Supporting Information

Immobilization of Manganese Dioxide Nanoparticles on Modified Poly 2,4-dichlorostyrene Microspheres: An Highly Efficient and Recyclable Catalyst for Borrowing Hydrogen Reactions

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1. General methods and materials:

All of the reactions dealing with air and/or moisture-sensitive reactions were carried out under an atmosphere of nitrogen using oven/flame-dried glassware and standard syringe/ Schlenk tube. Unless otherwise noted, all commercial reagents and solvents were obtained from the commercial provider and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker Advance III HD 400 or 101 MHz spectrometers. Chemical shifts were reported relative to internal tetramethylsilane (δ 0.00 ppm) or $CDCl_3$ (δ 7.26 ppm) for ^{1}H NMR and $CDCl_3$ (δ 77.0 ppm) for ^{13}C NMR. Flash column chromatography was performed on 230-430 mesh silica gel. Analytical thin layer chromatography was performed with precoated glass baked plates (250μ) and visualized by fluorescence. HRMS were recorded on LTQ-FTUHRA spectrometer. The crystal structures were characterized with powder X-ray diffraction (XRD) on a Bruker D8 Advance X-ray diffractometer. TEM was recorded on a transmission electron microscope (JEM–2100, JEOL, Japan), operating at 200 kV. SEM image and EDS spectra was performed on a HITACHI S-4800 field-emission scanning electron microscope. XPS data were recorded with electron energy analyzer (ESCALAB 250Xi, Thermo Fisher Co, USA).

2. Synthesis of catalysts

The polyvinylpyrrolidone (1.400 g), azoisobutyronitrile (0.100 g), and isopropanol (80 mL) were separately weighed into a 250 ml Schlenk bottle, fully dissolved, and heated to 70 °C under nitrogen. fully dissolved, and heated to 70 ^{o}C under nitrogen. After completion of the reaction, 2,4-dichlorostyrene (10.0 g) was added, and polymerization was carried out for 24 hours while stirring at room temperature. The modified poly 2,4-dichlorostyrene microspheres (PDCS) were collected by centrifugation, washed three times with water and ethanol, sonicated, and finally freeze-dried for 12 hours.

The modified poly 2,4-dichlorostyrene microspheres (0.100 g), $KMnO_4$ (0.005 g), 20 mL of deionized water were added to a 100 mL round bottom flask and magnetically stirred for 10 minutes at room temperature to form a homogeneous solution. The solution was then transferred to a 40 mL teflon reactor and crystallized for 10 hours in an electrothermally heated constant temperature blast drying oven at 120 ^{o}C. After cooling to room temperature, remove the kettle, collected by centrifugation, and the impurities were removed by washing with deionized water for 3 to 4 times. Vacuum freeze-drying gave the product α-MnO_2@PDCS nanocatalyst.

The synthesis of other MnO_2 catalysts.

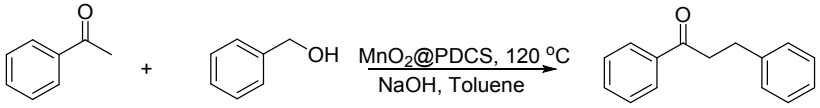
(**α-MnO_2-PS**) The polystyrene microspheres (0.100 g), $KMnO_4$ (0.005 g), 20 mL of deionized water were added to a 100 mL round bottom flask and magnetically stirred for 10 minutes at room temperature to form a homogeneous solution. The solution was then transferred to a 40 mL teflon reactor and crystallized for 10 hours in an electrothermally heated constant temperature blast drying oven at 120 °C. After cooling to room temperature, remove the kettle, collected by centrifugation, and the impurities were removed by washing with deionized water for 3 to 4 times. Vacuum freeze-drying gave the product α-MnO_2@PCS nanocatalyst.

(**α-MnO_2-PCS**) The poly 4-cyanostyrene microspheres (0.100 g), $KMnO_4$ (0.005 g), 20 mL of deionized water were added to a 100 mL round bottom flask and magnetically stirred for 10 minutes at room temperature to form a homogeneous solution. The solution was then transferred to a 40 mL teflon reactor and crystallized for 10 hours in an electrothermally heated constant temperature blast drying oven at 120 °C. After cooling to room temperature, remove the kettle, collected by centrifugation, and the impurities were removed by washing with deionized water for 3 to 4 times. Vacuum freeze-drying gave the product α-MnO_2@PCS nanocatalyst.

(**α-MnO_2-PBS**) The poly 4-bromostyrene microspheres (0.100 g), $KMnO_4$ (0.005 g), 20 mL of deionized water were added to a 100 mL round bottom flask and magnetically stirred for 10 minutes at room temperature to form a homogeneous solution. The solution was then transferred to a 40 mL teflon reactor and crystallized for 10 hours in an electrothermally heated constant temperature blast drying oven at 120 °C. After cooling to room temperature, remove the kettle, collected by centrifugation, and the impurities were removed by washing with deionized water for 3 to 4 times. Vacuum freeze-drying gave the product α-MnO_2@PCS nanocatalyst.

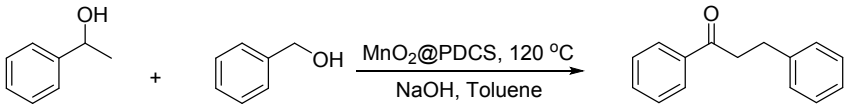
(**α-MnO_2-PNS**) The poly 4-nitrostyrene microspheres (0.100 g), $KMnO_4$ (0.005 g), 20 mL of deionized water were added to a 100 mL round bottom flask and magnetically stirred for 10 minutes at room temperature to form a homogeneous solution. The solution was then transferred to a 40 mL teflon reactor and crystallized for 10 hours in an electrothermally heated constant temperature blast drying oven at 120 °C. After cooling to room temperature, remove the kettle, collected by centrifugation, and the impurities were removed by washing with deionized water for 3 to 4 times. Vacuum freeze-drying gave the product α-MnO_2@PCS nanocatalyst.

3. General procedure for the alkylation of acetophenone with alcohol



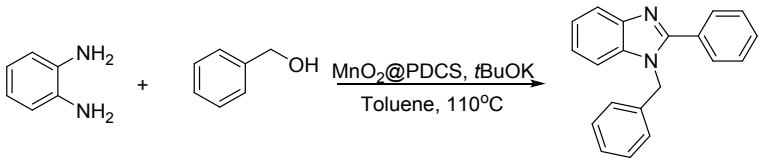
To 20 mL Schlenk tube was added α-MnO_2@PDCS (15 mg), alcohol (1.2 mmol), acetophenone (1.0 mmol), NaOH (1.0 mmol) and toluene (2.5 mL). The mixture was heated under 120 °C for 12 h and TLC method was used to track and detect the reaction mixture. After the reaction, the solvent was removed by rotating evaporation, and the reaction mixture was separated by column chromatography with gradient elution method. The corresponding eluents were collected and combined with spin-dry solvents. (Petroleum ether /ethyl acetate (v/v = 40:1))

3.1 General procedure for cross-coupling of secondary and primary alcohols



To 20 mL Schlenk tube was added α-MnO_2@PDCS (15 mg), primary alcohol (1.2 mmol), Secondary alcohol (2.0 mmol), NaOH (1.0 mmol) and toluene (2.5 mL). The mixture was heated under 120 °C for 18 h and then cooled to room temperature. and TLC method was used to track and detect the reaction mixture. After the reaction, the solvent was removed by rotating evaporation, and the reaction mixture was separated by column chromatography with gradient elution method The corresponding eluents were collected and combined with spin-dry solvents. (Petroleum ether /ethyl acetate (v/v = 40:1)).

3.2 Representative procedure for the preparation of 6a



To 20 mL Schlenk tube was added α-MnO_2@PDCS (15 mg), alcohol (1.10 mmol), amine (0.50 mmol) and potassium *tert*-butoxide (0.75 mmol) and toluene (3.0 mL). The mixture was heated under 110 °C for 24 h and then cooled to room temperature. and TLC method was used to track and detect the reaction mixture. After the reaction, the solvent was removed by rotating evaporation, and the reaction mixture was separated by column chromatography with gradient elution method. The corresponding eluents were collected and combined with spin-dry solvents. (Petroleum ether /ethyl acetate (v/v = 60:1)).

4. **Other characterizations of catalysts.**

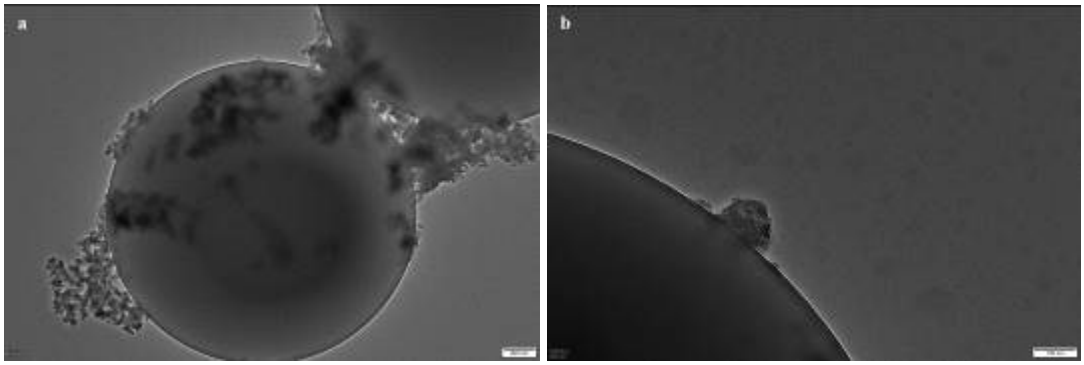
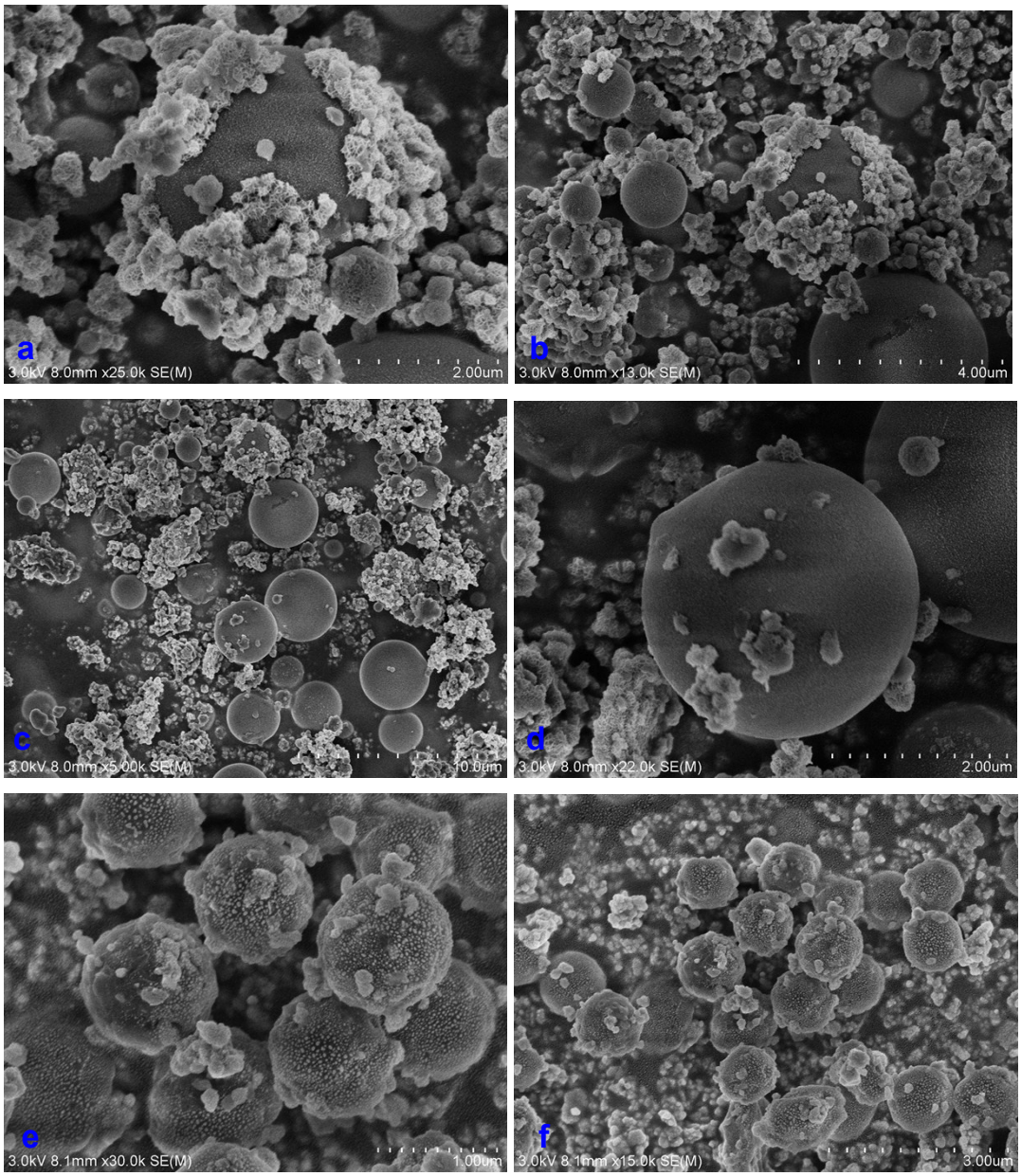


Fig.S1. TEM images of (a), (b) α-MnO_2-PDCS.



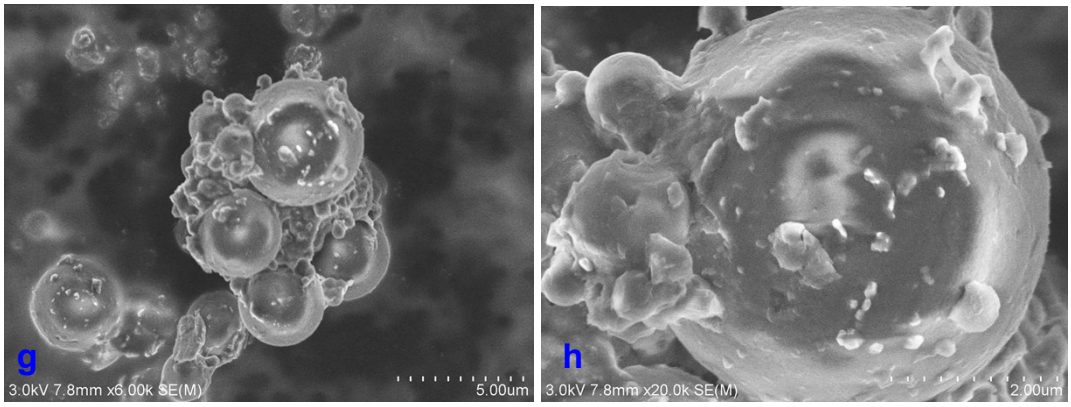
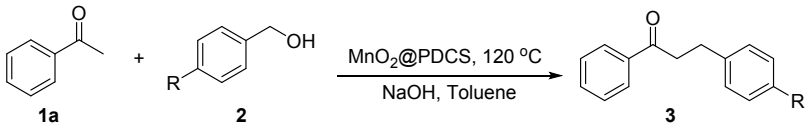


Fig.S2. SEM images of (a), (b) α-MnO_2-PS; (c), (d) α-MnO_2-PCS; (e), (f) α-MnO_2-PBS; (g), (h) α-MnO_2-PNS;

5. Hammett plot and mechanism studies.

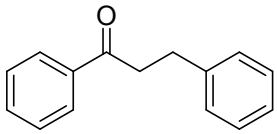


Experimental procedure: To 20 mL Schlenk tube was added α-MnO_2@PDCS (15 mg), alcohol (1.2 mmol), acetophenone (1.0 mmol), NaOH (1.0 mmol) and toluene (2.5 mL). The mixture was heated under 120 °C for 1 h. After centrifugation and recovery the catalyst, the water mixture was diluted by water (5.0 mL) and extracted with EtOAc (3 x 10 mL). Next, the yield of product **3** was determined by GC.

R	H	Me	OMe	F	CF_3
Yield	12 %	19%	16%	7 %	5 %

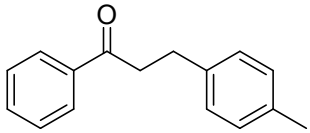
6. Analytical data of the obtained compounds

(1) 1,3-diphenylpropan-1-one (3a)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.94 (m, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.35 – 7.33 (m, 4H), 7.31 (t, *J* = 7.7 Hz, 1H), 3.41 (t, *J* = 7.7 Hz, 2H), 3.20 – 3.08 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.16, 141.42, 137.03, 132.99, 128.73, 128.54, 128.58, 128.07, 126.19, 40.53, 30.18.

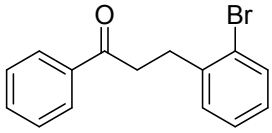
（2）1-phenyl-3-(*p*-tolyl)propan-1-one (3b)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.1 Hz, 2H), 7.59 – 7.52 (m, 1H), 7.48 (t, *J* = 7.6 Hz, 2H),

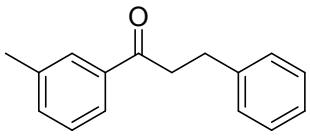
7.21(q, J = 8.1 Hz, 4H), 3.29– 3.16 (m, 2H), 3.11 – 3.04 (m, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.43, 138.26, 136.89, 135.70, 133.11, 129.17, 128.58, 128.35, 127.99, 40.68, 29.81, 21.09.

(3) 3-(2-bromophenyl)-1-phenylpropan-1-one (3c)



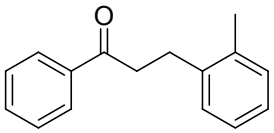
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 7.89 (m, 2H), 7.62 (t, J = 7.4 Hz, 2H), 7.51 (t, J = 7.6 Hz, 2H), 7.41 (dd, J = 7.6, 1.7 Hz, 1H), 7.31 (td, J = 7.5, 1.1 Hz, 1H), 7.08 (td, J = 7.7, 1.7 Hz, 1H), 3.41 – 3.33 (m, 2H), 3.30 – 3.05 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.01, 140.68, 136.76, 133.09, 132.95, 130.87, 128.59, 128.07, 127.96, 127.72, 124.39, 38.56, 30.78.

(4) 3-phenyl-1-(*m*-tolyl)propan-1-one (3d)



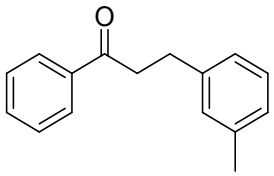
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.9 Hz, 2H), 7.45 – 7.30 (m, 2H), 7.28 (m, 4H), 7.09 (t, J = 5.3 Hz, 1H), 3.28 (m, 2H), 3.16 – 2.99(m, 2H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.52, 141.43, 138.38, 136.87, 133.79, 128.99, 128.87, 128.49, 128.51, 126.08, 125.31, 40.49, 30.28, 21.43.

(5) 1-phenyl-3-(*o*-tolyl)propan-1-one (3e)



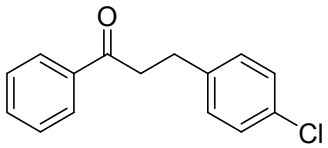
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, J = 8.3, 1.3 Hz, 2H), 7.71 – 7.50 (m, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.31 – 7.09 (m, 4H), 3.28 (dd, J = 9.0, 6.4 Hz, 2H), 3.06 (dd, J = 9.0, 6.7 Hz, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.41, 139.37, 136.89, 135.97, 132.99, 130.41, 128.6, 128.56, 128.12, 126.26, 126.18, 39.06, 27.61, 19.42.

(6) 1-phenyl-3-(*m*-tolyl)propan-1-one (3f)



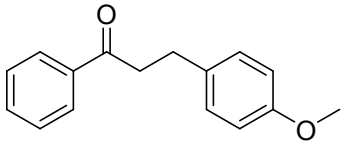
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.94 (m, 2H), 7.64 – 7.52 (m, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.30 (t, J = 7.5 Hz, 1H), 7.03 (dd, J = 14.2, 9.4 Hz, 3H), 3.41 – 3.31 (m, 2H), 3.09 – 2.99 (m, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.40, 141.31, 138.08, 136.87, 133.00, 129.32, 128.69, 128.53, 128.11, 127.08, 125.56, 40.63, 29.98, 21.54.

(7) 3-(4-chlorophenyl)-1-phenylpropan-1-one (3g)



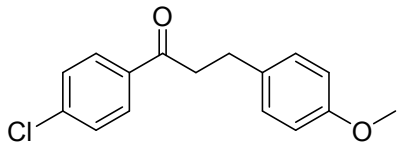
^{1}H NMR (400 MHz, CDCl3) δ 8.03 – 7.90 (m, 2H), 7.64 – 7.54 (m, 1H), 7.49 – 7.38 (m, 2H), 7.33 – 7.21(m, 2H), 7.25 – 7.09 (m, 2H), 3.29 (t, *J* = 7.5 Hz, 2H), 3.11 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, CDCl3) δ 198.87, 139.80, 136.84, 133.21, 131.93, 130.41, 129.95, 128.73, 127.98, 40.21, 29.39.

(8) 3-(4-methoxyphenyl)-1-phenylpropan-1-one (3h)



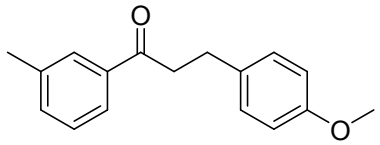
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.5 Hz, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.25 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 8.6 Hz, 2H), 3.79 (s, 3H), 3.38 (t, *J* = 7.7 Hz, 2H), 3.11 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.50, 159.98, 137.00, 133.45, 133.11, 129.43, 128.70, 127.99, 114.01, 55.27, 40.84, 29.28.

(9) 1-(4-chlorophenyl)-3-(4-methoxyphenyl)propan-1-one (3i)



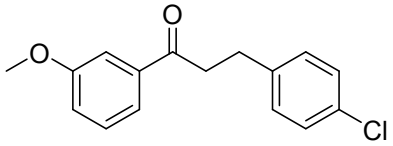
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.80 (m, 2H), 7.53 – 7.37 (m, 2H), 7.21 – 7.18 (m, 2H), 6.93 – 6.79 (m, 2H), 3.76 (s, 3H), 3.31 (t, *J* = 7.6 Hz, 2H), 2.97 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.04, 158.13, 139.52, 135.31, 133.11, 129.52, 129.41, 128.87, 114.05, 55.35, 40.73, 29.18.

（10）3-(4-methoxyphenyl)-1-(*m*-tolyl)propan-1-one (3j)



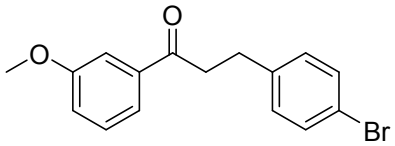
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 10.2 Hz, 2H), 7.39– 7.29 (m, 2H), 7.17 (d, *J* = 8.6 Hz, 2H), 6.93(d, *J* = 8.6 Hz, 2H), 3.87 (s, 3H), 3.34 (t, *J* = 7.7 Hz, 2H), 3.11 (t, *J* = 7.6 Hz, 2H), 2.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.64, 158.11, 138.43, 137.08, 133.79, 133.38, 129.39, 128.59, 128.47, 125.27, 114.02, 55.31, 40.82, 29.44, 21.41.

(11) 3-(4-chlorophenyl)-1-(3-methoxyphenyl)propan-1-one (3k)



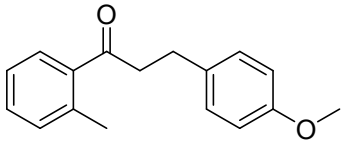
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.43 (m, 2H), 7.41 (t, *J* = 7.9 Hz, 1H), 7.33 (dd, *J* = 8.1, 2.7 Hz, 2H), 7.16 (s, 2H), 7.09 (dd, *J* = 8.2, 2.6 Hz, 1H), 3.01 (s, 3H), 3.34 (t, *J* = 7.5 Hz, 2H), 2.99 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.73, 159.88, 139.78, 138.21, 131.89, 129.79, 129.71, 128.65, 120.58, 119.70, 112.40, 55.50, 40.27, 29.50.

(12) 3-(4-bromophenyl)-1-(3-methoxyphenyl)propan-1-one (3l)



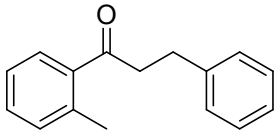
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61– 7.50 (m, 2H), 7.48 – 7.38 (m, 2H), 7.41 – 7.28 (m, 1H), 7.20 – 7.13 (m, 3H), 3.90 (s, 3H), 3.28 – 3.15 (m, 2H), 3.11 (dd, *J* = 9.5, 5.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.63, 159.98, 140.31, 138.25, 131.64, 130.31, 129.73, 120.70, 119.98, 119.59, 112.41, 55.50, 40.21, 29.48.

(13) 3-(4-methoxyphenyl)-1-(*o*-tolyl)propan-1-one (3m)



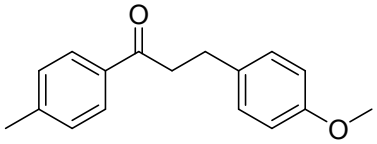
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.0 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.31 – 7.18 (m, 2H), 7.15 (d, *J* = 8.6 Hz, 2H), 6.91 (d, *J* = 8.6 Hz, 2H), 3.74 (s, 3H), 3.28 (t, *J* = 7.6 Hz, 2H), 2.99 (t, *J* = 7.6 Hz, 2H), 2.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 203.57, 157.99, 138.03, 138.06, 133.34, 131.87, 131.23, 129.40, 128.37, 125.71, 114.00, 55.34, 43.47, 29.54, 21.19.

(14) 3-phenyl-1-(*o*-tolyl)propan-1-one (3n)



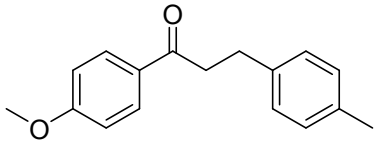
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.18 (dd, *J* = 17.6, 6.7 Hz, 5H), 3.17 (t, *J* = 7.6 Hz, 2H), 2.99 (t, *J* = 7.6 Hz, 2H), 2.51 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 203.38, 141.31, 138.29, 137.98, 131.98, 131.31, 128.60, 128.52, 128.38, 126.09, 125.68, 43.31, 30.40, 21.33.

（15）3-(4-methoxyphenyl)-1-(*p*-tolyl)propan-1-one (3o)



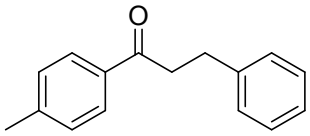
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.18 (d, *J* = 8.6 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 3.86 (s, 3H), 3.33 (t, *J* = 7.7 Hz, 2H), 2.98 (t, *J* = 7.7 Hz, 2H), 2.53 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.98, 158.13, 143.87, 134.45, 133.50, 129.37, 129.29, 128.27, 114.00, 55.31, 40.56, 29.38, 21.70.

(16) 1-(4-methoxyphenyl)-3-(*p*-tolyl)propan-1-one (3p)



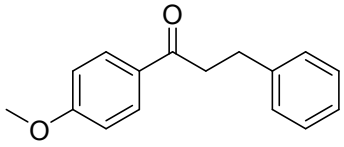
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.87 (m, 2H), 7.23 (q, *J* = 8.1 Hz, 4H), 7.05 – 6.87 (m, 2H), 3.91 (s, 3H), 3.30 (dd, *J* = 8.7, 6.8 Hz, 2H), 3.11 – 3.04 (m, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.03, 163.53, 138.30, 135.51, 130.40, 129.98, 129.29, 128.47, 113.83, 55.53, 40.29, 30.01, 21.10.

(17) 3-phenyl-1-(*p*-tolyl)propan-1-one (3q)



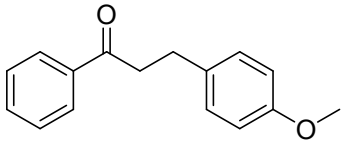
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.2 Hz, 2H), 7.41 – 7.29 (m, 2H), 7.27 – 7.19 (m, 4H), 7.21 (d, *J* = 7.0 Hz, 1H), 3.43 – 3.31 (m, 2H), 3.21 – 3.11 (m, 2H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.89, 143.92, 141.47, 134.50, 129.37, 128.48, 128.477, 128.25, 126.18, 40.41, 30.33, 21.71.

(18) 1-(4-methoxyphenyl)-3-phenylpropan-1-one (3r)



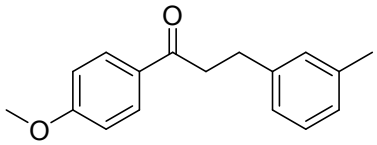
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.9 Hz, 2H), 7.40 (dt, *J* = 14.6, 7.2 Hz, 4H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.00 (d, *J* = 8.9 Hz, 2H), 3.94 (s, 3H), 3.40 (m, 2H), 3.15 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.79, 163.52, 141.56, 130.40, 128.98, 128.61, 128.51, 126.09, 113.83, 55.51, 40.09, 30.41.

(19) 3-(4-methoxyphenyl)-1-phenylpropan-1-one (3s)



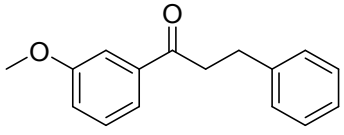
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.5 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.19 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.6 Hz, 2H), 3.79 (s, 3H), 3.28 (t, *J* = 7.7 Hz, 2H), 3.01 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.37, 157.98, 136.97, 133.29, 132.97, 129.34, 128.59, 127.98, 114.02, 55.27, 40.63, 29.27.

(20) 1-(4-methoxyphenyl)-3-(*m*-tolyl)propan-1-one (3t)



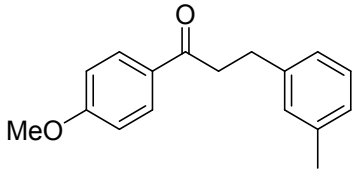
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.9 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.14 – 7.02 (m, 3H), 7.00(d, *J* = 8.9 Hz, 2H), 3.93 (s, 3H), 3.41 – 3.27 (m, 2H), 3.20 – 3.01 (m, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.79, 163.54, 141.40, 138.14, 130.42, 130.14, 129.34, 128.53, 126.92, 125.53, 113.82, 55.51, 40.23, 30.40, 21.53.

(21) 1-(3-methoxyphenyl)-3-phenylpropan-1-one (3u)



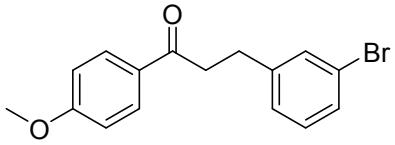
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.47 (m, 2H), 7.40 – 7.20 (m, 6H), 7.13 (dd, *J* = 8.2, 2.6 Hz, 1H), 3.93 (s, 3H), 3.41 (t, *J* = 7.7 Hz, 2H), 3.09 (t, *J* = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.11, 159.97, 141.28, 138.37, 129.57, 128.61, 128.54, 126.21, 120.75, 119.63, 112.41, 55.50, 40.61, 30.32.

(22) 1-(4-methoxyphenyl)-3-(*m*-tolyl)propan-1-one (3v)



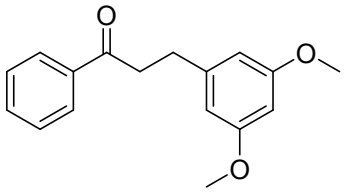
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.89 (m, 2H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.03 (dd, *J* = 14.1, 9.3 Hz, 3H), 6.97 – 6.87 (m, 2H), 3.91 (s, 3H), 3.31 (dd, *J* = 8.8, 6.8 Hz, 2H), 3.05 – 2.97 (m, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.91, 163.50, 141.47, 138.11, 130.40, 130.11, 129.31, 128.36, 126.91, 125.47, 113.81, 55.51, 40.27, 30.28, 21.45.

(23) 3-(3-bromophenyl)-1-(4-methoxyphenyl)propan-1-one (3w)



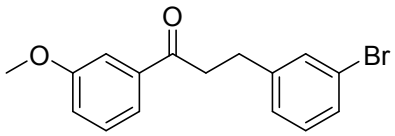
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.9 Hz, 1H), 7.50 (s, 1H), 7.41 (d, *J* = 7.3 Hz, 1H), 7.30 – 7.17 (m, 1H), 6.90 (d, *J* = 8.9 Hz, 1H), 3.84 (s, 2H), 3.31 (t, *J* = 7.7 Hz, 1H), 3.13 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.21, 163.63, 143.89, 131.98, 131.63, 130.27, 130.15, 129.25, 127.27, 122.56, 113.84, 55.52, 39.71, 29.91.

（24）3-(3,5-dimethoxyphenyl)-1-phenylpropan-1-one (3x)



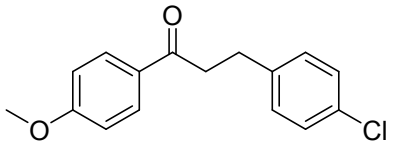
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.87 (m, 2H), 7.64 – 7.52 (m, 1H), 7.43 (dd, *J* = 10.5, 4.7 Hz, 2H), 6.48 (d, *J* = 2.3 Hz, 2H), 6.33 (t, *J* = 2.2 Hz, 1H), 3.85 (s, 6H), 3.40 (dd, *J* = 8.5, 6.9 Hz, 2H), 3.11 – 3.05 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.23, 161.08, 143.83, 136.91, 133.17, 128.72, 128.15, 106.58, 98.16, 55.31, 4033, 30.52.

(25) 3-(3-bromophenyl)-1-(3-methoxyphenyl)propan-1-one (3y)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.52(m, 2H), 7.43 (dd, *J* = 14.3, 6.5 Hz, 2H), 7.26 (t, *J* = 8.1 Hz, 2H), 7.15 (ddd, *J* = 19.9, 11.8, 6.7 Hz, 2H), 3.91 (s, 3H), 3.28 (t, *J* = 7.6 Hz, 2H), 3.11 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.53, 159.97, 143.73, 138.21, 131.57, 130.13, 129.73, 129.31, 127.27, 122.61, 120.71, 119.73, 112.40, 55.51, 40.17, 29.83.

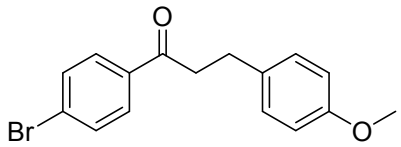
(26) 3-(4-chlorophenyl)-1-(4-methoxyphenyl)propan-1-one (3z)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.9 Hz, 2H), 7.34 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.03 (d, *J* = 8.9 Hz, 2H), 3.93 (s, 3H), 3.33 (t, *J* = 7.6 Hz, 2H), 2.98 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR

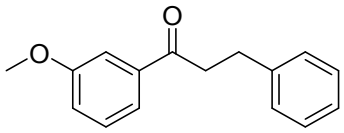
(101 MHz, $CDCl_3$) δ 197.55, 163.61, 140.00, 131.93, 130.42, 130.27, 129.93, 128.42, 113.81, 55.53, 39.84, 29.62

(27) 1-(4-bromophenyl)-3-(4-methoxyphenyl)propan-1-one (3aa)



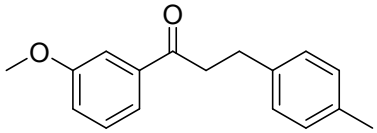
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 20.0, 7.7 Hz, 2H), 7.49 – 7.29 (m, 2H), 7.20 – 7.11 (m, 2H), 6.93 (t, *J* = 6.2 Hz, 2H), 3.87 (s, 3H), 3.41 – 3.28 (m, 2H), 3.11 – 3.08 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.43, 158.11, 137.01, 133.43, 133.12, 129.42, 128.67, 128.11, 114.02, 55.31, 40.63, 29.40.

(28) 1-(3-methoxyphenyl)-3-phenylpropan-1-one (3ab)



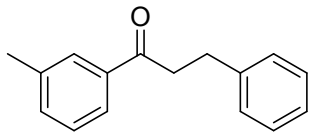
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.47 (m, 2H), 7.40 – 7.17 (m, 6H), 7.12 (dd, *J* = 8.2, 2.6 Hz, 1H), 3.93 (s, 3H), 3.40 (t, *J* = 7.7 Hz, 2H), 2.97 (t, *J* = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.11, 159.97, 141.38, 138.27, 129.59, 128.61, 128.53, 126.22, 120.75, 119.63, 112.41, 55.52, 40.63, 30.27.

(29) 1-(3-methoxyphenyl)-3-(*p*-tolyl)propan-1-one (3ac)



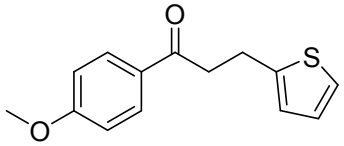
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 13.4, 5.1 Hz, 2H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.31 – 7.15 (m, 5H), 3.93 (s, 3H), 3.41 (t, *J* = 7.7 Hz, 2H), 3.09 – 3.11 (m, 2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.17, 159.94, 138.41, 138.30, 135.58, 129.56, 129.33, 128.40, 120.68, 119.62, 112.41, 55.50, 40.78, 29.88, 21.08.

(30) 3-phenyl-1-(*m*-tolyl)propan-1-one (3ad)



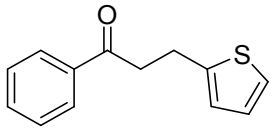
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.9 Hz, 2H), 7.45 – 7.32 (m, 2H), 7.28 (m, 4H), 7.20 (t, *J* = 5.3 Hz, 1H), 3.35 (m, 2H), 3.13 – 3.04 (m, 2H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.53, 141.42, 138.38, 137.00, 133.90, 129.11, 128.59, 128.59, 128.53, 126.18, 125.31, 40.69, 30.27, 21.43.

(31) 1-(4-methoxyphenyl)-3-(thiophen-2-yl)propan-1-one (3ae)



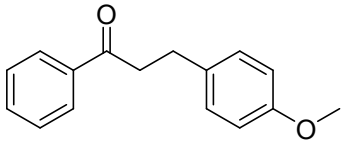
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.92 (m, 2H), 7.15 (dd, *J* = 5.1, 1.2 Hz, 1H), 6.99 – 6.92 (m, 3H), 6.88 (dd, *J* = 3.3, 0.7 Hz, 1H), 3.88 (s, 3H), 3.32 (dt, *J* = 5.6, 2.7 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.09, 163.63, 144.17, 130.38, 129.95, 126.92, 124.70, 123.41, 113.83, 55.52, 40.24, 24.50.

(32) 1-phenyl-3-(thiophen-2-yl)propan-1-one (3af)



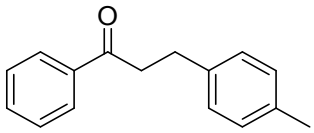
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.94 (m, 2H), 7.71 – 7.60 (m, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.21 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.02 (dd, *J* = 5.1, 3.4 Hz, 1H), 6.95 (dd, *J* = 3.4, 0.9 Hz, 1H), 3.38 – 3.35 (m, 2H), 3.33 – 3.26 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.51, 143.89, 136.81, 133.23, 128.70, 128.11, 126.92, 124.74, 123.36, 40.60, 24.27.

(33) 3-(4-methoxyphenyl)-1-phenylpropan-1-one (3ag)



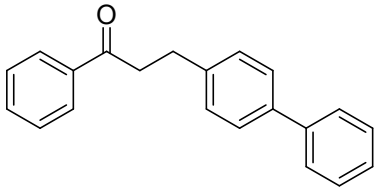
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.5 Hz, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 3.87 (s, 3H), 3.35 (t, *J* = 7.7 Hz, 2H), 3.11 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.46, 158.10, 136.97, 133.42, 133.13, 129.43, 128.58, 128.11, 114.02, 55.28, 40.79, 29.28.

(34) 1-phenyl-3-(*p*-tolyl)propan-1-one (3ah)



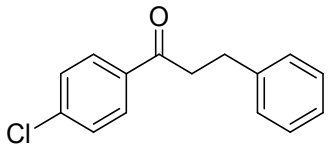
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.94 (m, 2H), 7.69 – 7.61 (m, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.18 (q, *J* = 8.1 Hz, 4H), 3.43 – 3.20(m, 2H), 3.17 – 3.04(m, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.42, 138.27, 136.95, 135.68, 133.12, 129.28, 128.59, 128.33, 128.13, 40.71, 29.75, 21.19.

(35) 3-([1,1'-biphenyl]-4-yl)-1-phenylpropan-1-one (3ai)



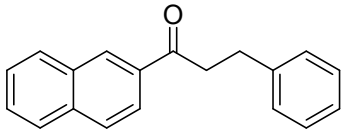
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.3 Hz, 2H), 7.72 – 7.54 (m, 5H), 7.53 (dd, *J* = 17.5, 7.9 Hz, 4H), 7.45 – 7.30 (m, 3H), 3.43 (t, *J* = 7.6 Hz, 2H), 3.21 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.19, 141.17, 140.52, 139.21, 136.97, 133.20, 128.98, 128.84, 128.71, 128.18, 127.37, 127.21, 127.18, 40.47, 29.82.

(36) 1-(4-chlorophenyl)-3-phenylpropan-1-one (3aj)



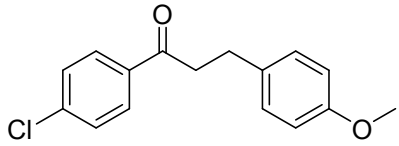
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.93 (m, 2H), 7.52 – 7.46 (m, 2H), 7.40 – 7.37 (m, 2H), 7.31 – 7.19 (m, 3H), 3.27 (t, *J* = 7.7 Hz, 2H), 3.11 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.08, 141.21, 139.48, 135.17, 129.52, 129.01, 128.63, 128.38, 126.31, 40.47, 30.11.

