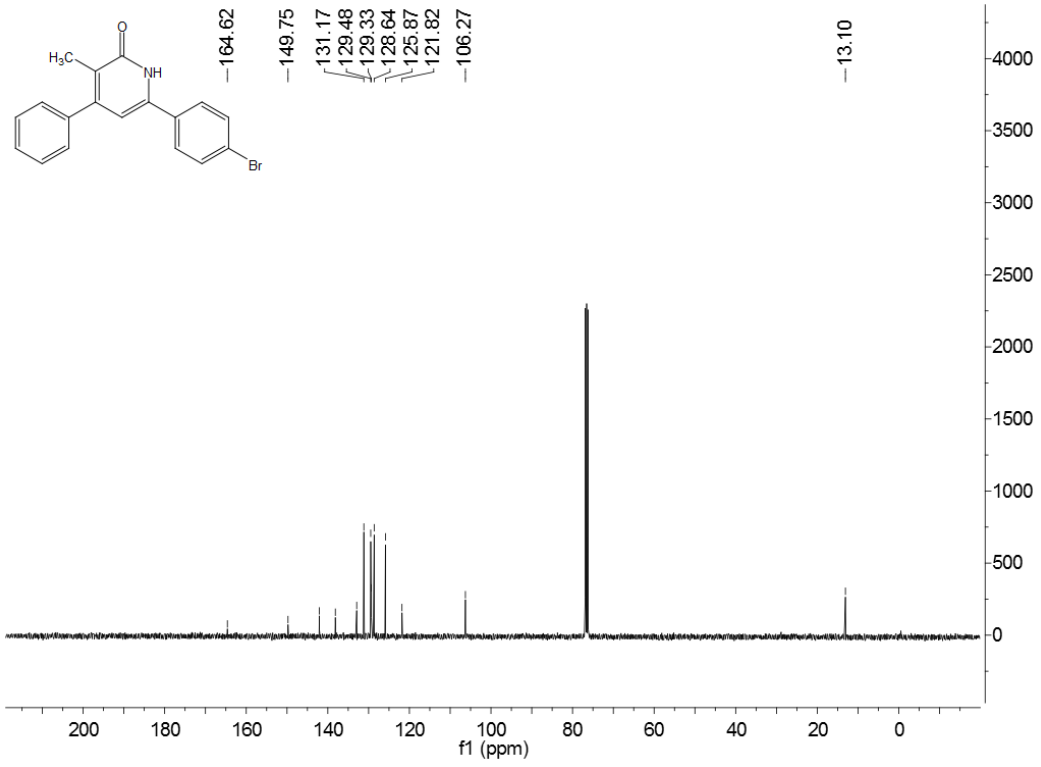
Compound **5j**


12.15
7.66
7.58
7.47
7.43
7.39
7.35
6.49
2.12
7.68
7.66
7.58
7.49
7.47
7.45
7.43
7.41
7.39
7.37
7.35
4.00
5.02
f1 (ppm)
1.07
4.00
3.01
2.00
1.00
3.03
f1 (ppm)
O
NH
H3C
Br

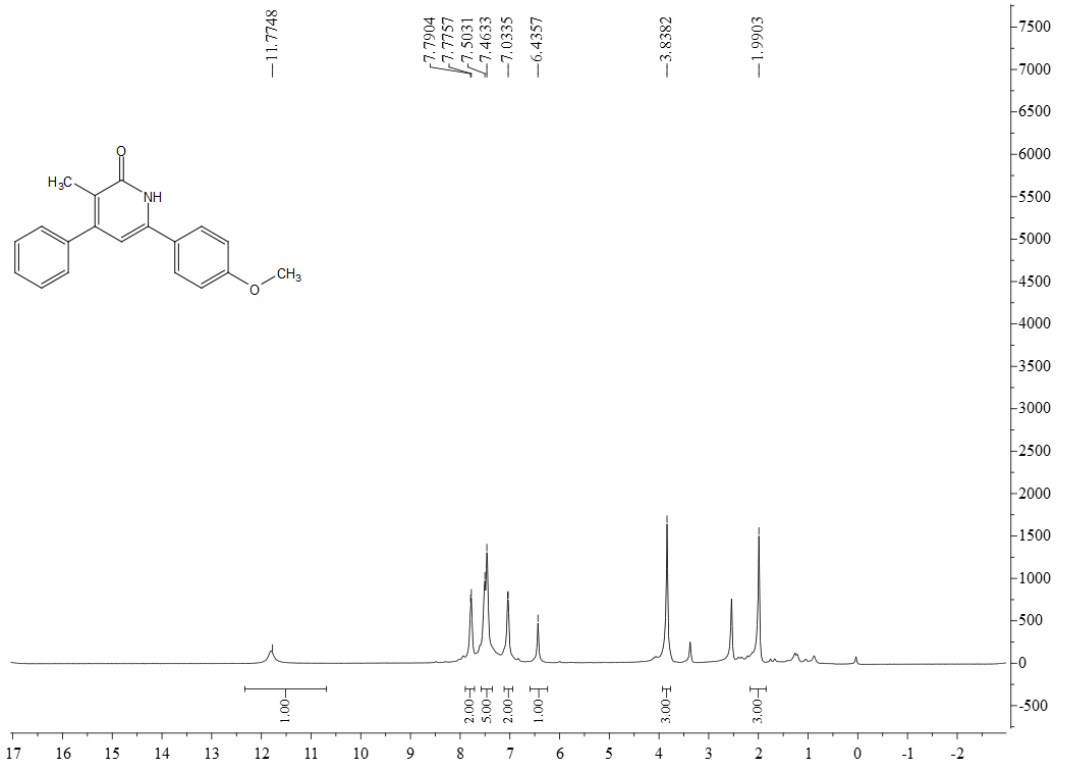

165.45
150.58
132.00
130.31
130.16
129.46
126.70
122.64
107.09
13.92
142.90
138.98
133.74
132.00
130.31
130.16
129.46
126.70
122.64
f1 (ppm)
f1 (ppm)
O
NH
H3C
Br

