

Supporting Information

Electrochemically Driven Cross-Electrophile Esterification of Alkyl Halides

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1. General Analytical	S2
2. General Reagent Information	S2
3. General Procedure for Electrochemically Driven Cross-Electrophile Esterification of Alkyl Halides	S3
4. Large Scale Reaction Procedure	S4
5. Optimization of Electrochemically Driven Cross-Electrophile Esterification of Alkyl Halides	S6
6. Control Experiments	S7
7. Cyclic Voltammetry	S10
8. Analytical Data of Substrates and Products	S11
9. NMR Spectra of Substrates and Products	S28
10. References	S87

General Analytical Information

Nuclear Magnetic Resonance spectra were recorded on a Bruker Avance 400 MHz instruments at ambient temperature. All ^1H NMR spectra were measured in part per million (ppm) relative to the signals of tetramethylsilane (TMS, 0.00 ppm) added into the deuterated chloroform (CDCl_3 , 7.30 ppm) unless otherwise stated. Data for ^1H NMR were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets), coupling constants, and integration. All ^{13}C NMR spectra were reported in ppm relative to tetramethylsilane (0.00 ppm) unless otherwise stated, and were obtained with complete ^1H decoupling. All GC analyses were performed on a Perkin-Elmer Clarus 400 GC system with an FID detector. High-resolution mass spectra were obtained with an AB Triple 5600 mass spectrometer by ESI on a TOF mass analyzer.

General Reagent Information

Unless otherwise noted, all chemicals used in the preparations of starting materials and in the electrochemically driven cross-electrophile esterification of alkyl halides were commercially available and were used as received without further purifications or prepared according to previous work. Solvents transferred to the glove box without exposure to air. Anhydrous dimethylacetamide (DMA) (99.8% purity) were purchased from China National Pharmaceutical Group Corporation.

General Procedure for Electrochemically Driven Cross-Electrophile Esterification of Alkyl Halides

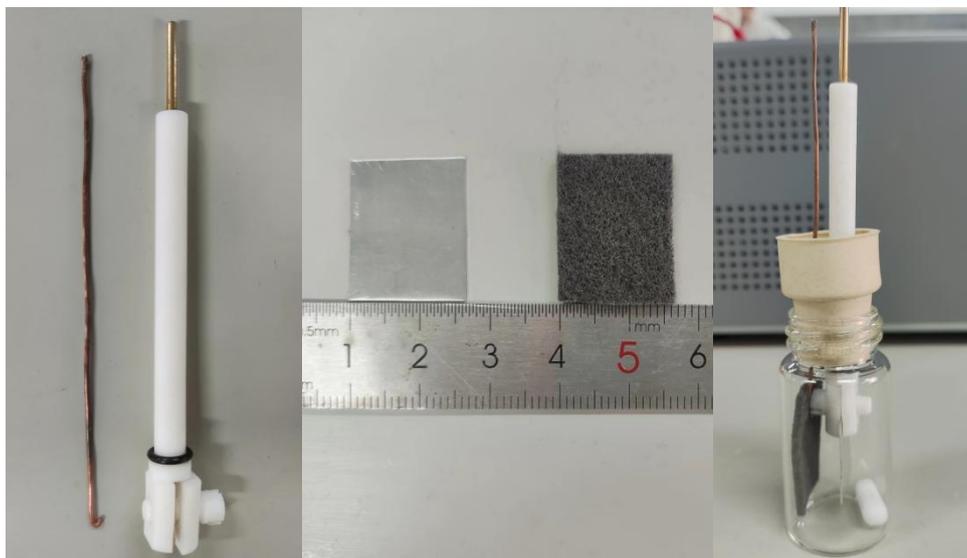


Figure S1 Hand-made electrochemical cell

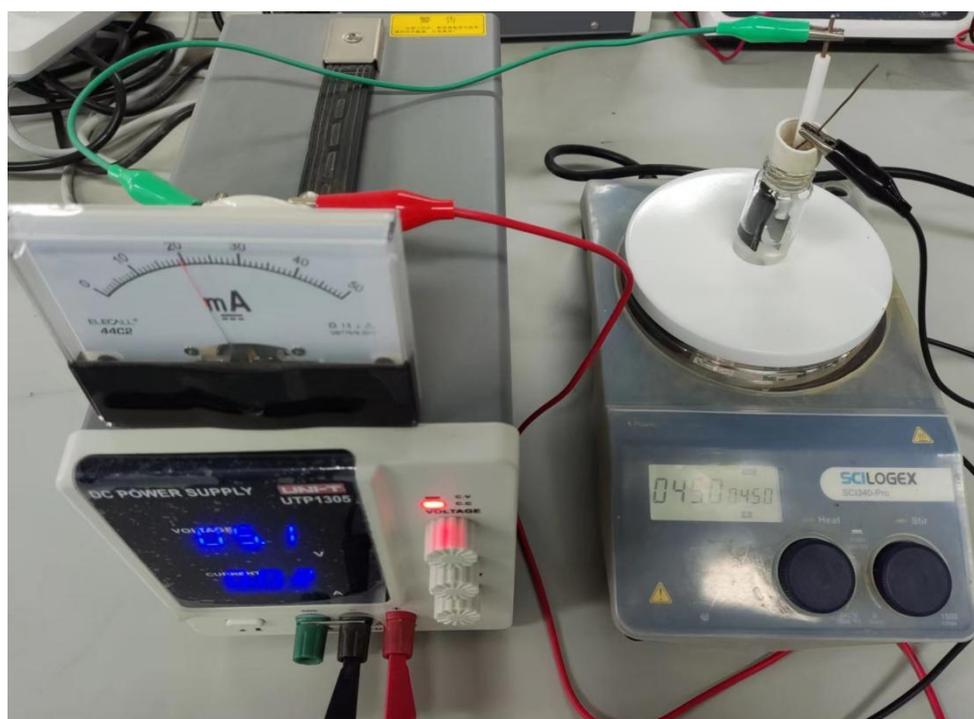
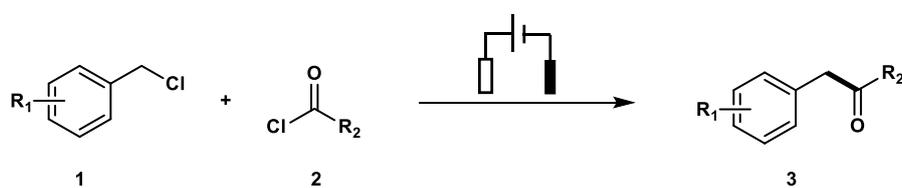


Figure S2 Electrochemical reactor

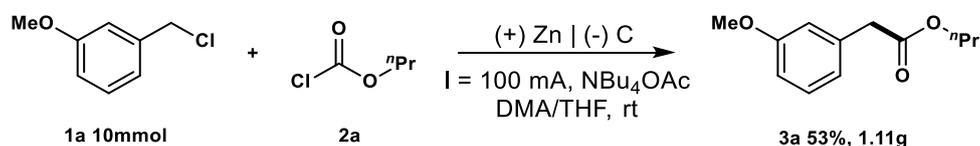


An oven-dried 20 mL re-sealable screw-cap test tube equipped with a Teflon-coated magnetic stir bar was charged with $n\text{Bu}_4\text{NOAc}$ (0.2 M) in the glove. Then DMA (4 mL), THF (2 mL), alkyl halides (0.5 mmol), alkyl halides (4.5eq), were added into the tube in turn. All these procedures were conducted in the glovebox. Screw the vial cap with electrode (Zn anode (16 mm X 20 mm), graphite felt cathode (16 mm X 20 mm)) onto the vial to finger tight and adapt the electrochemical cell. Then removed from the glove box. The reaction mixture was stirred and electrolyzed at a constant current (20 mA) at room temperature for 5h. After electrolysis, the product was extracted from the crude reaction mixture with ethyl acetate (4 X 30 mL). The organic layers were combined, and washed with brine (60 mL). Dried over Na_2SO_4 , filtered, and concentrated under reduced pressure. The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

Large Scale Reaction Procedure



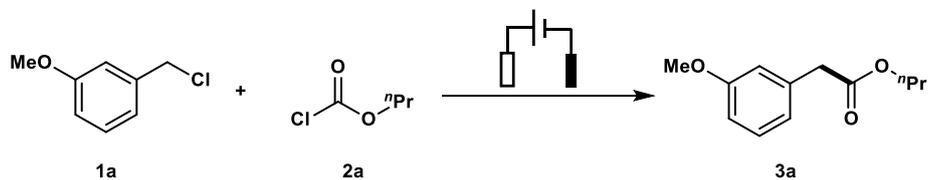
Figure S3 Scale reaction set-up



An oven-dried 100 mL three-necked flask equipped with a Teflon-coated magnetic stir bar was charged with $n\text{Bu}_4\text{NOAc}$ (0.2 M) in the glove. Then 40 mL DMA and 20 mL THF, 3-methoxybenzyl chloride **1a** (10 mmol), ClCOOPr **2a** (45 mmol) were added into the three-necked flask in turn. All these procedures were conducted in the glovebox. Screw the vial cap with electrode onto the vial to finger tight and adapt the electrochemical cell. Then removed from the glove box. The reaction mixture was stirred and electrolyzed at a constant current (100 mA) at room temperature for 12 h.

Optimizations of Electrochemically Driven Cross-Electrophile Esterification of Benzyl halides

Table 1. Screening of the Reaction Conditions

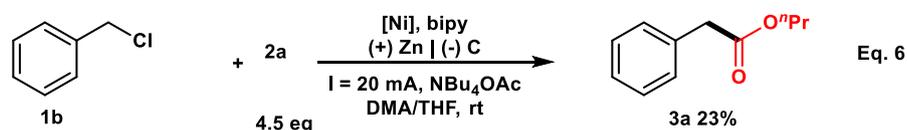
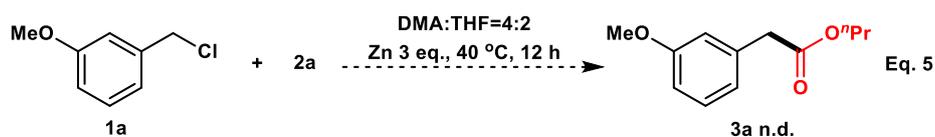
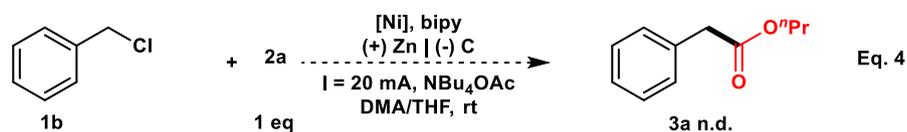
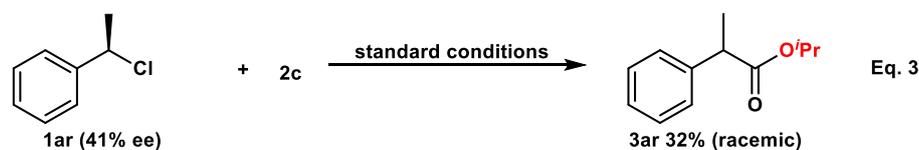
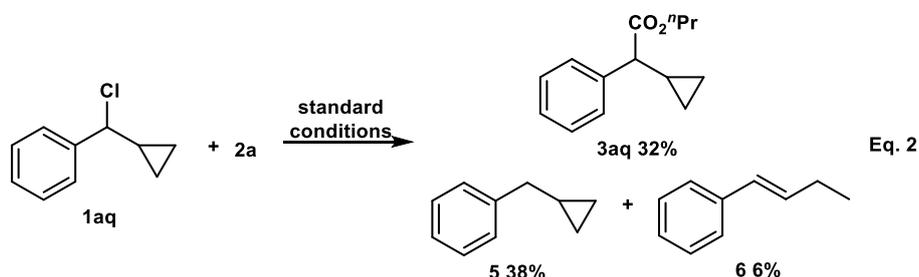


entry	deviation from standard conditions	yield 3a [%]
1	none	68 (78)^c
2 ^b	Zn powder	0
3	I = 10 mA	59
4	I = 15 mA	56
5	I = 25 mA	53
6	I = 30 mA	50
7	t = 4 h	53
8	t = 6h	58
9	Fe instead of Zn	61
10	Mg instead of Zn	30
11	Cu instead of Zn	25
12	Pt instead of graphite felt	31
13	Fe instead of graphite felt	42
14	Cu instead of graphite felt	36
15	Zn instead of graphite felt	58
16	ⁿ Bu ₄ NBr instead of ⁿ Bu ₄ NOAc	43
17	ⁿ Bu ₄ NI instead of ⁿ Bu ₄ NOAc	24
18	ⁿ Bu ₄ NCl instead of ⁿ Bu ₄ NOAc	0
19	ⁿ Bu ₄ NPF ₆ instead of ⁿ Bu ₄ NOAc	0
20	Et ₄ NCl instead of ⁿ Bu ₄ NOAc	0
21	DMA instead of DMA/THF	45
22	NMP instead of DMA/THF	28
23	DMA/1,4-Dioxane of DMA/THF	57
24	DMA/THF 3:3 instead of DMA/THF 4:2	53
25	DMA/THF 5:1 of DMA/THF 4:2	43
26	0.1 M ⁿ Bu ₄ NOAc	35
27	0.3 M ⁿ Bu ₄ NOAc	65
28	2 eq 2a	22
29	3 eq 2a	51
30	5 eq 2a	63
31	Without ⁿ Bu ₄ NOAc	0
32	Without current	0

^aReaction condition : 0.5 mmol **1a**, 4.5 eq **2a**, 0.2 M ⁿBu₄NOAc, DMA/THF = 4 ml:2 ml, Zn anode, graphite felt cathode, undivided cell, constant current of 20 mA, rt, 5h. Conversion was measured by GC using naphthalene as an internal standard. ^bNo electrode and electrolyte, 3 equiv. Zn powder. ^cIsolated yield.

Control Experiments

In order to gain a better understanding of the reaction's mechanism, we conducted several control experiments.



Eq. 1 followed the General Procedure, with adding free radical inhibitor, TEMPO. After reaction, no product was detected.

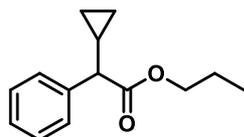
Eq. 2 followed the General Procedure using (chloro(cyclopropyl)methyl)benzene (0.5 mmol) and propyl chloroformate (4.5 eq) as the substrate. After purification, the yield of **3aq** is 32%, **5** is 38%, **6** is 6%

Eq. 3 followed the General Procedure using (R)-(1-chloroethyl)benzene (41% ee) (0.5 mmol) and isopropyl chloroformate (4.5 eq) as the substrate. After purification, the yield of **3ar** is 32%.

Eq. 4 followed the General Procedure using (chloromethyl)benzene (0.5 mmol) and propyl chlorocarbonate (1 eq) as the substrate. Add catalyst NiCl₂dme (10% mmol) and ligand bpy (15% mmol), After purification, the yield of **3a** is nd.

Eq. 5 Standard reaction without current, adding 3eq zinc powder reaction at 40°C for 12h reaction will not occur.

Eq. 6 followed the General Procedure using (chloromethyl)benzene (0.5 mmol) and propyl chlorocarbonate (4.5 eq) as the substrate. Add catalyst NiCl₂dme (10% mmol) and ligand bpy (15% mmol), After purification, the yield of **3a** is 23%.



Propyl 2-cyclopropyl-2-phenylacetate The product was purified by silica gel column chromatography, using PE/EA = 120/1 (v/v) as an eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.26 – 7.19 (m, 4H), 4.09 (t, *J* = 6.7 Hz, 2H), 3.63 (s, 2H), 2.68 (q, *J* = 7.6 Hz, 2H), 1.69 (h, *J* = 7.2 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H), 0.96 (t, *J* = 7.4 Hz, 3H).

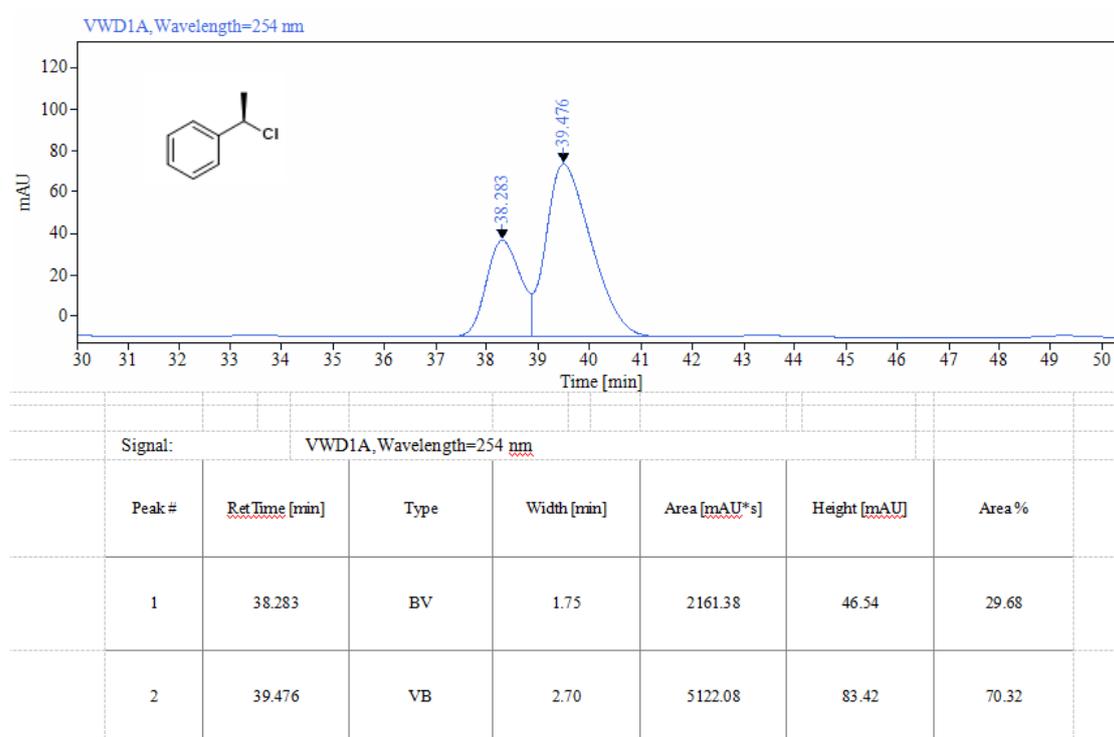
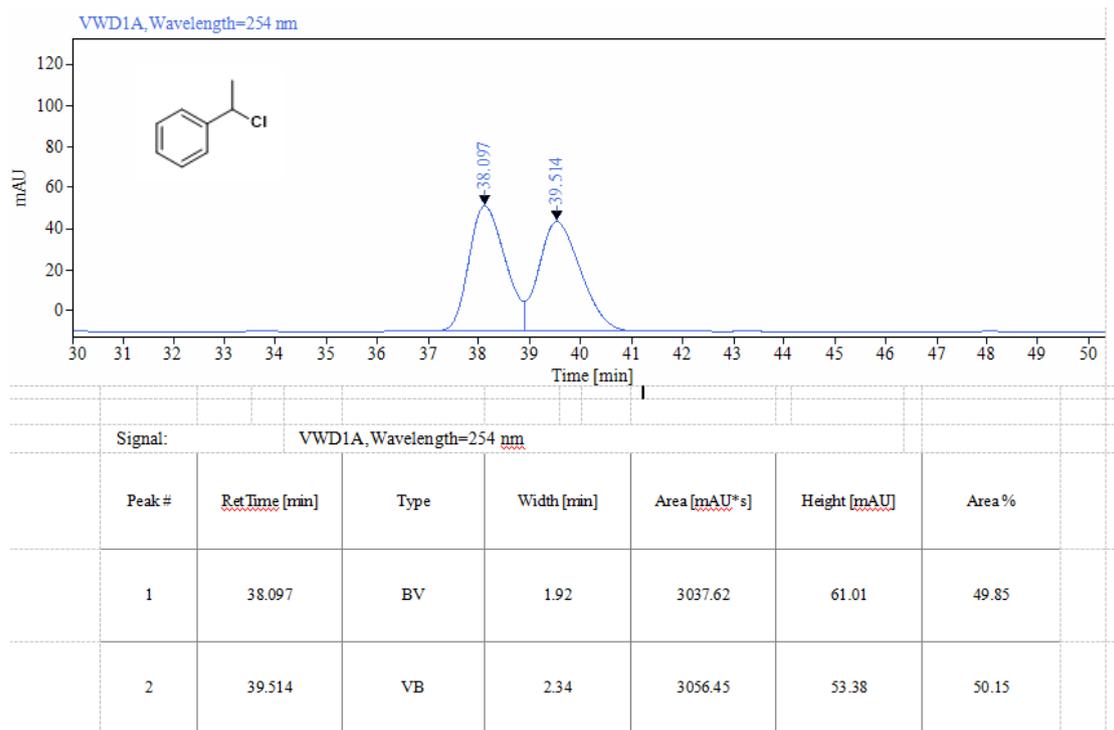
¹³C NMR (101 MHz, CDCl₃) δ 171.97, 143.01, 131.38, 129.19, 128.07, 66.44, 41.06, 28.52, 21.98, 15.62, 10.39.

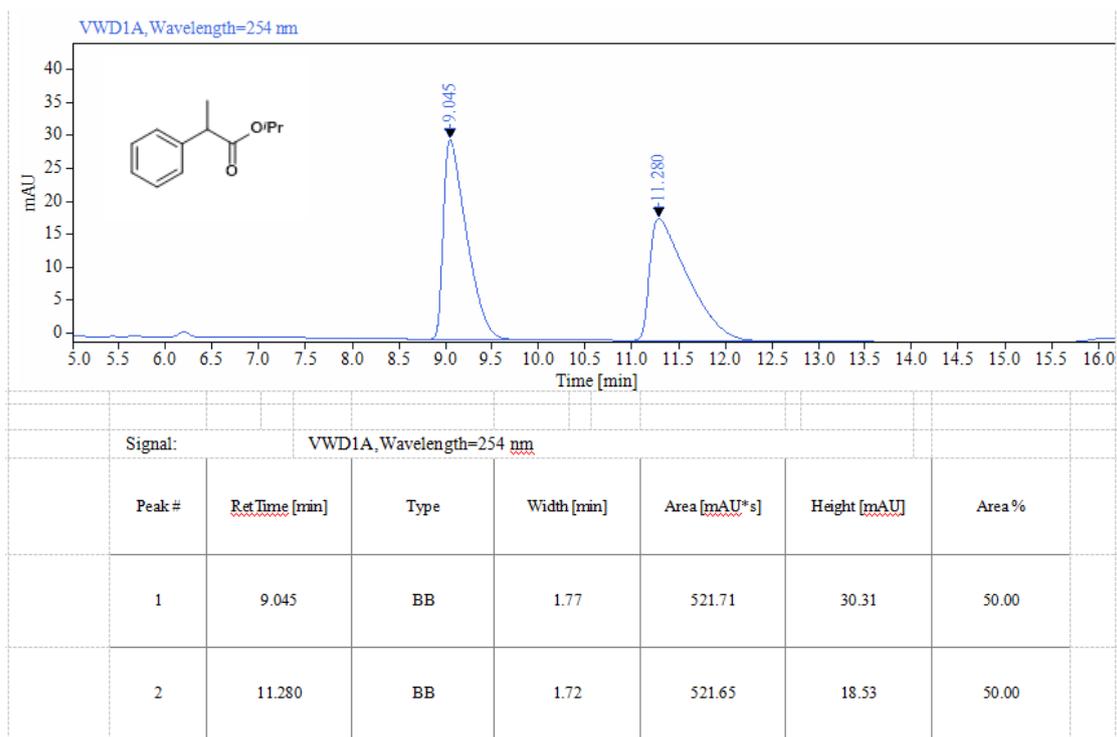


(cyclopropylmethyl)benzene and (E)-but-1-en-1-ylbenzene The product was purified by silica gel column chromatography, using PE/EA = 120/1 (v/v) as an eluent. According to the spectrum, **(cyclopropylmethyl)benzene : (E)-but-1-en-1-ylbenzene=7:1**.

¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.23 (m, 4H), 6.38 (d, *J* = 16.0 Hz, 1H), 6.27 (dt, *J* = 15.8, 6.3 Hz, 1H), 2.55 (d, *J* = 6.9 Hz, 14H), 2.23 (p, *J* = 7.4, 6.9 Hz, 2H), 1.09 (t, *J* = 7.5 Hz, 3H), 1.09 – 0.99 (m, 7H), 0.59 – 0.55 (m, 14H), 0.20 (q, *J* = 5.0 Hz, 14H).

¹³C NMR (101 MHz, CDCl₃) δ 142.15(major), 137.92(minor), 132.63(minor), 128.76(major), 128.45(major), 128.33(minor), 128.21(minor), 126.73(minor), 125.88(major), 125.80(minor), 40.33(major), 26.05(minor), 13.64(minor), 11.83(major), 4.64(major).





Cyclic Voltammetry

Cyclic voltammograms in solvent (10 mL) by using glassy carbon as the working electrode, Pt wire as the counter electrode and Ag/AgCl as the reference electrode under N₂ at room temperature. NMP (10mL) containing 0.1 M ⁿBu₄NBr was poured into the electro chemical cell in all experiments. The scan rate was 100 mV s⁻¹.

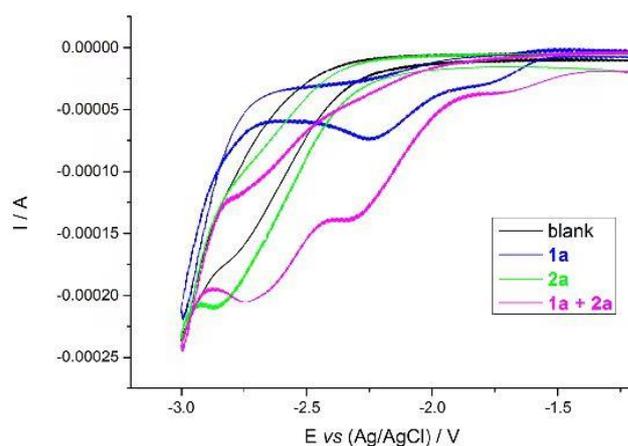
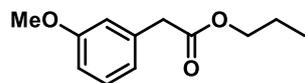


Figure S4: Cyclic voltammograms recorded on a glassy carbon electrode at 100 mVs⁻¹ in: black: NMP (10 mL), ⁿBu₄NBr (1 mol); **1a**: NMP (10 mL), ⁿBu₄NBr (1 mol), 3-methoxybenzyl chloride (0.1 mmol); **2a**: NMP (10 mL), ⁿBu₄NBr (1 mol), propyl chlorocarbonate (0.1 mmol); **1a+2a**: NMP

(10 mL), ⁿBu₄NBr (1 mol); **1a**: NMP (10 mL), ⁿBu₄NBr (1 mol), 3-methoxybenzyl chloride (0.1 mmol), propyl chlorocarbonate (0.1 mmol).

Analytical Data of Substrates and Products

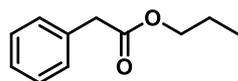


1-(4-(tert-butyl)phenyl)-2-(4-fluorophenyl)ethan-1-one Light yellow liquid (81.1 mg, 78% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.25 (m, 1H), 6.92 – 6.83 (m, 3H), 4.09 (t, *J* = 6.7 Hz, 2H), 3.83 (s, 3H), 3.63 (s, 2H), 1.72 – 1.63 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 171.61, 159.66, 135.61, 129.52, 121.62, 114.82, 112.63, 66.51, 55.20, 41.52, 21.96, 10.38.

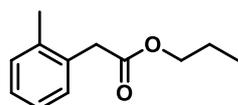
HRMS (ESI) *m/z*: [M + Li]⁺ Calcd for C₁₂H₁₆LiO₃⁺ 215.1254; Found 215.1239.



propyl 2-phenylacetate^[1] Light yellow liquid (47.2 mg, 53% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.29 (m, 5H), 4.09 (t, *J* = 6.7 Hz, 2H), 3.66 (s, 2H), 1.68 (h, *J* = 7.2 Hz, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

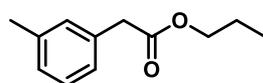
¹³C NMR (101 MHz, CDCl₃) δ 171.75, 134.21, 129.27, 128.56, 127.05, 66.49, 41.49, 21.97, 10.38.



propyl 2-(o-tolyl)acetate Light yellow liquid (63.4 mg, 66% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.26 – 7.18 (m, 4H), 4.10 (t, *J* = 6.7 Hz, 2H), 3.68 (s, 2H), 2.37 (s, 3H), 1.69 (h, *J* = 6.9 Hz, 2H), 0.95 (t, *J* = 7.4 Hz, 3H).

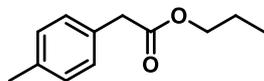
¹³C NMR (101 MHz, CDCl₃) δ 171.66, 136.84, 132.96, 130.33, 130.17, 127.36, 126.13, 66.44, 39.31, 21.99, 19.64, 10.38.



propyl 2-(m-tolyl)acetate Light yellow liquid (50.9 mg, 53% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 30/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.29 – 7.11 (m, 4H), 4.10 (t, $J = 6.7$ Hz, 2H), 3.63 (s, 2H), 2.39 (s, 3H), 1.74 – 1.64 (m, 2H), 0.96 (t, $J = 7.4$ Hz, 3H).

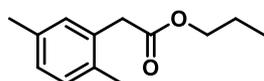
^{13}C NMR (101 MHz, CDCl_3) δ 171.86, 138.18, 134.09, 130.03, 128.45, 127.80, 126.28, 66.46, 41.41, 21.98, 21.40, 10.39.



propyl 2-(p-tolyl)acetate Light yellow liquid (56.6 mg, 59% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.23 – 7.16 (m, 4H), 4.08 (t, $J = 6.7$ Hz, 2H), 3.62 (s, 2H), 2.37 (s, 3H), 1.68 (h, $J = 7.2$ Hz, 2H), 0.95 (t, $J = 7.4$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.96, 136.64, 131.14, 129.25, 129.12, 66.44, 41.06, 21.97, 21.12, 10.39.

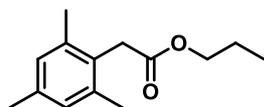


propyl 2-(2,5-dimethylphenyl)acetate Light yellow liquid (63.9 mg, 62% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.12 – 7.02 (m, 3H), 4.10 (t, $J = 6.7$ Hz, 2H), 3.64 (s, 2H), 2.34 (d, $J = 10.4$ Hz, 6H), 1.69 (h, $J = 7.2$ Hz, 2H), 0.96 (t, $J = 7.4$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.81, 135.53, 133.63, 132.69, 130.91, 130.22, 128.04, 66.42, 39.26, 22.00, 20.93, 19.15, 10.39.

HRMS (ESI) m/z : $[\text{M} + \text{Li}]^+$ Calcd for $\text{C}_{13}\text{H}_{18}\text{LiO}_2^+$ 213.1461; Found 213.1466.

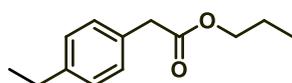


propyl 2-mesitylacetate Light yellow liquid (59.4 mg, 54% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 6.93 (s, 2H), 4.10 (t, $J = 6.7$ Hz, 2H), 3.71 (s, 2H), 2.34 (d, $J = 16.7$ Hz, 9H), 1.69 (h, $J = 7.1$ Hz, 2H), 0.97 (t, $J = 7.4$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.68, 137.02, 136.44, 128.91, 128.75, 66.34, 35.14, 22.03, 20.96, 20.28, 10.43.

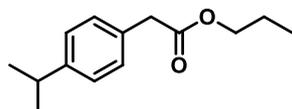
HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{14}\text{H}_{20}\text{NaO}_2^+$ 243.1356; Found 243.1368.



propyl 2-(4-ethylphenyl)acetate Light yellow liquid (55.6 mg, 54% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.26 – 7.19 (m, 4H), 4.09 (t, J = 6.7 Hz, 2H), 3.63 (s, 2H), 2.68 (q, J = 7.6 Hz, 2H), 1.69 (h, J = 7.2 Hz, 2H), 1.27 (t, J = 7.6 Hz, 3H), 0.96 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.97, 143.01, 131.38, 129.19, 128.07, 66.44, 41.06, 28.52, 21.98, 15.62, 10.39.

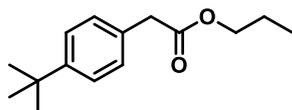


propyl 2-(4-isopropylphenyl)acetate Light yellow liquid (63.8 mg, 58% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.29 – 7.22 (m, 4H), 4.10 (t, J = 6.7 Hz, 2H), 3.64 (s, 2H), 2.93 (h, J = 6.9 Hz, 1H), 1.70 (h, J = 7.2 Hz, 2H), 1.29 (d, J = 7.0 Hz, 6H), 0.97 (t, J = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.98, 147.61, 131.51, 129.19, 126.64, 66.44, 41.03, 33.80, 24.04, 21.99, 10.40.

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{14}\text{H}_{20}\text{NaO}_2^+$ 243.1356; Found 243.1351.

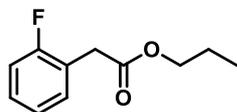


propyl 2-(4-(tert-butyl)phenyl)acetate Light yellow liquid (73.7 mg, 63% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.41 – 7.27 (m, 4H), 4.11 (t, J = 6.7 Hz, 2H), 3.65 (s, 2H), 1.70 (h, J = 7.1 Hz, 2H), 1.37 (s, 9H), 0.97 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.96, 149.86, 131.16, 128.93, 125.51, 66.44, 40.92, 34.49, 31.39, 21.99, 10.41.

HRMS (ESI) m/z : $[\text{M} + \text{Li}]^+$ Calcd for $\text{C}_{15}\text{H}_{22}\text{LiO}_2^+$ 241.1774; Found 241.1792.



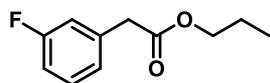
propyl 2-(2-fluorophenyl)acetate Light yellow liquid (51.0 mg, 52% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.32 – 7.26 (m, 2H), 7.16 – 7.07 (m, 2H), 4.11 (t, J = 6.7 Hz, 2H), 3.71 (d, J = 1.2 Hz, 2H), 1.68 (hept, J = 6.9 Hz, 2H), 0.94 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 170.85, 161.08 (d, J = 246.4 Hz), 131.45 (d, J = 4.0 Hz), 129.02 (d, J = 8.1 Hz), 124.10 (d, J = 3.7 Hz), 121.56 (d, J = 15.8 Hz), 115.36 (d, J = 21.7 Hz), 66.65, 34.59 (d, J = 3.2 Hz), 21.93, 10.31.

^{19}F NMR (377 MHz, CDCl_3) δ -117.27.

HRMS (ESI) m/z : $[\text{M} + \text{NH}_4]^+$ Calcd for $\text{C}_{11}\text{H}_{17}\text{FNO}_2^+$ 214.1238; Found 214.1246.



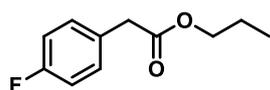
propyl 2-(3-fluorophenyl)acetate Light yellow liquid (49.0 mg, 50% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.34 – 7.29 (m, 1H), 7.10 – 6.97 (m, 3H), 4.09 (t, J = 6.7 Hz, 2H), 3.65 (s, 2H), 1.68 (h, J = 7.2 Hz, 2H), 0.94 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.13, 162.79 (d, J = 245.8 Hz), 136.44 (d, J = 7.9 Hz), 129.96 (d, J = 8.4 Hz), 124.99 (d, J = 2.9 Hz), 116.31 (d, J = 21.8 Hz), 114.04 (d, J = 21.0 Hz), 66.67, 41.09 (d, J = 1.8 Hz), 21.93, 10.34.

^{19}F NMR (377 MHz, CDCl_3) δ -113.25.

HRMS (ESI) m/z : $[\text{M} + \text{K}]^+$ Calcd for $\text{C}_{11}\text{H}_{13}\text{FKO}_2^+$ 235.0531; Found 235.0529.



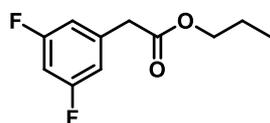
propyl 2-(4-fluorophenyl)acetate Light yellow liquid (43.1 mg, 44% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 1200/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.30 – 7.28 (m, 2H), 7.06 – 7.02 (m, 2H), 4.08 (t, J = 6.7 Hz, 2H), 3.62 (s, 2H), 1.67 (dtd, J = 14.1, 7.4, 6.7 Hz, 2H), 0.94 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.60, 161.98 (d, J = 245.2 Hz), 130.83 (d, J = 8.0 Hz), 129.89 (d, J = 3.3 Hz), 115.39 (d, J = 21.3 Hz), 66.57, 40.56, 21.94, 10.36.

^{19}F NMR (377 MHz, CDCl_3) δ -115.85.

HRMS (ESI) m/z : $[\text{M} + \text{K}]^+$ Calcd for $\text{C}_{11}\text{H}_{13}\text{FKO}_2^+$ 235.0531; Found 235.0545.



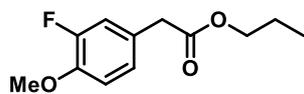
propyl 2-(3,5-difluorophenyl)acetate Light yellow liquid (73.8 mg, 69% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 6.88 – 6.83 (m, 2H), 6.75 (tt, J = 9.0, 2.4 Hz, 1H), 4.10 (t, J = 6.7 Hz, 2H), 3.63 (s, 2H), 1.68 (h, J = 7.2 Hz, 2H), 0.95 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 170.47, 162.92 (dd, J = 248.3, 12.9 Hz), 137.60 (t, J = 9.7 Hz), 112.54 – 112.02 (m), 102.66 (t, J = 25.2 Hz), 66.84, 40.95 (t, J = 2.0 Hz), 21.90, 10.32.

^{19}F NMR (377 MHz, CDCl_3) δ -110.02.

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{11}\text{H}_{13}\text{F}_2\text{O}_2^+$ 215.0878; Found 215.0881.



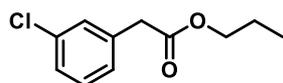
propyl 2-(3-fluoro-4-methoxyphenyl)acetate Light yellow liquid (58.8 mg, 52% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.08 – 6.90 (m, 3H), 4.07 (t, J = 6.7 Hz, 2H), 3.89 (s, 3H), 3.56 (s, 2H), 1.67 (h, J = 7.2 Hz, 2H), 0.94 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.49, 152.13 (d, J = 245.5 Hz), 146.68 (d, J = 10.6 Hz), 127.00 (d, J = 6.7 Hz), 125.00 (d, J = 3.6 Hz), 117.05 (d, J = 18.7 Hz), 113.29 (d, J = 2.2 Hz), 66.57, 56.23, 40.36 (d, J = 1.4 Hz), 21.93, 10.35.

^{19}F NMR (377 MHz, CDCl_3) δ -135.26.

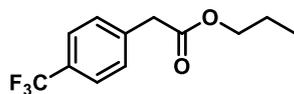
HRMS (ESI) m/z : $[\text{M} + \text{NH}_4]^+$ Calcd for $\text{C}_{12}\text{H}_{19}\text{FNO}_3^+$ 244.1344; Found 244.1354.



propyl 2-(3-chlorophenyl)acetate Light yellow liquid (78.4 mg, 74% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.34 – 7.26 (m, 3H), 7.20 (ddd, J = 5.5, 3.5, 1.6 Hz, 1H), 4.09 (t, J = 6.7 Hz, 2H), 3.62 (s, 2H), 1.68 (dtd, J = 14.1, 7.4, 6.6 Hz, 2H), 0.95 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.05, 136.03, 134.27, 129.76, 129.46, 127.51, 127.29, 66.69, 40.99, 21.93, 10.35.



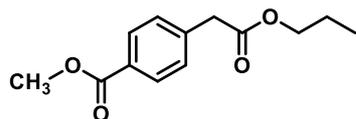
propyl 2-(4-(trifluoromethyl)phenyl)acetate Light yellow liquid (45.5 mg, 37% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, J = 8.0 Hz, 2H), 7.44 (d, J = 7.9 Hz, 2H), 4.10 (t, J = 6.7 Hz, 2H), 3.72 (s, 2H), 1.68 (h, J = 7.1 Hz, 2H), 0.95 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 170.89, 138.13, 129.69, 129.41 (q, J = 32.5 Hz), 125.47 (q, J = 3.8 Hz), 121.45 (d, J = 271.9 Hz), 66.78, 41.16, 21.91, 10.33.

^{19}F NMR (377 MHz, CDCl_3) δ -62.53.

HRMS (ESI) m/z : $[\text{M} + \text{Li}]^+$ Calcd for $\text{C}_{12}\text{H}_{13}\text{F}_3\text{LiO}_2^+$ 253.1022; Found 253.1047.

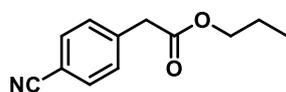


methyl 4-(2-oxo-2-propoxyethyl)benzoate Light yellow liquid (56.4 mg, 48% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.02 (d, $J = 8.3$ Hz, 2H), 7.39 (d, $J = 8.3$ Hz, 2H), 4.08 (t, $J = 6.7$ Hz, 2H), 3.93 (s, 3H), 3.70 (s, 2H), 1.71 – 1.60 (m, 2H), 0.92 (t, $J = 7.4$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 170.94, 166.89, 139.34, 129.83, 129.36, 128.96, 66.70, 52.12, 41.41, 21.91, 10.34.

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{17}\text{O}_4^+$ 237.1121; Found 237.1121.

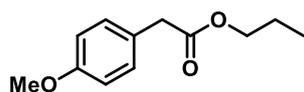


propyl 2-(4-cyanophenyl)acetate Light yellow liquid (42.6 mg, 42% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.61 (d, $J = 8.1$ Hz, 2H), 7.41 (d, $J = 8.1$ Hz, 2H), 4.06 (t, $J = 6.7$ Hz, 2H), 3.69 (s, 2H), 1.64 (h, $J = 7.1$ Hz, 2H), 0.90 (t, $J = 7.4$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 170.41, 139.54, 132.28, 130.20, 118.74, 111.03, 66.85, 41.30, 21.88, 10.33.

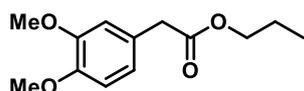
HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{12}\text{H}_{14}\text{NO}_2^+$ 240.1019; Found 240.1023.



propyl 2-(4-methoxyphenyl)acetate^[2] Light yellow liquid (55.1 mg, 53% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.24 (d, $J = 8.4$ Hz, 2H), 6.90 (d, $J = 8.6$ Hz, 2H), 4.08 (t, $J = 6.7$ Hz, 2H), 3.82 (s, 3H), 3.59 (s, 2H), 1.67 (h, $J = 7.2$ Hz, 2H), 0.95 (t, $J = 7.4$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 172.08, 158.63, 130.29, 126.28, 113.95, 66.41, 55.25, 40.55, 21.97, 10.40.

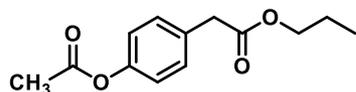


propyl 2-(3,4-dimethoxyphenyl)acetate Light yellow liquid (70.2 mg, 59% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 6.83 (d, $J = 5.3$ Hz, 3H), 4.06 (t, $J = 6.7$ Hz, 2H), 3.87 (d, $J = 6.4$ Hz, 6H), 3.56 (s, 2H), 1.65 (h, $J = 7.2$ Hz, 2H), 0.92 (t, $J = 7.4$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.93, 148.82, 148.04, 126.64, 121.37, 112.29, 111.09, 66.42, 55.85, 55.80, 40.97, 21.95, 10.38.

HRMS (ESI) m/z : $[\text{M} + \text{Li}]^+$ Calcd for $\text{C}_{13}\text{H}_{18}\text{LiO}_4^+$ 245.1360; Found 245.1356.

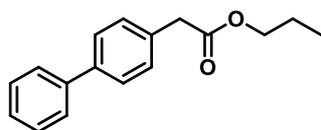


propyl 2-(4-acetoxyphenyl)acetate Light yellow liquid (61.4 mg, 52% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.33 (d, $J = 8.2$ Hz, 2H), 7.07 (d, $J = 8.3$ Hz, 2H), 4.08 (dd, $J = 7.2$, 6.2 Hz, 2H), 3.64 (s, 2H), 2.32 (d, $J = 1.0$ Hz, 3H), 1.67 (h, $J = 7.1$ Hz, 2H), 0.96 – 0.92 (m, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.46, 169.54, 149.69, 131.76, 130.32, 121.65, 66.57, 40.80, 21.93, 21.16, 10.37.

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{17}\text{O}_4^+$ 237.1121; Found 237.1131.

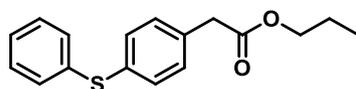


propyl 2-([1,1'-biphenyl]-4-yl)acetate Light yellow liquid (90.2 mg, 71% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.66 – 7.61 (m, 4H), 7.50 (dd, $J = 8.4$, 6.9 Hz, 2H), 7.42 (dd, $J = 8.5$, 6.8 Hz, 3H), 4.14 (t, $J = 6.7$ Hz, 2H), 3.73 (s, 2H), 1.72 (h, $J = 7.1$ Hz, 2H), 0.99 (t, $J = 7.4$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.77, 140.84, 140.03, 133.26, 129.74, 128.82, 127.35, 127.31, 127.12, 66.60, 41.11, 22.02, 10.45.

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{17}\text{H}_{18}\text{NaO}_2^+$ 277.1199; Found 277.1182.

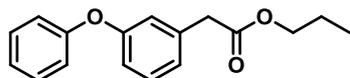


propyl 2-(3-(phenylthio)phenyl)acetate Light yellow liquid (85.8 mg, 60% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.38 – 7.26 (m, 9H), 4.10 (t, $J = 6.7$ Hz, 2H), 3.64 (s, 2H), 1.73 – 1.64 (m, 2H), 0.95 (t, $J = 7.4$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.45, 135.83, 134.37, 133.24, 131.33, 130.91, 130.18, 129.22, 127.04, 66.61, 40.99, 21.96, 10.40.

HRMS (ESI) m/z : $[M + Li]^+$ Calcd for $C_{17}H_{18}LiO_2S^+$ 293.1182; Found 293.1186.

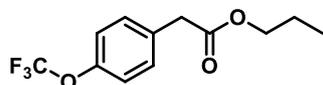


propyl 2-(3-phenoxyphenyl)acetate Light yellow liquid (82.4 mg, 61% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

1H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.13 (m, 4H), 7.09 – 6.95 (m, 5H), 4.10 (t, $J = 6.7$ Hz, 2H), 3.64 (s, 2H), 1.68 (h, $J = 7.1$ Hz, 2H), 0.96 (t, $J = 7.5$ Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.36, 157.43, 157.07, 136.08, 129.82, 129.80, 124.15, 123.37, 119.74, 119.04, 117.45, 66.56, 41.31, 21.98, 10.42.

HRMS (ESI) m/z : $[M + K]^+$ Calcd for $C_{17}H_{18}KO_3^+$ 309.0888; Found 309.0890.



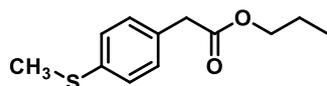
propyl 2-(4-(trifluoromethoxy)phenyl)acetate Light yellow liquid (65.5 mg, 50% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

1H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.33 (m, 2H), 7.22 – 7.19 (m, 2H), 4.09 (td, $J = 6.7, 3.8$ Hz, 2H), 3.66 (s, 2H), 1.72 – 1.63 (m, 2H), 0.94 (td, $J = 7.4, 2.0$ Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.25, 132.89, 130.68, 129.26, 128.54, 121.07, 66.67, 40.63, 21.92, 10.31.