(37) 1-(naphthalen-2-yl)-3-phenylpropan-1-one (3ak)



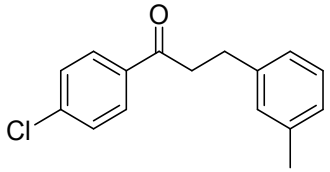
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.15 (d, *J* = 8.6 Hz, 1H), 8.00 – 7.93 (m, 2H), 7.74– 7.59 (m, 1H), 7.42 (dd, *J* = 4.7, 2.5 Hz, 2H), 7.38 – 7.27 (m, 4H), 3.52 (t, *J* = 7.8 Hz, 2H), 3.35 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.21, 141.53, 135.71, 134.33, 132.59, 129.83, 129.71, 129.23, 128.70, 128.61, 128.51, 127.93, 126.91, 126.33, 124.01, 40.63, 30.42.

(38) 1-(4-chlorophenyl)-3-(4-methoxyphenyl)propan-1-one (3al)



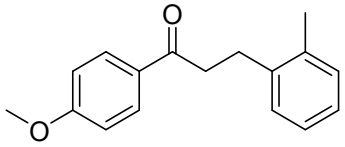
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.84 (m, 2H), 7.52 – 7.45 (m, 2H), 7.27 – 7.09 (m, 2H), 6.92 – 6.83 (m, 2H), 3.87 (s, 3H), 3.33 (t, *J* = 7.6 Hz, 2H), 3.28 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.21, 158.11, 139.53, 135.30, 133.15, 129.52, 129.41, 128.97, 114.08, 55.31, 40.73, 29.34.

(39) 1-(4-chlorophenyl)-3-(*m*-tolyl)propan-1-one (3am)



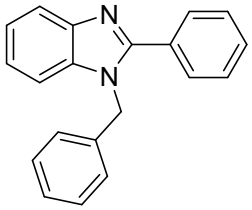
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.90 (m, 2H), 7.48 – 7.39 (m, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.09 (dd, *J* = 13.6, 5.8 Hz, 3H), 3.41 – 3.31 (m, 2H), 3.08 – 3.02 (m, 2H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.05, 141.12, 139.53, 138.23, 135.31, 129.60, 129.33, 128.99, 128.65, 127.12, 125.53, 40.60, 30.17, 21.54.

(40) 1-(4-methoxyphenyl)-3-(*o*-tolyl)propan-1-one (3an)



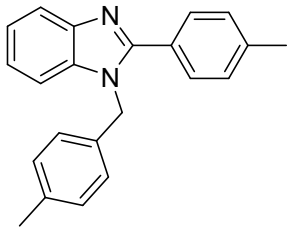
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.96 (m, 2H), 7.31 – 7.20 (m, 4H), 7.09 – 6.97 (m, 2H), 3.94 (s, 3H), 3.40 – 3.23 (m, 2H), 3.09 – 2.98 (m, 2H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.01, 163.57, 139.63, 135.98, 130.41, 130.40, 139.98, 128.84, 126.28, 126.25, 113.81, 55.51, 38.87, 27.82, 19.43.

(41) 1-benzyl-2-phenyl-1H-benzo[d]imidazole (6a).



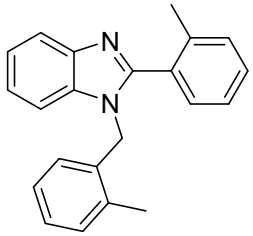
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.0 Hz, 1H), 7.75 – 7.70 (m, 2H), 7.53 – 7.45 (m, 3H), 7.38 – 7.31 (m, 4H), 7.24 (td, *J* = 7.8, 1.3 Hz, 2H), 7.17 – 7.10 (m, 2H), 5.48 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ =154.21, 143.26, 136.50, 136.21, 130.22, 130.02, 129.43, 129.19, 128.82, 127.79, 126.09, 123.11, 122.68, 120.11, 110.65, 48.49.

(42) 1-(4-methylbenzyl)-2-(*p*-tolyl)-1H-benzo[d]imidazole (6b)



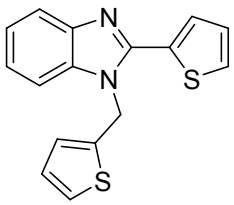
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.01 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.1 Hz, 2H), 7.40 – 7.32 (m, 3H), 7.29– 7.22 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 5.51 (s, 2H), 2.51 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 154.43, 143.32, 140.15, 137.56, 136.23, 133.41, 129.68, 129.51, 129.19, 127.17, 125.88, 122.81, 122.63, 119.90, 110.60, 48.32, 21.50, 21.20.

(43) 1-(2-methylbenzyl)-2-(*o*-tolyl)-1H-benzo[d]imidazole (6c).



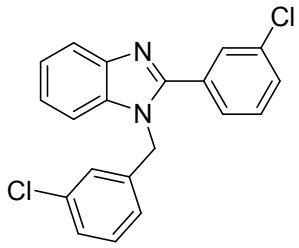
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.01 (d, *J* = 8.0 Hz, 1H), 7.50– 7.47 (m, 4H), 7.39– 7.20 (m, 5H), 7.16 (td, *J* = 8.0, 2.5 Hz, 1H), 6.80 (d, *J* = 7.7 Hz, 1H), 5.29 (s, 2H), 2.38 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 154.01, 143.32, 138.46, 135.25, 135.02, 134.09, 131.02, 130.73, 130.49, 129.98, 129.93, 127.67, 126.46, 126.21, 125.73, 122.97, 122.49, 120.16, 110.74, 45.92, 19.89, 19.13.

(44) 2-(thiophen-2-yl)-1-(thiophen-2-ylmethyl)-1H-benzo[d]imidazole (6d).



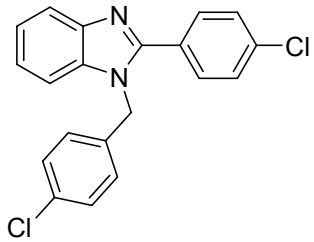
^{1}H NMR (400 MHz, DMSO): δ = 7.88 (d, *J* = 5.1 Hz, 1H), 7.80 – 7.72 (m, 3H), 7.45 (d, *J* = 5.0 Hz, 1H), 7.33 (ddd, *J* = 13.1, 7.6, 5.6 Hz, 3H), 7.08 (d, *J* = 3.3 Hz, 1H), 7.10 – 6.98 (m, 1H), 5.97 (s, 2H). ^{13}C NMR (101 MHz, DMSO): δ = 147.23, 143.93, 139.90, 136.40, 132.48, 130.18, 128.90, 128.41, 127.59, 126.60, 126.48, 123.40, 123.11, 119.53, 111.33, 43.62.

(45) 1-(3-chlorobenzyl)-2-(3-chlorophenyl)-1H-benzo[d]imidazole (6e).



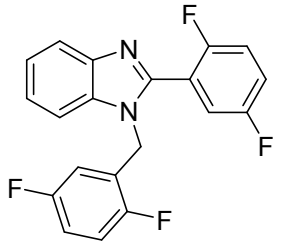
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.91 (d, *J* = 8.0 Hz, 1H), 7.81 (t, *J* = 1.8 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.50 – 7.42 (m, 2H), 7.39 – 7.32 (m, 3H), 7.31 – 7.30 (m, 1H), 7.22 (s, 1H), 7.01 (d, *J* = 7.1 Hz, 1H), 5.50 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ= 152.58, 143.20, 138.27, 136.00, 135.31, 135.08, 131.76, 130.52, 130.21, 130.11, 129.58, 128.39, 127.14, 126.31, 124.19, 123.73, 123.20, 120.43, 110.38, 48.00.

(46) 1-(4-chlorobenzyl)-2-(4-chlorophenyl)-1H-benzo[d]imidazole (6f).



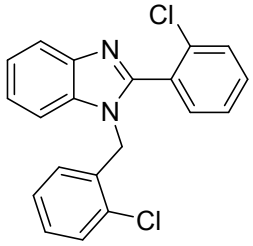
^{1}H NMR (400 MHz, DMSO): δ= 7.81 – 7.75 (m, 3H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.58 – 7.43 (m, 1H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.35 – 7.28 (m, 2H), 7.08 (d, *J* = 8.4 Hz, 2H), 5.69 (s, 2H). ^{13}C NMR (101 MHz, DMSO): δ = 152.58, 143.17, 138.30, 136.41, 136.32, 135.31, 132.68, 131.63, 131.31, 130.28, 129.49, 129.27, 128.51, 123.50, 122.96, 120.01, 111.61, 47.40.

(47) 1-(2,5-difluorobenzyl)-2-(2,5-difluorophenyl)-1H-benzo[d]imidazole (6g).



^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.91 (d, *J* = 7.2 Hz, 1H), 7.45 – 7.33 (m, 4H), 7.30 – 7.21 (m, 2H), 7.10 (td, *J* = 9.9, 4.4 Hz, 1H), 7.08 – 6.93 (m, 1H), 6.57 – 6.51 (m, 1H), 5.42 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 158.80, 156.13, 148.02, 143.31, 135.20, 124.60, 123.91, 123.17, 120.55, 119.95, 117.49, 116.78, 116.21, 115.14, 114.90, 110.42, 42.24.

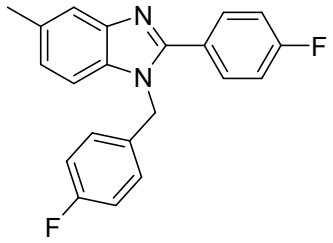
(48) 1-(2-chlorobenzyl)-2-(2-chlorophenyl)-1H-benzo[d]imidazole (6h).



^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.95 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.1 Hz, 1H), 7.53 – 7.41 (m,

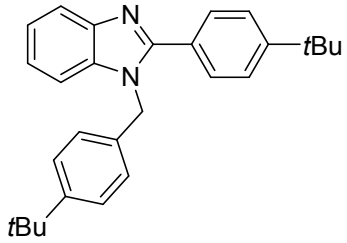
2H), 7.38 – 7.29 (m, 4H), 7.26 – 7.08 (m, 2H), 7.07 (t, *J* = 7.2 Hz, 1H), 6.70 (d, *J* = 7.6 Hz, 1H), 5.52 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 151.58, 143.16, 134.86, 134.48, 133.41, 132.45, 132.20, 131.49, 1300.00, 129.79,129.68, 129.10, 127.89, 127.21, 127.01, 123.47, 122.79, 120.46, 110.58, 45.77.

(49) 1-(4-fluorobenzyl)-2-(4-fluorophenyl)-5-methyl-1H-benzo[d]imidazole (6i).



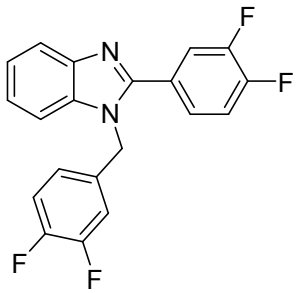
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82– 7.58 (m, 3H), 7.28 – 7.11(m, 3H), 7.09 (s, 1H), 7.10 – 7.00 (m, 4H), 5.40 (s, 2H), 2.58 (d, *J* = 20.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 163.76 163.58, 161.11, 153.07, 152.67, 143.50, 141.27, 136.19, 134.11, 133.4,2 132.68, 132.09, 131.19, 127.58, 126.43,124.80, 124.58, 119.90, 119.63, 116.10, 110.21, 109.94, 47.59, 21.90, 21.62.

(50) 1-(4-(*tert*-butyl)benzyl)-2-(4-(*tert*-butyl)phenyl)-1H-benzo[d]imidazole (6j).



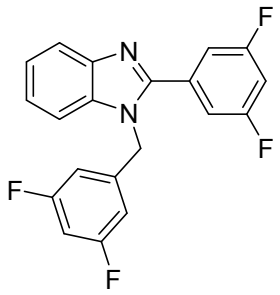
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.92 (d, *J* = 8.0 Hz, 1H), 7.78 (dt, *J* = 8.4, 2.0 Hz 2H), 7.58 (dt, *J* = 8.8, 2.0 Hz, 2H), 7.43 – 7.20 (m, 3H), 7.28 – 7.17 (m, 2H), 7.14 (d, *J* = 8.4 Hz, 2H), 5.56 (s, 2H), 1.43 (s, 9H), 1.41 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 154.37, 153.15, 150.71, 143.36, 136.20, 133.53, 129.10, 127.30, 126.00, 125.74, 122.82, 122.57, 119.90, 110.65, 48.20, 34.91, 34.60, 31.40,31.39.

(51) 1-(3,4-difluorobenzyl)-2-(3,4-difluorophenyl)-1H-benzo[d]imidazole (6k).



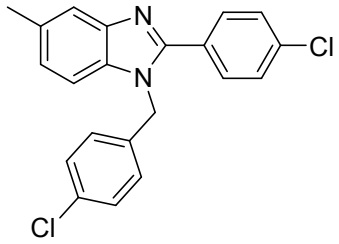
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.93 (d, *J* = 8.0 Hz, 1H), 7.65 – 7.48 (m, 1H), 7.43 – 7.30 (m, 4H), 7.28– 7.01 (m, 2H), 6.98 – 6.90 (m, 1H), 6.89 – 6.84 (m, 1H), 5.47 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 152.11, 150.48, 149.25, 142.70, 135.70, 133.15 – 132.57 (m), 126.69, 125.58, 124.01, 123.53, 121.95, 120.30, 119.26, 118.71, 118.05, 117.23, 115.92 – 115.17 (m), 115.30, 115.11, 110.27, 47.45.

(52) 1-(3,5-difluorobenzyl)-2-(3,5-difluorophenyl)-1H-benzo[d]imidazole (6l).



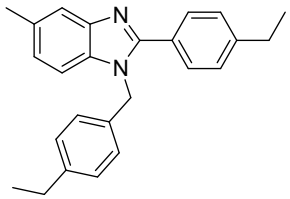
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.91 (d, *J* = 7.8 Hz, 1H), 7.43 – 7.34 (m, 2H), 7.27 – 7.10 (m, 3H), 7.00 (tt, *J* = 8.7, 2.3 Hz, 1H), 6.83 (tt, *J* = 8.7, 2.2 Hz, 1H), 6.71 – 6.53 (m, 2H), 5.40 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 163.41, 151.37, 143.03, 140.01, 135.98, 132.79, 124.09, 123.57, 120.56, 112.28, 110. 17, 109.05, 105.70, 104.13, 103.86, 103.60, 47.78

(53) 1-(4-chlorobenzyl)-2-(4-chlorophenyl)-5-methyl-1H-benzo[d]imidazole(6m)



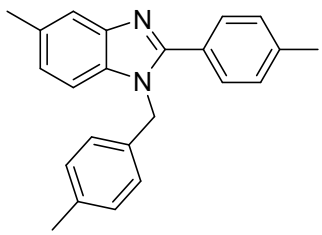
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.80– 7.57 (m, 3H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.33 – 7.19 (m, 2H), 7.20 – 6.95 (m, 4H), 5.40 (d, *J* = 6.8 Hz, 2H), 2.51 (dd, *J* = 21.1, 9.6 Hz, 3H). ^{13}C NMR (101MHz, $CDCl_3$): δ = 152.80, 152.41, 143.50, 141.30, 136.33, 136.20, 136.07, 134.90, 134.87, 134.12, 133.80, 133.68, 132.80, 132.76, 130.42, 130.29, 129.43, 129.38, 129.11, 128.60, 127.33, 127.29, 125.03, 124.72, 119.96, 119.71, 110.20, 109.78, 47.83, 47.59, 21.93, 21.63.

(54) 1-(4-ethylbenzyl)-2-(4-ethylphenyl)-5-methyl-1H-benzo[d]imidazole (6n)



^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87 – 7.65 (m, 3H), 7.38 (dd, *J* = 8.2, 4.2 Hz, 2H), 7.30 – 7.18 (m, 3H), 7.15– 7.05(m, 3H), 5.47 (s, 2H), 2.80 – 2.57 (m, 4H), 2.48 (d, *J* = 27.4 Hz, 3H), 1.35 – 1.19 (m, 6H). ^{13}CNMR (101MHz, $CDCl_3$): δ = 154.27, 153.93, 146.19, 146.15, 143.75, 143.73, 143.66, 141.49, 136.58, 134.39, 134.03, 133.97, 132.89, 132.25, 129.31, 129.29, 128.56, 128.58, 128.32, 128.31, 127.67, 126.11, 126.02, 124.38, 124.23, 119.70, 119.42, 110.41, 110.18, 48.27, 48.13,28.81, 28.57, 21.93, 21.73, 15.52, 15.43.

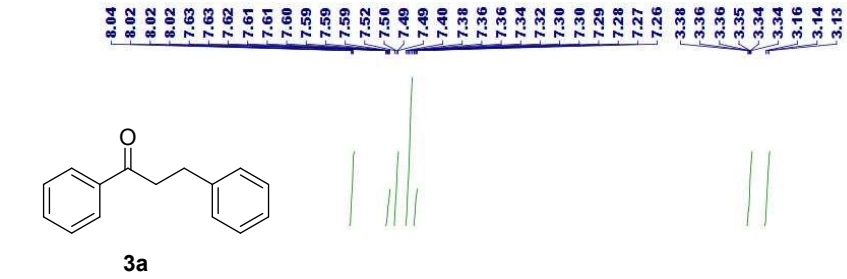
(55) 5-methyl-1-(4-methylbenzyl)-2-(*p*-tolyl)-1H-benzo[d]imidazole (6o)



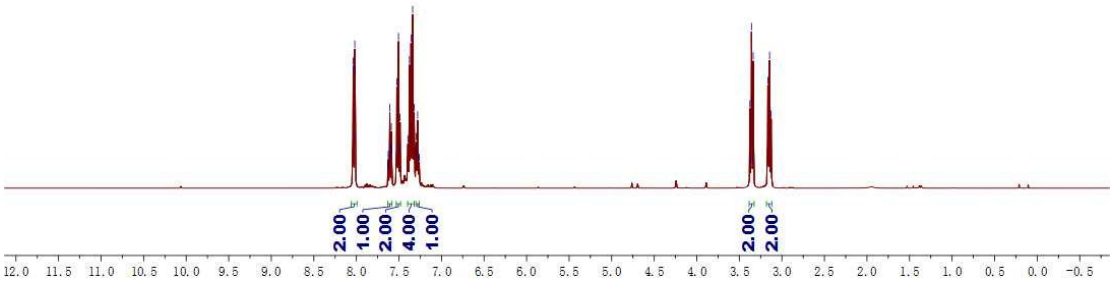
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.88 – 7.76 (m, 1H), 7.71 – 7.67 (m, 2H), 7.30 (dd, *J* = 7.9, 3.8 Hz,

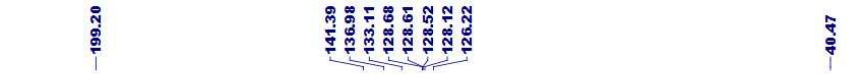
2H), 7.20– 7.00 (m, 6H), 5.41 (s, 2H), 2.52 (d, J = 31.6 Hz, 3H), 2.49 (s, 3H), 2.41 (d, J = 4.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 154.30, 153.90, 143.71, 141.50, 139.90, 139.87, 137.28, 137.38, 136.53, 134.38, 133.77, 133.78, 132.85, 132.19, 129.73,129.71, 129.53, 129.54, 129.24, 129.18, 127.52, 125.94, 125.81, 124.35, 124.27, 119.60, 119.45, 110.38, 110.17, 48.18, 48.09, 21.86, 21.69, 21.48, 21.13.

7. NMR spectra of obtained compounds



3a





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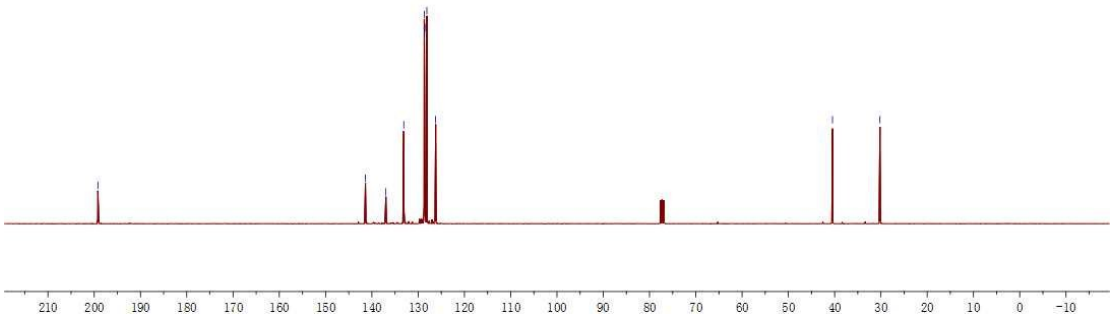

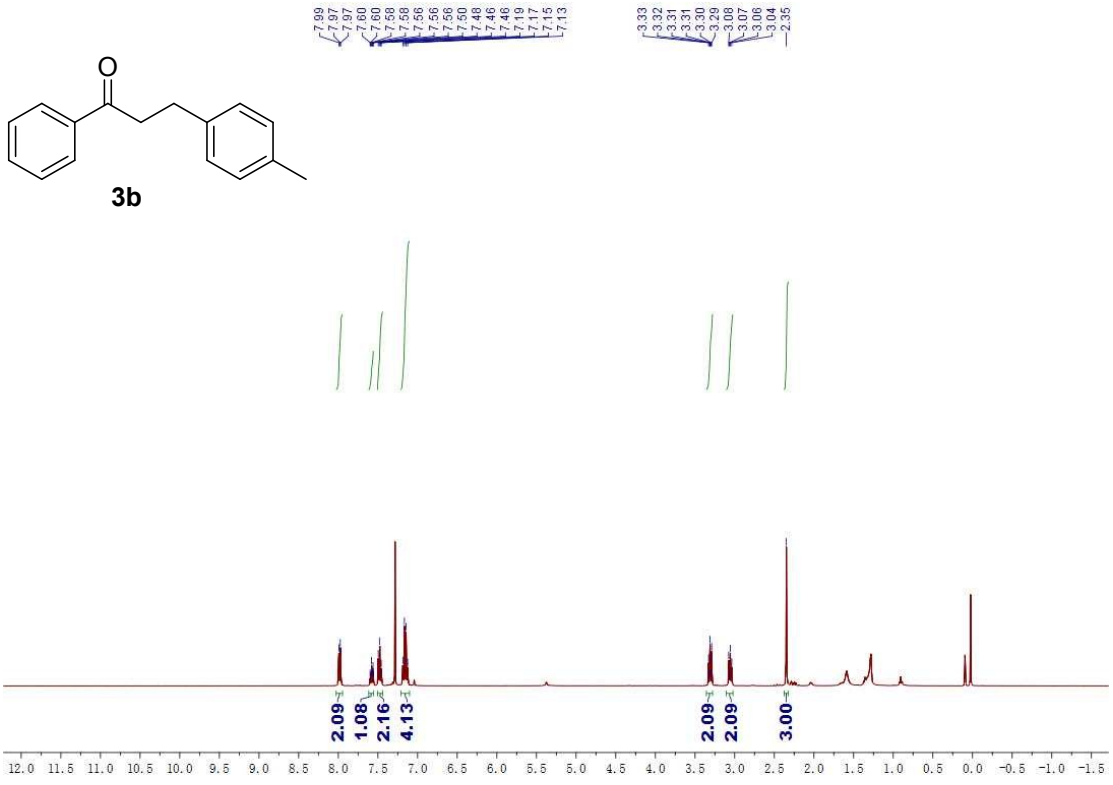
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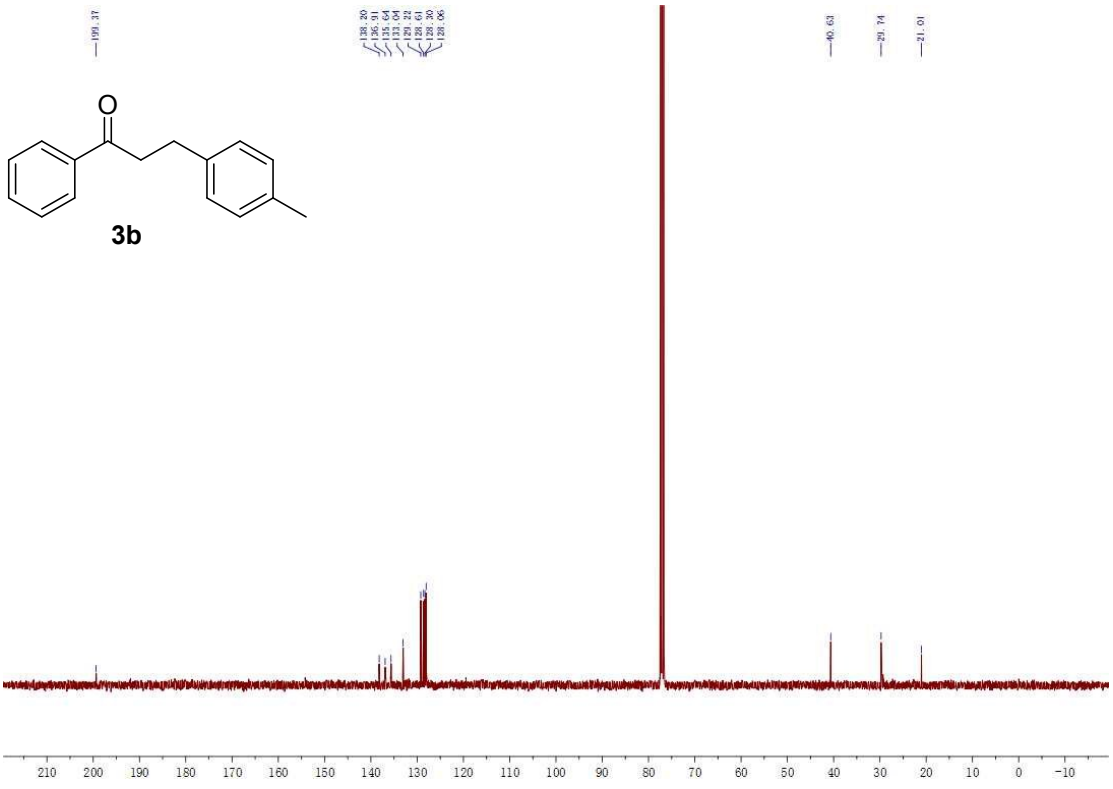
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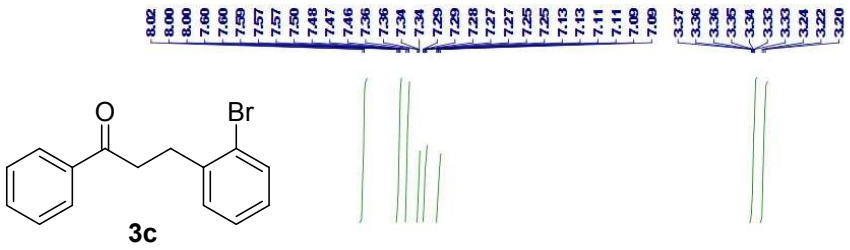
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7.13
7.13
7.11
7.11
7.09
7.09
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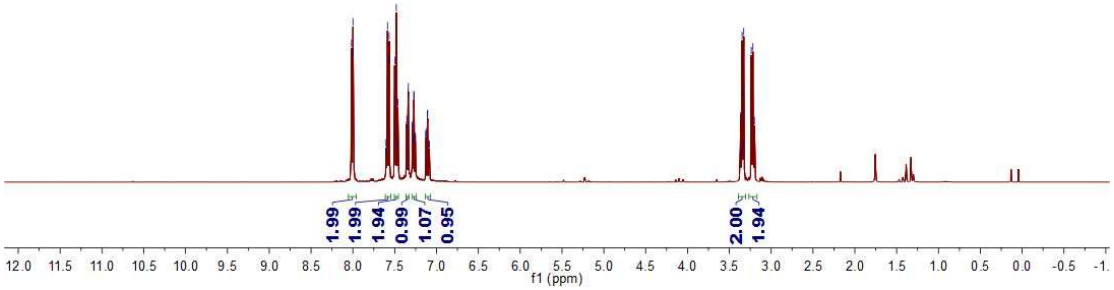
3.20
O
Br

3c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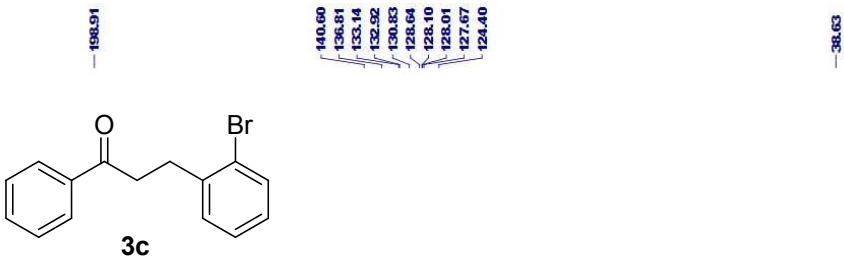
0.95
2.00
1.94
f1 (ppm)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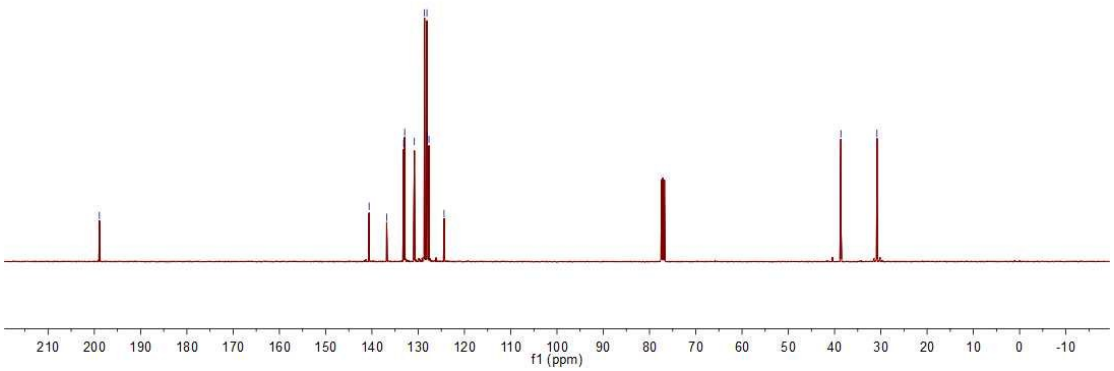
30.83
O
Br

3c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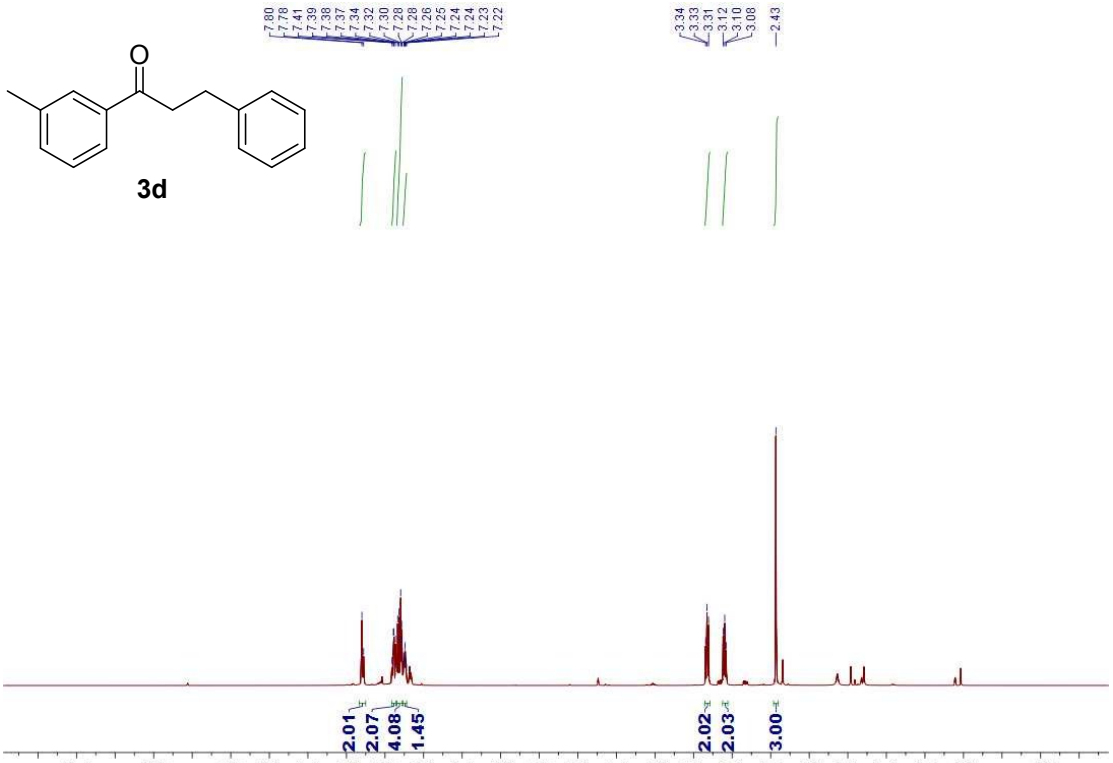
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3.34
3.33
3.31
3.12
3.10
3.08
2.43
O
3d
2.01
2.07
4.08
1.45
2.02
2.03
3.00
11.5
10.5
9.5
9.0
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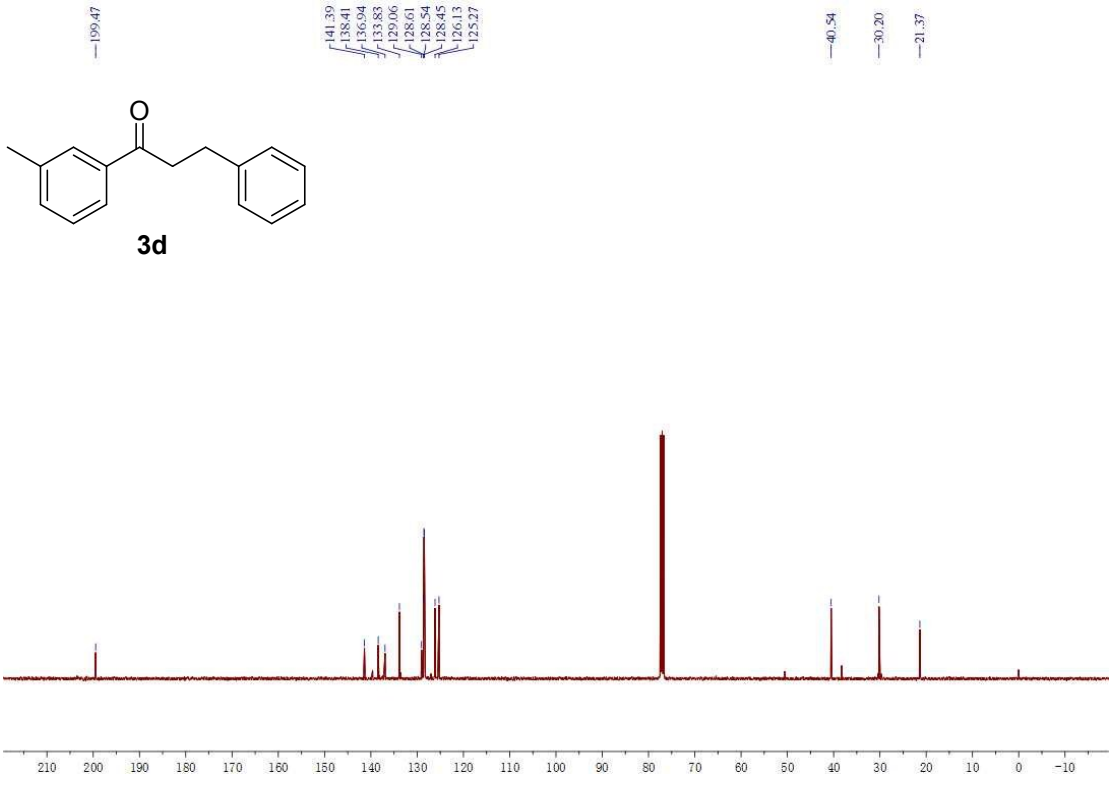
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126.13
125.27
40.54
30.20
21.37
O
3d
210
200
190
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100
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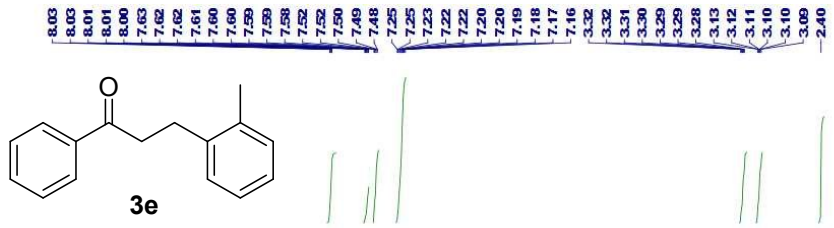
10
0
-10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7.58
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7.52
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7.23
7.22
7.22
7.20
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7.19
7.18
7.17
7.16
3.32
3.32
3.31
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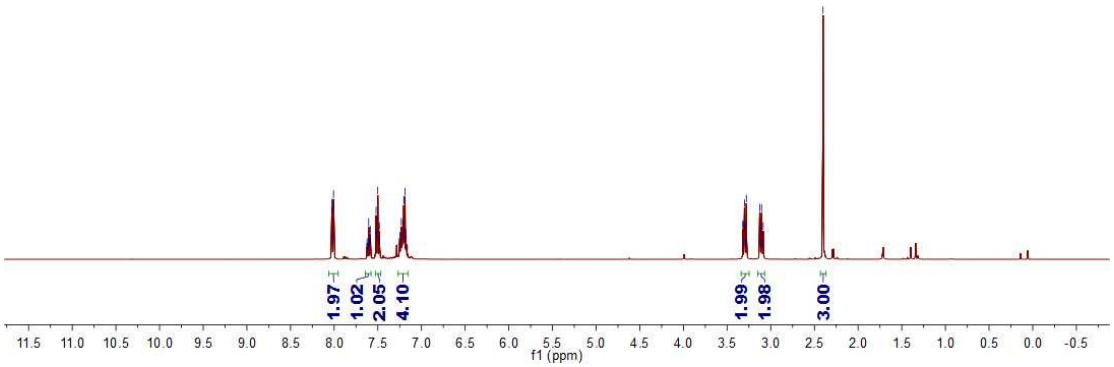
3.28
3.13
3.12
3.11
3.10
3.10
3.09
2.40