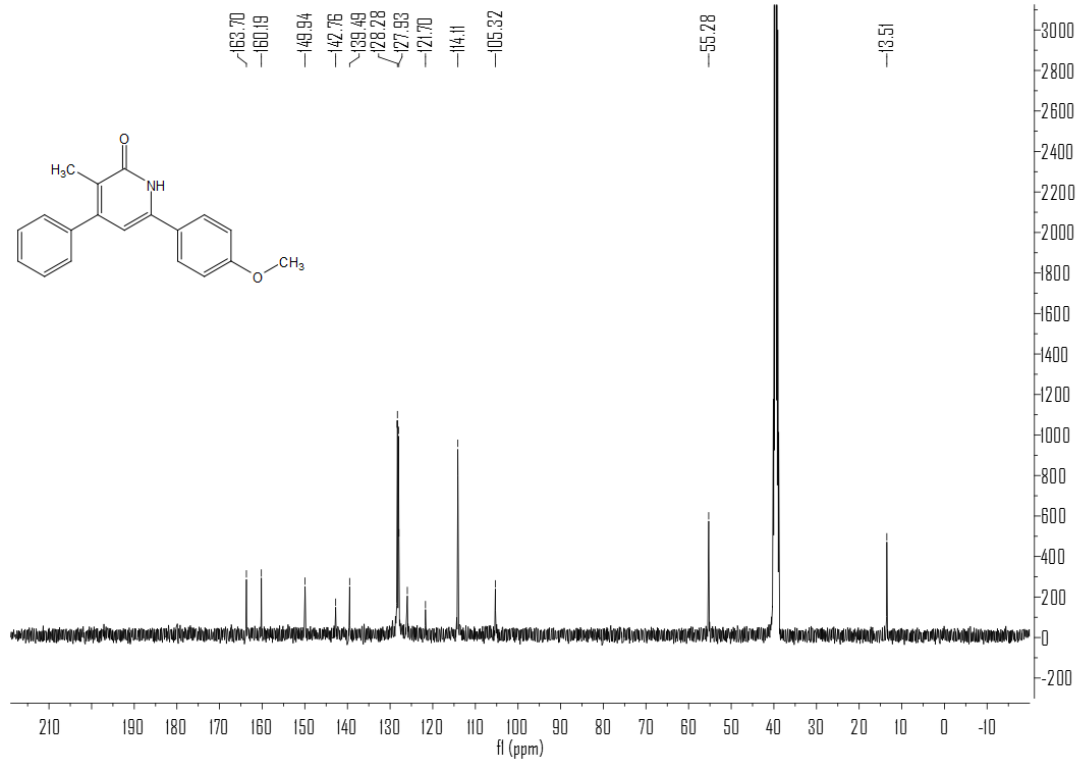
Compound **5k**


11.74
7.75
7.59
7.46
7.26
7.25
7.23
6.43
2.10
1.01
1.98
1.98
3.01
2.09
1.04
3.00
f1 (ppm)

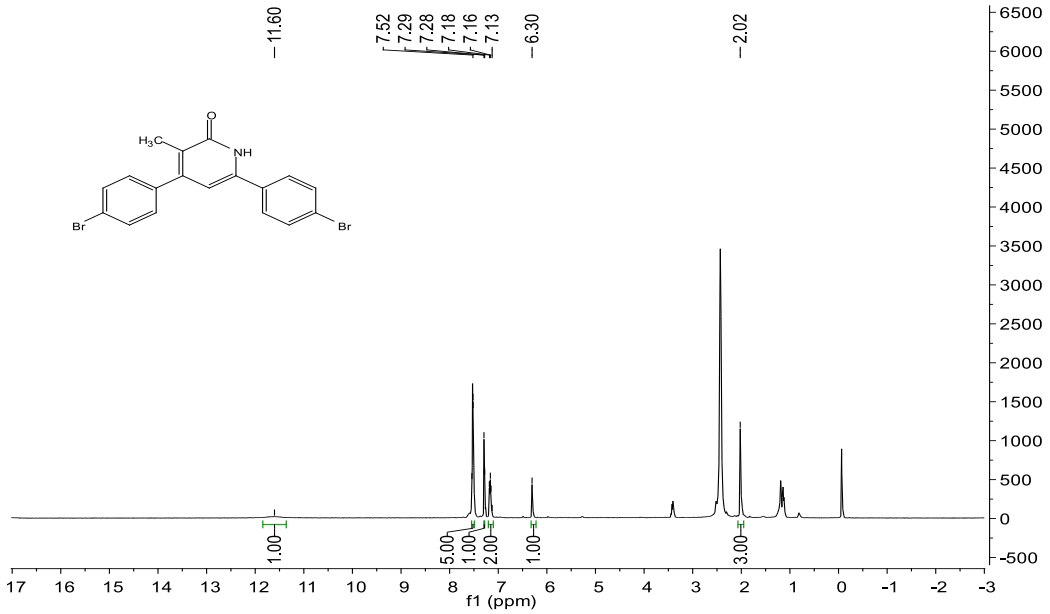

164.62
149.75
131.17
129.48
129.33
128.64
125.87
121.82
106.27
13.10
f1 (ppm)