^{19}F NMR (377 MHz, $CDCl_3$) δ -57.92.

HRMS (ESI) m/z : $[M + Li]^+$ Calcd for $C_{12}H_{13}F_3LiO_3^+$ 269.0971; Found 269.0990.

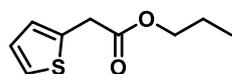


propyl 2-(4-(methylthio)phenyl)acetate Light yellow solid (67.2 mg, 60% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

1H NMR (400 MHz, $CDCl_3$) δ 7.24 (s, 4H), 4.08 (t, $J = 6.7$ Hz, 2H), 3.61 (s, 2H), 2.50 (s, 3H), 1.67 (dtd, $J = 14.1, 7.4, 6.6$ Hz, 2H), 0.94 (t, $J = 7.4$ Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.77, 130.69, 129.41, 126.51, 126.50, 66.19, 40.55, 21.62, 15.63, 10.44.

HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{12}H_{17}O_2S^+$ 225.0944; Found 225.0934.

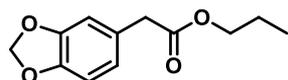


propyl 2-(thiophen-2-yl)acetate Light yellow liquid (50.6 mg, 55% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.33 – 7.29 (m, 1H), 7.19 – 7.18 (m, 1H), 7.08 (dd, $J = 4.9, 1.3$ Hz, 1H), 4.10 (td, $J = 6.7, 1.1$ Hz, 2H), 3.69 (s, 2H), 1.69 (h, $J = 7.1, 6.7$ Hz, 2H), 0.96 (td, $J = 7.5, 1.1$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.27, 133.77, 128.52, 125.69, 122.80, 66.54, 35.95, 21.97, 10.39.

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_9\text{H}_{12}\text{NaO}_2\text{S}^+$ 207.0450; Found 207.0455.

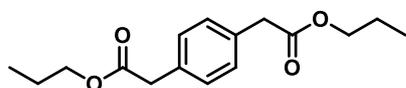


propyl 2-(benzo[d][1,3]dioxol-5-yl)acetate Light yellow liquid (48.8 mg, 44% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 6.82 – 6.74 (m, 3H), 5.97 (s, 2H), 4.07 (t, $J = 6.7$ Hz, 2H), 3.55 (s, 2H), 1.67 (h, $J = 7.2$ Hz, 2H), 0.95 (t, $J = 7.4$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.83, 147.72, 146.64, 127.76, 122.39, 109.73, 108.27, 101.02, 66.50, 41.04, 21.95, 10.38.

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{12}\text{H}_{15}\text{O}_4^+$ 223.0965; Found 223.0950.

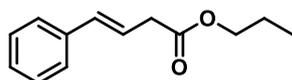


dipropyl 2,2'-(1,4-phenylene)diacetate White solid (44.48 mg, 32% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.27 (s, 4H), 4.08 (t, $J = 6.7$ Hz, 4H), 3.63 (s, 4H), 1.67 (dtd, $J = 14.1, 7.4, 6.7$ Hz, 4H), 0.94 (t, $J = 7.4$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.61, 132.97, 129.42, 66.47, 41.08, 21.95, 10.34.

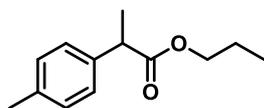
HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{23}\text{O}_4^+$ 279.1591; Found 279.1589.



propyl (E)-4-phenylbut-3-enoate Light yellow liquid (71.4 mg, 70% yield, E/Z=13:1). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, Chloroform- d) δ 7.42 – 7.18 (m, 5H), 6.54 (dt, $J = 15.9, 1.5$ Hz, 1H), 6.35 (dt, $J = 15.8, 7.1$ Hz, 1H), 4.13 (dt, $J = 10.1, 6.7$ Hz, 2H), 3.29 (dd, $J = 7.1, 1.4$ Hz, 1.5H), 1.79 (d, $J = 7.2$ Hz, 0.5H), 1.76 – 1.66 (m, 2H), 0.97 (dt, $J = 19.6, 7.4$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.68 (major), 167.24 (minor), 139.64 (major), 136.92 (major), 135.21 (minor), 135.05 (minor), 133.35 (major), 129.80 (minor), 128.54 (major), 127.92 (minor), 127.53 (major), 127.30 (minor), 126.29 (major), 121.92 (minor), 66.41 (major), 66.34 (minor), 38.48, 22.03 (minor), 21.99 (major), 10.46 (minor), 10.39 (major).

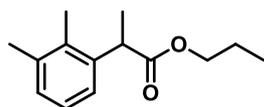


propyl 2-(p-tolyl)propanoate Light yellow liquid (62.8 mg, 61% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.29 – 7.17 (m, 4H), 4.07 (td, J = 6.7, 2.2 Hz, 2H), 3.74 (q, J = 7.2 Hz, 1H), 2.37 (s, 3H), 1.65 (dtd, J = 14.1, 7.4, 6.6 Hz, 2H), 1.53 (d, J = 7.2 Hz, 3H), 0.91 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 174.83, 137.75, 136.66, 129.27, 127.36, 66.29, 45.21, 21.96, 21.08, 18.61, 10.34.

HRMS (ESI) m/z : $[\text{M} + \text{Li}]^+$ Calcd for $\text{C}_{13}\text{H}_{18}\text{LiO}_2^+$ 213.1461; Found 213.1466.

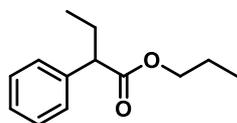


propyl 2-(2,3-dimethylphenyl)propanoate Light yellow liquid (69.3 mg, 63% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.17 – 7.08 (m, 3H), 4.07 (pd, J = 7.1, 6.5, 3.9 Hz, 3H), 2.32 (d, J = 15.8 Hz, 6H), 1.64 (h, J = 7.0 Hz, 2H), 1.51 (d, J = 7.1 Hz, 3H), 0.90 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 175.19, 139.23, 137.00, 134.26, 128.64, 125.75, 124.39, 66.30, 41.89, 21.95, 21.09, 18.10, 15.14, 10.33.

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{14}\text{H}_{20}\text{NaO}_2^+$ 243.1356; Found 243.1338.

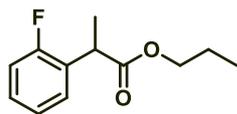


propyl 2-phenylbutanoate Light yellow liquid (46.4 mg, 45% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.37 – 7.26 (m, 5H), 4.16 – 3.99 (m, 2H), 3.49 (t, J = 7.7 Hz, 1H), 2.20 – 2.08 (m, 1H), 1.84 (dt, J = 13.6, 7.4 Hz, 1H), 1.64 (h, J = 7.1 Hz, 2H), 0.95-0.88 (m, 6H).

^{13}C NMR (101 MHz, CDCl_3) δ 174.19, 139.29, 128.51, 127.97, 127.11, 66.23, 53.63, 26.71, 21.96, 12.23, 10.33.

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{19}\text{O}_2^+$ 207.1380; Found 207.1385.

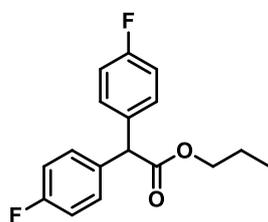


propyl 2-(2-fluorophenyl)propanoate Light yellow liquid (51.5 mg, 49% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.36 – 7.24 (m, 2H), 7.16 – 7.05 (m, 2H), 4.11 – 4.03 (m, 3H), 1.63 (h, $J = 7.2$ Hz, 2H), 1.54 (d, $J = 7.2$ Hz, 3H), 0.88 (t, $J = 7.4$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 174.02, 160.37 (d, $J = 245.9$ Hz), 128.67 (d, $J = 4.1$ Hz), 128.58 (d, $J = 8.4$ Hz), 128.00 (d, $J = 14.9$ Hz), 124.24 (d, $J = 3.6$ Hz), 115.40 (d, $J = 22.2$ Hz), 66.51, 38.49 (d, $J = 2.8$ Hz), 21.91, 17.50, 10.26.

$^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -118.25.



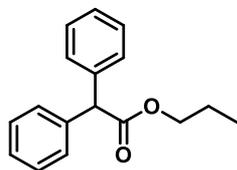
propyl 2,2-bis(4-fluorophenyl)acetate Light yellow liquid (130.5 mg, 90% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, Chloroform-*d*) δ 7.34 – 7.29 (m, 4H), 7.09 – 7.03 (m, 4H), 5.03 (s, 1H), 4.16 (t, $J = 6.7$ Hz, 2H), 1.69 (dtd, $J = 14.1, 7.4, 6.7$ Hz, 2H), 0.92 (t, $J = 7.4$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 172.38, 162.05 (d, $J = 246.2$ Hz), 134.44 (d, $J = 3.3$ Hz), 130.13 (d, $J = 8.0$ Hz), 115.54 (d, $J = 21.5$ Hz), 67.00, 55.56, 21.91, 10.33.

$^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -115.16.

HRMS (ESI) m/z : $[\text{M} + \text{NH}_4]^+$ Calcd for $\text{C}_{17}\text{H}_{20}\text{F}_2\text{NO}_2^+$ 308.1457; Found 308.1440.

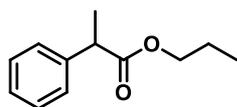


propyl 2,2-diphenylacetate Light yellow solid (95.3 mg, 75% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.44 – 7.29 (m, 10H), 5.13 (s, 1H), 4.20 (t, $J = 6.7$ Hz, 2H), 1.73 (h, $J = 7.2$ Hz, 2H), 0.96 (t, $J = 7.4$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 172.63, 138.87, 128.68, 128.63, 127.28, 66.85, 57.27, 22.00, 10.42.

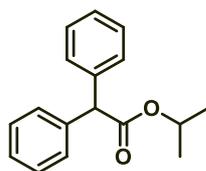
HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{17}\text{H}_{18}\text{NaO}_2^+$ 277.1199; Found 277.1200.



propyl 2-phenylpropanoate^[3] Light yellow liquid (48.0 mg, 50% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.27 (m, 5H), 4.06 (t, *J* = 6.7 Hz, 2H), 3.76 (q, *J* = 7.2 Hz, 1H), 1.68 – 1.59 (m, 2H), 1.54 (d, *J* = 7.2 Hz, 3H), 0.89 (t, *J* = 7.4 Hz, 3H).

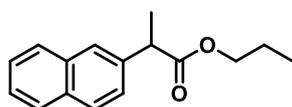
¹³C NMR (101 MHz, CDCl₃) δ 174.66, 140.71, 128.58, 127.50, 127.07, 66.34, 45.61, 21.94, 18.54, 10.31.



isopropyl 2,2-diphenylacetate^[4] Light yellow solid (90.2 mg, 71% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.29 (m, 10H), 5.15 (hept, *J* = 6.3 Hz, 1H), 5.05 (s, 1H), 1.29 (d, *J* = 6.3 Hz, 6H).

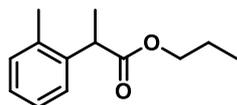
¹³C NMR (101 MHz, CDCl₃) δ 172.04, 138.93, 128.64, 128.58, 127.19, 68.66, 57.32, 21.73.



propyl 2-(naphthalen-2-yl)propanoate Light yellow liquid (75.0 mg, 62% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.88 – 7.81 (m, 4H), 7.55 – 7.48 (m, 3H), 4.10 (td, *J* = 6.7, 2.0 Hz, 2H), 3.95 (q, *J* = 7.1 Hz, 1H), 1.69-1.61 (m, 5H), 0.90 (t, *J* = 7.4 Hz, 3H).

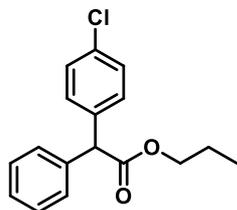
¹³C NMR (101 MHz, CDCl₃) δ 174.65, 138.19, 133.48, 132.58, 128.28, 127.83, 127.65, 126.15, 126.14, 125.83, 125.79, 66.45, 45.77, 21.97, 18.60, 10.36.



propyl 2-(o-tolyl)propanoate Light yellow liquid (57.7 mg, 56% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

¹H NMR (400 MHz, CDCl₃) δ 7.33 – 7.16 (m, 4H), 4.09 – 3.95 (m, 3H), 2.42 (s, 3H), 1.62 (ddd, *J* = 14.2, 7.5, 6.8 Hz, 2H), 1.52 (d, *J* = 7.2 Hz, 3H), 0.89 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 174.95, 139.26, 135.71, 130.43, 126.87, 126.48, 126.38, 66.30, 41.36, 21.94, 19.67, 17.87, 10.31.

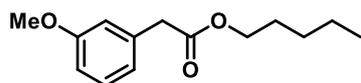


propyl 2-(4-chlorophenyl)-2-phenylacetate Light yellow liquid (111.7 mg, 98% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.42 – 7.32 (m, 9H), 5.07 (s, 1H), 4.19 (t, J = 6.7 Hz, 2H), 1.71 (h, J = 7.2 Hz, 2H), 0.95 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 172.26, 138.42, 137.38, 133.21, 130.10, 128.76, 128.75, 128.52, 127.48, 66.99, 56.55, 21.97, 10.40.

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{17}\text{H}_{17}\text{ClNaO}_2^+$ 311.0809; Found 311.0828.

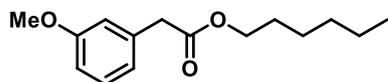


pentyl 2-(3-methoxyphenyl)acetate Light yellow liquid (74.3 mg, 63% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.29 – 7.25 (m, 1H), 6.92 – 6.83 (m, 3H), 4.12 (t, J = 6.7 Hz, 2H), 3.83 (s, 3H), 3.62 (s, 2H), 1.79 – 1.62 (m, 2H), 1.33 (tt, J = 4.8, 3.5 Hz, 4H), 0.94 – 0.90 (m, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.61, 159.67, 135.62, 129.51, 121.62, 114.82, 112.63, 65.08, 55.19, 41.54, 28.27, 28.03, 22.32, 13.99.

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{14}\text{H}_{20}\text{NaO}_3^+$ 259.1305; Found 259.1291.

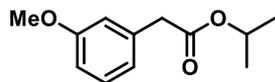


hexyl 2-(3-methoxyphenyl)acetate Light yellow liquid (76.3 mg, 61% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.29 – 7.25 (m, 1H), 6.92 – 6.83 (m, 3H), 4.12 (t, J = 6.7 Hz, 2H), 3.83 (s, 3H), 3.62 (s, 2H), 1.68 – 1.61 (m, 2H), 1.38 – 1.27 (m, 6H), 0.93 – 0.90 (m, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.61, 159.67, 135.62, 129.51, 121.61, 114.83, 112.62, 65.09, 55.17, 41.54, 31.41, 28.54, 25.54, 22.56, 14.02.

HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{15}\text{H}_{22}\text{NaO}_3^+$ 273.1461; Found 273.1446.

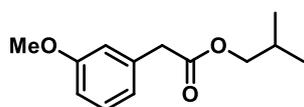


isopropyl 2-(3-methoxyphenyl)acetate Light yellow liquid (63.4 mg, 61% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.27 (t, $J = 7.8$ Hz, 1H), 6.91 – 6.83 (m, 3H), 5.05 (hept, $J = 6.3$ Hz, 1H), 3.83 (s, 3H), 3.59 (s, 2H), 1.27 (d, $J = 6.3$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.06, 159.65, 135.75, 129.49, 121.57, 114.75, 112.58, 68.24, 55.18, 41.77, 21.80.

HRMS (ESI) m/z : $[\text{M} + \text{K}]^+$ Calcd for $\text{C}_{12}\text{H}_{16}\text{KO}_3^+$ 247.0731; Found 247.0738.

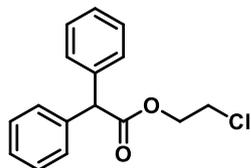


isobutyl 2-(3-methoxyphenyl)acetate Light yellow liquid (71.0 mg, 64% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.29 – 7.25 (m, 1H), 6.92 – 6.83 (m, 3H), 3.91 (d, $J = 6.7$ Hz, 2H), 3.83 (s, 3H), 3.64 (s, 2H), 1.95 (dp, $J = 13.4, 6.7$ Hz, 1H), 0.93 (d, $J = 6.8$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 171.57, 159.67, 135.63, 129.51, 121.65, 114.81, 112.66, 70.98, 55.19, 41.56, 27.72, 19.06.

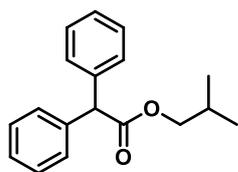
HRMS (ESI) m/z : $[\text{M} + \text{Li}]^+$ Calcd for $\text{C}_{13}\text{H}_{18}\text{LiO}_3^+$ 229.1411; Found 229.1419.



2-chloroethyl 2,2-diphenylacetate Light yellow liquid (69.9 mg, 51% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.42 – 7.31 (m, 10H), 5.15 (s, 1H), 4.45 (dd, $J = 6.3, 5.3$ Hz, 2H), 3.71 (dd, $J = 6.3, 5.2$ Hz, 2H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 172.19, 138.35, 128.70, 128.65, 127.44, 64.68, 56.95, 41.40.

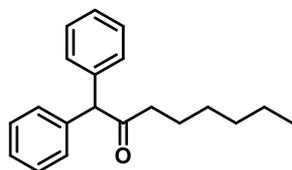


isobutyl 2,2-diphenylacetate Light yellow liquid (109.9 mg, 82% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.40 – 7.29 (m, 10H), 5.11 (s, 1H), 4.00 (d, $J = 6.6$ Hz, 2H), 1.98 (dp, $J = 13.4, 6.7$ Hz, 1H), 0.92 (d, $J = 6.7$ Hz, 6H).

^{13}C NMR (101 MHz, CDCl_3) δ 172.58, 138.83, 128.68, 128.59, 127.25, 71.29, 57.32, 27.75, 19.07.

HRMS (ESI) m/z : $[\text{M} + \text{K}]^+$ Calcd for $\text{C}_{18}\text{H}_{20}\text{KO}_2^+$ 307.1095; Found 307.1090.

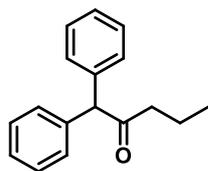


1,1-diphenylheptan-2-one Light yellow liquid (61.6 mg, 44% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.39 – 7.35 (m, 4H), 7.32 – 7.27 (m, 6H), 5.18 (s, 1H), 2.59 (t, $J = 7.4$ Hz, 2H), 1.67 – 1.60 (m, 2H), 1.34 – 1.25 (m, 6H), 0.90 (t, $J = 6.8$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 208.82, 138.53, 128.99, 128.69, 127.19, 64.14, 42.98, 31.58, 28.77, 23.98, 22.51, 14.08.

HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{20}\text{H}_{25}\text{O}^+$ 281.1900; Found 281.1905.

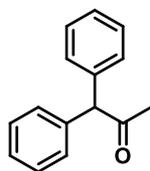


1,1-diphenylpentan-2-one Light yellow liquid (79.7 mg, 67% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.41 – 7.29 (m, 10H), 5.19 (s, 1H), 2.61 – 2.57 (m, 2H), 1.73 – 1.64 (m, 2H), 0.93 (td, $J = 7.4, 1.0$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 208.68, 138.54, 129.00, 128.71, 127.21, 64.15, 44.88, 17.47, 13.69.

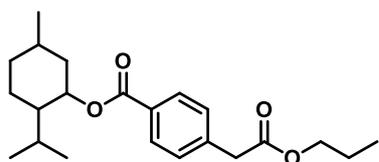
HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{17}\text{H}_{19}\text{O}^+$ 239.1430; Found 239.1419.



1,1-diphenylpropan-2-one^[5] Light yellow liquid (66.2 mg, 63% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.44 – 7.26 (m, 10H), 5.18 (s, 1H), 2.30 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 206.62, 138.32, 129.03, 128.78, 127.32, 65.08, 30.14.

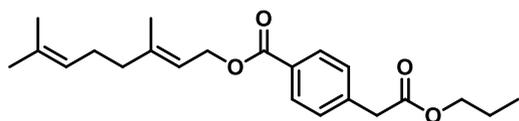


2-isopropyl-5-methylphenyl 4-(2-oxo-2-propoxyethyl)benzoate White solid (139.8 mg, 79% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 8.03 (d, $J = 8.3$ Hz, 2H), 7.39 – 7.37 (m, 2H), 4.95 (td, $J = 10.9, 4.4$ Hz, 1H), 4.08 (t, $J = 6.7$ Hz, 2H), 3.70 (s, 2H), 2.14 (dtd, $J = 12.0, 3.9, 1.7$ Hz, 1H), 1.98 (pd, $J = 7.0, 2.8$ Hz, 1H), 1.78 – 1.54 (m, 6H), 1.14 (dtd, $J = 15.4, 12.4, 9.7$ Hz, 2H), 0.96 – 0.92 (m, 10H), 0.81 (d, $J = 7.0$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 170.92, 165.83, 139.09, 129.81, 129.71, 129.27, 74.81, 66.66, 47.29, 41.40, 40.98, 34.34, 31.45, 26.52, 23.66, 22.05, 21.93, 20.77, 16.54, 10.33.

HRMS (ESI) m/z : $[\text{M} + \text{Li}]^+$ Calcd for $\text{C}_{22}\text{H}_{32}\text{LiO}_4^+$ 367.2455; Found 367.2468.

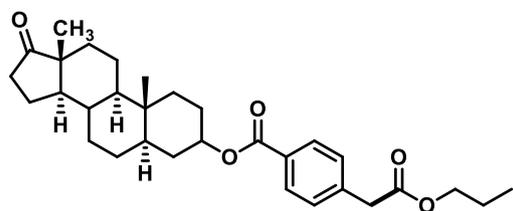


(E)-3,7-dimethylocta-2,6-dien-1-yl 4-(2-oxo-2-propoxyethyl)benzoate White solid (75.2 mg, 42% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 8.05 – 8.02 (m, 2H), 7.40 – 7.37 (m, 2H), 5.51 – 5.47 (m, 1H), 5.15 – 5.11 (m, 1H), 4.86 (d, $J = 7.0$ Hz, 2H), 4.09 (t, $J = 6.7$ Hz, 2H), 3.70 (s, 2H), 2.17 – 2.10 (m, 4H), 1.79 (d, $J = 1.3$ Hz, 3H), 1.71 (d, $J = 1.4$ Hz, 3H), 1.69 – 1.66 (m, 2H), 1.64 (d, $J = 1.2$ Hz, 3H), 0.93 (t, $J = 7.5$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 170.93, 166.44, 142.38, 139.18, 131.85, 129.85, 129.38, 129.27, 123.75, 118.39, 66.68, 61.89, 41.46, 39.56, 26.32, 25.68, 21.92, 17.71, 16.57, 10.32, 1.04.

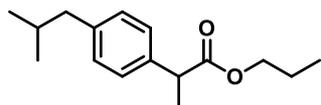
HRMS (ESI) m/z : $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{22}\text{H}_{30}\text{NaO}_4^+$ 381.2036; Found 381.2052.



(5R,9R,10R,13R,14R)-10,13-dimethyl-17-oxohexadecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-(2-oxo-2-propoxyethyl)benzoate White solid (158 mg, 64% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

^1H NMR (400 MHz, CDCl_3) δ 7.91 (d, $J = 8.3$ Hz, 2H), 7.28 (d, $J = 8.2$ Hz, 2H), 4.86 (tt, $J = 11.4, 4.9$ Hz, 1H), 3.98 (t, $J = 6.7$ Hz, 2H), 3.60 (s, 2H), 2.40 – 2.33 (m, 1H), 2.05 – 1.95 (m, 1H), 1.87 (ddd, $J = 12.1, 8.7, 6.0$ Hz, 2H), 1.77 – 1.66 (m, 4H), 1.65 – 1.50 (m, 5H), 1.49 – 1.37 (m, 3H), 1.31 – 1.18 (m, 7H), 0.81 – 0.78 (m, 10H).

^{13}C NMR (101 MHz, CDCl_3) δ 221.41, 171.03, 165.96, 139.19, 129.86, 129.75, 129.33, 74.17, 66.75, 54.39, 51.43, 47.88, 44.78, 41.50, 36.82, 35.95, 35.79, 35.12, 34.12, 31.60, 30.90, 28.38, 27.60, 21.99, 21.87, 20.57, 13.91, 12.38, 10.43.



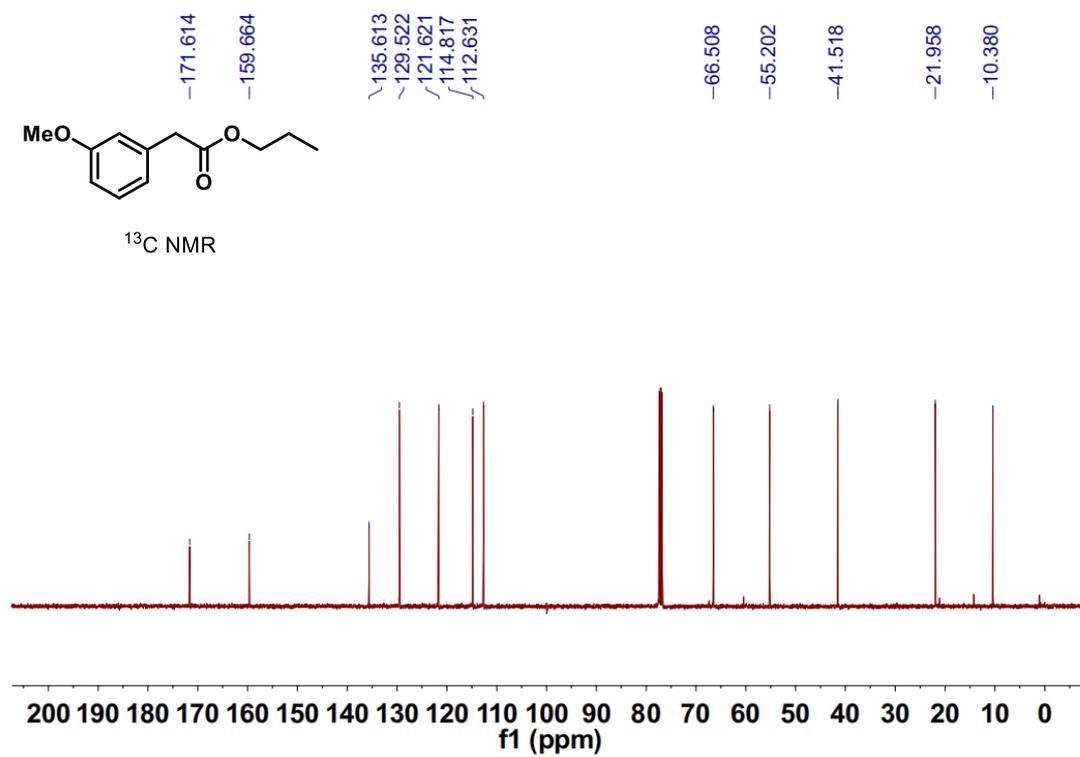
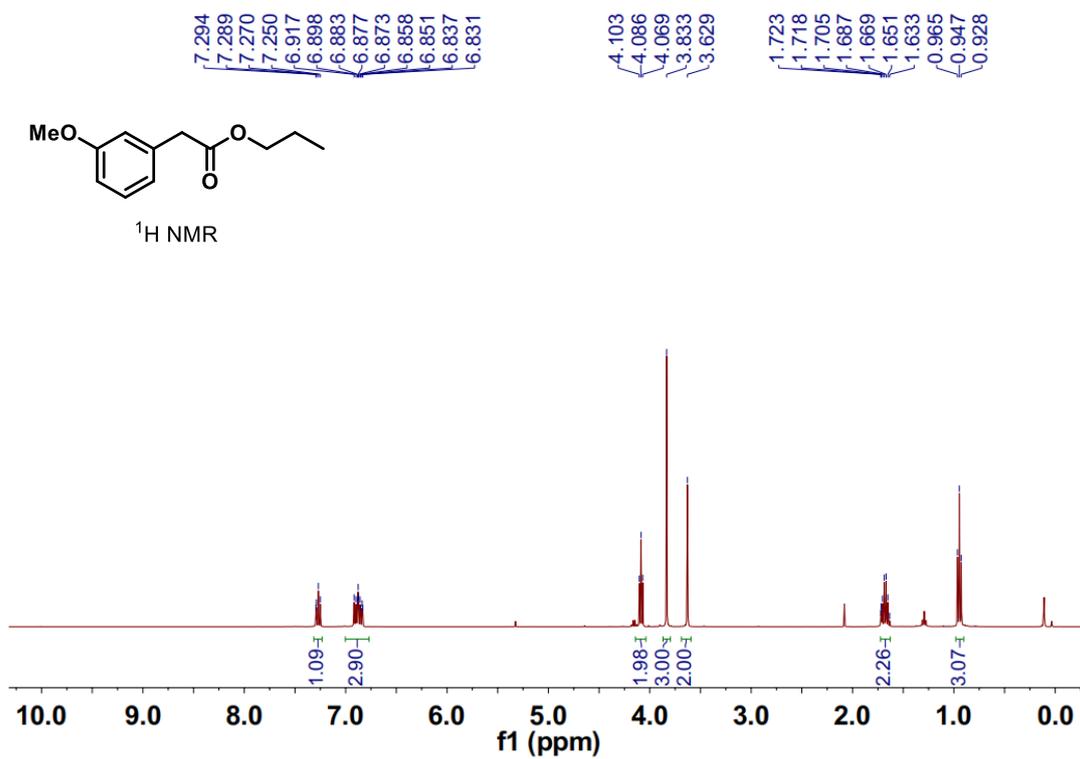
propyl 2-(4-isobutylphenyl)propanoate White solid (71.9 mg, 58% yield). The product was purified by silica gel column chromatography, using petroleum ether /EA = 120/1 (v/v) as an eluent.

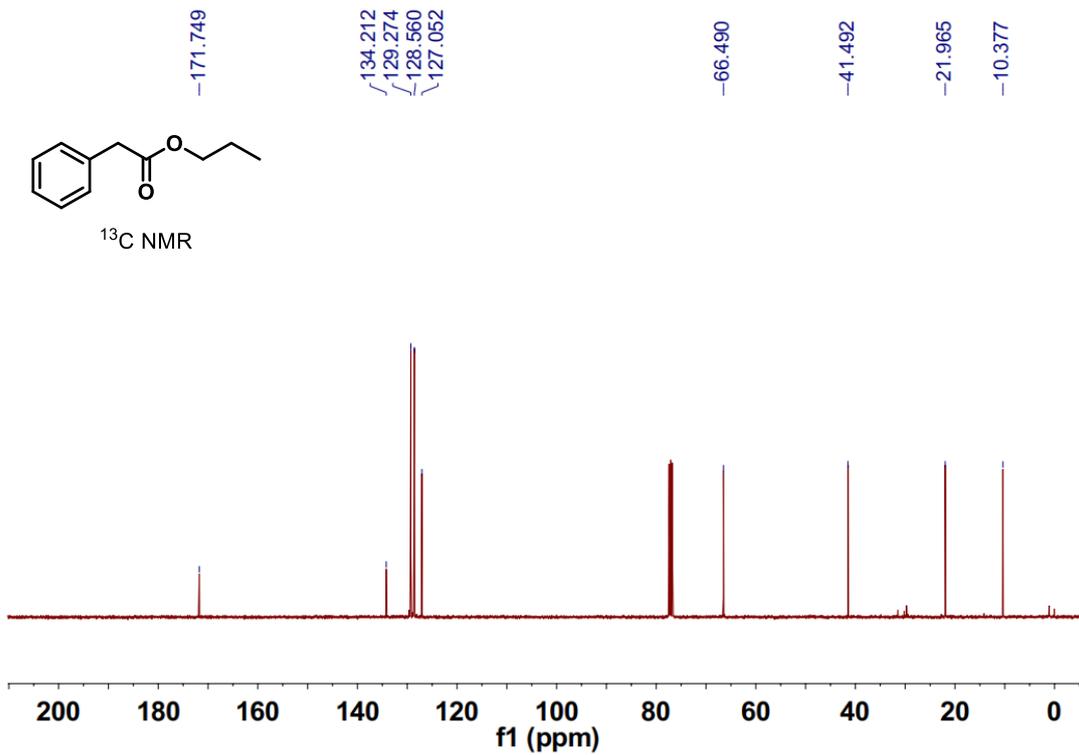
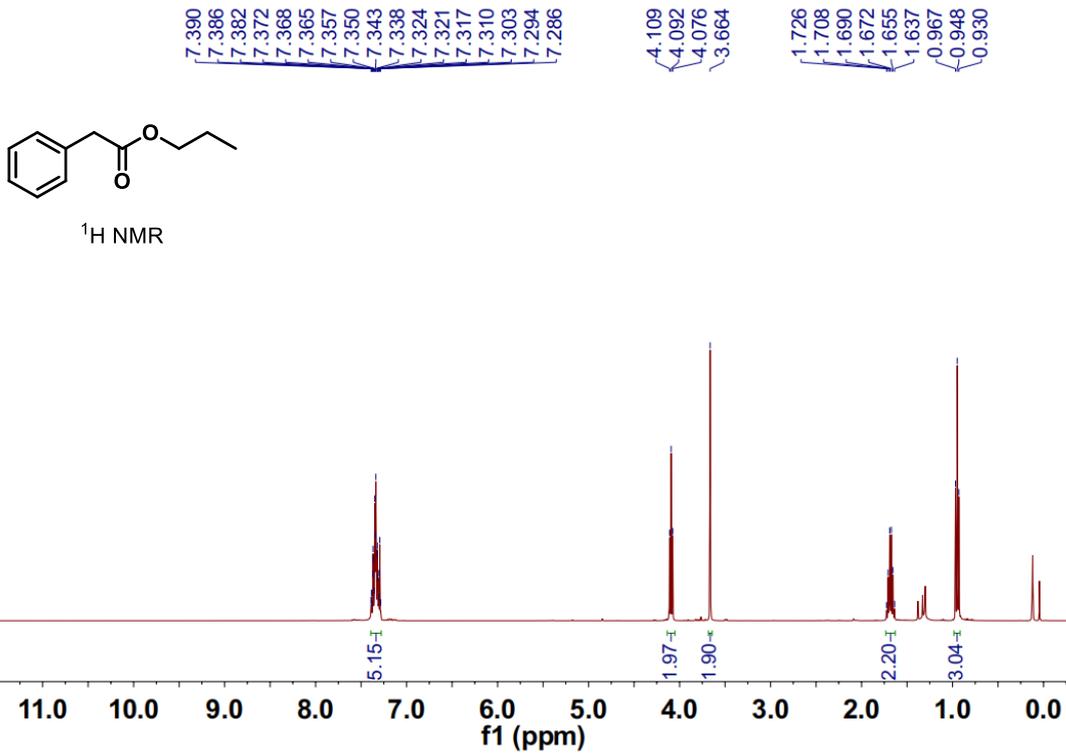
^1H NMR (400 MHz, CDCl_3) δ 7.25 – 7.19 (m, 2H), 7.10 – 7.08 (m, 2H), 4.02 (t, $J = 6.7$ Hz, 2H), 3.69 (d, $J = 7.2$ Hz, 1H), 2.45 – 2.43 (m, 2H), 1.83 (dq, $J = 13.6, 6.8$ Hz, 1H), 1.59 (h, $J = 7.4$ Hz, 2H), 1.49 (d, $J = 7.2$ Hz, 3H), 0.90 – 0.82 (m, 9H).

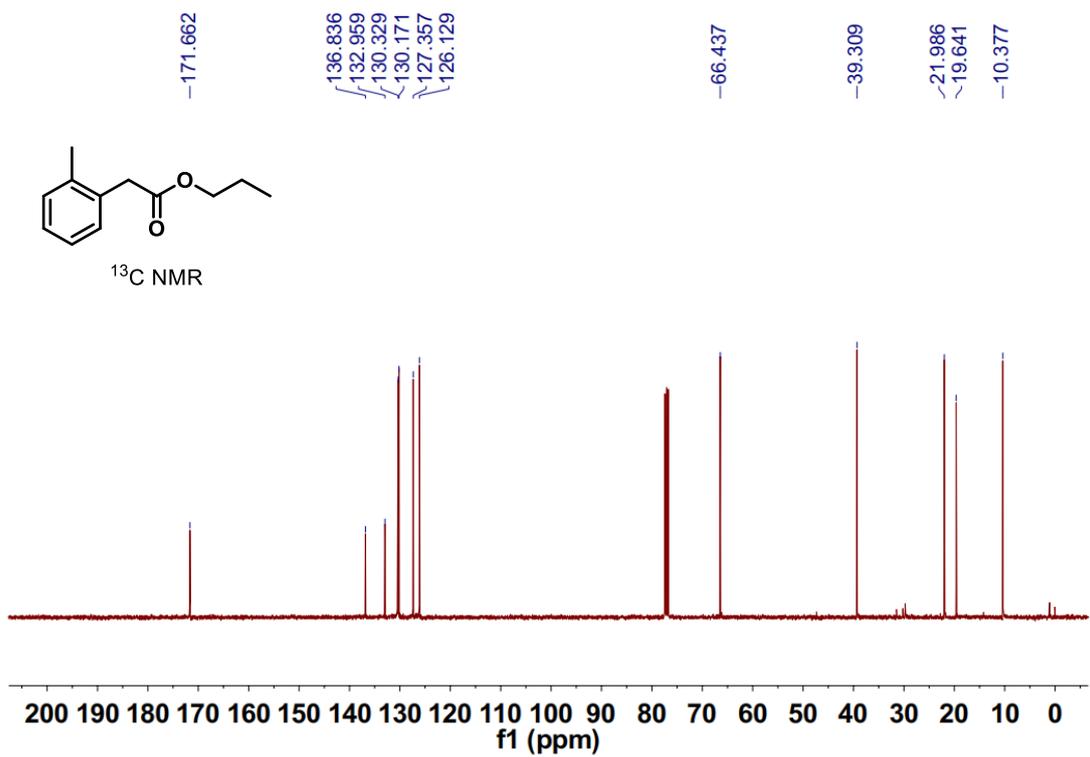
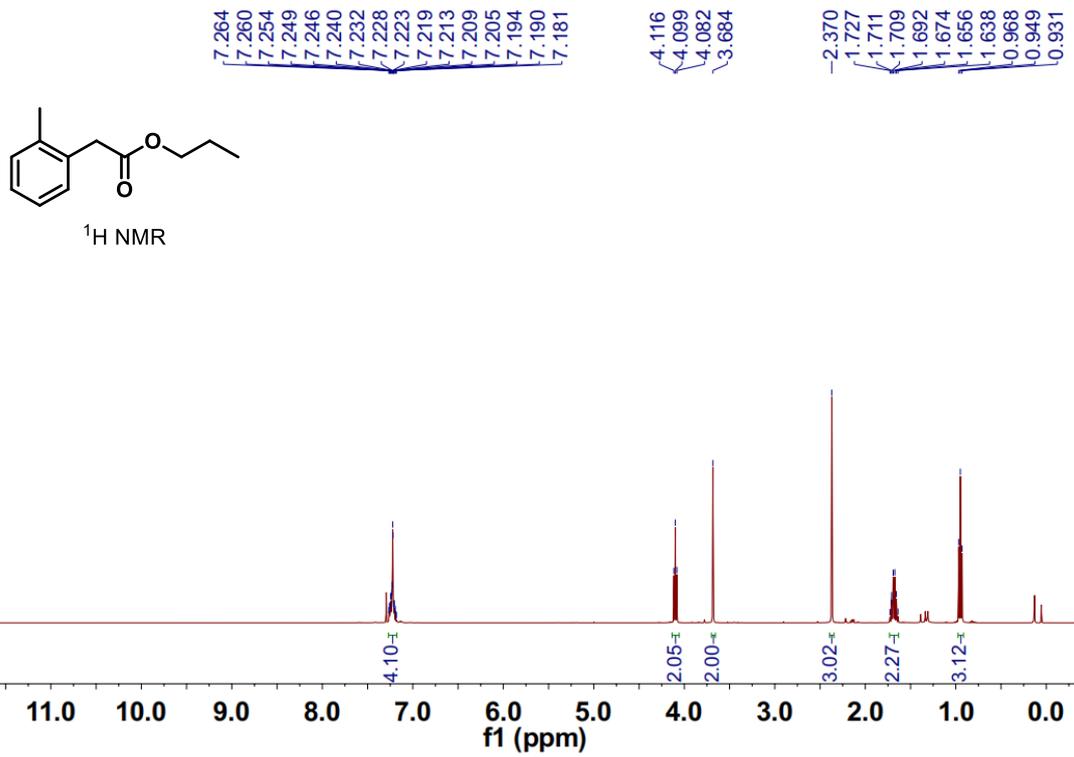
^{13}C NMR (101 MHz, CDCl_3) δ 174.92, 140.52, 138.01, 129.35, 127.24, 66.30, 45.30, 45.13, 30.29, 22.46, 22.02, 18.57, 10.35.

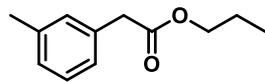
HRMS (ESI) m/z : $[\text{M} + \text{Li}]^+$ Calcd for $\text{C}_{16}\text{H}_{24}\text{LiO}_2^+$ 255.1931; Found 255.1943.