3e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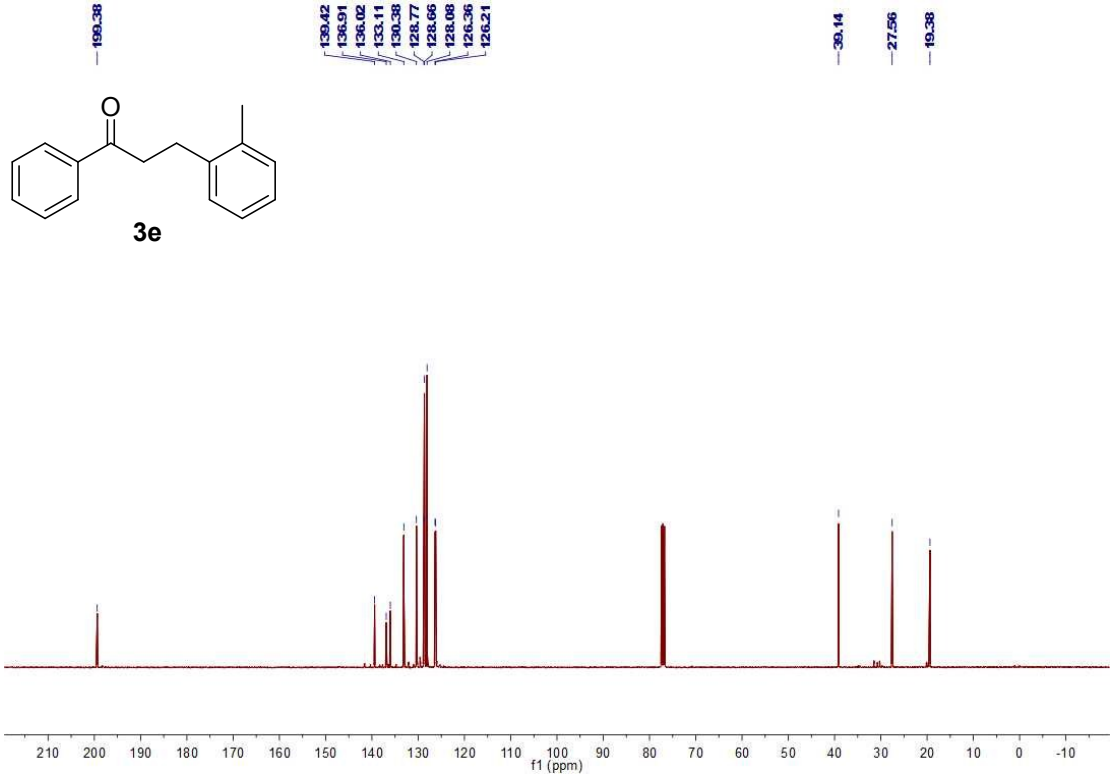
1.02
2.05
4.10
1.99
1.98
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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130.38
128.77
128.66
128.08
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126.21
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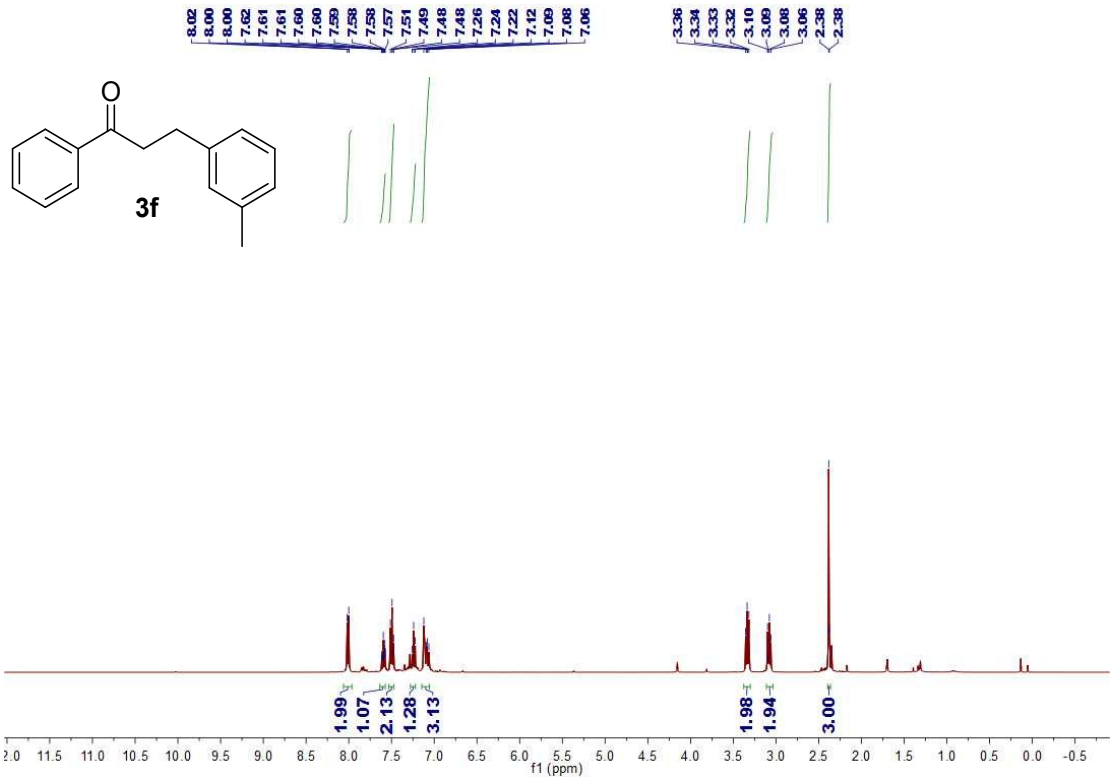
27.56
19.38
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3e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7.06
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3.32
3.10
3.09
3.08
3.06
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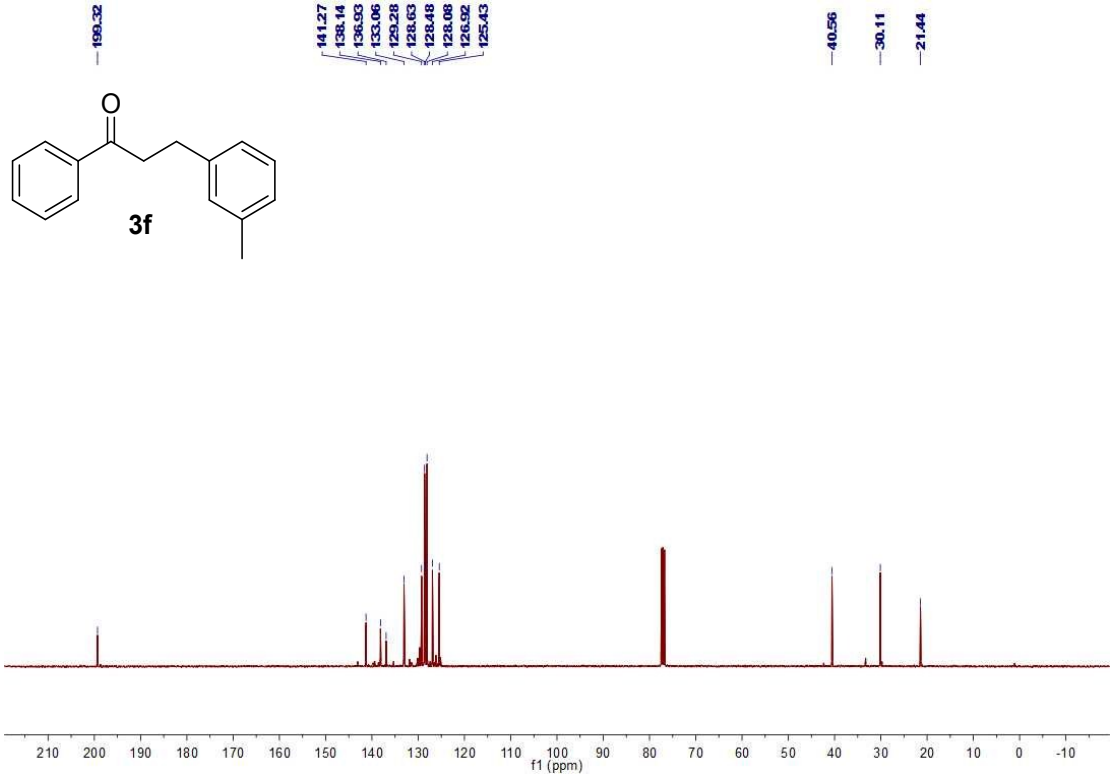
3.13
1.98
1.94
3.00
f1 (ppm)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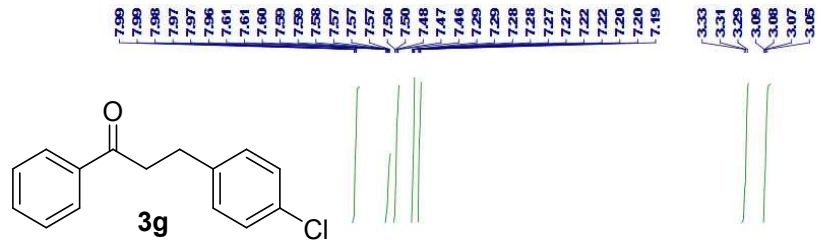
30.11
21.44
O
3f
f1 (ppm)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7.50
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7.27
7.22
7.22
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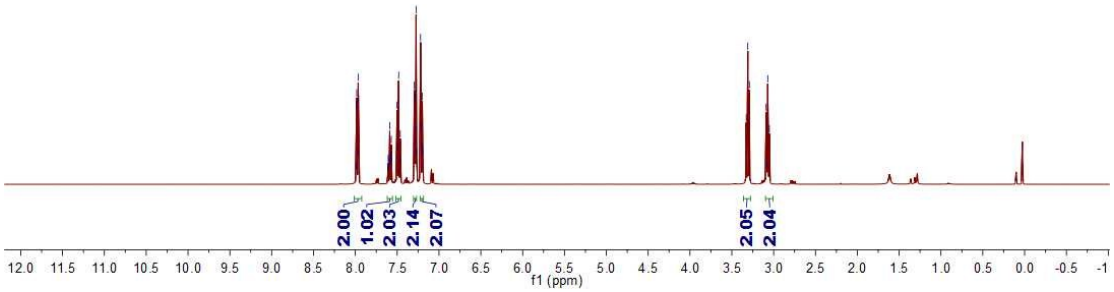
3.33
3.31
3.29
3.09
3.08
3.07
3.05
O
3g
Cl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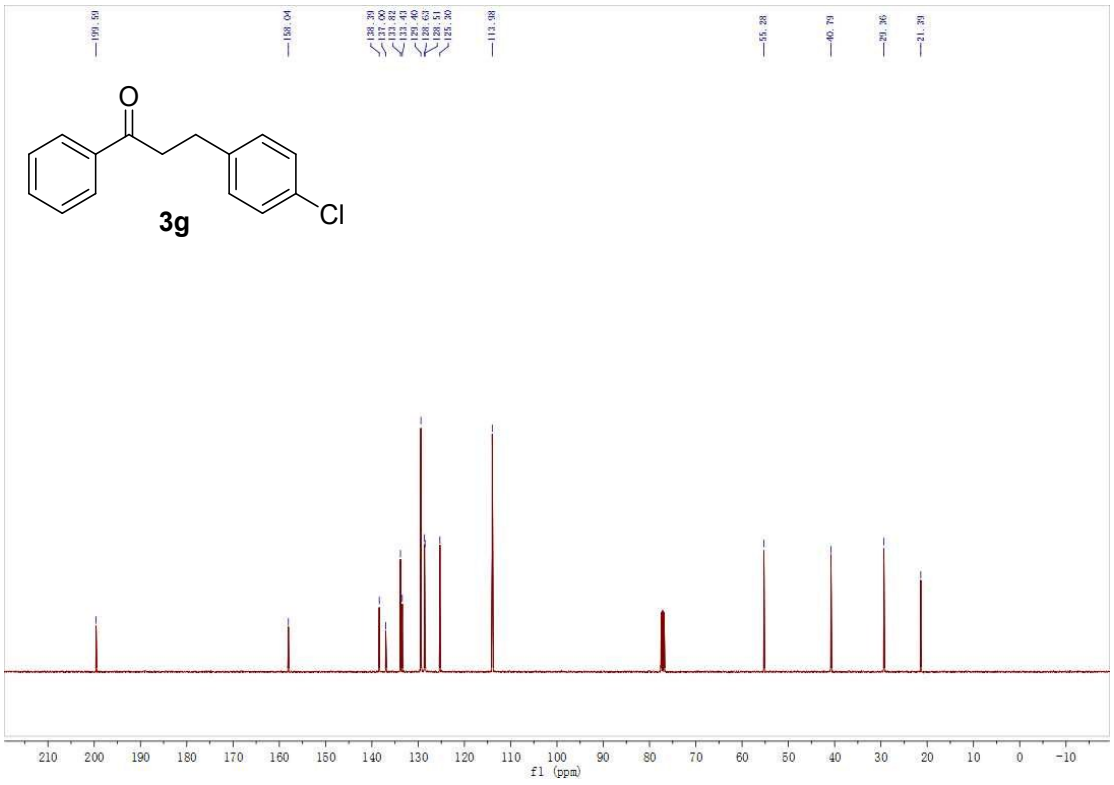
2.03
2.14
2.07
2.05
2.04
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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128.51
125.30
113.98
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40.79
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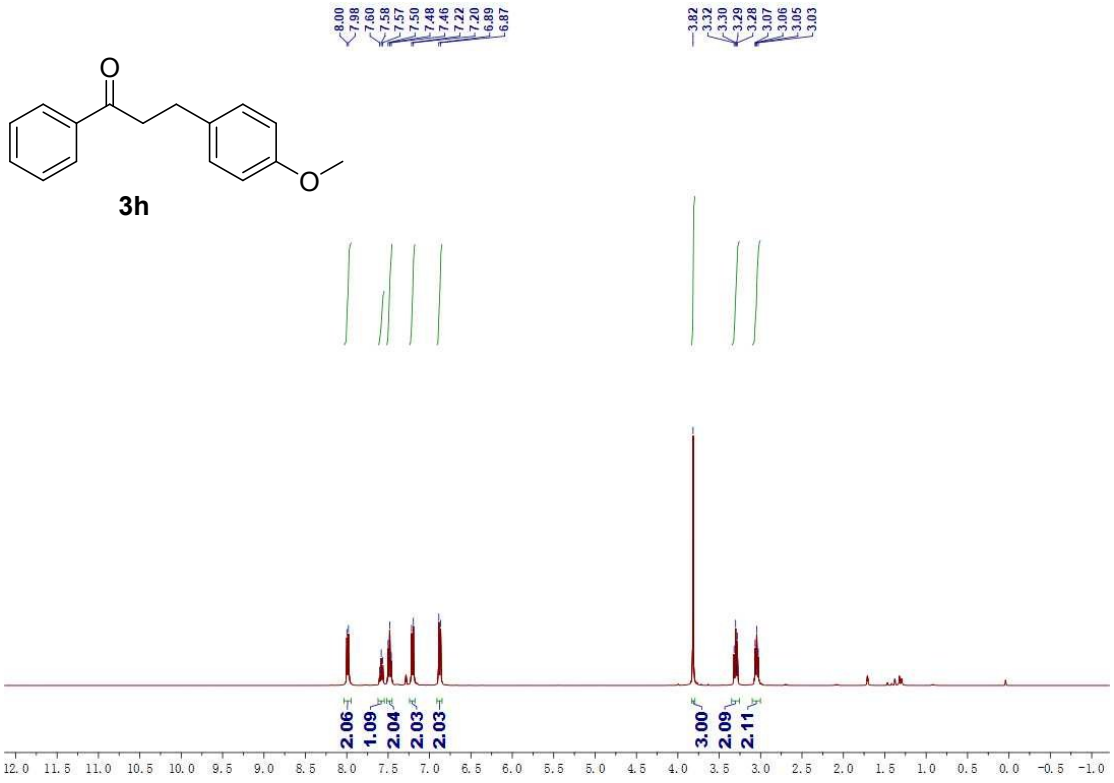
21.39
O
3g
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.87
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3.32
3.30
3.29
3.28
3.07
3.06
3.05
3.03
O
O
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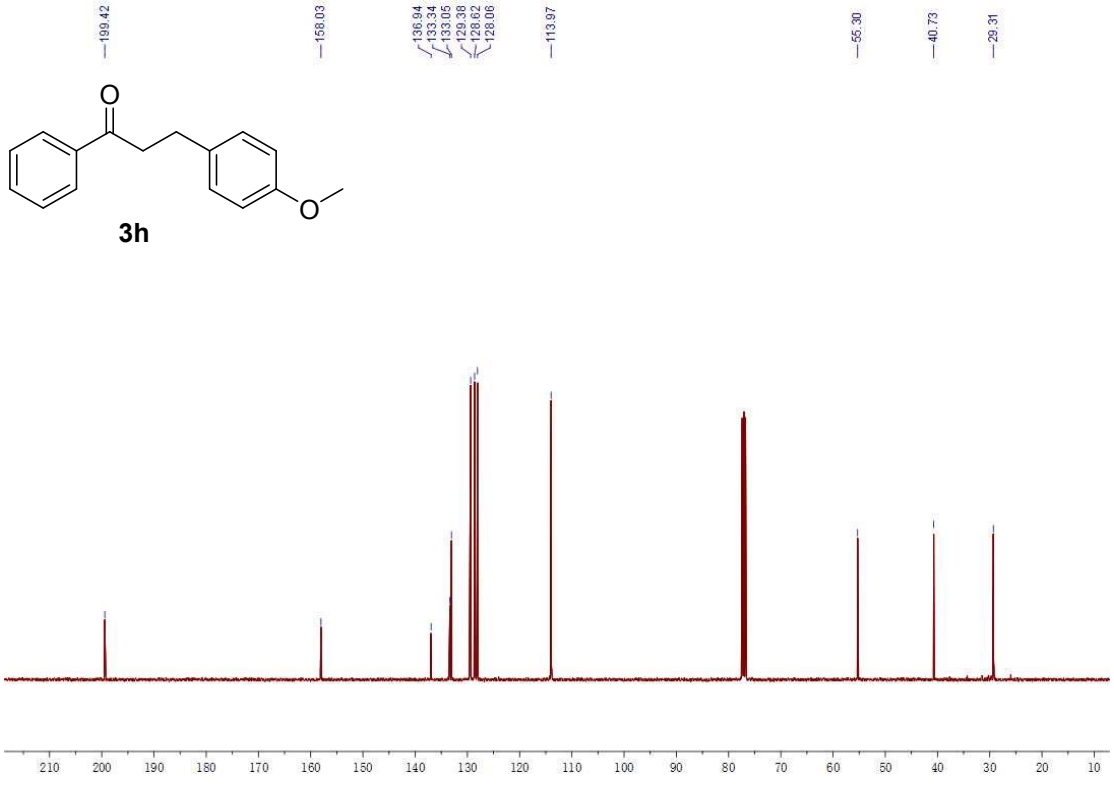
1.09
2.04
2.03
2.03
3.00
2.09
2.11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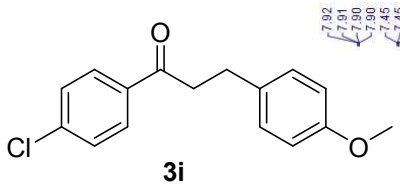
O
O
3h


O
Cl
O

3i

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6.87
6.86
6.86
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3.28
3.26
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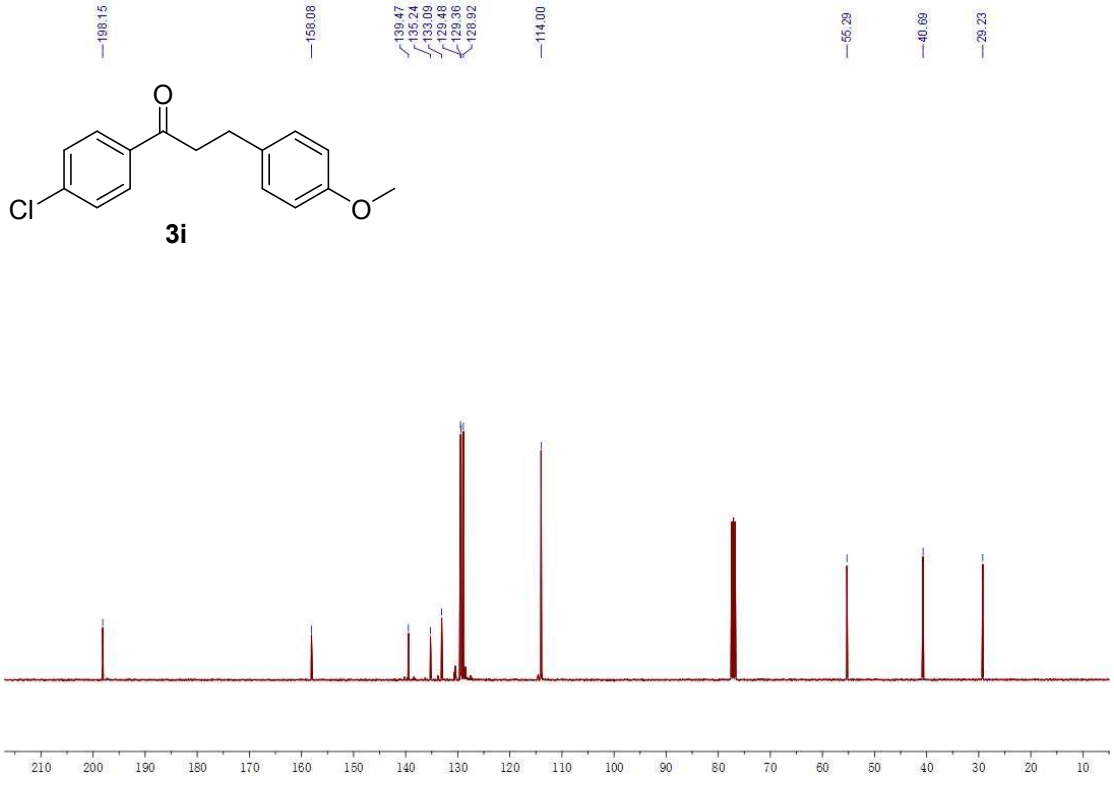
2.06
2.08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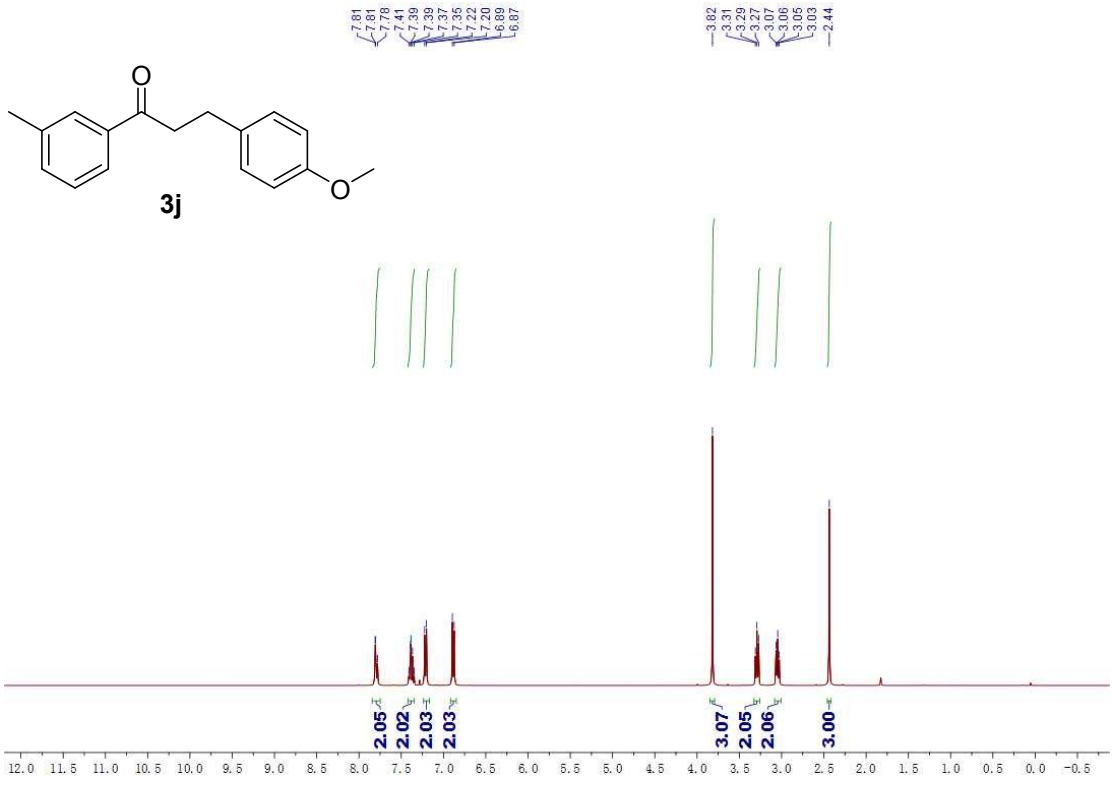
O
Cl
O

3i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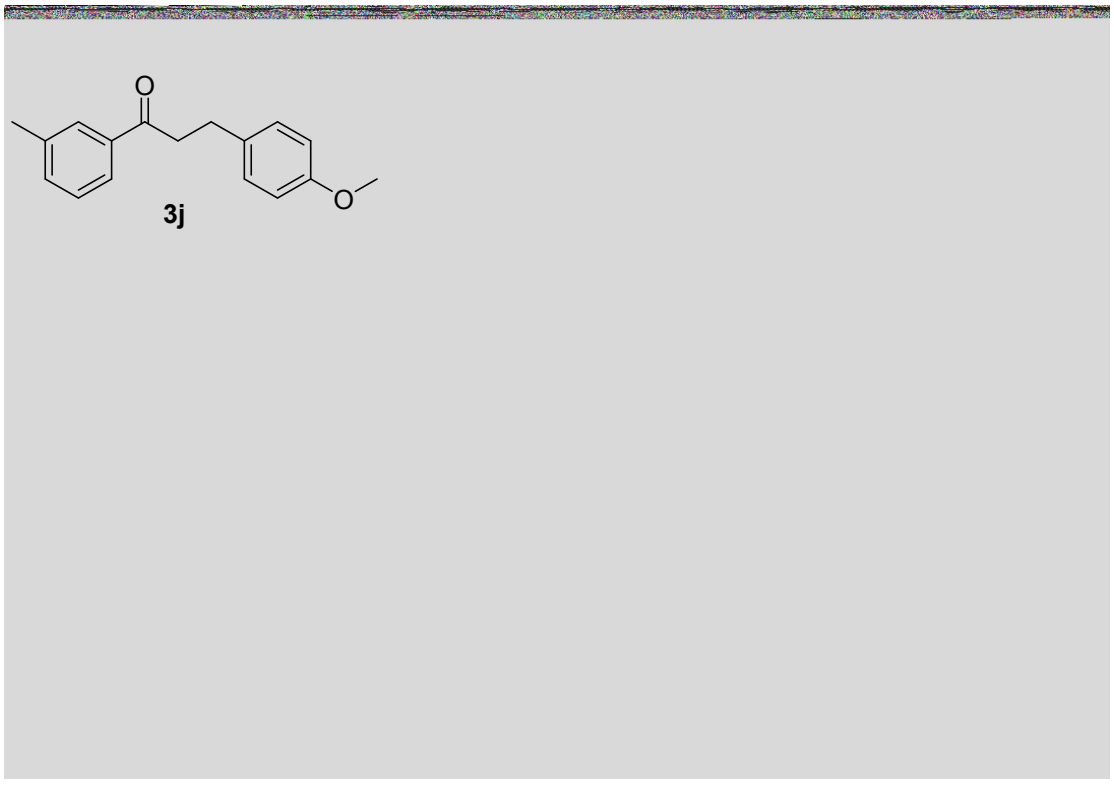
3.29
3.27
3.07
3.06
3.05
3.03
2.44
O
O
3j
2.05
2.02
2.03
2.03
3.07
2.05
2.06
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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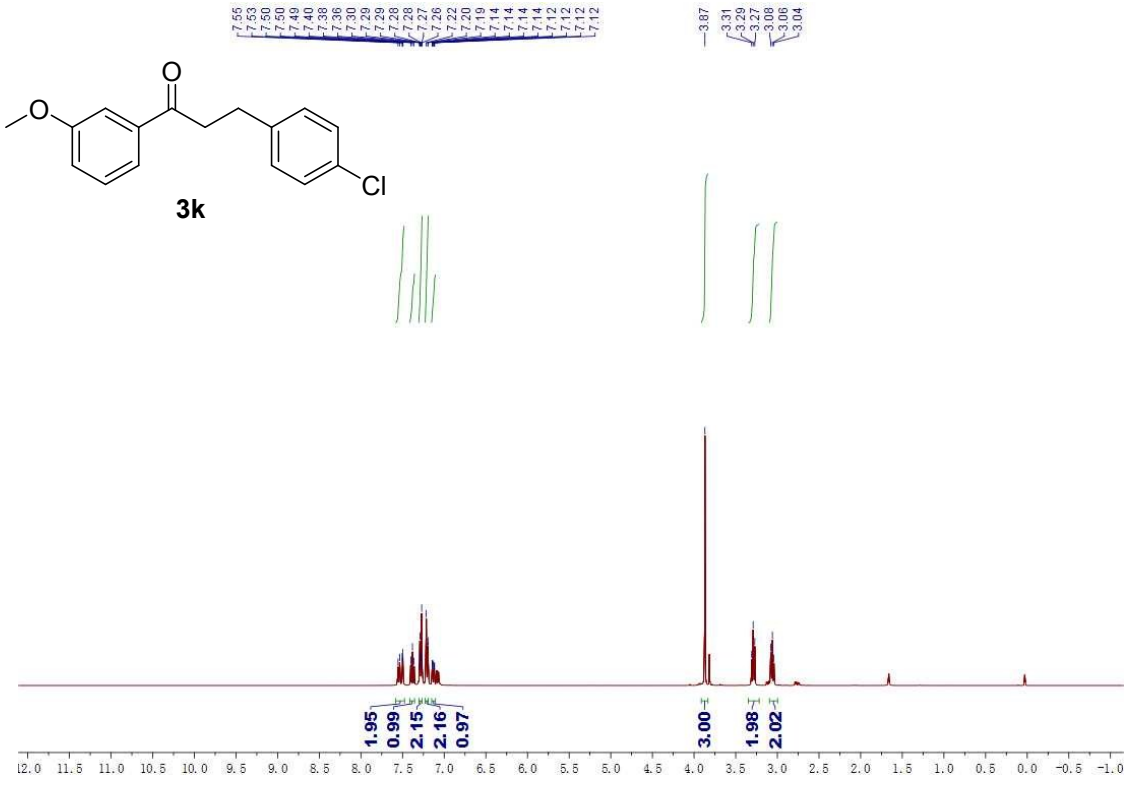
3j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7.14
7.14
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7.12
7.12
7.12
3.87
3.31
3.29
3.27
3.08
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O
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2.16
0.97
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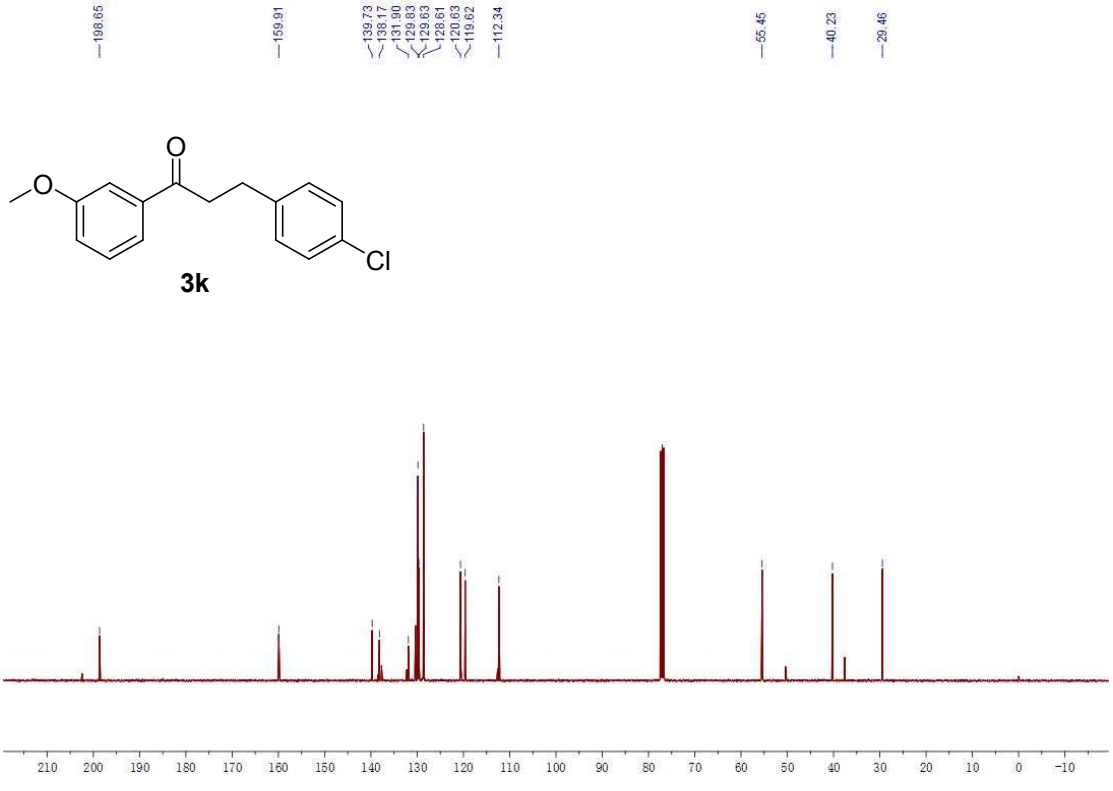
1.98
2.02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O
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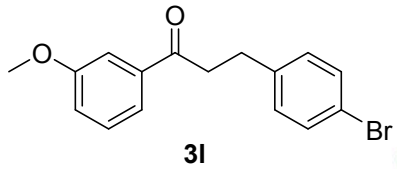
Cl
3k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O
Br

3l

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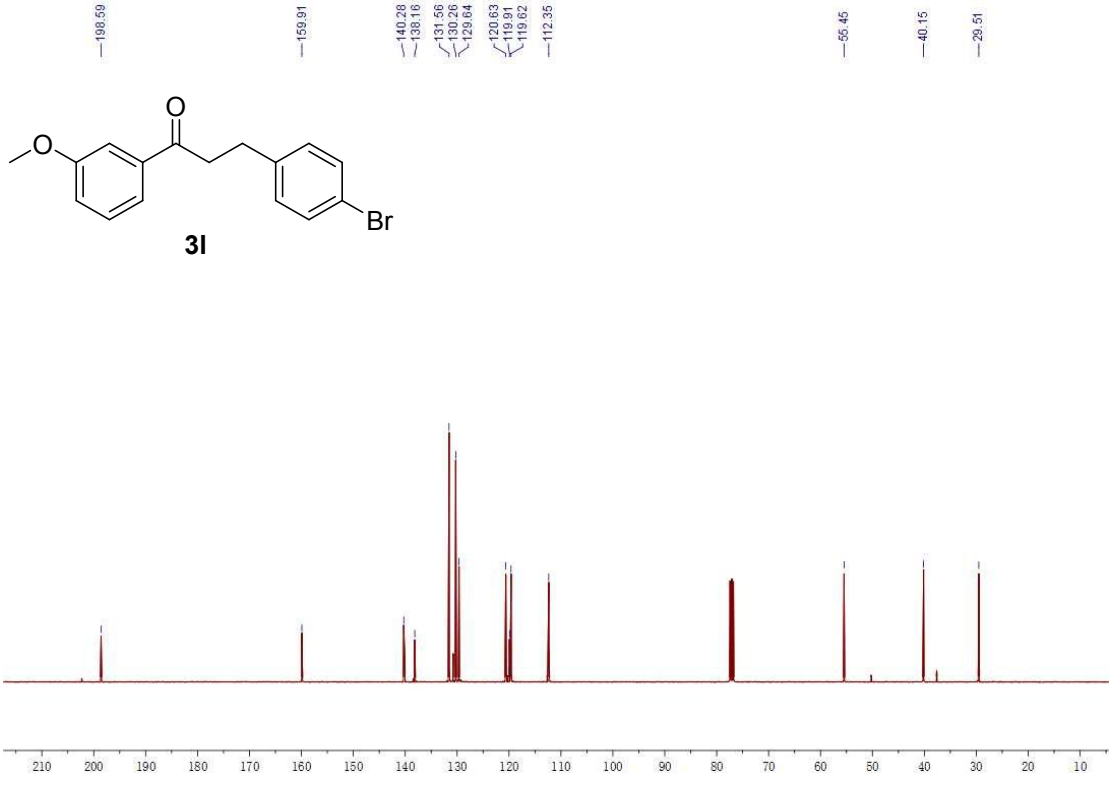
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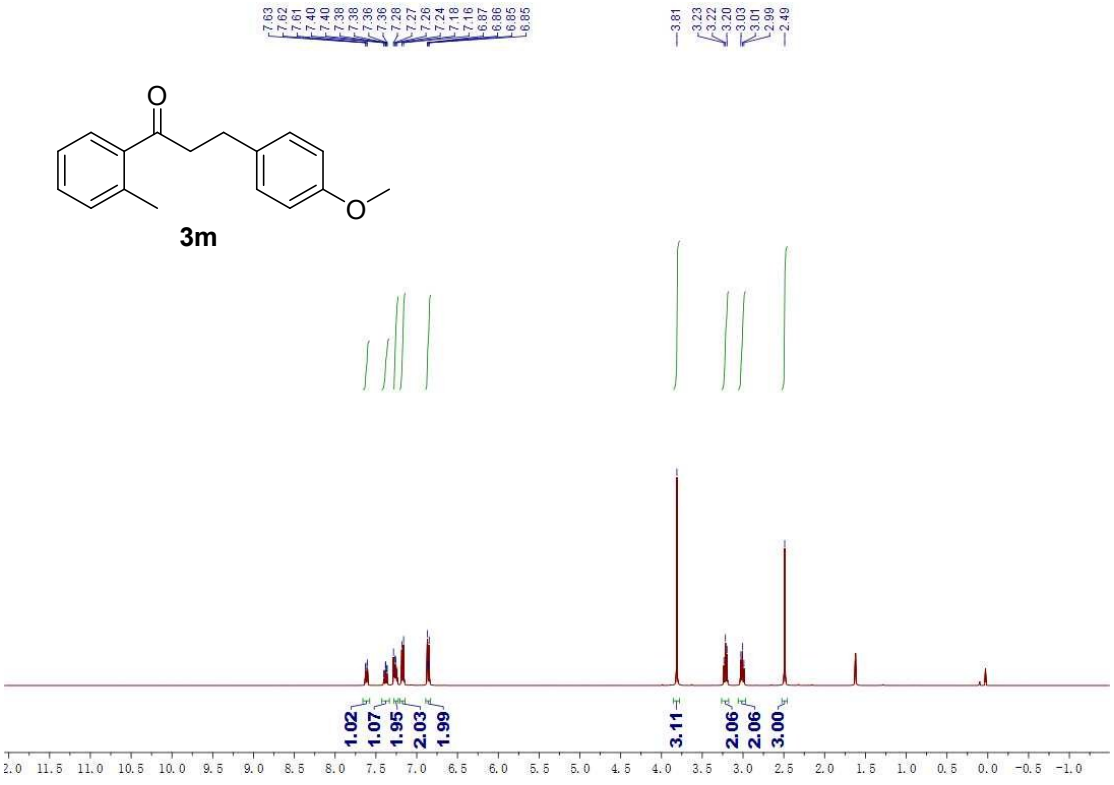
29.51