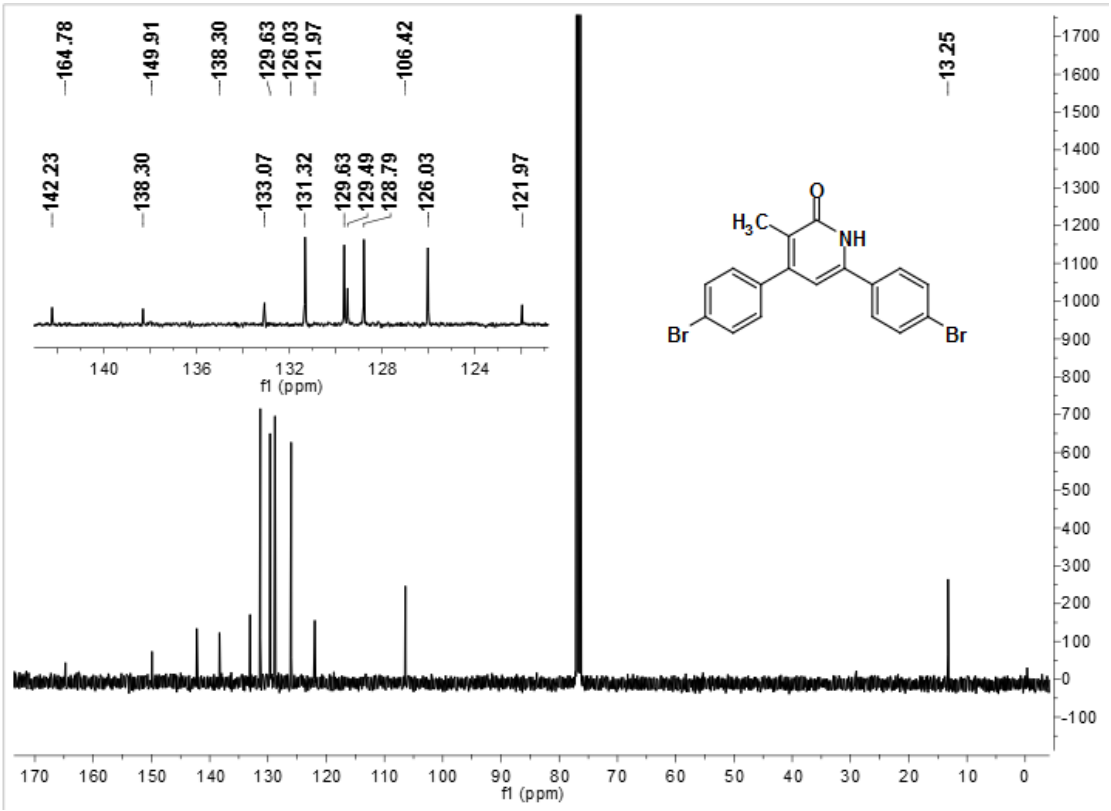
Compound **5l**


11.7748
7.7904
7.7757
7.5031
7.4633
7.0335
6.4357
3.8382
1.9903
1.00
2.00
5.00
2.00
1.00
3.00
3.00
O
H3C
NH
O
CH3

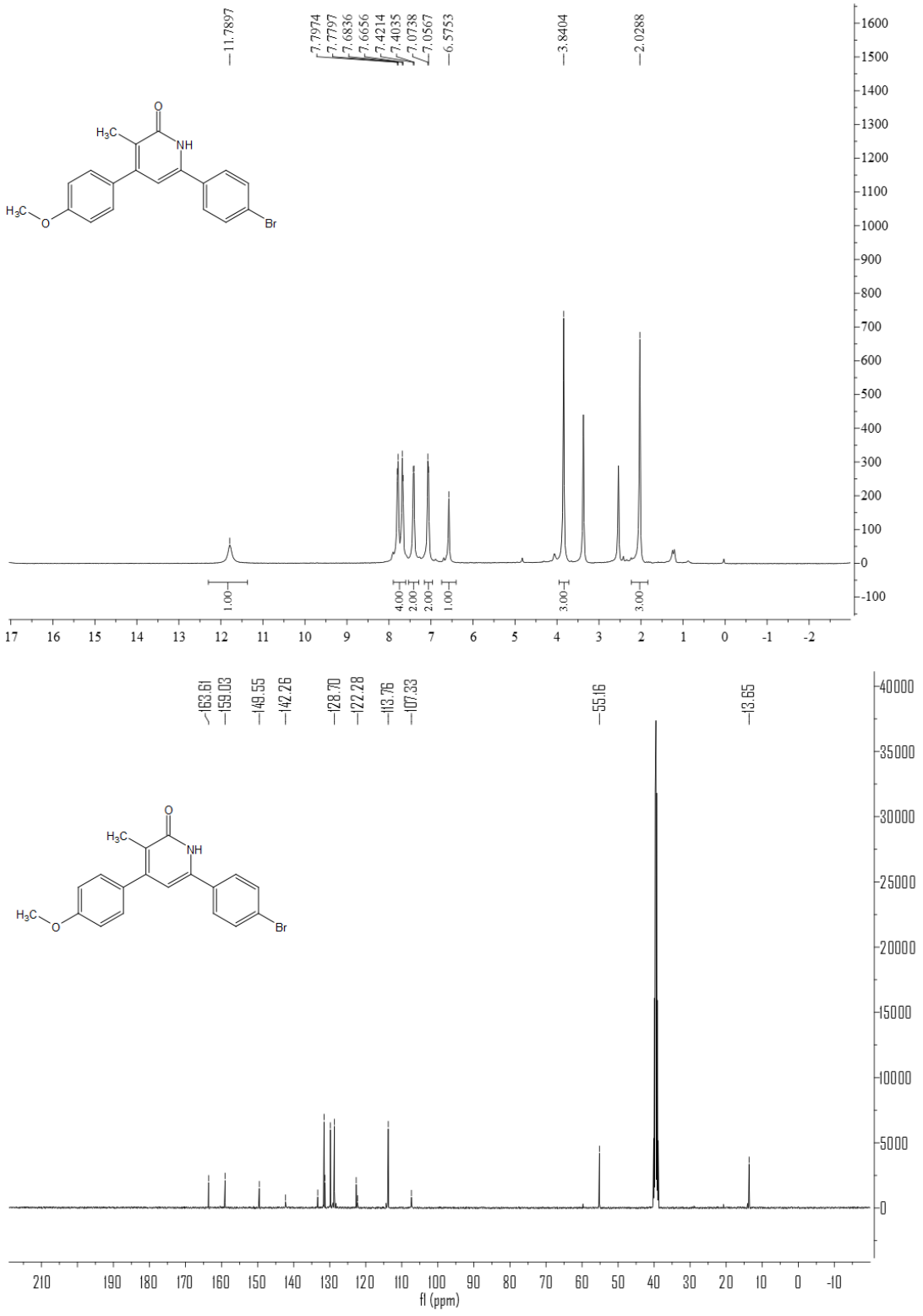

163.70
160.19
149.94
