Supplementary Information (SI) for ChemComm.

Selective Nucleophilic Addition of Aryllithium Reagents to α-ketonitriles giving ketones under microflow Conditions.

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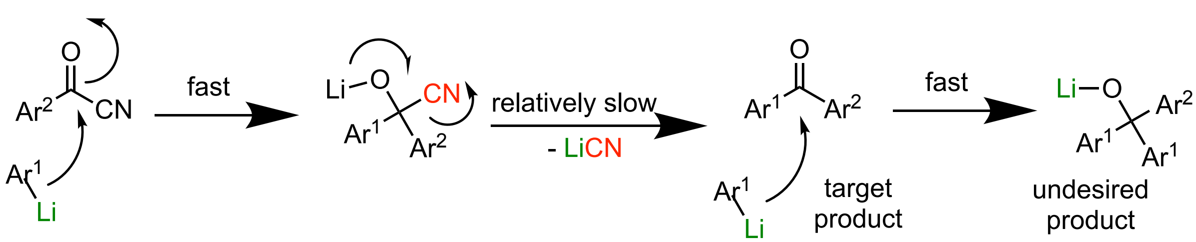
General

Abbreviations. residence time of microtube reactor R*n* (t_n), and inner diameter of tubes and mixers (ϕ).

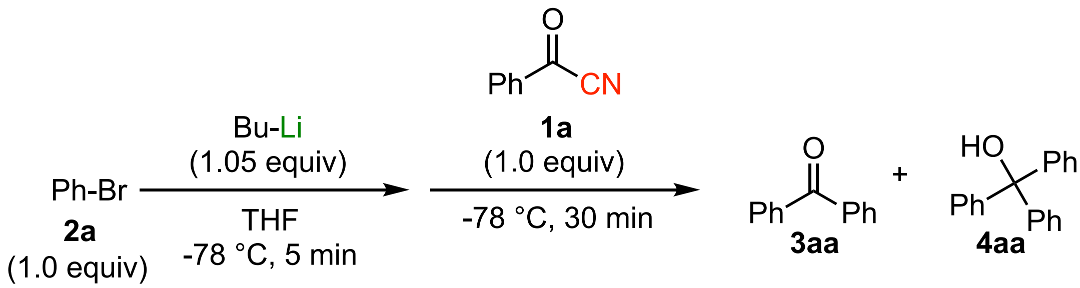
General. ^{1}H and ^{13}C NMR spectra were recorded on a JEOL ECZ-400S spectrometer (^{1}H 400 MHz, ^{13}C 100 MHz). Chemical shifts are recorded using Me_4Si (0.0 ppm) signals as an internal standard for ^{1}H NMR, and methine signal of $CHCl_3$ for ^{13}C NMR (77.0 ppm) unless otherwise noted. NMR yields were calculated by ^{1}H NMR analyses using 1,1,2,2-tetrachloroethane (TCE) as an internal standard. GC analyses were performed on a SHIMADZU GC-2025 gas chromatograph equipped with a flame ionization detector using a fused silica capillary column (column, Rtx-200; 0.25 mm × 30 m). GC yields were calculated by GC analyses with *n*-dodecane as an internal standard using calibration lines derived from commercial or isolated compounds with the internal standards. GC-MS analysis was performed on a SHIMADZU GCMS-QP2020 NX. Merck pre-coated silica gel F_{254} plates (thickness 0.25 mm) were used for TLC analyses. Preparative GPC separation was performed on a JAI HPLC 9021 equipped with JAIGEL-1H and -2H columns. All batch reactions were carried out in a flame-dried glassware under argon atmosphere unless otherwise noted.

Flow Synthesis. Stainless steel (SUS304) T-shaped micromixers with inner diameter of 500 μm and 250 μm were manufactured by Sanko Seiki Co., Inc. Stainless steel (SUS316) microtube reactors with 1000 μm inner diameter and PTFE tubes with inner diameter of 1000 μm were purchased from GL Sciences. The syringe pumps (Harvard PHD ULTRA) equipped with gastight syringes (SGE 50MR-LL-GT or 100MR-LL-GT) were used for introduction of the solutions into the micromixer systems *via* stainless steel fittings (GL Sciences, 1/16 OUW). Flow microreactor system is composed with stainless steel pre-cooling units (**P1**, **P2**, etc.), stainless steel microtube reactors (**R1**, **R2**, etc.), T-shaped micromixers (**M1**, **M2**, etc.), and, if necessary, PTFE tube with inner diameter of 1000 μm. The solution of *n*-butyllithium was prepared by dilution of those commercial solution with dehydrated *n*-hexane.

Reaction pathways for nucleophilic addition of Ar1Li to acyl cyanide Ar2COCN:

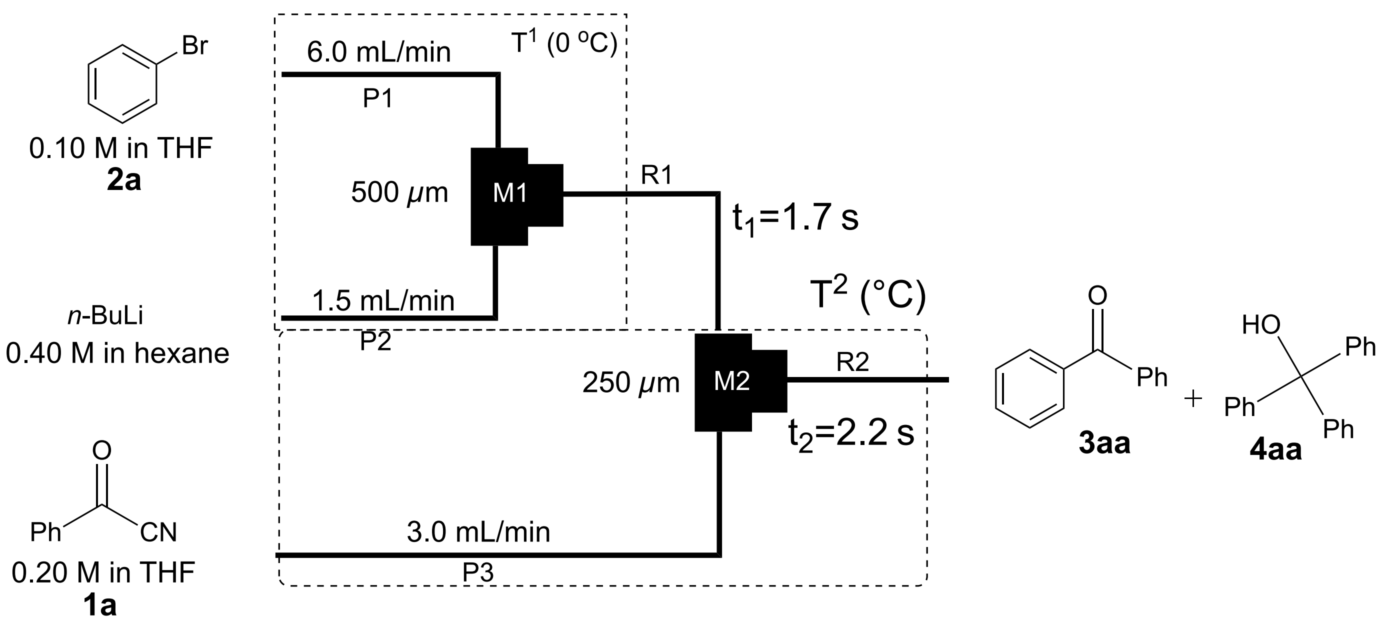


General Procedure for Br-Li Exchange Reaction of Bromobenzene Followed by the Reaction with benzoyl cyanide in a Macrobatch Systems.



A solution of *n*-BuLi (0.42 M in *n*-hexane, 1.0 mL) was added to a mixture solution of bromobenzene **(2a)** (0.10 M in THF, 4.0 mL) at T_1 = –78 °C at regular pace for 1.0 min. After stirring for 5 min, a solution of benzoyl cyanide **1a** (0.20 M in THF, 4.0 mL) was added to this mixture at a regular pace for 30 s. After stirring at T_2 °C for 30 min, a solution of ammonium chloride (10% in water, 1.0 mL) was added into the reaction mixture reached room temperature, yields of benzophenone **(3aa)** and triphenylmethanol (4**aa**) were determined by GC analysis using an internal standard (dodecane). Dodecane as an internal standard was added to an aliquot of the product solution after work up. Gas chromatography (GC) and NMR analysis of the crude product revealed the formation of the desired product, benzophenone 15% yield, because of selective nucleophilic addition of the aryl lithium species to the carbonyl group of benzoyl cyanide, accompanied by elimination of the cyano group as a leaving group. In addition to the major product, minor side products were observed, primarily arising from overreaction at the carbonyl group of the initially formed benzophenone, leading to the formation of triphenylmethanol 42% yield.

Effect of Temperature for Br-Li Exchange Reaction of Bromobenzene Followed by the Reaction with benzoyl cyanide in the Flow Microreactor System.



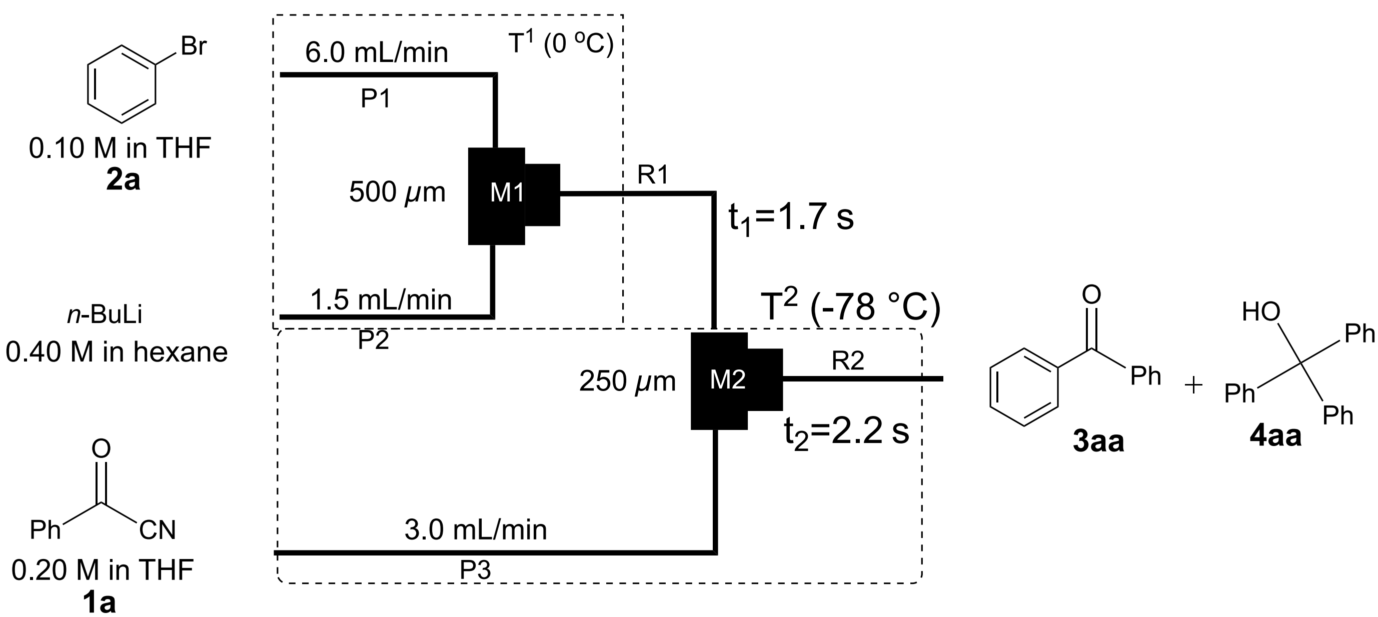
A flow microreactor system consisting of two T-shaped micromixers (**M1** and **M2**), two microtube reactors (**R1** and **R2**), and three tube pre-cooling units (**P1** (inner diameter ϕ = 1000 μm, length L = 100 cm), **P2** (ϕ = 1000 μm, length L = 50 cm) and **P3** (ϕ = 1000 μm, length L = 50 cm)) was used. A solution of bromobenzene **(2a)** (0. 1 M in THF) (flow rate: 6.0 mL min^{-1}) and a solution of *n*-BuLi (0.40 M in hexane) (flow rate: 1.50 mL min^{-1}) were introduced to **M1** (ϕ =500 μm) by syringe pumps. The resulting solution was passed through **R1** (ϕ =1000 μm, length L = 50 cm) and was mixed with a solution of benzoyl cyanide **(1a)**

(0. 20 M in THF) (flow rate: 3.0 mL min^{-1}) in **M2** (ϕ =250 μm). The resulting solution was passed through **R2** (ϕ =1000 μm, length L = 200 cm). After a steady state was reached, an aliquot of the product solution was collected for 30 s and was treated with 10% aqueous NH_4Cl solution. Yields of benzophenone **(3aa)** and triphenylmethanol (4**aa**) were determined by GC analysis using an internal standard (dodecane). Dodecane as an internal standard was added to an aliquot of the product solution after work up. The results are summarized in Table S-1.

T_2 (°C)	t_1 (s)	t_2 (s)	Conversion of **2a** (%)	Yield (%)	
				3aa	**4aa**
-78	1.7	2.2	100	90	0
-60	1.7	2.2	100	84	0
-40	1.7	2.2	100	73	0
-20	1.7	2.2	100	66	0
0	1.7	2.2	100	58	0

Table S-1 Reaction of benzoyl cynaide with phenyllithium generated from bromobenzene using a flow microreactor system. The Effect of Temperature.

Effect of Mixing for Br-Li Exchange Reaction of Bromobenzene Followed by the Reaction with Benzoyl Cyanide in the Flow Microreactor System.

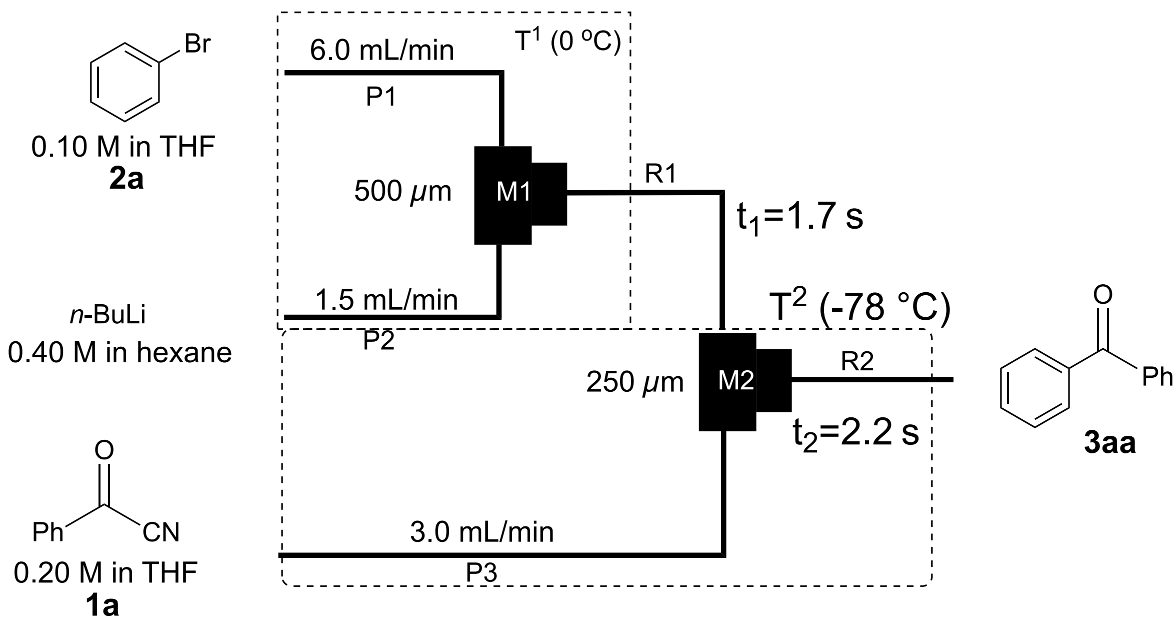


A flow microreactor system consisting of two T-shaped micromixers (**M1** and **M2**), two microtube reactors (**R1** and **R2**), and three tube pre-cooling units (**P1** (inner diameter ϕ = 1000 μm, length L = 100 cm), **P2** (ϕ = 1000 μm, length L = 50 cm) and **P3** (ϕ = 1000 μm, length L = 50 cm)) was used. A solution of bromobenzene **(2a)** (0. 1 M in THF) (flow rate: 6.0 mL min^{-1}) and a solution of *n*-BuLi (0.40 M in hexane) (flow rate: 1.50 mL min^{-1}) were introduced to **M1** (ϕ =500 μm) by syringe pumps. The resulting solution was passed through **R1** (ϕ =1000 μm, length L = 50 cm) and was mixed with a solution of Benzoyl Cyanide **(1a)** (0. 20 M in THF) (flow rate: 3.0 mL min^{-1}) in **M2** (ϕ =250, 500 and 1000 μm). The resulting solution was passed through **R2** (ϕ =1000 μm, length L = 200 cm). After a steady state was reached, an aliquot of the product solution was collected for 30 s and was treated with 10% aqueous NH_4Cl solution. Yields of benzophenone **(3aa)** and triphenylmethanol (4**aa**) were determined by GC analysis using an internal standard (dodecane). Dodecane as an internal standard was added to an aliquot of the product solution after work up. The results are summarized in Table S-2.

Inner diameter of **M2** (μm)	Total flow rate at **M2** (mL min^{-1})	Conversion of **2a** (%)	Yield	
			3aa	**4aa**
250	10.5	100	90	0
500	10.5	100	54	0
1000	10.5	100	42	0

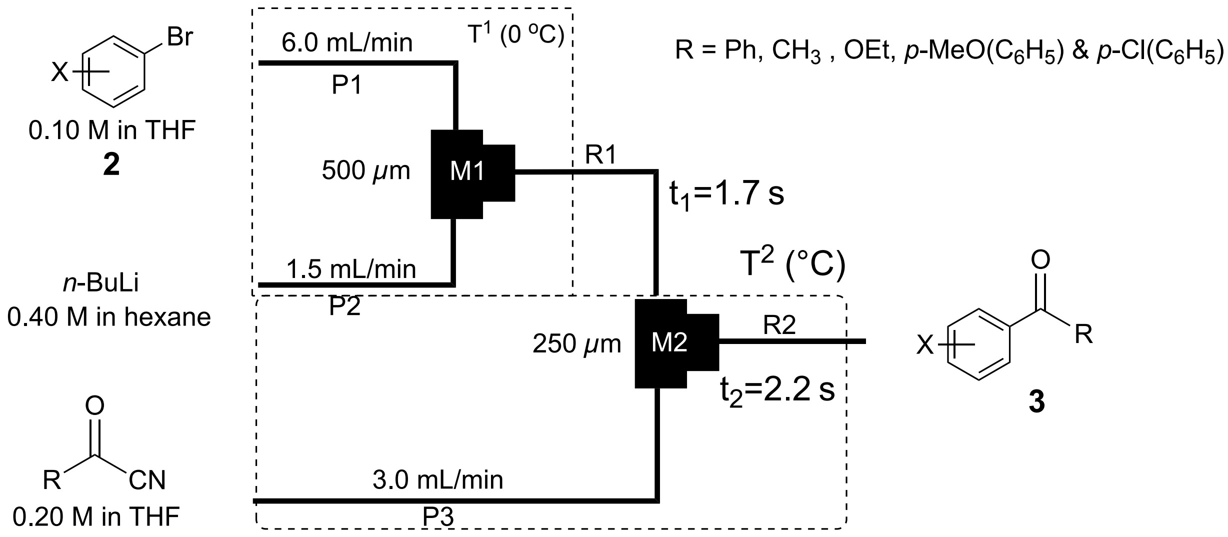
Table S-2 Reaction of Benzoyl Cyanide with phenyllithium generated from bromobenzene using a flow microreactor system. The Effect of Mixing. The reactions were carried out at $T = -78$ °C.

Gram-scale synthesis for Br-Li Exchange Reaction of Bromobenzene Followed by the Reaction with Benzoyl Cyanide in the Flow Microreactor System.



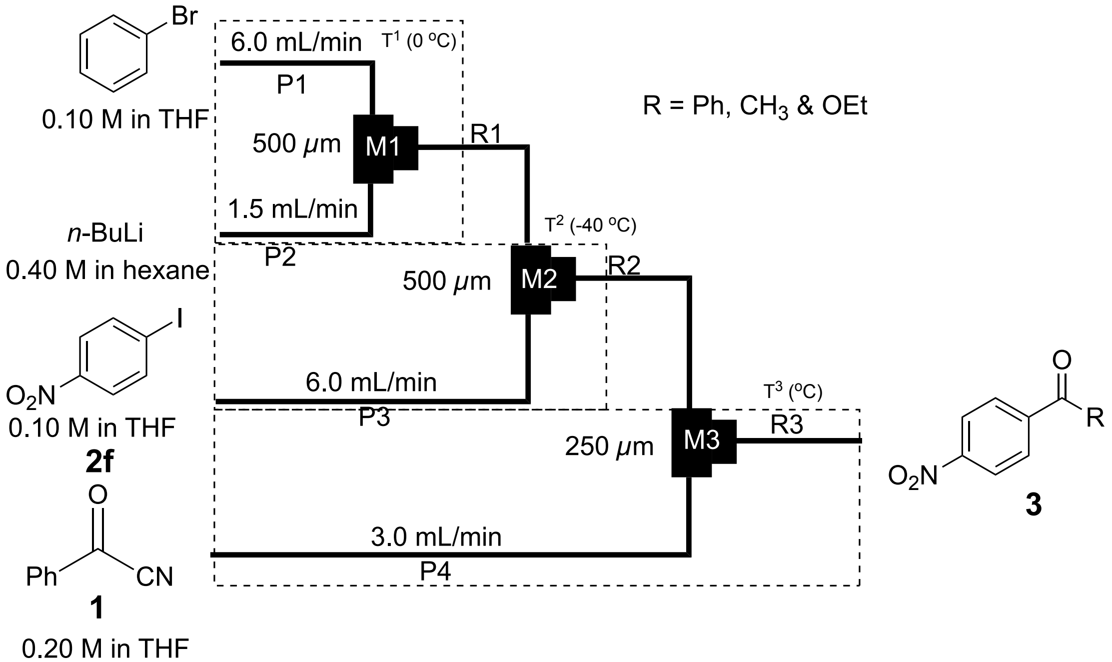
A flow microreactor system consisting of two T-shaped micromixers (**M1** and **M2**), two microtube reactors (**R1** and **R2**), and three tube pre-cooling units (**P1** (inner diameter ϕ = 1000 μm, length L = 100 cm), **P2** (ϕ = 1000 μm, length L = 50 cm) and **P3** (ϕ = 1000 μm, length L = 50 cm)) was used. A solution of bromobenzene **(2a)** (0. 1 M in THF) (100 ml) (flow rate: 6.0 mL min^{-1}) and a solution of *n*-BuLi (0.40 M in hexane) (30 ml) (flow rate: 1.50 mL min^{-1}) were introduced to **M1** (ϕ =500 μm) by syringe pumps. The resulting solution was passed through **R1** (ϕ =1000 μm, length L = 50 cm) and was mixed with a solution of Benzoyl Cyanide **(1a)** (0. 20 M in THF) (50 ml) (flow rate: 3.0 mL min^{-1}) in **M2** (ϕ =250μm). The resulting solution was passed through **R2** (ϕ =1000 μm, length L = 200 cm). After the system reached a steady state, the product stream was collected over an extended continuous operation period and subsequently quenched with 10% aqueous NH_4Cl solution. The yield of benzophenone (**3aa**) was determined by GC analysis using dodecane as an internal standard, which was added to an aliquot of the product solution after workup. The product was further purified by column chromatography. Continuous operation under these conditions enabled gram-scale production, thereby demonstrating the practical scalability and robustness of the flow process.

