

Supplementary Information

Selective C(sp³)–C(sp³) reduction and metathesis of ketones

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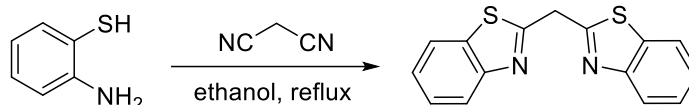
1. General information

All reagents were used directly without purification unless stated otherwise. All manipulations involving air- and moisture-sensitive organometallic compounds were performed under dinitrogen atmosphere using Schlenk techniques or an Mbraun glovebox. Toluene and tetrahydrofuran (THF) were taken from a solvent purification system (PS-400-5, Unilab Mbraun, Inc.). Analytical thin layer chromatography was performed on 0.25 silica gel 60-F254. The products were purified by flash column chromatography (300-400 mesh). Visualization was carried out with UV light. ^1H NMR and ^{13}C NMR spectra of organic compounds were recorded on a JEOL ECA-400 NMR spectrometer (FT, 400 MHz for ^1H ; 100 MHz for ^{13}C) in CDCl_3 at room temperature. All chemical shift values are quoted in ppm referenced to an internal tetramethylsilane standard for ^1H NMR. Chemical shifts of ^{13}C NMR are reported relative to CDCl_3 (δ 77.16). The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants (J) was reported in Hz unit. GC-MS analyses were measured on a Focus GC-ISQ MS instrument. High resolution mass spectrometry (HRMS) spectra were obtained on a micro TOF II Instrument using ESI ionization sources. MALDI-TOF (matrix-assisted laser desorption ionization time-of-flight) spectra was recorded in the linear, positive mode by using a Bruker Daltonics ultrafleXtreme MALDI-TOF/TOF instrument. DHB (2,5-Dihydroxybenzoic acid) was used as the matrix. Gel Permeation Chromatography (GPC) was used to obtain molecular weight (M_n and M_w) and polydispersity index (PDI) of polymers or mother liquor using an Agilent Technologies 1260 Infinity equipped with three columns (Agilent PLgel (5 μm , 103 $\text{\AA}$), Agilent PLgel (5 μm , 106 $\text{\AA}$) and Agilent PLgel (10 μm , MIXED BLS)) in a column oven with one differential refractometer. THF (HPLC Grade) was used as the eluent with a flow rate of 1 mL/min. Polystyrene standards (from Agilent Technologies, $M_n = 162 \sim 6.57 \times 10^6 \text{ g mol}^{-1}$) were used for calibration. The single crystal X-ray diffraction studies were carried out on a Bruker Kappa APEX-II CCD diffractometer equipped with Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$).

2. Synthesis and characterization of substrates

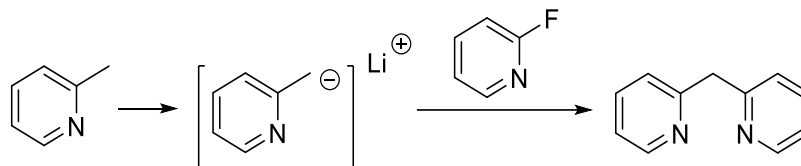
2.1 General procedures for preparation of heteroaryl- and dihydrooxazolyl-substituted ketones (1 - 5, 23 and 24)

Synthesis of bis(benzothiazol-2-yl)methane (11)¹



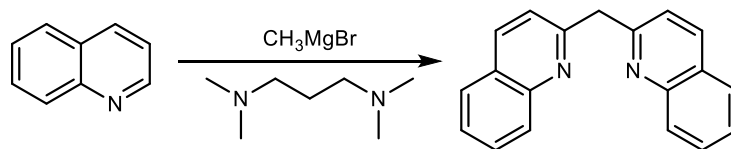
2-Aminothiophenol (10.0 g, 80.0 mmol) and malononitrile (2.64 g, 40.0 mmol) were dissolved in ethanol (40 mL). The reaction mixture was heated to reflux for 6 h, cooled to room temperature, and stored in the fridge at -32 °C. The resulting precipitate was filtered, washed with hexane (2 × 50 mL) and dried under reduced pressure. A yellow powder was obtained upon recrystallisation from ethanol in 69% yield. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.07 (d, *J* = 7.2 Hz, 2H), 7.87 (d, *J* = 7.9 Hz, 2H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 2H), 4.98 (s, 2H).

Synthesis of di(pyridin-2-yl)methane (12)¹



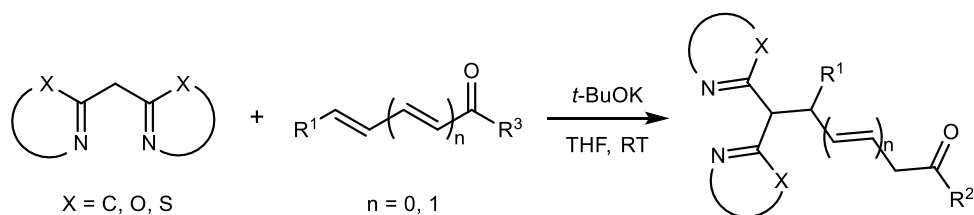
A reported procedure was followed: 2-methylpyridine (931 mg, 10.0 mmol) was dissolved in 20 mL of THF in a 100 mL Schlenk flask equipped with a stir bar and reflux condenser. The solution was cooled to -78 °C under N₂ atmosphere and 2.5 M *n*-BuLi (8.0 mL, 20.0 mmol) was added dropwise. The solution was stirred for one hour, and then warmed to -20 °C, whereupon 2-fluoropyridine (971 mg, 10 mmol) was added dropwise. The mixture was subsequently heated to reflux for 25 minutes, and then hydrolyzed with ice. The aqueous layer was separated and extracted three times with 20 mL CH₂Cl₂. The combined organic layer was dried over Na₂SO₄, filtered and evaporated. The crude product was purified by silica gel column chromatography with the eluent 1:1 ethyl acetate/petroleum ether, yielding yellow oil. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.55 (d, *J* = 4.5 Hz, 2H), 7.61 (td, *J* = 7.7, 1.6 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 2H), 7.15 – 7.11 (m, 2H), 4.35 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 159.42, 149.45, 136.60, 123.58, 121.48, 47.30.

Synthesis of di(2-quinoly)lmethane (13)¹



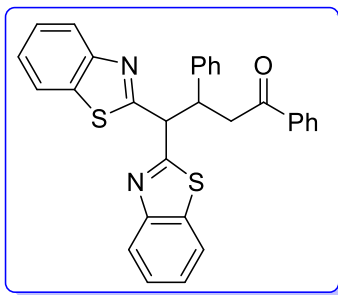
Quinoline (2.58 g, 20.0 mmol), 3.0 M methylmagnesium bromide (20.0 mL, 60.0 mmol), N,N,N',N'-tetramethylethylenediamine (0.30 mL, 2.0 mmol), and 15 mL toluene were added to a pressure flask under N₂ atmosphere. The flask was sealed and heated at 140 °C (oil bath temperature) overnight. The reaction mixture was then cooled to room temperature, carefully quenched by a saturated sodium sulfite solution, and extracted three times with ethyl acetate. The combined organic layer was washed with brine, dried over Na₂SO₄, filtered and condensed to a dark orange oil by rotary evaporation. The crude product was purified by silica gel column chromatography with the eluent 1:1 ethyl acetate/petroleum ether, yielding light brown oil. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.11 (d, *J* = 8.5 Hz, 2H), 8.02 (d, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.2 Hz, 2H), 7.70 (t, *J* = 7.7 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 4.74 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 159.54, 147.98, 136.61, 129.56, 129.07, 127.58, 126.95, 126.16, 121.94, 49.11.

Synthesis and characterization of heteroaryl- and dihydrooxazolyl-substituted ketones (1-4, 23 and 24)



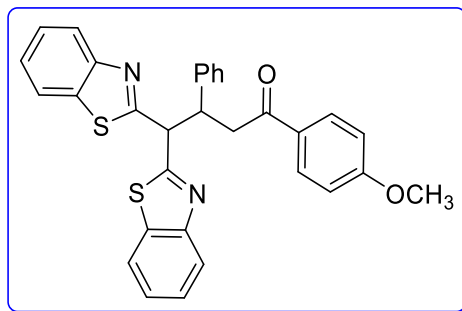
General procedures: To a stirred solution of the corresponding methylene-bridged diheterocycle (5.0 mmol) in THF (15 mL) at room temperature was added *t*-BuOK (5.0 mmol). Then, corresponding ketone (5.0 mmol) was added to the reaction mixture in one portion. The reaction mixture was extracted with ethyl acetate. The organic layer was washed with brine, dried over anhydrous Na₂SO₄, further purified on silica gel chromatography to afford the target ketones.

4,4-Bis(benzo[d]thiazol-2-yl)-1, 3-diphenylbutan-1-one (1a)



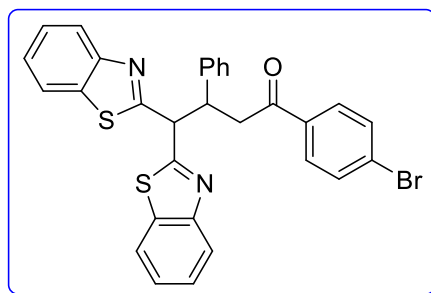
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.00 (t, $J = 9.6$ Hz, 2H), 7.84 (d, $J = 8.0$ Hz, 1H), 7.77 (d, $J = 7.6$ Hz, 1H), 7.71 (d, $J = 7.9$ Hz, 1H), 7.48 – 7.26 (m, 9H), 7.13 (t, $J = 7.2$ Hz, 1H), 7.06 – 7.02 (m, 1H), 5.44 (d, $J = 10.9$ Hz, 1H), 4.77 (t, $J = 8.7$ Hz, 1H), 3.66 – 3.47 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 197.39, 169.31, 168.61, 152.79, 152.64, 140.65, 136.83, 135.77, 135.22, 132.89, 128.40, 128.38, 128.36, 128.00, 126.98, 126.14, 125.91, 125.37, 125.04, 123.25, 123.18, 121.69, 121.47, 55.16, 47.23, 43.14.

4,4-Bis(benzo[d]thiazol-2-yl)-1-(4-methoxyphenyl)-3-phenylbutan-1-one (1b)



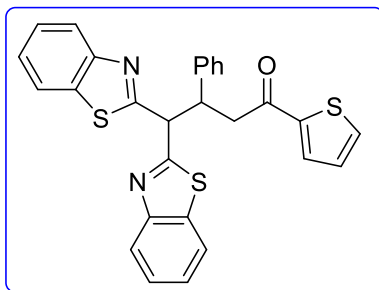
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.01 (dd, $J = 18.0, 7.2$ Hz, 2H), 7.77 (td, $J = 23.6, 6.4$ Hz, 1H), 7.46 – 7.31 (m, 6H), 7.13 – 7.03 (m, 3H), 6.81 (d, $J = 6.8$ Hz, 2H), 5.44 (d, $J = 10.4$ Hz, 1H), 4.75 (s, 1H), 3.80 (s, 3H), 3.60 – 3.40 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 195.99, 169.44, 168.74, 163.35, 152.85, 152.71, 140.79, 135.85, 135.30, 130.34, 130.05, 128.42, 126.97, 126.15, 125.94, 125.39, 125.07, 123.30, 123.23, 121.75, 121.51, 113.56, 55.44, 55.28, 47.50, 42.82.

4,4-Bis(benzo[d]thiazol-2-yl)-1-(4-bromophenyl)-3-phenylbutan-1-one (1c)



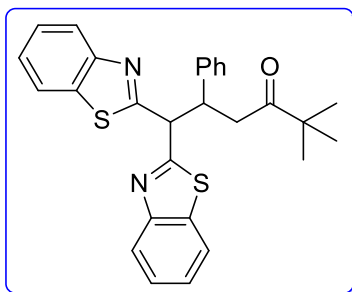
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.00 (dd, $J = 8.0, 3.9$ Hz, 2H), 7.83 (d, $J = 7.9$ Hz, 1H), 7.70 (d, $J = 7.9$ Hz, 1H), 7.62 (d, $J = 8.5$ Hz, 2H), 7.46 – 7.45 (m, 3H), 7.42 – 7.35 (m, 2H), 7.30 (t, $J = 7.8$ Hz, 3H), 7.14 (t, $J = 7.5$ Hz, 2H), 7.05 (t, $J = 7.3$ Hz, 1H), 5.42 (d, $J = 10.8$ Hz, 1H), 4.78 – 4.72 (m, 1H), 3.53 – 3.52 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 196.51, 169.24, 168.48, 152.78, 152.60, 140.51, 135.75, 135.48, 135.19, 131.67, 129.56, 128.50, 128.31, 128.09, 127.12, 126.21, 125.98, 125.46, 125.12, 123.22, 123.20, 121.73, 121.51, 55.10, 47.34, 43.15.

4,4-Bis(benzo[d]thiazol-2-yl)-3-phenyl-1-(thiophen-2-yl)butan-1-one (1d)



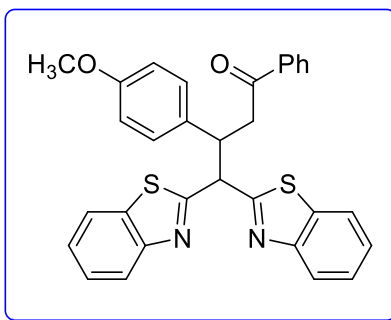
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.01 (dd, $J = 16.8, 8.1$ Hz, 2H), 7.84 (d, $J = 8.0$ Hz, 1H), 7.71 (d, $J = 7.9$ Hz, 1H), 7.61 – 7.60 (m, 1H), 7.51 – 7.44 (m, 2H), 7.42 – 7.28 (m, 5H), 7.13 (t, $J = 7.5$ Hz, 2H), 7.06 – 7.00 (m, 2H), 5.44 (d, $J = 11.0$ Hz, 1H), 4.74 (td, $J = 10.4, 3.6$ Hz, 1H), 3.55 – 3.38 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 190.21, 169.22, 168.49, 152.79, 152.62, 144.19, 140.33, 135.79, 135.21, 133.59, 131.91, 128.44, 128.33, 127.86, 127.06, 126.15, 125.92, 125.38, 125.05, 123.22, 123.19, 121.71, 121.47, 55.01, 47.51, 43.88.

6,6-Bis(benzo[d]thiazol-2-yl)-2,2-dimethyl-5-phenylhexan-3-one (1e)



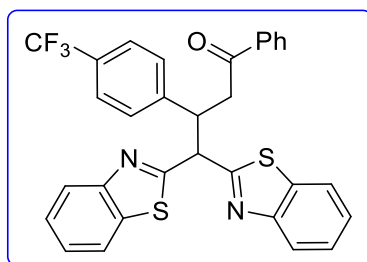
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.07 (d, $J = 8.1$ Hz, 1H), 7.96 (d, $J = 8.2$ Hz, 1H), 7.85 (d, $J = 8.0$ Hz, 1H), 7.70 (d, $J = 8.0$ Hz, 1H), 7.48 (td, $J = 7.2, 0.8$ Hz, 1H), 7.40 – 7.36 (m, 2H), 7.29 – 7.25 (m, 3H), 7.15 – 7.12 (m, 2H), 7.07 – 7.03 (m, 1H), 5.41 (d, $J = 11.2$ Hz, 1H), 4.60 – 4.54 (m, 1H), 3.22 (dd, $J = 17.0, 9.8$ Hz, 1H), 2.79 (dd, $J = 17.0, 3.3$ Hz, 1H), 0.84 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 212.81, 169.56, 168.79, 152.74, 152.60, 140.85, 135.79, 135.21, 128.46, 128.28, 126.86, 126.11, 125.85, 125.33, 124.98, 123.25, 123.16, 121.73, 121.45, 54.69, 46.95, 44.08, 41.49, 25.75.

4,4-Bis(benzo[d]thiazol-2-yl)-3-(4-methoxyphenyl)-1-phenylbutan-1-one (1f)



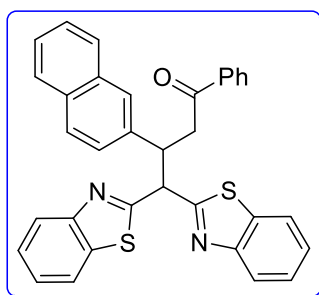
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.00 (dd, $J = 12.8, 8.1$ Hz, 2H), 7.84 (d, $J = 8.0$ Hz, 1H), 7.78 – 7.76 (m, 2H), 7.72 (d, $J = 8.0$ Hz, 1H), 7.48 – 7.44 (m, 2H), 7.42 – 7.33 (m, 4H), 7.31 – 7.27 (m, 1H), 7.22 (d, $J = 8.7$ Hz, 2H), 6.66 (d, $J = 8.7$ Hz, 2H), 5.40 (d, $J = 10.8$ Hz, 1H), 4.70 (td, $J = 10.1, 4.0$ Hz, 1H), 3.65 (s, 3H), 3.61 – 3.43 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 197.62, 169.44, 168.82, 158.31, 152.85, 152.71, 136.95, 135.81, 135.32, 132.88, 132.63, 129.40, 128.41, 128.05, 126.15, 125.92, 125.38, 125.04, 123.29, 123.22, 121.72, 121.51, 113.83, 55.41, 55.02, 46.60, 43.37.

4,4-Bis(benzo[d]thiazol-2-yl)-1-phenyl-3-(4-(trifluoromethyl)phenyl)butan-1-one (1g)



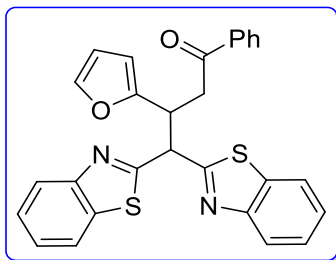
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.01 (dd, $J = 17.2, 8.0$ Hz, 2H), 7.85 (dd, $J = 8.0, 0.4$ Hz, 1H), 7.79 – 7.76 (m, 2H), 7.73 (dd, $J = 8.0, 0.4$ Hz, 1H), 7.51 – 7.46 (m, 4H), 7.45 – 7.29 (m, 7H), 5.44 (d, $J = 10.8$ Hz, 1H), 4.87 (td, $J = 10.1, 3.9$ Hz, 1H), 3.69 – 3.51 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 196.92, 168.71, 167.98, 152.75, 152.65, 144.95, 136.54, 135.69, 135.14, 133.15, 128.80, 128.48, 127.96, 126.27, 126.11, 125.54, 125.38, 125.34, 125.30, 123.33, 123.25, 121.73, 121.54, 54.63, 46.71, 42.80.

4,4-Bis(benzo[d]thiazol-2-yl)-3-(naphthalen-2-yl)-1-phenylbutan-1-one (1h)



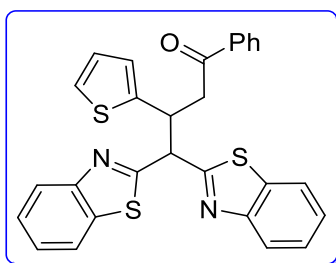
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.03 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 8.1 Hz, 1H), 7.85 (d, J = 7.7 Hz, 1H), 7.79 – 7.75 (m, 3H), 7.66 – 7.64 (m, 4H), 7.53 – 7.43 (m, 3H), 7.39 – 7.30 (m, 6H), 7.26 – 7.22 (m, 1H), 5.60 (d, J = 10.8 Hz, 1H), 5.00 – 4.94 (m, 1H), 3.72 (dd, J = 16.7, 9.5 Hz, 1H), 3.58 (dd, J = 16.9, 3.5 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 197.38, 169.40, 168.60, 152.83, 152.75, 138.36, 136.88, 135.87, 135.26, 133.29, 132.96, 132.49, 128.43, 128.21, 128.06, 127.91, 127.61, 127.52, 126.38, 126.21, 125.97, 125.85, 125.66, 125.45, 125.10, 123.35, 123.24, 121.77, 121.53, 55.13, 47.19, 43.43.

4,4-Bis(benzo[d]thiazol-2-yl)-3-(furan-2-yl)-1-phenylbutan-1-one (1i)



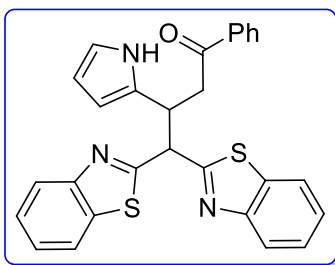
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.99 (dd, J = 8.1, 3.6 Hz, 2H), 7.83 (d, J = 7.9 Hz, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.62 (d, J = 8.5 Hz, 2H), 7.48 – 7.45 (m, 3H), 7.42 – 7.35 (m, 2H), 7.31 – 7.28 (m, 2H), 7.14 (t, J = 7.5 Hz, 2H), 7.05 (t, J = 7.3 Hz, 1H), 5.42 (d, J = 10.8 Hz, 1H), 4.78 – 4.72 (m, 1H), 3.53 – 3.51 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 196.54, 169.22, 168.49, 152.82, 152.65, 140.52, 135.79, 135.56, 135.23, 131.69, 129.57, 128.51, 128.32, 128.09, 127.13, 126.21, 125.99, 125.46, 125.13, 123.23, 121.73, 121.51, 55.14, 47.36, 43.17.

4,4-Bis(benzo[d]thiazol-2-yl)-1-phenyl-3-(thiophen-2-yl)butan-1-one (1j)



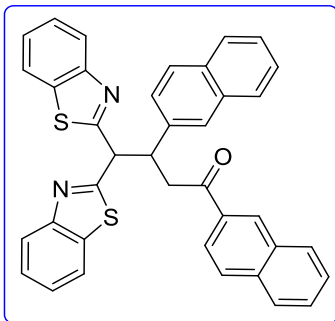
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.06 – 8.01 (m, 2H), 7.85 – 7.82 (m, 3H), 7.76 (d, J = 8.0 Hz, 1H), 7.51 – 7.42 (m, 3H), 7.39 – 7.31 (m, 4H), 7.01 (d, J = 5.0 Hz, 1H), 6.86 (d, J = 3.2 Hz, 1H), 6.73 – 6.71 (m, 1H), 5.44 (d, J = 10.1 Hz, 1H), 5.12 (td, J = 9.6, 3.9 Hz, 1H), 3.69 (dd, J = 17.0, 9.3 Hz, 1H), 3.53 (dd, J = 17.0, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 197.07, 168.72, 168.35, 152.88, 152.63, 143.93, 136.75, 135.78, 135.33, 133.03, 128.44, 128.05, 126.58, 126.26, 126.15, 126.01, 125.42, 125.16, 124.16, 123.28, 121.69, 121.52, 55.83, 43.63, 42.64.

4,4-Bis(benzo[d]thiazol-2-yl)-1-phenyl-3-(1H-pyrrol-2-yl)butan-1-one (1k)



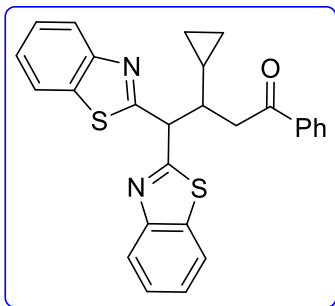
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 9.47 (s, 1H), 8.03 (dd, $J = 17.4, 8.2$ Hz, 2H), 7.86 (d, $J = 8.0$ Hz, 2H), 7.78 (dd, $J = 15.2, 8.0$ Hz, 2H), 7.53 – 7.44 (m, 3H), 7.40 – 7.32 (m, 4H), 6.62 (s, 1H), 5.96 – 5.95 (m, 1H), 5.92 (s, 1H), 5.60 (d, $J = 8.4$ Hz, 1H), 4.83 – 4.78 (m, 1H), 3.65 (dd, $J = 17.8, 7.5$ Hz, 1H), 3.51 (dd, $J = 17.8, 5.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.77, 169.82, 169.22, 152.71, 152.57, 136.84, 135.76, 135.57, 133.21, 130.91, 128.52, 128.09, 126.15, 126.05, 125.41, 125.24, 123.26, 123.20, 121.66, 117.28, 107.94, 106.71, 53.41, 42.26, 39.23.

4,4-Bis(benzo[d]thiazol-2-yl)-1,3-di(naphthalen-2-yl)butan-1-one (1l)



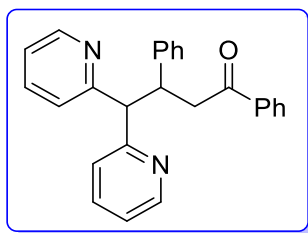
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.30 (s, 1H), 8.00 (dd, $J = 19.3, 8.1$ Hz, 2H), 7.86 – 7.73 (m, 6H), 7.69 – 7.64 (m, 4H), 7.57 – 7.42 (m, 4H), 7.39 – 7.31 (m, 4H), 7.26 – 7.22 (m, 1H), 5.65 (d, $J = 10.9$ Hz, 1H), 5.06 – 5.00 (m, 1H), 3.86 – 3.72 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 197.35, 169.45, 168.58, 152.83, 152.73, 138.35, 135.88, 135.47, 135.24, 134.18, 133.28, 132.49, 132.37, 129.75, 129.55, 128.37, 128.25, 127.88, 127.68, 127.62, 127.50, 126.64, 126.33, 126.19, 125.95, 125.85, 125.65, 125.45, 125.09, 123.83, 123.32, 123.23, 121.75, 121.51, 55.20, 47.49, 43.56.

4,4-Bis(benzo[d]thiazol-2-yl)-3-cyclopropyl-1-phenylbutan-1-one (1m)



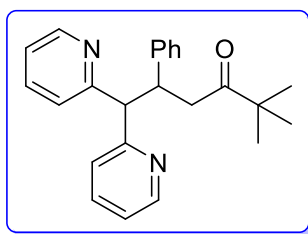
Yellow liquid. ^1H NMR (400 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 8.04 (t, $J = 7.5$ Hz, 2H), 7.91 – 7.89 (m, 2H), 7.86 – 7.80 (m, 2H), 7.52 – 7.43 (m, 3H), 7.41 – 7.30 (m, 4H), 7.15 (s, 0.25H, minor isomer), 5.37 (d, $J = 7.9$ Hz, 0.75H, major isomer), 3.53 – 3.40 (m, 1H), 3.34 – 3.17 (m, 1H), 3.07 – 3.02 (m, 0.25H, minor isomer), 2.76 – 2.69 (m, 0.75H, major isomer), 1.24 – 1.17 (m, 0.25H, minor isomer), 1.05 – 0.96 (m, 0.75H, major isomer), 0.39 – 0.32 (m, 0.75H, major isomer), 0.31 – 0.24 (m, 1H), 0.15 – -0.01 (m, 2H), -0.10 – -0.16 (m, 0.25H, minor isomer); ^{13}C NMR (100 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 201.21, 199.29, 175.91, 175.37, 169.45, 169.11, 152.99, 152.97, 137.28, 136.88, 135.96, 135.91, 135.57, 135.49, 133.41, 132.90, 128.54, 128.49, 128.22, 126.10, 125.93, 125.29, 125.20, 125.02, 123.38, 123.28, 123.21, 121.84, 121.76, 121.60, 53.95, 51.32, 46.78, 41.80, 40.17, 15.46, 11.54, 6.11, 5.55, 4.32, 3.12. Ratio of diastereoisomers (major to minor): 3.0.

1,3-Diphenyl-4,4-di(pyridin-2-yl)butan-1-one (2a)



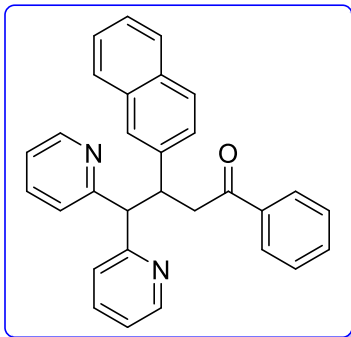
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.59 (s, 1H), 8.40 (s, 1H), 7.75 – 7.70 (m, 3H), 7.64 – 7.60 (m, 1H), 7.47 – 7.44 (m, 1H), 7.36 – 7.34 (m, 3H), 7.20 (s, 3H), 7.12 (s, 1H), 7.06 (t, $J = 7.0$ Hz, 2H), 6.97 – 6.94 (m, 1H), 6.87 (s, 1H), 4.67 (s, 2H), 3.42 – 3.37 (m, 1H), 3.13 (d, $J = 16.1$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.65, 161.12, 160.62, 149.33, 148.95, 142.28, 137.07, 136.70, 135.89, 132.66, 128.42, 128.32, 128.03, 127.95, 126.09, 123.95, 123.77, 122.00, 121.23, 62.13, 45.65, 43.94.

2,2-Dimethyl-5-phenyl-6,6-di(pyridin-2-yl)hexan-3-one (2b)



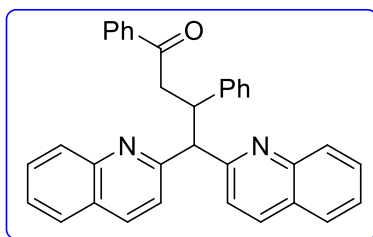
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.56 (s, 1H), 8.38 (s, 1H), 7.73 – 7.71 (m, 1H), 7.64 – 7.62 (m, 1H), 7.32 – 7.30 (m, 1H), 7.19 – 7.07 (m, 6H), 6.98 – 6.97 (m, 1H), 6.86 (s, 1H), 4.64 – 4.48 (m, 2H), 3.05 (dd, $J = 16.8, 10.1$ Hz, 1H), 2.40 (d, $J = 16.8$ Hz, 1H), 0.79 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 213.71, 161.42, 160.86, 149.21, 148.96, 142.83, 136.67, 135.84, 128.56, 127.87, 125.96, 123.79, 123.70, 121.89, 121.16, 61.65, 45.11, 44.03, 41.95, 25.75.

3-(Naphthalen-2-yl)-1-phenyl-4,4-di(pyridin-2-yl)butan-1-one (2c)



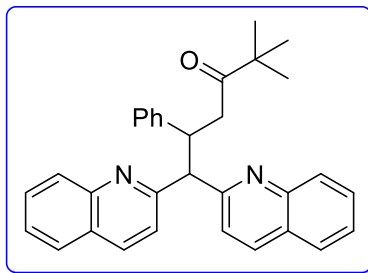
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.64 (s, 1H), 8.40 (s, 1H), 7.77 – 7.76 (m, 3H), 7.67 – 7.61 (m, 5H), 7.47 (d, J = 6.8 Hz, 2H), 7.35 – 7.29 (m, 6H), 7.16 (s, 1H), 6.84 (s, 1H), 4.94 – 4.82 (m, 2H), 3.56 – 3.50 (m, 1H), 3.24 (d, J = 16.3 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.55, 161.21, 160.56, 149.39, 149.01, 140.05, 137.11, 136.75, 135.96, 133.25, 132.68, 132.13, 128.34, 128.05, 127.73, 127.63, 127.42, 126.68, 125.47, 125.13, 124.01, 123.80, 122.05, 121.31, 62.09, 45.63, 44.07.

1,3-Diphenyl-4,4-di(quinolin-2-yl)butan-1-one (3a)



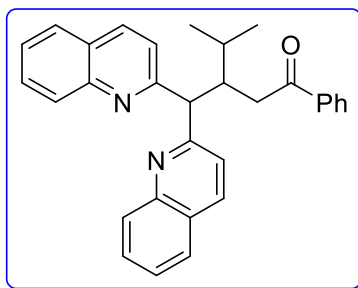
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.14 (d, J = 8.5 Hz, 1H), 8.08 – 8.05 (m, 2H), 7.97 (d, J = 8.6 Hz, 1H), 7.81 – 7.68 (m, 5H), 7.64 – 7.58 (m, 2H), 7.50 – 7.29 (m, 9H), 7.03 (t, J = 7.5 Hz, 2H), 6.91 (t, J = 7.2 Hz, 1H), 5.11 – 5.03 (m, 2H), 3.48 (dd, J = 15.9, 8.7 Hz, 1H), 3.30 – 3.25 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.79, 161.40, 160.67, 147.72, 142.38, 137.03, 136.64, 135.82, 132.65, 129.39, 129.19, 129.02, 128.62, 128.25, 128.07, 127.96, 127.57, 127.34, 127.24, 126.68, 126.22, 126.14, 125.83, 122.06, 63.33, 45.36, 44.16.

2,2-Dimethyl-5-phenyl-6,6-di(quinolin-2-yl)hexan-3-one (3b)



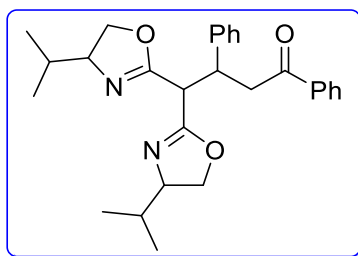
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.15 (d, $J = 8.5$ Hz, 1H), 8.06 (t, $J = 7.9$ Hz, 2H), 8.01 (d, $J = 8.6$ Hz, 1H), 7.76 (dd, $J = 12.1, 8.3$ Hz, 2H), 7.70 (t, $J = 7.7$ Hz, 1H), 7.63 – 7.58 (m, 2H), 7.49 (t, $J = 7.5$ Hz, 1H), 7.40 – 7.33 (m, 4H), 7.04 (t, $J = 7.5$ Hz, 2H), 6.92 (t, $J = 7.4$ Hz, 1H), 5.02 (d, $J = 11.9$ Hz, 1H), 4.90 (t, $J = 11.2$ Hz, 1H), 3.17 (dd, $J = 16.9, 10.0$ Hz, 1H), 2.52 (d, $J = 16.8$ Hz, 1H), 0.76 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 213.92, 161.67, 160.83, 147.78, 147.70, 143.00, 136.57, 135.77, 129.35, 129.28, 129.24, 128.99, 128.76, 127.87, 127.56, 127.34, 127.27, 126.68, 126.20, 126.00, 125.80, 122.28, 121.78, 62.89, 44.72, 44.03, 42.15, 25.78.

3-(Di(quinolin-2-yl)methyl)-4-methyl-1-phenylpentan-1-one (3c)



Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.17 (d, $J = 8.2$ Hz, 1H), 8.01 (d, $J = 8.4$ Hz, 1H), 7.92 – 7.81 (m, 3H), 7.74 – 7.62 (m, 5H), 7.58 – 7.53 (m, 2H), 7.50 – 7.46 (m, 1H), 7.38 – 7.30 (m, 2H), 7.19 (t, $J = 7.0$ Hz, 2H), 4.72 (d, $J = 11.9$ Hz, 1H), 4.00 – 3.96 (m, 1H), 3.04 (dd, $J = 16.5, 5.3$ Hz, 1H), 2.87 (dd, $J = 16.7, 5.2$ Hz, 1H), 1.82 – 1.79 (m, 1H), 0.94 – 0.92 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 200.33, 161.66, 161.66, 150.44, 148.09, 147.44, 137.03, 136.22, 132.29, 129.56, 129.23, 129.04, 129.00, 127.98, 127.89, 127.82, 127.46, 127.34, 126.99, 126.03, 125.88, 122.41, 122.21, 61.67, 43.53, 36.84, 28.75, 21.64, 16.37.

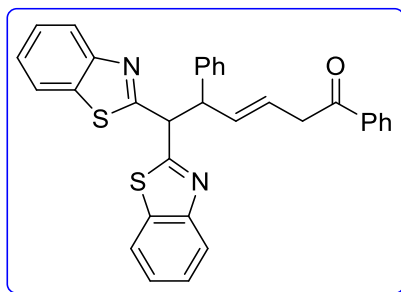
4,4-Bis(4-isopropyl-4,5-dihydrooxazol-2-yl)-1,3-diphenylbutan-1-one (4)



Yellow solid. ^1H NMR (400 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 7.88 (d, $J = 7.3$ Hz, 2H), 7.44 (t, $J = 7.4$ Hz, 1H), 7.34 (t, $J = 7.5$ Hz, 2H), 7.23 – 7.20 (m, 2H), 7.15 (t, $J = 7.4$ Hz, 2H), 7.07 (t, $J = 7.3$ Hz, 1H), 4.26 – 4.10 (m, 2H), 4.02 – 3.82 (m, 4H), 3.78 – 3.57 (m, 3H), 3.36 – 3.27 (m, 1H), 1.75 – 1.66 (m, 1H), 1.50 – 1.12 (m, 1H), 0.91 – 0.82 (m, 6H), 0.69 – 0.47 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 197.63, 197.58, 197.56, 163.41, 163.36, 163.20, 162.71, 162.67, 162.62, 162.57, 140.96, 140.89, 140.49, 140.39, 136.80, 136.77, 136.75, 132.81, 128.41, 128.37, 128.24, 128.13, 128.10, 126.91, 126.87, 126.78, 126.75, 72.11, 72.07, 71.88, 71.63, 71.58, 71.53, 70.47, 70.42, 70.39, 70.31, 70.21, 70.16, 69.71,

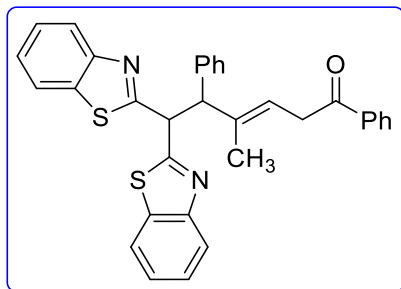
69.68, 45.71, 45.62, 45.43, 45.32, 43.58, 43.53, 43.50, 43.44, 41.71, 41.55, 41.51, 41.47, 32.61, 32.47, 32.43, 32.05, 32.03, 31.99, 31.97, 18.74, 18.71, 18.52, 18.44, 18.41, 18.30, 18.28, 18.19, 18.12, 17.74, 17.70, 17.59, 17.55.

(E)-6,6-Bis(benzo[d]thiazol-2-yl)-1,5-diphenylhex-3-en-1-one (23a)



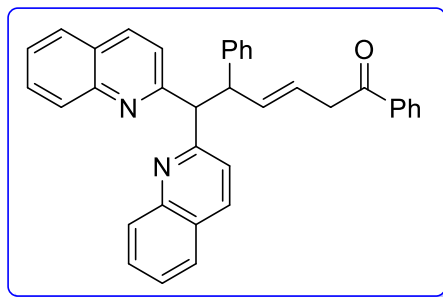
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.05 (d, $J = 8.1$ Hz, 2H), 7.90 – 7.80 (m, 4H), 7.54 – 7.32 (m, 7H), 7.18 – 7.13 (m, 5H), 6.47 (d, $J = 15.8$ Hz, 1H), 6.30 (dd, $J = 15.8, 8.8$ Hz, 1H), 5.39 (d, $J = 8.9$ Hz, 1H), 4.31 – 4.24 (m, 1H), 3.46 – 3.30 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 197.88, 168.85, 168.68, 152.88, 152.85, 152.84, 136.97, 136.86, 135.59, 133.43, 133.03, 128.81, 128.51, 128.31, 128.13, 127.38, 126.36, 126.14, 126.06, 125.35, 125.22, 123.32, 123.26, 121.65, 121.60, 53.56, 44.73, 41.82.

(E)-6,6-Bis(benzo[d]thiazol-2-yl)-4-methyl-1,5-diphenylhex-3-en-1-one (23b)



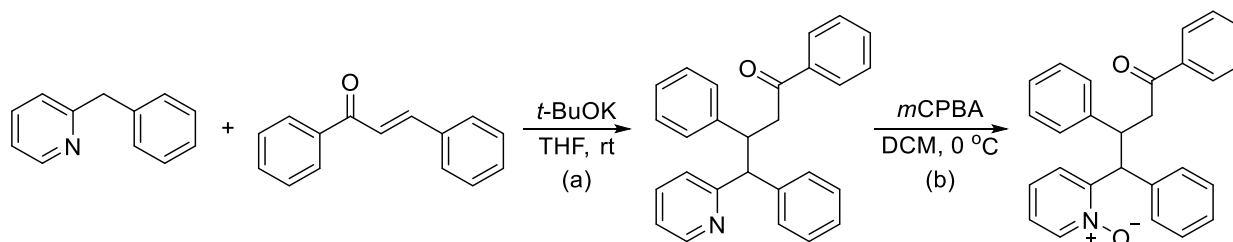
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.04 (dd, $J = 8.0, 4.1$ Hz, 2H), 7.88 – 7.86 (m, 3H), 7.80 (d, $J = 7.6$ Hz, 1H), 7.54 – 7.39 (m, 6H), 7.37 – 7.31 (m, 1H), 7.15 – 7.05 (m, 3H), 6.80 (d, $J = 7.2$ Hz, 2H), 6.30 (s, 1H), 5.28 (d, $J = 11.0$ Hz, 1H), 4.29 – 4.23 (m, 1H), 3.34 – 3.30 (m, 2H), 1.87 (d, $J = 1.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.20, 169.13, 168.68, 152.86, 152.83, 137.45, 136.99, 135.84, 135.74, 135.38, 132.96, 130.50, 128.70, 128.57, 128.45, 128.24, 127.83, 126.26, 126.09, 125.48, 125.24, 123.33, 123.24, 121.76, 121.61, 53.23, 51.67, 41.08, 15.10.

(E)-1,5-Diphenyl-6,6-di(quinolin-2-yl)hex-2-en-1-one (24)



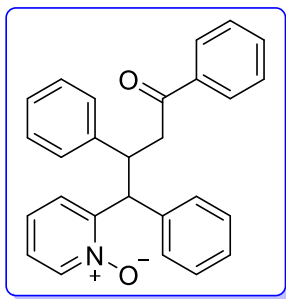
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.16 (d, J = 8.6 Hz, 1H), 8.11 (d, J = 8.5 Hz, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.95 – 7.91 (m, 3H), 7.76 – 7.60 (m, 6H), 7.50 (t, J = 7.3 Hz, 2H), 7.45 – 7.38 (m, 3H), 7.12 – 7.02 (m, 5H), 6.29 (d, J = 15.9 Hz, 1H), 6.18 (dd, J = 15.9, 8.7 Hz, 1H), 4.87 (d, J = 10.6 Hz, 1H), 4.62 – 4.56 (m, 1H), 3.28 – 3.12 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.17, 161.08, 160.96, 147.89, 147.76, 137.30, 137.17, 136.57, 136.21, 132.77, 132.03, 131.00, 129.47, 129.27, 129.23, 129.19, 128.40, 128.34, 128.15, 127.61, 127.49, 127.15, 127.03, 126.88, 126.27, 126.14, 126.04, 122.48, 121.88, 62.22, 43.09, 43.04.

Synthesis and characterization of Pyridine N-Oxide-substituted ketone (5)



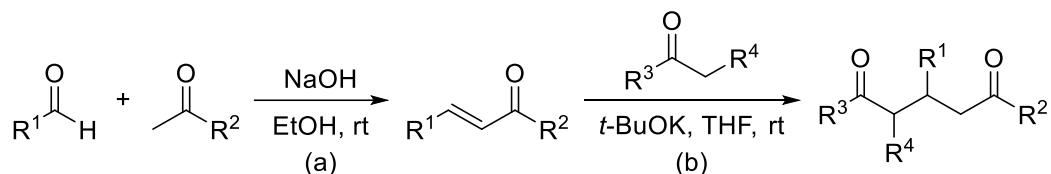
General procedures: (a) To a stirred solution of 2-benzylpyridine (5.0 mmol) in THF (15 mL) at room temperature was added $t\text{-BuOK}$ (5.0 mmol). Then, (*E*)-chalcone (5.0 mmol) was added to the reaction mixture in one portion. The reaction mixture was extracted with ethyl acetate. The organic layer was washed with brine, dried over anhydrous Na_2SO_4 , further purified on silica gel chromatography to afford 1,3,4-triphenyl-4-(pyridin-2-yl)butan-1-one. (b) To a stirred solution of 1,3,4-triphenyl-4-(pyridin-2-yl)butan-1-one (2.0 mmol) in DCM (10 mL) at 0 °C was slowly added *m*-chloroperbenzoic acid (2.4 mmol, 1.2 equiv). The mixture was quenched by saturated Na_2SO_3 and extracted with DCM (3×10 mL), the organic layer was washed with brine, dried over anhydrous Na_2SO_4 , further purified on silica gel chromatography to afford the targeted ketone.

2-(4-Oxo-1,2,4-triphenylbutyl)pyridine 1-oxide (5)



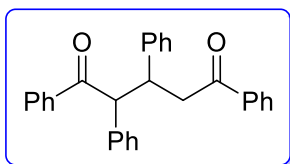
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.02 (d, J = 6.4 Hz, 1H), 7.65 (dd, J = 17.1, 7.5 Hz, 4H), 7.47 – 7.43 (m, 2H), 7.38 – 7.30 (m, 6H), 7.21 (t, J = 7.3 Hz, 1H), 7.14 (t, J = 7.6 Hz, 2H), 7.01 (t, J = 7.9 Hz, 2H), 6.88 – 6.85 (m, 1H), 5.71 (d, J = 12.9 Hz, 1H), 4.43 – 4.37 (m, 1H), 3.41 (dd, J = 16.9, 9.9 Hz, 1H), 3.10 (dd, J = 16.8, 2.6 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.49, 153.14, 142.13, 139.38, 139.22, 137.02, 132.91, 128.99, 128.93, 128.52, 128.39, 127.98, 127.91, 127.48, 126.69, 125.06, 124.97, 123.01, 47.04, 44.86, 43.67. HRMS: for $[\text{M}+\text{H}]^+$ calcd. 394.1802, found: 394.1792.

2.2 General procedures for the synthesis of 1,5-diketone substrates (6 - 9)



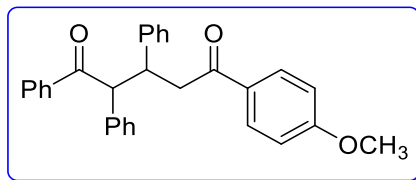
General procedures: (a) Corresponding benzaldehyde (10.0 mmol) was dissolved in ethanol (20 mL). Then aqueous NaOH (2.0 equiv) was added dropwise followed by slow addition of the corresponding ketone (10.0 mmol). The mixture was stirred at room temperature until the complete consumption of the starting materials (monitored by TLC). The reaction mixture was diluted with water. The precipitate was collected by filtration and washed with water and EtOH in sequence. (b) To a well stirred solution of carbonyl compounds (5.0 mmol) and THF (10 mL) at room temperature was added *t*-BuOK (5.0 mmol). Then, α,β -unsaturated ketone (5.0 mmol) was added to the reaction mixture in one portion. After completion of the reaction, the reaction was quenched by addition of saturated NH_4Cl solution and extracted with CH_2Cl_2 . The combined organic extracts were washed with brine, dried over anhydrous Na_2SO_4 , filtered, concentrated and purified on silica gel chromatography to afford the corresponding compounds.

1,2,3,5-Tetraphenylpentane-1,5-dione (6a)



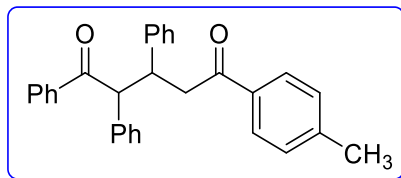
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.80 (d, $J = 7.5$ Hz, 2H), 7.65 (d, $J = 7.4$ Hz, 2H), 7.51 (d, $J = 7.3$ Hz, 2H), 7.48 – 7.40 (m, 2H), 7.35 – 7.29 (m, 7H), 7.26 – 7.22 (m, 2H), 7.16 (t, $J = 7.4$ Hz, 2H), 7.05 (t, $J = 7.4$ Hz, 1H), 7.05 (m, 2H), 5.16 (d, $J = 10.9$ Hz, 1H), 4.39 (t, $J = 10.3$ Hz, 1H), 3.24 – 3.06 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.70, 142.54, 137.23, 137.0, 132.71, 129.24, 129.16, 128.48, 128.47, 128.39, 128.36, 128.31, 128.25, 127.90, 127.78, 126.54, 58.67, 44.66, 42.84.

5-(4-Methoxyphenyl)-1,2,3-triphenylpentane-1,5-dione (6b)



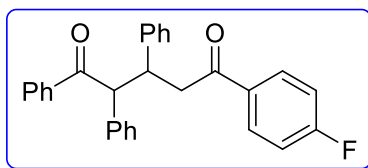
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.80 (d, $J = 7.4$ Hz, 2H), 7.65 (d, $J = 8.5$ Hz, 2H), 7.52 (d, $J = 7.1$ Hz, 2H), 7.41 – 7.22 (m, 9H), 7.16 (t, $J = 7.3$ Hz, 2H), 7.08 – 7.00 (m, 1H), 6.81 (d, $J = 8.5$ Hz, 2H), 5.17 (d, $J = 10.8$ Hz, 1H), 4.40 – 4.35 (m, 1H), 3.85 – 3.81 (m, 3H), 3.18 – 3.00 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.81, 197.24, 163.23, 142.65, 137.29, 137.17, 132.72, 130.36, 130.22, 129.28, 129.17, 128.42, 128.32, 128.28, 127.77, 126.52, 113.54, 58.71, 55.44, 44.90, 42.47.

1,2,3-Triphenyl-5-(*p*-tolyl)pentane-1,5-dione (6c)



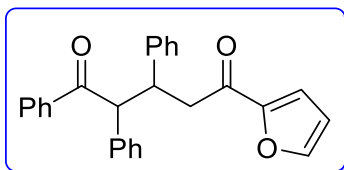
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.82 (d, $J = 7.8$ Hz, 2H), 7.55 (dd, $J = 16.5, 7.7$ Hz, 4H), 7.43 (t, $J = 8.0$ Hz, 1H), 7.37 – 7.30 (m, 6H), 7.28 – 7.24 (m, 1H), 7.19 – 7.10 (m, 4H), 7.06 (t, $J = 8.0$ Hz, 1H), 5.19 (d, $J = 10.9$ Hz, 1H), 4.42 – 4.36 (m, 1H), 3.22 – 3.04 (m, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.78, 198.36, 143.48, 142.61, 137.28, 137.15, 134.79, 132.72, 129.27, 129.17, 129.07, 128.42, 128.33, 128.28, 128.07, 127.78, 126.53, 58.69, 44.79, 42.75, 21.58.

5-(4-Fluorophenyl)-1,2,3-triphenylpentane-1,5-dione (6d)



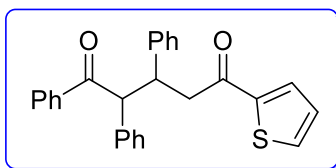
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.81 – 7.79 (m, 2H), 7.70 – 7.65 (m, 2H), 7.52 – 7.50 (m, 2H), 7.44 – 7.39 (m, 1H), 7.36 – 7.29 (m, 6H), 7.26 – 7.23 (m, 1H), 7.19 – 7.15 (m, 2H), 7.09 – 6.97 (m, 3H), 5.16 (d, J = 10.8 Hz, 1H), 4.37 (td, J = 10.3, 3.9 Hz, 1H), 3.20 – 3.03 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.46, 197.03, 165.34 (d, J = 253.3 Hz), 142.27, 136.94, 136.82, 133.44, 133.41, 132.67, 130.44 (d, J = 9.1 Hz), 129.08, 128.30, 128.25, 128.19, 128.05, 127.71, 126.50, 115.31 (d, J = 21.0 Hz), 58.48, 44.57, 42.58.

5-(Furan-2-yl)-1,2,3-triphenylpentane-1,5-dione (6e)



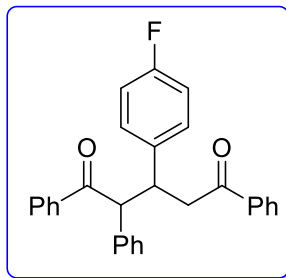
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.82 (d, J = 7.4 Hz, 2H), 7.53 (d, J = 6.8 Hz, 2H), 7.44 – 7.40 (m, 2H), 7.33 – 7.22 (m, 7H), 7.17 (t, J = 6.9 Hz, 2H), 7.06 (t, J = 6.7 Hz, 1H), 6.91 (s, 1H), 6.39 (s, 1H), 5.18 (d, J = 10.9 Hz, 1H), 4.42 – 4.38 (t, J = 8.3 Hz, 1H), 3.12 – 2.89 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.61, 187.67, 152.83, 145.95, 142.34, 137.17, 136.96, 132.74, 129.26, 129.11, 128.41, 128.33, 128.20, 127.76, 126.58, 116.72, 112.05, 58.54, 44.57, 42.63.

1,2,3-Triphenyl-5-(thiophen-2-yl)pentane-1,5-dione (6f)



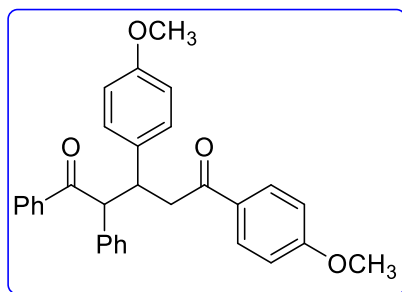
White solid. ^1H NMR (400 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 8.05 (d, J = 7.6 Hz, 0.98H, minor isomer), 7.84 (d, J = 7.6 Hz, 1.02H), 7.81 (d, J = 3.8 Hz, 0.51H, major isomer), 7.58 (d, J = 4.9 Hz, 0.49H, minor isomer), 7.53 (t, J = 7.0 Hz, 2H), 7.46 – 7.42 (m, 2H), 7.37 – 7.24 (m, 4H), 7.18 (t, J = 7.6 Hz, 1H), 7.13 – 7.00 (m, 6H), 5.22 (d, J = 10.9 Hz, 0.51H, major isomer), 5.05 (d, J = 10.4 Hz, 0.49H, minor isomer), 4.40 (td, J = 10.4, 4.0 Hz, 0.51H, major isomer), 4.27 (td, J = 10.0, 3.9 Hz, 0.49H, minor isomer), 3.49 – 3.34 (m, 0.98H, minor isomer), 3.15 – 3.00 (m, 1.02H, major isomer). Ratio of diastereoisomers (major to minor): 1.0; ^{13}C NMR (100 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 199.45, 191.35, 144.47, 142.29, 140.73, 137.06, 136.88, 133.48, 133.36, 133.14, 132.76, 132.15, 131.61, 129.22, 129.17, 128.94, 128.72, 128.64, 128.48, 128.40, 128.35, 128.31, 128.17, 128.03, 127.83, 127.79, 127.03, 126.60, 126.47, 58.97, 58.31, 46.14, 45.02, 44.11, 43.51. Ratio of diastereoisomers (major to minor): 1.0.

3-(4-Fluorophenyl)-1,2,5-triphenylpentane-1,5-dione (6g)



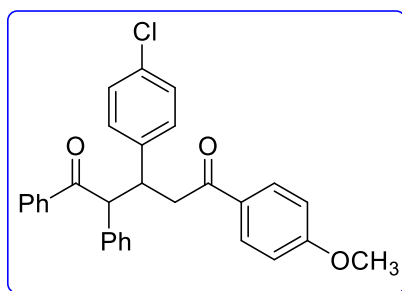
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.83 (d, $J = 7.8$ Hz, 2H), 7.68 (d, $J = 7.9$ Hz, 2H), 7.54 – 7.44 (m, 4H), 7.39 – 7.26 (m, 9H), 6.88 (t, $J = 8.3$ Hz, 2H), 5.14 (d, $J = 10.8$ Hz, 1H), 4.43 – 4.37 (m, 1H), 3.24 – 3.07 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.60, 162.41 (d, $J = 243.4$ Hz), 138.30, 137.08, 136.90, 132.91, 129.78 (d, $J = 8.0$ Hz), 129.27, 129.16, 128.50, 128.46, 128.31, 127.92, 127.89, 115.18 (d, $J = 21.0$ Hz), 58.78, 43.95, 42.79.

3,5-Bis(4-methoxyphenyl)-1,2-diphenylpentane-1,5-dione (6h)



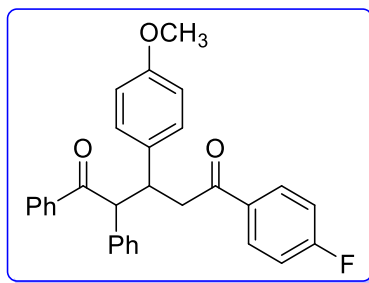
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.82 (d, $J = 7.7$ Hz, 2H), 7.67 (d, $J = 8.5$ Hz, 2H), 7.52 (d, $J = 7.4$ Hz, 2H), 7.44 – 7.41 (m, 1H), 7.36 – 7.24 (m, 7H), 6.82 (d, $J = 8.3$ Hz, 2H), 6.70 (d, $J = 8.2$ Hz, 2H), 5.13 (d, $J = 10.7$ Hz, 1H), 4.33 (t, $J = 8.7$ Hz, 1H), 3.83 (s, 3H), 3.68 (s, 3H), 3.15 – 2.98 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.91, 197.42, 163.19, 157.97, 137.24, 134.59, 132.72, 130.32, 130.22, 129.19, 129.13, 128.41, 128.33, 127.72, 113.71, 113.51, 58.90, 55.41, 55.05, 44.13, 42.57.

3-(4-Chlorophenyl)-5-(4-methoxyphenyl)-1,2-diphenylpentane-1,5-dione (6i)



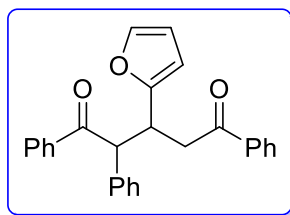
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.80 (d, $J = 7.7$ Hz, 2H), 7.64 (d, $J = 8.6$ Hz, 2H), 7.48 (d, $J = 7.5$ Hz, 2H), 7.42 (t, $J = 7.2$ Hz, 1H), 7.34 – 7.22 (m, 7H), 7.12 (d, $J = 8.2$ Hz, 2H), 6.81 (d, $J = 8.6$ Hz, 2H), 5.11 (d, $J = 10.8$ Hz, 1H), 4.33 (td, $J = 10.4, 3.4$ Hz, 1H), 3.80 (s, 3H), 3.14 – 3.06 (m, 1H), 3.02 – 2.97 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.43, 196.88, 163.35, 141.27, 137.01, 136.84, 132.90, 132.13, 130.16, 129.67, 129.23, 129.14, 128.49, 128.43, 128.33, 127.87, 113.59, 58.55, 55.43, 44.17, 42.19.

5-(4-Fluorophenyl)-3-(4-methoxyphenyl)-1,2-diphenylpentane-1,5-dione (6j)



White solid. ^1H NMR (400MHz, CDCl_3) δ (ppm) 7.81 (dd, $J = 8.2, 2.0$ Hz, 2H), 7.70 – 7.66 (m, 2H), 7.51 – 7.48 (m, 2H), 7.44 – 7.40 (m, 1H), 7.32 (q, $J = 7.7$ Hz, 4H), 7.26 – 7.21 (m, 3H), 7.00 (t, $J = 8.6$ Hz, 2H), 6.70 (dd, $J = 8.6, 1.8$ Hz, 2H), 5.10 (dd, $J = 10.8, 5.8$ Hz, 1H), 4.36 – 4.28 (m, 1H), 3.68 – 3.67 (m, 3H), 3.16 – 2.99 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 198.60, 197.23, 165.34 (d, $J = 253.0$ Hz), 157.90, 136.9 (d, $J = 4.5$ Hz), 134.20, 132.66, 130.46 (d, $J = 9.4$ Hz), 129.05, 129.00, 128.30, 128.20, 127.67, 115.42 (d, $J = 21.8$ Hz), 113.62, 58.72, 54.94, 43.84, 42.71.

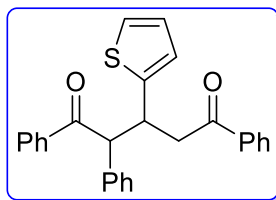
3-(Furan-2-yl)-1,2,5-triphenylpentane-1,5-dione (6k)



Gray solid. ^1H NMR (400 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 8.05 (d, $J = 7.7$ Hz, 0.9H, minor isomer), 7.95 – 7.92 (m, 2H), 7.76 (d, $J = 7.6$ Hz, 1.1H, major isomer), 7.56 – 7.22 (m, 9H), 7.18 – 7.13 (m, 3H), 6.14 (s, 0.55H, major isomer), 6.07 – 6.03 (m, 1H), 5.72 (s, 0.45H, minor isomer), 5.28 (d, $J = 10.4$ Hz, 0.55H, major isomer), 5.17 (d, $J = 10.1$ Hz, 0.45H, minor isomer), 4.54 (td, $J = 9.9, 3.1$ Hz, 0.55H, major isomer), 4.38 (td, $J = 9.7, 3.2$ Hz, 0.45H, minor isomer), 3.52 (dd, $J = 15.6, 10.0$ Hz, 0.45H, minor isomer), 3.36 (dd, $J = 15.8, 3.2$ Hz, 0.45H, minor isomer), 3.23 (dd, $J = 16.4, 9.6$ Hz, 0.55H, major isomer), 3.07 (dd, $J = 16.4, 3.2$ Hz, 0.55H, major isomer). Ratio of diastereoisomers (major to minor): 1.2; ^{13}C NMR (100 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 198.81, 198.74, 198.43, 198.15, 155.11, 154.00, 141.00, 140.93, 137.04, 136.98, 136.83, 136.79, 136.42, 133.19, 132.94, 132.88, 132.87, 129.14, 128.80, 128.64, 128.62, 128.51, 128.47, 128.41,

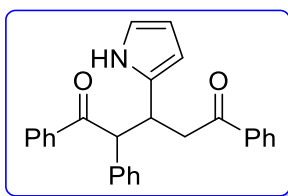
128.20, 127.93, 127.80, 127.26, 110.29, 109.96, 107.62, 107.11, 57.05, 56.00, 41.23, 39.88, 39.35, 37.96. Ratio of diastereoisomers (major to minor): 1.2.

1,2,5-Triphenyl-3-(thiophen-2-yl)pentane-1,5-dione (6l)



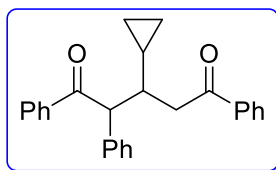
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.91 (d, $J = 7.7$ Hz, 2H), 7.73 (d, $J = 7.7$ Hz, 2H), 7.50 – 7.44 (m, 4H), 7.39 – 7.31 (m, 6H), 7.28 – 7.22 (m, 1H), 7.01 (d, $J = 5.1$ Hz, 1H), 6.93 (d, $J = 3.6$ Hz, 1H), 6.79 – 6.77 (m, 1H), 5.24 (d, $J = 10.7$ Hz, 1H), 4.78 (td, $J = 10.0, 3.9$ Hz, 1H), 3.23 (dd, $J = 16.5, 9.5$ Hz, 1H), 3.14 – 3.09 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.47, 198.36, 145.99, 137.18, 137.04, 136.75, 132.86, 129.20, 129.12, 128.47, 128.42, 127.92, 127.87, 126.57, 125.87, 123.32, 59.36, 43.46, 39.90.

1,2,5-Triphenyl-3-(1H-pyrrol-2-yl)pentane-1,5-dione (6m)



Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.89 (s, 1H), 7.91 (d, $J = 7.3$ Hz, 2H), 7.75 (d, $J = 7.2$ Hz, 2H), 7.51 – 7.34 (m, 8H), 7.30 – 7.26 (m, 2H), 7.19 (t, $J = 7.3$ Hz, 1H), 6.57 – 6.56 (m, 1H), 5.93 (q, $J = 2.8$ Hz, 1H), 5.86 (s, 1H), 5.20 (d, $J = 10.8$ Hz, 1H), 4.45 (td, $J = 10.7, 3.3$ Hz, 1H), 3.31 (dd, $J = 17.7, 9.3$ Hz, 1H), 3.01 (dd, $J = 17.7, 3.3$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.81, 199.33, 137.01, 136.86, 136.81, 133.36, 132.96, 132.80, 129.08, 128.81, 128.41, 128.36, 127.76, 127.60, 116.50, 107.48, 104.49, 57.45, 42.10, 36.93.

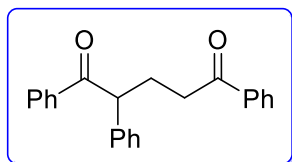
3-Cyclopropyl-1,2,5-triphenylpentane-1,5-dione (6n)



White solid. ^1H NMR (400 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 8.01 (dd, $J = 14.4, 7.9$ Hz, 4H), 7.55 – 7.51 (m, 1H), 7.49 – 7.34 (m, 7H), 7.26 (t, $J = 7.3$ Hz, 2H), 7.22 – 7.18 (m, 1H), 5.05 (d, $J = 8.5$ Hz, 1H), 3.32 – 3.27 (m, 1H), 3.16 – 3.10 (m, 1H), 2.23 – 2.16 (m, 1H), 0.82 – 0.73 (m, 1H), 0.29 – 0.22 (m, 1H), 0.09 – 0.01 (m, 1H), -0.06 – -0.12 (m, 1H), -0.37 – -0.44 (m, 1H). Ratio of diastereoisomers (major to minor): 1.0; ^{13}C NMR (100 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 200.84, 200.54, 200.39, 199.97,

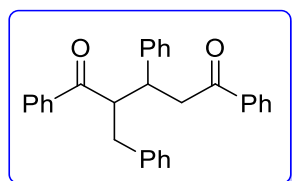
137.76, 137.73, 137.67, 137.47, 137.40, 137.10, 132.89, 132.87, 132.83, 132.75, 129.40, 129.23, 128.76, 128.74, 128.60, 128.57, 128.54, 128.52, 128.46, 128.27, 128.22, 128.05, 127.30, 127.14, 57.81, 57.01, 44.58, 44.11, 42.59, 41.82, 15.60, 14.63, 6.23, 5.91, 4.56, 3.74. Ratio of diastereoisomers (major to minor): 1.1.

1,2,5-Triphenylpentane-1,5-dione (6o)



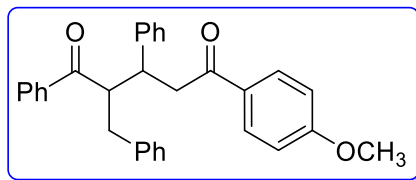
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) δ 7.99 – 7.97 (m, 2H), 7.91 – 7.89 (m, 2H), 7.56 – 7.36 (m, 6H), 7.33 – 7.27 (m, 4H), 7.25 – 7.18 (m, 1H), 4.78 (t, J = 7.3 Hz, 1H), 3.06 – 2.89 (m, 2H), 2.63 – 2.55 (m, 1H), 2.33 – 2.24 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.93, 199.65, 139.18, 136.86, 136.68, 133.07, 132.96, 129.08, 128.81, 128.59, 128.55, 128.36, 128.06, 127.26, 52.48, 36.01, 28.34.

2-Benzyl-1,3,5-triphenylpentane-1,5-dione (6p)



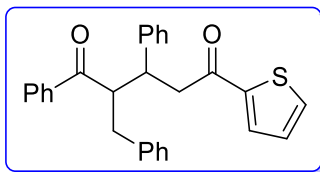
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.89 – 7.86 (m, 2H), 7.64 – 7.61 (m, 2H), 7.57 – 7.53 (m, 1H), 7.45 – 7.40 (m, 3H), 7.31 – 7.29 (m, 1H), 7.28 – 7.27 (m, 2H), 7.26 – 7.24 (m, 2H), 7.23 – 7.21 (m, 1H), 7.17 – 7.12 (m, 3H), 7.09 – 7.05 (m, 3H), 4.23 – 4.18 (m, 1H), 4.00 – 3.95 (m, 1H), 3.62 – 3.48 (m, 2H), 3.29 (dd, J = 13.3, 10.8 Hz, 1H), 2.97 (dd, J = 13.3, 3.3 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 202.92, 198.18, 142.01, 139.73, 138.06, 137.05, 133.05, 132.65, 128.94, 128.55, 128.47, 128.38, 128.10, 128.00, 127.92, 126.79, 126.13, 54.17, 42.91, 39.64, 34.55.

2-Benzyl-5-(4-methoxyphenyl)-1,3-diphenylpentane-1,5-dione (6q)



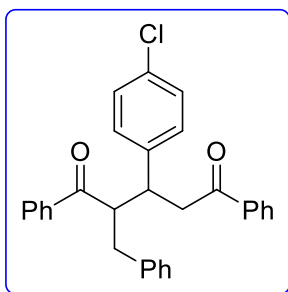
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.82 (d, J = 8.7 Hz, 2H), 7.72 (d, J = 7.9 Hz, 2H), 7.47 (t, J = 7.2 Hz, 1H), 7.35 – 7.20 (m, 7H), 7.12 – 6.98 (m, 5H), 6.90 (d, J = 8.7 Hz, 2H), 4.24 – 4.19 (m, 1H), 3.93 – 3.88 (m, 1H), 3.87 (s, 3H), 3.36 – 3.24 (m, 2H), 3.00 – 2.94 (m, 1H), 2.77 (dd, J = 13.3, 3.5 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 204.25, 196.76, 163.37, 141.57, 139.36, 138.50, 132.87, 130.40, 130.02, 128.91, 128.57, 128.41, 128.34, 128.27, 128.21, 126.99, 126.12, 113.67, 55.45, 53.59, 44.94, 42.28, 37.44.

2-Benzyl-1,3-diphenyl-5-(thiophen-2-yl)pentane-1,5-dione (6r)



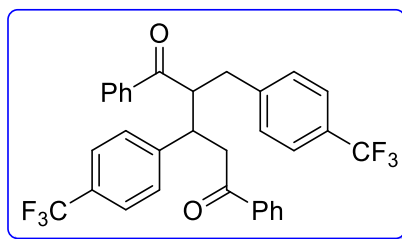
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.74 (d, $J = 7.2$ Hz, 2H), 7.64 (s, 1H), 7.57 (d, $J = 4.5$ Hz, 1H), 7.48 (t, $J = 6.7$ Hz, 1H), 7.36 – 7.23 (m, 7H), 7.11 – 6.99 (m, 6H), 4.27 – 4.23 (m, 1H), 3.93 – 3.90 (m, 1H), 3.34 – 3.23 (m, 2H), 3.01 – 2.95 (m, 1H), 2.81 – 2.78 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 204.11, 191.07, 144.29, 141.26, 139.26, 138.42, 133.68, 132.97, 132.06, 128.94, 128.67, 128.47, 128.35, 128.31, 128.25, 128.09, 127.15, 126.19, 53.34, 45.06, 43.35, 37.47.

2-Benzyl-3-(4-chlorophenyl)-1,5-diphenylpentane-1,5-dione (6s)



White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.81 (d, $J = 7.6$ Hz, 2H), 7.72 (d, $J = 7.7$ Hz, 2H), 7.55 (t, $J = 7.3$ Hz, 1H), 7.49 (t, $J = 7.3$ Hz, 1H), 7.43 (t, $J = 7.6$ Hz, 2H), 7.35 (t, $J = 7.7$ Hz, 2H), 7.29 – 7.26 (m, 2H), 7.20 (d, $J = 8.4$ Hz, 2H), 7.13 – 7.04 (m, 3H), 6.98 (d, $J = 7.2$ Hz, 2H), 4.18 (td, $J = 9.8, 4.0$ Hz, 1H), 3.92 – 3.87 (m, 1H), 3.39 – 3.28 (m, 2H), 2.97 (dd, $J = 13.3, 10.2$ Hz, 1H), 2.74 (dd, $J = 13.4, 3.9$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 203.89, 197.92, 140.13, 138.97, 138.27, 136.74, 133.13, 133.07, 132.71, 129.70, 128.87, 128.77, 128.60, 128.51, 128.36, 128.20, 128.05, 126.27, 53.33, 43.97, 42.39, 37.49.

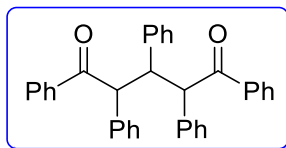
1,5-Diphenyl-2-(4-(trifluoromethyl)benzyl)-3-(4-(trifluoromethyl)phenyl)pentane-1,5-dione (6t)



White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.80 (d, $J = 7.4$ Hz, 2H), 7.71 (d, $J = 7.5$ Hz, 2H), 7.55 – 7.48 (m, 4H), 7.41 (t, $J = 7.7$ Hz, 2H), 7.34 (t, $J = 7.9$ Hz, 6H), 7.06 (d, $J = 8.0$ Hz, 2H), 4.26 – 4.20 (m, 1H), 3.99 (q, $J = 7.6$ Hz, 1H), 3.39 (d, $J = 7.0$ Hz, 2H), 3.02 (dd, $J = 13.4, 10.2$ Hz, 1H), 2.76 (dd, $J = 13.4, 3.9$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 202.66, 197.41, 145.33, 142.88, 137.63, 136.39, 133.35, 133.23, 129.08,

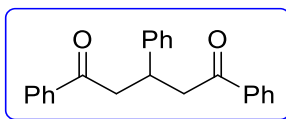
128.61, 128.55, 128.37, 128.02, 127.86, 125.48(d, $J = 3.97$ Hz), 125.46, 125.16, 125.12, 52.36, 43.97, 41.87, 36.79.

1,2,3,4,5-Pentaphenylpentane-1,5-dione (6u)



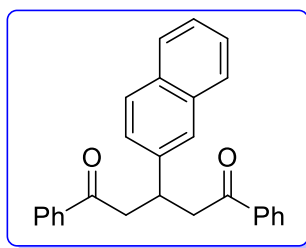
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.73 (d, $J = 7.7$ Hz, 2H), 7.63 (d, $J = 7.7$ Hz, 2H), 7.45 (d, $J = 7.4$ Hz, 2H), 7.40 – 7.33 (m, 2H), 7.24 (t, $J = 7.5$ Hz, 4H), 7.15 – 7.11 (m, 4H), 7.07 – 6.98 (m, 8H), 6.94 – 6.91 (m, 1H), 5.26 (d, $J = 10.5$ Hz, 1H), 5.09 (d, $J = 7.5$ Hz, 1H), 4.91 (dd, $J = 10.3, 7.7$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 198.55, 198.31, 140.38, 137.18, 136.78, 136.54, 136.29, 132.54, 132.41, 130.35, 130.20, 129.95, 128.77, 128.34, 128.29, 128.20, 127.99, 127.71, 127.45, 126.71, 126.07, 58.78, 56.01, 50.85.

1,3,5-Triphenylpentane-1,5-dione (6v)

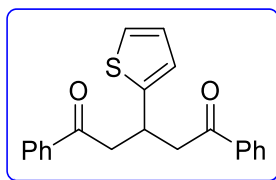


White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.96 – 7.94 (m, 4H), 7.57 – 7.53 (m, 2H), 7.47 – 7.43 (m, 4H), 7.29 – 7.26 (m, 4H), 7.21 – 7.16 (m, 1H), 4.12 – 4.04 (m, 1H), 3.53 – 3.47 (m, 2H), 3.40 – 3.33 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.58, 143.85, 136.98, 133.07, 128.63, 128.59, 128.15, 127.48, 126.70, 44.92, 37.22.

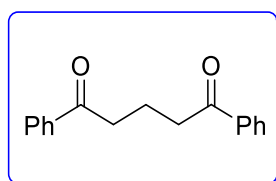
3-(Naphthalen-2-yl)-1,5-diphenylpentane-1,5-dione (6w)



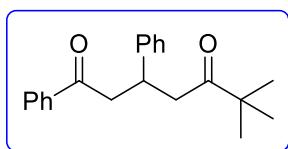
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.98 – 7.95 (m, 4H), 7.80 – 7.76 (m, 3H), 7.72 (s, 1H), 7.55 (t, $J = 7.4$ Hz, 2H), 7.49 – 7.40 (m, 7H), 4.27 (quint, $J = 7.0$ Hz, 1H), 3.59 (dd, $J = 16.7, 6.9$ Hz, 2H), 3.47 (dd, $J = 16.7, 7.1$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.52, 141.35, 136.92, 133.53, 133.14, 132.44, 128.63, 128.39, 128.18, 127.76, 127.63, 126.02, 125.94, 125.55, 44.95, 37.27.

1,5-Diphenyl-3-(thiophen-2-yl)pentane-1,5-dione (6x)

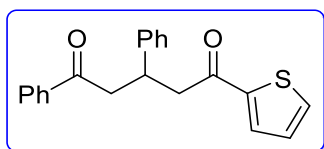
Brown solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.97 (d, $J = 7.4$ Hz, 4H), 7.56 (t, $J = 7.4$ Hz, 2H), 7.46 (t, $J = 7.4$ Hz, 4H), 7.11 (d, $J = 4.1$ Hz, 1H), 6.89 – 6.87 (m, 2H), 4.47 – 4.40 (m, 1H), 3.53 (dd, $J = 16.9, 6.8$ Hz, 2H), 3.43 (dd, $J = 16.9, 6.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.08, 147.47, 136.78, 133.17, 128.61, 128.12, 126.71, 124.26, 123.32, 45.58, 32.39.

1,5-Diphenylpentane-1,5-dione (6y)

White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.98 (d, $J = 7.4$ Hz, 4H), 7.55 (t, $J = 7.3$ Hz, 2H), 7.45 (t, $J = 7.6$ Hz, 4H), 3.12 (t, $J = 6.9$ Hz, 4H), 2.21 (dd, $J = 13.9, 6.9$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.86, 136.88, 133.08, 128.62, 128.08, 37.61, 18.75.

6,6-Dimethyl-1,3-diphenylheptane-1,5-dione (6z)

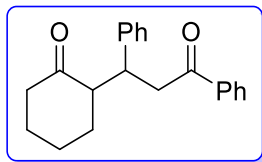
Yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.97 – 7.94 (m, 2H), 7.56 (tt, $J = 8.0, 2.0$ Hz, 2H), 7.48 – 7.44 (m, 2H), 7.31 – 7.25 (m, 4H), 7.22 – 7.17 (m, 1H), 3.98 – 3.91 (m, 1H), 3.44 – 3.38 (m, 1H), 3.32 – 3.27 (m, 1H), 2.96 (d, $J = 6.9$ Hz, 2H), 1.08 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 213.86, 198.58, 143.95, 136.80, 132.90, 128.46, 128.39, 128.04, 127.39, 126.45, 44.50, 44.01, 42.83, 36.62, 26.04.

1,3-Diphenyl-5-(thiophen-2-yl)pentane-1,5-dione (6aa)

Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.94 (d, $J = 7.8$ Hz, 2H), 7.76 (d, $J = 3.7$ Hz, 1H), 7.60 (d, $J = 4.9$ Hz, 1H), 7.55 (t, $J = 7.3$ Hz, 1H), 7.44 (t, $J = 7.6$ Hz, 2H), 7.29 – 7.26 (m, 4H), 7.22 – 7.17 (m, 1H), 7.11 (t, $J = 4.3$ Hz, 1H), 4.10 – 4.03 (m, 1H), 3.55 – 3.49 (m, 1H), 3.45 – 3.34 (td, 2H), 3.31 – 3.25 (m, 1H); ^{13}C NMR

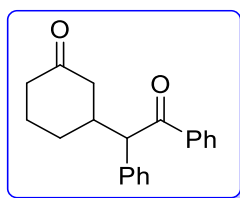
(100 MHz, CDCl₃) δ (ppm) 198.50, 191.49, 144.34, 143.53, 136.92, 133.70, 133.12, 132.14, 128.66, 128.61, 128.15, 127.47, 126.79, 45.64, 44.67, 37.59.

2-(3-Oxo-1,3-diphenylpropyl)cyclohexan-1-one (7a)



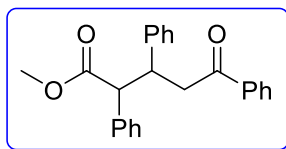
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.93 (d, J = 7.5 Hz, 2H), 7.53 (t, J = 7.3 Hz, 1H), 7.43 (t, J = 7.6 Hz, 2H), 7.30 – 7.17 (m, 5H), 3.76 (td, J = 9.7, 4.0 Hz, 1H), 3.52 (dd, J = 16.2, 4.0 Hz, 1H), 3.26 (dd, J = 16.2, 9.5 Hz, 1H), 2.76 (td, J = 10.0, 5.1 Hz, 1H), 2.57 – 2.51 (m, 1H), 2.45 – 2.38 (m, 1H), 2.02 – 1.98 (m, 1H), 1.83 – 1.52 (m, 4H), 1.33 – 1.24 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 213.58, 198.79, 142.06, 137.09, 132.80, 128.48, 128.45, 128.37, 128.17, 126.61, 55.83, 44.23, 42.32, 41.14, 32.45, 28.53, 24.12.

3-(2-Oxo-1,2-diphenylethyl)cyclohexan-1-one (7b)



White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.95 (dd, J = 15.8, 7.5 Hz, 2H), 7.49 (q, J = 7.5 Hz, 1H), 7.39 (q, J = 7.8 Hz, 2H), 7.34 – 7.19 (m, 5H), 4.43 (d, J = 9.6 Hz, 1H), 2.85 – 2.74 (m, 1H), 2.60 – 2.56 (m, 1H), 2.39 – 2.36 (m, 0.50H), 2.29 – 2.21 (m, 1H), 2.13 – 1.90 (m, 3H), 1.75 – 1.68 (m, 0.50H), 1.63 – 1.60 (m, 1H), 1.46 – 1.22 (m, 1H). Ratio of diastereoisomers (major to minor): 1.0; ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 210.97, 210.43, 199.04, 198.80, 137.09, 136.93, 136.36, 133.12, 133.07, 129.10, 129.00, 128.79, 128.63, 128.59, 128.53, 127.59, 127.49, 59.29, 58.92, 46.78, 45.52, 41.64, 41.49, 41.45, 41.33, 30.51, 28.52, 24.87, 24.55. Ratio of diastereoisomers (major to minor): 1.0.

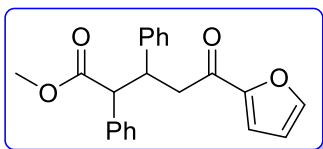
Methyl 5-oxo-2,3,5-triphenylpentanoate (8a)



White solid. ¹H NMR (400 MHz, CDCl₃) major + minor diastereoisomers δ (ppm) 7.91 – 7.89 (m, 1.33H, major isomer), 7.69 – 7.64 (m, 0.67H, minor isomer), 7.54 (t, J = 7.8 Hz, 1H), 7.48 – 7.26 (m, 5H), 7.20 – 7.00 (m, 7H), 4.23 – 4.11 (m, 1H), 4.03 – 3.98 (m, 1H), 3.70 (s, 2H, major isomer), 3.56 (dd, J = 16.2, 9.6 Hz, 0.67H, major isomer), 3.42 (dd, J = 16.2, 4.1 Hz, 0.67H, major isomer), 3.39 (s, 1H, minor isomer), 3.26 (dd, J = 16.6,

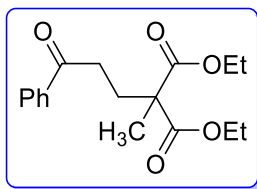
10.3 Hz, 0.33H, minor isomer), 2.96 (dd, $J = 16.6, 3.3$ Hz, 0.33H, minor isomer). Ratio of diastereoisomers (major to minor): 2.0; ^{13}C NMR (100 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 198.11, 197.94, 173.60, 172.74, 141.76, 140.66, 136.92, 136.84, 136.71, 132.96, 132.82, 128.95, 128.77, 128.63, 128.52, 128.36, 128.24, 128.10, 127.84, 127.22, 126.89, 126.51, 57.98, 57.49, 52.17, 51.77, 45.04, 44.51, 43.28, 42.53. Ratio of diastereoisomers (major to minor): 2.0.

Methyl 5-(furan-2-yl)-5-oxo-2,3-diphenylpentanoate (8b)



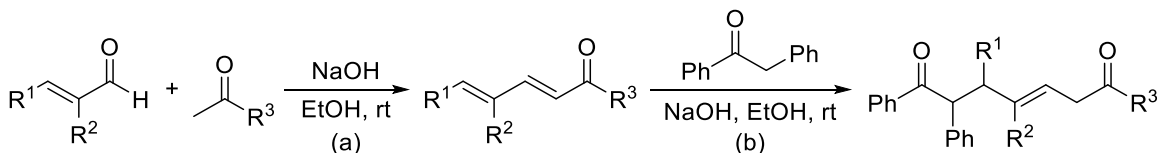
Yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.53 (d, $J = 7.9$ Hz, 2H), 7.42 (s, 1H), 7.38 – 7.35 (m, 4H), 7.31 – 7.24 (m, 3H), 7.18 – 7.14 (m, 1H), 6.90 (d, $J = 3.5$ Hz, 1H), 6.38 – 6.37 (m, 1H), 4.16 (td, $J = 11.6, 3.6$ Hz, 1H), 3.99 (d, $J = 11.7$ Hz, 1H), 3.38 (s, 3H), 3.10 (dd, $J = 16.2, 10.3$ Hz, 1H), 2.78 (dd, $J = 16.1, 3.7$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 187.20, 172.73, 152.70, 146.05, 141.56, 136.76, 128.93, 128.83, 128.40, 128.15, 128.01, 126.97, 116.79, 112.11, 57.96, 51.79, 44.42, 42.37.

Diethyl 2-methyl-2-(3-oxo-3-phenylpropyl)malonate (9)



Yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.94 (d, $J = 7.5$ Hz, 2H), 7.53 (t, $J = 7.3$ Hz, 1H), 7.43 (t, $J = 7.6$ Hz, 2H), 4.17 (qd, $J = 6.8, 1.6$ Hz, 4H), 3.02 (t, $J = 8.0$ Hz, 2H), 2.8 (t, $J = 8.0$ Hz, 2H), 1.46 (s, 3H), 1.22 (t, $J = 7.1$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.88, 171.93, 136.66, 133.03, 128.55, 127.98, 61.27, 52.97, 33.94, 30.00, 20.51, 13.98.

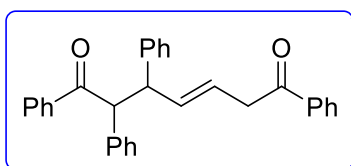
2.3 General procedures for the synthesis of unsaturated 1,7-diketone substrates (21)



General procedures: (a) To a mixture of ketone (10.0 mmol) and NaOH (2.0 equiv) in EtOH (20 mL) was added cinnamaldehyde (10.0 mmol). After stirring at room temperature for 2 h, the reaction mixture was diluted with water. The precipitate was collected by filtration and washed with water and EtOH. (b) To a solution of 2-

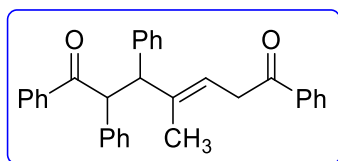
phenylacetophenone (5.0 mmol) in EtOH (20 mL) NaOH (5.0 mmol) was added. After stirring for 10 min, the conjugated dienone (5.0 mmol) was added. The resulting mixture was stirred for 3 h at room temperature and quenched with saturated NH₄Cl solution. Then, the mixture was extracted with ethyl acetate (3 × 30 mL). The organic phase was collected and dried with anhydrous Na₂SO₄, evaporated and purified by flash column chromatography to afford the target product.

(E)-1,5,6,7-Tetraphenylhept-2-ene-1,7-dione (21a)



White solid. ¹H NMR (400 MHz, CDCl₃) major + minor diastereoisomers δ (ppm) 8.11 – 8.09 (m, 0.42H, minor isomer), 8.05 – 8.03 (m, 2H), 7.86 – 7.84 (m, 1.58H, major isomer), 7.58 – 7.34 (m, 10H), 7.31 – 7.22 (m, 5H), 7.19 – 7.15 (m, 1H), 6.53 (d, *J* = 15.9 Hz, 0.79H, major isomer), 6.40 (dd, *J* = 15.9, 8.5 Hz, 0.79H, major isomer), 6.21 (d, *J* = 15.9 Hz, 0.21H, minor isomer), 6.13 (dd, *J* = 15.9, 8.2 Hz, 0.21H), 5.17 (d, *J* = 9.6 Hz, 0.79H, major isomer), 5.08 (d, *J* = 9.0 Hz, 0.21H), 4.02 – 3.88 (m, 1H), 3.42 (dd, *J* = 15.9, 4.3 Hz, 0.21H, minor isomer), 3.29 (dd, *J* = 15.9, 8.2 Hz, 0.21H, minor isomer), 3.16 (dd, *J* = 16.5, 3.9 Hz, 0.79H, major isomer), 3.03 (dd, *J* = 16.5, 8.3 Hz, 0.79H, major isomer). Ratio of diastereoisomers (major to minor): 3.8; ¹³C NMR (100 MHz, CDCl₃) major + minor diastereoisomers δ (ppm) 199.37, 199.09, 199.00, 137.13, 137.04, 136.98, 136.91, 132.99, 132.89, 132.80, 132.22, 131.92, 130.52, 129.97, 129.09, 129.02, 129.00, 128.71, 128.66, 128.45, 128.39, 128.16, 127.86, 127.53, 127.27, 127.06, 126.98, 126.18, 126.06, 57.36, 56.89, 42.70, 42.60, 42.19, 41.33. Ratio of diastereoisomers (major to minor): 3.8.

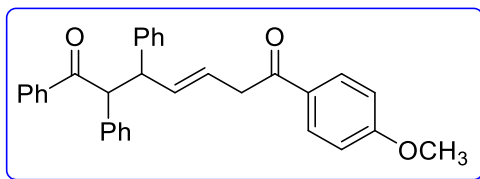
(E)-4-Methyl-1,5,6,7-tetraphenylhept-2-ene-1,7-dione (21b)



Yellow solid. ¹H NMR (400 MHz, CDCl₃) major + minor diastereoisomers δ (ppm) 8.13 – 8.10 (m, 2H), 8.04 – 8.00 (m, 1.04H), 7.80 – 7.76 (m, 0.96H), 7.62 – 7.50 (m, 4H), 7.48 – 7.38 (m, 5H), 7.31 – 7.24 (m, 2H), 7.22 – 7.18 (m, 2H), 7.17 – 7.10 (m, 1H), 6.98 (d, *J* = 7.4 Hz, 0.96H, minor isomer), 6.81 (d, *J* = 7.4 Hz, 1.04H, major isomer), 6.41 (s, 0.48H, minor isomer), 6.00 (s, 0.52H, major isomer), 5.07 (d, *J* = 10.8 Hz, 0.48H, minor isomer), 4.91 (d, *J* = 10.8 Hz, 0.52H, major isomer), 3.97 – 3.89 (m, 1H), 3.48 (dd, *J* = 14.1, 3.7 Hz, 0.52H, major isomer), 3.10 (dd, *J* = 14.0, 11.2 Hz, 0.48H, minor isomer), 3.02 (d, *J* = 7.2 Hz, 1H), 1.89 (s, 1.44H, minor isomer), 1.71 (s, 1.56H, major isomer). Ratio of diastereoisomers (major to minor): 1.1; ¹³C NMR (100 MHz, CDCl₃) major + minor diastereoisomers δ (ppm) 199.46, 199.26, 199.16, 198.91, 138.14, 137.75, 137.72, 137.32, 137.17,

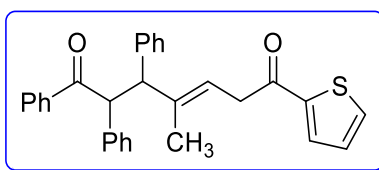
137.07, 136.98, 136.93, 136.90, 136.27, 133.18, 132.87, 132.83, 132.74, 129.47, 129.15, 129.07, 128.84, 128.73, 128.64, 128.62, 128.59, 128.56, 128.48, 128.44, 128.39, 128.27, 128.07, 127.98, 127.77, 127.74, 127.71, 127.25, 126.02, 125.94, 57.15, 56.63, 49.53, 48.64, 42.12, 41.09, 16.56, 15.31. Ratio of diastereoisomers (major to minor): 1.1.

(E)-1-(4-Methoxyphenyl)-5,6,7-triphenylhept-2-ene-1,7-dione (21c)



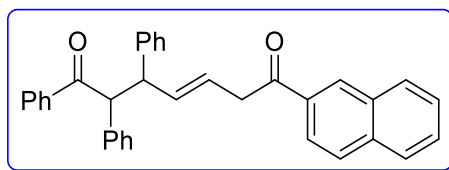
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.96 (d, $J = 7.3$ Hz, 2H), 7.78 (d, $J = 8.7$ Hz, 2H), 7.48 – 7.43 (m, 3H), 7.37 (t, $J = 7.6$ Hz, 2H), 7.30 (t, $J = 7.5$ Hz, 2H), 7.23 (d, $J = 7.4$ Hz, 1H), 7.20 (d, $J = 4.3$ Hz, 2H), 7.16 – 7.11 (m, 1H), 6.87 (d, $J = 8.8$ Hz, 2H), 6.41 (d, $J = 15.9$ Hz, 1H), 6.30 (dd, $J = 15.9, 8.4$ Hz, 1H), 5.07 (d, $J = 9.6$ Hz, 1H), 3.88 – 3.80 (m, 4H), 3.04 (dd, $J = 16.3, 4.0$ Hz, 1H), 2.88 (dd, $J = 16.2, 8.3$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.16, 197.71, 163.29, 137.24, 137.08, 132.85, 132.14, 130.66, 130.28, 130.25, 129.10, 129.01, 128.56, 128.50, 128.26, 127.53, 127.06, 126.25, 113.59, 56.95, 55.41, 42.88, 41.03.

(E)-4-Methyl-5,6,7-triphenyl-1-(thiophen-2-yl)hept-2-ene-1,7-dione (21d)



White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.97 (d, $J = 6.6$ Hz, 2H), 7.57 – 7.47 (m, 5H), 7.42 – 7.34 (m, 4H), 7.26 (s, 1H), 7.19 – 7.17 (m, 2H), 7.12 – 7.06 (m, 2H), 6.93 (d, $J = 6.5$ Hz, 2H), 6.41 (s, 1H), 5.04 (d, $J = 10.7$ Hz, 1H), 3.87 (d, $J = 6.2$ Hz, 1H), 2.88 (d, $J = 5.8$ Hz, 2H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.92, 192.05, 144.69, 138.19, 137.86, 137.42, 136.97, 133.51, 132.93, 131.72, 129.25, 129.15, 128.81, 128.63, 128.50, 128.37, 127.98, 127.82, 126.09, 56.57, 49.06, 41.79, 16.86.

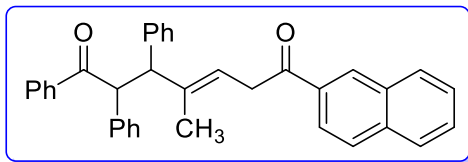
(E)-1-(Naphthalen-2-yl)-5,6,7-triphenylhept-2-ene-1,7-dione (21e)



White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.27 (s, 1H), 7.97 (d, $J = 7.3$ Hz, 2H), 7.90 – 7.83 (m, 4H), 7.60 – 7.52 (m, 2H), 7.47 (t, $J = 8.4$ Hz, 3H), 7.40 – 7.31 (m, 4H), 7.24 – 7.11 (m, 6H), 6.44 (d, $J = 15.9$ Hz, 1H), 6.33 (dd, $J = 15.9, 8.4$ Hz, 1H), 5.11 (d, $J = 9.6$ Hz, 1H), 3.92 (qd, $J = 8.6, 3.9$ Hz, 1H), 3.25 (dd, $J = 16.2, 3.9$ Hz, 1H), 3.05 (dd, $J = 16.2, 8.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.21, 199.11, 137.30,

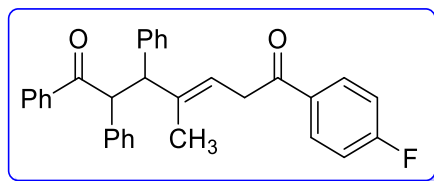
137.23, 137.13, 135.50, 134.54, 132.91, 132.47, 132.41, 130.54, 129.68, 129.55, 129.19, 129.13, 128.61, 128.56, 128.39, 128.31, 127.76, 127.67, 127.16, 126.72, 126.32, 123.88, 57.07, 43.07, 41.60.

(E)-4-Methyl-1-(naphthalen-2-yl)-5,6,7-triphenylhept-2-ene-1,7-dione (21f)



White solid. ^1H NMR (400 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 8.70 (s, 0.44H, minor isomer), 8.21 (s, 0.56H, major isomer), 8.14 – 8.09 (m, 2H), 8.02 – 7.99 (m, 1H), 7.96 – 7.87 (m, 3H), 7.65 – 7.41 (m, 8H), 7.38 – 7.31 (m, 2H), 7.28 – 7.08 (m, 5H), 6.96 (d, $J = 7.2$ Hz, 1.12H, major isomer), 6.77 (d, $J = 7.2$ Hz, 0.88H, minor isomer), 6.39 (s, 0.56H, major isomer), 5.96 (s, 0.44H, minor isomer), 5.07 (d, $J = 10.9$ Hz, 0.56H, major isomer), 4.92 (d, $J = 10.8$ Hz, 0.44H, minor isomer), 3.99 – 3.91 (m, 1H), 3.60 (dd, $J = 13.9, 3.7$ Hz, 0.44H, minor isomer), 3.20 – 3.14 (m, 1H), 3.06 (dd, $J = 14.7, 10.5$ Hz, 0.56H, major isomer), 1.88 (d, $J = 1.4$ Hz, 1.68H, major isomer), 1.72 (d, $J = 1.3$ Hz, 1.32H, minor isomer). Ratio of diastereoisomers (major to minor): 1.3; ^{13}C NMR (100 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 199.47, 199.37, 199.20, 198.96, 138.12, 137.82, 137.45, 137.14, 137.09, 136.36, 135.60, 135.49, 134.53, 134.30, 133.26, 132.96, 132.74, 132.50, 130.35, 129.88, 129.69, 129.63, 129.52, 129.34, 129.23, 128.95, 128.85, 128.78, 128.76, 128.74, 128.69, 128.66, 128.46, 128.38, 127.91, 127.85, 127.79, 127.34, 126.73, 126.67, 126.11, 126.01, 124.32, 124.03, 57.29, 56.76, 49.92, 49.27, 42.33, 41.32, 16.58, 15.40. Ratio of diastereoisomers (major to minor): 1.3.

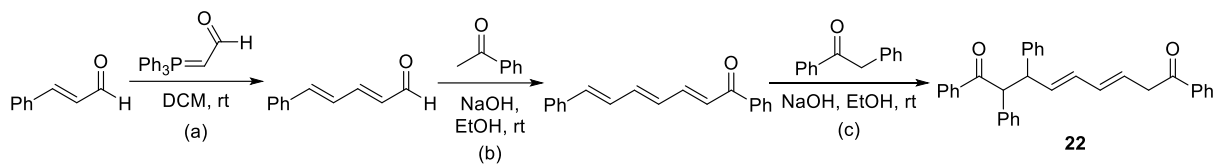
(E)-1-(4-Fluorophenyl)-4-methyl-5,6,7-triphenylhept-2-ene-1,7-dione (21g)



White solid. ^1H NMR (400 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 8.19 – 8.13 (m, 2H), 8.05 (d, $J = 7.3$ Hz, 1H), 7.81 (dd, $J = 8.7, 5.4$ Hz, 1H), 7.63 (d, $J = 7.4$ Hz, 1H), 7.54 – 7.38 (m, 5H), 7.31 – 7.13 (m, 6H), 7.11 – 7.06 (m, 1H), 7.01 (d, $J = 7.3$ Hz, 0.94H, minor isomer), 6.84 (d, $J = 7.3$ Hz, 1.06H, major isomer), 6.46 (s, 0.47H, minor isomer), 6.02 (s, 0.53H, major isomer), 5.10 (d, $J = 10.8$ Hz, 0.47H, minor isomer), 4.93 (d, $J = 10.8$ Hz, 0.53H, major isomer), 3.99 – 3.89 (m, 1H), 3.48 (dd, $J = 13.9, 3.6$ Hz, 0.53H, major isomer), 3.09 (dd, $J = 13.8, 11.3$ Hz, 0.47H, minor isomer), 3.02 (d, $J = 7.2$ Hz, 1.41H, minor isomer), 1.93 (s, 1H), 1.75 (s, 1.59H, major isomer). Ratio of diastereoisomers (major to minor): 1.1; ^{13}C NMR (100 MHz, CDCl_3) major + minor diastereoisomers δ (ppm) 199.39, 198.90, 197.86, 197.64, 166.89 (d, $J = 253.9$ Hz), 166.57 (d, $J = 253.9$ Hz), 136.97, 136.11, 133.32, 132.98, 131.23 (d, $J = 9.1$ Hz), 130.73 (d, $J = 9.2$ Hz), 129.67, 129.24, 129.18, 129.00, 128.88, 128.80, 128.75, 128.66, 128.59, 128.37, 127.89, 127.82, 127.40, 126.13 (d, $J = 8.3$ Hz), 115.75

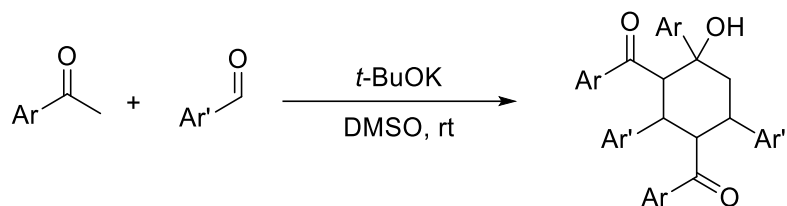
(d, $J = 21.7$ Hz), 115.60 (d, $J = 21.7$ Hz), 57.21, 56.71, 49.83, 48.77, 42.19, 41.06, 16.64, 15.23. Ratio of diastereoisomers (major to minor): 1.1.

2.4 Synthesis and characterization of (2*E*, 4*E*)-1,7,8,9-tetraphenylnona-2,4-diene-1,9-dione (**22**)



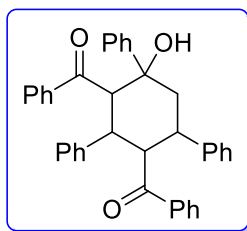
General procedures: (a) To a mixture of cinnamaldehyde (10.0 mmol) in CH_2Cl_2 (20 mL) was added 2-(triphenyl-15-phosphaneylidene)acetaldehyde (10.0 mmol). After stirring at room temperature for 2 h, the reaction was quenched by addition of saturated NH_4Cl solution and extracted with CH_2Cl_2 . The combined organic extracts were washed with brine, dried over anhydrous Na_2SO_4 , filtered, concentrated and purified on silica gel chromatography to afford the intermediate (2*E*,4*E*)-5-phenylpenta-2,4-dienal for the next step. (b) Corresponding aldehyde (5.0 mmol) was dissolved in ethanol (20 mL). Then aqueous NaOH (2.0 equiv) was added dropwise followed by slow addition of acetophenone (5.0 mmol). The reaction mixture was diluted with water. The precipitate was collected by filtration and washed with water and EtOH in sequence, giving the intermediate 1,7-diphenylhepta-2,4,6-trien-1-one. (c) To a solution of 2-phenylacetophenone (5.0 mmol) in EtOH (20 mL) was added NaOH (5.0 mmol). After stirring for 10 min, the conjugated trienone (5.0 mmol) was added. The resulting mixture was stirred for 3 h at room temperature and quenched with saturated NH_4Cl solution. The mixture was extracted with ethyl acetate (3×30 mL). The organic phase was collected and dried with anhydrous Na_2SO_4 , evaporated and purified by flash column chromatography to afford the target product **20** as yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.96 (d, $J = 7.3$ Hz, 2H), 7.78 (d, $J = 7.3$ Hz, 2H), 7.53 – 7.46 (m, 2H), 7.42 – 7.37 (m, 5H), 7.32 – 7.20 (m, 8H), 7.17 – 7.14 (m, 1H), 6.57 (dd, $J = 15.6, 10.4$ Hz, 1H), 6.37 (d, $J = 15.6$ Hz, 1H), 6.23 (dd, $J = 15.0, 10.5$ Hz, 1H), 5.86 (dd, $J = 15.0, 8.6$ Hz, 1H), 4.99 (d, $J = 9.7$ Hz, 1H), 3.83 – 3.76 (m, 1H), 3.04 (dd, $J = 16.5, 3.6$ Hz, 1H), 2.87 (dd, $J = 16.3, 8.5$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.19, 199.06, 137.39, 137.27, 137.24, 136.99, 134.83, 132.90, 131.58, 129.08, 128.82, 128.59, 128.54, 128.49, 127.99, 127.61, 127.23, 126.21, 57.04, 42.47, 41.36.

2.5 General procedure for the synthesis of substituted cyclohexanols (28)



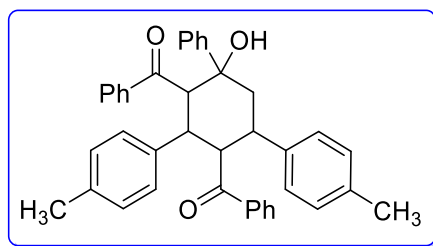
A catalytic amount of *t*-BuOK (0.060 mol) was added to a solution of ketone (9.0 mmol) and aldehyde (6.0 mmol) in DMSO (2 mL). After stirring at room temperature for 5 min, the dark brown mixture was washed with diluted HCl (10%, 10 mL) and extracted with DCM (2 × 10 mL). The combined organic layer was dried over Na₂SO₄, and the solvent was removed under reduced pressure. The crude product was crystallized in EtOH/hexane (5:1).

2,4-Dibenzoyl-1,3,5-triphenylcyclohexanol (28a)



White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.82 (d, *J* = 7.0 Hz, 2H), 7.49 (d, *J* = 7.0 Hz, 2H), 7.29 (s, 3H), 7.24 - 7.19 (m, 3H), 7.15 - 7.09 (m, 9H), 7.03 - 7.00 (m, 3H), 6.84 (s, 3H), 5.75 (d, *J* = 11.9 Hz, 1H), 5.24 (s, 1H), 4.40 (s, 1H), 4.20 (t, *J* = 14.4 Hz, 2H), 3.44 (t, *J* = 13.2 Hz, 1H), 2.08 (d, *J* = 13.3 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 208.29, 206.84, 146.87, 141.69, 140.19, 139.27, 138.28, 132.87, 131.93, 128.78, 128.24, 128.17, 128.07, 127.80, 127.74, 127.68, 127.40, 126.93, 126.59, 125.19, 75.95, 52.76, 50.18, 48.06, 42.24, 38.38.

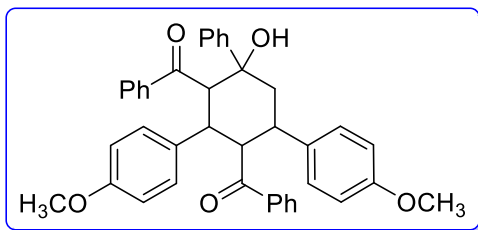
2,4-Dibenzoyl-1-phenyl-3,5-di(*p*-tolyl)cyclohexanol (28b)



White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.78 (d, *J* = 7.5 Hz, 2H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.29 - 7.23 (m, 3H), 7.18 (t, *J* = 7.1 Hz, 1H), 7.12 - 7.05 (m, 7H), 7.02 - 6.95 (m, 4H), 6.86 (d, *J* = 7.7 Hz, 2H), 6.62 (d, *J*

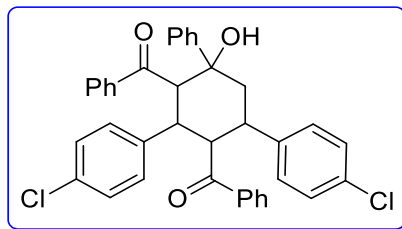
= 7.7 Hz, 2H), 5.70 (d, J = 12.0 Hz, 1H), 5.17 (s, 1H), 4.35 (t, J = 4.4 Hz, 1H), 4.17 – 4.08 (m, 2H), 3.41 – 3.34 (m, 1H), 2.12 (s, 3H), 2.05 – 2.00 (m, 1H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 208.35, 207.11, 146.97, 140.33, 138.73, 138.30, 136.32, 135.96, 132.76, 131.73, 128.86, 128.71, 128.62, 128.21, 128.12, 127.73, 127.60, 127.50, 126.84, 125.21, 75.97, 53.01, 50.36, 47.60, 41.88, 38.59, 20.81, 20.71.

3,5-Bis(4-methoxyphenyl)-2,4-dibenzoyl-1-phenylcyclohexanol (28c)



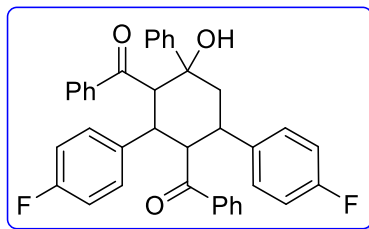
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.79 (d, J = 7.6 Hz, 2H), 7.47 (d, J = 7.6 Hz, 2H), 7.32 – 7.25 (m, 4H), 7.22 (d, J = 7.1 Hz, 1H), 7.15 – 7.10 (m, 7H), 7.05 (t, J = 7.6 Hz, 2H), 7.00 (d, J = 8.5 Hz, 2H), 6.62 (d, J = 8.5 Hz, 2H), 6.37 (d, J = 8.5 Hz, 2H), 5.68 (d, J = 12.0 Hz, 1H), 5.22 (s, 1H), 4.37 – 4.35 (m, 1H), 4.15 – 4.08 (m, 2H), 3.65 (s, 3H), 3.52 (s, 3H), 3.35 (t, J = 13.3 Hz, 1H), 2.02 (dd, J = 13.6, 3.1 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 208.50, 207.23, 158.20, 158.13, 146.95, 140.20, 138.30, 133.96, 132.82, 131.92, 131.46, 129.81, 128.67, 128.59, 128.14, 127.80, 127.74, 127.50, 126.87, 125.17, 113.63, 113.41, 75.98, 55.14, 54.95, 53.06, 50.47, 47.17, 41.43, 38.79.

3,5-Bis(4-chlorophenyl)-2,4-dibenzoyl-1-phenylcyclohexanol (28d)



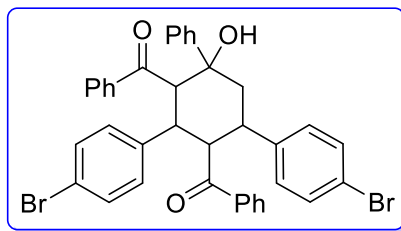
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.75 (d, J = 7.6 Hz, 2H), 7.45 (d, J = 7.7 Hz, 2H), 7.32 – 7.25 (m, 4H), 7.15 – 7.11 (m, 6H), 7.08 – 7.00 (m, 7H), 6.80 (d, J = 8.3 Hz, 2H), 5.66 (d, J = 12.0 Hz, 1H), 5.15 (s, 1H), 4.34 – 4.32 (m, 1H), 4.17 – 4.10 (m, 2H), 3.32 (t, J = 13.2 Hz, 1H), 2.04 – 1.99 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 207.78, 206.10, 146.40, 140.03, 139.59, 137.99, 137.73, 133.15, 132.76, 132.51, 132.36, 130.07, 129.05, 128.35, 128.23, 128.08, 127.98, 127.94, 127.38, 127.07, 125.05, 75.76, 52.01, 50.04, 47.27, 41.54, 38.32.

3,5-Bis(4-fluorophenyl)-2,4-dibenzoyl-1-phenylcyclohexanol (28e)



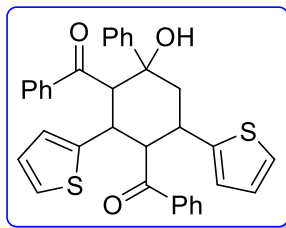
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.77 (d, $J = 7.5$ Hz, 2H), 7.45 (d, $J = 7.5$ Hz, 2H), 7.32 – 7.23 (m, 4H), 7.18 – 7.10 (m, 7H), 7.08 – 7.02 (m, 4H), 6.76 (t, $J = 8.7$ Hz, 2H), 6.52 (t, $J = 8.6$ Hz, 2H), 5.66 (d, $J = 12.0$ Hz, 1H), 5.21 (d, $J = 2.2$ Hz, 1H), 4.34 (t, $J = 4.6$ Hz, 1H), 4.18 – 4.10 (m, 2H), 3.33 (td, $J = 13.5, 2.2$ Hz, 1H), 2.02 (dd, $J = 13.7, 3.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 208.13, 206.48, 162.73, 160.29, 146.57, 139.76, 138.15, 137.34, 135.00, 133.09, 132.42, 130.36, 130.28, 129.20, 129.12, 128.24, 128.06, 127.94, 127.39, 127.05, 125.08, 115.15, 115.05, 114.94, 114.84, 75.85, 52.47, 50.26, 47.20, 41.42, 38.57.

3,5-Bis(4-bromophenyl)-2,4-dibenzoyl-1-phenylcyclohexanol (28f)



White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.75 (d, $J = 7.3$ Hz, 2H), 7.46 – 7.44 (m, 2H), 7.32 – 7.24 (m, 4H), 7.18 (d, $J = 8.4$ Hz, 1H), 7.13 – 7.10 (m, 4H), 7.08 – 7.05 (m, 4H), 6.95 (s, 4H), 5.66 (d, $J = 12.0$ Hz, 1H), 5.13 (d, $J = 2.1$ Hz, 1H), 4.33 (t, $J = 4.6$ Hz, 1H), 4.17 – 4.08 (m, 2H), 3.32 (td, $J = 13.5, 2.0$ Hz, 1H), 2.01 (dd, $J = 13.8, 3.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 207.80, 206.11, 146.36, 140.53, 139.59, 138.24, 137.99, 133.20, 132.58, 131.33, 131.22, 130.42, 129.44, 128.26, 128.11, 128.04, 127.98, 127.42, 127.11, 125.06, 120.97, 120.52, 75.76, 51.93, 50.01, 47.34, 41.63, 38.25.

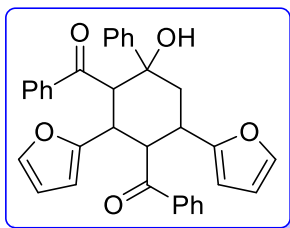
3,5-Bis(thiophen-2-yl)-2,4-dibenzoyl-1-phenylcyclohexanol (28g)



White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.73 – 7.71 (m, 2H), 7.55 – 7.53 (m, 2H), 7.38 – 7.36 (m, 2H), 7.32 – 7.28 (m, 2H), 7.24 (t, $J = 7.8$ Hz, 2H), 7.14 (q, $J = 7.5$ Hz, 4H), 7.06 (t, $J = 7.3$ Hz, 1H), 6.87 (dd, $J = 5.1, 1.0$ Hz, 1H), 6.75 (d, $J = 3.4$ Hz, 1H), 6.71 (dd, $J = 5.0, 0.7$ Hz, 1H), 6.65 (dd, $J = 5.0, 3.6$ Hz, 1H), 6.62 (d, $J =$

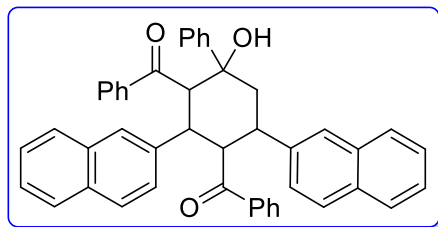
2.9 Hz, 1H), 6.42 (dd, $J = 5.1, 3.6$ Hz, 1H), 5.71 (d, $J = 11.8$ Hz, 1H), 5.17 (d, $J = 2.4$ Hz, 1H), 4.56 (t, $J = 4.7$ Hz, 1H), 4.48 (dd, $J = 11.8, 4.3$ Hz, 1H), 4.39 (dt, $J = 12.5, 4.0$ Hz, 1H), 3.24 (td, $J = 13.6, 2.5$ Hz, 1H), 2.17 (dd, $J = 13.7, 3.5$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 207.64, 206.15, 146.06, 144.96, 141.69, 140.03, 137.88, 133.03, 132.24, 128.34, 128.17, 127.87, 127.79, 127.61, 127.00, 126.70, 126.46, 126.29, 125.09, 124.31, 123.79, 123.20, 75.73, 52.62, 51.34, 42.29, 40.05, 37.42.

3,5-Bis(furan-2-yl)-2,4-dibenzoyl-1-phenylcyclohexanol (28h)



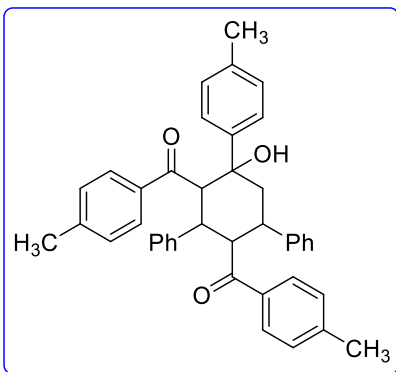
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.70 (d, $J = 7.7$ Hz, 2H), 7.60 (d, $J = 7.8$ Hz, 2H), 7.53 (d, $J = 7.7$ Hz, 2H), 7.36 (dt, $J = 21.0, 7.4$ Hz, 2H), 7.28 – 7.16 (m, 6H), 7.07 (t, $J = 7.3$ Hz, 1H), 6.99 (s, 1H), 6.75 (s, 1H), 6.03 – 5.79 (m, 4H), 5.69 (d, $J = 11.9$ Hz, 1H), 5.29 (s, 1H), 4.67 (t, $J = 4.4$ Hz, 1H), 4.27 (dd, $J = 11.9, 4.0$ Hz, 1H), 4.14 (dd, $J = 8.9, 3.8$ Hz, 1H), 3.06 (t, $J = 13.3$ Hz, 1H), 2.08 (dd, $J = 13.8, 3.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 207.81, 204.78, 155.34, 152.84, 146.25, 141.26, 140.93, 139.13, 137.34, 133.10, 132.15, 128.32, 128.14, 127.99, 127.90, 127.57, 126.94, 125.05, 109.95, 109.89, 107.75, 105.46, 75.40, 48.88, 46.83, 40.18, 37.87, 35.62.

3,5-Bis(naphthalen-2-yl)-2,4-dibenzoyl-1-phenylcyclohexanol (28i)



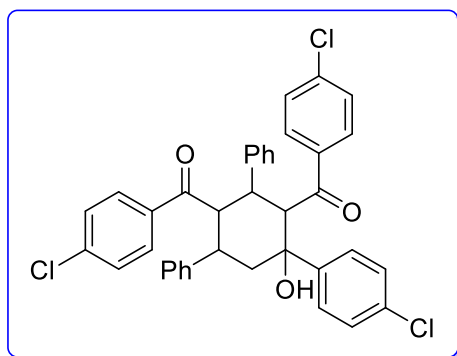
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.88 (d, $J = 7.3$ Hz, 2H), 7.70 – 7.67 (m, 2H), 7.63 – 7.58 (m, 2H), 7.54 (d, $J = 8.5$ Hz, 1H), 7.49 – 7.46 (m, 4H), 7.40 – 7.30 (m, 6H), 7.28 – 7.22 (m, 4H), 7.15 – 7.02 (m, 5H), 6.95 (t, $J = 7.4$ Hz, 1H), 6.76 (t, $J = 7.8$ Hz, 2H), 5.92 (d, $J = 12.0$ Hz, 1H), 5.31 (s, 1H), 4.61 (t, $J = 4.5$ Hz, 1H), 4.46 – 4.36 (m, 2H), 3.62 – 3.55 (m, 1H), 2.21 (dd, $J = 13.7, 3.3$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 208.28, 206.78, 146.87, 139.96, 139.22, 138.27, 136.90, 133.34, 132.94, 132.28, 132.24, 131.85, 128.27, 128.18, 128.03, 127.88, 127.82, 127.70, 127.56, 127.36, 127.28, 127.04, 126.73, 126.57, 126.09, 125.79, 125.53, 125.36, 125.28, 76.08, 52.59, 50.33, 48.28, 42.48, 38.69.

2,4-Bis(4-methylbenzoyl)-3,5-diphenyl-1-(*p*-tolyl)cyclohexanol (28j)



White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.66 (d, $J = 8.0$ Hz, 2H), 7.40 (d, $J = 8.1$ Hz, 2H), 7.20 (d, $J = 7.5$ Hz, 2H), 7.07 – 7.05 (m, 6H), 7.00 – 6.90 (m, 5H), 6.82 – 6.77 (m, 5H), 5.68 (d, $J = 12.0$ Hz, 1H), 5.28 (s, 1H), 4.32 (t, $J = 4.5$ Hz, 1H), 4.18 – 4.09 (m, 2H), 3.37 (t, $J = 13.3$ Hz, 1H), 2.22 (d, $J = 8.3$ Hz, 6H), 2.15 (s, 3H), 2.00 (dd, $J = 13.7, 3.3$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 207.78, 206.29, 144.12, 143.65, 142.55, 141.92, 139.42, 137.76, 136.24, 135.85, 128.77, 128.42, 128.39, 128.15, 127.93, 127.75, 127.54, 126.73, 126.45, 125.07, 75.83, 52.46, 49.74, 48.13, 42.34, 38.77, 21.51, 21.36, 20.88.

2,4-Bis(4-chlorobenzoyl)-3,5-diphenyl-1-(4-chlorophenyl)cyclohexanol (28k)



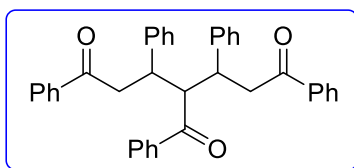
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.69 (d, $J = 8.4$ Hz, 2H), 7.41 (d, $J = 8.5$ Hz, 2H), 7.24 (d, $J = 8.5$ Hz, 2H), 7.17 – 7.12 (m, 4H), 7.08 (t, $J = 7.5$ Hz, 2H), 7.03 – 6.96 (m, 7H), 6.86 – 6.85 (m, 3H), 5.60 (d, $J = 11.8$ Hz, 1H), 5.15 (s, 1H), 4.28 (t, $J = 4.5$ Hz, 1H), 4.15 – 4.08 (m, 2H), 3.27 (t, $J = 13.2$ Hz, 1H), 2.00 (dd, $J = 13.7, 3.2$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 206.55, 205.62, 145.36, 141.20, 139.86, 138.79, 138.64, 138.22, 136.21, 132.94, 129.49, 128.78, 128.58, 128.39, 128.30, 128.11, 127.59, 127.30, 126.90, 126.60, 75.67, 52.64, 49.87, 47.94, 42.14, 38.35.

2.6 General procedure for synthesis of triketone substrates (27)



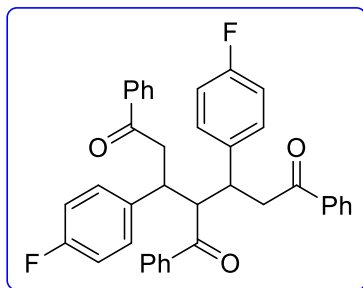
General procedure: To a stirred solution of corresponding substrate **28** (1.0 mmol) in toluene (5 mL) at 0 °C was added concentrated sulfuric acid (5.0 mmol) dropwise. The reaction mixture was subsequently heated to 80 °C for 1 h, then hydrolyzed with ice. The aqueous layer was separated and extracted three times with 20 mL CH₂Cl₂. The combined organic layer was dried over anhydrous Na₂SO₄, filtered and evaporated. The crude product was purified by silica gel column chromatography with the eluent 1:10 ethyl acetate/petroleum ether, affording the corresponding compounds.

4-Benzoyl-1,3,5,7-tetraphenylheptane-1,7-dione (27a)



White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.75 – 7.73 (m, 4H), 7.55 – 7.53 (m, 2H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.43 (t, *J* = 7.4 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 4H), 7.25 (t, *J* = 7.6 Hz, 2H), 7.18 – 7.08 (m, 10H), 4.38 (t, *J* = 7.4 Hz, 1H), 3.85 – 3.80 (m, 2H), 3.47 (dd, *J* = 16.7, 10.9 Hz, 2H), 3.30 (dd, *J* = 16.7, 3.3 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 204.07, 197.98, 141.54, 138.90, 136.96, 133.03, 132.87, 128.72, 128.46, 128.34, 128.29, 128.03, 127.94, 127.00, 56.20, 42.17, 40.54.

4-Benzoyl-3,5-bis(4-fluorophenyl)-1,7-diphenylheptane-1,7-dione (27b)



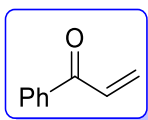
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.75 (d, *J* = 7.7 Hz, 4H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.52 – 7.45 (m, 3H), 7.37 (t, *J* = 7.6 Hz, 4H), 7.30 (t, *J* = 7.7 Hz, 2H), 7.09 (q, *J* = 5.2 Hz, 4H), 6.85 (t, *J* = 8.5 Hz, 4H), 4.33 (t, *J* = 7.4 Hz, 1H), 3.84 – 3.78 (m, 2H), 3.44 (dd, *J* = 16.9, 10.8 Hz, 2H), 3.28 (dd, *J* = 16.8, 3.4 Hz, 2H); ¹³C

NMR (100 MHz, CDCl₃) δ (ppm) 203.66, 197.74, 161.66 (d, J = 244.2 Hz), 138.64, 137.25 (d, J = 3.4 Hz), 136.80, 133.38, 133.08, 129.41 (d, J = 7.9 Hz), 128.54, 128.28, 127.98, 115.6 (d, J = 21.2 Hz), 56.03, 41.42, 40.59.

2.7 General procedures for the synthesis of poly(phenyl vinyl ketone) (29)

General procedure: (a) To a CHCl₃ (80 mL) solution of 3-chloropropiophenone (6.00 g, 35.6 mmol, 1.0 equiv) was added dropwise triethyl amine (12.0 mL, 85.4 mmol, 2.4 equiv) under nitrogen atmosphere. After stirring for 18 h, the reaction mixture was orderly washed with 0.1 N HCl aq. (2 $\times$ 40 mL), distilled water (2 $\times$ 40 mL), saturated NaHCO₃ aq. (2 $\times$ 40 mL), and brine (1 $\times$ 40 mL). The organic layer was dried over anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography with 1:5 ethyl acetate/petroleum ether to give phenyl vinyl ketone as yellowish oil in 90% yield.² ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.92 (d, J = 7.8 Hz, 2H), 7.56 – 7.52 (m, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.13 (dd, J = 17.1, 10.6 Hz, 1H), 6.43 – 6.39 (m, 1H), 5.89 (d, J = 10.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 190.98, 137.28, 133.00, 132.39, 130.13, 128.69, 128.63. (b) To a stirred solution of phenyl vinyl ketone (4.30 g, 32.5 mmol) in benzene (12 mL) was added azobisisobutyronitrile (1-2 mol%). After stirring at 50 °C overnight, the reaction mixture was poured into EtOH (30 mL). The white viscous polymer was isolated by decantation, washed with ethyl acetate (1 $\times$ 5 mL), and petroleum ether (2 $\times$ 10 mL), and then dried under vacuum at 60 °C, affording **27** as a white solid.

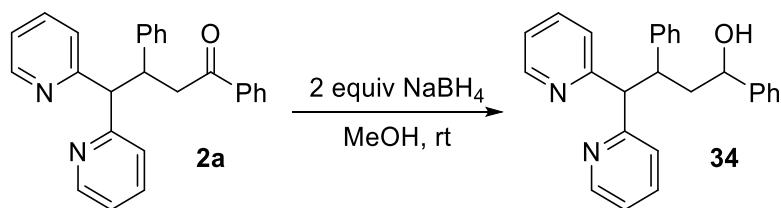
1-Phenylprop-2-en-1-one (41) (CAS: 768-03-6)²



Colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.92 (d, J = 7.8 Hz, 2H), 7.56 – 7.52 (m, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.13 (dd, J = 17.1, 10.6 Hz, 1H), 6.43 – 6.39 (m, 1H), 5.89 (d, J = 10.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 190.98, 137.28, 133.00, 132.39, 130.13, 128.69, 128.63.

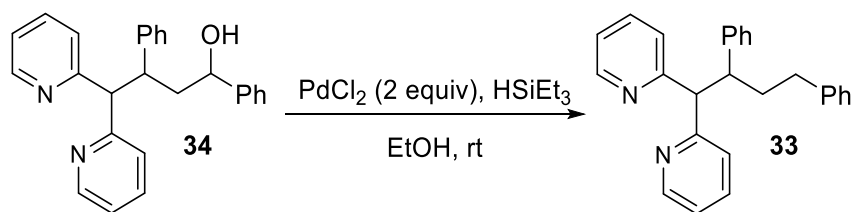
2.8 General procedures for the synthesis of di(2-pyridyl)methane derivatives (33 - 35)

Synthesis and characterization of **34**



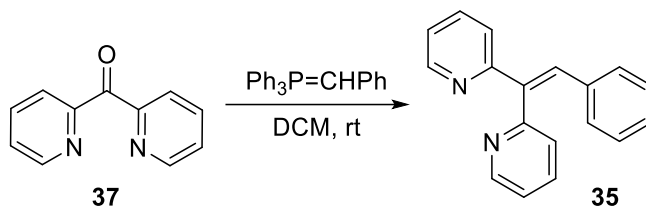
2a (10.0 mmol) was dissolved in MeOH (50 mL) and cooled to 0 °C. Then, NaBH₄ (20.0 mmol) was added slowly and the mixture was stirred until the complete consumption of the starting materials (monitored by TLC). The reaction mixture was diluted with water and extracted with CH₂Cl₂. The combined organic extracts were washed with brine, dried over anhydrous Na₂SO₄, filtered, concentrated and purified on silica gel chromatography, affording the product **34** as white solid. ¹H NMR (400 MHz, CDCl₃) major + minor diastereoisomers δ (ppm) 8.53 (dd, *J* = 12.3, 4.4 Hz, 1H), 8.25 (d, *J* = 4.2 Hz, 1H), 7.59 – 7.40 (m, 2H), 7.31 – 7.18 (m, 5H), 7.16 – 7.08 (m, 6H), 7.06 – 7.03 (m, 2H), 6.83 – 6.77 (m, 1H), 4.57 (dd, *J* = 24.7, 11.6 Hz, 1H), 4.42 – 4.38 (m, 1H), 4.36 – 4.32 (m, 0.50H), 3.72 – 3.66 (m, 0.50H), 3.63 (s, 0.50H), 3.21 (s, 0.50H), 2.26 – 1.89 (m, 2H). Ratio of diastereoisomers (major to minor): 1.0; ¹³C NMR (100 MHz, CDCl₃) major + minor diastereoisomers δ (ppm) 161.37, 161.35, 161.13, 160.82, 149.10, 148.96, 148.70, 145.70, 143.96, 142.80, 142.70, 136.73, 136.61, 135.96, 135.82, 128.77, 128.61, 128.32, 128.16, 128.13, 128.08, 127.54, 126.91, 126.55, 126.12, 126.08, 125.40, 124.50, 123.95, 123.84, 123.55, 121.82, 121.09, 121.05, 72.72, 71.42, 62.22, 62.01, 46.55, 46.06, 45.00, 43.27. Ratio of diastereoisomers (major to minor): 1.0.

Synthesis and characterization of **33**



PdCl₂ (2.0 mmol) was added to a solution of substrate **34** (1.0 mmol) and HSiEt₃ (2.0 mmol) in EtOH (5 mL). The mixture was stirred at 60 °C under nitrogen atmosphere for 6 h and quenched with saturated NH₄Cl solution (2 mL). Then, the mixture was extracted with ethyl acetate (3 × 5 mL). The organic phase was collected and dried with anhydrous Na₂SO₄, evaporated and purified by flash column chromatography using hexane/ethyl acetate as eluent to give **33** as yellow solid (255.1 mg, 70%). ¹H NMR (400 MHz, CDCl₃) δ 8.59 – 8.57 (m, 1H), 8.35 – 8.34 (m, 1H), 7.62 – 7.54 (m, 2H), 7.31 (td, *J* = 7.7, 1.8 Hz, 1H), 7.23 – 7.09 (m, 9H), 7.07 – 7.03 (m, 1H), 6.96 – 6.93 (m, 2H), 6.85 (ddd, *J* = 7.4, 4.9, 1.1 Hz, 1H), 4.53 (d, *J* = 11.6 Hz, 1H), 3.89 (td, *J* = 11.2, 3.5 Hz, 1H), 2.43 – 2.28 (m, 2H), 1.96 – 1.78 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 161.55, 161.21, 149.25, 148.72, 142.82, 142.27, 136.44, 135.80, 128.60, 128.28, 128.10, 128.01, 125.95, 125.53, 123.79, 123.72, 121.70, 121.02, 62.79, 49.50, 36.04, 33.48.

Synthesis and characterization of 35

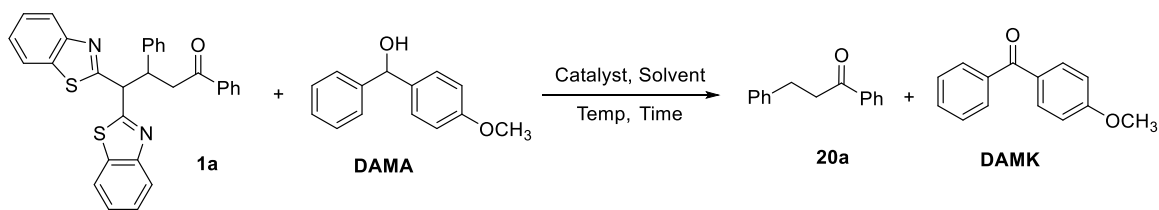


37 (10.0 mmol) was added to a solution of $\text{Ph}_3\text{P=CHPh}$ (20.0 mmol) in DCM (20.0 mL). The resulting mixture was stirred at room temperature until the complete consumption of **37** (monitored by TLC). The reaction mixture was diluted with water and extracted with DCM. The combined organic extracts were washed with brine, dried over anhydrous Na_2SO_4 , filtered, concentrated and purified on silica gel chromatography, affording **35** as white solid (1.55 g, 60%). ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.72 – 8.70 (m, 1H), 8.60 – 8.58 (m, 1H), 7.89 (s, 1H), 7.57 (td, $J = 7.7, 1.8$ Hz, 1H), 7.50 (td, $J = 7.8, 1.9$ Hz, 1H), 7.22 – 7.17 (m, 2H), 7.09 – 7.07 (m, 4H), 7.00 – 6.95 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 158.43, 157.70, 150.18, 149.28, 140.26, 136.85, 136.38, 136.33, 132.44, 129.73, 128.01, 127.56, 125.92, 122.43, 122.26, 122.14.

3. Studies on C–C bond hydrogenolysis reactions

3.1 Development of the C–C bond hydrogenolysis procedure

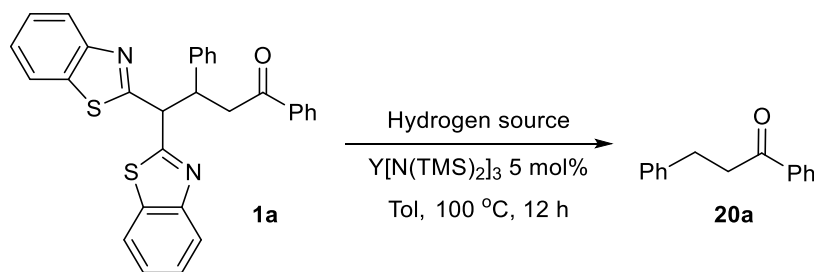
Table S1. Optimization of the reaction conditions^a



Entry	Catalyst	Solvent	(1a : DAMA) ^d	Temp (°C)	Time (h)	20a (%)
1	Y[N(TMS) ₂] ₃ , Y-1	Toluene	1:1	100	12	89
2	La[N(TMS) ₂] ₃	Toluene	1:1	100	12	86
3	Sm[N(TMS) ₂] ₃	Toluene	1:1	100	12	87
4	Lu[N(TMS) ₂] ₃	Toluene	1:1	100	12	85
5 ^b	YCl ₃	Toluene	1:1	100	12	0
6 ^b	Y(OTf) ₃	Toluene	1:1	100	12	0
7	--	Toluene	1:1	100	12	0
8	CuBr	Toluene	1:1	100	12	0
9	Pd(PPh ₃) ₄	Toluene	1:1	100	12	0
10	Y[N(TMS) ₂] ₃	Toluene	1:1	80	12	67
11	Y[N(TMS) ₂] ₃	Toluene	1:1	110	12	83
12	Y[N(TMS) ₂] ₃	Toluene	1:1	100	24	87
13	Y[N(TMS) ₂] ₃	Toluene	1:1	100	6	65
14 ^c	Y[N(TMS) ₂] ₃	Toluene	1:1	100	12	45
15	Y[N(TMS) ₂] ₃	Toluene	1:1.2	100	12	83
16	Y[N(TMS) ₂] ₃	Toluene	1:2	100	12	53
17	Y[N(TMS) ₂] ₃	THF	1:1	100	12	56
18	Y[N(TMS) ₂] ₃	Hexane	1:1	100	12	84

^aReaction conditions: **1a** (0.50 mmol), **DAMA** (0.50-2.0 mmol), catalyst (5 mol%), solvent (2 mL), under N₂ atmosphere, isolated yield. ^bCatalyst loading 10 mol%. ^cCatalyst loading 1 mol%. ^dmole ratio.

Table S2. Optimization of the hydrogen sources^a



Entry	Hydrogen source	20a (%)
1	PhCH ₂ NH ₂	31%
2	diisobutylamine	33%
3	diethylamine	25%
4	<i>n</i> -butylamine	19%
5	<i>N</i> -benzyl-isobutylamine	29%
6	methanol	trace
7	ethanol	trace
8	Isopropanol (solvent)	trace
9 ^b	H ₂	22%
10	phenylsilane	38%
11 ^c	diphenylmethanol	84% (¹ H NMR)

Conditions: ^aReactions were carried out with **1a** (0.50 mmol), hydrogen source (0.50 mmol), **Y-1** (0.025 mmol), toluene (2 mL) at 100 °C under N₂, isolated yield. ^b6 atm H₂. ^cThe dehydrogenative product benzophenone is hard to separate from **20a**, thus **DAMA** was selected as the compromised hydrogen source.

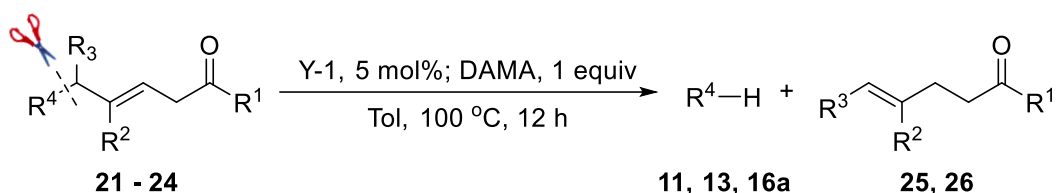
3.2 General procedure for C–C hydrogenolysis of monoketone substrates (1 - 5)

In a glovebox, to a 25 ml capped Schlenk tube equipped with a magnetic stir bar were added **DAMA** (107 mg, 0.50 mmol), ketone substrate (0.50 mmol), **Y-1** (14 mg, 5 mol%) and toluene (2.0 mL). The mixture was heated at the indicated temperature for 12 h. Subsequently, the reaction mixture was cooled to room temperature and quenched with saturated NH₄Cl solution (2 mL). The mixture was extracted with ethyl acetate (3 × 5 mL). The combined organic layer was dried with anhydrous Na₂SO₄, filtered, evaporated and purified by flash column chromatography using petroleum ether/ethyl acetate as eluent, affording the corresponding hydrogenolysis products.

3.3 General procedure for C–C hydrogenolysis of 1,5-diketone substrates (6 - 9)

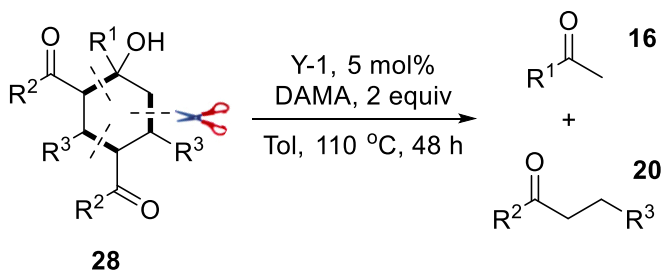
A catalytic amount of $Y[N(TMS)_2]_3$ (5 mol%) was added to a solution of **DAMA** (0.50 mmol) and 1,5-diketone (0.50 mmol) in toluene (2 mL). The mixture was stirred at 60 °C for 6 h, then quenched with saturated NH_4Cl solution (2 mL), and extracted with ethyl acetate (3×5 mL). The organic phase was collected and dried with anhydrous Na_2SO_4 , evaporated and purified by flash column chromatography using hexane/ethyl acetate as eluent, giving the corresponding C–C hydrogenolysis products.

3.4 General procedures for C–C hydrogenolysis of unsaturated ketone substrates (21 - 24)



A catalytic amount of $Y[N(TMS)_2]_3$ (5 mol%) was added to a solution of (4-methoxyphenyl)phenylmethanol (0.50 mmol) and unsaturated ketone compound (0.50 mmol) in toluene (2 mL). The mixture was stirred at 100 °C for 12 h and then quenched with saturated NH_4Cl solution (2 mL). The mixture was extracted with ethyl acetate (3×5 mL). The organic layer was collected and dried with anhydrous Na_2SO_4 , evaporated and purified by flash column chromatography using petroleum ether/ethyl acetate as eluent to give the corresponding C–C hydrogenolysis products.

3.5 General procedures for hydrogenolytic retro-[2+2+2]-cycloreversion of 2,4-diacetylcyclohexanols (28)

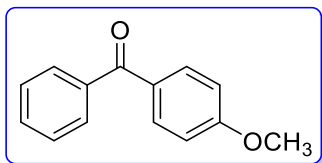


In a glovebox, a dried Schlenk tube was charged with **Y-1** (14 mg, 5 mol%), **DAMA** (107 mg, 0.50 mmol), substituted cyclohexanol (0.50 mmol) and toluene (2.0 mL). Then, the tube was sealed and removed out from the glove box. After stirring at 110 °C for 48 h, the resulting mixture was quenched with saturated NH_4Cl solution (2 mL). Then the mixture was extracted with ethyl acetate (3×5 mL). The combined organic phase was dried

with anhydrous Na₂SO₄, evaporated and all volatiles were removed under reduced pressure. The crude products were purified by flash column chromatography using petroleum ether/ethyl acetate as eluent.