142.76
139.49
128.28
127.93
121.70
114.11
105.32
55.28
13.51
O
H3C
NH
O
CH3
f1 (ppm)

Compound **5m**

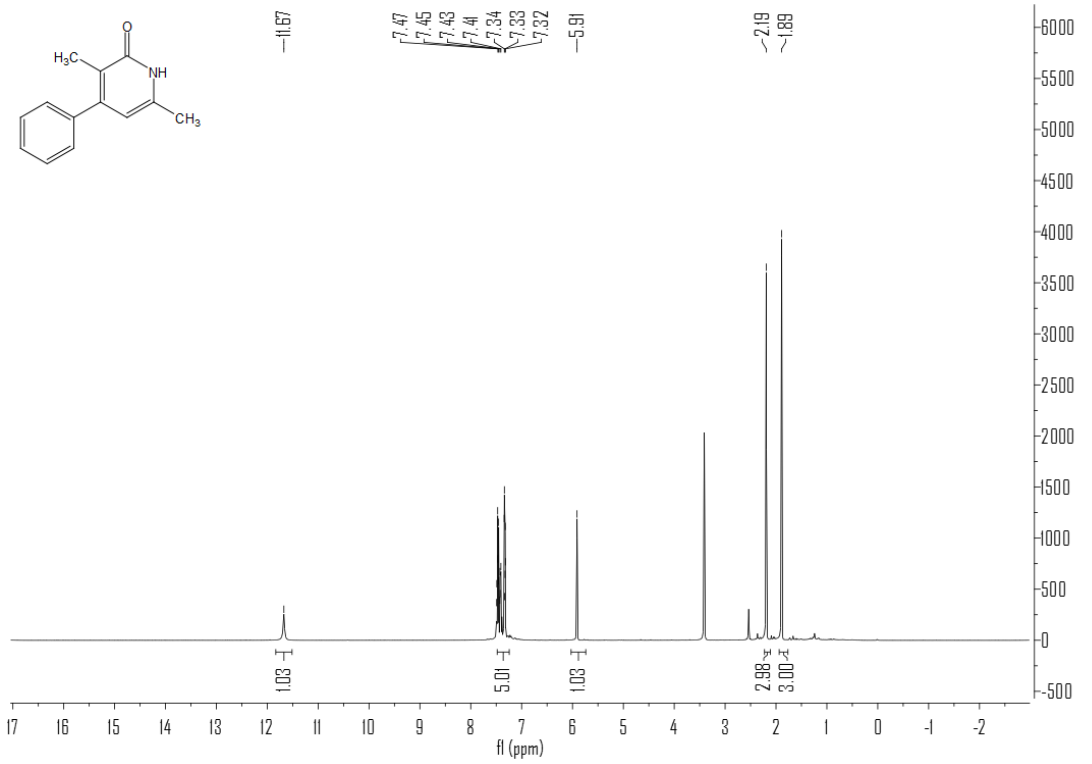

11.60
7.52
7.29
7.28
7.18
7.16
7.13
6.30
2.02
1.00
5.00
1.00
2.00
1.00
3.00
f1 (ppm)