NMR Spectra of Substrates and Products

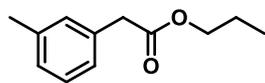
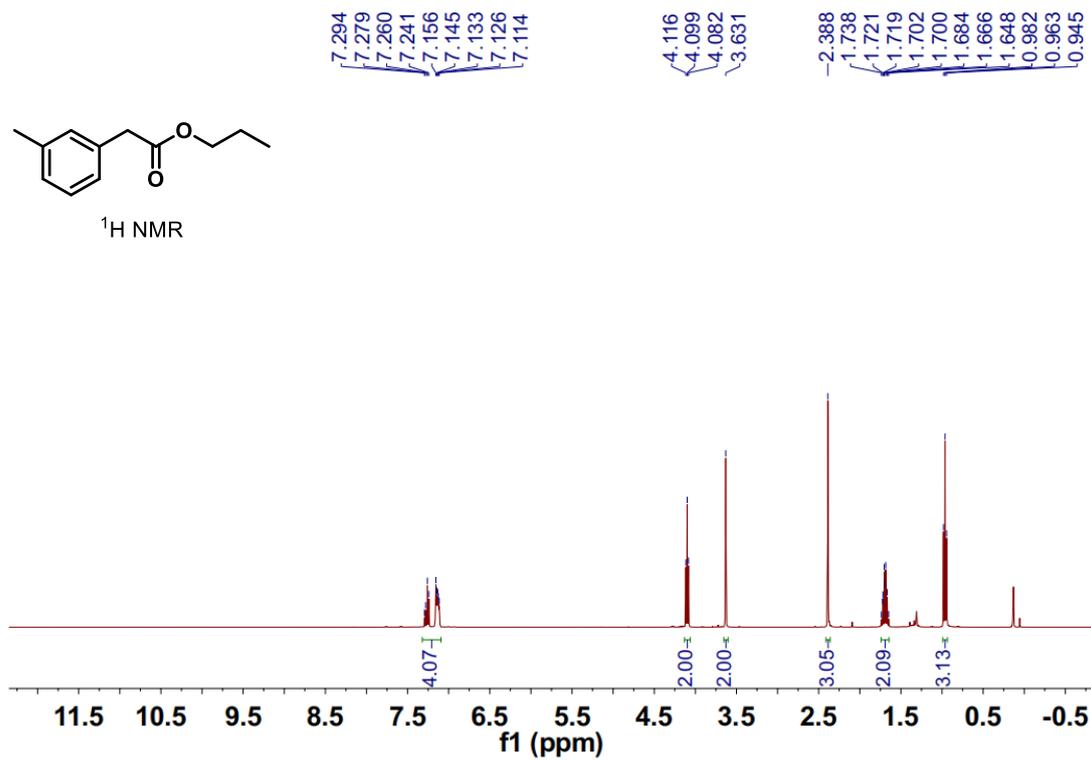




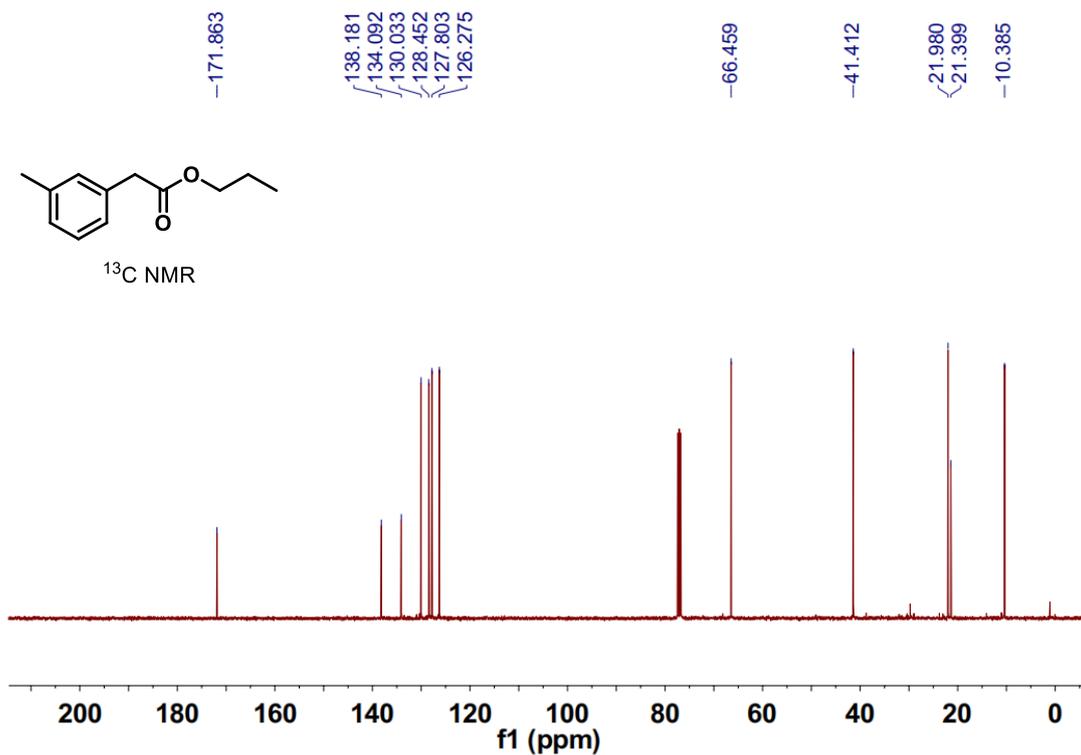


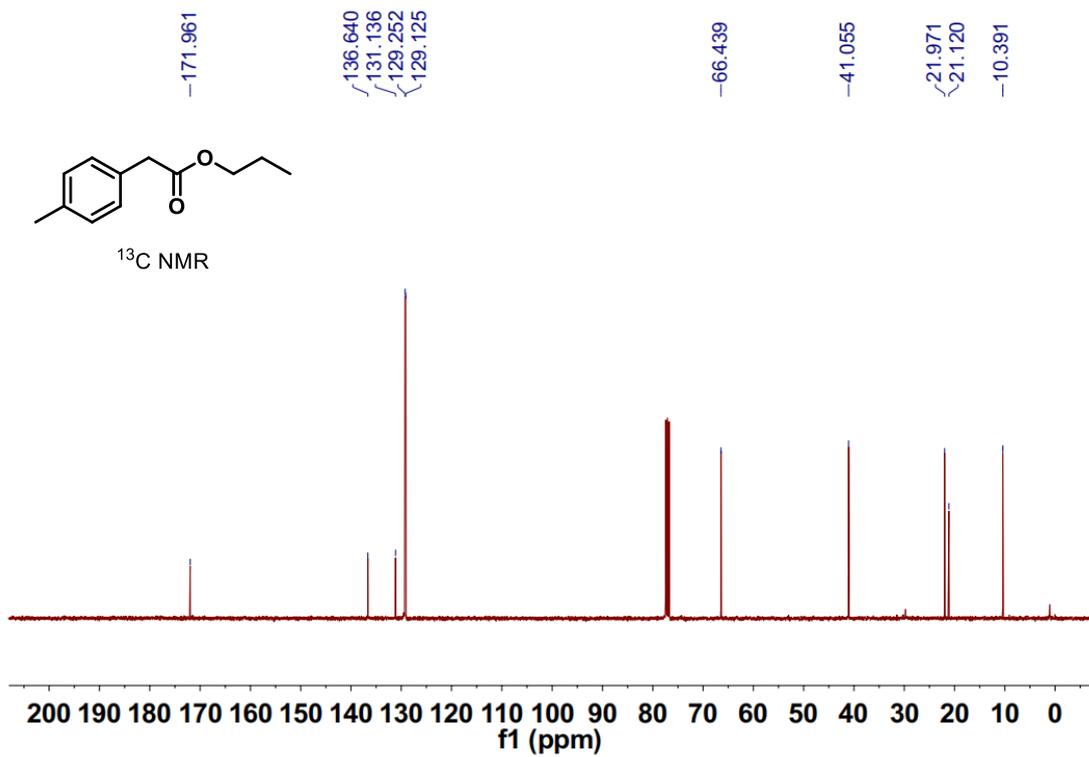
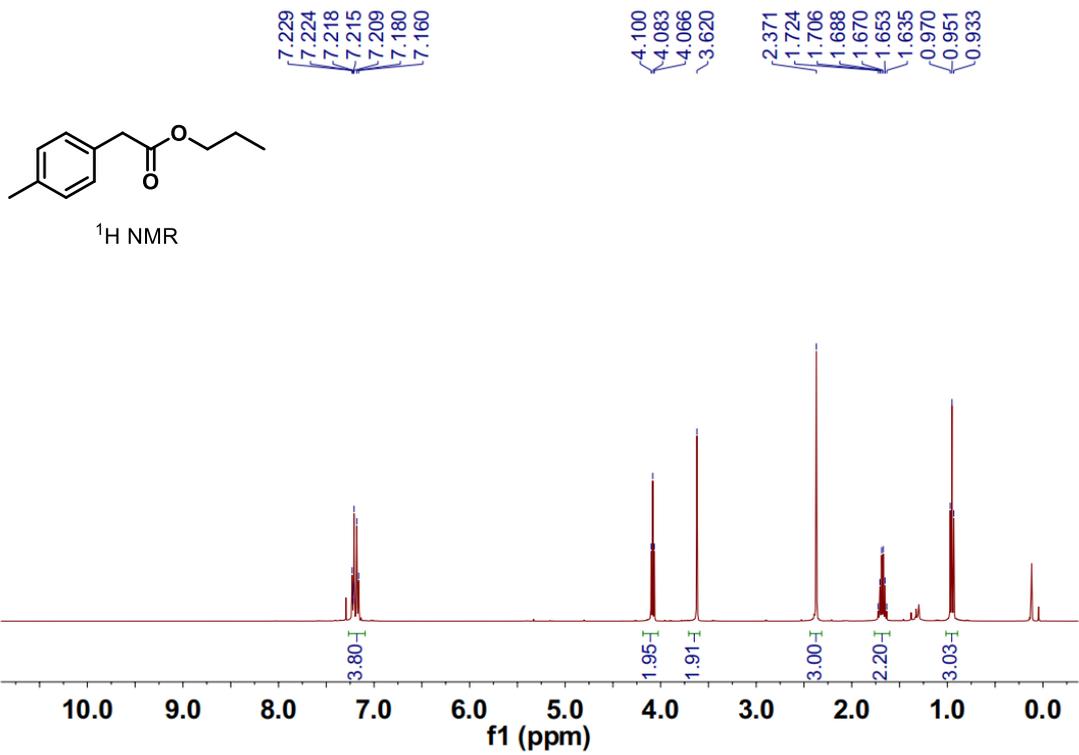


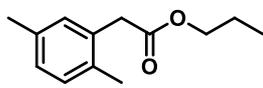
¹H NMR



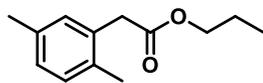
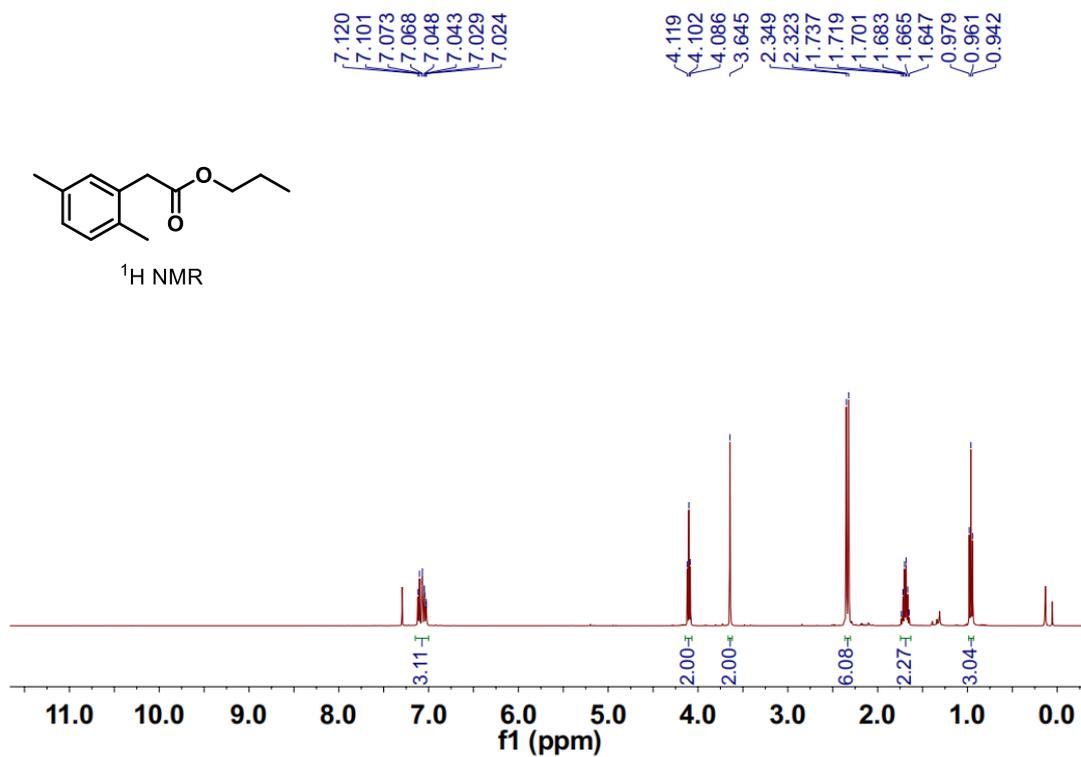
¹³C NMR



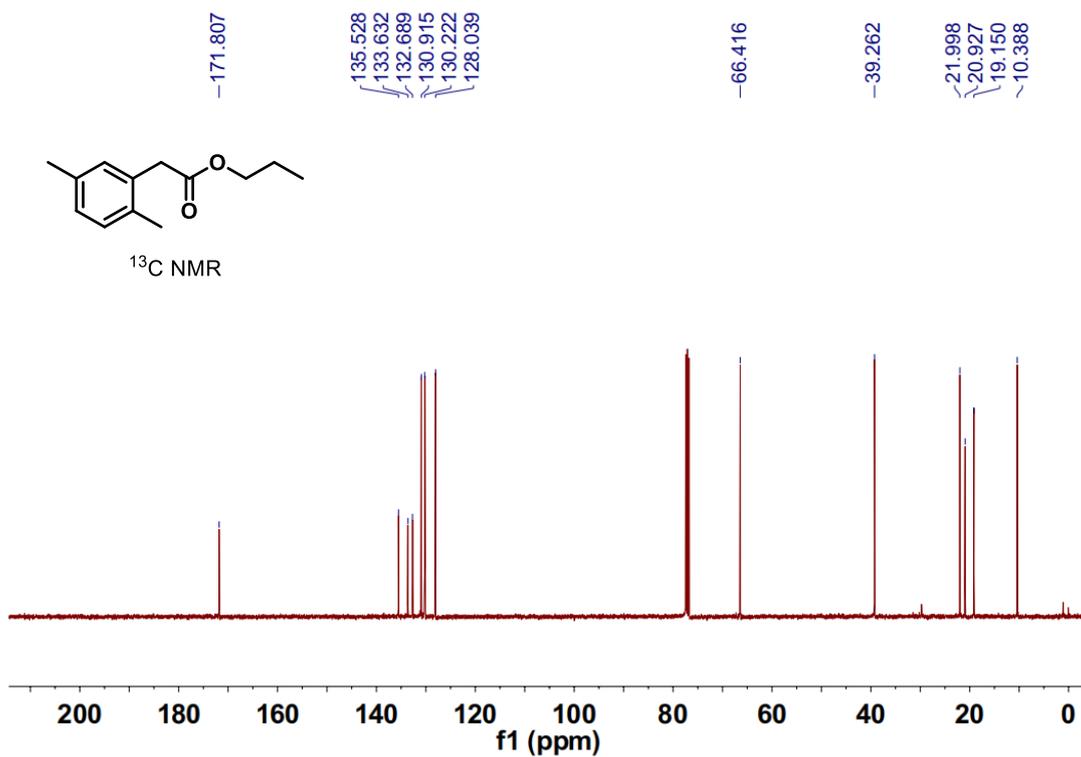


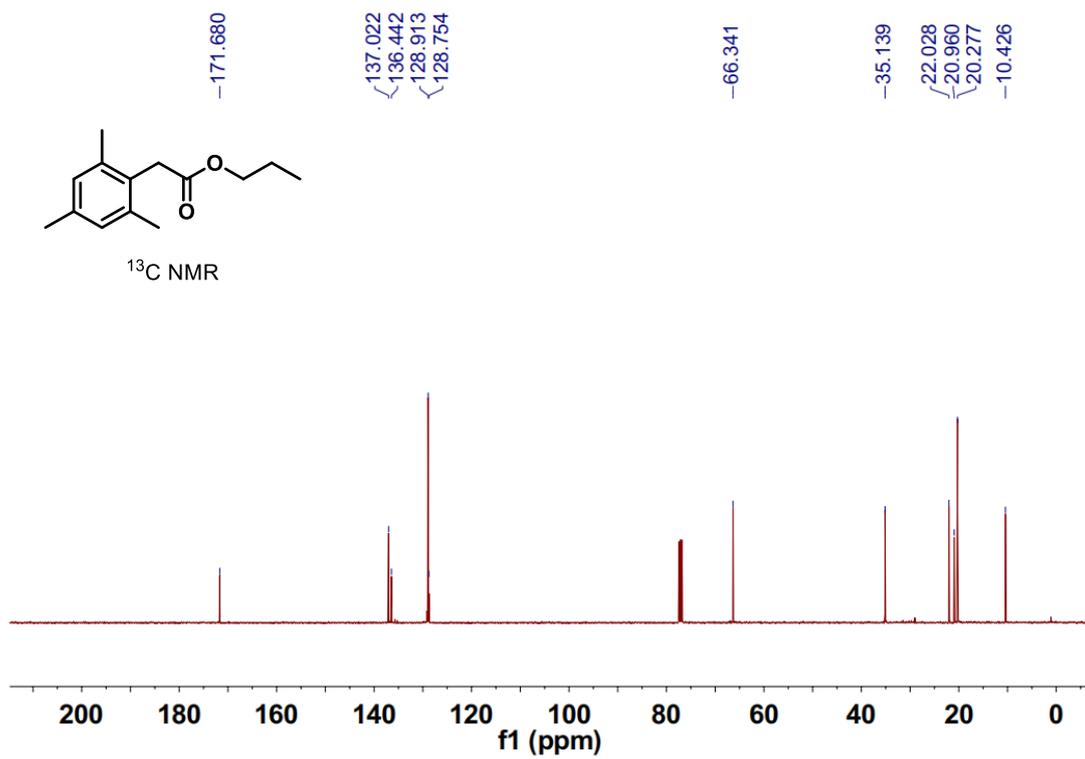
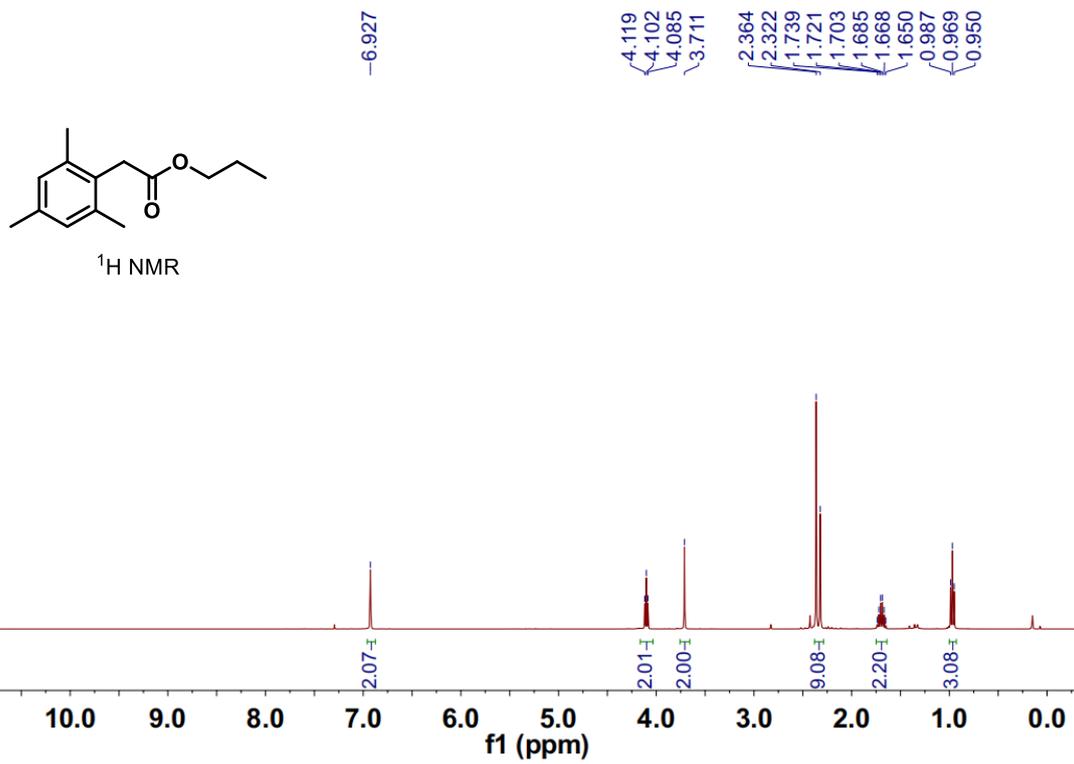


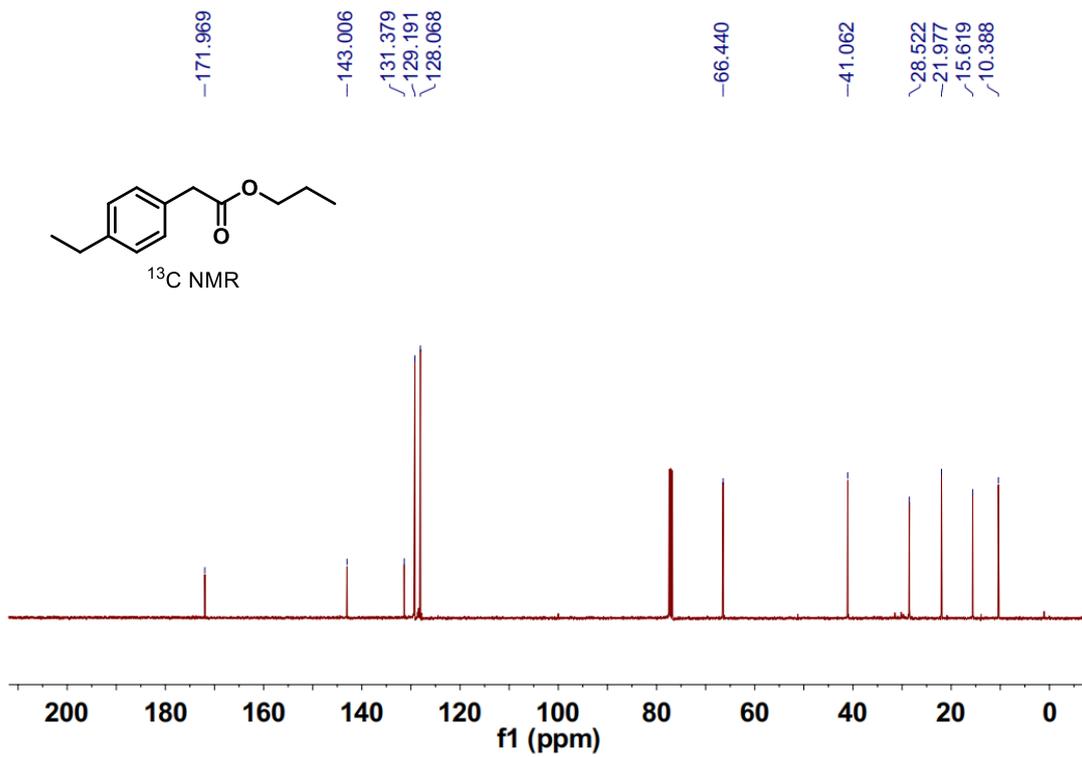
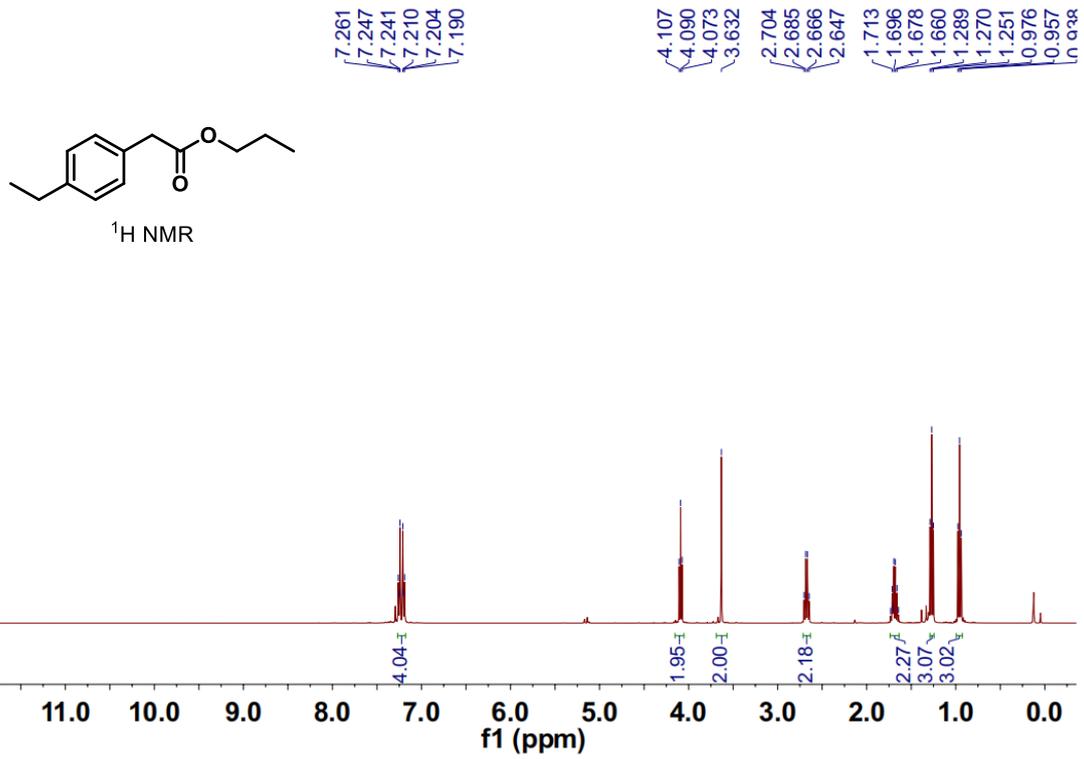
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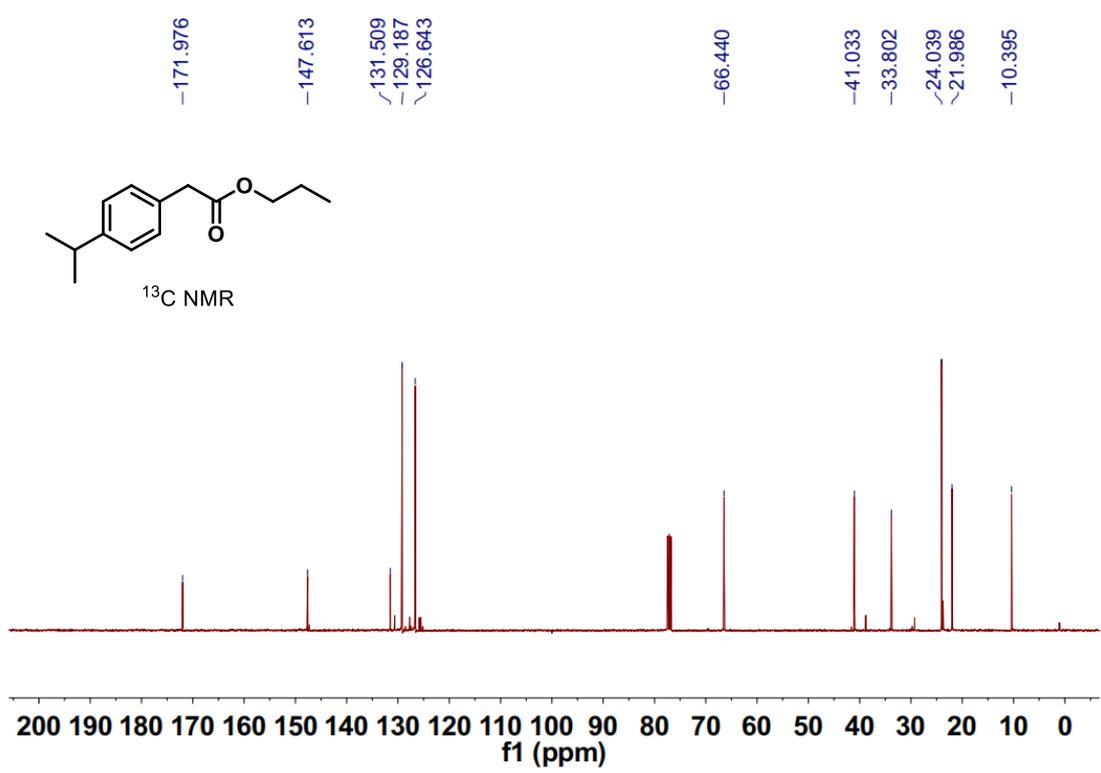
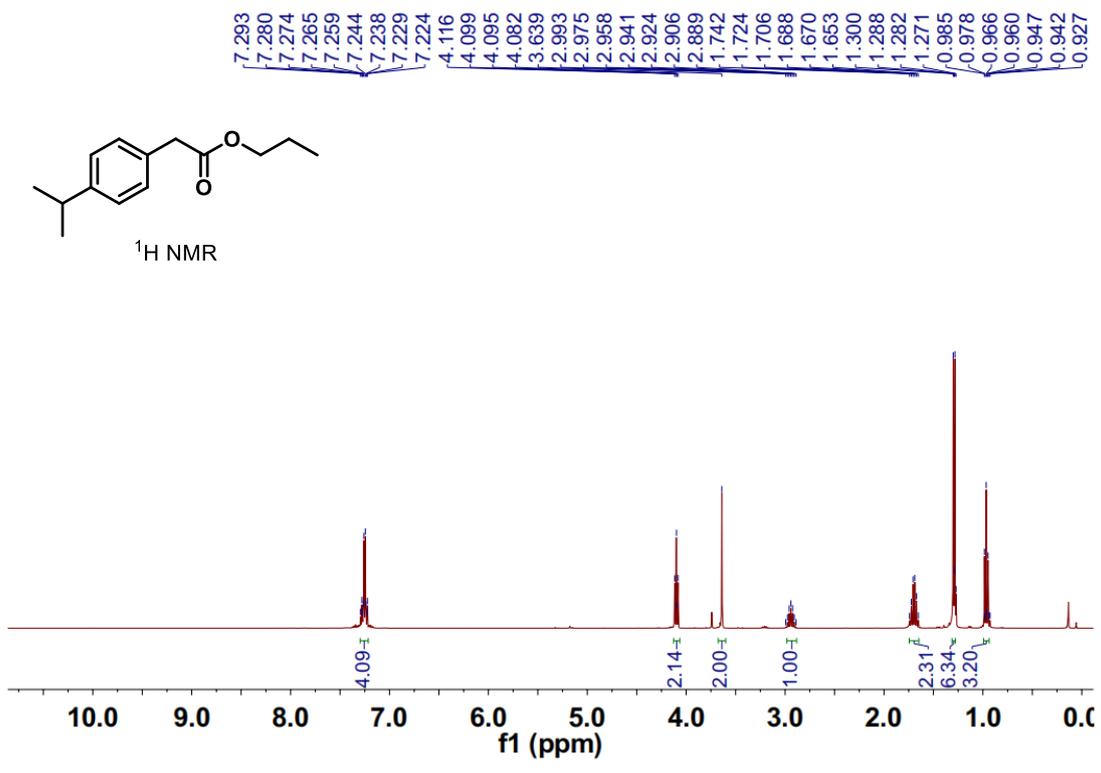


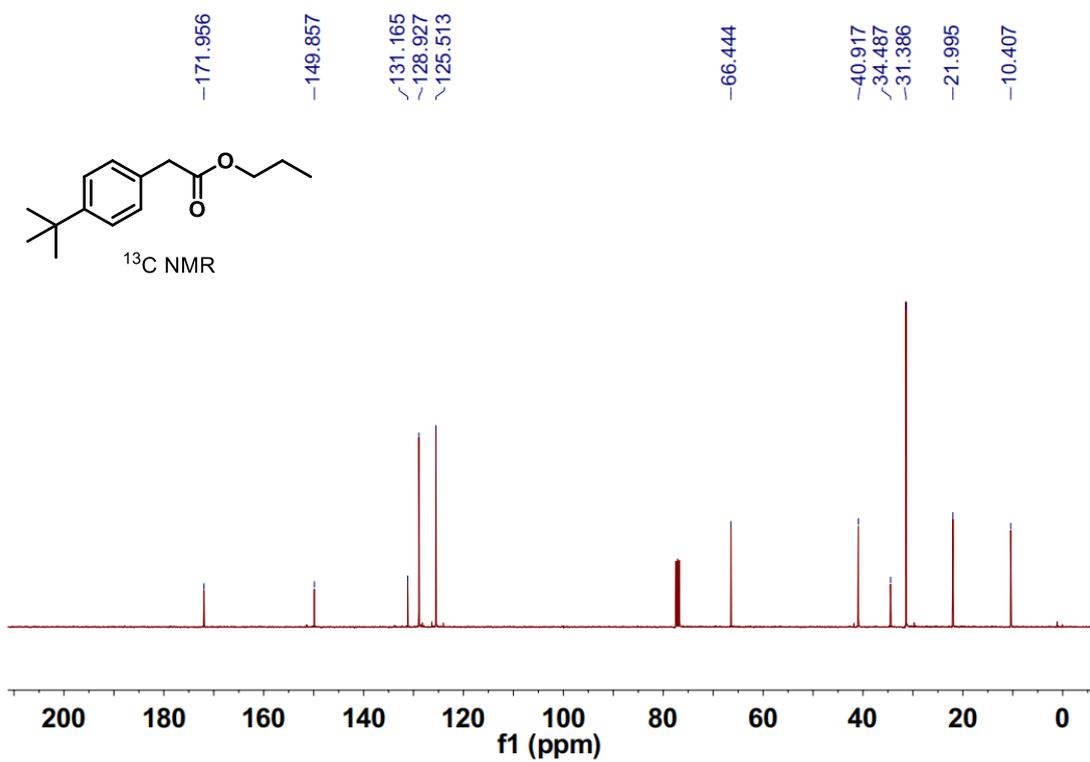
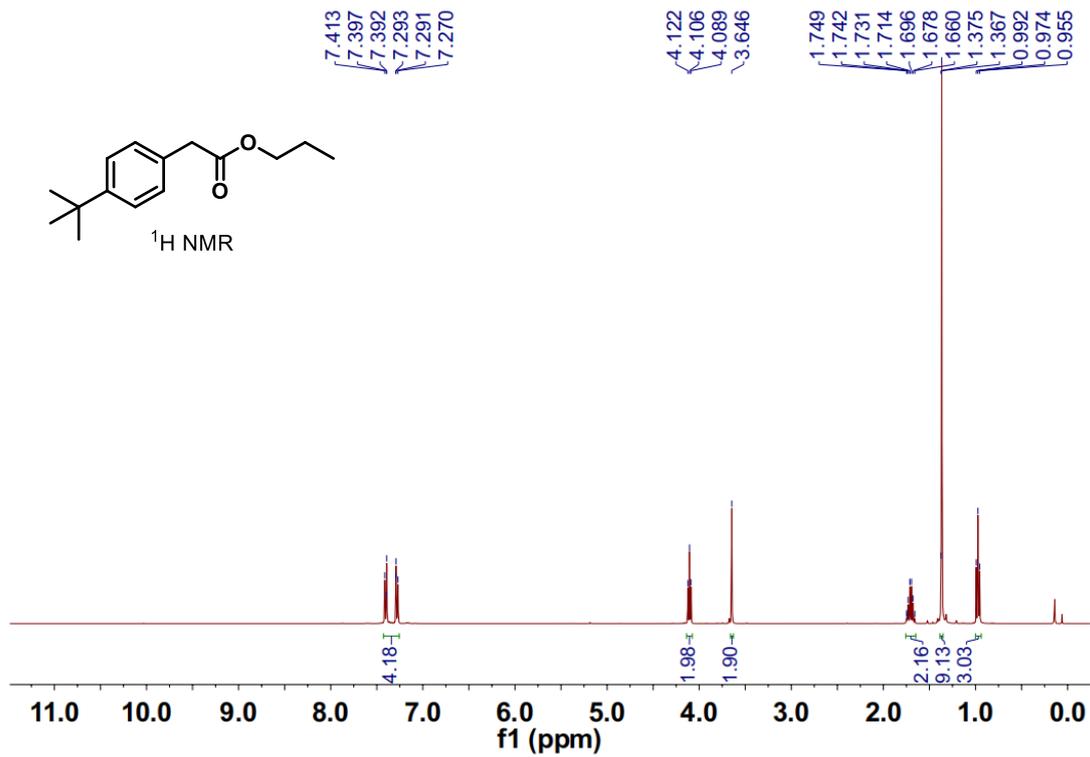
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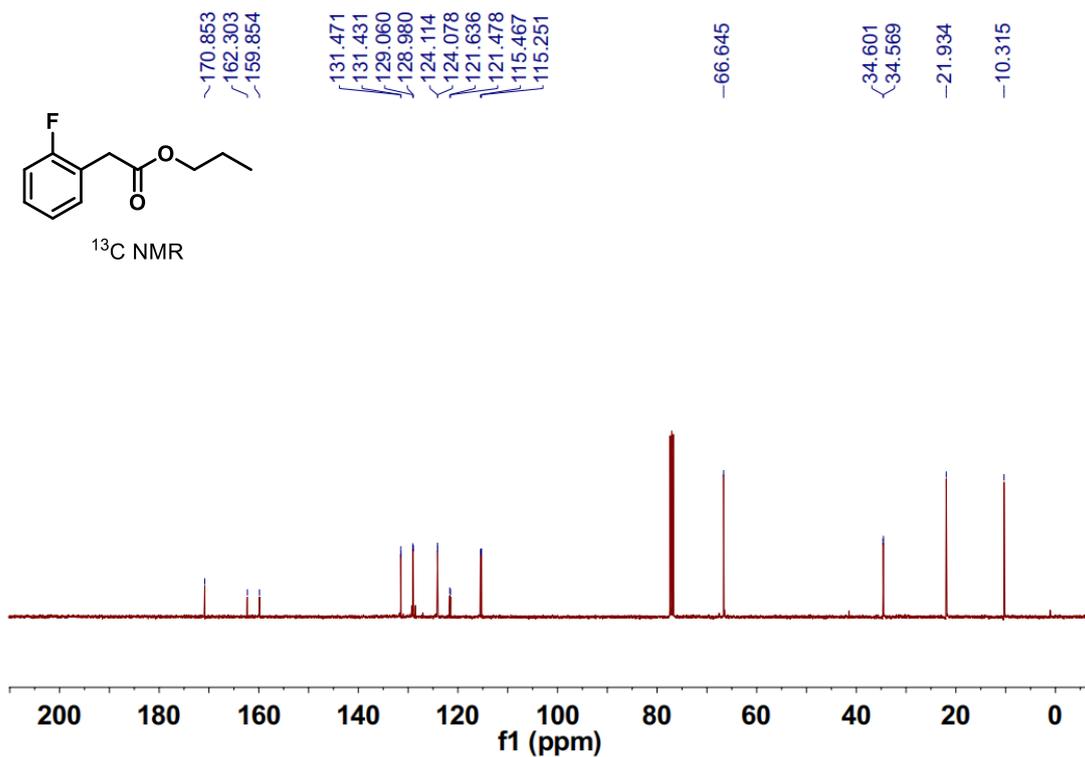
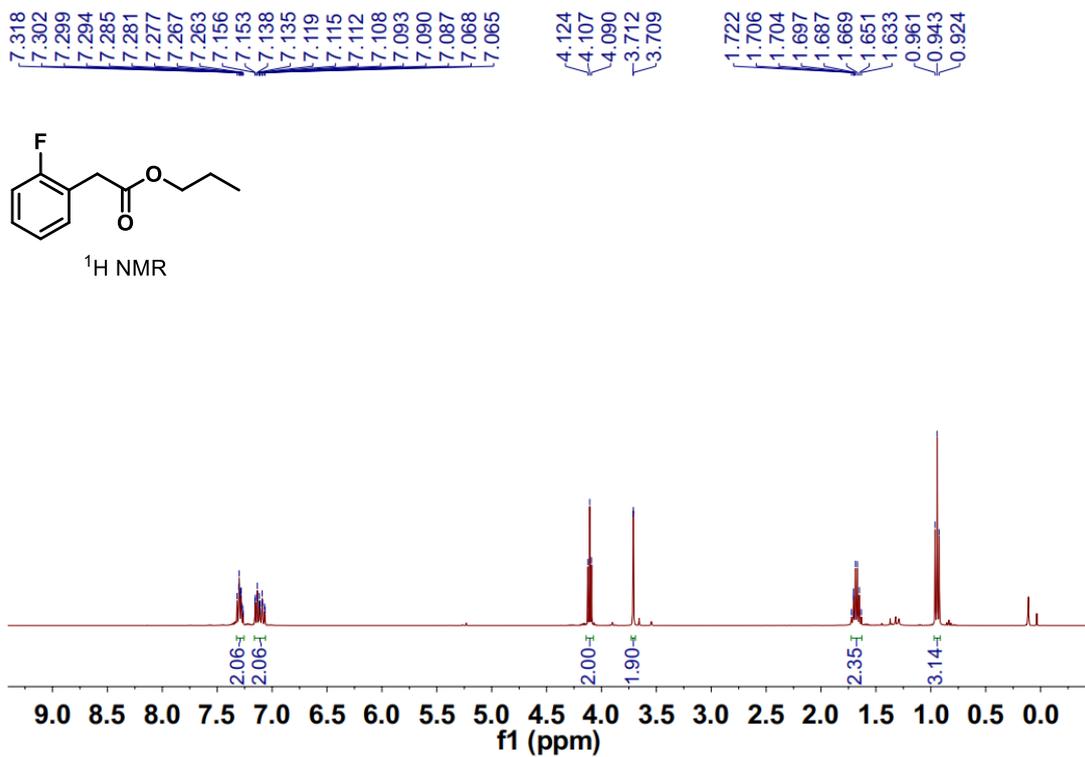


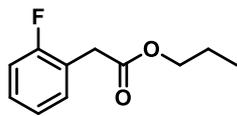




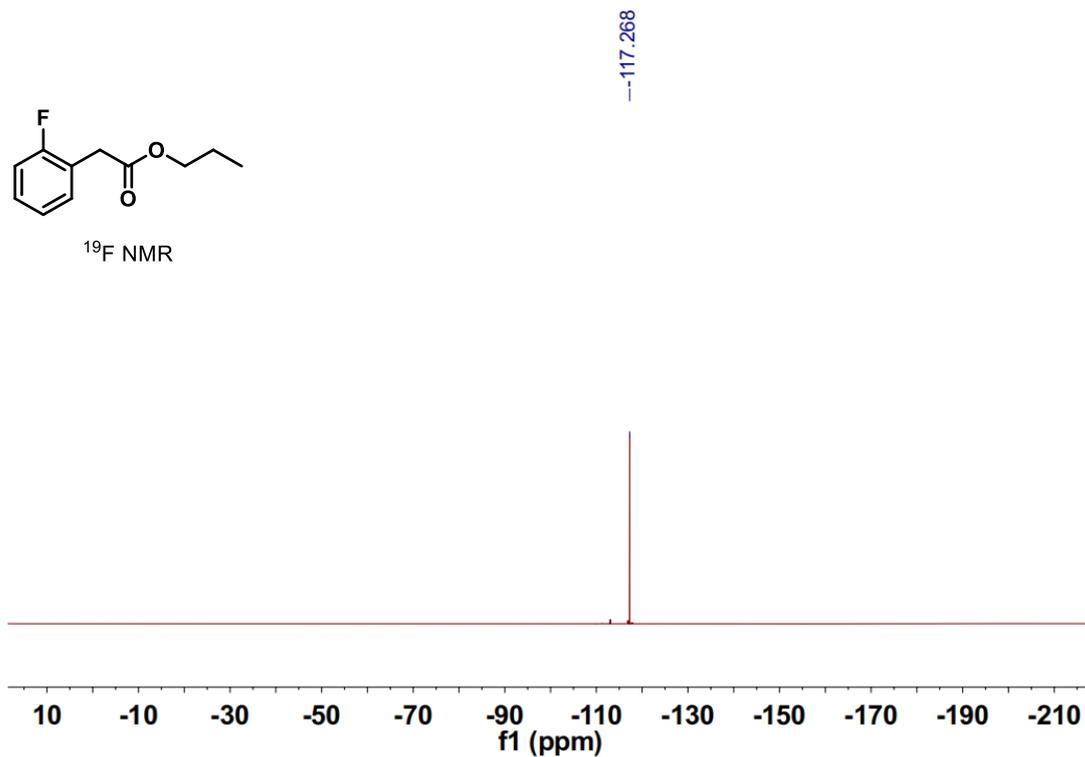




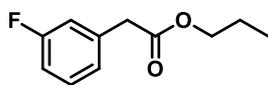




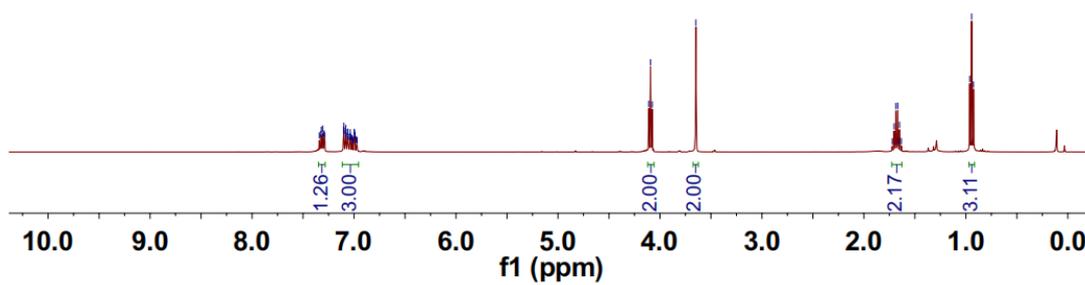
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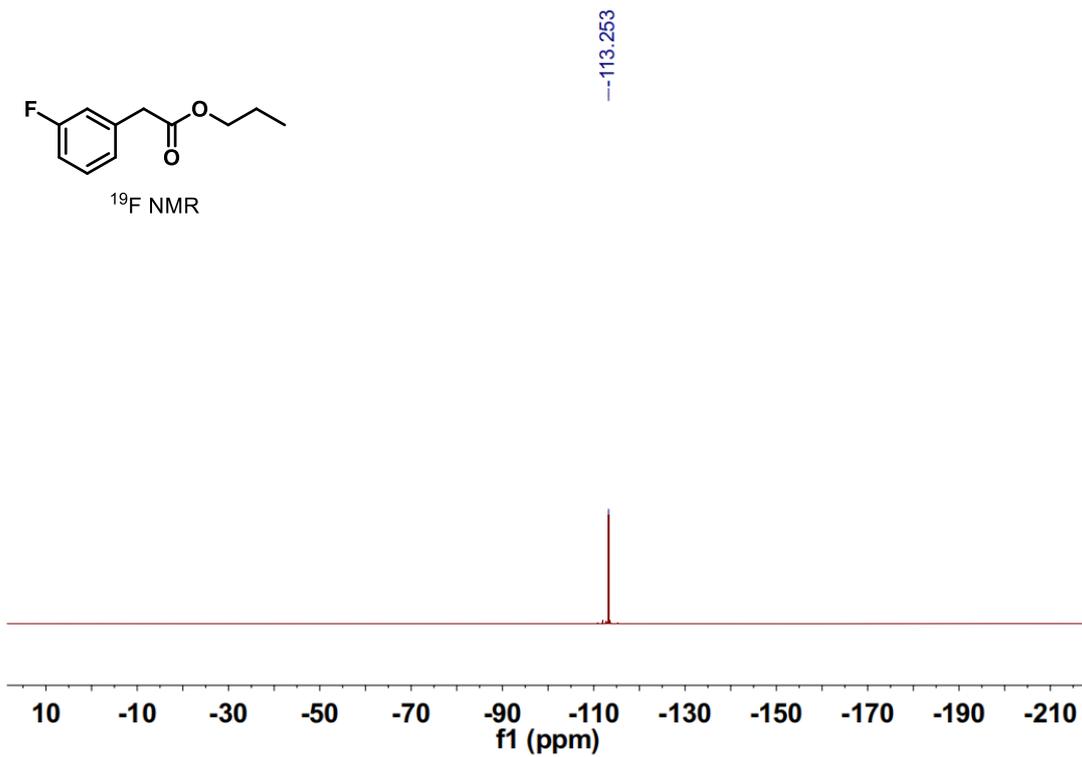
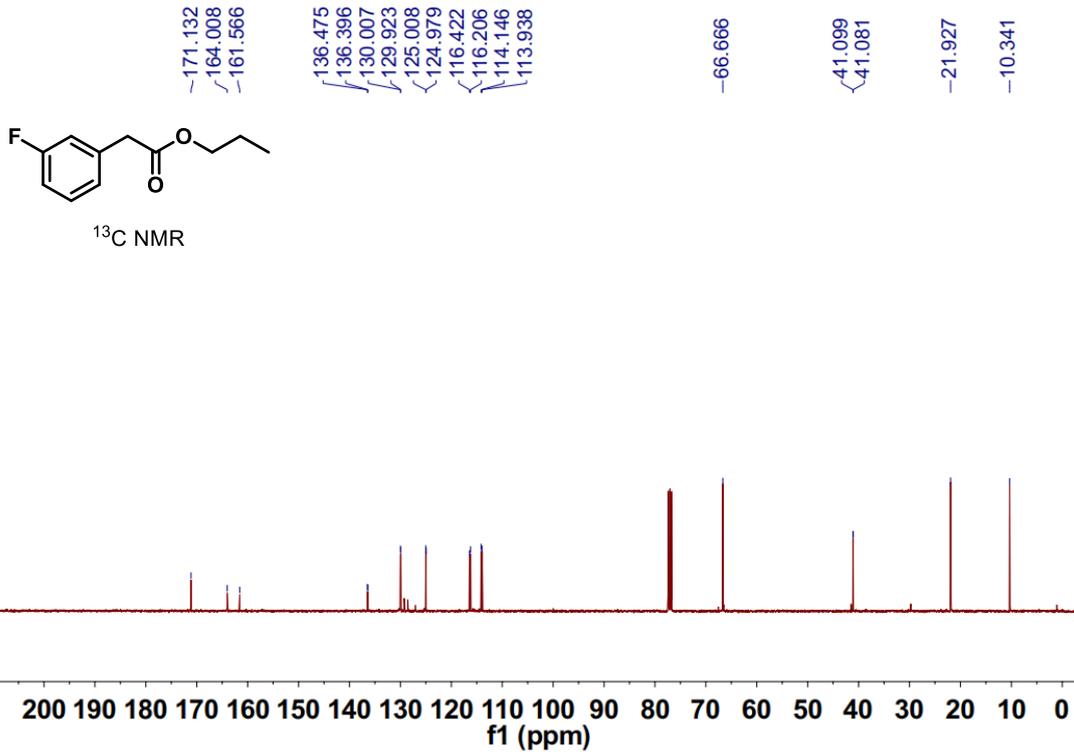


