Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting information

Controllable Carbonyl-Assisted C(sp^3)–C(sp^3) Bond Reduction and Reorganization

Shengke Wang,[#a] Yitu Wang,[#a] Kun Hu,[a] Kai Wang[a] and Xigeng Zhou[*ab]

[a]Department of Chemistry, Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Fudan University, Shanghai 200438, China.
[b]State Key Laboratory of Organometallic Chemistry, Shanghai 200032, China.
[#]These authors contributed equally.

Email: xgzhou@fudan.edu.cn

Table of Contents

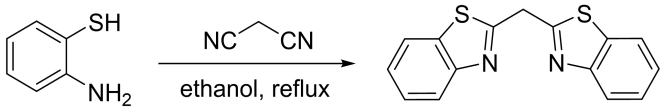
1. General information

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. ^{1}H NMR and ^{13}C NMR spectra of organic compounds were recorded on a JEOL ECA-400 NMR spectrometer (FT, 400 MHz for ^{1}H; 100 MHz for ^{13}C) in $CDCl_3$ at room temperature. All chemical shift values are quoted in ppm referenced to $CDCl_3$ (δ 7.26) for ^{1}H NMR. 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 Å), Agilent PLgel (5 μm, 106 Å) 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, Mn = 162 ~ 6.57 × 106 g/mol) 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*α radiation (λ = 0.71073 Å).

2. Synthesis and characterization of substrates

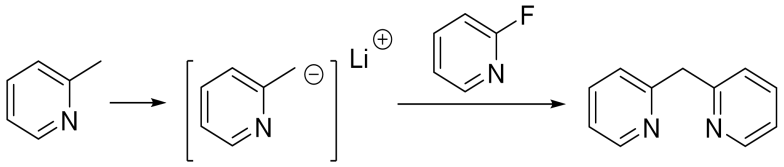
2.1 General procedures for preparation of heteroaryl- and dihydrooxazolyl-substituted ketones (1 - 5, 23 and 24)

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



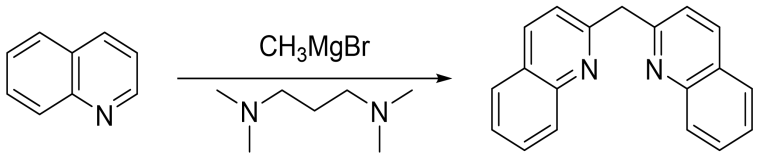
Aminothiophenol (10.0 g, 80.0 mmol) and malononitrile (2.64 g, 40.0 mmol) were dissolved in ethanol (40 mL). The reaction mixture was refluxed for 6 h, cooled to room temperature, and stored in the fridge at -32 °C. The resulting precipitate was filtered, washed with hexane (2 × 50 mL) and dried under reduced pressure. A yellow powder was obtained upon recrystallisation from ethanol in 69% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.62, 153.10, 135.83, 126.25, 125.36, 123.19, 121.66, 38.94.

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 N_2 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, 10.0 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 CH_2Cl_2. The combined organic layer was dried over Na_2SO_4, 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. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.42, 149.45, 136.60, 123.58, 121.48, 47.30.

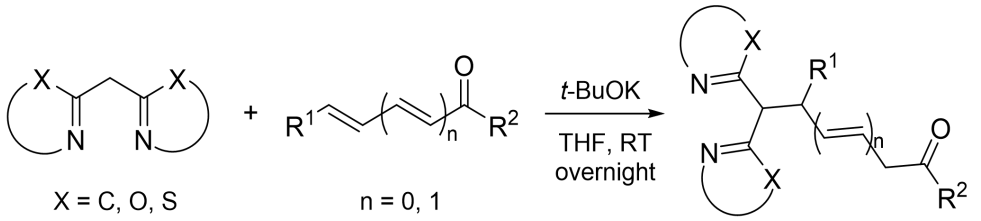
Synthesis of di(2-quinolyl)methane (13)[1]



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 N_2 atmosphere. After stirring 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 Na_2SO_4, filtered and condensed to afford a dark orange oil. The crude product was purified by silica gel column chromatography with the eluent 1:1 ethyl acetate/petroleum

ether, yielding light brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)

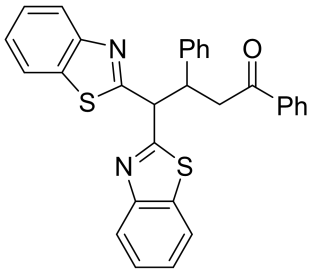


X = C, O, S — **11 - 14**

n = 0, 1 — **1 - 4, 23, 24**

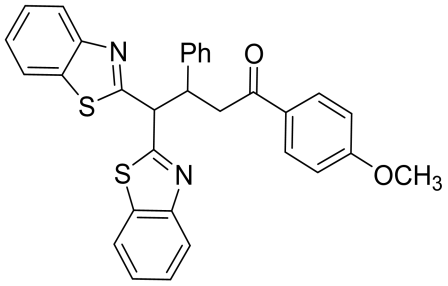
General procedures: To a mixture of methylene-bridged diheterocycle (**11 - 14**) (5.0 mmol) and *t*-BuOK (5.0 mmol) in THF (15 mL) was added the corresponding enone (5.0 mmol). Stirring at room temperature overnight and extracted with ethyl acetate (3 × 30 mL). The organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered and condensed, the residue was further purified on silica gel chromatography to afford the target ketones (**1 - 4, 23, 24**).

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



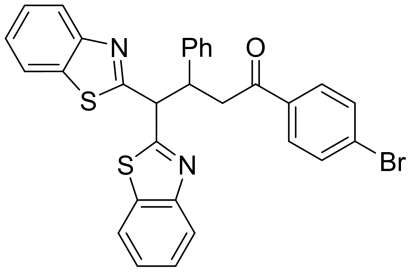
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (t, J = 9.6 Hz, 2H), 7.84 (d, J = 8.0 Hz, 1H), 7.77 (d, J = 7.6 Hz, 1H), 7.71 (d, J = 7.9 Hz, 1H), 7.48 – 7.26 (m, 9H), 7.13 (t, J = 7.2 Hz, 1H), 7.06 – 7.02 (m, 1H), 5.44 (d, J = 10.9 Hz, 1H), 4.77 (t, J = 8.7 Hz, 1H), 3.66 – 3.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



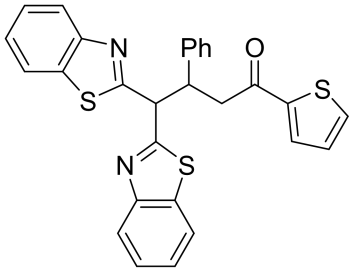
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, J = 18.0, 7.2 Hz, 2H), 7.77 (td, J = 23.6, 6.4 Hz, 1H), 7.46 – 7.31 (m, 6H), 7.13 – 7.03 (m, 3H), 6.81 (d, J = 6.8 Hz, 2H), 5.44 (d, J = 10.4 Hz, 1H), 4.75 (s, 1H), 3.80 (s, 3H), 3.60 – 3.40 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.99, 169.44, 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)



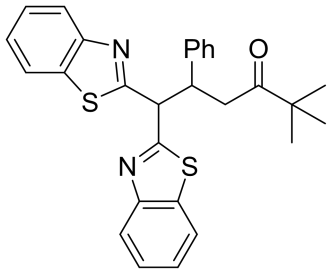
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 8.0, 3.9 Hz, 2H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.46 – 7.45 (m, 3H), 7.42 – 7.35 (m, 2H), 7.30 (t, *J* = 7.8 Hz, 3H), 7.14 (t, *J* = 7.5 Hz, 2H), 7.05 (t, *J* = 7.3 Hz, 1H), 5.42 (d, *J* = 10.8 Hz, 1H), 4.78 – 4.72 (m, 1H), 3.53 – 3.52 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



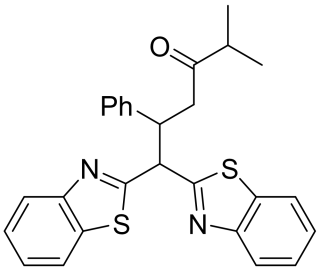
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, *J* = 16.8, 8.1 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.61 – 7.60 (m, 1H), 7.51 – 7.44 (m, 2H), 7.42 – 7.28 (m, 5H), 7.13 (t, *J* = 7.5 Hz, 2H), 7.06 – 7.00 (m, 2H), 5.44 (d, *J* = 11.0 Hz, 1H), 4.74 (td, *J* = 10.4, 3.6 Hz, 1H), 3.55 – 3.38 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



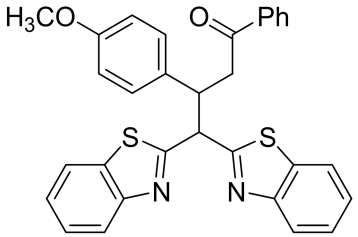
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.1 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.48 (td, *J* = 7.2, 0.8 Hz, 1H), 7.40 – 7.36 (m, 2H), 7.29 – 7.25 (m, 3H), 7.15 – 7.12 (m, 2H), 7.07 – 7.03 (m, 1H), 5.41 (d, *J* = 11.2 Hz, 1H), 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 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.

6,6-bis(benzo[d]thiazol-2-yl)-2-methyl-5-phenylhexan-3-one (1f)



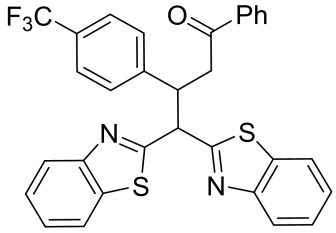
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.2 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.45 (m, 1H), 7.41 - 7.35 (m, 2H), 7.28 (d, *J* = 7.4 Hz, 3H), 7.15 (t, *J* = 7.5 Hz, 2H), 7.06 (t, *J* = 7.3 Hz, 1H), 5.36 (d, *J* = 11.1 Hz, 1H), 4.54 (td, *J* = 12.0, 4.0 Hz, 3H), 1H), 3.09 (dd, *J* = 16.6, 9.6 Hz, 1H), 2.87 (dd, *J* = 16.6, 4.0 Hz, 1H), 2.38 – 2.26 (m, 1H), 0.78 (dd, *J* = 11.4, 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.74, 169.41, 168.62, 152.77, 152.61, 140.75, 135.80, 135.19, 128.39, 128.30, 126.95, 126.13, 125.88, 125.35, 125.01, 123.22, 123.17, 121.72, 121.45, 54.84, 47.02, 45.07, 41.16, 17.66, 17.36.

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



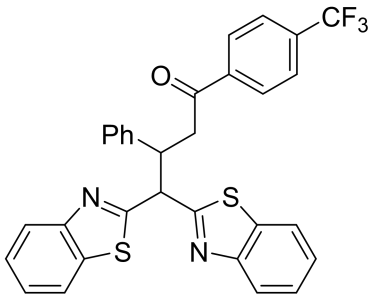
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 12.8, 8.1 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.78 – 7.76 (m, 2H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.48 – 7.44 (m, 2H), 7.42 – 7.33 (m, 4H), 7.31 – 7.27 (m, 1H), 7.22 (d, *J* = 8.7 Hz, 2H), 6.66 (d, *J* = 8.7 Hz, 2H), 5.40 (d, *J* = 10.8 Hz, 1H), 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 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 (1h)



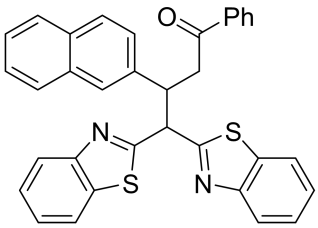
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, *J* = 17.2, 8.0 Hz, 2H), 7.85 (dd, *J* = 8.0, 0.4 Hz, 1H), 7.79 – 7.76 (m, 2H), 7.73 (dd, *J* = 8.0, 0.4 Hz, 1H), 7.51 – 7.46 (m, 4H), 7.45 – 7.29 (m, 7H), 5.44 (d, *J* = 10.8 Hz, 1H), 4.87 (td, *J* = 10.1, 3.9 Hz, 1H), 3.69 – 3.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.92, 168.71, 167.98, 152.75, 152.65, 144.95, 136.54, 135.69, 135.14, 133.15, 129.08 (d, *J* = 32.0 Hz), 128.80, 128.48, 127.96, 126.27, 125.54, 125.38, 125.34, 125.30, 124.72 (d, *J* = 278.0 Hz), 123.25, 121.73, 121.54, 54.63, 46.71, 42.80; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.58.

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



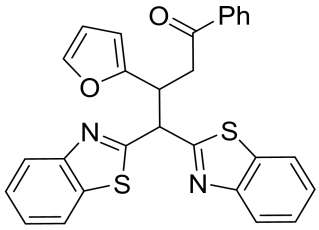
Light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.94 (m, 2H), 7.84 (d, *J* = 8.0 Hz, 3H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 2H), 7.49 – 7.35 (m, 3H), 7.33 – 7.27 (m, 3H), 7.14 (t, *J* = 7.4 Hz, 2H), 7.06 (t, *J* = 7.3 Hz, 1H), 5.41 (d, *J* = 10.8 Hz, 1H), 4.81 – 4.70 (m, 1H), 3.66 – 3.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.65, 169.18, 168.40, 152.83, 152.62, 140.47, 139.50, 135.79, 135.23, 134.18 (d, *J* = 33.0 Hz), 128.56, 128.34, 127.20, 126.89 (d, *J* = 280.0 Hz), 126.24, 126.02, 125.49, 125.17, 123.22, 121.72, 121.51, 55.12, 47.33, 43.50; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.15.

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



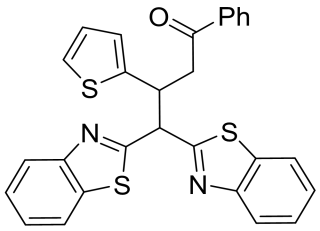
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.79 – 7.75 (m, 3H), 7.66 – 7.64 (m, 4H), 7.53 – 7.43 (m, 3H), 7.39 – 7.30 (m, 6H), 7.26 – 7.22 (m, 1H), 5.60 (d, *J* = 10.8 Hz, 1H), 5.00 – 4.94 (m, 1H), 3.72 (dd, *J* = 16.7, 9.5 Hz, 1H), 3.58 (dd, *J* = 16.9, 3.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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 (1k)



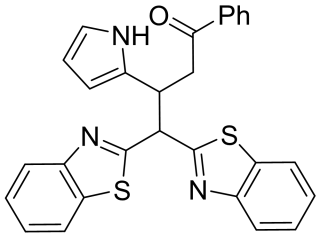
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 8.1, 3.6 Hz, 2H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.48 – 7.45 (m, 3H), 7.42 – 7.35 (m, 2H), 7.31 – 7.28 (m, 2H), 7.14 (t, *J* = 7.5 Hz, 2H), 7.05 (t, *J* = 7.3 Hz, 1H), 5.42 (d, *J* = 10.8 Hz, 1H), 4.78 – 4.72 (m, 1H), 3.53 – 3.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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 (1l)



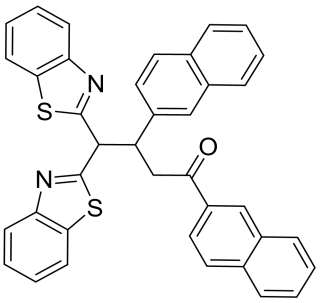
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 8.01 (m, 2H), 7.85 – 7.82 (m, 3H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.42 (m, 3H), 7.39 – 7.31 (m, 4H), 7.01 (d, *J* = 5.0 Hz, 1H), 6.86 (d, *J* = 3.2 Hz, 1H), 6.73 – 6.71 (m, 1H), 5.44 (d, *J* = 10.1 Hz, 1H), 5.12 (td, *J* = 9.6, 3.9 Hz, 1H), 3.69 (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 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 (1m)



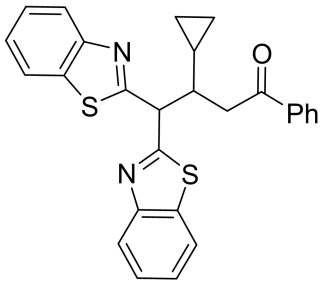
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.47 (s, 1H), 8.03 (dd, *J* = 17.4, 8.2 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.78 (dd, *J* = 15.2, 8.0 Hz, 2H), 7.53 – 7.44 (m, 3H), 7.40 – 7.32 (m, 4H), 6.62 (s, 1H), 5.96 – 5.95 (m, 1H), 5.92 (s, 1H), 5.60 (d, *J* = 8.4 Hz, 1H), 4.83 – 4.78 (m, 1H), 3.65 (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 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 (1n)



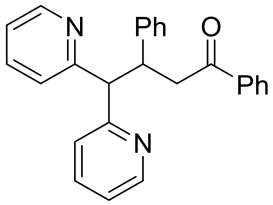
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 8.00 (dd, *J* = 19.3, 8.1 Hz, 2H), 7.86 – 7.73 (m, 6H), 7.69 – 7.64 (m, 4H), 7.57 – 7.42 (m, 4H), 7.39 – 7.31 (m, 4H), 7.26 – 7.22 (m, 1H), 5.65 (d, *J* = 10.9 Hz, 1H), 5.06 – 5.00 (m, 1H), 3.86 – 3.72 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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 (1o)



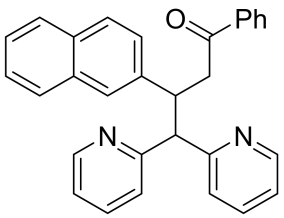
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 8.04 (t, *J* = 7.5 Hz, 2H), 7.91 – 7.89 (m, 2H), 7.86 – 7.80 (m, 2H), 7.52 – 7.43 (m, 3H), 7.41 – 7.30 (m, 4H), 7.15 (s, 0.25H, minor isomer), 5.37 (d, *J* = 7.9 Hz, 0.75H, major isomer), 3.53 – 3.40 (m, 1H), 3.34 – 3.17 (m, 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 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)



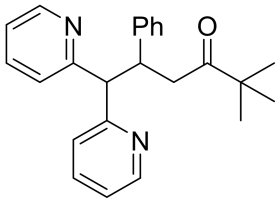
Light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 8.40 (s, 1H), 7.75 – 7.70 (m, 3H), 7.64 – 7.60 (m, 1H), 7.47 – 7.44 (m, 1H), 7.36 – 7.34 (m, 3H), 7.20 (s, 3H), 7.12 (s, 1H), 7.06 (t, *J* = 7.0 Hz, 2H), 6.97 – 6.94 (m, 1H), 6.87 (s, 1H), 4.67 (s, 2H), 3.42 – 3.37 (m, 1H), 3.13 (d, *J* = 16.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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.

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



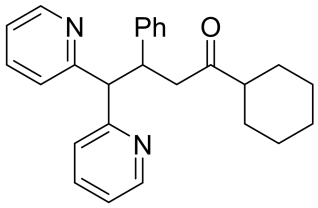
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (s, 1H), 8.40 (s, 1H), 7.77 – 7.76 (m, 3H), 7.67 – 7.61 (m, 5H), 7.47 (d, *J* = 6.8 Hz, 2H), 7.35 – 7.29 (m, 6H), 7.16 (s, 1H), 6.84 (s, 1H), 4.94 – 4.82 (m, 2H), 3.56 – 3.50 (m, 1H), 3.24 (d, *J* = 16.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.55, 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.

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



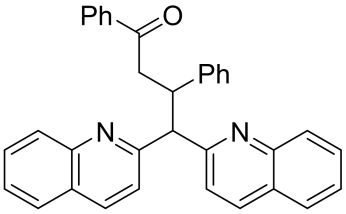
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 8.38 (s, 1H), 7.73 – 7.71 (m, 1H), 7.64 – 7.62 (m, 1H), 7.32 – 7.30 (m, 1H), 7.19 – 7.07 (m, 6H), 6.98 – 6.97 (m, 1H), 6.86 (s, 1H), 4.64 – 4.48 (m, 2H), 3.05 (dd, *J* = 16.8, 10.1 Hz, 1H), 2.40 (d, *J* = 16.8 Hz, 1H), 0.79 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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.

1-cyclohexyl-3-phenyl-4,4-di(pyridin-2-yl)butan-1-one (2d)



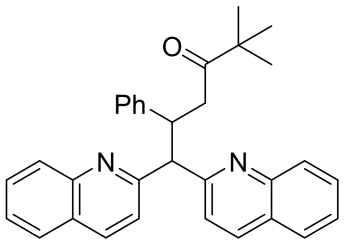
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.7 Hz, 1H), 8.38 (d, *J* = 4.7 Hz, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.65 – 7.58 (td, J = 7.6, 1.5 Hz, 1H), 7.32 (td, *J* = 7.7, 1.5 Hz, 1H), 7.18 (t, *J* = 6.6 Hz, 3H), 7.14 – 7.04 (m, 3H), 6.98 (t, *J* = 7.3 Hz, 1H), 6.90 – 6.84 (m, 1H), 4.57 (d, *J* = 11.8 Hz, 1H), 4.53 – 4.42 (m, 1H), 2.88 (dd, *J* = 16.2, 9.9 Hz, 1H), 2.51 (dd, *J* = 16.2, 3.5 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.63 – 1.50 (m, 3H), 1.47 – 1.38 (m, 2H), 1.14 – 0.99 (m, 4H), 0.95 – 0.83 (dt, *J* = 12.3, 7.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.31, 161.23, 160.72, 149.24, 148.95, 142.69, 136.64, 135.88, 128.42, 127.97, 126.06, 123.88, 123.78, 121.90, 121.21, 61.90, 51.00, 45.97, 45.21, 27.92, 27.72, 25.77, 25.60, 25.43.

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



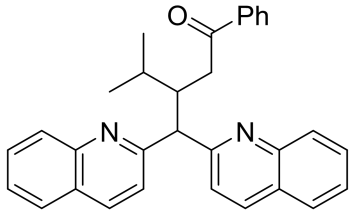
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.5 Hz, 1H), 8.08 – 8.05 (m, 2H), 7.97 (d, *J* = 8.6 Hz, 1H), 7.81 – 7.68 (m, 5H), 7.64 – 7.58 (m, 2H), 7.50 – 7.29 (m, 9H), 7.03 (t, *J* = 7.5 Hz, 2H), 6.91 (t, *J* = 7.2 Hz, 1H), 5.11 – 5.03 (m, 2H), 3.48 (dd, *J* = 15.9, 8.7 Hz, 1H), 3.30 – 3.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



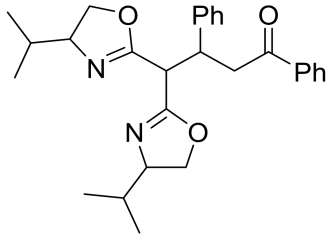
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.5 Hz, 1H), 8.06 (t, *J* = 7.9 Hz, 2H), 8.01 (d, *J* = 8.6 Hz, 1H), 7.76 (dd, *J* = 12.1, 8.3 Hz, 2H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.63 – 7.58 (m, 2H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.40 – 7.33 (m, 4H), 7.04 (t, *J* = 7.5 Hz, 2H), 6.92 (t, *J* = 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 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)



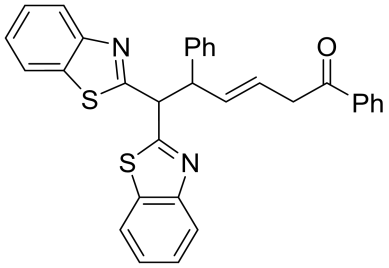
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.2 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.92 – 7.81 (m, 3H), 7.74 – 7.62 (m, 5H), 7.58 – 7.53 (m, 2H), 7.50 – 7.46 (m, 1H), 7.38 – 7.30 (m, 2H), 7.19 (t, *J* = 7.0 Hz, 2H), 4.72 (d, *J* = 11.9 Hz, 1H), 4.00 – 3.96 (m, 1H), 3.04 (dd, *J* = 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 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)



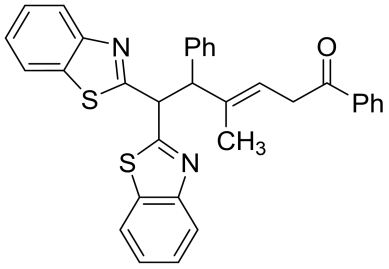
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 7.88 (d, *J* = 7.3 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.23 – 7.20 (m, 2H), 7.15 (t, *J* = 7.4 Hz, 2H), 7.07 (t, *J* = 7.3 Hz, 1H), 4.26 – 4.10 (m, 2H), 4.02 – 3.82 (m, 4H), 3.78 – 3.57 (m, 3H), 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 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. Ratio of diastereoisomers (major to minor): 1.1.

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



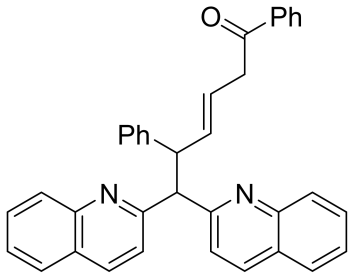
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.1 Hz, 2H), 7.90 – 7.80 (m, 4H), 7.54 – 7.32 (m, 7H), 7.18 – 7.13 (m, 5H), 6.47 (d, *J* = 15.8 Hz, 1H), 6.30 (dd, *J* = 15.8, 8.8 Hz, 1H), 5.39 (d, *J* = 8.9 Hz, 1H), 4.31 – 4.24 (m, 1H), 3.46 – 3.30 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



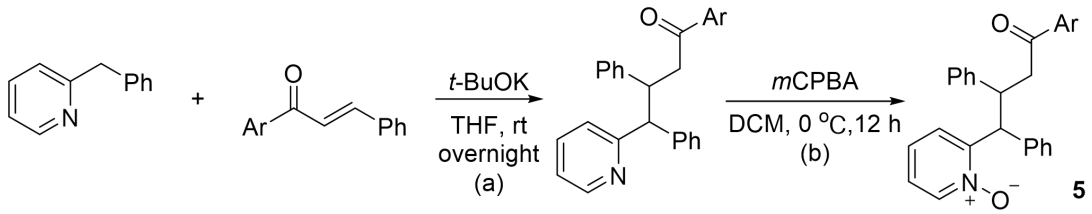
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 8.0, 4.1 Hz, 2H), 7.88 – 7.86 (m, 3H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.54 – 7.39 (m, 6H), 7.37 – 7.31 (m, 1H), 7.15 – 7.05 (m, 3H), 6.80 (d, *J* = 7.2 Hz, 2H), 6.30 (s, 1H), 5.28 (d, *J* = 11.0 Hz, 1H), 4.29 – 4.23 (m, 1H), 3.34 – 3.30 (m, 2H), 1.87 (d, *J* = 1.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



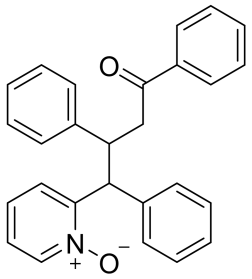
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.6 Hz, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.95 – 7.91 (m, 3H), 7.76 – 7.60 (m, 6H), 7.50 (t, *J* = 7.3 Hz, 2H), 7.45 – 7.38 (m, 3H), 7.12 – 7.02 (m, 5H), 6.29 (d, *J* = 15.9 Hz, 1H), 6.18 (dd, *J* = 15.9, 8.7 Hz, 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 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)



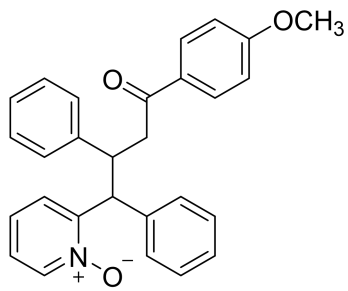
General procedures: (a) To a stirred solution of 2-benzylpyridine (5.0 mmol) in THF (15 mL) at room temperature was added *t*-BuOK (5.0 mmol). Then, (*E*)-chalcone (5.0 mmol) was added to the reaction mixture in one portion. The reaction mixture was extracted with ethyl acetate. The organic layer was 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 ℃ 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 (5a)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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 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 $[M+H]^+$ calcd. 394.1802, found: 394.1792.

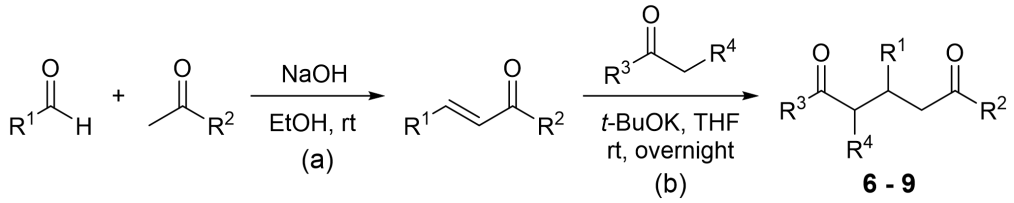
2-(4-(4-methoxyphenyl)-4-oxo-1,2-diphenylbutyl)pyridine 1-oxide (5b)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 8.27 – 8.07 (m, 1H), 7.98 – 7.73 (m, 1H), 7.79 – 7.59 (m, 2.64H, major isomer), 7.53 – 7.41 (m, 1.36H, minor isomer), 7.37 – 6.95 (m, 10H), 6.89 – 6.75 (m, 2H), 5.72 (d, J = 12.6 Hz, 1H), 4.50 – 4.29 (t, J = 10.8 Hz, 1H), 3.90 – 3.65 (m, 3H), 3.52 (dd, J = 16.9, 8.5 Hz, 0.36H, minor isomer), 3.37 (dd, J = 16.4, 9.9 Hz, 0.64H, major isomer), 3.05 – 2.95 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$)

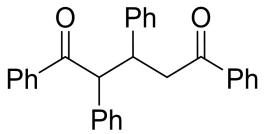
major + minor diastereoisomers δ 197.05, 196.95, 163.41, 163.30, 153.30, 142.32, 142.10, 139.95, 139.47, 139.28, 139.13, 132.42, 130.28, 130.18, 129.02, 128.97, 128.89, 128.46, 128.43, 128.24, 128.20, 127.95, 127.47, 126.73, 126.63, 126.37, 126.01, 125.40, 125.05, 123.55, 123.03, 113.48, 55.38, 47.05, 44.32, 43.78, 43.25. Ratio of diastereoisomers (major to minor): 1.8. HRMS: for $[M+Na]^+$ calcd. 446.1727, found: 446.1728.

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



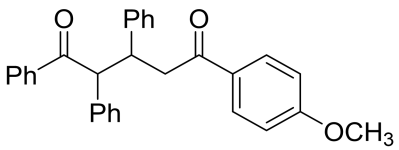
General procedures: (a) To an ethanol (20 mL) solution of aldehyde (R^1CHO, 10.0 mmol) aqueous NaOH (10%, 1.5 mL) was added dropwise followed by slow addition of the corresponding ketone (R^2COMe,10.0 mmol). The mixture was stirred at room temperature until the complete consumption of the starting materials (monitored by TLC). The reaction mixture was diluted with water and the precipitate was collected by filtration and washed with water and EtOH in sequence, affording corresponding α,β-unsaturated ketone. (b) Then, the resulting α,β-unsaturated ketone (5.0 mmol) was added to a reaction mixture of another carbonyl compound (5.0 mmol) and *t*-BuOK (5.0 mmol) in THF at room temperature. After completion of the reaction, the reaction was quenched by addition of saturated NH_4Cl solution and extracted with DCM. The combined organic extract was washed with brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified on silica gel chromatography to afford the corresponding 1,5-diketone (**6 - 9**).

1,2,3,5-Tetraphenylpentane-1,5-dione (6a) (CAS: 61764-77-0)



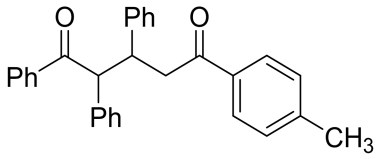
White solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.5 Hz, 2H), 7.65 (d, *J* = 7.4 Hz, 2H), 7.51 (d, *J* = 7.3 Hz, 2H), 7.48 – 7.40 (m, 2H), 7.35 – 7.29 (m, 7H), 7.26 – 7.22 (m, 2H), 7.16 (t, *J* = 7.4 Hz, 2H), 7.05 (t, *J* = 7.4 Hz, 1H), 7.05 (m, 2H), 5.16 (d, *J* = 10.9 Hz, 1H), 4.39 (t, *J* = 10.3 Hz, 1H), 3.24 – 3.06 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



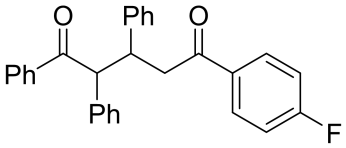
White solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.4 Hz, 2H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 7.1 Hz, 2H), 7.41 – 7.22 (m, 9H), 7.16 (t, *J* = 7.3 Hz, 2H), 7.08 – 7.00 (m, 1H), 6.81 (d, *J* = 8.5 Hz, 2H), 5.17 (d, *J* = 10.8 Hz, 1H), 4.40 – 4.35 (m, 1H), 3.85 – 3.81 (m, 3H), 3.18 – 3.00 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



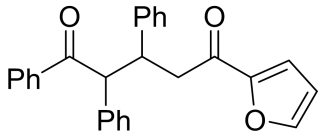
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.8 Hz, 2H), 7.55 (dd, *J* = 16.5, 7.7 Hz, 4H), 7.43 (t, *J* = 8.0 Hz,1H), 7.37 – 7.30 (m, 6H), 7.28 – 7.24 (m, 1H), 7.19 – 7.10 (m, 4H), 7.06 (t, *J* = 8.0 Hz, 1H), 5.19 (d, *J* = 10.9 Hz, 1H), 4.42 – 4.36 (m, 1H), 3.22 – 3.04 (m, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



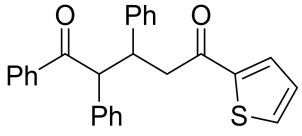
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.79 (m, 2H), 7.70 – 7.65 (m, 2H), 7.52 – 7.50 (m, 2H), 7.44 – 7.39 (m, 1H), 7.36 – 7.29 (m, 6H), 7.26 – 7.23 (m, 1H), 7.19 – 7.15 (m, 2H), 7.09 – 6.97 (m, 3H), 5.16 (d, *J* = 10.8 Hz, 1H), 4.37 (td, *J* = 10.3, 3.9 Hz, 1H), 3.20 – 3.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.70.

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



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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 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.

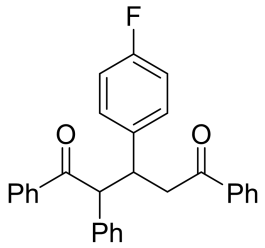
1,2,3-Triphenyl-5-(thiophen-2-yl)pentane-1,5-dione (6f)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 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

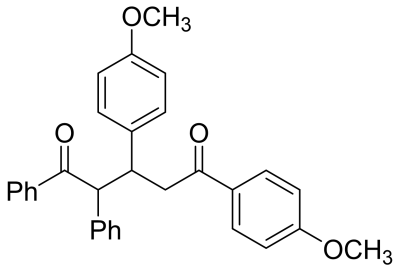
diastereoisomers δ 199.45, 191.35, 144.47, 142.29, 140.73, 137.06, 136.88, 133.48, 133.36, 133.14, 132.76, 132.15, 131.61, 129.22, 129.17, 128.94, 128.72, 128.64, 128.48, 128.40, 128.35, 128.31, 128.17, 128.03, 127.83, 127.79, 127.03, 126.60, 126.47, 58.97, 58.31, 46.14, 45.02, 44.11, 43.51. Ratio of diastereoisomers (major to minor): 1.0.

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



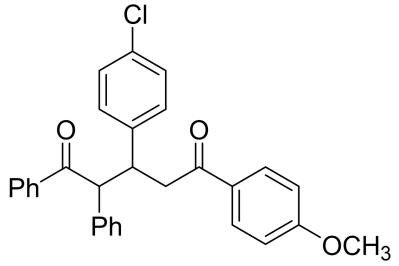
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.8 Hz, 2H), 7.68 (d, *J* = 7.9 Hz, 2H), 7.54 – 7.44 (m, 4H), 7.39 – 7.26 (m, 9H), 6.88 (t, *J* = 8.3 Hz, 2H), 5.14 (d, *J* = 10.8 Hz, 1H), 4.43 – 4.37 (m, 1H), 3.24 – 3.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.60, 162.41 (d, *J* = 243.4 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; ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.36.

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



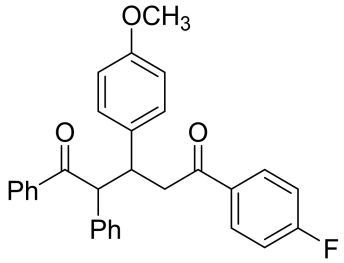
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.7 Hz, 2H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 7.4 Hz, 2H), 7.44 – 7.41 (m, 1H), 7.36 – 7.24 (m, 7H), 6.82 (d, *J* = 8.3 Hz, 2H), 6.70 (d, *J* = 8.2 Hz, 2H), 5.13 (d, *J* = 10.7 Hz, 1H), 4.33 (t, *J* = 8.7 Hz, 1H), 3.83 (s, 3H), 3.68 (s, 3H), 3.15 – 2.98 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



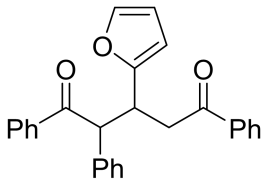
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.7 Hz, 2H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.48 (d, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.2 Hz, 1H), 7.34 – 7.22 (m, 7H), 7.12 (d, *J* = 8.2 Hz, 2H), 6.81 (d, *J* = 8.6 Hz, 2H), 5.11 (d, *J* = 10.8 Hz, 1H), 4.33 (td, *J* = 10.4, 3.4 Hz, 1H), 3.80 (s, 3H), 3.14 – 3.06 (m, 1H), 3.02 – 2.97 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



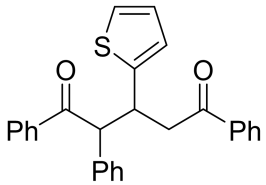
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 8.2, 2.0 Hz, 2H), 7.70 – 7.66 (m, 2H), 7.51 – 7.48 (m, 2H), 7.44 – 7.40 (m, 1H), 7.32 (q, *J* = 7.7 Hz, 4H), 7.26 – 7.21 (m, 3H), 7.00 (t, *J* = 8.6 Hz, 2H), 6.70 (dd, *J* = 8.6, 1.8 Hz, 2H), 5.10 (dd, *J* = 10.8, 5.8 Hz, 1H), 4.36 – 4.28 (m, 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; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.76.

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



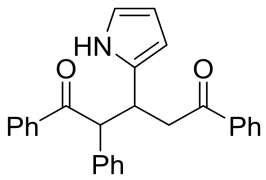
Gray solid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 8.05 (d, *J* = 7.7 Hz, 0.9H, minor isomer), 7.95 – 7.92 (m, 2H), 7.76 (d, *J* = 7.6 Hz, 1.1H, major isomer), 7.56 – 7.22 (m, 9H), 7.18 – 7.13 (m, 3H), 6.14 (s, 0.55H, major isomer), 6.07 – 6.03 (m, 1H), 5.72 (s, 0.45H, minor isomer), 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 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)



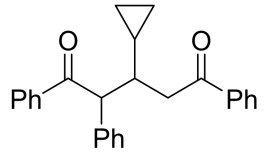
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.7 Hz, 2H), 7.73 (d, *J* = 7.7 Hz, 2H), 7.50 – 7.44 (m, 4H), 7.39 – 7.31 (m, 6H), 7.28 – 7.22 (m, 1H), 7.01 (d, *J* = 5.1 Hz, 1H), 6.93 (d, *J* = 3.6 Hz, 1H), 6.79 – 6.77 (m, 1H), 5.24 (d, *J* = 10.7 Hz, 1H), 4.78 (td, *J* = 10.0, 3.9 Hz, 1H), 3.23 (dd, *J* = 16.5, 9.5 Hz, 1H), 3.14 – 3.09 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



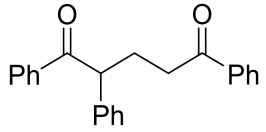
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (s, 1H), 7.91 (d, *J* = 7.3 Hz, 2H), 7.75 (d, *J* = 7.2 Hz, 2H), 7.51 – 7.34 (m, 8H), 7.30 – 7.26 (m, 2H), 7.19 (t, *J* = 7.3 Hz, 1H), 6.57 – 6.56 (m, 1H), 5.93 (q, *J* = 2.8 Hz, 1H), 5.86 (s, 1H), 5.20 (d, *J* = 10.8 Hz, 1H), 4.45 (td, *J* = 10.7, 3.3 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 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)



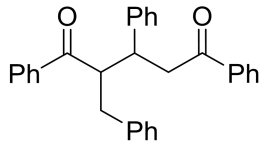
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 8.01 (dd, *J* = 14.4, 7.9 Hz, 4H), 7.55 – 7.51 (m, 1H), 7.49 – 7.34 (m, 7H), 7.26 (t, *J* = 7.3 Hz, 2H), 7.22 – 7.18 (m, 1H), 5.05 (d, *J* = 8.5 Hz, 1H), 3.32 – 3.27 (m, 1H), 3.16 – 3.10 (m, 1H), 2.23 – 2.16 (m, 1H), 0.82 – 0.73 (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 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. ^{1}H NMR (400 MHz, $CDCl_3$) 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 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.

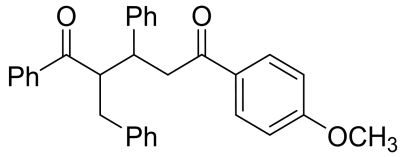
2-Benzyl-1,3,5-triphenylpentane-1,5-dione (6p)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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

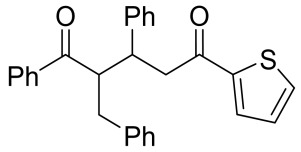
(dd, J = 13.3, 3.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.92, 198.18, 142.01, 139.73, 138.06, 137.05, 133.05, 132.65, 128.94, 128.55, 128.47, 128.38, 128.10, 128.00, 127.92, 126.79, 126.13, 54.17, 42.91, 39.64, 34.55.

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



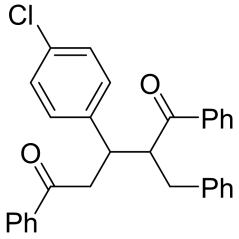
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.7 Hz, 2H), 7.72 (d, J = 7.9 Hz, 2H), 7.47 (t, J = 7.2 Hz, 1H), 7.35 – 7.20 (m, 7H), 7.12 – 6.98 (m, 5H), 6.90 (d, J = 8.7 Hz, 2H), 4.24 – 4.19 (m, 1H), 3.93 – 3.88 (m, 1H), 3.87 (s, 3H), 3.36 – 3.24 (m, 2H), 3.00 – 2.94 (m, 1H), 2.77 (dd, J = 13.3, 3.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



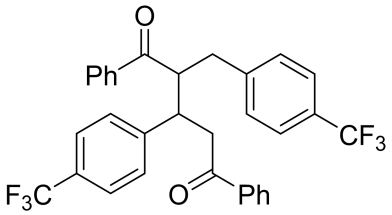
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.2 Hz, 2H), 7.64 (s, 1H), 7.57 (d, J = 4.5 Hz, 1H), 7.48 (t, J = 6.7 Hz, 1H), 7.36 – 7.23 (m, 7H), 7.11 – 6.99 (m, 6H), 4.27 – 4.23 (m, 1H), 3.93 – 3.90 (m, 1H), 3.34 – 3.23 (m, 2H), 3.01 – 2.95 (m, 1H), 2.81 – 2.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



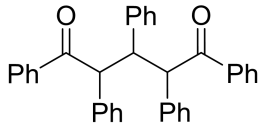
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, J = 7.6 Hz, 2H), 7.72 (d, J = 7.7 Hz, 2H), 7.55 (t, J = 7.3 Hz, 1H), 7.49 (t, J = 7.3 Hz, 1H), 7.43 (t, J = 7.6 Hz, 2H), 7.35 (t, J = 7.7 Hz, 2H), 7.29 – 7.26 (m, 2H), 7.20 (d, J = 8.4 Hz, 2H), 7.13 – 7.04 (m, 3H), 6.98 (d, J = 7.2 Hz, 2H), 4.18 (td, 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 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)



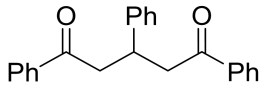
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.4 Hz, 2H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.55 – 7.48 (m, 4H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.34 (t, *J* = 7.9 Hz, 6H), 7.06 (d, *J* = 8.0 Hz, 2H), 4.26 – 4.20 (m, 1H), 3.99 (q, *J* = 7.6 Hz, 1H), 3.39 (d, *J* = 7.0 Hz, 2H), 3.02 (dd, *J* = 13.4, 10.2 Hz, 1H), 2.76 (dd, *J* = 13.4, 3.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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) (567-80-6)



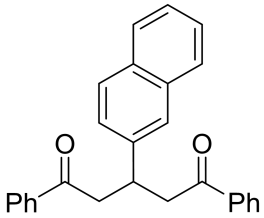
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.7 Hz, 2H), 7.63 (d, *J* = 7.7 Hz, 2H), 7.45 (d, *J* = 7.4 Hz, 2H), 7.40 – 7.33 (m, 2H), 7.24 (t, *J* = 7.5 Hz, 4H), 7.15 – 7.11 (m, 4H), 7.07 – 6.98 (m, 8H), 6.94 – 6.91 (m, 1H), 5.26 (d, *J* = 10.5 Hz, 1H), 5.09 (d, *J* = 7.5 Hz, 1H), 4.91 (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) (6263-84-9)



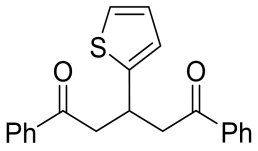
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.94 (m, 4H), 7.57 – 7.53 (m, 2H), 7.47 – 7.43 (m, 4H), 7.29 – 7.26 (m, 4H), 7.21 – 7.16 (m, 1H), 4.12 – 4.04 (m, 1H), 3.53 – 3.47 (m, 2H), 3.40 – 3.33 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.58, 143.85, 136.98, 133.07, 128.63, 128.59, 128.15,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

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



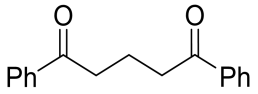
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.95 (m, 4H), 7.80 – 7.76 (m, 3H), 7.72 (s, 1H), 7.55 (t, *J* = 7.4 Hz, 2H), 7.49 – 7.40 (m, 7H), 4.27 (quint, *J* = 7.0 Hz, 1H), 3.59 (dd, *J* = 16.7, 6.9 Hz, 2H), 3.47 (dd, *J* = 16.7, 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.52, 141.35, 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)



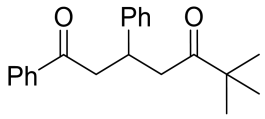
Brown solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.4 Hz, 4H), 7.56 (t, *J* = 7.4 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 4H), 7.11 (d, *J* = 4.1 Hz, 1H), 6.89 – 6.87 (m, 2H), 4.47 – 4.40 (m, 1H), 3.53 (dd, *J* = 16.9, 6.8 Hz, 2H), 3.43 (dd, *J* = 16.9, 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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) (6263-83-8)



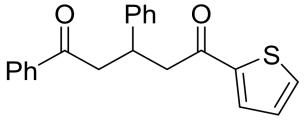
White solid.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.4 Hz, 4H), 7.55 (t, *J* = 7.3 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 4H), 3.12 (t, *J* = 6.9 Hz, 4H), 2.21 (dd, *J* = 13.9, 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.86, 136.88, 133.08, 128.62, 128.08, 37.61, 18.75.

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



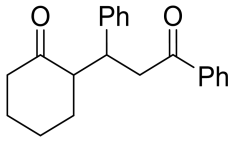
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.94 (m, 2H), 7.56 (tt, *J* = 8.0, 2.0 Hz, 2H), 7.48 – 7.44 (m, 2H), 7.31 – 7.25 (m, 4H), 7.22 – 7.17 (m, 1H), 3.98 – 3.91 (m, 1H), 3.44 – 3.38 (m, 1H), 3.32 – 3.27 (m, 1H), 2.96 (d, *J* = 6.9 Hz, 2H), 1.08 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) 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. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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, $CDCl_3$) δ 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.

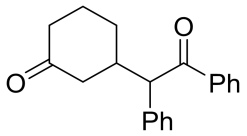
2-(3-Oxo-1,3-diphenylpropyl)cyclohexan-1-one (7a)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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),

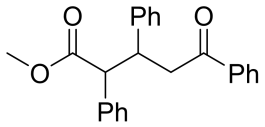
1.33 – 1.24 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 213.58, 198.79, 142.06, 137.09, 132.80, 128.48, 128.45, 128.37, 128.17, 126.61, 55.83, 44.23, 42.32, 41.14, 32.45, 28.53, 24.12.

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



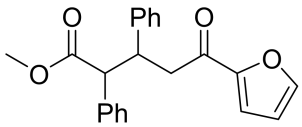
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 15.8, 7.5 Hz, 2H), 7.49 (q, *J* = 7.5 Hz, 1H), 7.39 (q, *J* = 7.8 Hz, 2H), 7.34 – 7.19 (m, 5H), 4.43 (d, *J* = 9.6 Hz, 1H), 2.85 – 2.74 (m, 1H), 2.60 – 2.56 (m, 1H), 2.39 – 2.36 (m, 0.50H), 2.29 – 2.21 (m, 1H), 2.13 – 1.90 (m, 3H), 1.75 – 1.68 (m, 0.50H), 1.63 – 1.60 (m, 1H), 1.46 – 1.22 (m, 1H). Ratio of diastereoisomers (major to minor): 1.0; ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



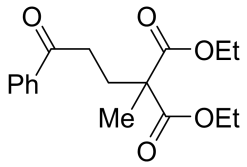
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 7.91 – 7.89 (m, 1.33H, major isomer), 7.69 – 7.64 (m, 0.67H, minor isomer), 7.54 (t, *J* = 7.8 Hz, 1H), 7.48 – 7.26 (m, 5H), 7.20 – 7.00 (m, 7H), 4.23 – 4.11 (m, 1H), 4.03 – 3.98 (m, 1H), 3.70 (s, 2H, major isomer), 3.56 (dd, *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 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. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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 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.

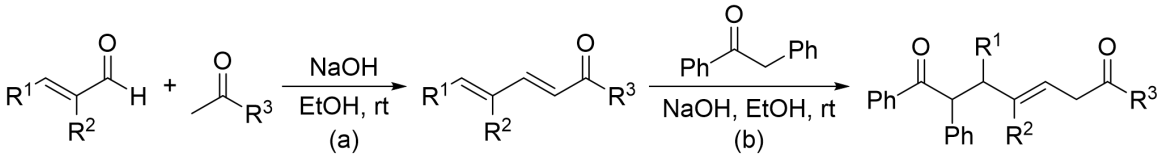
Diethyl 2-methyl-2-(3-oxo-3-phenylpropyl)malonate (9)



Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.5 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H),

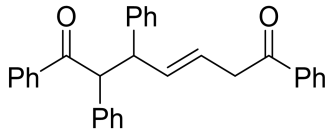
4.17 (qd, *J* = 6.8, 1.6 Hz, 4H), 3.02 (t, *J* = 8.0 Hz, 2H), 2.8 (t, *J* = 8.0 Hz, 2H), 1.46 (s, 3H), 1.22 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.88, 171.93, 136.66, 133.03, 128.55, 127.98, 61.27, 52.97, 33.94, 30.00, 20.51, 13.98.

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



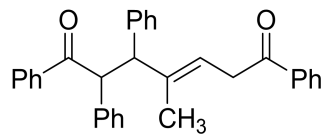
General procedures: (a) To a mixture of ketone (10.0 mmol) and NaOH (2.0 equiv) in EtOH (20 mL) was added cinnamaldehyde (10.0 mmol). After stirring at room temperature for 2 h, the reaction mixture was diluted with water. The precipitate was collected by filtration and washed with water and EtOH. (b) To a solution of 2-phenylacetophenone (5.0 mmol) in EtOH (20 mL) was added NaOH (5.0 mmol). After stirring for 10 min at room temperature, to the mixture was added conjugated dienone (5.0 mmol). The resulting mixture was continued to stir for 3 h at room temperature and then quenched with saturated NH_4Cl solution. Then, 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.

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



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 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; ^{13}C NMR (100 MHz, $CDCl_3$) major + minor diastereoisomers δ 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.

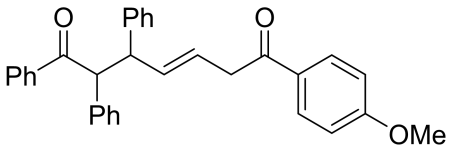
(*E*)-4-Methyl-1,5,6,7-tetraphenylhept-2-ene-1,7-dione (21b)



Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 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,

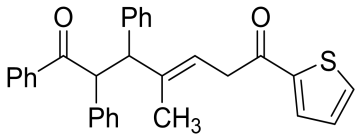
0.52H, major isomer), 3.97 – 3.89 (m, 1H), 3.48 (dd, *J* = 14.1, 3.7 Hz, 0.52H, major isomer), 3.10 (dd, *J* = 14.0, 11.2 Hz, 0.48H, minor isomer), 3.02 (d, *J* = 7.2 Hz, 1H), 1.89 (s, 1.44H, minor isomer), 1.71 (s, 1.56H, major isomer). Ratio of diastereoisomers (major to minor): 1.1; ^{13}C NMR (100 MHz, $CDCl_3$) major + minor diastereoisomers δ 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)



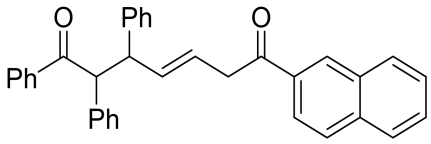
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.3 Hz, 2H), 7.78 (d, *J* = 8.7 Hz, 2H), 7.48 – 7.43 (m, 3H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.23 (d, *J* = 7.4 Hz, 1H), 7.20 (d, *J* = 4.3 Hz, 2H), 7.16 – 7.11 (m, 1H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.41 (d, *J* = 15.9 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 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)



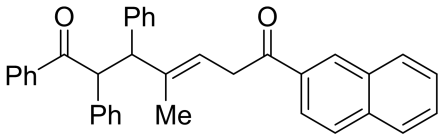
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 6.6 Hz, 2H), 7.57 – 7.47 (m, 5H), 7.42 – 7.34 (m, 4H), 7.26 (s, 1H), 7.19 – 7.17 (m, 2H), 7.12 – 7.06 (m, 2H), 6.93 (d, *J* = 6.5 Hz, 2H), 6.41 (s, 1H), 5.04 (d, *J* = 10.7 Hz, 1H), 3.87 (d, *J* = 6.2 Hz, 1H), 2.88 (d, *J* = 5.8 Hz, 2H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



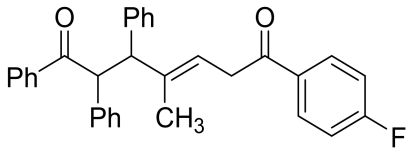
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.97 (d, *J* = 7.3 Hz, 2H), 7.90 – 7.83 (m, 4H), 7.60 – 7.52 (m, 2H), 7.47 (t, *J* = 8.4 Hz, 3H), 7.40 – 7.31 (m, 4H), 7.24 – 7.11 (m, 6H), 6.44 (d, *J* = 15.9 Hz, 1H), 6.33 (dd, *J* = 15.9, 8.4 Hz, 1H), 5.11 (d, *J* = 9.6 Hz, 1H), 3.92 (qd, *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 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)



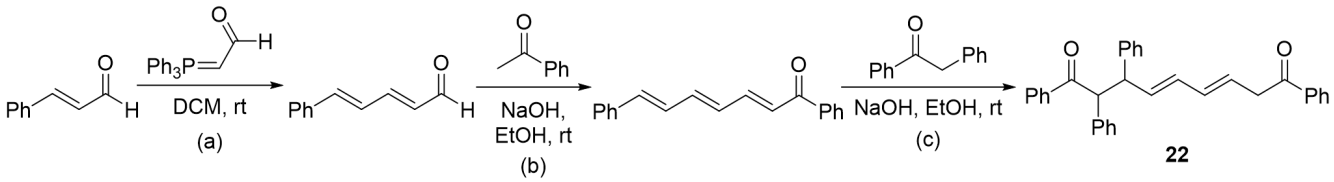
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 8.70 (s, 0.44H, minor isomer), 8.21 (s, 0.56H, major isomer), 8.14 – 8.09 (m, 2H), 8.02 – 7.99 (m, 1H), 7.96 – 7.87 (m, 3H), 7.65 – 7.41 (m, 8H), 7.38 – 7.31 (m, 2H), 7.28 – 7.08 (m, 5H), 6.96 (d, *J* = 7.2 Hz, 1.12H, major isomer), 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 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. ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 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 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; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.69.

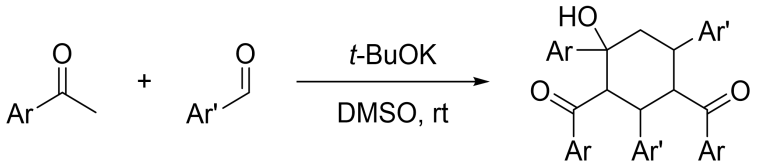
2.4 Synthesis and characterization of (2*E*, 4*E*)-1,7,8,9-tetraphenylnona-2,4-diene-1,9-dione (22)



General procedures: (a) To a mixture of cinnamaldehyde (10.0 mmol) in CH_2Cl_2 (20 mL) was added 2-

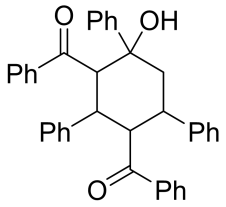
(triphenylphosphaneylidene)acetaldehyde (10.0 mmol). After stirring at room temperature for 2 h, the reaction was quenched by addition of saturated NH_4Cl solution and extracted with CH_2Cl_2. The combined organic extract was washed with brine, dried over anhydrous Na_2SO_4, filtered, concentrated and purified on silica gel chromatography to afford the intermediate (2*E*,4*E*)-5-phenylpenta-2,4-dienal for the next step. (b) was dissolved in ethanol (20 mL). Then, to an ethanol solution of corresponding aldehyde (5.0 mmol) was added dropwise aqueous NaOH (2.0 equiv) followed by slow addition of acetophenone (5.0 mmol). At completion of the reaction, it 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. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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 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)



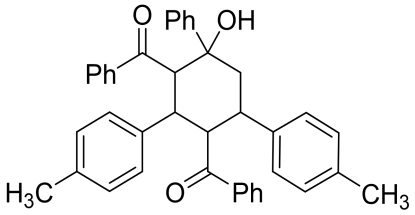
A catalytic amount of *t*-BuOK (0.060 mol) was added to a solution of ketone (9.0 mmol) and aldehyde (6.0 mmol) in DMSO (2 mL). After stirring at room temperature for 5 min, the dark brown mixture was washed with diluted HCl (10%, 10 mL) and extracted with DCM (2 × 10 mL). The combined organic layer was dried over Na_2SO_4, 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)



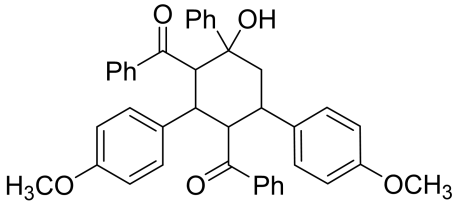
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.0 Hz, 2H), 7.49 (d, *J* = 7.0 Hz, 2H), 7.29 (s, 3H), 7.24 - 7.19 (m, 3H), 7.15 – 7.09 (m, 9H), 7.03 – 7.00 (m, 3H), 6.84 (s, 3H), 5.75 (d, *J* = 11.9 Hz, 1H), 5.24 (s, 1H), 4.40 (s, 1H), 4.20 (t, *J* = 14.4 Hz, 2H), 3.44 (t, *J* = 13.2 Hz, 1H), 2.08 (d, *J* = 13.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



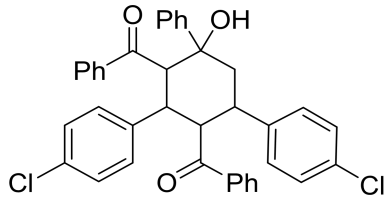
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.5 Hz, 2H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.29 – 7.23 (m, 3H), 7.18 (t, *J* = 7.1 Hz, 1H), 7.12 – 7.05 (m, 7H), 7.02 – 6.95 (m, 4H), 6.86 (d, *J* = 7.7 Hz, 2H), 6.62 (d, *J* = 7.7 Hz, 2H), 5.70 (d, *J* = 12.0 Hz, 1H), 5.17 (s, 1H), 4.35 (t, *J* = 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 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)



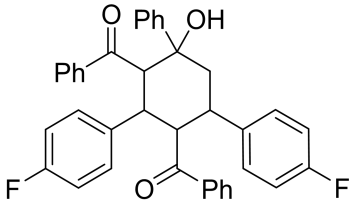
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.6 Hz, 2H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.32 – 7.25 (m, 4H), 7.22 (d, *J* = 7.1 Hz, 1H), 7.15 – 7.10 (m, 7H), 7.05 (t, *J* = 7.6 Hz, 2H), 7.00 (d, *J* = 8.5 Hz, 2H), 6.62 (d, *J* = 8.5 Hz, 2H), 6.37 (d, *J* = 8.5 Hz, 2H), 5.68 (d, *J* = 12.0 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 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)



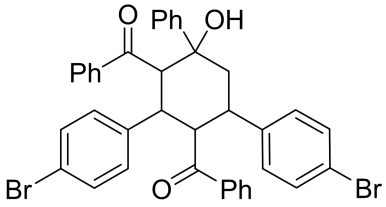
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.45 (d, *J* = 7.7 Hz, 2H), 7.32 – 7.25 (m, 4H), 7.15 – 7.11 (m, 6H), 7.08 – 7.00 (m, 7H), 6.80 (d, *J* = 8.3 Hz, 2H), 5.66 (d, *J* = 12.0 Hz, 1H), 5.15 (s, 1H), 4.34 – 4.32 (m, 1H), 4.17 – 4.10 (m, 2H), 3.32 (t, *J* = 13.2 Hz, 1H), 2.04 – 1.99 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



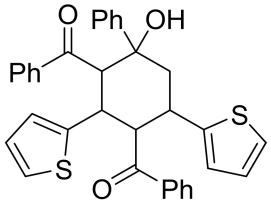
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.5 Hz, 2H), 7.45 (d, *J* = 7.5 Hz, 2H), 7.32 – 7.23 (m, 4H), 7.18 – 7.10 (m, 7H), 7.08 – 7.02 (m, 4H), 6.76 (t, *J* = 8.7 Hz, 2H), 6.52 (t, *J* = 8.6 Hz, 2H), 5.66 (d, *J* = 12.0 Hz, 1H), 5.21 (d, *J* = 2.2 Hz, 1H), 4.34 (t, *J* = 4.6 Hz, 1H), 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 208.13, 206.48, 161.51 (d, *J* = 244.0 Hz), 146.57, 139.76, 138.15, 137.34, 135.00, 133.09, 132.42, 130.32 (d, *J* = 8.0 Hz), 129.16 (d, *J* = 8.0 Hz), 128.24, 128.06, 127.94, 127.39, 127.05, 125.08, 115.05 (d, *J* = 21.0 Hz), 114.95 (d, *J* = 21.0 Hz), 75.85, 52.47, 50.26, 47.20, 41.42, 38.57; ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.26, -116.19.

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



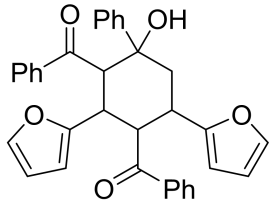
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.3 Hz, 2H), 7.46 – 7.44 (m, 2H), 7.32 – 7.24 (m, 4H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.13 – 7.10 (m, 4H), 7.08 – 7.05 (m, 4H), 6.95 (s, 4H), 5.66 (d, *J* = 12.0 Hz, 1H), 5.13 (d, *J* = 2.1 Hz, 1H), 4.33 (t, *J* = 4.6 Hz, 1H), 4.17 – 4.08 (m, 2H), 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 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)



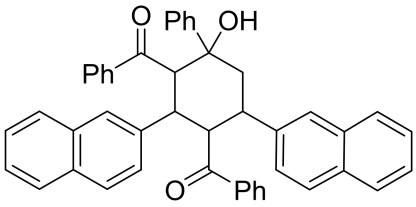
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.71 (m, 2H), 7.55 – 7.53 (m, 2H), 7.38 – 7.36 (m, 2H), 7.32 – 7.28 (m, 2H), 7.24 (t, *J* = 7.8 Hz, 2H), 7.14 (q, *J* = 7.5 Hz, 4H), 7.06 (t, *J* = 7.3 Hz, 1H), 6.87 (dd, *J* = 5.1, 1.0 Hz, 1H), 6.75 (d, *J* = 3.4 Hz, 1H), 6.71 (dd, *J* = 5.0, 0.7 Hz,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



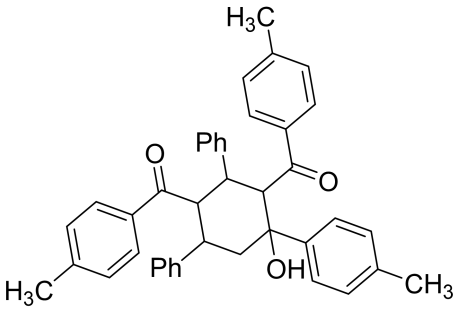
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.7 Hz, 2H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.53 (d, *J* = 7.7 Hz, 2H), 7.36 (dt, *J* = 21.0, 7.4 Hz, 2H), 7.28 – 7.16 (m, 6H), 7.07 (t, *J* = 7.3 Hz, 1H), 6.99 (s, 1H), 6.75 (s, 1H), 6.03 – 5.79 (m, 4H), 5.69 (d, *J* = 11.9 Hz, 1H), 5.29 (s, 1H), 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 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)



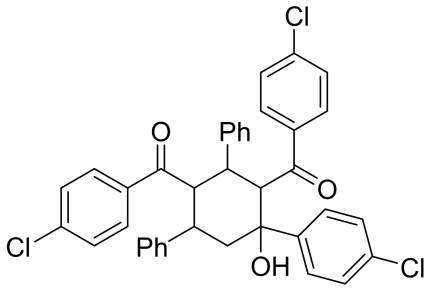
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.3 Hz, 2H), 7.70 – 7.67 (m, 2H), 7.63 – 7.58 (m, 2H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.49 – 7.46 (m, 4H), 7.40 – 7.30 (m, 6H), 7.28 – 7.22 (m, 4H), 7.15 – 7.02 (m, 5H), 6.95 (t, *J* = 7.4 Hz, 1H), 6.76 (t, *J* = 7.8 Hz, 2H), 5.92 (d, *J* = 12.0 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 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. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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 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)

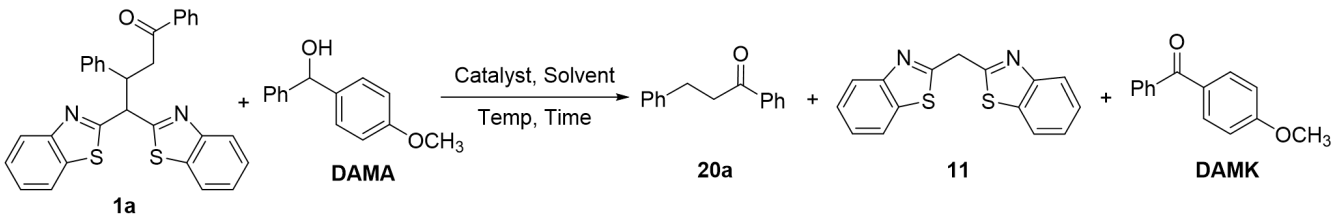


White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.5 Hz, 2H), 7.24 (d, *J* = 8.5 Hz, 2H), 7.17 – 7.12 (m, 4H), 7.08 (t, *J* = 7.5 Hz, 2H), 7.03 – 6.96 (m, 7H), 6.86 – 6.85 (m, 3H), 5.60 (d, *J* = 11.8 Hz, 1H), 5.15 (s, 1H), 4.28 (t, *J* = 4.5 Hz, 1H), 4.15 – 4.08 (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 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.

3. Studies on C–C bond hydrogenolysis reactions

3.1 Development of the C–C bond hydrogenolysis procedure

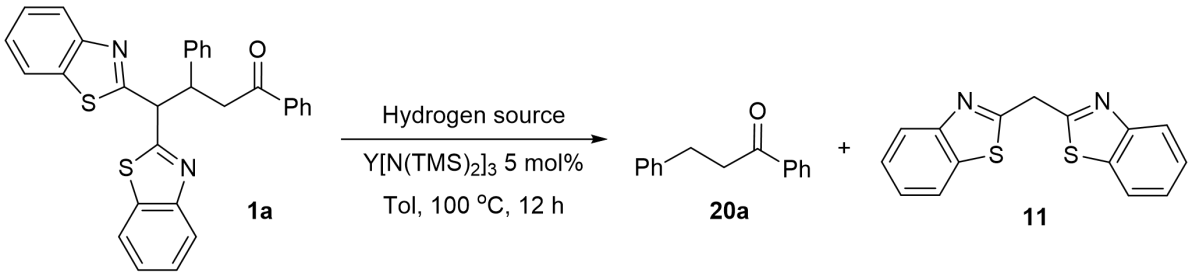
Table S1. Optimization of the reaction conditions[a]



Entry	Catalyst	Solvent	(**1a** : **DAMA**)[d]	Temp (°C)	Time (h)	**20a** (%)	**11** (%)
1	$Y[N(TMS)_2]_3$, **Y-1**	Toluene	1:1	100	12	89	86
2	$La[N(TMS)_2]_3$	Toluene	1:1	100	12	86	85
3	$Sm[N(TMS)_2]_3$	Toluene	1:1	100	12	87	83
4	$Lu[N(TMS)_2]_3$	Toluene	1:1	100	12	85	86
5[b]	YCl_3	Toluene	1:1	100	12	0	0
6[b]	$Y(OTf)_3$	Toluene	1:1	100	12	0	0
7	--	Toluene	1:1	100	12	0	0
8	CuBr	Toluene	1:1	100	12	0	0
9	$KN(TMS)_2$	Toluene	1:1	100	12	4	15
10	^{t}BuOK	Toluene	1:1	100	12	trace	20
11	$Pd(PPh_3)_4$	Toluene	1:1	100	12	0	0
12	$Y[N(TMS)_2]_3$	Toluene	1:1	80	12	67	66
13	$Y[N(TMS)_2]_3$	Toluene	1:1	110	12	83	80
14[c]	$Y[N(TMS)_2]_3$	Toluene	1:1	100	24	87	82
15	$Y[N(TMS)_2]_3$	Toluene	1:1	100	6	65	60
16	$Y[N(TMS)_2]_3$	Toluene	1:1	100	12	45	49
17	$Y[N(TMS)_2]_3$	Toluene	1:1.2	100	12	83	80
18	$Y[N(TMS)_2]_3$	Toluene	1:2	100	12	53	51
19	$Y[N(TMS)_2]_3$	THF	1:1	100	12	56	52
20	$Y[N(TMS)_2]_3$	Hexane	1:1	100	12	84	86

[a]Reaction conditions: **1a** (0.50 mmol), **DAMA** (0.5 - 2.0 mmol), catalyst (5 mol%), solvent (2 mL), at 100 °C under N_2 atmosphere, isolated yield. [b]Catalyst loading 10 mol%. [c]Catalyst loading 1 mol%. [d]Mole ratio.

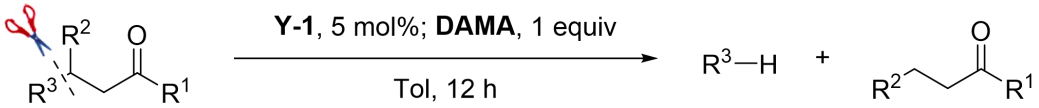
Table S2. Optimization of the hydrogen sources[a]



Entry	Hydrogen source	**20a** (%)	**11** (%)
1	$PhCH_2NH_2$	31%	25
2	diisobutylamine	33%	28
3	diethylamine	25%	24
4	*n*-butylamine	19%	14
5	*N*-benzyl-isobutylamine	29%	17
6	methanol	trace	trace
7	ethanol	trace	trace
8	Isopropanol (solvent)	trace	trace
9[b]	H_2	22%	18
10	phenylsilane	38%	34
11[c]	diphenylmethanol	84% (^{1}H NMR)	81

[a]Reactions 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 N_2, isolated yield. [b]6 atm H_2. [c]The dehydrogenative product benzophenone is hard to separate from **20a**, thus **DAMA** was selected as the compromised hydrogen source.

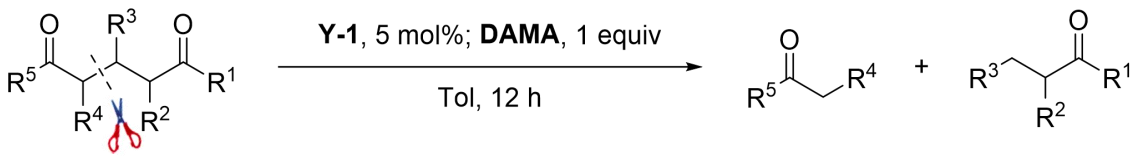
3.2 General procedure for C–C hydrogenolysis of monoketone substrates (1 - 5)



1 - 5 **11 - 15** **20**

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 NH_4Cl solution (2 mL). The mixture was extracted with ethyl acetate (3 × 5 mL). The combined organic layer was dried with anhydrous Na_2SO_4, 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)

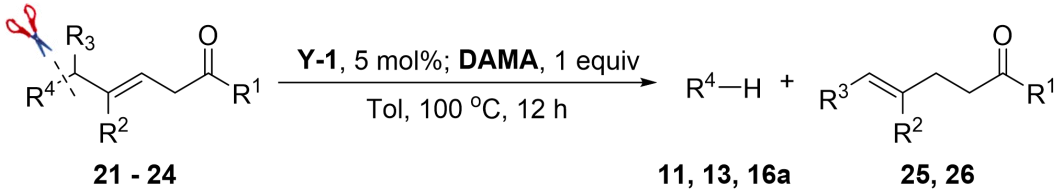


6 - 9 **16 - 19** **20**

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.

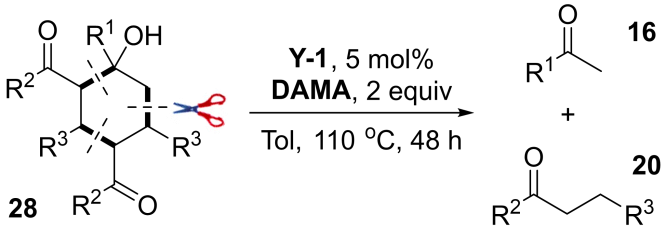
3.4 General procedures for C–C hydrogenolysis of unsaturated ketone substrates (21 - 24)



21 - 24 **11, 13, 16a** **25, 26**

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 ℃ 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, filtered, evaporated and purified by flash column chromatography using petroleum ether/ethyl acetate as eluent to give the corresponding C–C hydrogenolysis products.

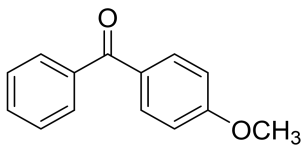
3.5 General procedures for hydrogenolytic [2+2+2]-cycloreversion of 2,4-diacylcyclohexanols (28)



In a glovebox, a dried Schlenk tube was charged with **Y-1** (14 mg, 5 mol%), **DAMA** (214 mg, 1.0 mmol), substituted cyclohexanol **28** (0.50 mmol) and toluene (2.0 mL). Then, the tube was sealed and removed out from the glove box. After stirring at 110 ℃ for 48 h, the resulting mixture was quenched with saturated NH_4Cl solution (2 mL) and extracted with ethyl acetate (3 × 5 mL). The combined organic phase was dried with anhydrous Na_2SO_4, and filtered and all volatiles were removed under reduced pressure. The crude products were purified by flash column chromatography using petroleum ether/ethyl acetate as eluent.

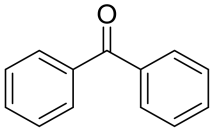
3.6 Characterization of products

(4-Methoxyphenyl)phenylmethanone (DAMK) (CAS: 611-94-9)[2]



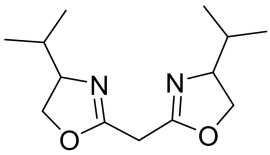
White solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.8 Hz, 2H), 7.75 (d, J = 7.1 Hz, 2H), 7.56 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.5 Hz, 2H), 6.96 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.55, 163.20, 138.25, 132.54, 131.87, 130.12, 129.70, 128.16, 113.53, 55.47.

Benzophenone (43) (CAS: 119-61-9)[3]



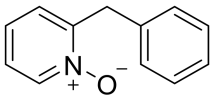
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.80 (m, 4H), 7.61 – 7.57 (dd, *J* = 10.6, 4.3 Hz, 2H), 7.48 (t, *J* = 7.5 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.77, 137.63, 132.43, 130.08, 128.29.

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



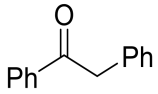
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.24 (t, *J* = 8.5 Hz, 2H), 3.99 – 3.88 (m, 4H), 3.31 – 3.25 (m, 2H), 1.77 – 1.69 (m, 2H), 0.92 (d, *J* = 6.7 Hz, 6H), 0.84 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.51, 161.47, 72.13, 72.09, 70.52, 70.49, 32.40, 28.33, 28.30, 18.63, 18.59, 17.94.

2-benzylpyridine 1-oxide (15) (CAS: 20531-86-6)[5]



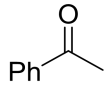
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 8.20 (m, 1H), 7.30 – 7.26 (m, 2H), 7.22 – 7.20 (m, 3H), 7.07 – 7.05 (m, 2H), 6.89 – 6.86 (m, 1H), 4.19 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.86, 139.33, 136.27, 129.66, 128.83, 127.03, 125.82, 125.57, 123.60, 36.48.

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



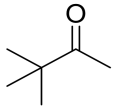
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.6 Hz, 2H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.3 Hz, 2H), 7.35 (t, *J* = 7.1 Hz, 2H), 7.31 – 7.26 (m, 3H), 4.31 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.65, 136.66, 134.58, 133.18, 129.50, 128.70, 128.67, 128.65, 126.91, 45.53.

Acetophenone (16b) (CAS: 98-86-2)[7]



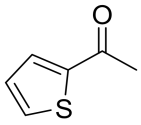
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.2 Hz, 2H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.00, 137.09, 133.05, 128.53, 128.25, 26.50.

3,3-Dimethylbutan-2-one (16c) (CAS: 75-97-8)[7]



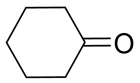
Colorless liquid. For reduction of substrate **6z**, yield was 71% (35.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.03 (s, 3H), 1.04 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 213.99, 44.16, 26.25, 24.53.

1-(Thiophen-2-yl)ethan-1-one (16d) (CAS: 88-15-3)[7]



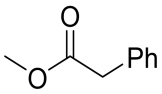
Yellow liquid. For reduction of substrate **6aa**, yield was 43% (27.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 3.7 Hz, 1H), 7.57 (d, J = 4.9 Hz, 1H), 7.06 (t, J = 4.3 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.70, 144.52, 133.80, 132.56, 128.16, 26.85.

Cyclohexanone (17) (CAS: 108-94-1)[8]



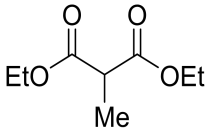
Colorless liquid. For reduction of substrate **7a**, yield was 64% (31.4 mg); For reduction of substrate **7b**, yield was 74% (36.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.27 (t, J = 6.5 Hz, 4H), 1.83 – 1.77 (m, 4H), 1.69 – 1.65 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.02, 41.93, 26.99, 24.95.

Methyl 2-phenylacetate (18) (CAS: 101-41-7)[9]



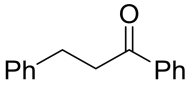
Colorless liquid. For reduction of substrate **8a**, yield was 78% (58.6 mg); For reduction of substrate **8b**, yield was 80% (60.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 5H), 3.71 (s, 3H), 3.65 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.05, 134.06, 129.30, 128.63, 127.15, 52.03, 41.22.

Diethyl 2-methylmalonate (19) (CAS: 609-08-5)[10]



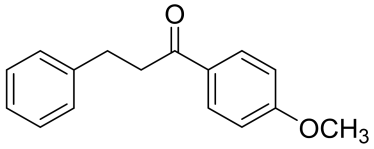
Colorless liquid. For reduction of substrate **9**, yield was 76% (66.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.16 (q, J = 6.8 Hz, 4H), 3.39 (q, J = 7.1 Hz, 1H), 1.38 (d, J = 7.2 Hz, 3H), 1.24 (t, J = 7.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.96, 61.11, 46.00, 13.85, 13.33.

1,3-Diphenylpropan-1-one (20a) (CAS: 1083-30-3)[11]



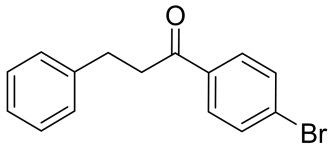
White solid. For reduction of substrate **1a**, yield was 89% (93.6 mg); For reduction of substrate **2a**, yield was 86% (90.4 mg); For reduction of substrate **3a**, yield was 89% (93.6 mg); For reduction of substrate **4**, yield was 79% (83.1 mg); For reduction of substrate **5a**, yield was 77% (81.0 mg); For reduction of substrate **6a**, yield was 90% (94.6 mg); For reduction of substrate **6p**, yield was 88% (92.5 mg); For reduction of substrate **6v**, yield was 77% (81.0 mg); For reduction of substrate **6z**, yield was 74% (77.8 mg); For reduction of substrate **6aa**, yield was 46% (48.4 mg); For reduction of substrate **7a**, yield was 89% (93.6 mg); For reduction of substrate **8a**, yield was 81% (85.2 mg); For reduction of substrate **27a**, yield was 77% (85.2 mg); For reduction of substrate **8a**, yield was 81% (85.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) 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); ^{13}C NMR (100 MHz, $CDCl_3$) 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)[11]



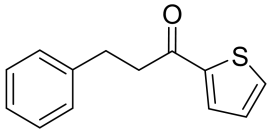
Light yellow solid. For reduction of substrate **1b**, yield was 82% (98.5 mg); For reduction of substrate **5b**, yield was 82% (98.5 mg); For reduction of substrate **6b**, yield was 77% (92.5 mg); For reduction of substrate **6q**, yield was 83% (99.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.90 (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) ^{13}C NMR (100 MHz, $CDCl_3$) 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)[11]



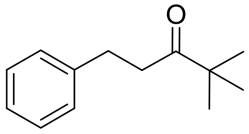
White solid. For reduction of substrate **1c**, yield was 82% (118.6 mg); For reduction of substrate **1c**, yield was 82% (118.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 2H), 7.33 – 7.20 (m, 5H), 3.27 (t, *J* = 7.6 Hz, 2H), 3.07 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 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]



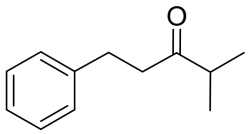
Pale yellow solid. For reduction of substrate **1d**, yield was 85% (91.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.68 (m, 1H), 7.63 – 7.62 (m, 1H), 7.32 – 7.19 (m, 5H), 7.12 – 7.10 (m, 1H), 3.26 – 3.22 (m, 2H), 3.07 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.17, 144.21, 141.03, 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]



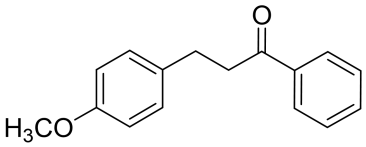
Yellow solid. For reduction of substrate **1e**, yield was 82% (78.0 mg); For reduction of substrate **2c**, yield was 82% (74.2 mg); For reduction of substrate **3b**, yield was 83% (79.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.26 (m, 2H), 7.21 – 7.17 (m, 3H), 2.91 – 2.87 (m, 2H), 2.83 – 2.78 (m, 2H), 1.12 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 214.89, 141.62, 128.45, 128.42, 126.03, 44.09, 38.49, 30.13, 26.33.

4-methyl-1-phenylpentan-3-one (20f) (CAS: 5195-24-4)[11]



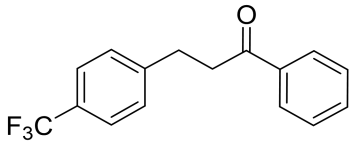
Yellow oil. For reduction of substrate **1f**, yield was 88% (77.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.15 (m, 5H), 2.95 – 2.86 (m, 2H), 2.81 – 2.73 (m, 2H), 2.63 – 2.51 (m, 1H), 1.07 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 213.75, 141.38, 128.46, 128.34, 126.05, 77.35, 77.03, 76.71, 41.97, 41.03, 29.86, 29.71, 18.13.

3-(4-Methoxyphenyl)-1-phenylpropan-1-one (20g) (CAS: 1669-49-4)[11]



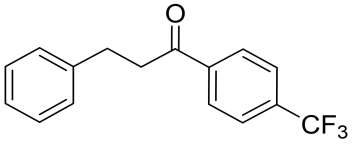
White solid. For reduction of substrate **1g**, yield was 82% (98.5 mg); For reduction of substrate **28c**, yield was 71% (85.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.94 (m, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 3.79 (s, 3H), 3.27 (t, *J* = 7.7 Hz, 2H), 3.02 (t, *J* = 7.6 Hz, 2H); ^{13}C 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 (20h)[11]



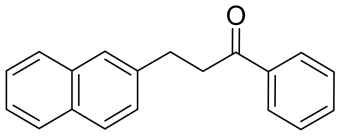
White solid. For reduction of substrate **1h**, yield was 78% (108.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.95 (m, 2H), 7.59 – 7.54 (m, 3H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 3.33 (t, *J* = 7.5 Hz, 2H), 3.14 (t, *J* = 7.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.56, 145.49, 136.71, 133.29, 128.85, 128.72, 128.05, 125.47 (q, *J* = 3.5 Hz), 124.33 (d, *J* = 270.0 Hz), 38.77, 28.72.

1-Phenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one (20i)[11]



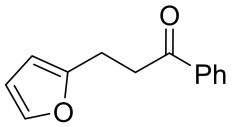
Light yellow solid. For reduction of substrate **1i**, yield was 78% (108.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.1 Hz, 2H), 7.73 (d, *J* = 8.3 Hz, 2H), 7.36 – 7.29 (m, 2H), 7.29 – 7.20 (m, 3H), 3.34 (t, *J* = 7.6 Hz, 2H), 3.10 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.20, 140.89, 139.53, 134.39 (d, *J* = 32.0 Hz), 128.63, 128.43, 128.38, 126.32, 125.71 (q, *J* = 3.0 Hz), 123.63 (d, *J* = 272.0 Hz), 40.74, 29.95; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.10.

3-(Naphthalen-2-yl)-1-phenylpropan-1-one (20j)[11]



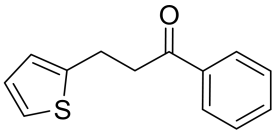
White solid. For reduction of substrate **1j**, yield was 85% (110.6 mg); For reduction of substrate **28i**, yield was 67% (87.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.98 (m, 2H), 7.82 (t, *J* = 7.7 Hz, 3H), 7.71 (s, 1H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.49 – 7.40 (m, 5H), 3.40 (t, *J* = 7.7 Hz, 2H), 3.25 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 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 (20k) (CAS: 2207-63-8)[12]



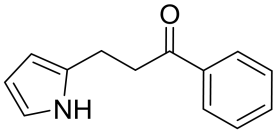
White solid. For reduction of substrate **1k**, yield was 85% (85.1 mg); For reduction of substrate **28h**, yield was 74% (74.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.97 (m, 2H), 7.57 (tt, *J* = 7.2, 1.6 Hz, 1H), 7.49 – 7.45 (m, 2H), 7.31 (d, *J* = 1.1 Hz, 1H), 6.29 (dd, *J* = 3.1, 1.9 Hz, 1H), 6.05 (dd, *J* = 3.1, 0.8 Hz, 1H), 3.36 – 3.32 (m, 2H), 3.10 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 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 (20l) (CAS: 71777-98-5)[12]



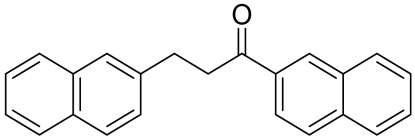
White solid. For reduction of substrate **1l**, yield was 85% (91.9 mg); For reduction of substrate **28g**, yield was 75% (81.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.9 Hz, 1H), 7.57 (t, *J* = 7.1, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 5.1 Hz, 1H), 6.94 – 6.92 (m, 1H), 6.87 (d, *J* = 3.1 Hz, 1H), 3.39 – 3.36 (m, 1H), 3.32 – 3.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 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 (20m) (CAS: 20948-44-1)[13]



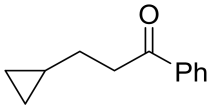
Brown solid. For reduction of substrate **1m**, yield was 26% (25.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (s, 1H), 7.97 (d, *J* = 7.8 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 6.67 (d, *J* = 1.3 Hz, 1H), 6.10 (d, *J* = 2.7 Hz, 1H), 5.95 (s, 1H), 3.35 (t, *J* = 6.4 Hz, 2H), 3.06 (t, *J* = 6.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 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 (20n) (CAS: 1221964-57-3)[14]



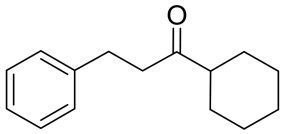
White solid. For reduction of substrate **1n**, yield was 84% (130.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.06 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.95 – 7.87 (m, 3H), 7.83 – 7.79 (m, 3H), 7.74 (s, 1H), 7.62 – 7.53 (m, 2H), 7.48 – 7.42 (m, 3H), 3.54 (t, *J* = 7.7 Hz, 2H), 3.30 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 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 (20o)[15]



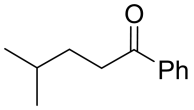
Colorless liquid. For reduction of substrate **1o**, yield was 82% (71.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.1 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 2H), 3.07 (t, *J* = 7.1 Hz, 2H), 1.63 (q, *J* = 7.0 Hz, 2H), 0.78 – 0.75 (m, 1H), 0.43 (d, *J* = 7.5 Hz, 2H), 0.07 (d, *J* = 4.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.42, 137.07, 132.86, 128.51, 128.03, 38.65, 29.50, 10.68, 4.61.

1-cyclohexyl-3-phenylpropan-1-one (20p) (CAS: 43125-06-0)[14]



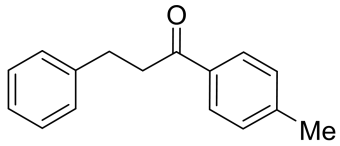
Yellow oil. For reduction of substrate **2d**, yield was 89% (96.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.14 (m, 5H), 2.88 (t, *J* = 8.0 Hz, 2H), 2.76 (t, *J* = 8.0 Hz, 2H), 2.38 – 2.26 (m, 1H), 1.85 – 1.72 (m, 4H), 1.68 – 1.63 (d, *J* = 9.7 Hz, 1H), 1.36 – 1.17 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 213.14, 141.40, 128.41, 128.30, 125.98, 50.95, 42.21, 29.71, 28.38, 25.81, 25.62.

4-Methyl-1-phenylpentan-1-one (20q) (CAS: 2050-07-9)[11]



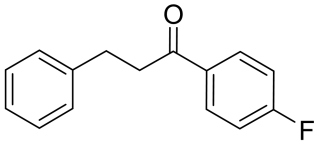
Yellow liquid. For reduction of substrate **3c**, yield was 80% (70.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.95 (m, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 2.99 – 2.95 (m, 2H), 1.65 – 1.61 (m, 3H), 0.95 (d, *J* = 6.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.83, 137.11, 132.89, 128.58, 128.09, 36.67, 33.28, 27.90, 22.47.

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



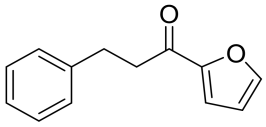
White solid. For reduction of substrate **6c**, yield was 78% (87.5 mg); For reduction of substrate **28j**, yield was 66% (74.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.1 Hz, 1H), 7.34 – 7.21 (m, 4H), 3.30 (t, *J* = 8.4 Hz, 1H), 3.08 (t, *J* = 7.6 Hz, 1H), 2.43 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 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 (20s) (CAS: 41938-64-1)[11]



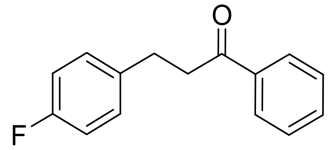
Colorless liquid. For reduction of substrate **6d**, yield was 81% (92.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.98 (m, 1H), 7.34 – 7.21 (m, 2H), 7.16 – 7.11 (m, 1H), 3.29 (t, *J* = 7.7 Hz, 1H), 3.09 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.62, 165.76 (d, *J* = 254.6 Hz), 141.15, 133.37 (d, *J* = 5.2Hz), 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 (20t) (CAS: 2976-01-4)[11]



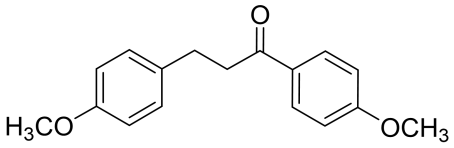
Brown liquid. For reduction of substrate **6e**, yield was 75% (75.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 1.0 Hz, 1H), 7.32 – 7.17 (m, 6H), 6.52 (dd, *J* = 3.5, 1.7 Hz, 1H), 3.19 – 3.13 (m, 2H), 3.09 – 3.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.50, 152.71, 146.32, 140.99, 128.53, 128.42, 126.19, 117.01, 112.21, 40.17, 29.98.

3-(4-Fluorophenyl)-1-phenylpropan-1-one (20u) (CAS: 41865-46-7)[11]



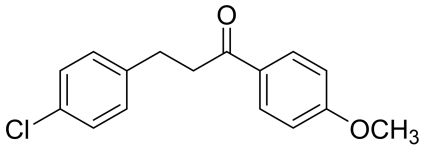
White solid. For reduction of substrate **6f**, yield was 80% (91.3 mg); For reduction of substrate **27b**, yield was 74% (84.5 mg); For reduction of substrate **28e**, yield was 70% (79.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.95 (m, 2H), 7.59 – 7.55 (m, 1H), 7.48 – 7.44 (m, 2H), 7.23 – 7.20 (m, 2H), 7.01 – 6.96 (m, 2H), 3.29 (t, *J* = 7.5 Hz, 2H), 3.06 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.99, 161.36 (d, *J* = 242.0 Hz), 136.88, 136.85, 136.78, 133.11, 129.81 (d, *J* =5.79 Hz), 128.61, 127.99, 115.22 (d, *J* = 15.8 Hz), 40.39, 29.24.

1,3-Bis(4-methoxyphenyl)propan-1-one (20v) (CAS: 20615-47-8)[14]



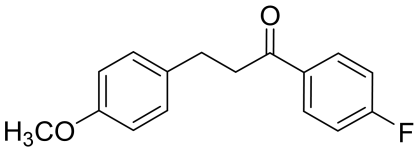
Pale yellow solid. For reduction of substrate **6h**, yield was 79% (106.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.92 (m, 2H), 7.17 (d, *J* = 8.6 Hz, 2H), 6.94 – 6.90 (m, 2H), 6.86 – 6.82 (m, 2H), 3.86 (s, 3H), 3.79 (s, 3H), 3.23 – 3.19 (m, 2H), 3.00 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) 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 (20w) (CAS: 111302-55-7)[16]



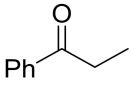
White solid. For reduction of substrate **6i**, yield was 78% (107.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) 7.95 – 7.91 (m, 2H), 7.26 – 7.24 (m, 2H), 7.18 (d, *J* = 8.3 Hz, 2H), 6.94 – 6.91 (m, 2H), 3.87 (s, 3H), 3.23 (t, *J* = 7.6 Hz, 2H), 3.03 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.43, 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 (20x)[17]



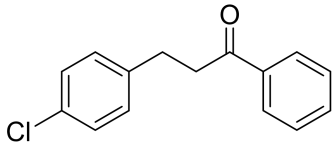
White solid. For reduction of substrate **6j**, yield was 81% (104.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.95 (m, 2H), 7.18 – 7.09 (m, 4H), 6.86 – 6.82 (m, 2H), 3.79 (s, 3H), 3.26 – 3.22 (m, 2H), 3.02 – 2.99 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.76, 165.67 (d, *J* = 253.0 Hz), 158.01, 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 (20y) (CAS: 93-55-0)[18]



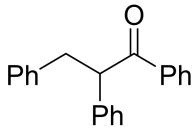
Yellow liquid. For reduction of substrate **6o**, yield was 22% (14.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.95 (m, 2H), 7.56 – 7.43 (m, 3H), 3.02 – 2.97 (m, 2H), 1.22 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.40, 136.69, 132.61, 128.31, 127.71, 31.49, 7.97.

3-(4-Chlorophenyl)-1-phenylpropan-1-one (20z) (CAS: 5739-39-9)[11]



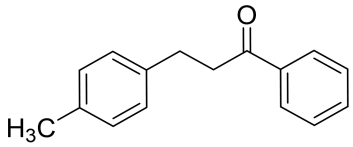
White solid. For reduction of substrate **6s**, yield was 81% (99.1 mg); For reduction of substrate **28d**, yield was 72% (88.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.94 (m, 2H), 7.56 (t, *J* = 7.3 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.26 (t, *J* = 4.1 Hz, 3H), 7.18 (d, *J* = 8.3 Hz, 2H), 3.28 (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 (20aa) (CAS: 4842-45-9)[12]



White solid. For reduction of substrate **6u**, yield was 75% (101.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 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 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.

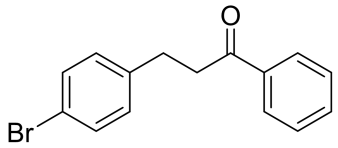
1-Phenyl-3-(p-tolyl)propan-1-one (20ab) (CAS: 1669-50-7)[11]



White solid. For reduction of substrate **28b**, yield was 69% (77.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 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* =

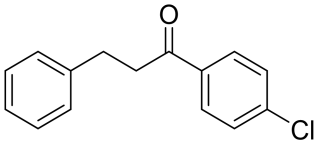
7.7 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.36, 138.21, 136.94, 135.63, 133.02, 129.22, 128.60, 128.30, 128.06, 40.61, 29.74, 21.00.

3-(4-Bromophenyl)-1-phenylpropan-1-one (20ac) (CAS: 52168-41-9)[11]



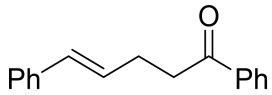
White solid. For reduction of substrate **28f**, yield was 75% (108.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.3 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 2H), 7.13 (d, *J* = 8.3 Hz, 2H), 3.28 (t, *J* = 7.5 Hz, 2H), 3.03 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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 (20ad) (CAS: 5739-37-7)[11]



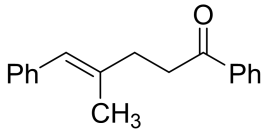
White solid. For reduction of substrate **28k**, yield was 68% (76.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.84 (m, 2H), 7.48 – 7.37 (m, 2H), 7.30 – 7.17 (m, 5H), 3.30 – 3.22 (m, 2H), 3.04 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.96, 141.03, 139.48, 135.13, 129.43, 128.90, 128.55, 128.39, 126.20, 40.41, 30.02.

(*E*)-1,5-Diphenylpent-4-en-1-one (25a) (CAS: 28069-36-5)[19]



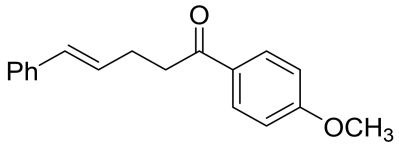
White solid. For reduction of substrate **21a**, yield was 80% (94.5 mg); For reduction of substrate **21a**, yield was 81% (95.7 mg); For reduction of substrate **24**, yield was 83% (98.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.7 Hz, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.7 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)[20]



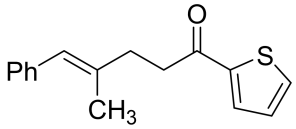
Yellow solid. For reduction of substrate **21b**, yield was 79% (98.9 mg); For reduction of substrate **23b**, yield was 79% (98.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.99 (m, 2H), 7.60 – 7.56 (m, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.24 – 7.18 (m, 3H), 6.34 (s, 1H), 3.23 – 3.19 (m, 2H), 2.62 (t, *J* = 7.6 Hz, 2H), 1.92 (d, *J* = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)[19]



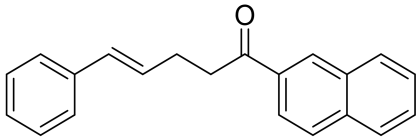
Yellow solid. For reduction of substrate **21c**, yield was 75% (99.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.9 Hz, 2H), 7.36 (d, *J* = 7.3 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 6.95 (d, *J* = 8.9 Hz, 2H), 6.47 (d, *J* = 15.8 Hz, 1H), 6.35 – 6.27 (m, 1H), 3.86 (s, 3H), 3.10 (t, *J* = 7.4 Hz, 2H), 2.66 (q, *J* = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



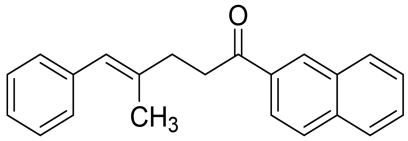
Yellow liquid. For reduction of substrate **21d**, yield was 78% (100.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.77 (m, 1H), 7.64 (d, *J* = 4.8 Hz, 1H), 7.36 – 7.32 (m, 2H), 7.26 – 7.20 (m, 3H), 7.16 – 7.14 (m, 1H), 6.37 (s, 1H), 3.19 – 3.11 (m, 2H), 2.65 (t, *J* = 7.6 Hz, 2H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)[19]



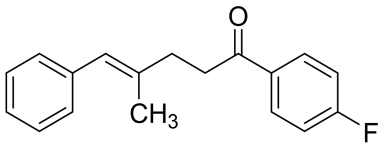
White solid. For reduction of substrate **21e**, yield was 82% (117.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 8.07 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.90 (t, *J* = 8.6 Hz, 2H), 7.63 – 7.54 (m, 2H), 7.37 (t, *J* = 7.2 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)



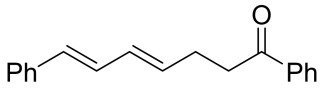
White solid. For reduction of substrate **21f**, yield was 82% (123.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.07 (d, *J* = 8.6 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.90 (t, *J* = 8.8 Hz, 2H), 7.63 – 7.55 (m, 2H), 7.35 – 7.31 (m, 2H), 7.26 – 7.18 (m, 3H), 6.38 (s, 1H), 3.36 – 3.32 (m, 2H), 2.74 – 2.64 (m, 2H), 1.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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): $[M+H]^+$ calcd for 301.1587, found 301.1591.

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



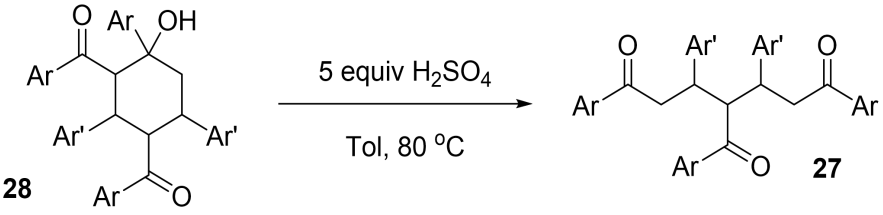
Yellow solid. For reduction of substrate **21g**, yield was 77% (118.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 8.01 (m, 2H), 7.33 (t, *J* = 8.6 Hz, 2H), 7.26 – 7.21 (m, 3H), 7.19 – 7.13 (t, *J* = 8.6 Hz, 2H), 6.34 (s, 1H), 3.20 – 3.16(m, 2H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.93 (d, *J* = 0.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.39. HRMS (m/z): $[M+H]^+$ calcd for 269.1336, found 269.1344.

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



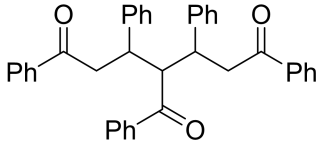
Yellow liquid. For reduction of substrate **22**, yield was 78% (102.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.7 Hz, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.38 (d, *J* = 7.7 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 6.76 (dd, *J* = 15.6, 10.4 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 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): $[M+H]^+$ calcd for 262.1358, found 262.1355.

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 ℃ was added concentrated sulfuric acid (5.0 mmol) dropwise. The reaction mixture was subsequently heated to 80 ℃ for 1 h, then hydrolyzed with ice. The aqueous layer was separated and extracted three times with 20 mL CH_2Cl_2. The combined organic layer was dried over anhydrous Na_2SO_4, 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.

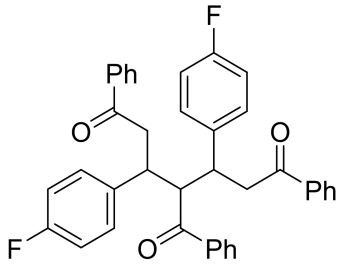
4-Benzoyl-1,3,5,7-tetraphenylheptane-1,7-dione (27a)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)

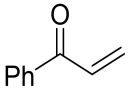


White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.7 Hz, 4H), 7.60 (d, J = 7.8 Hz, 2H), 7.52 – 7.45 (m, 3H), 7.37 (t, J = 7.6 Hz, 4H), 7.30 (t, J = 7.7 Hz, 2H), 7.09 (q, J = 5.2 Hz, 4H), 6.85 (t, J = 8.5 Hz, 4H), 4.33 (t, J = 7.4 Hz, 1H), 3.84 – 3.78 (m, 2H), 3.44 (dd, J = 16.9, 10.8 Hz, 2H), 3.28 (dd, J = 16.8, 3.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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; ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.45.

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

General procedure: (a) To a $CHCl_3$ (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 × 40 mL), distilled water (2 × 40 mL), saturated $NaHCO_3$ aq. (2 × 40 mL), and brine (1 × 40 mL). The organic layer was dried over anhydrous Na_2SO_4, 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 (**40**) as yellowish oil in 91% yield (4.30 g).[21] ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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 ℃ overnight, the reaction mixture was poured into EtOH (30 mL). The white viscous polymer was isolated by decantation, washed with ethyl acetate (1 × 5 mL), and petroleum ether (2 × 10 mL), and then dried under vacuum at 60 ℃, affording **29** as a white solid in 80% yield (3.44 g).

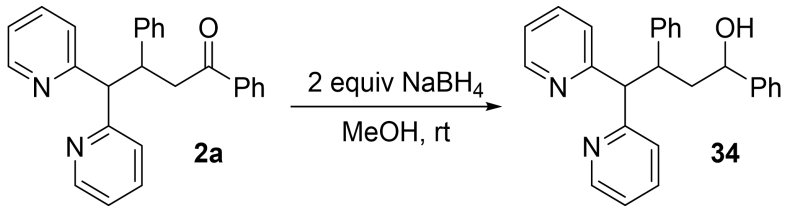
1-Phenylprop-2-en-1-one (**40**) (CAS: 768-03-6)[21]



Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.98, 137.28, 133.00, 132.39, 130.13, 128.69, 128.63.

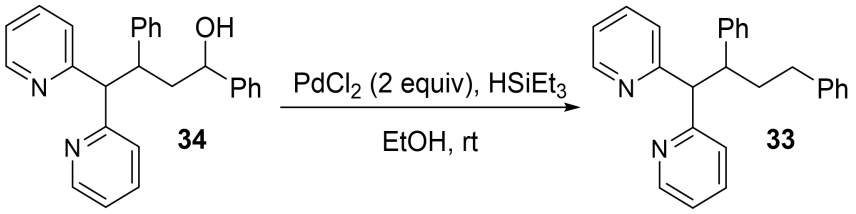
2.8 General procedures for the synthesis of di(2-pyridyl)methane derivatives (33 - 34)

Synthesis and characterization of 34



2a (10.0 mmol) was dissolved in MeOH (50 mL) and cooled to 0 ℃. Then, $NaBH_4$ (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 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, affording the product **34** as white solid in equivalent yield (3.81 g). ^{1}H NMR (400 MHz, $CDCl_3$) major + minor diastereoisomers δ 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; ^{13}C NMR (100 MHz, $CDCl_3$) major + minor diastereoisomers δ 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. HRMS (m/z): $[M+H]^+$ calcd for 381.1961, found 381.1979.

Synthesis and characterization of 33



$PdCl_2$ (2.0 mmol) was added to a solution of substrate **34** (1.0 mmol) and $HSiEt_3$ (2.0 mmol) in EtOH (5 mL). The mixture was stirred at 60 ℃ under nitrogen atmosphere for 6 h and quenched with saturated NH_4Cl solution (2 mL). Then, the mixture was 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 to give **33** as yellow solid (255.1 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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.

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

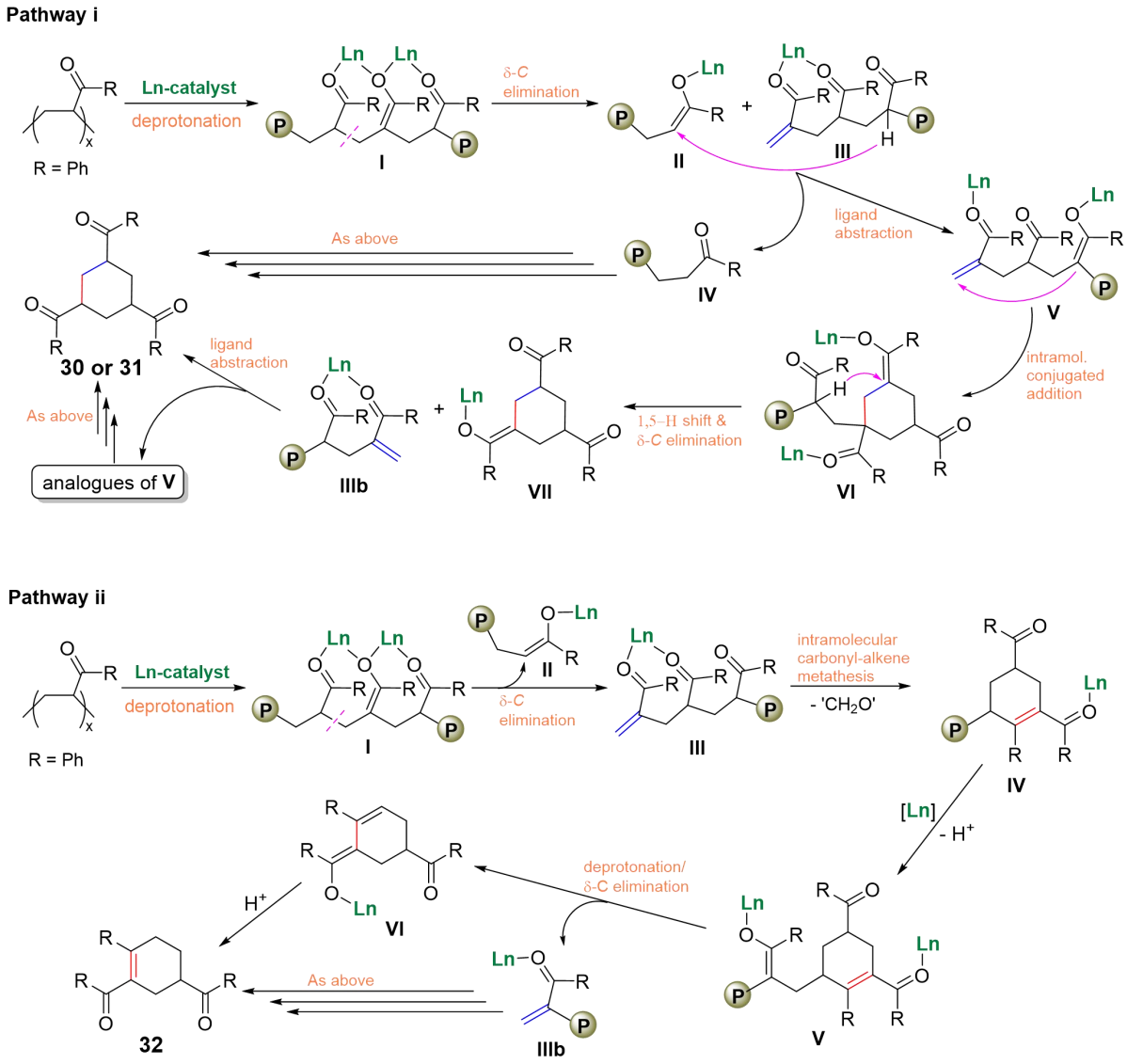
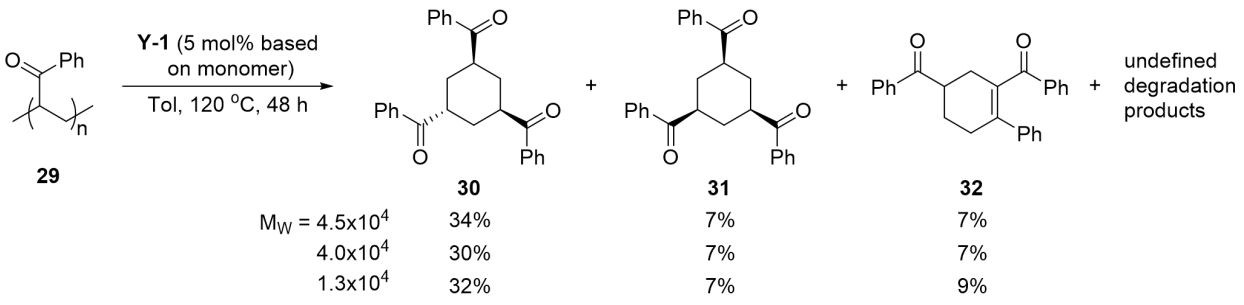


Figure S1. Proposed pathways for the formation of compounds **30 - 32.**

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 metal-block at 120 ℃ for 48 h, 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 Na_2SO_4, 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 ^{1}H 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.



29

	30	**31**	**32**
M_W = 4.5x10^4	34%	7%	7%
4.0x10^4	30%	7%	7%
1.3x10^4	32%	7%	9%

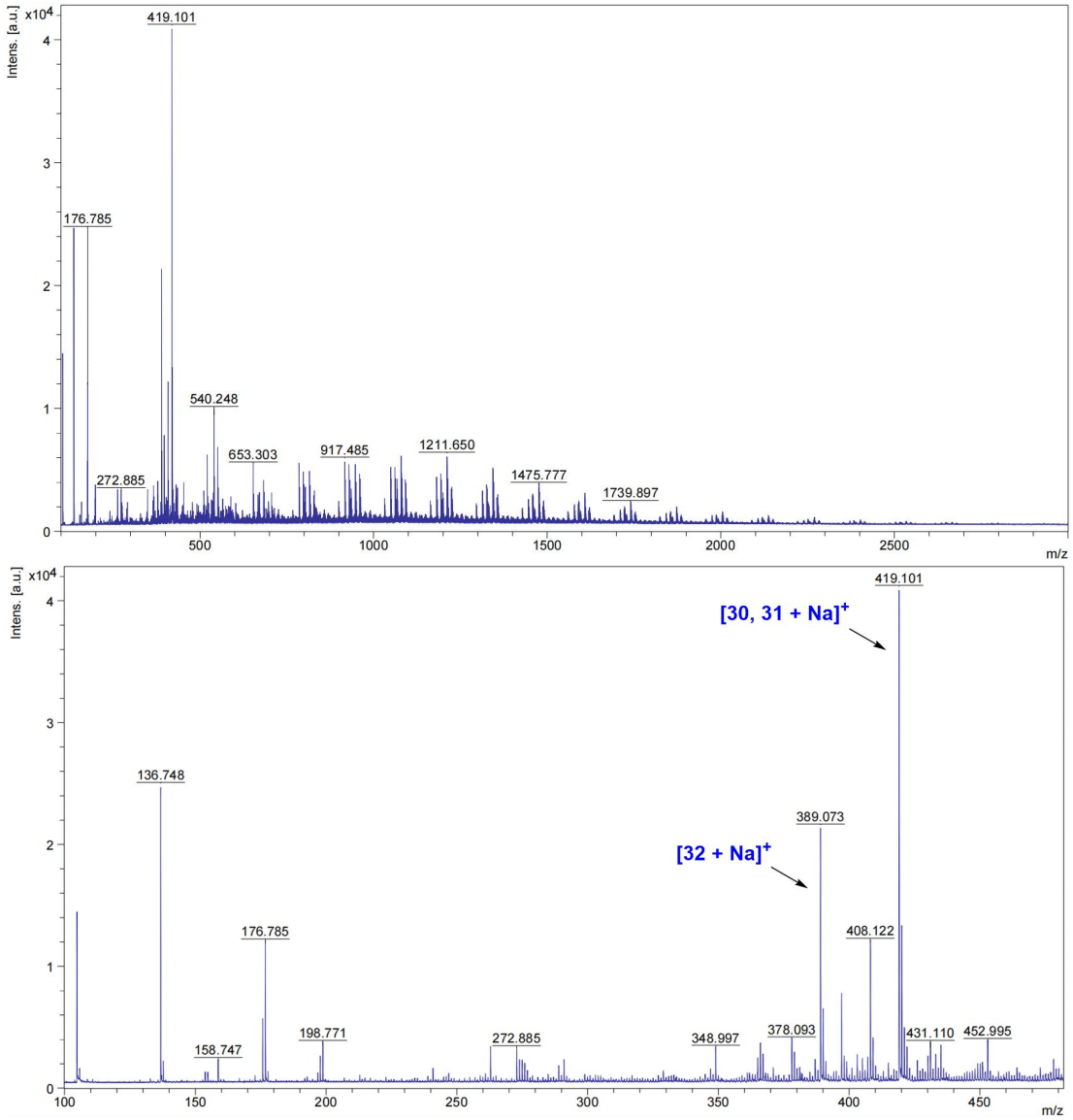


Figure S2. MALDI-TOF analysis of degradation products of sample **II**. The spectrum was acquired in linear, positive mode with DHB (matrix).

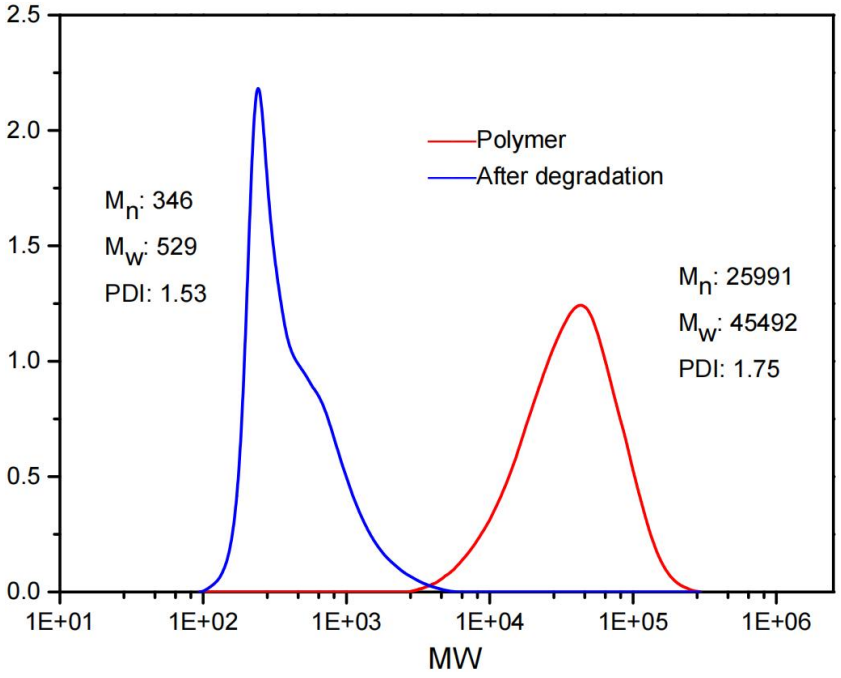


Figure S3. GPC profiles of sample **I** (red) and its degradation products (blue).

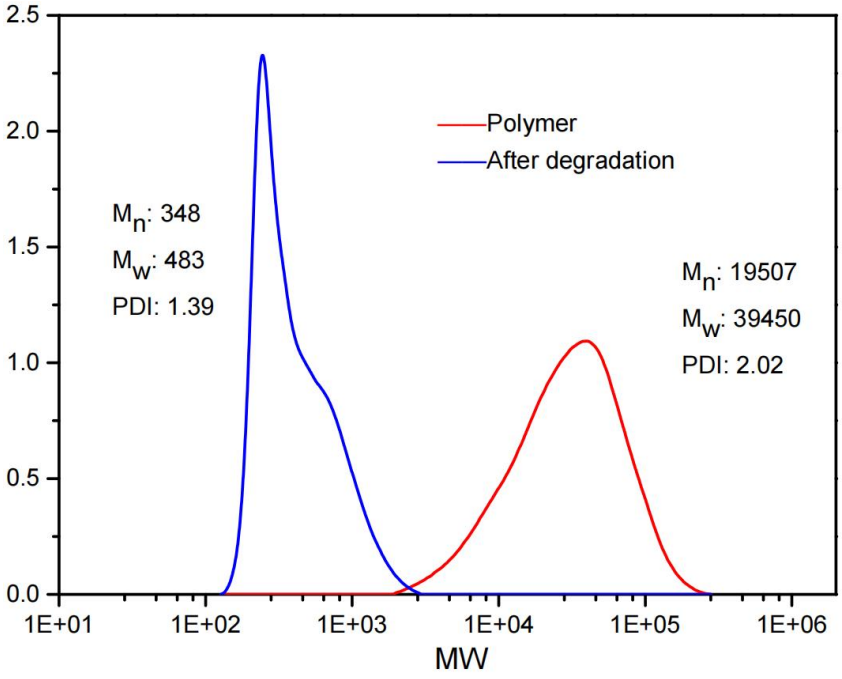


Figure S4. GPC profiles of sample **II** (red) and its degradation products (blue).

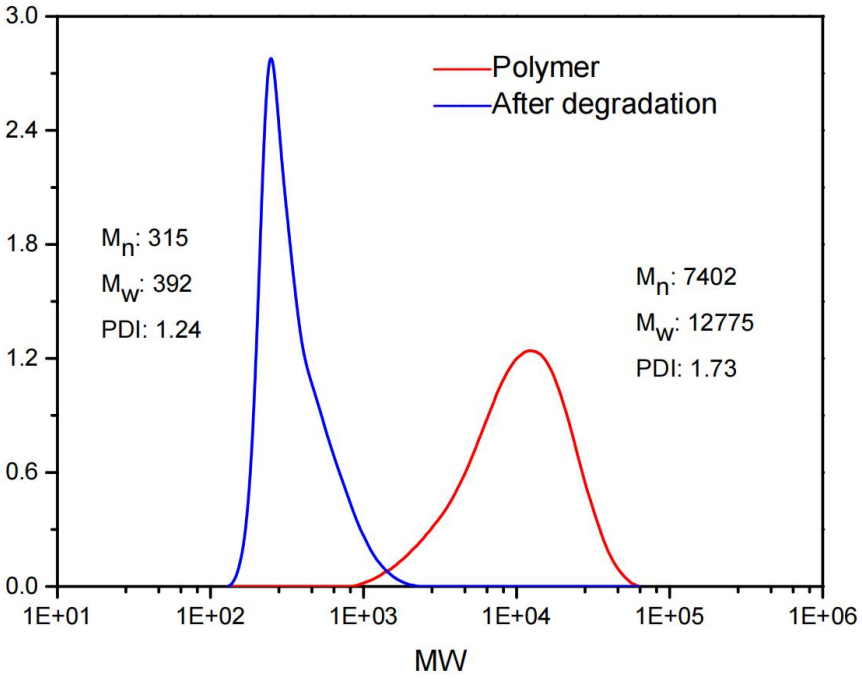
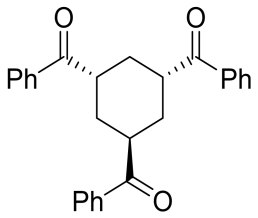


Figure S5. GPC profiles of sample **III** (red) and its degradation products (blue).

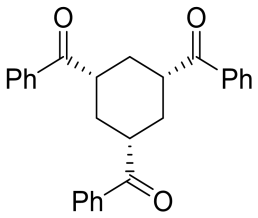
Characterization of products

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



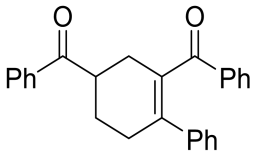
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.94 (m, 6H), 7.60 (t, *J* = 7.3 Hz, 1H), 7.53 – 7.49 (m, 4H), 7.40 (t, *J* = 7.7 Hz, 4H), 3.97 – 3.94 (m, 1H), 3.87 (tt, *J* = 12.1, 2.9 Hz, 2H), 2.41 (d, *J* = 13.7 Hz, 2H), 2.12 (d, *J* = 13.5 Hz, 1H), 1.92 (td, *J* = 13.3, 5.5 Hz, 2H), 1.81 (q, *J* = 12.3 Hz, 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 $[M+H]^+$ calcd. 397.1798, found: 397.1801.

r-1,1,*cis*-3,*cis*-5-tribenzoylcyclohexane (31)[22]



^{1}H NMR (400 MHz, $CDCl_3$) 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). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.35, 135.94, 133.16, 128.78, 128.24, 44.48, 31.47.

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



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) 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). ^{13}C NMR (100 MHz, $CDCl_3$) 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.

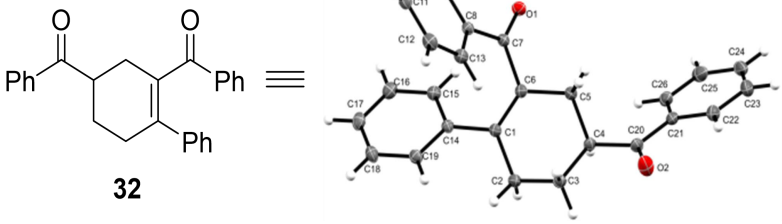


Figure S6. Molecular structure of 32 (Thermal ellipsoids at 30% level; all the hydrogen atoms are omitted for clarity). Selected bond lengths (Å) and bond angles (deg): C7−O1 1.22(1), C1−C2 1.51(2), C1−C6 1.34(2), C2−C3 1.52(2), C3 – C4 1.52(2), C4 – C5 1.54(2), C5 – C6 1.51(2), C4 – C20 1.52(2), C20 – 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

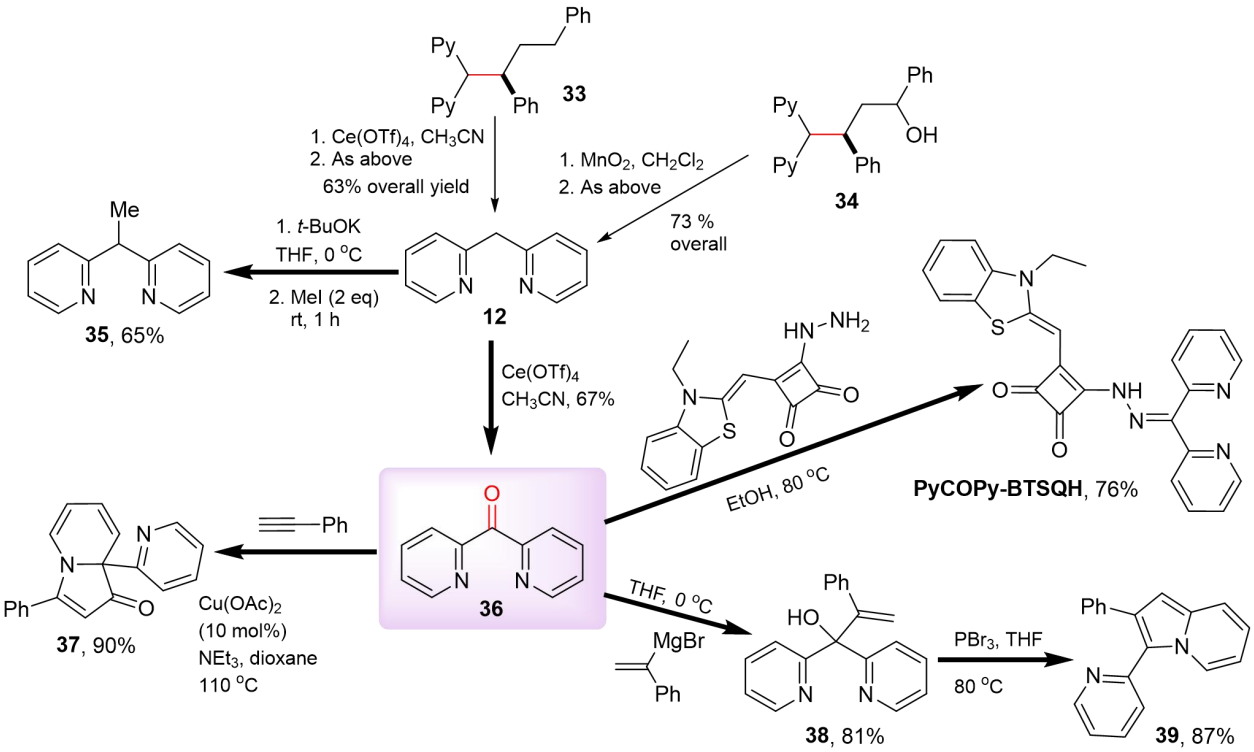
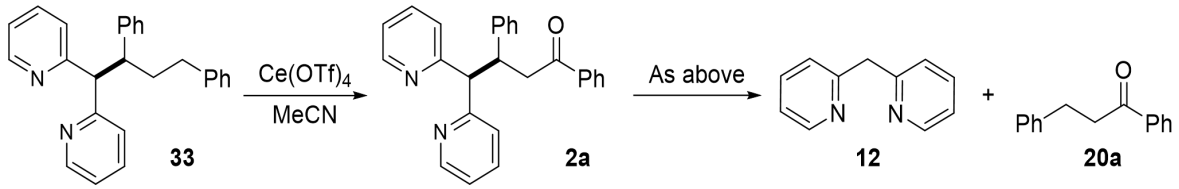


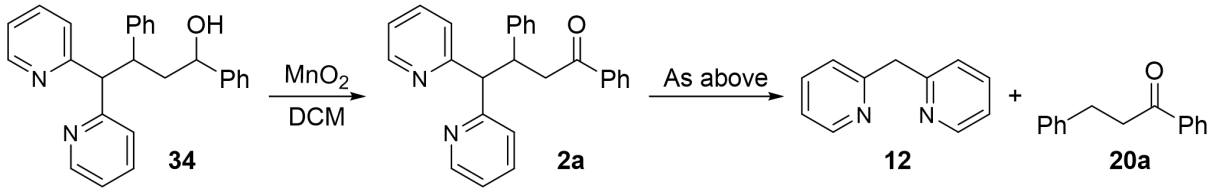
Figure S7. Representative examples of applications of the C–C hydrogenolysis protocol in side chain reduction and late-stage modification of 1,1-di(pyridin-2-yl)alkanes.

Two-step removal of alkyl from 33



To a stirred solution of **33** (5.0 mmol) in CH_3CN/H_2O (v/v = 2:1, 3 mL) was added $Ce(OTf)_4$ (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%).

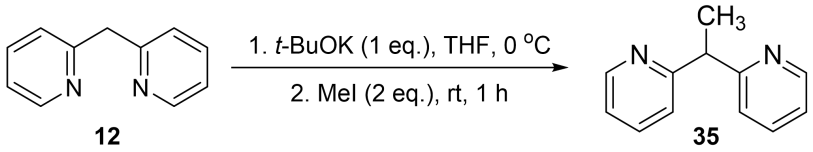
Two-step removal of β-hydroxyalkyl from 34



MnO_2 (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

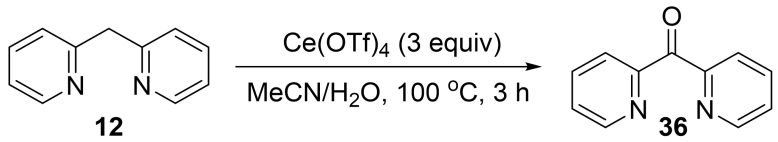
through a Celite Pad, and MnO_2 was washed by DCM (5 × 3 mL). The combined organic layer was concentrated to afford the crude product. The final purification was accomplished by flash chromatography (silica gel, with a mixture of petroleum ether/ethyl acetate = 1:1 as eluent) to give **2a** (1.62 g, 86%).

Synthesis and characterization of 1,1-dipyridylethane (35) (CAS: 29280-41-9)[23]



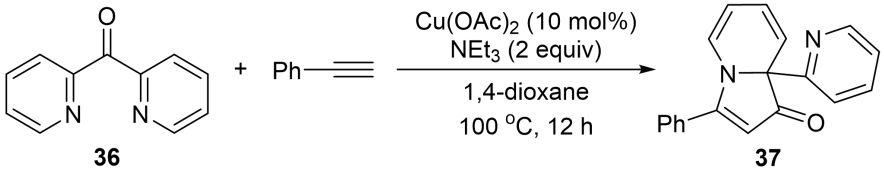
Di(pyridin-2-yl)methane **12** (1.0 mmol) was dissolved in 5 mL of THF in a 20 mL Schlenk flask equipped with a stir bar. The solution was cooled to 0 °C and *t*-BuOK (1.0 mmol) was added slowly. After stirring for 15 min, methyl iodide (2.0 mmol) was added dropwise. The reaction was subsequently warmed to room temperature for 1 h, and hydrolyzed with ice. The aqueous layer was separated and extracted three times with CH_2Cl_2. The combined organic layer was dried over anhydrous Na_2SO_4, filtered and evaporated. The crude product was purified by silica gel column chromatography with 1:1 ethyl acetate/petroleum ether as an eluent, yielding **35** as light yellow liquid (119.8 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 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 (36) (CAS:19437-26-4)[24]



Cerium(IV) trifluoromethanesulfonate (3.0 mmol) was added at once to a vigorously stirred solution of substrate **12** (0.50 mmol) in MeCN/H_2O (1:1 v/v 5 ml) at rt. The mixture was stirred at 100 °C for 3 h, quenched with saturated NH_4Cl solution (5 mL) and extracted with ethyl acetate (3 × 5 mL). The combined organic layer was dried with anhydrous Na_2SO_4, filtered, evaporated and purified by flash column chromatography using hexane/ethyl acetate as eluent, giving **36** as white solid (61.7 mg, 67%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.00, 154.33, 149.18, 136.75, 126.40, 125.23. HRMS (m/z): $[M+H]^+$ calcd for 184.0637, found 184.1980.

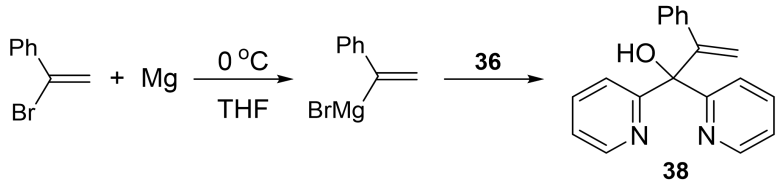
Synthesis of 3-phenyl-8a-(pyridin-2-yl)indolizin-1(8aH)-one (37)[25]



To a Teflon screw-cock vial containing a stir bar, **36** (0.30 mmol), phenylacetylene (0.60 mmol), $Cu(OAc)_2$ (0.03 mmol), NEt_3 (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 **37** as dark brown solid in 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 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.

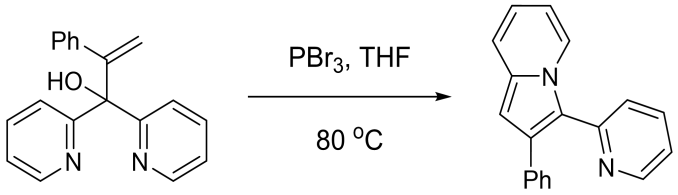
Synthesis of 2-phenyl-1,1-di(pyridin-2-yl)prop-2-en-1-ol (38)



38

Di(pyridin-2-yl)methanone **36** (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 NH_4Cl aqueous solution and extracted with Et_2O. The combined organic extracts were washed with brine, dried over anhydrous $MgSO_4$, filtered, concentrated and purified on silica gel chromatography with 1:5 ethyl acetate/petroleum ether as eluent, giving the allylic alcohol **38**. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.06, 153.78, 147.40, 140.83, 136.40, 128.54, 127.56, 126.92, 123.15, 122.22, 118.71, 81.42.