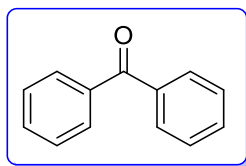
3.6 Characterization of products

(4-Methoxyphenyl)phenylmethanone (DAMK) (CAS: 611-94-9)³



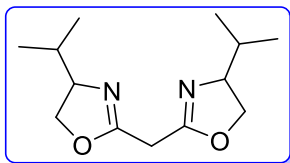
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.83 (d, *J* = 8.8 Hz, 2H), 7.75 (d, *J* = 7.1 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 195.55, 163.20, 138.25, 132.54, 131.87, 130.12, 129.70, 128.16, 113.53, 55.47.

Benzophenone (44) (CAS: 119-61-9)⁴



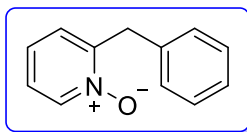
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.82 – 7.80 (m, 4H), 7.61 – 7.57 (dd, *J* = 10.6, 4.3 Hz, 2H), 7.48 (t, *J* = 7.5 Hz, 4H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 196.77, 137.63, 132.43, 130.08, 128.29.

Bis(4-isopropyl-4,5-dihydrooxazol-2-yl)methane (14) (CAS: 131833-90-4)⁵



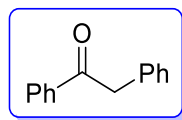
Yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 4.24 (t, *J* = 8.5 Hz, 2H), 3.99 – 3.88 (m, 4H), 3.31 – 3.25 (m, 2H), 1.77 – 1.69 (m, 2H), 0.92 (d, *J* = 6.7 Hz, 6H), 0.84 (d, *J* = 6.8 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 161.51, 161.47, 72.13, 72.09, 70.52, 70.49, 32.40, 28.33, 28.30, 18.63, 18.59, 17.94.

2-benzylpyridine 1-oxide (15)



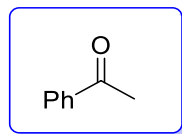
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.22 – 8.20 (m, 1H), 7.30 – 7.26 (m, 2H), 7.22 – 7.20 (m, 3H), 7.07 – 7.05 (m, 2H), 6.89 – 6.86 (m, 1H), 4.19 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 151.86, 139.33, 136.27, 129.66, 128.83, 127.03, 125.82, 125.57, 123.60, 36.48.

1,2-Diphenylethan-1-one (16a) (CAS: 451-40-1)⁶



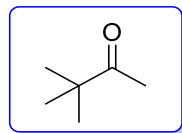
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.04 (d, *J* = 7.6 Hz, 2H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.3 Hz, 2H), 7.35 (t, *J* = 7.1 Hz, 2H), 7.31 – 7.26 (m, 3H), 4.31 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 197.65, 136.66, 134.58, 133.18, 129.50, 128.70, 128.67, 128.65, 126.91, 45.53.

Acetophenone (16b) (CAS: 98-86-2)



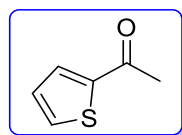
Colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.89 (d, *J* = 7.2 Hz, 2H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 2.51 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 198.00, 137.09, 133.05, 128.53, 128.25, 26.50.

3,3-Dimethylbutan-2-one (16c) (CAS: 75-97-8)



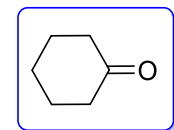
Colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ 2.03 (s, 3H), 1.04 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 213.99, 44.16, 26.25, 24.53.

1-(Thiophen-2-yl)ethan-1-one (16d) (CAS: 88-15-3)



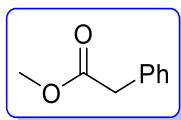
Yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.63 (d, *J* = 3.7 Hz, 1H), 7.57 (d, *J* = 4.9 Hz, 1H), 7.06 (t, *J* = 4.3 Hz, 1H), 2.49 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 190.70, 144.52, 133.80, 132.56, 128.16, 26.85.

Cyclohexanone (17) (CAS: 108-94-1)⁷



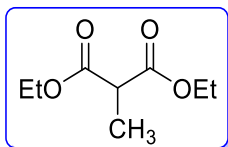
Colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 2.27 (t, *J* = 6.5 Hz, 4H), 1.83 – 1.77 (m, 4H), 1.69 – 1.65 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 212.02, 41.93, 26.99, 24.95.

Methyl 2-phenylacetate (18) (CAS: 101-41-7)⁸



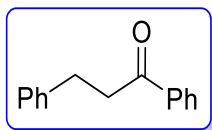
Colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.37 – 7.27 (m, 5H), 3.71 (s, 3H), 3.65 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 172.05, 134.06, 129.30, 128.63, 127.15, 52.03, 41.22.

Diethyl 2-methylmalonate (19) (CAS: 609-08-5)⁹



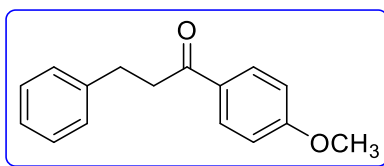
Colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 4.16 (q, *J* = 6.8 Hz, 4H), 3.39 (q, *J* = 7.1 Hz, 1H), 1.38 (d, *J* = 7.2 Hz, 3H), 1.24 (t, *J* = 7.0 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 169.96, 61.11, 46.00, 13.85, 13.33.

1,3-Diphenylpropan-1-one (20a) (CAS: 1083-30-3)¹⁰



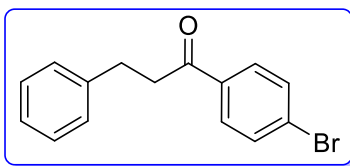
White solid. ¹H NMR (400 MHz, CDCl₃) δ 7.97 (d, *J* = 7.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.34 – 7.26 (m, 4H), 7.22 (t, *J* = 7.0 Hz, 1H), 3.35 – 3.29 (m, 2H), 3.09 (t, *J* = 7.7 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 199.26, 141.31, 136.91, 133.07, 128.62, 128.55, 128.44, 128.06, 126.15, 40.46, 30.16.

1-(4-Methoxyphenyl)-3-phenylpropan-1-one (20b) (CAS: 5739-38-8)¹⁰



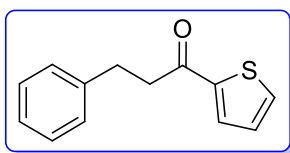
Light yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 7.94 – 7.90 (m, 2H), 7.30 – 7.16 (m, 5H), 6.92 – 6.88 (m, 2H), 3.84 (s, 3H), 3.25 – 3.20 (m, 2H), 3.04 (t, *J* = 8.4 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 197.84, 163.48, 141.49, 130.33, 130.02, 128.53, 128.45, 126.10, 113.76, 55.47, 40.12, 30.36.

1-(4-Bromophenyl)-3-phenylpropan-1-one (20c) (CAS: 1669-51-8)¹⁰



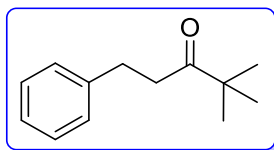
White solid. ¹H NMR (400 MHz, CDCl₃) δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 2H), 7.33 – 7.20 (m, 5H), 3.27 (t, *J* = 7.6 Hz, 2H), 3.07 (t, *J* = 7.6 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 198.18, 141.04, 135.60, 131.93, 129.58, 128.58, 128.41, 128.23, 126.24, 40.40, 30.06.

3-Phenyl-1-(thiophen-2-yl)propan-1-one (20d) (CAS: 40027-94-9)¹¹



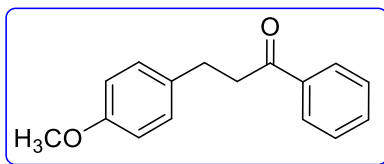
Pale yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 7.70 – 7.68 (m, 1H), 7.63 – 7.62 (m, 1H), 7.32 – 7.19 (m, 5H), 7.12 – 7.10 (m, 1H), 3.26 – 3.22 (m, 2H), 3.07 (t, *J* = 8.0 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 192.17, 144.21, 141.03, 133.56, 131.83, 128.57, 128.45, 128.11, 126.24, 41.16, 30.42.

4,4-Dimethyl-1-phenylpentan-3-one (20e) (CAS: 5195-24-4)¹²



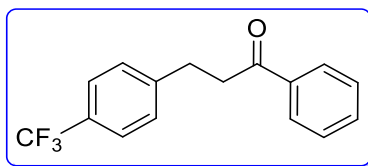
Yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 7.30 – 7.26 (m, 2H), 7.21 – 7.17 (m, 3H), 2.91 – 2.87 (m, 2H), 2.83 – 2.78 (m, 2H), 1.12 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 214.89, 141.62, 128.45, 128.42, 126.03, 44.09, 38.49, 30.13, 26.33.

3-(4-Methoxyphenyl)-1-phenylpropan-1-one (20f) (CAS: 1669-49-4)¹³



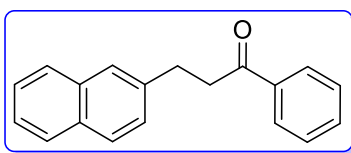
White solid. ¹H NMR (400 MHz, CDCl₃) δ 7.97 – 7.94 (m, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 3.79 (s, 3H), 3.27 (t, *J* = 7.7 Hz, 2H), 3.02 (t, *J* = 7.6 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 199.41, 158.03, 136.94, 133.34, 133.04, 129.37, 128.61, 128.06, 113.97, 55.29, 40.72, 29.31.

1-Phenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one (20g)¹³



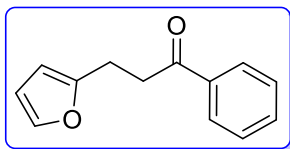
White solid. ¹H NMR (400 MHz, CDCl₃) δ 7.97 – 7.95 (m, 2H), 7.59 – 7.54 (m, 3H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 3.33 (t, *J* = 7.5 Hz, 2H), 3.14 (t, *J* = 7.4 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 198.56, 145.49, 136.71, 133.29, 128.85, 128.72, 128.05, 125.47 (q, *J* = 3.5 Hz), 122.98, 38.77, 28.72.

3-(Naphthalen-2-yl)-1-phenylpropan-1-one (20h)¹³



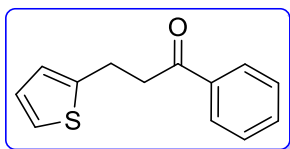
White solid. ¹H NMR (400 MHz, CDCl₃) δ 8.00 – 7.98 (m, 2H), 7.82 (t, *J* = 7.7 Hz, 3H), 7.71 (s, 1H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.49 – 7.40 (m, 5H), 3.40 (t, *J* = 7.7 Hz, 2H), 3.25 (t, *J* = 7.6 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 199.18, 138.81, 136.91, 133.66, 133.10, 132.13, 128.64, 128.13, 128.08, 127.64, 127.48, 127.18, 126.53, 126.04, 125.34, 40.37, 30.30.

3-(Furan-2-yl)-1-phenylpropan-1-one (20i) (CAS: 2207-63-8)¹⁴



White solid. ¹H NMR (400 MHz, CDCl₃) δ 7.99 – 7.97 (m, 2H), 7.57 (tt, *J* = 7.2, 1.6 Hz, 1H), 7.49 – 7.45 (m, 2H), 7.31 (d, *J* = 1.1 Hz, 1H), 6.29 (dd, *J* = 3.1, 1.9 Hz, 1H), 6.05 (dd, *J* = 3.1, 0.8 Hz, 1H), 3.36 – 3.32 (m, 2H), 3.10 (t, *J* = 7.6 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 198.66, 154.78, 141.11, 136.79, 133.13, 128.63, 128.04, 110.25, 105.32, 77.33, 77.02, 76.70, 36.94, 22.54.

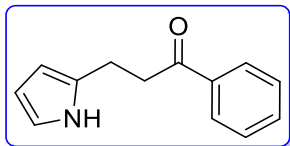
1-Phenyl-3-(thiophen-2-yl)propan-1-one (20j) (CAS: 71777-98-5)¹⁴



White solid. ¹H NMR (400 MHz, CDCl₃) δ 7.98 (d, *J* = 7.9 Hz, 1H), 7.57 (t, *J* = 7.1, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 5.1 Hz, 1H), 6.94 – 6.92 (m, 1H), 6.87 (d, *J* = 3.1 Hz, 1H), 3.39 – 3.36 (m, 1H), 3.32 – 3.29 (m,

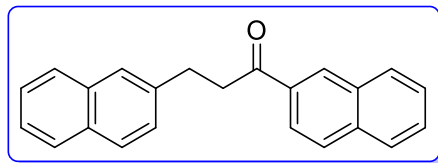
1H); ¹³C NMR (100 MHz, CDCl₃) δ 198.60, 143.9, 136.8, 133.16, 128.64, 128.04, 126.86, 124.68, 123.38, 40.56, 24.24.

1-Phenyl-3-(1H-pyrrol-2-yl)propan-1-one (20k) (CAS: 20948-44-1)¹⁴



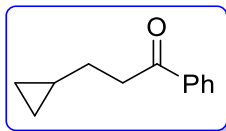
Brown solid. ¹H NMR (400 MHz, CDCl₃) δ 8.61 (s, 1H), 7.97 (d, *J* = 7.8 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 6.67 (d, *J* = 1.3 Hz, 1H), 6.10 (d, *J* = 2.7 Hz, 1H), 5.95 (s, 1H), 3.35 (t, *J* = 6.4 Hz, 2H), 3.06 (t, *J* = 6.3 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 200.69, 136.78, 133.36, 131.75, 128.69, 128.06, 116.77, 107.90, 105.43, 39.45, 21.55.

1,3-Di(naphthalen-2-yl)propan-1-one (20l)¹⁵



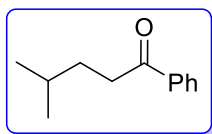
White solid. ¹H NMR (400 MHz, CDCl₃) δ 8.49 (s, 1H), 8.06 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.95 – 7.87 (m, 3H), 7.83 – 7.79 (m, 3H), 7.74 (s, 1H), 7.62 – 7.53 (m, 2H), 7.48 – 7.42 (m, 3H), 3.54 (t, *J* = 7.7 Hz, 2H), 3.30 (t, *J* = 7.7 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 199.13, 138.88, 135.63, 134.24, 133.70, 132.57, 132.16, 129.73, 129.58, 128.51, 128.19, 127.80, 127.67, 127.50, 127.23, 126.80, 126.57, 126.07, 125.36, 123.89, 40.49, 30.45.

3-Cyclopropyl-1-phenylpropan-1-one (20m)¹⁶



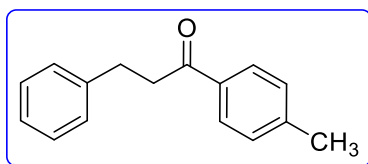
Colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.97 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.1 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 2H), 3.07 (t, *J* = 7.1 Hz, 2H), 1.63 (q, *J* = 7.0 Hz, 2H), 0.78 – 0.75 (m, 1H), 0.43 (d, *J* = 7.5 Hz, 2H), 0.07 (d, *J* = 4.3 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 200.42, 137.07, 132.86, 128.51, 128.03, 38.65, 29.50, 10.68, 4.61.

4-Methyl-1-phenylpentan-1-one (20n) (CAS: 2050-07-9)¹²



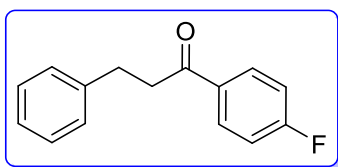
Yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.97 – 7.95 (m, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 2.99 – 2.95 (m, 2H), 1.65 – 1.61 (m, 3H), 0.95 (d, *J* = 6.2 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 200.83, 137.11, 132.89, 128.58, 128.09, 36.67, 33.28, 27.90, 22.47.

3-Phenyl-1-(p-tolyl)propan-1-one (20o) (CAS: 5012-90-8)¹¹



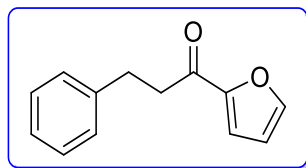
White solid. ¹H NMR (400 MHz, CDCl₃) δ 7.88 (d, *J* = 8.1 Hz, 1H), 7.34 – 7.21 (m, 4H), 3.30 (t, *J* = 8.4 Hz, 1H), 3.08 (t, *J* = 7.6 Hz, 1H), 2.43 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 198.92, 143.85, 141.44, 134.45, 129.31, 128.54, 128.46, 128.20, 126.13, 40.36, 30.26, 21.65.

1-(4-Fluorophenyl)-3-phenylpropan-1-one (20p) (CAS: 41938-64-1)¹¹



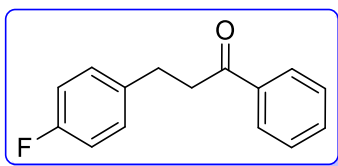
Colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ 8.02 – 7.98 (m, 1H), 7.34 – 7.21 (m, 2H), 7.16 – 7.11 (m, 1H), 3.29 (t, *J* = 7.7 Hz, 1H), 3.09 (t, *J* = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 197.62, 165.76 (d, *J* = 254.6 Hz), 141.15, 133.37 (d, *J* = 5.2 Hz), 130.65 (d, *J* = 9.3 Hz), 128.56, 128.41, 126.21, 115.69 (d, *J* = 21.8 Hz), 40.36, 30.13.

1-(Furan-2-yl)-3-phenylpropan-1-one (20q) (CAS: 2976-01-4)¹¹



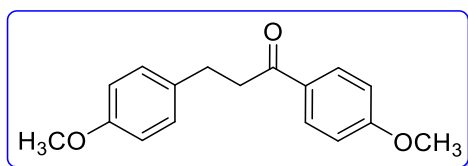
Brown liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.57 (d, *J* = 1.0 Hz, 1H), 7.32 – 7.17 (m, 6H), 6.52 (dd, *J* = 3.5, 1.7 Hz, 1H), 3.19 – 3.13 (m, 2H), 3.09 – 3.04 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 188.50, 152.71, 146.32, 140.99, 128.53, 128.42, 126.19, 117.01, 112.21, 40.17, 29.98.

3-(4-Fluorophenyl)-1-phenylpropan-1-one (20r) (CAS: 41865-46-7)¹⁷



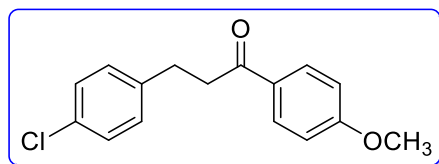
White solid, ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.97 – 7.95 (m, 2H), 7.59 – 7.55 (m, 1H), 7.48 – 7.44 (m, 2H), 7.23 – 7.20 (m, 2H), 7.01 – 6.96 (m, 2H), 3.29 (t, *J* = 7.5 Hz, 2H), 3.06 (t, *J* = 7.5 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 198.99, 161.36 (*J* = 181.8 Hz), 136.85, 136.83 (*J* = 7.73 Hz), 133.11, 129.81 (*J* = 5.79 Hz), 128.61, 127.99, 115.22 (*J* = 15.8 Hz), 40.39, 29.24.

1,3-Bis(4-methoxyphenyl)propan-1-one (20s) (CAS: 20615-47-8)¹⁸



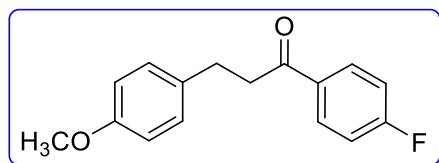
Pale yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 7.96 – 7.92 (m, 2H), 7.17 (d, *J* = 8.6 Hz, 2H), 6.94 – 6.90 (m, 2H), 6.86 – 6.82 (m, 2H), 3.86 (s, 3H), 3.79 (s, 3H), 3.23 – 3.19 (m, 2H), 3.00 (t, *J* = 7.2 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 197.98, 163.46, 158.00, 133.51, 130.32, 130.04, 129.37, 113.95, 113.75, 55.45, 55.26, 40.34, 29.51.

3-(4-Chlorophenyl)-1-(4-methoxyphenyl)propan-1-one (20t) (CAS: 111302-55-7)¹⁹



White solid. ¹H NMR (400 MHz, CDCl₃) 7.95 – 7.91 (m, 2H), 7.26 – 7.24 (m, 2H), 7.18 (d, *J* = 8.3 Hz, 2H), 6.94 – 6.91 (m, 2H), 3.87 (s, 3H), 3.23 (t, *J* = 7.6 Hz, 2H), 3.03 (t, *J* = 7.6 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 197.43, 163.56, 139.94, 131.83, 130.30, 129.83, 128.58, 113.79, 55.48, 39.78, 29.59.

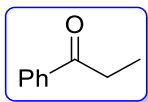
1-(4-Fluorophenyl)-3-(4-methoxyphenyl)propan-1-one (20u)²⁰



White solid. ¹H NMR (400 MHz, CDCl₃) δ 8.00 – 7.95 (m, 2H), 7.18 – 7.09 (m, 4H), 6.86 – 6.82 (m, 2H), 3.79 (s, 3H), 3.26 – 3.22 (m, 2H), 3.02 – 2.99 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 197.76, 165.67 (d, *J* = 253.0

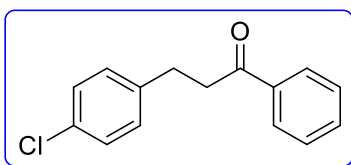
Hz), 158.01, 133.32 (d, $J = 3.0$ Hz), 133.13, 130.64 (d, $J = 9.1$ Hz), 129.34, 115.63 (d, $J = 21.7$ Hz), 113.94, 55.21, 40.57, 29.22.

Propiophenone (20v) (CAS: 93-55-0)²¹



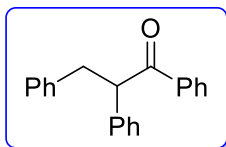
Yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.97 – 7.95 (m, 2H), 7.56 – 7.43 (m, 3H), 3.02 – 2.97 (m, 2H), 1.22 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 200.40, 136.69, 132.61, 128.31, 127.71, 31.49, 7.97.

3-(4-Chlorophenyl)-1-phenylpropan-1-one (20w) (CAS: 5739-39-9)¹⁰



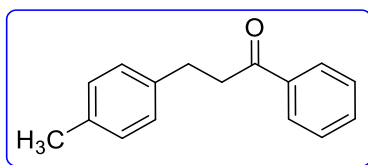
White solid. ^1H NMR (400 MHz, CDCl_3) δ 7.96 – 7.94 (m, 2H), 7.56 (t, $J = 7.3$ Hz, 1H), 7.46 (t, $J = 7.8$ Hz, 2H), 7.26 (t, $J = 4.1$ Hz, 3H), 7.18 (d, $J = 8.3$ Hz, 2H), 3.28 (t, $J = 7.5$ Hz, 2H), 3.04 (t, $J = 7.5$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 198.86, 139.75, 136.80, 133.16, 132.20, 131.90, 129.82, 128.64, 128.02, 40.14, 29.40.

1,2,3-Triphenylpropan-1-one (20x) (CAS: 4842-45-9)²²



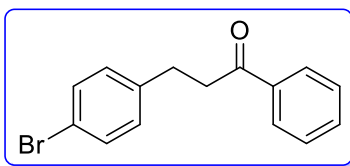
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.91 (d, $J = 7.5$ Hz, 2H), 7.46 (t, $J = 7.3$ Hz, 1H), 7.36 (t, $J = 7.7$ Hz, 2H), 7.30 – 7.13 (m, 8H), 7.10 (d, $J = 7.0$ Hz, 2H), 4.83 (t, $J = 7.3$ Hz, 1H), 3.58 (dd, $J = 13.7$, 7.5 Hz, 1H), 3.08 (dd, $J = 13.7$, 7.0 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.27, 139.81, 139.11, 136.79, 132.85, 129.15, 128.91, 128.70, 128.49, 128.32, 128.24, 127.16, 126.14, 55.95, 40.15.

1-Phenyl-3-(p-tolyl)propan-1-one (20y) (CAS: 1669-50-7)¹³



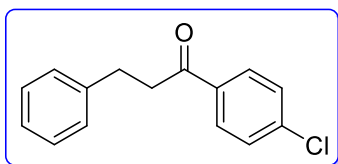
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.97 (d, $J = 7.5$ Hz, 2H), 7.56 (t, $J = 7.3$ Hz, 1H), 7.46 (t, $J = 7.6$ Hz, 2H), 7.14 (q, $J = 7.9$ Hz, 4H), 3.29 (t, $J = 7.7$ Hz, 2H), 3.04 (t, $J = 7.7$ Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.36, 138.21, 136.94, 135.63, 133.02, 129.22, 128.60, 128.30, 128.06, 40.61, 29.74, 21.00.

3-(4-Bromophenyl)-1-phenylpropan-1-one (20z) (CAS: 52168-41-9)¹⁷



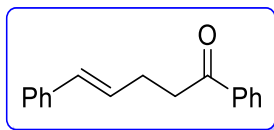
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.95 (d, *J* = 7.3 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 2H), 7.13 (d, *J* = 8.3 Hz, 2H), 3.28 (t, *J* = 7.5 Hz, 2H), 3.03 (t, *J* = 7.5 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 198.83, 140.29, 136.75, 133.20, 131.57, 130.27, 128.67, 128.03, 119.91, 40.08, 29.44.

1-(4-Chlorophenyl)-3-phenylpropan-1-one (20aa) (CAS: 5739-37-7)¹⁷



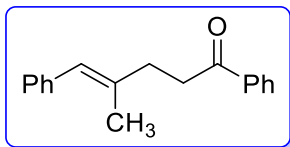
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.93 – 7.84 (m, 2H), 7.48 – 7.37 (m, 2H), 7.30 – 7.17 (m, 5H), 3.30 – 3.22 (m, 2H), 3.04 (t, *J* = 7.6 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 197.96, 141.03, 139.48, 135.13, 129.43, 128.90, 128.55, 128.39, 126.20, 40.41, 30.02.

(*E*)-1,5-Diphenylpent-4-en-1-one (25a) (CAS: 28069-36-5)²³



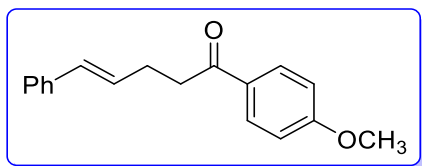
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.99 (d, *J* = 7.7 Hz, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.34 (d, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 6.47 (d, *J* = 15.9 Hz, 1H), 6.34 – 6.26 (m, 1H), 3.16 (t, *J* = 7.3 Hz, 2H), 2.66 (q, *J* = 7.2 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 199.36, 137.44, 136.89, 133.06, 130.78, 129.12, 128.61, 128.49, 128.04, 127.06, 126.01, 38.25, 27.49.

(*E*)-4-Methyl-1,5-diphenylpent-4-en-1-one (25b)²⁴



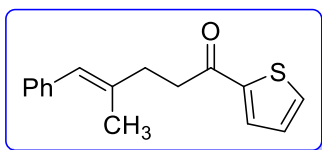
Yellow solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.01 – 7.99 (m, 2H), 7.60 – 7.56 (m, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.24 – 7.18 (m, 3H), 6.34 (s, 1H), 3.23 – 3.19 (m, 2H), 2.62 (t, *J* = 7.6 Hz, 2H), 1.92 (d, *J* = 1.4 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 199.75, 138.19, 137.62, 136.96, 133.01, 128.79, 128.61, 128.06, 128.02, 126.02, 125.50, 37.33, 34.92, 17.95.

(E)-1-(4-Methoxyphenyl)-5-phenylpent-4-en-1-one (25c)²⁵



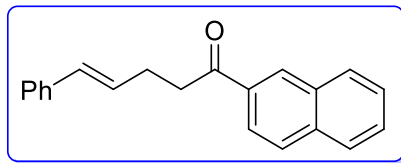
Yellow solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.98 (d, *J* = 8.9 Hz, 2H), 7.36 (d, *J* = 7.3 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 6.95 (d, *J* = 8.9 Hz, 2H), 6.47 (d, *J* = 15.8 Hz, 1H), 6.35 – 6.27 (m, 1H), 3.86 (s, 3H), 3.10 (t, *J* = 7.4 Hz, 2H), 2.66 (q, *J* = 6.9 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 197.92, 163.49, 137.56, 130.71, 130.36, 130.06, 129.41, 128.54, 127.08, 126.07, 113.79, 55.49, 37.93, 27.76.

(E)-4-Methyl-5-phenyl-1-(thiophen-2-yl)pent-4-en-1-one (25d)



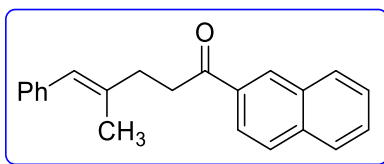
Yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.78 – 7.77 (m, 1H), 7.64 (d, *J* = 4.8 Hz, 1H), 7.36 – 7.32 (m, 2H), 7.26 – 7.20 (m, 3H), 7.16 – 7.14 (m, 1H), 6.37 (s, 1H), 3.19 – 3.11 (m, 2H), 2.65 (t, *J* = 7.6 Hz, 2H), 1.94 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 192.64, 144.30, 138.16, 137.39, 133.60, 131.85, 128.83, 128.14, 128.07, 126.10, 125.71, 38.13, 35.27, 17.94. HRMS (*m/z*): [*M*+*H*]⁺ calcd for 257.0995, found 257.0999.

(E)-1-(Naphthalen-2-yl)-5-phenylpent-4-en-1-one (25e)²⁵



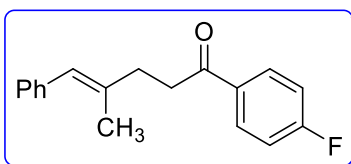
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.51 (s, 1H), 8.07 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.90 (t, *J* = 8.6 Hz, 2H), 7.63 – 7.54 (m, 2H), 7.37 (t, *J* = 7.2 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 6.52 (d, *J* = 15.8 Hz, 1H), 6.36 (dt, *J* = 15.8, 6.8 Hz, 1H), 3.30 (t, *J* = 7.4 Hz, 2H), 2.73 (q, *J* = 6.8 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 199.25, 137.51, 135.61, 134.29, 132.58, 130.88, 129.69, 129.58, 129.21, 128.52, 128.45, 127.80, 127.10, 126.79, 126.07, 123.90, 38.38, 27.69.

(E)-4-Methyl-1-(naphthalen-2-yl)-5-phenylpent-4-en-1-one (25f)



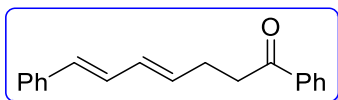
White solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.52 (s, 1H), 8.07 (d, $J = 8.6$ Hz, 1H), 7.99 (d, $J = 8.0$ Hz, 1H), 7.90 (t, $J = 8.8$ Hz, 2H), 7.63 – 7.55 (m, 2H), 7.35 – 7.31 (m, 2H), 7.26 – 7.18 (m, 3H), 6.38 (s, 1H), 3.36 – 3.32 (m, 2H), 2.74 – 2.64 (m, 2H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.68, 138.26, 137.72, 135.61, 134.36, 132.60, 129.66, 129.57, 128.85, 128.50, 128.43, 128.07, 127.80, 126.79, 126.07, 125.61, 123.95, 37.47, 35.12, 18.04. HRMS (m/z): $[\text{M}+\text{H}]^+$ calcd for 301.1587, found 301.1591.

(E)-1-(4-Fluorophenyl)-4-methyl-5-phenylpent-4-en-1-one (25g)



Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 8.05 – 8.01 (m, 2H), 7.33 (t, $J = 8.6$ Hz, 2H), 7.26 – 7.21 (m, 3H), 7.19 – 7.13 (t, $J = 8.6$ Hz, 2H), 6.34 (s, 1H), 3.20 – 3.16 (m, 2H), 2.63 (t, $J = 7.6$ Hz, 2H), 1.93 (d, $J = 0.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 198.09, 165.75 (d, $J = 254.2$ Hz), 138.19, 137.50, 130.72 (d, $J = 9.3$ Hz), 128.84, 128.09, 127.66, 126.12, 125.66, 115.73 (d, $J = 21.9$ Hz), 37.29, 34.93, 17.98. HRMS (m/z): $[\text{M}+\text{H}]^+$ calcd for 269.1336, found 269.1344.

(4E, 6E)-1,7-diphenylhepta-4,6-dien-1-one (26)



Yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ (ppm) 7.98 (d, $J = 7.7$ Hz, 2H), 7.57 (t, $J = 7.3$ Hz, 1H), 7.48 (t, $J = 7.4$ Hz, 2H), 7.38 (d, $J = 7.7$ Hz, 2H), 7.31 (t, $J = 7.3$ Hz, 2H), 7.21 (t, $J = 7.2$ Hz, 1H), 6.76 (dd, $J = 15.6, 10.4$ Hz, 1H), 6.48 (d, $J = 15.7$ Hz, 1H), 6.30 (dd, $J = 15.0, 10.5$ Hz, 1H), 5.94 – 5.87 (m, 1H), 3.12 (t, $J = 7.3$ Hz, 2H), 2.61 (q, $J = 7.2$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ (ppm) 199.30, 137.51, 136.94, 133.66, 133.09, 131.49, 130.84, 129.02, 128.65, 128.60, 128.08, 127.28, 126.23, 38.19, 27.34. HRMS (m/z): $[\text{M}+\text{H}]^+$ calcd for 262.1358, found 262.1355.

4. General procedure for cyclizative degradation of poly(phenyl vinyl ketone) (29)

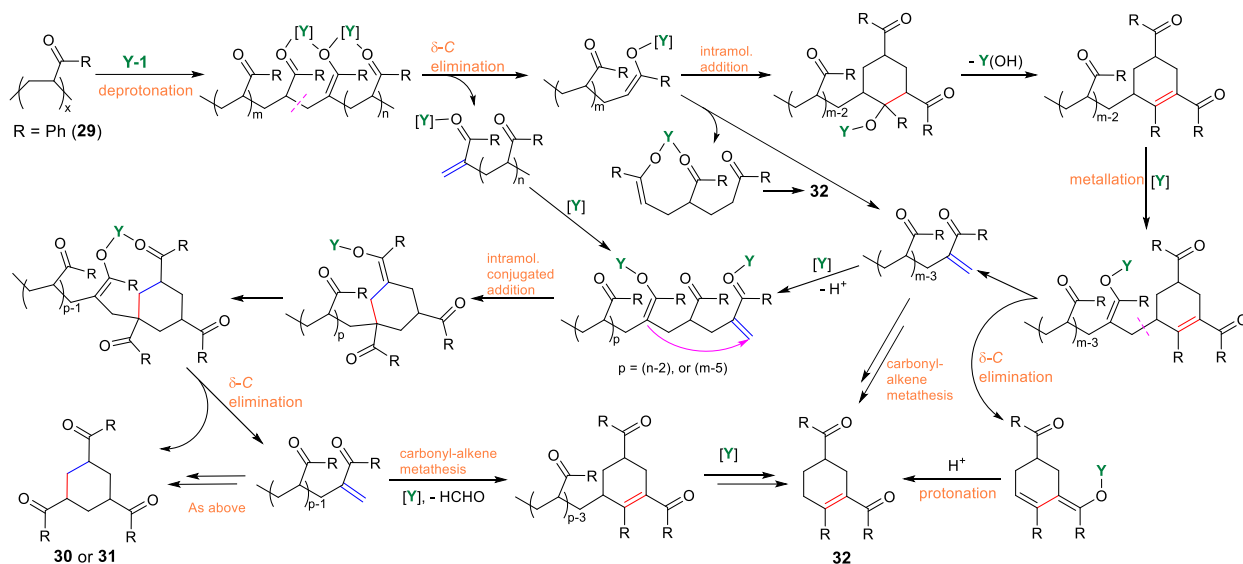
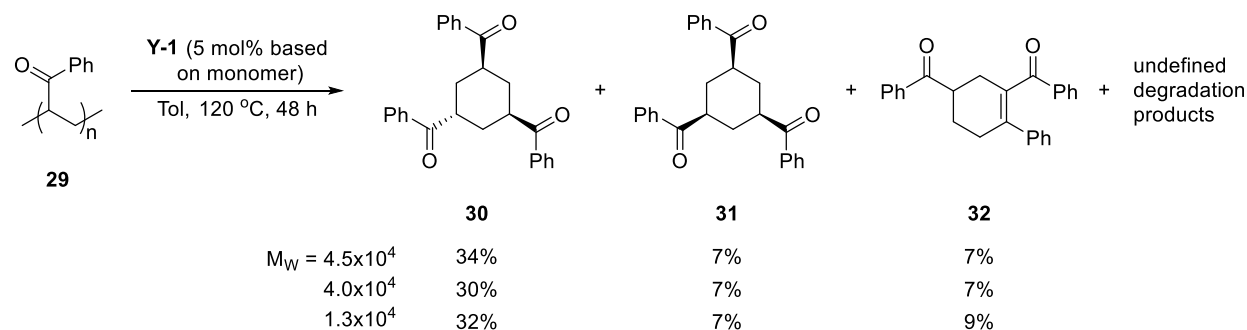


Fig. S1. Proposed pathways for the formation of compounds **30** - **32**

To a 10 mL Schlenk tube equipped with a stir bar was charged with dried **29** (0.106 g), **Y-1** (23 mg, 5 mol% based on monomer) and toluene (2.0 mL) in the glove box. Then, the tube was sealed and removed out from the glove box. After being heated in a pie-block at 120 °C for 2 days, the reaction was quenched by the addition of 0.10 M HCl and adjusted to pH = 6, extracted with ethyl acetate (3 × 20 mL). The combined organic layer was washed with brine (1 × 20 mL), dried over Na₂SO₄, filtered and evaporated. The crude products were purified by column chromatography over silica gel (ethyl acetate/petroleum ether, from 1:10 to 1:3) to give the pure products **30** - **32**. The residue was a complex mixture. Attempts to further isolate and characterize structurally more components from the residue have been unsuccessful. Yield of each component was determined by ¹H NMR of crude product using 1,3,5-trimethoxybenzene as internal standard. Crystals of **32** suitable to X-ray single diffraction analysis were obtained by its recrystallization in ethyl acetate.



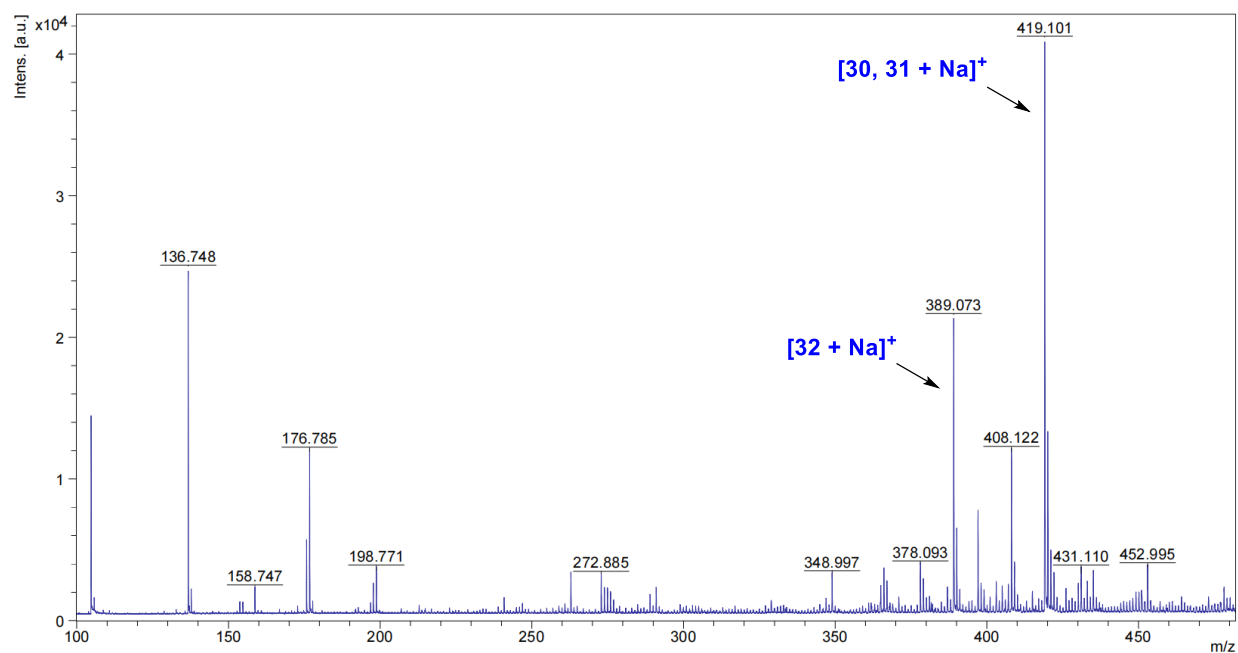
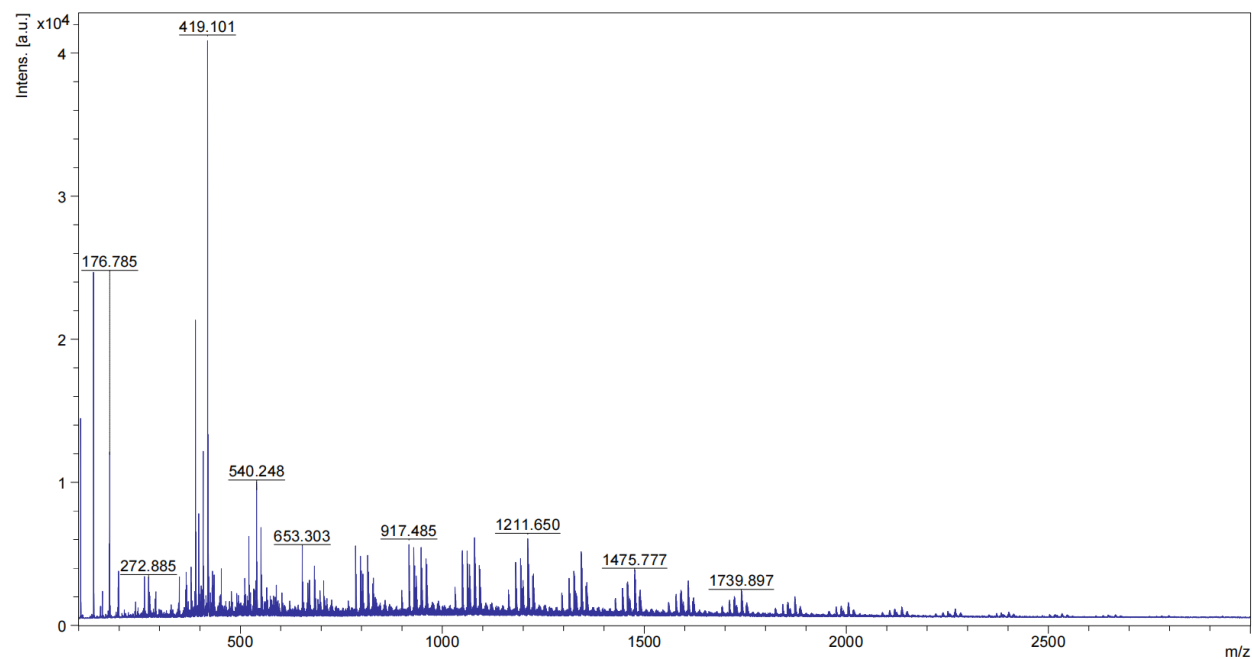


Fig. S2. MALDI-TOF analysis of degradation products of sample **II**. The spectrum was acquired in linear, positive mode with DHB (matrix).

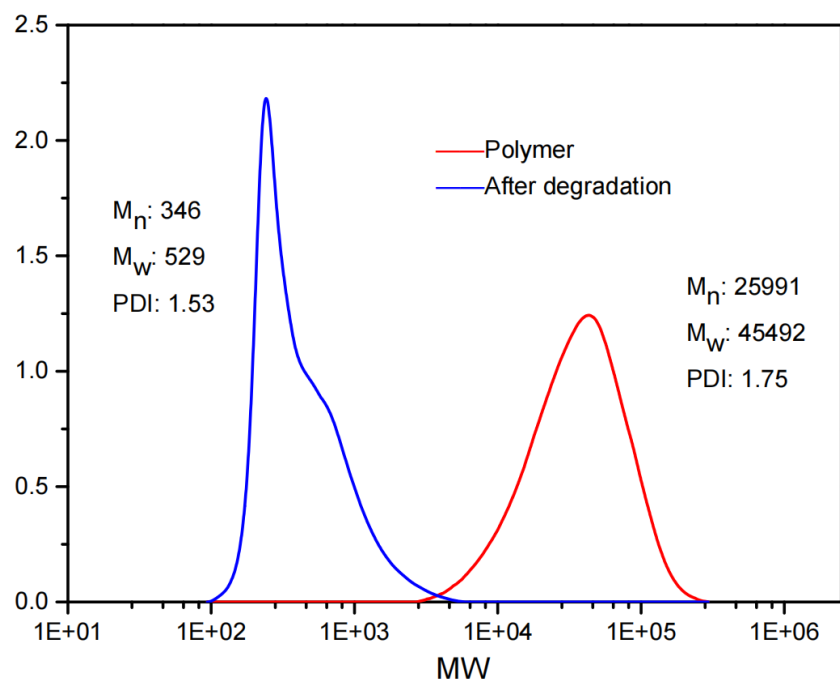


Fig. S3. GPC profiles of sample **I** (red) and its degradation products (blue).

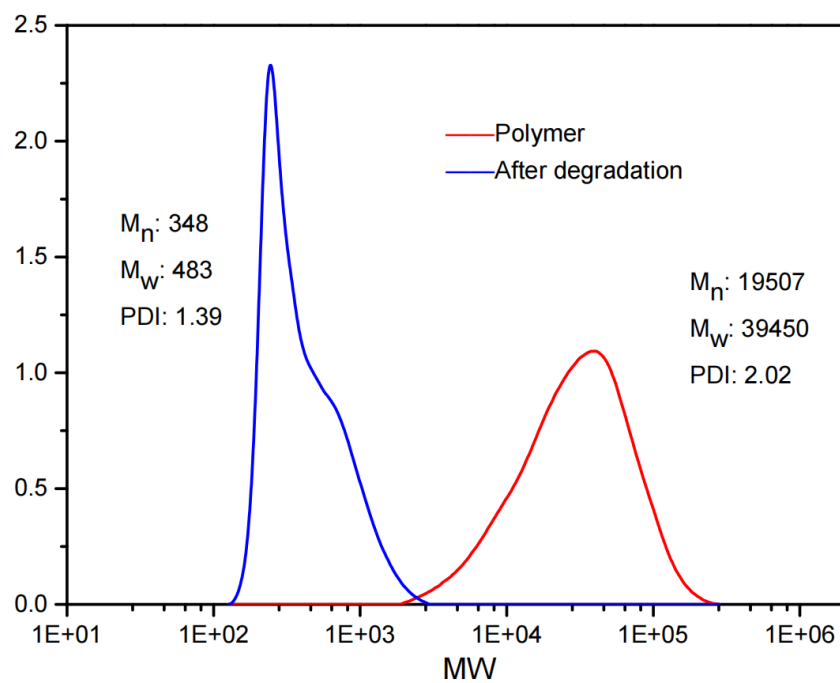


Fig. S4. GPC profiles of sample **II** (red) and its degradation products (blue).

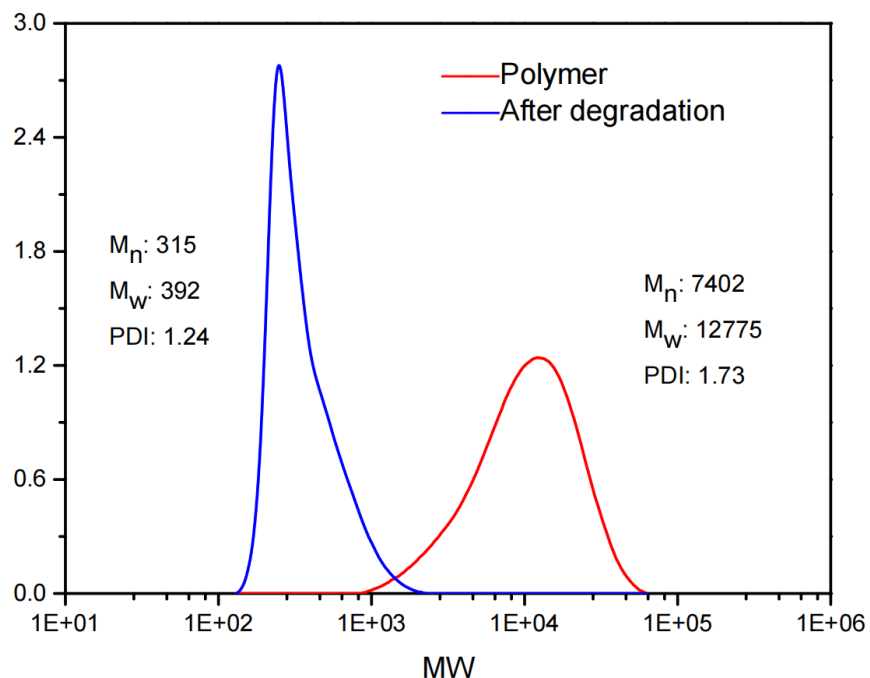
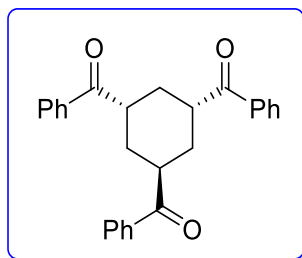


Fig. S5. GPC profiles of sample **III** (red) and its degradation products (blue).

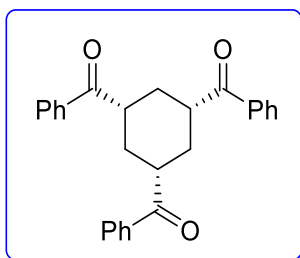
Characterization of products

r-1,1,cis-3,trans-5-tribenzoylcyclohexane (30)



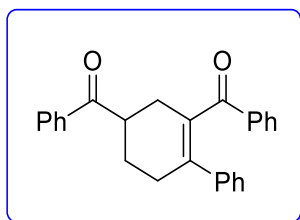
^1H NMR (400 MHz, CDCl_3) δ 8.00 – 7.94(m, 6H), 7.60 (t, J = 7.3 Hz, 1H), 7.53 – 7.49 (m, 4H), 7.40 (t, J = 7.7 Hz, 4H), 3.97 – 3.94 (m, 1H), 3.87 (tt, J = 12.1, 2.9 Hz, 2H), 2.41 (d, J = 13.7 Hz, 2H), 2.12 (d, J = 13.5 Hz, 1H), 1.92 (td, J = 13.3, 5.5 Hz, 2H), 1.81 (q, J = 12.3 Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 204.24, 202.26, 135.95, 135.65, 133.22, 133.03, 128.89, 128.65, 128.39, 128.34, 40.64, 40.54, 31.06, 30.29. HRMS: for $[\text{M}+\text{H}]^+$ calcd. 397.1798, found: 397.1801.

r-1,1,cis-3,cis-5-tribenzoylcyclohexane (31)²⁶



¹H NMR (400 MHz, CDCl₃) δ 7.95 (d, *J* = 8.1 Hz, 6H), 7.56 (t, *J* = 7.2 Hz, 3H), 7.47 (t, *J* = 7.5 Hz, 6H), 3.66 (t, *J* = 12.1 Hz, 3H), 2.22 (d, *J* = 13.4 Hz, 3H), 1.84 (q, *J* = 12.6 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 201.35, 135.94, 133.16, 128.78, 128.24, 44.48, 31.47.

1,5-dibenzoyl-2-phenylcyclohexene (32)



¹H NMR (400 MHz, CDCl₃) δ 8.03 (d, *J* = 7.3 Hz, 2H), 7.72 (d, *J* = 7.3 Hz, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 2H), 7.14 – 7.00 (m, 5H), 3.87 – 3.73 (m, 1H), 2.91 – 2.54 (m, 4H), 2.25 (dd, *J* = 9.1, 4.7 Hz, 1H), 2.12 – 2.01 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 202.51, 200.59, 140.93, 139.47, 136.73, 136.00, 133.95, 133.18, 132.55, 129.27, 128.78, 128.36, 128.02, 127.99, 127.95, 127.45, 40.88, 30.61, 30.48, 25.97. HRMS: for [M+H]⁺ calcd. 367.1333, found: 367.1697.

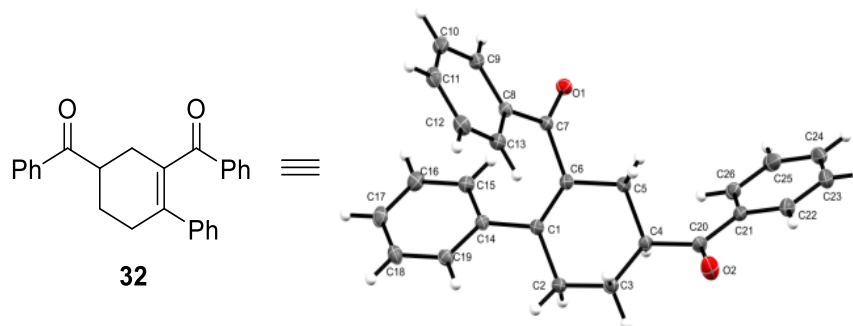


Fig. S6. Molecular structure of 32 (Thermal ellipsoids at 30% level; all the hydrogen atoms are omitted for clarity). Selected bond lengths (Å) and bond angles (deg): C7–O1 1.22(1), C1–C2 1.51(2), C1–C6 1.34(2), C2–C3 1.52(2), C3–C4 1.52(2), C4–C5 1.54(2), C5–C6 1.51(2), C4–C20 1.52(2), C20–O2 1.21(2), C11–C12–C13 113.0(1), O1–C7–C6 120(1), O1–C7–C8 120(1), C5–C6–C1 124(1), O2–C20–C4 121(1), O2–C20–C21 120(1).

5. Applications of the C–C hydrogenolysis reaction in the late-stage modification of the side-chain of 2-substituted pyridines

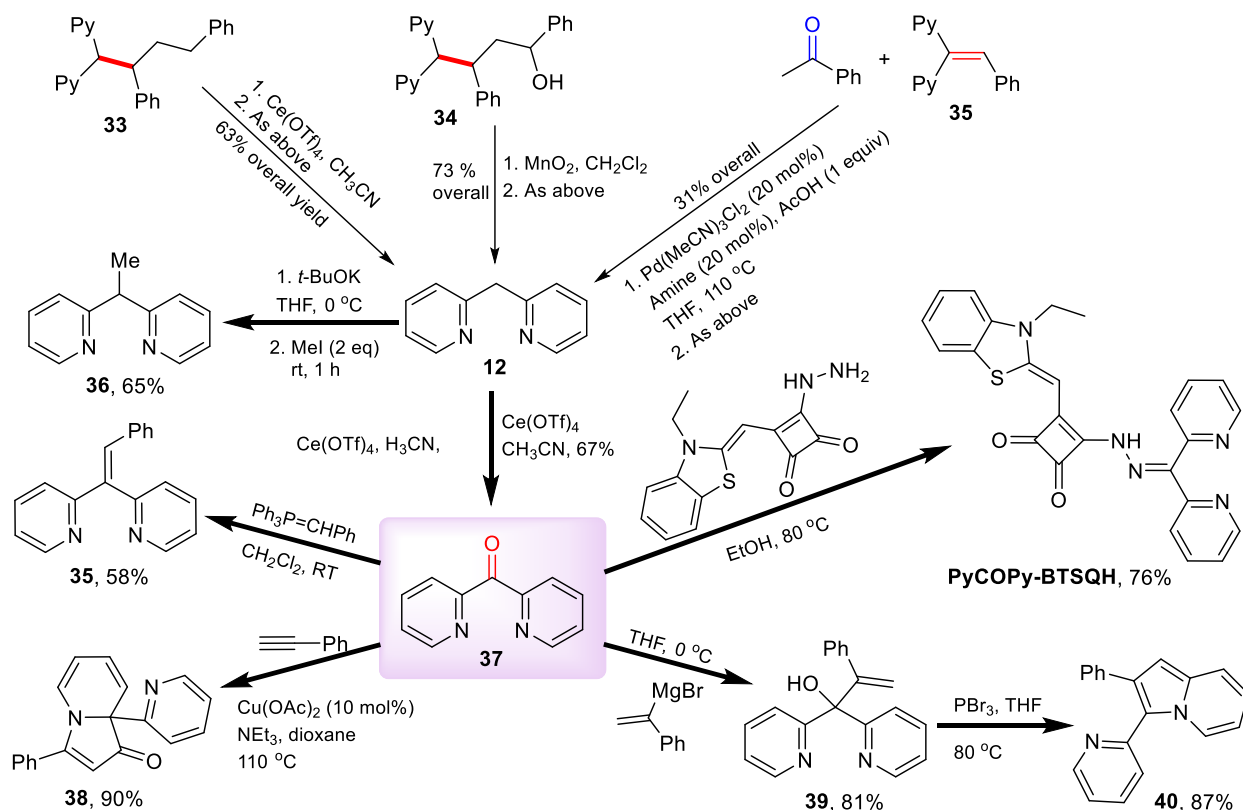
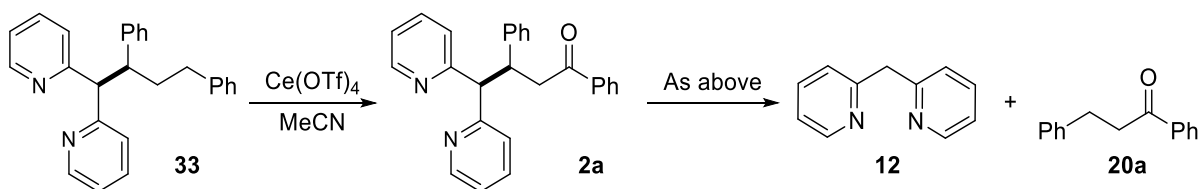


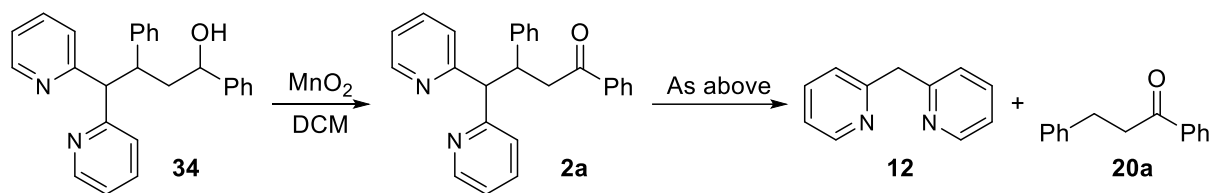
Fig. S7. Representative examples of applications of the C–C hydrogenolysis protocol in side chain reduction and late-stage modification of 1,1-di(pyridin-2-yl)alkanes.

Two-step removal of alkyl from **33**



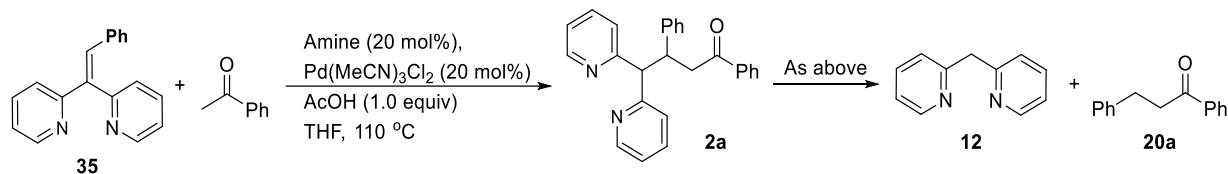
To a stirred solution of **33** (5.0 mmol) in $\text{CH}_3\text{CN}/\text{H}_2\text{O}$ (v/v = 2:1, 3 mL) was added $\text{Ce}(\text{OTf})_4$ (20 mmol). The resulting mixture was stirred at room temperature until the complete consumption of **33** (monitored by TLC). The reaction mixture was diluted with water and extracted with DCM. The combined organic extracts were washed with brine, dried over anhydrous Na_2SO_4 , filtered, concentrated and purified on silica gel chromatography, affording the product **2a** (1.40 g, 74%).

Two-step removal of β -hydroxyalkyl from **34**



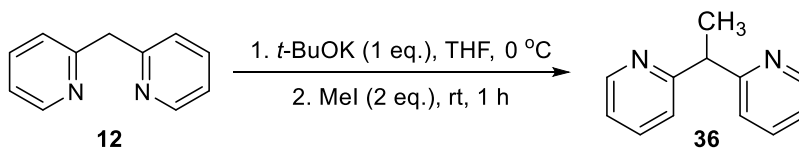
MnO₂ (50.0 mmol) was added to the solution of **34** (5.0 mmol) in DCM (20 mL). The resulting mixture was stirred at room temperature until the complete consumption of **34** (monitored by TLC). Then, the reaction mixture was filtered through a Celite Pad, and MnO₂ was washed by DCM (5 × 3 mL). The combined organic layer was concentrated to afford the crude product. The final purification was accomplished by flash chromatography (silica gel, with a mixture of petroleum ether/ethyl acetate = 1:1 as eluent) to give **2a** (1.62 g, 86%).

Two-step hydrodealkyldination of **35**



The mixture of **35** (1.0 mmol), Pd(MeCN)₃Cl₂ (0.20 mmol), *tert*-butyl (2-aminocyclohexyl)carbamate (0.20 mmol), acetophenone (6.0 mmol) and AcOH (1.0 mmol) in THF (2 mL) was heated at 110 °C for 24 h under N₂ atmosphere. Then, the solution was evaporated and the residue was purified by flash column chromatography (PE/EA = 1:1) on silica gel to afford the desired product **2a** (0.136 g, 36%).

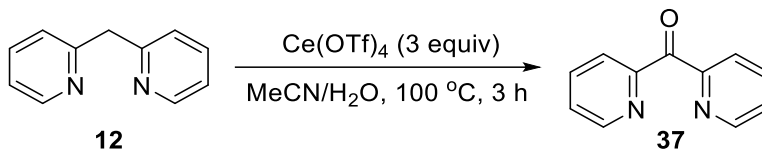
Synthesis and characterization of 1,1-dipyridylethane (**36**) (CAS: 29280-41-9)²⁷



Di(pyridin-2-yl)methane **12** (1.0 mmol) was dissolved in 5 mL of THF in a 20 mL Schlenk flask equipped with a stir bar. The solution was cooled to 0 °C and *t*-BuOK (1.0 mmol) was added slowly. After stirring for 15 min, methyl iodide (2.0 mmol) was added dropwise. The reaction was subsequently warmed to room temperature for 1 h, and hydrolyzed with ice. The aqueous layer was separated and extracted three times with CH₂Cl₂. The combined organic layer was dried over anhydrous Na₂SO₄, filtered and evaporated. The crude product was

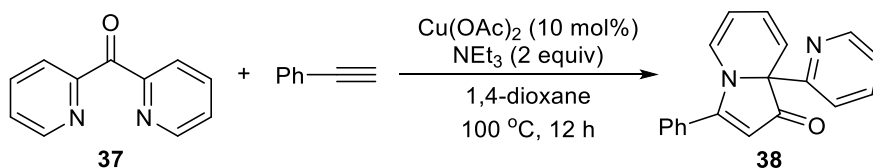
purified by silica gel column chromatography with 1:1 ethyl acetate/petroleum ether as an eluent, yielding **36** as light yellow liquid (119.8 mg, 65%). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.55 – 8.54 (m, 2H), 7.59 (td, *J* = 7.7, 1.8 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.12 – 7.09 (m, 2H), 4.46 (q, *J* = 7.2 Hz, 1H), 1.76 (d, *J* = 7.2 Hz, 3H).

Synthesis of di(2-pyridyl)methanone (**37**) (CAS:19437-26-4)²⁸



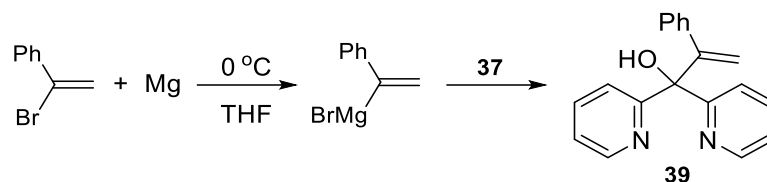
Cerium(IV) trifluoromethanesulfonate (3.0 mmol) was added at once to a vigorously stirred solution of substrate **12** (0.50 mmol) in MeCN/H₂O (1:1 v/v 5 ml) at rt. The mixture was stirred at 100 °C for 3 h, quenched with saturated NH₄Cl solution (5 mL) and extracted with ethyl acetate (3 × 5 mL). The combined organic layer was dried with anhydrous Na₂SO₄, filtered, evaporated and purified by flash column chromatography using hexane/ethyl acetate as eluent, giving **37** as white solid (61.7 mg, 67%). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.70 (d, *J* = 4.7 Hz, 2H), 8.05 (d, *J* = 7.8 Hz, 2H), 7.86 – 7.82 (m, 2H), 7.45 – 7.42 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 193.00, 154.33, 149.18, 136.75, 126.40, 125.23. HRMS (*m/z*): [M+H]⁺ calcd for 184.0637, found 184.1980.

Synthesis of 3-phenyl-8a-(pyridin-2-yl)indolizin-1(8aH)-one (**38**)²⁹



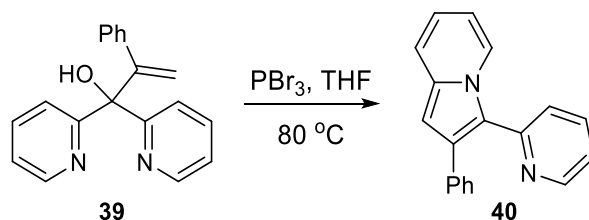
To a Teflon screw-cock vial containing a stir bar, **37** (0.30 mmol), phenylacetylene (0.60 mmol), Cu(OAc)₂ (0.03 mmol), NEt₃ (0.60 mmol) and 1,4-dioxane (2 mL) were added. The reaction mixture was heated at 110 °C for 12 hours. After cooling down to room temperature, volatiles were removed. The residue was purified by flash chromatography on a short silica gel to provide the target product **38** as dark brown solid in 90% yield. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.57 – 8.56 (m, 1H), 7.65 – 7.61 (m, 3H), 7.52 – 7.47 (m, 4H), 7.14 (ddd, *J* = 7.4, 4.8, 1.0 Hz, 1H), 6.70 (d, *J* = 7.2 Hz, 1H), 6.44 (d, *J* = 9.2 Hz, 1H), 6.09 (dd, *J* = 9.2, 5.4 Hz, 1H), 5.34 – 5.30 (m, 1H), 5.19 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 199.17, 175.21, 158.61, 149.48, 136.77, 131.18, 129.38, 129.05, 128.12, 124.51, 123.47, 122.68, 121.98, 120.15, 108.81, 99.40, 73.76.

Synthesis of 2-phenyl-1,1-di(pyridin-2-yl)prop-2-en-1-ol (**39**)



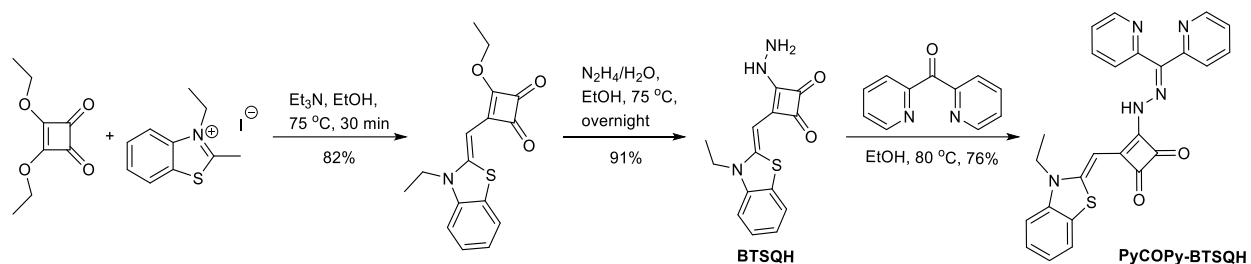
Di(pyridin-2-yl)methanone **37** (2.0 mmol) was slowly added to a stirred solution of (1-phenylvinyl)magnesium bromide (2.0 mmol) in THF, which was maintained an internal temperature below 5 °C. After stirring for 15 min, the reaction was allowed to warm to rt and stirred for additional 1 h. Then, the reaction was quenched by adding saturated NH₄Cl aqueous solution and extracted with Et₂O. The combined organic extracts were washed with brine, dried over anhydrous MgSO₄, filtered, concentrated and purified on silica gel chromatography with 1:5 ethyl acetate/petroleum ether as eluent, giving the allylic alcohol **39**. White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.51 (d, *J* = 4.7 Hz, 2H), 7.91 (d, *J* = 8.0 Hz, 2H), 7.64 (t, *J* = 7.5 Hz, 2H), 7.35 – 7.33 (m, 2H), 7.15 – 7.12 (m, 5H), 6.92 (s, 1H), 5.49 (s, 1H), 4.86 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 162.06, 153.78, 147.40, 140.83, 136.40, 128.54, 127.56, 126.92, 123.15, 122.22, 118.71, 81.42.

Synthesis of 2-phenyl-3-(pyridin-2-yl)indolizine (**40**)



To a solution of **39** (144 mg, 0.50 mmol) in THF (2.0 mL) was added PBr₃ (1.5 mmol). The mixture was stirred at room temperature for 0.5 h, and then heated at 80 °C for 2 h. After cooling in an ice water bath, the reaction was quenched by water. The pH of the mixture was adjusted to 11 by the addition of sodium carbonate, and the mixture was then extracted with ethyl acetate. The combined organic layer was dried over anhydrous Na₂SO₄, and evaporated in vacuum. The residue was purified on silica gel chromatography to give **40** (118 mg, 87%) as dark green solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.68 (d, *J* = 4.6 Hz, 1H), 8.13 (d, *J* = 9.1 Hz, 1H), 7.92 (d, *J* = 6.9 Hz, 1H), 7.45 – 7.26 (m, 7H), 7.03 (t, *J* = 6.3 Hz, 2H), 6.84 – 6.80 (m, 1H), 6.58 – 6.55 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 155.25, 149.32, 135.48, 135.42, 132.65, 129.51, 128.91, 128.40, 126.73, 124.98, 124.33, 119.67, 119.59, 119.49, 112.25, 111.72, 112.23.

Synthesis of (Z)-3-(2-(di(pyridin-2-yl)methylene)hydrazino)-4-((3-ethylbenzo[d]thiazol-2(3H)-ylidene)methyl) cyclobut-3-ene-1,2-dione (PyCOPy-BTSQH)³⁰



3-Ethoxy-4-((3-ethylbenzothiazol-2(3H)-ylidene)methyl)cyclobut-3-ene-1,2-dione (monosubstituted ethyl squarate) was prepared by reaction of diethyl squarate with *N*-ethyl benzothiazolium iodide in ethanol in the presence of triethylamine in 52% yield. In the next step, to an ethanol (30 mL) solution of monosubstituted ethyl squarate (301 mg, 1.0 mmol) was added hydrazine hydrate (1.0 mL). Reaction mixture was stirred at 75 °C overnight. Then volatile compounds were evaporated and the residue was suspended in methanol-diethyl ether mixture (1:1 v/v, 50 mL), filtered, washed with additional portion of methanol-diethyl ether mixture (1:1 v/v, 50 mL) and dried under vacuum at 50 °C. 3-((*N*-ethyl-1,3-benzothiazole-2(3H)-ylidene)methyl)-4-hydrazinylcyclobut-3-en-1,2-dione **BTSQH** was obtained as orange-red powder. **BTSQH** (1.0 mmol) and **37** (1.0 mmol) were dissolved in ethanol (10 mL). The mixture was heated at 75 °C overnight, then cooled to room temperature and concentrated under vacuum. The residue was purified by flash chromatography on a short silica gel to give **PyCOPy-BTSQH** as dark brown powder in 76% yield. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.72 (d, *J* = 4.3 Hz, 1H), 8.67 (d, *J* = 4.5 Hz, 1H), 7.91 – 7.79 (m, 3H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.41 – 7.32 (m, 3H), 7.27 – 7.20 (m, 2H), 7.02 – 6.95 (m, 2H), 6.36 (s, 1H), 3.97 (q, *J* = 7.1 Hz, 2H), 1.26 (t, *J* = 7.1 Hz, 3H).

6. Mechanism studies

6.1 Proposed intermediates for C–C bond cleavage

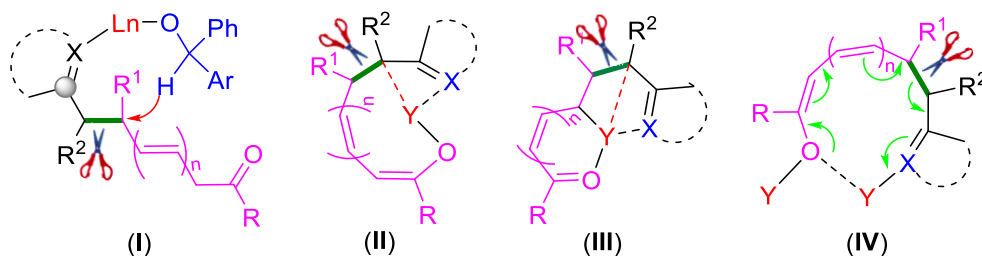


Fig. S8. Four main possible mechanisms for C–C cleavage include (1) a direct nucleophilic substitution via H-transfer from yttrium alkoxide (**I**); (2) C–H activation followed by a remote C-elimination assisted by the directing groups via a monometallic pathway (**II**); (3) β-C elimination paralleling with a β-agostic complex intermediate (**III**); and (4) a C–H activation followed by remote C-elimination assisted by the directing group and the dimetallic cooperation (**IV**).

6.2 Synthesis, structural characterization and reactivity of yttrium complex intermediates

To elucidate the mechanism of the Y-catalyzed transfer hydrogenolysis of remote and unstrained C–C bonds of ketones with alcohol, we firstly performed several stoichiometric reactions of pre-catalyst **Y-1** with two representative substrates to support the involvement of a dinuclear yttrium enolate intermediate in C–C bond cleavage and the nucleophile trapping as a driving force.

6.2.1 Reaction of **Y-1** with **9**

Complex **Y-2** was structurally characterized by single-crystal X-ray diffraction analysis (Fig. S10). The formation of **Y-2** might be attributed to the replacement of two $\text{N}(\text{TMS})_2$ ligands of **Y-1** by enolate groups followed by δ -C elimination and sequential mono- and di-insertion of the extracting α,β -unsaturated ketones into the remaining Y–N bond (Fig. S9). The result demonstrates that the addition of the extruded enone to the Y–N bond rather than the electrophile trapping of the resulting malonate anion plays a key role in driving the C–C cleavage.

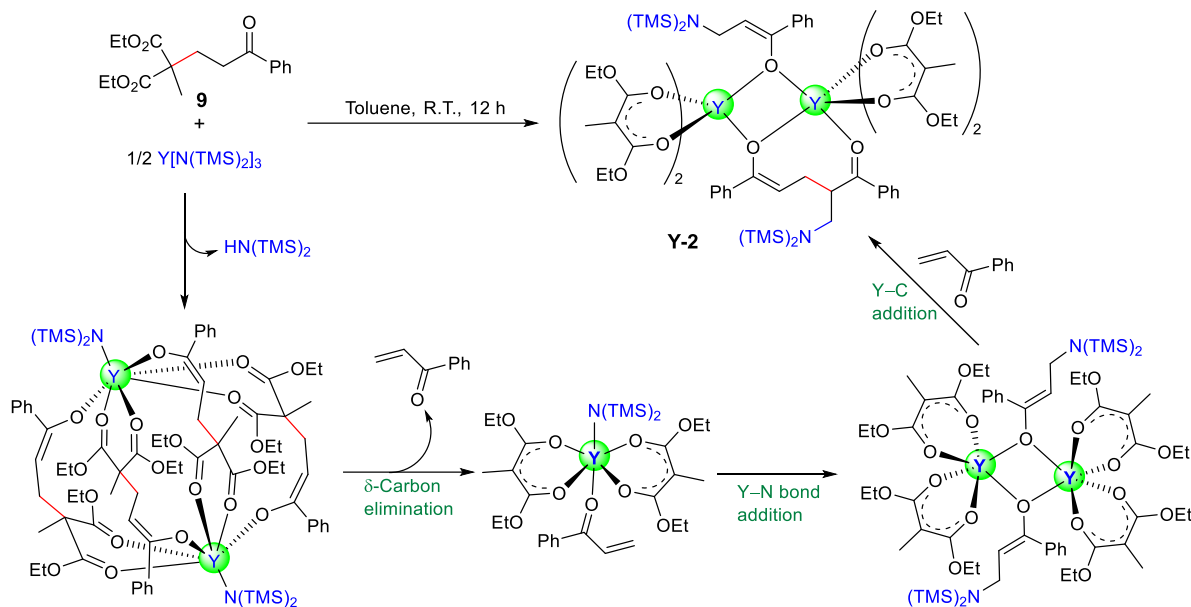


Fig. S9. Isolation of the intermediate **Y-2** involving a C–H activation of substrate **9** followed by δ -carbon elimination and subsequent addition of the resulting enone to yttrium species. A mixture of **Y-1** (569 mg, 1.0 mmol) and **9** (612 mg, 2.0 mmol) in 5 mL toluene was stirred at room temperature for 12 h. Removal of volatiles afforded **Y-2** as orange powder (487 mg, 61%). Diffusion of toluene into a THF solution of **Y-2** gave range crystals.

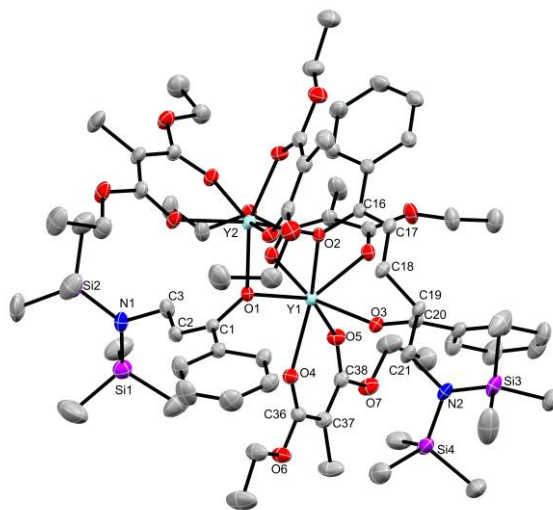


Fig. S10. Molecular structure of complex **Y-2** (thermal ellipsoids at 30% level; all the hydrogen atoms are omitted for clarity). Selected bond lengths (Å) and bond angles (deg): Y1–Y2 3.728(1), Y1–O1 2.276(2), Y1–O2 2.243(2), Y2–O1 2.324(2), Y2–O2 2.327(2), Y2–O3 2.318(2), Y1–O3 2.318(2), Y1–O4 2.243(2), Y1–O5 2.228(2), O1–C1 1.371(3), O2–C16 1.371(3), O3–C20 1.235(3), O4–C36 1.268(3), O5–C38 1.268(3), O6–C36 1.355(3), O7–C38 1.345(3), C36–C37 1.388(4), C37–C38 1.389(4), C1–C2 1.330(4), C1–C4 1.477(4), C2–C3 1.504(4), C16–C17 1.340(4), C17–C18 1.493(4), C18–C19 1.550(3), C19–C20 1.507(4), C19–C21 1.547(4), Y1–O1–Y2 108.3(1), Y1–O2–Y2 109.3(1), C1–O1–Y1 119.5(2), O4–C36–C37 128.1(3).

6.2.2 Verification of the viability for δ -carbon elimination of **Y-2**

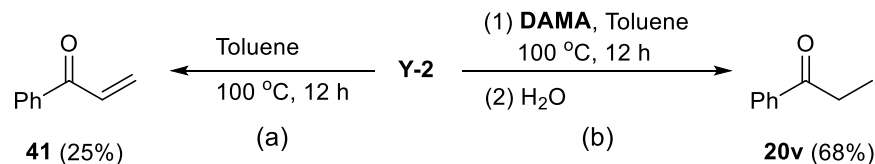


Fig. S11. Confirmation of the feasibility of the C(sp³)–C(sp³) bond cleavage via δ -carbon elimination of dinuclear yttrium enolate intermediate: (a) **Y-2** (125 mg, 0.10 mmol) and toluene (3 mL) were added to a Schlenk tube equipped with a magnetic stirring bar and a Teflon cap. After heating at 100 °C for 12 h, the reaction mixture was quenched with water (2 mL), and extracted with ethyl acetate (3 $\times$ 5 mL). The combined organic layers were dried over Na₂SO₄, filtered and evaporated under reduced pressure. Purification by flash column chromatography on silica gel with PE/EA (20:1) as eluent, gave 1-Phenylprop-2-en-1-one **41** as colourless liquid (3.3 mg, 25% yield). (b) A mixture of **Y-2** (125 mg, 0.10 mmol) and **DAMA** (21.4 mg, 0.10 mmol) in toluene (3 mL) was added to a Schlenk tube equipped with a Teflon cap. After heating at 100 °C for 12 h, the reaction mixture was quenched with water (2 mL), and extracted with ethyl acetate (3 $\times$ 5 mL). The combined organic layer was dried over Na₂SO₄, filtered and evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel with ethyl acetate/petroleum ether as eluent to give the desired product **20v** (9.0 mg, 68% based on the anionic diketone ligand).

Remarkably, the formation of **41** from thermal decomposition of **Y-2** provides a direct observation of the dimetallic cooperation-driven δ -carbon elimination from the enolate ligand. Furthermore, treatment of **Y-2** with **DAMA** at 100 °C led to the isolation of **20v** in moderate yield, indicating that the in situ trapping of the resulting enone **41** with **DAMA** is in favour of the C–C cleavage. The intermediacy of **Y-2** in the δ -carbon elimination demonstrates that the interaction of two Y³⁺ centers with a 5-carbonylpentenolate group precedes the δ -carbon elimination event and the exogenous hydrogen source is not necessary for the C–C activation step, which seems to exclude both the electrophilic C–C cleavage to a hydrogen donor (**I**) and the role of monometallic δ - or β -agostic complex intermediate (**II** and **III**) in this process.

6.2.3 Further insight into the factors that affect the δ -carbon elimination of yttrium enolate intermediates

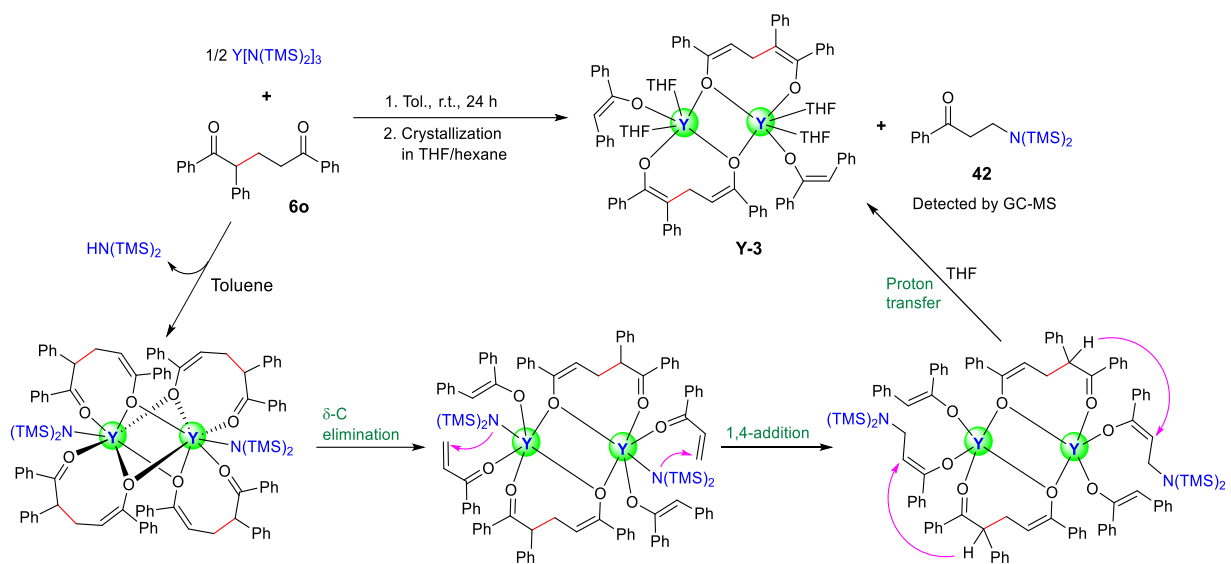


Fig. S12. Stoichiometric reaction of Y-1 with 6o. A mixture of **Y-1** (569 mg, 1.0 mmol) and **6o** (656 mg, 2.0 mmol) in toluene (5 mL) was stirred at room temperature for 24 h. Removal of volatiles afforded red powder. Diffusion of toluene into a THF solution of the orange powder gave **Y-3** as red crystals (534 mg, 71%). GC–MS analysis of the crude organic products indicated the formation of a significant amount of 3-(bis(trimethylsilyl)amino)-1-phenylpropan-1-one **42** (73% GC-content), 293 [M^+].

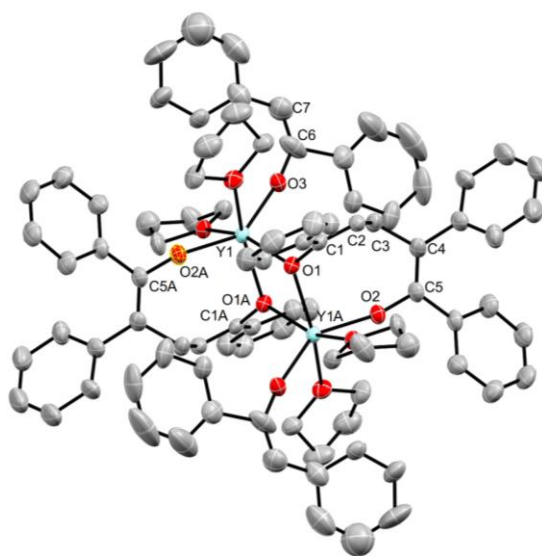


Fig. S13. Molecular structure of complex Y-3 (Thermal ellipsoids at 30% level; all the hydrogen atoms are omitted clarity). Selected bond lengths (Å) and bond angles (deg): Y1–Y1A 3.733(1), Y1–O1 2.281(4), Y1–O1A 2.274(4), Y1A–O2 2.105(4), Y1–O3

2.136(4), O1–C1 1.383(7), O2–C5 1.336(8), O3–C6 1.288(9), C1–C2 1.328(9), C2–C3 1.495(9), C3–C4 1.525(9), C4–C5 1.345(10), C6–C7 1.210(15). Y1–O1–Y1A 110.1(2), C2–C1–O1 121.1(5), C1–C2–C3 126.3(6), O2–C5–C4 121.2(6).

6.2.4 Reaction of Y-3 with DAMA

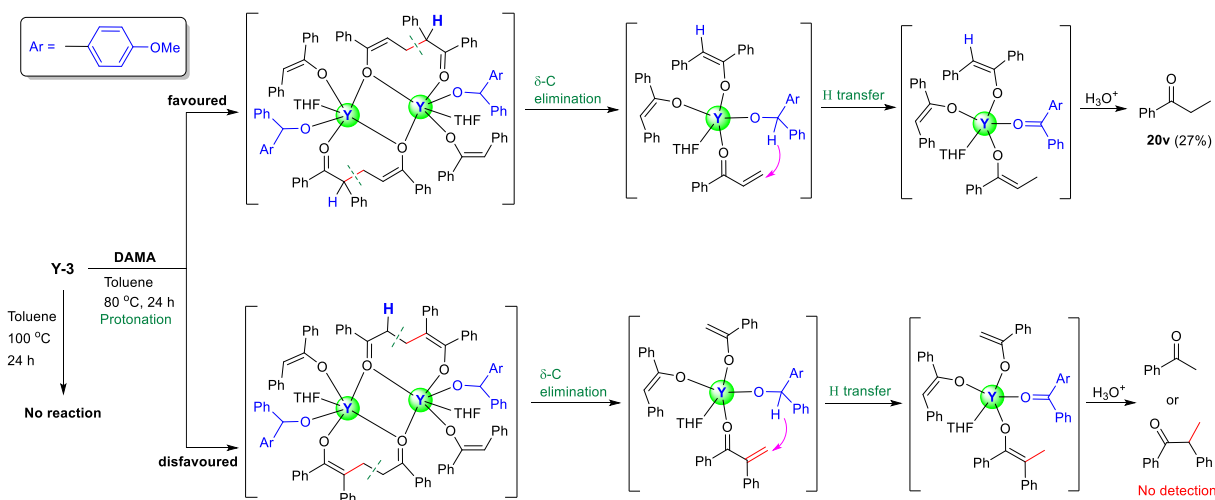


Fig. S14. Deprotonation effect and monodeprotonation regioselectivity of 1,5-diketone. A mixture of **Y-3** (150 mg, 0.10 mmol) and **DAMA** (43 mg, 0.20 mmol) in toluene (3 mL) was heated at 80 °C for 24 h, quenched with water (2 mL), and extracted with ethyl acetate (3 $\times$ 5 mL). The combined organic layer was dried over anhydrous Na_2SO_4 , filtered and evaporated. Purification of the residue by flash column chromatography on silica gel, eluting with PE/EA (20:1), gave propiophenone **20v** in 27% yield, without the observation of PhCOCH_3 or $\text{PhCOCH}(\text{Ph})\text{CH}_3$.

In contrast to **Y-2**, no reaction occurred when a toluene solution of **Y-3** was directly heated to 100 °C. It seems clear that only the monoanionic 5-oxo-1,4,5-triphenylpentenolate ligand bound to two Y^{3+} ions can undergo the δ -carbon elimination under current conditions, and the deprotonation of **6o** takes place preferentially at the position bearing less substituents adjacent to the carbonyl, which is consistent with the observations in substrate examination.

6.2.5 Examination of catalytic activation of Y-3

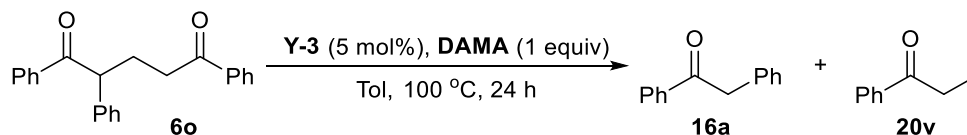


Fig. S15. Y-3-catalyzed C–C hydrogenolysis of 6o with DAMA: According to the procedure described previously, treatment of a mixture of **6o** (164 mg, 0.50 mmol) and **DAMA** (107 mg, 0.50 mmol) with **Y-3** (37.6 mg, 0.025 mmol) at 100 °C afforded **16a**

(22.5 mg, 23%) and **20v** (17 mg, 25%), respectively. This indicates that the activity of **Y-3** for catalytic reaction of **6o** with **DAMA** was nearly as same as that of **Y-1**.

These results suggest that the δ -C elimination is only suitable for the ketone-substituted enolate yttrium, while the 1,5-dienolate dianion yttrium intermediate is inert to C–C cleavage and must be protonated partly before the δ -elimination can take place. On the other hand, the results further support the mechanism (IV), but are inconsistent with mechanisms I–III.

6.2.6 Insight into the bonding mode of bis(2-benzothiazolyl)methyl anion to the Y^{3+} ion

The X-ray structural data of **Y-4**, which can model the di(2-heteroaryl)methyl yttrium intermediates formed in the C–C reduction, illustrate that the bis(2-benzothiazolyl)methyl anion ligand acts as a N,N-bidentate ligand to connect the Y^{3+} unit, and the negative charge is delocalized on the yttridacycle (Fig. S17). This hints that the assistance of such N,N-bidentate directing group systems for remote carbon elimination of yttrium enolate species possibly lies on their chelating coordination to another metal center and thus stabilizes the dative Y–C bond through the charge delocalization, where the proximity of a metal to the targeted carbon atom seem to be not prerequisite for the C–C cleavage. Attempts to isolate the metal complex intermediates from reaction of **Y-1** with **1a** have been unsuccessful.

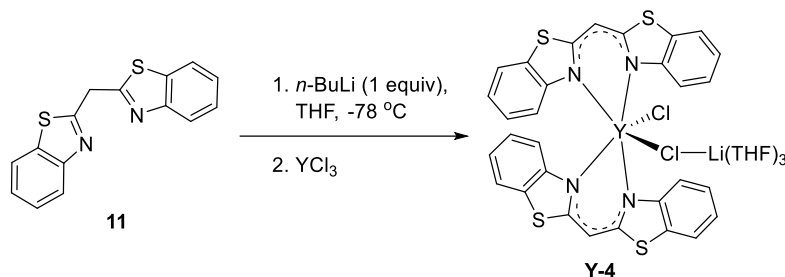


Fig. S16. Synthesis of the model complex for stabilizing the Y–C bond by the directing group. To a THF solution of compound **11** (282 mg, 1.0 mmol) was slowly added *n*-BuLi (2.5 M solution in hexane, 1.0 mmol) at $-78\text{ }^{\circ}\text{C}$ under N_2 atmosphere. After stirring at $-78\text{ }^{\circ}\text{C}$ for 1 h, the mixture was warmed to $-20\text{ }^{\circ}\text{C}$, and then added to a suspension of YCl_3 (98 mg, 0.50 mmol) in THF (3 mL). The reaction mixture was slowly warmed to room temperature and continued to stir for 12 h. Removing THF gave brown powder. Then the mixture was extracted with toluene and recrystallized in a toluene/THF afforded **Y-4** as brown crystals (327 mg, 69%).

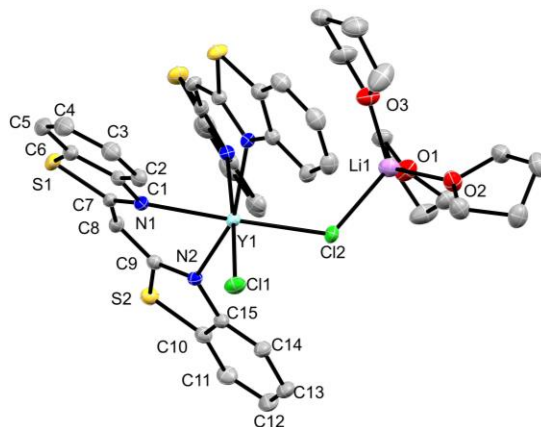


Fig. S17. Molecular structure of complex Y-4 (Thermal ellipsoids at 30% level; all the hydrogen atoms are omitted clarity). Selected bond lengths (Å): Y1–N1 2.397(2), Y1–N2 2.397(2), Y1–Cl1 2.558(1), Y1–Cl2 2.610(1), N1–C1 1.400(3), N1–C7 1.342(3), N2–C9 1.351(3), N2–C15 1.401(3), S1–C6 1.737(3), S1–C7 1.767(2), S2–C9 1.767(2), S2–C10 1.745(3), C1–C6 1.400(3), C7–C8 1.395(3), C8–C9 1.394(3), C10–C15 1.408(3), C11–C12 1.383(4).

6.2.7 Confirmation of the feasibility of Y(OCHPh₂)₃ as a key active intermediate

Preparation of Y(OCHPh₂)₃ (Y-4): To a stirred solution of **Y-1** (569 mg, 1.0 mmol) in toluene (20 mL) was added Ph₂CHOH (552 mg, 3.0 mmol). After stirring at room temperature for 12 hours, the volatiles were removed and washed by hexane (3 × 3 mL), and dried under reduced pressure, affording a white powder of **Y-4** (574 mg, 90%).

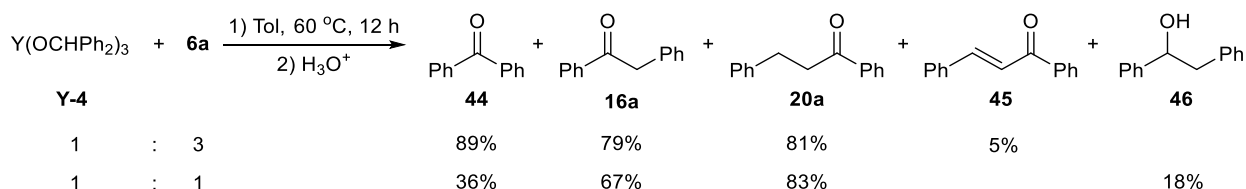


Fig. S18. Reaction of Y(OCHPh₂)₃ toward 6a: To a well stirred solution of **Y-4** (638 mg, 1.0 mmol) in toluene (5 mL) at room temperature was added **6a** (3.0 or 1.0 mmol). The reaction was subsequently heated to 60 °C for 12 h and quenched by addition of saturated NH₄Cl solution and extracted with DCM. The combined organic extracts were washed with brine, dried over anhydrous Na₂SO₄, filtered, concentrated and purified on silica gel chromatography, affording the corresponding compounds as shown above.

As shown in Fig. S18, treatment of Y(OCHPh₂)₃ with **6a** led to the formation of the expected transfer hydrogenolysis products **16a** and **20a**. Significantly, the intermediate **45** and the further reduction product **46** were respectively observed depending on the different stoichiometric ratio, which exclude the C–C cleavage

process involving mechanism **I** but support a catalytic cycle involving the abstraction of an alkoxide ligand with the ketone substrate followed by δ -C elimination and sequential H-transfer. However, attempts to isolate the yttrium complex from reaction of $Y(OCHPh_2)_3$ with **6a** have been unsuccessful so far.

6.2.8 Examination of the effects of both deprotonation capacity of substrates and basicity of catalysts on the C–C hydrogenolysis

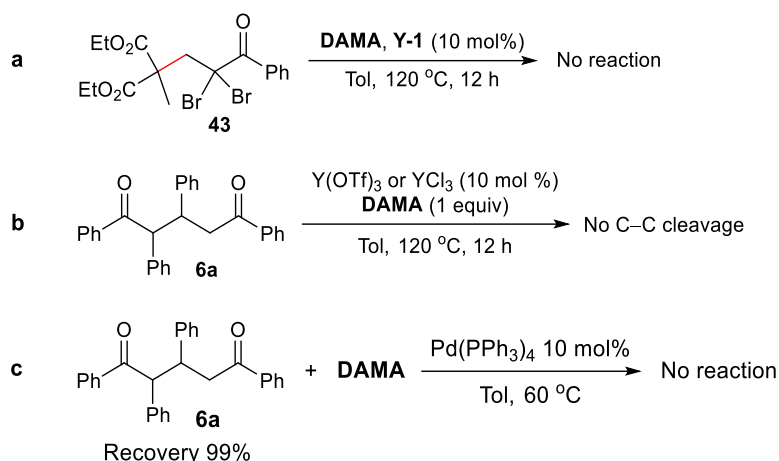
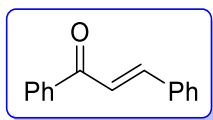


Fig. S19. Unsuccessful reactions.

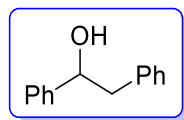
Notably, no products derived from the C–C bond cleavage were obtained even with a prolonged heating at 120 °C when the substrate **43** without the presence of an active α -C–H bond was used. It has also proven that no $C(sp^3)$ – $C(sp^3)$ cleavage reaction of **6a** took place under otherwise identical conditions when **Y-1** was replaced by insufficiently alkaline $Y(OTf)_3$ or YCl_3 or $Pd(PPh_3)_4$. These observations implied that deprotonation of ketones to form the corresponding yttrium enolate species might be an essential step for C–C bond cleavage, and mechanism **I** is unlikely.

(*E*)-Chalcone (**45**) (CAS: 94-41-7)⁷



Yellow solid. 1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.04 – 8.02 (m, 2H), 7.82 (d, J = 15.7 Hz, 1H), 7.66 – 7.64 (m, 2H), 7.61 – 7.56 (m, 2H), 7.53 – 7.49 (m, 2H), 7.43 – 7.42 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.54, 144.86, 138.25, 134.92, 132.84, 130.60, 129.01, 128.68, 128.55, 128.50, 122.12.

1,2-Diphenylethan-1-ol (46) (CAS: 614-29-9)³¹



White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.37 (d, *J* = 4.3 Hz, 4H), 7.34 – 7.29 (m, 3H), 7.27 – 7.24 (m, 1H), 7.21 (d, *J* = 7.0 Hz, 2H), 4.92 – 4.88 (m, 1H), 3.08 – 2.98 (m, 2H), 2.07 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 143.86, 138.10, 129.56, 128.54, 128.45, 127.65, 126.65, 125.95, 75.37, 46.12.

6.3 Deuterium labeling experiments

The C–C hydrogenolysis mechanism was further investigated through deuterium-labeling experiments. When *O*-*d*-**DAMA** was used, deuterium was found only at the α-position of the products **20a-d** and **16a-d**. Employing *C*-*d*-**DAMA** as the hydrogen source afforded **20a-d'** in 80% yield with 98% deuterium incorporation at the β-position. Therefore, it can be concluded that the deuterium at the α-position might result from protonation of yttrium enolate species with *O*-*d*-**DAMA**, whereas the deuterium at the β-position is more likely to come from direct D-transfer between α,β-unsaturated ketone and Y(OCD(C₆H₄OMe-*p*))Ph species through an eight-membered azametallacycle intermediate.

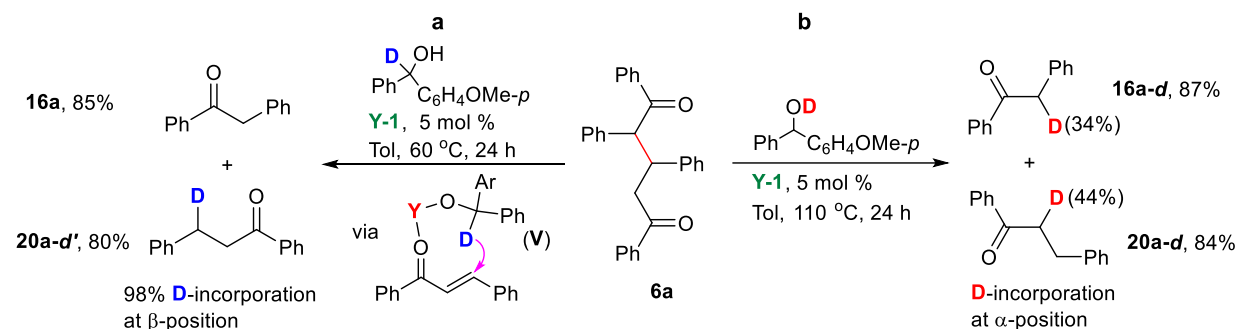
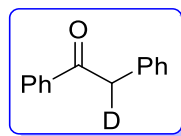


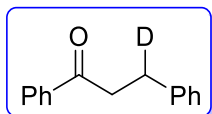
Fig. S20. **a**, A catalytic amount of **Y-1** (5 mol%) was added to a solution of **6a** (0.50 mmol) and *C*-*d*-(4-methoxyphenyl)(phenyl)methanol (0.50 mmol) in toluene (2 mL). The resulting mixture was stirred at 60 °C for 24 h and quenched with saturated NH₄Cl solution (2 mL). Then the mixture was extracted with ethyl acetate (3 × 5 mL). The organic phase was collected and dried with anhydrous Na₂SO₄, evaporated and purified by flash column chromatography using hexane/ethyl acetate as eluent, affording **16a** in 85% yield and **20a-d'** (D 98%) in 80% yield. **b**, A catalytic amount of **Y-1** (5 mol%) was added to a solution of **6a** (0.50 mmol) and *O*-*d*-(4-methoxyphenyl)(phenyl)methanol (0.50 mmol) in toluene (2 mL). The resulting mixture was stirred at 110 °C for 24 h and quenched with saturated NH₄Cl solution (2 mL). Then the mixture was extracted with ethyl acetate (3 × 5 mL). The organic phase was collected and dried with anhydrous Na₂SO₄, evaporated and purified by flash column chromatography using petroleum ether/ethyl acetate as eluent to afford the pure substrate **16a-d** (D 34%) in 87% yield and **20a-d** (D 44%) in 84% yield.

1,2-Diphenylethan-1-one-2-d (16a-d) (CAS: 84369-12-0)³²



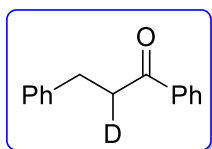
White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.03 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.1 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.36 – 7.28 (dd, *J* = 18.5, 6.6 Hz, 5H), 4.30 – 4.27 (d, *J* = 10.7 Hz, 1.64H).

1,3-Diphenylpropan-1-one-3-d (20a-d') (CAS: 93698-11-4)³³



White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.97 – 7.94 (m, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.32 – 7.19 (m, 5H), 3.32 – 3.28 (t, *J* = 7.5 Hz, 2H), 3.09 – 3.03 (m, 1H).

1,3-Diphenylpropan-1-one-2-d (20a-d)³³



White solid. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 7.97 (d, *J* = 7.7 Hz, 2H), 7.56 (t, *J* = 7.3 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.33 – 7.27 (m, 3H), 7.23 – 7.18 (m, 2H), 3.33 – 3.29 (m, 1.55H), 3.08 (t, *J* = 7.4 Hz, 2H).

6.4 ¹H NMR-monitoring the reaction of 6p and DAMA

In order to better understand the mechanism of the C–C hydrogenolysis, the reaction of **6p** with **DAMA** using **Y-1** as a catalyst was monitored by ¹H NMR spectroscopy. The ¹H NMR monitoring data (Fig. S21) reveal that addition of 10 mol% **Y-1** to a solution of **DAMA** in benzene-*d*₆ at room temperature led to the complete liberation of (Me₃Si)₂N ligand from the precatalyst rapidly, giving the free (Me₃Si)₂NH, and **Y-1** was cleanly converted into Y(OCHPh(C₆H₄Me-*p*))₃ within 5 minutes. When **6p** was added, the characteristic peaks of the target products **20a** and **DAMK** immediately appeared at 2.77 and 3.17 ppm, respectively. The C–C hydrogenolysis was significantly accelerated at 80 °C. Subsequent decrease of **6p** is consistent with the formation of **20a**. After 6 h at 80 °C the catalytic reaction reaches > 95% completion.

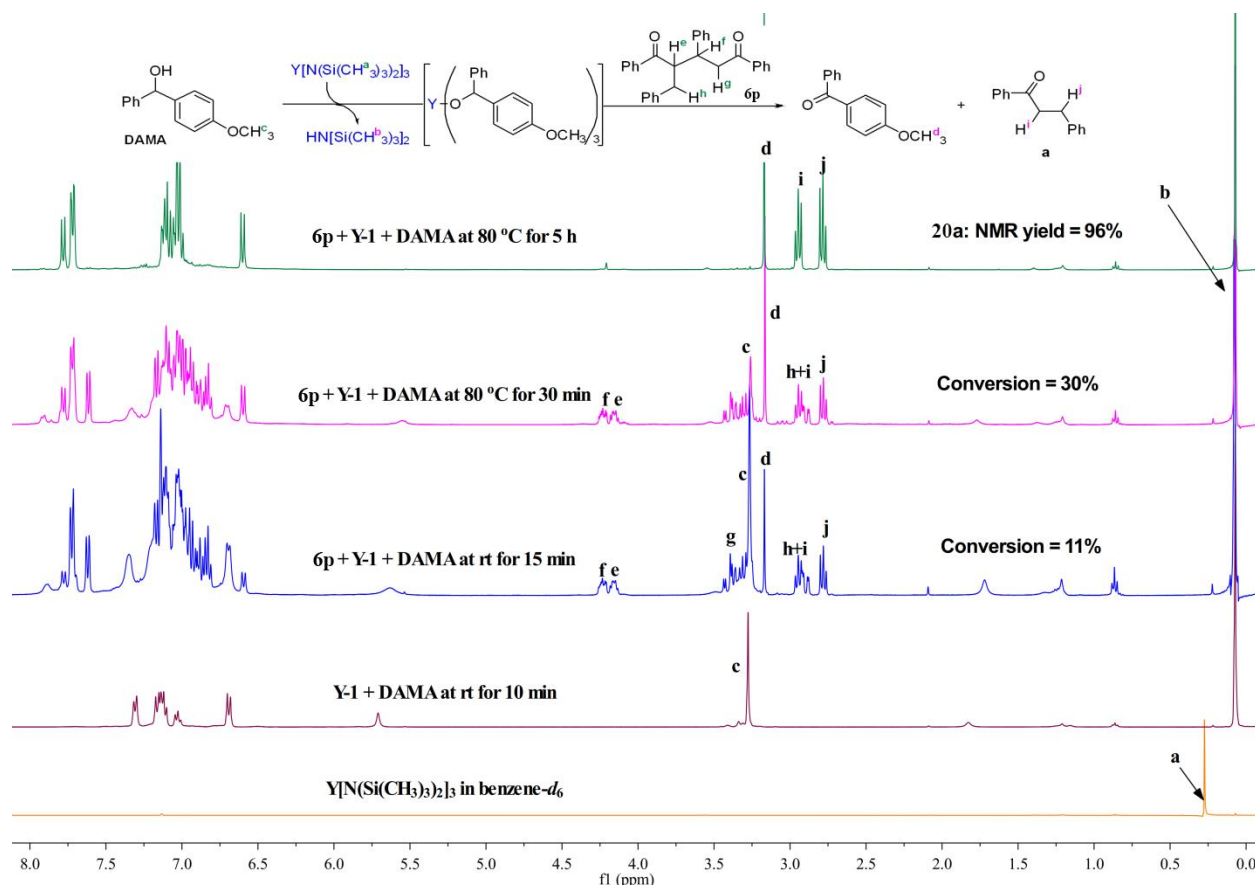


Fig. S21. ^1H NMR spectra for the progress of the reaction of **6p** with $\text{Y}(\text{OCHPh}_2)_3$ as catalyst. **Method A:** In a glovebox, **Y-1** (5.6 mg, 0.010 mmol) was weighed into a NMR tube equipped with a Teflon valve (J-Young). Then, a solution of **DAMA** (21.4 mg, 0.010 mmol) in benzene- d_6 (0.5 mL) was added via syringe. After 30 min, 0.10 mmol **6p** was added. Subsequently, the reaction mixture was heated at 80 °C. The reaction was monitored by ^1H NMR technique, and the experimental conditions and the actual conversion for transformation of **6p** into **20a** were listed.

Taking into consideration the differentiation of the deprotonation capacity between **6p** and **DAMA**, a different feeding sequence was used (Fig. S22). The ^1H NMR monitoring data reveals that **6p** abstracted the amido ligand more slowly than **DAMA**, leading to the liberation of only part $\text{N}(\text{SiMe}_3)_2$ ligands from $\text{Y}[\text{N}(\text{SiMe}_3)_2]_3$ at room temperature in 15 minutes. Notably, heating the solution at 80 °C can lead to the complete liberation of the amido ligands and the formation of a significant amount of **20a** and chalcone, indicating that the Y-mediated C–C cleavage of ketone does not depend on the presence of alcohol. When **DAMA** was added, the C–C hydrogenolysis reaction of the remaining ketone proceeded smoothly in accompany with the reduction of the previously formed chalcone, giving **20a** and **DAMK** with yields comparable to those of **method A**.

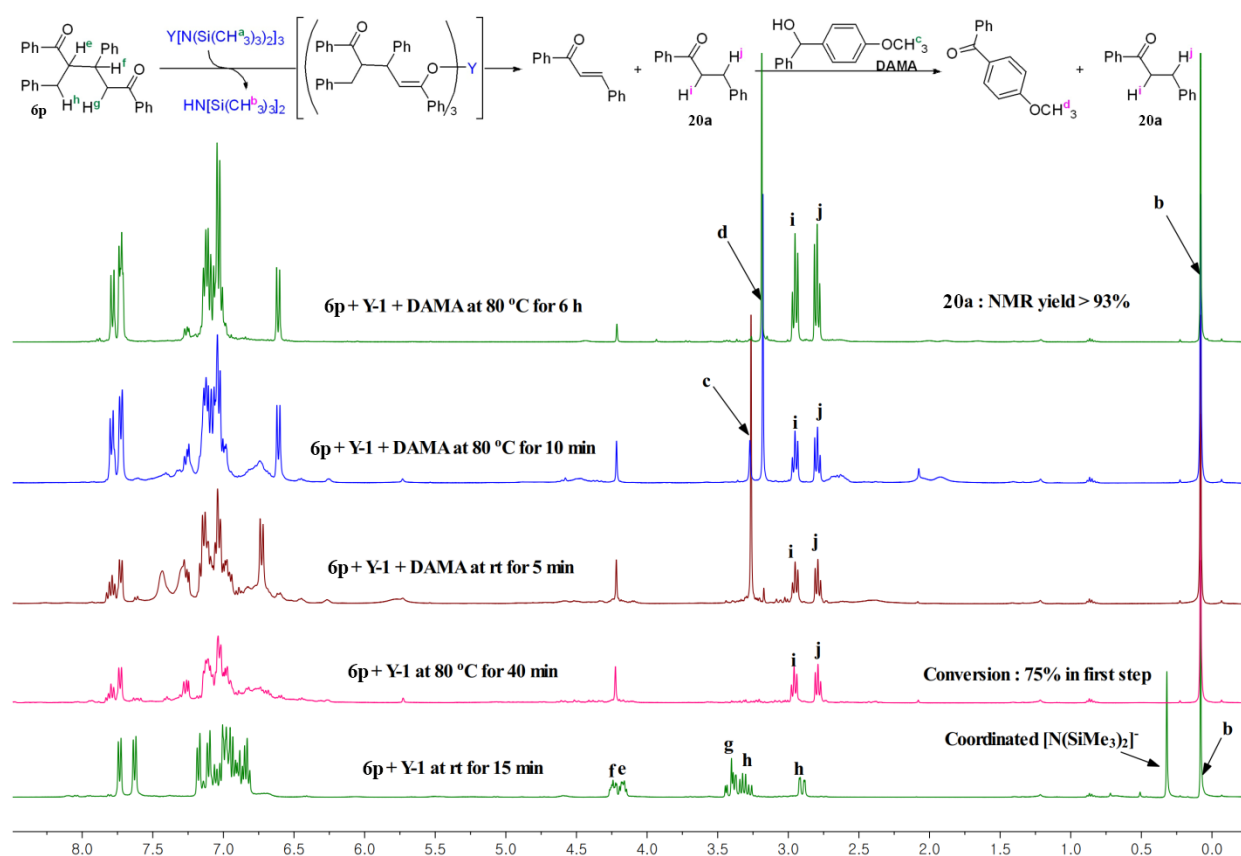


Fig. S22. ^1H NMR spectra for the progress of the reaction of **6p** with **DAMA** using **Y-1** as catalyst. **Method B:** To a solution of **6p** (40.8 mg, 0.10 mmol) in benzene- d_6 (0.50 mL) filled in a J-Young NMR tube, was added **Y-1** (5.6 mg, 0.010 mmol). After heating at 80 °C for 40 mins, the solution was cooled to room temperature and **DAMA** (21.4 mg, 0.10 mmol) was added. Then, the mixture continued to be heated at 80 °C. The reaction was monitored by ^1H NMR technique following the signal of the methylene group (H^f) formation, and the experimental conditions and the actual conversion of **6p** were listed.

In addition, when **Y-1** was directly added to a mixture of **6p** and **6p** in $\text{C}_6\text{D}_5\text{CD}_3$, the ^1H NMR monitoring data (Fig. S23) are very similar to those observed in **Method A**. Therefore, taking into account these results, initial displacement of amido ligands of **Y-1** by alkoxide groups followed by deprotonation of ketone by yttrium alkoxide intermediate and sequential δ -carbon elimination seems most likely, though the possibility that the mixed alkoxide/enolate intermediate is initially generated by competing deprotonation of **DAMA** and **6p** cannot be excluded at this stage.

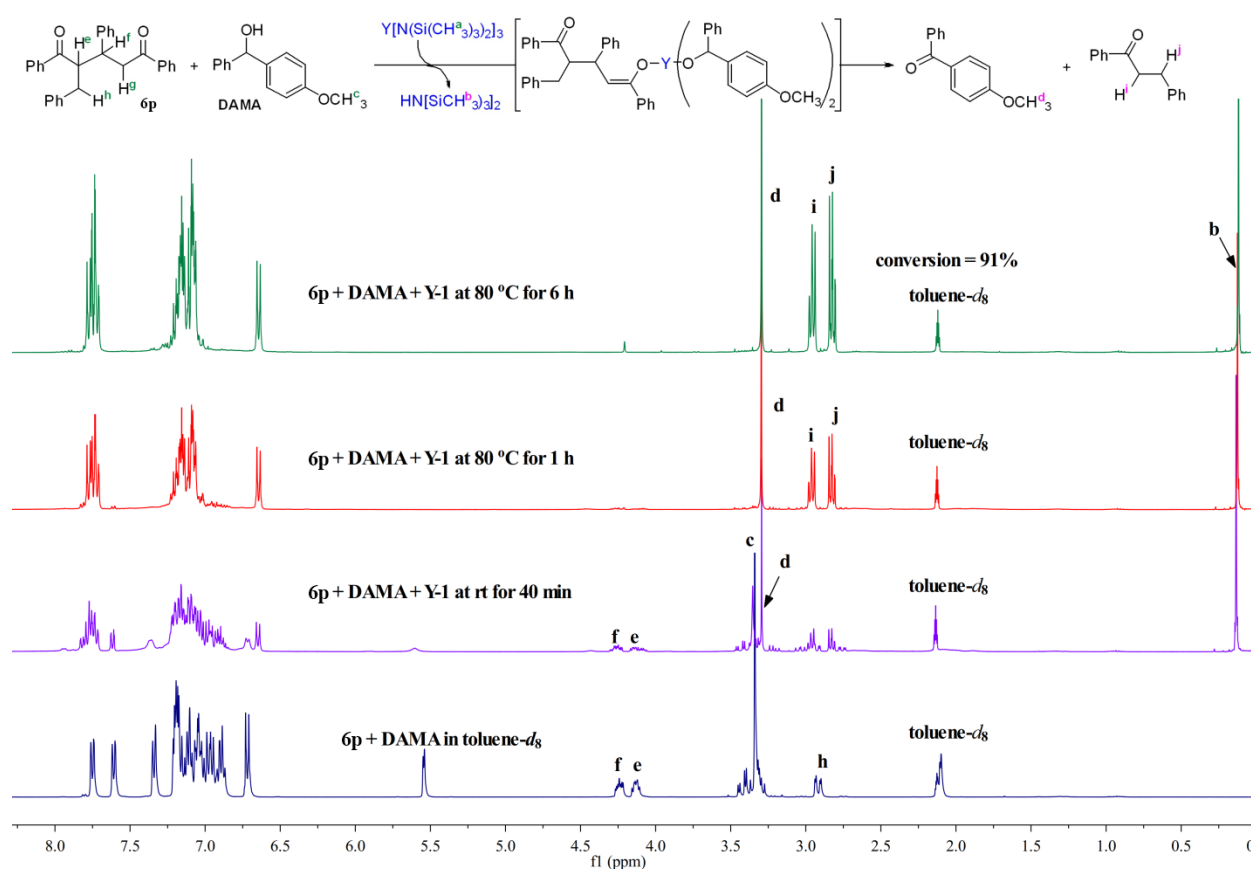


Fig. S23. ^1H NMR spectra for the progress of the reaction of **6p** with **DAMA** using **Y-1** as catalyst. **Method C:** In a glovebox, **Y-1** (5.6 mg, 0.010 mmol) was transferred to a NMR tube equipped with a Teflon valve (J-Young). Then, a mixture of **DAMA** (21.4 mg, 0.10 mmol) and **6p** (40.8 mg, 0.10 mmol) in toluene- d_8 (0.50 mL) was added. The reaction progress was detected by ^1H NMR technique following the shift of the signal of the methyl group from 3.34 to 3.29 ppm upon transfer from **DAMA** to **DAMK**, and the experimental conditions and the actual conversion for the transformation of **6p** into **20a** were listed.

6.5 Kinetic experiment

To further confirm that the δ -carbon elimination of yttrium enolates takes place via a bimetallic pathway rather than a monometallic one, early-stage kinetics of catalytic C–C bond cleavage of **6v** in the absence of **DAMA** and kinetics of the hydrogenolysis reaction of **6v** with **DAMA** were respectively studied. The results showed that the C–C bond cleavage step was second-order in yttrium when the transform ratio was under 30%. However, the pseudo-first-order chemical reaction model for the overall **Y-1** catalyzed C–C hydrogenolysis of **6v** with **DAMA** provided a better correlation of data. Namely, the reaction might be initiated by turnover-limiting deprotonation of ketone, subsequent fast δ -C elimination from a binuclear Y^{3+} enolate intermediate affords the enone and a new enolate complex intermediate.

6.5.1 Kinetic experiment for the C–C cleavage of **6v** catalyzed by **Y-1**

To a solution of **6v** (32.8 mg, 0.10 mmol) and 1,3,5-trimethoxybenzene (internal standard, 16.8 mg, 0.10 mmol) in toluene (2.0 mL) different loading of **Y-1** was added. The resulting mixture was stirred at 323 K, which was then quenched by H₂O. GC-MS analysis was carried out to monitor the accumulation of **16b** (Fig. S24).

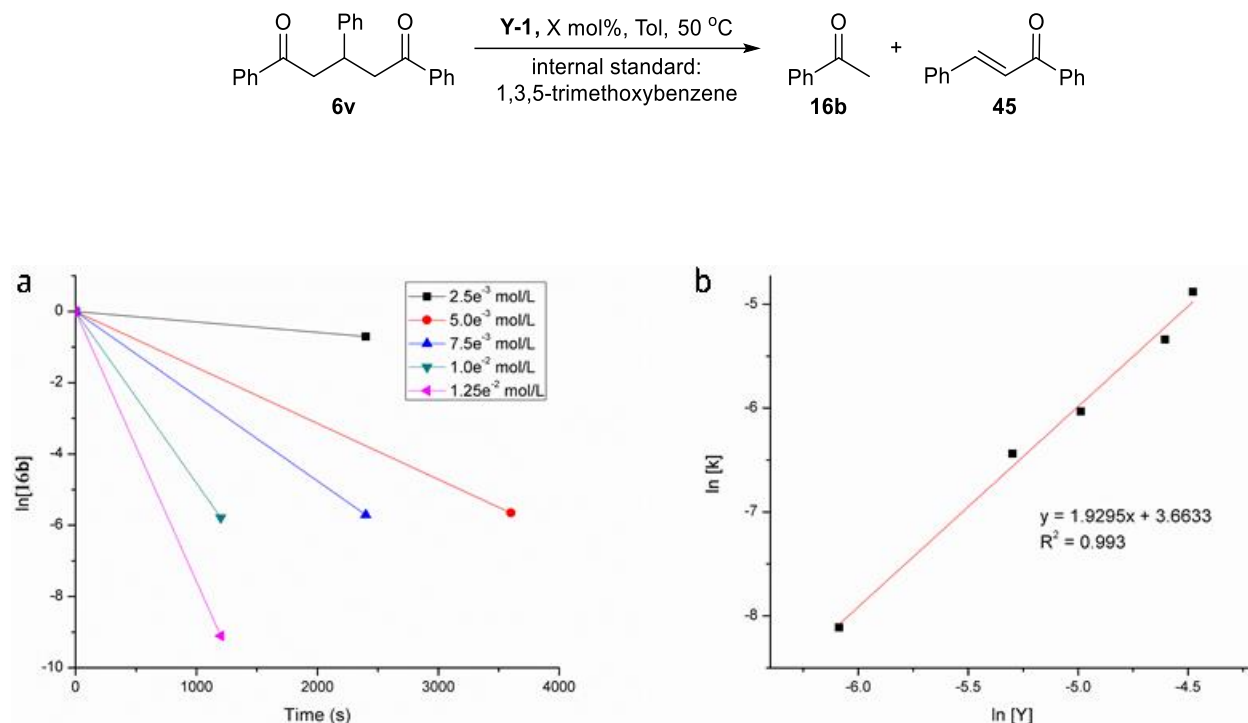


Fig. S24. Plots of the C–C cleavage reaction of **6v** catalyzed by **Y[N(TMS)₂]₃** at various loading of catalysts. **a.** Kinetic analysis plots for the reaction order between reaction rate constant and catalyst loading. **b.** The dynamic order of the metal for the reaction extracted from the plot is second-order reaction.

6.5.2 Kinetic experiment for the C–C hydrogenolysis reaction of **6v** with **DAMA** catalyzed by **Y-1**

To a mixture of 1,3,5-trimethoxybenzene (16.8 mg, 0.10 mmol) (internal standard), **6v** (32.8 mg, 0.10 mmol) and **DAMA** (21.4 mg, 0.10 mmol) in toluene (2.0 mL) a different loading of **Y-1** was added. The resulting mixture was stirred at 323 K, which was then quenched by H₂O. GC-MS analysis was carried out to monitor the accumulation of **16b** (Fig. S25).

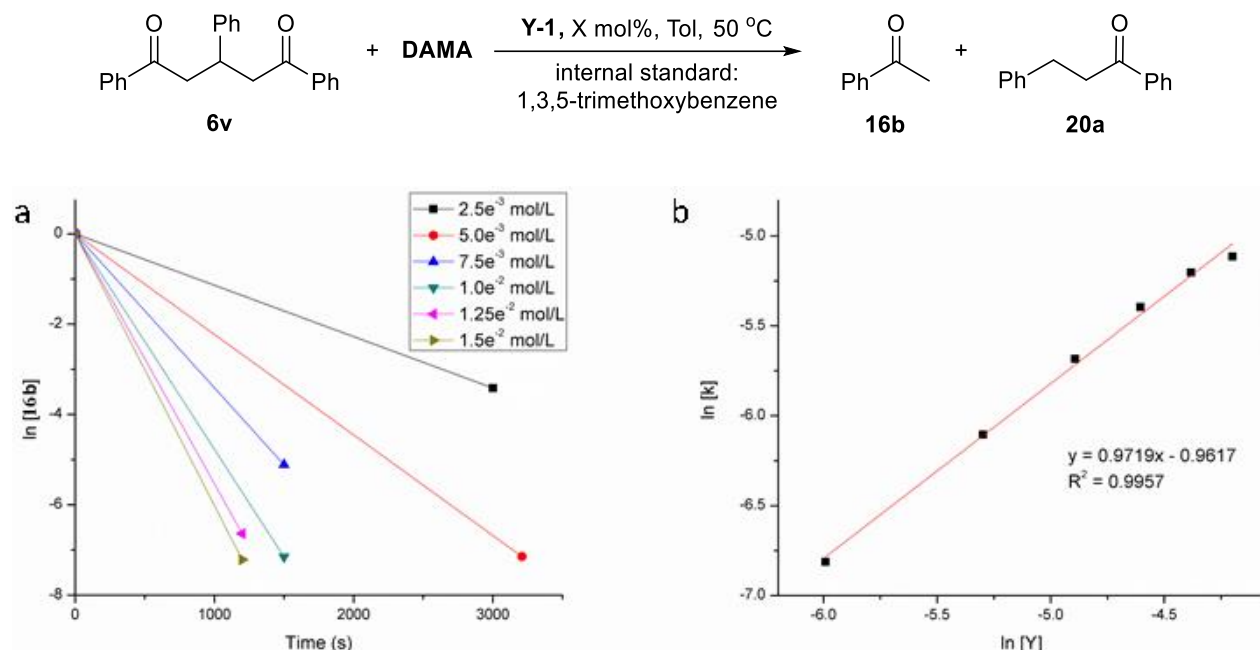


Fig. S25. Plots of the reaction between **6v** and **DAMA** at various loading of catalysts. **a**, Kinetic analysis plots for the reaction order between reaction rate constant and catalyst loading. **b**, The dynamic order of the metal for the reaction extracted from the plot is first-order reaction.

7. Determination of Molecular Structures of **Y-2**, **Y-3**, **Y-4**, **25f** and **32**

X-ray diffraction data for compounds **Y-2**, **Y-3**, **Y-4**, **25f** and **32** were collected on a SMART APEX CCD diffractometer (graphite-monochromated MoK α radiation, ϕ - ω scan technique, $\lambda = 0.71073$ Å). The intensity data were integrated by means of the SAINT program. SADABS was used to perform area-detector scaling and absorption corrections. The structure was solved by direct methods and was refined against F^2 using all reflections with the aid of the SHELXTL package. All non-hydrogen atoms were found from the difference Fourier syntheses and refined anisotropically. The H atoms were included in calculated positions with isotropic thermal parameters related to those of the supporting carbon atoms but were not included in the refinement. All calculations were performed using the Bruker Smart program. CCDC 2059440 (**Y-2**), 2059410 (**Y-3**), 2059442 (**Y-4**), 2059441 (**25f**) and 2116113 (**32**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (+44)-1223-336033; or deposit@ccdc.cam.ac.uk).

Table S3. Crystal and Data Collection Parameters of Complexes Y-2, Y-3, Y-4, 25f and 32.

	Y-2	Y-3	Y-4	25f	32
Empirical formula	C ₇₁ H ₁₁₂ N ₂ O ₁₉ Si ₄ Y ₂	C ₉₀ H ₉₀ O ₁₀ Y ₂	C ₄₂ H ₄₂ Cl ₂ LiN ₄ O ₃ S ₄ Y	C ₂₂ H ₂₀ O	C ₂₆ H ₂₂ O ₂
Molecular weight	1587.80	1509.43	945.78	300.38	366.43
Temperature (K)	173(2)	173(2)	173(2)	302(2)	173
Wavelength (Å)	1.34138	1.34138	1.34138	1.34138	1.34138
Crystal system	Triclinic	Monoclinic	Triclinic	Orthorhombic	monoclinic
Space group	<i>P</i> -1	<i>P</i> 2 ₁ /n	<i>P</i> -1	<i>P</i> bca	<i>P</i> 2 ₁ /c
<i>a</i> (Å)	13.5161(9)	12.360(10)	10.4735(14)	10.7579(7)	14.5793(5)
<i>b</i> (Å)	19.1767(13)	15.060(3)	11.7513(16)	8.3156(5)	8.3322(3)
<i>c</i> (Å)	19.7668(14)	23.844(5)	19.441(3)	37.093(3)	15.6350(6)
α (deg)	99.233(3)	90	74.410(5)	90	90
β (deg)	105.369(3)	100.70(3)	77.603(5)	90	97.1300(10)
γ (deg)	94.899(3)	90	68.154(4)	90	90
<i>V</i> (Å ³)	4832.0(6)	4361(4)	2121.5(5)	3318.3(4)	1884.62(12)
<i>Z</i>	2	2	2	8	4
Density (calculated)	1.091Mg/m ³	1.149 Mg/m ³	1.481 Mg/m ³	1.203 Mg/m ³	1.291 Mg/m ³
Absorption coefficient	1.6763 mm ⁻¹	1.461 mm ⁻¹	3.482 mm ⁻¹	0.356 mm ⁻¹	0.404 mm ⁻¹
<i>F</i> (000)	1676	1576	972	1280	776
Crystal size (mm ³)	0.16×0.10×0.10	0.18×0.17×0.15	0.16×0.08×0.08	0.23×0.16×0.04	0.30×0.14×0.05
θ range for data collection	7.446 to 105.992°	6.07 to 121.492°	7.208 to 105.986°	8.266 to 105.996°	9.92 to 116.976°
Index ranges <i>h</i> , <i>k</i> , <i>l</i>	-16 ≤ <i>h</i> ≤ 16 -22 ≤ <i>k</i> ≤ 22 -23 ≤ <i>l</i> ≤ 23	-16 ≤ <i>h</i> ≤ 13 -19 ≤ <i>k</i> ≤ 15 -25 ≤ <i>l</i> ≤ 30	-12 ≤ <i>h</i> ≤ 12 -13 ≤ <i>k</i> ≤ 12 -23 ≤ <i>l</i> ≤ 23	-9 ≤ <i>h</i> ≤ 12 -9 ≤ <i>k</i> ≤ 9 -44 ≤ <i>l</i> ≤ 37	-18 ≤ <i>h</i> ≤ 17 -10 ≤ <i>k</i> ≤ 10 -19 ≤ <i>l</i> ≤ 19
Reflections collected	54331	36513	25750	15401	22426
Independent reflections	16984 [<i>R</i> _{int} = 0.0532]	9873 [<i>R</i> _{int} = 0.1385]	7447 [<i>R</i> _{int} = 0.0422]	2910 [<i>R</i> _{int} = 0.0243]	4057 [<i>R</i> _{int} = 0.0594, <i>R</i> _{sigma} = 0.0420]
Completeness to θ	99.5% (θ = 52.996)	99.3% (θ = 52.998)	99.4% (θ = 52.993)	99.3% (θ = 52.998)	99.9% (θ = 53.549)
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. & min. transmission	0.7508 and 0.5531	0.7518 & 0.5691	0.7508 and 0.6373	0.9705 and 0.8255	0.752 and 0.572
Refinement method	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²
Data/restraints/parameters	16984/0/907	9873/87/461	7447/0/514	2910/0/209	4057/0/253
Goodness-of-fit on <i>F</i> ²	1.030	0.957	1.134	0.990	1.045
Final <i>R</i> indices [<i>I</i> > 2σ (<i>I</i>)]	<i>R</i> ₁ = 0.0424 <i>wR</i> ₂ = 0.1149	<i>R</i> ₁ = 0.0814 <i>wR</i> ₂ = 0.1935	<i>R</i> ₁ = 0.0284 <i>wR</i> ₂ = 0.0826	<i>R</i> ₁ = 0.0349 <i>wR</i> ₂ = 0.0921	<i>R</i> ₁ = 0.0438 <i>wR</i> ₂ = 0.1108
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0518 <i>wR</i> ₂ = 0.1219	<i>R</i> ₁ = 0.1377 <i>wR</i> ₂ = 0.2247	<i>R</i> ₁ = 0.0339 <i>wR</i> ₂ = 0.0943	<i>R</i> ₁ = 0.0383 <i>wR</i> ₂ = 0.0959	<i>R</i> ₁ = 0.0504 <i>wR</i> ₂ = 0.1168
Extinction coefficient	n/a	n/a	n/a	n/a	n/a
Largest diff. peak and hole (e·Å ⁻³)	1.03 and -0.7	1.2 and -0.83	0.46 and -0.72	0.11 and -0.11	0.22 and -0.24

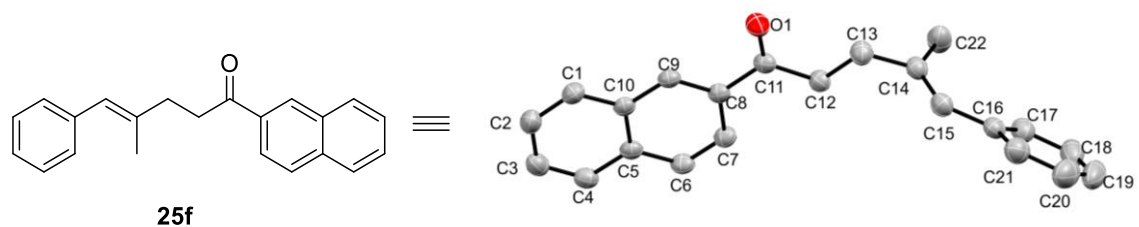


Fig. S26. Molecular structure of compound 25f (Thermal ellipsoids at 30% level; all the hydrogen atoms are omitted for clarity). Selected bond lengths (Å) and bond angles (deg): C11–O1 1.220(1), C8–C11 1.494(2), C11–C12 1.507(2), C12–C13 1.514(2), C13–C14 1.509(2), C14–C15 1.327(2), C14–C22 1.496(2), C15–C16 1.468(2); C11–C12–C13 113.0(1), O1–C11–C12 120.5(1), O1–C11–C8 120.2(1).

8. Computational Details and discussion

All DFT calculations were performed with Gaussian 09³⁴. Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional^{35,36} and the Stuttgart effective core potential for Y³⁷ and Si³⁸ augmented with a polarization functions ($\zeta_f = 1.000$ for Y and $\zeta_d = 0.284$ for Si). For the other elements (H, C, N, and O), Pople's double- ζ basis set 6-31G (d,p)³⁹ was used. Calculations of vibrational frequencies were systematically done in order to characterize the nature of stationary points. The electron density and partial charge distribution were examined in terms of localized electron-pair bonding units using the NBO program⁴⁰ available in Gaussian 09.

The computed reaction profile is rather complicated and was then splitted in three main parts of the reaction. The first part of the reaction (Fig. S27) corresponds to the active catalyst formation.

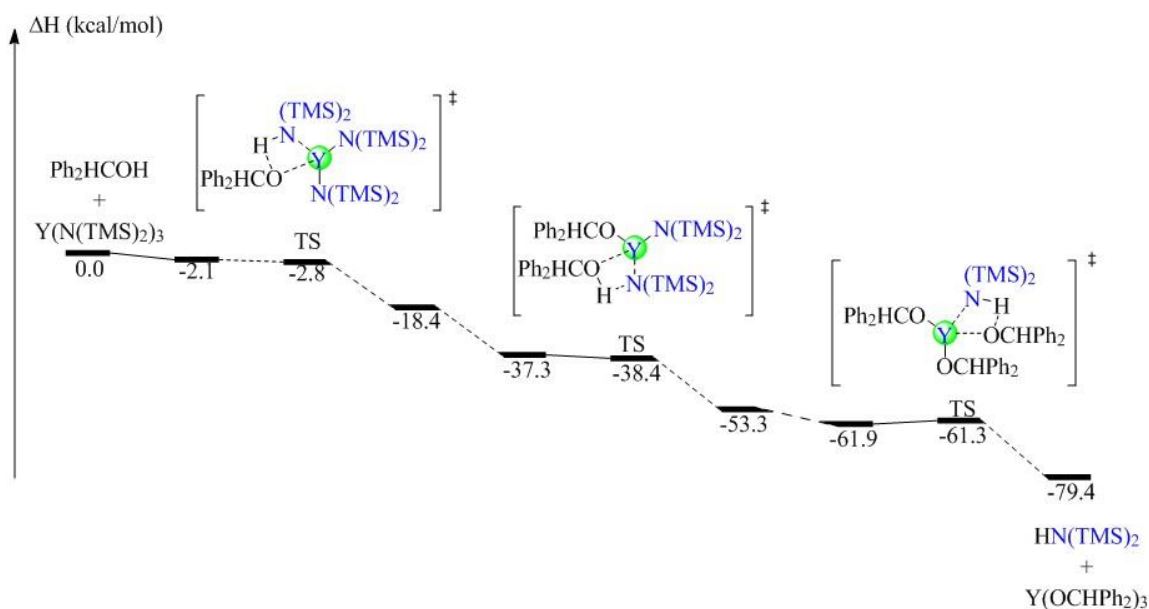


Fig. S27. DFT Computed Enthalpy Profile at room temperature for the formation of the active catalyst $\text{Y}(\text{OCHPh}_2)_3$ from $\text{Y}(\text{N}(\text{TMS})_2)_3$.

The reaction is a step-wise replacement of the trimethylsilylamido ligands by alkoxide upon a proton transfer from the alcohol to the amido ligand. These reactions requires no barrier and are strongly exothermic as expected with an oxophilic metal such as yttrium.

The second part of the reaction is the breaking of the C-C bond. The calculations were carried out with substrate **21a** (Fig. S28).

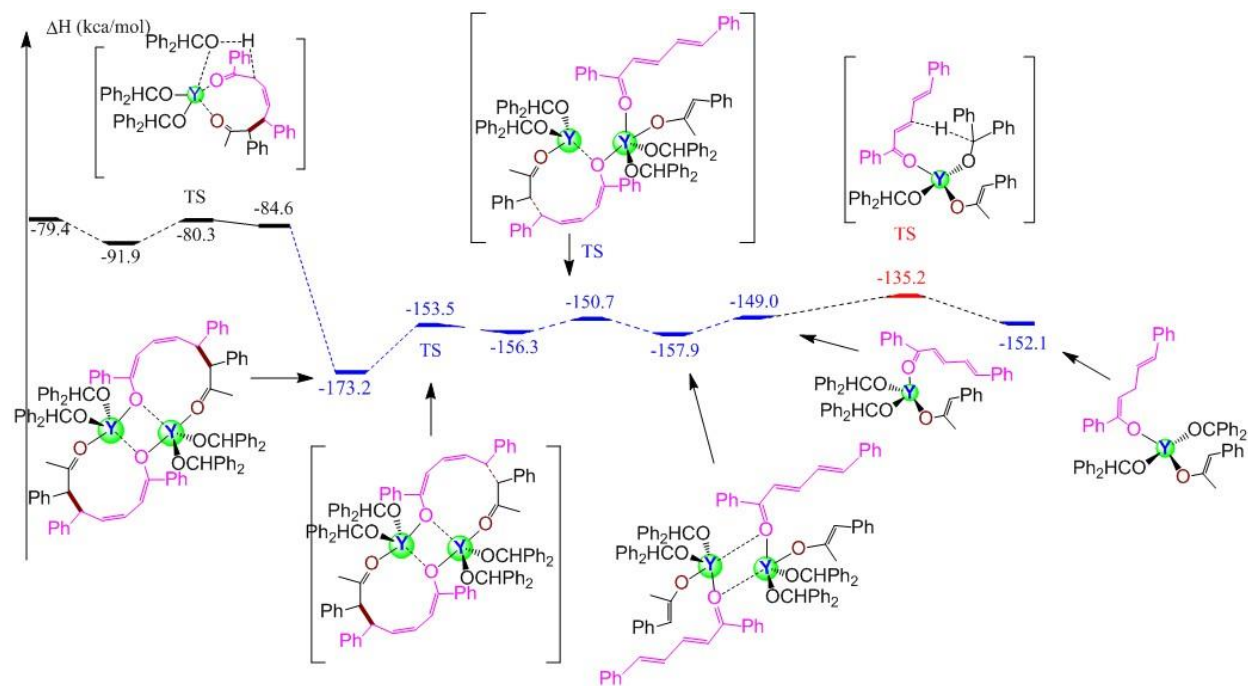


Fig. S28: DFT Computed Enthalpy Profile at room temperature for the C–C bond breaking of substrate **21a** catalyzed by $\text{Y}(\text{OCHPh}_2)_3$.