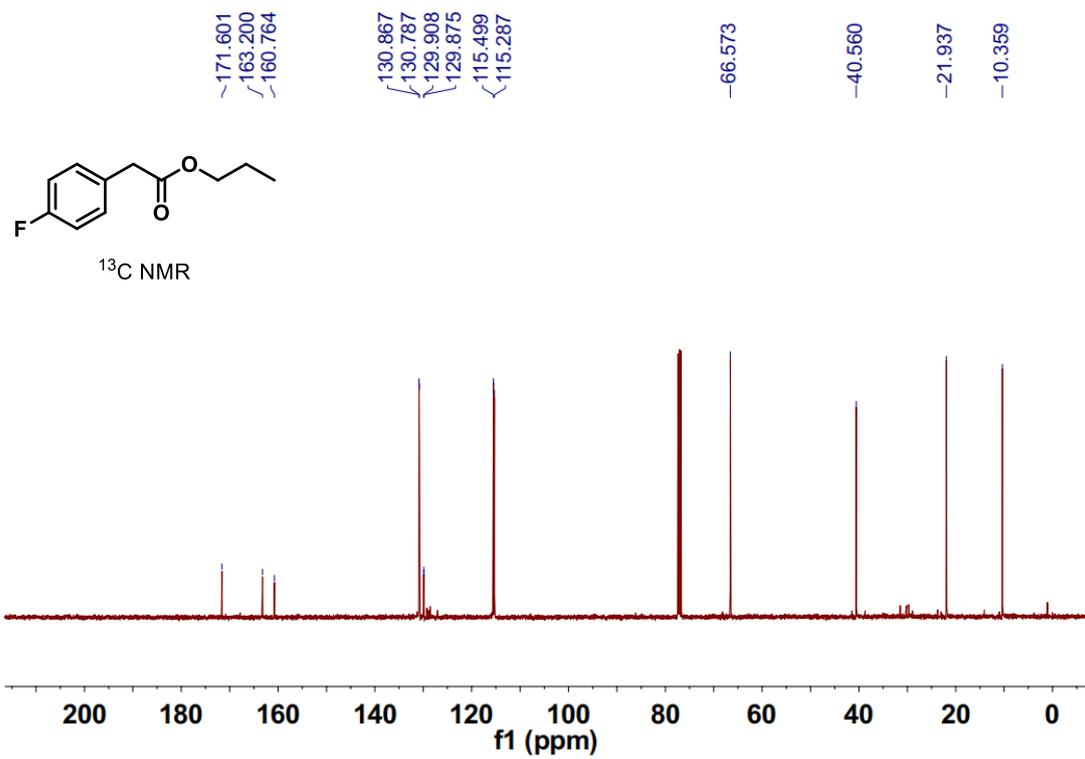
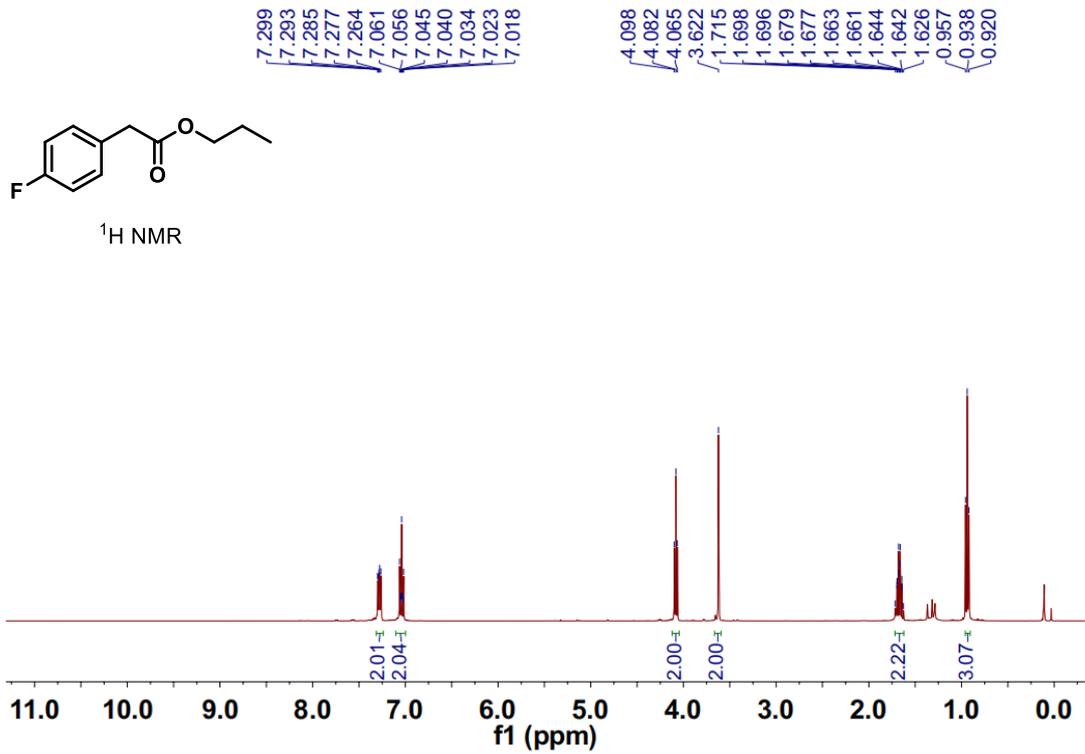
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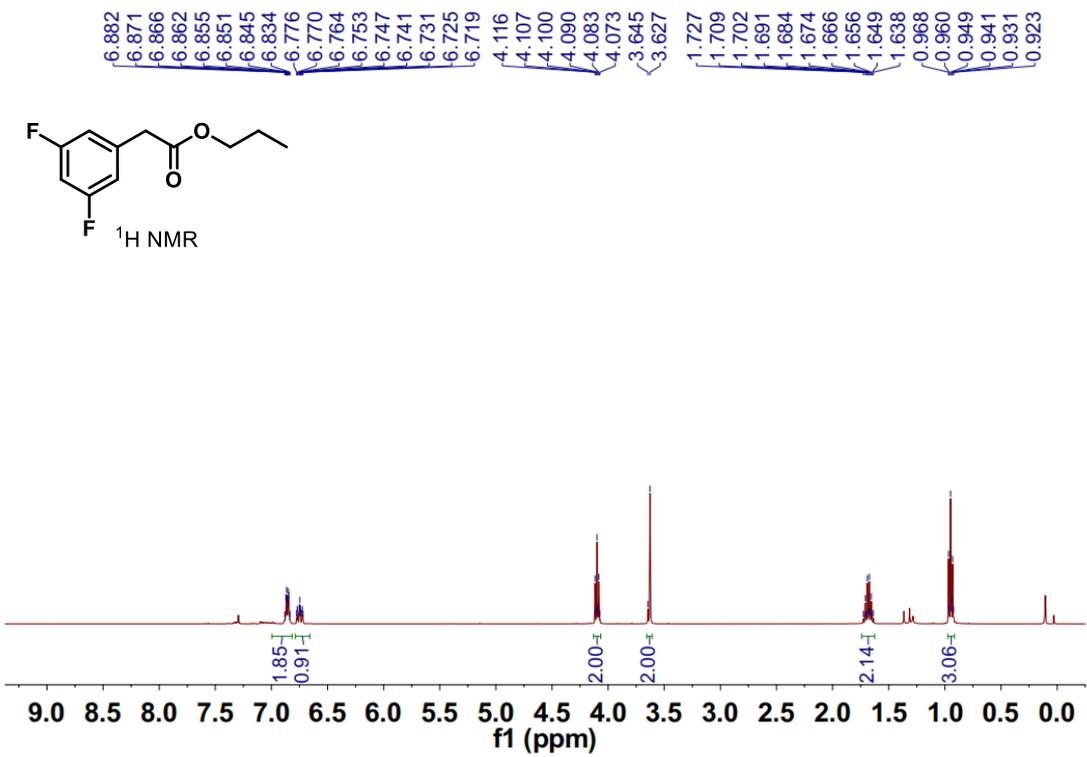
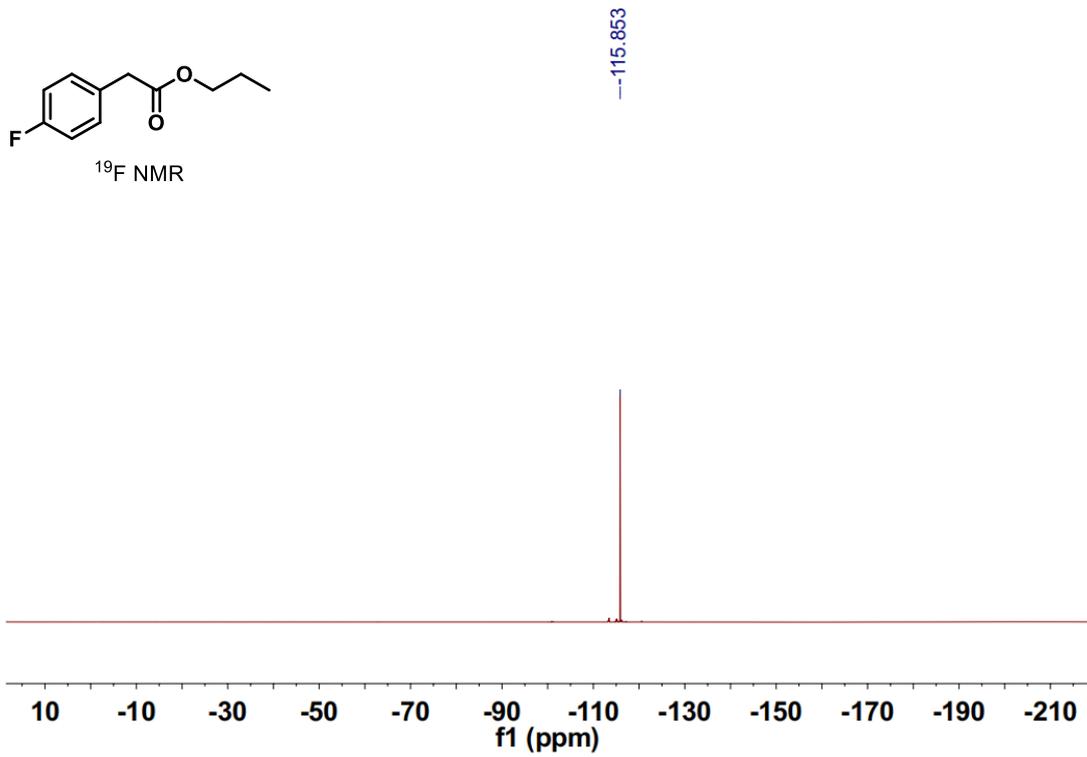


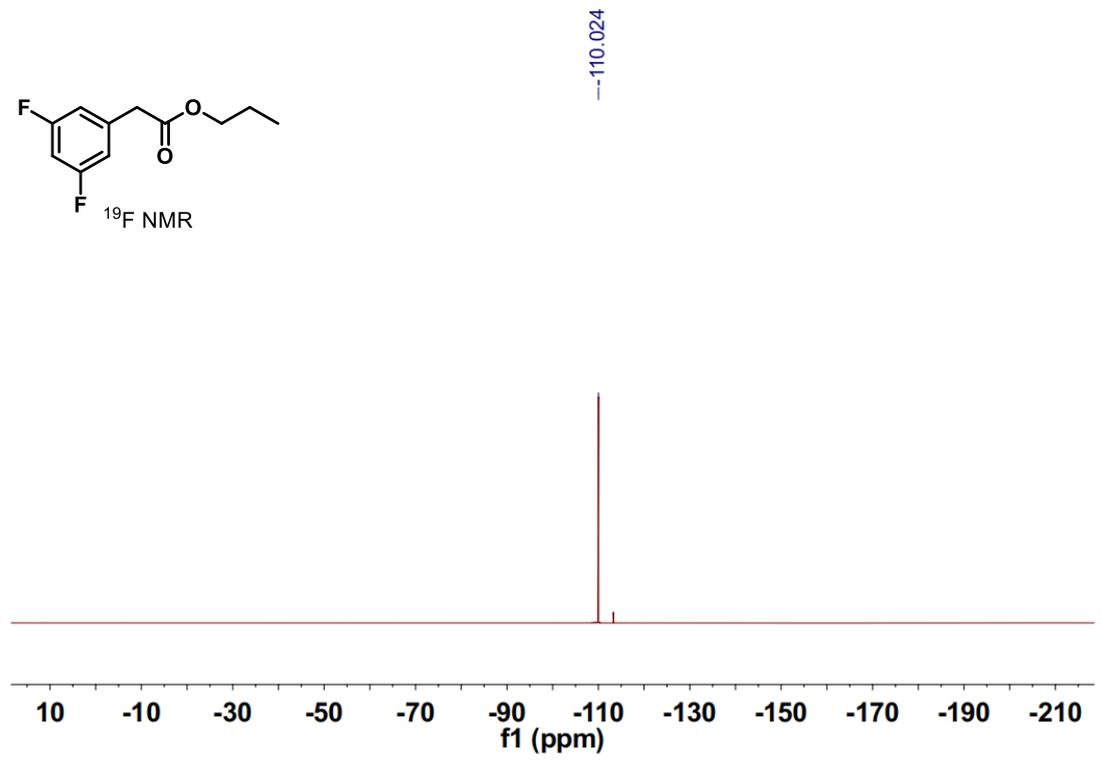
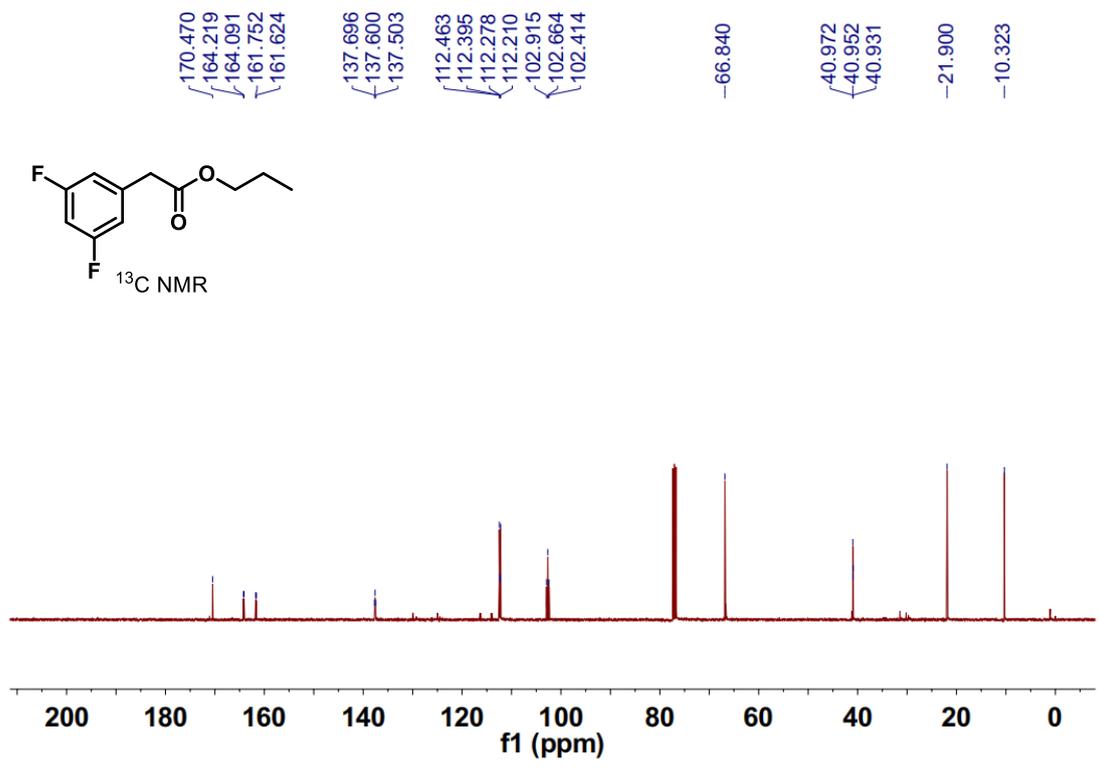
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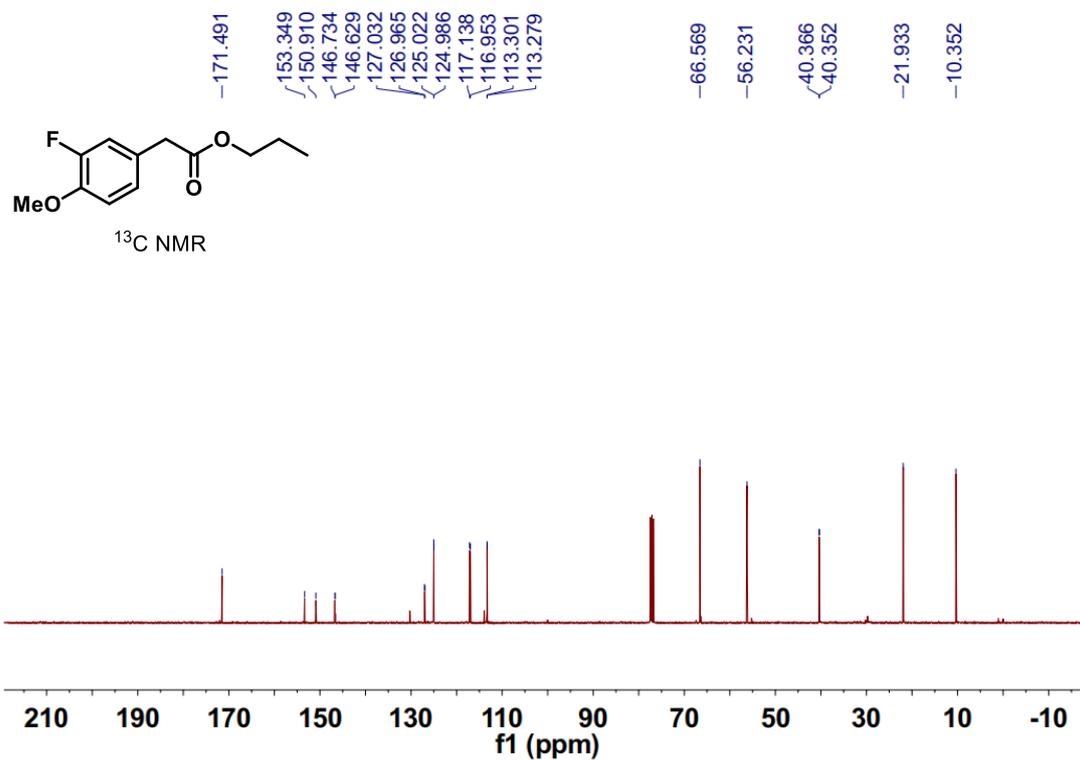
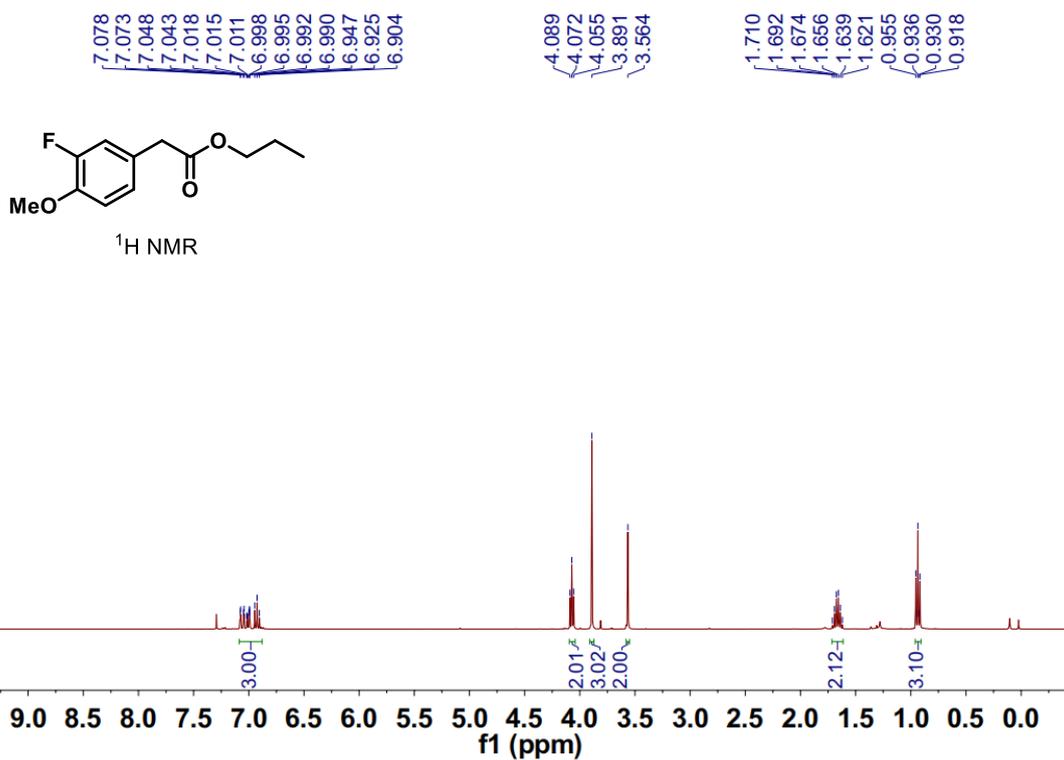


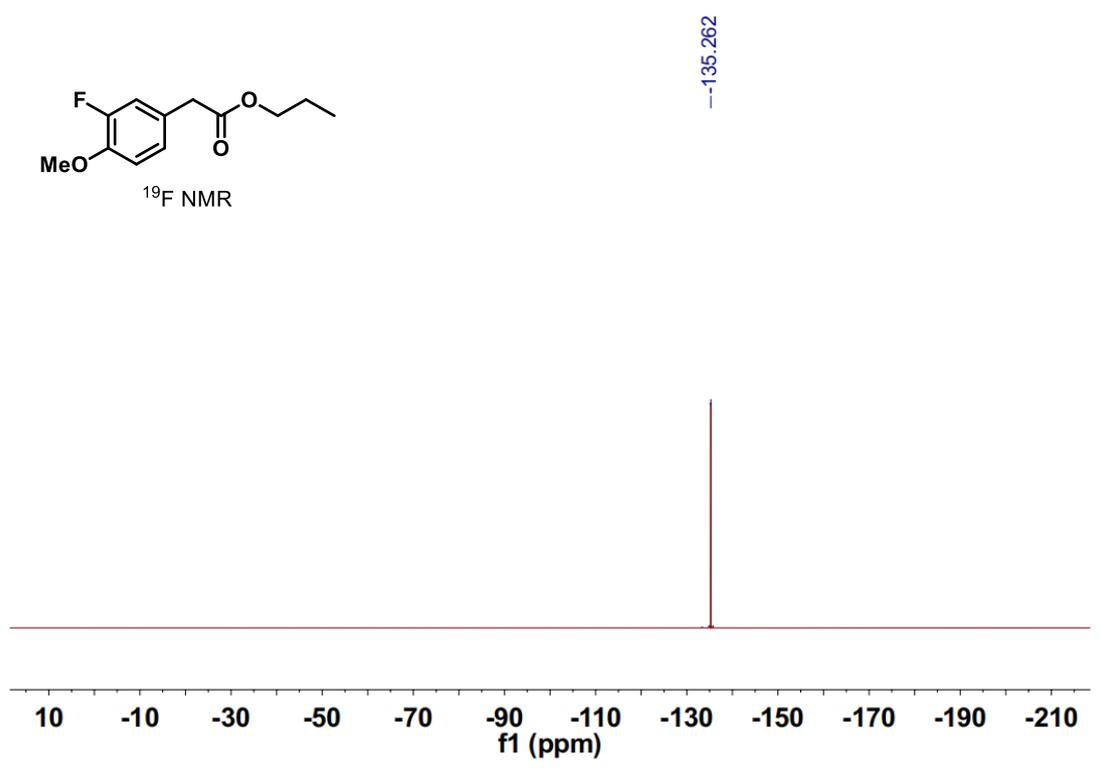
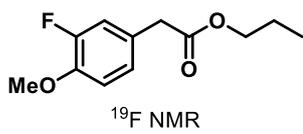




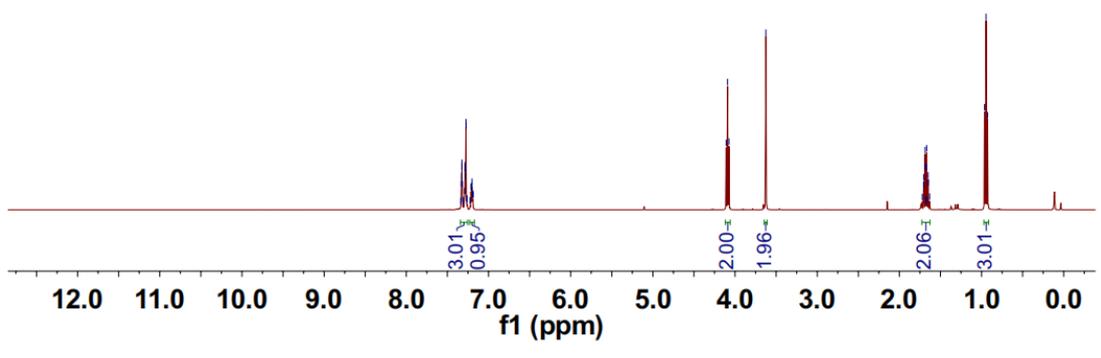
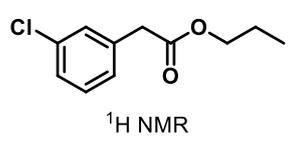


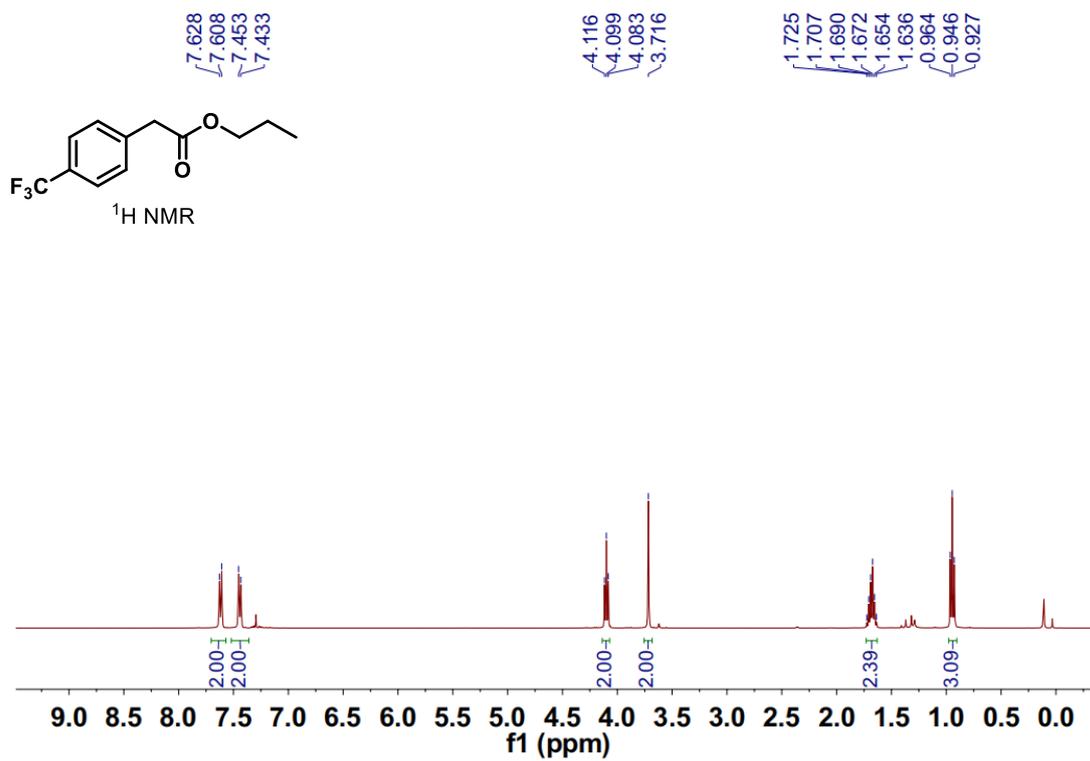
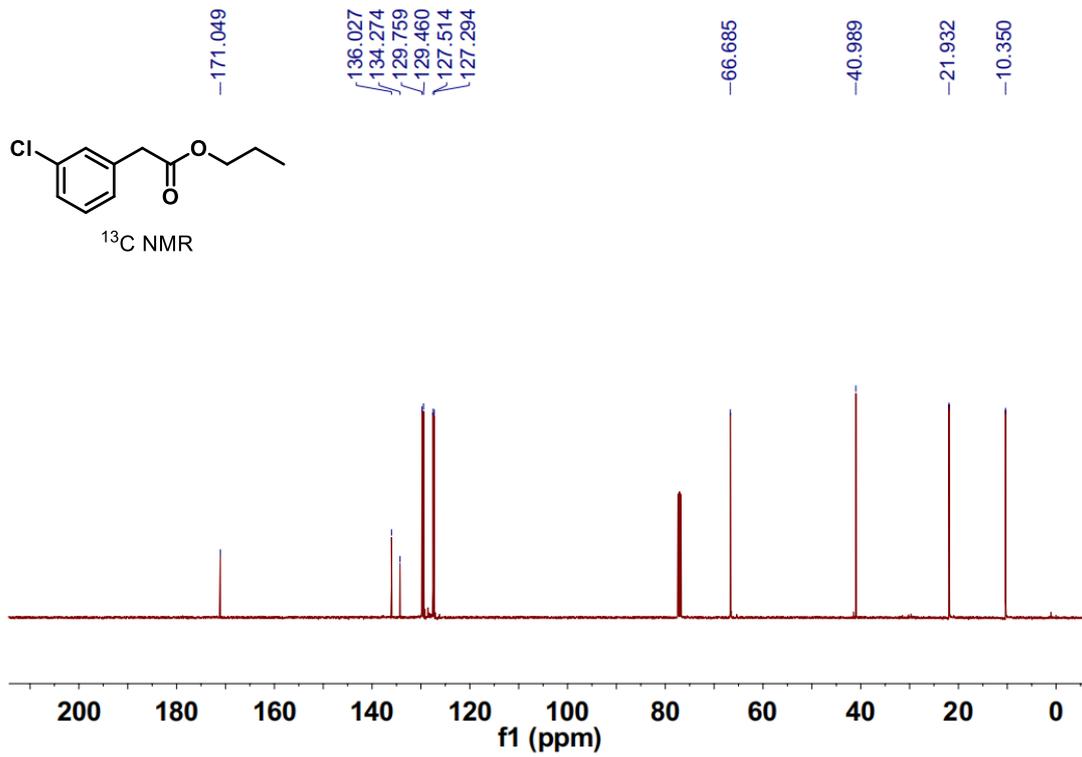


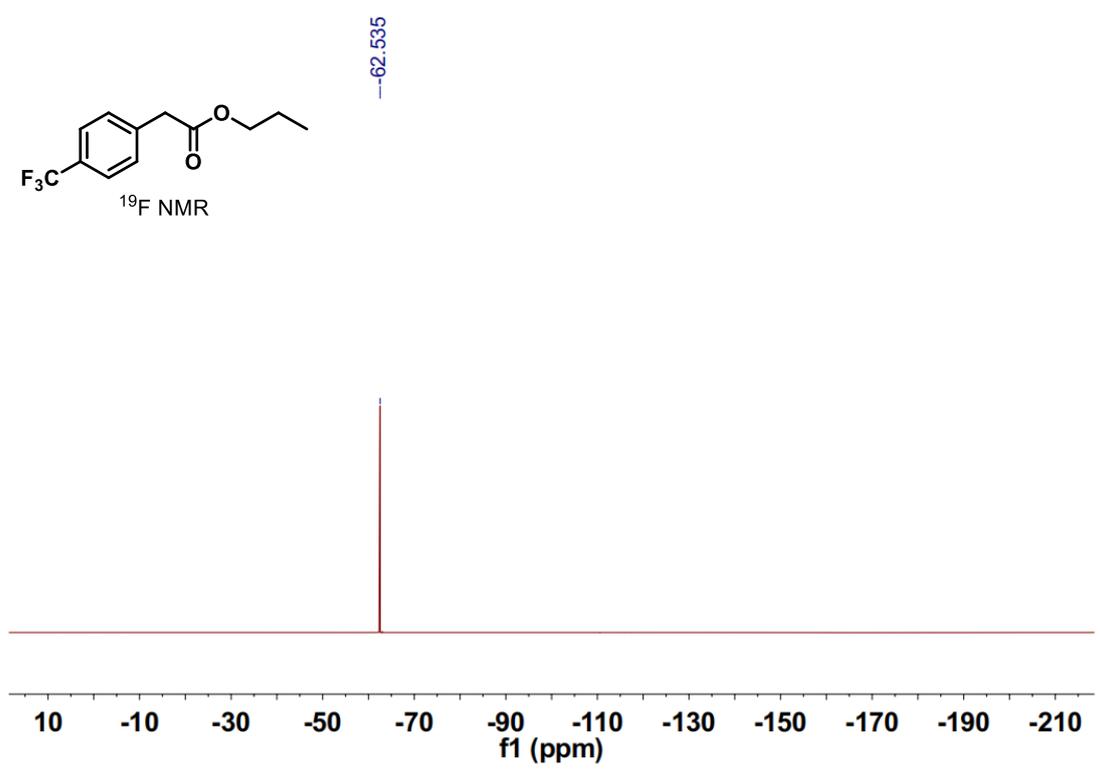
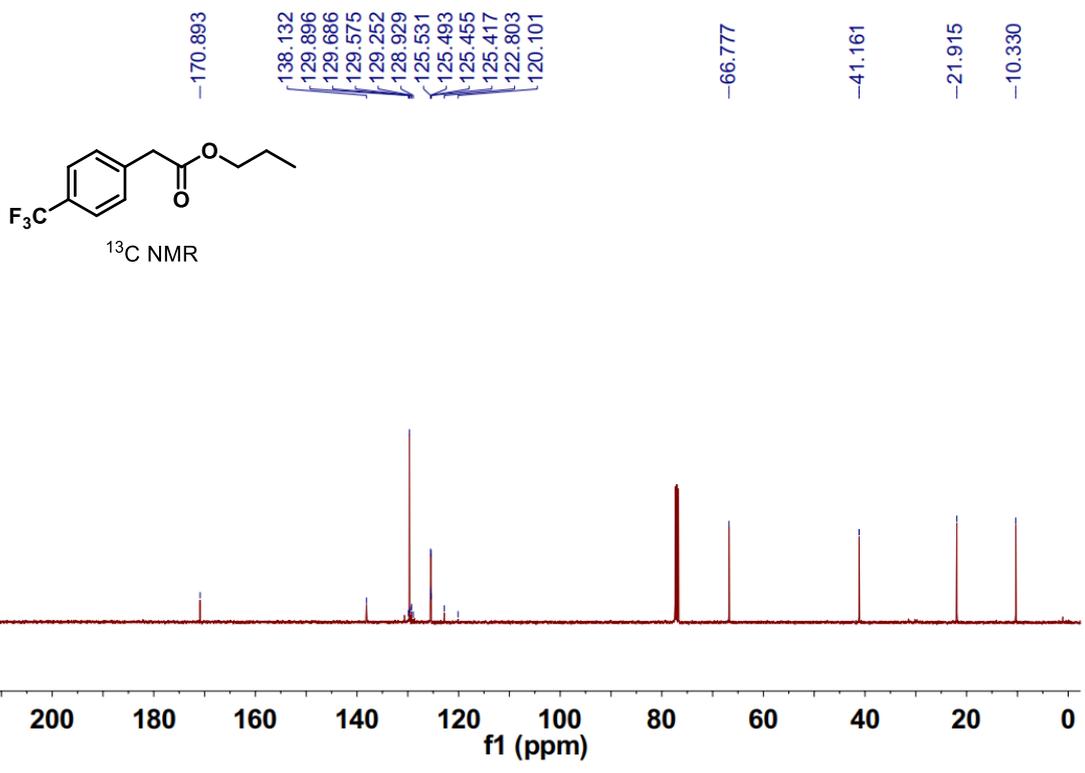


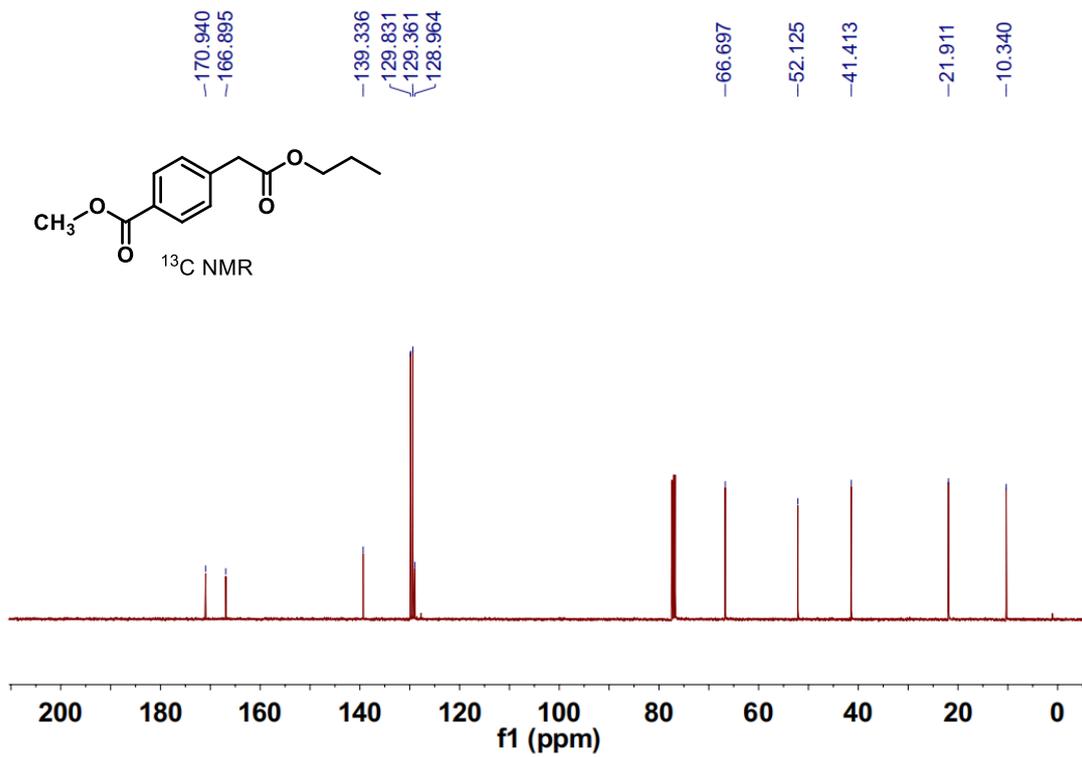
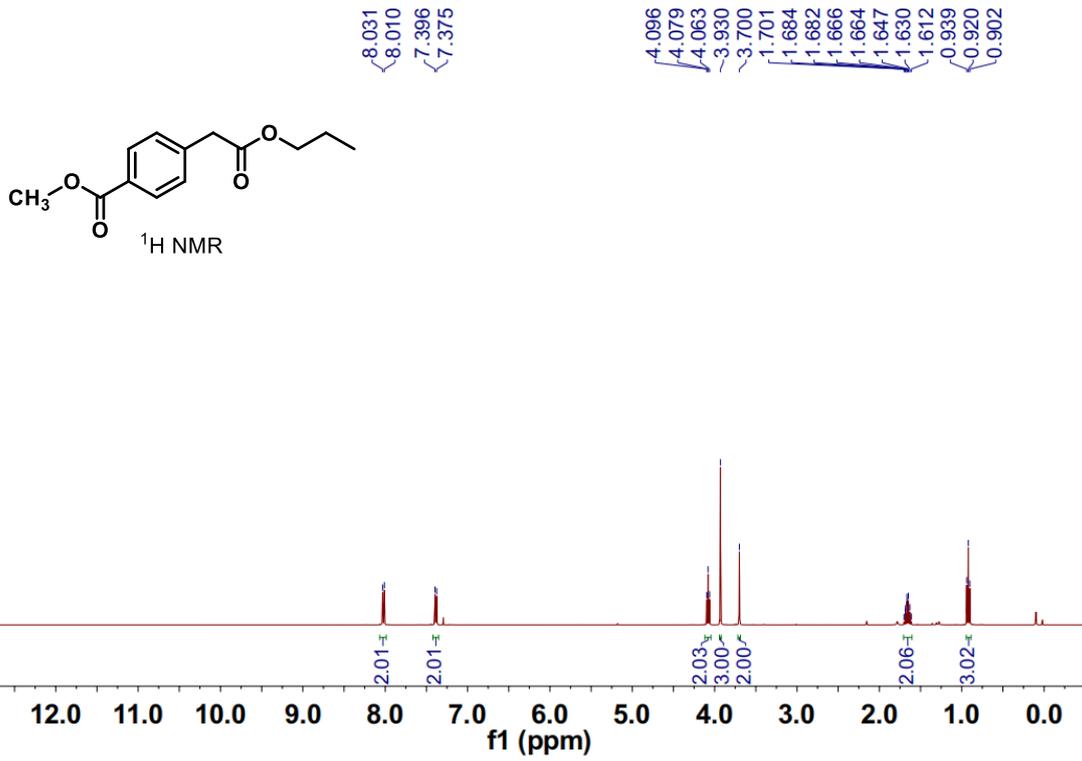


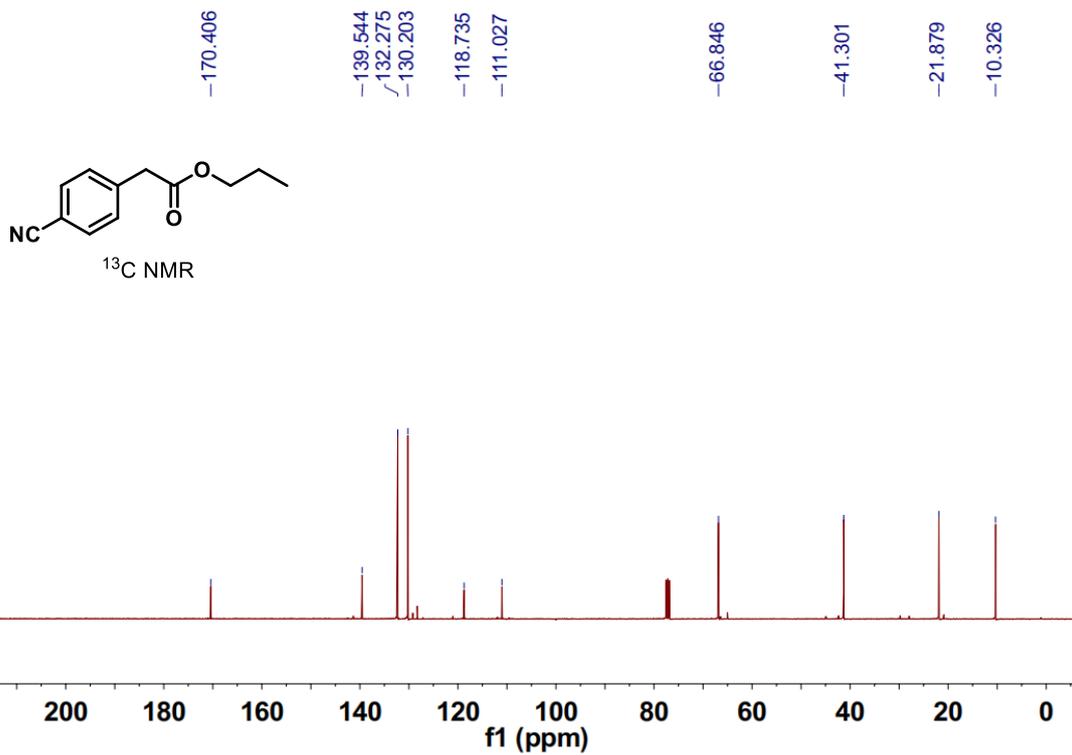
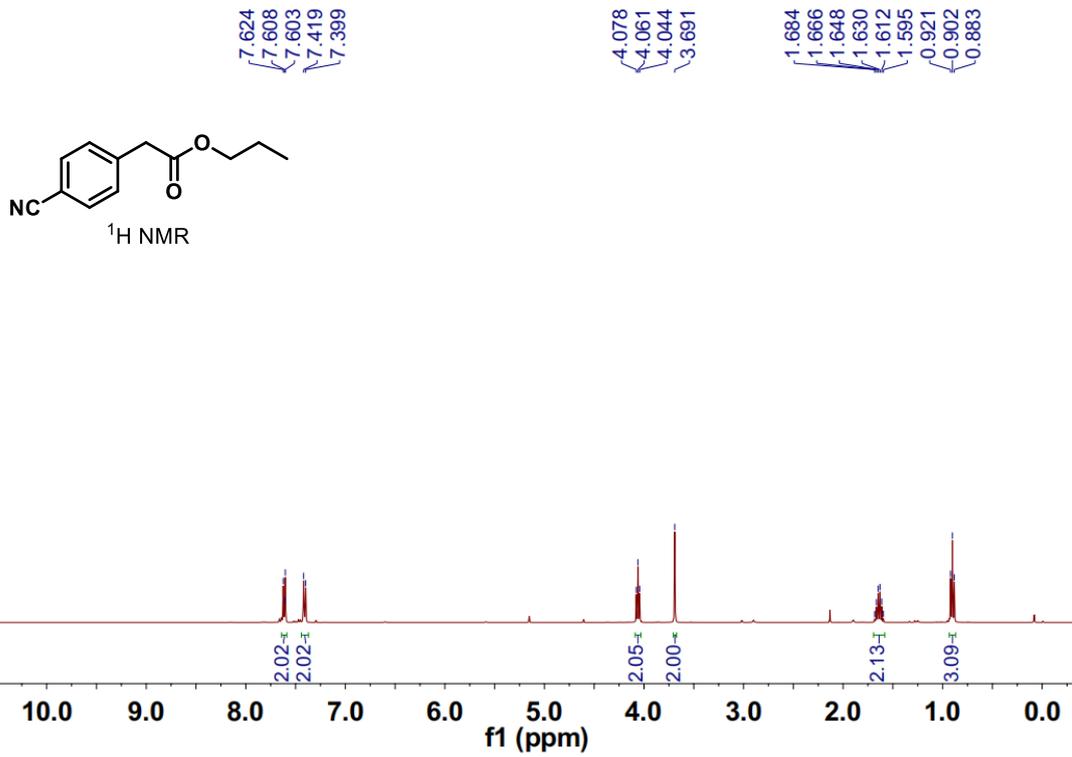
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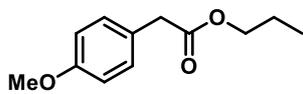




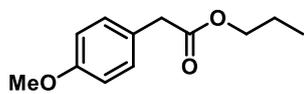
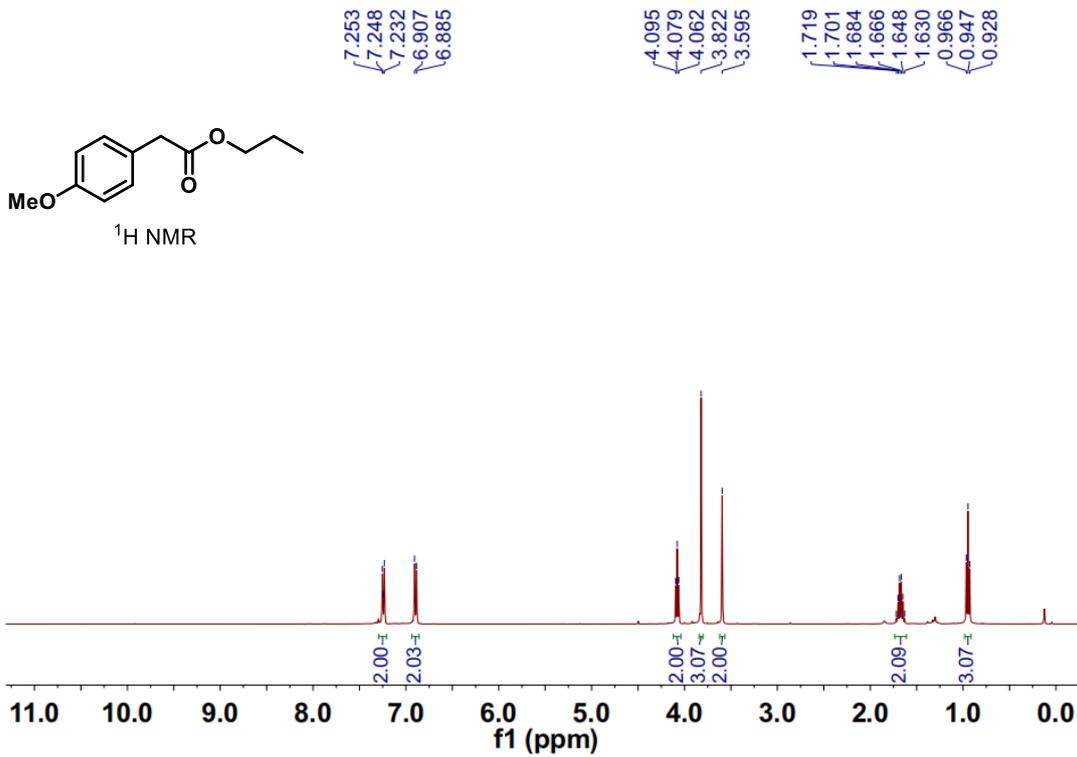