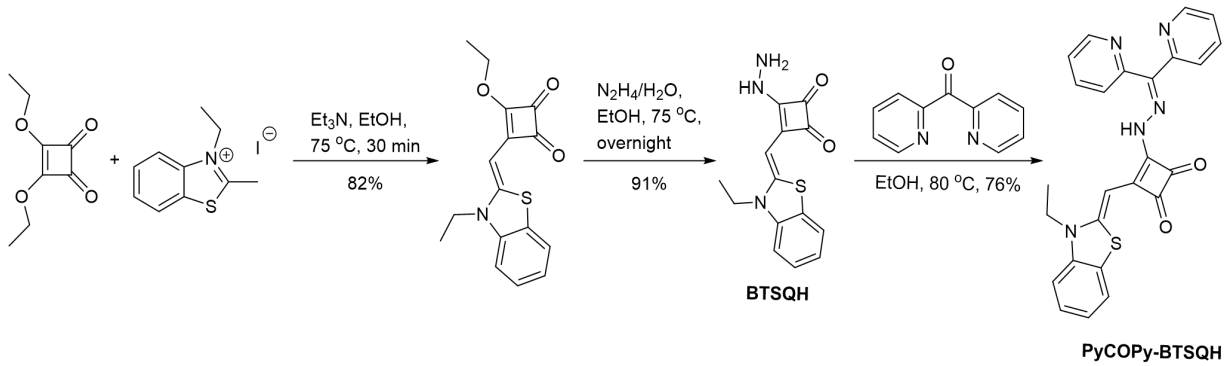
Synthesis of 2-phenyl-3-(pyridin-2-yl)indolizine (39)



38 **39**

To a solution of **38** (144 mg, 0.50 mmol) in THF (2.0 mL) was added PBr_3 (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 Na_2SO_4, and evaporated in vacuum. The residue was purified on silica gel chromatography to give **39** (118 mg, 87%) as dark green solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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)[26]



3-Ethoxy-4-((3-ethylbenzothiazol-2(3*H*)-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(3*H*)-ylidene)methyl)-4-hydrazinylcyclobut-3-en-1,2-dione **BTSQH** was obtained as orange-red powder. **BTSQH** (1.0 mmol) and **36** (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. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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

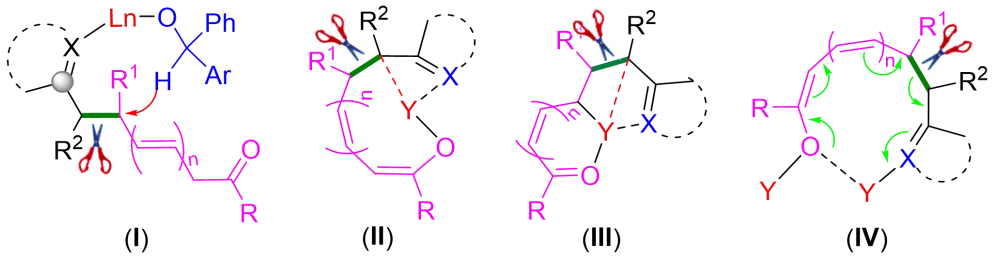


Figure S8. Four main possible mechanisms for C – C cleavage include (1) a direct nucleophilic substitution via H-transfer from yttrium alkoxide (**I**); (2) C – H activation followed by a remote C-elimination assisted by the directing groups via a monometallic pathway (**II**); (3) β-C elimination paralleling 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

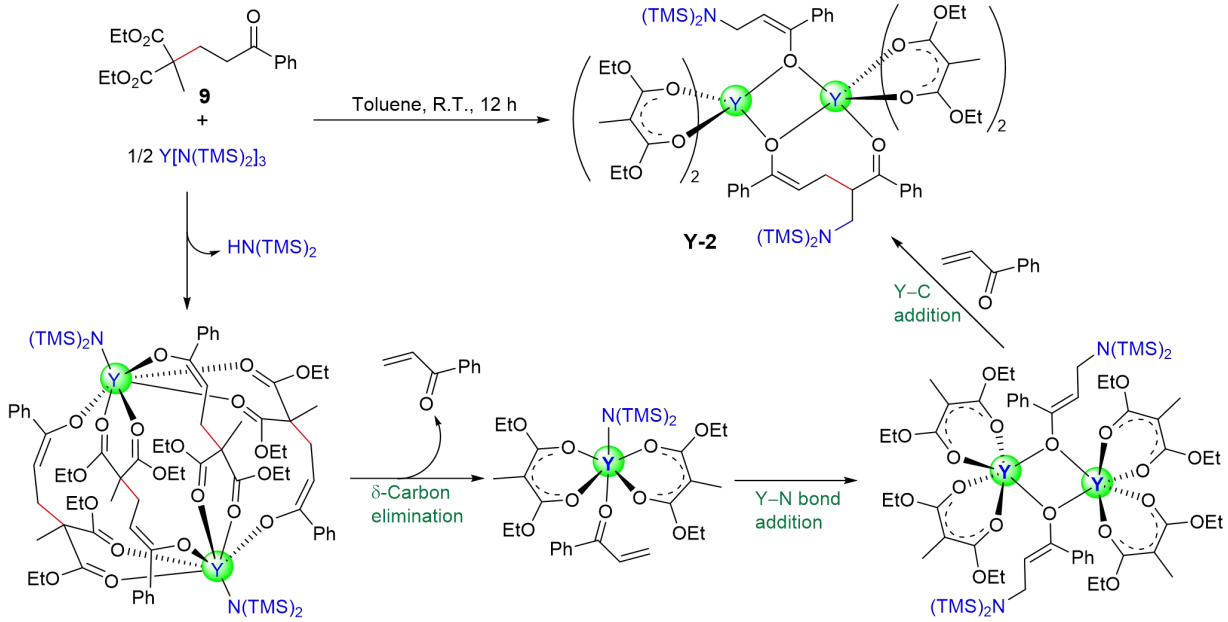


Figure S9. Isolation of the intermediate Y-2 involving a C–H activation of substrate 9 followed by δ-carbon elimination and subsequent addition of the resulting enone to yttrium species. A mixture of **Y-1** (569 mg, 1.0 mmol) and **9** (612 mg, 2.0 mmol) in 5 mL toluene was stirred at room temperature 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.

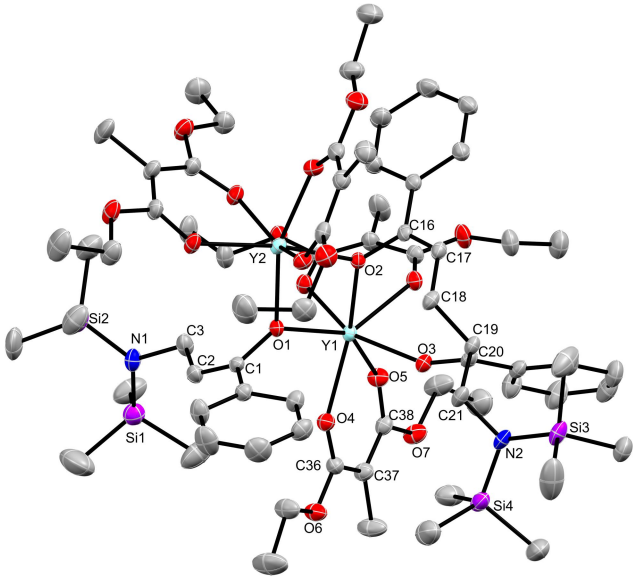


Figure S10. Molecular structure of complex **Y-2** (thermal ellipsoids at 30% level; all the hydrogen atoms are omitted for clarity). Selected bond lengths (Å) and bond angles (deg): Y1−Y2 3.728(1), Y1−O1 2.276(2), Y1−O2 2.243(2), Y2−O1 2.324(2), Y2−O2 2.327(2), Y2−O3 2.318(2), Y1−O3 2.318(2), Y1−O4 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).

Complex **Y-2** was structurally characterized by single-crystal X-ray diffraction analysis (Figure S10). The formation of **Y-2** might be attributed to the replacement of two $N(TMS)_2$ 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 (Figure 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.

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

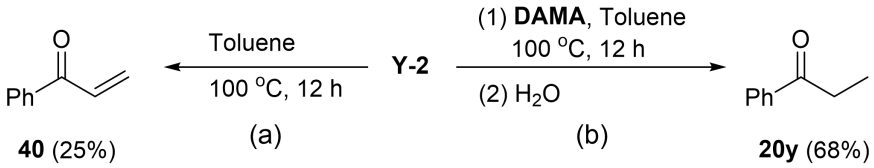


Figure S11. Confirmation of the feasibility of the C(sp^3)−C(sp^3) bond cleavage via δ-carbon elimination of dinuclear yttrium enolate intermediate: (a) **Y-2** (125 mg, 0.10 mmol) and toluene (3 mL) were added to a Schlenk tube equipped with a magnetic stirring bar and a Teflon cap. After heating at 100 °C for 12 h, the reaction mixture was quenched with water (2 mL), and extracted with ethyl acetate (3 × 5 mL). The combined organic layers were dried over Na_2SO_4, 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 **40** 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 × 5 mL). The combined organic layer was dried over Na_2SO_4, 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 **20y** (9.0 mg, 68% based on the anionic diketone ligand).

Remarkably, the formation of **40** 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 **20y** in moderate yield, indicating that the in situ trapping of the resulting enone **40** 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 Y^{3+} 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

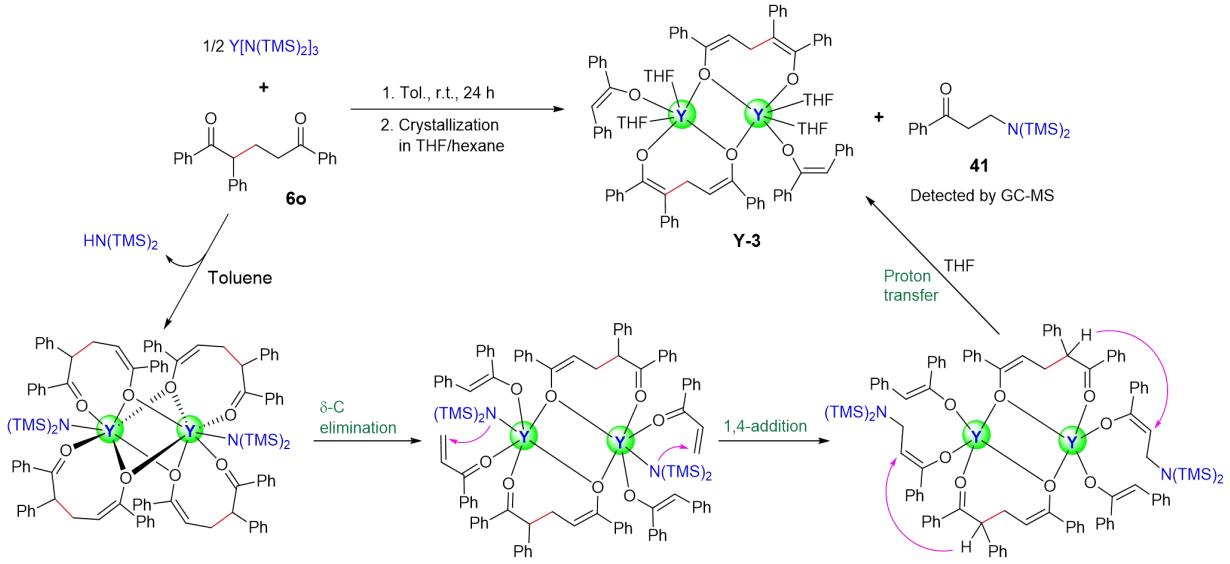


Figure S12. Stoichiometric reaction of Y-1 with 6o. A mixture of **Y-1** (569 mg, 1.0 mmol) and **6o** (656 mg, 2.0 mmol) in toluene (5 mL) was stirred at room temperature for 24 h. Removal of volatiles afforded red powder. Diffusion of toluene into a THF solution of the orange powder gave **Y-3** as 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 **41** (73% GC-content), 293 [M^+].

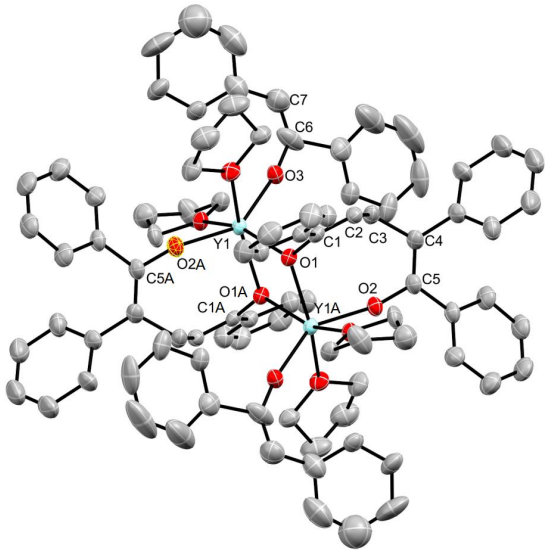


Figure S13. Molecular structure of complex **Y-3** (Thermal ellipsoids at 30% level; all the hydrogen atoms are omitted clarity). Selected bond lengths (Å) and bond angles (deg): Y1−Y1A 3.733(1), Y1−O1 2.281(4), Y1−O1A 2.274(4), Y1A−O2 2.105(4), Y1−O3 2.136(4), O1−C1 1.383(7), O2−C5 1.336(8), O3−C6 1.288(9), 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

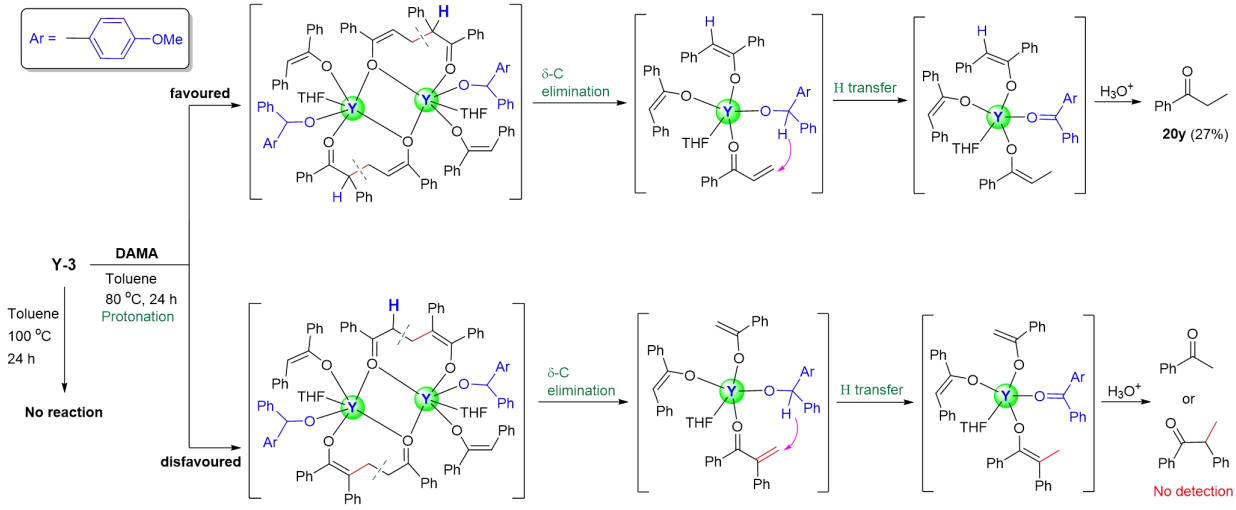


Figure S14. Deprotonation effect and monodeprotonation regioselectivity of 1,5-diketone. A mixture of **Y-3** (150 mg, 0.10 mmol) and **DAMA** (43 mg, 0.20 mmol) in toluene (3 mL) was heated at 80 ℃ for 24 h, quenched with water (2 mL), and extracted with ethyl acetate (3 × 5 mL). The combined organic 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 **20y** in 27% yield, without the observation of $PhCOCH_3$ or $PhCOCH(Ph)CH_3$. In contrast to **Y-2**, no reaction occurred when a toluene solution of **Y-3** was directly heated to 100 ℃. 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

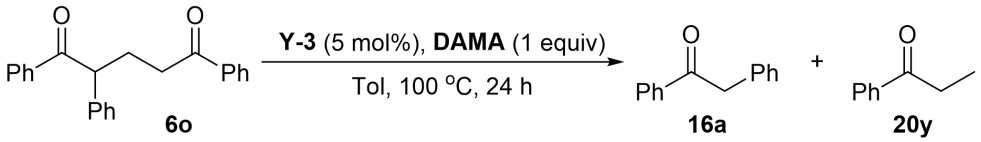


Figure S15. Y-3-catalyzed C–C hydrogenolysis of 6o with DAMA: According to the procedure described previously, treatment of a mixture of **6o** (164 mg, 0.50 mmol) and **DAMA** (107 mg, 0.50 mmol) with **Y-3** (37.6 mg, 0.025 mmol) at 100 °C afforded **16a** (22.5 mg, 23%) and **20y** (17 mg, 25%), respectively. 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 (Figure 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.

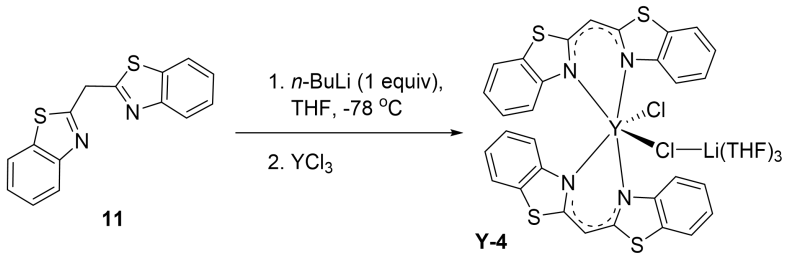


Figure S16. Synthesis of the model complex for stabilizing the Y–C bond by the directing group. To a THF solution of compound **11** (282 mg, 1.0 mmol) was slowly added *n*-BuLi (2.5 M solution in hexane, 1.0 mmol) at -78 °C under N_2 atmosphere. After stirring at -78 °C for 1 h, the mixture was warmed to -20 °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%).

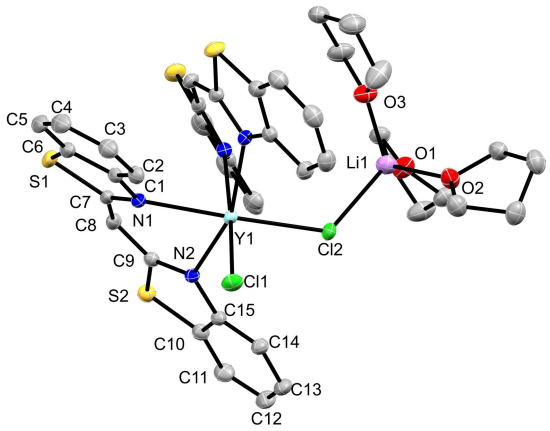
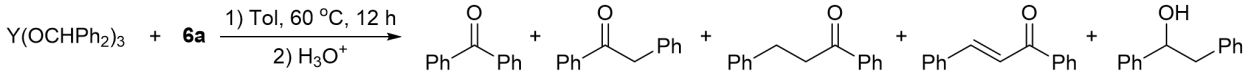


Figure S17. Molecular structure of complex Y-4 (Thermal ellipsoids at 30% level; all the hydrogen atoms are omitted clarity). Selected bond lengths (Å): Y1−N1 2.397(2), Y1−N2 2.397(2), Y1−Cl1 2.558(1), Y1−Cl2 2.610(1), N1−C1 1.400(3), N1−C7 1.342(3), N2−C9 1.351(3), N2−C15 1.401(3), S1−C6 1.737(3), S1−C7 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 $Y(OCHPh_2)_3$ as a key active intermediate

Preparation of $Y(OCHPh_2)_3$ (Y-4): To a stirred solution of **Y-1** (569 mg, 1.0 mmol) in toluene (20 mL) was added Ph_2CHOH (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%).



Y-4		6a	43	16a	20a	44	45
1	:	3	89%	79%	81%	5%	
1	:	1	36%	67%	83%		18%

Figure S18. Reaction of $Y(OCHPh_2)_3$ 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 ℃ for 12 h and quenched by addition of saturated NH_4Cl solution 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 corresponding compounds as shown above.

As shown in Figure S18, treatment of $Y(OCHPh_2)_3$ with **6a** led to the formation of the expected transfer hydrogenolysis products **16a** and **20a**. Significantly, the intermediate **44** and the further reduction product **45** 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

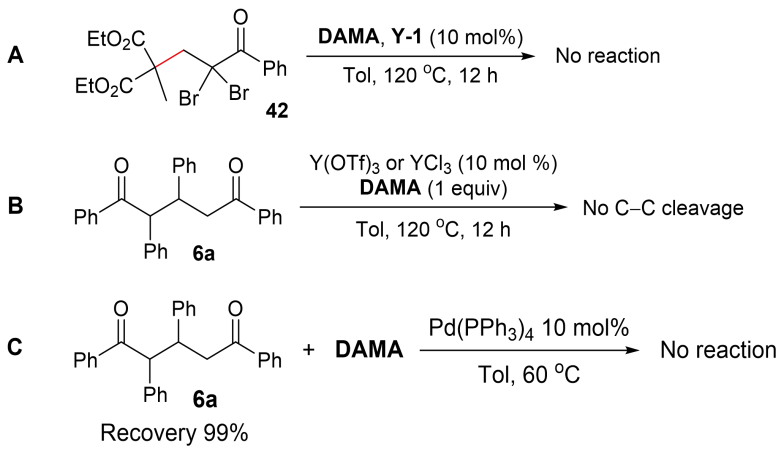
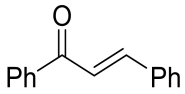


Figure S19. Unsuccessful reactions.

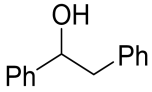
Notably, no products derived from the C–C bond cleavage were obtained even with a prolonged heating at 120 °C when the substrate **42** without the presence of an active α-C–H bond was used. It has also proven that no $C(sp^3)-C(sp^3)$ cleavage reaction of **6a** took place under otherwise identical 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 (44) (CAS: 94-41-7)



Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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 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 (45) (CAS: 614-29-9)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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); ^{13}C NMR (100 MHz, $CDCl_3$) δ 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

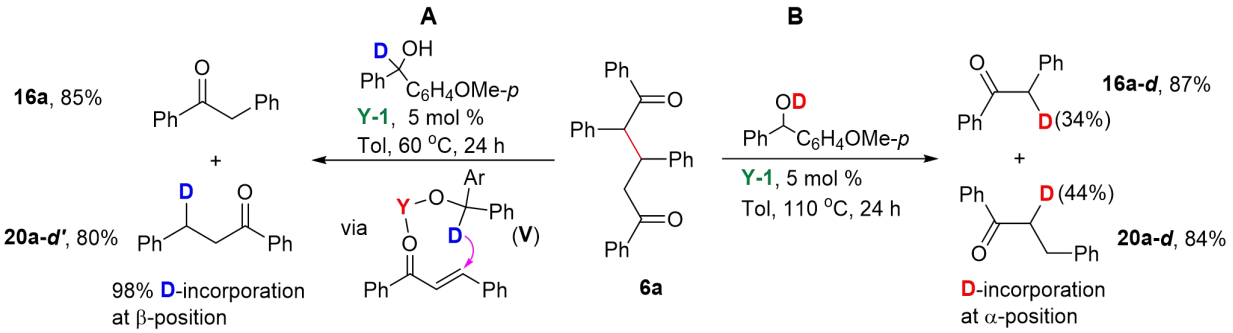
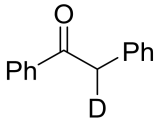


Figure S20. (A) A catalytic amount of **Y-1** (5 mol%) was added to a solution of **6a** (0.50 mmol) and *C-d*-(4-methoxyphenyl) (phenyl)methanol (0.50 mmol) in toluene (2 mL). The resulting mixture was stirred at 60 ℃ for 24 h and quenched with saturated NH_4Cl solution (2 mL). Then the mixture was 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, 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 ℃ for 24 h and quenched with saturated NH_4Cl solution (2 mL). Then the mixture was 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 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.

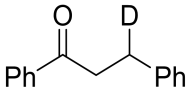
The C−C hydrogenolysis mechanism was further investigated through deuterium-labeling experiments. When ***O-d*-DAMA** was used, deuterium was found only at the α-position of the products **20a-*d*** and **16a-*d***. Employing ***C-d*-DAMA** as the hydrogen source afforded **20a-*d'*** in 80% yield with 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(C_6H_4OMe-*p*)Ph species through an eight-membered azametalacycle intermediate.

1,2-Diphenylethan-1-one-2-*d* (16a-d) (CAS: 84369-12-0)[27]



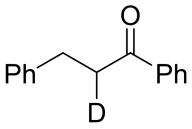
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.1 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.36 – 7.28 (dd, *J* = 18.5, 6.6 Hz, 5H), 4.30 – 4.27 (d, *J* = 10.7 Hz, 1.64H).

1,3-Diphenylpropan-1-one-3-d (20a-d') (CAS: 93698-11-4)[28]



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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)[28]



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 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 ^{1}H NMR-monitoring the reaction of 6p and DAMA

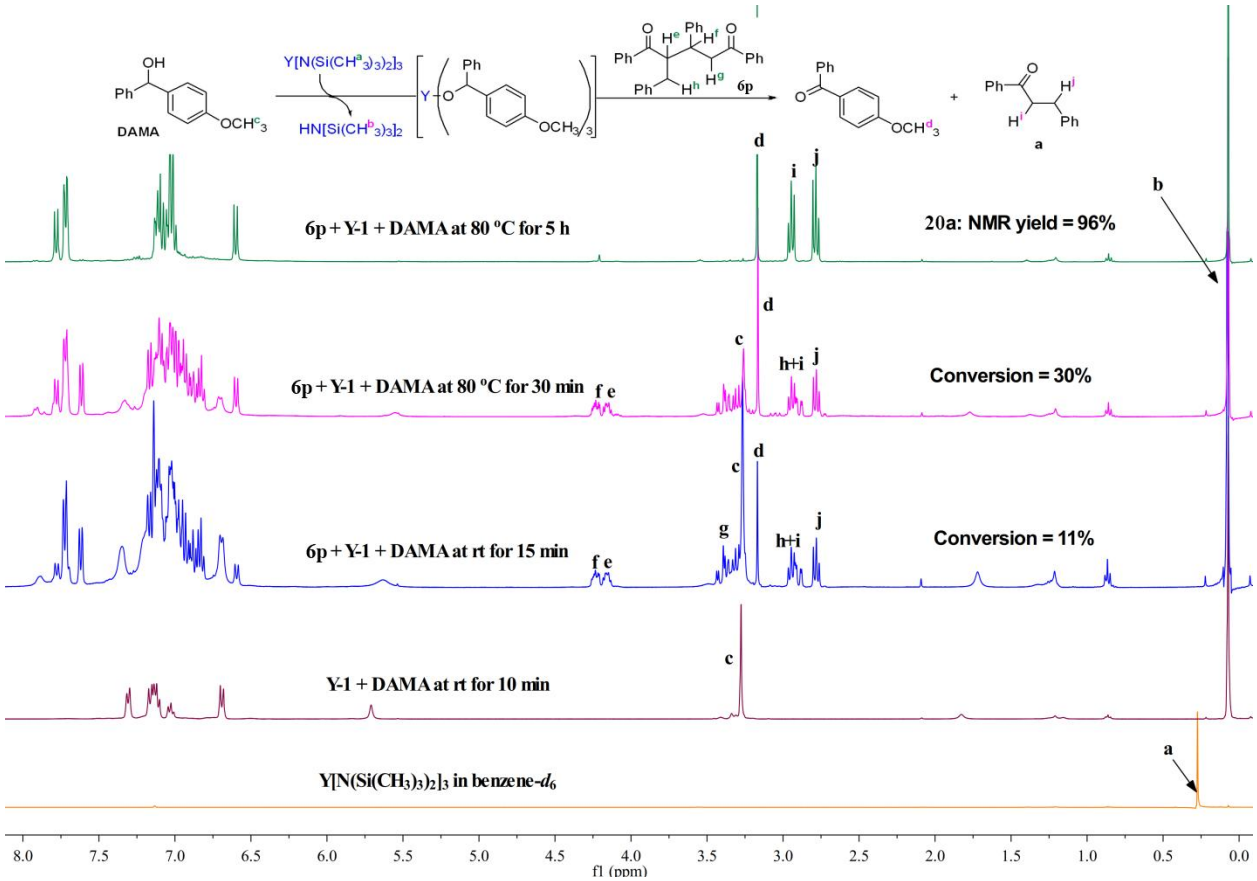


Figure S21. ^{1}H NMR spectra for the progress of the reaction of **6p** with **Y(OCHPh$_2$)$_3$** as catalyst. **Method A:** In a glovebox, **Y-1** (5.6 mg, 0.010 mmol) was weighed into a NMR tube equipped with a Teflon valve (J-Young). Then, a solution of **DAMA** (21.4 mg, 0.010 mmol) in benzene-d_6 (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 ^{1}H 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 (Figure S22). The ^{1}H NMR monitoring data reveals that **6p** abstracted the amido ligand more slowly than **DAMA**, leading to the liberation of only part $N(SiMe_3)_2$ ligands from $Y[N(SiMe_3)_2]_3$ 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**. In addition, the rate of carbon-carbon cleavage seems to be faster without the presence of **DAMA** than with the presence of **DAMA** (**method A** *vs* **method B**), which might be attributed to the fact that abstraction of OCHPh(C_6H_4OMe-*p*) ligand from yttrium alkoxide complex intermediates with **6p** is more difficult than abstraction of $N(SiMe_3)_2$ and enolate ligands from corresponding amido and enolate complexes.

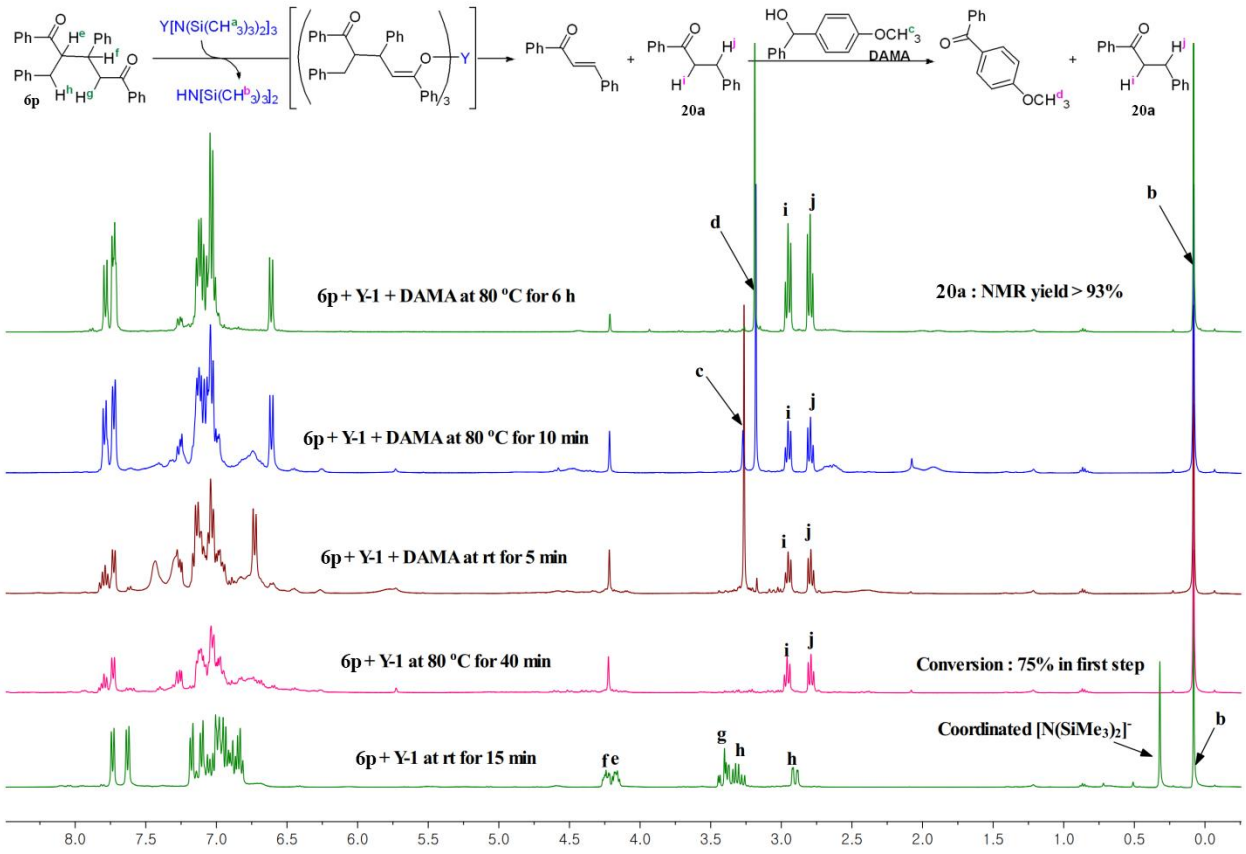


Figure S22. ^{1}H NMR spectra for the progress of the reaction of **6p** with **DAMA** using **Y-1** as catalyst. **Method B:** To a solution of **6p** (40.8 mg, 0.10 mmol) in benzene-d_6 (0.50 mL) filled in a J-Young NMR tube, was added **Y-1** (5.6 mg, 0.010 mmol). After heating at 80 °C for 40 mins, 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 ^{1}H NMR technique following the signal of the methylene group (H^j) formation, and the experimental conditions and the actual conversion of **6p** were listed.

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 ^{1}H NMR spectroscopy. The ^{1}H NMR monitoring data (Figure 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 $(Me_3Si)_2N$ ligand from the precatalyst rapidly, giving the free $(Me_3Si)_2NH$, and **Y-1** was cleanly converted into $Y(OCHPh(C_6H_4Me\text{-}p))_3$ 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.

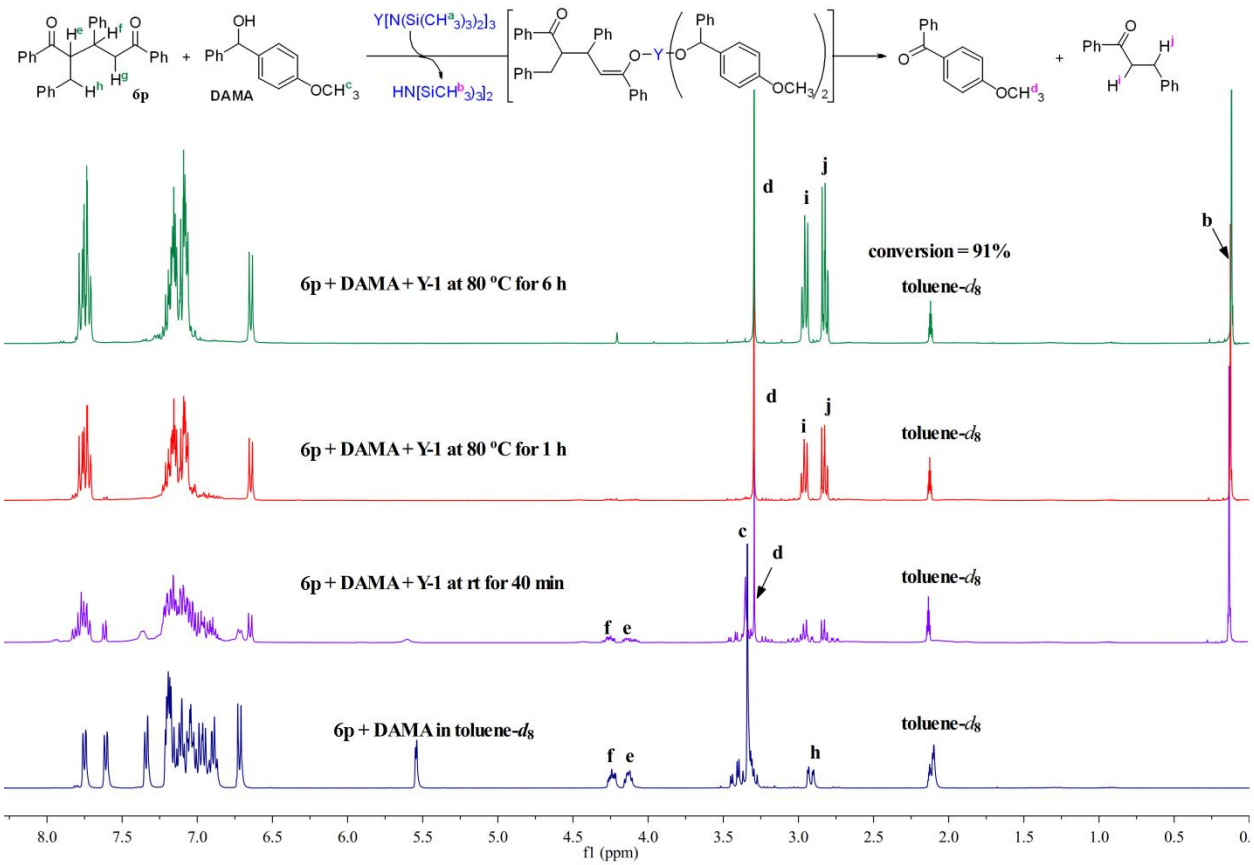


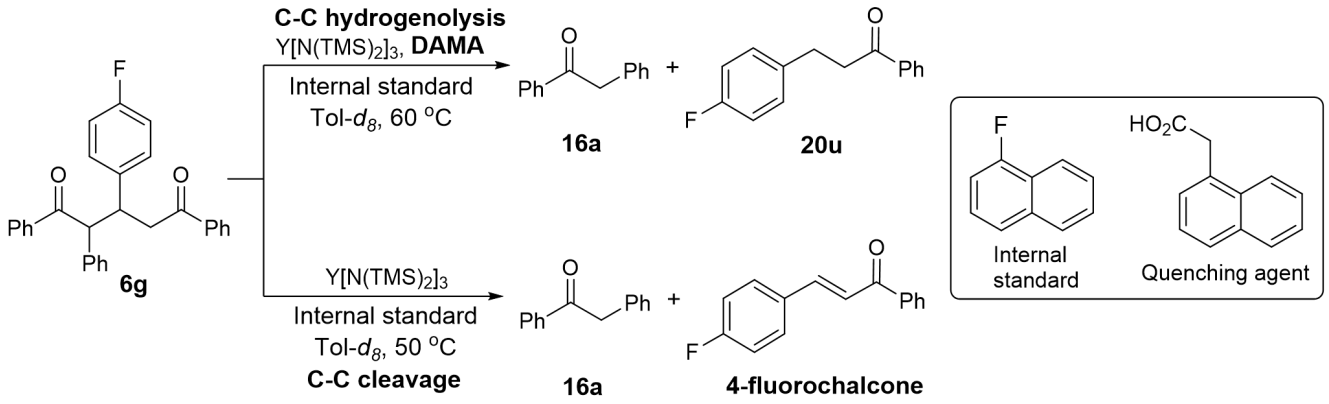
Figure S23. ^{1}H NMR spectra for the progress of the reaction of **6p** with **DAMA** using **Y-1** as catalyst. **Method C:** In a glovebox, **Y-1** (5.6 mg, 0.010 mmol) was transferred to a NMR tube equipped with a Teflon valve (J-Young). Then, a mixture of **DAMA** (21.4 mg, 0.10 mmol) and **6p** (40.8 mg, 0.10 mmol) in toluene-d_8 (0.50 mL) was added. The reaction progress was detected by ^{1}H 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.

When **Y-1** was directly added to a mixture of **6p** and **6p** in toluene-d_8, the ^{1}H NMR monitoring data (Figure 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.

6.5 Kinetic experiment

6.5.1 General information

The kinetic orders for each reactant were measured by initial rate method. The generation rate of dihydrochalcone **20u** was used to calculate the initial rate of hydrogenolysis reaction and the generation rate of 4-fluorochalcone was used to calculate the initial rates of C−C bond cleavage reaction. The yields of **20u** and 4-fluorochalcone were determined by comparing the intergration of the peak at -117.2 ppm and -109.7 ppm with that of the peak of 1-fluoronaphthalene at -123.4 ppm from the ^{19}F NMR spectra of the reaction mixture. All reactions were run in the glovebox.



6.5.2 Initial rate *vs* *c*(Y[N(TMS)$_2$]$_3$) of hydrogenolysis reaction

In a glovebox, a different amount of **Y-1** (3.8 mg (6.7 mol%), 5.7 mg (10 mol%), 7.1 mg (12.5 mol%), 8.6 mg (15 mol%), 11.4 mg (20 mol%)) and 1-fluoronapthalene (internal standard) were added into to a Schlenk tube with Teflon valve and a magnetic stir bar. Then, to which a dry toluene-d_8 (3 mL) solution of substrate **6g** (42.2 mg, 0.10 mmol) and **DAMA** (21.4 mg, 0.10 mmol) was added. The Schlenk tube was sealed and quickly heated at 60 °C in a pre-heated metal block. About 0.4 mL of the reaction mixture was taken out according to the interval time shown in **Table S3.1-3.5** and injected into a NMR tube filled with the quenching agent (2-(naphthalen-1-yl)acetic acid), and analyzed by ^{19}F NMR spectroscopy to periodically determine the yield of **20u**. First order rate dependence on *c*(Y[N(TMS)$_2$]$_3$) was observed.

Table S3.1 Initial rate vs *c*(Y[N(TMS)$_2$]$_3$) (0.0022 M)

c(Y[N(TMS)$_2$]$_3$) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0022	3.9	5	0.000889	0.000178
		9	0.001601	
		13	0.002223	
		17	0.003024	
		21	0.003735	

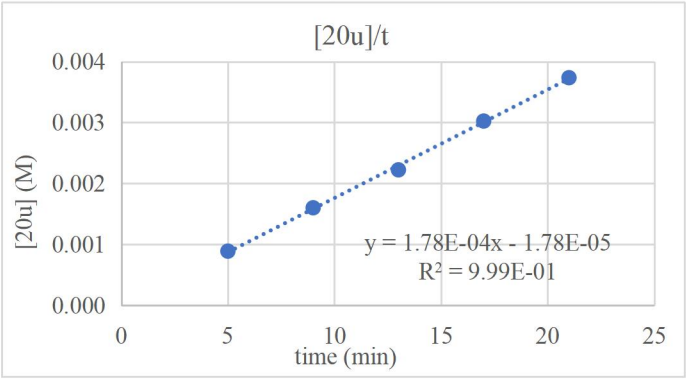


Table S3.2 Initial rate vs $c(Y[N(TMS)_2]_3)$ (0.0033 M)

$c(Y[N(TMS)_2]_3)$ (M)	Internal standard (mg)	Time (min)	c(**20u**) (M)	Initial rate (M/min)
0.0033	4.2	4	0.001245	0.000244
		8	0.002490	
		12	0.003639	
		16	0.004406	
		20	0.005172	

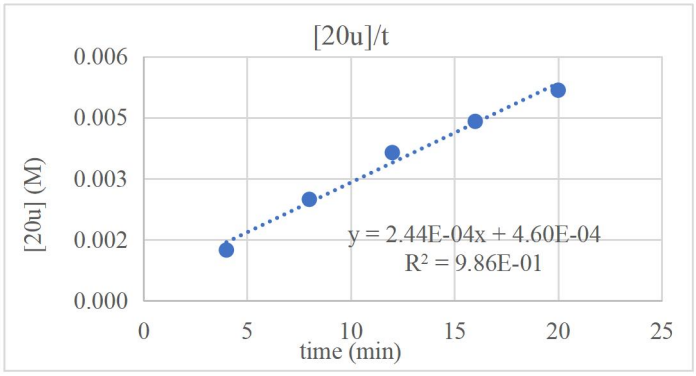


Table S3.3 Initial rate vs $c(Y[N(TMS)_2]_3)$ (0.0042 M)

$c(Y[N(TMS)_2]_3)$ (M)	Internal standard (mg)	Time (min)	c(**20u**) (M)	Initial rate (M/min)
0.0042	4.4	3	0.001003	0.000328
		6	0.002107	
		9	0.003311	
		12	0.004114	
		15	0.004916	

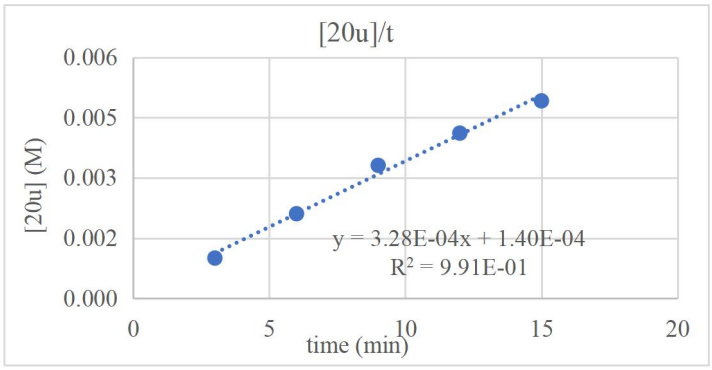


Table S3.4 Initial rate vs $c(Y[N(TMS)_2]_3)$ (0.0042 M)

$c(Y[N(TMS)_2]_3)$ (M)	Internal standard (mg)	Time (min)	c(**20u**) (M)	Initial rate (M/min)
0.0050	4.3	4	0.001373	0.000379
		7	0.002844	
		10	0.004118	
		13	0.005001	
		16	0.005981	

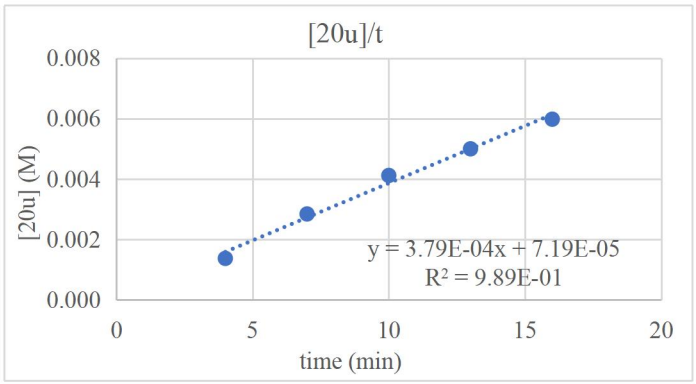


Table S3.5 Initial rate vs $c(Y[N(TMS)_2]_3)$ (0.0042 M)

$c(Y[N(TMS)_2]_3)$ (M)	Internal standard (mg)	Time (min)	c(**20u**) (M)	Initial rate (M/min)
0.0067	3.8	3	0.001300	0.000491
		6	0.002773	
		9	0.004073	
		12	0.005719	
		15	0.007192	

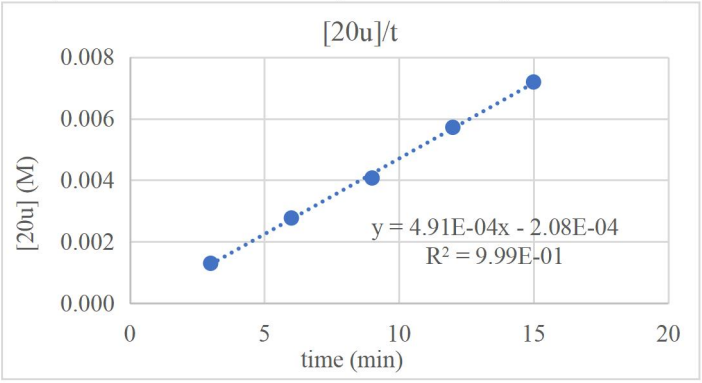
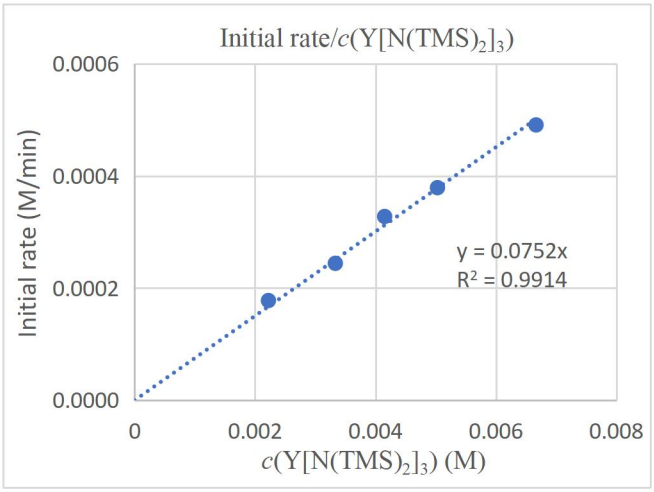
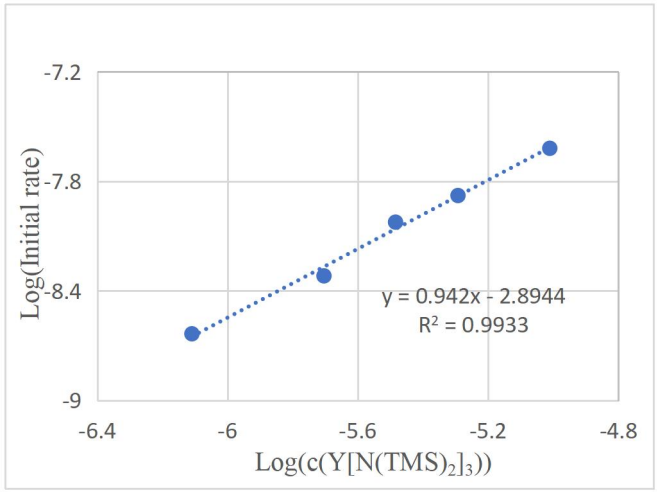


Table S3.6 Kinetic order for $c(Y[N(TMS)_2]_3)$ of hydrogenolysis reaction

$c(Y[N(TMS)_2]_3)$ (M)	Initial rate (M/min)	Log($c(Y[N(TMS)_2]_3)$)	Log(Initial rate)
0.0022	0.000178	-6.1094	-8.6345
0.0033	0.000244	-5.7039	-8.3174
0.0042	0.000328	-5.4843	-8.0232
0.0050	0.000379	-5.2926	-7.8776
0.0067	0.000491	-5.0108	-7.6190





6.5.3 Initial rate *vs* *c*(DAMA) of hydrogenolysis reaction

In a glovebox, **Y-1** (5.7 mg, 10 mol%) and 1-fluoronapthalene (internal standard) were added to the Schlenk tube with Teflon valve and a magnetic stir bar. Then, to which a dry toluene-d_8 (3 mL) solution of substrate **6g** (42.2 mg, 0.10 mmol), **DAMA** (12.7 mg (0.060 mmol), 17.2 mg (0.08 mmol), 21.4 mg (0.10 mmol), 25.3 mg (0.12 mmol), 30.0 mg (0.14 mmol)) was added. The Schlenk tube was reassembled and quickly heated at 60 °C in a pre-heated metal block. About 0.4 mL of the reaction mixture was taken out according to the interval time shown in **Table S4.1-4.5**, injected into a NMR tube filled with 2-(naphthalen-1-yl)acetic acid, and analyzed by ^{19}F NMR spectroscopy to periodically determine the yield of **20u**. Zero order rate dependence on *c*(DAMA) was observed.

Table S4.1 Initial rate vs *c*(DAMA) (0.0198 M)

c(DAMA) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0198	4.5	3	0.001026	0.000236
		6	0.001950	
		9	0.002668	
		12	0.003284	
		15	0.003899	

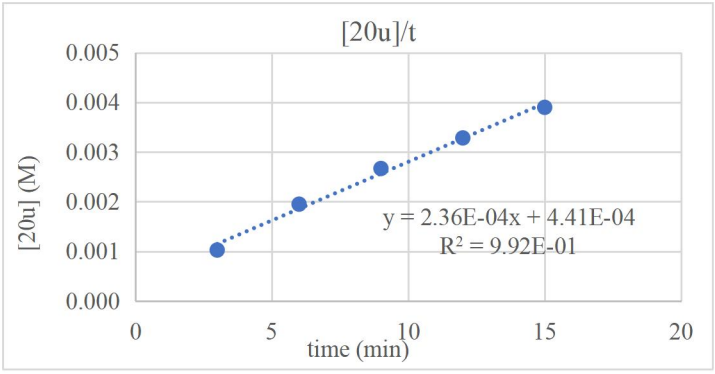


Table S4.2 Initial rate vs *c*(DAMA) (0.0268 M)

c(DAMA) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0268	4.0	3	0.000821	0.000240
		6	0.001733	
		9	0.002463	
		12	0.003101	
		15	0.003740	

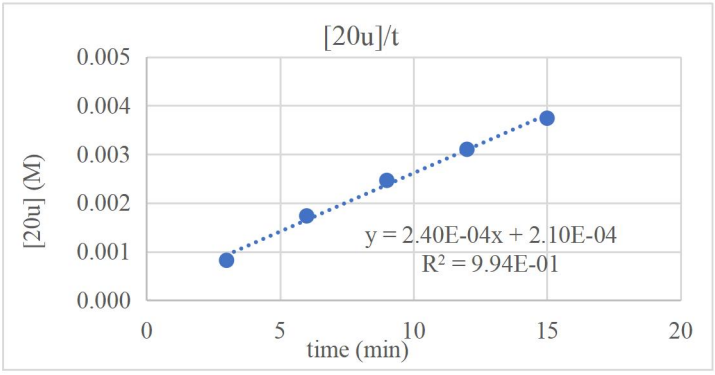


Table S4.3 Initial rate vs *c*(DAMA) (0.0333 M)

c(DAMA) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0333	4.2	4	0.001245	0.000244
		8	0.002490	
		12	0.003639	
		16	0.004406	
		20	0.005172	

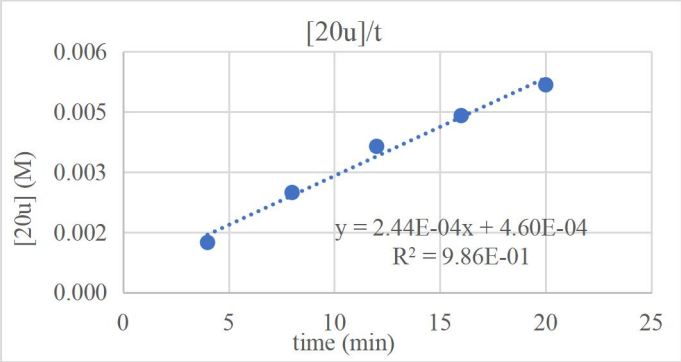


Table S4.4 Initial rate vs *c*(DAMA) (0.0394 M)

c(DAMA) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0394	4.1	3	0.000748	0.000249
		6	0.001683	
		9	0.002431	
		12	0.003179	
		15	0.003740	

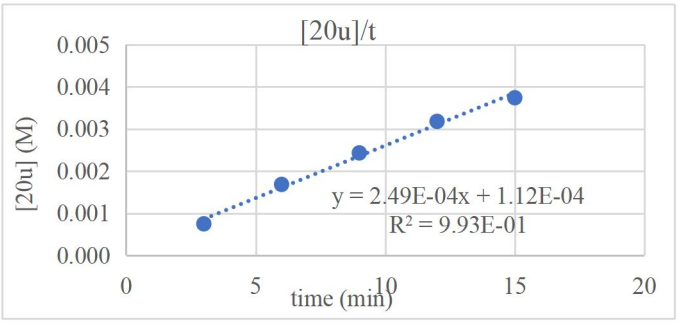


Table S4.5 Initial rate vs *c*(DAMA) (0.0467 M)

c(DAMA) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0467	4.1	3	0.000654	0.000243
		6	0.001309	
		9	0.002057	
		12	0.002805	
		15	0.003553	

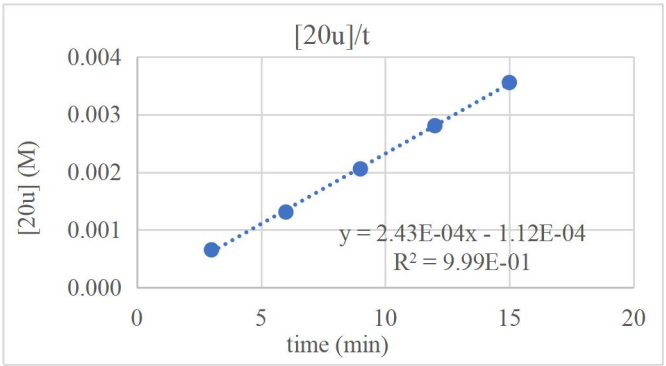
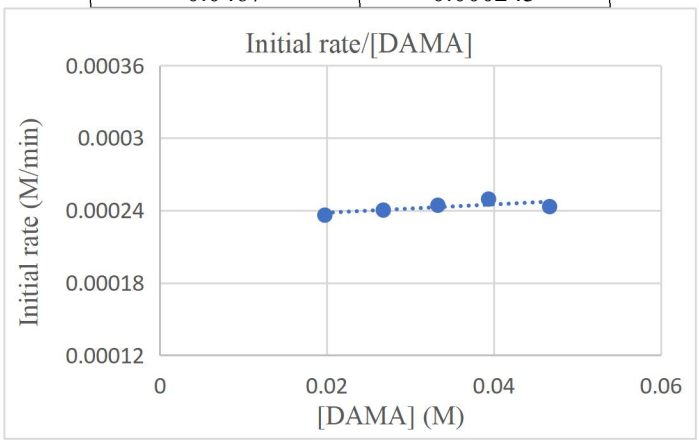


Table S4.6 Kinetic order for *c*(DAMA) of hydrogenolysis reaction

c(DAMA) (M)	Initial rate (M/min)
0.0198	0.000236
0.0268	0.000240
0.0333	0.000244
0.0394	0.000249
0.0467	0.000243



6.5.2 Initial rate *vs* *c*(substrate 6g) of hydrogenolysis reaction

In a glovebox, **Y-1** (5.7 mg, 10 mol%) and 1-fluoronapthalene (internal standard) were injected to the Schlenk tube with Teflon valve and a magnetic stir bar. Then, a dry toluene-d_8 (3 mL) solution of substrate **6g** (38.8 mg (0.80 mmol), 42.2 mg (0.10 mmol), 51.4 mg (0.12 mmol), 60.2 mg (0.14 mmol), 67.4 mg (0.16 mmol)), and **DAMA** (21.4 mg, 0.10 mmol) were added. The Schlenk tube was reassembled and quickly heated at 60 °C in a pre-heated metal block. About 0.4 mL of the reaction mixture was taken out according to the interval time shown in **Table S5.1-5.5**, injected into a NMR tube filled with the quenching agent (2-(naphthalen-1-yl)acetic acid), and then analyzed by ^{19}F NMR spectroscopy to periodically determine the yield of **20u**. First order rate dependence on *c*(**6g**) was observed.

Table S5.1 Initial rate vs *c*(**6g**) (0.0267 M)

c(**6g**) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0267	4.1	4	0.001122	0.000199
		8	0.001870	
		12	0.002524	
		16	0.002992	
		20	0.003553	

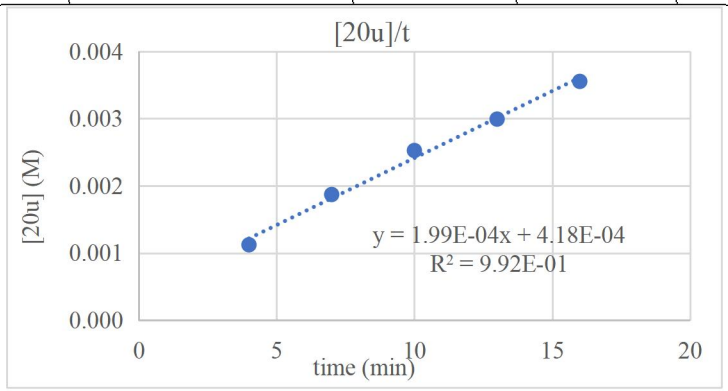


Table S5.2 Initial rate vs *c*(**6g**) (0.0333 M)

c(**6g**) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0333	4.2	4	0.001245	0.000244
		8	0.002490	
		12	0.003639	
		16	0.004406	
		20	0.005172	

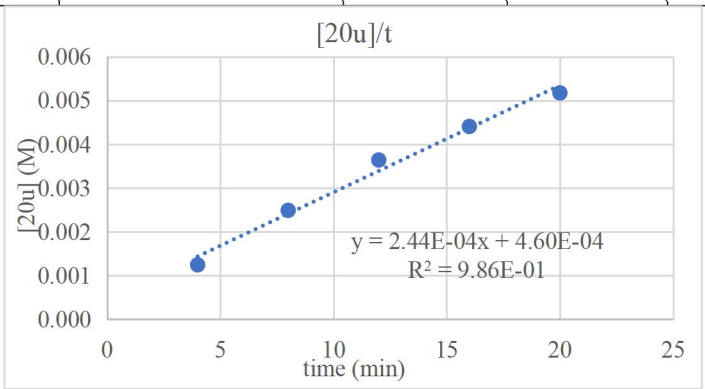


Table S5.3 Initial rate vs *c*(**6g**) (0.0406 M)

c(**6g**) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0406	4.4	3	0.001003	0.000294
		6	0.001806	
		9	0.002910	
		12	0.003612	
		15	0.004515	

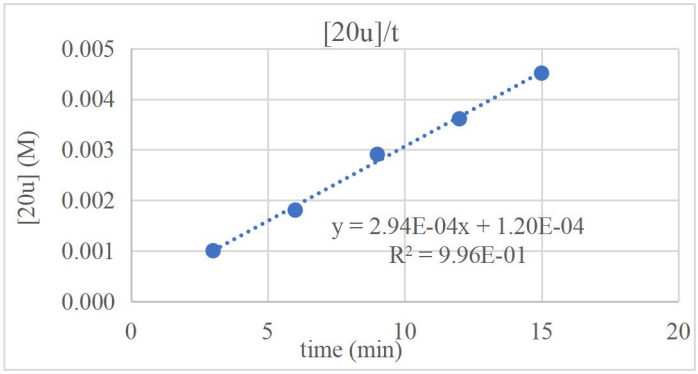


Table S5.4 Initial rate vs *c*(**6g**) (0.0475 M)

c(**6g**) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0475	4.1	3	0.001589	0.000343
		6	0.003085	
		9	0.004020	
		12	0.004955	
		15	0.005797	

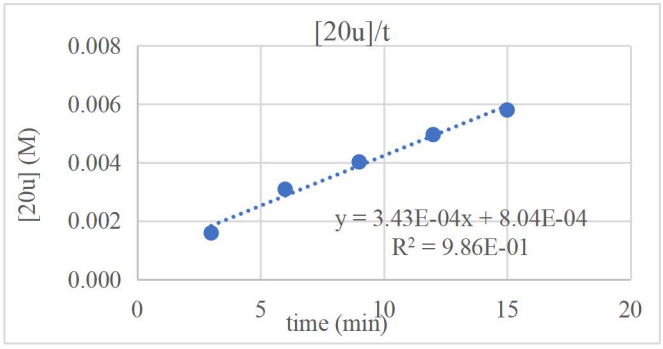


Table S5.5 Initial rate vs *c*(**6g**) (0.0532 M)

c(**6g**) (M)	Internal standard (mg)	Time (min)	*c*(**20u**) (M)	Initial rate (M/min)
0.0532	4.5	3	0.001026	0.000380
		6	0.002052	
		9	0.003386	
		12	0.004618	
		15	0.005439	

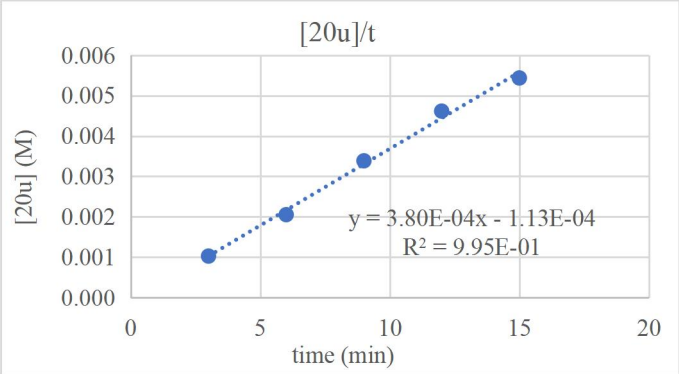
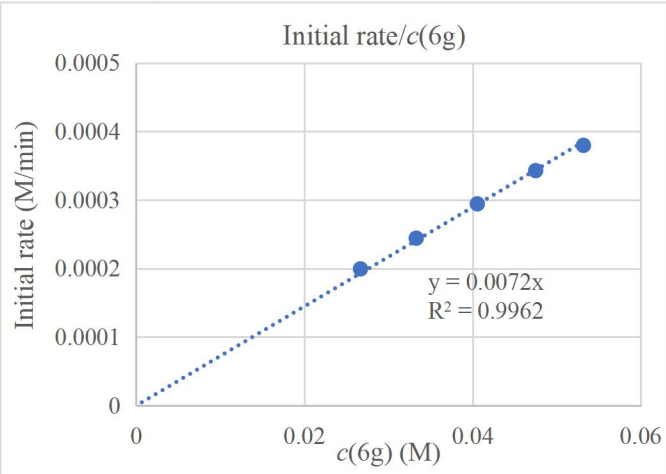
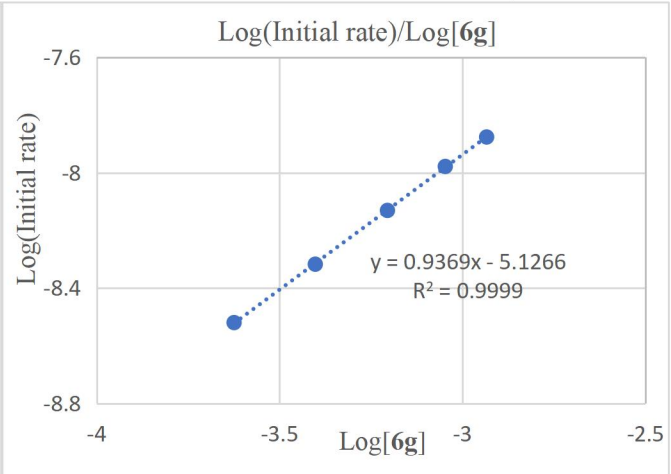


Table S5.6 Kinetic order for *c*(**6g**) of hydrogenolysis reaction

c(**6g**) (M)	Initial rate (M/min)	Log[**6g**]	Log(Initial rate)
0.0267	0.000199	-3.6243	-8.5199
0.0333	0.000244	-3.4024	-8.3174
0.0406	0.000294	-3.2052	-8.1308
0.0475	0.000343	-3.0471	-7.9783
0.0532	0.000380	-2.9342	-7.8762





6.5.5 Initial rate *vs* *c*(Y[N(TMS)$_2$]$_3$) of C–C bond cleavage reaction

In a glovebox, substrate **6g** (42.2 mg, 0.10 mmol), 1-fluoronapthalene (internal standard) and 3.0 mL toluene-d_8 were added to a Schlenk tube with Teflon valve and a magnetic stir bar. The Schlenk tube was sealed and heated at 50 °C in a pre-heated metal block until substrate **6g** was completely dissolved. Then, 1.0 mL of toluene-d_8 solution of **Y-1** (0.0023 M (2.3 mol%), 0.0034 M (3.4 mol%), 0.0042 M (4.2 mol%), 0.0056 M (5.6 mol%)) was injected to the Schlenk tube. About 0.4 mL of the reaction mixture was taken out according to the interval time shown in **Table S6.1-6.4** and injected into a NMR tube filled with 2-(naphthalen-1-yl)acetic acid. The insulting mixture was then analyzed by ^{19}F NMR to determine the yield of 4-fluorochalcone. Half-order rate dependence on *c*(Y[N(TMS)$_2$]$_3$) was observed.

Table S6.1 Initial rate vs $c(Y[N(TMS)_2]_3)$ (0.00057 M)

$c(Y[N(TMS)_2]_3)$ (M)	Internal standard (mg)	Time (min)	c(4-fluorochalcone) (M)	Initial rate (M/min)
0.00057	4.0	3	0.001095	0.000195
		5	0.001505	
		7	0.001916	
		9	0.002258	
		11	0.002668	

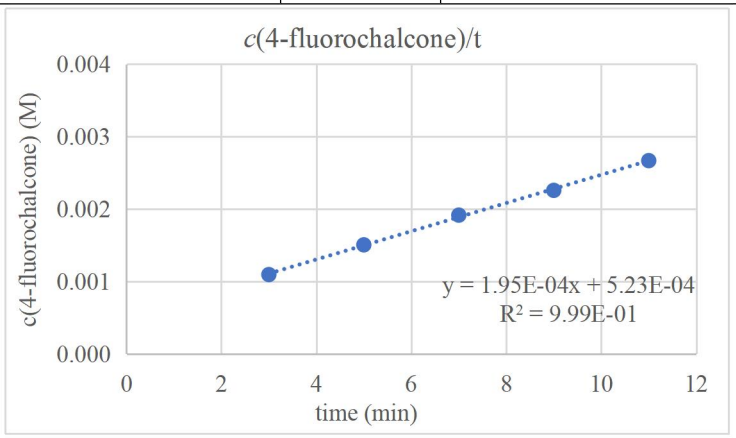


Table S6.2 Initial rate vs $c(Y[N(TMS)_2]_3)$ (0.00086 M)

$c(Y[N(TMS)_2]_3)$ (M)	Internal standard (mg)	Time (min)	c(4-fluorochalcone) (M)	Initial rate (M/min)
0.00086	4.0	2	0.000821	0.000250
		4	0.001573	
		6	0.001916	
		8	0.002463	
		10	0.002873	

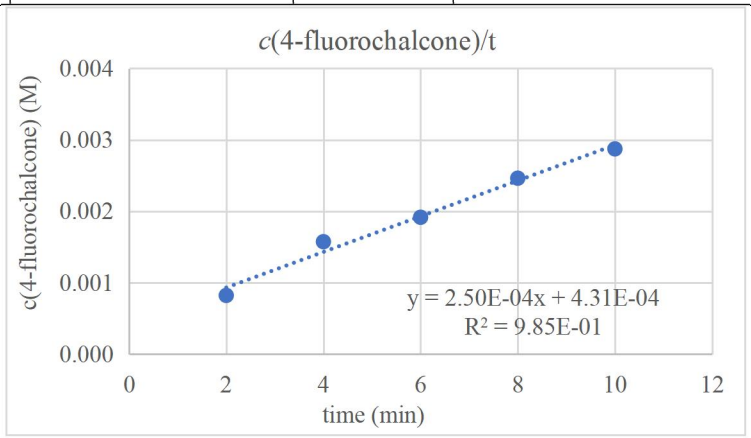


Table S6.3 Initial rate vs $c(Y[N(TMS)_2]_3)$ (0.00105 M)

$c(Y[N(TMS)_2]_3)$ (M)	Internal standard (mg)	Time (min)	c(4-fluorochalcone) (M)	Initial rate (M/min)
0.00105	4.4	2	0.000903	0.000275
		4	0.001656	
		6	0.002182	
		8	0.002634	
		10	0.003161	

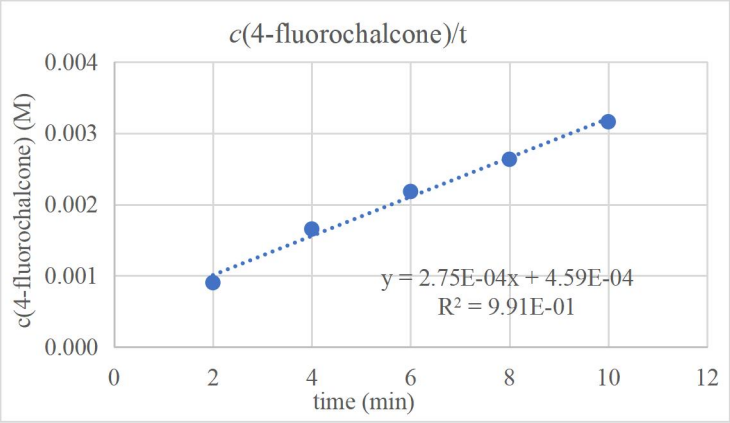


Table S6.4 Initial rate vs $c(Y[N(TMS)_2]_3)$ (0.00140 M)

$c(Y[N(TMS)_2]_3)$ (M)	Internal standard (mg)	Time (min)	c(4-fluorochalcone) (M)	Initial rate (M/min)
0.00140	4.6	2	0.001337	0.000330
		4	0.002045	
		6	0.002832	
		7.5	0.003226	
		9	0.003619	

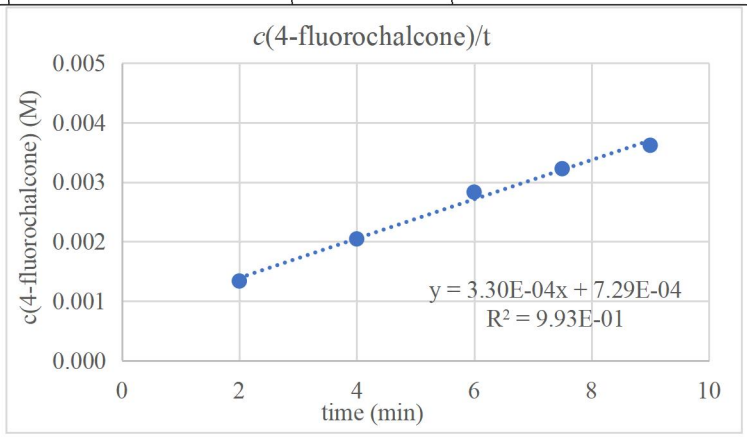
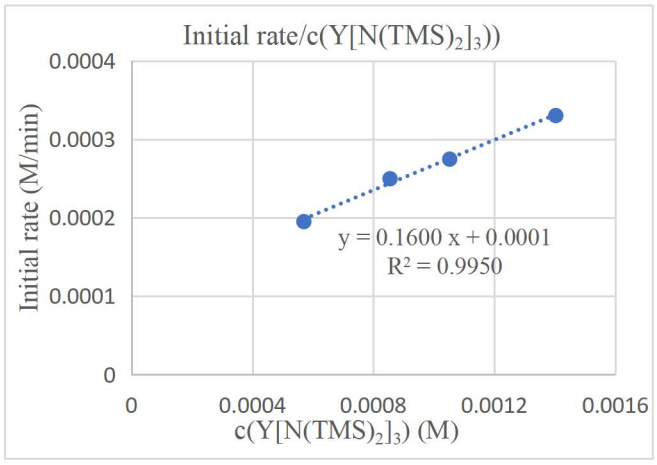
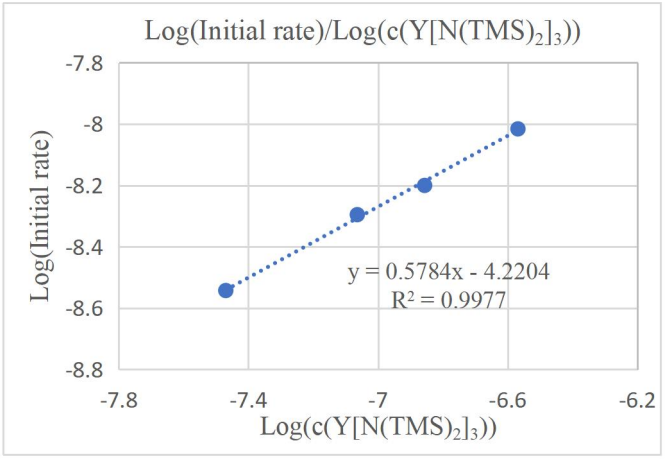


Table S6.5 Kinetic order for $c(Y[N(TMS)_2]_3)$ of C–C bond cleavage reaction

$c(Y[N(TMS)_2]_3)$ (M)	Initial rate (M/min)	Log($c(Y[N(TMS)_2]_3)$)	Log(Initial rate)
0.00057	0.000195	-8.24	-9.32
0.00086	0.000250	-7.47	-8.54
0.00105	0.000275	-7.06	-8.30
0.00140	0.000330	-6.86	-8.20





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 Mo*K*α radiation, ϕ-ω scan technique, λ = 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).

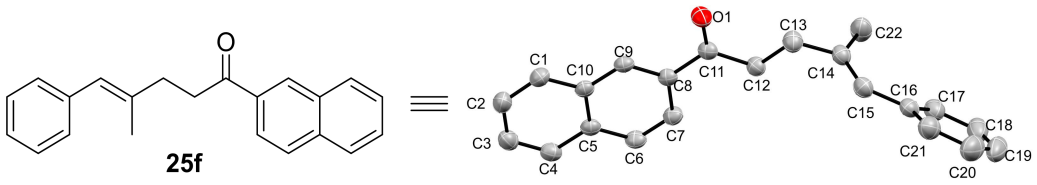


Figure S24. Molecular structure of compound 25f (Thermal ellipsoids at 30% level; all the hydrogen atoms are omitted for clarity). Selected bond lengths (Å) and bond angles (deg): C11–O1 1.220(1), C8–C11 1.494(2), C11–C12 1.507(2), C12–C13 1.514(2), C13–C14 1.509(2), C14–C15 1.327(2), C14–C22 1.496(2), C15–C16 1.468(2); C11–C12–C13 113.0(1), O1–C11–C12 120.5(1), O1–C11–C8 120.2(1).

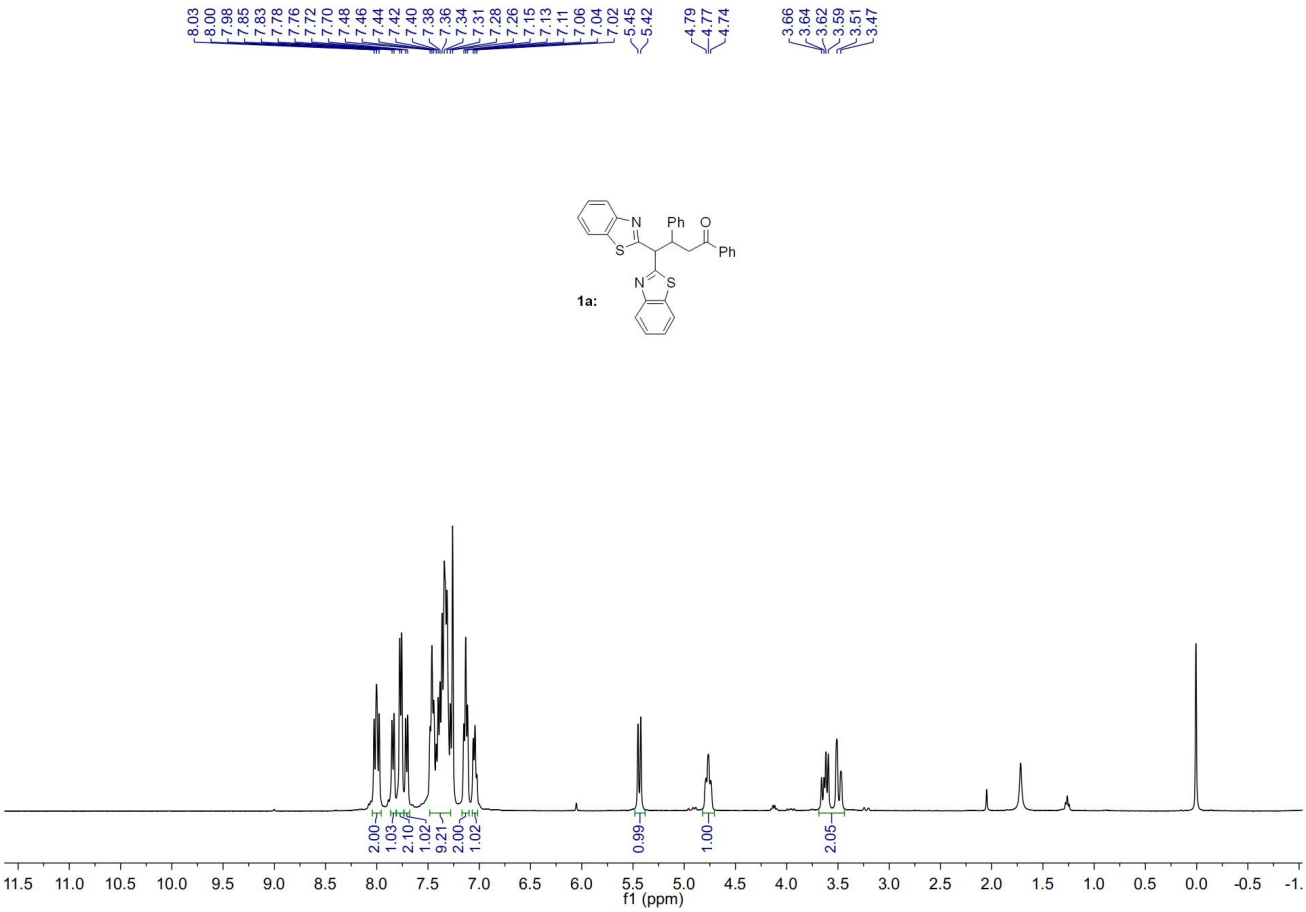
Table S6. Crystal and Data Collection Parameters of Complexes Y-2, Y-3, Y-4, 25f and 32.

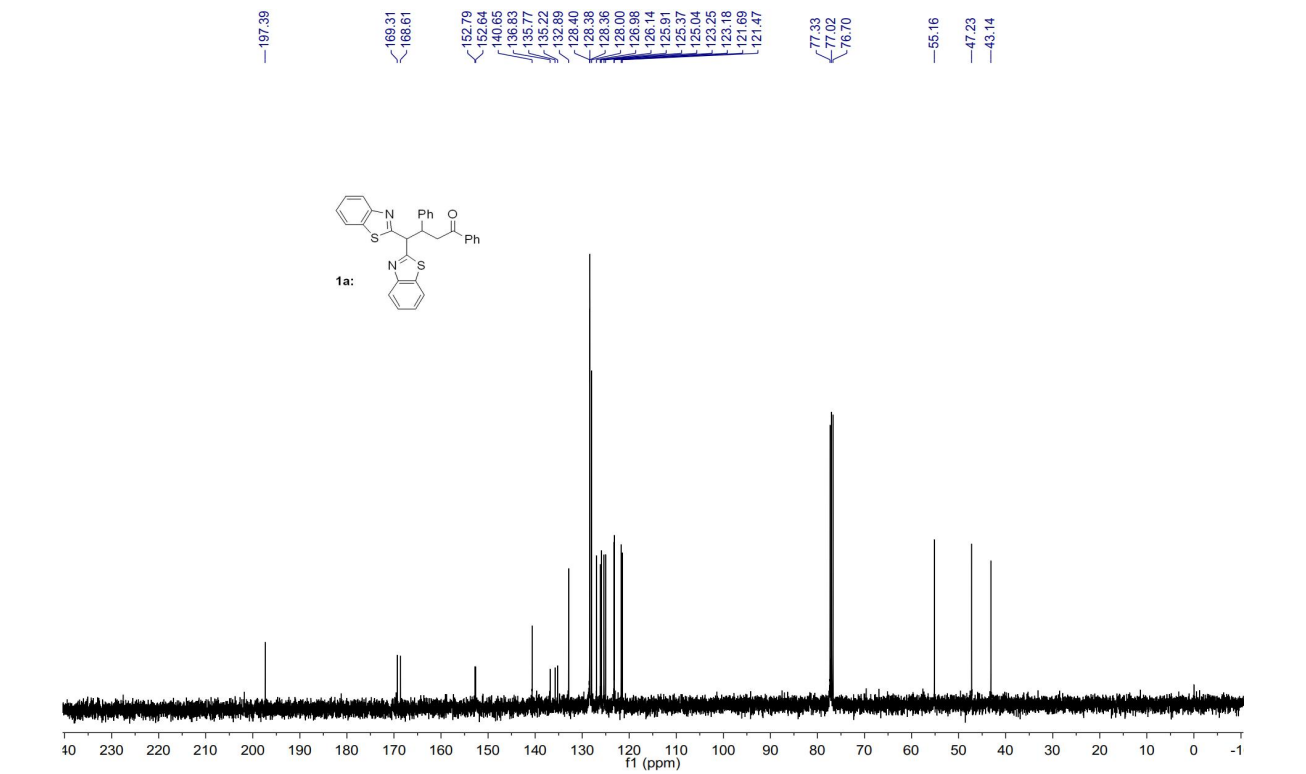
	Y-2	Y-3	Y-4	25f	32
Empirical formula	$C_{71}H_{112}N_2O_{19}Si_4Y_2$	$C_{90}H_{90}O_{10}Y_2$	$C_{42}H_{42}Cl_2LiN_4O_3S_4Y$	$C_{22}H_{20}O$	$C_{26}H_{22}O_2$
Molecular weight	1587.80	1509.43	945.78	300.38	366.43
Temperature (K)	173(2)	173(2)	173(2)	302(2)	173
Wavelength (Å)	1.34138	1.34138	1.34138	1.34138	1.34138
Crystal system	Triclinic	Monoclinic	Triclinic	Orthorhombic	monoclinic
Space group	*P*-1	$P2_1/n$	*P*-1	*P*bca	$P2_1/c$
a (Å)	13.5161(9)	12.360(10)	10.4735(14)	10.7579(7)	14.5793(5)
b (Å)	19.1767(13)	15.060(3)	11.7513(16)	8.3156(5)	8.3322(3)
c (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
V (Å^3)	4832.0(6)	4361(4)	2121.5(5)	3318.3(4)	1884.62(12)
Z	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}
F(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 *h*, *k*, *l*	$-16 \le h \le 16$ $-22 \le k \le 22$ $-23 \le l \le 23$	$-16 \le h \le 13$ $-19 \le k \le 15$ $-25 \le l \le 30$	$-12 \le h \le 12$ $-13 \le k \le 12$ $-23 \le l \le 23$	$-9 \le h \le 12$ $-9 \le k \le 9$ $-44 \le l \le 37$	$-18 \le h \le 17$ $-10 \le k \le 10$ $-19 \le l \le 19$
Reflections collected	54331	36513	25750	15401	22426
Independent reflections	16984[R_{int} = 0.0532]	9873[R_{int} = 0.1385]	7447[R_{int} = 0.0422]	2910[R_{int} = 0.0243]	4057[R_{int} = 0.0594, R_{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. transmision	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 F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	16984/0/907	9873/87/461	7447/0/514	2910/0/209	4057/0/253
Goodness-of-fit on F^2	1.030	0.957	1.134	0.990	1.045
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0424 wR_2 = 0.1149	R_1 = 0.0814 wR_2 = 0.1935	R_1 = 0.0284 wR_2 = 0.0826	R_1 = 0.0349 wR_2 = 0.0921	R_1 = 0.0438 wR_2 = 0.1108
R indices (all data)	R_1 = 0.0518 wR_2 = 0.1219	R_1 = 0.1377 wR_2 = 0.2247	R_1 = 0.0339 wR_2 = 0.0943	R_1 = 0.0383 wR_2 = 0.0959	R_1 = 0.0504 wR_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

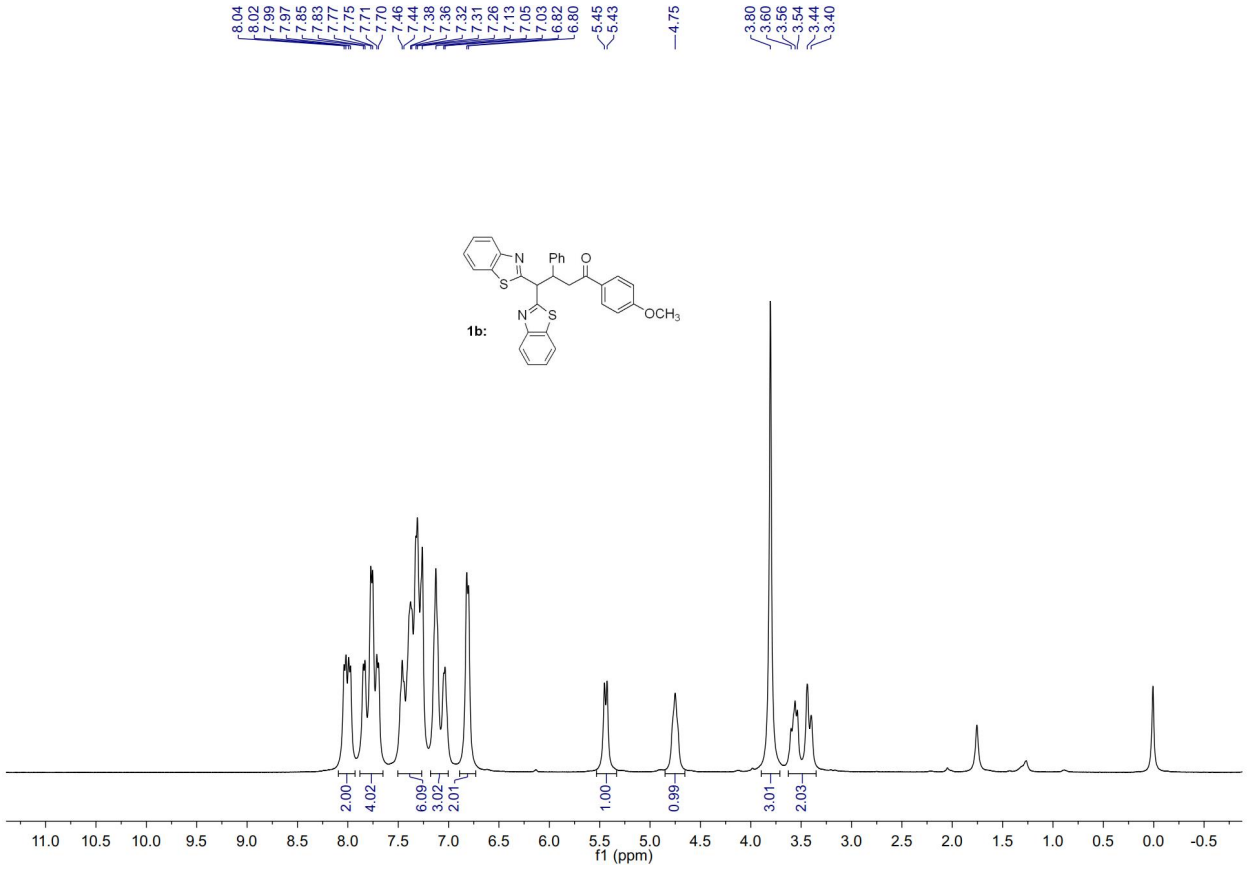
8. References

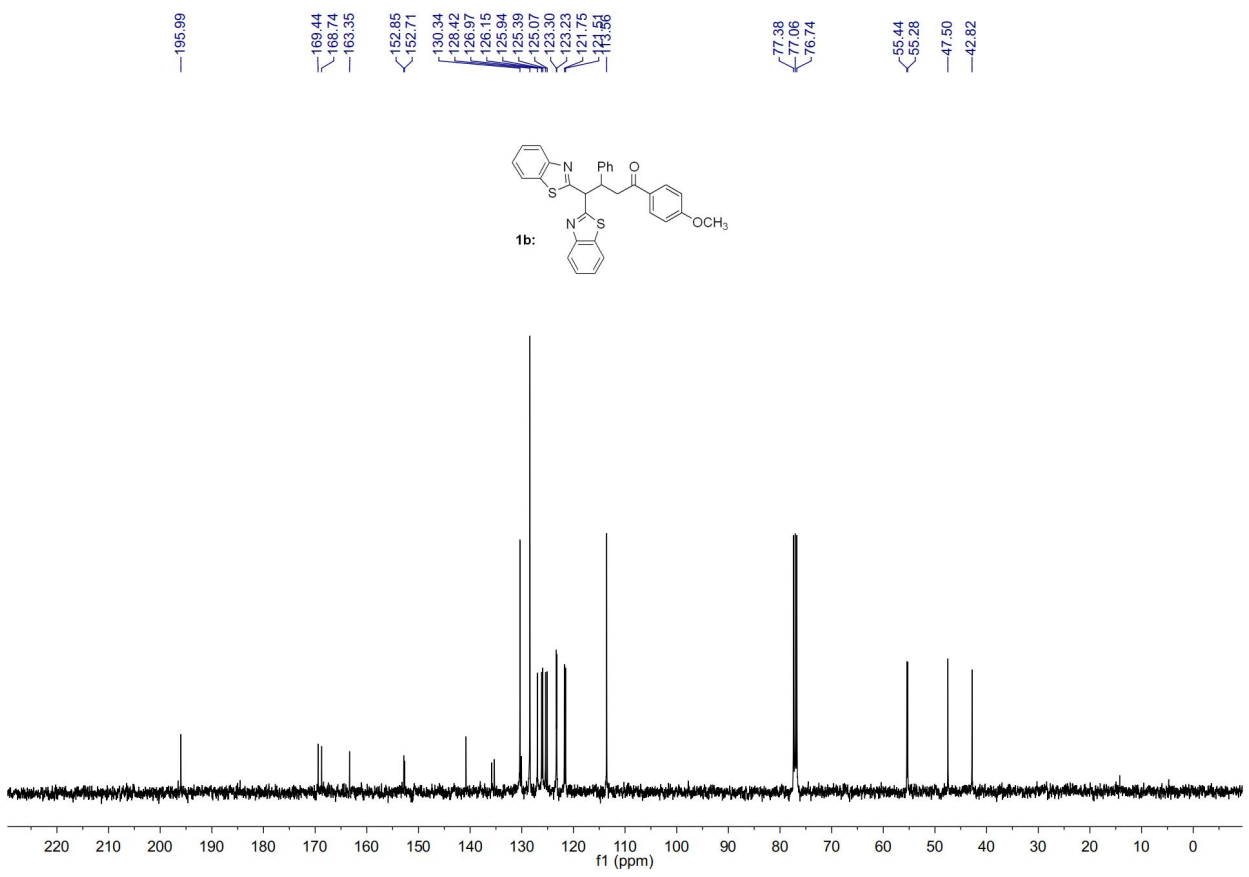
1. J. H. Golden, J. W. Facendola, S. M. R. Daniel, C. Q. Baez, P. I. Djurovich and M. E. Thompson, *J. Org. Chem.*, 2017, **82**, 7215–7222.
2. X. Peng, Y. liu, Q. Shen, D. Chen, X. Chen, Y. Fu, J. Wang, X. Zhang, H. Jiang and J. Li. *J. Org. Chem.,* 2022, 87, 18, 11958–11967
3. T. Matsuyama, T.i Yatabe, T. Yabe and Kazuya Yamaguchi, *ACS Catal.,* 2022, **12**, 13600–13608.
4. Y. Grell, N. Demirel, K. Harms and E. Meggers, *Organometallics,* 2019, **38**, 3852–3859.
5. E. Kianmehr, N. Faghih and K. M. Khan, *Org. Lett.*, 2015, **17**, 414–417.
6. S. Mao, Y. -R. Gao, X, -Q. Zhu, D. -D. Guo and Y. -Q. Wang, *Org. Lett.,* 2015*,* **17**, 1692–1695.
7. L. Shen, X. Han, B. Dong, Y. Yang, J. Yang and F. Li, *ACS Appl. Polym. Mater.*, 2022, **4**, 7408–7416.
8. Y. Zhu, B. Zhao and Y. Shi, *Org. Lett.,* 2013, **15**, 992–995.
9. C. Volpe, S. Meninno, A. Roselli, M. Mancinelli, A. Mazzanti and A. Lattanzi, *Adv. Synth. Catal.,* 2020, **362**, 5457–5466.
10. M. F. Vansco, B. Marchetti, N. Trongsiriwat, T. Bhagde, G. Wang, P. J. Walsh, S. J. Klipppenstein and M. I. Lester, *J. Am. Chem. Soc.,* 2019, **141**, 15058–15069.
11. B. Ding, Z. Zhang, Y. Liu, M. Sugiya, T. Imamoto and W. Zhang, *Org. Lett.,* 2013, **15**, 3690–3693.
12. X. -N. Cao, X. -M. Wan, F. -L. Yang, K. Li, X. -Q. Hao, T. J. Shao, X. Zhu and M. -P. Song, *J. Org. Chem.,* 2018, **83**, 3657–3668.
13. H. -C. Li, C. An, G. Wu, G. -X. Li, X. -B. Huang, W. -X. Gao, J. -C. Ding, Y. -B. Zhou, M. -C. Liu and H. -Y. Wu, *Org. Lett.,* 2018, **20**, 5573–5577.
14. Z. Luo, X. Zhang, Z. -Q. Liu, C. -M. Hong, Q. -H. Li and T. -L. Liu, *Org. Lett.,* 2022, 24, 8072–8076.
15. S. Usugi, T. Tsuritani, H. Yorimitsu, H. Shinokubo and K. Oshima. *B. Chem. Soc. Jpn.,* 2002, **75**, 841–845.
16. T. Ramar, M. A. M. Subbaiah and A. Ilangovan, *J. Org. Chem.,* 2020, **85**, 7711–7727.
17. C. W. Downey, S. E. Covington, D. C.Obenschain, E. Halliday, J. T. Rague. D. N. Confair, *Tetrahedron Lett.,* 2014, **55**, 5213–5215.
18. M. Lee, H. Jung, D. Kim,J. -W. Park and S. Chang., *J. Am. Chem. Soc.,* 2020, **142**, 11999–12004.
19. M. C. Belhomme, D. Wang and K. J. Szabo, *Org. Lett.,* 2016, **18**, 2503–2506.
20. H. T. Chang, T. T. Jayanth, C. C. Wang and C.-H. Cheng, *J. Am. Chem. Soc.,* 2007, **129**, 12032–12041.
21. S. Chanthamath, S. Takaki, K. Shibatomi and S. Iwasa, *Angew. Chem. Int. Ed.,* 2013, **52**, 5818–5821.
22. Z. Li, L. He, R. Fu, G. Song, W. Song, D. Xie, J. Yang, Tetrahedron, 2016, 72, 4321–4328.
23. N. S. W. Jonasson and J. L. Daumann, *Chem. Eur. J.*, 2019, **25**, 12091–12097.
24. A. Maji, S. Rana, Akanksha and D. Maiti, *Angew. Chem., Int. Ed.*, 2014, **53**, 2428–2432.
25. B. -Q. Hu, L. -X. Wang, G. Shen, Y. -L. Tang and L. Yang, *RSC Adv.*, 2015, **5**, 100097–100101.
26. C. W. D'Acunto, R. Kaplánek, H. Gbelcová, Z. Kejík, T. Bříza, L. Vasina, M. Havlík, T. Ruml and V. Král, *Eur. J.Med. Chem.*, 2018, **150**, 140–155.
27. J. W. Labadie and J. K. Stille, *J. Am. Chem. Soc.*, 1983, *105*, 6129–6137.
28. H. -X. Zheng, Z. -F. Xiao, C. -Z. Yao, Q. -Q. Li, X. -S. Ning, Y. -B. Kang and Y. Tang, *Org. Lett.*, 2015, **17**, 6102–6105.

9. Copies of ^{1}H and ^{13}C NMR Spectra

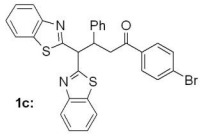


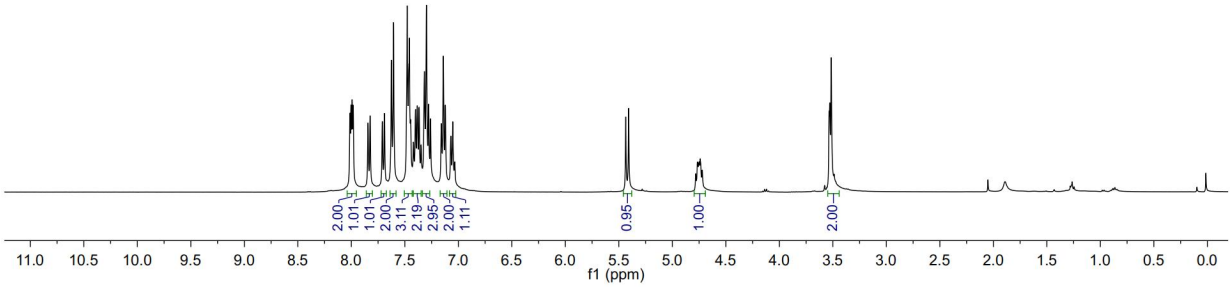



8.04
8.02
7.99
7.97
7.85
7.83
7.77
7.75
7.71
7.70
7.46
7.44
7.38
7.36
7.32
7.31
7.26
7.13
7.05
7.03
6.82
6.80
5.45
5.43
4.75
3.80
3.60
3.56
3.54
3.44
3.40
Ph
O
N
S
OCH3
1b:
2.00
4.02
6.09
3.02
2.01
1.00
0.99
3.01
2.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

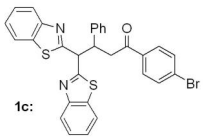

195.99
169.44
168.74
163.35
152.85
152.71
130.34
128.42
126.97
126.15
125.94
125.39
125.07
123.30
123.23
121.75
77.38
77.06
76.74
55.44
55.28
47.50
42.82
Ph
O
N
S
OCH3
1b:
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

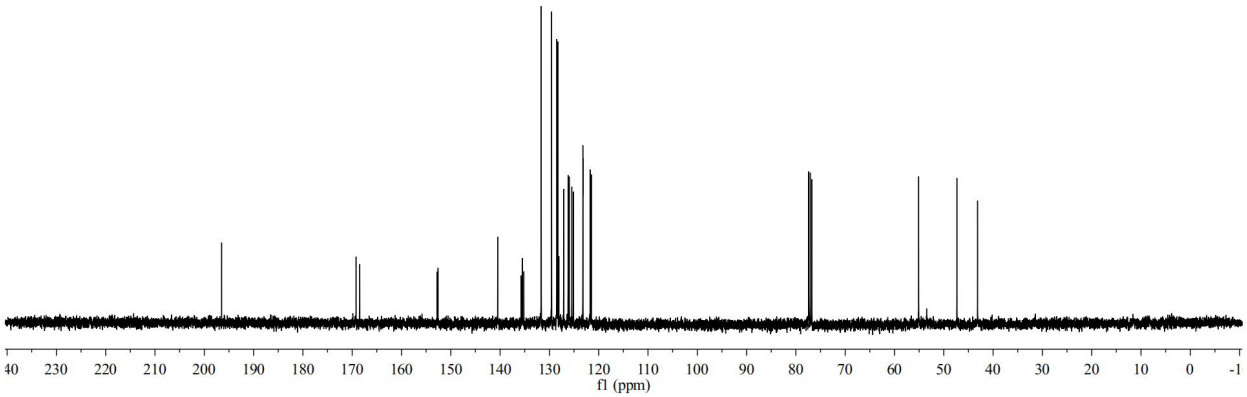

8.01
8.00
7.99
7.98
7.84
7.82
7.71
7.69
7.63
7.60
7.48
7.46
7.46
7.45
7.42
7.40
7.38
7.37
7.35
7.32
7.30
7.28
7.26
7.16
7.14
7.12
7.07
7.05
7.03
5.44
5.41
4.78
4.77
4.76
4.75
4.75
4.74
4.72
3.53
3.53
3.52

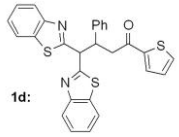

N
Ph
O
S
Br
N
S
1c:

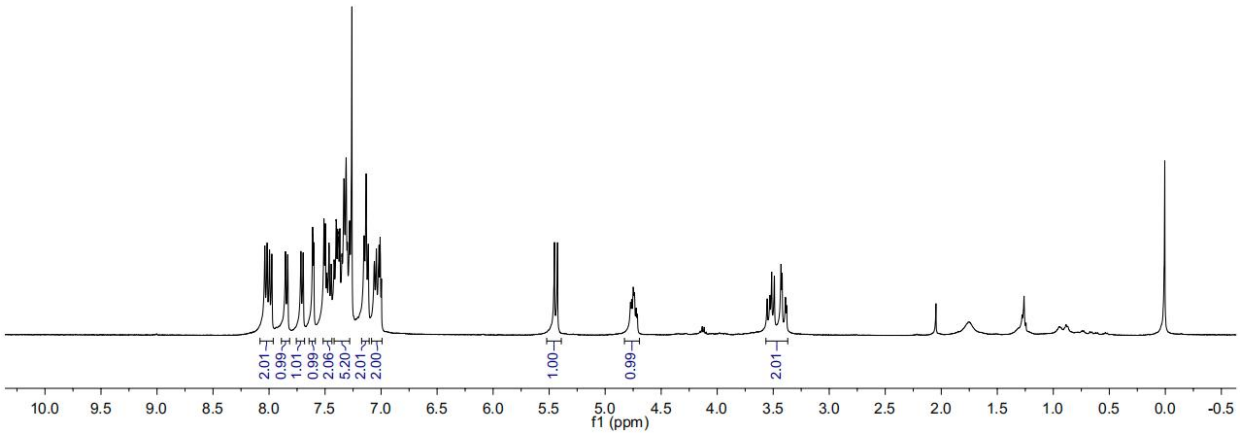

2.00
1.01
1.01
2.00
3.11
2.19
2.95
2.00
1.11
0.95
1.00
2.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

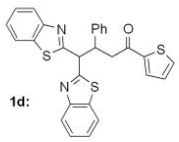

196.51
169.24
168.48
152.78
152.60
140.51
135.75
135.48
135.19
131.67
129.56
128.50
128.31
128.09
127.12
126.21
125.98
125.46
125.12
123.22
123.20
121.73
121.51
77.42
77.10
76.78
55.10
47.34
43.15

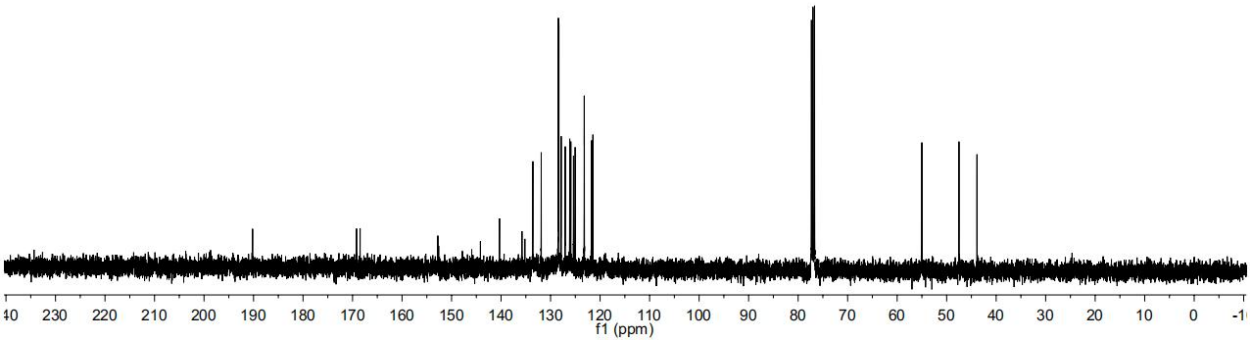

N
Ph
O
S
Br
N
S
1c:

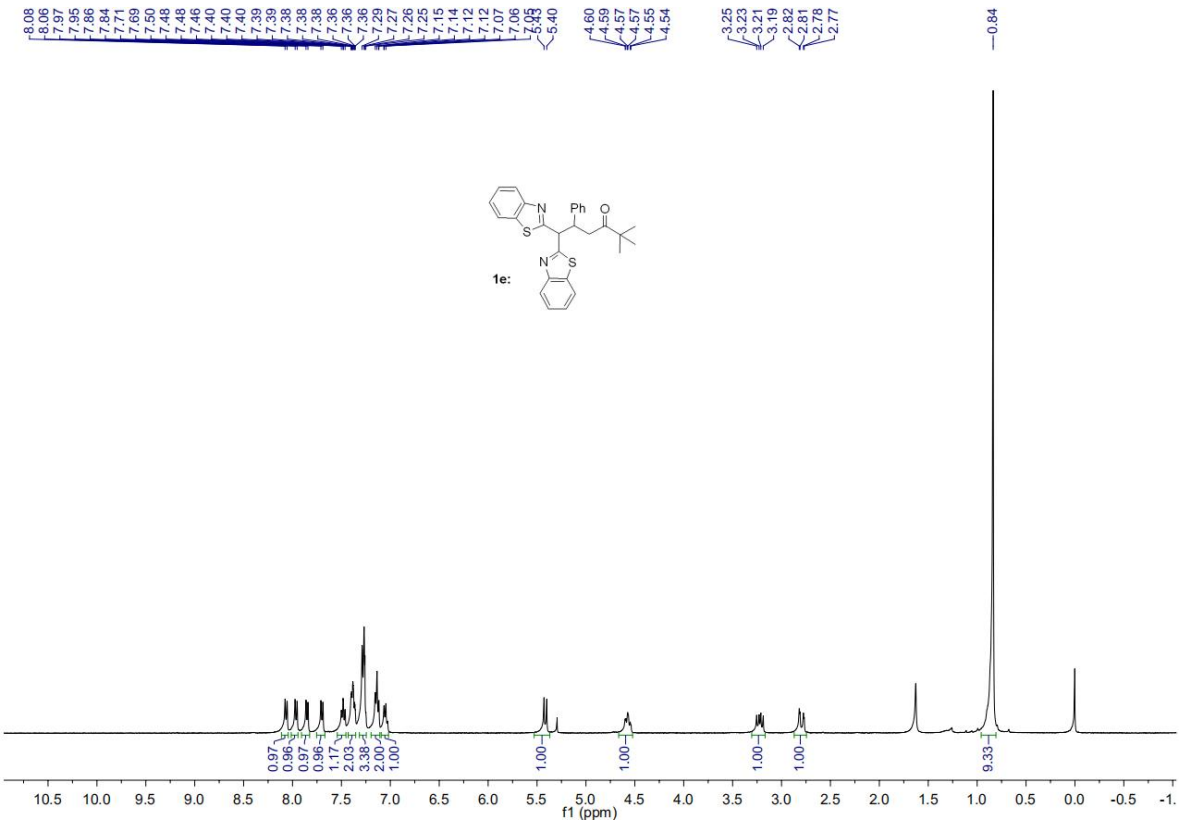

40
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

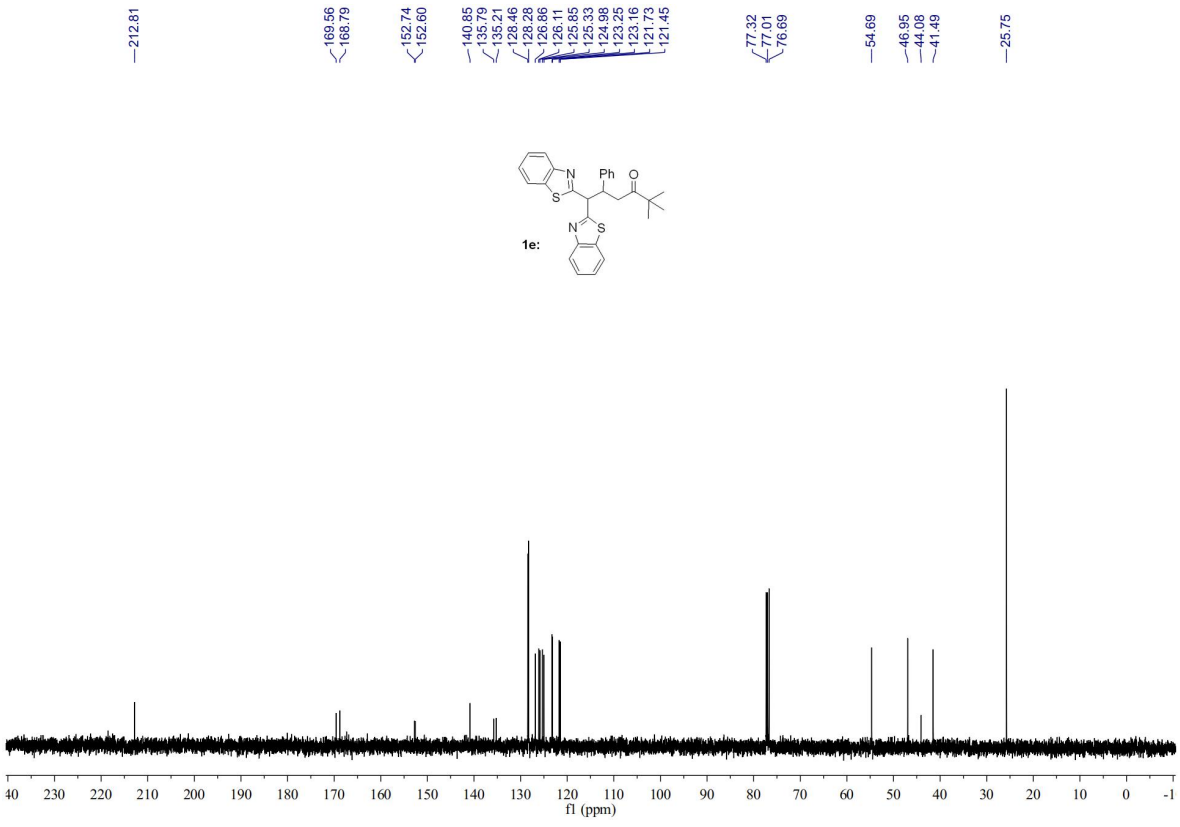

Ph
O
N
S
S
N
S
1d:


2.01
0.99
1.01
0.99
2.06
5.20
2.01
2.00
1.00
0.99
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

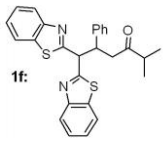

Ph
O
N
S
S
N
S
1d:

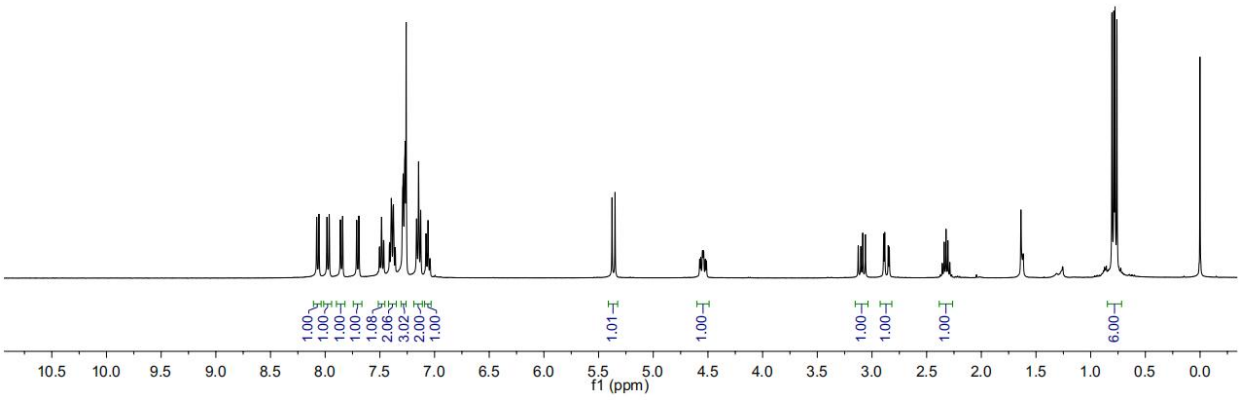

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


1e:
f1 (ppm)

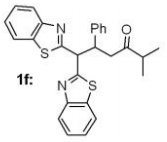

1e:
f1 (ppm)

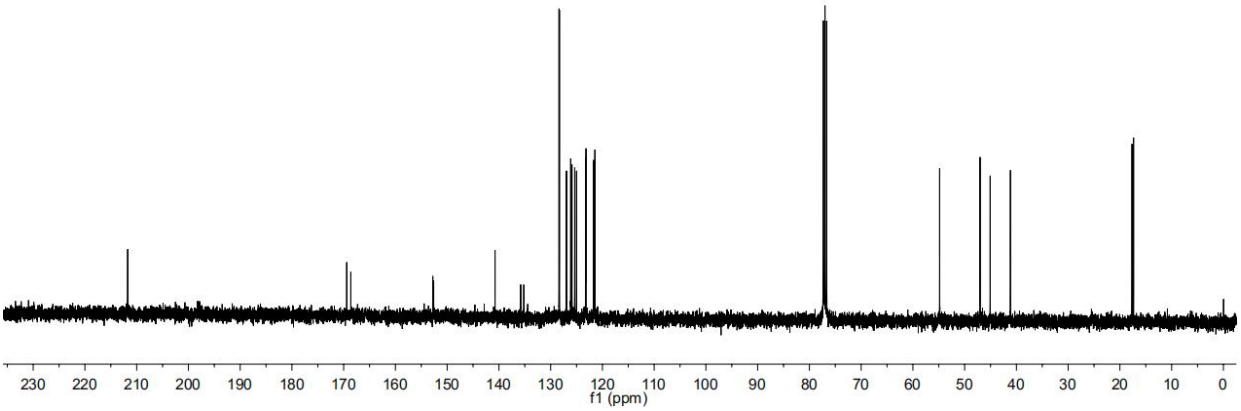

8.08
8.06
7.98
7.96
7.86
7.84
7.71
7.69
7.50
7.50
7.48
7.47
7.46
7.41
7.40
7.38
7.36
7.36
7.29
7.27
7.26
7.16
7.15
7.13
7.08
7.06
7.04
5.38
5.35
4.58
4.57
4.55
4.54
4.52
4.51
3.13
3.10
3.08
3.06
2.89
2.88
2.85
2.84
2.37
2.36
2.34
2.32
2.31
2.29
2.27
0.81
0.79
0.78
0.76

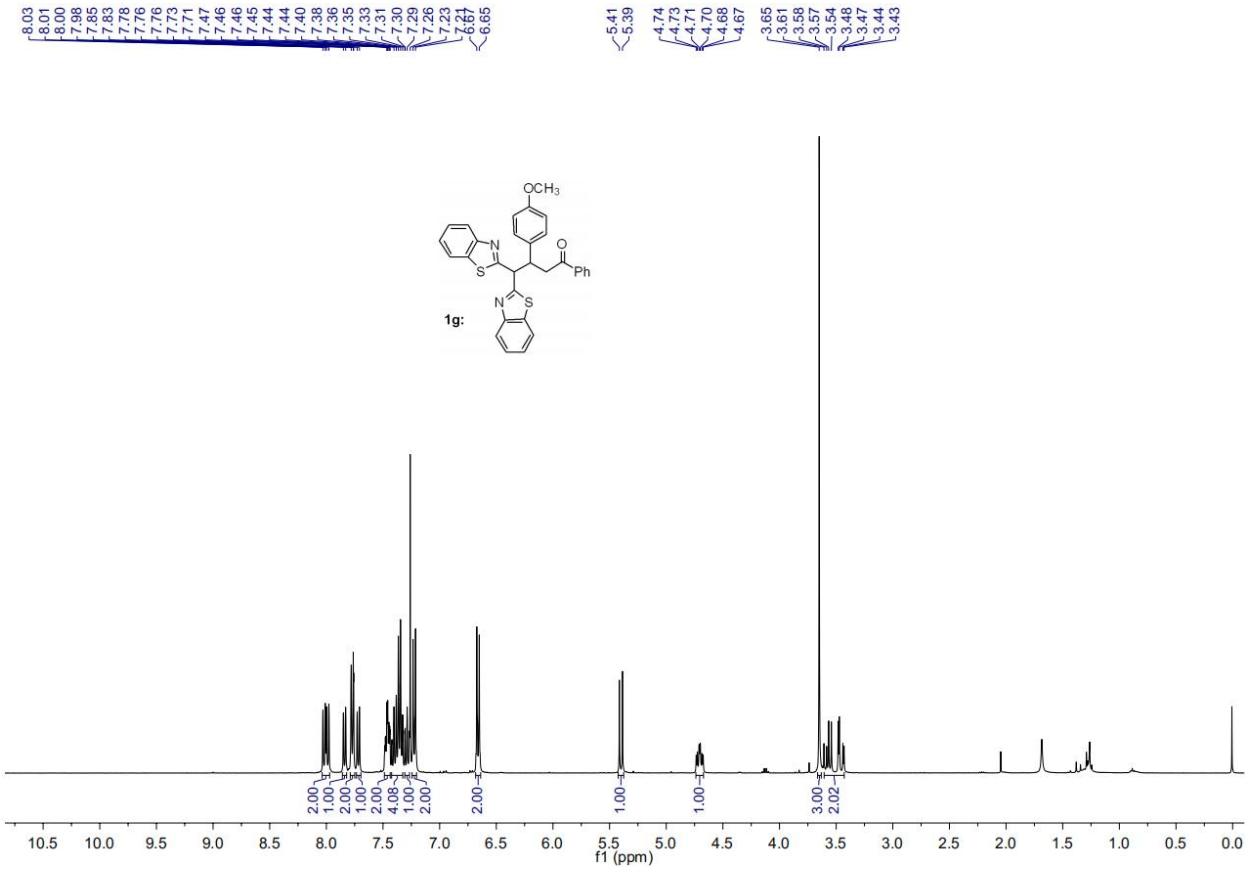

Ph
O
N
S
1f:
N
S

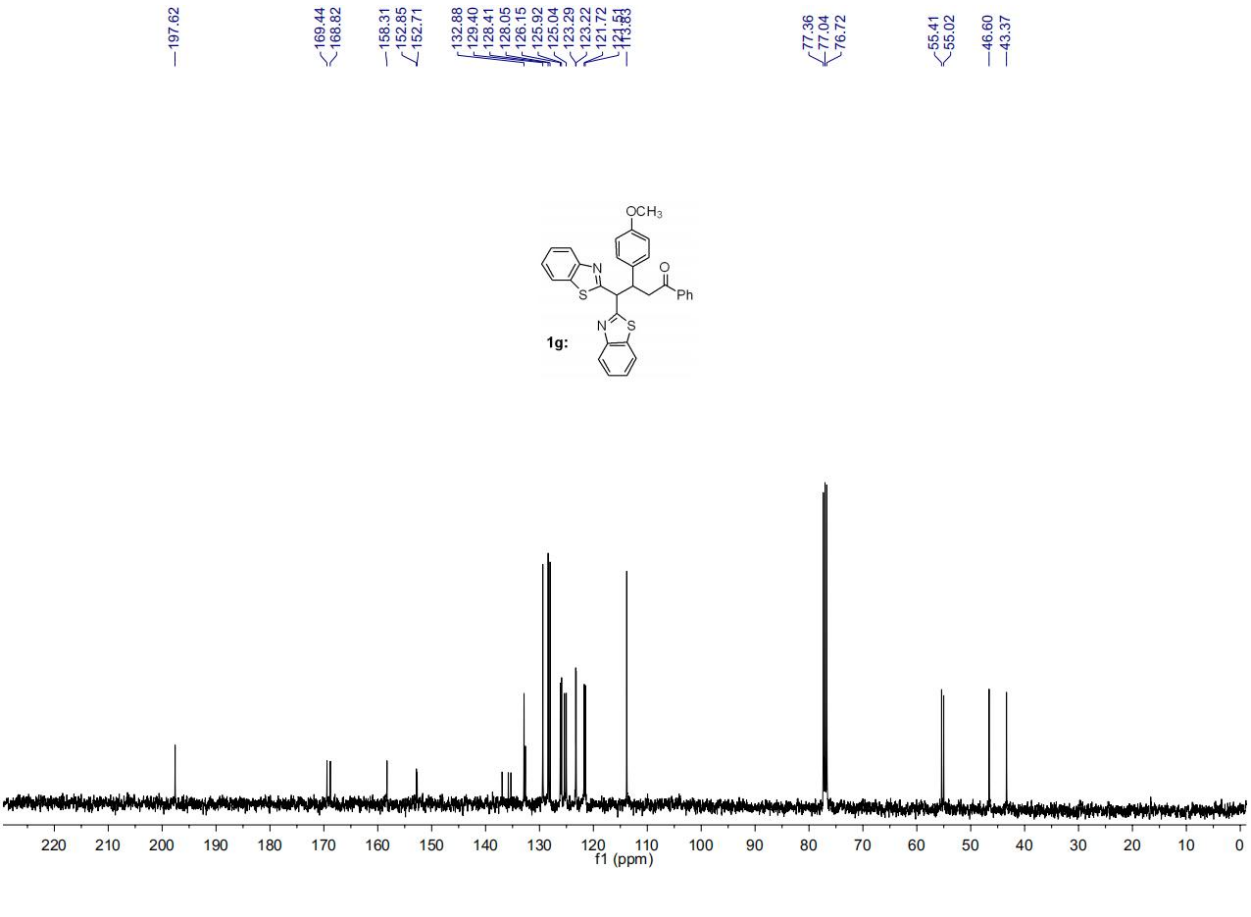

1.00
1.00
1.00
1.00
1.08
2.06
3.02
2.00
1.00
1.01
1.00
1.00
1.00
1.00
6.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


211.74
169.41
168.62
152.77
152.61
140.75
135.80
135.19
128.39
128.30
126.95
126.13
125.88
125.35
125.01
123.22
123.17
121.72
121.45
77.31
76.99
76.67
54.84
47.02
45.07
41.16
17.66
17.36

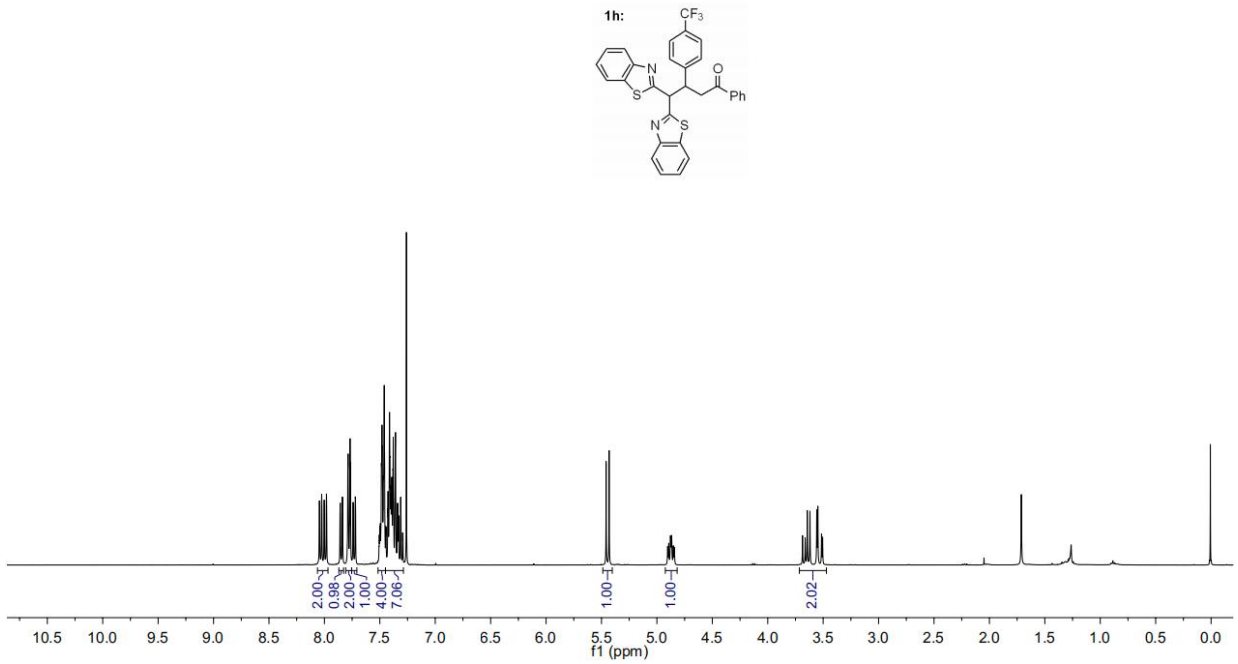

Ph
O
N
S
1f:
N
S


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

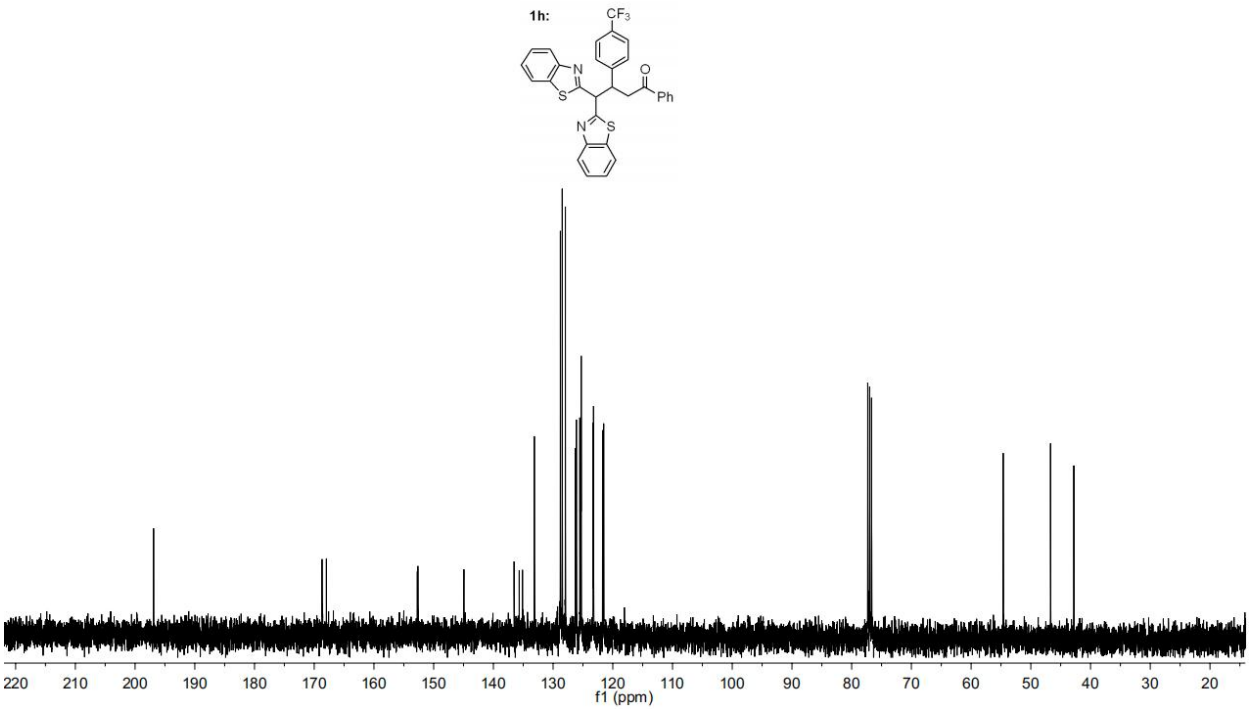

8.03
8.01
8.00
7.98
7.85
7.83
7.78
7.76
7.76
7.73
7.71
7.47
7.46
7.46
7.45
7.44
7.44
7.40
7.38
7.36
7.35
7.33
7.31
7.30
7.29
7.26
7.23
6.67
6.65
5.41
5.39
4.74
4.73
4.71
4.70
4.68
4.67
3.65
3.61
3.58
3.57
3.54
3.48
3.47
3.44
3.43
OCH3
N
S
O
Ph
N
S
1g:
2.00
1.00
2.00
1.00
2.00
4.08
1.00
2.00
2.00
1.00
1.00
3.00
2.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

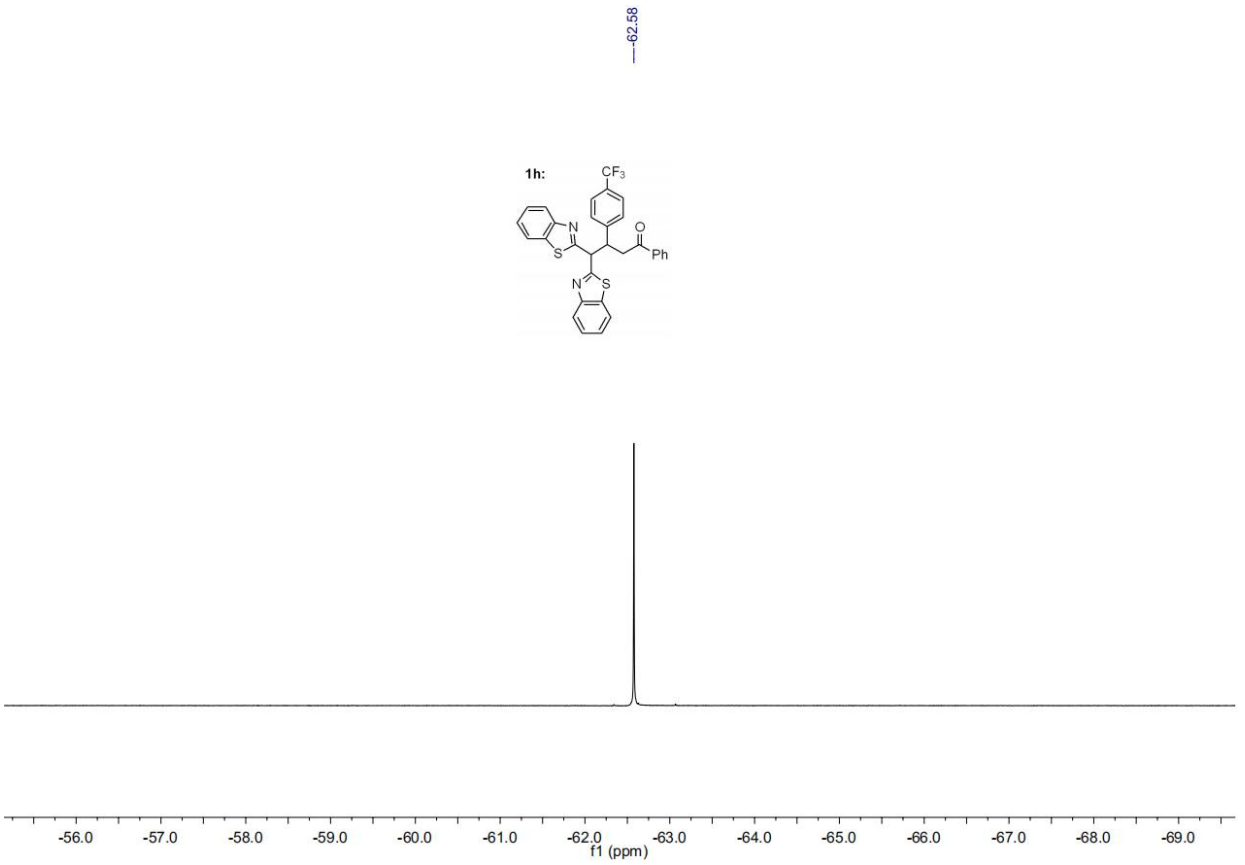

197.62
169.44
168.82
158.31
152.85
152.71
132.88
129.40
128.41
128.05
126.15
125.92
125.04
123.29
123.22
121.72
121.51
113.83
77.36
77.04
76.72
55.41
55.02
46.60
43.37
OCH3
N
S
O
Ph
N
S
1g:
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.04
8.02
8.00
7.98
7.86
7.86
7.84
7.84
7.79
7.77
7.76
7.74
7.74
7.72
7.72
7.49
7.48
7.48
7.47
7.47
7.46
7.43
7.43
7.41
7.41
7.41
7.40
7.40
7.39
7.38
7.38
7.36
7.34
7.31
7.31
5.46
5.43
4.90
4.89
4.88
4.87
4.85
4.84
3.69
3.66
3.64
3.62
3.56
3.55
3.51
3.51

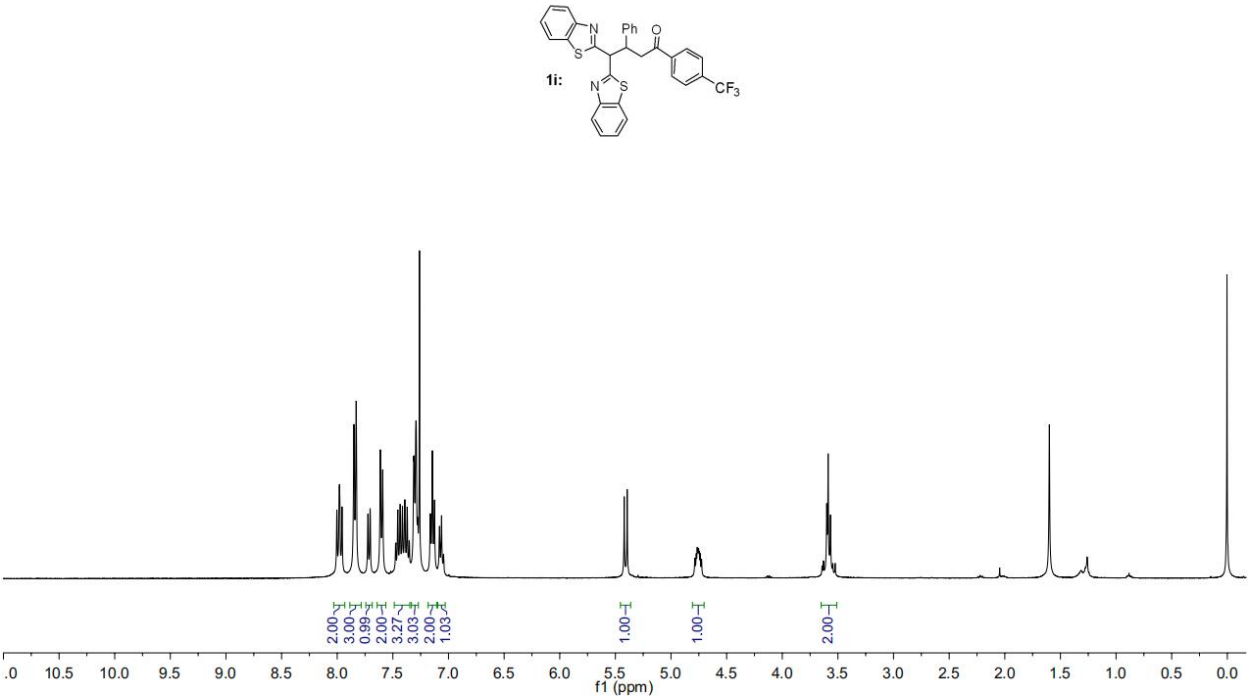

1h:
CF3
N
S
O
Ph
N
S
2.00
0.98
2.00
1.00
4.00
7.06
1.00
1.00
2.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