O
O
Br

3l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7.16
6.87
6.86
6.85
6.85
3.81
3.23
3.22
3.20
3.03
3.01
2.99
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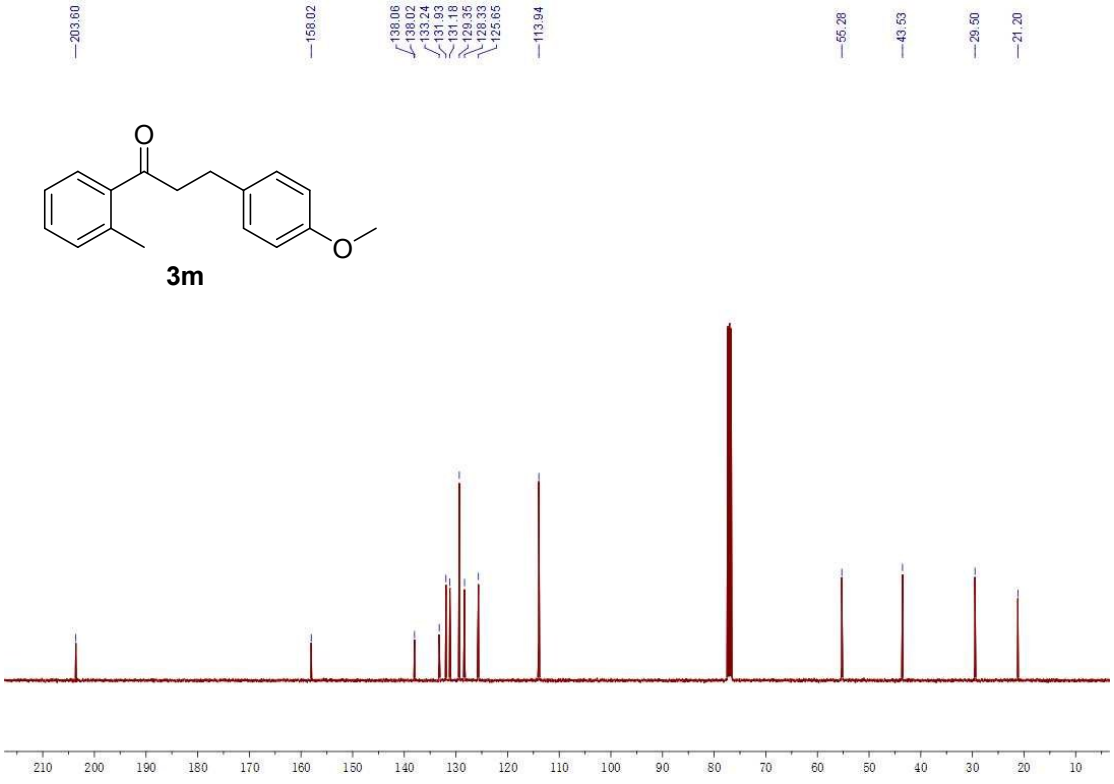
2.06
3.00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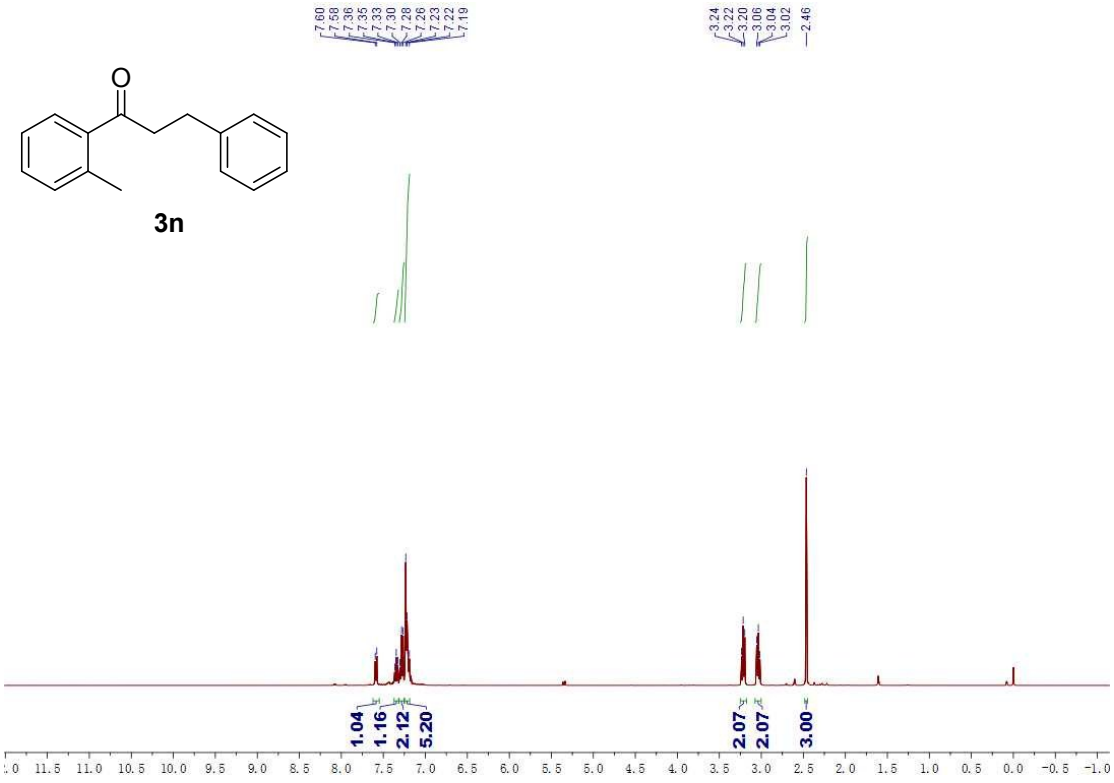
O
3m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3.20
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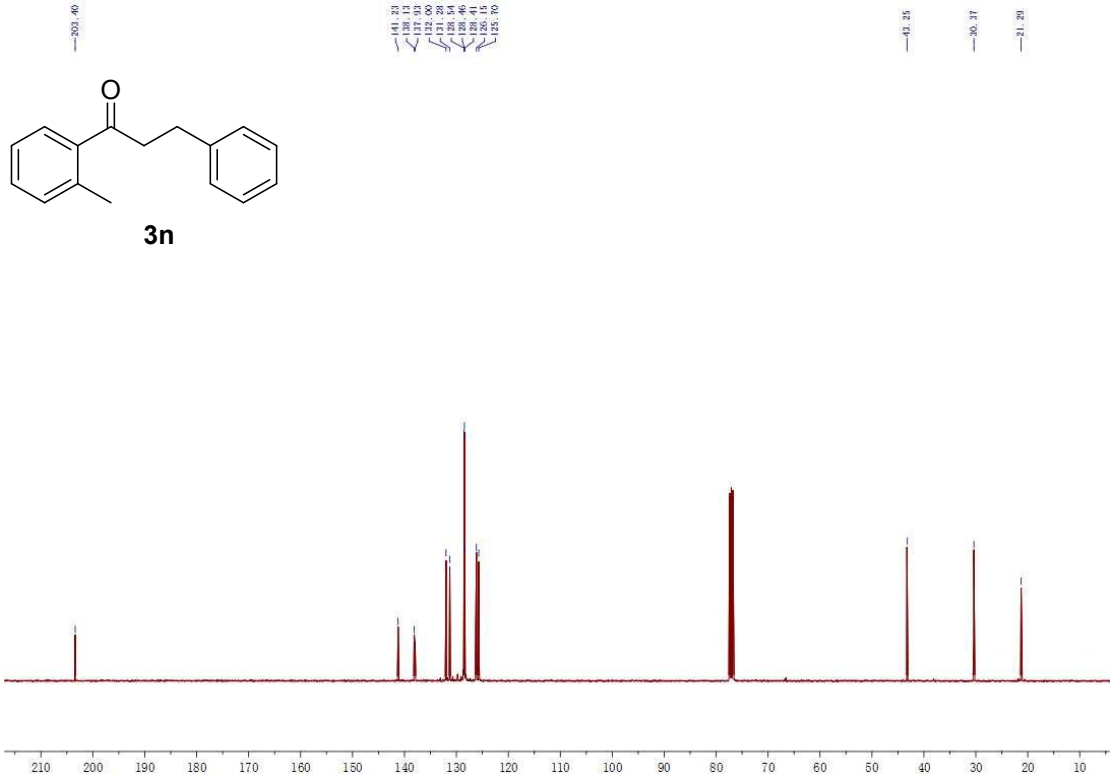
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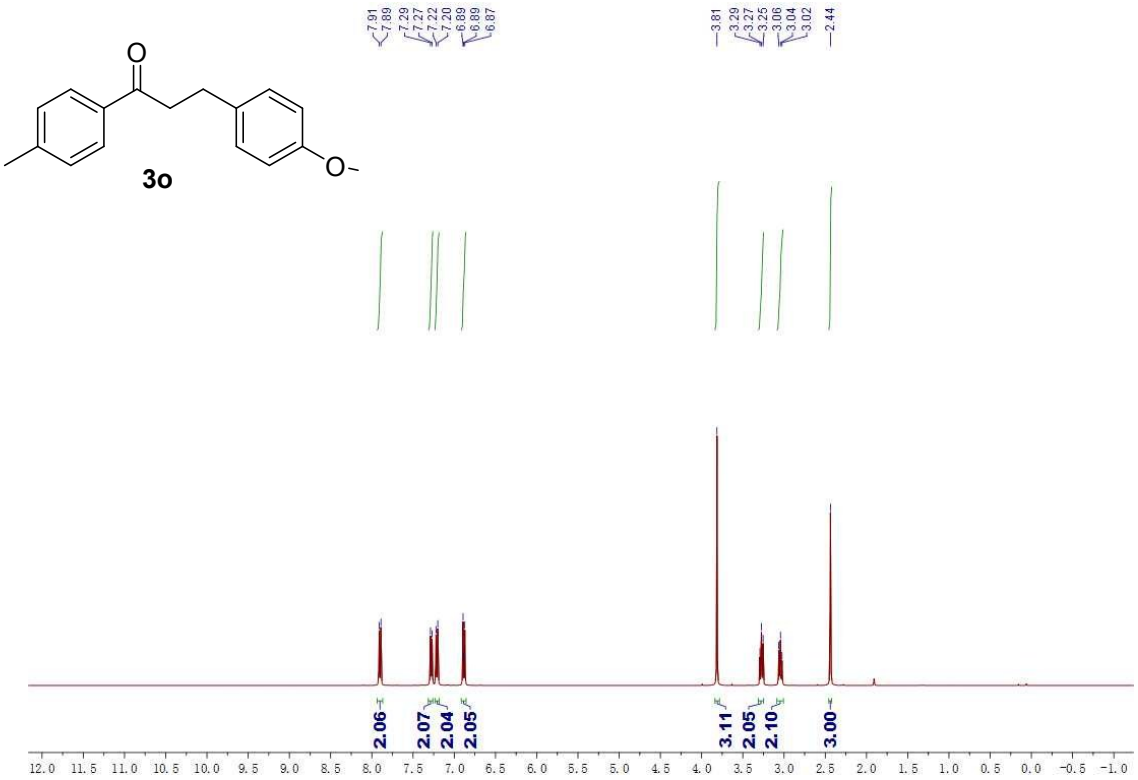
O
3n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3.06
3.04
3.02
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O
O
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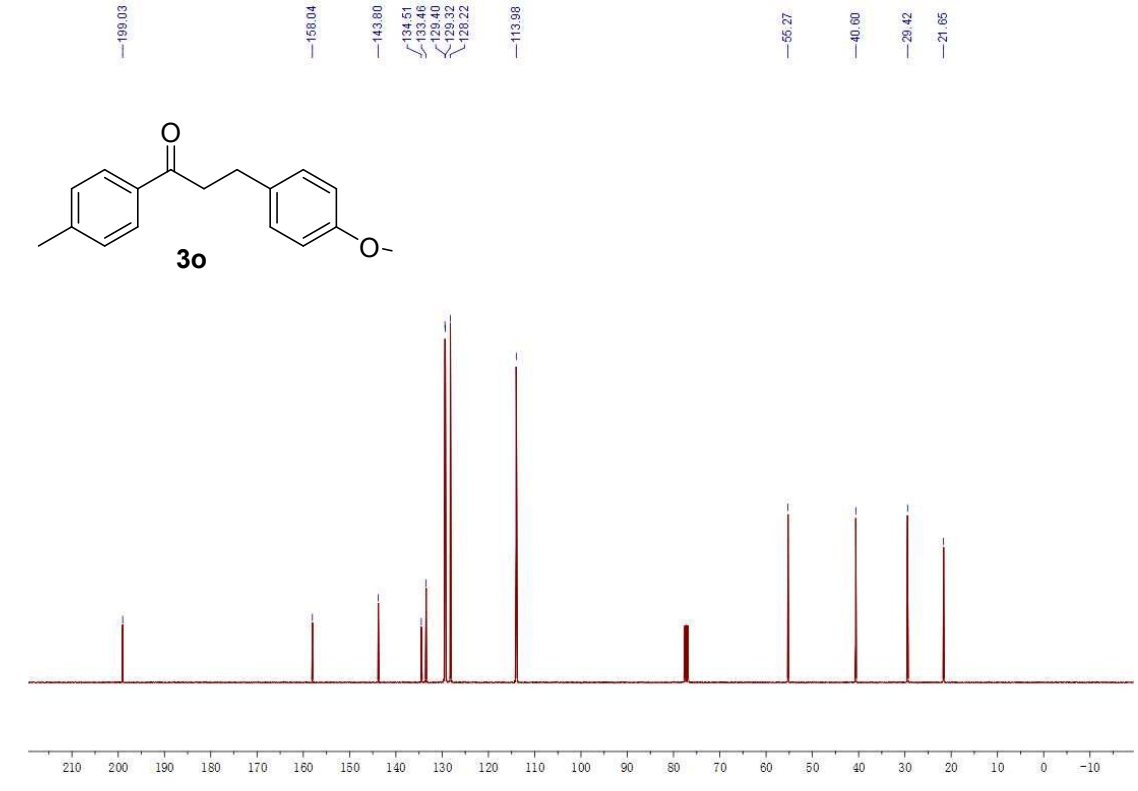
3.00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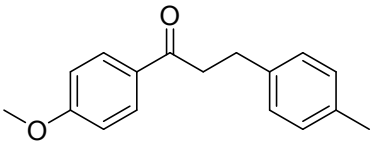
O
3o



3p

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3.25
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2.03
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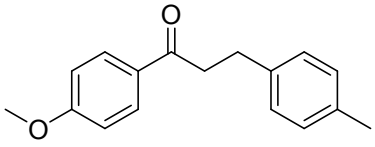
3.00



3p

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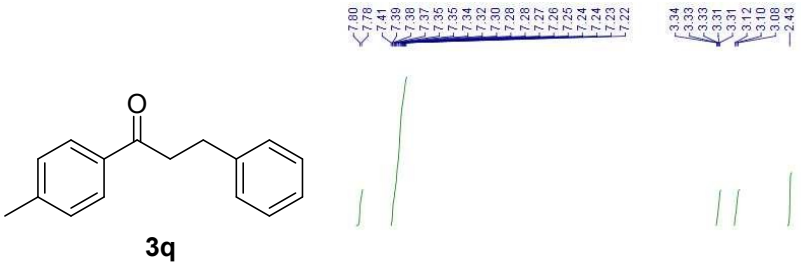
21.03



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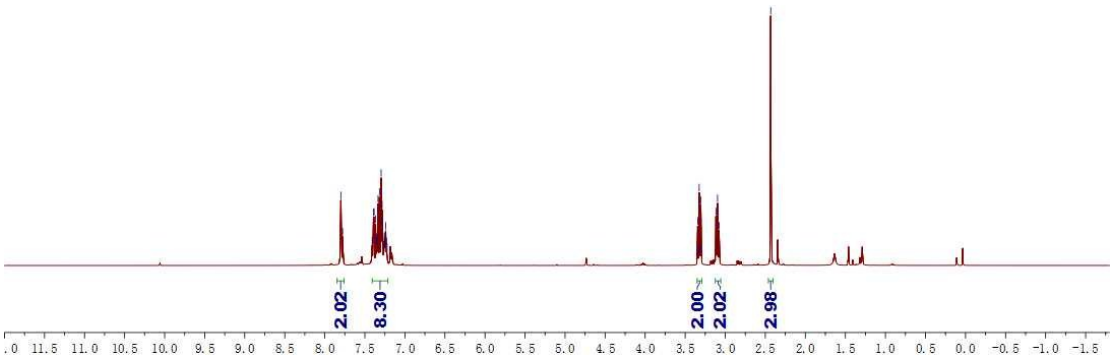

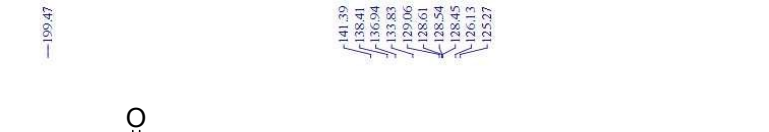

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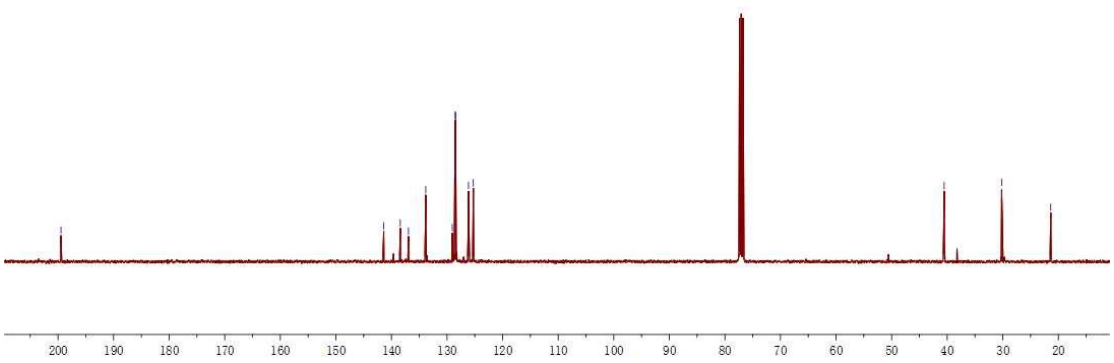

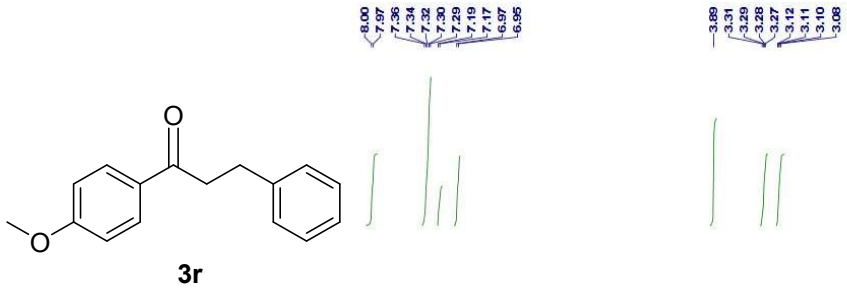
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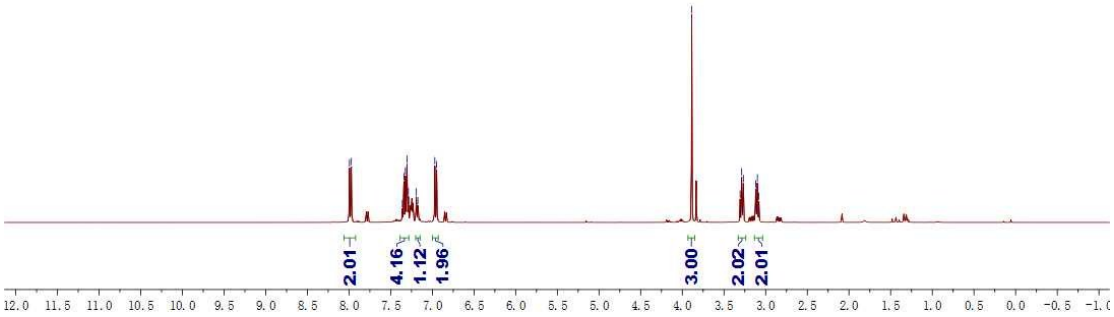
3.31
3.29
3.28
3.27
3.12
3.11
3.10
3.08
O
O

3r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4.16
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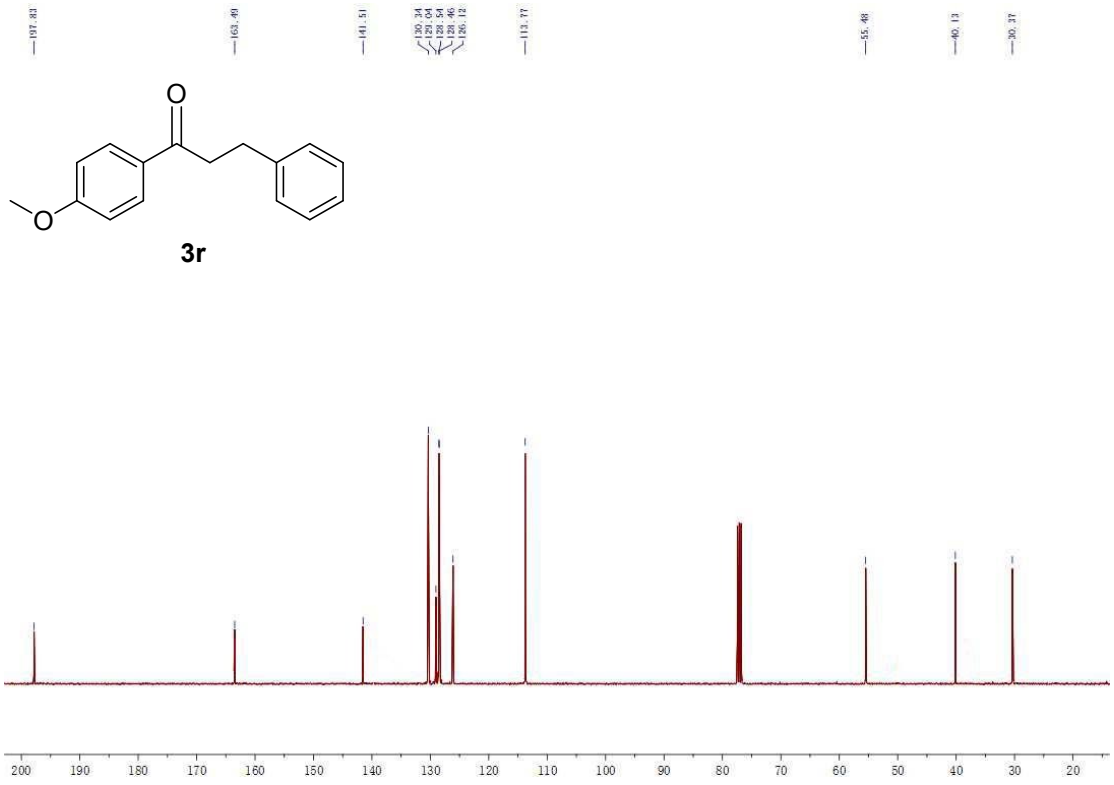
1.96
3.00
2.02
2.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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30.37
O
O
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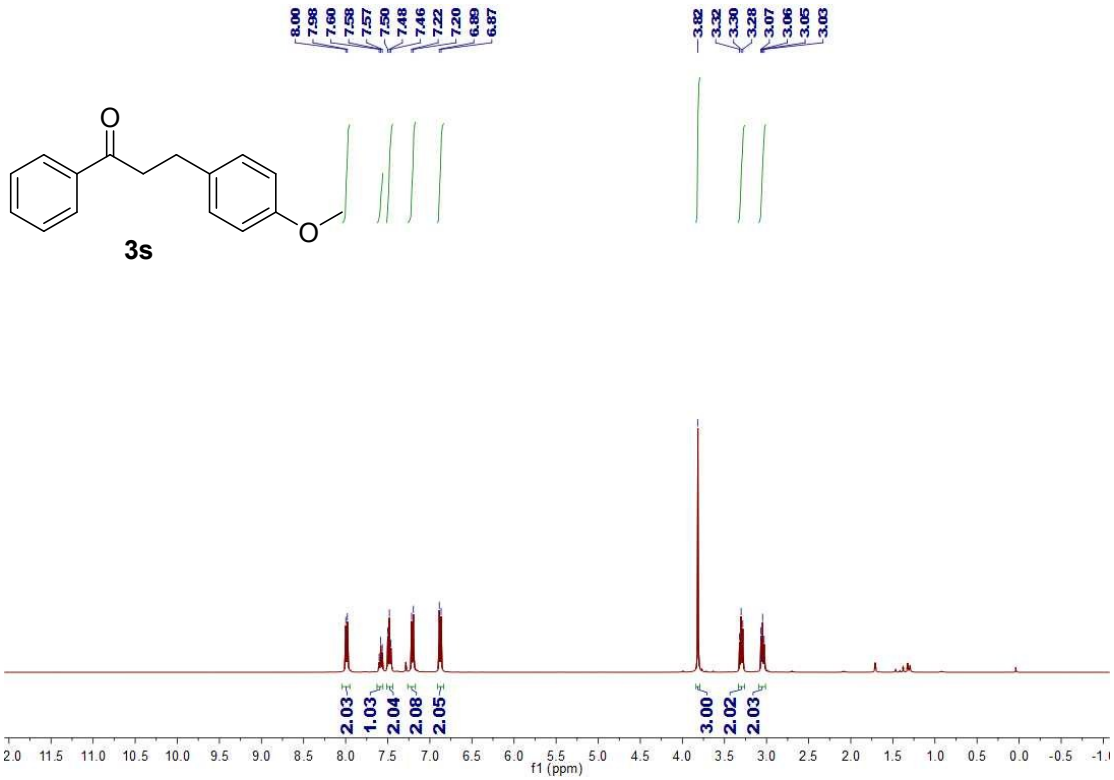
3r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6.87
3.82
3.32
3.30
3.28
3.07
3.06
3.05
3.03
O
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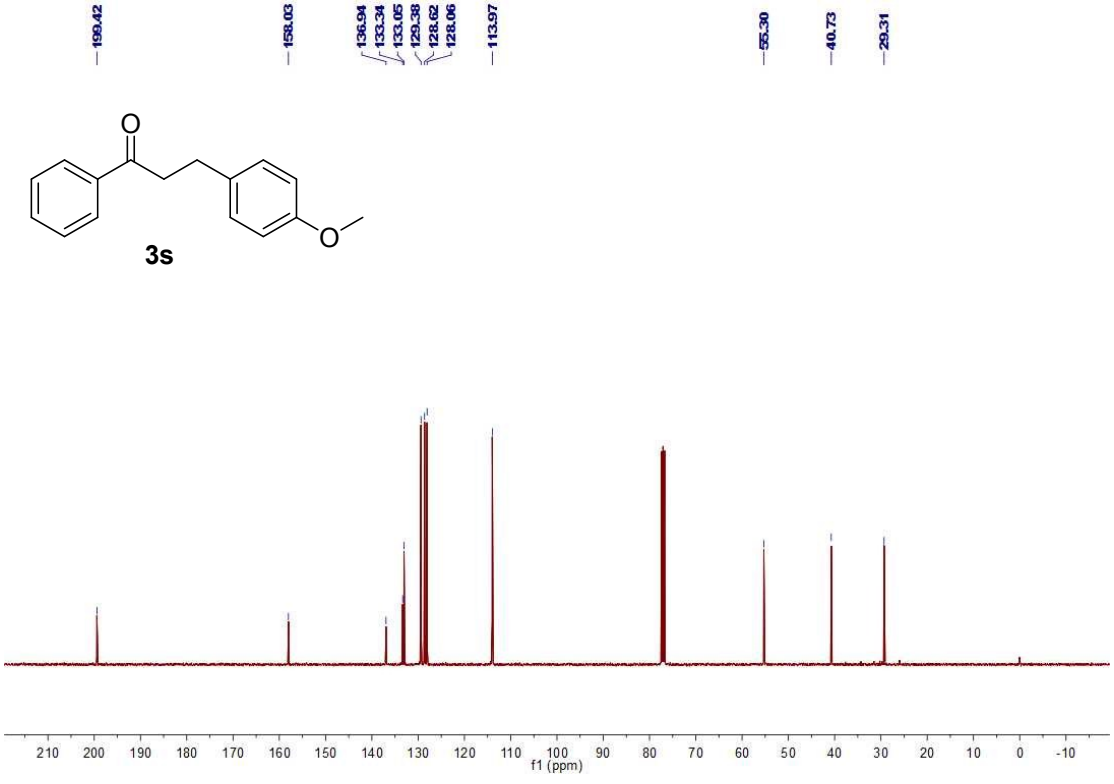
2.03
1.03
2.04
2.08
2.05
3.00
2.02
2.03
f1 (ppm)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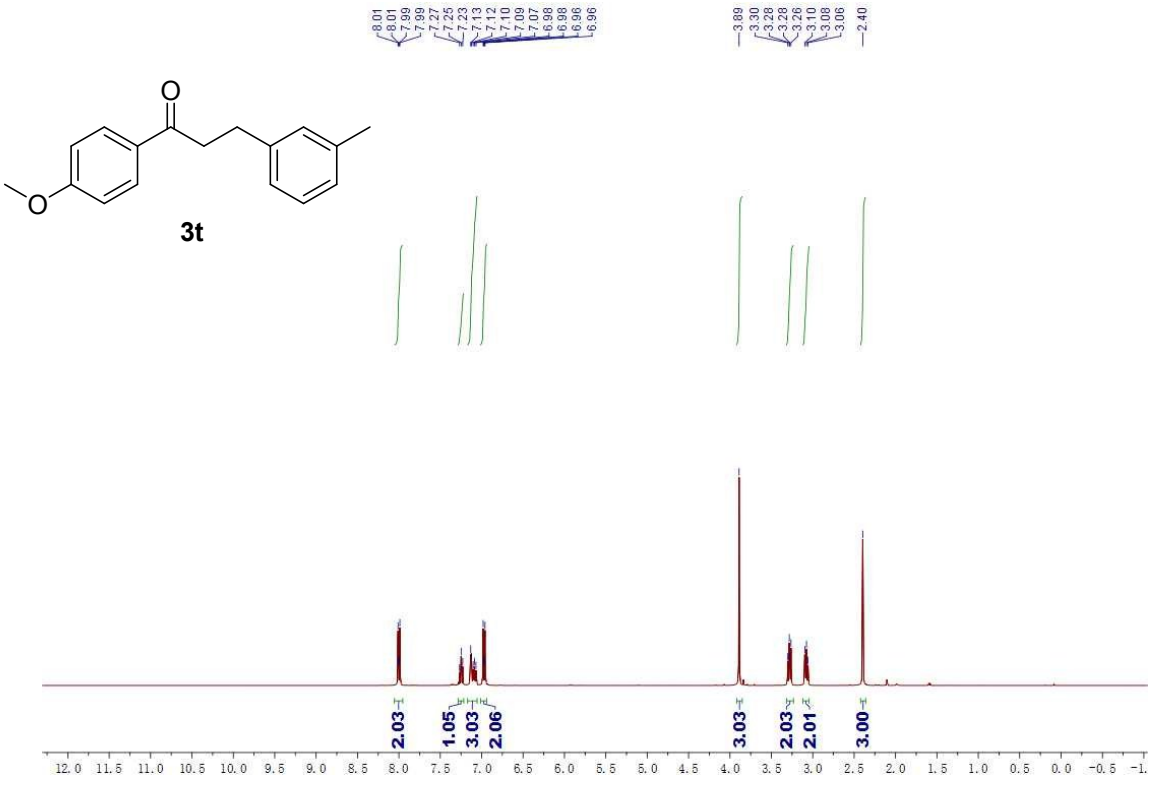
128.06
113.97
55.30
40.73
29.31
O
O
3s
f1 (ppm)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7.07
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6.98
6.96
6.96
3.89
3.30
3.28
3.28
3.26
3.10
3.08
3.06
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O
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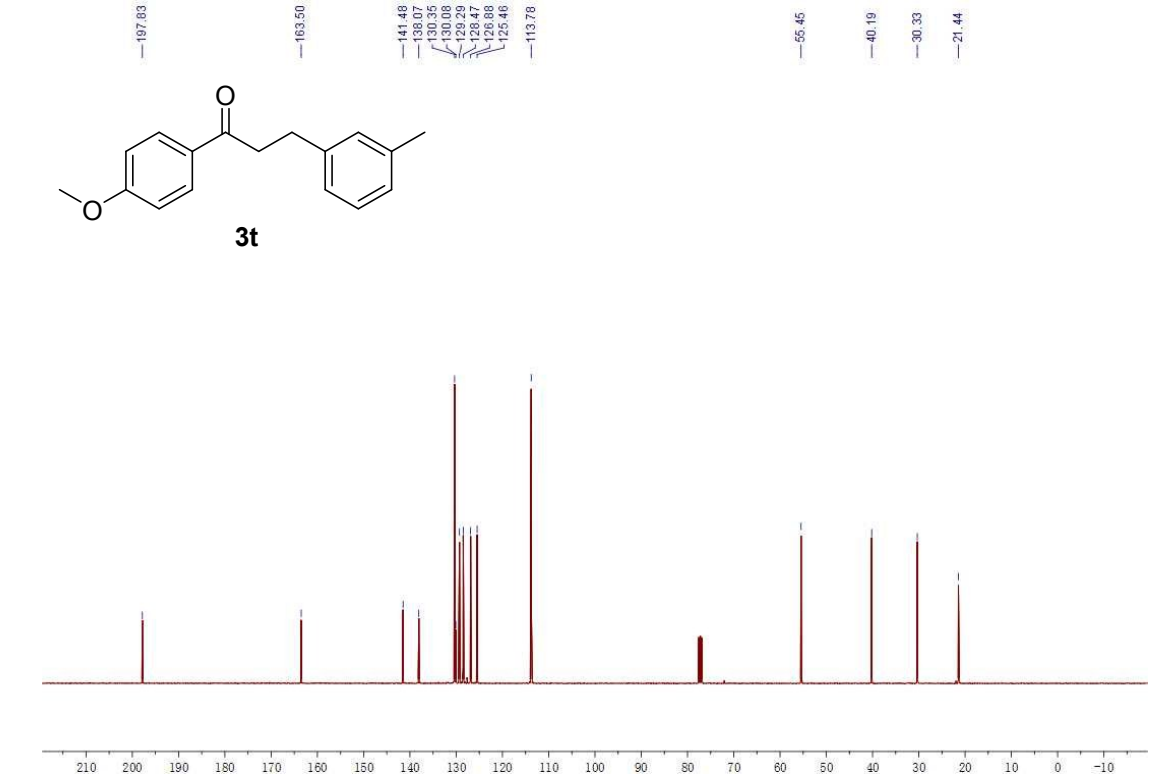
1.05
3.03
2.06
3.03
2.03
2.01
3.00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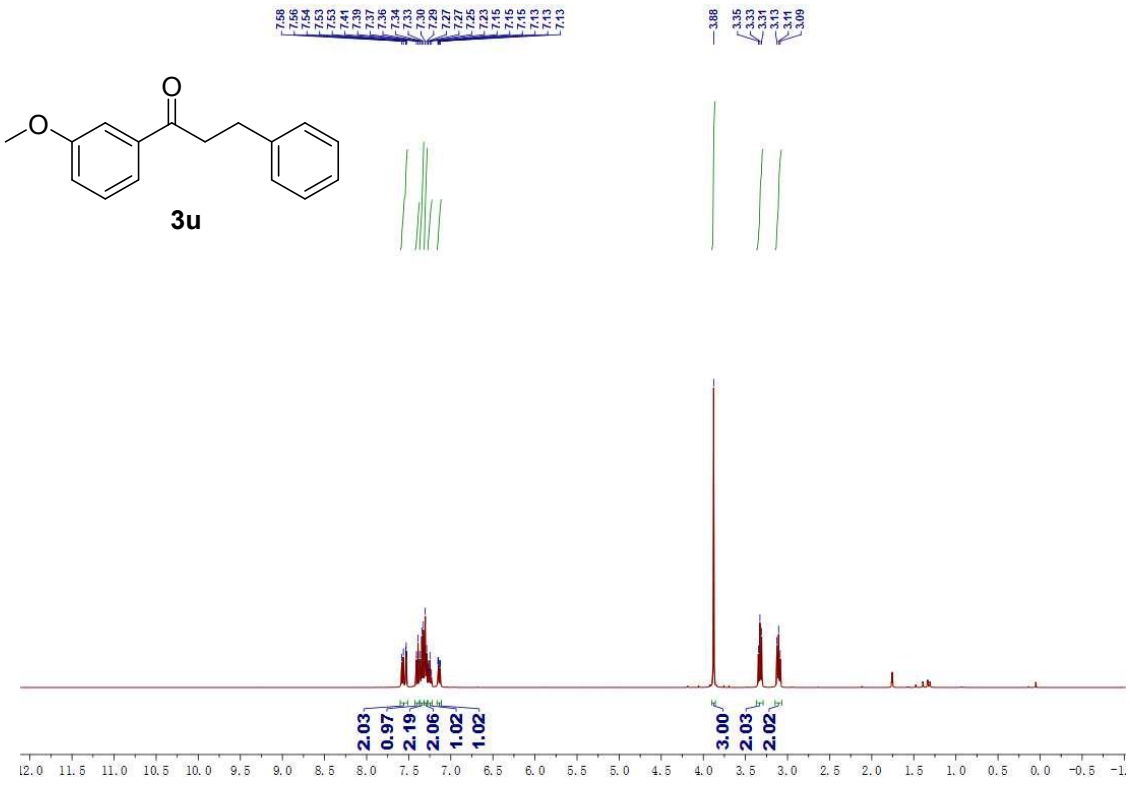
40.19
30.33
21.44
O
O
3t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1.02
1.02
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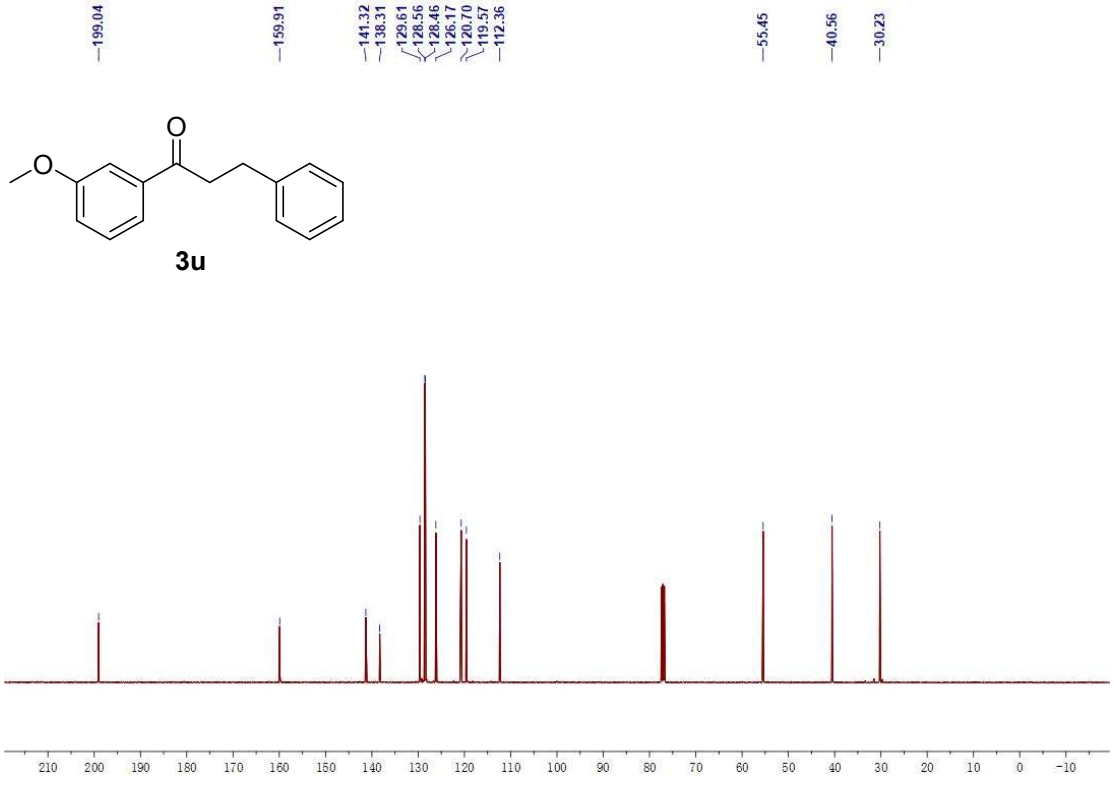
2.02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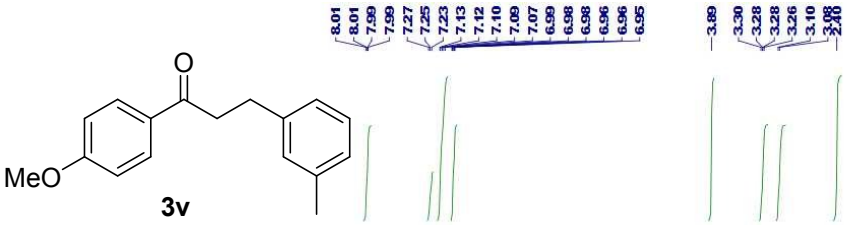
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7.10
7.09
7.07
6.99
6.98
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6.95
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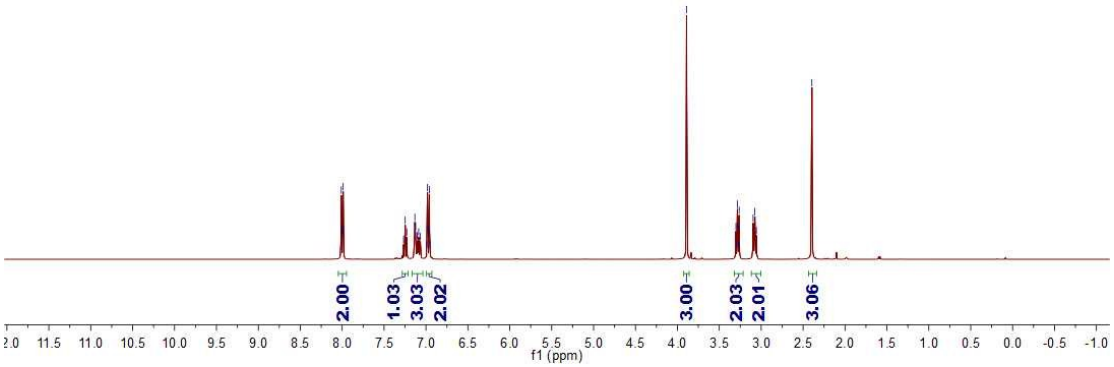
3.30
3.28
3.28
3.26
3.10
O
MeO
3v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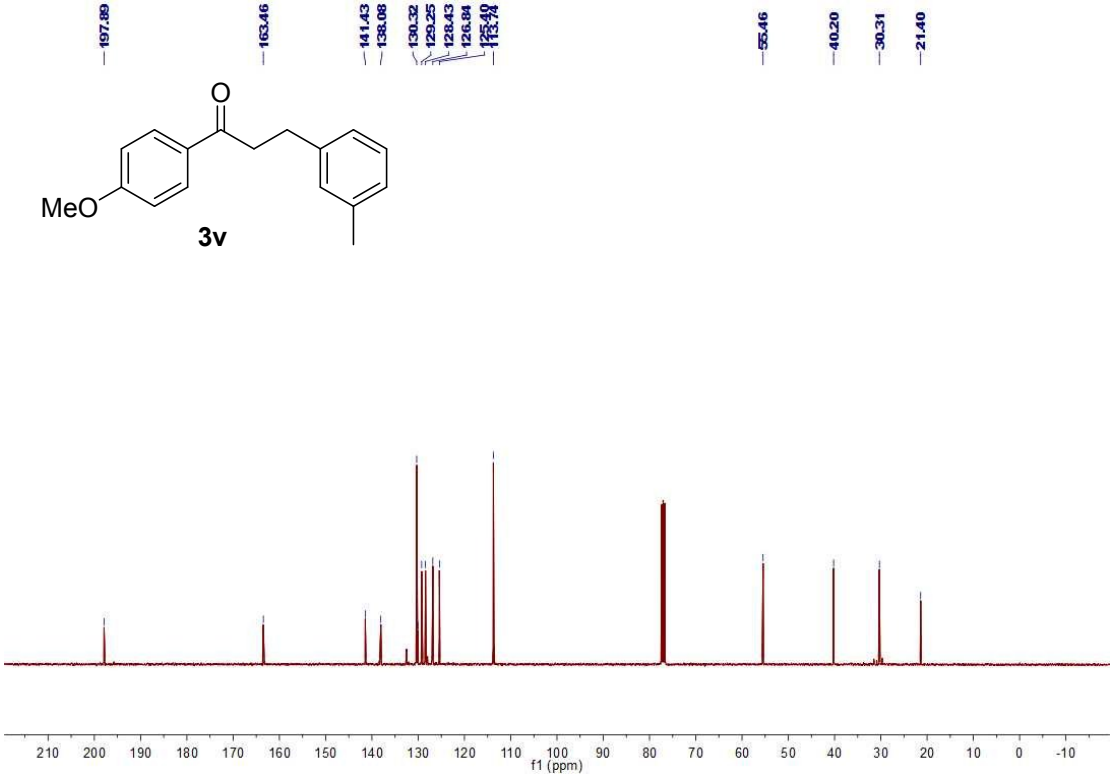
3.06
f1 (ppm)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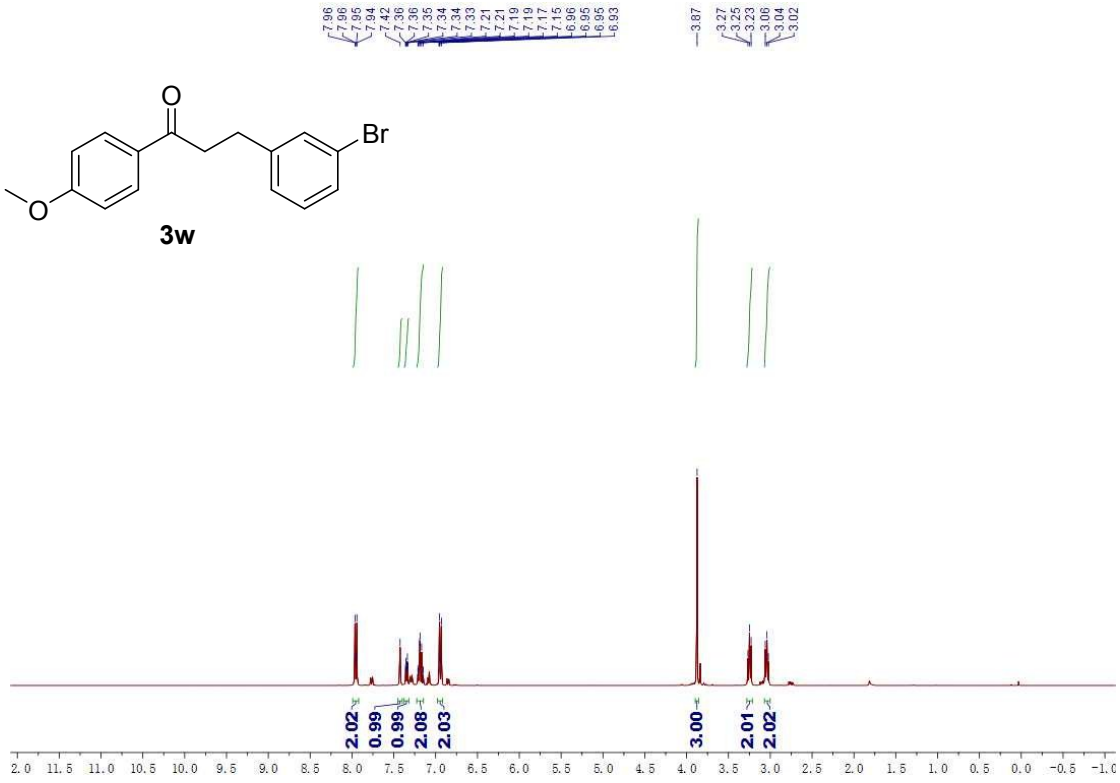
21.40
O
MeO
3v
f1 (ppm)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6.93
3.87
3.27
3.25
3.23
3.06
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Br
O
3w
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0.99
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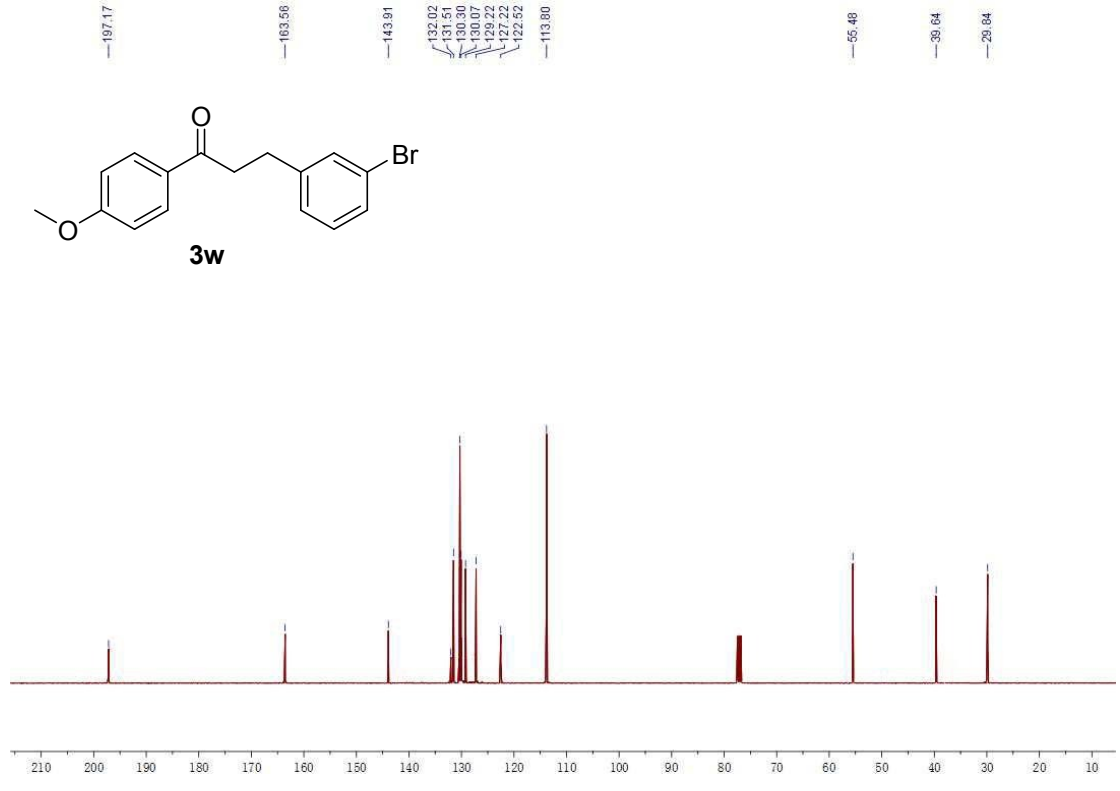
3.00
2.01
2.02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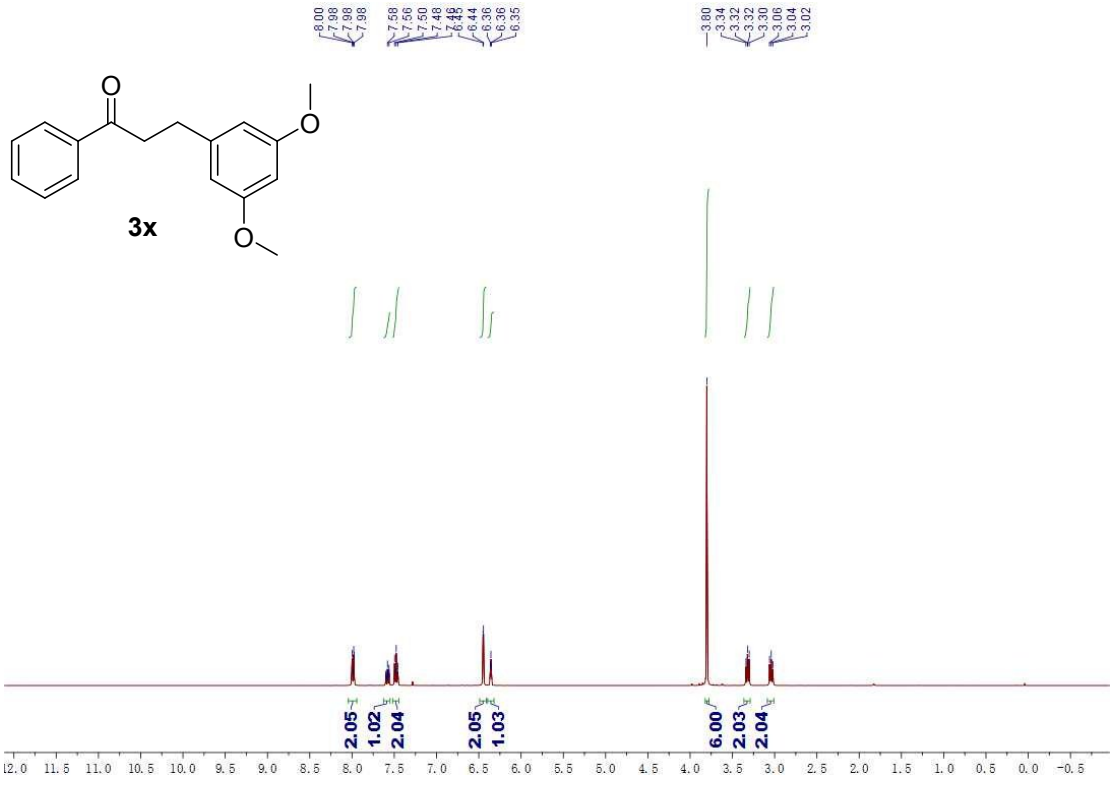
39.64
29.84
O
Br
O
3w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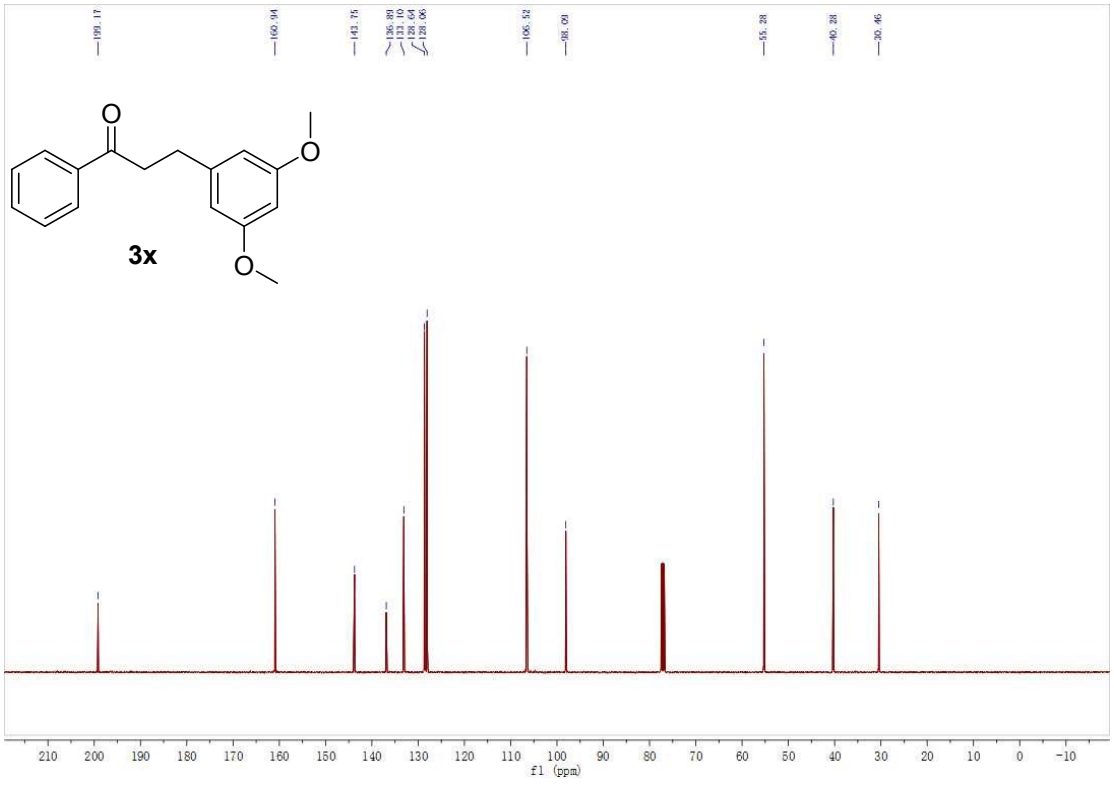
6.35
3.80
3.34
3.32
3.32
3.30
3.06
3.04
3.02
O
O
O
3x
2.05
1.02
2.04
2.05
1.03
6.00
2.03
2.04
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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O
O
O
3x
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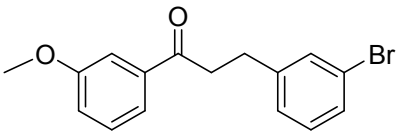
f1 (ppm)