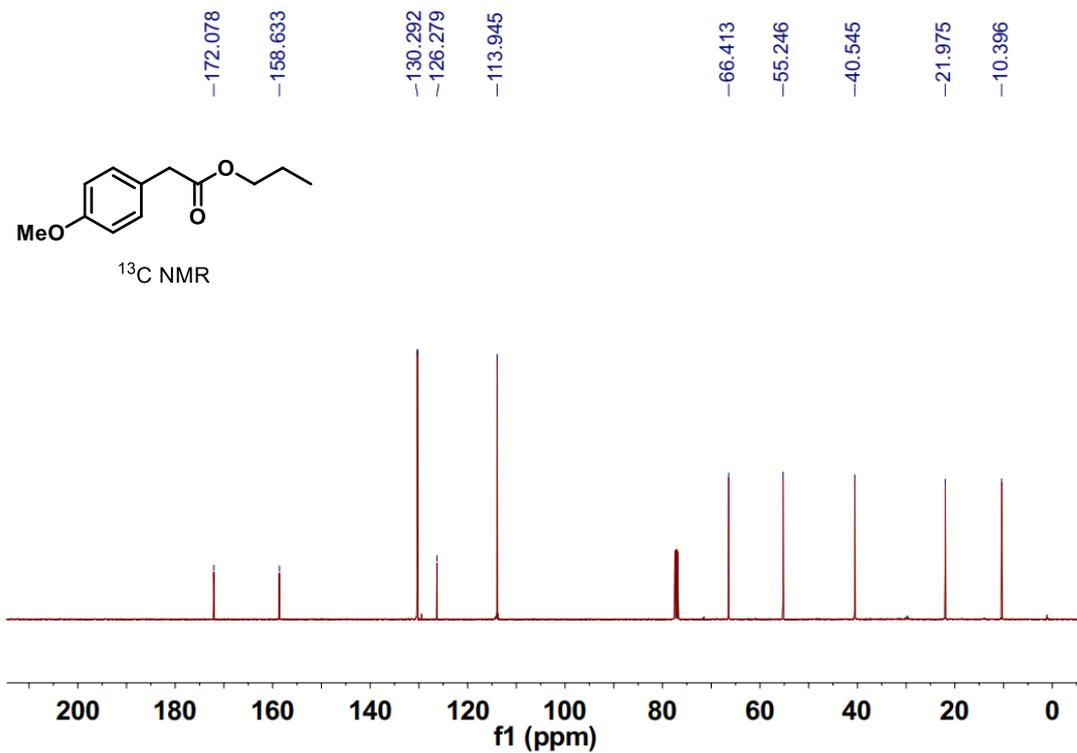


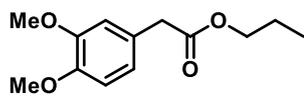


¹H NMR

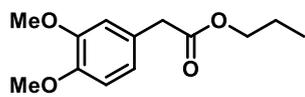
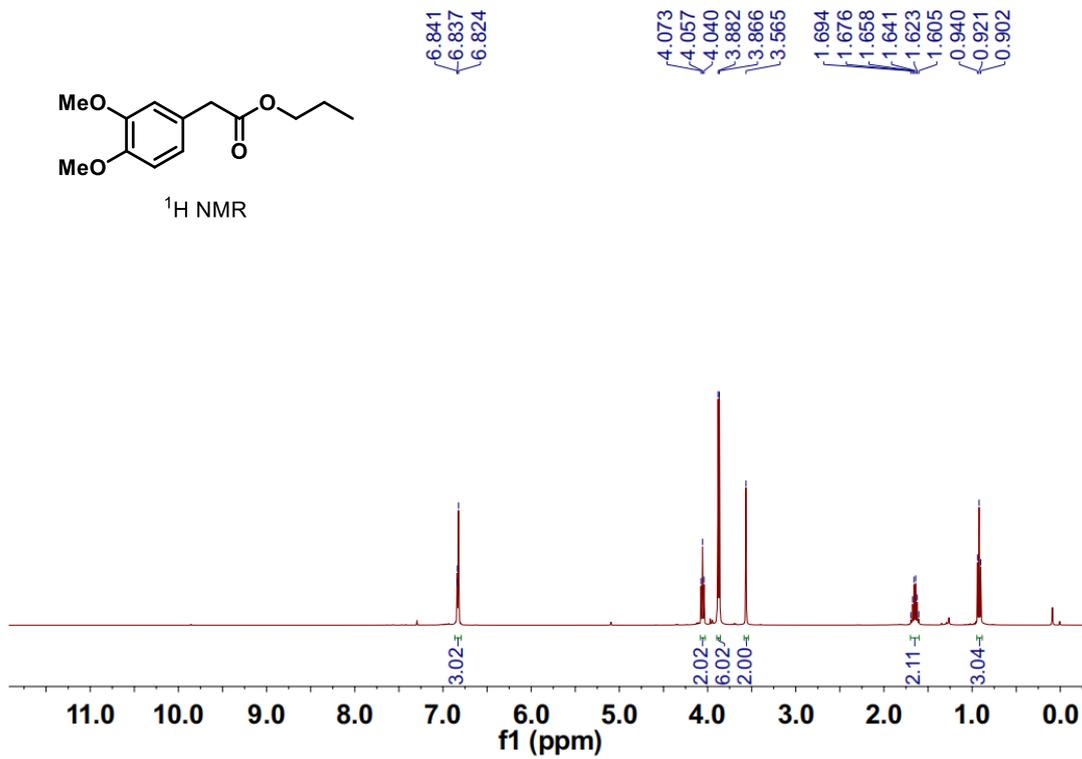


¹³C NMR

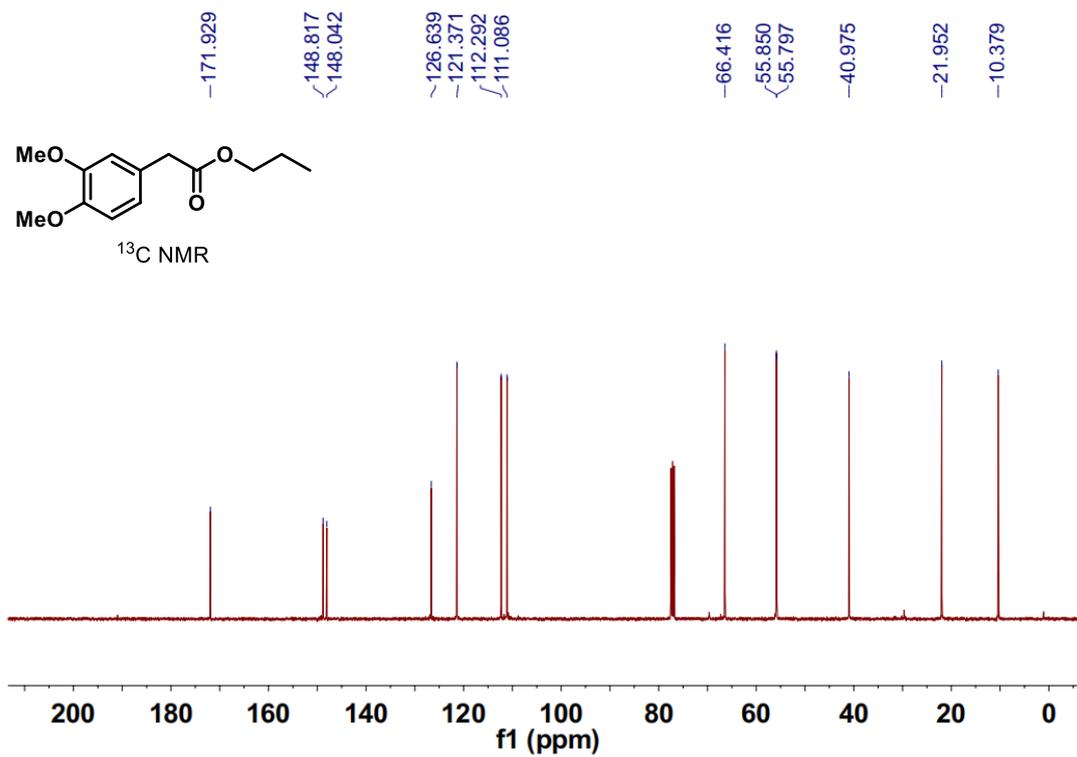


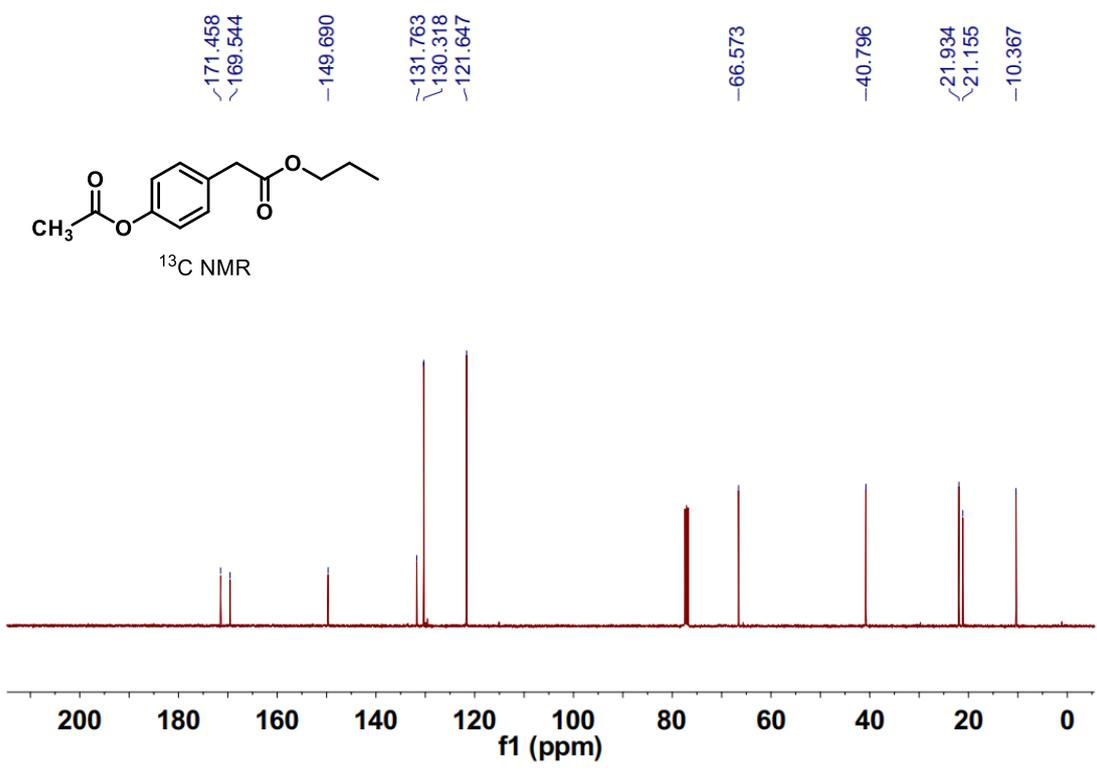
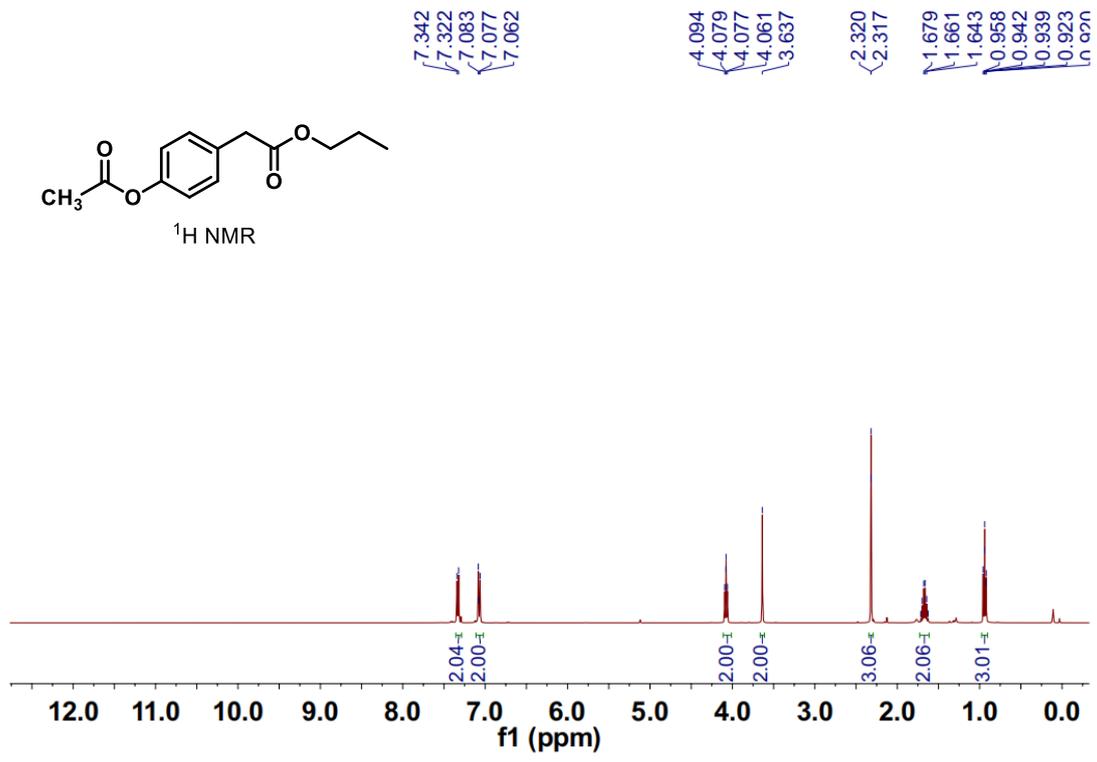
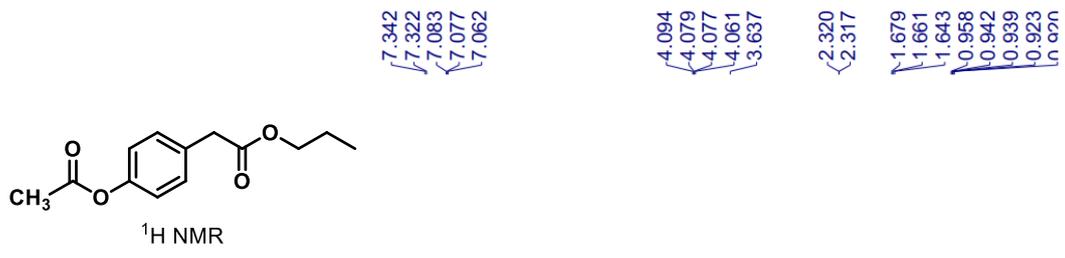


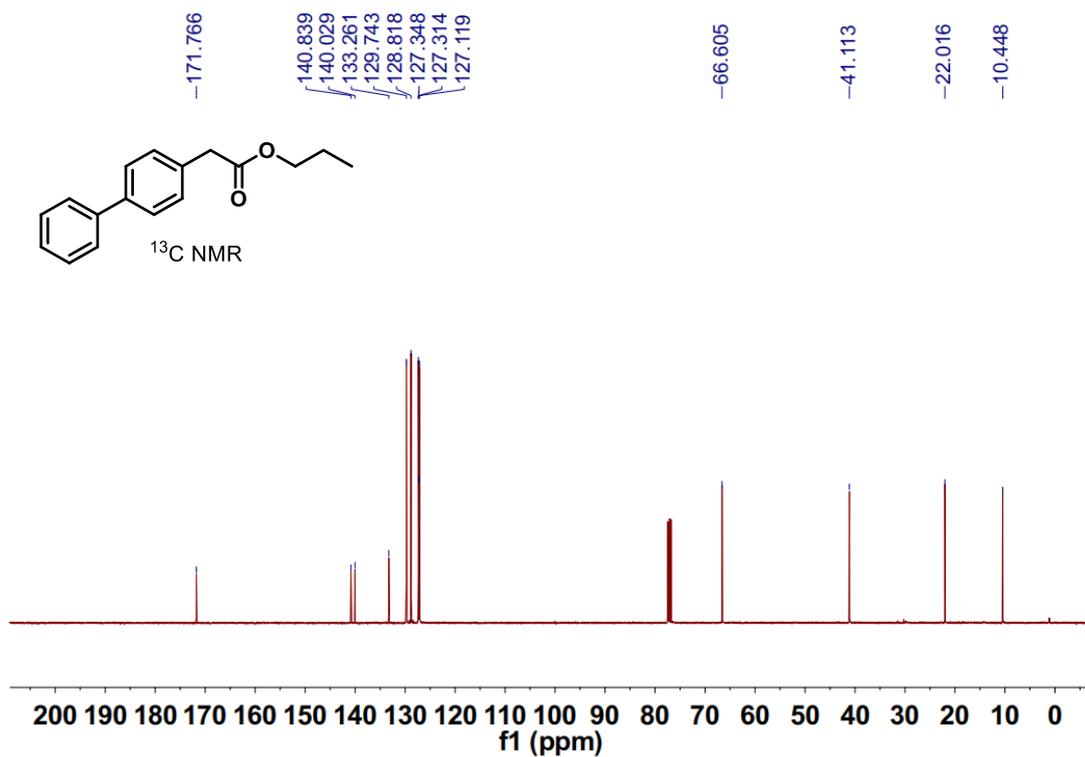
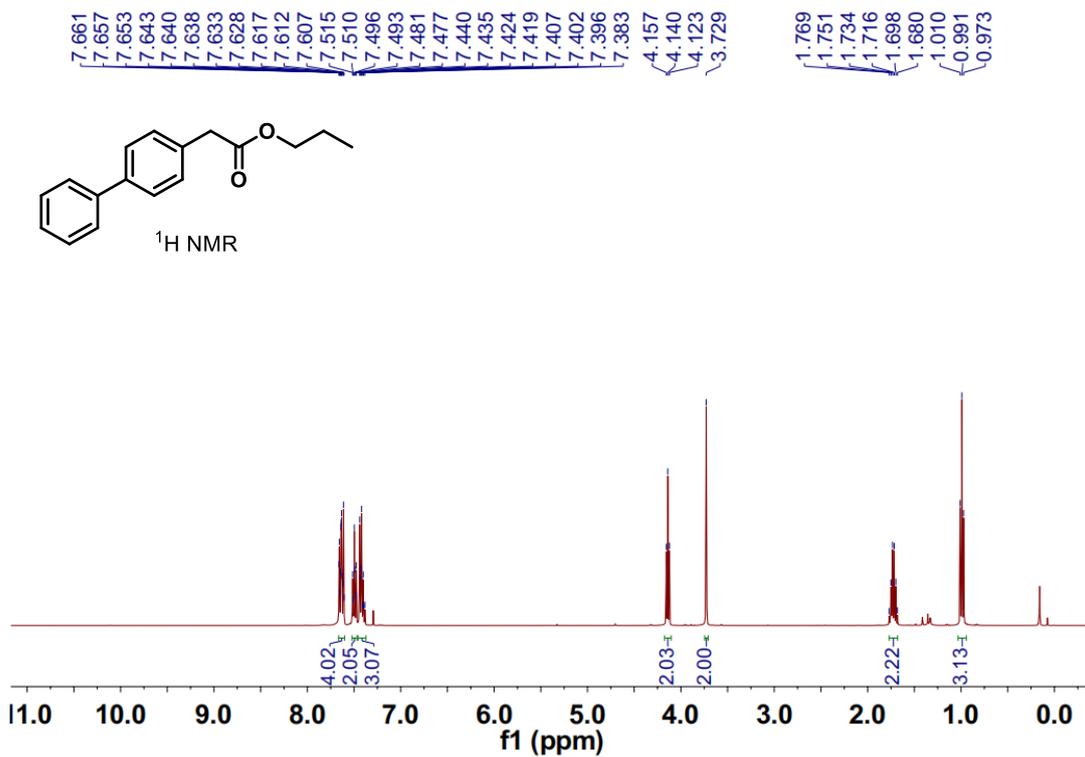
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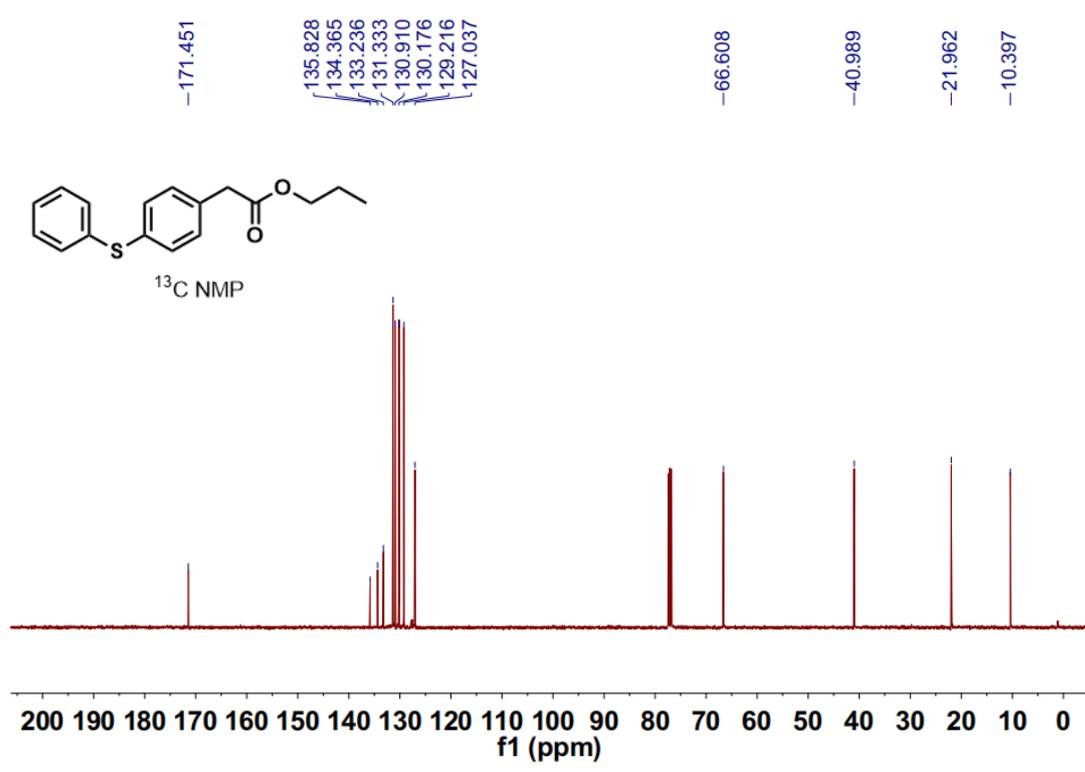
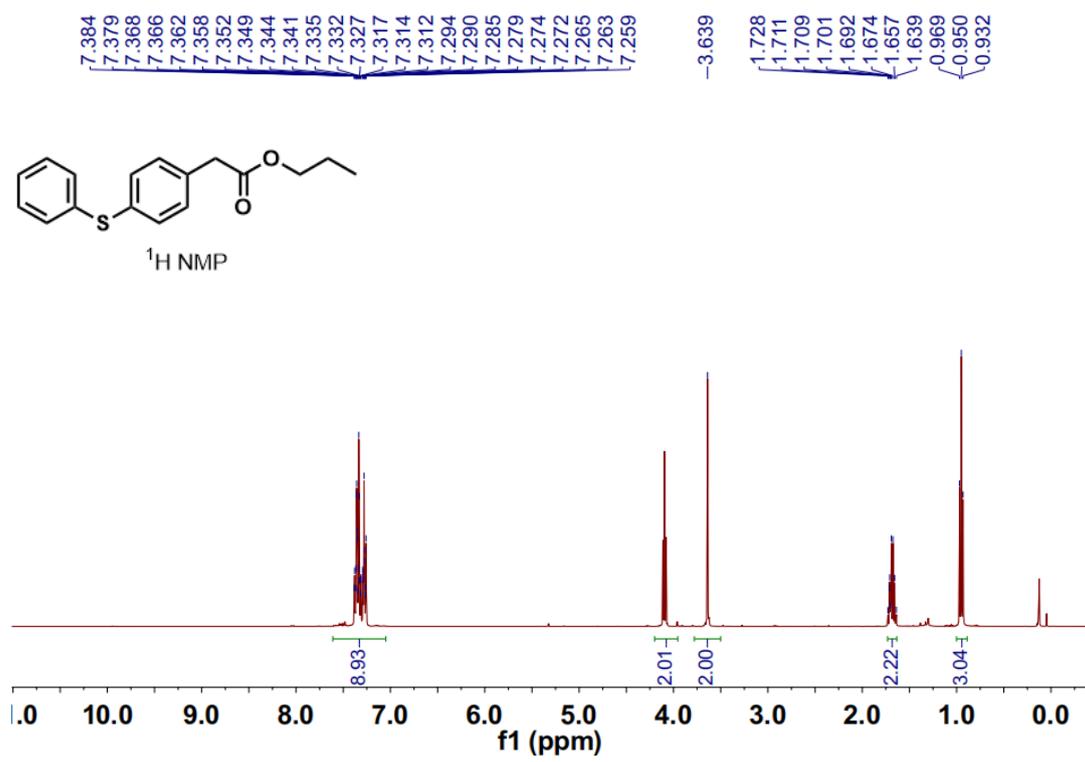


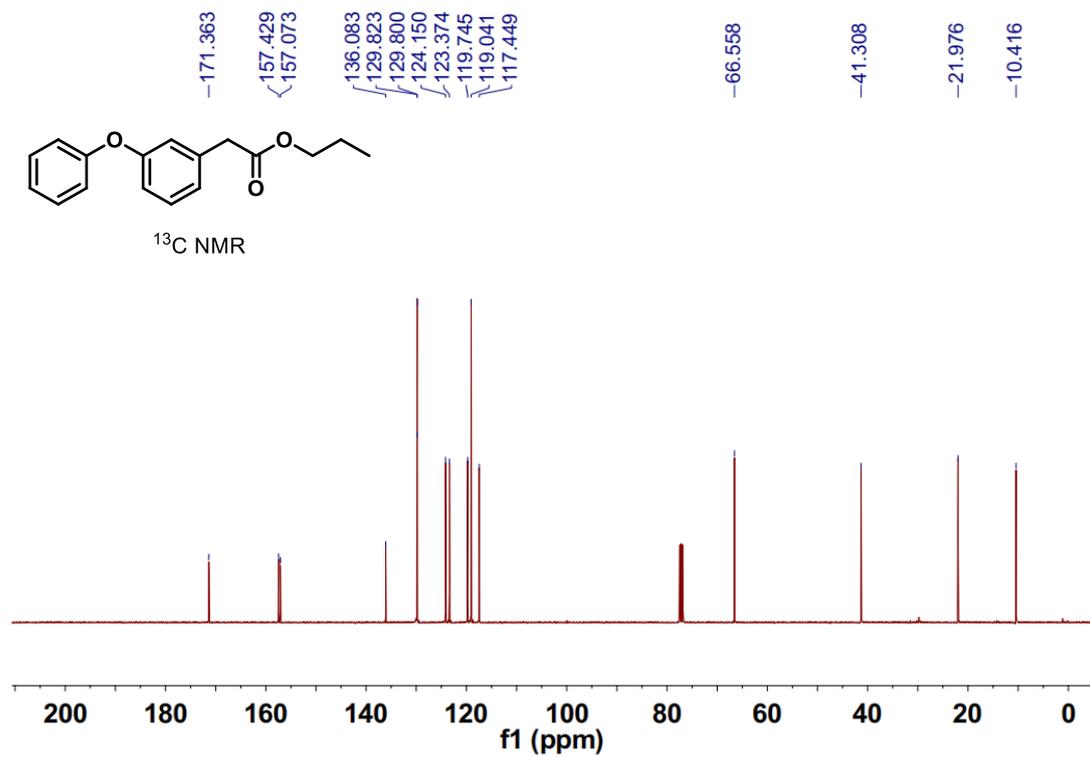
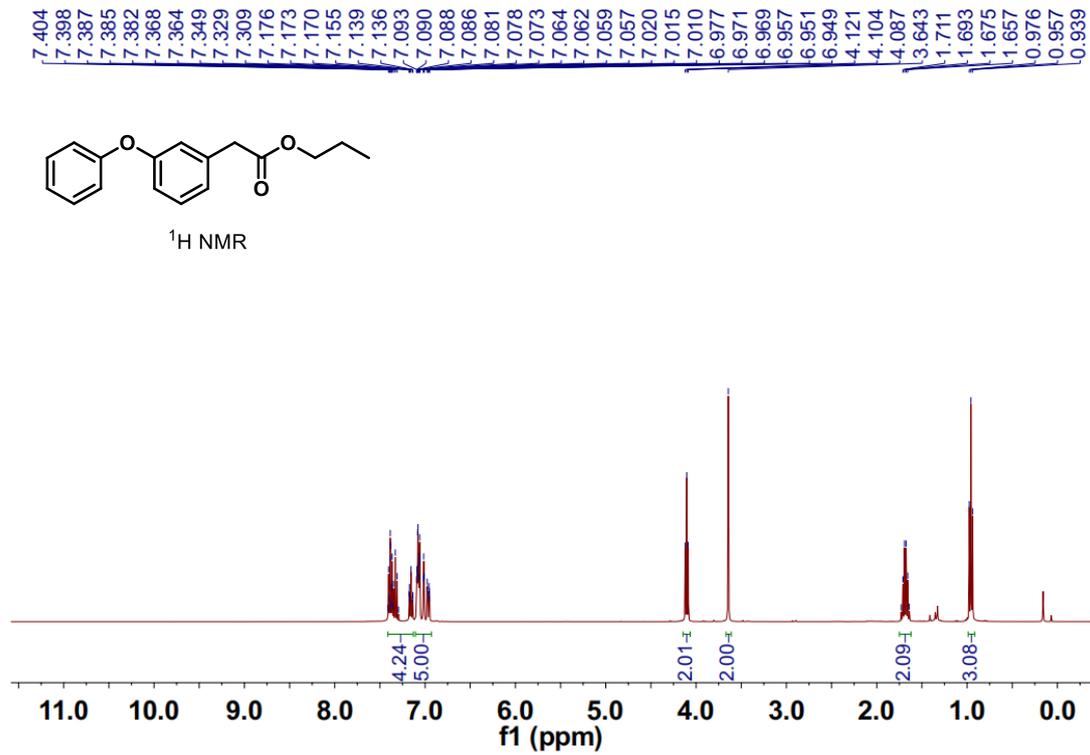
¹³C NMR

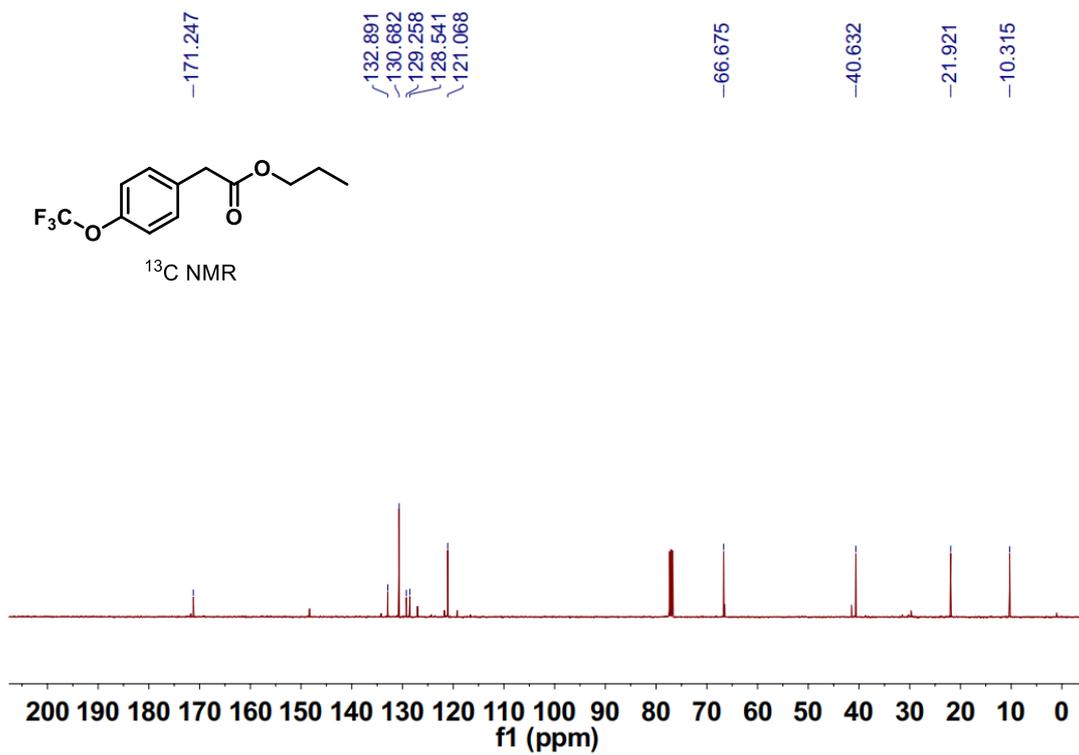
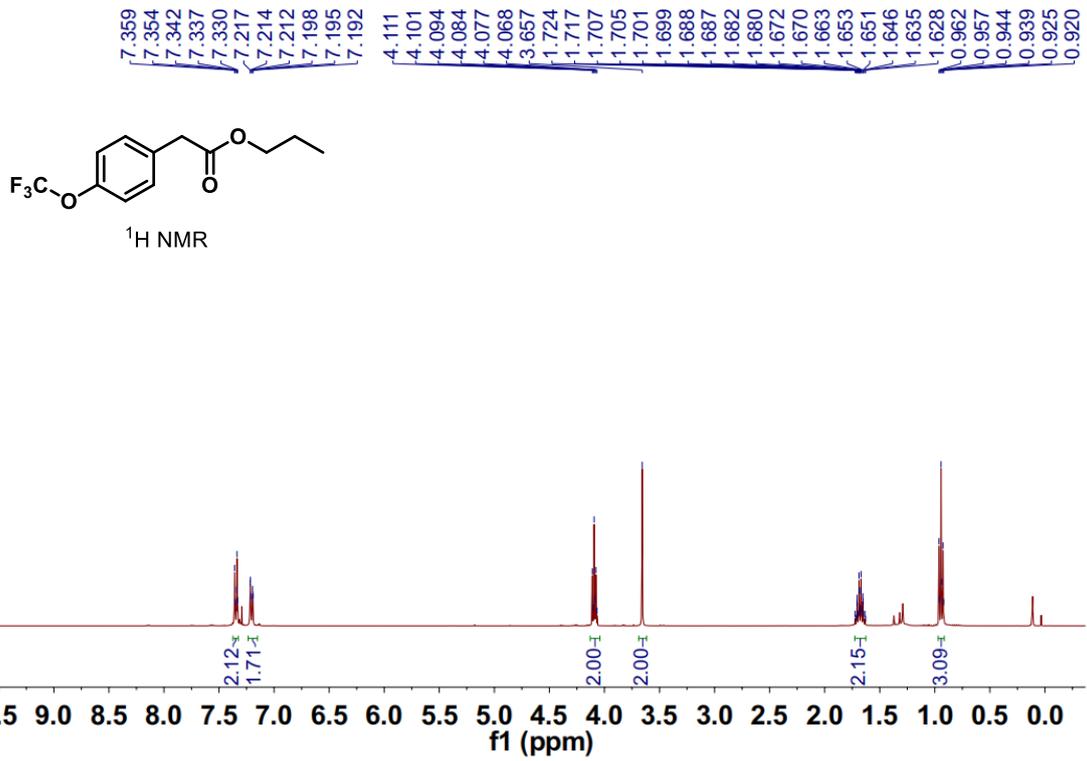


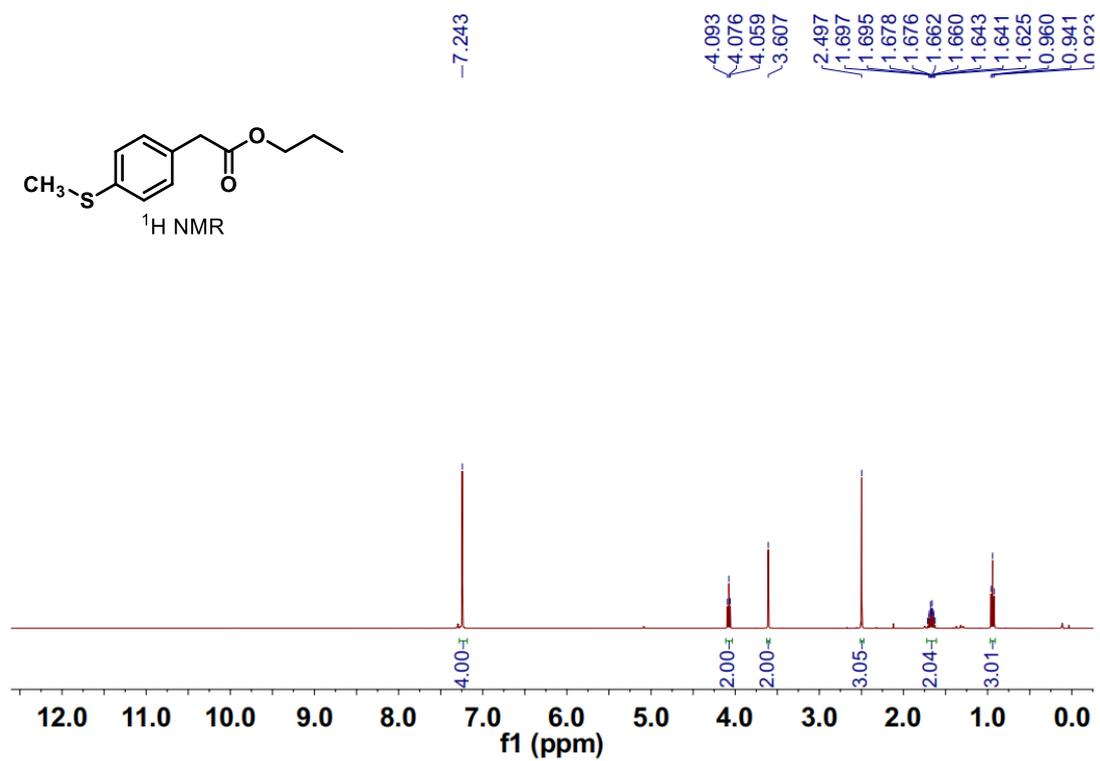
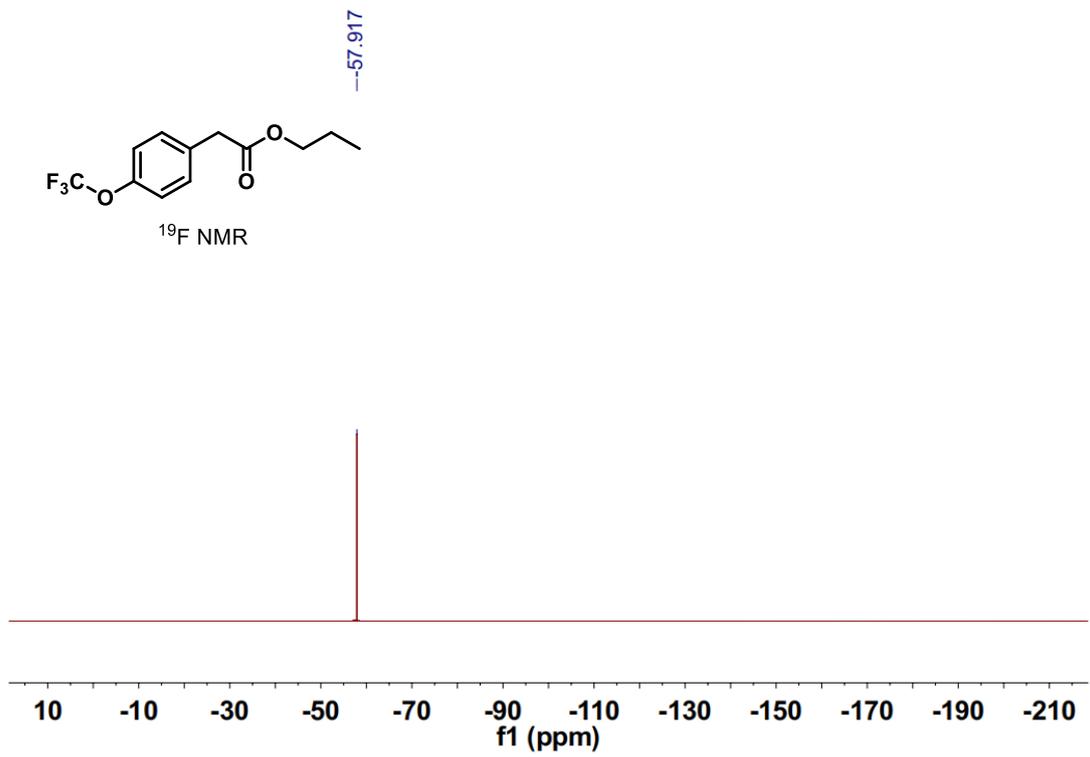


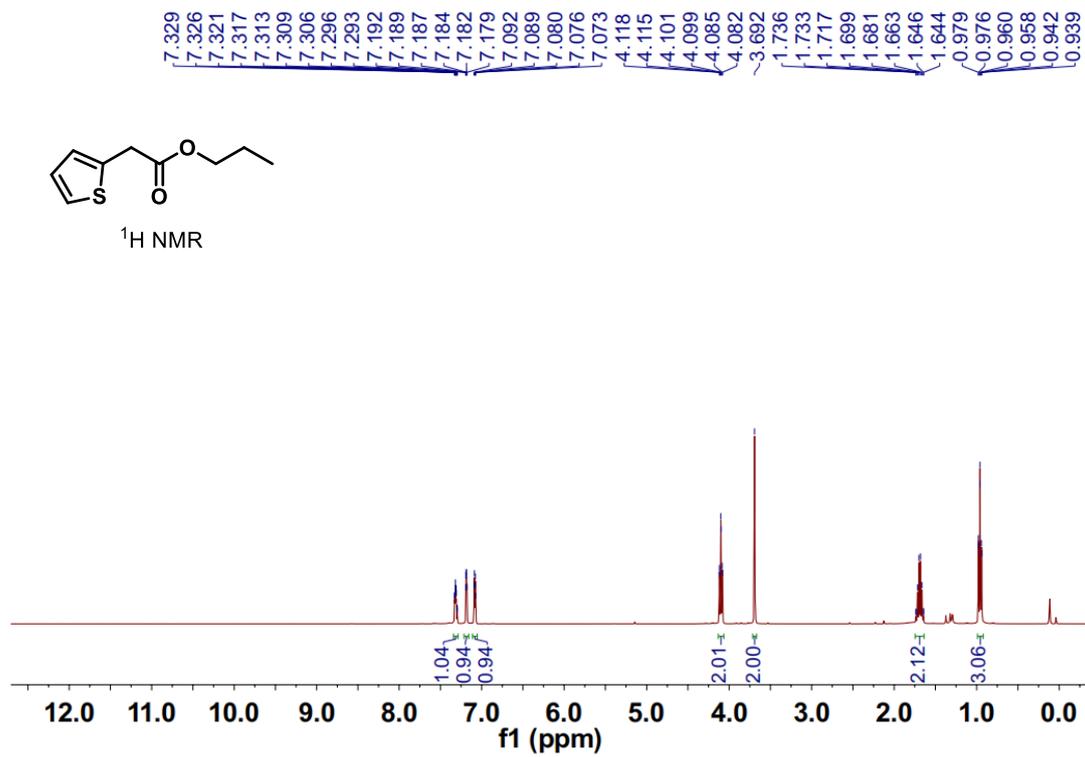
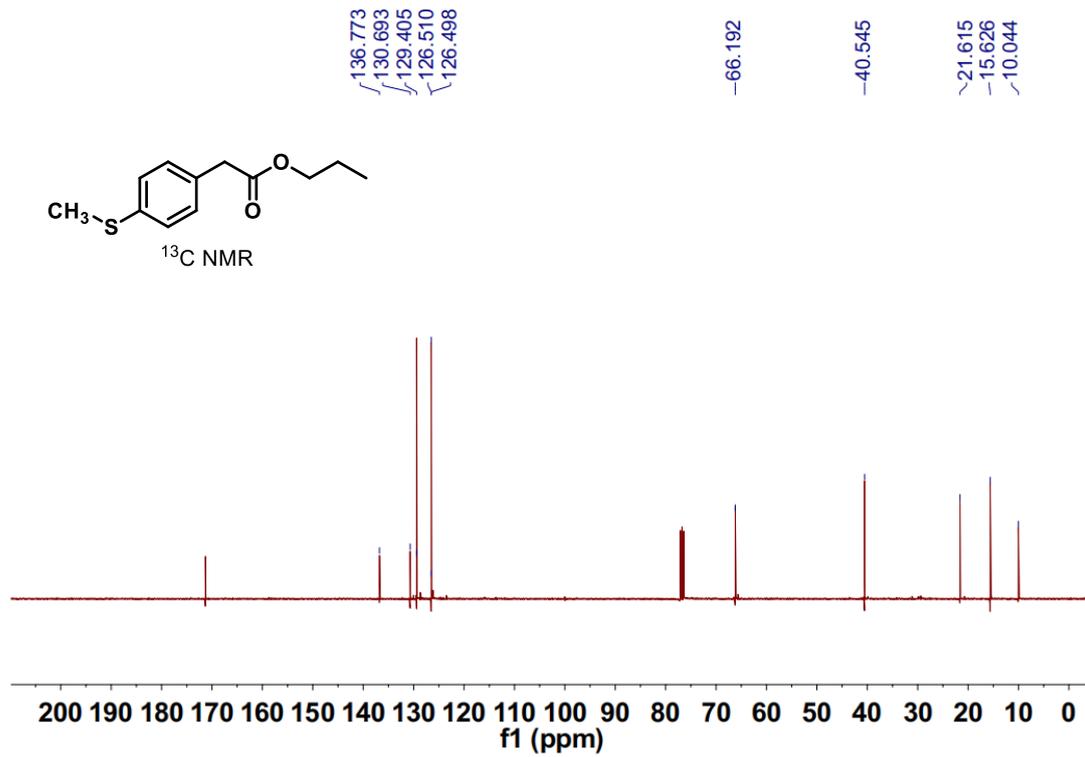