Typical Procedure for X-Li Exchange Reaction of Halobenzene Followed by the Reaction with α-Cyano Carbonyl Compounds in the Flow Microreactor System.



A flow microreactor system consisting of two T-shaped micromixers (**M1** and **M2**), two microtube reactors (**R1** and **R2**), and three tube pre-cooling units (**P1** (inner diameter ϕ = 1000 μm, length L = 100 cm), **P2** (ϕ = 1000 μm, length L = 50 cm) and **P3** (ϕ = 1000 μm, length L = 50 cm)) was used. A solution of halobenzene **(2)** (0. 1 M in THF) (flow rate: 6.0 mL min^{-1}) and a solution of *n*-BuLi (0.40 M in hexane) (flow rate: 1.50 mL min^{-1}) were introduced to **M1** (ϕ =500 μm) by syringe pumps. The resulting solution was passed through **R1** (ϕ =1000 μm, length L = 50 cm) and was mixed with a solution of α-Cyano Carbonyl Compounds **(1)** (0. 20 M in THF) (flow rate: 3.0 mL min^{-1}) in **M2** (ϕ =250 μm). The resulting solution was passed through **R2** (ϕ =1000 μm, length L = 200 cm). After a steady state was reached, an aliquot of the product solution was collected for 30 s and was treated with 10% aqueous NH_4Cl solution. Yields of desired products were determined by GC analysis using an internal standard or isolation by column chromatography. Dodecane as an internal standard was added to an aliquot of the product solution after work up.

General Procedure for I-Li Exchange Reaction of 1-iodo-4-nitrobenzene Followed by the Reaction with α-Cyano Carbonyl Compounds in the Flow Microreactor System.



A flow microreactor system consisting of three T-shaped micromixers (**M1**, **M2** and **M3**), three microtube reactors (**R1**, **R2** and **R3**), and four tube pre-cooling units (**P1** (inner diameter ϕ = 1000 μm, length L = 100 cm), **P2** (ϕ = 1000 μm, length L = 50 cm), **P3** (ϕ = 1000 μm, length L = 100 cm) and **P4** (ϕ = 1000 μm, length L = 50 cm)) was used. A solution of bromobenzene (0. 1 M in THF) (flow rate: 6.0 mL min^{-1}) and a solution of *n*-BuLi (0.40 M in hexane) (flow rate: 1.50 mL min^{-1}) were introduced to **M1** (ϕ =500 μm) by syringe pumps. The resulting solution was passed through **R1** (ϕ =1000 μm, length L = 50 cm) and was mixed with a solution of 1-iodo-4-nitrobenzene **(2f)** (0. 10 M in THF) (flow rate: 6.0 mL min^{-1}) in **M2** (ϕ =500 μm). The resulting solution was passed through **R2** (ϕ =1000 μm, length L = 3.50 cm) and was mixed with a solution of α-Cyano Carbonyl Compounds **(1)** (0.20 M in THF) (flow rate: 3.0 mL min^{-1}) in **M3** (ϕ =250 μm). The resulting solution was passed through **R3** (ϕ =1000 μm, length L = 200 cm). After a steady state was reached, an aliquot of the product solution was collected for 30 s and was treated with 10% aqueous NH_4Cl solution. Yields of desired products (**3**) were determined by GC analysis using an internal standard (dodecane). Dodecane as an internal standard was added to an aliquot of the product solution after work up. The results are summarized in Table S-3.

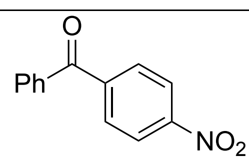
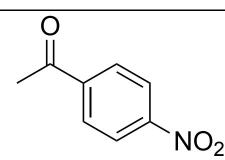
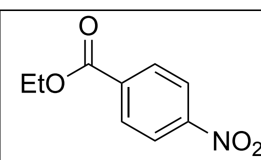
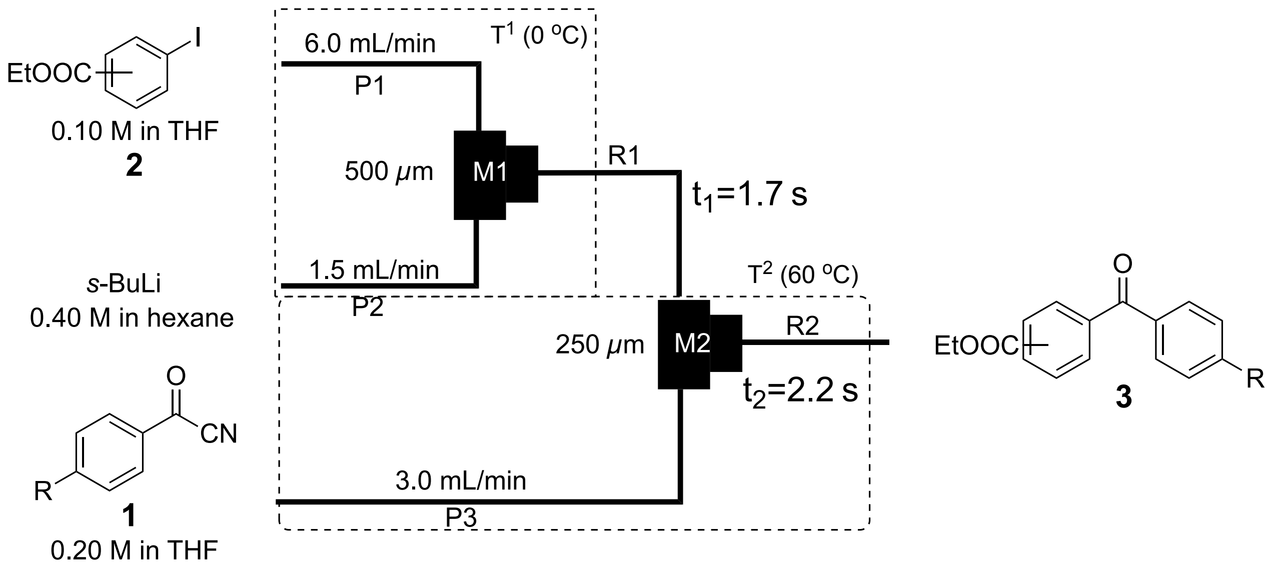
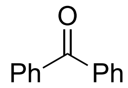
T (°C)	t_3 (s)	Conversion (%)	 (%)	 (%)	 (%)
-78	5.7	100	77	61	62
-60	5.7	100	72	57	52
-40	5.7	100	44	47	45
-20	5.7	100	40	41	39
0	5.7	100	37	38	33

Table S-3 Reaction of α-Cyano Carbonyl Compounds with (4-nitrophenyl)lithium generated from 1-iodo-4-nitrobenzene using a flow microreactor system.

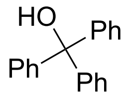
Typical Procedure for X-Li Exchange Reaction of Halobenzene Followed by the Reaction with α-Cyano Carbonyl Compounds in the Flow Microreactor System.



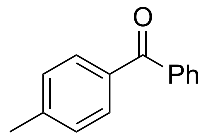
A flow microreactor system consisting of two T-shaped micromixers (**M1** and **M2**), two microtube reactors **(R1** and **R2**), and three tube pre-cooling units (**P1** (inner diameter ϕ = 1000 μm, length L = 100 cm), **P2** (ϕ = 1000 μm, length L = 50 cm) and (**P3** (inner diameter ϕ = 1000 μm, length L = 50 cm)) was used. A solution ethyl iodobenzoates (**2)** (0. 1 M in THF) (flow rate: 6.0 mL min^{-1}) and a solution of *s*-BuLi (0.40 M in hexane) (flow rate: 1.50 mL min^{-1}) were introduced to **M1** (ϕ =500 μm) by syringe pumps. The resulting solution was passed through **R1** (ϕ =1000 μm, length L = 50 cm) and was mixed with a solution of of α-Cyano Carbonyl Compounds **(1)** (0. 20 M in THF) (flow rate: 3.0 mL min^{-1}) in **M2** (ϕ =250 μm). The resulting solution was passed through **R2** (ϕ =1000 μm, length L = 200 cm). After a steady state was reached, an aliquot of the product solution was collected for 30 s and was treated with 10% aqueous NH_4Cl solution. Yields of desired products were determined by GC analysis using an internal standard or isolation by column chromatography. Dodecane as an internal standard was added to an aliquot of the product solution after work up.



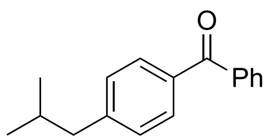
benzophenone ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80–7.78 (m, 4 H), 7.6 (tt, *J* = 7.4 Hz, 2 H), 7.46 ppm (t, *J* = 7.6 Hz, 4 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 196.7, 137.6, 132.4, 130.0, 128.2 ppm. GC-MS (EI) *m/z* Calcd for $C_{13}H_{10}O$ $[Na]^{+}$ 182.08352; Found: 182.08326.



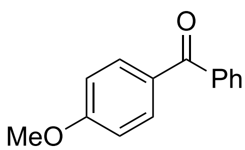
triphenylmethanol ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.19 (m, 15H), 2.85 (s, 1H); ^{13}C NMR (100MHz, $CDCl_3$) δ 146.9, 128.03, 1.28.0 127.3, 82.1. ppm. GC-MS (EI) *m/z* Calcd for $C_{19}H_{16}O$ $[Na]^{+}$ 283.18363; Found: 283.12437.



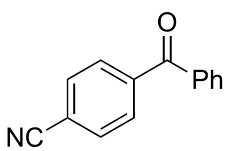
phenyl(p-tolyl)methanone ^{1}H NMR (400 MHz, $CDCl_3$):δ 7.78–7.75 (m, 2 H), 7.73 (d, *J* = 8.0 Hz, 2 H), 7.56 (tt, *J* = 7.4, 1.3 Hz, 1 H), 7.46 (t,*J* = 7.5 Hz, 2 H), 7.26 (d, *J* = 8.0 Hz, 2 H), 2.42 ppm (s, 3 H); ^{13}C NMR (100 MHz,$CDCl_3$): δ 196.5, 143.2, 137.9, 134.8, 132.1, 130.3, 129.9, 129.0, 128.2, 21.6 ppm. GC-MS (EI) *m/z* Calcd for $C_{14}H_{12}O$ $[Na]^{+}$ 219.09574; Found: 219.09548.



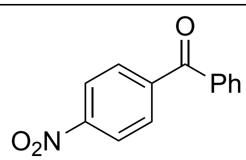
(4-isobutylphenyl)(phenyl)methanone ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.6 Hz, 2H), 7.77 (d, *J* = 7.9 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 2H), 2.58 (d, *J* = 7.2 Hz, 2H), 2.01 – 1.89 (m, 1H), 0.96 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.55, 146.99, 137.95, 135.13, 132.19, 130.20, 129.97, 129.04, 128.23, 45.44, 30.18, 22.40 ppm. GC-MS (EI) *m/z* Calcd for $C_{17}H_{18}O$ $[Na]^{+}$ 261.14685; Found: 261.14659.



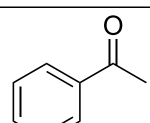
(4-methoxyphenyl)(phenyl)methanone ^{1}H NMR (400 MHz, $CDCl_3$):δ 7.81 (d, *J* = 8.0 Hz, 2 H), 7.75–7.72 (m, 2 H), 7.54 (tt, *J* = 8.0, 2.0 Hz, 1 H),7.47–7.43 (m, 2 H), 6.94 (d, *J* = 8.0 Hz, 2 H), 3.87 (s, 3 H).^{13}C NMR(100 MHz, $CDCl_3$): δ 195.6, 163.2, 138.3, 132.6, 131.9, 130.2, 129.7,128.2,113.6,55.5 ppm. GC-MS (EI) *m/z* Calcd for $C_{14}H_{12}O_2$ $[Na]^{+}$ 235.08352; Found: 235.08326.



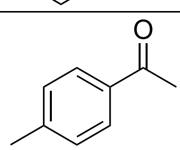
4-benzoylbenzonitrile ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.84 (m, 2H), 7.82 – 7.75 (m, 4H), 7.64 (tt, *J* =7.5, 1.4 Hz, 1H), 7.56 – 7.46 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9, 141.2, 136.3,133.3, 132.1, 130.2, 130.0, 128.6, 117.9, 115.6. ppm. GC-MS (EI) *m/z* Calcd for $C_{14}H_9NO$ $[Na]^{+}$ 230.07463; Found: 230.07437.



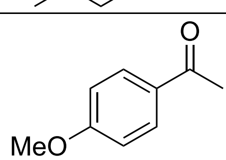
(4-nitrophenyl)(phenyl)methanone ^{1}H NMR (400 MHz, $CDCl_3$):δ 8.32 (d, *J* = 8.8 Hz, 2 H), 7.92 (d, *J* = 8.8 Hz, 2 H), 7.79–7.77 (m, 2 H), 7.64 (tt, *J* =7.4, 1.3 Hz, 1 H), 7.51 ppm (t, *J* = 7.7 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ194.8, 149.8, 142.9, 136.3, 133.5, 130.7, 130.1, 128.7, 123.5 ppm. GC-MS (EI) *m/z* Calcd for $C_{13}H_9NO_3$ $[Na]^{+}$ 250.06574; Found: 250.06548.



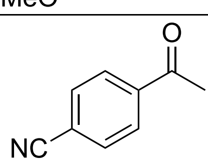
acetophenone ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.96 (m, 2H), 7.55 (t, *J* = 7.7 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 2H), 2.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.1, 137.0, 133.1, 128.5, 128.3, 26.6. ppm. GC-MS (EI) *m/z* Calcd for C_8H_8O $[Na]^{+}$ 143.06685; Found: 143.06659.



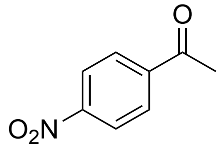
1-(p-tolyl)ethan-1-one ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 4.55 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.11, 144.10, 134.92, 129.45, 128.65, 26.75, 21.85. ppm. GC-MS (EI) *m/z* Calcd for $C_9H_{10}O$ $[Na]^{+}$ 157.07352; Found: 157.07326.



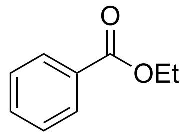
1-(4-methoxyphenyl)ethan-1-one ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 9.0 Hz, 2H), 6.92 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H), 2.54 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.00, 163.64, 130.75, 130.46, 113.83, 55.62, 26.50. ppm. GC-MS (EI) *m/z* Calcd for $C_9H_{10}O_2$ $[Na]^{+}$ 173.07354; Found: 173.07328.



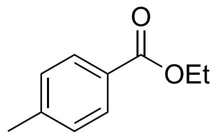
4-acetylbenzonitrile ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 8.4 Hz, 2H), 2.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 139.9, 132.5, 128.7, 117.9, 116.4, 26.7. ppm. GC-MS (EI) *m/z* Calcd for C_9H_7NO $[Na]^{+}$ 168.05361; Found: 168.05335.



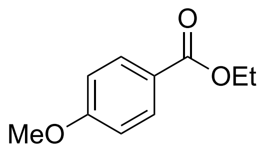
1-(4-nitrophenyl)ethan-1-one ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.6 Hz, 2H), 8.12 (d, *J* = 8.6 Hz, 2H), 2.69 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.3, 141.4, 129.3, 123.8, 27.0. ppm. GC-MS (EI) *m/z* Calcd for $C_8H_7NO_3$ $[Na]^+$ 188.05371; Found: 188.05345.



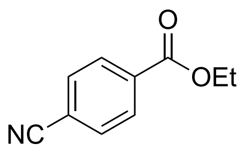
ethyl benzoate ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.04 (dt, *J* = 8.5, 1.9 Hz, 2H), 7.44 (m, 3H), 7.35-7.45 (t, 2H), 4.35 (q, *J* = 7.2 Hz, 2H), 1.36 (t, *J* = 7.2Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 166.51, 132.77, 130.48, 129.50, 128,28, 60.88, 14.29. ppm. GC-MS (EI) *m/z* Calcd for $C_9H_{10}O_2$ $[Na]^+$ 173.05372; Found: 173.05346.



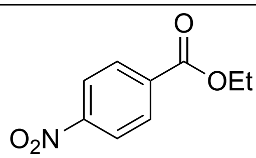
ethyl 4-methylbenzoate ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ = 7.93 (d, *J* = 7.9 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 4.36 (q, *J* = 7.1 Hz, 2H), 2.40 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 166.82, 143.51, 129.66, 129.12, 127.87, 60.85, 21.73, 14.45. ppm. GC-MS (EI) *m/z* Calcd for $C_{10}H_{12}O_2$ $[Na]^+$ 187.05382; Found: 187.05356.



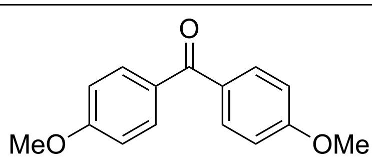
ethyl 4-methoxybenzoate ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ = 8.00 (d, *J* = 8.9 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 3.85 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 166.52, 163.36, 131.65, 123.07, 113.65, 60.75, 55.52, 14.50. ppm. GC-MS (EI) *m/z* Calcd for $C_{10}H_{12}O_3$ $[Na]^+$ 203.05371; Found: 203.05345.



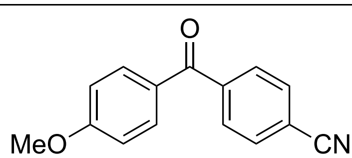
ethyl 4-cyanobenzoate ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.7 Hz, 2H), 7.74 (d, *J* = 8.7 Hz, 2H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.96, 134.32, 132.19, 130.08, 118.03, 116.30, 61.84, 14.26. ppm. GC-MS (EI) *m/z* Calcd for $C_{10}H_9NO_2$ $[Na]^+$ 198.05360; Found: 198.05334.



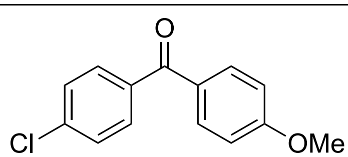
ethyl 4-nitrobenzoate ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ = 8.33 – 8.16 (m, 4H), 4.43 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 164.82, 138.79, 135.97, 130.79, 123.62, 62.09, 14.35. ppm. GC-MS (EI) *m/z* Calcd for $C_9H_9NO_4$ $[Na]^+$ 218.05349; Found: 218.05323.



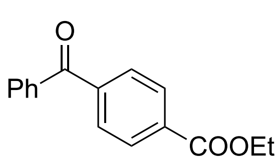
bis(4-methoxyphenyl)methanone ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.83 (d, *J* = 9.0 Hz, 1H), 6.92 – 7.02 (d, *J* = 8.9 Hz, 2H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.82, 162.91, 132.33, 130.85, 113.54, 77.26, 55.54. ppm. GC-MS (EI) *m/z* Calcd for $C_{15}H_{14}O_3$ $[Na]^+$ 265.05338; Found: 265.05312.



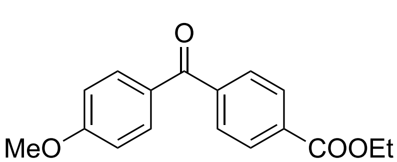
4-(4-methoxybenzoyl)benzonitrile ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ = 7.79 (q, *J* = 8.0 Hz, 6H), 6.98 (d, *J* = 8.6 Hz, 2H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ = 193.9, 164.1, 142.3, 132.8, 132.3, 130.1, 129.1, 118.3, 115.3, 114.1, 55.8. ppm. GC-MS (EI) *m/z* Calcd for $C_{15}H_{11}NO_2$ $[Na]^+$ 260.05327; Found: 260.05301.



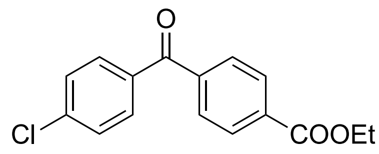
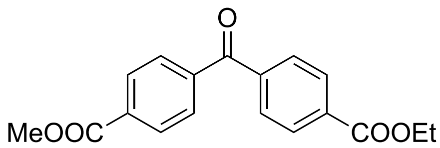
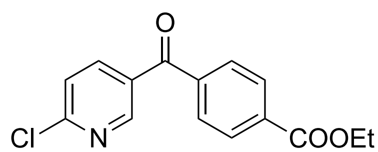
(4-chlorophenyl)(4-methoxyphenyl)methanone ^{1}H NMR (400MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.8 Hz, 2H), 7.72 (d, *J* = 8.7 Hz, 2H), 7.46 (d, *J* =8.6 Hz, 2H), 6.98 (d, *J* = 8.9 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4, 163.5, 138.4, 136.7, 132.6, 131.3, 129.9, 128.7, 113.8, 77.2, 55.7. ppm. GC-MS (EI) *m/z* Calcd for $C_{14}H_{11}ClO_2$ $[Na]^+$ 269.05371; Found: 269.05345.

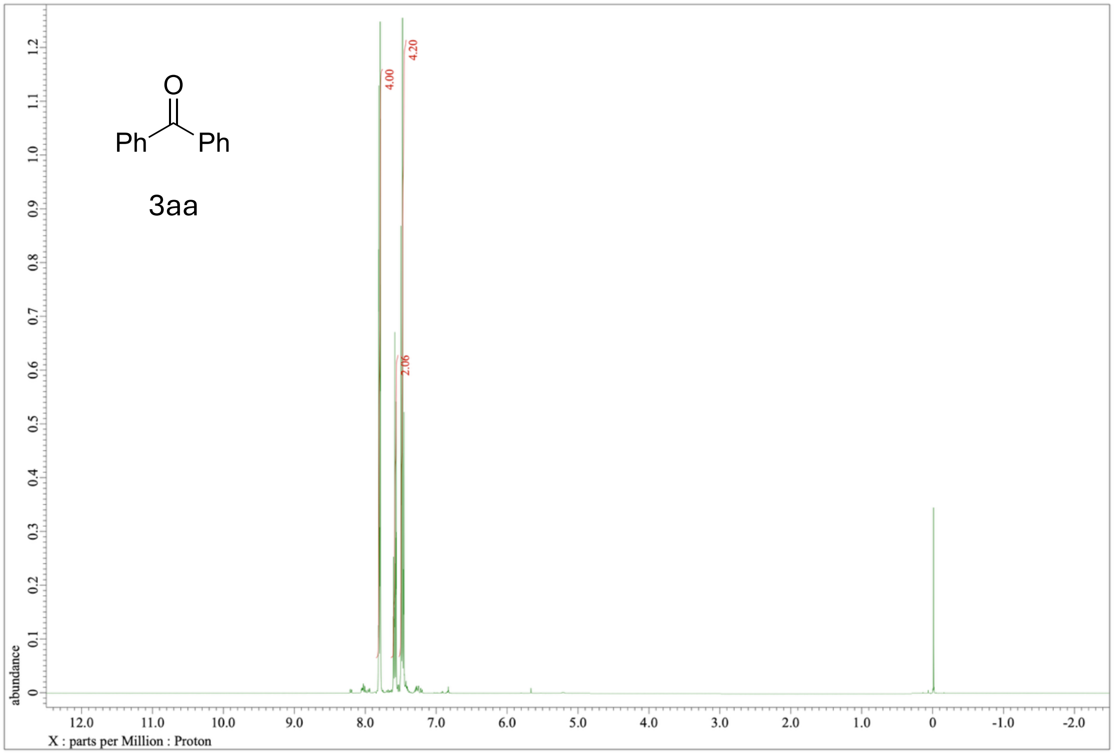


ethyl 4-benzoylbenzoate ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.4 Hz, 2H), 7.80 (d, *J* = 8.4 Hz, 2H), 7.78 - 7.75 (m, 2H), 7.59 - 7.55 (m, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 4.39 (d, *J* = 7.2 Hz, 2H), 1.39 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.9, 165.7, 141.2, 136.9, 133.6, 132.9, 130.1, 129.7, 129.5, 128.4, 61.4, 14.3. ppm. GC-MS (EI) *m/z* Calcd for $C_{16}H_{14}O_3$ $[Na]^+$ 277.05382; Found: 277.05356.



ethyl 4-(4-methoxybenzoyl)benzoate ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 6.8 Hz, 1.6 Hz, 2H), 7.84-7.77 (m, 4H), 6.97 (dd, *J* = 6.8 Hz, 2.0 Hz, 2H), 4.42 (q, *J* = 7.1 Hz, 2H), 3.90 (s, 3H),1.42 (t, *J* = 7.19 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.2, 166.3, 164.0, 142.4, 133.5, 133.0, 130.0, 129.9, 114.1, 61.8, 55.9, 14.7. ppm. GC-MS (EI) *m/z* Calcd for $C_{17}H_{15}O_4$ $[Na]^+$ 307.05393; Found: 307.05367.