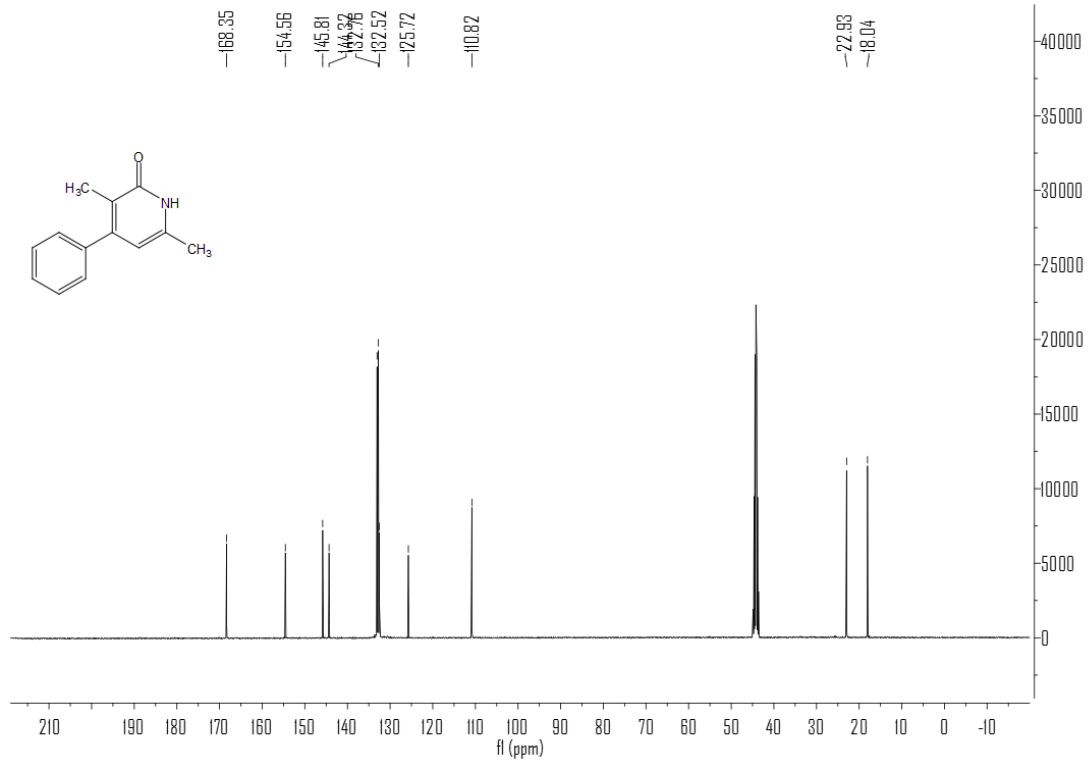

164.78
149.91
138.30
129.63
126.03
121.97
106.42
13.25
142.23
138.30
133.07
131.32
129.63
129.49
128.79
126.03
121.97
f1 (ppm)
f1 (ppm)