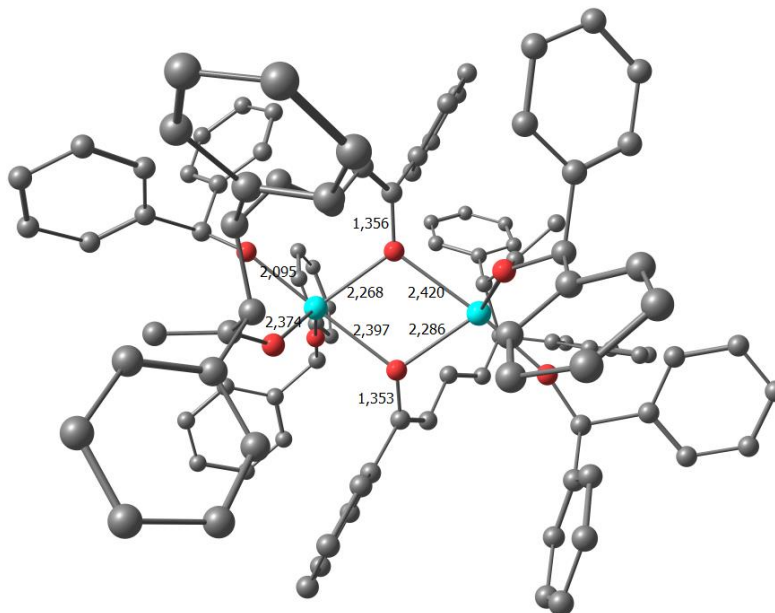


Fig. S29. DFT optimized geometry of the dimer. The main distances are given in Å.

The C–C hydrogenolysis begins with the coordination of **21a** to the yttrium center. This coordination is ensured by the two terminal carbonyl groups and is favourable by 12.5 kcal/mol. The system is thus readily

undergoing an intramolecular α -H abstraction of **21a** by one alcoholate, with an accessible barrier of 11.6 kcal/mol. This alcohol elimination is endothermic by 7.3 kcal/mol from the adduct so that this step is not very efficient, and may be the turnover-limiting as shown in dynamic experiments. However, this can be overcome by the dimerization of the complex, that drives the thermodynamic of the reaction (becoming exothermic by more than 80 kcal/mol from the adduct). In this dimer, the alcoholate coming from the former substrate **21a** is bridging two yttrium centers (see Fig. S28) but one Y–O distance is shorter than the other one, indicating an asymmetric structure. Moreover, the carbonyl of the coordinated substrate is interacting with the yttrium center for which the Y–O distance is the shortest, in line with the formation of a real dimer. The bridging interaction of the alcoholate is thus formed by a Y–O bond (see Fig. S29) and a dative interaction between the oxygen lone pair of the alcoholate (that are the HOMO and HOMO-1, Fig. S30) and the second yttrium center. This dative interaction is strong enough to stabilize the complex so that the rest of the reactivity is expected to occur at the dimer.

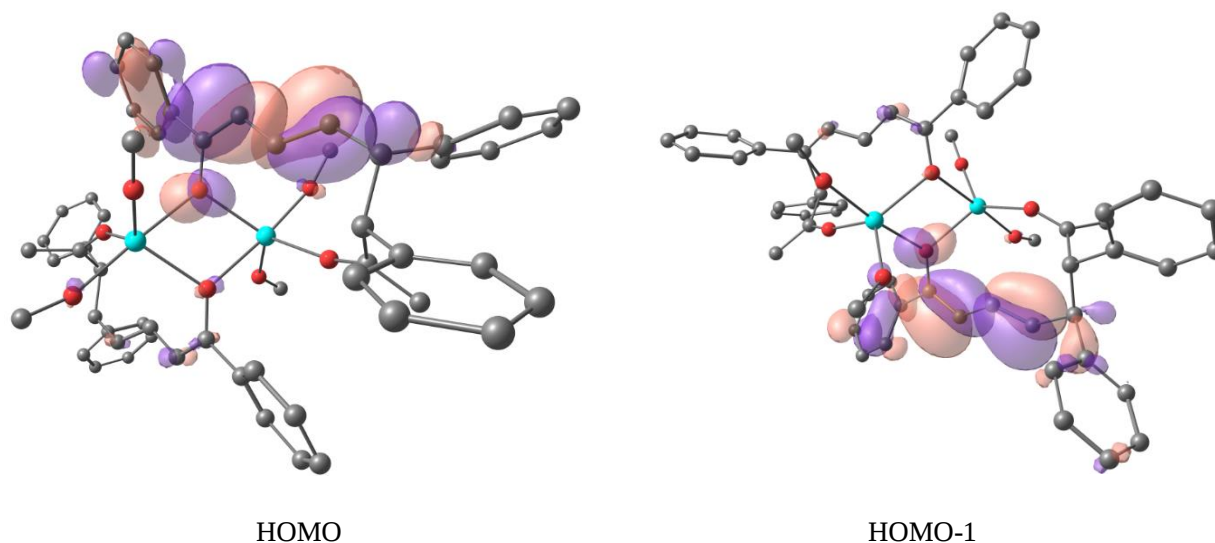


Fig. S30. 3D-depiction of the HOMO and HOMO-1 of the dimer species.

It should be noted that the subsequent C–C bond breaking was computed on the monomer but was found not to be competitive thermodynamically. The two C–C bond breaking occur in a step-wise manner. The first C–C bond breaking implies a barrier of 19.7 kcal/mol whereas the second barrier is only 5.6 kcal/mol. The C–C bond breaking leads to the formation of an alkoxide ligand and a ketone both interacting with a yttrium center, in a dimeric form. This dimer is loosely bonded as the ketone is ensuring the interaction between the two yttrium and its formation is endothermic by 15.4 kcal/mol with respect to the previous dimer. This loosely bonded dimer easily splits out into two monomers that readily undergoes an intramolecular proton transfer from one OCHPh₂ ligand to the ketone (barrier of 13.8 kcal/mol). This yields the formation of a benzophenone molecule and a slightly

more stable trisalcoholate by 3.1 kcal/mol. The latter binds an alcohol molecule to form a stable adduct, that pulls down the reaction in energy (Fig. S28).

Indeed, from the alcohol adduct, sequential proton transfer/product liberation/alcohol coordination can occur to generate all the experimentally observed products. Two pathways (a and b in Fig. S31) were considered depending on the first product that is generated but of course both pathways are equivalent. The barriers for the two proton transfers from the alcohol are low 3 and 5 kcal/mol) and the regeneration of the catalyst is thermodynamically favored (-184/-187 kcal/mol). The benzophenone molecule can then be replaced by a molecule of substrate **21a**, that undergoes a proton transfer to regenerate the dimer, restarting the C–C bond breaking process in a catalytic way. These results verify the mechanistic probe experiments and are consistent with the catalytic cycle shown in Fig. S32, where the bimetallic synergy-driven remote C–C bond cleavage shows a different mechanism from the previous β -carbon of metal alkoxide complexes.

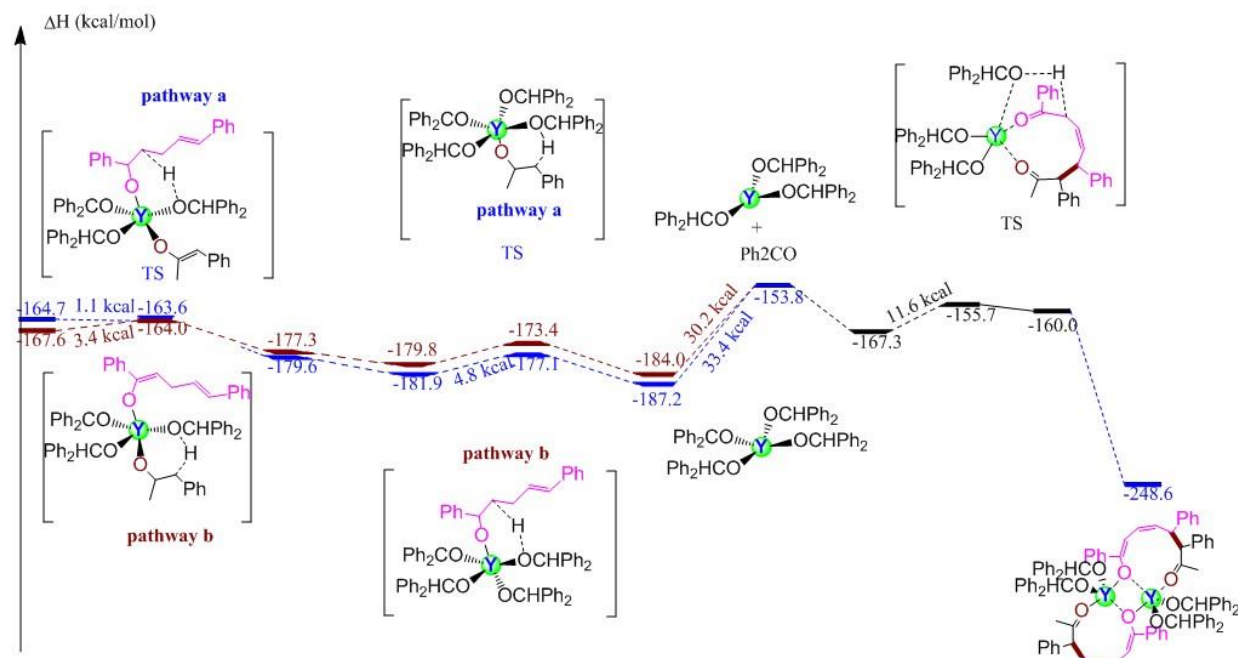


Fig. S31. DFT Computed Enthalpy Profile at room temperature for the liberation of the products and catalyst regeneration.

9. Proposed mechanism for remote C–C hydrogenolysis of ketones

Based on these results, a plausible mechanism for the rare earth-catalysed transfer hydrogenolysis of remote and unstrained C–C bonds of ketones with alcohol is outlined in Fig. S32. First, abstraction of amido ligands with alcohol formed the intermediate **A**. Then, deprotonation of ketone **1** occurs to give a dinuclear yttrium enolate intermediate **B**. **B** undergoes the δ -C elimination to form α,β -unsaturated ketone adduct **C**. Next, intramolecular H-transfer of the alkoxide ligand with the coordinated enone via eight-membered cyclic transition state leads to the formation of **D**. Finally, protonolysis of **D** with another alcohol affords the corresponding C–C bond hydrogenolysis products and regenerates the active intermediate **A**.

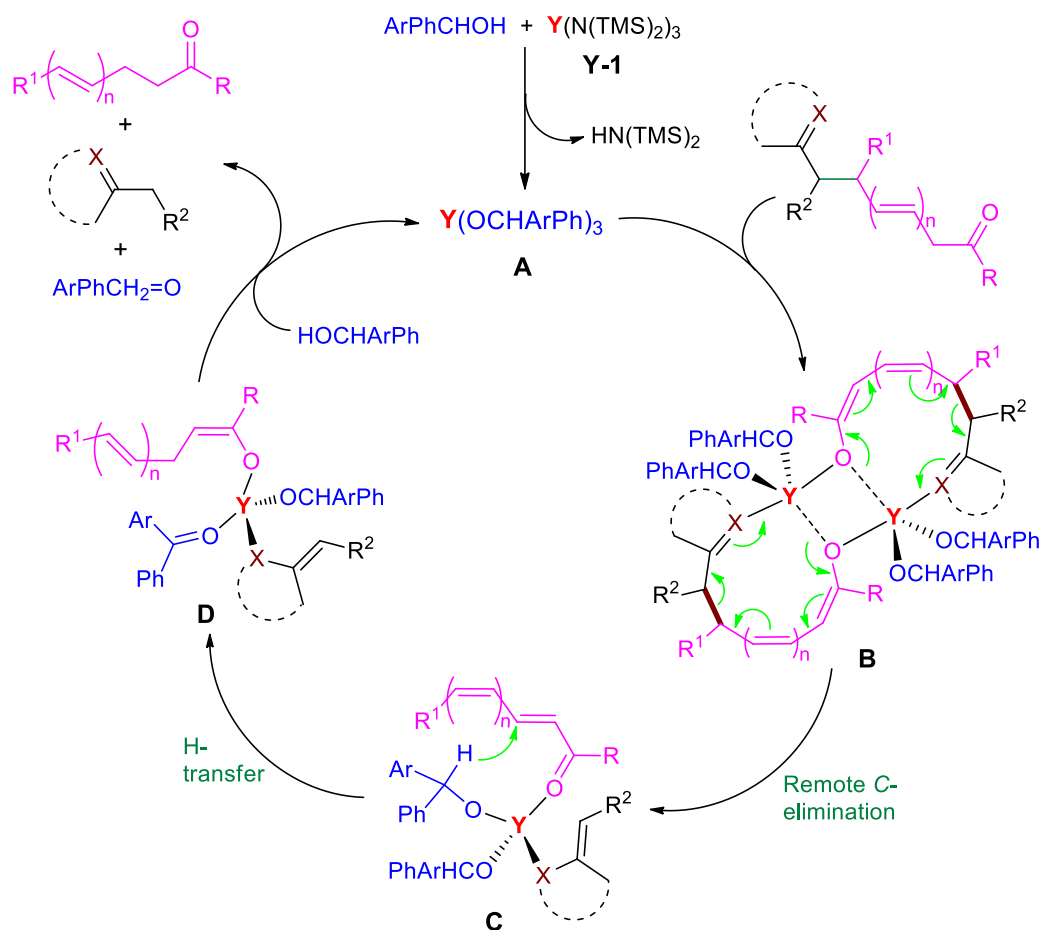
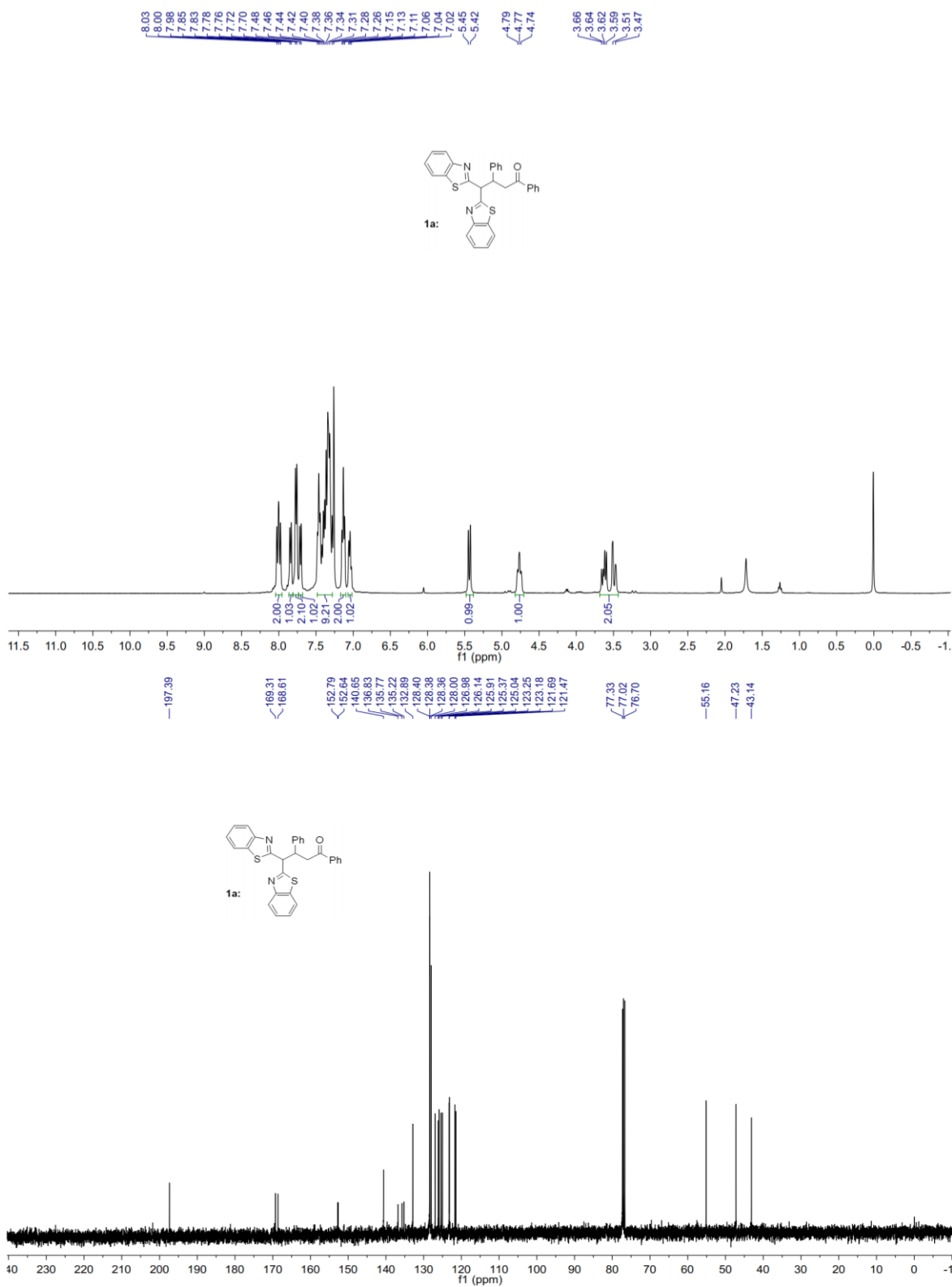
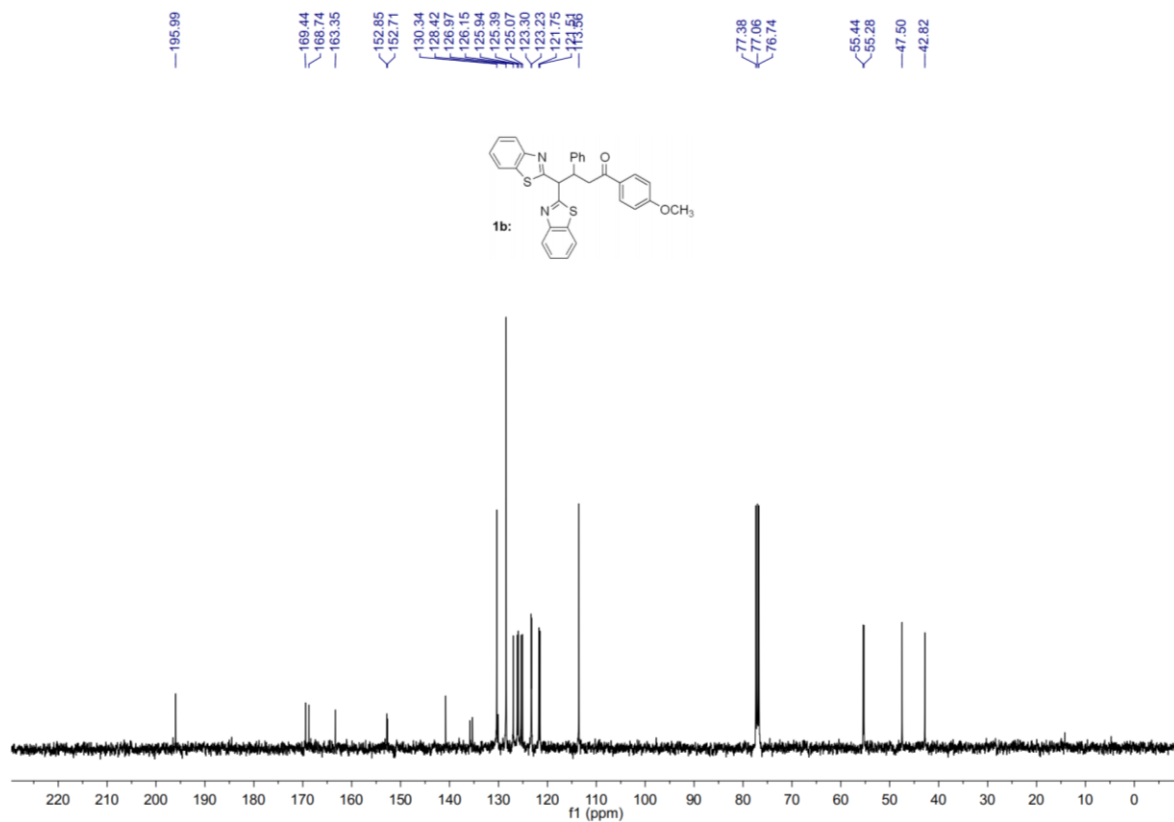
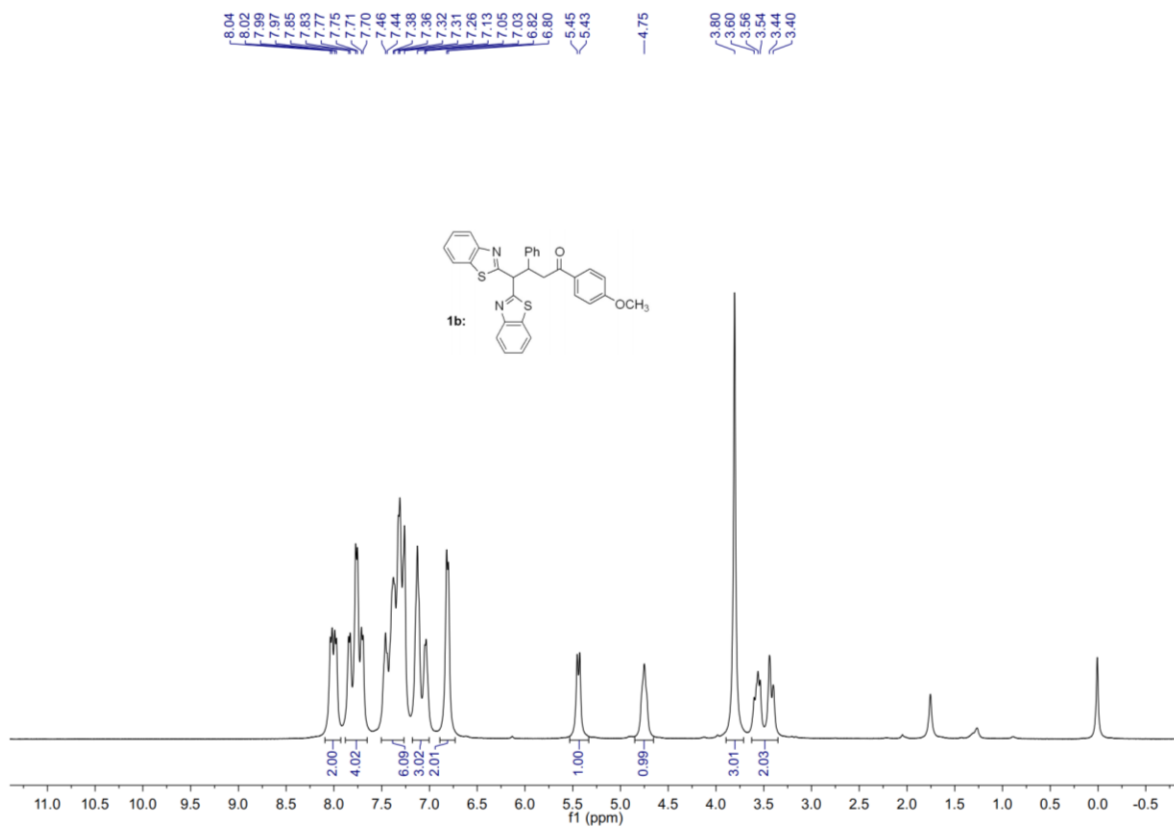
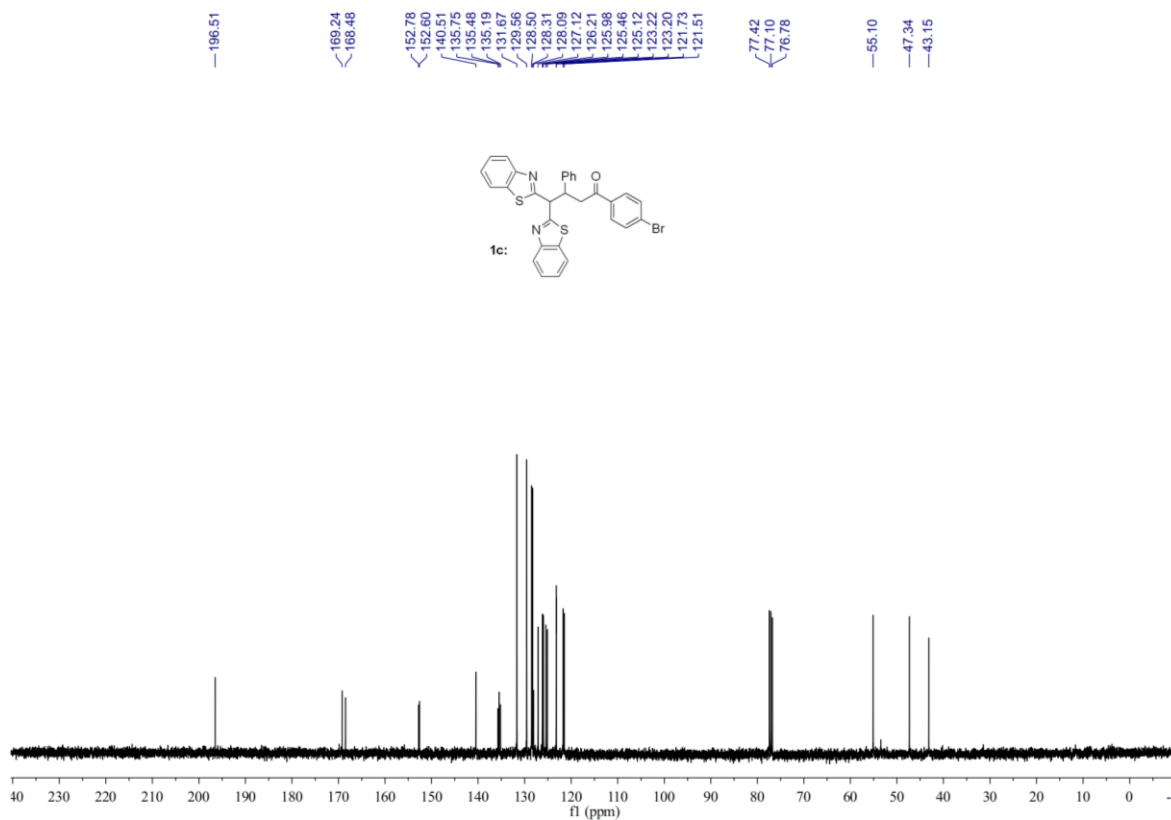
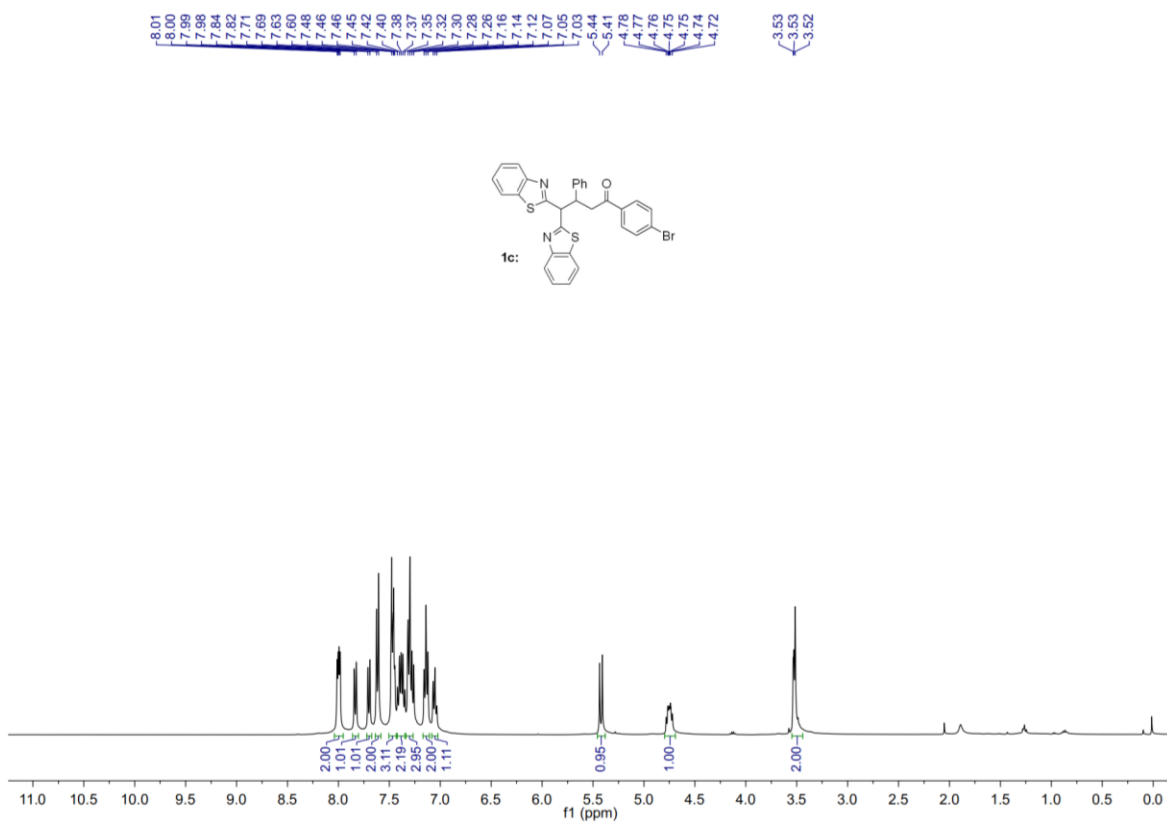


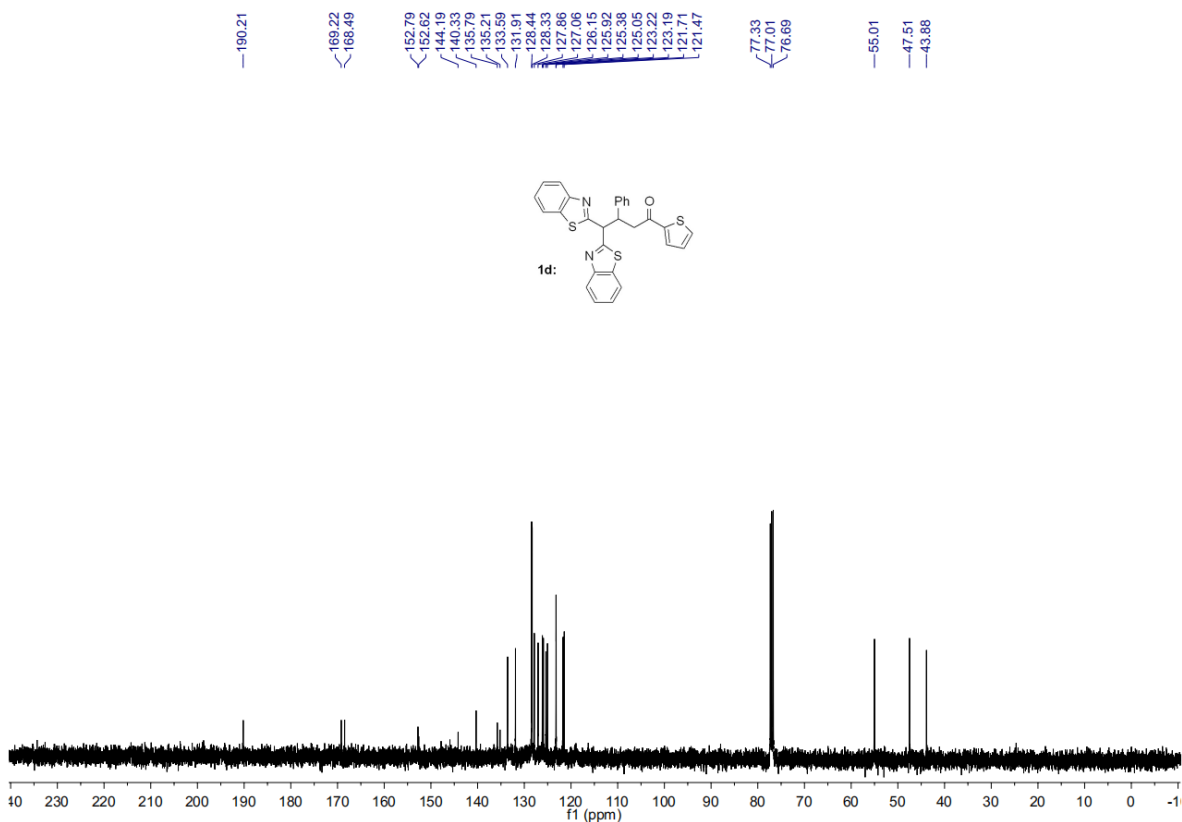
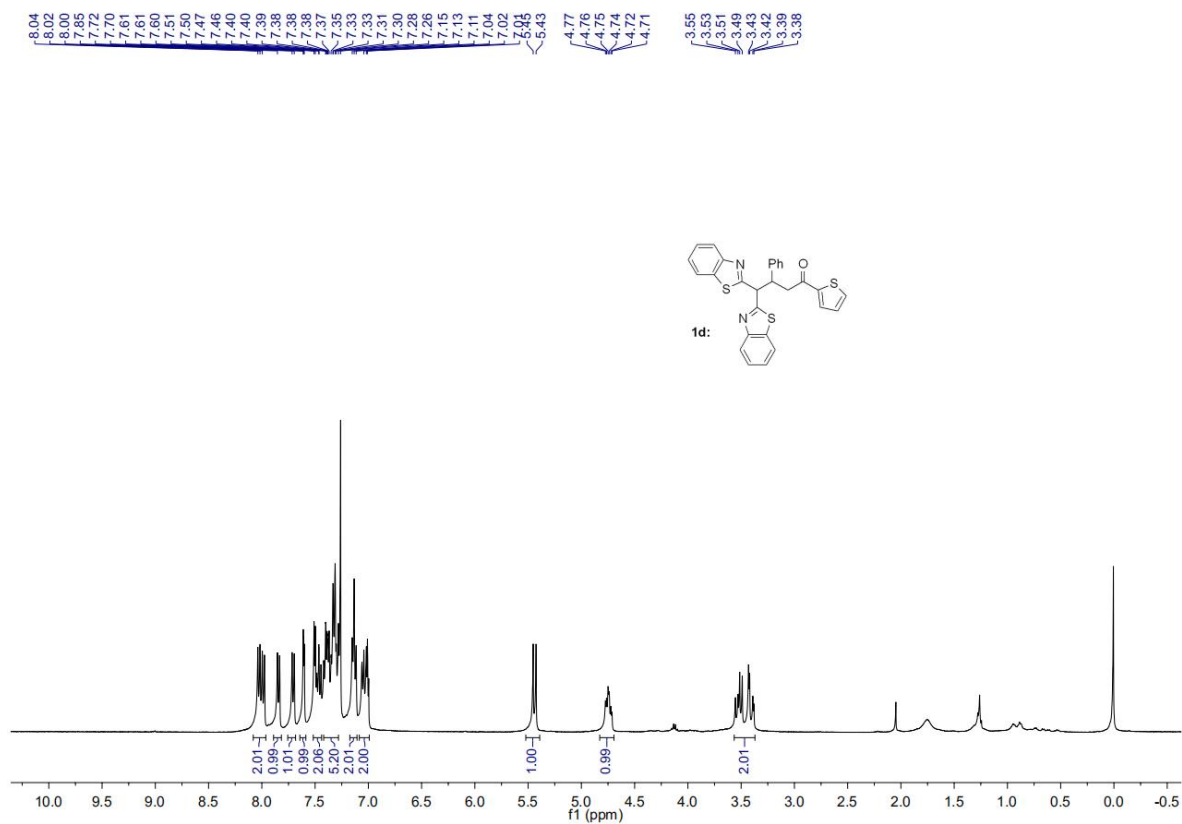
Fig. S32. Proposed mechanism for remote C–C hydrogenolysis of ketones catalyzed by **Y-1**.

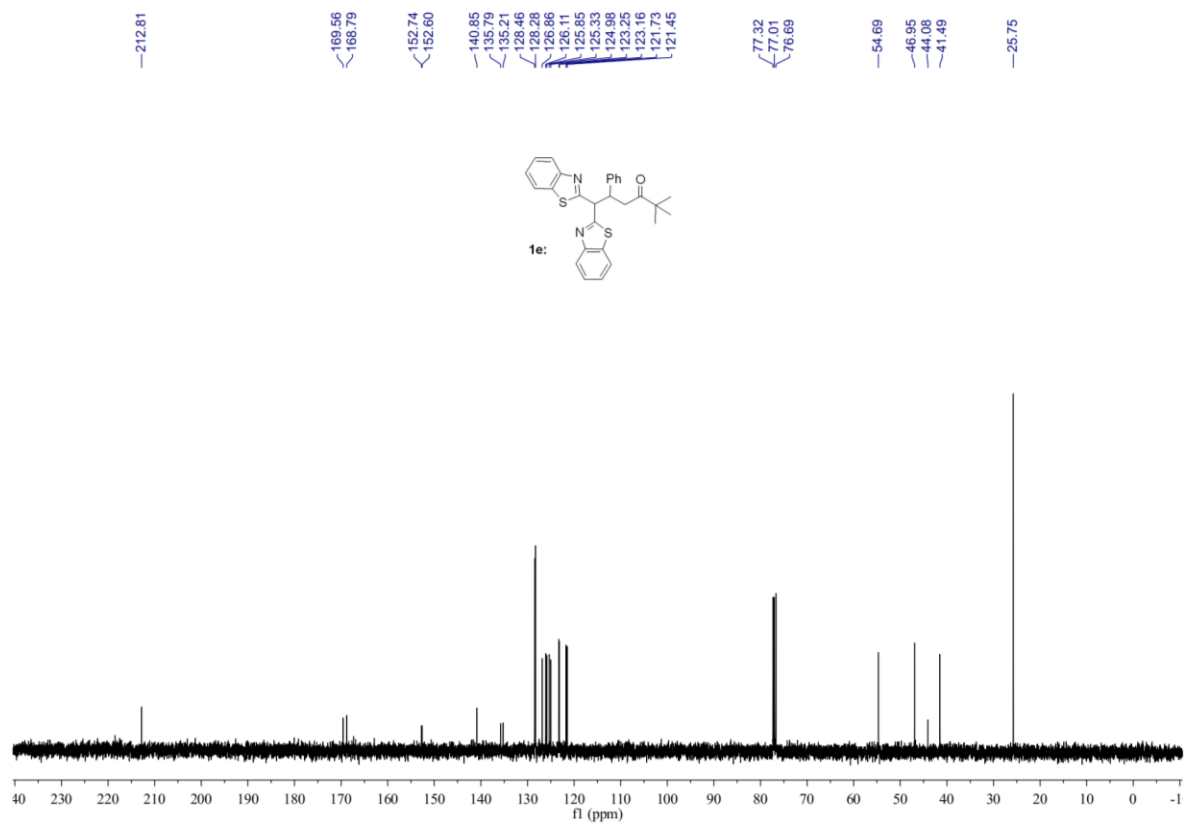
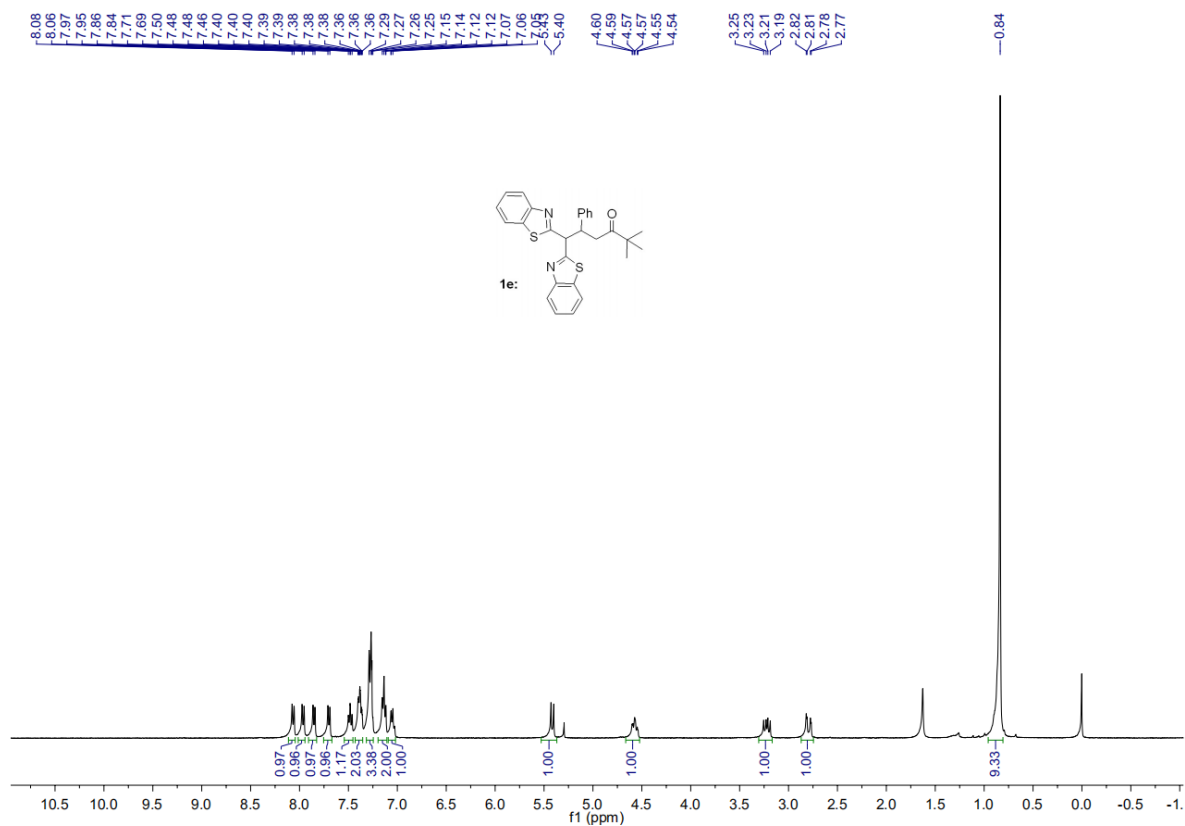
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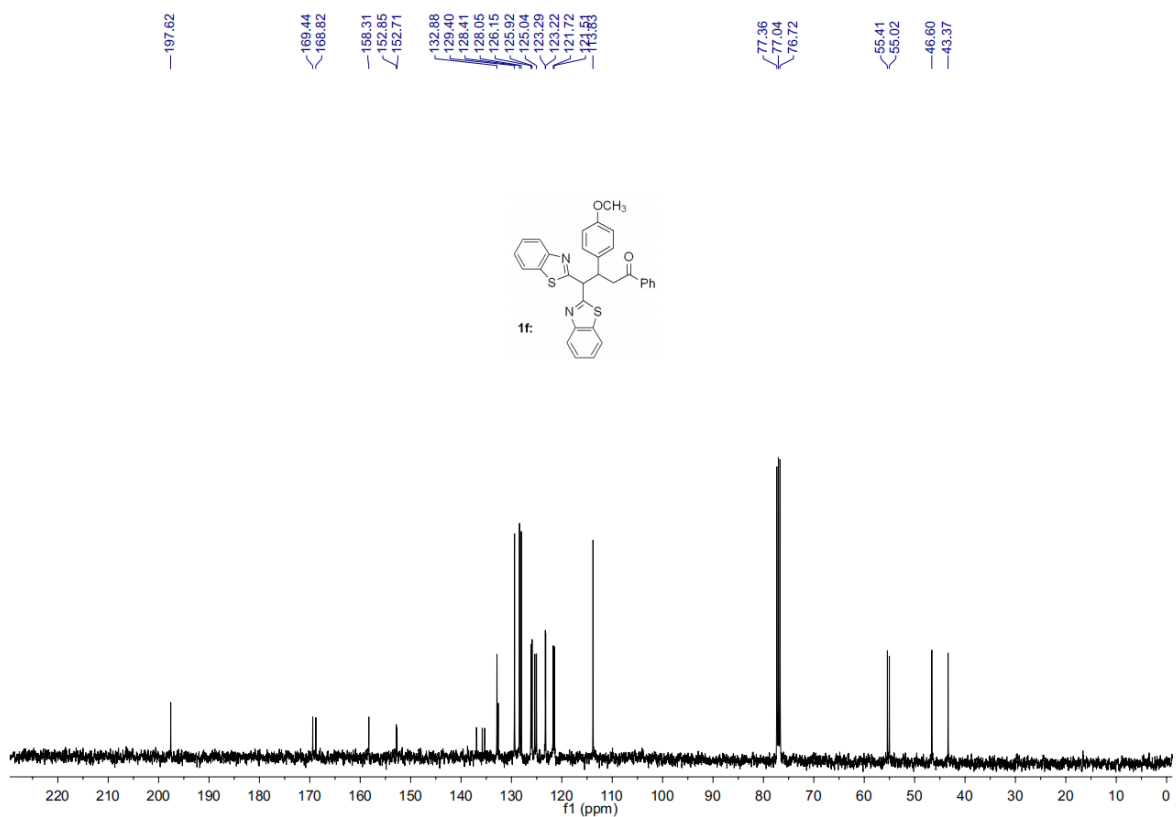
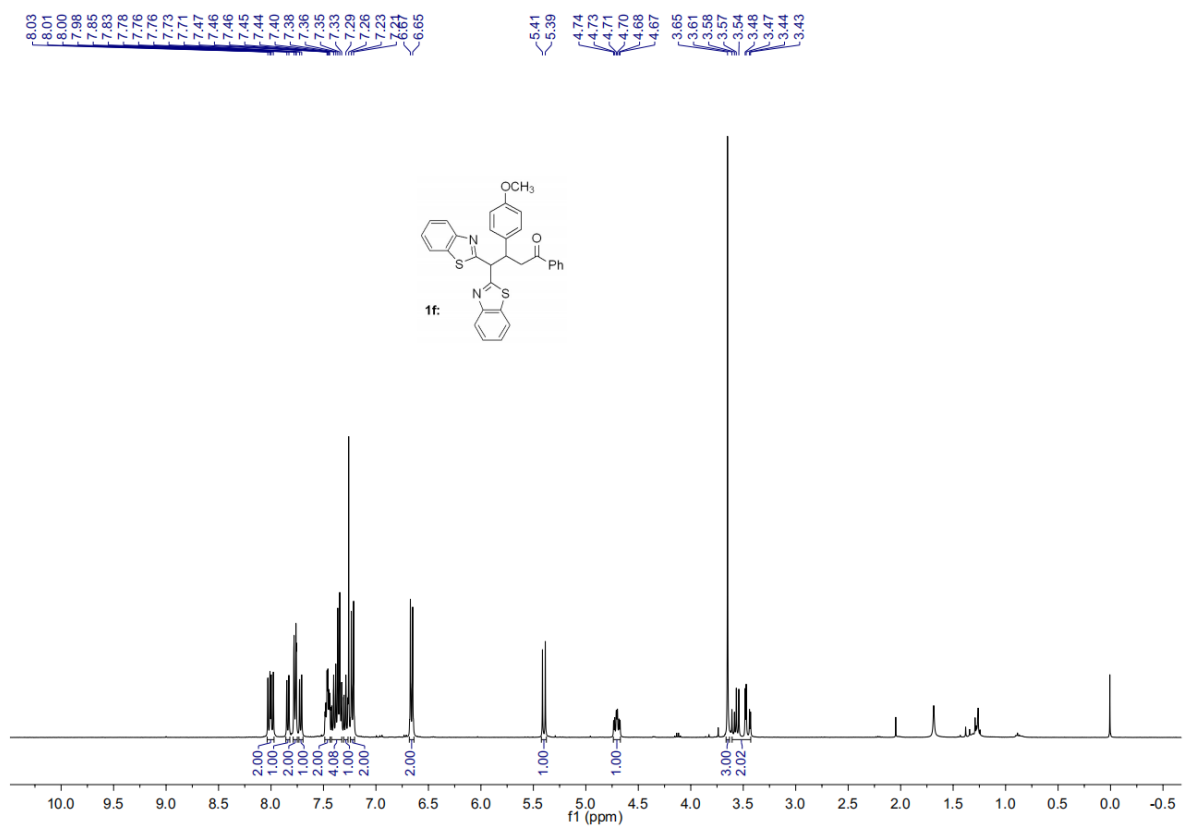


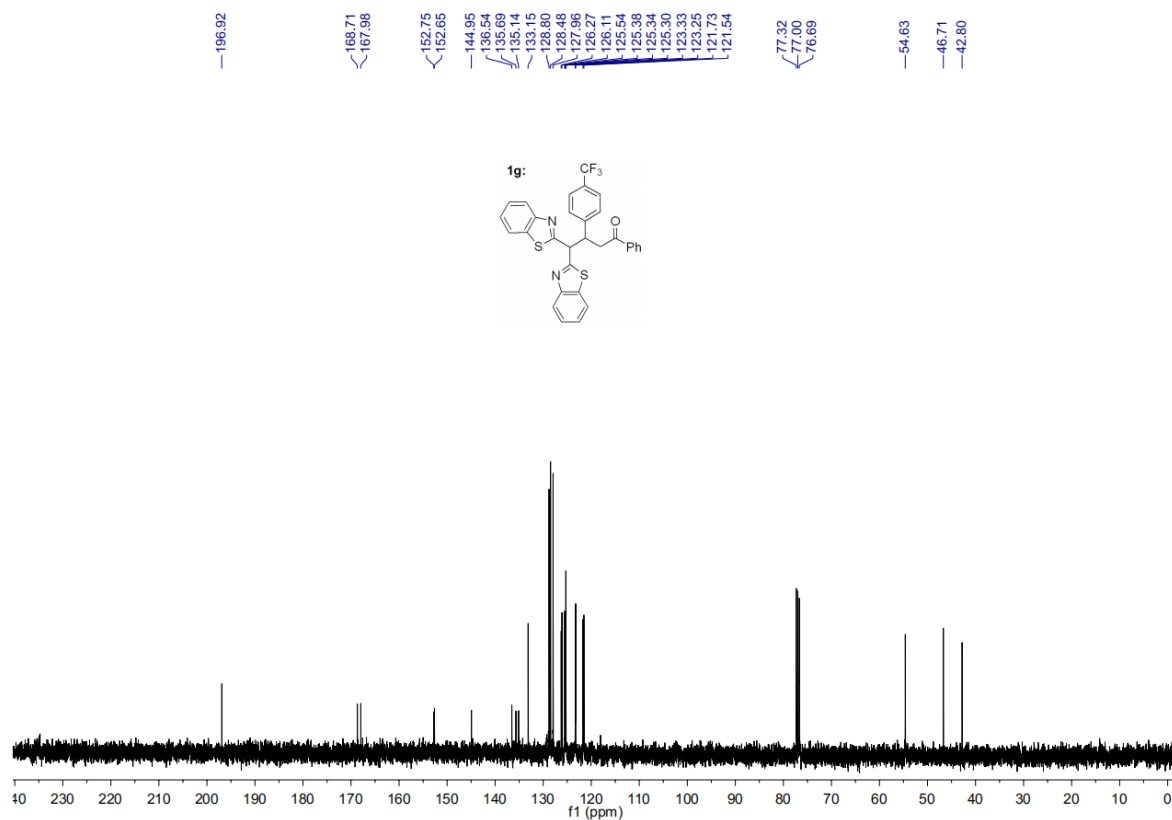
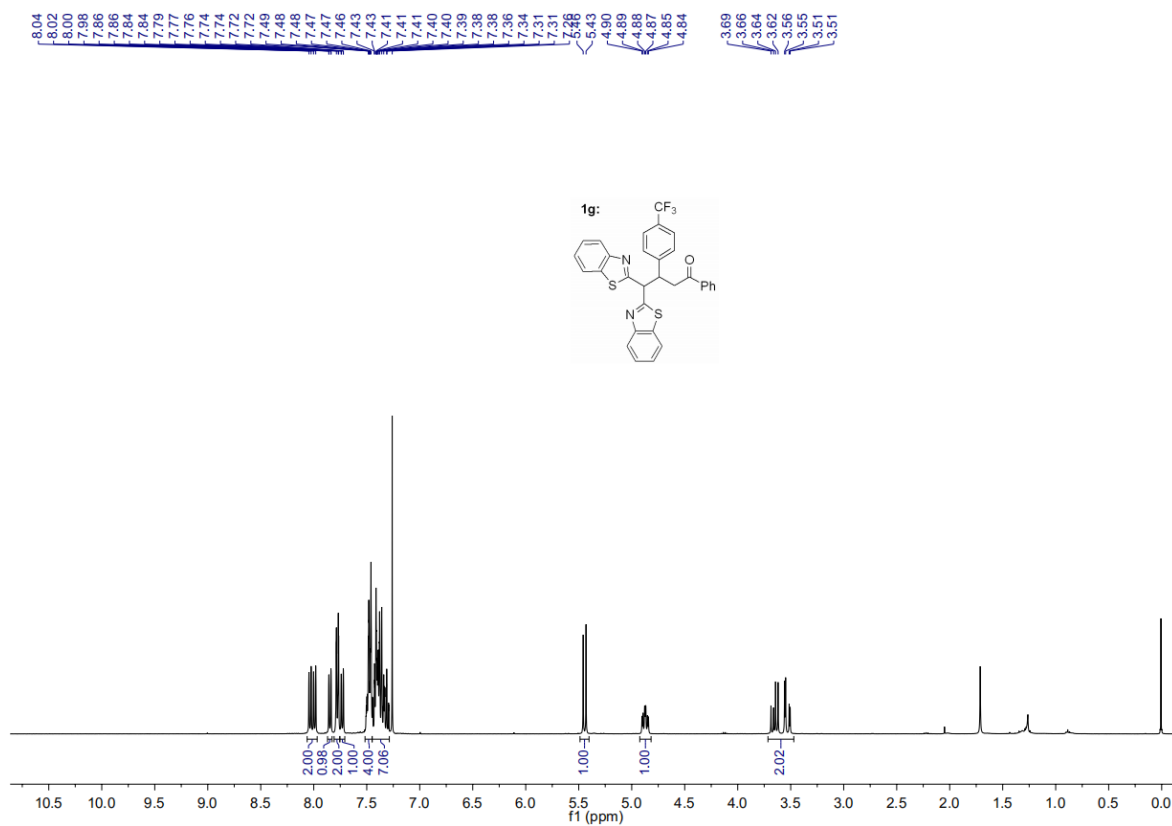


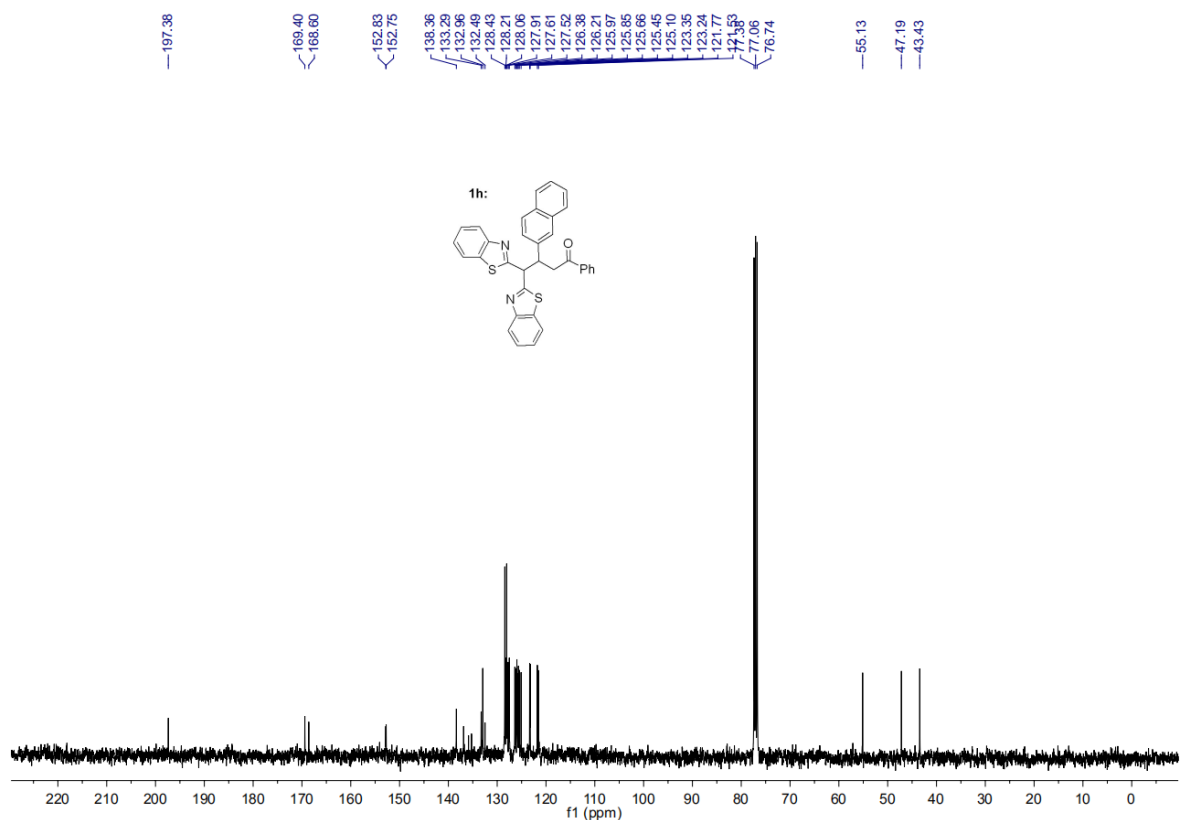
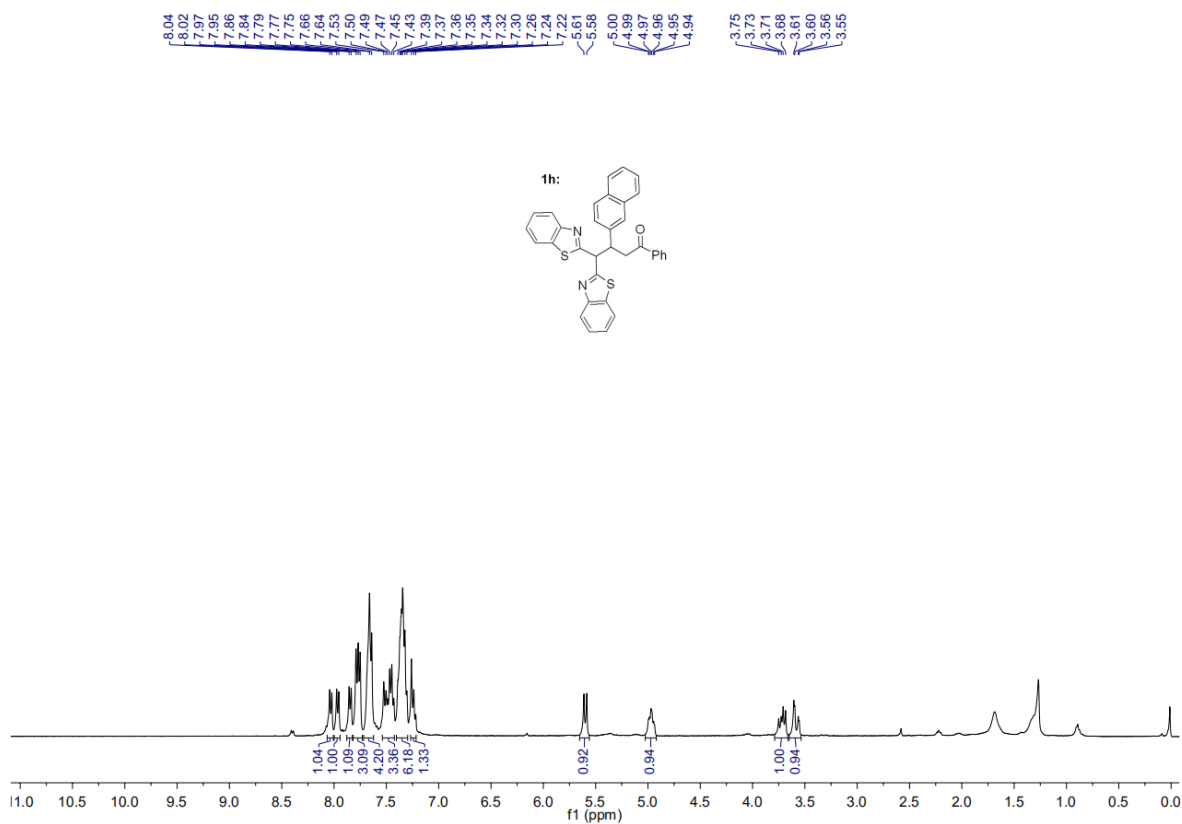


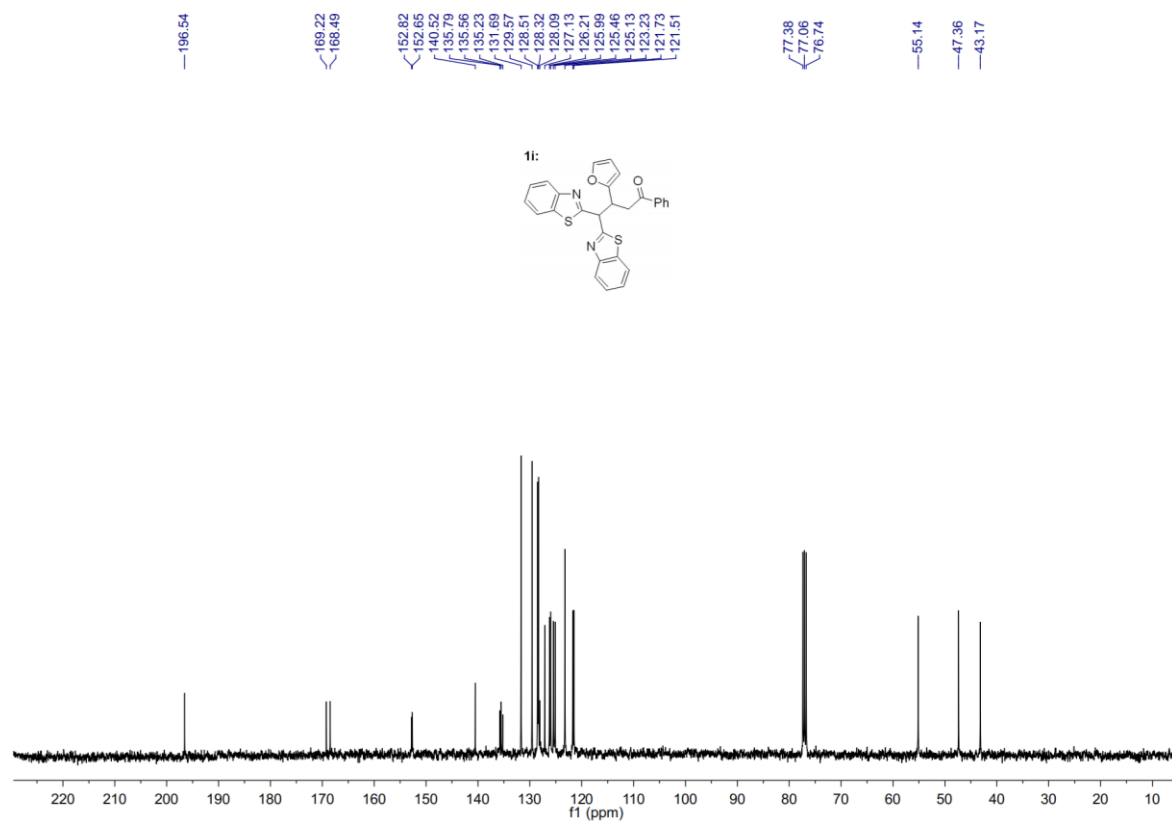
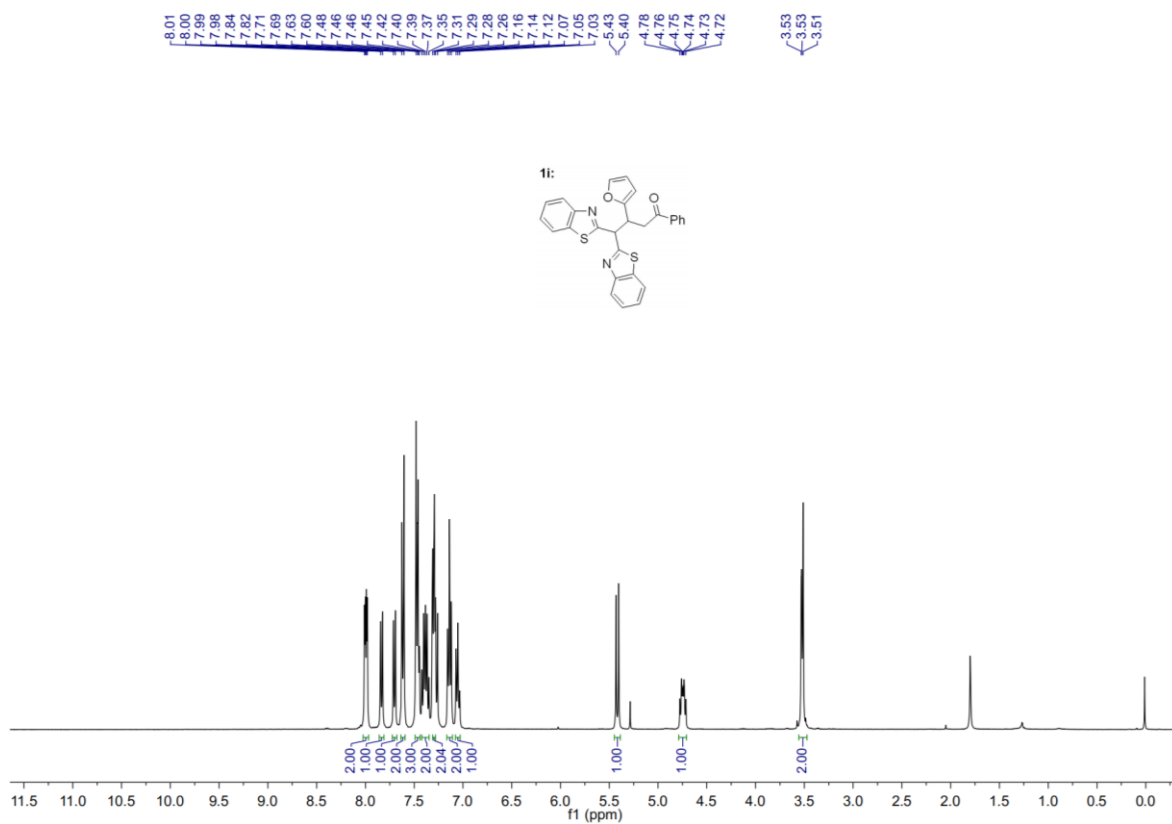


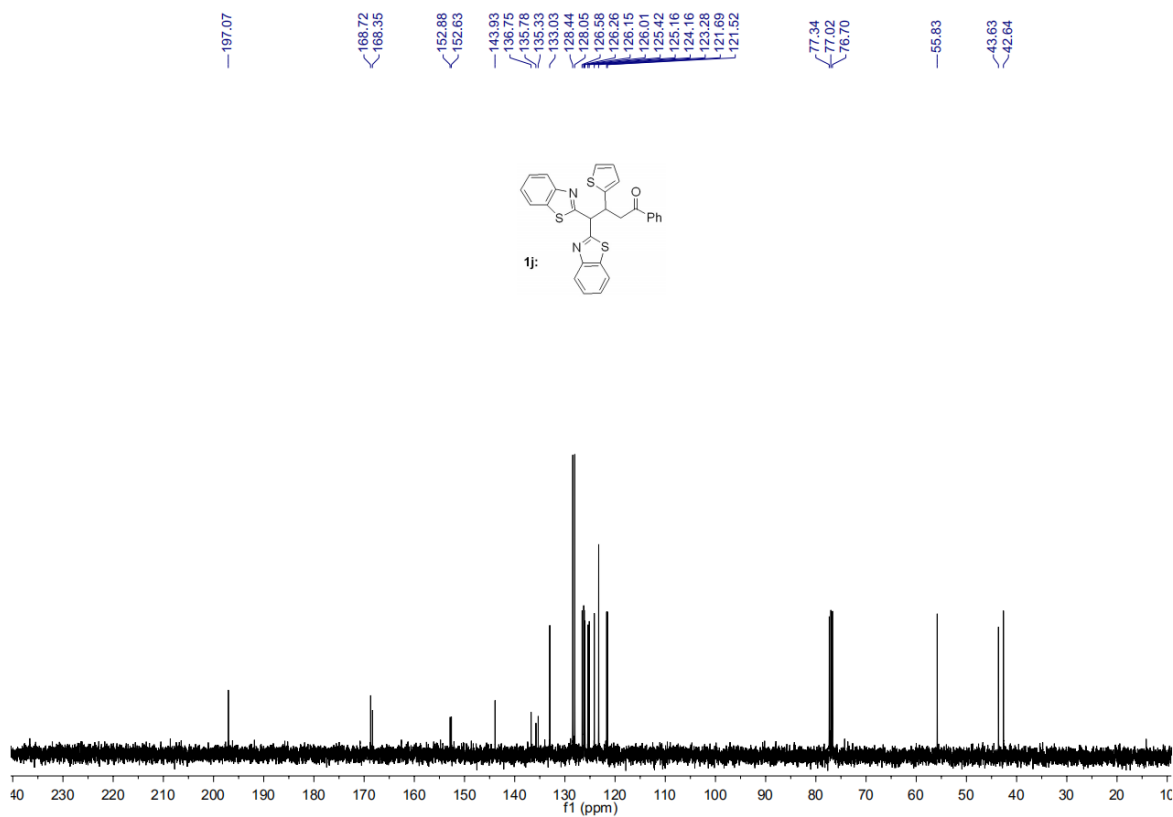
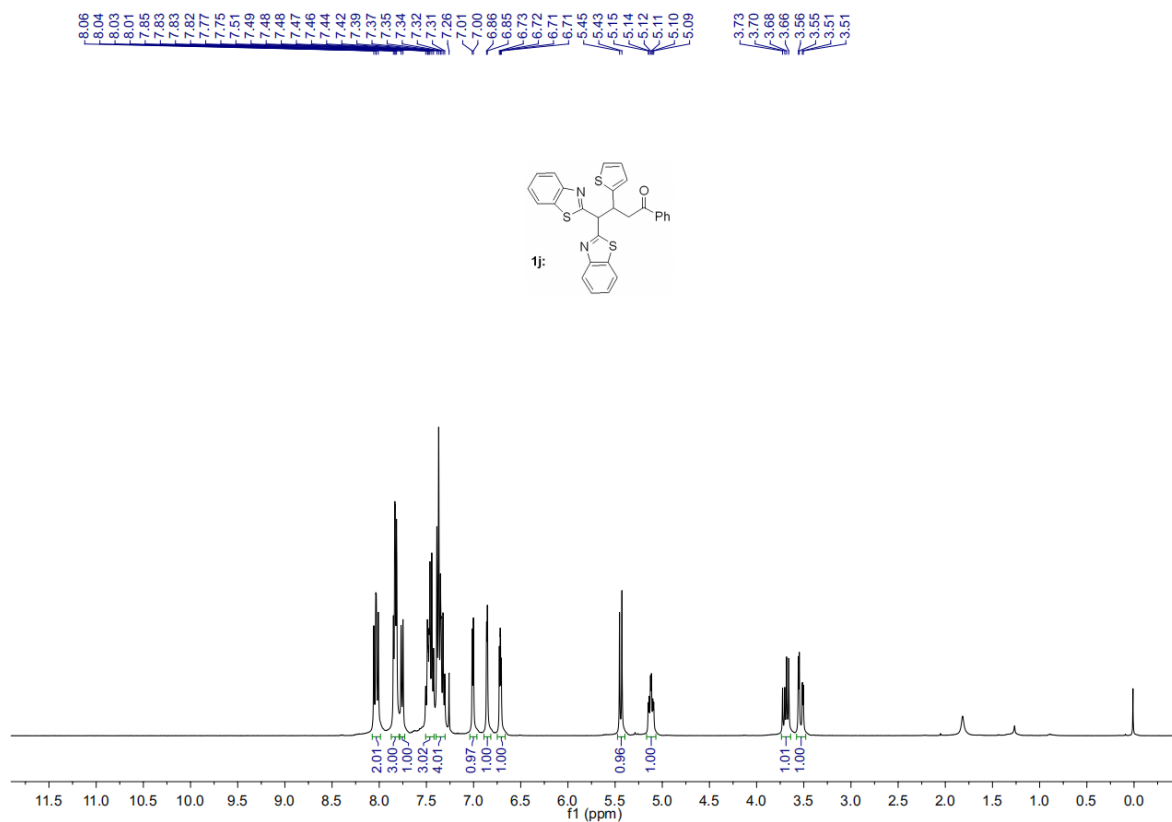


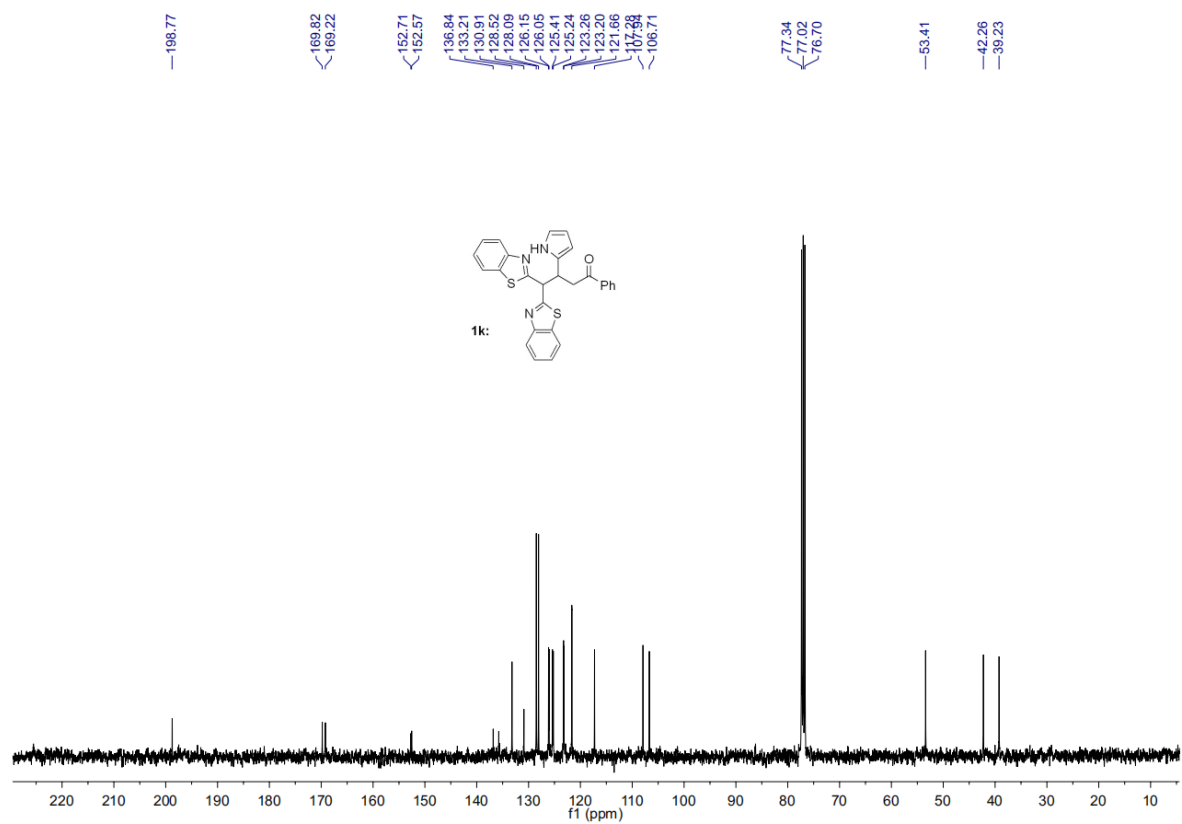
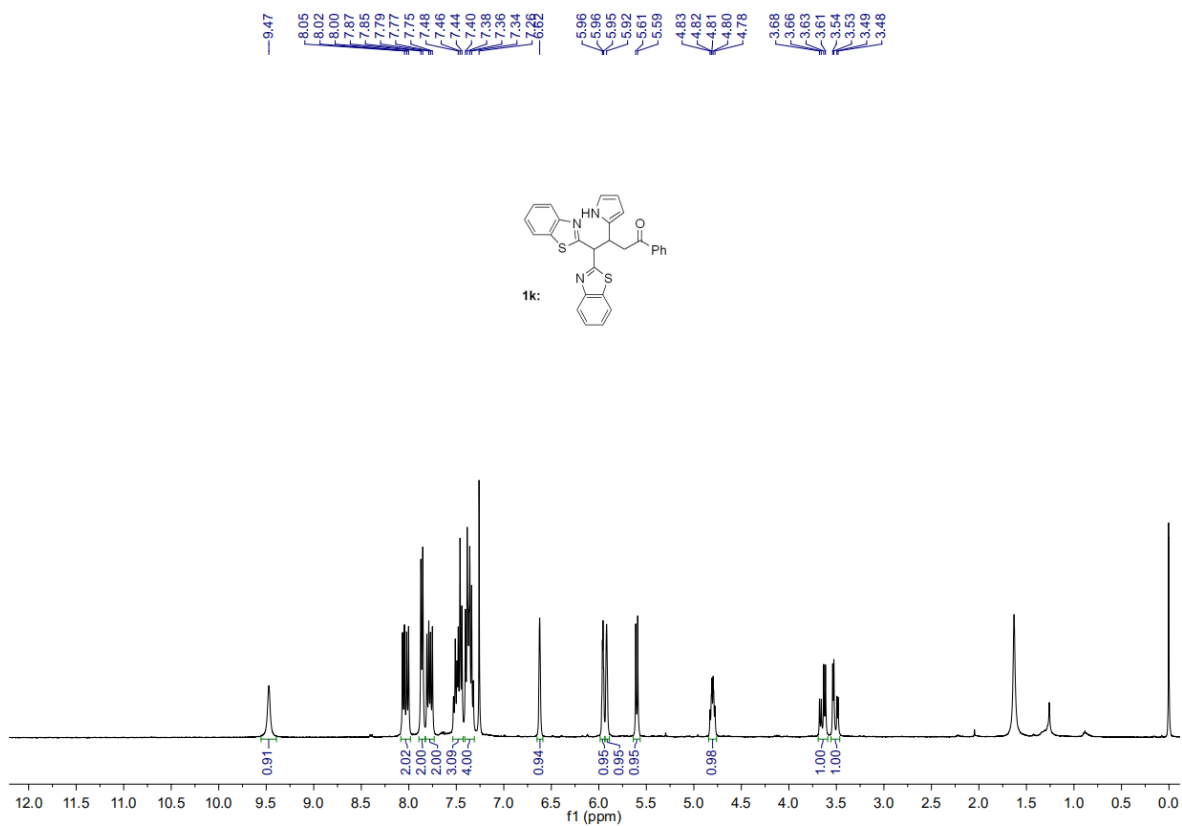


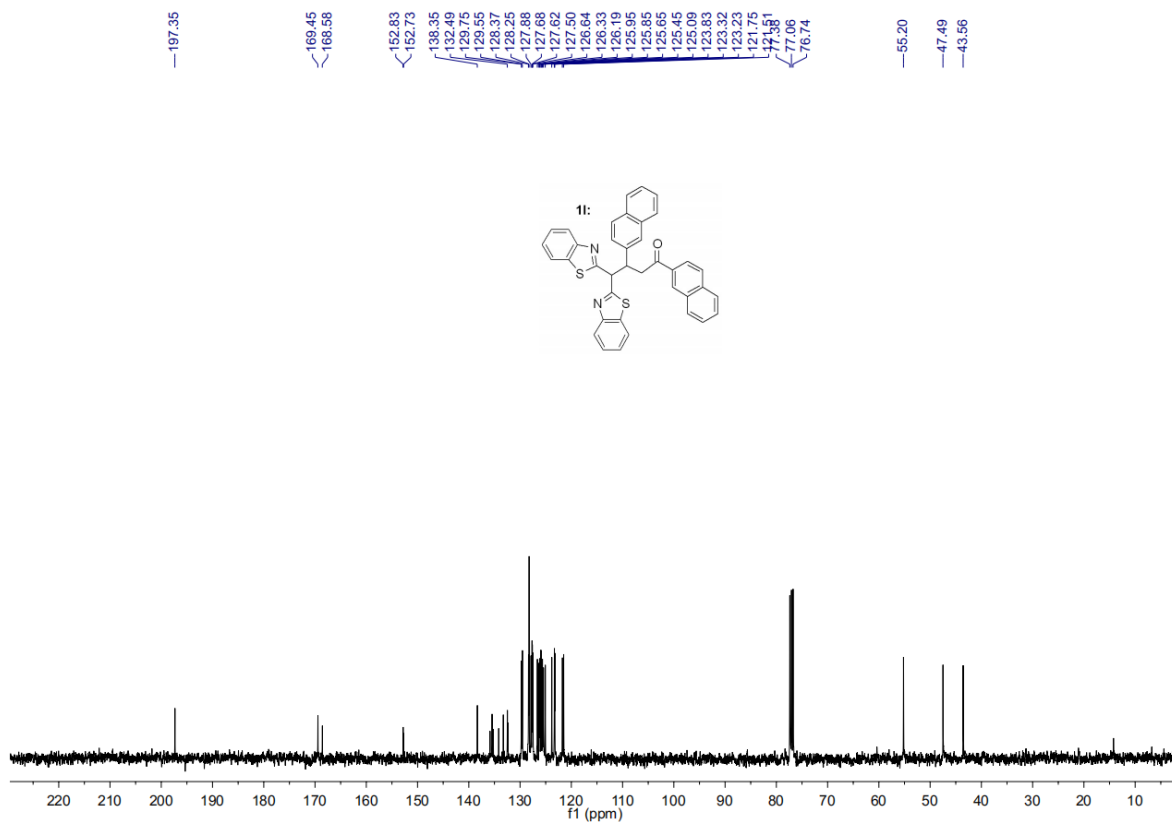
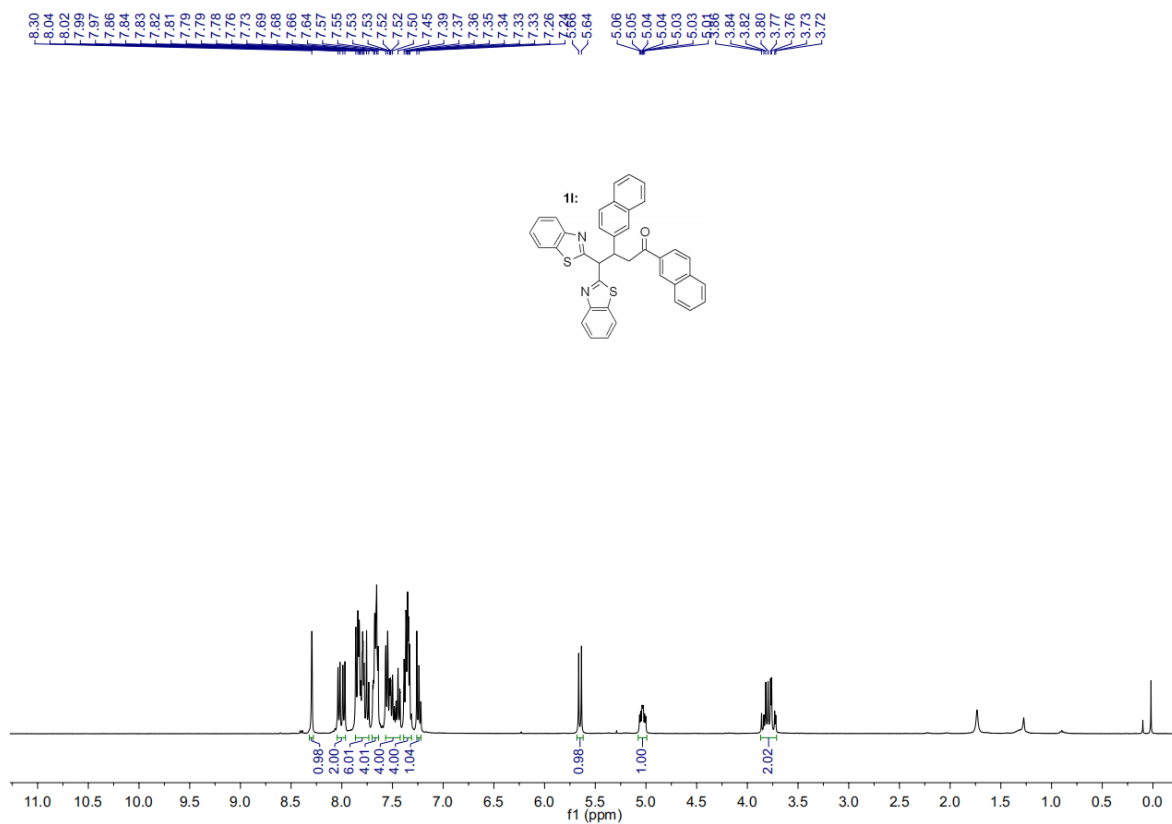


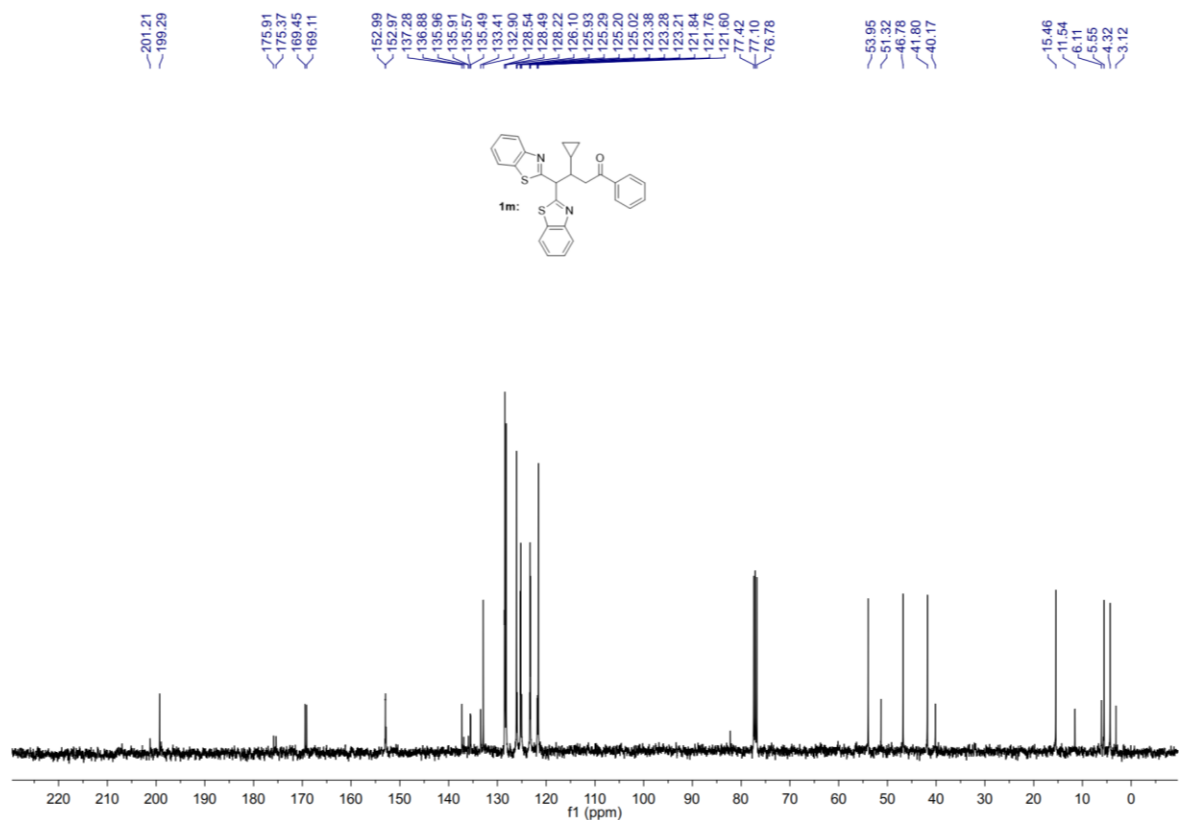
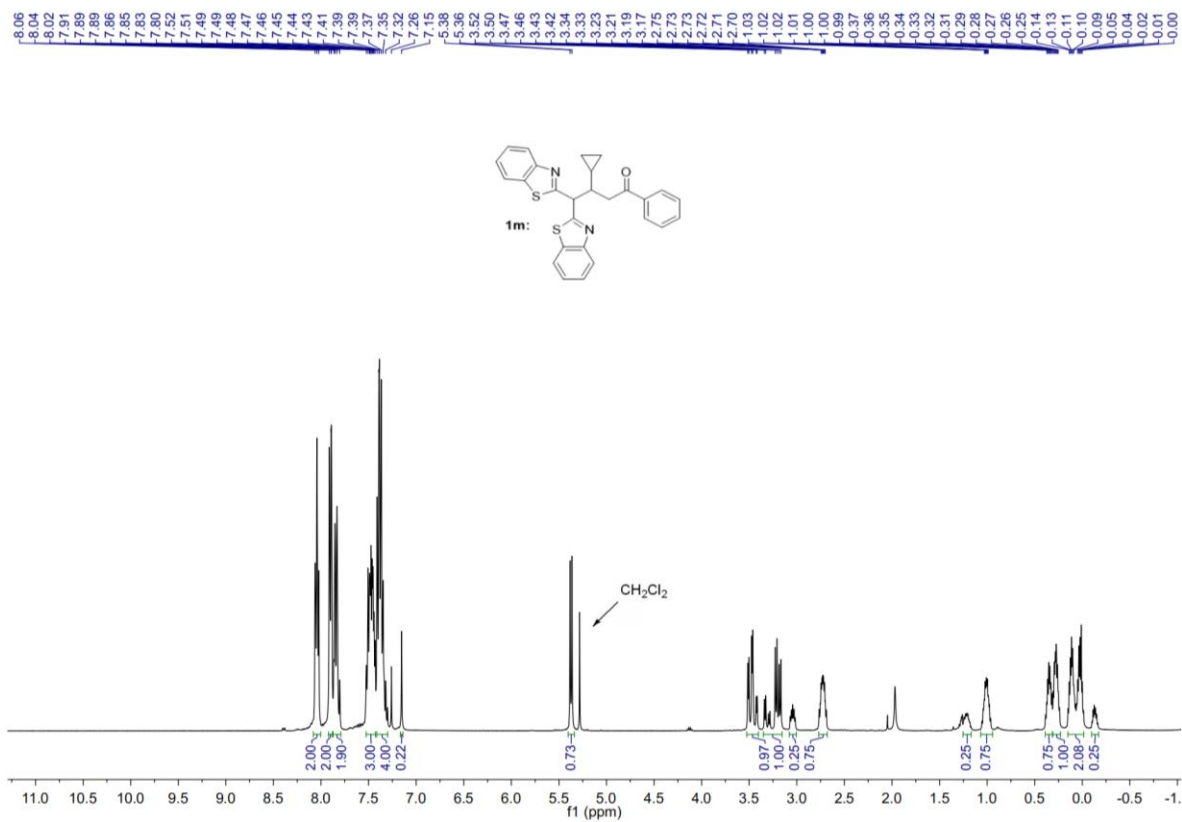


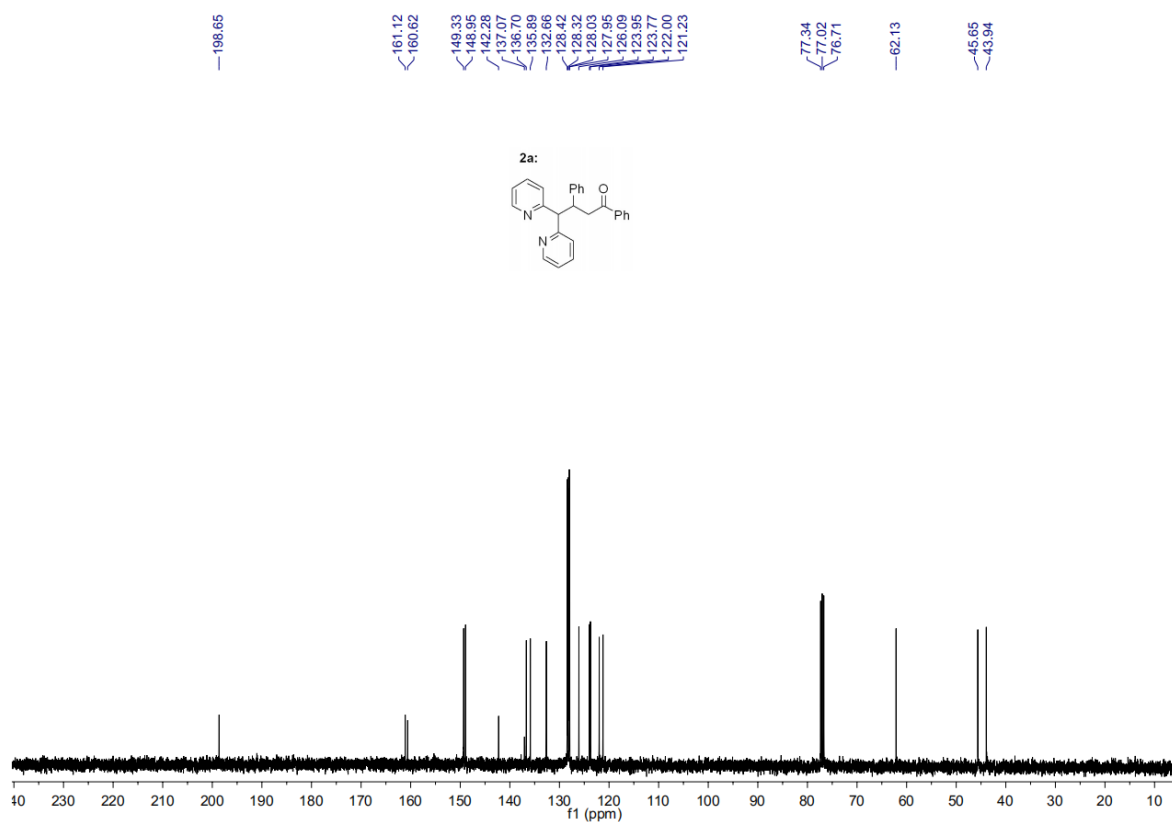
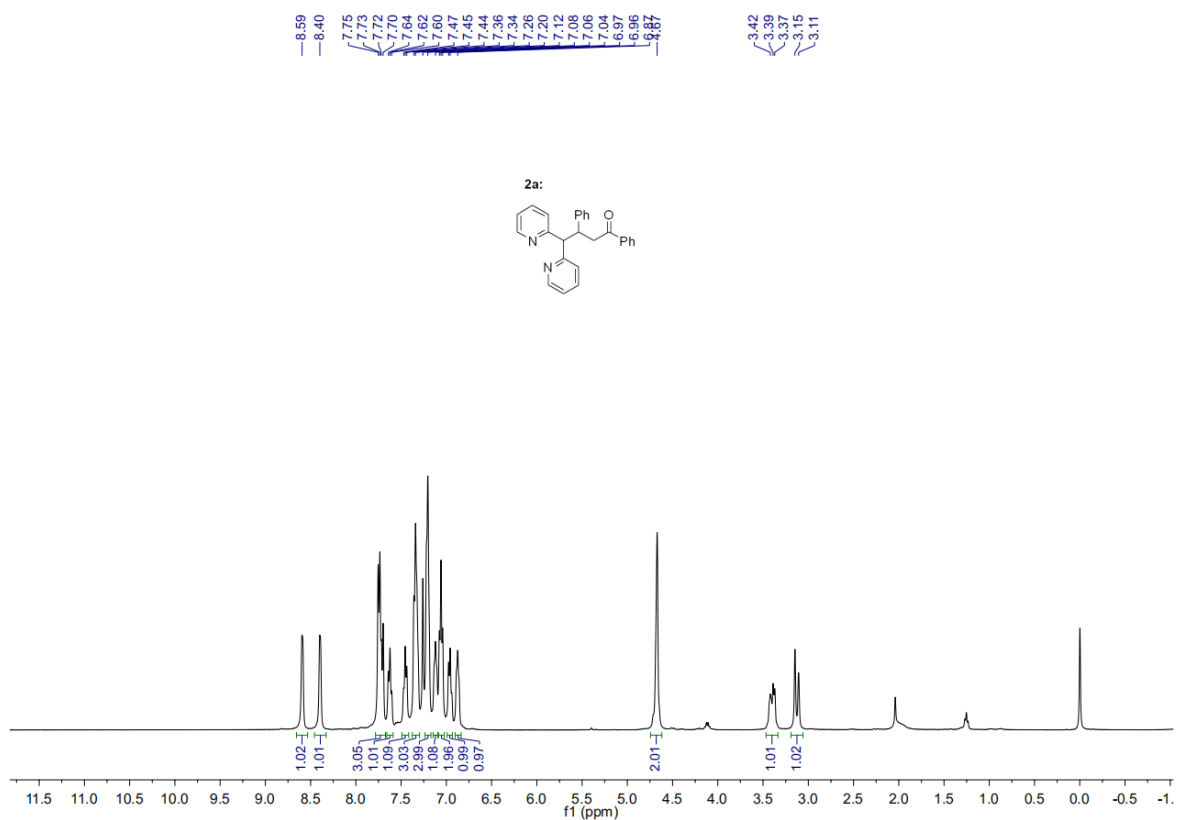


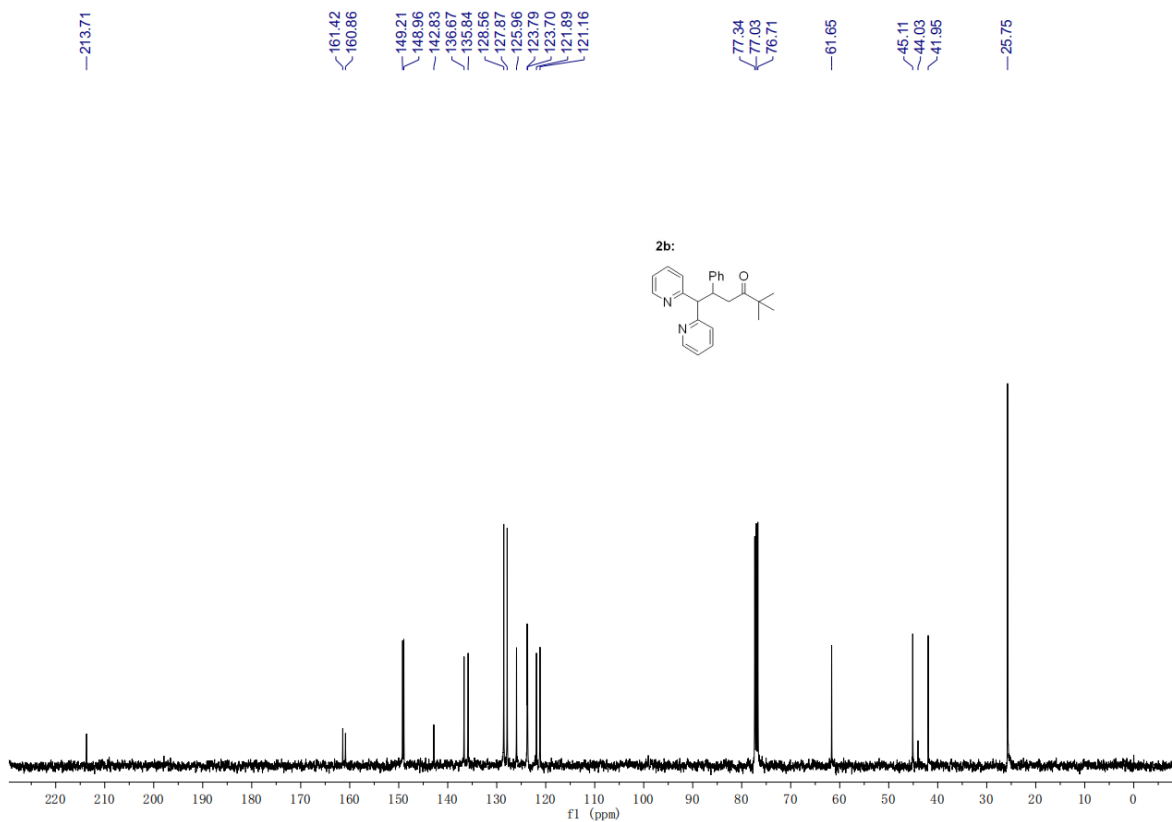
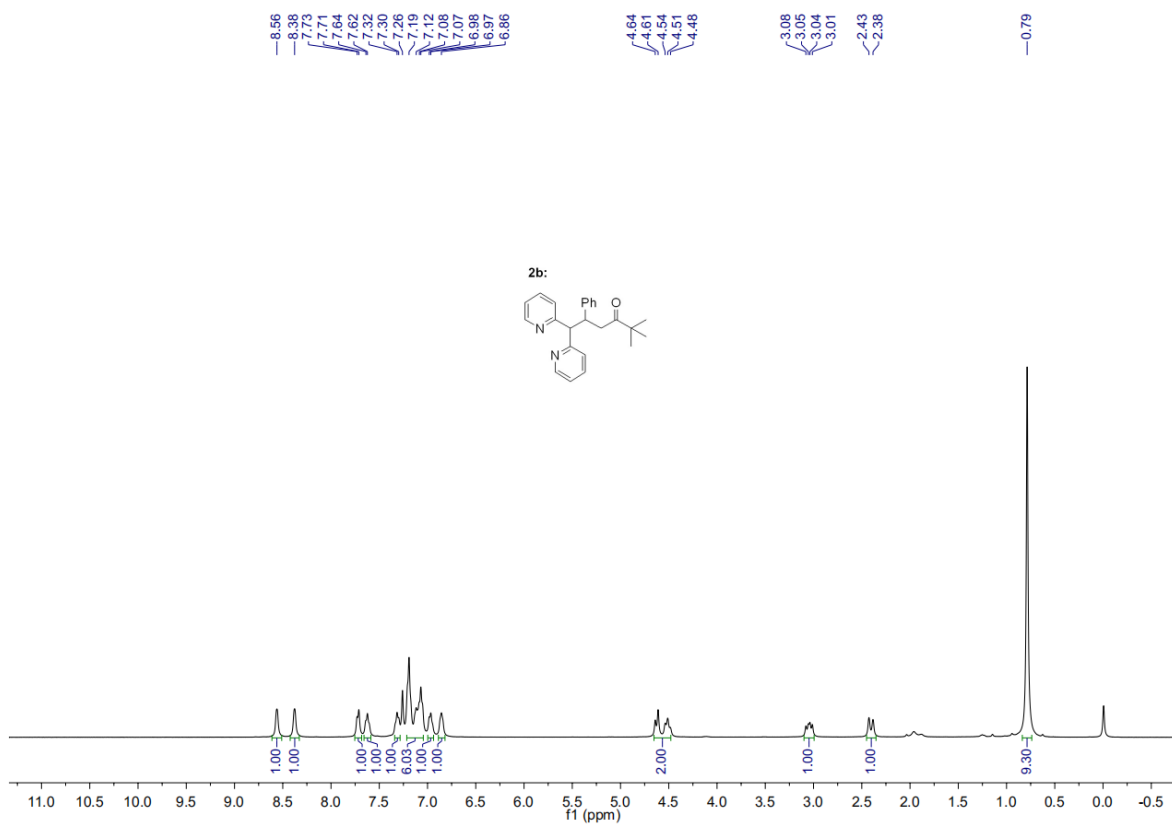


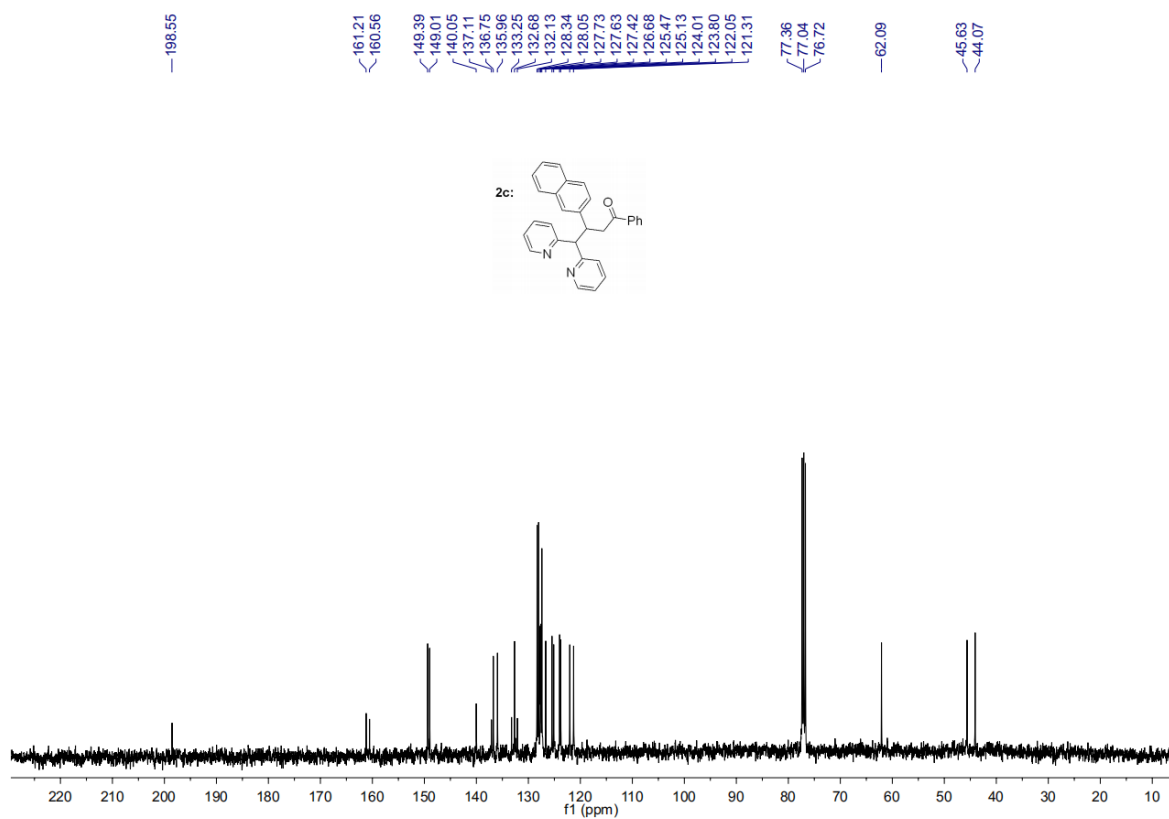
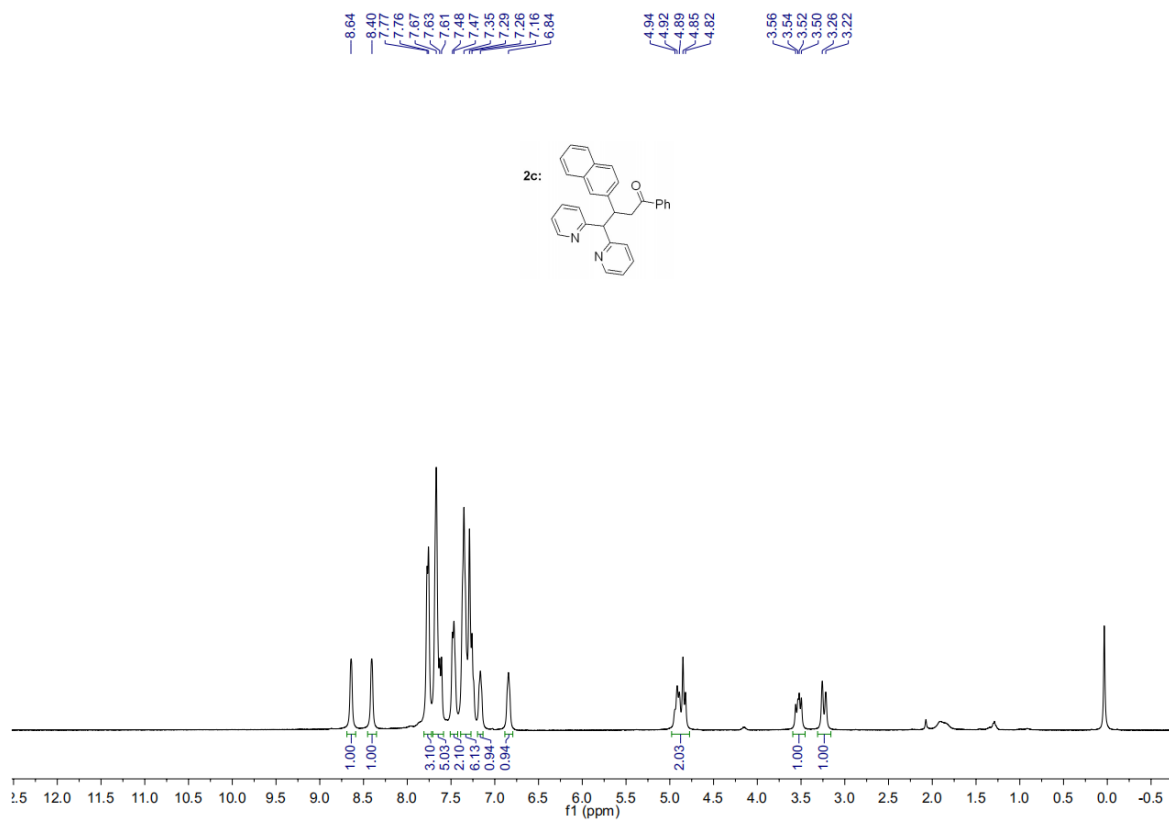


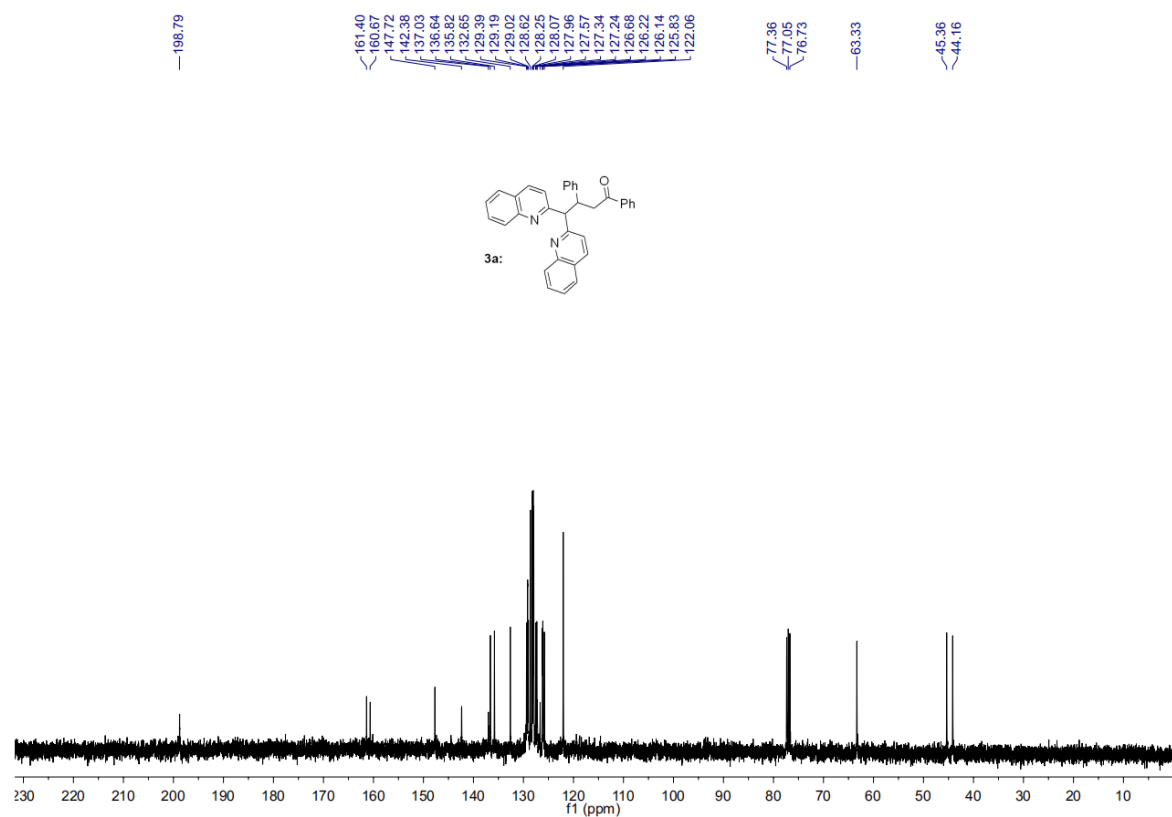
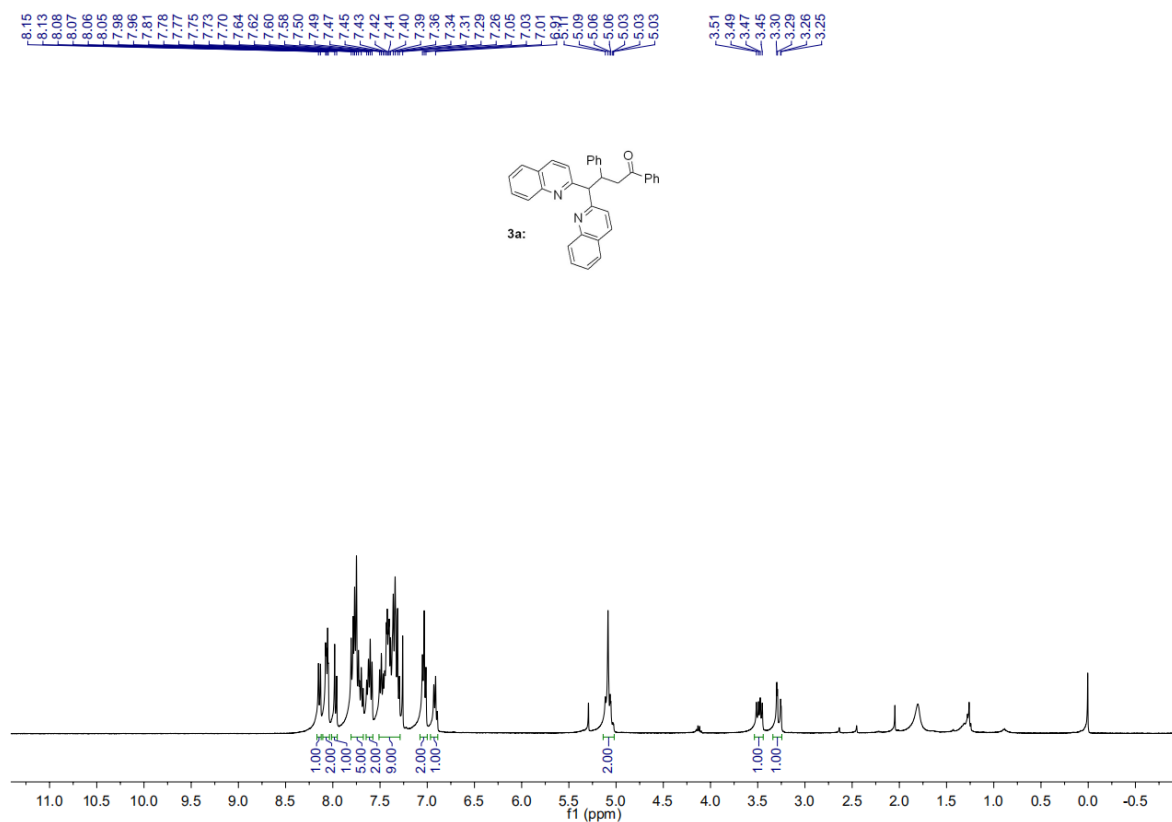


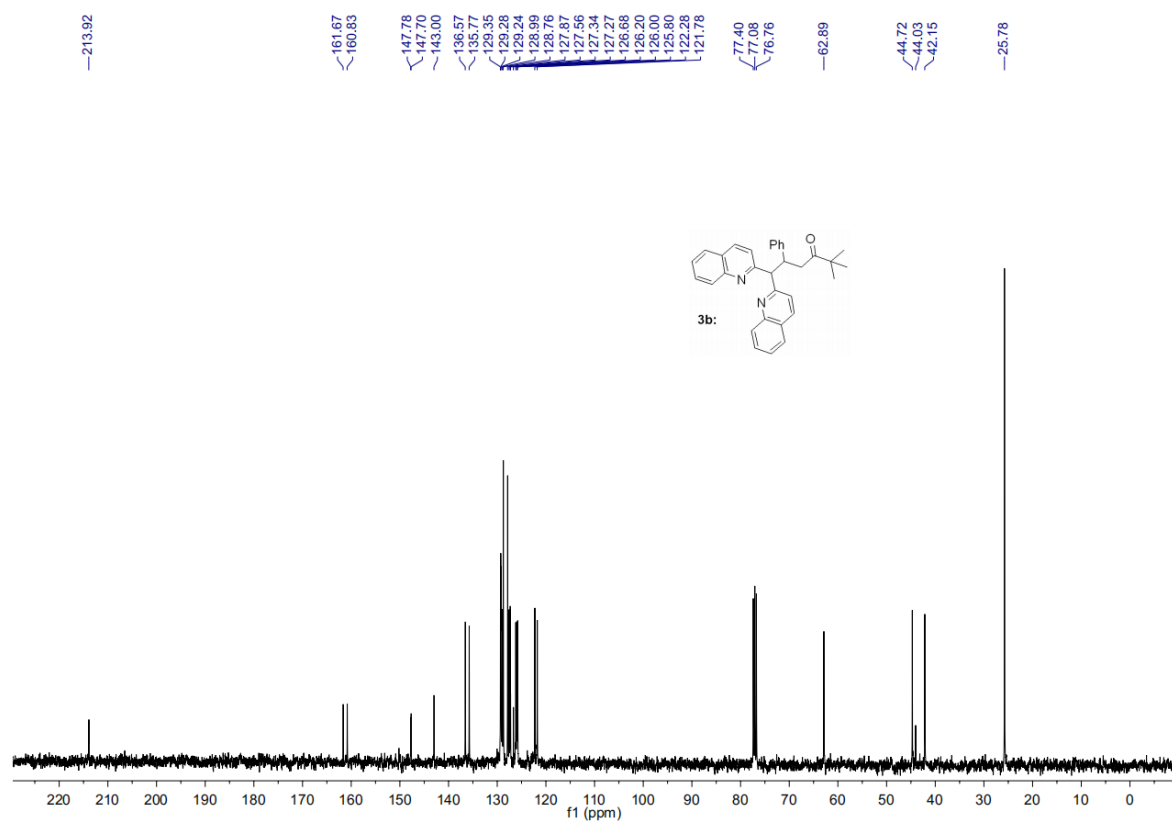
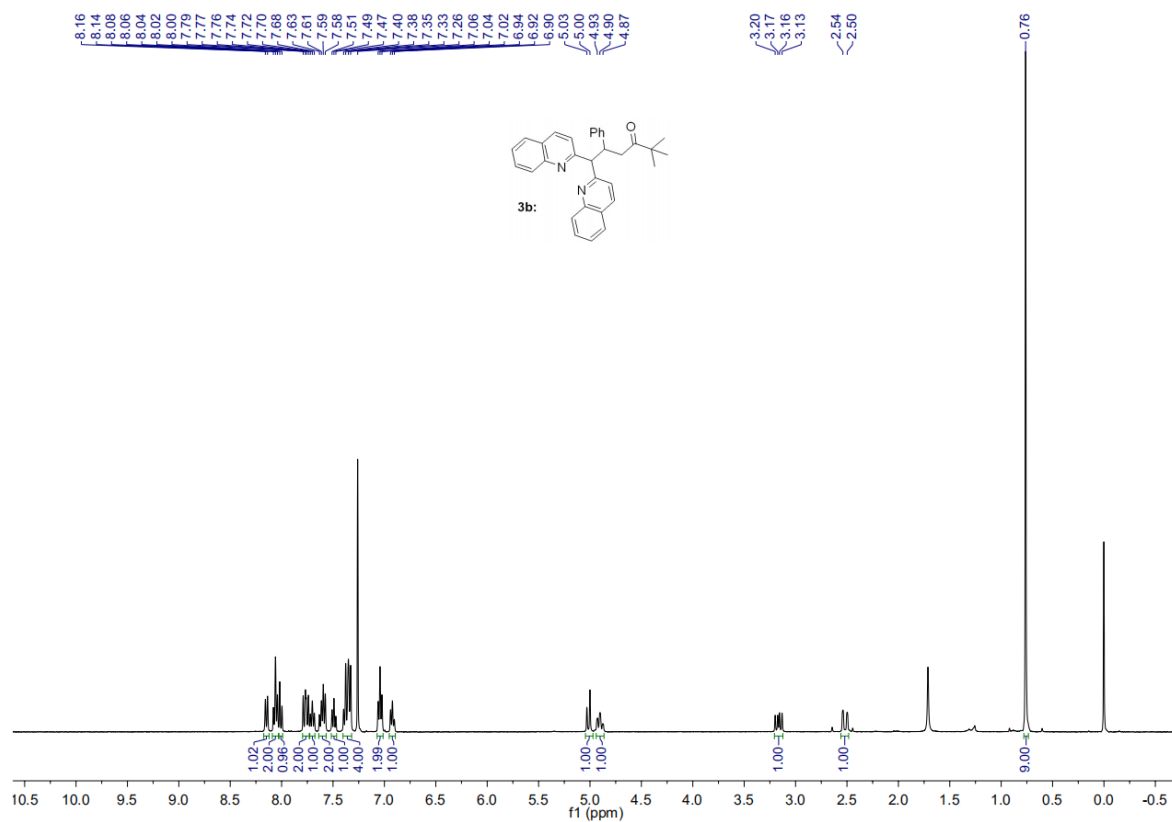


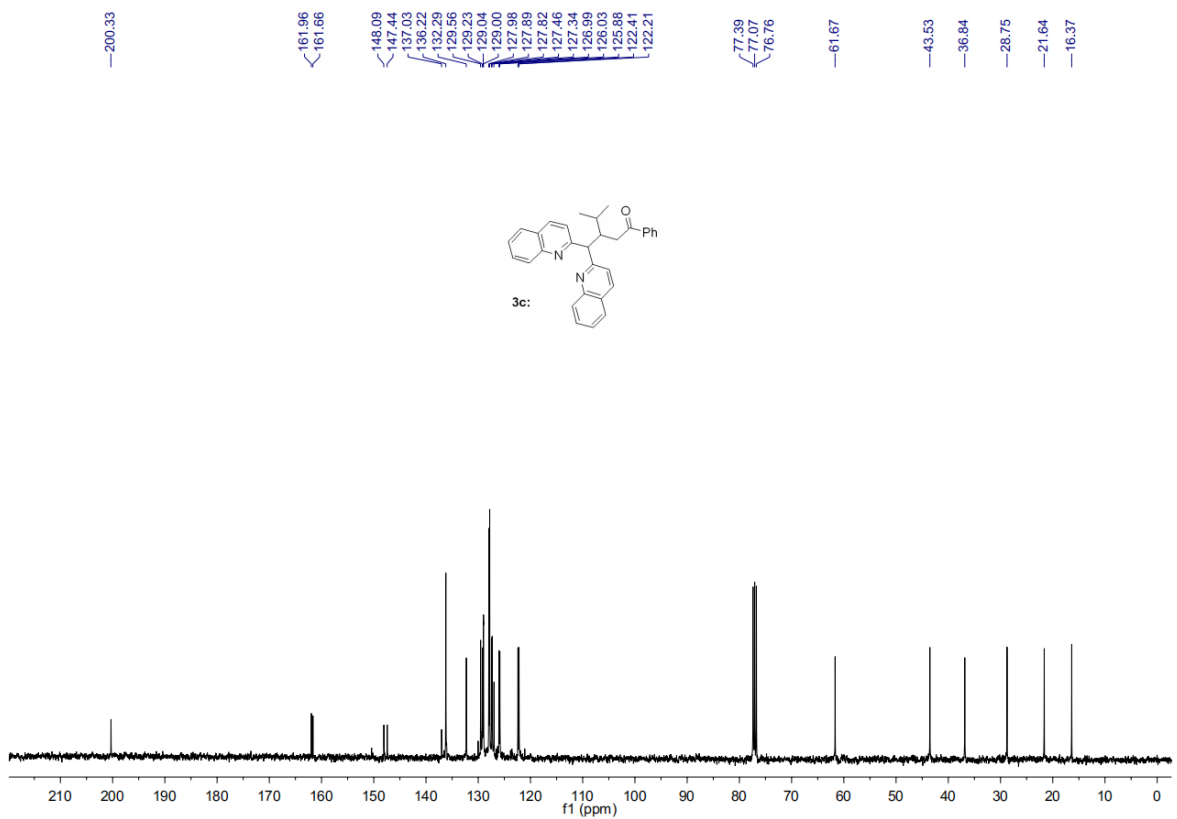
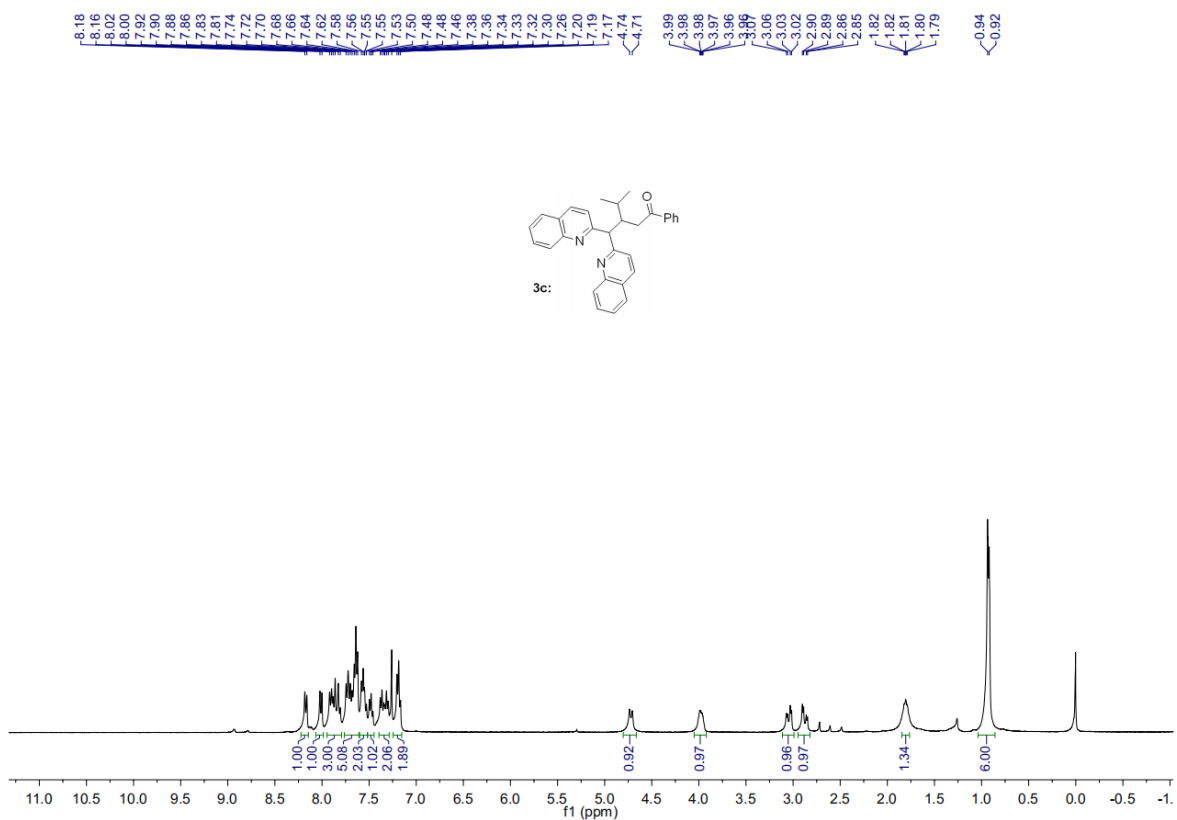




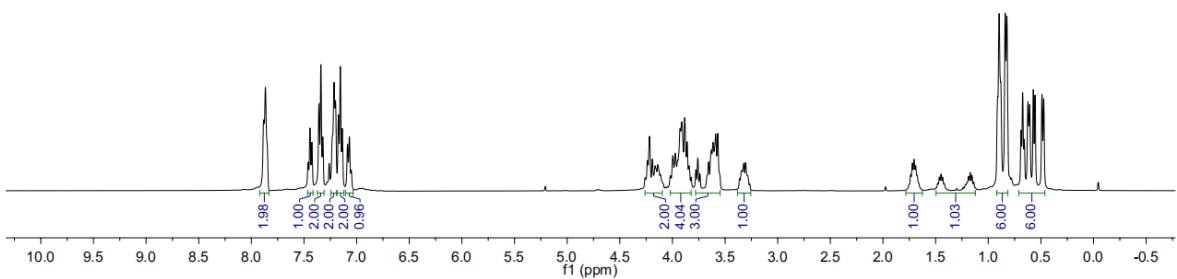
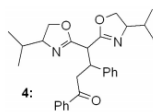




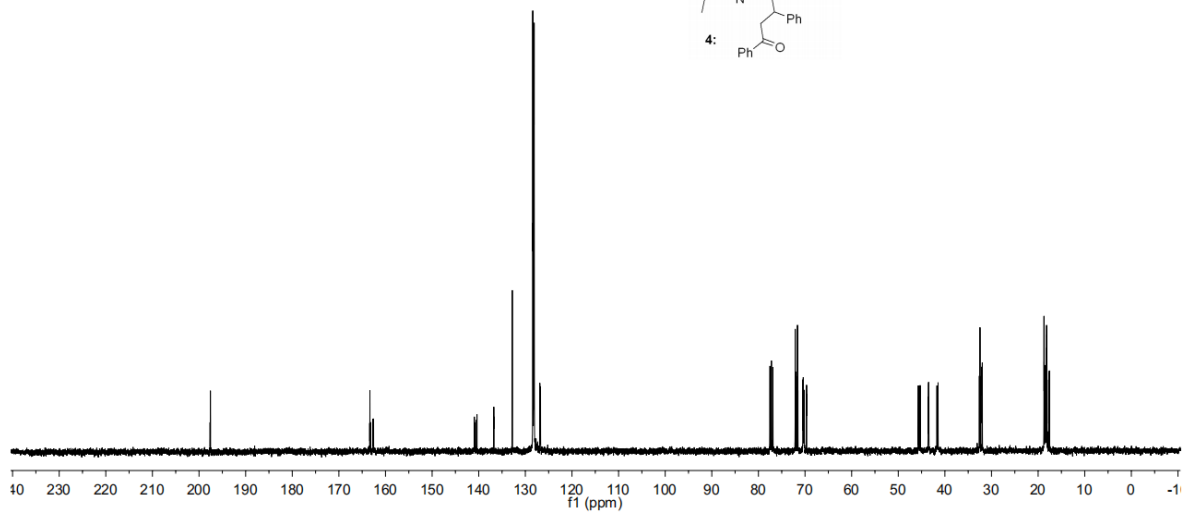
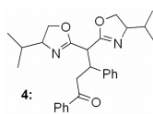


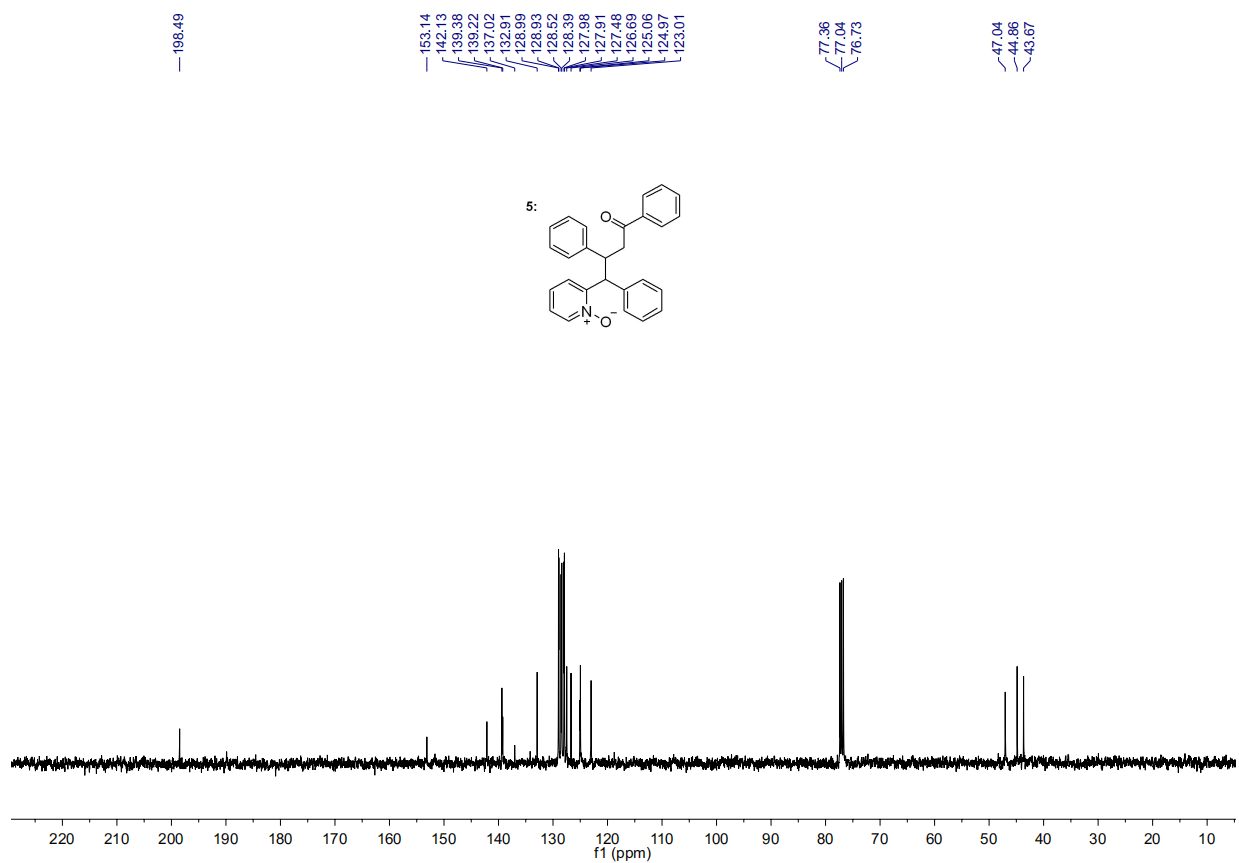
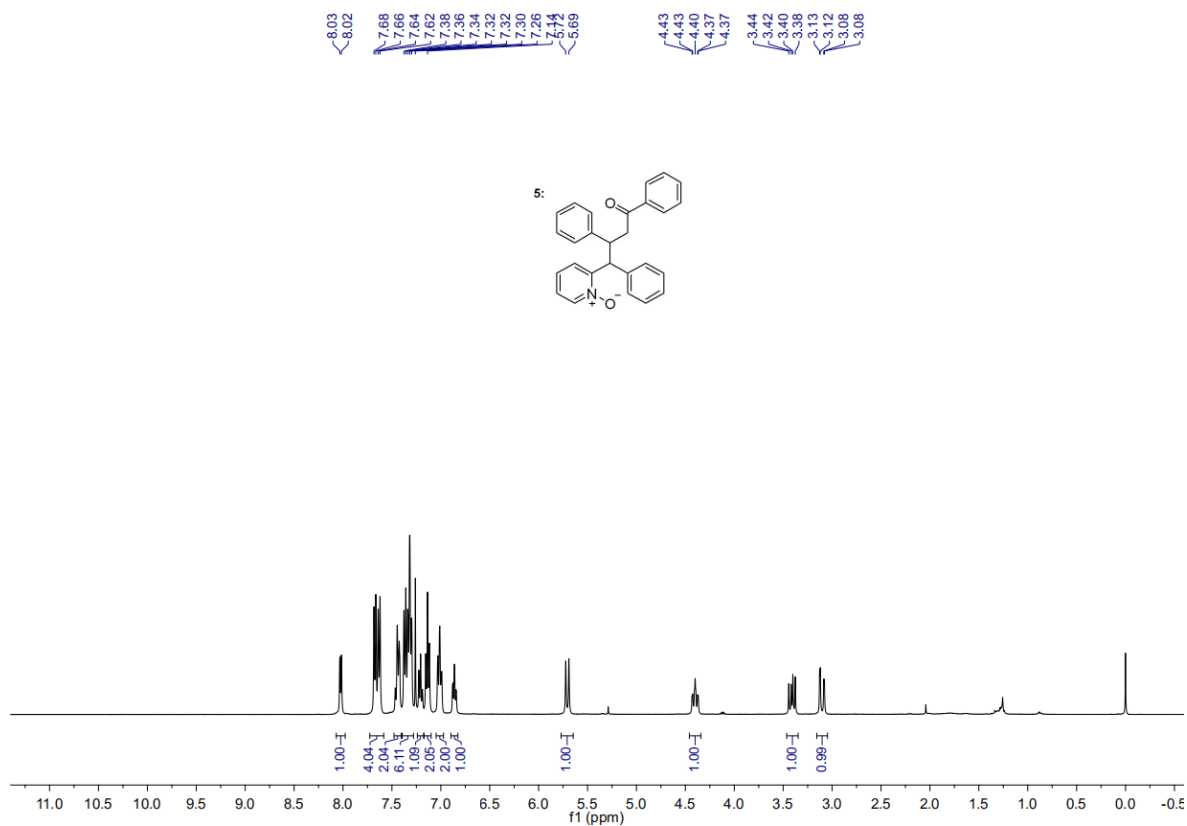