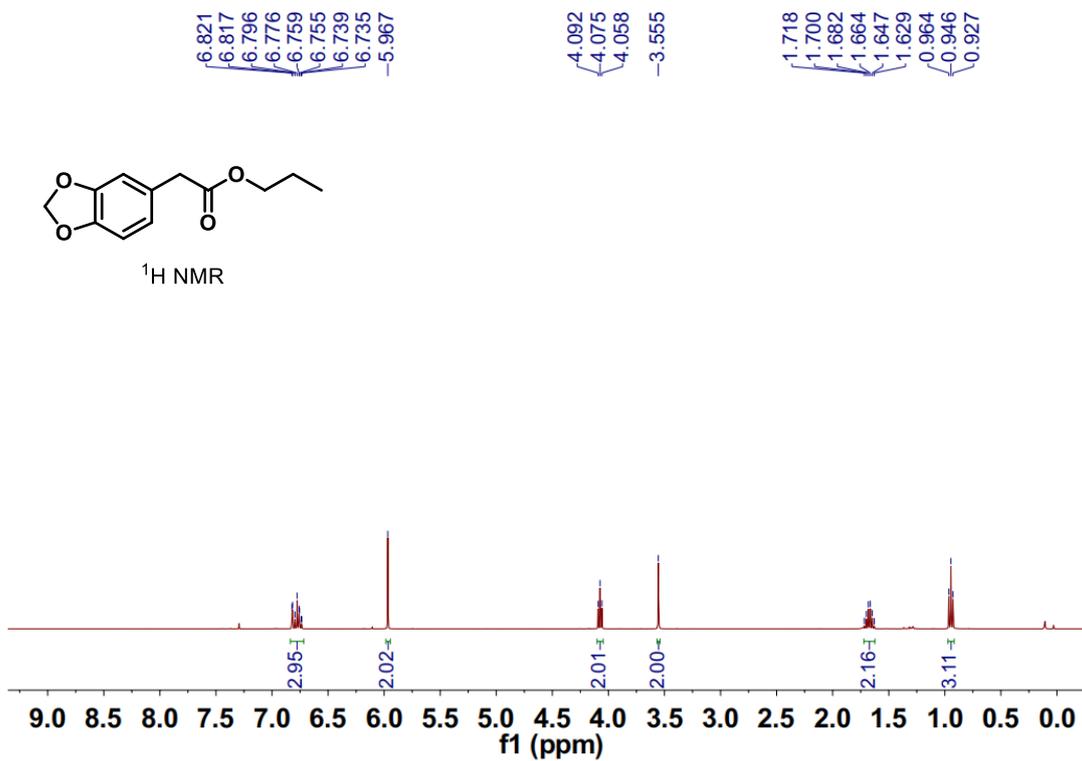
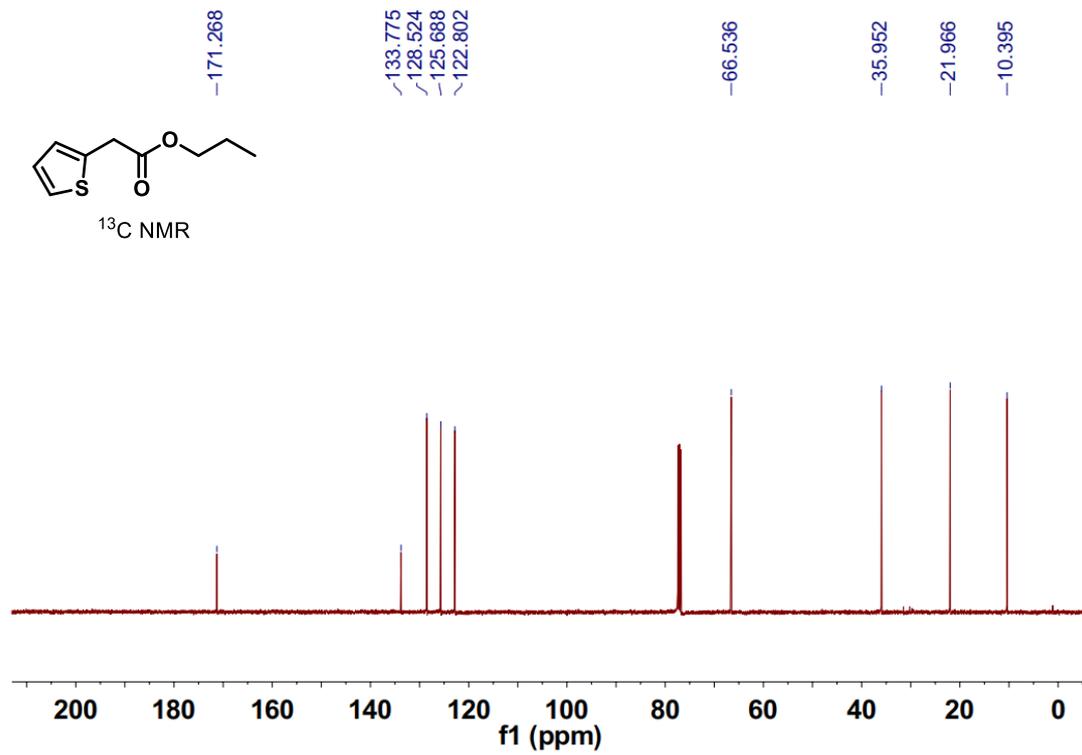


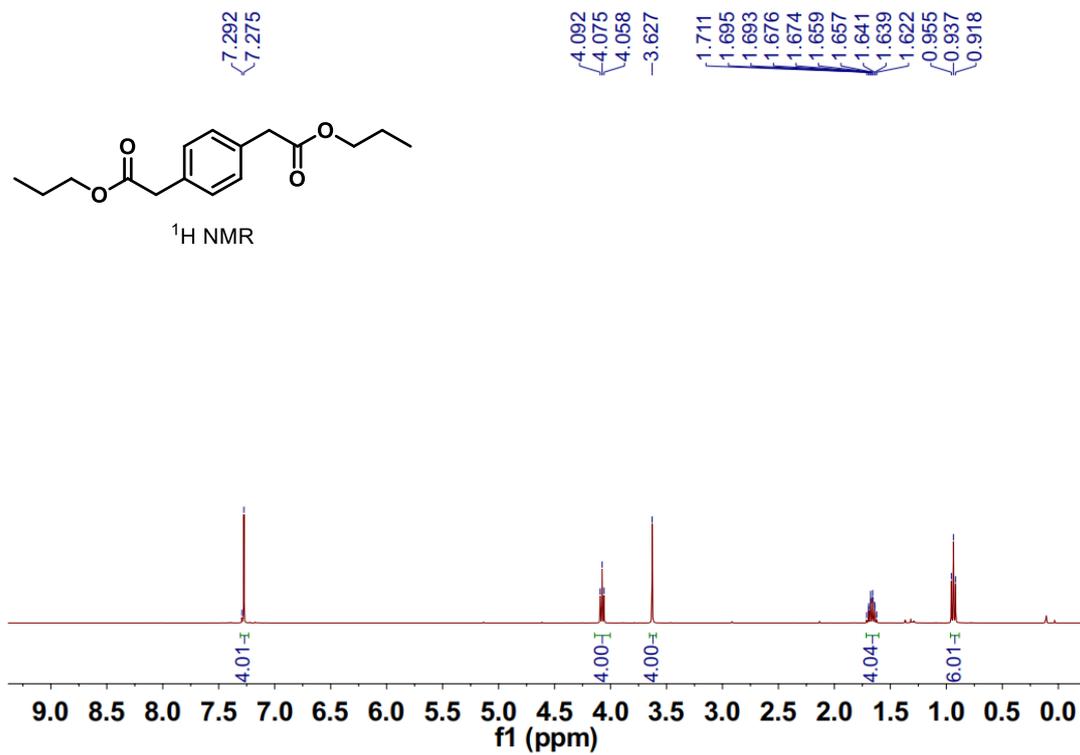
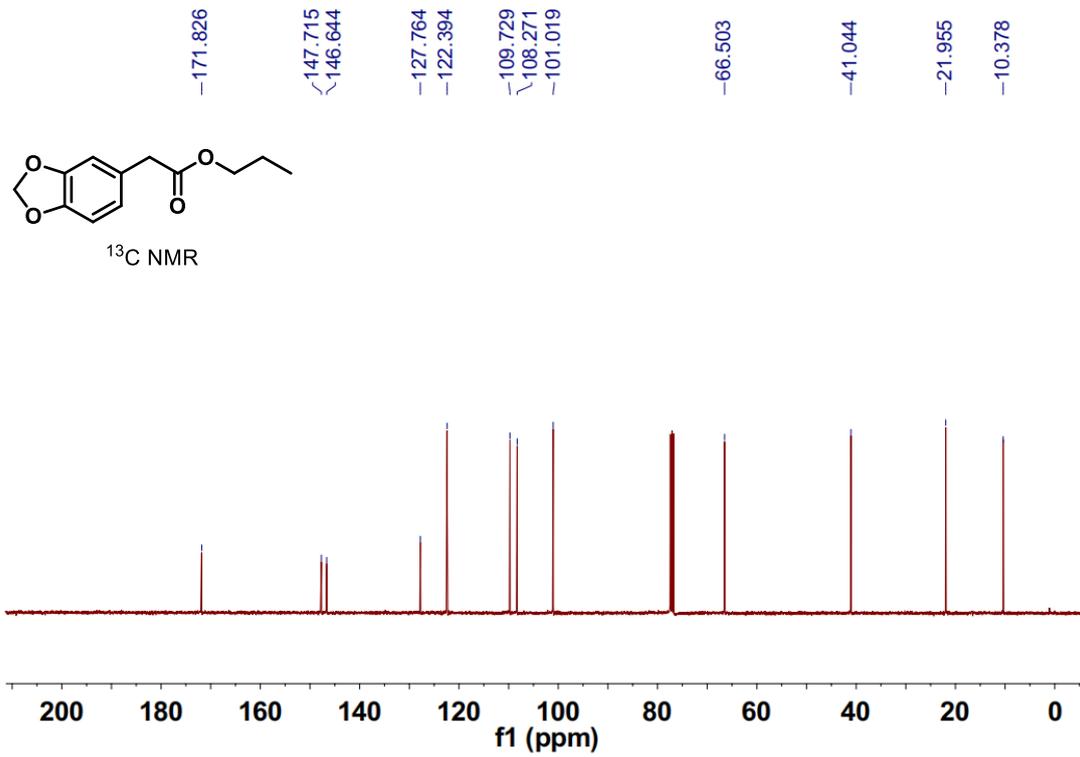


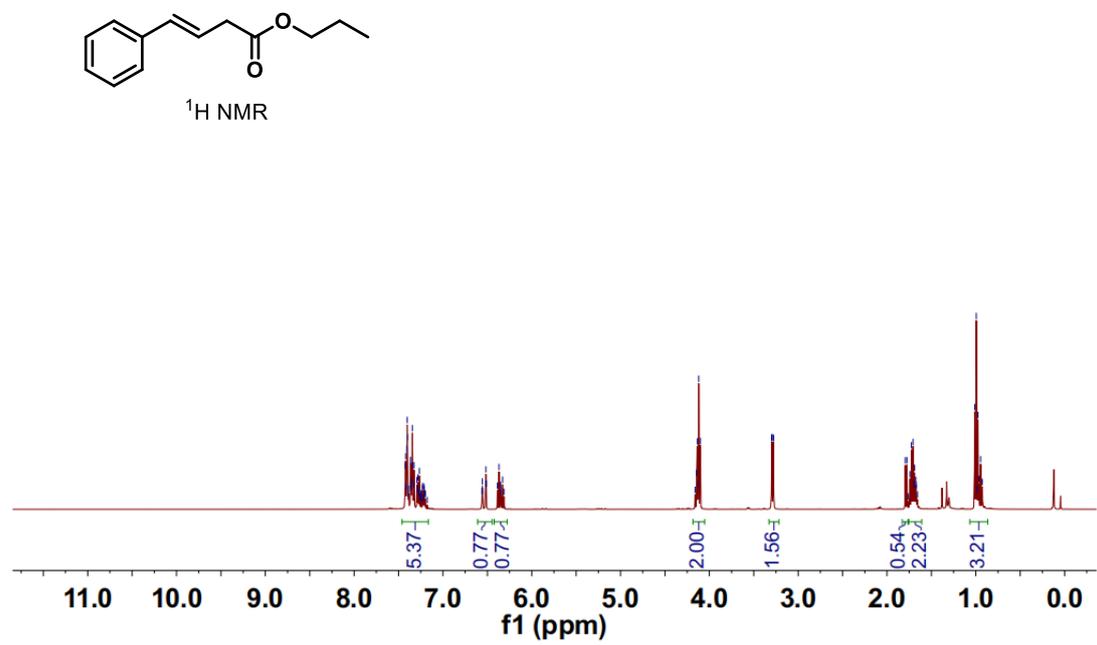
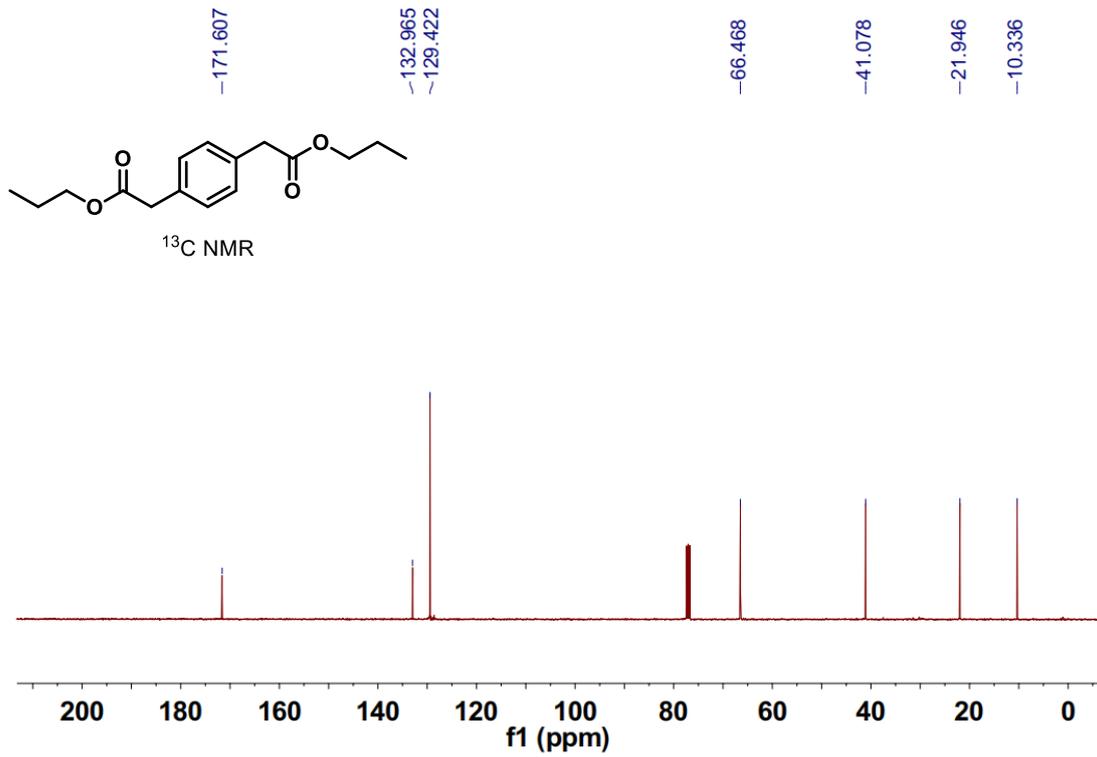


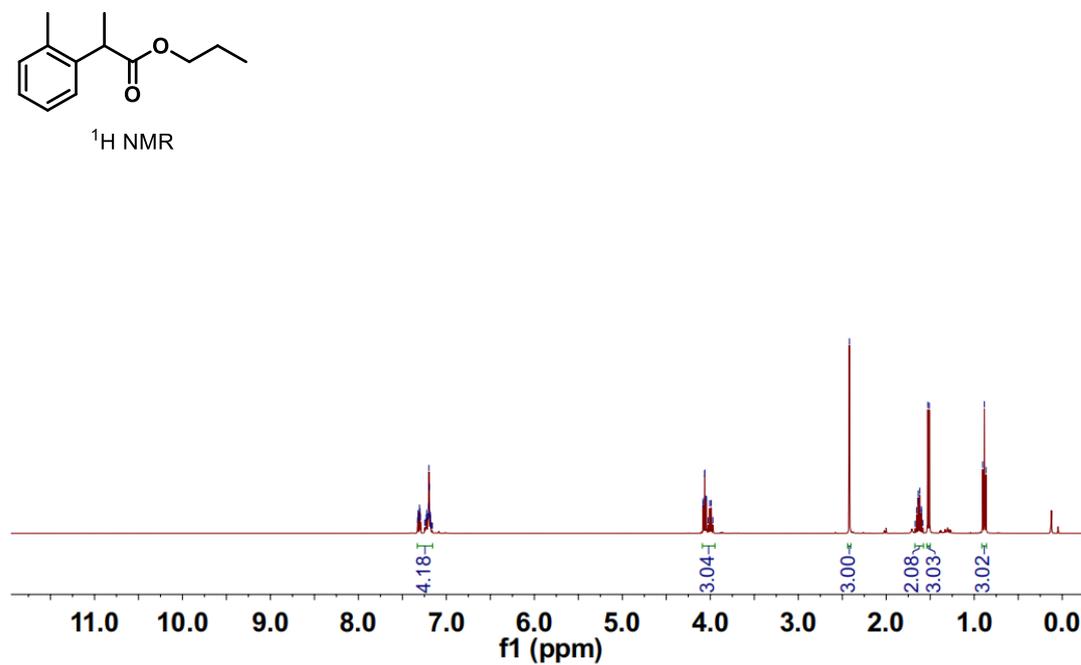
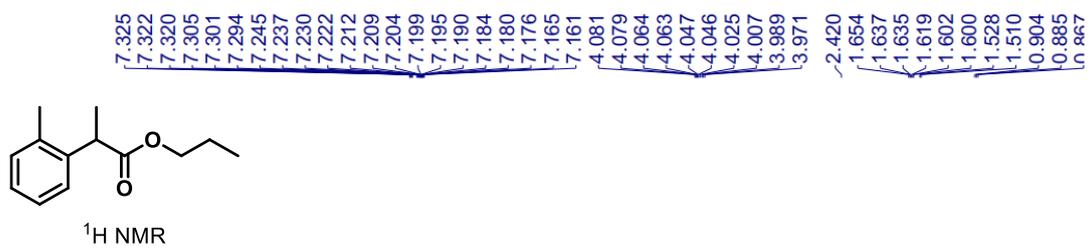
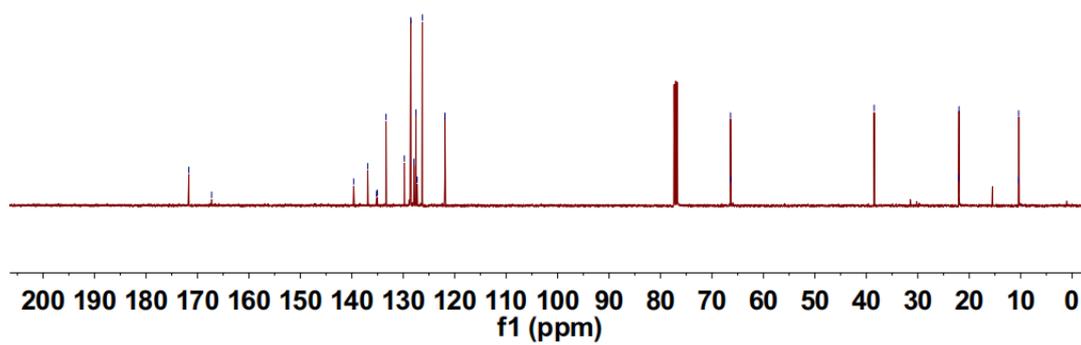
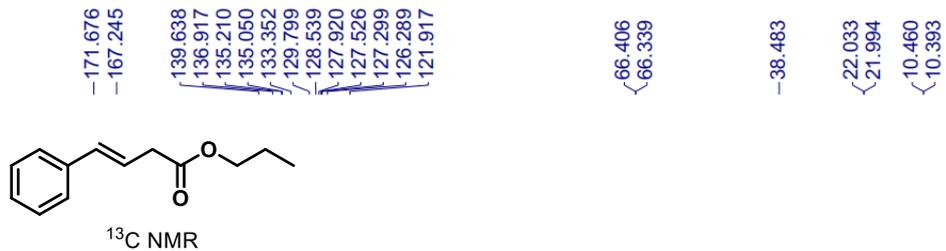


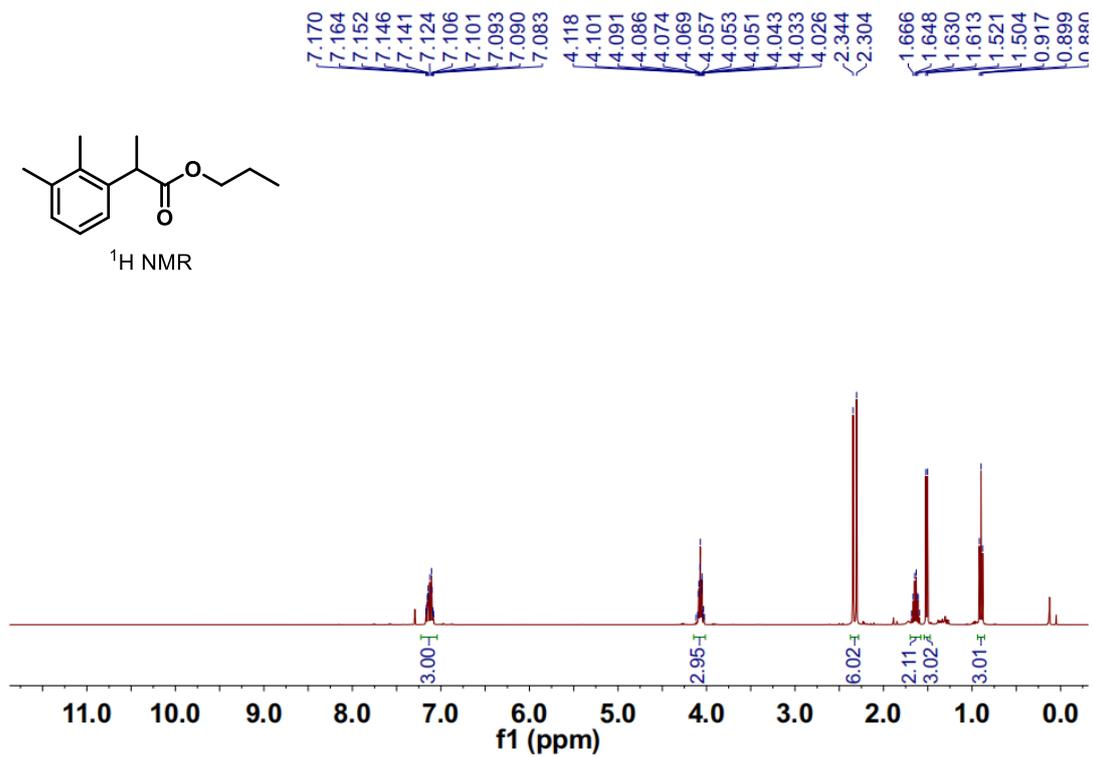
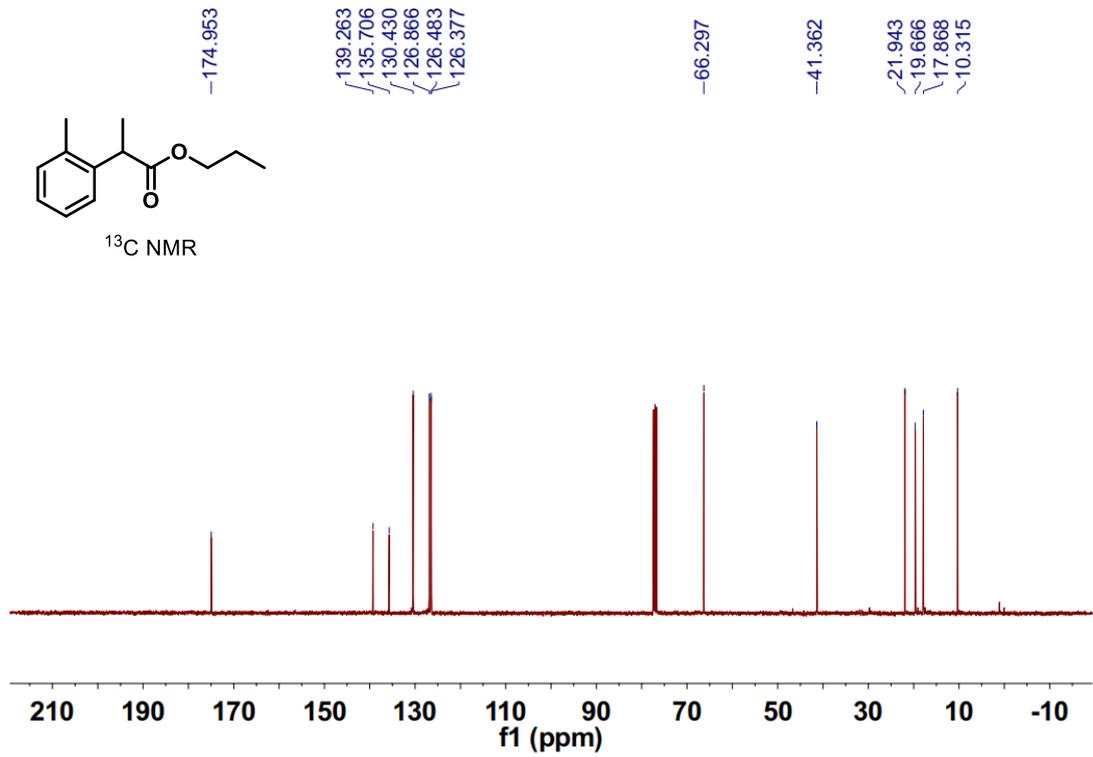


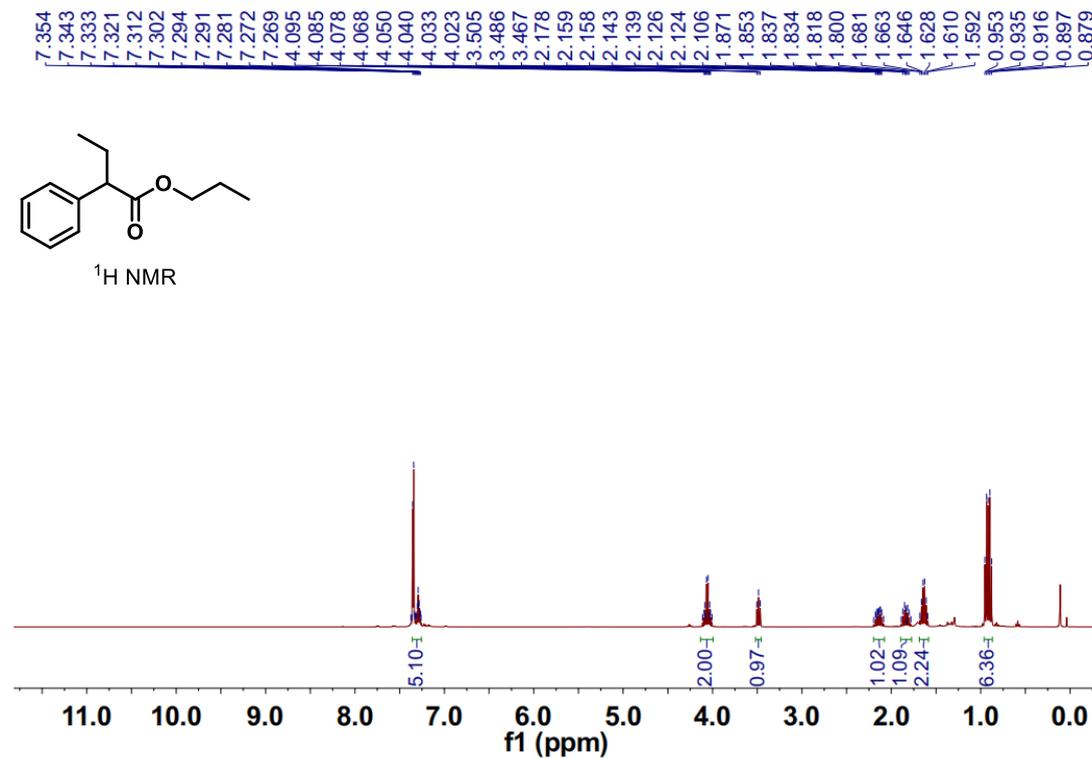
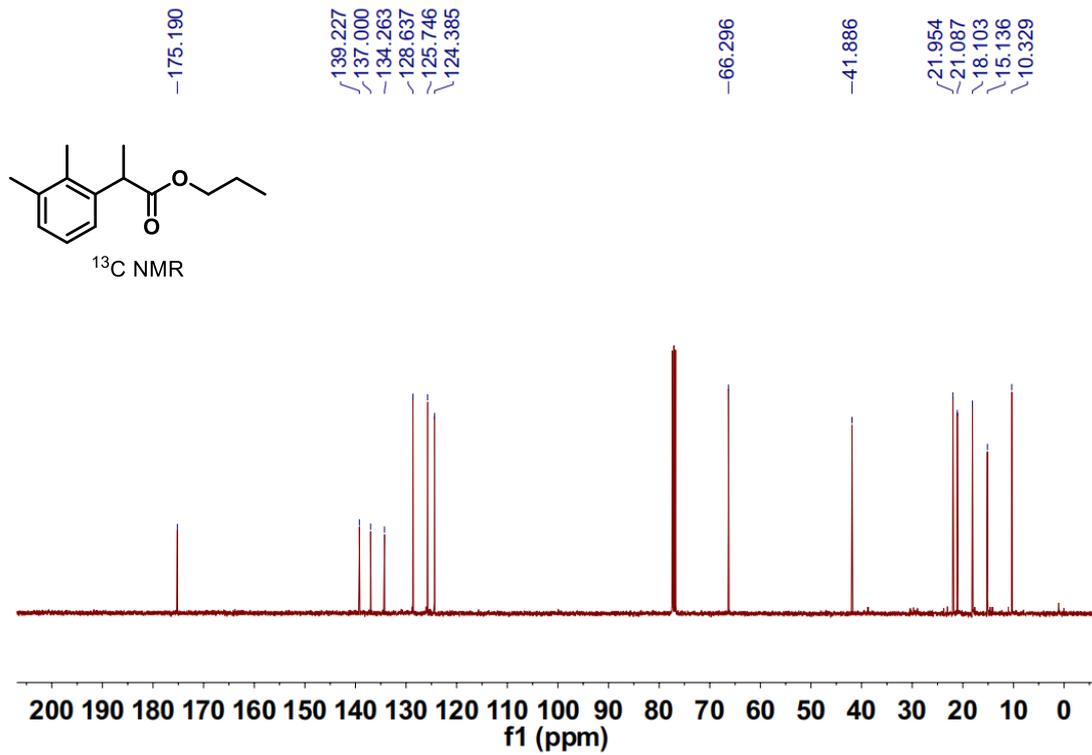


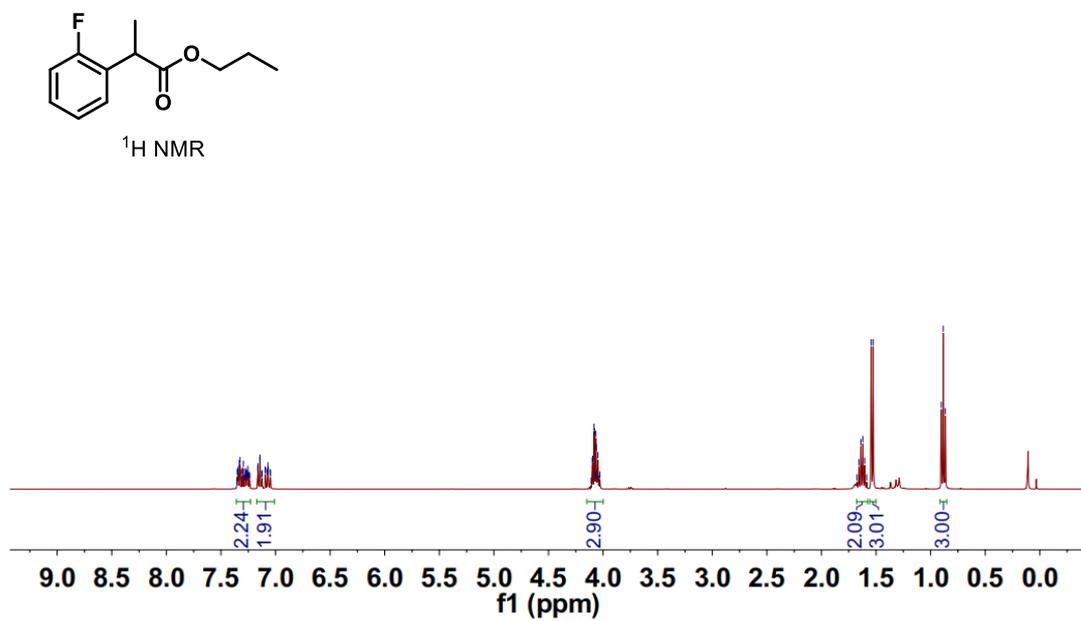
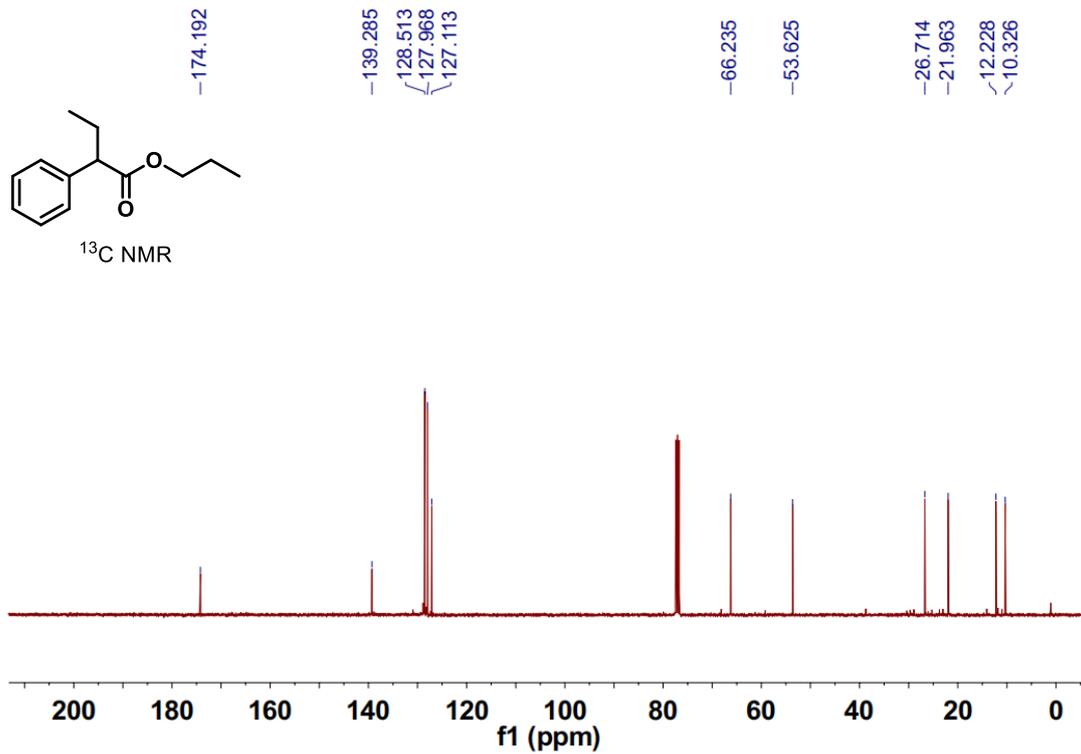


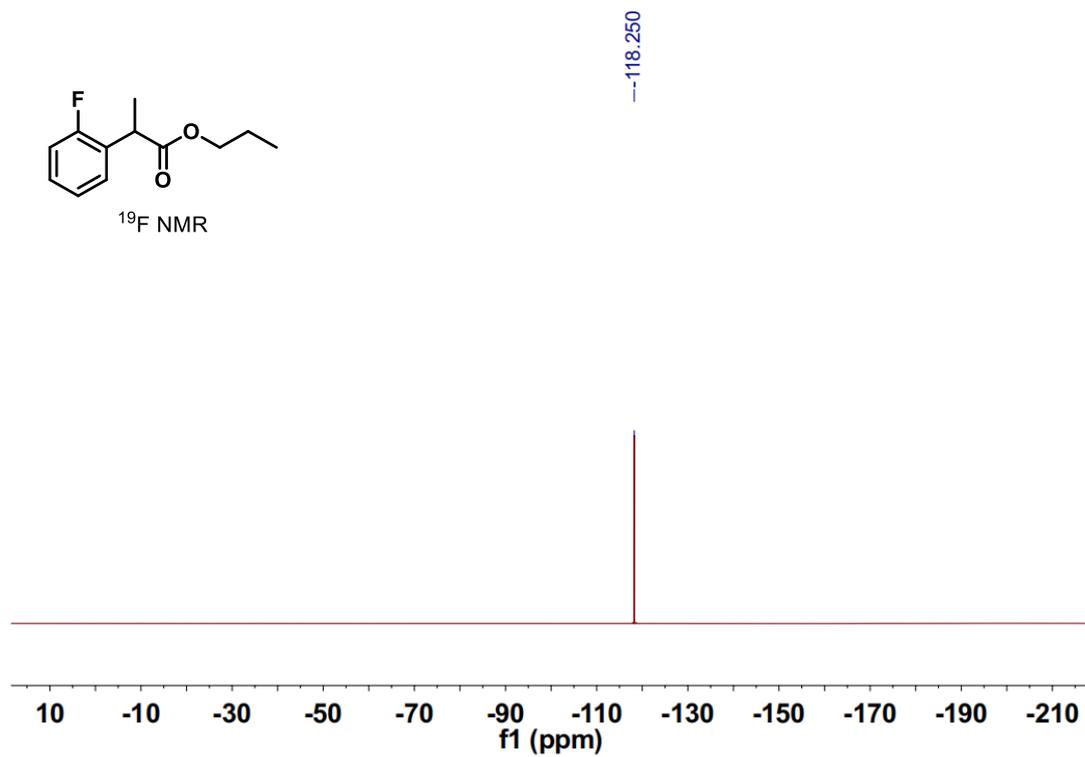
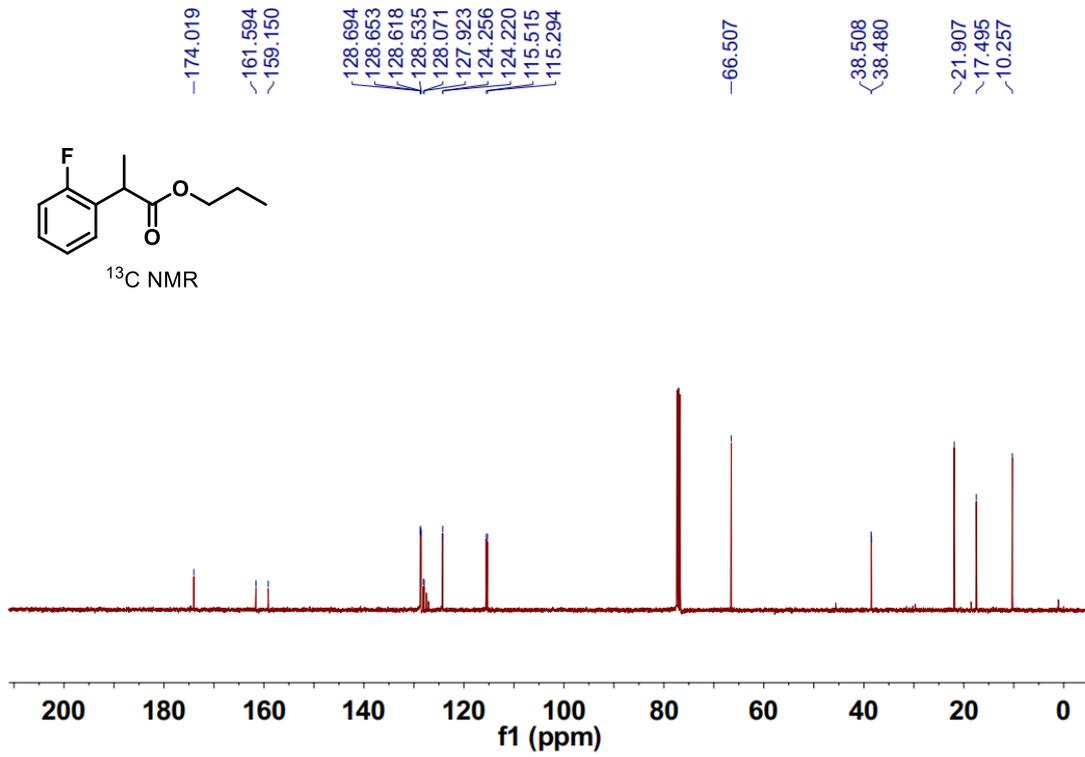


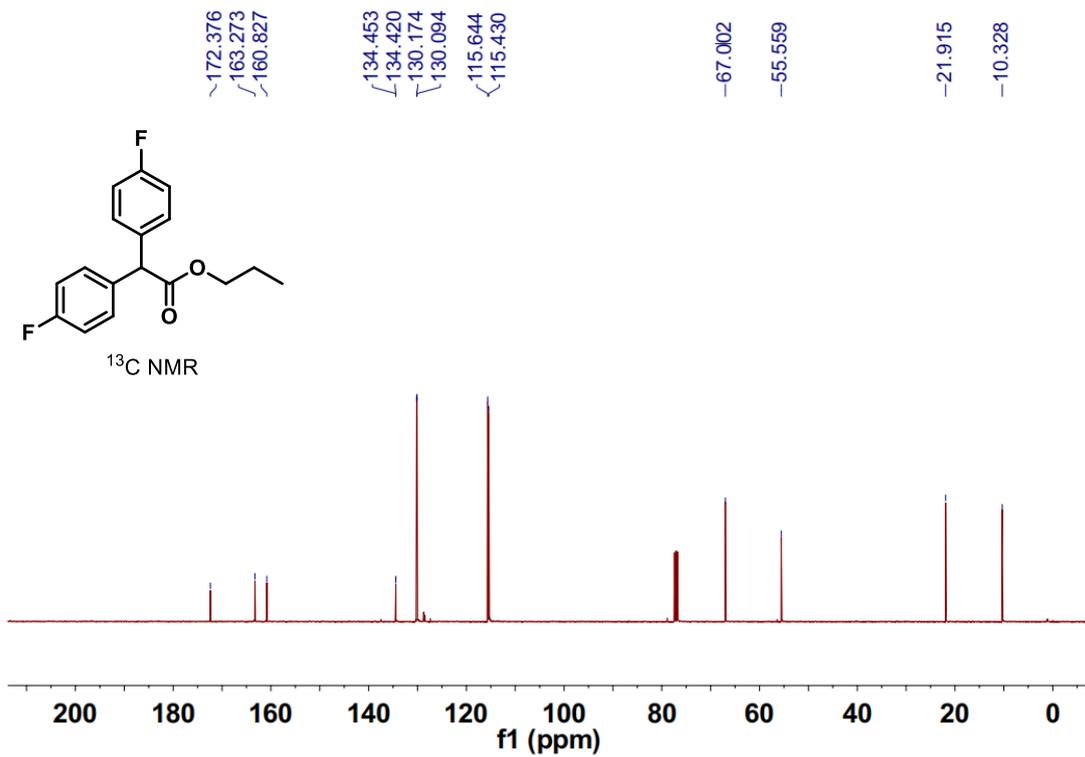
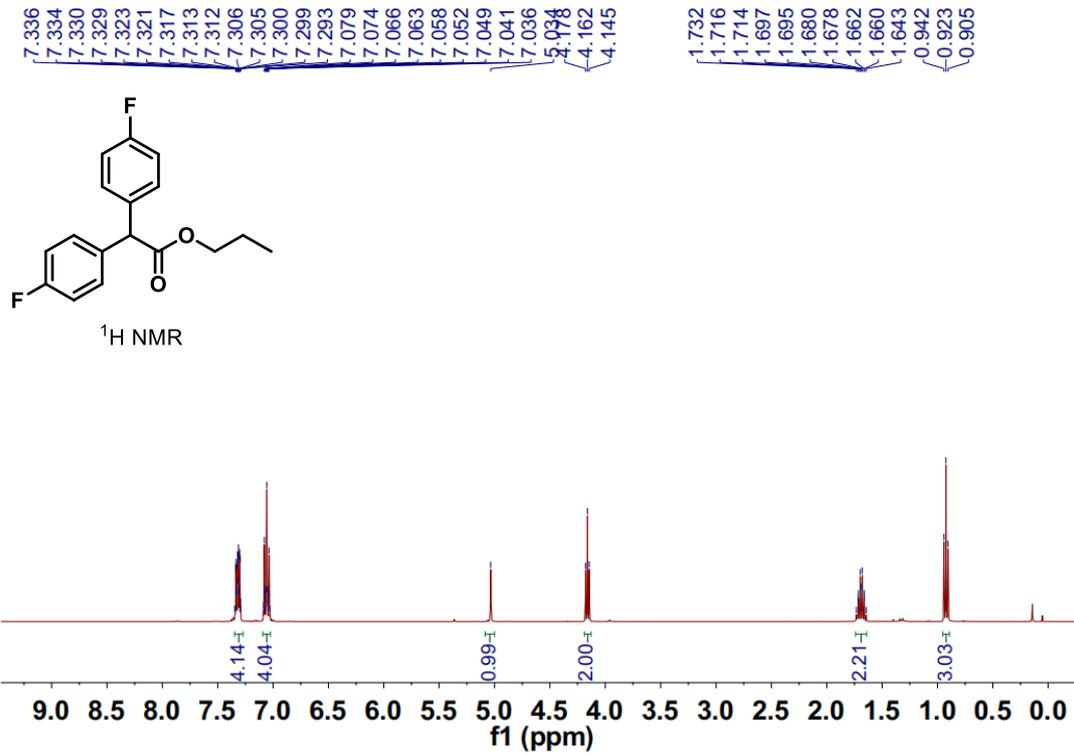


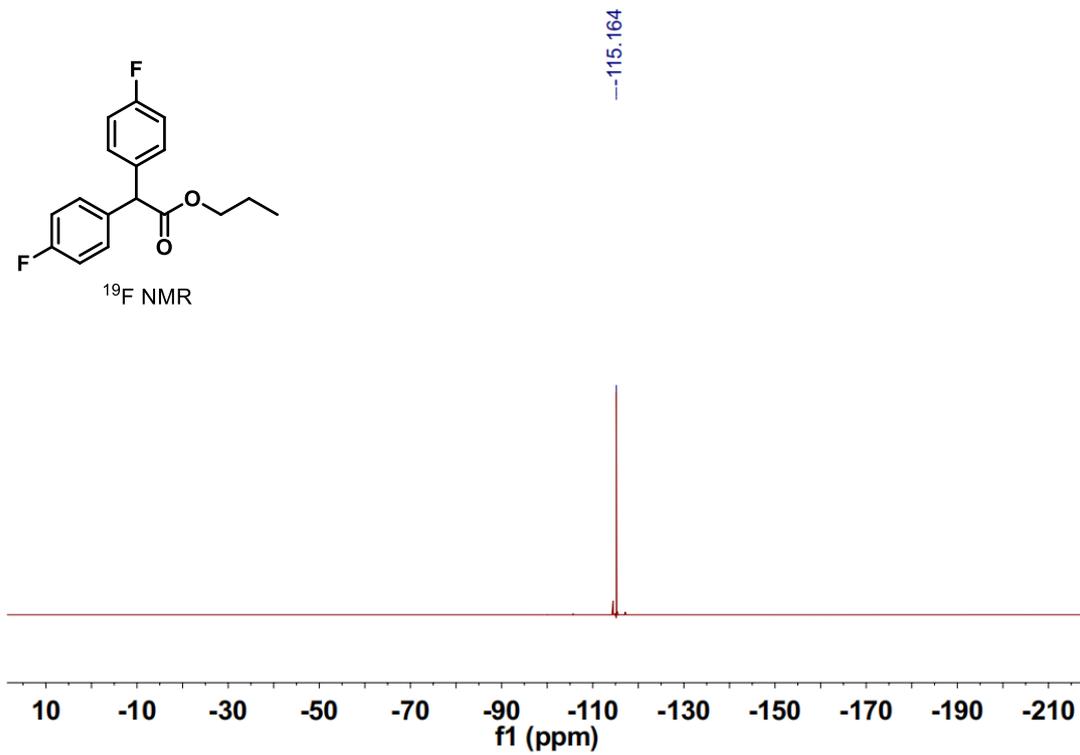
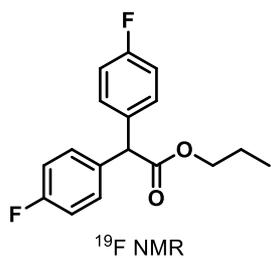