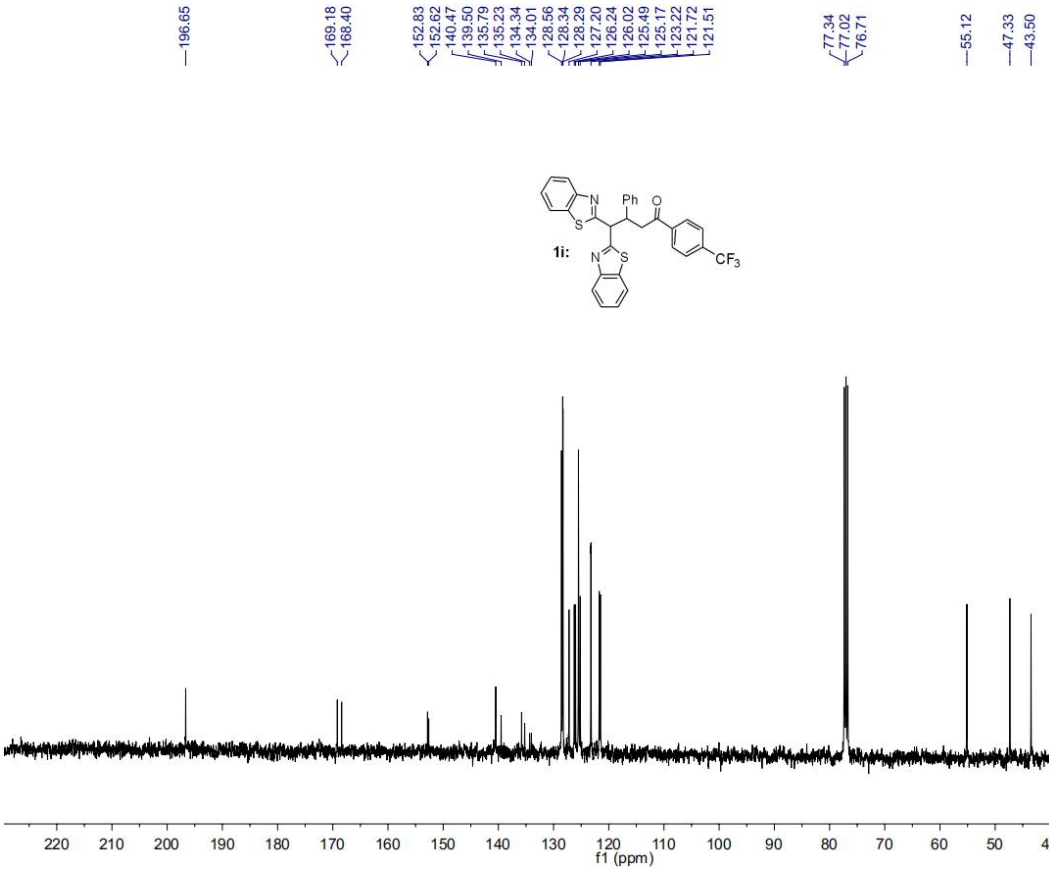

196.92
168.71
167.98
152.75
152.65
144.95
136.54
135.69
135.14
133.15
129.24
128.92
128.80
128.48
127.96
126.27
126.11
125.54
125.38
125.34
125.30
123.33
123.25
121.73
121.54
77.32
77.00
76.69
54.63
46.71
42.80

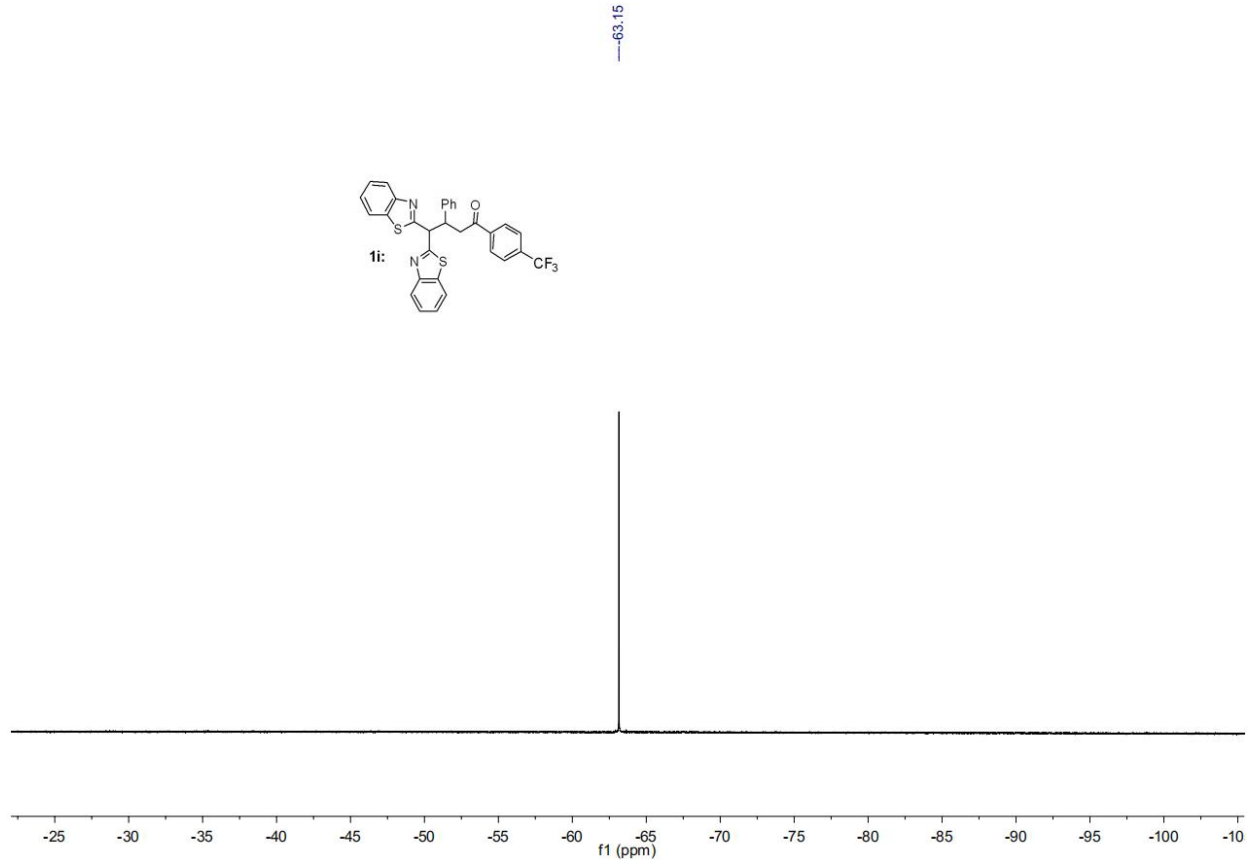

1h:
CF3
N
S
O
Ph
N
S
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)


-62.58
1h:
CF3
N
S
O
Ph
N
S
-56.0
-57.0
-58.0
-59.0
-60.0
-61.0
-62.0
-63.0
-64.0
-65.0
-66.0
-67.0
-68.0
-69.0
f1 (ppm)

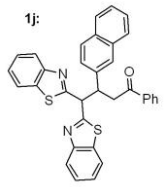

8.00
7.98
7.96
7.85
7.83
7.72
7.70
7.61
7.59
7.48
7.47
7.46
7.43
7.41
7.39
7.37
7.35
7.31
7.31
7.29
7.28
7.26
7.16
7.14
7.13
7.08
7.06
7.04
5.42
5.39
4.79
4.77
4.76
4.76
4.75
4.74
4.73
3.64
3.63
3.60
3.59
3.57
3.55
3.52

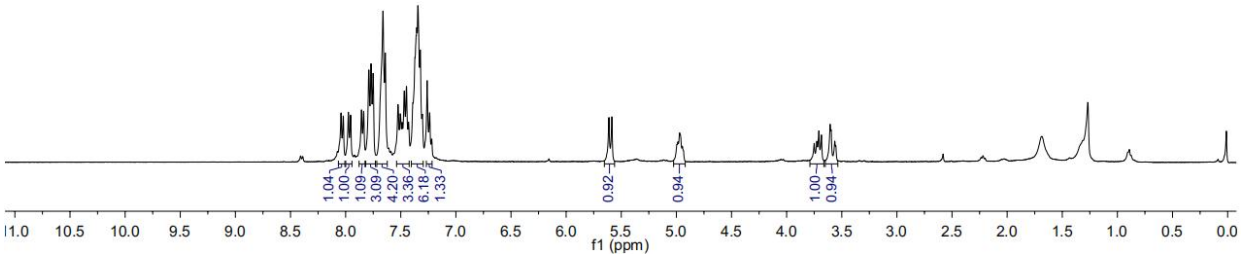

1i:
N
S
Ph
O
N
S
CF3
2.00
3.00
0.99
2.00
3.27
3.03
2.00
1.03
1.00
1.00
2.00
.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


196.65
169.18
168.40
152.83
152.62
140.47
139.50
135.79
135.23
134.34
134.01
128.56
128.34
128.29
127.20
126.24
126.02
125.49
125.17
123.22
121.72
121.51
77.34
77.02
76.71
55.12
47.33
43.50
1i:
Ph
O
N
S
CF3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

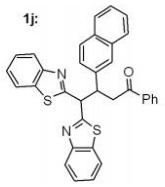

-63.15
1i:
Ph
O
N
S
CF3
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-10
f1 (ppm)


8.04
8.02
7.97
7.95
7.86
7.84
7.79
7.77
7.75
7.66
7.64
7.53
7.50
7.49
7.47
7.45
7.43
7.39
7.37
7.36
7.35
7.34
7.32
7.30
7.26
7.24
7.22
5.61
5.58
5.00
4.99
4.97
4.96
4.95
4.94
3.75
3.73
3.71
3.68
3.61
3.60
3.56
3.55


1j:
N
S
O
Ph
N
S

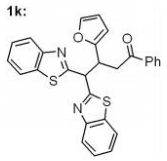

1.04
1.00
1.09
3.09
4.20
3.36
6.18
1.33
0.92
0.94
1.00
0.94
f1 (ppm)

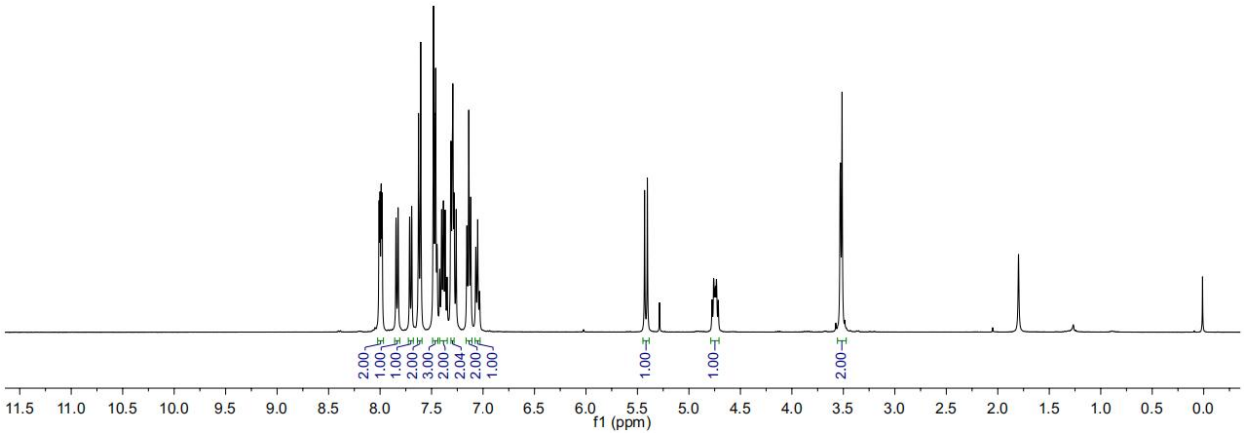

197.38
169.40
168.60
152.83
152.75
138.36
133.29
132.96
132.49
128.43
128.21
128.06
127.91
127.61
127.52
126.38
126.21
125.97
125.85
125.66
125.45
125.10
123.35
123.24
121.77
121.53
77.38
77.06
76.74
55.13
47.19
43.43


1j:
N
S
O
Ph
N
S

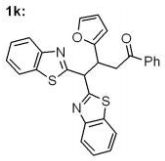
f1 (ppm)

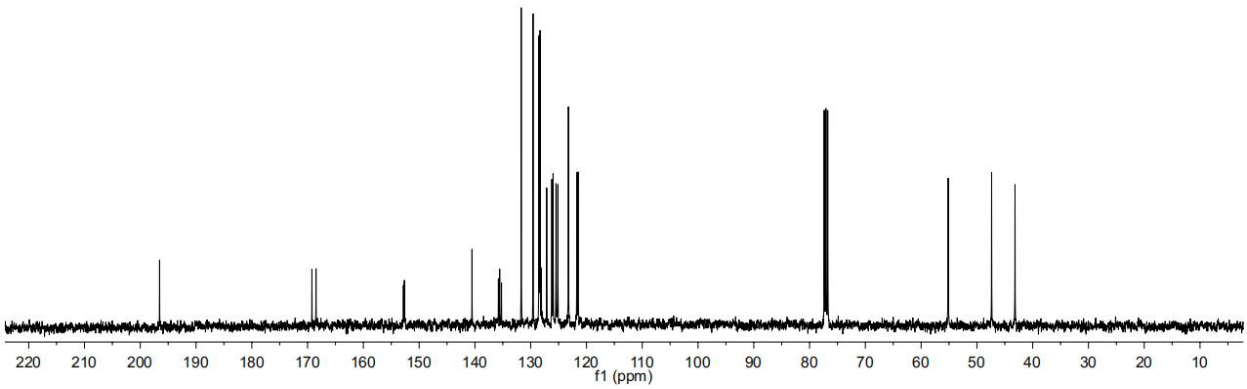

8.01
8.00
7.99
7.98
7.84
7.82
7.71
7.69
7.63
7.60
7.48
7.46
7.46
7.45
7.42
7.40
7.39
7.37
7.35
7.31
7.29
7.28
7.26
7.16
7.14
7.12
7.07
7.05
7.03
5.43
5.40
4.78
4.76
4.75
4.74
4.73
4.72
3.53
3.53
3.51


1k:
Ph

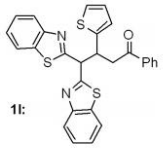

2.00
1.00
1.00
2.00
3.00
2.00
2.04
2.00
1.00
1.00
1.00
2.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


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
77.38
77.06
76.74
55.14
47.36
43.17

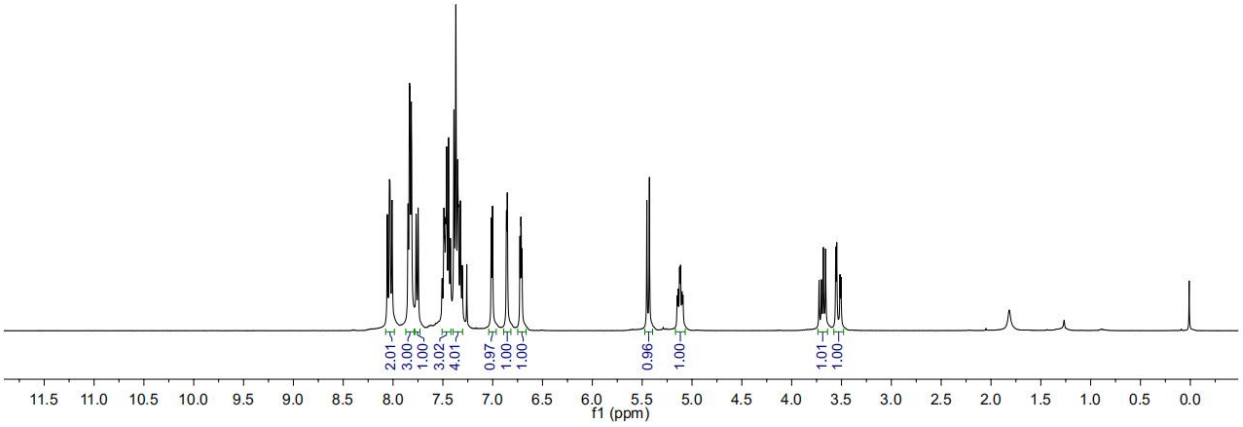

1k:
Ph


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

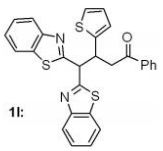

8.06
8.04
8.03
8.01
7.85
7.83
7.83
7.82
7.77
7.75
7.51
7.49
7.48
7.48
7.47
7.46
7.44
7.42
7.39
7.37
7.35
7.34
7.32
7.31
7.26
7.01
7.00
6.86
6.85
6.73
6.72
6.71
6.71
5.45
5.43
5.15
5.14
5.12
5.11
5.10
5.09
3.73
3.70
3.68
3.66
3.56
3.55
3.51
3.51


S
N
S
O
Ph
N
S

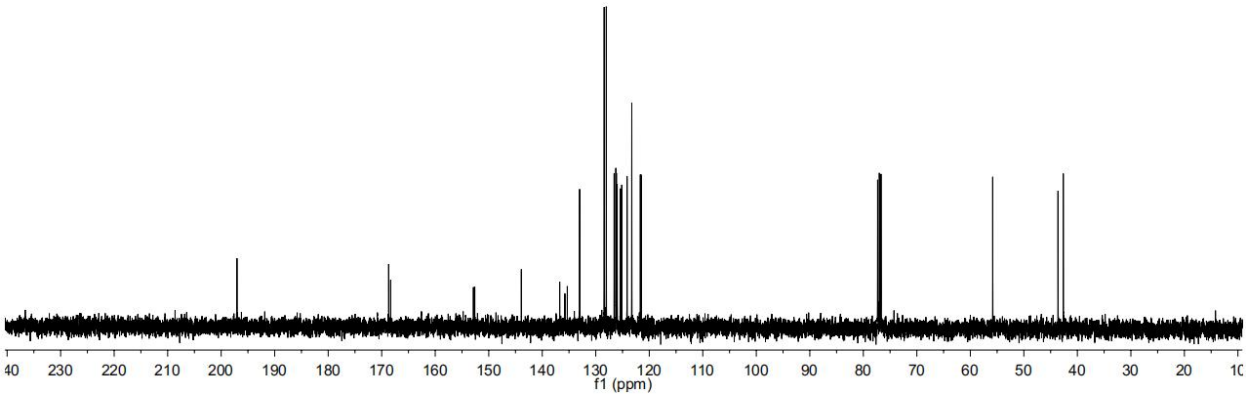
1l:

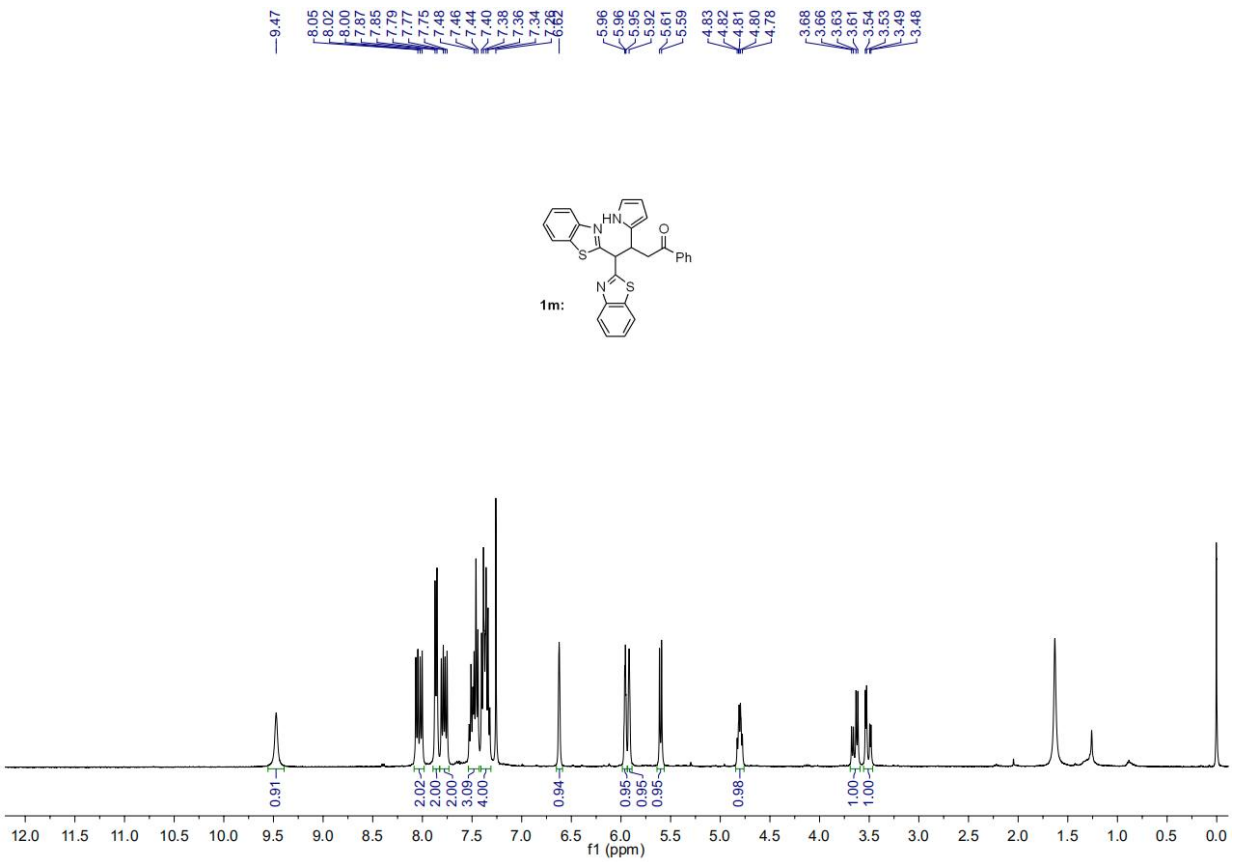

2.01
3.00
1.00
3.02
4.01
0.97
1.00
1.00
0.96
1.00
1.01
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

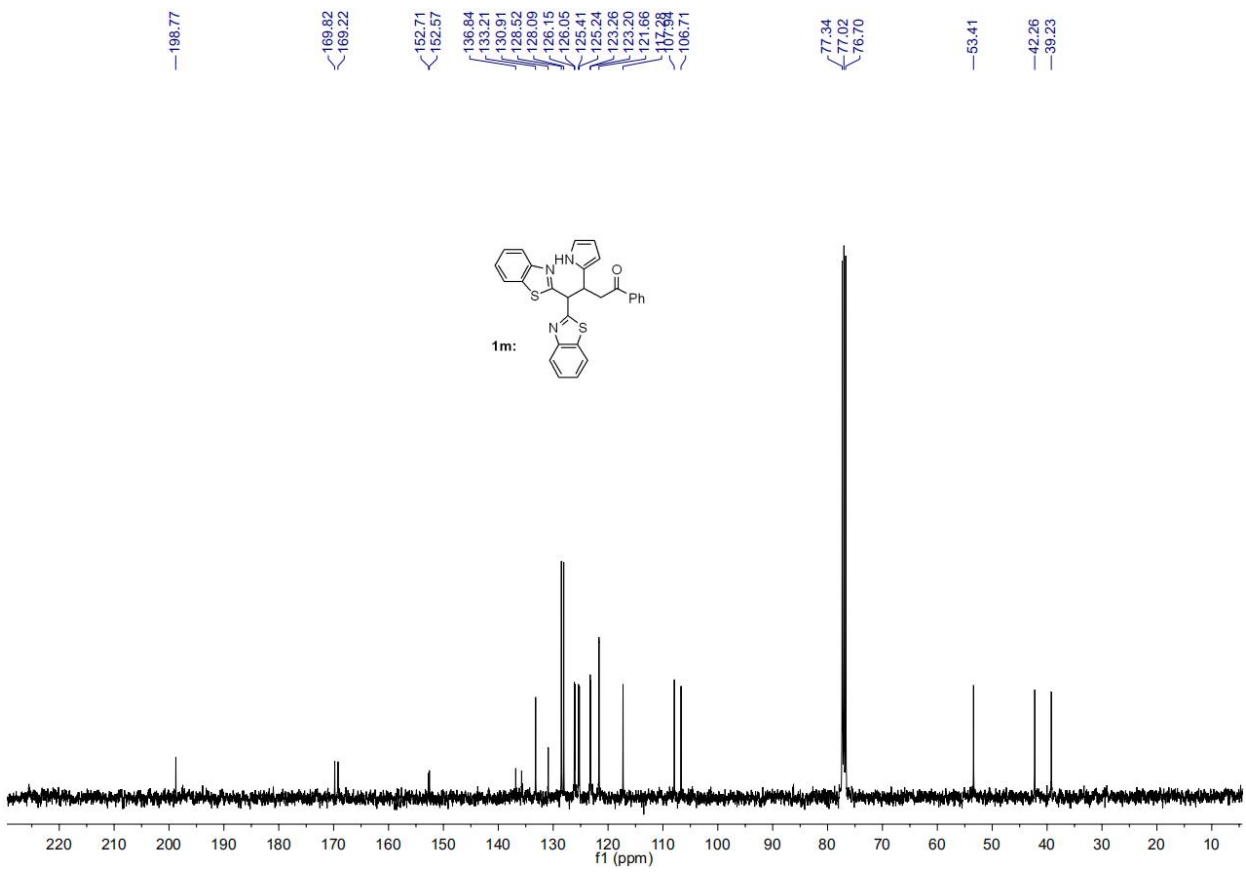

197.07
168.72
168.35
152.88
152.63
143.93
136.75
135.78
135.33
133.03
128.44
128.05
126.58
126.26
126.15
126.01
125.42
125.16
124.16
123.28
121.69
121.52
77.34
77.02
76.70
55.83
43.63
42.64

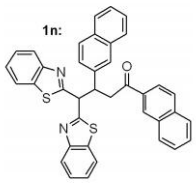

S
N
S
O
Ph
N
S

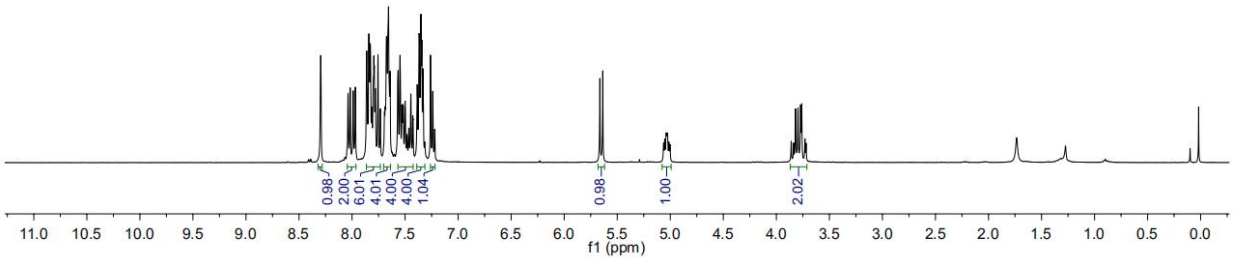
1l:

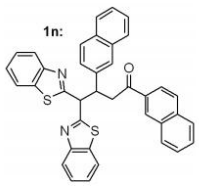

40 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

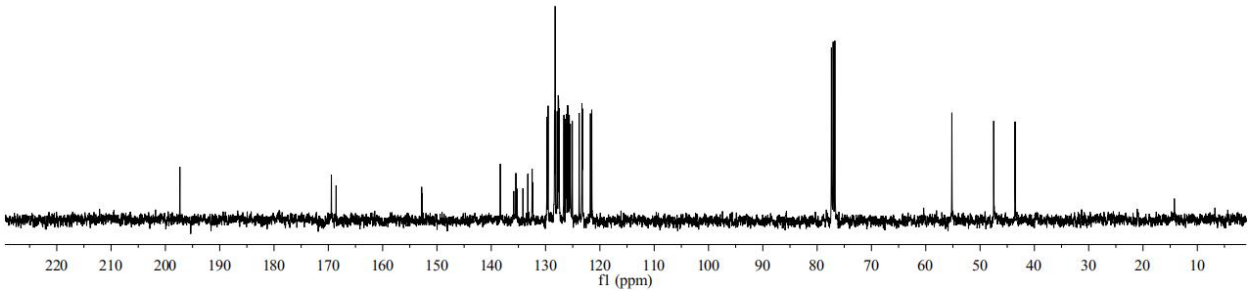

9.47
8.05
8.02
8.00
7.87
7.85
7.79
7.77
7.75
7.48
7.46
7.44
7.40
7.38
7.36
7.34
6.62
5.96
5.96
5.95
5.92
5.61
5.59
4.83
4.82
4.81
4.80
4.78
3.68
3.66
3.63
3.61
3.54
3.53
3.49
3.48
1m:
0.91
2.02
2.00
2.00
3.09
4.00
0.94
0.95
0.95
0.95
0.98
1.00
1.00
f1 (ppm)


198.77
169.82
169.22
152.71
152.57
136.84
133.21
130.91
128.52
128.09
126.15
126.05
125.41
125.24
123.26
123.20
121.66
107.94
106.71
77.34
77.02
76.70
53.41
42.26
39.23
1m:
f1 (ppm)

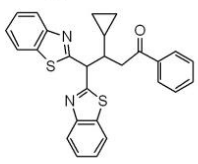

1n:

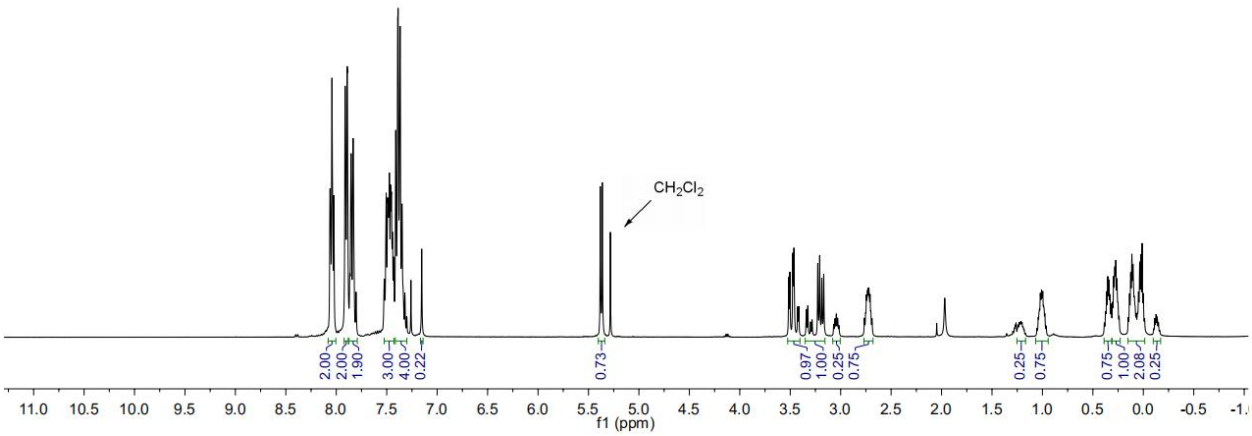

0.98
2.00
6.01
4.01
4.00
4.00
1.04
0.98
1.00
2.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


1n:

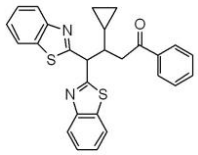

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

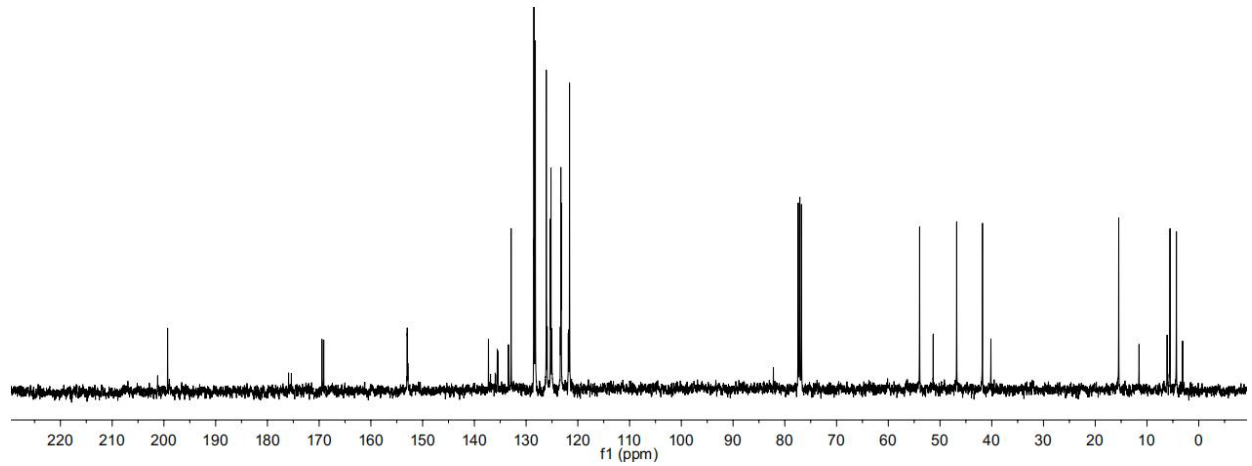
1o:

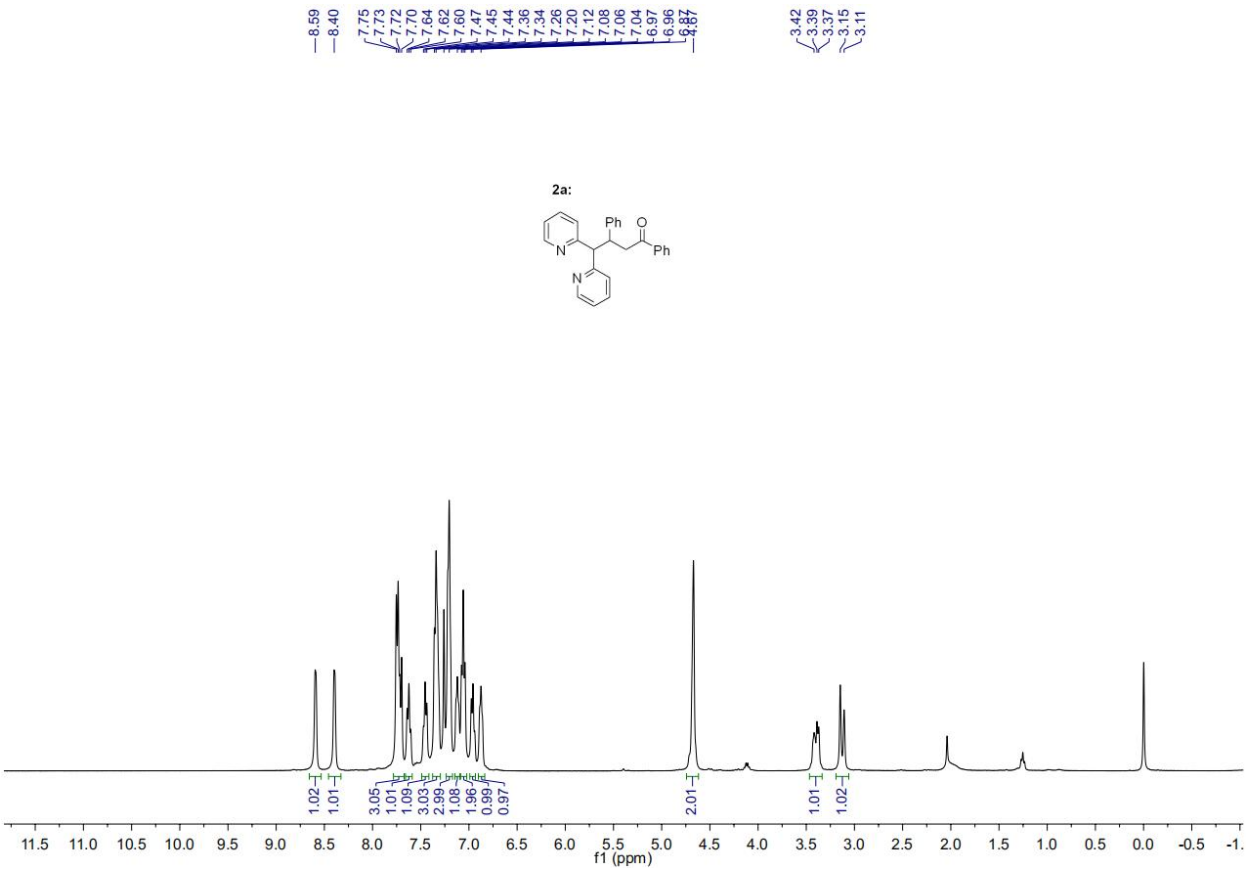


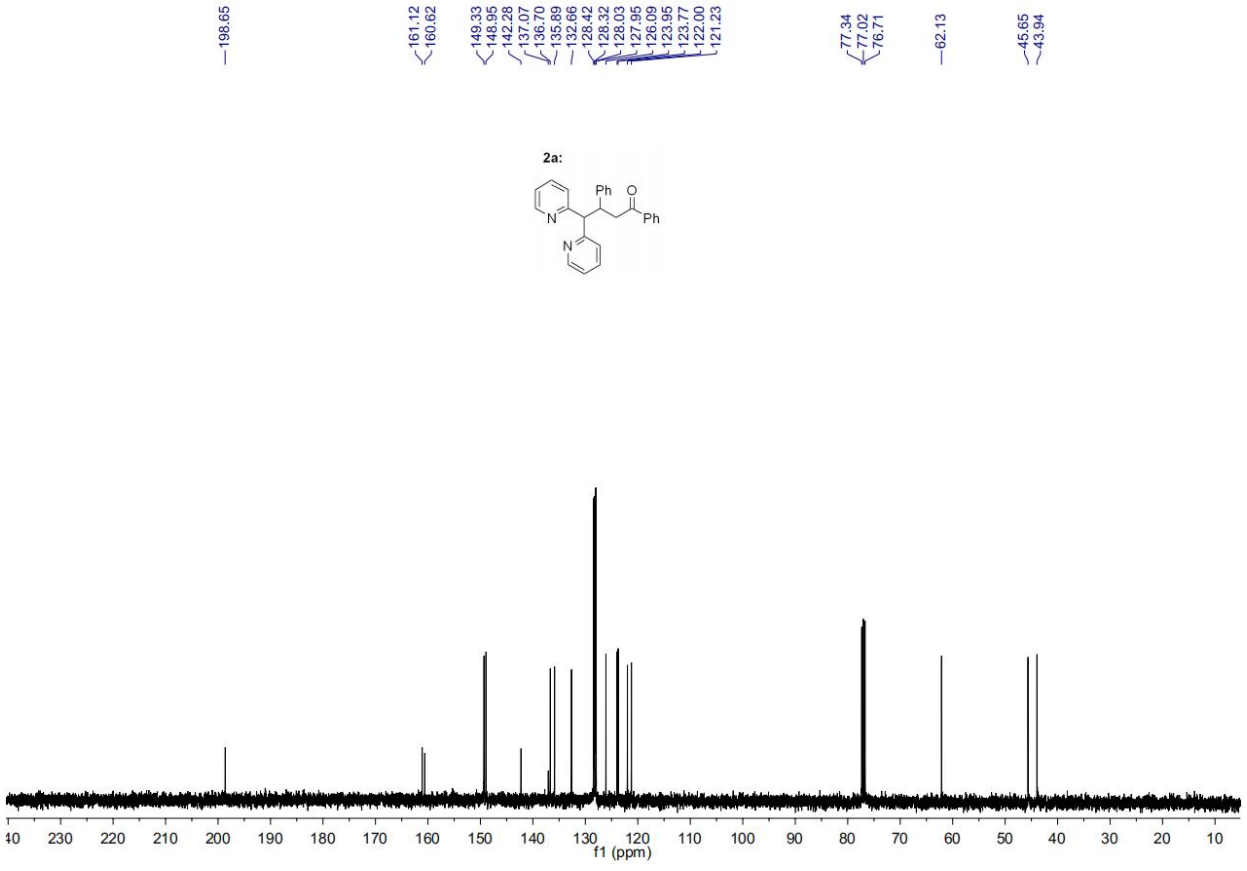

CH2Cl2
2.00
2.00
1.90
3.00
4.00
0.22
0.73
0.97
1.00
0.25
0.75
0.25
0.75
0.75
1.00
2.08
0.25
f1 (ppm)

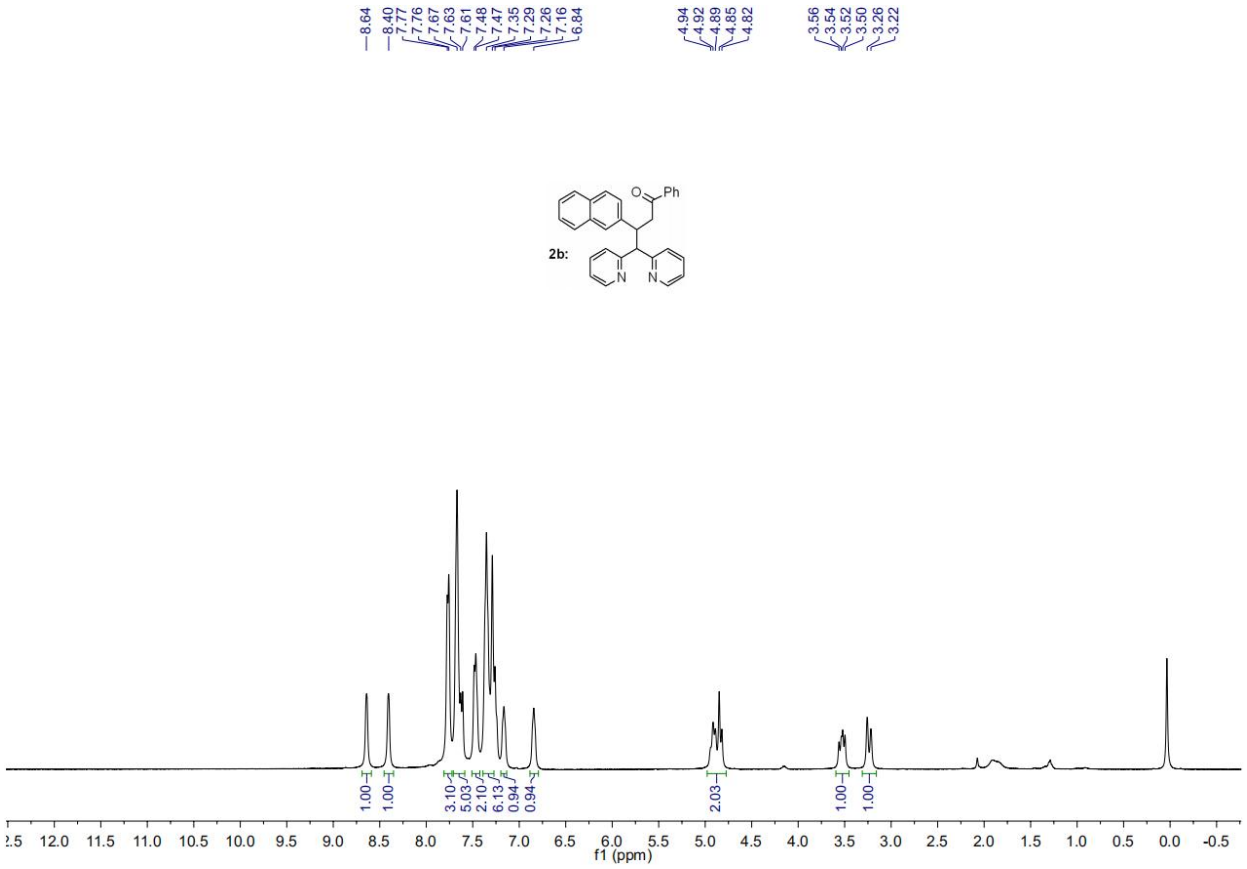
1o:

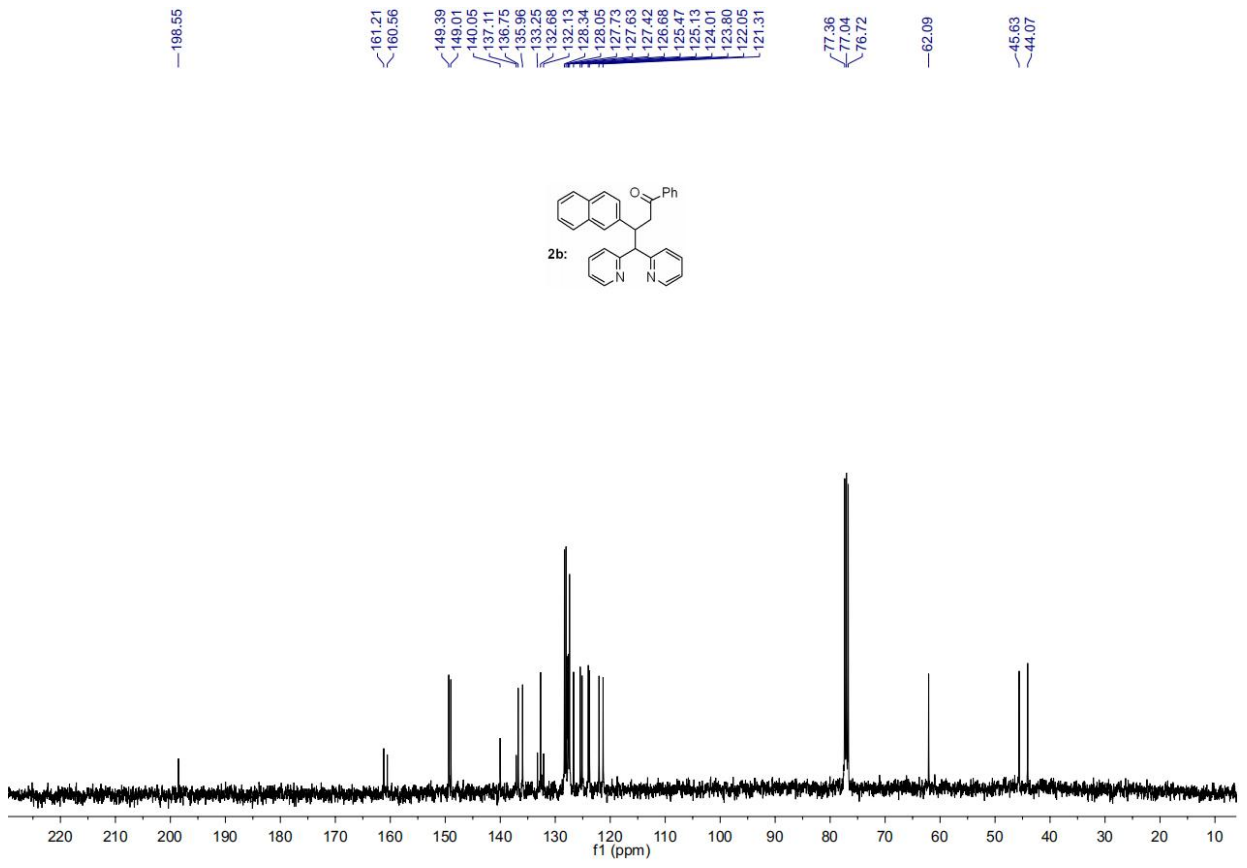


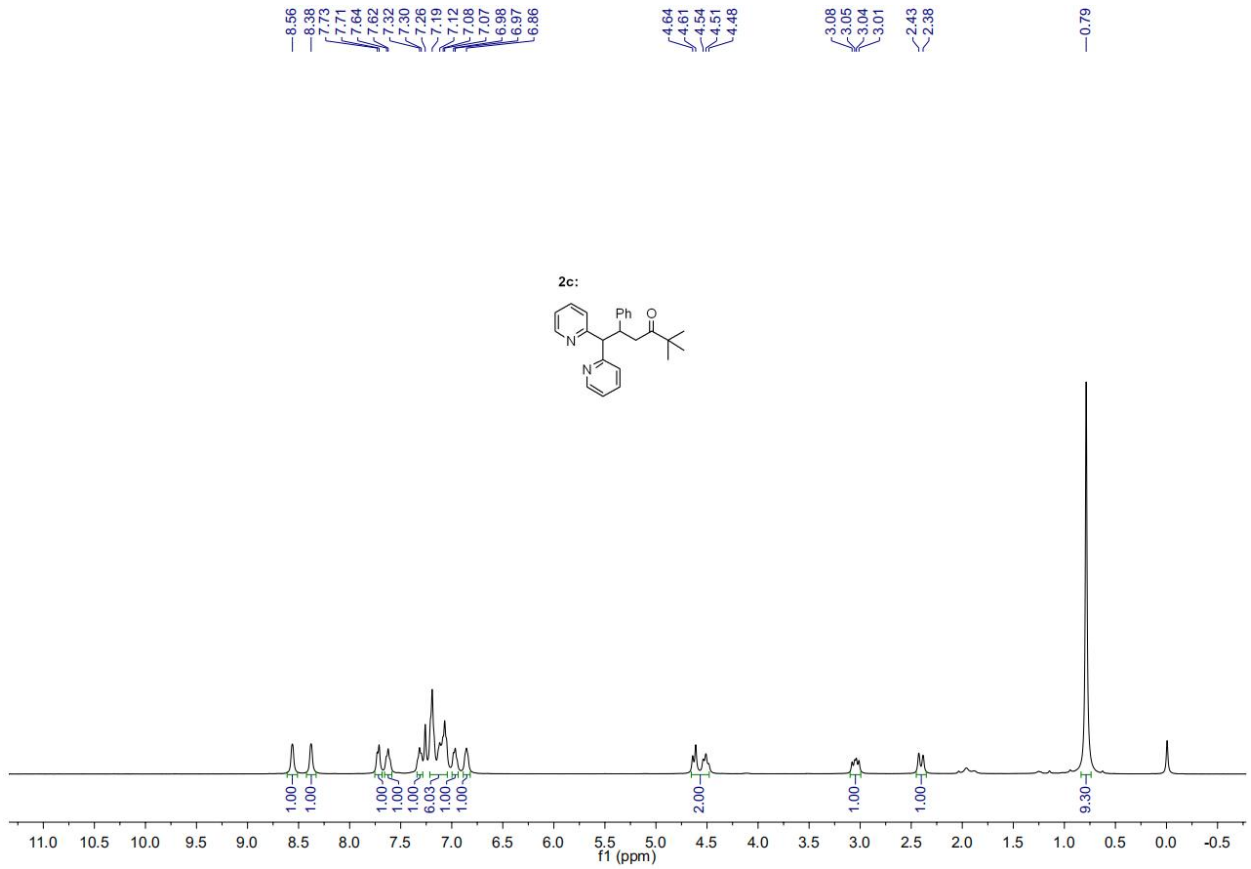

f1 (ppm)

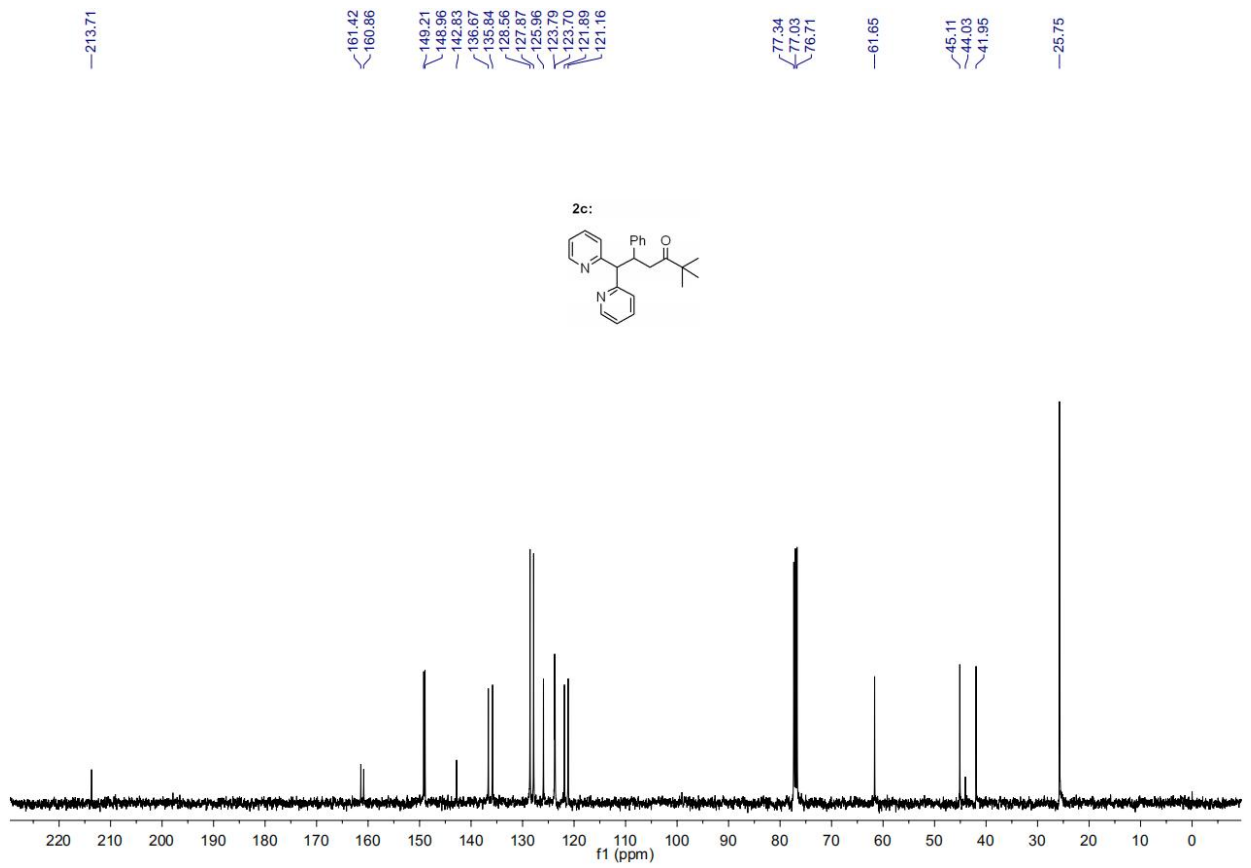

8.59
8.40
7.75
7.73
7.72
7.70
7.64
7.62
7.60
7.47
7.45
7.44
7.36
7.34
7.26
7.20
7.12
7.08
7.06
7.04
6.97
6.96
3.42
3.39
3.37
3.15
3.11
2a:
Ph
O
Ph
N
N
1.02
1.01
3.05
1.01
1.09
3.03
2.99
1.08
1.96
0.99
0.97
2.01
1.01
1.02
f1 (ppm)


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
77.34
77.02
76.71
62.13
45.65
43.94
2a:
Ph
O
Ph
N
N
f1 (ppm)


8.64
8.40
7.77
7.76
7.67
7.63
7.61
7.48
7.47
7.35
7.29
7.26
7.16
6.84
4.94
4.92
4.89
4.85
4.82
3.56
3.54
3.52
3.50
3.26
3.22
O
Ph
2b:
N
N
1.00
1.00
3.10
5.03
2.10
6.13
0.94
0.94
2.03
1.00
1.00
f1 (ppm)

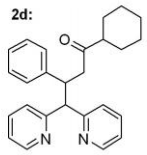

198.55
161.21
160.56
149.39
149.01
140.05
137.11
136.75
135.96
133.25
132.68
132.13
128.34
128.05
127.73
127.63
127.42
126.68
125.47
125.13
124.01
123.80
122.05
121.31
77.36
77.04
76.72
62.09
45.63
44.07
O
Ph
2b:
N
N
f1 (ppm)

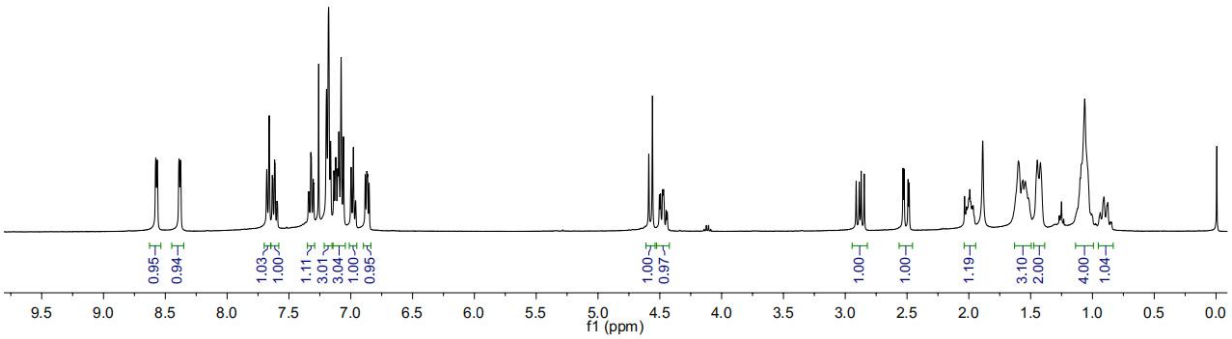

8.56
8.38
7.73
7.71
7.64
7.62
7.32
7.30
7.26
7.19
7.12
7.08
7.07
6.98
6.97
6.86
4.64
4.61
4.54
4.51
4.48
3.08
3.05
3.04
3.01
2.43
2.38
0.79
2c:
Ph
O
N
N
1.00
1.00
1.00
1.00
1.00
6.03
1.00
1.00
2.00
1.00
1.00
9.30
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


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
77.34
77.03
76.71
61.65
45.11
44.03
41.95
25.75
2c:
Ph
O
N
N
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.58
8.57
8.39
8.38
7.68
7.66
7.63
7.63
7.62
7.61
7.32
7.32
7.26
7.20
7.18
7.16
7.14
7.12
7.11
7.10
7.08
7.06
7.00
6.98
6.88
6.87
6.87
4.56
4.50
4.49
4.48
4.47
4.45
4.44
2.91
2.89
2.87
2.85
2.53
2.52
2.49
2.03
2.00
1.99
1.60
1.56
1.45
1.01
0.94
0.91
0.88
0.88
0.85
0.85

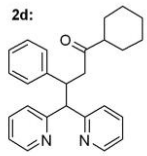
2d:

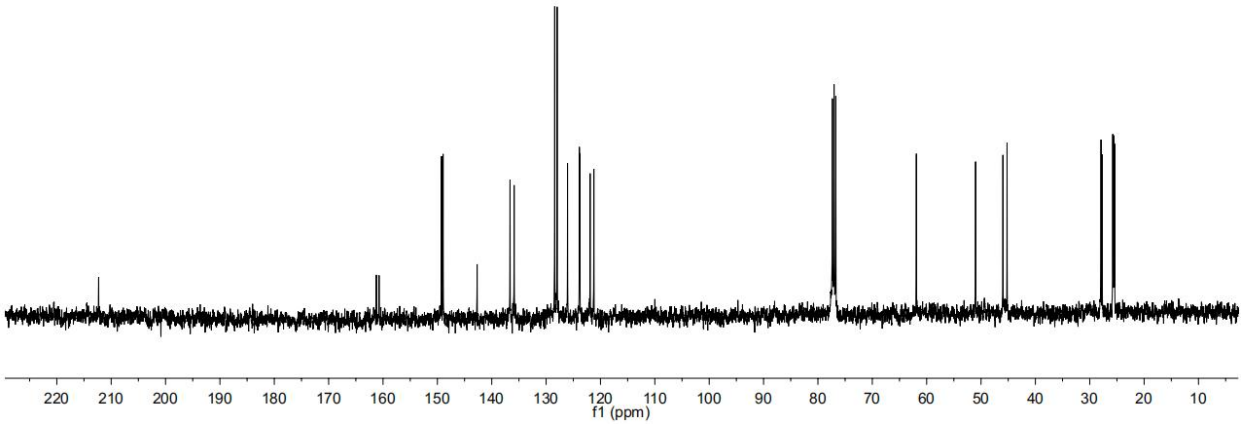


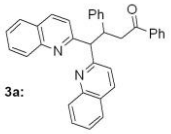

0.95
0.94
1.03
1.00
1.11
3.01
3.04
1.00
0.95
1.00
0.97
1.00
1.00
1.19
3.10
2.00
4.00
1.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


212.31
161.23
160.72
149.24
148.95
142.69
136.64
135.88
128.42
127.97
126.06
123.88
123.78
121.90
121.21
77.35
77.03
76.71
61.90
51.00
45.97
45.21
27.92
27.72
25.77
25.60
25.43

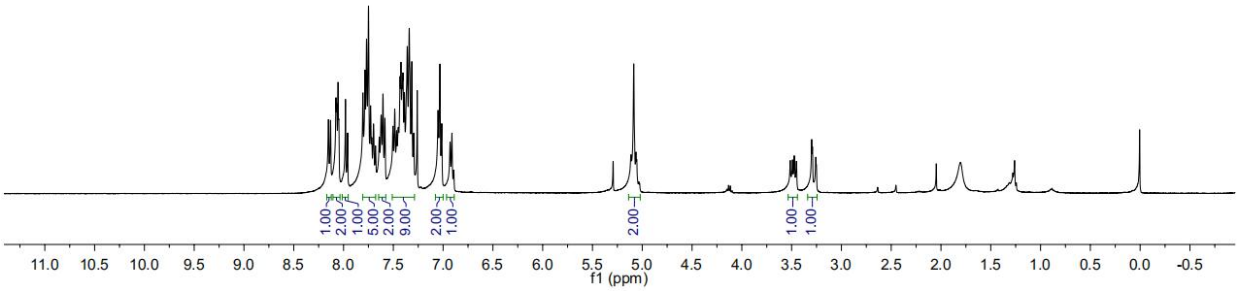
2d:

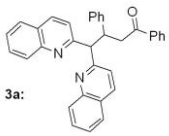



220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

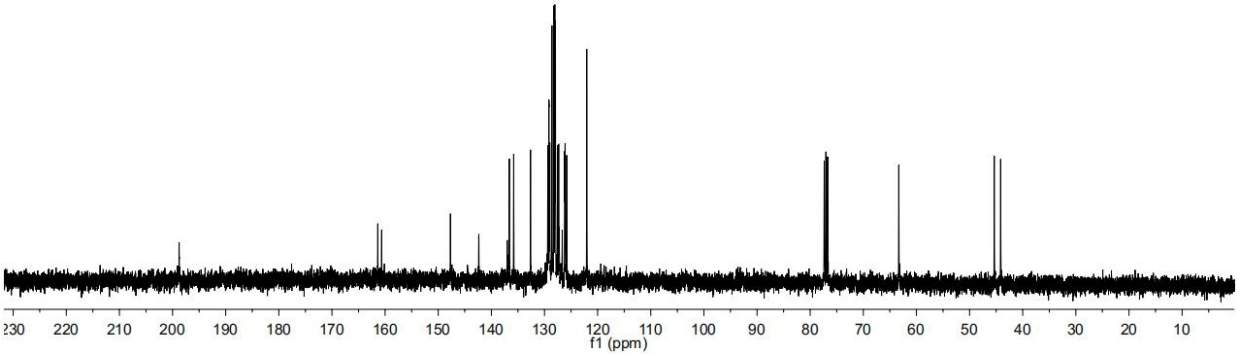

Ph
O
Ph
N
N

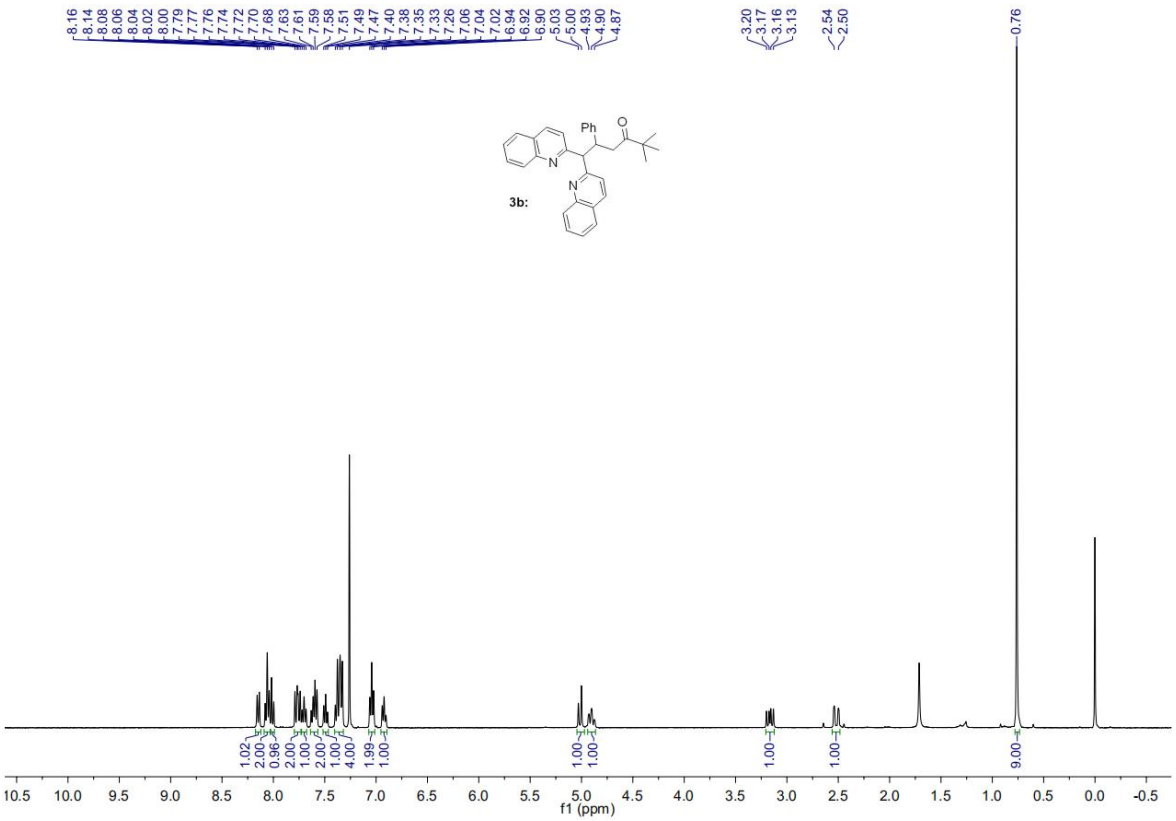
3a:

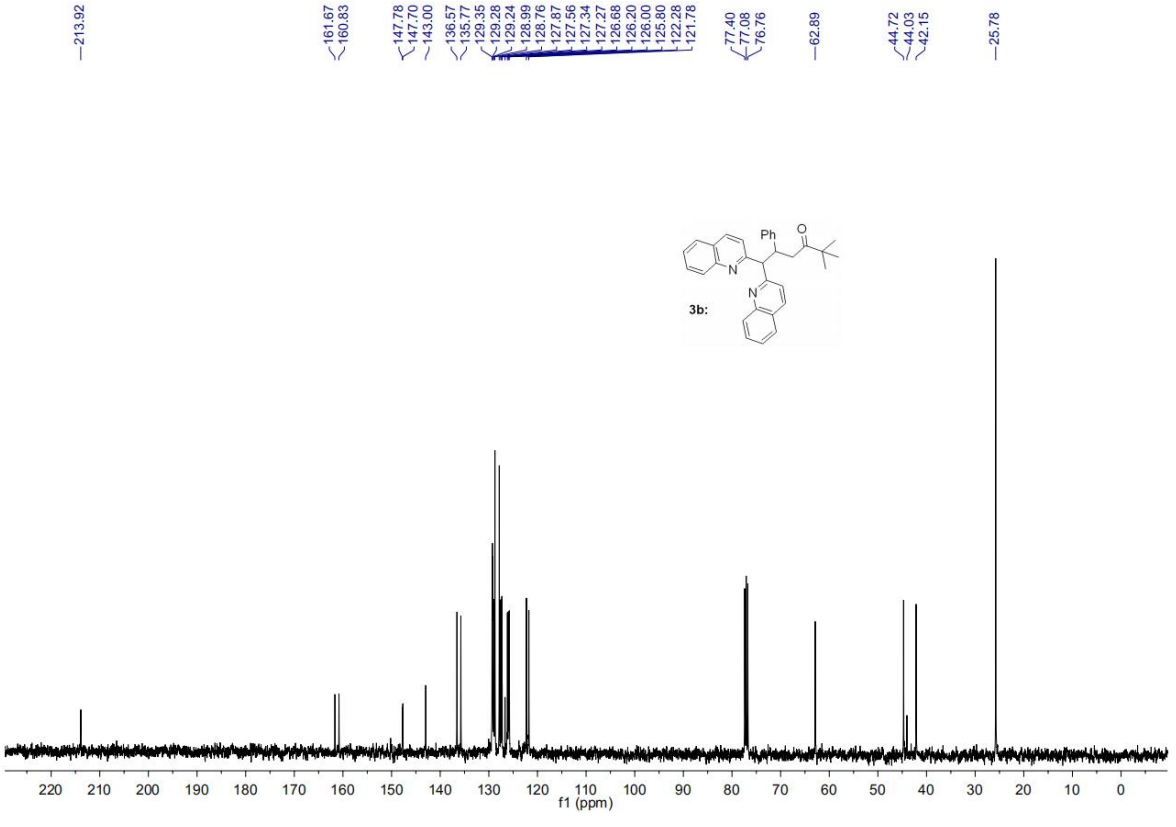

1.00
2.00
1.00
5.00
2.00
9.00
2.00
1.00
2.00
1.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

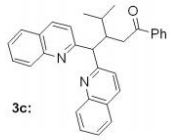

Ph
O
Ph
N
N

3a:

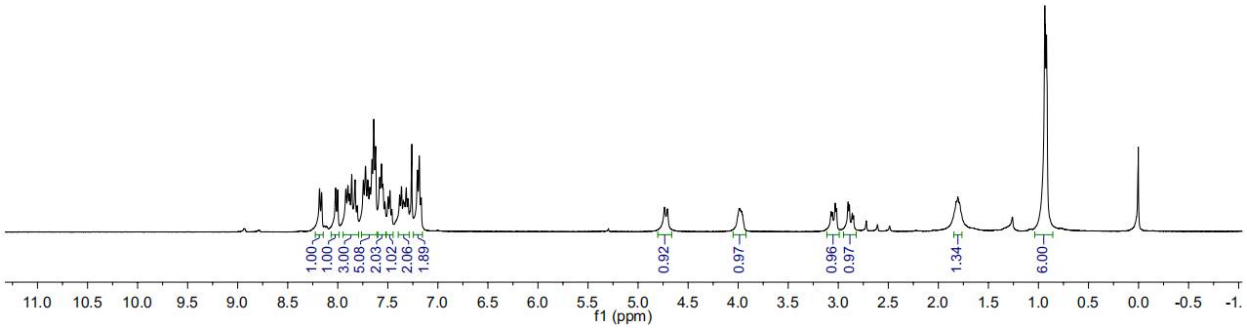

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

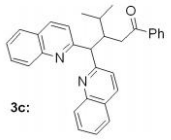

8.16
8.14
8.08
8.06
8.04
8.02
8.00
7.79
7.77
7.76
7.74
7.72
7.70
7.68
7.63
7.61
7.59
7.58
7.51
7.49
7.47
7.40
7.38
7.35
7.33
7.26
7.06
7.04
7.02
6.94
6.92
6.90
5.03
5.00
4.93
4.90
4.87
3.20
3.17
3.16
3.13
2.54
2.50
0.76
Ph
O
N
N
3b:
1.02
2.00
0.96
2.00
1.00
2.00
1.00
4.00
1.99
1.00
1.00
1.00
1.00
1.00
9.00
f1 (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
77.40
77.08
76.76
62.89
44.72
44.03
42.15
25.78
Ph
O
N
N
3b:
f1 (ppm)

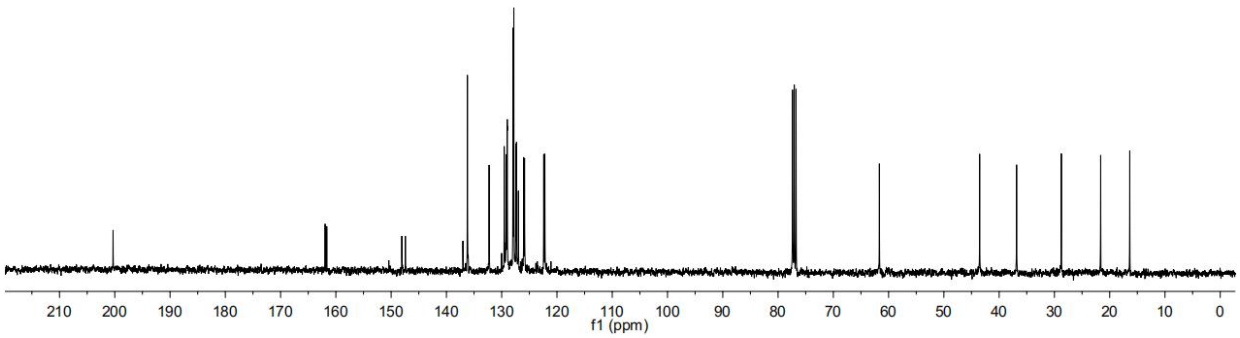

O
Ph
N
N

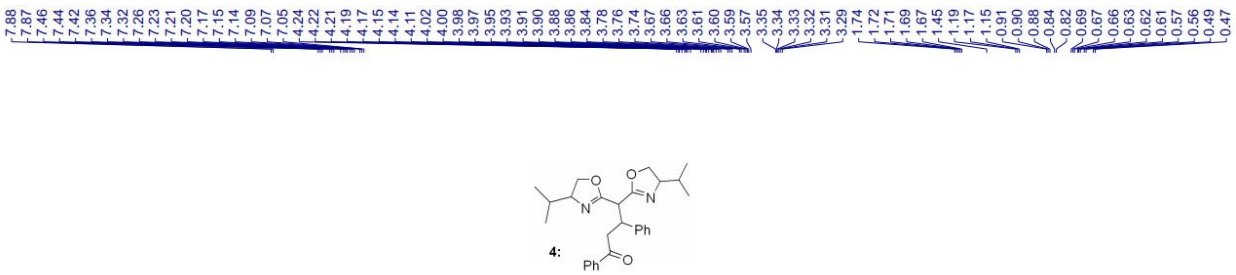
3c:


1.00
1.00
3.00
5.08
2.03
1.02
2.06
1.89
0.92
0.97
0.96
0.97
1.34
6.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

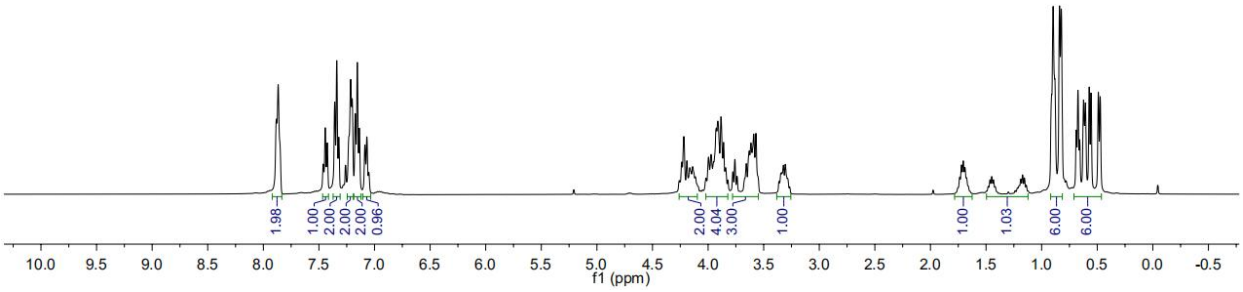

O
Ph
N
N

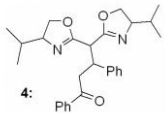
3c:


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



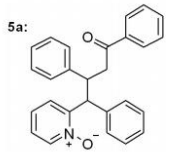
4:
Ph
Ph
O
N
O
N

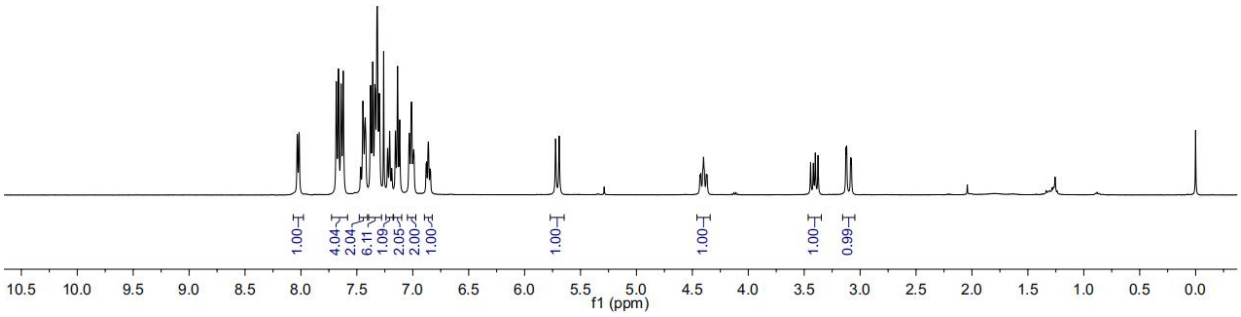

1.98
1.00
2.00
2.00
2.00
0.96
2.00
4.04
3.00
1.00
1.00
1.03
6.00
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


4:
Ph
Ph
O
N
O
N

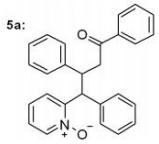
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

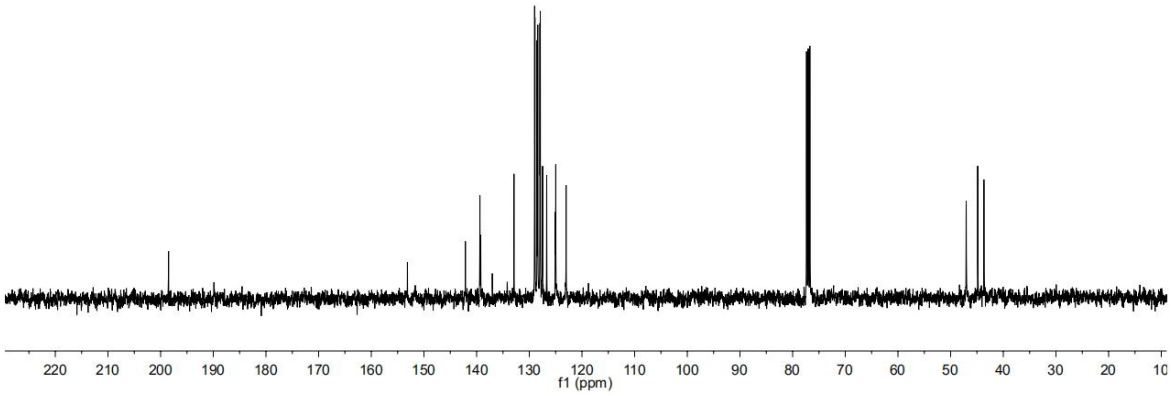

8.03
8.02
7.68
7.66
7.64
7.62
7.45
7.38
7.36
7.34
7.32
7.32
7.30
7.30
7.26
7.14
7.12
5.69
4.43
4.43
4.40
4.37
4.37
3.44
3.42
3.40
3.38
3.13
3.12
3.08
3.08

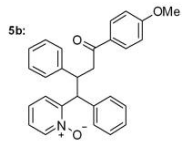

5a:

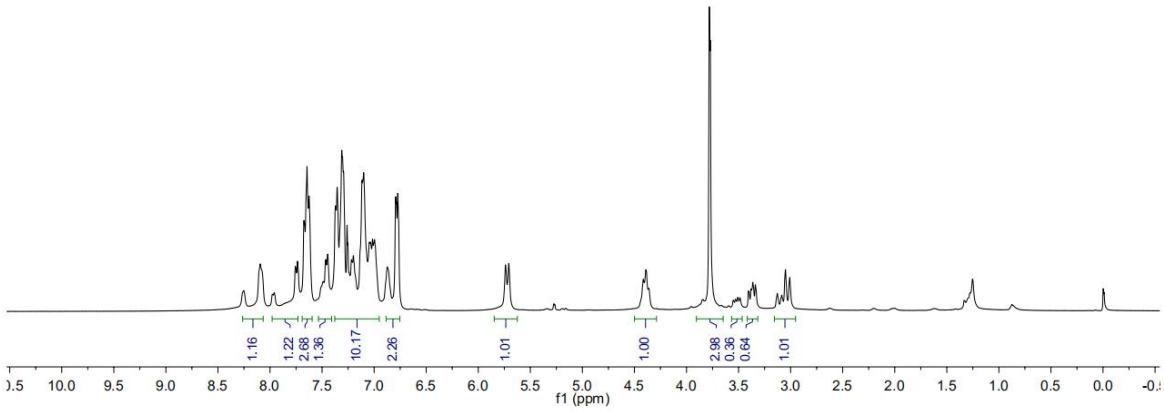

1.00
4.04
2.04
6.11
1.09
2.05
2.00
1.00
1.00
1.00
1.00
0.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

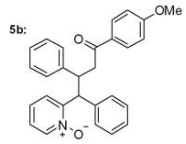

198.49
153.14
142.13
139.38
139.22
137.02
132.91
128.99
128.93
128.52
128.39
127.98
127.91
127.48
126.69
125.06
124.97
123.01
77.36
77.04
76.73
47.04
44.86
43.67

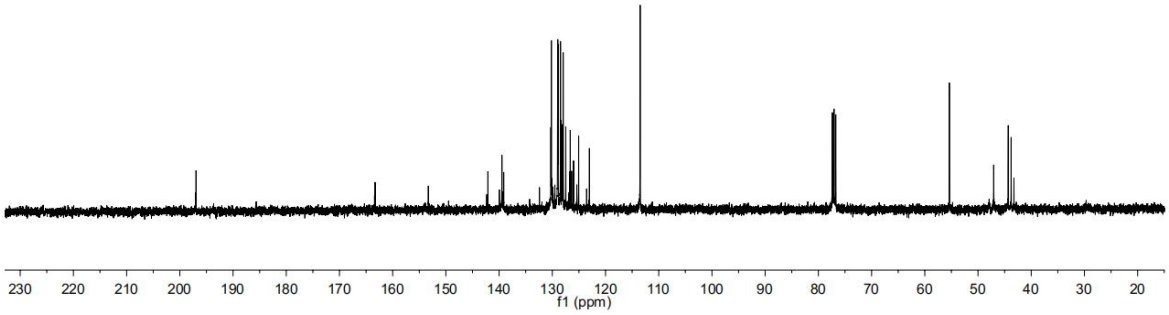

5a:

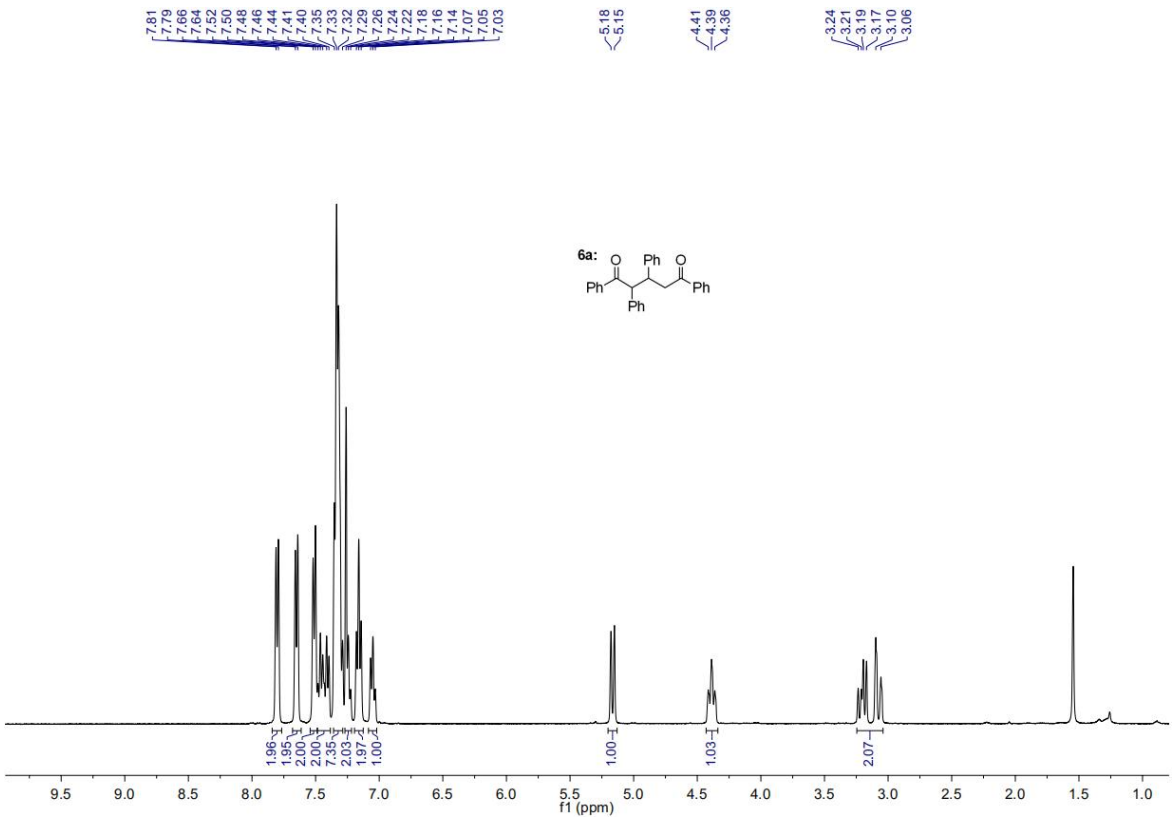

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

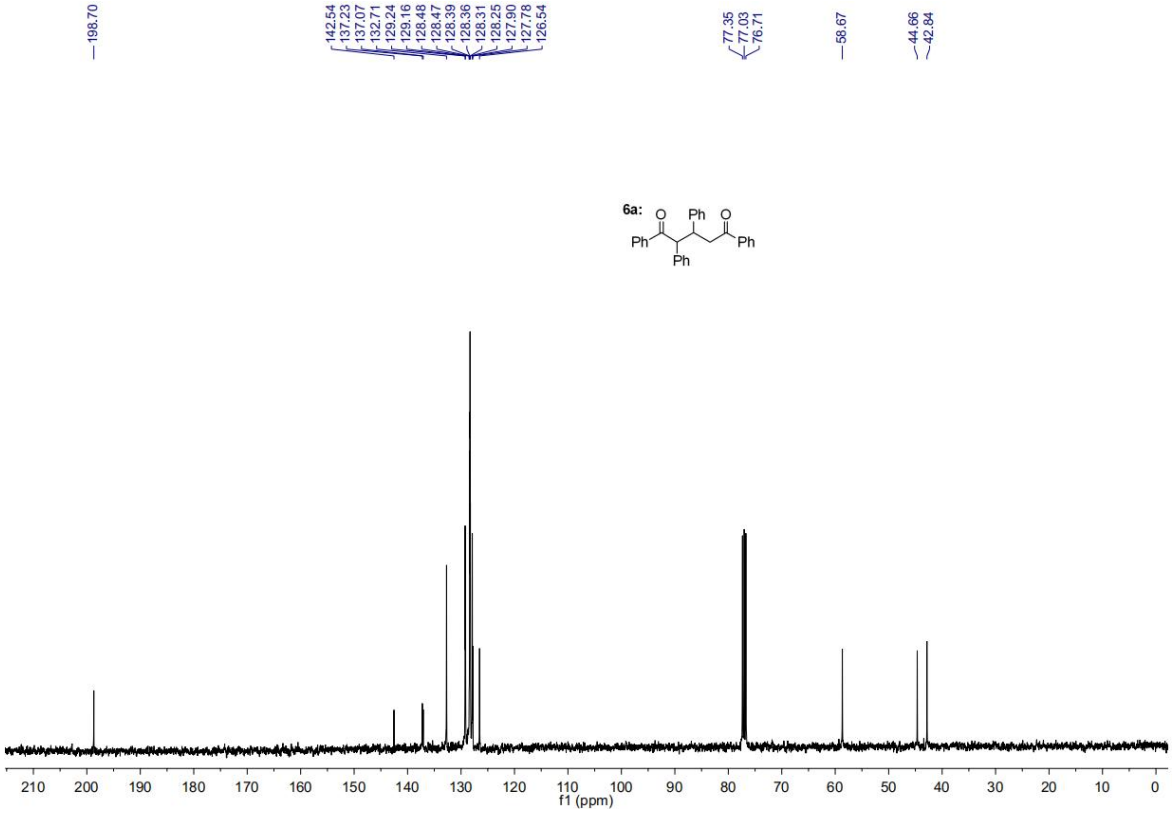

5b:
OMe
O
N
O


1.16
1.22
2.68
1.36
10.17
2.26
1.01
1.00
2.98
0.36
0.64
1.01
f1 (ppm)

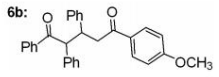

5b:
OMe
O
N
O

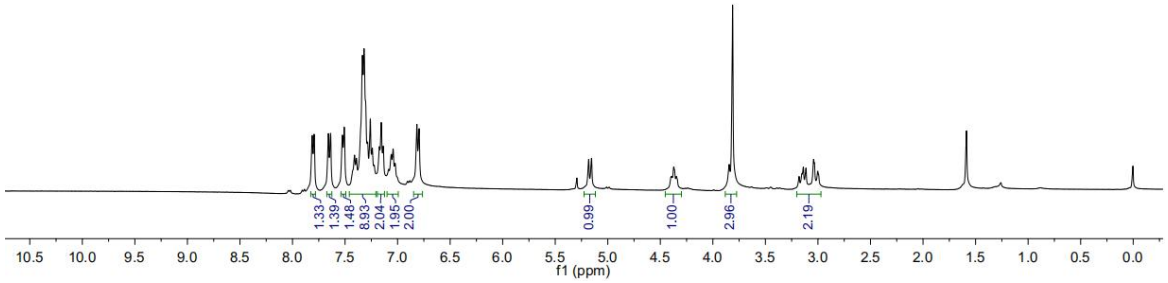

f1 (ppm)


7.81
7.79
7.66
7.64
7.52
7.50
7.48
7.46
7.44
7.41
7.40
7.35
7.33
7.32
7.29
7.26
7.24
7.22
7.18
7.16
7.14
7.07
7.05
7.03
5.18
5.15
4.41
4.39
4.36
3.24
3.21
3.19
3.17
3.10
3.06
6a:
1.96
1.95
2.00
2.00
7.35
2.03
1.97
1.00
1.00
1.03
2.07
f1 (ppm)

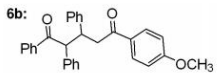

198.70
142.54
137.23
137.07
132.71
129.24
129.16
128.48
128.47
128.39
128.36
128.31
128.25
127.90
127.78
126.54
77.35
77.03
76.71
58.67
44.66
42.84
6a:
f1 (ppm)

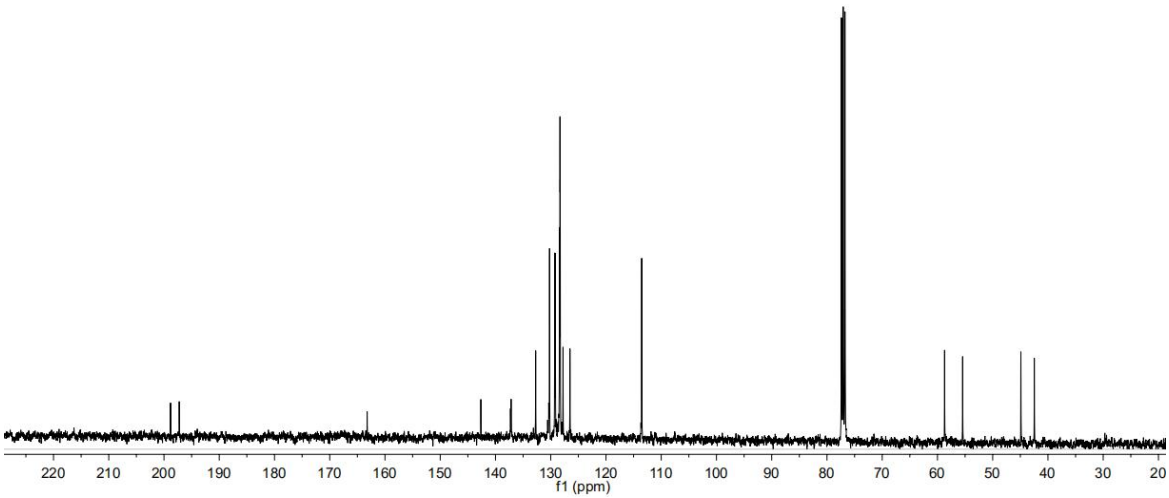

7.81
7.80
7.66
7.64
7.53
7.51
7.41
7.39
7.34
7.32
7.29
7.26
7.24
7.22
7.17
7.16
7.14
7.08
7.06
7.04
7.02
7.00
6.82
6.80
5.18
5.16
4.40
4.39
4.37
4.35
3.85
3.81
3.18
3.15
3.14
3.12
3.04
3.00


6b:
O
Ph
Ph
O
Ph
OCH3


1.33
1.39
1.48
8.93
2.04
1.95
2.00
0.99
1.00
2.96
2.19
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

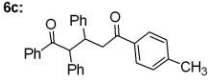

198.81
197.24
163.23
142.65
137.29
137.17
132.72
130.36
130.22
129.28
129.17
128.42
128.32
128.28
127.77
126.52
113.54
77.38
77.06
76.74
58.71
55.44
44.90
42.47

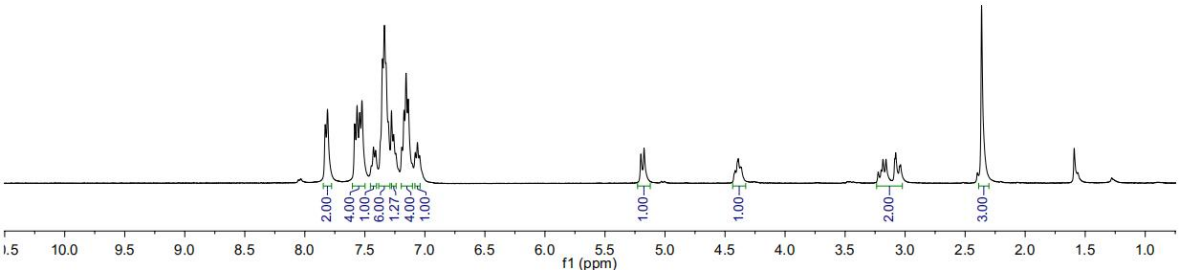

6b:
O
Ph
Ph
O
Ph
OCH3


220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


7.83
7.81
7.58
7.56
7.54
7.52
7.45
7.43
7.41
7.37
7.35
7.34
7.32
7.30
7.28
7.26
7.24
7.22
7.19
7.17
7.16
7.14
7.10
7.08
7.06
7.04
5.20
5.17
4.42
4.40
4.39
4.37
4.36
3.22
3.20
3.18
3.16
3.09
3.08
3.05
3.04
2.36

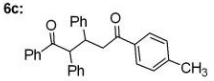
6c:


O
Ph
Ph
O
Ph
CH3

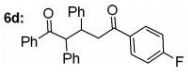

2.00
4.00
1.00
6.00
1.27
4.00
1.00
1.00
1.00
2.00
3.00
f1 (ppm)

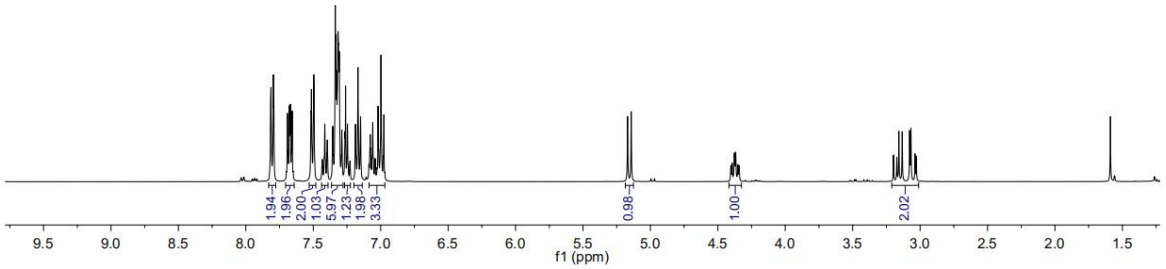

198.78
198.36
143.48
142.61
137.28
137.15
134.79
132.72
129.27
129.17
129.07
128.42
128.33
128.28
128.07
127.78
126.53
77.38
77.06
76.74
58.69
44.79
42.75
21.58

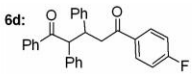
6c:


O
Ph
Ph
O
Ph
CH3

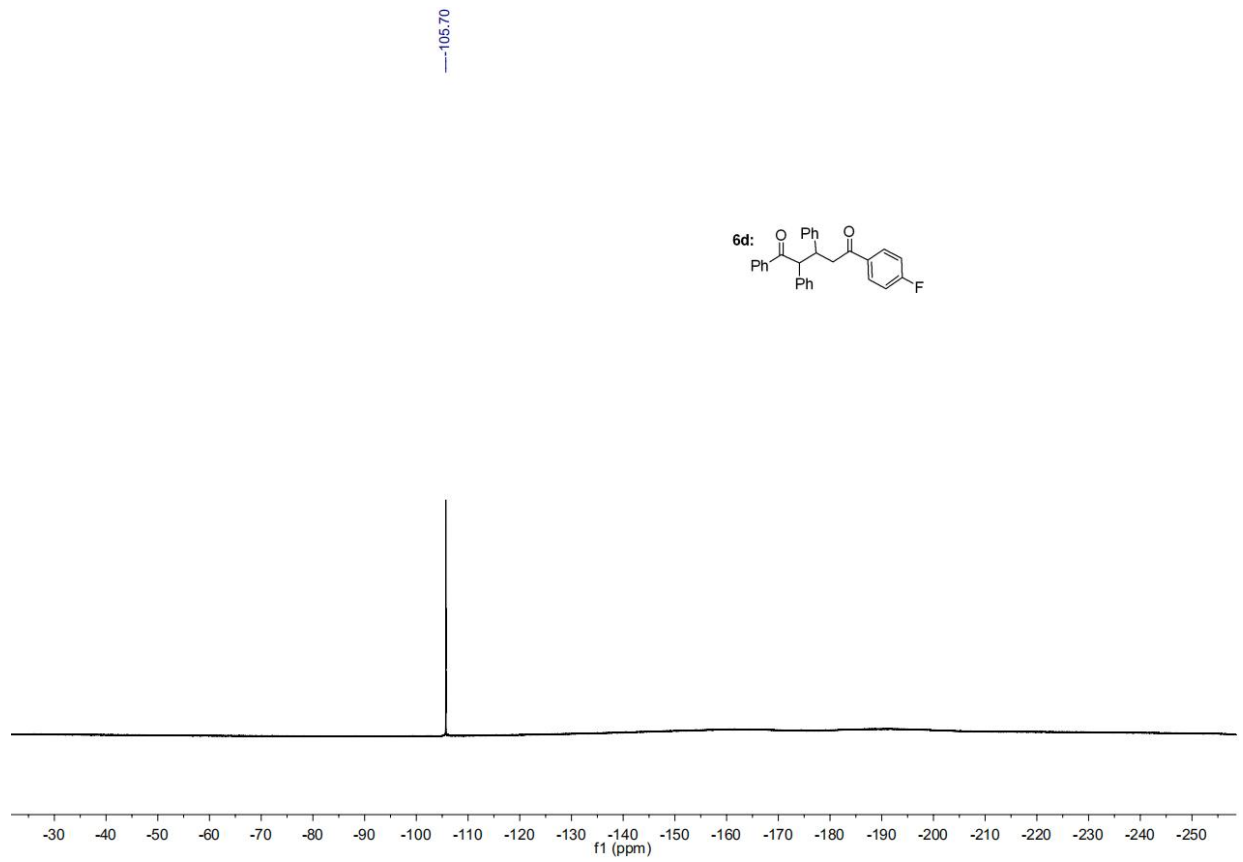
f1 (ppm)

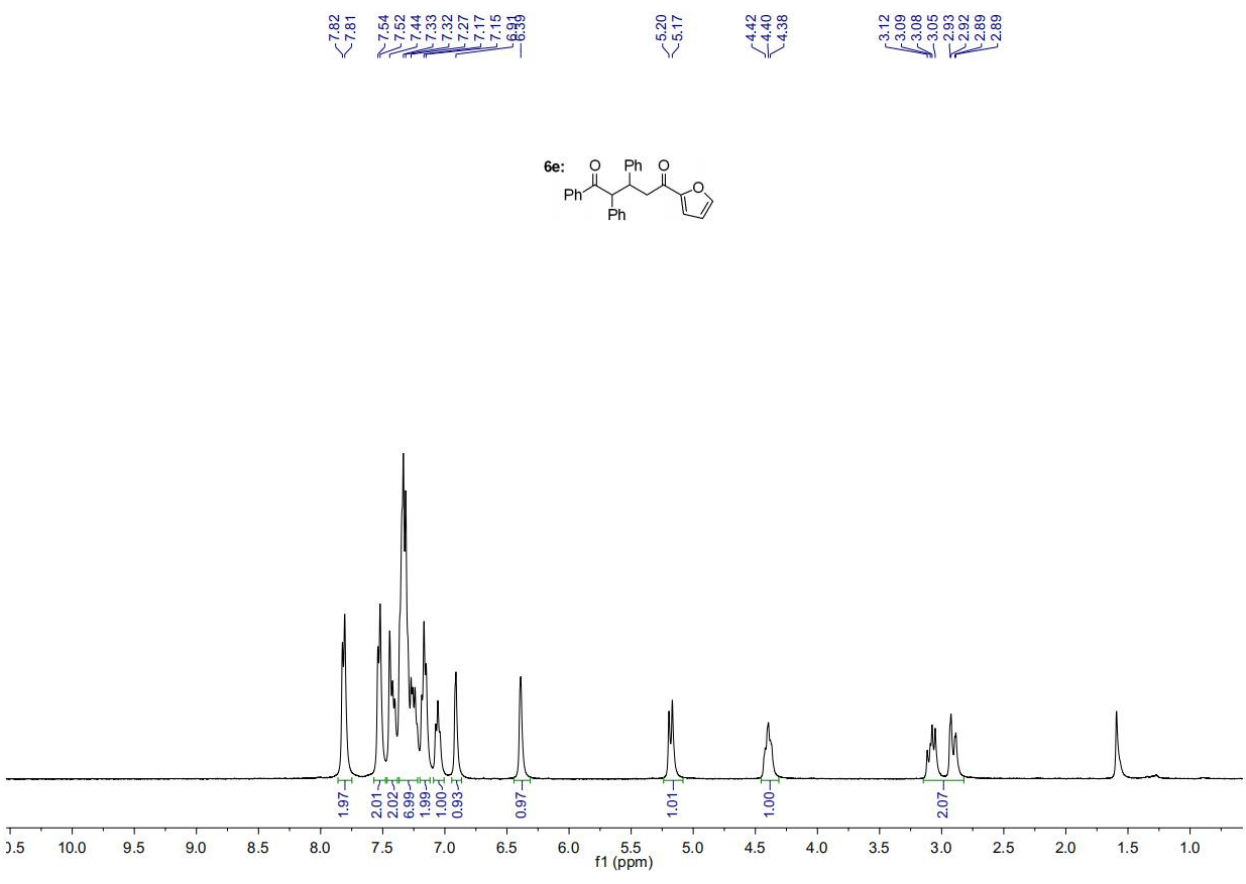

6d:
O
Ph
Ph
Ph
O
F

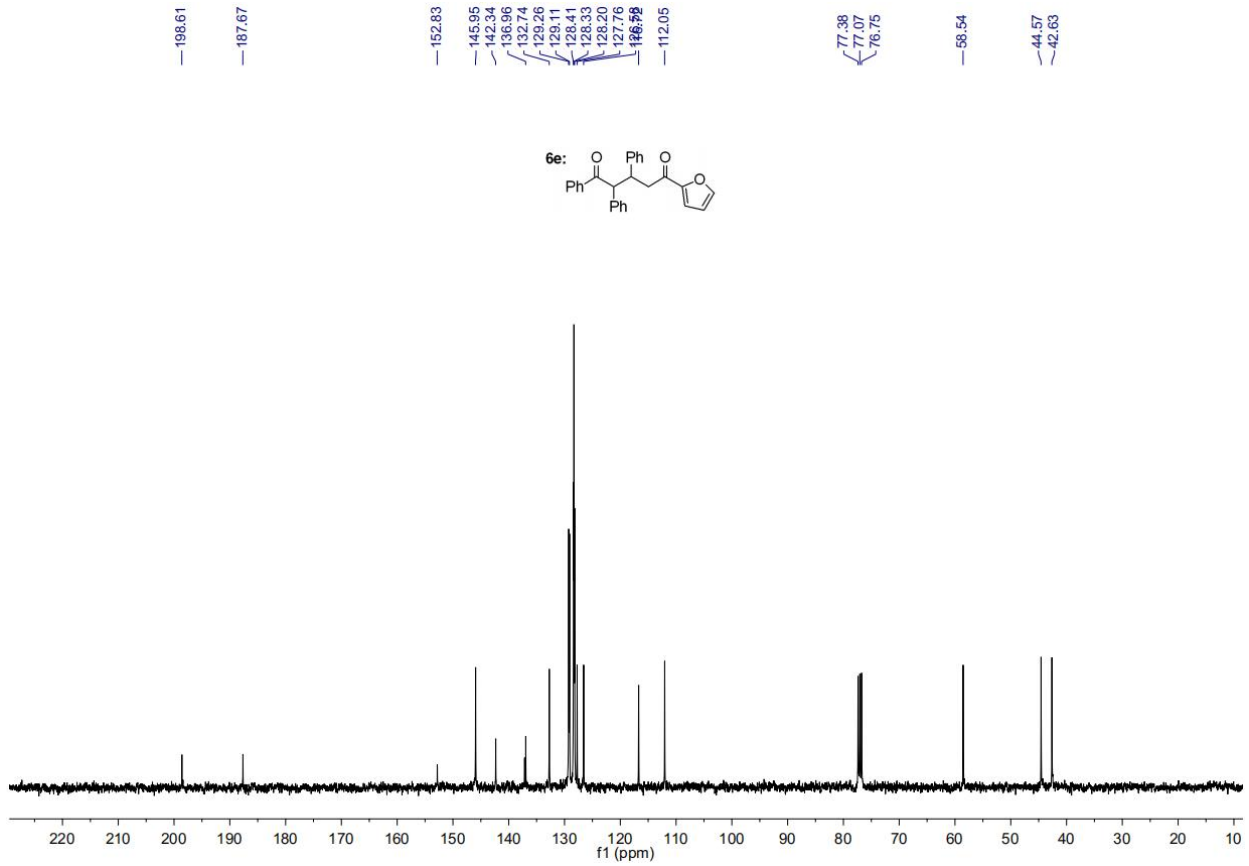

1.94
1.96
2.00
1.03
5.97
1.23
1.98
3.33
0.98
1.00
2.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

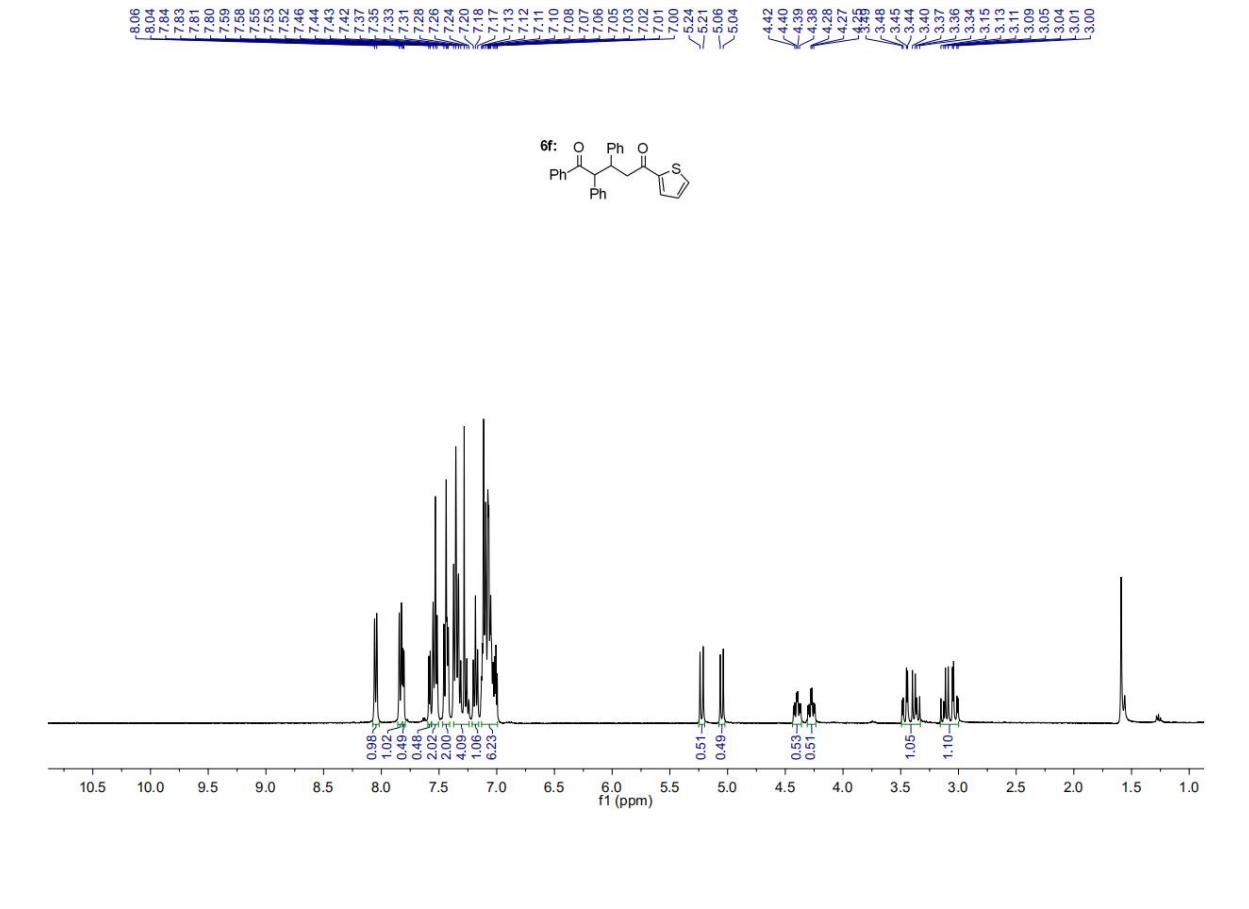

6d:
O
Ph
Ph
Ph
O
F

220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


-105.70
6d:
Ph
O
Ph
O
Ph
Ph
F
-30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250
f1 (ppm)

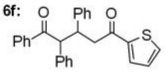

7.82
7.81
7.54
7.52
7.44
7.33
7.32
7.27
7.17
7.15
6.99
6.99
5.20
5.17
4.42
4.40
4.38
3.12
3.09
3.08
3.05
2.93
2.92
2.89
2.89
6e:
O
Ph
Ph
O
Ph
O
1.97
2.01
2.02
6.99
1.99
1.00
0.93
0.97
1.01
1.00
2.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)

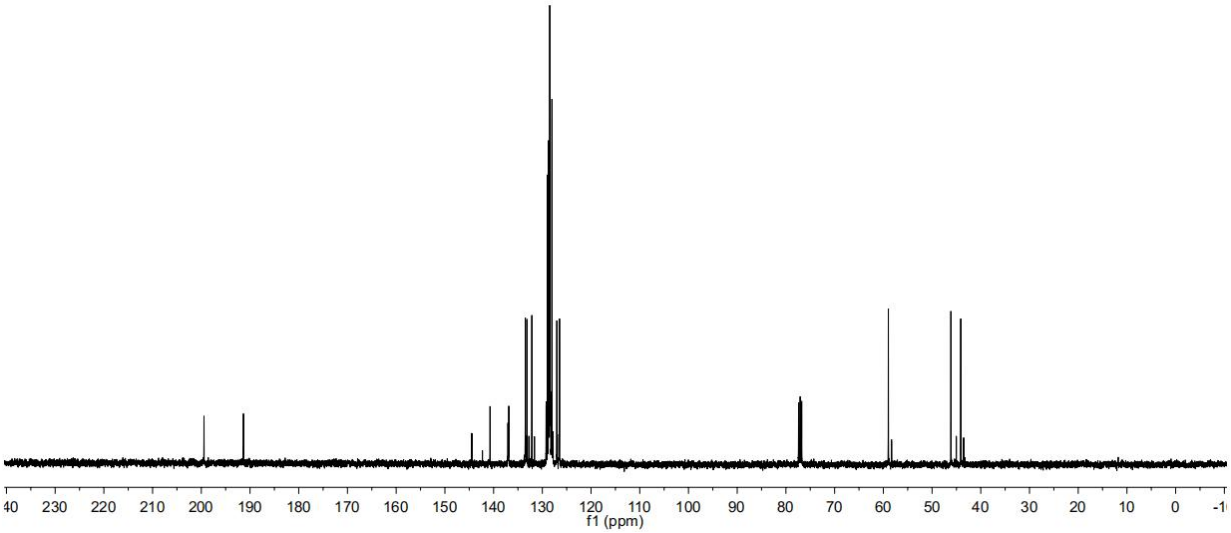

198.61
187.67
152.83
145.95
142.34
136.96
132.74
129.26
129.11
128.41
128.33
128.20
127.76
112.05
77.38
77.07
76.75
58.54
44.57
42.63
6e:
Ph
O
Ph
O
Ph
O
f1 (ppm)


6f:
Ph
O
Ph
O
Ph
S
0.98
1.02
0.49
0.48
2.02
2.00
4.09
1.06
6.23
0.51
0.49
0.53
0.51
1.05
1.10
f1 (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
77.39
77.08
76.76
58.97
58.31
46.14
45.02
44.11
43.51

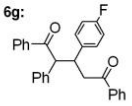
6f:

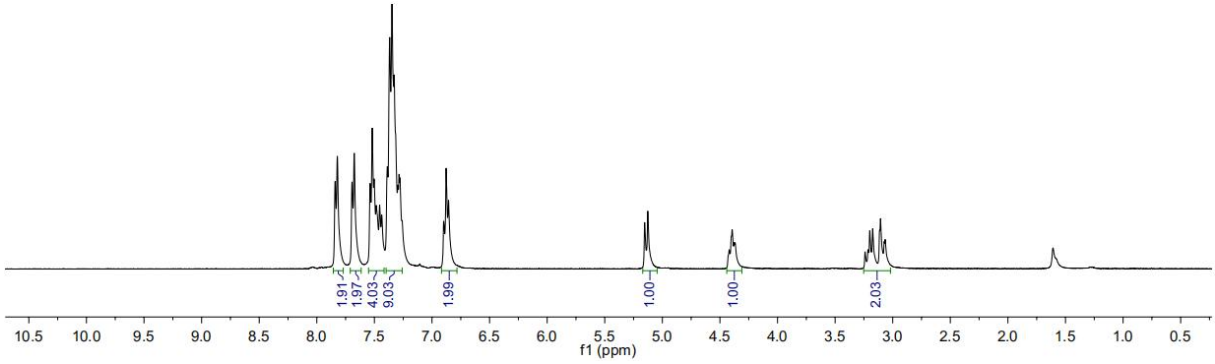

O
Ph
Ph
O
Ph
S


40 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


7.84
7.82
7.69
7.67
7.54
7.52
7.50
7.48
7.47
7.45
7.44
7.39
7.37
7.35
7.33
7.31
7.30
7.29
7.28
7.26
6.90
6.88
6.86
5.15
5.13
4.43
4.42
4.40
4.39
4.38
4.37
3.24
3.22
3.20
3.17
3.12
3.11
3.07
3.07

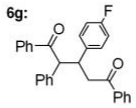
6g:

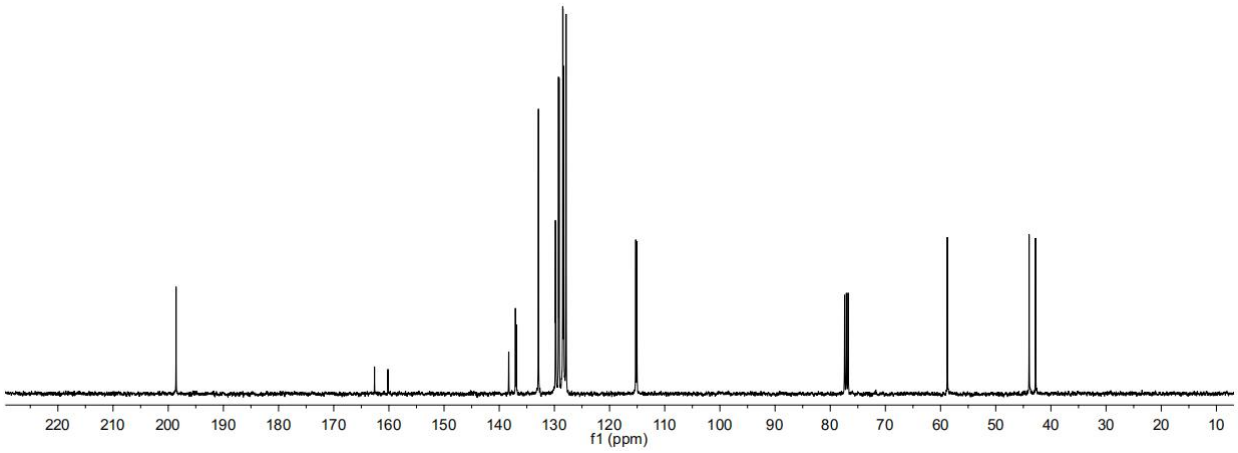

F
Ph
O
Ph
O
Ph


1.91
1.97
4.03
9.03
1.99
1.00
1.00
2.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

198.60
162.63
160.19
138.30
137.08
136.90
132.91
129.83
129.75
129.27
129.16
128.50
128.46
128.31
127.92
127.89
115.27
115.06
77.41
77.09
76.77
58.78
43.95
42.79

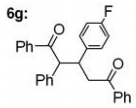
6g:

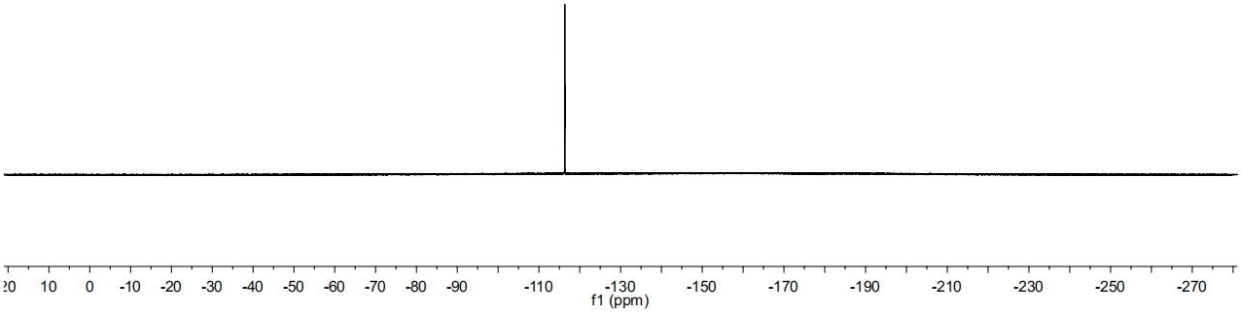




-116.36

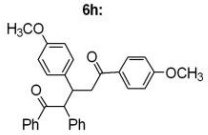
6g:

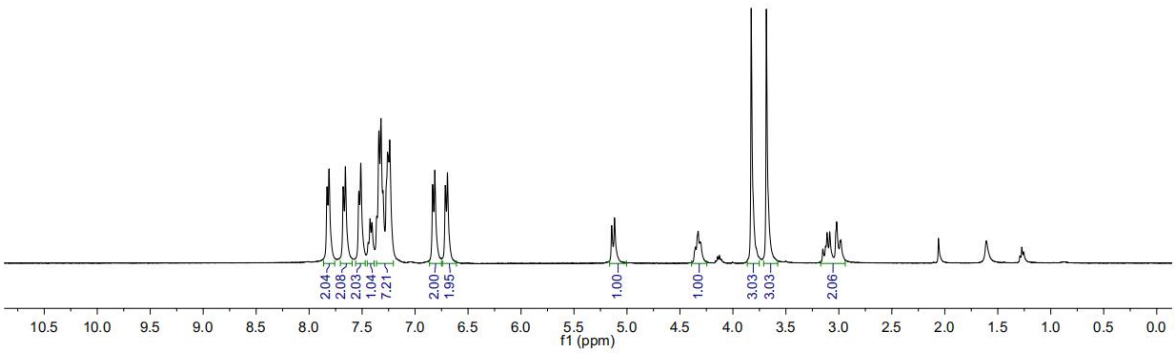





7.83
7.81
7.68
7.66
7.53
7.51
7.44
7.43
7.41
7.36
7.34
7.32
7.30
7.26
7.24
6.83
6.81
6.71
6.69
5.14
5.12
4.35
4.33
4.31
3.83
3.68
3.15
3.13
3.11
3.09
3.02
2.99
2.98

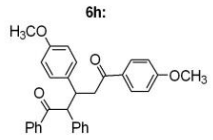
6h:


H3CO
O
OCH3
O
Ph
Ph

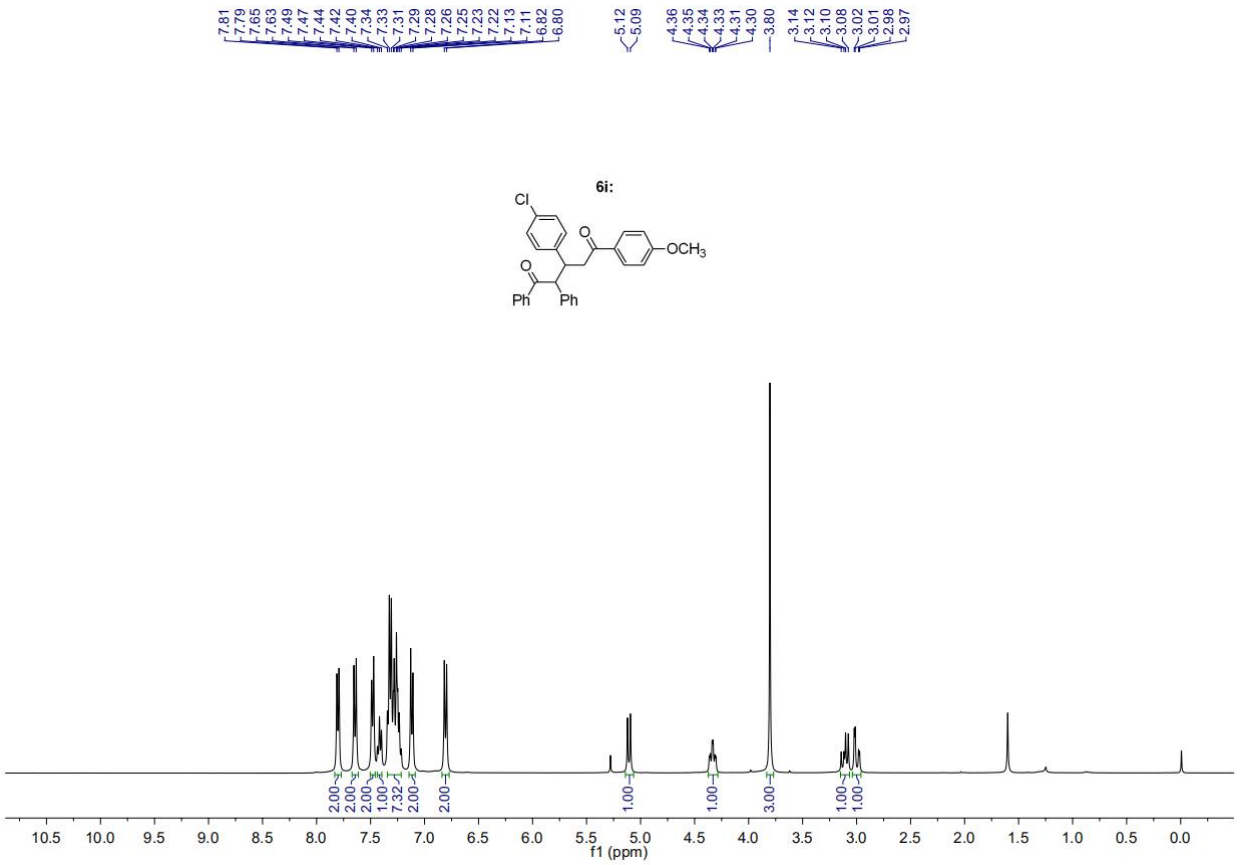

2.04
2.08
2.03
1.04
7.21
2.00
1.95
1.00
1.00
3.03
3.03
2.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

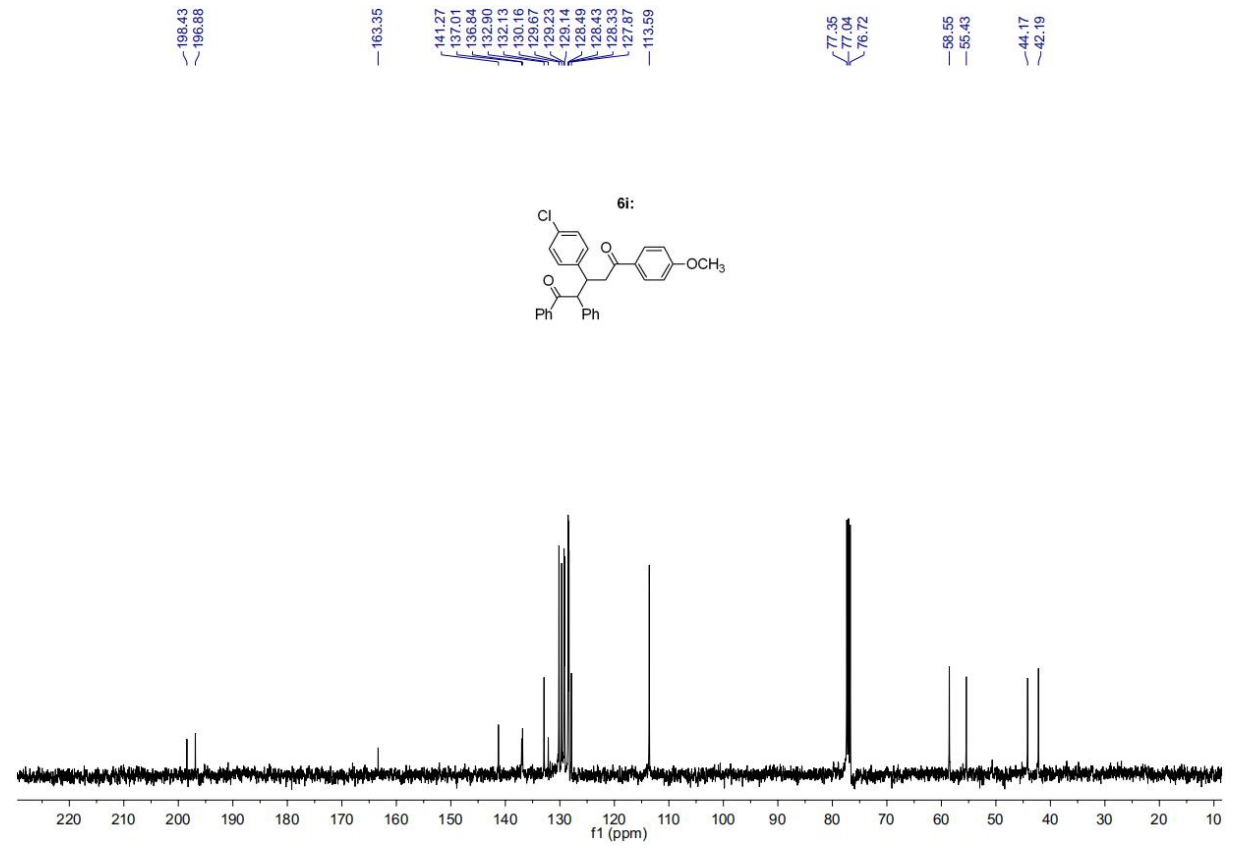

198.91
197.42
163.19
157.97
137.24
134.59
132.72
130.32
130.22
129.19
129.13
128.41
128.33
127.72
113.71
113.51
77.39
77.07
76.75
58.90
55.41
55.05
44.13
42.57

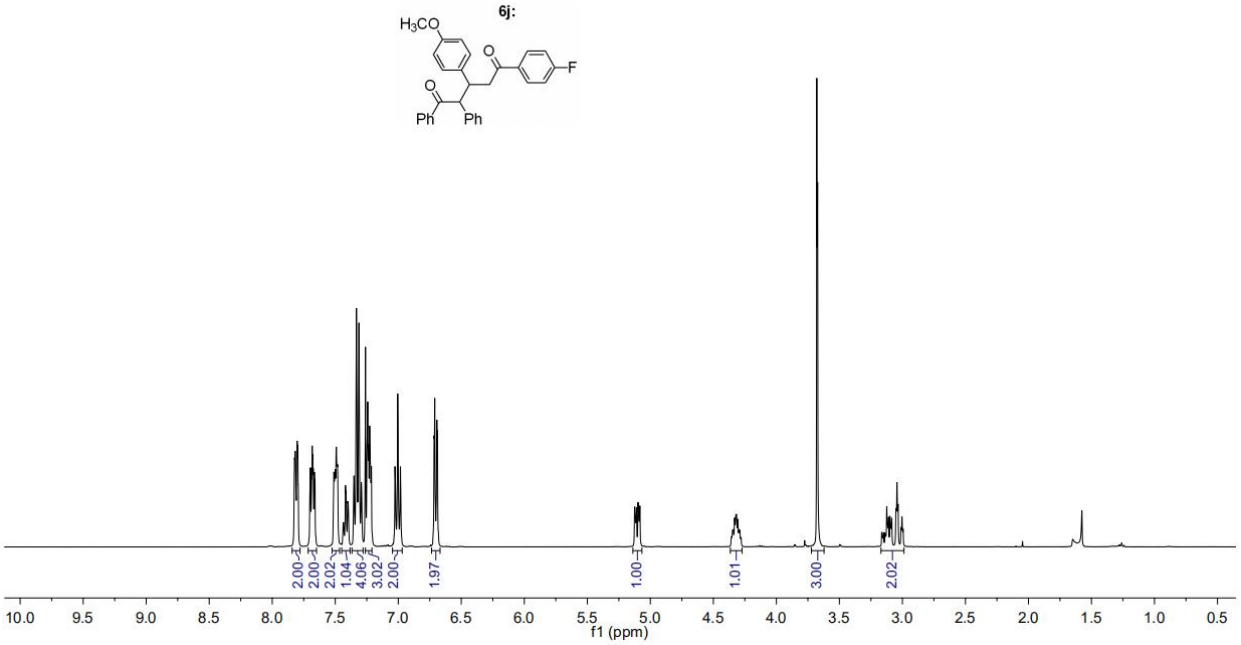
6h:

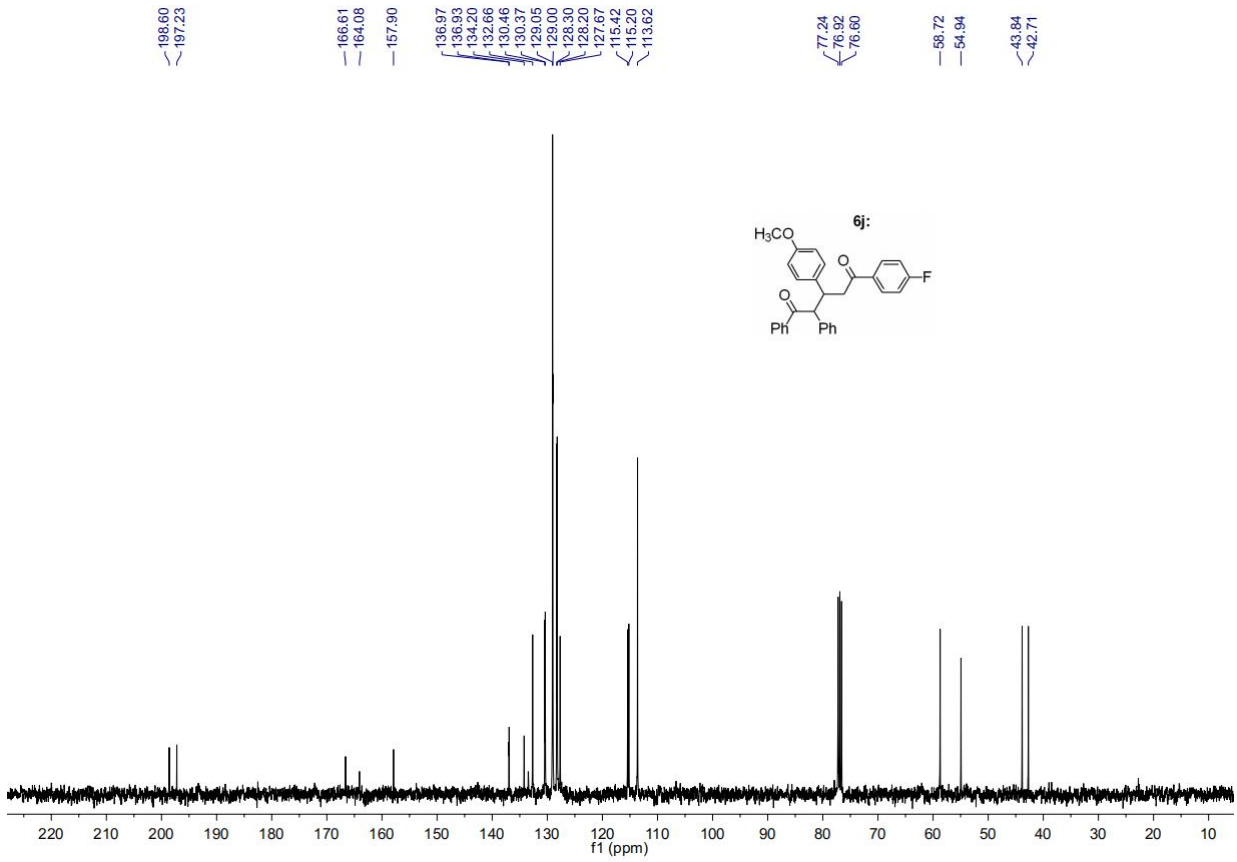

H3CO
O
OCH3
O
Ph
Ph

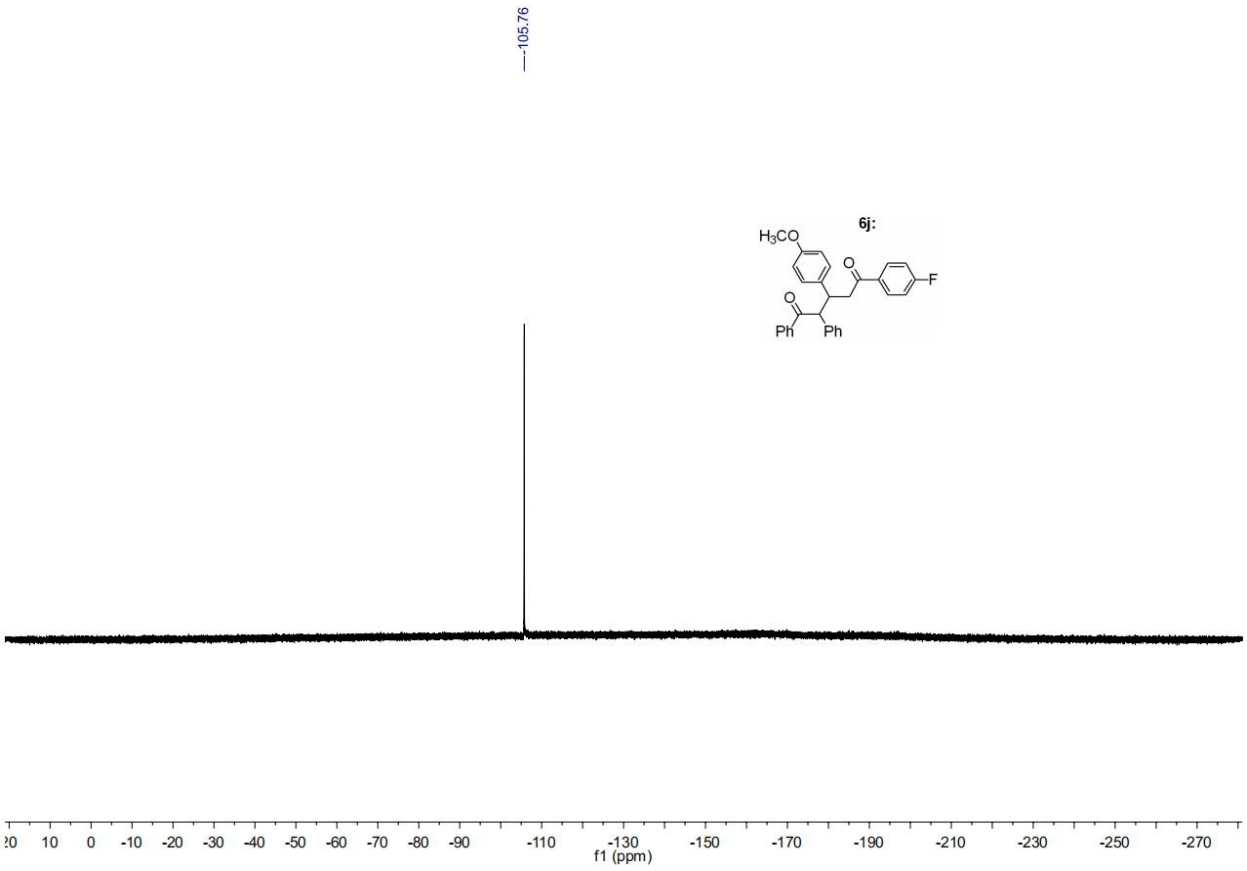
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30
f1 (ppm)


7.81
7.79
7.65
7.63
7.49
7.47
7.44
7.42
7.40
7.34
7.33
7.31
7.29
7.28
7.26
7.25
7.23
7.22
7.13
7.11
6.82
6.80
5.12
5.09
4.36
4.35
4.34
4.33
4.31
4.30
3.80
3.14
3.12
3.10
3.08
3.02
3.01
2.98
2.97
6i:
Cl
O
OCH3
O
Ph
Ph
2.00
2.00
2.00
1.00
7.32
2.00
2.00
1.00
1.00
3.00
1.00
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