	**ethyl 4-(4-chlorobenzoyl)benzoate** ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.2 Hz, 2H), 7.79 (d, *J* = 8.6 Hz, 2H), 7.74 (d, *J* = 8.7 Hz, 2H), 7.46 (d, *J* = 8.7 Hz, 2H), 4.41 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.8, 165.7, 140.8, 139.5, 135.2, 133.8, 131.4, 129.5 (2C), 128.8, 61.5, 14.3. ppm. GC-MS (EI) *m/z* Calcd for $C_{16}H_{13}ClO_3$ $[Na]^+$ 288.05371; Found: 288.05345.
	**ethyl 4-(4-(methoxycarbonyl)benzoyl)benzoate** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.3 Hz, 2H), 8.19 (d, *J* = 8.3 Hz, 2H), 8.07 (s, 1H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.65 (t, *J* = 7.8 Hz, 1H), 4.07 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 195.3, 166.1, 165.9, 140.6, 140.4, 134.0, 133.9, 129.8, 129.7, 129.6, 129.5, 61.5, 52.5, 14.3. ppm. GC-MS (EI) *m/z* Calcd for $C_{18}H_{16}O_5$ $[Na]^+$ 335.05324; Found: 335.05318.
	**ethyl 4-(6-chloronicotinoyl)benzoate** ^{1}H NMR (400 MHz, $CDCl_3$) δ. 8.78 (d, *J* = 2.4 Hz, 1H), 8.20 (ABq, *J* = 8.5 Hz, 2H), 8.12 (dd, *J* = 2.4, 8.3 Hz, 1H), 7.85 (ABq, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.3 Hz, 1H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.44 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 193.0, 165.5, 155.4, 151.2, 139.8, 134.5, 131.4, 129.8, 129.6, 124.5, 61.6, 14.3.ppm. GC-MS (EI) *m/z* Calcd for $C_{15}H_{12}ClNO_3$ $[Na]^+$ 312.05378; Found: 312.05356.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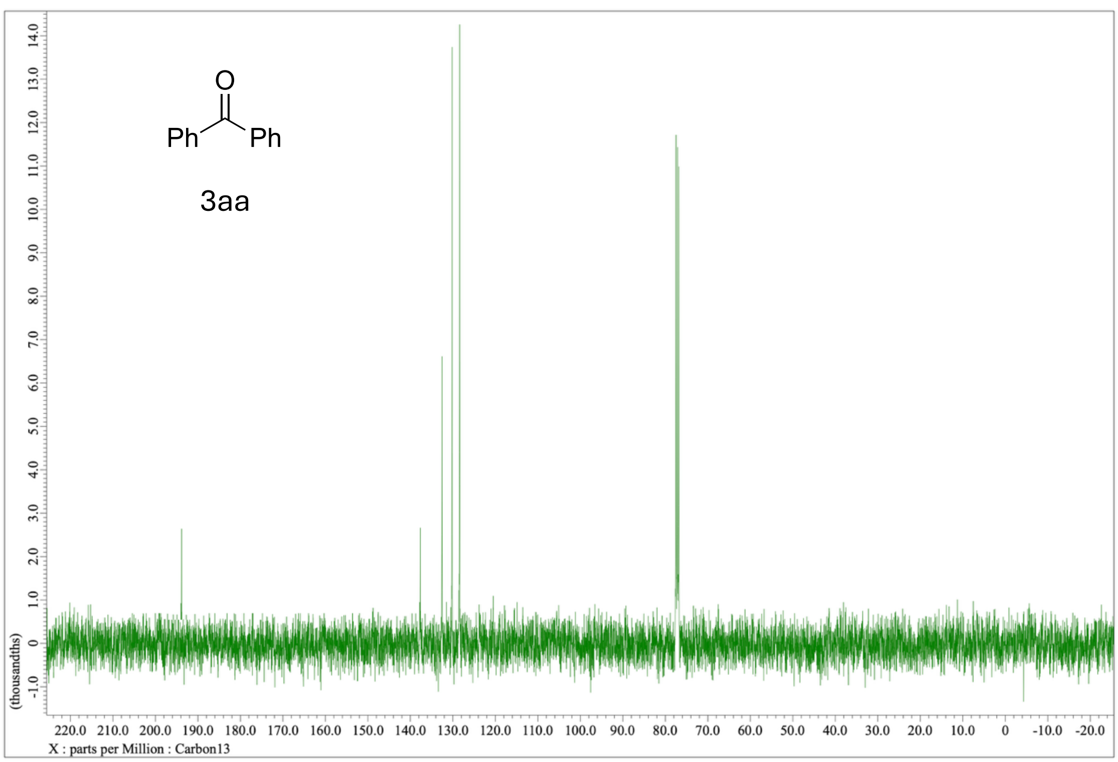
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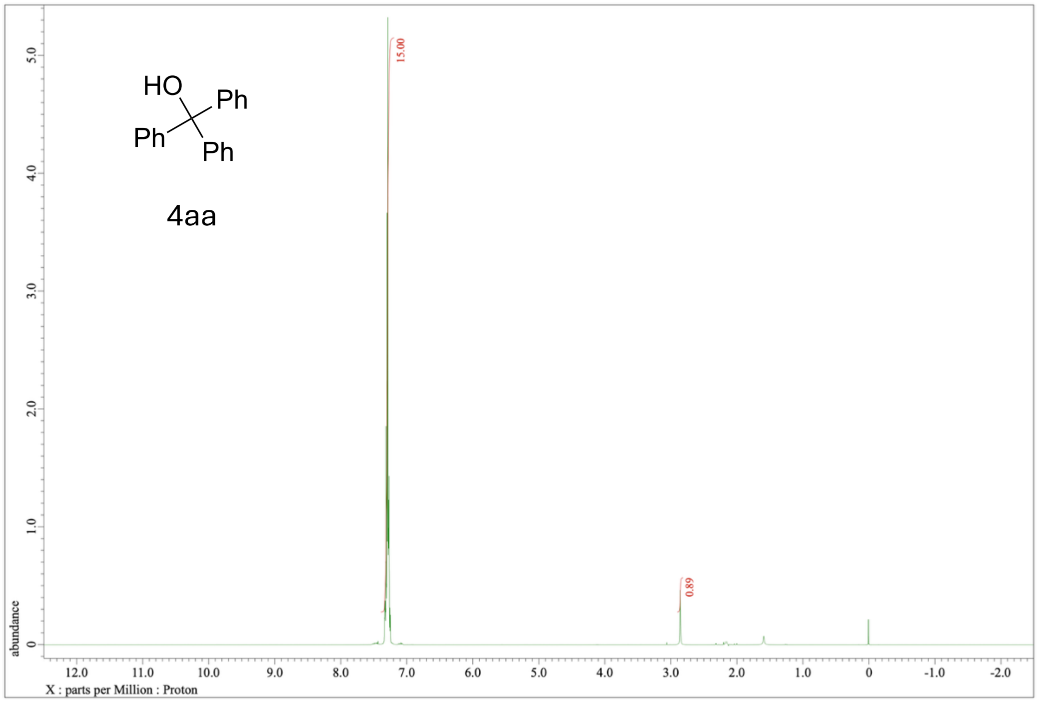
X : parts per Million : Carbon13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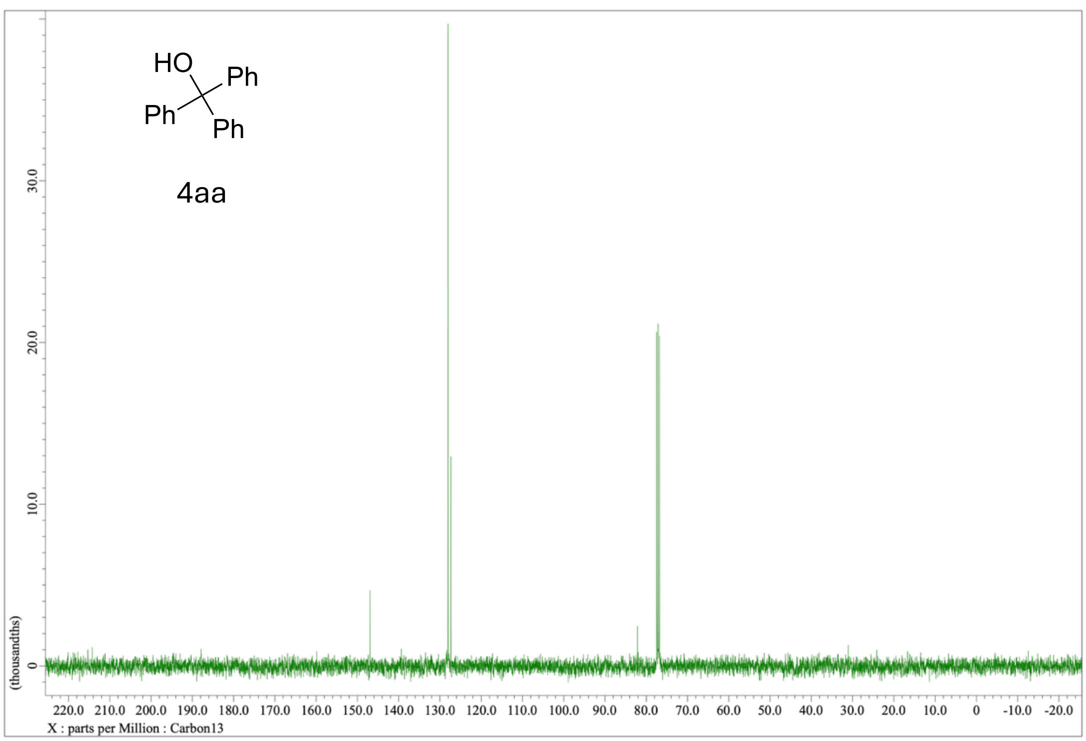
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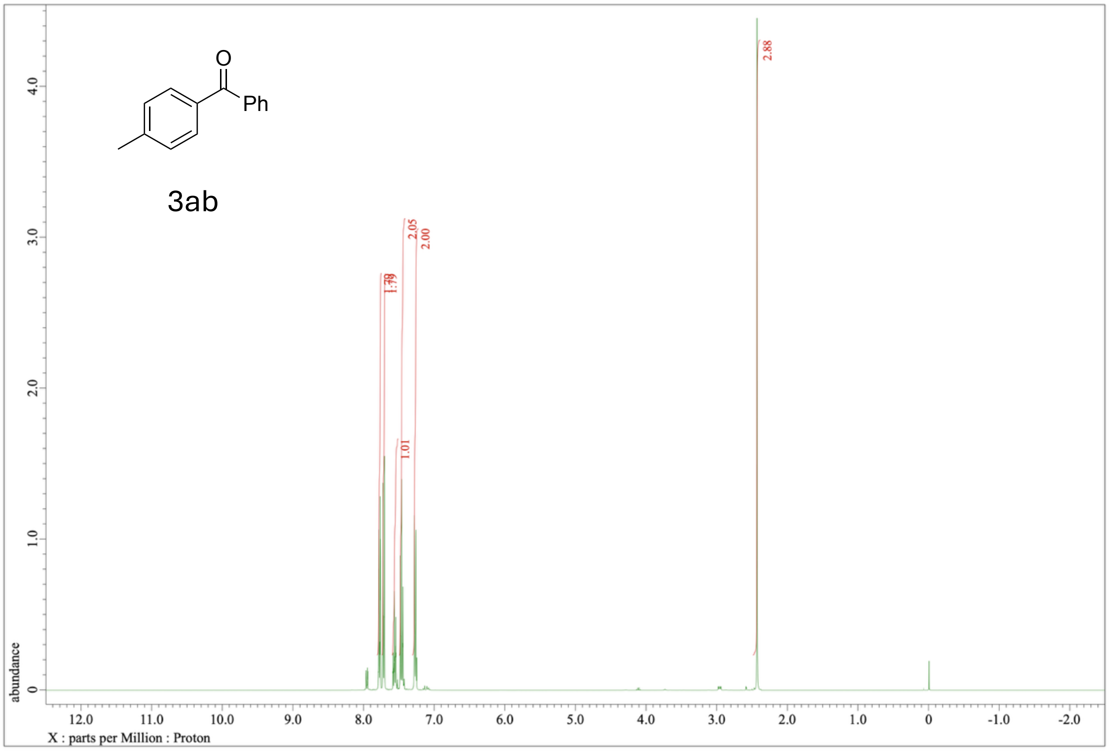
Ph
Ph
Ph
4aa
(thousandths)
X : parts per Million : Carbon13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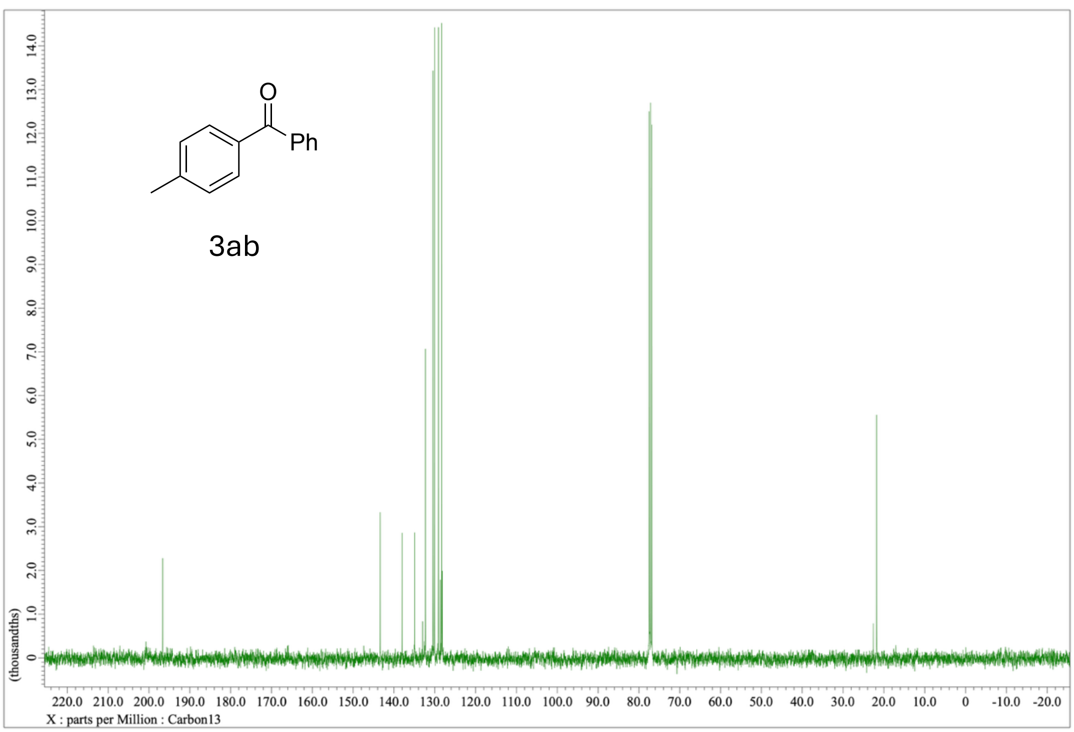
2.00
1.01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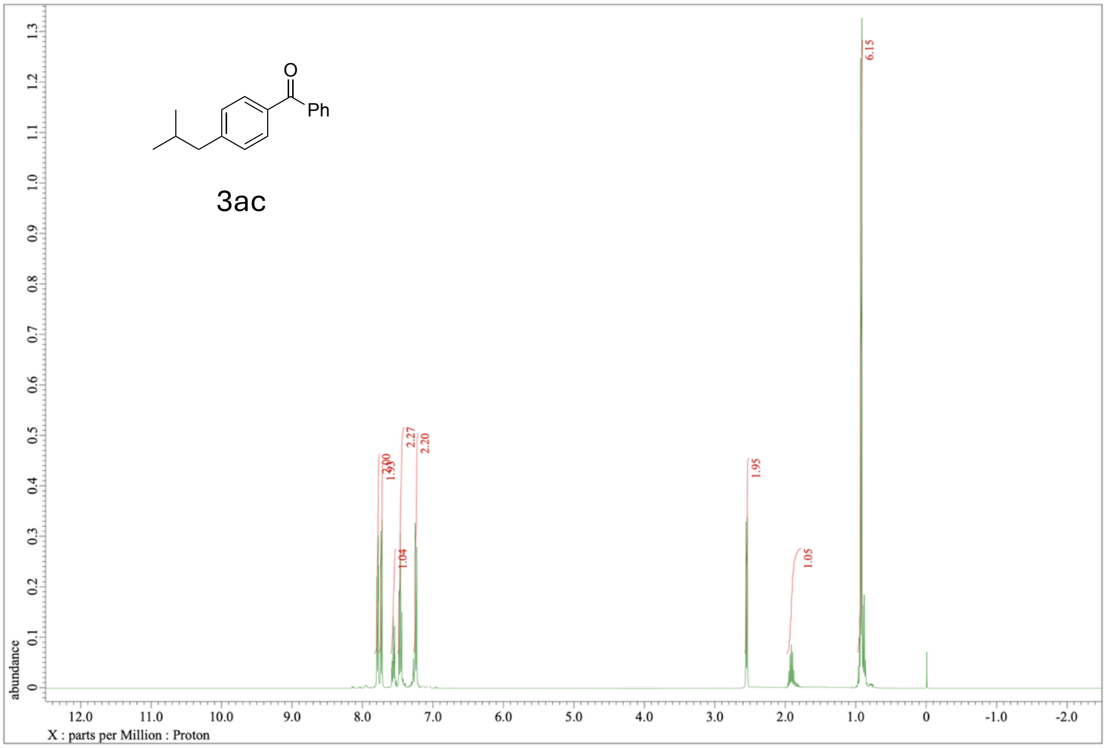
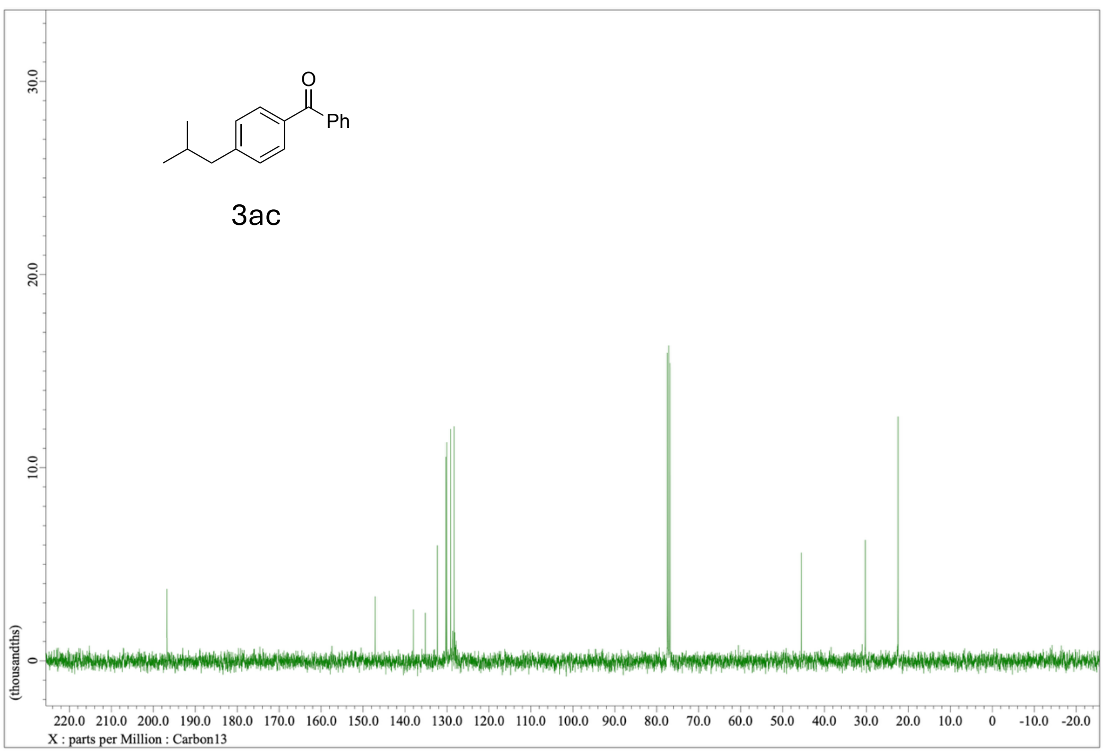
(thousandths)
X : parts per Million : Carbon13