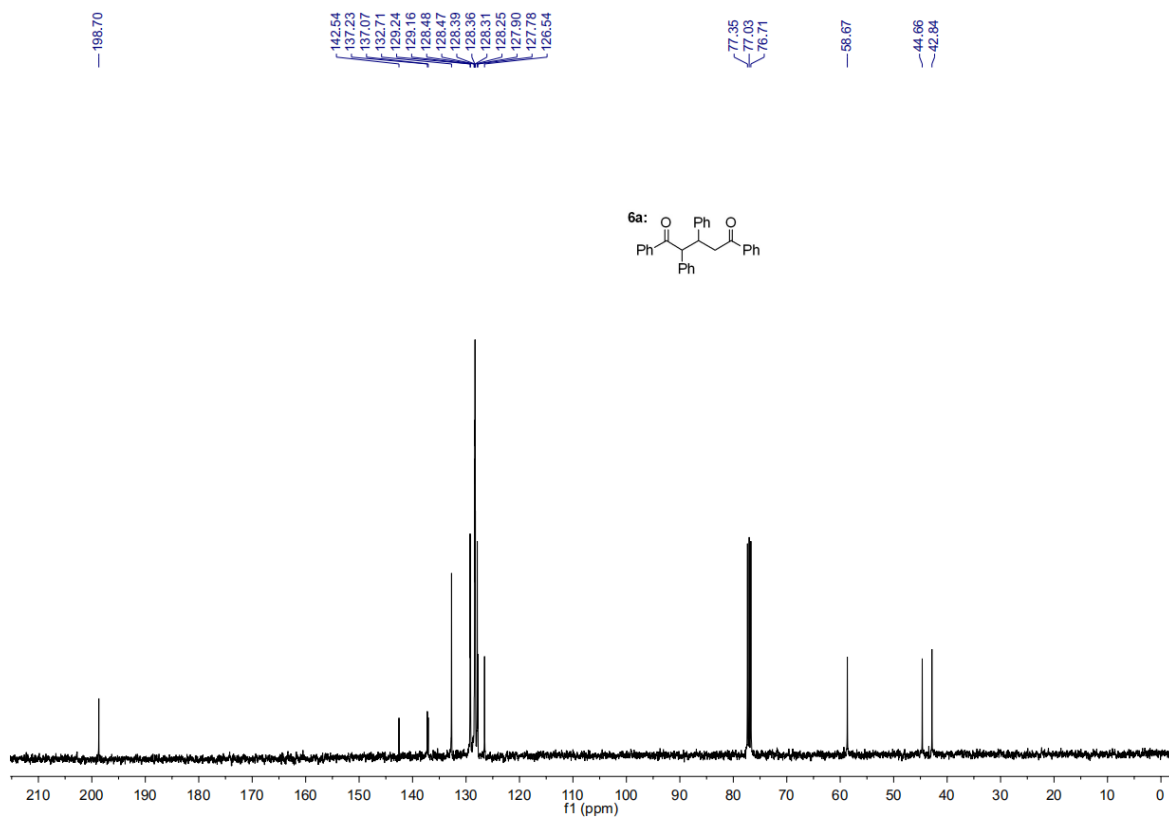
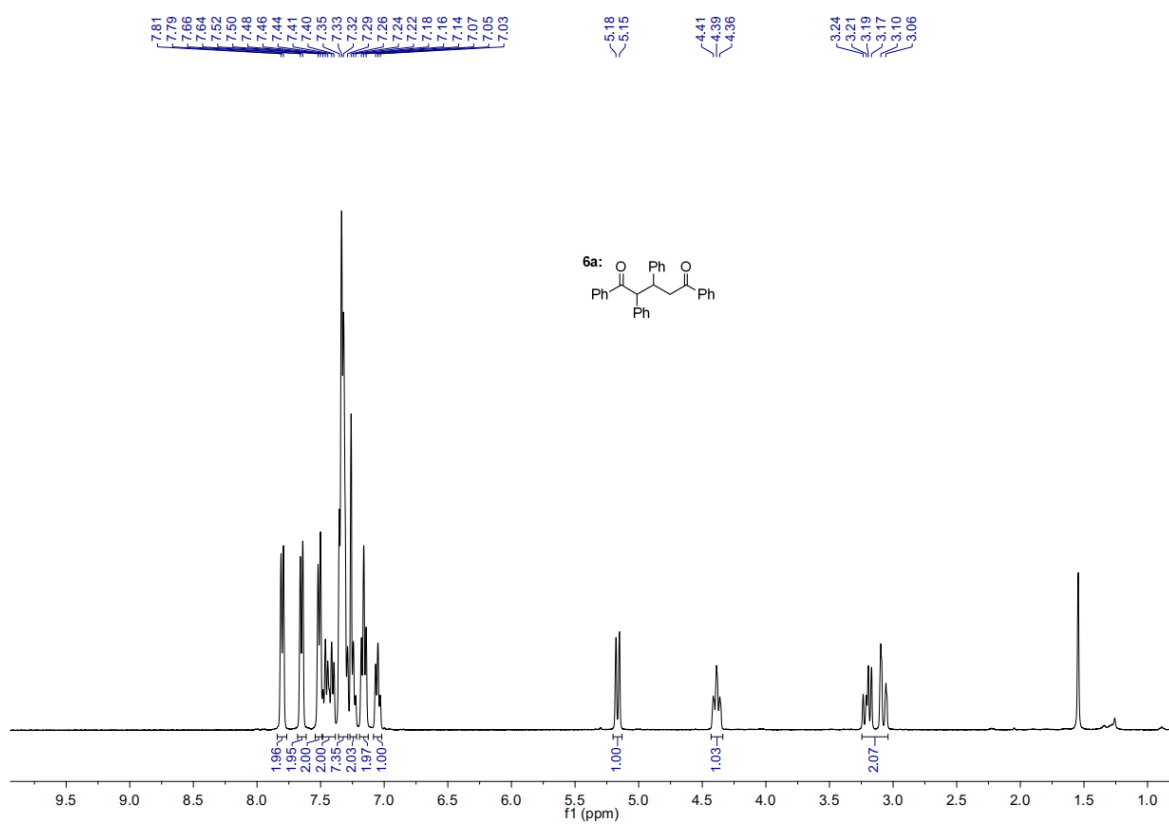
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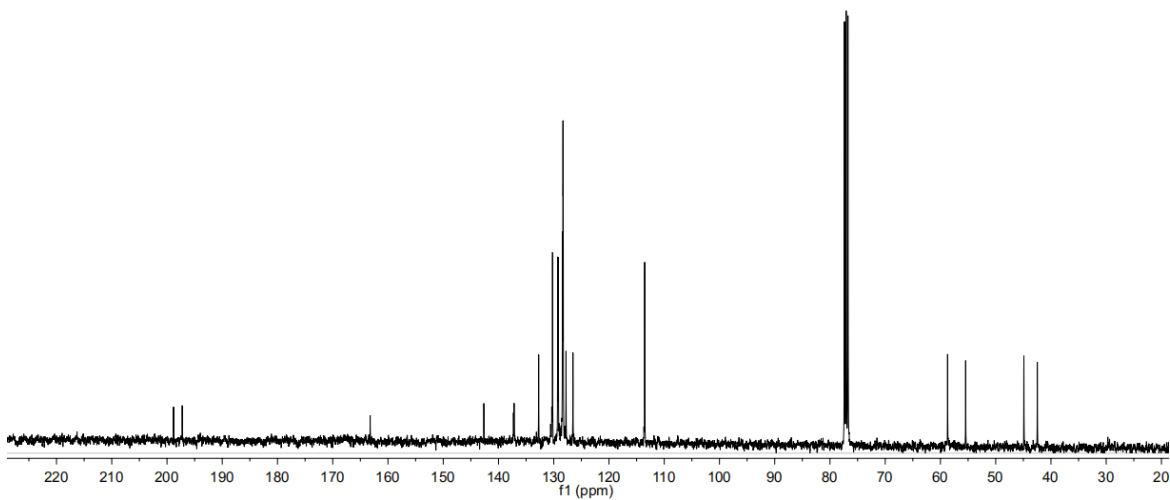
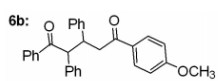
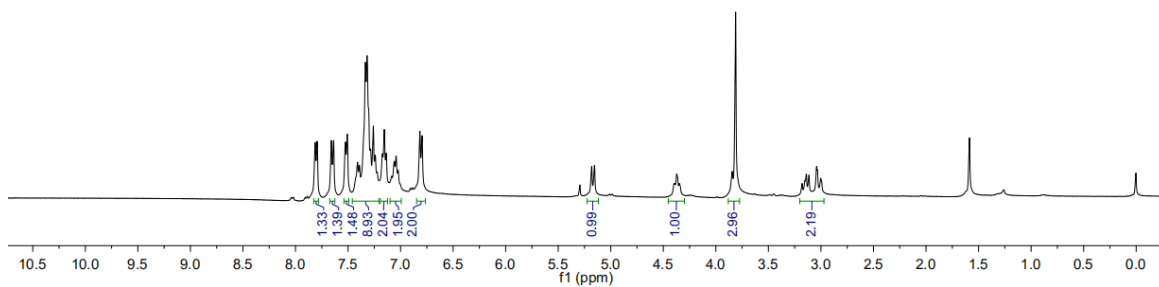
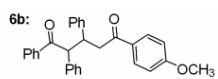


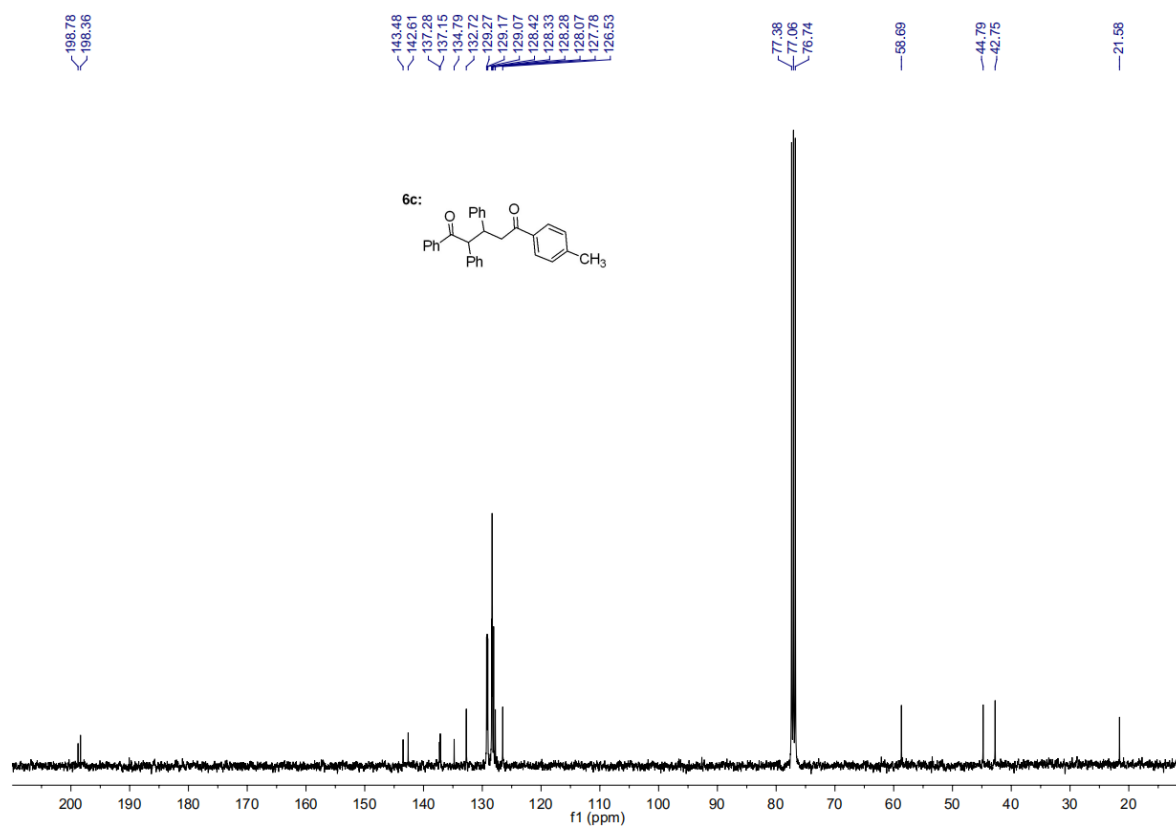
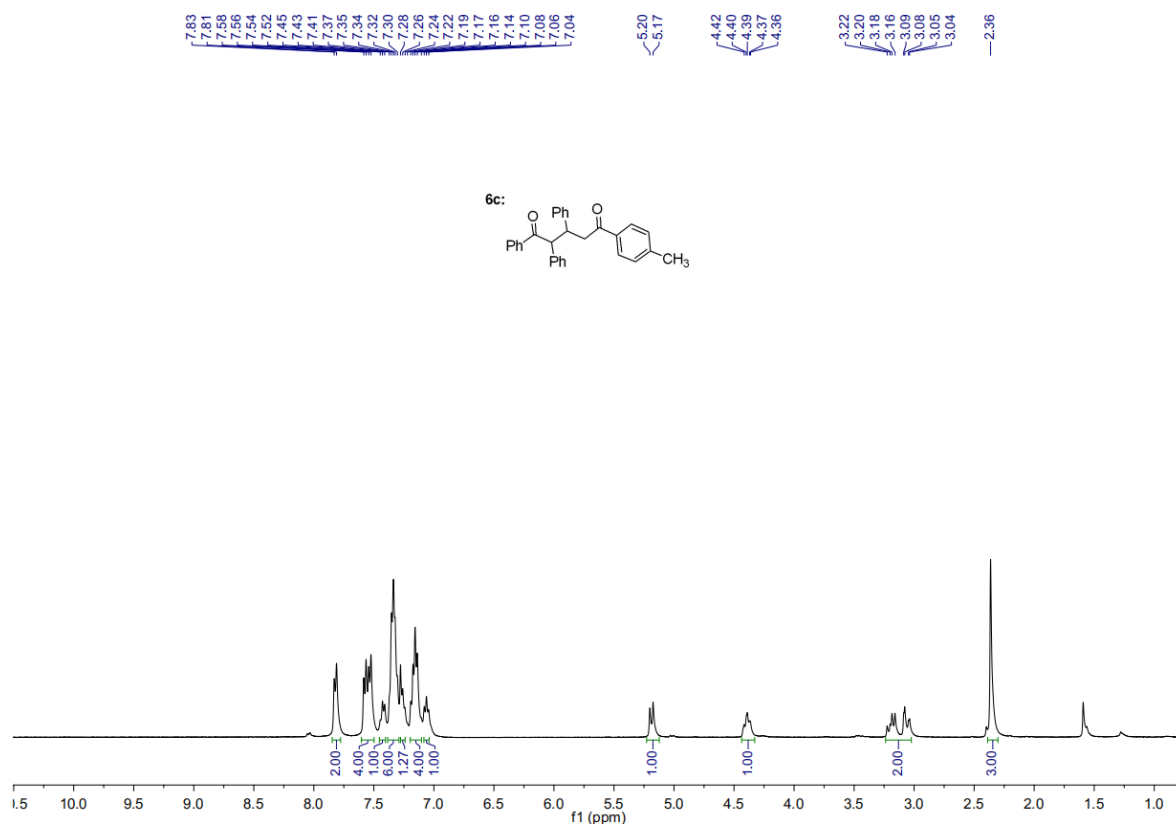
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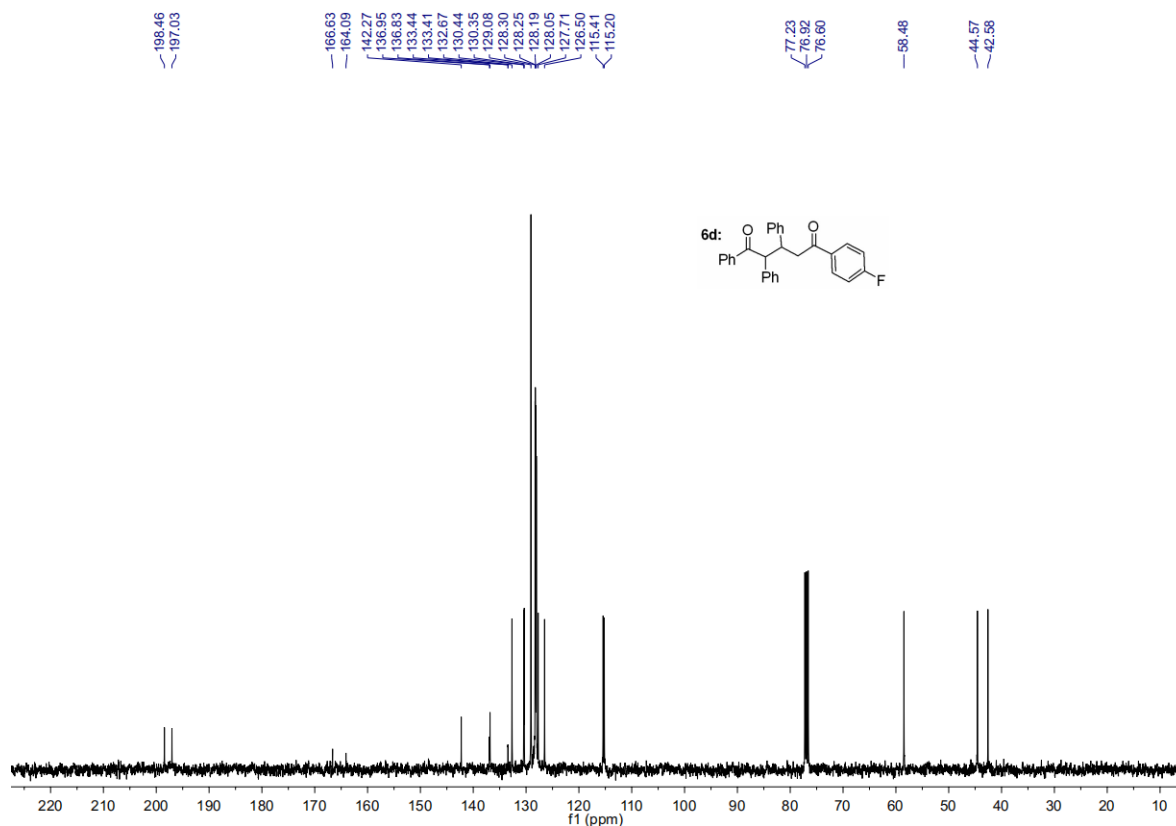
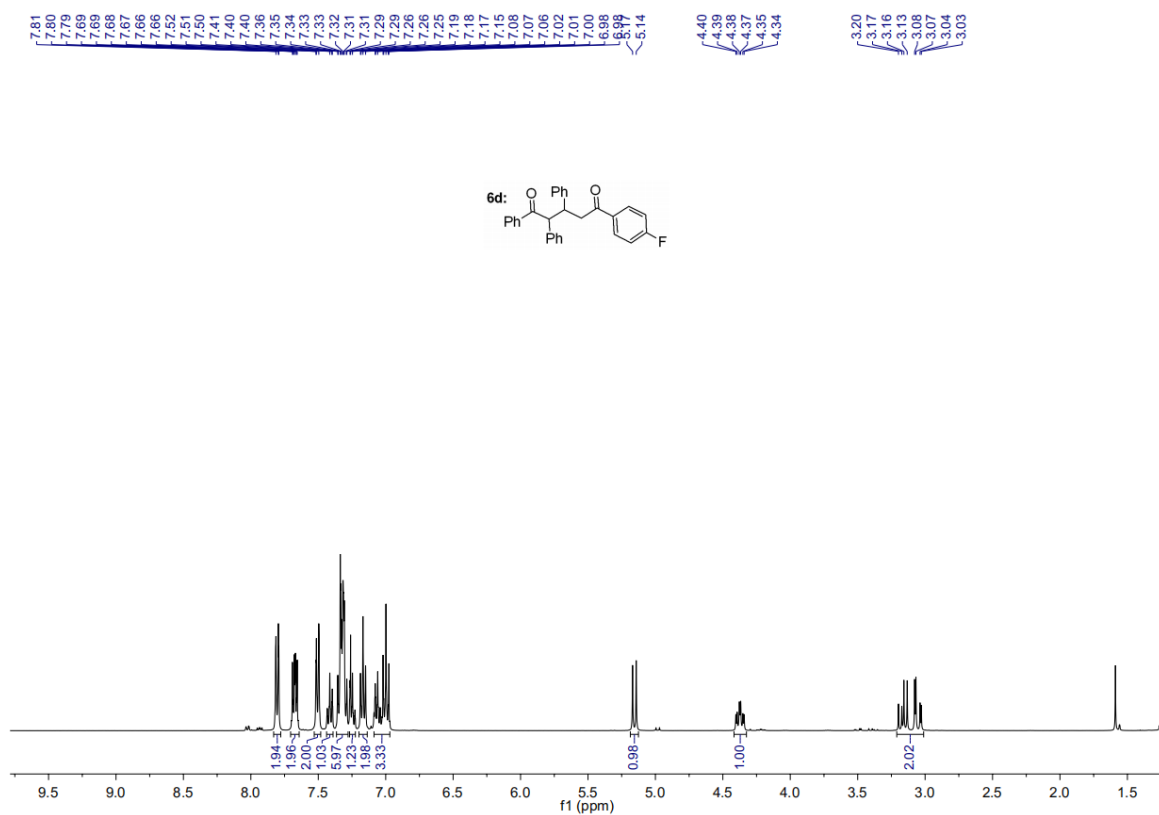


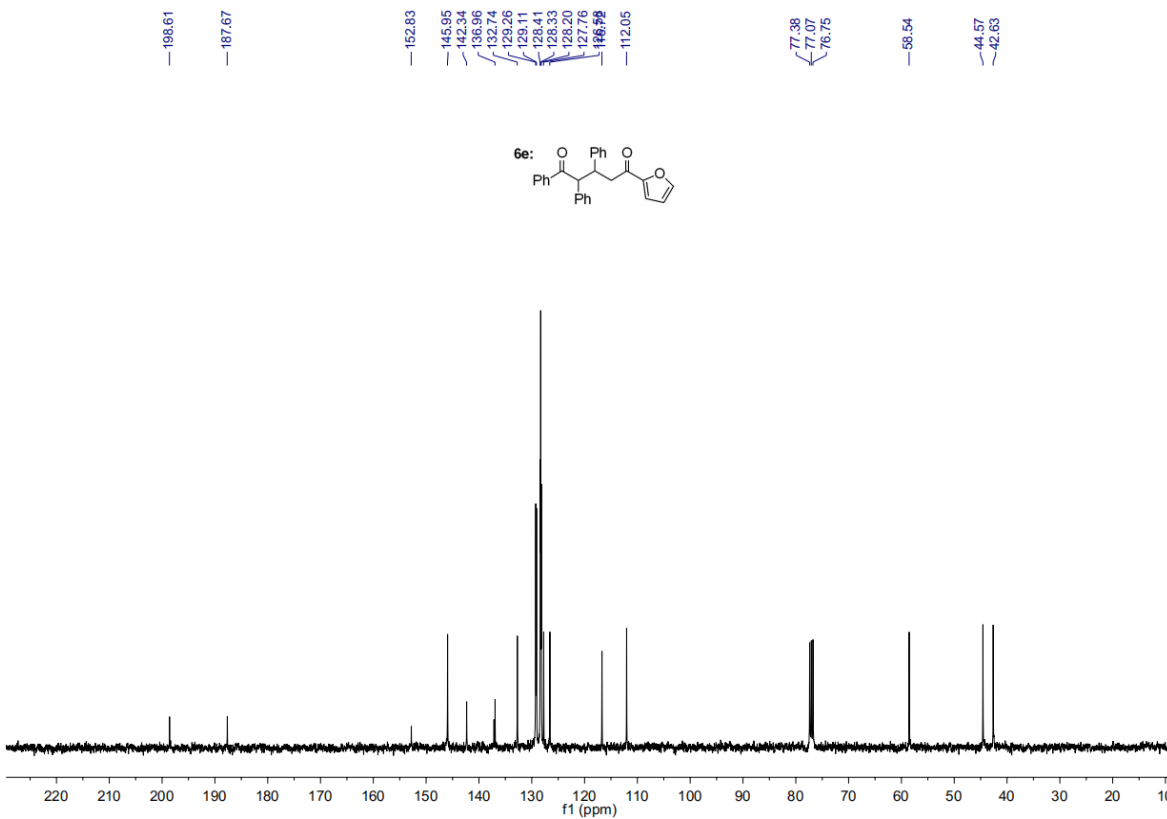
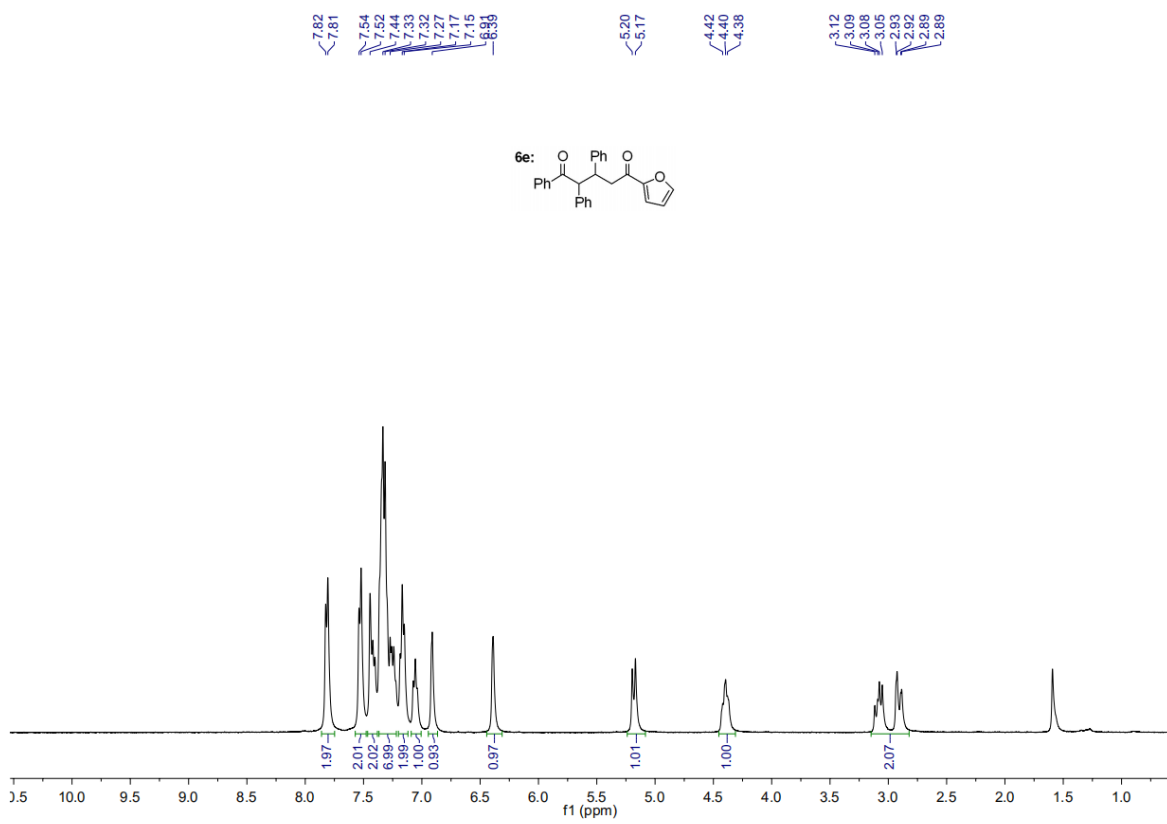


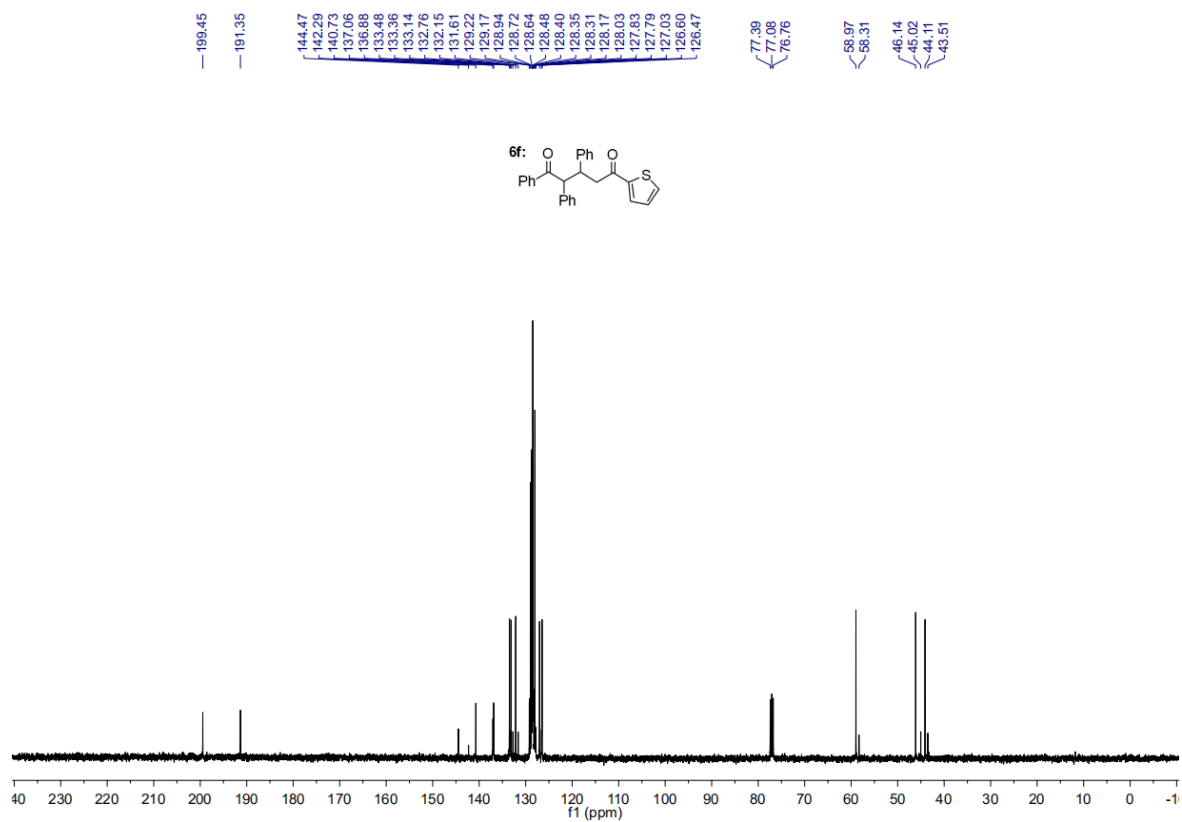
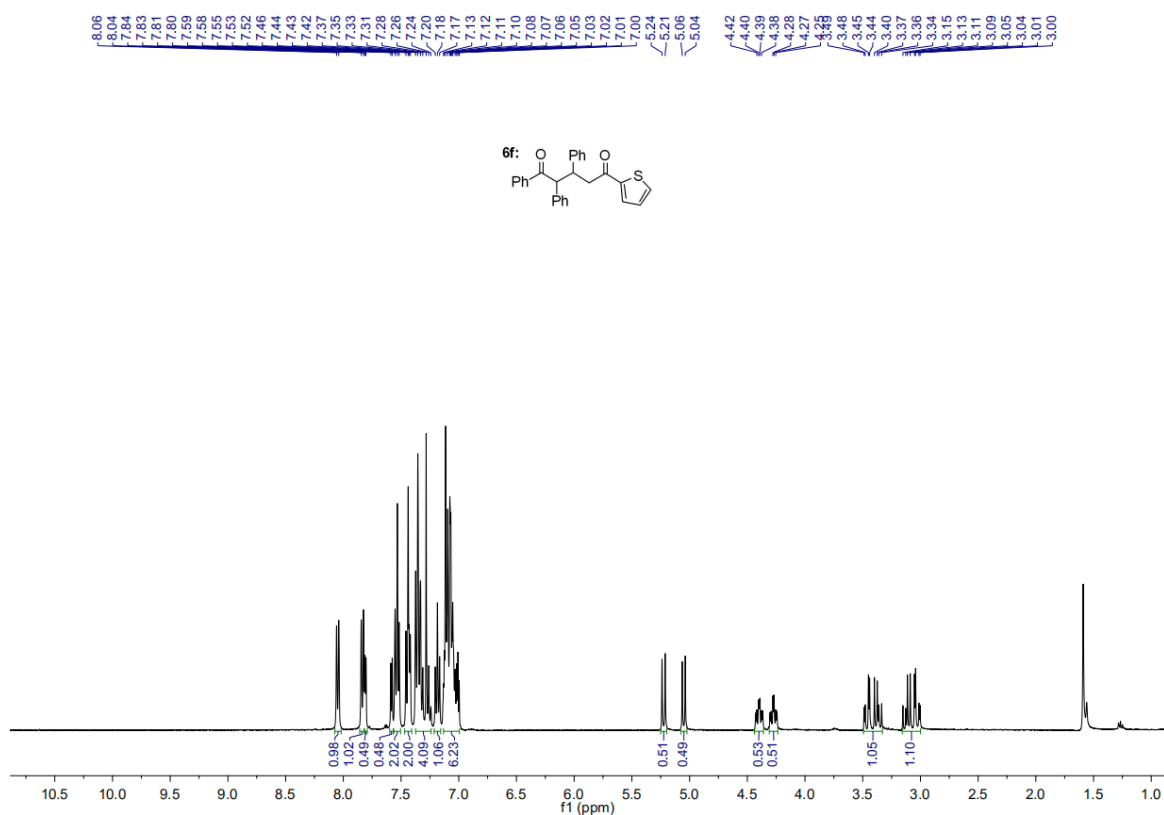


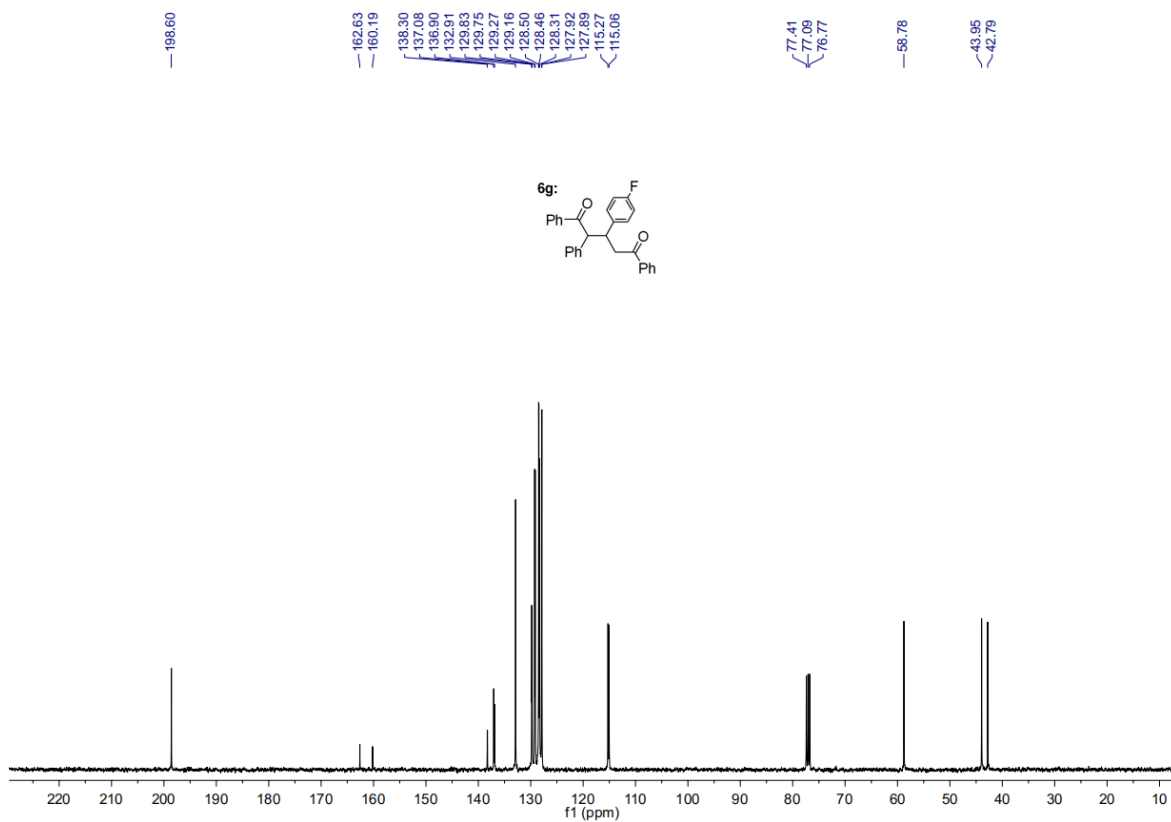
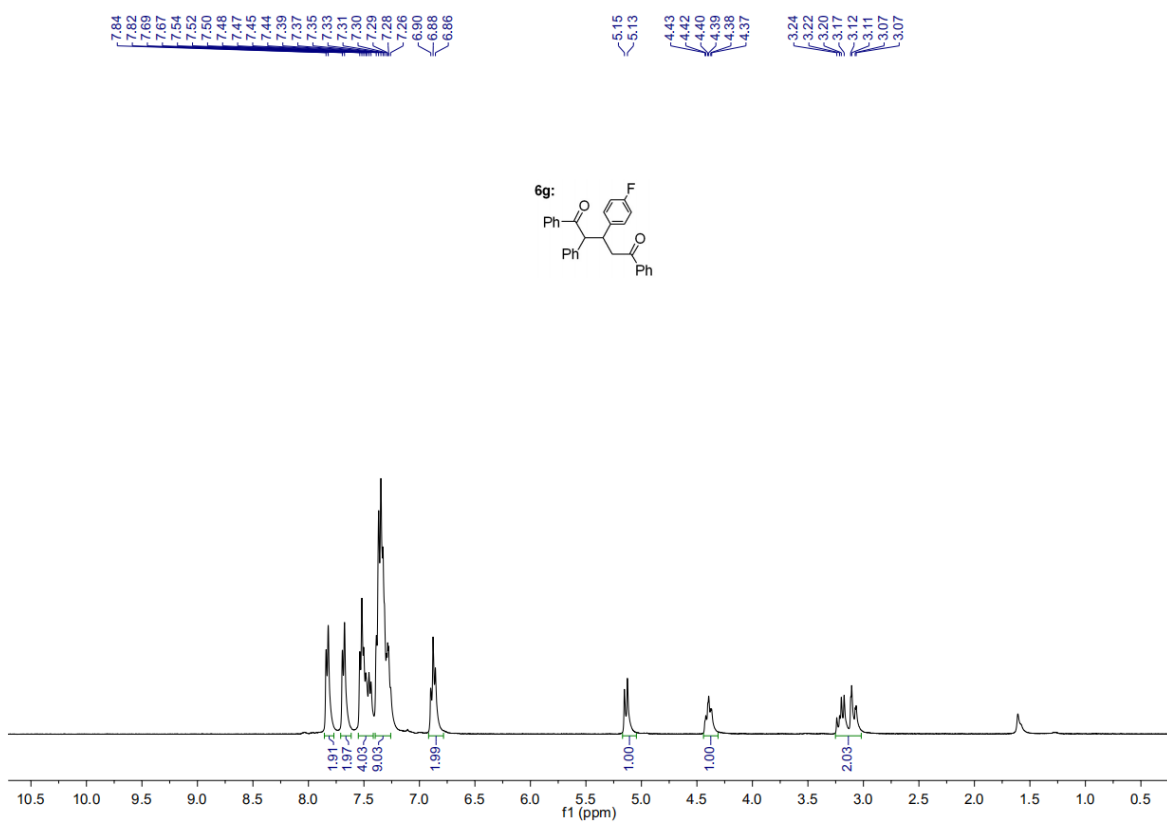


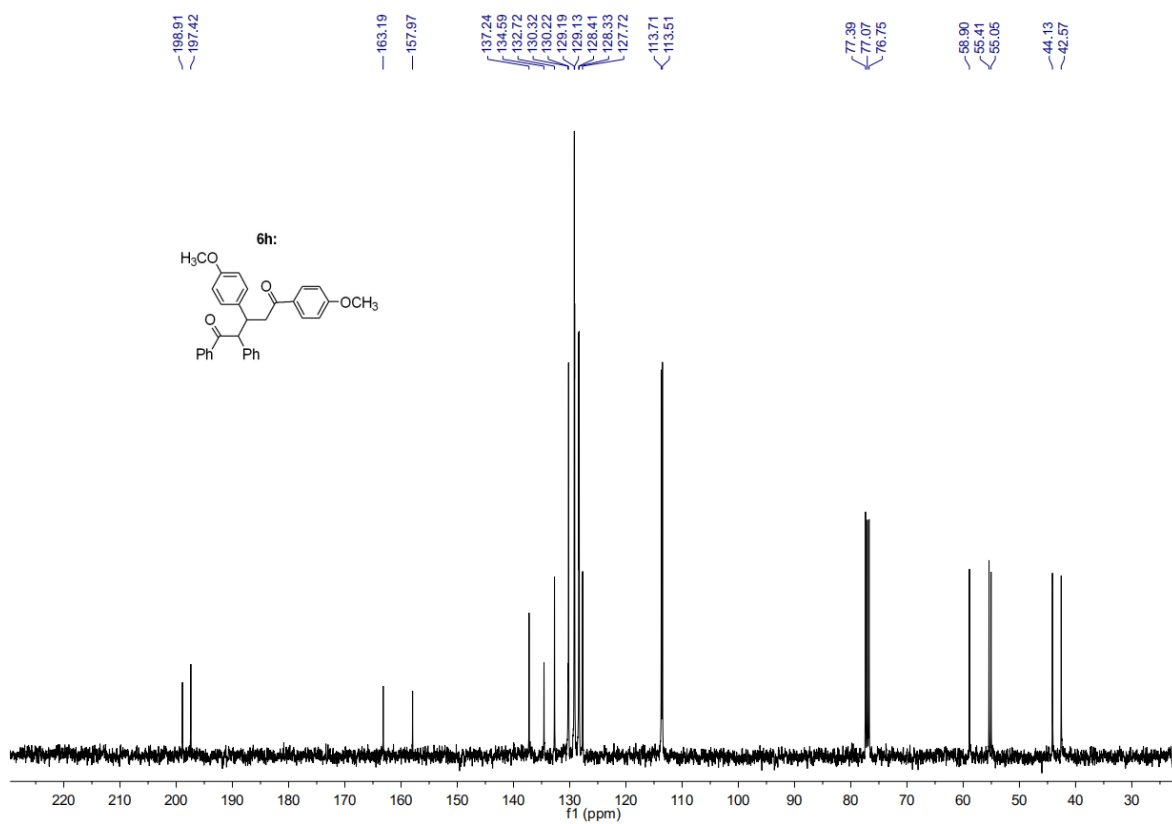
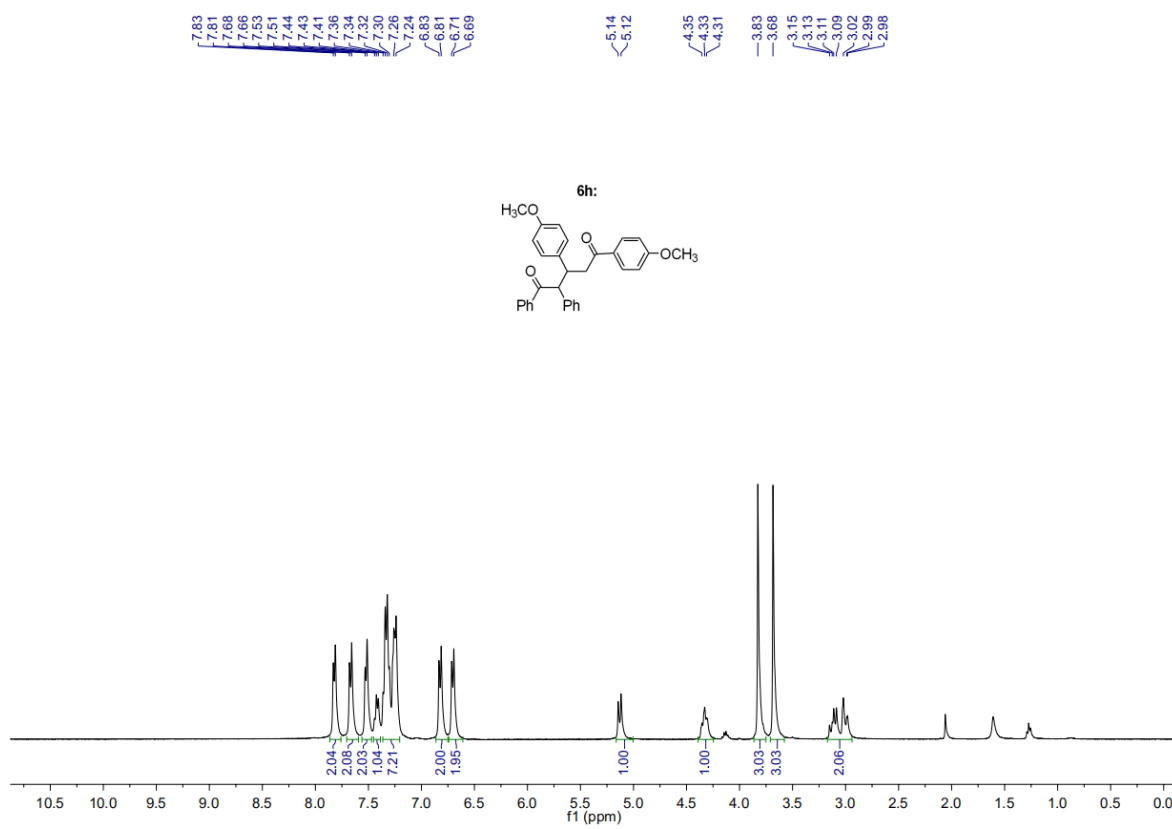


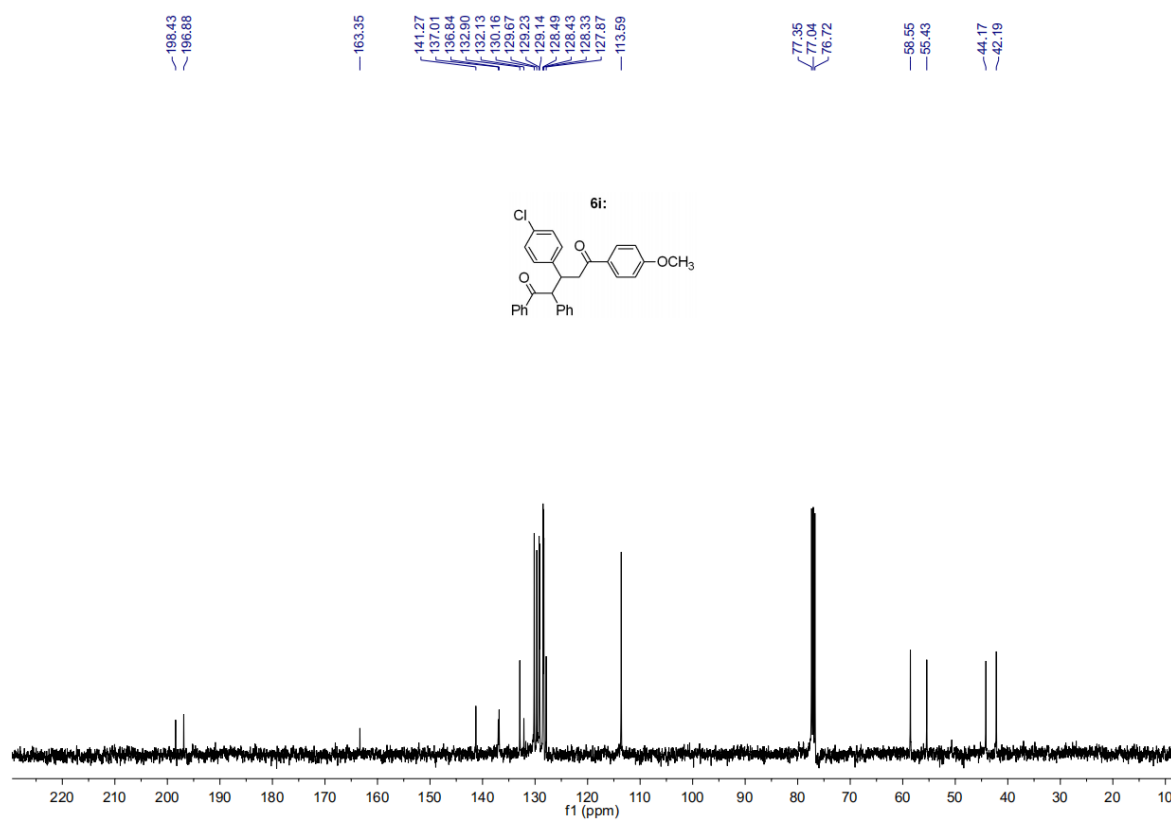
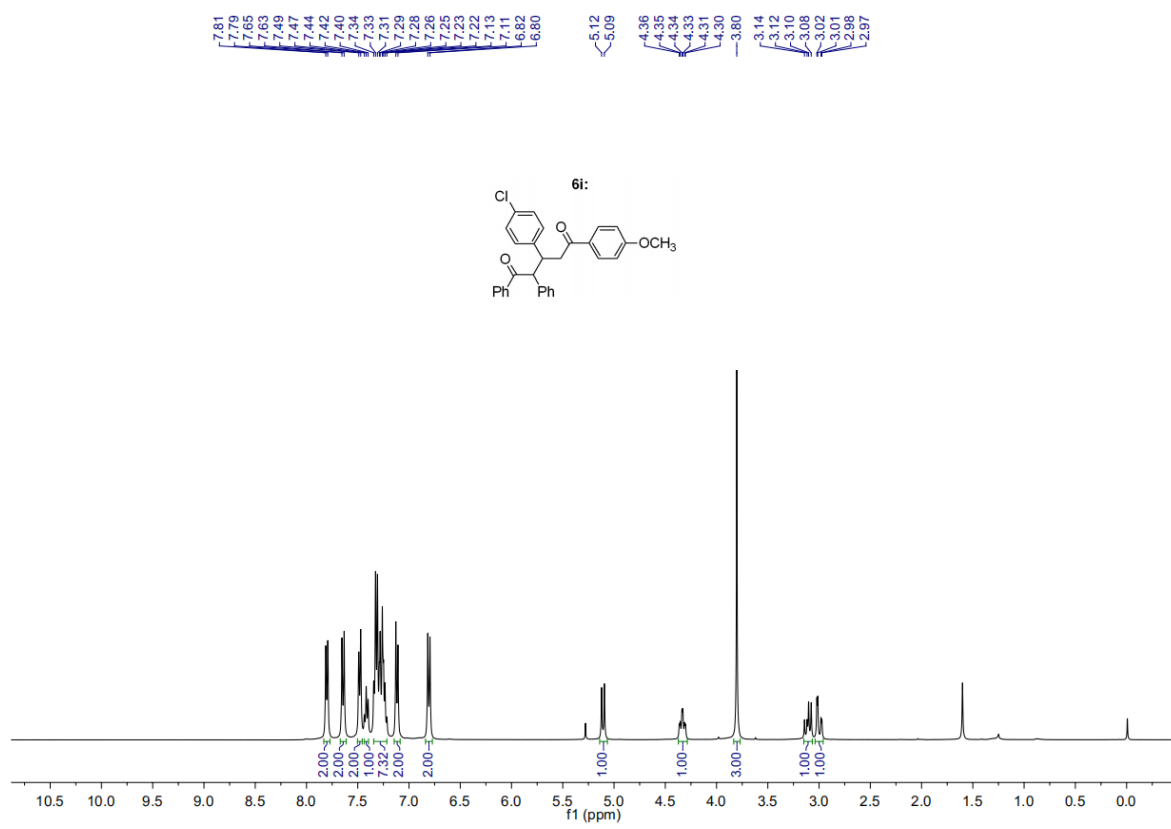


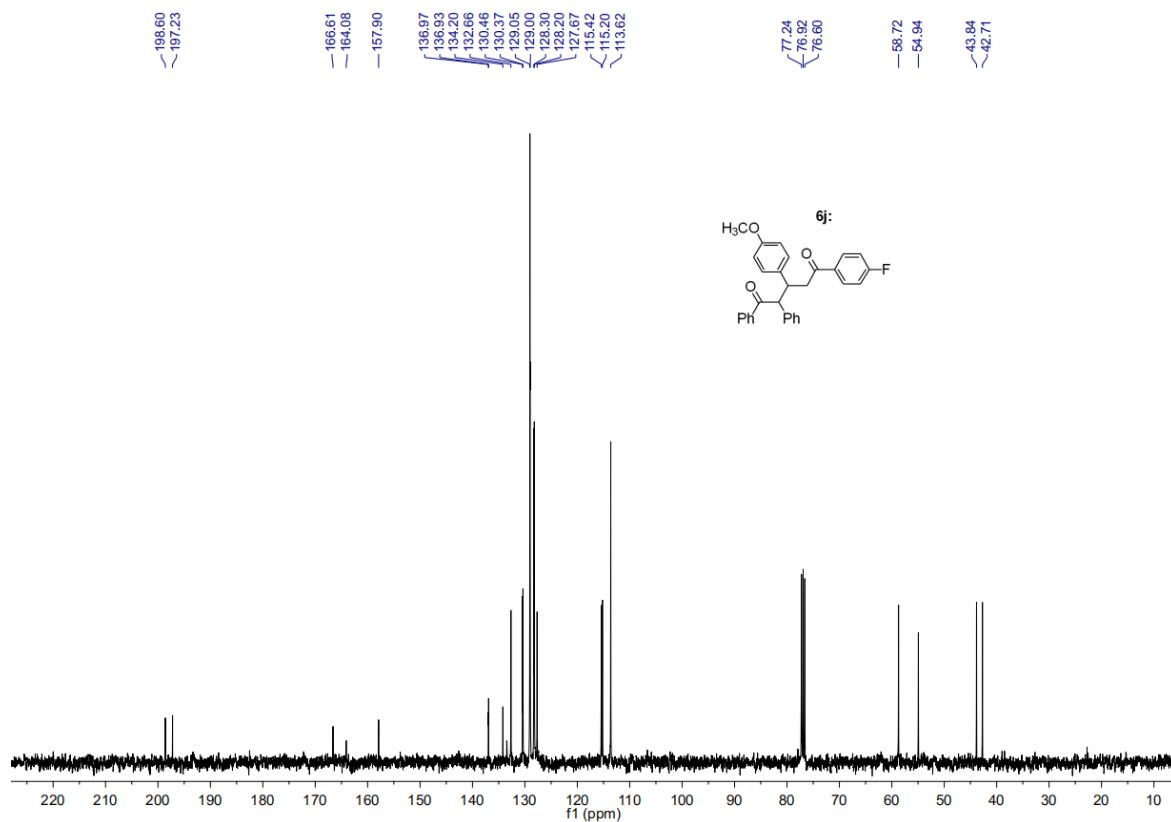
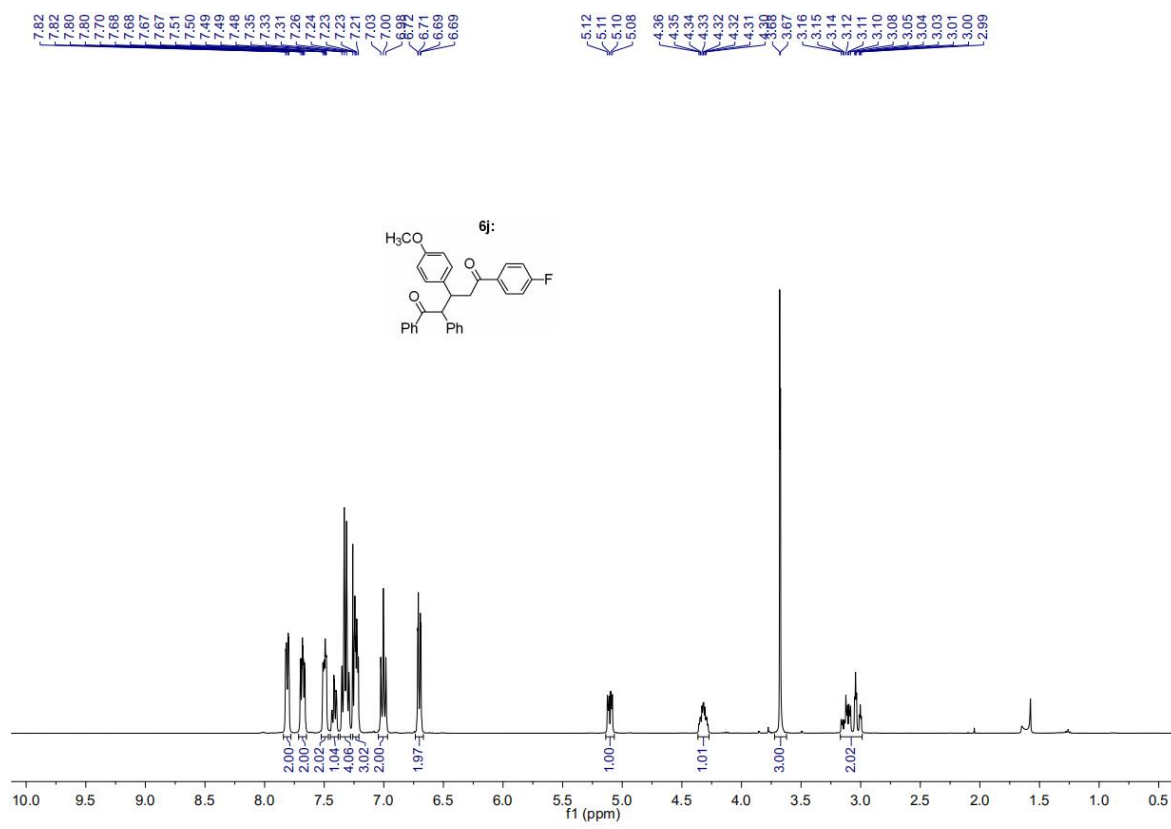


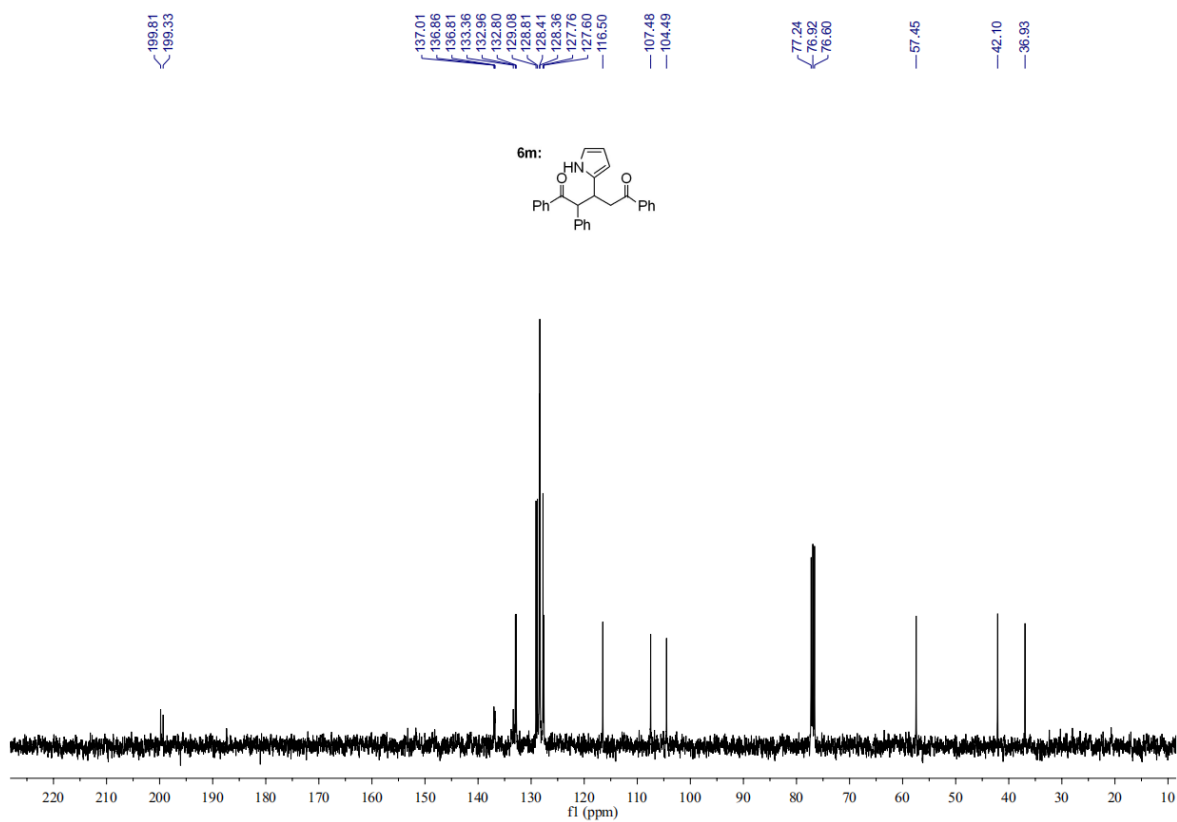
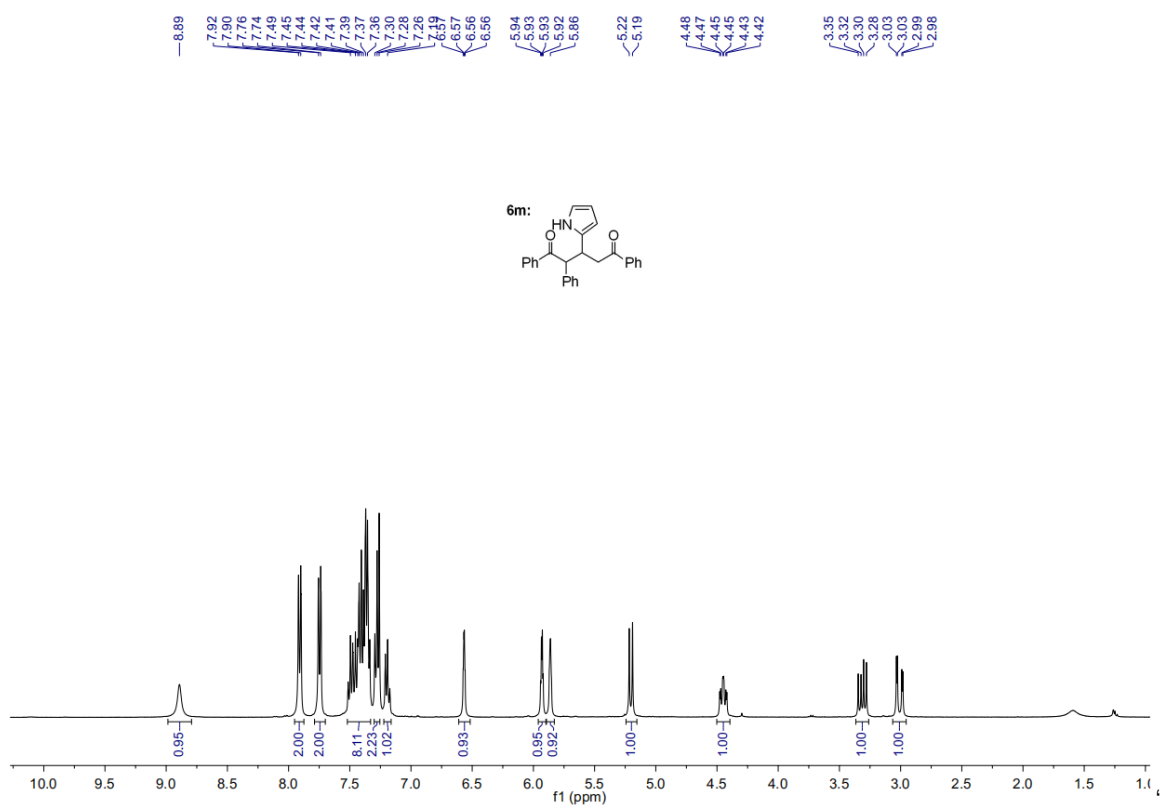


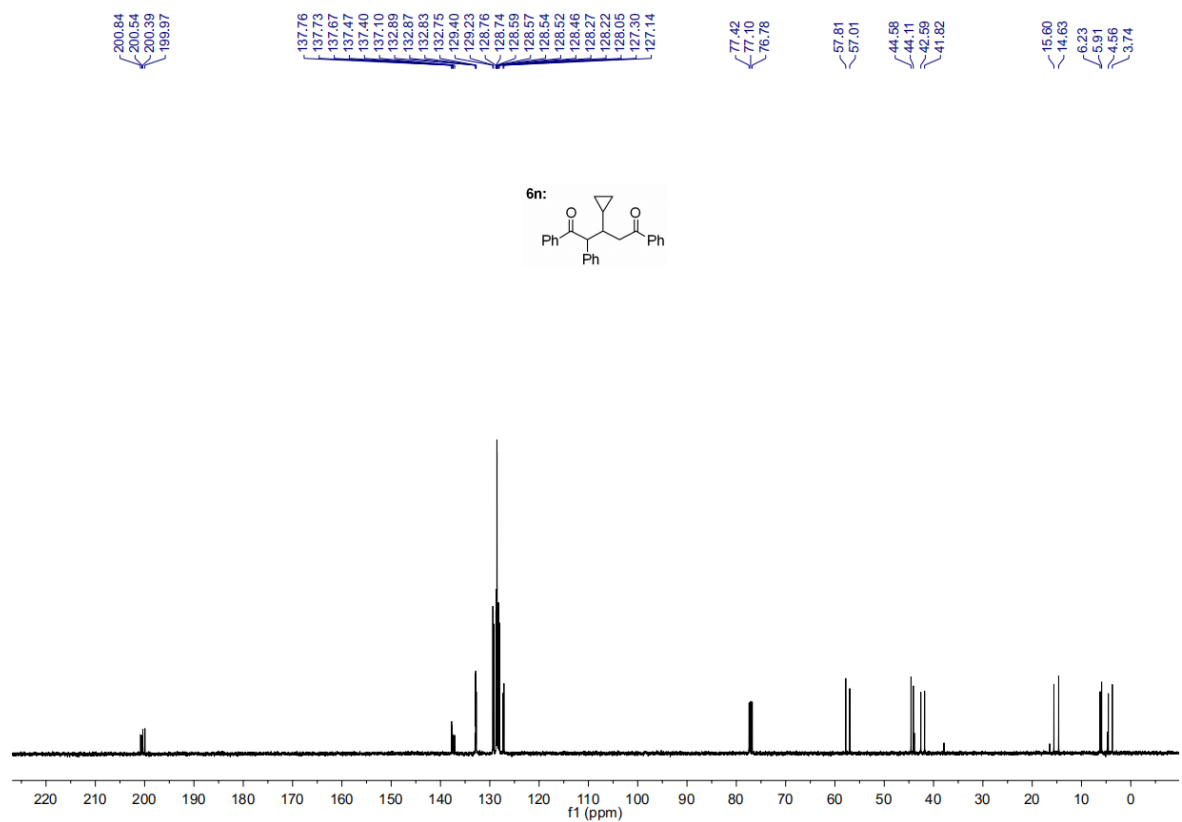
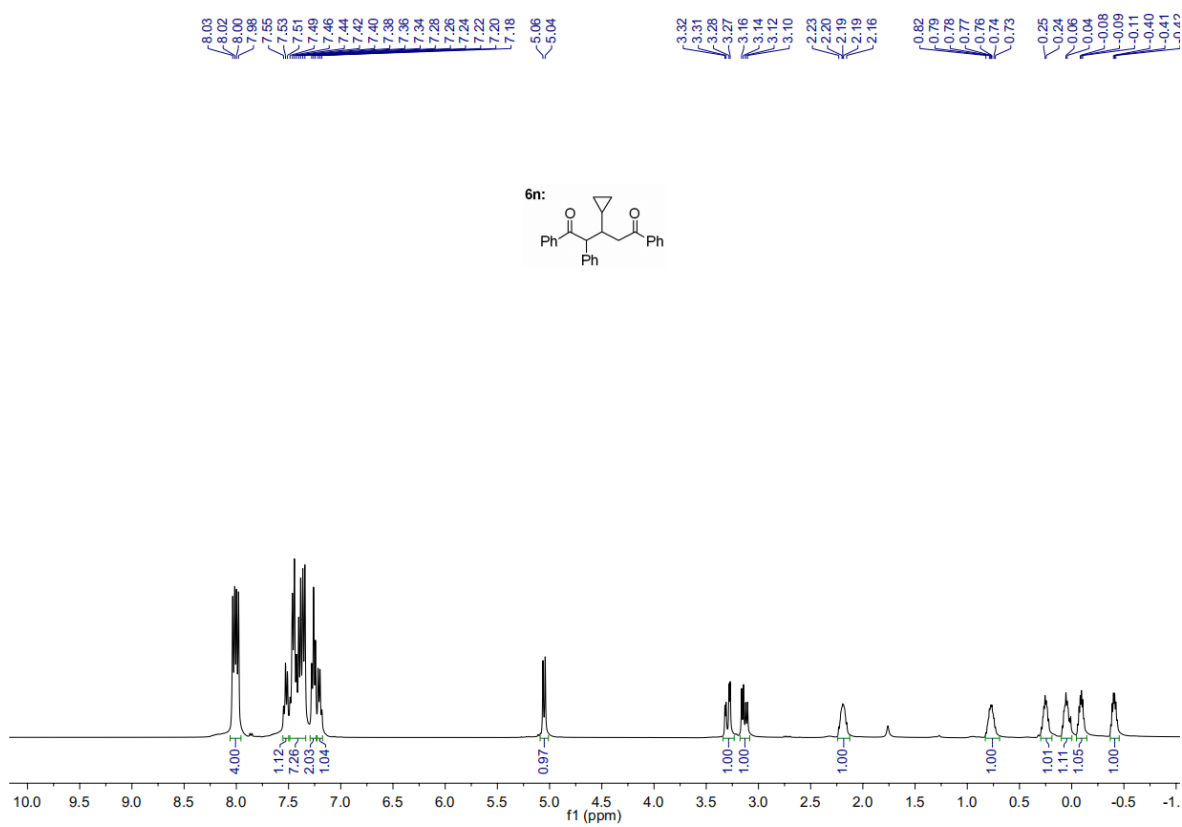


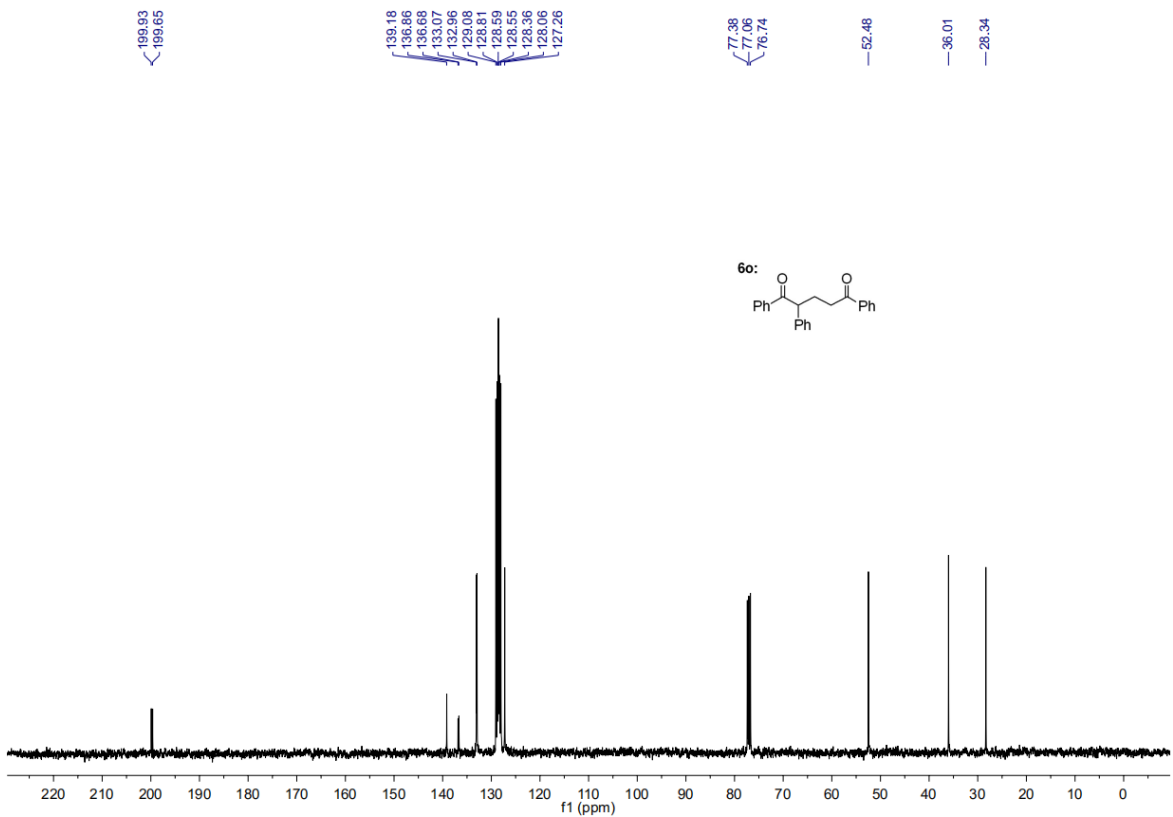
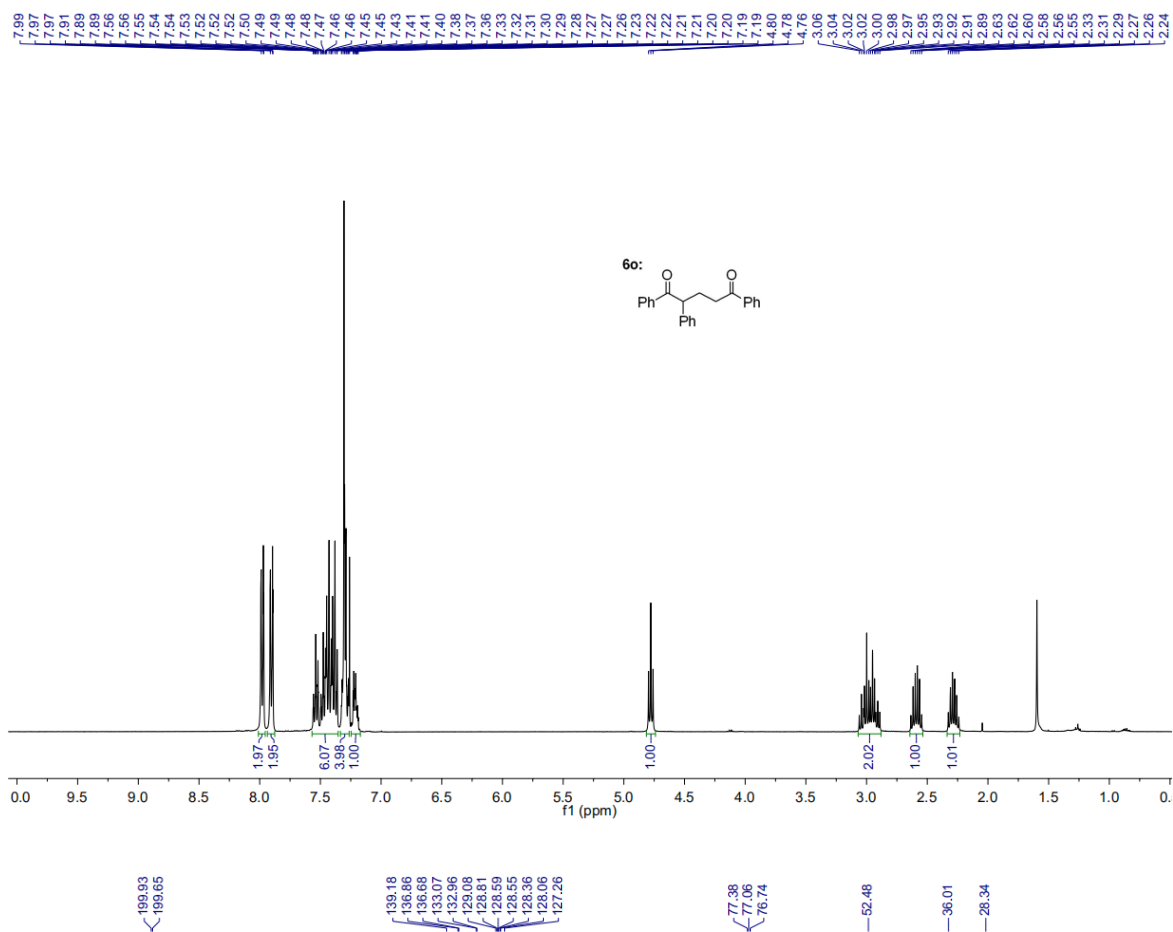


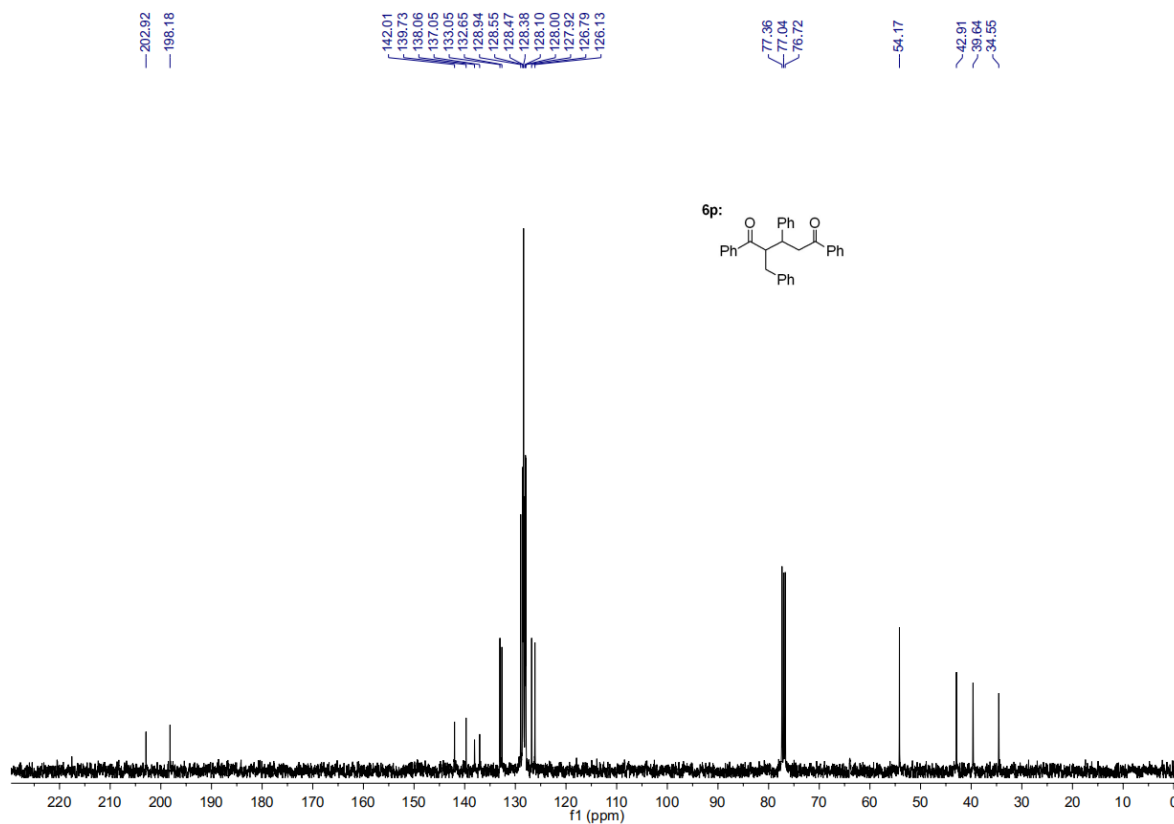
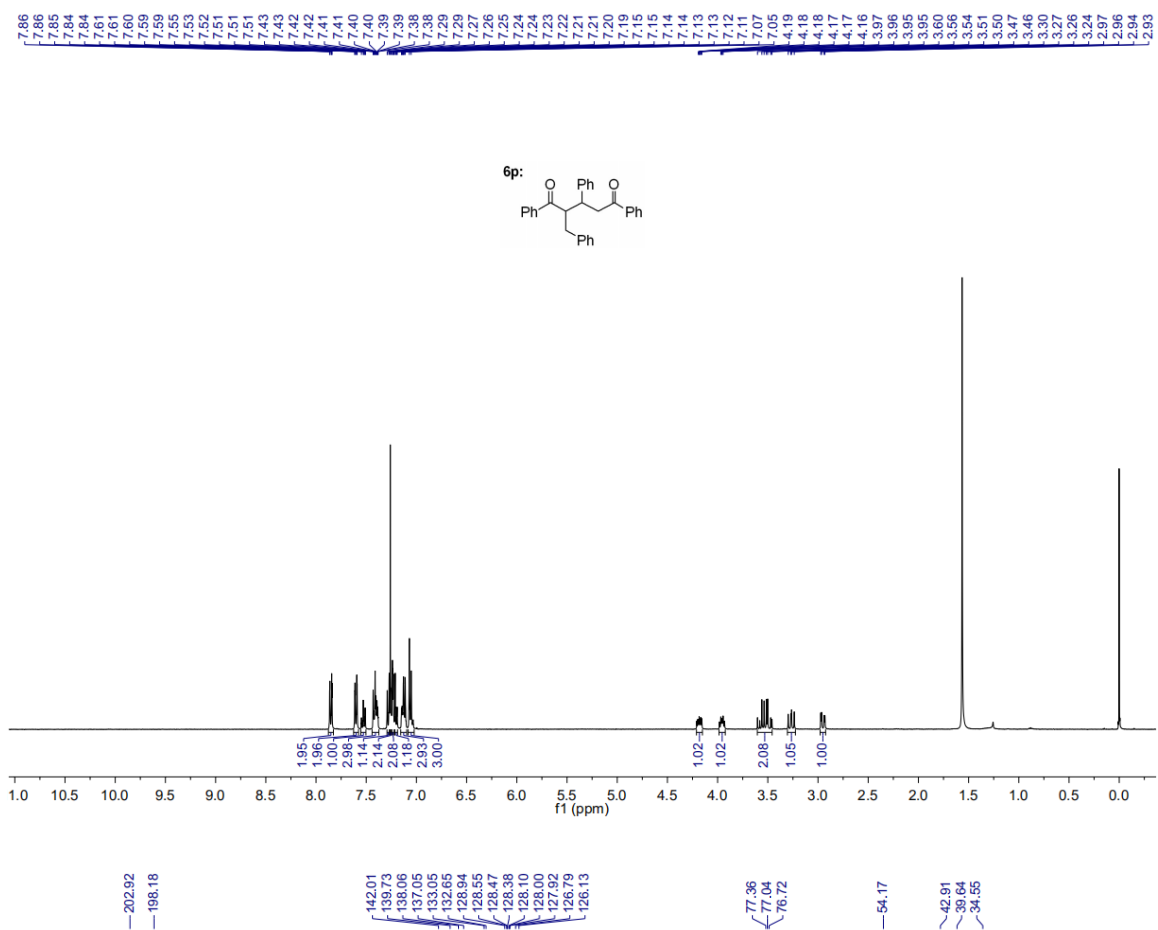


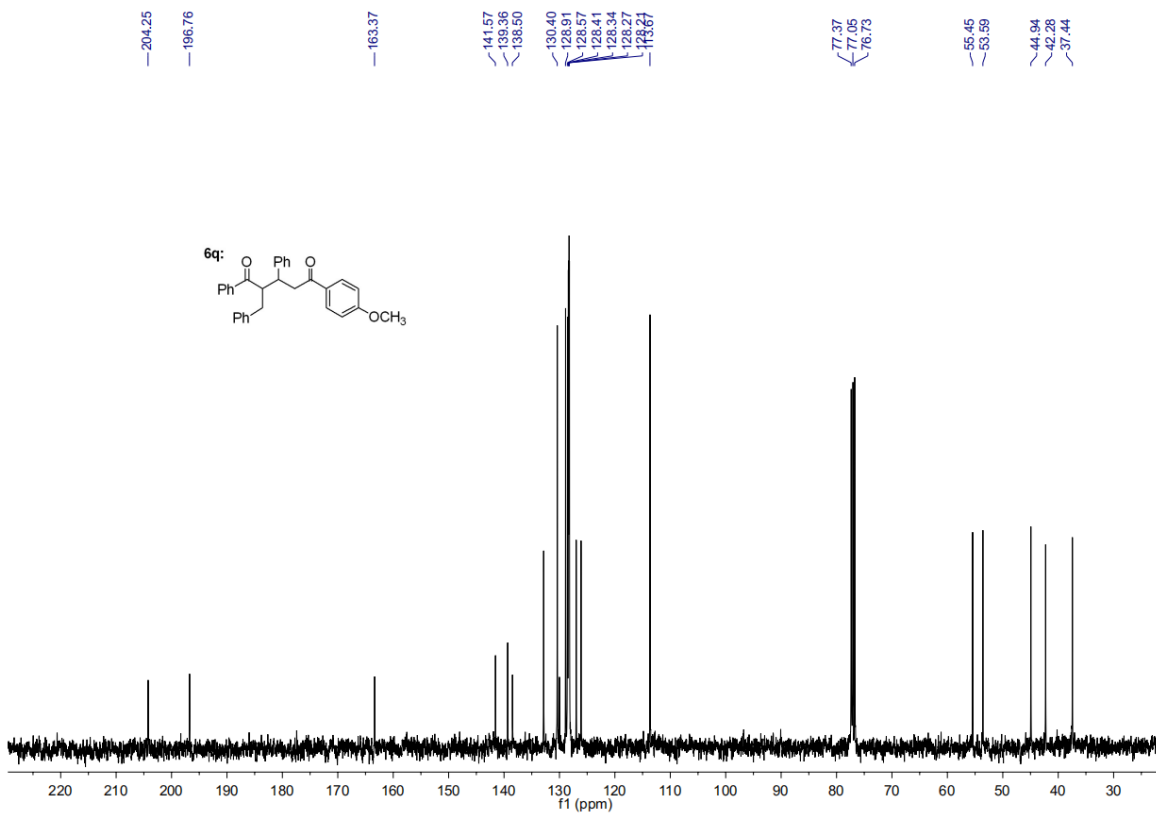
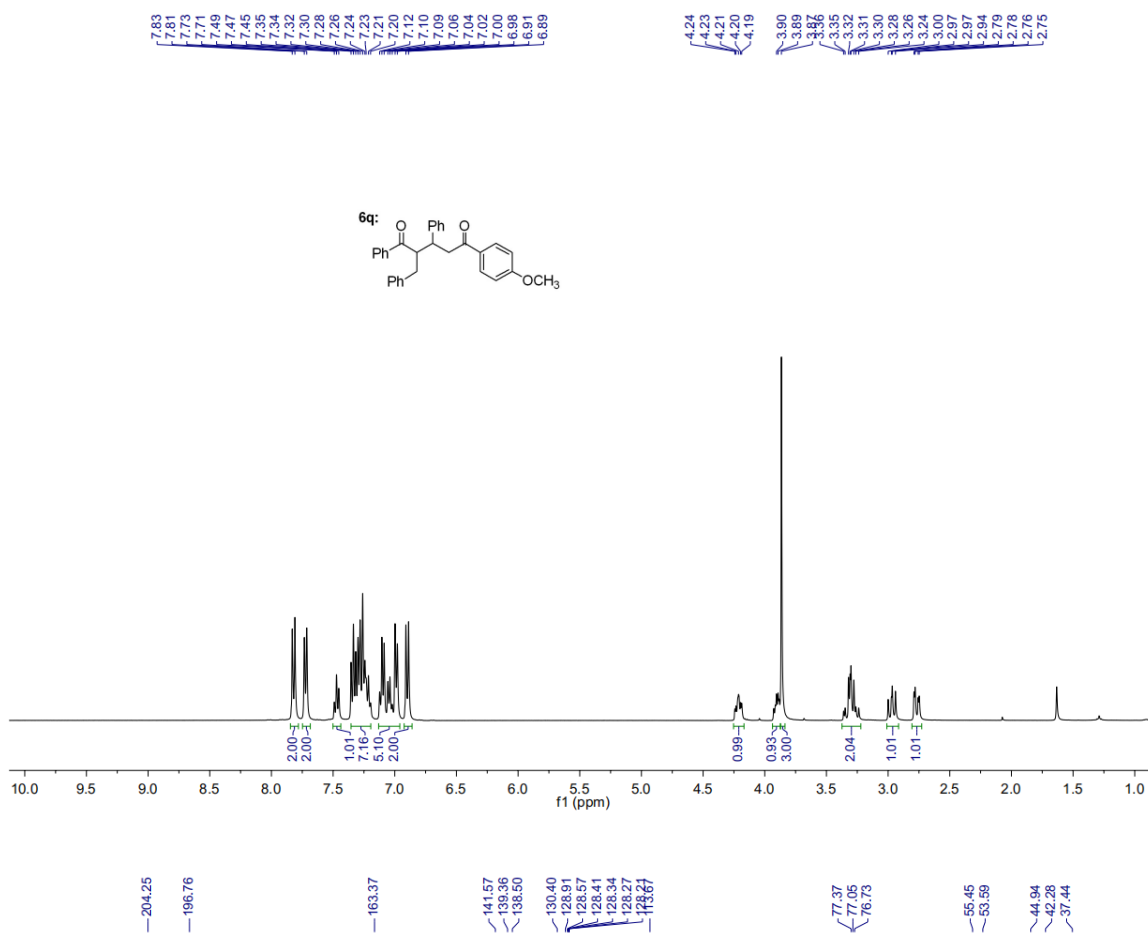


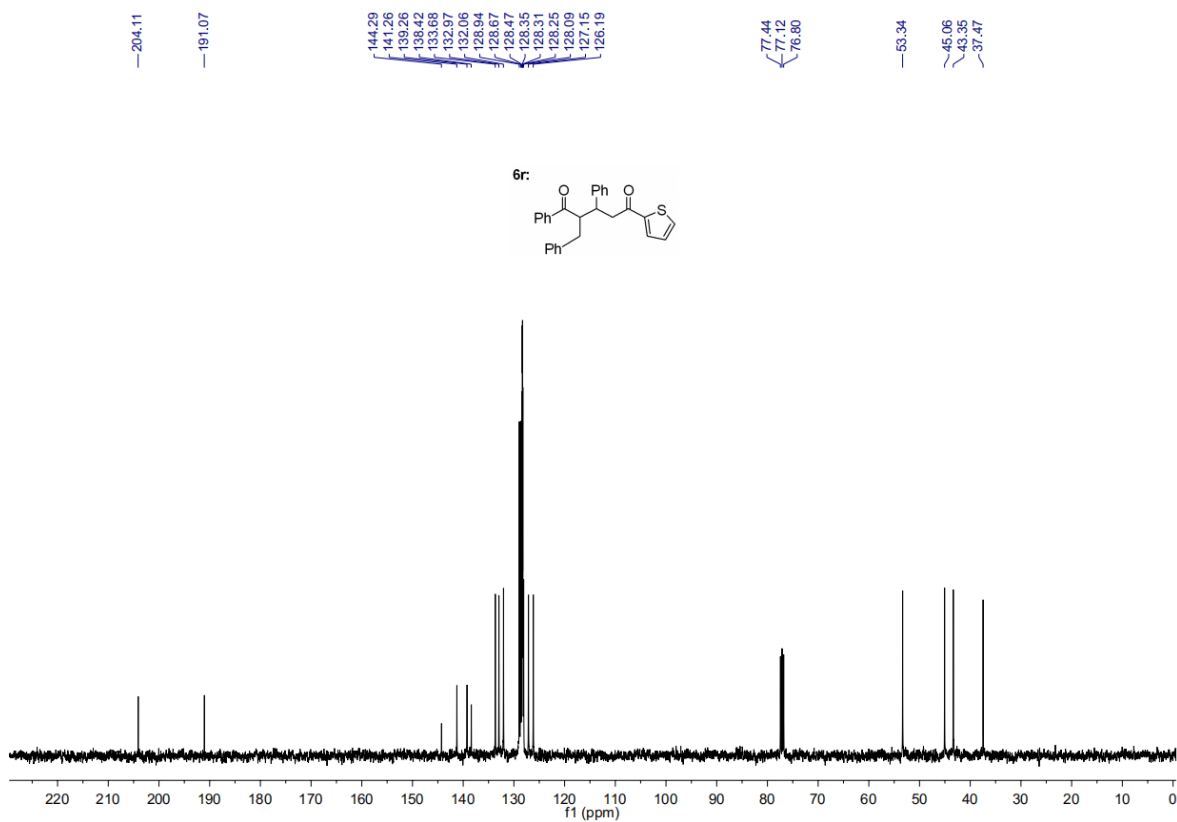
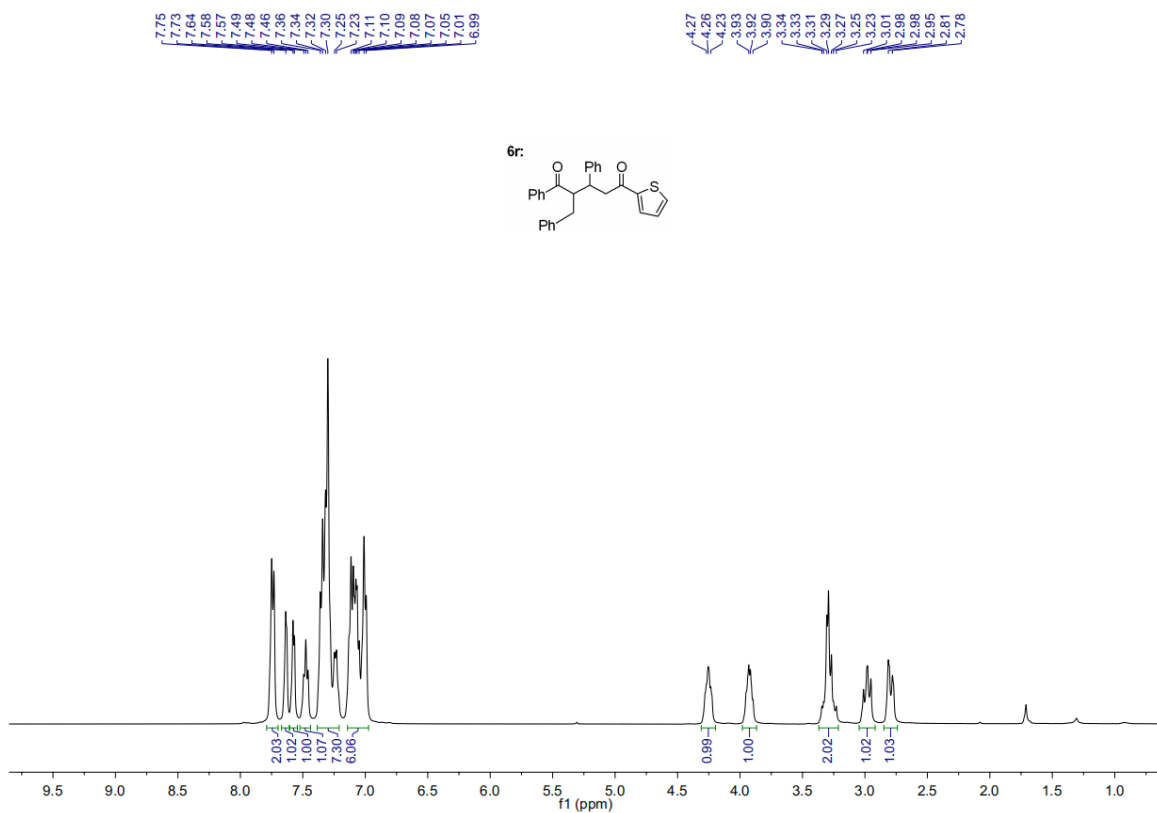


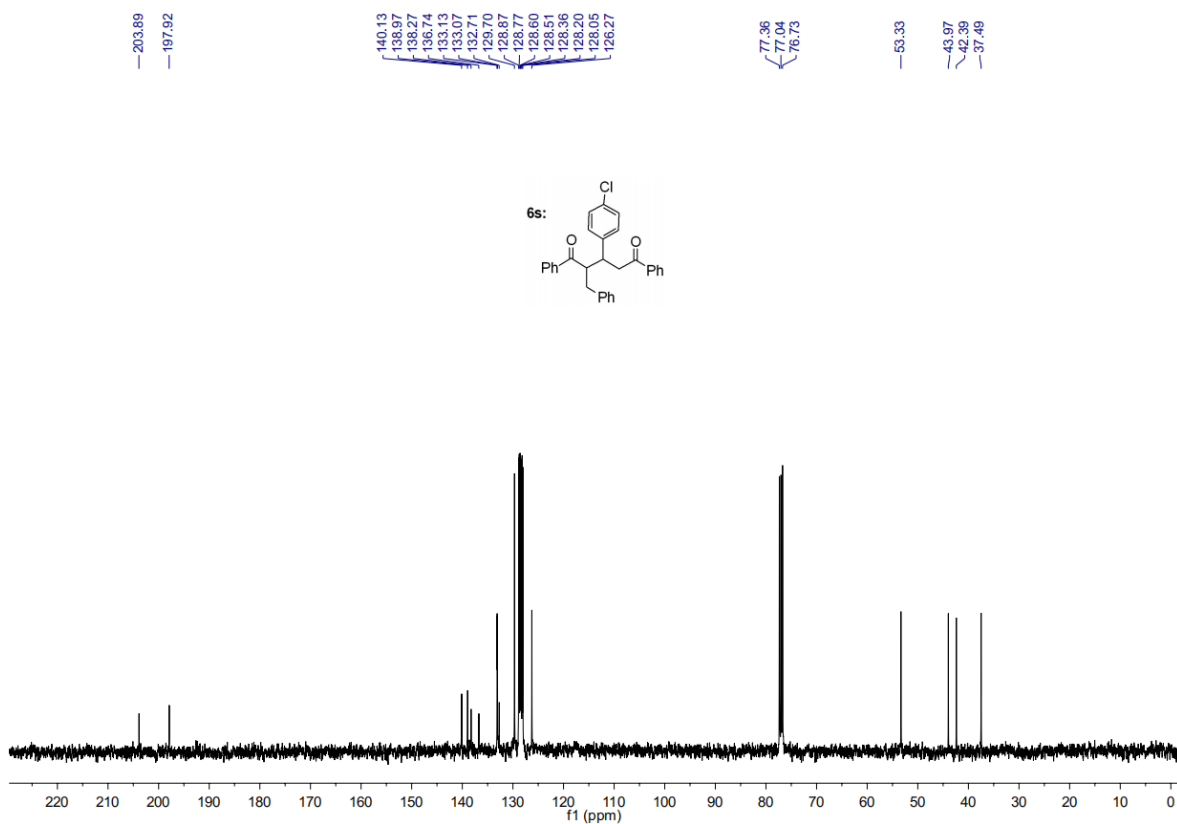
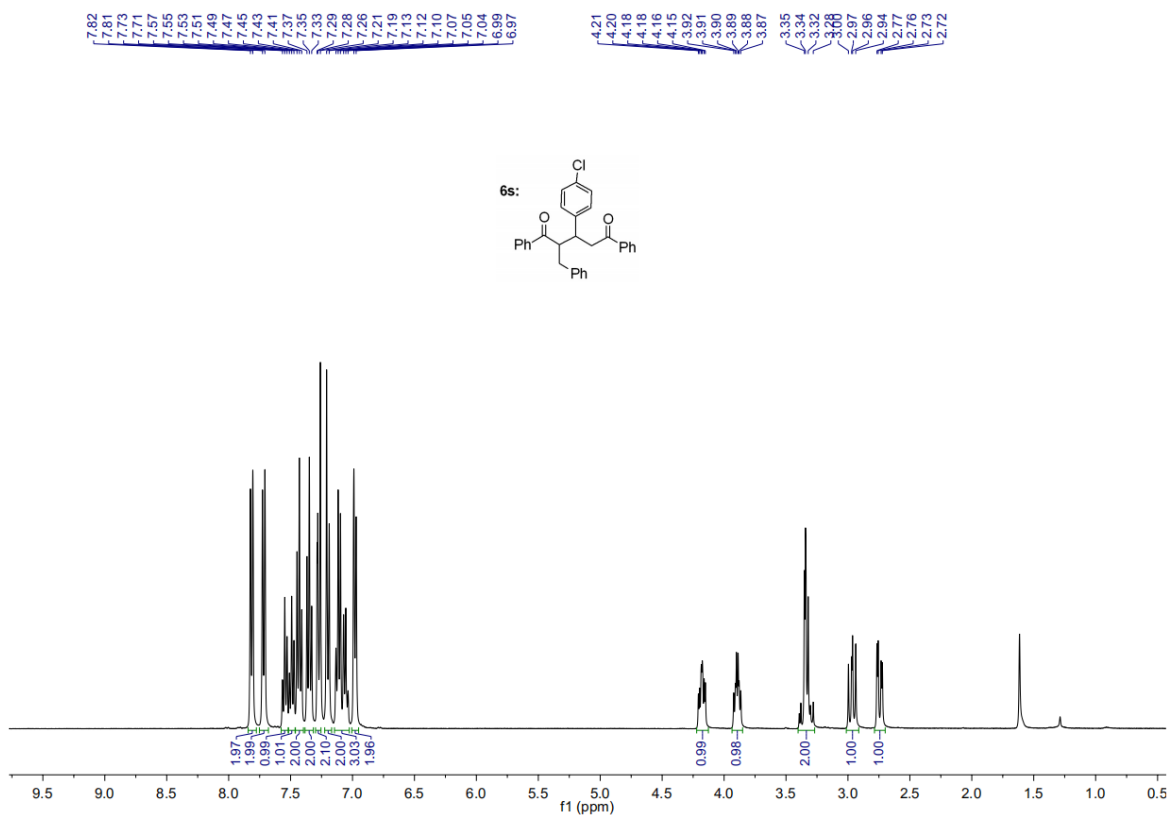


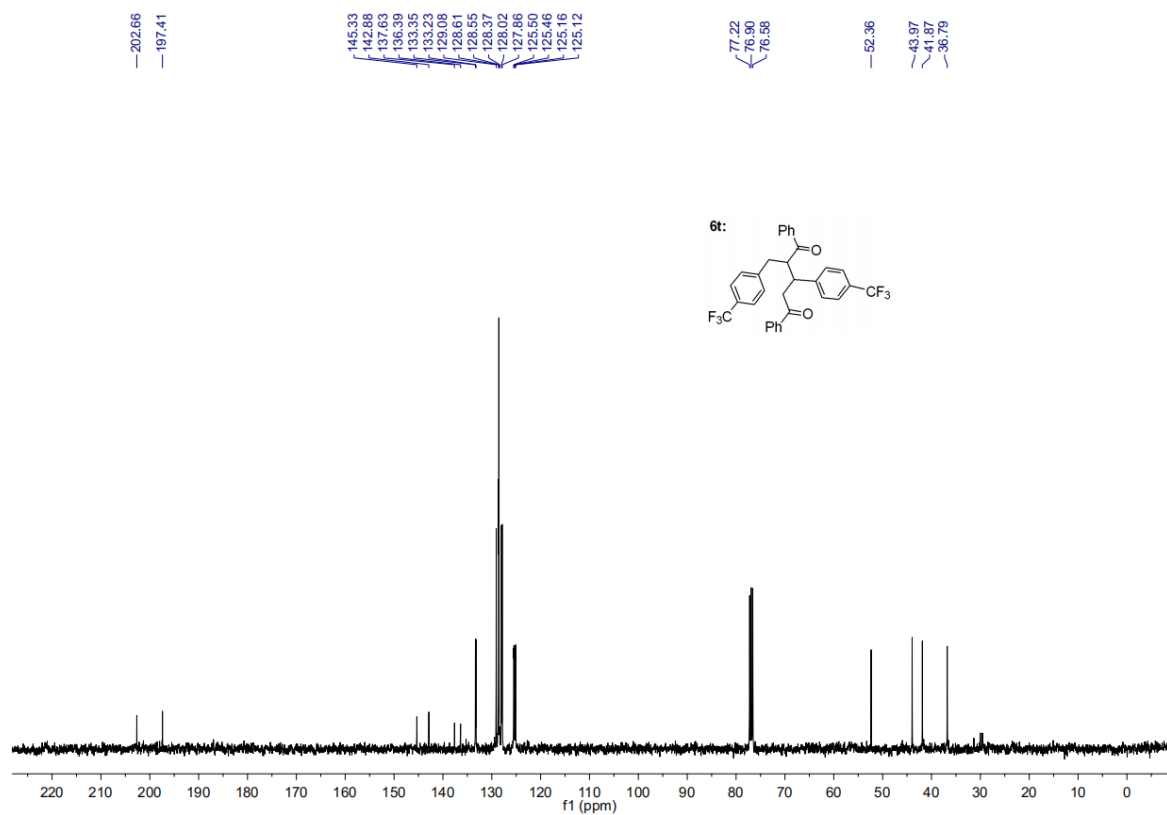
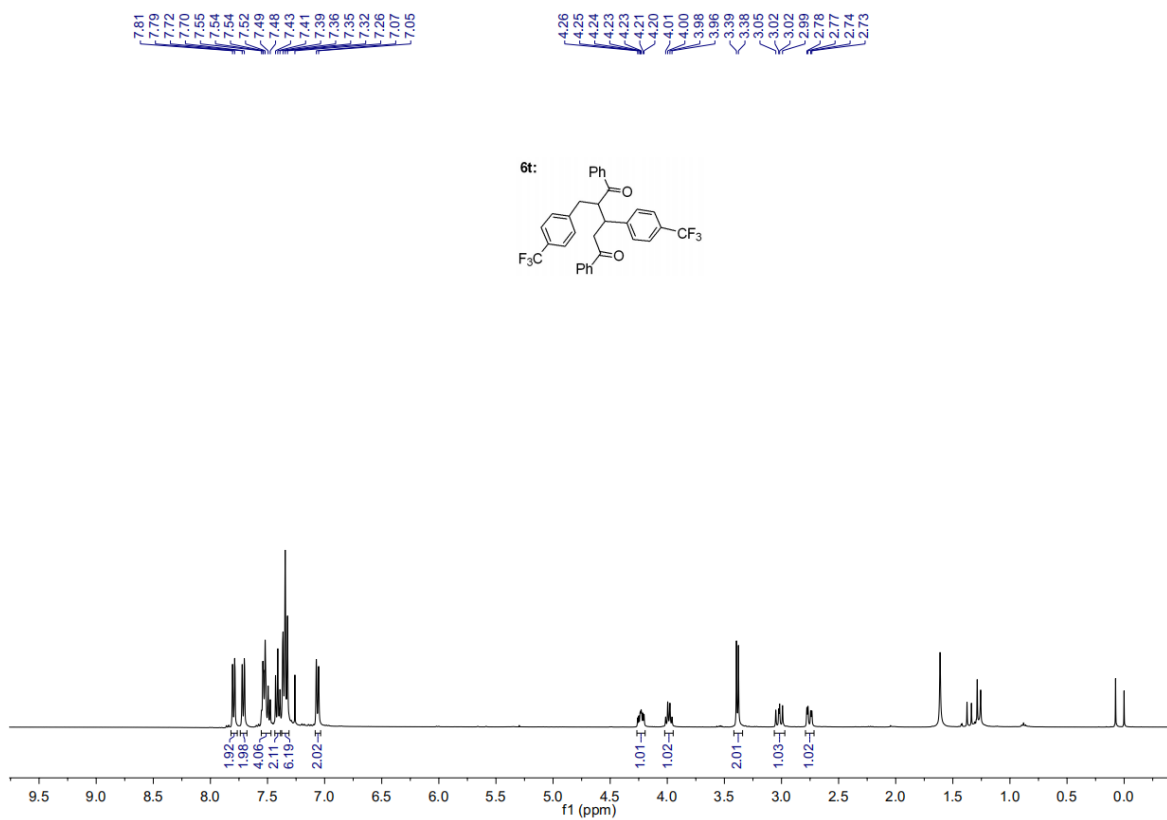


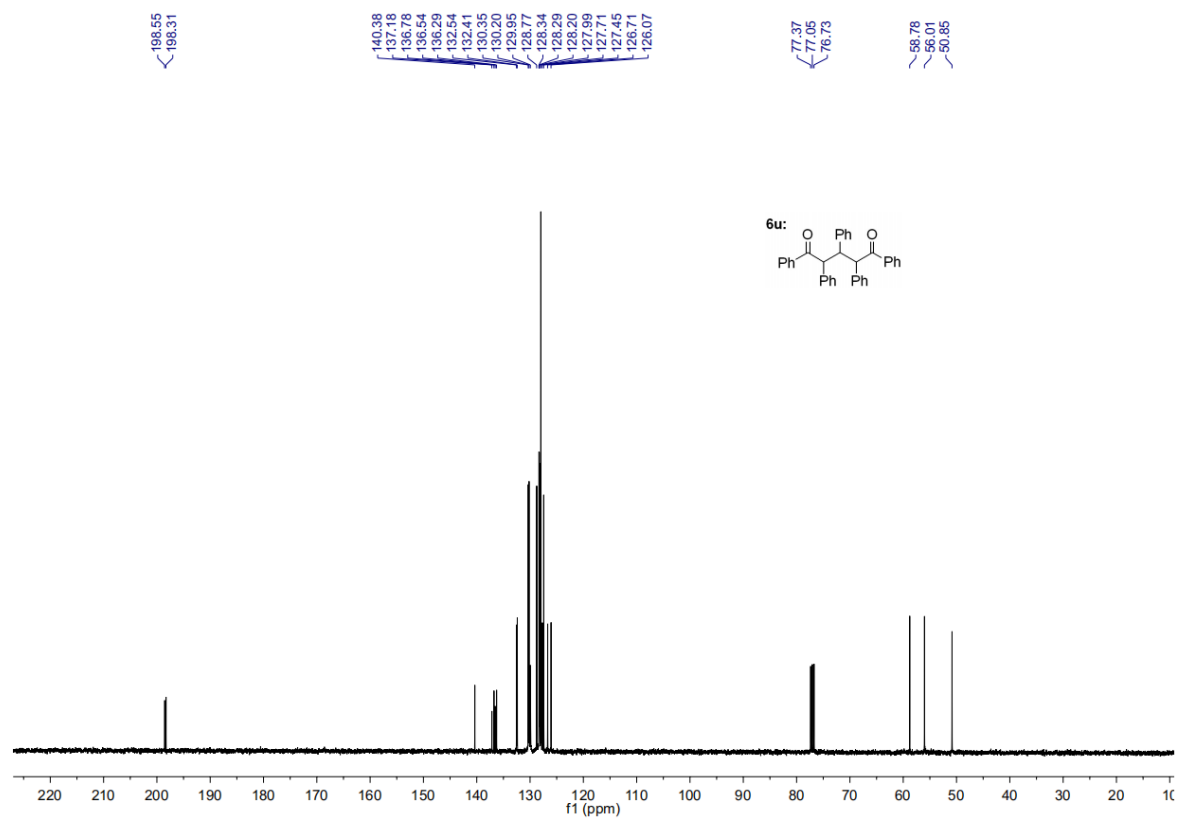
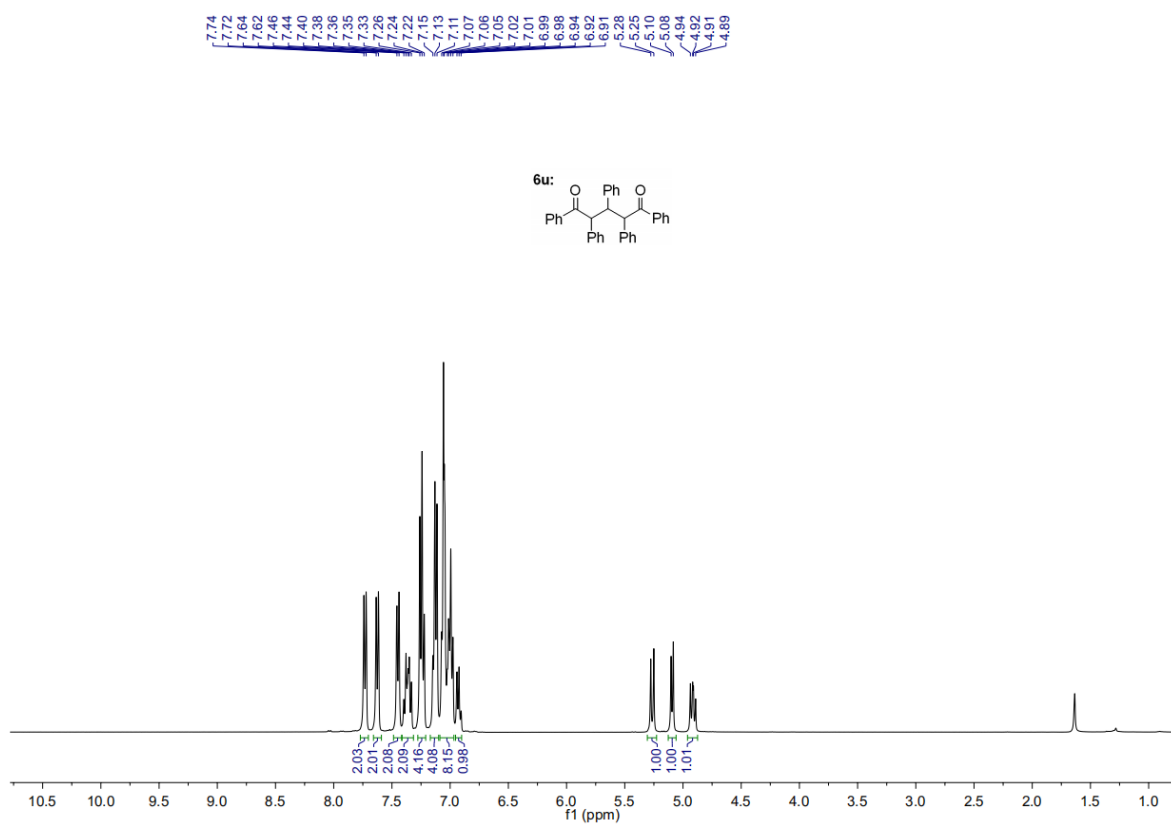






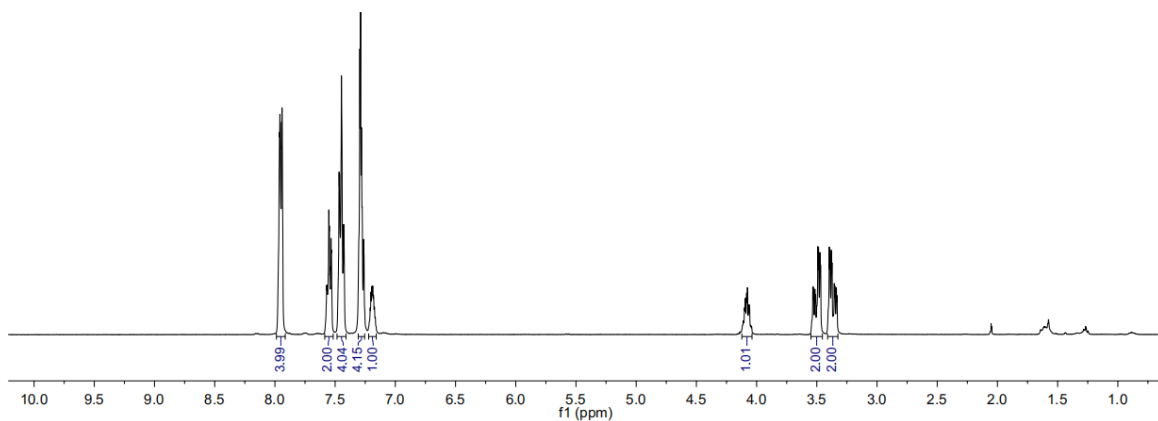
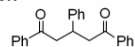






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6v:



— 198.58

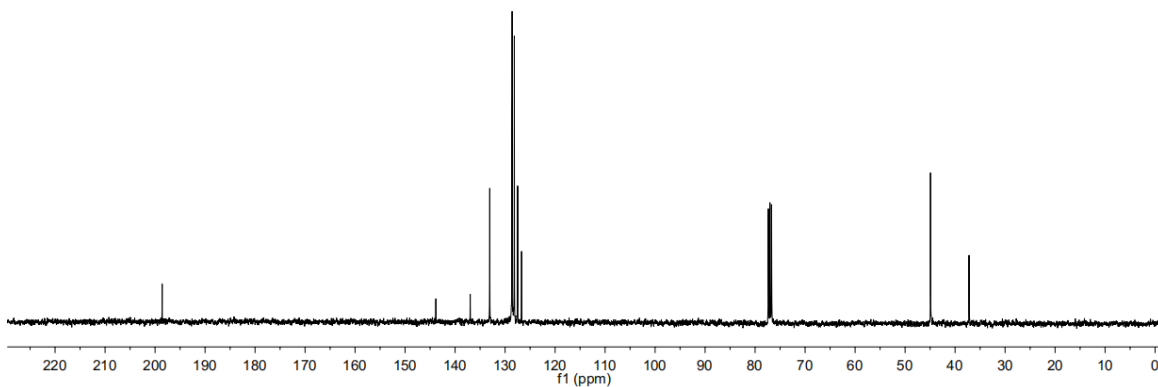
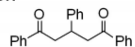
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— 138.98
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— 44.92

— 37.22

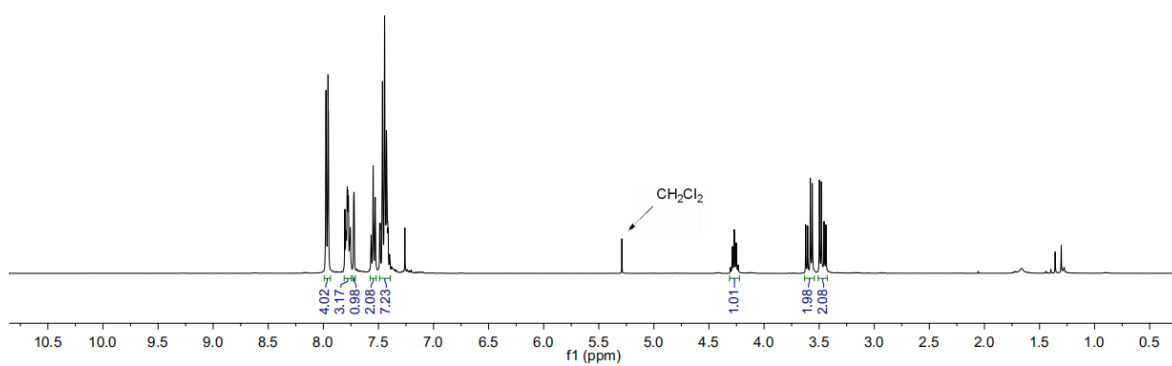
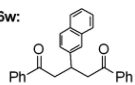
6v:



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6w:



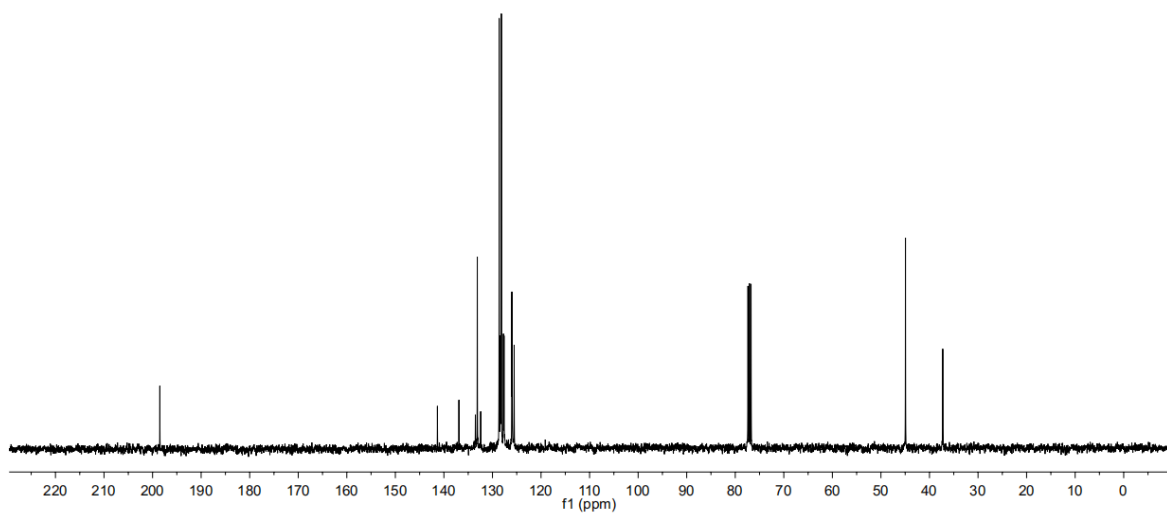
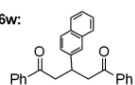
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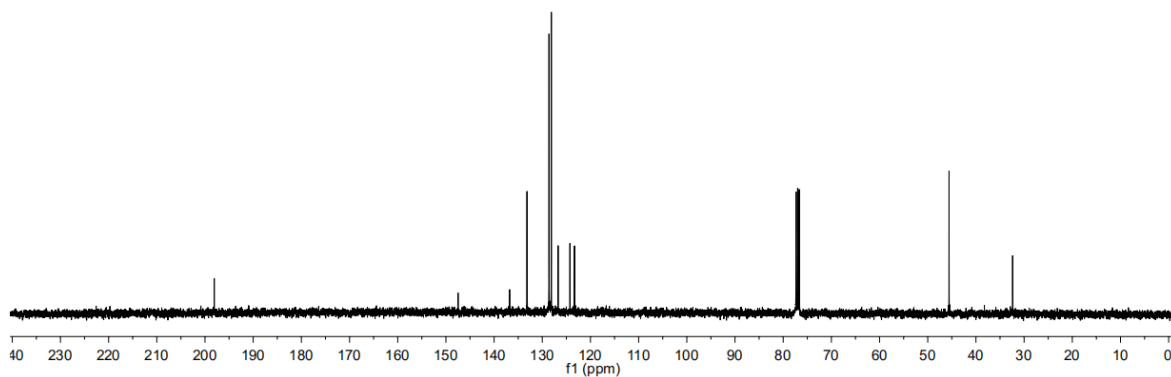
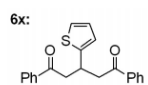
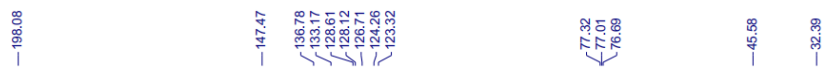
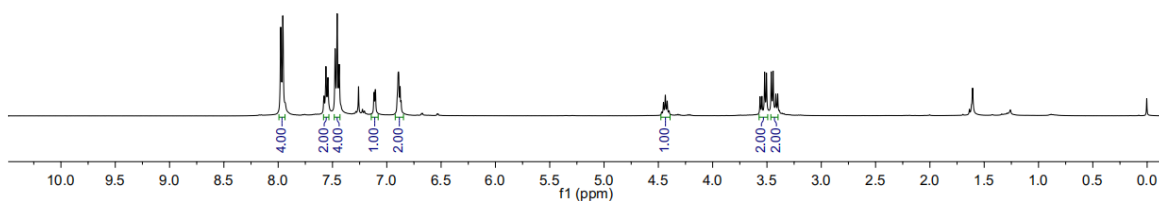
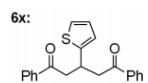
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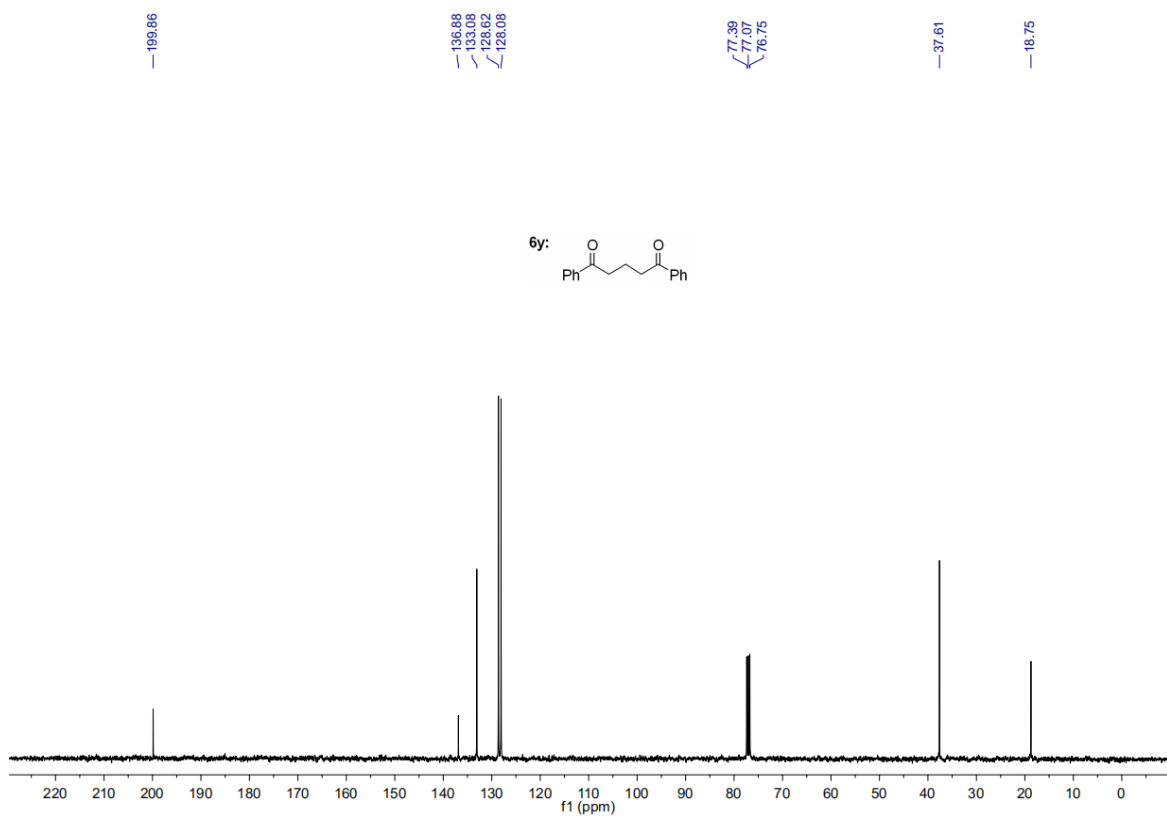
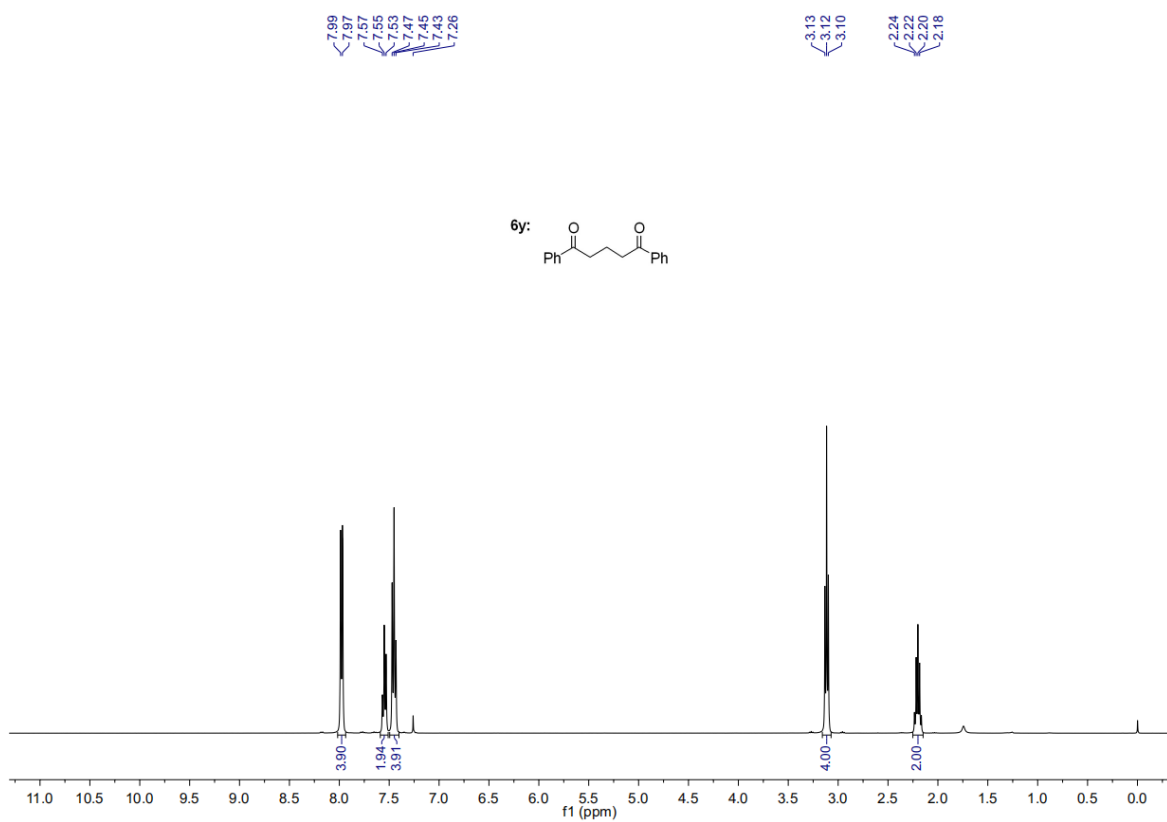
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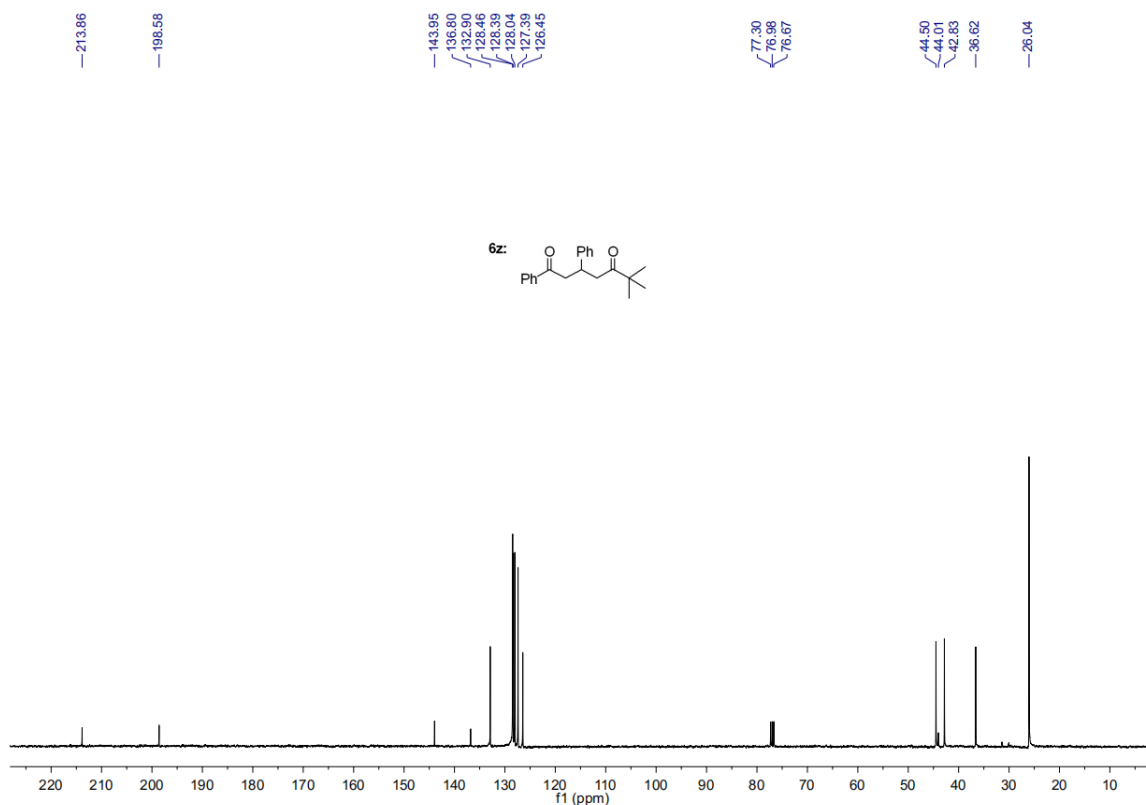
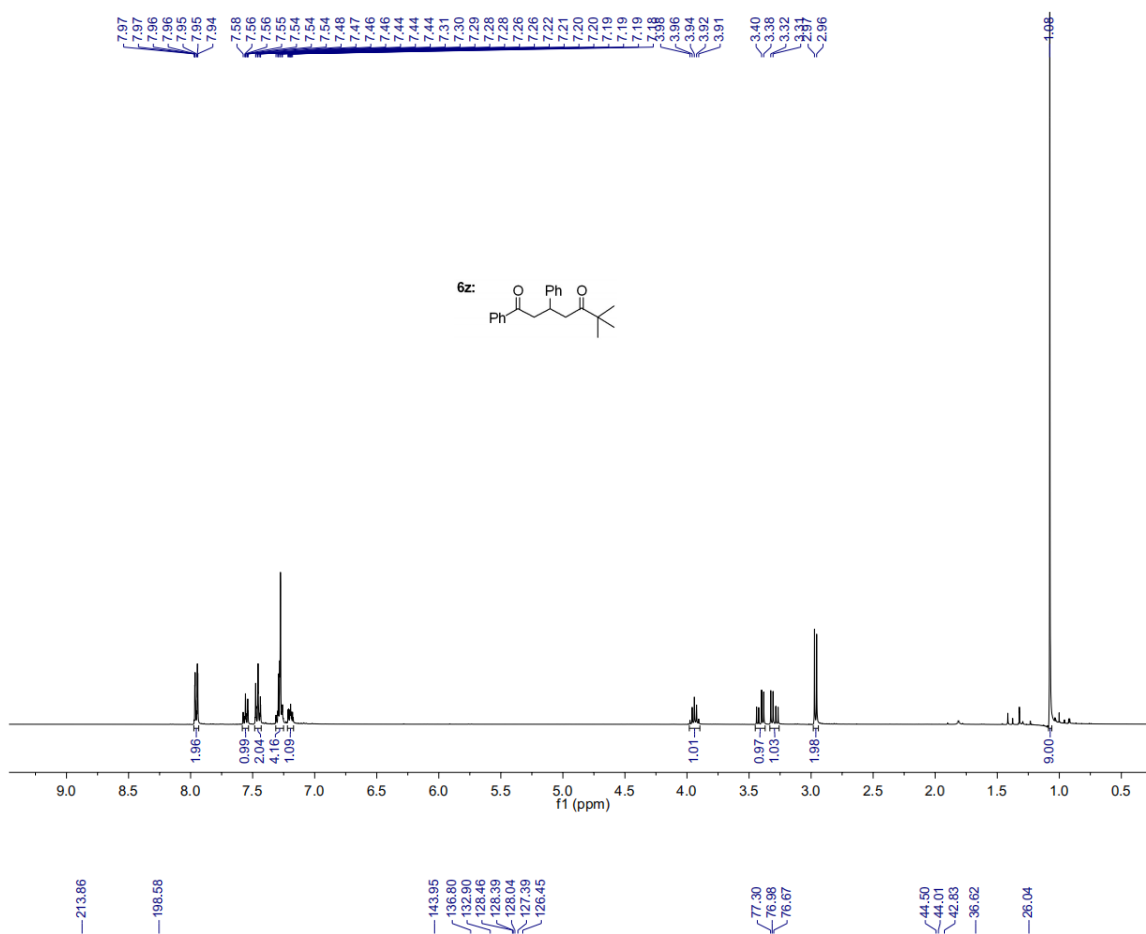
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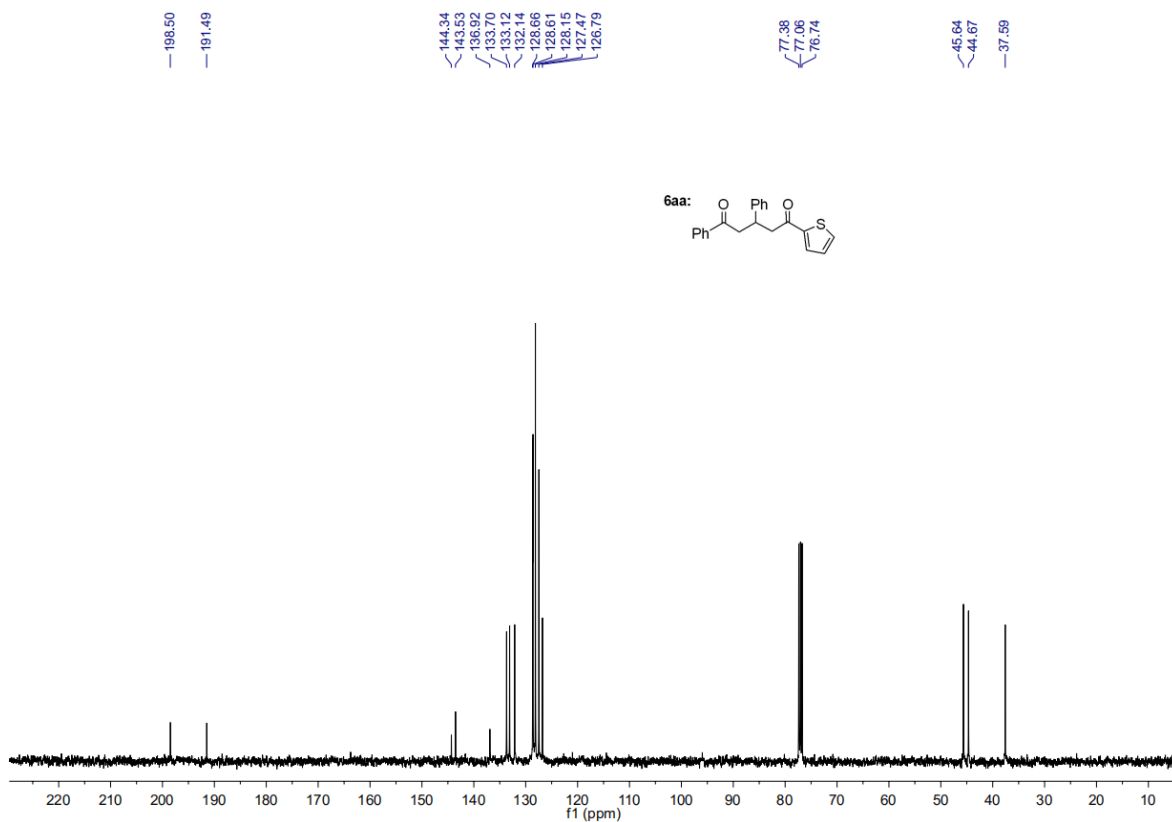
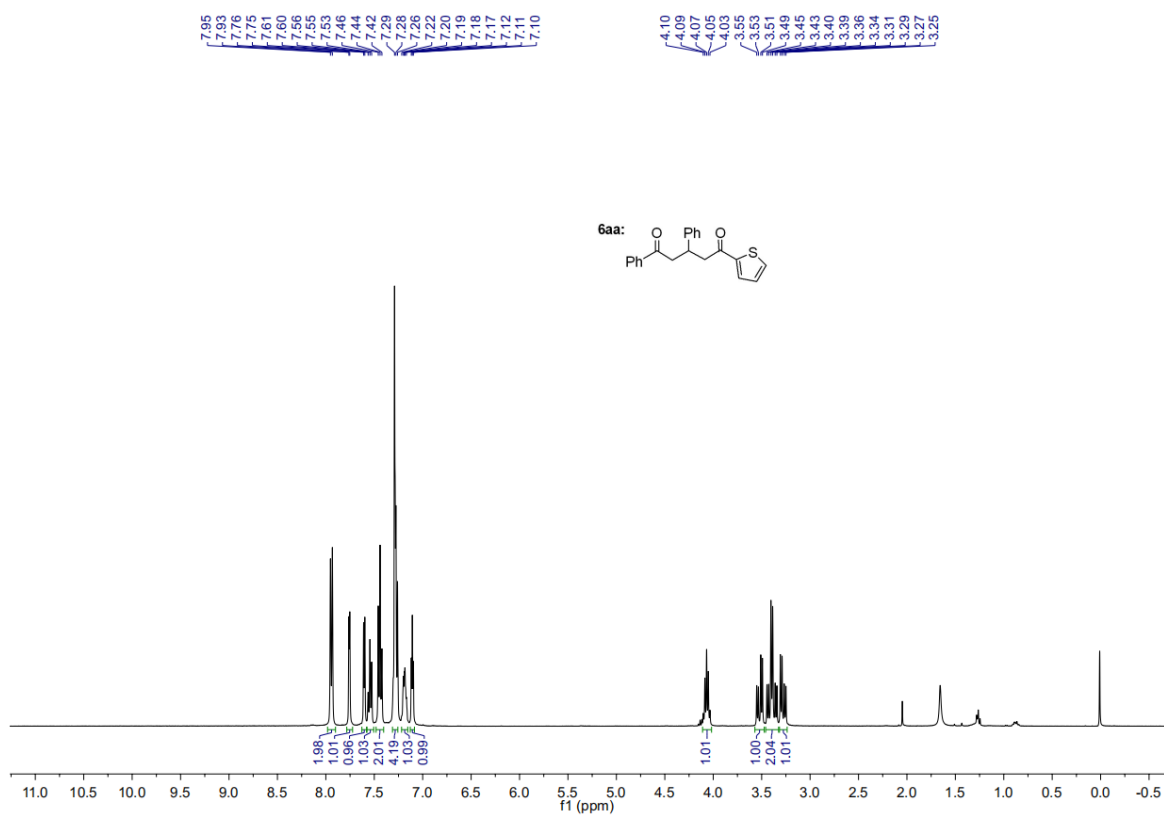
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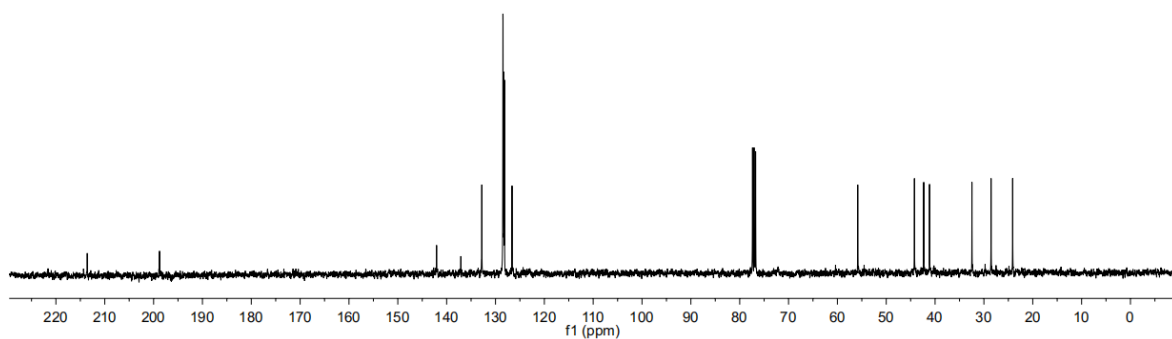
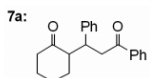
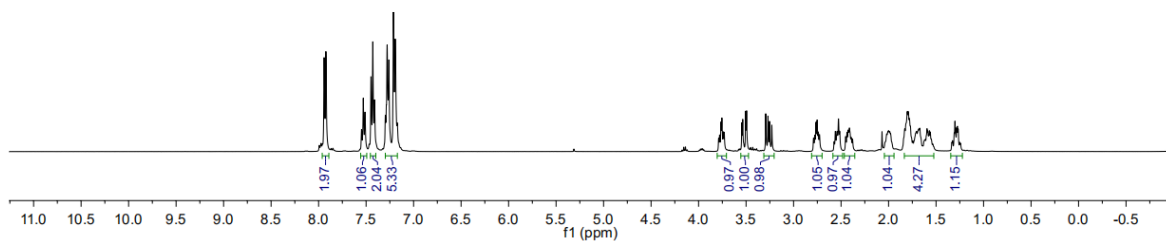
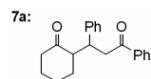
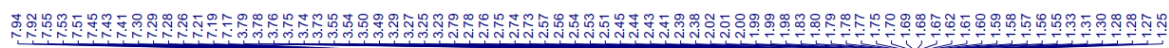


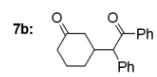
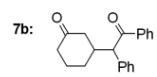