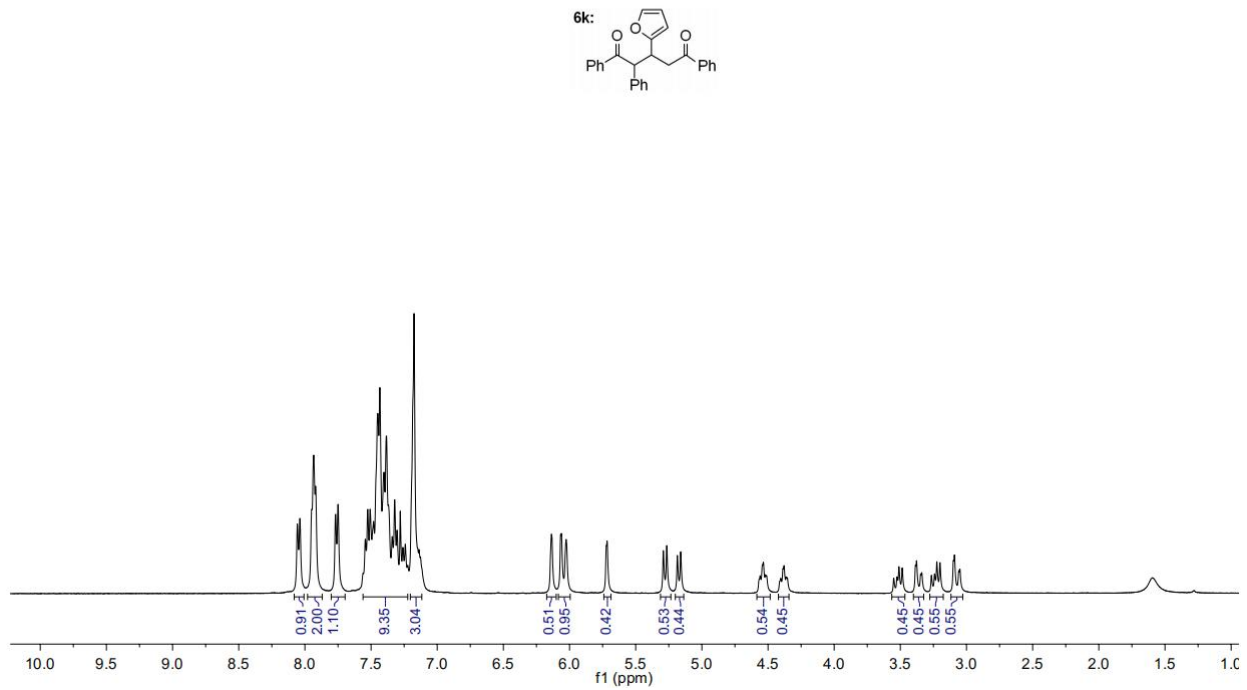

198.43
196.88
163.35
141.27
137.01
136.84
132.90
132.13
130.16
129.67
129.23
129.14
128.49
128.43
128.33
127.87
113.59
77.35
77.04
76.72
58.55
55.43
44.17
42.19
6i:
Cl
O
OCH3
O
Ph
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


6j:
H3CO
O
F
O
Ph
Ph
2.00
2.00
2.02
1.04
4.06
3.02
2.00
1.97
1.00
1.01
3.00
2.02
f1 (ppm)


6j:
H3CO
O
F
O
Ph
Ph
f1 (ppm)

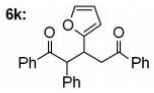

-105.76
6j:
H3CO
O
F
O
Ph
Ph
f1 (ppm)

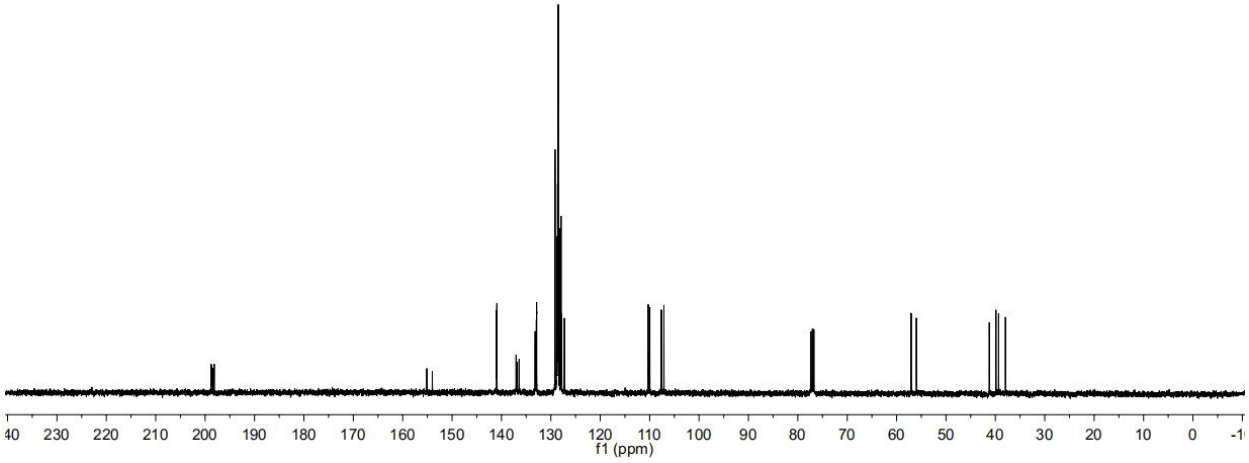

8.06
8.04
7.95
7.93
7.92
7.77
7.75
7.56
7.54
7.53
7.51
7.48
7.45
7.43
7.40
7.38
7.37
7.34
7.32
7.30
7.28
7.26
7.24
7.22
7.18
7.14
7.13
6.14
6.07
6.06
6.03
5.72
5.29
5.27
5.19
5.16
4.56
4.54
4.54
4.52
4.51
4.39
4.38
3.52
3.51
3.49
3.39
3.38
3.35
3.34
3.27
3.24
3.22
3.20
3.10
3.09
3.06
3.05

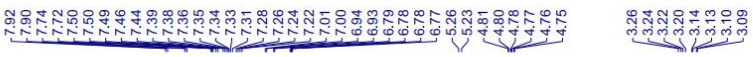

6k:
O
O
Ph
Ph
Ph
0.91
2.00
1.10
9.35
3.04
0.51
0.95
0.42
0.53
0.44
0.54
0.45
0.45
0.45
0.55
0.55
f1 (ppm)


198.81
198.74
198.43
198.15
155.11
154.00
140.93
132.88
129.14
128.80
128.64
128.62
128.51
128.47
128.41
128.20
110.29
109.96
107.62
107.11
77.38
77.06
76.74
57.05
56.00
41.23
39.88
39.35
37.96

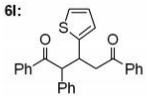
6k:

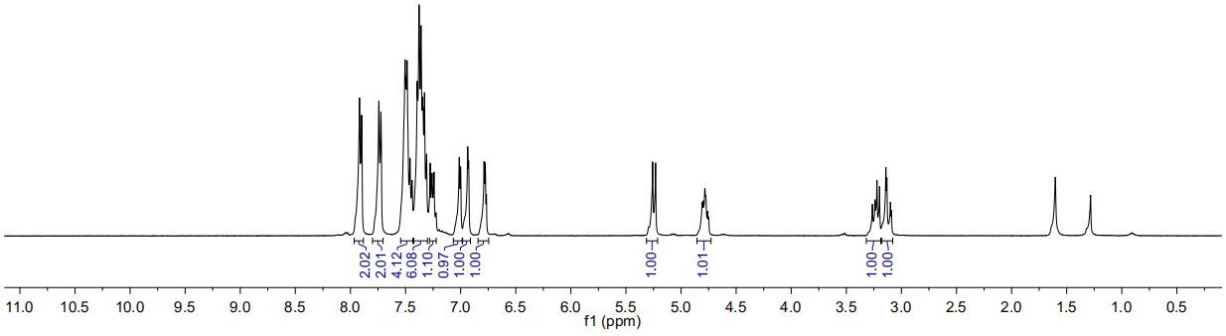

O
O
Ph
O
Ph
Ph

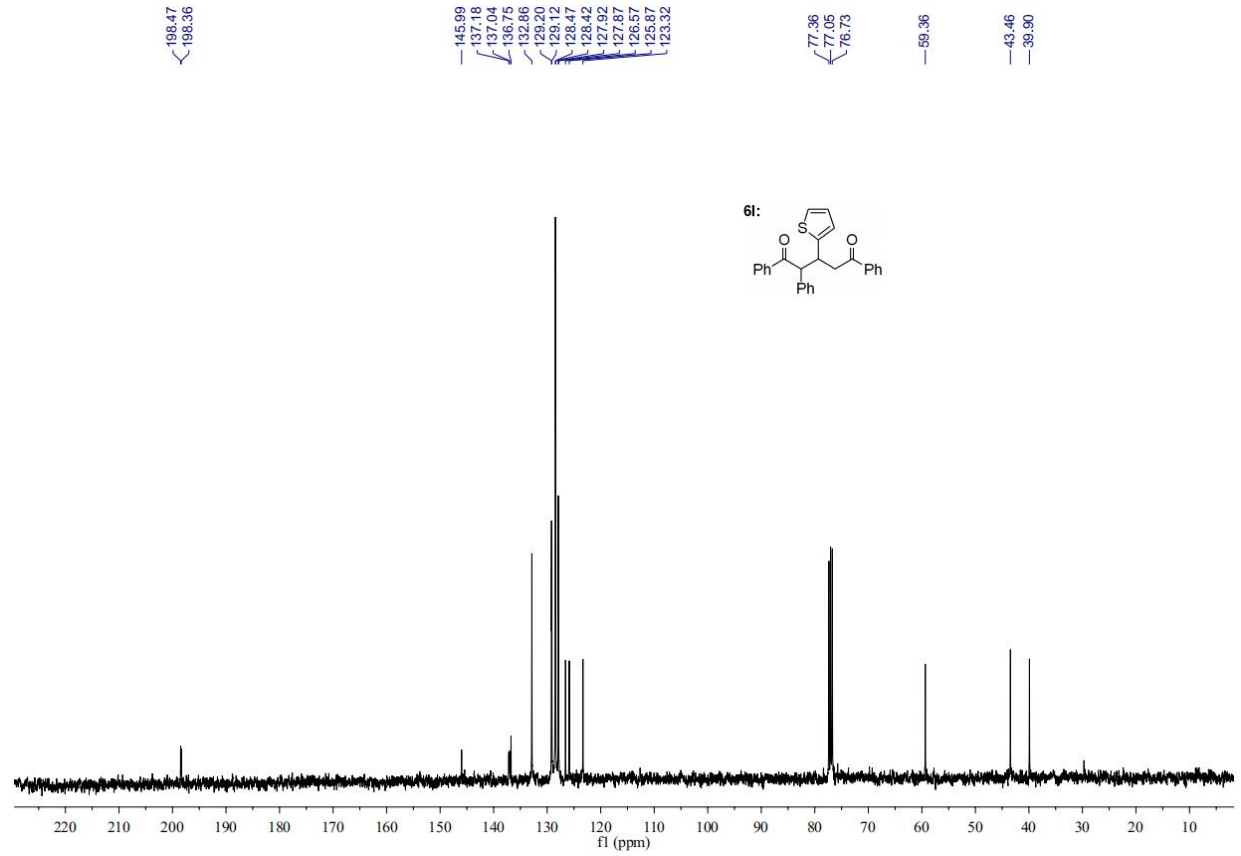

40 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

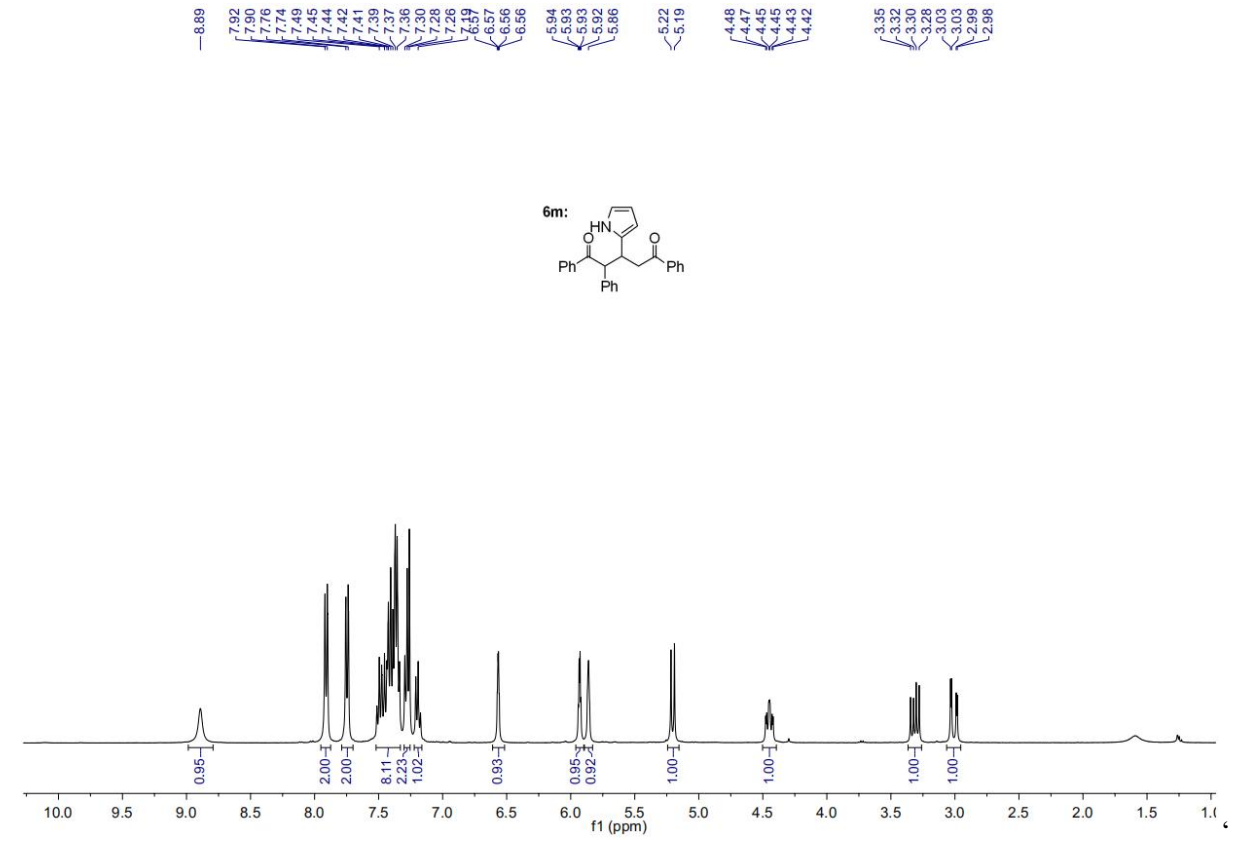

7.92
7.90
7.74
7.72
7.50
7.50
7.49
7.46
7.44
7.39
7.38
7.36
7.35
7.34
7.33
7.31
7.28
7.26
7.24
7.22
7.01
7.00
6.94
6.93
6.79
6.78
6.77
5.26
5.23
4.81
4.80
4.78
4.77
4.76
4.75
3.26
3.24
3.22
3.20
3.14
3.13
3.10
3.09

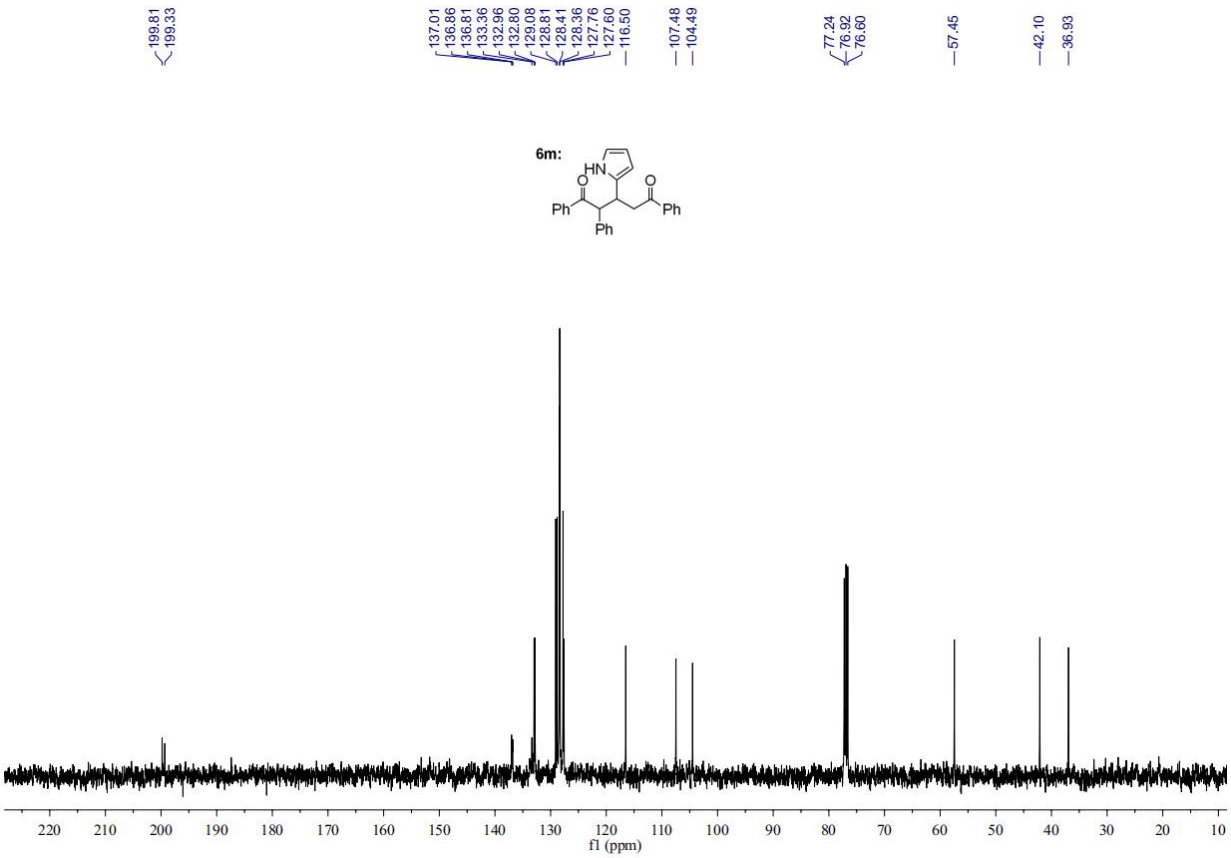
6l:

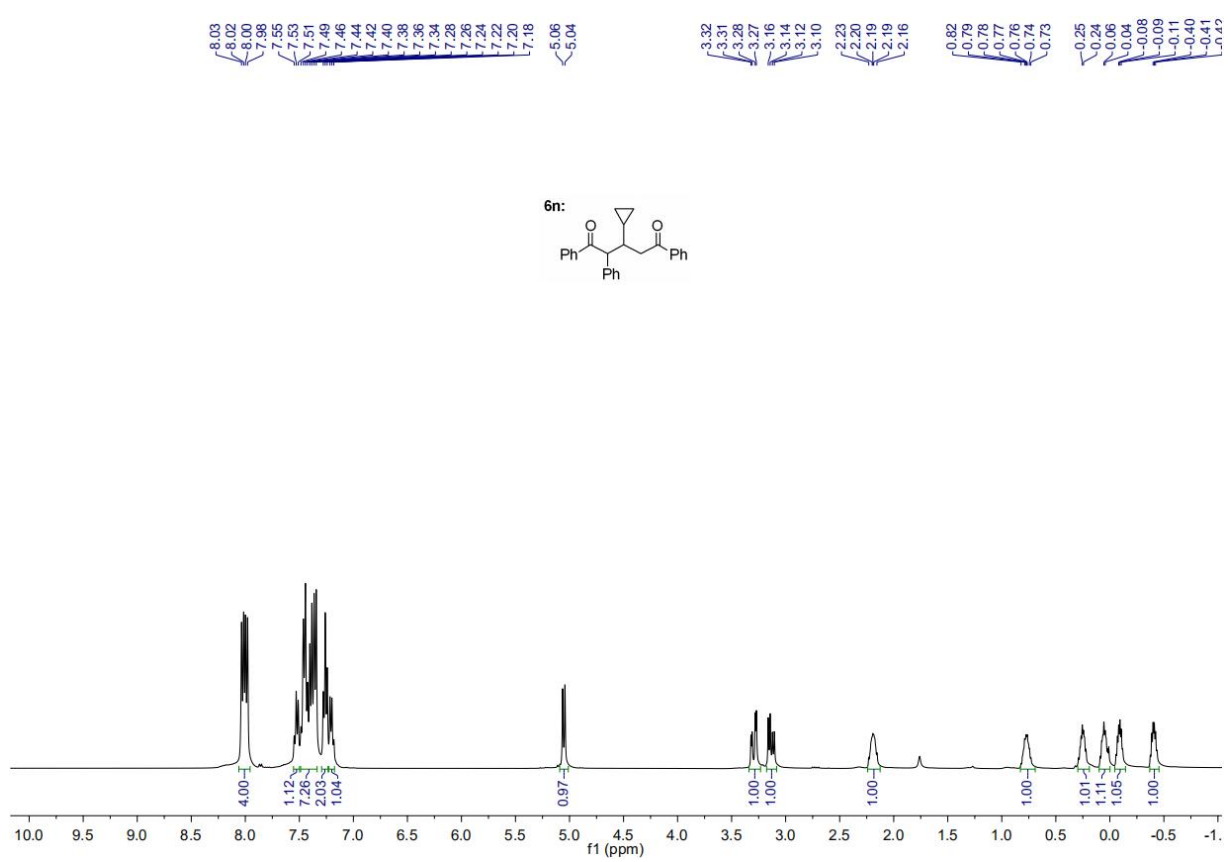

S
O
Ph
O
Ph
Ph


2.02
2.01
4.12
6.08
1.10
0.97
1.00
1.00
1.00
1.01
1.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (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
77.36
77.05
76.73
59.36
43.46
39.90
6l:
S
O
Ph
Ph
O
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

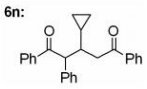

8.89
7.92
7.90
7.76
7.74
7.49
7.45
7.44
7.42
7.41
7.39
7.37
7.36
7.30
7.28
7.26
7.19
6.57
6.56
6.56
5.94
5.93
5.93
5.92
5.86
5.22
5.19
4.48
4.47
4.45
4.45
4.43
4.42
3.35
3.32
3.30
3.28
3.03
3.03
2.99
2.98
6m:
HN
O
Ph
Ph
O
Ph
0.95
2.00
2.00
8.11
2.23
1.02
0.93
0.95
0.92
1.00
1.00
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)

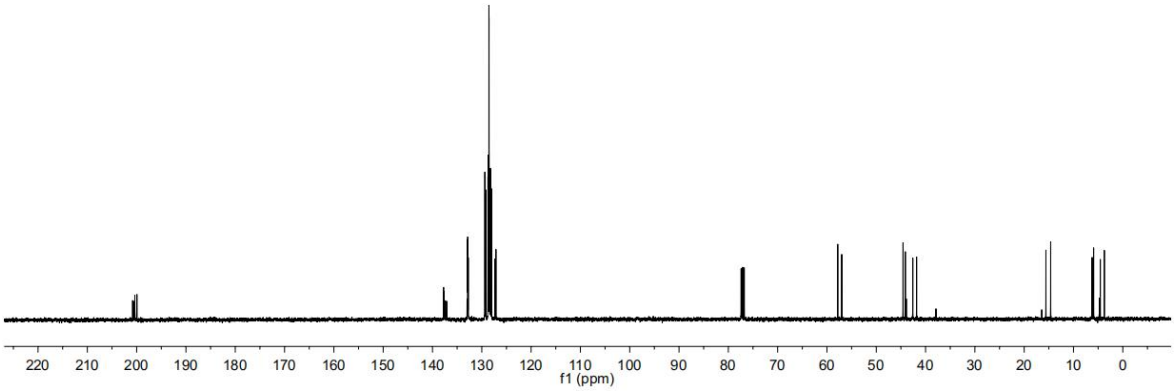

199.81
199.33
137.01
136.86
136.81
133.36
132.96
132.80
129.08
128.81
128.41
128.36
127.76
127.60
116.50
107.48
104.49
77.24
76.92
76.60
57.45
42.10
36.93
6m:
HN
O
O
Ph
Ph
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.03
8.02
8.00
7.98
7.55
7.53
7.51
7.49
7.46
7.44
7.42
7.40
7.38
7.36
7.34
7.28
7.26
7.24
7.22
7.20
7.18
5.06
5.04
3.32
3.31
3.28
3.27
3.16
3.14
3.12
3.10
2.23
2.20
2.19
2.19
2.16
0.82
0.79
0.78
0.77
0.76
0.74
0.73
0.25
0.24
0.06
0.04
-0.08
-0.09
-0.11
-0.40
-0.41
6n:
O
O
Ph
Ph
Ph
4.00
1.12
7.26
2.03
1.04
0.97
1.00
1.00
1.00
1.00
1.01
1.11
1.05
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


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
128.59
128.57
128.54
128.52
128.46
128.27
128.22
128.05
127.30
127.14
77.42
77.10
76.78
57.81
57.01
44.58
44.11
42.59
41.82
15.60
14.63
6.23
5.91
4.56
3.74

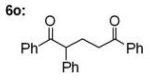
6n:


O
O
Ph
Ph
Ph

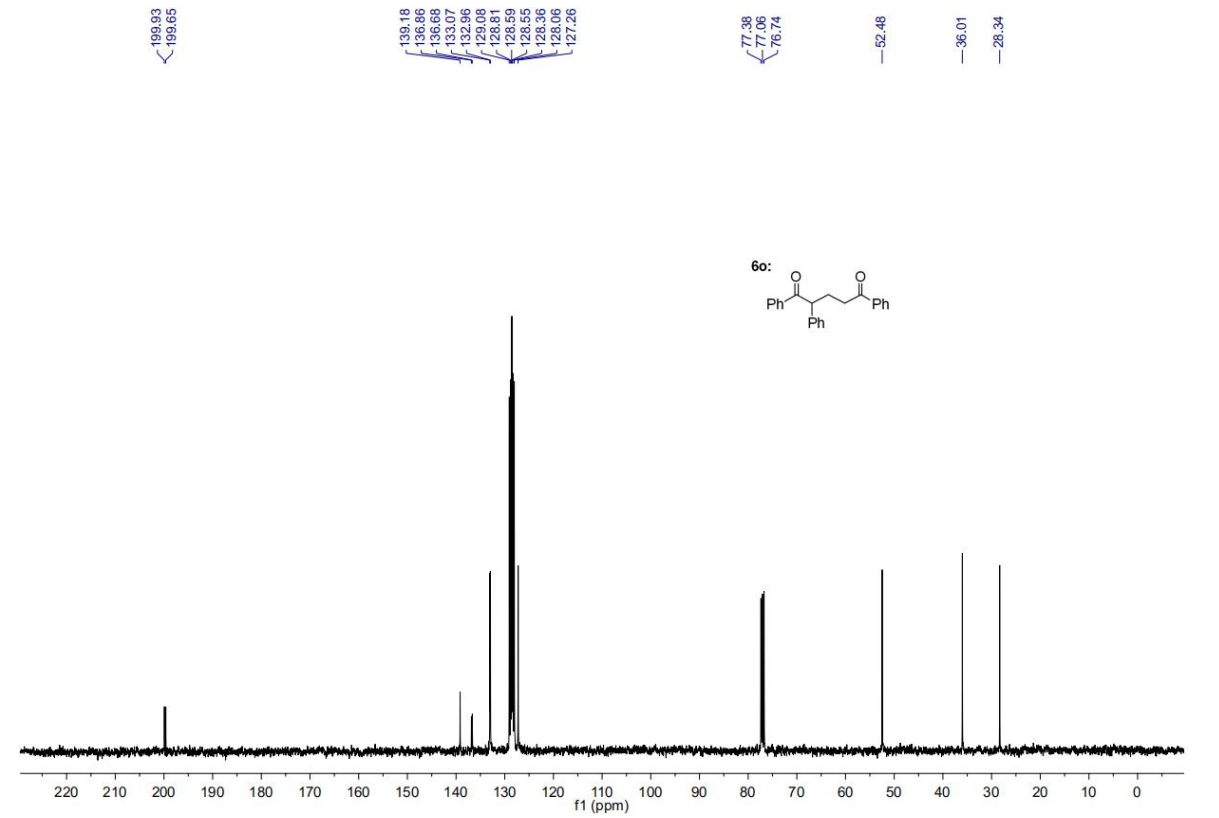

220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.99
7.97
7.97
7.91
7.89
7.89
7.56
7.56
7.55
7.54
7.54
7.53
7.52
7.52
7.52
7.50
7.49
7.49
7.48
7.48
7.47
7.46
7.46
7.45
7.45
7.43
7.41
7.41
7.40
7.38
7.37
7.36
7.33
7.32
7.31
7.30
7.29
7.28
7.27
7.27
7.26
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.19
7.19
4.80
4.78
4.76
3.06
3.04
3.02
3.02
3.00
2.98
2.97
2.95
2.93
2.92
2.91
2.89
2.63
2.62
2.60
2.58
2.56
2.55
2.33
2.31
2.29
2.27
2.26
2.24

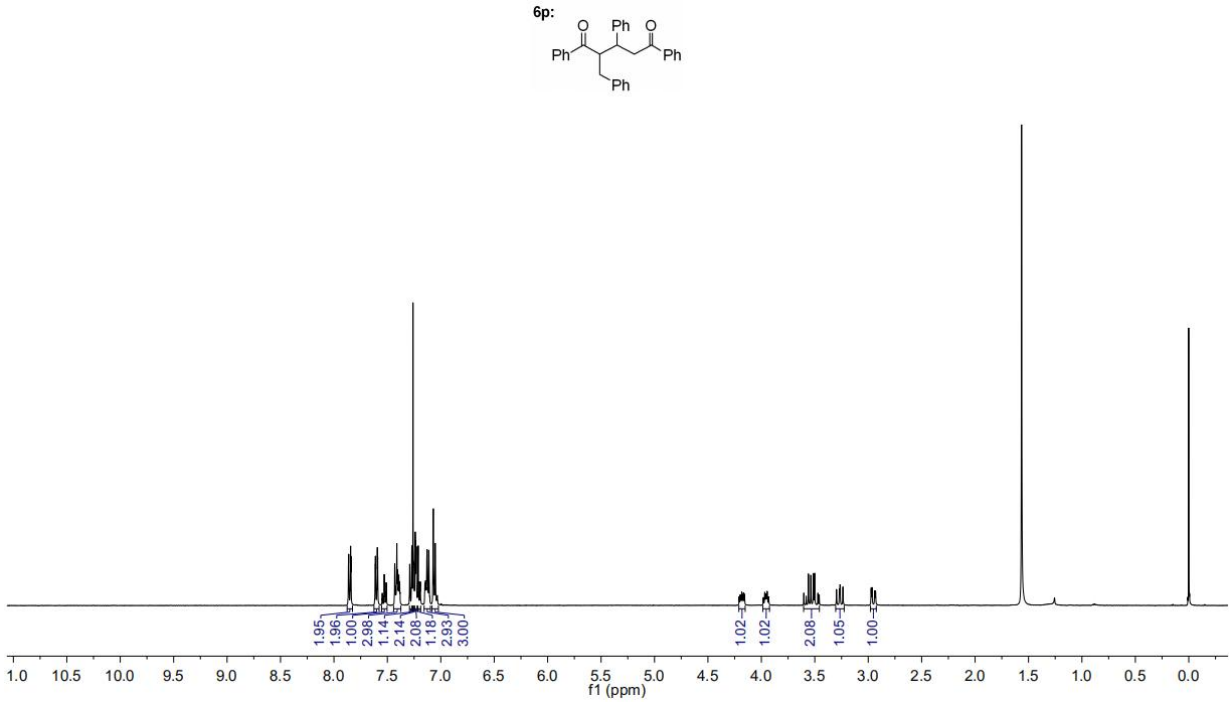
6o:

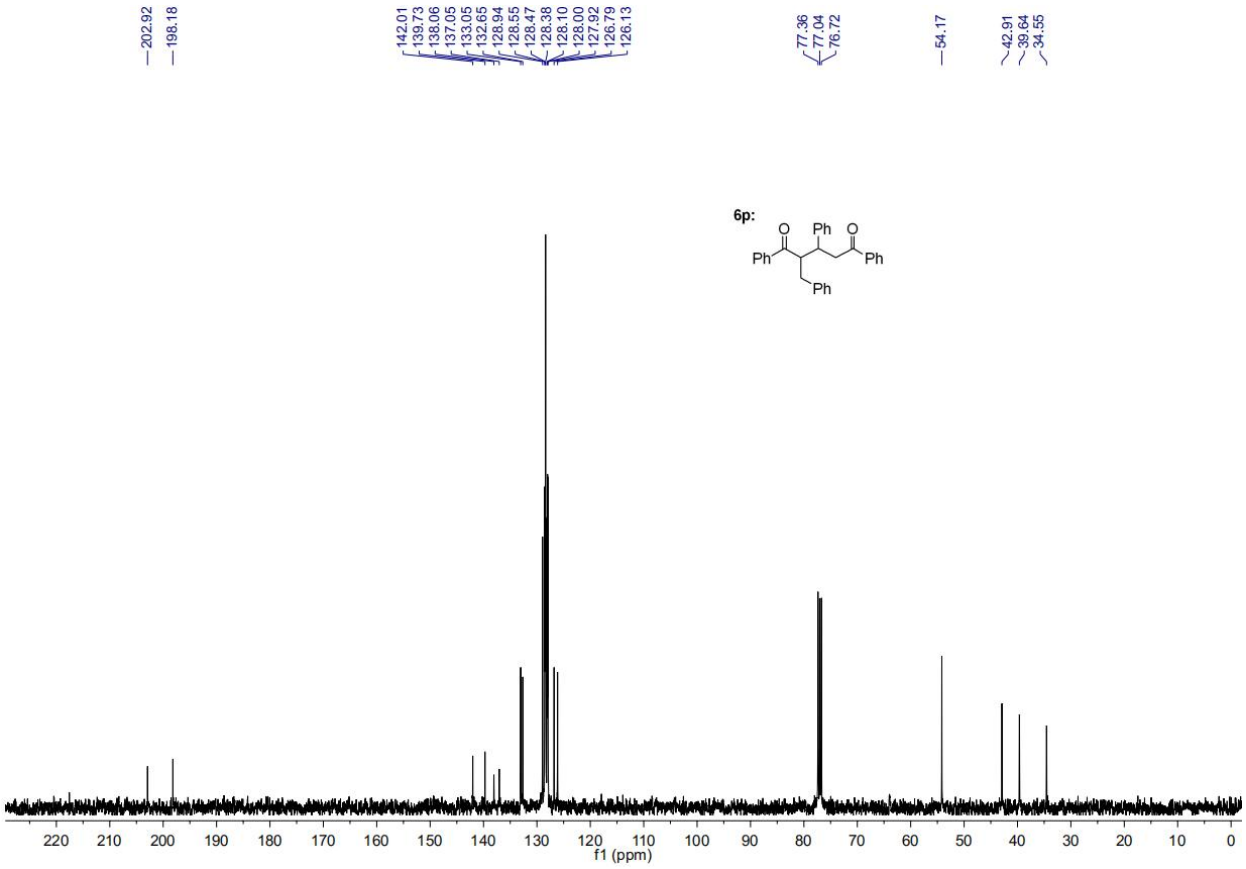

O
O
Ph
Ph
Ph

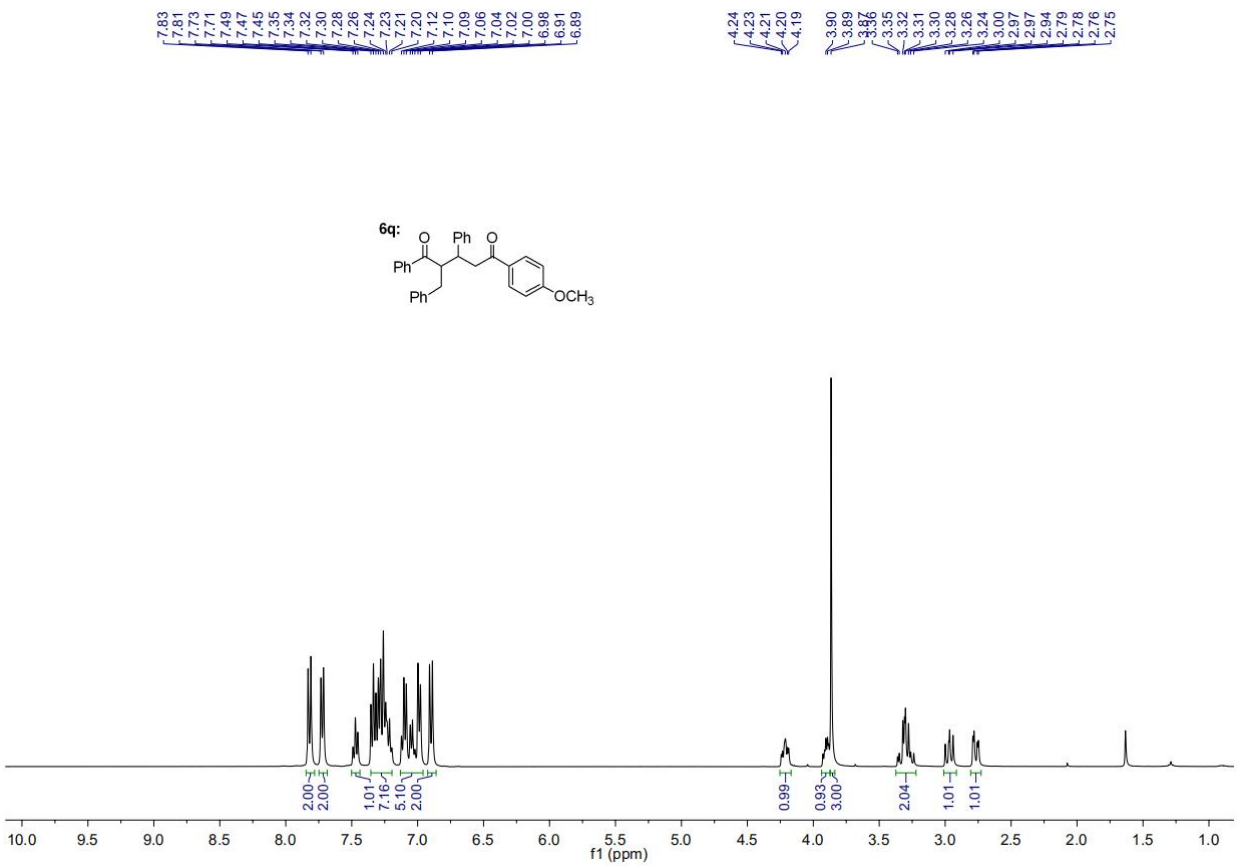
1.97
1.95
6.07
3.98
1.00
1.00
2.02
1.00
1.01
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

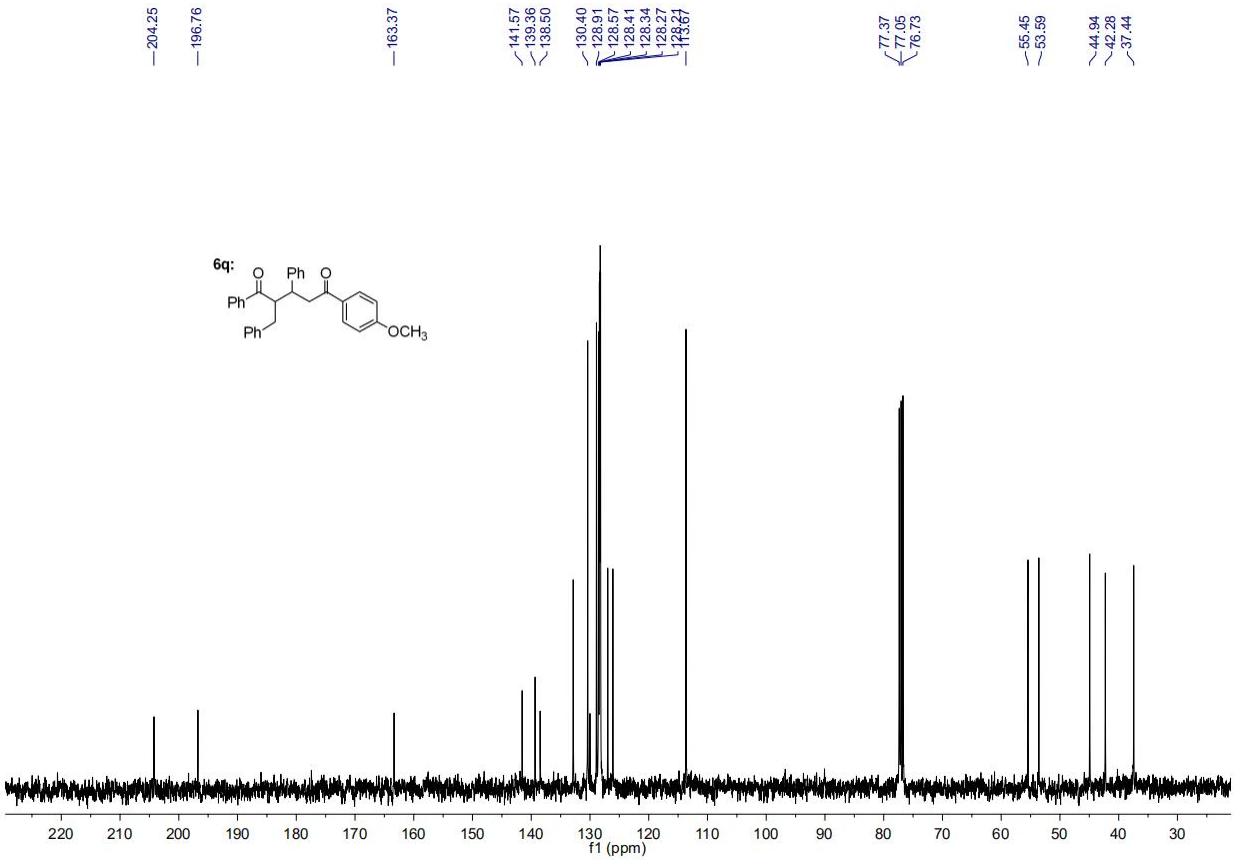

199.93
199.65
139.18
136.86
136.68
133.07
132.96
129.08
128.81
128.59
128.55
128.36
128.06
127.26
77.38
77.06
76.74
52.48
36.01
28.34
6o:
Ph
O
O
Ph
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.86 7.86 7.85 7.84 7.84 7.61 7.61 7.60 7.59 7.59 7.55 7.53 7.52 7.51 7.51 7.51 7.43 7.42 7.42 7.41 7.41 7.40 7.40 7.39 7.39 7.38 7.38 7.29 7.29 7.27 7.26 7.25 7.24 7.24 7.23 7.22 7.21 7.21 7.20 7.19 7.15 7.15 7.14 7.14 7.13 7.13 7.12 7.11 7.07 7.05 4.19 4.18 4.18 4.17 4.16 3.97 3.96 3.95 3.95 3.60 3.56 3.54 3.51 3.50 3.47 3.46 3.30 3.27 3.26 3.24 2.97 2.96 2.94 2.93

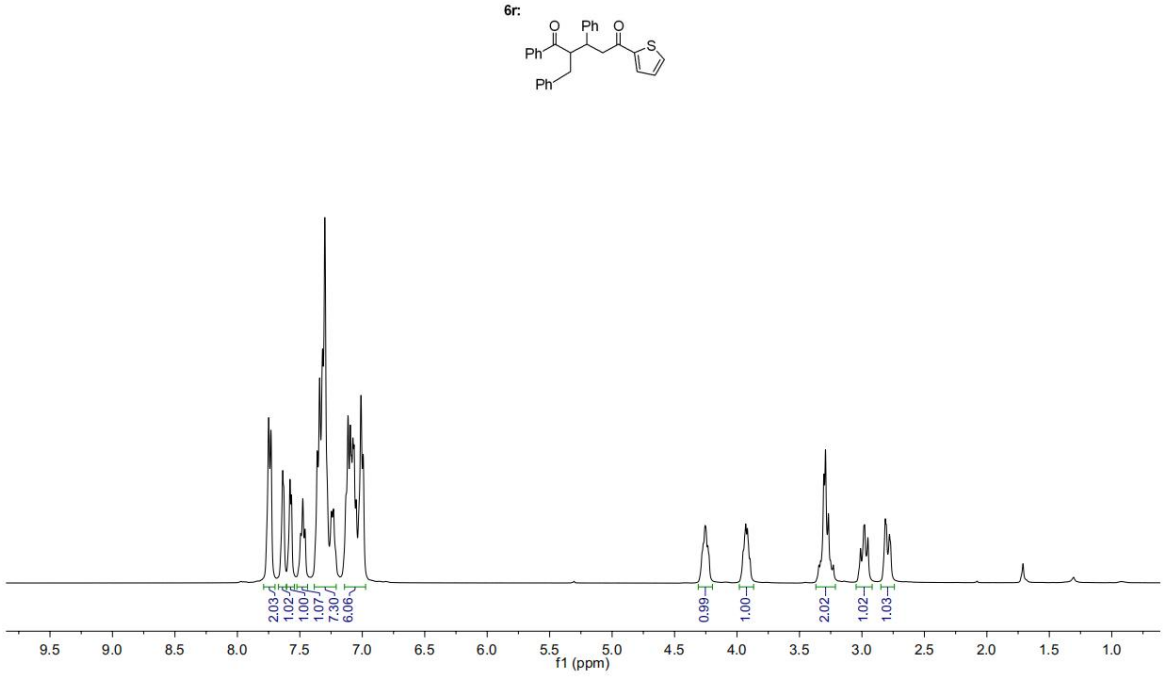

6p:
Ph
O
Ph
O
Ph
Ph
1.95 1.96 1.00 2.98 1.14 2.14 2.08 1.18 2.93 3.00
1.02 1.02 2.08 1.05 1.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

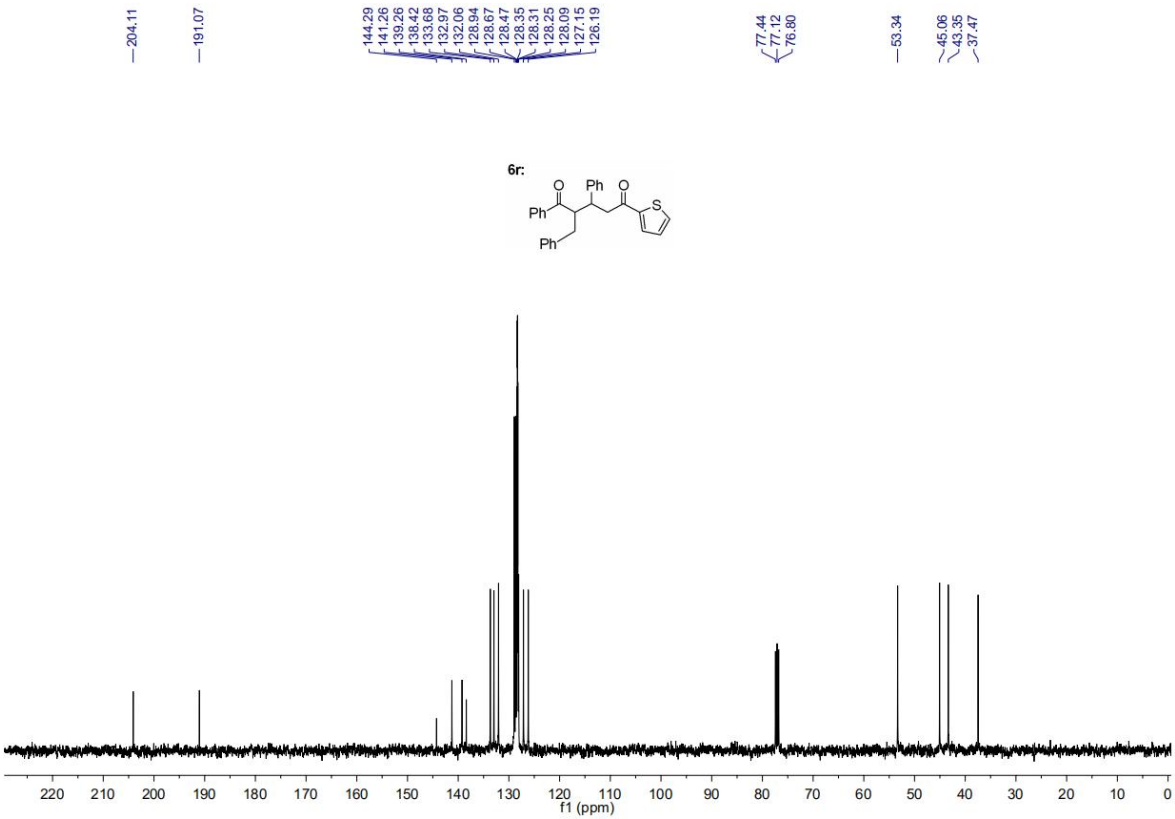

202.92
198.18
142.01
139.73
138.06
137.05
133.05
132.65
128.94
128.55
128.47
128.38
128.10
128.00
127.92
126.79
126.13
77.36
77.04
76.72
54.17
42.91
39.64
34.55
6p:
O
Ph
Ph
O
Ph
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

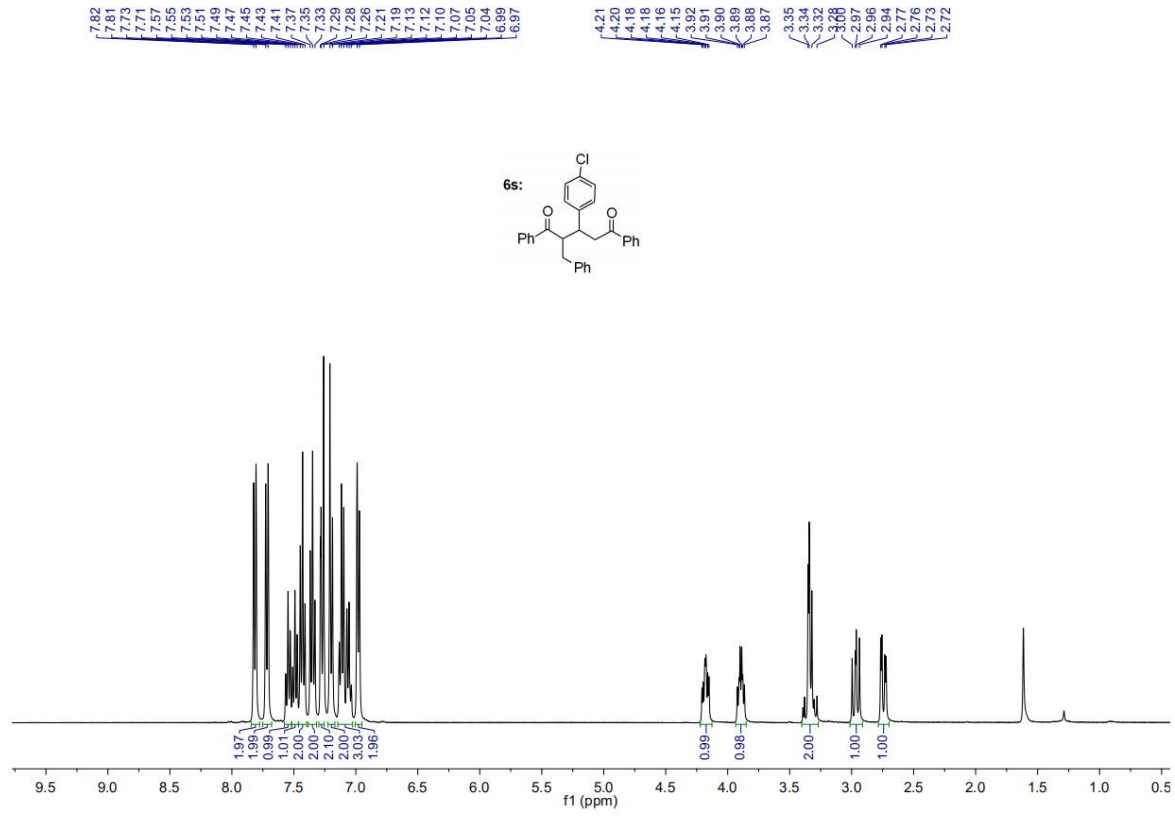

7.83
7.81
7.73
7.71
7.49
7.47
7.45
7.35
7.34
7.32
7.30
7.28
7.26
7.24
7.23
7.21
7.20
7.12
7.10
7.09
7.06
7.04
7.02
7.00
6.98
6.91
6.89
4.24
4.23
4.21
4.20
4.19
3.90
3.89
3.87
3.86
3.35
3.32
3.31
3.30
3.28
3.26
3.24
3.00
2.97
2.97
2.94
2.79
2.78
2.76
2.75
6q:
O
Ph
Ph
O
Ph
OCH3
2.00
2.00
1.01
7.16
5.10
2.00
0.99
0.93
3.00
2.04
1.01
1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)


204.25
196.76
163.37
141.57
139.36
138.50
130.40
128.91
128.57
128.41
128.34
128.27
128.21
113.67
77.37
77.05
76.73
55.45
53.59
44.94
42.28
37.44
6q:
Ph
O
Ph
O
Ph
OCH3
f1 (ppm)


7.75
7.73
7.64
7.58
7.57
7.49
7.48
7.46
7.36
7.34
7.32
7.30
7.25
7.23
7.11
7.10
7.09
7.08
7.07
7.05
7.01
6.99
4.27
4.26
4.23
3.93
3.92
3.90
3.34
3.33
3.31
3.29
3.27
3.25
3.23
3.01
2.98
2.98
2.95
2.81
2.78

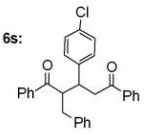

6r:
O
Ph
O
S
Ph
Ph
2.03
1.02
1.00
1.07
7.30
6.06
0.99
1.00
2.02
1.02
1.03
f1 (ppm)

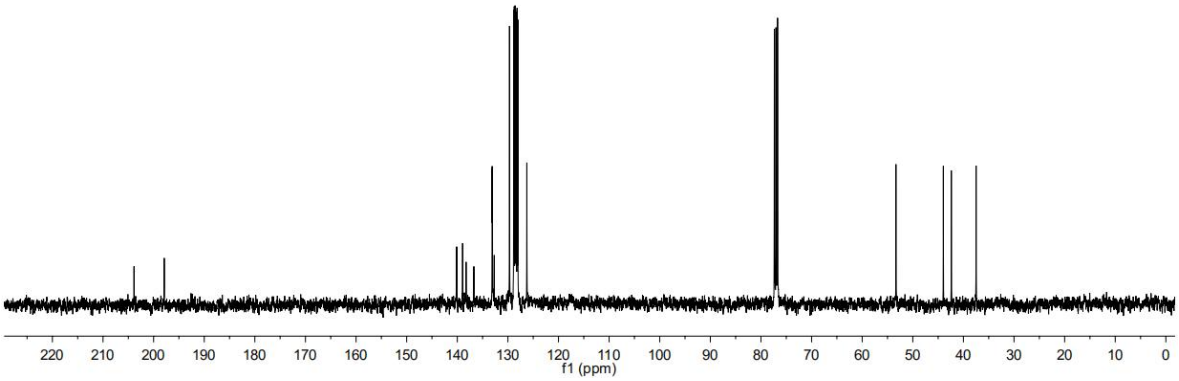

204.11
191.07
144.29
141.26
139.26
138.42
133.68
132.97
132.06
128.94
128.67
128.47
128.35
128.31
128.25
128.09
127.15
126.19
77.44
77.12
76.80
53.34
45.06
43.35
37.47
6r:
Ph
O
Ph
O
S
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.82
7.81
7.73
7.71
7.57
7.55
7.53
7.51
7.49
7.47
7.45
7.43
7.41
7.37
7.35
7.33
7.29
7.28
7.26
7.21
7.19
7.13
7.12
7.10
7.07
7.05
7.04
6.99
6.97
4.21
4.20
4.18
4.18
4.16
4.15
3.92
3.91
3.90
3.89
3.88
3.87
3.35
3.34
3.32
2.97
2.96
2.94
2.77
2.76
2.73
2.72
6s:
Cl
O
Ph
O
Ph
Ph
1.97
1.99
0.99
1.01
2.00
2.00
2.10
2.00
3.03
1.96
0.99
0.98
2.00
1.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (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
77.36
77.04
76.73
53.33
43.97
42.39
37.49

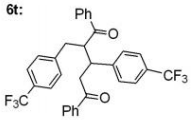
6s:

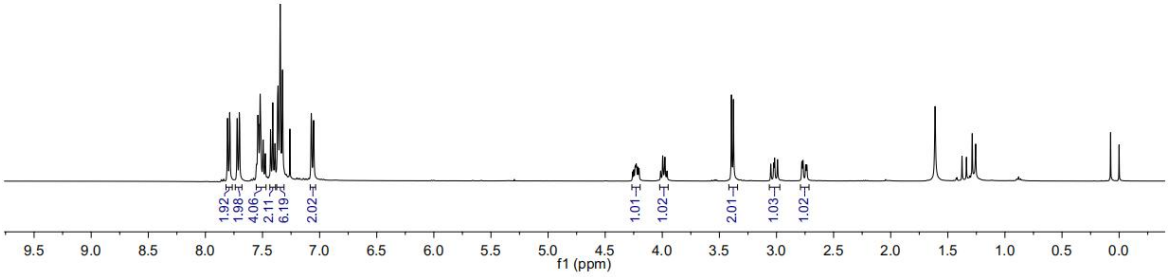

Cl
O
Ph
O
Ph
Ph

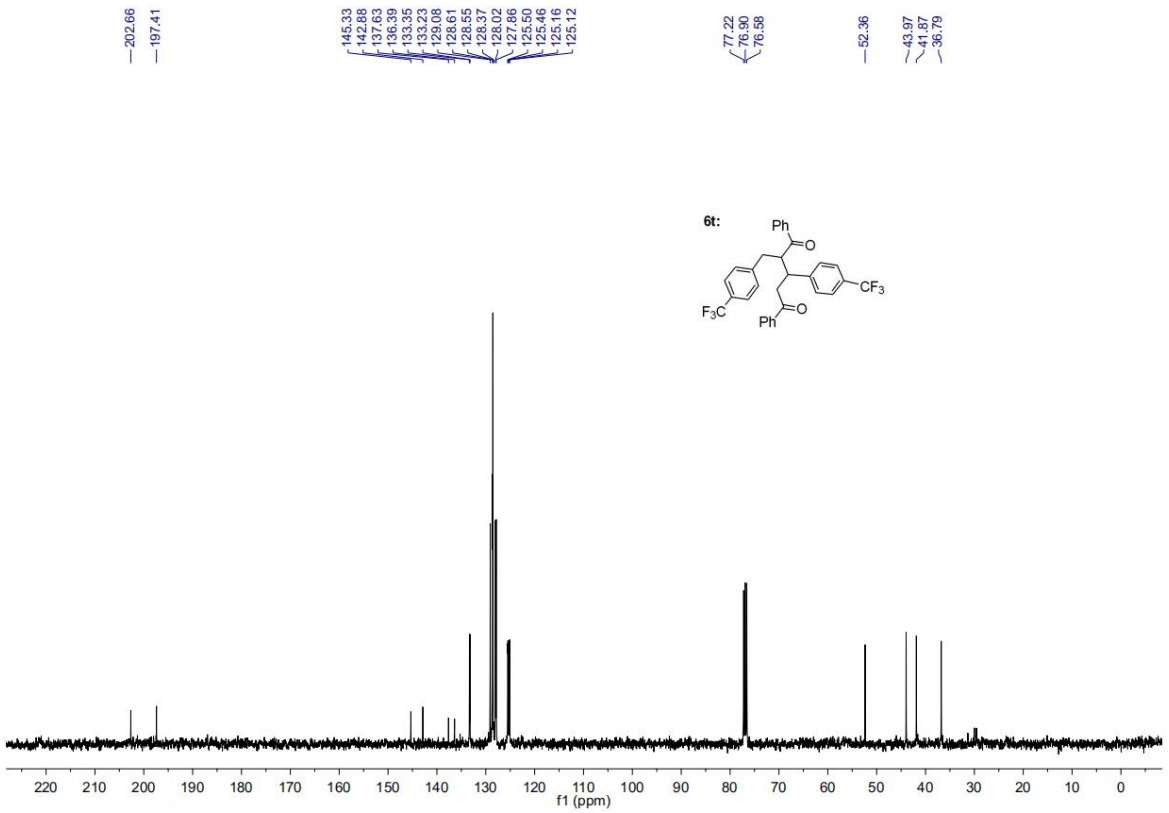

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.81
7.79
7.72
7.70
7.55
7.54
7.54
7.52
7.49
7.48
7.43
7.41
7.39
7.36
7.35
7.32
7.26
7.07
7.05
4.26
4.25
4.24
4.23
4.23
4.21
4.20
4.01
4.00
3.98
3.96
3.39
3.38
3.05
3.02
3.02
2.99
2.78
2.77
2.74
2.73

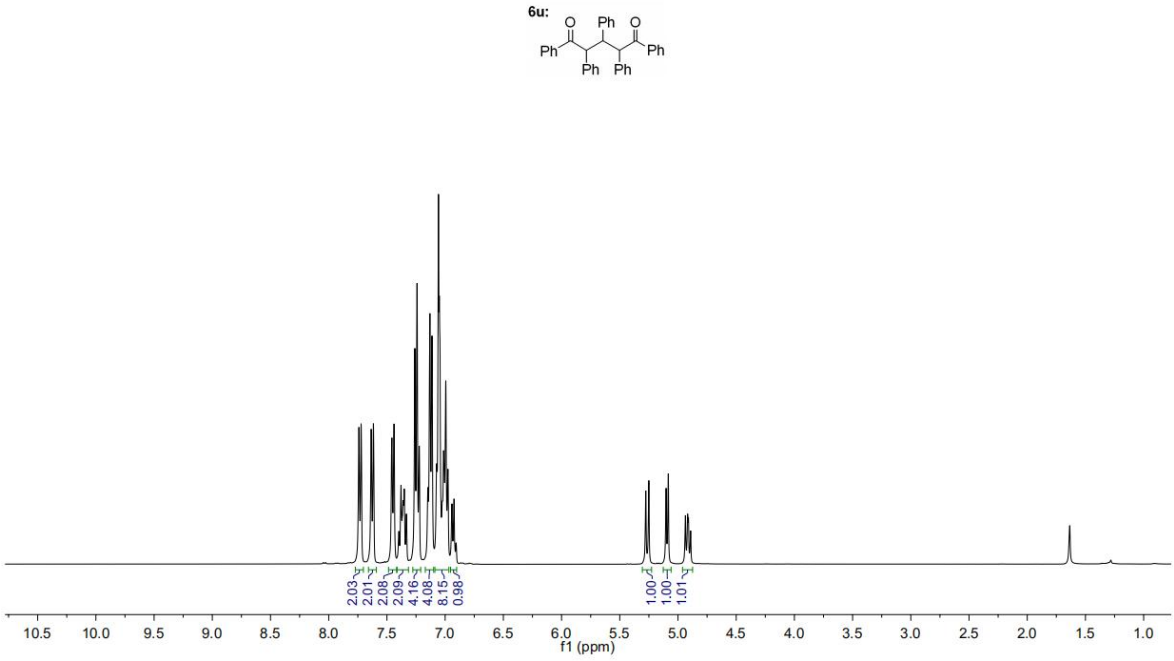
6t:

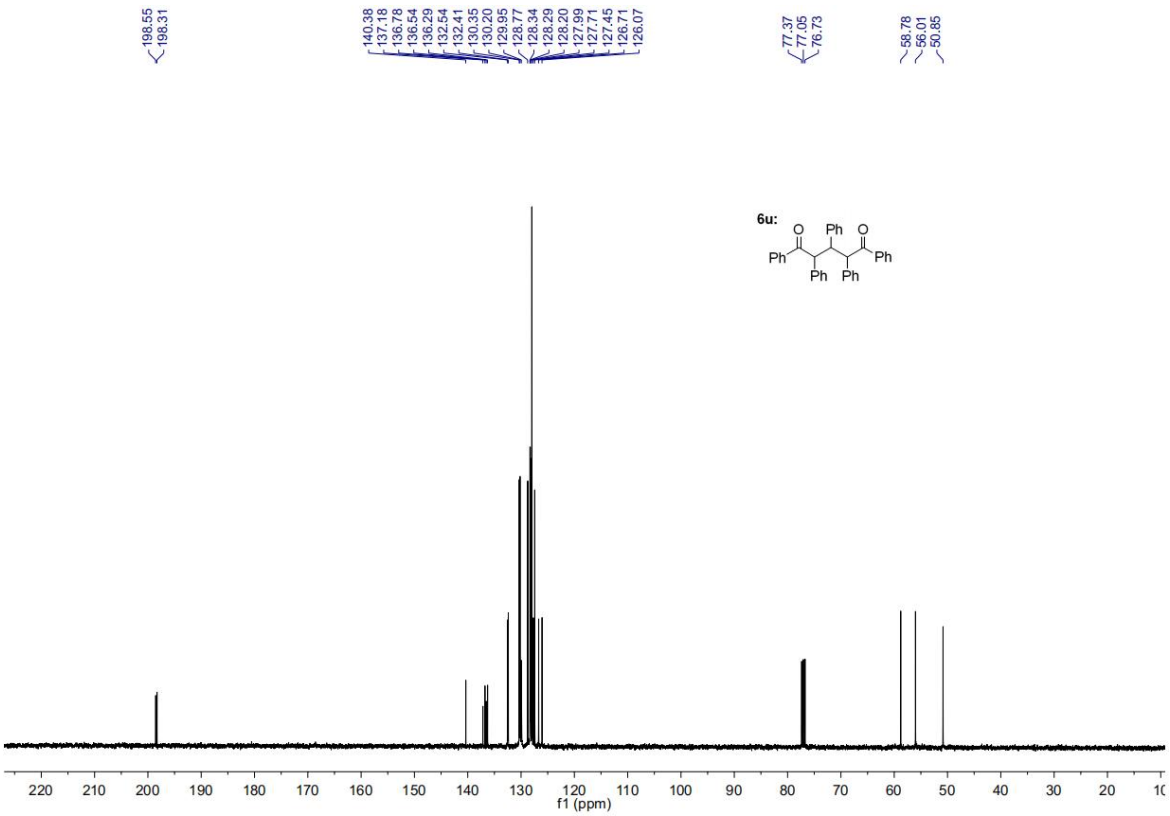

Ph
O
CF3
F3C
Ph
O

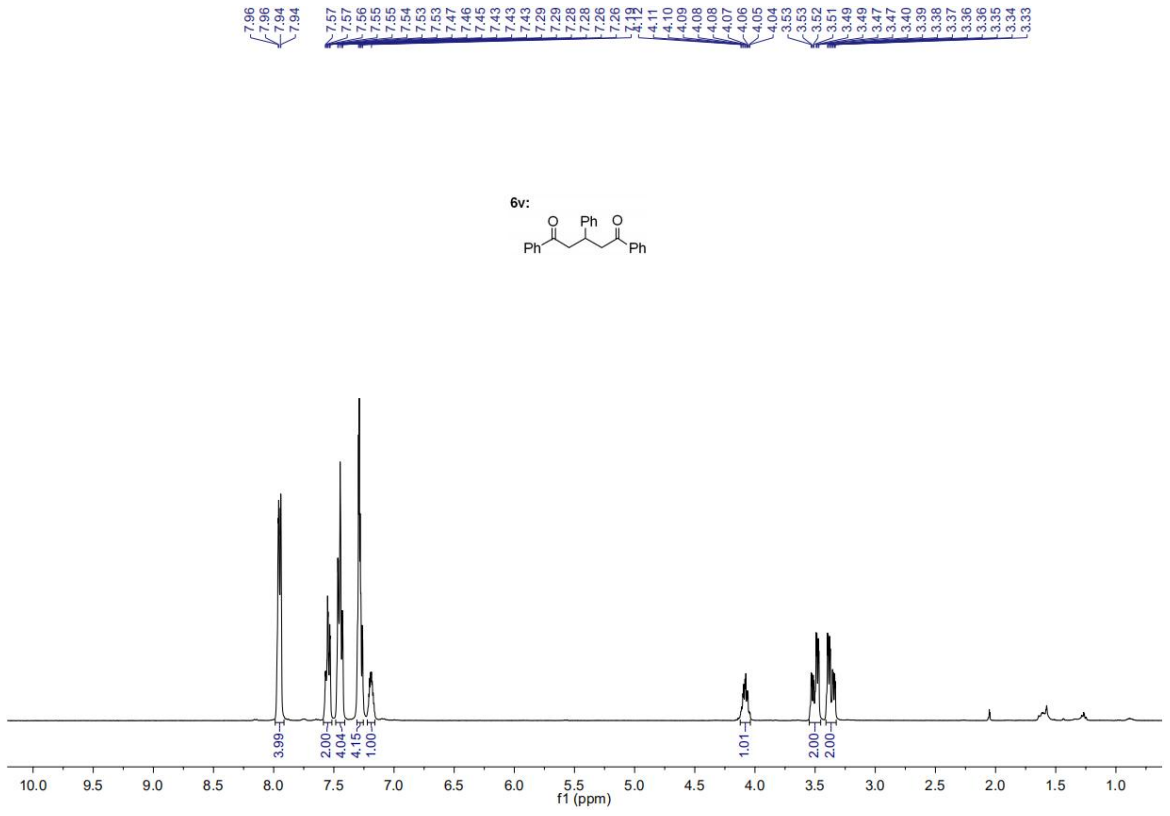

1.92
1.98
4.06
2.11
6.19
2.02
1.01
1.02
2.01
1.03
1.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


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
125.50
125.46
125.16
125.12
77.22
76.90
76.58
52.36
43.97
41.87
36.79
6t:
Ph
O
CF3
F3C
O
Ph
f1 (ppm)


7.74
7.72
7.64
7.62
7.46
7.44
7.40
7.38
7.36
7.35
7.33
7.26
7.24
7.22
7.15
7.13
7.11
7.07
7.06
7.05
7.02
7.01
6.99
6.98
6.94
6.92
6.91
5.28
5.25
5.10
5.08
4.94
4.92
4.91
4.89

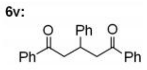

6u:
O
Ph
Ph
O
Ph
Ph
Ph
2.03
2.01
2.08
2.09
4.16
4.08
8.15
0.98
1.00
1.00
1.01
f1 (ppm)

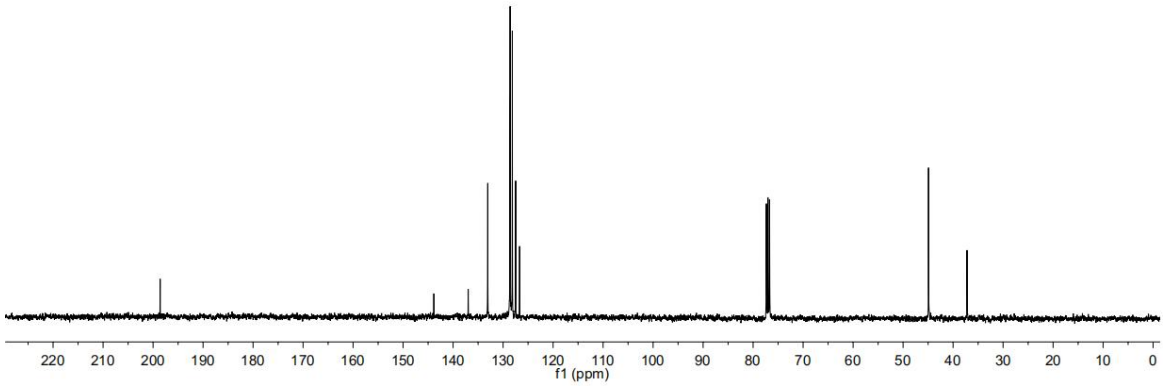

198.55
198.31
140.38
137.18
136.78
136.54
136.29
132.54
132.41
130.35
130.20
129.95
128.77
128.34
128.29
128.20
127.99
127.71
127.45
126.71
126.07
77.37
77.05
76.73
58.78
56.01
50.85
6u:
Ph
O
Ph
O
Ph
Ph
Ph
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


7.96
7.96
7.94
7.94
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.53
7.47
7.46
7.45
7.43
7.43
7.43
7.29
7.29
7.28
7.28
7.26
7.26
4.12
4.11
4.10
4.09
4.08
4.08
4.07
4.06
4.05
4.04
3.53
3.53
3.52
3.51
3.49
3.49
3.47
3.47
3.40
3.39
3.38
3.37
3.36
3.36
3.35
3.34
3.33
6v:
O
Ph
O
Ph
Ph
3.99
2.00
4.04
4.15
1.00
1.01
2.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

198.58
143.85
136.98
133.07
128.63
128.59
128.15
127.48
126.70
77.35
77.03
76.71
44.92
37.22

6v:

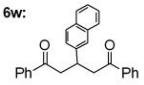


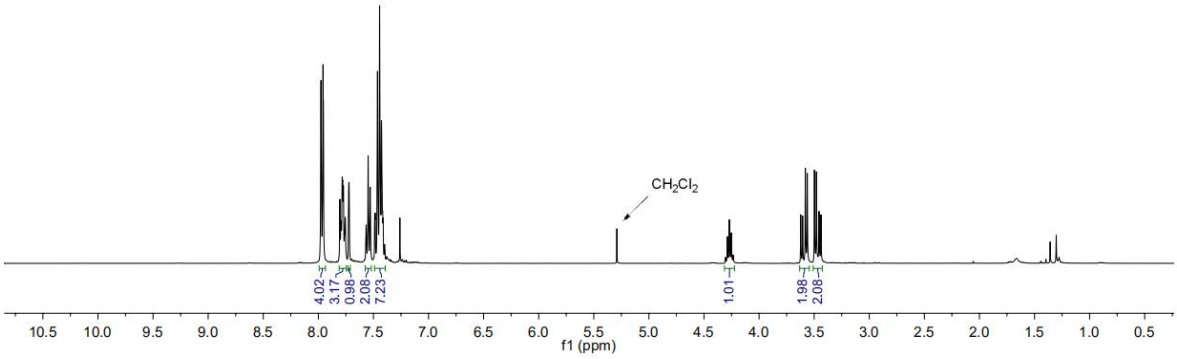


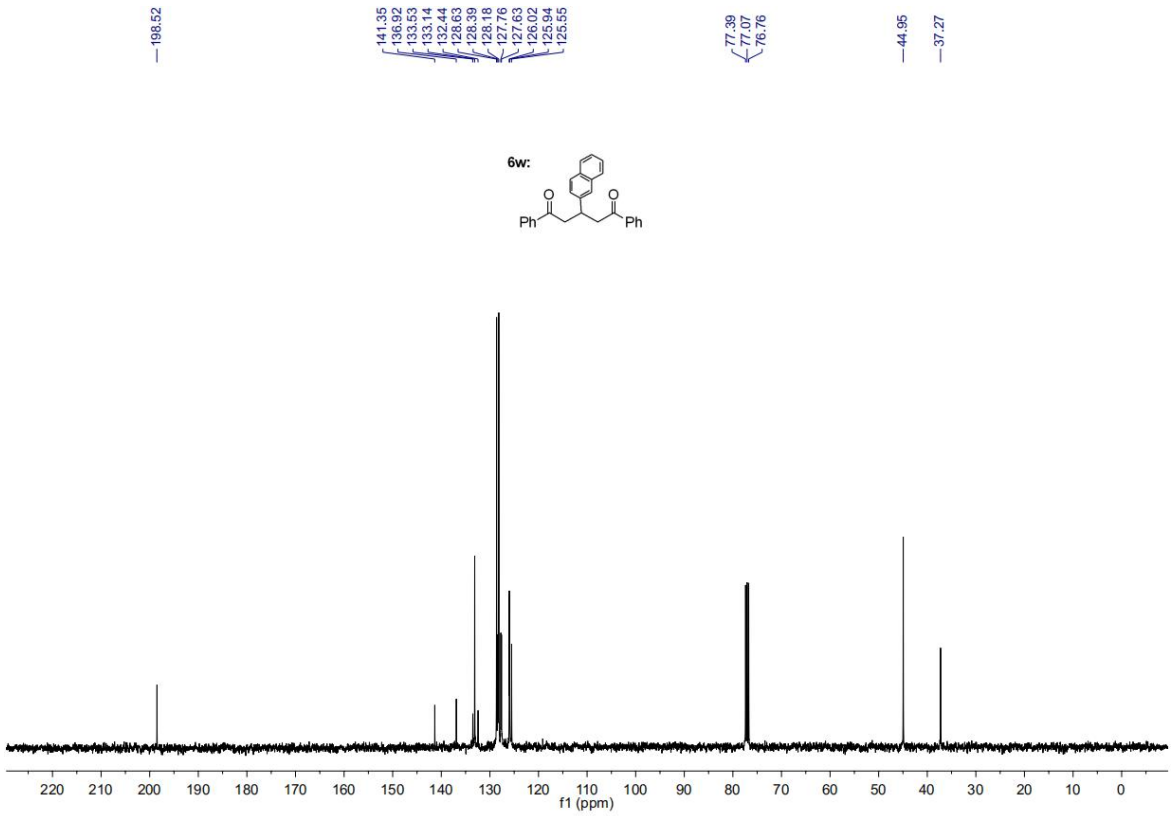
7.98
7.96
7.95
7.80
7.79
7.78
7.78
7.77
7.76
7.72
7.57
7.55
7.53
7.49
7.48
7.46
7.44
7.44
7.43
7.42
7.41
7.40
7.40
7.26

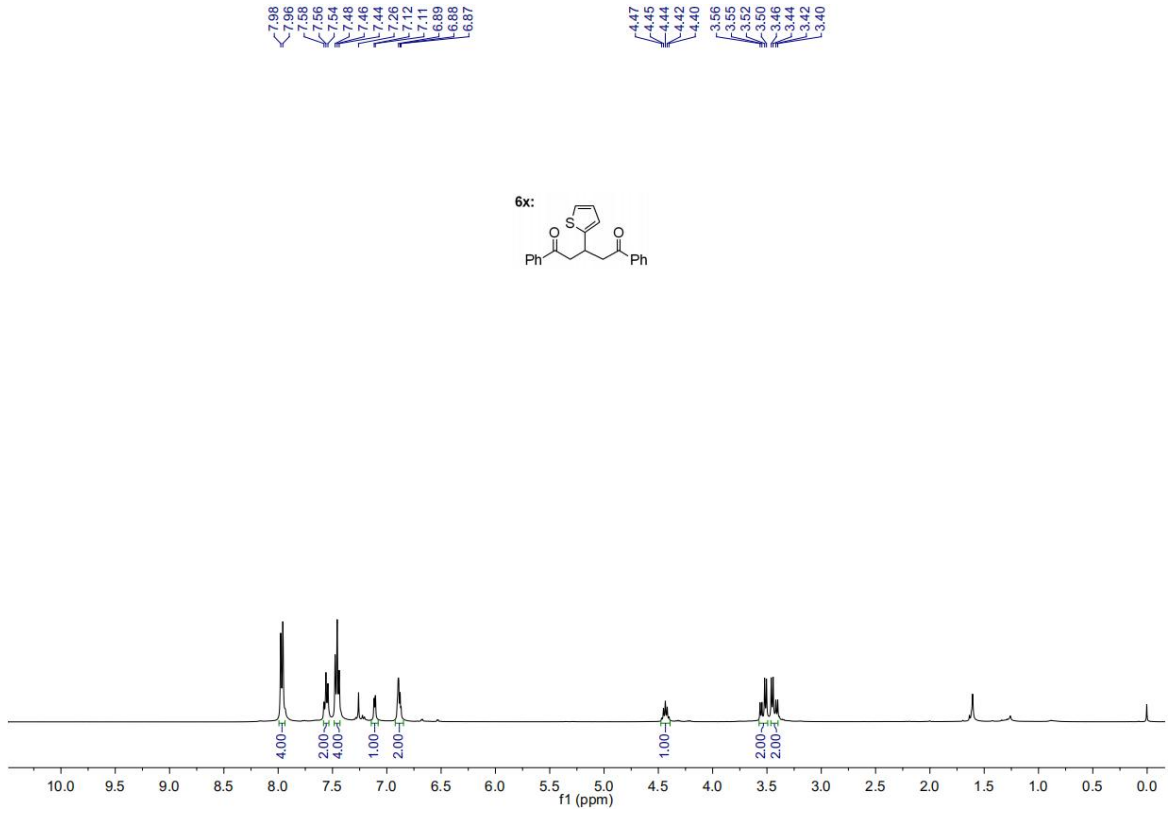
4.31
4.29
4.27
4.25
4.24
3.62
3.60
3.58
3.56
3.50
3.48
3.46
3.44

6w:



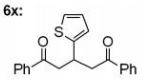


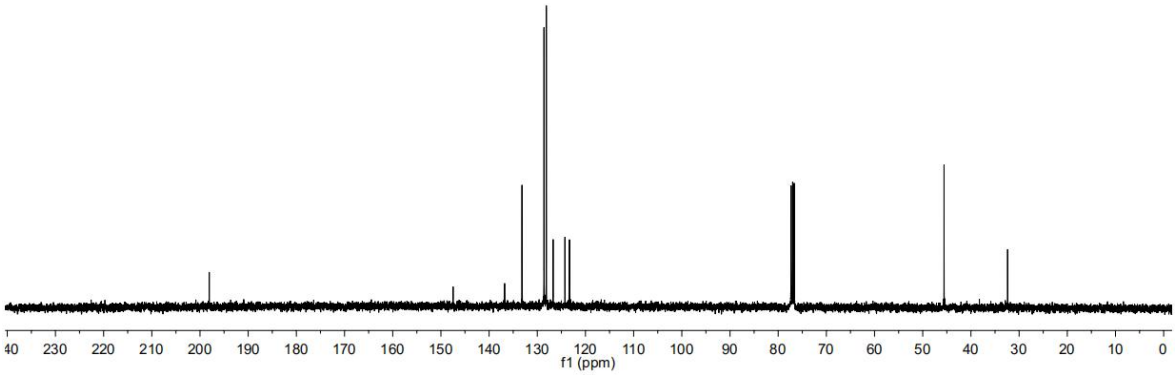

198.52
141.35
136.92
133.53
133.14
132.44
128.63
128.39
128.18
127.76
127.63
126.02
125.94
125.55
77.39
77.07
76.76
44.95
37.27
6w:
Ph
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.98
7.96
7.58
7.56
7.54
7.48
7.46
7.44
7.26
7.12
7.11
6.89
6.88
6.87
4.47
4.45
4.44
4.42
4.40
3.56
3.55
3.52
3.50
3.46
3.44
3.42
3.40
6x:
S
Ph
Ph
4.00
2.00
4.00
1.00
2.00
1.00
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

198.08
147.47
136.78
133.17
128.61
128.12
126.71
124.26
123.32
77.32
77.01
76.69
45.58
32.39

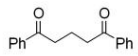
6x:

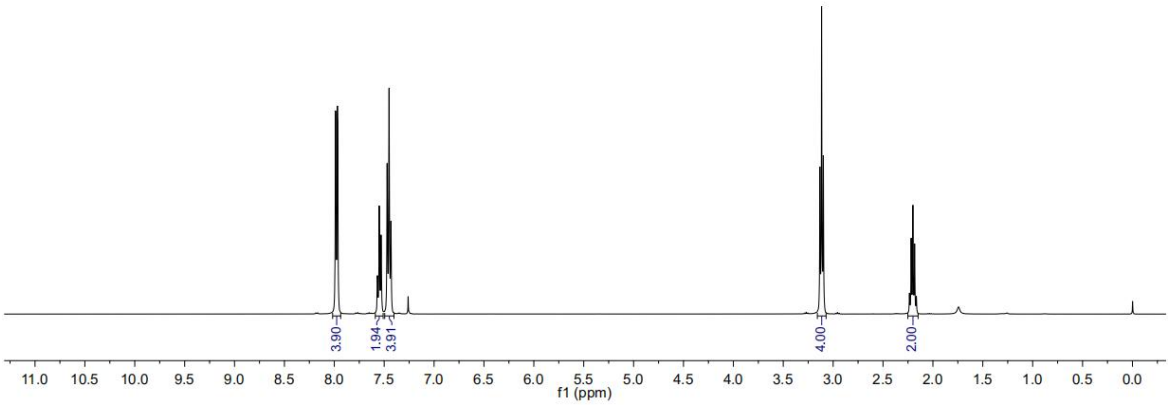


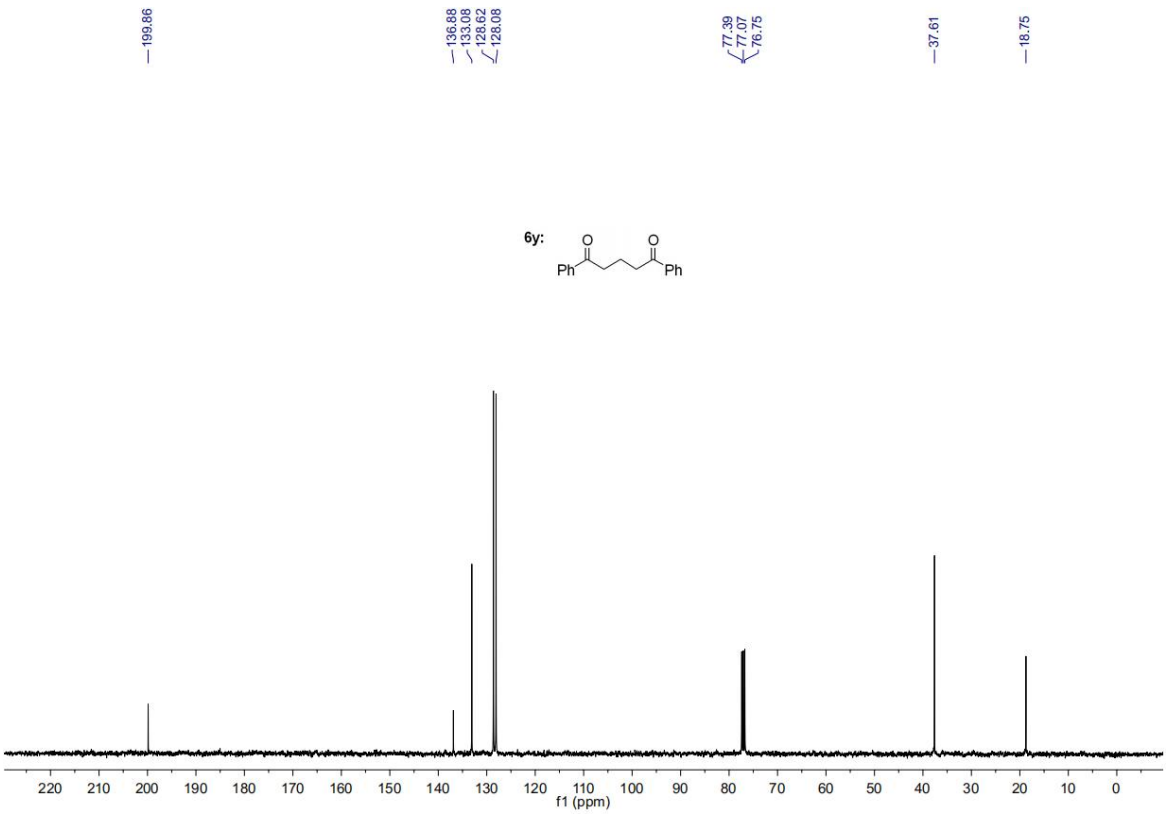


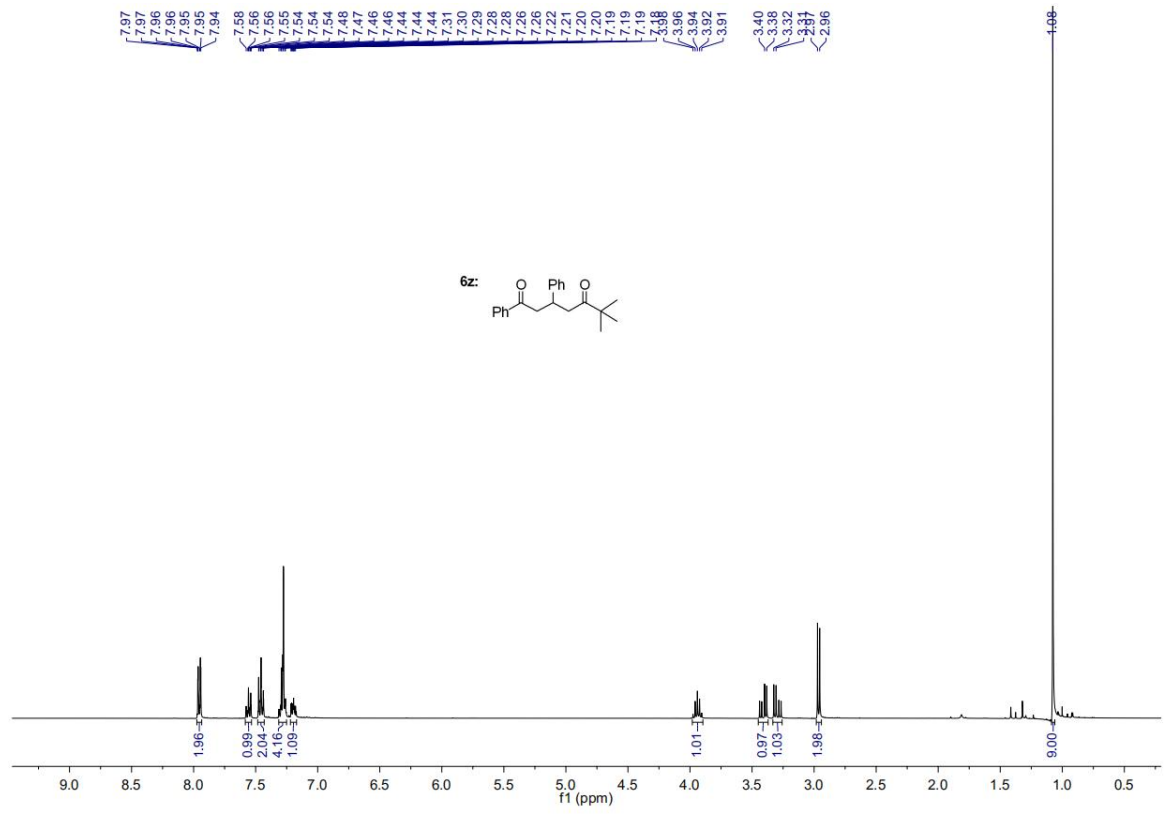
7.99
7.97
7.57
7.55
7.53
7.47
7.45
7.43
7.26
3.13
3.12
3.10
2.24
2.22
2.20
2.18

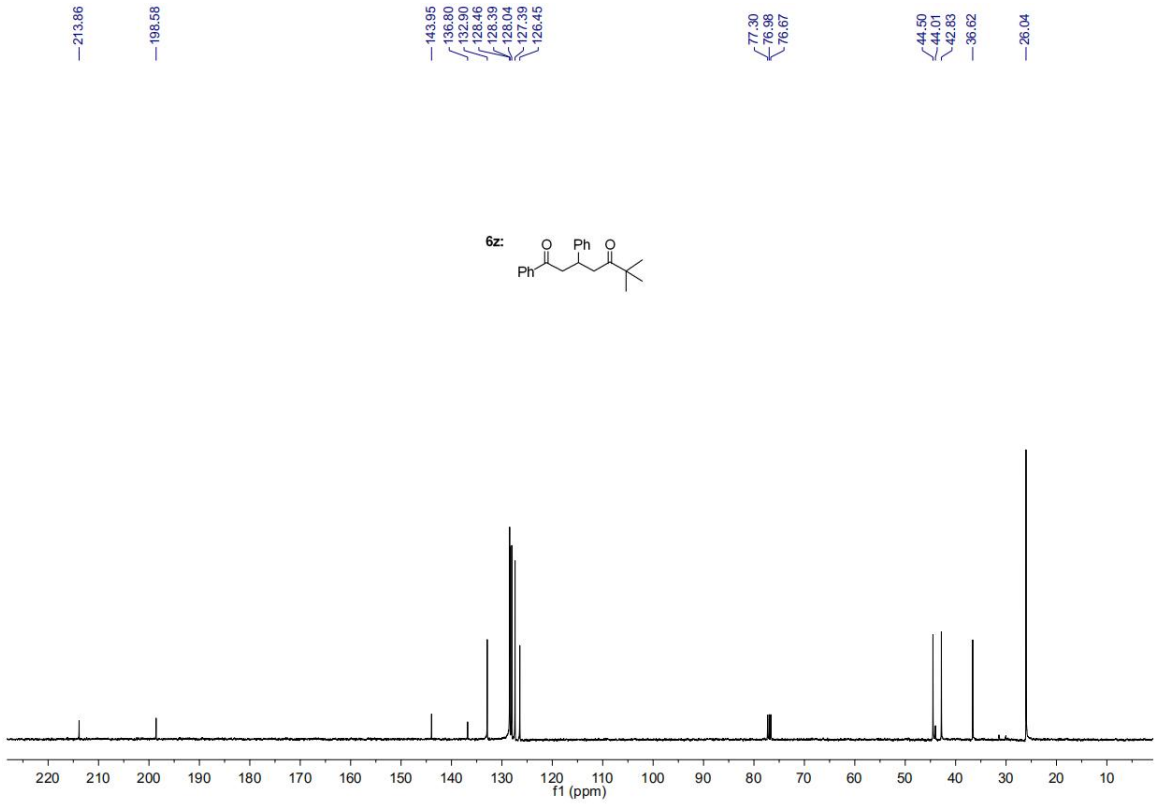
6y:

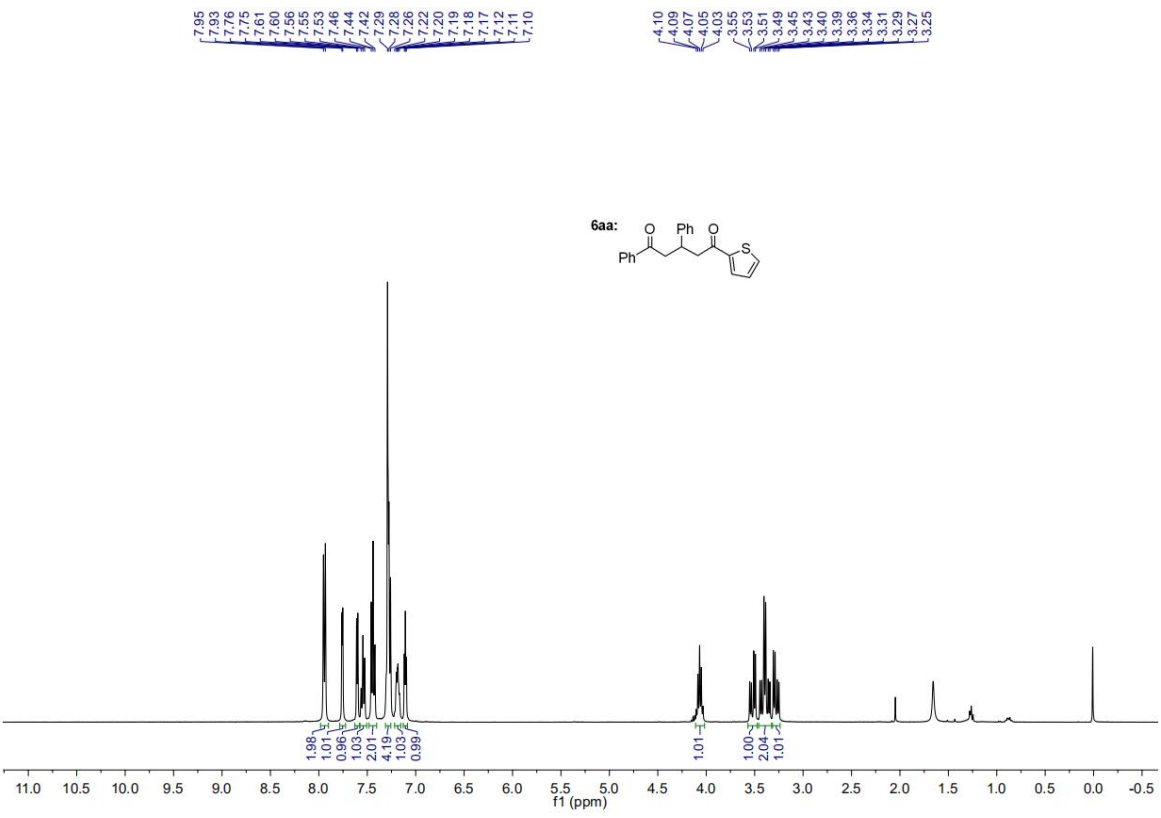





199.86
136.88
133.08
128.62
128.08
77.39
77.07
76.75
37.61
18.75
6y:
Ph
O
O
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

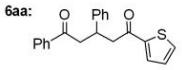

7.97
7.96
7.95
7.94
7.58
7.56
7.55
7.54
7.48
7.47
7.46
7.44
7.31
7.30
7.29
7.28
7.26
7.22
7.21
7.20
7.19
3.96
3.94
3.92
3.91
3.40
3.38
3.32
2.96
1.08
6z:
Ph
O
Ph
O
1.96
0.99
2.04
4.16
1.09
1.01
0.97
1.03
1.98
9.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

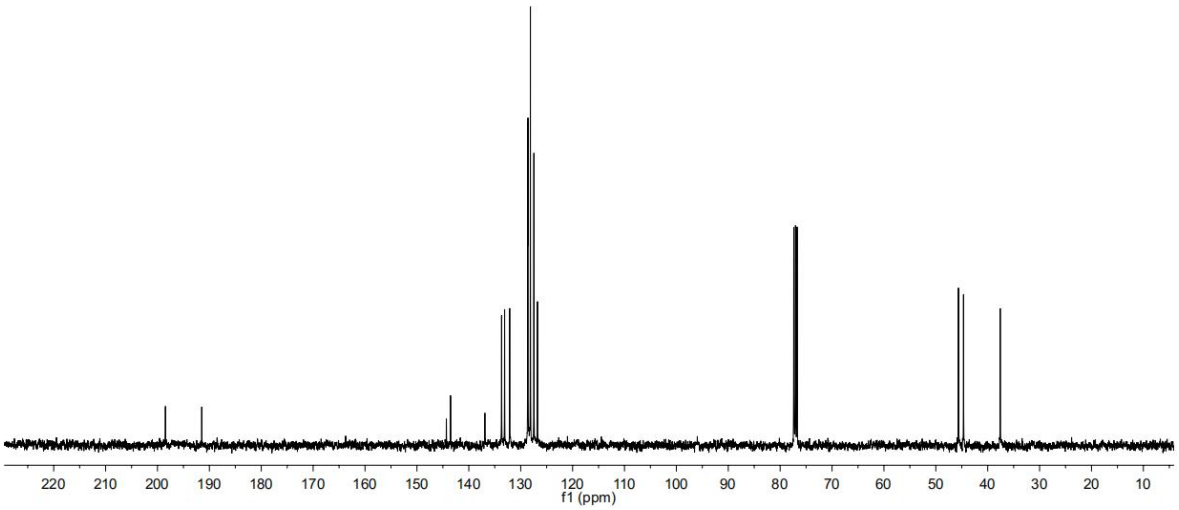

213.86
198.58
143.95
136.80
132.90
128.46
128.39
128.04
127.39
126.45
77.30
76.98
76.67
44.50
44.01
42.83
36.62
26.04
6z:
O
Ph
O
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.95
7.93
7.76
7.75
7.61
7.60
7.56
7.55
7.53
7.46
7.44
7.42
7.29
7.28
7.26
7.22
7.20
7.19
7.18
7.17
7.12
7.11
7.10
4.10
4.09
4.07
4.05
4.03
3.55
3.53
3.51
3.49
3.45
3.43
3.40
3.39
3.36
3.34
3.31
3.29
3.27
3.25
6aa:
O
Ph
O
Ph
S
1.98
1.01
0.96
1.03
2.01
4.19
1.03
0.99
1.01
1.00
2.04
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

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
77.38
77.06
76.74
45.64
44.67
37.59

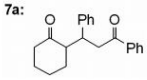
6aa:

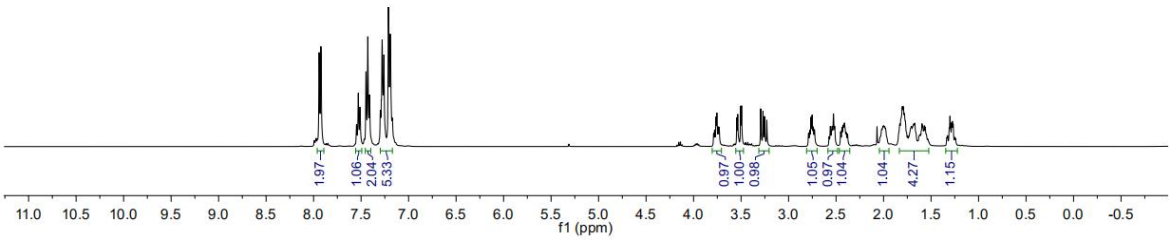




7.94
7.92
7.55
7.53
7.51
7.45
7.43
7.41
7.30
7.29
7.28
7.26
7.21
7.19
7.17
3.79
3.78
3.76
3.75
3.74
3.73
3.55
3.54
3.50
3.49
3.29
3.27
3.25
3.23
2.79
2.78
2.76
2.75
2.74
2.73
2.57
2.56
2.54
2.53
2.51
2.45
2.44
2.43
2.41
2.39
2.38
2.02
2.01
2.00
1.99
1.99
1.98
1.83
1.80
1.79
1.78
1.77
1.75
1.70
1.69
1.68
1.67
1.62
1.61
1.60
1.59
1.58
1.57
1.56
1.55
1.33
1.31
1.30
1.28
1.28
1.27
1.25

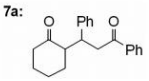
7a:

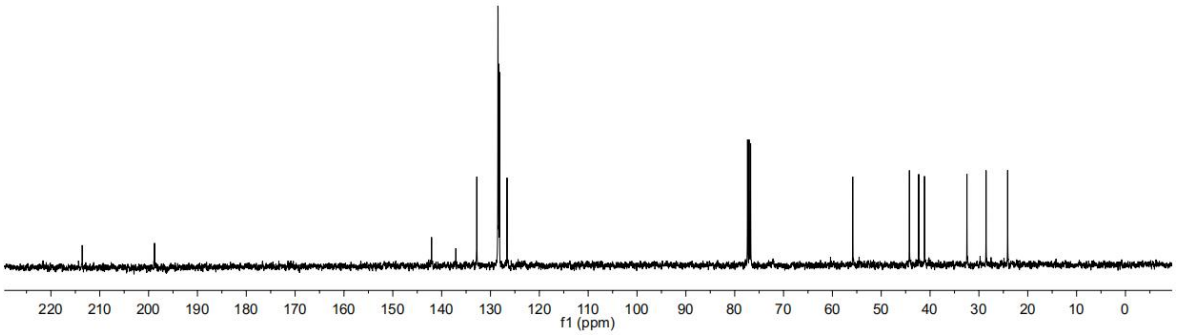




213.58
198.79
142.06
137.09
132.80
128.48
128.45
128.37
128.17
126.61
77.38
77.06
76.74
55.83
44.23
42.32
41.14
32.45
28.53
24.12

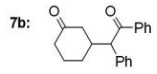
7a:

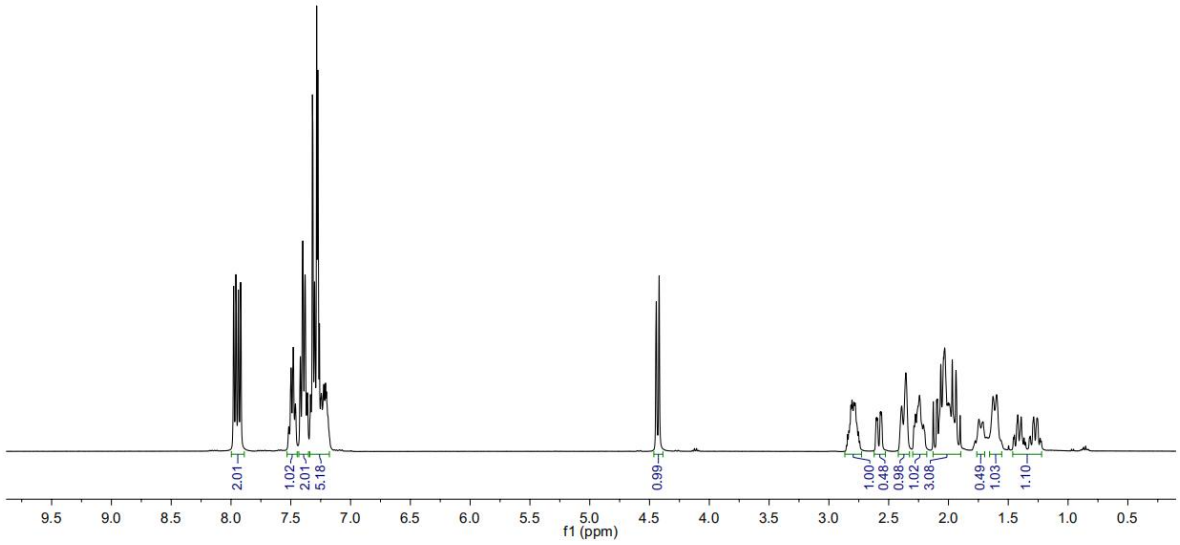


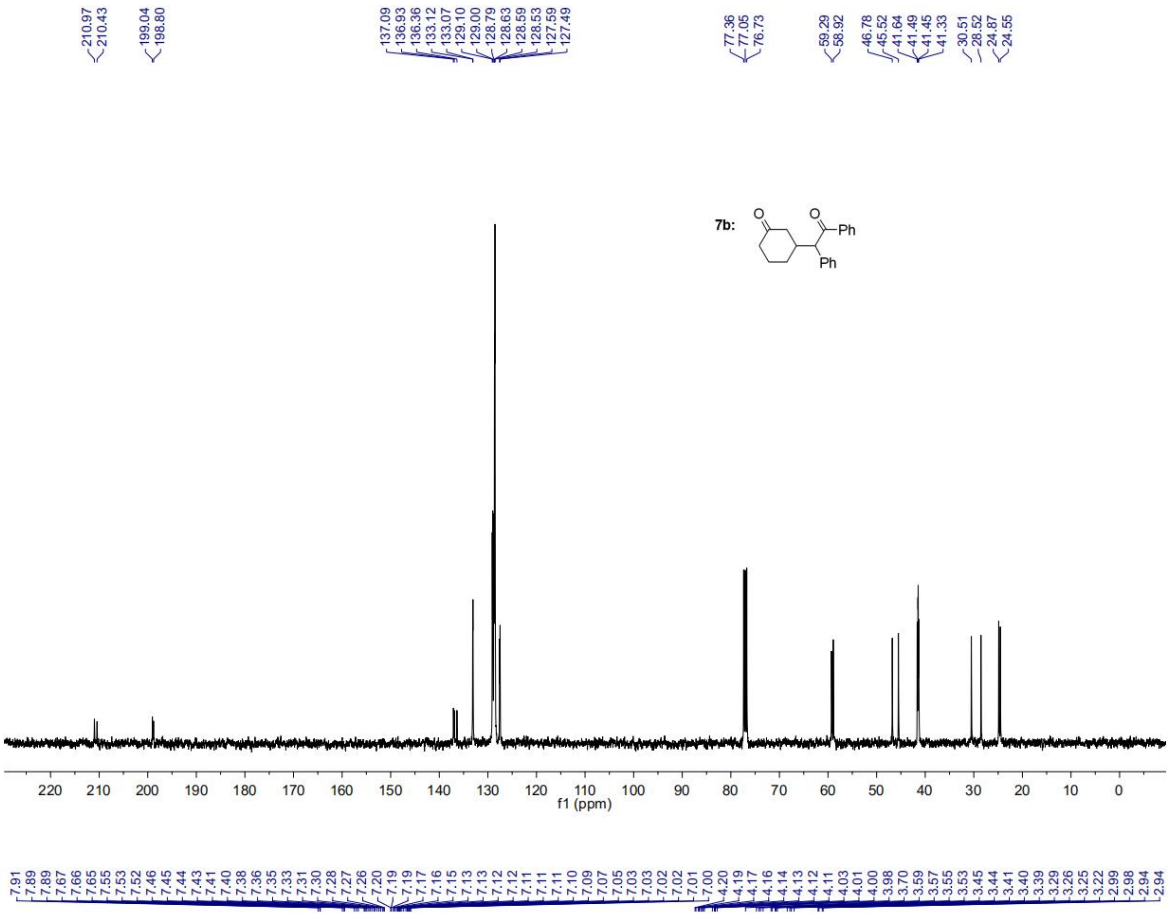


7.98 7.96 7.94 7.92 7.52 7.50 7.48 7.46 7.42 7.40 7.38 7.36 7.34 7.32 7.30 7.28 7.27 7.26 7.25 7.24 7.24 7.22 7.21 7.20 7.19
4.44 4.42 2.84 2.83 2.82 2.82 2.81 2.80 2.79 2.78 2.75 2.60 2.60 2.59 2.57 2.57 2.56 2.39 2.36 2.29 2.28 2.26 2.24 2.21 2.13 2.10 2.09 2.06 2.04 2.03 2.01 2.00 1.99 1.97 1.94 1.90 1.75 1.71 1.69 1.68 1.63 1.60 1.46 1.45 1.42 1.39 1.37 1.32 1.32 1.29 1.26 1.26

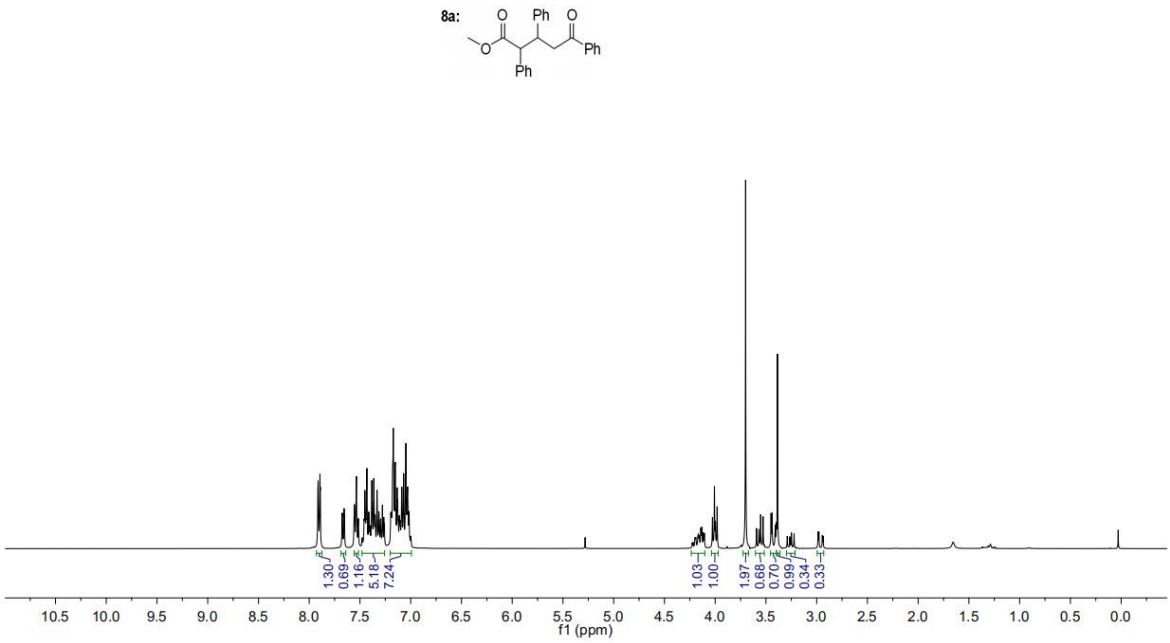
7b:

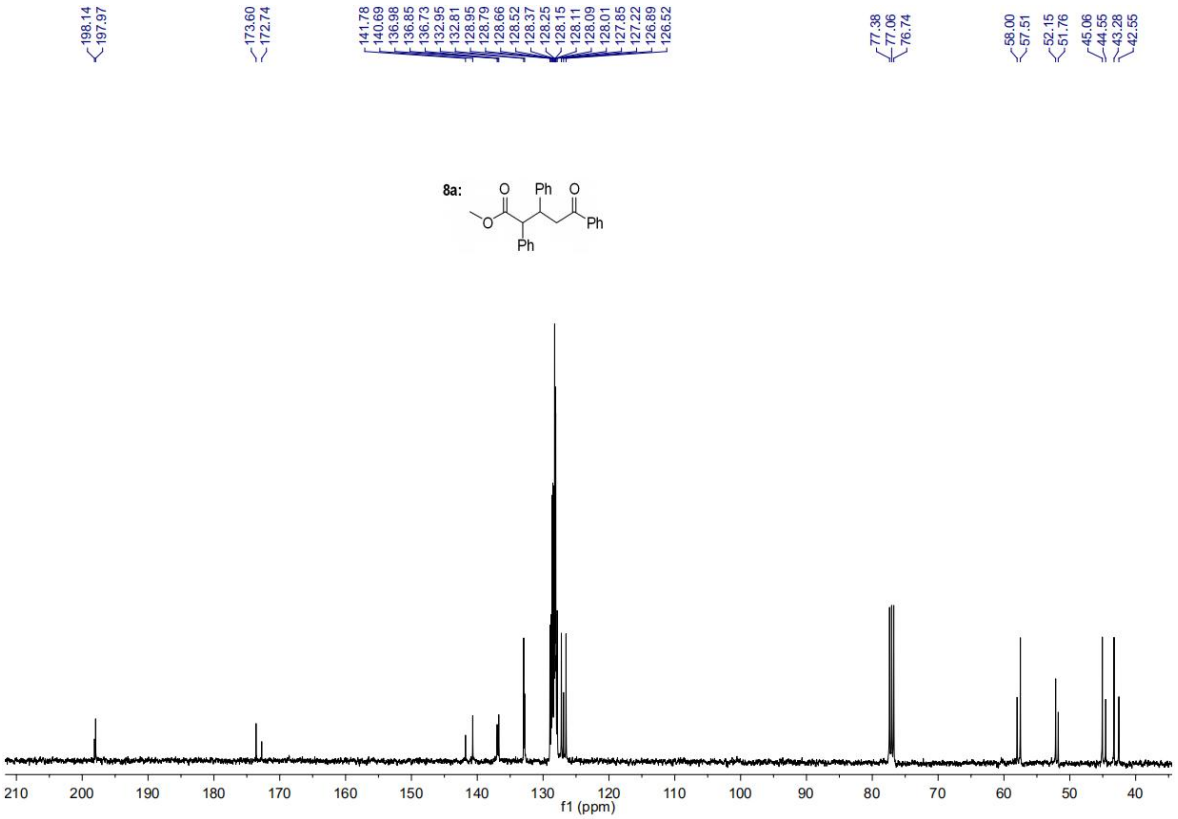


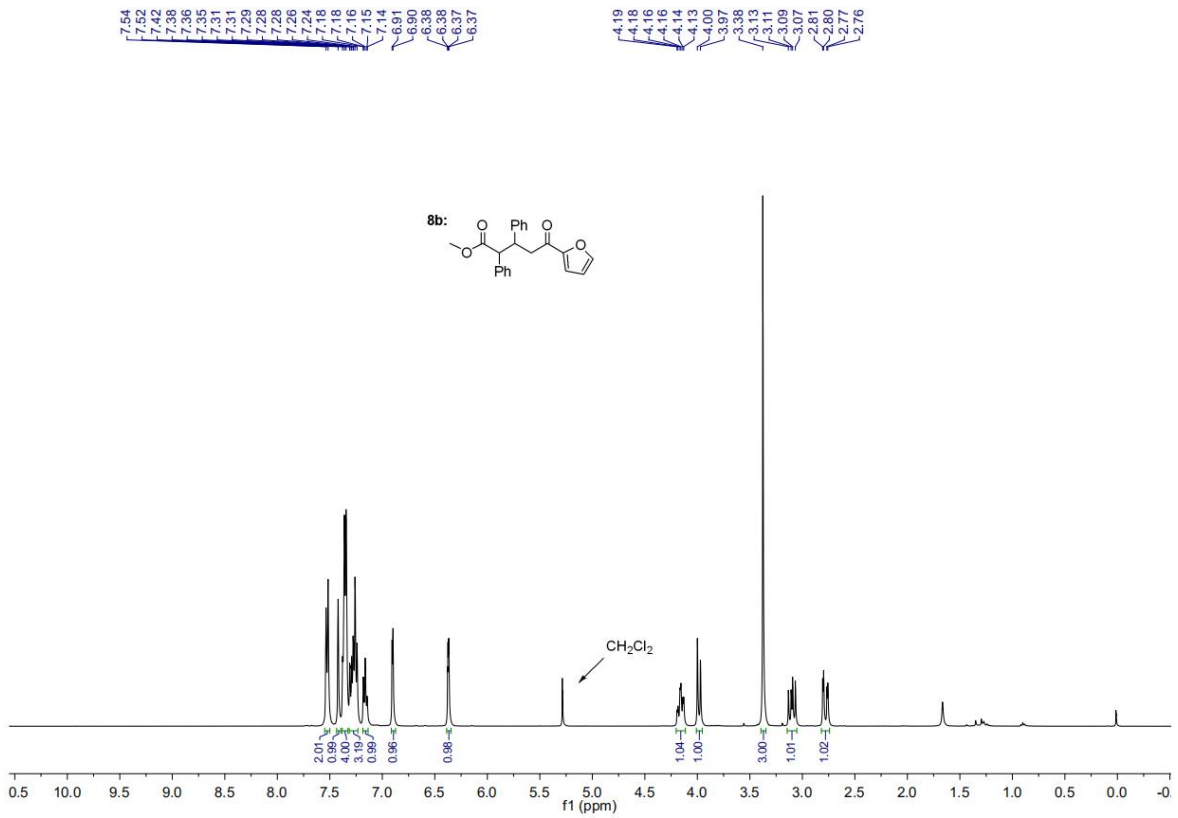


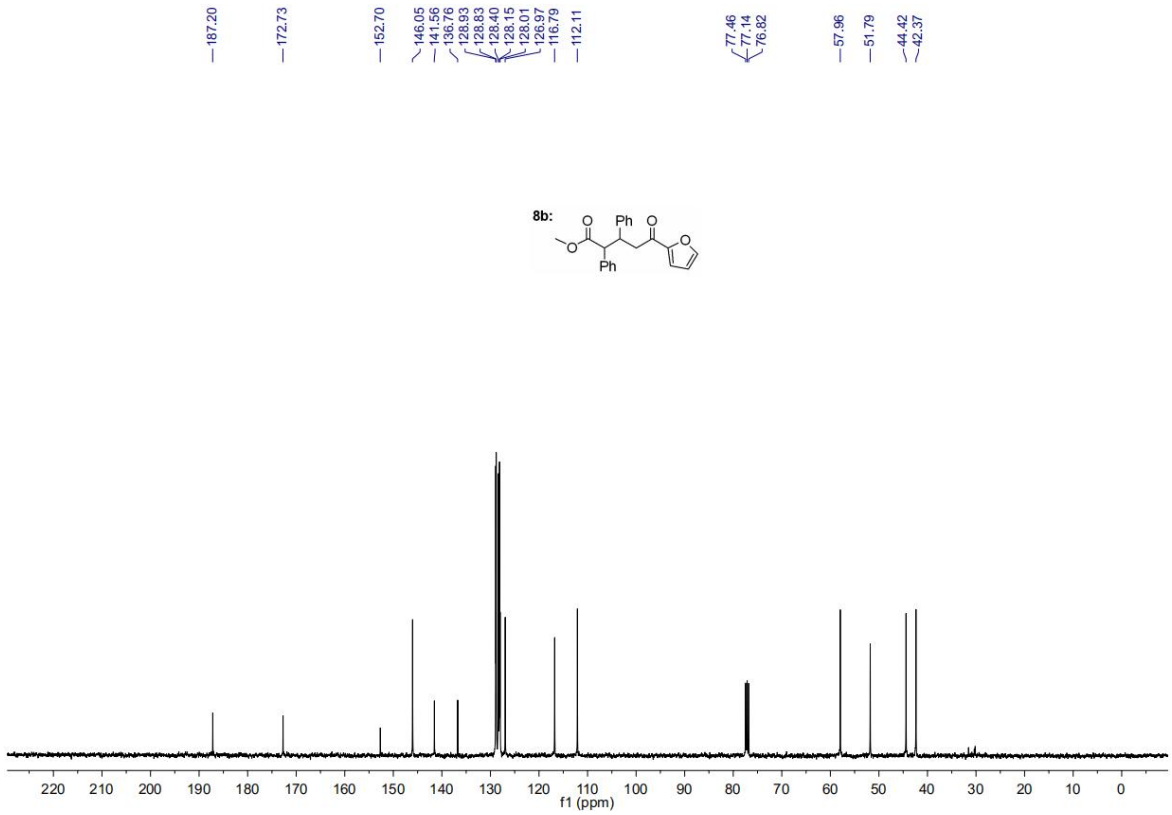

210.97
210.43
199.04
198.80
137.09
136.93
136.36
133.12
133.07
129.10
129.00
128.79
128.63
128.59
128.53
127.59
127.49
77.36
77.05
76.73
59.29
58.92
46.78
45.52
41.64
41.49
41.45
41.33
30.51
28.52
24.87
24.55
7b:
Ph
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

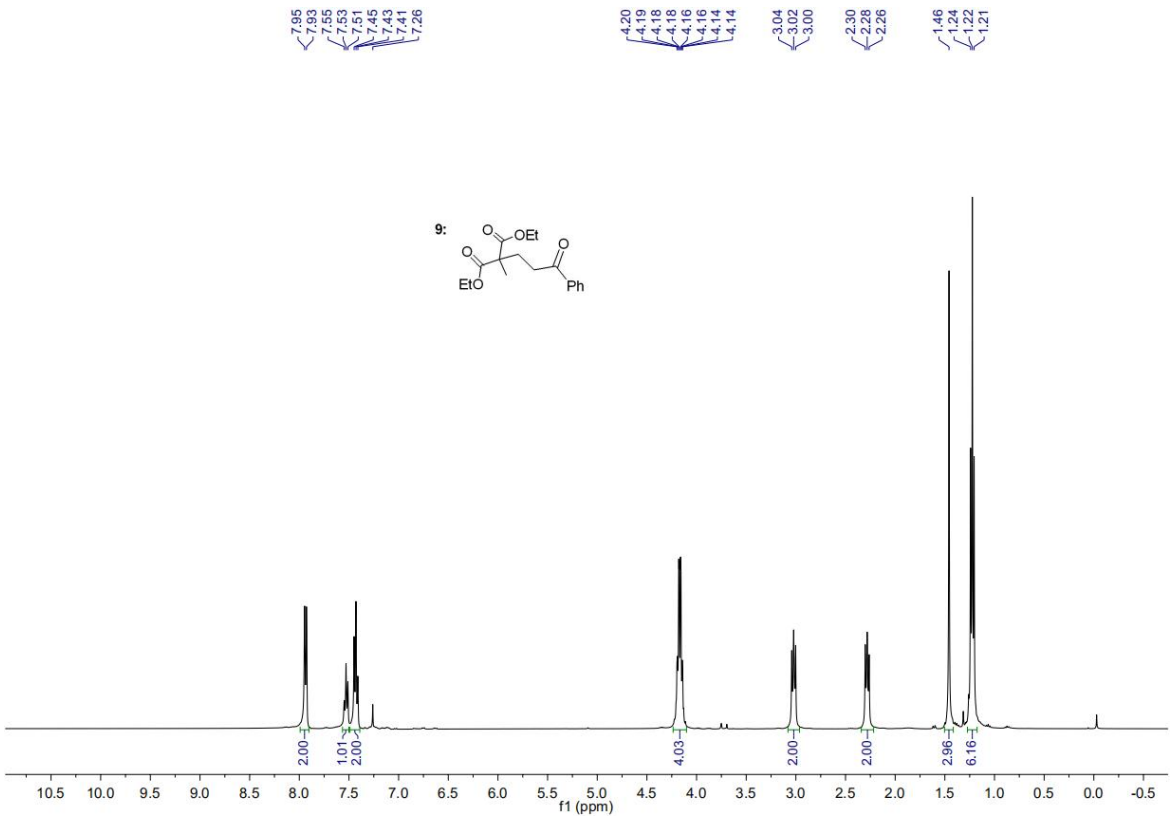
7.91
7.89
7.89
7.67
7.66
7.65
7.55
7.53
7.52
7.46
7.45
7.44
7.43
7.41
7.40
7.38
7.36
7.35
7.33
7.31
7.30
7.28
7.27
7.26
7.20
7.19
7.19
7.17
7.16
7.15
7.13
7.13
7.12
7.12
7.11
7.11
7.11
7.10
7.09
7.07
7.05
7.03
7.03
7.02
7.02
7.01
7.00
4.20
4.19
4.17
4.16
4.14
4.13
4.12
4.11
4.03
4.01
4.00
3.98
3.70
3.59
3.57
3.55
3.53
3.45
3.44
3.41
3.40
3.39
3.29
3.26
3.25
3.22
2.99
2.98
2.94
2.94

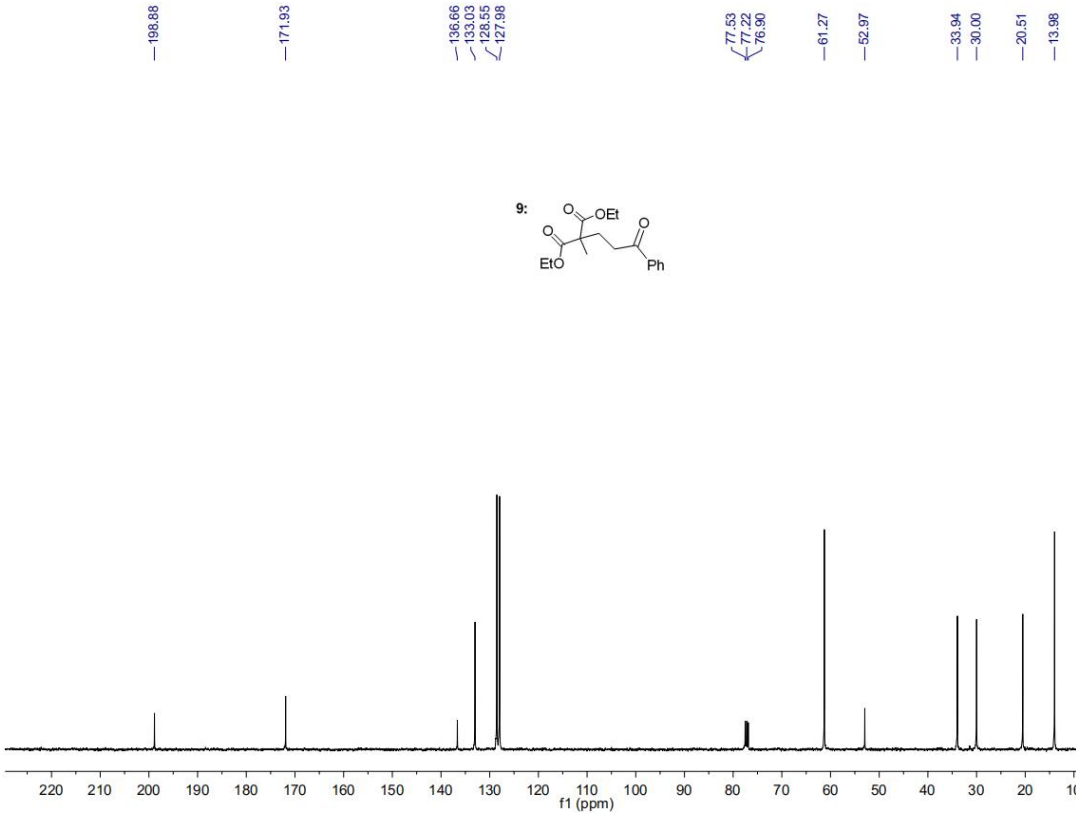

8a:
O
Ph
O
O
Ph
Ph
1.30
0.69
1.16
5.18
7.24
1.03
1.00
1.97
0.68
0.70
0.99
0.34
0.33
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

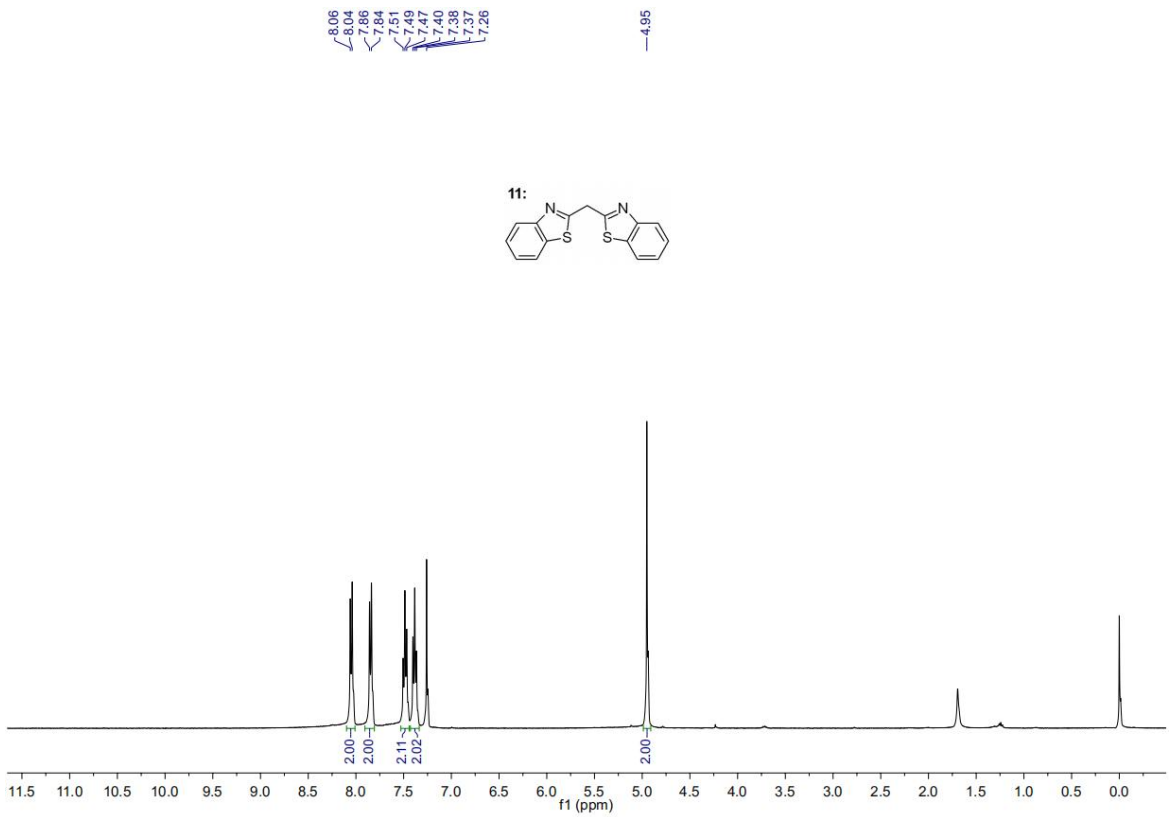

198.14
197.97
173.60
172.74
141.78
140.69
136.98
136.85
136.73
132.95
132.81
128.95
128.79
128.66
128.52
128.37
128.25
128.15
128.11
128.09
128.01
127.85
127.22
126.89
126.52
77.38
77.06
76.74
58.00
57.51
52.15
51.76
45.06
44.55
43.28
42.55
8a:
O
Ph
O
O
Ph
Ph
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)

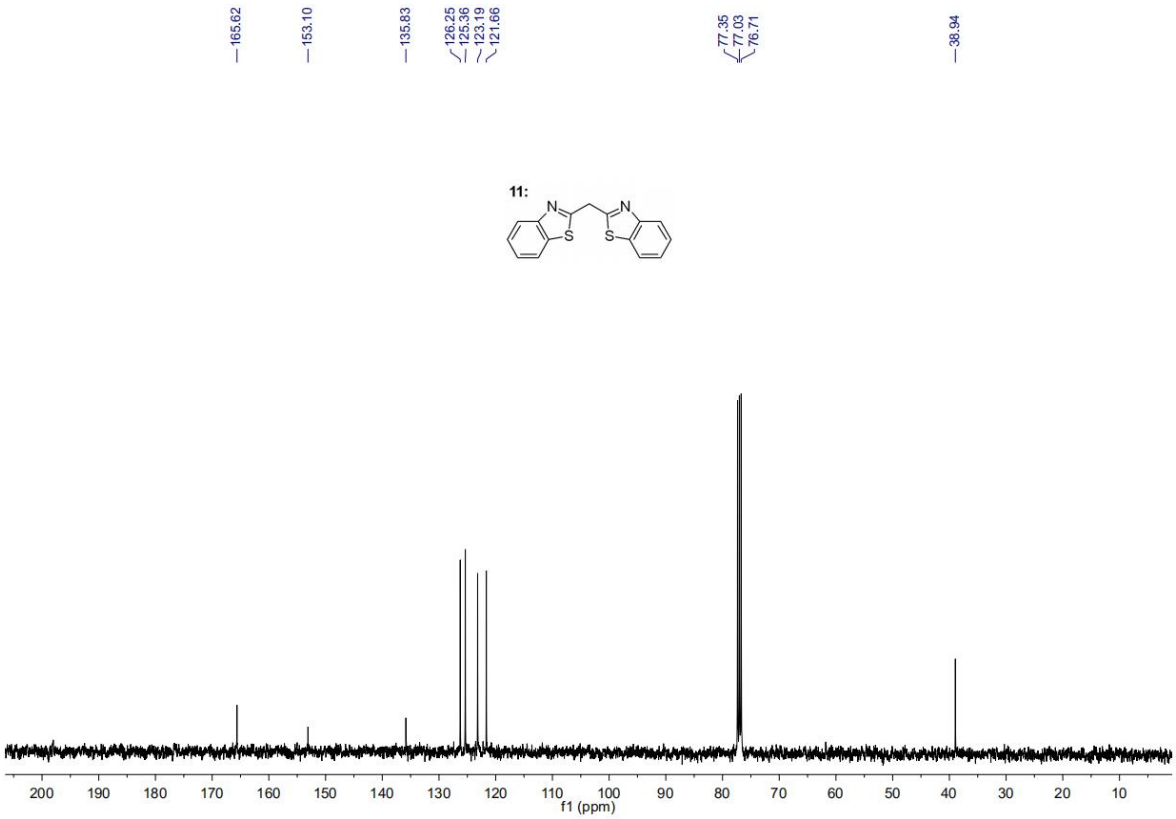

7.54
7.52
7.42
7.38
7.36
7.35
7.31
7.31
7.29
7.28
7.28
7.26
7.24
7.18
7.18
7.16
7.15
7.14
6.91
6.90
6.38
6.38
6.37
6.37
4.19
4.18
4.16
4.16
4.14
4.13
4.00
3.97
3.38
3.13
3.11
3.09
3.07
2.81
2.80
2.77
2.76
8b:
O
Ph
O
O
Ph
CH2Cl2
2.01
0.99
4.00
3.19
0.99
0.96
0.98
1.04
1.00
3.00
1.01
1.02
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

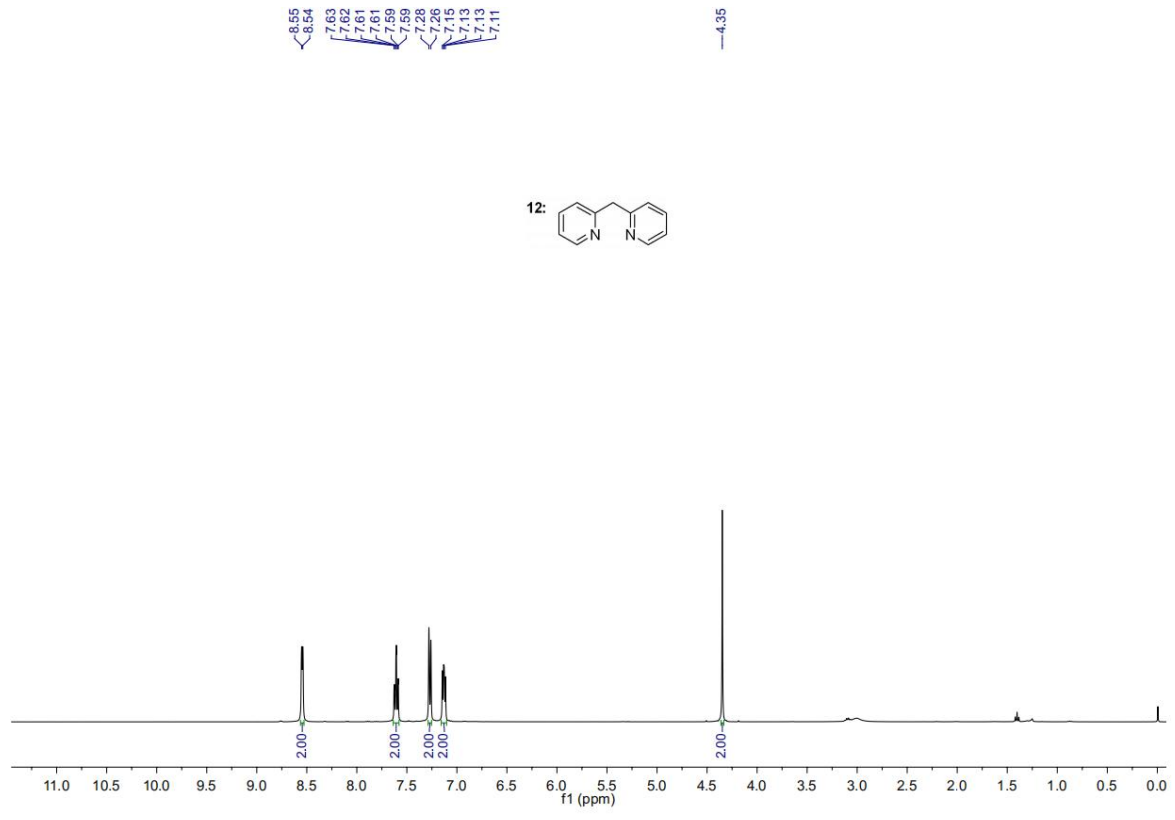

187.20
172.73
152.70
146.05
141.56
136.76
128.93
128.83
128.40
128.15
128.01
126.97
116.79
112.11
77.46
77.14
76.82
57.96
51.79
44.42
42.37
8b:
Ph
Ph
f1 (ppm)