3ac
abundance
X : parts per Million : Proton



3ac
(thousandths)
X : parts per Million : Carbon13


MeO
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Ph
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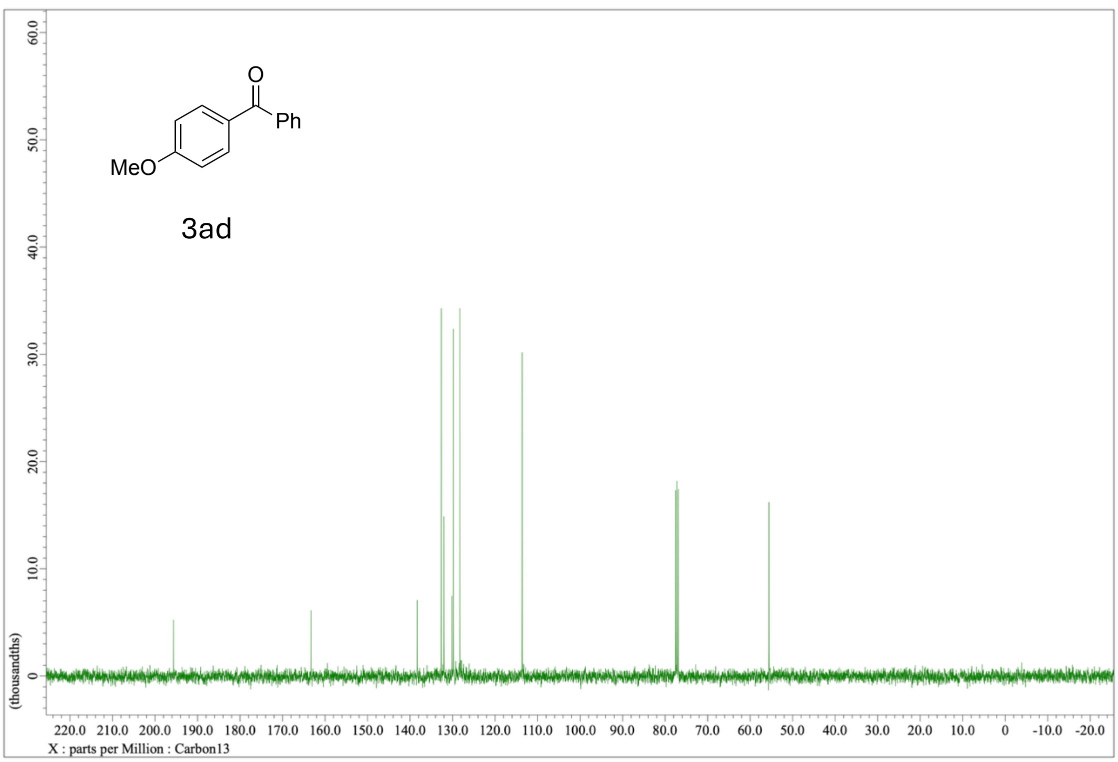
abundance
X : parts per Million : Proton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Ph
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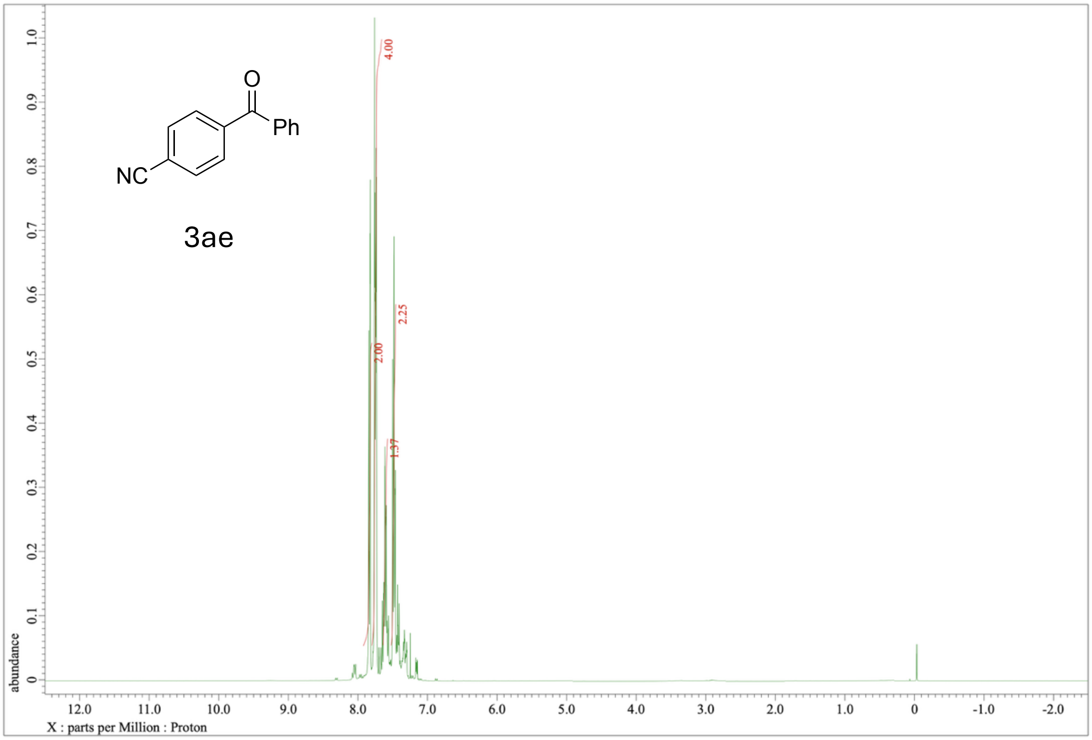
(thousandths)
X : parts per Million : Carbon13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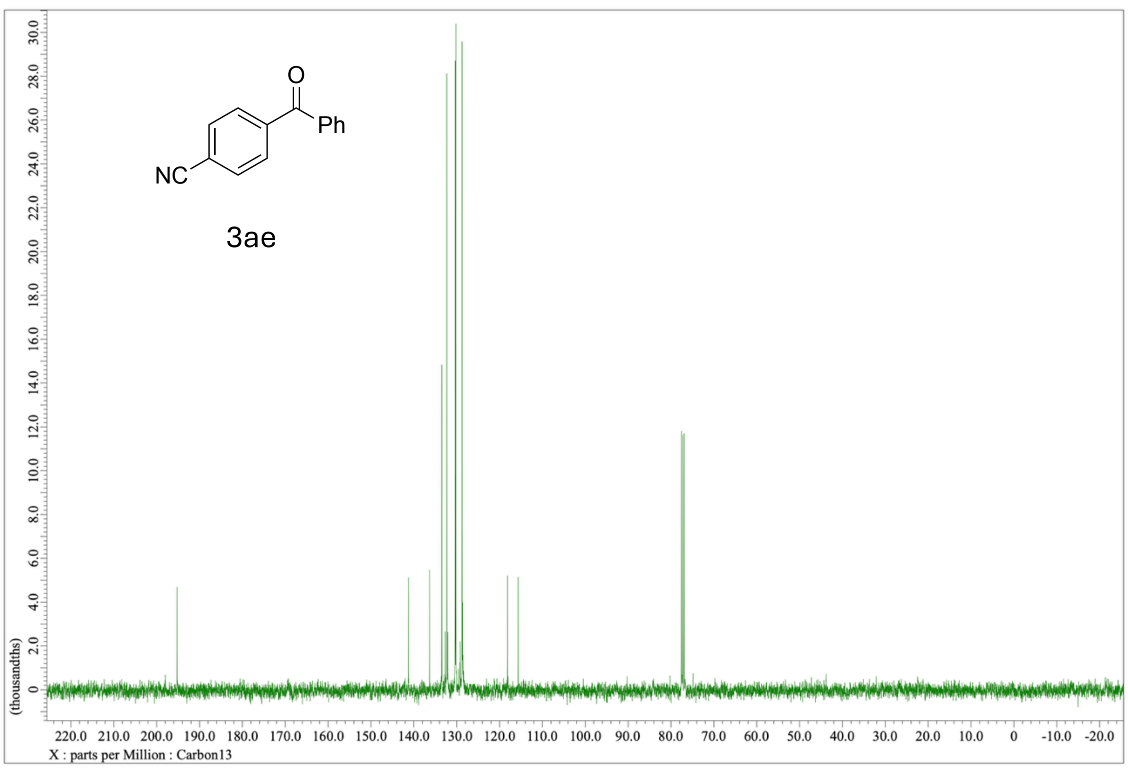
X : parts per Million : Proton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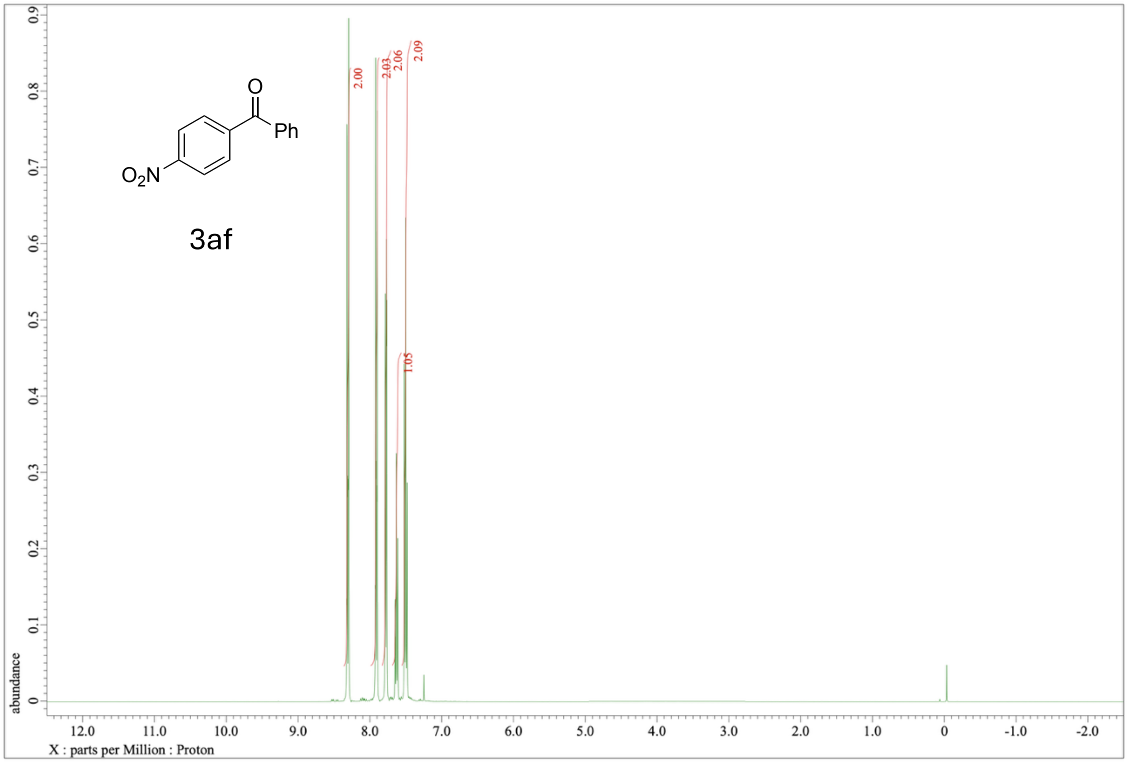
(thousandths)
X : parts per Million : Carbon13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O₂N
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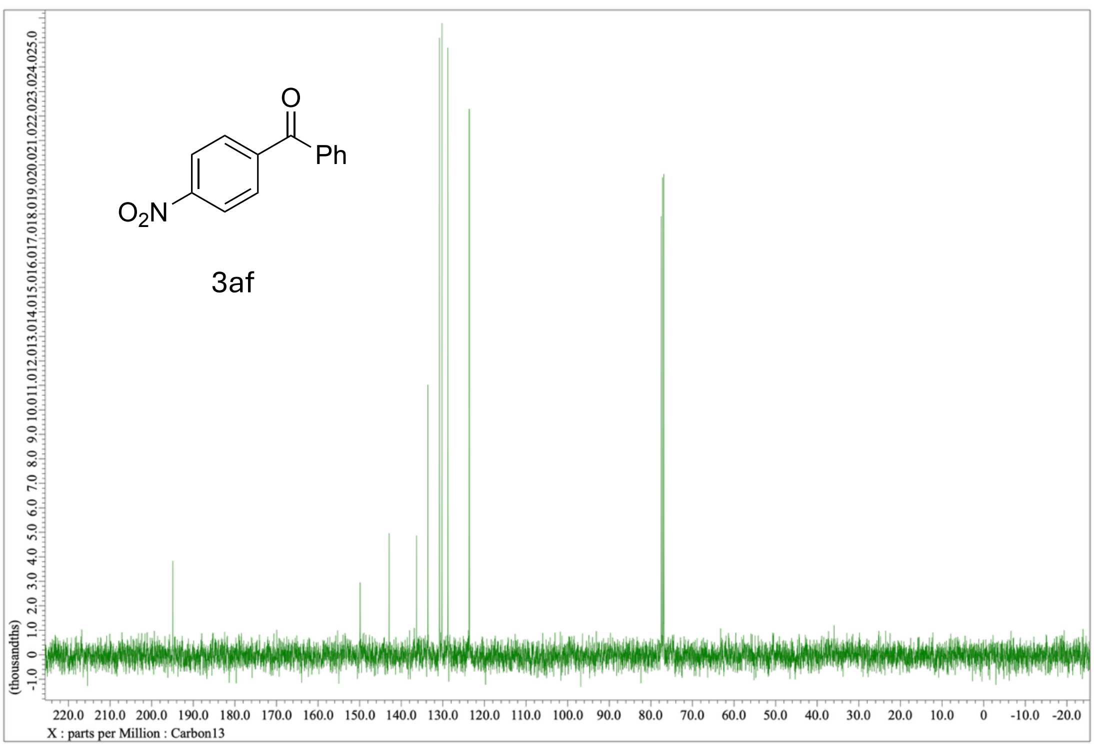
X : parts per Million : Proton
abundance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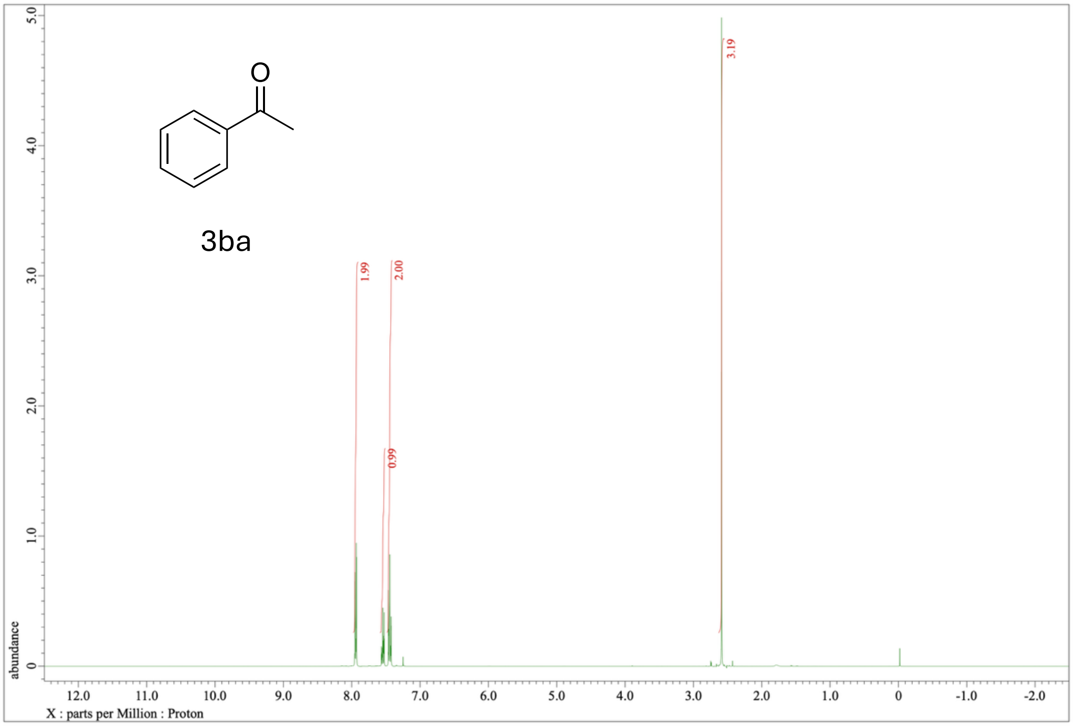
X : parts per Million : Carbon13
(thousandths)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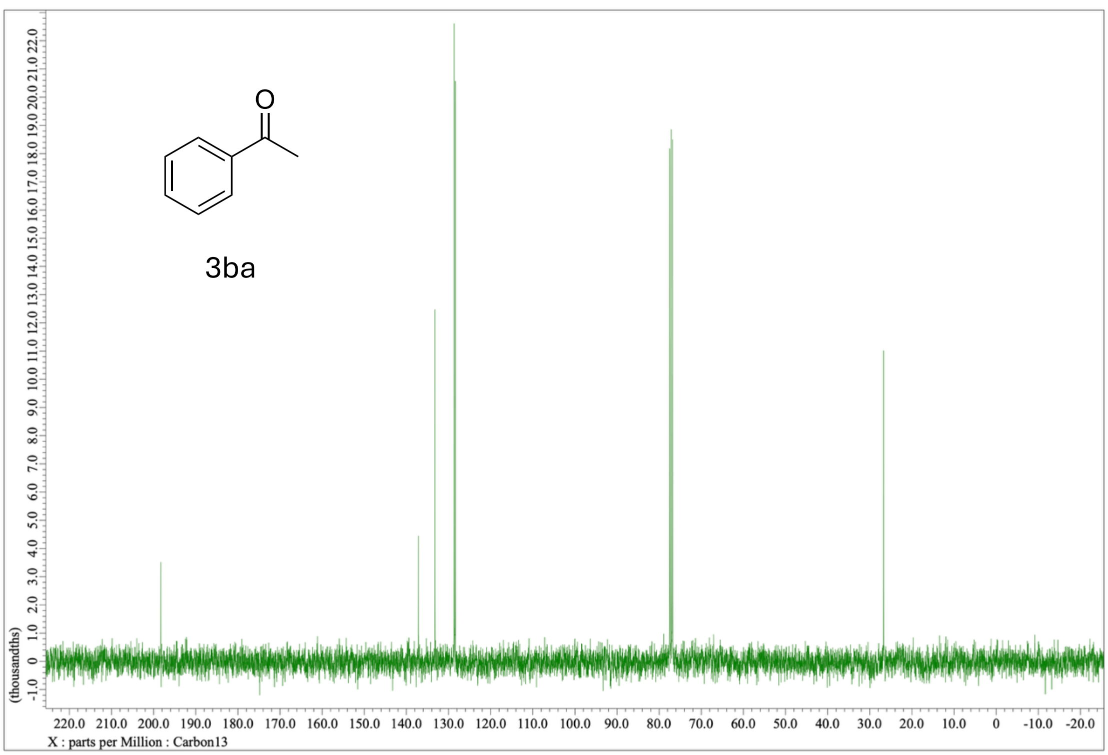
abundance
X : parts per Million : Proton


3ba
(thousandths)
X : parts per Million : Carbon13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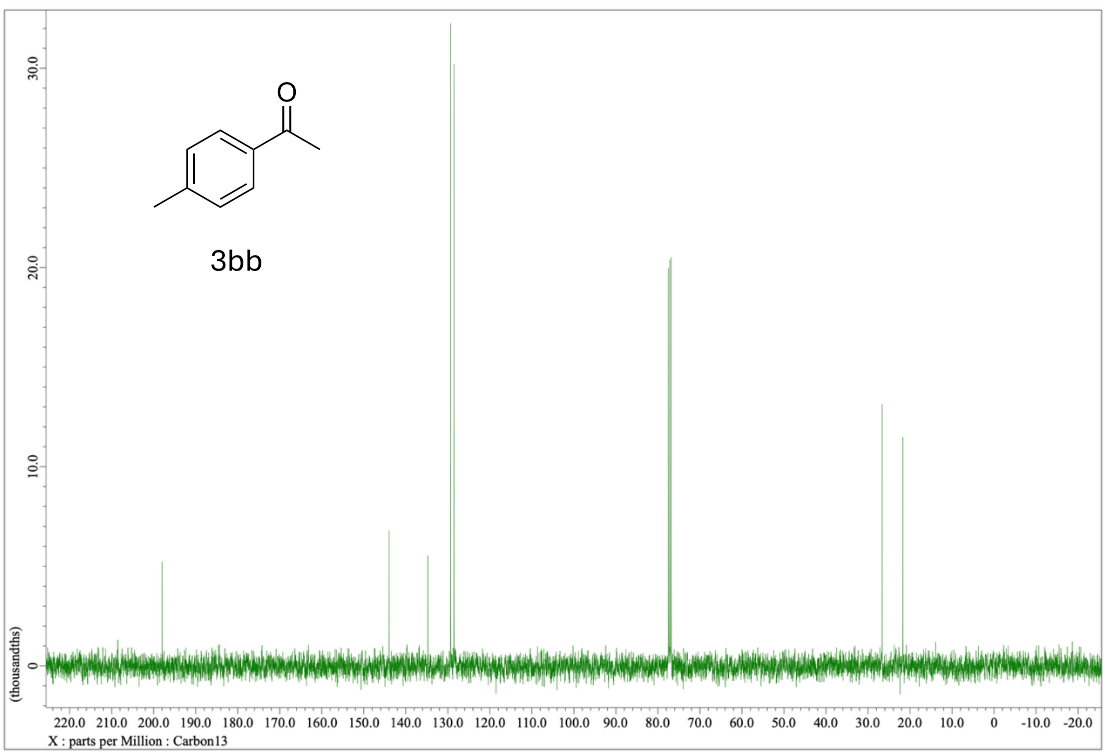
2.01
3.21
3.23
abundance
X : parts per Million : Proton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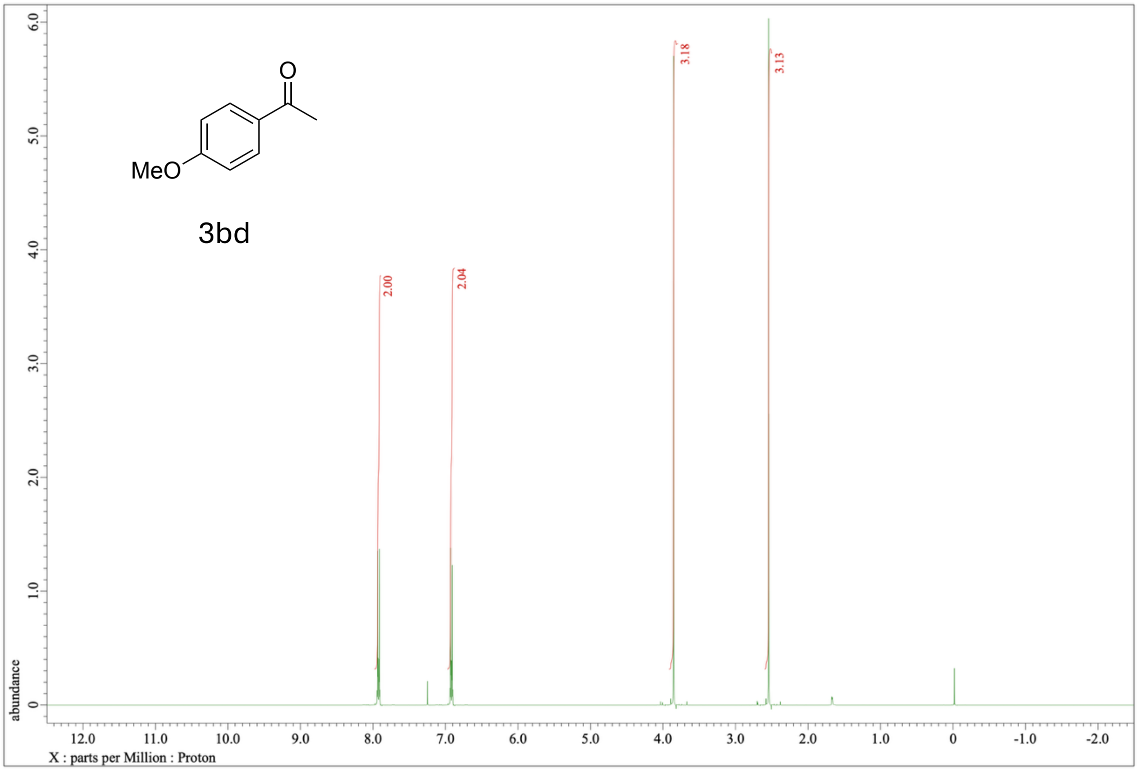
(thousandths)
X : parts per Million : Carbon13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3bd
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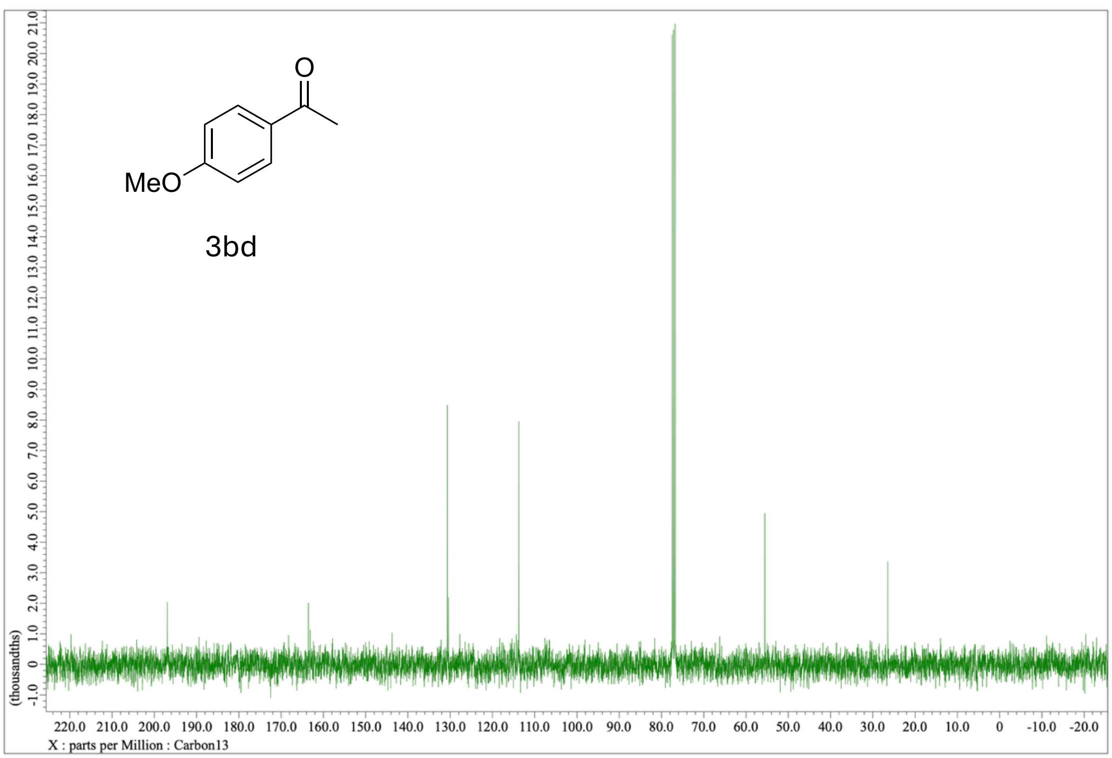
3.18
3.13
abundance
X : parts per Million : Proton