Compound **5n**

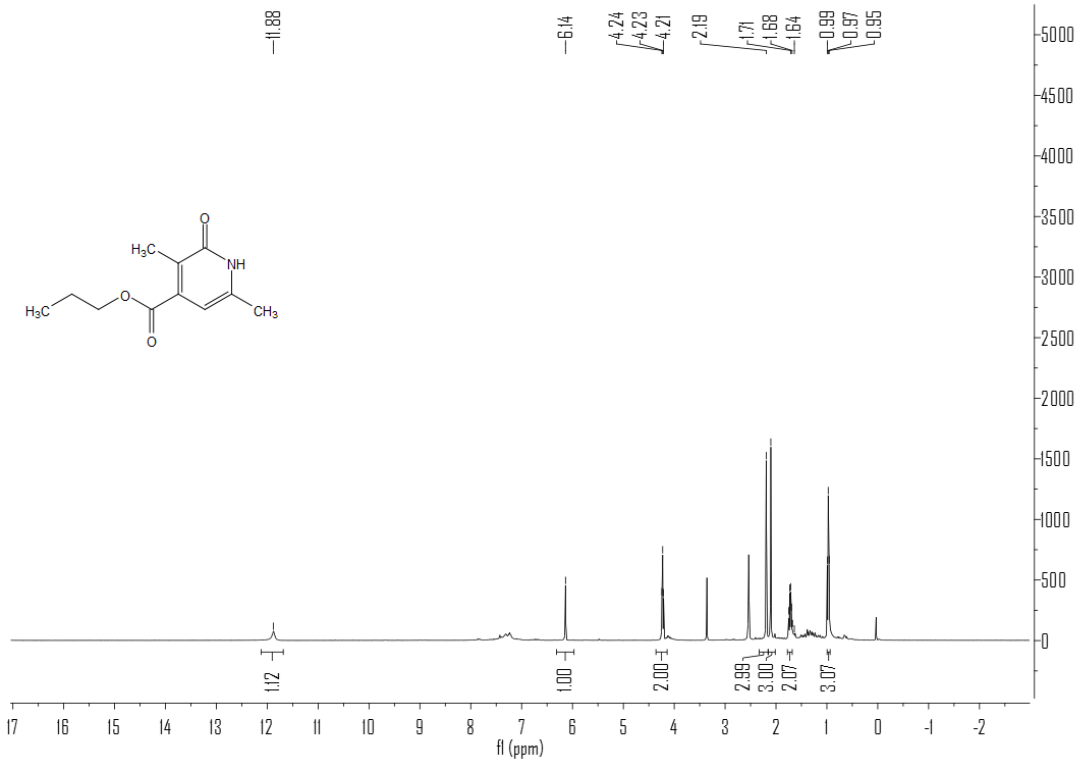

11.7897
7.7974
7.7797
7.6836
7.6656
7.4214
7.4035
7.0738
7.0567
6.5753
3.8404
2.0288
1.00
4.00
2.00
2.00
1.00
3.00
3.00
O
H3C
NH
H3C
O
Br
163.61
159.03
149.55
142.26
128.70
122.28
113.76
107.33
55.16
13.65
f1 (ppm)

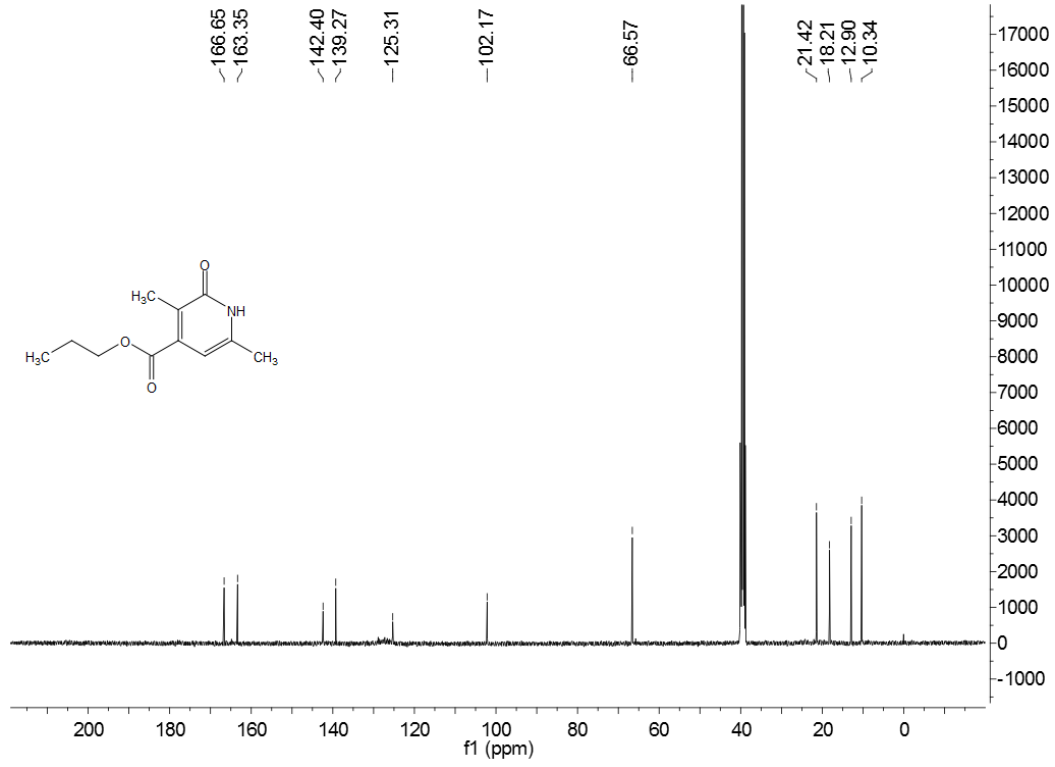
Compound **5o**


11.67
7.47
7.45
7.43
7.41
7.34
7.33
7.32
5.91
2.19
1.89
1.03
5.01
1.03
2.98
3.00
f1 (ppm)