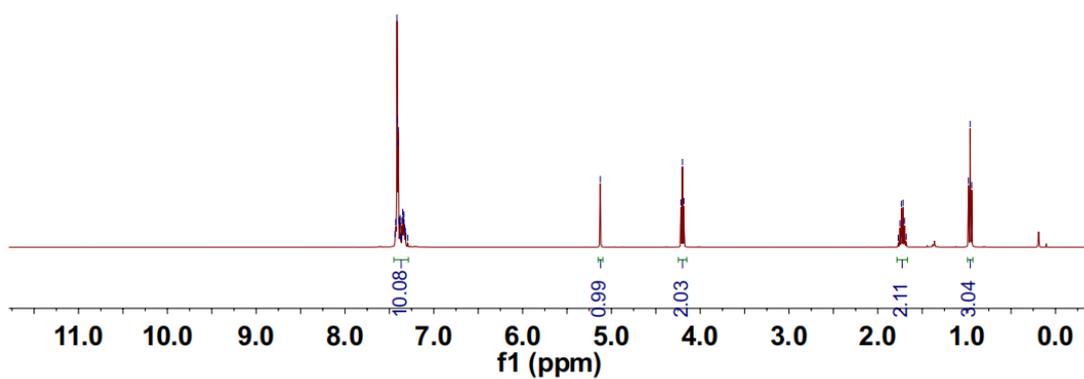
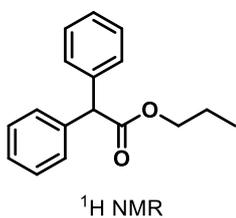


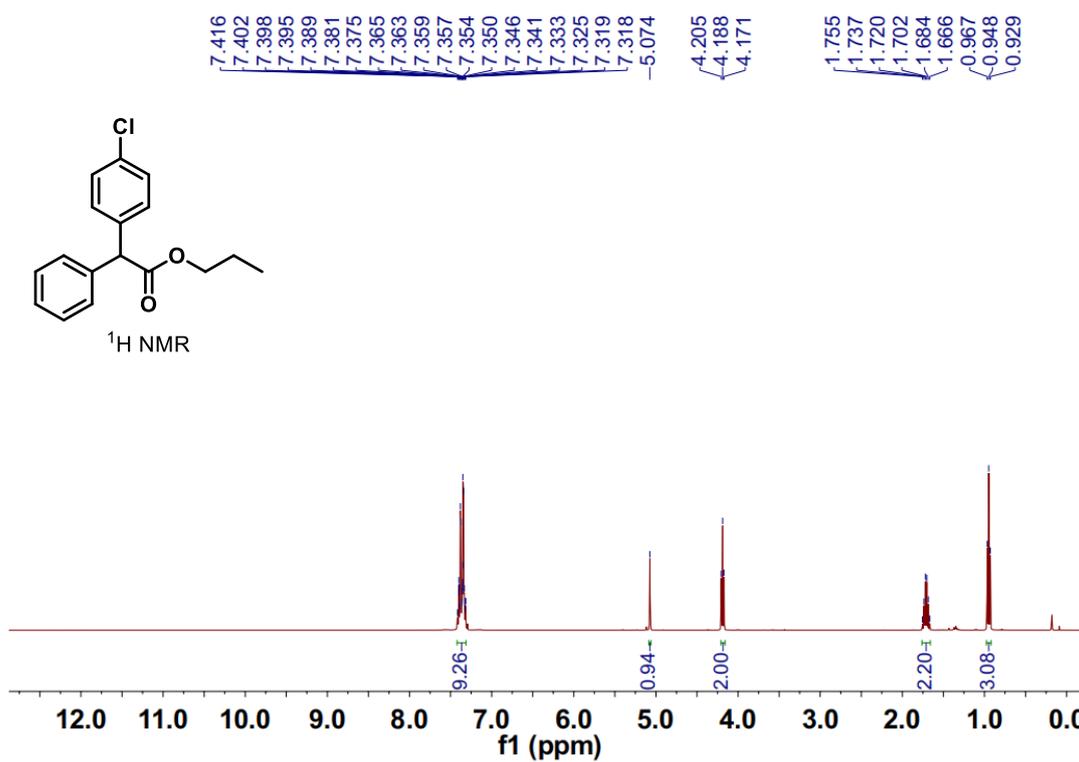
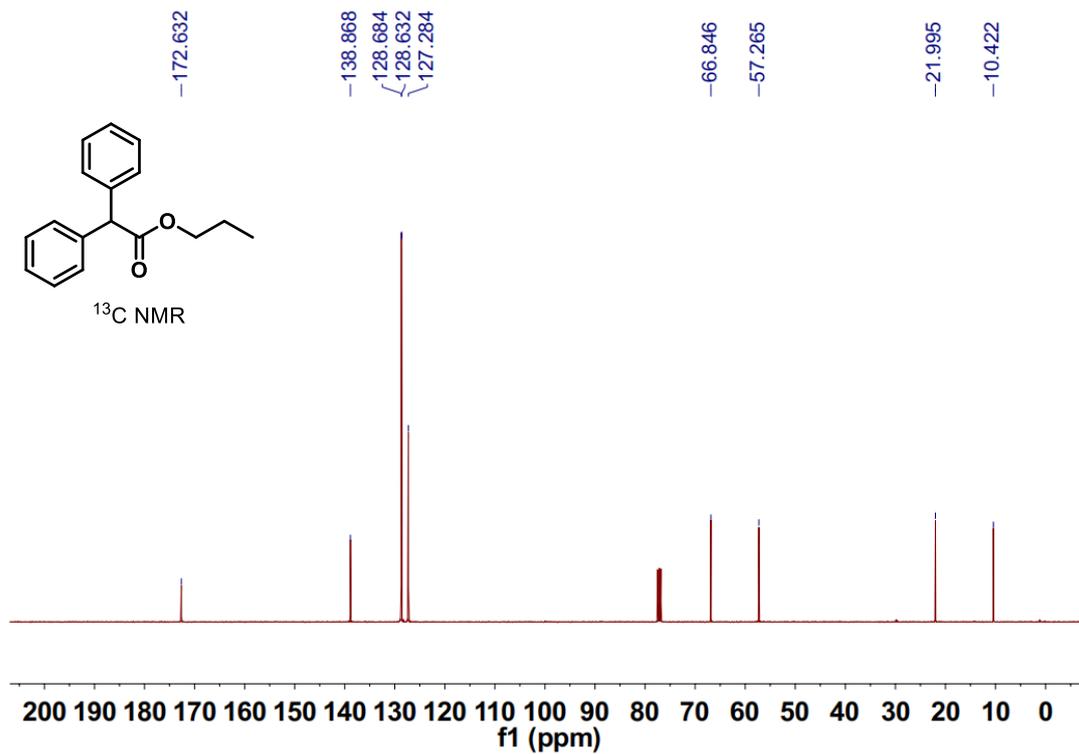


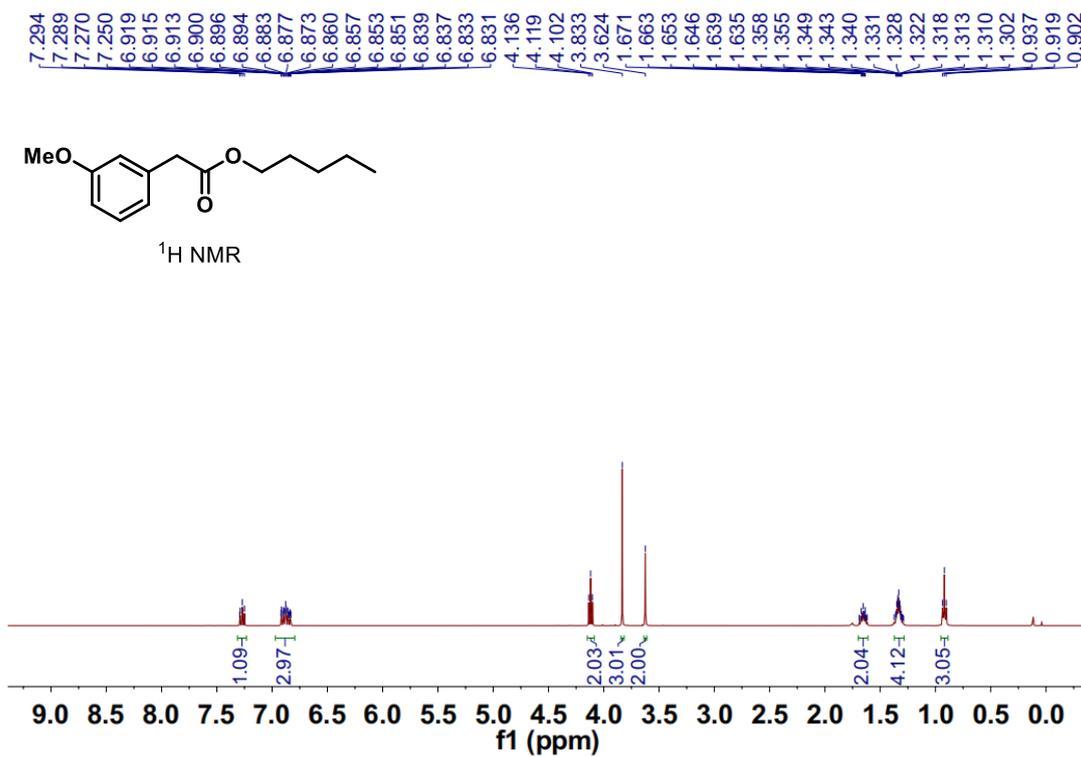
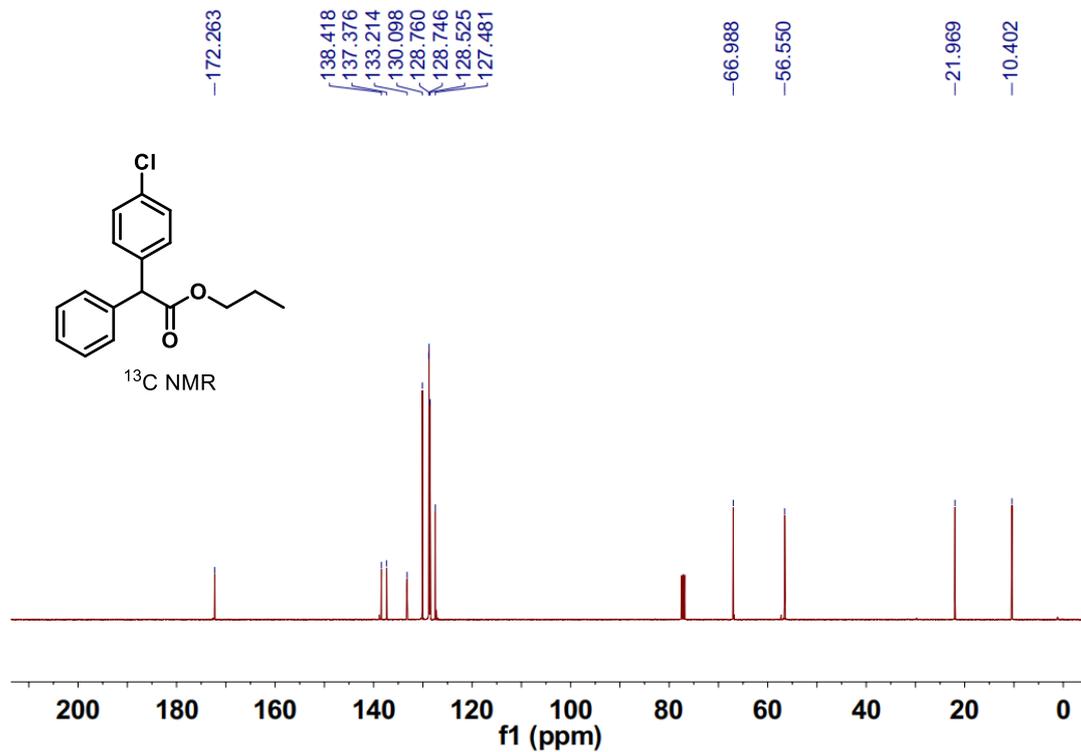


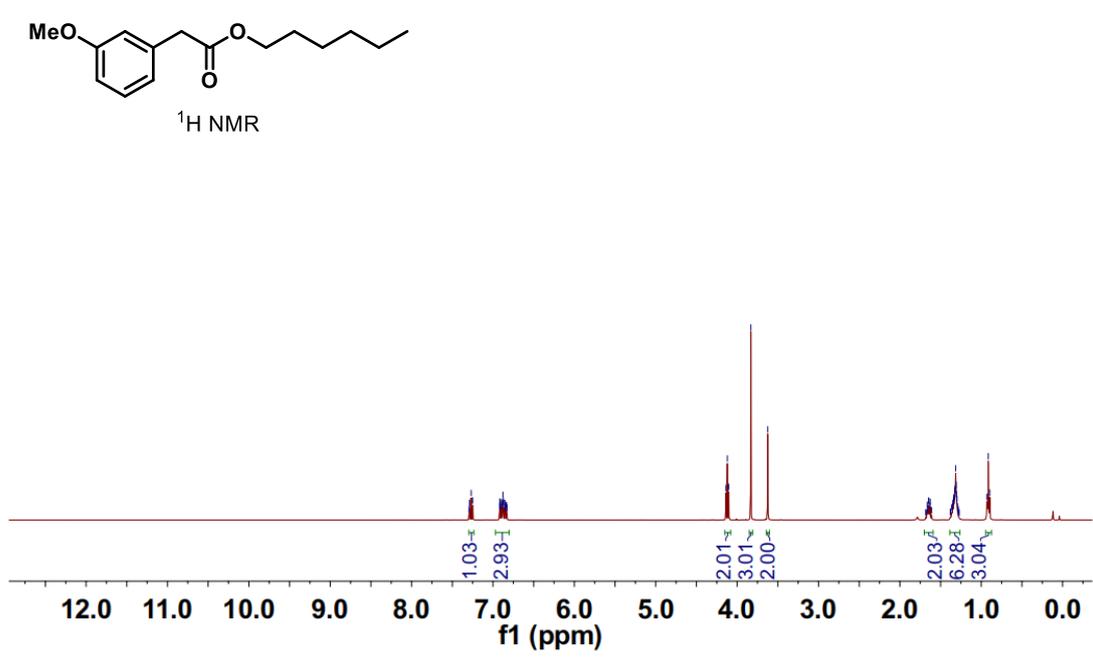
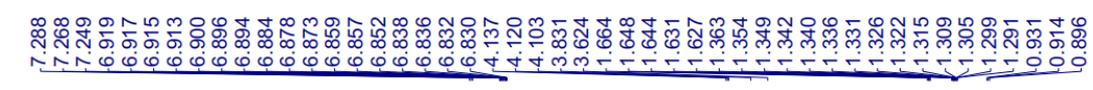
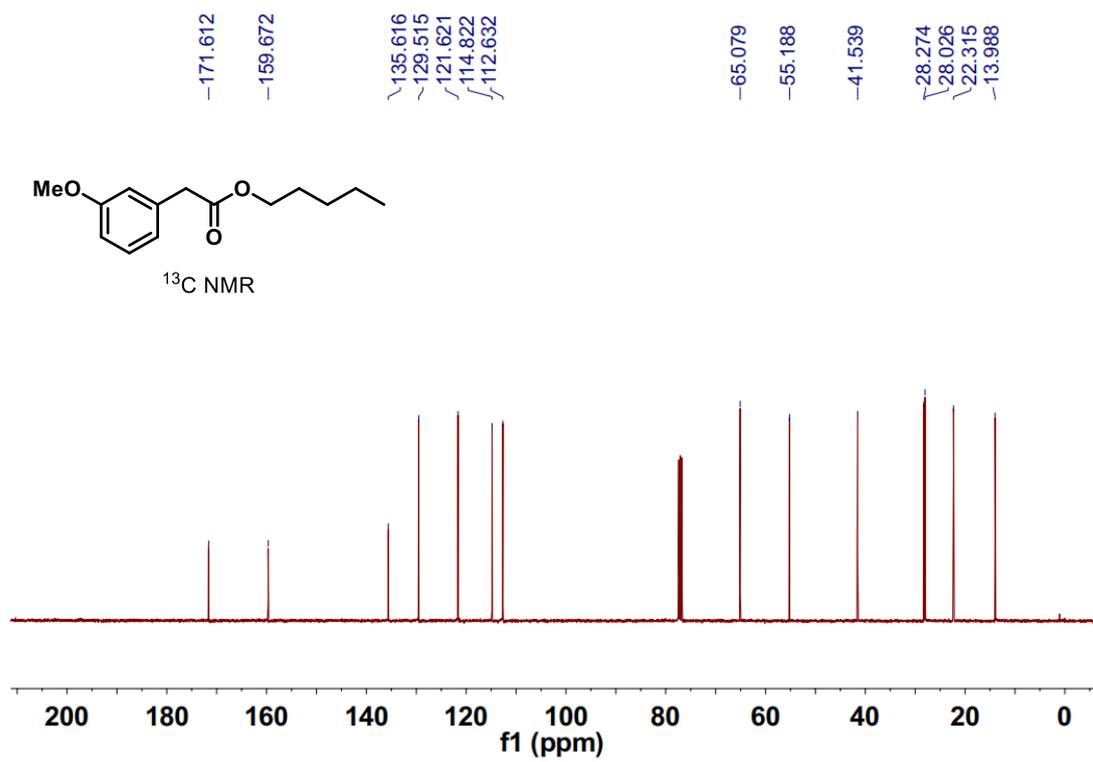


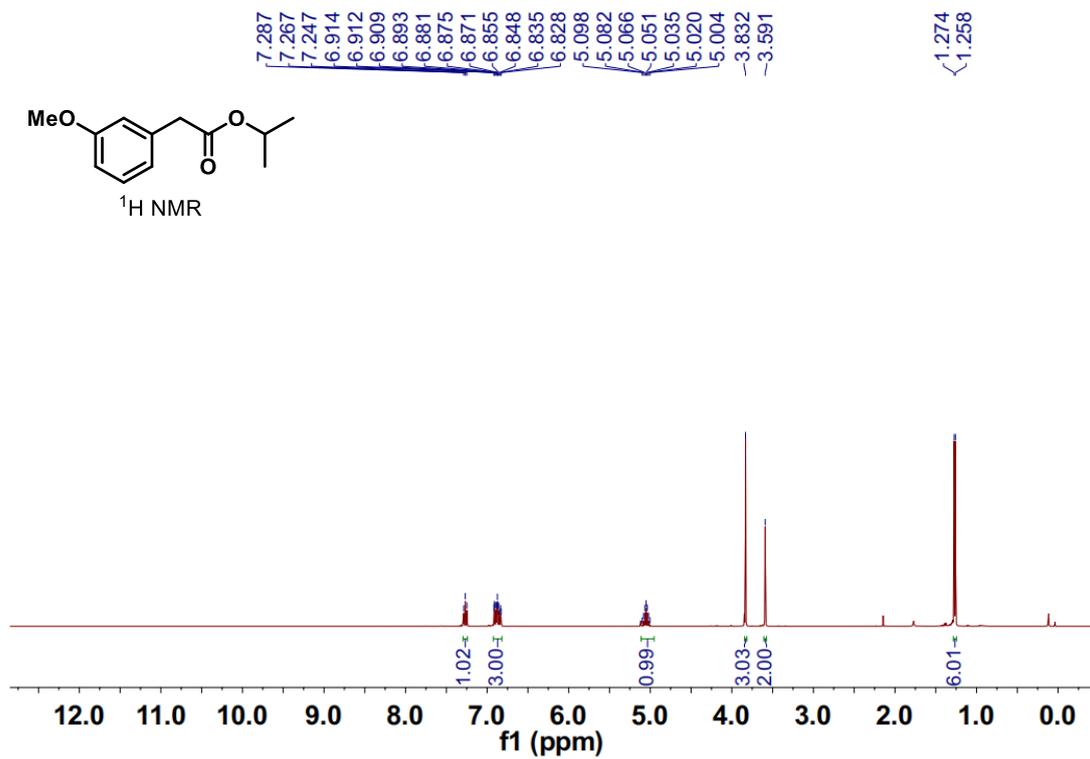
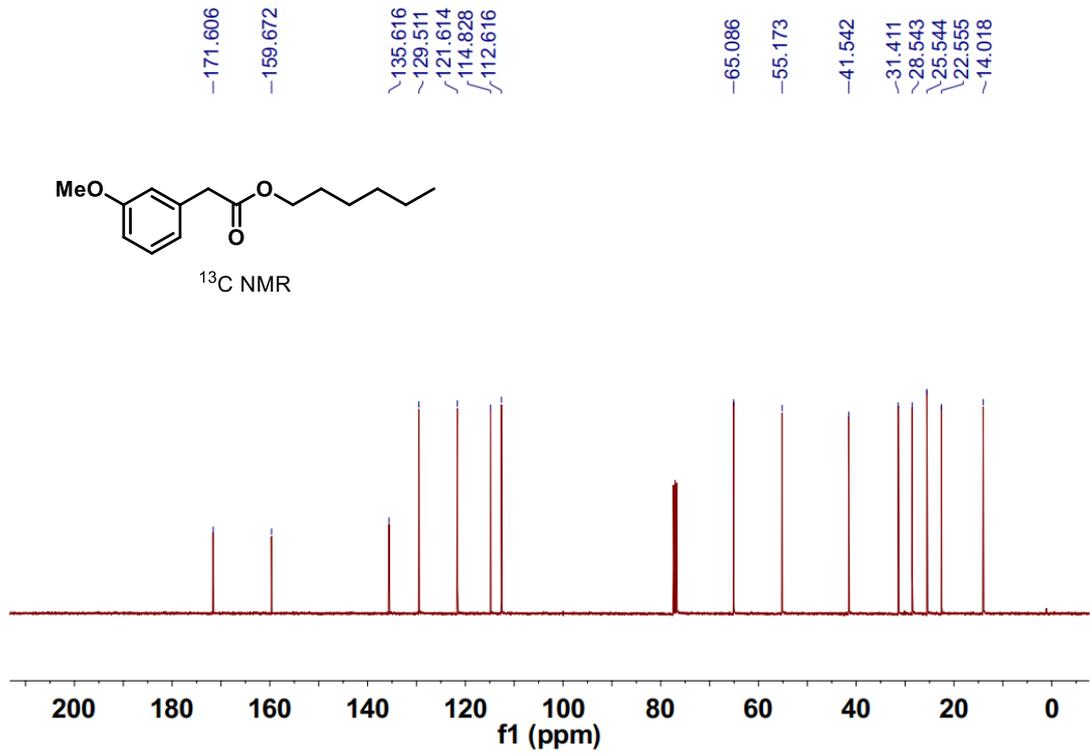
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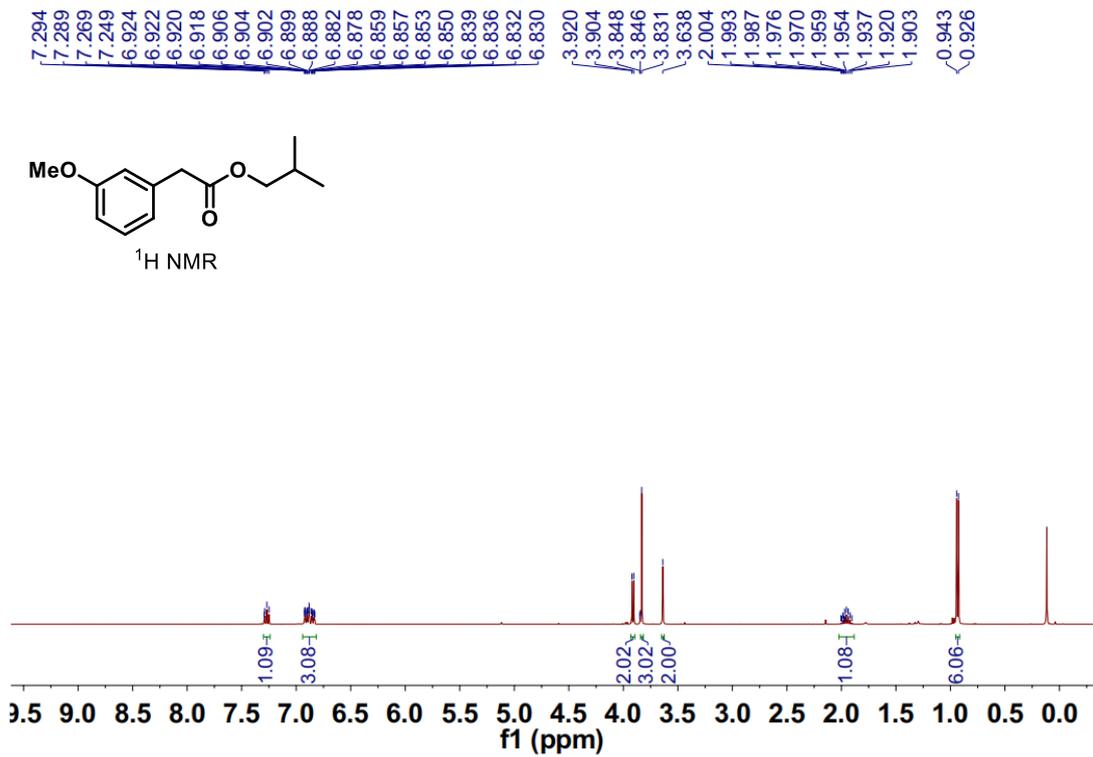
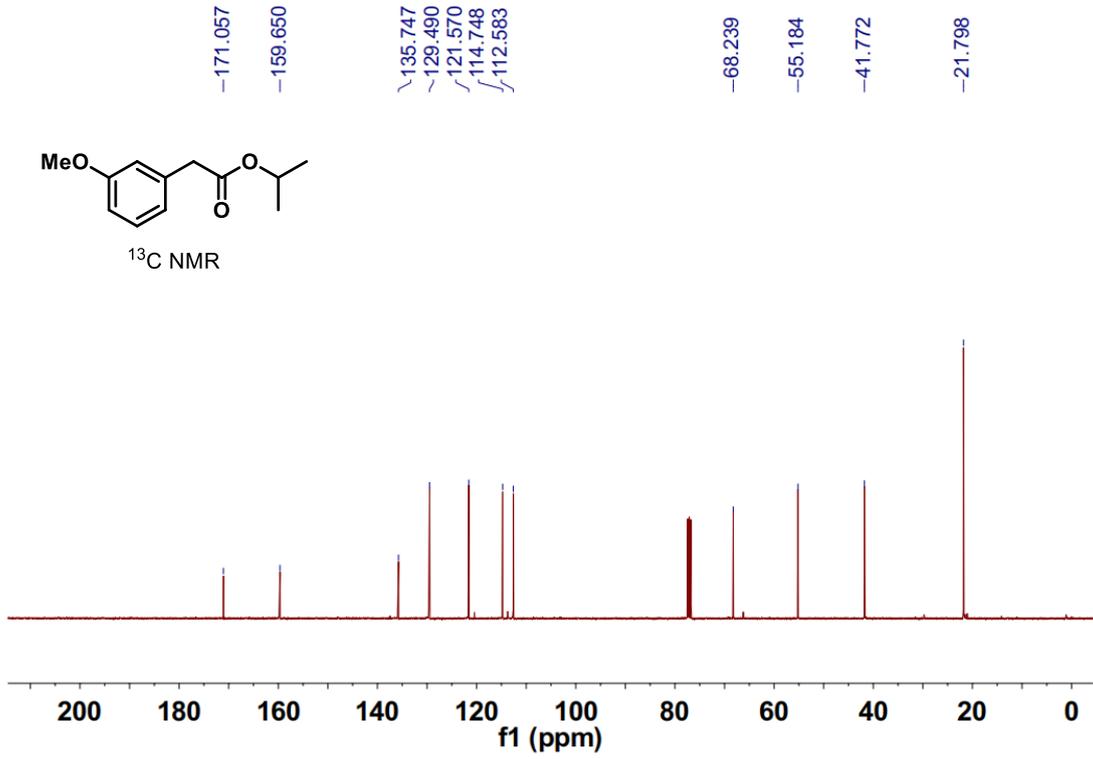


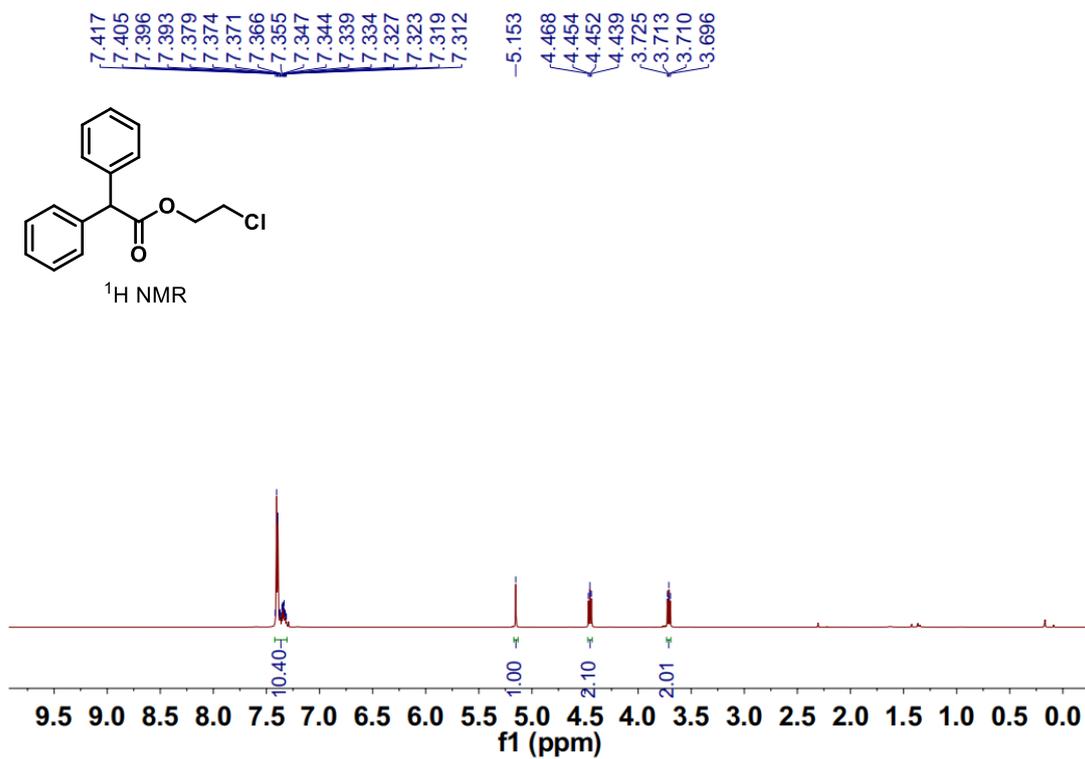
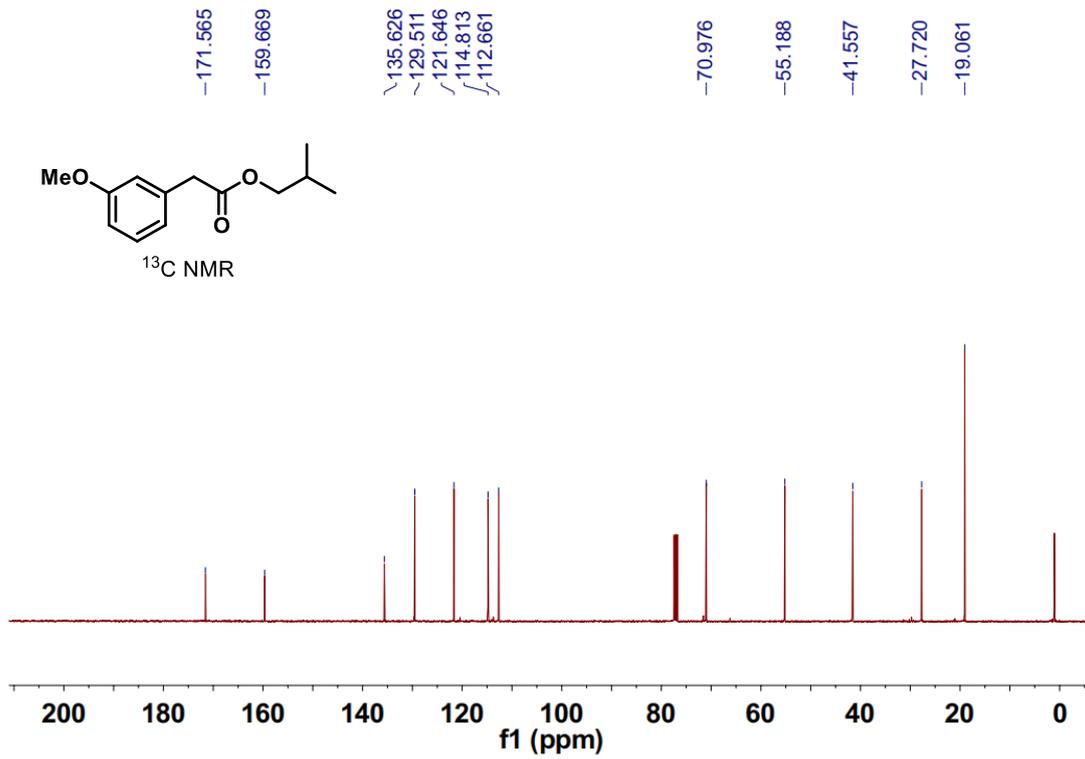


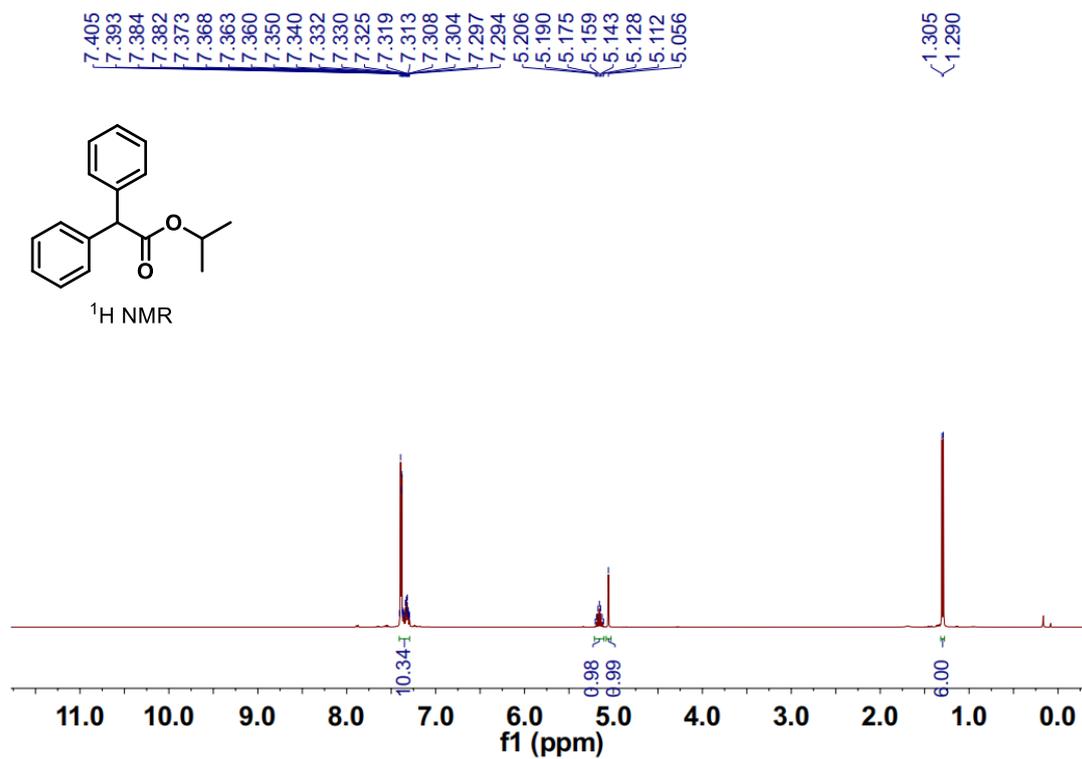
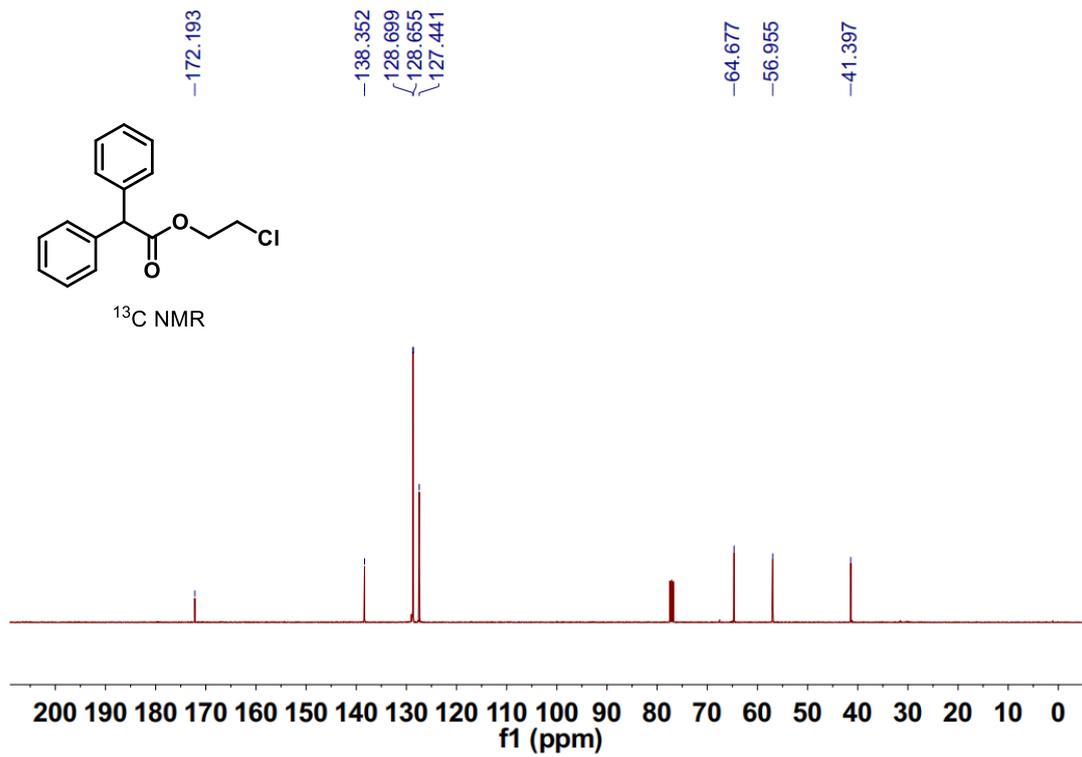


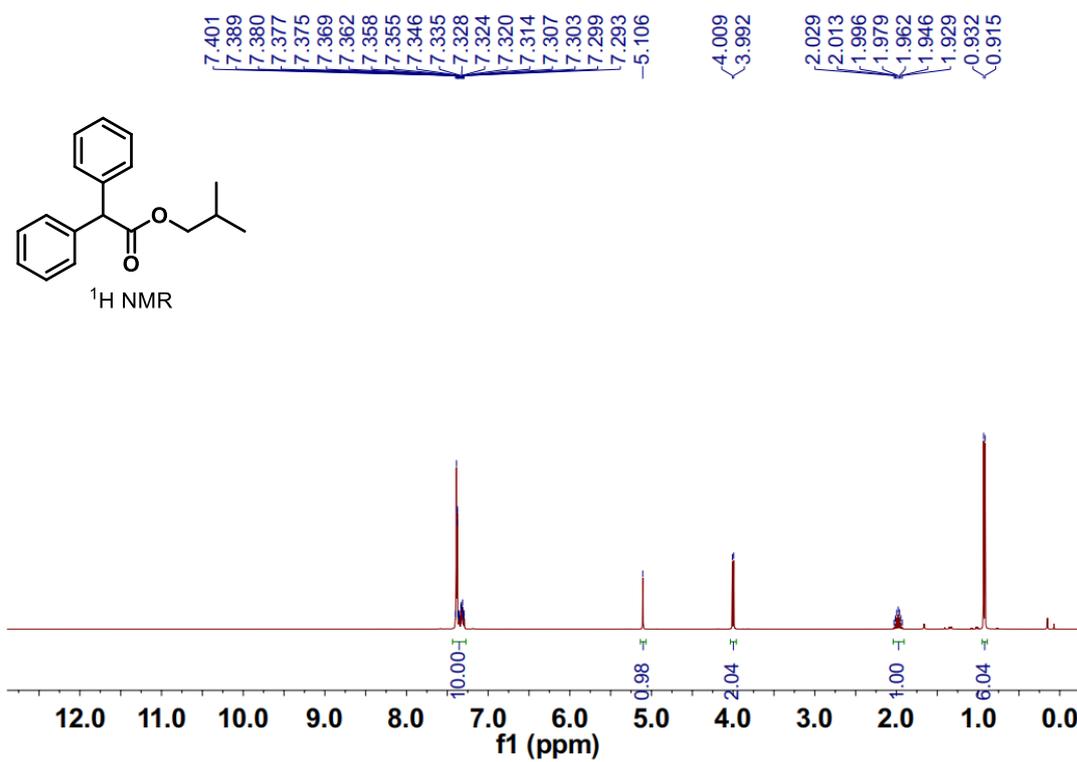
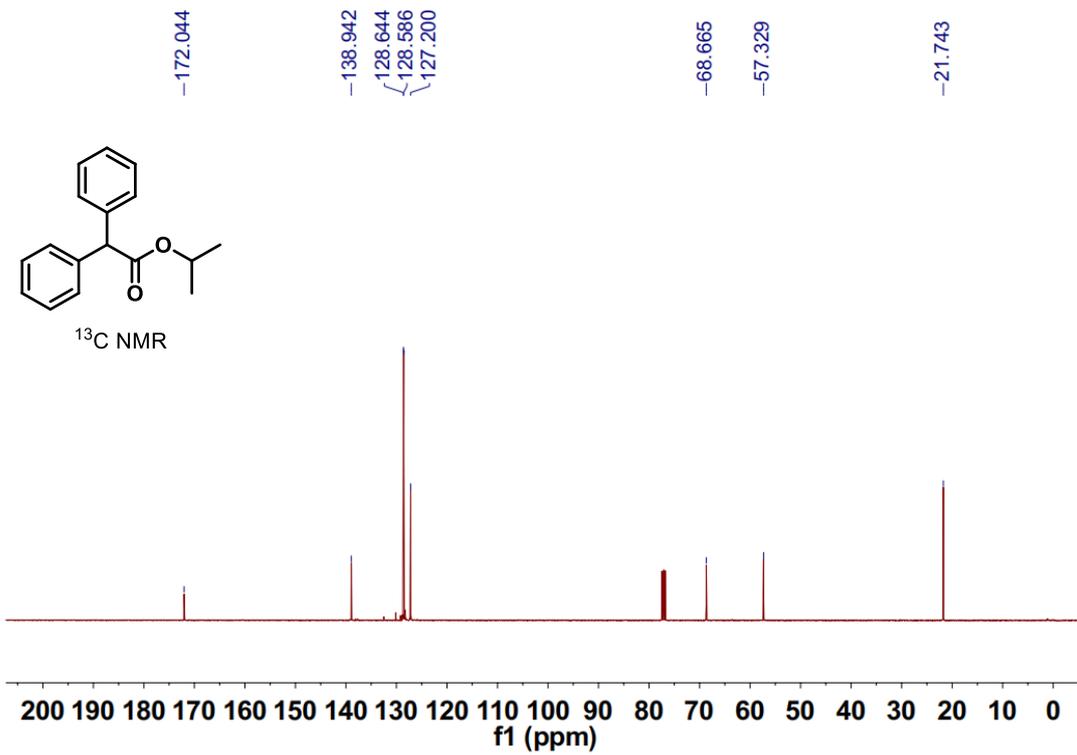