MeO
O
3bd
(thousandths)
X : parts per Million : Carbon13


NC
O
3be
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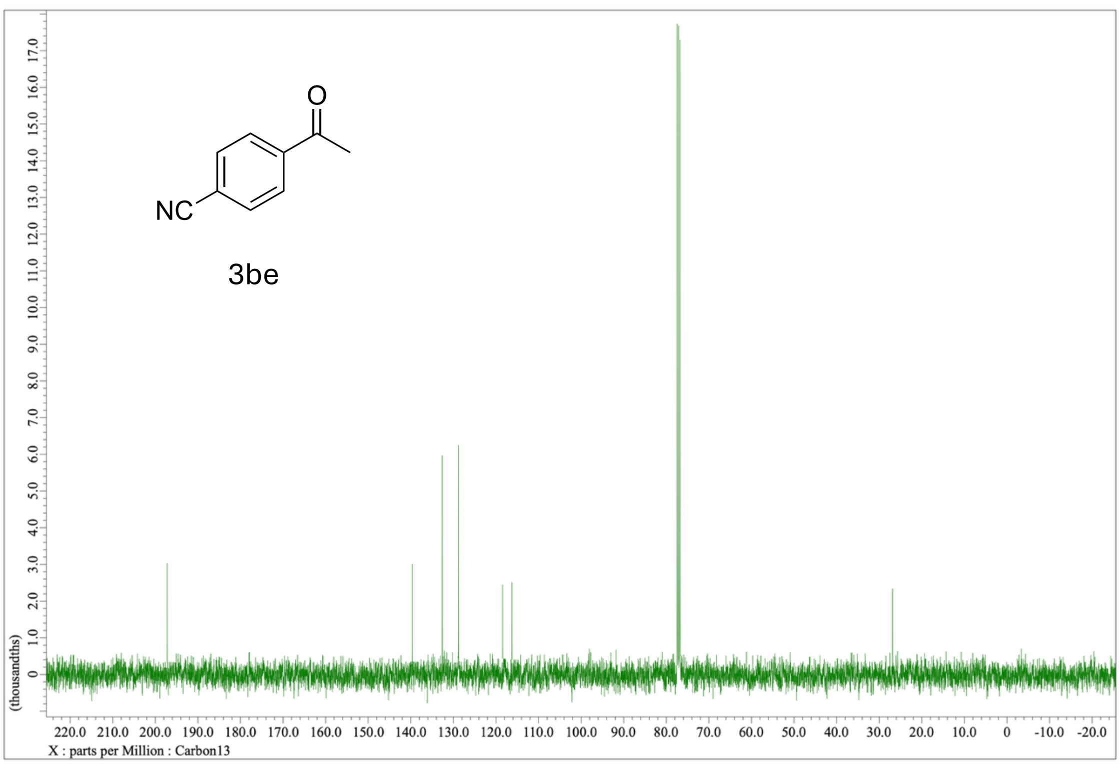
2.06
3.19
abundance
X : parts per Million : Proton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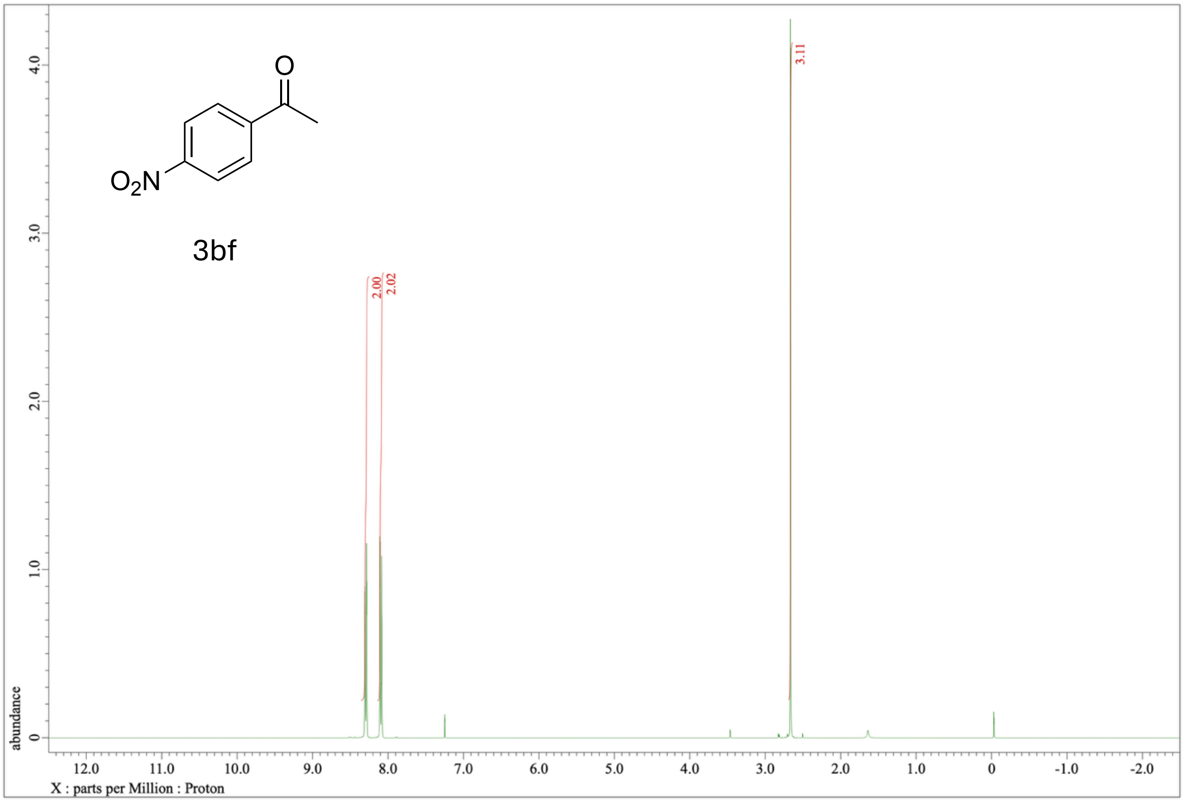
O
3be
(thousandths)
X : parts per Million : Carbon13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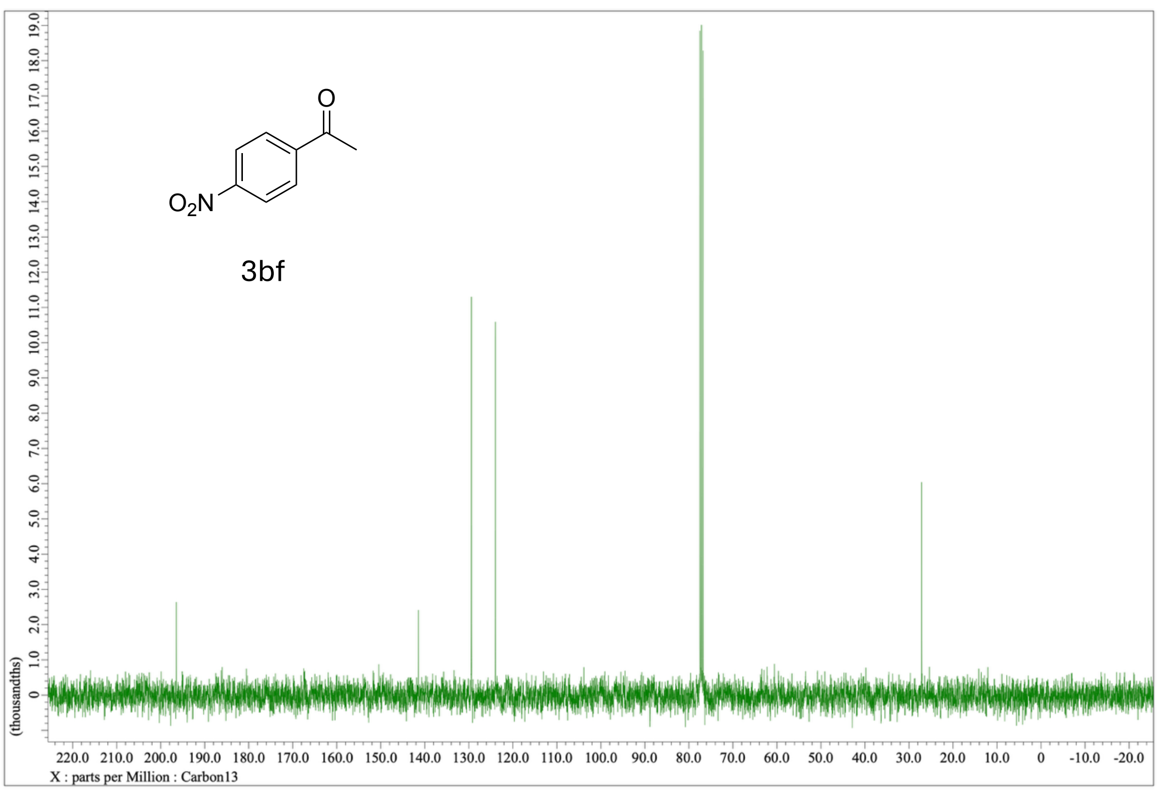
2.02
3.11
abundance
X : parts per Million : Proton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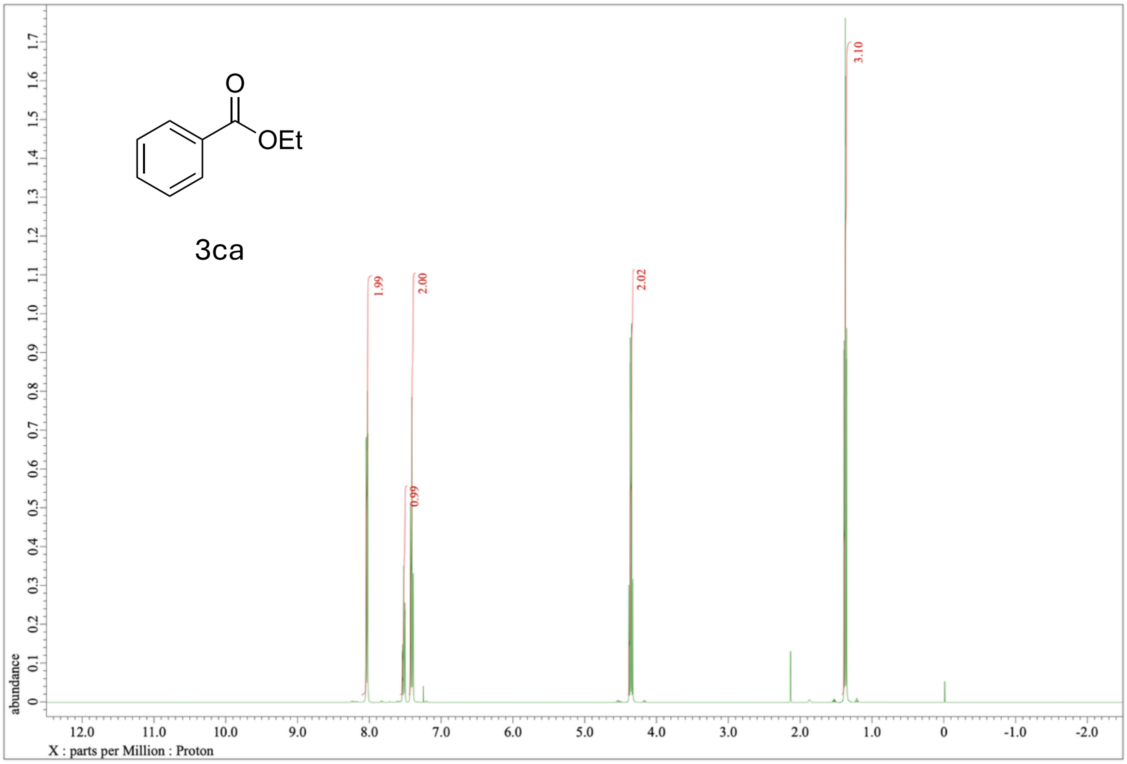
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abundance
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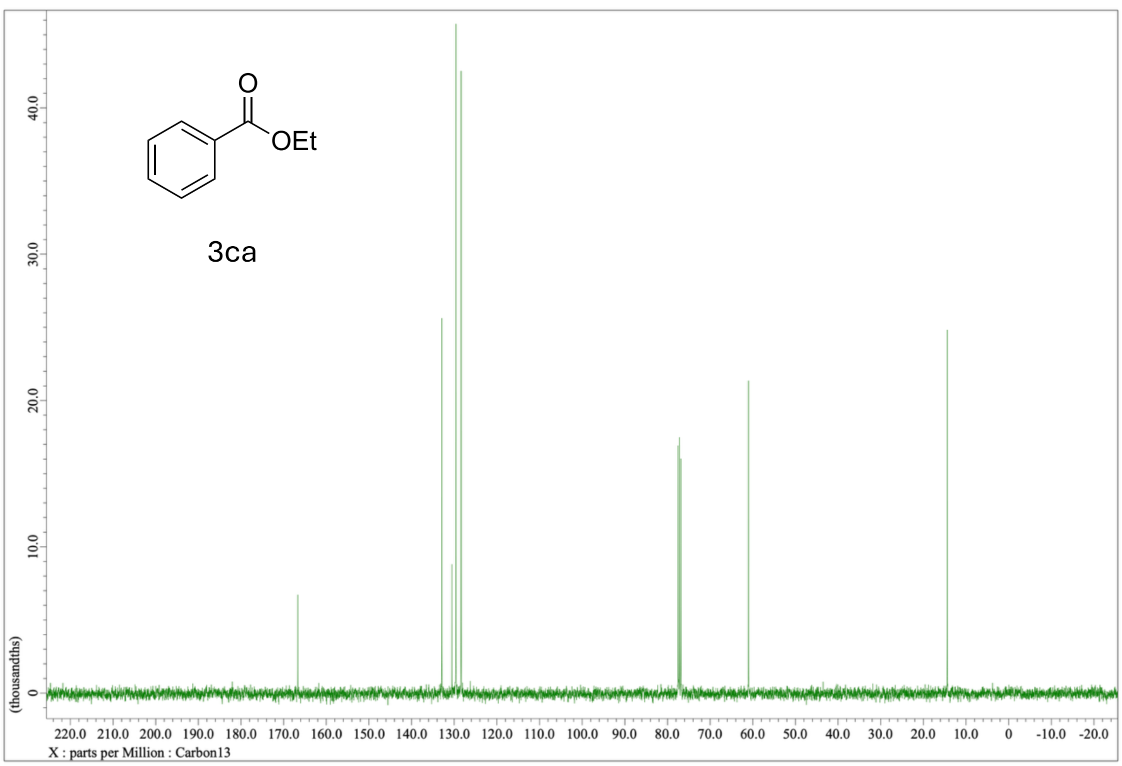
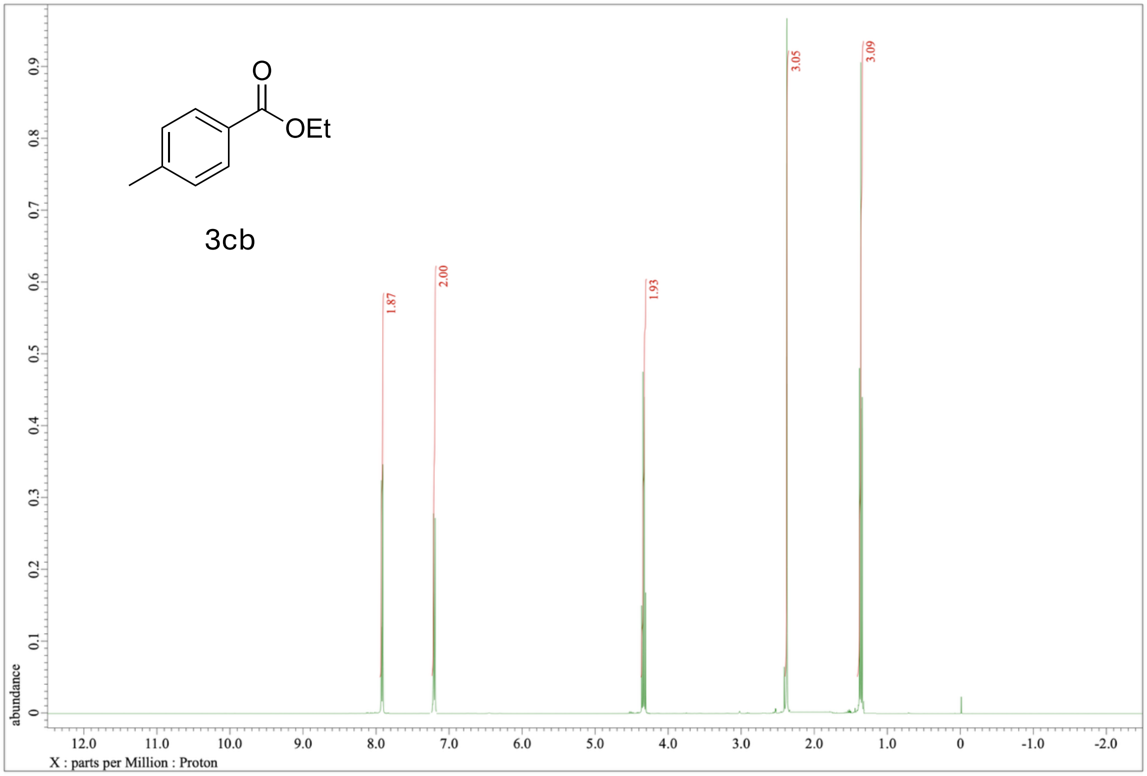
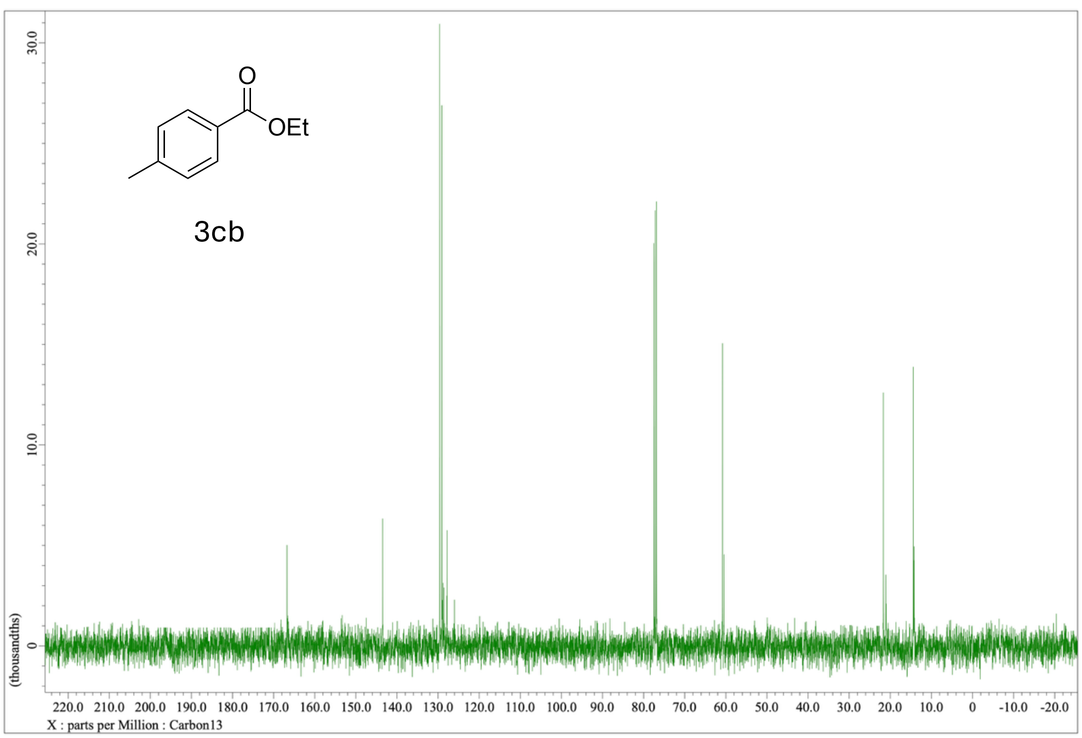
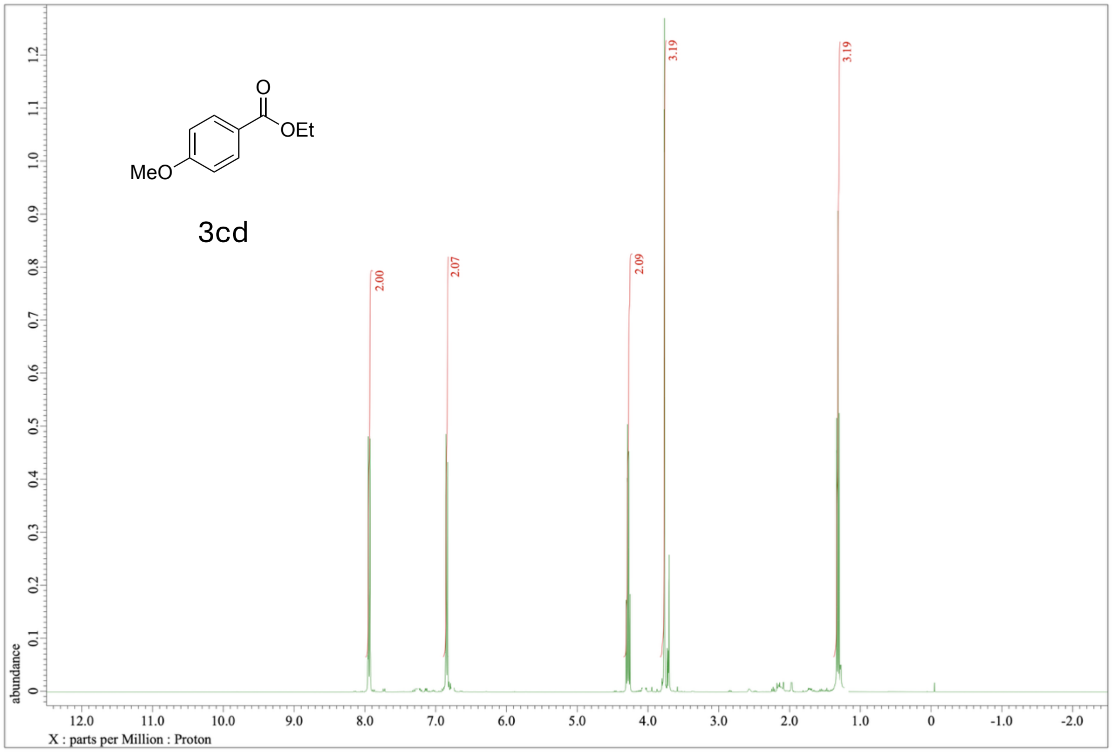
0.99
2.02
3.10
X : parts per Million : Proton