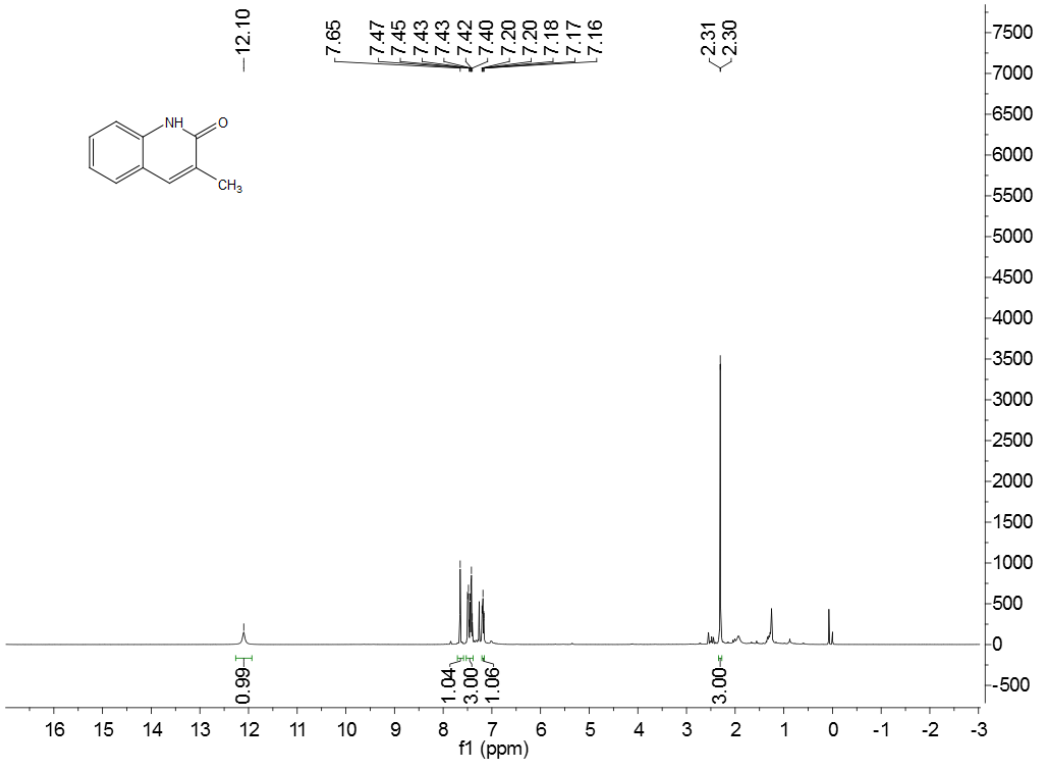

168.35
154.56
145.81
144.32
132.76
132.52
125.72
110.82
22.93
18.04
f1 (ppm)

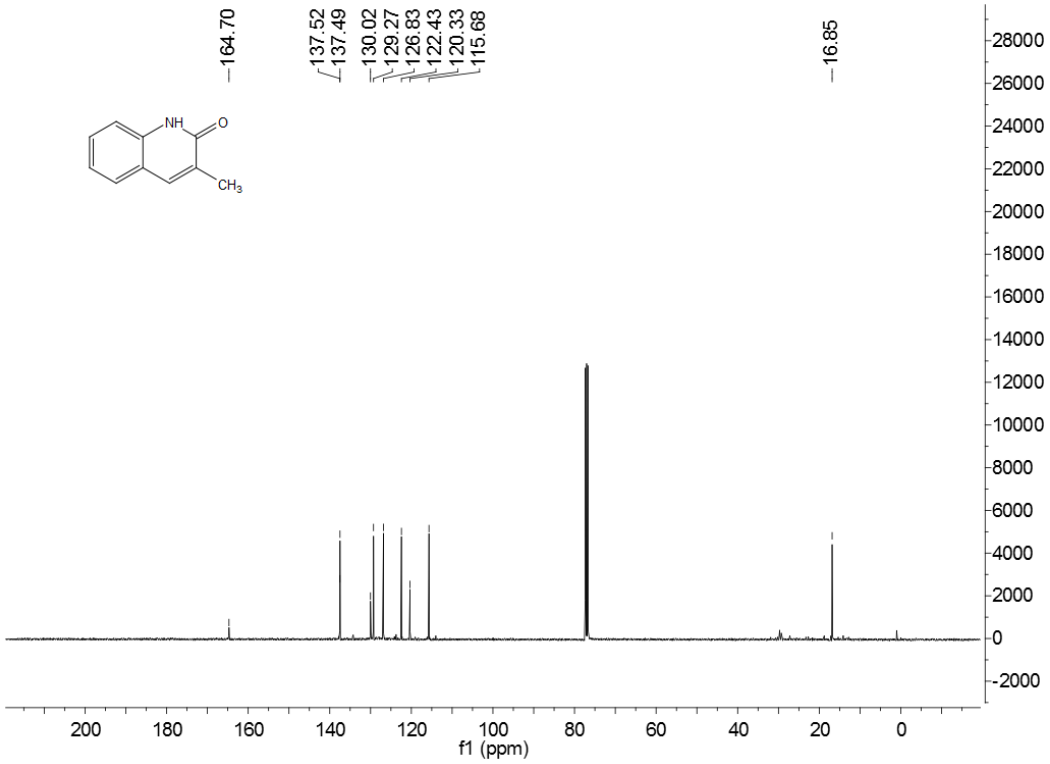
Compound **5p**


11.88
6.14
4.24
4.23
4.21
2.19
1.71
1.68
1.64
0.99
0.97
0.95
1.12
1.00
2.00
2.99
3.00
2.07
3.07
f1 (ppm)