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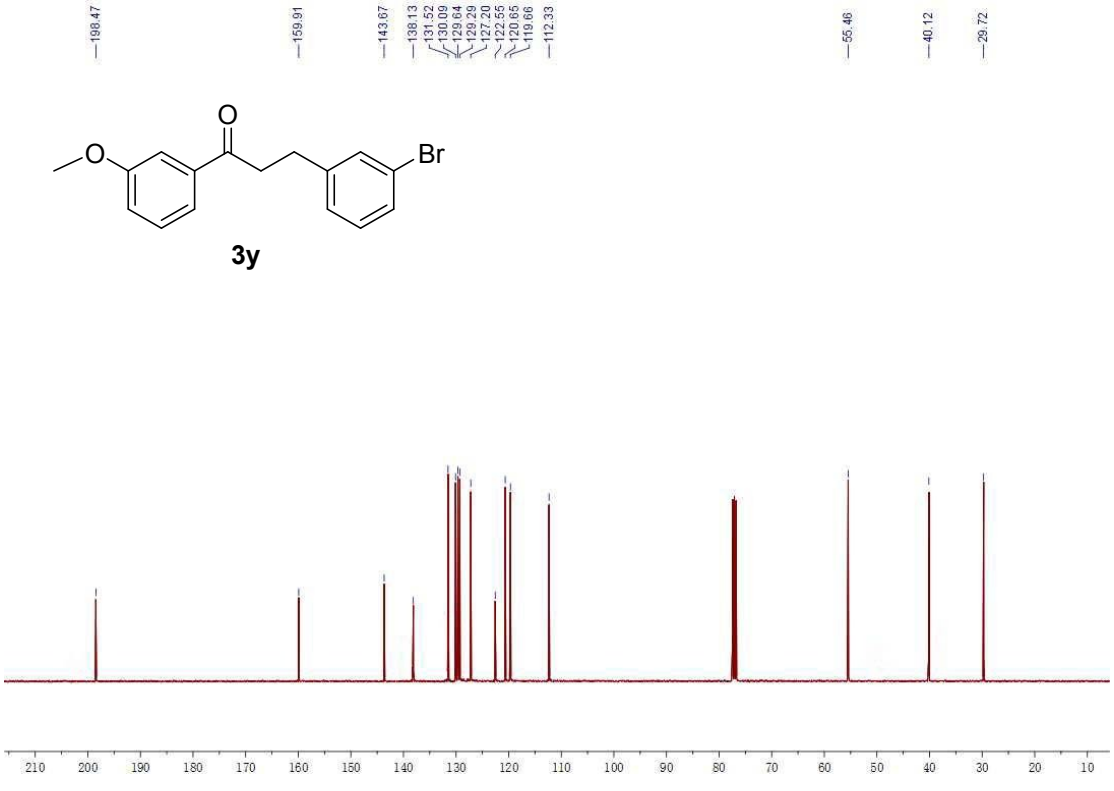

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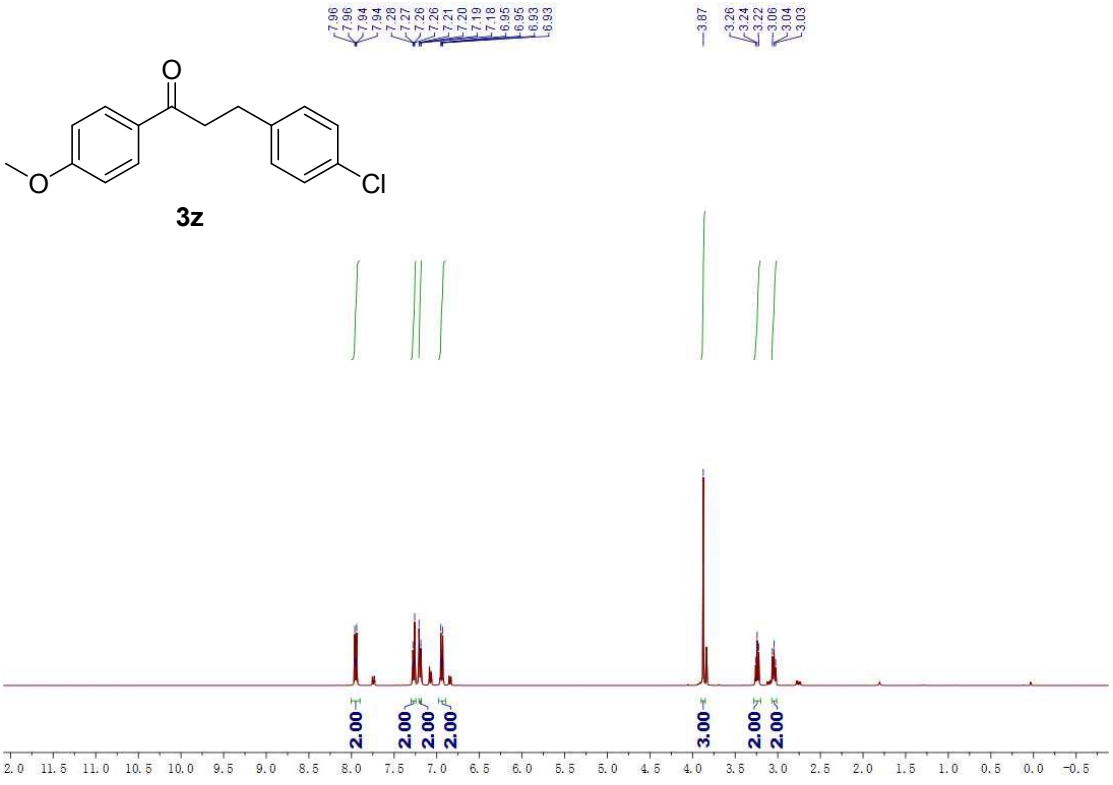
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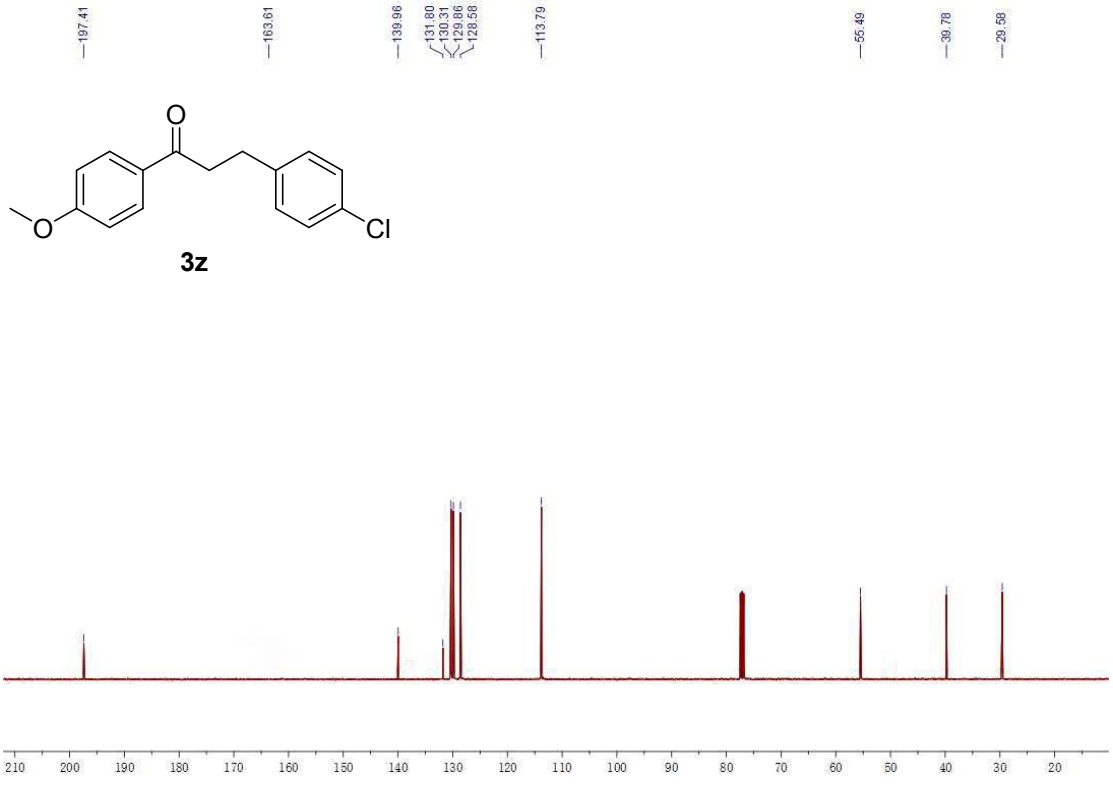
6.95
6.95
6.93
6.93
3.87
3.26
3.24
3.22
3.06
3.04
3.03
O
O
Cl
3z
2.00
2.00
2.00
2.00
3.00
2.00
2.00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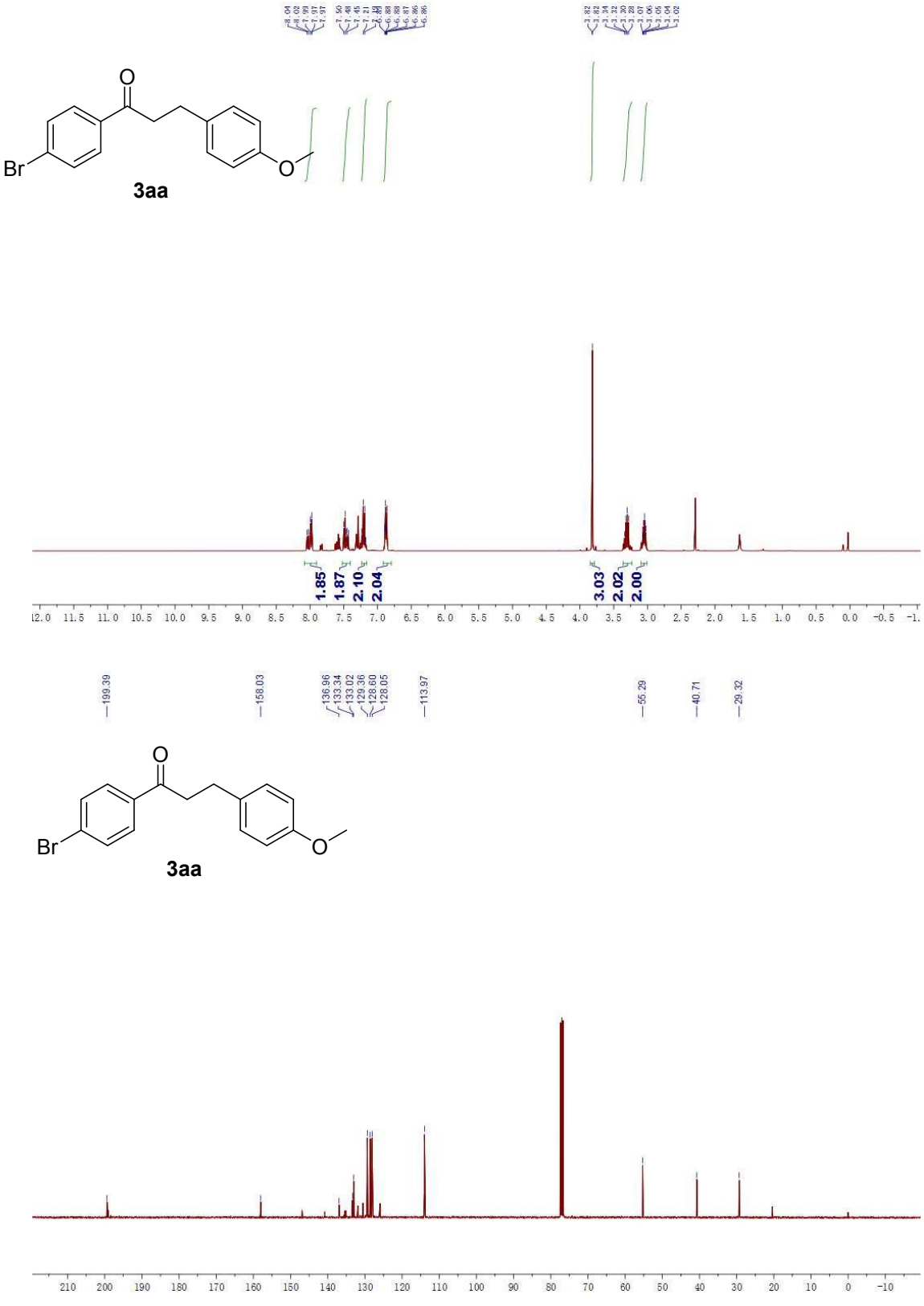
O
O
Cl
3z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Br
O
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3.03
2.02
2.00
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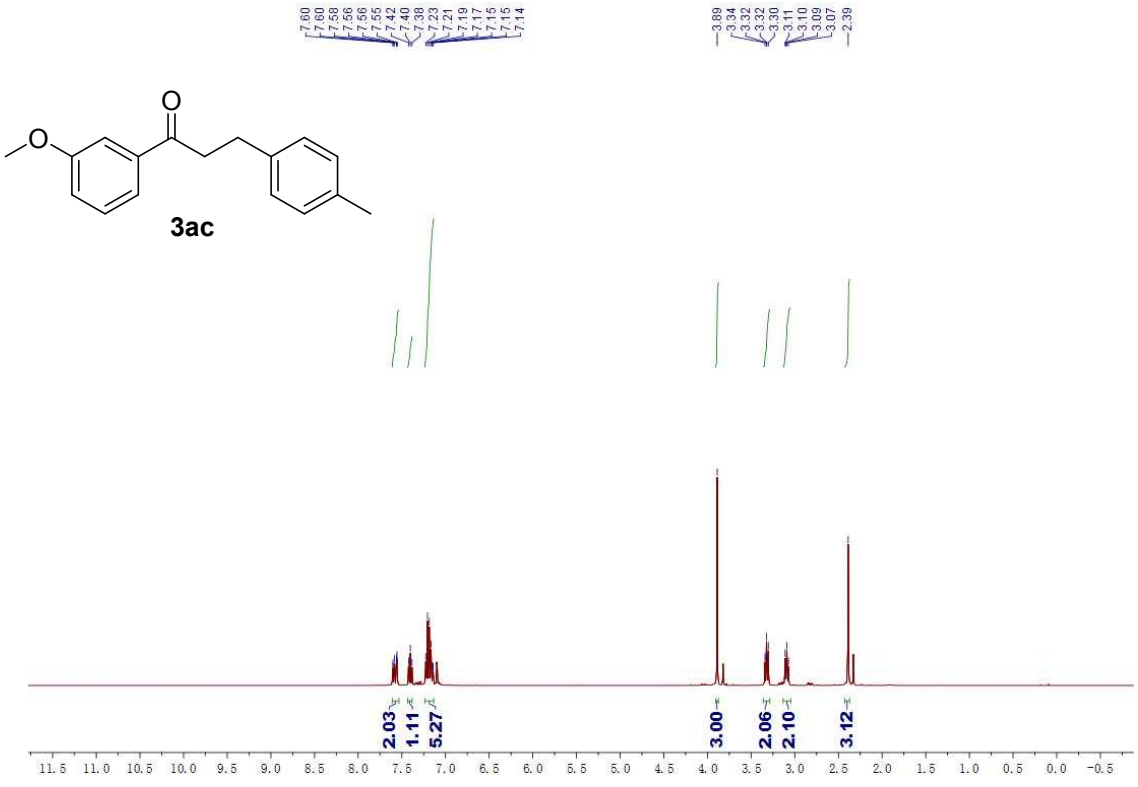
129.36
128.60
128.05
113.97
55.29
40.71
29.32
O
Br
O
3aa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7.19
7.17
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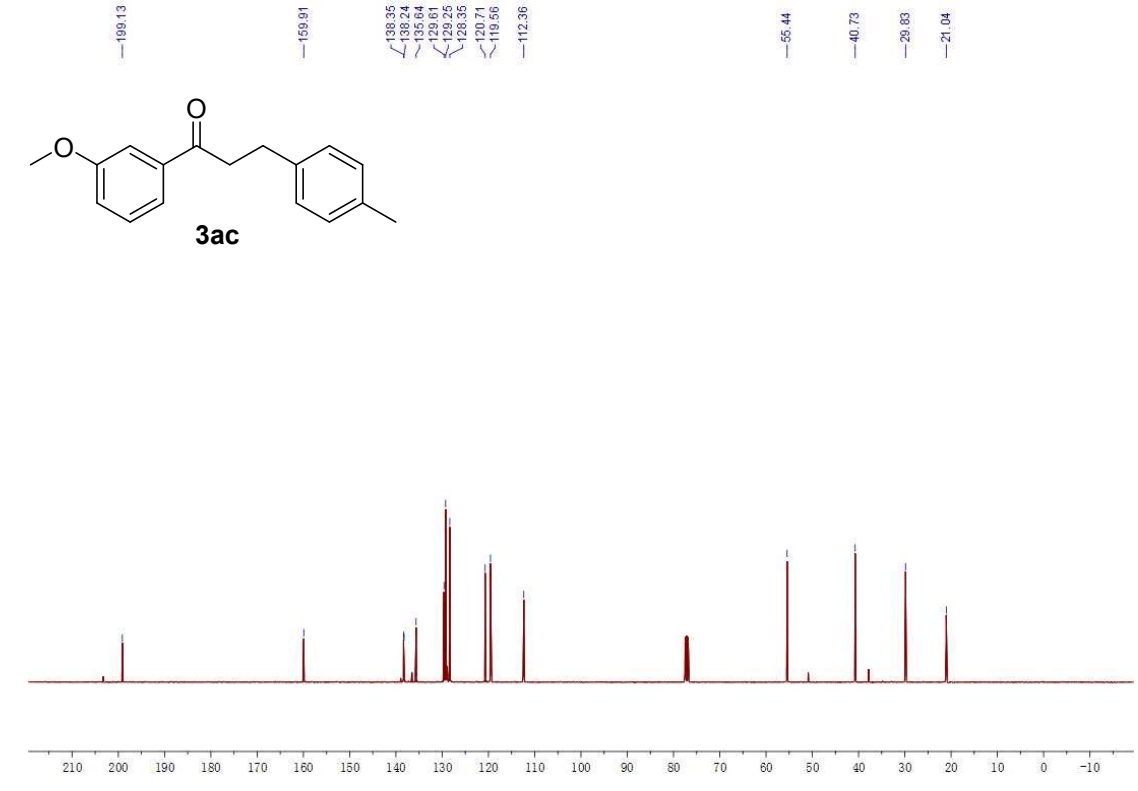
7.15
7.14
3.89
3.34
3.32
3.32
3.30
3.11
3.10
3.09
3.07
2.39
O
O
3ac
2.03
1.11
5.27
3.00
2.06
2.10
3.12
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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129.61
129.25
128.35
120.71
119.56
112.36
55.44
40.73
29.83
21.04
O
O
3ac
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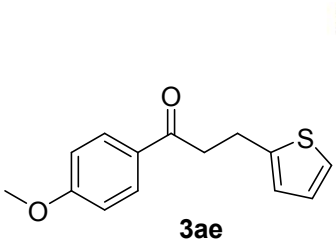
O
S
O

3ae

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7.97
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7.15
7.14
7.14
6.97
6.96
6.96
6.95
6.93
6.89
6.89
6.88
6.88
3.88
3.33
3.33
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3.31
3.31
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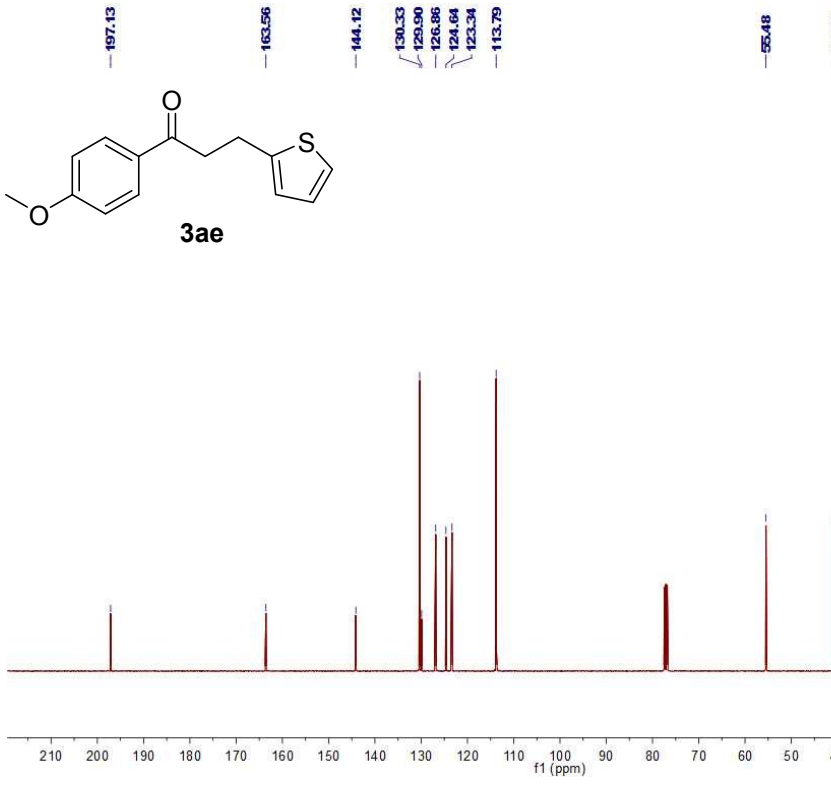
2.98
0.98
3.03
4.00
f1 (ppm)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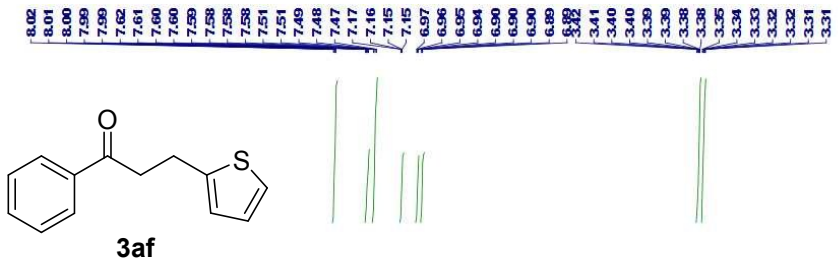
40.19
24.41
f1 (ppm)

O
S
O

3ae



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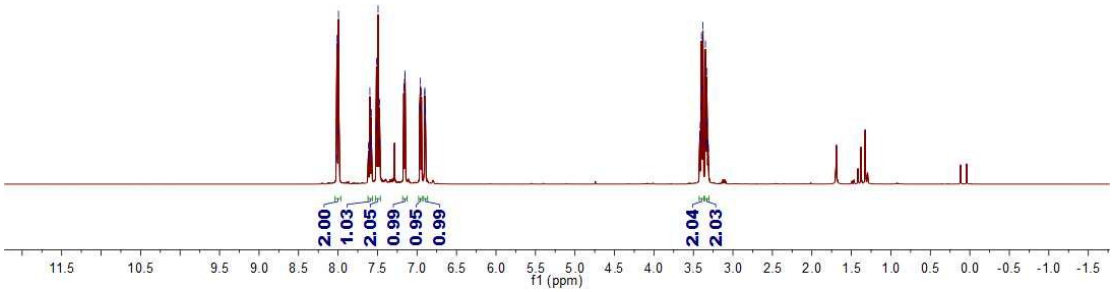

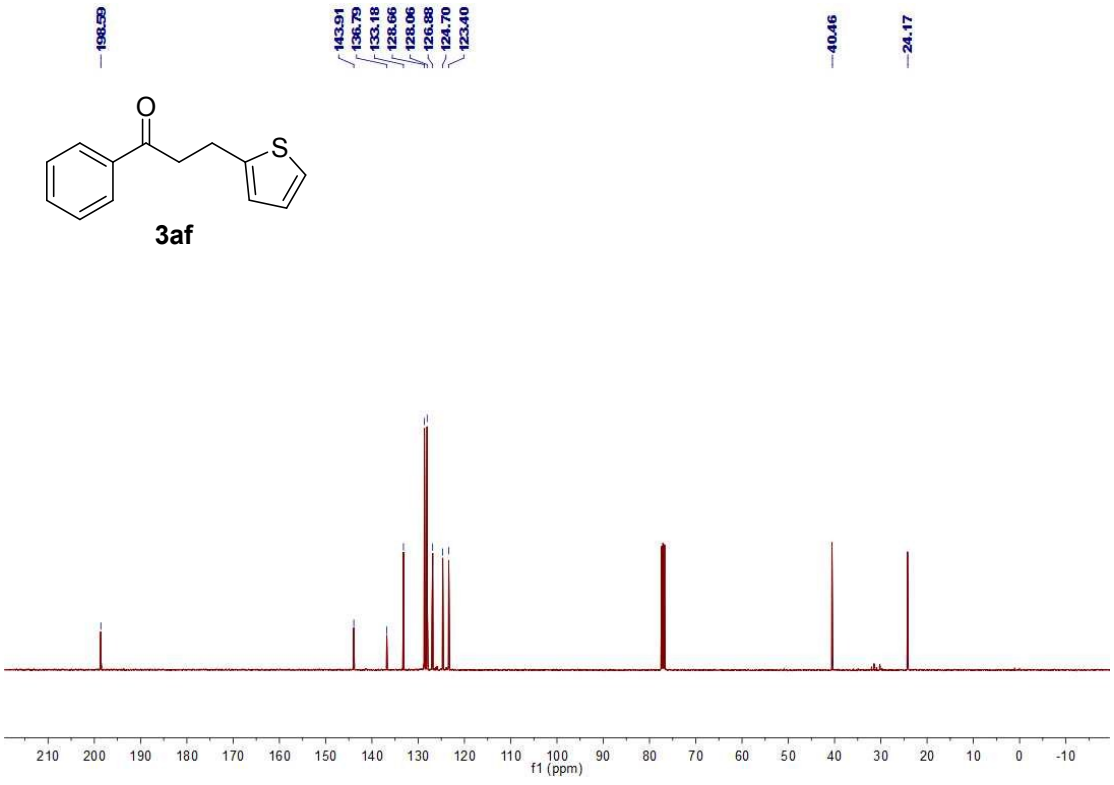

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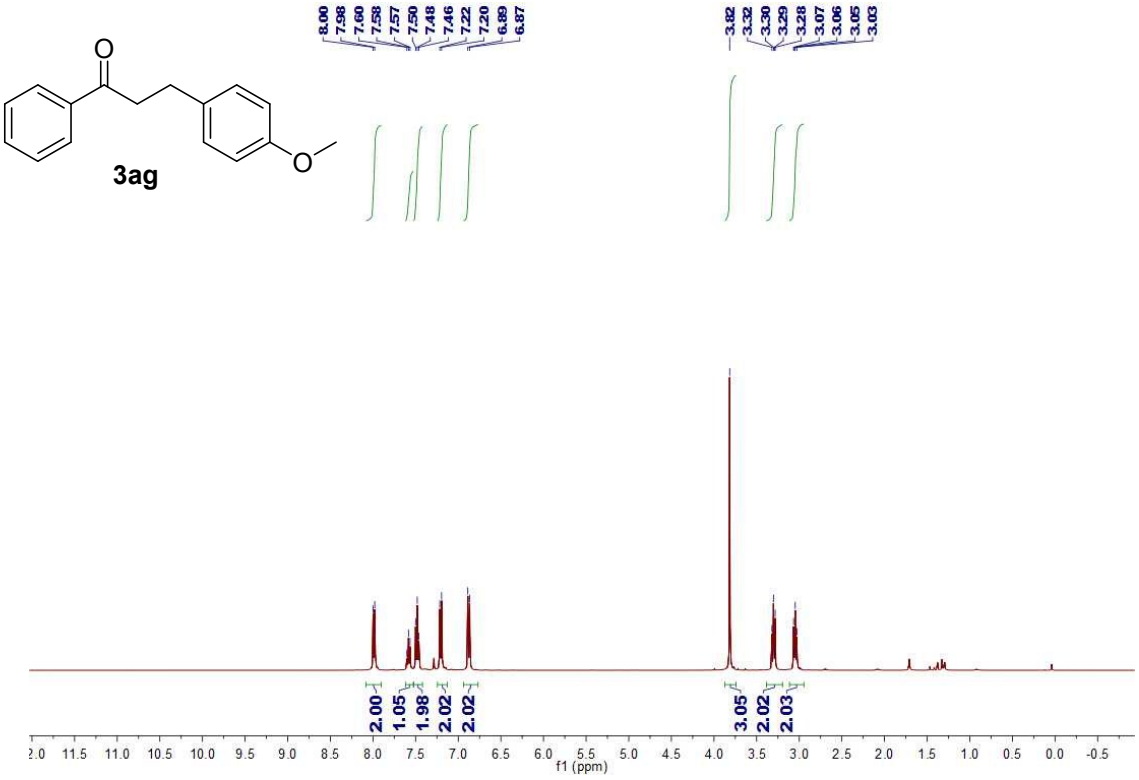
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7.22
7.20
6.89
6.87
3.82
3.32
3.30
3.29
3.28
3.07
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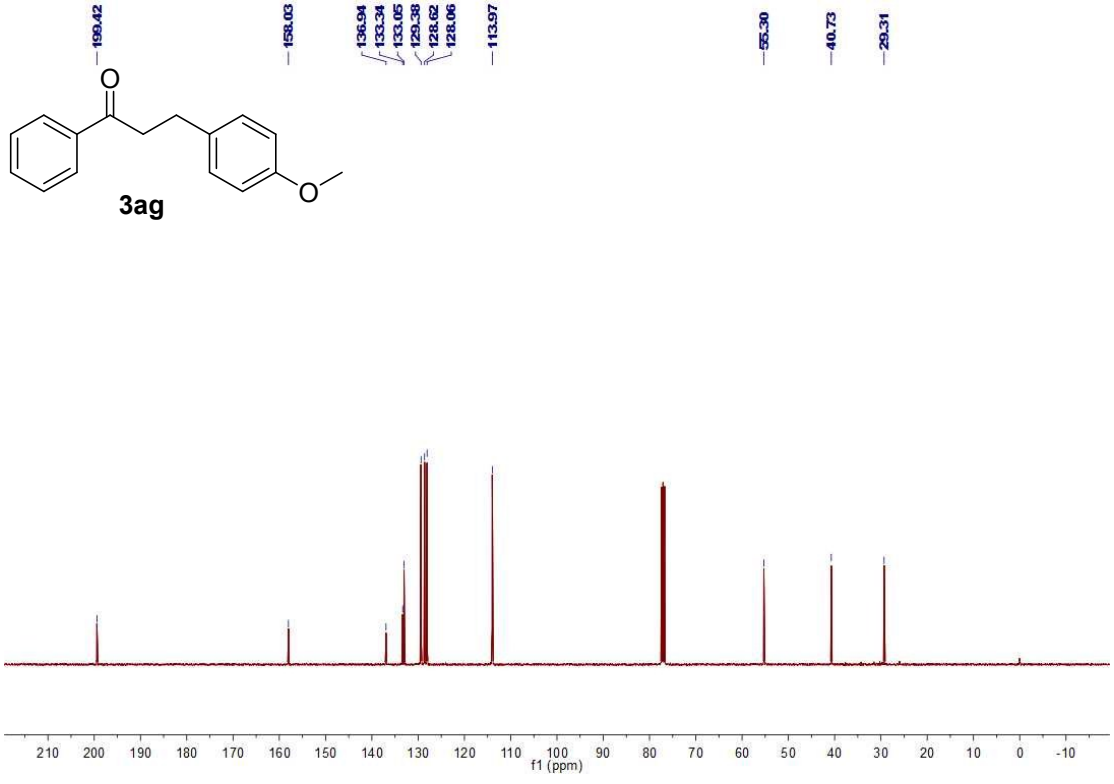
2.00
1.05
1.98
2.02
2.02
3.05
2.02
2.03
f1 (ppm)