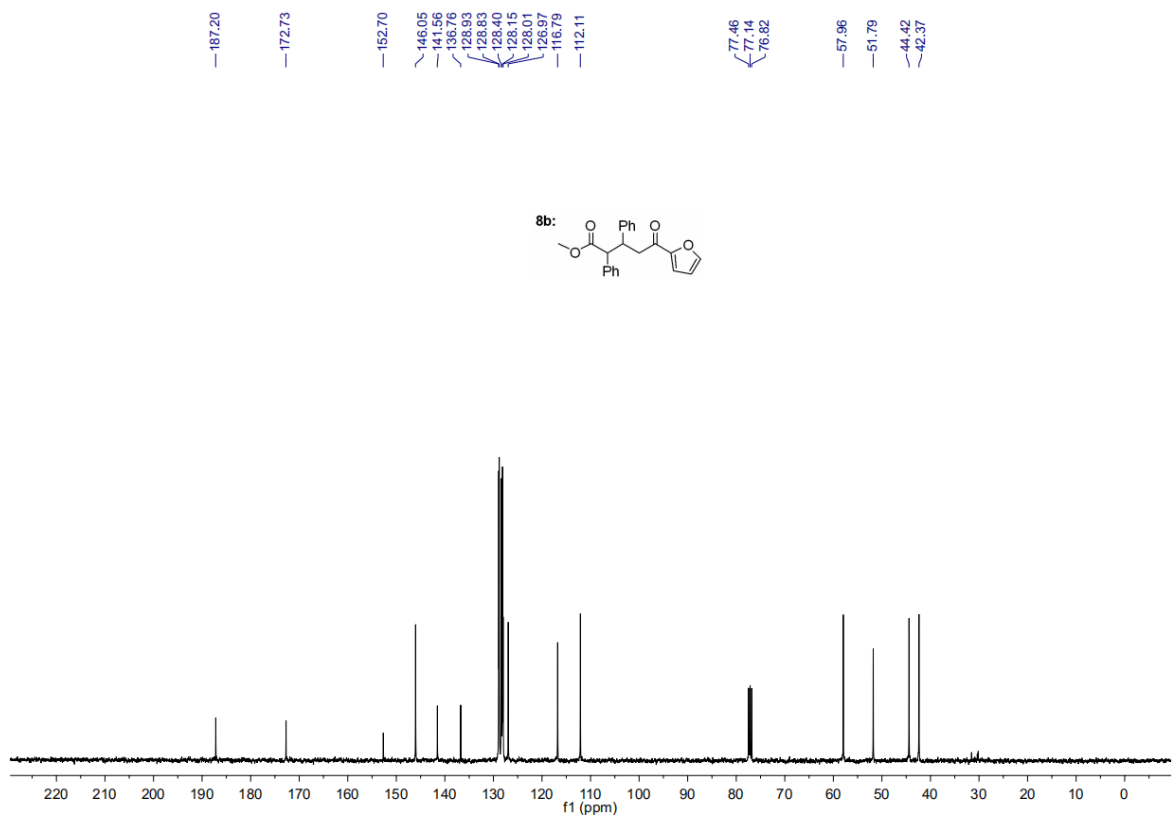
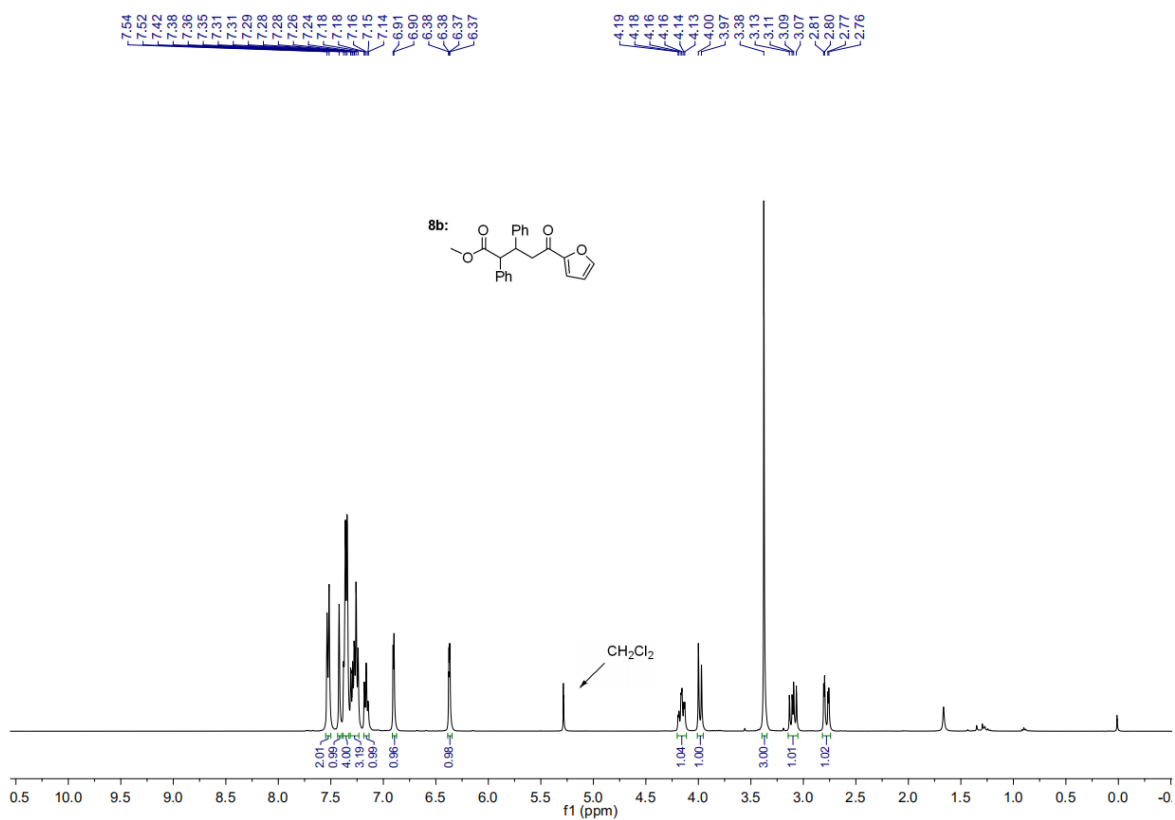


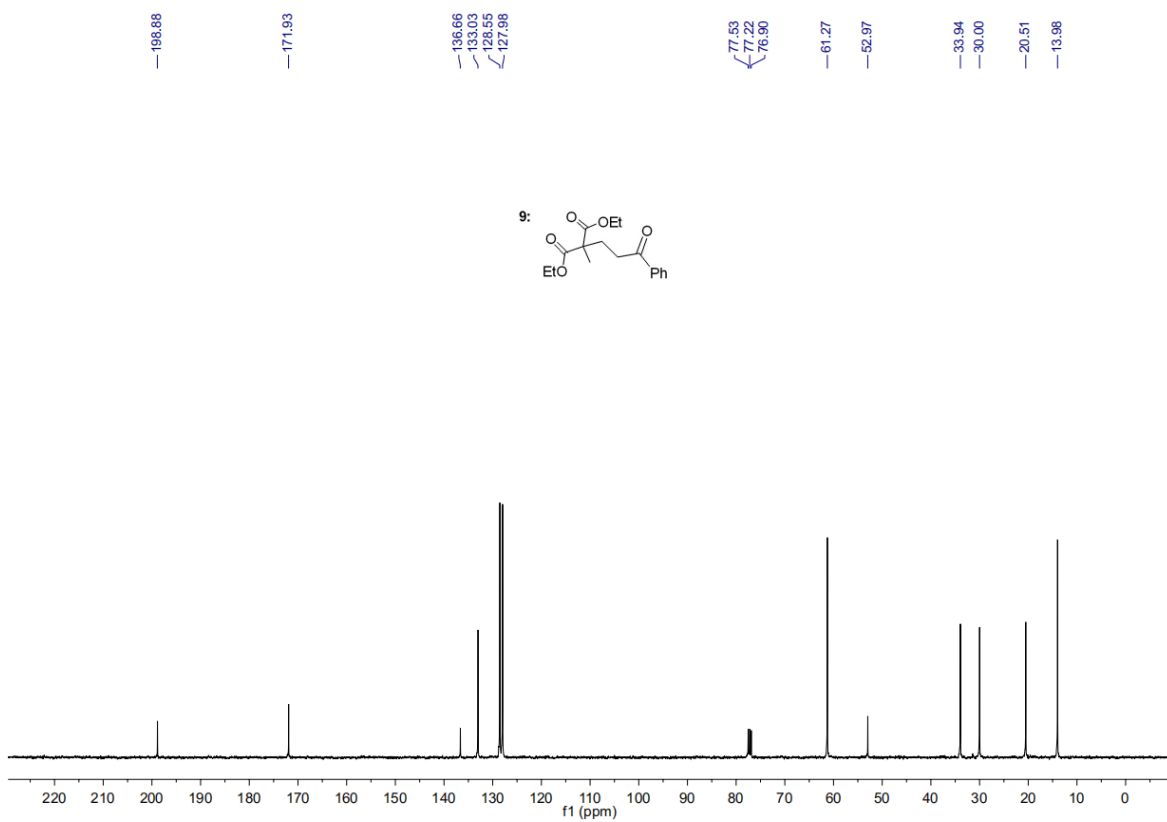
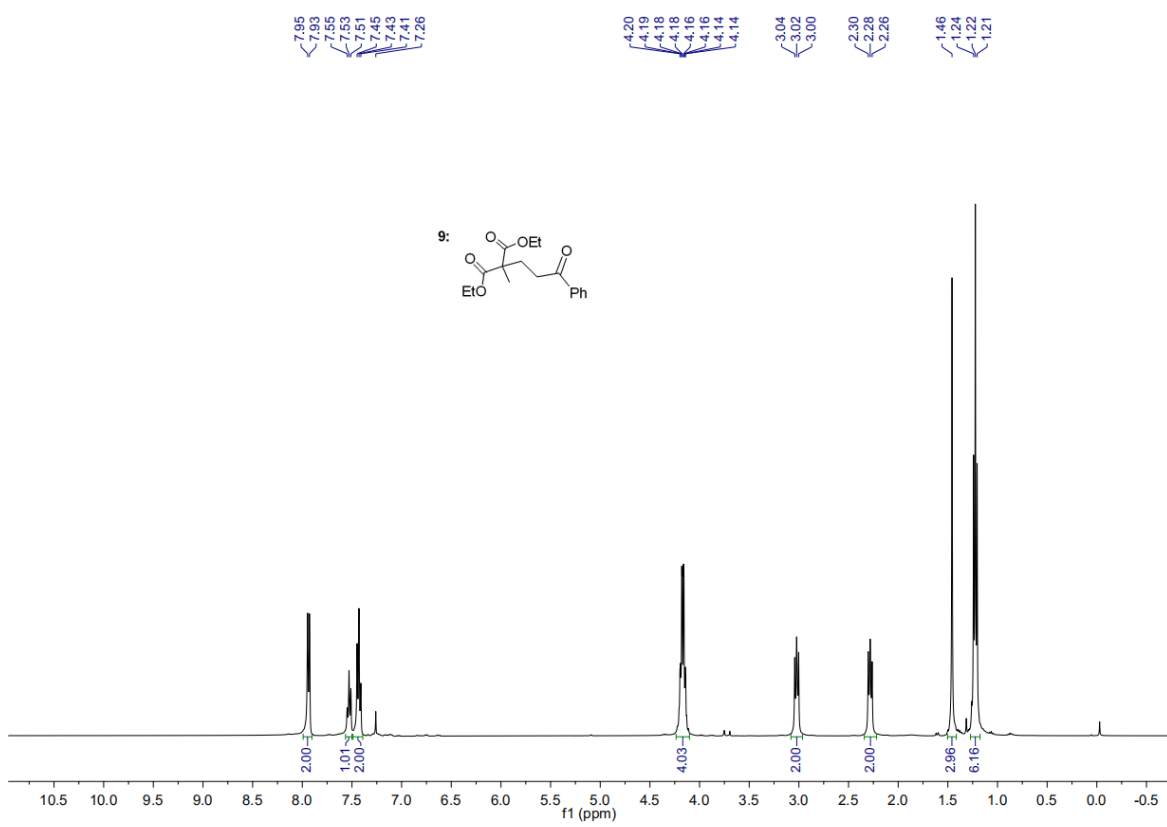


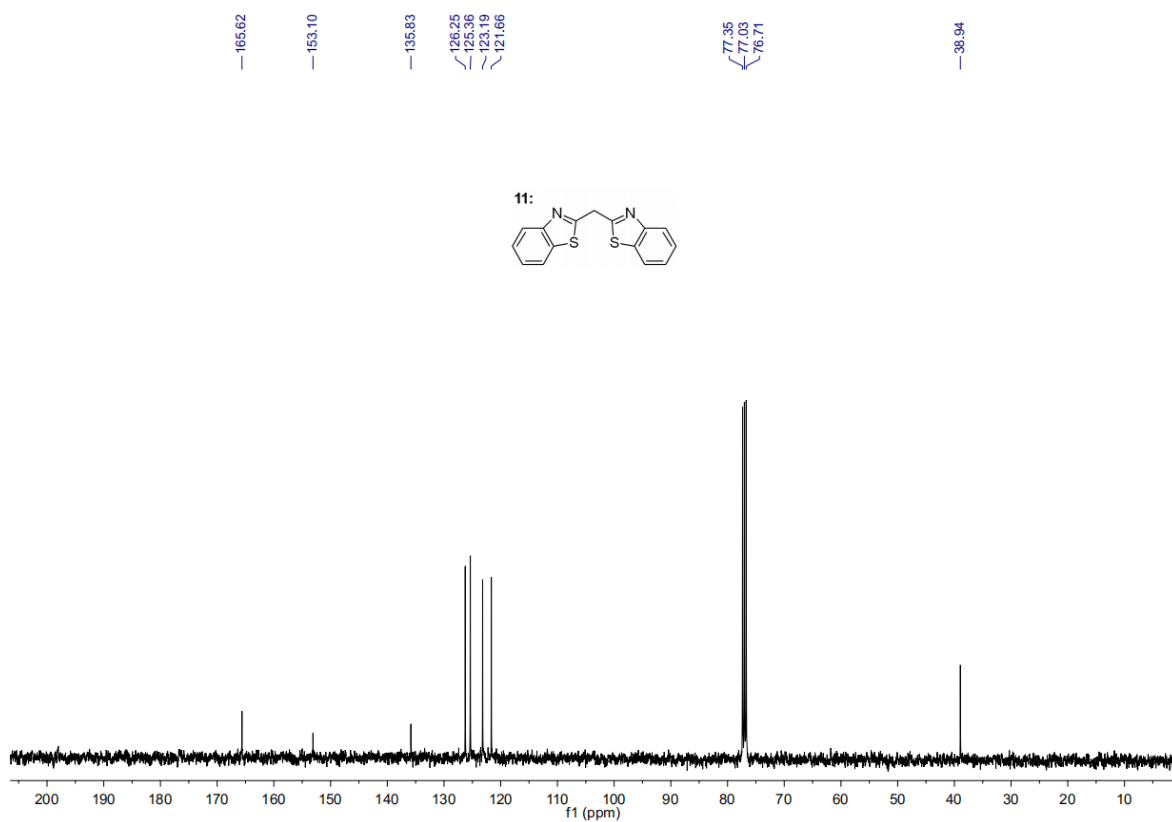
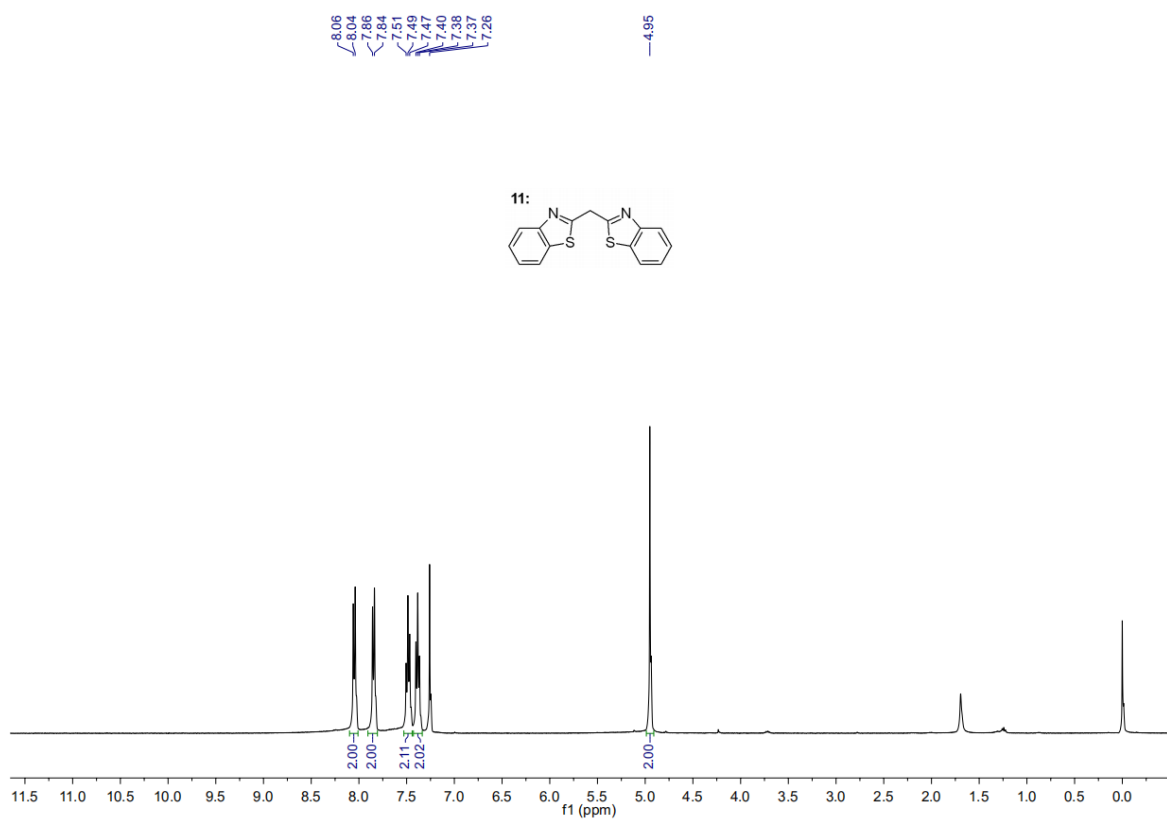




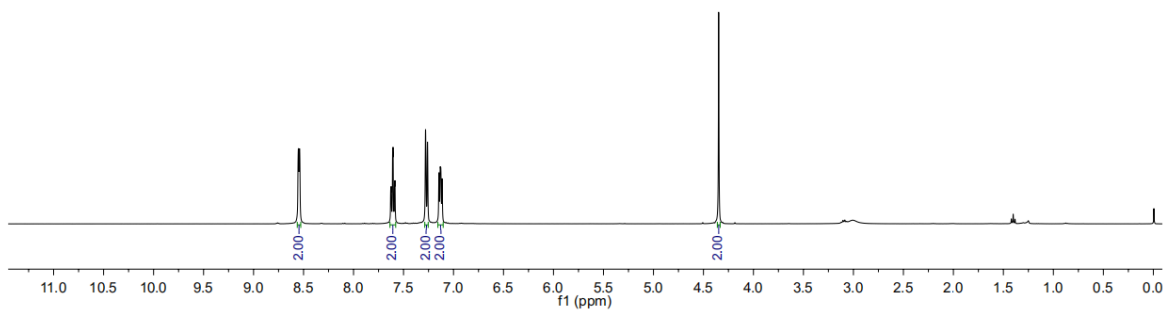
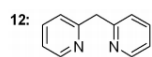




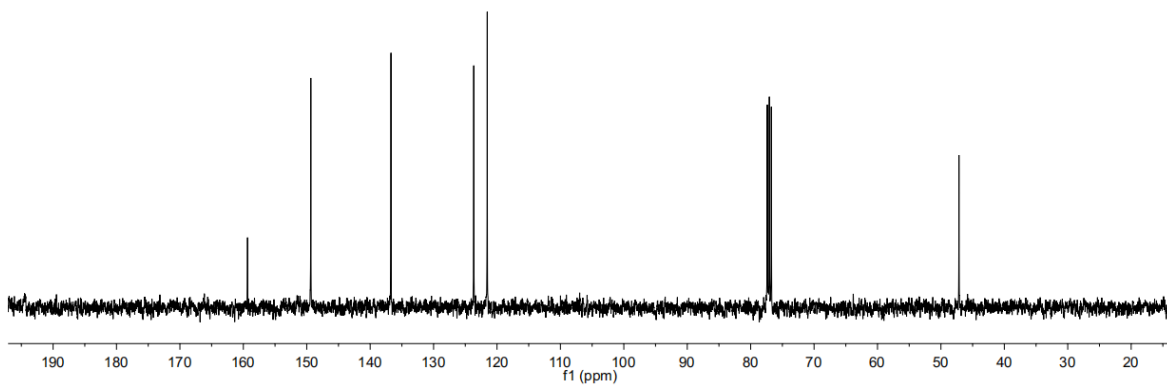
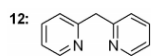


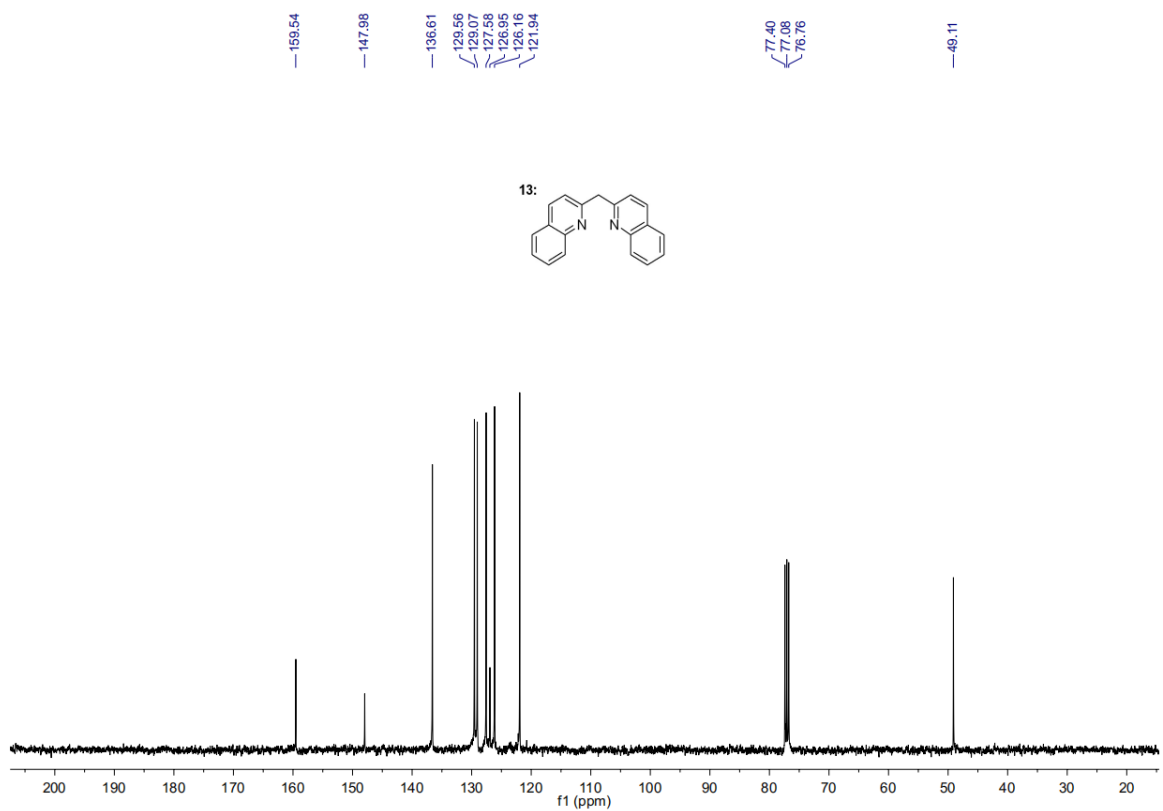
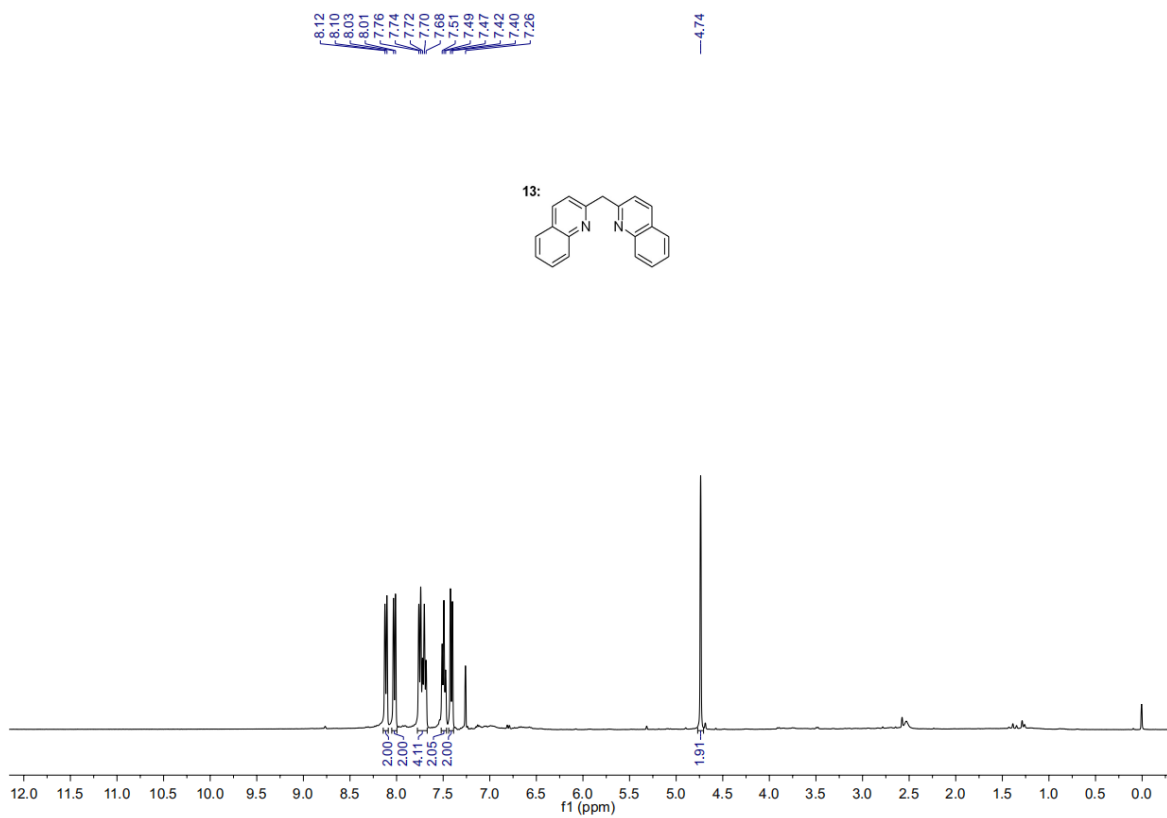


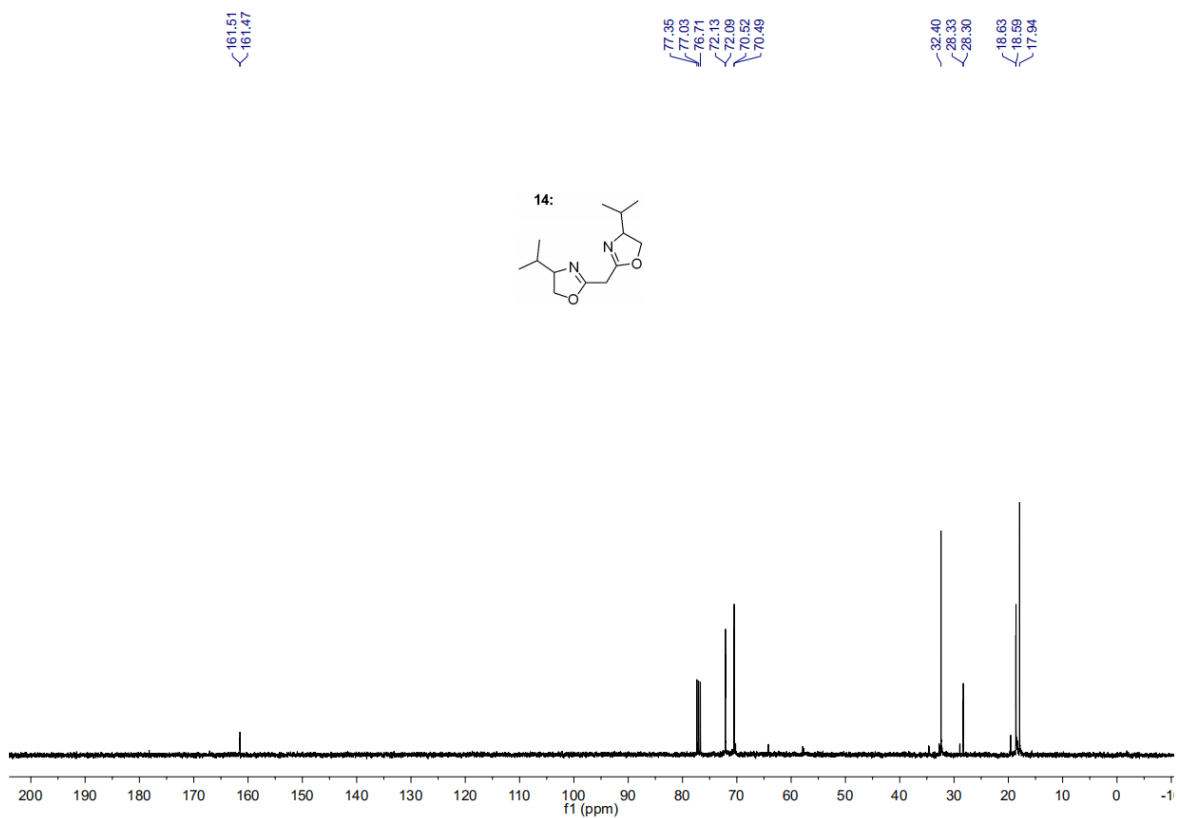
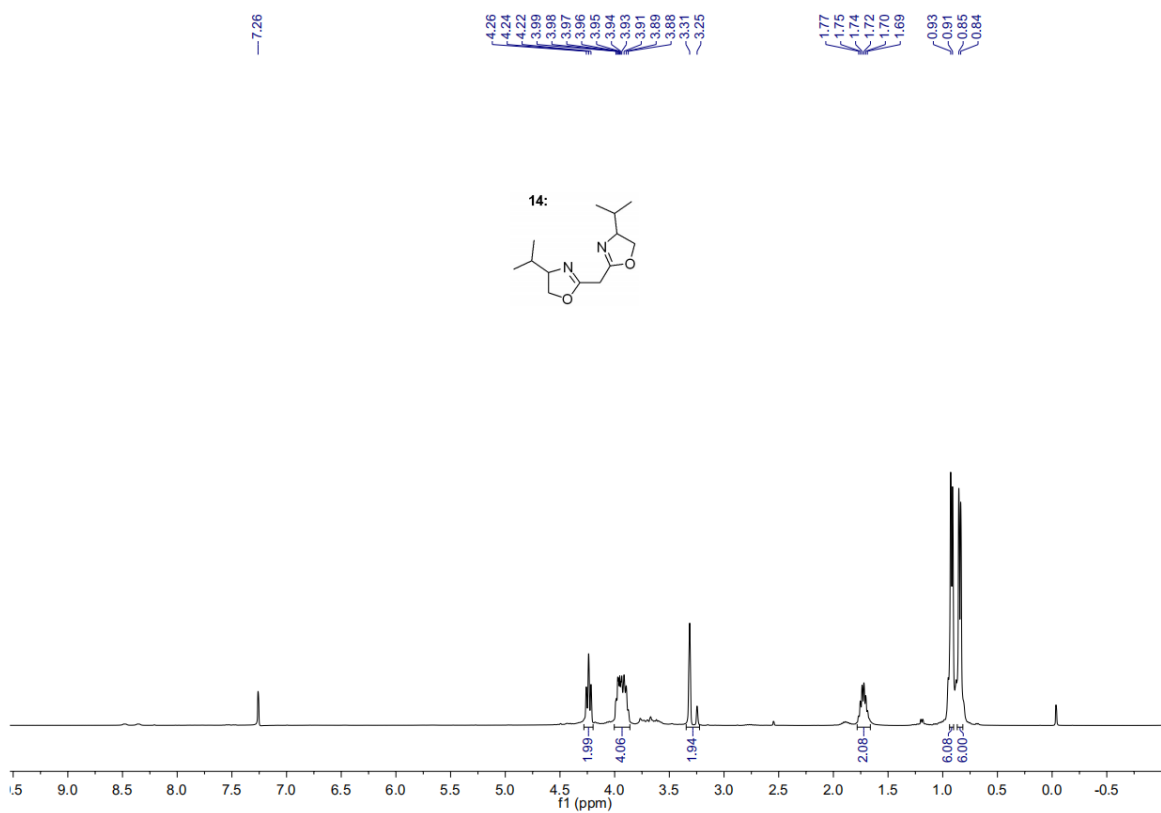
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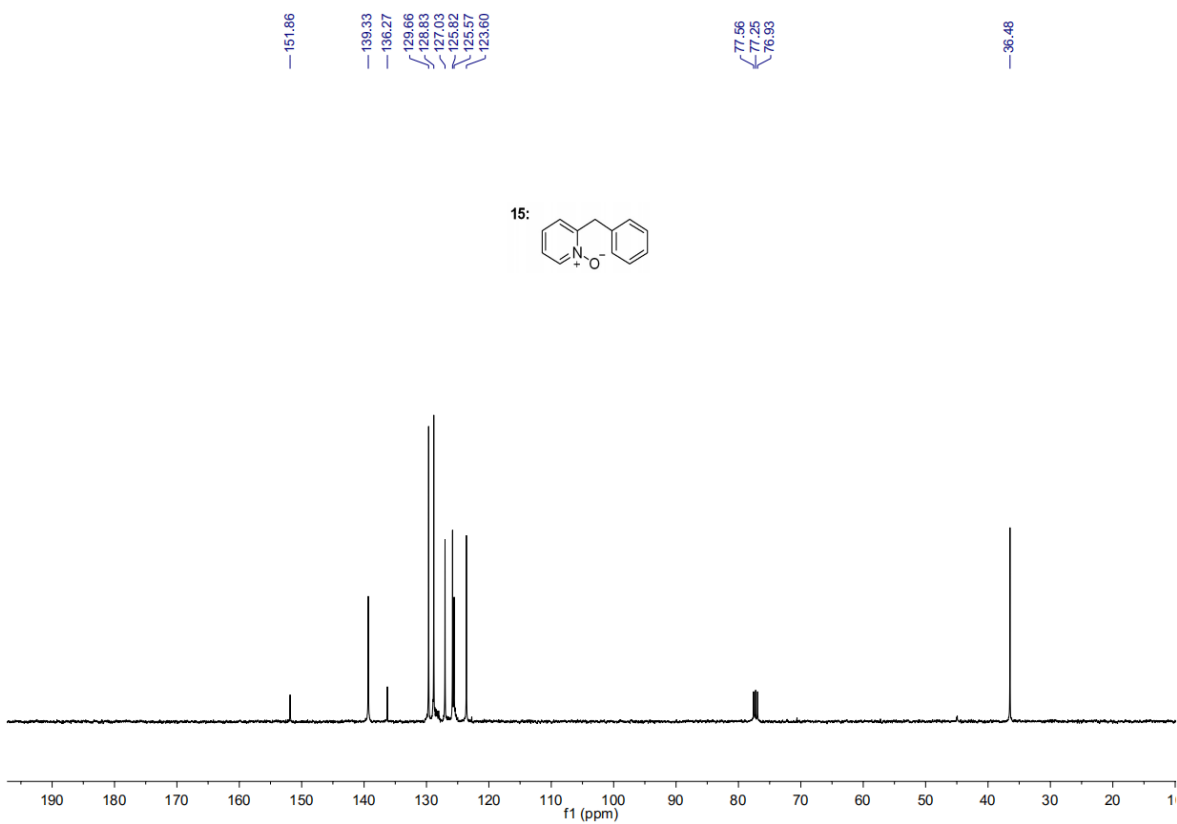
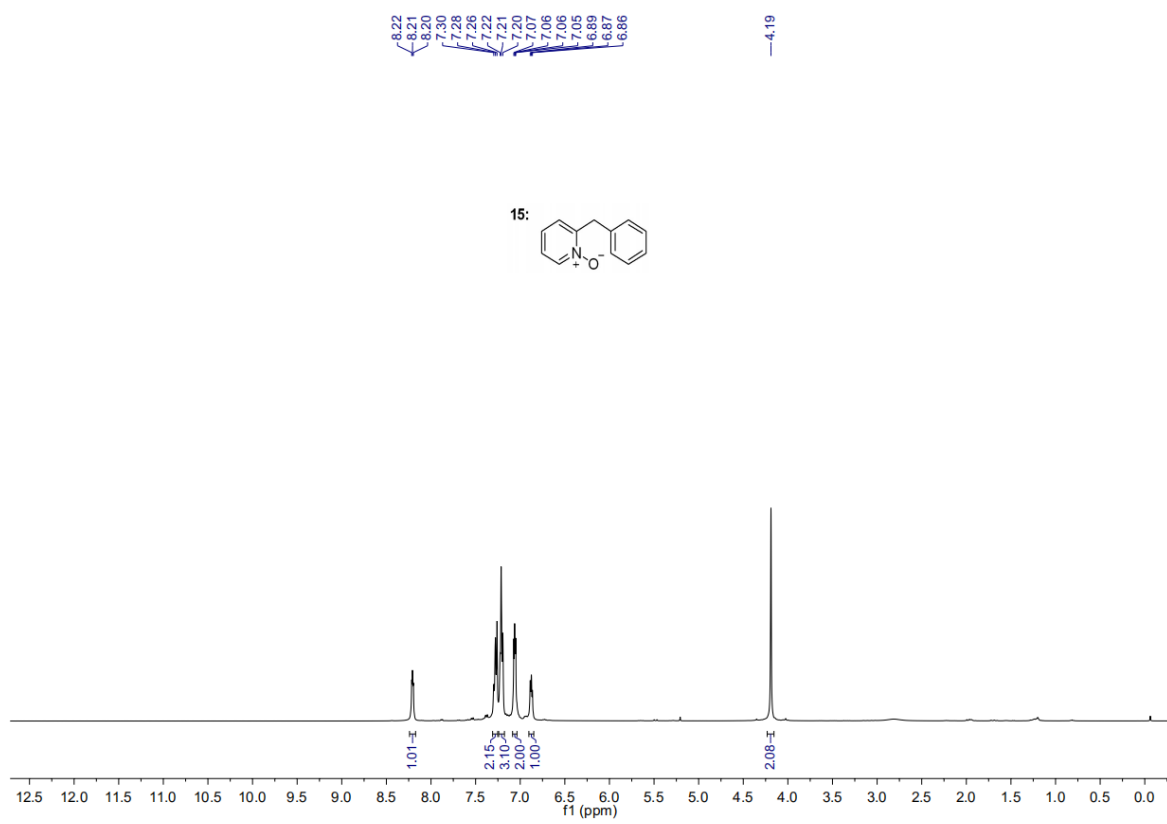


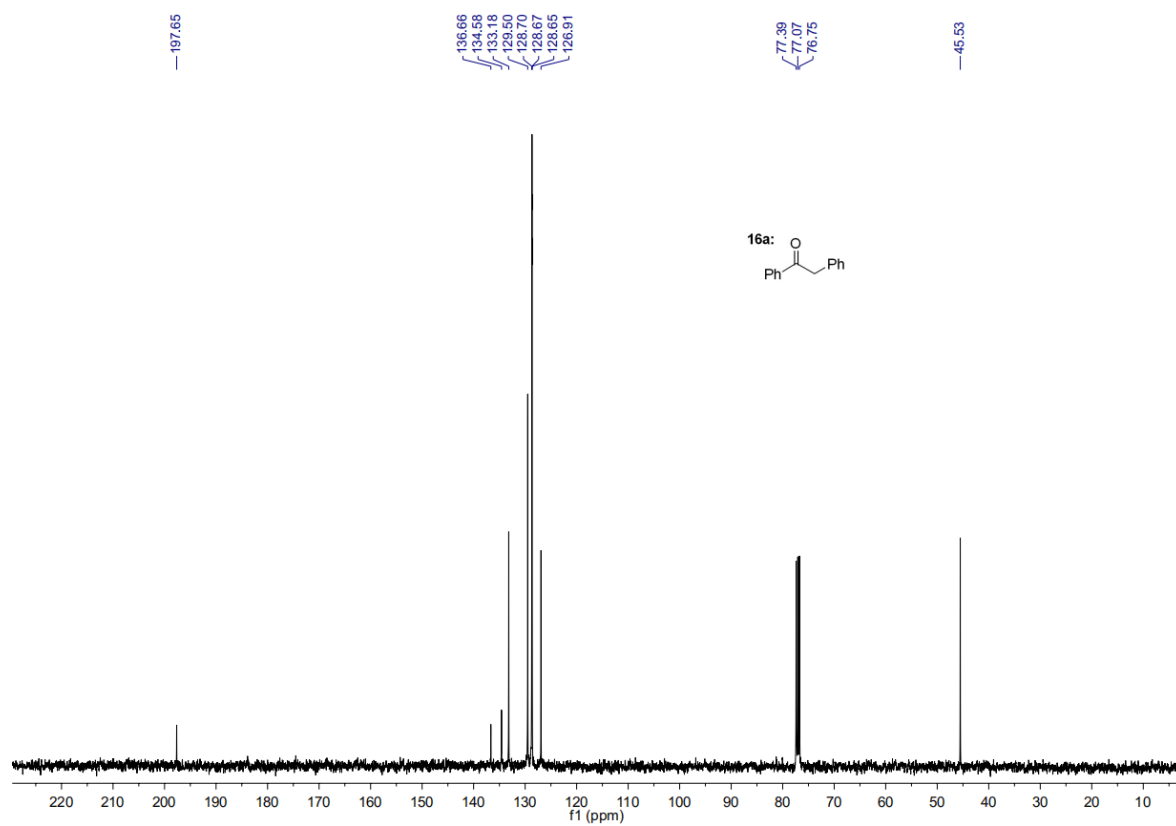
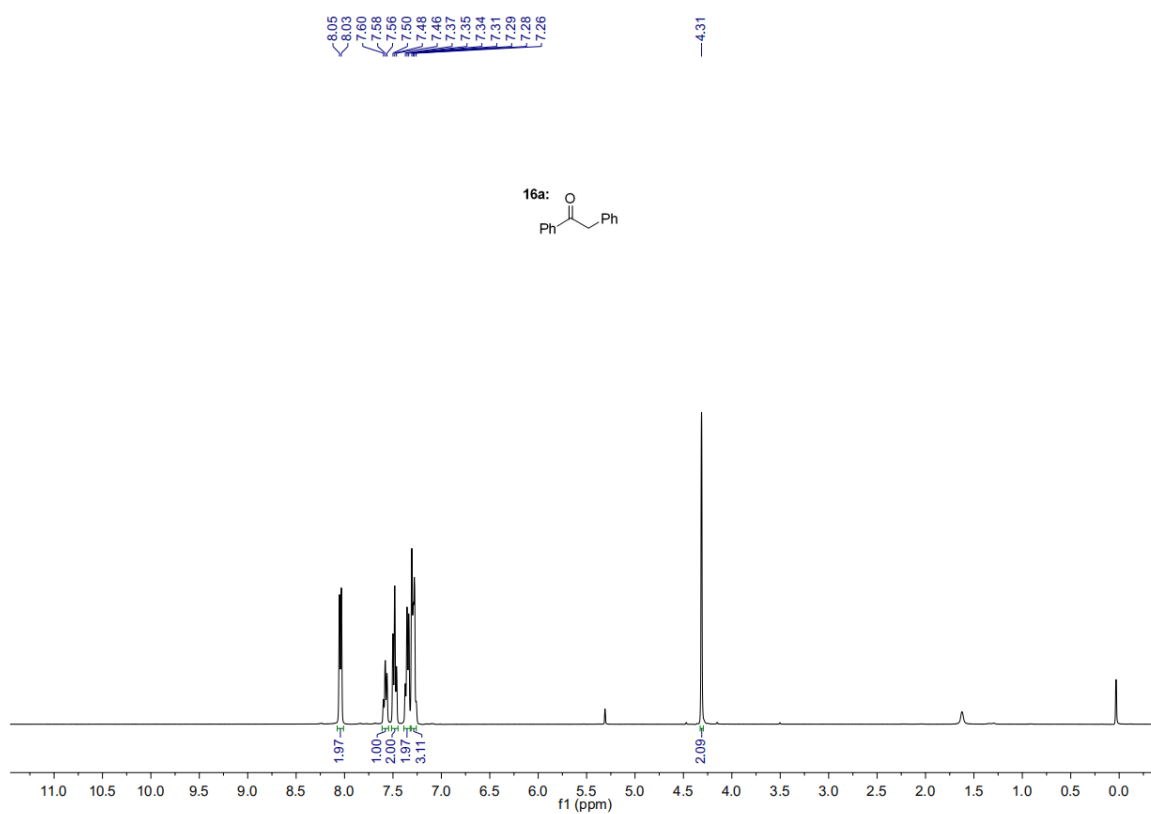
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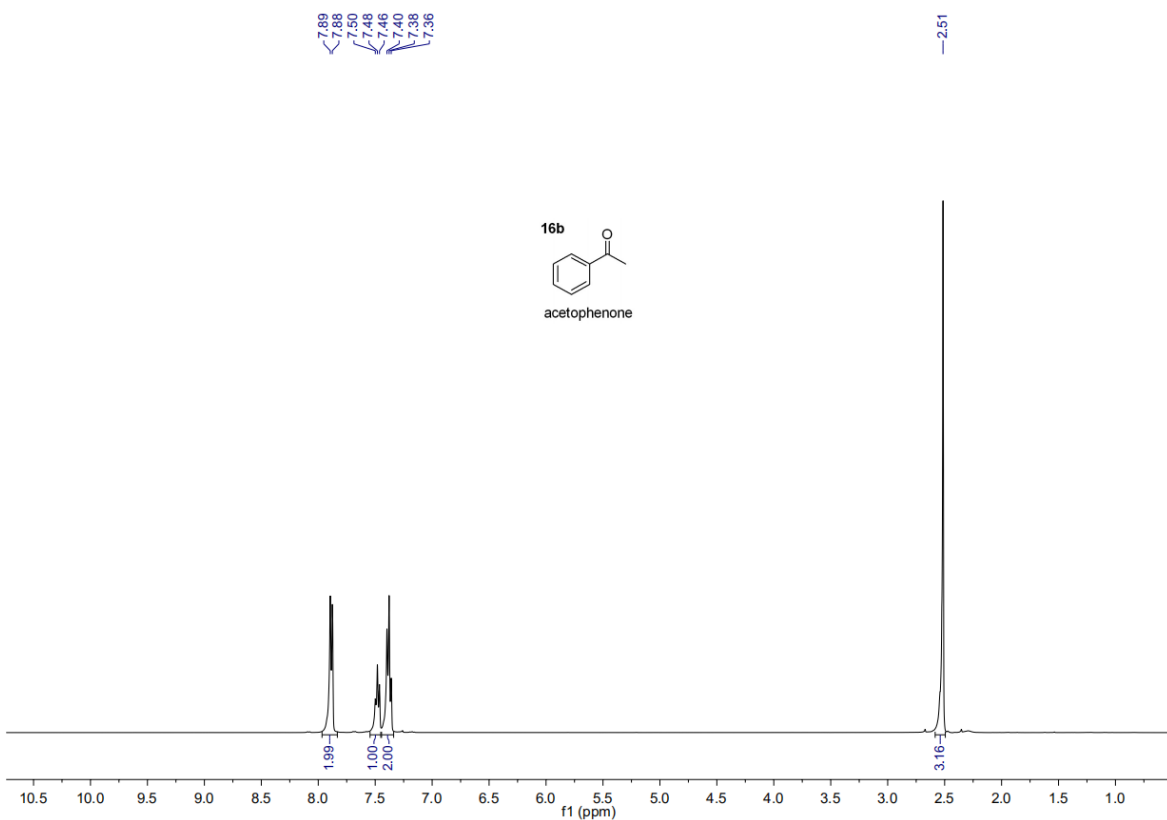
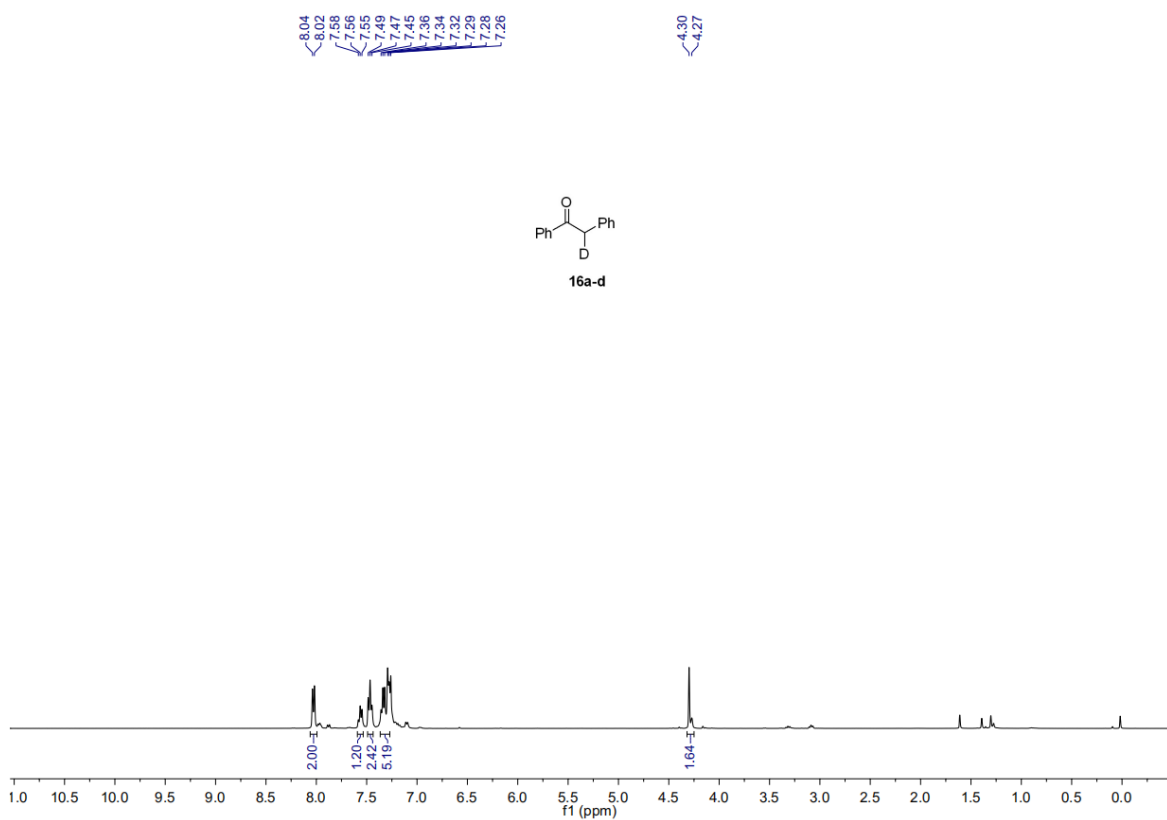


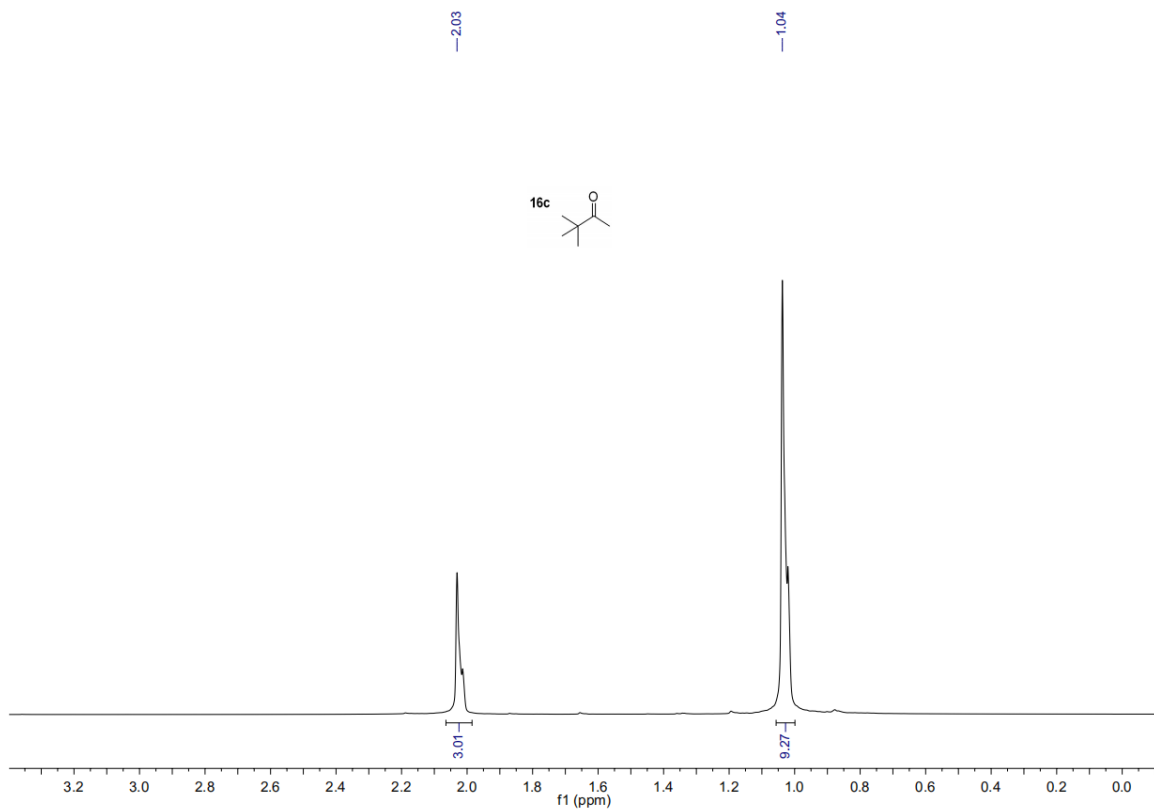
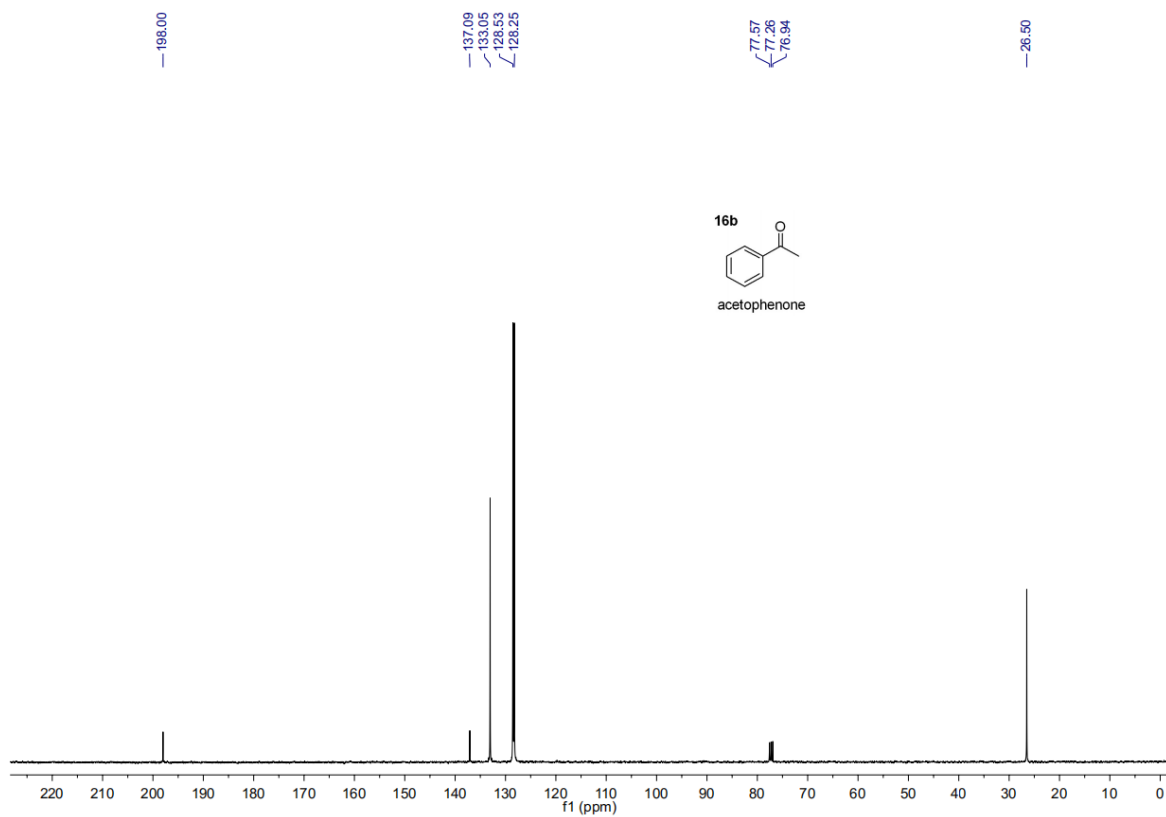


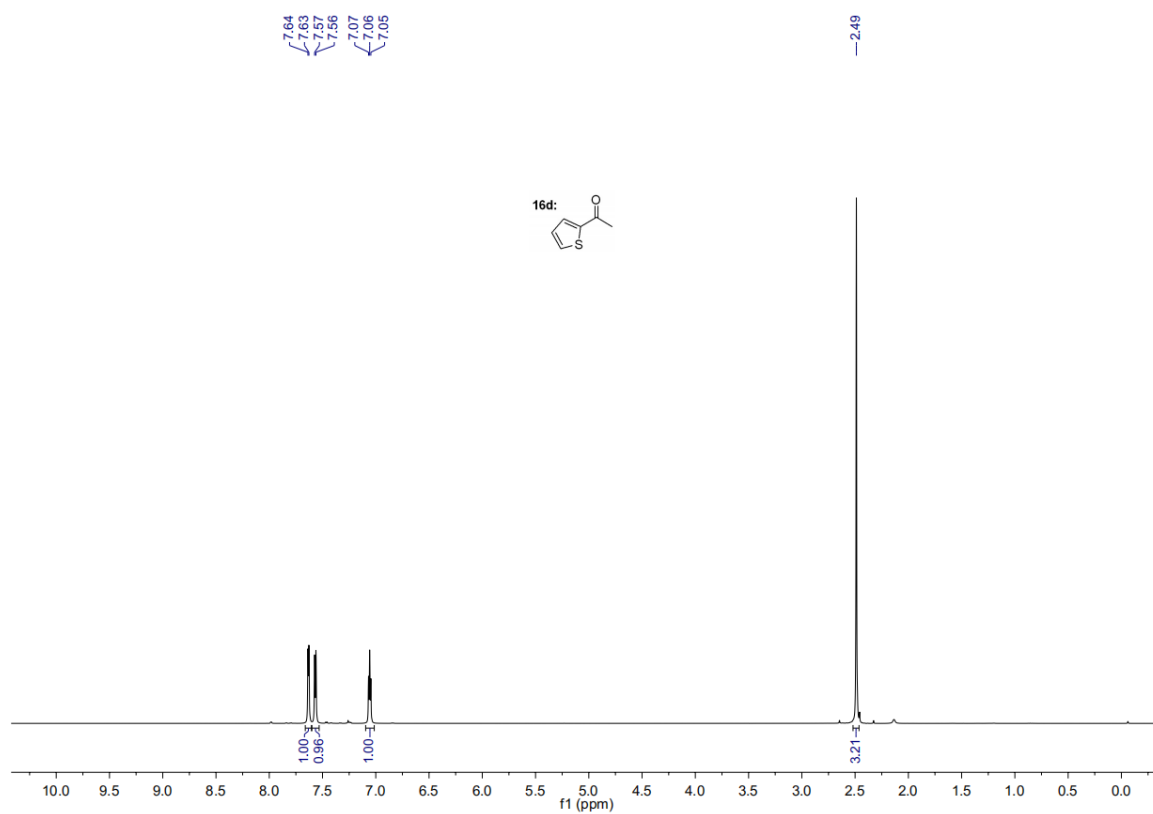
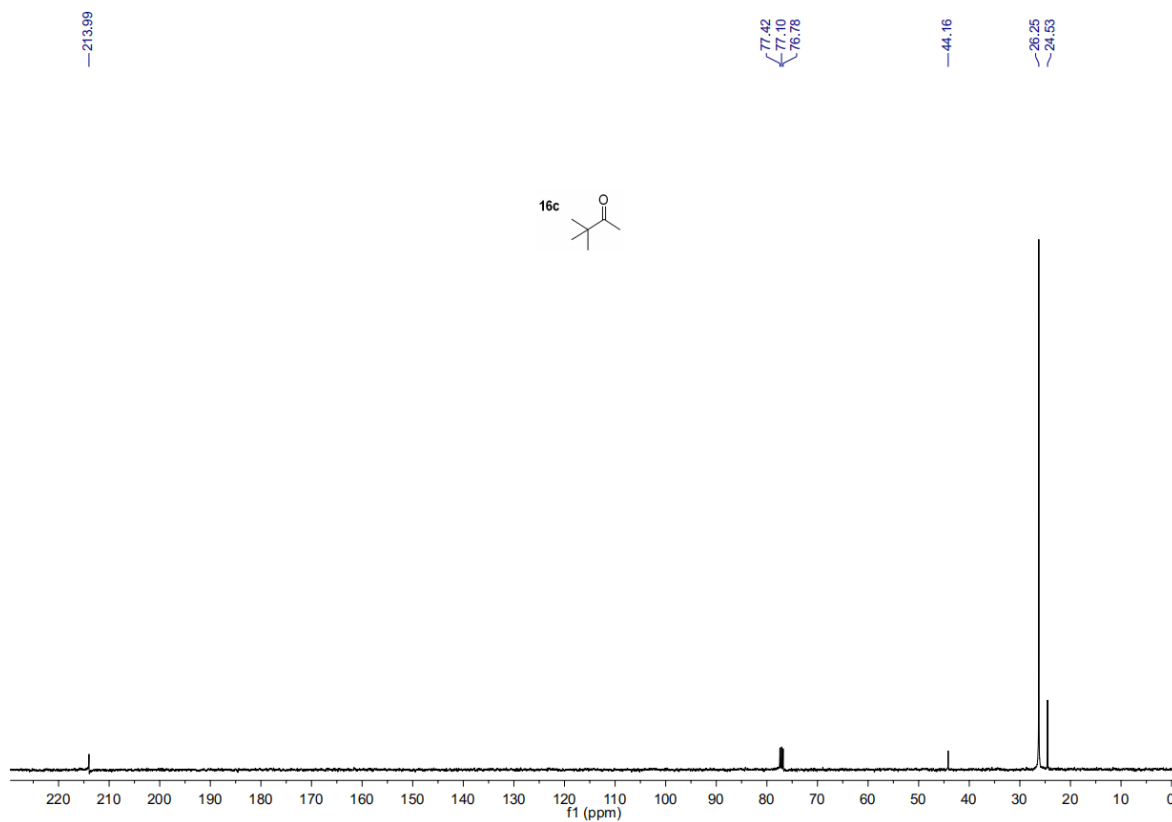


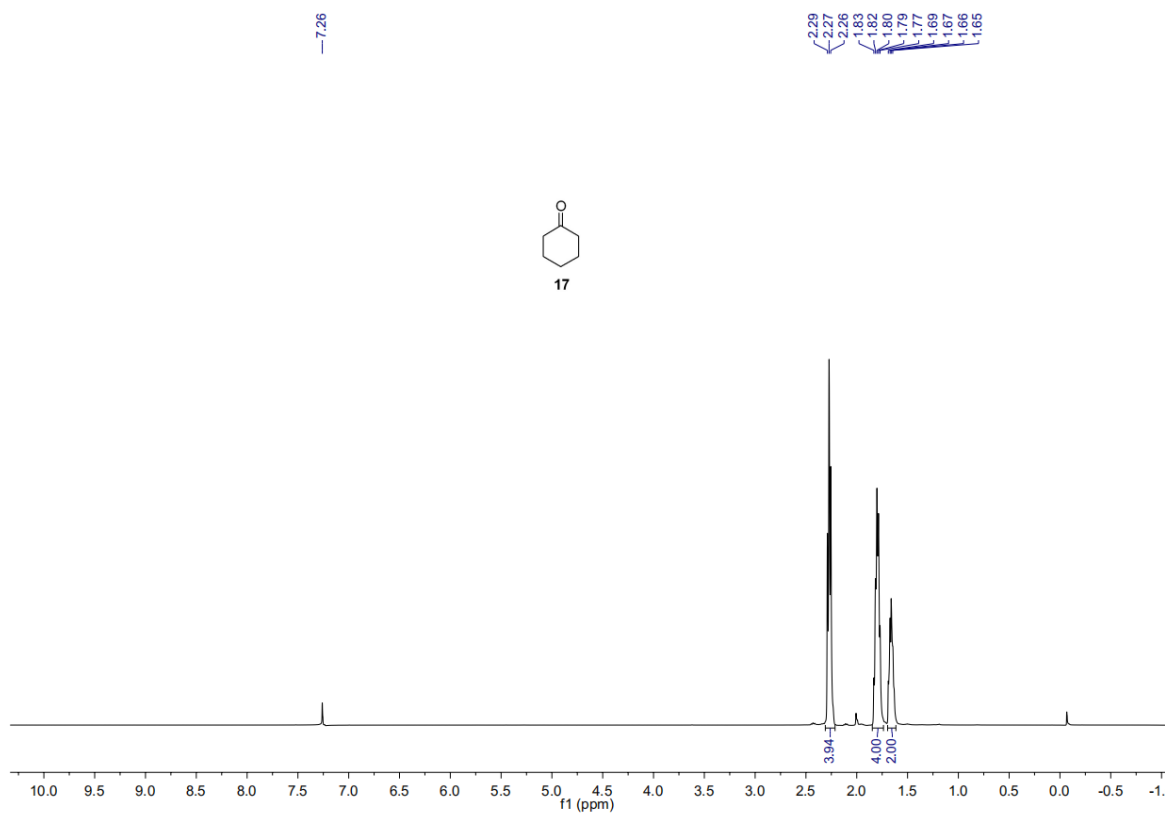
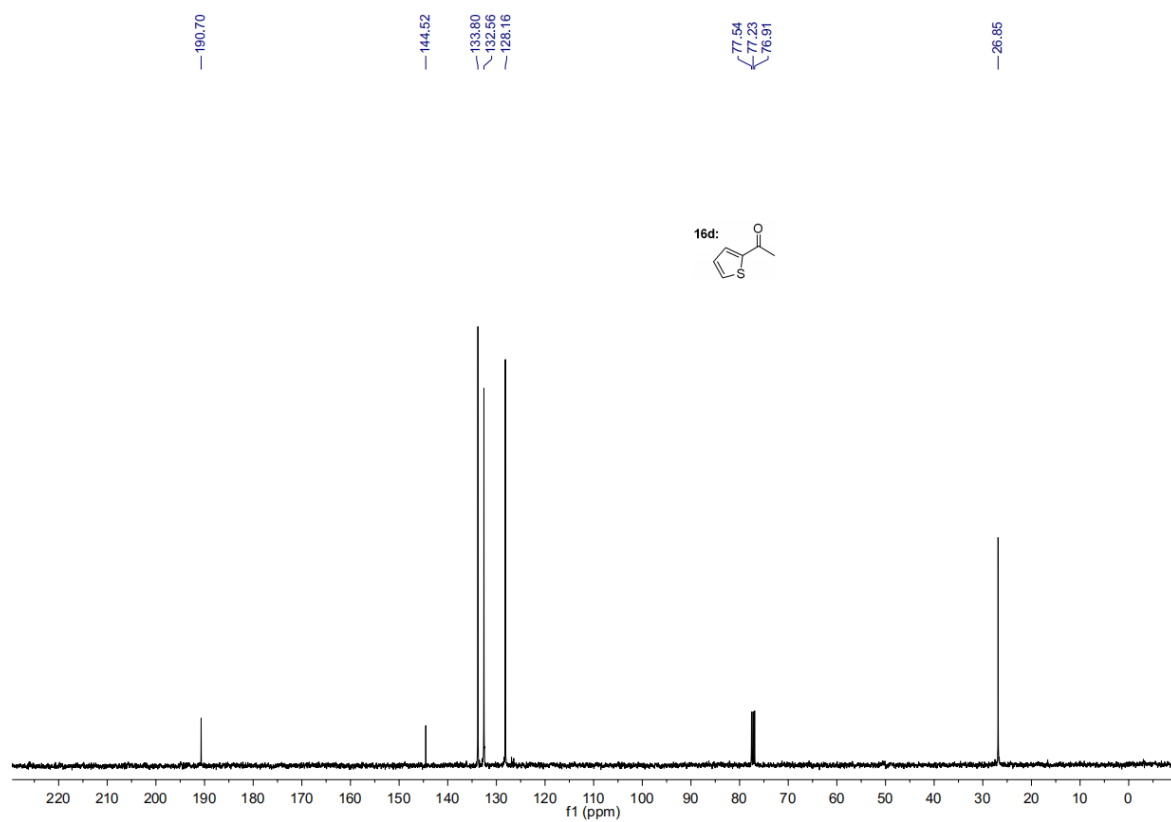


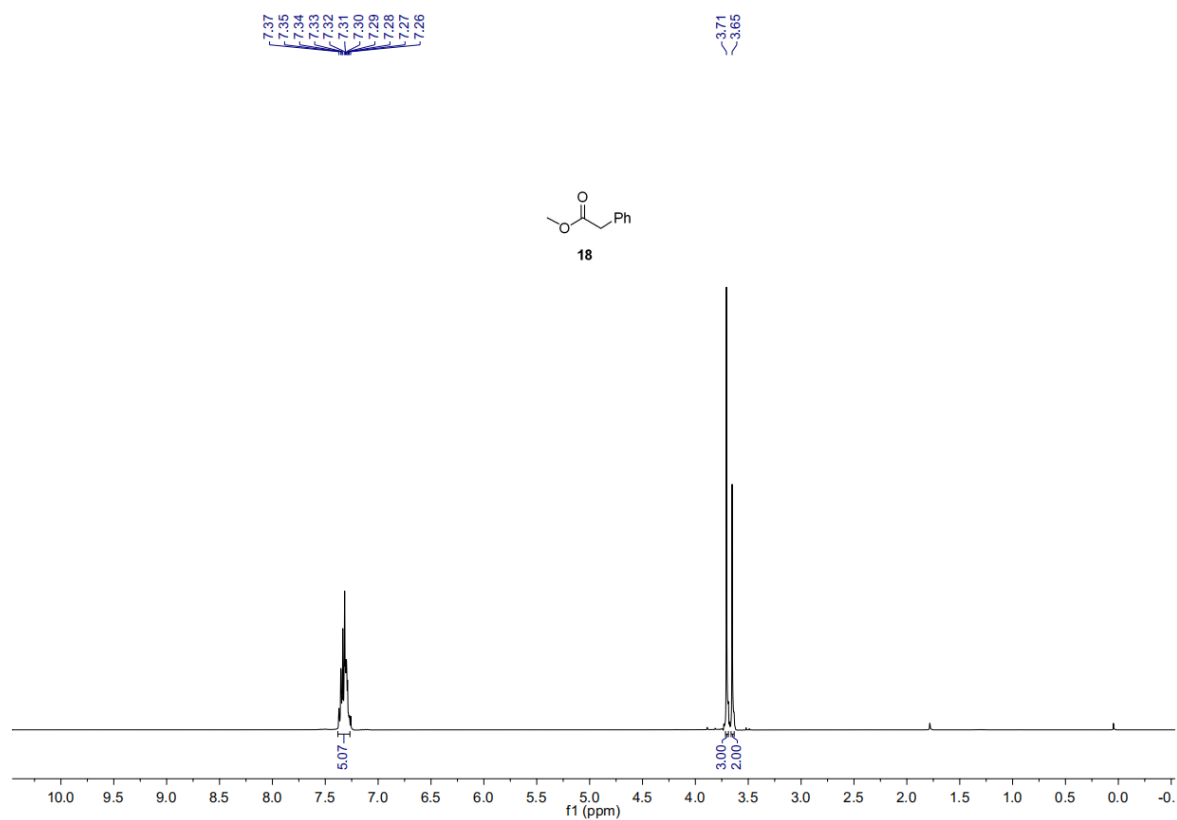
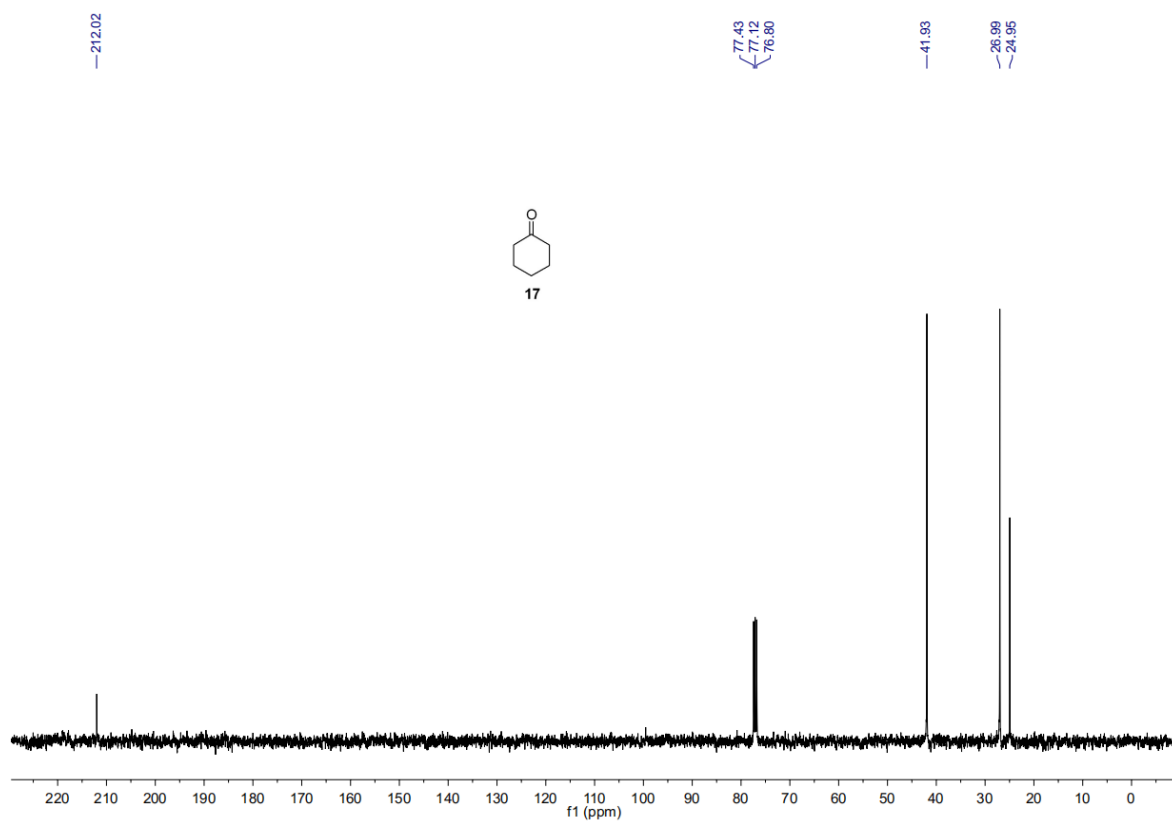


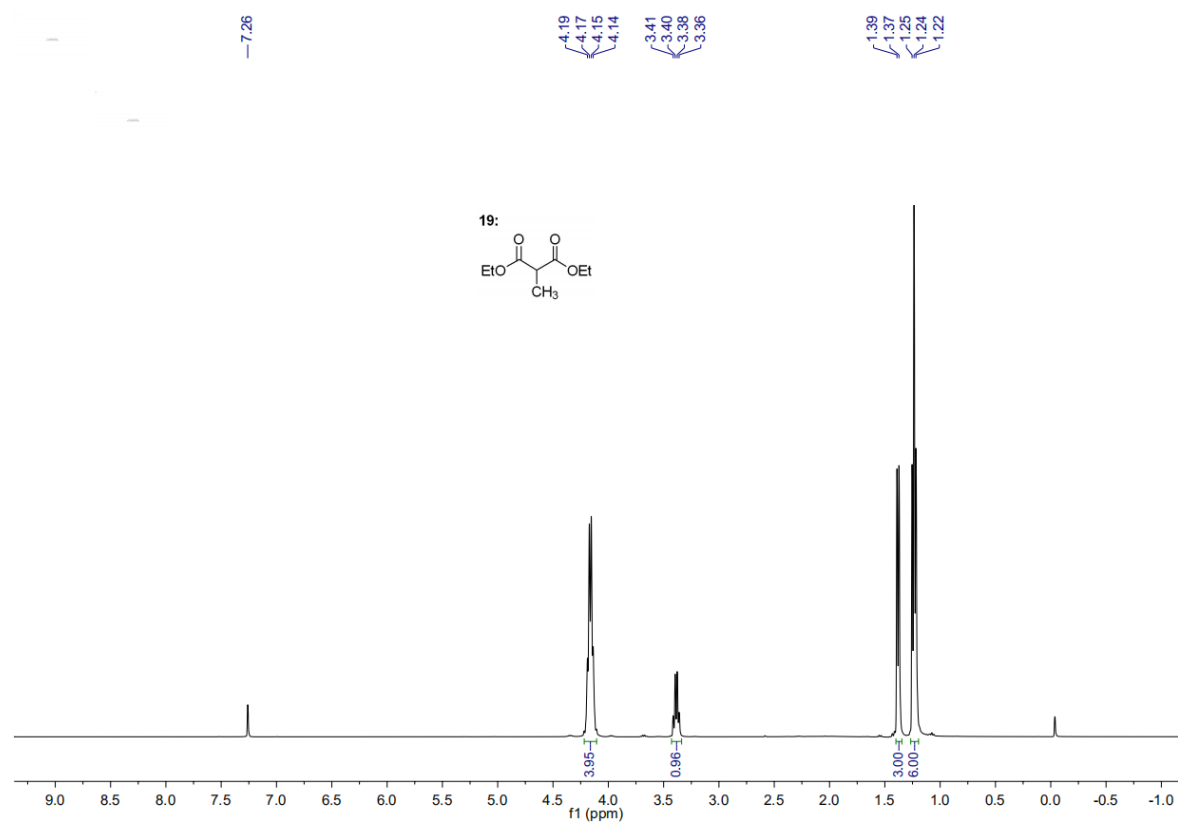
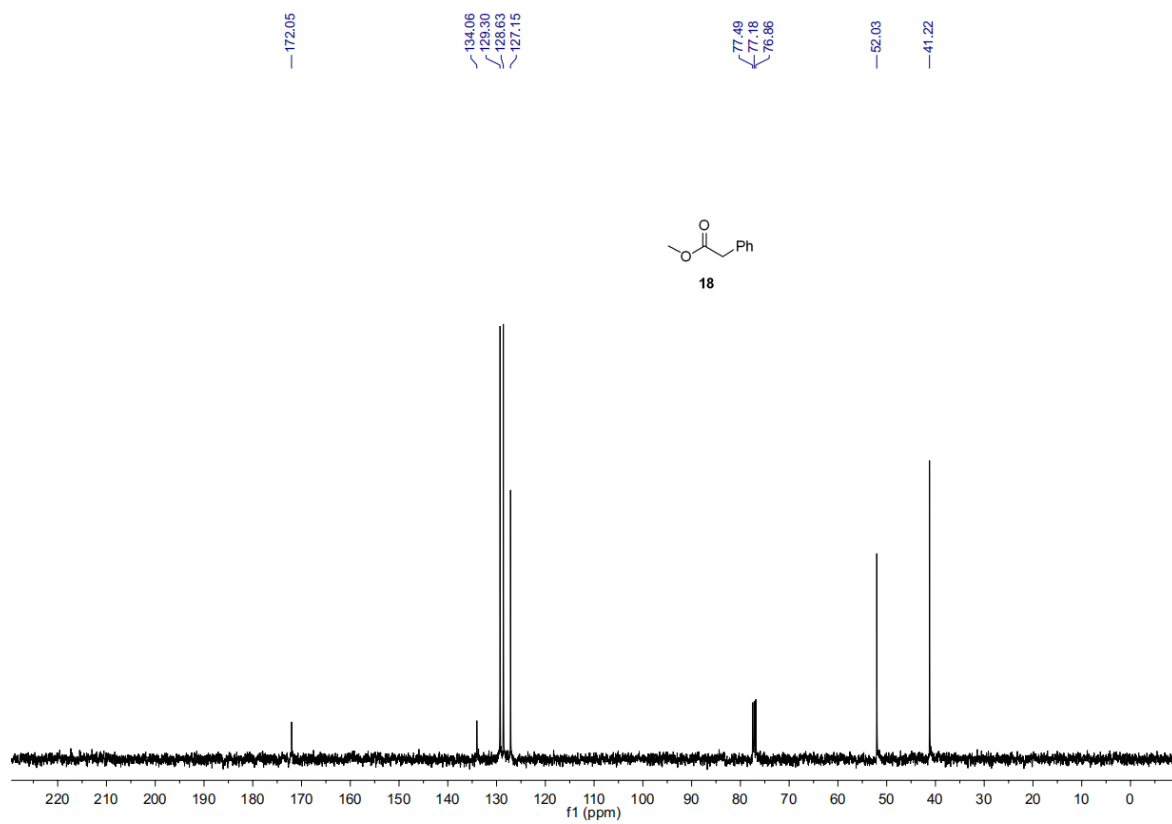


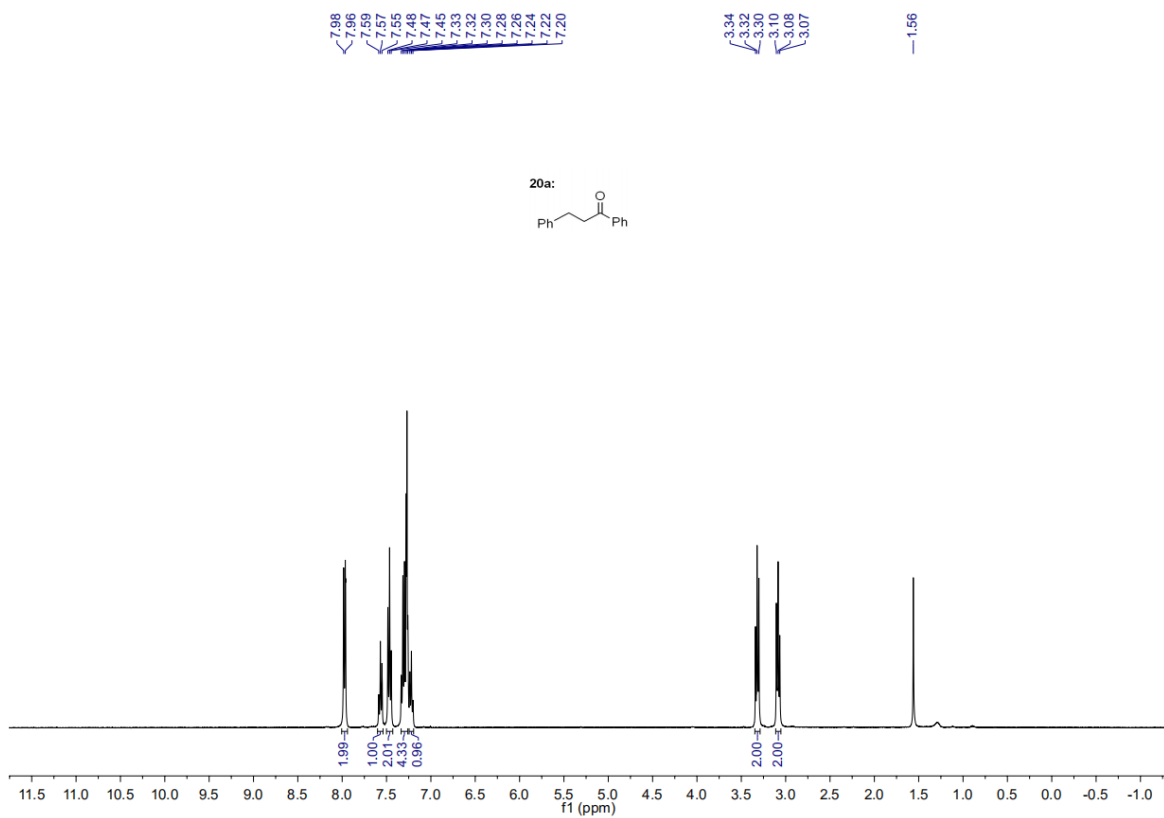
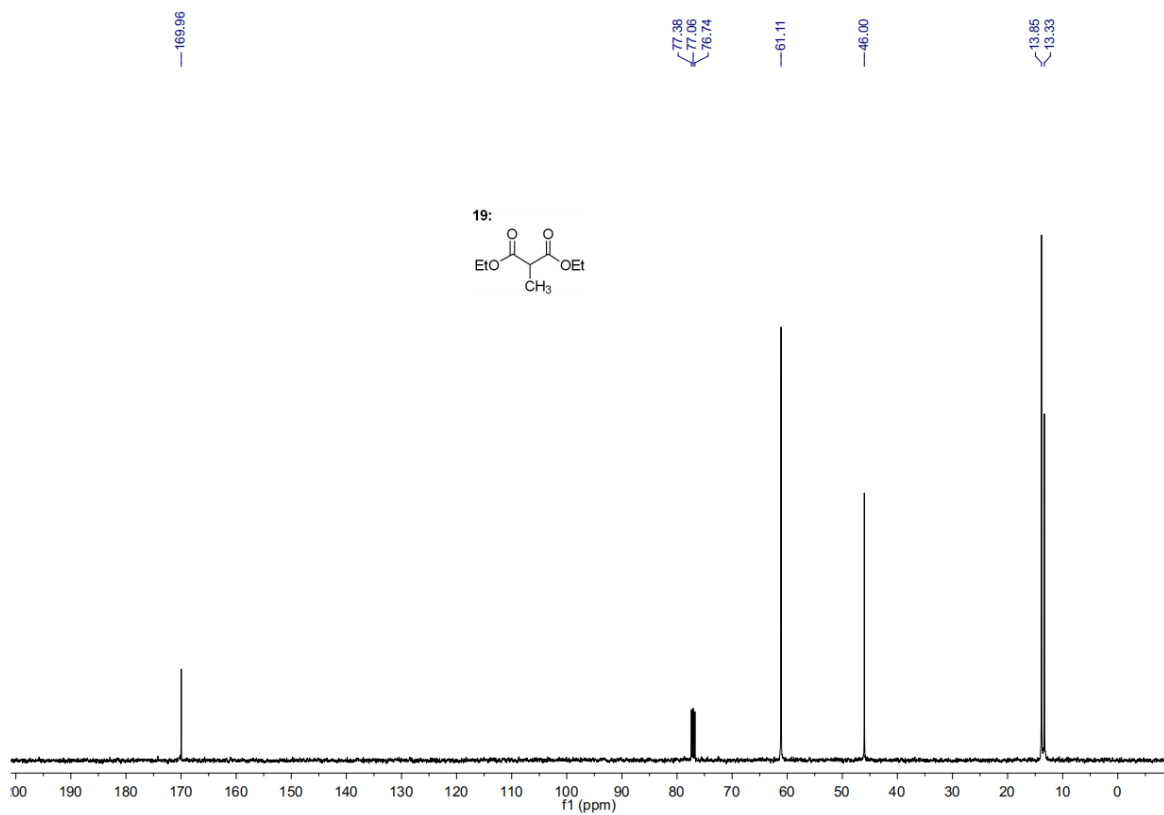


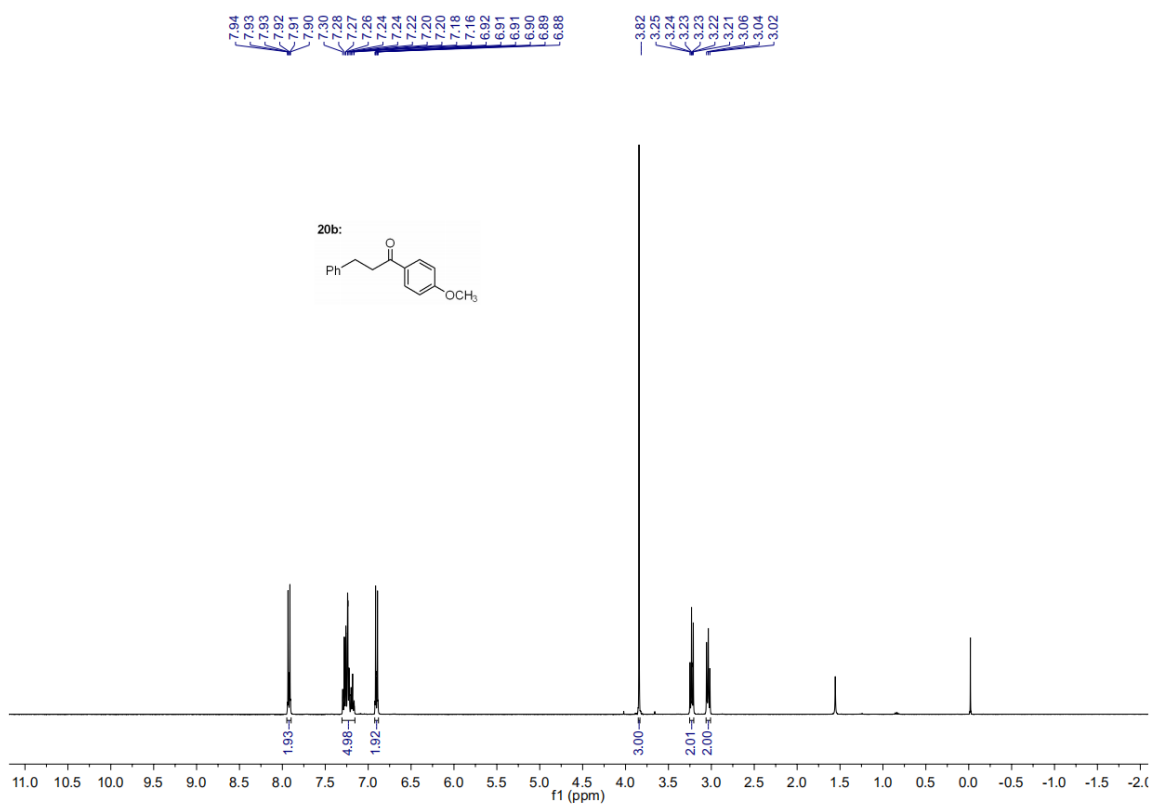
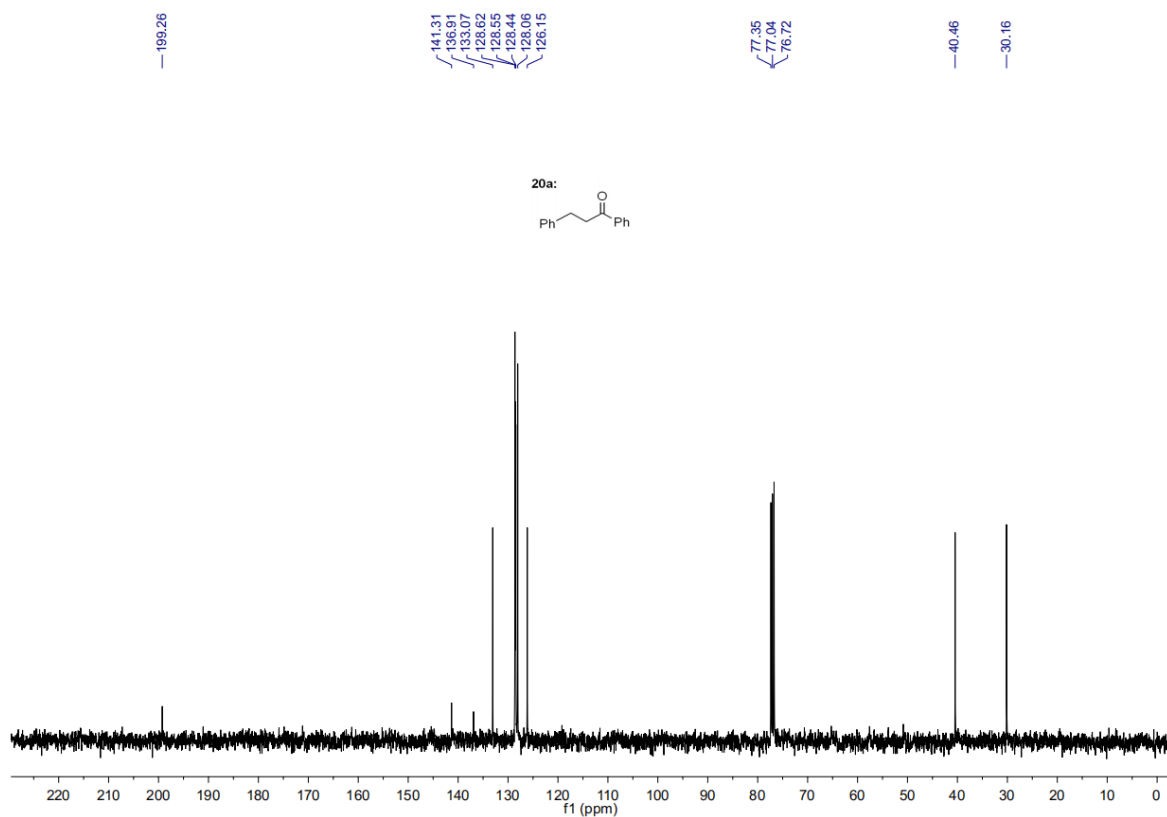


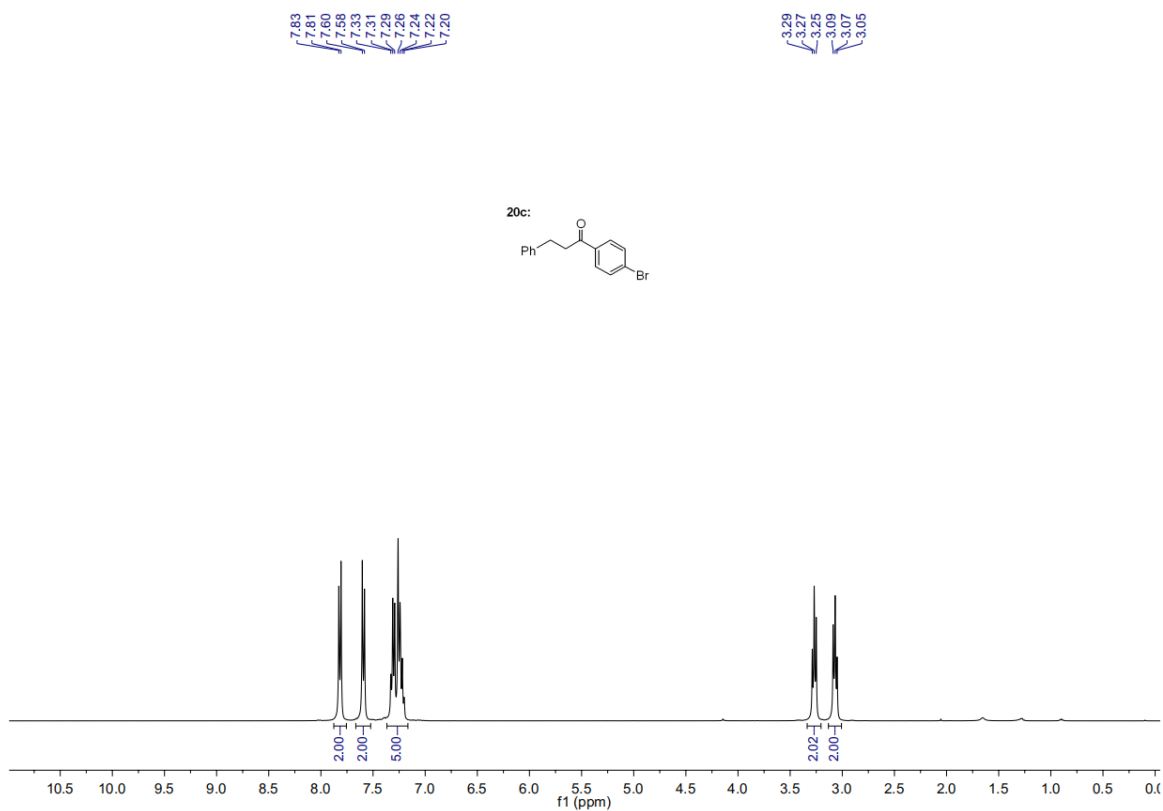
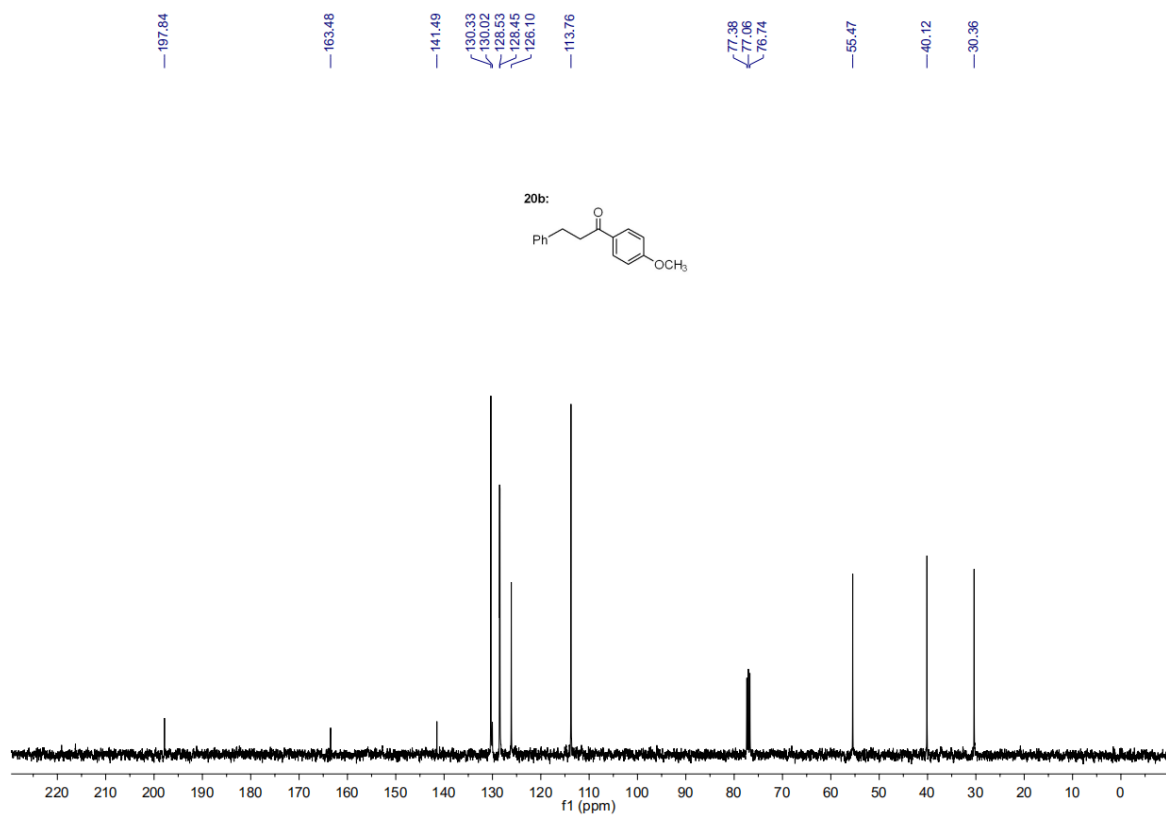


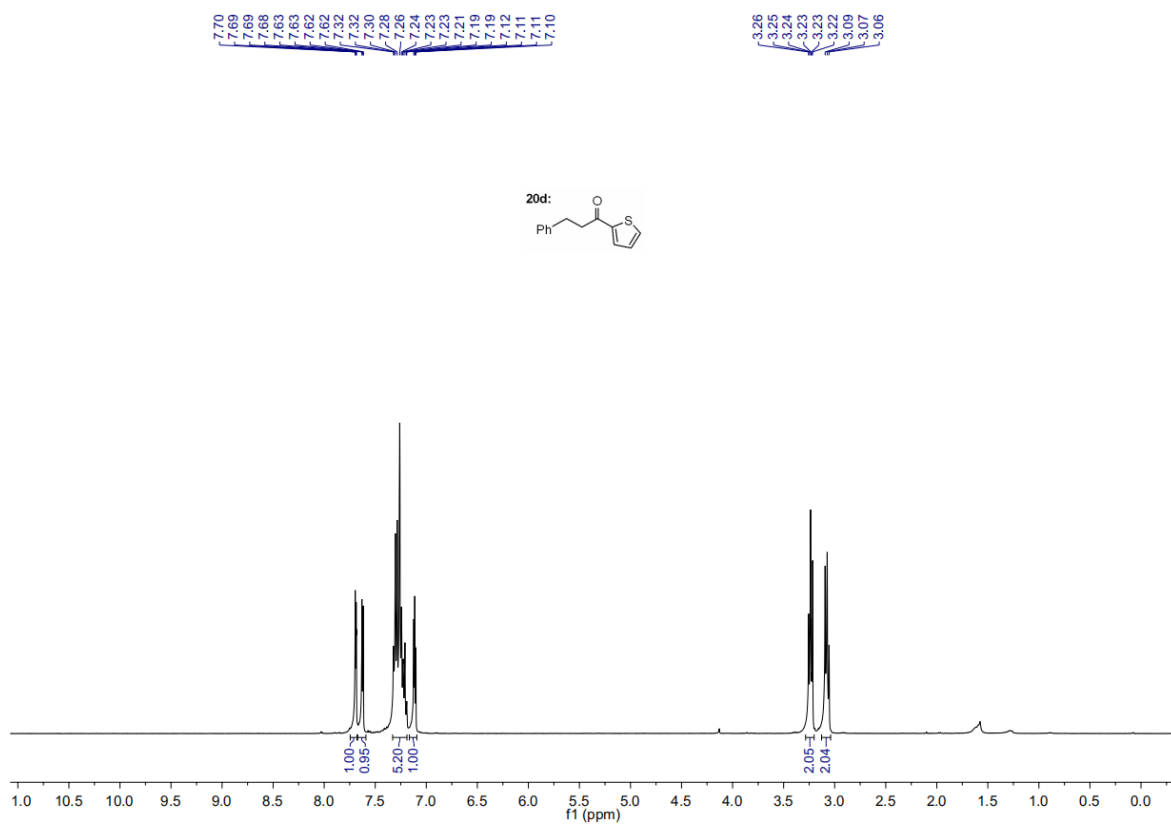
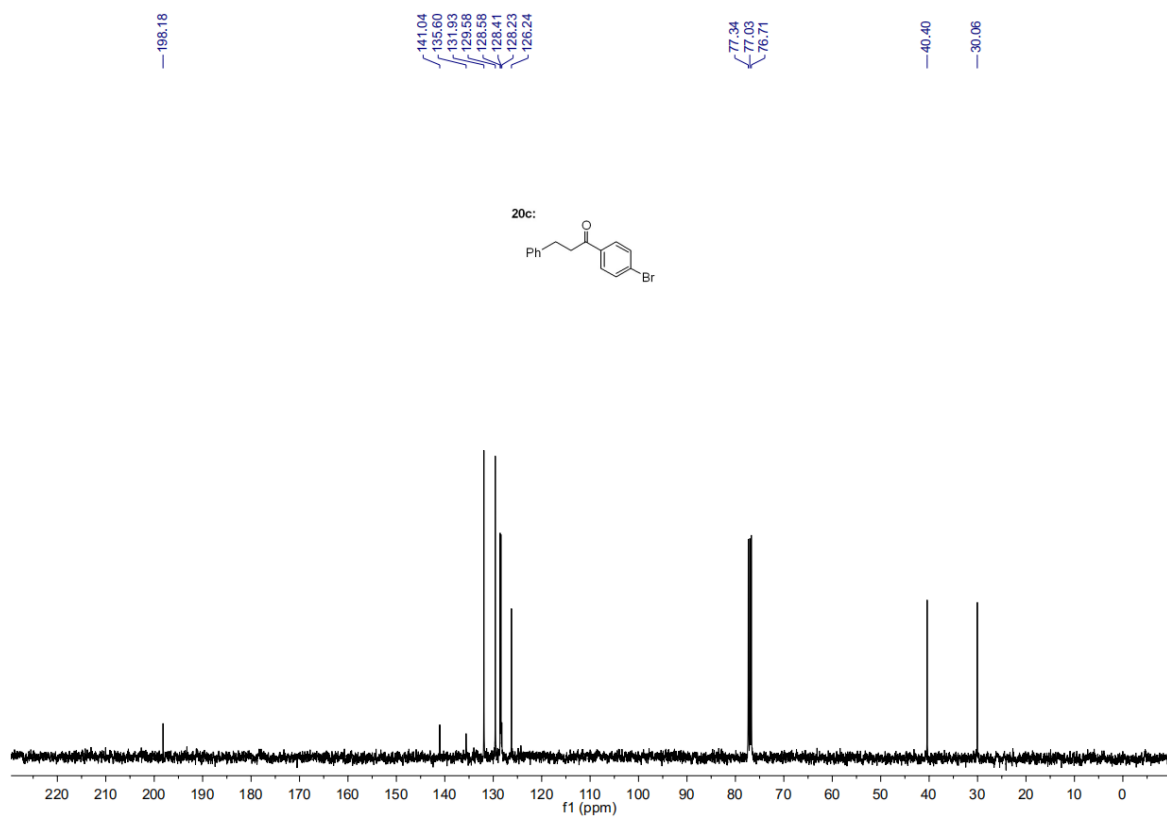


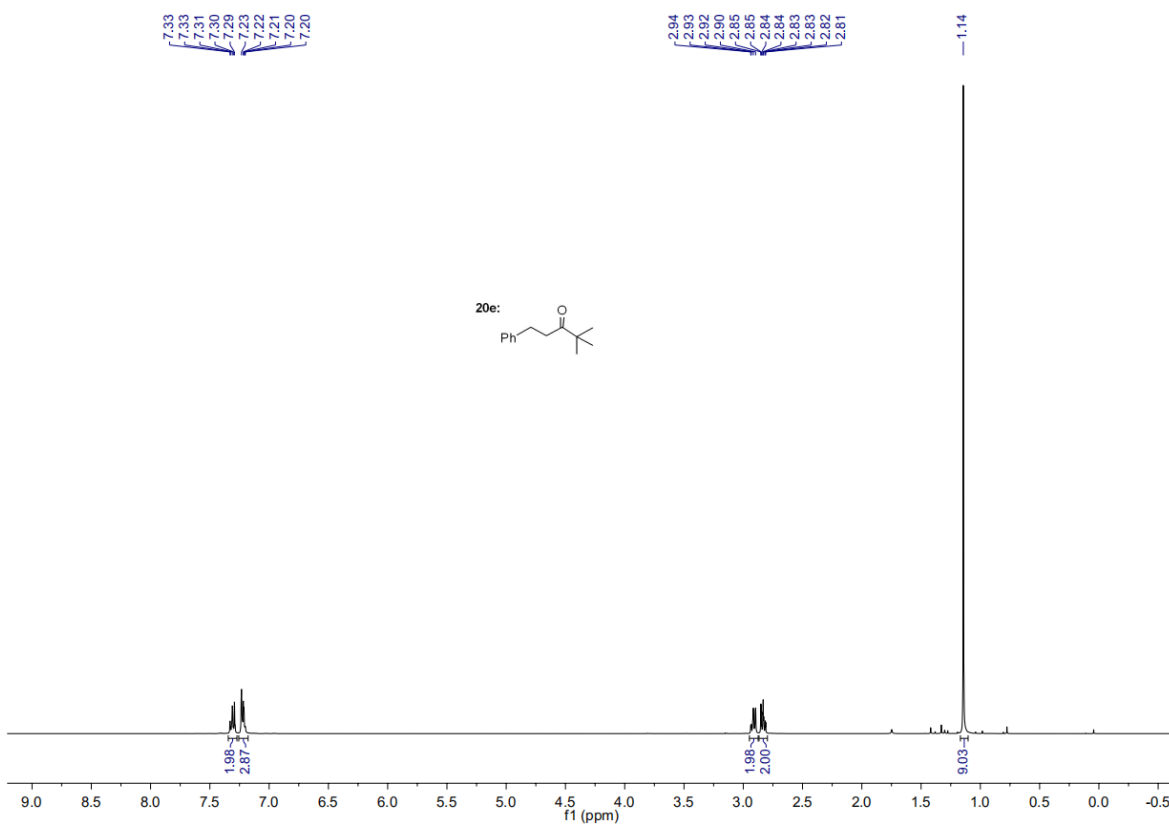
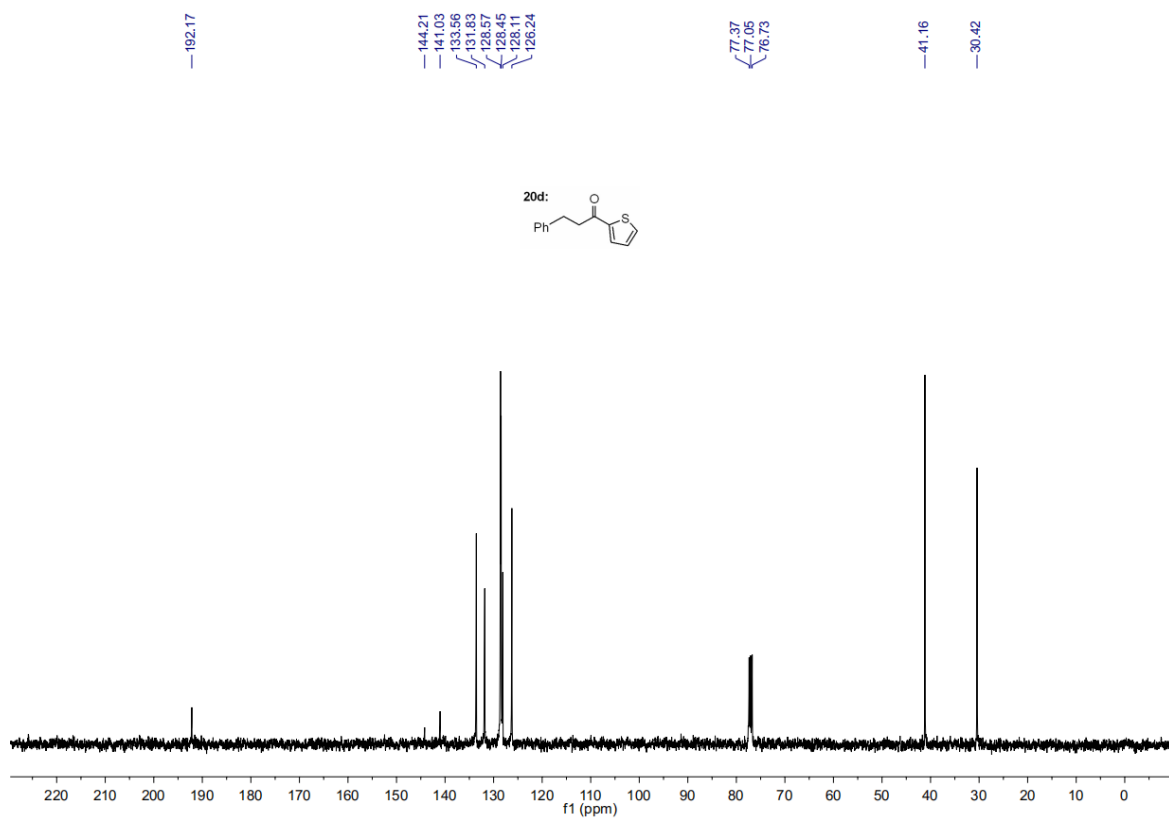


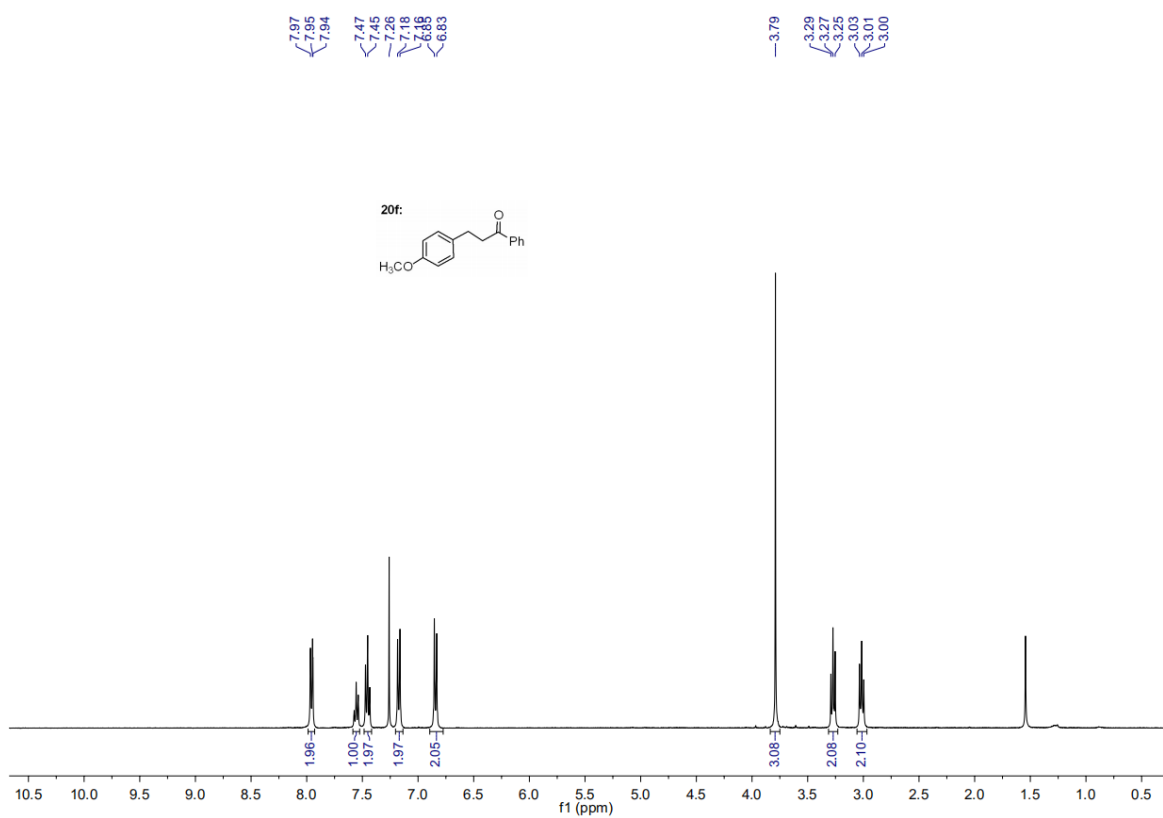
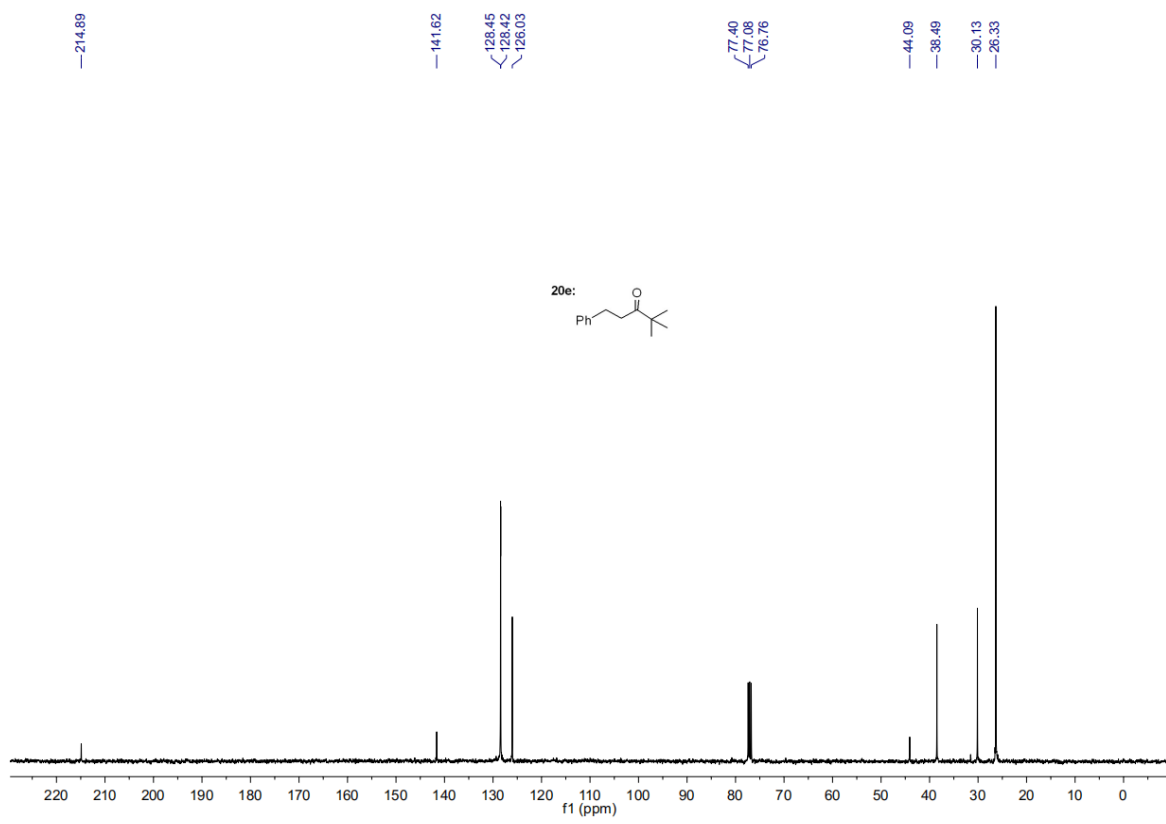


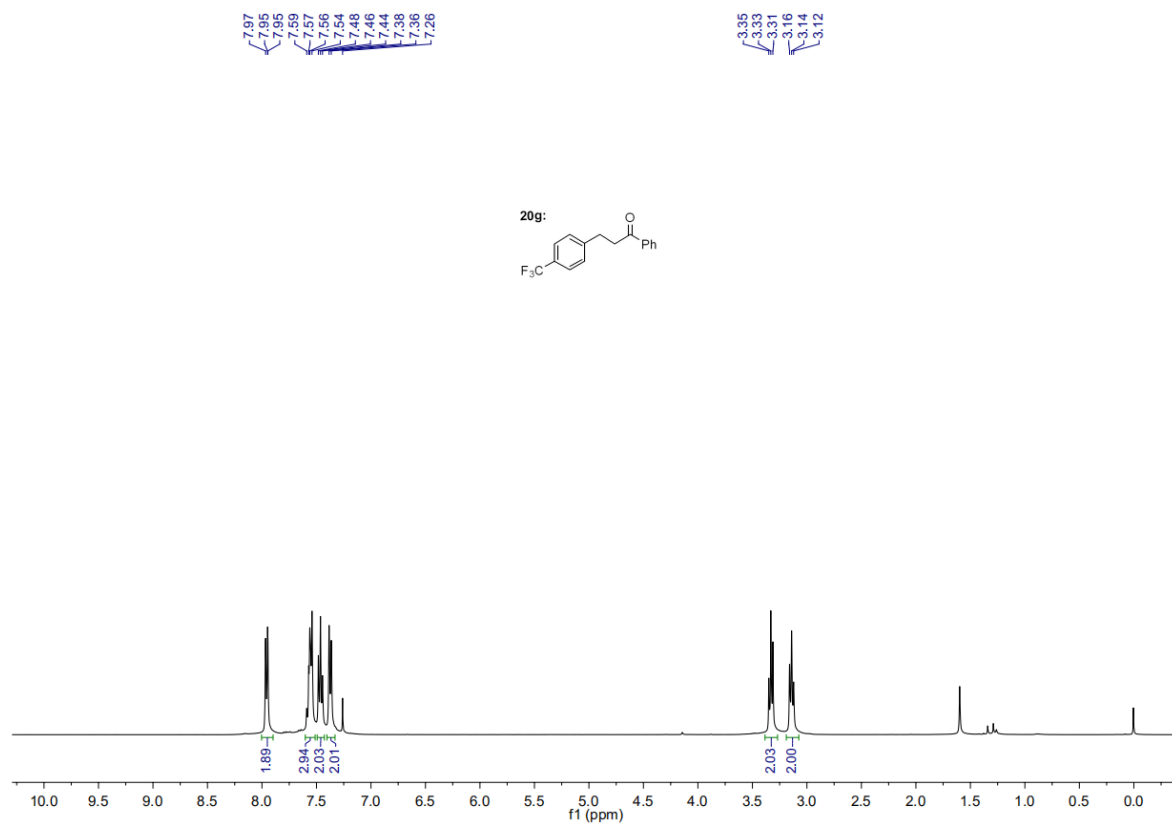
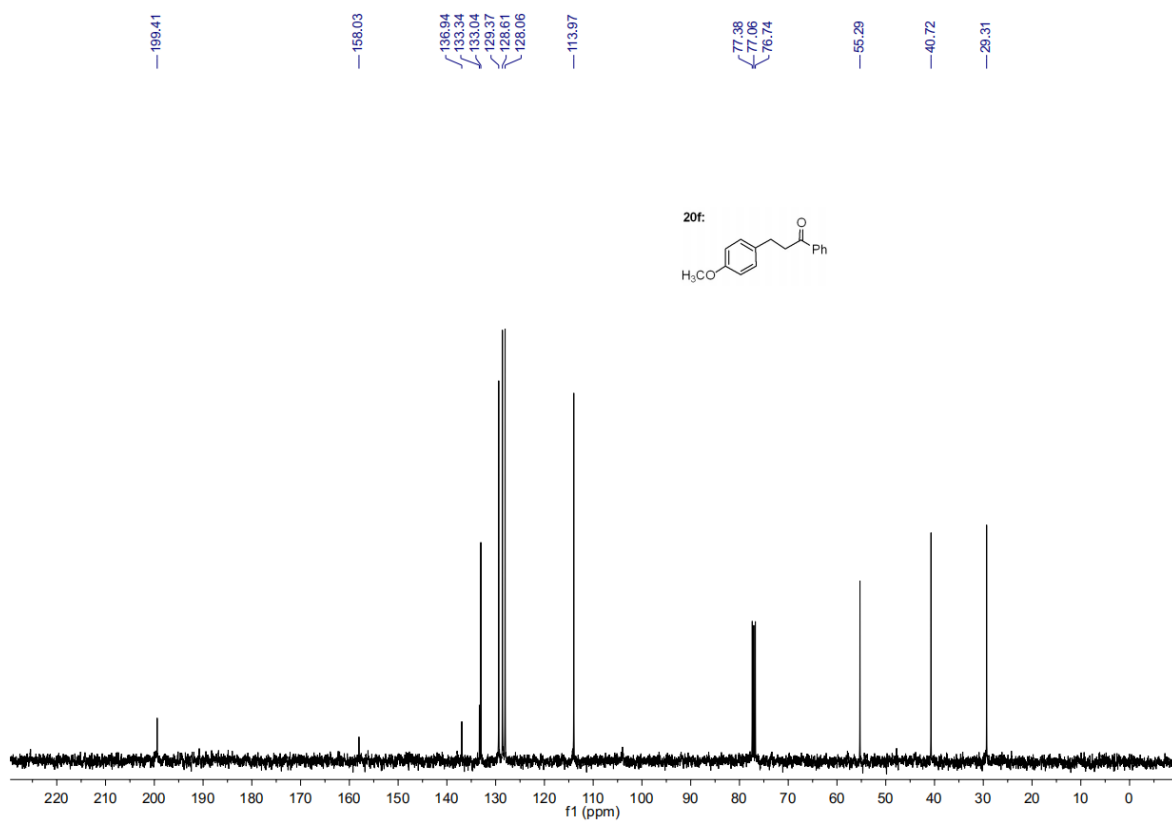


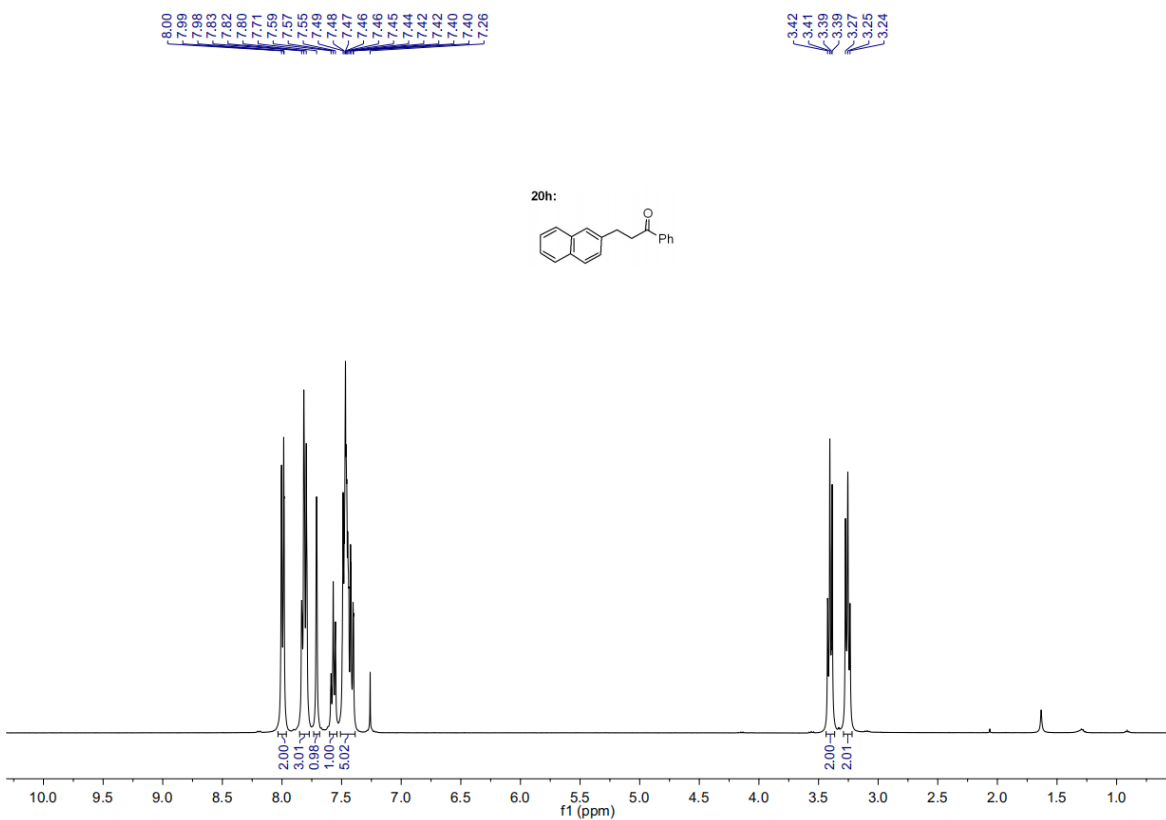
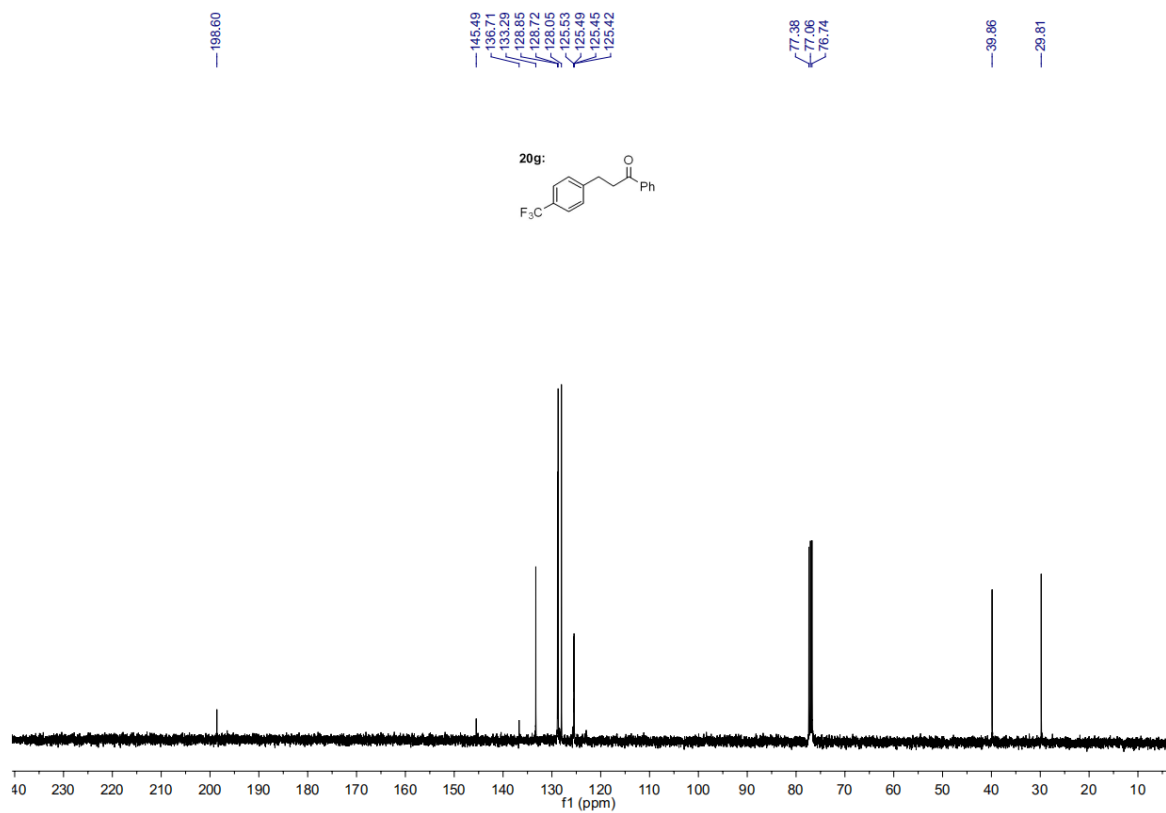


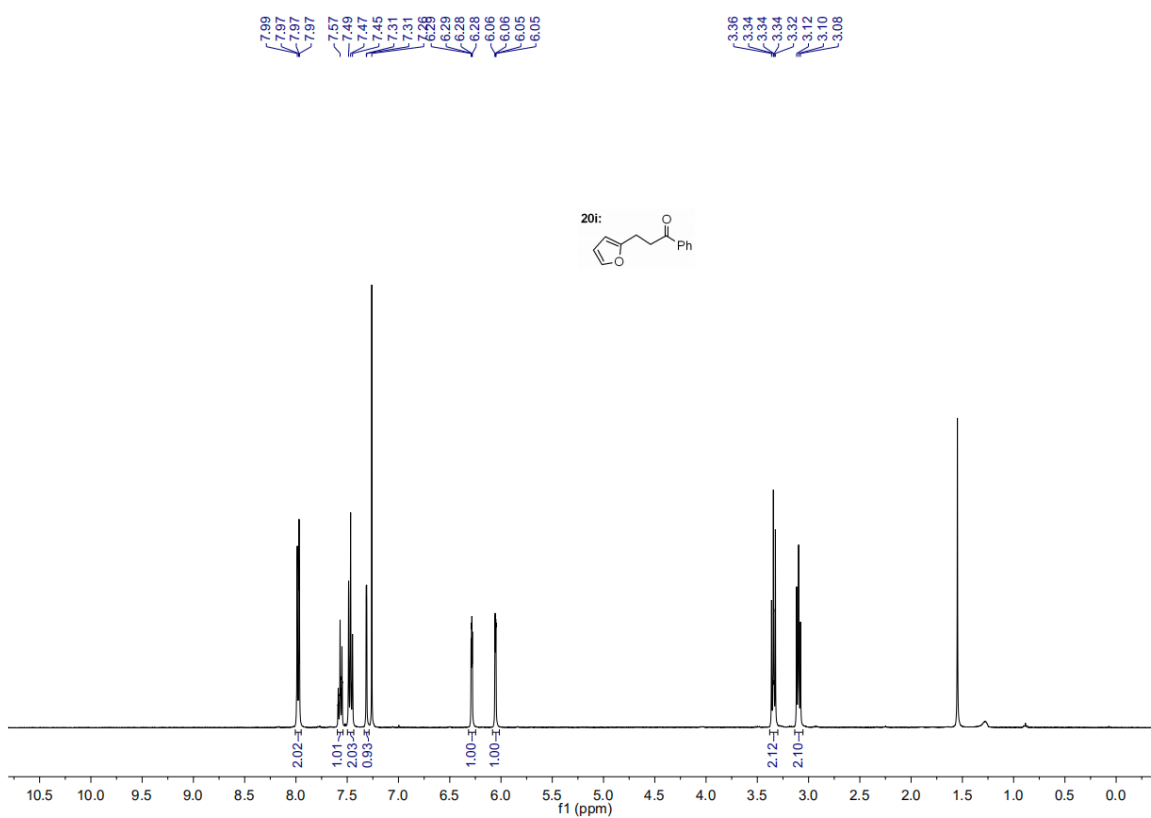
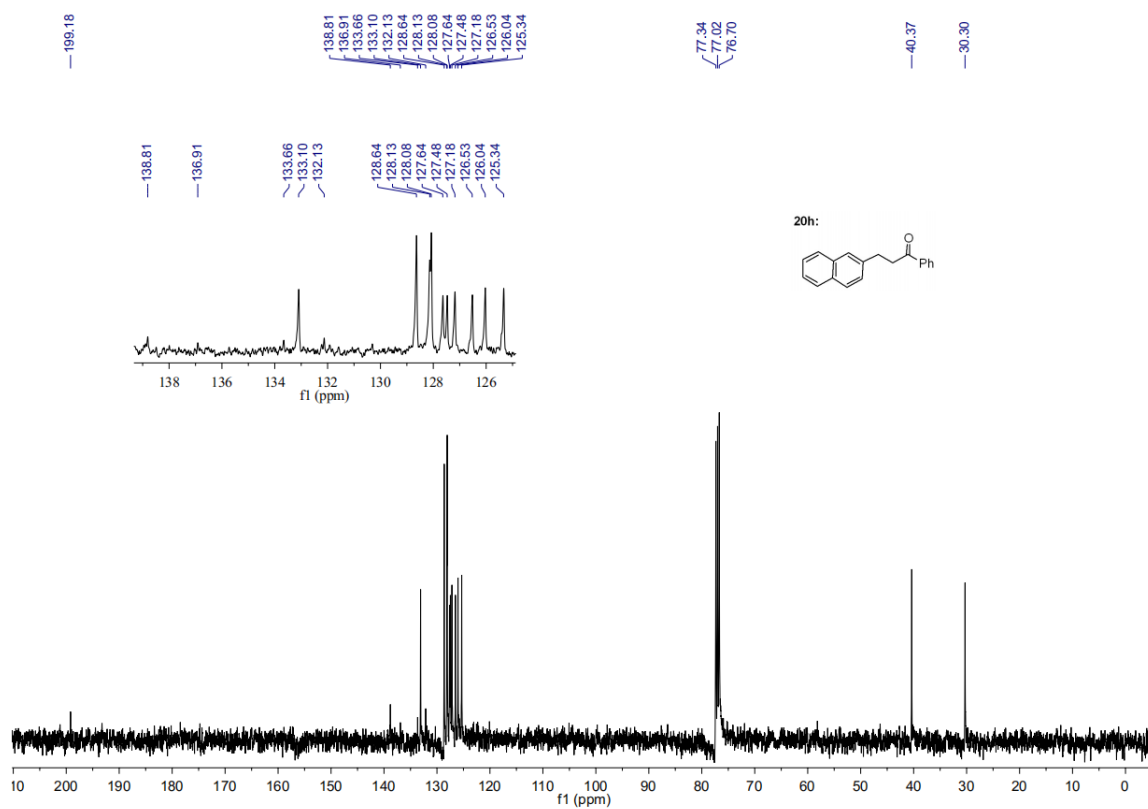


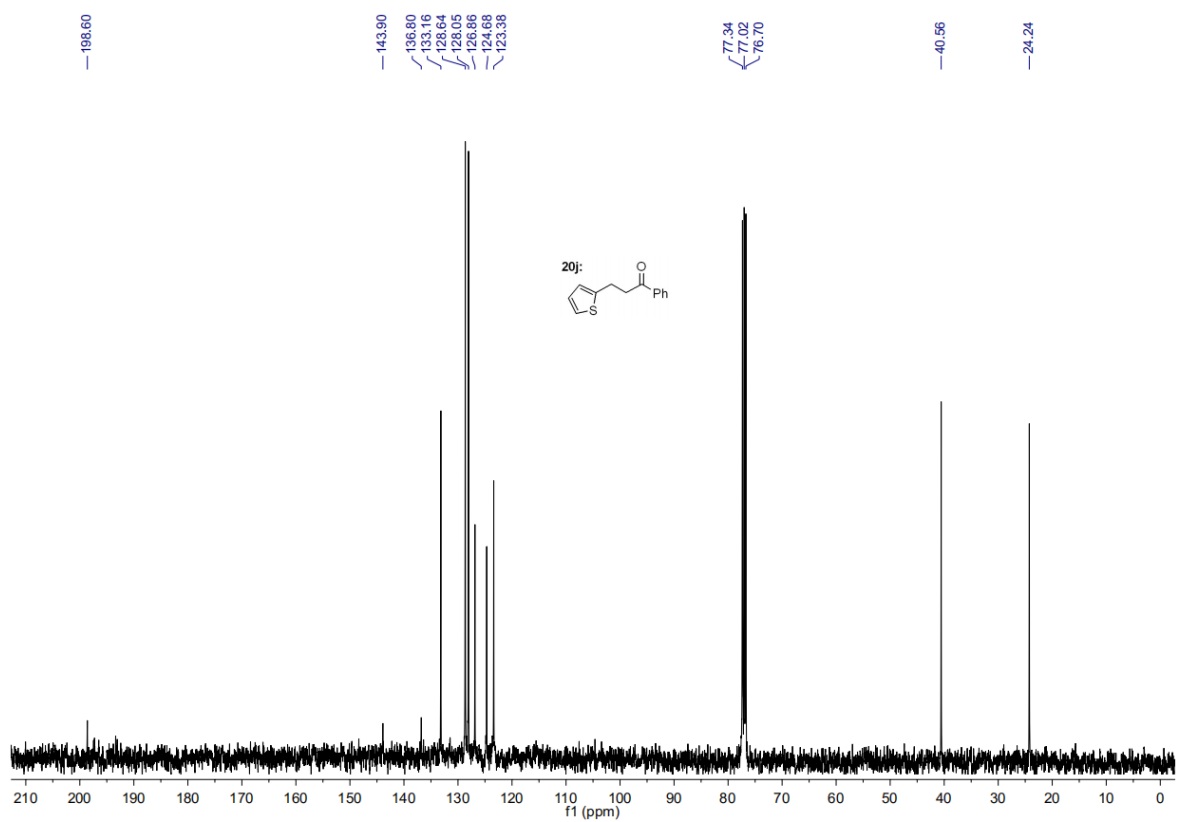
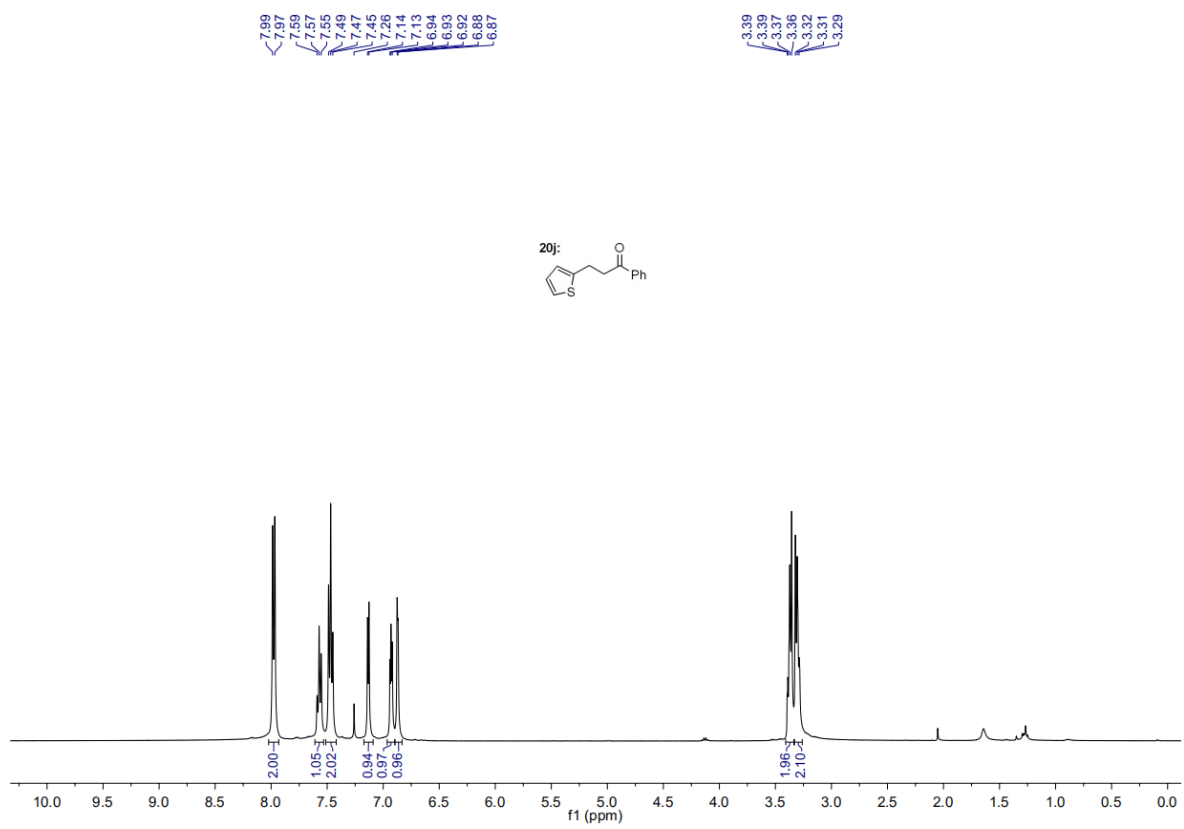