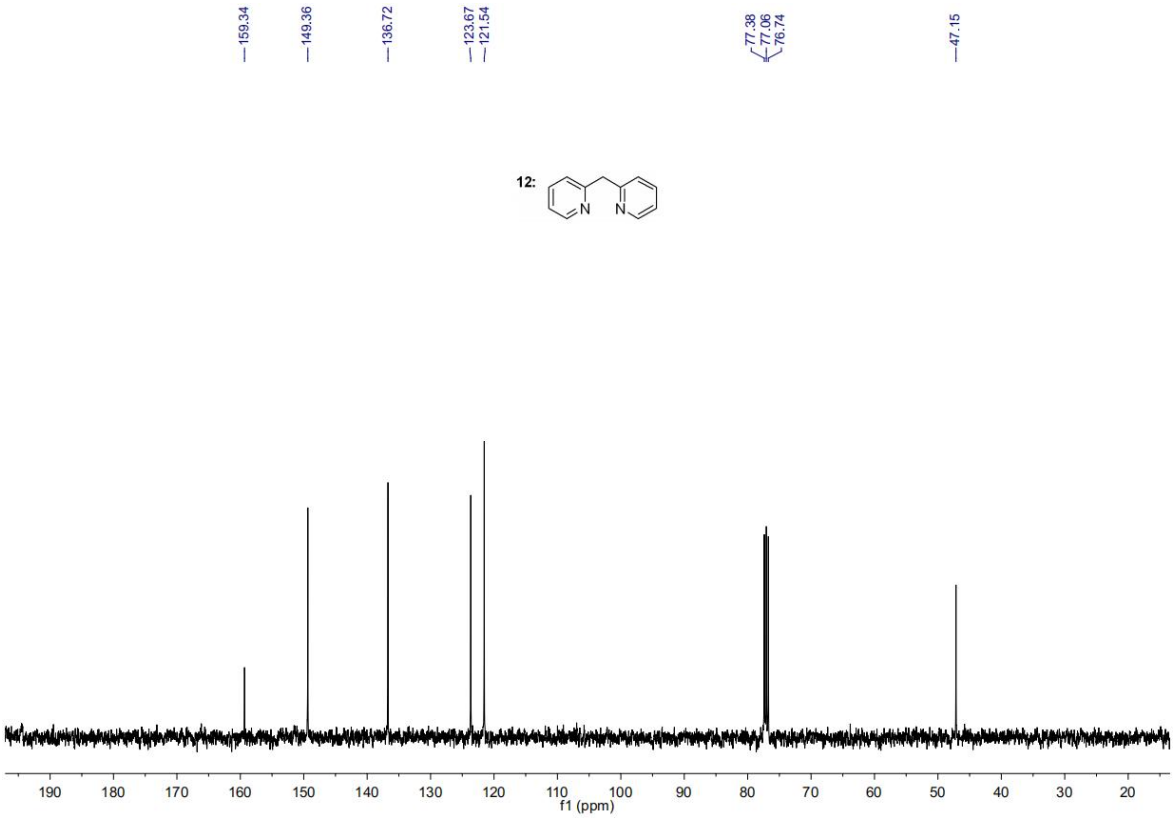

7.95
7.93
7.55
7.53
7.51
7.45
7.43
7.41
7.26
4.20
4.19
4.18
4.18
4.16
4.16
4.14
4.14
3.04
3.02
3.00
2.30
2.28
2.26
1.46
1.24
1.22
1.21
9:
OEt
EtO
Ph
2.00
1.01
2.00
4.03
2.00
2.00
2.96
6.16
f1 (ppm)

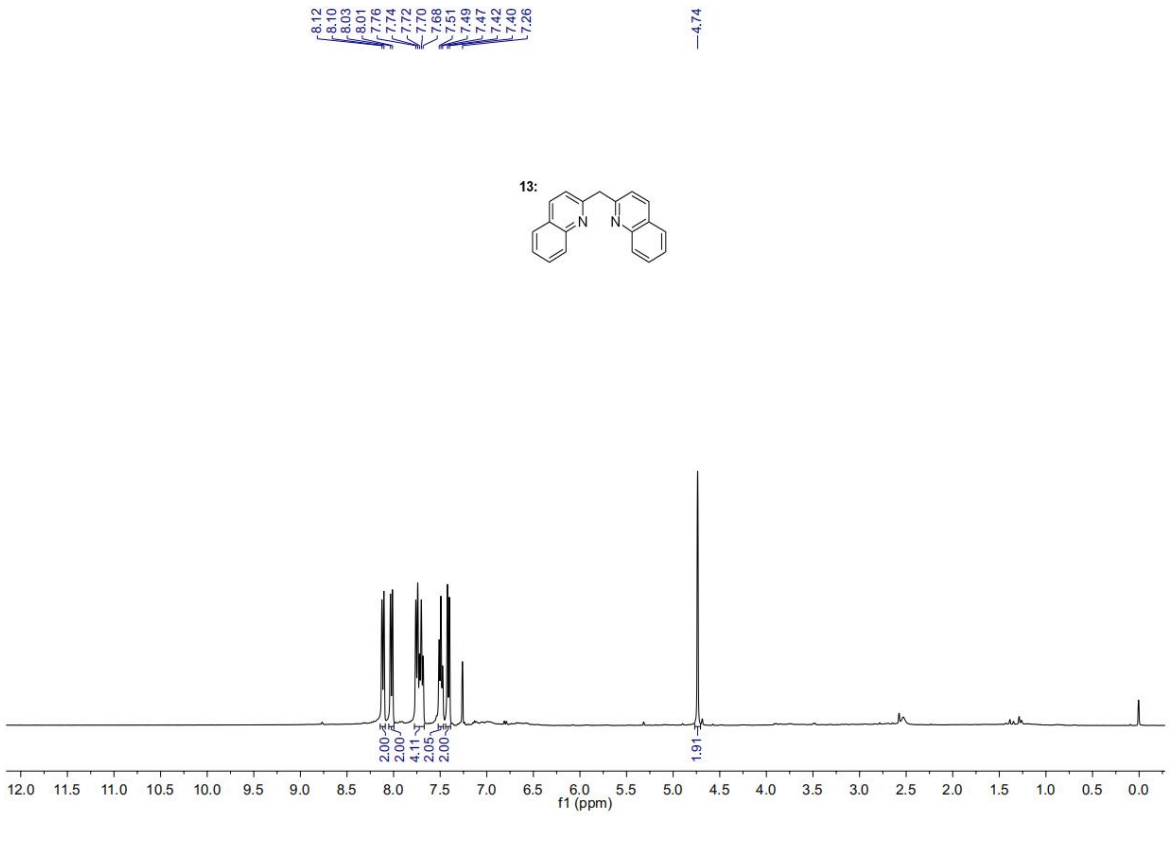

198.88
171.93
136.66
133.03
128.55
127.98
77.53
77.22
76.90
61.27
52.97
33.94
30.00
20.51
13.98
9:
OEt
EtO
Ph
f1 (ppm)


8.06
8.04
7.86
7.84
7.51
7.49
7.47
7.40
7.38
7.37
7.26
4.95
11:
2.00
2.00
2.11
2.02
2.00
f1 (ppm)


165.62
153.10
135.83
126.25
125.36
123.19
121.66
77.35
77.03
76.71
38.94
11:
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

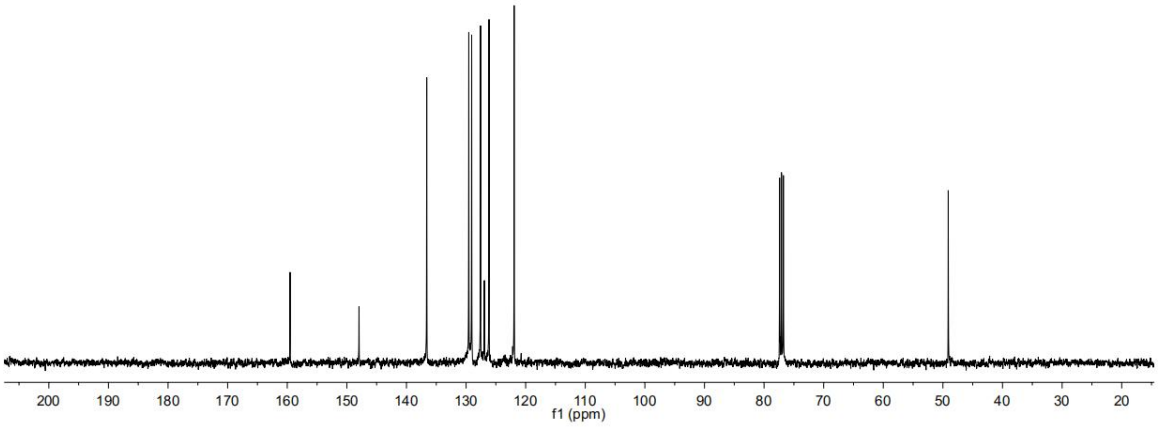

8.55
8.54
7.63
7.62
7.61
7.61
7.59
7.59
7.28
7.26
7.15
7.13
7.11
4.35
12:
2.00
2.00
2.00
2.00
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


159.34
149.36
136.72
123.67
121.54
77.38
77.06
76.74
47.15
12:
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)


8.12
8.10
8.03
8.01
7.76
7.74
7.72
7.70
7.68
7.51
7.49
7.47
7.42
7.40
7.26
4.74
13:
2.00
2.00
4.11
2.05
2.00
1.91
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

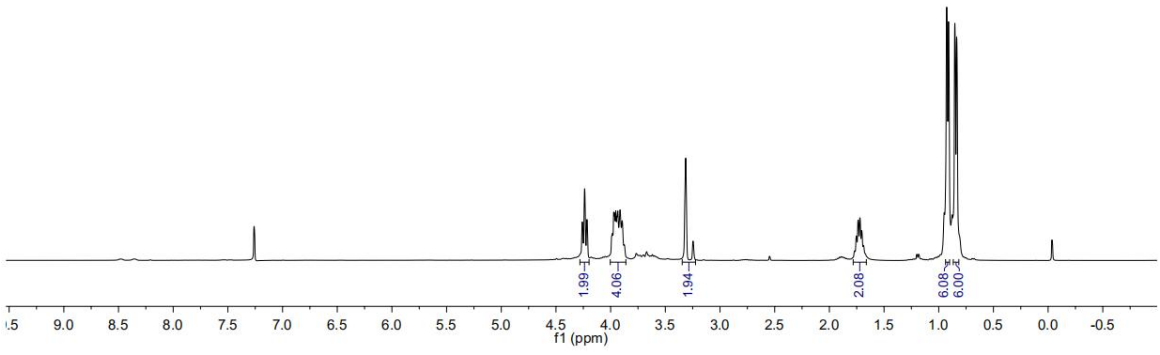
159.54
147.98
136.61
129.56
129.07
127.58
126.95
126.16
121.94
77.40
77.08
76.76
49.11

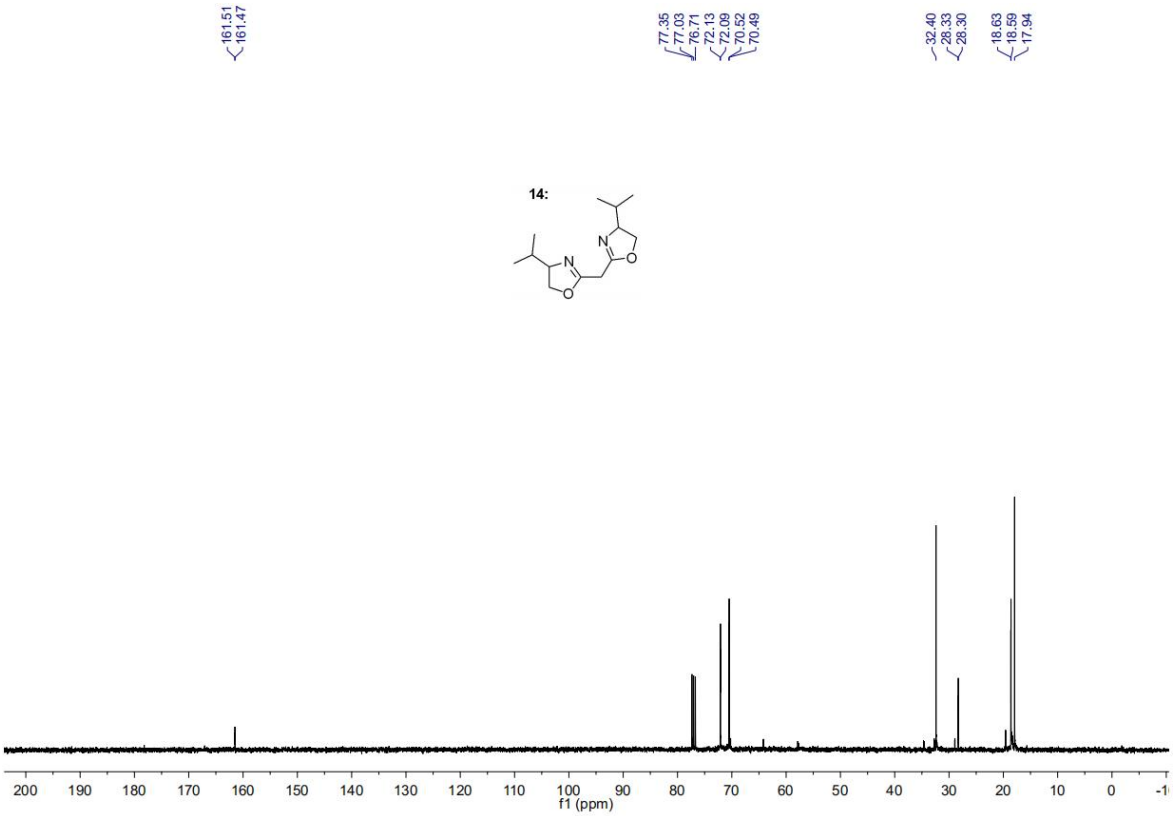
13:

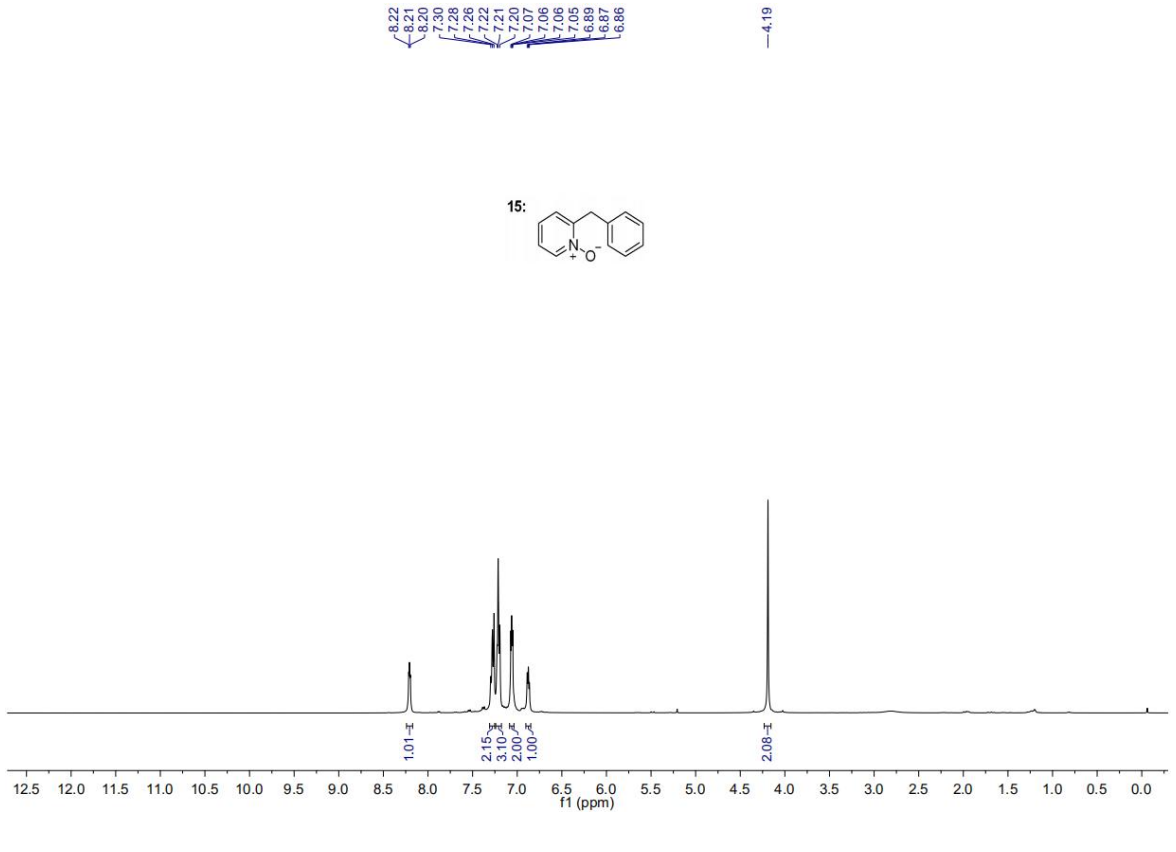


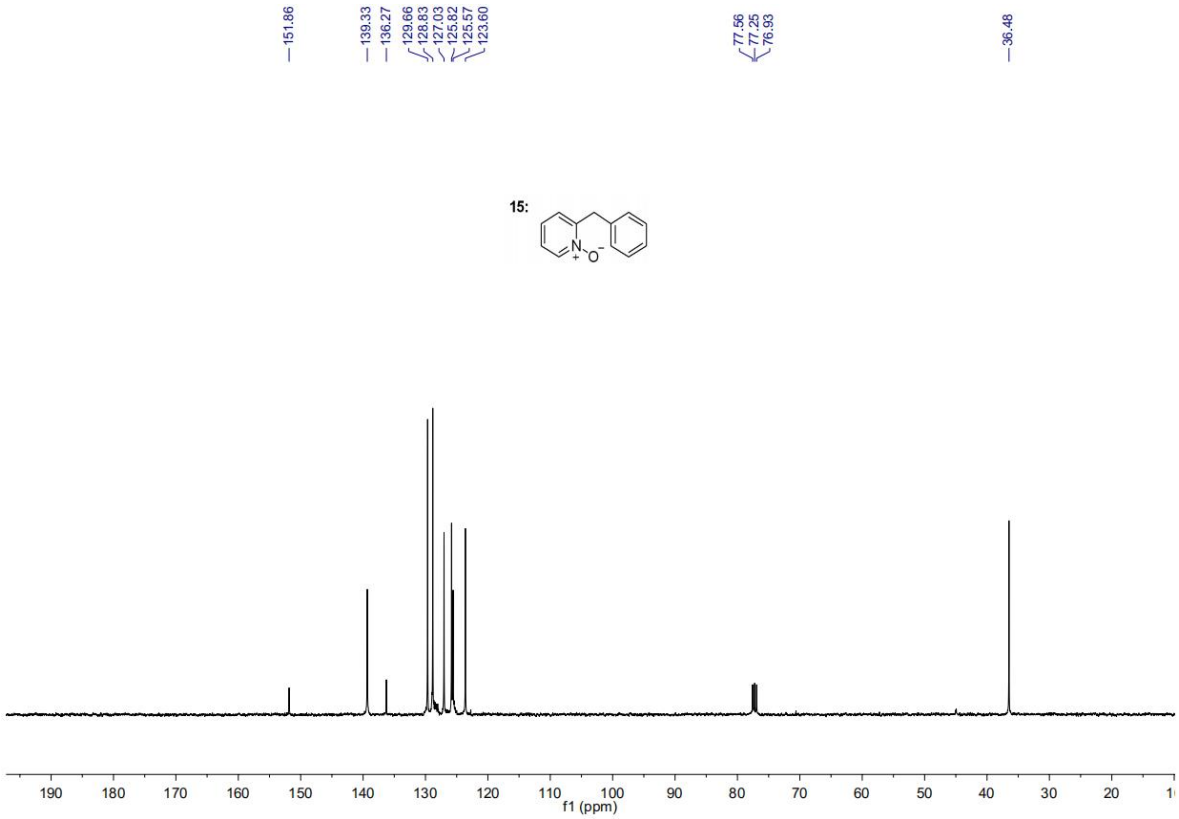
7.26
4.26
4.24
4.22
3.99
3.98
3.97
3.96
3.95
3.94
3.93
3.91
3.89
3.88
3.31
3.25
1.77
1.75
1.74
1.72
1.70
1.69
0.93
0.91
0.85
0.84

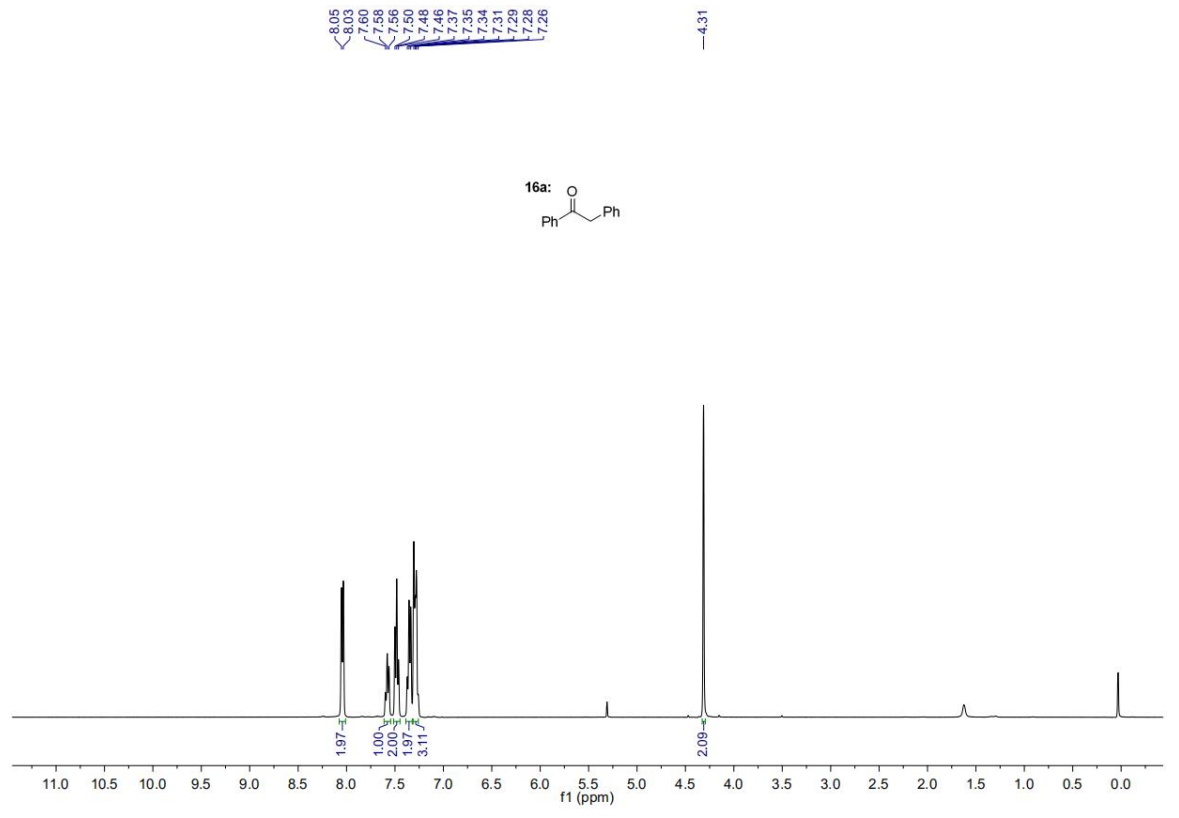
14:

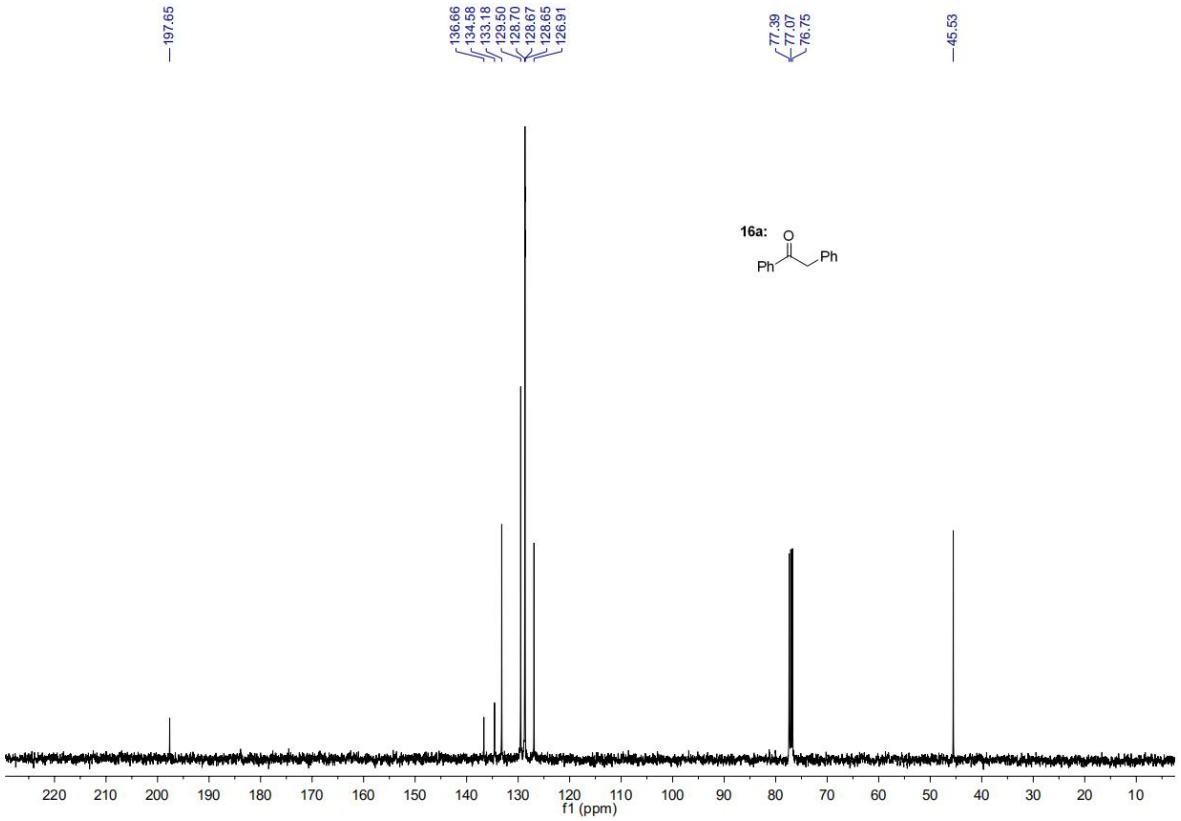


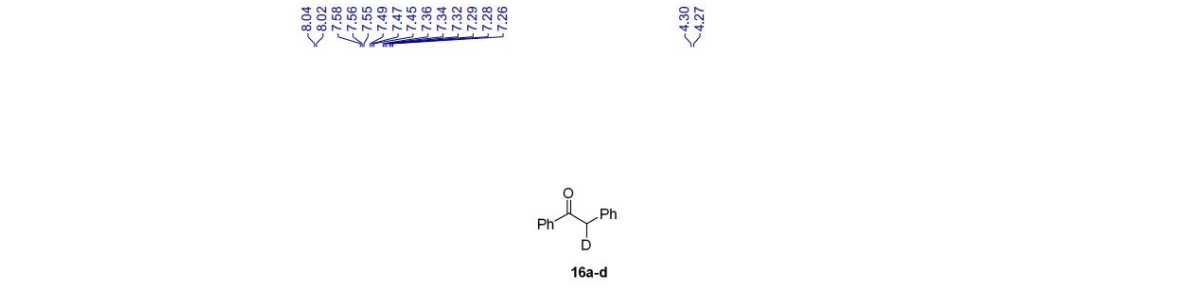

161.51
161.47
77.35
77.03
76.71
72.13
72.09
70.52
70.49
32.40
28.33
28.30
18.63
18.59
17.94
14:
f1 (ppm)


8.22
8.21
8.20
7.30
7.28
7.26
7.22
7.21
7.20
7.07
7.06
7.06
7.05
6.89
6.87
6.86
4.19
15:
1.01
2.15
3.10
2.00
1.00
2.08
f1 (ppm)


151.86
139.33
136.27
129.66
128.83
127.03
125.82
125.57
123.60
77.56
77.25
76.93
36.48
15:
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)

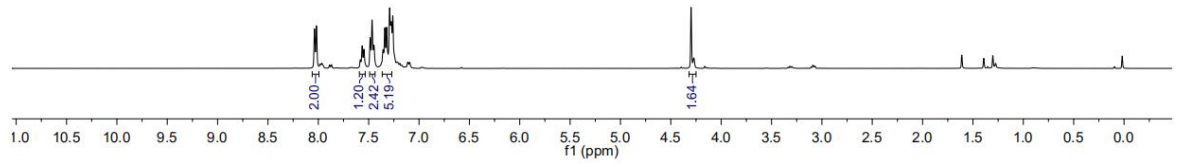

8.05
8.03
7.60
7.58
7.56
7.50
7.48
7.46
7.37
7.35
7.34
7.31
7.29
7.28
7.26
4.31
16a:
O
Ph
Ph
1.97
1.00
2.00
1.97
3.11
2.09
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

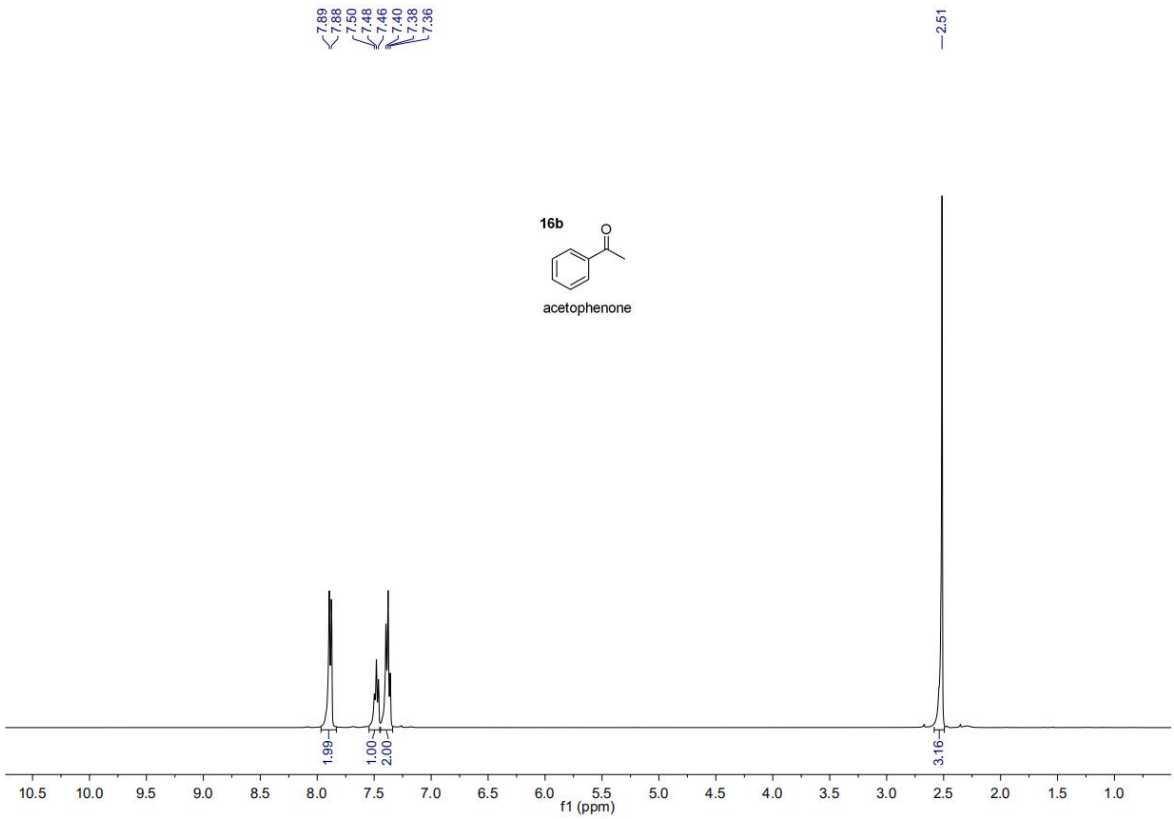

197.65
136.66
134.58
133.18
129.50
128.70
128.67
128.65
126.91
77.39
77.07
76.75
45.53
16a:
Ph
O
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

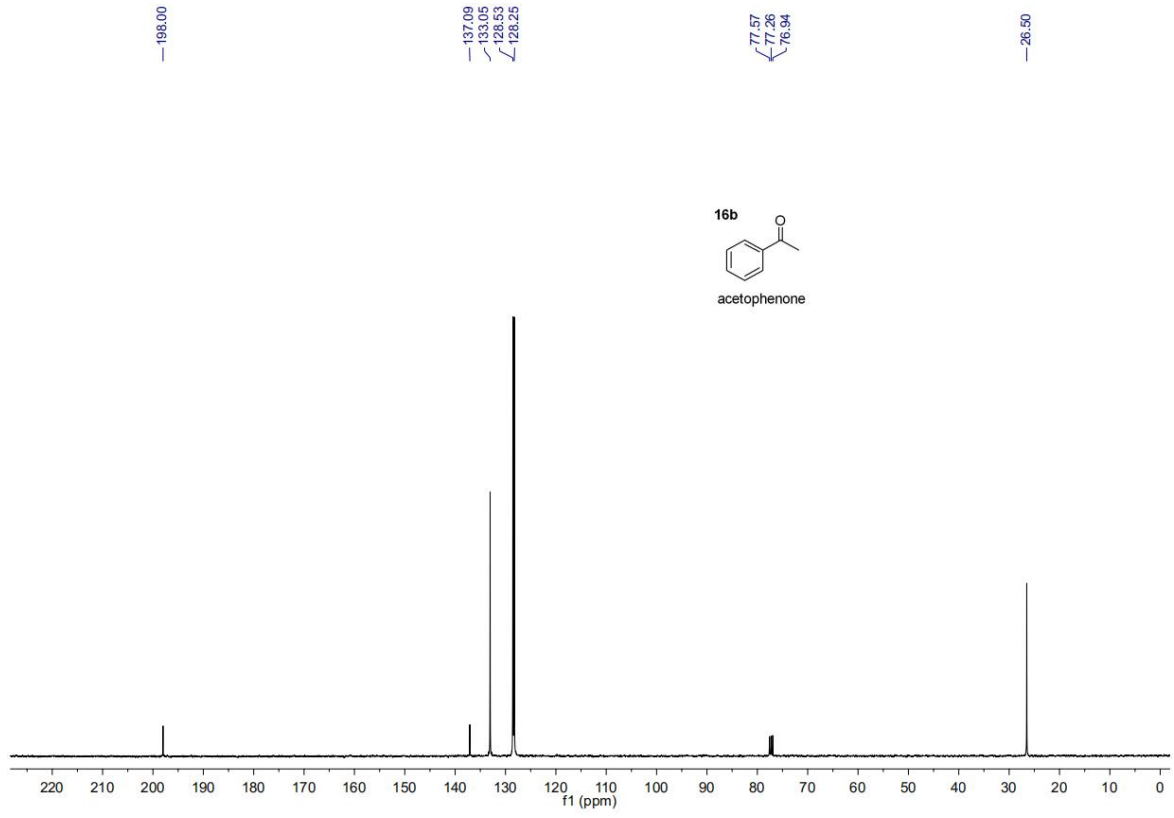

8.04
8.02
7.58
7.56
7.55
7.49
7.47
7.45
7.36
7.34
7.32
7.29
7.28
7.26
4.30
4.27

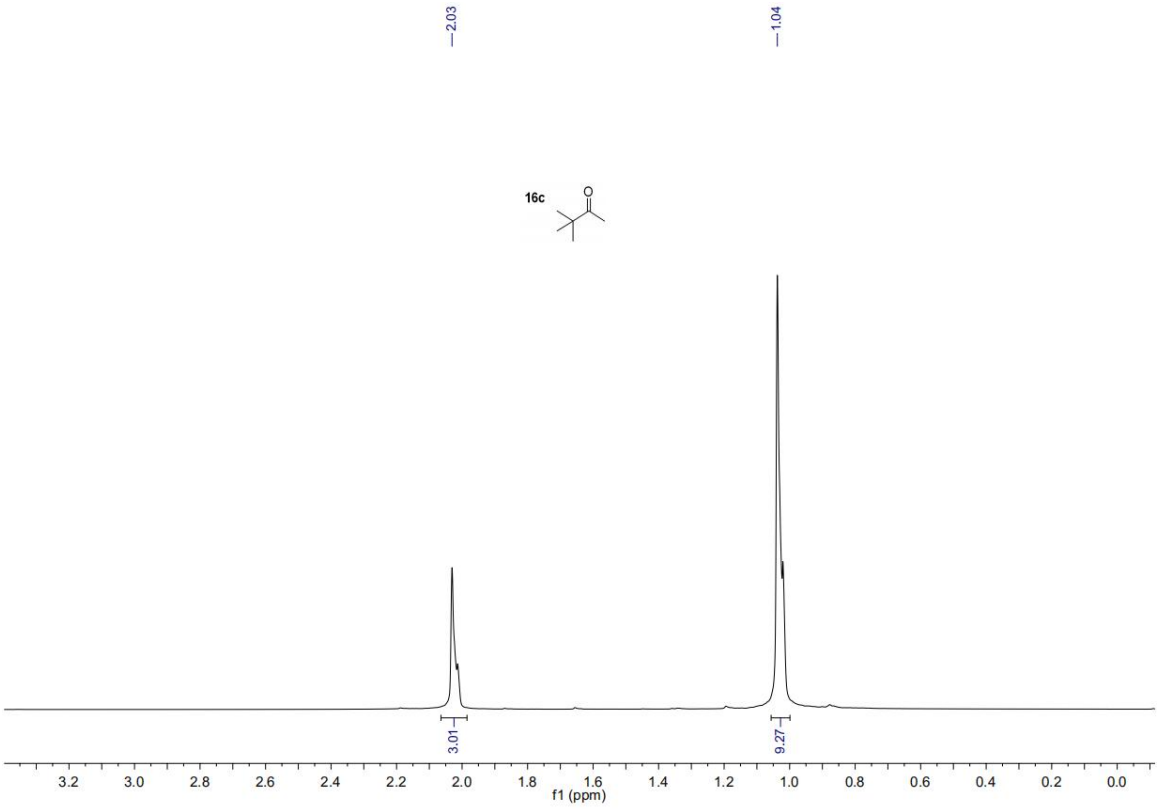
O
Ph
Ph
D

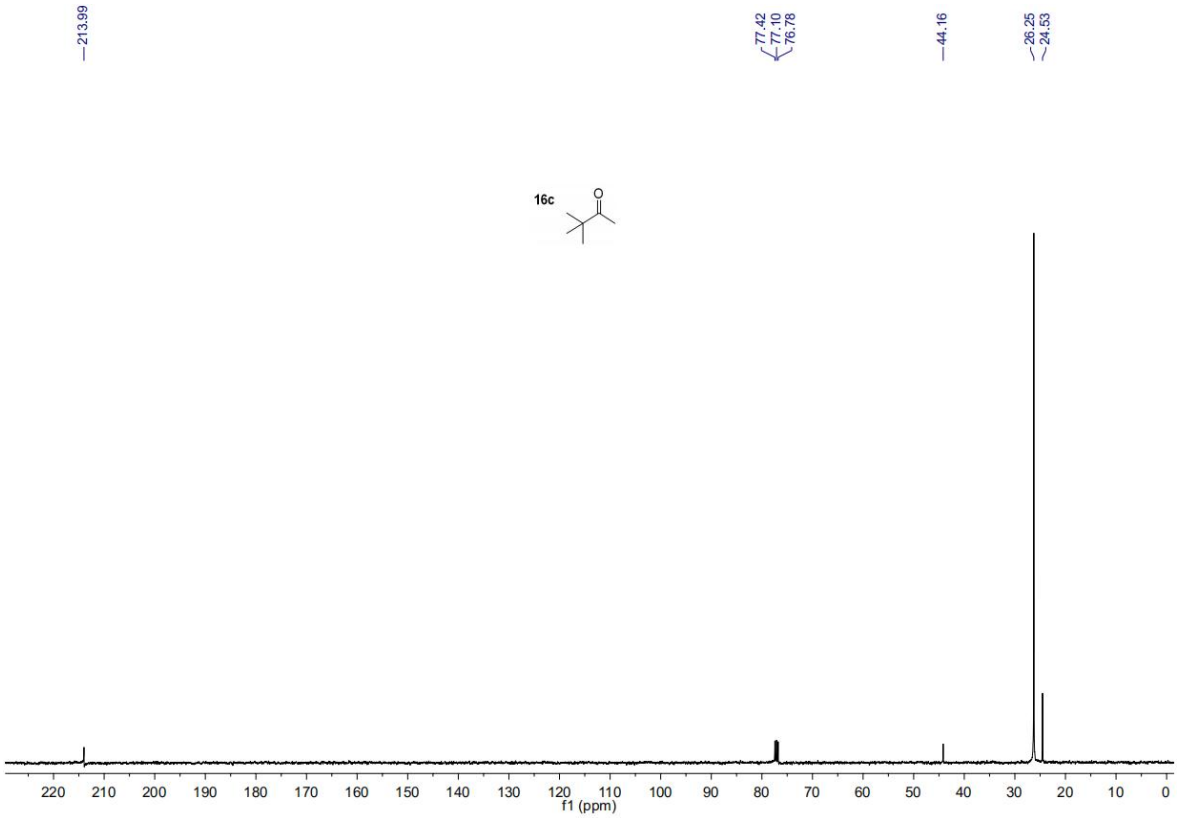
16a-d

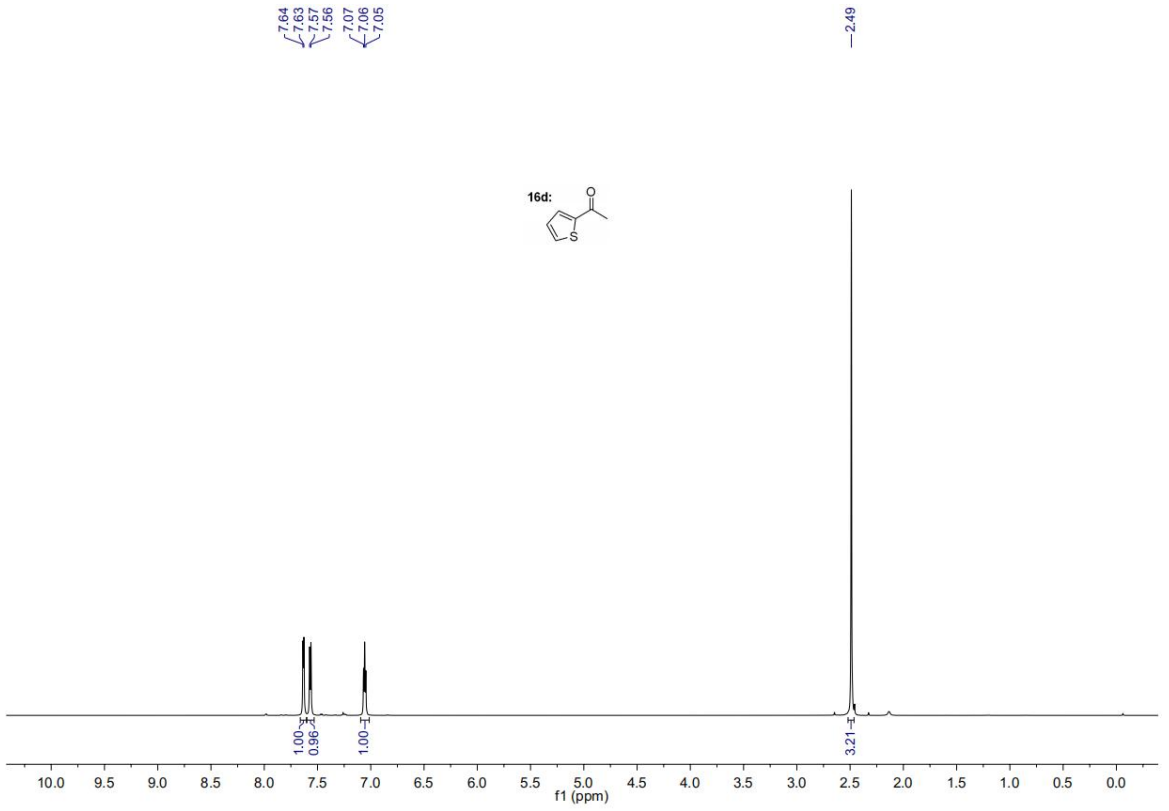

2.00
1.20
2.42
5.19
1.64
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

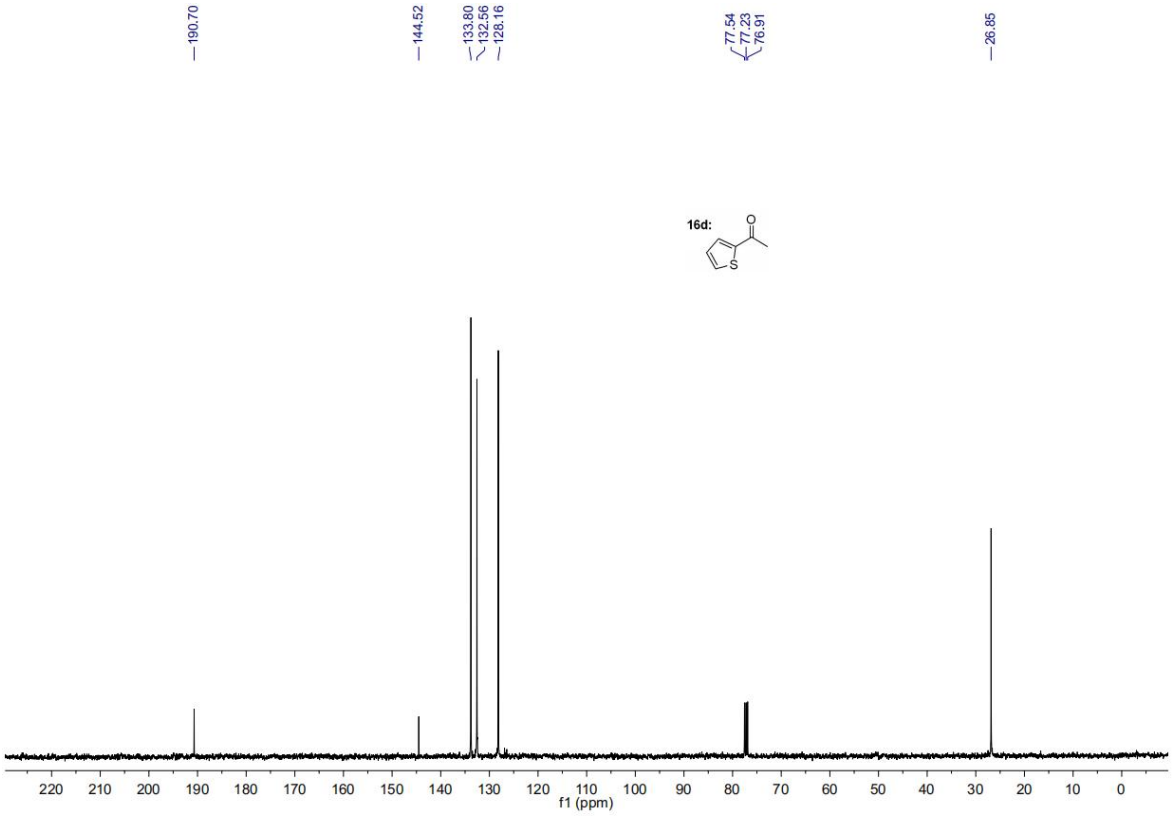

7.89
7.88
7.50
7.48
7.46
7.40
7.38
7.36
2.51
16b
acetophenone
1.99
1.00
2.00
3.16
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)

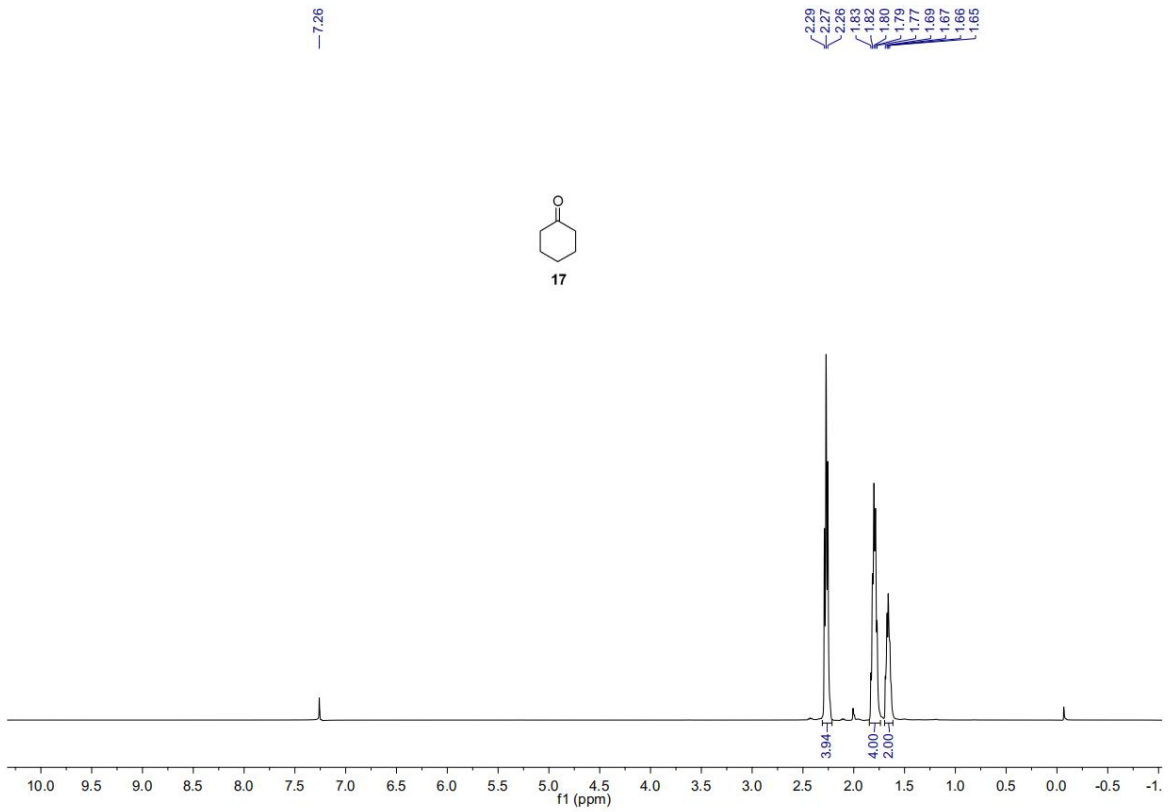

198.00
137.09
133.05
128.53
128.25
77.57
77.26
76.94
26.50
16b
acetophenone
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

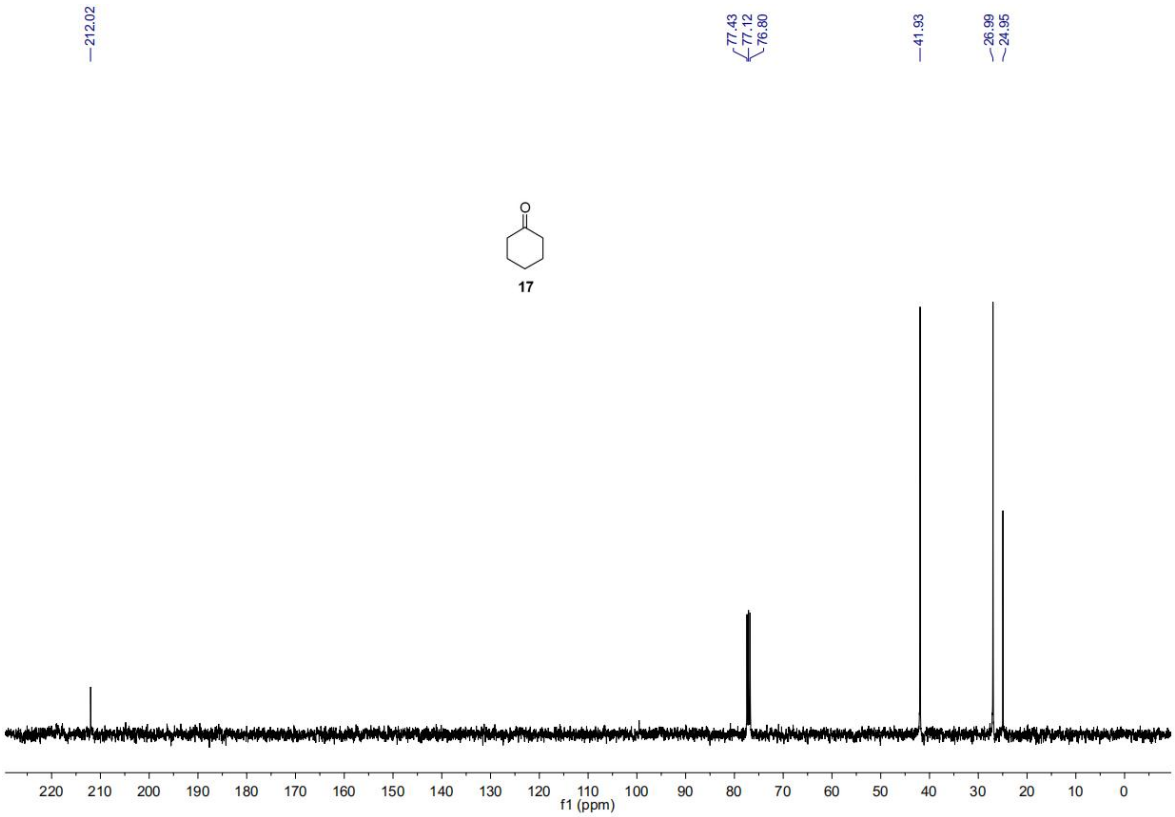

2.03
1.04
16c
3.01
9.27
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
f1 (ppm)

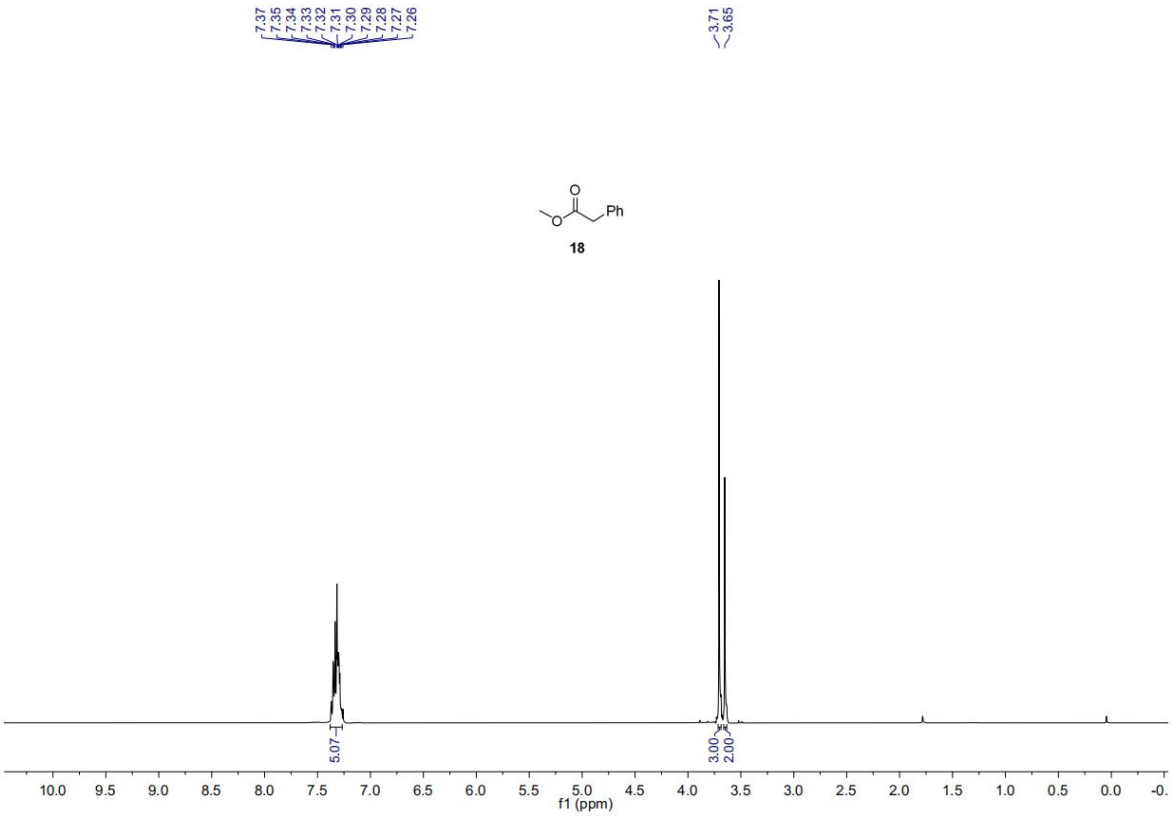

213.99
77.42
77.10
76.78
44.16
26.25
24.53
16c
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

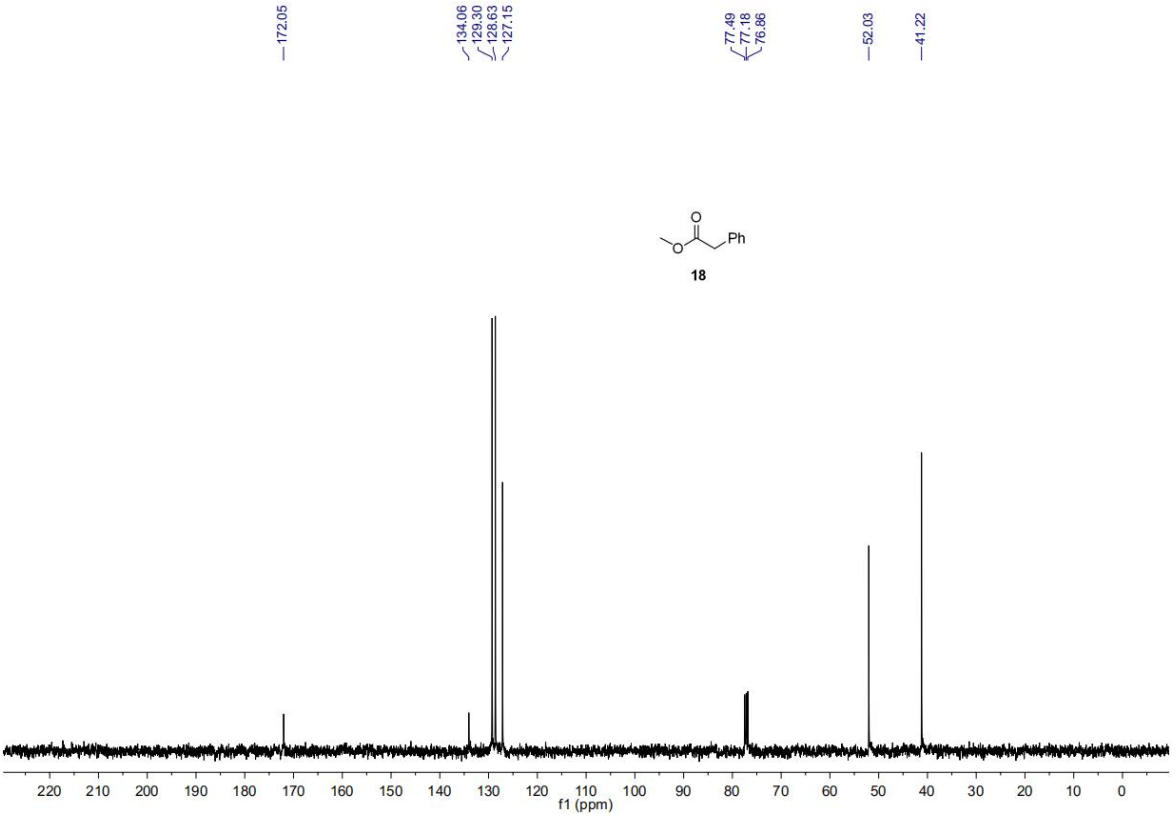

7.64
7.63
7.57
7.56
7.07
7.06
7.05
2.49
16d:
1.00
0.96
1.00
3.21
f1 (ppm)

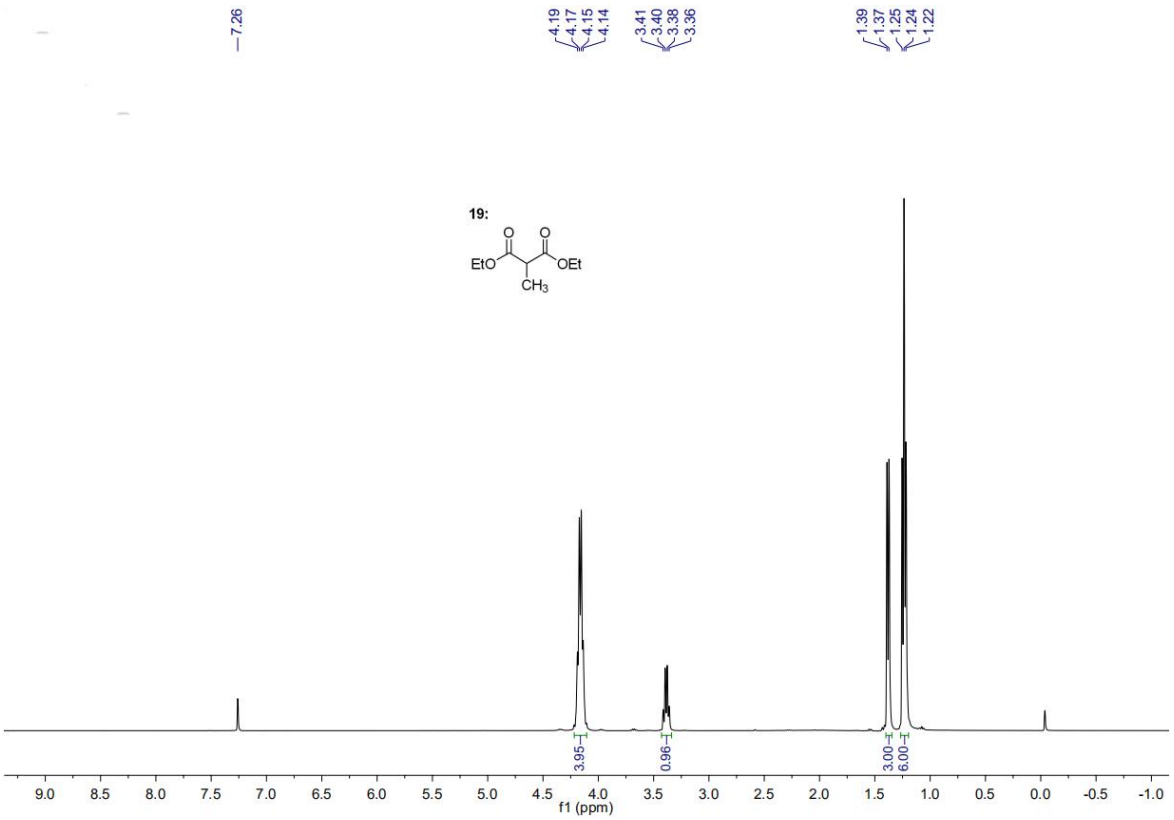

190.70
144.52
133.80
132.56
128.16
77.54
77.23
76.91
26.85
16d:
f1 (ppm)

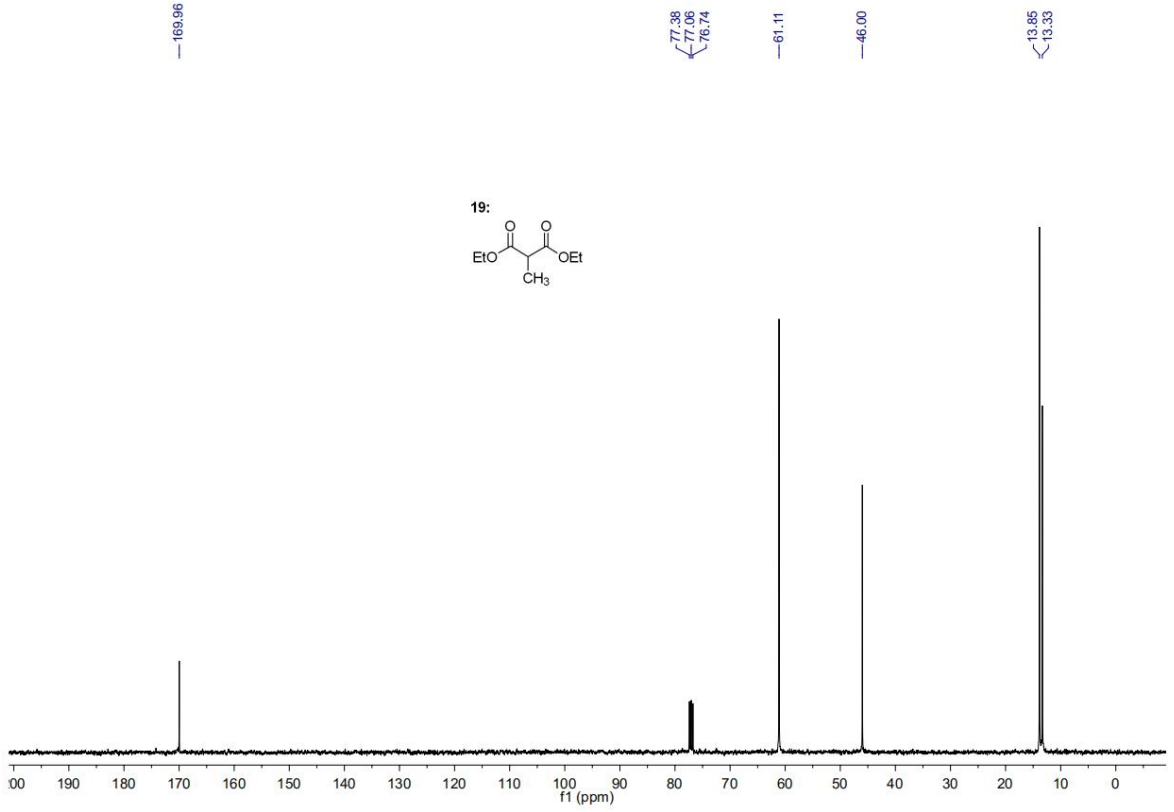

7.26
2.29
2.27
2.26
1.83
1.82
1.80
1.79
1.77
1.69
1.67
1.66
1.65
17
3.94
4.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

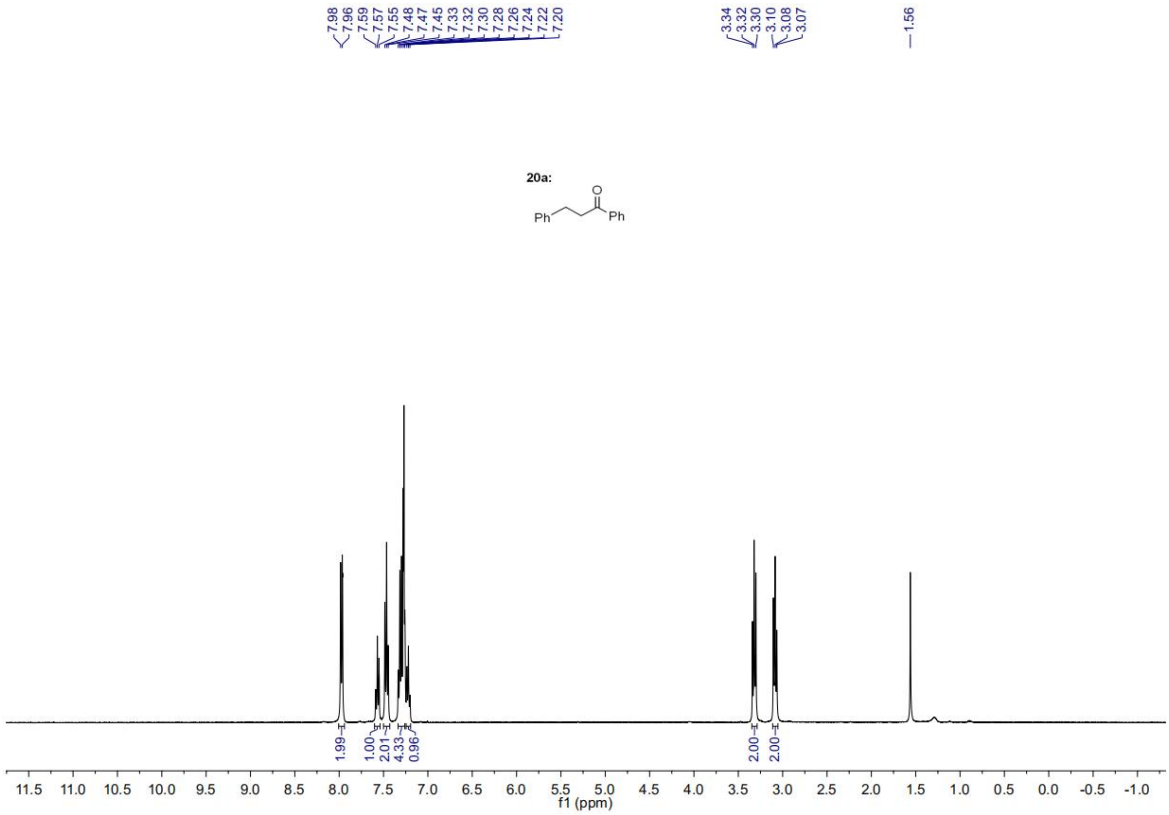

212.02
77.43
77.12
76.80
41.93
26.99
24.95
17
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

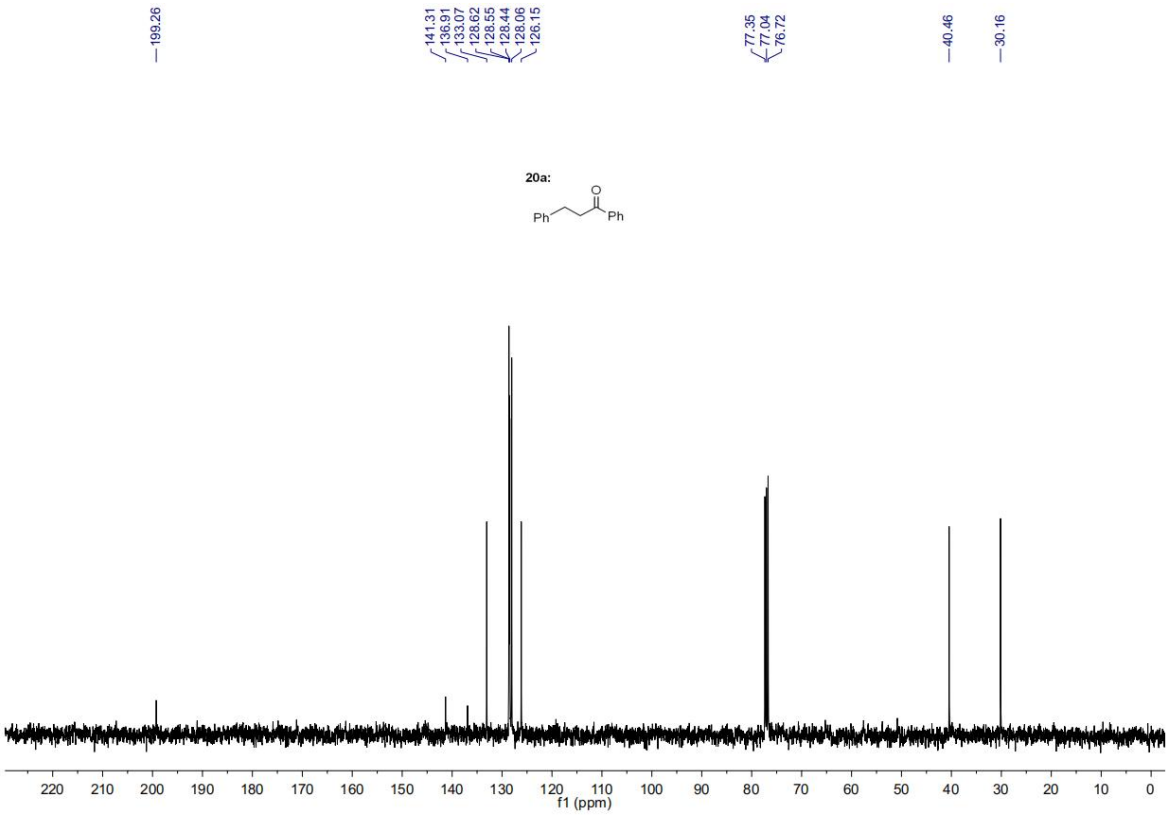

7.37
7.35
7.34
7.33
7.32
7.31
7.30
7.29
7.28
7.27
7.26
3.71
3.65
Ph
18
5.07
3.00
2.00
f1 (ppm)

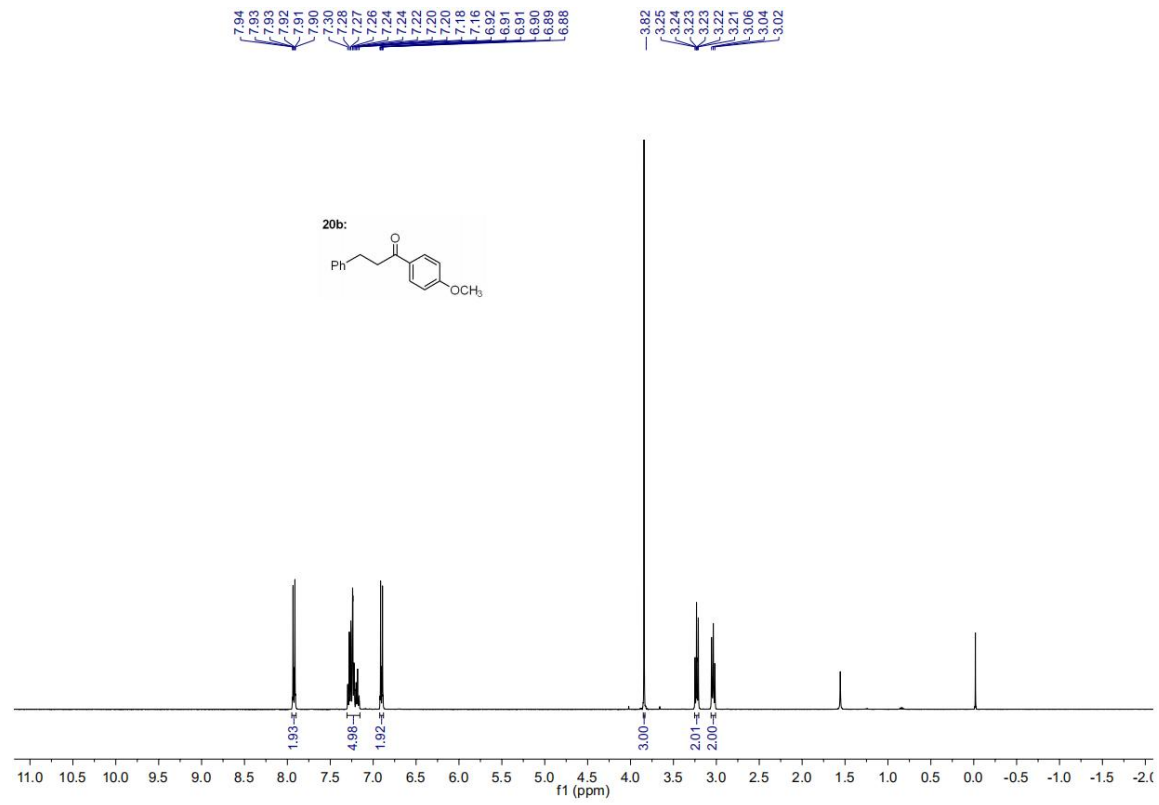

172.05
134.06
129.30
128.63
127.15
77.49
77.18
76.86
52.03
41.22
Ph
18
f1 (ppm)

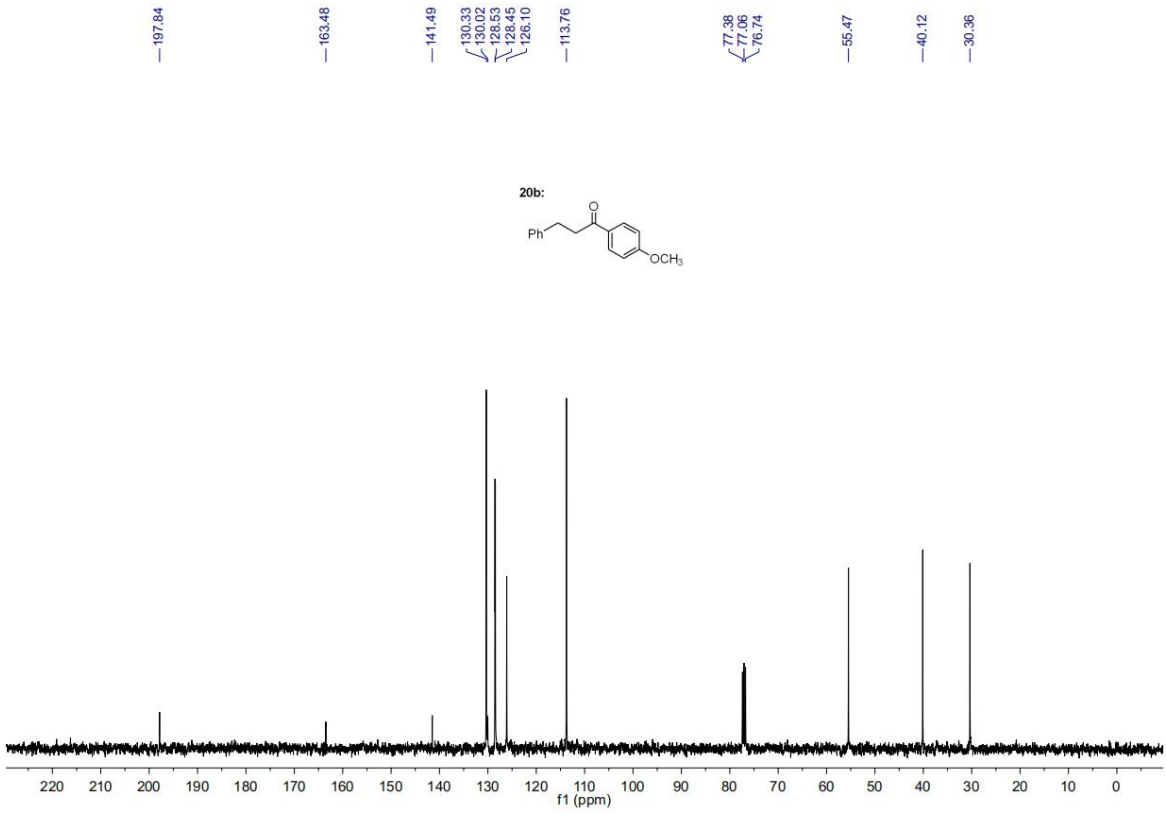

7.26
4.19
4.17
4.15
4.14
3.41
3.40
3.38
3.36
1.39
1.37
1.25
1.24
1.22
19:
EtO
OEt
CH3
3.95
0.96
3.00
6.00
f1 (ppm)

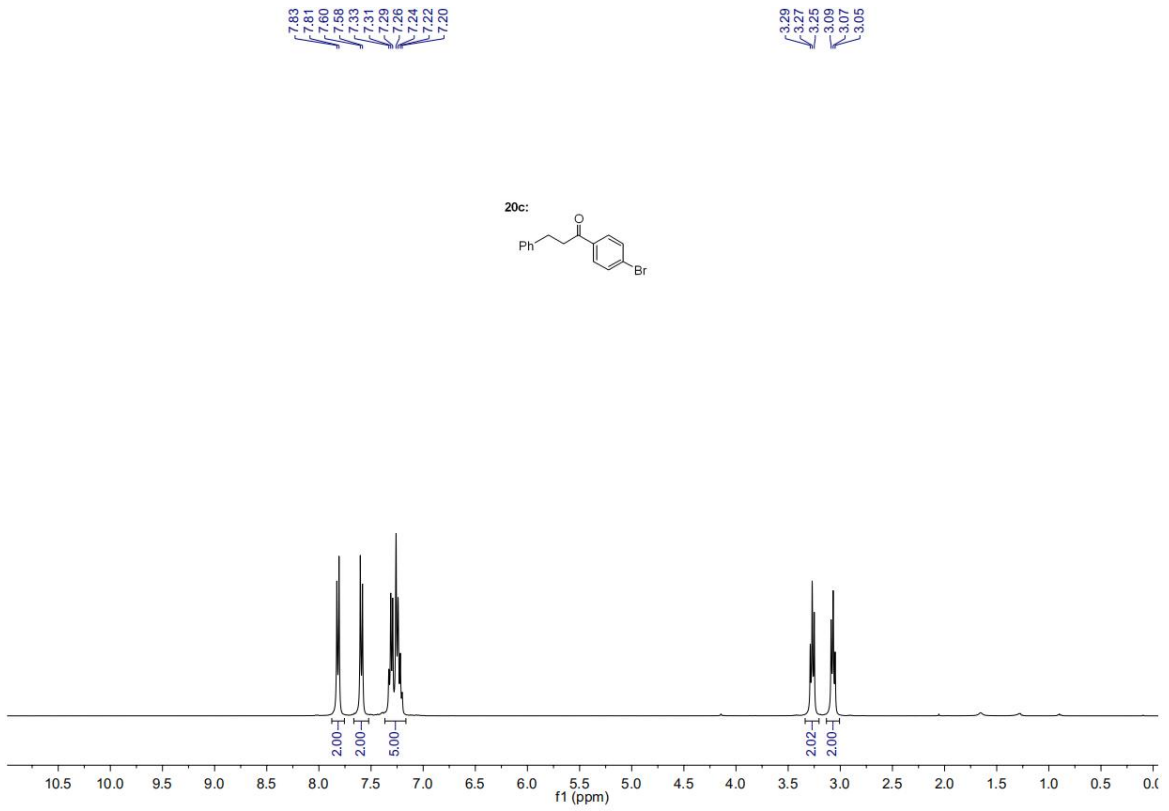

169.96
77.38
77.06
76.74
61.11
46.00
13.85
13.33
19:
EtO
OEt
CH3
f1 (ppm)

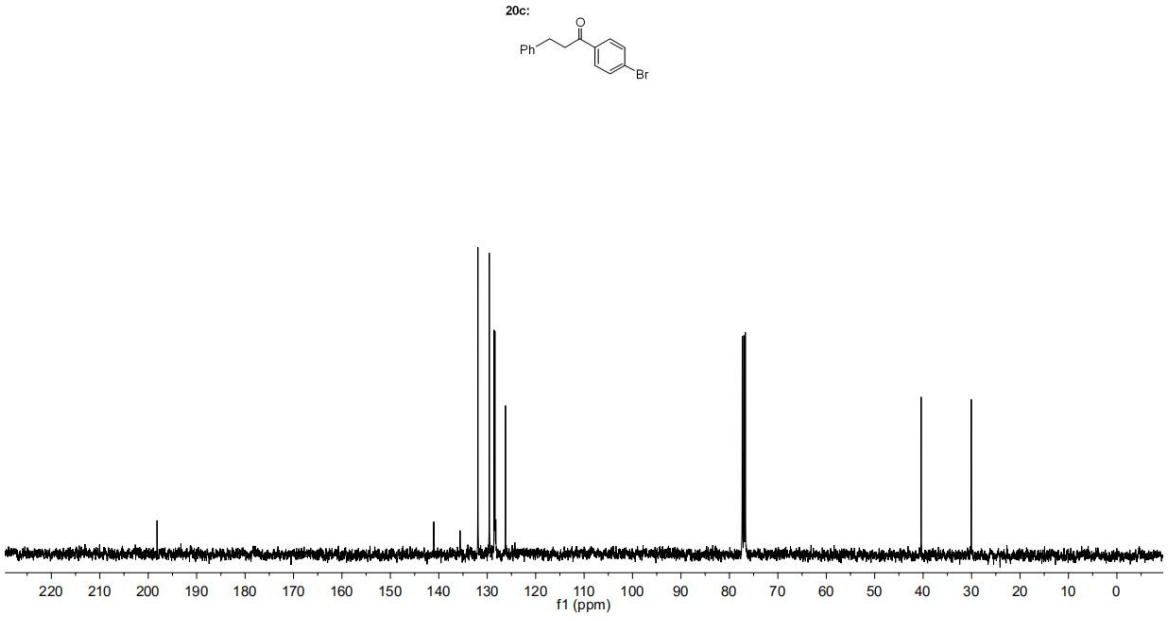

7.98
7.96
7.59
7.57
7.55
7.48
7.47
7.45
7.33
7.32
7.30
7.28
7.26
7.24
7.22
7.20
3.34
3.32
3.30
3.10
3.08
3.07
1.56
20a:
Ph
Ph
1.99
1.00
2.01
4.33
0.96
2.00
2.00
f1 (ppm)


199.26
141.31
136.91
133.07
128.62
128.55
128.44
128.06
126.15
77.35
77.04
76.72
40.46
30.16
20a:
Ph
Ph
f1 (ppm)

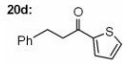

7.94
7.93
7.93
7.92
7.91
7.90
7.30
7.28
7.27
7.26
7.24
7.24
7.24
7.22
7.20
7.20
7.18
7.16
6.92
6.91
6.91
6.90
6.89
6.88
3.82
3.25
3.24
3.23
3.23
3.22
3.21
3.06
3.04
3.02
20b:
Ph
OCH3
1.93
4.98
1.92
3.00
2.01
2.00
f1 (ppm)

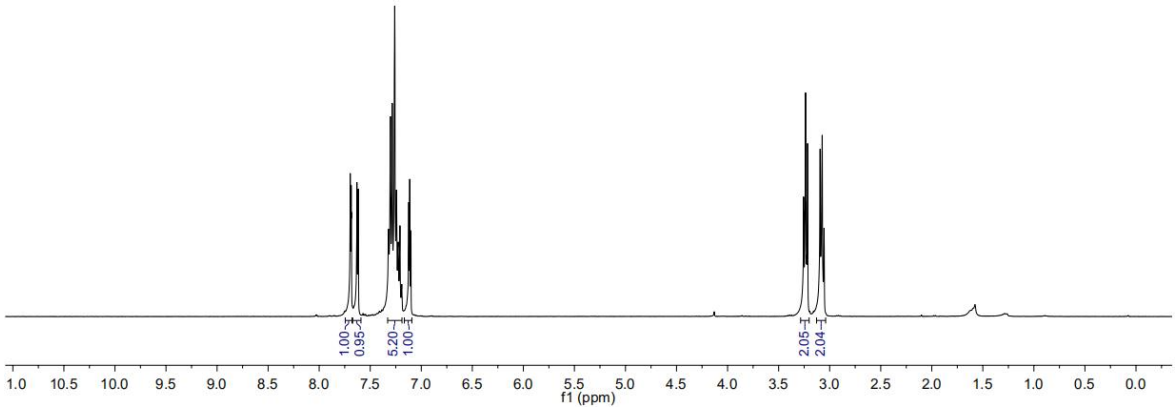

197.84
163.48
141.49
130.33
130.02
128.53
128.45
126.10
113.76
77.38
77.06
76.74
55.47
40.12
30.36
20b:
Ph
OCH3
f1 (ppm)


7.83
7.81
7.60
7.58
7.33
7.31
7.29
7.26
7.24
7.22
7.20
3.29
3.27
3.25
3.09
3.07
3.05
20c:
Ph
O
Br
2.00
2.00
5.00
2.02
2.00
f1 (ppm)

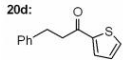

198.18
141.04
135.60
131.93
129.58
128.58
128.41
128.23
126.24
77.34
77.03
76.71
40.40
30.06
20c:
Ph
O
Br
f1 (ppm)

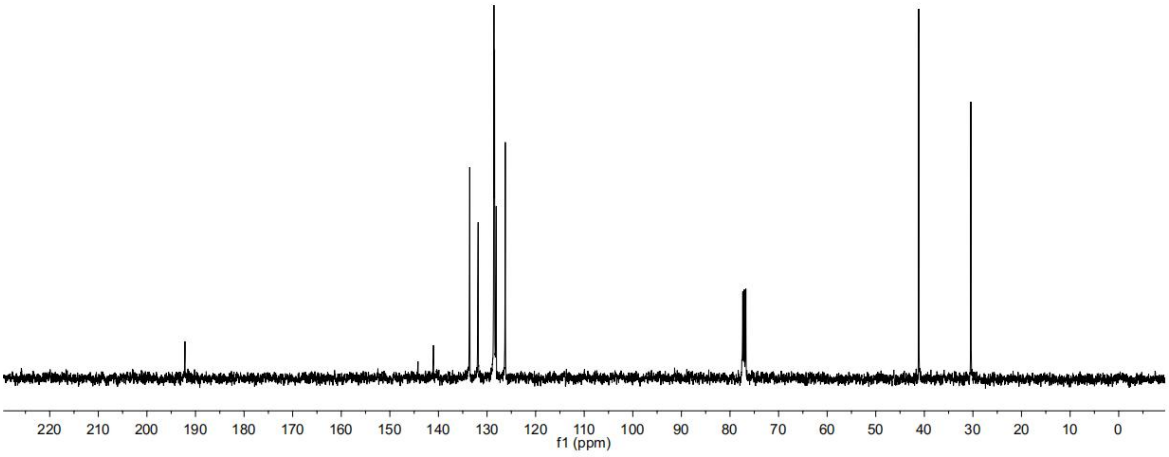

7.70
7.69
7.69
7.68
7.63
7.63
7.62
7.62
7.32
7.32
7.30
7.28
7.26
7.24
7.23
7.23
7.21
7.19
7.12
7.11
7.11
7.10
3.26
3.25
3.24
3.23
3.23
3.22
3.09
3.07
3.06

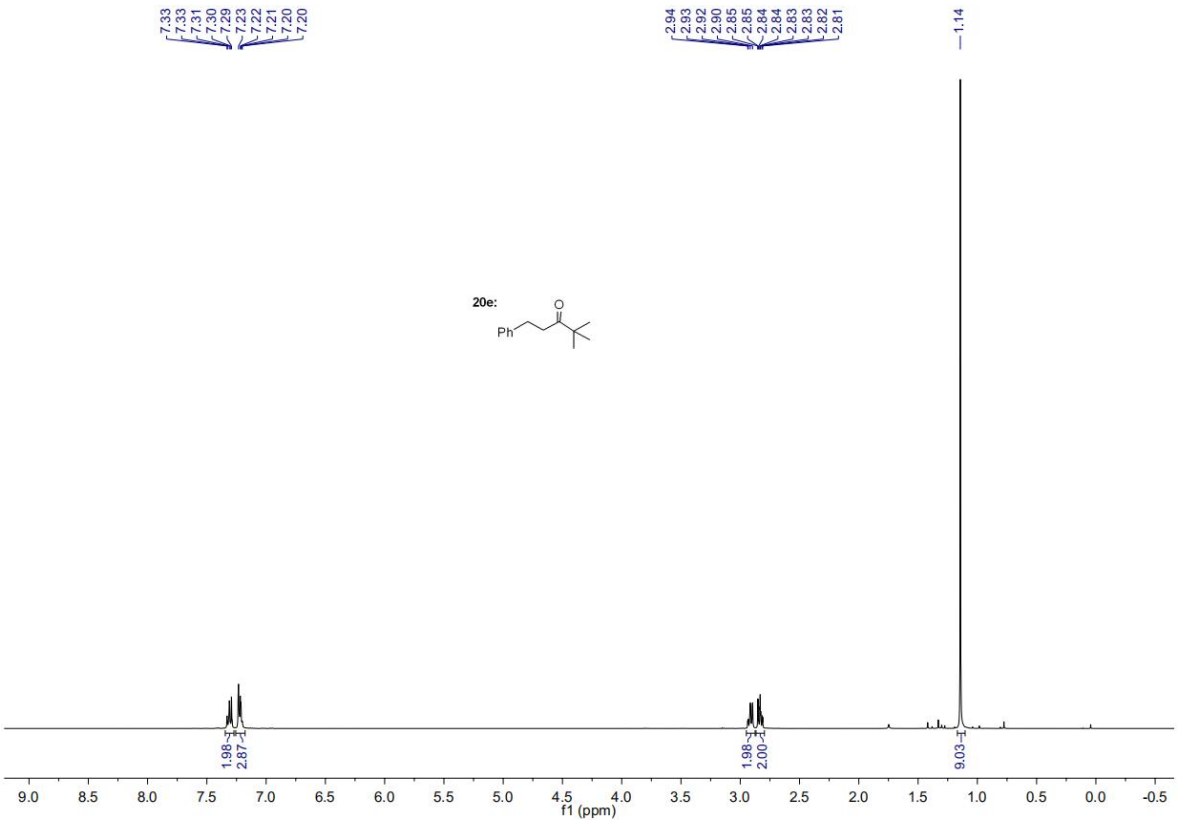

20d:
Ph
O
S

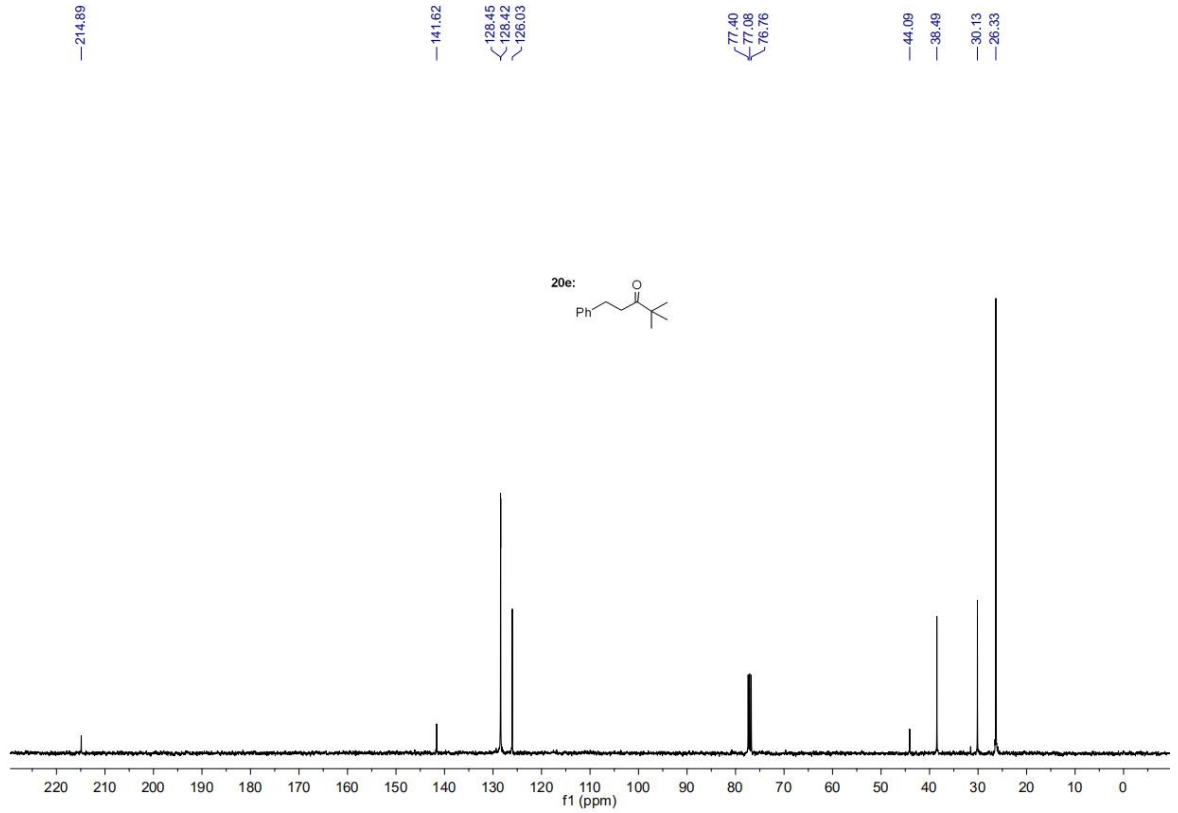

1.00
0.95
5.20
1.00
2.05
2.04
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

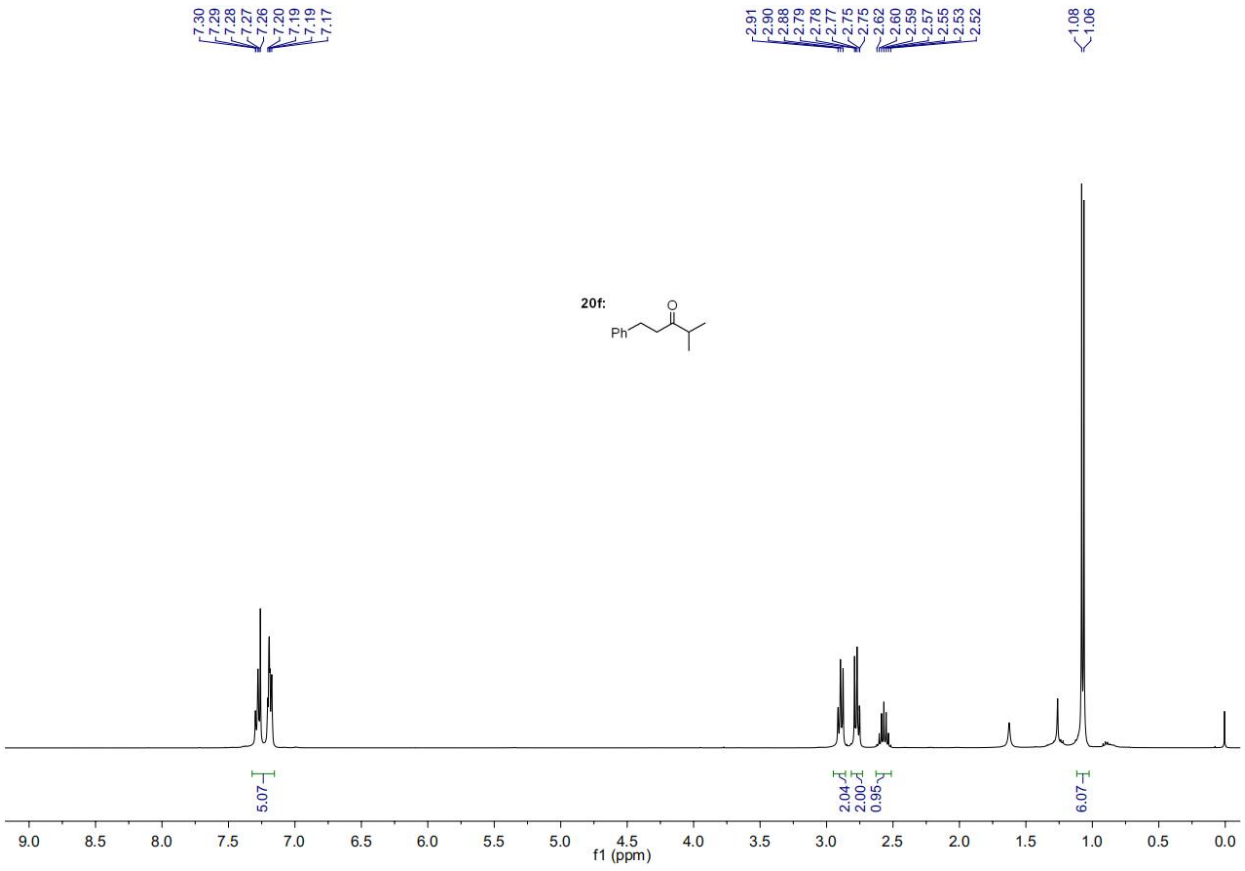

192.17
144.21
141.03
133.56
131.83
128.57
128.45
128.11
126.24
77.37
77.05
76.73
41.16
30.42

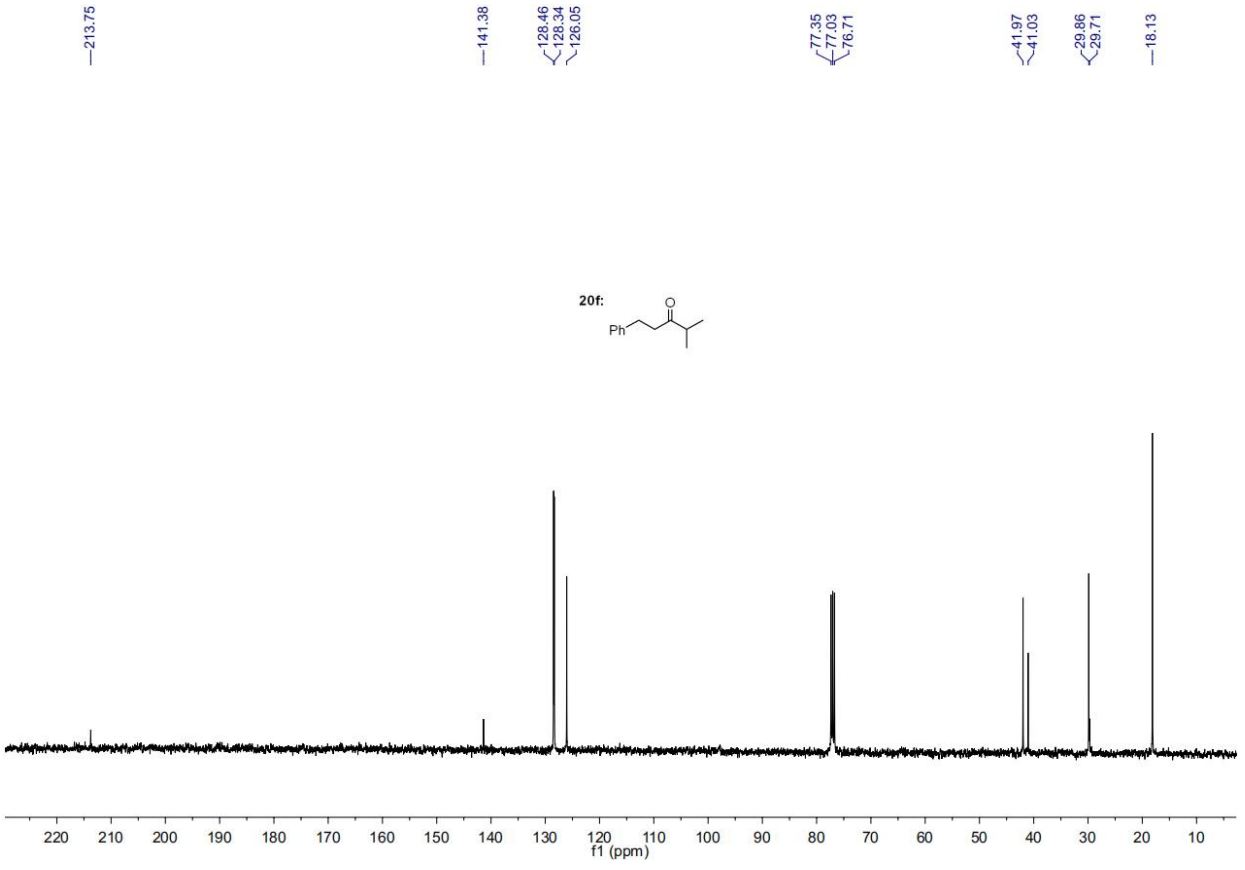

20d:
Ph
O
S

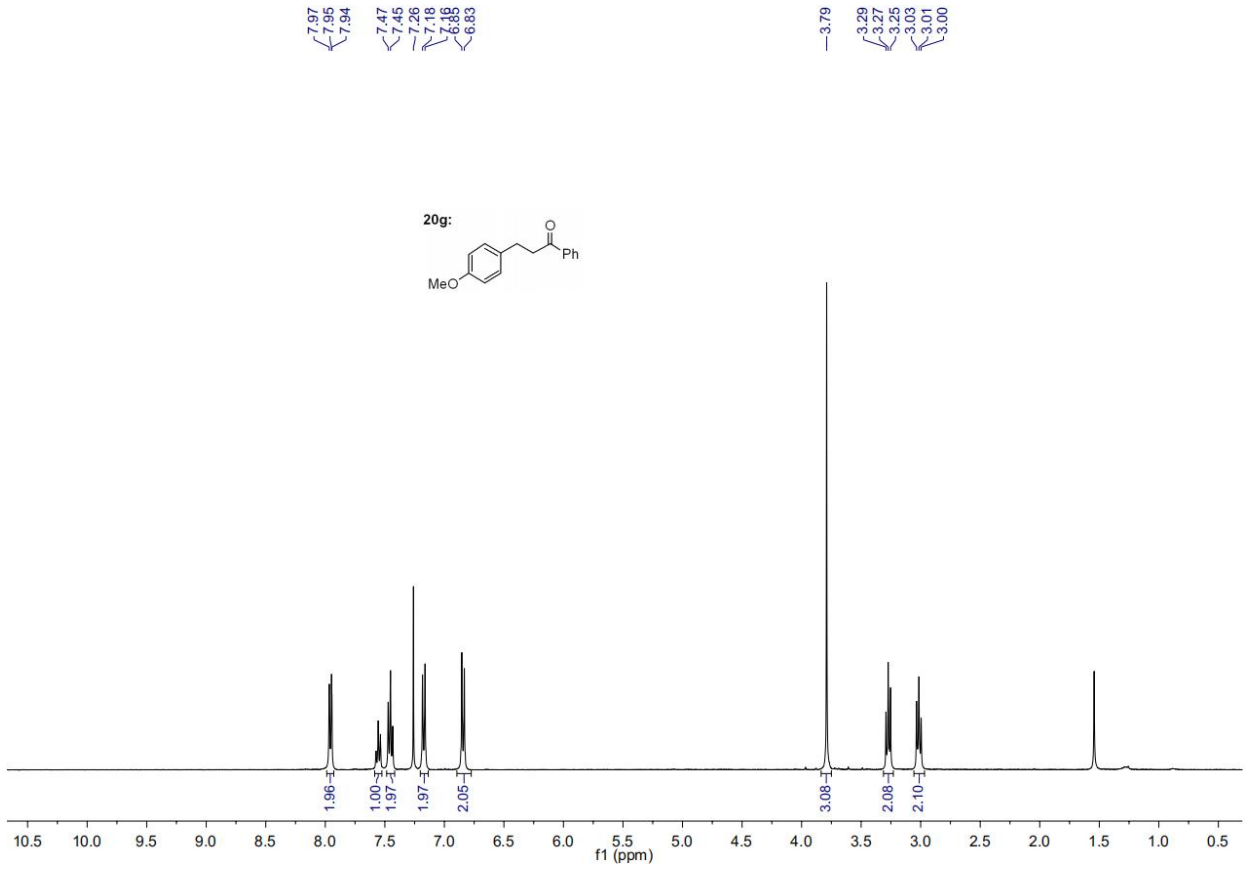

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

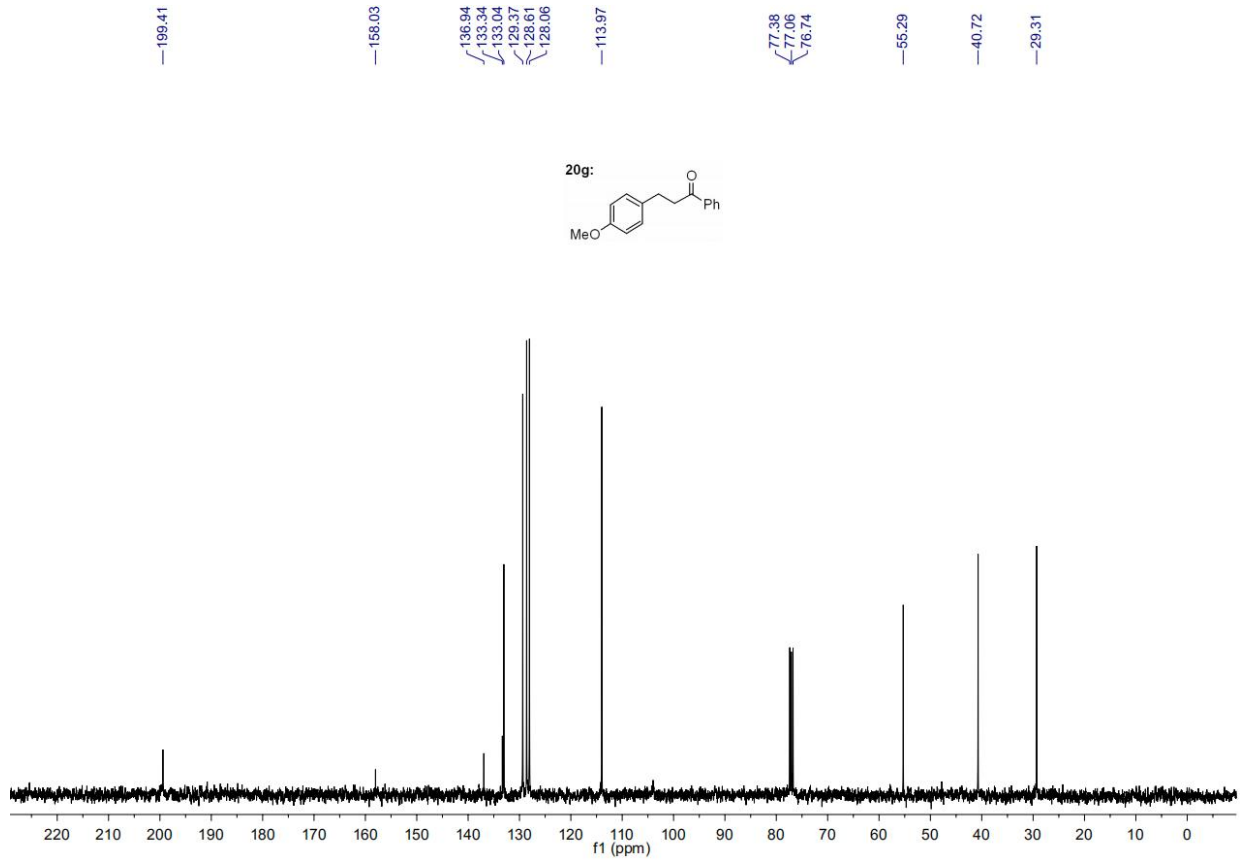

7.33
7.33
7.31
7.30
7.29
7.23
7.22
7.21
7.20
7.20
2.94
2.93
2.92
2.90
2.85
2.85
2.84
2.84
2.83
2.83
2.82
2.81
1.14
20e:
Ph
O
1.98
2.87
1.98
2.00
9.03
f1 (ppm)

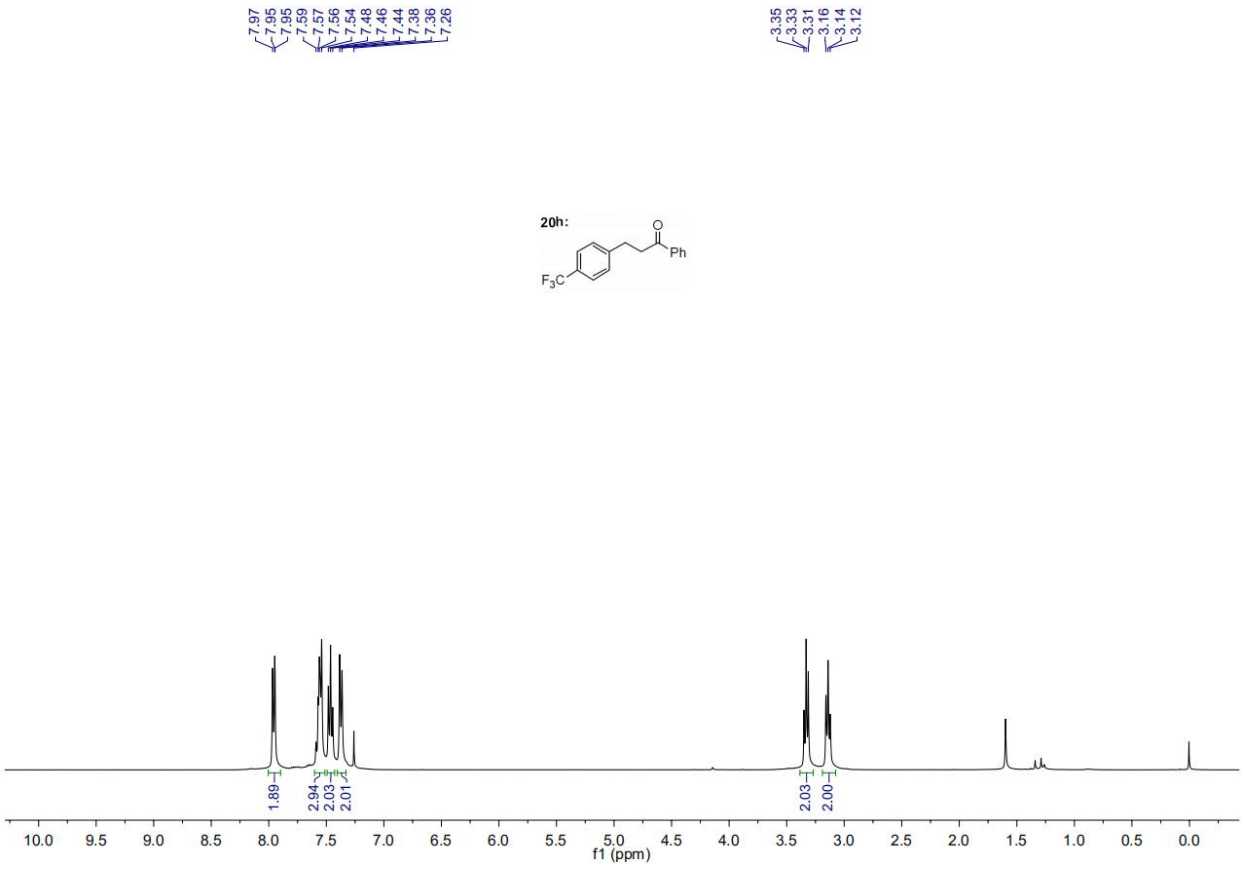

214.89
141.62
128.45
128.42
126.03
77.40
77.08
76.76
44.09
38.49
30.13
26.33
20e:
Ph
O
f1 (ppm)

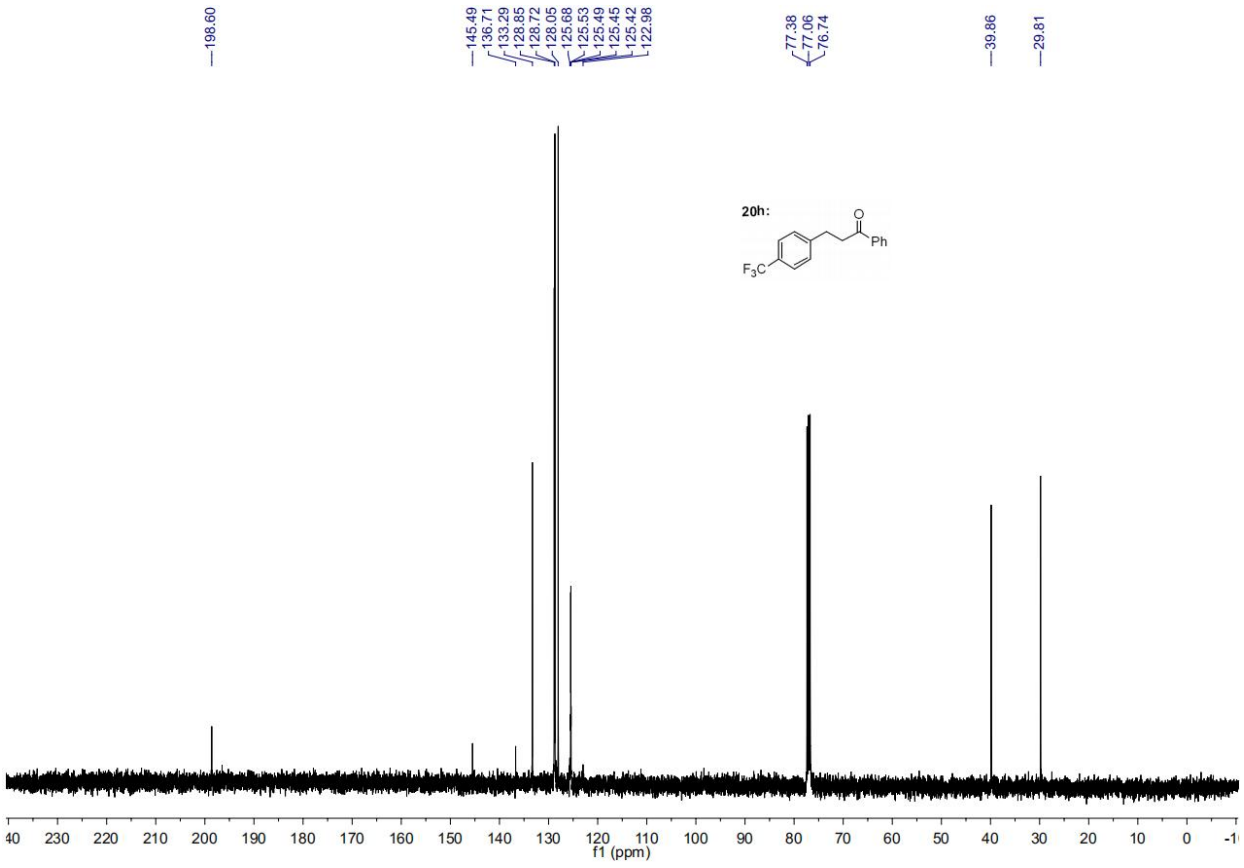

7.30
7.29
7.28
7.27
7.26
7.20
7.19
7.17
2.91
2.90
2.88
2.79
2.78
2.77
2.75
2.75
2.62
2.60
2.59
2.57
2.55
2.53
2.52
1.08
1.06
20f:
Ph
O
5.07
2.04
2.00
0.95
6.07
f1 (ppm)

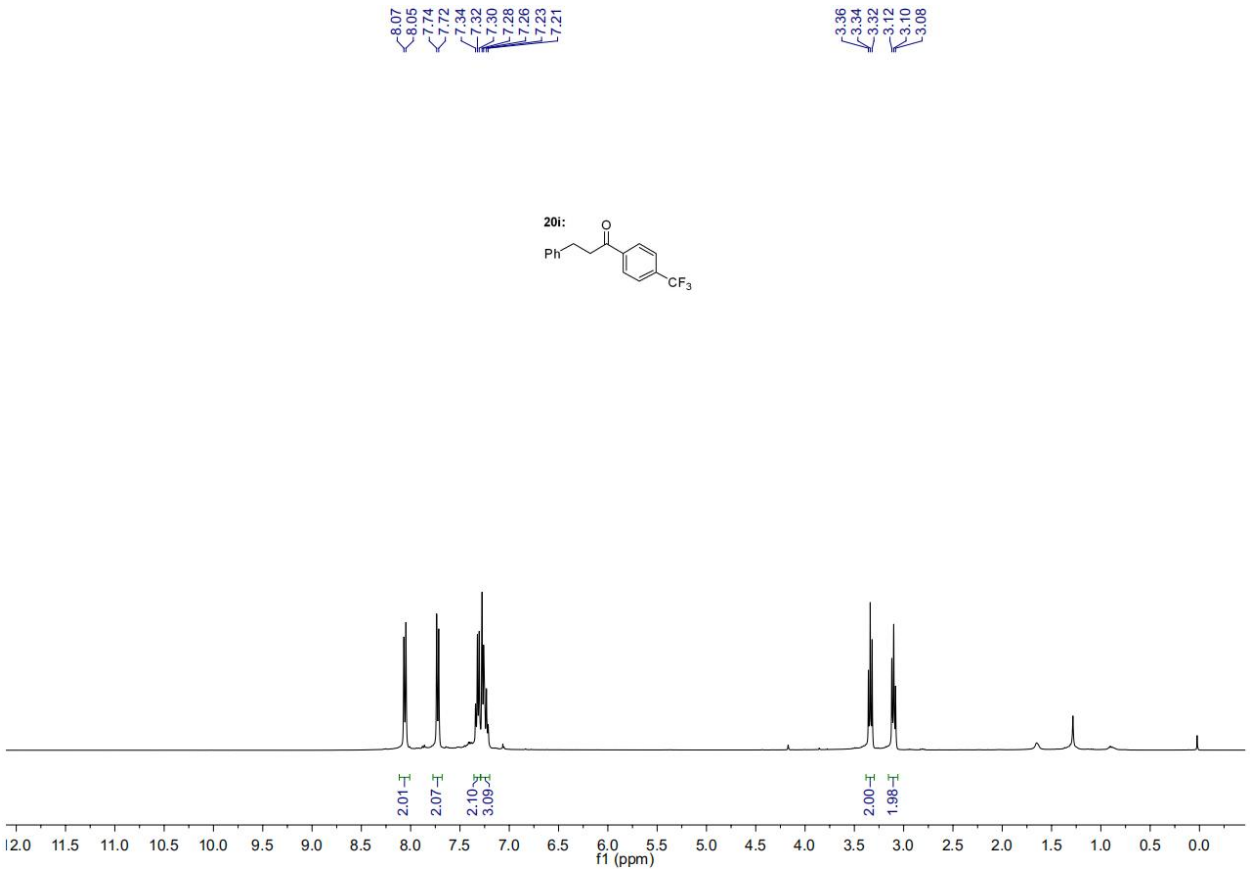

213.75
141.38
128.46
128.34
126.05
77.35
77.03
76.71
41.97
41.03
29.86
29.71
18.13
20f:
Ph
O
f1 (ppm)

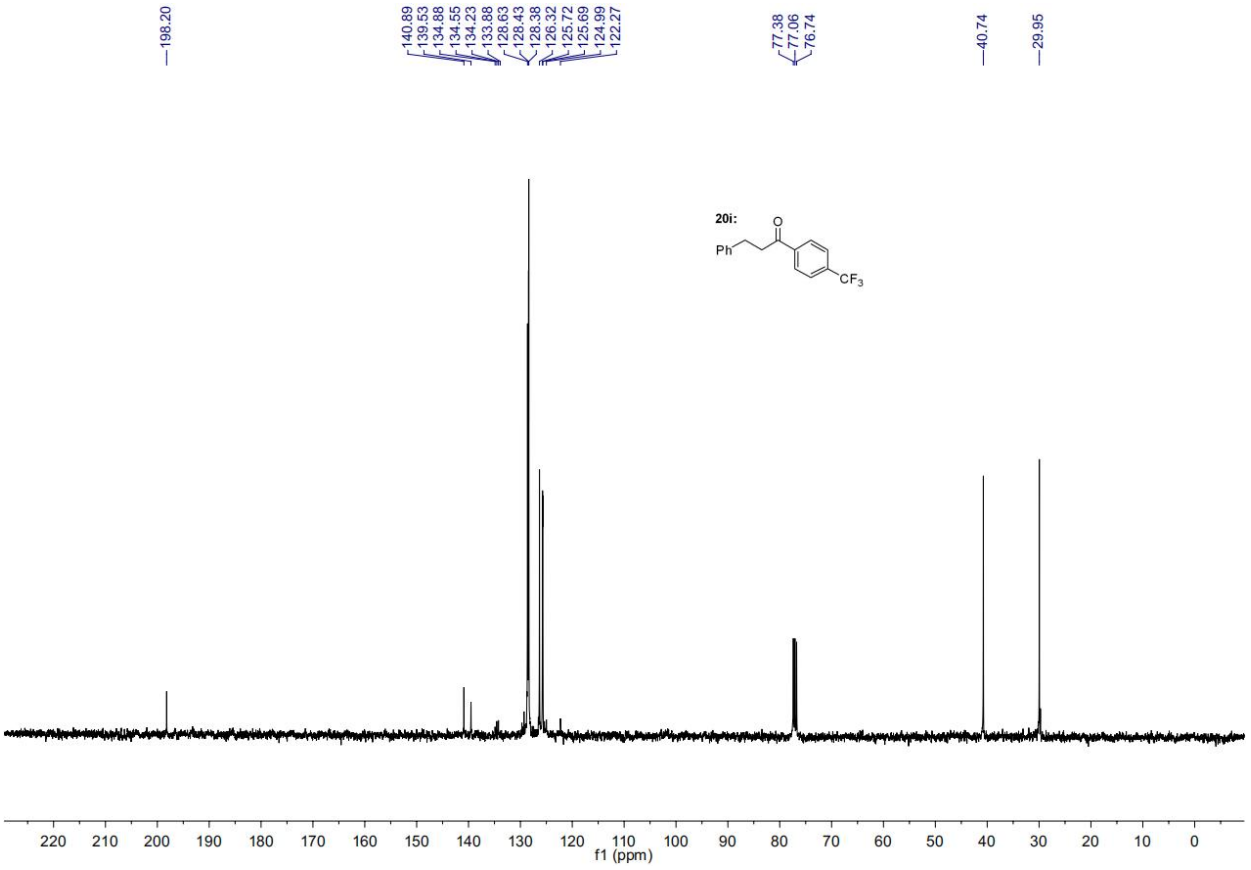

7.97
7.95
7.94
7.47
7.45
7.26
7.18
6.85
6.83
3.79
3.29
3.27
3.25
3.03
3.01
3.00
20g:
O
Ph
MeO
1.96
1.00
1.97
1.97
2.05
3.08
2.08
2.10
f1 (ppm)

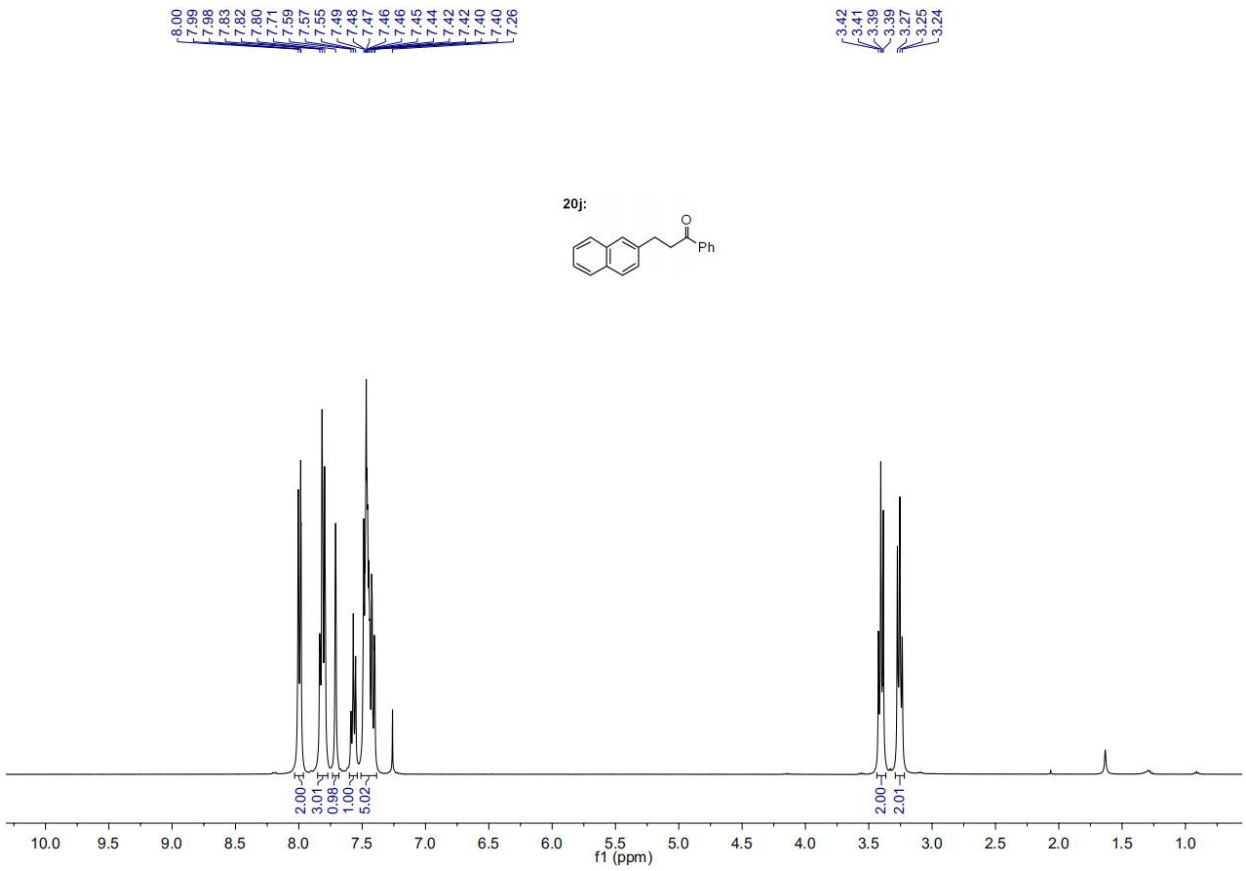

199.41
158.03
136.94
133.34
133.04
129.37
128.61
128.06
113.97
77.38
77.06
76.74
55.29
40.72
29.31
20g:
O
Ph
MeO
f1 (ppm)

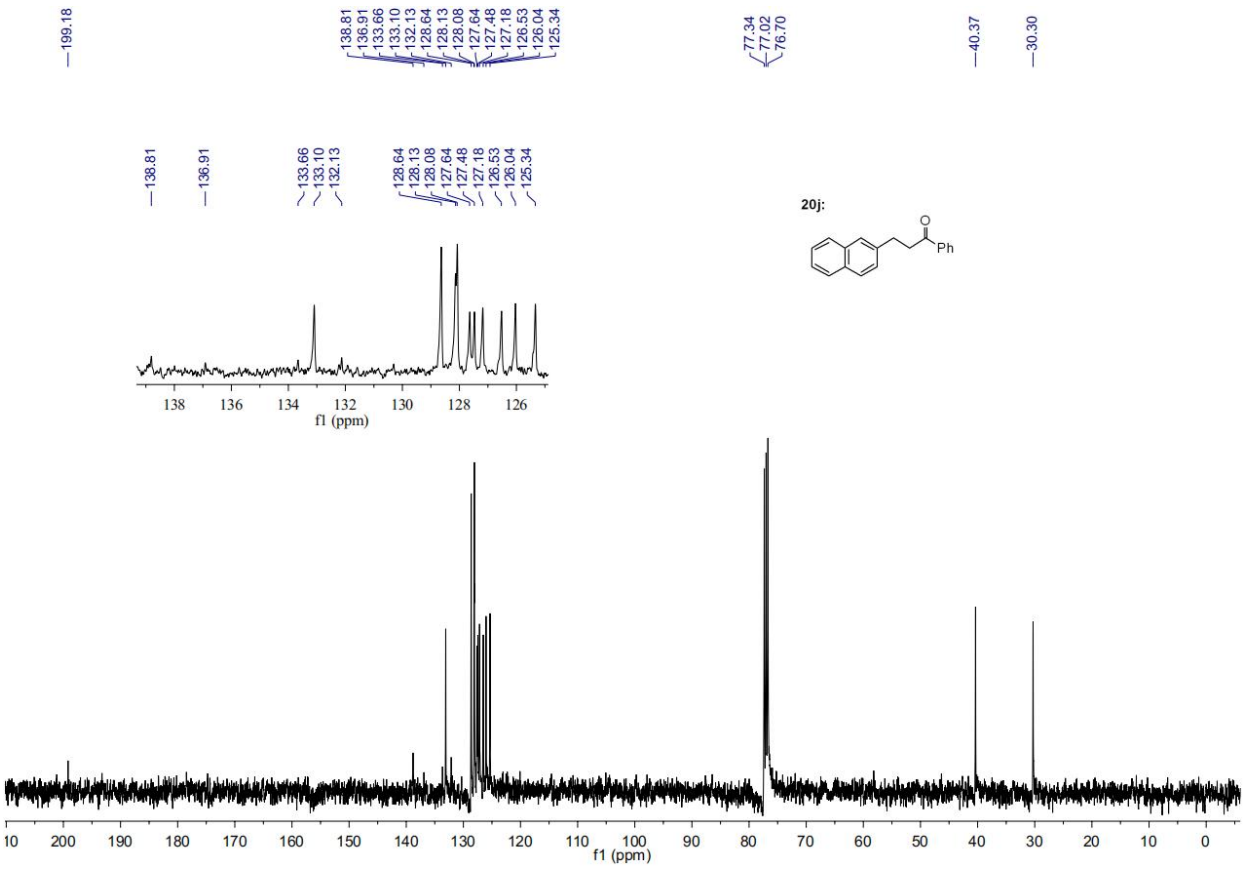

7.97
7.95
7.95
7.59
7.57
7.56
7.54
7.48
7.46
7.44
7.38
7.36
7.26
3.35
3.33
3.31
3.16
3.14
3.12
20h:
Ph
F3C
1.89
2.94
2.03
2.01
2.03
2.00
f1 (ppm)

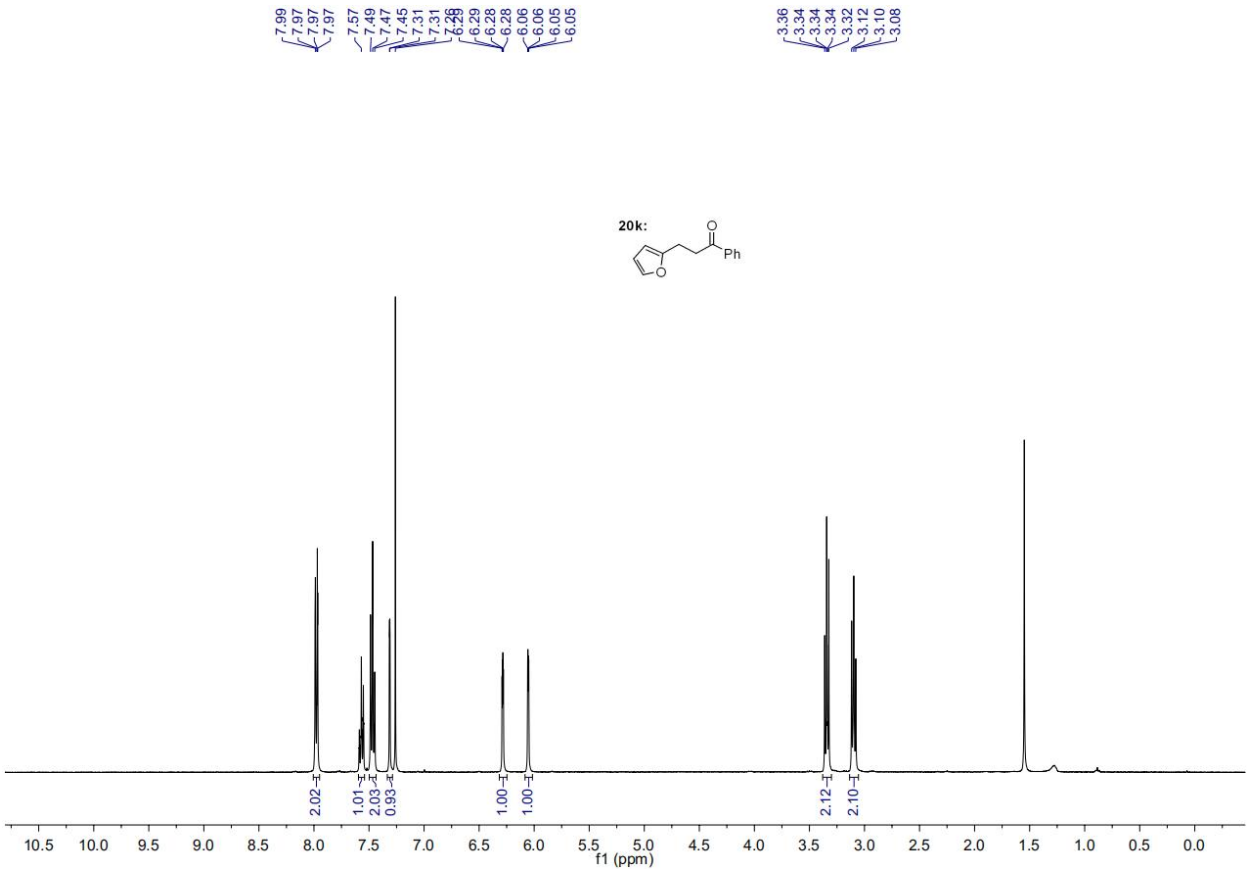

198.60
145.49
136.71
133.29
128.85
128.72
128.05
125.68
125.53
125.49
125.45
125.42
122.98
77.38
77.06
76.74
39.86
29.81
20h:
Ph
F3C
f1 (ppm)