3ag
190.42
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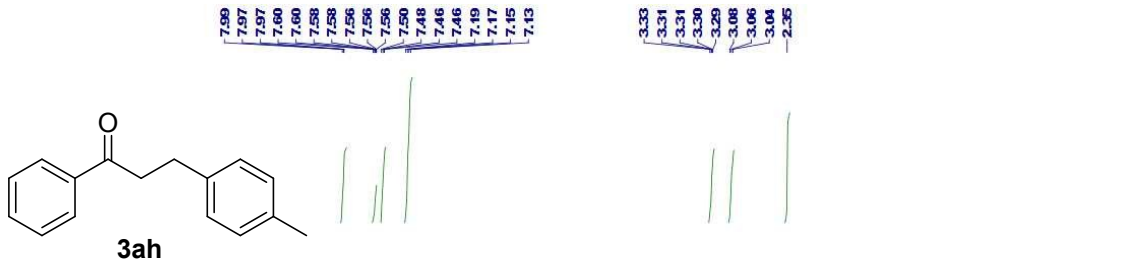
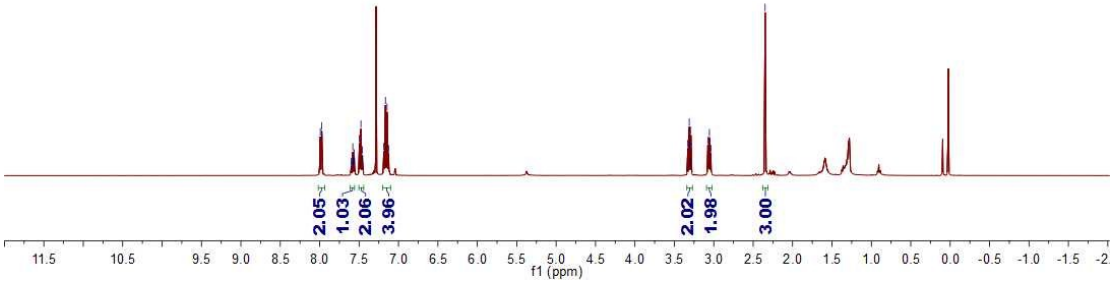
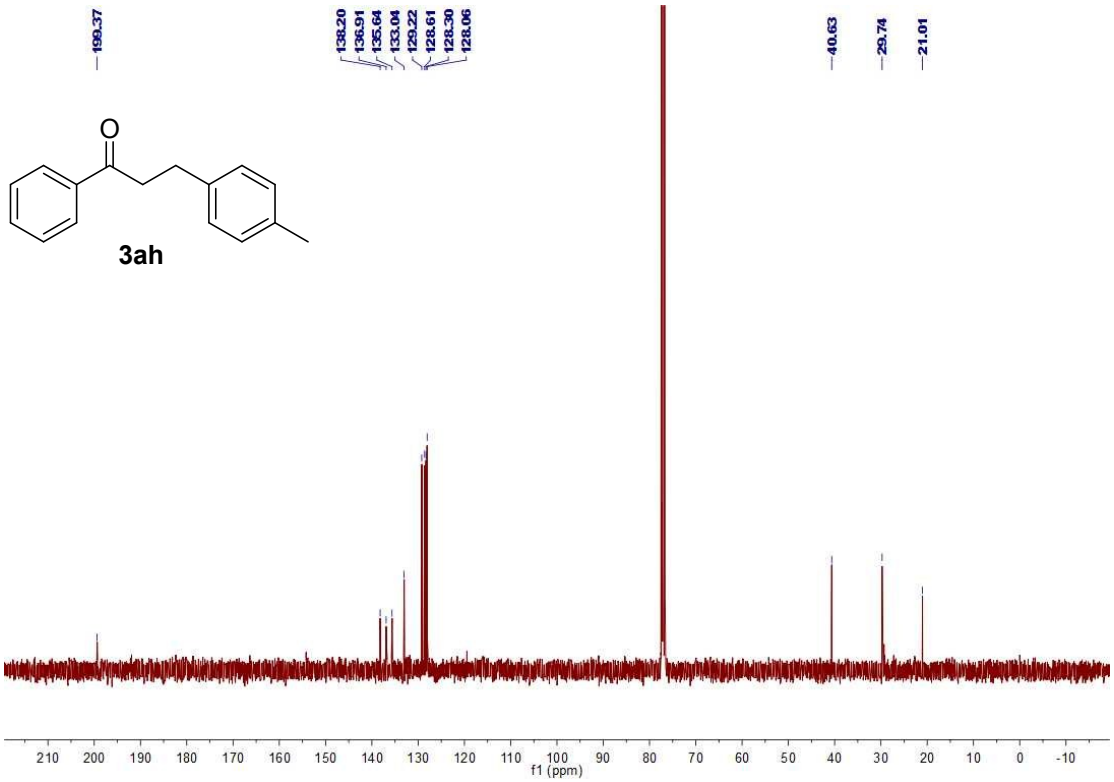
133.34
133.05
129.38
128.62
128.06
113.97
55.30
40.73
29.31
f1 (ppm)

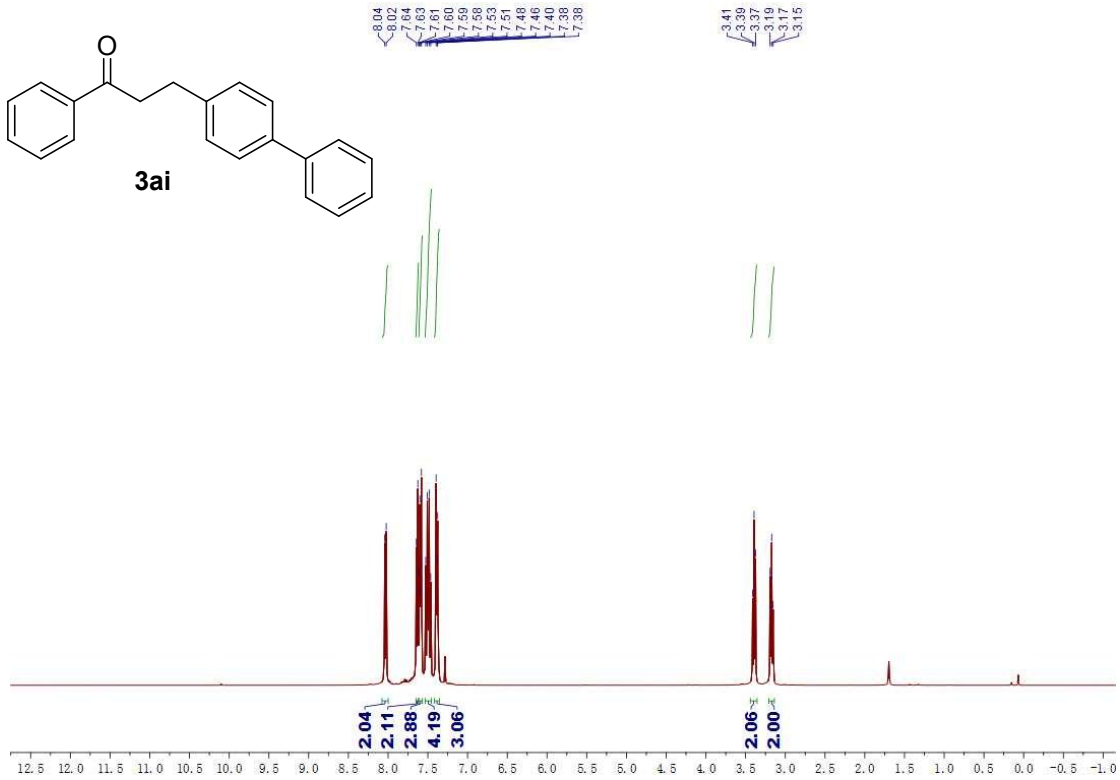

7.99
7.97
7.97
7.60
7.60
7.58
7.58
7.56
7.56
7.56
7.50
7.48
7.46
7.46
7.19
7.17
7.15
7.13
3.33
3.31
3.31
3.30
3.29
3.08
3.06
3.04
2.35
O

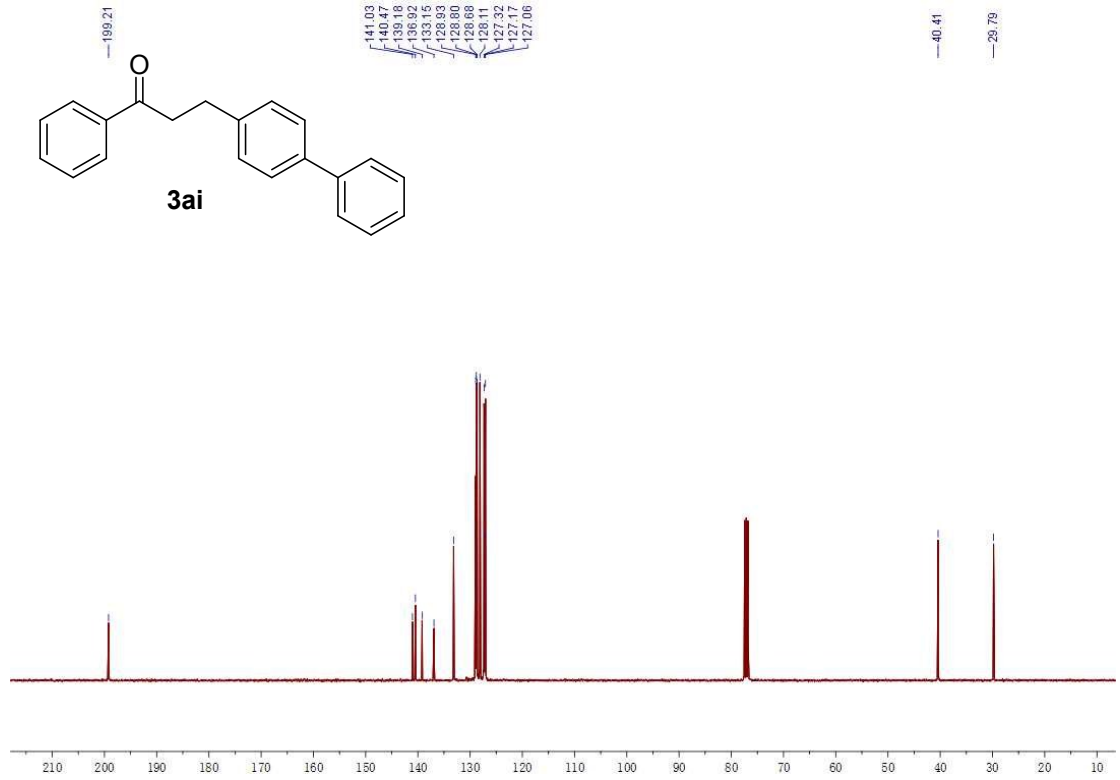
3ah


2.05
1.03
2.06
3.96
2.02
1.98
3.00
f1 (ppm)


199.37
138.20
136.91
135.64
133.04
129.22
128.61
128.30
128.06
40.63
29.74
21.01
O
f1 (ppm)

3ah


3ai
8.04
8.02
7.64
7.63
7.61
7.60
7.59
7.58
7.53
7.51
7.48
7.46
7.40
7.38
7.38
3.41
3.39
3.37
3.19
3.17
3.15
2.04
2.11
2.88
4.19
3.06
2.06
2.00


3ai
199.21
141.03
140.47
139.18
136.92
133.15
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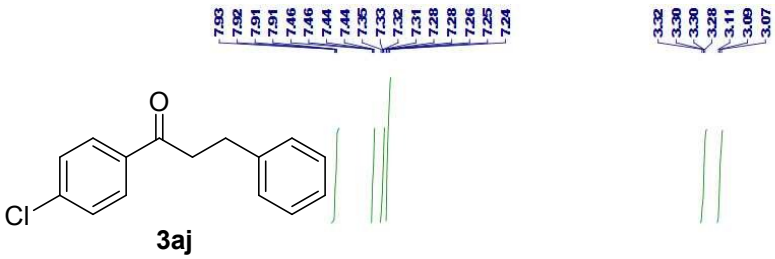
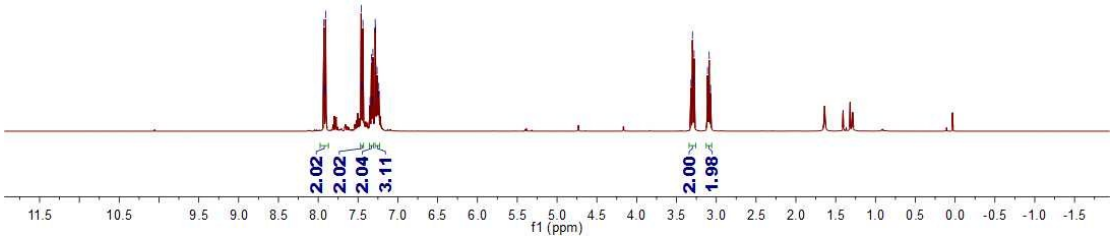
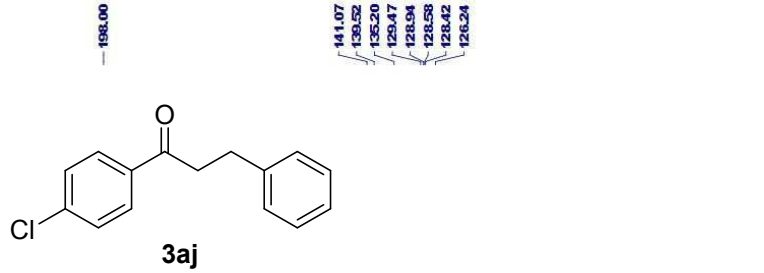
128.68
128.11
127.32
127.17
127.06
40.41
29.79

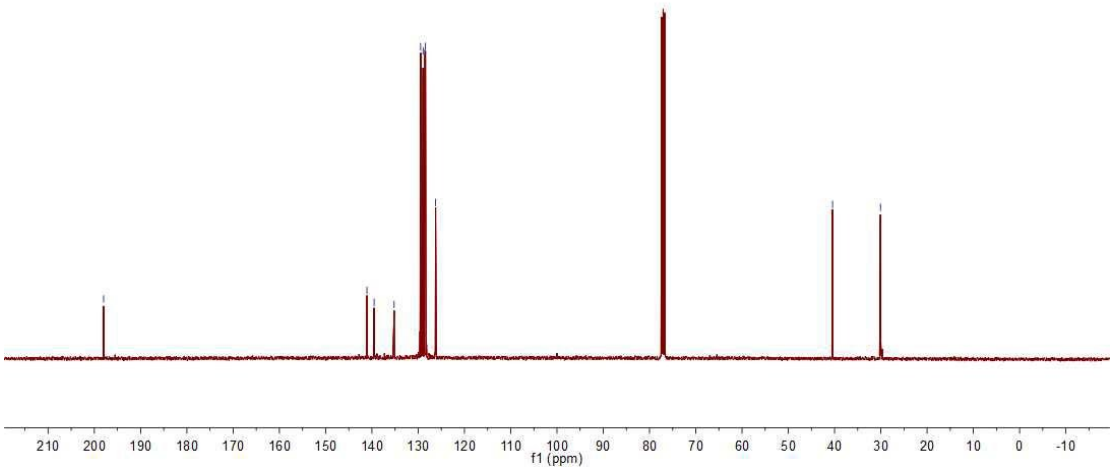

7.93
7.92
7.91
7.91
7.46
7.46
7.44
7.44
7.35
7.33
7.32
7.31
7.28
7.28
7.26
7.25
7.24
3.32
3.30
3.30
3.28
3.11
3.09
3.07
O
Cl

3aj


2.02
2.02
2.04
3.11
2.00
1.98
11.5
10.5
9.5
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
-0.5
-1.0
-1.5
f1 (ppm)


198.00
141.07
139.52
135.20
129.47
128.94
128.58
128.42
126.24
40.43
30.07
O
Cl

3aj


210
200
190
180
170
160
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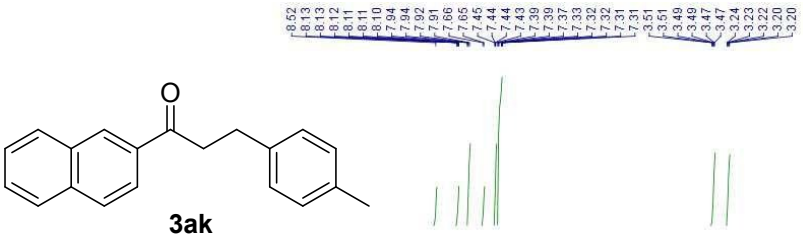
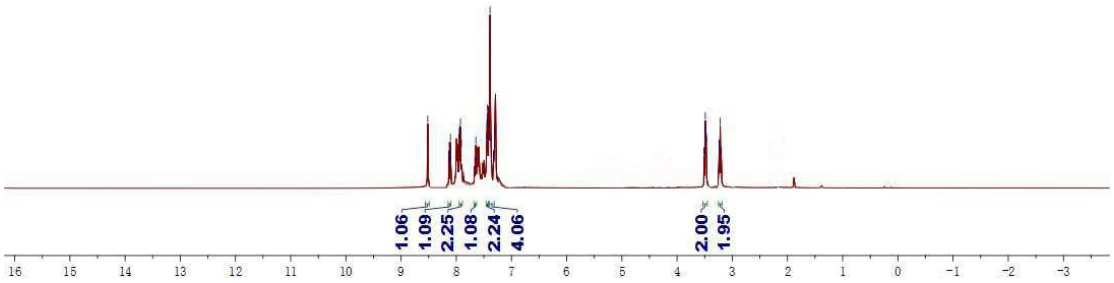
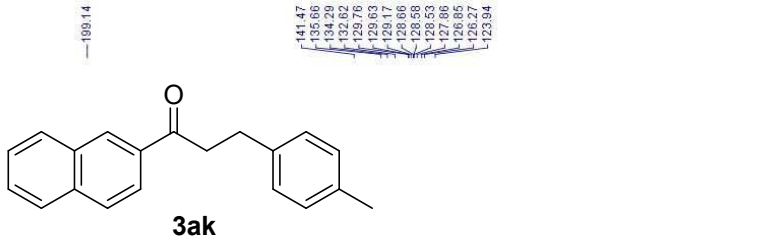
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.52
8.13
8.13
8.12
8.11
8.11
8.10
7.94
7.94
7.92
7.91
7.66
7.65
7.45
7.44
7.44
7.43
7.39
7.39
7.37
7.33
7.32
7.32
7.31
7.31
3.51
3.51
3.49
3.49
3.47
3.47
3.24
3.23
3.22
3.20
3.20
O

3ak


1.06
1.09
2.25
1.08
2.24
4.06
2.00
1.95
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3


199.14
141.47
135.66
134.29
132.62
129.76
129.63
129.17
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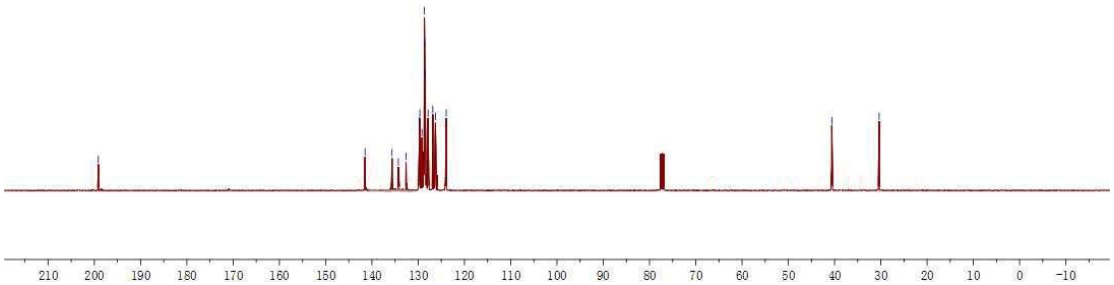
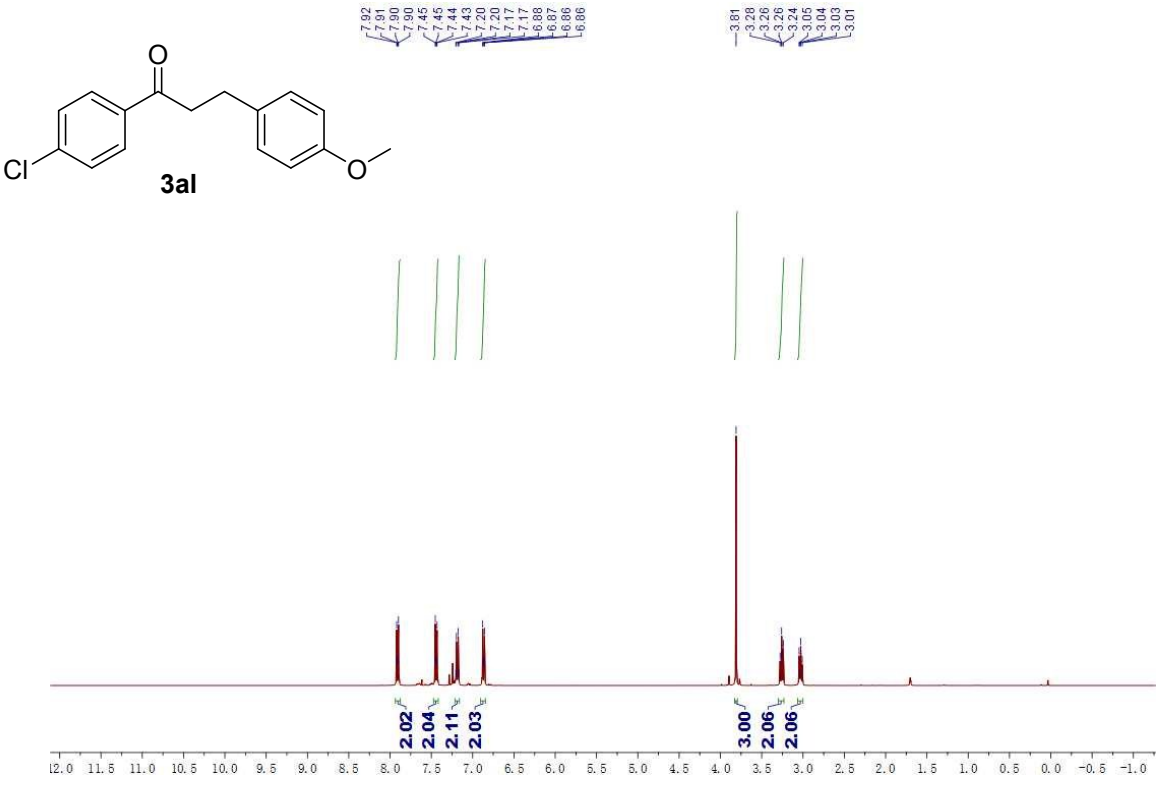
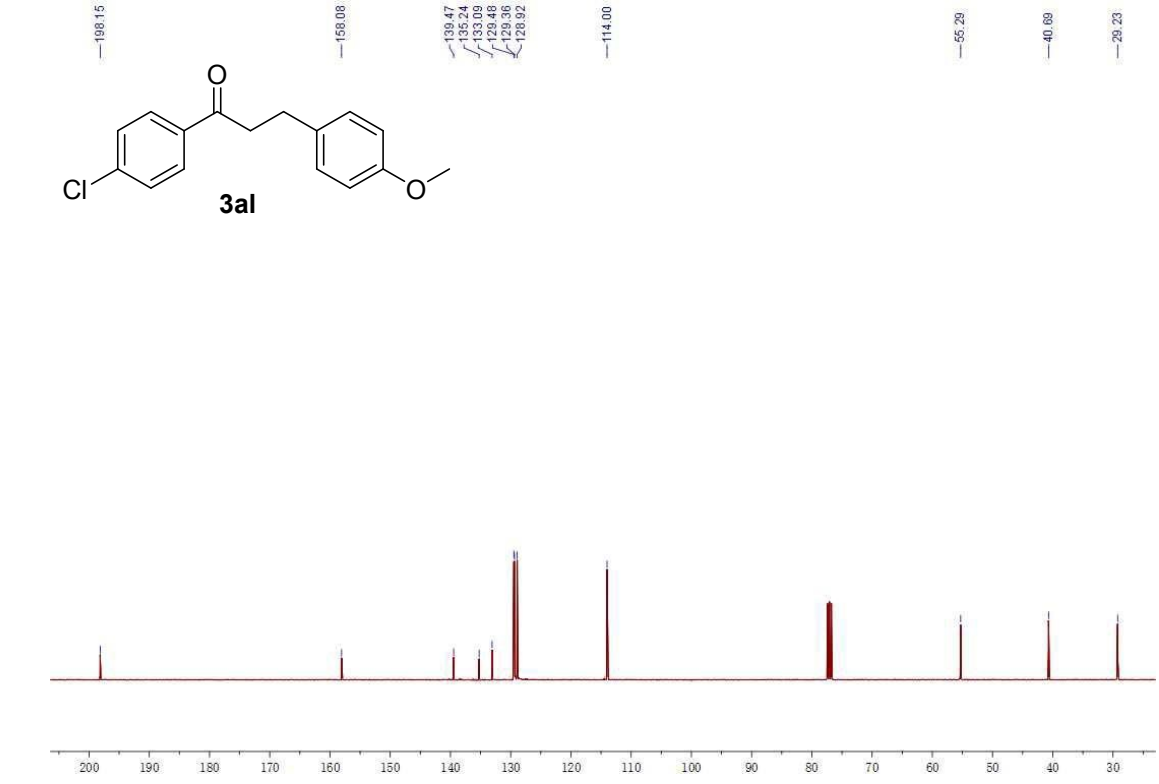
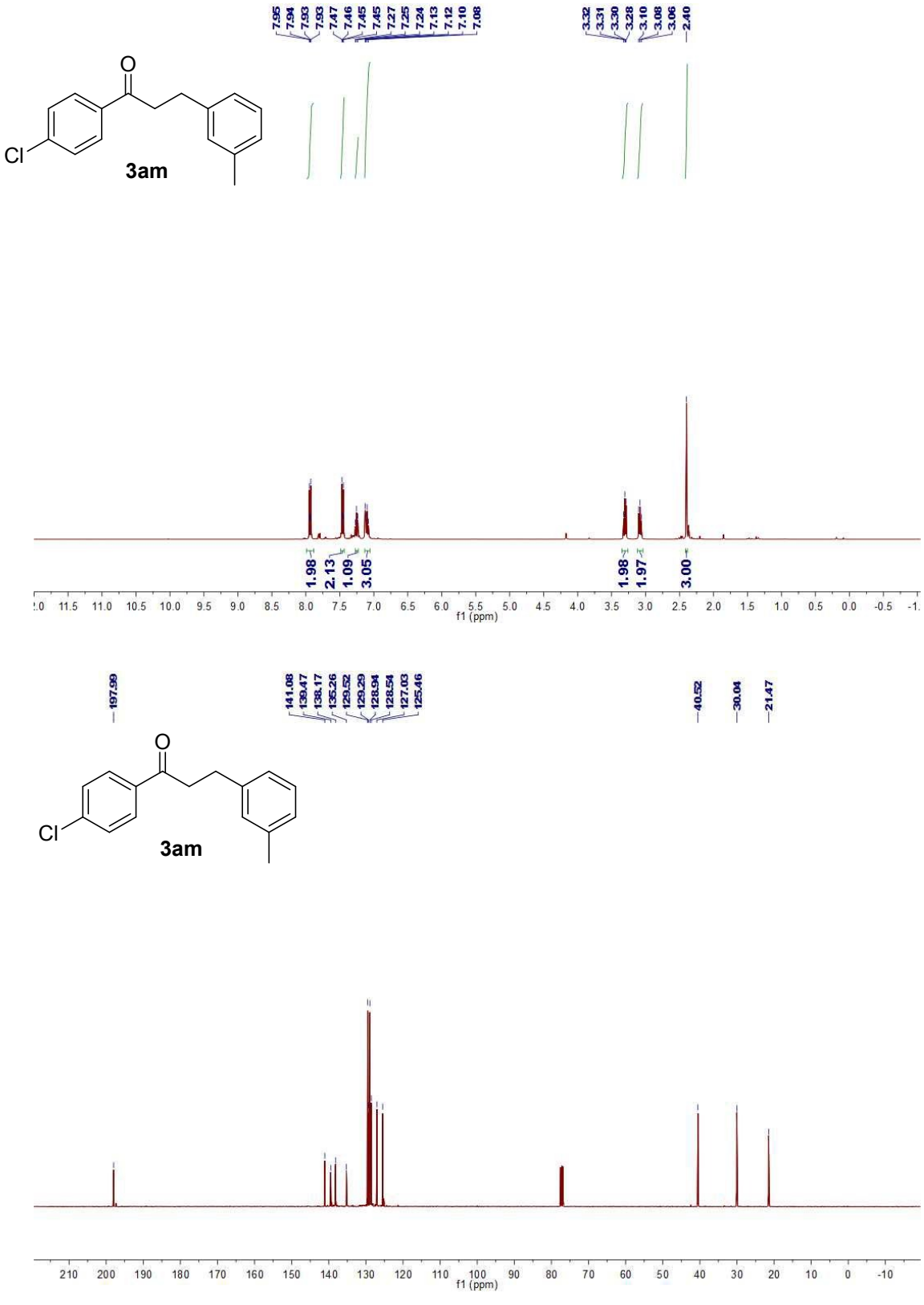
128.58
128.53
127.86
126.85
126.27
123.94
40.59
30.37
O

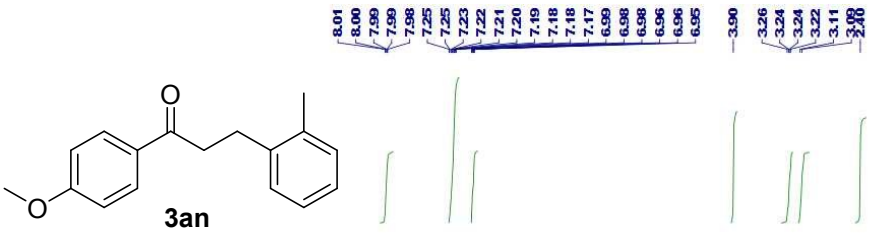
3ak


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10

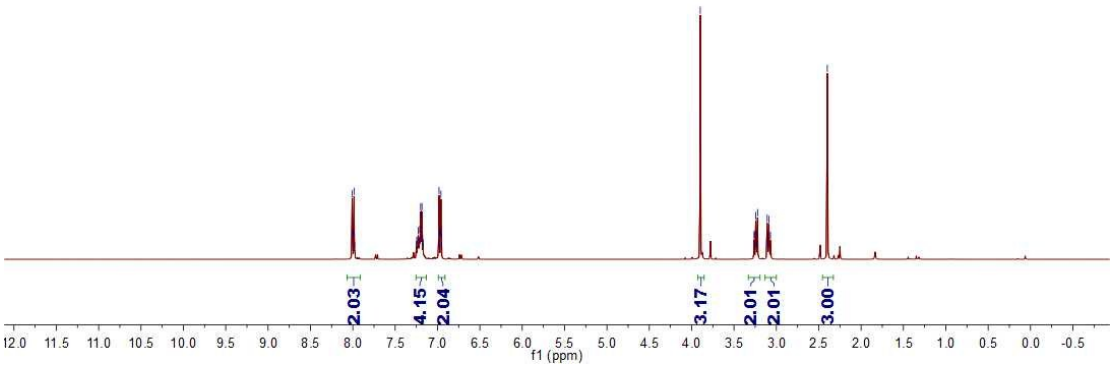

7.92
7.91
7.90
7.90
7.45
7.44
7.43
7.20
7.17
7.17
6.88
6.87
6.86
6.86
3.81
3.28
3.26
3.26
3.24
3.05
3.04
3.03
3.01
O
Cl
O
3al
2.02
2.04
2.11
2.03
3.00
2.06
2.06


198.15
158.08
139.47
135.24
133.09
129.48
129.36
128.92
114.00
55.29
40.69
29.23
O
Cl
O
3al

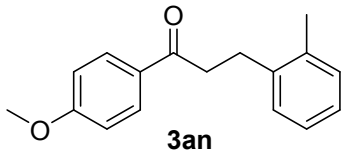

7.95
7.94
7.93
7.93
7.47
7.46
7.45
7.45
7.27
7.25
7.24
7.13
7.12
7.10
7.08
3.32
3.31
3.30
3.28
3.10
3.08
3.06
2.40
O
Cl
3am
1.98
2.13
1.09
3.05
1.98
1.97
3.00
f1 (ppm)
197.99
141.08
138.47
138.17
135.26
129.52
129.29
128.94
128.54
127.03
125.46
40.52
30.04
21.47
O
Cl
3am
f1 (ppm)


8.01
8.00
7.99
7.99
7.98
7.25
7.25
7.23
7.22
7.21
7.20
7.19
7.18
7.18
7.17
6.99
6.98
6.98
6.96
6.96
6.95
3.90
3.26
3.24
3.24
3.22
3.11
3.08
2.40
O
O

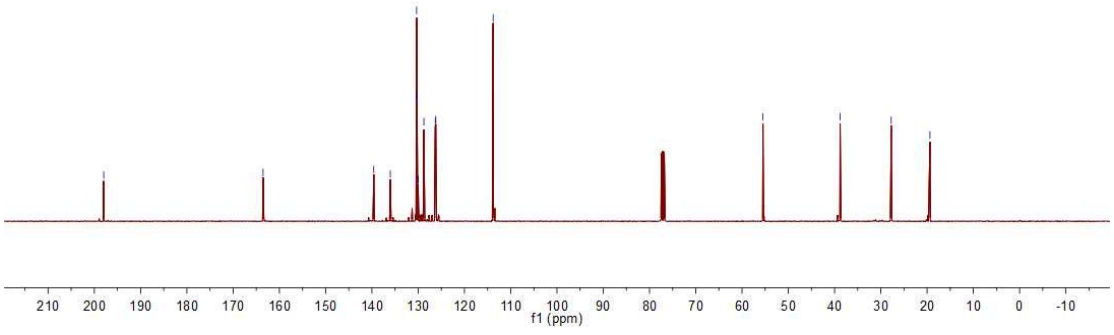
3an

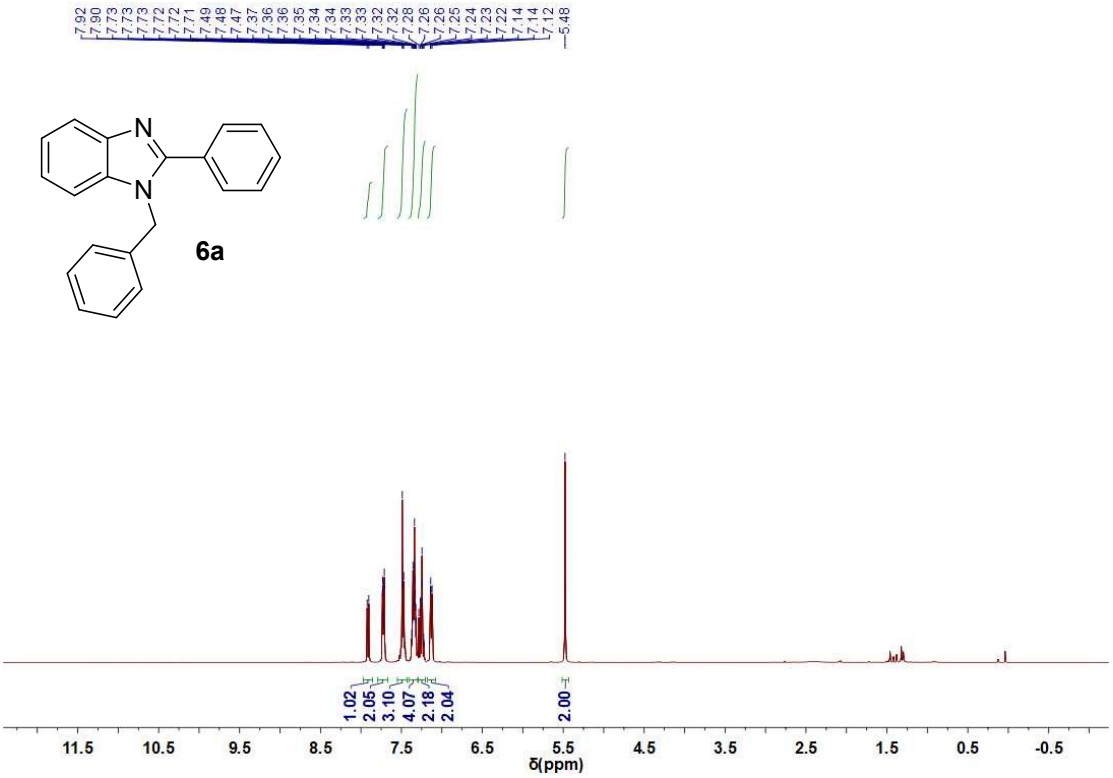

2.03
4.15
2.04
3.17
2.01
2.01
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

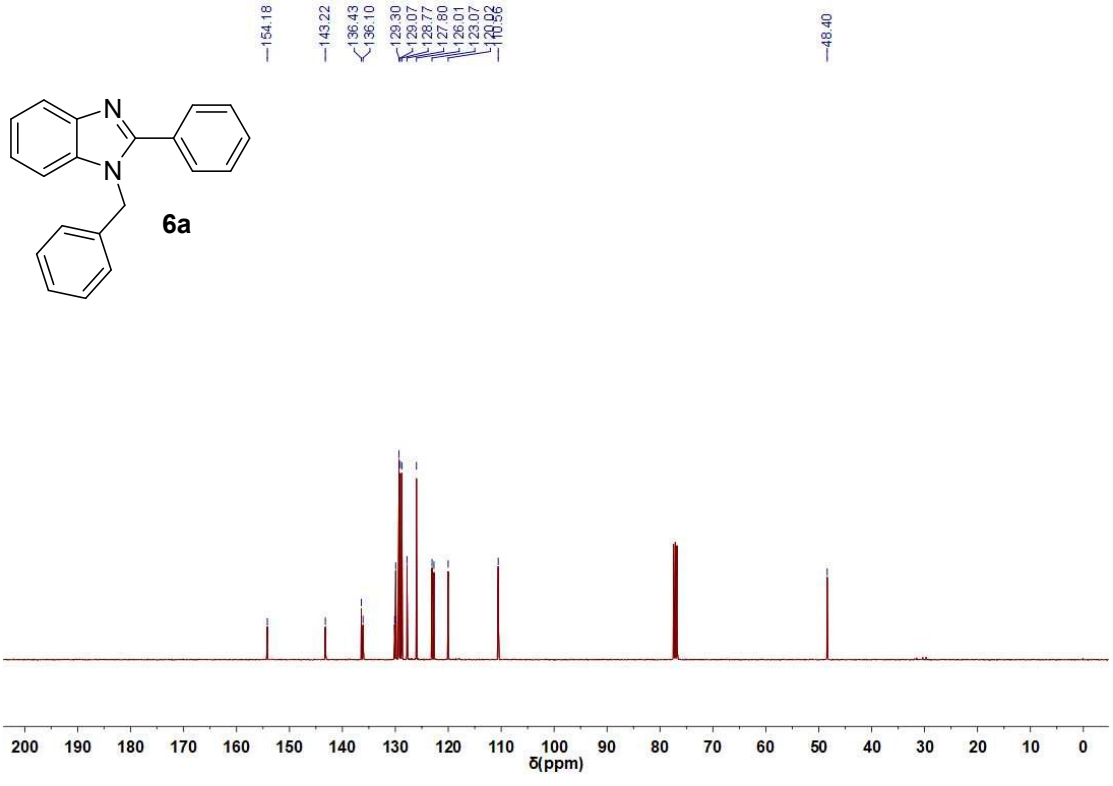

197.97
163.52
139.60
136.02
130.36
130.34
130.01
128.77
126.31
126.19
113.79
55.48
38.80
27.76
19.38