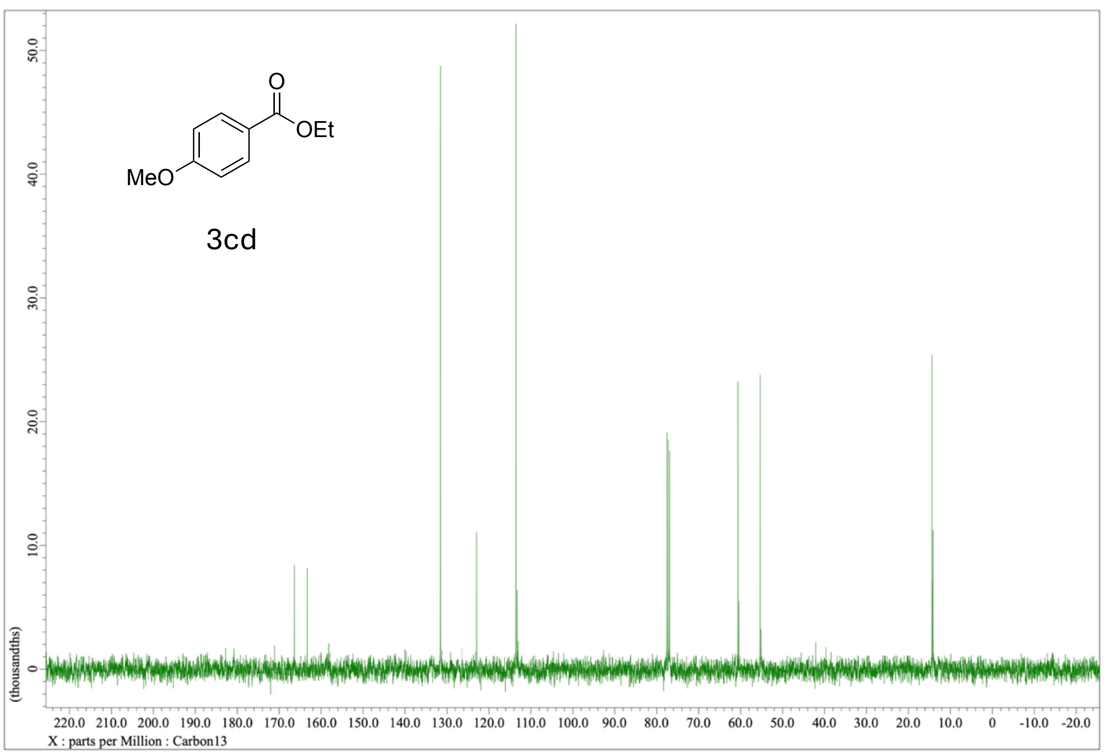

O
OEt
3ca
(thousandths)
X : parts per Million : Carbon13


OEt
3cb
1.87
2.00
1.93
3.05
3.09
abundance
X : parts per Million : Proton

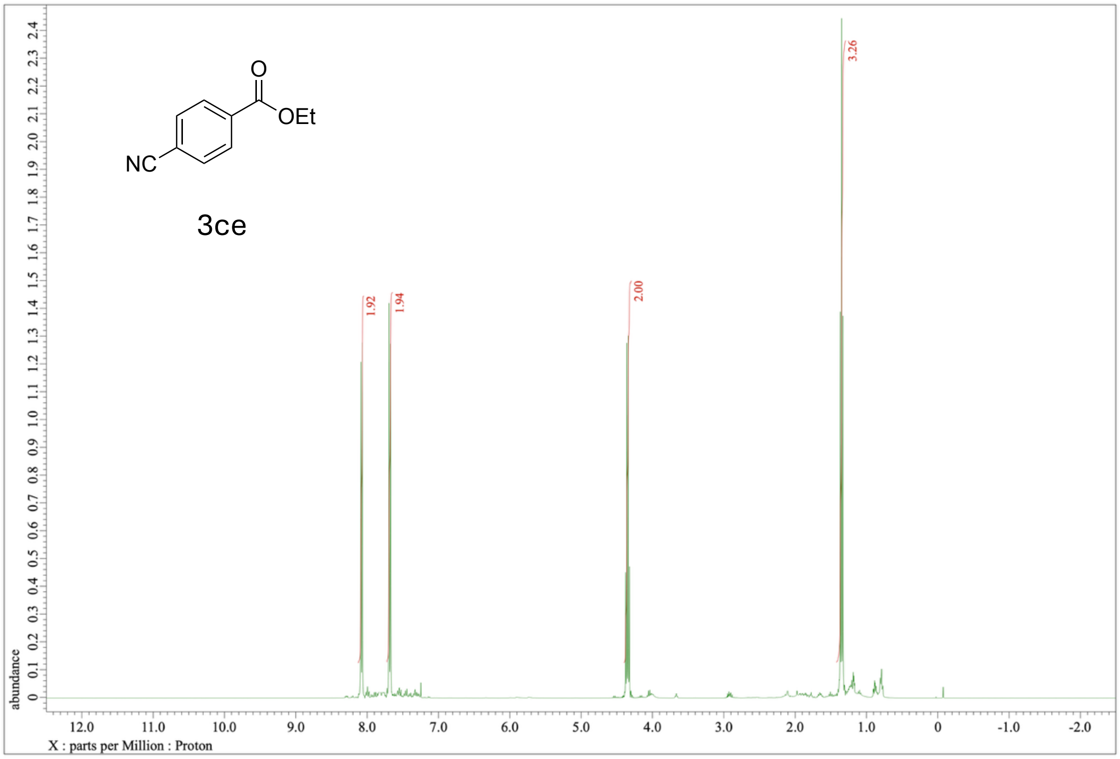

OEt
3cb
(thousandths)
X : parts per Million : Carbon13


O
OEt
MeO
2.00
2.07
2.09
3.19
3.19
abundance
X : parts per Million : Proton

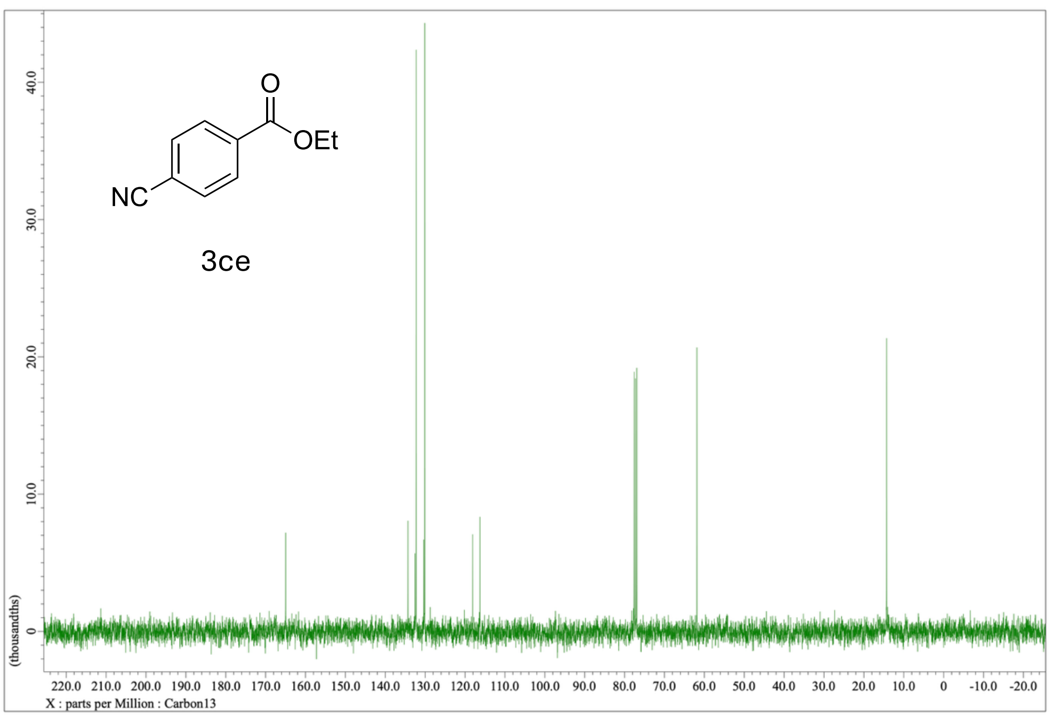
3cd


O
OEt
MeO
(thousandths)
X : parts per Million : Carbon13

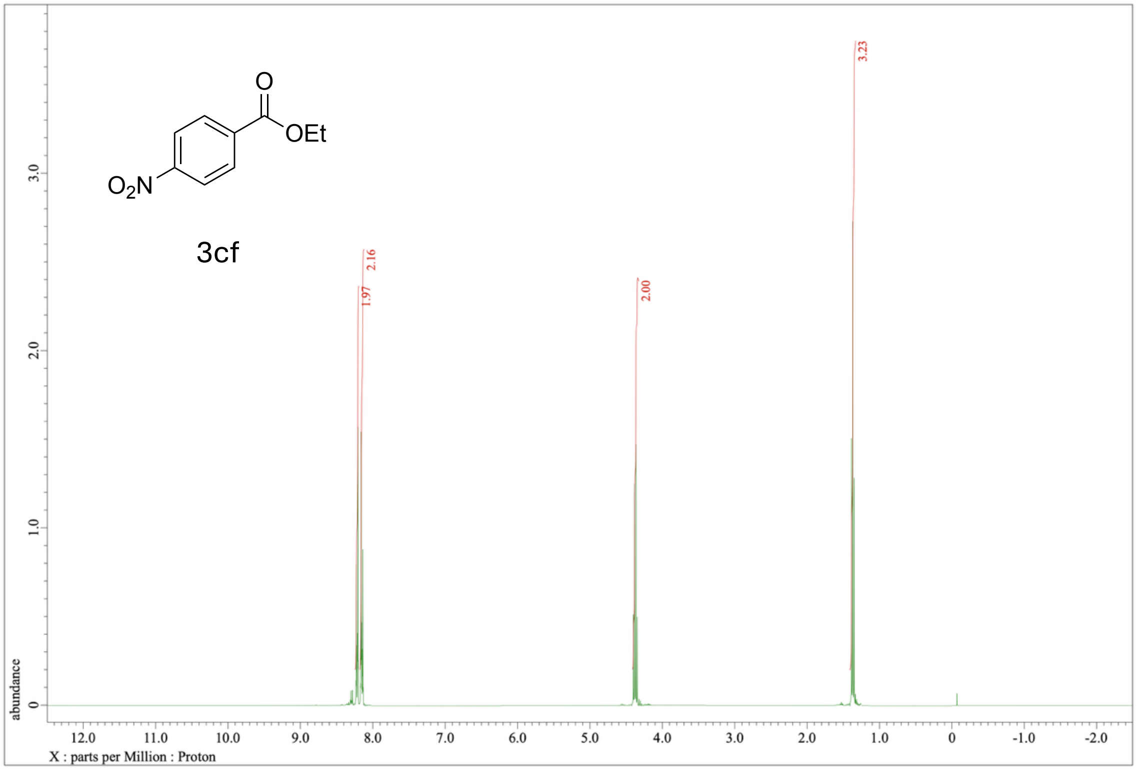
3cd

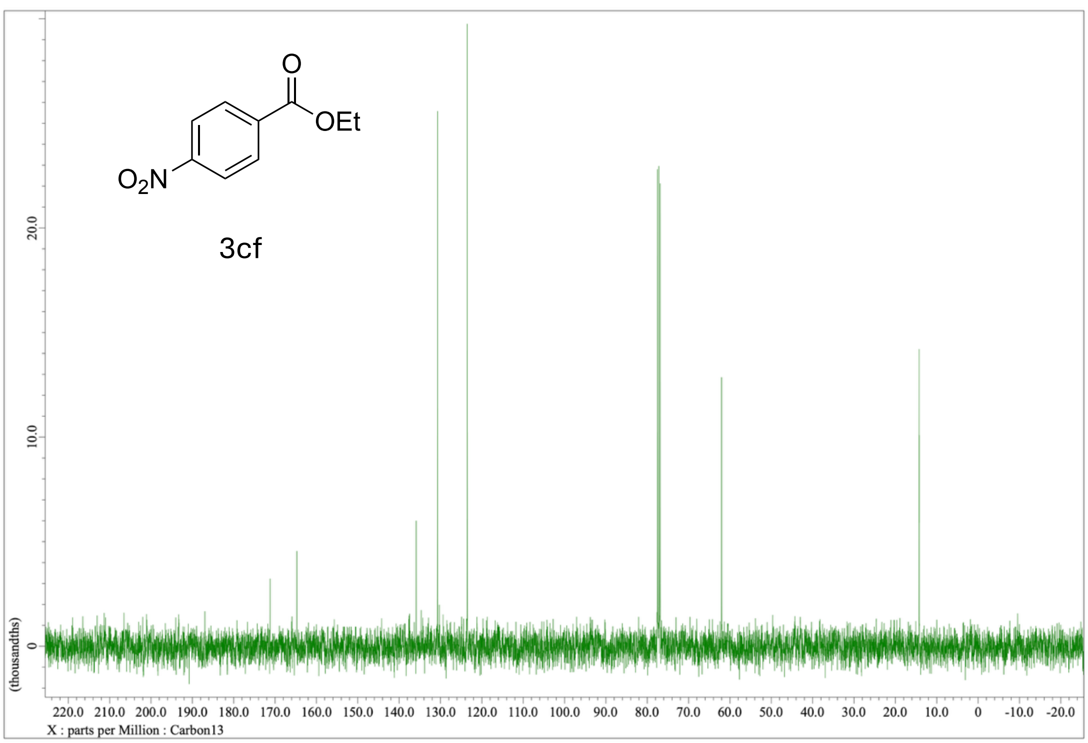


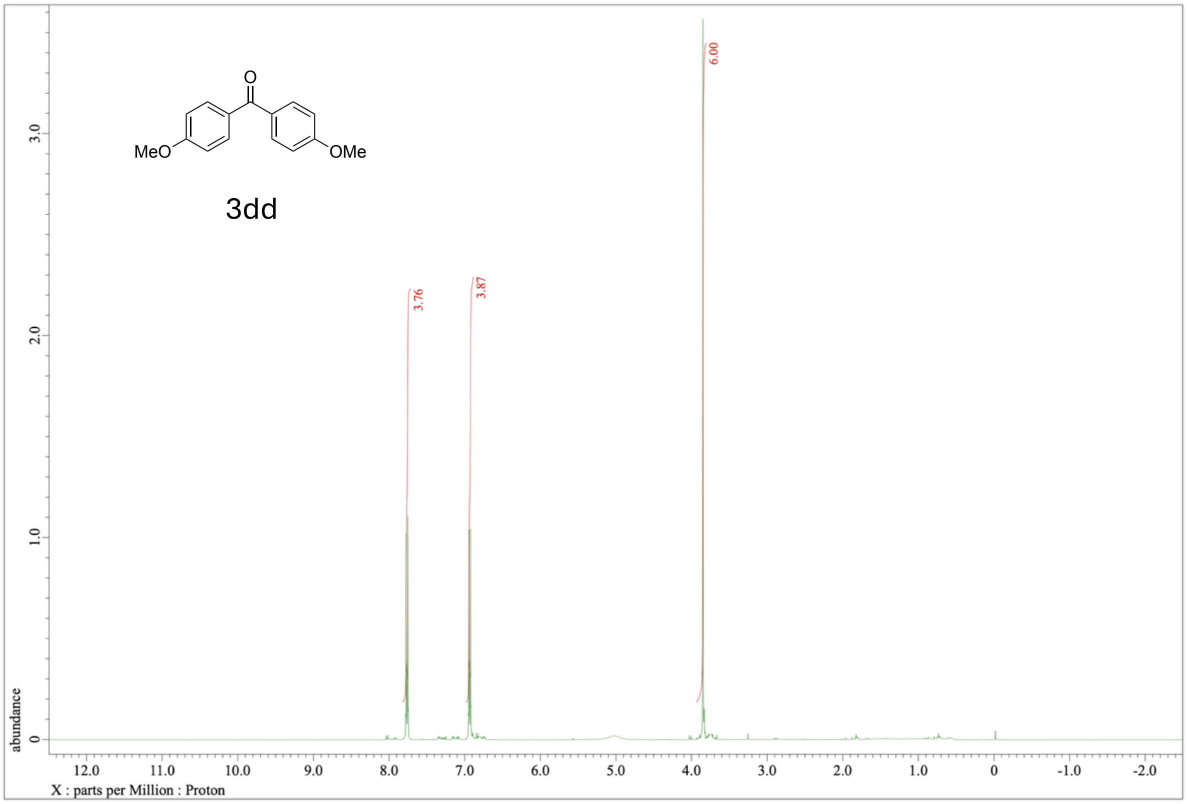
O
OEt
NC
3ce
1.92
1.94
2.00
3.26
abundance
X : parts per Million : Proton



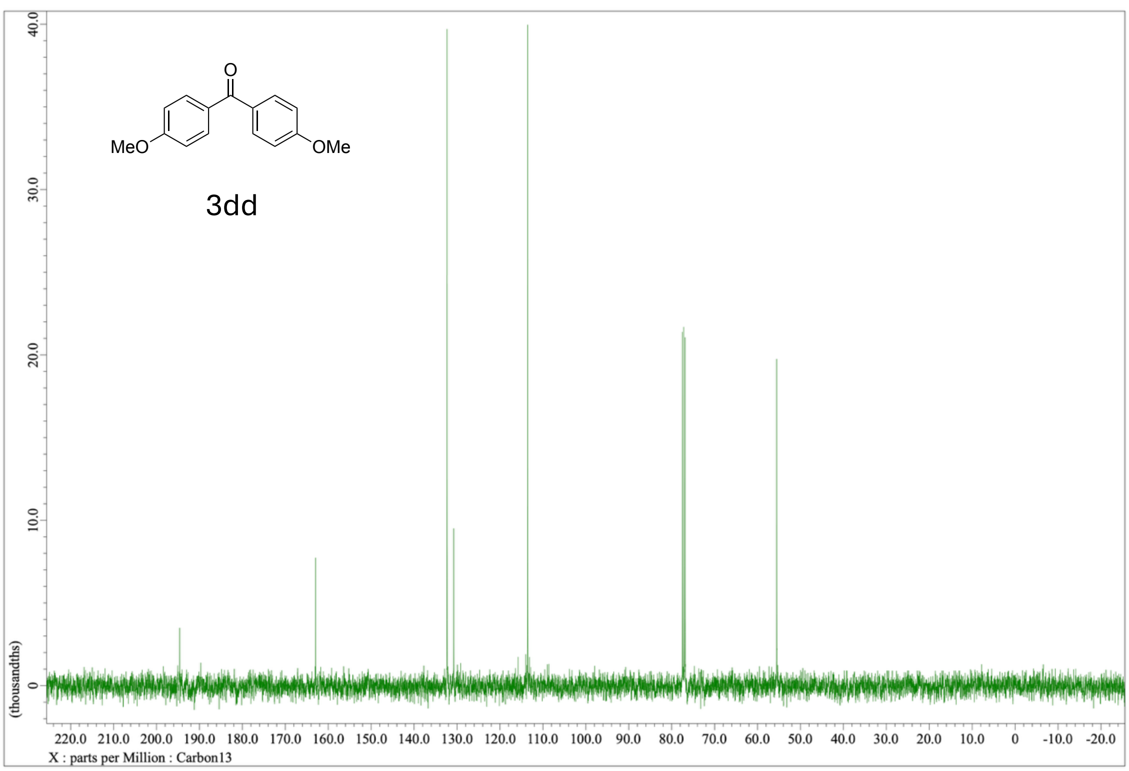
O
OEt
NC
3ce
(thousandths)
X : parts per Million : Carbon13


O
OEt
O2N
3cf
1.97
2.16
2.00
3.23
abundance
X : parts per Million : Proton


O
OEt
O2N
3cf
(thousandths)
X : parts per Million : Carbon13

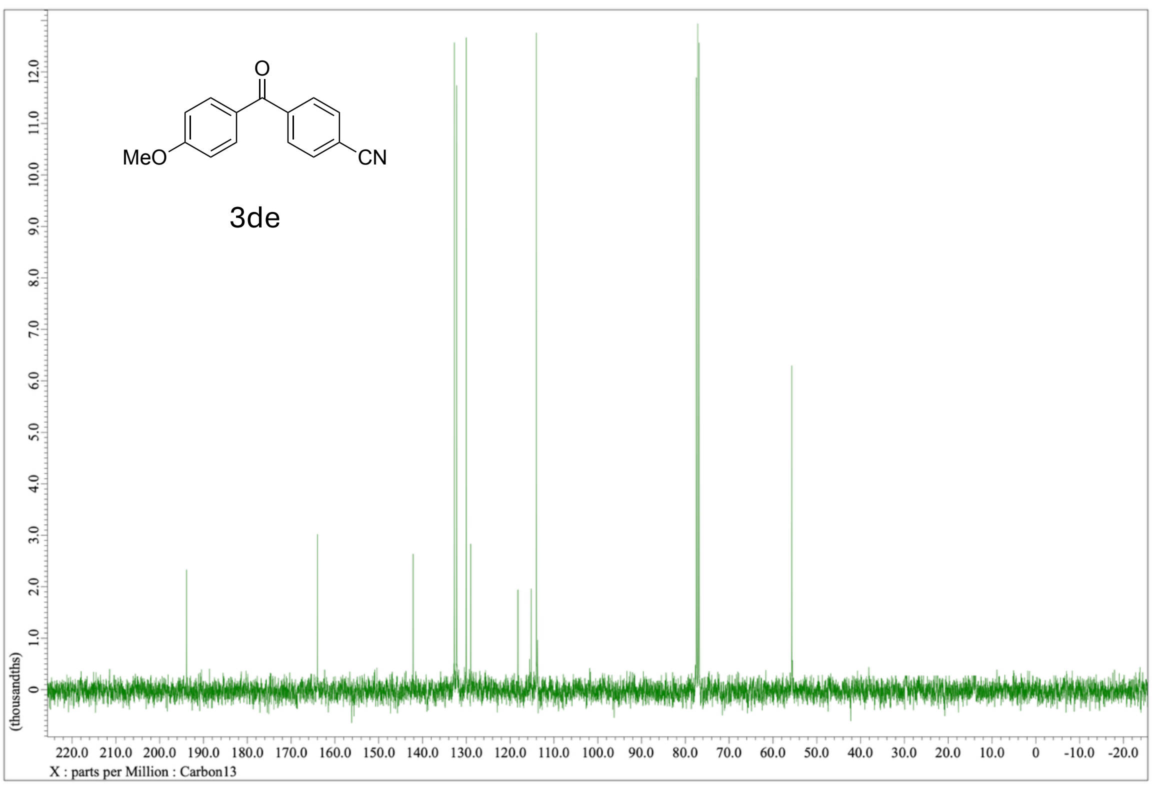


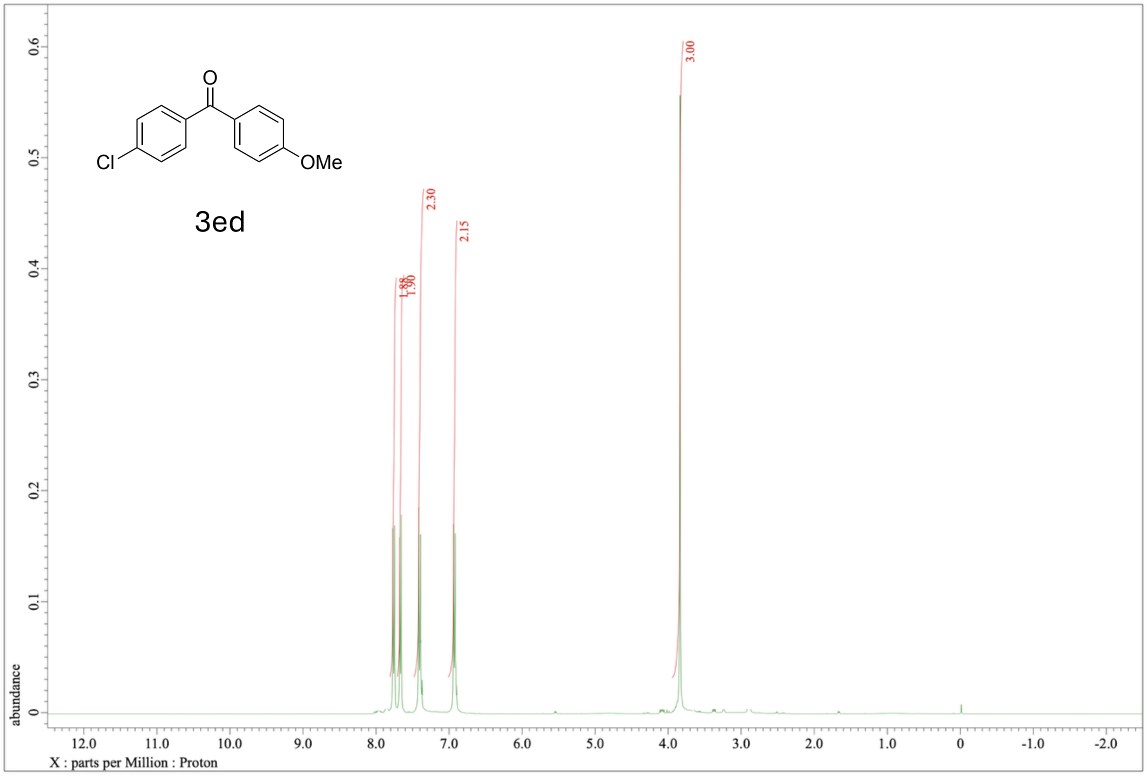
3dd
MeO
OMe
O
abundance
X : parts per Million : Proton
3.76
3.87
6.00