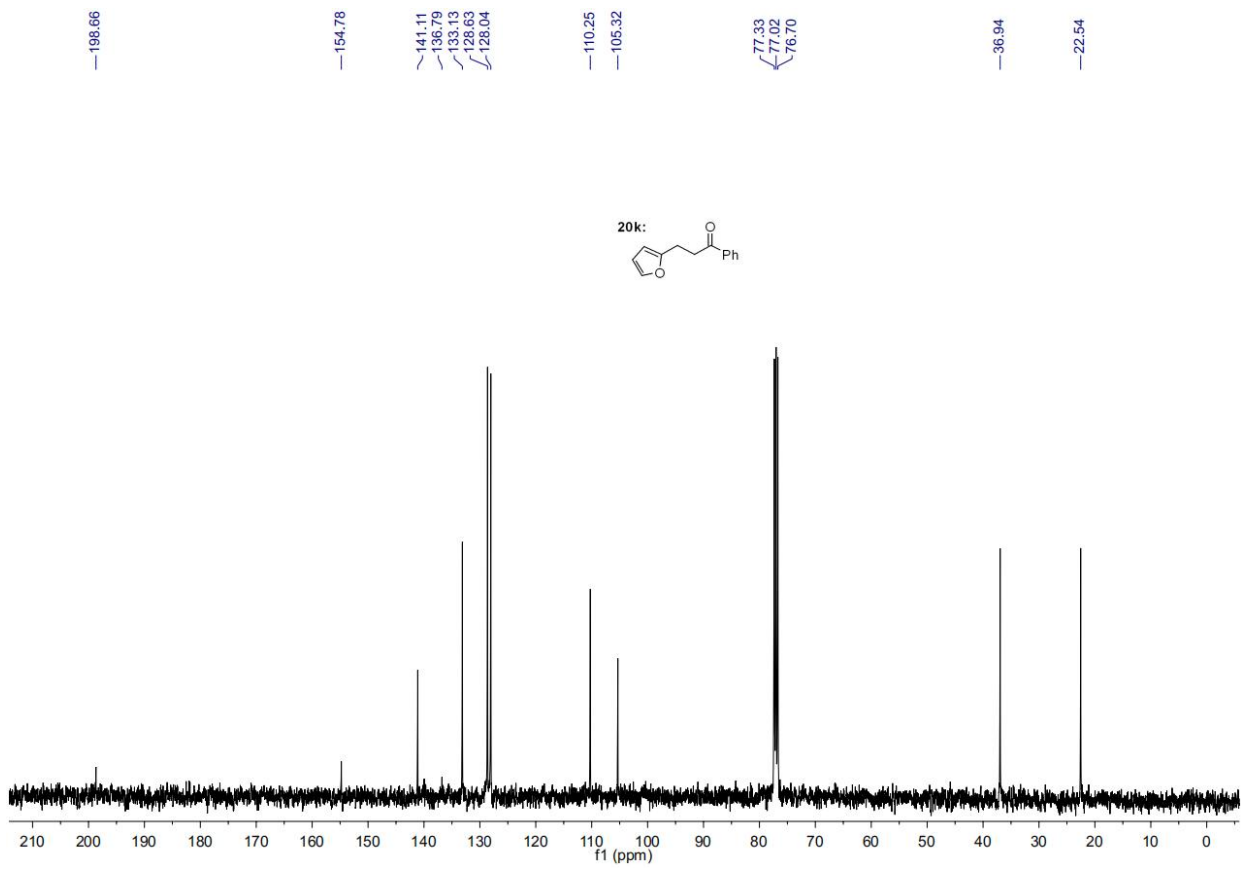

8.07
8.05
7.74
7.72
7.34
7.32
7.30
7.28
7.26
7.23
7.21
3.36
3.34
3.32
3.12
3.10
3.08
20i:
Ph
O
CF3
2.01
2.07
2.10
3.09
2.00
1.98
f1 (ppm)

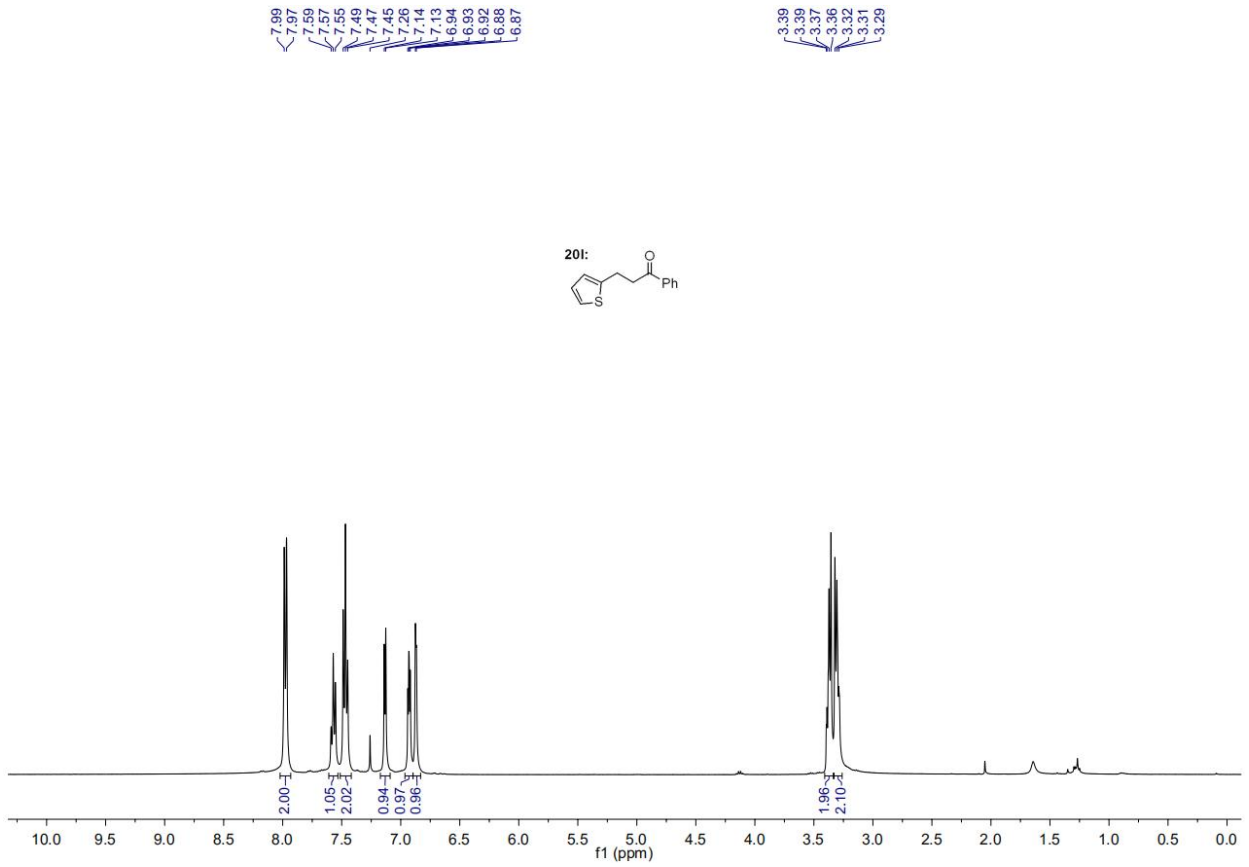

198.20
140.89
139.53
134.88
134.55
134.23
133.88
128.63
128.43
128.38
126.32
125.72
125.69
124.99
122.27
77.38
77.06
76.74
40.74
29.95
20i:
Ph
O
CF3
f1 (ppm)

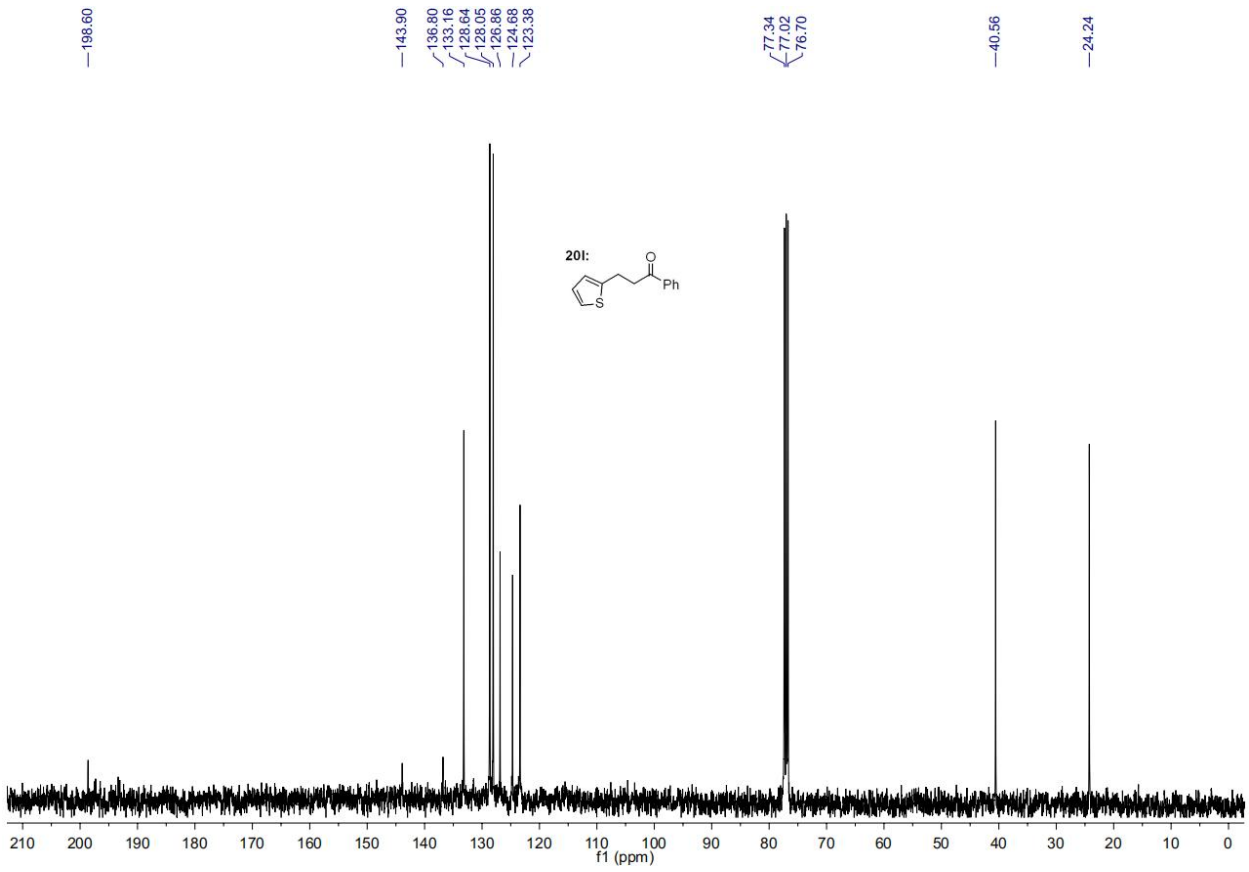

8.00
7.99
7.98
7.83
7.82
7.80
7.71
7.59
7.57
7.55
7.49
7.48
7.47
7.46
7.46
7.45
7.44
7.42
7.42
7.40
7.40
7.26
3.42
3.41
3.39
3.39
3.27
3.25
3.24
20j:
O
Ph
2.00
3.01
0.98
1.00
5.02
2.00
2.01
f1 (ppm)

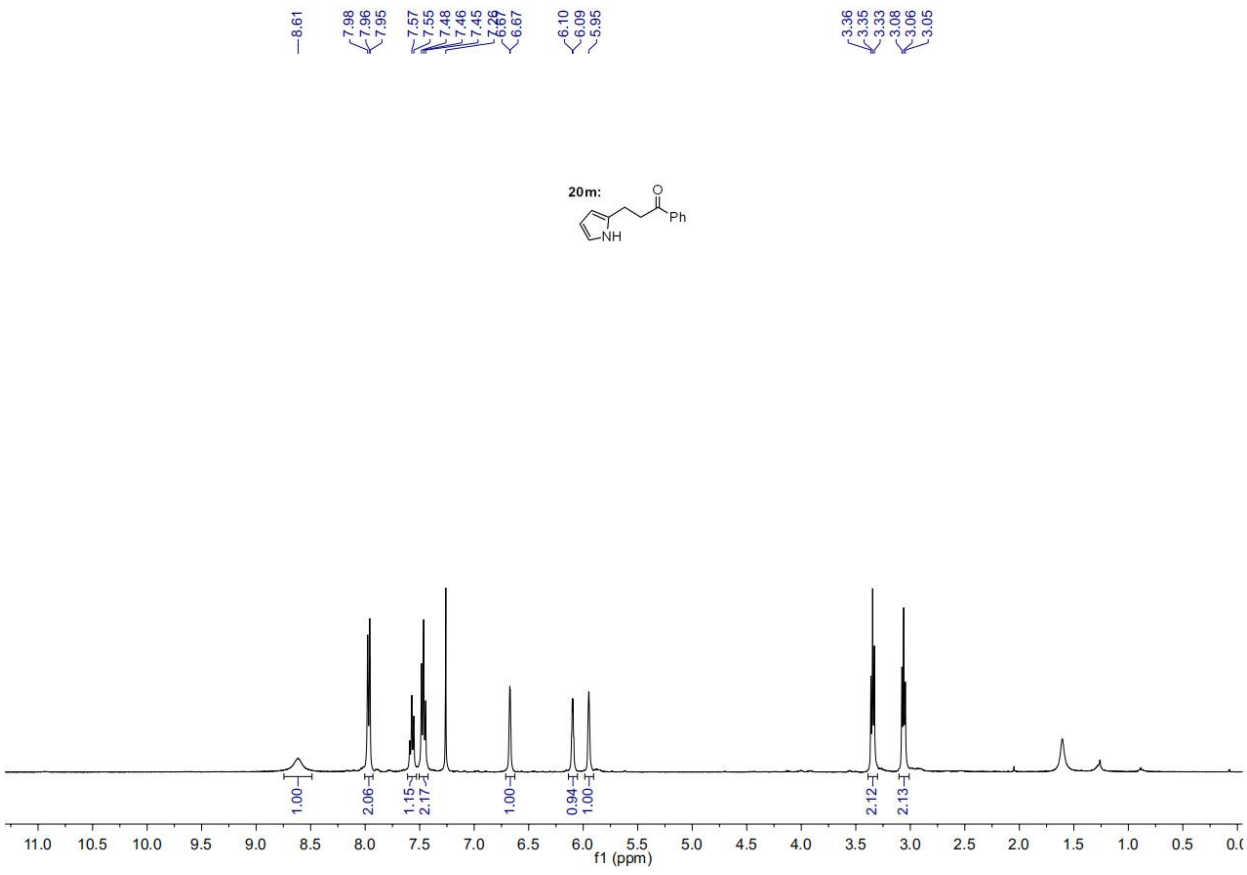

199.18
138.81
136.91
133.66
133.10
132.13
128.64
128.13
128.08
127.64
127.48
127.18
126.53
126.04
125.34
77.34
77.02
76.70
40.37
30.30
20j:
O
Ph
f1 (ppm)

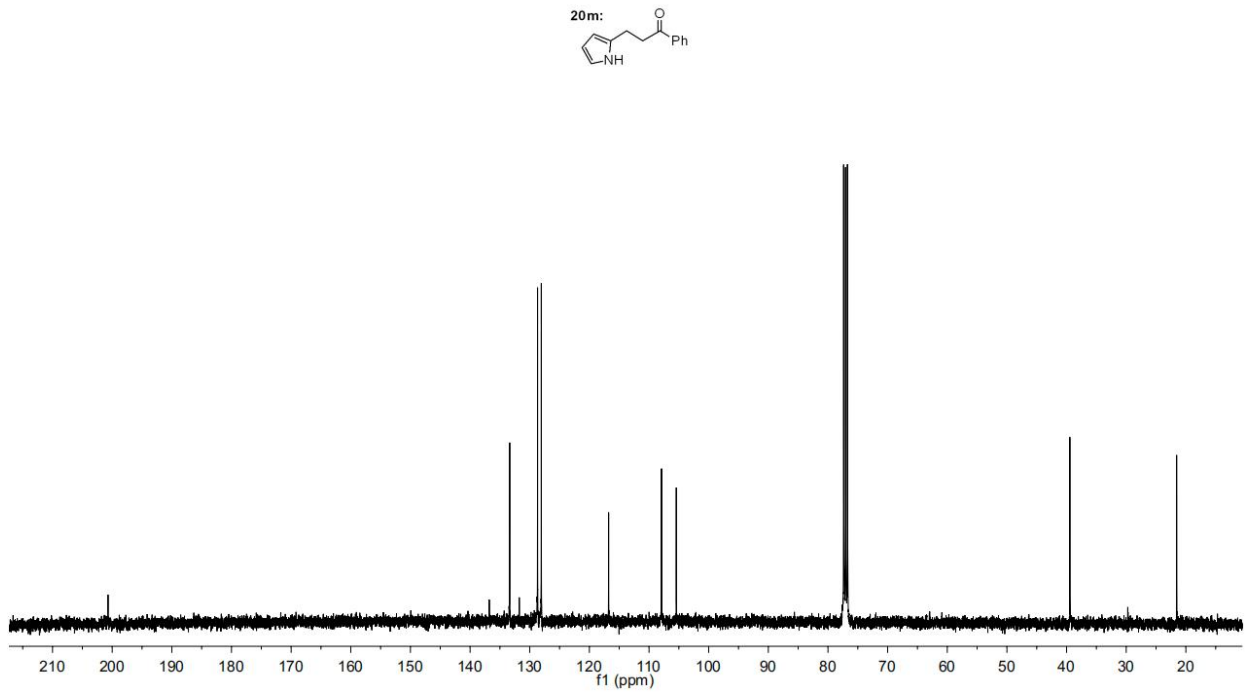

7.99
7.97
7.97
7.97
7.57
7.49
7.47
7.45
7.31
7.31
6.29
6.29
6.28
6.28
6.06
6.06
6.05
6.05
3.36
3.34
3.34
3.34
3.32
3.12
3.10
3.08
20k:
O
Ph
O
2.02
1.01
2.03
0.93
1.00
1.00
2.12
2.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


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

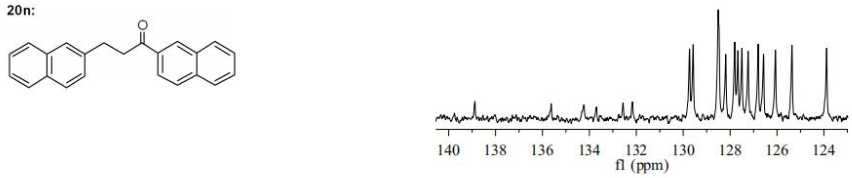

7.99
7.97
7.59
7.57
7.55
7.49
7.47
7.45
7.26
7.14
7.13
6.94
6.93
6.92
6.88
6.87
3.39
3.39
3.37
3.36
3.32
3.31
3.29
20l:
O
Ph
S
2.00
1.05
2.02
0.94
0.97
0.96
1.96
2.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

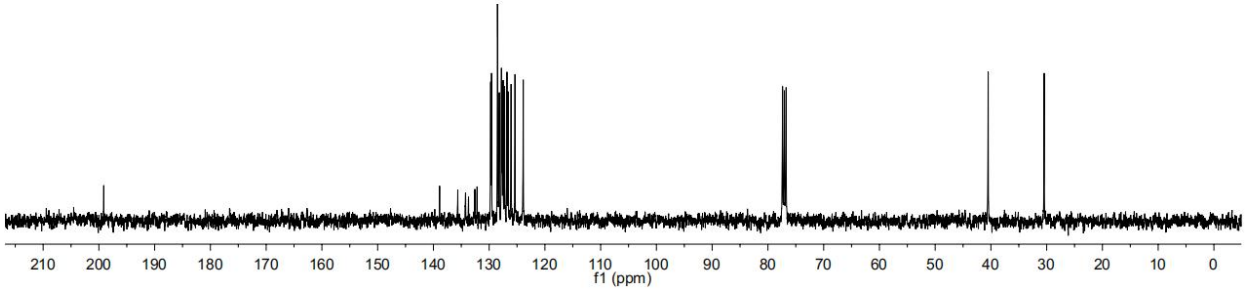

198.60
143.90
136.80
133.16
128.64
128.05
126.86
124.68
123.38
77.34
77.02
76.70
40.56
24.24
20l:
O
Ph
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.61
7.98
7.96
7.95
7.57
7.55
7.48
7.46
7.45
6.67
6.67
6.10
6.09
5.95
3.36
3.35
3.33
3.08
3.06
3.05
20m:
O
Ph
NH
1.00
2.06
1.15
2.17
1.00
0.94
1.00
2.12
2.13
f1 (ppm)

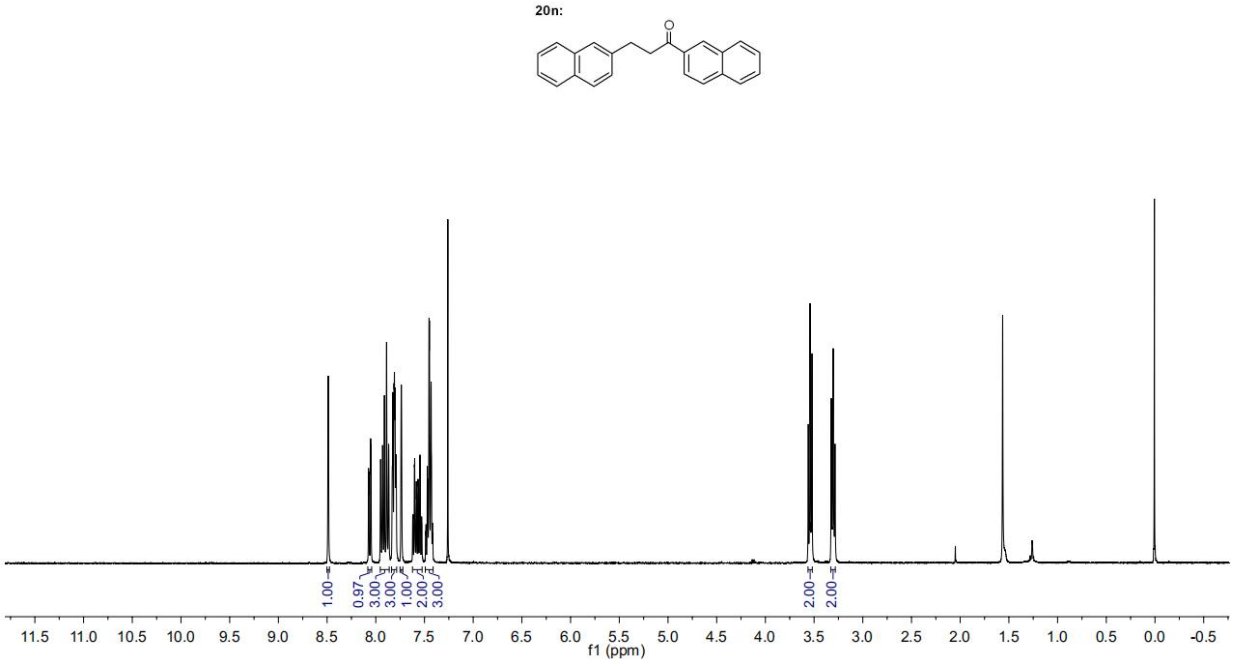

200.69
136.78
133.36
131.75
128.69
128.06
116.77
107.90
105.43
77.38
77.06
76.74
39.45
21.55
20m:
O
Ph
NH
f1 (ppm)

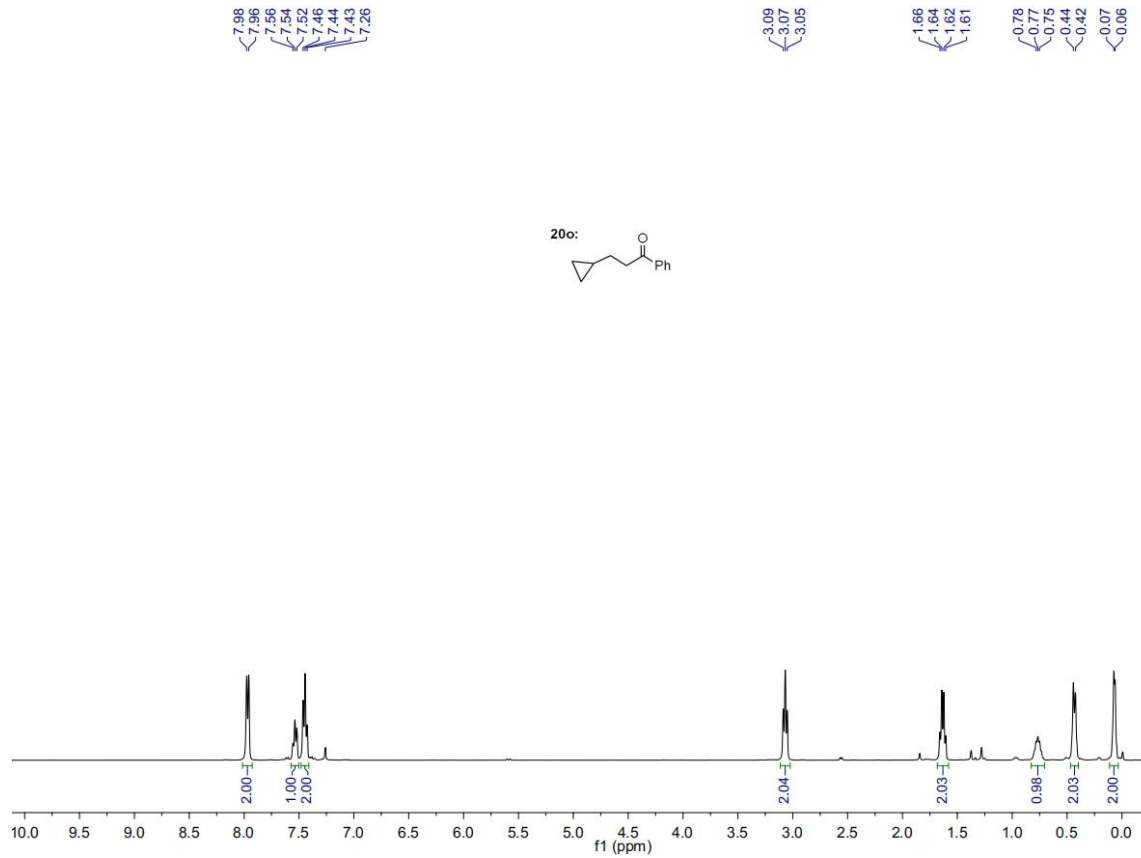

199.13
138.88
135.63
134.24
133.70
132.57
132.16
129.73
129.58
128.51
128.19
127.80
127.67
127.50
127.23
126.80
126.57
126.07
125.36
123.89
77.37
77.05
76.73
40.49
30.45

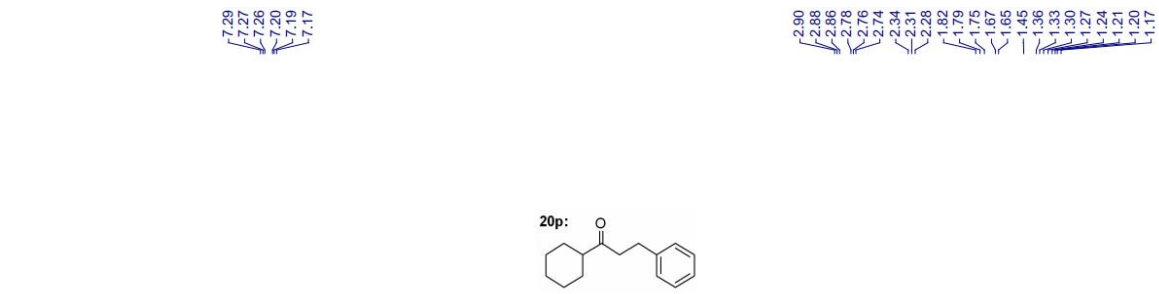

20n:
138.88
135.63
134.24
133.70
132.57
132.16
129.73
129.58
128.51
127.80
127.67
127.50
127.23
126.80
126.57
126.07
125.36
123.89
140 138 136 134 132 130 128 126 124
f1 (ppm)

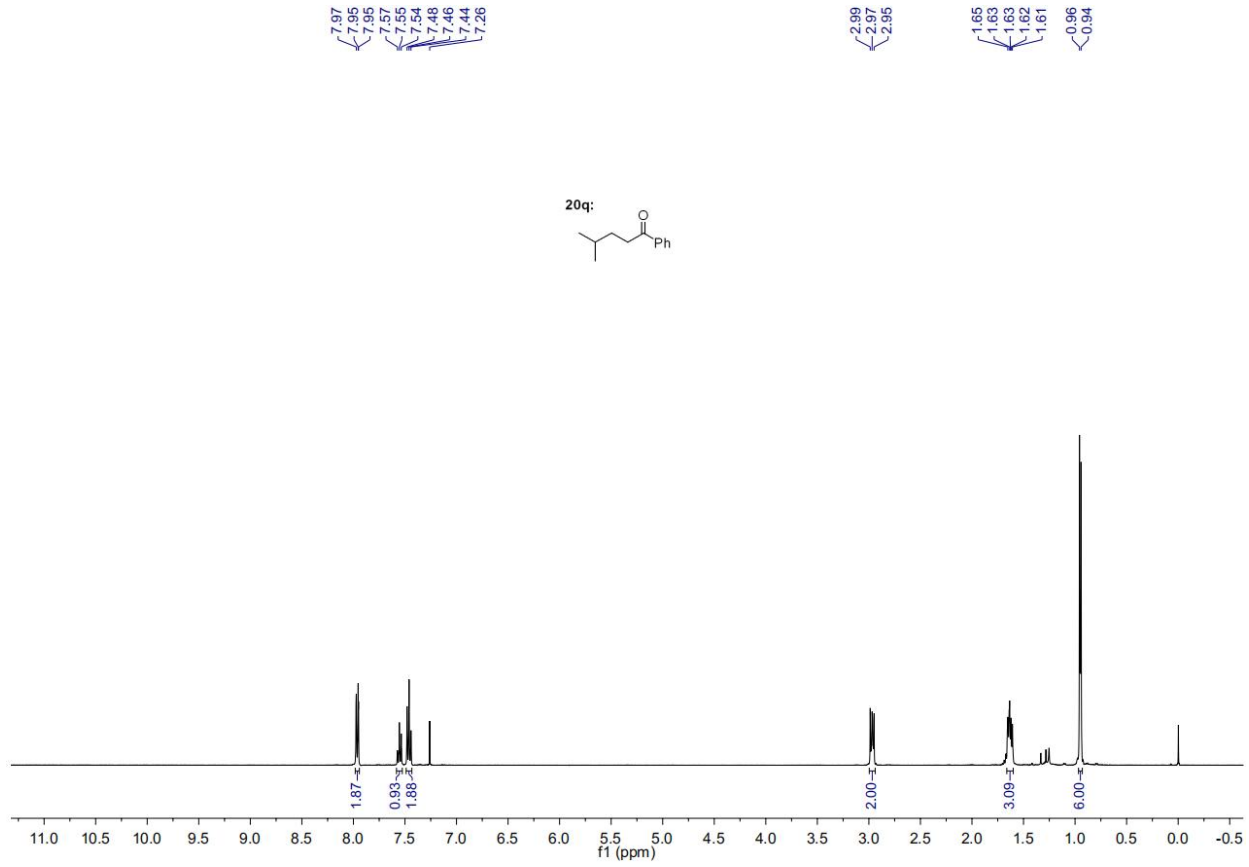

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

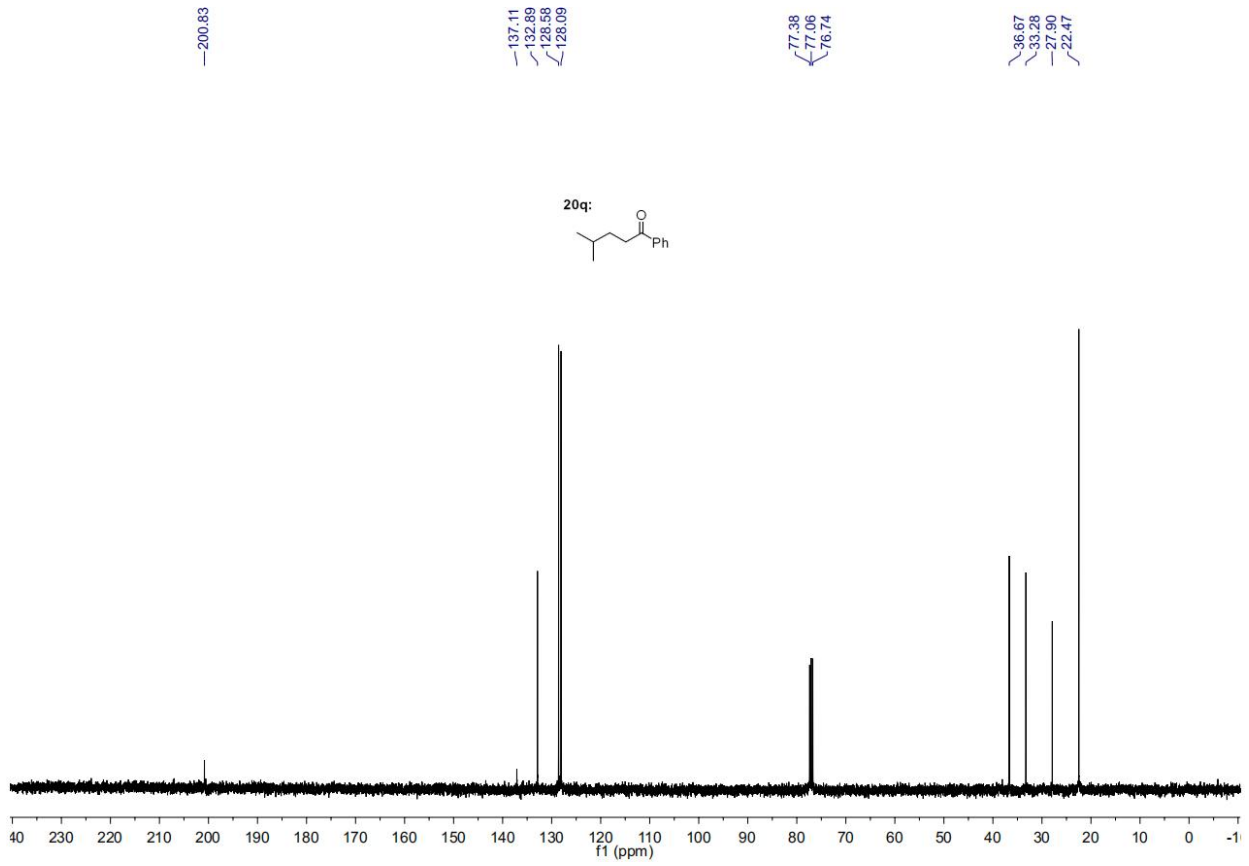

8.49
8.07
8.07
8.05
8.05
7.95
7.93
7.91
7.89
7.87
7.83
7.82
7.81
7.81
7.80
7.79
7.74
7.60
7.60
7.58
7.57
7.56
7.55
7.47
7.47
7.45
7.45
3.54
3.52
3.32
3.30
3.29

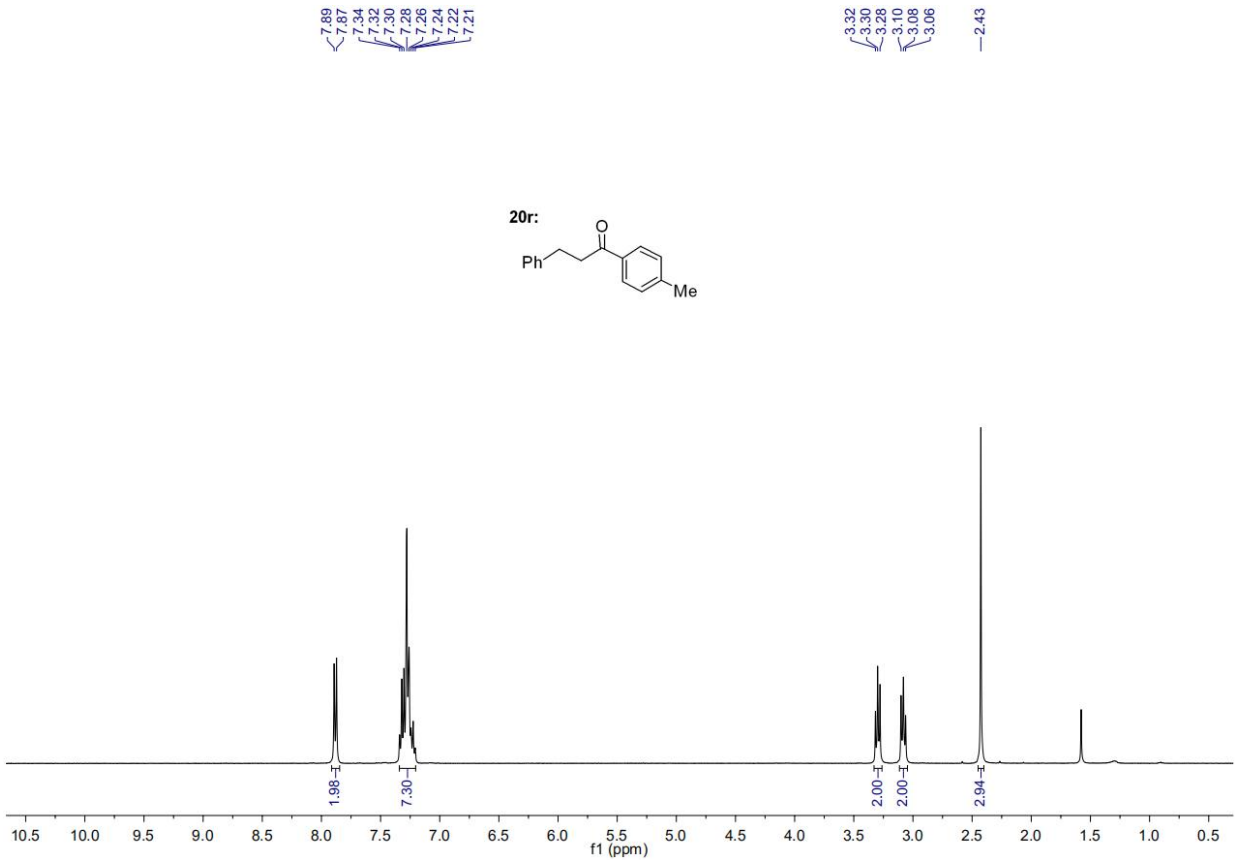

20n:
1.00
0.97
3.00
3.00
1.00
2.00
3.00
2.00
2.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

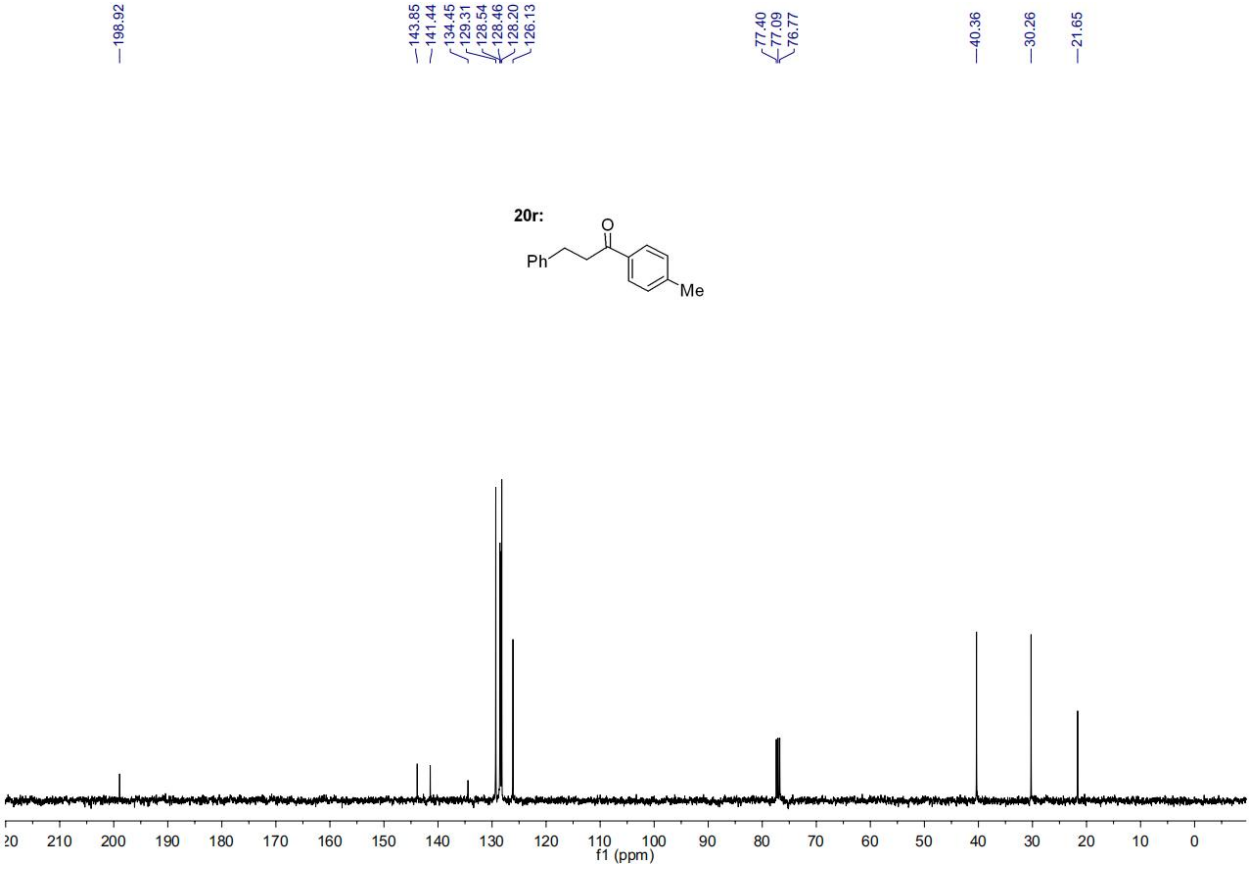

7.98
7.96
7.56
7.54
7.52
7.46
7.44
7.43
7.26
3.09
3.07
3.05
1.66
1.64
1.62
1.61
0.78
0.77
0.75
0.44
0.42
0.07
0.06
20o:
Ph
2.00
1.00
2.00
2.04
2.03
0.98
2.03
2.00
f1 (ppm)
200.42
137.07
132.86
128.51
128.03
77.38
77.06
76.75
38.65
29.50
10.68
4.61
20o:
Ph
f1 (ppm)


7.29
7.27
7.26
7.20
7.19
7.17
2.90
2.88
2.86
2.78
2.76
2.74
2.34
2.31
2.28
1.82
1.79
1.75
1.67
1.65
1.45
1.36
1.33
1.30
1.27
1.24
1.21
1.20
1.17
20p:
5.24
2.00
1.85
1.00
4.11
1.00
5.47
f1 (ppm)
213.14
141.40
128.41
128.30
125.98
77.31
77.00
76.68
50.95
42.21
29.71
28.38
25.81
25.62
20p:
f1 (ppm)

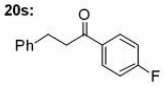

7.97
7.95
7.95
7.57
7.55
7.54
7.48
7.46
7.44
7.26
2.99
2.97
2.95
1.65
1.63
1.63
1.62
1.61
0.96
0.94
20q:
O
Ph
1.87
0.93
1.88
2.00
3.09
6.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

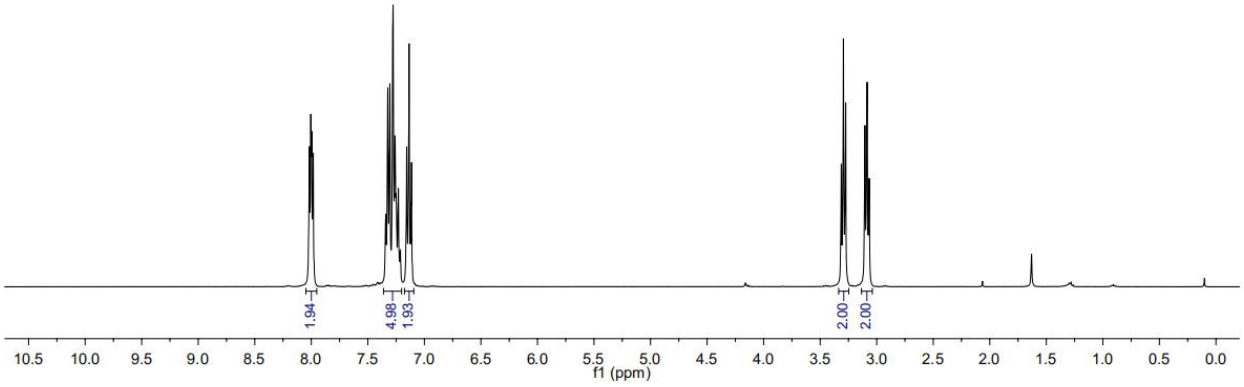

200.83
137.11
132.89
128.58
128.09
77.38
77.06
76.74
36.67
33.28
27.90
22.47
20q:
O
Ph
40 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


7.89
7.87
7.34
7.32
7.30
7.28
7.26
7.24
7.22
7.21
3.32
3.30
3.28
3.10
3.08
3.06
2.43
20r:
Ph
O
Me
1.98
7.30
2.00
2.00
2.94
f1 (ppm)

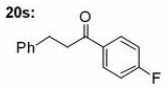

198.92
143.85
141.44
134.45
129.31
128.54
128.46
128.20
126.13
77.40
77.09
76.77
40.36
30.26
21.65
20r:
Ph
O
Me
f1 (ppm)

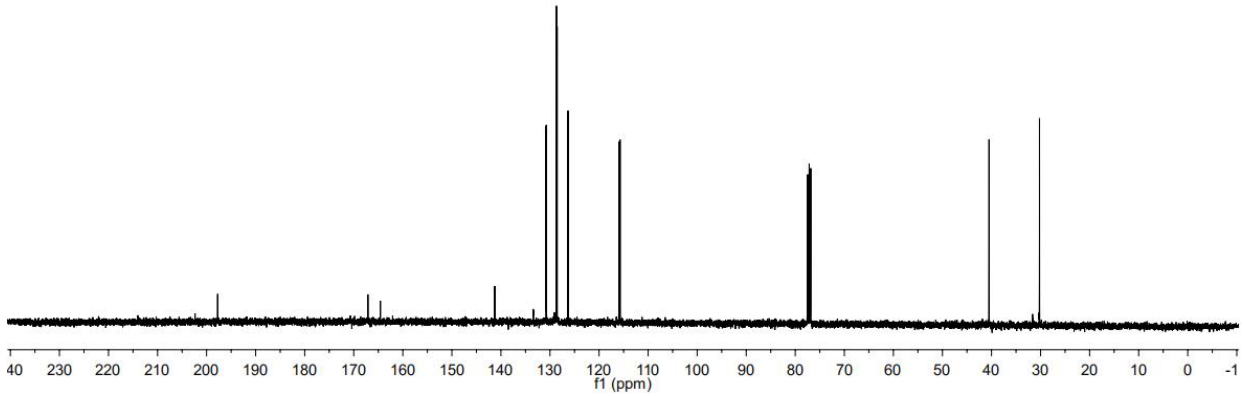

8.02
8.01
8.00
8.00
8.00
7.99
7.98
7.34
7.32
7.31
7.28
7.26
7.25
7.23
7.22
7.21
7.16
7.15
7.14
7.14
7.12
7.11
3.31
3.29
3.27
3.10
3.08
3.07


20s:
O
Ph
F


1.94
4.98
1.93
2.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


197.75
167.11
164.58
141.25
133.41
130.82
130.73
128.68
128.54
115.92
115.71
77.48
77.16
76.84
40.50
30.21

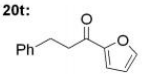

20s:
O
Ph
F

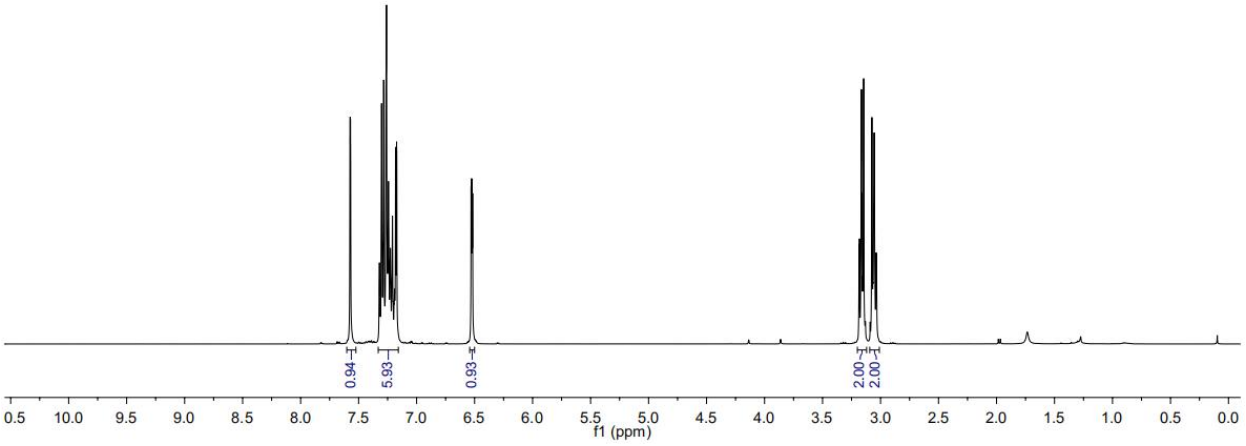

40
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


7.57
7.57
7.32
7.30
7.29
7.28
7.26
7.26
7.24
7.23
7.23
7.21
7.20
7.19
7.19
7.18
7.18
7.17
7.17
6.53
6.53
6.52
6.52


3.19
3.18
3.16
3.16
3.15
3.15
3.13
3.09
3.07
3.07
3.07
3.05
3.04

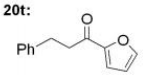
20t:

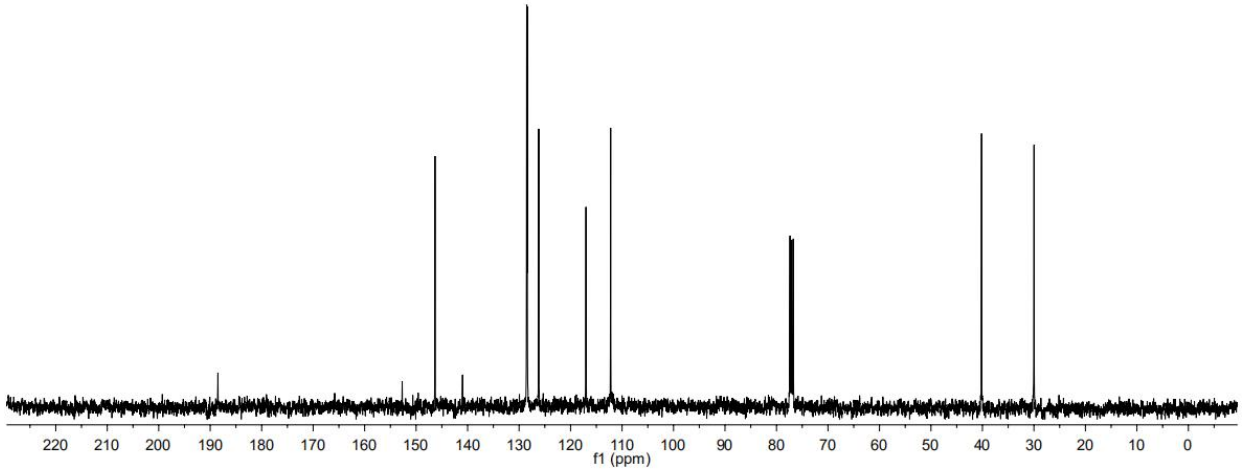

O
Ph
O

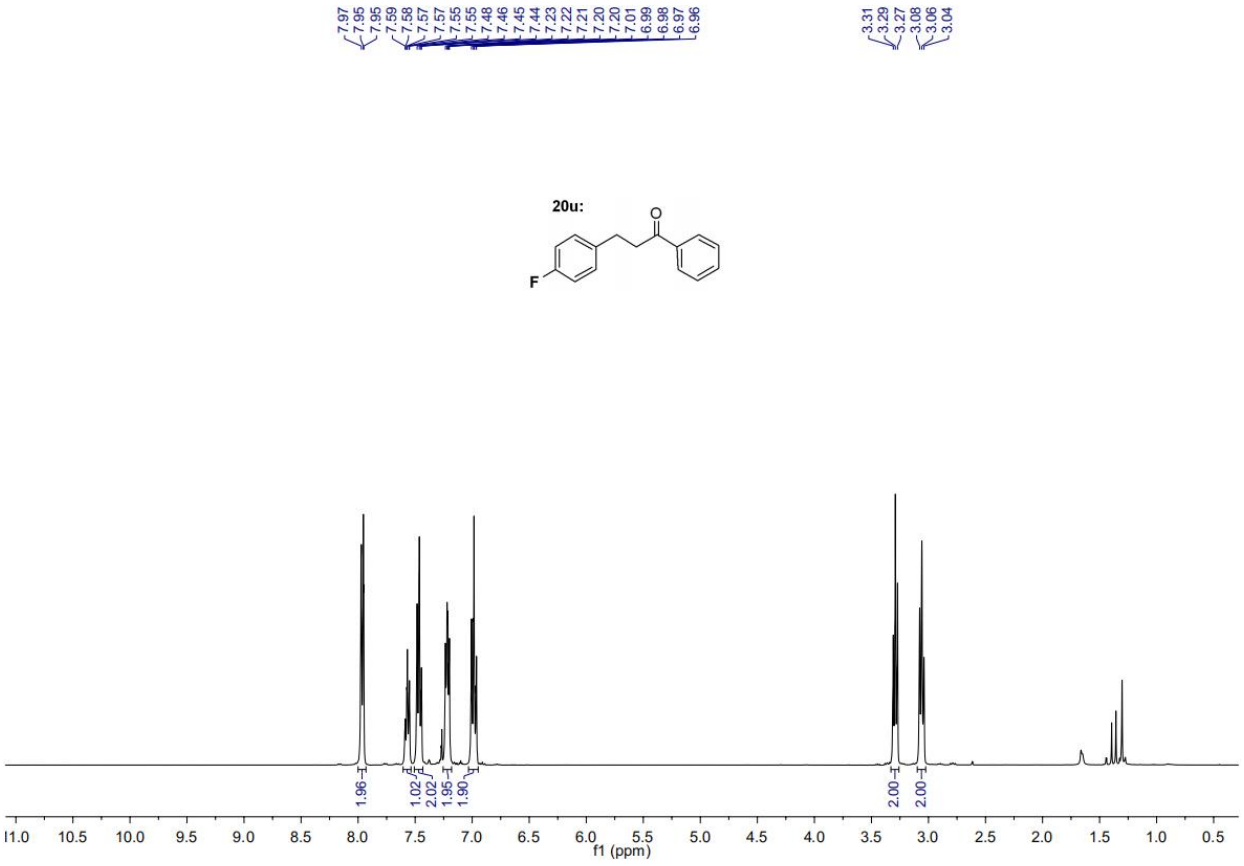

0.94
5.93
0.93
2.00
2.00
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

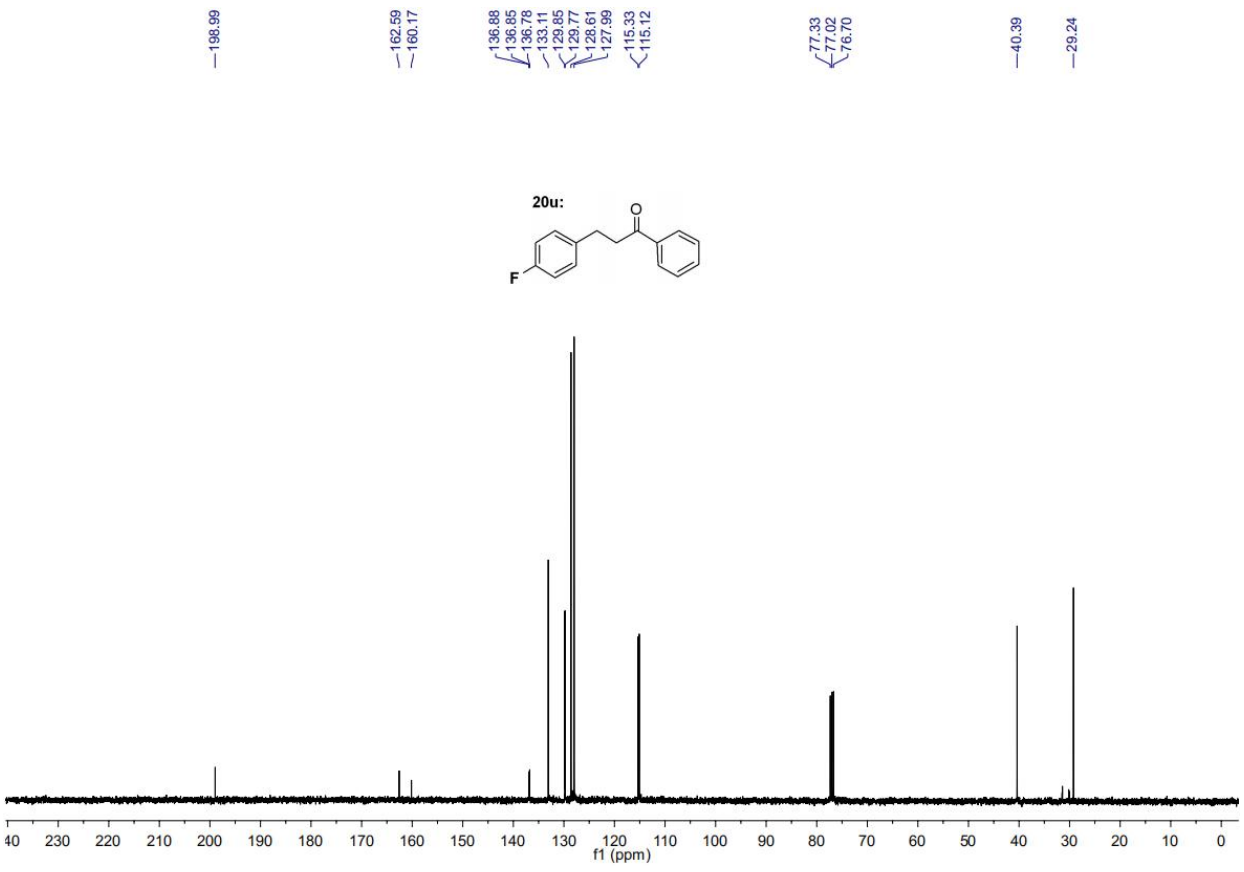

188.50
152.71
146.32
140.99
128.53
128.42
126.19
117.01
112.21
77.38
77.06
76.74
40.17
29.98

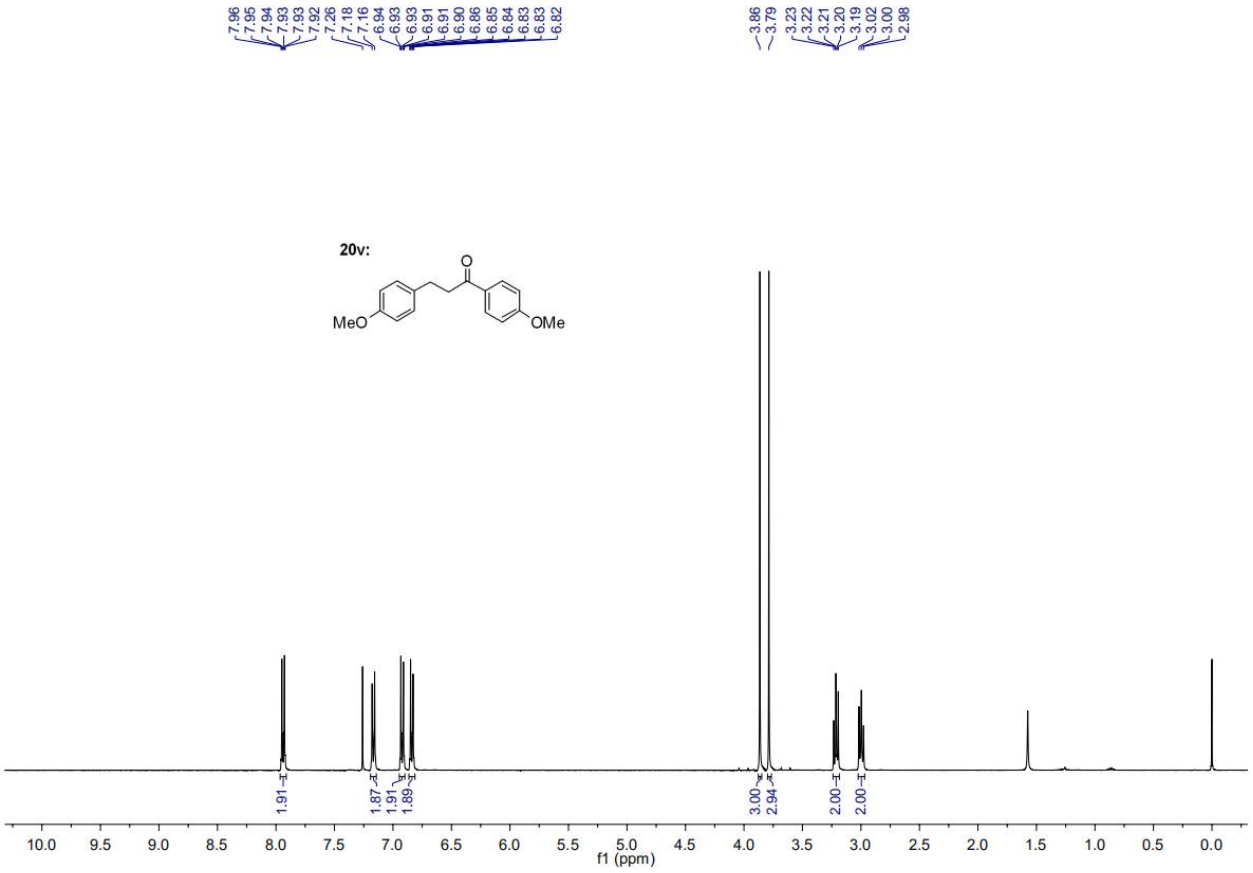
20t:

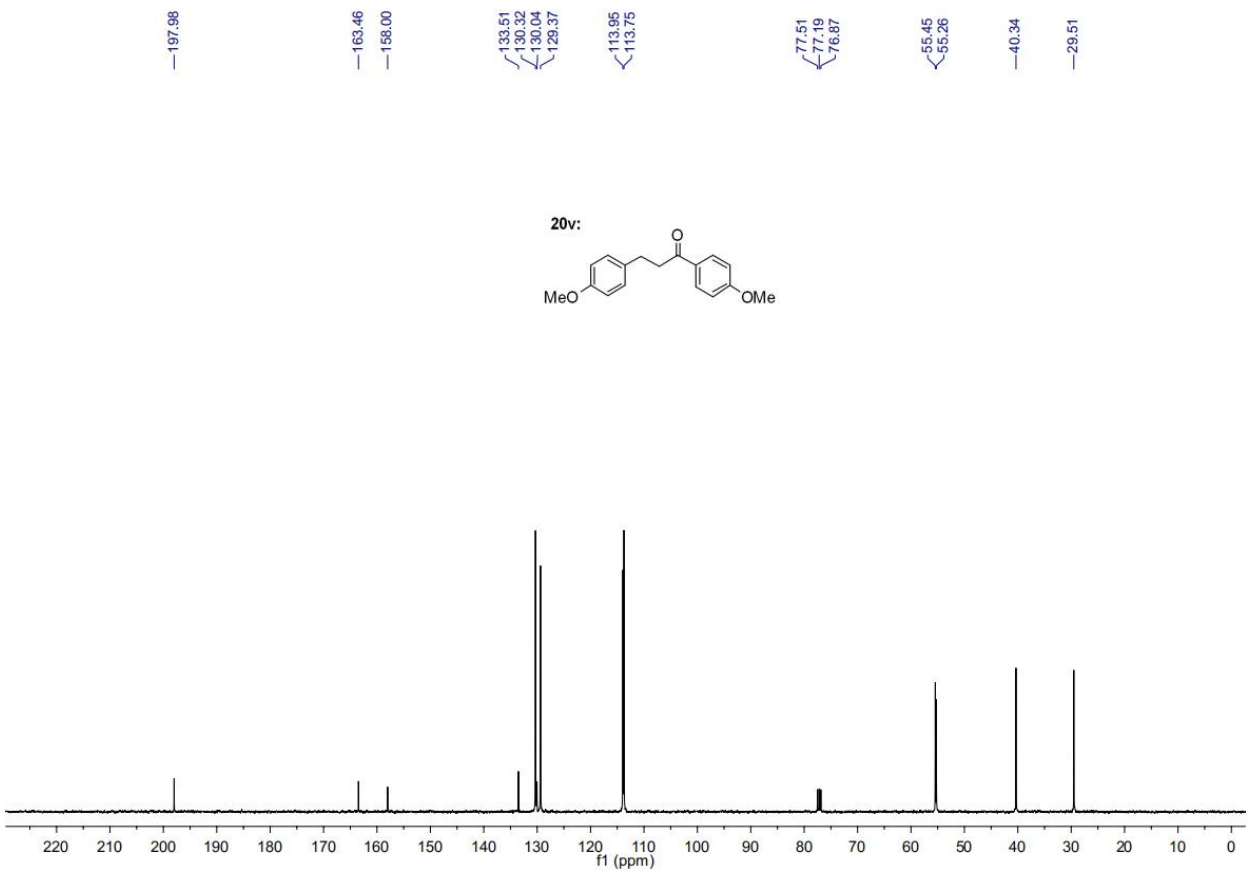

O
Ph
O

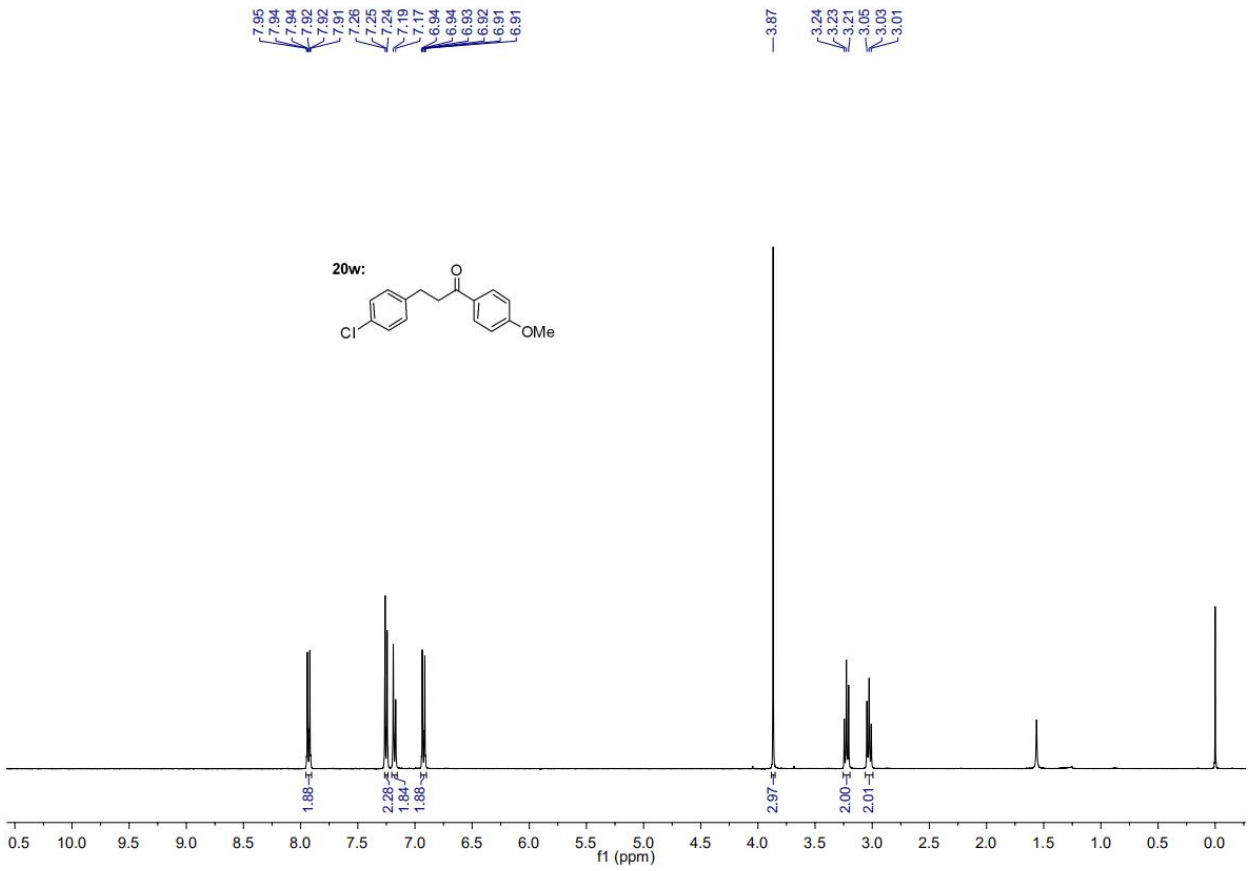

220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

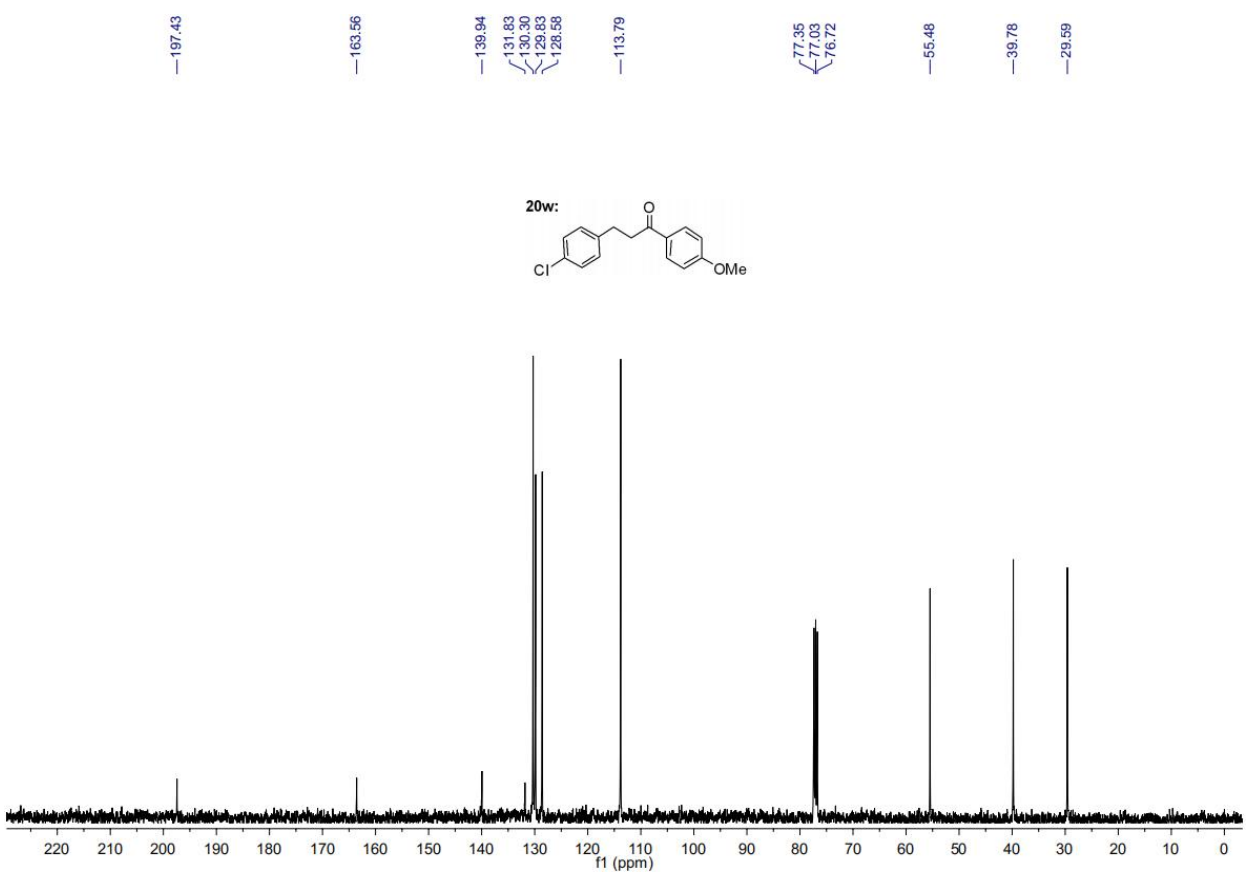

7.97
7.95
7.95
7.59
7.58
7.57
7.57
7.55
7.55
7.48
7.46
7.45
7.44
7.23
7.22
7.21
7.20
7.20
7.01
6.99
6.98
6.97
6.96
3.31
3.29
3.27
3.08
3.06
3.04
20u:
F
1.96
1.02
2.02
1.95
1.90
2.00
2.00
f1 (ppm)

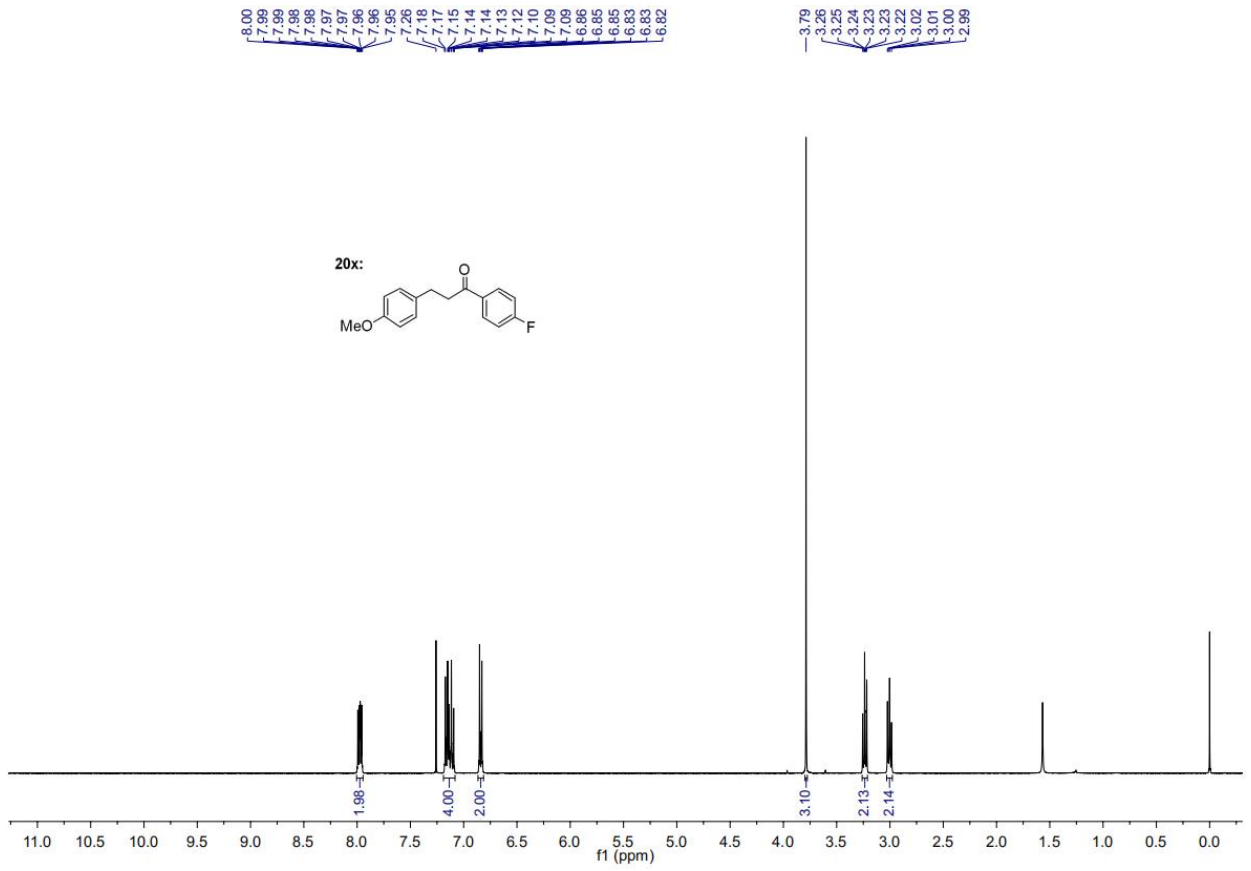

198.99
162.59
160.17
136.88
136.85
136.78
133.11
129.85
129.77
128.61
127.99
115.33
115.12
77.33
77.02
76.70
40.39
29.24
20u:
F
f1 (ppm)

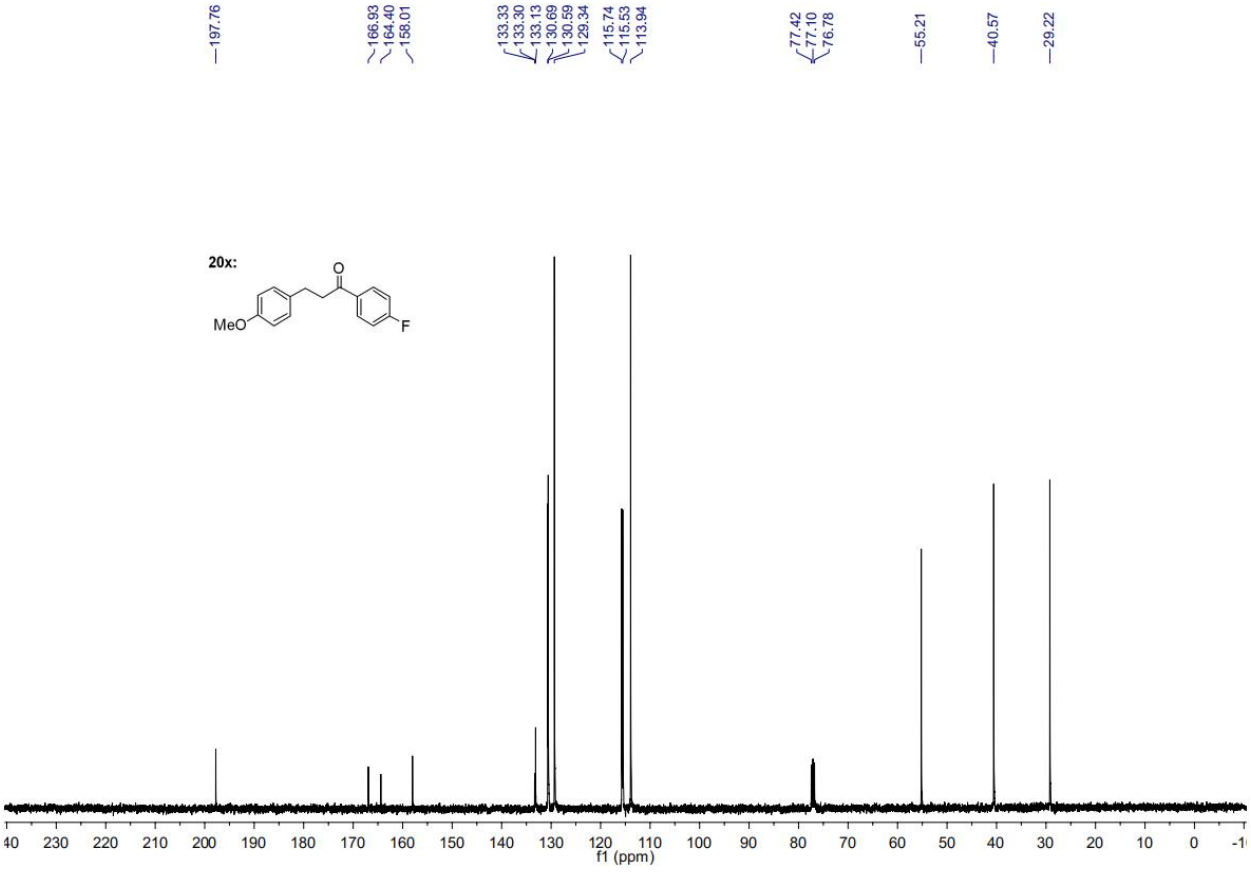

7.96
7.95
7.94
7.93
7.93
7.92
7.26
7.18
7.16
6.94
6.93
6.93
6.91
6.91
6.90
6.86
6.85
6.84
6.83
6.82
3.86
3.79
3.23
3.22
3.21
3.20
3.19
3.02
3.00
2.98
20v:
MeO
OMe
1.91
1.87
1.91
1.89
3.00
2.94
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

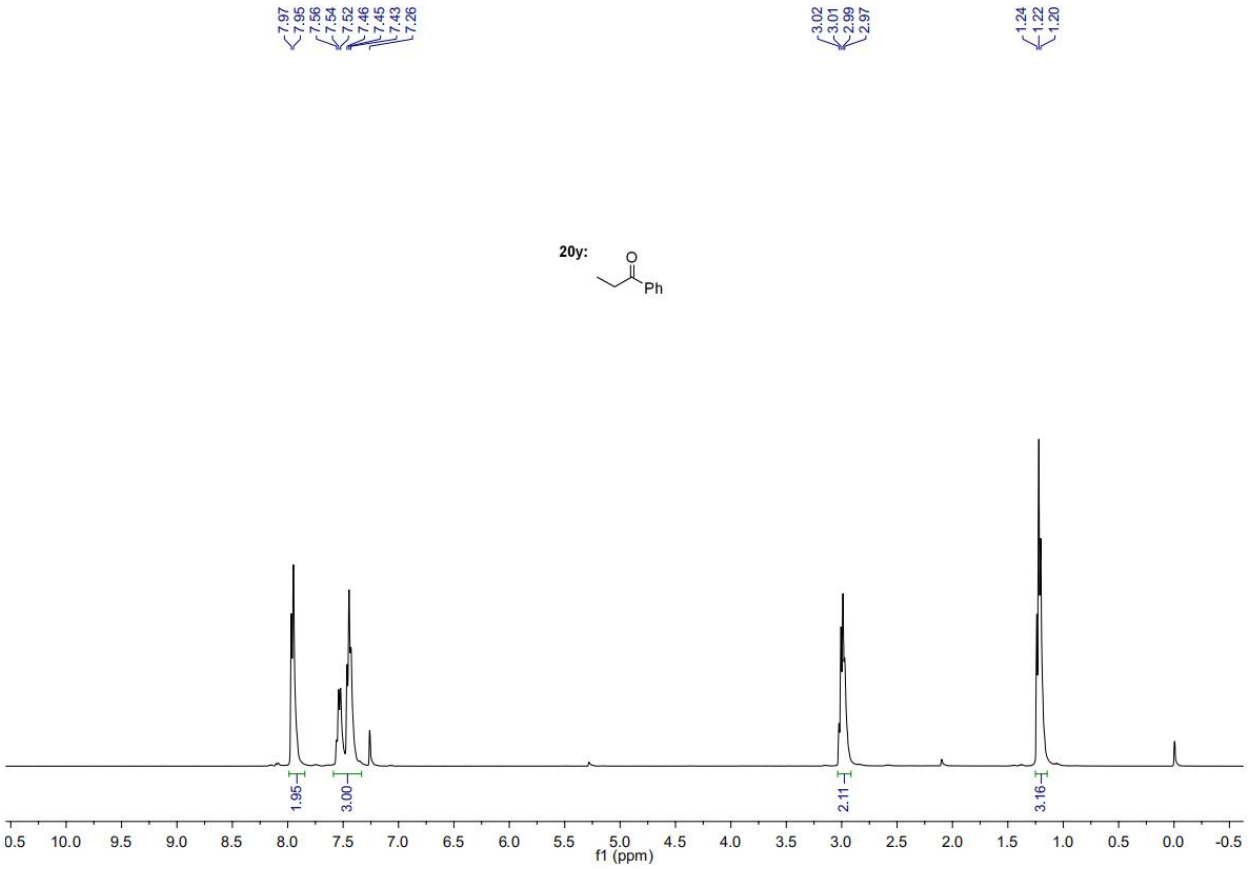

197.98
163.46
158.00
133.51
130.32
130.04
129.37
113.95
113.75
77.51
77.19
76.87
55.45
55.26
40.34
29.51
20v:
MeO
OMe
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

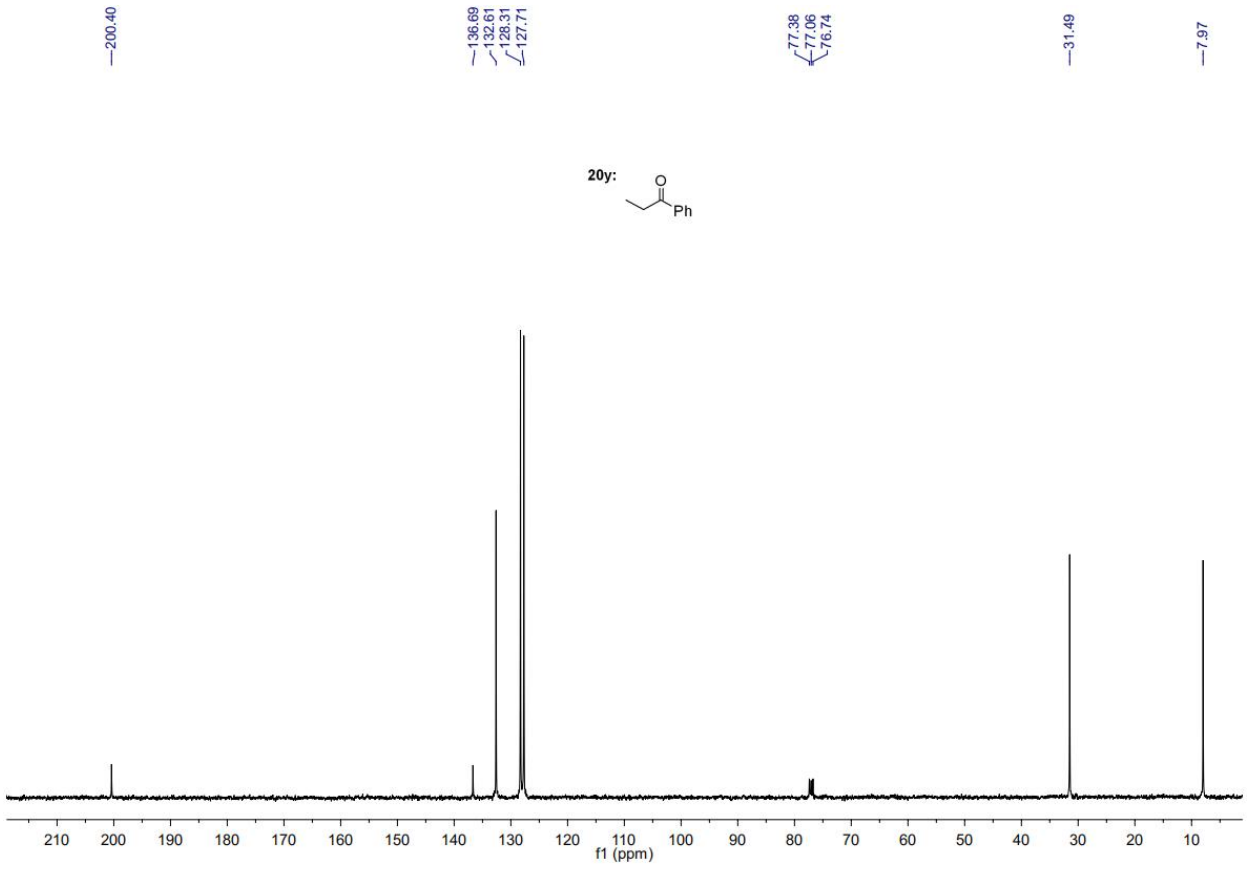

7.95
7.94
7.94
7.92
7.92
7.91
7.26
7.25
7.24
7.19
7.17
6.94
6.94
6.93
6.92
6.91
6.91
3.87
3.24
3.23
3.21
3.05
3.03
3.01
20w:
O
Cl
OMe
1.88
2.28
1.84
1.88
2.97
2.00
2.01
f1 (ppm)

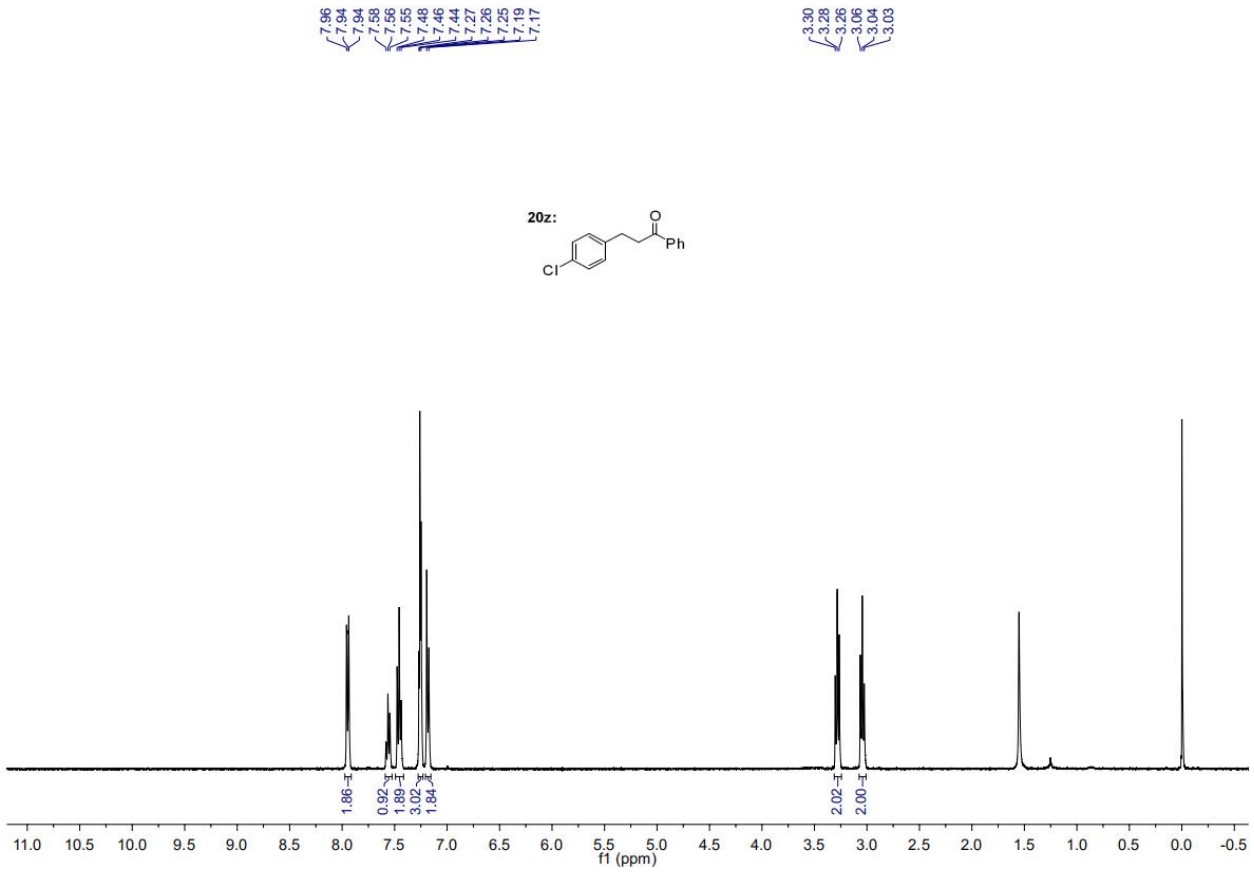

197.43
163.56
139.94
131.83
130.30
129.83
128.58
113.79
77.35
77.03
76.72
55.48
39.78
29.59
20w:
O
Cl
OMe
f1 (ppm)

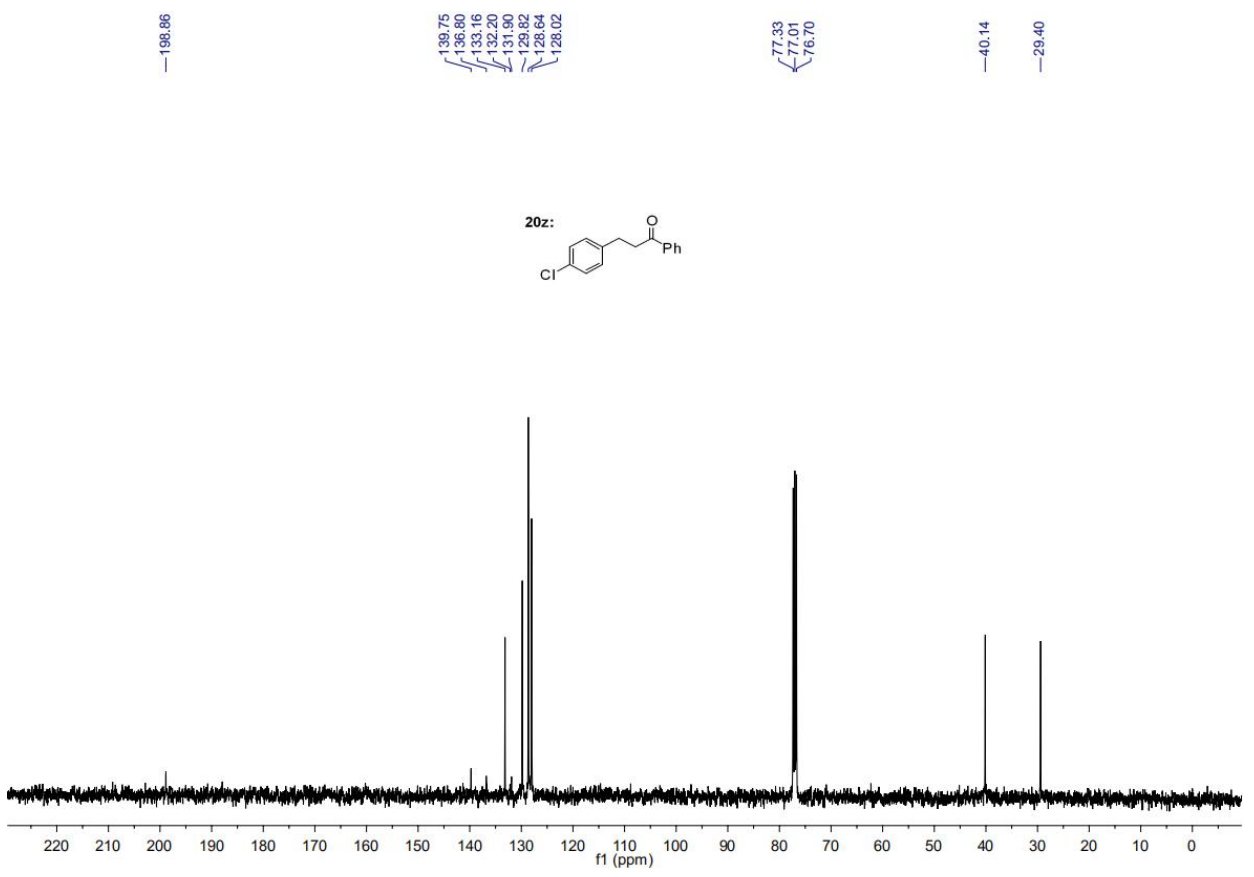

8.00
7.99
7.99
7.98
7.98
7.97
7.97
7.96
7.96
7.95
7.26
7.18
7.17
7.15
7.14
7.14
7.13
7.12
7.10
7.09
7.09
6.86
6.85
6.85
6.83
6.83
6.82
3.79
3.26
3.25
3.24
3.23
3.23
3.22
3.02
3.01
3.00
2.99
20x:
MeO
F
1.98
4.00
2.00
3.10
2.13
2.14
f1 (ppm)

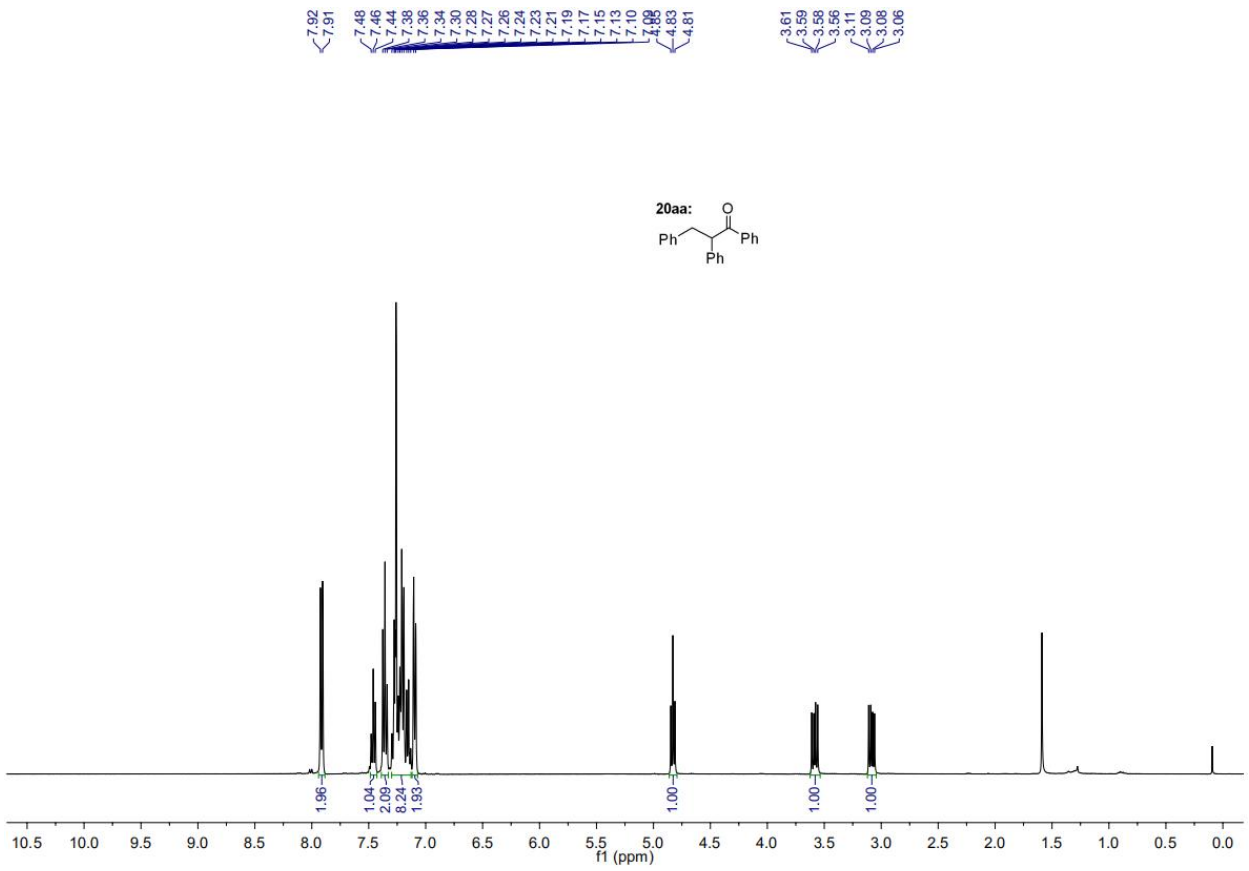

197.76
166.93
164.40
158.01
133.33
133.30
133.13
130.69
130.59
129.34
115.74
115.53
113.94
77.42
77.10
76.78
55.21
40.57
29.22
20x:
MeO
F
f1 (ppm)

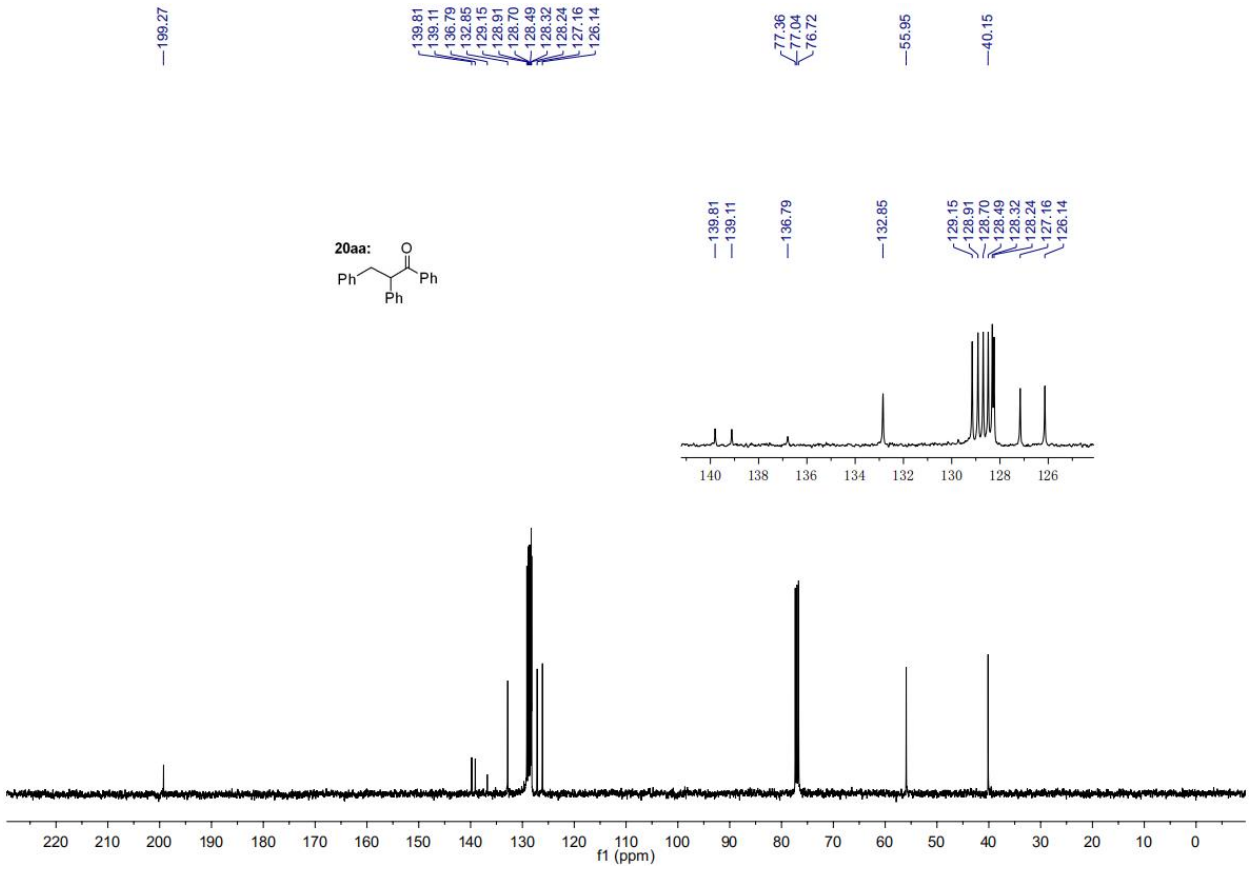

7.97
7.95
7.56
7.54
7.52
7.46
7.45
7.43
7.26
3.02
3.01
2.99
2.97
1.24
1.22
1.20
20y:
O
Ph
1.95
3.00
2.11
3.16
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

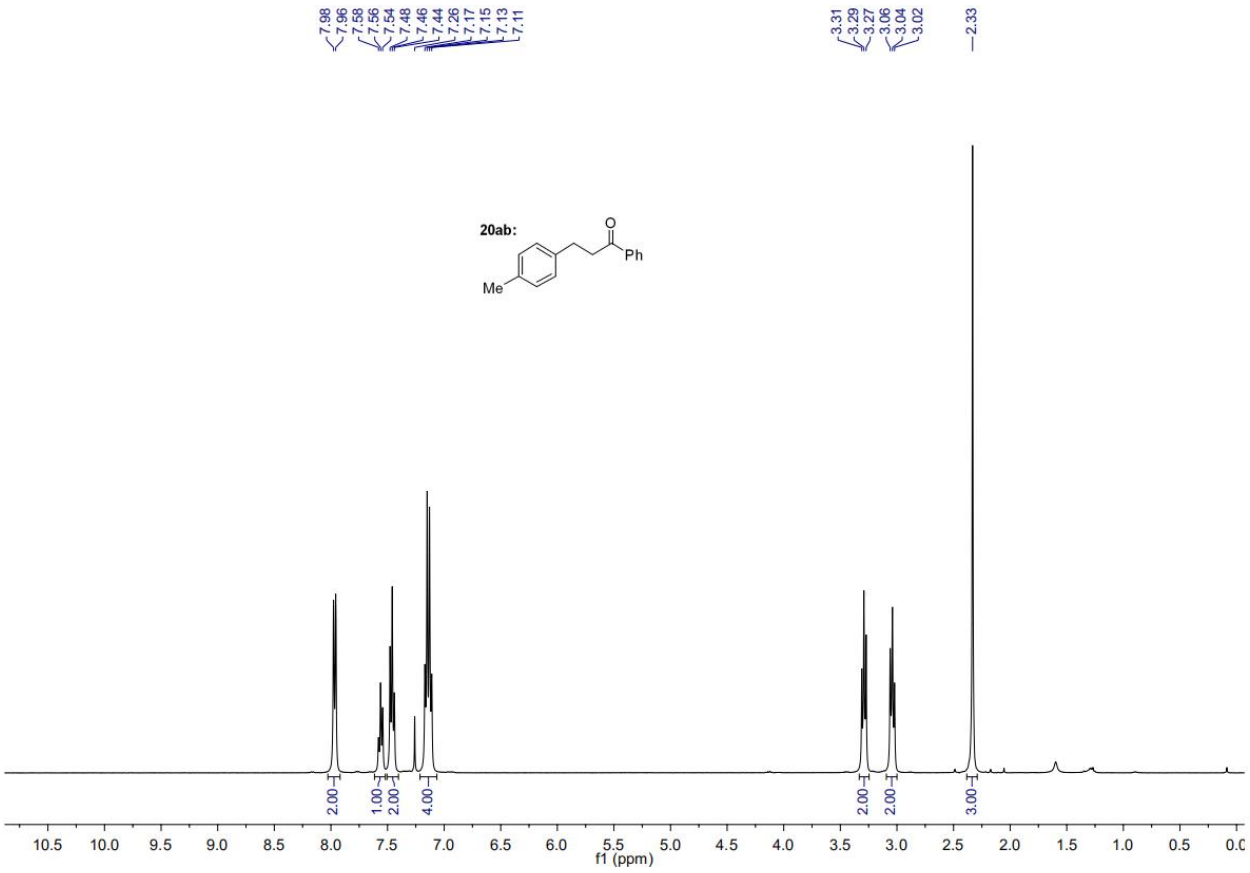

200.40
136.69
132.61
128.31
127.71
77.38
77.06
76.74
31.49
7.97
20y:
O
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

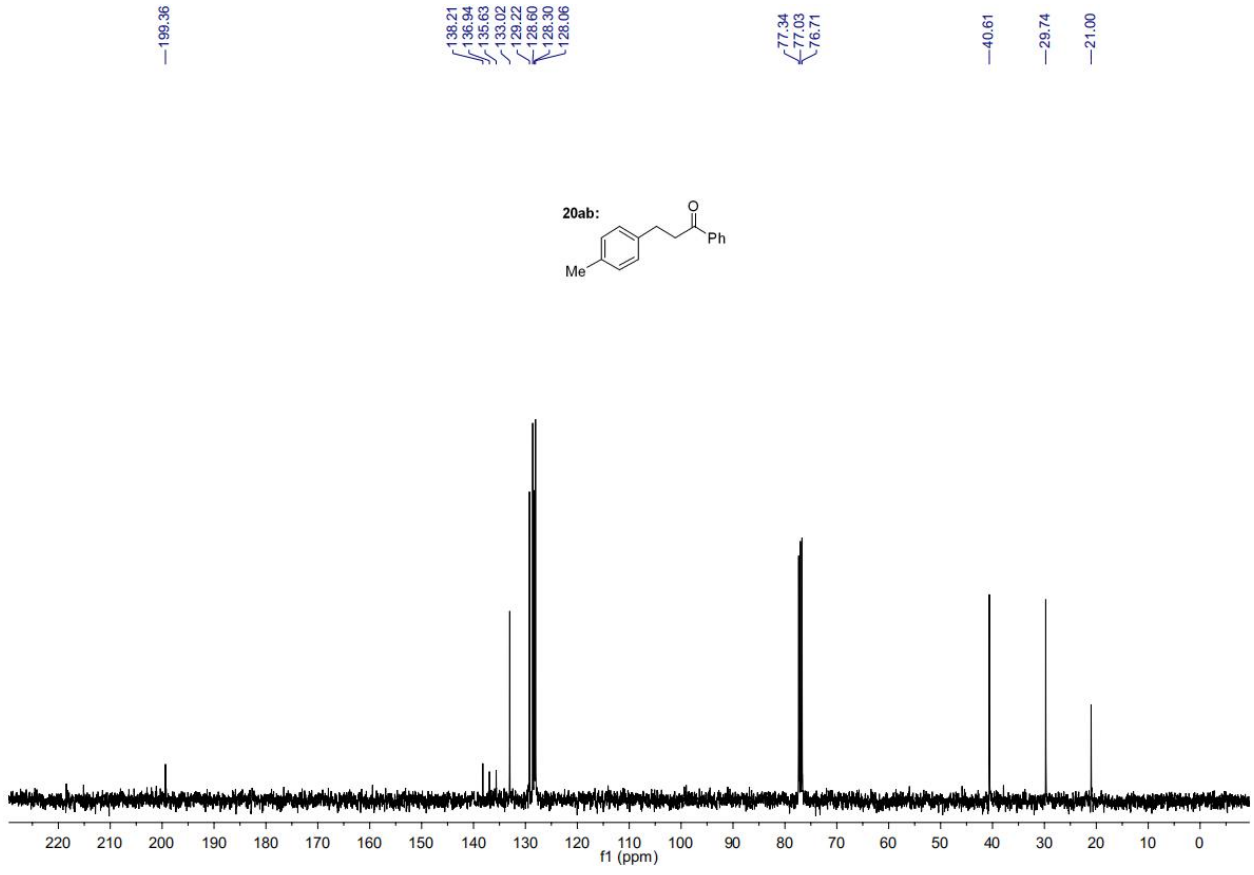

7.96
7.94
7.94
7.58
7.56
7.55
7.48
7.46
7.44
7.27
7.26
7.25
7.19
7.17
3.30
3.28
3.26
3.06
3.04
3.03
20z:
O
Ph
Cl
1.86
0.92
1.89
3.02
1.84
2.02
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

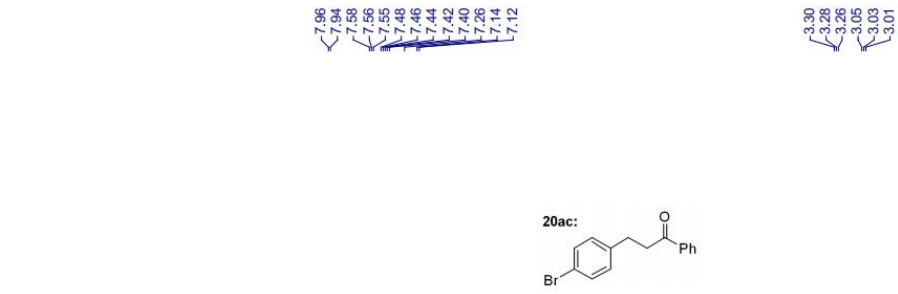

198.86
139.75
136.80
133.16
132.20
131.90
129.82
128.64
128.02
77.33
77.01
76.70
40.14
29.40
20z:
O
Ph
Cl
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

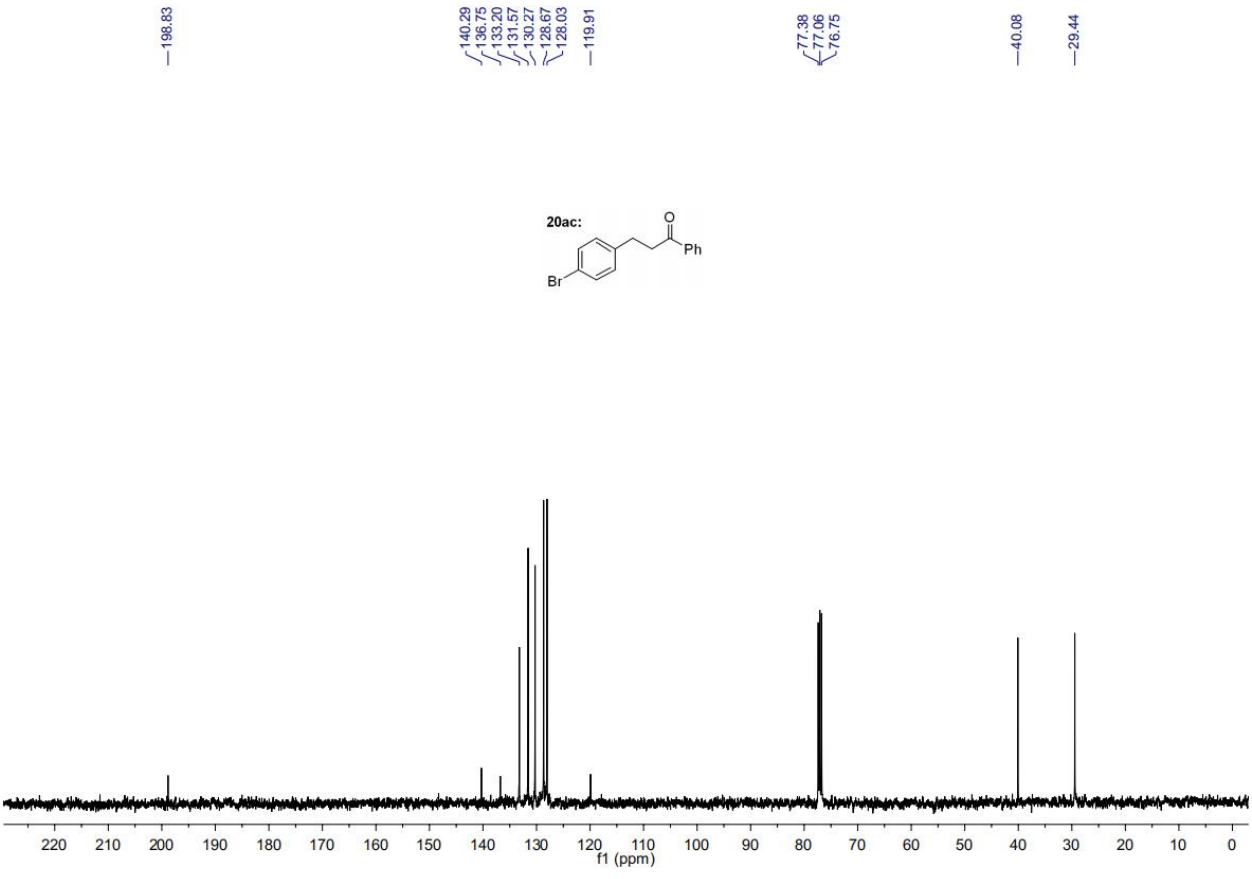

7.92
7.91
7.48
7.46
7.44
7.38
7.36
7.34
7.30
7.28
7.27
7.26
7.24
7.23
7.21
7.19
7.17
7.15
7.13
7.10
4.83
4.81
3.61
3.59
3.58
3.56
3.11
3.09
3.08
3.06
20aa:
Ph
Ph
Ph
1.96
1.04
2.09
8.24
1.93
1.00
1.00
1.00
f1 (ppm)


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
77.36
77.04
76.72
55.95
40.15
20aa:
Ph
Ph
Ph
f1 (ppm)

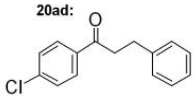

7.98
7.96
7.58
7.56
7.54
7.48
7.46
7.44
7.26
7.17
7.15
7.13
7.11
3.31
3.29
3.27
3.06
3.04
3.02
2.33
20ab:
O
Ph
Me
2.00
1.00
2.00
4.00
2.00
2.00
3.00
f1 (ppm)

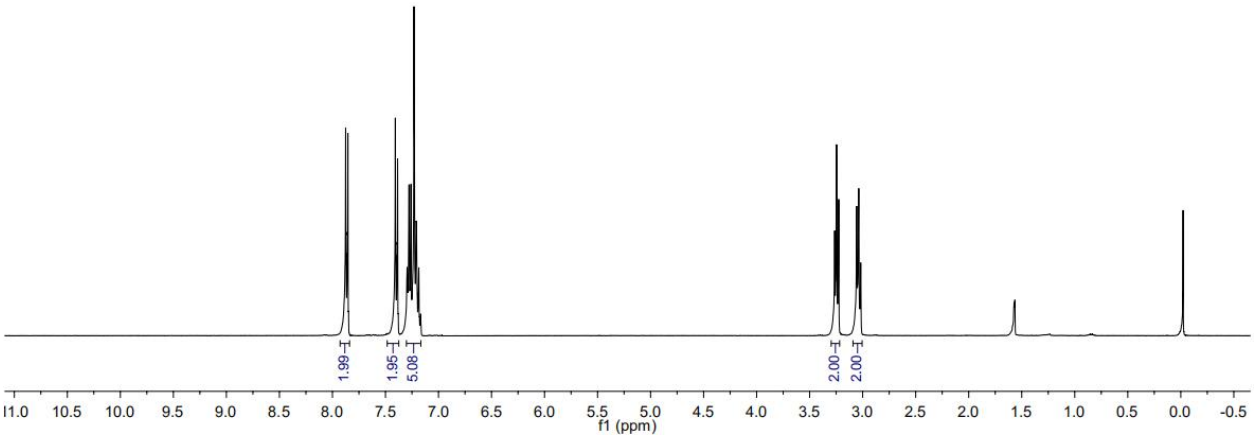

199.36
138.21
136.94
135.63
133.02
129.22
128.60
128.30
128.06
77.34
77.03
76.71
40.61
29.74
21.00
20ab:
O
Ph
Me
f1 (ppm)


7.96
7.94
7.58
7.56
7.55
7.48
7.46
7.44
7.42
7.40
7.26
7.14
7.12
3.30
3.28
3.26
3.05
3.03
3.01
20ac:
O
Ph
Br
2.00
1.00
2.00
2.00
2.00
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

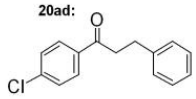

198.83
140.29
136.75
133.20
131.57
130.27
128.67
128.03
119.91
77.38
77.06
76.75
40.08
29.44
20ac:
O
Ph
Br
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

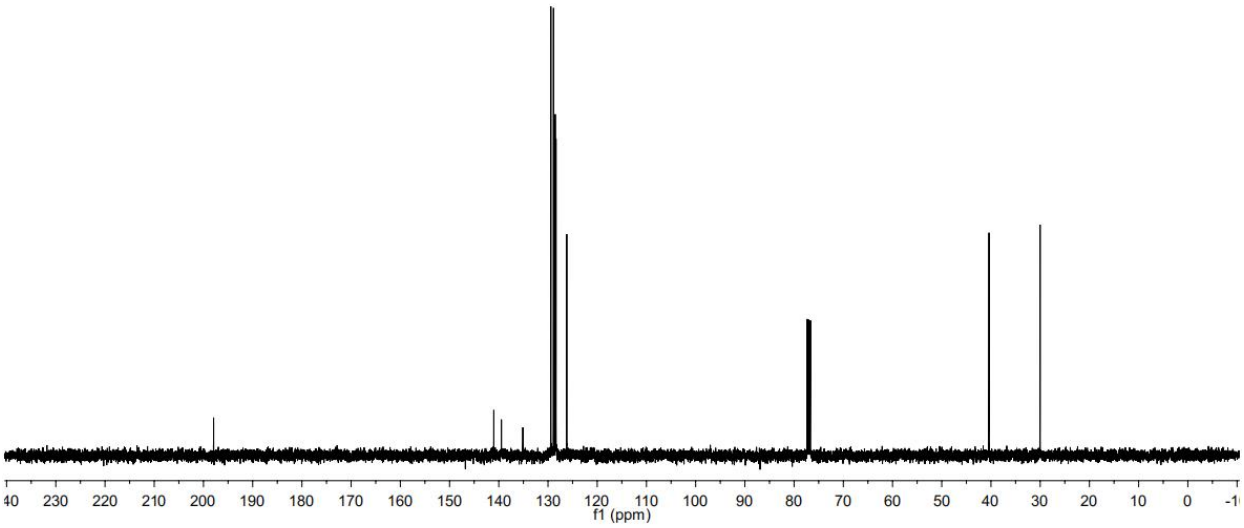

7.88
7.87
7.86
7.85
7.85
7.41
7.40
7.39
7.39
7.38
7.30
7.29
7.28
7.26
7.23
7.21
7.19
7.18
7.17
7.17
3.26
3.25
3.25
3.23
3.23
3.06
3.04
3.02

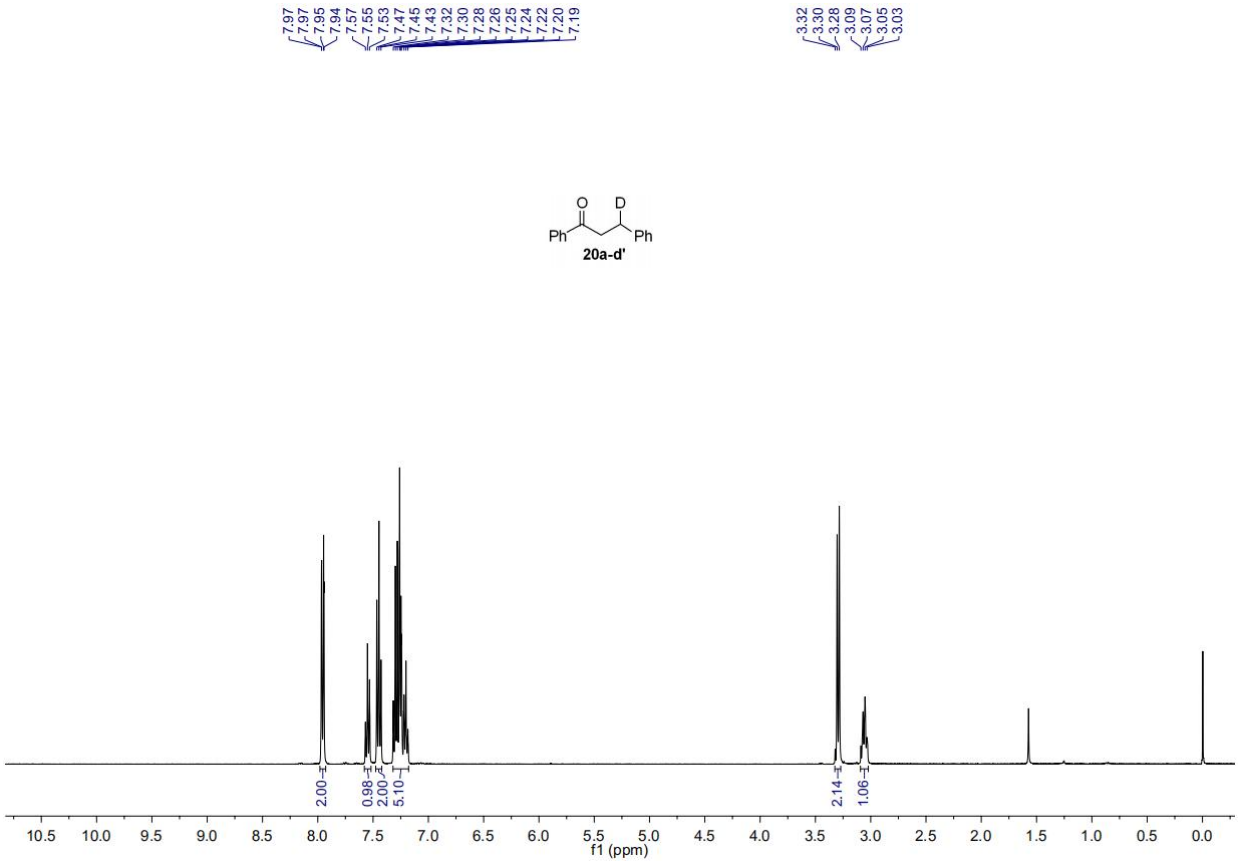

20ad:
O
Cl

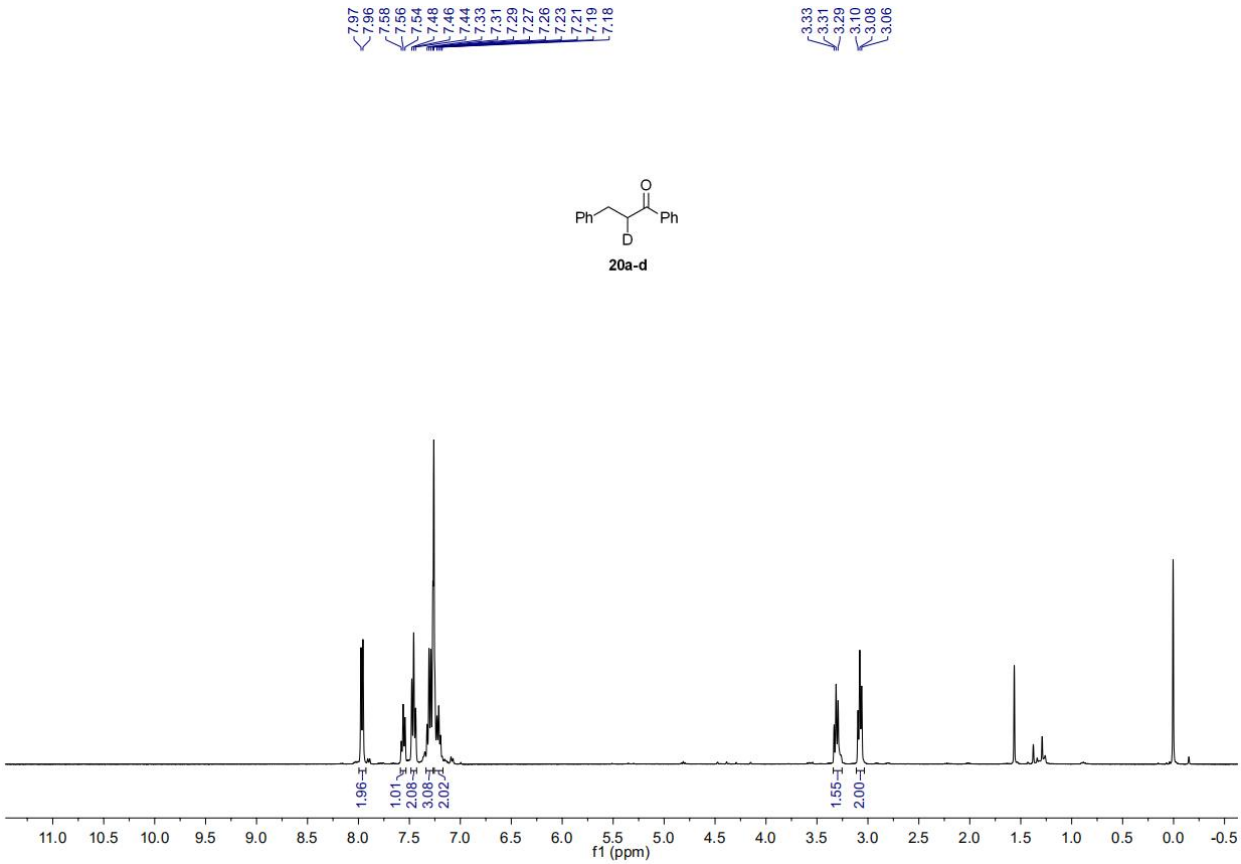

1.99
1.95
5.08
2.00
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

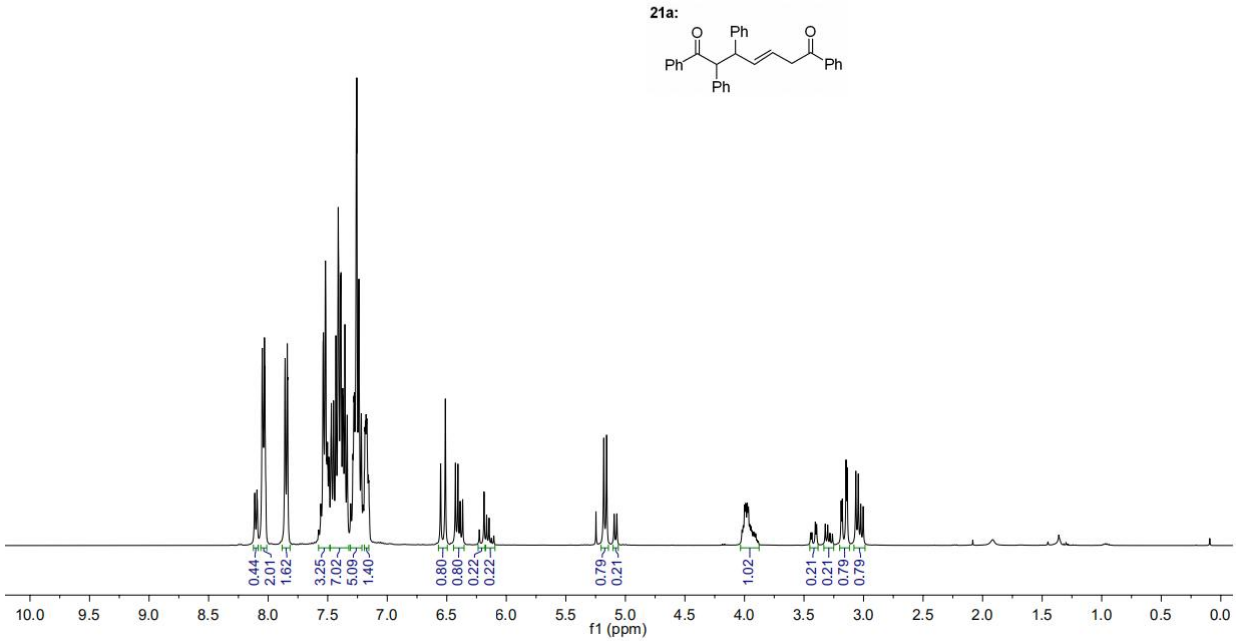

197.96
141.03
139.48
135.13
129.43
128.90
128.55
128.39
126.20
77.33
77.01
76.69
40.41
30.02

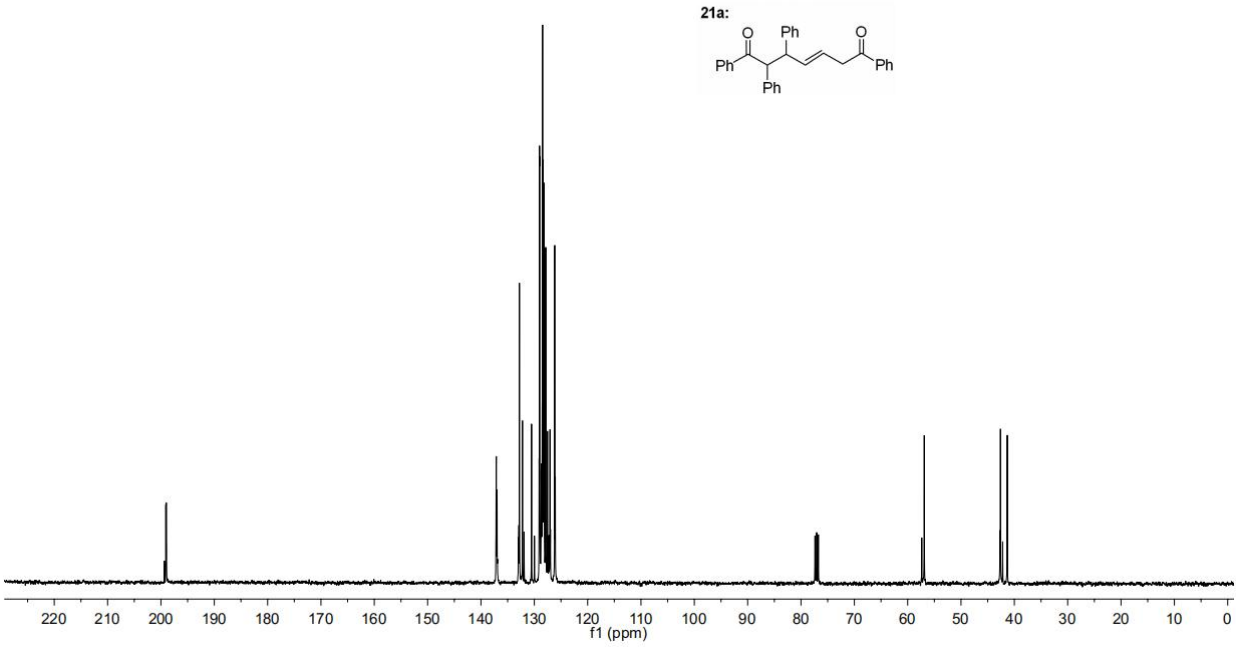

20ad:
O
Cl


40 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

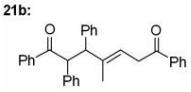

7.97
7.97
7.95
7.94
7.57
7.55
7.53
7.47
7.45
7.43
7.32
7.30
7.28
7.26
7.25
7.24
7.22
7.20
7.19
3.32
3.30
3.28
3.09
3.07
3.05
3.03
O
D
Ph
Ph
20a-d'
2.00
0.98
2.00
5.10
2.14
1.06
f1 (ppm)

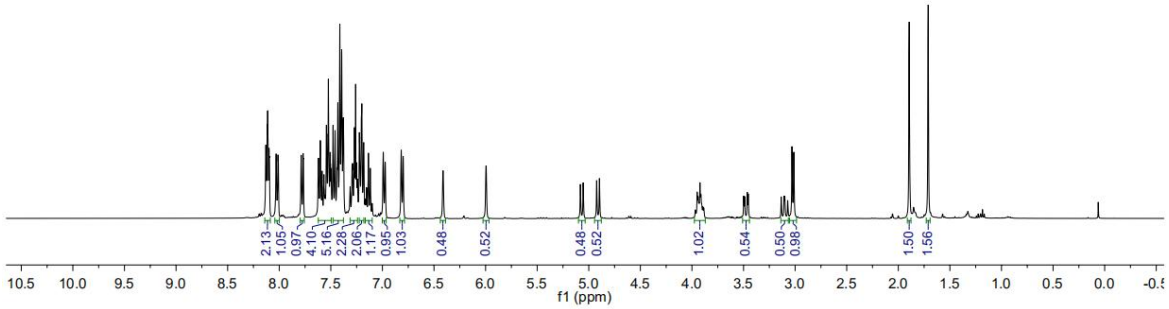

7.97
7.96
7.58
7.56
7.54
7.48
7.46
7.44
7.33
7.31
7.29
7.27
7.26
7.23
7.21
7.19
7.18
3.33
3.31
3.29
3.10
3.08
3.06
O
Ph
Ph
D
20a-d
1.96
1.01
2.08
3.08
2.02
1.55
2.00
f1 (ppm)

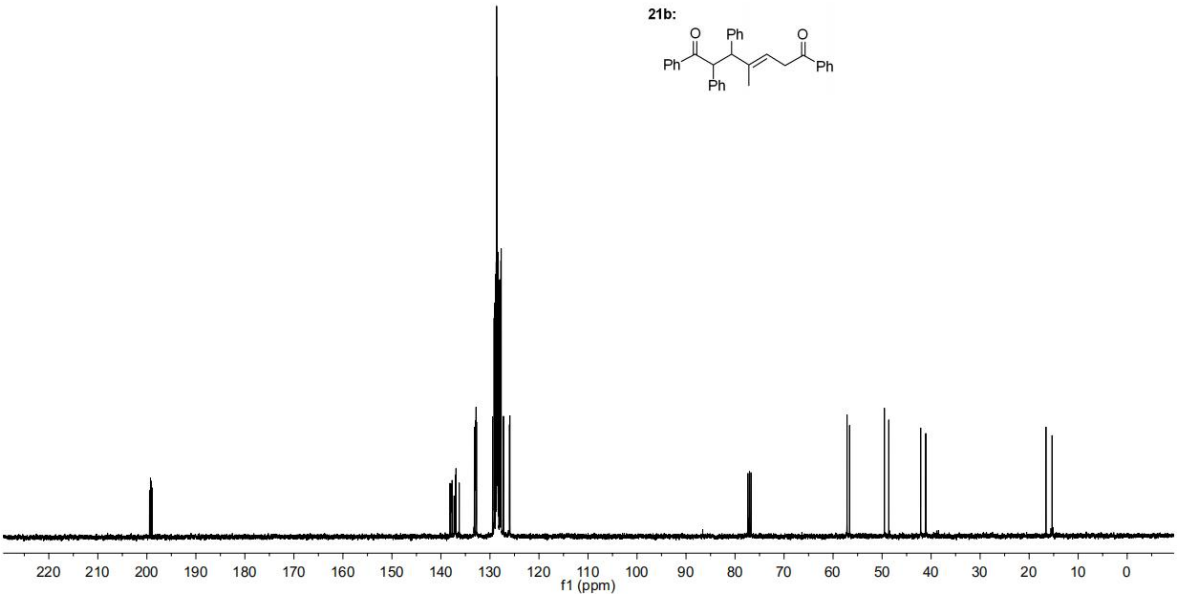

21a:
O
Ph
O
Ph
Ph
Ph
0.44
2.01
1.62
3.25
7.02
5.09
1.40
0.80
0.80
0.22
0.22
0.79
0.21
1.02
0.21
0.21
0.79
0.79
f1 (ppm)


21a:
O
Ph
O
Ph
Ph
Ph
f1 (ppm)

21b:

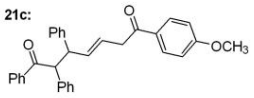


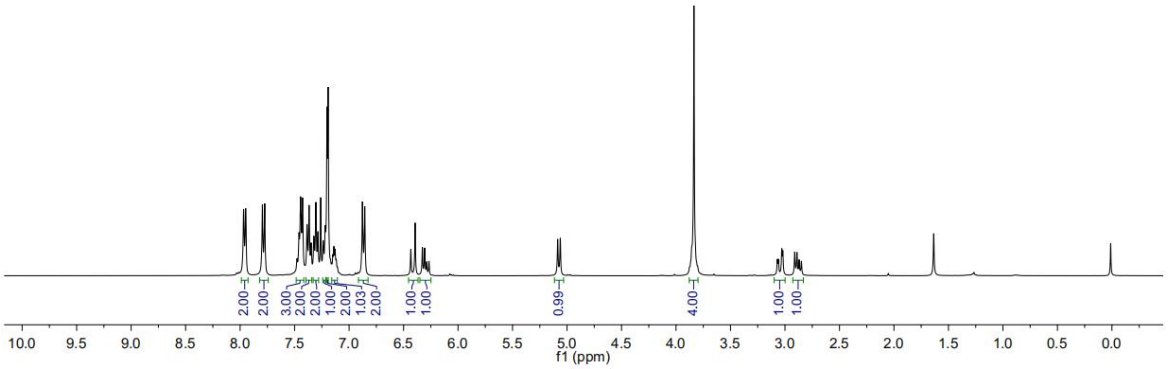

2.13
1.05
0.97
4.10
5.16
2.28
2.06
1.17
0.95
1.03
0.48
0.52
0.48
0.52
1.02
0.54
0.50
0.98
1.50
1.56
f1 (ppm)


f1 (ppm)


7.97
7.95
7.80
7.77
7.44
7.43
7.30
7.26
7.20
7.19
6.39
6.33
6.31
6.29
6.27
5.09
5.06
3.84
3.07
3.06
3.03
3.02
2.91
2.89
2.87
2.85

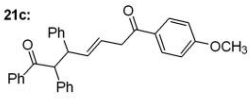
21c:

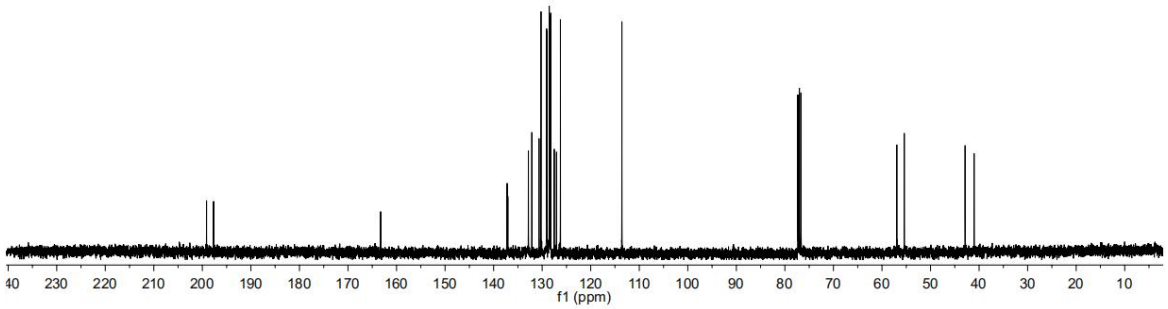

Ph
O
OCH3
Ph
Ph

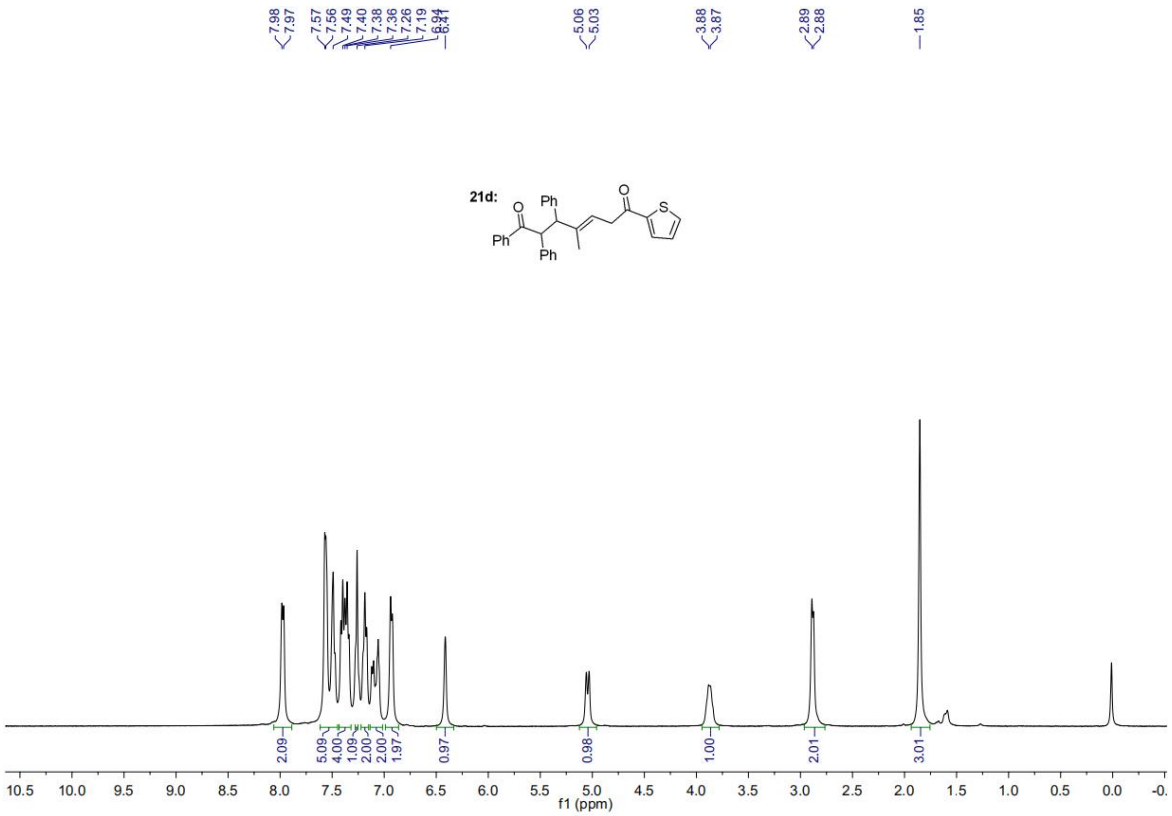

2.00
2.00
3.00
2.00
2.00
1.00
2.00
1.03
2.00
1.00
1.00
0.99
4.00
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

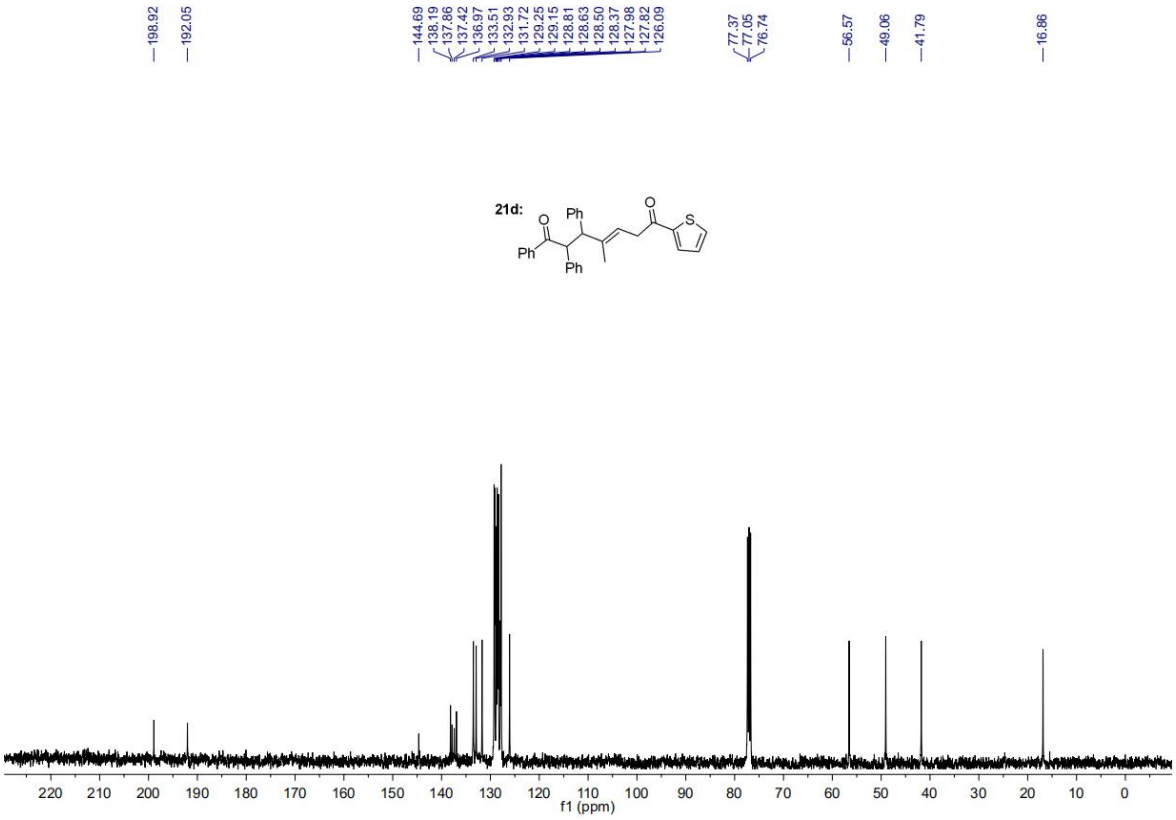

199.16
197.71
163.29
137.24
137.08
132.85
132.14
130.66
130.28
130.25
129.10
129.01
128.56
128.50
128.26
127.53
127.06
126.25
113.59
77.34
77.02
76.70
56.95
55.41
42.88
41.03

21c:


Ph
O
OCH3
Ph
Ph

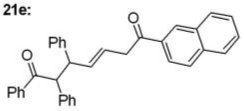

40 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

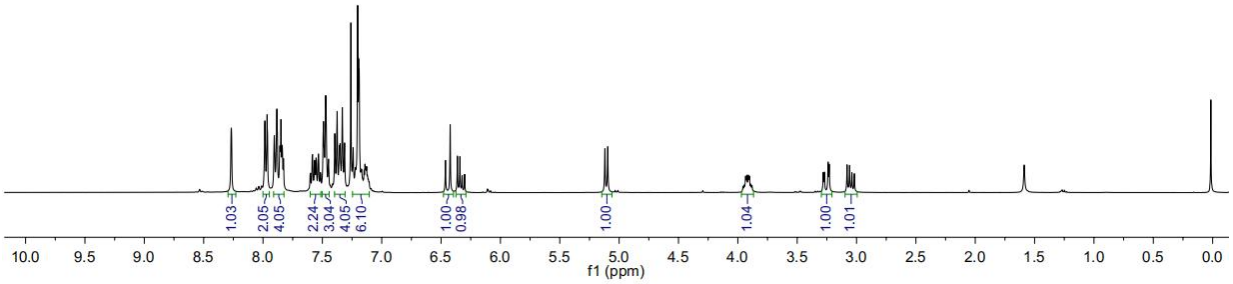

7.98
7.97
7.57
7.56
7.49
7.40
7.38
7.36
7.26
7.19
6.94
6.41
5.06
5.03
3.88
3.87
2.89
2.88
1.85
21d:
Ph
Ph
Ph
O
O
S
2.09
5.09
4.00
1.09
2.00
2.00
1.97
0.97
0.98
1.00
2.01
3.01
f1 (ppm)


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
77.37
77.05
76.74
56.57
49.06
41.79
16.86
21d:
Ph
Ph
Ph
O
O
S
f1 (ppm)


8.27
7.97
7.88
7.85
7.47
7.38
7.33
7.26
7.20
7.19
6.42
6.36
6.34
6.32
6.30
5.12
5.10
3.96
3.95
3.93
3.93
3.91
3.90
3.89
3.88
3.28
3.27
3.24
3.23
3.08
3.06
3.04
3.02

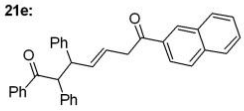
21e:

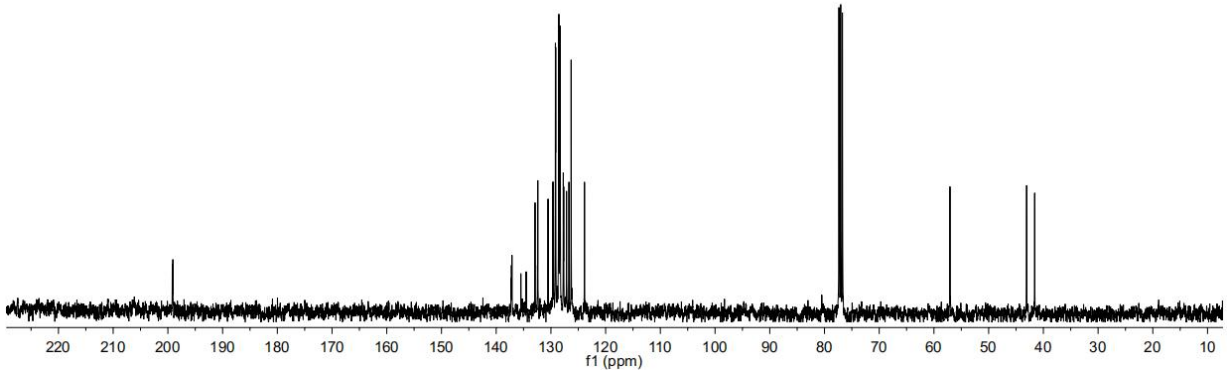

O
Ph
Ph
O
Ph

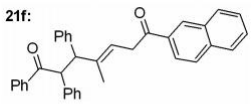

1.03
2.05
4.05
2.24
3.04
4.05
6.10
1.00
0.98
1.00
1.04
1.00
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

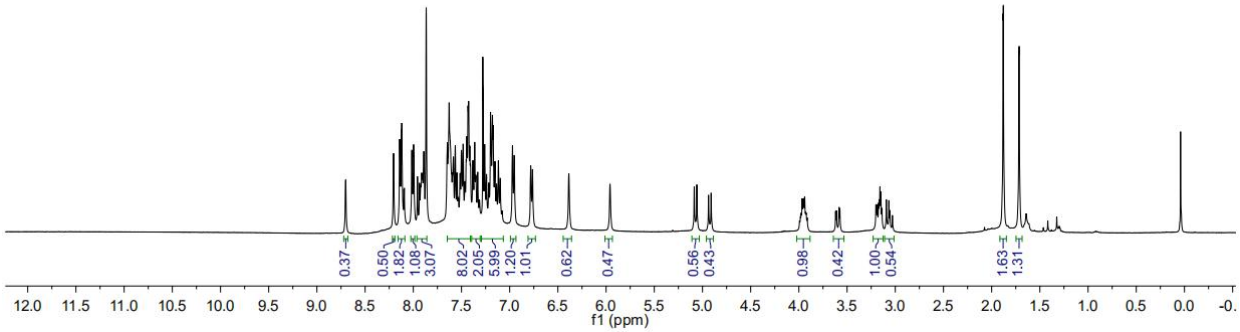

199.21
199.11
137.30
137.23
137.13
135.50
134.54
132.91
132.47
132.41
130.54
129.68
129.55
129.19
129.13
128.61
128.56
128.39
128.31
127.76
127.67
127.16
126.72
126.32
123.88
77.37
77.05
76.73
57.07
43.07
41.60

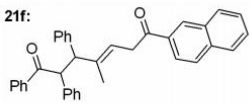
21e:

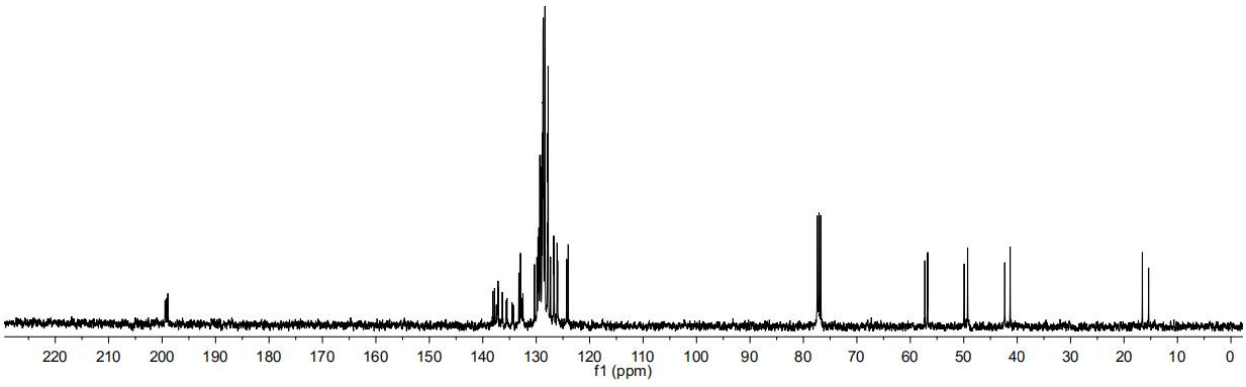

O
Ph
Ph
O
Ph

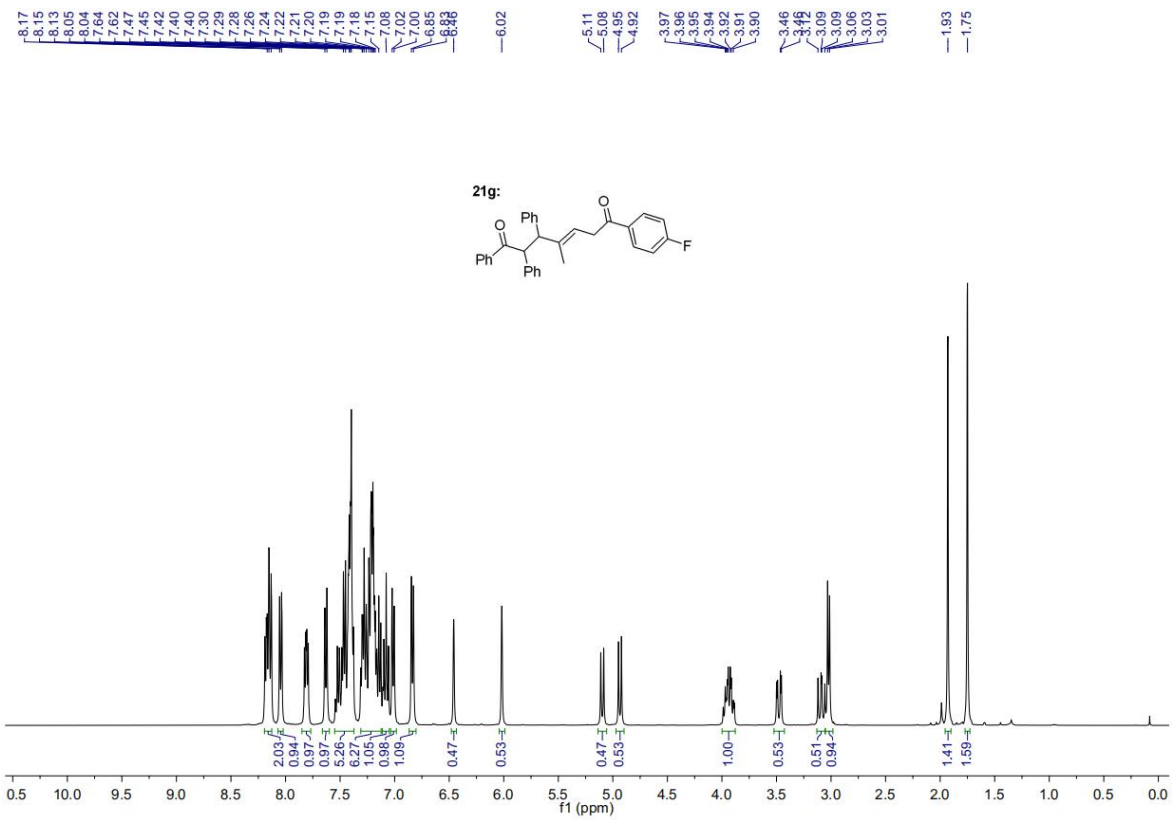

220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

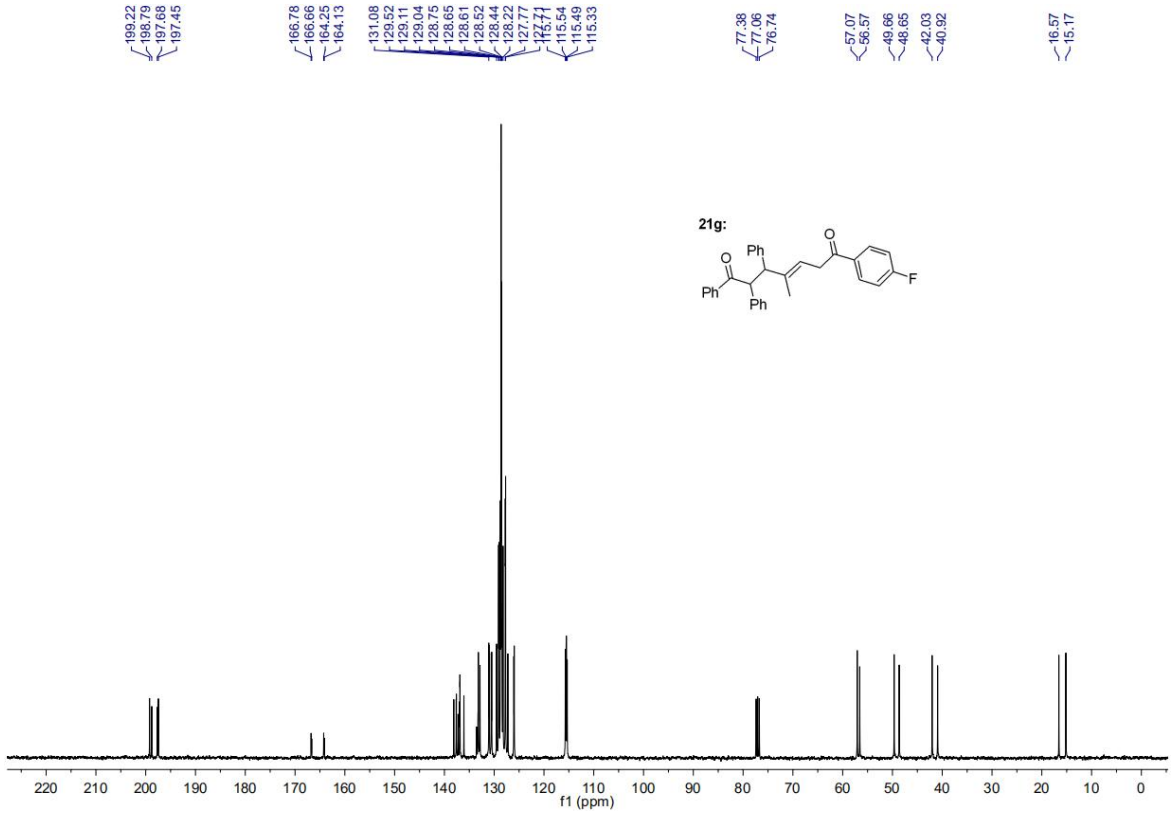

21f:
Ph
O
Ph
O
Ph

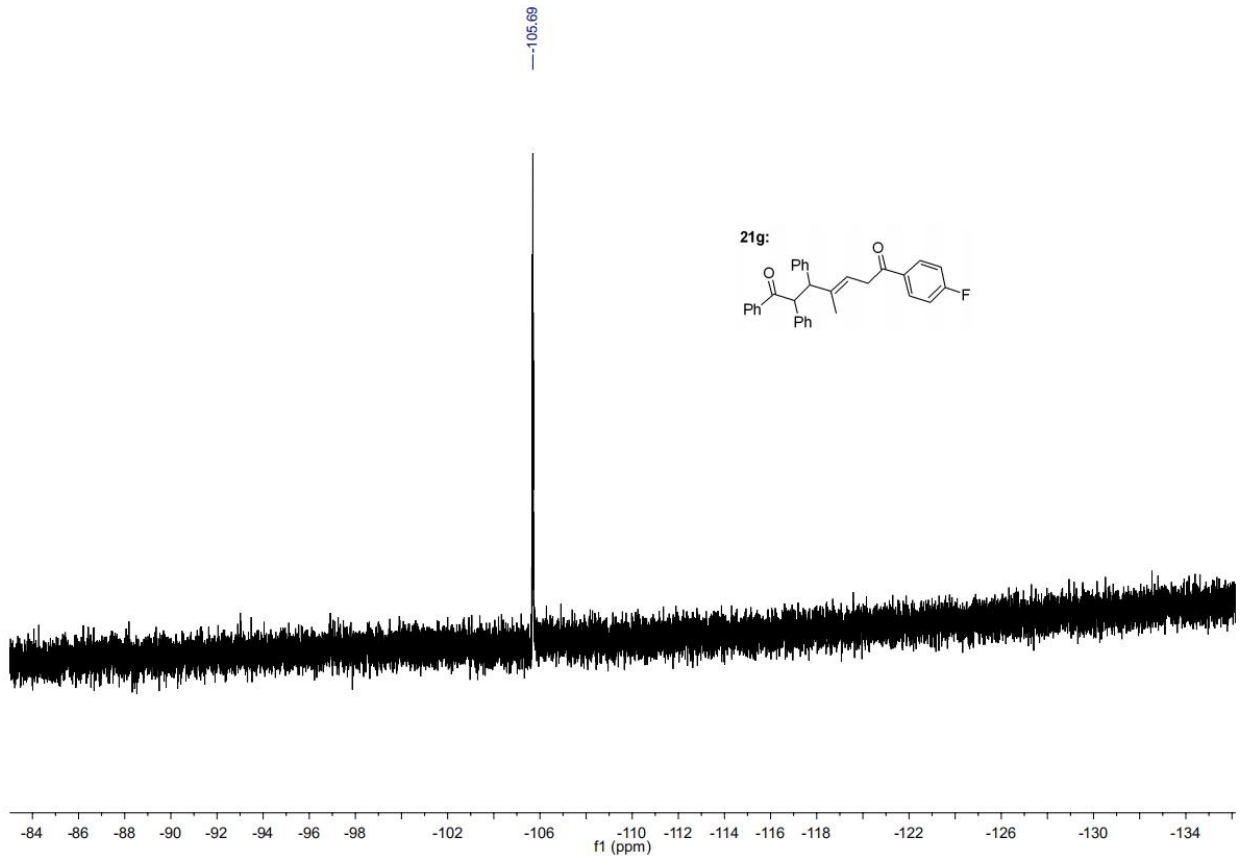

0.37
0.50
1.82
1.08
3.07
8.02
2.05
5.99
1.20
1.01
0.62
0.47
0.56
0.43
0.98
0.42
1.00
0.54
1.63
1.31
f1 (ppm)


21f:
Ph
O
Ph
O
Ph

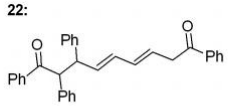

f1 (ppm)

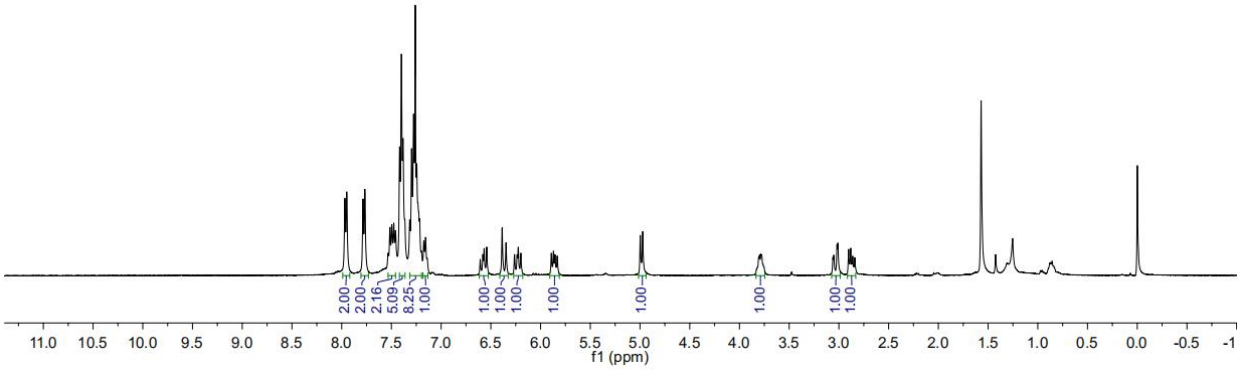

21g:
Ph
O
Ph
Ph
O
F
f1 (ppm)

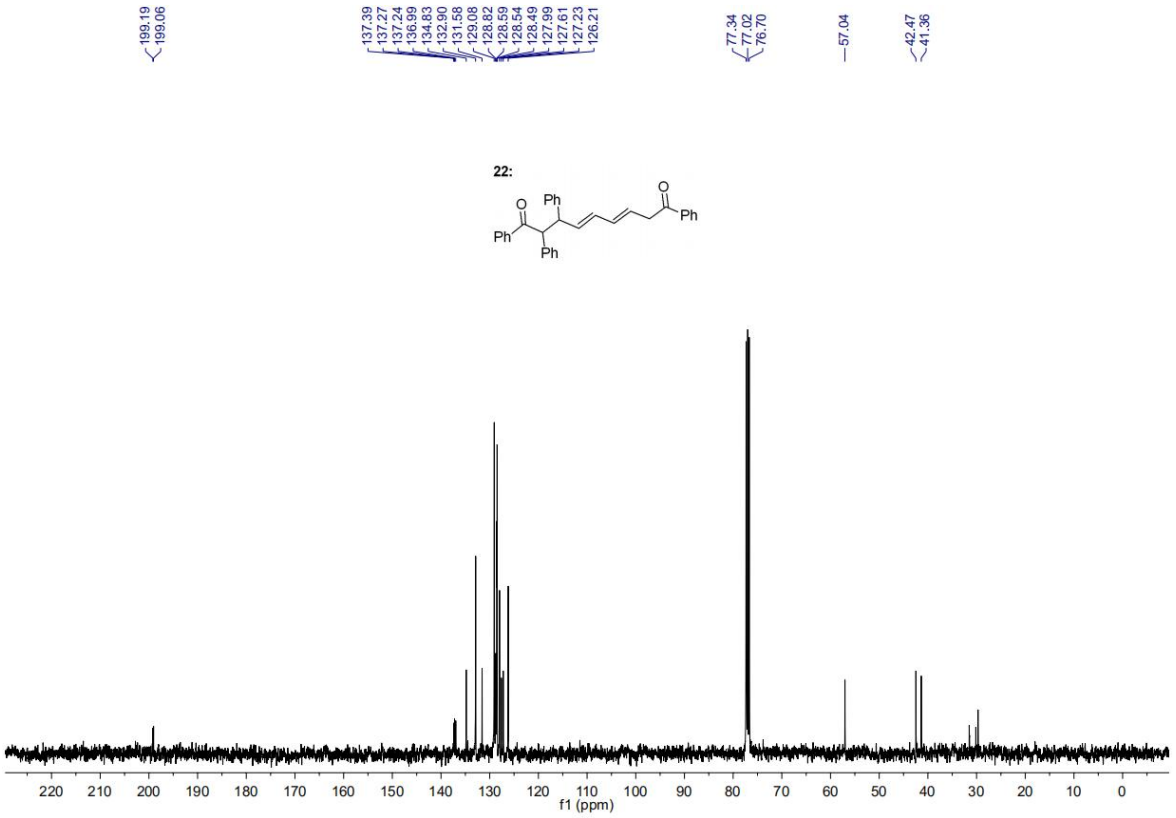

21g:
Ph
O
Ph
Ph
O
F
f1 (ppm)

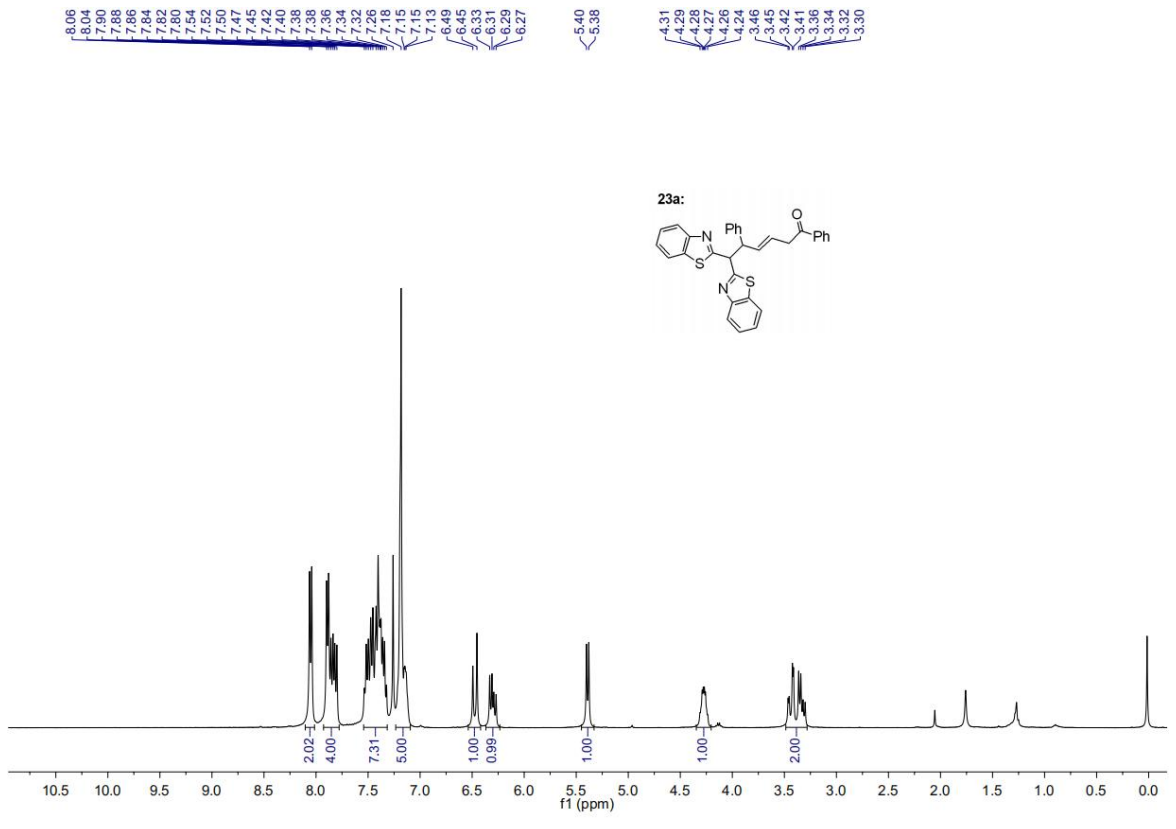

-105.69
21g:
Ph
O
Ph
Ph
O
F
-84 -86 -88 -90 -92 -94 -96 -98 -102 -106 -110 -112 -114 -116 -118 -122 -126 -130 -134
f1 (ppm)


7.97 7.95 7.79 7.77 7.53 7.52 7.50 7.48 7.46 7.42 7.40 7.38 7.37 7.32 7.30 7.28 7.26 7.24 7.23 7.23 7.22 7.20 7.17 7.16 7.14
6.58 6.57 6.54 6.39 6.35 6.26 6.22 6.20 5.89 5.87 5.00 4.97
3.83 3.82 3.81 3.80 3.78 3.78 3.76 3.76 3.06 3.05 3.02 3.01 2.90 2.88 2.86 2.84


22:
O
Ph
Ph
Ph
O
Ph

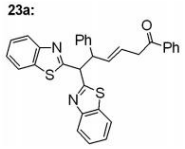

2.00 2.00 2.16 5.09 8.25 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

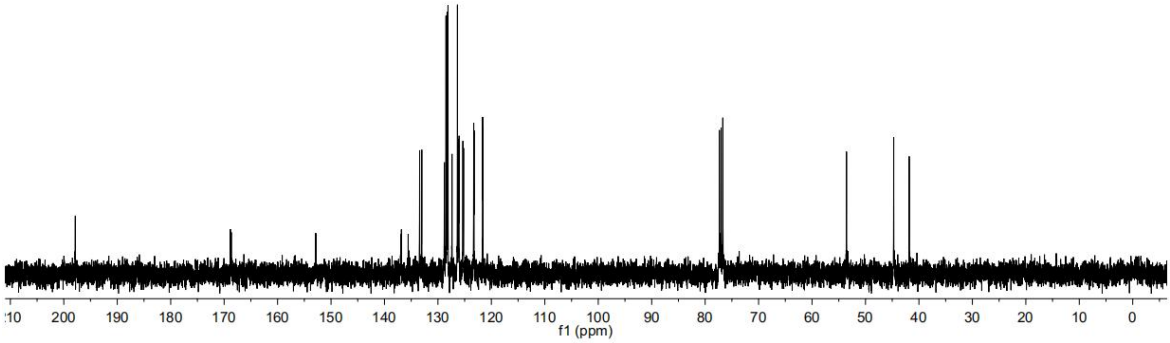

199.19
199.06
137.39
137.27
137.24
136.99
134.83
132.90
131.58
129.08
128.82
128.59
128.54
128.49
127.99
127.61
127.23
126.21
77.34
77.02
76.70
57.04
42.47
41.36
22:
Ph
O
Ph
Ph
Ph
O
Ph
f1 (ppm)


8.06
8.04
7.90
7.88
7.86
7.84
7.82
7.80
7.54
7.52
7.50
7.47
7.45
7.42
7.40
7.38
7.36
7.34
7.32
7.26
7.18
7.15
7.13
6.49
6.45
6.33
6.31
6.29
6.27
5.40
5.38
4.31
4.29
4.28
4.27
4.26
4.24
3.46
3.45
3.42
3.41
3.36
3.34
3.32
3.30
23a:
N
S
Ph
O
Ph
N
S
2.02
4.00
7.31
5.00
1.00
0.99
1.00
1.00
2.00
f1 (ppm)


197.88
168.85
168.68
152.88
152.85
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
77.34
77.02
76.70
53.56
44.73
41.82

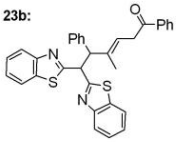
23a:

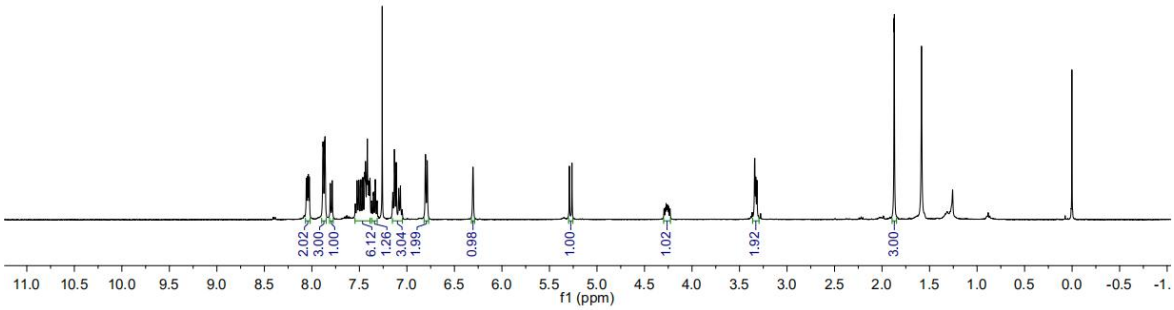

Ph
O
Ph
N
S
S
N

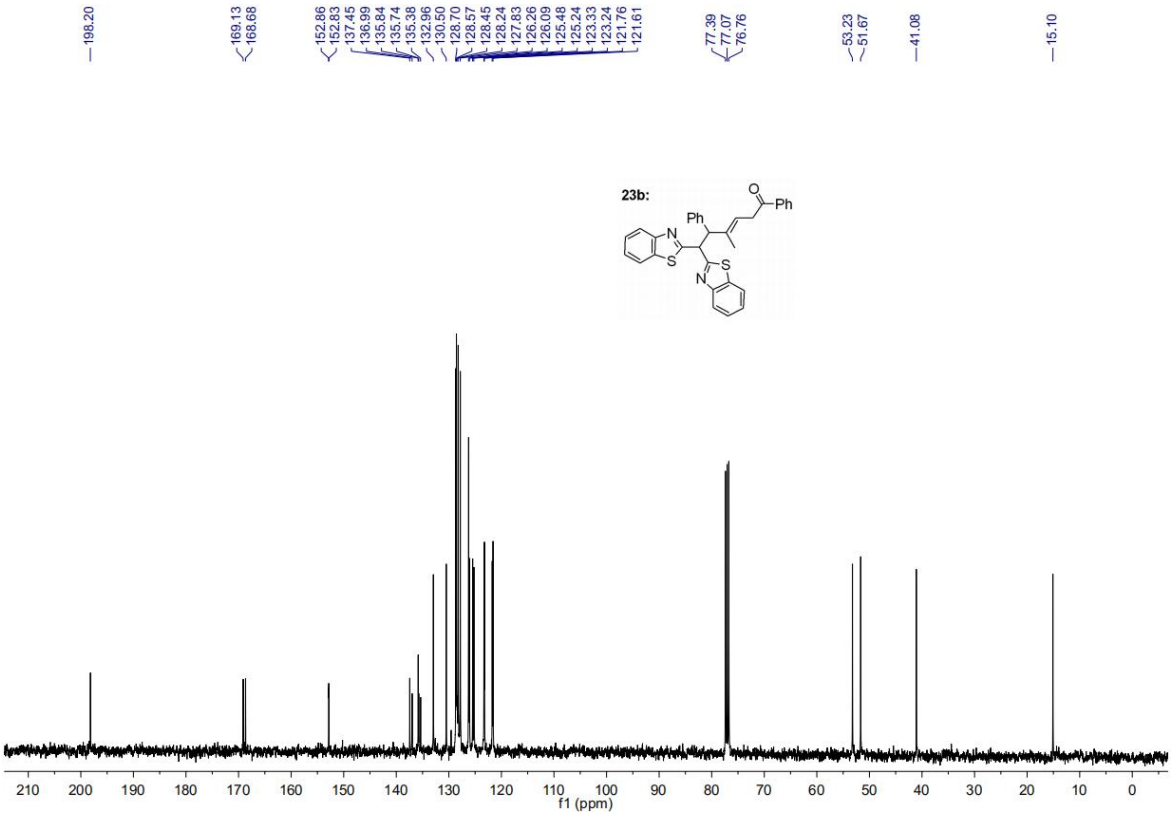

f1 (ppm)

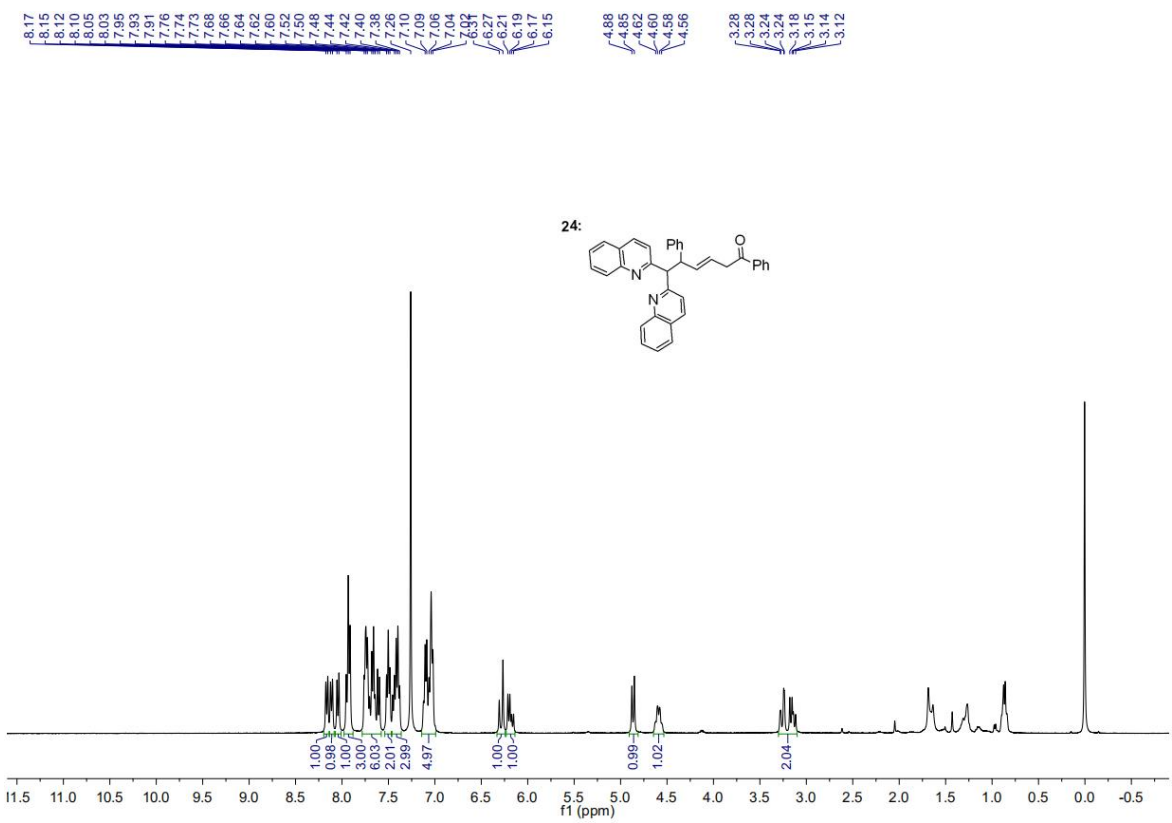

8.06
8.05
8.04
8.03
7.88
7.88
7.87
7.86
7.81
7.79
7.52
7.51
7.48
7.46
7.44
7.44
7.44
7.43
7.42
7.41
7.41
7.40
7.39
7.33
7.26
7.13
7.11
7.07
6.80
6.78
6.30
5.29
5.26
4.29
4.28
4.27
4.27
4.26
4.25
4.24
4.24
4.23
3.34
3.34
3.33
3.32
3.30
1.87
1.87

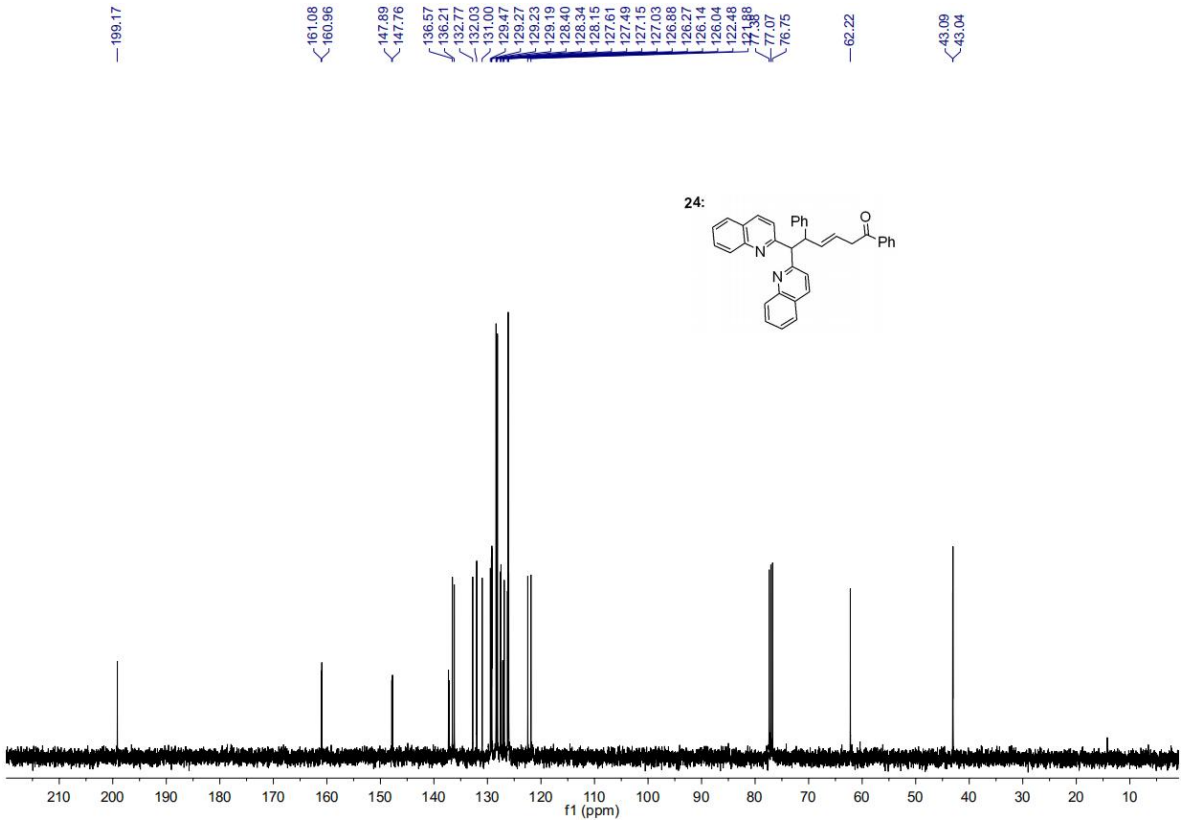
23b:

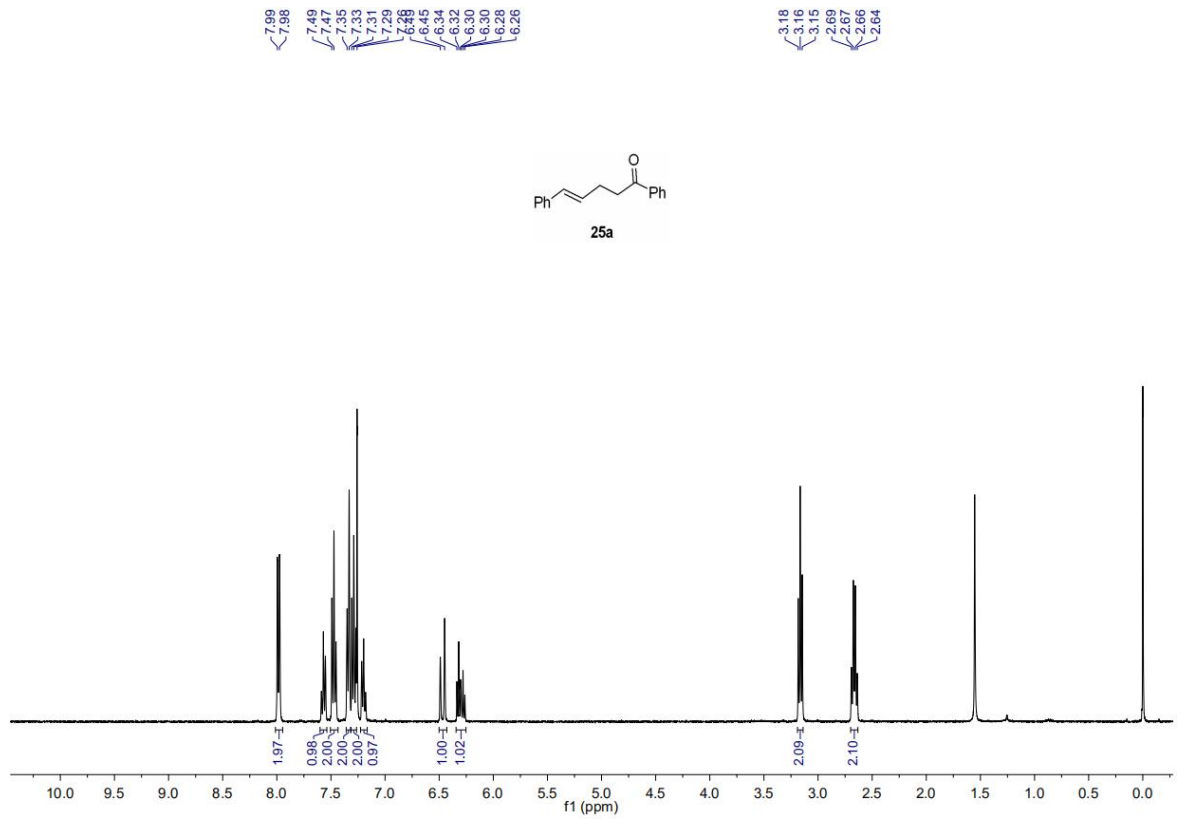

O
Ph
Ph
N
S
S
N

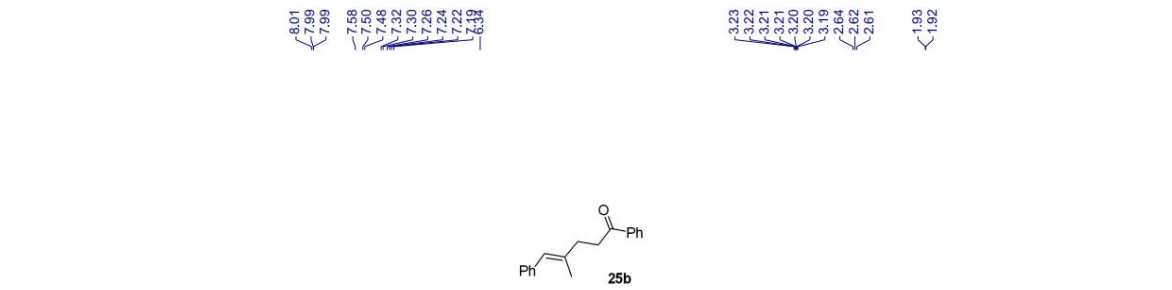

2.02
3.00
1.00
6.12
1.26
3.04
1.99
0.98
1.00
1.02
1.92
3.00
f1 (ppm)

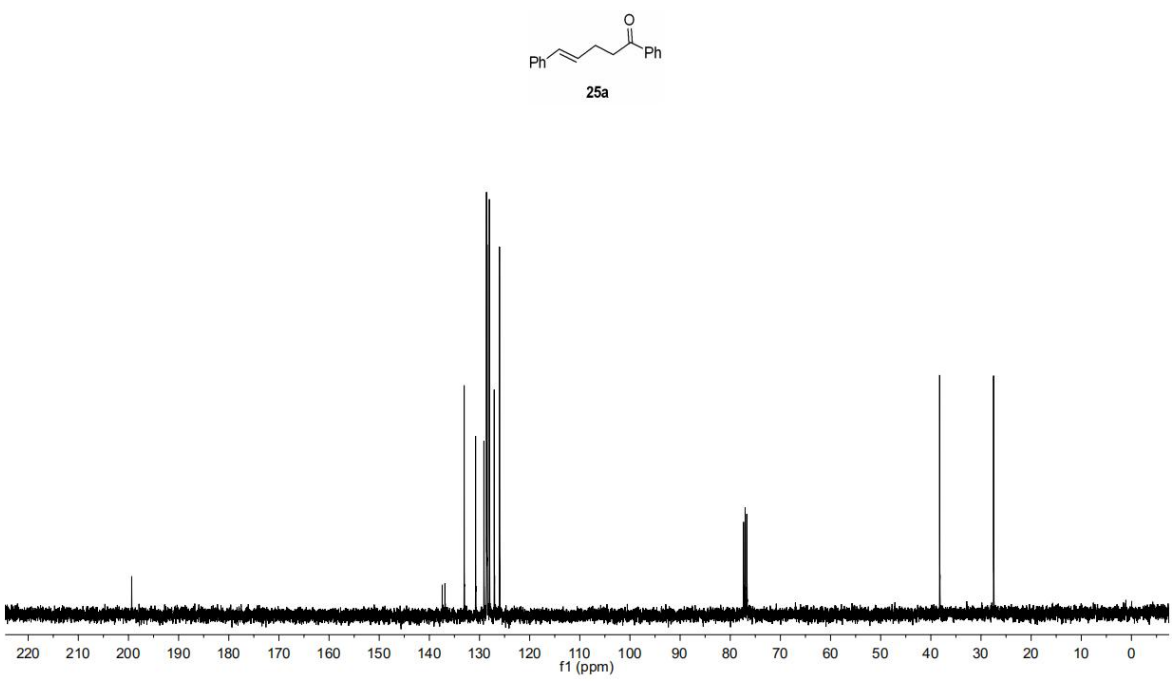

198.20
169.13
168.68
152.86
152.83
137.45
136.99
135.84
135.74
135.38
132.96
130.50
128.70
128.57
128.45
128.24
127.83
126.26
126.09
125.48
125.24
123.33
123.24
121.76
121.61
77.39
77.07
76.76
53.23
51.67
41.08
15.10
23b:
Ph
O
Ph
N
S
S
N
f1 (ppm)

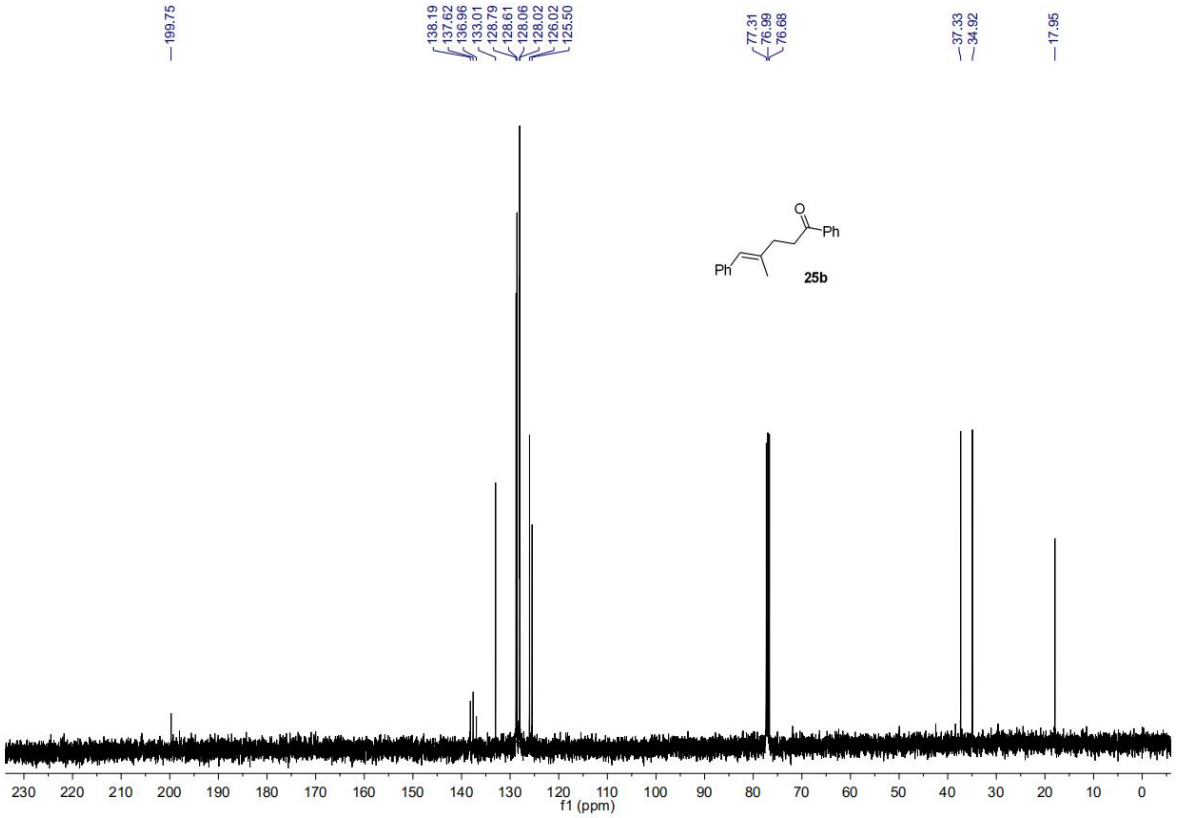

8.17
8.15
8.12
8.10
8.05
8.03
7.95
7.93
7.91
7.76
7.74
7.73
7.68
7.66
7.64
7.62
7.60
7.52
7.50
7.48
7.44
7.42
7.40
7.38
7.26
7.10
7.09
7.06
7.04
7.02
6.31
6.27
6.21
6.19
6.17
6.15
4.88
4.85
4.62
4.60
4.58
4.56
3.28
3.28
3.24
3.24
3.18
3.15
3.14
3.12
24:
Ph
O
Ph
N
N
1.00
0.98
1.00
3.00
6.03
2.01
2.99
4.97
1.00
1.00
0.99
1.02
2.04
f1 (ppm)

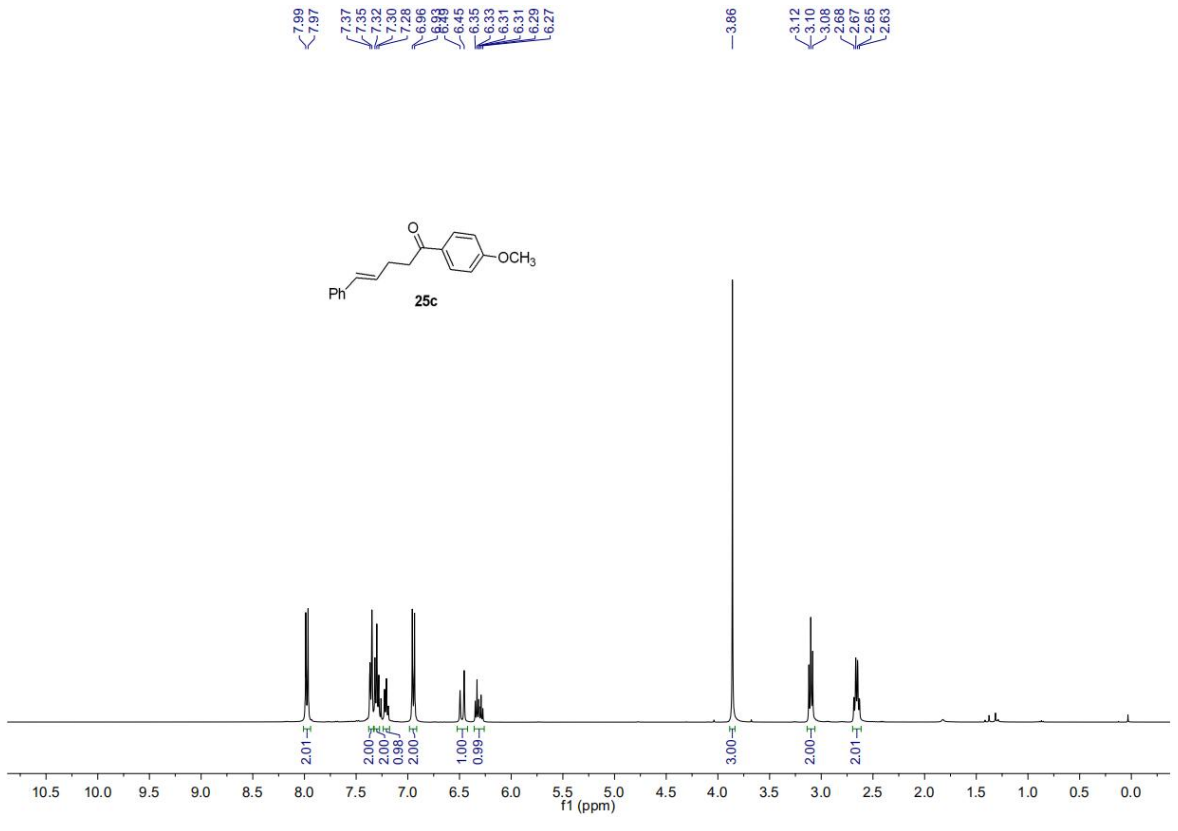

199.17
161.08
160.96
147.89
147.76
136.57
136.21
132.77
132.03
131.00
129.47
129.27
129.23
129.19
128.40
128.34
128.15
127.61
127.49
127.15
127.03
126.88
126.27
126.14
126.04
122.48
77.07
76.75
62.22
43.09
43.04
24:
Ph
O
Ph
N
N
f1 (ppm)

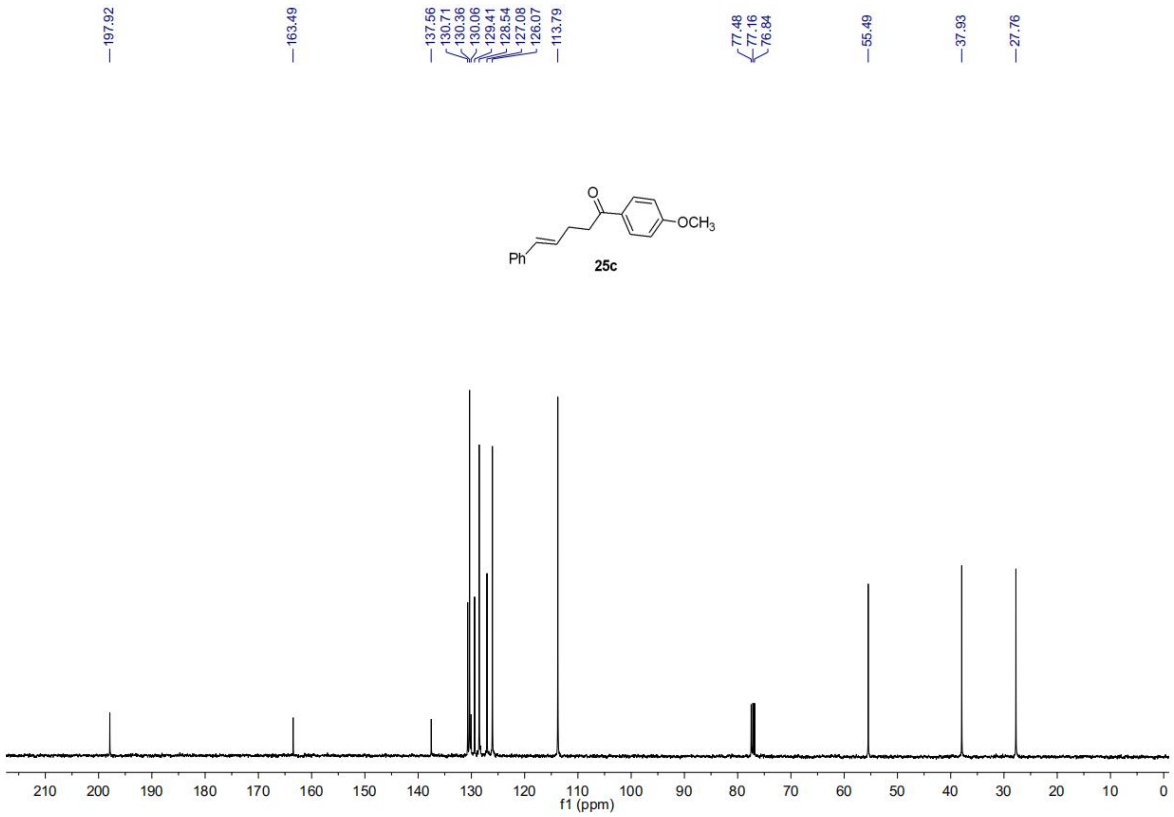

7.99
7.98
7.49
7.47
7.35
7.33
7.31
7.29
6.45
6.34
6.32
6.30
6.28
6.26
3.18
3.16
3.15
2.69
2.67
2.66
2.64
O
Ph
Ph
25a
1.97
0.98
2.00
2.00
2.00
0.97
1.00
1.02
2.09
2.10
f1 (ppm)

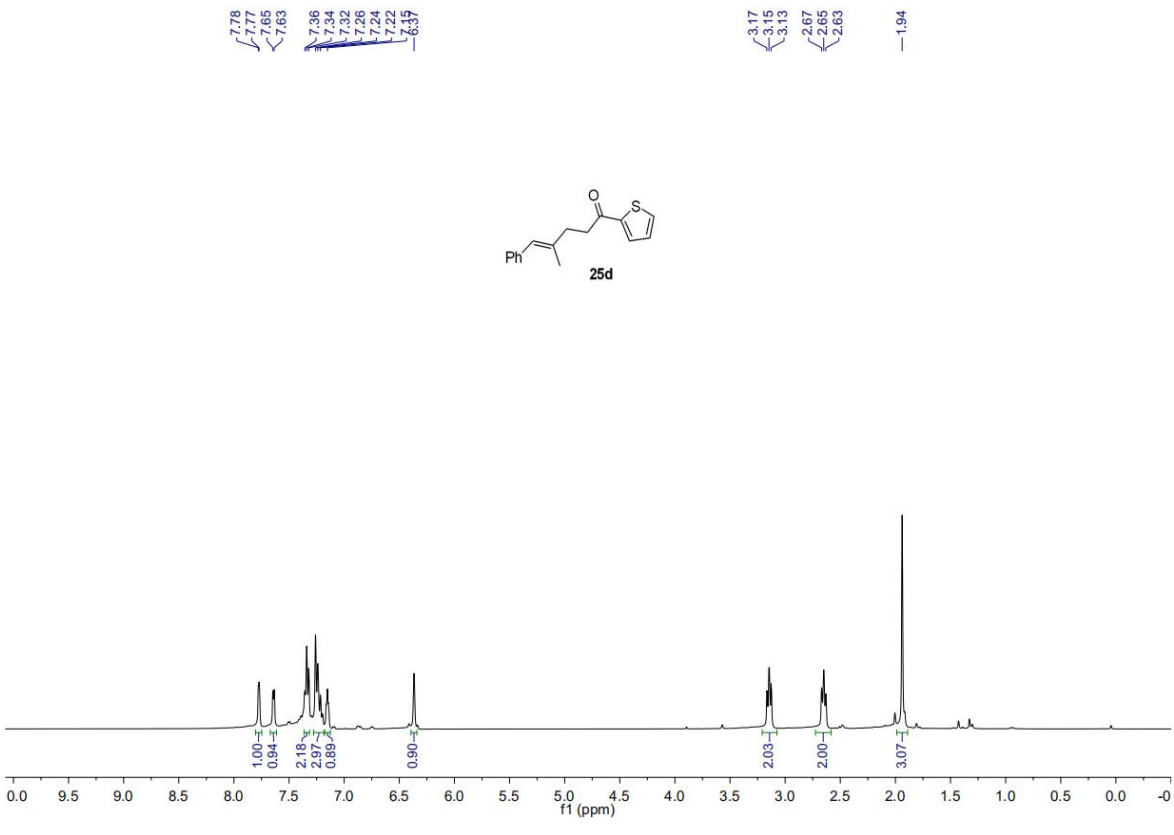

8.01
7.99
7.99
7.58
7.50
7.48
7.32
7.30
7.26
7.24
7.22
7.19
6.34
3.23
3.22
3.21
3.21
3.20
3.20
3.19
2.64
2.62
2.61
1.93
1.92
O
Ph
Ph
25b
2.00
1.02
2.04
2.23
3.17
1.00
2.00
2.00
2.97
f1 (ppm)

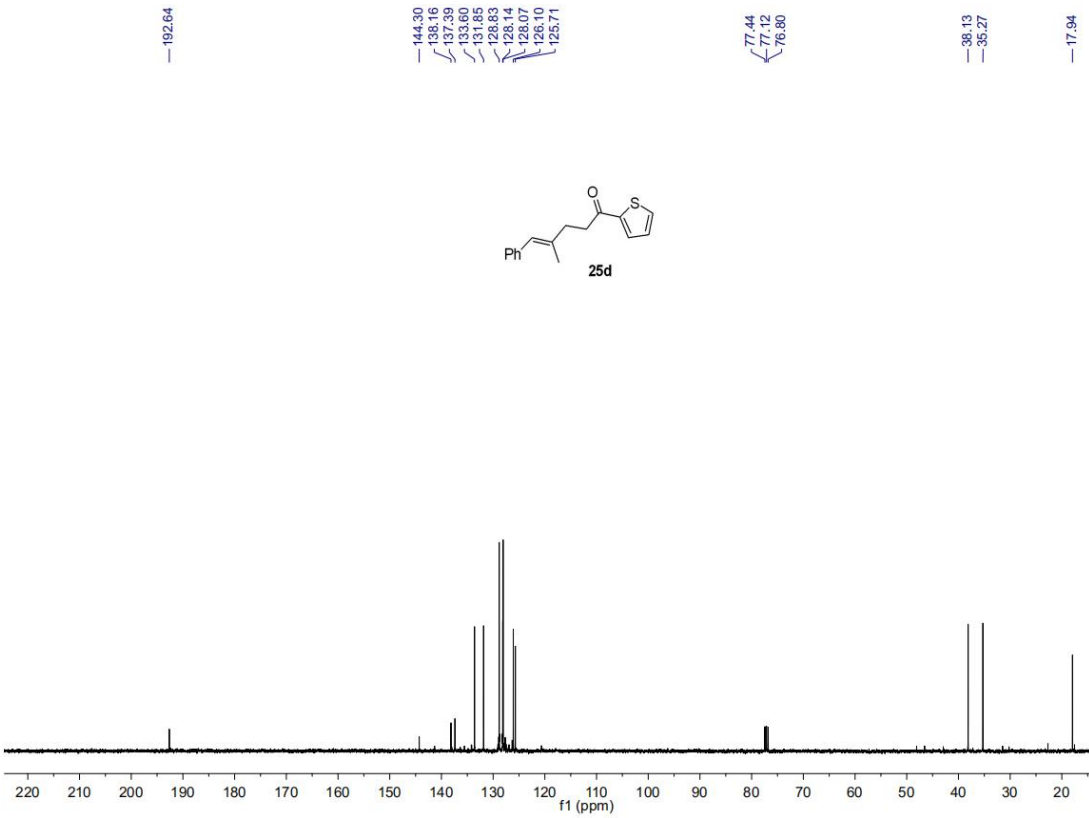

199.36
137.44
136.89
133.06
130.78
129.12
128.61
128.49
128.04
127.06
126.01
77.34
77.03
76.71
38.25
27.49
O
Ph
Ph
25a
f1 (ppm)

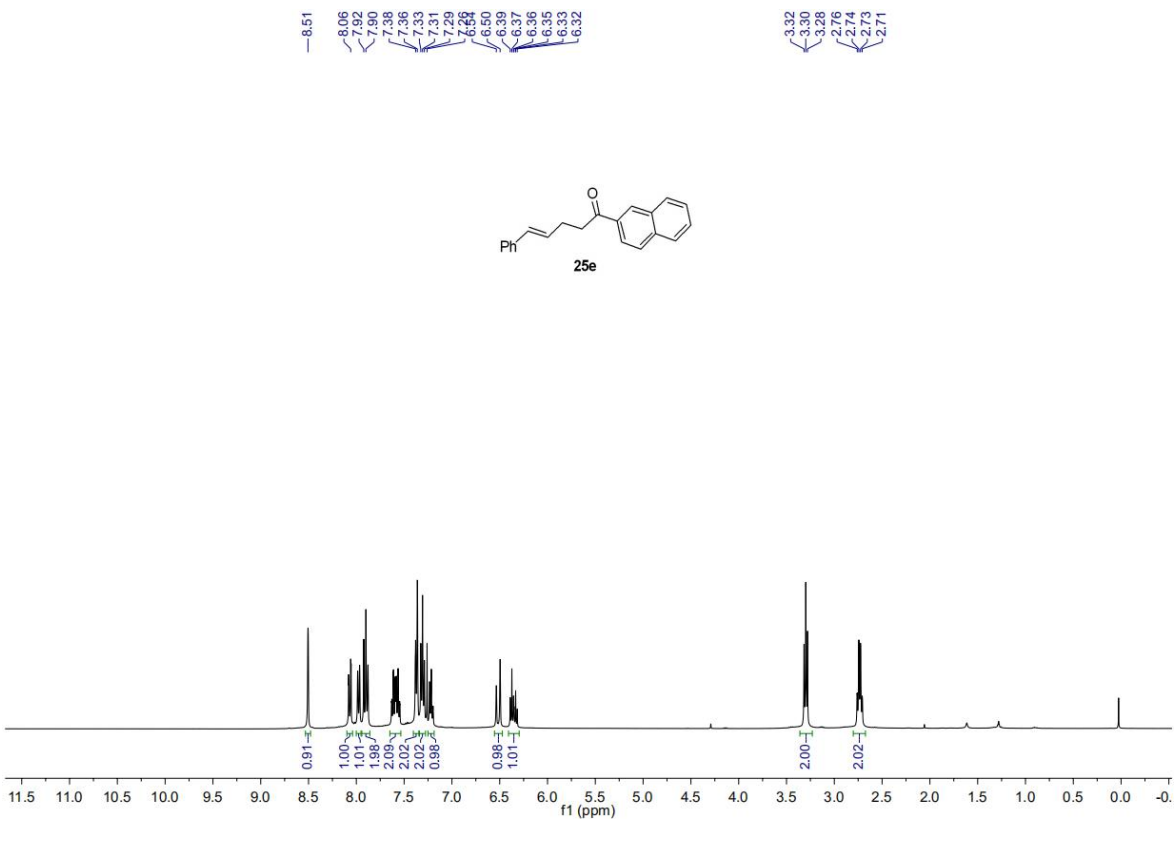

199.75
138.19
137.62
136.96
133.01
128.79
128.61
128.06
128.02
126.02
125.50
77.31
76.99
76.68
37.33
34.92
17.95
O
Ph
Ph
25b
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

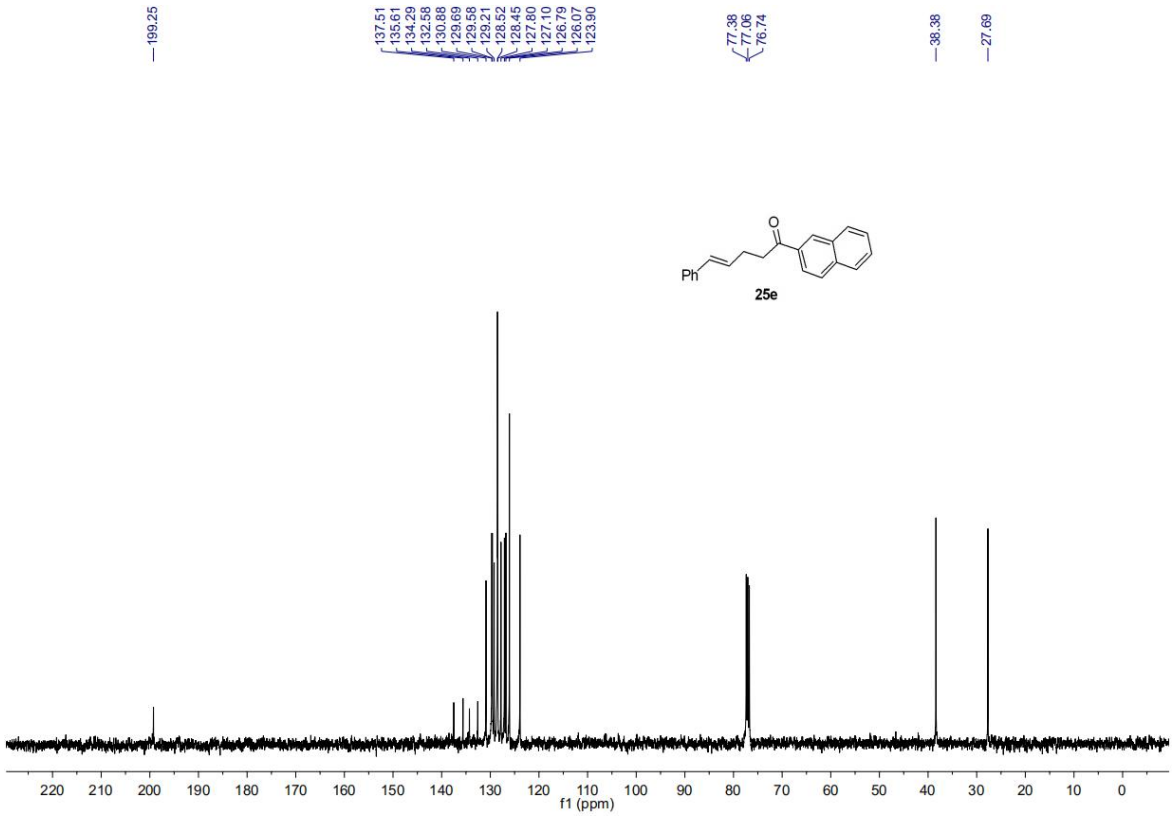

7.99
7.97
7.37
7.35
7.32
7.30
7.28
6.96
6.45
6.35
6.33
6.31
6.31
6.29
6.27
3.86
3.12
3.10
3.08
2.68
2.67
2.65
2.63
O
OCH3
Ph
25c
2.01
2.00
2.00
0.98
2.00
1.00
0.99
3.00
2.00
2.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

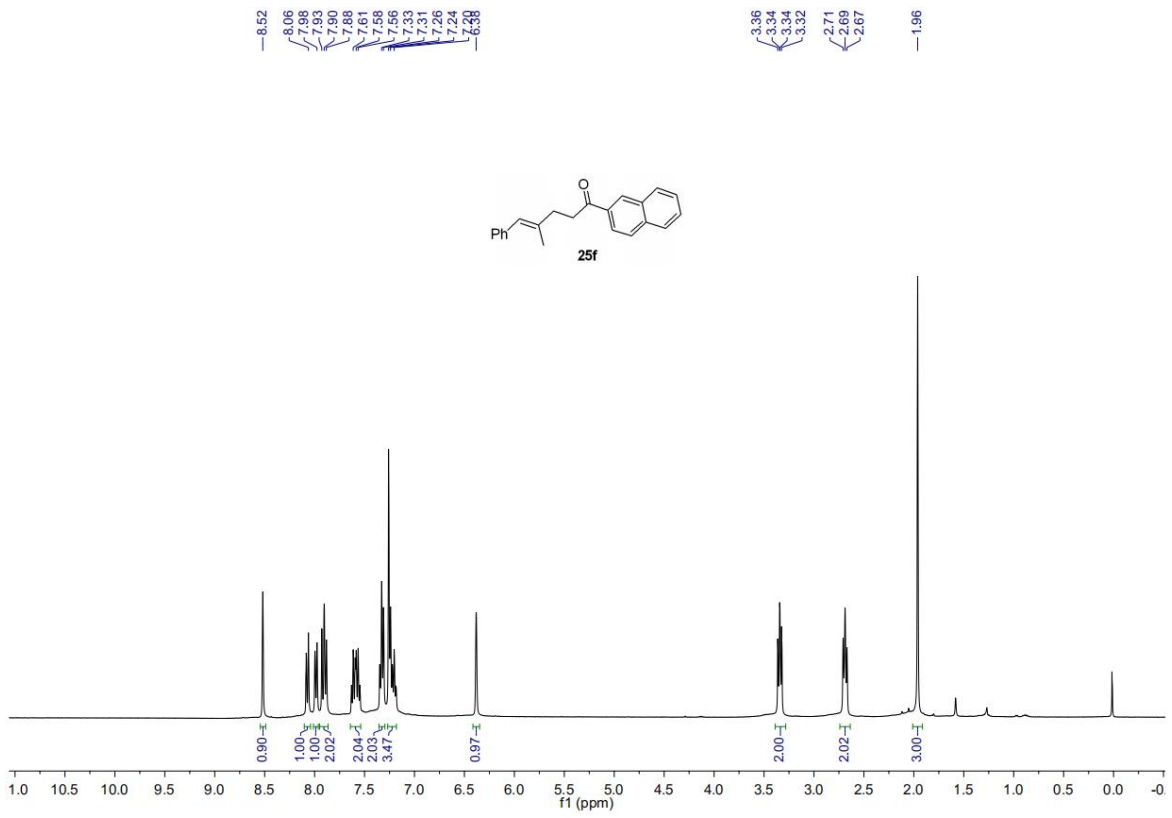

197.92
163.49
137.56
130.71
130.36
130.06
129.41
128.54
127.08
126.07
113.79
77.48
77.16
76.84
55.49
37.93
27.76
O
OCH3
Ph
25c
f1 (ppm)


7.78
7.77
7.65
7.63
7.36
7.34
7.32
7.26
7.24
7.22
6.37
3.17
3.15
3.13
2.67
2.65
2.63
1.94
O
S
Ph
25d
1.00
0.94
2.18
2.97
0.89
0.90
2.03
2.00
3.07
f1 (ppm)

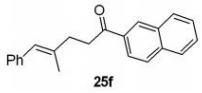

192.64
144.30
138.16
137.39
133.60
131.85
128.83
128.14
128.07
126.10
125.71
77.44
77.12
76.80
38.13
35.27
17.94
O
S
Ph
25d
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.51
8.06
7.92
7.90
7.38
7.36
7.33
7.31
7.29
6.50
6.39
6.37
6.36
6.35
6.33
6.32
3.32
3.30
3.28
2.76
2.74
2.73
2.71
O
Ph
25e
0.91
1.00
1.01
1.98
2.09
2.02
2.02
0.98
0.98
1.01
2.00
2.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

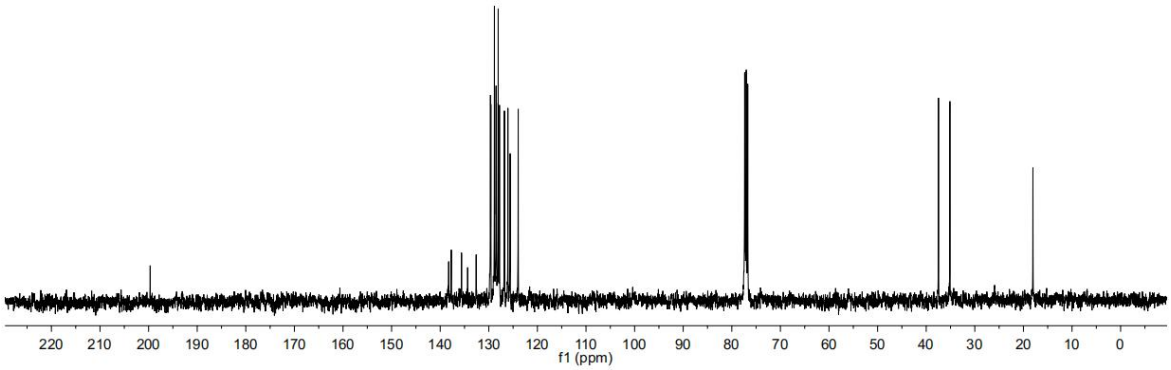

199.25
137.51
135.61
134.29
132.58
130.88
129.69
129.58
129.21
128.52
128.45
127.80
127.10
126.79
126.07
123.90
77.38
77.06
76.74
38.38
27.69
O
Ph
25e
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.52
8.06
7.98
7.93
7.90
7.88
7.61
7.58
7.56
7.33
7.31
7.26
7.24
7.20
6.38
3.36
3.34
3.34
3.32
2.71
2.69
2.67
1.96
O
Ph
25f
0.90
1.00
1.00
2.02
2.04
2.03
3.47
0.97
2.00
2.02
3.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

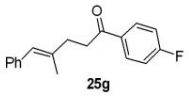

199.68
138.26
137.72
135.61
134.36
132.60
129.66
129.57
128.85
128.50
128.43
128.07
127.80
126.79
126.07
125.61
123.95
77.35
77.04
76.72
37.47
35.12
18.04


O
Ph

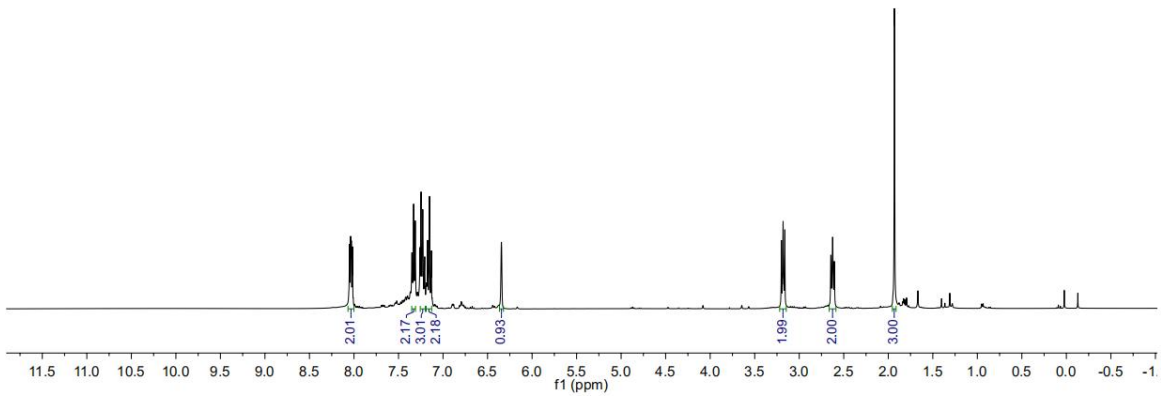
25f

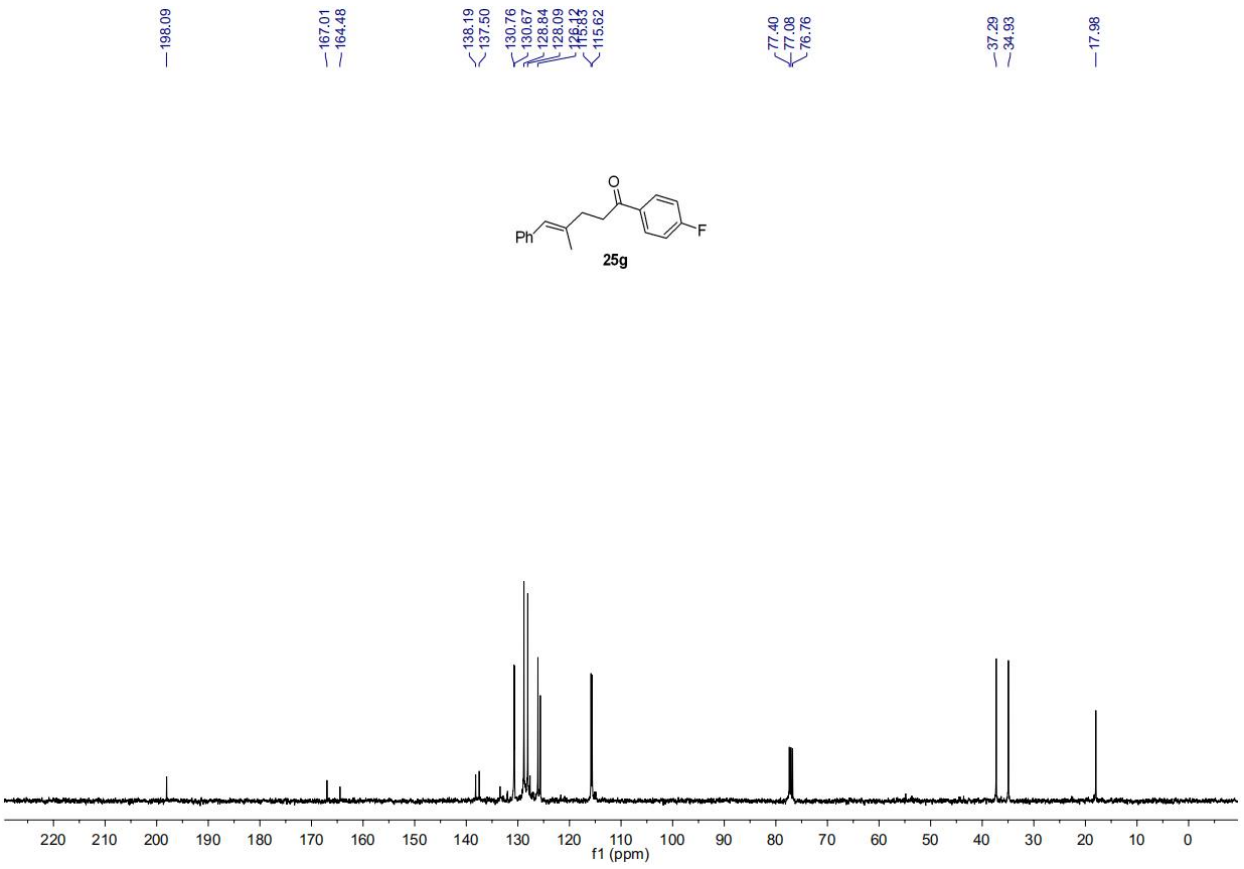

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

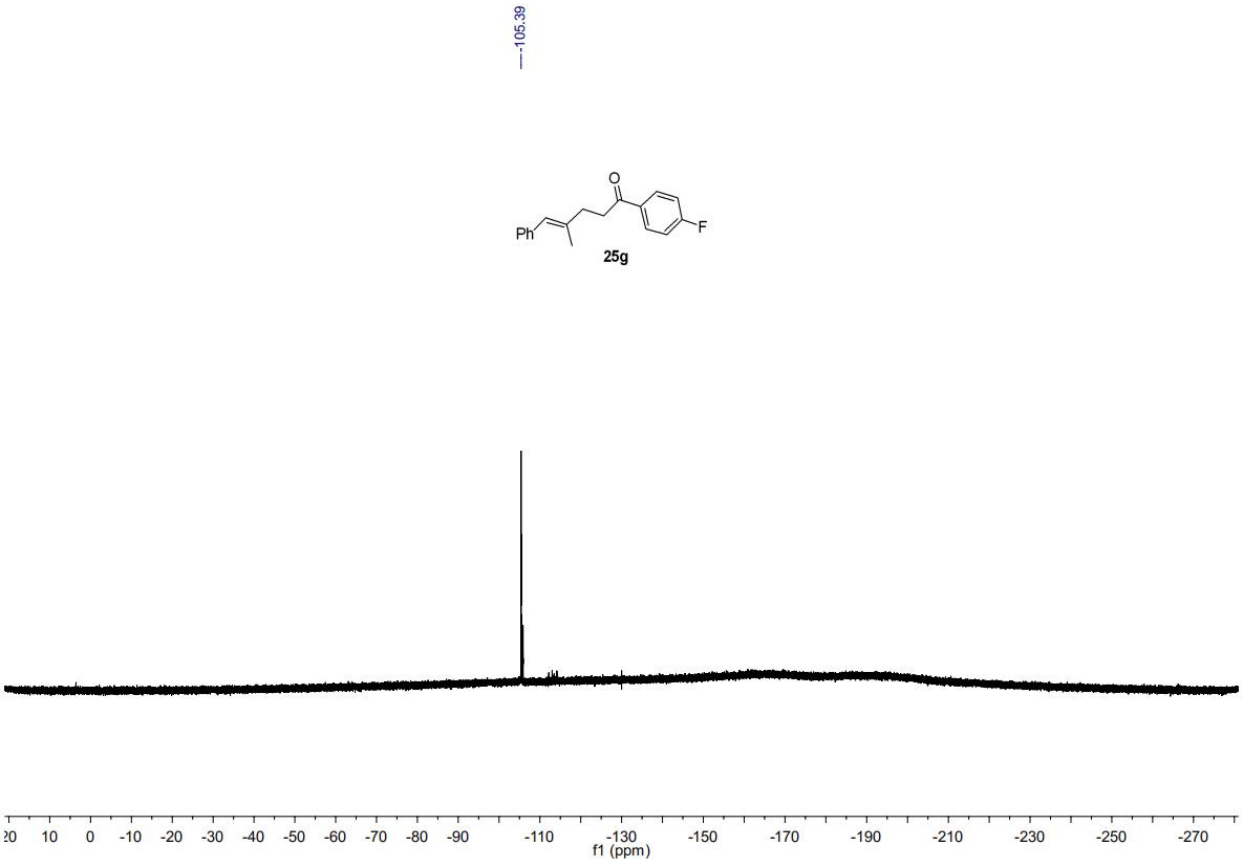

8.05
8.05
8.04
8.03
8.02
8.02
8.01
7.33
7.31
7.26
7.25
7.23
7.17
7.15
6.34
3.20
3.18
3.17
3.16
2.64
2.63
2.61
1.93
1.93

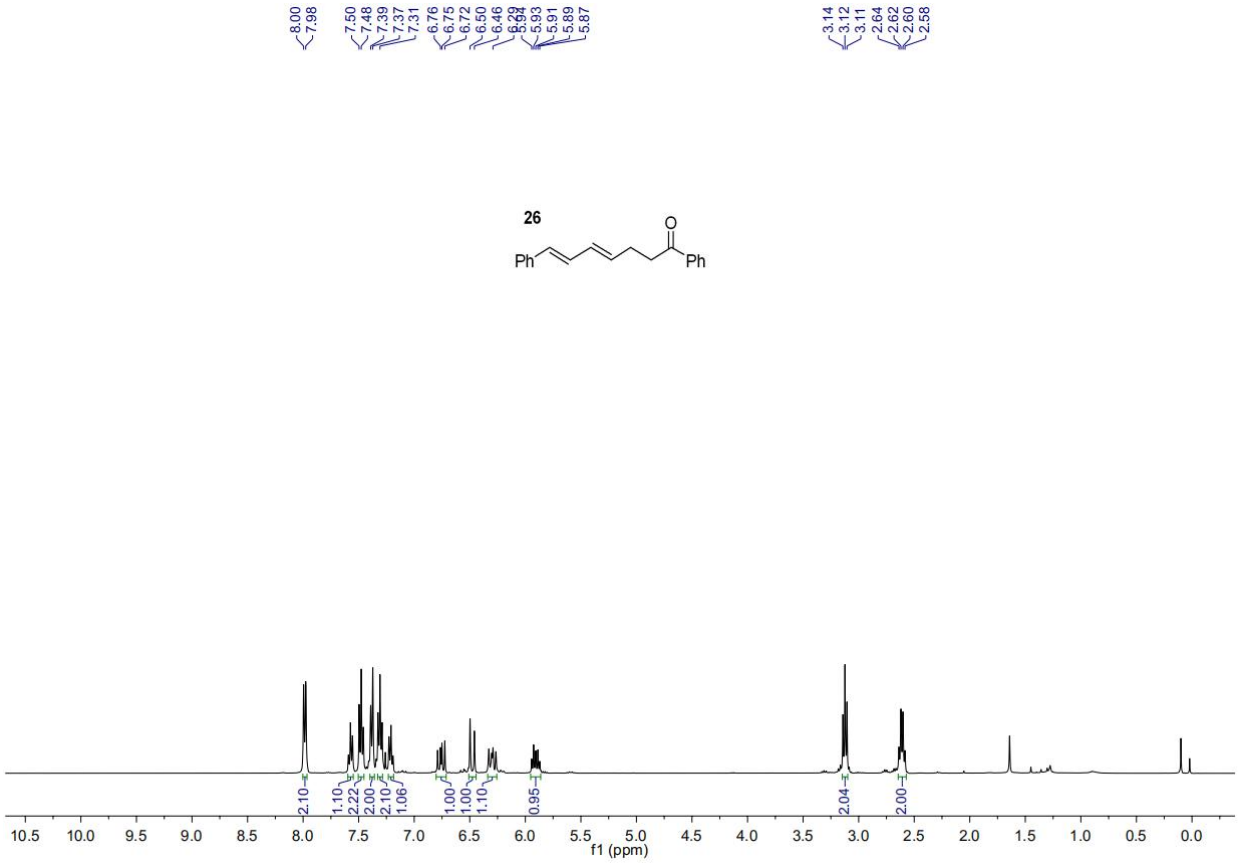

O
Ph
F

25g


2.01
2.17
3.01
2.18
0.93
1.99
2.00
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

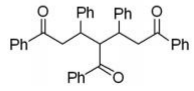

198.09
167.01
164.48
138.19
137.50
130.76
130.67
128.84
128.09
126.12
115.83
115.62
77.40
77.08
76.76
37.29
34.93
17.98
O
Ph
F
25g
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

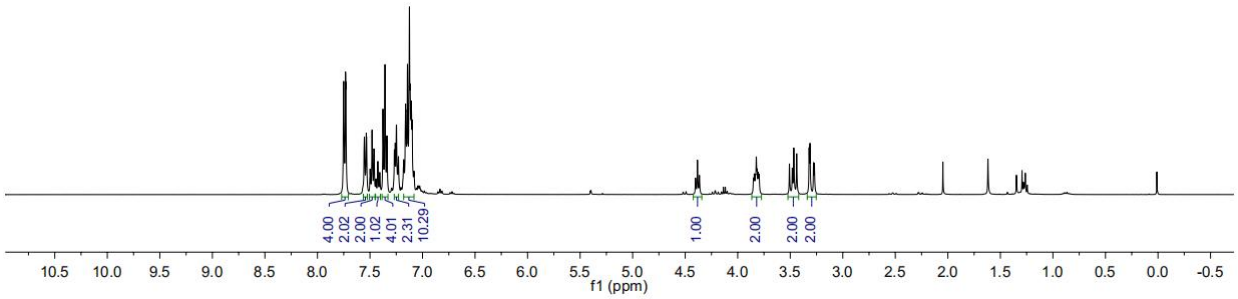

-105.39
O
Ph
F
25g
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)


8.00
7.98
7.50
7.48
7.39
7.37
7.31
6.76
6.75
6.72
6.50
6.46
5.93
5.91
5.89
5.87
3.14
3.12
3.11
2.64
2.62
2.60
2.58
26
O
Ph
Ph
2.10
1.10
2.22
2.00
2.10
1.06
1.00
1.00
1.10
0.95
2.04
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (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
77.39
77.08
76.76
38.19
27.34
26
O
Ph
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.75
7.73
7.73
7.55
7.54
7.53
7.50
7.48
7.46
7.44
7.43
7.41
7.38
7.36
7.34
7.27
7.26
7.25
7.23
7.18
7.16
7.16
7.15
7.14
7.12
7.12
7.11
7.10
7.09
7.08
4.40
4.38
4.36
3.85
3.84
3.83
3.82
3.82
3.80
3.80
3.51
3.48
3.47
3.44
3.32
3.31
3.28
3.27

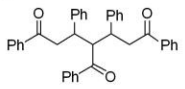
27a:

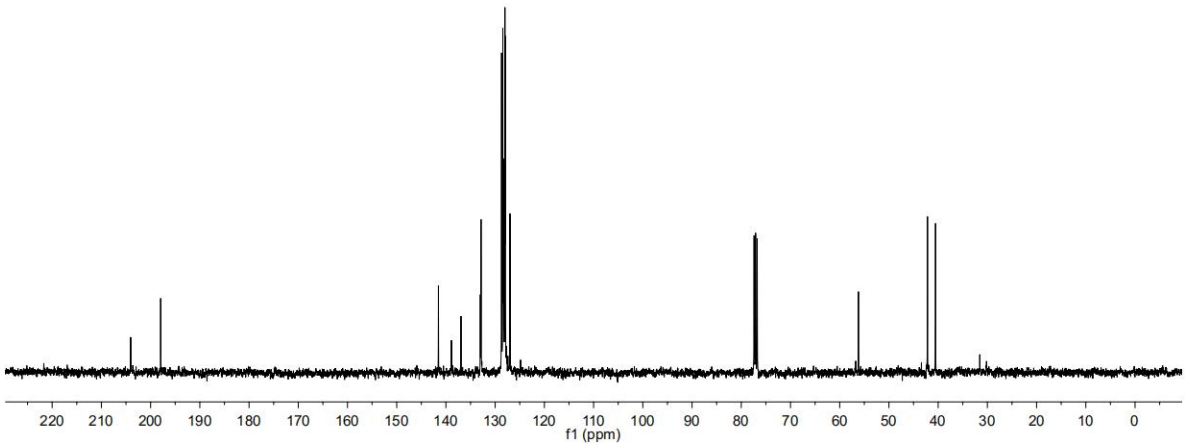

O
Ph
Ph
O
Ph
Ph
Ph
O

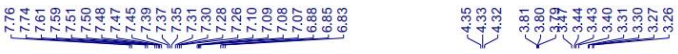

4.00
2.02
2.00
1.02
4.01
2.31
10.29
1.00
2.00
2.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


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
77.40
77.09
76.77
56.20
42.17
40.54

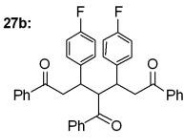
27a:

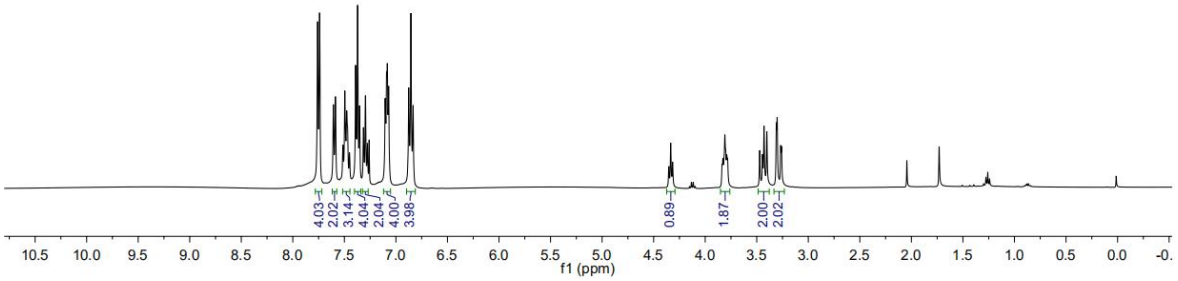

O
Ph
Ph
O
Ph
Ph
Ph
O


220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.76
7.74
7.61
7.59
7.51
7.50
7.48
7.47
7.45
7.39
7.37
7.35
7.31
7.30
7.28
7.26
7.10
7.09
7.08
7.07
6.88
6.85
6.83
4.35
4.33
4.32
3.81
3.80
3.47
3.44
3.43
3.40
3.31
3.30
3.27
3.26

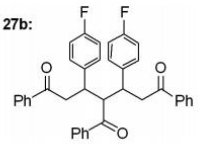
27b:

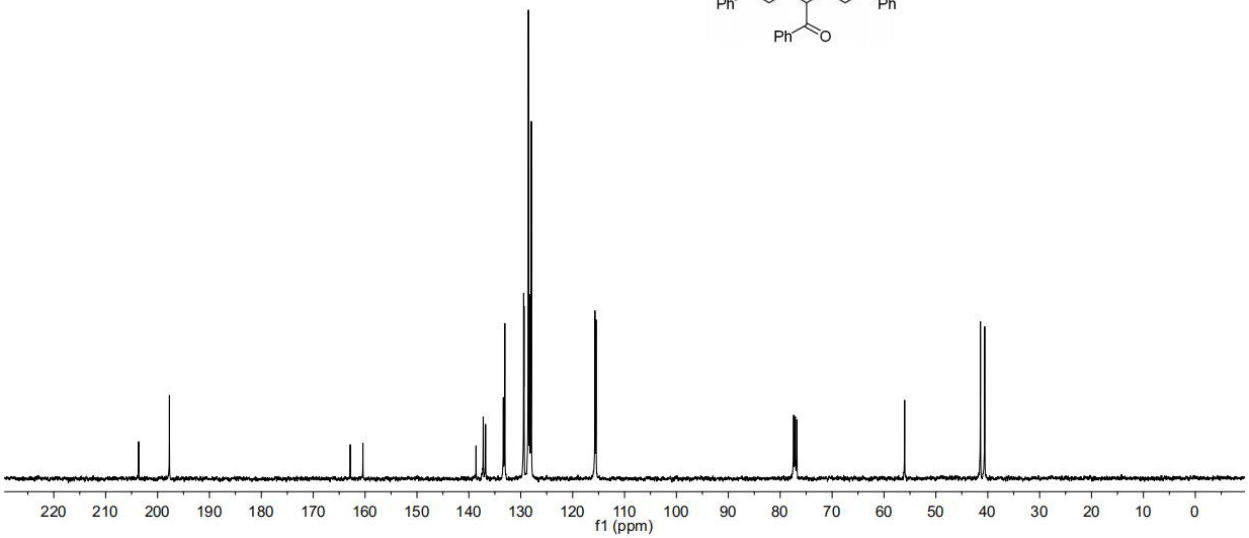

F
F
O
Ph
O
Ph
Ph
O

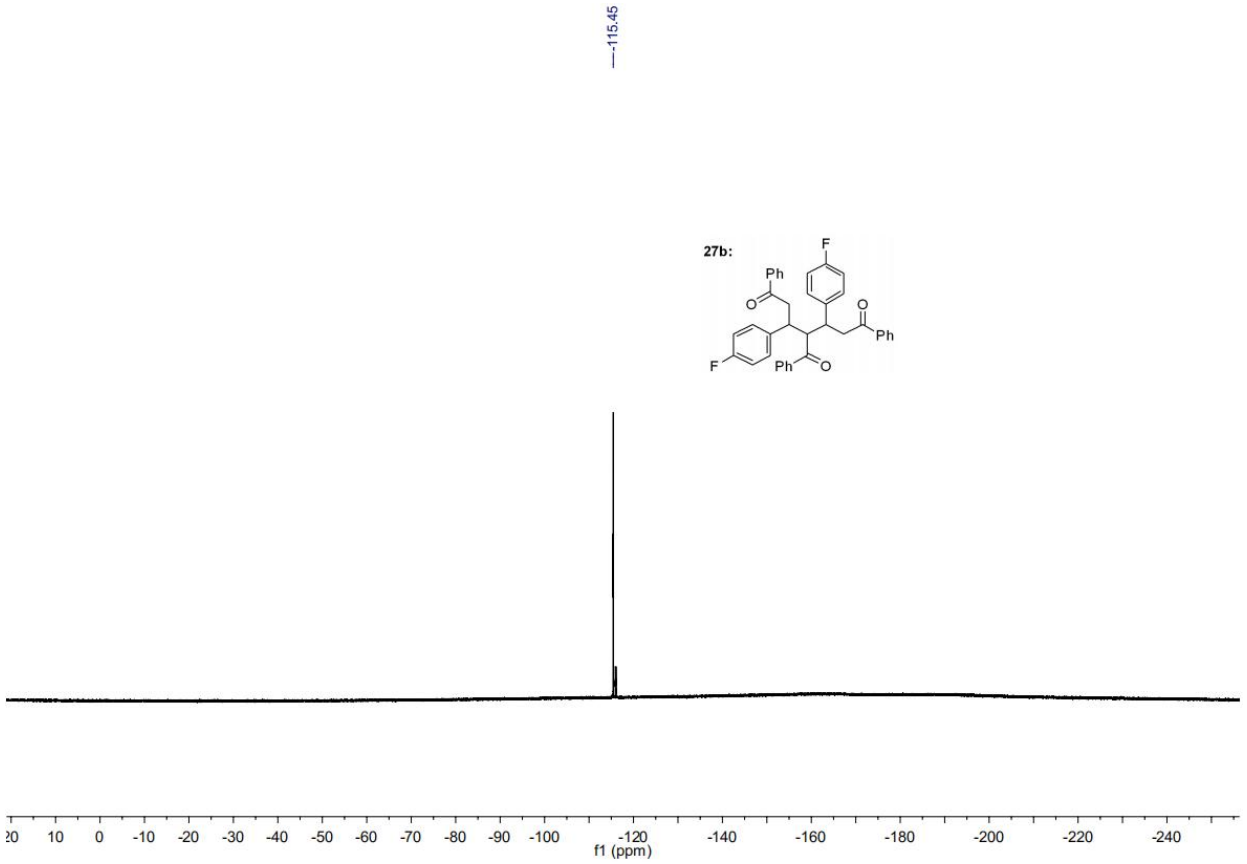

4.03
2.02
3.14
4.04
2.04
4.00
3.98
0.89
1.87
2.00
2.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


203.66
197.74
162.88
160.44
138.64
137.26
137.23
136.80
133.38
133.08
129.46
129.38
128.54
128.28
127.98
115.71
115.50
77.42
77.10
76.78
56.03
41.42
40.59

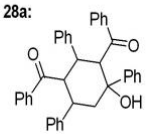
27b:

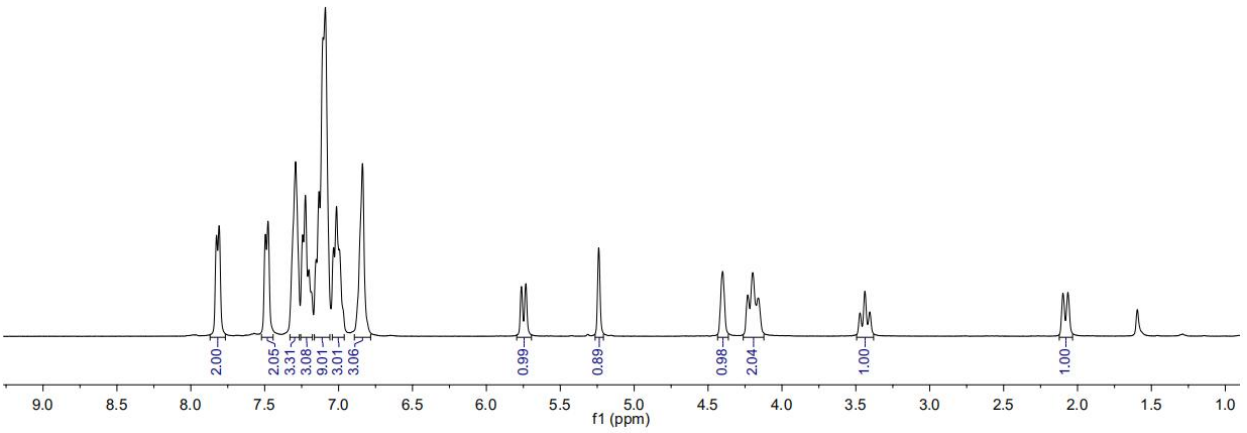

F
F
O
Ph
O
Ph
Ph
O

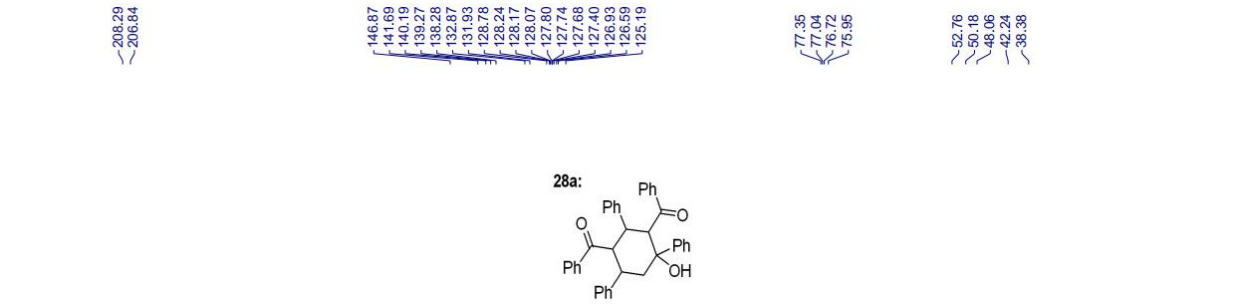

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

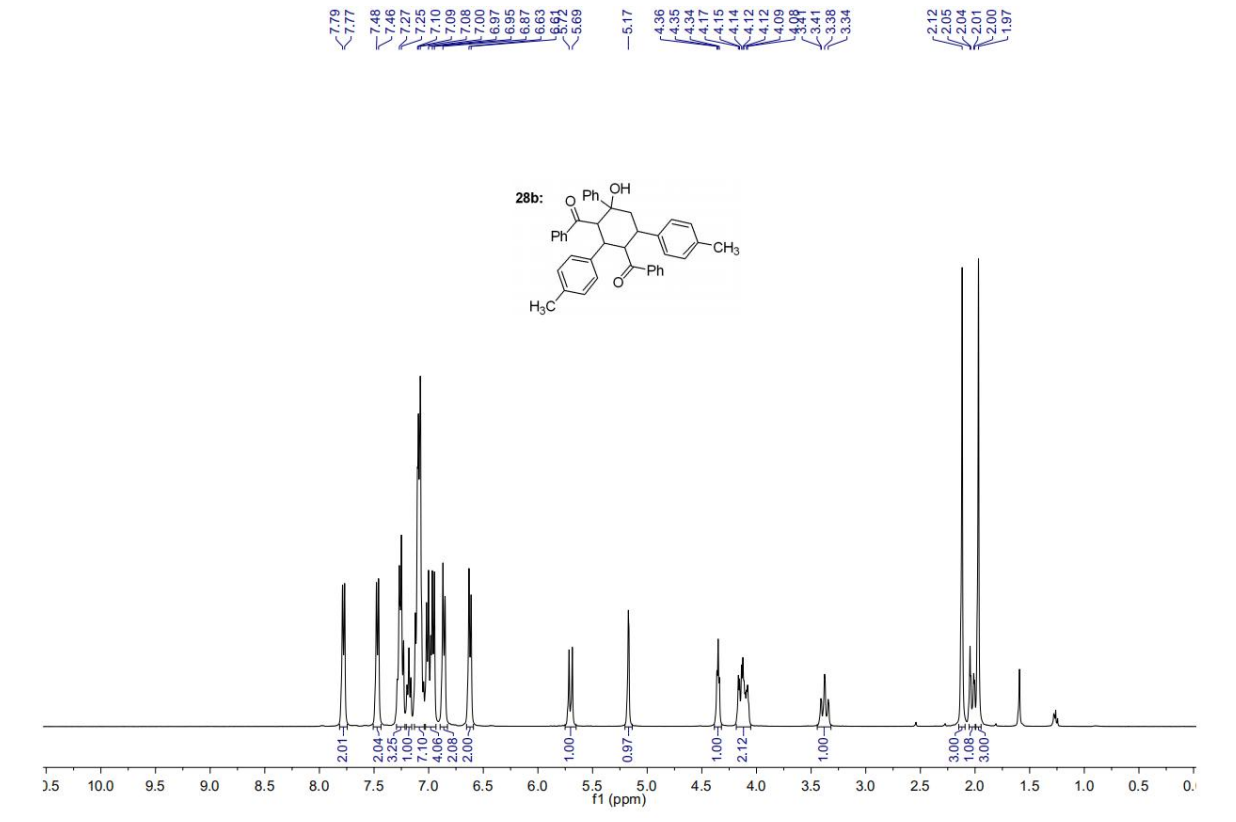

-115.45
27b:
f1 (ppm)

7.83
7.81
7.50
7.48
7.29
7.24
7.22
7.20
7.19
7.15
7.13
7.11
7.09
7.03
7.01
7.00
6.84
5.76
5.73
5.24
4.40
4.23
4.20
4.16
3.47
3.44
3.41
2.10
2.07


28a:

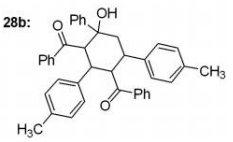

2.00
2.05
3.31
3.08
9.01
3.01
3.06
0.99
0.89
0.98
2.04
1.00
1.00
f1 (ppm)

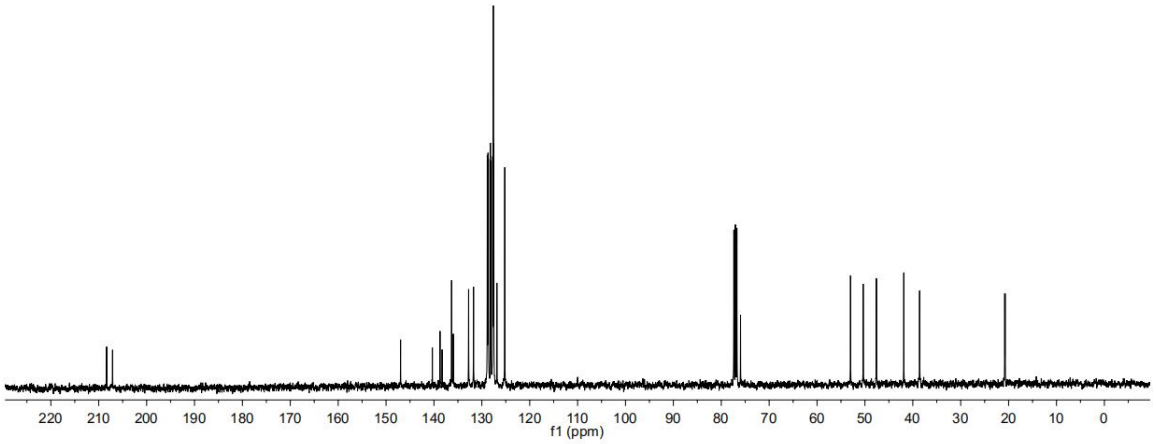

208.29
206.84
146.87
141.69
140.19
139.27
138.28
132.87
131.93
128.78
128.24
128.17
128.07
127.80
127.74
127.68
127.40
126.93
126.59
125.19
77.35
77.04
76.72
75.95
52.76
50.18
48.06
42.24
38.38
28a:
Ph
Ph
O
Ph
Ph
O
Ph
OH
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.79
7.77
7.48
7.46
7.27
7.25
7.10
7.09
7.08
7.00
6.97
6.95
6.87
6.63
6.61
5.72
5.69
5.17
4.36
4.35
4.34
4.17
4.15
4.14
4.12
4.12
4.09
4.08
3.41
3.38
3.34
2.12
2.05
2.04
2.01
2.00
1.97
28b:
Ph
OH
O
Ph
CH3
O
Ph
H3C
2.01
2.04
3.25
1.00
7.10
4.06
2.08
2.00
1.00
0.97
1.00
2.12
1.00
3.00
1.08
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (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
77.37
77.05
76.74
75.97
53.01
50.36
47.60
41.88
38.59
20.81
20.71

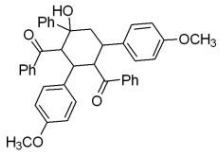
28b:

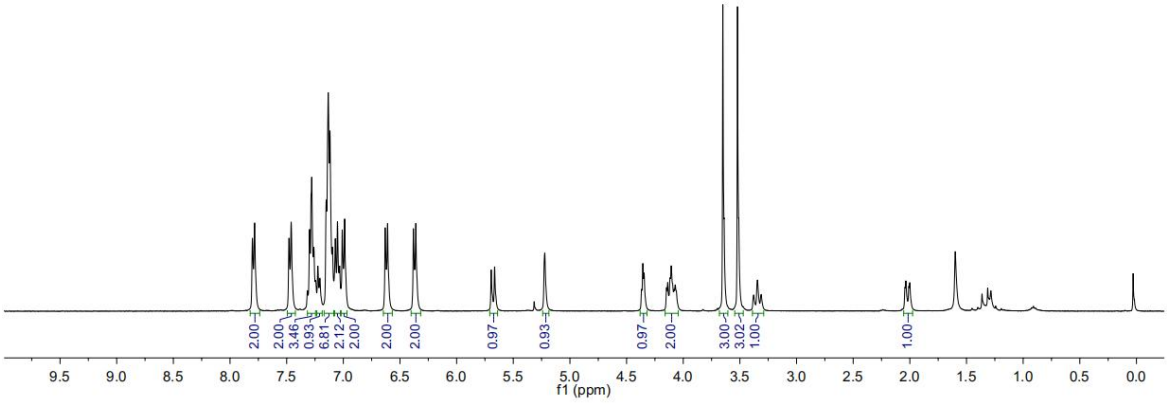

Ph
OH
O
Ph
CH3
O
Ph
H3C


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.80
7.78
7.28
7.15
7.13
7.12
7.05
6.63
6.61
6.38
6.36
5.69
5.66
5.22
4.37
4.36
4.35
4.15
4.14
4.12
4.11
4.08
3.65
3.52
3.38
3.35
3.31
2.04
2.04
2.01
2.00

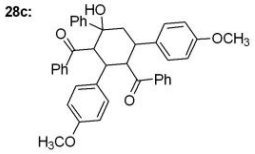
28c:

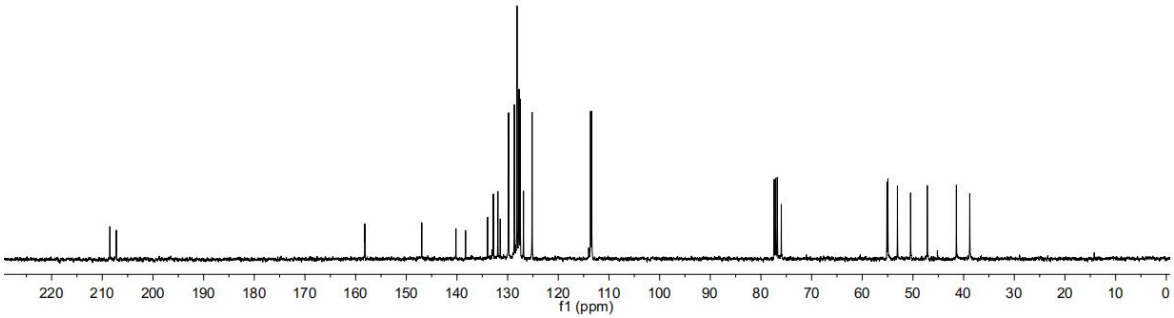

HO
Ph
O
Ph
OCH3
O
Ph
H3CO


2.00
2.00
3.46
0.93
6.81
2.12
2.00
2.00
2.00
0.97
0.93
0.97
2.00
3.00
3.02
1.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


208.50
207.23
158.20
158.13
146.95
131.92
129.81
128.67
128.14
127.80
127.74
127.50
126.67
113.41
77.40
77.08
76.76
75.98
55.14
54.95
53.06
50.47
47.17
41.43
38.79

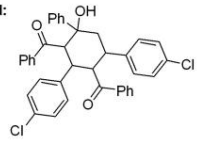
28c:

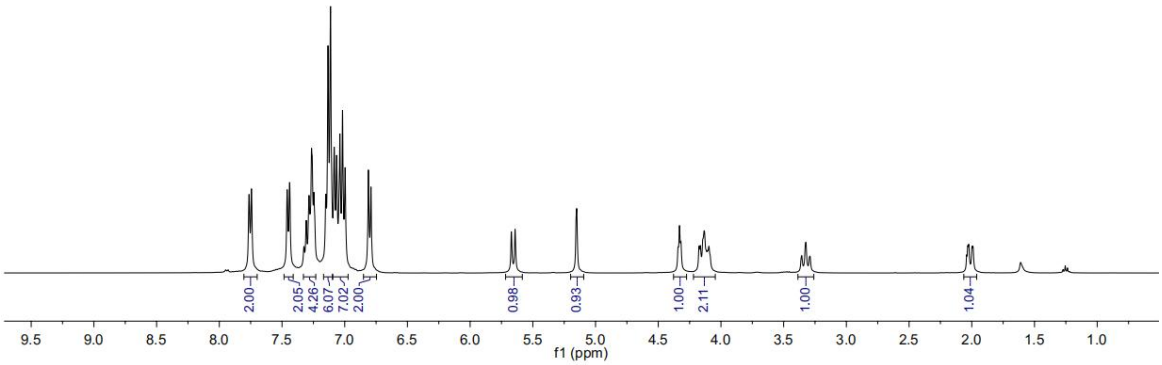

HO
Ph
O
Ph
OCH3
Ph
O
H3CO


220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.76
7.74
7.46
7.44
7.28
7.26
7.25
7.15
7.13
7.11
7.08
7.06
7.04
7.02
7.00
6.81
5.64
5.15
4.34
4.33
4.32
4.17
4.16
4.13
4.11
4.10
3.36
3.32
3.29
2.04
2.03
2.02
2.00
1.99

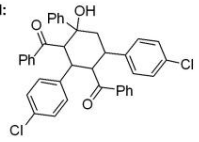
28d:

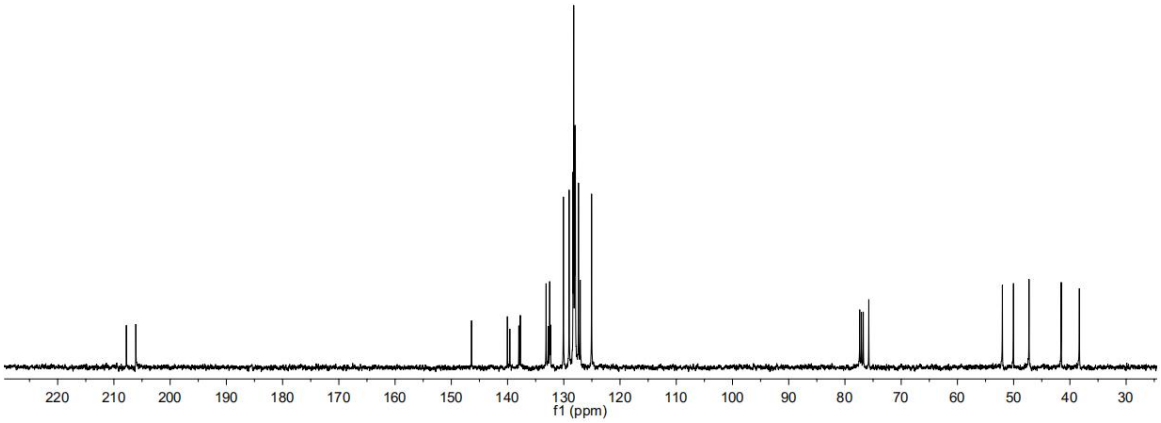

Ph
OH
O
Ph
Cl
Ph
O
Cl


2.00
2.05
4.26
6.07
7.02
2.00
0.98
0.93
1.00
2.11
1.00
1.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (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
77.38
77.06
76.74
75.76
52.01
50.04
47.27
41.54
38.32

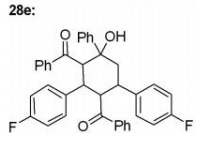
28d:

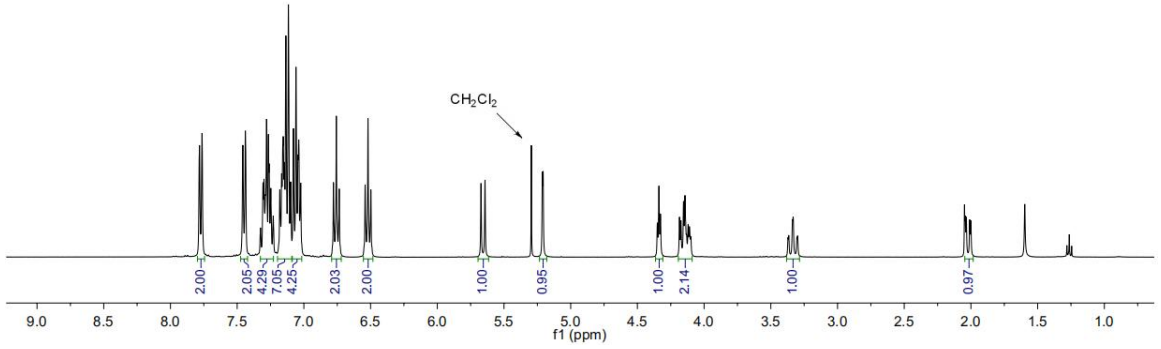


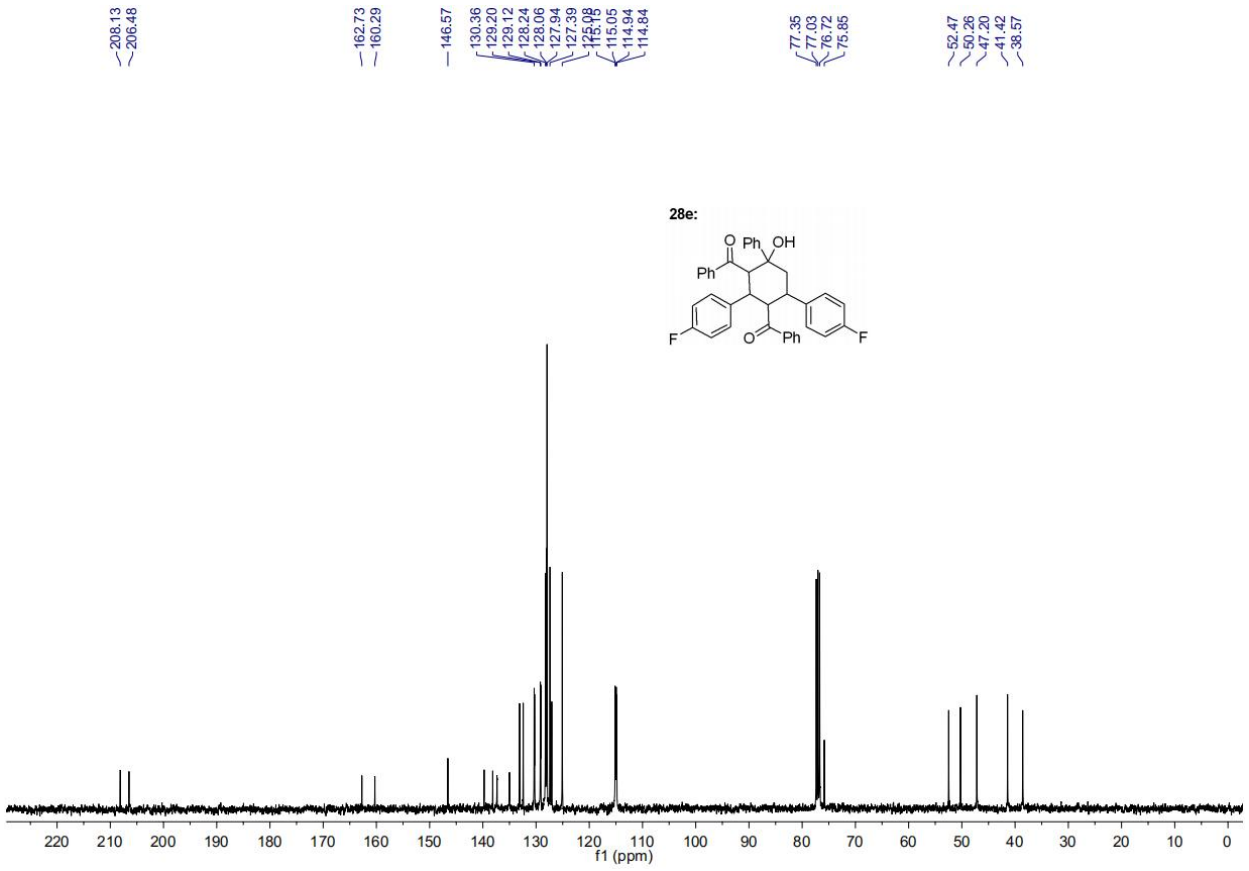


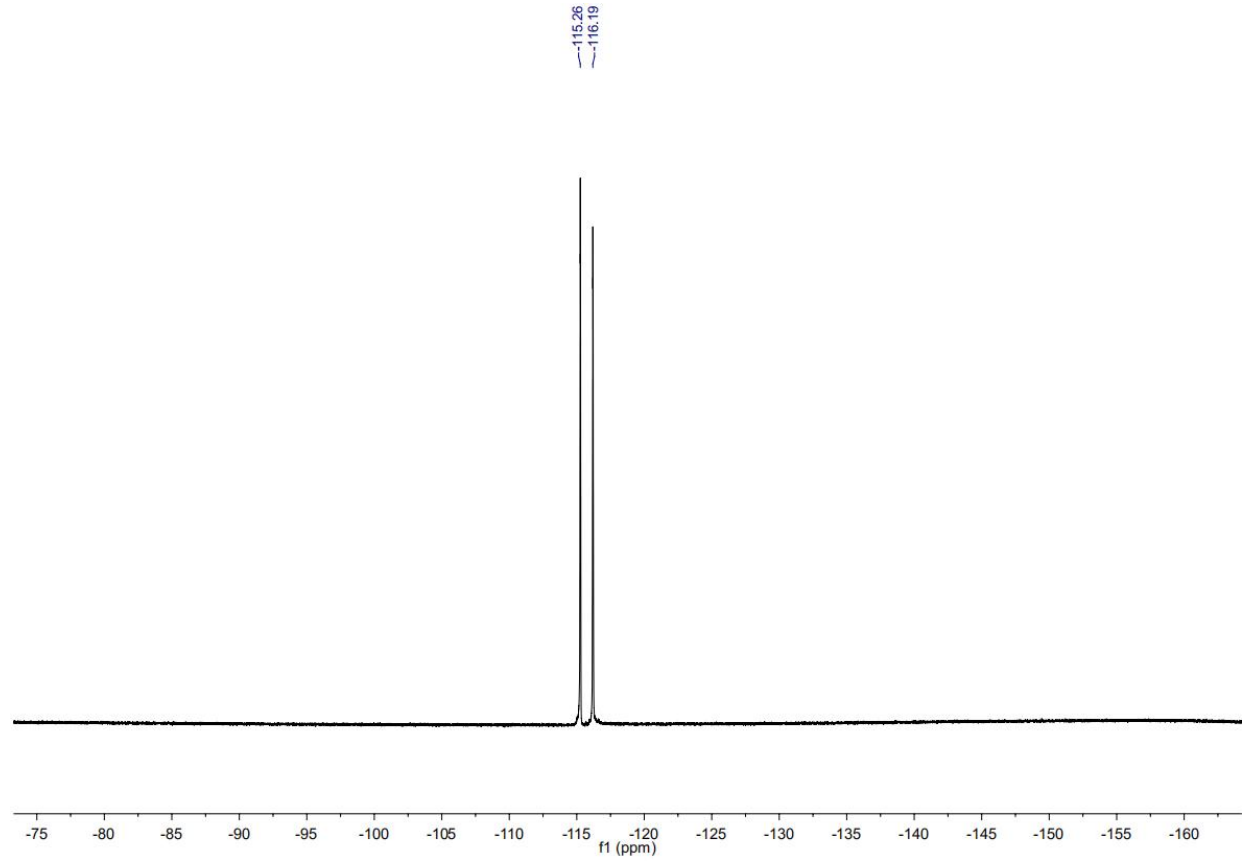
7.78
7.76
7.44
7.28
7.13
7.12
7.08
6.78
6.76
6.73
6.54
6.52
6.50
5.67
5.64
5.21
5.21
4.35
4.34
4.33
4.18
4.17
4.15
4.14
4.13
4.12
4.11
4.10
3.37
3.37
3.34
3.33
3.30
3.30
2.04
2.03
2.01
2.00