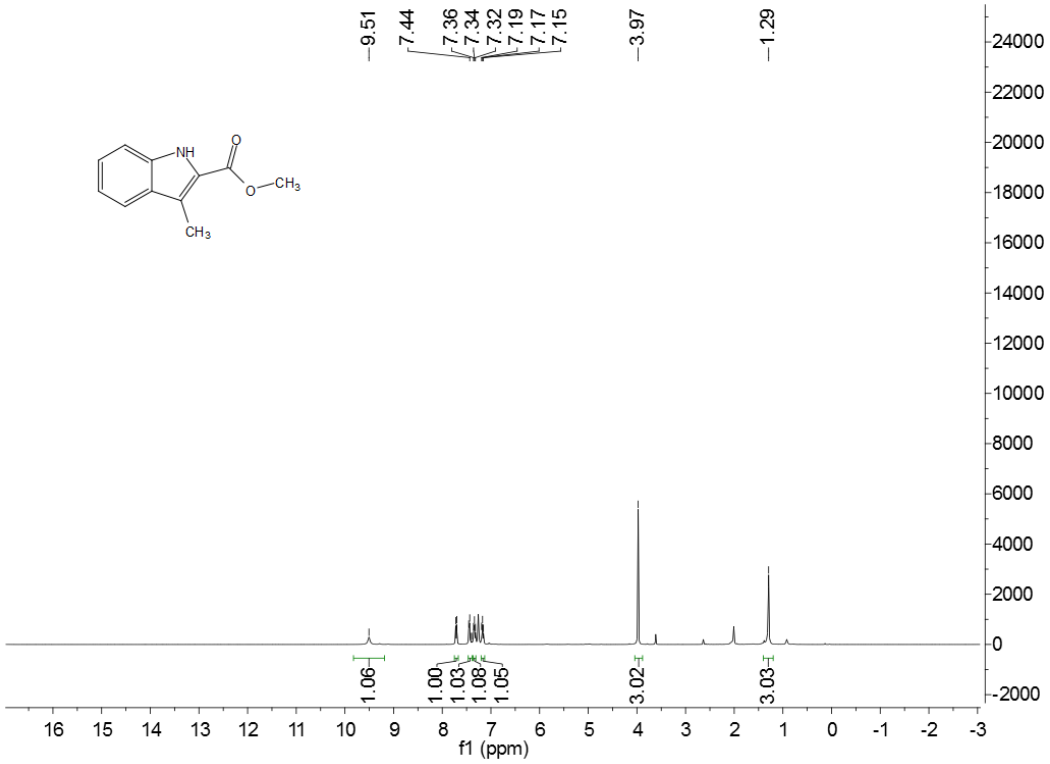

166.65
163.35
142.40
139.27
125.31
102.17
66.57
21.42
18.21
12.90
10.34
f1 (ppm)

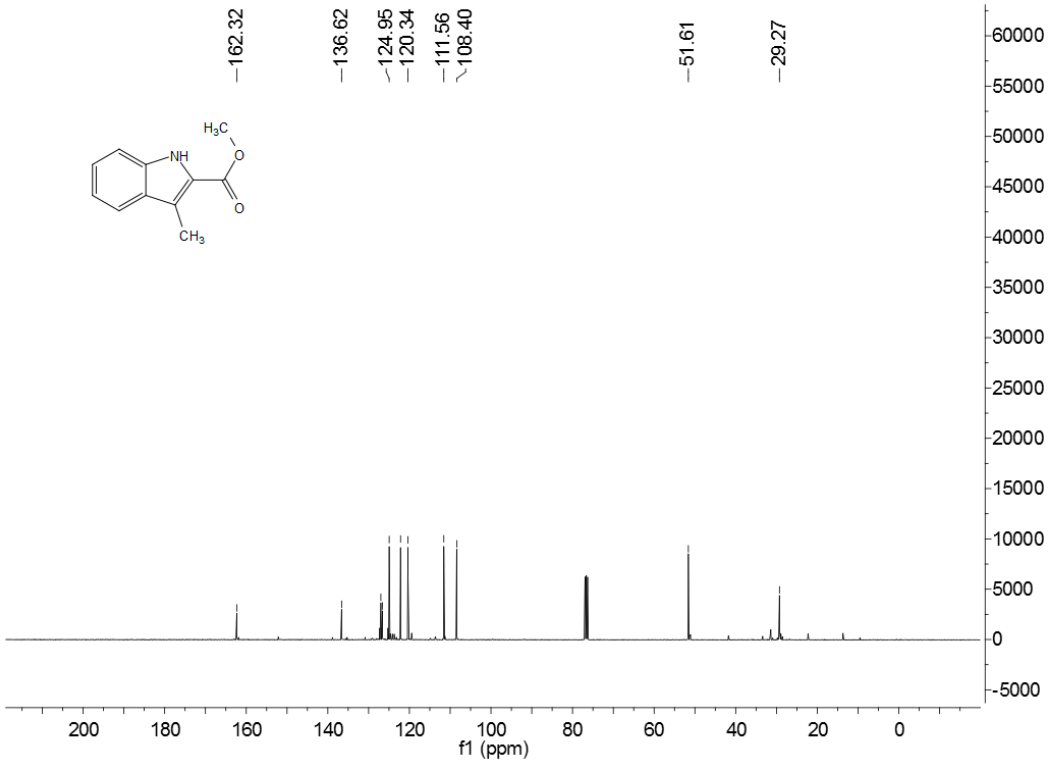
Compound **5q**


12.10
7.65
7.47
7.45
7.43
7.43
7.42
7.40
7.20
7.20
7.18
7.17
7.16
2.31
2.30
NH
O
CH3
0.99
1.04
3.00
1.06
3.00
f1 (ppm)


164.70
137.52
137.49
130.02
129.27
126.83
122.43
120.33
115.68
16.85
NH
O
CH3
f1 (ppm)

Compound **5r**


9.51
7.44
7.36
7.34
7.32
7.19
7.17
7.15
3.97
1.29
NH
O
O
CH3
CH3
1.06
1.00
1.03
1.08
1.05
3.02
3.03
f1 (ppm)


162.32
136.62
124.95
120.34
111.56
108.40
51.61
29.27
H3C
NH
O
O
CH3
f1 (ppm)