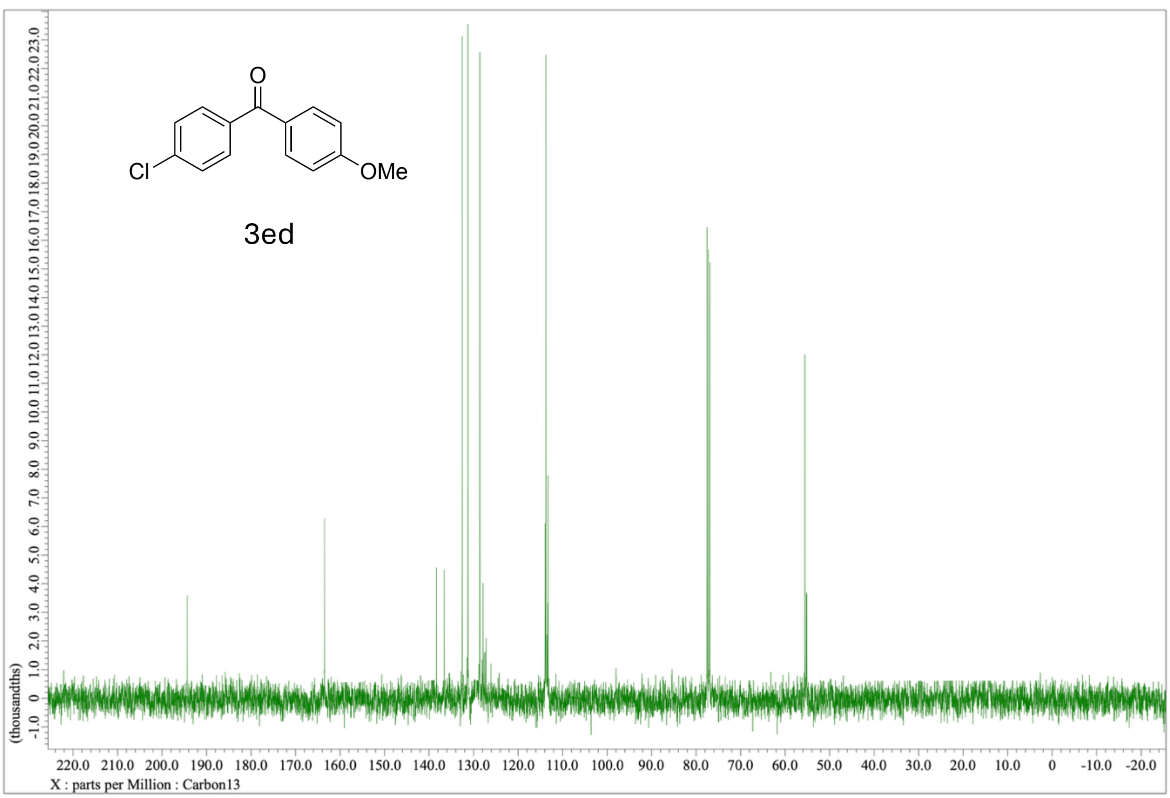
3dd
MeO
OMe
O
(thousandths)
X : parts per Million : Carbon13


MeO
CN
3de
5.83
1.87
3.00
abundance
X : parts per Million : Proton

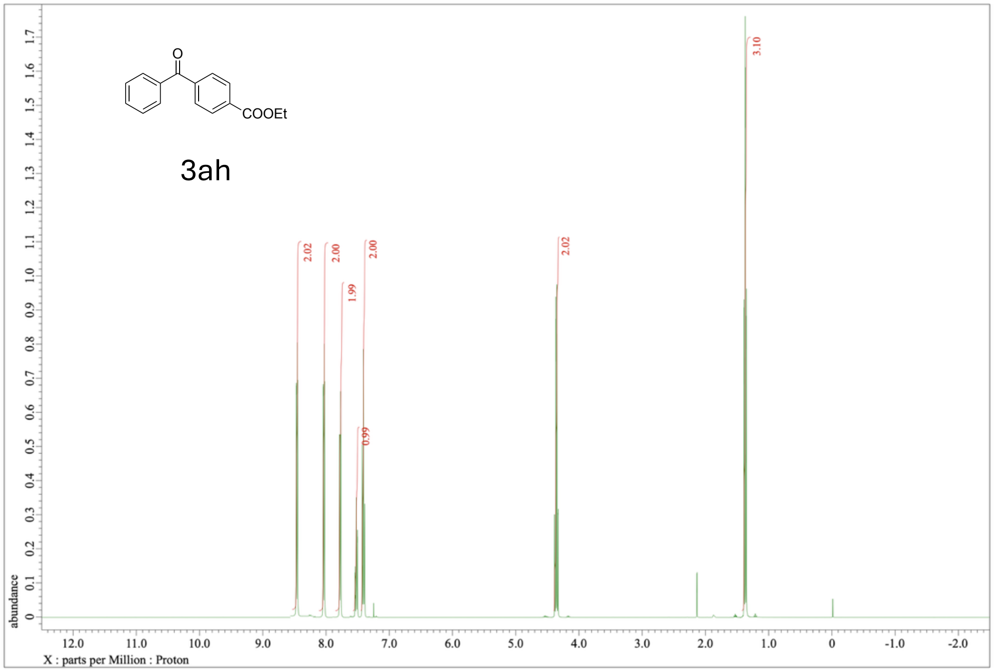

MeO
CN
3de
(thousandths)
X : parts per Million : Carbon13



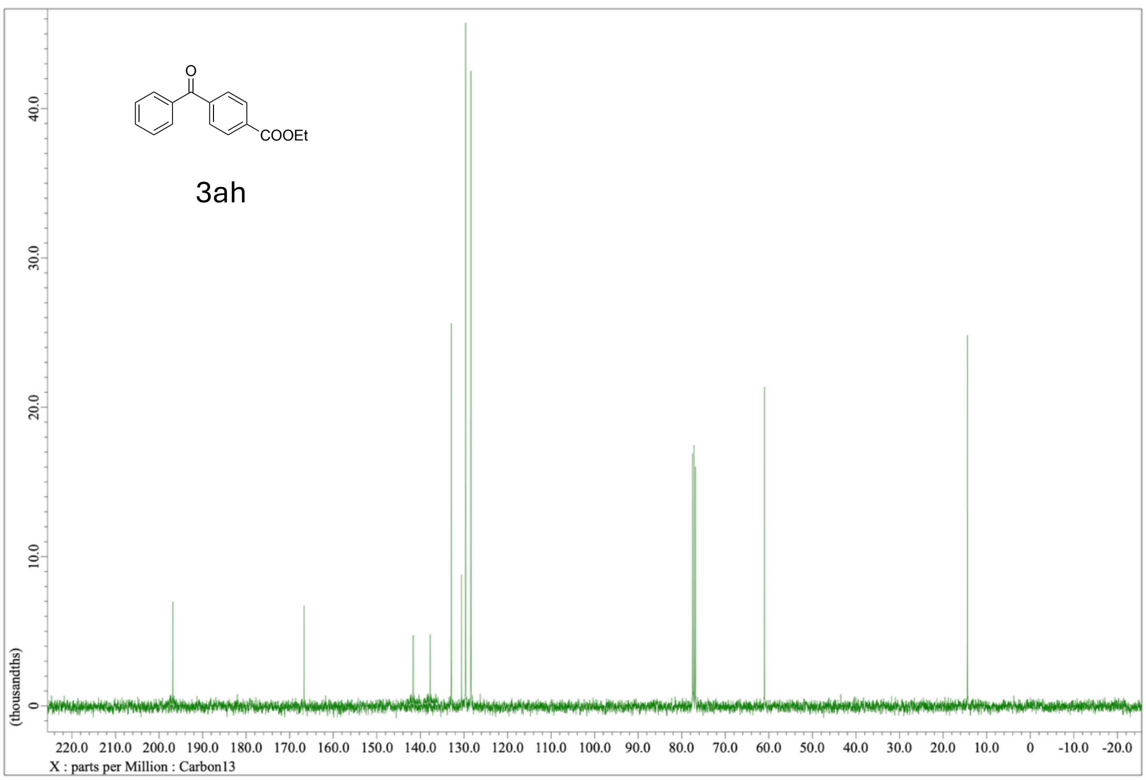
O
Cl
OMe
3ed
3.00
2.30
2.15
1.88
1.90
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
X : parts per Million : Proton



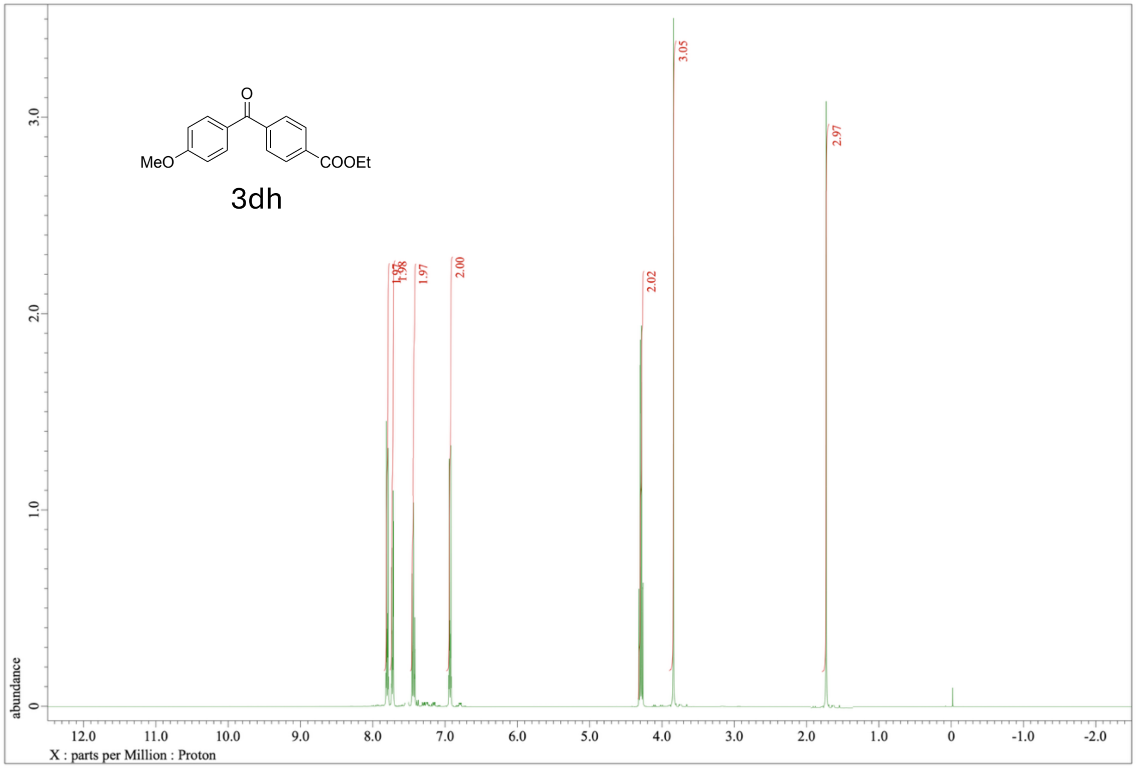
O
Cl
OMe
3ed
(thousandths)
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

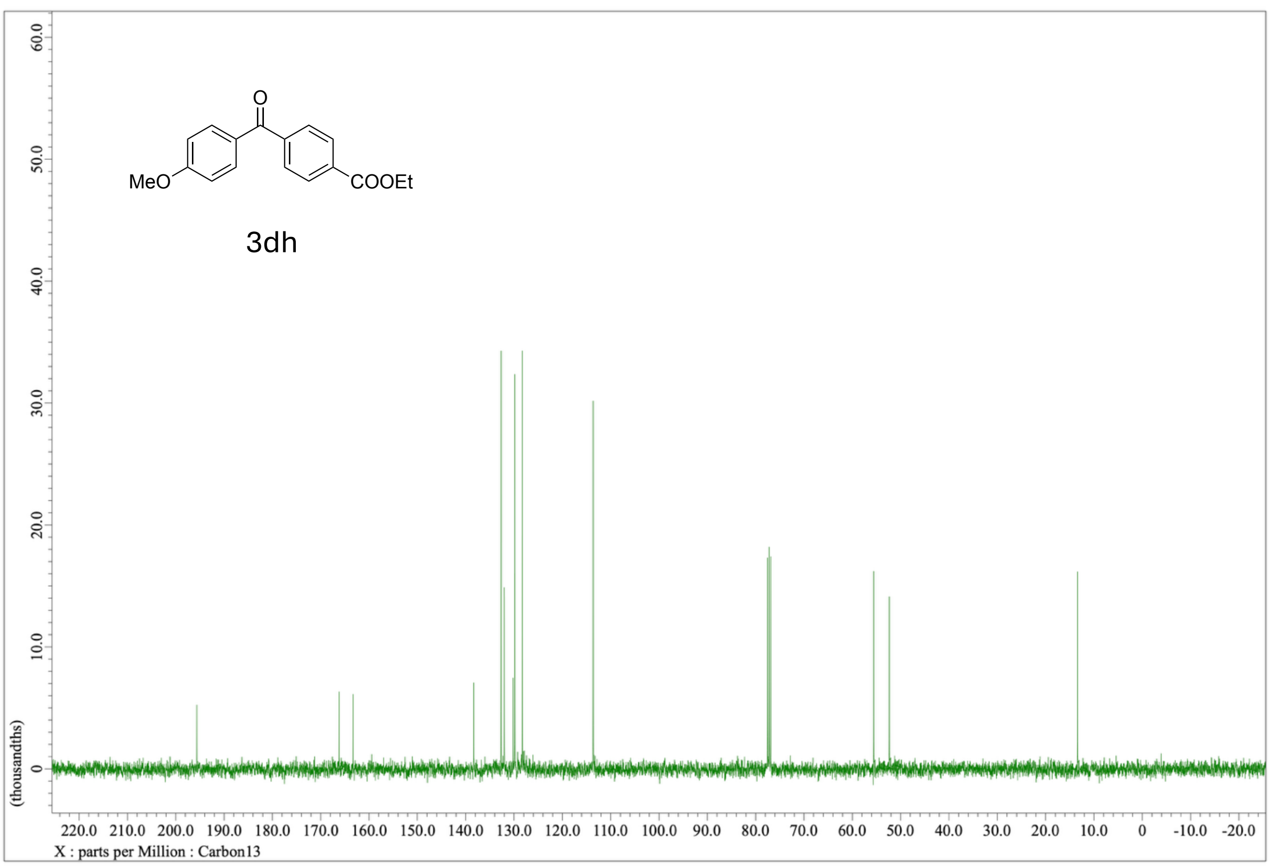


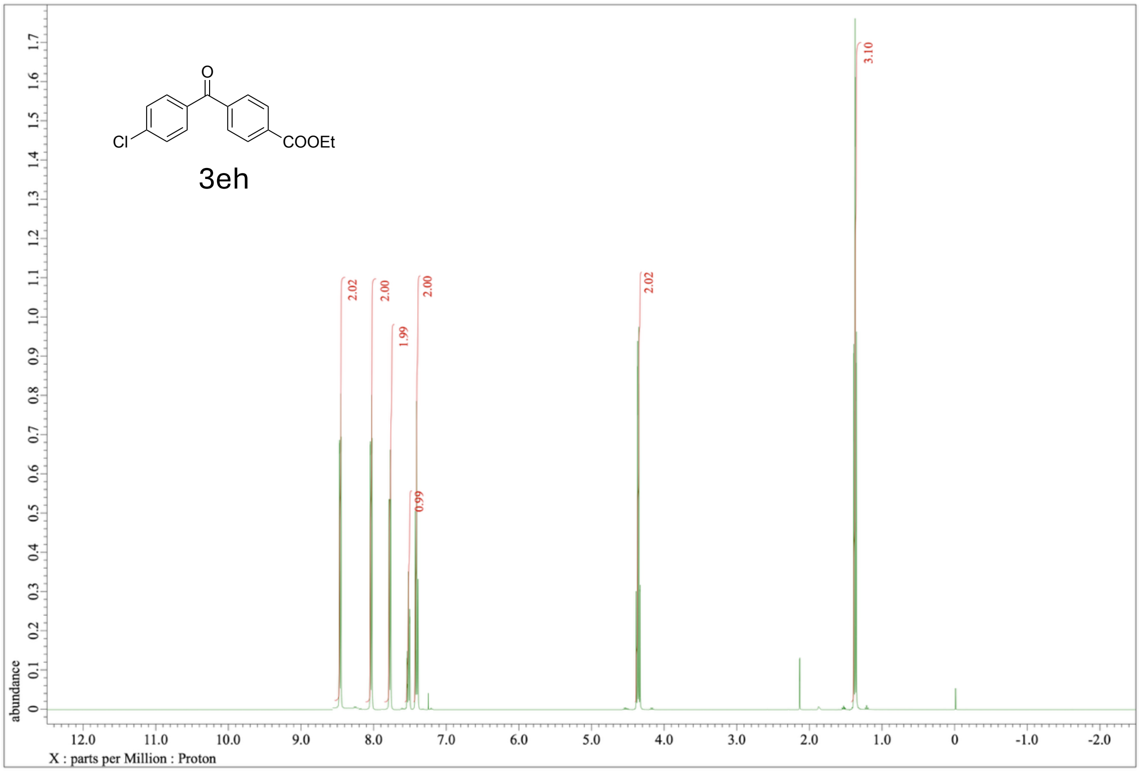
COOEt
3ah
X : parts per Million : Proton
abundance
2.02
2.00
1.99
2.00
0.99
2.02
3.10



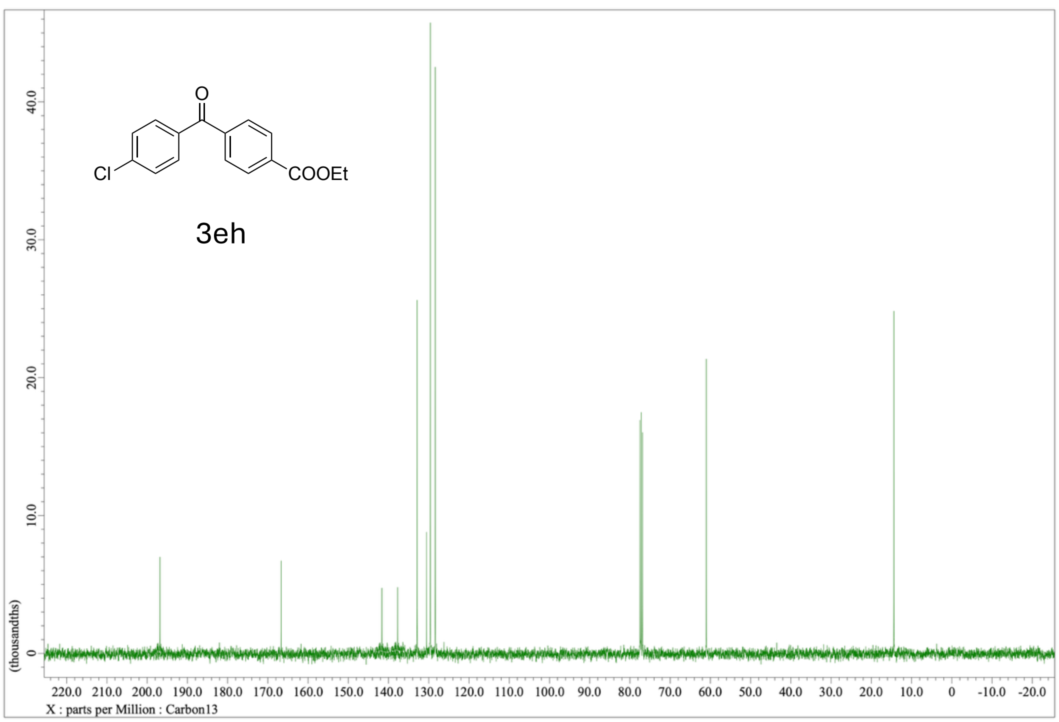
COOEt
3ah
X : parts per Million : Carbon13
(thousandths)


MeO
COOEt
3dh
abundance
X : parts per Million : Proton
1.97
1.98
1.97
2.00
2.02
3.05
2.97