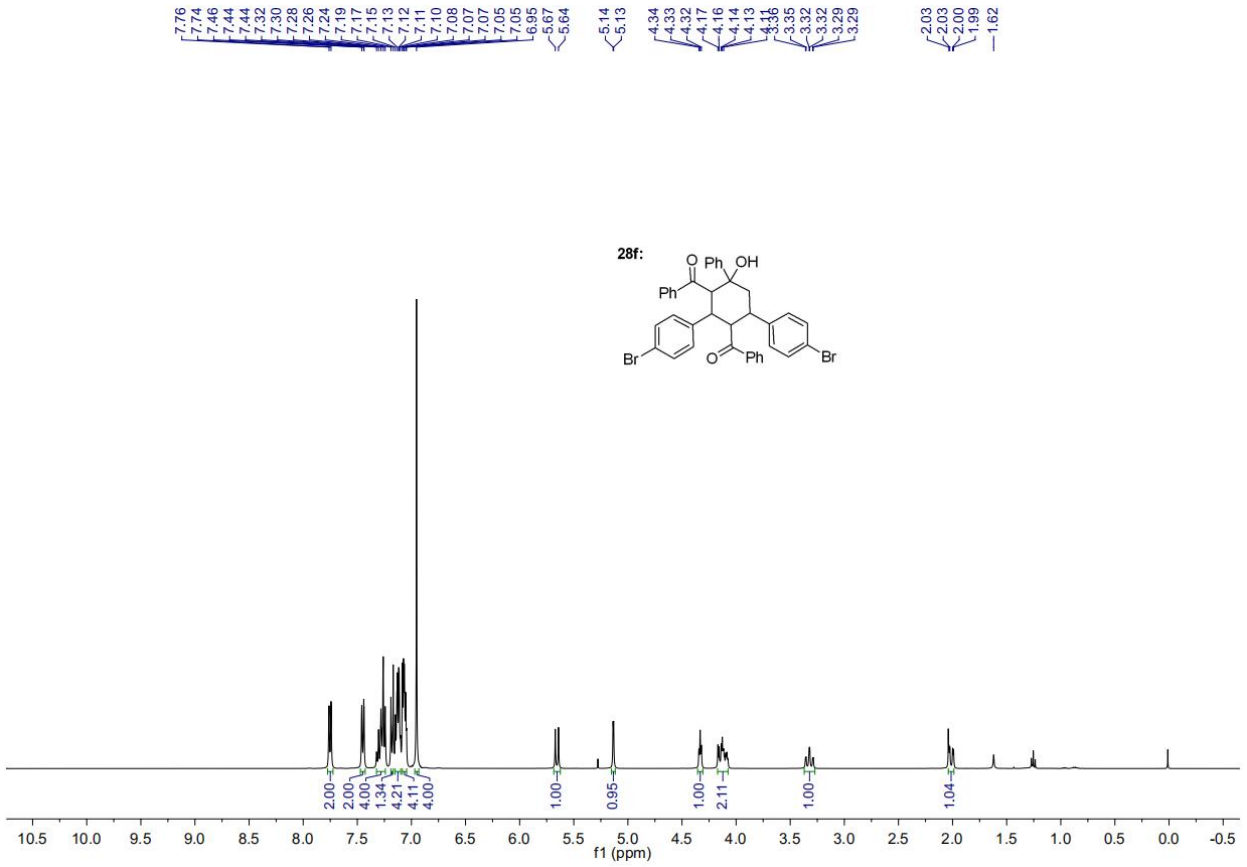
28e:

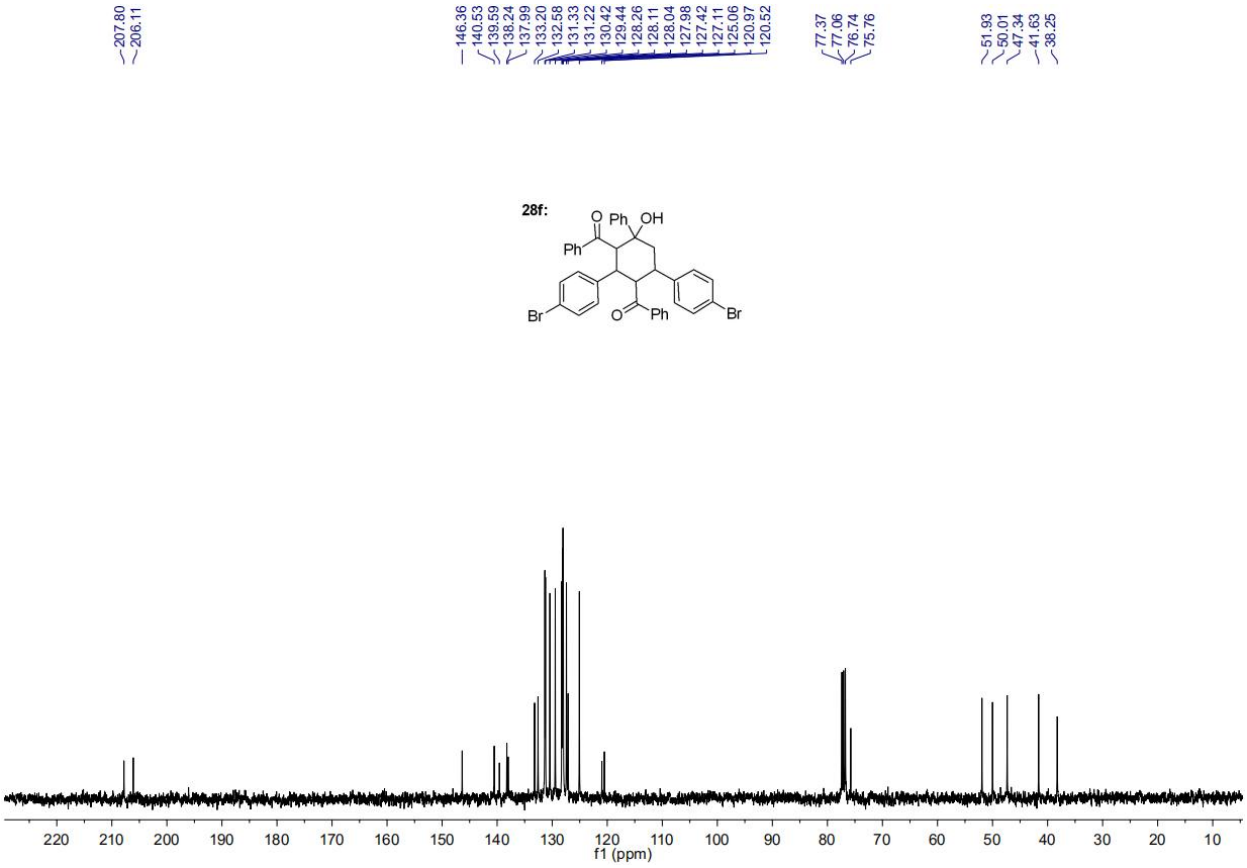


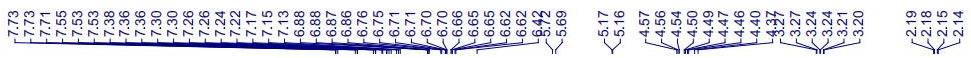



208.13
206.48
162.73
160.29
146.57
130.36
129.20
129.12
128.24
128.06
127.94
127.39
125.08
115.15
115.05
114.94
114.84
77.35
77.03
76.72
75.85
52.47
50.26
47.20
41.42
38.57
28e:
O
Ph
OH
Ph
F
O
Ph
F
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

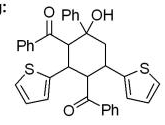

-115.26
-116.19
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

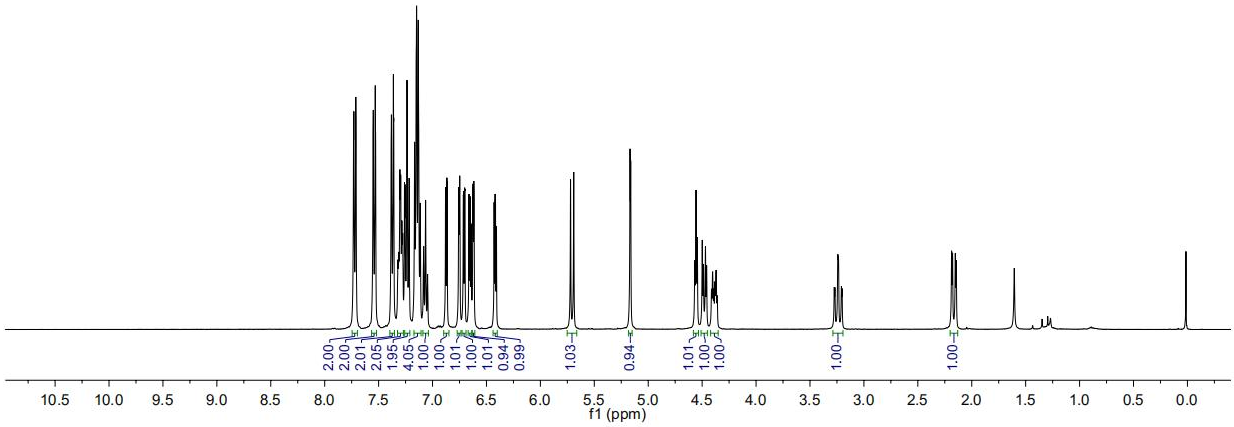

28f:
Ph
OH
O
Ph
Br
O
Ph
Br
2.00
2.00
4.00
1.34
4.21
4.11
4.00
1.00
0.95
1.00
2.11
1.00
1.04
f1 (ppm)


28f:
Ph
OH
O
Ph
Br
O
Ph
Br
f1 (ppm)

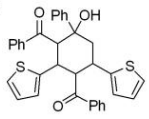


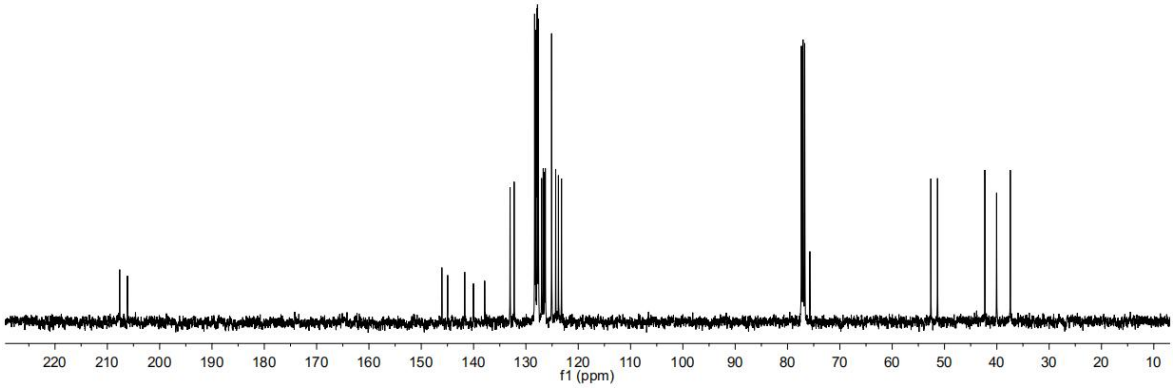
28g:





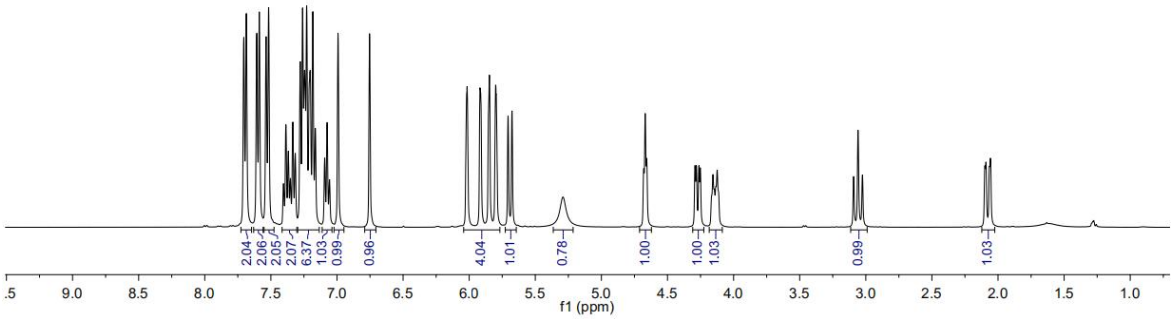
28g:





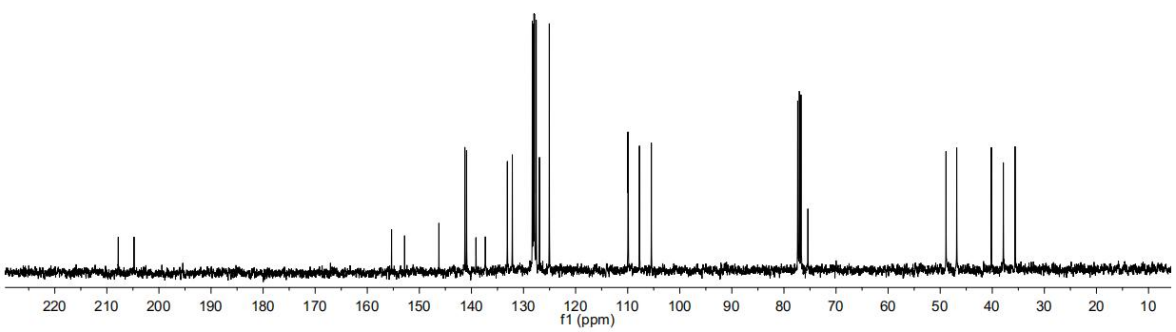

7.71
7.69
7.61
7.59
7.54
7.52
7.39
7.37
7.35
7.33
7.32
7.28
7.26
7.24
7.23
7.21
7.21
7.20
7.18
7.16
7.09
7.07
6.02
6.01
5.92
5.91
5.91
5.85
5.85
5.80
5.79
5.71
5.68
4.68
4.67
4.66
4.29
4.28
4.26
4.25
4.16
4.15
4.13
4.12
3.09
3.06
3.03
2.10
2.09
2.06
2.06

28h:

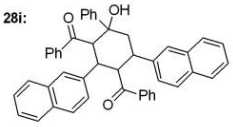

2.04
2.06
2.05
2.07
6.37
1.03
0.99
0.96
4.04
1.01
0.78
1.00
1.00
1.03
0.99
1.03
f1 (ppm)

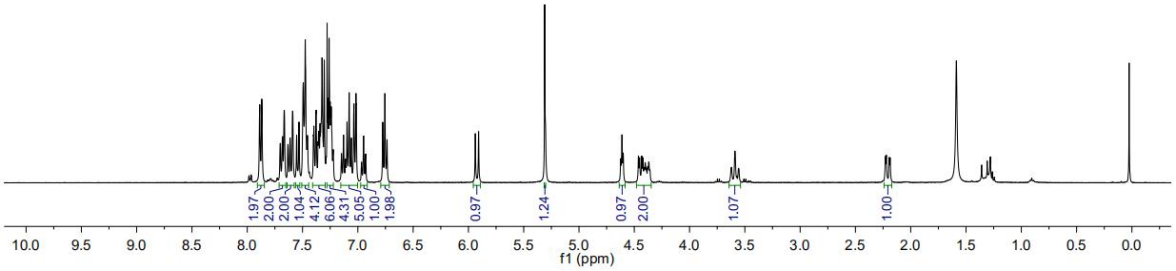

207.81
204.78
155.34
152.84
146.25
141.26
140.93
137.34
133.10
132.15
128.32
128.14
127.99
127.90
127.57
126.94
109.89
107.75
105.46
77.36
77.05
76.73
75.40
48.88
46.83
40.18
37.87
35.62

28h:

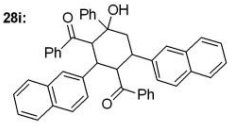

f1 (ppm)

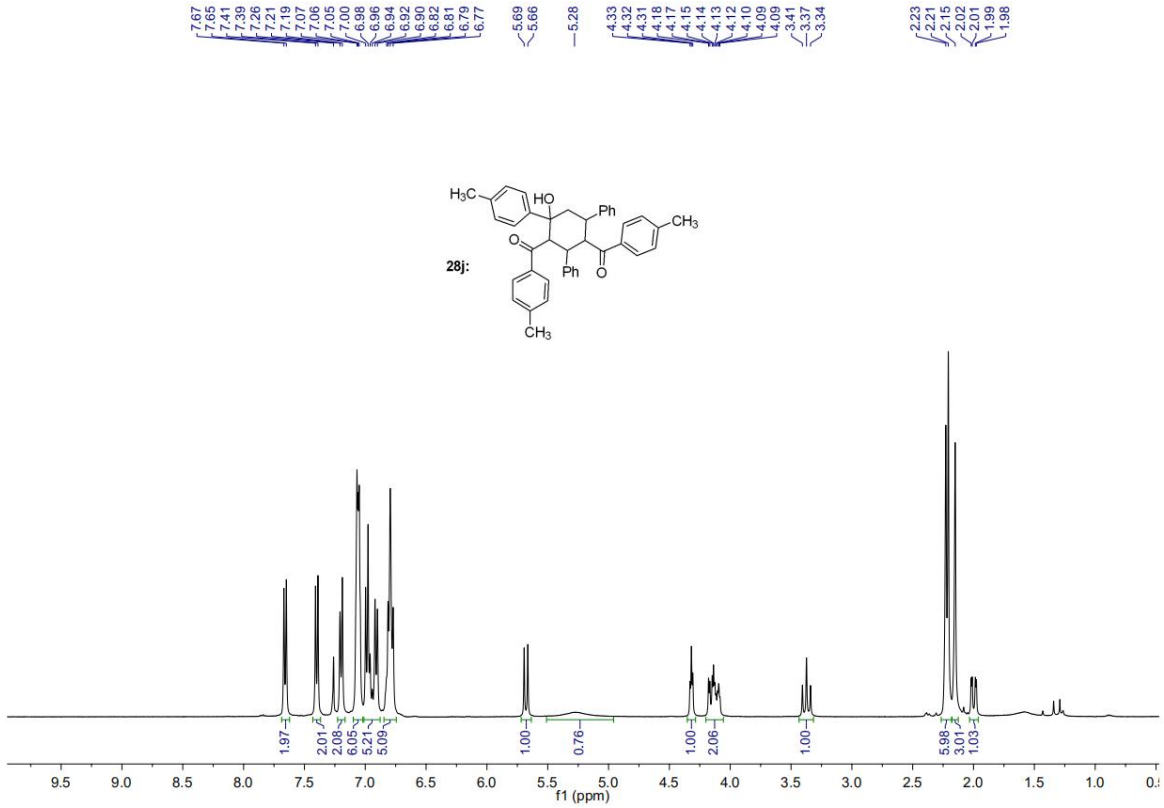
28i:

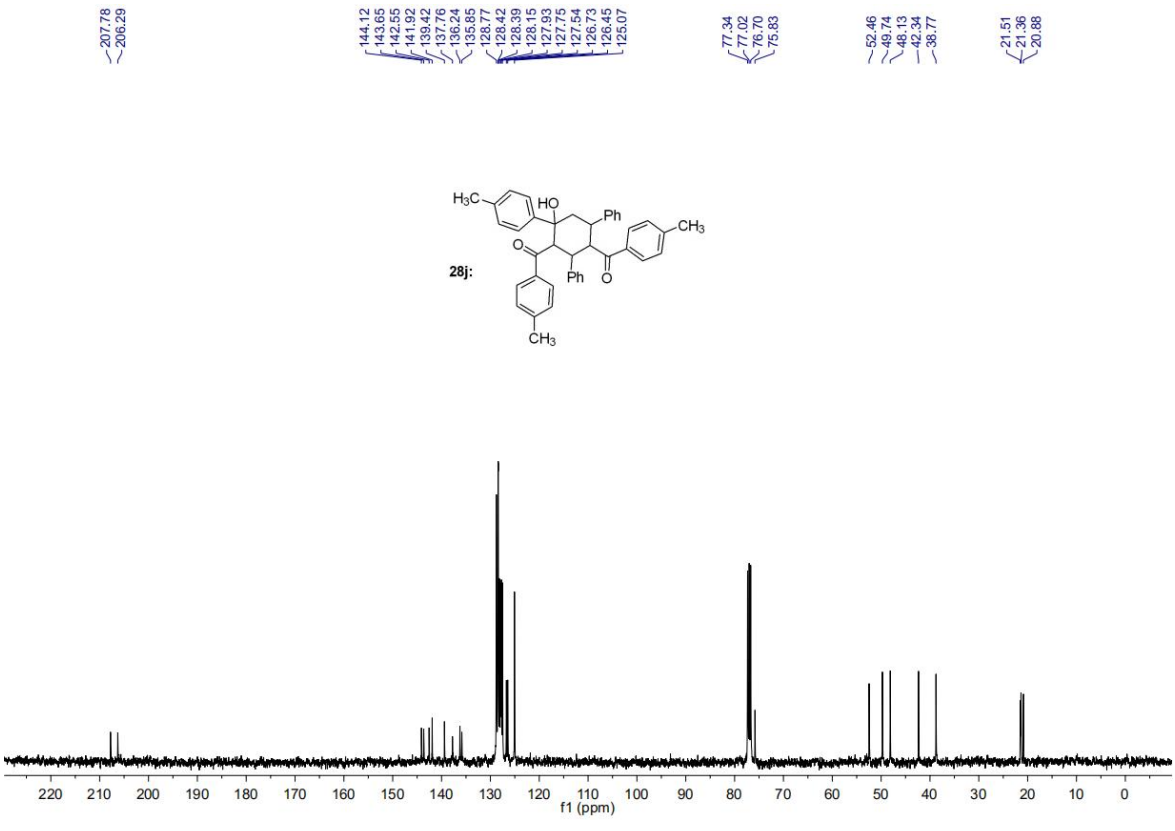


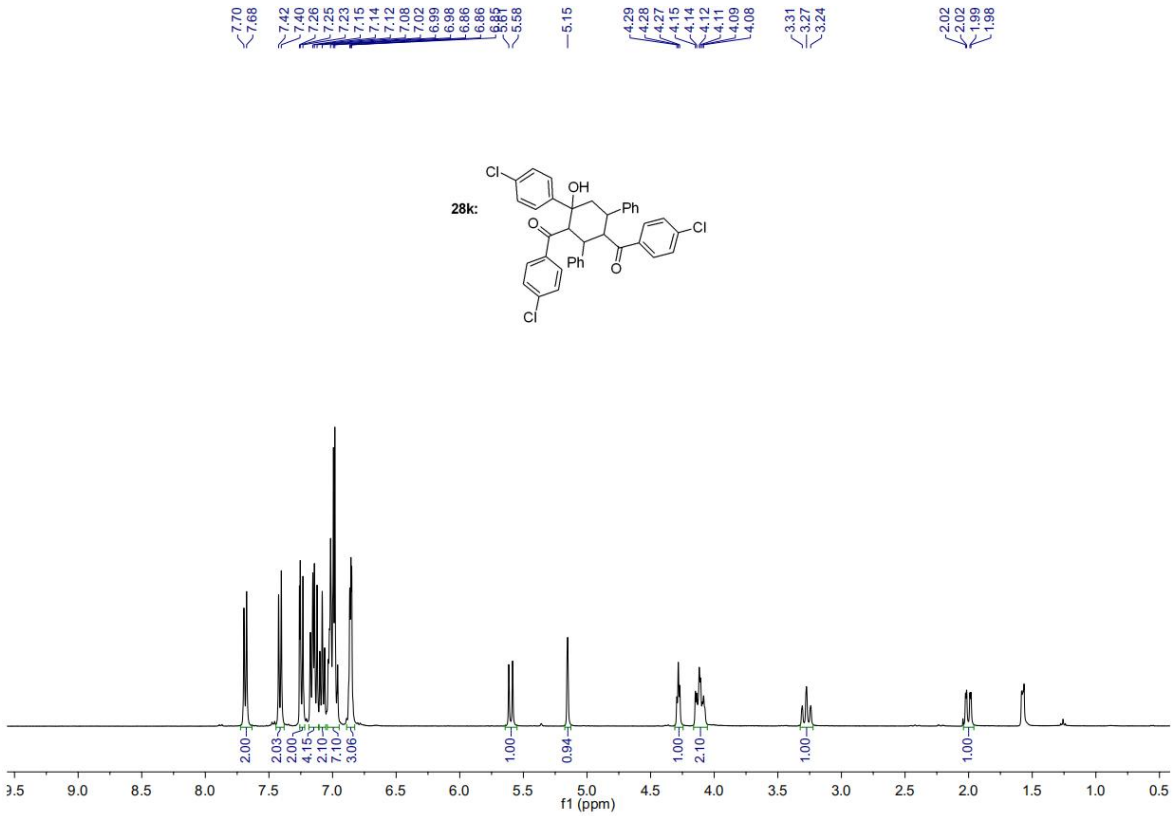


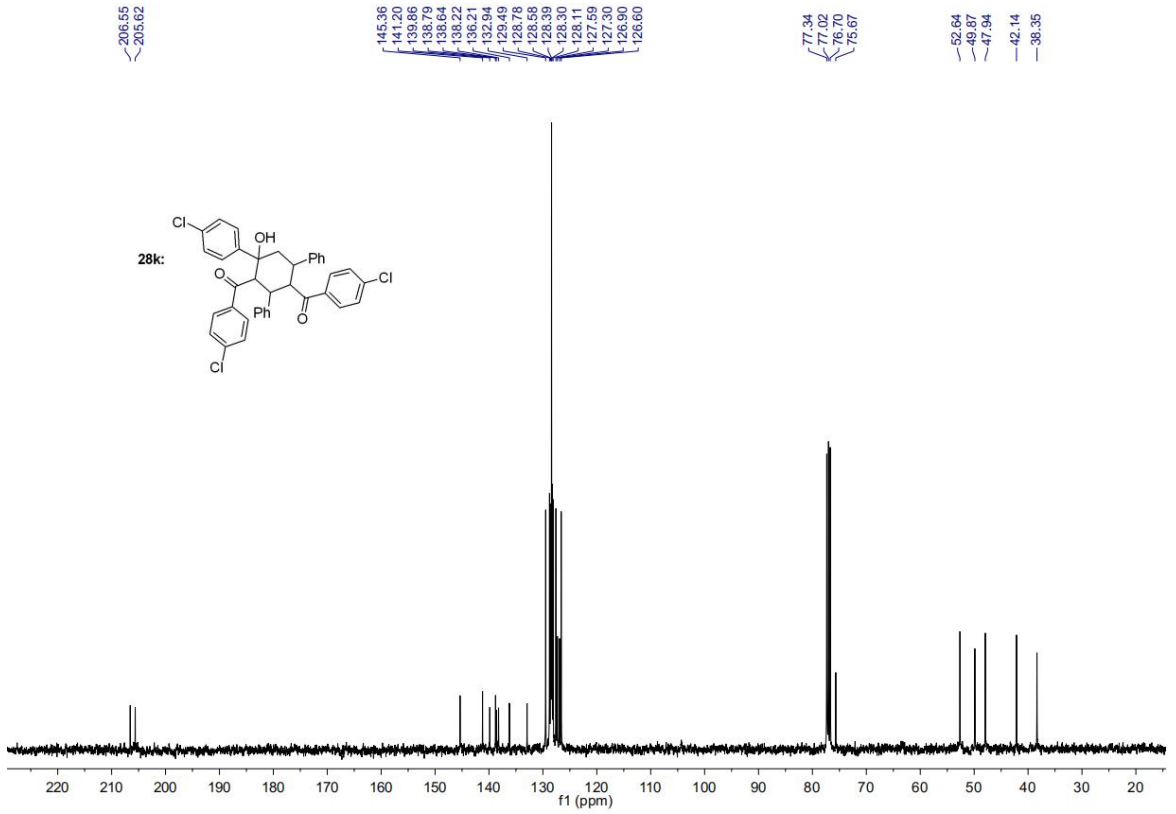
28i:

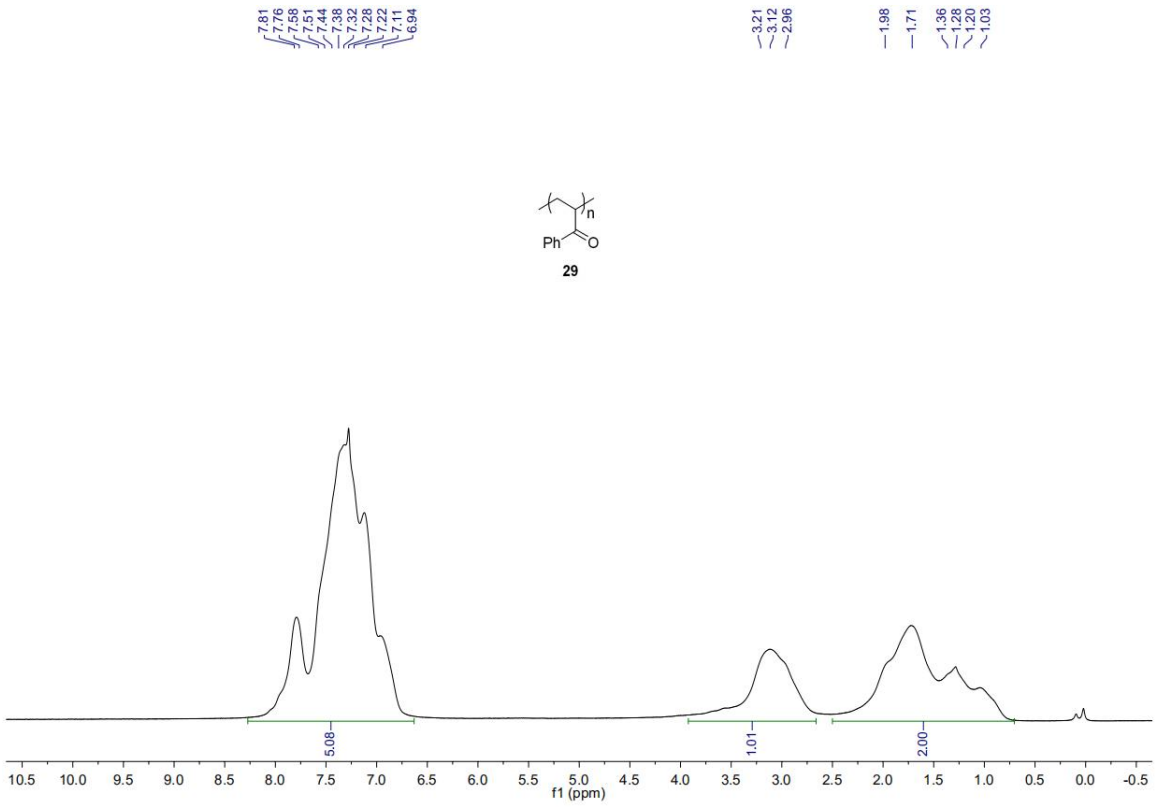


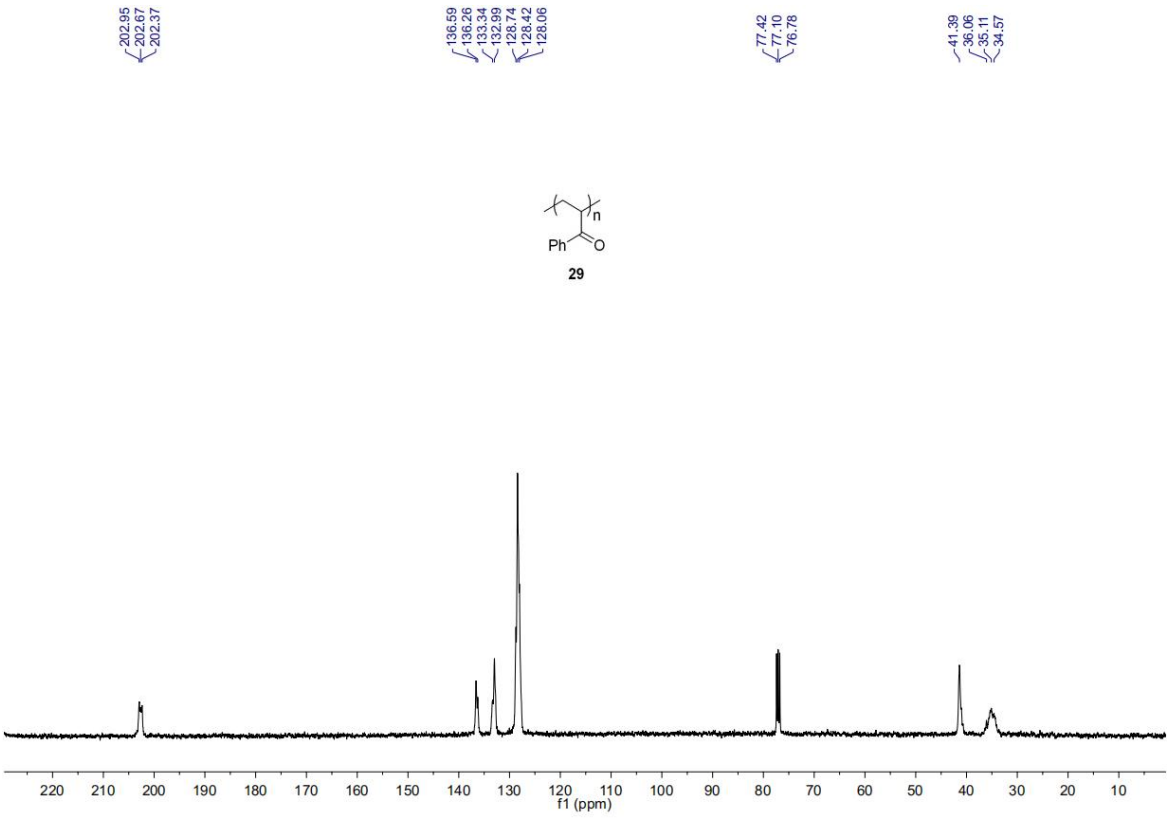

7.67
7.65
7.41
7.39
7.26
7.21
7.19
7.07
7.06
7.05
7.00
6.98
6.96
6.94
6.92
6.90
6.82
6.81
6.79
6.77
5.69
5.66
5.28
4.33
4.32
4.31
4.18
4.17
4.15
4.14
4.13
4.12
4.10
4.09
4.09
3.41
3.37
3.34
2.23
2.21
2.15
2.02
2.01
1.99
1.98
H3C
HO
Ph
CH3
O
28j:
Ph
O
CH3
1.97
2.01
2.08
6.05
5.21
5.09
1.00
0.76
1.00
2.06
1.00
5.98
3.01
1.03
f1 (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
77.34
77.02
76.70
75.83
52.46
49.74
48.13
42.34
38.77
21.51
21.36
20.88
H3C
HO
Ph
CH3
O
28j:
Ph
O
CH3
f1 (ppm)


28k:
Cl
OH
Ph
O
Ph
Cl
O
Cl
f1 (ppm)

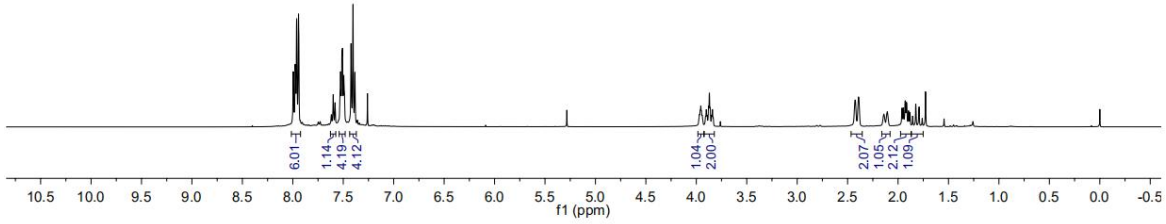

28k:
Cl
OH
Ph
O
Ph
Cl
O
Cl
f1 (ppm)


7.81
7.76
7.58
7.51
7.44
7.38
7.32
7.28
7.22
7.11
6.94
3.21
3.12
2.96
1.98
1.71
1.36
1.28
1.20
1.03
n
Ph
O
29
5.08
1.01
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


202.95
202.67
202.37
136.59
136.26
133.34
132.99
128.74
128.42
128.06
77.42
77.10
76.78
41.39
36.06
35.11
34.57
n
Ph
O
29
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

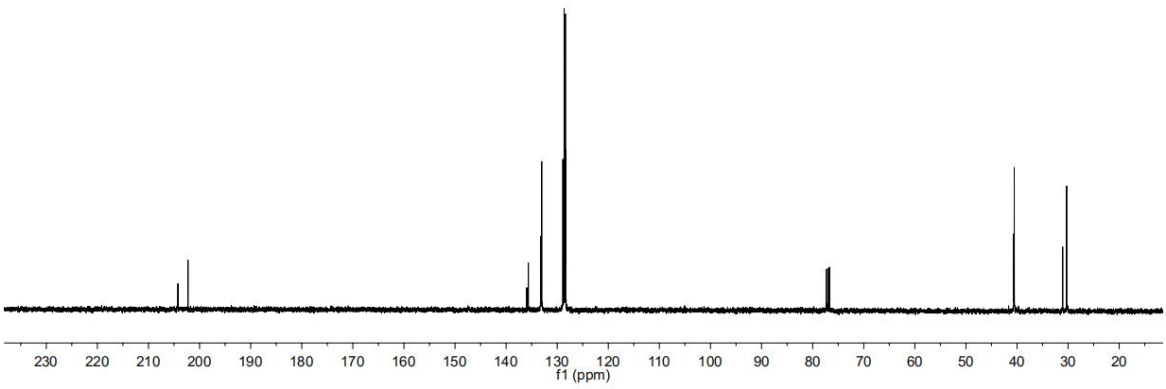

8.00
7.98
7.96
7.94
7.62
7.60
7.58
7.53
7.51
7.51
7.49
7.42
7.40
7.38
3.97
3.96
3.96
3.95
3.94
3.91
3.90
3.89
3.88
3.87
3.86
3.85
3.84
3.83
2.43
2.39
2.14
2.11
1.96
1.95
1.93
1.92
1.90
1.88
1.86
1.82
1.79
1.76

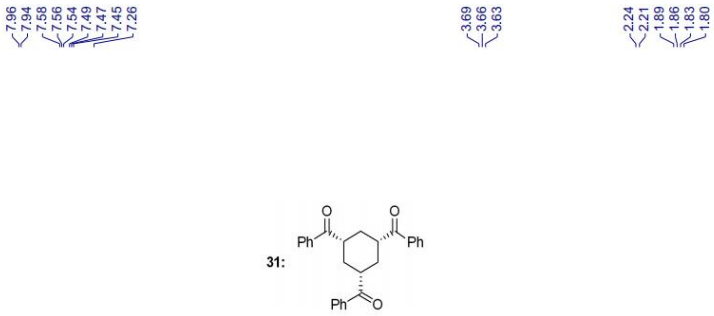
30:

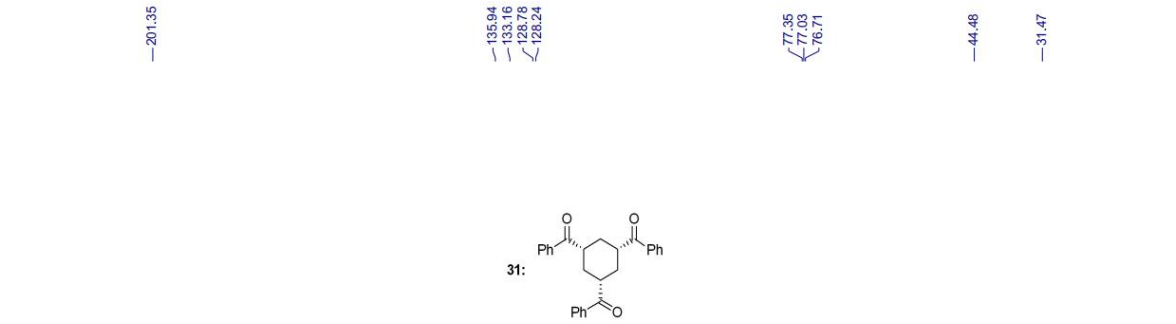

6.01
1.14
4.19
4.12
1.04
2.00
2.07
1.05
2.12
1.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


204.24
202.26
135.95
135.65
133.22
133.03
128.89
128.65
128.39
128.34
77.35
77.03
76.71
40.64
40.54
31.06
30.29

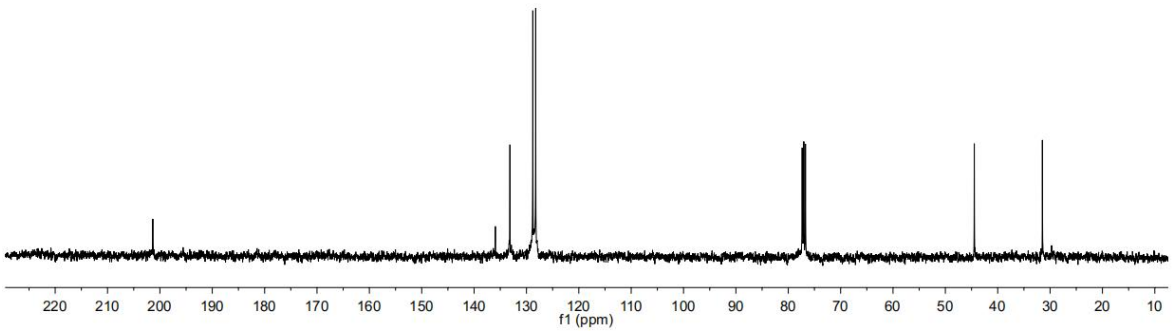
30:


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)


7.96
7.94
7.58
7.56
7.54
7.49
7.47
7.45
7.26
3.69
3.66
3.63
2.24
2.21
1.89
1.86
1.83
1.80
31:
Ph
Ph
Ph
O
O
O
5.85
3.31
6.31
3.00
3.09
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

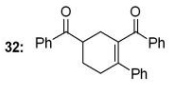

201.35
135.94
133.16
128.78
128.24
77.35
77.03
76.71
44.48
31.47

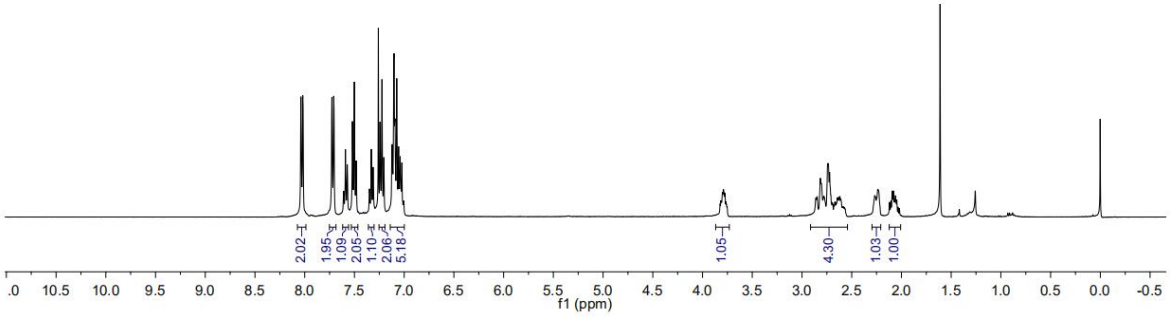
31:
Ph
Ph
Ph
O
O
O


220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.04
8.02
7.73
7.71
7.61
7.59
7.57
7.52
7.50
7.48
7.35
7.33
7.31
7.26
7.24
7.22
7.20
7.12
7.10
7.09
7.07
7.06
7.04
7.03
7.02
7.01
3.82
3.82
3.81
3.80
3.79
3.77
3.77
3.76
3.75
2.82
2.81
2.74
2.74
2.27
2.25
2.24
2.23
2.12
2.11
2.09
2.08
2.07
2.06
2.05
2.05
2.03
2.02

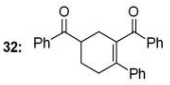
32:

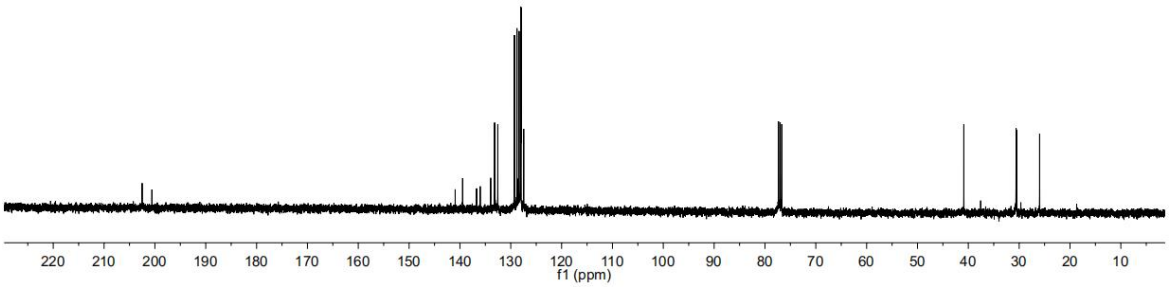

O
O
Ph
Ph
Ph

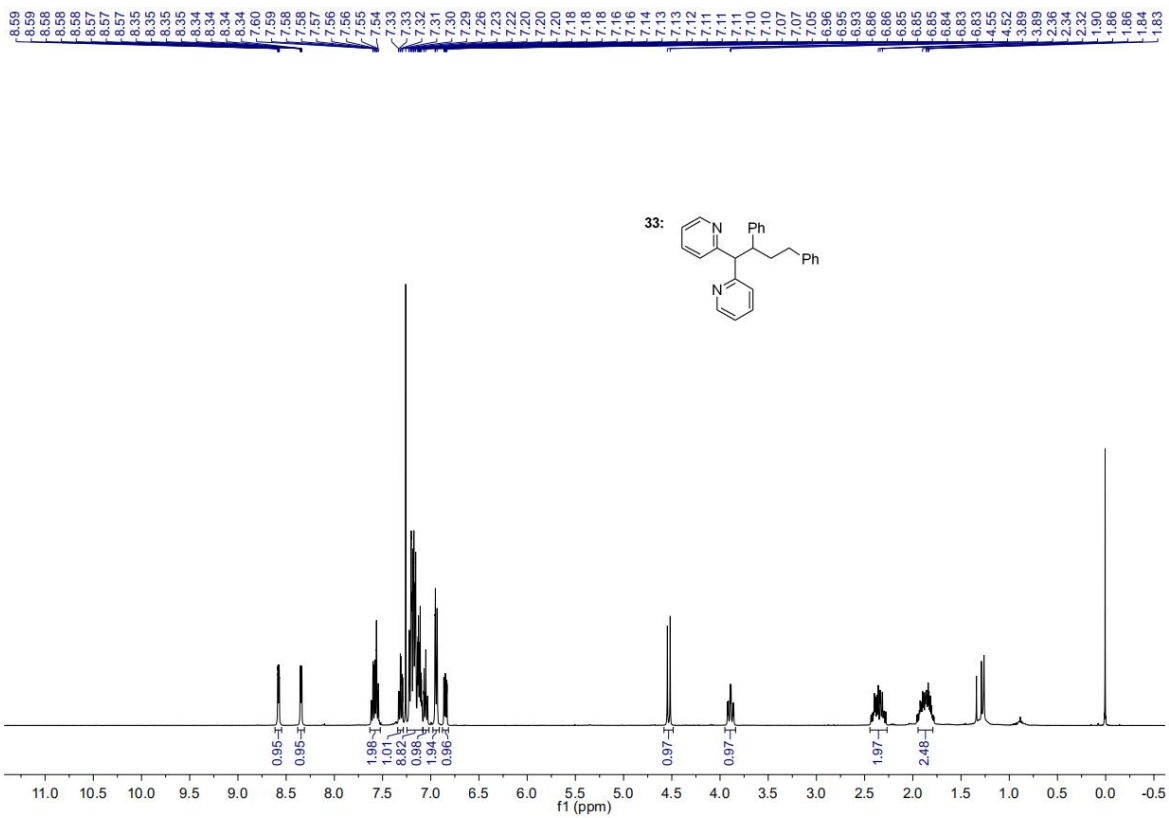

2.02
1.95
1.09
2.05
1.10
2.06
5.18
1.05
4.30
1.03
1.00
.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

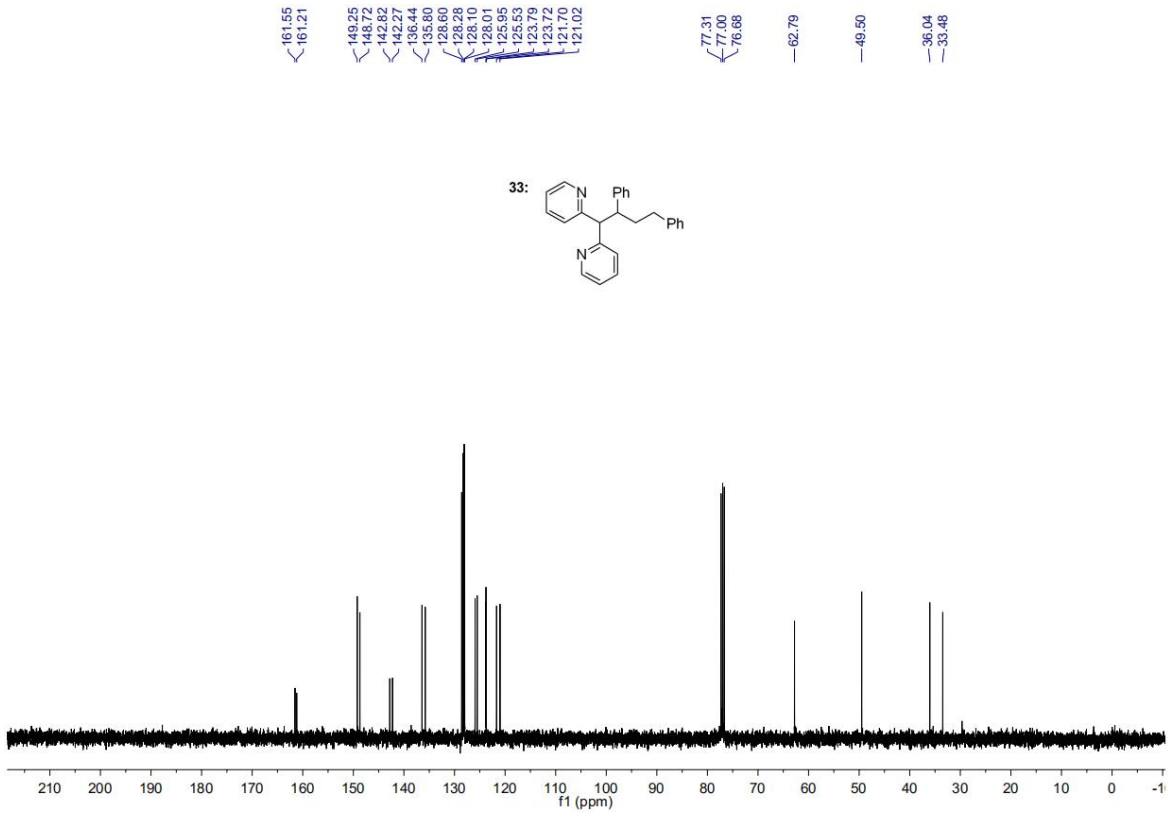

202.51
200.59
140.93
139.47
136.73
136.00
133.95
133.18
132.55
129.27
128.78
128.36
128.02
127.99
127.95
127.45
77.32
77.01
76.69
40.88
30.61
30.48
25.97

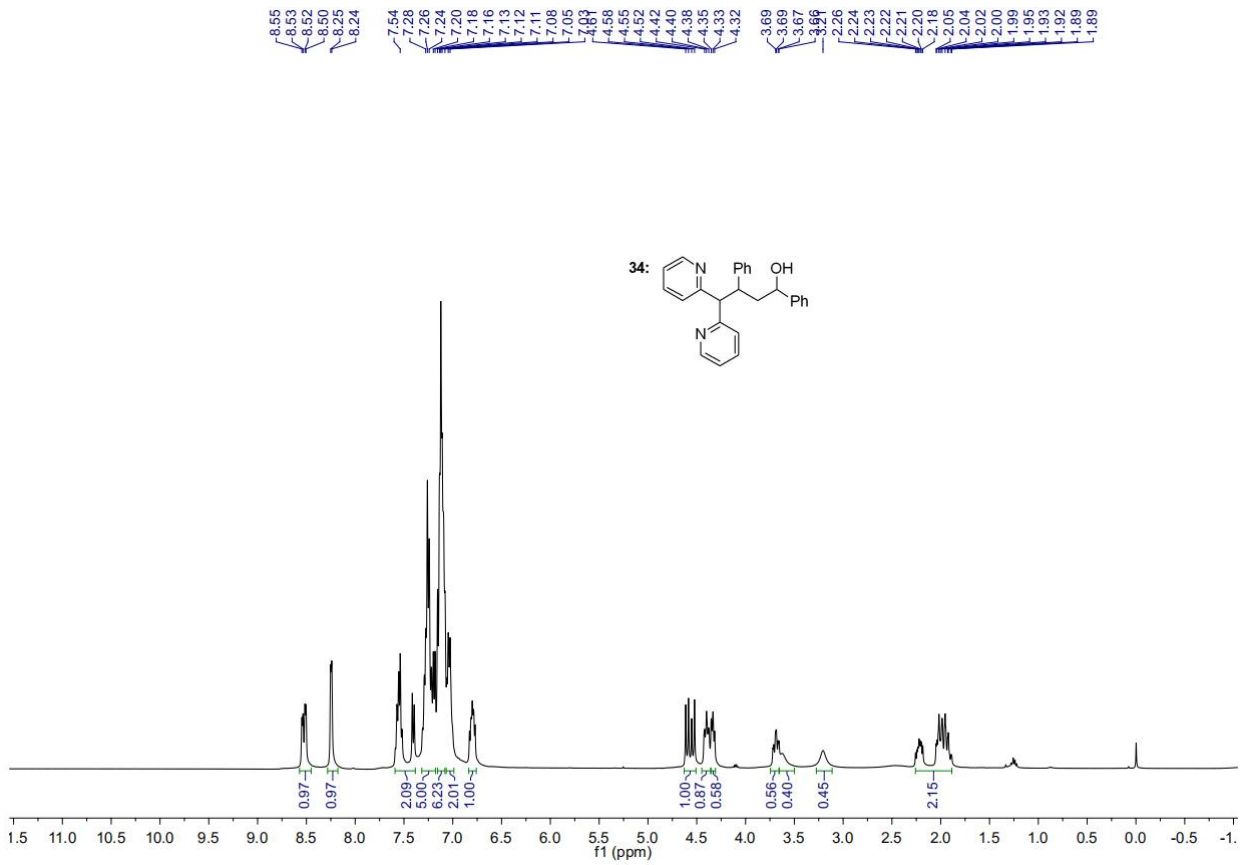
32:

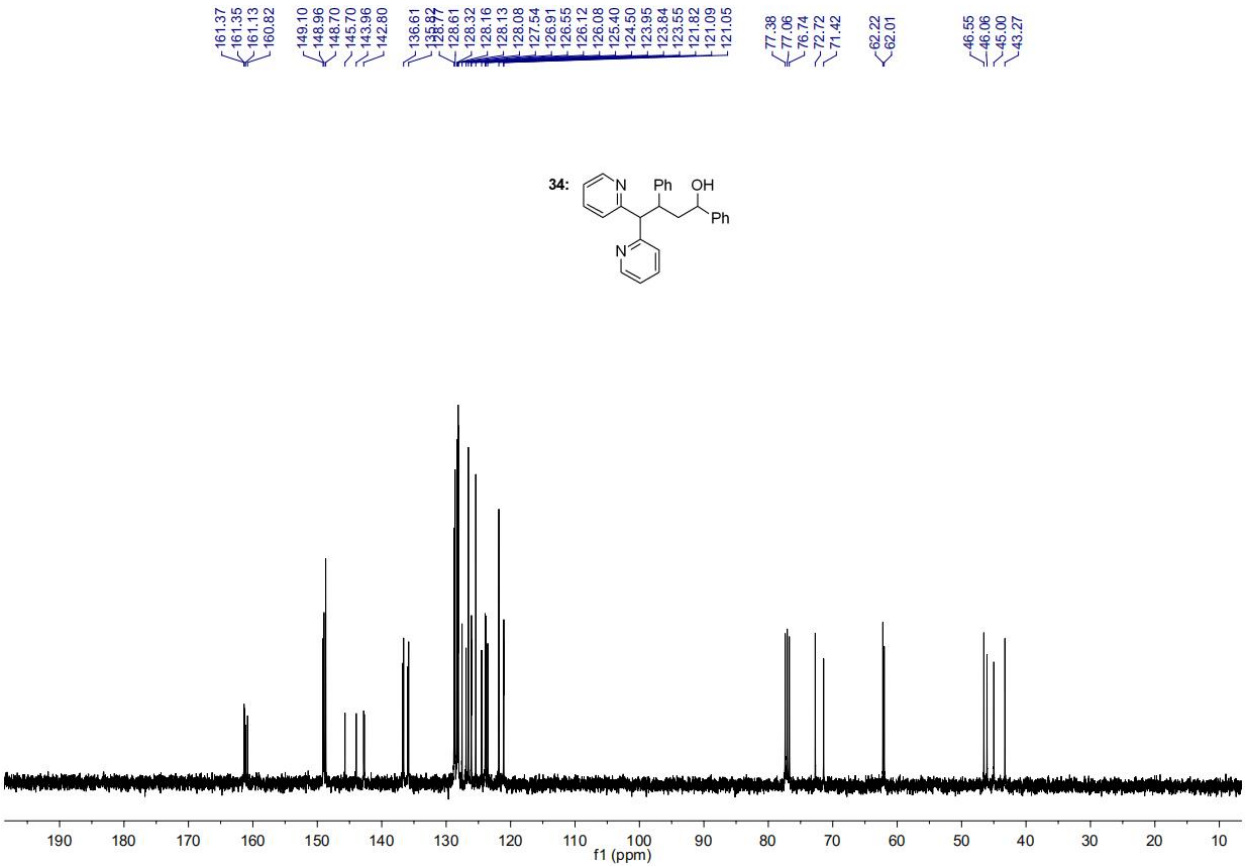

O
O
Ph
Ph
Ph

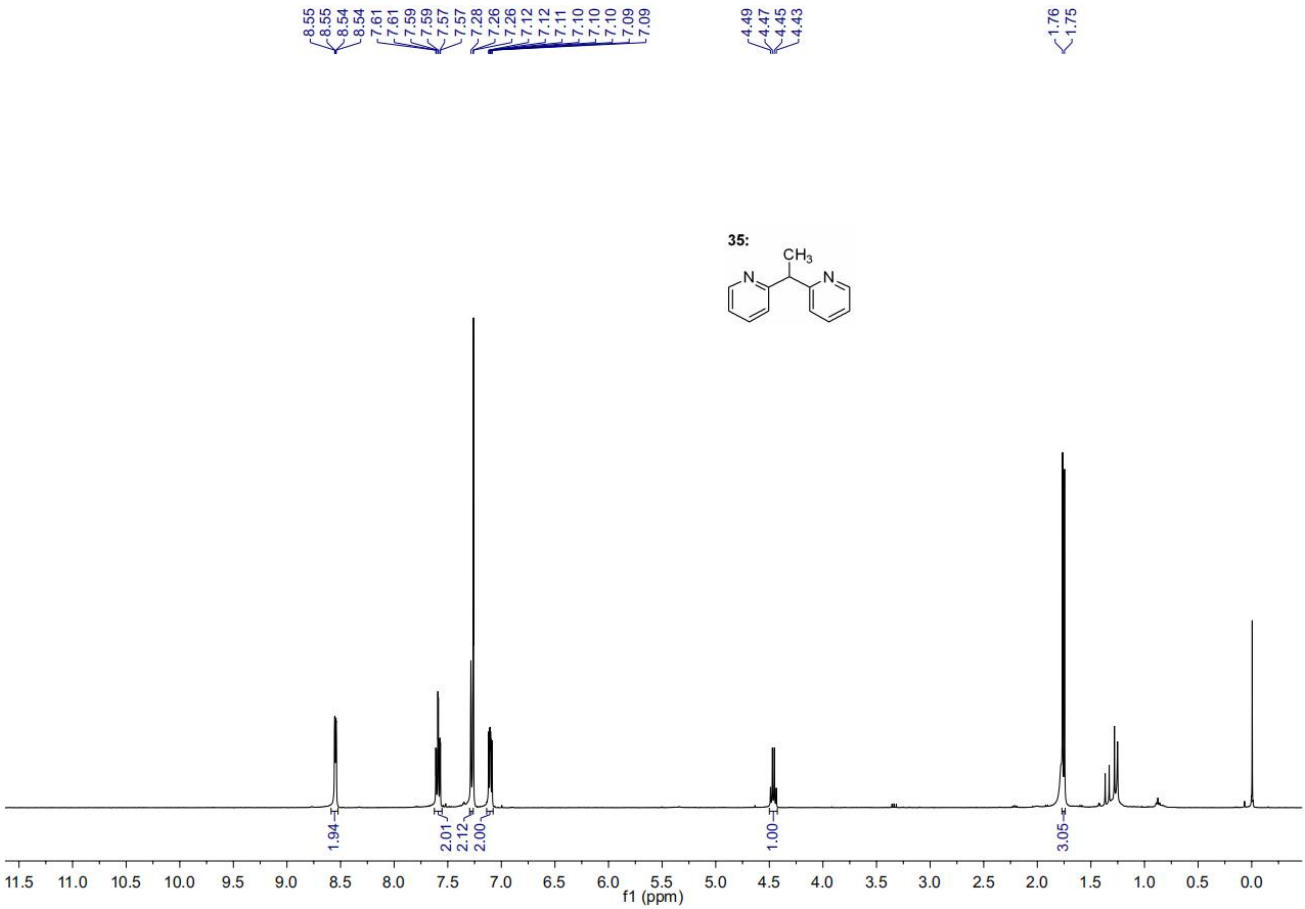

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

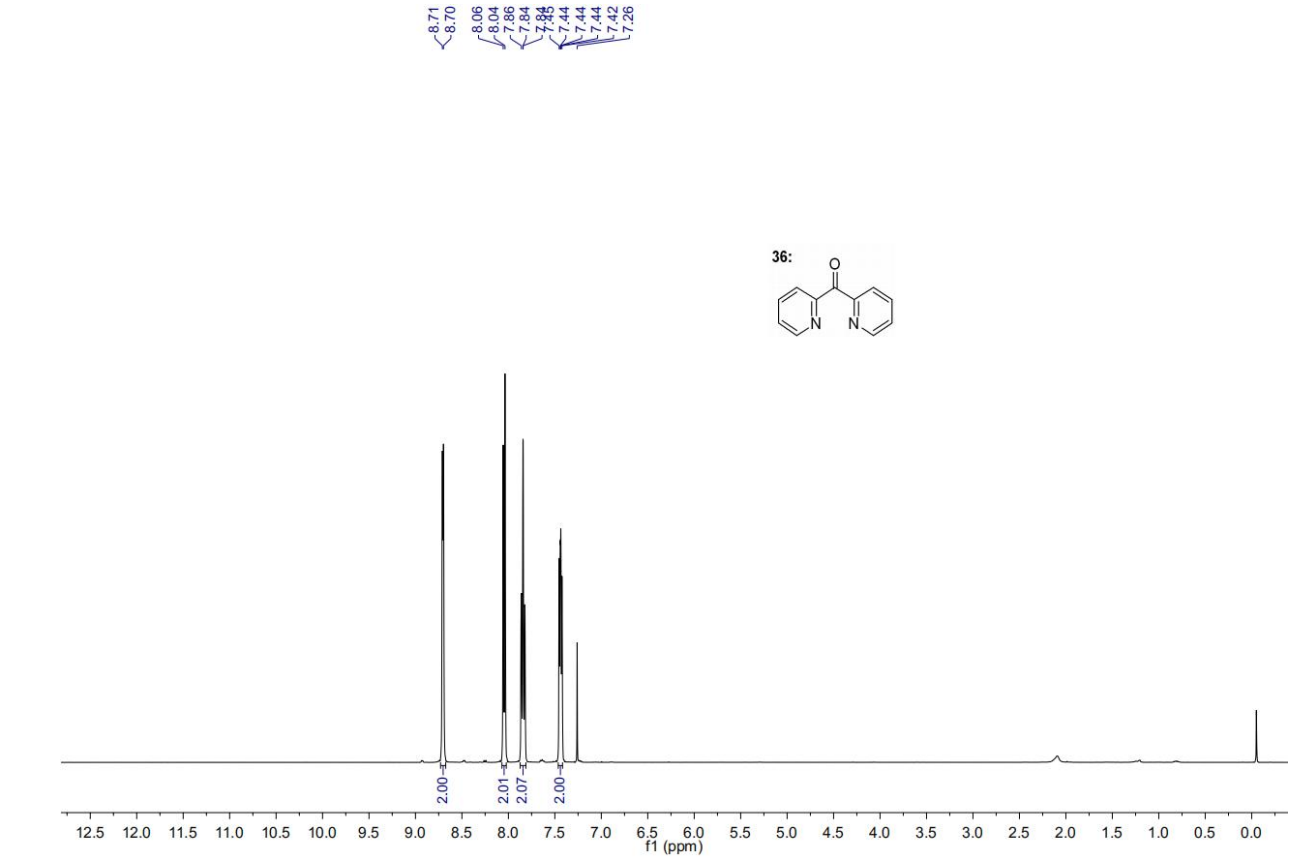

33:
N
Ph
Ph
N
0.95
0.95
1.98
1.01
8.82
0.98
1.94
0.96
0.97
0.97
1.97
2.48
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

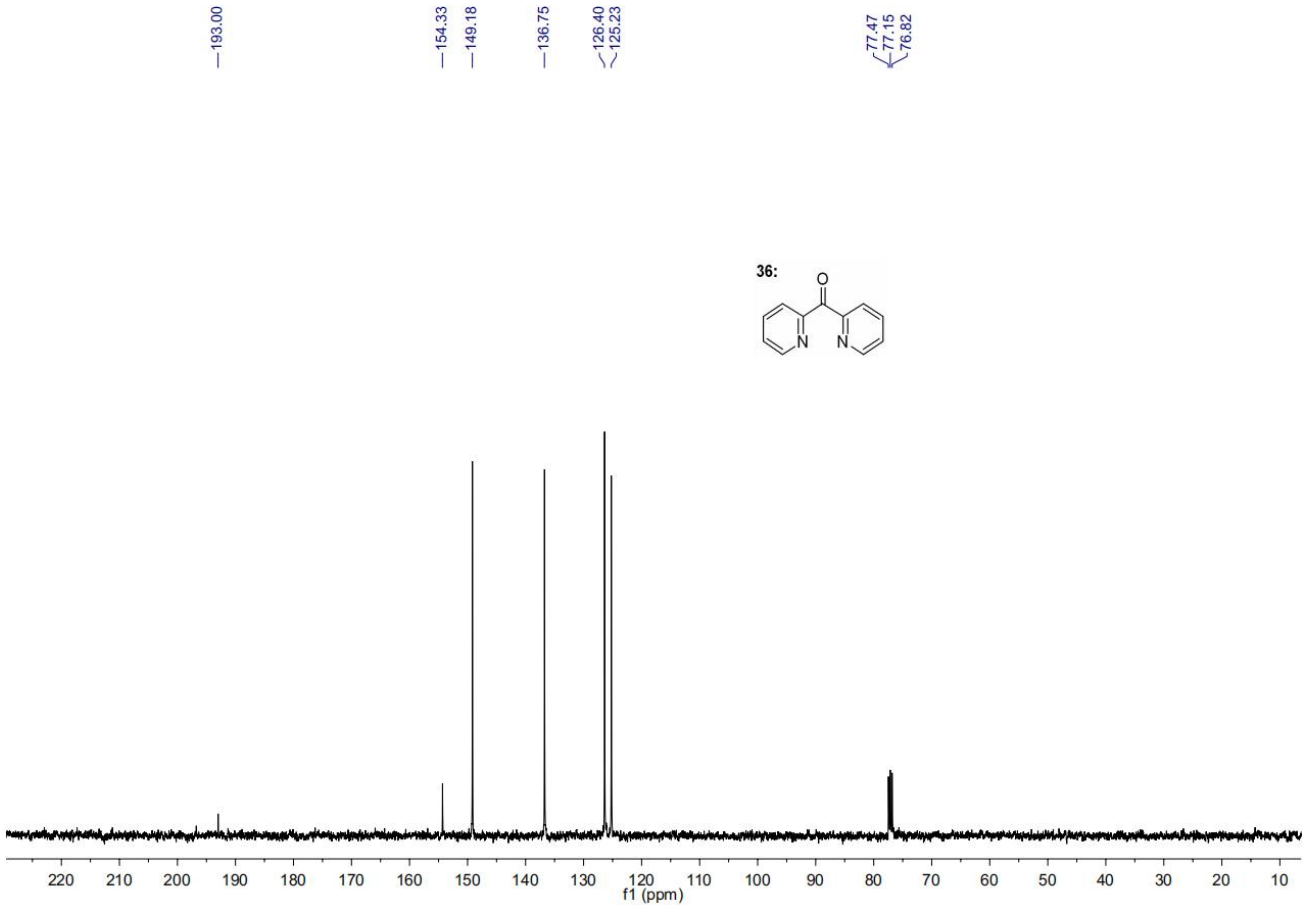

161.55
161.21
149.25
148.72
142.82
142.27
136.44
135.80
128.60
128.28
128.10
128.01
125.95
125.53
123.79
123.72
121.70
121.02
77.31
77.00
76.68
62.79
49.50
36.04
33.48
33:
N
Ph
Ph
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

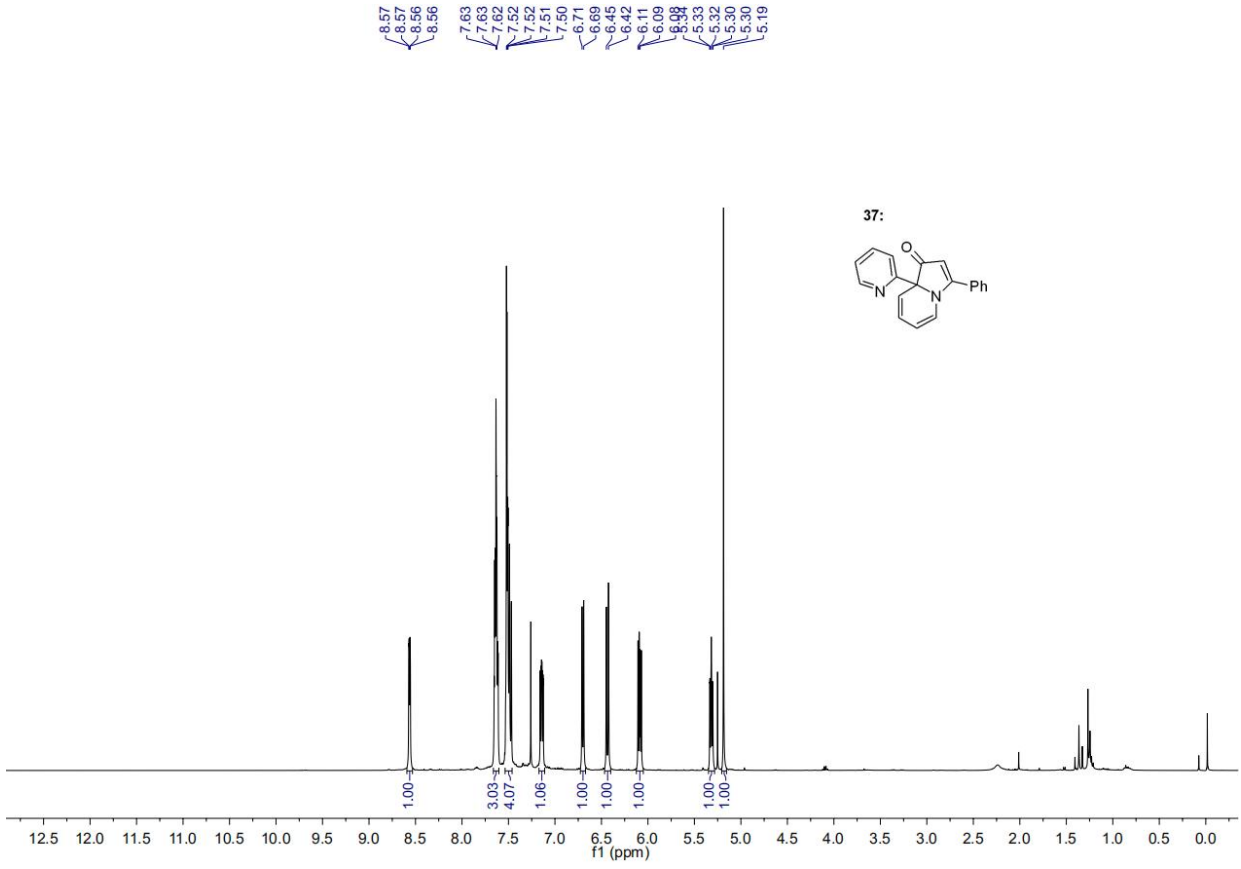

34:
Ph
OH
Ph
N
N
f1 (ppm)

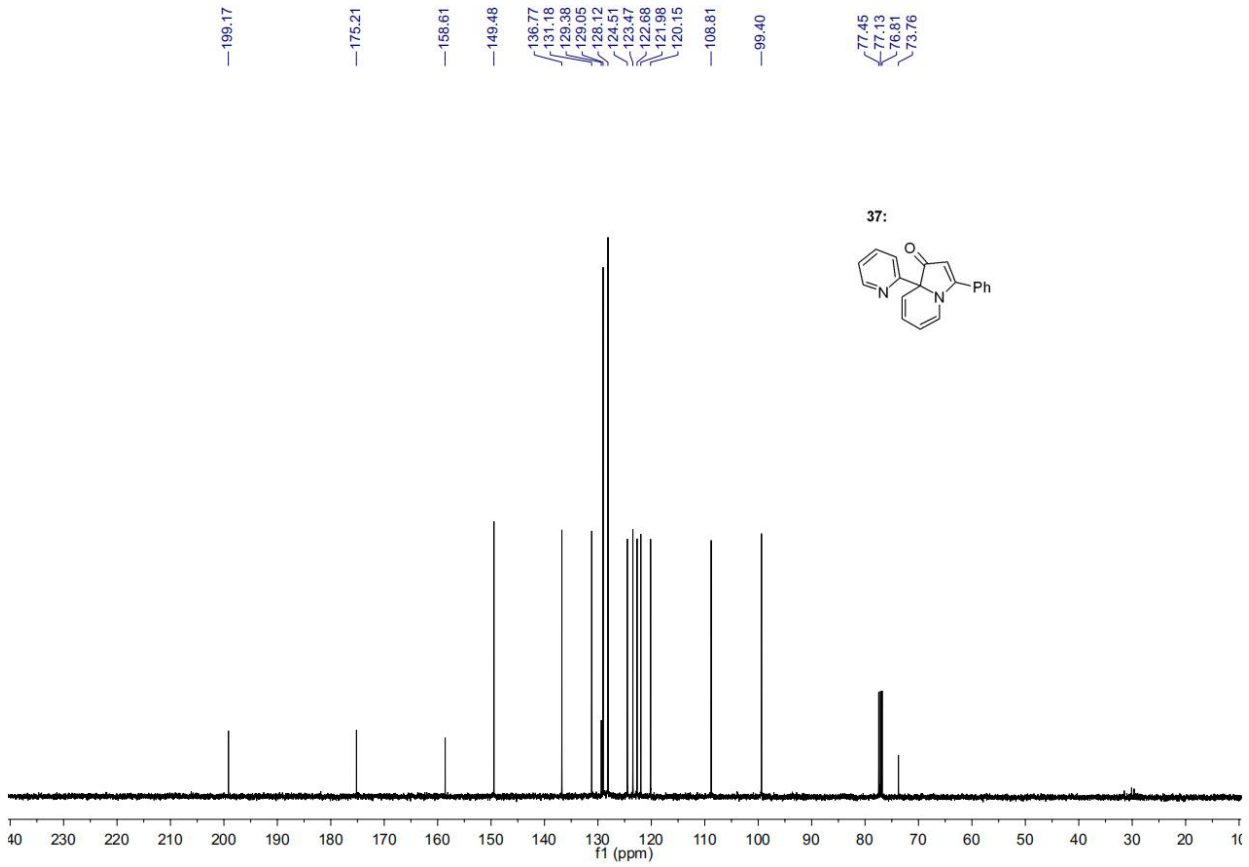

34:
Ph
OH
Ph
N
N
f1 (ppm)

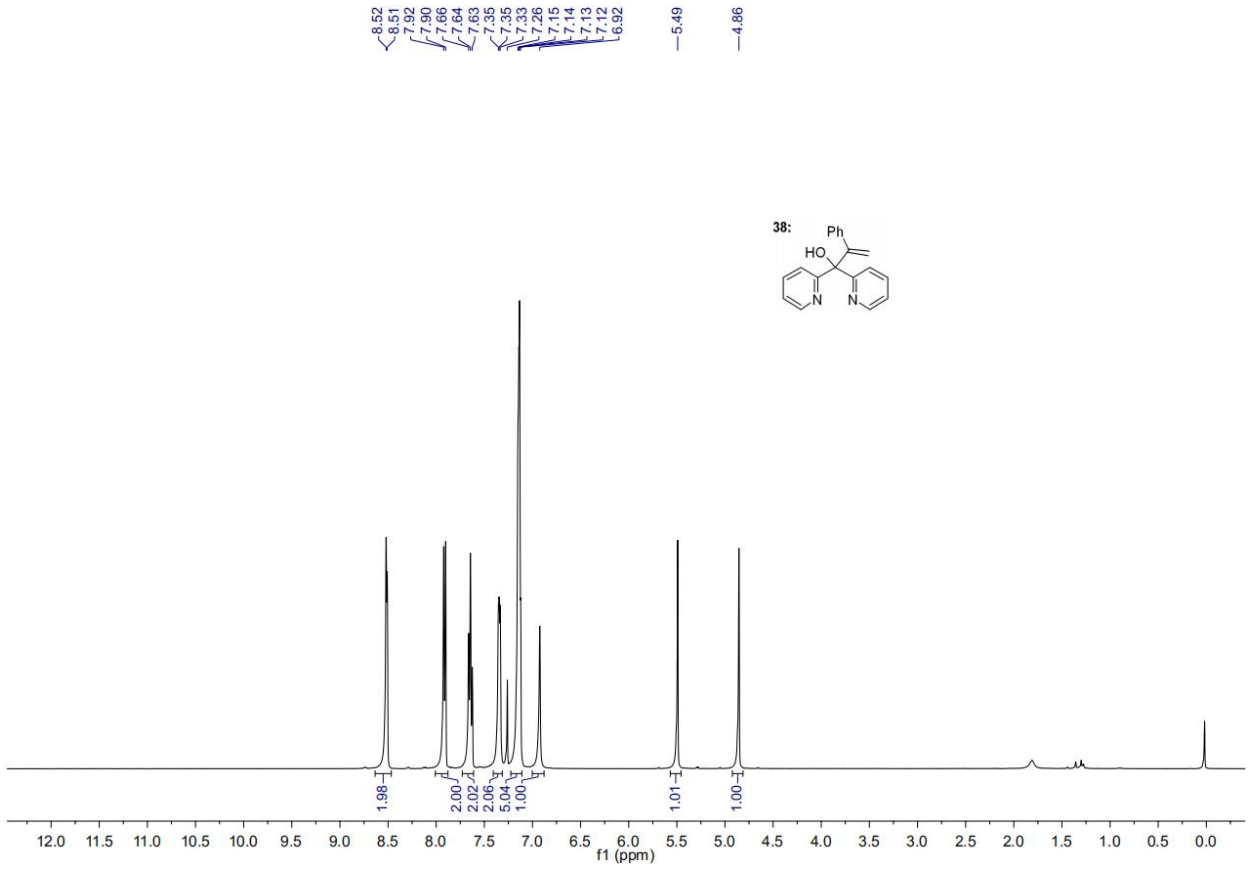

8.55
8.55
8.54
8.54
7.61
7.61
7.59
7.59
7.57
7.57
7.28
7.26
7.12
7.12
7.11
7.10
7.10
7.09
7.09
4.49
4.47
4.45
4.43
1.76
1.75
35:
CH3
N
N
1.94
2.01
2.12
2.00
1.00
3.05
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

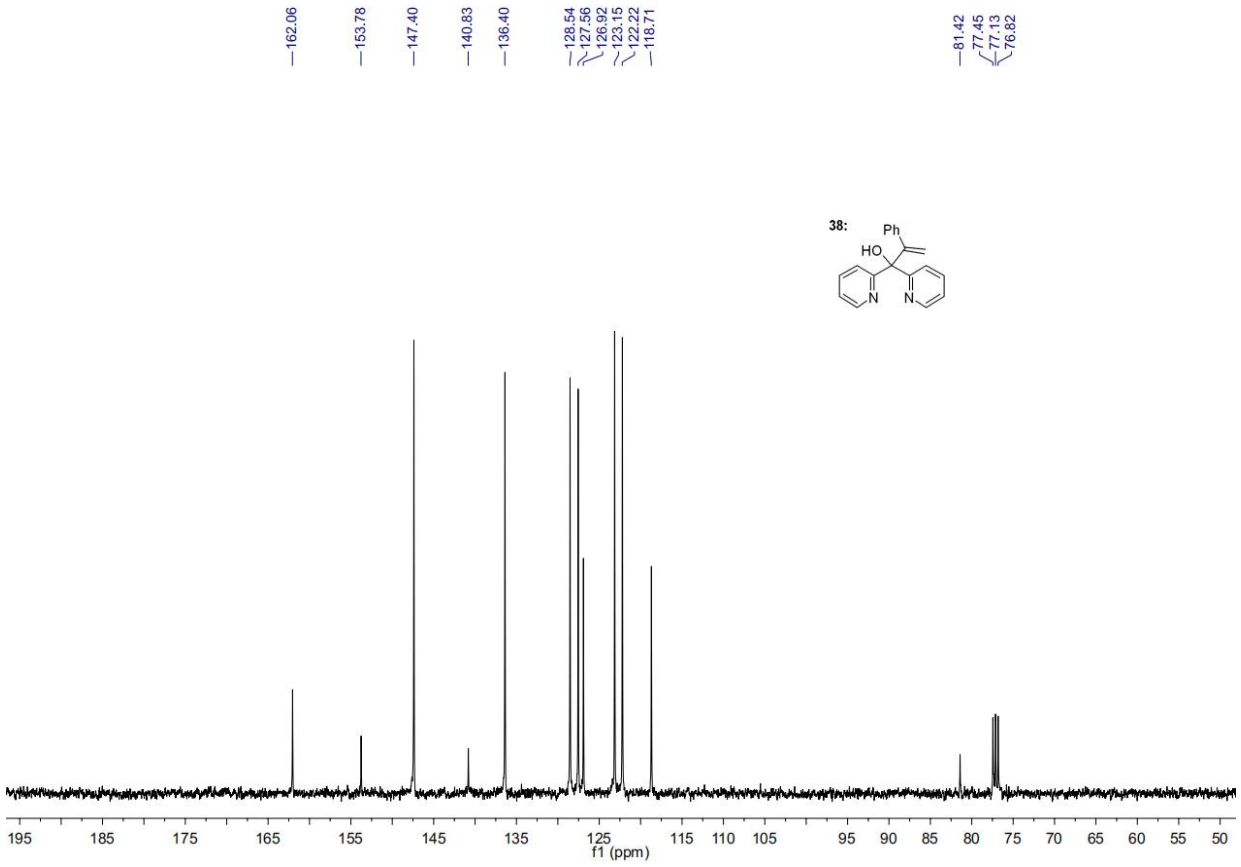

8.71
8.70
8.06
8.04
7.86
7.84
7.44
7.44
7.44
7.42
7.26
36:
O
N
N
2.00
2.01
2.07
2.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

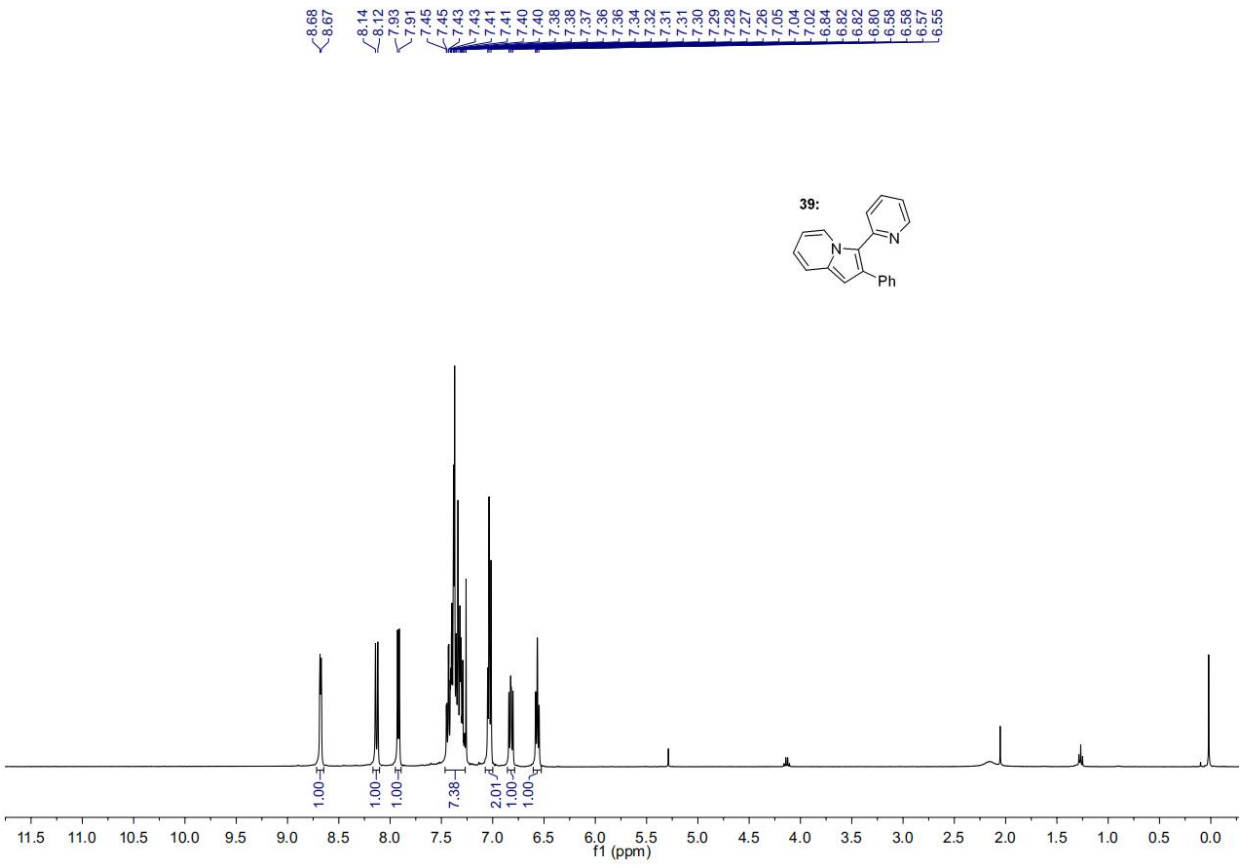

193.00
154.33
149.18
136.75
126.40
125.23
77.47
77.15
76.82
36:
O
N
N
f1 (ppm)

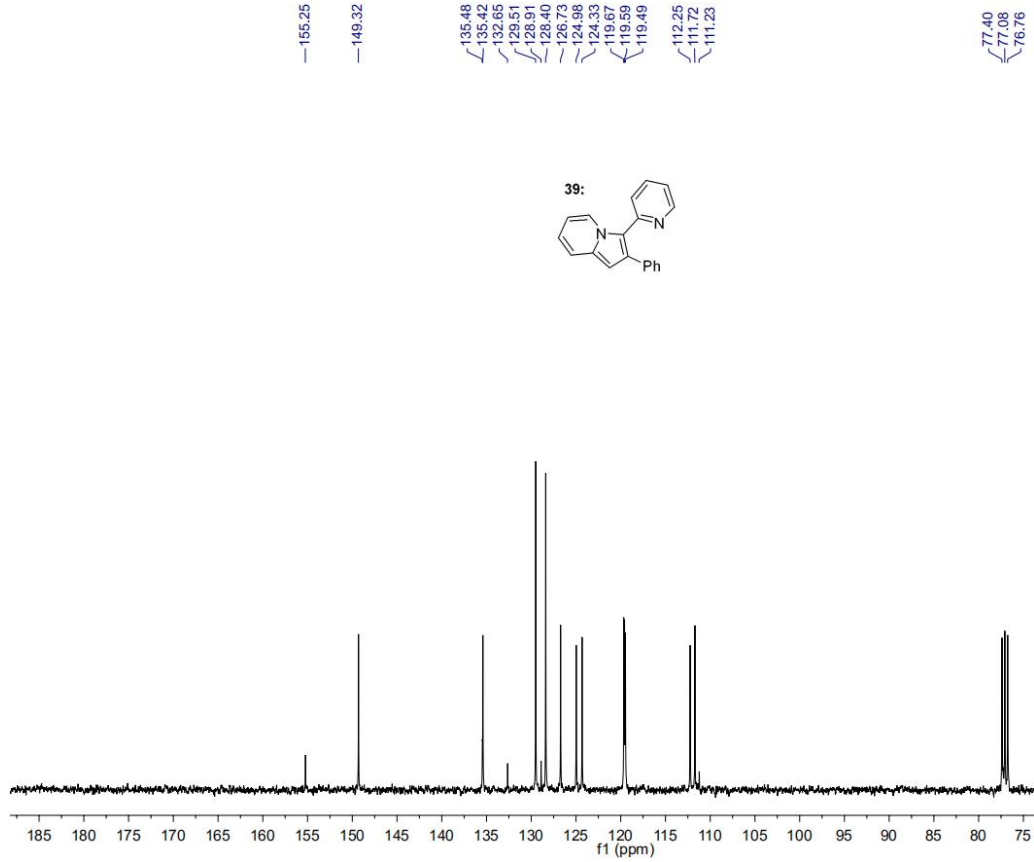

8.57
8.57
8.56
8.56
7.63
7.63
7.62
7.52
7.52
7.51
7.50
6.71
6.69
6.45
6.42
6.11
6.09
5.33
5.32
5.30
5.30
5.19
37:
O
N
N
Ph
1.00
3.03
4.07
1.06
1.00
1.00
1.00
1.00
1.00
f1 (ppm)

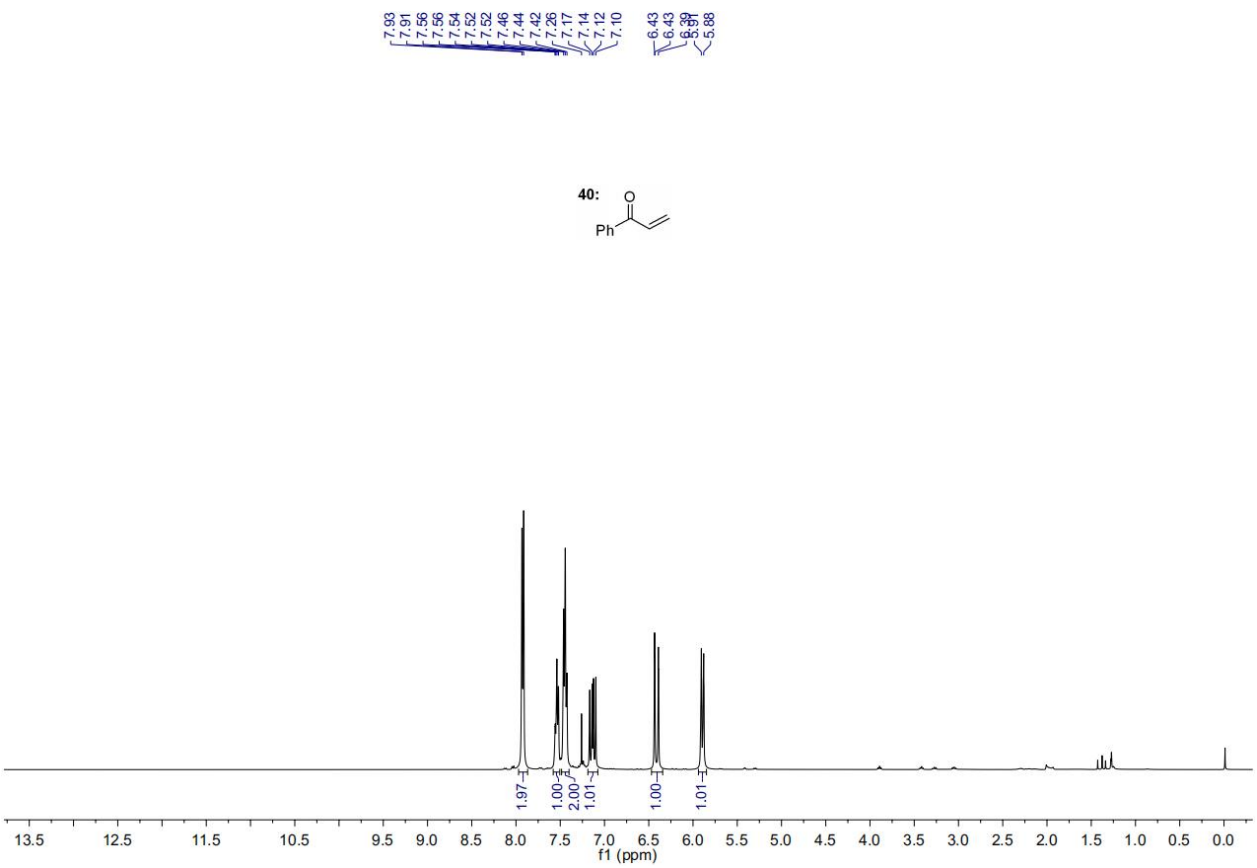

199.17
175.21
158.61
149.48
136.77
131.18
129.38
129.05
128.12
124.51
123.47
122.68
121.98
120.15
108.81
99.40
77.45
77.13
76.81
73.76
37:
O
N
N
Ph
f1 (ppm)

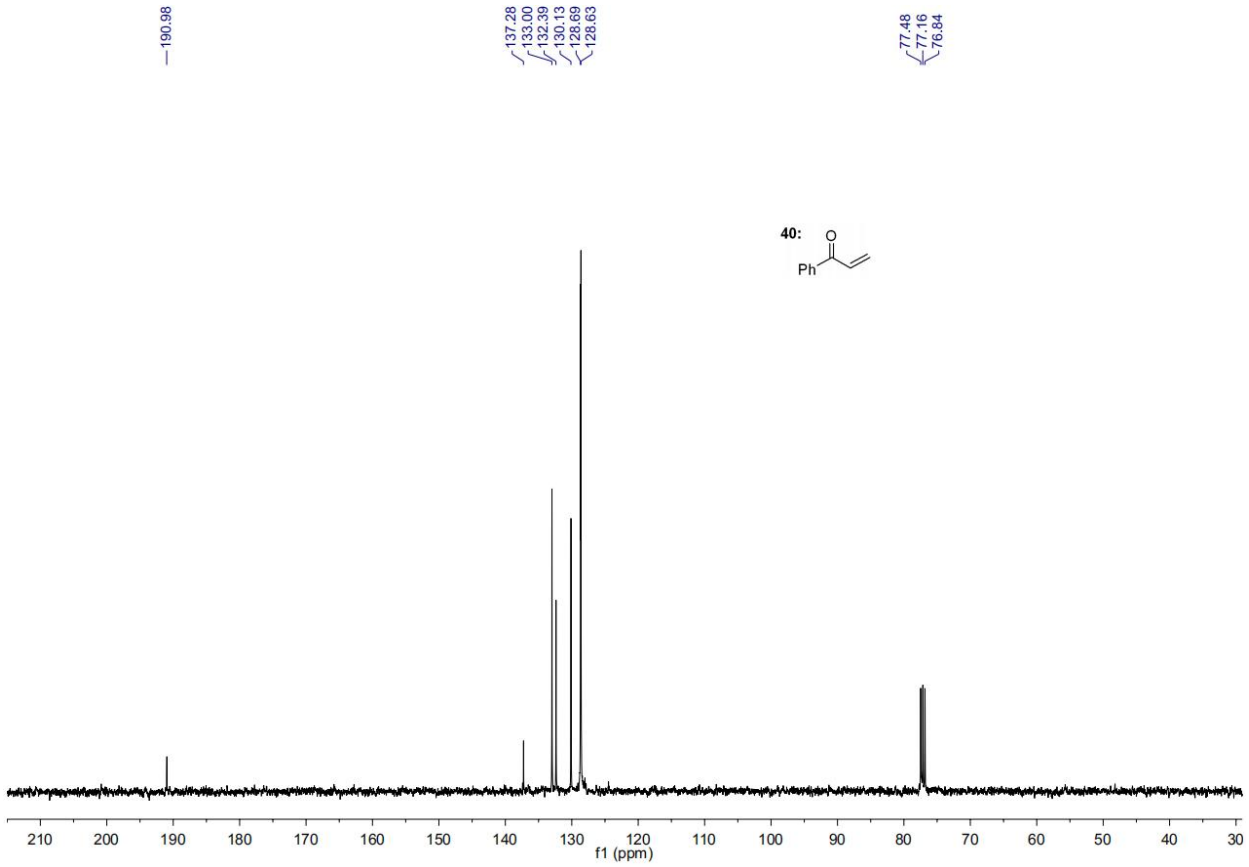

8.52
8.51
7.92
7.90
7.66
7.64
7.63
7.35
7.35
7.33
7.26
7.15
7.14
7.13
7.12
6.92
5.49
4.86
38:
Ph
HO
N
N
1.98
2.00
2.02
2.06
5.04
1.00
1.01
1.00
f1 (ppm)

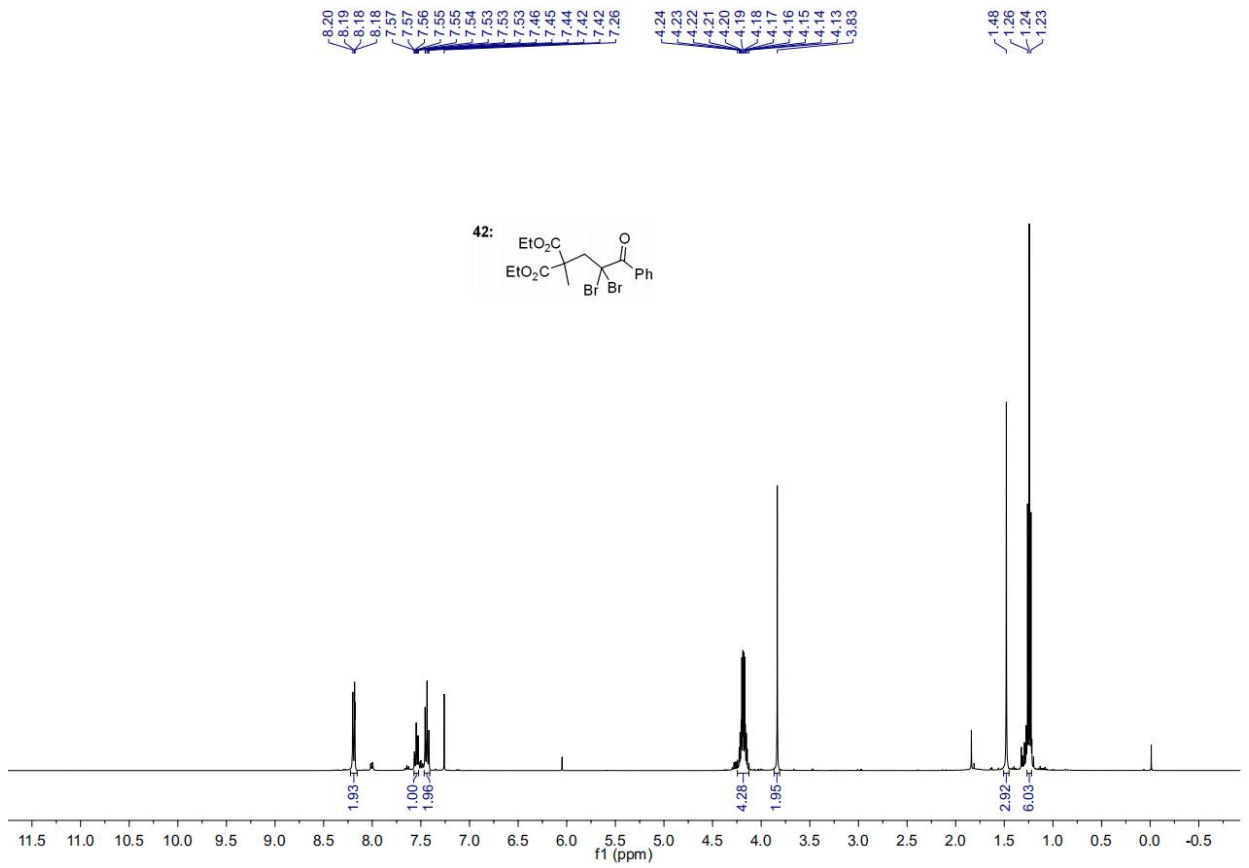

162.06
153.78
147.40
140.83
136.40
128.54
127.56
126.92
123.15
122.22
118.71
81.42
77.45
77.13
76.82
38:
Ph
HO
N
N
195 185 175 165 155 145 135 125 115 110 105 95 90 85 80 75 70 65 60 55 50
f1 (ppm)

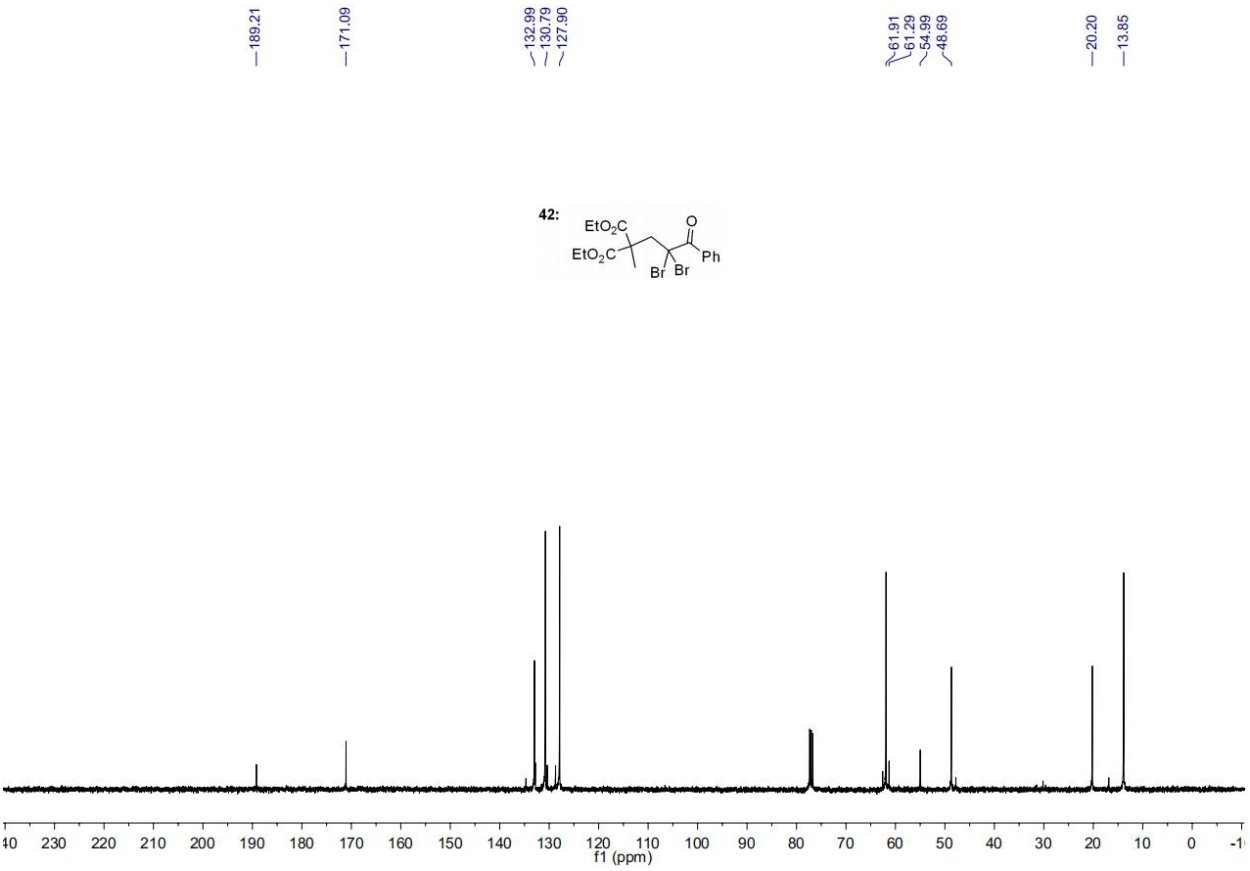

8.68
8.67
8.14
8.12
7.93
7.91
7.45
7.43
7.41
7.40
7.38
7.37
7.36
7.34
7.32
7.31
7.30
7.29
7.28
7.27
7.26
7.05
7.04
7.02
6.84
6.82
6.80
6.58
6.57
6.55
39:
N
N
Ph
1.00
1.00
1.00
7.38
2.01
1.00
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

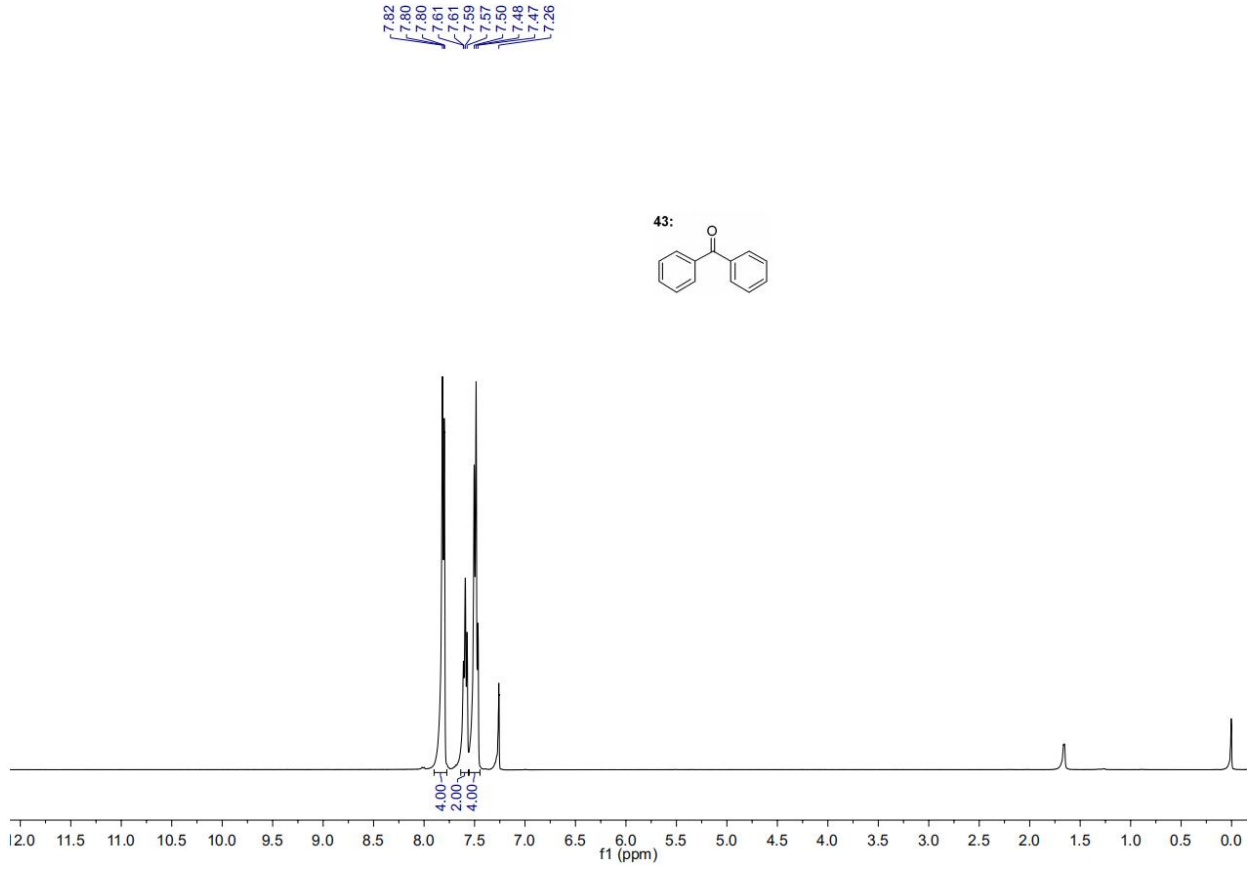

155.25
149.32
135.48
135.42
132.65
129.51
128.91
128.40
126.73
124.98
124.33
119.67
119.59
119.49
112.25
111.72
111.23
77.40
77.08
76.76
39:
N
N
Ph
185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55
f1 (ppm)

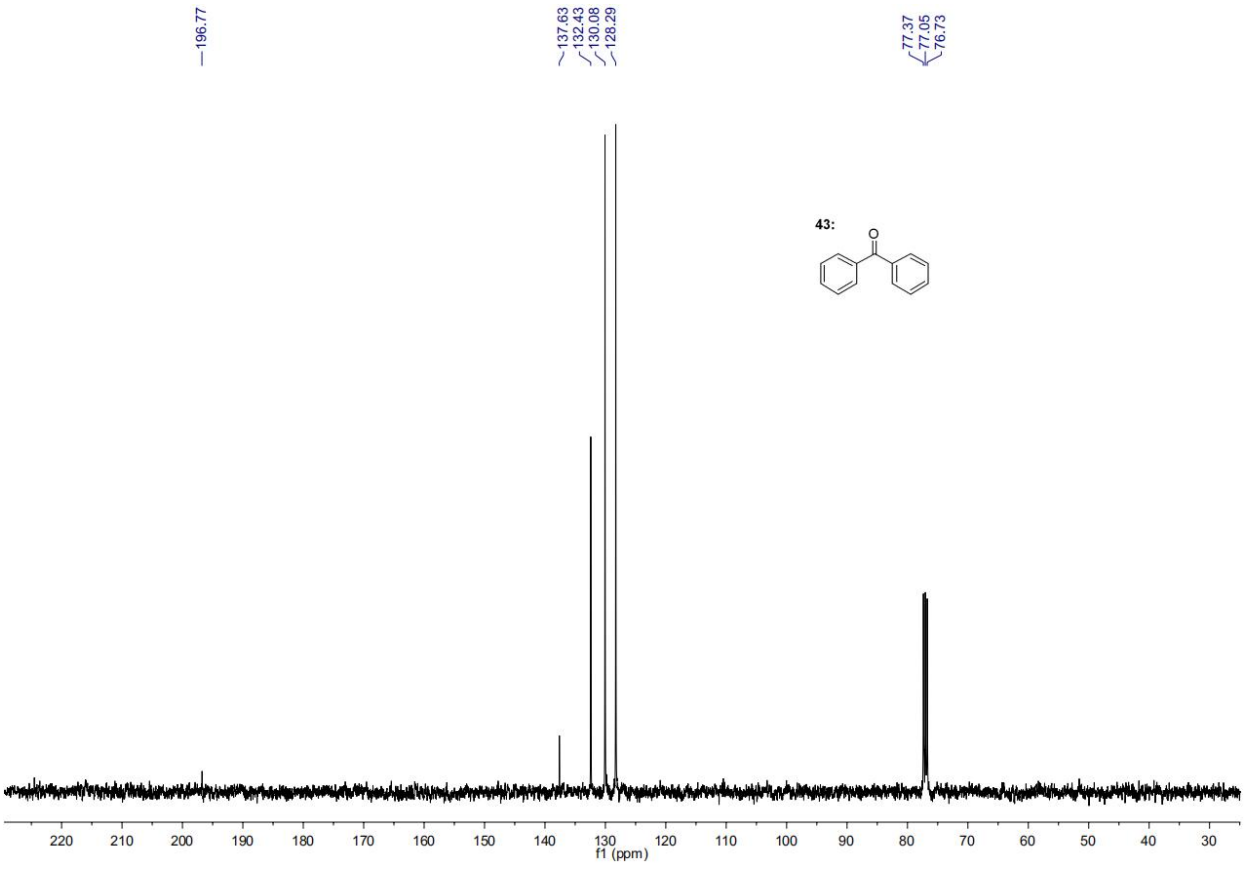

7.93
7.91
7.56
7.56
7.54
7.52
7.52
7.46
7.44
7.42
7.26
7.17
7.14
7.12
7.10
6.43
6.43
5.88
40:
O
Ph
1.97
1.00
2.00
1.01
1.00
1.01
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


190.98
137.28
133.00
132.39
130.13
128.69
128.63
77.48
77.16
76.84
40:
Ph
f1 (ppm)

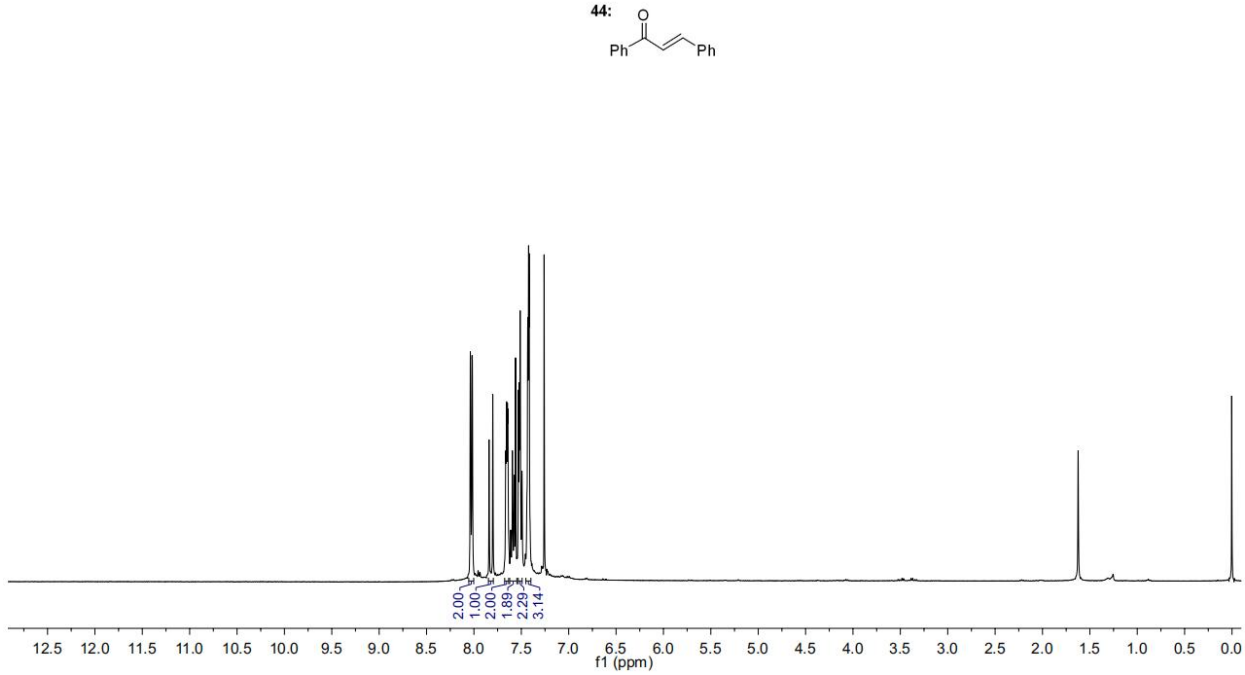

8.20
8.19
8.18
8.18
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.53
7.53
7.46
7.45
7.44
7.42
7.42
7.26
4.24
4.23
4.22
4.21
4.20
4.19
4.18
4.17
4.16
4.15
4.14
4.13
3.83
1.48
1.26
1.24
1.23
42:
EtO2C
EtO2C
O
Ph
Br
Br
1.93
1.00
1.96
4.28
1.95
2.92
6.03
f1 (ppm)

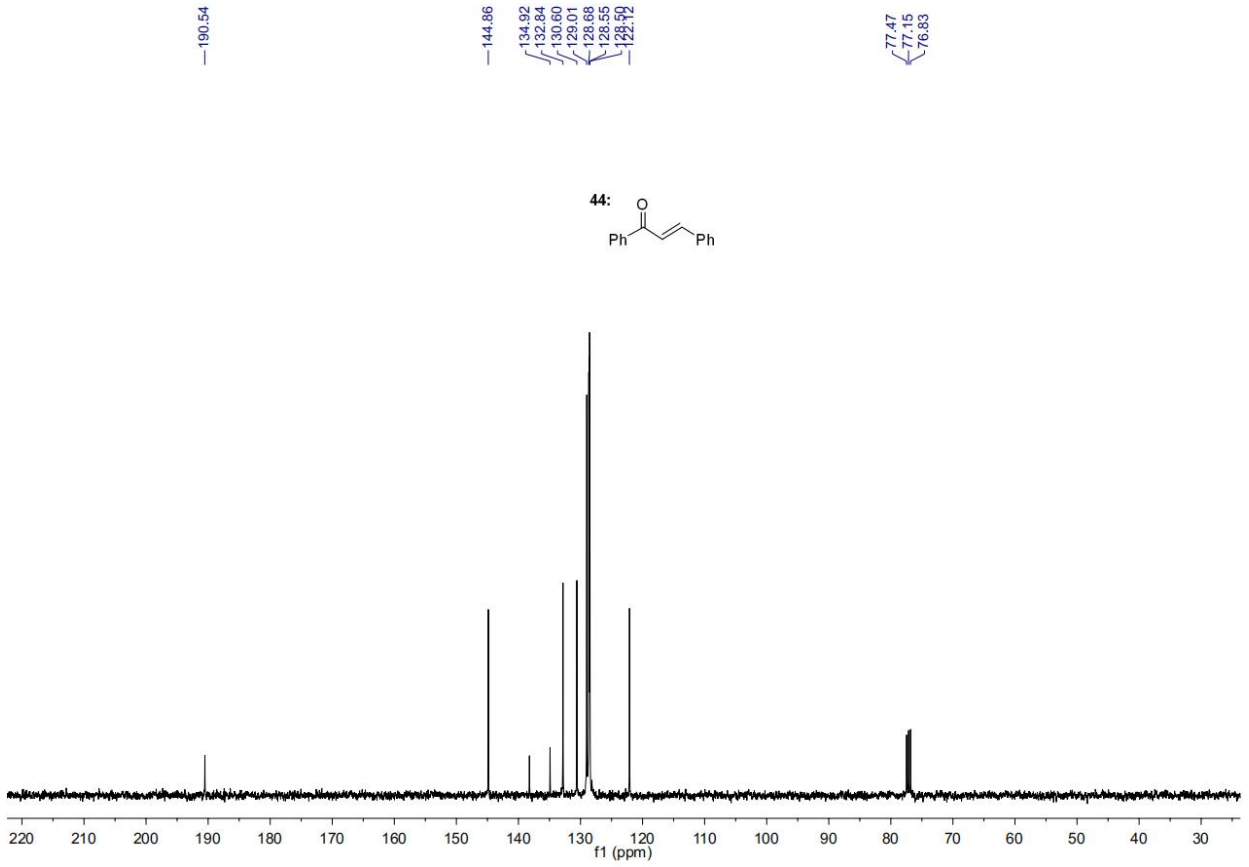

189.21
171.09
132.99
130.79
127.90
61.91
61.29
54.99
48.69
20.20
13.85
42:
EtO2C
EtO2C
O
Ph
Br
Br
f1 (ppm)

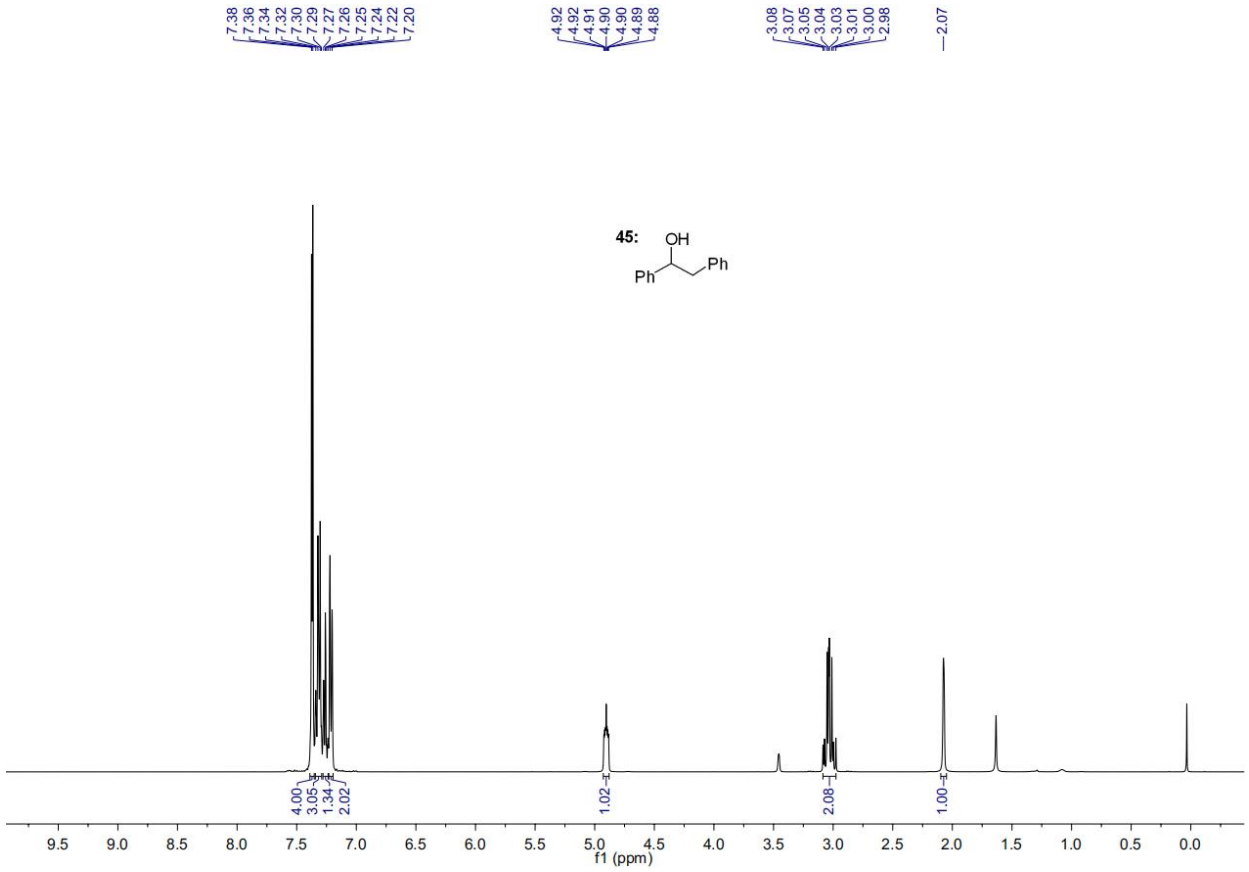

7.82
7.80
7.80
7.61
7.61
7.59
7.57
7.50
7.48
7.47
7.26
43:
O
4.00
2.00
4.00
f1 (ppm)

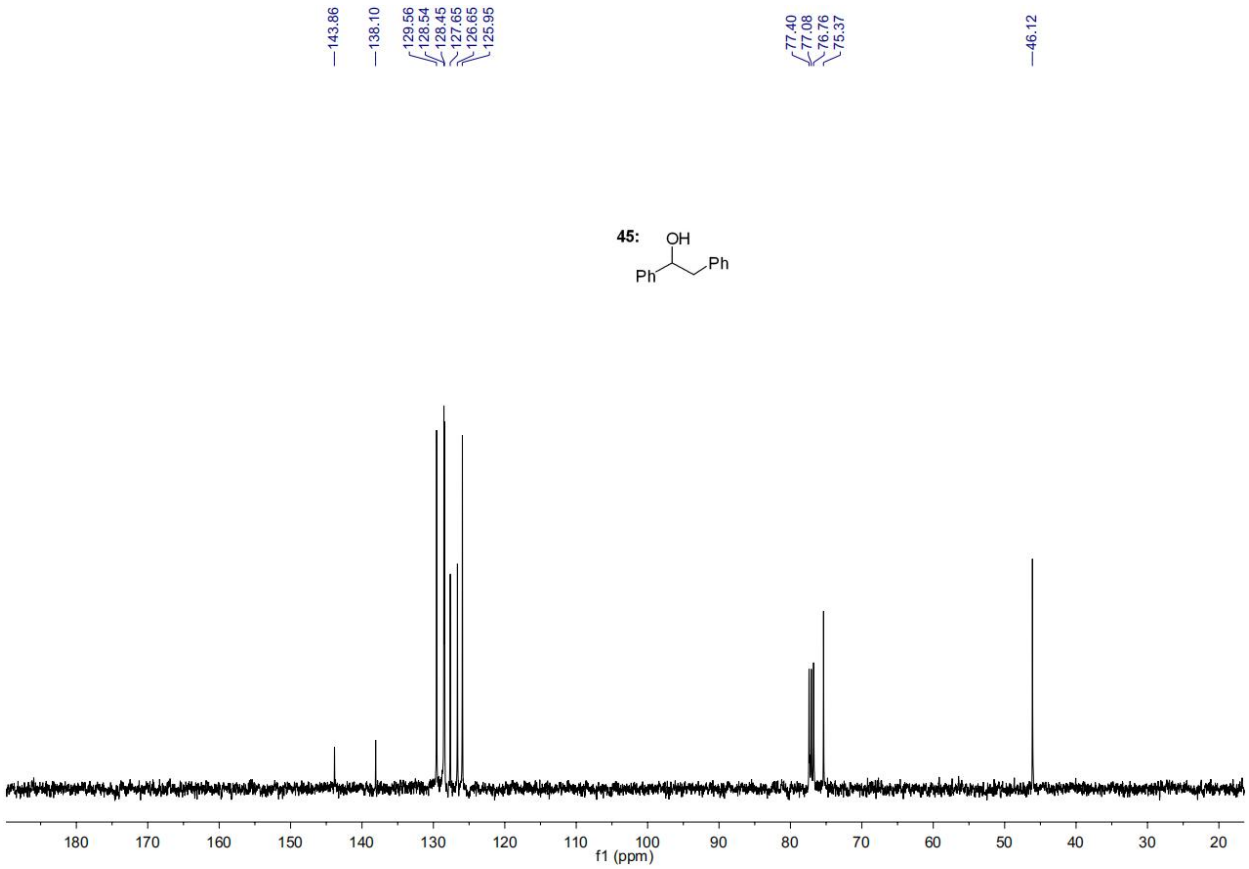

196.77
137.63
132.43
130.08
128.29
77.37
77.05
76.73
43:
f1 (ppm)

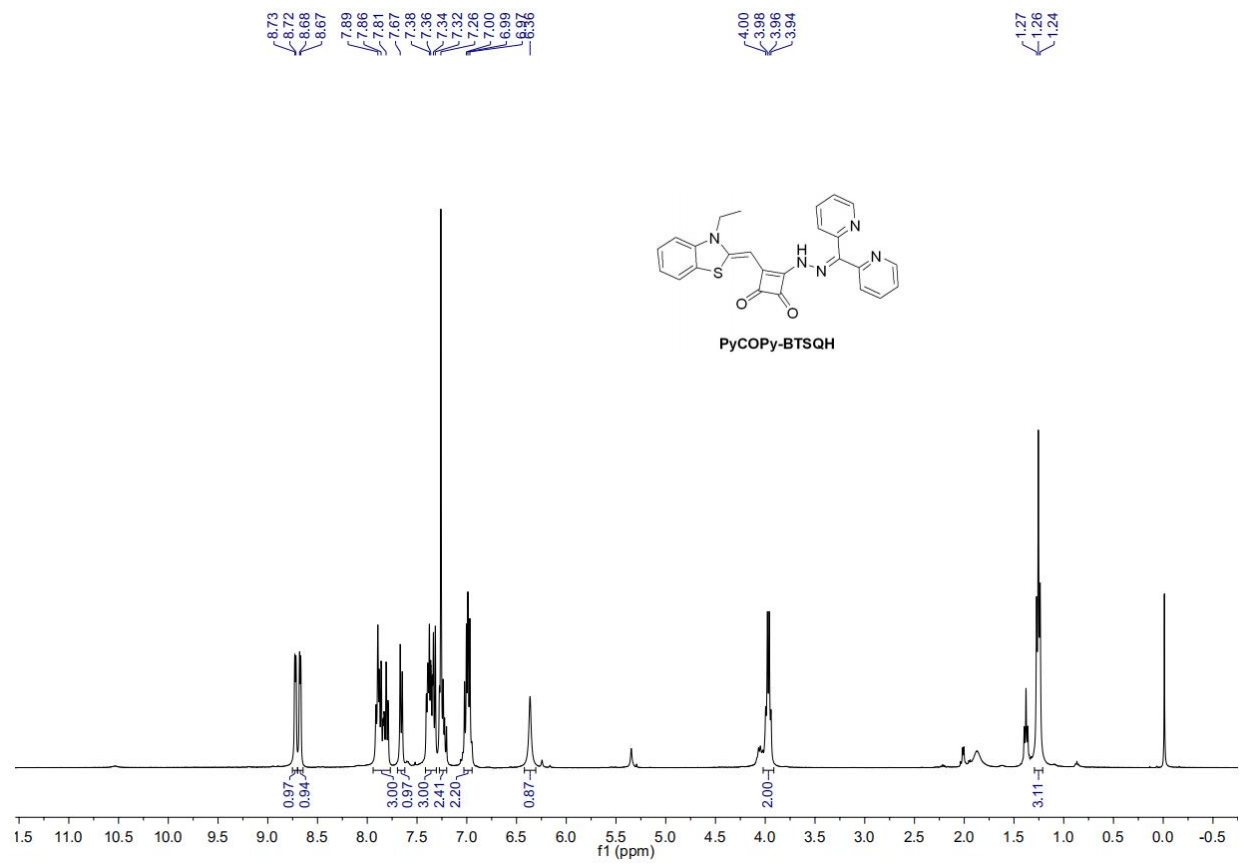

8.04
8.02
8.02
7.84
7.80
7.66
7.66
7.65
7.64
7.61
7.59
7.58
7.56
7.53
7.52
7.51
7.49
7.43
7.42
7.42
7.26

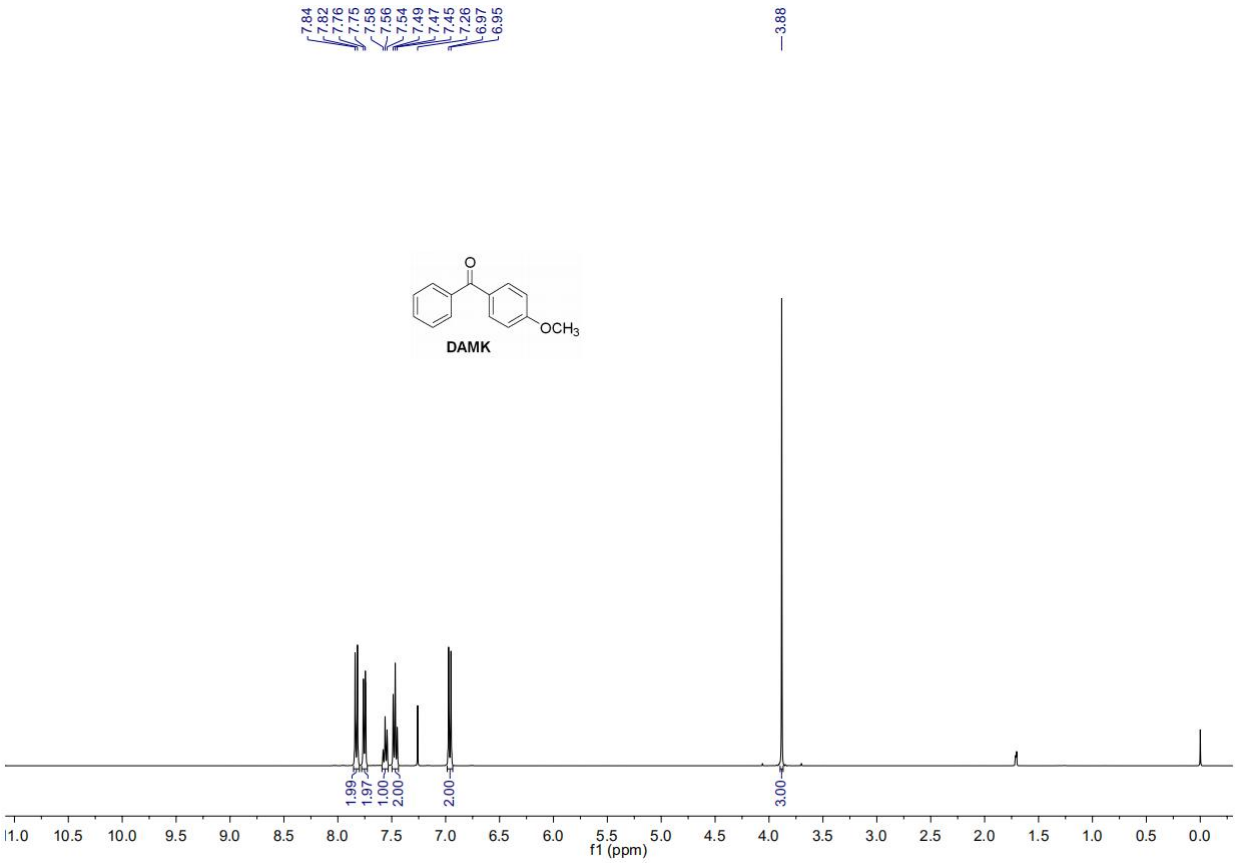

44:
O
Ph
Ph
2.00
1.00
2.00
1.89
2.29
3.14
f1 (ppm)

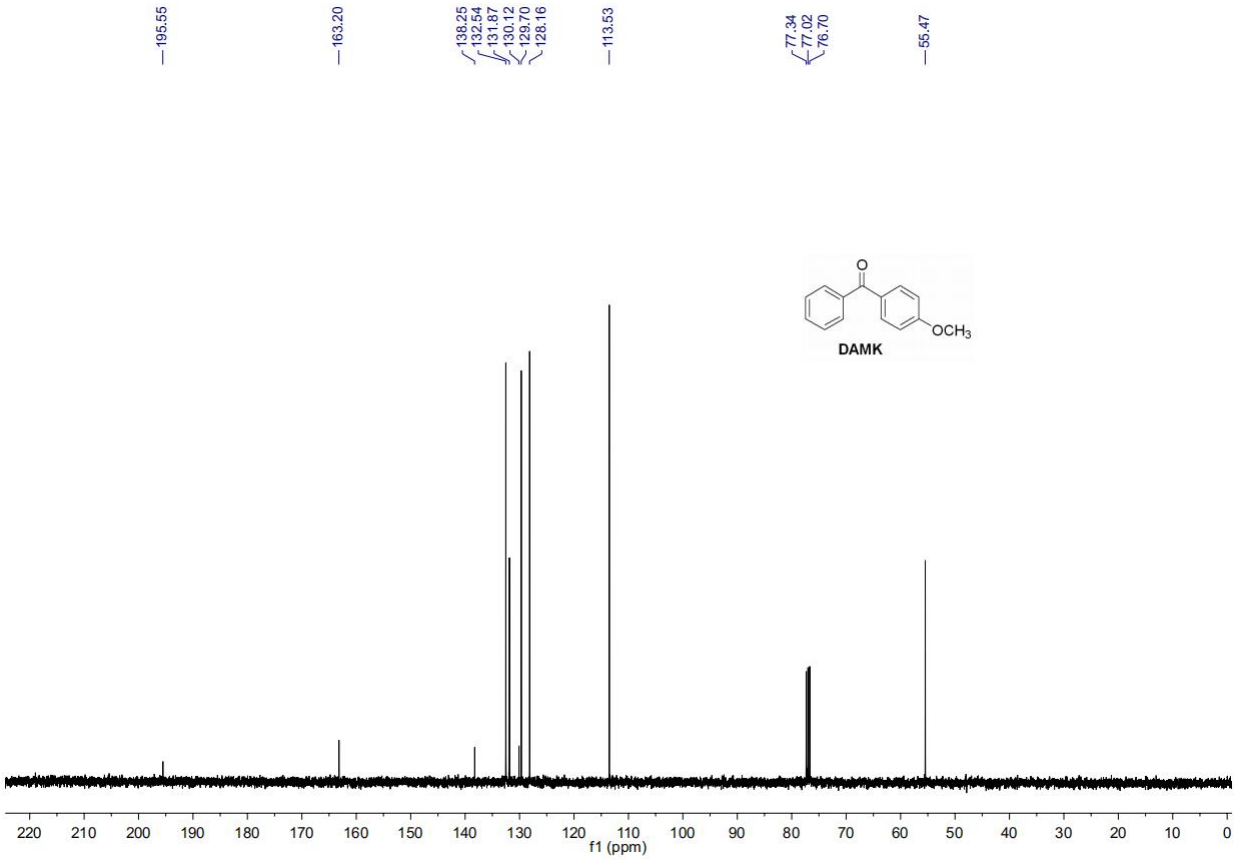

190.54
144.86
134.92
132.84
130.60
129.01
128.68
128.55
128.50
122.12
77.47
77.15
76.83
44:
O
Ph
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30
f1 (ppm)


7.38
7.36
7.34
7.32
7.30
7.29
7.27
7.26
7.25
7.24
7.22
7.20
4.92
4.92
4.91
4.90
4.90
4.89
4.88
3.08
3.07
3.05
3.04
3.03
3.01
3.00
2.98
2.07
45:
OH
Ph
Ph
4.00
3.05
1.34
2.02
1.02
2.08
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


143.86
138.10
129.56
128.54
128.45
127.65
126.65
125.95
77.40
77.08
76.76
75.37
46.12
45:
OH
Ph
Ph
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


8.73
8.72
8.68
8.67
7.89
7.86
7.81
7.67
7.38
7.36
7.34
7.32
7.26
7.00
6.99
6.97
6.96
4.00
3.98
3.96
3.94
1.27
1.26
1.24
PyCOPy-BTSQH
0.97
0.94
3.00
0.97
3.00
2.41
2.20
0.87
2.00
3.11
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


7.84
7.82
7.76
7.75
7.58
7.56
7.54
7.49
7.47
7.45
7.26
6.97
6.95
3.88
DAMK
1.99
1.97
1.00
2.00
2.00
3.00
f1 (ppm)


195.55
163.20
138.25
132.54
131.87
130.12
129.70
128.16
113.53
77.34
77.02
76.70
55.47
DAMK
f1 (ppm)