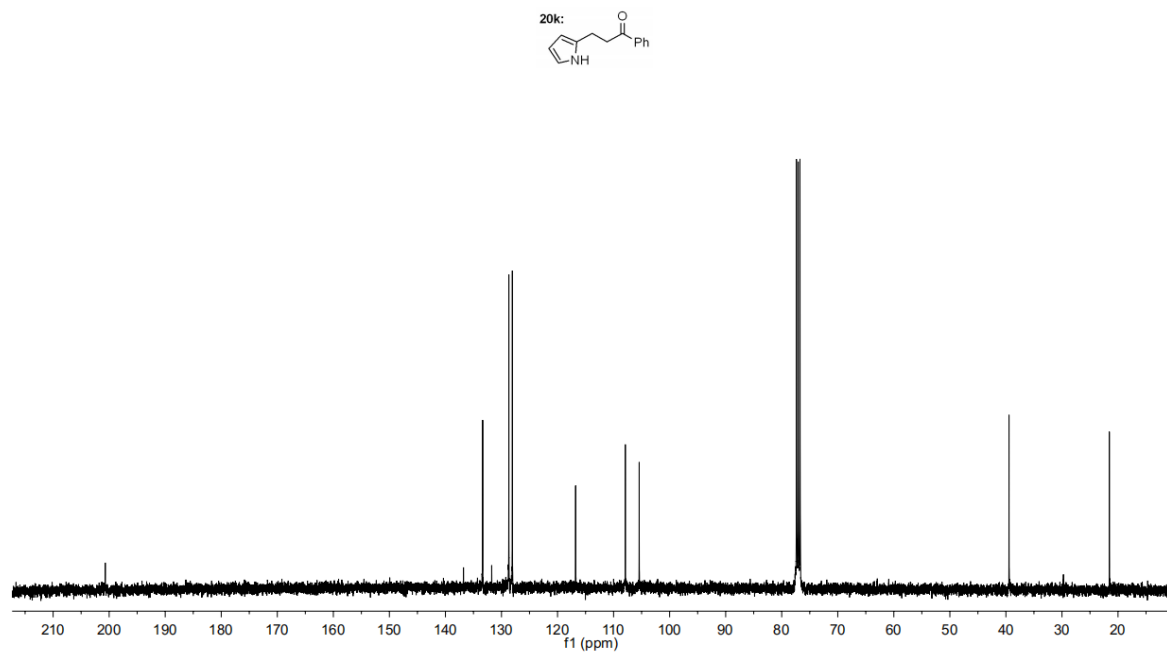
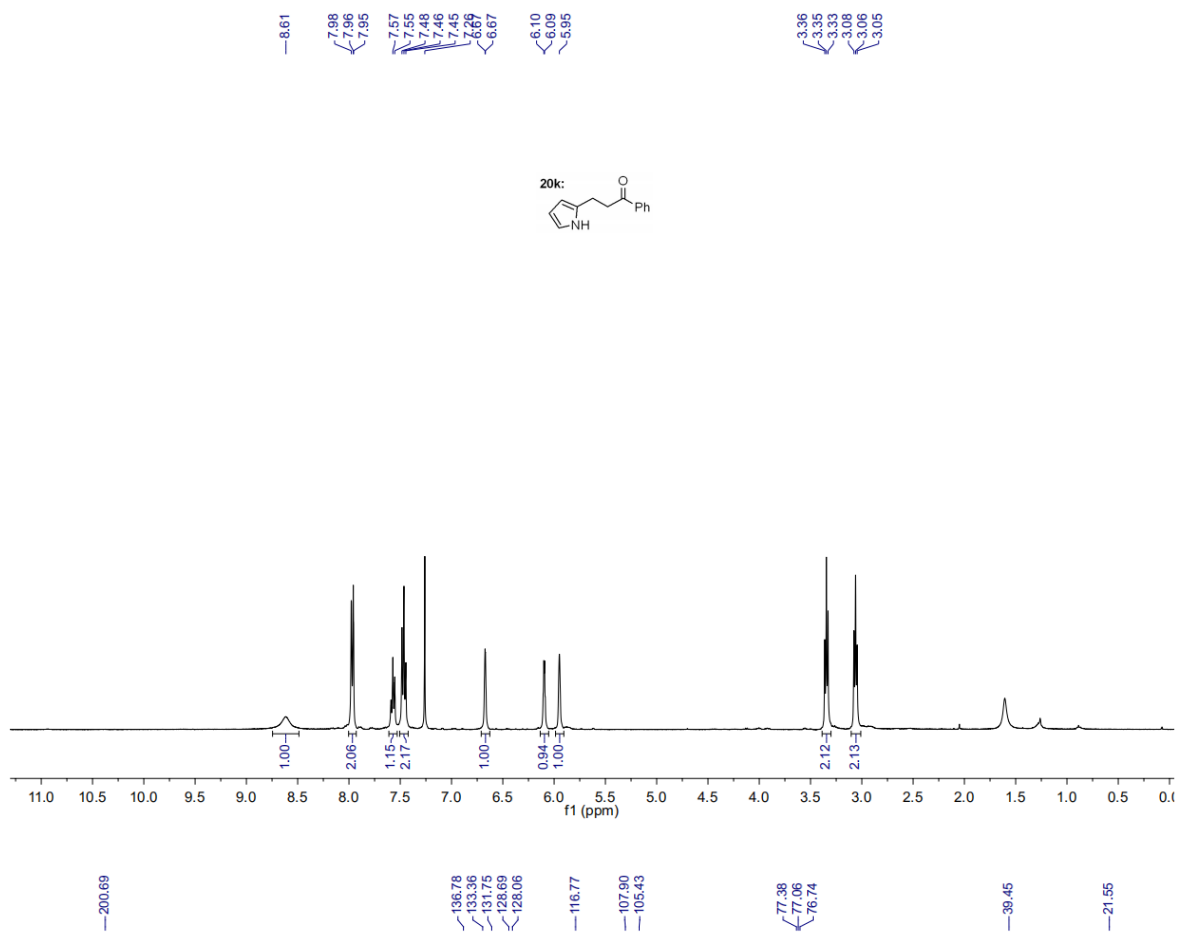


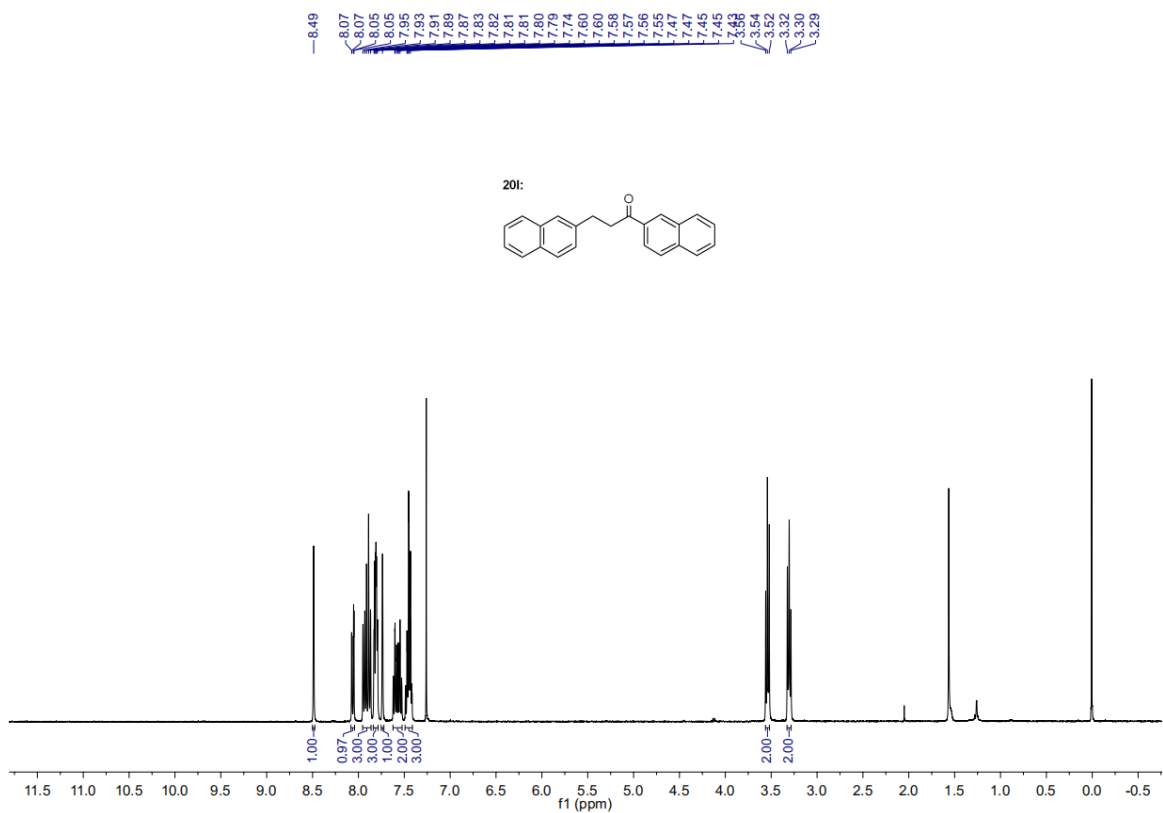
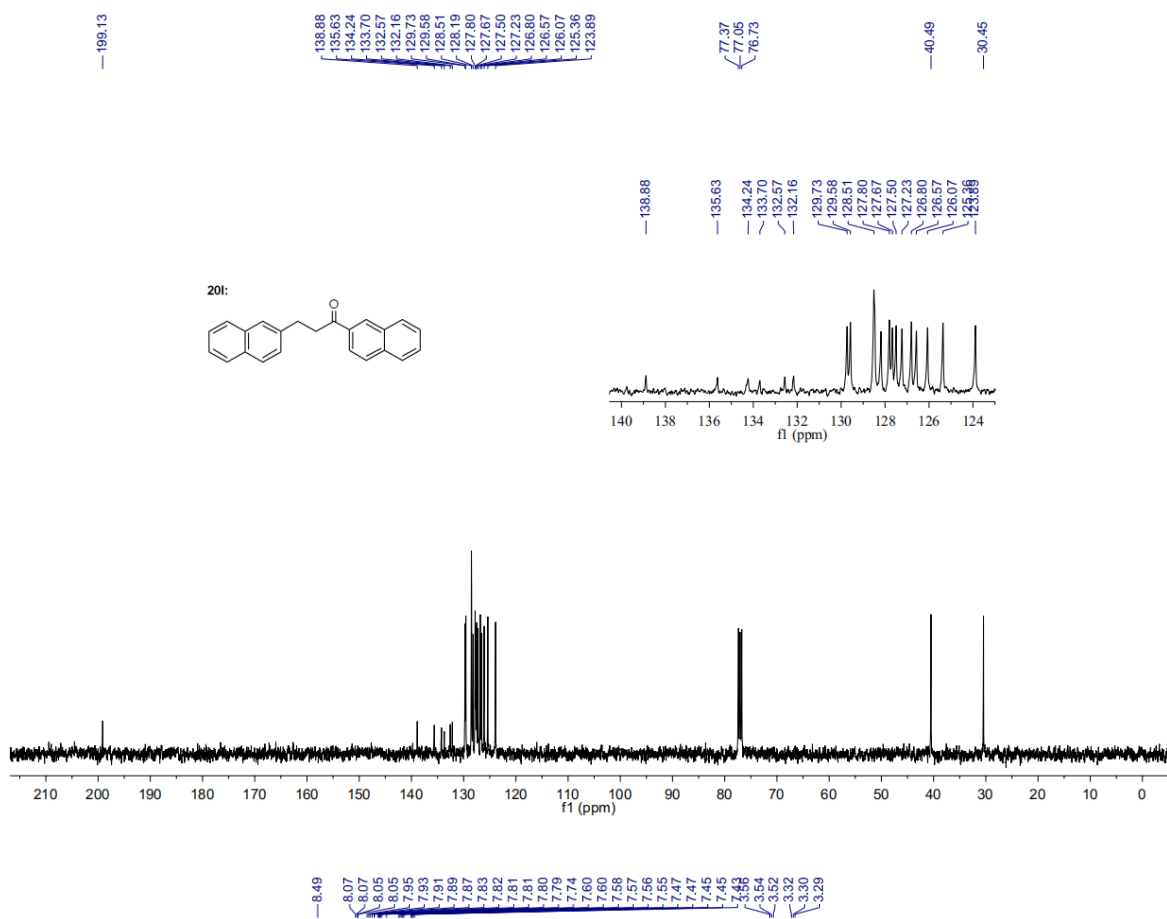


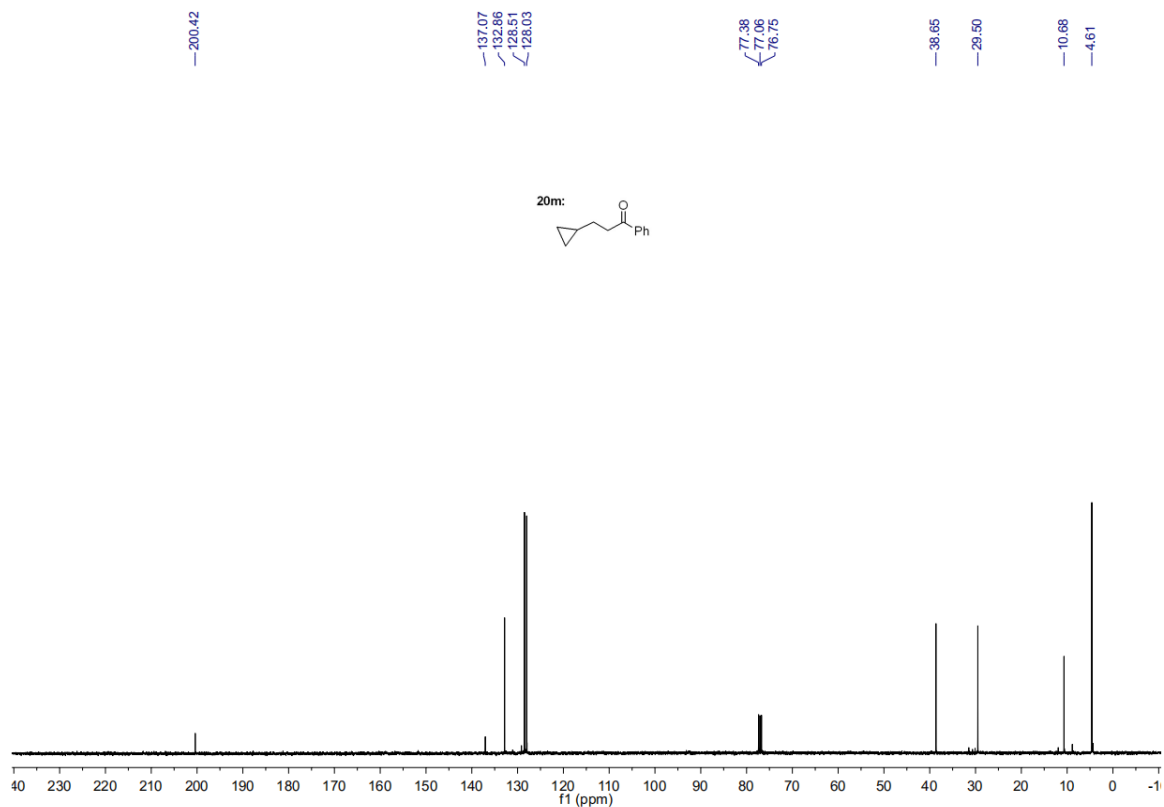
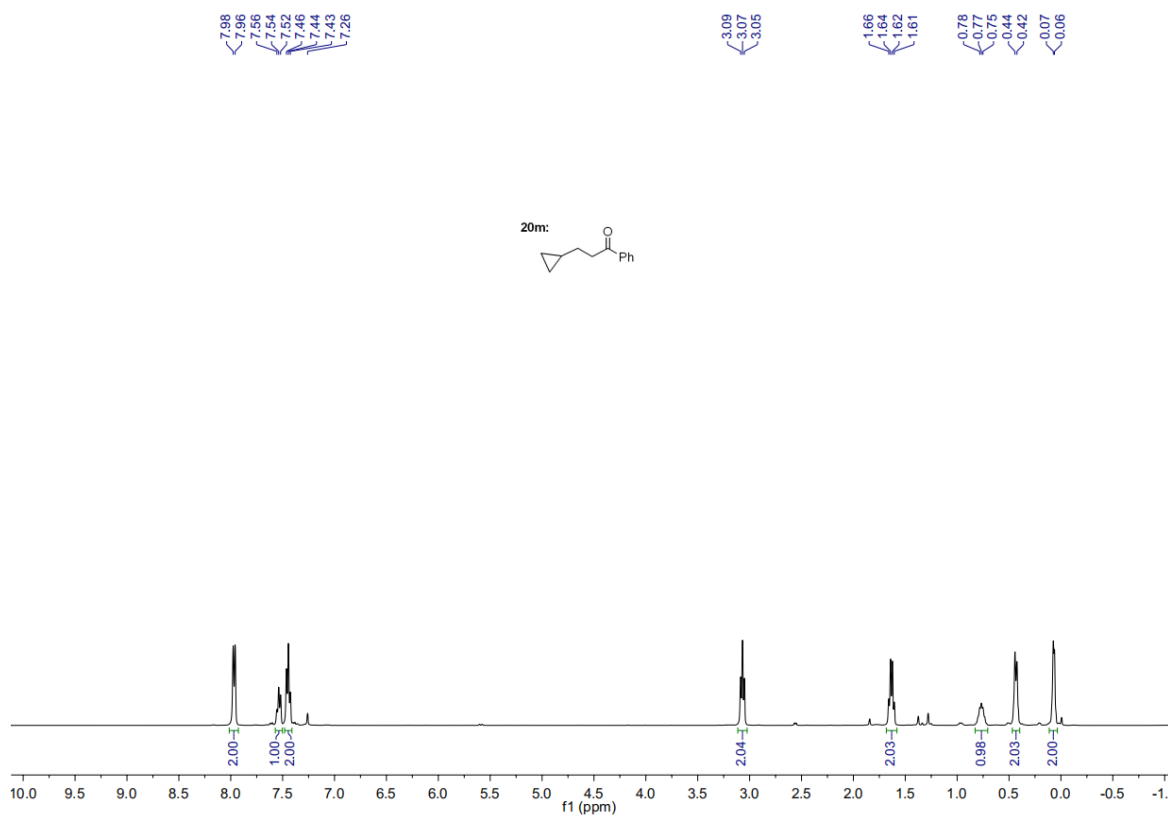


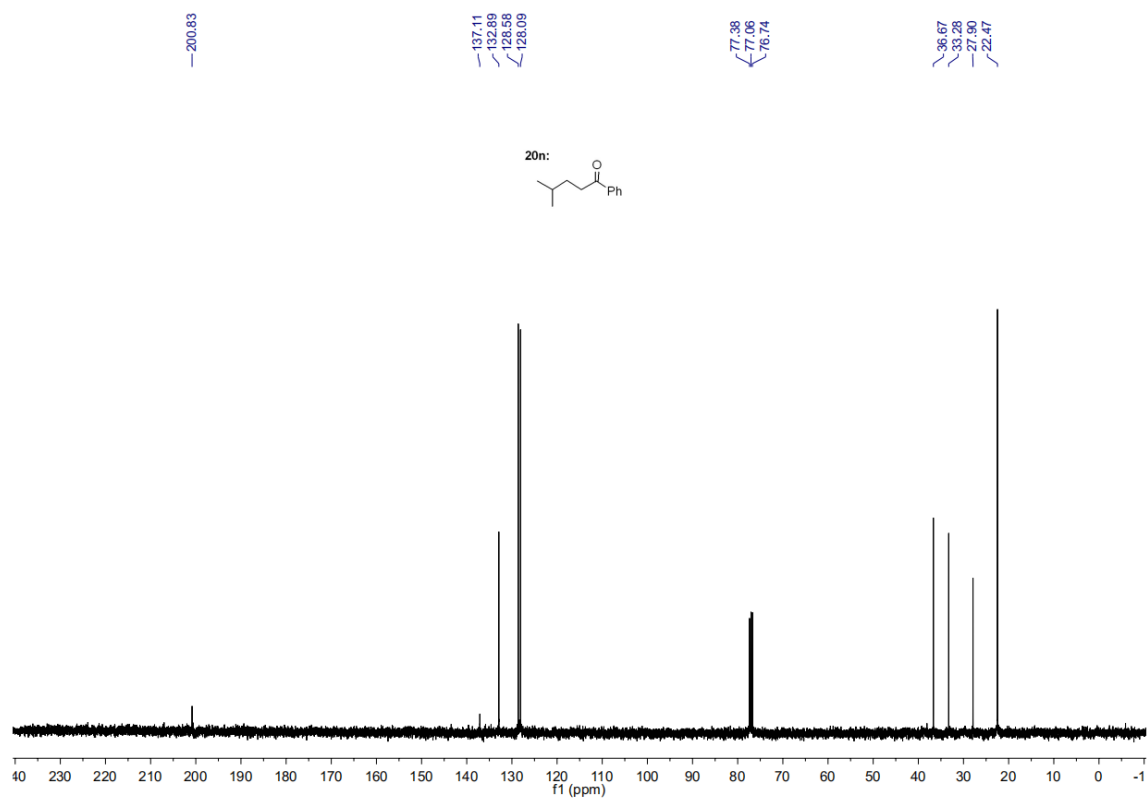
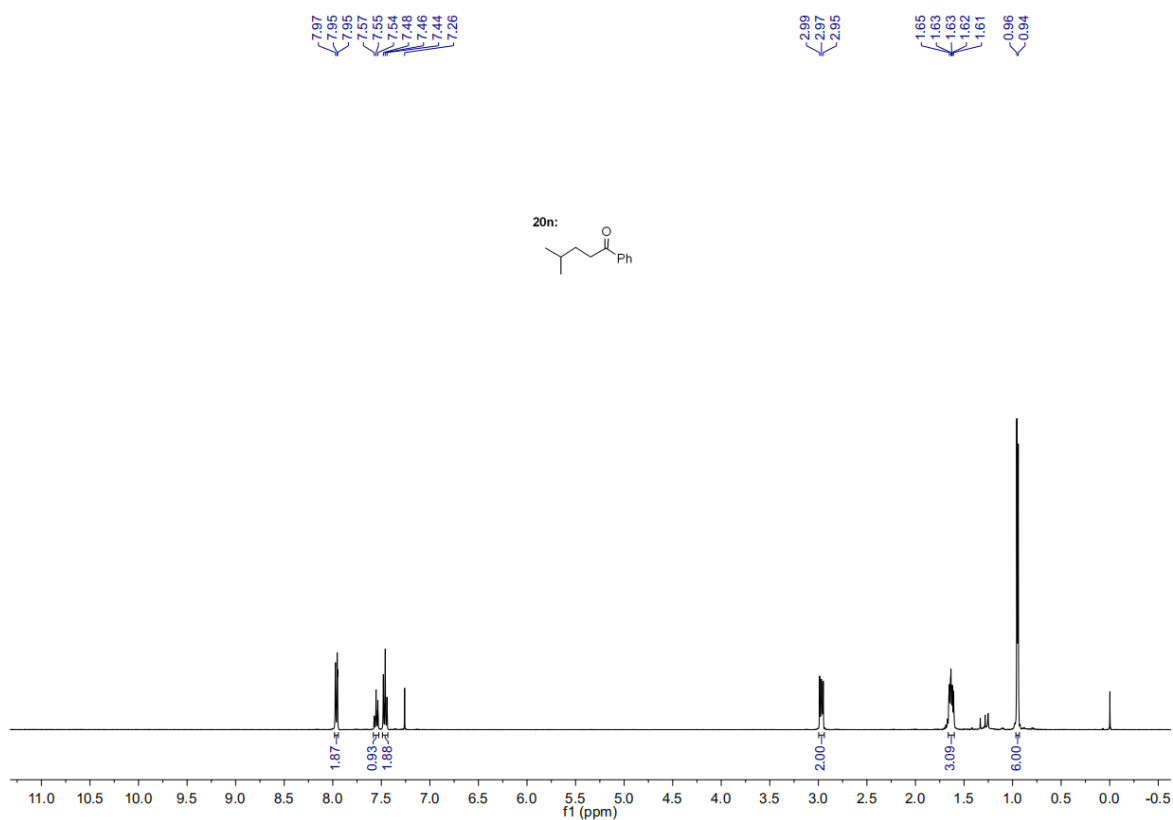


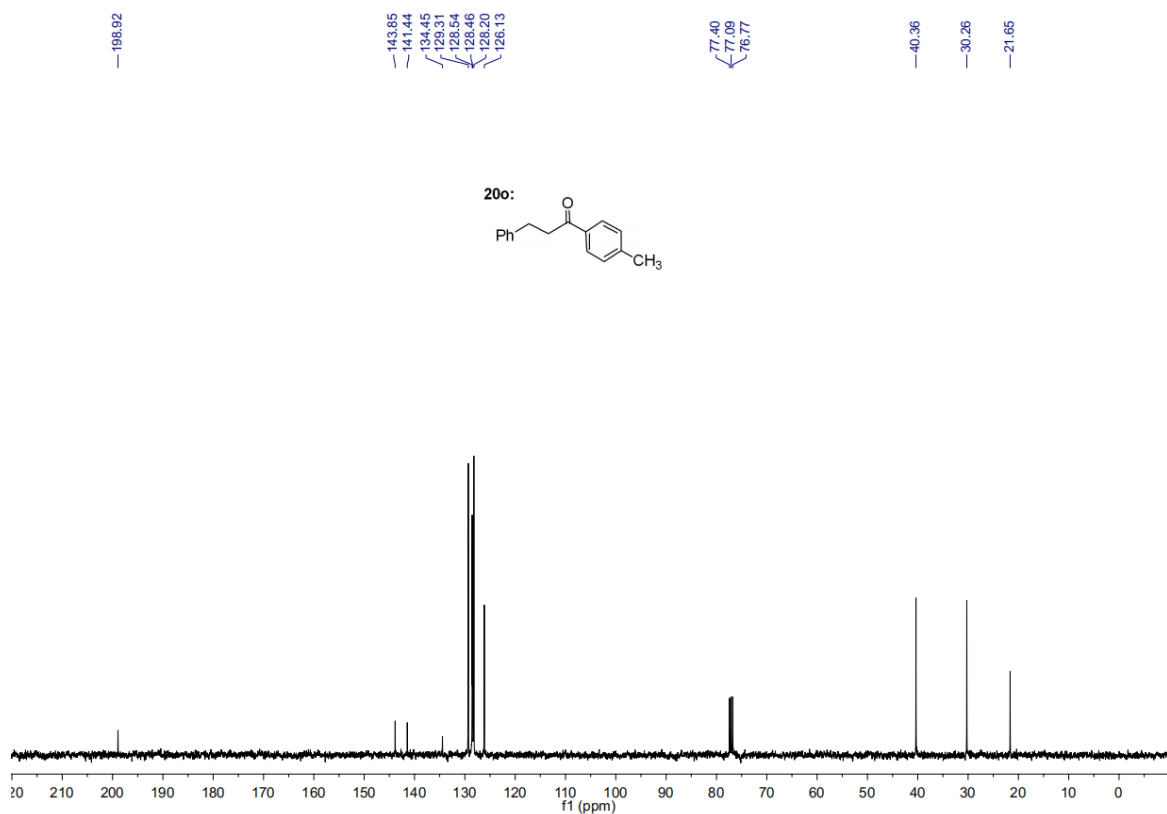
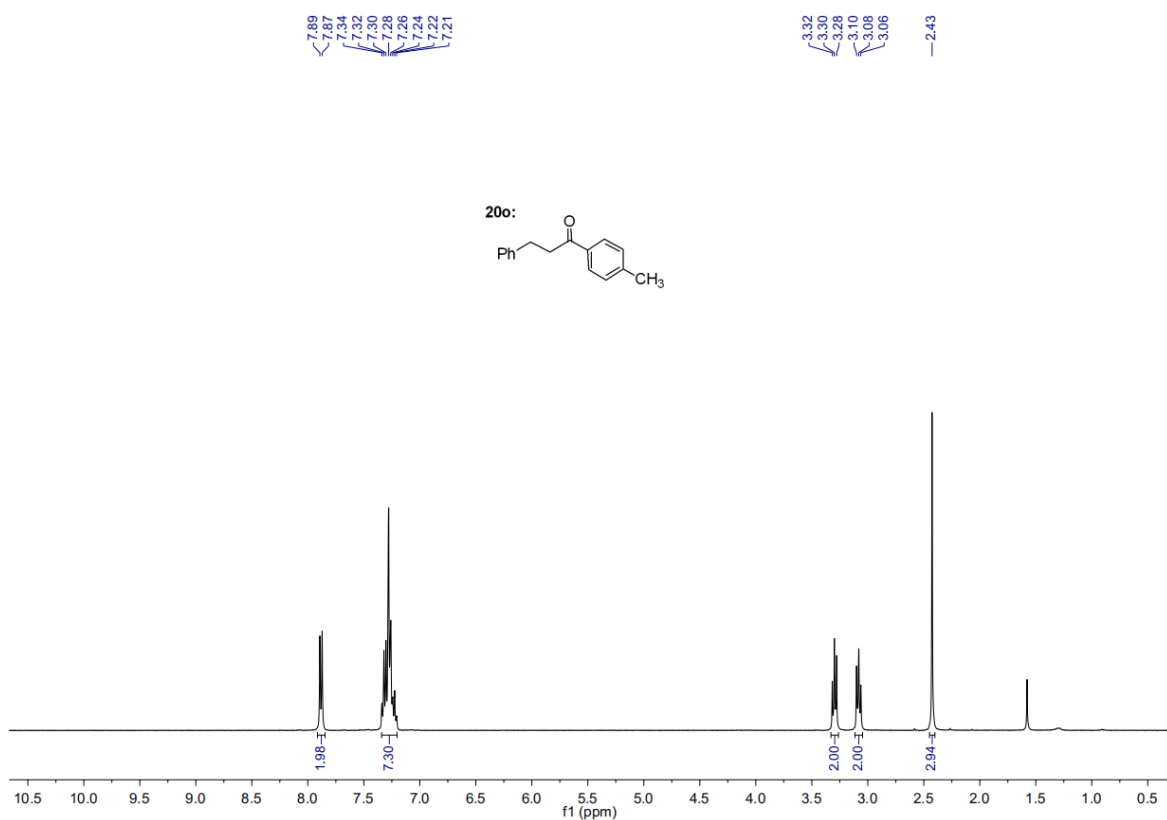








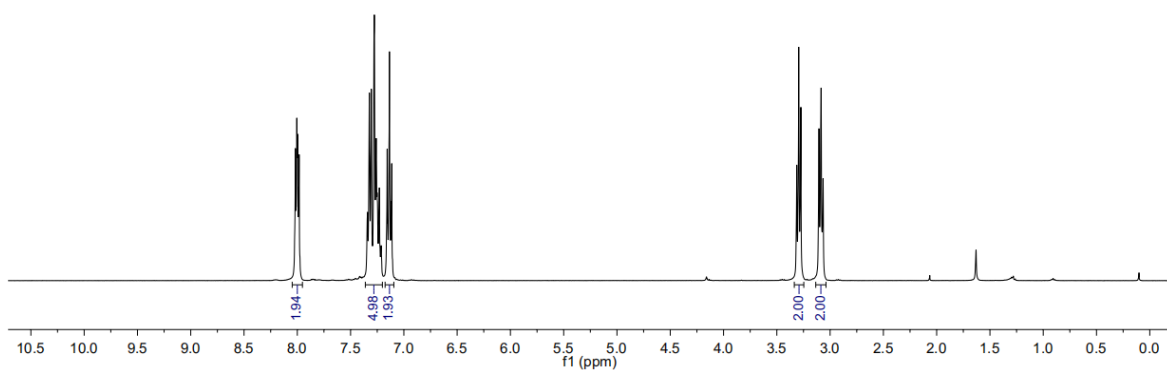
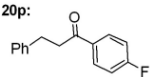




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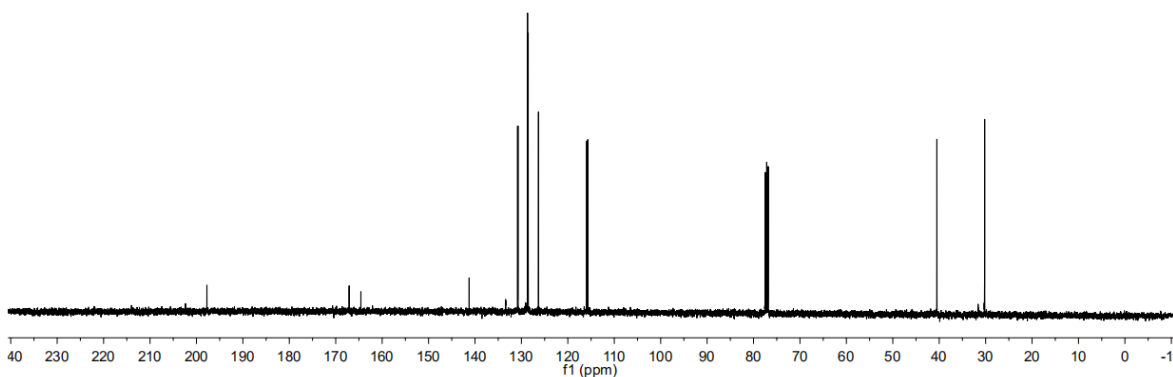
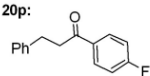
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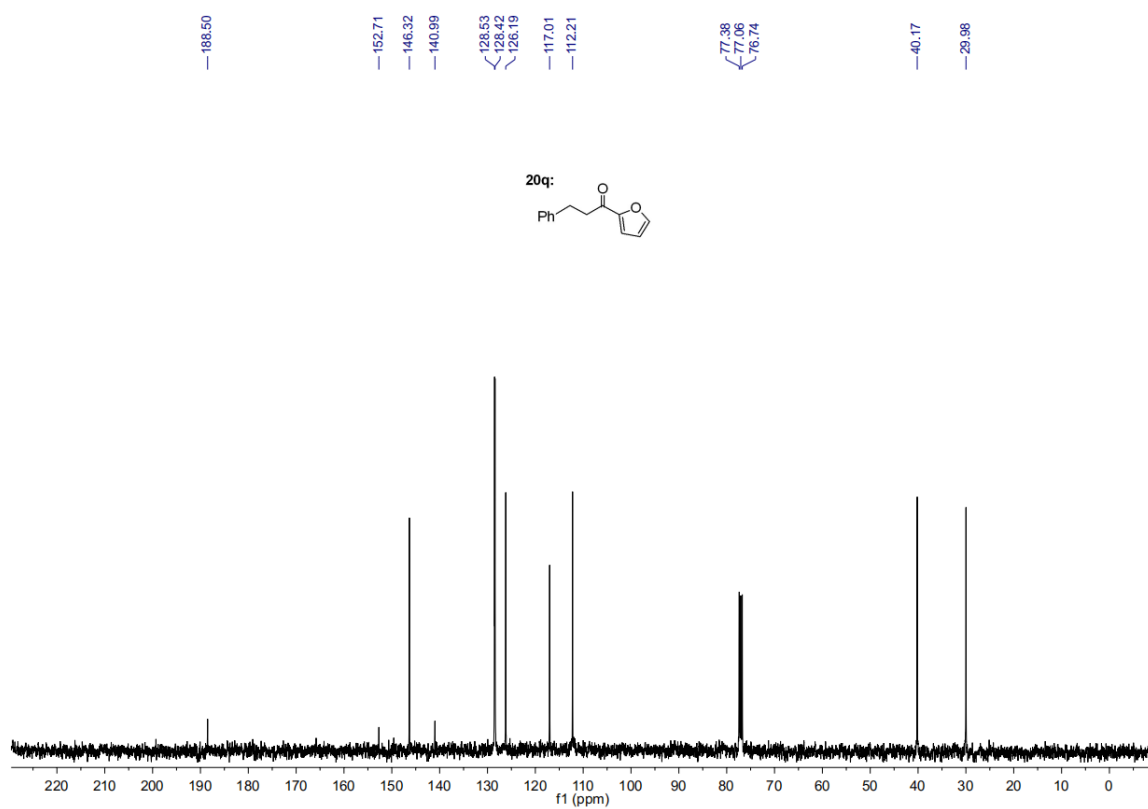
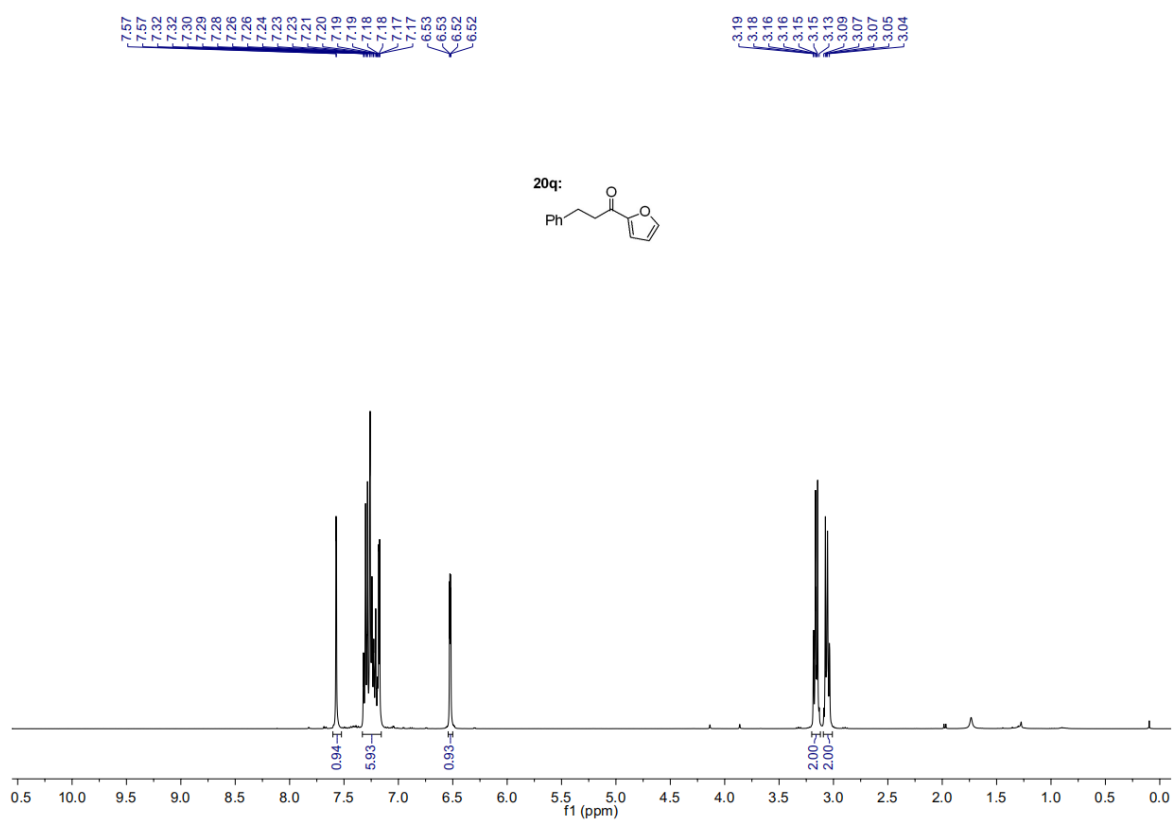
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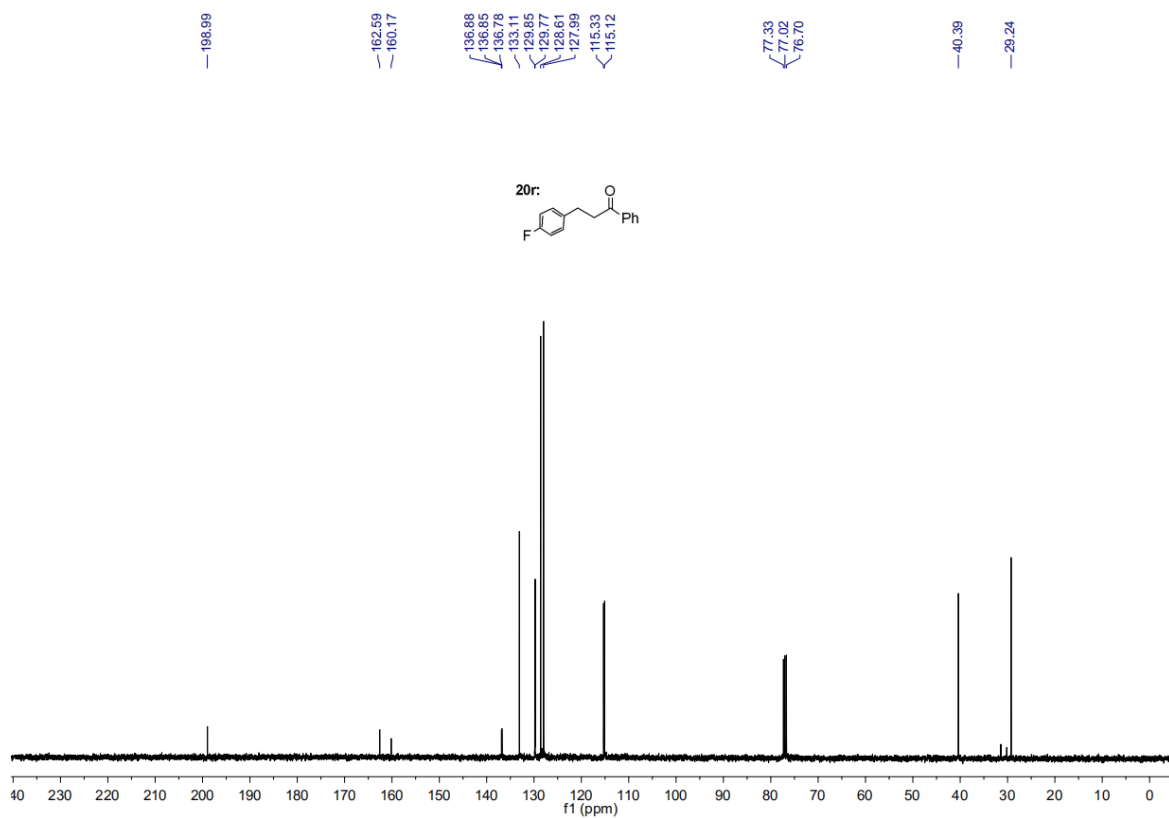
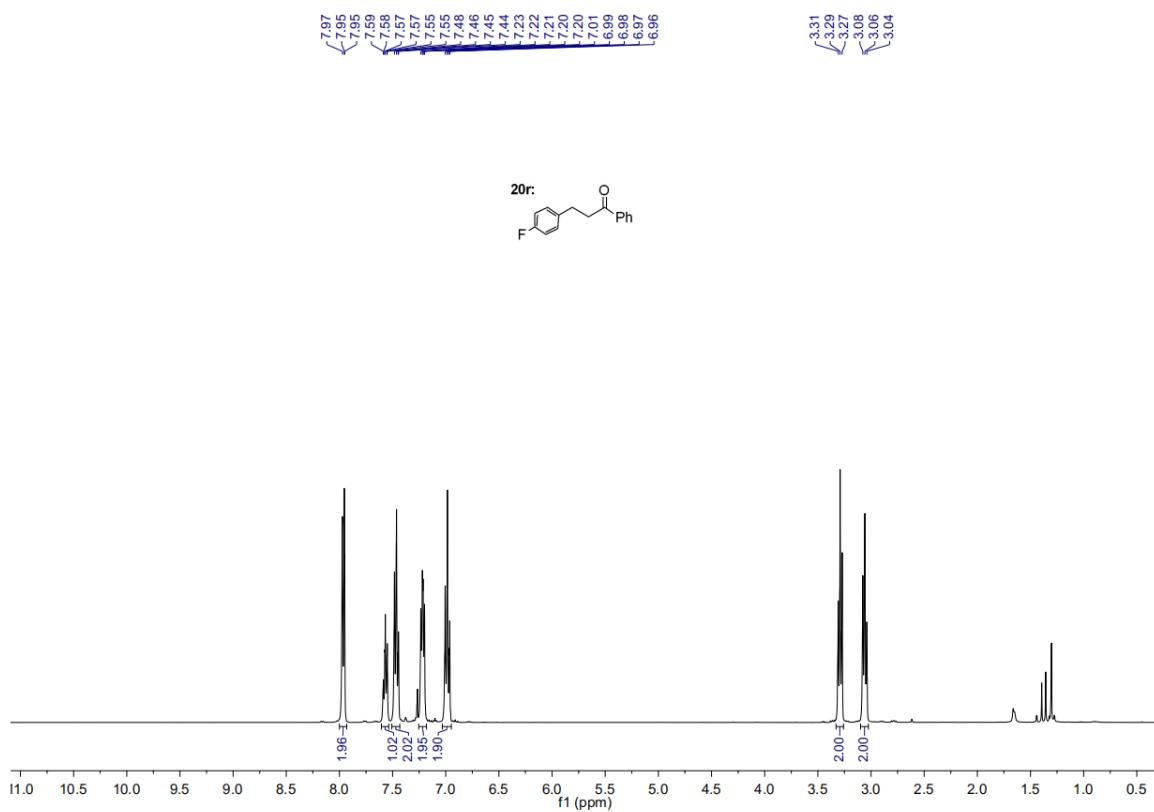
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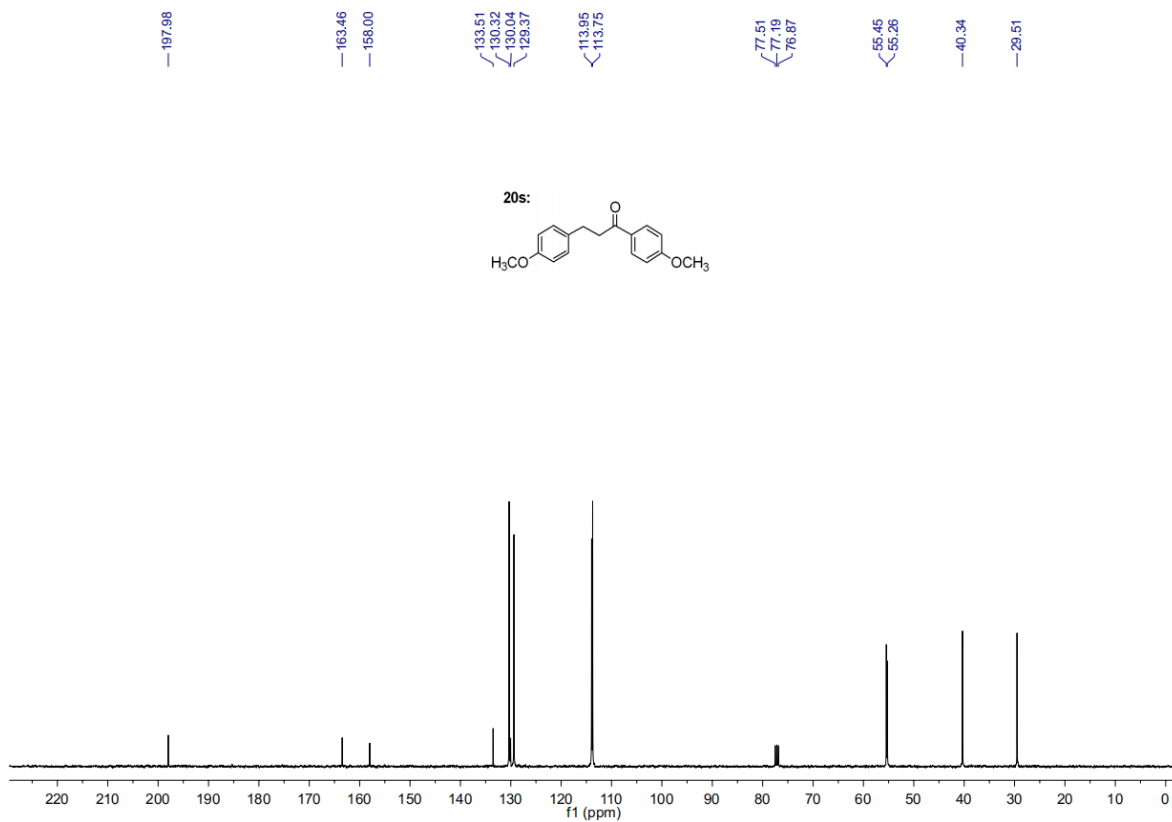
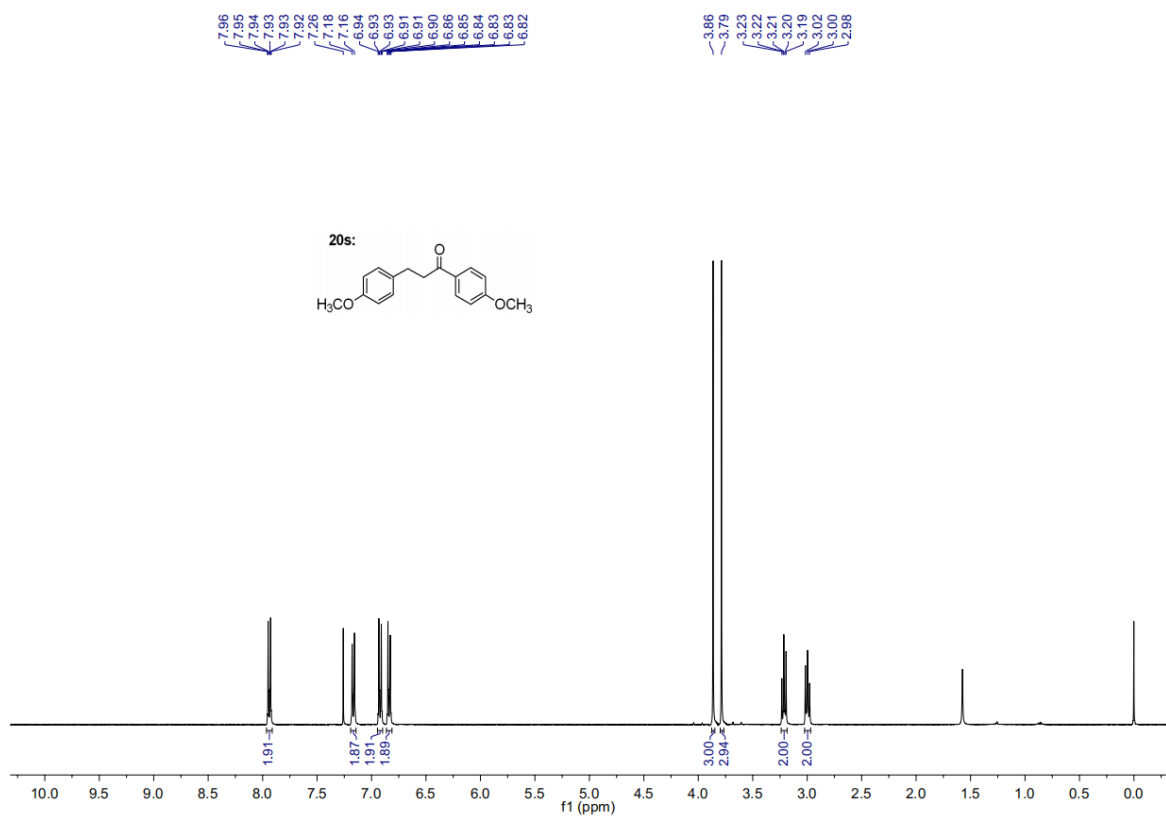
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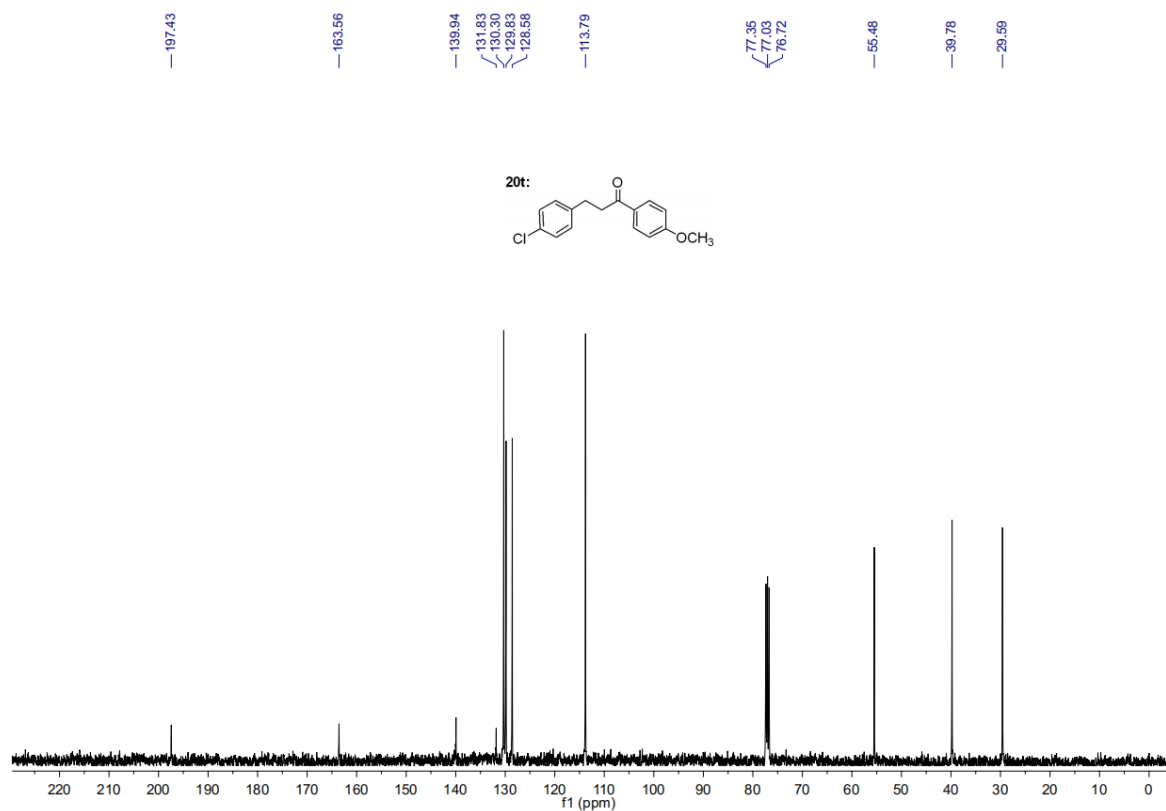
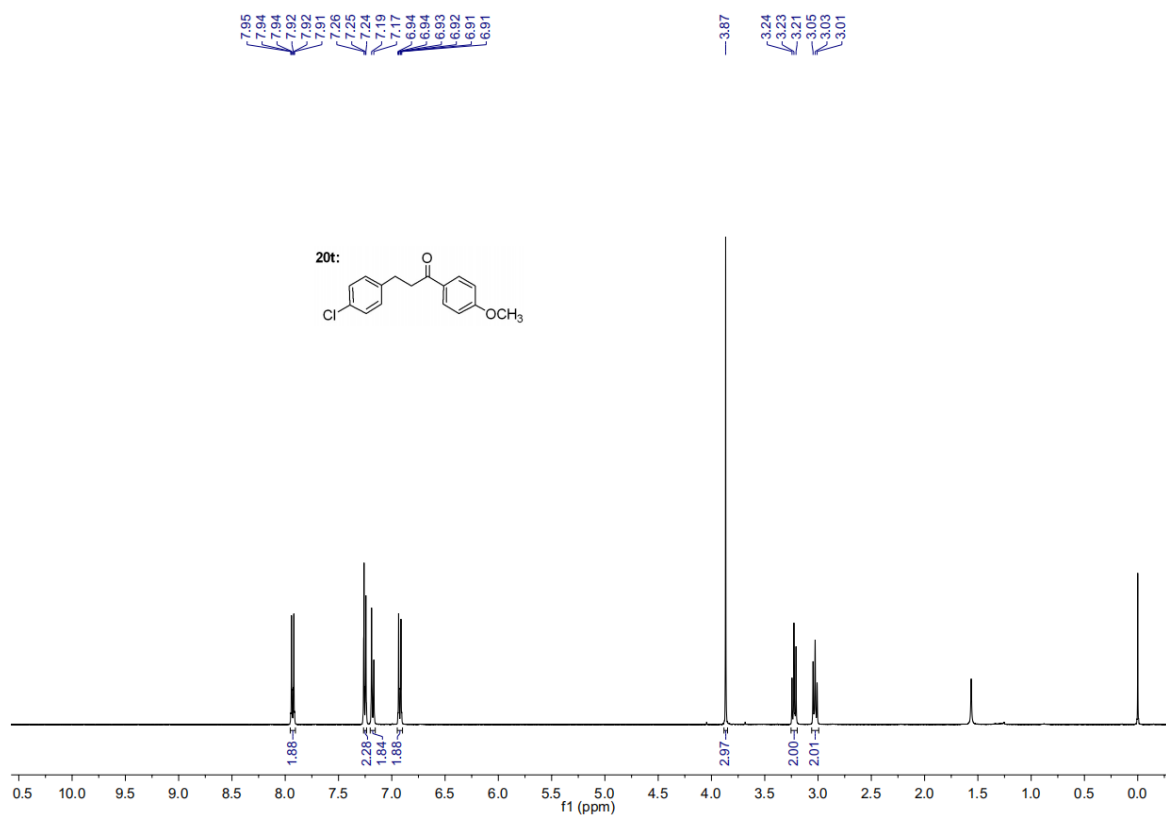
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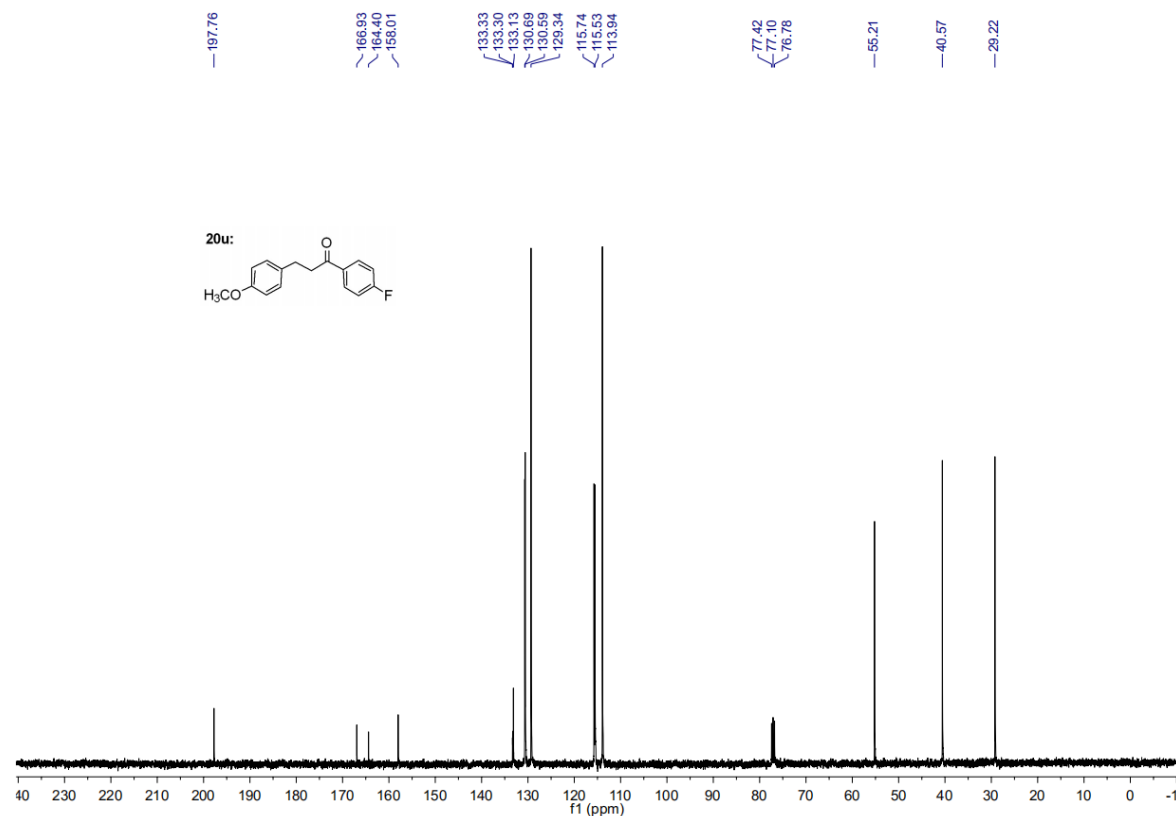
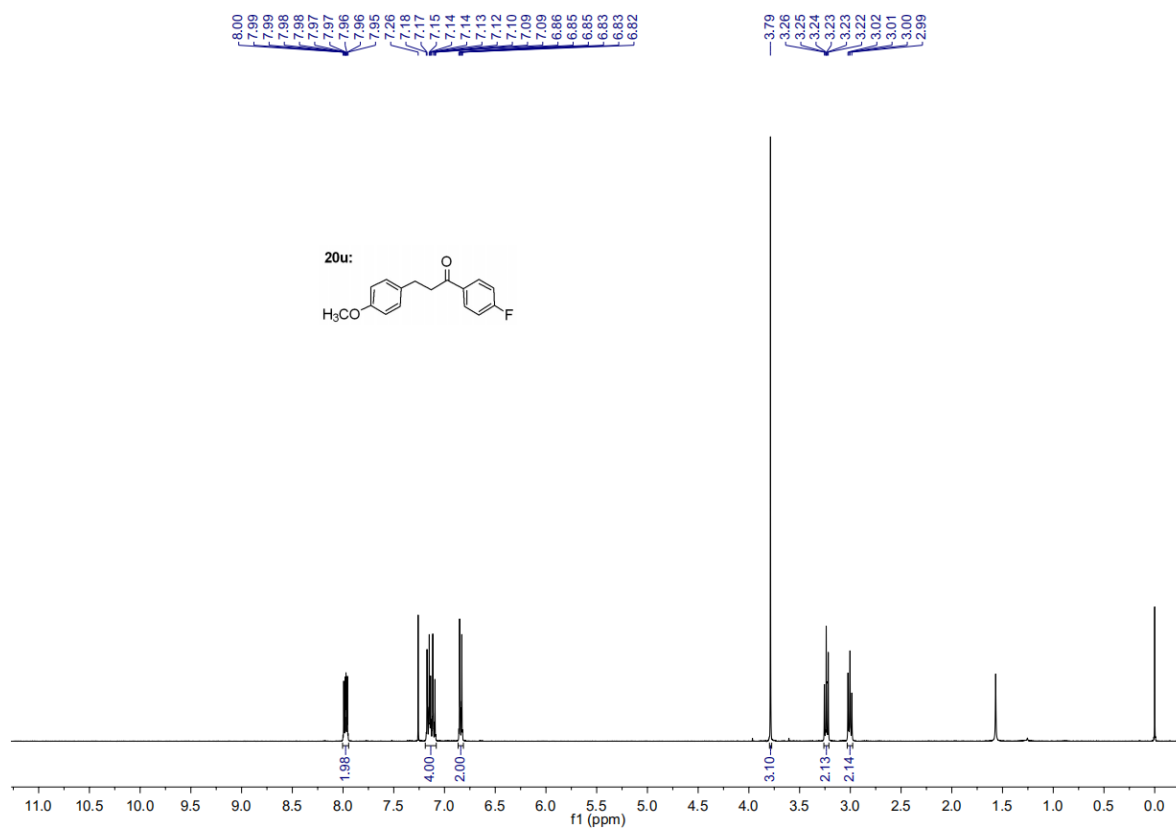


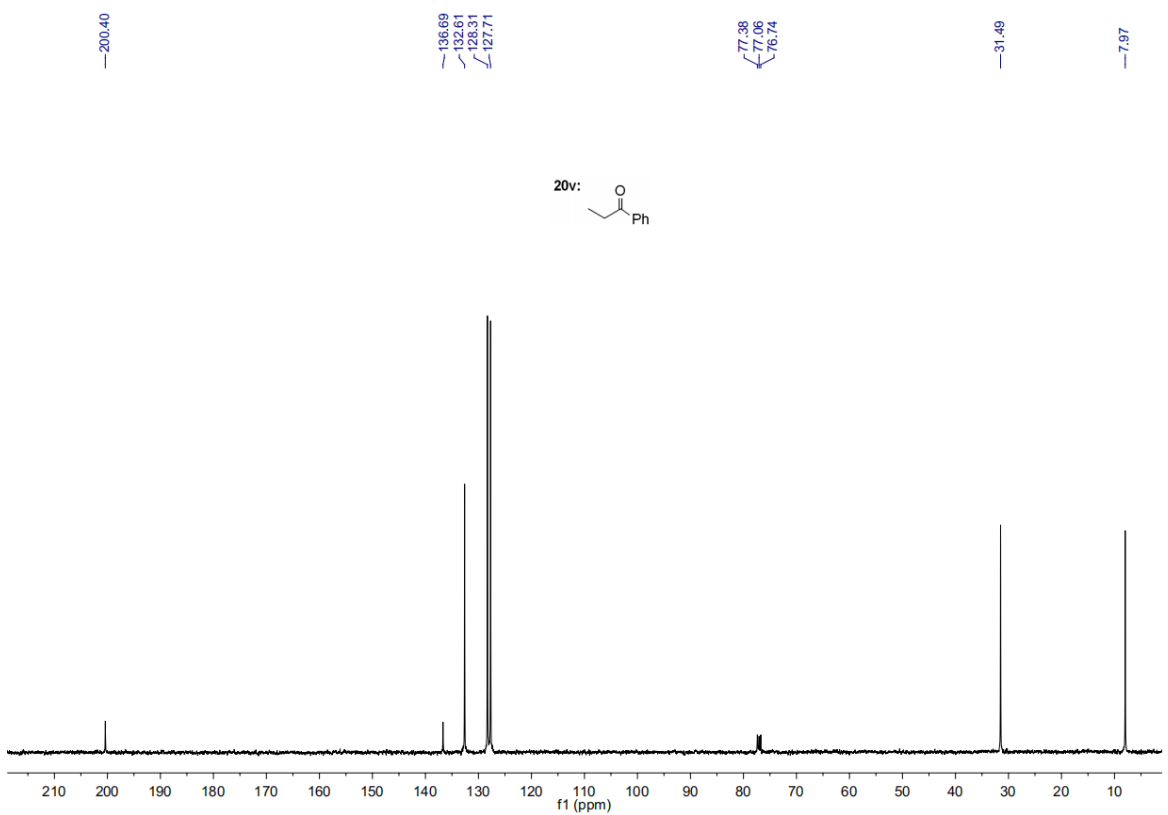
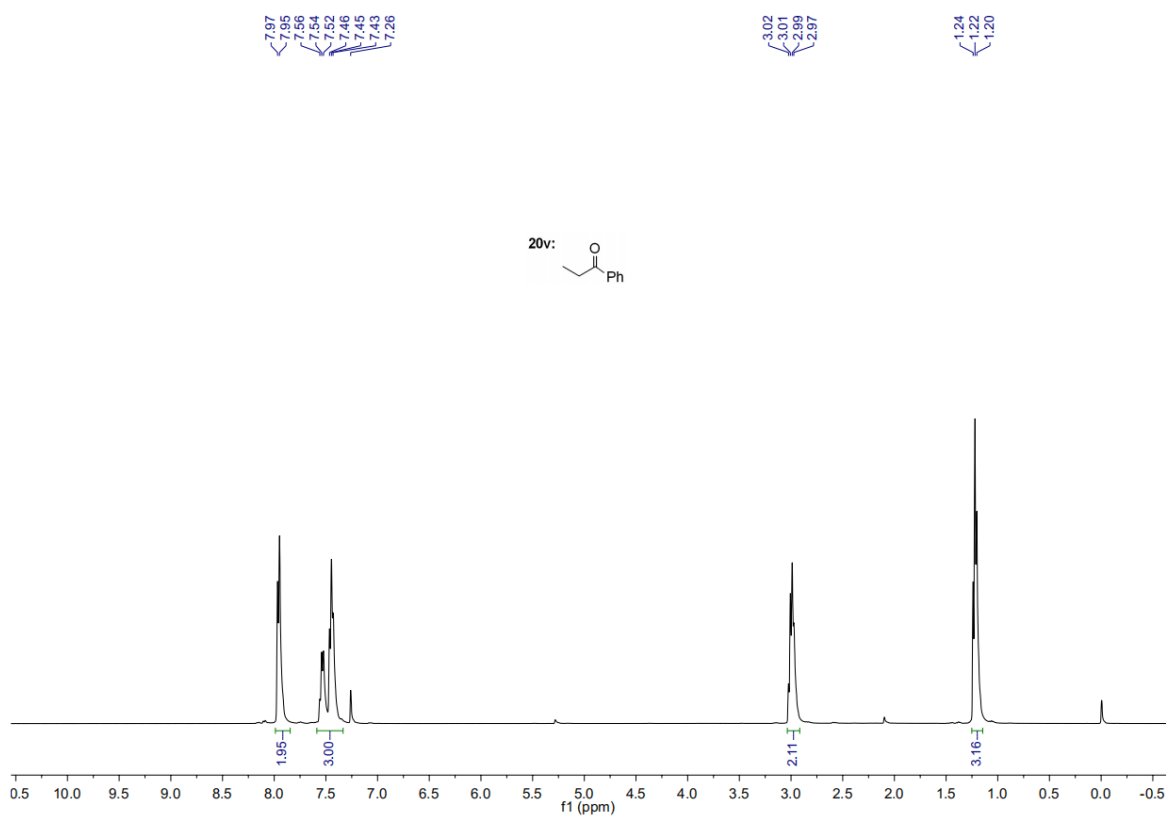






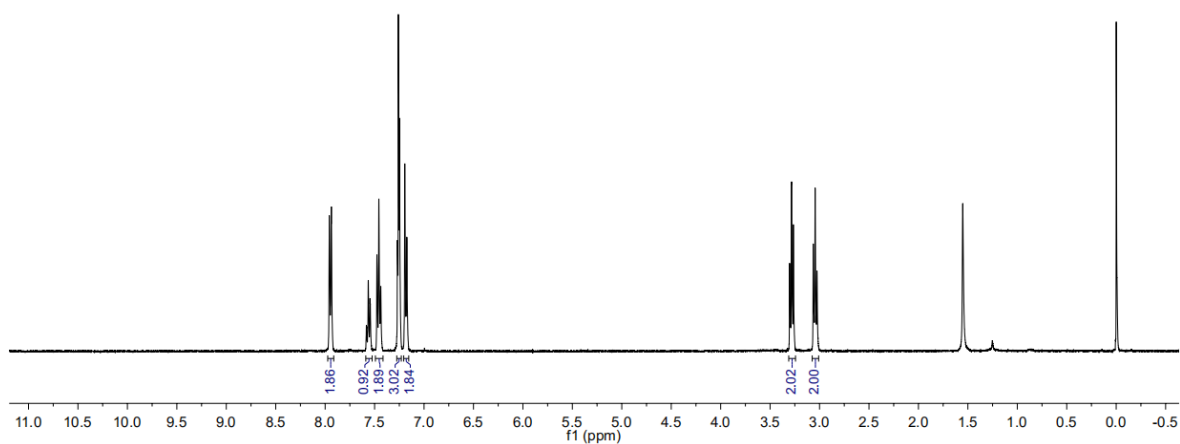
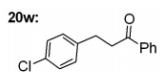






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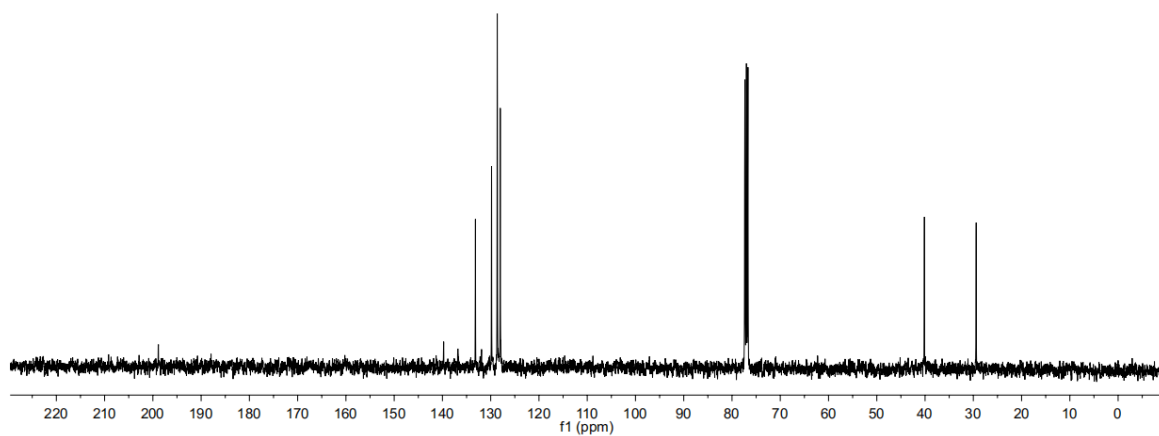
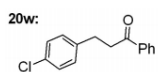


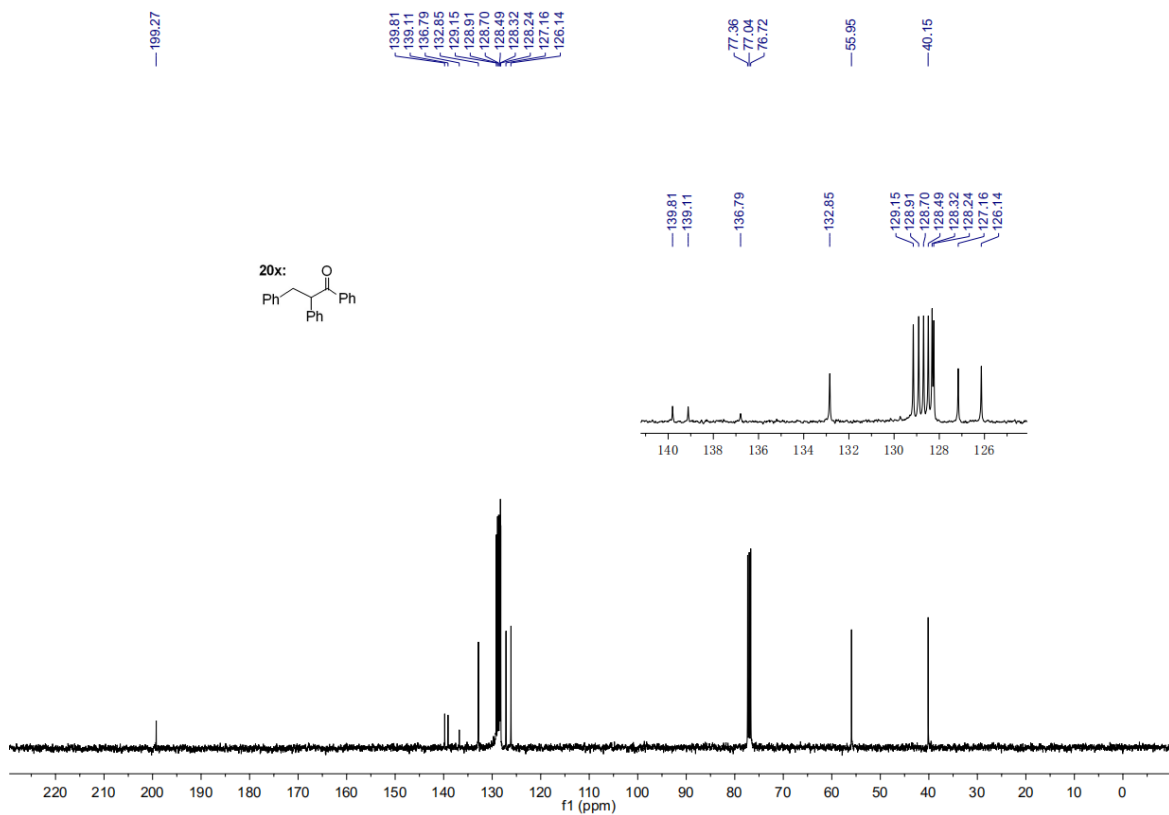
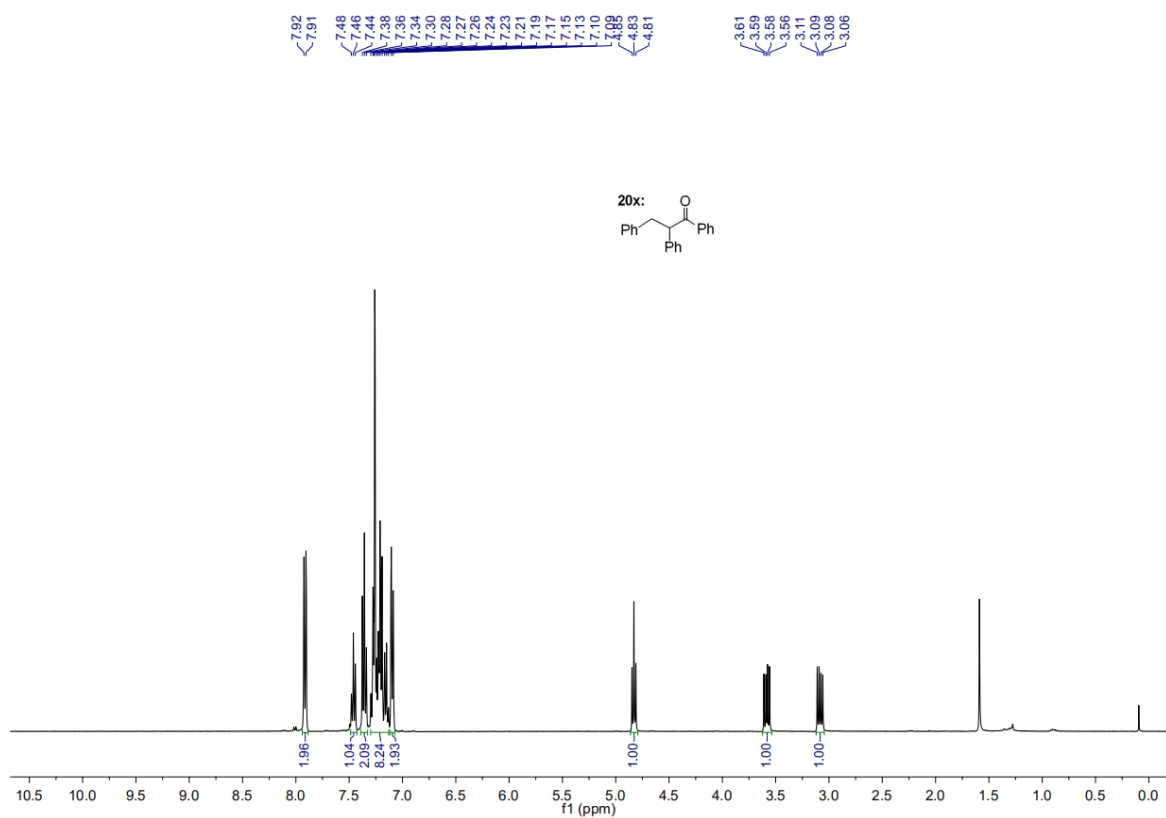
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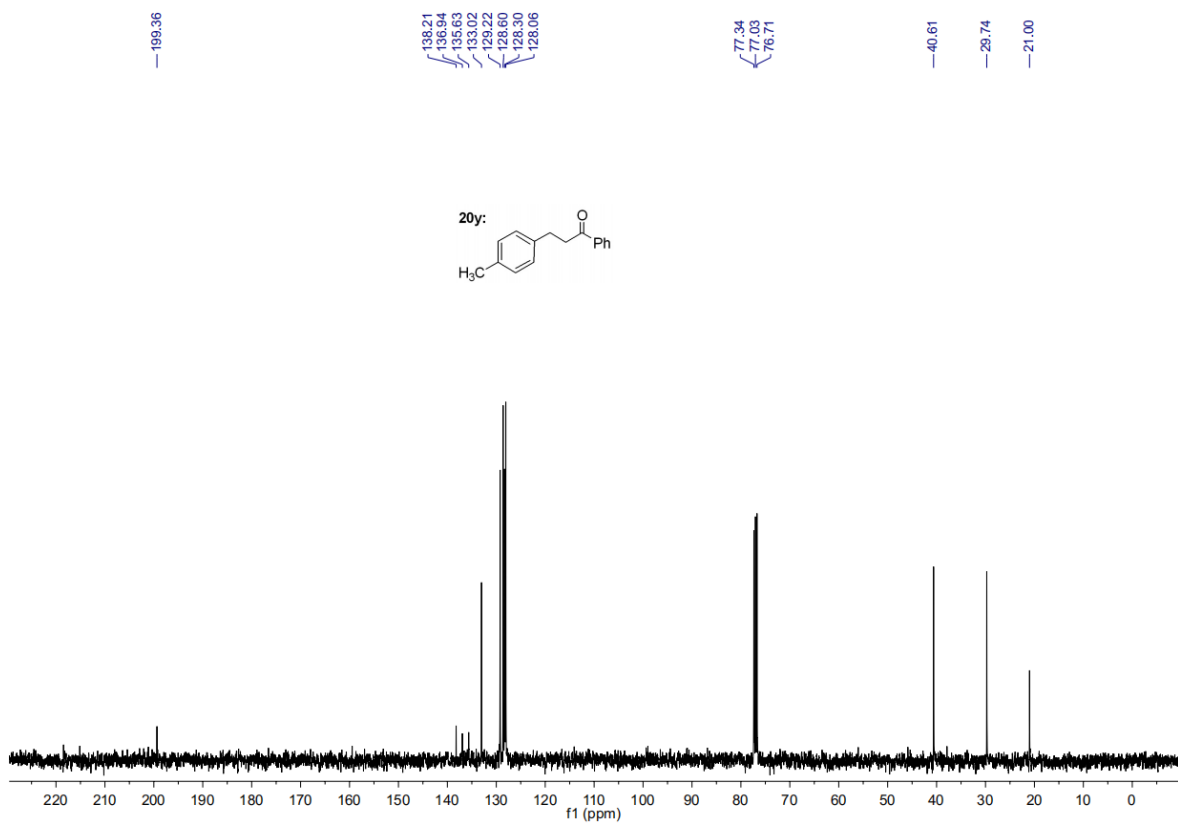
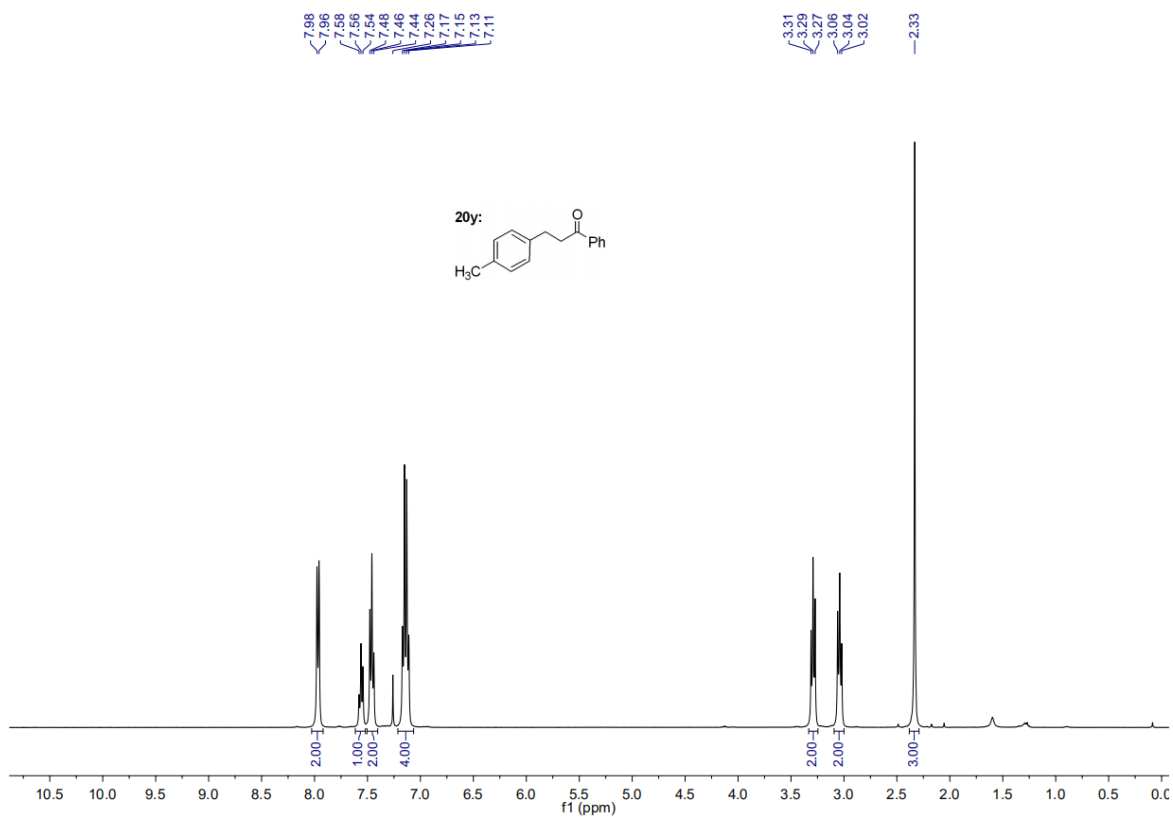
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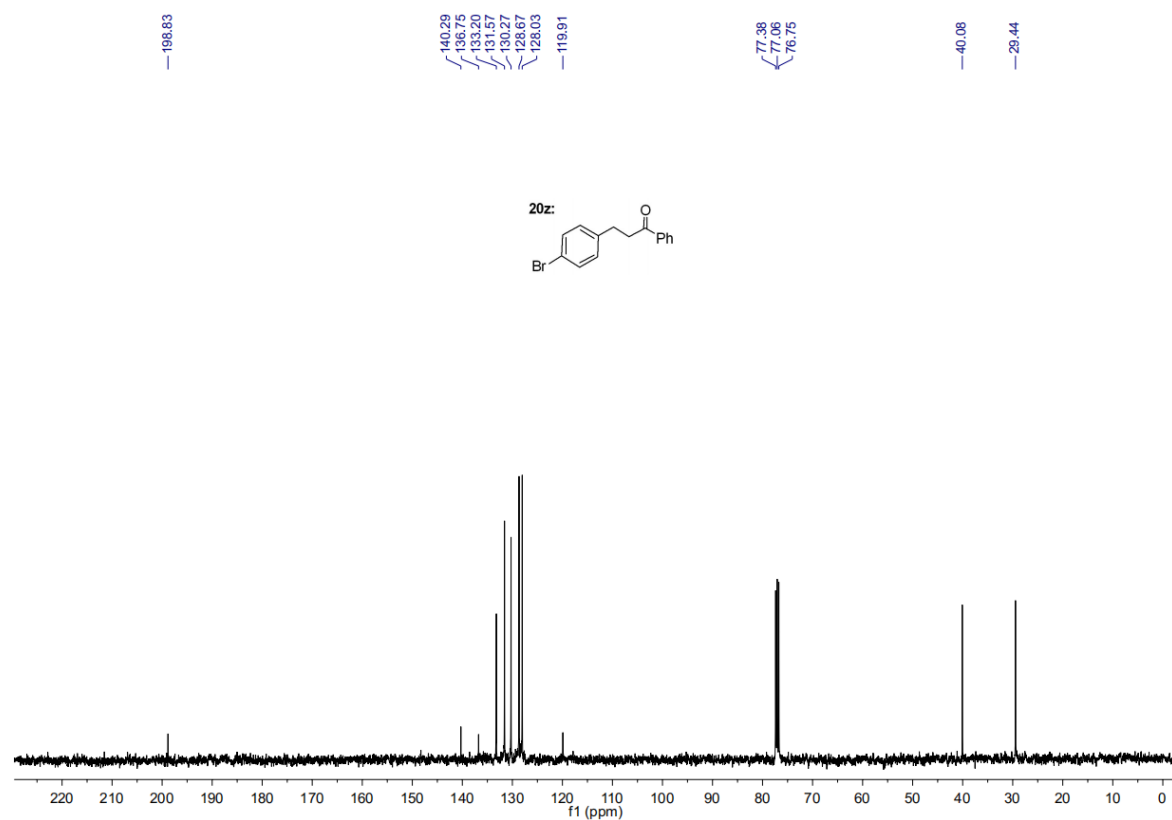
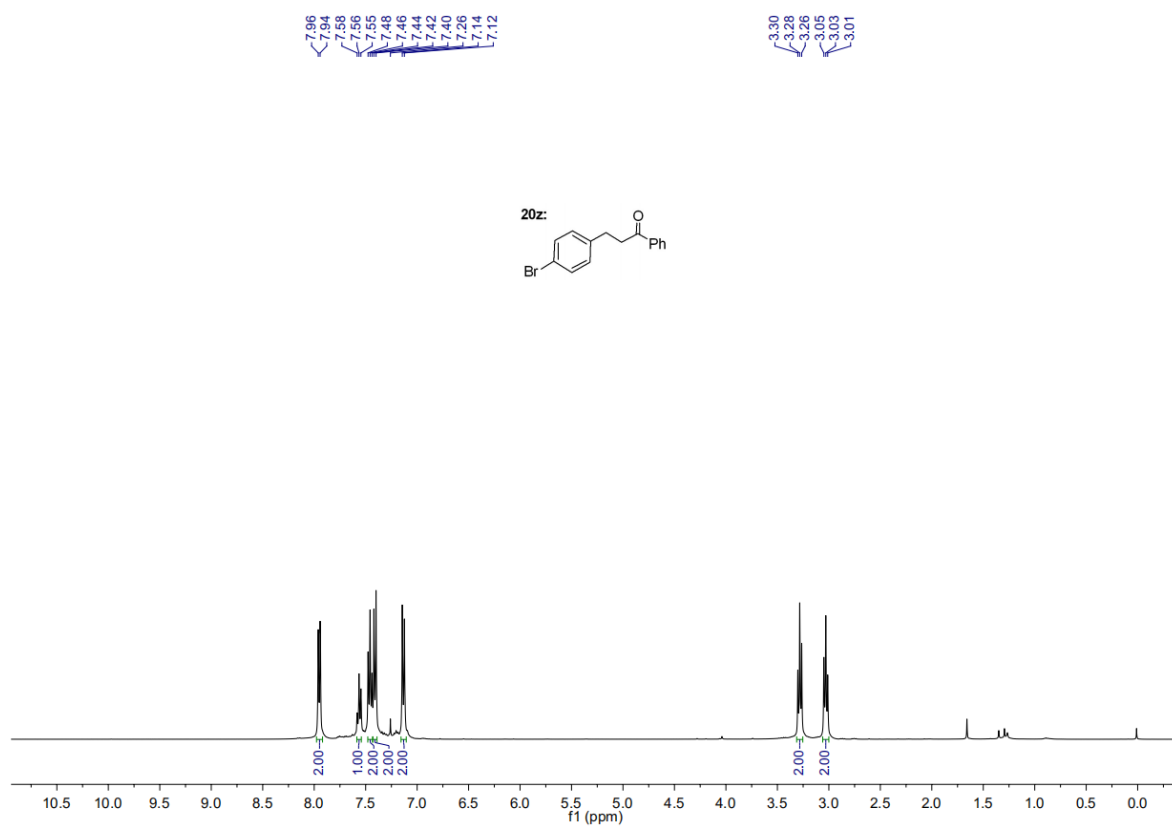
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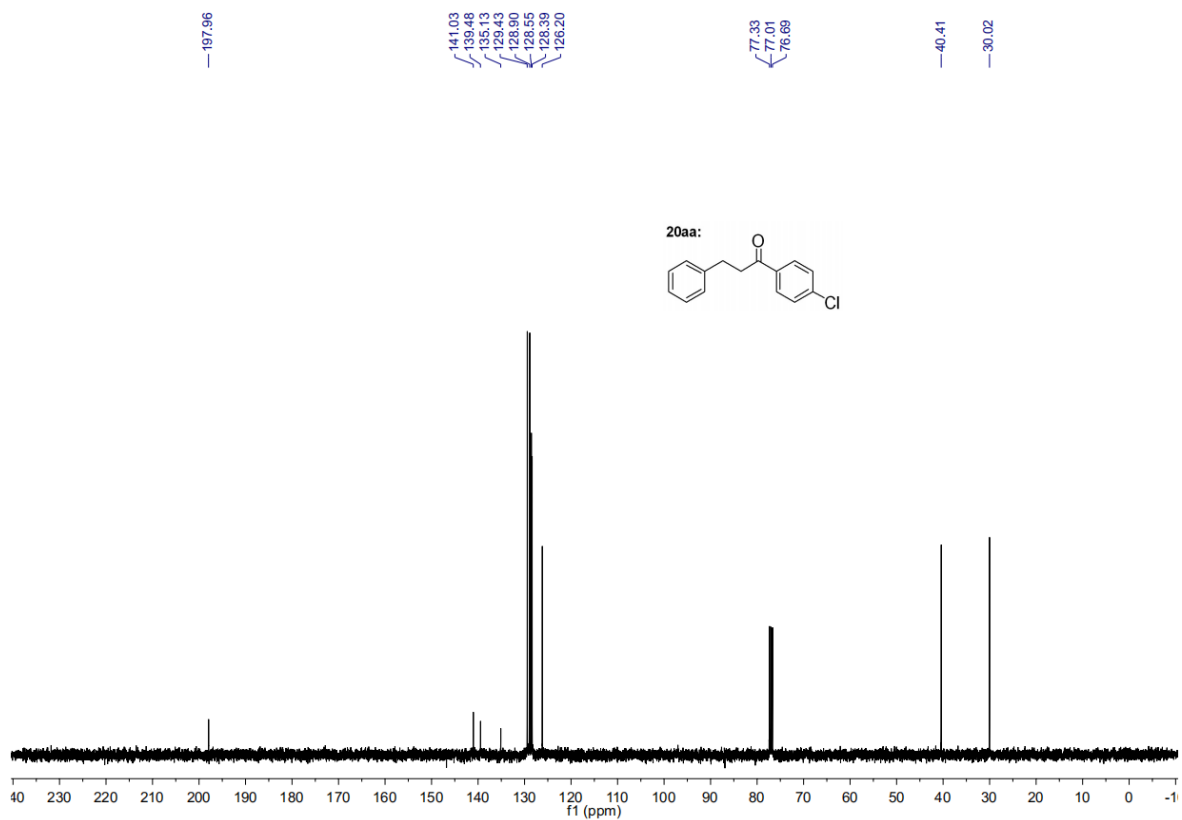
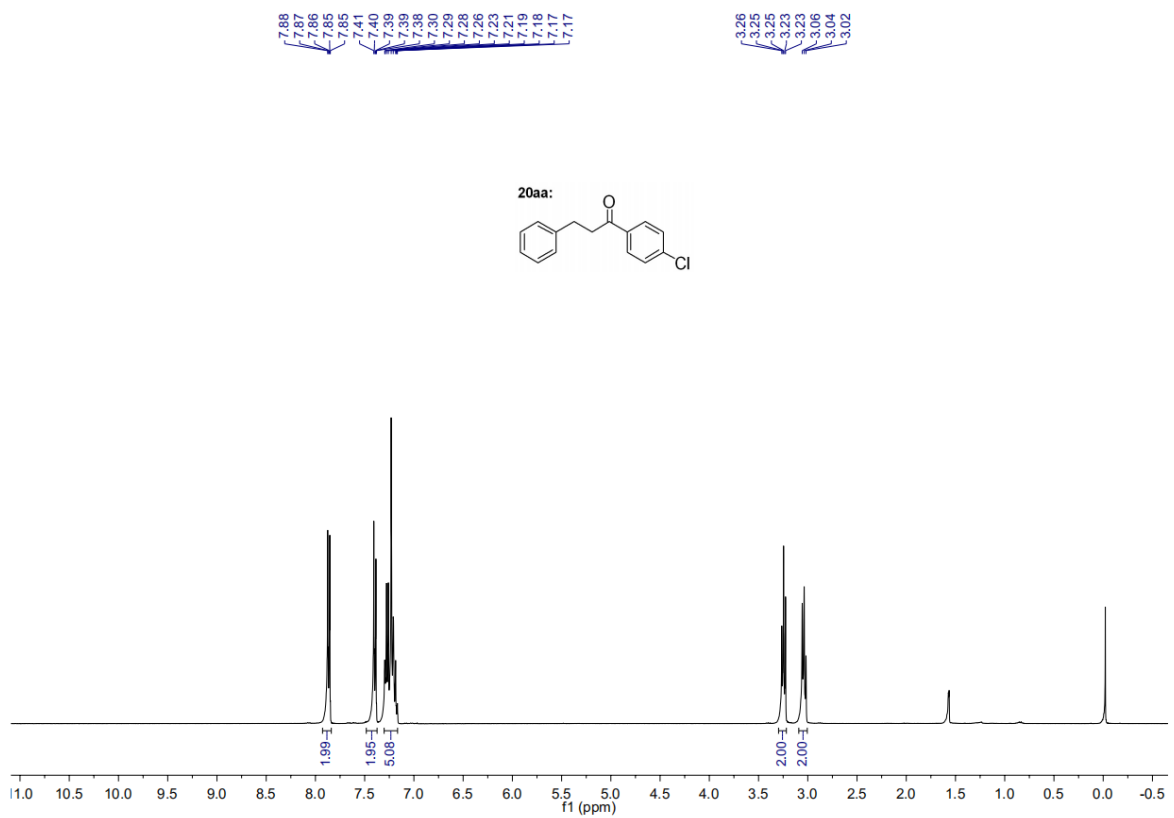
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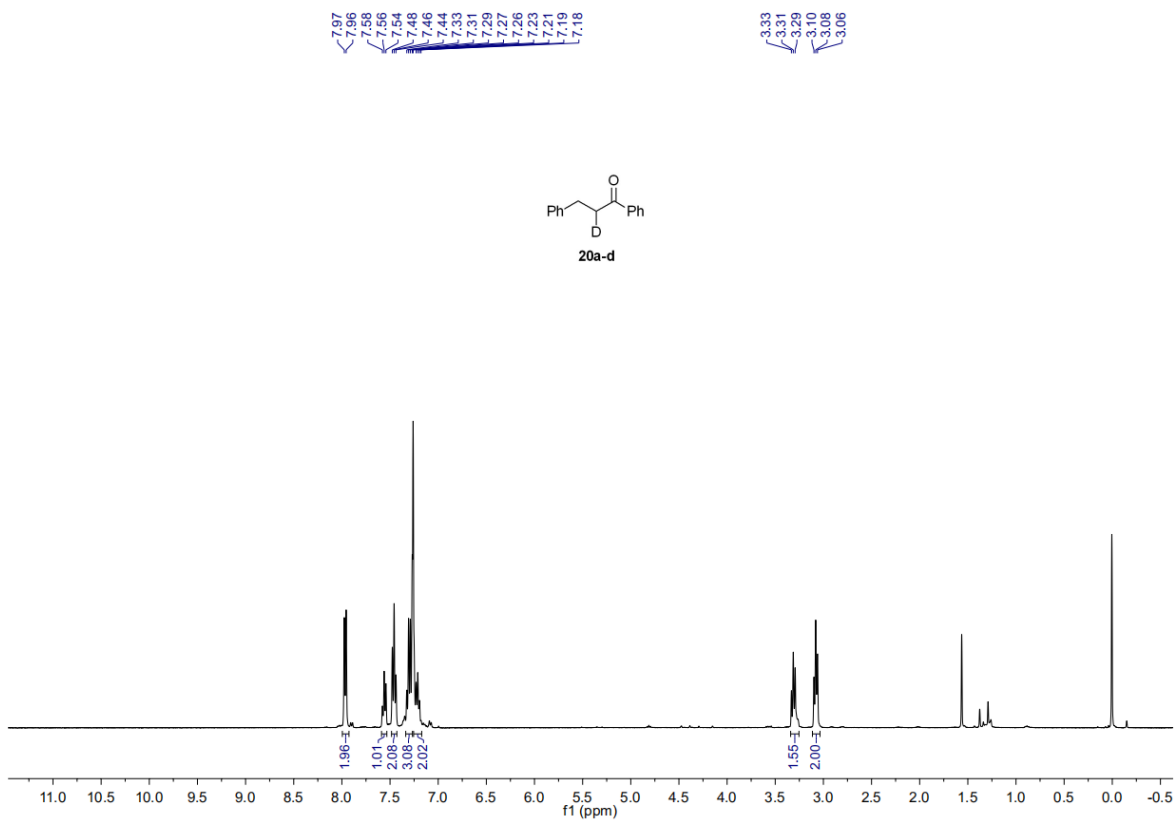
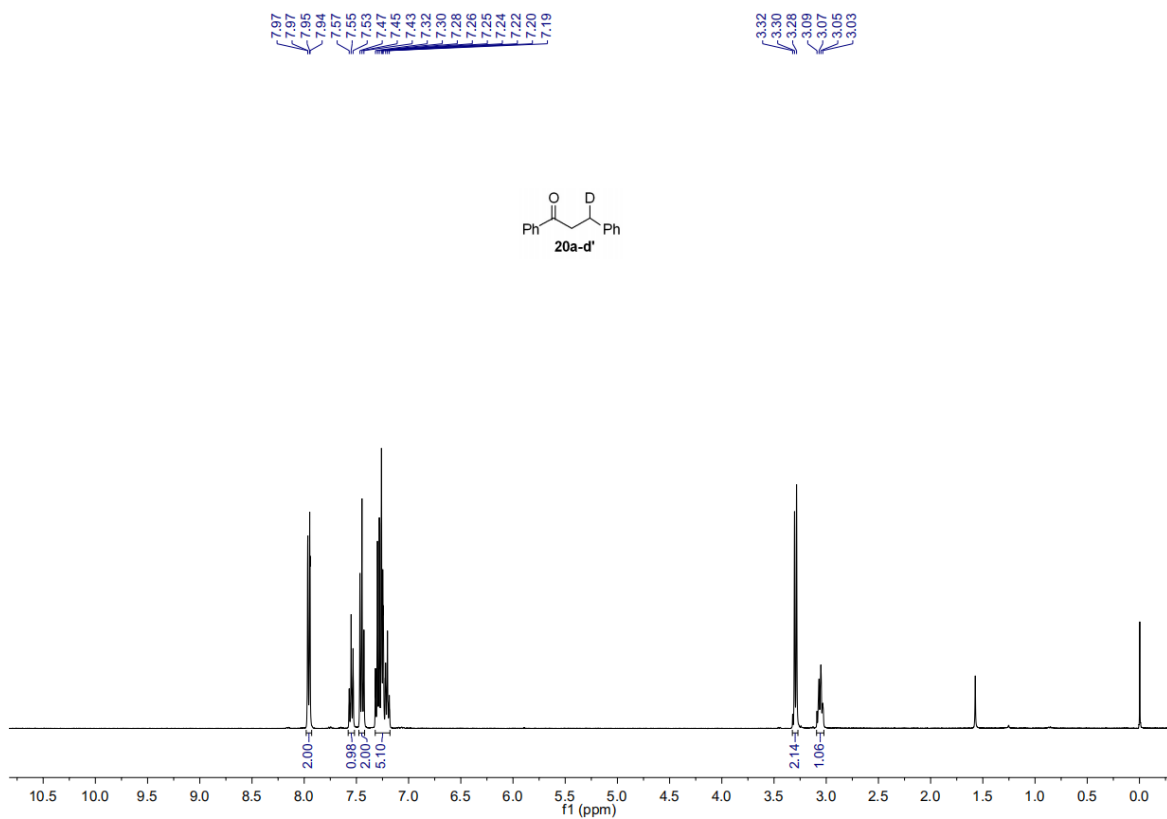


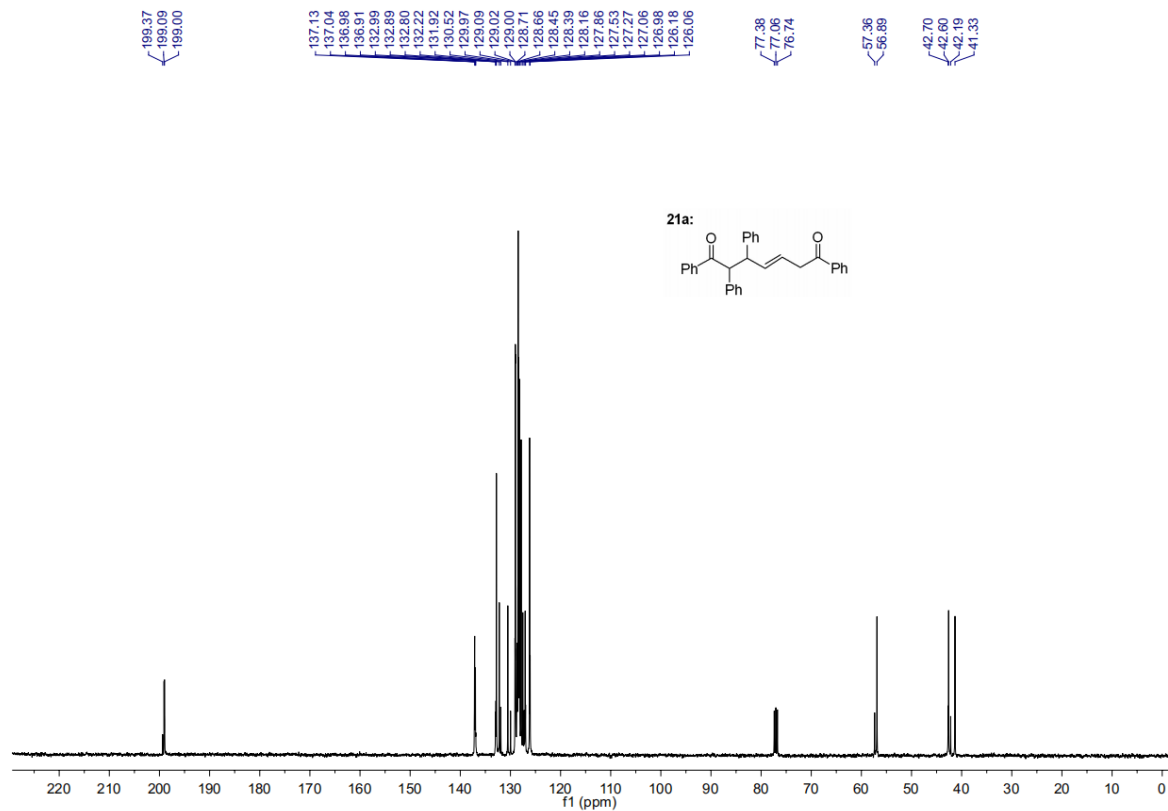
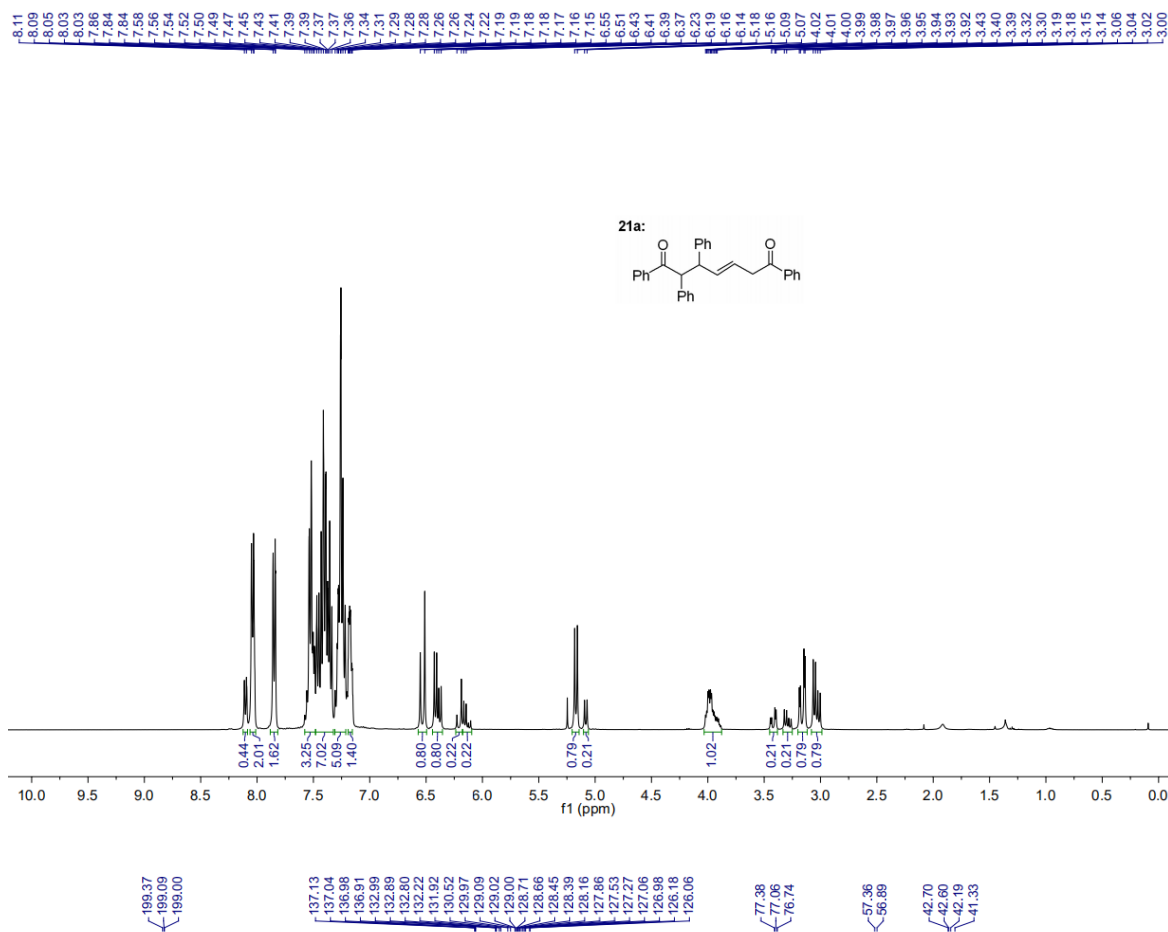






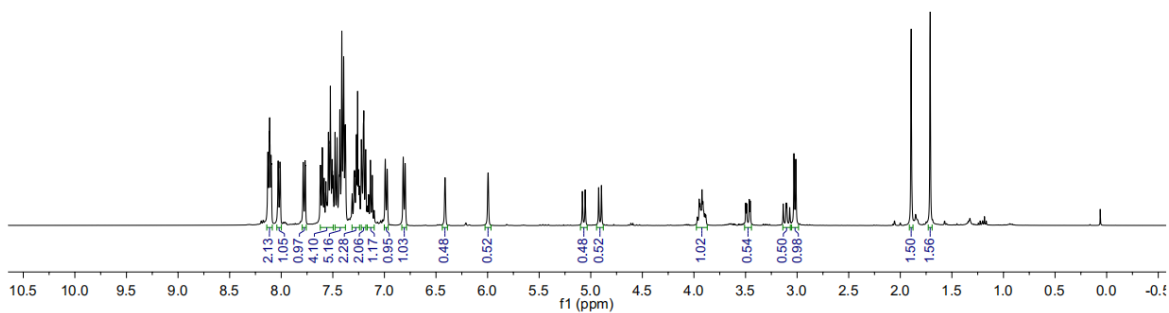
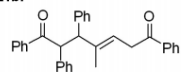






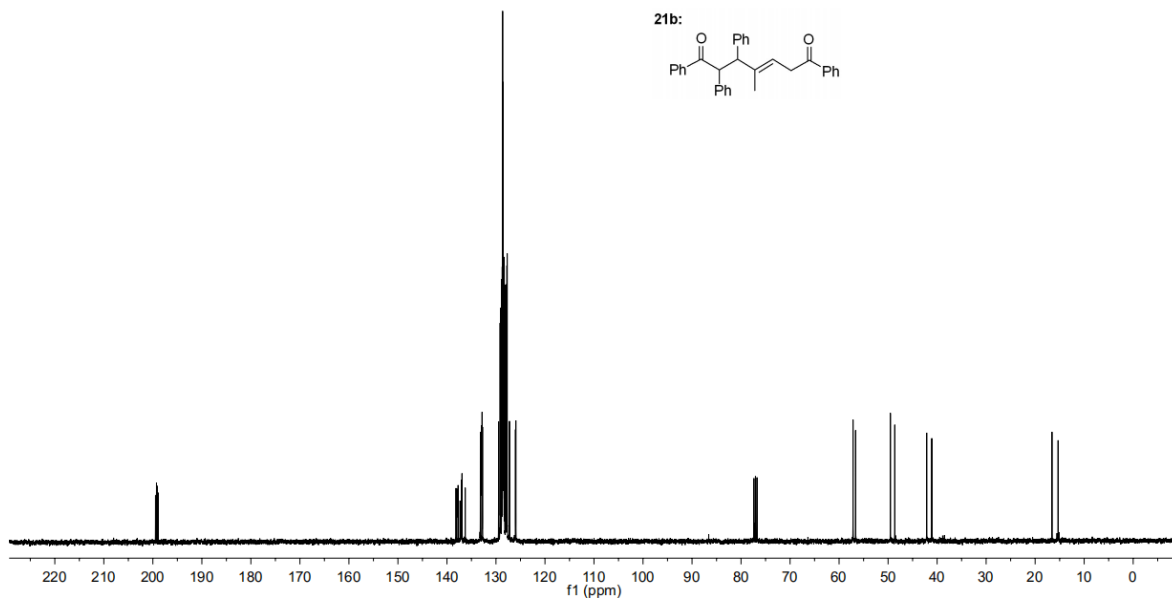
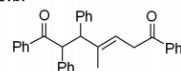
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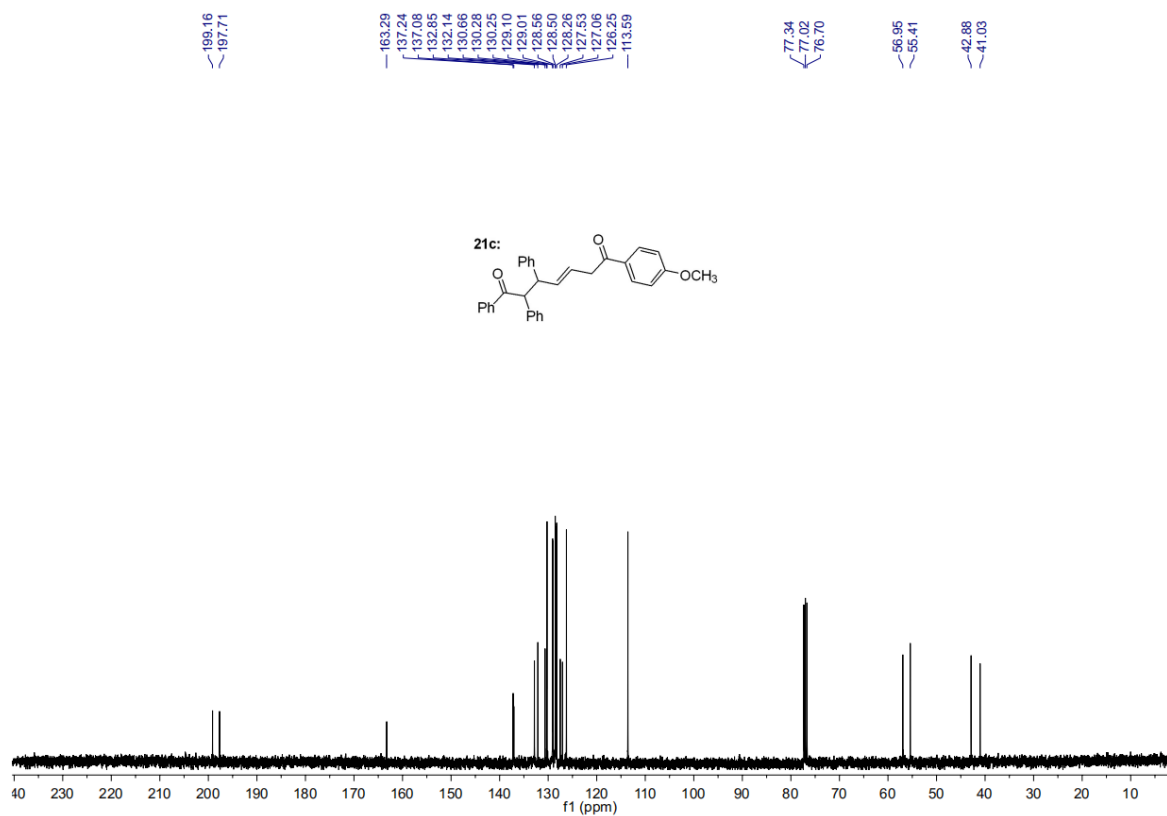
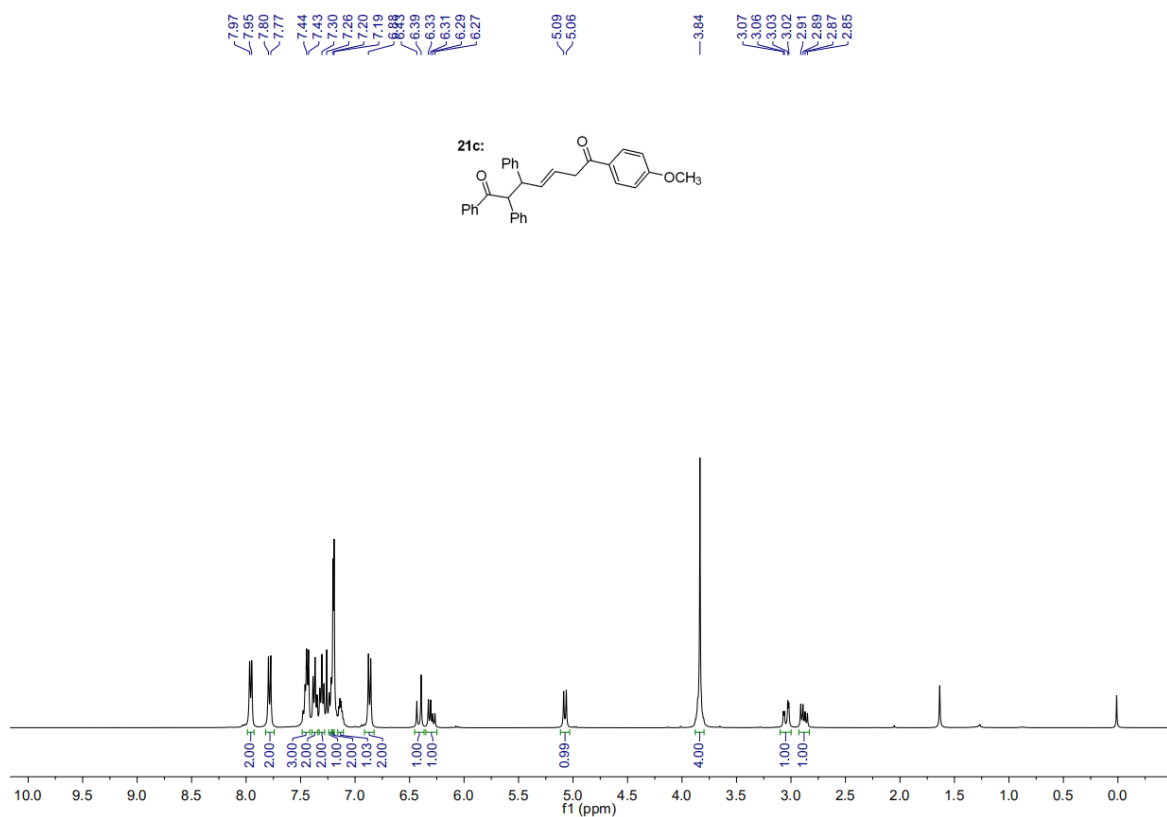
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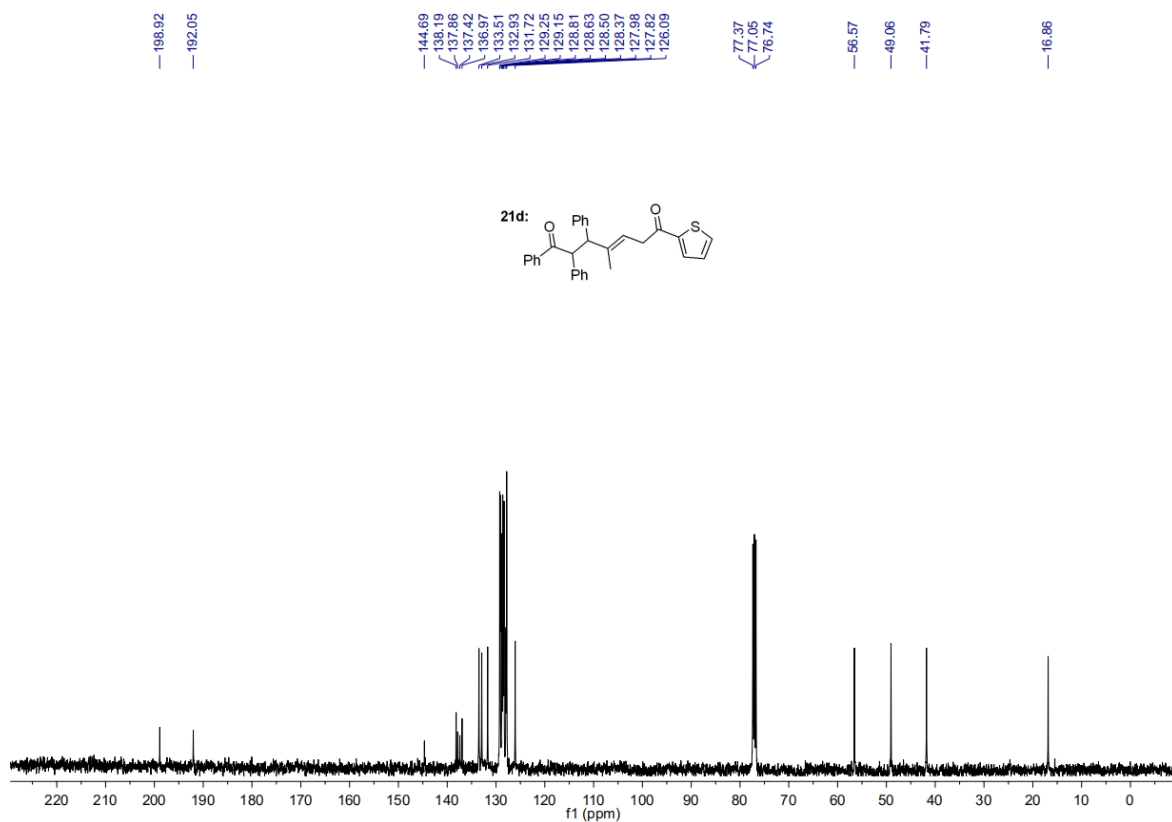
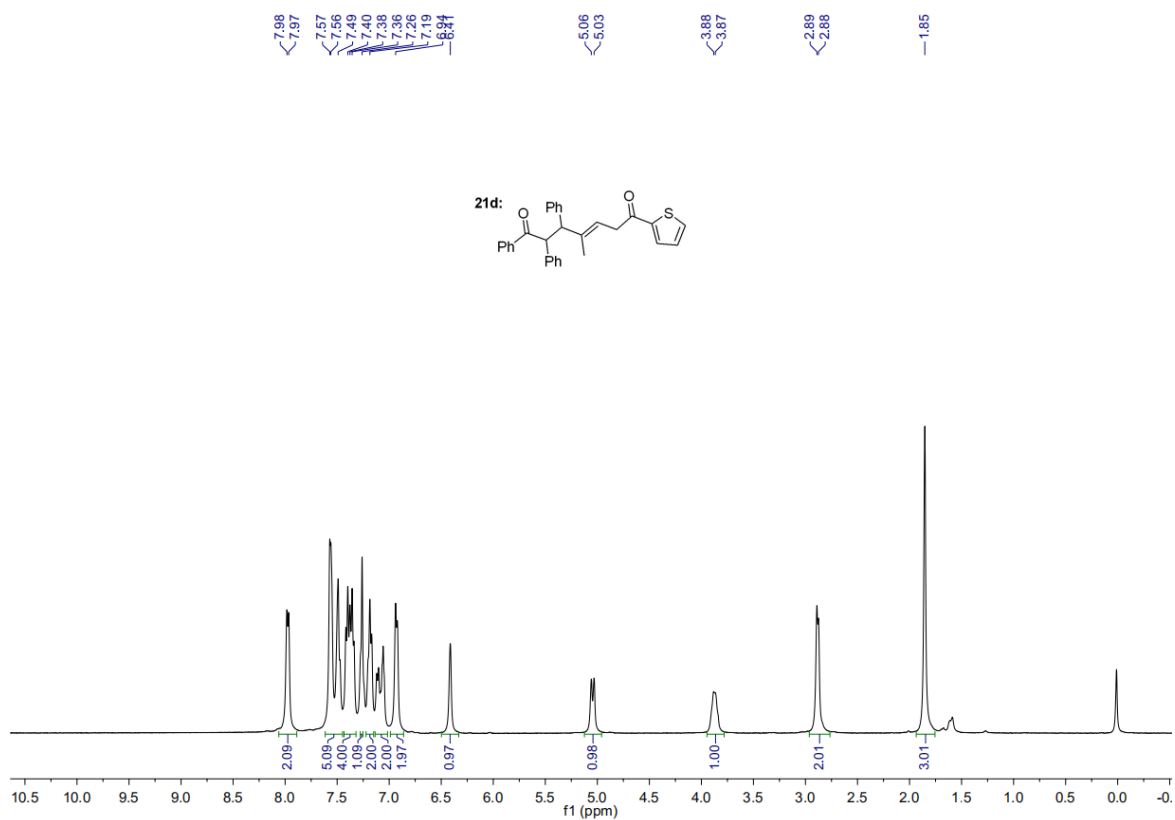


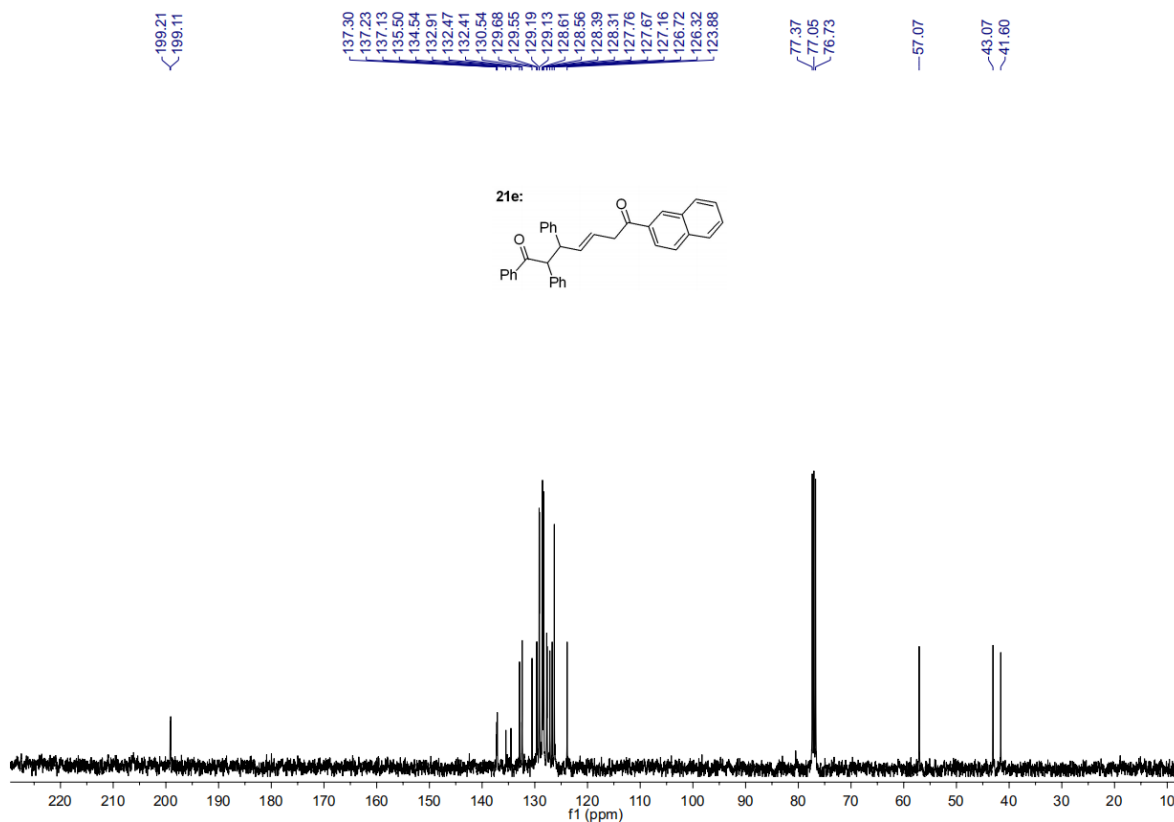
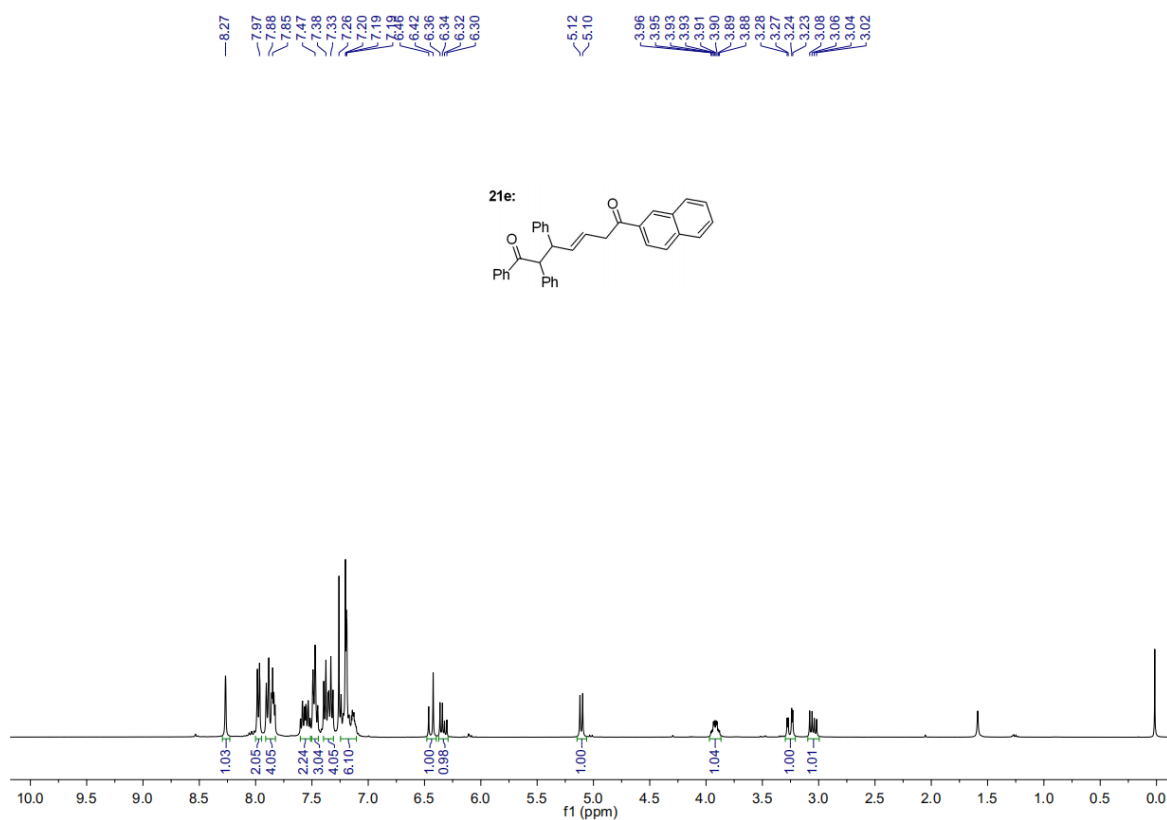
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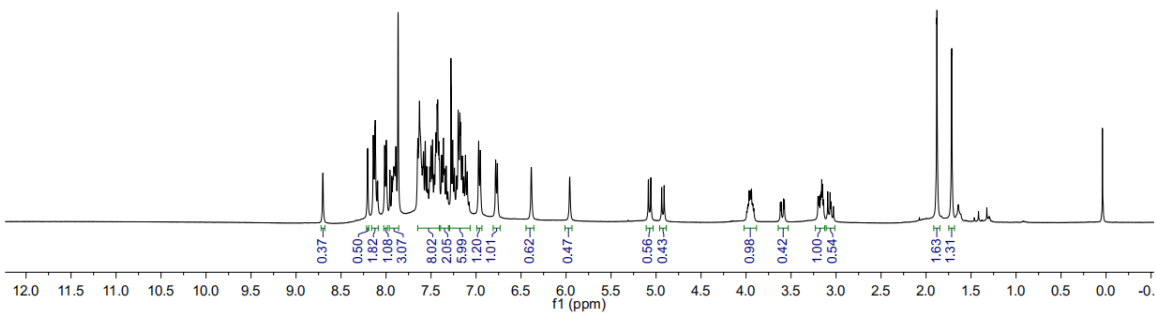
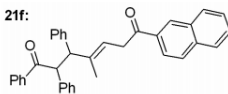






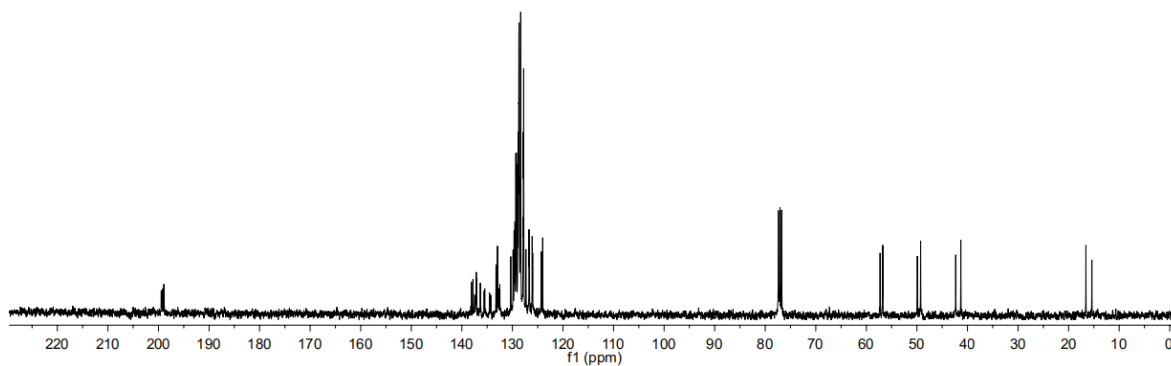
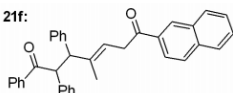
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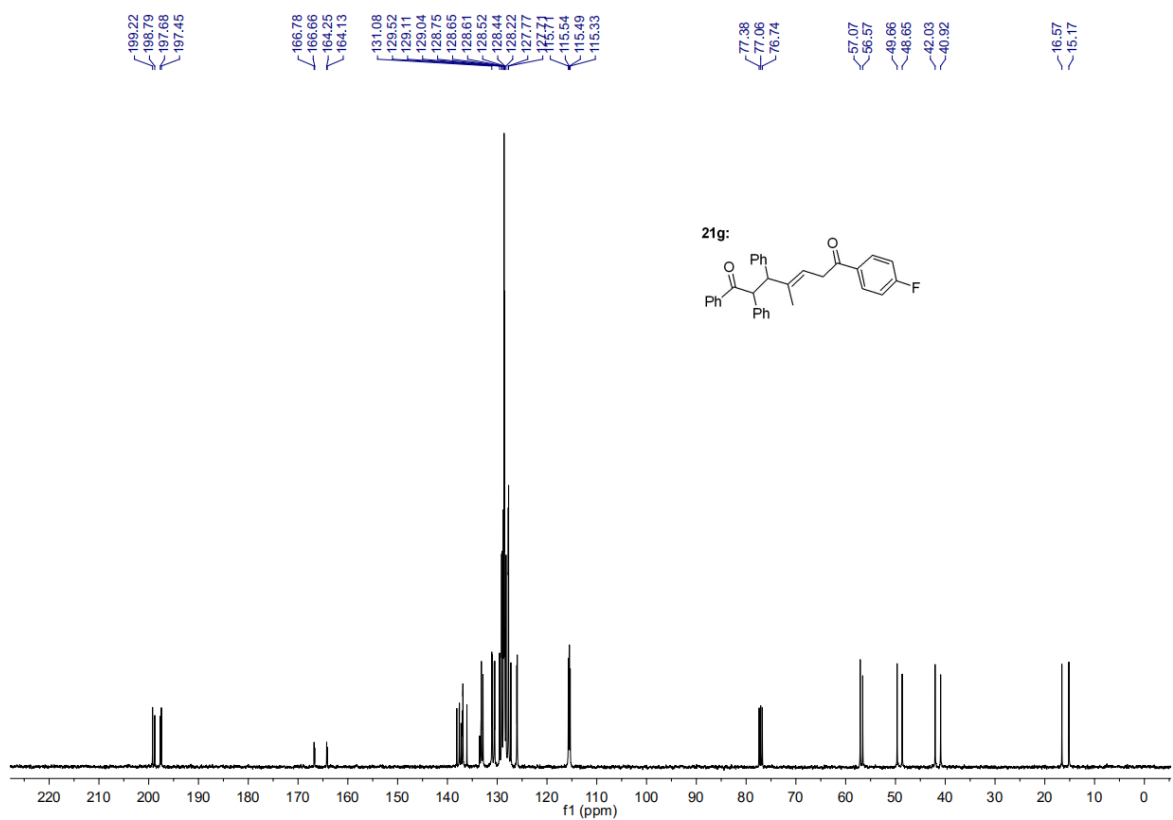
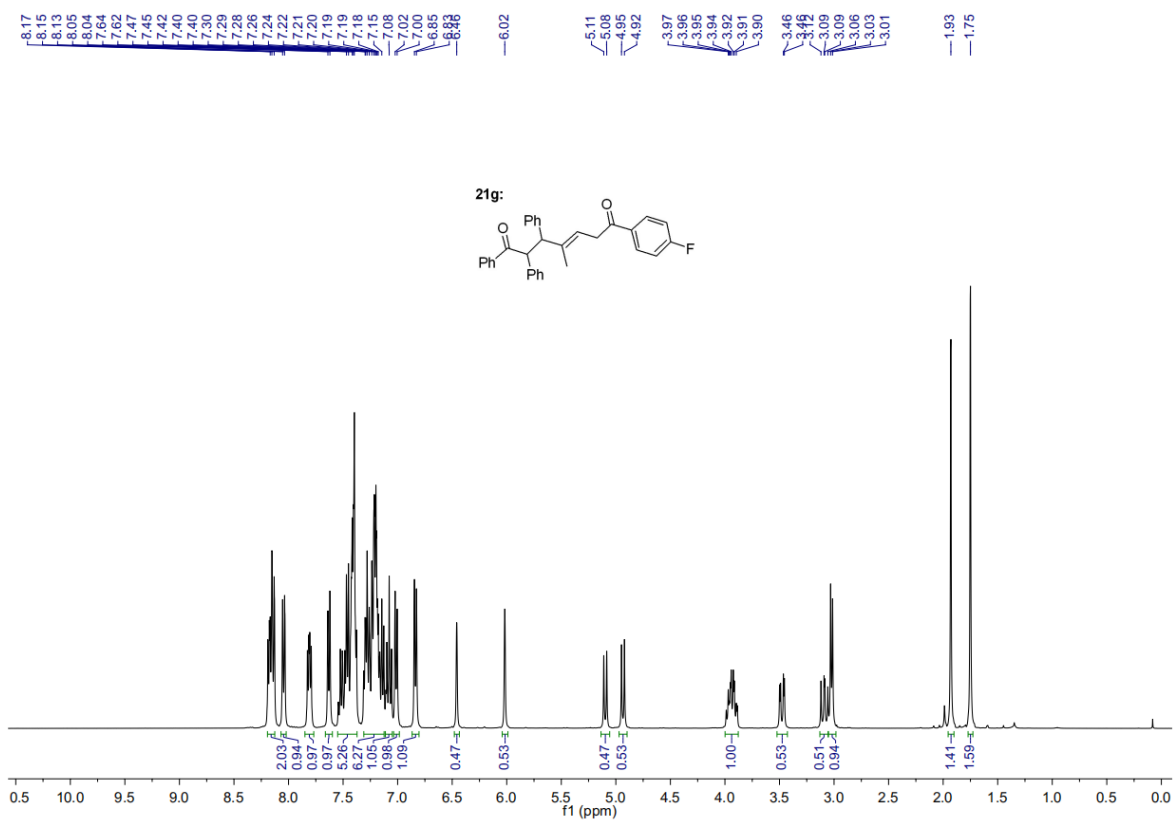
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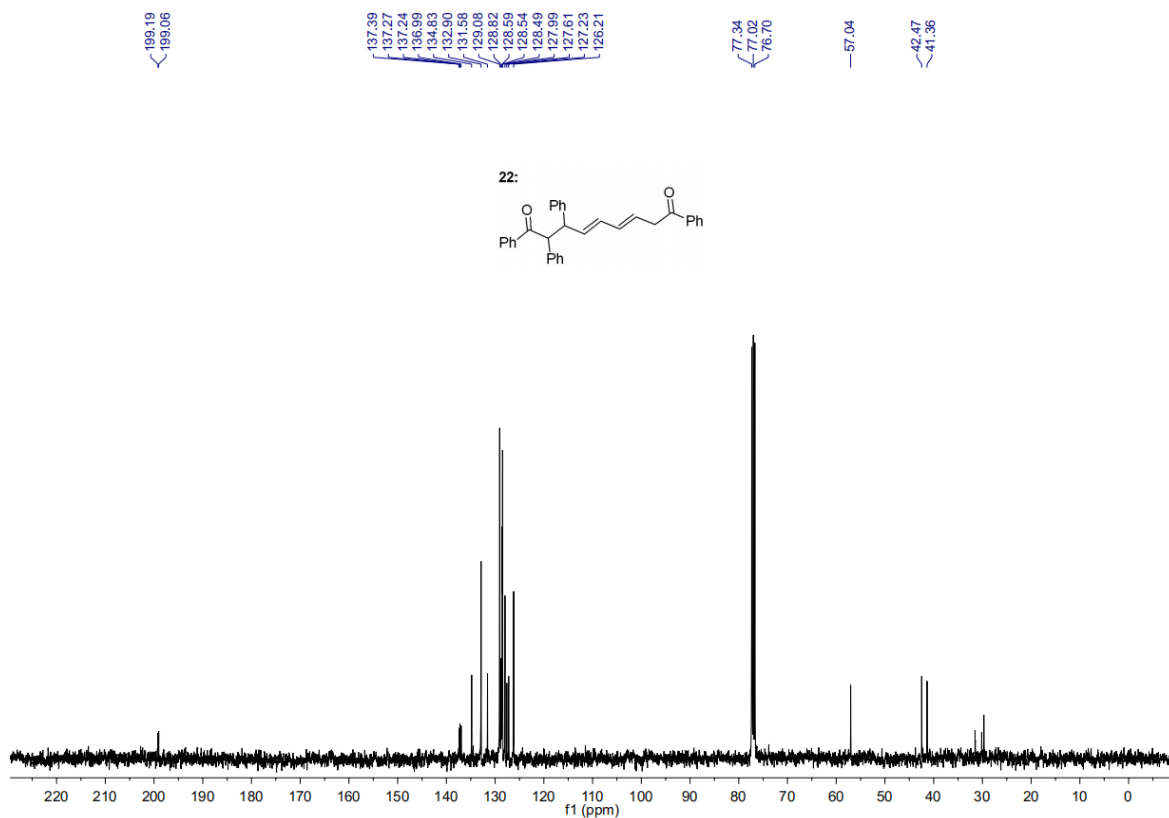
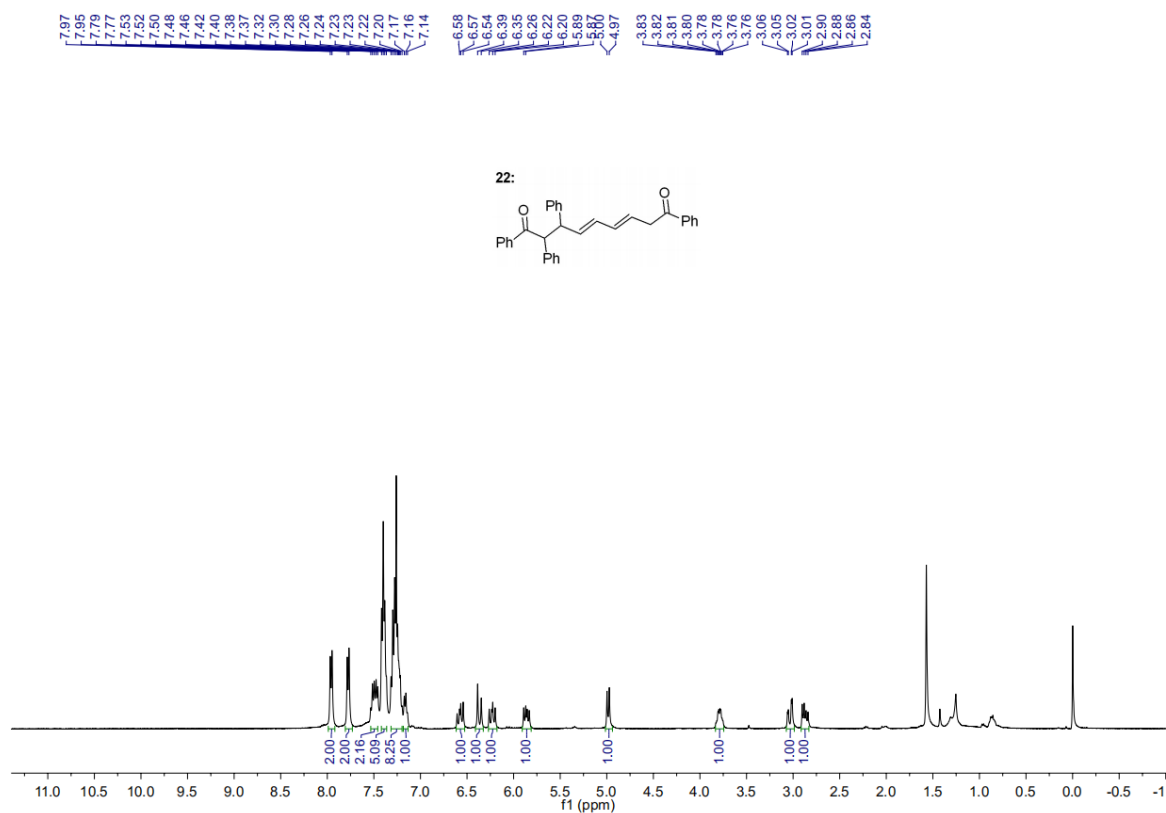