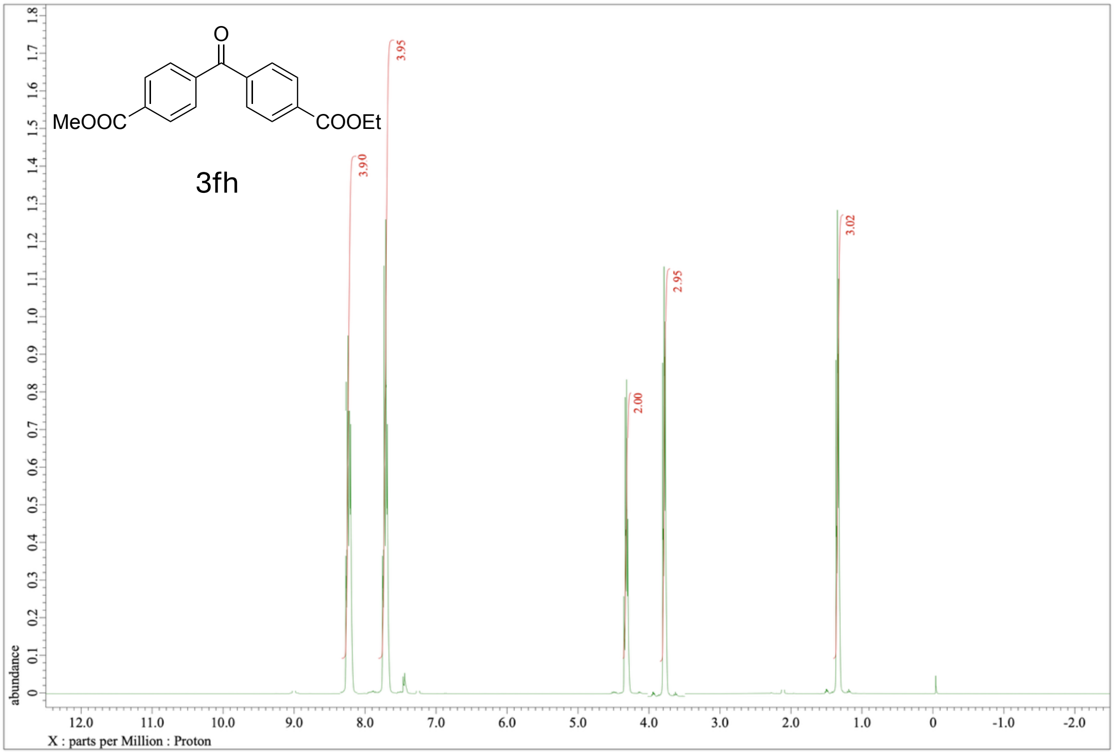

MeO
COOEt
3dh
(thousandths)
X : parts per Million : Carbon13

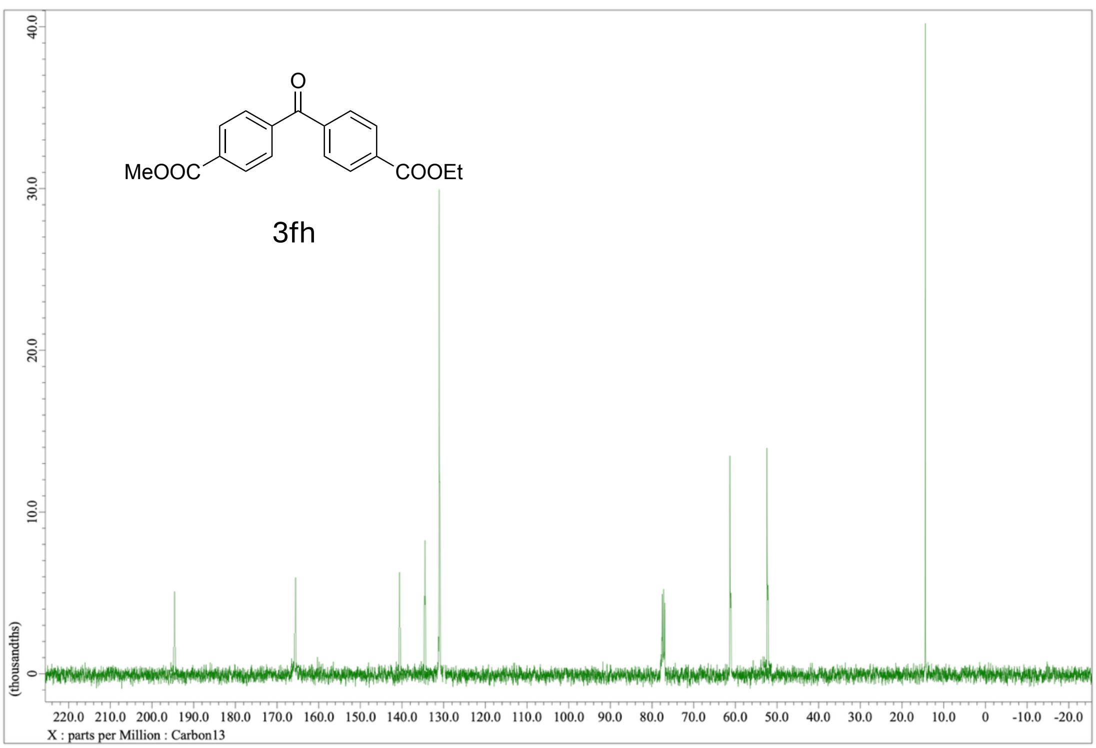


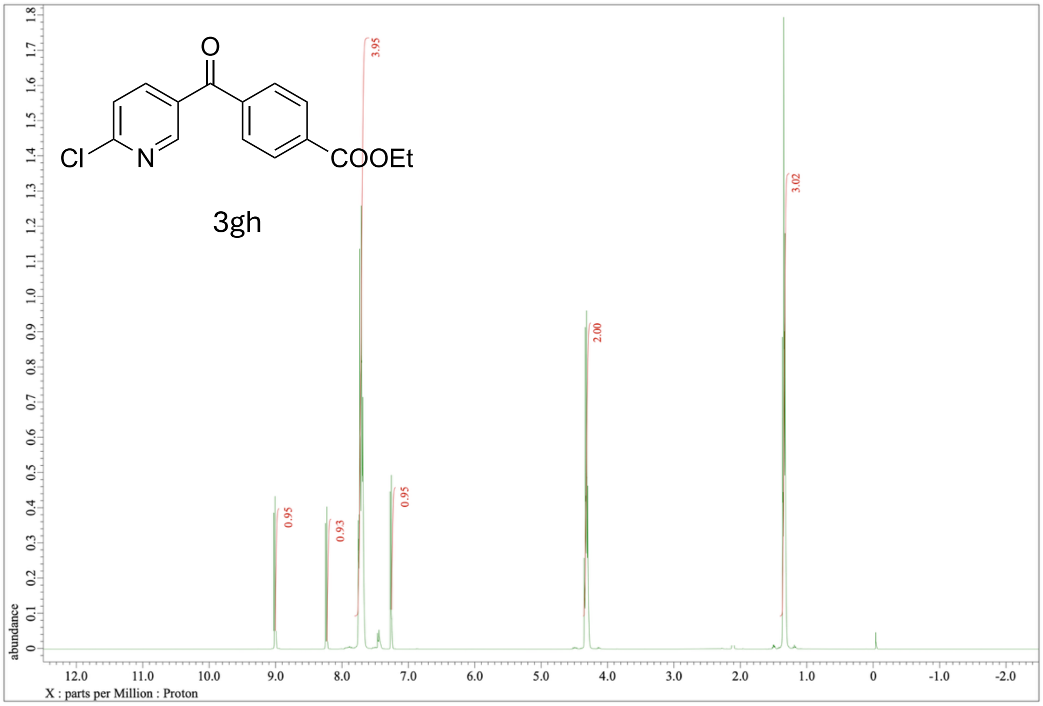
O
Cl
COOEt
3eh
2.02
2.00
1.99
2.00
0.99
2.02
3.10
abundance
X : parts per Million : Proton

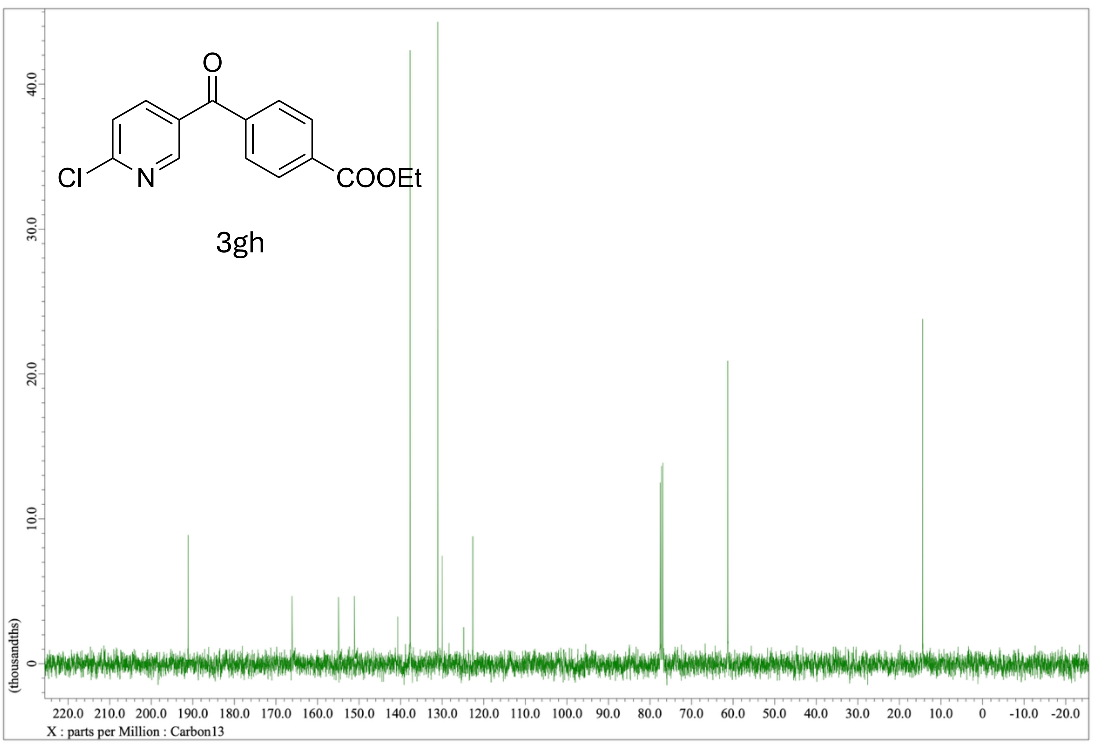


O
Cl
COOEt
3eh
(thousandths)
X : parts per Million : Carbon13

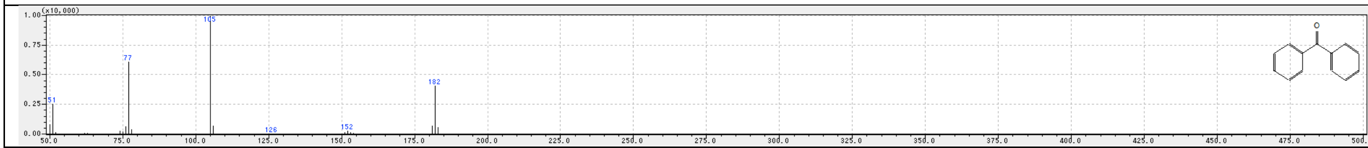

MeOOC
COOEt
3fh
3.90
3.95
2.00
2.95
3.02
abundance
X : parts per Million : Proton


MeOOC
COOEt
3fh
(thousandths)
X : parts per Million : Carbon13

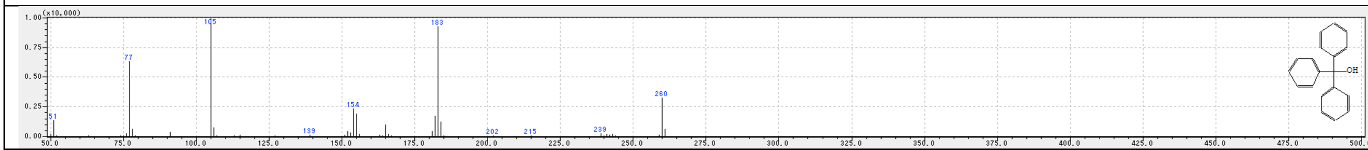

O
Cl
N
COOEt
3gh
3.95
3.02
2.00
0.95
0.93
0.95
abundance
X : parts per Million : Proton


O
Cl
N
COOEt
3gh
(thousandths)
X : parts per Million : Carbon13

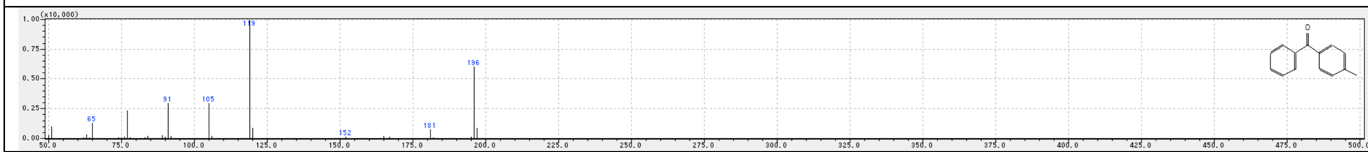
3aa



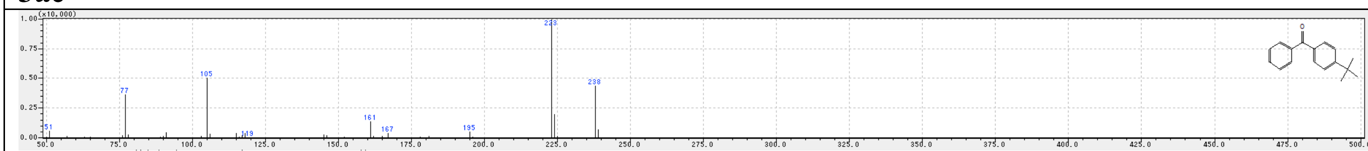
4aa



3ab



3ac



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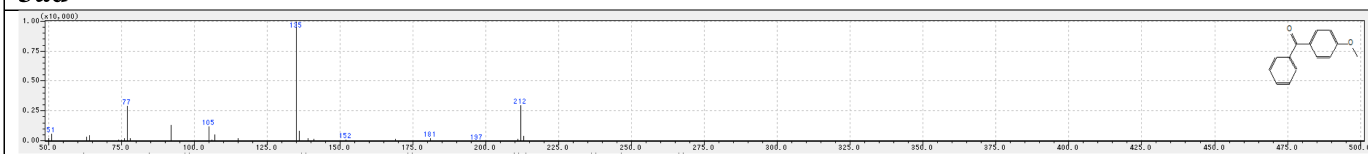
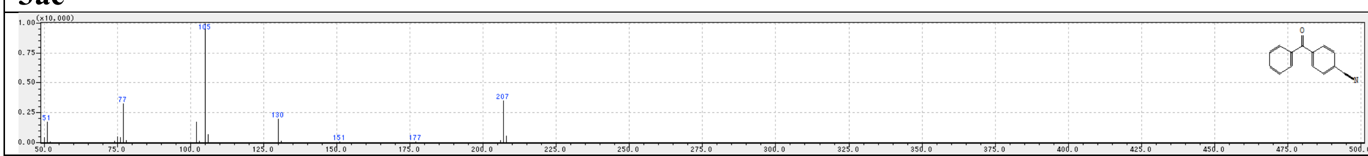


3ae



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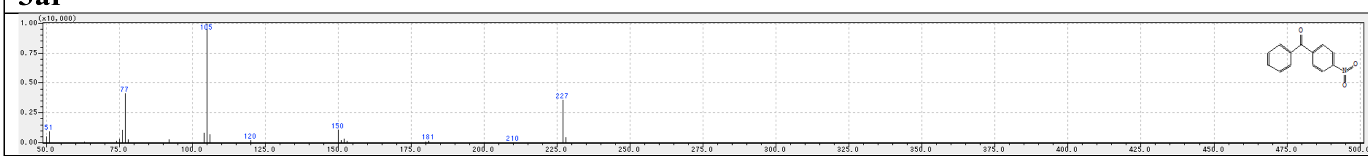

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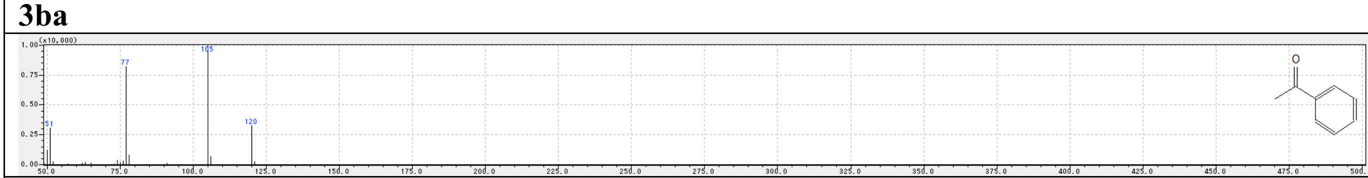

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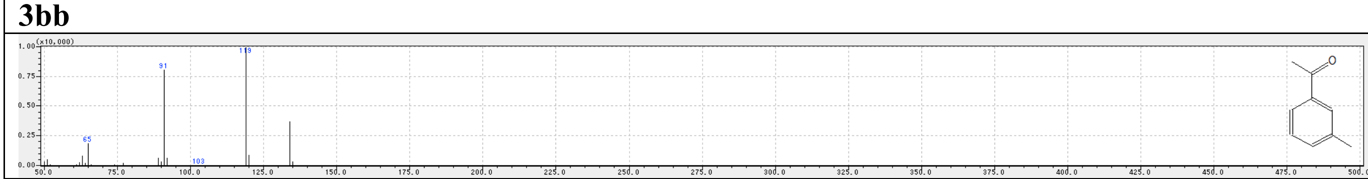

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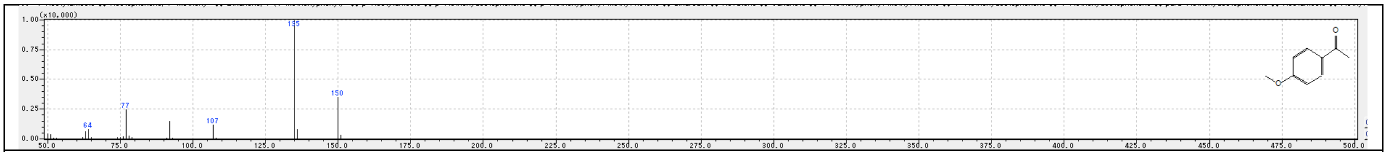

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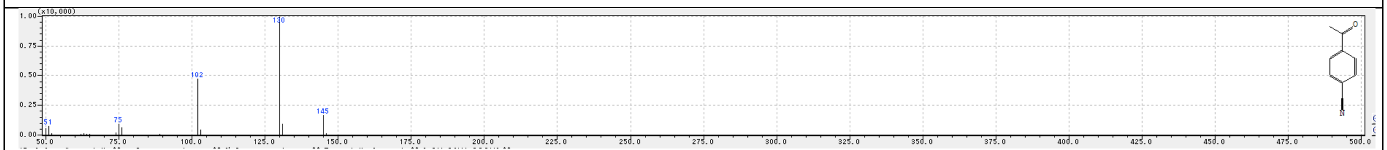
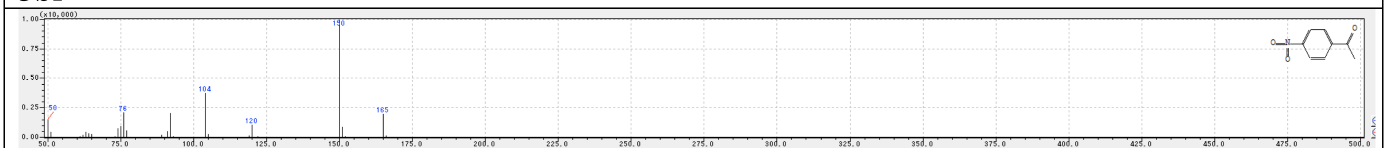
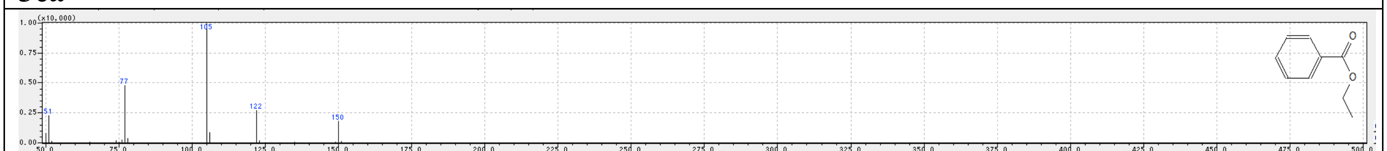


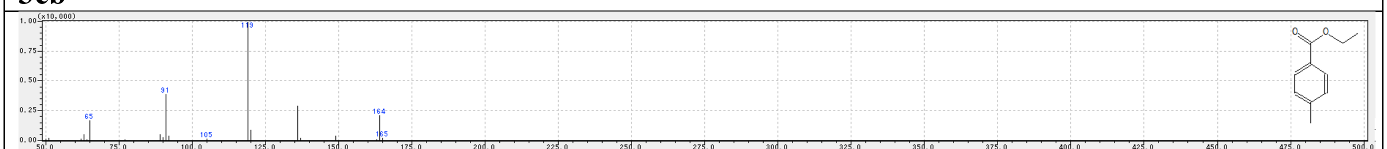
3bf



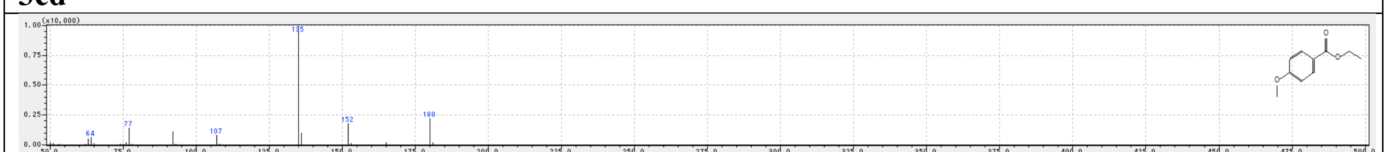
3ca



3cb



3cd



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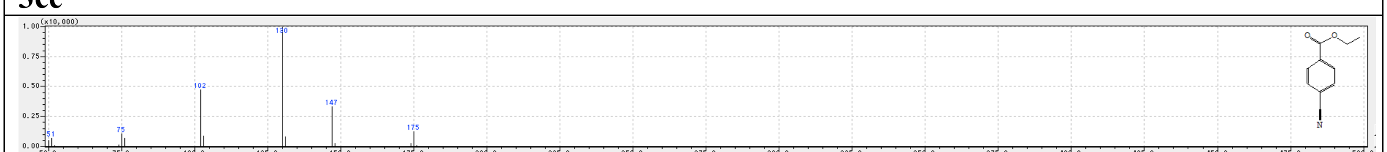

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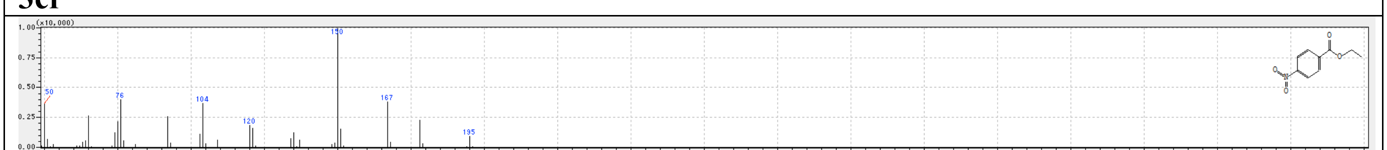
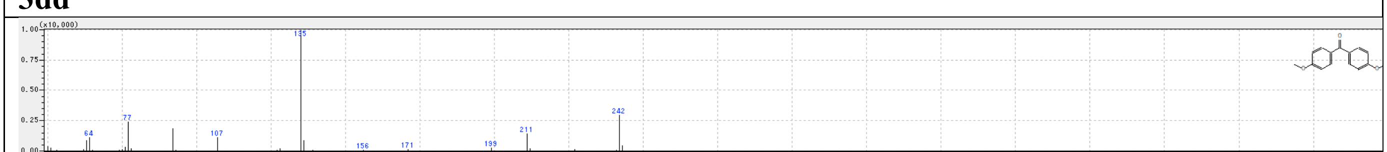


3dd



3ah