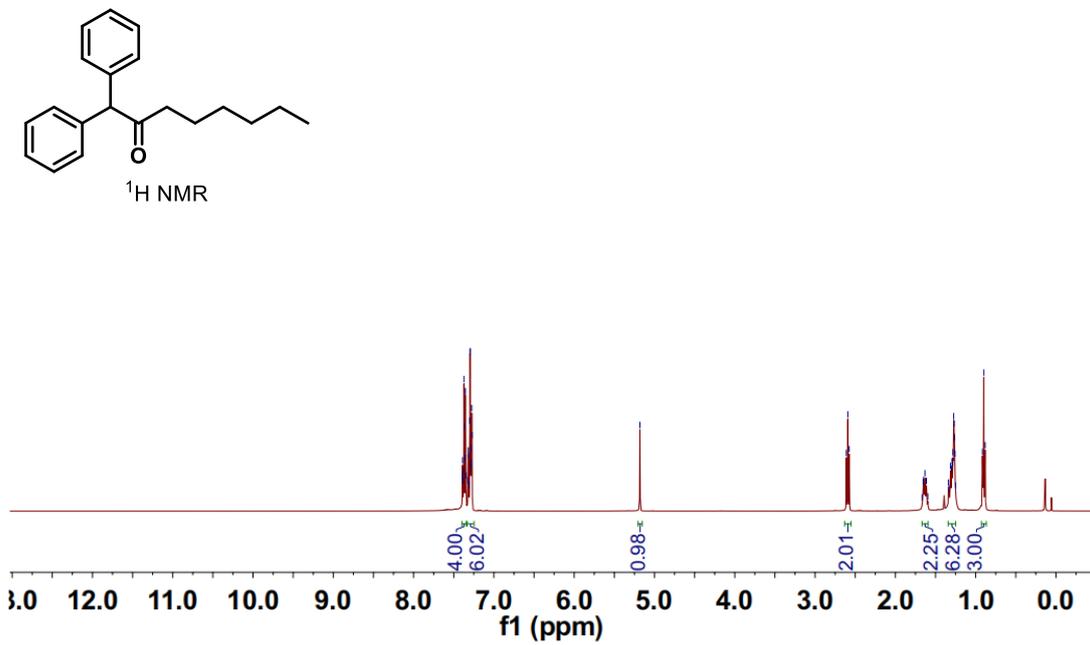
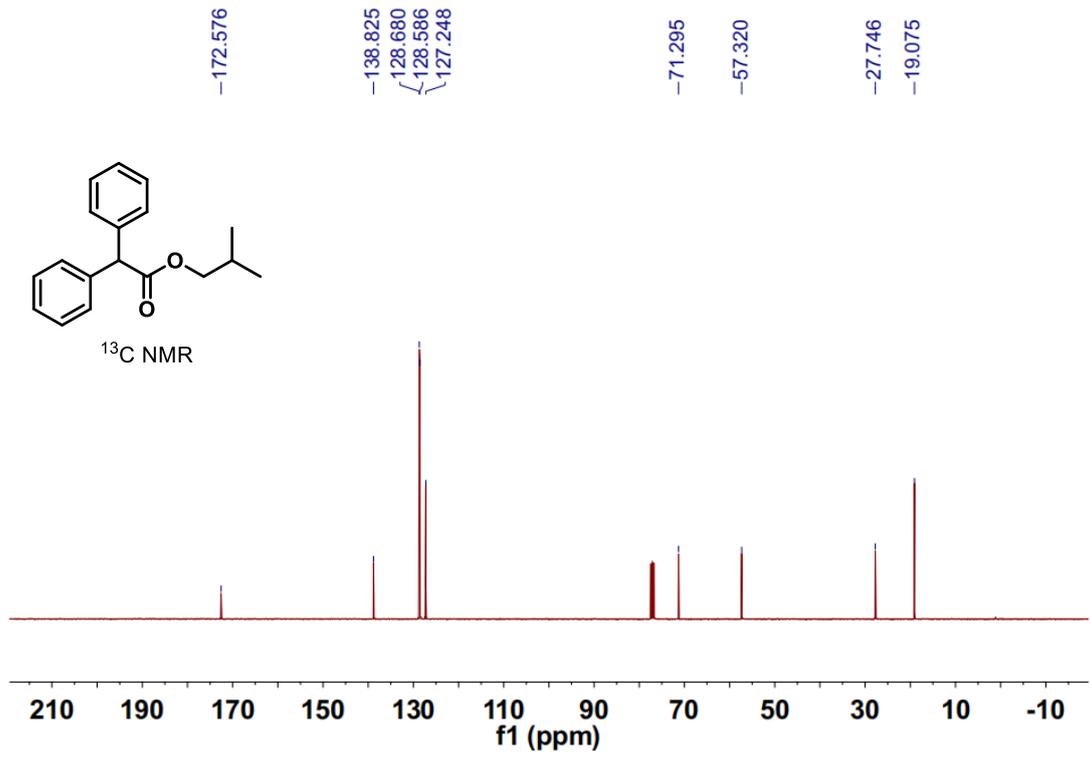


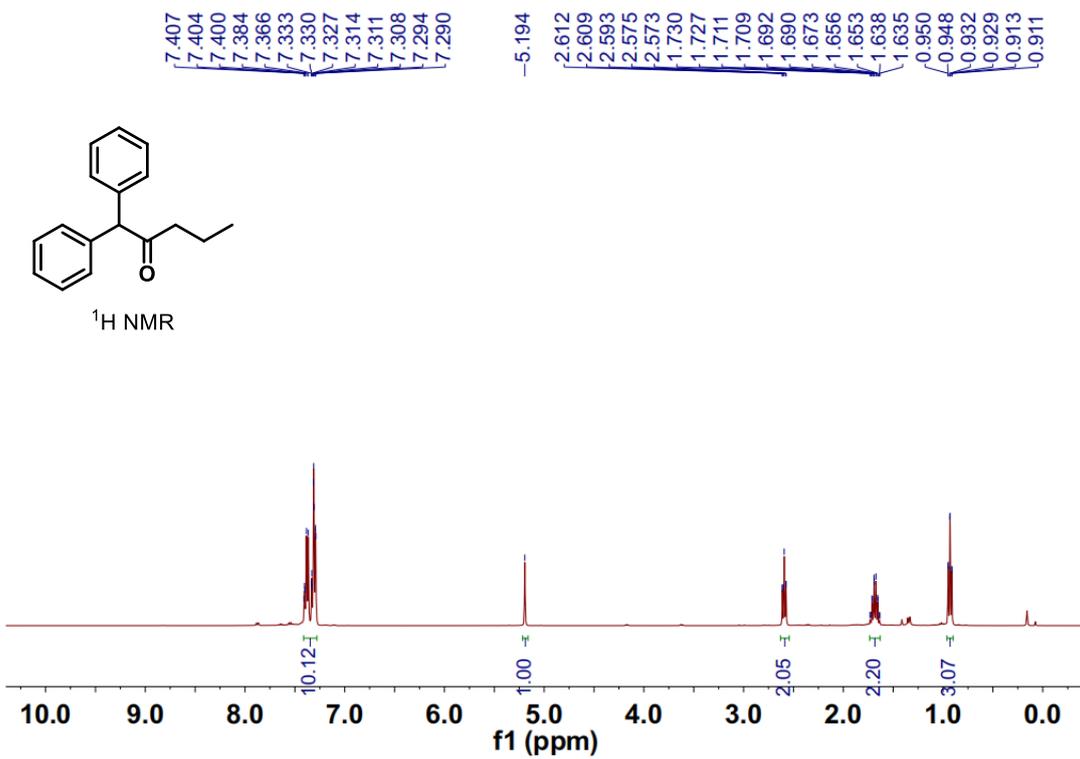
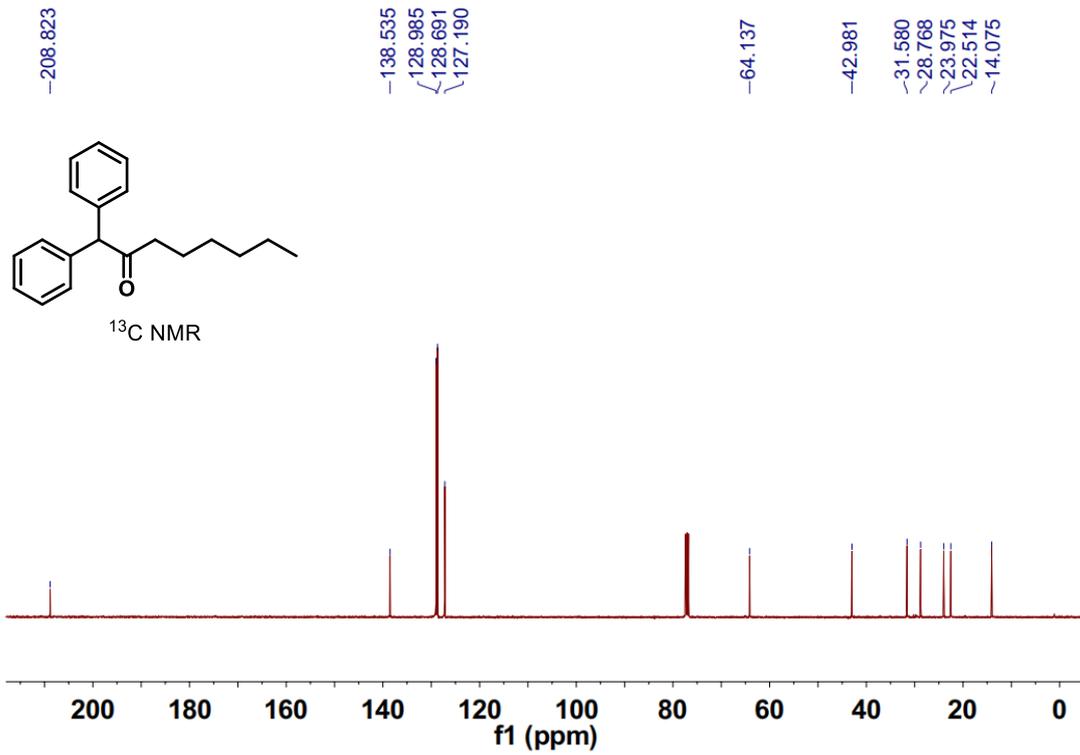


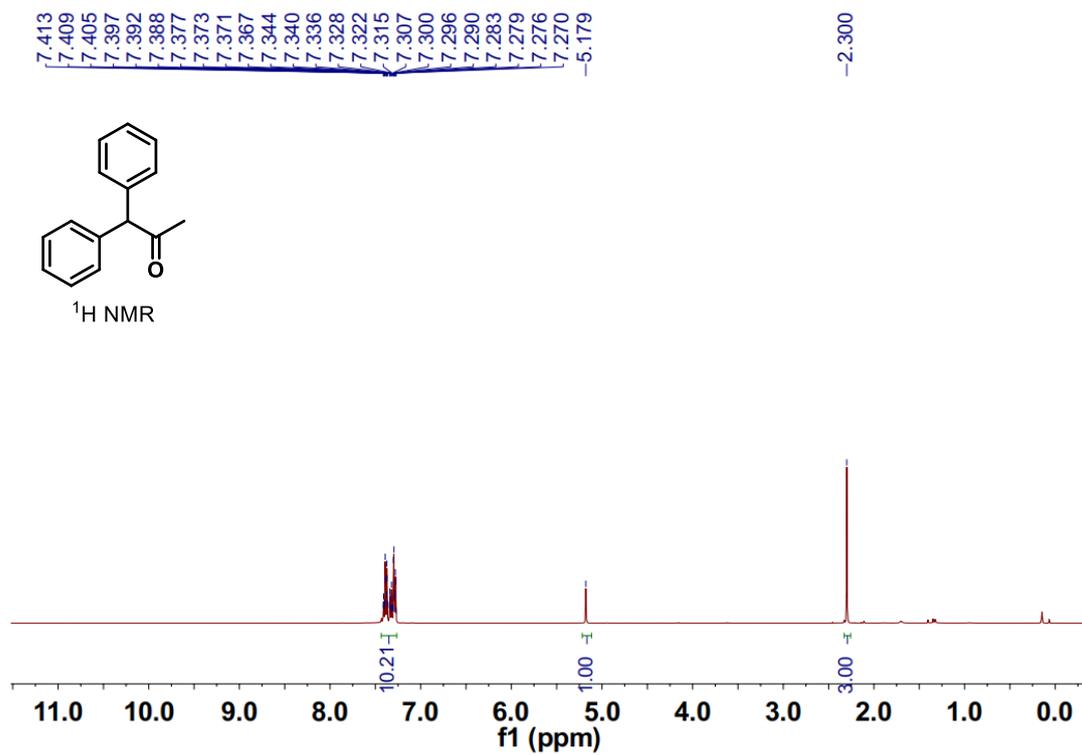
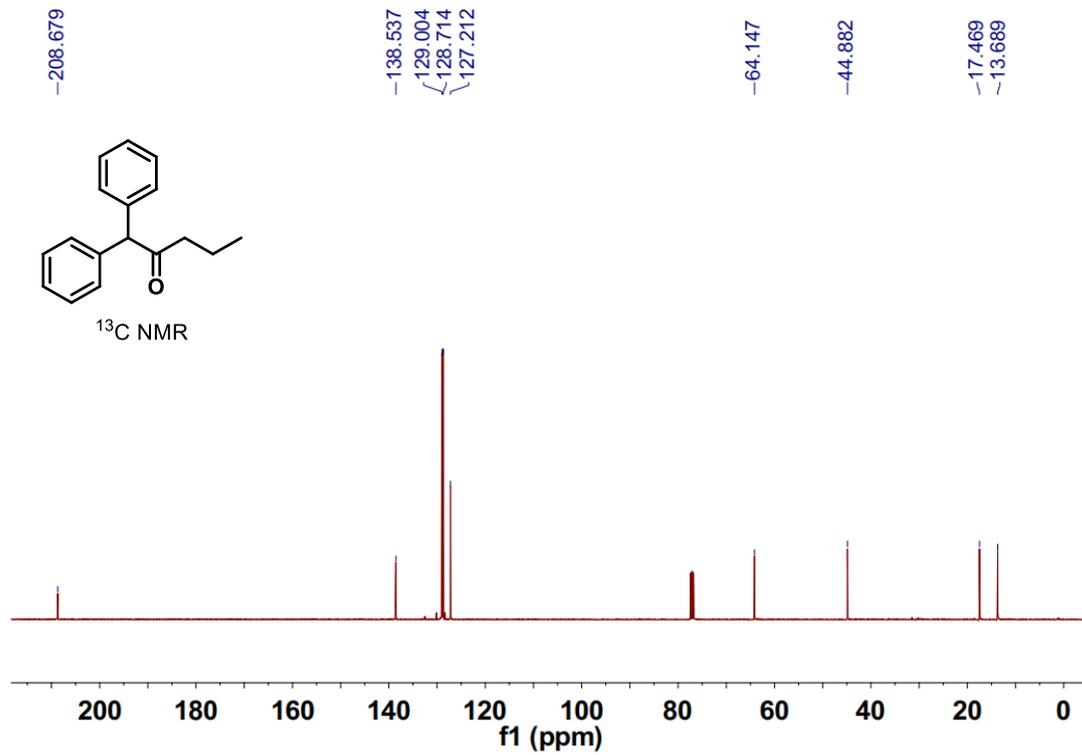


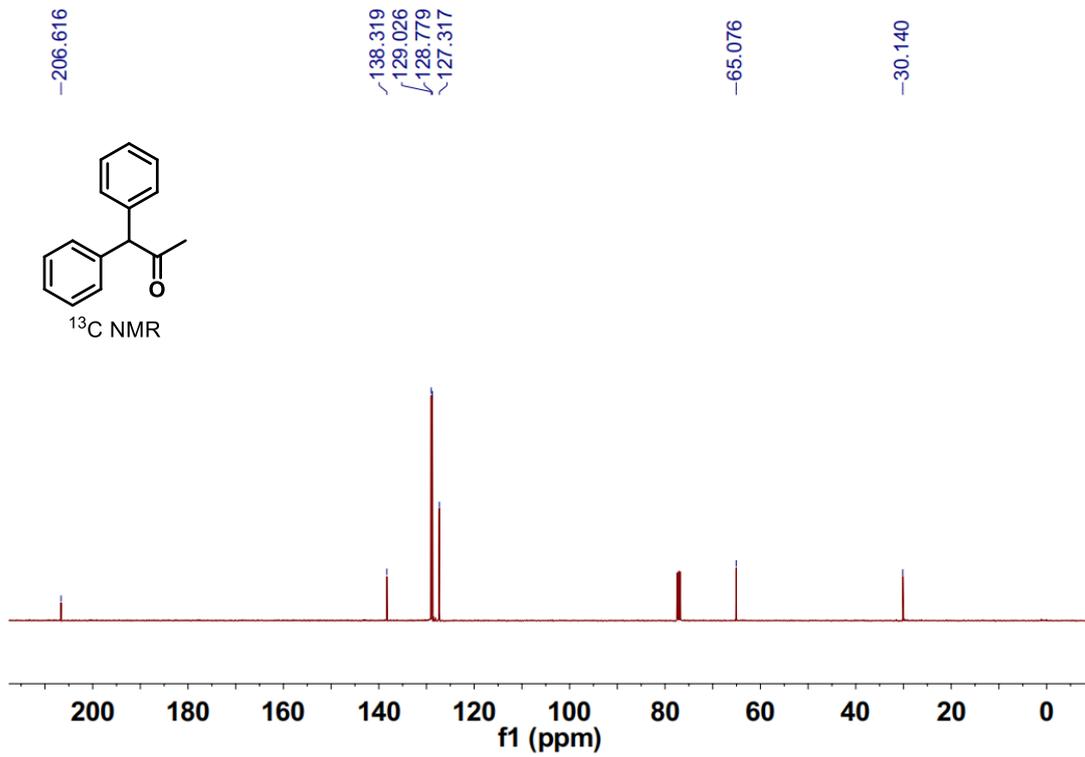




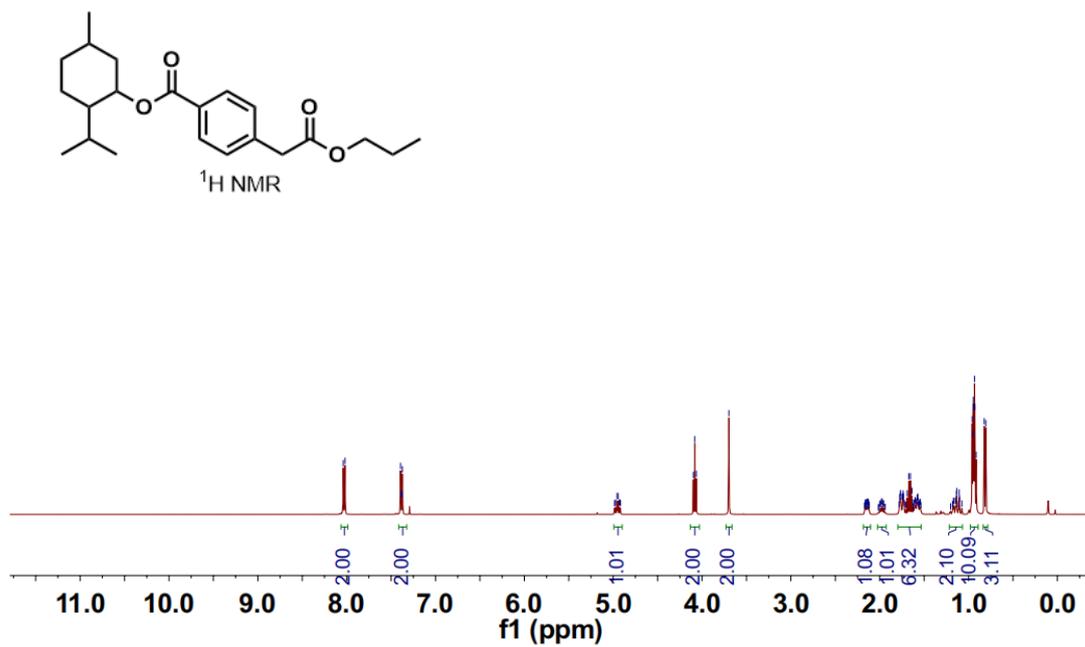


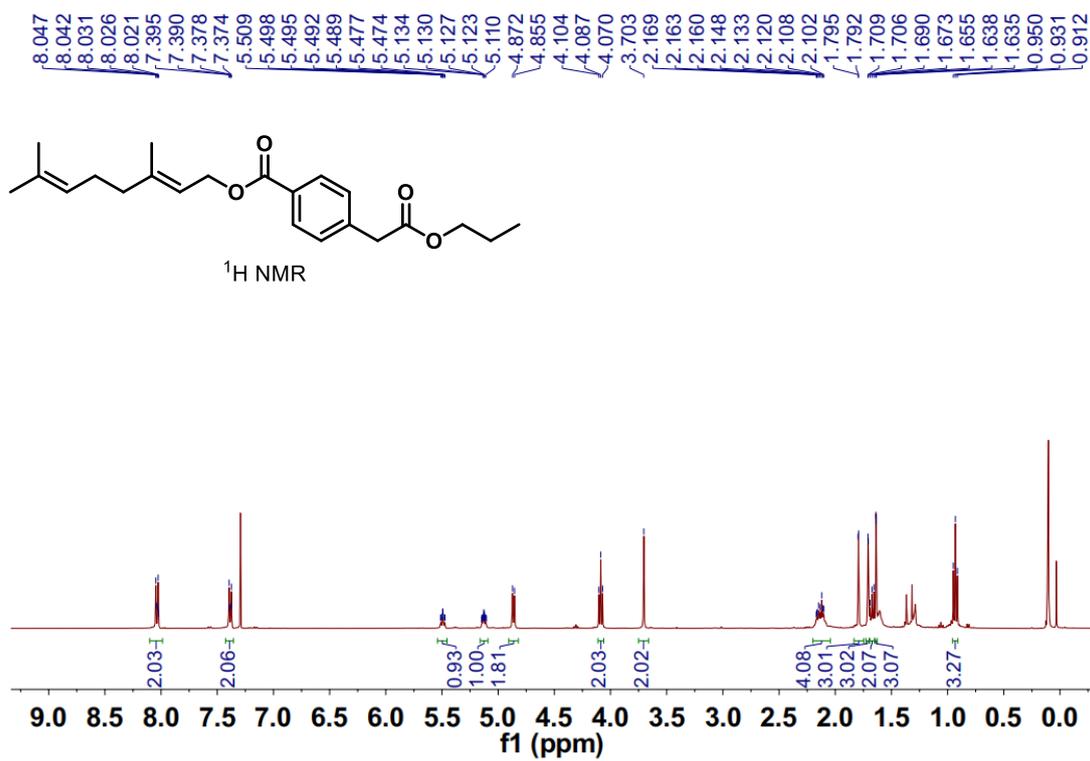
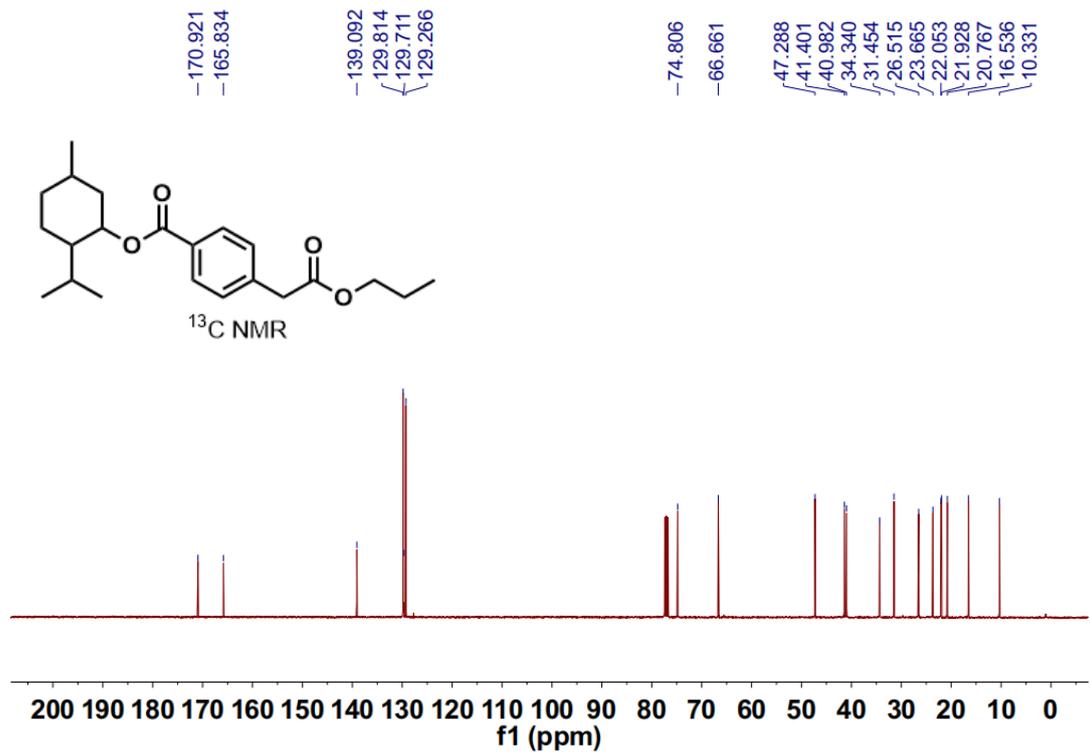


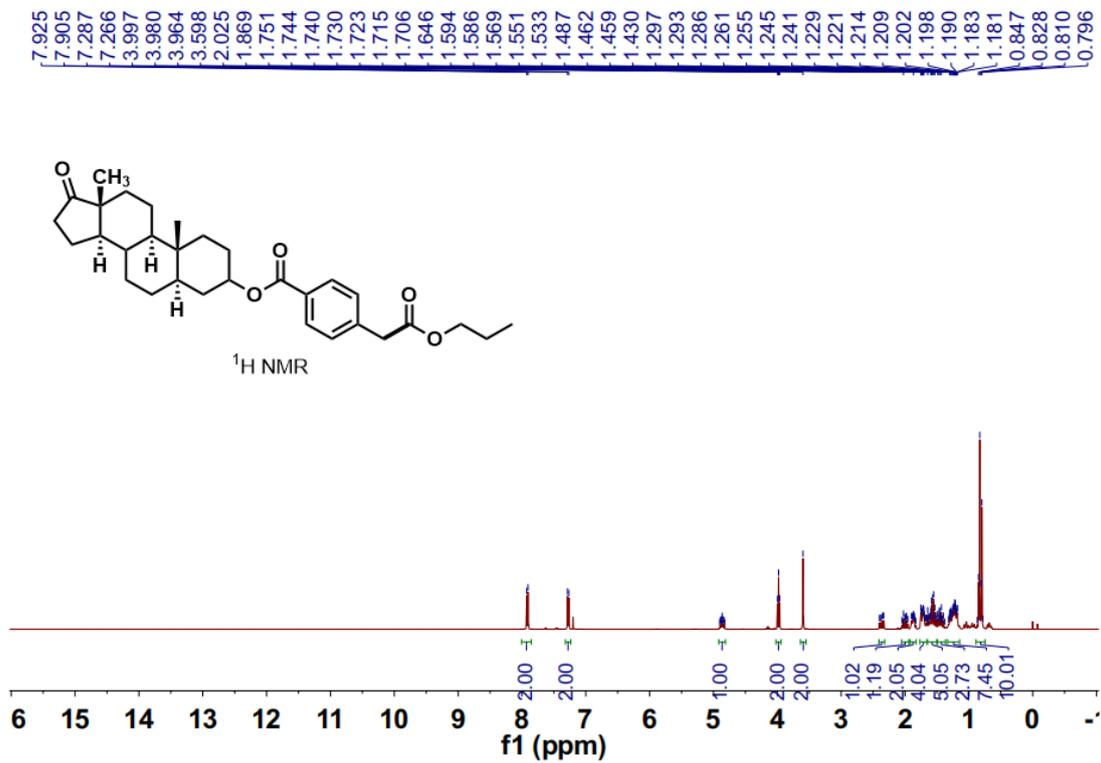
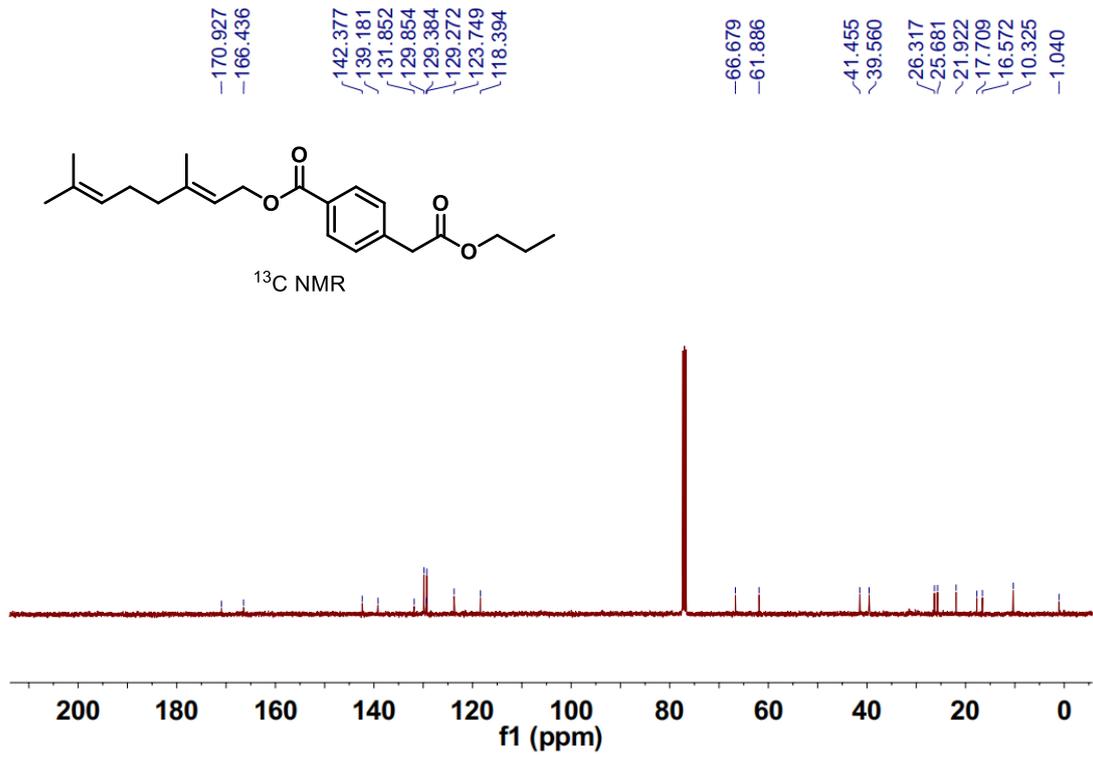


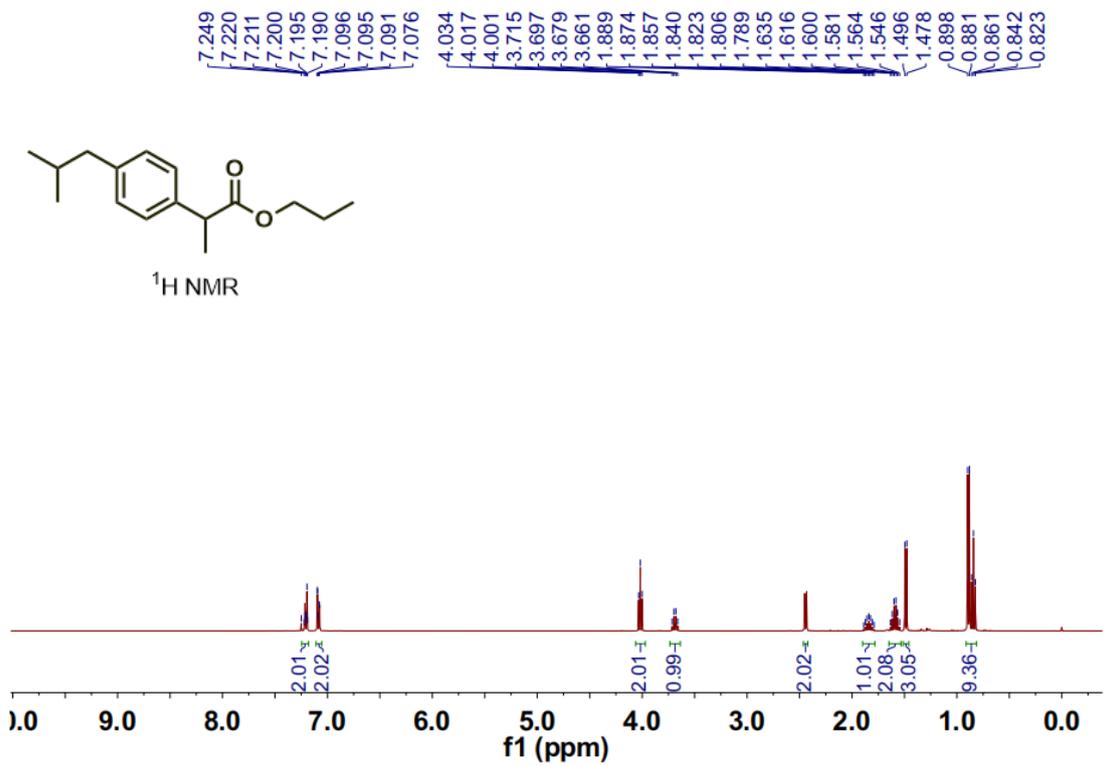
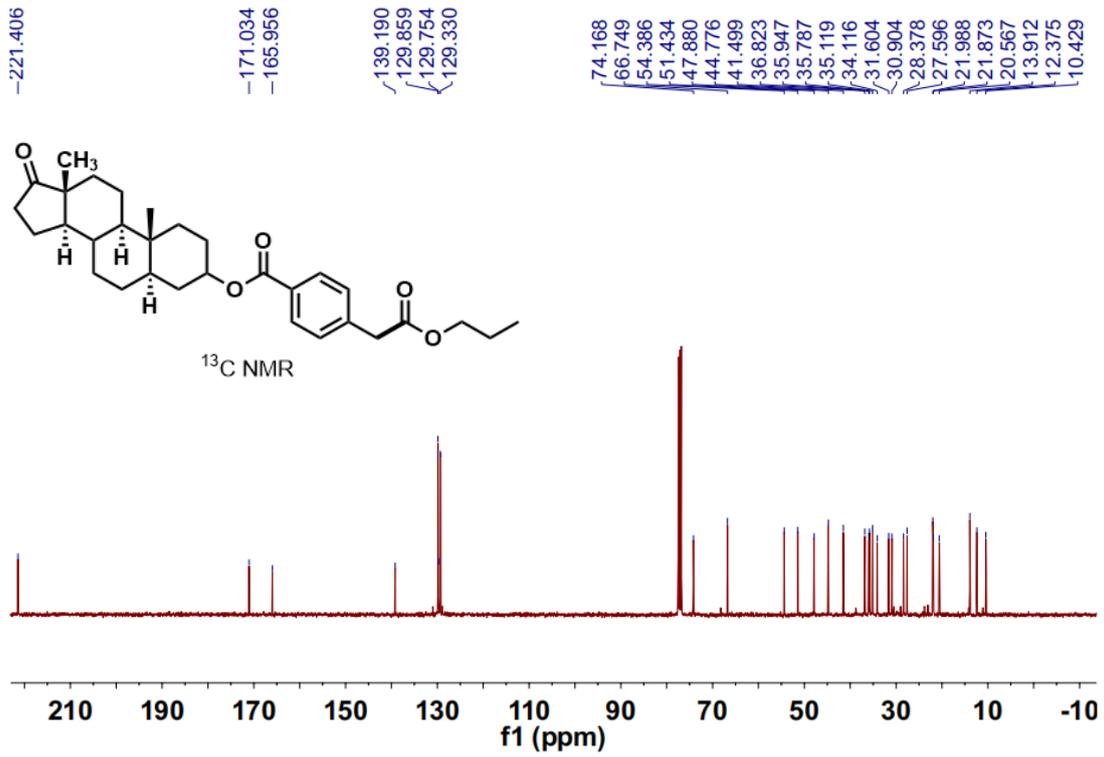


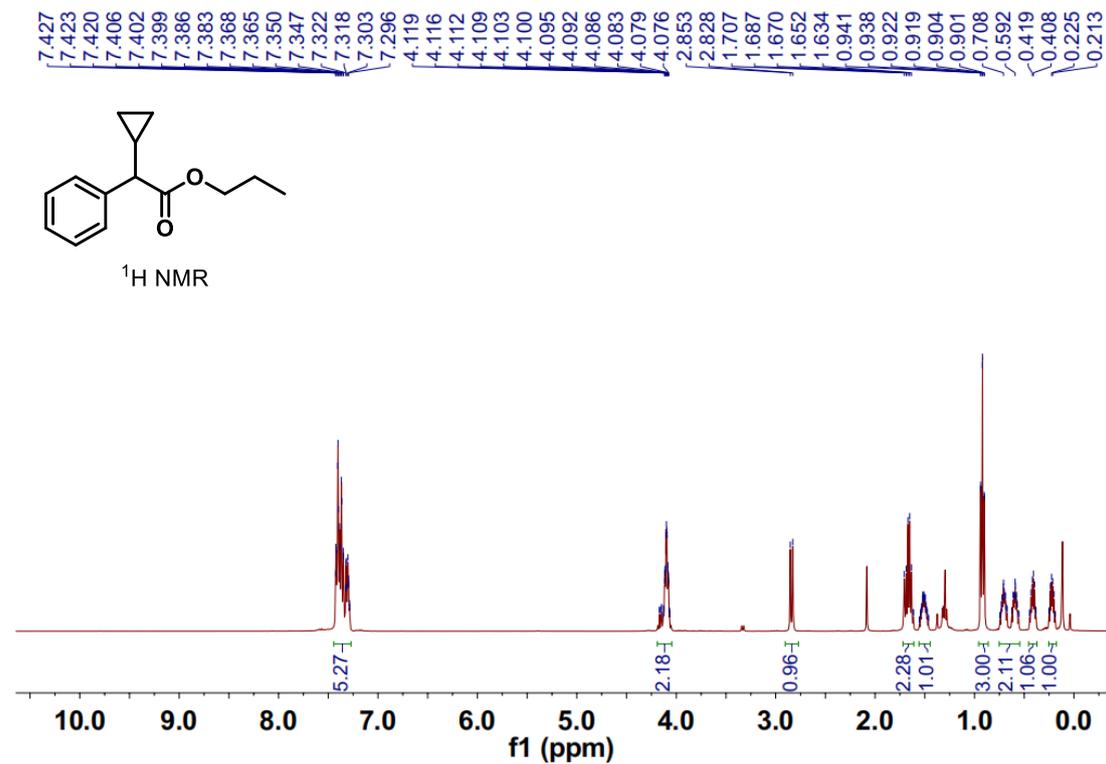
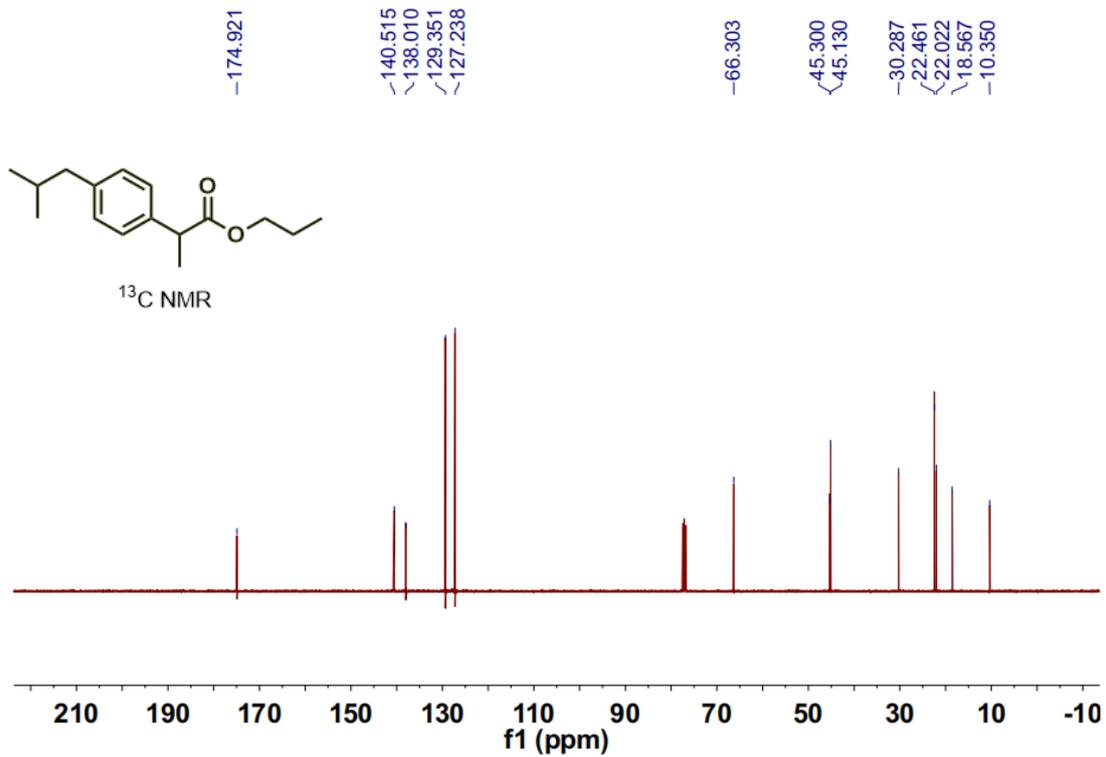
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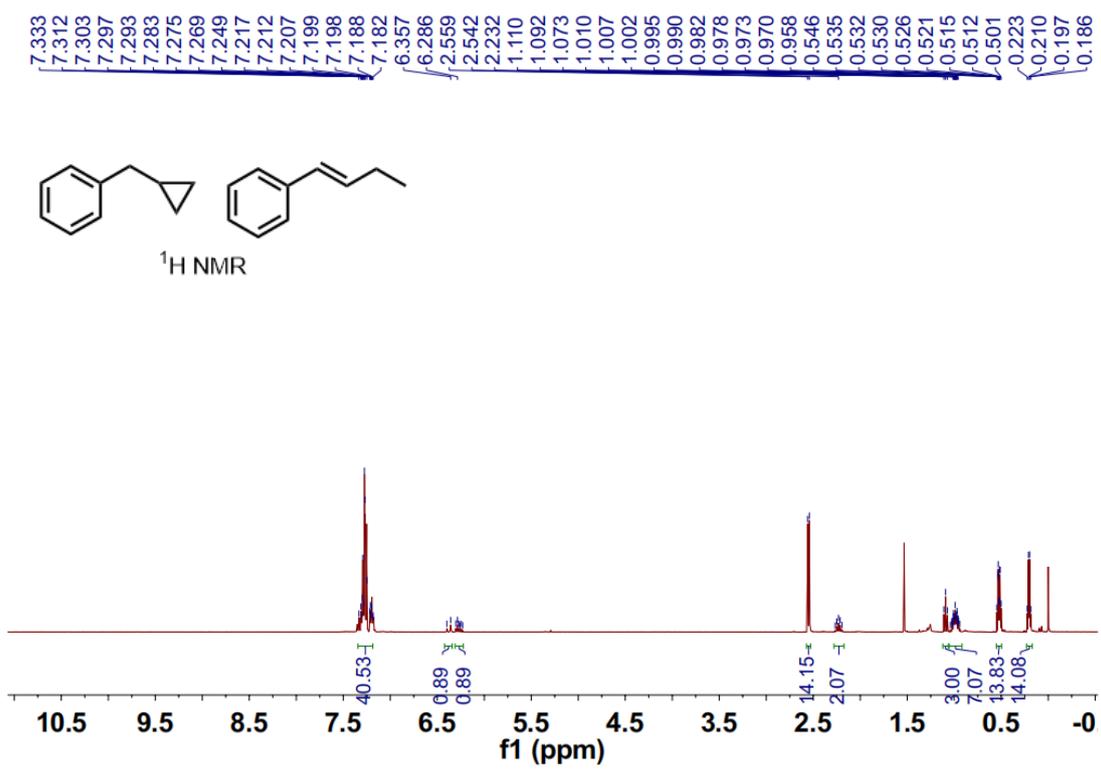
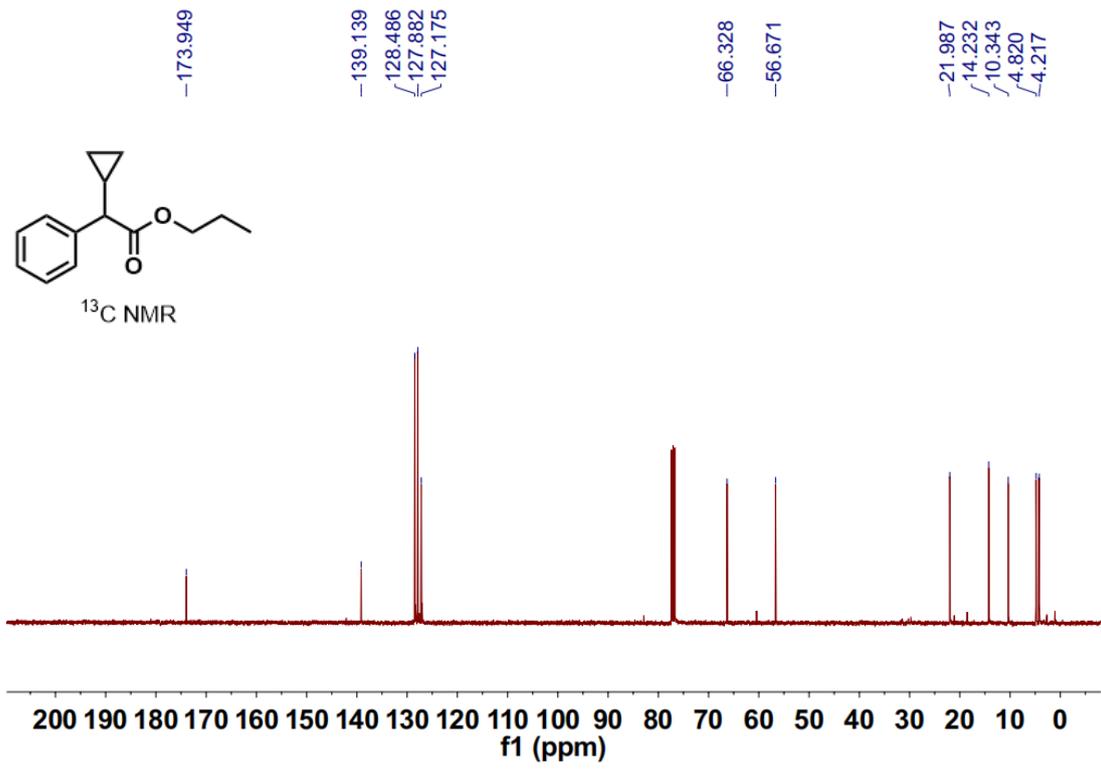


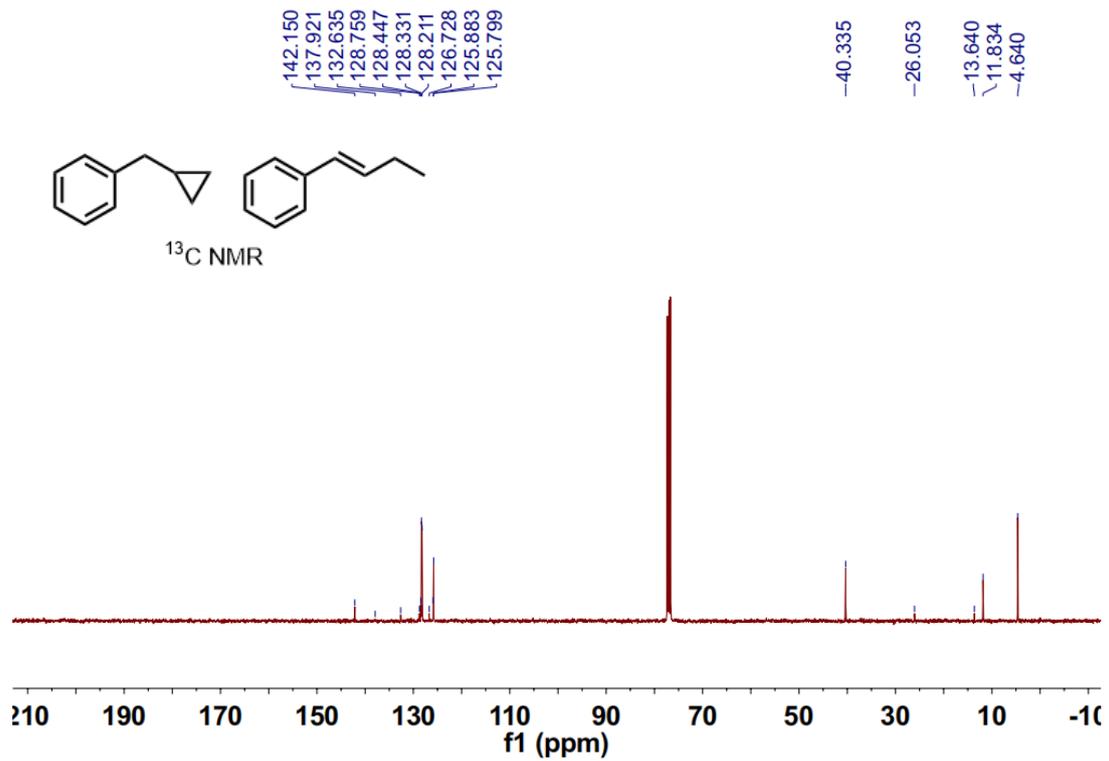












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