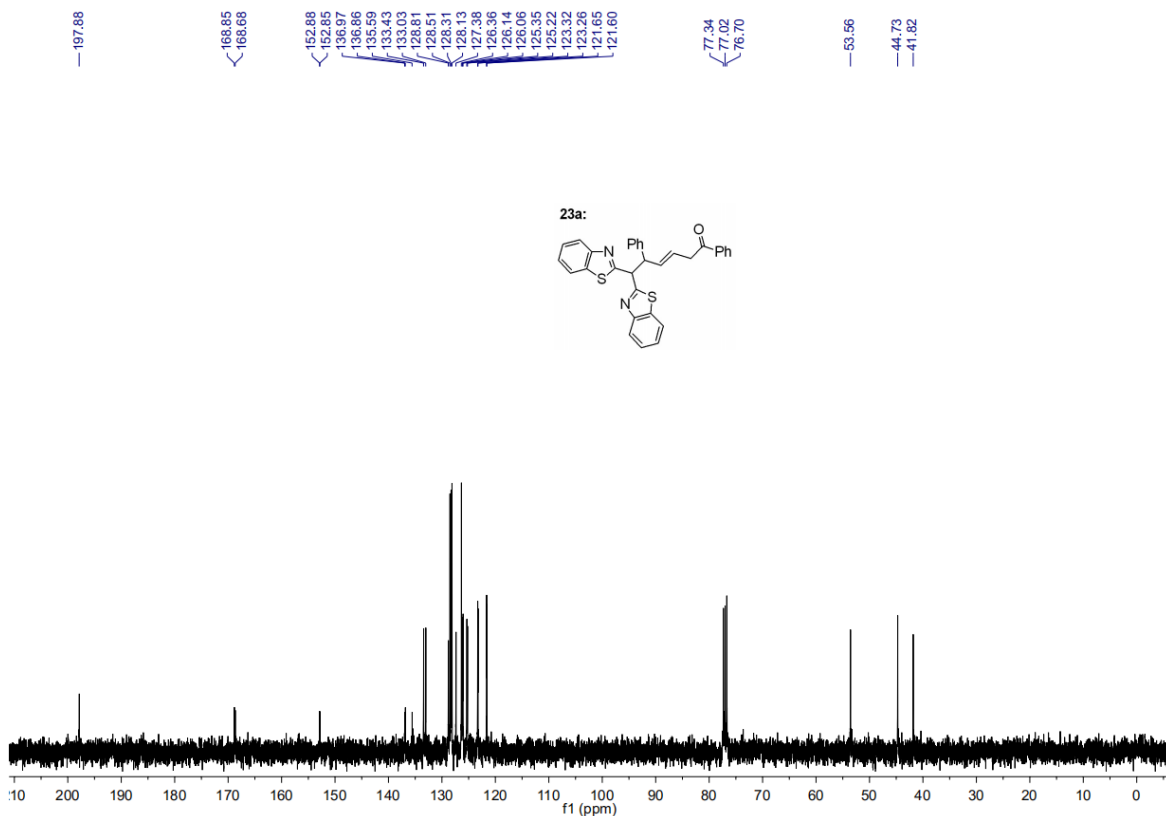
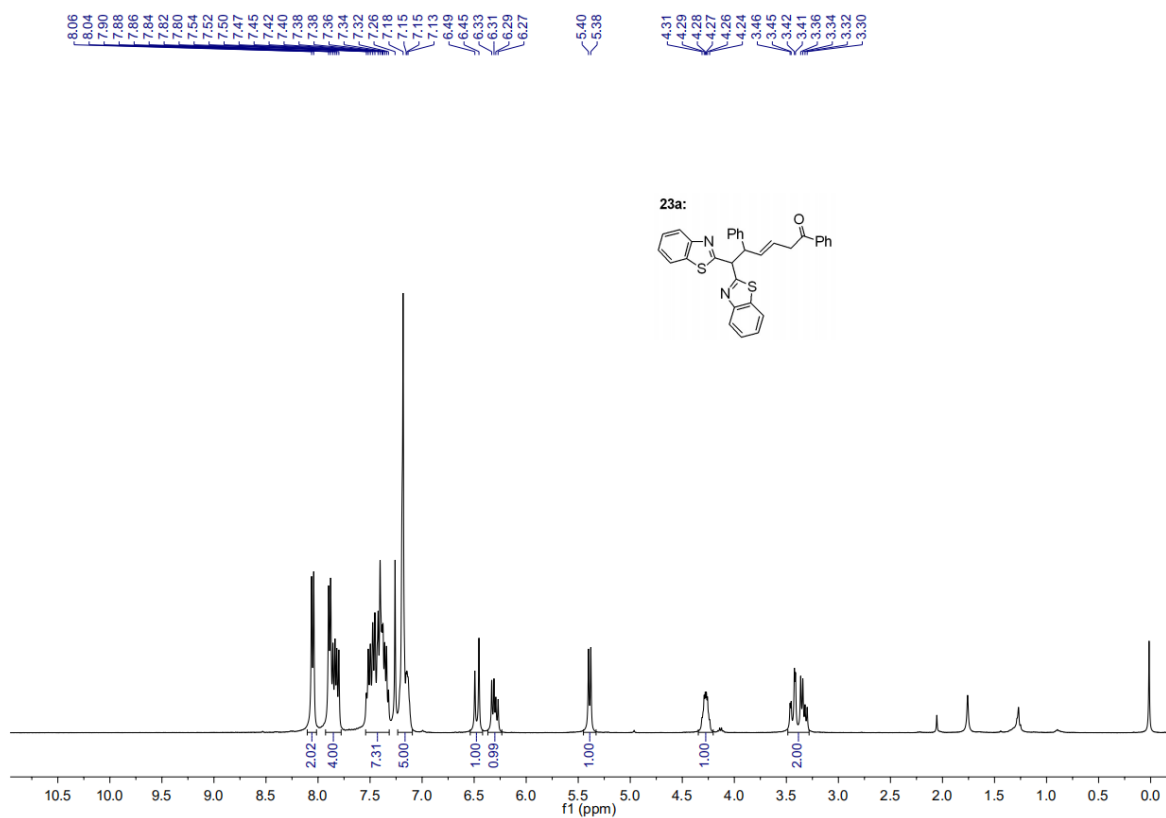
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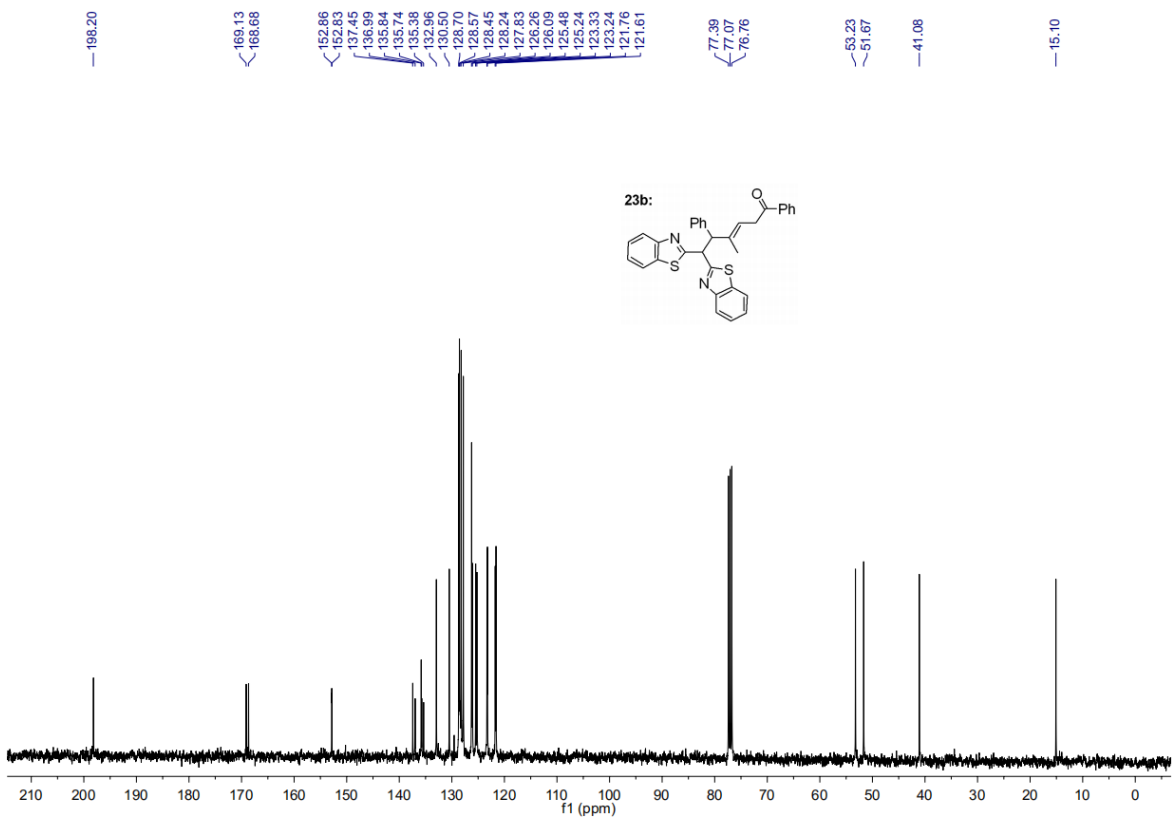
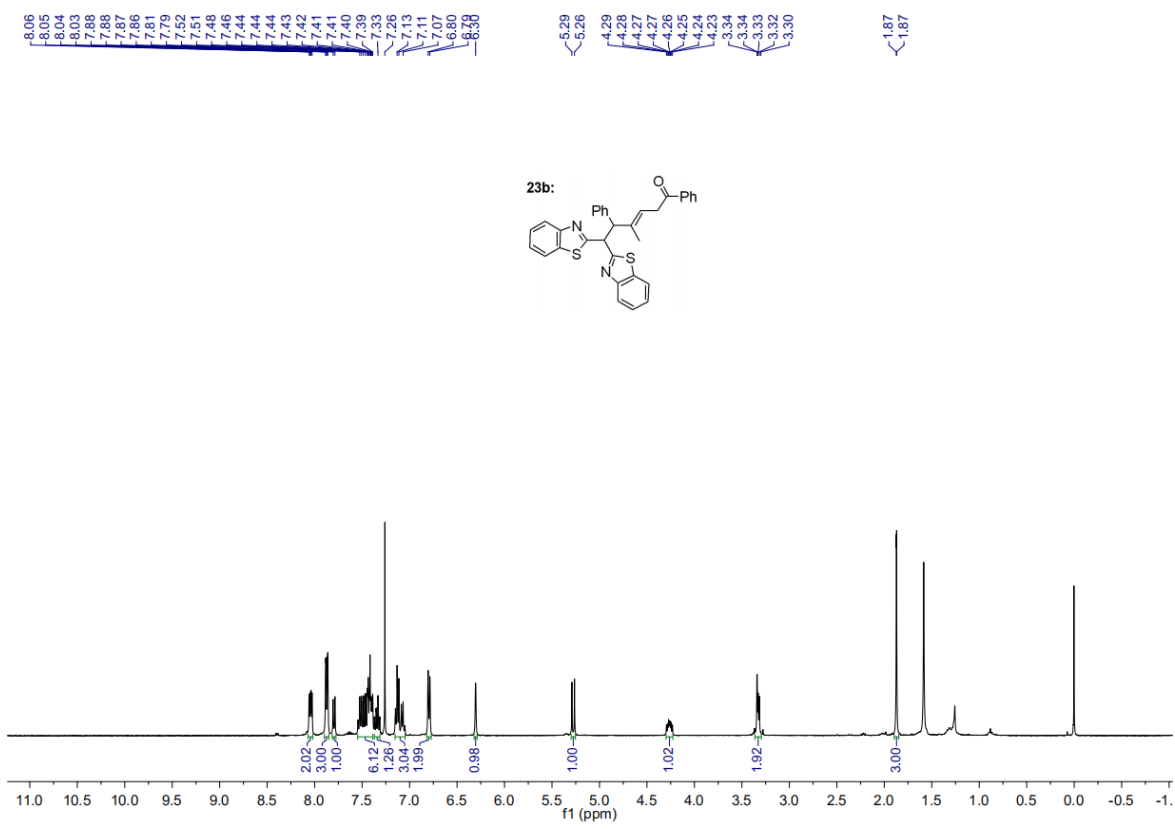
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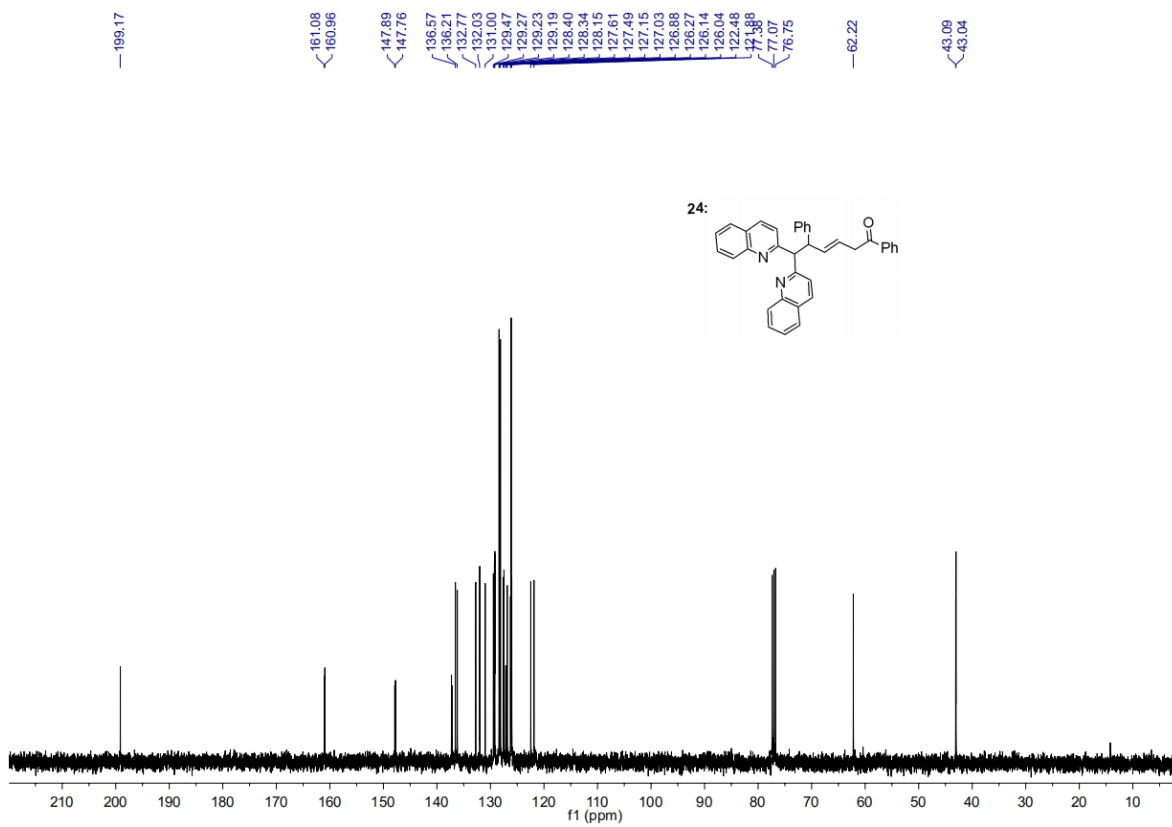
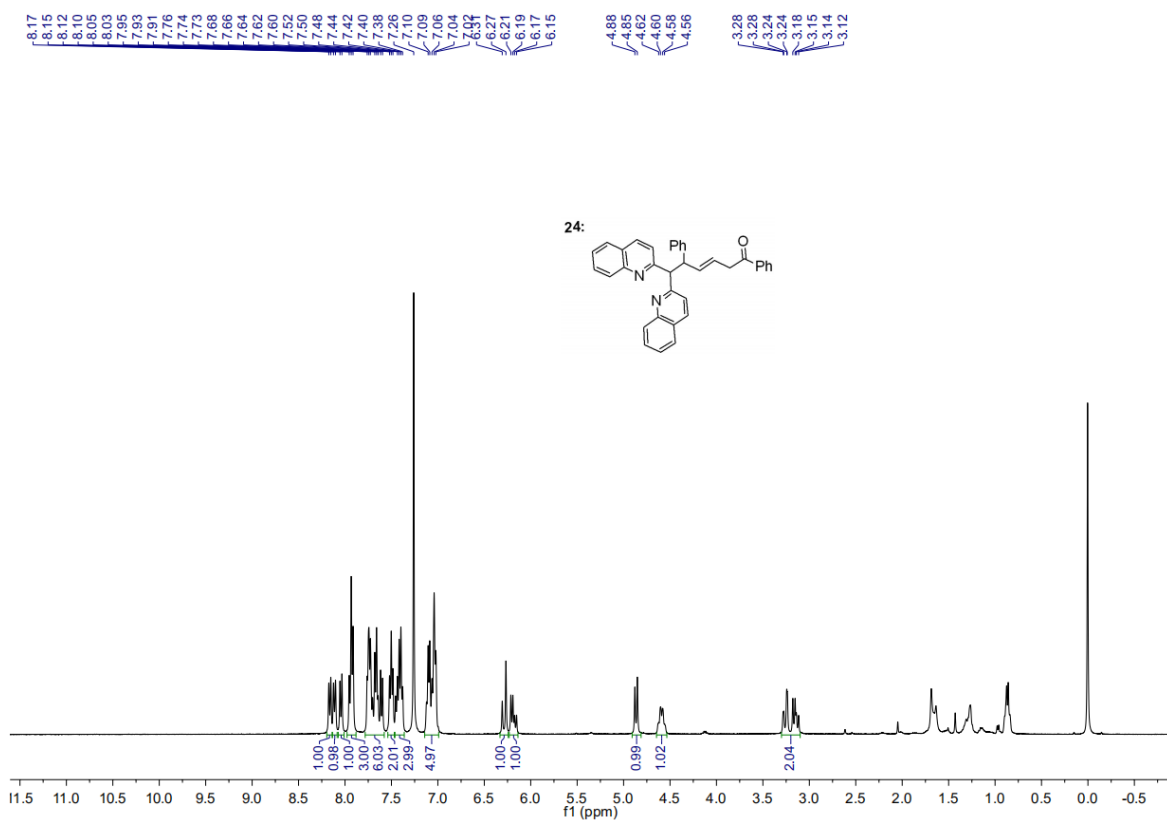


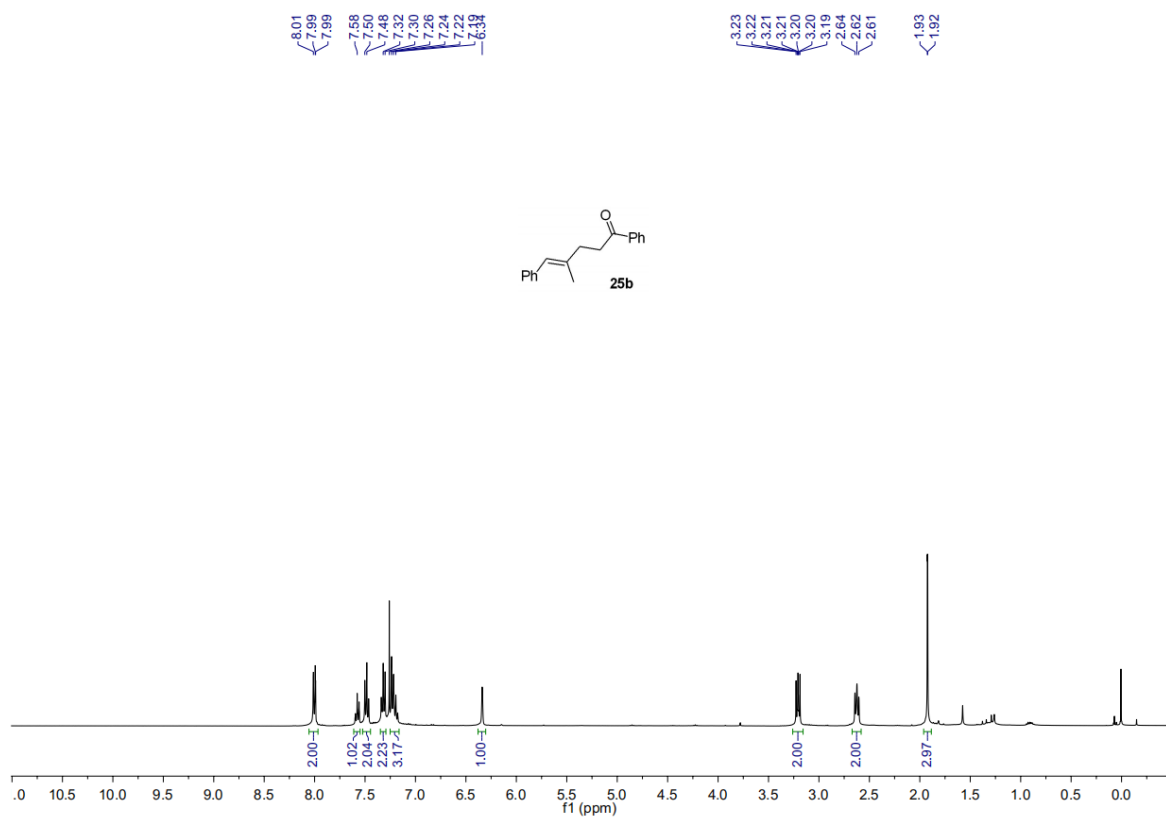
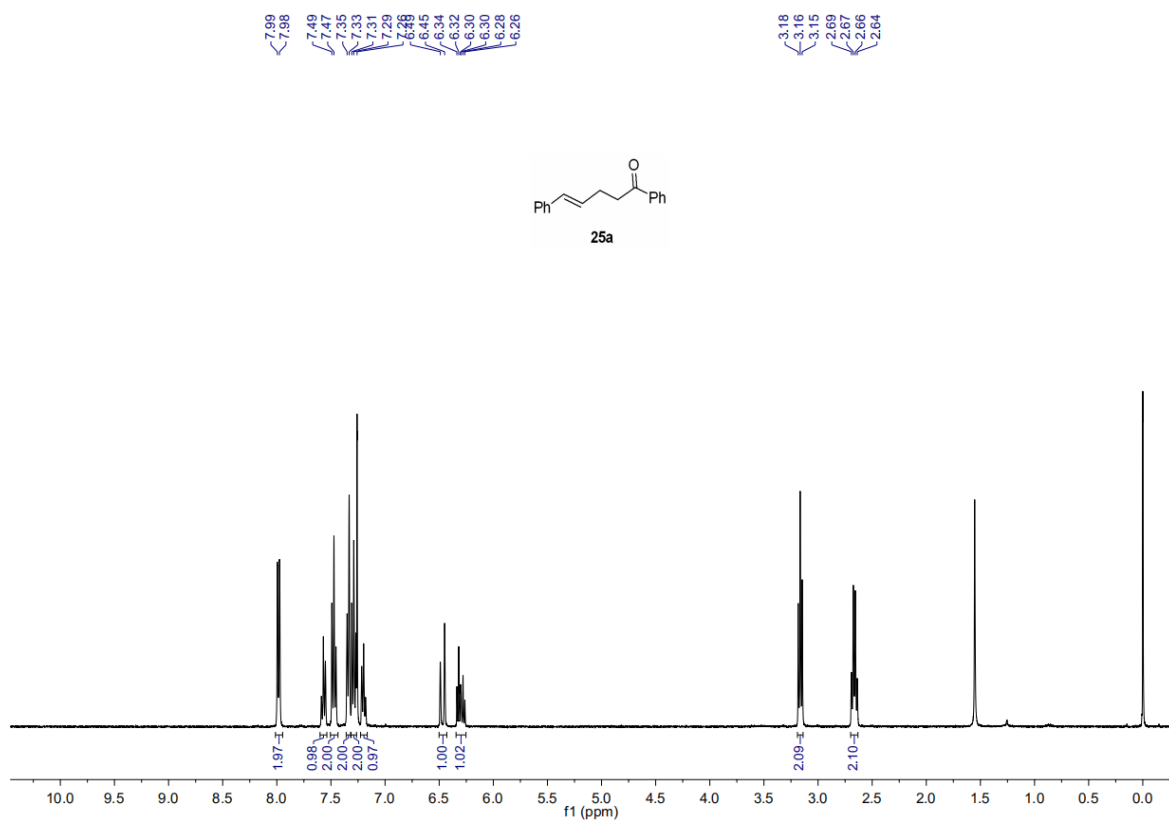


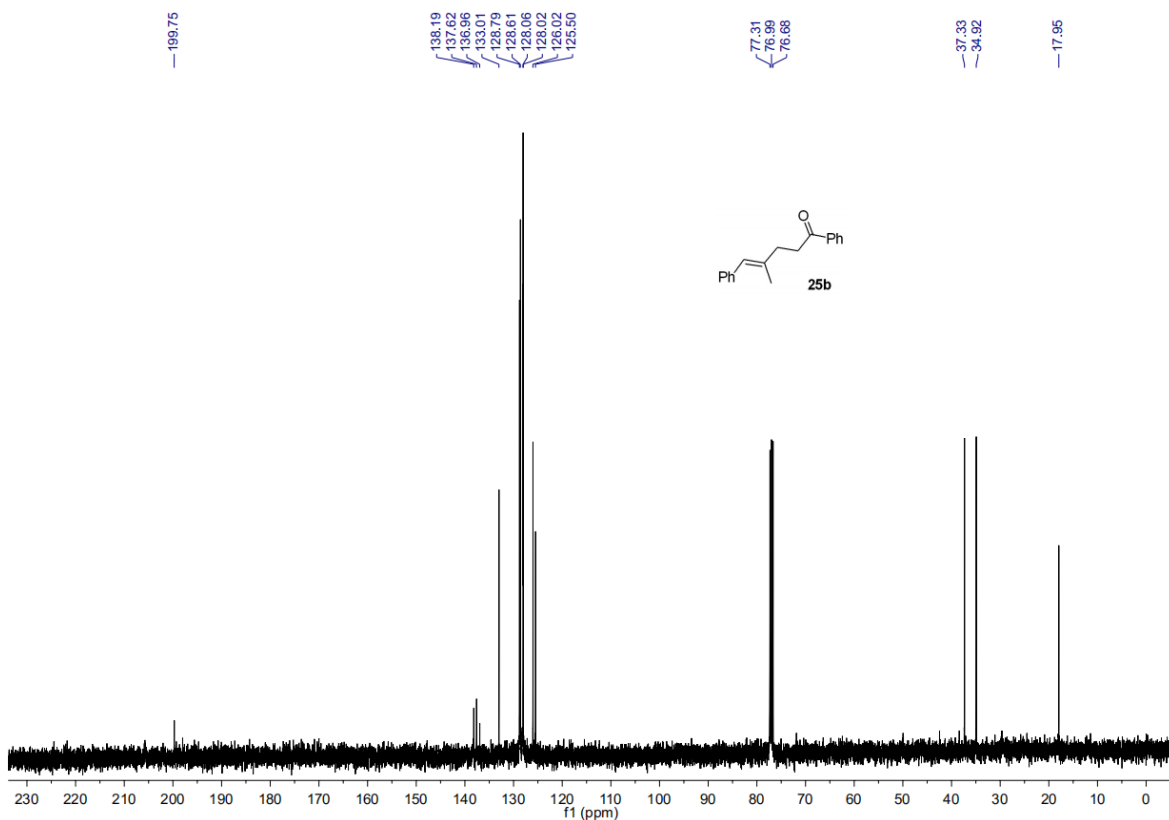
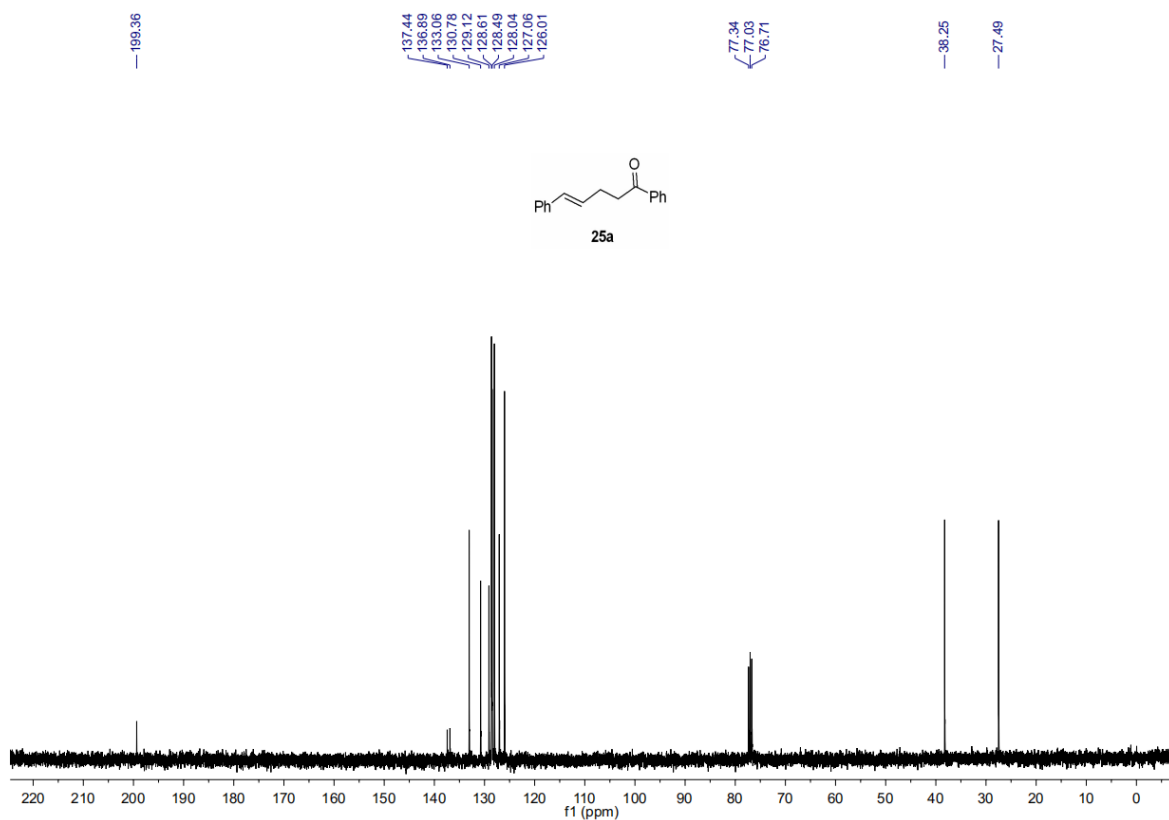


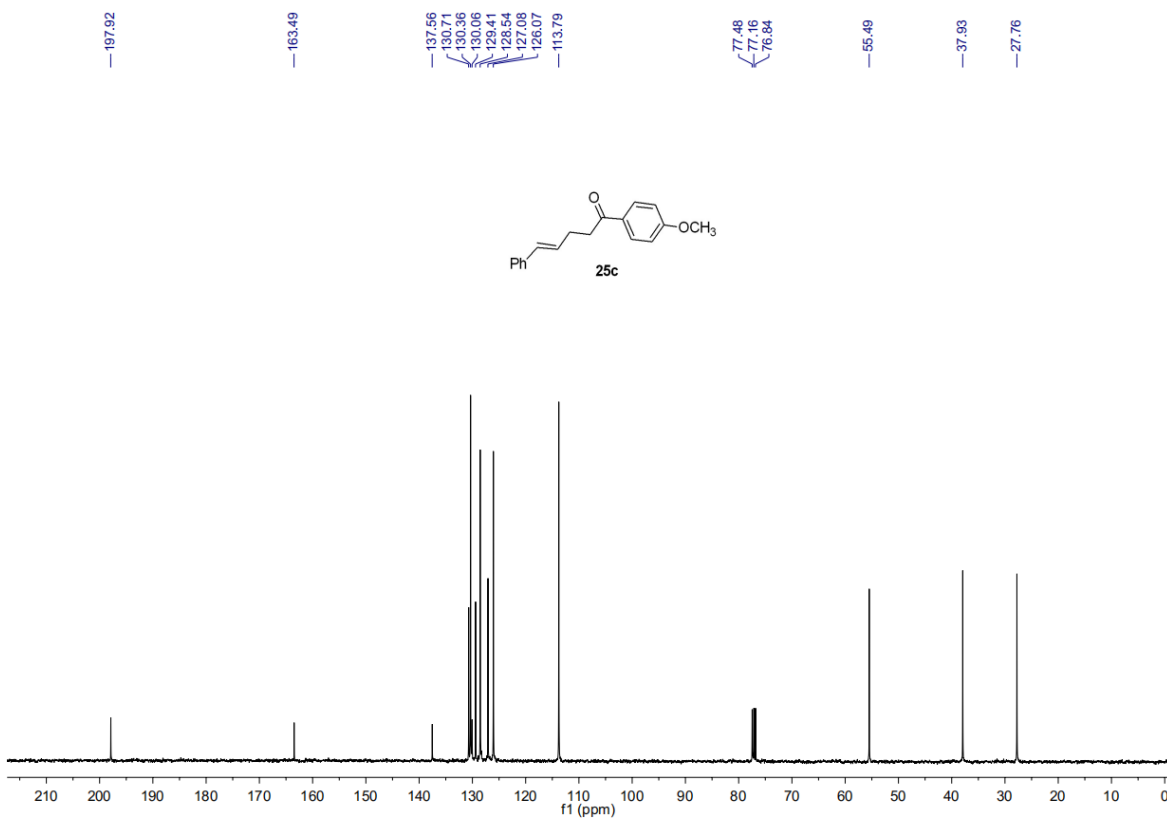
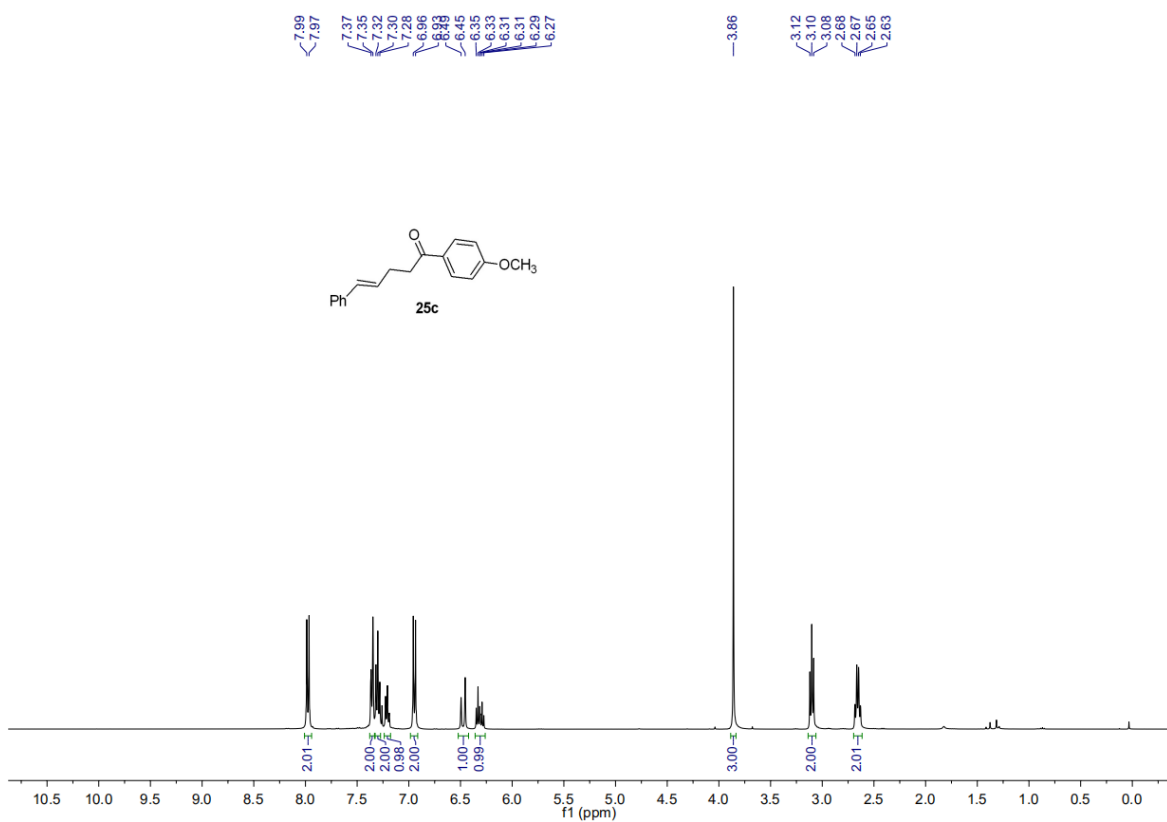


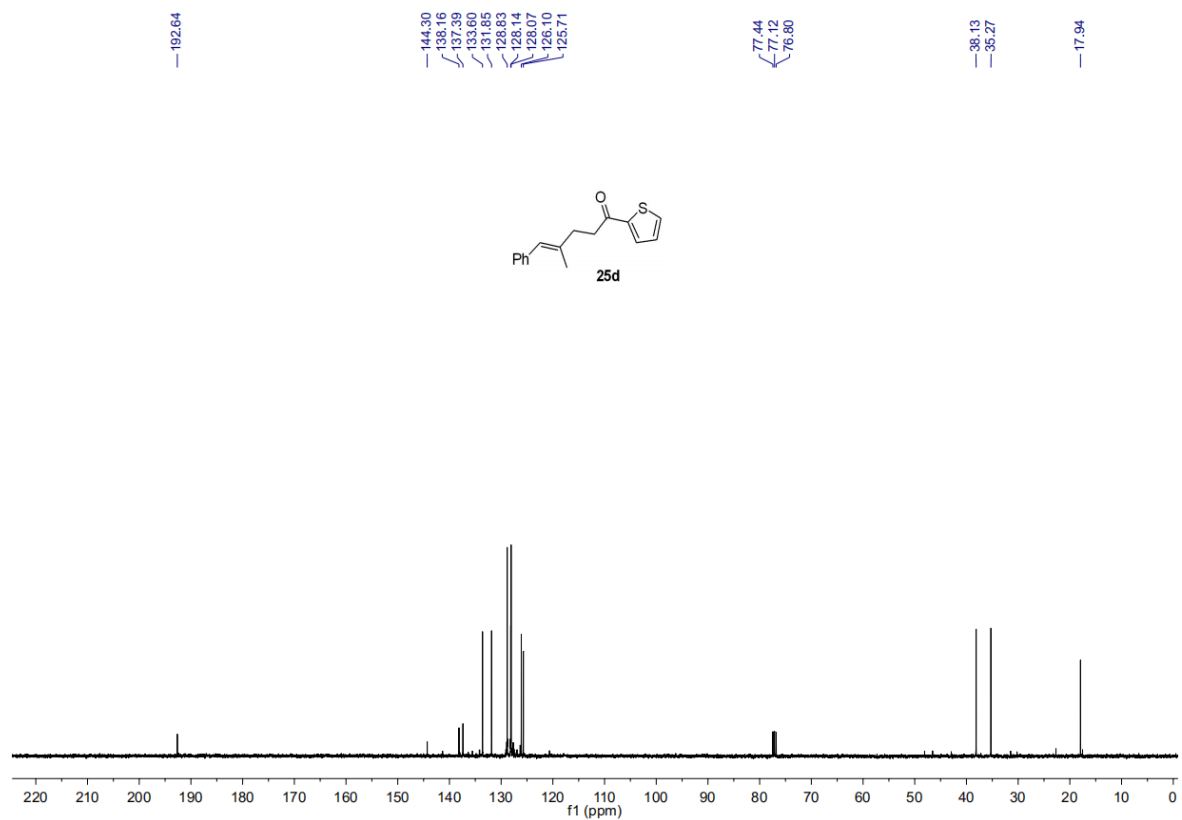
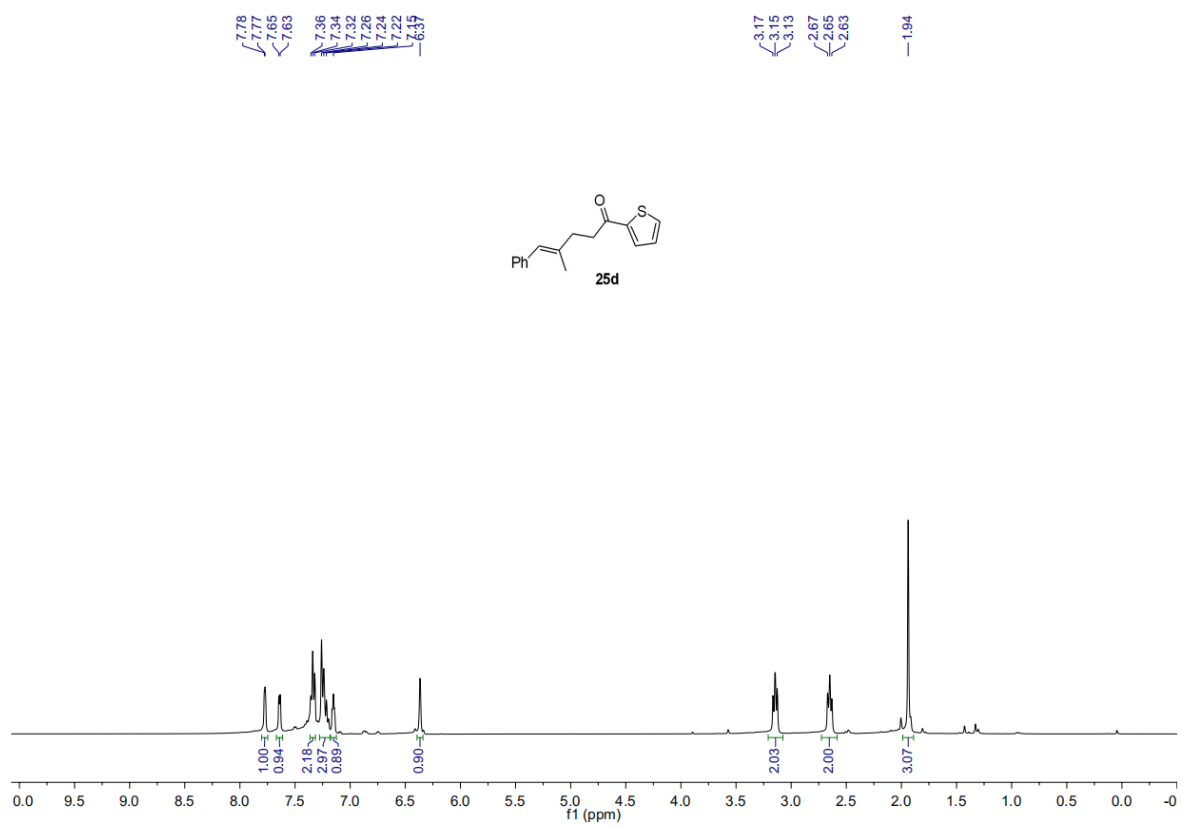


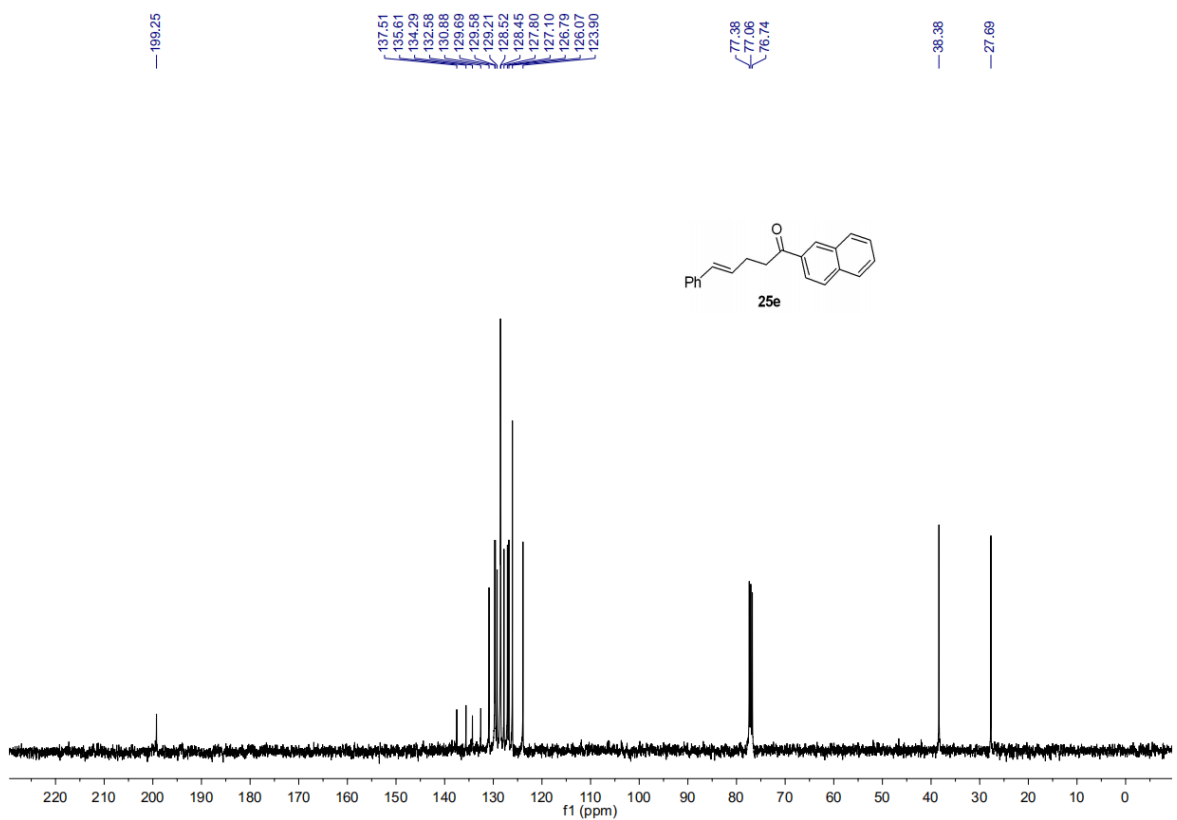
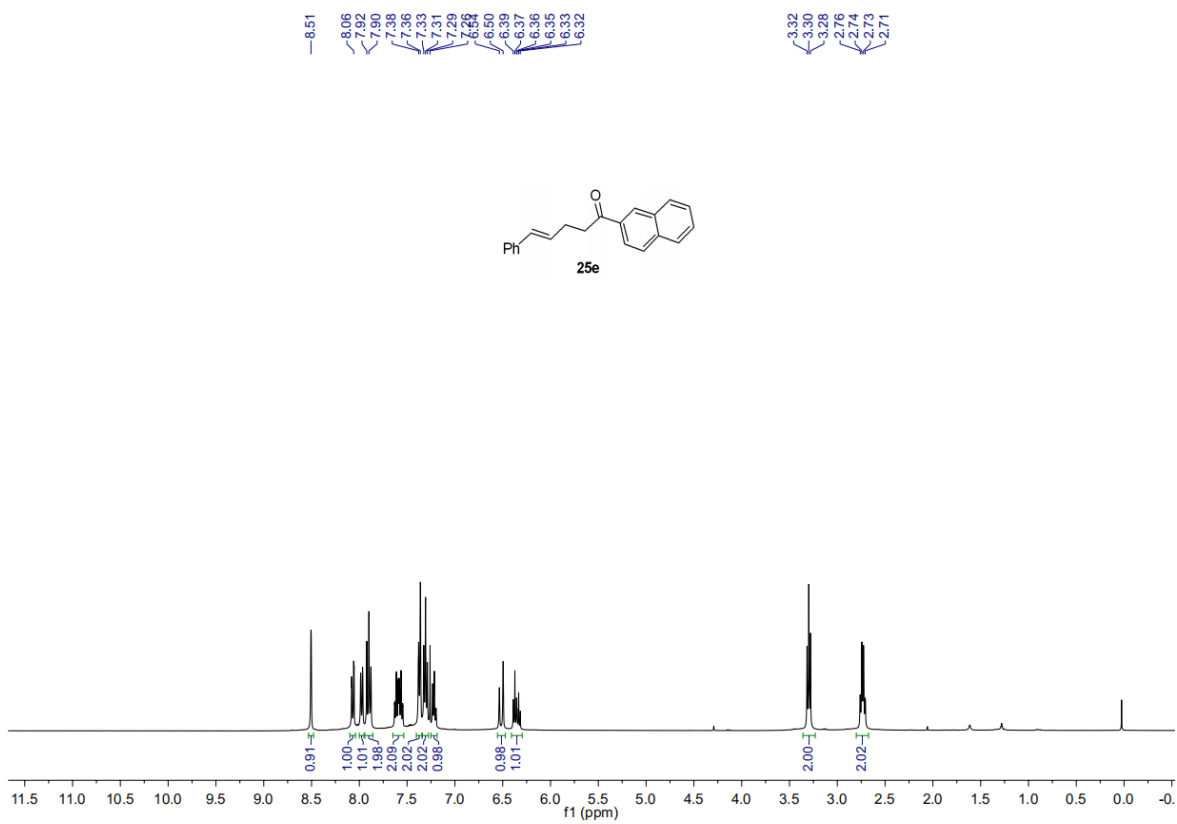


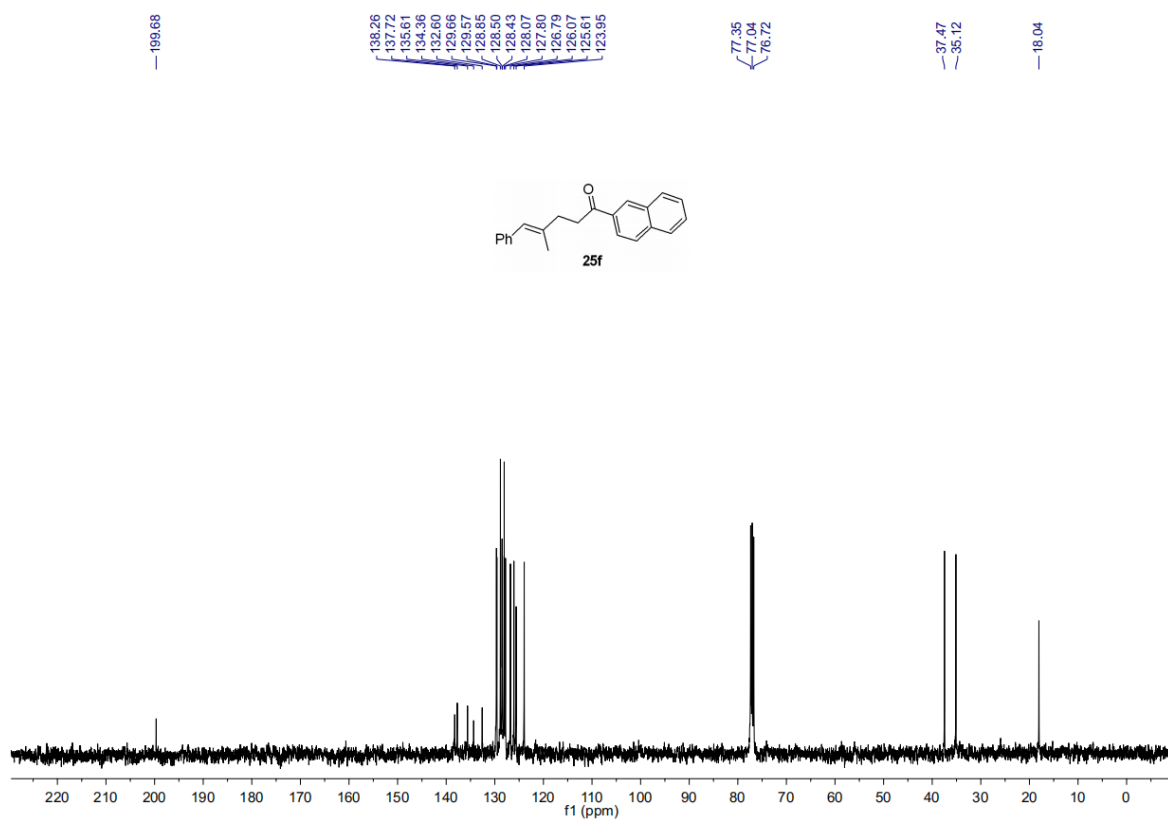
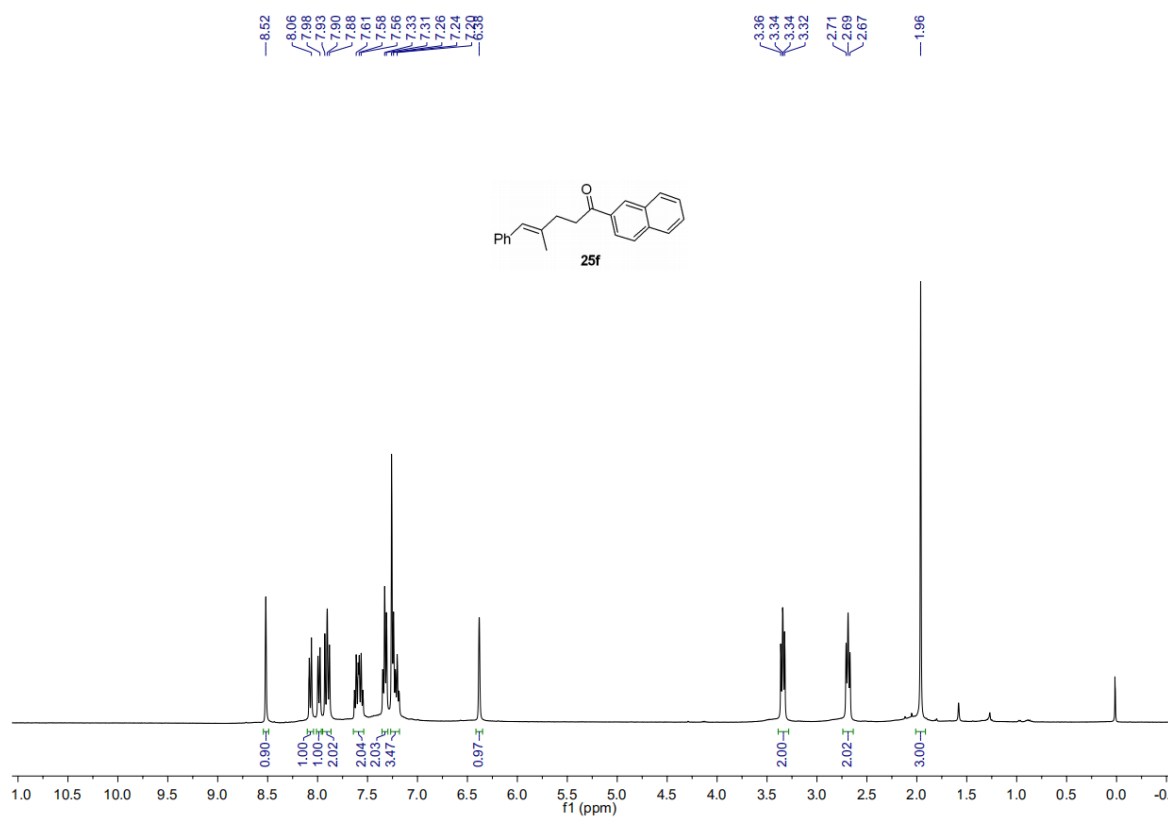




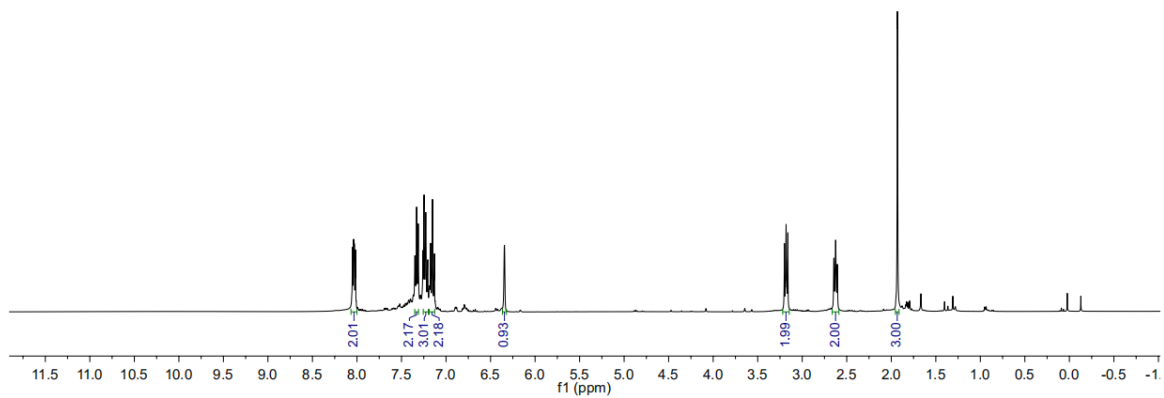
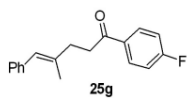




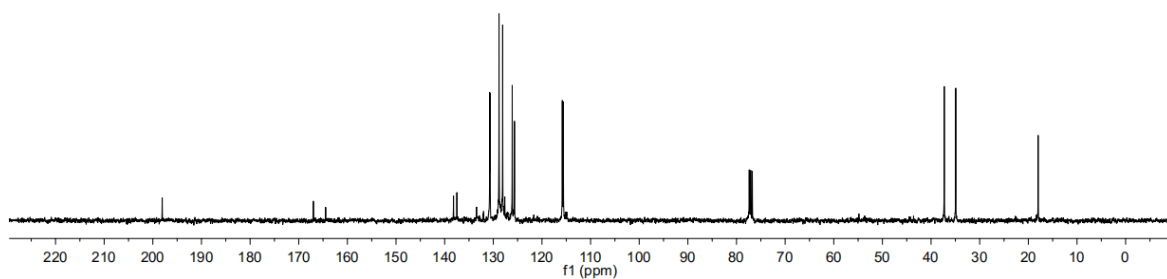
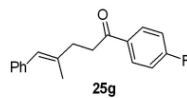


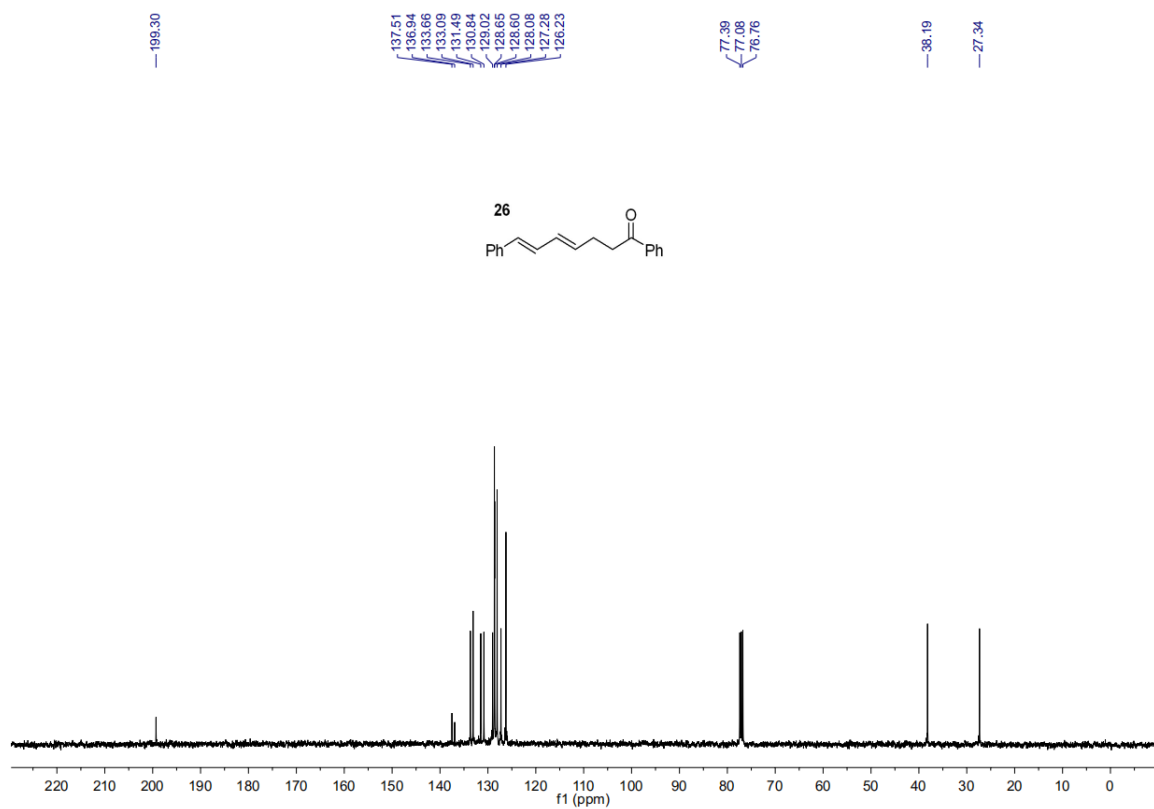
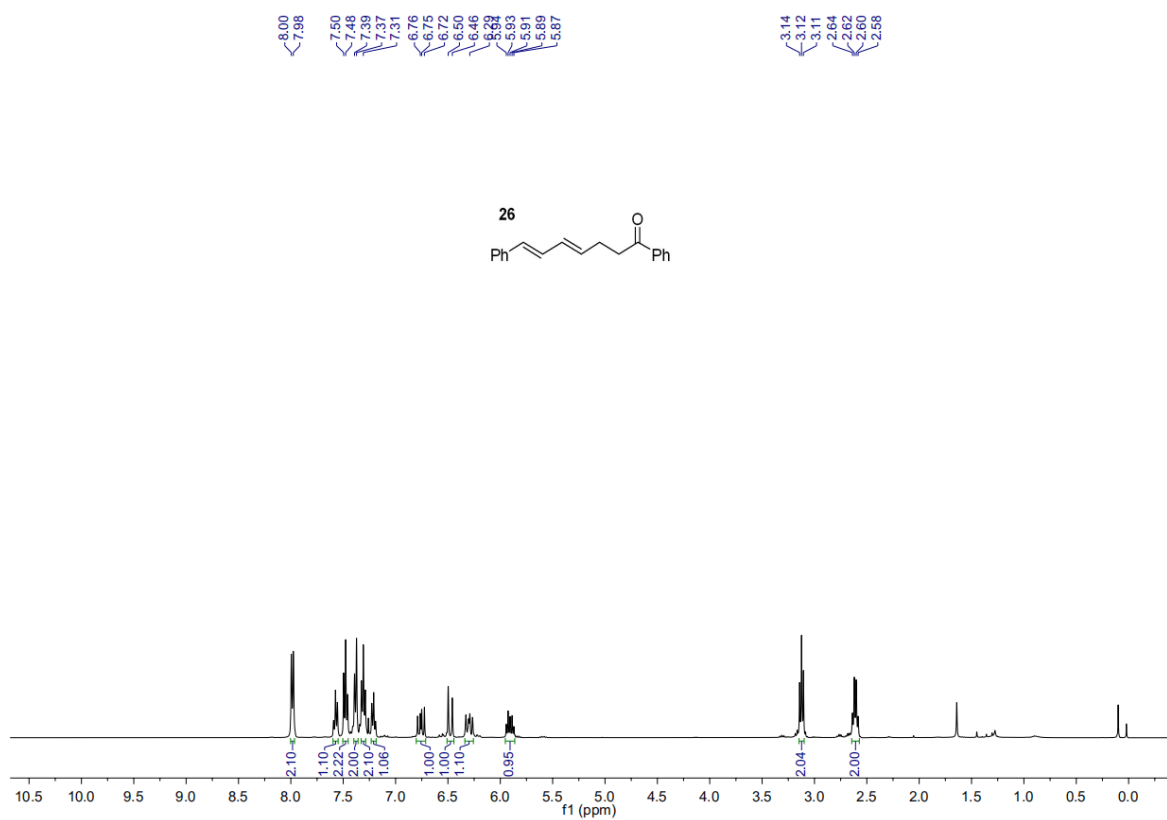


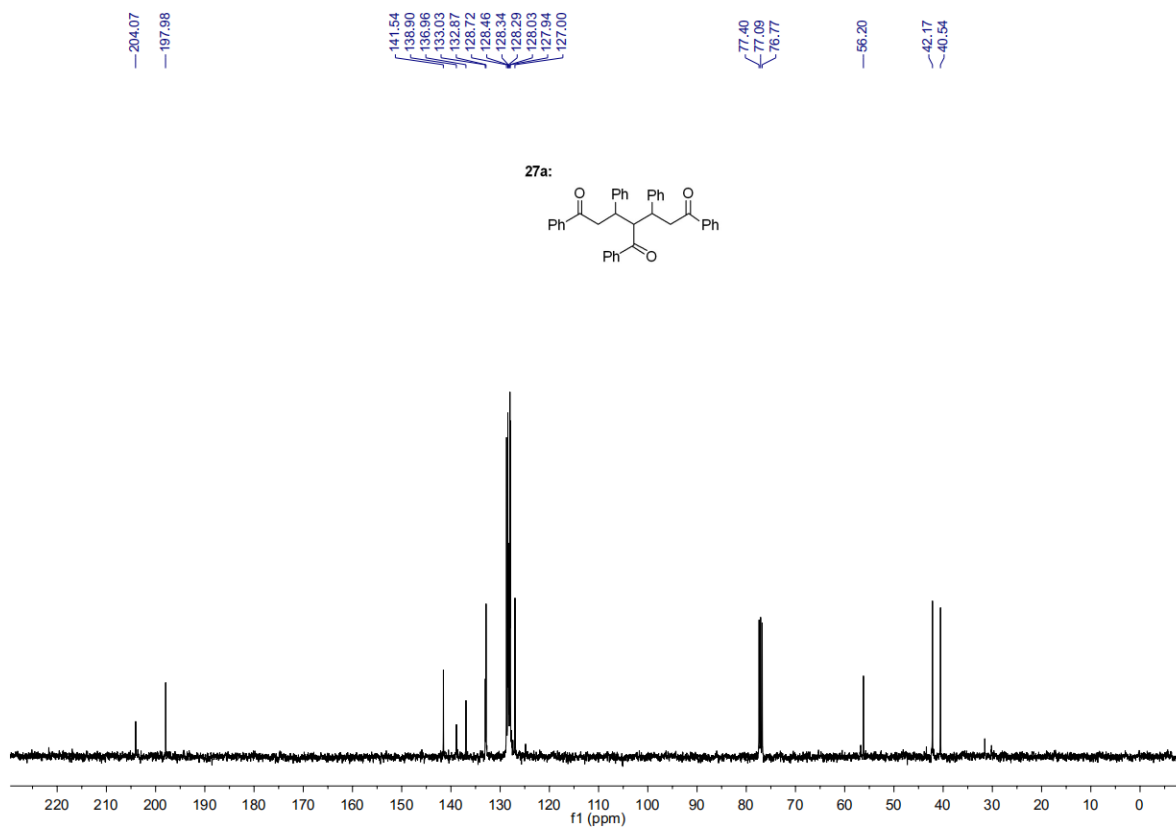
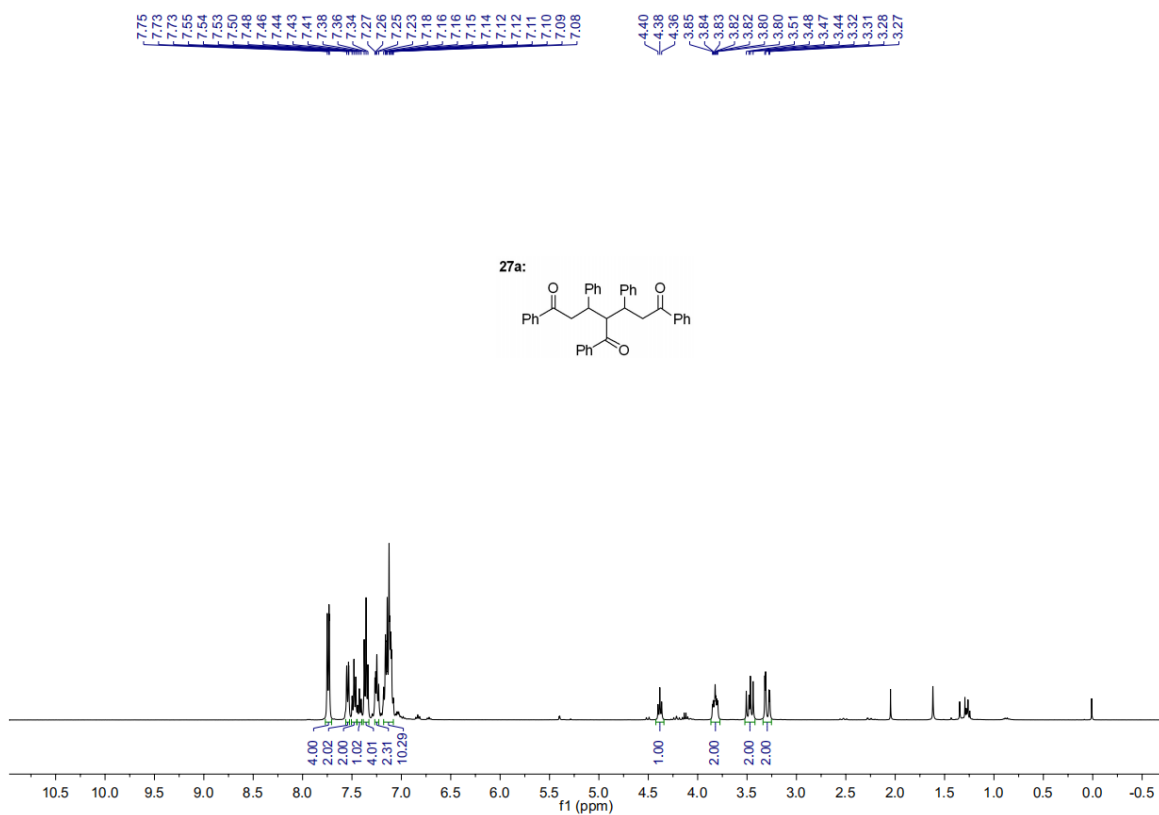
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1.93
1.93

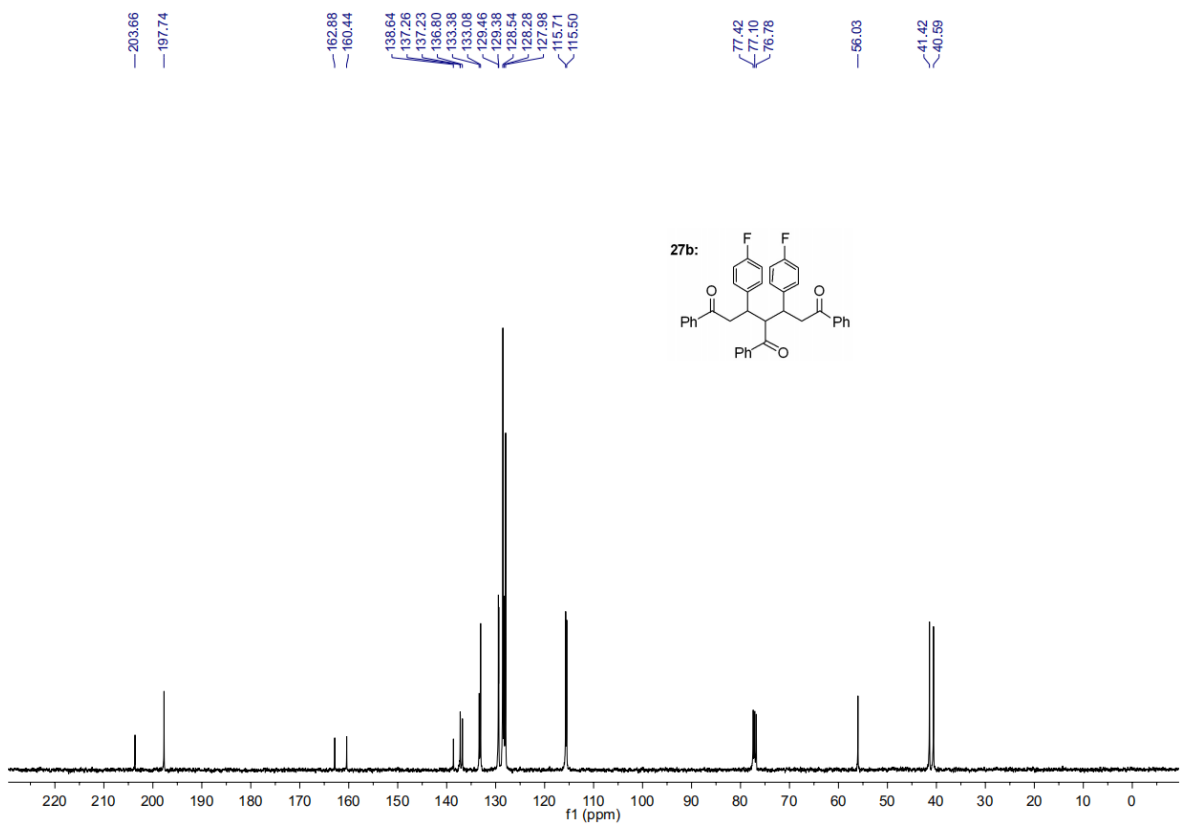
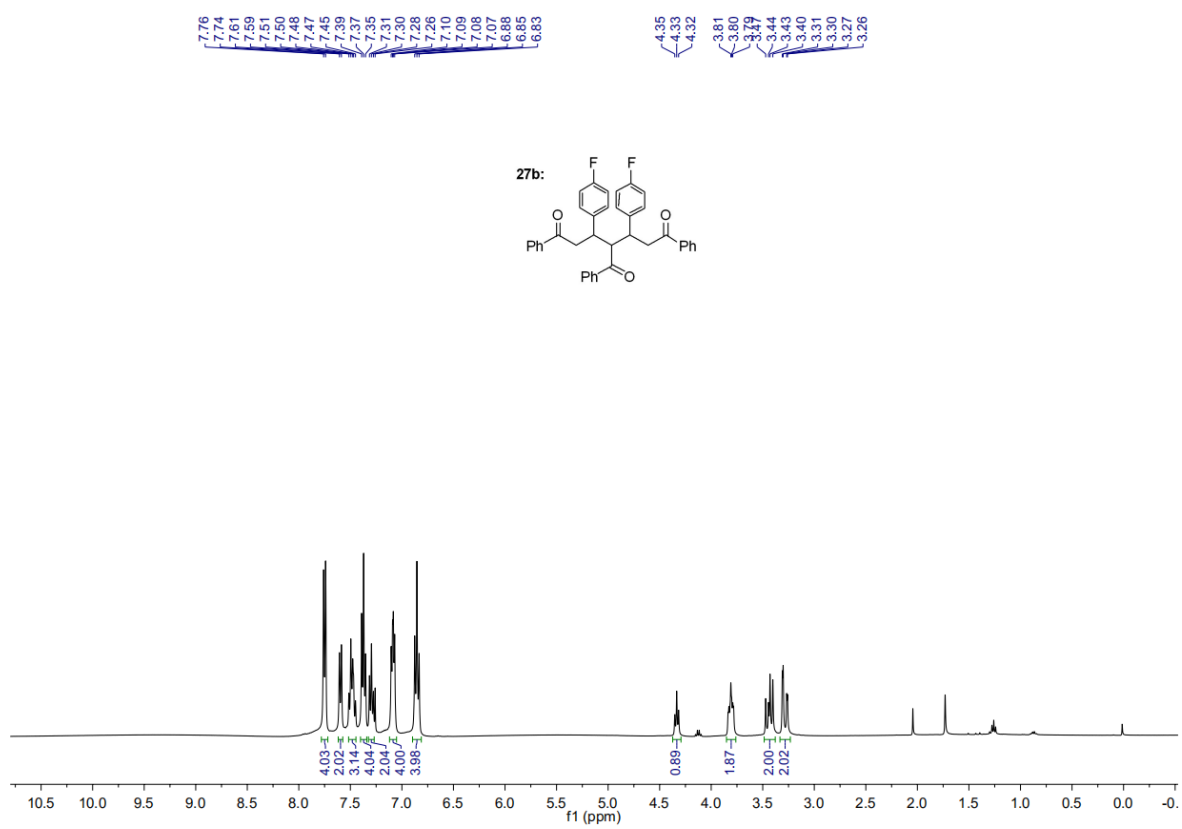


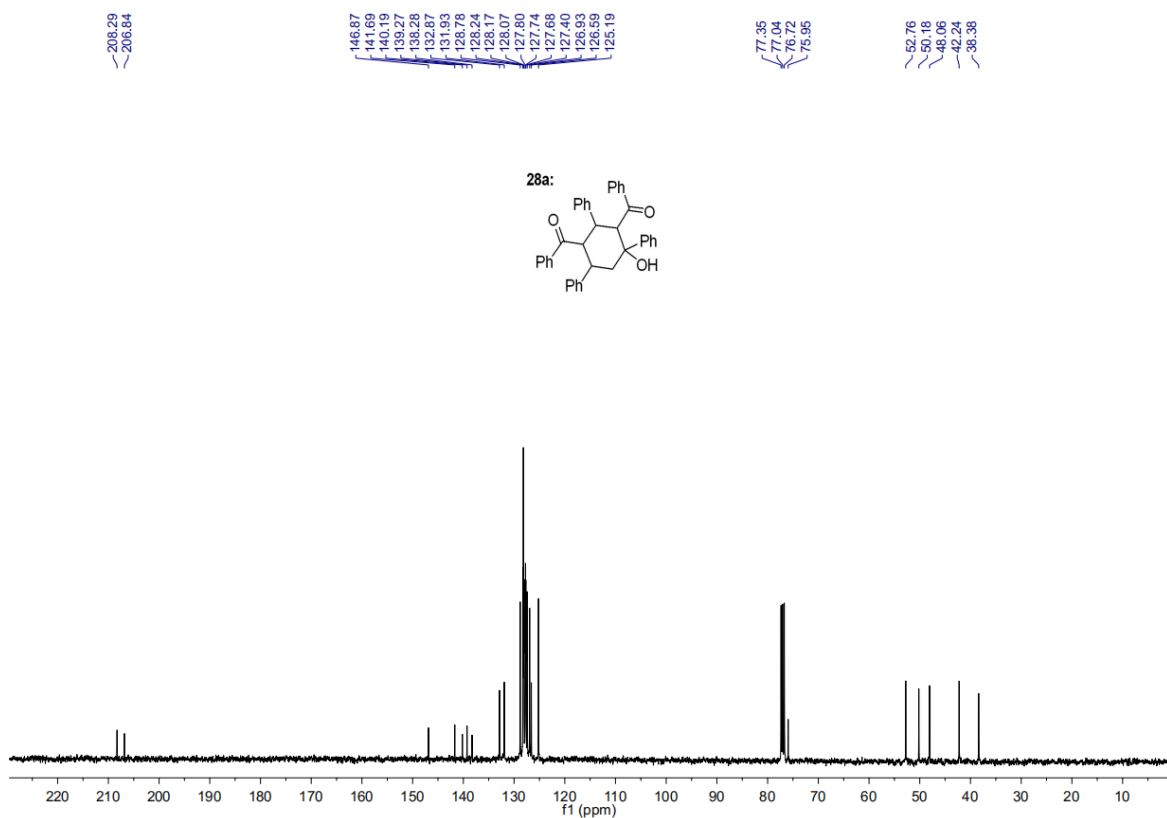
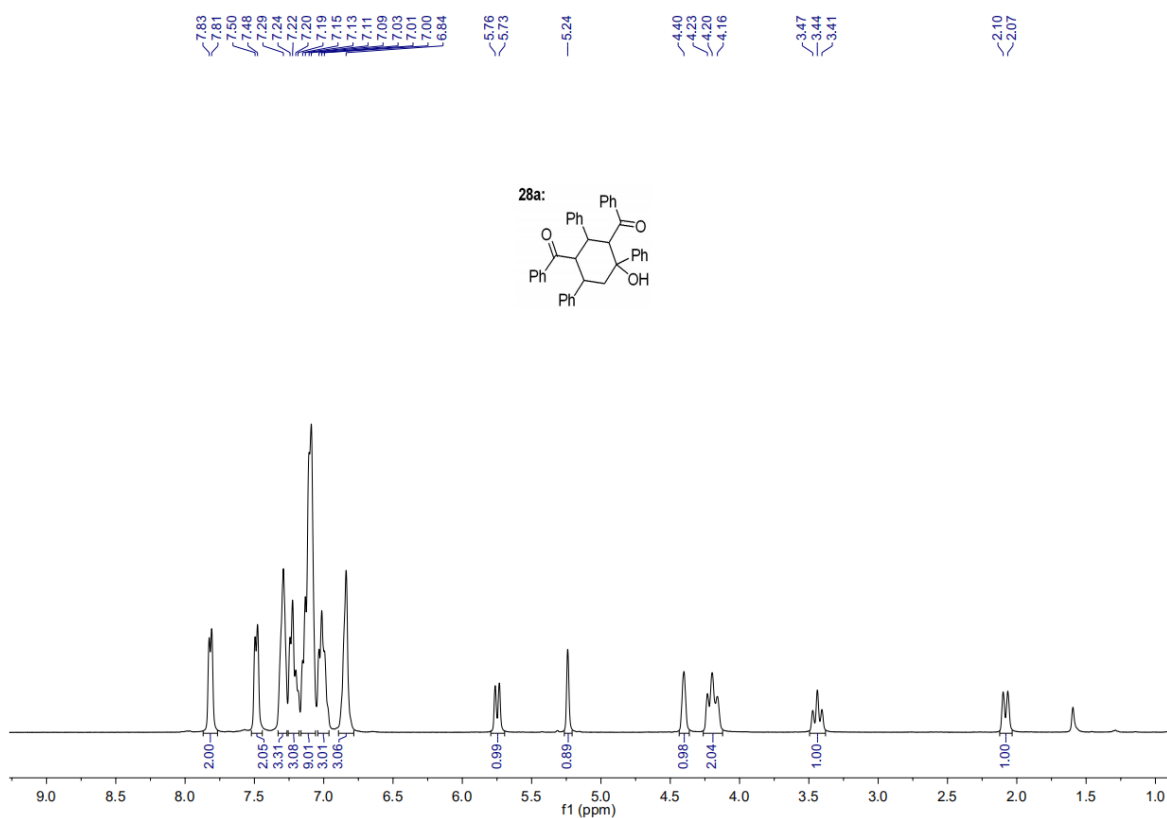
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34.93
17.98

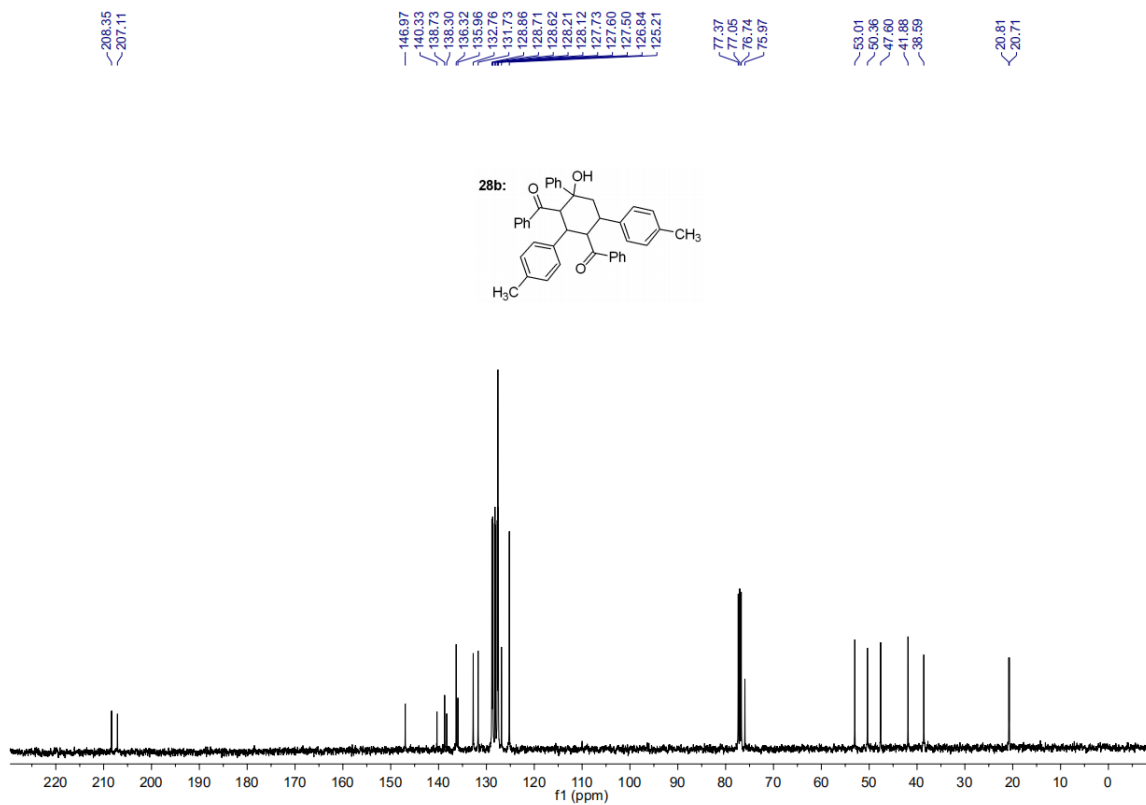
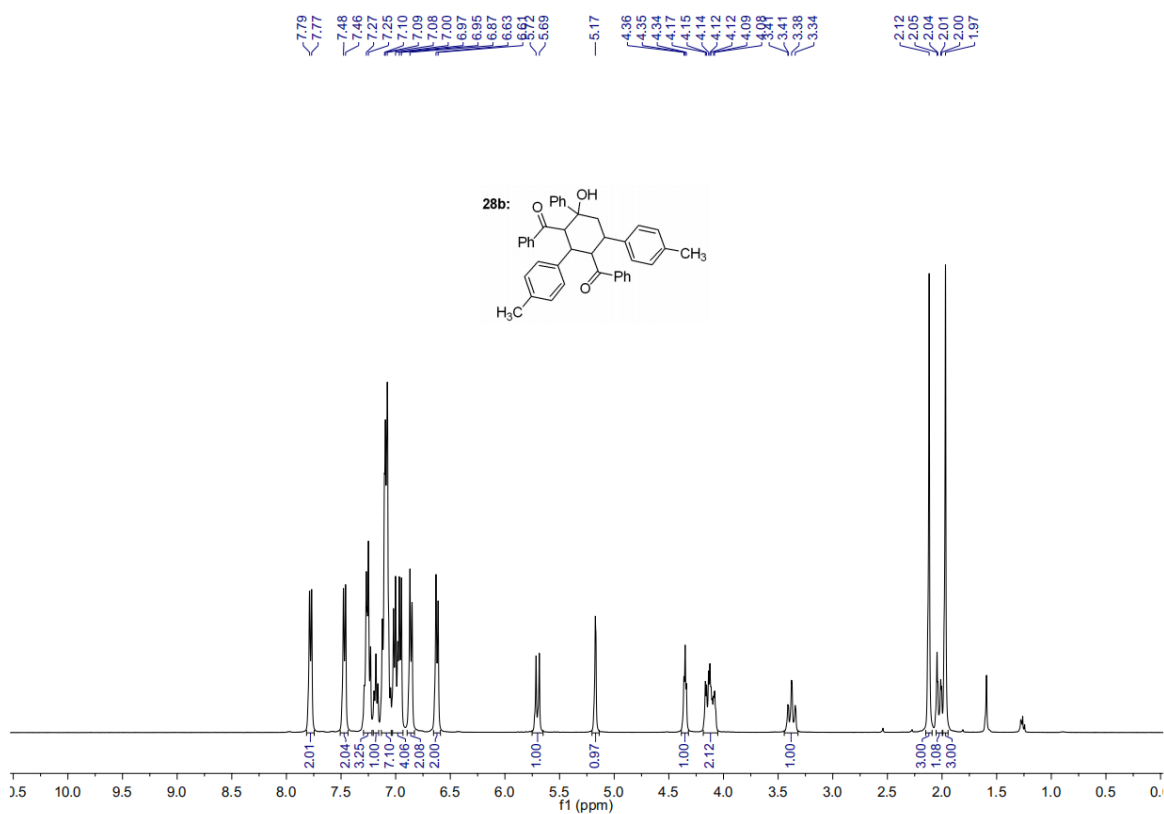


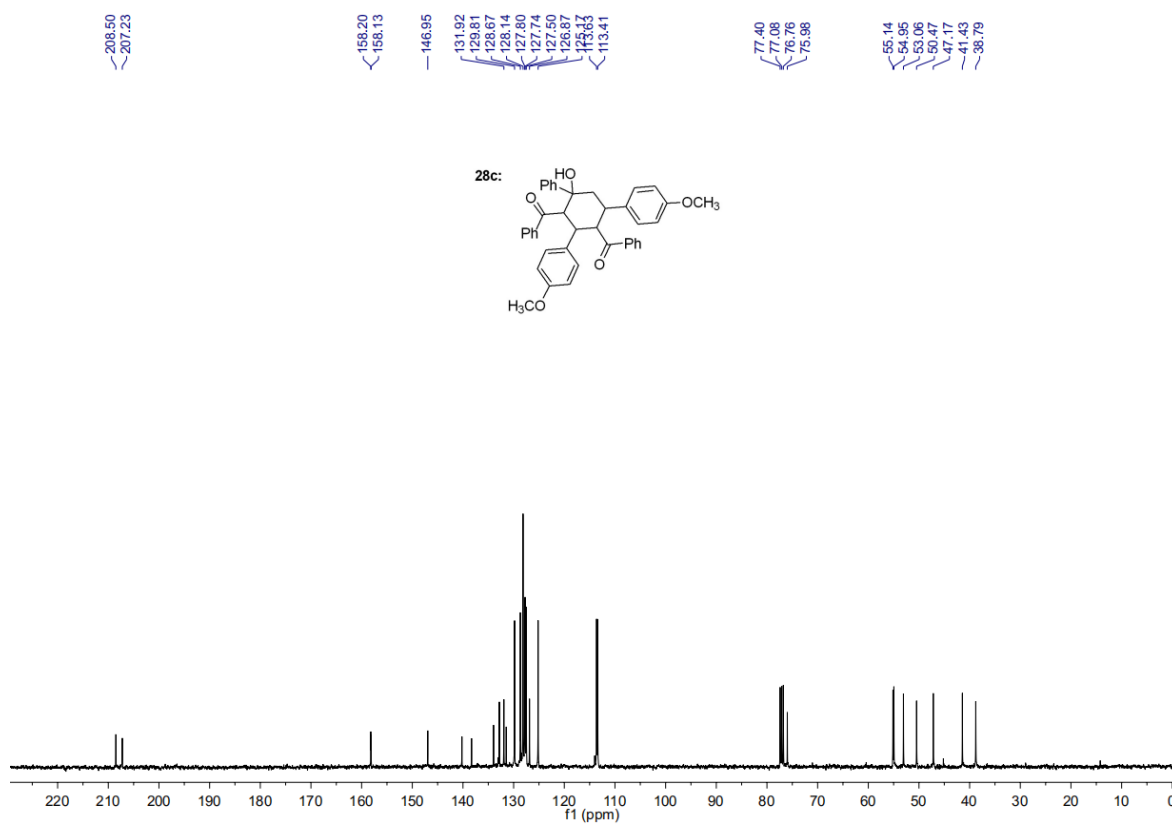
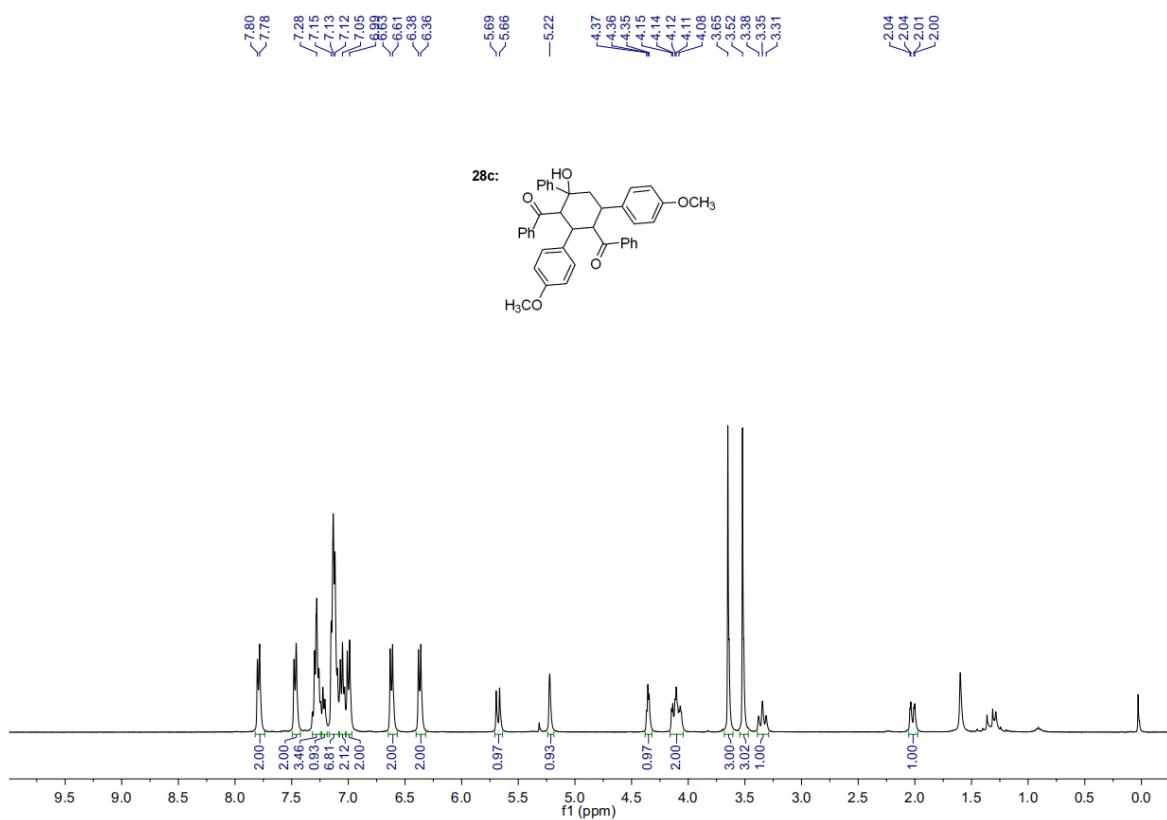


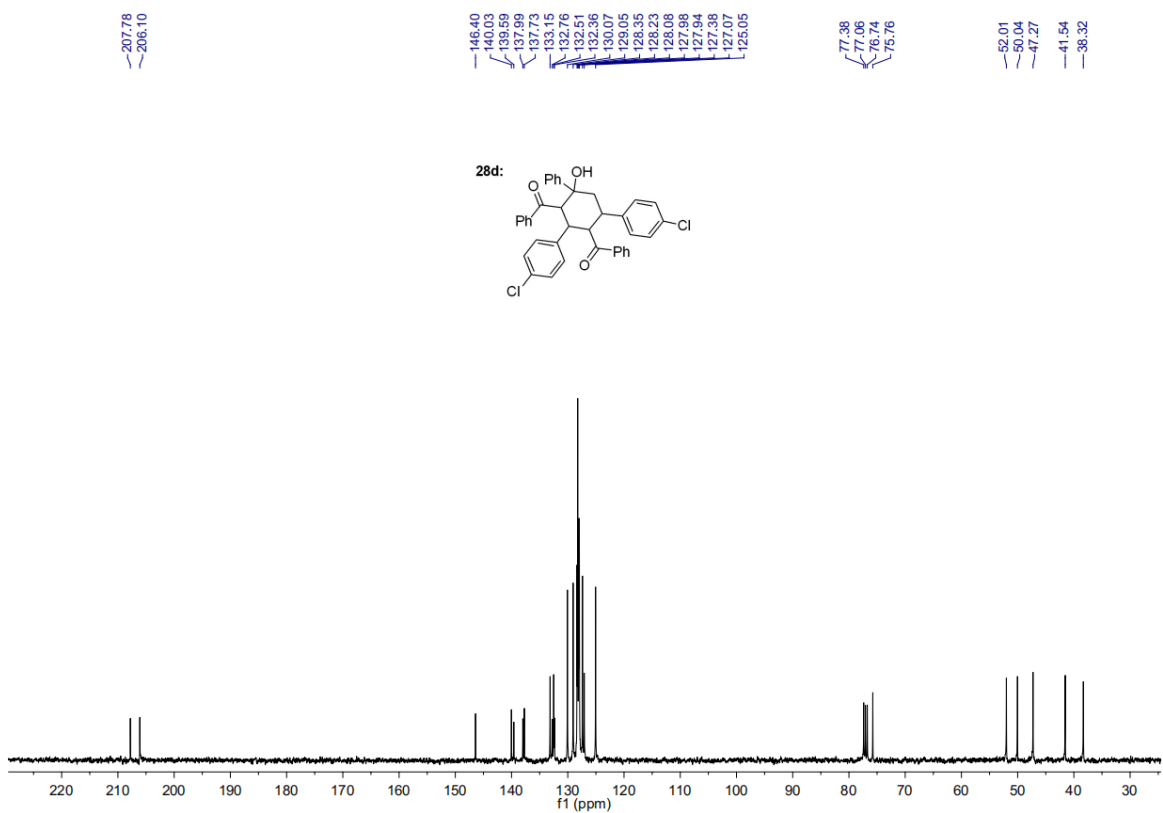
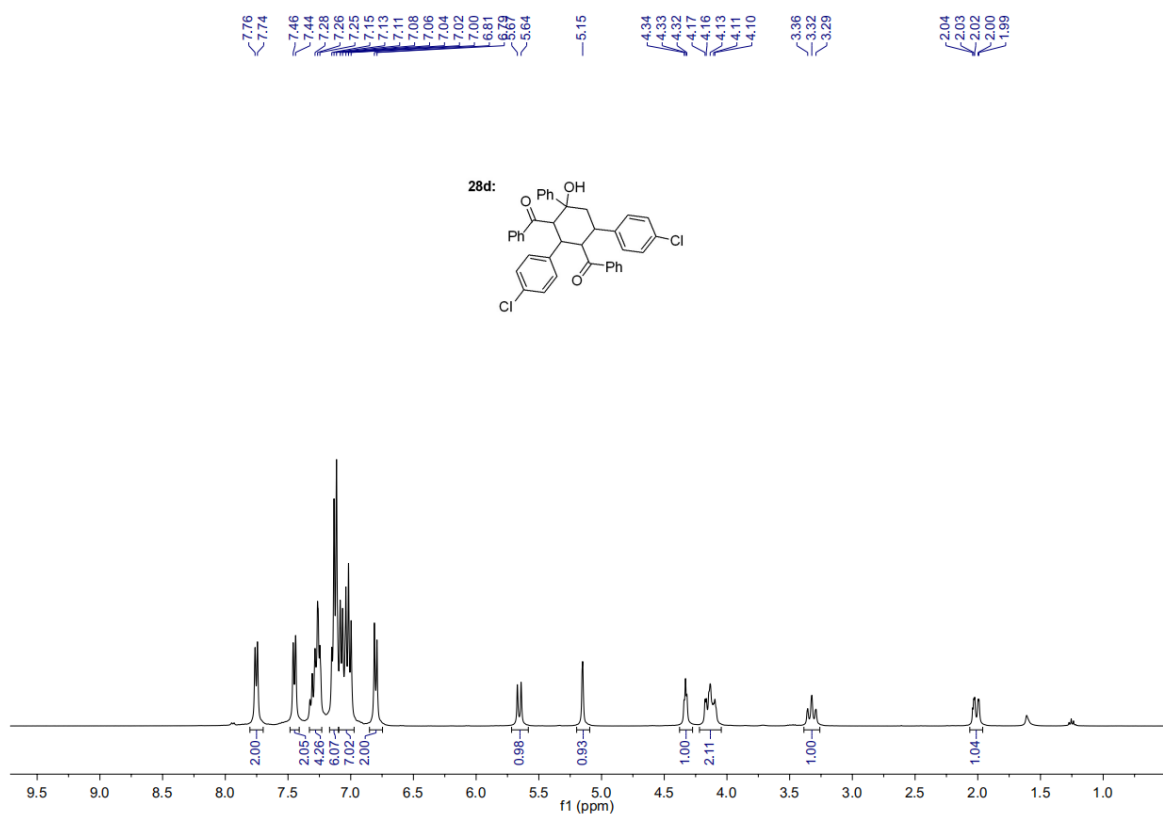


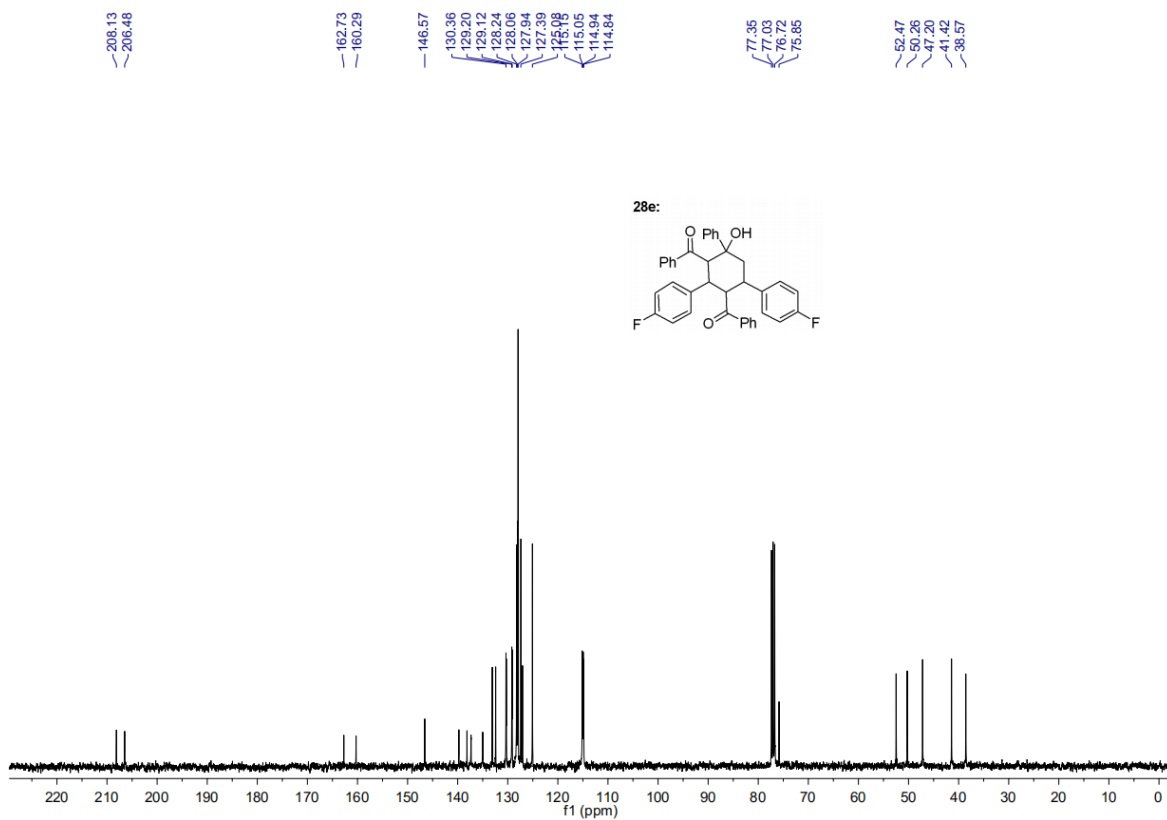
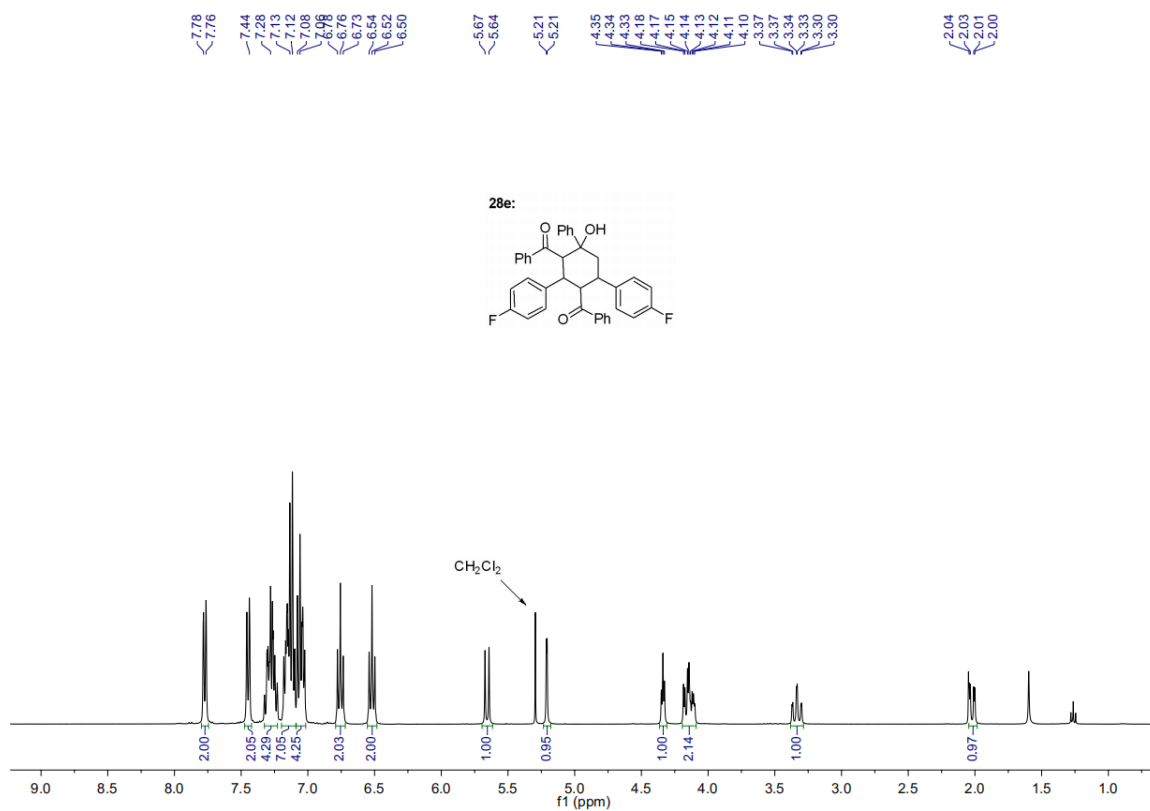


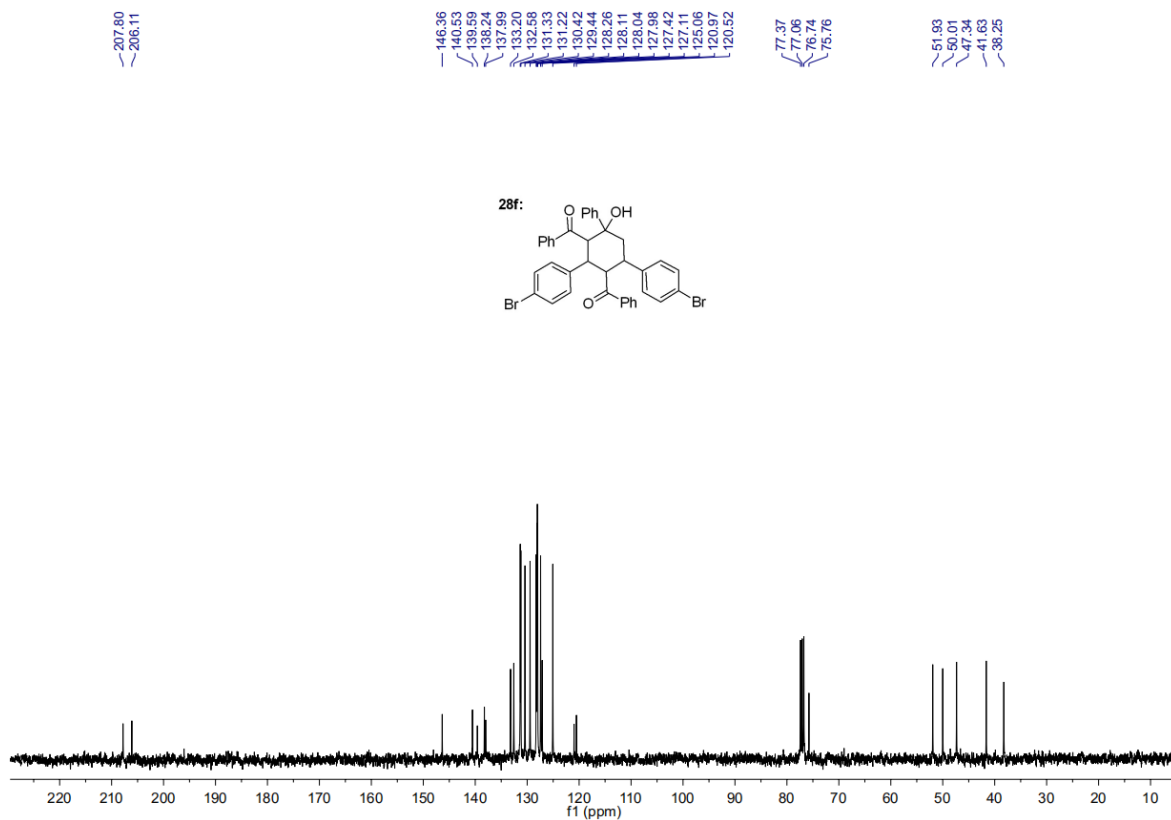
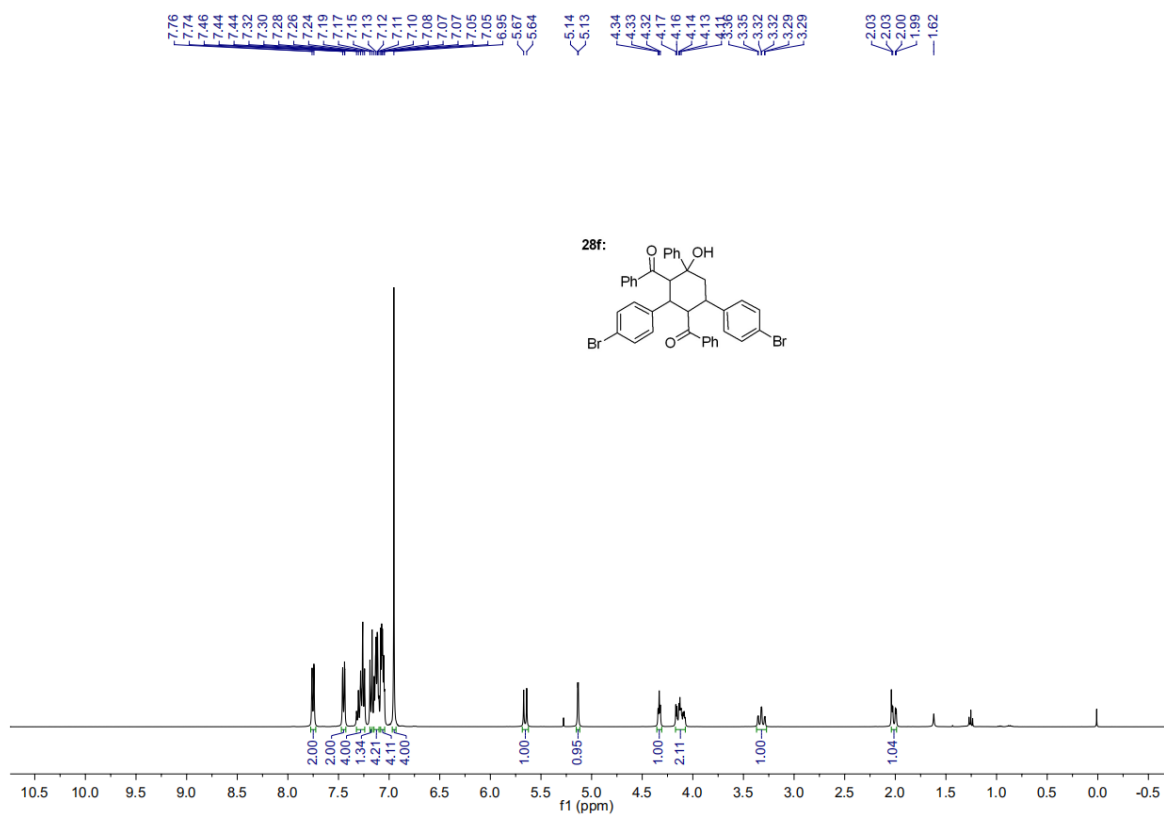


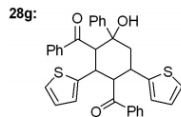
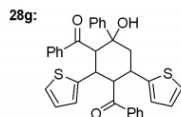


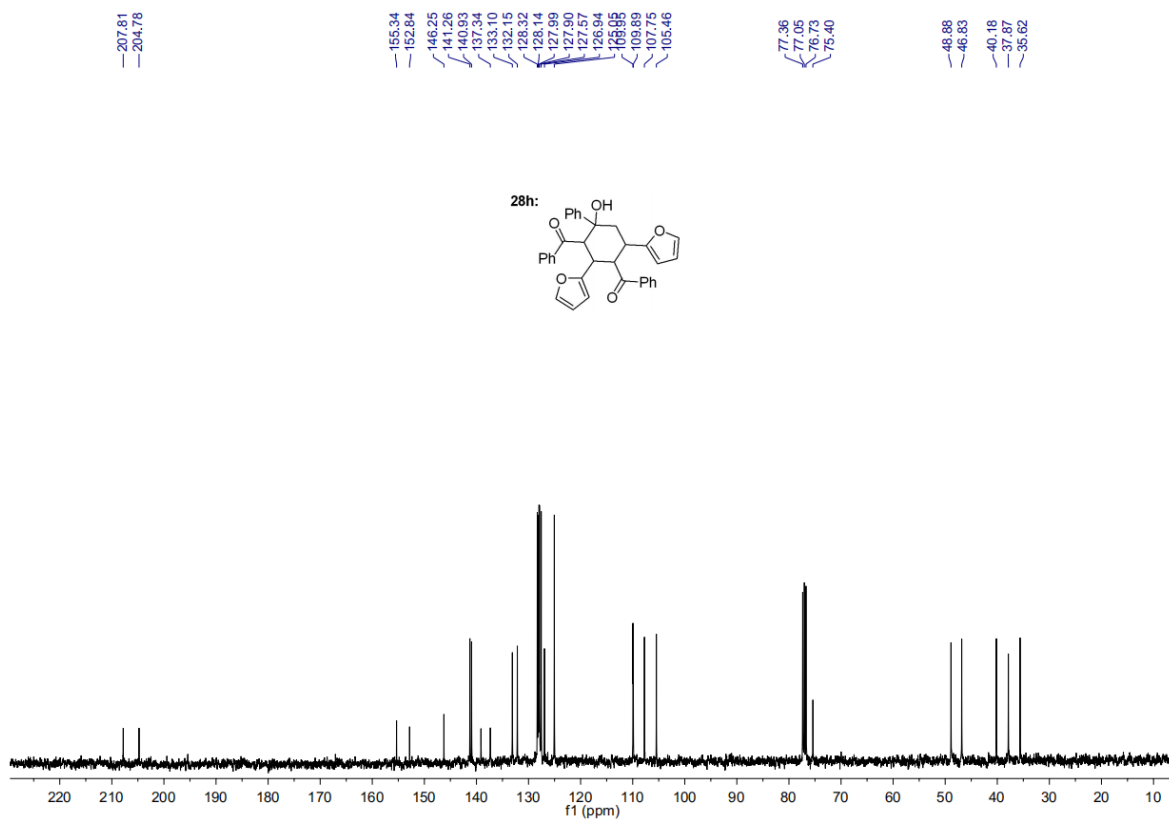
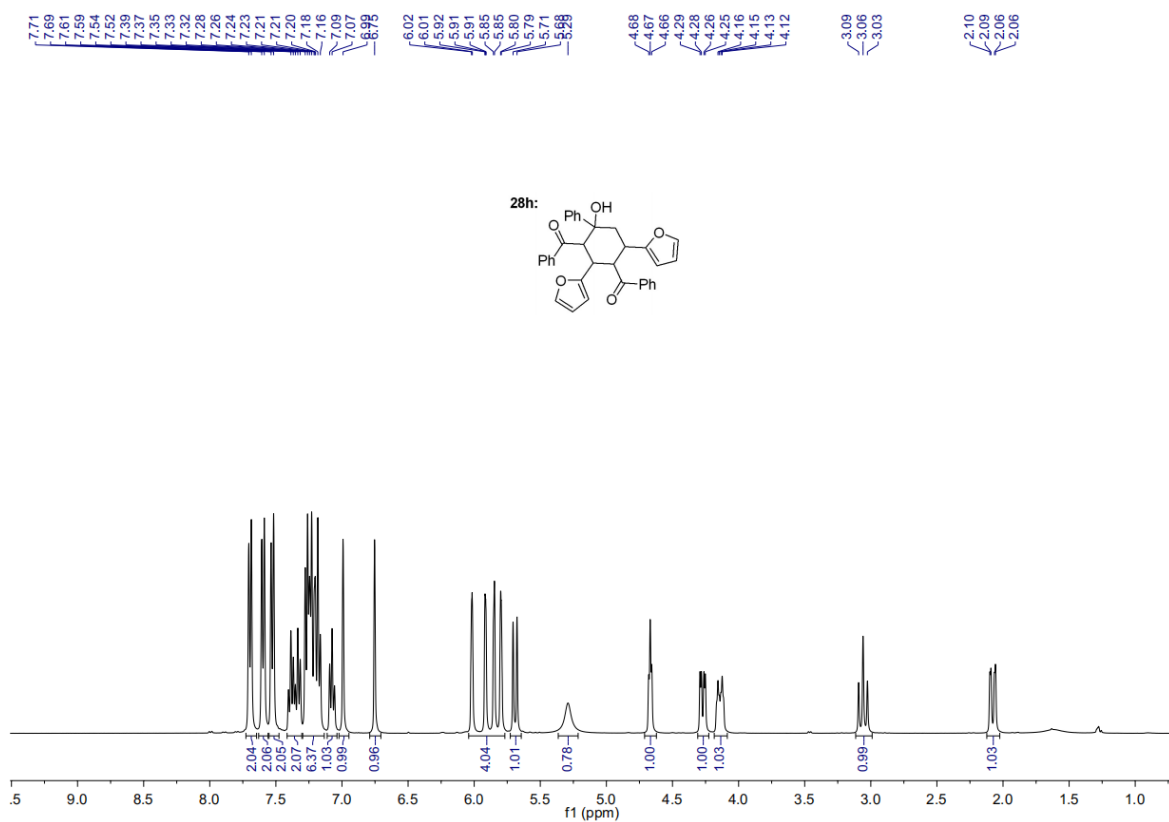






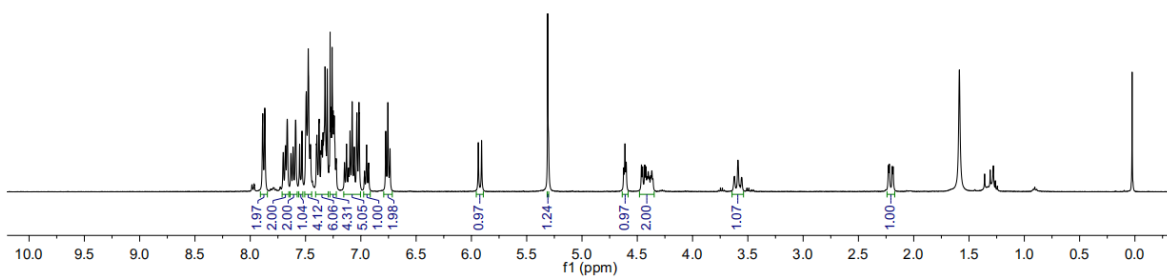
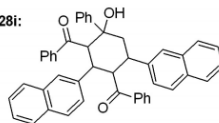








28i:

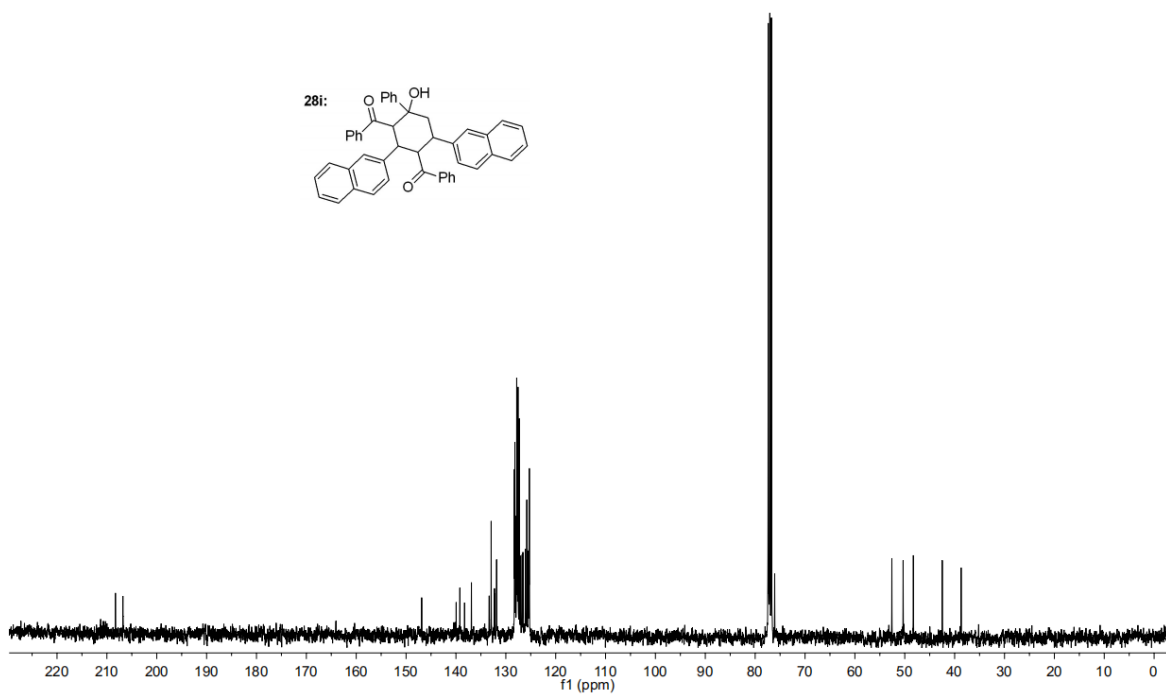
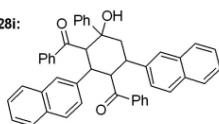