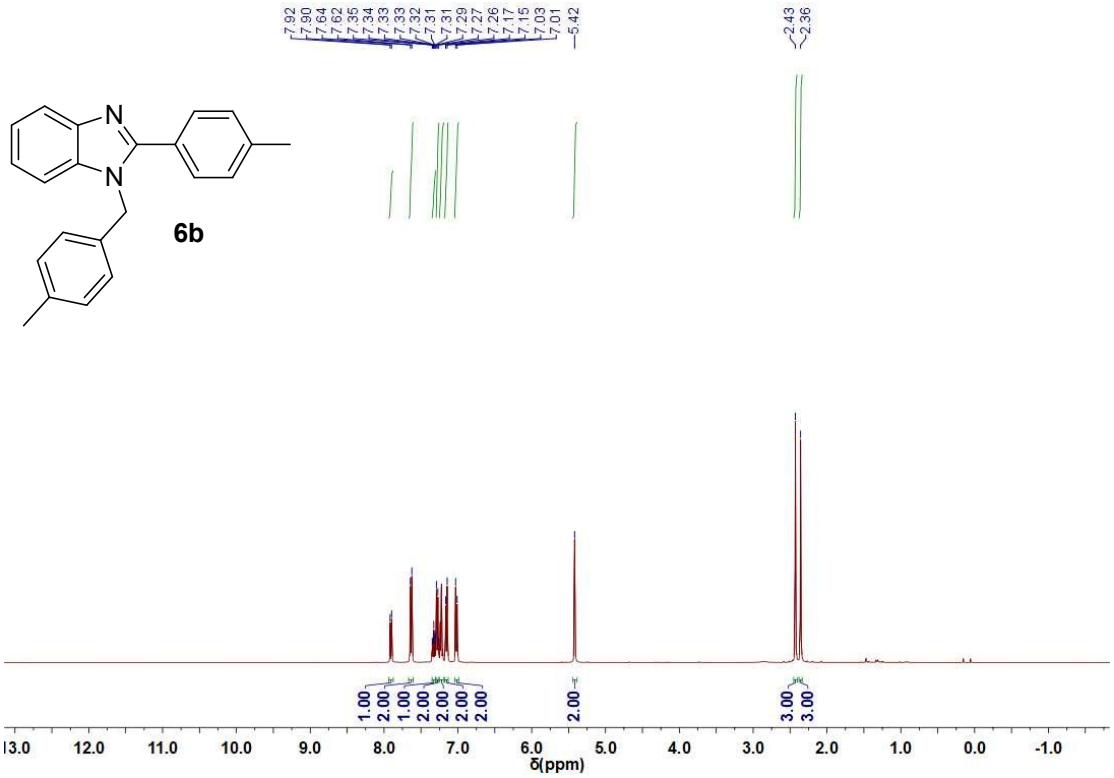

O
O

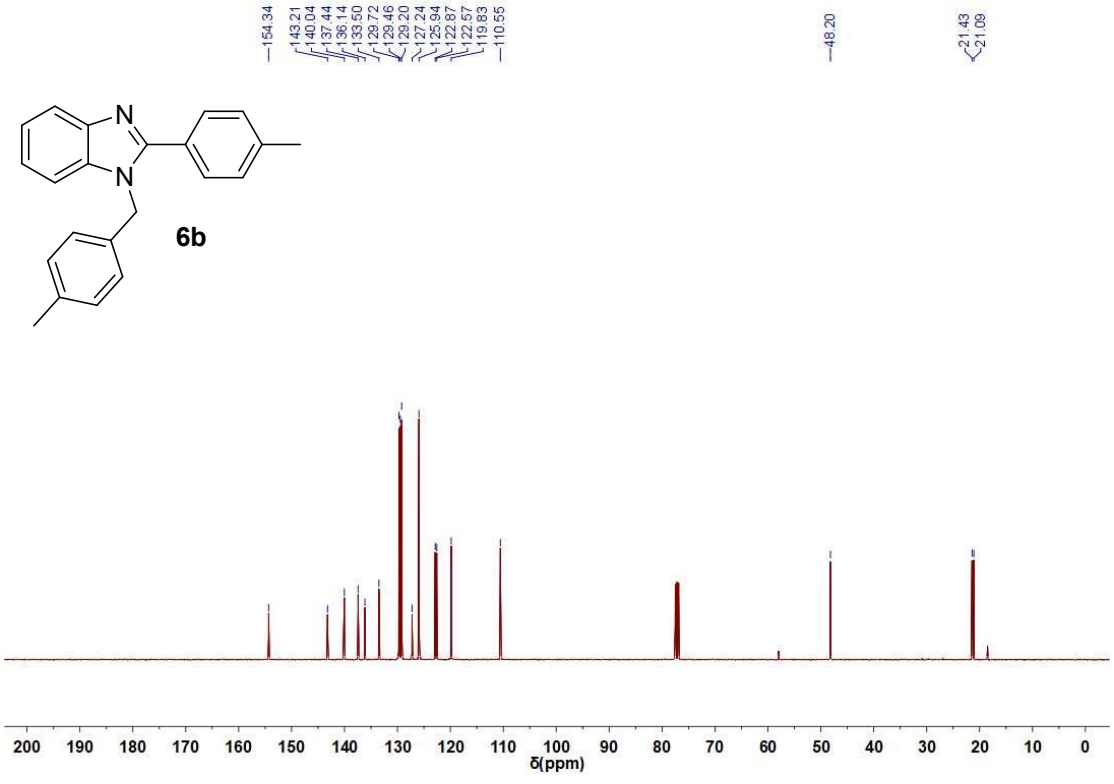
3an

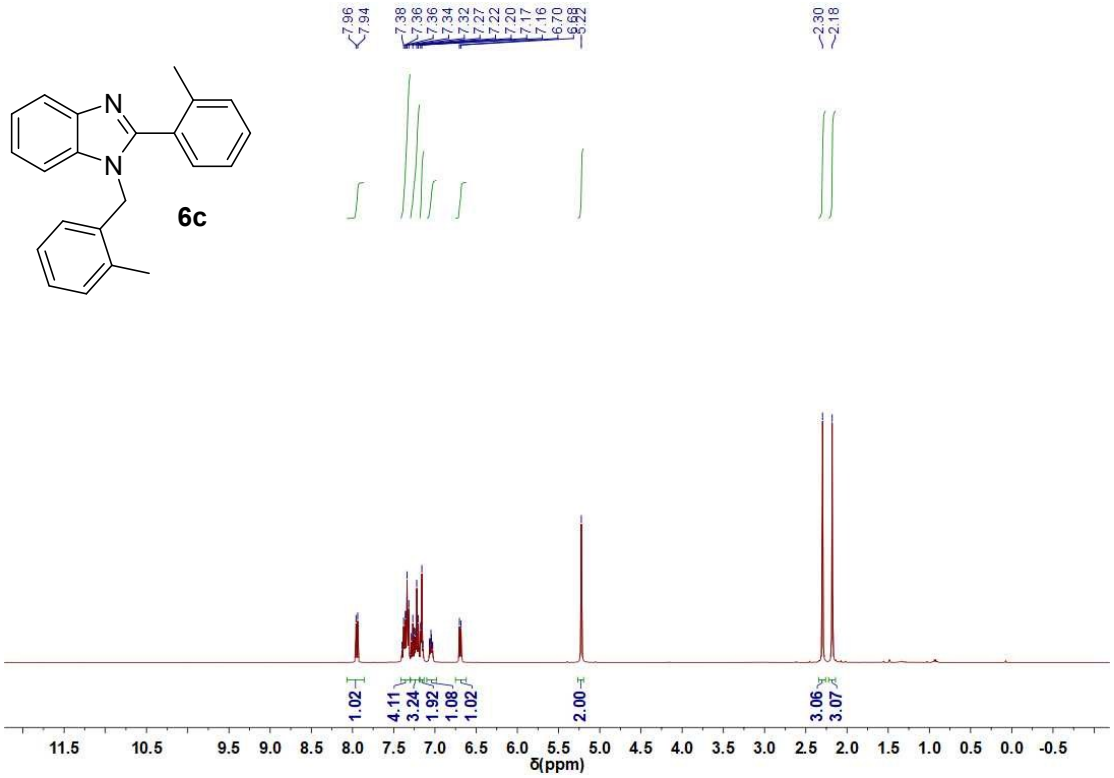

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

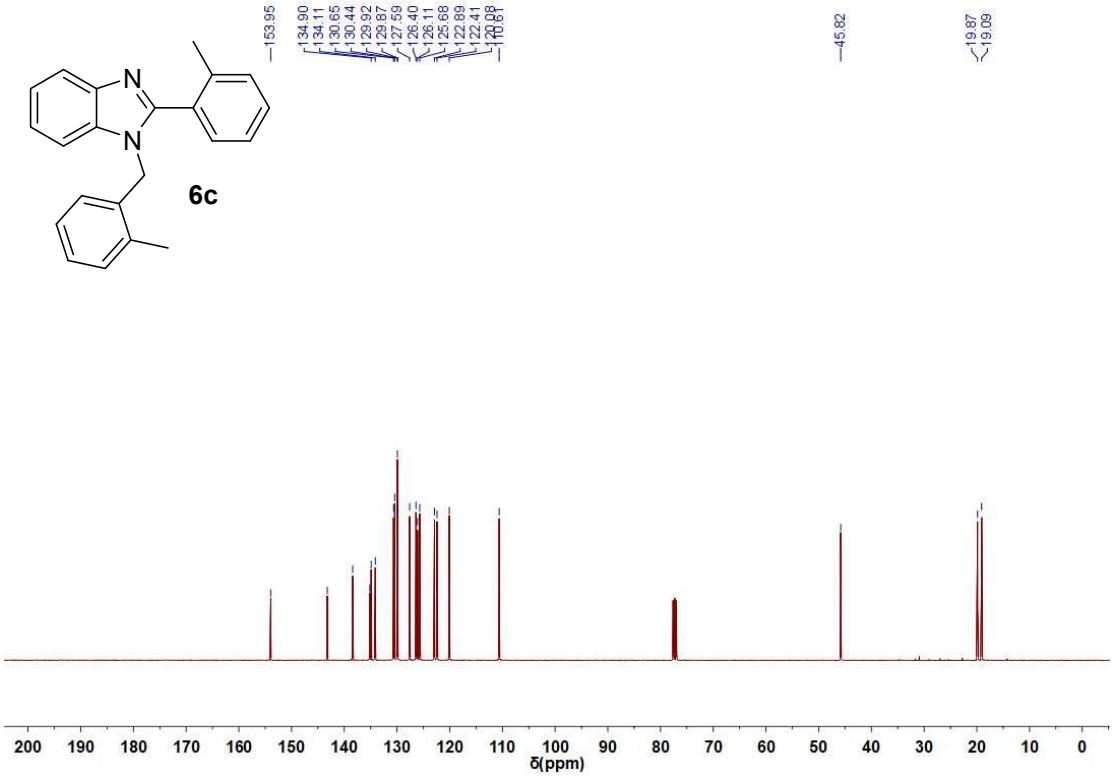

7.92
7.90
7.73
7.73
7.73
7.72
7.72
7.71
7.49
7.48
7.47
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.28
7.26
7.26
7.25
7.24
7.23
7.22
7.14
7.14
7.12
5.48
N
N
6a
1.02
2.05
3.10
4.07
2.18
2.04
2.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
δ(ppm)

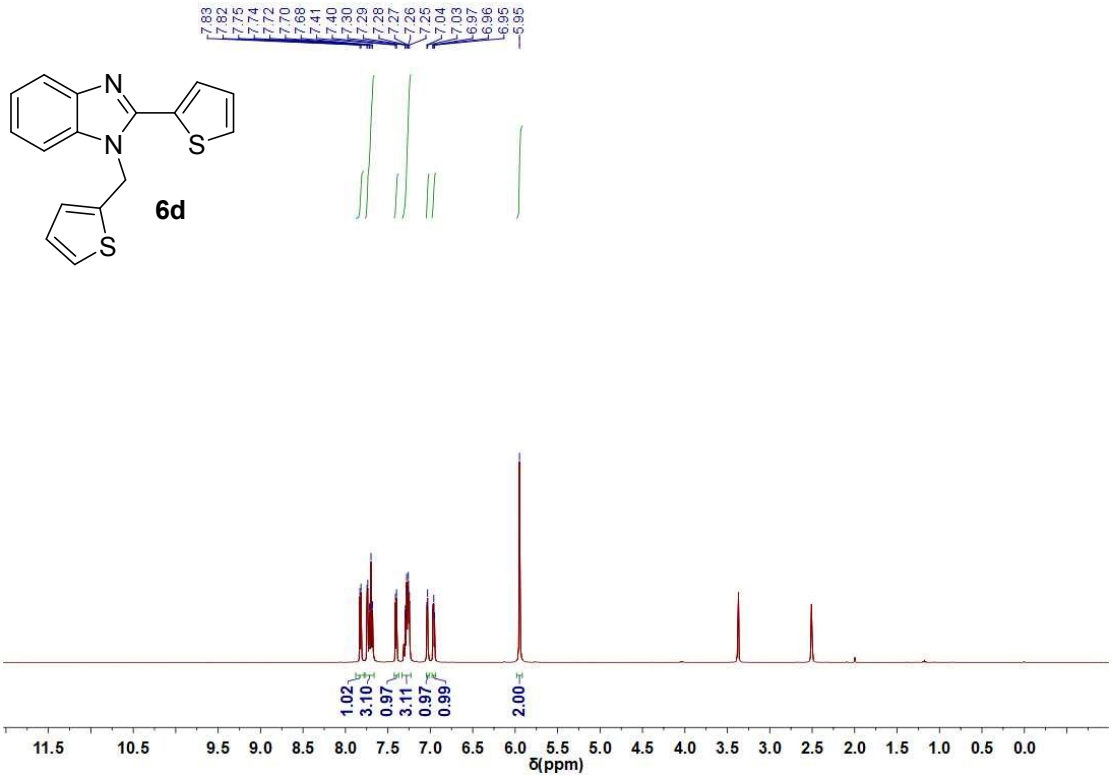

154.18
143.22
136.43
136.10
129.30
129.07
128.77
127.80
126.01
123.07
120.82
110.56
48.40
N
N
6a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ(ppm)

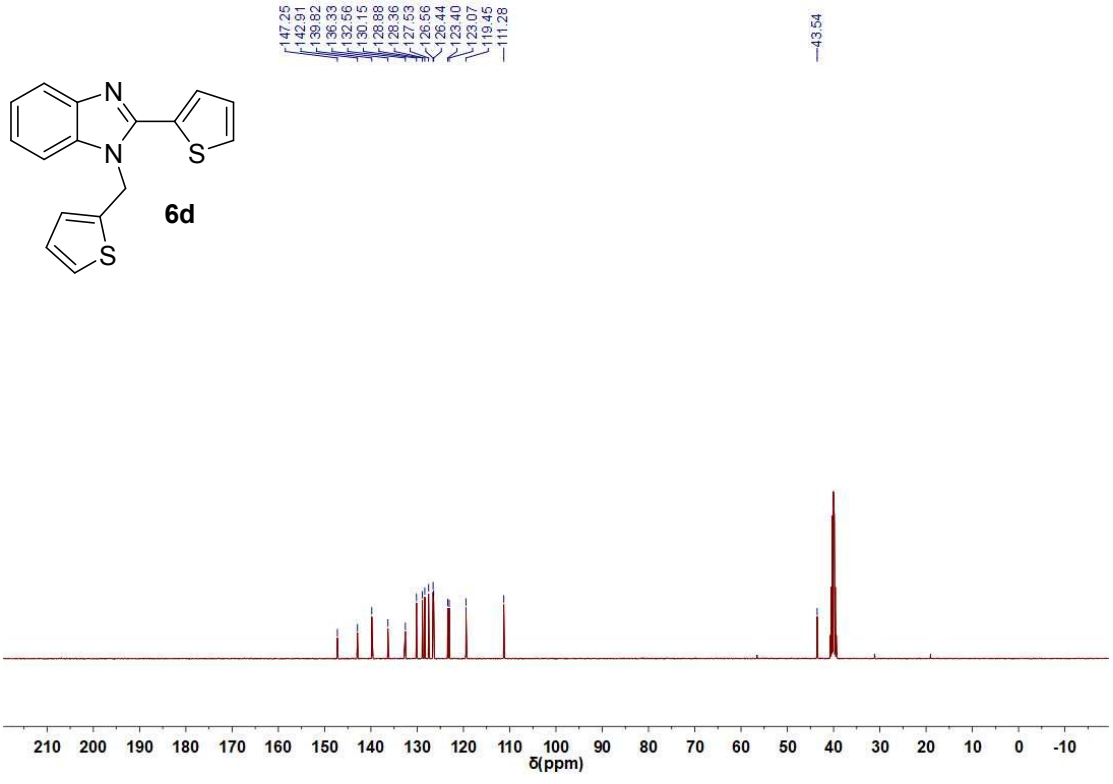

7.92
7.90
7.64
7.62
7.35
7.34
7.33
7.33
7.32
7.31
7.31
7.29
7.27
7.26
7.17
7.15
7.03
7.01
5.42
2.43
2.36
N
N
6b
1.00
2.00
1.00
2.00
2.00
2.00
2.00
3.00
3.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
δ(ppm)

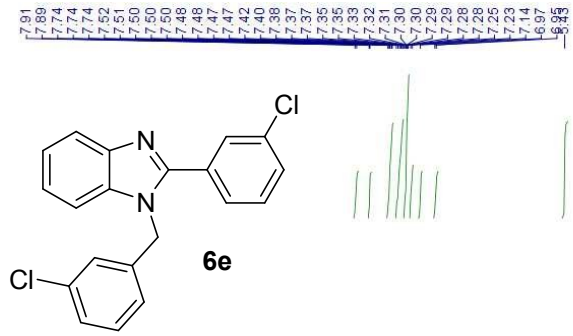

154.34
143.21
140.04
137.44
136.14
133.50
129.72
129.46
129.20
127.24
125.84
122.87
122.57
119.83
110.55
48.20
21.43
21.09
N
N
6b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ(ppm)

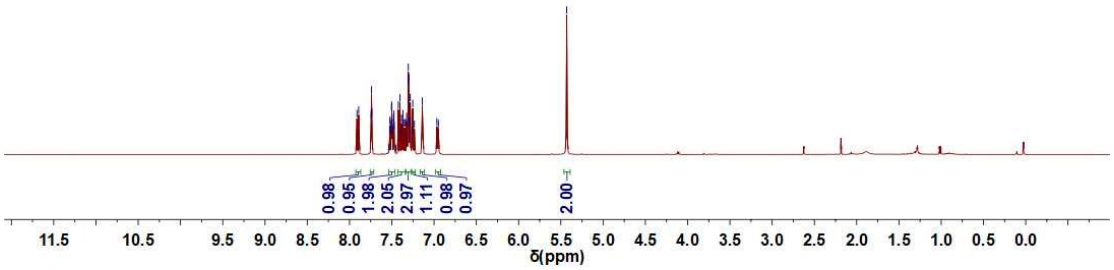

6c
7.96
7.94
7.38
7.36
7.36
7.34
7.32
7.27
7.22
7.20
7.17
7.16
6.70
6.68
6.22
2.30
2.18
1.02
4.11
3.24
1.92
1.08
1.02
2.00
3.06
3.07
δ(ppm)

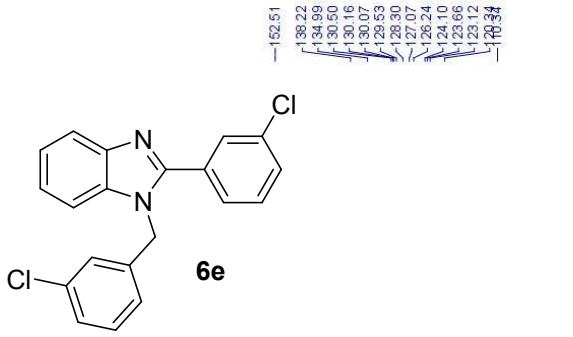

6c
153.95
134.90
134.11
130.65
130.44
129.92
129.87
127.59
126.40
126.11
125.68
122.89
122.41
120.08
110.61
45.82
19.87
19.09
δ(ppm)

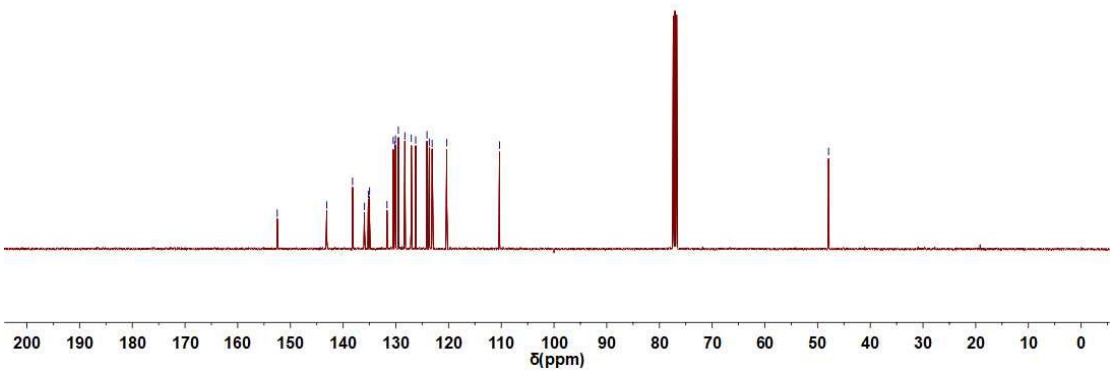

7.83
7.82
7.75
7.74
7.72
7.70
7.68
7.41
7.40
7.30
7.29
7.28
7.27
7.26
7.25
7.04
7.03
6.97
6.96
6.95
5.95
N
N
S
S
6d
1.02
3.10
0.97
3.11
0.97
0.99
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ(ppm)

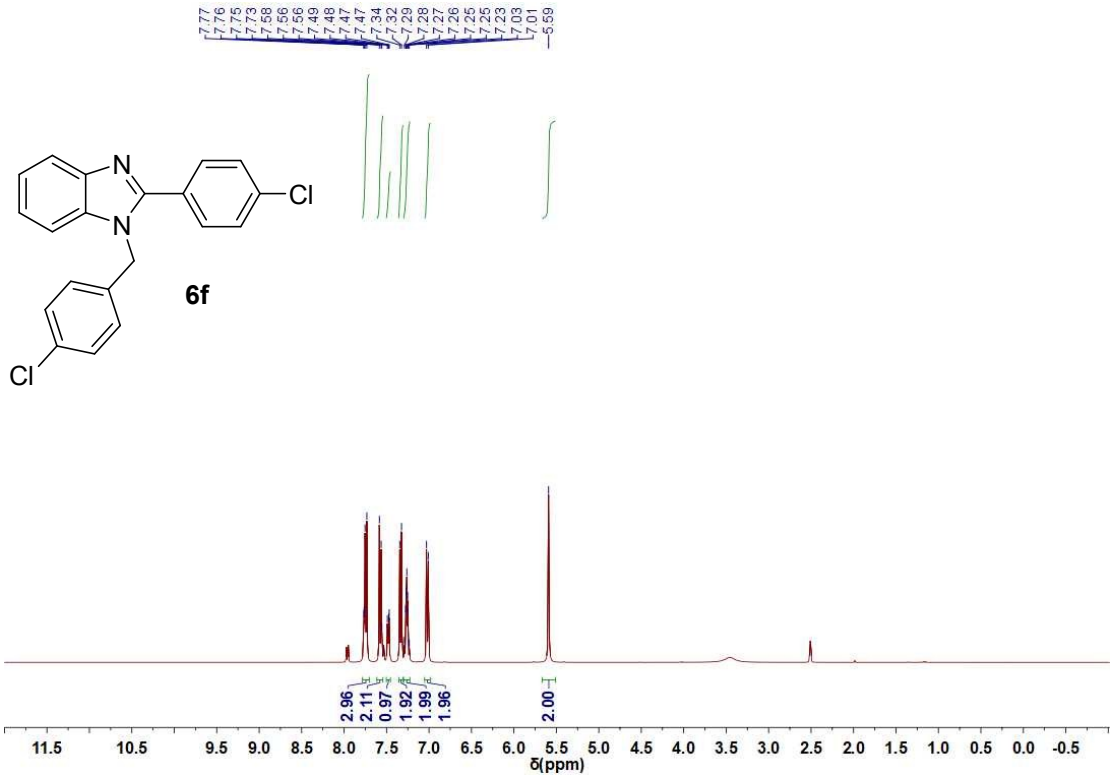

147.25
142.91
139.82
136.33
132.56
130.15
128.88
128.36
127.53
126.56
126.44
123.40
123.07
119.45
111.28
43.54
N
N
S
S
6d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
δ(ppm)


Cl
N
N
Cl
6e


0.98
0.95
1.98
2.05
2.97
1.11
0.98
0.97
2.00
δ(ppm)


Cl
N
N
Cl
6e


δ(ppm)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7.76
7.75
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7.56
7.56
7.49
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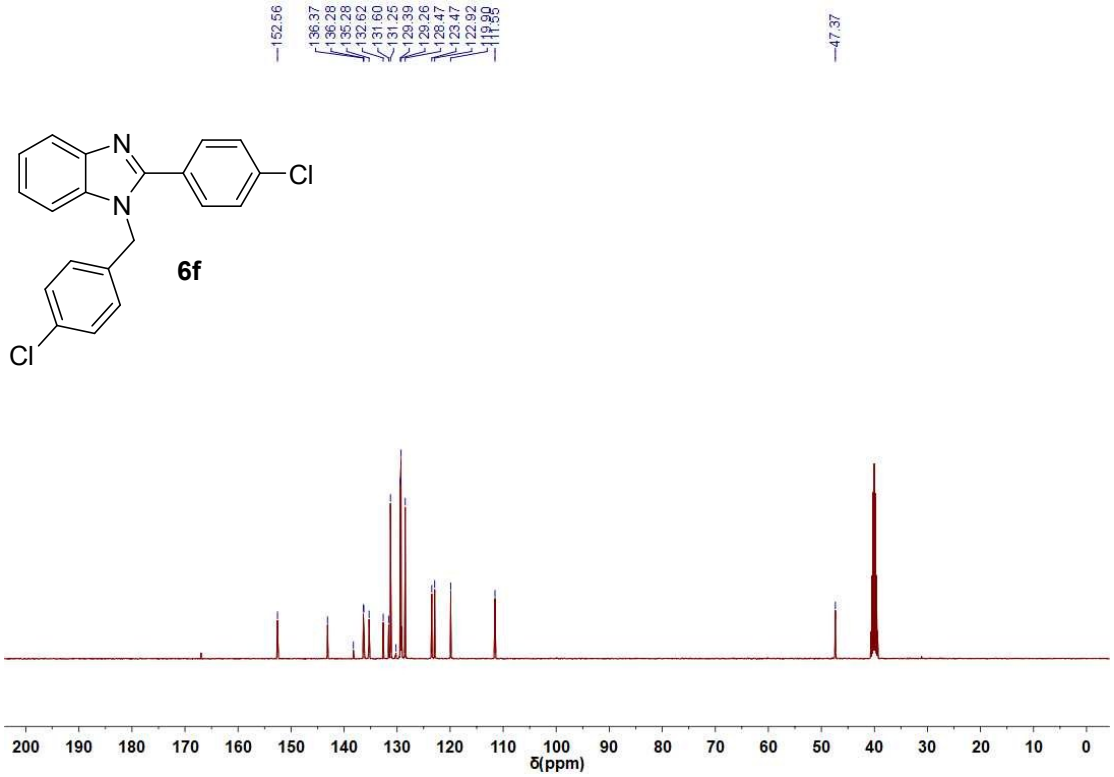
7.47
7.47
7.34
7.32
7.29
7.28
7.27
7.26
7.25
7.25
7.23
7.03
7.01
5.59
N
N
Cl
Cl
6f
2.96
2.11
0.97
1.92
1.99
1.96
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
δ(ppm)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136.37
136.28
135.28
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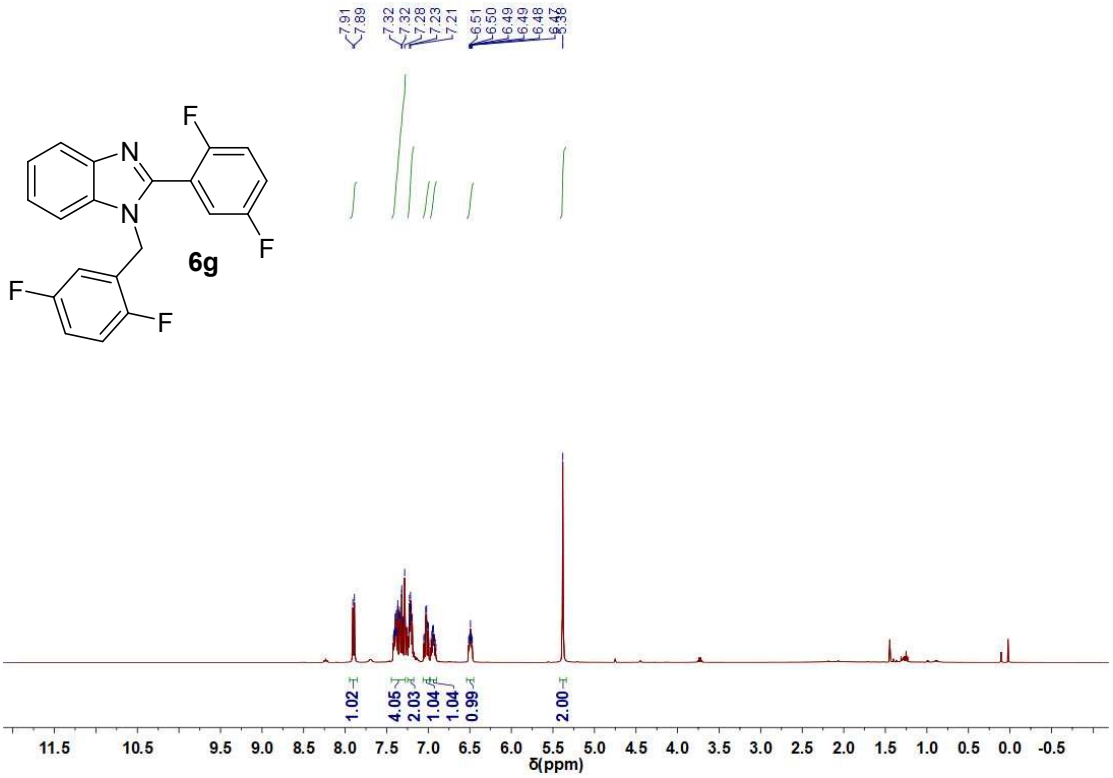
131.60
131.25
129.39
129.26
128.47
123.47
122.92
119.90
111.58
47.37
N
N
Cl
Cl
6f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ(ppm)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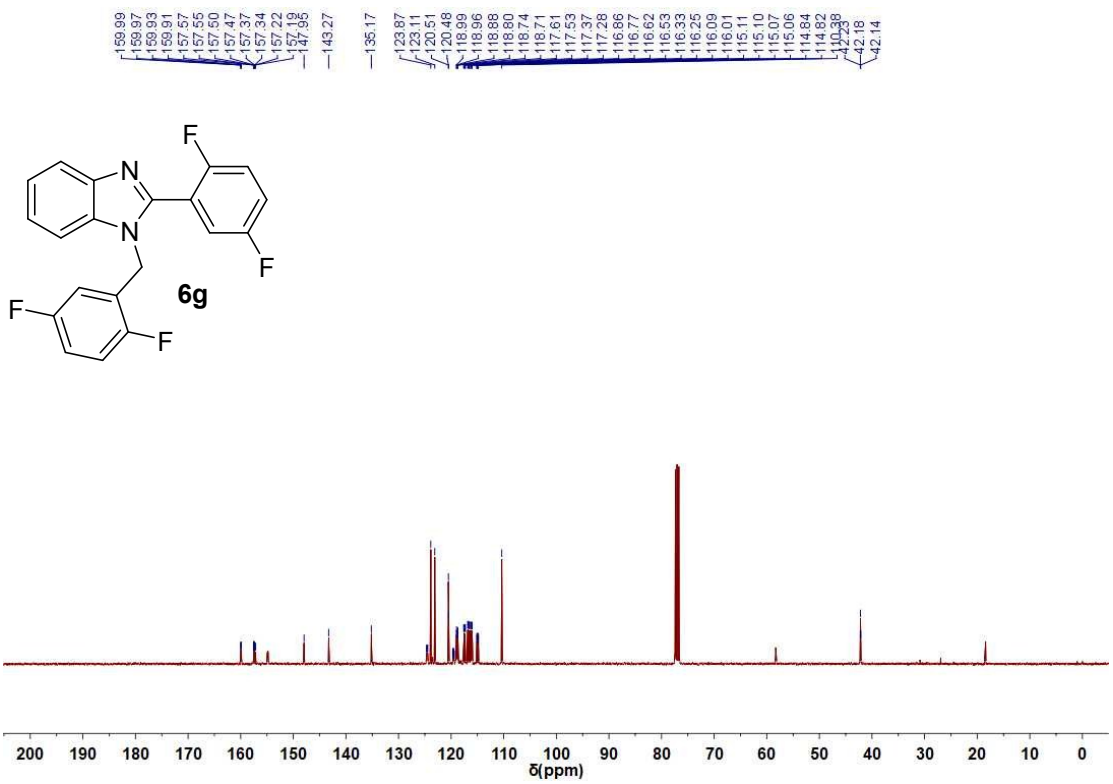
7.89
7.32
7.32
7.28
7.23
7.21
6.51
6.50
6.49
6.49
6.48
6.47
6.38
F
N
N
F
6g
F
F
1.02
4.05
2.03
1.04
1.04
0.99
2.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
δ(ppm)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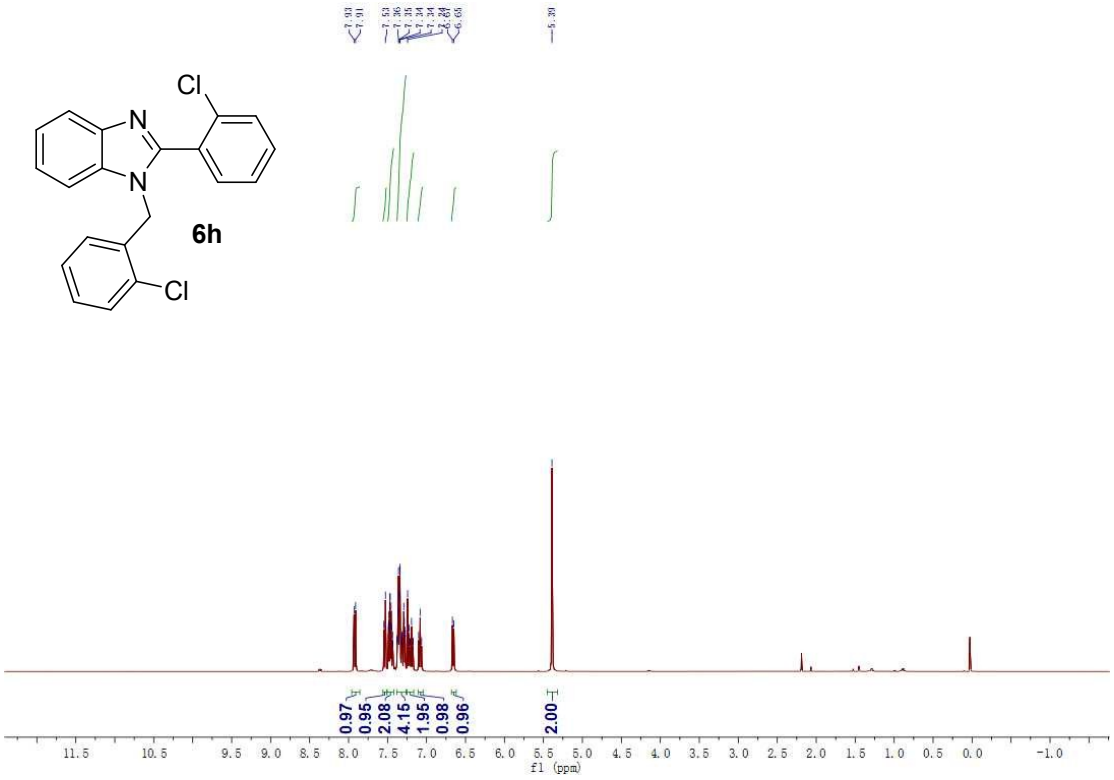
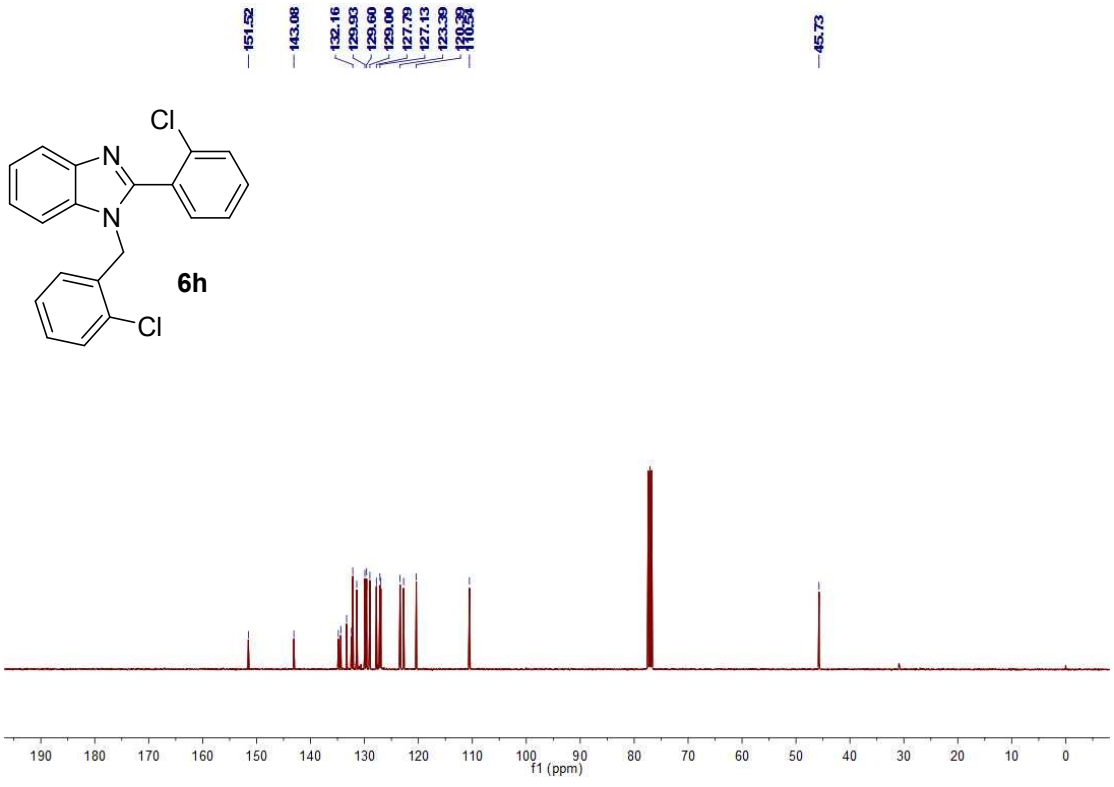
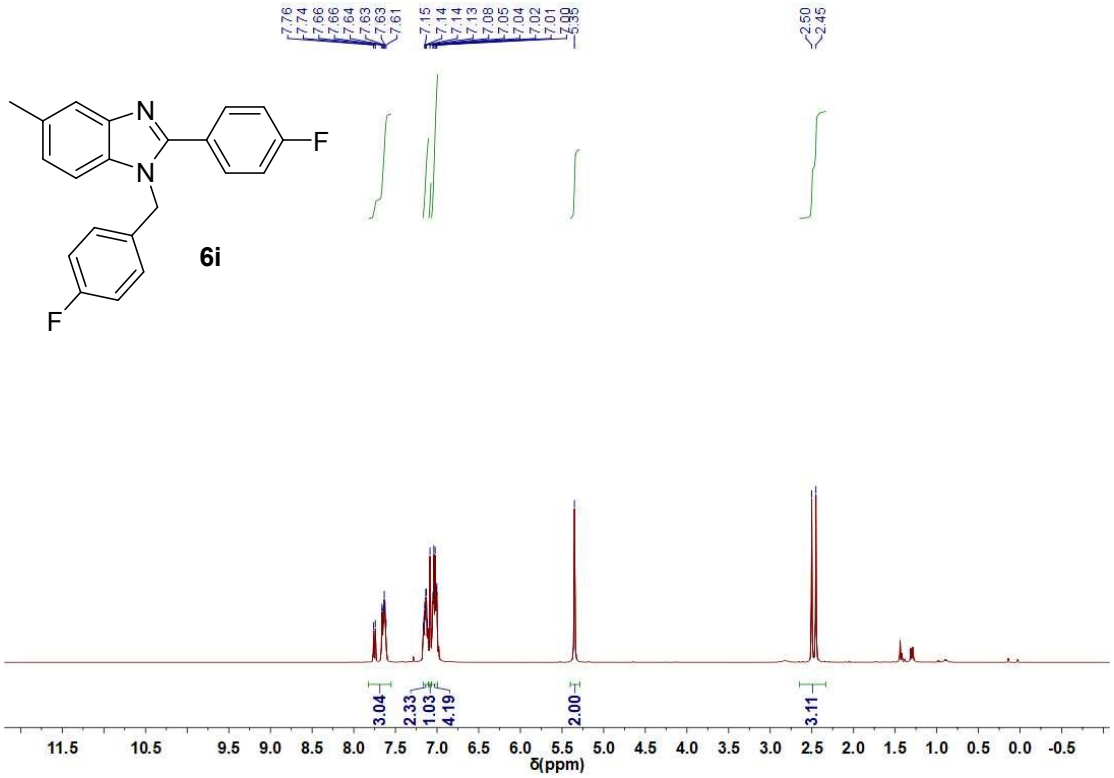
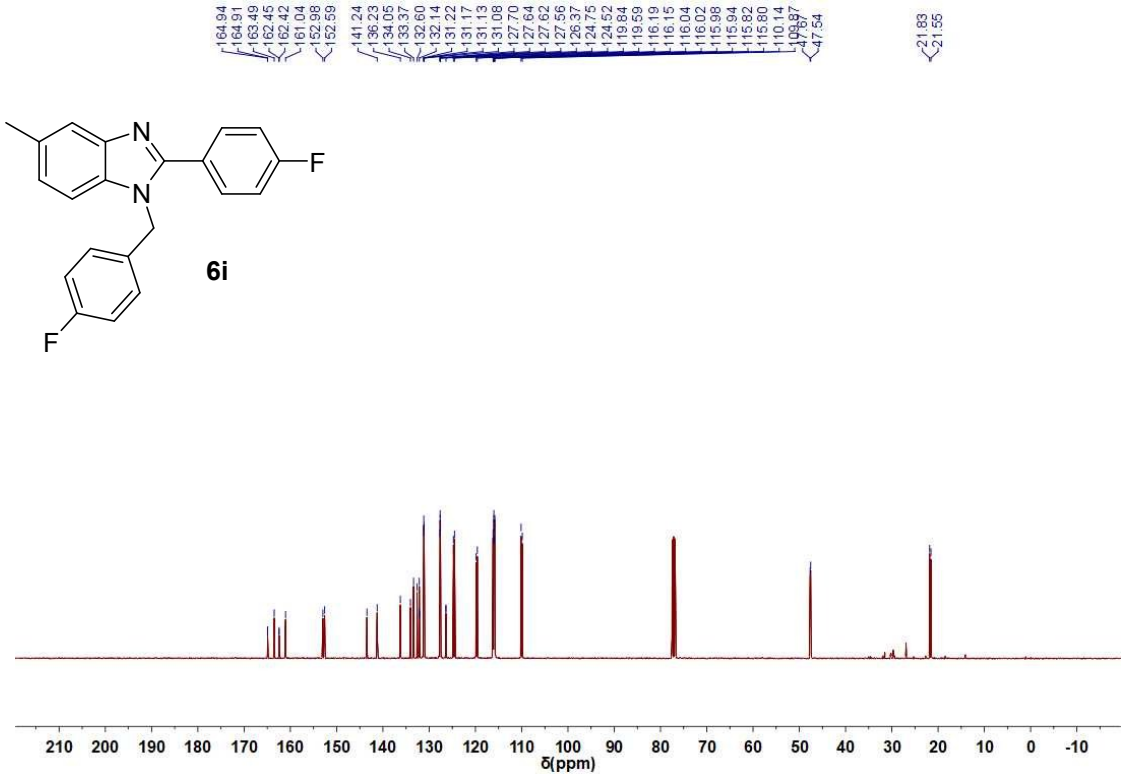
159.97
159.93
159.91
157.57
157.55
157.50
157.47
157.37
157.34
157.22
157.19
147.95
143.27
135.17
123.87
123.11
120.51
120.48
118.99
118.96
118.88
118.80
118.74
118.71
117.61
117.53
117.37
117.28
116.86
116.77
116.62
116.53
116.33
116.25
116.09
116.01
115.11
115.10
115.07
115.06
114.84
114.82
110.38
42.23
42.18
42.14
F
N
N
F
6g
F
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ(ppm)