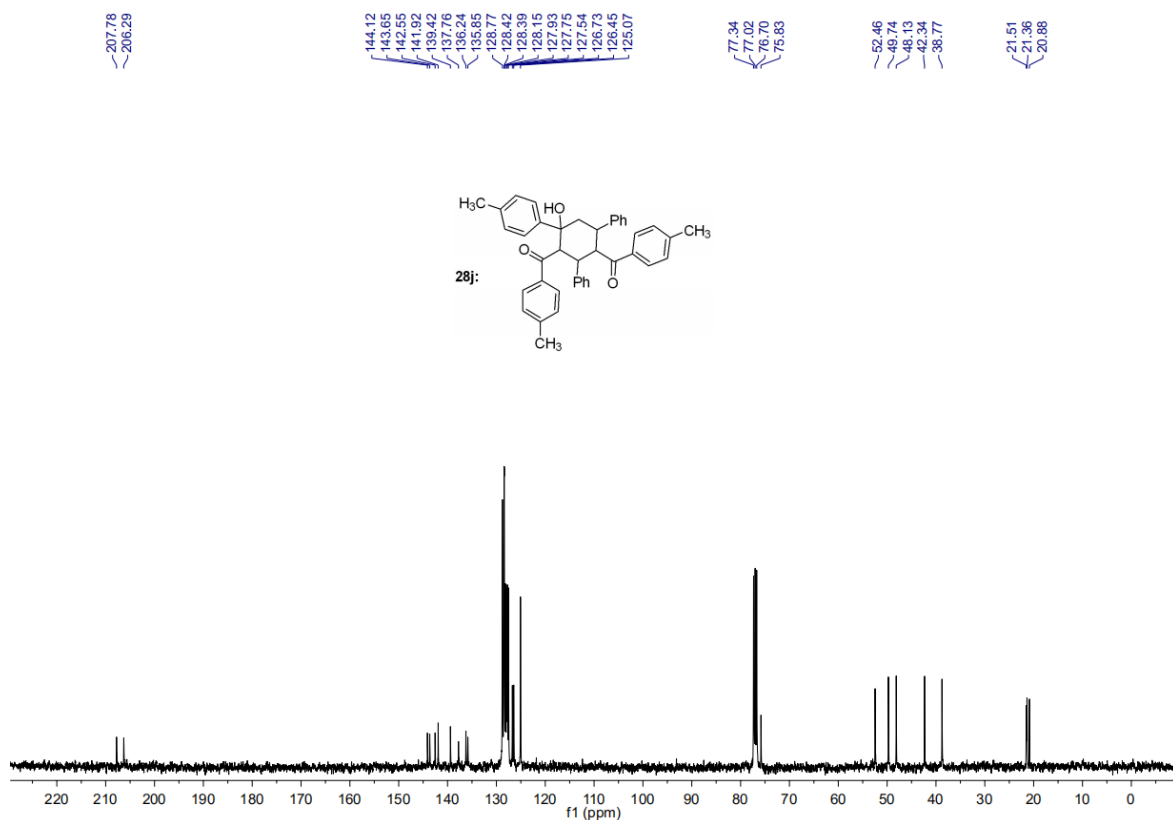
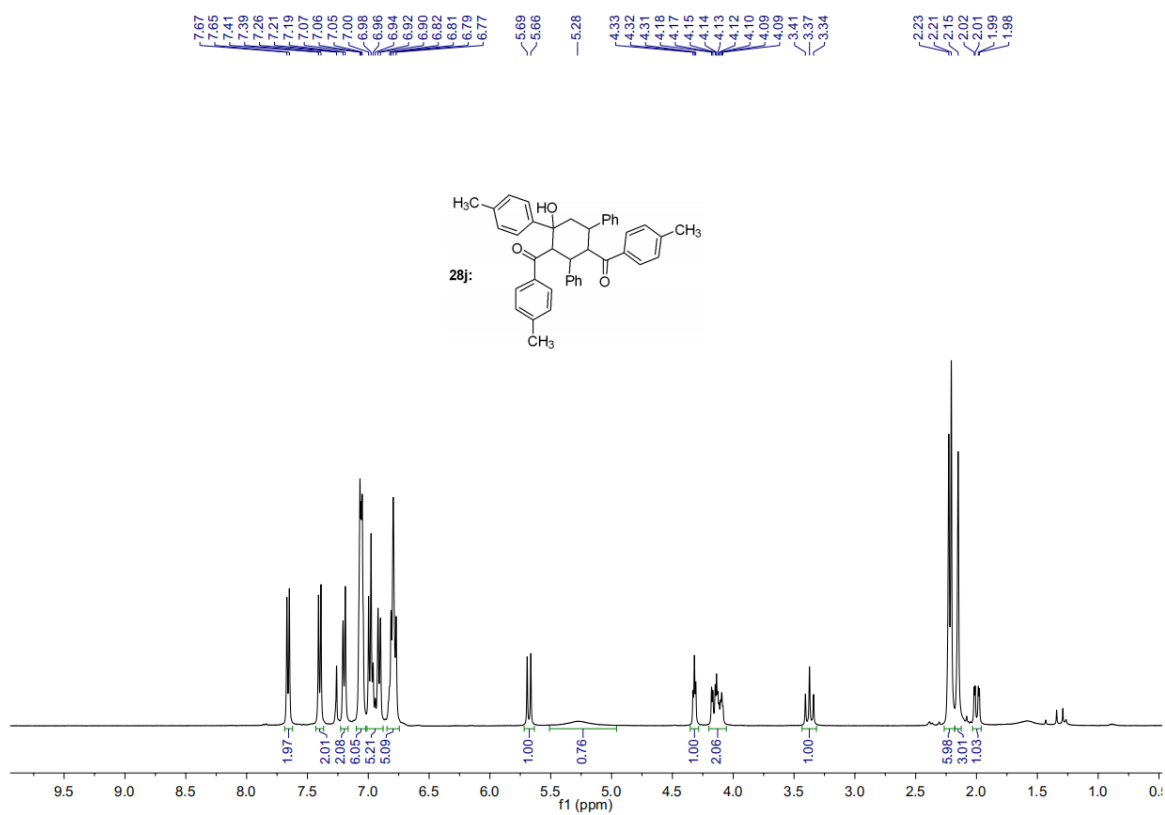
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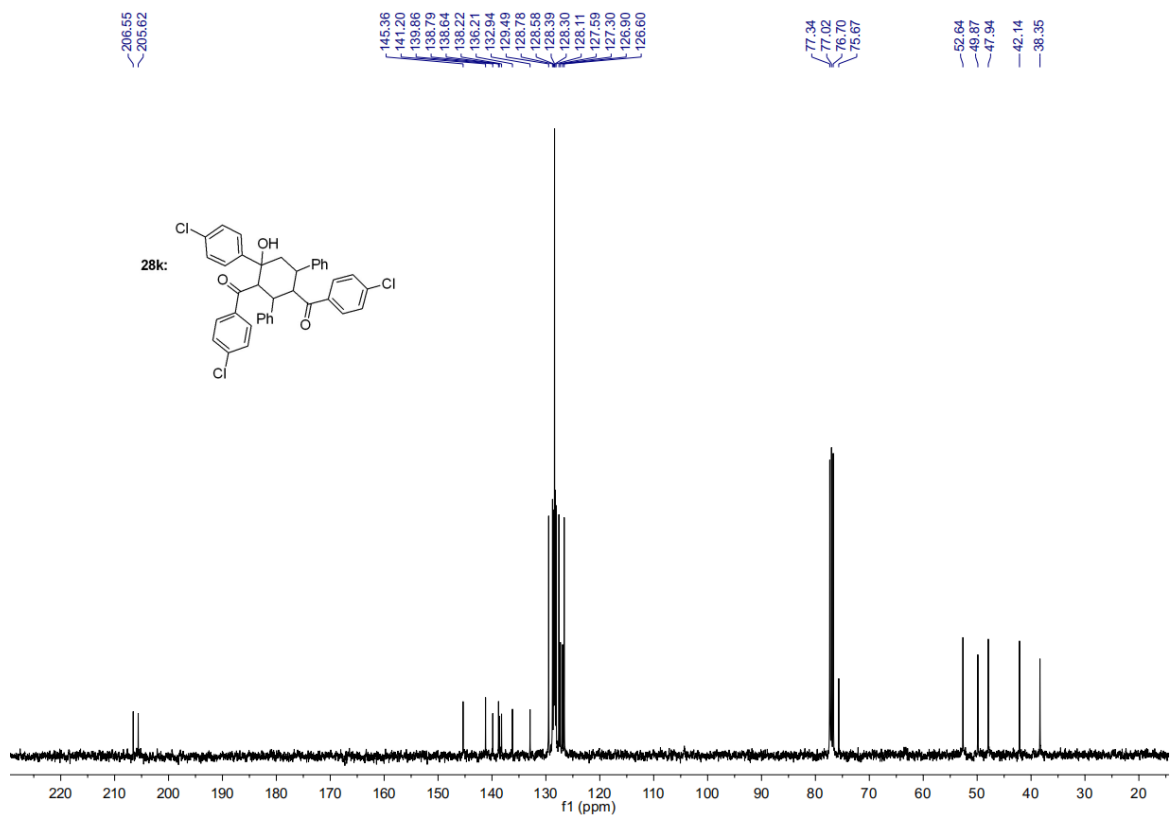
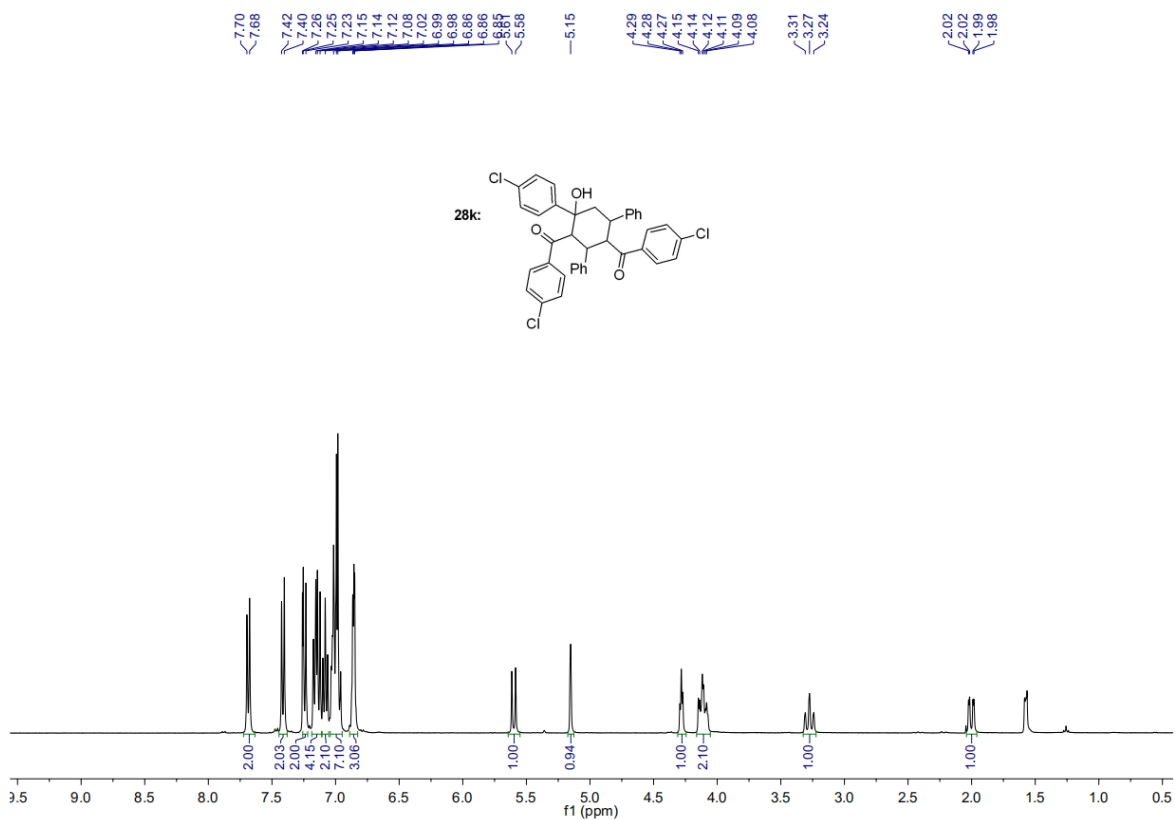
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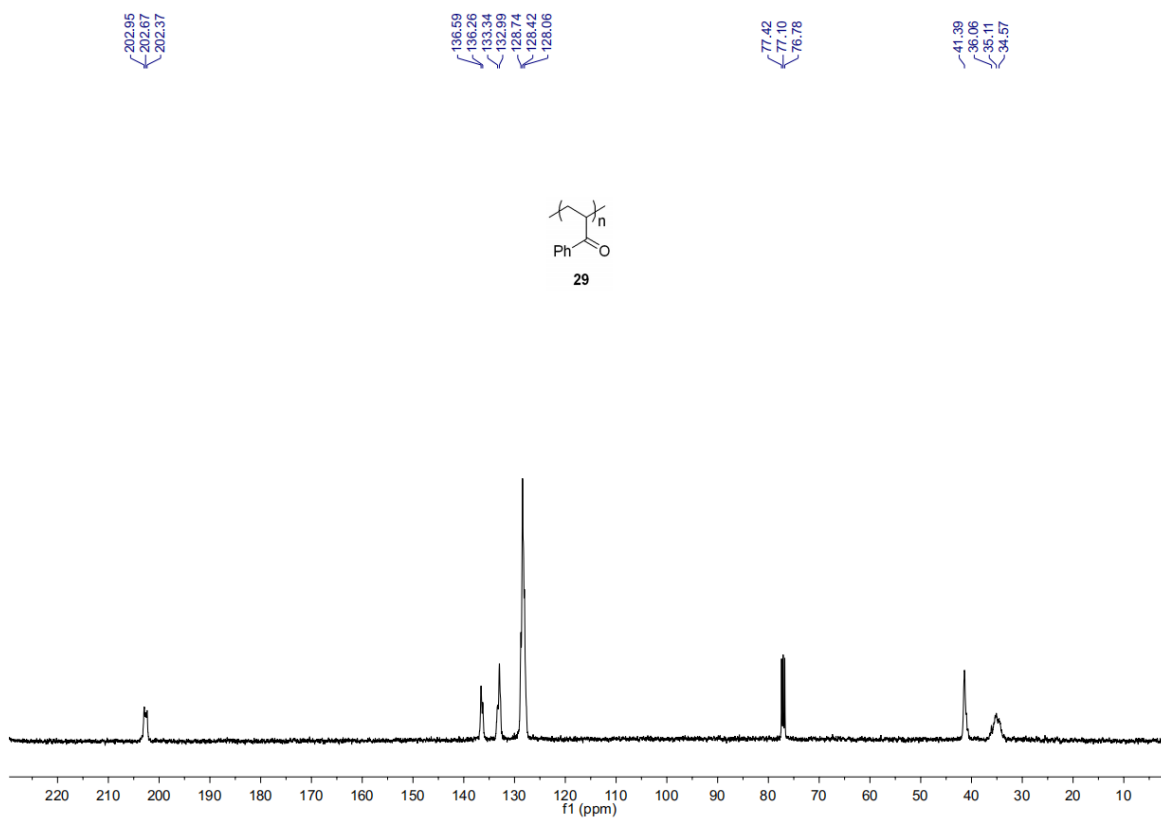
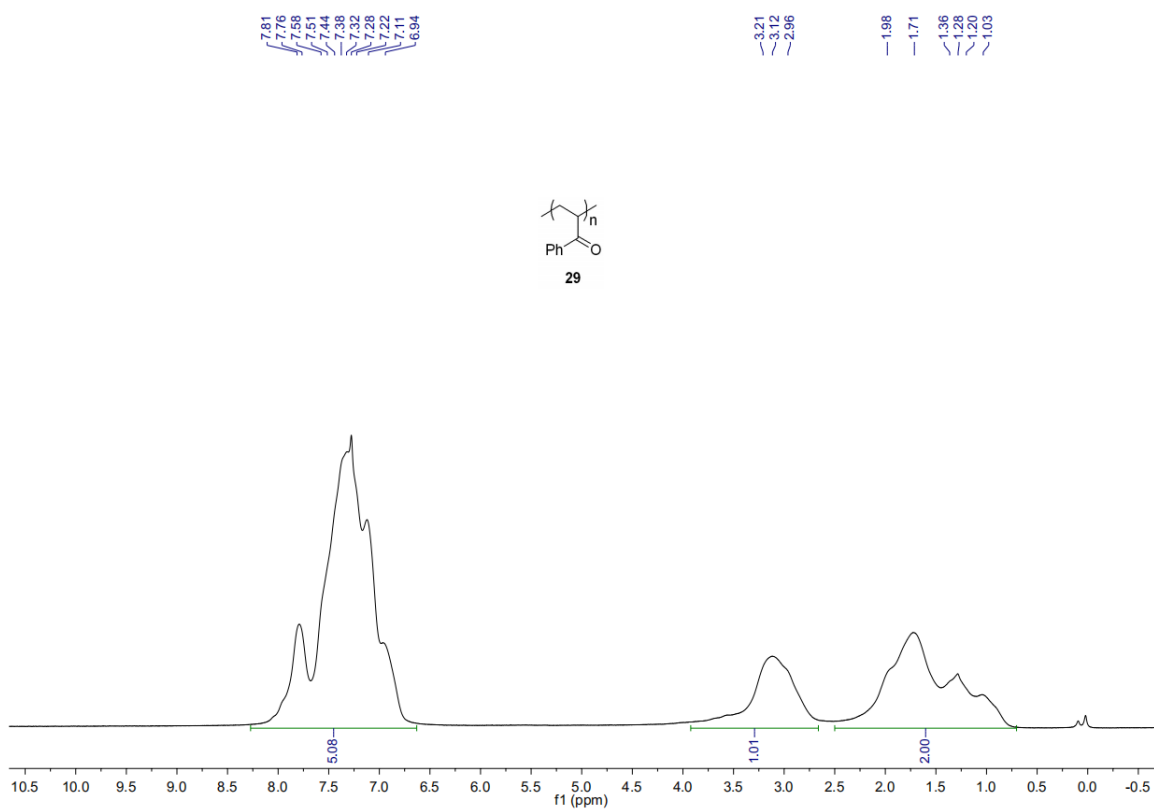
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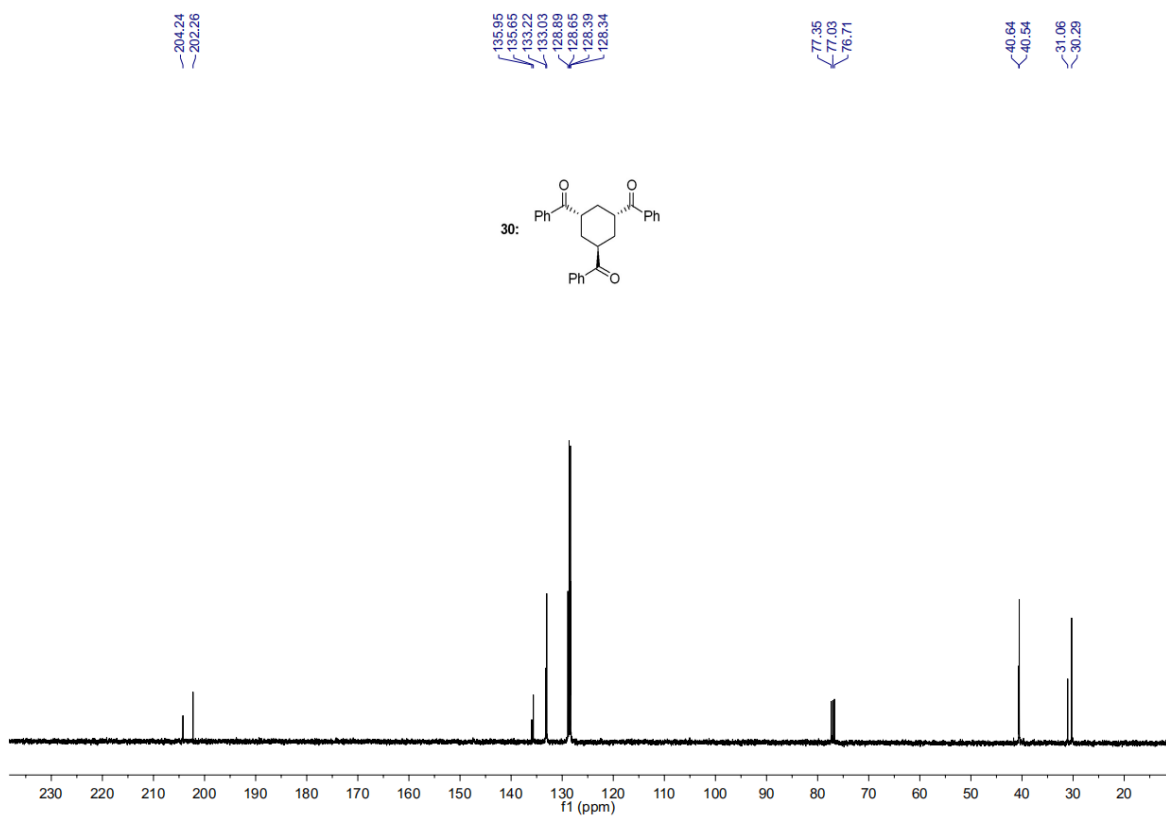
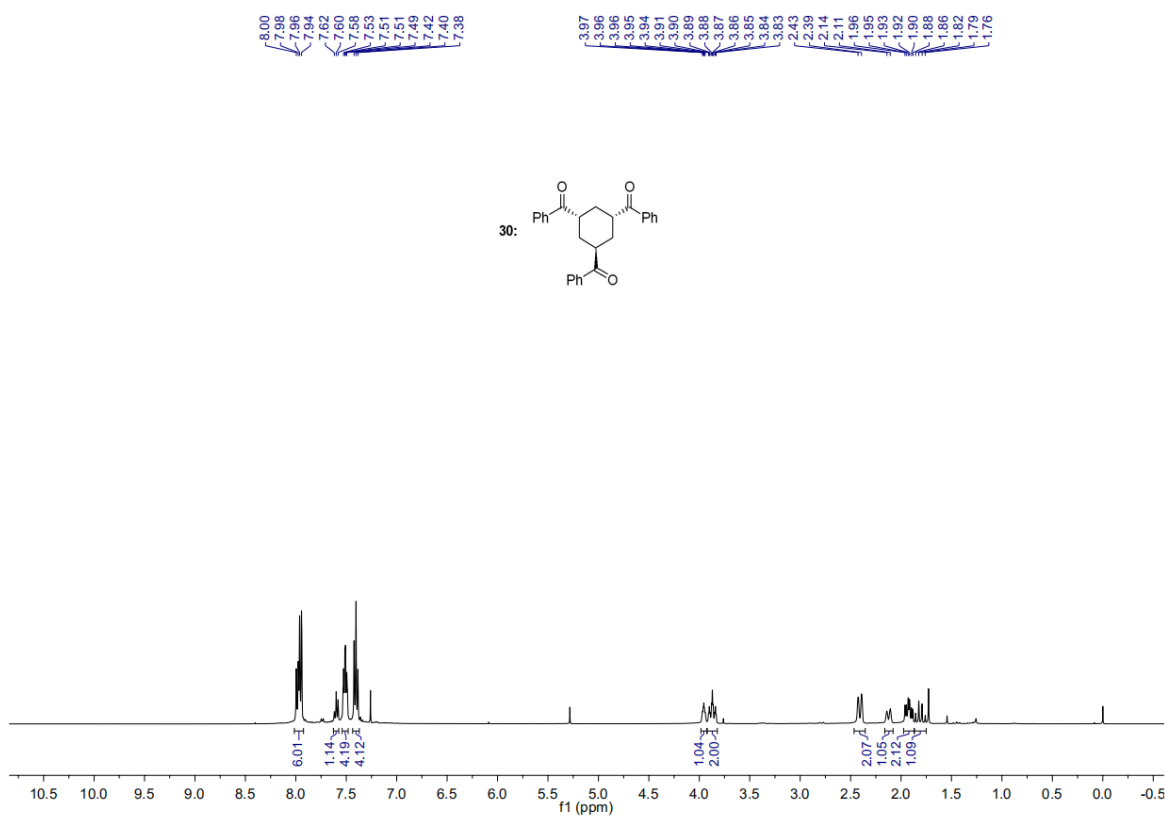
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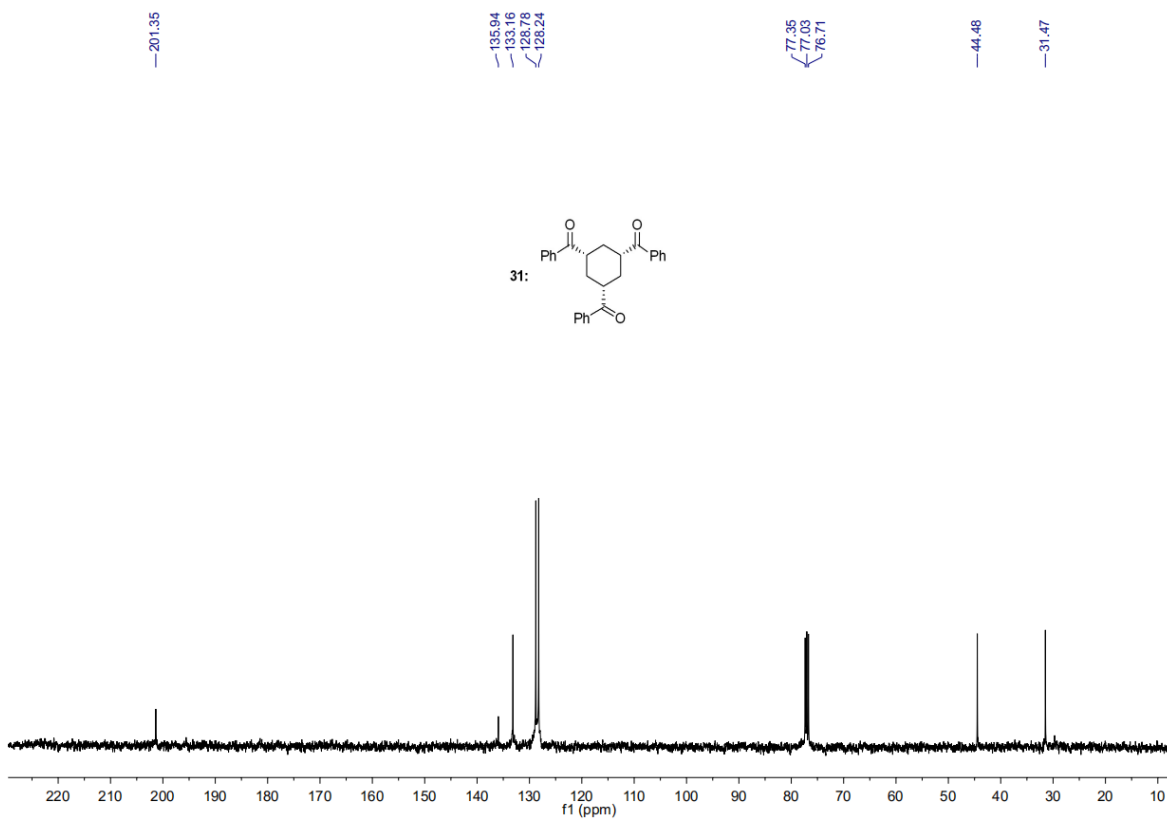
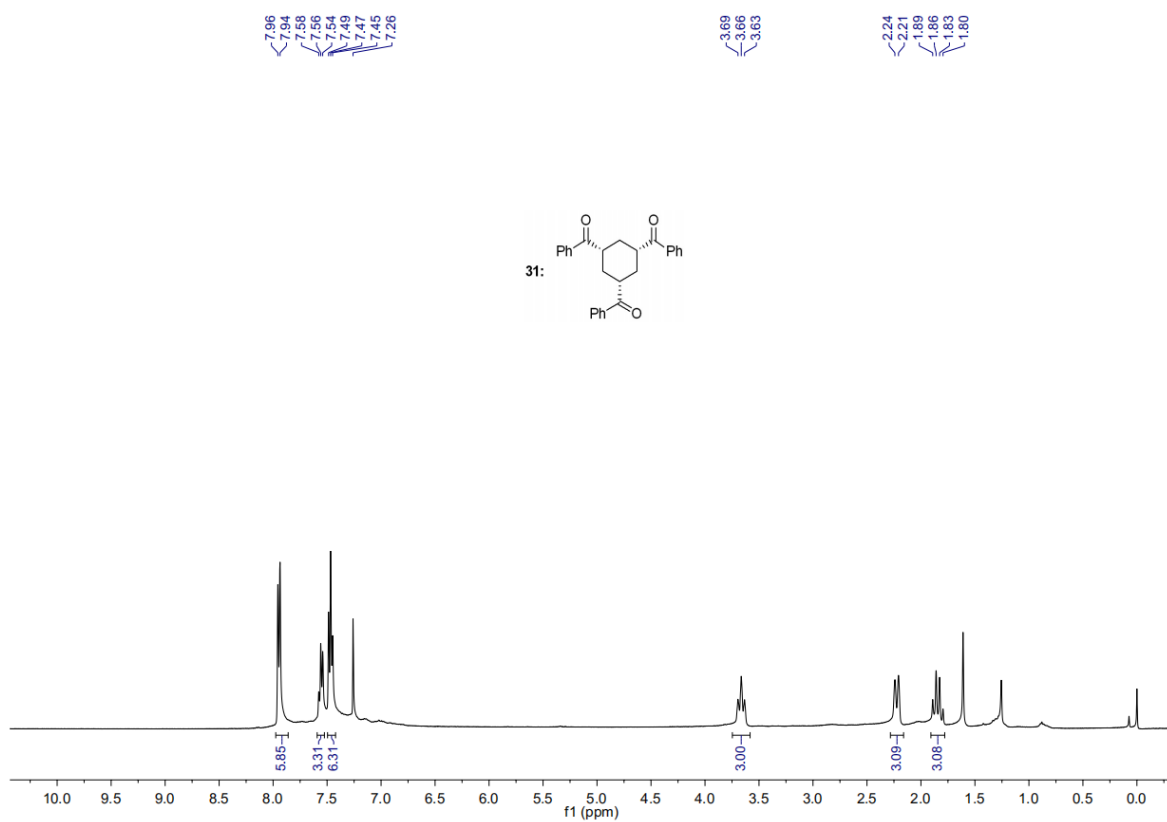


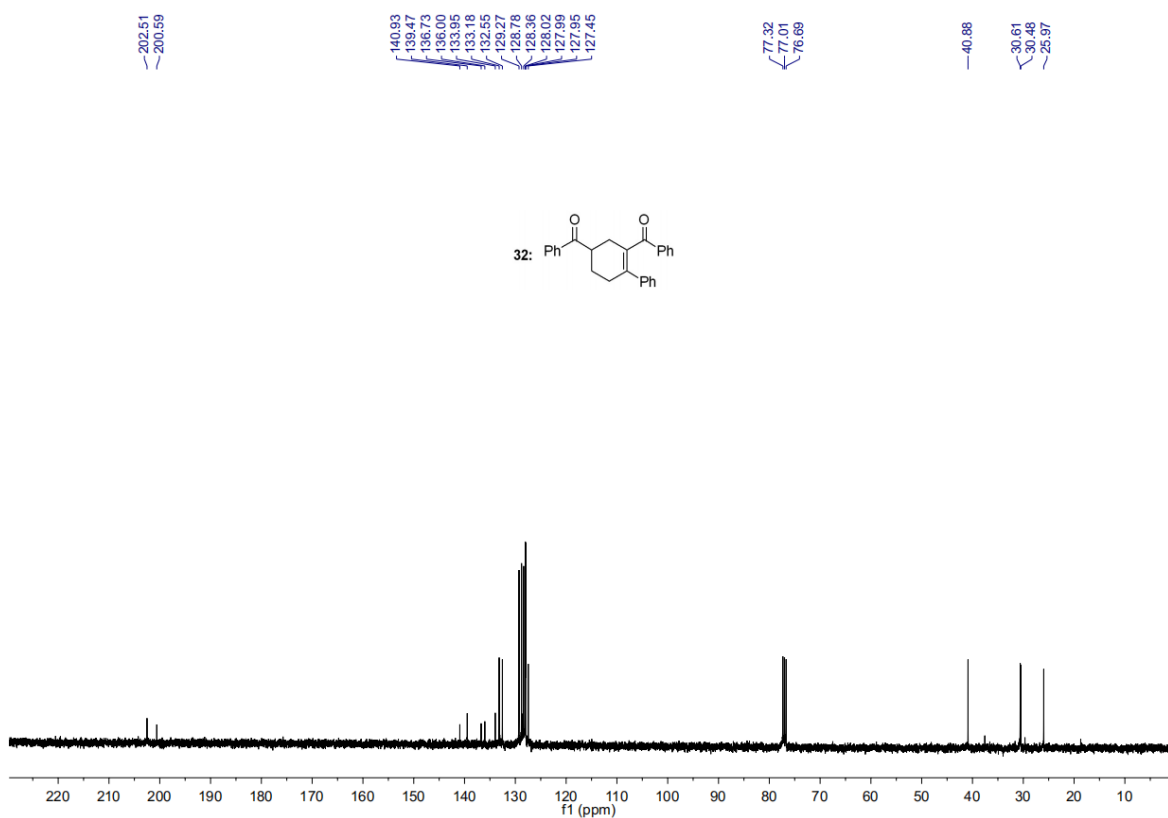
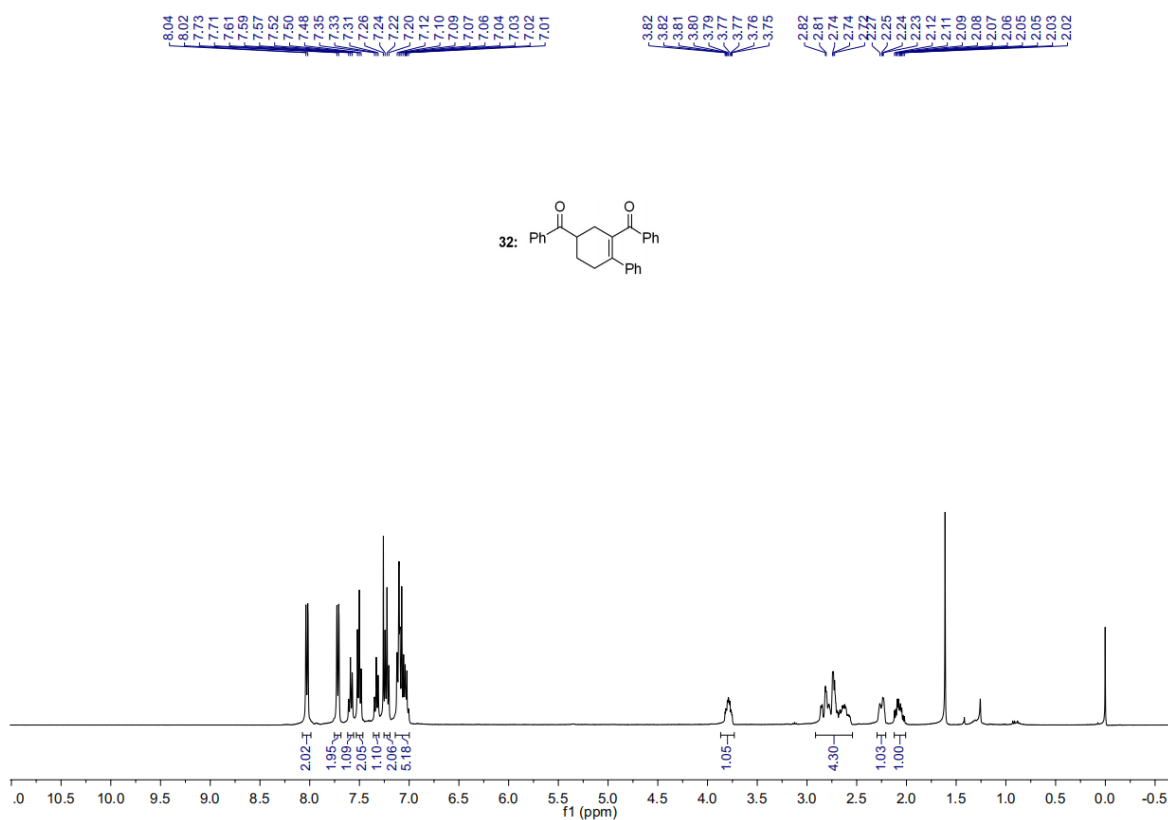


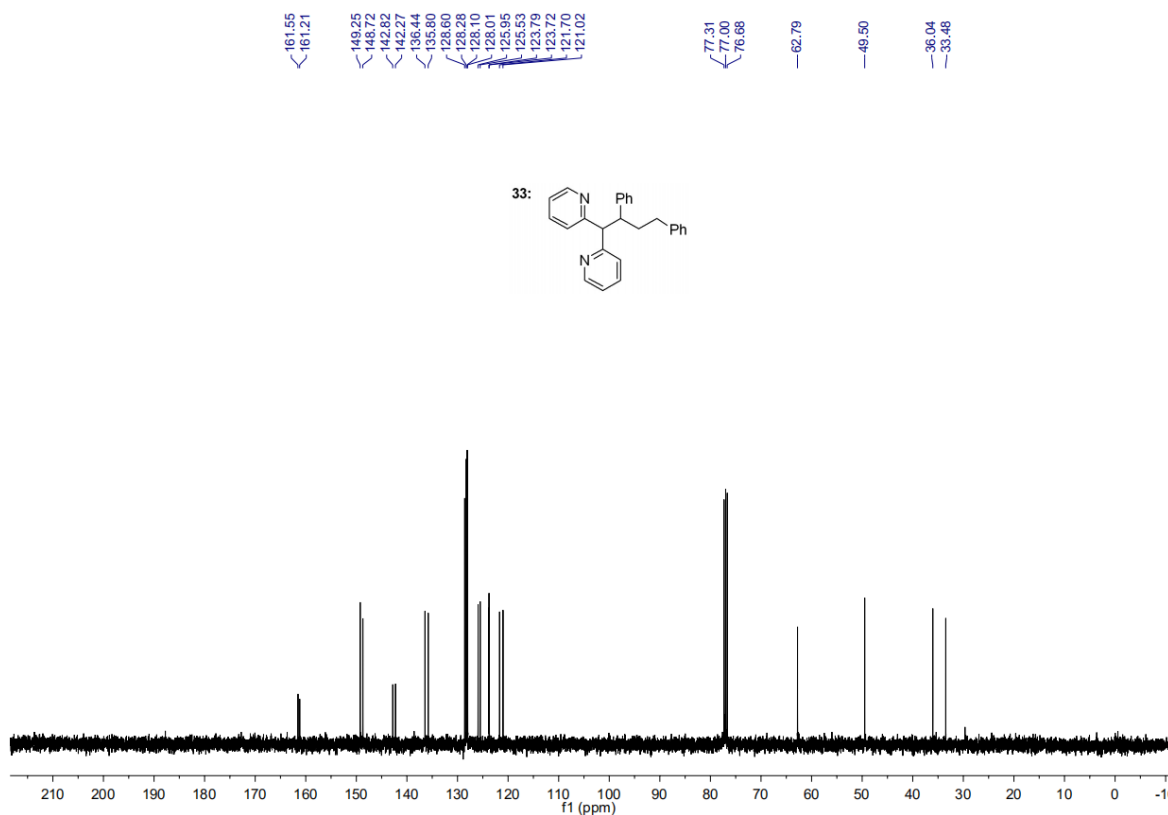
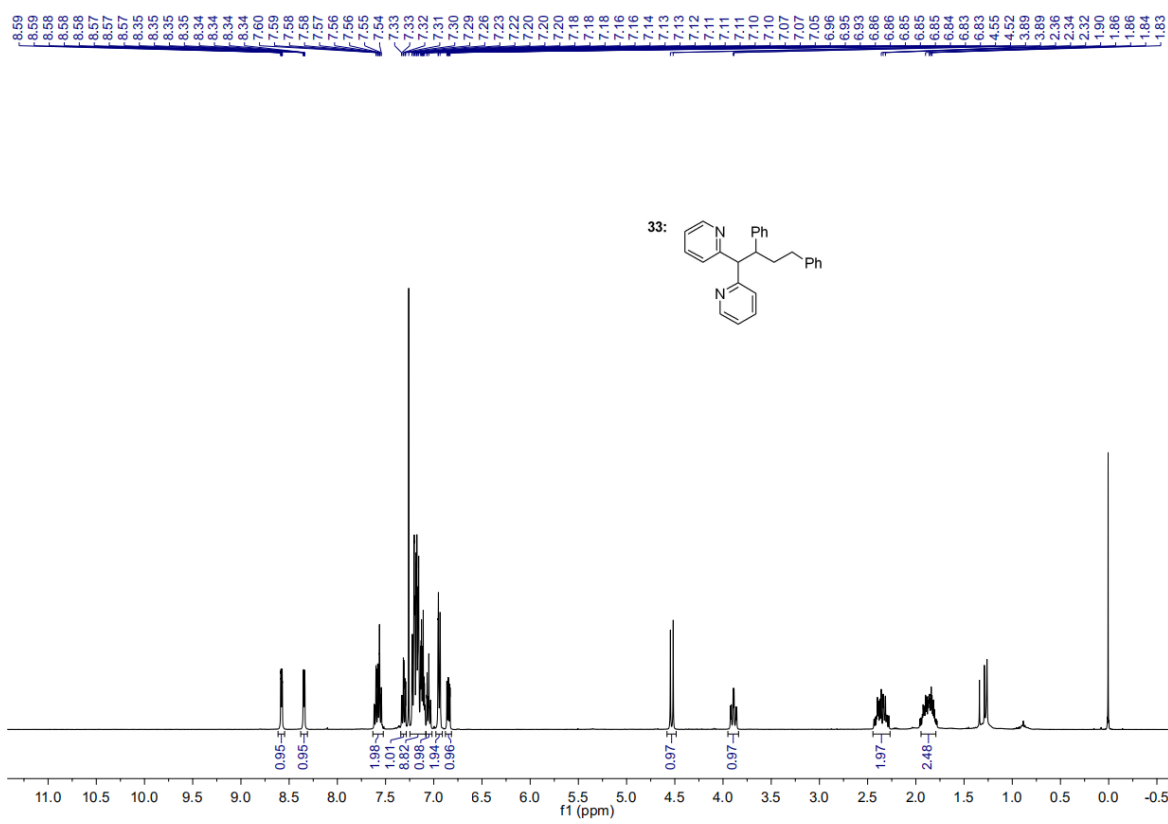


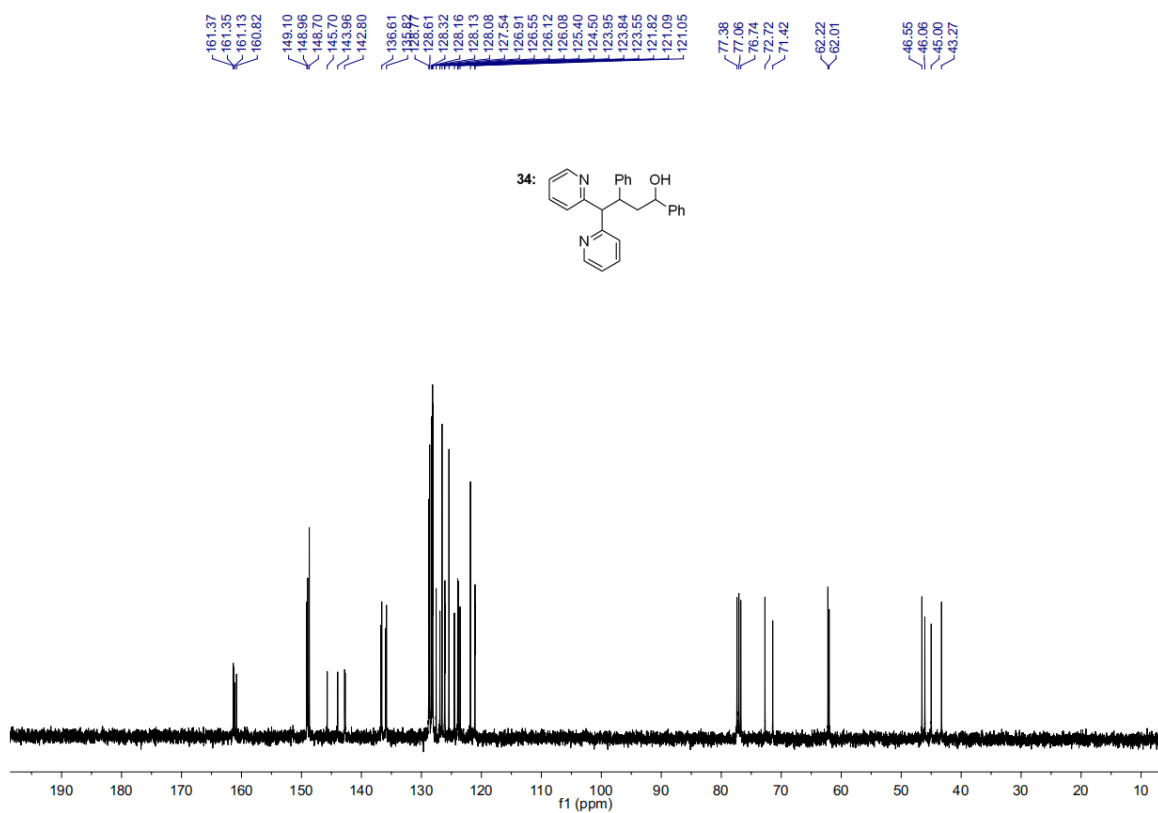
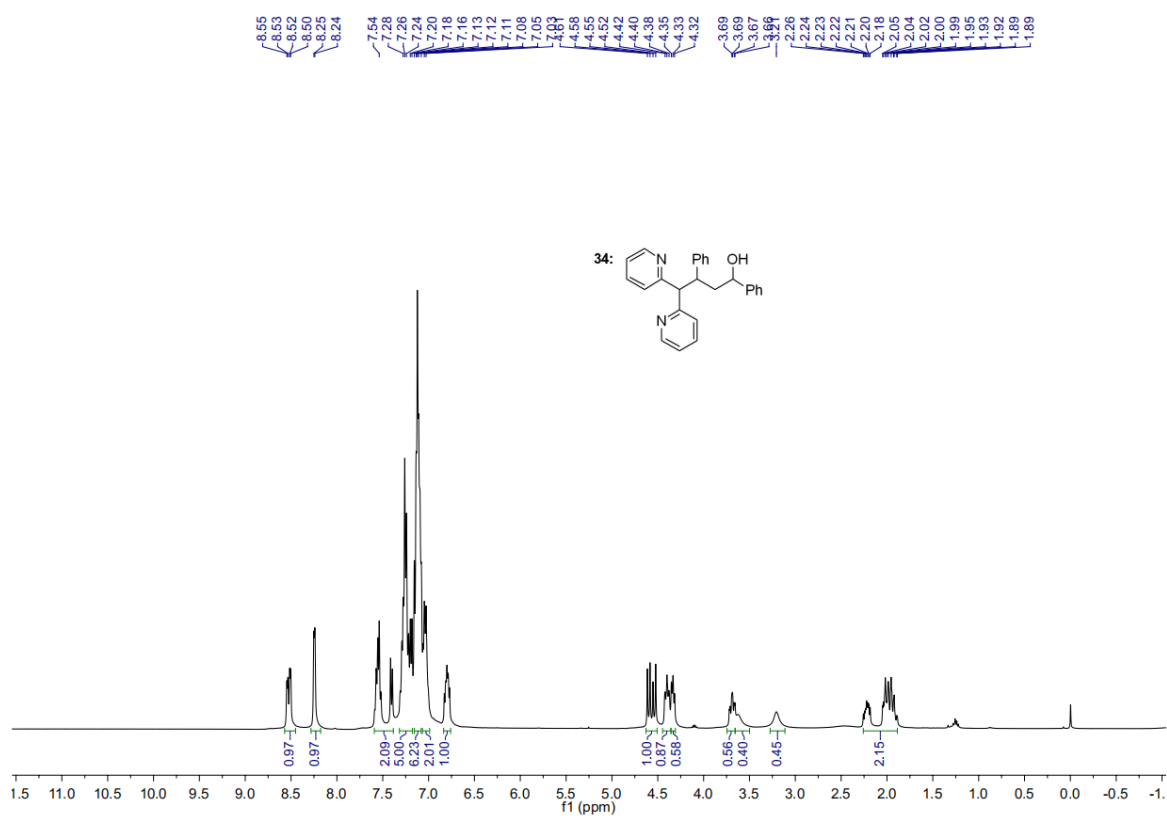


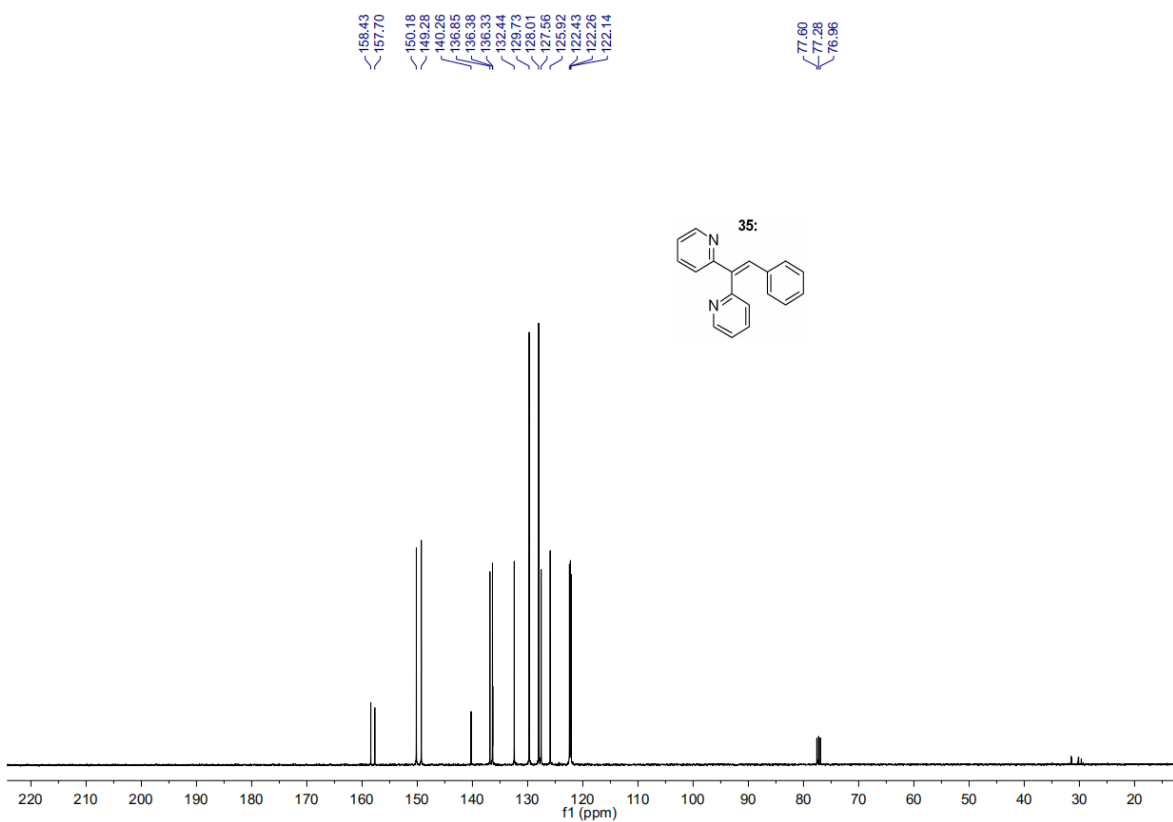
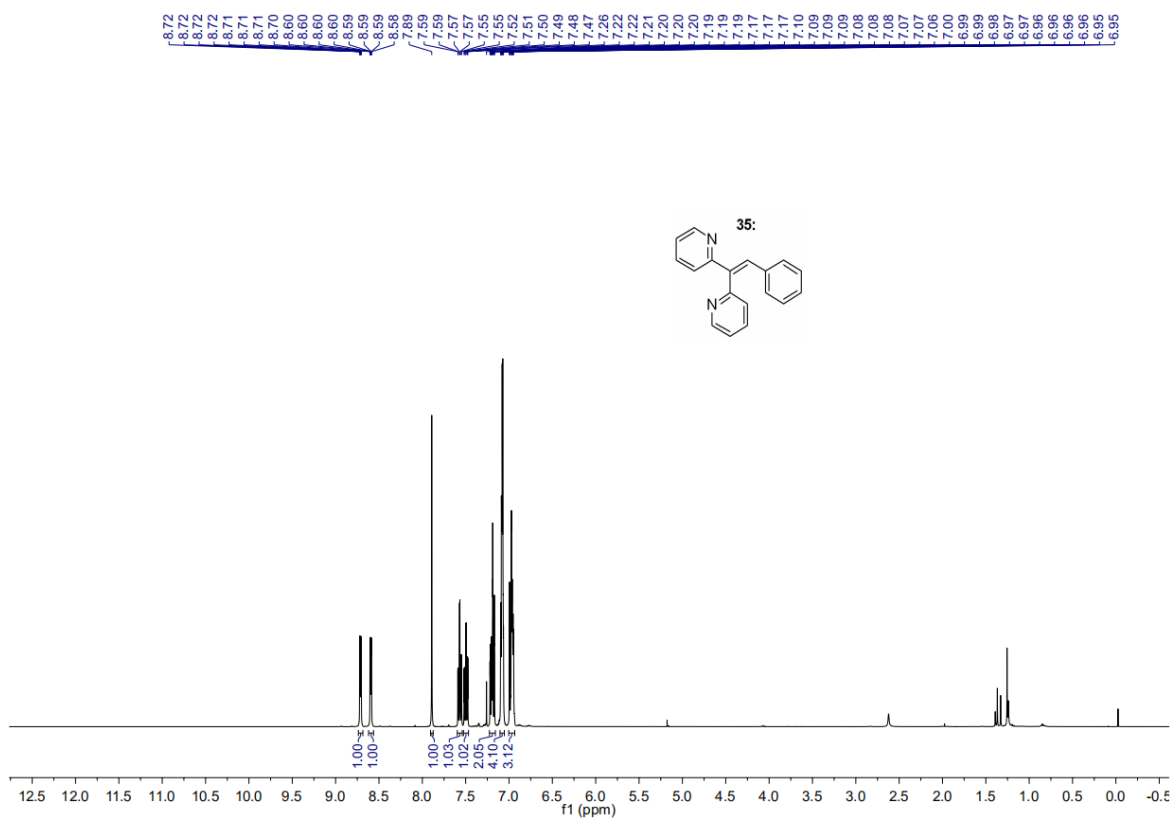


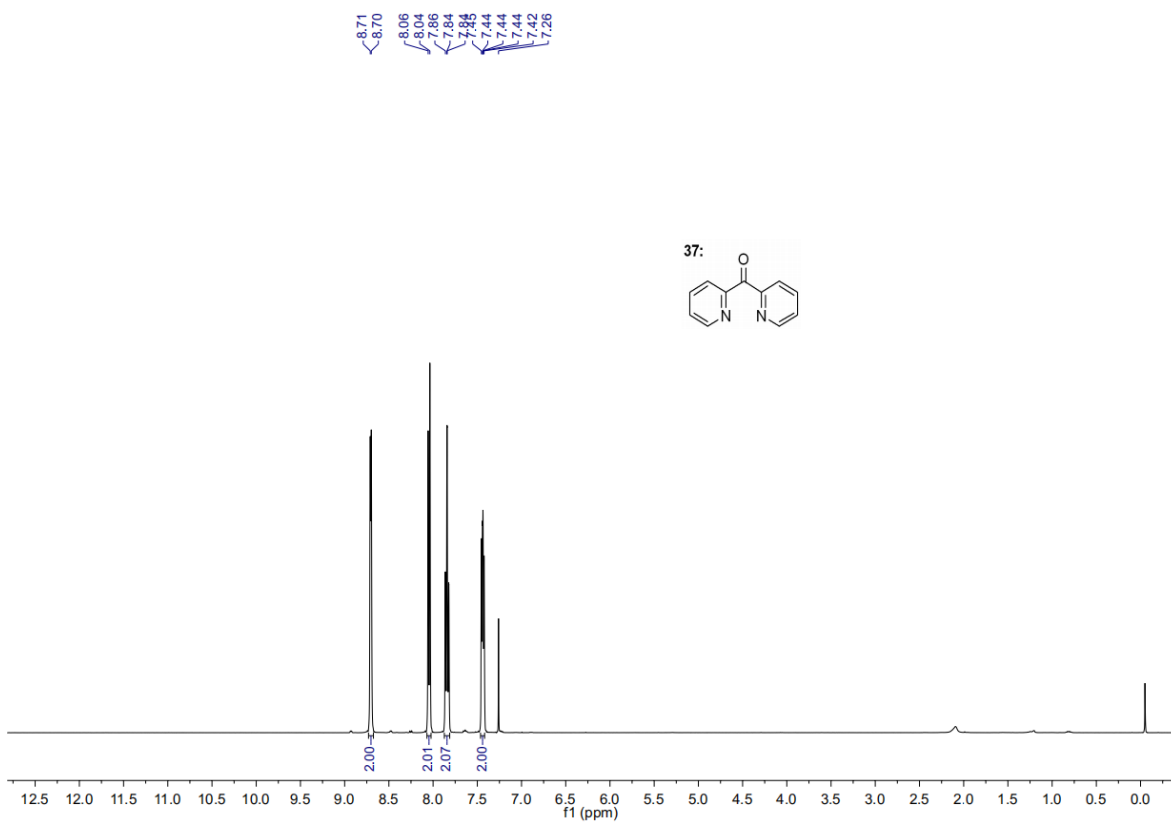
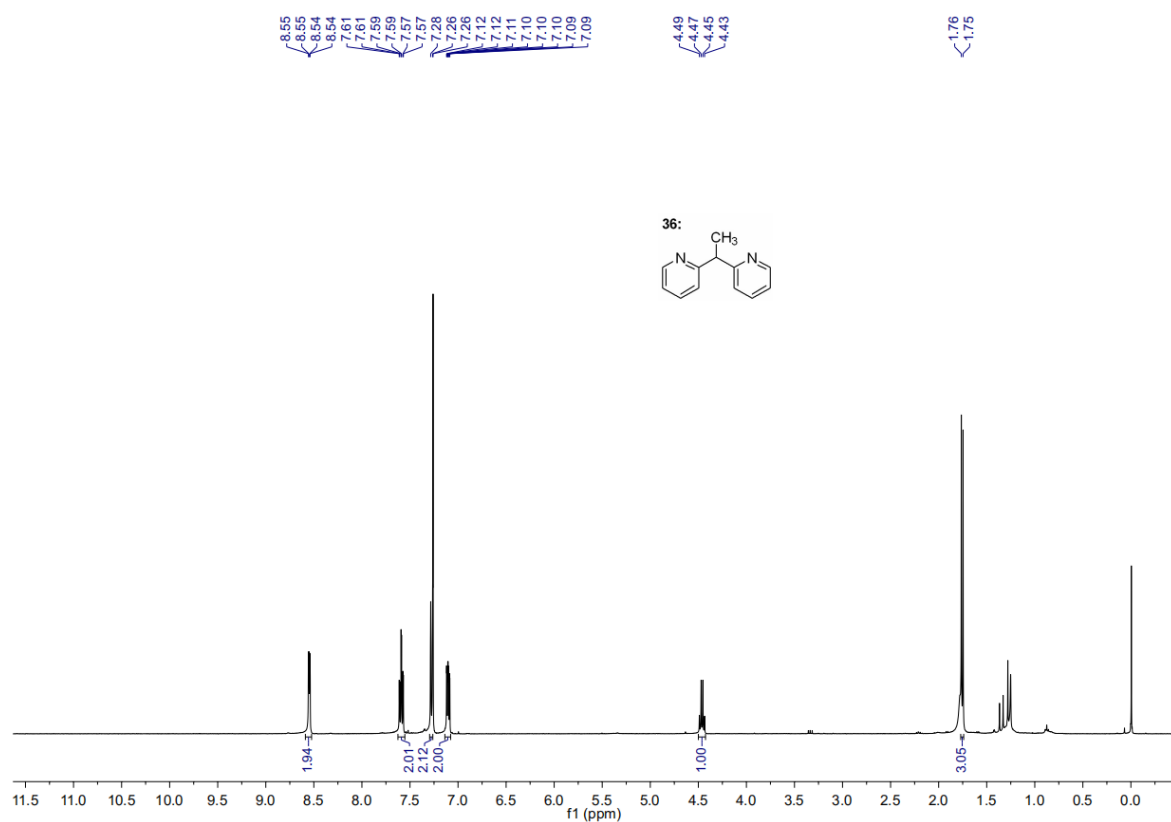


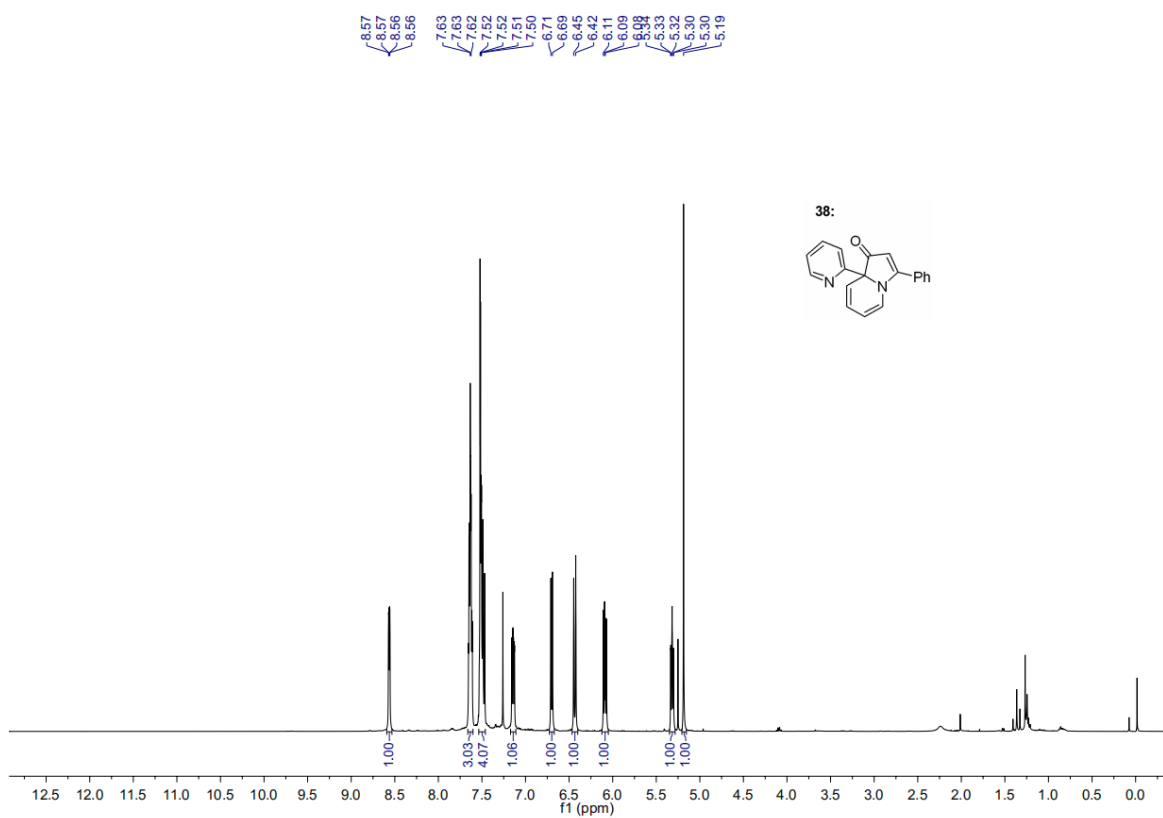
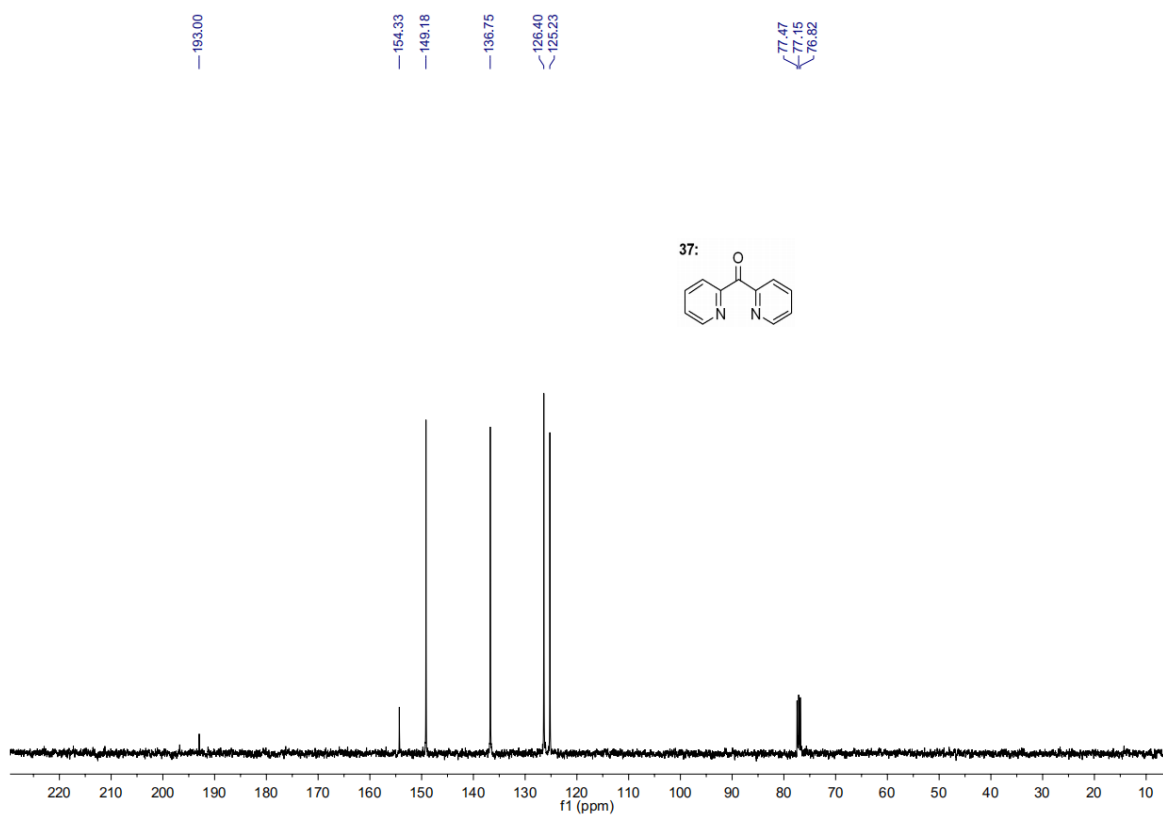


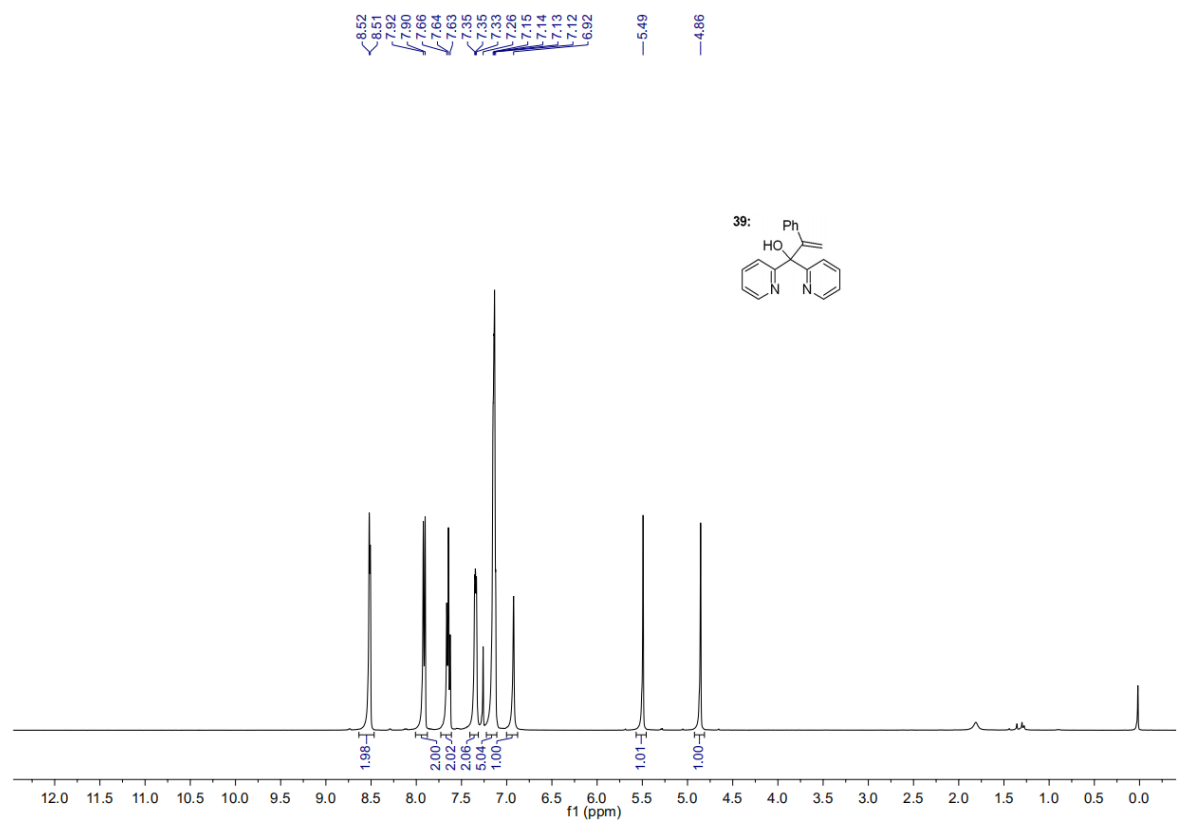
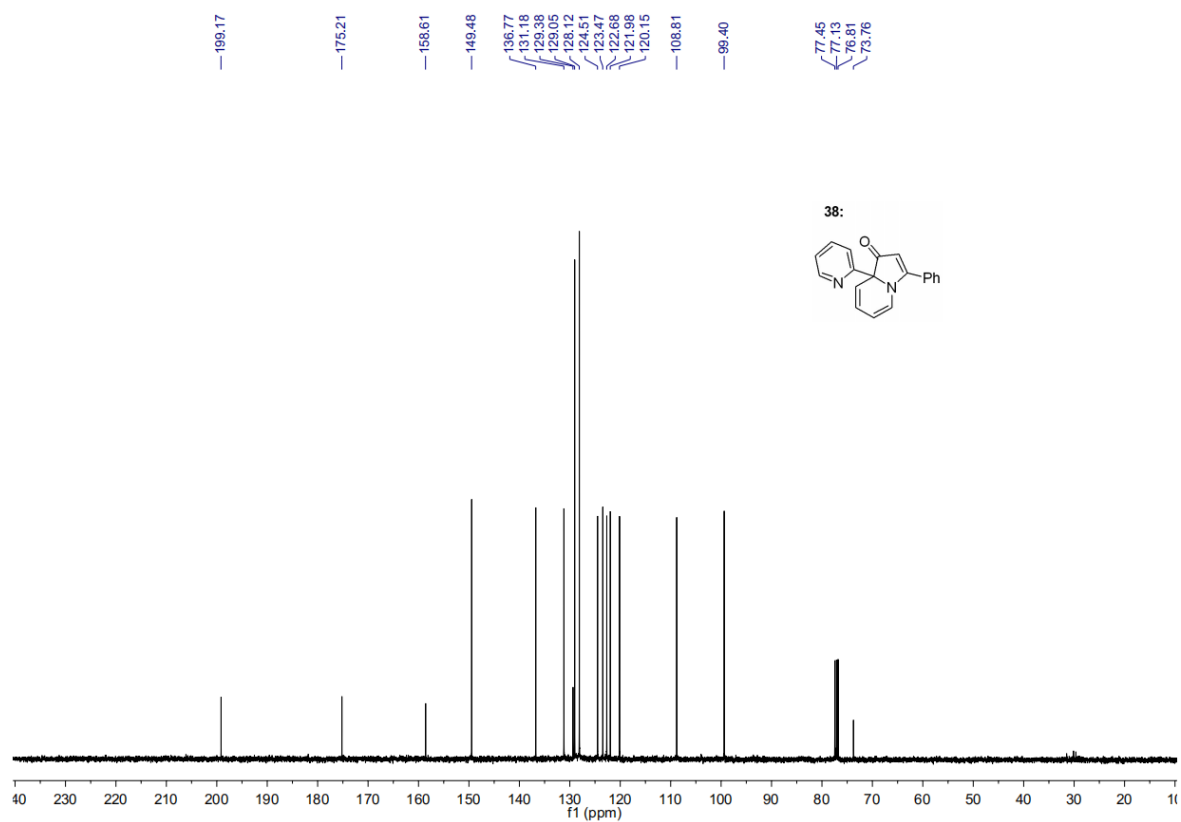


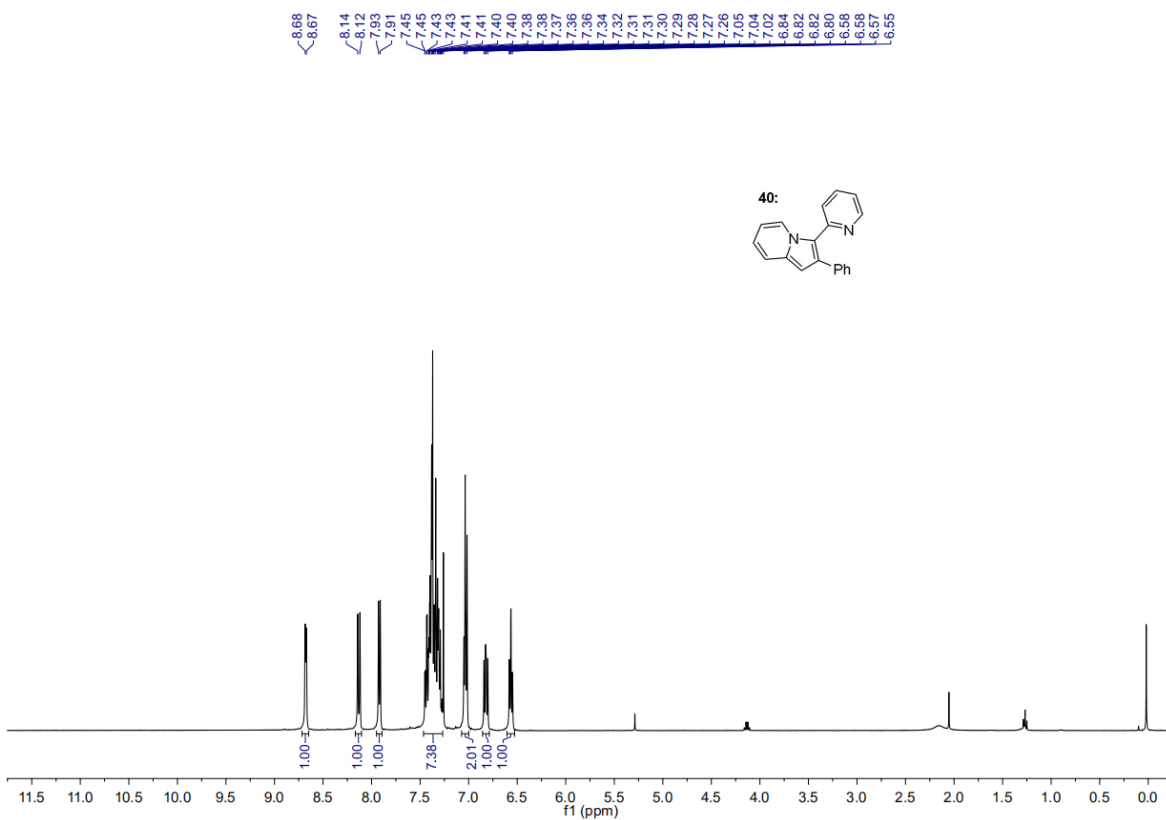
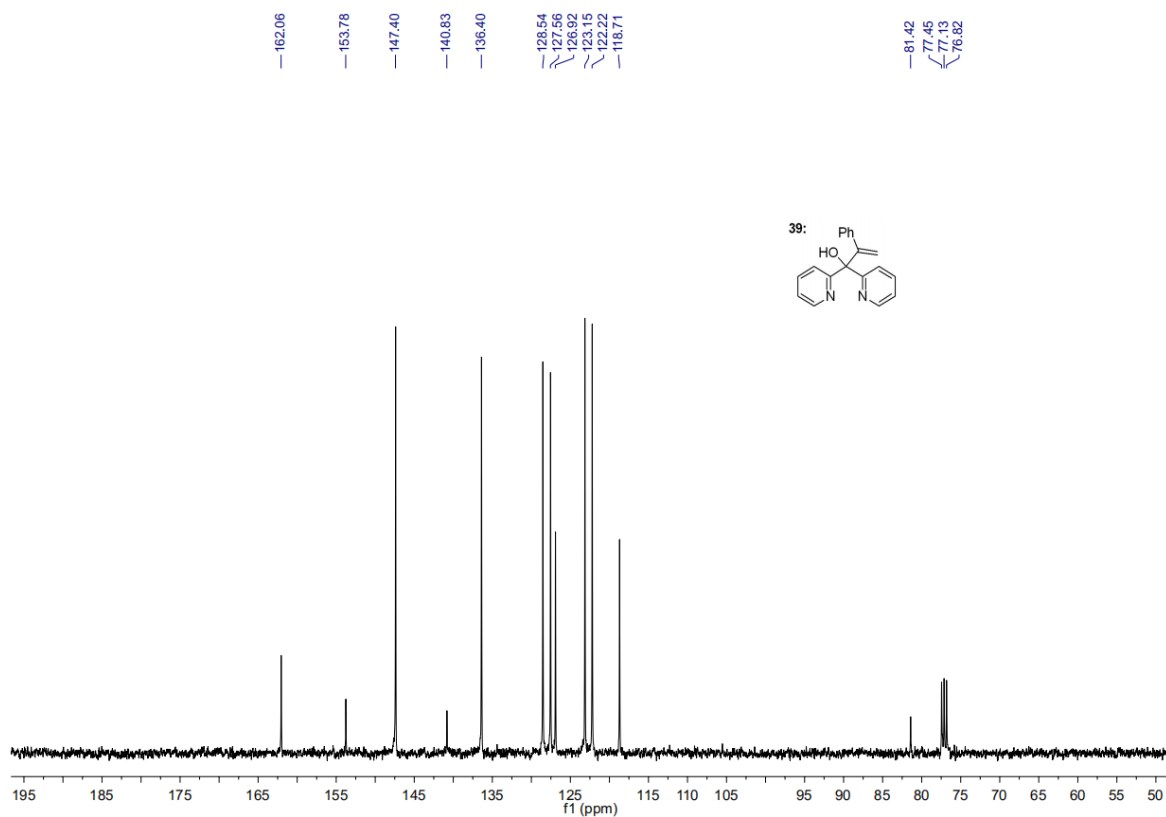


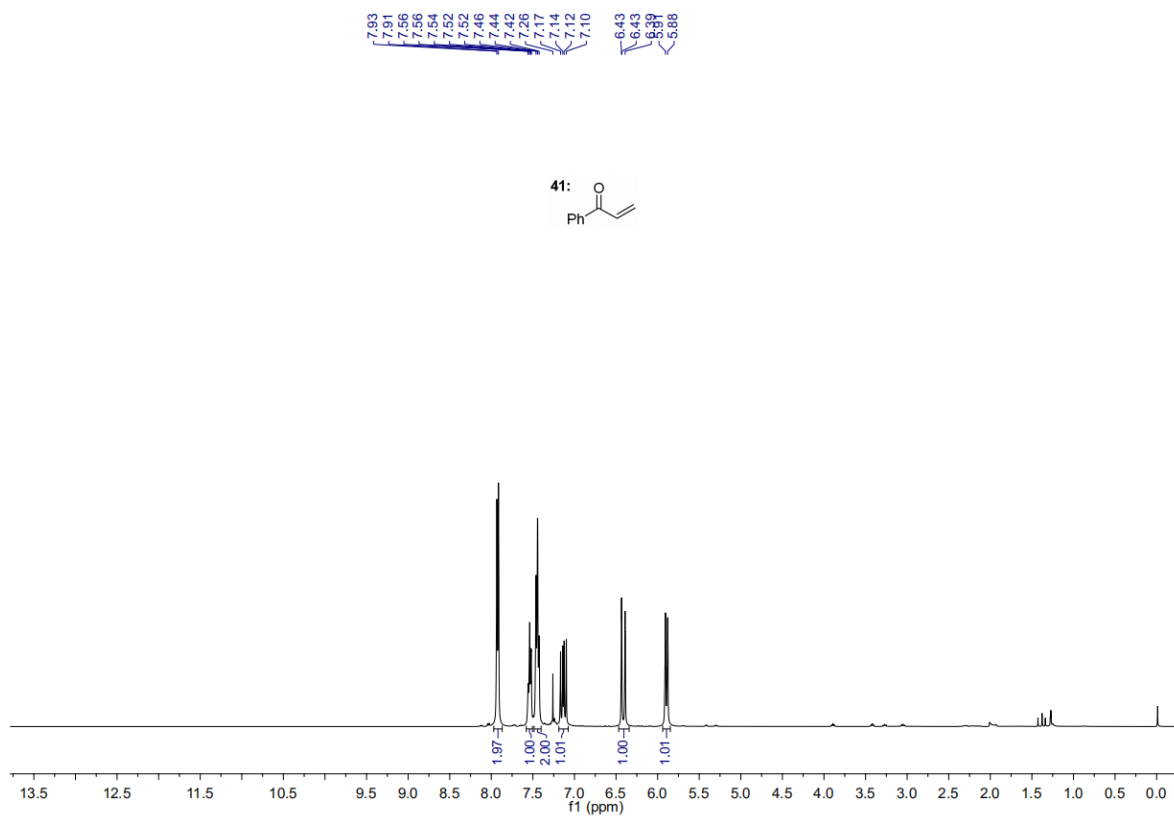
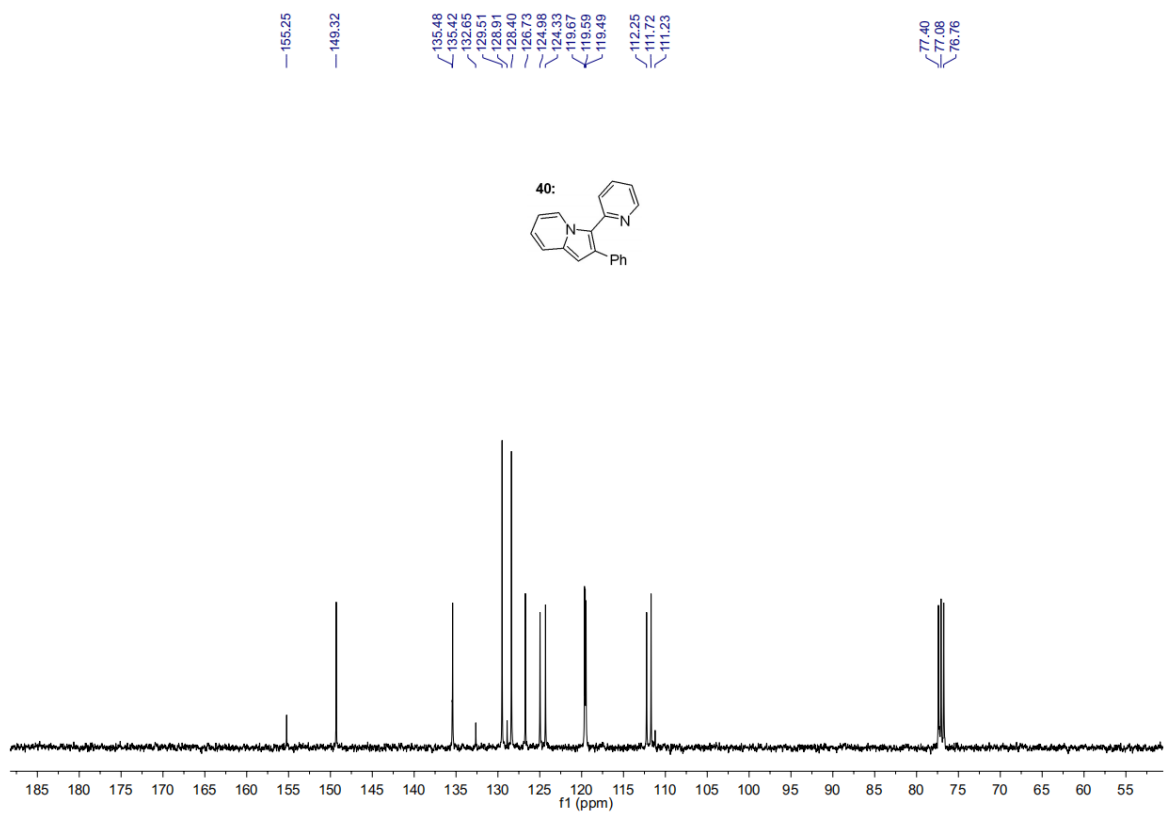


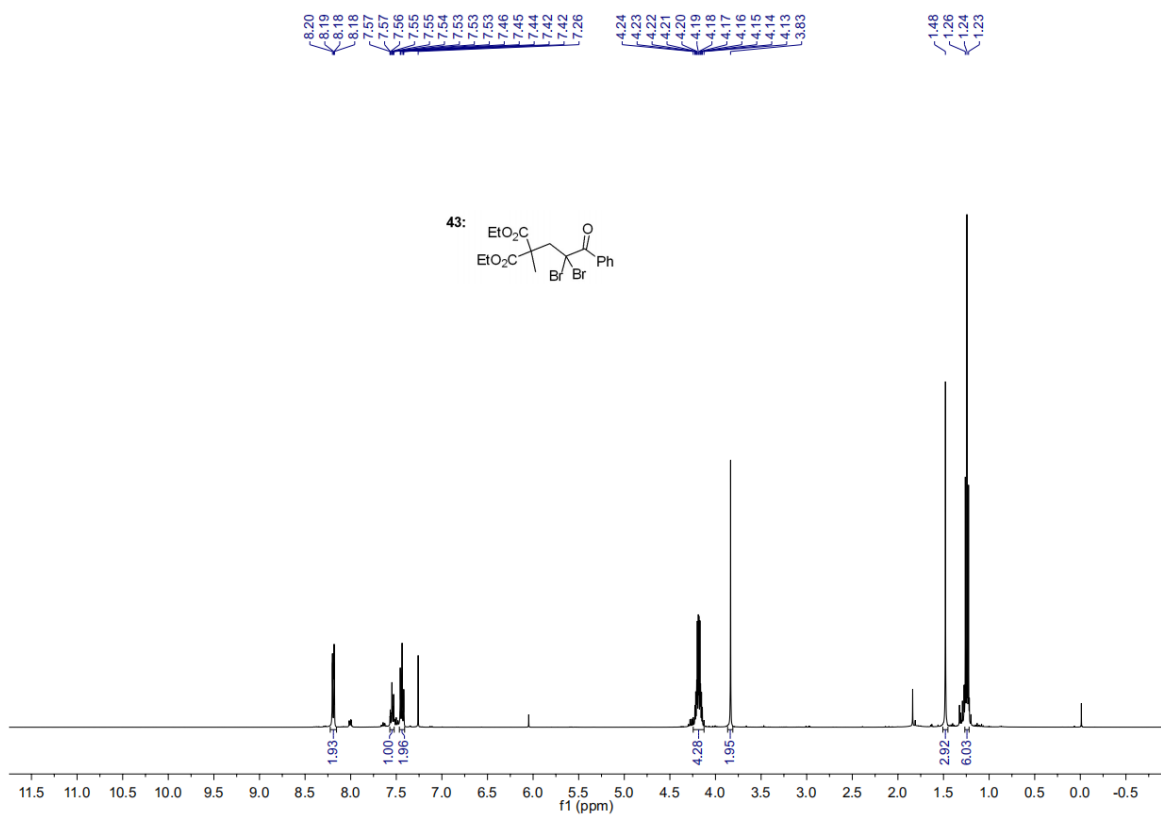
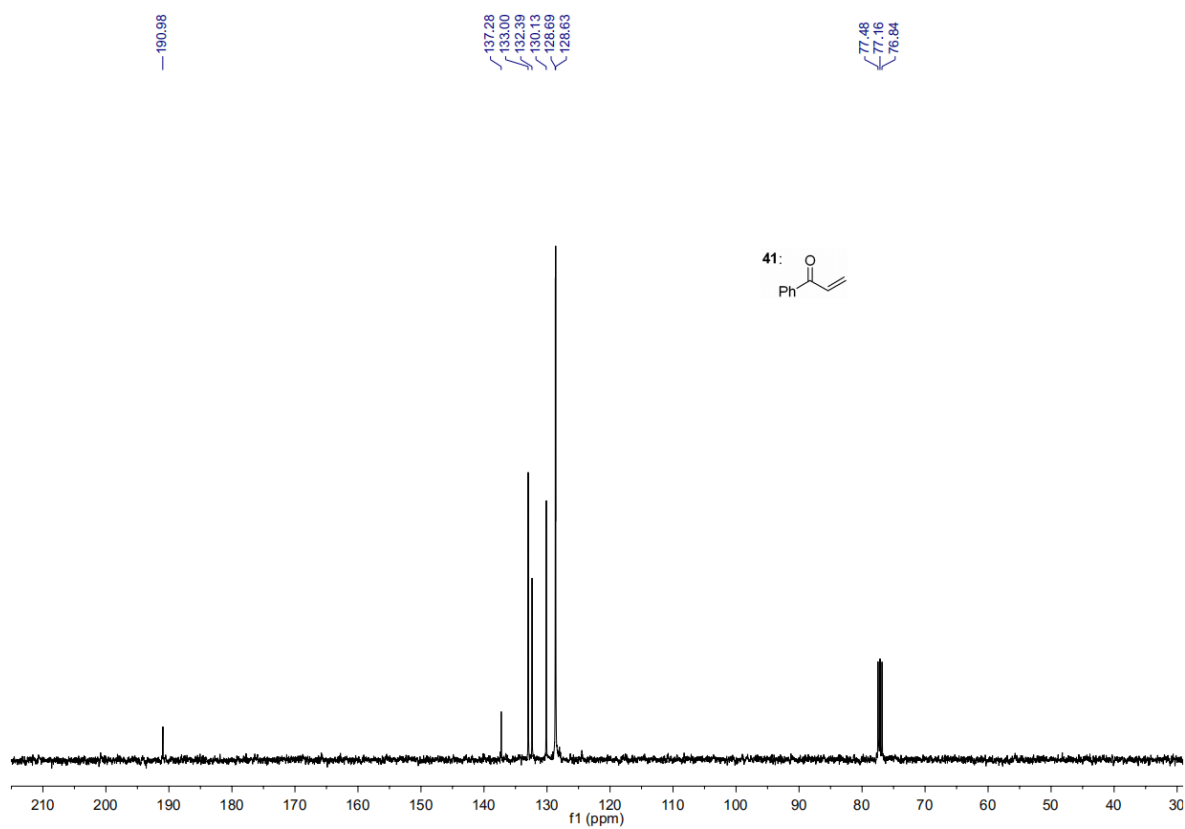


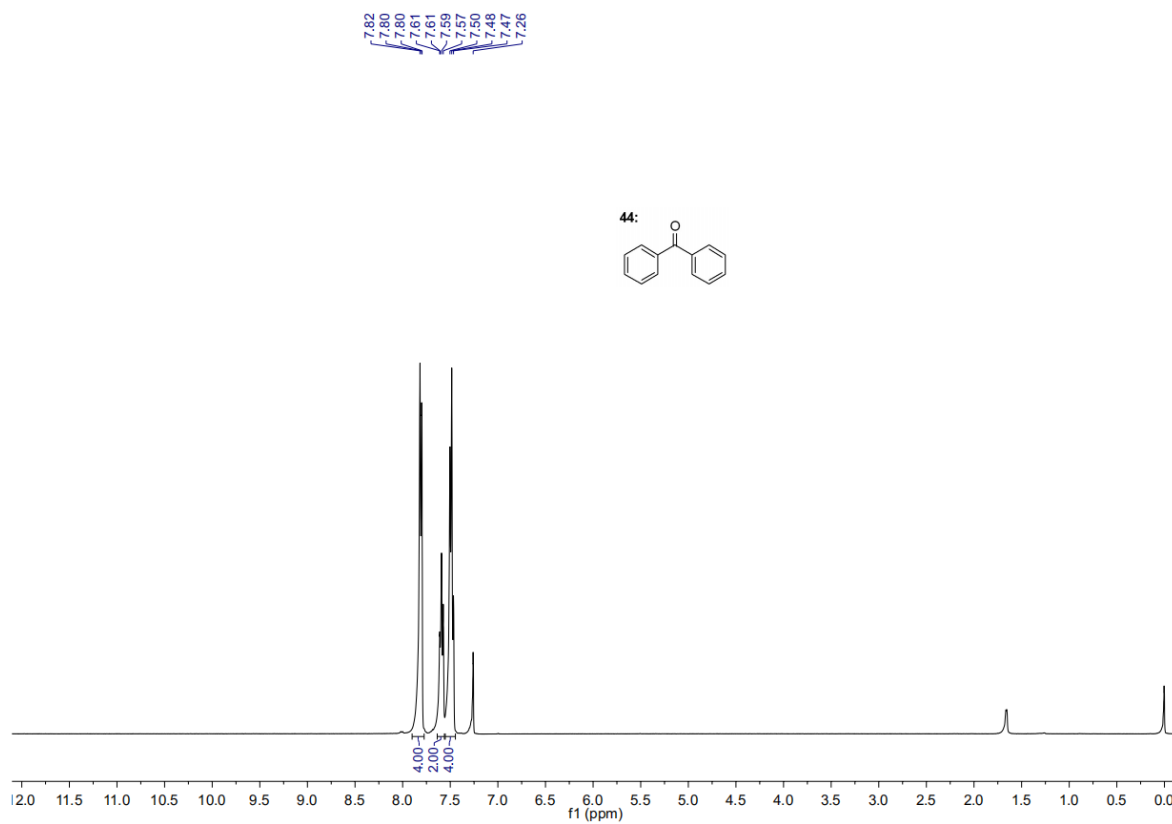
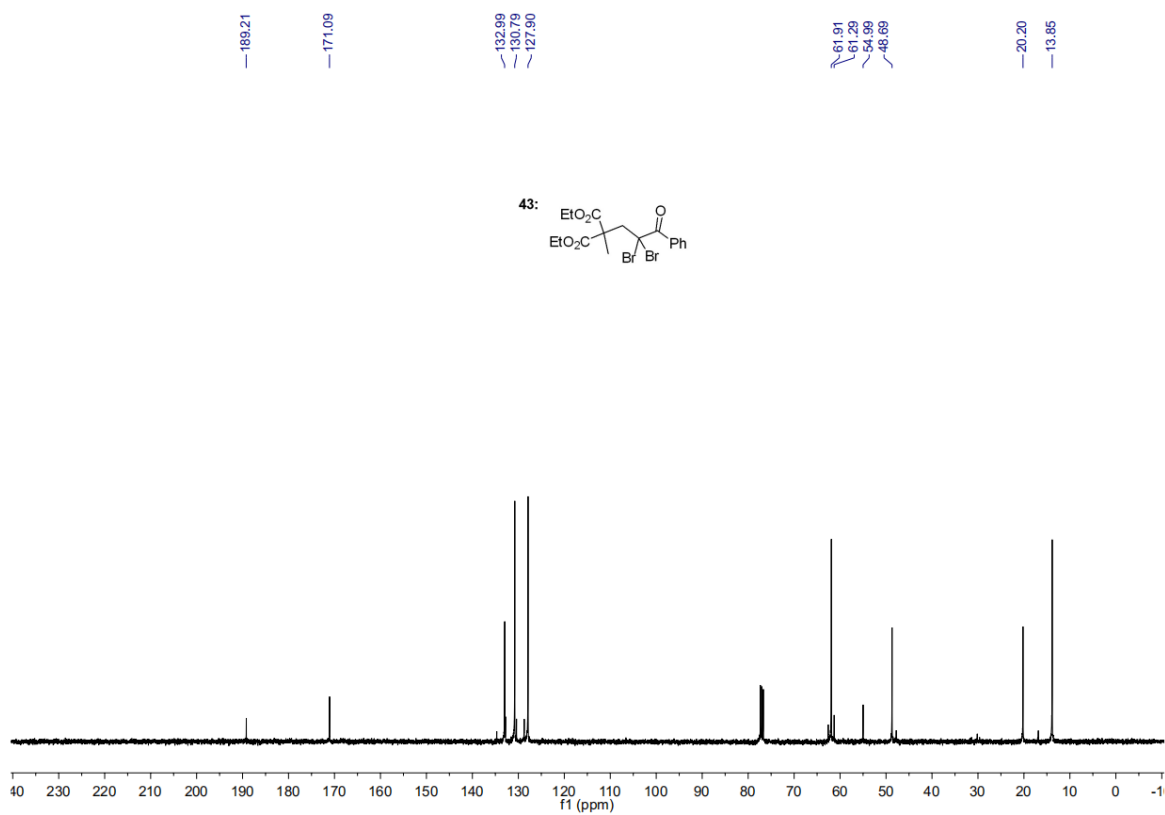


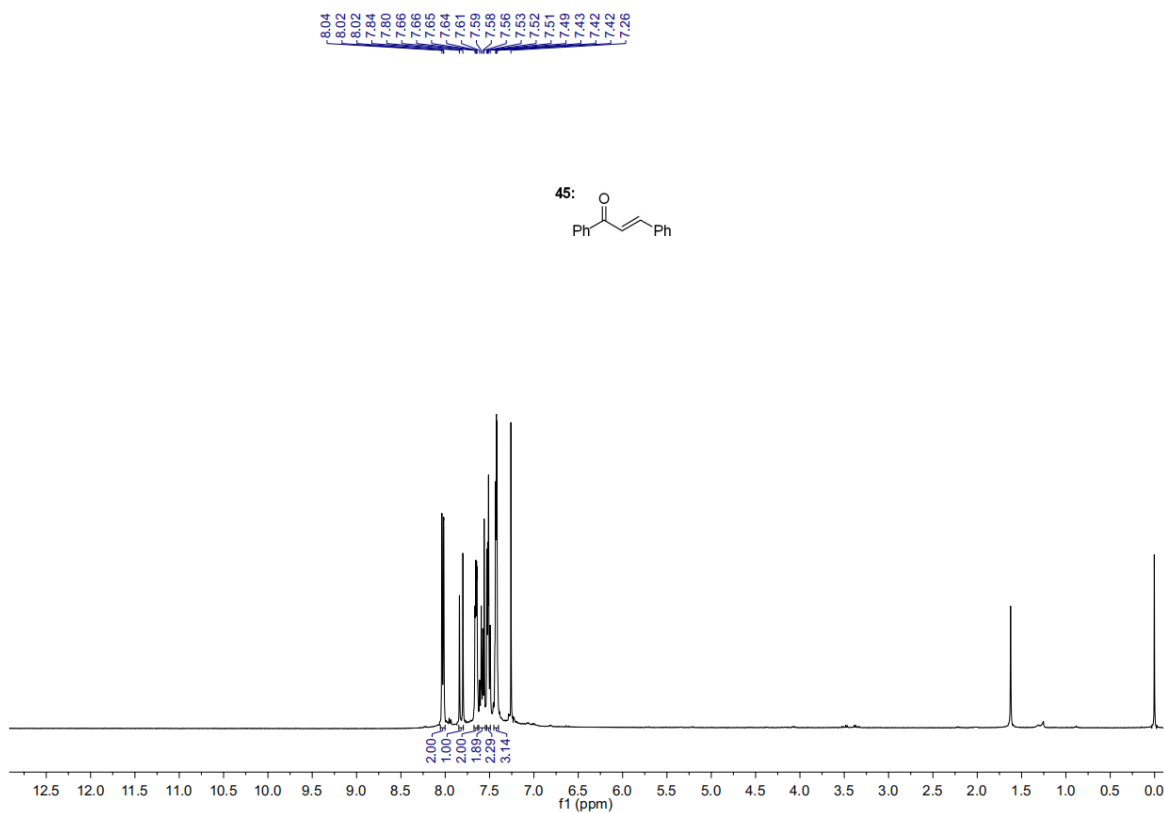
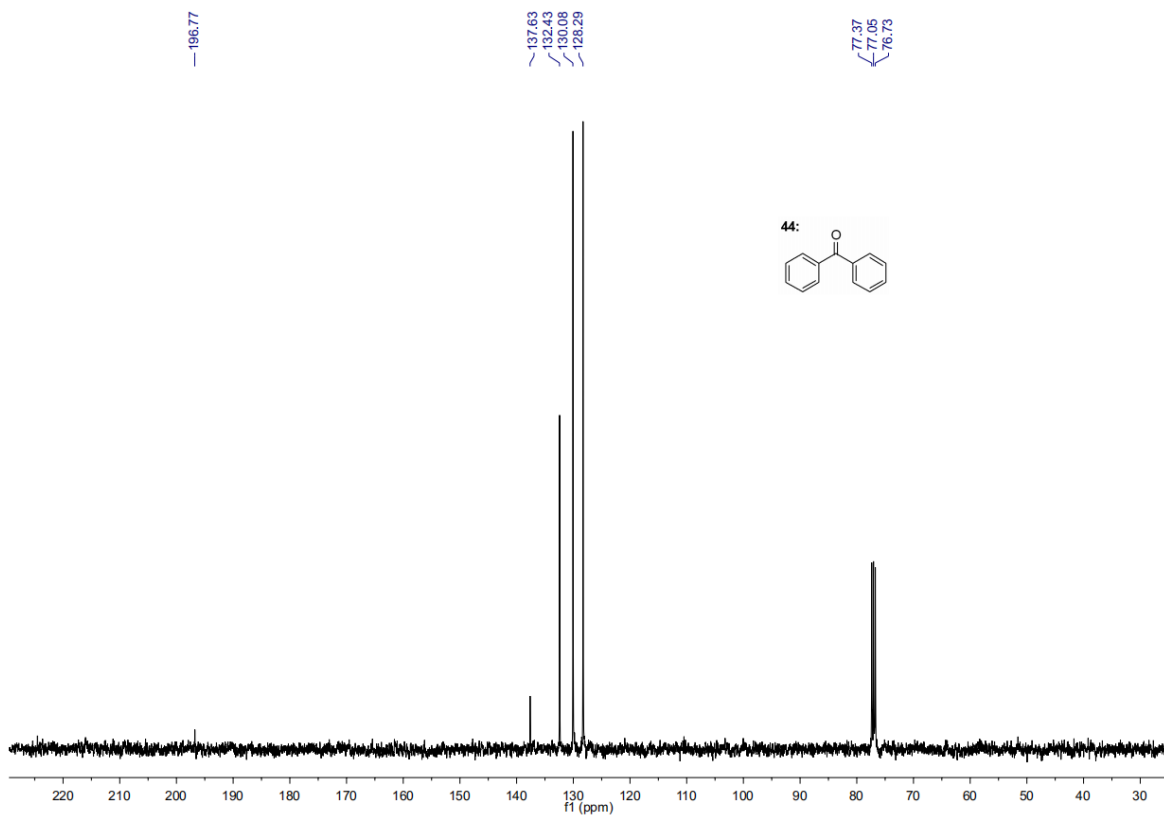


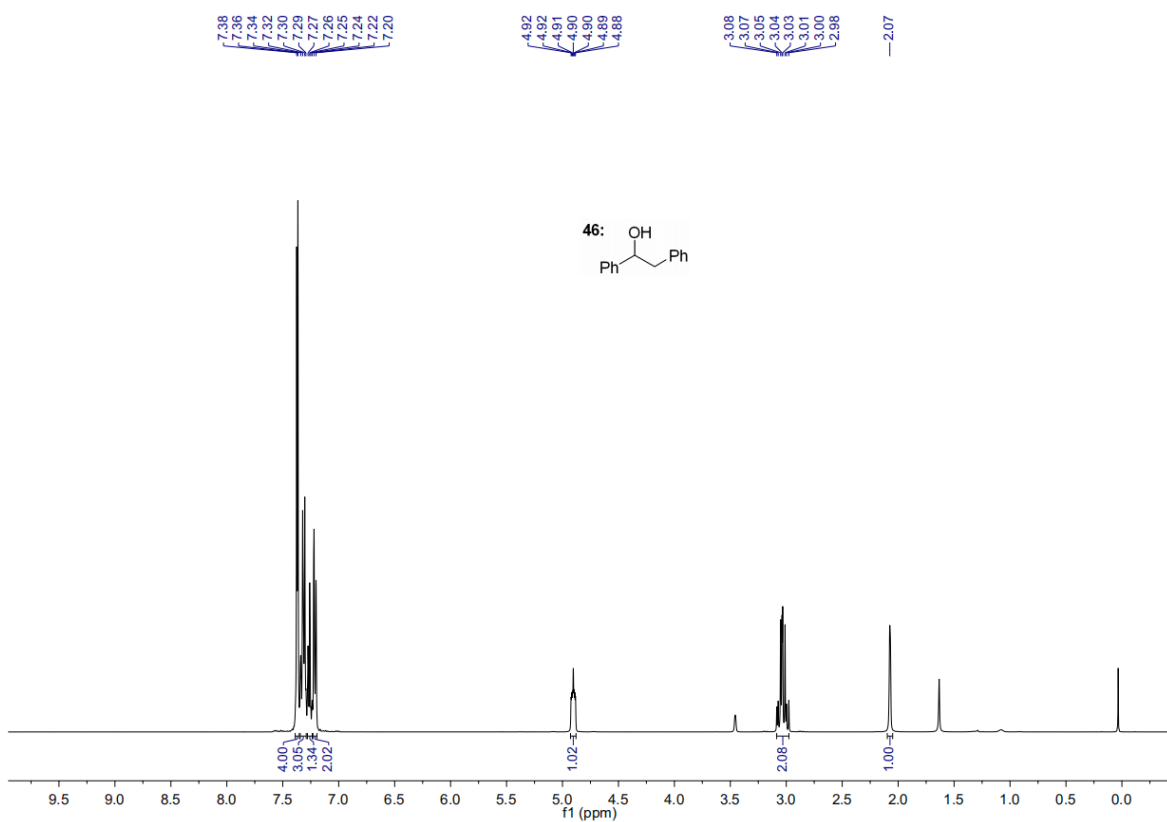
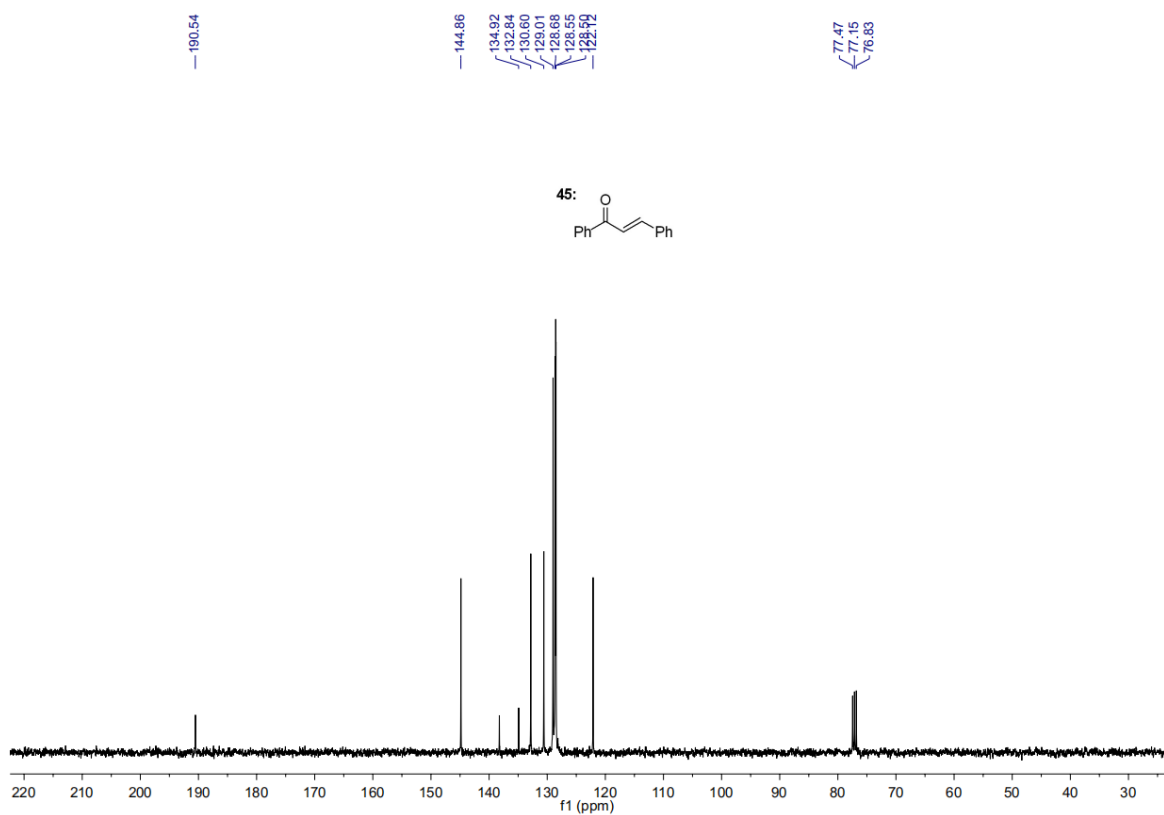


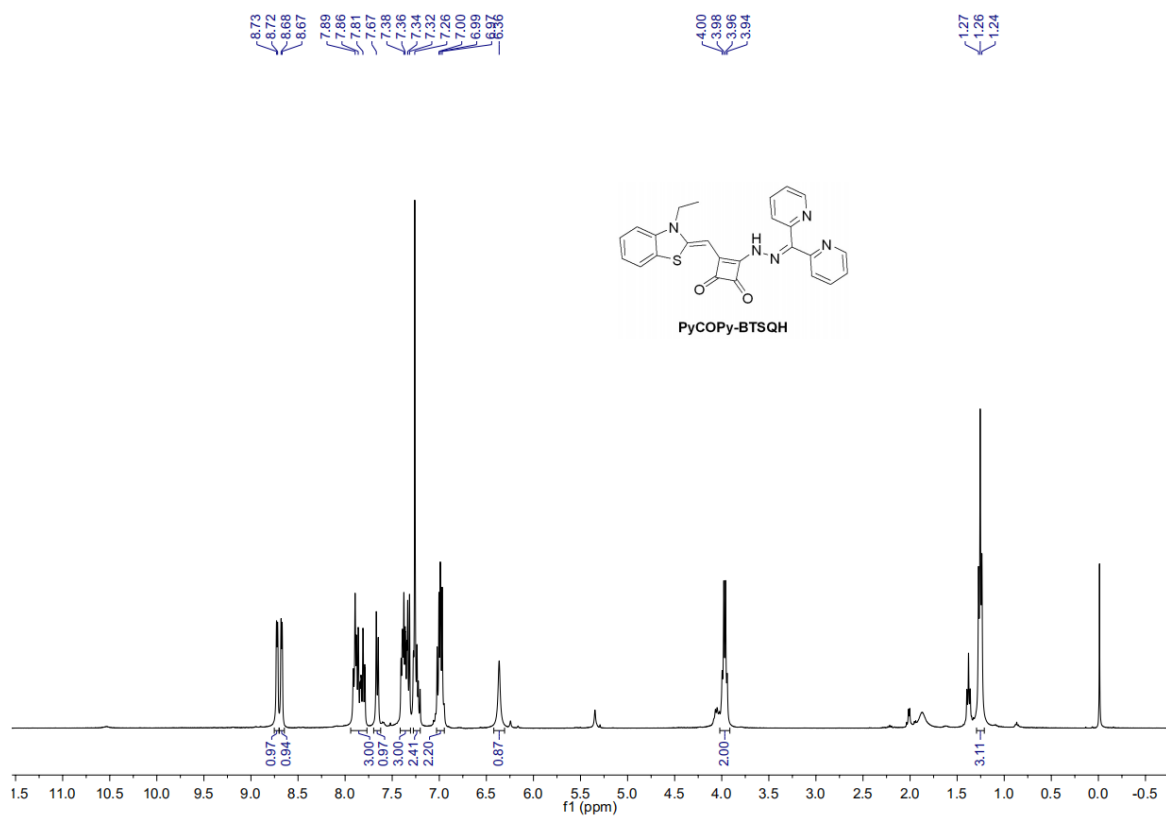
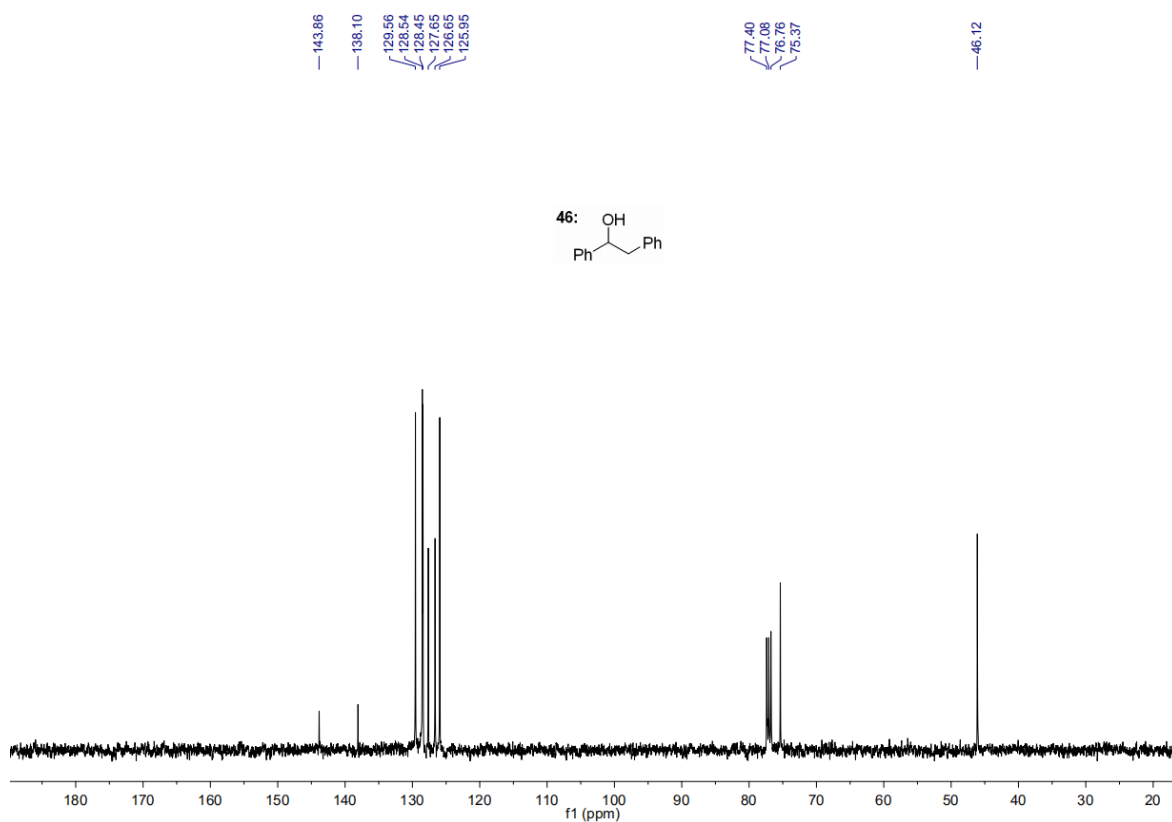


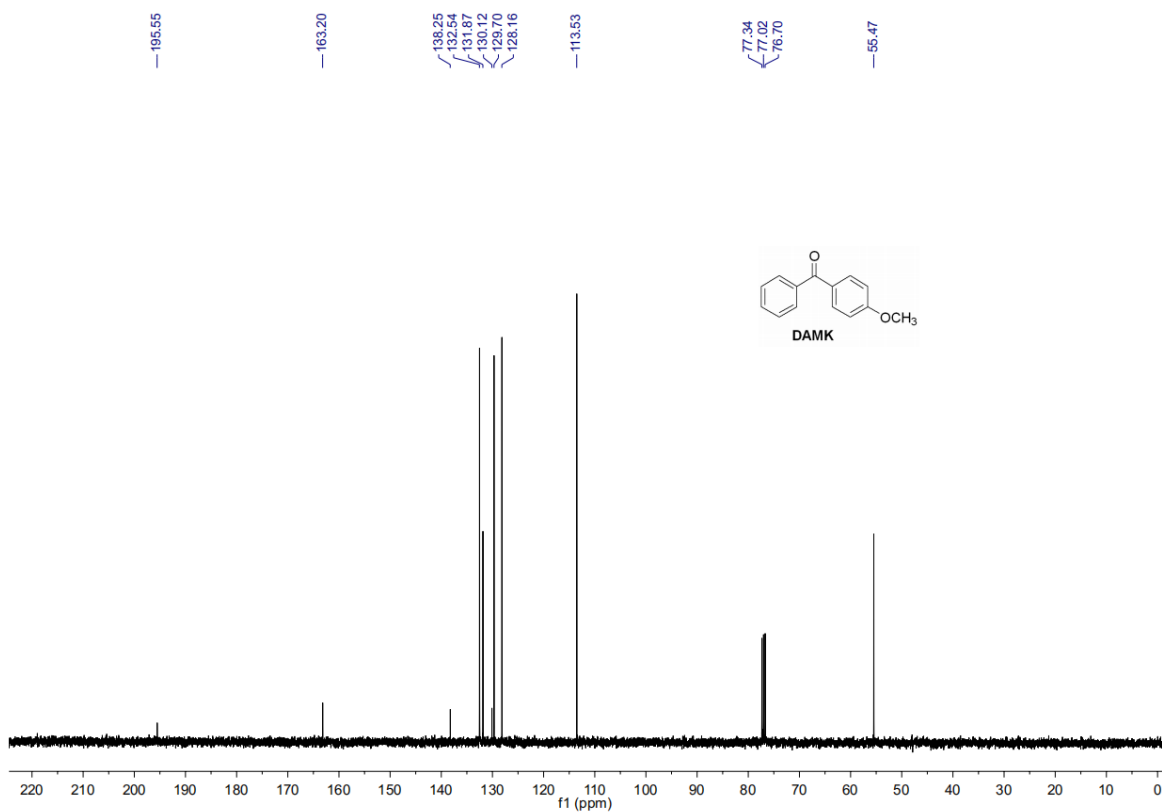
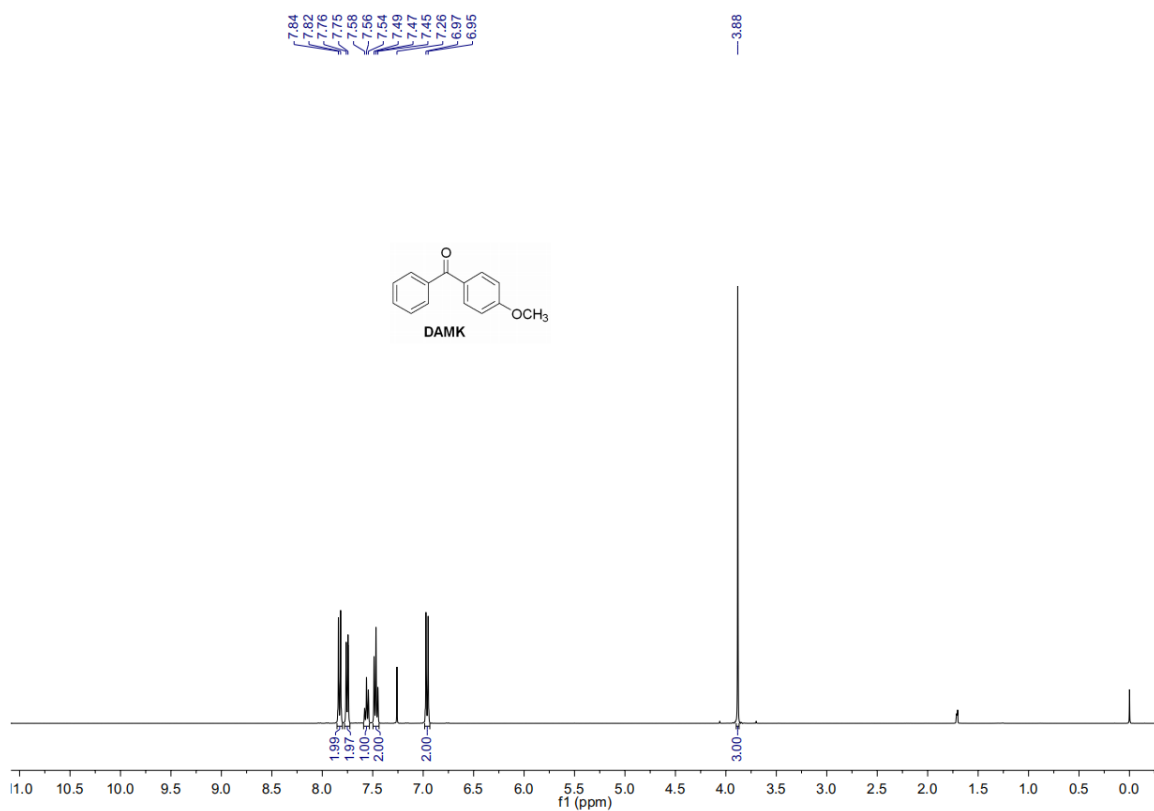




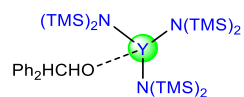








11. Cartesian coordinates of all optimized structures



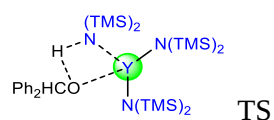
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Si	-2.88595900	1.92264600	0.16779100
Si	-2.60571700	-0.18597000	-1.94092900
C	-4.66742100	1.35224900	0.51426300
H	-5.17354000	2.13364000	1.09681300
H	-5.25437900	1.20070100	-0.39855400
H	-4.71208000	0.42586700	1.09912300
C	-2.18576600	2.36645700	1.87003800
H	-2.21534600	1.50580700	2.55061700
H	-1.15068800	2.72251900	1.84616600
H	-2.80081200	3.15734700	2.31949700
C	-3.06560500	3.52886300	-0.82681400
H	-2.10112300	3.93887800	-1.14438000
H	-3.66780000	3.37802500	-1.72962700
H	-3.56782600	4.29383900	-0.21980700
C	-1.30909000	-1.24263800	-2.83631400
H	-1.76017100	-1.65376400	-3.74940800
H	-0.40350700	-0.70173500	-3.12659800
H	-1.00143900	-2.10048000	-2.22455500

C	-3.52539800	0.87287300	-3.21770200
H	-3.82730700	0.24393400	-4.06547100
H	-4.43955300	1.30887000	-2.79778800
H	-2.91366700	1.69134800	-3.60916500
C	-3.88141800	-1.46239200	-1.33623700
H	-3.46165000	-2.16055100	-0.60197900
H	-4.77073600	-1.00606700	-0.89175400
H	-4.21108500	-2.06765300	-2.19145800
N	1.34839100	1.83635800	1.41941000
N	1.72906100	0.55002100	-2.02649700
Si	1.90748300	3.41812000	0.91973200
Si	1.73395500	1.34759800	3.05615100
Si	2.99281900	-0.62935100	-1.81529900
Si	1.70303600	1.48137000	-3.51074900
C	3.56667200	1.61178600	3.48535900
H	3.86375800	2.66660500	3.46777000
H	3.77131600	1.23358900	4.49561500
H	4.22280800	1.07240300	2.79091600
C	0.70717100	2.21388100	4.39568700
H	0.99188800	1.82727700	5.38337600
H	0.84815100	3.29882500	4.41199600
H	-0.36312500	2.02030500	4.26059100
C	1.40930400	-0.49842700	3.34249700
H	0.35710700	-0.76110100	3.18969600

H	2.03386600	-1.14906300	2.71989800
H	1.64502700	-0.73087300	4.38916300
C	3.69289100	3.41301100	0.29093200
H	3.97841700	4.39952400	-0.09693400
H	4.39874500	3.15169300	1.08738000
H	3.81609000	2.68618100	-0.51892100
C	1.78589400	4.77828600	2.23877200
H	2.43337100	4.60740200	3.10587700
H	2.09194400	5.73216500	1.78855600
H	0.75934400	4.89960900	2.60389600
C	0.78305900	4.04404200	-0.47696600
H	0.63711100	3.35331200	-1.31767500
H	-0.20331300	4.30665500	-0.07905000
H	1.20917700	4.95459300	-0.91809200
C	2.98984300	-1.15560500	0.01937300
H	3.20317100	-0.31752600	0.69367800
H	2.06814900	-1.65208400	0.35771800
H	3.78492400	-1.89758000	0.17017600
C	4.75128400	-0.01435600	-2.16002900
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H	4.89130300	0.27359400	-3.20825000
H	5.00679200	0.85152000	-1.53889000
C	2.74576900	-2.22610700	-2.80817000
H	3.46995200	-2.98939100	-2.49275900

H	1.73791000	-2.63260200	-2.66434500
H	2.88409700	-2.06657400	-3.88273900
C	2.91581200	2.93925300	-3.49201600
H	3.95379900	2.60717900	-3.37664200
H	2.84854200	3.49235800	-4.43828300
H	2.70304200	3.64210300	-2.67974300
C	2.13833400	0.45747900	-5.05205800
H	3.17182200	0.09156200	-5.04851500
H	1.47571600	-0.40796300	-5.17227900
H	2.02312500	1.08749000	-5.94410100
C	-0.02072200	2.18583600	-3.86921500
H	-0.51931300	2.64005600	-3.00574700
H	0.05811400	2.96139100	-4.64239700
H	-0.68401500	1.40443400	-4.25524600
H	-1.45108000	-1.16941400	0.37171300
C	-0.52688300	-2.70449200	1.35418300
H	0.50376700	-2.77015700	1.71580800
C	-1.45081900	-2.71385700	2.55799800
C	-1.29686500	-3.73934700	3.50011400
C	-2.45301000	-1.76235400	2.75668700
C	-2.12564900	-3.80994800	4.61487400
H	-0.52231100	-4.48966400	3.35549700
C	-3.28766600	-1.83496400	3.87422600
H	-2.59007700	-0.94350600	2.05584800

C	-3.12734500	-2.85644400	4.80546800
H	-1.98792000	-4.60946900	5.33815200
H	-4.06048200	-1.08361000	4.01342300
H	-3.77443900	-2.90951700	5.67686300
C	-0.76623200	-3.85285800	0.38675800
C	0.30002600	-4.32119800	-0.39032400
C	-2.02249900	-4.44947800	0.23901600
C	0.11366800	-5.35204300	-1.30810000
H	1.28537300	-3.87530900	-0.27620800
C	-2.21180000	-5.47972900	-0.68117700
H	-2.85293000	-4.11978900	0.85723700
C	-1.14620600	-5.93189900	-1.45742800
H	0.95268100	-5.70450600	-1.90204900
H	-3.19398300	-5.93314700	-0.78568200
H	-1.29399000	-6.73899400	-2.17020900



Y	8.19047100	13.96377200	8.48504600
O	7.16259900	12.07713600	9.30559800
N	5.77185400	13.80197700	8.17178800
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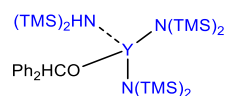
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H	2.87000100	13.50887200	9.84040700
C	5.51899500	15.28748300	10.74454600
H	5.51264000	14.37568500	11.35409300
H	6.55277800	15.65039300	10.70225400
H	4.92671100	16.04461000	11.27496900
C	4.67283000	16.64852400	8.13117200
H	5.64468700	17.00050700	7.77032900
H	4.00344900	16.59695300	7.26596000
H	4.27523700	17.41509000	8.80940900
C	6.38845700	12.08978400	5.78136200
H	5.97476800	11.74671700	4.82382300
H	7.29247300	12.66828300	5.56659500
H	6.69096000	11.19631000	6.34100100
C	4.22347000	14.29060700	5.56147100
H	3.96663900	13.78347400	4.62215700
H	3.28735600	14.67117100	5.98689300
H	4.85483800	15.14944700	5.31531200
C	3.73474900	11.76886200	7.15226500
H	4.14075500	10.94825700	7.75362200
H	2.87700700	12.19177700	7.68464000
H	3.35741900	11.32568400	6.22083500

N	9.10899400	15.22855200	10.08958200
N	9.46973200	13.92213000	6.64502400
Si	9.65827400	16.81110900	9.57831200
Si	9.51668600	14.74190500	11.72640600
Si	10.72359500	12.72997500	6.85475300
Si	9.43566300	14.85047200	5.15887900
C	11.35931500	14.99472100	12.11814200
H	11.66125800	16.04823500	12.09781900
H	11.58039900	14.61341500	13.12373900
H	12.00052000	14.45353800	11.41130500
C	8.52626900	15.62945600	13.07903300
H	8.83707800	15.25080500	14.06194500
H	8.67124600	16.71382600	13.08216800
H	7.45256900	15.43553100	12.97626100
C	9.17111800	12.90373200	12.02550400
H	8.11543000	12.65466300	11.87526800
H	9.78286200	12.23712700	11.40725800
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H	8.36791500	16.72383000	7.35662700
H	7.53258900	17.68404600	8.59707100
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C	9.85144500	13.81686400	3.62023900
H	10.88395200	13.44812500	3.61711900

H	9.18542600	12.95250500	3.51303900
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C	7.71068700	15.56111000	4.81404400
H	7.23998500	16.06574700	5.66575900
H	7.78300300	16.30210100	4.00702100
H	7.02570300	14.77652800	4.47605100
H	6.26150900	12.64303300	8.92662200
C	7.10333800	10.81846700	9.98957700
H	8.11228300	10.67503500	10.39529200
C	6.15054800	10.83660300	11.16903400
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C	4.91332400	11.48528600	11.11792500
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C	6.85035100	9.66241000	9.02359500
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C	7.72637400	8.19138000	7.29616300

H	8.86367200	9.73732300	8.25769600
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C	6.49642700	7.53733000	7.21573500
H	8.55428600	7.88056600	6.66411800
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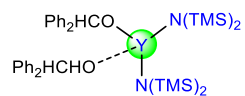
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C	-2.38174600	2.49524700	1.82398500
H	-2.60866100	1.71850800	2.56456500
H	-1.29380200	2.62571600	1.81157300
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H	-3.28524100	4.45116500	-0.47816000
C	-1.51515700	-1.33636800	-2.67585000
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C	-3.58346500	0.92090400	-3.21595300
H	-3.84808900	0.33469100	-4.10551100
H	-4.50201100	1.40292900	-2.86374800
H	-2.88417900	1.69916000	-3.53284600
C	-4.24763100	-1.39636200	-1.33733200
H	-3.91259500	-2.03336000	-0.51195400
H	-5.13735000	-0.85043100	-1.00811800
H	-4.54941600	-2.06284600	-2.15558100
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Si	3.10120000	-0.74860800	-1.78022200
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C	3.49298800	1.83195100	3.61839800
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C	1.72759800	-0.57495600	3.43568000
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C	-0.26823200	-2.59678400	1.30600500
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C	-0.58083200	-3.69764000	0.28995600
C	0.46247700	-4.28556400	-0.43253500
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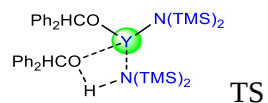
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Si	2.41951600	3.04113900	1.00451600
Si	1.89274200	0.90660500	3.07230600
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H	3.97298600	2.11836400	3.86572300
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C	1.22215200	-6.11691900	-2.06879300
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C	-5.36263500	0.44668700	-1.52893500
H	-6.00802800	2.44413700	-2.03059200
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N	9.22457400	15.31908600	10.71646000
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Si	9.50763300	14.68504400	12.33884700
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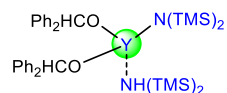
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H	10.17915200	19.15382400	11.06019900
H	8.73727700	18.36628900	11.72582500
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H	9.33614400	16.64527700	7.78942200
H	8.17387700	17.63049300	8.69599800
H	9.74269200	18.30473100	8.24227400

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H	10.56744400	11.91209900	9.00322100
H	12.18365300	12.46302100	8.64926300
C	11.99474500	14.61407800	6.33920900
H	13.01249700	14.25366700	6.53732600
H	11.92253400	14.81873100	5.26473400
H	11.86408400	15.56706900	6.86332200
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H	12.01923500	11.48644600	5.81327800
H	10.36560500	10.95046000	6.16114400
H	10.69224600	11.97567400	4.75273300
C	9.17111000	14.92605500	4.04999600
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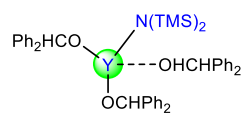
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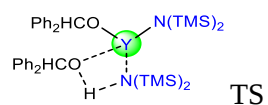
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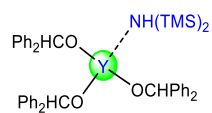
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Si	4.51576000	12.48626400	7.90919300
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H	2.95449800	10.56420200	7.64812700
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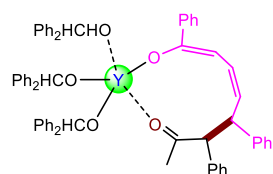
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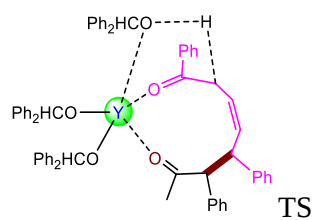
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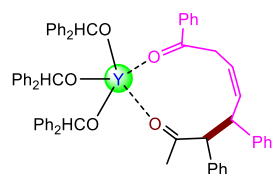
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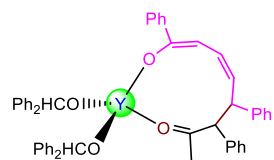
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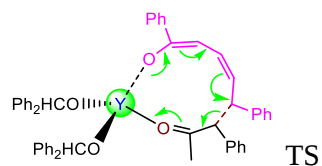
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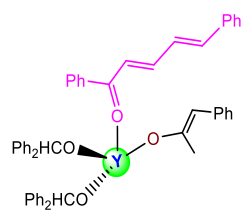
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C	2.40336800	3.23962900	1.27111300
H	1.94829800	3.72341200	2.15339100
C	3.03891900	-0.61103800	-2.63960900
C	4.16920300	0.07191000	-3.09272200
C	3.21428200	-1.74195900	-1.83252300
C	5.45241200	-0.36208700	-2.75260400
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C	4.49108300	-2.17579600	-1.48753500
H	2.33924700	-2.28394500	-1.48165100
C	5.61636800	-1.48697000	-1.94818500
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C	-0.85514100	-2.74614500	-4.29168400
H	-0.61954600	-1.59915400	-2.47509600
C	-0.35054700	-3.01078200	-5.56260000
H	1.19619900	-2.53791100	-6.99034400
H	-1.74867600	-3.26002500	-3.94345300
H	-0.84457400	-3.73046100	-6.21086800
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C	3.05813000	4.01830100	-1.06090700
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H	3.55536300	3.06201200	-1.20548500
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H	2.42634700	6.93481100	-2.69823600
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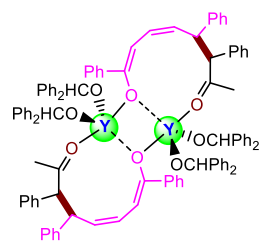
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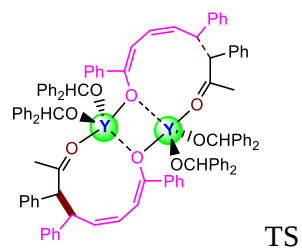
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O	-4.72700100	-3.73180700	-0.81667000
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H	-5.93514900	1.27075100	3.65778400
C	-8.47375500	-0.34187600	1.22556600
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C	-7.44816400	-5.68065200	-4.53915600
H	-9.28314900	-4.79198100	-3.84040800

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C	-4.93060100	-8.19649700	1.55363700
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H	-5.59114400	-2.52682000	7.02057300
H	-5.43191800	-5.54547700	3.95669100
C	-8.79914900	0.85081100	1.87414900
H	-8.12313300	2.35749900	3.25895600
H	-9.18379900	-0.79793200	0.53890200
H	-7.85516700	-5.96066500	-5.50778600
H	-4.71470700	-9.10749700	2.10681600
H	-5.70028000	-4.92366100	6.35744200
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H	-5.75041500	-2.95805500	-3.59517200
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O	-3.81711300	-1.26391800	-2.57486200
C	-3.07034200	-1.70521600	-4.80428900
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H	-2.32190300	-5.10597200	-4.26237900
C	-1.75329500	-3.60945400	-2.90337700

H	-1.68813800	-2.54167600	-2.70363100
C	-1.22449800	-4.46507200	-1.86576300
C	-1.03957600	-4.06735100	-0.57621000
O	-1.43590500	-2.85014900	-0.12744200
H	-0.99283900	-5.49632200	-2.11774700
C	-0.43574200	-4.97599300	0.42648000
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C	2.13343700	0.19006200	-3.52159900
C	4.65149600	0.45259500	-4.67745400
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C	2.38065000	1.21633200	-4.43800000
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H	1.58650800	1.91719300	-4.68588200
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C	2.01167700	2.84443900	-0.85152600
C	0.35129200	4.89605800	0.04076300
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H	2.66161000	2.04682600	-1.20123300
C	0.92513300	4.97262600	-1.22573000
H	-0.30358400	5.68913900	0.39356700
H	2.21078000	3.99116600	-2.65611400
H	0.72833000	5.83034200	-1.86463000
C	3.22542800	1.56450100	1.70245500
C	3.74470200	2.58469100	2.50950500
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C	5.09641900	2.61413400	2.84327000
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C	5.44866900	0.59843100	1.57265400
H	3.69247300	-0.21622100	0.61145700
C	5.95673600	1.61808300	2.37511400
H	5.48082400	3.41711600	3.46816900

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H	2.47754200	-4.62261100	3.58348300
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H	3.10645700	-3.51892800	2.31892400
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C	-0.00045200	-1.62112000	4.91676600
C	-0.65239500	-0.50745500	4.12963000
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C	-1.26461500	-0.56693300	2.93102100
H	-1.31910800	-1.52462500	2.41696800
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C	-4.07273900	3.69870600	0.15050800
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C	-0.89973400	-5.05951000	5.15984800
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H	-1.74920500	-4.90311800	4.49830300
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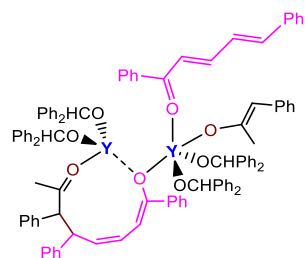
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H	0.66944600	-1.29243000	3.64685200
C	1.28656700	0.23424900	5.00617300
C	0.73887700	1.34370300	4.13437300
H	0.76828900	2.32630800	4.60641400
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C	-0.34192100	2.32095400	2.11673500
C	-0.59241400	2.20948800	0.78065300
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H	-0.53829700	3.26727300	2.61120900
C	-1.20486900	3.28786500	-0.02372500
C	-1.99707000	4.28920200	0.56348700
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C	-2.54522500	5.30583200	-0.21191200
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C	-1.55693000	4.34188100	-2.18792500
H	-0.40191400	2.55762300	-1.88642600
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H	-3.16477300	6.06376600	0.26079100
H	-1.37976000	4.35182800	-3.26015500
H	-2.76095700	6.13225000	-2.19435500

C	2.41768900	0.74911400	5.88186700
C	2.40685700	0.50913600	7.26139300
C	3.46169800	1.51675600	5.34822000
C	3.42147000	0.99880900	8.08279100
H	1.59382000	-0.06832500	7.69563000
C	4.48165500	2.00268800	6.16521700
H	3.47315700	1.75433000	4.28625500
C	4.46591000	1.74212000	7.53537000
H	3.39098300	0.80301400	9.15175000
H	5.28079800	2.59139600	5.72338100
H	5.25730000	2.12632900	8.17396700
C	1.69709600	-2.31556400	5.17761500
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C	2.75213500	-2.50524900	6.08181500
C	0.68862300	-4.37124900	6.00424800
H	-0.17887000	-3.13379700	4.48405400
C	2.77938800	-3.61680200	6.92325300
H	3.55461100	-1.77981200	6.15129300
C	1.75058500	-4.55606500	6.88643400
H	-0.13048700	-5.08354900	5.96791000
H	3.60894100	-3.74177200	7.61469500
H	1.77447000	-5.42092000	7.54445700
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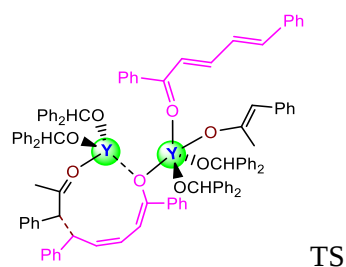
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C	-4.67203300	1.48117900	0.40721800
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C	-3.79229500	-3.99071300	0.20323700
C	-3.26013200	-3.29785600	2.57661100
H	-4.57362800	2.29300900	-0.33598600
C	-4.79602700	2.16225100	1.76858700
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C	-2.85175800	-4.70648700	-0.54234500
C	-3.58437900	-2.39310300	3.59543300
C	-2.83407400	-4.58024500	2.93826200
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H	-5.88543500	-3.79467500	0.66986500
C	-3.24642500	-5.76968100	-1.35532100
H	-1.80810500	-4.41377200	-0.48272700
C	-3.49398700	-2.75769000	4.93801000
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C	-2.74731900	-4.95235900	4.28057200
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H	-4.90069300	-6.95152300	-2.07893800
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H	-3.36985600	-2.83276500	-3.98207900
H	-4.91353400	-1.97156800	-4.19101800
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O	-2.39814900	-0.65819800	-2.49984100
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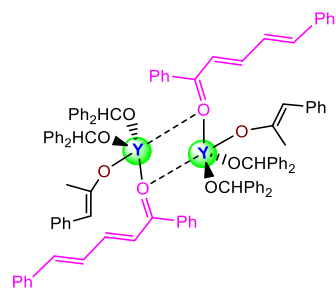
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H	3.25910600	-5.47555700	6.07660800
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H	5.29063900	-4.64635400	7.25796900
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O	-2.28729300	-2.27382500	0.36747400
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C	-3.19687200	-2.96967600	1.16257900
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H	-4.06632600	-2.32684300	1.39006000
C	-3.75112100	-4.21414100	0.47330100

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C	-5.02518400	1.93436500	1.96250600
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H	-3.26671900	-6.21423600	-2.24235300
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H	-3.81080900	-2.29151000	-4.39962500
H	-5.39818100	-1.49629100	-4.29160900
H	-4.59155400	-2.10475700	-2.83020200
C	-3.72889200	-0.30060500	-3.57242600

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C	-4.00986000	0.86503300	-4.23233700
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C	-0.95947400	-0.88237700	-5.45337400
H	-1.25223100	-1.83760200	-5.88733700
C	-0.40736300	-0.92413500	-4.14340600
H	-0.33669600	0.00665900	-3.58999500
C	-0.00164000	-2.08430600	-3.52447300
C	0.35731600	-2.12126100	-2.15090200
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C	0.92972300	-3.34961900	-1.57321500
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H	-2.32801700	-2.08550100	5.68534400

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C	-0.85507800	1.61961100	-5.93634100
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C	-1.66406900	2.66322200	-6.42813900
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C	-5.51377100	2.42491600	-5.41382300
C	-6.25212600	0.52422700	-7.29332600
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C	-6.41603500	2.75632800	-6.41861100
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H	-6.82512000	3.76348500	-6.46185100
H	-7.50789900	2.05972500	-8.14931000



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C	3.89736900	-0.63986400	-4.10523500
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C	5.72849200	-1.42970000	-1.18052400

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H	5.94307600	0.59771700	-1.87103700
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C	4.78047300	4.75903500	-4.09480300
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H	4.98758400	2.42190900	0.49283900
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H	3.68922300	6.32341500	3.26684000
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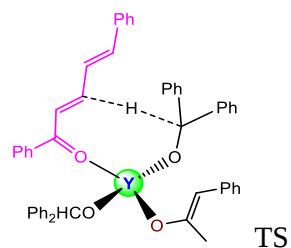
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H	3.96424000	-4.72739300	8.01396300
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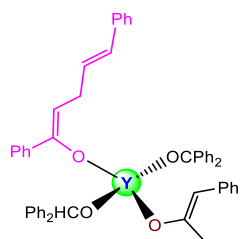
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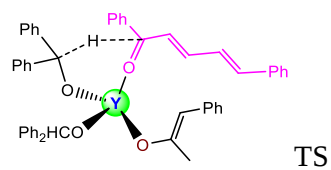
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H	3.48653300	-2.09475800	-3.81828600
C	1.40816000	0.82097300	-5.31569100
H	0.95515100	1.35280600	-3.28279800

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H	2.00887000	0.04308600	-7.23405000
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C	2.93155800	5.13049500	-0.45544400
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C	3.20419600	6.30446600	0.24257400
H	2.93326500	7.36573400	2.10107100

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H	1.56261500	-6.97439600	4.26203900
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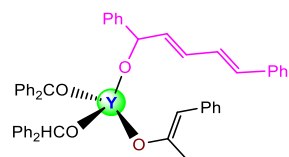
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C	2.33602700	2.60271600	-4.10407300
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H	-2.11755900	-4.33130600	-4.98018600
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C	2.01001400	6.08695600	1.41559600
C	1.67273800	4.81438400	-0.59740800
C	2.61117100	7.10336500	0.67899000
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C	2.27735100	5.83167600	-1.33913700
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H	2.97326000	7.99541600	1.18480500
H	2.37419500	5.72330200	-2.41703200
H	3.21604800	7.77310200	-1.28190200
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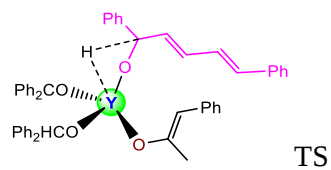
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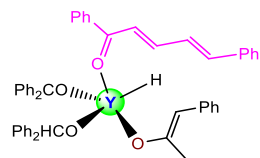
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C	-2.90885600	1.53945900	-3.24639700
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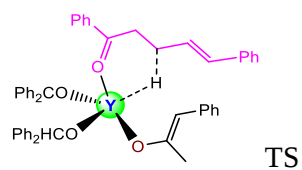
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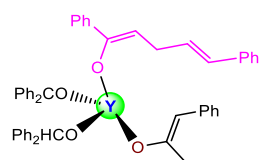
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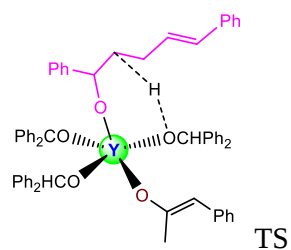
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C	-2.65994100	-1.61755900	-1.54895400
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O	-2.21504400	-0.22840200	0.30241800
C	-3.62145900	0.68780200	-1.39744200
C	-4.59610400	0.50974400	-2.39214000
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C	-5.32278600	1.59027200	-2.88234600
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H	-6.07716900	1.42713500	-3.64843200
H	-3.98970600	4.05170400	-0.95752200
H	-5.67692600	3.71580600	-2.75723100
C	-4.69032500	-5.55565600	0.27323600
C	-5.29048700	-5.81403200	1.51646700
C	-5.10011600	-6.33141700	-0.82521300
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C	-0.43729500	-0.95074700	7.38030900
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C	0.49973700	-3.53776300	-4.41304900

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C	1.33193700	-4.46392100	-3.78483300
H	2.75448300	-4.78809300	-2.19682000
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H	1.38432400	-5.48623500	-4.15031300
H	-0.79935100	-0.73861300	-1.61971900
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Y	-0.00730300	0.11898200	0.57538400
O	2.33720900	0.51523800	0.68054000
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H	-0.59915300	-3.03283500	-2.43443800
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C	5.82091000	1.03945600	0.22430600
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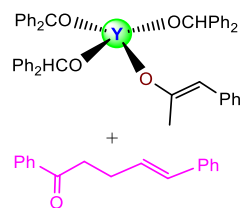
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C	5.15344600	0.93728800	4.50109800
H	5.39860800	1.98759200	2.64354100
C	3.41163700	-0.74356500	4.55407200
H	2.29172200	-0.99813800	2.73652300
C	4.43782300	-0.04263100	5.19099900
H	5.93586800	1.49876700	5.00441200
H	2.83897300	-1.49479500	5.08994400
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H	0.82079900	5.46601300	0.61705300
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H	0.56455100	2.73632300	3.91538100
C	2.77914900	5.26772800	3.38999100
H	2.77464700	6.56879600	1.67163500
H	2.52433500	3.82324100	4.97245700
H	3.63445500	5.75075200	3.85664400
C	-1.90255000	3.56330500	2.39291100
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H	3.28127700	2.78631600	-5.79499500
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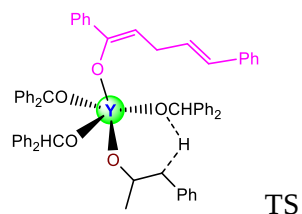
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H	1.61486800	2.50061100	-1.98081400
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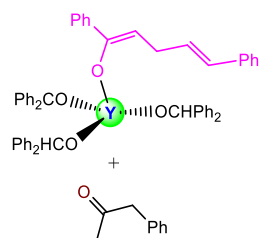
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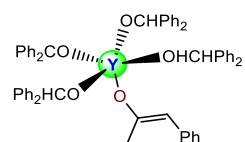
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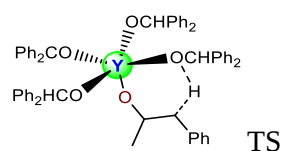
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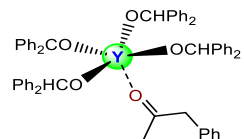
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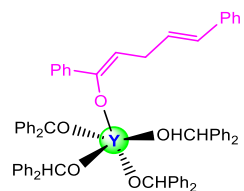
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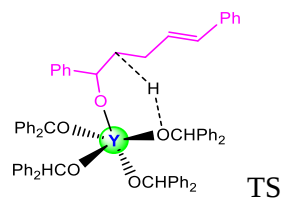
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H	-0.59346000	-0.74435600	-6.40913100
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C	-8.39309000	1.16332600	0.28814300
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C	-10.76794100	1.40042900	0.78939700
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C	-9.61478000	-0.62403400	1.39780000
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H	-11.71312100	-0.27360000	1.76908700
H	-7.25461400	2.80732200	-0.54517300
O	0.34537200	-1.18516400	-0.80908600
C	1.37691000	-2.02996200	-1.17187300
H	1.65946100	-1.85571800	-2.22671200
C	0.96054400	-3.49895000	-1.07257300
C	0.35914900	-3.98768400	0.09370000
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C	-0.01626000	-5.32522200	0.19290300
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C	0.80306200	-5.72342600	-2.03851000
H	1.63750600	-4.01325400	-3.04974000
C	0.20465600	-6.19920500	-0.87397700
H	-0.48012400	-5.68856600	1.10696300
H	0.97769500	-6.39468700	-2.87626800
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C	3.89773700	-2.11357800	-0.86277000
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C	5.05347400	-1.94128200	-0.10361900
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H	5.86645800	-1.32185700	1.79665400
H	-3.53725300	-0.65971000	-1.58768300
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C	-3.05905800	-2.46218100	-0.79392100
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H	-6.58983800	-3.33764600	-3.74321700
H	-5.10777000	-4.52844900	-5.34511100
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O	0.36989500	1.79656500	-1.24358900
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C	2.49079200	4.53115200	-0.36741400

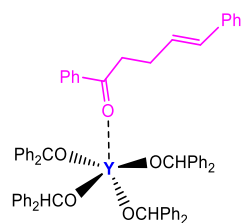
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C	3.70814500	2.54715900	1.18022800
H	2.45316600	1.15664100	0.12032900
C	4.05844300	3.88779800	1.35189900
H	3.69811800	5.92410900	0.73789500
H	4.18127900	1.77070200	1.77395600
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C	-2.41377400	2.51419200	2.83079500
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C	-3.51249700	4.16318000	4.23449000
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H	-5.30003600	1.69740600	-0.79707600
C	-4.48146800	-0.02778400	-1.82233700
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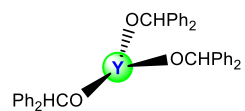
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C	3.28395400	-1.78967300	0.37639300
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C	2.86326700	-1.47428700	1.66954300
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C	-4.44115100	-5.00930400	2.94896900
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H	-1.80182700	-4.67729300	-4.96857200
H	-5.79647800	-4.37696900	-3.40495300
H	-4.26328200	-4.79603400	-5.31798200
H	-5.42371300	-0.75548700	-2.09068500

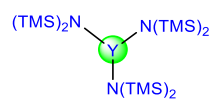


Y	-1.49410600	2.02138500	-0.59695000
O	-0.94719200	3.38193000	0.84889200
C	-0.59154300	4.59119100	1.43343300
H	-1.48745200	5.05237600	1.88667100
C	-0.08620300	5.55853800	0.36584600
C	-0.80863000	6.70740000	0.03808100
C	1.08938400	5.27640100	-0.34211900
C	-0.37162100	7.56125200	-0.97671900

H	-1.72549400	6.93550000	0.57930300
C	1.52535100	6.12200700	-1.35841600
H	1.66861100	4.39248000	-0.08357500
C	0.79480900	7.26873600	-1.67924800
H	-0.94608000	8.45228900	-1.21873700
H	2.44113100	5.89123400	-1.89753400
H	1.13735200	7.93083100	-2.47056900
C	0.42893200	4.41806800	2.55804300
C	0.77818300	5.51610900	3.35385300
C	1.02224000	3.18360900	2.82209200
C	1.70164200	5.38267900	4.38639700
H	0.32724600	6.48681800	3.15495900
C	1.95175500	3.04693600	3.85507800
H	0.74656900	2.32908600	2.21184900
C	2.29458100	4.14445900	4.64084800
H	1.96103400	6.24643900	4.99416400
H	2.40708300	2.07748800	4.04584200
H	3.01681500	4.03880500	5.44665400
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C	1.00099000	-0.11704700	-1.55898600
H	1.82607200	0.01145800	-0.83548800
C	1.61154700	0.02538000	-2.95139700
C	2.71417100	-0.76143000	-3.30691500
C	1.10642000	0.93249100	-3.88281000

C	3.29582600	-0.64492300	-4.56575900
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H	4.15251700	-1.26291500	-4.82427300
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C	-0.50384200	-2.05411800	-2.23210200
C	0.17064200	-3.48829400	0.05921400
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H	-1.80597600	-3.70210900	-2.69781300
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C	-3.53337800	-0.00845000	-0.70343000
C	-4.10441100	1.19003300	1.75076200
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C	-3.19592100	-0.65853600	0.48887900
H	-3.30935000	-0.47968400	-1.65785700
C	-3.47934300	-0.05786900	1.72009300
H	-4.32111300	1.66735300	2.70259600
H	-2.70373200	-1.62646700	0.44705100
H	-3.21115500	-0.55808200	2.64638100



N	4.21856300	11.07252300	11.24698600
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Si	3.23963000	10.66941400	9.87134000
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C	2.52219600	9.64036600	13.32007200
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Si	6.58564800	14.69843400	11.44537500
Si	8.54301200	10.50805800	8.52236800
Si	7.41835900	8.24226700	10.24393300
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H	7.28446900	9.59810000	6.54071300
C	10.38995100	10.51043000	8.93162900
H	10.78855800	9.49047000	8.97432400
H	10.95778700	11.05444700	8.16558100
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H	8.71298000	12.73911700	7.43621800
H	7.03202400	12.45843500	7.79957800

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