Cl
N
N
6h
Cl
0.97
0.95
2.08
4.15
1.95
0.98
0.96
2.00
f1 (ppm)


151.52
143.08
132.16
129.93
129.60
129.00
127.79
127.13
123.39
45.73
Cl
N
N
6h
Cl
f1 (ppm)


7.76
7.74
7.66
7.66
7.64
7.63
7.63
7.61
7.15
7.14
7.14
7.13
7.08
7.05
7.04
7.02
7.01
6.99
2.50
2.45
N
N
F
F
6i
3.04
2.33
1.03
4.19
2.00
3.11
11.5
10.5
9.5
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
-0.5
δ(ppm)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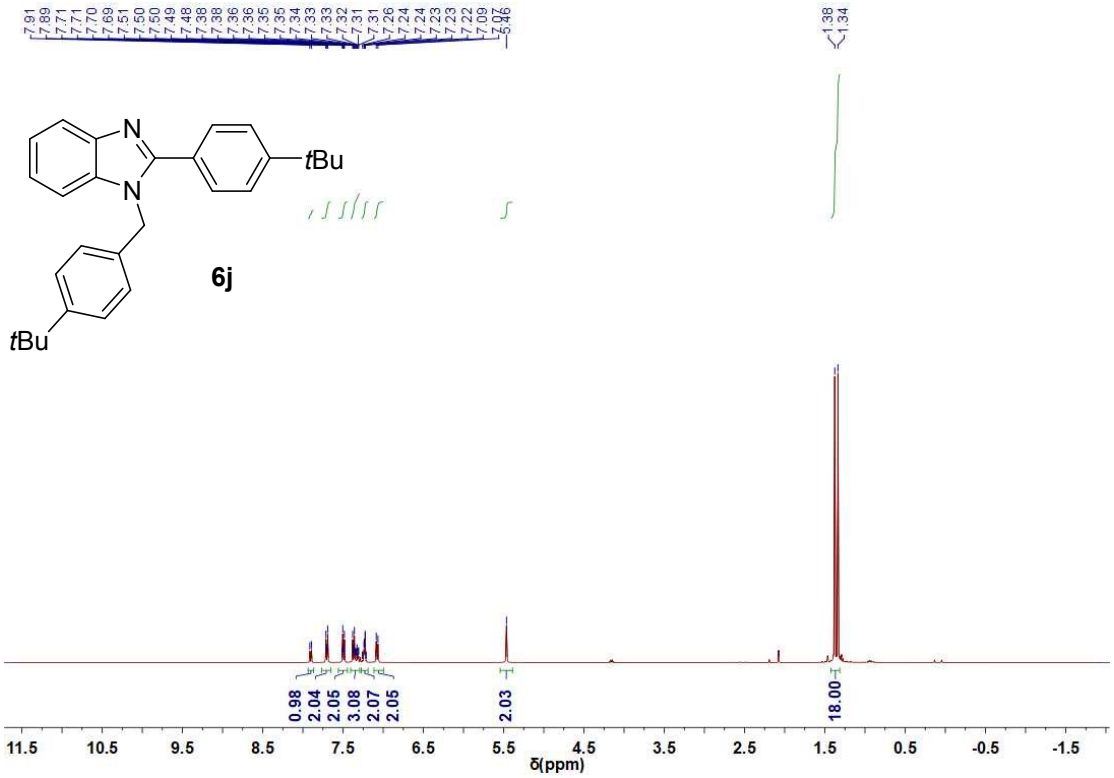
164.91
163.49
162.45
162.42
161.04
152.98
152.59
141.24
136.23
134.05
133.37
132.60
132.14
131.22
131.17
131.13
131.08
127.70
127.64
127.62
127.56
126.37
124.75
124.52
119.84
119.59
116.19
116.15
116.04
116.02
115.98
115.94
115.82
115.80
110.14
109.87
47.67
47.54
21.83
21.55
N
N
F
F
6i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
δ(ppm)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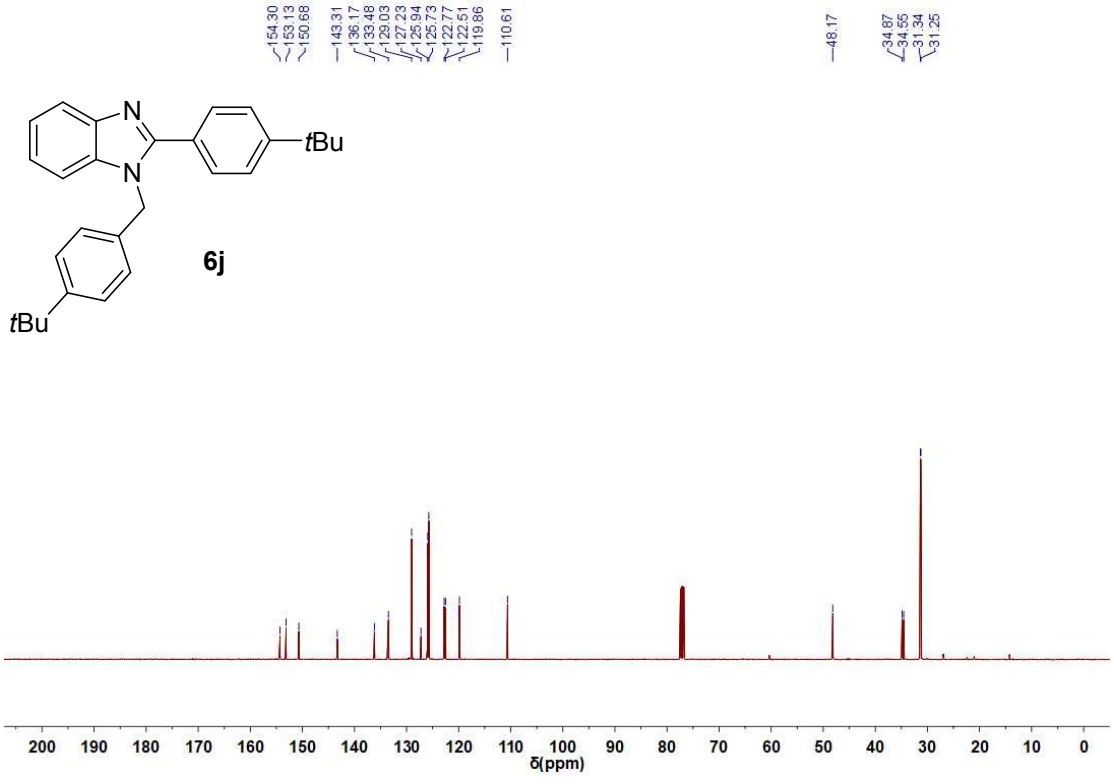
7.71
7.71
7.70
7.69
7.51
7.50
7.50
7.49
7.48
7.38
7.38
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.31
7.31
7.26
7.24
7.24
7.23
7.23
7.22
7.09
7.07
5.46
1.38
1.34
N
N
tBu
tBu
6j
0.98
2.04
2.05
3.08
2.07
2.05
2.03
18.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
δ(ppm)


154.30
153.13
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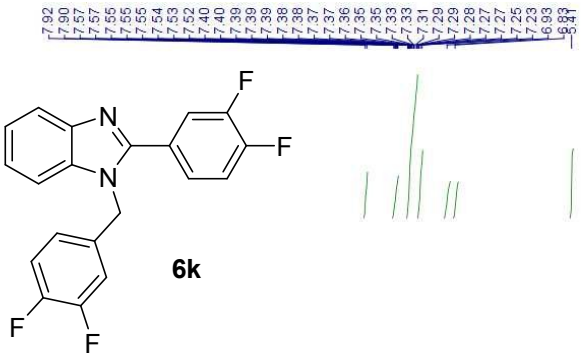
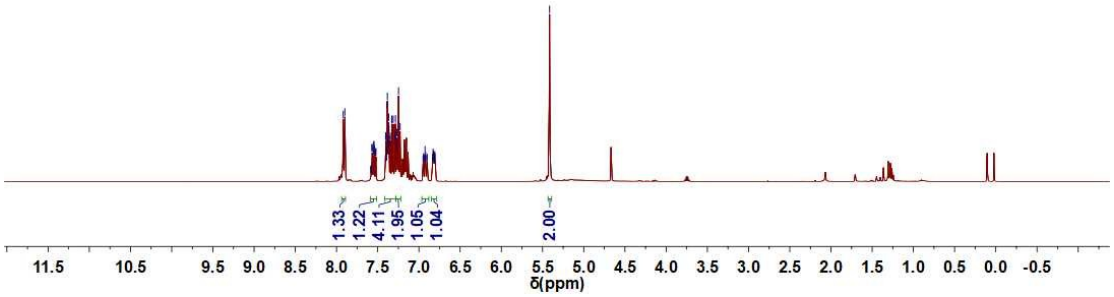
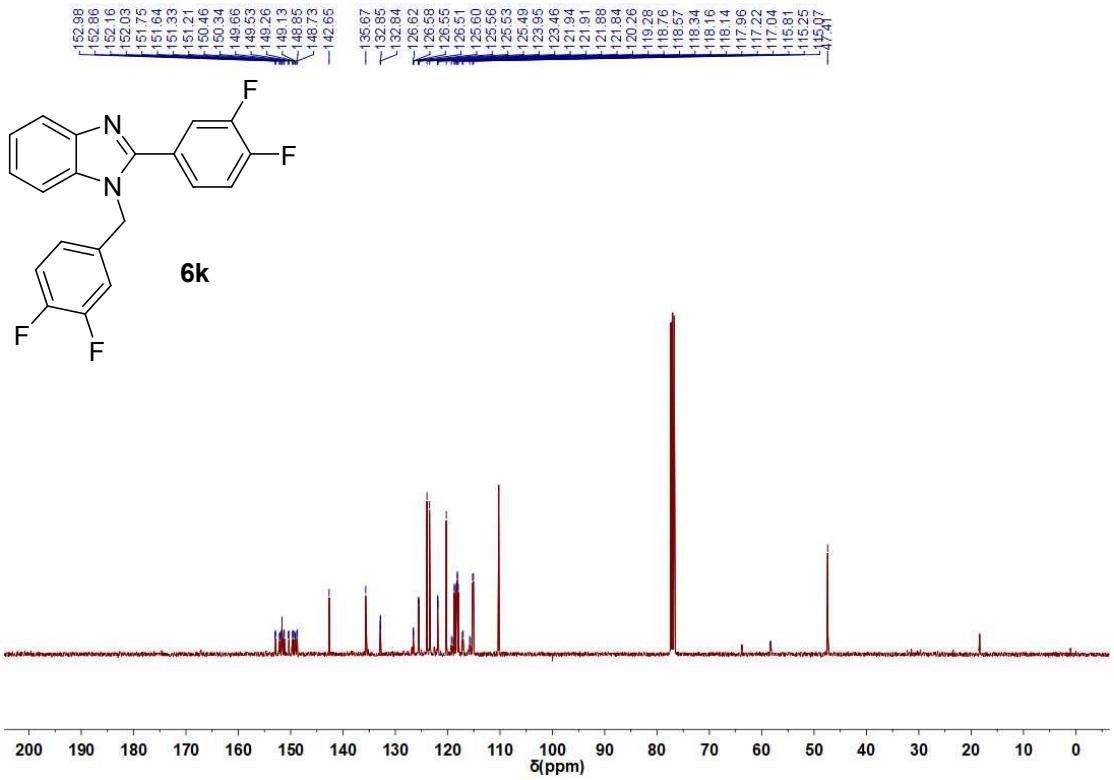
143.31
136.17
133.48
129.03
127.23
125.94
125.73
122.77
122.51
119.86
110.61
48.17
34.87
34.55
31.34
31.25
N
N
tBu
tBu
6j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ(ppm)

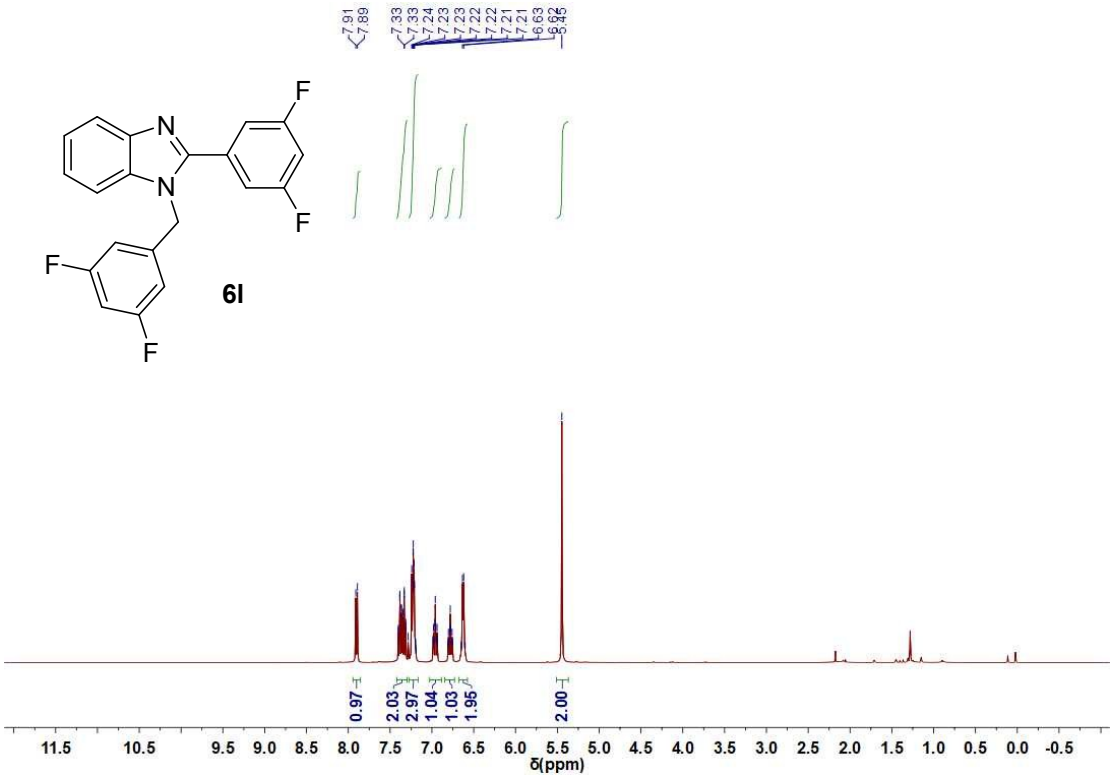


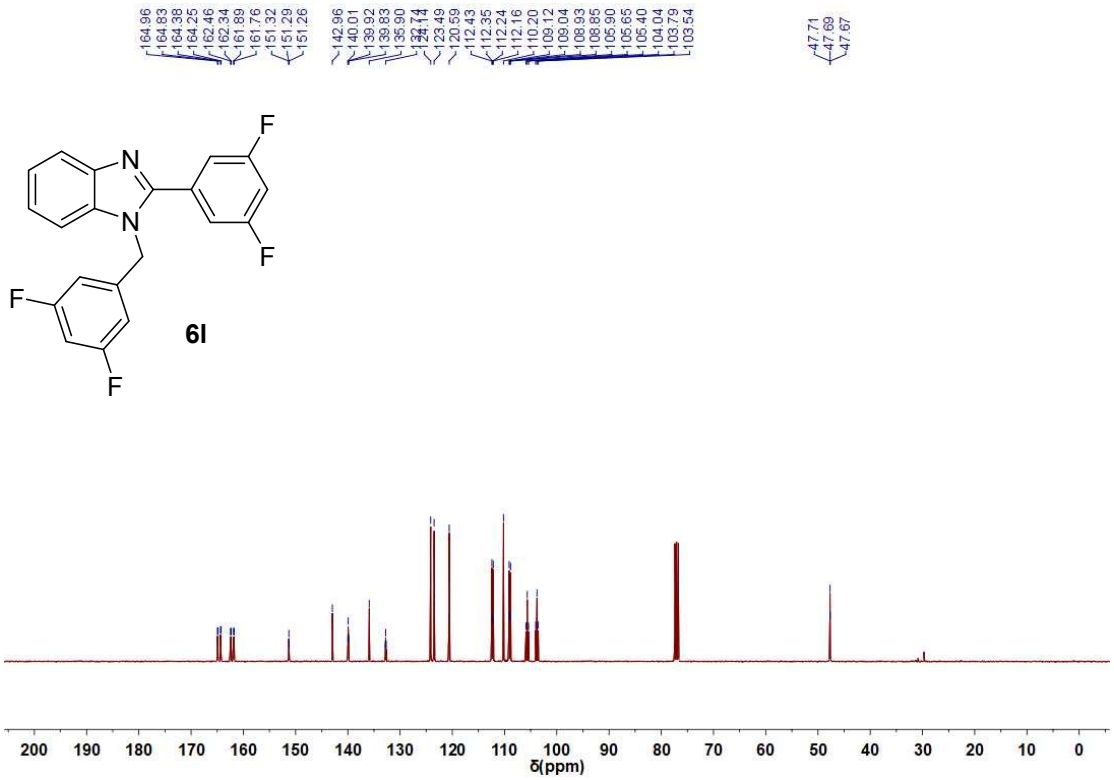
6k





6k


7.91
7.89
7.33
7.33
7.24
7.23
7.23
7.22
7.22
7.21
7.21
6.63
6.62
5.45
F
N
N
F
F
F
6l
0.97
2.03
2.97
1.04
1.03
1.95
2.00
11.5
10.5
9.5
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
-0.5
δ(ppm)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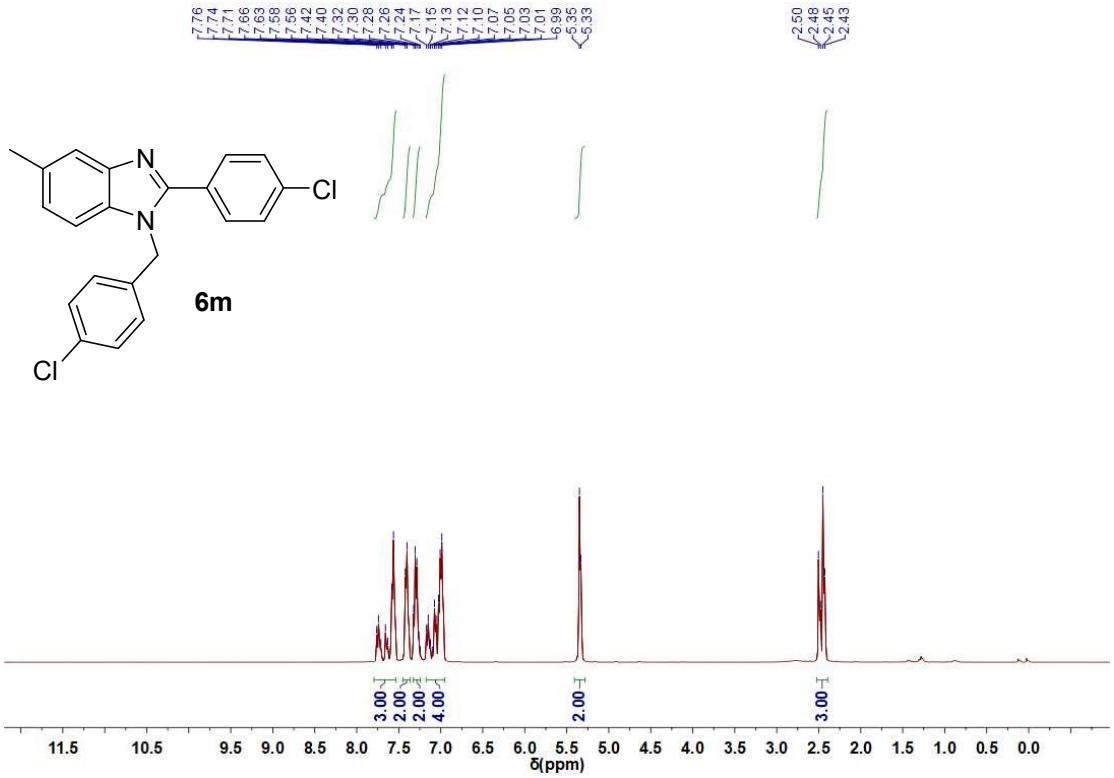
161.89
161.76
151.32
151.29
151.26
142.96
140.01
139.92
139.83
135.90
123.49
120.59
112.43
112.35
112.24
112.16
110.20
109.12
109.04
108.93
108.85
105.90
105.65
105.40
104.04
103.79
103.54
47.71
47.69
47.67
F
N
N
F
F
F
6l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ(ppm)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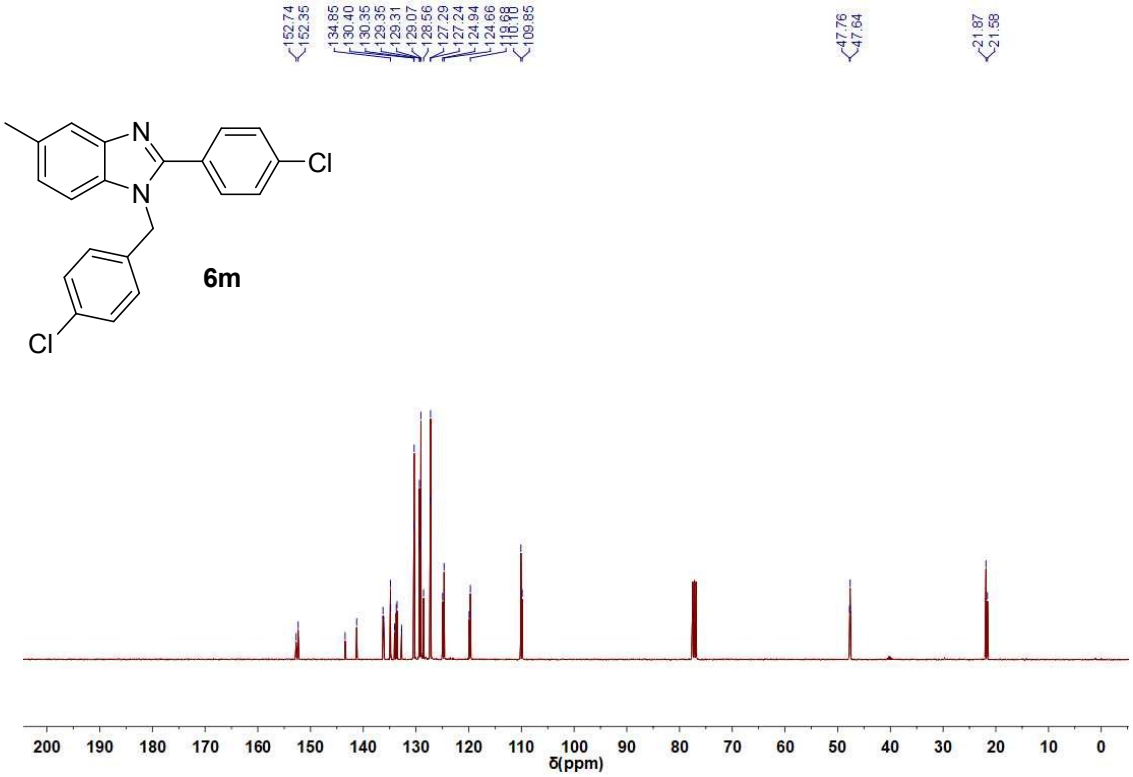
7.40
7.32
7.30
7.28
7.26
7.24
7.17
7.15
7.13
7.12
7.10
7.07
7.05
7.03
7.01
6.99
5.35
5.33
2.50
2.48
2.45
2.43
N
N
Cl
Cl
6m
3.00
2.00
2.00
4.00
2.00
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ(ppm)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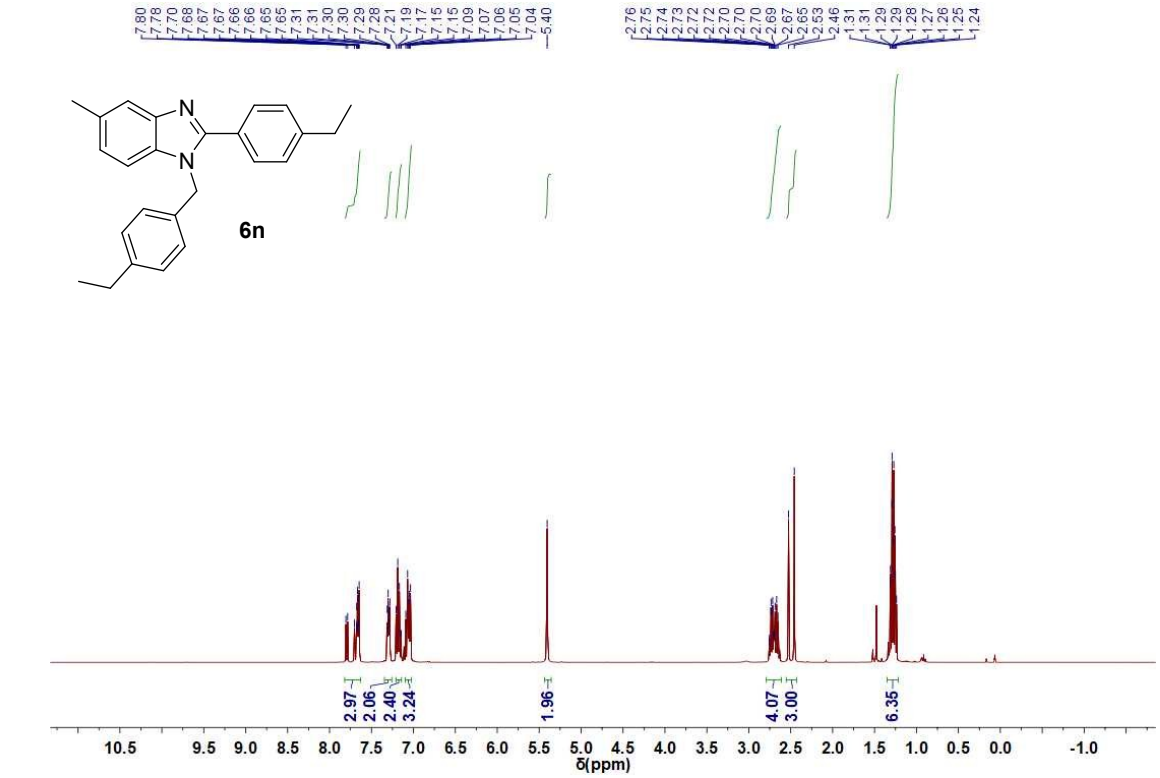
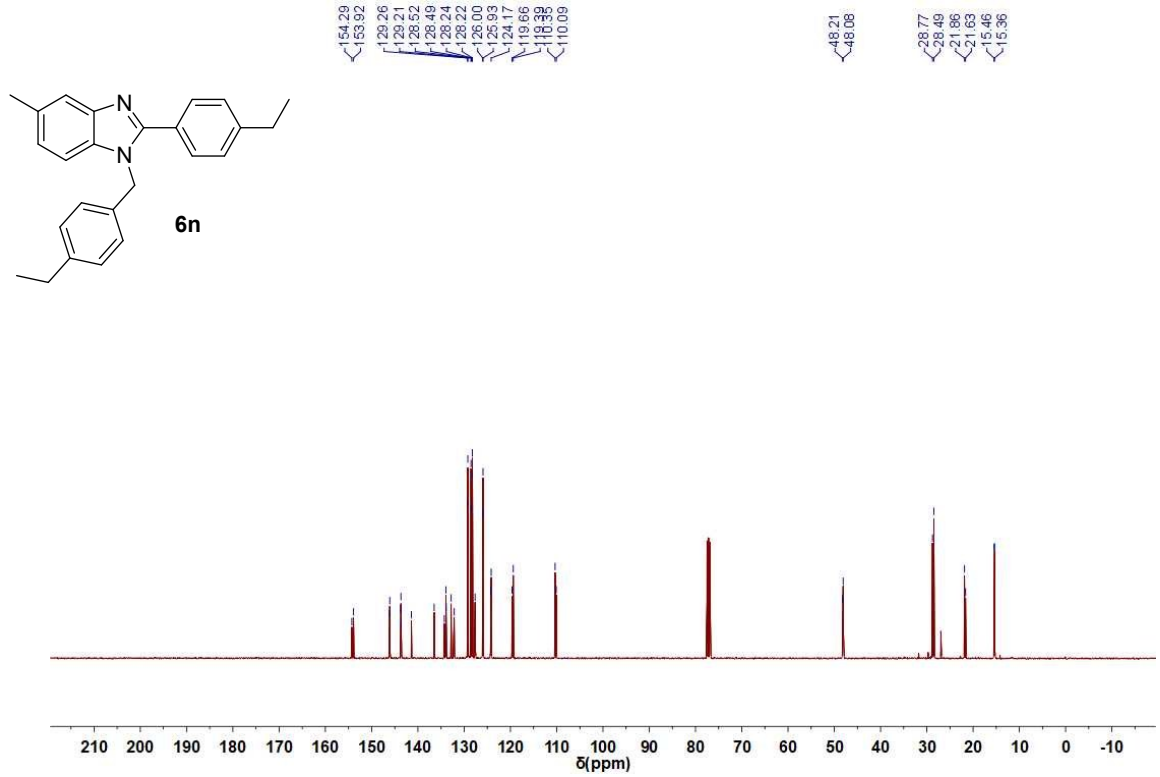
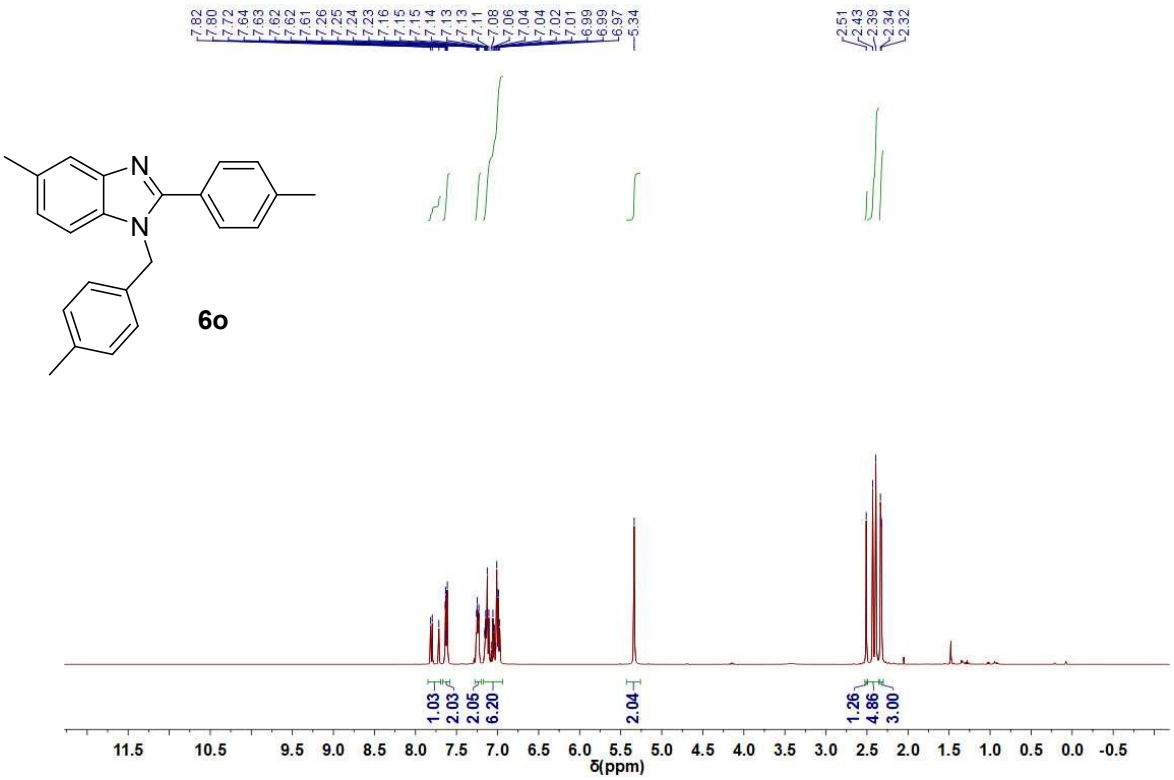
152.35
134.85
130.40
130.35
129.35
129.31
129.07
128.56
127.29
127.24
124.94
124.66
110.10
109.85
47.76
47.64
21.87
21.58
N
N
Cl
Cl
6m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ(ppm)


7.80 7.78 7.70 7.68 7.67 7.67 7.66 7.66 7.65 7.65 7.31 7.31 7.30 7.30 7.29 7.28 7.21 7.19 7.17 7.15 7.15 7.09 7.07 7.06 7.05 7.04 5.40
2.76 2.75 2.74 2.73 2.72 2.72 2.70 2.70 2.69 2.67 2.65 2.53 2.46 1.31 1.31 1.29 1.29 1.28 1.27 1.26 1.25 1.24
N
N
6n
2.97
2.06
2.40
3.24
1.96
4.07
3.00
6.35
10.5 9.5 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 -1.0
δ(ppm)


154.29 153.92 129.26 129.21 128.52 128.49 128.24 128.22 126.00 125.93 124.17 119.66 119.39 118.39 110.09
48.21 48.08
28.77 28.49 21.86 21.63 15.46 15.36
N
N
6n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
δ(ppm)


7.82
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7.64
7.63
7.62
7.62
7.61
7.26
7.25
7.24
7.23
7.16
7.15
7.15
7.14
7.13
7.13
7.11
7.08
7.06
7.04
7.04
7.02
7.01
6.99
6.99
6.97
5.34
2.51
2.43
2.39
2.34
2.32
N
N
6o
1.03
2.03
2.05
6.20
2.04
1.26
4.86
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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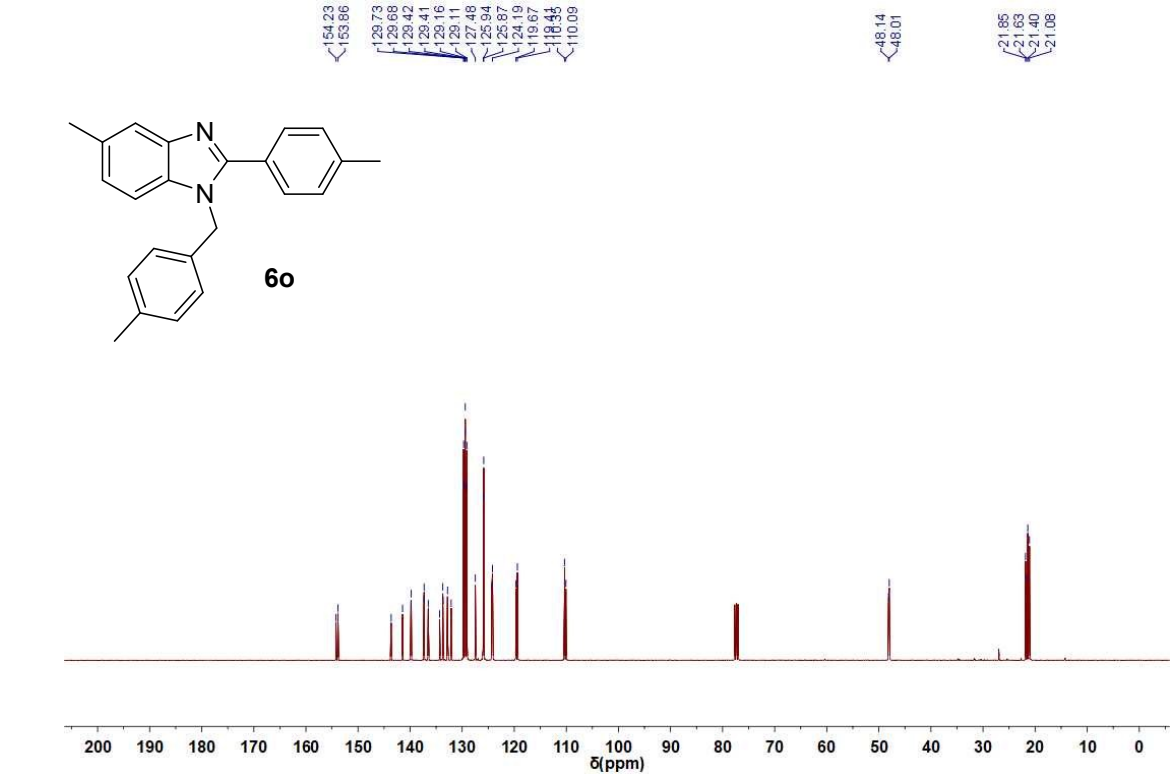
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
δ(ppm)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129.41
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129.11
127.48
125.94
125.87
124.19
119.67
118.44
118.35
110.09
48.14
48.01
21.85
21.63
21.40
21.08
N
N
6o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ(ppm)